On the spectral and wave propagation properties of the surface Maryland model

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(Received 3 June 2002; accepted 19 September 2002)

We study the discrete Schrödinger operator H in $\mathbb{Z}^d$ with the surface potential of the form $V(\mathbf{x})=g\,\delta(x_1)\tan\pi(\alpha\cdot x_2+\omega)$, where for $x\in\mathbb{Z}^d$ we write $\mathbf{x}=(x_1,x_2)$, $x_1\in\mathbb{Z}^{d_1}$, $x_2\in\mathbb{Z}^{d_2}$, $\alpha\in\mathbb{R}^{d_2}$, $\omega\in[0,1)$. We first consider the case where the components of the vector α are rationally independent, i.e., the case of the quasi-periodic potential. We prove that the spectrum of H on the interval $[-d,d]$ (coinciding with the spectrum of the discrete Laplacian) is absolutely continuous. Then we show that generalized eigenfunctions, corresponding to this interval, have the form of volume (bulk) waves, which are oscillating and nondecreasing (or slow decreasing) in all variables. They are the sum of the incident plane wave and of an infinite number of reflected or transmitted plane waves, scattered by the subspace $\mathbb{Z}^{d_2}$. These eigenfunctions are orthogonal, complete and verify a natural analog of the Lippmann–Schwinger equation. We discuss also the case where $d_1=d_2=1$ and $\alpha=p/q$ is a rational number, i.e., a q-periodic surface potential. In this case we show that the spectrum is absolutely continuous and besides the volume (Bloch) waves there are also the surface waves, whose amplitude decays exponentially as $|x_1|\to\infty$. The part of the spectrum corresponding to the surface waves consists of a finite number of bands. For large q the bands outside of $[-d,d]$ are exponentially small in q, and converge in a natural sense to the pure point spectrum that was found [B. Khoruzhenko and L. Pastur, Phys. Rep. **288**, 109–125 (1997)] in the case of the Diophantine α's. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1521798]

I. INTRODUCTION

The progress of the last decades in spectral theory of differential and finite difference operators with random ergodic and almost periodic coefficients in the whole space makes natural the study of operators with same type of coefficients, supported on a subspace only. Being of evident interest from the point of view of wave physics, they provide a class of operators ''intermediate'' between operators whose coefficients decay in all coordinates (scattering theory) and operators, having coefficients of the same order of magnitude in all coordinates. We mention recent papers, Refs. 2, 6, 8–15, and 19, devoted to the study of the spectral and related properties of these operators. They are either defined on the half-space by random, almost periodic or periodic boundary conditions or have the same type of coefficients supported on certain subspaces of $\mathbb{R}^d$ or $\mathbb{Z}^d$.

As in Ref. 19 we consider here the discrete Schrödinger operator

$$H=H_0+V \tag{1.1}$$

acting on $l^2(\mathbb{Z}^d)$, where

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$$(H_0\Psi)(\mathbf{x}) = -\frac{1}{2}\sum_{|\mathbf{x}-\mathbf{y}|=1}\Psi(\mathbf{y}), \tag{1.2}$$

is the discrete Laplacian,

$$V(\mathbf{x}) = \delta(x_1)v(x_2), \quad \mathbf{x}=(x_1,x_2), \quad x_1\in\mathbb{Z}^{d_1}, \quad x_2\in\mathbb{Z}^{d_2}, \quad d_1+d_2=d, \tag{1.3}$$

with

$$v(x_2) = g\tan\pi(\alpha\cdot x_2+\omega) \tag{1.4}$$

the multiplication operator (''surface'' potential), whose support is the subspace $\mathbb{Z}^{d_2}$ of the space $\mathbb{Z}^d$, and

$$d_1,d_2\in\mathbb{N}, \ \ g>0, \ \ \alpha\in\mathbb{R}^{d_2}, \ \ \omega\in[0,1) \tag{1.5}$$

are the parameters determining the potential.

It was shown in Ref. 19 that for any $g\neq 0$, $\omega\in[0,1)$, and for $\alpha\in\mathbb{R}^{d_2}$, satisfying the Diophantine condition, i.e., there exists $\varepsilon>0$ such that

$$|\alpha\cdot x_2-m|\geqslant \text{const}/|x_2|^{d_2+\varepsilon}, \quad \forall x_2\in\mathbb{Z}^{d_2}\backslash\{0\}, \quad \forall m\in\mathbb{Z}, \tag{1.6}$$

the spectrum of $H=H_0+V$, lying outside the spectrum $[-d,d]$ of the discrete Laplacian (1.2), is pure point, dense, of multiplicity one, and the respective eigenfunctions decay exponentially at infinity.

The ''volume'' version of this operator, corresponding to the case $d_1=0$, has been studied previously in Refs. 5 and 26. The operator has a complete system of exponentially decaying eigenfunctions, corresponding to the pure point dense spectrum of multiplicity one occupying the whole real axis. This spectral structure is caused by strong and irregular fluctuations of the quasi-periodic potential (1.3). It is the extreme case of the strong localization regime, which in general appears either if, for a fixed energy, the amplitude of the potential (random or almost periodic) is large enough or, if for a fixed potential, the energy is close enough to the spectrum edges (see Ref. 22 for related results and references).

In the case $d_1=1$ the support of the potential is the hyper-plane $\mathbb{Z}^{d-1}$ of the space $\mathbb{Z}^d$. This is why it is natural to call the respective operator (1.1)–(1.5) the surface Maryland model. This operator is closely related to the boundary value problem (3.5), considered in Refs. 15, 11, and 14. We may also call the operator (1.1)–(1.5), for $d_1\geqslant 2$, the subspace Maryland model.

These models can be analyzed in great detail, thereby providing examples of spectral types which are only partly known for general random or almost periodic function v in (1.3). All these versions of the Maryland model have an absolutely continuous component of the spectrum. This component was first indicated in Ref. 15, and then was studied in Ref. 11 in the context of the boundary value problem defined by (1.4) and by formula (3.5) below. It was proven that if the components of the vector $\alpha\in\mathbb{R}^{d_2}$ are rationally independent, this part of the spectrum of H is purely absolutely continuous and also that the properly defined wave operators corresponding to this part exist and are complete. Besides, it was proven in Ref. 14 that the surface states (see Refs. 15 and 14 for definitions) are absent.

In this article we develop several general ideas and results of the theory by considering the explicitly soluble model, defined by formulas (1.1)–(1.5). We begin by showing that the Green function of the model can be written in a rather convenient form (Sec. II). By using this form we study first the quasi-periodic case of rationally independent components of the vector α in (1.3) (Sec. III). We prove that the spectrum of the operator is purely absolutely continuous on the interval $[-d,d]$ (on the spectrum of discrete Laplacian) and that the wave operators corresponding to this part of the spectrum exist (these facts were proved in Refs. 11 and 14 by other methods). Then we find an explicit form of the generalized eigenfunctions (polynomially bounded

solutions of the respective equation), corresponding to this part of the spectrum. These eigenfunctions possess properties similar to those of the Sommerfeld solutions of scattering theory. Along the x_2 direction, they behave like Bloch–Floquet solutions. They are orthogonal and complete on the interval $[-d,d]$ of the spectrum. As they do not decay in the longitudinal coordinates x_1 we call them volume states. We consider also the case of rationally dependent components of the vector α in (1.4), where the respective surface potential is periodic in x_2, restricting ourselves to the technically simplest case of $d_1=d_2=1$, where $\alpha=p/q$ is a rational number (Sec. IV). In this case the whole spectrum is absolutely continuous. It consists of the interval $[-2,2]$ as in the quasiperiodic case, and of a certain number of intervals, some of them possibly intersecting $[-2,2]$. Generalized eigenfunctions, corresponding to the interval $[-2,2]$, do not decay in the longitudinal coordinates x_1. However, the generalized eigenfunctions, corresponding to other intervals, decay exponentially in x_1, being of the Bloch–Floquet form in the longitudinal coordinate x_2 as those of the interval $[-2,2]$. This type of surface states (see Definition 3.1 below) was discovered by Rayleigh in the problem of oscillation of the homogeneous elastic half-space (see, e.g., Ref. 21), and since then was found and studied in a number of problems, described by differential and finite difference equations whose coefficients are strongly varying in coordinates x_1 (see, e.g., Refs. 19, 20 for a list of references on respective physics results and applications, and Refs. 7, 16, and 17 for spectral analysis of certain periodic cases). We analyze also the case where $\alpha_n=p_n/q_n$ approaches an irrational α as $n\to\infty$, and we show that there exists a certain continuity of the spectrum in this asymptotic regime. In particular, the width of surface bands lying outside of $[-2,2]$ is exponentially small in q_n as $n\to\infty$, and the bands approach the dense set of eigenvalues, found in Ref. 19.

II. GENERALITIES

Recall that we are studying the self-adjoint operator H, acting in $l^2(\mathbb{Z}^d)$ and defined in (1.1)–(1.5). The operator is self-adjoint as the sum of the multiplication self-adjoint operator V of (1.3), and of the bounded self-adjoint operator H_0 of (1.2). We will use an analogue of the Cayley transform introduced in Ref. 5 for the ''volume'' potential ($d_1=0$) and in Ref. 19 for the ''surface'' case ($d_1=1$), in both cases to study the pure point spectrum for the Diophantine α's [see (1.6)].

To put the subsequent simple argument in a more general context, we rewrite the potential (1.3) as

$$V(\mathbf{x})=v(x_2)\chi_S(\mathbf{x}), \tag{2.1}$$

where χ_S is the indicator of the subspace $S=\mathbb{Z}^{d_2}$ and we assume that $g>0$ (the case $g<0$ can be treated analogously). We define the orthogonal projection P of $l^2(\mathbb{Z}^d)$:

$$(P\Phi)(\mathbf{x})=\chi_S(\mathbf{x})\Phi((0,x_2)), \tag{2.2}$$

and we write the potential (2.1) in the form

$$V=Pv P. \tag{2.3}$$

Here and in the following we use lower cases to denote operators acting on $l^2(S)$ defined by the restriction on $Pl^2(\mathbb{Z}^d)$ of the corresponding operator.

We use as a starting point the well known formulas for the resolvent $G(z)=(H-z)^{-1}$ of a self-adjoint operator $H=H_0+V$:

$$G(z)=G_0(z)-G_0(z)T(z)G_0(z), \Im z\neq 0 \tag{2.4}$$

with

$$G_0(z)=(H_0-z)^{-1}, \quad T(z)=V-T(z)G_0(z)V. \tag{2.5}$$

It follows from (2.3) and from (2.5) that the operator $T(z)$ has the form

$$T(z)=Pt(z)P, \tag{2.6}$$

where the operator $t(z)$, acting on $l^2(S)$, satisfies the equation

$$t(z)=v-t(z)\gamma_0(z)v, \tag{2.7}$$

in which $\gamma_0(z)$ is defined from the restriction of $G_0(z)$ to the subspace $Pl^2(\mathbb{Z}^d)$. The formal solution of the equation is

$$t(z)=v(1+\gamma_0(z)v)^{-1}=(v^{-1}+\gamma_0(z))^{-1}. \tag{2.8}$$

Let u be the unitary operator in $l^2(S)$ defined by the relation:

$$(u\psi)(x_2)=e^{-2i\pi\alpha.x_2}\psi(x_2), \quad x_2\in S. \tag{2.9}$$

Then, by using the Euler formula for the function $x\mapsto\tan x$ and the notations above, we can write the potential (1.4) as

$$v=\frac{g}{i}\cdot\frac{1-\sigma u}{1+\sigma u}, \tag{2.10}$$

where

$$\sigma=e^{-2i\pi\omega}. \tag{2.11}$$

Formulas (1.3)–(2.11) motivate the following abstract statement.

Lemma 2.1: Let H be a self-adjoint operator, acting on $l^2(\mathbb{Z}^d)$, and having the form $H=H_0+V$, where H_0 is a self-adjoint operator and V is given by formulas (2.3) and (2.10) in which S is any subset of $\mathbb{Z}^d$ and $|\sigma|\leqslant 1$. Define the following operators in $l^2(S)$,

$$b(z)=(g\gamma_0(z)-i)(g\gamma_0(z)+i)^{-1}, \tag{2.12}$$

assuming that $b(z)$ is bounded. If the operator $g\gamma_0(z)+i$ is invertible and if, for some z, $\Im z>0$, we have

$$||b(z)||<1, \tag{2.13}$$

then the operator $t(z)$, defined in (2.6) and in (2.8), can be represented in the form

$$t(z)=g(1-\sigma u)(1-\sigma b(z)u)^{-1}(g\gamma_0(z)+i)^{-1}, \tag{2.14}$$

or in the form

$$t(z)=g(g\gamma_0(z)+i)^{-1}\left[1-2i\sigma u\sum_{l=0}^{q-1}(\sigma b(z)u)^l(1-(\sigma b(z)u)^q)^{-1}(g\gamma_0(z)+i)^{-1}\right], \tag{2.15}$$

where σ is defined in (2.11), and $q\geqslant 1$ is an integer.

Proof: Note that the conditions $||b(z)||<1$ and $|\sigma|\leqslant 1$ allow us to define the operator $(1-\sigma b(z)u)^{-1}$ by the Neumann–Liouville series. Consider first the case, where the modulus of the complex number σ in (2.10) is strictly less than 1. In this case the operator $(1+\sigma u)^{-1}$ is well defined and we obtain from (2.10), and from (2.12),

$$1+\gamma_0 v=[i(1+\sigma u)+g\gamma_0(1-\sigma u)](i(1+\sigma u))^{-1}$$
$$=(g\gamma_0+i)(1-(g\gamma_0-i)(g\gamma_0+i)^{-1}\sigma u)(i(1+\sigma u))^{-1},$$

or $1+\gamma_0 v=(g\gamma_0+i)(1-b(z)\sigma u)(i(1+\sigma u))^{-1}$, where the operators $\gamma_0(z)$ and $b(z)$ are defined in (2.12). Formulas (2.7), (2.10), and the hypotheses of the lemma lead to (2.14) for $|\sigma|<1$. According to inequality (2.13) the Neumann–Liouville series for $(1-b(z)\sigma u)^{-1}$ converges for $|\sigma|=1$, and since the operator $(1+\sigma u)^{-1}$ is not present in formula (2.14), we can make the limit $|\sigma|\to 1$ in the formula, proved for $|\sigma|<1$, and obtain representation (2.14) in the case $|\sigma|=1$.

Proposition 2.1: Let H be the self-adjoint operator defined in Lemma 2.1 and $G(z)=(H-z)^{-1}$, $\Im z>0$ be its resolvent. Assume that z is such that the conditions of Lemma 2.1 hold. Then $G(z)$ can be represented as follows:

$$G(z)=G_0(z)-gG_0(z)P(g\gamma_0(z)+i)^{-1}PG_0(z)+2igG_0(z)P(g\gamma_0(z)+i)^{-1}$$
$$\times\sigma u\sum_{l=0}^{q-1}(\sigma b(z)u)^l(1-(\sigma b(z)u)^q)^{-1}(g\gamma_0(z)+i)^{-1}PG_0(z), \tag{2.16}$$

where $q\geqslant 1$ is an integer, u is defined in (2.9) and the operators $\gamma_0(z)$, $b(z)$ are defined in (2.12).

Proof: The proposition follows easily from (2.4), and from Lemma 2.1.

Remarks. (1) In formula (2.10) the unitary operator σu can be viewed as the Cayley transform of v (see Ref. 1 for the definition of the Cayley transform). Likewise, the contraction operator $b(z)$ can be viewed as the Cayley transform of the dissipative operator $i\gamma_0(z)$ ($\Re i\gamma_0>0$). Hence, we can say that the passage from the operators v^{-1} and $\gamma_0(z)$ in (2.8) to their Cayley transforms σu and $b(z)$ in the case of the potential (1.3) and (1.4) leads to formulas (2.14)–(2.16). This will allow us to study the absolutely continuous spectrum of the operator H for any $d_1\geqslant 0$, as it was done in papers Refs. 22 and 19 for the pure point spectrum, despite that the subsequent techniques to study the resolvent (2.16) are different in these two cases.

(2) Integrate formula (2.16) with respect to $\omega\in[0,1)$ and denote this operation by $\langle\cdots\rangle$. We obtain

$$\langle G(z)\rangle=G_0(z)-gG_0(z)P(g\gamma_0(z)+i)^{-1}PG_0(z).$$

In view of the general formula (2.8), valid for any surface potential v, we can interpret the equality $\langle t(z)\rangle=g(g\gamma_0(z)+i)^{-1}=(-(ig)^{-1}+\gamma_0(z))^{-1}$ as the fact that $\langle G(z)\rangle$ is the resolvent of the Schrödinger operator whose surface potential is the complex constant $V(\mathbf{x})=-ig\chi_S(\mathbf{x})$. This fact plays an important role in the interpretation of results of analysis of the point spectrum of H outside $[-d,d]$ in Ref. 19. Similar fact is known also in the case of the volume potential (2.3), i.e., for the case $S=\mathbb{Z}^d$.[5]

Now we are going to show that the above proposition is applicable to the operator defined by (1.1)–(1.5) where S is chosen as Z^{d_2}. To check the conditions of the lemma and the proposition we will use the Fourier transformation which we define as follows:

$$\hat{\Phi}(\mathbf{k})=\sum_{\mathbf{x}\in\mathbb{Z}^\nu}e^{-2i\pi\mathbf{x}\cdot\mathbf{k}}\Phi(\mathbf{x}),\quad \mathbf{k}\in\mathbb{T}^\nu,\qquad \Phi(\mathbf{x})=\int_{\mathbb{T}^\nu}d\mathbf{k}e^{2i\pi\mathbf{x}\cdot\mathbf{k}}\hat{\Phi}(\mathbf{k}),\quad \mathbf{x}\in\mathbb{Z}^\nu, \tag{2.17}$$

where $\mathbb{T}^\nu=[0,1)^\nu$ is the ν-dimensional unit torus.

By using the Fourier transformation we can write the following representation of the Green function $G_0^{(\nu)}(\mathbf{x}-\mathbf{y};z)$ of the ν-dimensional Laplacian [operator (1.2) for $d=\nu$]:

$$G_0^{(\nu)}(\mathbf{x}-\mathbf{y};z)=\int_{\mathbb{T}^\nu}d\mathbf{k}\frac{e^{2i\pi\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{E_\nu(\mathbf{k})-z},\quad \Im z\neq 0, \tag{2.18}$$

where

$$E_\nu(\mathbf{k}) = -\sum_{i=1}^{\nu} \cos 2\pi k_i, \quad (k_1 \ldots, k_\nu) = \mathbf{k} \in \mathbb{T}^\nu. \tag{2.19}$$

These formulas imply that the operator $\gamma_0(z)$ of (2.12) has the following matrix in $l^2(\mathbb{Z}^{d_2})$:

$$\gamma_0(x_2 - y_2; z) = G_0^{(d)}((0,x_2) - (0,y_2); z), \tag{2.20}$$

i.e., $\gamma_0(z)$ is a convolution operator in $l^2(\mathbb{Z}^{d_2})$. In view of (2.18) we have

$$\gamma_0(x_2; z) = \int_{\mathbb{T}^{d_2}} dk_2 e^{2i\pi k_2 \cdot x_2} \int_{\mathbb{T}^{d_1}} \frac{dk_1}{E_d(\mathbf{k}) - z}, \tag{2.21}$$

or

$$\gamma_0(x_2; z) = \int_{\mathbb{T}^{d_2}} dk_2 e^{2i\pi k_2 \cdot x_2} G_0^{(d_1)}(0, z - E_{d_2}(k_2)). \tag{2.22}$$

We shall denote

$$\hat{\gamma}_0(k_2; z) := G_0^{(d_1)}(0, z - E_{d_2}(k_2)), \tag{2.23}$$

i.e., $\hat{\gamma}_0(k_2; z)$ is the symbol, representing the operator $\gamma_0(z)$ in $L^2(\mathbb{T}^{d_2})$ as a multiplication operator. These formulas allow us to show that the hypotheses of Lemma 2.1 and Proposition 2.1 are valid for any z, $\Im z > 0$ (see Lemma 5.2). Besides, we have the following.

Lemma 2.2: Let $b(z)$ and u be the operators, defined by (2.12) and (2.9). Then for any integer $m \geqslant 1$,

$$((b(z)u)^m \varphi(k_2) = \left(\prod_{l=0}^{m-1} \hat{b}(k_2 + l\alpha; z) \right) \hat{\varphi}(k_2 + m\alpha), \quad k_2 \in \mathbb{T}^{d_2}, \tag{2.24}$$

where $\hat{\varphi}$ denotes the Fourier transform of $\varphi \in l^2(\mathbb{Z}^{d_2})$ and

$$\hat{b}(k_2; z) = \frac{g\hat{\gamma}_0(k_2; z) - i}{g\hat{\gamma}_0(k_2; z) + i} \tag{2.25}$$

where $\hat{\gamma}_0(k_2, z)$ is defined in (2.23).

Proof: It follows from (2.9) that the operator u is the shift by α in the space $L^2(\mathbb{T}^{d_2})$:

$$\widehat{(u\varphi)}(k_2) = \hat{\varphi}(k_2 + \alpha). \tag{2.26}$$

From this and the fact that $b(z)$ of (2.12) is the multiplication by the function $\hat{b}(k_2; z)$ of (2.25) in the space $L^2(\mathbb{T}^{d_2})$ we prove the lemma.

We will obtain now a representation of the Green function of H which will be central in the subsequent spectral analysis of the absolutely continuous spectrum of the operator.

Theorem 2.1: *Let H be the operator, defined by (1.1)–(1.5). Then the Green function of H [the matrix in $l^2(\mathbb{Z}^d)$ of its resolvent $G(z) = (H - z)^{-1}$] can be written in the following form for $\Im z > 0$:*

$$G(\mathbf{x}, \mathbf{y}; z) = G_0^{(d)}(\mathbf{x} - \mathbf{y}; z) + \sum_{m=0}^{\infty} \int_{\mathbb{T}^{d_2}} dk_2 e^{2i\pi k_2 \cdot (x_2 - y_2)} t_m(k_2; z)$$
$$\times G_0^{(d_1)}(x_1; z - E_{d_2}(k_2)) G_0^{(d_1)}(y_1; z - E_{d_2}(k_2 + m\alpha)) e^{-2i\pi m\alpha \cdot y_2}, \tag{2.27}$$

where

$$t_m(k_2;z)=\frac{g}{g\,\hat\gamma_0(k_2;z)+i}\begin{cases}-1, & m=0,\\ 2i\sigma(g\,\hat\gamma_0(k_2+\alpha;z)+i)^{-1}, & m=1,\\ 2i\sigma^m(g\,\hat\gamma_0(k_2+m\alpha;z)+i)^{-1}\prod_{l=1}^{m-1}\hat b(k_2+l\alpha;z), & m\geqslant 2,\end{cases} \tag{2.28}$$

$G_0^{(d_1)}(x_1;z)$ is the Green function (2.18) of the d_1-dimensional Laplacian, $E_{d_2}(k_2)$ is defined in (2.19) for $\nu=d_2$, and $\hat\gamma_0(k_2;z)$, $\hat b(k_2;z)$ are defined respectively in (2.23) and (2.25).

Besides, the (generalized) kernel of the operator $T(z)$ of (2.4) and of Lemma 2.1 has the following form in $L^2(\mathbb{T}^d)$:

$$T(\mathbf{k},\mathbf{p};z)=\sum_{m=0}^{\infty} t_m(k_2;z)\,\delta(k_2+m\alpha-p_2), \tag{2.29}$$

where $t_m(k_2;z)$ is defined in (2.28). In particular, the kernel is independent of the components $k_1,p_1\in\mathbb{T}^{d_1}$ of its arguments $\mathbf{k},\mathbf{p}\in\mathbb{T}^d$.

Remark: Formulas (2.27) and (2.29) have to be compared with the formulas for respective quantities for point potential: $V(\mathbf{x})=v\,\delta(\mathbf{x})$, $(d_2=0)$ and for the constant surface potential: $V(\mathbf{x})=v\,\delta(x_1)$, $v=\text{const}$. In the first case we have

$$G(\mathbf{x},\mathbf{y};z)=G_0^{(d)}(\mathbf{x}-\mathbf{y};z)-\frac{v}{1+v\,G_0^{(d)}(0;z)}G_0^{(d)}(\mathbf{x};z)G_0^{(d)}(\mathbf{y};z), \tag{2.30}$$

and

$$T(\mathbf{k},\mathbf{p};z)=\frac{v}{1+v\,G_0^{(d)}(0;z)}, \tag{2.31}$$

while in the second case,

$$\begin{aligned}G(\mathbf{x},\mathbf{y};z)=G_0^{(d)}(\mathbf{x}-\mathbf{y};z)-v\int_{\mathbb{T}^{d_2}}dk_2\frac{e^{2i\pi k_2\cdot(x_2-y_2)}}{1+v\,G_0^{(d_1)}(0;z-E_{d_2}(k_2))}\\ \times G_0^{(d_1)}(x_1;z-E_{d_2}(k_2))\;\;G_0^{(d_1)}(y_1;z-E_{d_2}(k_2)),\end{aligned} \tag{2.32}$$

and

$$T(\mathbf{k},\mathbf{p};z)=\frac{v\,\delta(k_2-p_2)}{1+v\,G_0^{(d_1)}(0;z-E_{d_2}(k_2))}. \tag{2.33}$$

In particular the term, corresponding to $m=0$ in (2.27), coincides with the second of (2.32) in which v is replaced by ig.

Proof of Theorem 2.1: According to Lemma 5.2, $\|b(z)\|<1$ for $\Im z>0$. Hence we can write the operator $(1-\sigma bu)^{-1}$ in (2.14) for $q=1$ as the Neumann–Liouville series in powers of σbu. Applying Lemma 2.2 to each term of the series, we get (2.27) after simple algebra. Formula (2.29) follows from (2.4) and (2.27). Theorem 2.1 is then proved.

Remark: Formulas (2.27) and (2.29) are the basic tools of spectral and scattering analysis of the operator (1.1) presented in this article. An advantage of these formulas is that they are valid for all values of the spectral parameter $z=E+i\varepsilon$, up to the real values $z=E\pm i0$, for $|E|<d$, in the case of α's with rationally independent components [quasi-periodic in x_2 potential $V(\mathbf{x})$] and they are valid for all $E\in\mathbb{R}$ in the case of α's with rational components [periodic in x_2 potential $V(\mathbf{x})$].

One more general fact, concerning the operator H and necessary in the sequel, is given by the following theorem.

Theorem 2.2: *Let $H=H_0+V$ be the operator defined by (1.1), (1.2) and (2.1). Then its spectrum $\sigma(H)$ contains the interval $[-d,d]=\sigma(H_0)$ for all $g\in\mathbb{R}$, $\alpha\in\mathbb{R}^{d_2}$ and $\omega\in[0,1]$.*

Proof: We will apply the H. Weyl criterion, according to which $E\in\mathbb{R}$ belongs to the spectrum of a self-adjoint operator H if and only if there exists a sequence $\{\Psi_n\}_{n\in\mathbb{N}}$ of vectors of respective Hilbert space such that $\|\Psi_n\|=1$, and that $\lim_{n\to\infty}\|(H-E)\Psi_n\|=0$.

Denote by $\mathbf{1}_r$ the indicator of the ball $\{\mathbf{x}\in\mathbb{Z}^d:|\mathbf{x}|\leqslant r\}$ and set for all $\mathbf{k}\in\mathbb{T}^d$

$$\Psi_n(\mathbf{x})=\mathbf{1}_n(\mathbf{x})(1-\delta(x_1))e^{2i\pi\mathbf{k}.\mathbf{x}}/N_n;\quad N_n^2=\sum_{\mathbf{x}\in\mathbb{Z}^d}|\mathbf{1}_n(\mathbf{x})(1-\delta(x_1))|^2=O(n^d),\quad n\to\infty.$$

It is easy to find that

$$(H\Psi_n)(\mathbf{x})=\begin{cases}E_d(\mathbf{k})\Psi_n(\mathbf{x}), & |\mathbf{x}|\leqslant n-2,|x_1|\geqslant 2;\\ A_n(\mathbf{x}), & n-2\leqslant|\mathbf{x}|\leqslant n+2;\\ b_n(\mathbf{x}), & |x_1|\leqslant 1;\\ 0, & |\mathbf{x}|\geqslant n+3,\end{cases}$$

where $\|A_n\|=O(n^{-1/2})$, $\|b_n\|=O(n^{-d_1/2})$ as $n\to\infty$. This proves the theorem.

III. ABSOLUTE CONTINUOUS SPECTRUM IN THE ALMOST PERIODIC CASE

In this section we assume that the vector $\alpha\in\mathbb{R}^{d_2}$ from (1.3) has rationally independent components, i.e., that the relation $\alpha_1 r_1+\cdots+\alpha_{d_2}r_{d_2}=0$ with rational coefficients $r_1,\ldots,r_{d_2}$ implies that all these coefficients are equal to zero.

Theorem 3.1: *Let $H=H_0+V$ be the self-adjoint operator defined by (1.1)–(1.5) in which the vector $\alpha\in\mathbb{R}^{d_2}$ has rationally independent components. Then H has purely absolutely continuous spectrum on the interval $(-d,d)$.*

Proof: According to the general principles (see, e.g., Ref. 24), it suffices to prove that for any vector $\Phi\in l^2(\mathbb{Z}^d)$ of a dense set the limit $\Im(G(E+i0)\Phi,\Phi)$ exists and is bounded for all $E\in(-d,d)$. Restricting ourselves to the vectors concentrated at a point $\mathbf{x}\in\mathbb{Z}^d$, i.e., to the vectors $\delta_{\mathbf{x}}=\{\delta(\mathbf{x}-\mathbf{y})\}_{\mathbf{y}\in\mathbb{Z}^d}$, we have to prove that for any $\mathbf{x}\in\mathbb{Z}^d$ the limit $\Im G(\mathbf{x},\mathbf{x};E+i0)$ exists and is bounded for all $E\in(-d,d)$. We shall prove more, namely that $G(\mathbf{x},\mathbf{y};E+i0)$ exists and is bounded for all $E\in(-d,d)$ and all $\mathbf{x},\mathbf{y}\in\mathbb{Z}^d$. In view of Theorem 2.1, we have to prove that the series of (2.27) converges not only for $\Im z>0$ but also for $\Im z=0$.

Since the vector α has rationally independent components, we have uniformly in $k_2\in\mathbb{T}^{d_2}$ and for any $\gamma>0$ (see, e.g., Ref. 3),

$$\lim_{m\to\infty}\sharp\{l\in\mathbb{Z}:\ \{k_2+l\alpha\}\in K_\gamma(E),\ \ 1\leqslant l\leqslant m\}m^{-1}=|K_\gamma(E)|,\tag{3.1}$$

where $\{k_2+l\alpha\}$ is the d_2-dimensional vector, whose components are the fractional parts of components of the vector $k_2+l\alpha$,

$$K_\gamma(E)=\{k_2\in\mathbb{T}^{d_2}:\ E-E_{d_2}(k_2)\in[-d_1+\gamma,d_1-\gamma]\},\tag{3.2}$$

and $|K_\gamma(E)|$ denotes the Lebesgue measure of the set $K_\gamma(E)\subset\mathbb{T}^{d_2}$. It is easy to check that for any $|E|<d$ there exists $\gamma>0$ such that $K_\gamma(E)$ is an open set of $\mathbb{T}^{d_2}$. According to Lemma 5.3, in this case there exists $\delta>0$ such that $|\hat{b}(k_2,E+i0)|\leqslant 1-\delta,\forall k_2\in K_\gamma(E)$, and according to (3.1), there exists $m_0>0$ such that

$$\sharp\{l\in\mathbb{Z}:\ \{k_2+l\alpha\}\in K_\gamma(E),\ \ 1\leqslant l\leqslant m\}\geqslant\frac{m}{2}|K_\gamma(E)|$$

for all $m \geqslant m_0$. Hence we have the following bound for the product on the r.h.s. of (2.27):

$$\left| \prod_{l=1}^{m-1} \hat{b}(k_2 + l\alpha; E + i0) \right| \leqslant (1-\delta)^{m|K_\gamma(E)|/2}, \quad m \geqslant m_0, \tag{3.3}$$

and the series in the r.h.s. of (2.27) converges uniformly in $k_2 \in \mathbb{T}^{d_2}$. Besides, by using bound (3.3) and Lemma 5.5, it can be shown that for $|E| \leqslant d - \gamma$, $\gamma > 0$, the series is bounded in k_2 and E, hence we can integrate the series with respect to k_2. Theorem is proved.

Remarks: (1) Another form to express (3.1)–(3.3) is to write the relation:

$$\lim_{m\to\infty} \left| \prod_{l=1}^{m-1} \hat{b}(k_2 + l\alpha; E + i0) \right|^{1/m} = \exp\left\{ \int_{\mathbb{T}^{d_2}} dq_2 \log|\hat{b}(q_2; E + i0)| \right\}, \tag{3.4}$$

valid uniformly in $k_2 \in \mathbb{T}^{d_2}$ (see Ref. 3) and showing that if $|E| \leqslant d - \gamma$, $\gamma > 0$, then the integral on the r.h.s. is negative, thus the product on the l.h.s. is exponentially decaying in m as $m \to \infty$.

(2) Theorem 3.1 reveals a fairly simple mathematical mechanism responsible for the absolutely continuous spectrum for the ''subspace'' potential (1.3) and (1.4) with $d_1 \geqslant 1$ (recall that in the ''volume'' case $d_1 = 0$, $d_2 = d$, the absolutely continuous spectrum is absent, moreover if α is Diophantine, then the spectrum is pure point[5]). The mechanism is the positiveness of the imaginary part of $\hat{\gamma}_0(k_2; E + i0) = G_0^{(d_1)}(0, E + i0 - E(k_2))$ in a certain domain of (E, k_2). This is most transparent in the ''genuine surface'' case $d_1 = 1$, where $G_0^{(1)}(0, E + i0)$ is pure imaginary if $|E| < 1$ and is pure real if $|E| \geqslant 1$ [see formula (3.37) below]. In the latter case $|\hat{b}(k_2; E + i0))| = 1$ and the series (2.27) diverges for a dense set of energies (see Ref. 19). This leads to the pure point spectrum everywhere outside of the spectrum $\sigma(H_0)$ of the Laplacian (similarly to the volume case,[5] where the analog of $\hat{\gamma}_0(k_2; E)$ in (2.25) is real for all $E \in \mathbb{R}$). In the former case $|\hat{b}(k_2; E + i0))|$ is strictly less than 1 for any $E \in (-d, d)$ on an open set of $k_2 \in \mathbb{T}^{d_2}$, the series is convergent and the spectrum inside of $\sigma(H_0) = [-d, d]$ is pure absolutely continuous.

As usual in scattering theory, a fact of primary interest is the existence and completeness of wave operators $\Omega_\pm = \mathrm{s} \cdot \lim_{t \to \mp\infty} e^{itH} e^{-itH_0} \mathcal{E}_0(\Delta)$, where $\mathcal{E}_0$ is the resolution of identity of H_0, and Δ is an interval of the spectral axis. In the next theorem we prove these properties in our case.

We mention first that in Refs. 8, 9, 11, and 14, the scattering theory was developed for the operator H_1, acting in $l^2(\mathbb{Z}^d_+)$, $\mathbb{Z}^d_+ = \{(x_1, x_2) \in \mathbb{Z}^d; x_1 \geqslant 0, x_2 \in \mathbb{Z}^{d-1}\}$, and defined as

$$(H_1\Psi)(\mathbf{x}) = \begin{cases} \displaystyle\sum_{|\mathbf{x}-\mathbf{y}|=1} \Psi(\mathbf{y}), & x_1 \geqslant 1; \\ \Psi(1, x_2) + \displaystyle\sum_{|x_2 - y_2|=1} \Psi(0, y_2) + v(x_2)\Psi(0, x_2), & x_1 = 0, \end{cases} \tag{3.5}$$

for certain random and almost periodic surface potentials v. The operator can be viewed as a boundary value problem for the discrete Laplacian in $l^2(\mathbb{Z}^d_+)$ with the boundary condition $\Psi(-1, x_2) = v(x_2)\Psi(0, x_2), x_2 \in \mathbb{Z}^{d-1}$. The ''unperturbed'' operator H_0 here is the discrete Dirichlet Laplacian, corresponding to $v \equiv 0$ in (3.5). The operator H_1 is closely related to our operator H of (1.1) for the surface case $d_1 = 1$, $d_2 = d - 1$ via standard Green's formulas.

Theorem 3.2: *Under the conditions of Theorem 3.1, the wave operators $\Omega_\pm$ for the pair (H, H_0), defined by (1.1)–(1.5), exist and are complete for any closed interval $\Delta = [a, b] \subset (-d, d)$.*

Proof: Existence of wave operators is a rather general fact. It was proved in Ref. 8 for a general surface perturbation v in (3.5). In our case the proof is practically the same. Thus we have to prove the completeness. Mimicking the argument of Refs. 11 and 14, developed for the boundary value problem (3.5), it is easy to reduce the proof of completeness to the proof of the relation:

$$\sup_{\varepsilon>0, E\in[a,b]} \sum_{x_2\in\mathbb{Z}^{d_2}} |G((x_1,x_2),\mathbf{y};E\pm i\varepsilon)|^2<\infty \tag{3.6}$$

for any fixed $x_1\in\mathbb{Z}^{d_1}$, $\mathbf{y}\in\mathbb{Z}^d$ and $[a,b]\subset(-d,d)$. Our formulas (2.27) and (2.28) for the Green function of H can be written in the form

$$G((x_1,x_2),\mathbf{y};z)=\int_{\mathbb{T}^{d_2}} dk_2 e^{2i\pi k_2\cdot x_2} G((x_1,k_2),\mathbf{y};z),$$

where

$$G((x_1,k_2),\mathbf{y};z)=G_0^{(d_1)}(x_1-y_1;z-E_{d_2}(k_2))\sum_{m=0}^{\infty} t_m(k_2,z)G_0^{(d_1)}(x_1;z-E_{d_2}(k_2))$$
$$\times G_0^{(d_1)}(y_1;z-E_{d_2}(k_2+m\alpha))e^{2i\pi y_2\cdot(k_2+m\alpha)}. \tag{3.7}$$

Thus, applying the Parseval equality for the Fourier transform with respect to the variable x_2, we can present the sum in (3.6) as

$$\int_{\mathbb{T}^{d_2}} dk_2 |G((x_1,k_2),\mathbf{y};E+i\varepsilon)|^2. \tag{3.8}$$

We have shown in the proof of Theorem 3.1 that the series (3.7) converges uniformly in $k_2\in\mathbb{T}^{d_2}$ for $z=E+i\varepsilon$, $E\in[a,b]\subset(-d,d)$; $\varepsilon>0$. Hence the integral in (3.8) is finite for these values of E and ε. This proves (3.6).

In the next theorem we construct a family of generalized eigenfunctions of H, relating them to the Green function of the operator, as in the conventional scattering theory.[23,25]

Theorem 3.3: *Let $G(\mathbf{x},\mathbf{y};z)$ be the Green function of the operator $H=H_0+V$, defined by (1.1)–(1.5), in which the vector α is rationally independent. Set*

$$G(\mathbf{x},\mathbf{k};z)=\sum_{\mathbf{y}\in\mathbb{Z}^d} G(\mathbf{x},\mathbf{y};z)e^{2i\pi\mathbf{k}\cdot\mathbf{y}},\quad \mathbf{k}\in\mathbb{T}^d, \tag{3.9}$$

$$\Psi_z(\mathbf{x},\mathbf{k})=(E_d(\mathbf{k})-z)G(\mathbf{x},\mathbf{k};z), \tag{3.10}$$

and

$$\dot{\mathbb{T}}^{d_2}=\mathbb{T}^{d_2}\setminus\{\overbrace{(0,0,\ldots,0)}^{d_2-\text{times}},\overbrace{(\pi,\pi,\ldots,\pi)}^{d_2-\text{times}}\};\quad \dot{\mathbb{T}}^d=\mathbb{T}^{d_1}\times\dot{\mathbb{T}}^{d_2}. \tag{3.11}$$

Then, for $z=E_d(\mathbf{k})\mp i\varepsilon$, the limits

$$\Psi_\pm(\mathbf{x},\mathbf{k})=\lim_{\varepsilon\to+0}\Psi_z(\mathbf{x},\mathbf{k})|_{z=E_d(\mathbf{k})\mp i\varepsilon}=\lim_{\varepsilon\to+0}\pm i\varepsilon G(\mathbf{x},\mathbf{k};E_d(\mathbf{k})\mp i\varepsilon), \tag{3.12}$$

exist for all $\mathbf{k}\in\dot{\mathbb{T}}^d$, are bounded in $\mathbf{x}\in\mathbb{Z}^d$ for any $\mathbf{k}\in\dot{\mathbb{T}}^d$, are continuous in $\mathbf{k}$ varying in any compact set of $\dot{\mathbb{T}}^d$, and have the form

$$\Psi_\pm(\mathbf{x},\mathbf{k})=e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\sum_{m=0}^{\infty} t_m(k_2-m\alpha;z)G_0^{(d_1)}(x_1;z-E_{d_2}(k_2-m\alpha))|_{z=E_d(\mathbf{k})\mp i0}e^{2i\pi(k_2-m\alpha)\cdot x_2}, \tag{3.13}$$

where the coefficients $t_m(k_2,z)$ are defined in (2.28).

Moreover:

(i) the functions $\Psi_{\pm}(\mathbf{x},\mathbf{k})$ *satisfy the Schrödinger equation in* $\mathbf{x}$ *for any* $\mathbf{k}\in\dot{\mathbb{T}}^d$:

$$((H_0+V)\Psi_{\pm})(\mathbf{x},\mathbf{k})=E_d(\mathbf{k})\Psi_{\pm}(\mathbf{x},\mathbf{k}). \tag{3.14}$$

(ii) The functions $\Psi_{\pm}(\mathbf{x},\mathbf{k})$ *are the unique solutions of the equation:*

$$\Psi_{\pm}(\mathbf{x},\mathbf{k})=e^{2i\pi\mathbf{k}\cdot\mathbf{x}}-\sum_{\mathbf{y}\in\mathbb{Z}^d} G_0^{(d)}(\mathbf{x}-\mathbf{y};E_d(\mathbf{k})\mp i0)V(\mathbf{y})\Psi_{\pm}(\mathbf{y},\mathbf{k}), \tag{3.15}$$

for any $\mathbf{k}\in\dot{\mathbb{T}}^d$ *in the class of sequences* $\Psi=\{\Psi(\mathbf{x})\}_{\mathbf{x}\in\mathbb{Z}^d}$ *whose restrictions* $\psi=\{\Psi(0,x_2)\}_{x_2\in\mathbb{Z}^{d_2}}$ *and the sequences* $\{(1+\sigma e^{-2i\pi\alpha\cdot x_2})\psi(x_2)\}_{x_2\in\mathbb{Z}^{d_2}}$ *are representable as the Fourier transforms of measures of bounded variation on* $\mathbb{T}^{d_2}$, *and the sum of the r.h.s. of (3.15) is understood as the generalized convolution of respective functions and measures.*

(iii) The families $\{\Psi_{\pm}(\cdot,\mathbf{k})\}_{\mathbf{k}\in\dot{\mathbb{T}}^d}$ *are orthonormalized, i.e., if for any continuous function* $\hat{\Phi}$ *of compact support in* $\dot{\mathbb{T}}^d$ *we set*

$$\Phi_{\pm}(\mathbf{x})=\int_{\dot{\mathbb{T}}^d}\Psi_{\pm}(\mathbf{x},\mathbf{k})\hat{\Phi}(\mathbf{k})d\mathbf{k}, \tag{3.16}$$

then for any two such functions $\hat{\Phi}^{(1)}$ *and* $\hat{\Phi}^{(2)}$ *we have*

$$\sum_{\mathbf{x}\in\mathbb{Z}^d}\Phi_{\pm}^{(1)}(\mathbf{x})\overline{\Phi_{\pm}^{(2)}(\mathbf{x})}=\int_{\dot{\mathbb{T}}^d}d\mathbf{k}\hat{\Phi}^{(1)}(\mathbf{k})\overline{\hat{\Phi}^{(2)}(\mathbf{k})}. \tag{3.17}$$

(iv) The functions $\Psi_{\pm}:\mathbb{Z}^d\times\dot{\mathbb{T}}^d\to\mathbb{C}$ *are the kernels of the wave operators* $\Omega_{\pm}$, *whose existence and completeness are proved in Theorem 3.2, i.e., for any* $\Phi\in l^2(\mathbb{Z}^d)$ *such that the support of its Fourier transform* $\hat{\Phi}$ *is a compact set in* $\dot{\mathbb{T}}^d$ *we have*

$$(\Omega_{\pm}\Phi)(\mathbf{x})=\int_{\dot{\mathbb{T}}^d}\Psi_{\pm}(\mathbf{x},\mathbf{k})\hat{\Phi}(\mathbf{k})d\mathbf{k}. \tag{3.18}$$

Proof: We use again our basic formulas (2.27) and (2.28) for the resolvent of H. Making the Fourier transform of (2.27) with respect to $\mathbf{y}$ and multiplying the result by $E_d(\mathbf{k})-z$, we present (3.10) in the form

$$\Psi_z(\mathbf{x},\mathbf{k})=e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\sum_{m=0}^{\infty} t_m(k_2-m\alpha;z)G_0^{(d_1)}(x_1;z-E_{d_2}(k_2-m\alpha))e^{2i\pi(k_2-m\alpha)\cdot x_2}. \tag{3.19}$$

Each term in this series is continuous in k_2 and z, $\Im z>0$ and can be extended to real $z=E+i0$, $E\in[a,b]$, if the closed interval $[a,b]$ lies strictly inside $(-d,d)$. According to bound (3.3), the series converges uniformly in $k_2\in\dot{\mathbb{T}}^{d_2}$ and $a\leqslant\Re z\leqslant b$, $\Im z\geqslant 0$, hence it defines a continuous function in this domain. This allows us to perform the limits (3.12) for $k_2\in\dot{\mathbb{T}}^{d_2}$ and to obtain formula (3.13).

Our limitation $\mathbf{k}\in\dot{\mathbb{T}}^d$, where $\dot{\mathbb{T}}^d$, is defined in (3.11), is necessary because for $\mathbf{k}\in\mathbb{T}^d\backslash\dot{\mathbb{T}}^d$ and for the respective two values of $E=\pm d$ we cannot guarantee the validity of bound (3.3), thus the convergence of the series in formula (3.13).

Let us prove now property (i) of $\Psi_{\pm}(\mathbf{x},\mathbf{k})$. We have obviously

$$\sum_{|\mathbf{t}-\mathbf{x}|=1} H_0(\mathbf{x}-\mathbf{t})G(\mathbf{t},\mathbf{y};z)-EG(\mathbf{x},\mathbf{y};z)+V(\mathbf{x})G(\mathbf{x},\mathbf{y};z)=i\varepsilon G(\mathbf{x},\mathbf{y};z)+\delta(\mathbf{x}-\mathbf{y}).$$

The definition (3.10) of $\Psi_z(\mathbf{x},\mathbf{k})$ and an easy justification of the interchange of the multiplication by $V(\mathbf{x})$ and of the Fourier transformation in $\mathbf{y}$ in the third term of the l.h.s. lead to the equality

$$\sum_{|\mathbf{t}-\mathbf{x}|=1} H_0(\mathbf{x}-\mathbf{t})\Psi_z(\mathbf{t},\mathbf{k})-E\Psi_z(\mathbf{x},\mathbf{k})+V(\mathbf{x})\Psi_z(\mathbf{x},\mathbf{k})=i\varepsilon(\Psi_z(\mathbf{x},\mathbf{k})+e^{2i\pi\mathbf{k}\cdot\mathbf{x}}).$$

Now, in view of relation (3.12), the limit of the r.h.s. of the last equality is zero as $\varepsilon\to 0$, and we get (3.14).

Let us prove now assertion (*ii*) of the theorem, i.e., that $\Psi_{\pm}(\mathbf{x},\mathbf{k})$ satisfy (the Lippmann–Schwinger) equation (3.15). We remark first that any solution Ψ of (3.15) is uniquely determined by its restriction $\psi(x_2)=\Psi((0,x_2))$ to the subspace $\mathbb{Z}^{d_2}$, and that ψ verifies the equation, which can be symbolically written as

$$\psi(x_2)=e^{2i\pi k_2\cdot x_2}-(\gamma_0 v\,\psi)(x_2),\quad x_2\in\mathbb{Z}^{d_2}. \tag{3.20}$$

Hence we have to verify that the restriction $\psi(x_2,\mathbf{k})$ of (3.13) to $\mathbb{Z}^{d_2}$ satisfies (3.20). By using (3.19 and (3.13), we can write the restriction symbolically in the form

$$\psi=\{1-(g\gamma_0+i)^{-1}g\gamma_0[1-2i\sigma u(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}]\}e_2\big|_{z=E_d(\mathbf{k})\mp i0}, \tag{3.21}$$

where $e_2(x_2)=e^{2i\pi k_2\cdot x_2}$ and we used definition (2.12) of γ_0. The symbols γ_0, b and u in the formula denote now not operators on $l^2(\mathbb{Z}^{d_2})$ or in $L^2(\mathbb{T}^{d_2})$, defined in (2.12) and in (2.9), but just operations acting on sequences (functions of $x_2\in\mathbb{Z}^{d_2}$) and representable as Fourier transforms of measures of bounded variation depending on the parameter $z=E(\mathbf{k})\mp i0$, $\mathbf{k}\in\dot{\mathbb{T}}^{d_2}$. In order words, they belong to the linear manifold:

$$\mathcal{L}_{\mathbf{k}}=\left\{f(x_2),x_2\in\mathbb{Z}^{d_2}: f(x_2)=\int_{\mathbb{T}^{d_2}} e^{2i\pi p_2\cdot x_2}M_{\mathbf{k}}(dp_2);\quad \text{Var } M_{\mathbf{k}}<\infty\right\}. \tag{3.22}$$

The operations b and γ_0 are multiplications of $M_{\mathbf{k}}$ by $\hat{b}(p_2,z)$ and by $\hat{\gamma}_0(p_2,z)$ with $z=E_d(\mathbf{k})\mp i0$, and u is the shift by α of the measure. The operation $(1-bu)^{-1}$ is defined by the series $\Sigma_{m=0}^{\infty}(bu)^m$, whose terms are given by (2.24), and which converges for all $\mathbf{k}\in\dot{\mathbb{T}}^d$. By using these facts and a simple algebra, we can rewrite (3.21) as

$$\psi=i(1+\sigma u)(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}e_2\big|_{z=E_d(\mathbf{k})\mp i0}. \tag{3.23}$$

Hence we have for the r.h.s. of (3.20):

$$e_2-\gamma_0 v\,\psi=e_2-g\gamma_0(1-\sigma u)(1+\sigma u)^{-1}(1+\sigma u)(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}e_2$$

or

$$e_2-\gamma_0 v\,\psi=\{1-g\gamma_0(1-\sigma u)(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}\}e_2,$$

meaning that the complex spectral parameter z is replaced by $E(\mathbf{k})\mp i0$. The r.h.s. of the relation coincides with ψ. To prove this fact we have to repeat the arguments leading to (3.13) and (3.21), but starting from formula (2.14) for the operator $T(z)$ instead of formula (2.15). Thus we have proved that (3.13) solves (3.15).

Let us prove that (3.13) is the unique solution of (3.15) in $\mathcal{L}_{\mathbf{k}}$ and such that their multiplication by $(1+\sigma e^{2\pi ik_2\cdot x_2})$ belongs also to $\mathcal{L}_{\mathbf{k}}$. Consider the homogeneous equation, corresponding to (3.15):

$$\chi=\gamma_0 v\,\chi \tag{3.24}$$

on the same manifold, and write the equality $\chi=(1+u)\varphi$, where φ also belongs to (3.22). Then we obtain the following equation for φ:

$$(1+g\gamma_0)(1-\sigma bu)\varphi=0,$$

where the symbols γ_0, b, and u are again understood as operations in the class $\mathcal{L}_{\mathbf{k}}$. Applying to this relation the operation $(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}$,which is well defined in $\mathcal{L}_{\mathbf{k}}$, we obtain $\varphi=0$.

According to the above considerations the second term in the r.h.s. of (3.15) is the Fourier transform of the product of $G_0^{(d_1)}(x_1;E_d(\mathbf{k})-E_{d_2}(k_2)+i0)$ [the Fourier transform of $G_0^{(d)}(\mathbf{x};z)|_{z=E_d(\mathbf{k})+i0}$ in x_2] and of the measure $M_{\mathbf{k}}$, corresponding to $v\psi$:

$$\int_{\mathbb{T}^{d_2}} G_0^{(d_1)}(x_1;E_d(\mathbf{k})-E_{d_2}(p_2)+i0)M_{\mathbf{k}}(dp_2). \tag{3.25}$$

In view of (2.10), and (3.23) we have

$$\begin{aligned} v\psi&=g(1-\sigma u)(1-\sigma bu)^{-1}(g\gamma_0+i)^{-1}e_2|_{z=E_d(\mathbf{k})\mp i0}\\ &=g(g\gamma_0+i)^{-1}\left(1-2i\sum_{m=0}^{\infty}\sigma u(\sigma bu)^m(g\gamma_0+i)^{-1}e_2\right)\Bigg|_{z=E_d(\mathbf{k})\mp i0}. \end{aligned} \tag{3.26}$$

By using this relation and the notations introduced in Lemma 2.1 and in Theorem 2.1, we obtain that the measure corresponding to the second term of the r.h.s. of (3.15) is

$$\sum_{m=0}^{\infty} t_m(k_2-m\alpha;E_d(\mathbf{k})\pm i0)\,\delta(k_2-m\alpha-p_2).$$

Combining these formulas we obtain (3.15).

Let us prove now the orthogonality of $\Psi_{\pm}(\mathbf{x},\mathbf{k})$, corresponding to different $\mathbf{k}$'s, i.e., relation (3.17). It is clear that it is sufficient to prove (3.17) for $\Phi^{(1)}=\Phi^{(2)}$. The proof is rather technical and we outline only its scheme, considering, say, Φ_-.

The first step is the proof of the relation

$$\lim_{\varepsilon\to+0}\sum_{\mathbf{x}\in\mathbb{Z}^d}|\Phi_-(\mathbf{x})-\Phi_\varepsilon(\mathbf{x})|^2=0, \tag{3.27}$$

where [cf. (3.16)]

$$\Phi_\varepsilon(\mathbf{x})=\int_{\mathbb{T}^d}\Psi_{E_d(\mathbf{k})+i\varepsilon}(\mathbf{x},\mathbf{k})\hat{\Phi}(\mathbf{k})d\mathbf{k}, \tag{3.28}$$

and $\Psi_z(\mathbf{x},\mathbf{k})$ is defined in (3.10), i.e., $\Psi_{E_d(\mathbf{k})+i\epsilon}(\mathbf{x},\mathbf{k})=-i\varepsilon G(\mathbf{x},\mathbf{k};E_d(\mathbf{k})+i\varepsilon)$. The proof is based on formulas (3.19) and (3.13), and on the continuity of $G_0^{(d)}(\mathbf{x},E+i\varepsilon)$ with respect to $\varepsilon>0$. It is given in Lemma 3.1 below.

The second step is the proof of the relation

$$\lim_{\varepsilon\to+0}\sum_{\mathbf{x}\in\mathbb{Z}^d}|\hat{\Phi}_\varepsilon(\mathbf{x})|^2=\int_{\mathbb{T}^d}|\hat{\Phi}(\mathbf{k})|^2d\mathbf{k}, \tag{3.29}$$

which implies (3.17). We will just sketch a proof of this relation.

Write the resolvent identity for the pair $G(\overline{z}')$ and $G(z'')$:

$$\sum_{\mathbf{t}\in\mathbb{Z}^d} G(\mathbf{t},\mathbf{y};z'')\overline{G(\mathbf{t},\mathbf{x};z')}=(\overline{z}'-z'')^{-1}(G(\mathbf{t},\mathbf{x};\overline{z}')-G(\mathbf{t},\mathbf{y};z'')). \tag{3.30}$$

Replace on the r.h.s. of the identity G by $G_0-G_0TG_0$ [see (2.4)]. We obtain after a simple algebra

$$G_0'G_0''+(\overline{z}'-z'')^{-1}(G_0'T'G_0'-G_0''T''G_0''), \tag{3.31}$$

where $G_0'=(H_0-\overline{z}')^{-1}$, $G_0''=(H_0-z'')^{-1}$ and T' and T'', are the T-operators for the spectral parameters $\overline{z}'$ and z'', respectively. Now we make the Fourier transformation with respect to $\mathbf{x}$ and $\mathbf{y}$, multiplying (3.30) and (3.31) by $e^{2i\pi\mathbf{p}\cdot\mathbf{y}-2i\pi\mathbf{k}\cdot\mathbf{x}}$ and summing the result over $\mathbf{x},\mathbf{y}\in\mathbb{Z}^d$. The l.h.s. of the obtained relation is $(\Psi_{z''},\Psi_{z'})$. As for the r.h.s., it can be written symbolically as

$$\delta(\mathbf{k}-\mathbf{p})-T(\mathbf{k},\mathbf{p};\overline{z}')\left(\frac{1}{E_d(\mathbf{p})-\overline{z}'}-\frac{1}{z''-\overline{z}'}\right)-T(\mathbf{k},\mathbf{p};z'')\left(\frac{1}{E_d(\mathbf{k})-z''}-\frac{1}{\overline{z}'-z''}\right), \tag{3.32}$$

where $T(\mathbf{k},\mathbf{p};z)$ is the kernel in $L^2(\mathbb{T}^d)$ of the T-operator, whose expression is given in Theorem 2.1. Setting in (3.32) $z'=E_d(\mathbf{p})+i\varepsilon$ and $z''=E_d(\mathbf{k})+i\varepsilon$, we obtain

$$\delta(\mathbf{k}-\mathbf{p})-(T(\mathbf{k},\mathbf{p};E_d(\mathbf{k})+i\varepsilon)+T(\mathbf{k},\mathbf{p};E_d(\mathbf{p})+i\varepsilon))\times\left(\frac{1}{E_d(\mathbf{p})-E_d(\mathbf{k})+i\varepsilon}-\frac{1}{E_d(\mathbf{p})-E_d(\mathbf{k})+2i\varepsilon}\right).$$

After multiplication by $\hat{\Phi}(\mathbf{k})\overline{\hat{\Phi}(\mathbf{p})}$, where $\hat{\Phi}(\mathbf{k})$ is a smooth function whose compact support is strictly inside $\dot{\mathbb{T}}^d$, and after the subsequent integration with respect to $\mathbf{k},\mathbf{p}\in\mathbb{T}^d$, the second term of the last expression tends (weakly) to zero as $\varepsilon\to 0$. We use the explicit form (2.29) of the kernel $T(\mathbf{k},\mathbf{p};z)$ to prove that $T(\mathbf{k},\mathbf{p};E+i\varepsilon)$ is weakly bounded in $\varepsilon\geqslant 0$, if $\mathbf{k}$, $\mathbf{p}$ are strictly inside of $\dot{\mathbb{T}}^d$ and $|E|<d$. After that we are left to prove that the expression in the parentheses tends weakly to zero as $\varepsilon\to 0$. This proves assertion (*iii*) of the theorem.

Let us prove assertion (*iv*), according to which the solutions $\Psi_{\pm}(\mathbf{x},\mathbf{k})$ are the kernels of the wave operators $\Omega_{\pm}$, whose existence and completeness are proved in Theorem 3.2 (see also Ref. 14 for similar results). We will base the proof on the formula (see Ref. 23):

$$\Omega_{\pm}\Phi=\mathrm{s}-\lim_{\varepsilon\to\mp 0}\int_{-\infty}^{\infty} G(E+i\varepsilon)\mathcal{E}_0(dE)\Phi,$$

where $\mathcal{E}_0$ is the resolution of identity of the Laplacian H_0 of (1.2), and $G(z)=(H-z)^{-1}$. In the $(\mathbf{x},\mathbf{k})$ representation, usual in the scattering theory, this formula can be written as follows:

$$(\Omega_{\pm}\Phi)(\mathbf{x})=\mathrm{s}-\lim_{\varepsilon\to\mp 0}(\Omega_{\varepsilon}\Phi)(\mathbf{x}), \tag{3.33}$$

where

$$(\Omega_{\varepsilon}\Phi)(\mathbf{x})=\int_{\mathbb{T}^d}\Psi_{E_d(\mathbf{k})+i\varepsilon}(\mathbf{x},\mathbf{k})\hat{\Phi}(\mathbf{k})d\mathbf{k}, \tag{3.34}$$

and $\Psi_z(\mathbf{x},\mathbf{k})$ is defined in (3.10).

According to general principles, it suffices to prove (3.33) for a dense set of vectors of $L^2(\mathbb{T}^d)$. We choose a set of functions of the form $\hat{\Phi}((k_1,k_2))=\hat{\Phi}_1(k_1)\hat{\Phi}_2(k_2)$, where $\hat{\Phi}_{1,2}$ are smooth and the support of $\hat{\Phi}_1$ does not contain the critical points of E_{d_1}. Denoting the r.h.s. of (3.34) by $\Phi_{\varepsilon}(\mathbf{x})$, we have to prove the relations:

(a) $\lim_{\varepsilon\to\mp 0}\Phi_\varepsilon(\mathbf{x})=\Phi_\pm(\mathbf{x})$;
(b) $\lim_{\varepsilon\to\mp 0}\Sigma_{\mathbf{x}\in\mathbb{Z}^d}|\Phi_\varepsilon(\mathbf{x})-\Phi_\pm(\mathbf{x})|^2=0$,

where $\Phi_\pm(\mathbf{x})$ are defined in (3.16). Both facts are proved in the Lemma 3.1 below. Theorem 3.3 is proved.

Remarks: (1). Functions $\Psi_\pm(\mathbf{x},\mathbf{k})$ are analogs of the Sommerfeld solutions, which appear in the scattering theory for potentials decaying in all directions and which provide a complete set of generalized eigenfunctions for the part of the spectrum that coincides with the spectrum of the Laplacian.[23,25] Likewise, (3.15) is an analog of the Lippmann–Schwinger equation of scattering theory.

(2). According to formula (3.13), $\Psi_\pm(\mathbf{x},\mathbf{k})$ depends on the component x_2 of $\mathbf{x}=(x_1,x_2)$, $x_1\in\mathbb{Z}^{d_1}$, $x_2\in\mathbb{Z}^{d_2}$ via the product of $e^{ik_2\cdot x_2}$ and of a one-periodic function of the argument $\alpha\cdot x_2$, i.e., of a quasi-periodic function of $x_2\in\mathbb{Z}^{d_2}$ [recall that we assume in this section that the components of the vector α in (1.4) are rationally independent]. This fact is in agreement with the widely accepted idea, according to which generalized eigenfunctions of absolutely continuous spectrum of differential and finite difference operators with almost periodic coefficients have the ''almost Bloch'' form, i.e., the form of the product of a plane wave and an almost periodic function with the same frequencies as the coefficients (see, e.g., Ref. 22).

(3). According to formula (2.18), if $|E|>\nu$, the Green function $G_0^{(\nu)}(\mathbf{x};E+i0)$ of the ν-dimensional Laplacian decays exponentially and if $|E|<\nu$ it decays as $1/|x|^{(\nu-1)/2}$ for $\nu\geqslant 2$ [in the one-dimensional case for $|E|<1$, $G_0^{(1)}(x;E+i0)$ behaves as $e^{i\eta(E)|x|}$, where $\eta(E)$ is a real valued function, see formulas (3.37) and (3.38) below]. As m varies the expression $E_d(\mathbf{k})-E_{d_2}(k_2-m\alpha)$ has values inside $(-d_1,d_1)$ as well as outside this interval. Then the Green function

$$G_0^{(d_1)}(x_1;E_d(\mathbf{k})-E_{d_2}(k_2-m\alpha)),$$

entering the expression (3.13), may be exponentially decaying or slowly decaying (i.e., as $1/|x|^{(\nu-1)/2}$). In other words, we can write, say, for Ψ_-,

$$\Psi_-(\mathbf{x},\mathbf{k})=e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\Psi_{\mathrm{vol}}(\mathbf{x},\mathbf{k})+\Psi_{\mathrm{surf}}(\mathbf{x},\mathbf{k}), \tag{3.35}$$

where Ψ_{vol} is the part of the sum in (3.13) containing only slow decaying terms, and Ψ_{surf} is the part containing the exponentially decaying terms.

Recall now the definition of the surface states according to Ref. 15 (for other definitions see Refs. 4, 10, and 14).

Definition 3.1: Let Ψ_E be a generalized eigenfunction, corresponding to a point E of the spectrum of the operator H of (1.1)–(1.3). We say that Ψ_E is a surface state, if for any $\varepsilon>0$ we have

$$\sup_{x_2\in\mathbb{Z}^{d_2}}(1+|x_2|^{d_2/2+\varepsilon})^{-1}\sum_{x_1\in\mathbb{Z}^{d_1}}|\Psi_E((x_1,x_2))|^2<\infty. \tag{3.36}$$

Since the part $e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\Psi_{\mathrm{vol}}(\mathbf{x},\mathbf{k})$ of the solution (3.35) $\Psi(\mathbf{x},\mathbf{k})$ is not decaying in the x_1-direction, the solution is not a ''surface'' state but a ''volume'' state. Hence, we can say that Theorem 3.3 above implies the existence of the volume states for all $E\in(-d,d)$. Theorem 3.4 below implies that these generalized eigenfunctions are complete in the interval $(-d,d)$. We conclude that there is no surface states in the interval $(-d,d)$ of the spectrum of the operator H in the considered case of quasi-periodic surface potential (1.3) and (1.4). However, despite that surface states are absent, the volume states (3.35) contain both a term, $e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\Psi^{\mathrm{vol}}(\mathbf{x},\mathbf{k})$ which slowly decays or even only oscillates in $|x_1|$, and a term, $\Psi_{\mathrm{surf}}(\mathbf{x},\mathbf{k})$, which exponentially decays in $|x_1|$. They are respectively the superposition of reflected or transmitted waves which propagate inside the bulk and of waves which propagate only along the subspace $\mathbb{Z}^{d_2}$.

(4) The scattering interpretation (3.35) of generalized eigenfunction (3.13) allows us to introduce transmission and reflection amplitudes and coefficients (the latter as square of the modulus of the former). Consider the simplest case of $d_1=1$ and recall that

$$G_0^{(1)}(x;z)=\frac{ie^{i\eta(z)|x|}}{\sin\eta(z)}=-\frac{e^{i\eta(z)|x|}}{\sqrt{z^2-1}}, \tag{3.37}$$

where $-\cos\eta=z$, or

$$\eta(z)=-i\log(-z+\sqrt{z^2-1}), \tag{3.38}$$

and we use the branch of the logarithm that has the cut along the negative semi-axis and the branch of $\sqrt{z^2-1}$ fixed by the condition $\sqrt{z^2-1}=z(1+O(z^{-1})), z\to\infty$. In particular $\Im\eta(z)\geqslant 0$ for $\Im z\geqslant 0$ and

$$\eta(E+i0)\in\begin{cases}(0,\pi), & |E|<1,\\ \pi+i\mathbb{R}_+, & E>1,\\ +i\mathbb{R}_+, & E<-1.\end{cases} \tag{3.39}$$

Combining these formulas and (3.13), we can present $\Psi_{\mathrm{vol}}(\mathbf{x},\mathbf{k})$ in (3.35) for $d_1=1$ as

$$\Psi_{\mathrm{vol}}(\mathbf{x},\mathbf{k})=\sum_m \Psi_m(\mathbf{k})e^{i\eta_m(\mathbf{k})|x_1|+2i\pi(k_2-\alpha m)\cdot x_2}, \tag{3.40}$$

where Σ_m denotes the sum of those terms in (3.13) for which $\eta_m(\mathbf{k}):=\eta(\lambda_m(\mathbf{k})+i0)$ is real, and $\lambda_m(\mathbf{k})$ is defined by the equation: $\lambda_m(\mathbf{k})=E_d(\mathbf{k})-E_{d-1}(k_2-m\alpha)$. Recall that in the one-dimensional scattering problem for the potential $v\,\delta(x)$, $x\in\mathbb{Z}$, the Sommerfeld solutions are [cf. (2.30) and (2.31)]

$$\Psi_-(x,k)=e^{2i\pi kx}-\frac{iv}{iv+\sin 2\pi k}e^{i\eta_-(k)|x|},$$

where $\eta_-(k)=\eta(\cos 2\pi k+i0)$, $k\in\mathbb{T}$. Hence in this case

$$t(k)=\frac{\sin 2\pi k}{iv+\sin 2\pi k},\quad r_-(k)=-\frac{iv}{iv+\sin 2\pi k}$$

are the transmission and the reflection amplitudes. This makes it natural to view

$$t_0=1+\Psi_0(\mathbf{k}),\quad r_0=\Psi_0(\mathbf{k}),$$

where $\Psi_0(\mathbf{k})$ is given by (3.40), as the transmission and the reflection amplitudes of the plane waves scattered by the surface potential (1.3) and propagating in direction $\mathbf{k}$ of the incident wave and in the opposite direction. Likewise it is natural to view the coefficients $\Psi_m(\mathbf{k})$, $m\geqslant 1$ of (3.40) as the transmission and the reflection amplitudes of the scattered plane waves propagating in the directions $((2\pi)^{-1}\eta_m,k_2+m\alpha)$ and $(-(2\pi)^{-1}\eta_m,k_2+m\alpha)$, respectively, to the right and to the left of the plane $x_1=0$. This scattering theory interpretation of the solutions (3.13) is in agreement with the form of the scattering matrix $\mathcal{S}$ in our case. We use the general formula [see Ref. 23, formula (4.2.30)]

$$\mathcal{S}=1-\mathcal{T},\quad \mathcal{T}=(-2i\pi)\ \mathrm{s}-\lim_{\substack{\varepsilon_1\to 0\\ \varepsilon_2\to 0}}\int \delta_{\varepsilon_2}(H_0-\lambda)T(\lambda+i\varepsilon_1)\mathcal{E}_0(dE), \tag{3.41}$$

where $\delta_\varepsilon(A)=(2i\pi)^{-1}[(A+i\varepsilon)^{-1}-(A-i\varepsilon)^{-1}]$, $T(z)$ is defined in (2.4), $\mathcal{E}_0$ is the resolution of identity of H_0, and the limits have to be carried out in the following order: first $\varepsilon_1\to 0$, second $\varepsilon_2\to 0$. Formula (3.41) implies that for any sufficiently smooth function $\hat{f}$ on $\mathbb{T}^d$ we have

$$(\mathcal{T}\hat{f})(\mathbf{k})=(-2i\pi)\ \ \mathrm{s}-\lim_{\substack{\varepsilon_1\to 0\\ \varepsilon_2\to 0}}\int_{T^d}\delta_{\varepsilon_2}(E_d(\mathbf{k})-E_d(\mathbf{p}))T(\mathbf{k},\mathbf{p};E_d(\mathbf{p})+i\varepsilon_1)\hat{f}(\mathbf{p})d\mathbf{p}.$$

By using formula (2.29) for the kernel of the T-operator, it can be shown that the generalized kernel $\mathcal{T}(\mathbf{k},\mathbf{p})$ of the $\mathcal{T}$-matrix of (3.41) is

$$\begin{aligned}\mathcal{T}(\mathbf{k},\mathbf{p})&=-2i\pi\delta(E_d(\mathbf{k})-E_d(\mathbf{p}))T(\mathbf{k},\mathbf{p};E_d(\mathbf{p})+i0)\\&=-2i\pi\delta(E_d(\mathbf{k})-E_d(\mathbf{p}))\sum_{m=0}^{\infty}t_m(k_2;E_d(\mathbf{k})+i0)\,\delta(k_2+m\alpha-p_2).\end{aligned}\tag{3.42}$$

Now we formulate and prove the lemma that was used in the proofs of assertions (*iii*) and (*iv*) of Theorem 3.3.

Lemma 3.1: Let $\hat{\Phi}_{1,2}:\mathbb{T}^{d_{1,2}}\to\mathbb{C}$ *be smooth functions. Assume that the support of* $\hat{\Phi}_1$ *does not contain the critical points of* E_{d_1}:

$$\mathrm{supp}\ \ \hat{\Phi}_1\cap\{k_1\in\mathbb{T}^{d_1}:\nabla_1 E_{d_1}(k_1)=0\}=\varnothing.\tag{3.43}$$

Set for $\varepsilon\neq 0$

$$\Phi_\varepsilon(\mathbf{x})=\int_{\mathbb{T}^d}\Psi_{E_d(\mathbf{k})+i\varepsilon}(\mathbf{x},\mathbf{k})\hat{\Phi}(\mathbf{k})d\mathbf{k},$$

where $\Psi_z(\mathbf{x},\mathbf{k})$ *is defined in (3.9), (3.10), and (3.19), and* $\hat{\Phi}(\mathbf{k})$ *is of the form* $\hat{\Phi}((k_1,k_2))=\hat{\Phi}(k_1)\hat{\Phi}(k_2)$. *Then*

$$\lim_{\varepsilon\to\mp 0}\sum_{\mathbf{x}\in\mathbb{Z}^d}|\Phi_\varepsilon(\mathbf{x})-\Phi_\pm(\mathbf{x})|^2=0,\tag{3.44}$$

where $\Phi_\pm(\mathbf{x},\mathbf{k})$ *are defined in (3.12) and (3.16).*

Proof: By using (3.19), we find that for any $\varepsilon\neq 0$

$$\begin{aligned}\Phi_\varepsilon(\mathbf{x})=\Phi(\mathbf{x})+\sum_{m=0}^{\infty}&\int_{\mathbb{T}^{d_1}}dp_1\hat{\Phi}_1(p_1)\int_{\mathbb{T}^{d_2}}dp_2 e^{2i\pi(k_2-m\alpha)\cdot x_2}\hat{\Phi}_2(p_2)\\&\times t_m(k_2,E_d(\mathbf{k})+i\varepsilon)G_0^{(d_1)}(x_1,E_d(\mathbf{k})-E_{d_2}(k_2-m\alpha)+i\varepsilon),\end{aligned}\tag{3.45}$$

where Φ is the Fourier transform of $\hat{\Phi}$. The integrals and the series in this formula converge and can be written in any order because of the bound (3.3) applicable in view of (3.43). The integral representation (2.18) for $G_0^{(d_1)}$ allows us to rewrite the last formula as follows:

$$\Phi_\varepsilon(\mathbf{x})=\Phi(\mathbf{x})+\int_{\mathbb{T}^d}e^{2i\pi\mathbf{k}\cdot\mathbf{x}}\hat{\Psi}_\varepsilon(\mathbf{k})d\mathbf{k},\tag{3.46}$$

where

$$\hat{\Psi}_\varepsilon(\mathbf{k})=\sum_{m=0}^{\infty}\int_{\mathbb{T}^{d_1}}dp_1\frac{\hat{\Phi}_1(p_1)\hat{\Phi}_2(k_2+m\alpha)}{E_d(\mathbf{k})-E_{d_1}(p_1)-E_{d_2}(k_2+m\alpha)+i\varepsilon}$$
$$\times t_m(k_2,E_{d_1}(p_1)+E_{d_2}(k_2+m\alpha)+i\varepsilon). \tag{3.47}$$

This series and the integral are convergent because the modulus of the denominator is bounded from below for $\varepsilon\neq 0$, and because of bound (3.3).

Now we will prove that for any $\mathbf{k}\in\mathbb{T}^d$, the limits $\lim_{\varepsilon\to\mp 0}\hat{\Psi}_\varepsilon(\mathbf{k})\equiv\hat{\Psi}_\mp(\mathbf{k})$ exist and that the convergence is bounded. Consider the case $\hat{\Psi}_-$ for the sake of definiteness. The building block of the coefficient $t_m(k_2,E+i\varepsilon)$ in (3.47) is the function $\hat{\gamma}_0(k_2,E+i\varepsilon)=G_0^{(d_1)}(0,E-E_{d_2}(k_2)+i\varepsilon))$. This function is real analytic in $k_2\in\dot{\mathbb{T}}^{d_2}$ [see (3.11) for the definition of $\dot{\mathbb{T}}^{d_2}$], and in $E\in(-d+\gamma,d-\gamma)$ for any fixed (small) $\gamma>0$ [see (2.18) and (2.19)]. By using identity (5.8) for $G_0^{(d_1)}$, we can write the mth term of formula (3.47) as

$$\int_0^\infty dt e^{-\varepsilon t-it(E_d(\mathbf{k})-E_{d_2}(k_2+m\alpha))}\hat{\Phi}_2(k_2+m\alpha)$$
$$\times\int_{\mathbb{T}^{d_1}}dp_1\hat{\Phi}_1(p_1)e^{-itE_{d_1}(p_1)}t_m(k_2,E_{d_1}(p_1)+E_{d_2}(k_2+m\alpha)+i\varepsilon)). \tag{3.48}$$

Since the support of $\hat{\Phi}_1$ does not contain critical points of E_{d_1} and since $G_m(k_2,E+i\varepsilon)$ is real analytic in $k_2\in\mathbb{T}^{d_2}$ and in $E\in(-d+\gamma,d-\gamma),\gamma>0$ for all $\varepsilon\geqslant 0$, we can integrate by parts twice in components of $p_1\in\mathbb{T}^{d_1}$, and obtain an expression of the form $t^{-2}\Phi_m(\mathbf{k},p_1,\varepsilon)$, where Φ_m is bounded in $\mathbf{k}\in\mathbb{T}^d$, $p_1\in\mathbb{T}^{d_1}$ and $\varepsilon>0$. This allows us to make the limit $\varepsilon\to+0$ in (3.48) and obtain a bounded in $\mathbf{k}$ expression.

Besides, Φ_m is a linear combination of the first and second partial derivatives in components of $p_1\in\mathbb{T}^{d_1}$ of the integrand in (3.48). The derivatives are a linear combination of products of bounded (and smooth) in $\mathbf{k}\in\mathbb{T}^d,p_1\in\mathbb{T}^{d_1}$ for $\varepsilon>0$, and independent of m functions, multiplied by the first and the second partial derivatives in components of $p_1\in\mathbb{T}^{d_1}$ of $\Pi_{l=1}^m\hat{b}(k_2+l\alpha,E_{d_1}(p_1)+E_{d_2}(k_2+m\alpha)+i\varepsilon))$. This leads to the bound $|\Phi_m(\mathbf{k},p_1,\varepsilon)|\leqslant c_1m^2e^{-c_2m}$ where $c_1,c_2>0$ and are independent of $m,\mathbf{k},p_1$ and ε. The bound allows us to make the limit $\varepsilon\to+0$ in (3.47) for any $\mathbf{k}\in\mathbb{T}^d$:

$$\lim_{\varepsilon\to+0}\hat{\Psi}_\varepsilon(\mathbf{k})=\hat{\Psi}_-(\mathbf{k}),$$

and to obtain the bound $|\Psi_\varepsilon(\mathbf{k})|\leqslant$const, valid for any $\varepsilon\geqslant 0$ and $\mathbf{k}\in\mathbb{T}^d$. Now the Lebesgue dominated convergence theorem and relation (3.12) proved above lead to the representation:

$$\Psi_-(\mathbf{x})=\Phi(\mathbf{x})+\int_{\mathbb{T}^d}e^{2i\pi\mathbf{k}.\mathbf{x}}\hat{\Psi}_-(\mathbf{k})d\mathbf{k}. \tag{3.49}$$

Subtracting this relation from (3.46) and applying to the result the Parseval equality, we obtain that

$$\sum_{\mathbf{x}\in\mathbb{Z}^d}|\Psi_\varepsilon(\mathbf{x})-\Psi_-(\mathbf{x})|^2=\int_{\mathbb{T}^d}|\hat{\Psi}_\varepsilon(\mathbf{k})-\hat{\Psi}_-(\mathbf{k})|^2d\mathbf{k}. \tag{3.50}$$

Thus (3.49) and the Lebesgue theorem imply (3.44). The lemma is proved.

Theorem 3.4: *Let $H=H_0+V$ be the self-adjoint operator on $l^2(\mathbb{Z}^d)$, defined by (1.1)–(1.5) in which the vector $\alpha\in\mathbb{R}^{d_2}$ has rationally independent components. Then the family $\{\Psi_z(\mathbf{x},\mathbf{k});\mathbf{x}\in\mathbb{Z}^d\}_{\mathbf{k}\in\dot{\mathbb{T}}^d}$, defined in Theorem 3.3 [see (3.9), (3.12), and (3.13)], is the complete system of generalized eigenfunctions of H in the part $(-d,d)$ of the spectrum of H, i.e.,*

(i) for any $f \in l^2(\mathbb{Z}^d)$, *the series*

$$F_{\pm}(\mathbf{k}) = \sum_{\mathbf{x} \in \mathbb{Z}^d} \overline{\Psi_{\pm}(\mathbf{x},\mathbf{k})} f(\mathbf{x}) \tag{3.51}$$

converges in $l^2(\mathbb{Z}^d)$;

(ii) if $\mathcal{E}_H(\Delta)$ *is the spectral projection of H, corresponding to the closed interval* $\Delta = [a,b] \subset (-d,d)$, *then*

$$\|\mathcal{E}_H(\Delta) f\|^2 = \int_{\mathbf{k} \in \dot{\mathbb{T}}^d : E_d(\mathbf{k}) \in \Delta} |F_{\pm}(\mathbf{k})|^2 d\mathbf{k}; \tag{3.52}$$

where $E_d(\mathbf{k})$ *is defined in (2.19)*;

(iii) the following relation is valid:

$$\|H\mathcal{E}_H(\Delta) f\|^2 = \int_{\mathbf{k} \in \dot{\mathbb{T}}^d : E_d(\mathbf{k}) \in \Delta} |E_d(\mathbf{k}) F_{\pm}(\mathbf{k})|^2 d\mathbf{k}. \tag{3.53}$$

Proof: We write the Hilbert identity for the Green function $G(\mathbf{x},\mathbf{y};z_{1,2})$, $\Im z_{1,2} \neq 0$:

$$G(\mathbf{x},\mathbf{y},z_1) - G(\mathbf{x},\mathbf{y},z_2) = (z_1 - z_2) \sum_{\mathbf{s} \in \mathbb{Z}^d} G(\mathbf{x},\mathbf{s};z_1) \overline{G(\mathbf{y},\mathbf{s};\overline{z_2})}. \tag{3.54}$$

By using the Parseval equality for the Fourier transform with respect to the variable $\mathbf{s}$ on the r.h.s. of this identity, we rewrite it as follows:

$$\int_{\mathbf{k} \in \mathbb{T}^d} d\mathbf{k} G(\mathbf{x},\mathbf{k},z_1) \overline{G(\mathbf{y},\mathbf{k},\overline{z_2})},$$

where $G(\mathbf{x},\mathbf{k},z)$ is the Fourier transform of $G(\mathbf{x},\mathbf{y},z)$ in the second variable $\mathbf{y}$, defined in (3.9). Multiply now resulting relation by $\overline{f(\mathbf{x})} f(\mathbf{y})$, where f has compact support in $\mathbb{Z}^d$ and sum over $\mathbf{x},\mathbf{y} \in \mathbb{Z}^d$. This yields

$$((G(z_1) - G(z_2)) f, f) = \int_{\dot{\mathbb{T}}^d} d\mathbf{k} \frac{z_1 - z_2}{(E_d(\mathbf{k}) - z_1)(E_d(\mathbf{k}) - z_2)} \overline{F_{z_1}(\mathbf{k})} F_{z_2}(\mathbf{k}),$$

where

$$F_z(\mathbf{k}) = \sum_{\mathbf{x} \in \mathbb{Z}^d} \overline{\Psi_z(\mathbf{x},\mathbf{k})} f(\mathbf{x}), \tag{3.55}$$

and $\Psi_z(\mathbf{x},\mathbf{k})$ is defined in (3.10). Setting $z_1 = \overline{z_2} = E + i\varepsilon, \varepsilon > 0$, we get

$$\frac{1}{\pi} \Im (G(E + i\varepsilon) f, f) = \frac{1}{\pi} \int_{\dot{\mathbb{T}}^d} d\mathbf{k} \frac{\varepsilon}{(E_d(\mathbf{k}) - E)^2 + \varepsilon^2} |F_{E+i\varepsilon}(\mathbf{k})|^2. \tag{3.56}$$

$\Delta = [a,b] \in (-d,d)$, we obtain on the l.h.s. of the resulting relation the expression $\|\mathcal{E}_H(\Delta) f\|^2$ can be continued in z to the real $z = E_d(\mathbf{k}) + i0 \in \Delta$, and that the continued function is uniformly continuous in $\mathbf{k} \in \{\mathbf{k} \in \dot{\mathbb{T}}^d : E_d(\mathbf{k}) \in \Delta\}$, where $\dot{\mathbb{T}}^d$ is defined in (3.11). Since f is of compact support in $\mathbb{Z}^d$, it suffices to show that $\Psi_z(\mathbf{x},\mathbf{k})$ possess this property for any fixed $\mathbf{x} \in \mathbb{Z}^d$. But this fact is proved Theorem 3.3. Thus we have established (ii) for the case where f's of finite support. The extension to f's belonging to $l^2(\mathbb{Z}^d)$ is based on the standard arguments of spectral theory [see, e.g., Refs. 25 and 24). This proves assertions (*i*) and (*ii*). As for assertion (*iii*), it follows from (*ii*) and from the spectral theorem.

IV. THE PERIODIC CASE

In this section we consider the operator $H=H_0+V$ of (1.1)–(1.5) in which $d_1=d_2=1$ and α is a rational number: $\alpha=p/q$, where q and $p<q$ are positive integers and p is not a divisor of q. In this case our potential v of (1.4) is q-periodic. We show that under these conditions the whole spectrum of H is absolutely continuous and we construct corresponding generalized eigenfunctions. It turns out that there are two types of generalized eigenfunctions. Both types have the Bloch–Floquet form in the longitudinal coordinates x_2 but behave differently in the transverse coordinate x_1. Similar spectral structure was found before in Refs. 7, 16, and 17 for the continuous Schödinger operator in $\mathbb{R}^d$, $d\leqslant 3$, whose potential is a periodic system of point scatterers in $\mathbb{R}^{d_2}$, $d_2=1,2$.

We will follow the same strategy as in the preceding section, namely the construction of generalized eigenfunctions based on the formulas for the Green function of Sec. II and on formulas (3.9), (3.10) and (3.12) of Theorem 3.3. Thus we have to analyze the behavior of the Green function as the spectral parameter tends to the real axis. Our first goal is to find the set of energies for which the limit $G(\mathbf{x},\mathbf{y},E+i0)$ exists and is bounded, i.e., the purely absolutely continuous part of the spectrum. We shall see that unlike the quasi-periodic case, where this set is $[-d,d]$, in the periodic case the whole spectrum is pure absolutely continuous. The spectrum which lies outside $[-d,d]$ consists of surface states only. As for the part in the interior of $[-d,d]$, it consists of the volume states whose energies occupy the whole interval $[-d,d]$, and of the surface states that may exist under certain conditions.

For any $z\in\mathbb{C},\Im z\neq 0$, and $m=1,\ldots,q$ define the function:

$$P_m(k_2;z)=\sigma^m\prod_{l=1}^{m}\hat{b}(k_2+l\alpha;z),\quad \forall k_2\in\mathbb{T}, \tag{4.1}$$

where σ and $\hat{b}$ are defined by (2.11), (2.12),(2.25) and $\mathbb{T}=(0,1]$. Then, by using Lemma 2.2, we obtain for $\alpha=p/q$

$$\sigma^q(\widehat{(bu)^q\varphi})(k_2)=\sigma^q\prod_{l=1}^{q}\hat{b}(k_2+l\alpha;z)\hat{\varphi}(k_2)=P_q(k_2;z)\hat{\varphi}(k_2), \tag{4.2}$$

where the operator u is defined in (2.9). We conclude that $\sigma^q(bu)^q$ is a multiplication operator by the function P_q in the space $L^2(\mathbb{T})$.

Theorem 4.1: *Let $H=H_0+V$ be the operator defined by (1.1)–(1.5) in which $d_1=d_2=1$ and $\alpha=p/q$, $p\in\mathbb{Z}$, $q\in\mathbb{Z}\{0\}$ is a rational parameter. Then the Green function $G(\mathbf{x},\mathbf{y};z)=(H-z)^{-1}(\mathbf{x},\mathbf{y})$, $\mathbf{x},\mathbf{y}\in\mathbb{Z}^2$ of H can be written in the form*

$$\begin{aligned}G(\mathbf{x},\mathbf{y};z)=G_0^{(2)}(\mathbf{x}-\mathbf{y};z)+\sum_{m=0}^{q}\int_{\mathbb{T}}dk_2e^{2i\pi k_2(x_2-y_2)}t_m(k_2;z)\\ \times G_0^{(1)}(x_1;z+\cos 2\pi k_2)G_0^{(1)}(y_1;z+\cos 2\pi(k_2+m\alpha))e^{-2i\pi m\alpha y_2},\end{aligned} \tag{4.3}$$

where

$$t_m(k_2;z)=\frac{g}{g\hat{\gamma}_0(k_2;z)+i}\times\begin{cases}-1, & m=0;\\ \dfrac{1}{1-P_q(k_2;z)}\dfrac{2i\sigma}{g\hat{\gamma}_0(k_2+\alpha;z)+i}, & m=1;\\ \dfrac{1}{1-P_q(k_2;z)}\dfrac{2i\sigma}{g\hat{\gamma}_0(k_2+m\alpha;z)+i}P_{m-1}(k_2;z), & m\geqslant 2,\end{cases} \tag{4.4}$$

$G_0^{(\nu)}(.;z)$, $\nu=1,2$ is the Green function (2.27) of the ν-dimensional discrete Laplacian, $\hat{\gamma}_0(.;z)$, and $\hat{b}(.;z)$ are defined in (2.22) and in (2.25).

The proof of the theorem is based on the same argument as that used in the proof of Theorem 2.1.

Formulas (4.3) and (4.4) suggest that the spectrum $\sigma(H)$ of H contains the set $S=\{E \in \mathbb{R}: \exists k_2 \in \mathbb{T}; P_q(k_2,E)=1\}$. We prove below that indeed, the limit $G(\mathbf{x},\mathbf{y},E+i0)$ exists and is bounded for all $E \in S\backslash D$ where D is a discrete set.

For any $1>\gamma>0$, $E \in \mathbb{R}$ and $l=1,\ldots,q$, define the sets

$$K_\gamma^l(E)=\{k_2 \in \mathbb{T}: E+\cos 2\pi(k_2+l\alpha) \in [-1+\gamma,1-\gamma]\}, \tag{4.5}$$

and

$$K_\gamma(E)=\bigcup_{l=1}^{q} K_\gamma^l(E), \quad K_\gamma^c(E)=\mathbb{T}\backslash K_\gamma(E). \tag{4.6}$$

It follows from formula (4.2), Lemma 5.3, and from the argument of the proof of Theorem 3.1 that for any $0<\gamma<1$ there exists $\delta(\gamma)>0$ such that the inequality $\sup_{\varepsilon>0}|P_q(k_2,E+i\varepsilon)|<1-\delta$ is valid uniformly in $k_2 \in K_\gamma(E)$. This means that the function $(1-P_q(k_2,E+i0))^{-1}$ is well defined and bounded on the sets

$$K(E)=\bigcup_{0<\gamma<1} K_\gamma(E),$$

and that possible singularities of this function which are given by the ''band-equation,''

$$P_q(k_2,E)=1, \tag{4.7}$$

where $P_q(k_2,E)=P_q(k_2,E+i0)$, are localized on $K^c(E)$. It is natural to think that energies, satisfying the band equation (4.7) for some $k_2 \in \mathbb{T}$, belong to the spectrum of H. The following proposition describes properties of solutions of the band equation.

Proposition 4.1: For any $2 \leqslant q<\infty$ the band equation (4.7) admits a finite number N_q' of positive solutions $0 \leqslant E_1(k_2)<\ldots<E_{N_q'}(k_2)<\infty$ (the positive energy band functions), and a finite number N_q'' of negative solutions $-\infty<E_{-N_q''}(k_2)<\ldots<E_{-1}(k_2) \leqslant 0$ (the negative energy band functions). The functions E_j, $j=-N_q'',\ldots,-1,1,\ldots,N_q'$ are $1/q$-periodic in k_2, and are real analytic in the interior of their respective domains $\mathcal{D}_j \subset \mathbb{T}$ (each domain $\mathcal{D}_j$ is a closed subset of $\mathbb{T}$). Moreover, the band functions are separated in the sense that

(i) for any $j=-N_q'',\ldots -1,1,\ldots N_q'$ there exists a finite subset $\mathcal{D}_j'$ of $\mathcal{D}_j$, such that for all $\mathbf{k} \in \mathbb{T}\times(\mathcal{D}_j\backslash\mathcal{D}_j')$ we have

$$|E_j(k_2)-E_2(\mathbf{k})|>0, \tag{4.8}$$

where $E_2(\mathbf{k})=-\cos 2\pi k_1-\cos 2\pi k_2$;

(ii) there exists a positive constant $\eta_q>0$ such that for any $j,j'=-N_q'',\ldots -1,1,\ldots N_q'$, $j \neq j'$ we have

$$\inf_{k_2 \in \mathcal{D}_j \cap \mathcal{D}_{j'}} |E_j(k_2)-E_{j'}(k_2)| \geqslant \eta_q>0. \tag{4.9}$$

The proof of the proposition will be given after the proof of Theorem 4.6.

The band function E_j, $j=-N_q'',\ldots,-1,1,\ldots,N_q'$ defined in Proposition 4.1 determines the band-gap structure of the spectrum of the periodic in x_2 operator H in the following sense.

Theorem 4.2: *Let $H=H_0+V$ be the operator defined in Theorem 4.1. Then for all rational parameter α, $g\neq 0$, and $\omega\in[0,1]$ the spectrum $\sigma(H)$ of H is a finite union of closed intervals (energy bands):*

$$\sigma(H)=\bigcup_{j=-N_q''}^{N_q'} \operatorname{Ran} E_j \cup [-2,2]. \tag{4.10}$$

The assertion that $(-d,d)$ is in the spectrum of H is a consequence of Theorem 2.2, the rest of the theorem will be proved after the proof of Theorem 4.5.

Let us now define the set $\mathcal{E}_c$ of critical energies as

$$\mathcal{E}_c=\left\{E\in\mathbb{R}:\exists j\in\{-N_q'',\ldots,N_q'\},\ \exists k_2\in\mathbb{T},\ E_j(k_2)=E \text{ and either } \frac{dE_j}{dk_2}(k_2)=0 \text{ or } k_2\in\partial\mathcal{D}_j\right\}.$$

Denote

$$D=\mathcal{E}_c\cup\{-d,d\}, \tag{4.11}$$

and notice that because of Proposition 4.1 D is a discrete subset of $\mathbb{R}$.

Theorem 4.3: *Let $H=H_0+V$ be the operator defined in Theorem 4.1, and let $G(\mathbf{x},\mathbf{y};z)$ be its Green function. Then for any rational α, $g\in\mathbb{R}$, and $\omega\in[0,1)$ the limit $G(\mathbf{x},\mathbf{y};E+i0)$ exists and is bounded for any $E\in\sigma(H)\backslash D$ and $\mathbf{x},\mathbf{y}\in\mathbb{Z}^2$, where D is defined in (4.11). In particular the spectrum of H is absolutely continuous.*

Proof: For any $E\in\sigma(H)\backslash D$ set $z=E+i\varepsilon$, $\varepsilon>0$ and fix $0<\gamma<1$. By using formula (4.3) we can write that

$$G(\mathbf{x},\mathbf{y};z)=G_{1,\gamma}(\mathbf{x},\mathbf{y};z)+G_{2,\gamma}(\mathbf{x},\mathbf{y};z),\quad \mathbf{x},\mathbf{y}\in\mathbb{Z}^2, \tag{4.12}$$

where

$$\begin{aligned}G_{1,\gamma}(\mathbf{x},\mathbf{y};z)=G_0^{(2)}(\mathbf{x}-\mathbf{y};z)+\int_{K_\gamma(E)} dk_2 e^{2i\pi k_2(x_2-y_2)}\sum_{m=0}^{q} t_m(k_2;z)\\ \times G_0^{(1)}(x_1;z+\cos 2\pi k_2)G_0^{(1)}(y_1;z+\cos 2\pi(k_2+m\alpha))e^{-2i\pi m\alpha y_2},\end{aligned} \tag{4.13}$$

$K_\gamma(E)$ and t_m are defined in (4.6) and in (4.4), and

$$G_{2,\gamma}(\mathbf{x},\mathbf{y};z)=G(\mathbf{x},\mathbf{y};z)-G_{1,\gamma}(\mathbf{x},\mathbf{y};z). \tag{4.14}$$

Since the inequality $\sup_{\varepsilon\geqslant 0}|P_q(k_2,E+i\varepsilon)|<1-\delta$ is valid uniformly on $K_\gamma(E)$ for some $\delta\varepsilon(0,1)$, the same arguments as in the proof of Theorem 3.1 imply that the limit $G_{1,\gamma}(\mathbf{x},\mathbf{y};E+i0)$ exists and is bounded.

Hence, to prove the theorem we have to show the same property for the term $G_{2,\gamma}(\mathbf{x},\mathbf{y};z)$ of (4.12). We first note that by Proposition 4.1 this term can be rewritten as

$$G_{2,\gamma}(\mathbf{x},\mathbf{y};z)=\int_{K_\gamma^c(E)} dk_2 \frac{g_{2,\gamma}(\mathbf{x},\mathbf{y},k_2;z)}{1-P_q(k_2;z)}, \tag{4.15}$$

where for any $0<\gamma<1$, $\varepsilon\geqslant 0$ and $(\mathbf{x},\mathbf{y})\in\mathbb{Z}^2\times\mathbb{Z}^2$, $g_{2,\gamma}(\mathbf{x},\mathbf{y},.;z)$ are smooth functions on $K_\gamma^c(E)$. Now in order to compute the integral on the r.h.s. of (4.15), consider the level sets

$$S_j=S_j(E,\gamma)=\{k_2\in K_\gamma^c(E):E_j(k_2)=E\},\quad j=-N_q'',\ldots,N_q',$$

and the following neighborhoods ν_j of S_j:

$$\nu_j = \nu_j(E,\gamma,\eta) = \{k_2 \in K_\gamma^c(E) : |E_j(k_2) - E| \leqslant \eta\}.$$

If η is small enough, then Proposition 4.1 implies the relation: $\nu_j \cap \nu_{j'} = \varnothing$ if $j \neq j'$. Thus to prove that $G_{2,\gamma}(\mathbf{x},\mathbf{y};E+i\varepsilon)$ exists and is bounded as $\varepsilon \to 0$, it suffices to show that this holds for

$$G_{2,\gamma,j}(\mathbf{x},\mathbf{y};E+i\varepsilon) = \int_{\nu_j} dk_2 \frac{g_{2,\gamma}(\mathbf{x},\mathbf{y},k_2;E+i\varepsilon)}{1-P_q(k_2;z)}, \quad j = -N_q'', \ldots, N_q'. \tag{4.16}$$

Since η is small enough and $E \notin D$, we can parametrize ν_j by the local coordinate $\tilde{E}$ defined by the relation $\tilde{E} = E_j(k_2)$. Denoting φ_j the respective change of variables and J_{φ_j} its Jacobian, we have

$$G_{2,\gamma,j}(\mathbf{x},\mathbf{y};E+i\varepsilon) = \int_{-\eta}^{\eta} d\tilde{E} \frac{g_{2,\gamma} \circ \varphi_j(\tilde{E})}{1-P_q \circ \varphi_j(\tilde{E})} J_{\varphi_j}, \quad j = -N_q'', \ldots, N_q'. \tag{4.17}$$

Suppose now that η and ε are so small that we can write

$$1 - P_q(\varphi_j(\tilde{E}), E+i\varepsilon) = (\tilde{E} - E - i\varepsilon) p_j(\tilde{E}; E+i\varepsilon), \tilde{E} \in [-\eta, \eta],$$

where p_j, $j = -N_q'', \ldots, N_q'$ are smooth and nonvanishing functions on the interval $[-\eta,\eta]$ such that

$$|p_j(.,E)| \geqslant C |\partial_E P_q(.,E)| + O(\eta) + O(\varepsilon)$$

for some strictly positive constant C. Moreover, it follows from the proof of Proposition 4.1 [see formula (4.46)] that

$$|\partial_E P_q(\varphi_j(\tilde{E}), E)| \neq 0, \quad \tilde{E} \in [-\eta, \eta].$$

Then standard arguments show that $G_{2,\gamma,j}(\mathbf{x},\mathbf{y};E+i0)$, $j = -N_q'', \ldots, N_q'$ exist and are bounded, hence $G_{2,\gamma}(\mathbf{x},\mathbf{y};E+i0)$ also exists and is bounded. The theorem is proved.

The last theorem together with the arguments of the proof of Theorem 3.2 lead to the following.

Theorem 4.4: *Under the conditions of Theorem 4.1, the wave operators* $\Omega_\pm$ *for the pair* (H,H_0) *defined in (1.1)–(1.5) with a rational* α *exist and are complete for any closed interval* $\Delta = [a,b] \subset (-d,d) \setminus \cup_{j=-N_q''}^{N_q'} \mathrm{Ran}\, E_j$.

Our next theorem shows that surface states (see Definition 3.1) exist and are bounded. They can be labeled by the "quasi-momentum" $k_2 \in \mathbb{T}/q$, such that respective eigenvalues are given by the band functions: $E = E_j(k_2)$. The "volume" states that do not belong to $l^2(\mathbb{Z})$ in x_1 are labeled by the "momentum" $\mathbf{k} \in \mathbb{T}^2$, such that the corresponding eigenvalues are given by the dispersion law of the Laplacian: $E = E_2(\mathbf{k}) = -(\cos 2\pi k_1 + \cos 2\pi k_2)$. We consider here only the nondegenerate case, i.e., the case where chosen pairs $(k_2, E = E_j(k_2))$, and $(\mathbf{k}, E = E_2(\mathbf{k}))$ are such that $E_j(k_2) \neq E_2(\mathbf{k})$. By Proposition 4.1 this property is valid for all energies except a finite set.

Consider the set

$$\mathbb{T}_j^2 = \{\mathbf{k} = (k_1,k_2) \in \dot{\mathbb{T}}^2, \ \ k_2 \in \mathbb{T}_j\}, \ \ j = -N_q'', \ldots, N_q',$$

where $\dot{\mathbb{T}}^2$ is defined in (3.11), $\mathbb{T}_j = \mathcal{D}_j \setminus \mathcal{D}_j'$, and $\mathcal{D}_j, \mathcal{D}_j'$ are defined in Proposition 4.1, and the set

$$\ddot{\mathbb{T}}^2 = \bigcup_{j=-N_q''}^{N_q'} \{\mathbf{k} = (k_1,k_2) \in \dot{\mathbb{T}}^2, \ k_2 \in \mathbb{T} \setminus \mathcal{D}_j'\}.$$

Hence the set of degenerate energies is

$$\mathcal{E}_c' = \{E \in \mathbb{R}, \exists \mathbf{k} = (k_1, k_2) \in \mathbb{T}^2, \exists j = -N_q'', \ldots, N_q', \ E = E_2(\mathbf{k}) = E_j(k_2)\}.$$

By Proposition 4.1 $\mathcal{E}_c'$ is a discrete set as well as the set

$$D' = D \cup \mathcal{E}_c',$$

where D is defined in (4.11).

Theorem 4.5: *Let $H = H_0 + V$ be the operator defined in Theorem 4.1, $G(\mathbf{x},\mathbf{y};z)$ be its Green function, and $G(\mathbf{x},\mathbf{k};z)$ be defined in (3.9). Then*

(i) for $z = E_2(\mathbf{k}) \mp i\varepsilon$ the limits

$$\Psi_{v,\pm}(\mathbf{x},\mathbf{k}) = \lim_{\varepsilon \to +0} \Psi_z(\mathbf{x},\mathbf{k})|_{z = E_2(\mathbf{k}) \mp i\varepsilon} = \lim_{\varepsilon \to +0} \pm i\varepsilon G(\mathbf{x},\mathbf{k};(E_2(\mathbf{k}) \mp i\varepsilon)), \tag{4.18}$$

exist for all $\mathbf{k} \in \ddot{\mathbb{T}}^2$, are bounded in $\mathbf{x} \in \mathbb{Z}^2$ for any $\mathbf{k} \in \ddot{\mathbb{T}}^2$, are continuous in $\mathbf{k}$ on any compact subset of $\ddot{\mathbb{T}}^2$ for any $\mathbf{x} \in \mathbb{Z}^2$, and satisfy the Schrödinger equation

$$((H_0 + V)\Psi_{v,\pm})(\mathbf{x},\mathbf{k}) = E_2(\mathbf{k})\Psi_{v,\pm}(\mathbf{x},\mathbf{k}). \tag{4.19}$$

(ii) For $z = E_j(k_2) \mp i\varepsilon$, $j = -N_q'', \ldots, N_q'$ the limits

$$\Psi_{s,j,\pm}(\mathbf{x},k_2) = \lim_{\varepsilon \to +0} \mp i\varepsilon I_j(\mathbf{k};z) G(\mathbf{x},\mathbf{k};(E_j(k_2) \mp i\varepsilon)),$$

in which

$$I_j(\mathbf{k};z) = (E_2(\mathbf{k}) - z)\left[\int_{\mathbb{T}} dk_1 \frac{1}{|(E_2(\mathbf{k}) - z)|^2}\right]^{1/2}$$

exist for any $\mathbf{k} = (k_1, k_2) \in \mathbb{T}_j^2$, are bounded in $\mathbf{x} \in \mathbb{Z}^2$ for any $k_2 \in \mathbb{T}_j$, are continuous in k_2 on any compact subset of $\mathbb{T}_j$ and satisfy the Schrödinger equation:

$$((H_0 + V)\Psi_{s,j,\pm})(\mathbf{x},k_2) = E_j(k_2)\Psi_{s,j,\pm}(\mathbf{x},k_2). \tag{4.20}$$

(iii) $\Psi_{s,j,\pm}(\cdot,k_2)$, $k_2 \in \mathbb{T}_j$ are surface states in the sense of Definition 3.1.

Remarks: (1) It can be shown that for all $\mathbf{k} \in \ddot{\mathbb{T}}^2$ such that $E_2(\mathbf{k}) \in (-d,d) \setminus \cup_{j=-N_q''}^{N_q'} \operatorname{Ran} E_j$ the function $\Psi_{v,\pm}$, defined by (4.18), is the unique solution of the integral equation:

$$\Psi(\mathbf{x},\mathbf{k}) = e^{2i\pi\mathbf{k}.\mathbf{x}} - \sum_{\mathbf{y} \in \mathbb{Z}^d} G_0^{(2)}(\mathbf{x} - \mathbf{y}; E_2(\mathbf{k}) \mp i0) V(\mathbf{y})\Psi(\mathbf{y},\mathbf{k}), \tag{4.21}$$

that has to be understood in the same way as in Theorem 3.3(ii). On the other hand, it is easy to check that for any $j = -N_q'', \ldots, N_q'$, $\mathbf{k} = (k_1, k_2) \in \mathbb{T}_j^2$ and $E_j(k_2) \notin [-d,d]$, $\Psi_{s,j,\pm}(\mathbf{x},k_2)$ is a solution of the homogeneous integral equation:

$$\Psi(\mathbf{x},k_2) = -\sum_{\mathbf{y} \in \mathbb{Z}^d} G_0^{(2)}(\mathbf{x} - \mathbf{y}; E_j(k_2) \mp i0) V(\mathbf{y})\Psi(\mathbf{y},k_2). \tag{4.22}$$

(2) One can view the above results from the point of view of the direct integral decomposition technique for finite difference operators with periodic coefficients.[4] Namely by using the periodicity in x_2 of the operator H with $\alpha = p/q$, we can write the direct integral decomposition

$$H=\int_{|k_2-1/2|\leqslant 1/2q}^{\oplus} H_q(k_2)dk_2. \tag{4.23}$$

Here $H_q(k_2)$ is the self-adjoint operator defined by the restriction of H to the linear manifold of functions $\Psi_{k_2}(\mathbf{x})=e^{2i\pi k_2 x_2}\Phi_{k_2}(\mathbf{x})$, where Φ_{k_2} is q-periodic in x_2. Thus $H_q(k_2)$ acts in the strip $\{x_1\in\mathbb{Z},\ 1\leqslant x_2\leqslant q\}$, and is the perturbation of the respective Laplacian by the q rank potential (1.3) with $1\leqslant x_2\leqslant q$. This implies that the spectrum of $H_q(k_2)$ consists of two parts. The first is the absolutely continuous component: the union of values of the functions $-\cos 2\pi k_1 - \cos 2\pi(k_2+l/q)$, $k_1\in\mathbb{T}$, $l=1,\ldots,q$ and $k_2\in[\frac{1}{2}+\frac{1}{2}q,1/2+1/2q)$ is fixed, the corresponding eigenfunctions are deformed plane waves in x_1. The second part is discrete spectrum, consisting of $N_q\leqslant q$ eigenvalues $E_j(k_2)$, lying outside of the above absolutely continuous spectrum, and having exponentially decaying in x_1 eigenfunctions. As k_2 varies in the direct integral the absolutely continuous spectrum of $H_q(k_2)$ gives rise to the volume states of the operator H, while the discrete spectrum of $H_q(k_2)$ gives rise to the surface states.

Proof of Theorem 4.5: Take $(E,\mathbf{k})\in\sigma(H)\times\ddot{\mathbb{T}}^2$, $z=E\pm i\varepsilon$, $\varepsilon>0$ and denote $\Psi_z(\mathbf{x},\mathbf{k})=(E-z)G(\mathbf{x},\mathbf{k};z)$, where $G(\mathbf{x},\mathbf{k};z)$ is defined in (3.9). We know from the proof of Theorem 3.3 that if for any $\mathbf{x}\in\mathbb{Z}^2$ the limit $\Psi_E(\mathbf{x},\mathbf{k})=\lim_{\varepsilon\to 0}\Psi_z(\mathbf{x},\mathbf{k})$ exists, then Ψ_E is a solution of the Schrödinger equation $H\Psi_E=E\Psi_E$. By Theorem 4.1 we can write the representation:

$$G(\mathbf{x},\mathbf{k},z)=\frac{1}{E_2(\mathbf{k})-z}\left[e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\sum_{m=0}^{q} t_m(k_2-m\alpha;z)G_0^{(1)}(x_1;z+\cos 2\pi(k_2-m\alpha))e^{2i\pi(k_2-m\alpha)x_2}\right]. \tag{4.24}$$

Choose first a pair $(\mathbf{k}\in\ddot{\mathbb{T}}^2, E=E_2(\mathbf{k}))$, as it was done in the proof of Theorem 3.3 for the quasi-periodic case. By Proposition 4.1 the denominator $1-P_q(E,k_2)$ in t_m of (4.4) is nonzero and we obtain from (4.25)

$$\Psi_{v,\pm}(\mathbf{x},\mathbf{k})=e^{2i\pi\mathbf{k}.\mathbf{x}}+\sum_{m=0}^{q} t_m(k_2-m\alpha;z)G_0^{(1)}(x_1;z+\cos 2\pi(k_2-m\alpha))\big|_{z=E_2(\mathbf{k})\mp i0}e^{2i\pi(k_2-m\alpha)x_2}. \tag{4.25}$$

This proves the first assertion of the theorem.

Consider now the case where $\mathbf{k}=(k_1,k_2)\in\mathbb{T}_j^2$, and $E=E_j(k_2)$ for some $j=-N_q'',\ldots,N_q'$. We know that the pair $(\mathbf{k},E)$ is such that $E+\cos 2\pi(k_2+l\alpha)\notin(-1,1)$ for any $l=1,\ldots,q$. Hence, by using the separability property (4.9) and the periodicity of the E_j's, given by Proposition 4.1, we find that $E+\cos 2\pi(k_2+l\alpha)\notin[-1,1]$ for any $l=1,\ldots,q$, i.e., all that these energies belong to the resolvent set of the one-dimensional Laplacian.

This observation implies the existence of the limit

$$\Psi_{s,j,\pm}(\mathbf{x},k_2)=\lim_{\varepsilon\to\mp 0}\left[I(\mathbf{k},z)\Psi_z(\mathbf{x},\mathbf{k})\right]\big|_{z=E_j(k_2)\mp i\varepsilon},$$

provided that the limit

$$\lim_{\varepsilon\to+0}\frac{\varepsilon}{1-P_q(k_2,E_j(k_2)\mp i\varepsilon)} \tag{4.26}$$

exists. This can be proved by using the relations

$$1-P_q(k_2,E_j(k_2)\mp i\varepsilon)=\pm i\varepsilon\partial_E P_q(k_2,E_j(k_2))+O(\varepsilon^2),$$

valid for sufficiently small ε, and the relation $\partial_E P_q\neq 0$. Now, it is easy to verify that

$$\Psi_{s,j,\pm}(\mathbf{x},k_2)=I_j(k_2)\sum_{m=1}^{q}\tilde{t}_m(k_2-m\alpha)G_0^{(1)}(x_1;E_j(k_2)+\cos 2\pi(k_2-m\alpha))e^{2i\pi(k_2-m\alpha)x_2}, \tag{4.27}$$

where

$$I_j(k_2)=\left[\int_{\mathbb{T}}dk_1\frac{1}{|(E_2(\mathbf{k})-z)|^2}\right]^{1/2}\Bigg|_{z=E_j(k_2)\mp i0},$$
$$\tilde{t}_1(k_2)=2i\sigma((g\hat{\gamma}_0(k_2;z)+i)\partial_E P_q(k_2,z)(g\hat{\gamma}_0(k_2+\alpha;z)+i))^{-1}|_{z=E_j(k_2)\mp i0}, \tag{4.28}$$

and for $m\geqslant 2$

$$\tilde{t}_m(k_2;E)=2ig\sigma((g\hat{\gamma}_0(k_2;z)+i)\partial_E P_q(k_2,z)(g\hat{\gamma}_0(k_2+m\alpha;z)+i))^{-1}$$
$$\times P_{m-1}(k_2;z)|_{z=E_j(k_2)\mp i0}. \tag{4.29}$$

By using the same argument as that in the proof of (4.19), we find that $\Psi_{s,j,\pm}$ satisfies (4.20). Let us prove now that $\Psi_{s,j,\pm}$ is a surface state. We know that $E+\cos 2\pi(k_2+l\alpha)\notin[-1,1]$ for any $l=1,\ldots,q$. Since all these energies are in the resolvent set of the one-dimensional Laplacian, each term of the sum of the r.h.s. of (4.27) decays exponentially with respect the transverse coordinate $x_1\in\mathbb{Z}$. Since the number of these terms is finite, we conclude that for any $x_2\in\mathbb{Z}$, $\Psi_{s,j,\pm}(.,x_2)\in l^2(\mathbb{Z})$ and is bounded in $x_2\in\mathbb{Z}$. The proof of the theorem is complete.

We can now use the last theorem, where we have constructed the generalized eigenfunctions (4.25) and (4.27), to prove Theorem 4.2.

Proof of Theorem 4.2: It follows from the proof of Theorem 4.3 that $\sigma(H)\subset[-d,d]\cup(\cup_{j=-N_q''}^{N_q'}\mathrm{Ran}\,E_j)$. Hence we have to prove the opposite inclusion. For the part $[-d,d]$ of the spectrum the inclusion was proved in Theorem 2.2. So assume that $E\in\cup_{j=-N_q''}^{N_q'}\mathrm{Ran}\,E_j\setminus[-d,d]$ is such that there exists a surface state $\Psi_s(\mathbf{x})$ satisfying the Schrödinger equation: $(H\Psi_s)(\mathbf{x})=E\Psi_s(\mathbf{x})$. We apply again the H. Weyl criterion, setting

$$\Psi_n(\mathbf{x})=1_n(x_2)\Psi_s(\mathbf{x})/N_n;\quad N_n=\|1_n\Psi_s\|_{l^2(\mathbb{Z}^2)},$$

where 1_r is the indicator of the ball $\{x_2\in\mathbb{Z}:|x_2|\leqslant n\}$. A straightforward calculation shows that $C_1n^{1/2}\leqslant N_n\leqslant C_2n^{1/2}$ as $n\to\infty$ for some strictly positive constants $C_{1,2}$, and that

$$(H\Psi_n)(\mathbf{x})=\begin{cases}E\Psi_n(\mathbf{x}), & |x_2|<n;\\ A_n(\mathbf{x}), & n\leqslant|x_2|\leqslant n+1;\\ E\Psi_n(\mathbf{x})=0, & |x_2|\geqslant n+2,\end{cases}$$

where $\|A_n\|_{l^2(\mathbb{Z}^2)}=O(n^{-1/2}),n\to\infty$. It is easy to check that Ψ_n is a Weyl sequence for H at the energy E. This proves the theorem.

Our next result concerns the completeness of the system of generalized eigenvectors (4.25) and (4.27), defined in Theorem 4.5.

Theorem 4.6: *Let $H=H_0+V$ be the self-adjoint operator in $l^2(\mathbb{Z}^2)$ defined in Theorem 4.1. Consider the family $\mathcal{F}=\{\Psi_v(\mathbf{x},\mathbf{k}),\ \mathbf{x}\in\mathbb{Z}^2\}_{\mathbf{k}\in\mathbb{T}^2}\cup_{j=-N_q''}^{N_q'}\{\Psi_{s,j}(\mathbf{x},k_2);\mathbf{x}\in\mathbb{Z}^2\}_{k_2\in\mathbb{T}_j}$, defined by (4.25) and (4.27). Then $\mathcal{F}$ is a complete system of generalized eigenfunctions of H in any sufficiently small interval Δ of $\sigma(H)$ such that $\Delta\cap D'=\varnothing$, i.e.,*

(i) for any $f\in l^2(\mathbb{Z}^2)$ the series

$$F_v(\mathbf{k})=\sum_{\mathbf{x}\in\mathbb{Z}^d}\overline{\Psi_v(\mathbf{x},\mathbf{k})}f(\mathbf{x}),\quad \mathbf{k}\in\ddot{\mathbb{T}}^2,$$

and

$$F_{s,j}(k_2)=\sum_{\mathbf{x}\in\mathbb{Z}^d}\overline{\Psi_{s,j}(\mathbf{x},k_2)}f(\mathbf{x}),\quad k_2\in\mathbb{T}_j,\quad j=-N_q'',\ldots,N_q',$$

converge in $l^2(\mathbb{Z}^2)$.

(ii) If $\mathcal{E}_H(\Delta)$ *is the spectral projection of* H *corresponding to the interval* $\Delta\in\sigma(H)$, *then*

$$\|\mathcal{E}_H(\Delta)f\|^2=\int_{\{\mathbf{k}\in\ddot{\mathbb{T}}^2:E_2(\mathbf{k})\in\Delta\}}|F_v(\mathbf{k})|^2d\mathbf{k}+\sum_{j=-N_q''}^{N_q'}\int_{\{k_2\in\mathbb{T}_j:E_j(k_2)\in\Delta\}}|F_{j,s}(k_2)|^2dk_2.$$

(iii) For the same interval we have

$$\|H\mathcal{E}_H(\Delta)f\|^2=\int_{\{\mathbf{k}\in\ddot{\mathbb{T}}^2:E_2(\mathbf{k})\in\Delta\}}|E_2(\mathbf{k})|^2|F_v(\mathbf{k})|^2d\mathbf{k}$$
$$+\sum_{j=-N_q''}^{N_q'}\int_{\{k_2\in\mathbb{T}_j:E_j(k_2)\in\Delta\}}|E_j(k_2)|^2|F_{s,j}(k_2)|^2dk_2.$$

Proof: For any compact interval $\Delta\subset\sigma(H)\backslash D'$ consider the sets

$$\nu=\{\mathbf{k}\in\ddot{\mathbb{T}}^2:E_2(\mathbf{k})\in\Delta\},\quad \nu_j=\{\mathbf{k}=(k_1,k_2)\in\mathbb{T}_j^2:E_j(k_2)\in\Delta\},\quad j=-N_q'',\ldots,N_q'.\tag{4.30}$$

Proposition 4.1 implies that there exists a constant $\eta>0$ such that

$$\min_j\inf_{\mathbf{k}\in\nu\cap\mathbb{T}_j^2}|E_2(\mathbf{k})-E_j(k_2)|,\ \min_j\inf_{\mathbf{k}\in\nu_j\cap\ddot{\mathbb{T}}^2}|E_2(\mathbf{k})-E_j(k_2)|\geqslant\eta.$$

Notice that η depends only on the dist(Δ,D'). Moreover, if Δ is sufficiently small, then the sets ν,ν_j, $j=-N_q'',\ldots,N_q'$ are disjoint. The subsequent argument uses this property of ν, and ν_j, $j=-N_q'',\ldots,N_q'$.

We will follow now the proof of Theorem 3.4. Hence we have to prove assertion (*ii*) first for a function f with compact support. We have for $z=E+i\varepsilon$, where $E\in\Delta$ and $\varepsilon>0$:

$$\frac{1}{\pi}\Im(G(z)f,f)=\frac{1}{\pi}\int_\nu d\mathbf{k}\frac{\varepsilon}{|(E_2(\mathbf{k})-z)|^2}|F_z(\mathbf{k})|^2$$
$$+\frac{1}{\pi}\sum_{j=-N_q''}^{N_q'}\int_{\nu_j}d\mathbf{k}\frac{\varepsilon}{|(E_j(k_2)-z)|^2}|F_z(\mathbf{k})|^2+O(\varepsilon),\tag{4.31}$$

where

$$F_z(\mathbf{k})=\sum_{\mathbf{x}\in\mathbb{Z}^d}\overline{\Psi_z(\mathbf{x},\mathbf{k})}f(\mathbf{x}),\quad \Psi_z(\mathbf{x},\mathbf{k})=(\tilde{E}-z)G(\mathbf{x},\mathbf{k};z),\tag{4.32}$$

$\tilde{E}=E_2(\mathbf{k})$ or $\tilde{E}=E_j(k_2)$ and $G(\mathbf{x},\mathbf{k};z)$ is defined by (3.9), (4.3), and (4.4). Since for every $\mathbf{k}=(k_1,k_2)\in\nu$ and $E\in\Delta$, $P_q(k_2,E)-1$ is not zero, the limit $\lim_{\varepsilon\to0}\Psi_{E+i\varepsilon}(\mathbf{x},\mathbf{k})$ exists for any $\mathbf{x}\in\mathbb{Z}^2$ uniformly in $\mathbf{k}=(k_1,k_2)\in\nu$ and in $E\in\Delta$. Applying to the first term of the r.h.s of (4.31) the operation $\lim_{\varepsilon\to0}\int_\Delta\ldots dE$, we get

$$\lim_{\varepsilon\to 0}\int_\Delta dE\,\frac{1}{\pi}\int_\nu d\mathbf{k}\frac{\varepsilon}{|(E_2(\mathbf{k})-z)|^2}|F_z(\mathbf{k})|^2=\int_{\{\mathbf{k}\in\ddot{\mathbb{T}}^2:E_2(\mathbf{k})\in\Delta\}}|F_v(\mathbf{k})|^2d\mathbf{k}. \tag{4.33}$$

So we are left with the second term of the r.h.s of (4.31). For every $j\in\{-N_q'',\ldots,N_q'\}$, $\mathbf{k}=(k_1,k_2)\in\nu_j$, and $E\in\Delta$, we have

$$\lim_{\varepsilon\to 0}F_{E+i\varepsilon}(\mathbf{k})=\sum_{\mathbf{x}\in\mathbb{Z}^d}\overline{\Psi(\mathbf{x},\mathbf{k};E)}f(\mathbf{x}), \tag{4.34}$$

where

$$\Psi(\mathbf{x},\mathbf{k},E)=\frac{(E_j(k_2)-E)}{E_2(\mathbf{k})-E}\Bigg[e^{2i\pi\mathbf{k}\cdot\mathbf{x}}+\sum_{m=0}^{q}t_m(k_2-m\alpha;E+i0)G_0^{(1)}(x_1;E+i0+\cos 2\pi(k_2-m\alpha))e^{2i\pi(k_2-m\alpha)x_2}\Bigg], \tag{4.35}$$

which in particular corresponds to $[(E_2(\mathbf{k})-E_j(k_2))I_j(k_2)]^{-1}\Psi_{s,j}(\mathbf{x},k_2)$ for $E=E_j(k_2)$. The limit (4.34) is also uniform in $\mathbf{k}=(k_1,k_2)\in\nu_j$ and in $E\in\Delta$. Applying again the same operation, $\lim_{\varepsilon\to 0}\int_\Delta\ldots dE$ to the jth term of the sum on the r.h.s. of (4.31), we get

$$\lim_{\varepsilon\to 0}\int_\Delta dE\,\frac{1}{\pi}\int_{\nu_j}d\mathbf{k}\frac{\varepsilon}{|(E_j(k_2)-z)|^2}|F_z(\mathbf{k})|^2=\int_{\{k_2\in\mathbb{T}_j:E_j(k_2)\in\Delta\}}|F_{j,s}(k_2)|^2dk_2. \tag{4.36}$$

Relations (4.33) and (4.36) imply assertions (*i*) and (*ii*) of the theorem for the case of a function f with compact support. The proofs of these assertions for an arbitrary function $f\in l^2(\mathbb{Z}^2)$, and the proof of assertion (*ii*) require standard means of spectral theory (see the proof of Theorem 3.4).

Proof of Proposition 4.1: According to (4.1), we can write Eq. (4.7) for $\alpha=p/q$ as

$$P_q(k_2,E)=\sigma^q\prod_{l=1}^{q}\hat{b}(k_2+l/q,E+i0)=1, \tag{4.37}$$

where

$$\hat{b}(k_2,z)=\frac{gG_0^{(1)}(0,z+\cos 2\pi k_2)-i}{gG_0^{(1)}(0,z+\cos 2\pi k_2)+i}. \tag{4.38}$$

Since the product on the l.h.s. of Eq. (4.37) is periodic in k_2 with period $1/q$, its solutions are also periodic in k_2 with period $1/q$, and we can restrict ourselves to the interval $[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$. By Lemmas 5.1 and 5.2 we have $|\hat{b}(k_2,z)|\leqslant 1$, $k_2\in\mathbb{T}$, $z\in\mathbb{C}$, thus the band equation (4.37) admits a solution if and only if the modulus of each factor $\hat{b}(k_2+l/q,E+i0)$, $l=1,\ldots,q$, on its l.h.s. is 1. Hence, we can write the representation

$$\hat{b}(k_2,E)=\exp\{2\pi i\phi(k_2,E)\}.$$

In what follows we will consider the case where E is positive (the arguments for negative E are similar and will be omitted). In this case we have from (3.37)

$$G_0^{(1)}(0,E+i0)=-\frac{1}{\sqrt{E^2-1}},\quad E>1,$$

and we can choose the phase $\phi(k_2,E)$ as

$$\phi(k_2,E)=1/\pi \arctan((1/g)\sqrt{(E+\cos 2\pi k_2)^2-1}). \tag{4.39}$$

For any $k_2\in[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$ ϕ is a non-negative and an increasing function of $E\geqslant 1-\cos 2\pi k_2$, satisfying the inequalities

$$0\leqslant \phi(k_2,E)<\tfrac{1}{2}.$$

The above formulas show that the l.h.s. of Eq. (4.37) is real analytic in the domain

$$\{(k_2,E):k_2\in[\tfrac{1}{2}-1/(2q),\tfrac{1}{2}+1/(2q)),\ \ E>1-\cos 2\pi k_2\},$$

hence solutions of the equation, if they exist, are real analytic in k_2 [notice that here the condition $E>1-\cos 2\pi k_2$ is equivalent to the conditions $E>1-\cos 2\pi(k_2+l\alpha),\forall l=1,..,q$].

We will use (4.37) in the form

$$\Phi_q(k_2,E)-q\omega=0 \pmod 1, \tag{4.40}$$

where

$$\Phi_q(k_2,E)=\sum_{l=1}^{q}\phi(k_2+l\alpha,E)=\sum_{l=0}^{q-1}\phi(k_2+l\alpha,E). \tag{4.41}$$

For any fixed $k_2\in[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$, $\Phi_q(k_2,E)$ is a positive and an increasing function of $E\geqslant 1-\cos 2\pi k_2$, bounded by $q/2$.

Fix now q and ω and denote by α_ω the integer part of the minimum

$$\min_{k_2\in[1/2-1/(2q),1/2+1/(2q))}\Phi_q(k_2,1-\cos 2\pi k_2)-q\omega.$$

For a fixed integer j denote by $E_j(k_2)$ the energy such that

$$\Phi_q(k_2,E_j(k_2))-q\omega=\alpha_\omega+j \tag{4.42}$$

and denote by $\mathcal{D}_j$ the set of $k_2\in\mathbb{T}$ such that (4.42) is satisfied. The sets $\mathcal{D}_j$, $j=-N_q'',\ldots,N_q'$ form an increasing family of the closed subsets of $\mathbb{T}$. For all j larger than some j_0, $\mathcal{D}_j$ coincides with $\mathbb{T}$.

Hence E_j is the jth energy band function and Ran E_j is the jth surface energy band. It is clear that the maximum value N_q' of j for which such a solution exists is such that $N_q'\leqslant q/2$. Since $\Phi_q(k_2,1-\cos 2\pi k_2)-q\omega$ is analytic in $k_2\in\mathbb{T}$, there may exist a discrete set $\mathcal{D}_j'$ of $k_2\in\mathbb{T}$, for which $\Phi_q(k_2,1-\cos 2\pi k_2)-q\omega$ is equal to the integer $\alpha_\omega+j$. Numerical experiments show that for small q there are at most two values of k_2 in the interval $[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$ for which this event occurs, so the number of points in $\mathcal{D}_1'$ is $2q$ and the other $\mathcal{D}_j'$ are empty. We have proved that if $k_2\in\mathbb{T}_j=\mathcal{D}_j\backslash\mathcal{D}_j'$, $E_j(k_2)$ exceeds $1-\cos 2\pi k_2$, then we have for all $\mathbf{k}\in\mathbb{T}_j^2$

$$E_j(k_2)>1-\cos 2\pi k_2\geqslant -\cos 2\pi k_1-\cos 2\pi k_2=E_2(\mathbf{k}), \tag{4.43}$$

i.e., the separation property (4.8) between the band of the volume states and the surface bands.

Let us now discuss separation between the surface bands $E_{-N_q''},\ldots E_{N_q'}$. We will use the relation

$$1=\Phi_q(k_2,E_{j+1}(k_2))-\Phi_q(k_2,E_j(k_2)), \tag{4.44}$$

implied by (4.40).

Consider first the energy range $E\geqslant\epsilon_m$ for some $\epsilon_m>2$. It follows from (4.40) that the maximum energy E_q for which the equation is soluble is finite (this is the upper edge of the spectrum of the operator H for a given q). Hence the partial derivative

$$\frac{\partial \Phi_q}{\partial E} = 1/\pi \sum_{l=0}^{q-1} \frac{g}{g^2 + [E + \cos 2\pi(k_2 + l/q)]^2 - 1} \frac{E + \cos 2\pi(k_2 + l/q)}{\sqrt{(E + \cos 2\pi(k_2 + l/q))^2 - 1}} \tag{4.45}$$

satisfies the inequalities:

$$0 < \frac{\partial \Phi_q}{\partial E} \leqslant \frac{q}{\pi g} \frac{E_q + 1}{\sqrt{(\epsilon_m - 2)\epsilon_m}} := (\eta_q')^{-1} < \infty.$$

This bound and (4.44) lead to the relations

$$1 = \int_{E(k_2)}^{E_{j+1}(k_2)} \frac{\partial \Phi_q(k_2, E)}{\partial E} dE \leqslant (E_{j+1}(k_2) - E_j(k_2))(\eta_q')^{-1}, \tag{4.46}$$

implying the separation property (4.9) in the case where $E_j(k_2) > 2$.

In the case, where

$$0 \leqslant 1 - \cos 2\pi k_2 \leqslant E_j(k_2) \leqslant 2, \quad k_2 \in [\tfrac{1}{2} - 1/(2q), \tfrac{1}{2} + 1/(2q)),$$

the r.h.s. of (4.45) can be infinite because of the contribution of the first term (for $E = 1 - \cos 2\pi k_2$), and of the second term [for $E = 1 - \cos 2\pi k_2$, and $k_2 = \frac{1}{2} - 1/(2q)$] or of the $(q-1)$th term [for $E = 1 - \cos 2\pi k_2$, and $k_2 = \frac{1}{2} + 1/(2q)$]. Since, however, each term in the phase (4.41) is non-negative and

$$\phi_q := \max_{k_2 \in [1/2 - 1/(2q), 1/2 + 1/(2q))} \phi(k_2, 2)$$

is strictly less than $\frac{1}{2}$, the contribution of these terms in the difference (4.44) is bounded from above by $2\phi_q < 1$, and we obtain from (4.44) the inequality

$$0 < 1 - 2\phi_q < \int_{E_j(k_2)}^{E_{j+1}(k_2)} \frac{\partial \tilde{\Phi}_q(k_2, E)}{\partial E} dE,$$

where $\tilde{\Phi}_q(k_2, E)$ is the sum in (4.41), in which the terms corresponding to $l = 0$ and to $l = 1$ if $k_2 \in [\frac{1}{2} - 1/(2q), \frac{1}{2})$, and to $l = q - 1$ if $k_2 \in [\frac{1}{2}, 1/2 + 1/(2q))$ are omitted. It is easy to check that the partial derivative of $\tilde{\Phi}_q(k_2, E)$ with respect to E is bounded from above by a constant $(\eta_q'')^{-1} < \infty$. This leads to the bound (4.46) in which $(\eta_q')^{-1}$ is replaced by $(\eta_q'')^{-1}$ and Φ_q by $\tilde{\Phi}_q$. The obtained bounds imply the separation property (4.9) with $\eta_q = \min\{\eta_q', \eta_q''\}$. Proposition 4.1 is proved.

Remark: It can be seen from the proof above that the distance between the bands increases as $|j|$ increases. Besides, the distance between the two first bands is of order $O(1/q)$ when q is large.

Denote from now on the operator of (1.1)–(1.4) as H_α. We conclude this section by discussing correspondence between the spectrums of the operators H_α with an irrational number α and with its rational approximations p_n/q_n:

$$\lim_{n \to \infty} \frac{p_n}{q_n} = \alpha. \tag{4.47}$$

It is easy to prove, by using the basic formula (2.16) for the resolvent, that under condition (4.47) H_{p_n/q_n} converges to H_α in the strong resolvent sense. Hence, according to general principles,[18] the spectrum $\sigma(H_{p_n/q_n})$ is upper semi-continuous in n in the limit (4.47). Here is a statement that

gives a more detailed behavior of $\sigma(H_{p/q})$ for large q. Recall that $\sigma(H_{p/q})$ is the union of the interval $[-2,2]$ and of $N_q''+N_q'$ surface bands, part of which can belong or intersect the interval $[-2,2]$.

Theorem 4.7: *Assume that q sufficiently large. Then there exists at most one negative surface energy band above $E=-2$ and at most one positive surface energy band below $E=2$. These bands, if they exist, have the width of order $O(1/q^2)$ as $q\to\infty$. The width of the surface energy bands lying in $(-\infty,-2)$ and in $(2,+\infty)$ are of order $O(\exp\{-\text{const}\cdot q\})$ as $q\to\infty$.*

Proof: We start from the dispersion equations (4.41) and (4.40) for the surface energy bands. Since the function $\Phi_q(k_2,E)$ has period $1/q$ in k_2, its Fourier series is

$$\Phi_q(k_2,E)=\sum_{n\in\mathbb{Z}}\hat{\Phi}_{q,n}(E)e^{-2\pi ik_2qn},$$

where

$$\hat{\Phi}_{q,n}(E)=q\sum_{l=0}^{q-1}\int_0^{1/q}dk_2e^{2\pi ik_2qn}\phi(k_2+l/q,E)=q\int_0^1 dk_2e^{2\pi ik_2qn}\phi(k_2,E):=q\hat{\phi}_{qn}(E),$$

and $\hat{\phi}_{qn}$ is the qnth Fourier coefficient of the function $\phi(.,E)$. Hence

$$\Phi_q(k_2,E)=q(\hat{\phi}_0(E)+\hat{\phi}_q(E)e^{-2\pi ik_2q}+\cdots). \tag{4.48}$$

According to (4.39), the function $\phi(\cdot,E)$ is analytic for $|E|>2$, thus its Fourier coefficient $\hat{\phi}_q(E)$ is of order $\exp\{-\text{const}\cdot q\}$ as $q\to\infty$. In addition, formula (4.40) implies the relation

$$\frac{dE_j}{dk_2}=\frac{\partial\Phi_q}{\partial k_2}\cdot\left(\frac{\partial\Phi_q}{\partial E}\right)^{-1}.$$

It follows now from (4.48) and from the exponential decay of the Fourier coefficient $\hat{\Phi}_{q,n}(E)$ that the upper bound for the derivative $\partial\Phi_q/\partial k_2$ is of order $O(q^2e^{-\text{const}\cdot q})$, while the lower bound for $\partial\Phi_q/\partial E$, which is reached for the highest energy band $E_{N_q'}(k_2)$, is of order $O(q)$. Thus the derivative dE_j/dk_2 is of order $O(qe^{-\text{const}\cdot q})$. Since $E_j(k_2)$ is periodic in k_2 with period $1/q$, then denoting respectively by $E_j^{\max}$, and by $E_j^{\min}$ the maximum and the minimum of the jth band function E_j, we see that $|E_j^{\max}-E_j^{\min}|$ is of the order $\exp\{-\text{const}\cdot q\}$ if $E_j^{\min}>2$.

Let us fix $k_2\in[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$. To see how many bands are in between the lowest possible energy $E=1-\cos 2\pi k_2$ and the energy, $E=2$, let us calculate $\delta\Phi=\Phi_q(k_2,2)-\Phi_q(k_2,1-\cos 2\pi k_2)$. We have

$$\delta\Phi=1/\pi\sum_{l=0}^{q-1}\int_{1-\cos 2\pi k_2}^{2}dE\,\frac{g}{g^2+(E+\cos 2\pi(k_2+l/q))^2-1}\,\frac{E+\cos 2\pi(k_2+l/q)}{\sqrt{(E+\cos 2\pi(k_2+l/q))^2-1}}.$$

Performing the integration for the different values of l and summing respective contributions we obtain that $\delta\Phi$ is of the order $(1/q)\log q$ as $q\to\infty$, thus $\delta\Phi\to 0$ as $q\to\infty$. Remembering that for each k_2 the energy of a band corresponds to an entire value of $\Phi_q+q\omega$, we deduce that for large q there is at most one band in the interval to the left of 2. Since the minimum of E_1 for $k_2\in[\frac{1}{2}-1/(2q),\frac{1}{2}+1/(2q))$ is larger than $1+\cos\pi/q$, the width of any band, lying inside the interval $[1+\cos\pi/q,2)$, is bounded by $\pi^2/2q^2$.

It can also occur that $E_1^{\max}>2$. In this case, the same argument as above shows that the part of the energy band in $(2,\infty)$ is exponentially small in q. Thus the total width in that case is at most of the order $1/q^2$.

Remark: The assertion of the theorem can be interpreted as a kind of continuity of the spectrum with respect to the limiting transition (4.47). Indeed, according to the theorem, the width

of the surface bands of H_{p_n/q_n}, lying outside the interval $[-d,d]$, is exponentially small in $q_n \to \infty$. It can also be shown that the gaps between these bands are of the order $1/q_n$. This is in agreement with the ''limiting'' form of this part of the spectrum of H_α for irrational α's, satisfying the Diophantine condition (1.6). Indeed, according to Ref. 19, the spectrum of H_α in this case is pure point and dense on $\mathbb{R}\backslash[-d,d]$. Here is one more manifestation of this continuity.

Recall that according to Ref. 19 the eigenvalues of H_α outside $[-d,d]$ are indexed by $x_2 \in \mathbb{Z}^{d_2}$, and for each $x_2 \in \mathbb{Z}^{d_2}$ the eigenvalue E_{x_2} is the unique solution of the equation

$$f(E_{x_2}) \equiv \alpha \cdot x_2 + \omega \pmod 1, \tag{4.49}$$

where $f:\mathbb{R}\backslash[-d,d]\to\mathbb{R}$ is the monotone increasing function, defined for $E>d$ as

$$f(E) = -\frac{1}{\pi}\int_{\mathbb{T}^{d_2}} dk_2 \arctan(g\,\gamma_0(k_2,E))^{-1}, \tag{4.50}$$

or, in view of (2.23) and (3.37), and for $d_2=1$

$$f(E) = -\frac{1}{\pi}\int_{\mathbb{T}^1} dk_2 \arctan g^{-1}\sqrt{(E+\cos 2\pi k_2)^2-1}. \tag{4.51}$$

On the other hand, we can write the band equation (4.40) as

$$\frac{1}{q_n}\Phi_q(k_2,E) = \frac{l}{q_n} + \omega \tag{4.52}$$

for some integer l. Choosing l in the form $l=p_n x_2 + m q_n$ for some integer m, we can write the last equation as

$$\frac{1}{q_n}\Phi_{q_n}(k_2,E) = \frac{p_n}{q_n}x_2 + \omega. \tag{4.53}$$

Recalling now the expression (4.41) for the function $\Phi_q(k_2,E)$, we conclude that for the limiting transition (4.47) and $E>2$ the equation (4.40), defining the surface bands of H_{p_n/q_n} outside $[-d,d]$, converges to the equation (4.49), defining the all eigenvalues of H_α for a Diophantine α outside $[-d,d]$.

V. AUXILIARY FACTS

We present here useful facts on the Green function (2.18) of the ν-dimensional Laplacian and on related quantities.

Lemma 5.1: Let $G_0^{(\nu)}(\mathbf{x}-\mathbf{y};z)$, $x,y\in\mathbb{Z}^\nu$, $\Im z\neq 0$, *be the Green function (2.18) of the* ν*-dimensional Laplacian (1.2). Write*

$$G_0^{(\nu)}(0;z) = R_\nu(z) + iI_\nu(z), \quad R_\nu, I_\nu \in \mathbb{R}. \tag{5.1}$$

Then
(i) for any $\varepsilon>0$, *and* $E\in\mathbb{R}$,

$$|R_\nu(E+i\varepsilon)|<\infty, \quad 0<I_\nu(E+i\varepsilon)<\infty; \tag{5.2}$$

(ii) the limits $R_\nu(E+i0)$ *and* $I_\nu(E+i0)$ *exist for* $|E|\neq\nu$, *satisfy inequality (5.2) for* $|E|<\nu$, *and* $I_\nu(E+i0)=0$ *if and only if* $|E|>\nu$.

Proof: The part (i) of the lemma follows from the integral representation (2.5). It is also easy to prove that the limits $R_\nu(E+i0)$ and $I_\nu(E+i0)$ exist and are finite for $|E|\neq\nu$ (in fact, for ν

$\geqslant 3$ they are finite even for $|E|=\nu$, see Lemma 5.4 below). Thus we have to prove that $I_\nu(E+i0)$ is strictly positive for $|E|<\nu$. By using (3.37), it easy to show that for $\nu=1$

$$\pi^{-1}I_1(E+i0):=\rho_1(E)=\begin{cases}(1-E^2)^{-1/2}, & |E|<1,\\ 0, & |E|>1,\end{cases}$$

and that $\pi^{-1}I_\nu(E+i0)$ is the νth convolution of ρ_1. These two observations imply that $\pi^{-1}I_\nu(E+i0)$ is strictly positive if $|E|<\nu$, and is zero for $|E|>\nu$. The lemma is proved.

Lemma 5.2: Let $\gamma_0(z)$ be the operator in $l(\mathbb{Z}^{d_2})$, defined as

$$\gamma_0(z)=P_{\mathbb{Z}^{d_2}}G_0^{(d)}(z)P_{\mathbb{Z}^{d_2}}, \quad d_2<d,$$

and

$$b(z)=\frac{g\gamma_0(z)-i}{g\gamma_0(z)+i}. \tag{5.3}$$

Then the operator $\gamma_0(z)+i$ is invertible for $\Im z\geqslant 0$, and the operator $b(z)$ is a contraction for $\Im z\neq 0$:

$$\|b(z)\|<1.$$

Proof: According to (2.18) and (2.22) $\gamma_0(z)$ is a convolution operator in $l^2(\mathbb{Z}^{d_2})$ and its symbol $\hat{\gamma}_0(k_2;z)$ satisfies the inequality $\Im\hat{\gamma}_0(k_2;z)\geqslant 0$, $\Im z\geqslant 0$. Since the symbol of $\gamma_0(z)+i$ is $\hat{\gamma}_0(k_2;z)+i$, we have that $|\hat{\gamma}_0(k_2;z)+i|\geqslant\Im(\hat{\gamma}_0(k_2;z)+i)\geqslant 1$. Hence $\gamma_0(z)+i$ is invertible and $||(\gamma_0(z)+i)^{-1}||\leqslant 1$.

The operator $b(z)$ is a rational function of $\gamma_0(z)$, thus its norm can be found as

$$\|b(z)\|=\sup_{k_2\in\mathbb{T}^{d_2}}|\hat{b}(k_2;z)|.$$

By using (5.1), we obtain that

$$|\hat{b}(k_2,z)|=\left.\frac{R_{d_1}^2+(I_{d_1}-1)^2}{R_{d_1}^2+(I_{d_1}+1)^2}\right|_{z\to z-E_{d_2}(k_2)}, \tag{5.4}$$

where R_ν and I_ν are defined in (5.1). This formula and Lemma 5.1 lead to (5.3).

Lemma 5.3: Let $\hat{b}(k_2;z)$ be defined by (2.25). Then

(i) $|\hat{b}(k_2;E+i0)|\leqslant 1$, $\forall E\in\mathbb{R}$;

(ii) for any $\gamma>0$ and $|E|\leqslant d-\gamma$ there exists an open set $K_\gamma(E)\subset\mathbb{T}^{d_2}$, such that

$$\hat{b}(k_2;E+i0)<1, \quad k_2\in K_\gamma(E). \tag{5.5}$$

Proof: The part (*i*) of the lemma follows from Lemma 5.1, and from (5.4). To prove assertion (*ii*) we have to find that for any $\gamma>0$ and $|E|<d-\gamma$ there exists an open set $K_\gamma(E)$ such that for $k_2\in K_\gamma(E)$, $|E-E_{d_2}(k_2)|<d_1$. Then $I_{d_1}(E+i0)$ will be strictly positive and $\hat{b}(k_2;E+i0)$ will be strictly less then 1 in view of (5.4). Since E_{d_2} is a continuous function in k_2 on $\mathbb{T}^{d_2}$, varying between $-d_2$ and d_2, respectively, open set $K_\gamma(E)$ always exists if $|E|<d$. The lemma is proved.

Lemma 5.4: Let $G_0^{(\nu)}(\mathbf{x};z)$ be the Green function of the ν-dimensional Laplacian and $g>0$. Then the expression

$$\frac{G_0^{(\nu)}(x;E+i0)}{gG_0^{(\nu)}(0;E+i0)+i} \tag{5.6}$$

is bounded in $x\in\mathbb{Z}^\nu$ *and in* $E\in\mathbb{R}$.

Proof: Consider first the one-dimensional case $\nu=1$. Then it follows from (3.37) that the expression (5.6) is

$$\frac{e^{i\eta(E+i0)|x|}}{g+\sin\eta(E+i0)},$$

and, according to (3.38) and (3.39), the modulus of the last expression is bounded by g^{-1}.

For $\nu\geqslant 2$ we will use the integral representation of $G_0^{(\nu)}(\mathbf{x};z)$ of (2.18), valid for $\Im z>0$:

$$G_0^{(\nu)}(x;z)=i\int_0^\infty dt e^{izt}\prod_{l=1}^{\nu} J_{x_l}(t)e^{i\pi x_l/2}, \tag{5.7}$$

where $x=\{x_l\}_{l=1}^{\nu}$, and $J_n(t)$ is the Bessel function of the order n:

$$J_n(t)=\frac{1}{2\pi}\int_0^{2\pi} e^{in\vartheta+it\sin\vartheta}d\vartheta.$$

The representation follows easily from (2.5), and from the identity

$$(\lambda-z)^{-1}=i\int_0^\infty dt e^{-it(\lambda-z)},\ \ \lambda\in\mathbb{R},\ \ \Im z>0. \tag{5.8}$$

By using the asymptotic formula

$$J_n(t)=\left(\frac{2}{\pi t}\right)^{1/2}\cos\left(t-\frac{(n+1/2)\pi}{2}\right)+O\left(\frac{1}{t}\right),\ \ t\to\infty, \tag{5.9}$$

we find that $\nu\geqslant 3$ $G_0^{(\nu)}(x;E+i0)$ is bounded in x and in E. Since, in addition, $|gG_0^{(\nu)}(0;E+i0)+i|\geqslant g\Im G_0^{(\nu)}(0;E+i0)+1\geqslant 1$ [recall that in view of (2.18) $\Im G_0^{(\nu)}(0;z)$ is non-negative], we obtain the assertion of the lemma for $\nu\geqslant 3$.

Thus, we are left with the case $\nu=2$. By using again (5.7) and (5.9), we find that $G_0^{(\nu)}(x;E+i0)$ is bounded in x and in E everywhere except $|E|=2$, and that in a sufficiently small neighborhood of $E=2$

$$G_0^{(\nu)}(x;E+i0)=A(x)\log|E-2|+B_\pm(x)+O(|E-z|),\ \ E-z\to 0,$$

where $A(x)$ and $B(x)$ are bounded in x, $A(0)\neq 0$, and $B_\pm(x)$ correspond to $\operatorname{sign}(E-2)$. The same asymptotic representation is valid in a neighborhood of $E=-2$. This shows that the ratio $G_0^{(\nu)}(x;E+i0)/G_0^{(\nu)}(0;E+i0)$ is bounded and continuous in $E\in\mathbb{R}$ for any $x\in\mathbb{Z}^\nu$. In addition we have

$$\left|\frac{G_0^{(\nu)}(0;E+i0)}{gG_0^{(\nu)}(0;E+i0)+i}\right|=\left|\frac{1}{g+i[G_0^{(\nu)}(0;E+i0)]^{-1}}\right|\leqslant\frac{1}{g-\Im[G_0^{(\nu)}(0;E+i0)]^{-1}}\leqslant g^{-1},$$

because

$$-\Im[G_0^{(\nu)}(0;E+i0)]^{-1}=\Im G_0^{(\nu)}(0;E+i0)/|G_0^{(\nu)}(0;E+i0)|^2\geqslant 0.$$

The lemma is proved.

Lemma 5.5: The expression

$$\frac{G_0^{(d_1)}(\mathbf{x};E-E_{d_2}(k_2)+i0)}{g\,\gamma_0(k_2,E+i0)+i}$$

is bounded in $E\in\mathbb{R}$, $k_2\in\mathbb{T}^{d_2}$, *and* $x\in\mathbb{Z}^{d_1}$.

Proof: According to (2.18), $\hat{\gamma}(k_2,z)=G_0^{(d_1)}(0;z-E_{d_2}(k_2))$. Hence, we can apply Lemma 5.4.

ACKNOWLEDGMENTS

L.P. would like to thank the Mathematics Department of the University of Wales, Swansea, where a part of the article was written.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

Asymptotics of information entropies of some Toda-like potentials

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(Received 10 May 2002; accepted 1 October 2002)

The spreading of the quantum probability density for the highly-excited states of a single-particle system with an exponential-type potential on the positive semiaxis is quantitatively determined in both position and momentum spaces by means of the Boltzmann–Shannon information entropy. This problem boils down to the calculation of the asymptotics of the entropy-like integrals of the modified Bessel function of the second kind (also called the Mcdonald function or Basset function). The dependence of the two physical entropies on the large quantum number n is given in detail. It is shown that the semiclassical (WKB) position–space entropy grows slower than the corresponding quantity of not only the harmonic oscillator but also the single-particle systems with any power-type potential of the form $V(x)=x^{2k}$, $x\in\mathbb{R}$ and $k\in\mathbb{N}$. The momentum–space entropy, calculated with a method based on the properties of the Mcdonald function, is rigorously found to have a behavior of the form $-\ln\ln n$, in strong contrast with the corresponding quantity of other one-dimensional systems known up to now (power-type potentials, infinite well).
 [DOI: 10.1063/1.1527223]

I. INTRODUCTION

The one-particle position and momentum probability densities are the basic elements for the quantum-mechanical description of the physical and chemical properties of the natural systems according to the density functional theory (DFT) initiated by Hohenberg and Kohn.[1,2] Indeed, all the fundamental and/or experimentally accessible quantities of these systems may be calculated by means of these densities in position and momentum spaces. However, its determination from the (wavefunction-based) Schrödinger equation of the system or even by means of the much simpler (density-based) Kohn-Sham equations of the DFT is an impossible analytical task. For this reason, often attention is focused on deriving not the densities themselves but certain specific properties of them (e.g., the spreading) directly from the Hamiltonian of the system.

Nowadays it is commonly accepted[3,4] that the spreading of the quantum probability densities in both position and momentum spaces are best measured not by the standard deviation but by the Boltzmann–Shannon information entropy. Moreover the uncertainty relation based on the information entropy of the densities (the entropic uncertainty relation) is valid for any quantum probability density, contrary to the Heisenberg uncertainty principle (which is based on the standard deviation of the densities) or any of its generalizations based on moments other than the standard deviation which yield nonuseful information or no information at all in certain cases.[3–5]

The analytical evaluation of the information entropies of quantum systems is a formidable

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task, even for one-dimensional single-particle systems whose Hamiltonian operator H has a discrete eigenvalue spectrum,

$$E_0<E_1<E_2\cdots \ . \tag{1}$$

The corresponding eigenfunctions (time-independent wavefunctions of the system) $\Psi_n(x)$, which satisfy

$$-\Psi_n''(x)+V(x)\Psi_n(x)=E_n\Psi_n(x), \tag{2}$$

will be assumed to be normalized to unity, i.e.,

$$\int_{\mathbb{R}}|\Psi_n(x)|^2\,dx=1. \tag{3}$$

The information entropy of the Born probability density associated with the wavefunction Ψ_n, $\rho(x)=|\Psi_n(x)|^2$, is defined by

$$S(\Psi_n)=-\int |\Psi_n(x)|^2\ln|\Psi_n(x)|^2\,dx, \tag{4}$$

which is called the position–space entropy of the system.

Analogously, the momentum-space entropy is given by

$$S(\hat{\Psi}_n)=-\int |\hat{\Psi}_n(p)|^2\ln|\hat{\Psi}_n(p)|^2\,dp, \tag{5}$$

where $\hat{\Psi}_n(p)$ is the Fourier transform of $\Psi_n(x)$, i.e.,

$$\hat{\Psi}_n(p)=\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\Psi_n(x)e^{-ixp}\,dx. \tag{6}$$

The entropic sum of this system, which measures the joint position–momentum uncertainty, is bounded from below according to the so-called entropic uncertainty relation of this system[8] is

$$S(\Psi_n)+S(\hat{\Psi}_n)\geqslant 1+\ln\pi, \tag{7}$$

which is a consequence of a well-known inequality in Fourier analysis, first conjectured by Hirschman[6] and then proved by Beckner[7] and Bialynicki-Birula and Mycielski.[8] This inequality strongly generalizes and improves[5,8] the Heisenberg–Kennard–Robertson uncertainty principle $\Delta x\,\Delta p\geqslant\hbar/2$.

Up until now the calculation of these information functionals has been undertaken only for the harmonic oscillator and the Coulomb potentials[9,10] as well as for the infinite well potential[11–13] and the power-type potentials.[11] In spite of the considerable effort done in recent years, it is not yet known the explicit form of these physical entropies for all quantum states of the three aforementioned prototype quantum-mechanical potentials except in the following cases.

(a) The position–space entropy for the ground and excited states of the infinite well potential of width L has the following constant value:[11,13] $\ln(2L)-1$.
(b) The momentum–space entropy of the Coulomb potential ($V=-1/|x|$) has the following decreasing logarithmic behavior with the quantum number n:[10] $-\ln n+\ln(8\pi)-2$.

The calculation of the other physical entropies boils down to the evaluation of entropy-like integrals of certain special functions, which are the Hermite polynomials for the harmonic oscillator in both complementary spaces, the Laguerre polynomials for the Coulomb potential in

position space and the trigonometric functions for the infinite well potential in momentum space. See Ref. 14 for a recent review. Up until now, these three quantities can only be explicitly calculated in the region of large quantum numbers ($n\to\infty$) by means of the semiclassical (WKB) approach[15,16] and/or a method based on the asymptotic behavior of the L^q norm of the involved polynomials, recently encountered.[17] As well, the two information entropies of the power-type potential $V(x)=x^{2k}$, $x\in\mathbb{R}$, $k\in\mathbb{N}$, have been recently calculated although again only for highly-excited states.[11] The asymptotic or high-energy region is of special interest because therein the transition from classical to quantum phenomena takes place, the correspondence limit operates and the chaotic dynamics can be analyzed. The following asymptotical ($n\to\infty$) results have been found.

(c) The position–and momentum–space entropy of the harmonic oscillator ($V=x^2/2$) behaves as $\frac{1}{2}\ln n+\ln(\pi\sqrt{2})-1$.[9,13,18]

(d) The momentum–space entropy of the infinite well potential of width L has the following constant value for all highly-excited states:[11,12] $-\ln(2L)+\ln(8\pi)+o(1)$.

(e) The position–space entropy of the power-type potential ($V=x^{2k}$, $k\in\mathbb{N}$) depends on the large quantum number n as $(1+k)^{-1}\ln(2n)+\sigma_k$, where σ_k is a known parameter.[11]

(f) The momentum–space entropy of the power-type potential depends for large values of n as $k(1+k)^{-1}\ln(2n)+\varepsilon_k$, where ε_k is a known parameter of k.[11]

(g) The position–space entropy of the Coulomb potential behaves as $2\ln n+\ln(4\pi)-2$ for all large quantum numbers.[19]

In this paper we shall investigate the position and momentum information entropies for the highly-excited states (i.e., when the quantum number n is large) of the single-particle system submitted to the Toda-like potential,

$$V(x)=\begin{cases} e^x, & \text{if } x\geqslant 0 \\ +\infty, & \text{otherwise.} \end{cases} \tag{8}$$

This system corresponds to the quantum SL(2) Toda chain of two particles[21,20] or, equivalently, to the motion of a particle on the positive semiaxis in the potential of the other particle, fixed at the origin. The bound states of this exponential potential are solutions of the Schrödinger equation (2), also known as Liouville equation in certain contexts,[21,20] with the following condition: $\Psi(x)=0$ for $x\leqslant 0$.

The eigenfunctions of the Toda-like potential (8) turn out to be the modified Bessel function of the first kind (also called the Mcdonald function or Basset function)[22–24] $K_\nu(z)$; see Sec. III. Then, the position–space entropy of the highly-excited states of this Toda-like system boils down to the calculation of the asymptotics of entropy-like integrals of the Macdonald function. The field of asymptotics of entropy-like integrals of special functions other than the classical orthogonal polynomials[17,14,18] has not yet been explored. Recently, the relevant role of these novel mathematical objects has been shown to explain certain characteristics of the quantum probability densities of some physical systems such as the (two-dimensional) circular membrane (entropy-like integral of Bessel functions of the first kind)[25] and the (one-dimensional) single-particle system with a general power-type potential,[11] particularly the linear potential (entropy-like integral of Airy functions).[13] Up until now, the asymptotics of these entropy-like integrals of nonpolynomial functions has been studied by means of the semiclassical (WKB) approximation.

The Toda chains, which apply when the interaction between particles depends exponentially on their mutual distance, play a relevant role in the theory of completely integrable systems. In classical mechanics, the Toda chain is the discrete analog of the wave Korteweg-de Vries equation. It is a completely integrable system solvable by means of the direct-inverse spectral problem for an operator of Jacobi-matrix type.[26] It is worthwhile to mention that the solution of a quantum Toda chain involves a new class of special functions, the Mcdonald or Whittaker functions of several variables.[21,20]

Here, we shall use the WKB method to find the position–space entropy of the Toda-like system above mentioned (see Sec. II). This method has been previously applied[13,27] to general potentials with two turning points, which led us to obtain a simple asymptotical relation between the quantum and classical Boltzmann–Shannon[13] and Renyi[27] information entropies, respectively. The information entropy in the momentum space is calculated in Sec. IV by a method which first shows the relationship between the momentum wavefunction of the system and the Mellin transform of the Mcdonald function, and then uses various asymptotical properties of this transform.

II. ASYMPTOTICS IN THE POSITION SPACE

Here we shall compute the position information entropy $S(\Psi_n)$ given by (4) for the wavefunctions of the highly excited states (i.e., the quantum states with a large quantum number n) of the Toda-like system described in the previous section, by means of the semiclassical (WKB) approximation.

For this purpose we will estimate the L^q norms of the WKB solution of the Schrödinger equation (2) for the Toda-like potential (8); then, an appropriate limit will lead us to the desired asymptotics.

Information on the sequence of energies E_n can be obtained from the well-known WKB quantization rule:[15,16] up to a vanishing summand, E_n satisfies

$$\frac{2}{\pi}\int_0^{\ln E_n}\sqrt{E_n-e^x}\,dx=2n+3/2,\quad n=0,1,2,\ldots,$$

or equivalently,

$$\sqrt{E_n}\ln(\sqrt{E_n}+\sqrt{E_n-1})-\sqrt{E_n-1}=\frac{\pi}{2}(n+3/4).$$

Asymptotically we have

$$t_n\ln t_n=\frac{\pi}{e}n\,,\quad t_n=\frac{2}{e}\sqrt{E_n}.$$

It is straightforward to see that

$$p_n=\sqrt{E_n}=\frac{\pi n}{2\ln n}(1+\epsilon_n+O(\epsilon_n^2))\,,\quad \epsilon_n=\frac{\ln\ln n}{\ln n}. \tag{9}$$

It is interesting to observe that the energy levels of the $SL(2)$ Toda chain grow faster than the corresponding levels of any power-type potential,[11] for which the potential is $V(x)=x^{2k}$ and $E_n\sim n^{2k/(1+k)}$, but slower than the corresponding energies of the infinite potential well, which are given by $\sqrt{E_n}=\pi n/2$. Here and below we write that $a_n\sim b_n$ when $a_n=b_n(1+o(1))$, $n\to\infty$.

If we denote

$$f_n(x)=\sqrt{E_n-e^x},$$

and

$$\Phi_n(x)=\int_x^{x_n}f_n(t)\,dt\,,\quad -x_n<x<x_n\,,\quad x_n=\ln E_n\,,$$

then the WKB solution of (2) on the interval of oscillatory behavior of Ψ_n, $(0,x_n)$, has the form

$$\Psi_n(x)=c_n\frac{\cos\{\Phi_n(x)-\pi/4\}}{\sqrt{f_n(x)}}, \tag{10}$$

where c_n is a normalization constant given by (3). Let us compute the L^q norm (Renyi entropy) of Ψ_n, that is,

$$N_n(q)=\int_{\mathbb{R}}|\Psi_n(x)|^{2q}\,dx.$$

From (10) it is easy to obtain that

$$\begin{aligned}N_n(q)&\sim c_n^{2q}\int_0^{x_n}|\cos(\Phi_n(x)-\pi/4)|^{2q}|f_n(x)|^{-q}\,dx\\&=c_n^{2q}\,x_n\int_0^1|\cos(\Phi_n(x_nt)-\pi/4)|^{2q}|f_n(x_n\,t)|^{-q}\,dt,\end{aligned} \tag{11}$$

where the definition of f_n and the substitution $x\mapsto x_nt$ have been used.

The function

$$\varphi(t)=\frac{1}{2n+3/2}\Phi_n(x_nt)$$

is continuous on $[0,1]$ and decreases monotonically from $\pi/2$ to 0. Thus, the inverse function $\omega=\varphi^{-1}$ on $[0,\pi/2]$ exists and the integral in (11) is

$$\int_0^{\pi/2}|\cos((2n+3/2)\,\varphi-\pi/4)|^{2q}|f_n(x_n\,\omega(\varphi))|^{-q}|\omega'(\varphi)|\,d\varphi.$$

We can use the analog of the Fejer's lemma, established by Aptekarev *et al.* Ref. 17, Lemma 2.1, by which this integral behaves as

$$\int_0^{\pi/2}|\cos(\varphi)|^{2q}d\varphi\,\frac{2}{\pi}\int_0^1|f_n(x_n\,t)|^{-q}\,dt.$$

Thus, if we denote

$$B(q)=\frac{2}{\pi}\int_0^{\pi/2}|\cos(\varphi)|^{2q}d\varphi\,,\quad h_n(q)=\int_0^{x_n}|f_n(x)|^{-q}\,dx, \tag{12}$$

then by (11),

$$N_n(q)\sim c_n^{2q}\,B(q)\,h_n(q).$$

Taking $q=1$ and keeping in mind that $N_n(1)=1$, we get

$$1\sim c_n^2\,B(1)\,h_n(1).$$

Finally, we arrive at

$$N_n(q)\sim\frac{B(q)}{B(1)^q}\,\frac{h_n(q)}{h_n(1)^q}. \tag{13}$$

It is well known and easy to verify that

$$S_n = S(\Psi_n) = -\frac{\partial}{\partial q} N_n(q)\Big|_{q=1} = -\frac{\partial}{\partial q} \ln N_n(q)\Big|_{q=1}.$$

In consequence,

$$S_n = -\frac{\partial}{\partial q} \ln B(q)\Big|_{q=1} + \ln B(1) - \frac{\partial}{\partial q} \ln h_n(q)\Big|_{q=1} + \ln h_n(1). \tag{14}$$

We compute each term in this formula separately. The integral $B(q)$ can be expressed in terms of the beta function $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$, namely

$$B(q) = \frac{1}{\pi} B(q+1/2, 1/2),$$

so that $B(1) = 1/2$ and

$$\frac{\partial}{\partial q} \ln B(q)\Big|_{q=1} = \{\psi(q+1/2) - \psi(q+1)\}|_{q=1} = \psi(3/2) - \psi(2) = 1 - 2\ln 2,$$

where $\psi(x) = \Gamma'(x)/\Gamma(x)$ is the digamma function. We have used here (Ref. 23, Sec. 11.1) that $\psi(3/2) = 2 - \gamma - 2\ln 2$ and $\psi(2) = 1 - \gamma$, where γ is the constant of Euler–Mascheroni.

Consider now the function $h_n(q)$, given in (12). After a suitable change of variables, this integral takes the form of the Markov function (Cauchy transform) of a simple Jacobi weight:

$$h_n(q) = (E_n - 1)^{-q/2} \int_0^1 \frac{x^{-q/2}}{\dfrac{E_n}{E_n - 1} - x}\, dx.$$

Then,

$$h_n(q) \sim E_n^{-q/2}\, \mathcal{F}_q(z_n),$$

where

$$\mathcal{F}_q(z) = \int_0^1 \frac{x^{-q/2}}{z - x}\, dx, \quad \text{and} \quad z_n = \frac{E_n}{E_n - 1}.$$

In particular,

$$h_n(1) \sim E_n^{-1/2}\, \mathcal{F}_1(z_n).$$

Observe that

$$\mathcal{F}_1(z) = \int_0^1 \frac{x^{-1/2}}{z - x}\, dx = \frac{1}{\sqrt{z}} \ln \frac{\sqrt{z} + 1}{\sqrt{z} - 1}$$

and that $z_n > 1$, $z_n \to 1$; in consequence,

$$\mathcal{F}_1(z_n) = \ln(4E_n) + o(1).$$

On the other hand,

$$\frac{\partial}{\partial q}\mathcal{F}_q(z_n)\bigg|_{q=1}=\frac{1}{2}\int_0^1\frac{\ln 1/x}{z-x}\frac{dx}{\sqrt{x}}=\frac{1}{\sqrt{z}}\{d(\sqrt{z})-d(-\sqrt{z})\},$$

where

$$d(z)=\int_0^1\frac{\ln 1/x}{z-x}dx=\sum_{n=1}^{\infty}\frac{1}{z^n}\frac{1}{n^2}$$

is the dilogarithm.[23] We have

$$\lim_{n\to\infty}\frac{\partial}{\partial q}\mathcal{F}_q(z_n)\bigg|_{q=1}=\lim_{z\to 1}\frac{1}{\sqrt{z}}\{d(\sqrt{z})-d(-\sqrt{z})\}=d(1)-d(-1). \tag{15}$$

Since

$$d(1)=\zeta(2)=\frac{\pi^2}{6},\quad d(-1)=-\frac{1}{2}\zeta(2)=-\frac{\pi^2}{12},$$

the limit in (15) is $\pi^2/4$.

Gathering in (14) all the formulas obtained above, we finally have the asymptotics for the entropy:

$$S_n=S(\Psi_n)=\ln\ln\left(\frac{\pi n}{\ln n}\right)^2+\ln 2-1+\frac{\pi^2}{4\ln\left(\frac{\pi n}{\ln n}\right)^2}+o\left(\frac{1}{\ln n}\right). \tag{16}$$

It is interesting to observe that this entropy grows slower than that of a single-particle system submitted to a power-type potential of the form $V(x)=x^{2k}$, for which $S_n\sim[1/(1+k)]\ln n$. On the other hand, now $S_n\to\infty$, unlike in the case of the potential well, for which the entropy is constant in all quantum states.

III. TODA-LIKE WAVE FUNCTIONS

In this section we shall determine the eigenfunctions of the Toda-like system with the exponential potential (8). It is well known[20] that the associated $SL(2)$ Toda equation reduces to the well-known Bessel equation. Let us recall the corresponding procedure for completeness.

Setting a new variable $z=2\exp(x/2)=2\sqrt{V(x)}$ in (8) and taking $y(z)=\Psi(x)$, we get

$$z^2y''+zy'-(z^2-4E)y=0,$$

which is the modified Bessel equation,

$$z^2y''+zy'-(z^2+\nu^2)y=0,$$

where $\nu^2=-4E$. For $\nu\notin\mathbb{Z}$, this equation has two linearly-independent solutions, I_ν and $I_{-\nu}$, where

$$I_\nu(z)=\sum_{n=0}^{\infty}\frac{1}{n!\,\Gamma(n+\nu+1)}\left(\frac{z}{2}\right)^{2n+\nu} \tag{17}$$

is the modified Bessel function of the first kind,[23] also called a Bessel's function of imaginary argument or hyperbolic Bessel function.[24]

The normalization condition (3) implies that

$$\int_2^{+\infty} |y_n(z)|^2 \frac{dz}{z} < +\infty.$$

The unique (up to a multiplicative constant) linear combination of the functions I_ν and $I_{-\nu}$ that is not exponentially increasing corresponds to the modified Bessel function of the second kind (or Mcdonald function),

$$K_\nu(z) = \frac{\pi}{2} \frac{I_{-\nu}(z) - I_\nu(z)}{\sin(\pi\nu)},$$

which is also called the Bessel's function of the second kind of imaginary argument, the modified Hankel function or even the Basset function.[24]

Thus, the $SL(2)$ Toda wave function has the form

$$\Psi_n(x) = C_n K_{\nu_n}(2\sqrt{V(x)}), \tag{18}$$

where the normalizing constant C_n is obtained from

$$C_n^2 \int_1^{+\infty} K_{\nu_n}^2(2\sqrt{V}) \frac{dV}{V} = 1. \tag{19}$$

The spectrum of values of the parameter ν is given by the boundary condition,

$$K_{\nu_n}(2\sqrt{V})\,|_{V=1} = 0.$$

As we have seen in (9), this condition must be satisfied for purely imaginary values of the index ν, namely,

$$\nu_n = \pm 2ip_n, \quad p_n = \sqrt{E_n}, \tag{20}$$

which agrees with the asymptotic behavior of the Mcdonald function for large values of the parameter ν.[22,24]

IV. ASYMPTOTICS IN THE MOMENTUM SPACE

Here the momentum–space entropy (5) of the Toda-like potential (8) shall be calculated for all quantum states with $n \to \infty$. From Eqs. (6) and (18), we have that the momentum wavefunction is

$$\hat{\Psi}_n(p) = \frac{1}{\sqrt{2\pi}} \int_1^{+\infty} C_n K_{\nu_n}(2\sqrt{V})\, V^{-ip} \frac{dV}{V}.$$

With an account of the Mellin's transform of the Mcdonald function (Ref. 28, Section 8.4.23) and Eq. (17), we have

$$\begin{aligned}
\mathcal{M}_\nu(s) &= \int_1^{+\infty} K_\nu(2\sqrt{x})\, x^{s-1}\, dx \\
&= \frac{1}{2}\Gamma\left(-\frac{\nu}{2}+s\right)\Gamma\left(\frac{\nu}{2}+s\right) + \frac{\Gamma(\nu)}{\nu-2s}\,{}_1F_2\left(\begin{matrix} -\nu/2+s \\ 1-\nu, 1-\nu/2+s \end{matrix}\middle| 1\right) \\
&\quad - \frac{\Gamma(-\nu)}{\nu+2s}\,{}_1F_2\left(\begin{matrix} \nu/2+s \\ 1+\nu, 1+\nu/2+s \end{matrix}\middle| 1\right),
\end{aligned}$$

where ${}_1F_2$ is the generalized hypergeometric series. In particular, for $\nu=\nu_n=2ip_n$ and $s=-ip$,

$$\mathcal{M}_{\nu_n}(-ip)=\frac{1}{2}\left(\Gamma(-ip+ip_n)\Gamma(-ip-ip_n)+\frac{\Gamma(2ip_n)}{ip+ip_n}+\frac{\Gamma(-2ip_n)}{ip-ip_n}\right)$$
$$-\frac{\Gamma(2ip_n)}{2}\sum_{k=1}^{\infty}\frac{1}{k!\,(1-2ip_n)_k}\frac{1}{k-(ip+ip_n)}$$
$$-\frac{\Gamma(-2ip_n)}{2}\sum_{k=1}^{\infty}\frac{1}{k!\,(1+2ip_n)_k}\frac{1}{k-(ip-ip_n)}, \tag{21}$$

where $(a)_k$ is the Pochhammer's symbol. The left hand side of this formula is an entire function; observe that on the right hand side we have a product of two gamma functions (which is meromorphic) minus the principal parts of its Laurent expansion.

When $n\to\infty$ the function $|\hat{\Psi}_n(p_n x)|^2 p_n$ behaves as a half-sum of Dirac deltas at $x=\pm 1$. Since

$$\hat{\Psi}_n(p)=\frac{C_n}{\sqrt{2\pi}}\mathcal{M}_{\nu_n}(-ip),$$

and with account of the symmetry of $\hat{\Psi}_n$ we obtain that

$$S(\hat{\Psi}_n)=-\int_{\mathbb{R}}|\hat{\Psi}_n(p)|^2\ln|\hat{\Psi}_n(p)|^2dp\sim-\ln|\hat{\Psi}_n(p_n)|^2=-2\{\ln C_n+\ln|\mathcal{M}_{\nu_n}(-ip_n)|\}-\ln(2\pi). \tag{22}$$

Thus, we need to establish the asymptotic behavior of $|\mathcal{M}_{\nu_n}(-ip_n)|$ and of the sequence of normalizing constants C_n.

Taking in (21) $z=ip_n-ip$ we obtain that

$$\mathcal{M}_{\nu_n}(-ip_n)=\lim_{z\to 0}\left\{\frac{1}{2}\Gamma(z)\Gamma(z-2ip_n)-\frac{1}{2z}\Gamma(-2ip_n)\right\}$$
$$-\frac{\Gamma(2ip_n)}{2}\sum_{k=1}^{\infty}\frac{1}{k!\,(1-2ip_n)_k}\frac{1}{2ip_n+k}-\frac{\Gamma(-2ip_n)}{2}\sum_{k=0}^{\infty}\frac{1}{k!\,(1+2ip_n)_k}\frac{1}{k}. \tag{23}$$

Since in a neighborhood of $z=0$,

$$\Gamma(z)=\frac{1}{z}-\gamma+O(z),\quad \Gamma(z-2ip_n)=\Gamma(-2ip_n)+z\Gamma'(-2ip_n)+O(z^2),$$

the limit in (23) is equal to

$$\psi(-2ip_n)-\gamma\sim\ln p_n.$$

On the other hand, the two series in (23) represent the integral Bessel functions of the first kind (Ref. 28, Appendix II.15) and are at the same time asymptotic expansions of these functions for $\nu\to\infty$. Thus, the series above behave as $O(1/p_n)$ for large n, and are infinitesimal with respect to $\ln p_n$. Finally, we have that

$$|\mathcal{M}_{\nu_n}(-ip_n)| \sim \tfrac{1}{2}|\Gamma(2ip_n)| \ln p_n,$$

or with account of the asymptotics of the gamma function (Stirling formula),

$$|\mathcal{M}_{\nu_n}(-ip_n)| \sim \frac{1}{2}\sqrt{\frac{\pi}{p_n}}\, e^{-\pi p_n} \ln p_n. \tag{24}$$

Now we study the normalizing constant C_n, satisfying (19) or, equivalently,

$$C_n^2 \int_4^{+\infty} K_{\nu_n}^2(\sqrt{x})\, \frac{dx}{x} = 1. \tag{25}$$

Once again we have to consider the Mellin transform, but now of K_ν^2. From Ref. 28, Section 8.4.23,

$$\mathcal{N}_\nu(s) = \int_0^{+\infty} K_\nu^2(\sqrt{x})\, x^{s-1}\, dx = \frac{\sqrt{\pi}}{2}\, \frac{\Gamma(s)\Gamma(s+\nu)\Gamma(s-\nu)}{\Gamma(s+1/2)},$$

and the integral in (25) is obtained subtracting from the formula above the principal parts of the Laurent series at the poles. Reasoning as in (23) we get

$$\begin{aligned} C_n^{-2} &\sim \lim_{s\to 0}\left\{ \mathcal{N}_{\nu_n}(s) - \frac{1}{s}\operatorname{res}_{s=0}\mathcal{N}_{\nu_n}(s) \right\} \\ &\sim \frac{1}{2}\frac{d}{ds}\{\Gamma(s+\nu_n)\Gamma(s-\nu_n)\}\big|_{s=0} \\ &= \tfrac{1}{2}\Gamma(\nu_n)\Gamma(-\nu_n)[\psi(\nu_n)+\psi(-\nu_n)]. \end{aligned}$$

The well-known asymptotics of the psi function and Stirling formula yield

$$C_n^2 \sim \frac{p_n}{\pi}\, e^{2\pi p_n}\, \frac{1}{\ln p_n}. \tag{26}$$

Finally, we can gather Eqs. (24) and (26) in (22) to obtain

$$S(\hat{\Psi}_n) \sim -\ln\left\{ \frac{1}{8\pi} \ln p_n \right\}.$$

With account of (9),

$$S(\hat{\Psi}_n) = -\ln\ln n + \ln(8\pi) + o(1). \tag{27}$$

We should notice that the entropy in momentum space gives a clear characterization of the known one-dimensional physical systems. For instance, $S(\hat{\Psi}_n)$ for the infinite potential well is constant, for the power-type potential $V(x)=x^{2k}$ it grows as $[k/(1+k)]\ln n$,[11] and the maximal $\ln n$ growth takes place for the Coulomb potential.[19] As we have shown, for the Toda-like potential (8), $S(\hat{\Psi}_n)\to -\infty$ as an iterated logarithm.

Finally, the combination of Eqs. (16) and (27) allows us to realize that the entropy sum is given by

$$S(\Psi_n) + S(\hat{\Psi}_n) \sim 5\ln 2 - 1 + \ln\pi, \tag{28}$$

which certainly fulfils the entropic uncertainty relation (7). This is most important since the entropy sum (a) is invariant under uniform scaling of the coordinates, (b) provides the net information content of the system and (c) measures the joint position-momentum uncertainty. We highlight that the entropy sum of the Toda-like system is asymptotically constant (i.e., it does not depend on the quantum number which characterizes the state of the system) because the position and momentum entropies have the same asymptotic behavior ($\ln \ln n$) but with opposite signs. This is characteristic of the exponential-type potential in contrast to the power-type and Coulomb potentials whose entropy sum has an increasing logarithmic behavior as the quantum number grows.

V. SUMMARY, CONCLUSION AND OPEN PROBLEMS

The spreading of the quantum probability of physical systems in position and momentum spaces may be quantitatively measured by the corresponding Boltzmann–Shannon information entropies. In general, however, the analytical determination of the explicit values of these quantities is an extremely difficult task. This is true even for one-dimensional single-particle systems, except for the infinite well potential at the position space[11,13] and for the Coulomb potential at the momentum space.[10] Then, ground state apart, most efforts have been concentrated in the high extreme of the spectrum where the wavefunctions of the highly-lying energy levels involve some special functions (orthogonal polynomials, Bessel functions, ...) with asymptotics under control; see the Introduction and Ref. 14. The high-energy part of the spectrum is most interesting because therein the transition of classical-to-quantum ideas takes place, the correspondence principle operates and chaotic phenomena may show up.

In this paper we consider a Toda-like system composed by a particle moving on the positive semiaxis under the exponential-type potential (8), which is equivalent to the quantum $SL(2)$ Toda chain of two particles.[20,21] The eigenfunctions of this system involve the Mcdonald or Basset function.[22,24] We have calculated the information entropies for the highly-excited states of the system in the two complementary spaces. The position entropy was determined in the framework of the semiclassical approximation, and the momentum entropy was calculated by means of only the asymptotic properties of the Mellin's transform of the Mcdonald function. Let us remark at this point that a most interesting open problem remains for the theorists of special functions: to find the expression (16), which gives the asymptotics of the position entropy of our Toda system, directly from the asymptotics of the Mcdonald function.

We have found that the position (momentum) entropy of the Toda-like potential (8) increases (decreases) without limit in a doubly logarithmic form as the quantum number n characterizing the state of the system tends to infinity. This means that the quantum probability density gets more and more diffused (localized) in position (momentum) space as the quantum number n grows. Moreover, the entropy sum or joint measure of the position–momentum uncertainty (which is invariant to uniform scaling of coordinates and provides the net information content of the system) has an absolute limit given by Eq. (28) for all ground and excited states of the system. This is because the position and momentum entropies have the same asymptotic behavior with the quantum number n (namely, $\ln \ln n$) but with opposite signs.

ACKNOWLEDGMENTS

This work was partially supported by the European Union Project No. INTAS-2000-272 and the Spanish research Grant No. BFM2001-3878-C02 (J.S.D. and A.M.F.) as well as by the Russian Grant No. RFFR 96-01-00730 and No. 96-15-96185 (V.N.S.). We belong to the Research Groups FQM-0207 (J.S.D.) and FQM-0229 (A.M.F.) of Andalucía (Spain).

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Spin coherent-state path integrals and the instanton calculus[a)]

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(Received 20 November 2001; accepted 19 September 2002)

We use an instanton approximation to the continuous-time spin coherent-state path integral to obtain the tunnel splitting of classically degenerate ground states. We show that provided the fluctuation determinant is carefully evaluated, the path integral expression is accurate to order $O(1/j)$. We apply the method to the LMG model and to the molecular magnet Fe_8 in a transverse field. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1521797]

I. INTRODUCTION

One of the most convincing demonstrations of quantum effects in a near-macroscopic system is provided by the dramatic oscillation[1] of the level splittings in the molecular magnet Fe_8 as function of an external magnetic field. This system is small enough that one can obtain all the energy levels by a trivial numerical diagonalization of a 21×21 Hamiltonian matrix, but little insight into the phenomenon can be obtained this way. However, by thinking of the spin vector as an almost classical object, the oscillations can be understood as quantum interference between competing tunneling paths for the large ($J=10$) spin between two classically degenerate minima.

The natural tool for studying tunneling in the semiclassical limit is the path integral. For spin this should be the spin [SU(2)] coherent-state path integral,[2,3] or its phase space relative.[4,5] It is easy to establish that this formalism gives a good qualitative description of the tunnelling process—[6–8] including the dramatic topological quenching of the tunneling[9] that makes the Fe_8 results so interesting. Unfortunately, a straightforward application of the spin coherent-state path integral to compute the semiclassical propagator[10] or the tunnel splitting[11] yields results that are incorrect beyond the leading exponential order. In other words, the first quantum corrections as $J\to\infty$ are incorrectly obtained.

This issue appears for other systems that involve, or can be modeled in terms of, large-J quantum mechanical spins. Examples include molecular rotors,[12,13] the Lipkin–Meshov–Glick model of certain collective excitations in nuclei,[14,15] and superdeformed rotating nuclei.[16] The large spin limit is also valuable as an approximate method for studying magnetic ordering[17,18] including ''order from disorder'' effects in such systems.[19] In all these cases the first quantum corrections are not known. Often they are fixed by heuristic or *ad hoc* considerations. Lieb[20] puts

[a)]This paper is dedicated to the memory of Victor Belinicher, who was lost when Siberia Airlines flight 1812 was shot down over the Black Sea, Oct. 4th, 2001. Victor made many contributions to physics, in particular to the spin tunnelling problem.

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rigorous bounds on the partition function of quantum spin systems, but he does not determine the $1/J$ corrections precisely.

In principle, a correct evaluation of the general spin propagator in the semiclassical limit should resolve all these difficulties. This propagator is a notoriously refractory object, however, and its parent, the spin path integral, has a reputation for being mathematically ill defined—or at least harder to deal with than the conventional Feynman path integral, whose mathematical subtleties have been well studied. Many authors have therefore sought other ways of attaining the semiclassical limit, but none applies to general Hamiltonians. For the calculation of spin tunnel splittings, although there do exist other path integral approaches which solve particular problems correctly,[21,22] the resulting calculations tend to be intricate, and the simplicity seen in the conventional Schrödinger particle case is lost. Further, they do not lead to generally applicable recipes.

Recently, however, it has begun to be appreciated that the problem with the spin coherent state calculation is simply that the fluctuation determinant has an ''anomaly,'' and that, once the ''extra phase'' provided by the anomaly is taken into account, the coherent state path integral gives correct answers. This extra phase seems to have been originally discovered in the 1980s by Solari,[23] but the significance of his result was not widely appreciated. It was then rediscovered by one of the present authors[24] and also by Vieira and Sacramento.[25] The interpretation of the extra phase as an ''anomaly'' is due to the remaining authors of the present article.[26]

The present article is another step in the larger program of developing the spin semiclassical limit. The discussions of the extra phase cited in the previous paragraph were restricted to the case of quantum evolution between generic values of the classical degrees of freedom. However, when we calculate the tunnel splitting, the endpoints of the instanton path lie at local minima of the classical energy and, just as in the Schrödinger particle case, the Jacobi fluctuation operator has a zero mode which makes the inverse of its determinant singular and the general formula for the propagator inapplicable. Thus our earlier work was not directly amenable to calculating the tunnel splitting. The present article fills this gap.

In the next section we provide a brief review of the spin coherent-state path integral, including the correction to the fluctuation determinant prefactor. In Secs. III and IV we discuss the complications that ensue when there is a zero mode and provide a general formula for the one-instanton contribution to the tunneling amplitude. In Sec. V we apply this formula to the relatively simple case of the Lipkin–Meshkov–Glick (LMG) model,[14] and in Sec. VI we evaluate the tunnel splitting for a realistic model of Fe_8.

As explained above, our aim is not to find formulas for the energy splittings that can be compared with experiment. After all, the splittings for both model Hamiltonians can easily be found numerically for moderate values of J, say $J \leqslant 20$.[27] Instead we are using these models as nontrivial test cases. It is our hope that our methods will prove practical in other situations—multispin problems, for example—where numerical work is not so easy.

II. SPIN COHERENT STATES

We follow the conventions in Ref. 26 and define our spin coherent states[28] to be

$$|z\rangle = \exp(z\hat{J}_+)|j,-j\rangle, \tag{2.1}$$

where $|j,-j\rangle$ is the lowest spin state in the $2j+1$-dimensional representation of SU(2) and $\hat{J}_+$ is the spin algebra ladder operator obeying

$$\hat{J}_+|j,m\rangle = \sqrt{j(j+1)-m(m+1)}\,|j,m+1\rangle. \tag{2.2}$$

The variable z is a stereographic coordinate on the unit sphere with $z=0$ at the south pole (spin down direction) and $z=\infty$ at the north pole (spin up).

These coherent states are not normalized, but depend holomorphicly on z. This means that matrix elements such as $\langle z'|\hat{O}|z\rangle$ are holomorphic functions of the variable z, and anti-holomorphic functions of the variable z'.

The inner product of two coherent states is

$$\langle z'|z\rangle=(1+\overline{z}'z)^{2j}, \tag{2.3}$$

and they satisfy the overcompleteness relation

$$\mathbf{1}=\frac{2j+1}{\pi}\int\frac{d^2z}{(1+\overline{z}z)^{2j+2}}|z\rangle\langle z|. \tag{2.4}$$

Here d^2z is shorthand for $dx\,dy$. The factor $1/(1+\overline{z}z)^2$ combines with this to make the invariant measure on the the two-sphere. The remaining factor in the integration measure, $1/(1+\overline{z}z)^{2j}$, serves to normalize the coherent states.

We may use the overcompleteness relation to derive a formal continuous-time path integral representation for the propagator

$$K(\overline{\zeta}_f,\zeta_i,T)=\langle\zeta_f|e^{-i\hat{H}T}|\zeta_i\rangle. \tag{2.5}$$

We insert N intermediate overcompleteness relations into (2.5) and consider the limit $N\to\infty$. This leads to the path integration formula[24]

$$K(\overline{\zeta}_f,\zeta_i,T)=\int_{\zeta_i}^{\overline{\zeta}_f}d\mu(\overline{z},z)\exp\{S(\overline{z}(t),z(t))\}, \tag{2.6}$$

where the path measure $d\mu$ is

$$d\mu(\overline{z}(t),z(t))=\lim_{N\to\infty}\prod_{n=1}^{N}\frac{2j+1}{\pi}\frac{d^2z_n}{(1+\overline{z}_nz_n)^2}, \tag{2.7}$$

and the action $S(\overline{z}(t),z(t))$ is

$$S(\overline{z}(t),z(t))=j\{\ln(1+\overline{\zeta}_fz(T))+\ln(1+\overline{z}(0)\zeta_i)\}+\int_0^T\left\{j\frac{\dot{\overline{z}}z-\overline{z}\dot{z}}{1+\overline{z}z}-iH(\overline{z},z)\right\}dt. \tag{2.8}$$

The c-number Hamiltonian, $H(\overline{z},z)$, is obtained from the operator $\hat{H}$ by

$$H(\overline{z},z)=\langle z|\hat{H}|z\rangle/\langle z|z\rangle. \tag{2.9}$$

The paths $z(t)$, $\overline{z}(t)$ obey the boundary conditions $z(0)=\zeta_i$, $\overline{z}(T)=\overline{\zeta}_f$, but $\overline{z}(0)$, $z(T)$, being actually $\overline{z}(0+\epsilon)$ and $z(T-\epsilon)$, are unconstrained, and are to be integrated over.[24]

The manipulations leading to the continuous time path integral are heuristic, but with careful treatment the formal path integral should be as useful as the familiar configuration space Feynman path integral. In particular the semiclassical, or large j, propagator can be obtained from a stationary phase approximation to the path integral.[26]

The stationary phase approximation requires us to seek "classical" trajectories for which S remains stationary as we vary the functions $z(t)$ and $\overline{z}(t)$. These stationary paths will generally be complex. If we write z as $x+iy$ and $\overline{z}=x-iy$, then, except in special cases, x and y are not real numbers. In particular there is no requirement that $\overline{z}(0)$ be the complex conjugate of $z(0)\equiv\zeta_i$, nor that $z(T)$ be the complex conjugate of $\overline{z}(T)\equiv\overline{\zeta}_f$. Bearing this in mind, we make variations about a chosen path, and keep track of all boundary contributions resulting from integrations by parts. We find that

$$\delta S=\frac{2jz(T)}{1+\overline{\zeta}_f z(T)}\,\delta\overline{z}(T)+\frac{2j\overline{z}(0)}{1+\overline{z}(0)\zeta_i}\,\delta z(0)$$
$$+\int_0^T\left\{\delta z(t)\left(\frac{2j\dot{\bar{z}}}{(1+\overline{z}z)^2}-i\frac{\partial H}{\partial z}\right)+\delta\overline{z}(t)\left(-\frac{2j\dot{z}}{(1+\overline{z}z)^2}-i\frac{\partial H}{\partial\overline{z}}\right)\right\}dt. \tag{2.10}$$

Demanding that this change in the action be zero requires the trajectory to obey Hamilton's equations

$$\dot{\bar{z}}=i\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial z},\quad \dot{z}=-i\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial\overline{z}}, \tag{2.11}$$

together with the conditions $\delta z(0)=0$ and $\delta\overline{z}(T)=0$. We can therefore impose the boundary conditions $z(0)=\zeta_i$, $\overline{z}(T)=\overline{\zeta}_f$, but $\overline{z}(0)$ and $z(T)$ are free to vary, and so are determined by the equations of motion. This is important because Hamilton's equations are first order in time and we cannot simultaneously impose initial and final conditions on their solutions.

The dynamically determined endpoints can also be read off from the Hamilton–Jacobi relations that follow from (2.10). These are

$$\frac{\partial S_{\rm cl}}{\partial\overline{\zeta}_f}=\frac{2jz(T)}{1+\overline{\zeta}_f z(T)},\quad \frac{\partial S_{\rm cl}}{\partial\zeta_i}=\frac{2j\overline{z}(0)}{1+\overline{z}(0)\zeta_i}. \tag{2.12}$$

The Hamilton–Jacobi relations also tell us that

$$\frac{\partial S_{\rm cl}}{\partial\overline{\zeta}_i}=\frac{\partial S_{\rm cl}}{\partial\zeta_f}=0, \tag{2.13}$$

showing that $S_{\rm cl}$ is a holomorphic function of ζ_i, and an anti-holomorphic function of ζ_f. These analyticity properties of $S_{\rm cl}$ coincide with those of K. This is reasonable since $\exp S_{\rm cl}$ is the leading approximation to K, and we would expect analyticity to be preserved term-by-term in the large j expansion. Finally, we have the Hamilton–Jacobi equation

$$\frac{\partial S_{\rm cl}}{\partial T}=-iH(\overline{\zeta}_f,z(T)). \tag{2.14}$$

In Ref. 26 we showed that after we compute the Gaussian integral over small fluctuations about the stationary phase path the resulting semiclassical approximation to the propagator is

$$K_{\rm scl}(\overline{\zeta}_f,\zeta_i,T)=\left(\frac{(1+\overline{\zeta}_f z(T))(1+\overline{z}(0)\zeta_i)}{2j}\frac{\partial^2 S_{\rm cl}}{\partial\zeta_i\partial\overline{\zeta}_f}\right)^{1/2}\exp\left\{S_{\rm cl}(\overline{\zeta}_f,\zeta_i,T)+\frac{i}{2}\int_0^T\phi_{\rm SK}(t)dt\right\}, \tag{2.15}$$

or a sum of such terms over a set of contributing classical paths. In this expression

$$\phi_{\rm SK}(\overline{z},z)=\frac{1}{2}\left(\frac{\partial}{\partial\overline{z}}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial z}+\frac{\partial}{\partial z}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial\overline{z}}\right) \tag{2.16}$$

is the ''extra-phase'' discovered by Solari, Kochetov, and Vieira and Sacramento.

The form (2.15) is valid only if the prefactor is finite. When we compute instanton contributions to tunneling there is a zero mode in the quadratic form for small fluctuations, and the

resulting divergent integral over this mode is to be replaced by an integral over a collective coordinate labeling the instant that the tunneling event occurred. This we will describe in the next section.

We conclude this section by writing the Solari–Kochetov phase in an alternative way that will prove useful later. We first write

$$\phi_{\mathrm{SK}}=\phi'_{\mathrm{SK}}-ia_{\mathrm{WZ}}, \tag{2.17}$$

where

$$\phi'_{\mathrm{SK}}=\frac{(1+\bar{z}z)^2}{2j}\frac{\partial^2 H}{\partial z\partial\bar{z}}, \tag{2.18}$$

$$a_{\mathrm{WZ}}=i\frac{1+\bar{z}z}{2j}\left(z\frac{\partial H}{\partial z}+\bar{z}\frac{\partial H}{\partial\bar{z}}\right). \tag{2.19}$$

Along the classical trajectory, the equations of motion allow us to trade in the partial derivatives $\partial H/\partial z$ and $\partial H/\partial\bar{z}$ for $\dot{\bar{z}}$ and $\dot{z}$, so that

$$a_{\mathrm{WZ}}(\tau)=\frac{\dot{\bar{z}}_{\mathrm{cl}}z_{\mathrm{cl}}-\dot{z}_{\mathrm{cl}}\bar{z}_{\mathrm{cl}}}{1+\bar{z}_{\mathrm{cl}}z_{\mathrm{cl}}}. \tag{2.20}$$

This is nothing but the Wess–Zumino or kinetic term in the classical action, and was anticipated in our notation. Hence,

$$\frac{i}{2}\int_0^T\phi_{\mathrm{SK}}(t)dt=\frac{1}{2}\int_0^T a_{\mathrm{WZ}}(t)dt+\frac{i}{2}\int_0^T\phi'_{\mathrm{SK}}(t)\,dt. \tag{2.21}$$

The advantage of this rewriting is that the integral of a_{WZ} is needed to find S_{cl} anyway, and it is generally easier to integrate ϕ'_{SK} than ϕ_{SK}. In fact, ϕ'_{SK} is essentially the Laplacian of the energy on the unit sphere,[29]

$$\phi'_{\mathrm{SK}}=\frac{1}{2j}\nabla^2_\Omega H. \tag{2.22}$$

III. DEALING WITH THE ZERO MODE

As is usual in calculating tunneling effects, it is convenient to perform the computations in Euclidean (imaginary) time. For the sake of symmetry we will take the time evolution as running from $-T/2$ to $T/2$ and the propagator (2.15) becomes

$$K(\bar{\zeta}_f,\zeta_i,T)=[D(T)]^{-1/2}\exp\left\{S_{\mathrm{cl}}+\frac{1}{2}\int_{-T/2}^{T/2}\phi_{\mathrm{SK}}d\tau\right\}, \tag{3.1}$$

where again ϕ_{SK} is the integrand of the Solari–Kochetov phase

$$\phi_{\mathrm{SK}}=\frac{1}{2}\left(\frac{\partial}{\partial\bar{z}}\frac{(1+\bar{z}z)^2}{2j}\frac{\partial H}{\partial z}+\frac{\partial}{\partial z}\frac{(1+\bar{z}z)^2}{2j}\frac{\partial H}{\partial\bar{z}}\right), \tag{3.2}$$

evaluated along $z_{\mathrm{cl}}(\tau)$, $\bar{z}_{\mathrm{cl}}(\tau)$, and $D(T)$ is the fluctuation determinant. The latter may be found by the ''shooting method.'' As explained in Ref. 26, this involves solving the equation

$$\hat{L}\Psi_L\equiv\begin{bmatrix}B(\tau) & -\partial_\tau+A(\tau)\\ \partial_\tau+A(\tau) & \overline{B}(\tau)\end{bmatrix}\begin{pmatrix}\psi_L\\ \overline{\psi}_L\end{pmatrix}=0, \tag{3.3}$$

where

$$A=\phi_{\mathrm{SK}}=\frac{1}{2}\left(\frac{\partial}{\partial\overline{z}}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial z}+\frac{\partial}{\partial z}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial\overline{z}}\right),$$

$$B=\frac{\partial}{\partial\overline{z}}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial\overline{z}}, \tag{3.4}$$

$$\overline{B}=\frac{\partial}{\partial z}\frac{(1+\overline{z}z)^2}{2j}\frac{\partial H}{\partial z},$$

with the initial condition

$$\Psi_L(-T/2)=\begin{pmatrix}\psi_L\\ \overline{\psi}_L\end{pmatrix}_{-T/2}=\begin{pmatrix}0\\ 1\end{pmatrix}. \tag{3.5}$$

Given the solution of this equation, we read off the determinant as $D(T)=\overline{\psi}_L(T/2)$. In real time, and when there are no problems with zero modes, this recipe leads to the prefactor appearing in (2.15).

Now assume that the coherent states $|z_i\rangle$ and $|z_f\rangle$ represent spins pointing along the directions of two equal-energy global minima of the Hamiltonian $\hat{H}$. Because the gradient of the energy vanishes at both ends, the classical path joining z_i to z_f has the character of an instanton: as the total time taken to traverse the path becomes longer and longer most of the motion still takes place in an ''instant,'' a fixed period short in duration compared to the total. When T becomes infinite, the epoch of this ''instant'' is arbitrary and this leads to a zero-eigenvalue mode in the fluctuation operator. Thus $D(T)$ is formally zero. The problem of dividing by the square root of zero is avoided by introducing a collective coordinate for the tunneling epoch, and the formal infinity in the one-instanton contribution to the propagator becomes a factor of T.

The classical instanton solution can be written $z_{\mathrm{cl}}(\tau-\tau_0)$, $\overline{z}_{\mathrm{cl}}(\tau-\tau_0)$ where τ_0 is the epoch at which the tunneling occurs. Since, in the large T limit, the action for the tunneling event is independent of τ_0, the normalized zero mode is

$$\Psi_0=\begin{pmatrix}\psi_0(\tau)\\ \overline{\psi}_0(\tau)\end{pmatrix}=\frac{\sqrt{g}}{1+\overline{z}_{\mathrm{cl}}z_{\mathrm{cl}}}\begin{pmatrix}\dot{z}_{\mathrm{cl}}(\tau)\\ \dot{\overline{z}}_{\mathrm{cl}}(\tau)\end{pmatrix}, \tag{3.6}$$

where g is chosen to make

$$\int_{-T/2}^{T/2}\Psi_0^t\Psi_0 d\tau=\int_{-T/2}^{T/2}(\psi_0^2+\overline{\psi}_0^2)d\tau=1. \tag{3.7}$$

The divergent Gaussian integration over the coefficient of the zero mode is replaced by an integral over possible tunneling epochs τ_0 by inserting a factor of

$$1=\frac{1}{\sqrt{2\pi\alpha}}\int_{-T/2}^{T/2}d\tau_0\left(\frac{\partial\mathcal{F}}{\partial\tau_0}\right)\exp-\frac{1}{2\alpha}\mathcal{F}^2(\tau_0) \tag{3.8}$$

into the path integral, with the choice

$$\mathcal{F}(\tau_0)=\int_{-T/2}^{T/2}d\tau'\frac{1}{1+\overline{z}_{\mathrm{cl}}z_{\mathrm{cl}}(\tau'-\tau_0)}\Psi_0^t(\tau'-\tau_0)\begin{pmatrix}z(\tau')\\ \overline{z}(\tau')\end{pmatrix}, \tag{3.9}$$

and then proceeding in a manner similar to that used for quantum mechanical instantons in the Feynman path integral:[30,31] we first set $z=z_{\mathrm{cl}}(\tau-\tau_0)+\delta z(\tau-\tau_0)$ and similarly $\overline{z}$. Next, after

observing that everything depends only on the combination $\tau-\tau_0$, we change variables $\tau-\tau_0 \rightarrow \tau$. The integral over τ_0 is then trivial and gives a factor of T. Meanwhile, after an integration by parts and ignoring the fuctuations of $(z,\overline{z})$ about $(z_{\rm cl},\overline{z}_{\rm cl})$ which are of higher order, the Jacobian factor becomes

$$\frac{\partial \mathcal{F}}{\partial \tau_0}=\int_{-T/2}^{T/2} d\tau' \Psi_0^t \frac{1}{1+\overline{z}_{\rm cl} z_{\rm cl}}\begin{pmatrix} \dot{z}_{\rm cl}(\tau') \\ \dot{\overline{z}}_{\rm cl}(\tau') \end{pmatrix}=\frac{1}{\sqrt{g}}. \tag{3.10}$$

The quadratic term in the exponent is a projector onto the zero mode and replaces the vanishing eigenvalue by $1/2j\alpha$. The net result is the replacement

$$[D(T)]^{-1/2}\rightarrow T\sqrt{\frac{j}{\pi g}}\left[\frac{D(T)}{\lambda_0}\right]^{-1/2}, \tag{3.11}$$

where $\lambda_0(T)$ is the eigenvalue that vanishes as T becomes large.

The desired ratio, $\mathrm{Det}'(\hat{L})=D(T)/\lambda_0$, is equal to $\overline{\psi}_L(T/2)/\lambda_0(T)$. We now turn to the evaluation of this ratio. As we shall see, we will not have to obtain $\overline{\psi}_L(T/2)$ and $\lambda_0(T)$ separately.

The eigenvalue problem is

$$\hat{L}\Psi_\lambda=\lambda\Psi_\lambda; \quad \Psi_\lambda=\begin{pmatrix} \psi_\lambda \\ \overline{\psi}_\lambda \end{pmatrix}, \tag{3.12}$$

where $\hat{L}$ is the same operator as in (3.3), but with boundary conditions $\psi_\lambda(-T/2)=\overline{\psi}_\lambda(T/2)=0$.

For finite T the shooting method solution, Ψ_L, is close to, but not quite equal to, the "small-eigenvalue" eigenfunction, Ψ_{λ_0}. Although Ψ_L obeys the boundary condition at $\tau=-T/2$, it does not quite obey the boundary condition at $\tau=+T/2$. In turn Ψ_{λ_0} is close to, but not quite equal to, the infinite-T zero-eigenvalue mode, Ψ_0.

Now Ψ_0 obeys the equation $\hat{L}\Psi_0=0$, but no particular boundary conditions at $\pm T/2$. There is a second solution of this equation, $\Xi_0=(\xi_0,\overline{\xi}_0)^t$. The Wronskian of these solutions

$$W(\Psi,\Xi)=\begin{vmatrix} \psi_0(\tau) & \xi_0(\tau) \\ \overline{\psi}_0(\tau) & \overline{\xi}_0(\tau) \end{vmatrix} \tag{3.13}$$

is independent of τ. Next we observe that the differential equation (3.12) can be converted to an integral equation

$$\begin{aligned}\Psi_\lambda(\tau)&=\Psi_L(\tau)+\lambda\int_{-T/2}^{\tau} d\tau' G(\tau,\tau')\Psi_\lambda(\tau') \\ &=\Psi_L(\tau)+\frac{\lambda}{W}\int_{-T/2}^{\tau} d\tau'[\Psi_0(\tau)\Xi_0^t(\tau')-\Xi_0(\tau)\Psi_0^t(\tau')]\Psi_\lambda(\tau').\end{aligned} \tag{3.14}$$

Since $\Psi_L(\tau)$ obeys the boundary conditions at $-T/2$, and the integral vanishes at this point, we can find the eigenvalues λ by requiring that the lower component of Ψ_λ vanishes at $\tau=T/2$. We are only interested in solutions where $\lambda=\lambda_0$ is very small. Because of this we can approximate the $\Psi_\lambda(\tau')$ appearing in the integral in (3.14) by the zeroth-order solution, Ψ_L. In this way we see that

$$\frac{\overline{\psi}_L(T/2)}{\lambda_0(T)}=-\frac{1}{W}\int_{-T/2}^{T/2} d\tau[\overline{\psi}_0(T/2)\Xi_0^t(\tau)-\overline{\xi}_0(T/2)\Psi_0^t(\tau)]\Psi_L(\tau). \tag{3.15}$$

The integral in (3.15) may be evaluated using only the asymptotic behavior of Ψ_0 and Ξ_0, which involve $z_{\rm cl}$ and $\overline{z}_{\rm cl}$. This asymptotic behavior depends only on the form of the Hamiltonian in the neighborhood of the endpoints.

In all cases we consider the instanton solutions have the property that $\overline{z}_{\rm cl}=z_{\rm cl}^*$ at their endpoints. Here the asterisk denotes a true complex conjugate as opposed to the formal conjugate denoted by the bar. The coincidence of the formal and true conjugate occurs because these endpoints lie on the real unit sphere.[32] Taking this observation into account, we parametrize the Hamiltonian in the vicinity of the initial stationary point in terms of two frequencies, $\omega_{1,2}$, as

$$H(\overline{z},z)\approx\frac{2j}{(1+z_i^*z_i)^2}\left[\omega_1(z-z_i)(\overline{z}-z_i^*)+\frac{1}{2}\omega_2(z-z_i)^2+\frac{1}{2}\omega_2^*(\overline{z}-z_i^*)^2\right]. \tag{3.16}$$

Since $H(\overline{z},z)$ is real, so is ω_1. Also, because the initial point is an energy minimum, we must have $\omega_1>|\omega_2|$. We can therefore define a real mean frequency, ω, by

$$\omega^2\equiv\omega_1^2-\omega_2\omega_2^*. \tag{3.17}$$

A similar expression holds at z_f with the same values of ω_1 and ω_2 provided the degeneracy in the Hamiltonian is due to some symmetry. (There might be an extra phase factor in ω_2, but this makes no difference to the subsequent calculation.)

As τ becomes large and negative, $B\to\omega_2$, $\overline{B}\to\omega_2^*$ and $A=\phi_{\rm SK}\to\omega_1$, so we see that

$$\begin{pmatrix}\psi_0\\ \overline{\psi}_0\end{pmatrix}\to\begin{pmatrix}\psi_{0-}\\ \overline{\psi}_{0-}\end{pmatrix}e^{\omega\tau};\quad \begin{pmatrix}\xi_0\\ \overline{\xi}_0\end{pmatrix}\to\begin{pmatrix}\xi_{0-}\\ \overline{\xi}_{0-}\end{pmatrix}e^{-\omega\tau}, \tag{3.18}$$

where

$$\begin{bmatrix}\omega_2 & -\omega+\omega_1\\ \omega+\omega_1 & \omega_2^*\end{bmatrix}\begin{pmatrix}\psi_{0-}\\ \overline{\psi}_{0-}\end{pmatrix}=0. \tag{3.19}$$

There is an analogous relation for $(\xi_{0-},\overline{\xi}_{0-})^t$. We can use the Wronskian to connect Ψ_{0-} with Ξ_{0-}, so everything can be expressed in terms of W and the normalization g. Similar remarks apply to Ψ_{0+} and Ξ_{0+}. If we write

$$\begin{pmatrix}\psi_L\\ \overline{\psi}_L\end{pmatrix}=\alpha\begin{pmatrix}\psi_0\\ \overline{\psi}_0\end{pmatrix}+\beta\begin{pmatrix}\xi_0\\ \overline{\xi}_0\end{pmatrix}, \tag{3.20}$$

and apply the boundary condition at $-T/2$, we can find α and β, and hence

$$\begin{pmatrix}\psi_L(\tau)\\ \overline{\psi}_L(\tau)\end{pmatrix}=\frac{1}{W}\left[-\xi_{0-}e^{\omega T/2}\begin{pmatrix}\psi_0(\tau)\\ \overline{\psi}_0(\tau)\end{pmatrix}+\psi_{0-}e^{-\omega T/2}\begin{pmatrix}\xi_0(\tau)\\ \overline{\xi}_0(\tau)\end{pmatrix}\right]. \tag{3.21}$$

Inserting this into (3.15) and noting that the $\psi_0\ \overline{\psi}_0$ terms dominate, we find

$$\frac{\overline{\psi}_L(T/2)}{\lambda_0(T)}=-\frac{1}{W^2}\xi_{0-}\overline{\xi}_{0+}e^{\omega T}\int_{-T/2}^{T/2}(\psi_0^2+\overline{\psi}_0^2)\,d\tau, \tag{3.22}$$

or

$$\frac{\overline{\psi}_L(T/2)}{\lambda_0(T)}=\frac{|\omega_2|^2}{\psi_{0-}\overline{\psi}_{0+}}\frac{e^{\omega T}}{4\omega^2}. \tag{3.23}$$

Thus the one-instanton contribution to the propagator is

$$K(\overline{z_f},z_i,T)=\exp\left\{S_{\rm cl}+\frac{1}{2}\int_{-T/2}^{T/2}\phi_{\rm SK}d\tau\right\}\sqrt{\frac{j}{\pi g}}\left[\frac{\psi_{0-}\overline{\psi}_{0+}}{|\omega_2|^2}\right]^{1/2}(2\omega Te^{-(1/2)\omega T}). \tag{3.24}$$

Note that ψ_0, $\overline{\psi}_0$ are proportional to $\sqrt{g}$, thus $\sqrt{g}$ drops out and we can simply put $g=1$ in the sequel. Let

$$\begin{aligned}\dot{z}_{\rm cl}&\approx\omega\zeta_-e^{\omega\tau},\quad \tau\to-\infty,\\ \dot{\bar{z}}_{\rm cl}&\approx\omega\overline{\zeta}_+e^{-\omega\tau},\quad \tau\to+\infty.\end{aligned} \tag{3.25}$$

Then

$$\psi_{0-}\overline{\psi}_{0+}=\frac{\omega^2\zeta_-\overline{\zeta}_+}{N} \tag{3.26}$$

with

$$N=(1+\overline{z}_iz_i)(1+\overline{z}_fz_f). \tag{3.27}$$

Using this we can write

$$K(\overline{z_f},z_i,T)=\exp\left\{S_{\rm cl}+\frac{1}{2}\int_{-T/2}^{T/2}\phi_{\rm SK}d\tau\right\}\sqrt{\frac{j}{\pi N}}\left[\frac{\overline{\zeta}_+\zeta_-}{|\omega_2|^2}\right]^{1/2}(2\omega^2Te^{-(1/2)\omega T}). \tag{3.28}$$

IV. EXTRACTING THE ENERGY SPLITTING

Again assume that the coherent states $|z_i\rangle$ and $|z_f\rangle$ represent spins pointing along the directions of two equal energy global minima of the Hamiltonian $\hat{H}$. Let $|\psi_{i,f}\rangle$ be the approximate (tunneling-ignored) energy eigenstates localized near these minima. These should have their phases chosen so that when tunneling *is* included the eigenstates become the linear combinations

$$|\psi_\pm\rangle=\frac{1}{\sqrt{2}}(|\psi_i\rangle\pm|\psi_f\rangle). \tag{4.1}$$

If the energies of these states are

$$E_\pm=E_{\rm av}\pm\tfrac{1}{2}\Delta, \tag{4.2}$$

and $a_\alpha\equiv\langle z_\alpha|\psi_\alpha\rangle$, then as T becomes large the coherent-state propagator,

$$K(\overline{z_f},z_i,T)=\langle z_f|e^{-\hat{H}T}|z_i\rangle, \tag{4.3}$$

is given by

$$\begin{aligned}K(\overline{z_f},z_i,T)&\approx a_fa_i^*e^{-E_{\rm av}T}\sinh\left(\frac{1}{2}\Delta T\right),\\ &=a_fa_i^*e^{-E_{\rm av}T}\left(\frac{1}{2}\Delta T+\frac{1}{6}\frac{\Delta^3T^3}{2^3}+\cdots\right).\end{aligned} \tag{4.4}$$

We will find the energy splitting, Δ, by evaluating K in the one-instanton approximation and comparing with this expression.

It is necessary to find expressions for the amplitudes a_i and a_f. These are obtained by looking at

$$K_f=\langle z_f|e^{-\hat{H}T}|z_f\rangle\approx|a_f|^2e^{-E_{\rm av}T}, \tag{4.5}$$

and

$$K_i=\langle z_i|e^{-\hat{H}T}|z_i\rangle\approx|a_i|^2e^{-E_{\rm av}T}, \tag{4.6}$$

both evaluated in the harmonic approximation. This evaluation is performed in the Appendix. This results in

$$K_f=(1+\overline{z}_fz_f)^{2j}\sqrt{\frac{2\omega}{\omega+\omega_1}}e^{-(1/2)(\omega-\omega_1)T} \tag{4.7}$$

and a similar expression for K_i. Thus

$$\frac{1}{2}\Delta=\frac{e^{S_{\rm cl}+(1/2)\int_{-T/2}^{T/2}(\phi_{\rm SK}-\omega_1)d\tau}}{[(1+\overline{z}_fz_f)^j(1+\overline{z}_iz_i)^j]}\sqrt{\frac{j}{\pi N}}[2\omega(\omega+\omega_1)]^{1/2}\omega\left[\frac{\overline{\zeta}_+\zeta_-}{|\omega_2|^2}\right]^{1/2}. \tag{4.8}$$

Now

$$\frac{2\omega(\omega+\omega_1)}{\omega_2^2}=\frac{2\omega}{\omega_1-\omega} \tag{4.9}$$

so finally

$$\Delta=2\omega\sqrt{P}e^I, \tag{4.10}$$

where

$$P=\frac{j}{\pi N}\frac{2\omega}{\omega_1-\omega}\overline{\zeta}_+\zeta_- \tag{4.11}$$

and

$$I=j\int_{-\infty}^{\infty}a_{\rm wz}(\tau)d\tau+\frac{1}{2}\int_{-\infty}^{\infty}(\phi_{\rm SK}-\omega_1)d\tau \tag{4.12}$$

$$=\left(j+\frac{1}{2}\right)\int_{-\infty}^{\infty}a_{\rm wz}(\tau)d\tau+\frac{1}{2}\int_{-\infty}^{\infty}(\phi'_{\rm SK}-\omega_1)d\tau, \tag{4.13}$$

where $a_{\rm wz}$ is the kinetic term

$$a_{\rm WZ}(\tau)=\frac{\dot{\overline{z}}_{\rm cl}z_{\rm cl}-\dot{z}_{\rm cl}\overline{z}_{\rm cl}}{1+\overline{z}_{\rm cl}z_{\rm cl}} \tag{4.14}$$

in the classical action—the boundary terms having canceled with the $(1+\overline{z}_fz_f)^j(1+\overline{z}_iz_i)^j$ in the denominator. In Eq. (4.13), we have used the alternative form (2.17) of the Solari–Kochetov phase.

V. THE LMG MODEL

In this section we will evaluate the tunnel splitting in the relatively simple case of the Lipkin–Meshkov–Glick (LMG) model.[14]

We will take the LMG Hamiltonian to be

$$\hat{H}=\frac{w}{\sqrt{2}(2j-1)}(\hat{J}_+^2+\hat{J}_-^2)+\frac{jw}{\sqrt{2}}, \tag{5.1}$$

with $w>0$. For half-integer j, the splitting vanishes due to Kramers' theorem, and we will indicate below how this comes about. Unless stated otherwise, we will be thinking of integer j in what follows. Since $\hat{J}_+^2+\hat{J}_-^2=2(\hat{J}_x^2-\hat{J}_y^2)$, we see that the classical minima lie along $\pm\hat{y}$. The Hamiltonian which appears in the path integral is

$$H(\bar{z},z)=\frac{\langle z|\hat{H}|z\rangle}{\langle z|z\rangle}=\sqrt{2}jw\frac{z^2+\bar{z}^2}{(1+\bar{z}z)^2}+\frac{jw}{\sqrt{2}}. \tag{5.2}$$

By setting $\partial H/\partial z=\partial H/\partial\bar{z}=0$, the classical minima are found to be at the points

$$(z,\bar{z})=(i,-i),\quad (-i,i), \tag{5.3}$$

which correspond to the $\pm\hat{y}$ directions of the Cartesian axes. The explicitly added constant in $\hat{H}$ is chosen to make $H(\bar{z},z)$ zero at these points.

Now we write down the equations of motion for the instantons

$$\dot{\bar{z}}=\sqrt{2}w\frac{z-\bar{z}^3}{(1+\bar{z}z)},$$

$$\dot{z}=-\sqrt{2}w\frac{\bar{z}-z^3}{(1+\bar{z}z)}. \tag{5.4}$$

We seek a solution which goes from $(z_i,\bar{z_i})=(-i,i)$ to $(z_f,\bar{z_f})=(i,-i)$. The two equations in (5.4) can be decoupled by exploiting the energy conservation condition $H(\bar{z},z)=0$ which follows from the Hamiltonian nature of the trajectory. This can be written as

$$2(z^2+\bar{z}^2)+1+2\bar{z}z+\bar{z}^2z^2=0, \tag{5.5}$$

and may be solved to yield z as a function of $\bar{z}$ and *vice versa*:

$$\bar{z}=-i\frac{\sqrt{2}z+i}{z+\sqrt{2}i},\quad z=-i\frac{\sqrt{2}\bar{z}+i}{\bar{z}+\sqrt{2}i}. \tag{5.6}$$

(Choosing the other solution of the quadratic equation yields instantons running in the opposite direction.) Substituting these formulas in the equations of motion yields

$$\dot{\bar{z}}=-iw(1+\bar{z}^2),\quad \dot{z}=iw(1+z^2). \tag{5.7}$$

These may be integrated by elementary means to yield

$$z_{\rm cl}(\tau)=i\frac{e^{2w\tau}-C}{e^{2w\tau}+C}=i\tanh w(\tau-\tau_0), \tag{5.8}$$

$$\bar{z}_{\rm cl}(\tau)=-i\frac{e^{2w\tau}-C'}{e^{2w\tau}+C'}=-i\tanh w(\tau-\tau_0'), \tag{5.9}$$

where $C=e^{2w\tau_0}$, $C'=e^{2w\tau_0'}$. These constants are not independent. Energy conservation requires

$$\frac{C'}{C}=\frac{\sqrt{2}-1}{\sqrt{2}+1}. \tag{5.10}$$

It is useful at this point to find the frequencies ω, ω_1 and ω_2. We have

$$\omega_1=\frac{(1+\overline{z}_i z_i)^2}{2j}\frac{\partial^2 H}{\partial z\partial\overline{z}}\bigg|_i, \quad \omega_2=\frac{(1+\overline{z}_i z_i)^2}{2j}\frac{\partial^2 H}{\partial z^2}\bigg|_i, \tag{5.11}$$

where the suffix i means that the derivatives are to be evaluated at the initial point. Carrying out the algebra, we obtain

$$\omega_1=\frac{3}{\sqrt{2}}w, \quad \omega_2=\frac{1}{\sqrt{2}}w. \tag{5.12}$$

Hence,

$$\omega=(\omega_1^2-\omega_2^2)^{1/2}=2w. \tag{5.13}$$

We can now evaluate the Wess–Zumino and Solari–Kochetov terms in the tunneling action (4.13). We denote

$$I_{\mathrm{WZ}}=\left(j+\frac{1}{2}\right)\int_{-\infty}^{\infty}a_{\mathrm{WZ}}(\tau), \tag{5.14}$$

$$I_{\mathrm{SK}}=\frac{1}{2}\int_{-\infty}^{\infty}(\phi'_{\mathrm{SK}}-\omega_1)d\tau. \tag{5.15}$$

Let us begin with I_{WZ}. If we make use of Eq. (5.7), we find

$$a_{\mathrm{WZ}}(\tau)=\frac{1}{1+\overline{z}z}(\dot{\overline{z}}z-\overline{z}\dot{z})=-iw(\overline{z}+z). \tag{5.16}$$

Substituting the explicit forms and performing the integration we get

$$I_{\mathrm{WZ}}=-\left(j+\frac{1}{2}\right)\ln(C/C')=-(2j+1)\ln(1+\sqrt{2}). \tag{5.17}$$

Now consider the Solari–Kochetov term. We find that

$$\phi'_{\mathrm{SK}}=-\frac{6w}{\sqrt{2}}\frac{(z^2+\overline{z}^2)}{(1+\overline{z}z)^2}. \tag{5.18}$$

By energy conservation this equals

$$\frac{3w}{\sqrt{2}}, \tag{5.19}$$

which is precisely equal to ω_1. Thus, I_{SK} vanishes, and the total tunneling action is

$$I=-(2j+1)\ln(1+\sqrt{2}). \tag{5.20}$$

We must now evaluate P. This consists of a product of various factors, all of which are to hand. Thus,

$$\frac{j}{\pi N}=\frac{j}{4\pi}. \tag{5.21}$$

The factors $\overline{\zeta}_+$ and ζ_- are found by differentiating the formulas (5.8) and (5.9) and examining the limits $\tau \to \pm\infty$. In this we way we get

$$\zeta_- \overline{\zeta}_+ = 4\frac{C'}{C}. \tag{5.22}$$

Finally,

$$\frac{2\omega}{\omega_1 - \omega} = 4\sqrt{2}(3+2\sqrt{2}). \tag{5.23}$$

Putting these together, we obtain

$$P = -\frac{4j}{\pi}(4+3\sqrt{2})\frac{C'}{C} = \frac{4j}{\pi}\sqrt{2}. \tag{5.24}$$

At this point we have almost all that we need to write down the answer for the tunnel splitting—except that we need to consider a second instanton. The trajectory (5.8) and (5.9) passes close to the north pole of the sphere. By symmetry there must be a second instanton which passes near the south pole. This is given by

$$z_{\rm cl} = i\coth w(\tau - \tau_0), \quad \overline{z}_{\rm cl} = -i\coth w(\tau - \tau_0'). \tag{5.25}$$

It is obvious by symmetry again that this instanton has exactly the same amplitude as the first, so the total amplitude (and thus the splitting) is obtained by simply doubling the answer from the first instanton. (For half-integer j, the amplitudes interfere destructively giving $\Delta = 0$.) Hence

$$\Delta = 16w\left(\frac{j}{\pi}\right)^{1/2} 2^{1/4} e^{-(2j+1)\ln(1+\sqrt{2})}. \tag{5.26}$$

This agrees with Refs. 21, 22, and 33. [In the last reference put $\xi^2 = 1/\sqrt{2}$ in Eqs. 4.31–4.34.] We show in Table I a comparison between this formula and numerical evaluation of Δ. The agreement gets better with increasing j, up to $j = 18$. After this value, Δ is close to the machine precision, and the error is largely in the numerical answer.[27]

For completeness, we note that the average energy is given by $E_{\rm av} = 1/2\,(\omega - \omega_1)$.

VI. APPLICATION TO FE_8

The LMG model is of interest to us primarily because it provides a check of our formalism against other well-confirmed calculations. In this section we will calculate the tunnel splitting for a family of models that includes a realistic approximation to the molecular magnet Fe_8. The spin-direction-dependent energy in Fe_8 is less symmetric than that of the LMG, and the relevant Hamiltonian includes an externally imposed magnetic field which serves to pull the classical minima off the equator of the unit sphere. It is the experimentally observed oscillations in the tunnel splitting as a function of the external field that makes this system interesting. The oscillations are a consequence of interference between the two distinct instanton trajectories and are accurately reproduced by our calculation.

We take as our Hamiltonian

$$\hat{H} = k_1 \hat{J}_z^2 + k_2 \hat{J}_y^2 - g\mu_B H \hat{J}_z, \tag{6.1}$$

with $k_1 > k_2 > 0$. We define $\lambda = k_2/k_1$, $H_c = 2k_1 j/g\mu_B$ and

$$h = H/H_c. \tag{6.2}$$

TABLE I. Comparison between numerical and analytic [Eq. (5.26)] results for the ground state tunnel splitting in the LMG model with $w=1$. Numbers in parentheses give the power of 10 multiplying the answer. The last column gives the deviation of the analytic answer from the numerical one. Note, however, that for $j=19$ and $j=20$, the splitting is getting close to the machine precision, and the error is largely in the numerical result.

j	Δ (numerical)	Δ (analytic)	Difference(%)
2	2.1878(−1)	1.8511(−1)	15.4
3	4.3279(−2)	3.8899(−2)	10.1
4	8.3587(−3)	7.7064(−3)	7.8
5	1.5781(−3)	1.4783(−3)	6.3
6	2.9339(−4)	2.7784(−4)	5.3
7	5.3948(−5)	5.1489(−5)	4.6
8	9.8372(−6)	9.4441(−6)	4.0
9	1.7820(−6)	1.7186(−6)	3.6
10	3.2111(−7)	3.1082(−7)	3.2
11	5.7611(−8)	5.5932(−8)	2.9
12	1.0298(−8)	1.0023(−8)	2.7
13	1.8352(−9)	1.7899(−9)	2.5
14	3.2618(−10)	3.1869(−10)	2.3
15	5.7836(−11)	5.6598(−11)	2.1
16	1.0233(−11)	1.0029(−11)	2.0
17	1.8157(−12)	1.7737(−12)	2.3
18	3.0813(−13)	3.1314(−13)	1.6
19	4.9021(−14)	5.5199(−14)	12.6
20	2.5766(−14)	9.7166(−15)	62.3

We will express all results in terms of the combinations λ and h. It is also convenient to define a $1/j$ corrected field $\tilde{h}$ and anisotropy $\tilde{k}_1$ by

$$\tilde{h}=jh\Big/\left(j-\frac{1}{2}\right),\quad \tilde{k}_1=k_1\left(j-\frac{1}{2}\right)\Big/ j. \tag{6.3}$$

We follow the same steps as in the LMG model. The ''classical'' Hamiltonian appearing in the path integral is

$$H(\bar{z},z)=\frac{\langle z|\hat{H}|z\rangle}{\langle z|z\rangle}=\tilde{k}_1 j^2\left[\frac{(1-\bar{z}z)^2-\lambda(z-\bar{z})^2-2\tilde{h}(1-\bar{z}^2z^2)}{(1+\bar{z}z)^2}\right]. \tag{6.4}$$

(We now use states in which $z=0$ corresponds to the north pole, as this is more convenient. Also, a constant $(k_1+k_2)\ j/2$ has been subtracted from the classical energy.) The energy minima are now at the points

$$\bar{z}=z=\pm z_0, \tag{6.5}$$

where z_0 is real and given by

$$z_0=[(1-\tilde{h})/(1+\tilde{h})]^{1/2}. \tag{6.6}$$

In Cartesian coordinates these minima lie in the xz plane—provided we confine ourselves to $\tilde{h}<1$, which we shall do. In fact, we will assume that

$$\tilde{h}<\sqrt{1-\lambda}. \tag{6.7}$$

At the two minima, the energy is

$$\epsilon_0=H(\bar{z}_0,z_0)=-\tilde{k}_1 j^2\tilde{h}^2. \tag{6.8}$$

The classical equations of motion are

$$\dot{\bar{z}}=\frac{\tilde{k}_1 j}{(1+\bar{z}z)}[-2\bar{z}(1-\bar{z}z)+\lambda(\bar{z}-z)(1+\bar{z}^2)+2\tilde{h}\bar{z}(1+\bar{z}z)],$$
$$\dot{z}=-\frac{\tilde{k}_1 j}{(1+\bar{z}z)}[-2z(1-\bar{z}z)+\lambda(z-\bar{z})(1+z^2)+2\tilde{h}z(1+\bar{z}z)]. \tag{6.9}$$

We wish to solve these subject to the boundary conditions $z_i=z(-\infty)=z_0$, $\bar{z}_f=z(\infty)=-z_0$. Note that $\bar{z}_i=z_i$, $z_f=\bar{z}_f$, so the instanton end points still lie on the real sphere, but the rest of the instanton does not. Once again the equations can be decoupled by exploiting the fact that energy is conserved along the instanton trajectory. In this case $H(\bar{z},z)=\epsilon_0$. This condition can be written as

$$(1-\bar{z}z)^2-\lambda(z-\bar{z})^2-2\tilde{h}(1-\bar{z}^2z^2)=-\tilde{h}^2(1+\bar{z}z)^2, \tag{6.10}$$

and may be solved to give

$$\bar{z}=\frac{\sqrt{\lambda}z\pm(1-\tilde{h})}{\sqrt{\lambda}\pm(1+\tilde{h})z}. \tag{6.11}$$

Substituting this in the equation of motion for $\dot{z}$, and simplifying, we get

$$\dot{z}=\pm\sqrt{\lambda}(1+\tilde{h})\tilde{k}_1 j(z_0^2-z^2). \tag{6.12}$$

We will see that to obtain instantons going from z_0 to $-z_0$, we must pick the minus sign in this equation. The other sign yields instantons running in the opposite direction.

It is now elementary to integrate Eq. (6.12), and use Eq. (6.11) to obtain the time dependence for both $z_{\rm cl}(\tau)$ and $\bar{z}_{\rm cl}(\tau)$. We find

$$z_{\rm cl}(\tau)=-z_0\tanh t, \tag{6.13}$$

$$\bar{z}_{\rm cl}(\tau)=-z_0\frac{\sqrt{\lambda}\tanh t+\sqrt{1-\tilde{h}^2}}{\sqrt{\lambda}+\sqrt{1-\tilde{h}^2}\tanh t}. \tag{6.14}$$

Here,

$$t=\omega\tau/2, \tag{6.15}$$

and the frequency ω is given by

$$\omega=2\tilde{k}_1 j[\lambda(1-\tilde{h}^2)]^{1/2}. \tag{6.16}$$

That this is the same ω that follows from Eqs. (3.16) and (3.17) shall be shown shortly. It can be seen that our solution corresponds to choosing the minus sign in Eq. (6.12) as asserted above. It is also useful to note that the solution (6.13) and (6.14) can be rewritten as

$$z_{\rm cl}=-z_0\tanh t,\quad \bar{z}_{\rm cl}=-z_0\coth(t+t_0), \tag{6.17}$$

where

$$\tanh t_0=\left(\frac{\lambda}{1-\tilde{h}^2}\right)^{1/2}. \tag{6.18}$$

Equations (6.12) and (6.11) possess a second solution,

$$z_{\rm cl}=-z_0\coth t,\quad \overline{z_{\rm cl}}=-z_0\tanh(t+t_0). \tag{6.19}$$

Formally, this new trajectory can be obtained from the first by the shift $t\to t+i\pi/2$. Alternatively, we could obtain it by switching the expressions for $z_{\rm cl}$ and $\overline{z_{\rm cl}}$ in Eqs. (6.13) and (6.14), which corresponds to reflection in the xz plane—a symmetry of the Hamiltonian—and then shifting t by $-t_0$.

Again we find the frequencies ω, ω_1 and ω_2. We note that

$$\omega_1=\frac{(1+\overline{z}_i z_i)^2}{2j}\frac{\partial^2 H}{\partial z\partial\overline{z}}\bigg|_i,\quad \omega_2=\frac{(1+\overline{z}_i z_i)^2}{2j}\frac{\partial^2 H}{\partial z^2}\bigg|_i, \tag{6.20}$$

where the suffix i means that the derivatives are to be evaluated at the initial point $\overline{z}=z=z_i$. Carrying out the algebra, we obtain

$$\omega_1=\tilde{k}_1 j(1-\tilde{h}^2+\lambda), \tag{6.21}$$

$$\omega_2=\tilde{k}_1 j(1-\tilde{h}^2-\lambda). \tag{6.22}$$

We now use Eq. (3.17) to show that ω is given by Eq. (6.16). The same frequencies are found at the final point $\overline{z}=z=z_f$.

We next evaluate and integrate the Wess–Zumino and Solari–Kochetov terms in the tunneling action, denoting these by $I_{\rm WZ}$ and $I_{\rm SK}$ as before. Since the calculations are somewhat lengthy, it is best to do the two terms separately. We begin with $I_{\rm WZ}$, considering instanton 1, i.e., that given by (6.13) and (6.14). After some algebra, we obtain

$$a_{\rm WZ}(\tau)=-\frac{\pi_2(\tanh t)}{\pi_3(\tanh t)}\frac{\omega}{2}\operatorname{sech}^2 t, \tag{6.23}$$

where π_2 and π_3 are polynomials of degree 2 and 3, whose explicit form we do not require. What we do need is the differential $a_{\rm WZ}d\tau$. If we make the substitution

$$v=\tanh t, \tag{6.24}$$

and factorize the polynomials π_2 and π_3, we obtain

$$\int_{-\infty}^{\infty}a_{\rm WZ}(\tau)d\tau=-\int_{-1}^{1}\frac{(v-v_3)(v-v_4)}{(v-v_1)(v-v_2)(v-v_5)}dv, \tag{6.25}$$

where

$$v_{1,2}=\frac{1}{\sqrt{\lambda}}\left(\frac{1+\tilde{h}}{1-\tilde{h}}\right)^{1/2}(-1\pm\sqrt{1-\lambda}), \tag{6.26}$$

$$v_{3,4}=\frac{-\sqrt{1-\tilde{h}^2}\pm\sqrt{1-\tilde{h}^2-\lambda}}{\sqrt{\lambda}}, \tag{6.27}$$

$$v_5=-\frac{\sqrt{\lambda}}{\sqrt{1-\tilde{h}^2}}. \tag{6.28}$$

The integral is best done by decomposing the integrand into partial fractions. We find

$$\frac{(v-v_3)(v-v_4)}{(v-v_1)(v-v_2)(v-v_5)}=\frac{1}{v-v_5}+\frac{\beta}{v-v_1}-\frac{\beta}{v-v_2}, \tag{6.29}$$

where

$$\beta=-\frac{\tilde{h}}{\sqrt{1-\lambda}}. \tag{6.30}$$

Thus,

$$\int_{-\infty}^{\infty} a_{\mathrm{WZ}}d\tau=-\left[\ln\left(\frac{1-v_5}{-1-v_5}\right)+\beta\ln\left(\frac{1-v_1}{-1-v_1}\right)-\beta\ln\left(\frac{1-v_2}{-1-v_2}\right)\right]. \tag{6.31}$$

The ratio involving v_5 is

$$\frac{1-v_5}{-1-v_5}=\frac{\sqrt{\lambda}+\sqrt{1-\tilde{h}^2}}{\sqrt{\lambda}-\sqrt{1-\tilde{h}^2}}\equiv\tilde{R}_1, \tag{6.32}$$

while the β terms combine to yield the logarithm of

$$\frac{1-v_1v_2+(v_2-v_1)}{1-v_1v_2-(v_2-v_1)}=\frac{\tilde{h}\sqrt{\lambda}+\sqrt{1-\lambda}\sqrt{1-\tilde{h}^2}}{\tilde{h}\sqrt{\lambda}-\sqrt{1-\lambda}\sqrt{1-\tilde{h}^2}}\equiv\tilde{R}_2. \tag{6.33}$$

Collecting together the various parts, we have

$$I_{\mathrm{WZ},1}=-\left(j+\frac{1}{2}\right)\ln\tilde{R}_1+\left(j+\frac{1}{2}\right)\frac{\tilde{h}}{\sqrt{1-\lambda}}\ln\tilde{R}_2. \tag{6.34}$$

We have added another suffix to show that this pertains to instanton 1.

The next step is to integrate the Solari–Kochetov term. For this we first need ϕ'_{SK}. From Eqs. (6.4) and (2.17) we find

$$\phi'_{\mathrm{SK}}=\frac{\tilde{k}_1 j}{(1+\overline{z}z)^2}[-2(1-4\overline{z}z+(\overline{z}z)^2)+\lambda((1+\overline{z}z)^2+3(\overline{z}-z)^2)+2\tilde{h}(1-\overline{z}^2z^2)]. \tag{6.35}$$

(The reader may verify that as $\tau\to\pm\infty$, $\phi'_{\mathrm{SK}}\to\omega_1$. This provides a check on our earlier calculation of ω_1.) After a little more work, we find

$$\phi'_{\mathrm{SK}}-\omega_1=\frac{\tilde{k}_1 j}{(1+\overline{z}z)^2}[-3(1-\overline{z}z)^2+3\lambda(\overline{z}-z)^2+2\tilde{h}(1-\overline{z}^2z^2)+\tilde{h}^2(1+\overline{z}z)^2]. \tag{6.36}$$

This quantity is the integrand in Eq. (5.15) for I_{SK}, and so it only needs to be evaluated along the instanton trajectories. We may simplify the calculation by using energy conservation to eliminate the term in λ. When this is done, we obtain

$$I_{\mathrm{SK}}=2\tilde{k}_1 j\tilde{h}\int_{-\infty}^{\infty}d\tau\frac{-(1-\tilde{h})+(1+\tilde{h})\overline{z}z}{1+\overline{z}z}. \tag{6.37}$$

The integrals are evaluated in the same way as I_{WZ}. With the same change of variables, and definitions of v_1 to v_5 as before, we get

$$I_{\mathrm{SK}}=-\frac{2\tilde{h}(1-\tilde{h}^2)^{1/2}}{\sqrt{\lambda}(1-\tilde{h})}\int_{-1}^{1}\frac{dv}{(v-v_1)(v-v_2)}=-\frac{\tilde{h}}{\sqrt{1-\lambda}}\int_{-1}^{1}\left[\frac{1}{v-v_1}-\frac{1}{v-v_2}\right]dv$$

$$=-\frac{\tilde{h}}{\sqrt{1-\lambda}}\ln\tilde{R}_2. \tag{6.38}$$

Note that this is $O(1/j)$ relative to the Wess–Zumino contribution. Adding together the two contributions, we obtain the total action

$$I=-\left(j+\frac{1}{2}\right)\ln\tilde{R}_1+\frac{jh}{\sqrt{1-\lambda}}\ln\tilde{R}_2. \tag{6.39}$$

In the second term we have used the formula $(j-1/2)\tilde{h}=jh$.

We now turn to the prefactor P. In evaluating this, we may ignore differences of order $1/j$, i.e., we may replace $\tilde{j}$ by j, $\tilde{h}$ by h, etc. The quantity consists of a product of various factors, all of which are already available. Thus,

$$\frac{j}{\pi N}=\frac{j}{\pi(1+z_0^2)^2}. \tag{6.40}$$

The factors $\bar{\zeta}_+$ and ζ_- are found by differentiating the formulas (6.13) and (6.14) and examining the limits $\tau\to\pm\infty$. In this we way we get

$$\zeta_-=-2z_0, \tag{6.41}$$

$$\bar{\zeta}_+=2z_0\frac{\sqrt{1-h^2}-\sqrt{\lambda}}{\sqrt{1-h^2}+\sqrt{\lambda}}. \tag{6.42}$$

Finally,

$$\frac{2\omega}{\omega_1-\omega}=4\frac{\sqrt{\lambda(1-h^2)}}{(1-h^2+\lambda)-2\sqrt{\lambda(1-h^2)}}=4\frac{\sqrt{\lambda(1-h^2)}}{[\sqrt{1-h^2}-\sqrt{\lambda}]^2}. \tag{6.43}$$

Making use of the identity

$$\frac{2z_0}{1+z_0^2}=(1-h^2)^{1/2}, \tag{6.44}$$

we obtain

$$P=-\frac{4j}{\pi}\frac{\lambda^{1/2}(1-h^2)^{3/2}}{1-h^2-\lambda}. \tag{6.45}$$

We can now obtain the contribution of instanton 1 to the tunneling amplitude by substituting Eqs. (6.39) and (6.45) in the general formula (4.10). Denoting this quantity by Δ_1, we have

$$\Delta_1=2\omega\sqrt{|P|}e^{I-i\pi/2}, \tag{6.46}$$

where the additional factor of $e^{-i\pi/2}$ arises from the fact that $P<0$.

It remains to obtain the tunneling amplitude Δ_2 from the second instanton. Because the two instantons are related by a complex shift in t, it is apparent that the actions $I_{1,2}$ (where we temporarily add suffixes to distinguish the two) and the prefactors $P_{1,2}$ will be given by the same

analytic expressions. However, the phases to be assigned to the actions and $\sqrt{P}$ are somewhat ambiguous. Unlike the case of a particle moving in one dimension, the prefactor in the general formula does not arise as the determinant of a Hermitian quadratic form, and there is no unambiguous way for factors of i to get partitioned between the prefactor and the exponent. The surest way of fixing the relative phases is to appeal to a physical argument. Alternatively, this can be regarded as fixing the signs of the amplitudes a_i and a_f.

For the Fe_8 Hamiltonian (6.4), let us work in the J_z basis $|j,m\rangle$ with the standard definition of the raising and lowering operators $J_\pm$, so that the matrix elements $\langle j,m\pm 1|J_\pm|j,m\rangle$ are all real. Then the matrix of $\hat{H}$ is completely real, and since it is Hermitian, all its eigenvalues and eigenvectors are also real. Second, since $z_i=z_0$ and $z_f=-z_0$ are real, the states $|z_{i,f}\rangle$ are real, i.e., all the matrix elements $\langle j,m|z_{i,f}\rangle$ are real. Thus the amplitudes a_i and a_f are real. It follows that the amplitude K is real, and so is the one-instanton contribution to it, i.e., $\Delta_1+\Delta_2$ is real. Therefore, we must have

$$\Delta_2=\Delta_1^*. \tag{6.47}$$

Equation (6.47) determines Δ_2, and the energy splitting Δ completely. However, it is still useful to investigate the origin of the phase difference in the actions a little more closely. As readers will have noticed already, the integrand in Eq. (6.25) is singular at $v=v_2$ and $v=v_5$, since for $\tilde{h}<\sqrt{1-\lambda}$,

$$v_1<-1, \quad -1<v_2<1, \quad -1<v_5<1. \tag{6.48}$$

Correspondingly, both $\tilde{R}_1$ and $\tilde{R}_2$ are negative, and both $\ln\tilde{R}_1$ and $\ln\tilde{R}_2$ must be interpreted to have an imaginary part of π modulo an integer multiple of 2π. The question is what the assignment should be for the two instantons. We can see this most easily by examining the difference $\Delta I_{\rm WZ}=I_{\rm WZ,2}-I_{\rm WZ,1}$. To this end, we note that the WZ one-form may be written as a complex one-form in the z plane,

$$a_{\rm WZ}d\tau=\frac{1}{1+z\overline{z}(z)}\left[z\frac{d\overline{z}}{dz}-\overline{z}(z)\right]dz\equiv F(z)dz, \tag{6.49}$$

with $\overline{z}(z)$ given by Eq. (6.11). Thus, $I_{\rm WZ}$ may be written as a z-plane contour integral of $F(z)$ from z_0 to $-z_0$. In fact, apart from a scale factor of z_0, the substitution (6.24) is tantamount to changing the integration variable to z, so we see that $F(z)$ has poles at z_0v_2 and z_0v_5 (the one at z_0v_1 does not matter). The two instantons go around these poles in opposite senses, so $\Delta I_{\rm WZ}$ is given by integrating $F(z)$ along a closed contour from z_0 to $-z_0$ and back to z_0:

$$\Delta I_{\rm WZ}=(2j+1)\oint F(z)dz. \tag{6.50}$$

The residues at the poles can be read off the partial fraction decomposition (6.29), yielding

$$I_{\rm WZ,2}-I_{\rm WZ,1}=(2j+1)\pi\left[1-\frac{\tilde{h}}{\sqrt{1-\lambda}}\right]. \tag{6.51}$$

This is precisely what we would obtain from Eq. (6.47), for that would have us assign $\pm i\pi$ for $\ln\tilde{R}_1$ (and $\ln\tilde{R}_2$) for the two instantons.

The energy splitting is given by

$$\Delta=\Delta_1+\Delta_2^*. \tag{6.52}$$

To compare with previous results, it is useful to rewrite this as follows. Consider the real part of the action, Eq. (6.39),

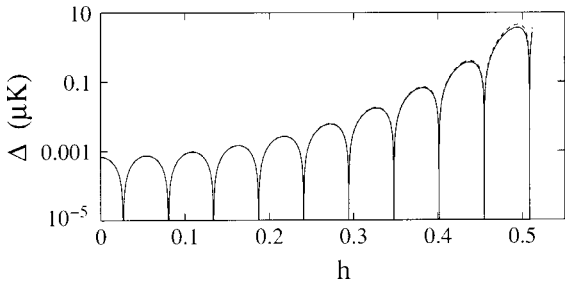

FIG. 1. Comparison between numerical (solid line) and analytic [Eq. (6.55), dashed line] results for the splitting between the two lowest levels in the Fe_8 model. The parameters are $k_1=0.321$ K, $k_2=0.229$ K, close to the measured values.

$$\Gamma_0 = -\operatorname{Re} I = \left(j+\frac{1}{2}\right)\ln|\tilde{R}_1| - \frac{jh}{\sqrt{1-\lambda}}\ln|\tilde{R}_2|. \tag{6.53}$$

The ratios $\tilde{R}_1$ and $\tilde{R}_2$ are defined in terms of the field $\tilde{h}$. If we write $\tilde{h}=h+O(1/j)$, and expand in powers of $1/j$, we discover that

$$\Gamma_0 = \left(j+\frac{1}{2}\right)\ln|R_1| - \frac{jh}{\sqrt{1-\lambda}}\ln|R_2| + O(j^{-1}), \tag{6.54}$$

where R_i is obtained from $\tilde{R}_i$ by simply deleting the tildes above the h's. Note that the corrections are of $O(1/j)$, not $O(1)$. These are beyond the accuracy to which we are working, so we simply drop them henceforth.

Thus, the complete expression for the splitting is

$$\Delta = \sqrt{\frac{8}{\pi}}\,\omega F^{1/2} e^{-\Gamma_0}\cos\Lambda. \tag{6.55}$$

We give the expressions for F, Γ_0 and Λ for ready reference:

$$F = 8j\,\frac{\lambda^{1/2}(1-h^2)^{3/2}}{1-h^2-\lambda}, \tag{6.56}$$

$$\Gamma_0 = \left(j+\frac{1}{2}\right)\ln\left[\frac{\sqrt{1-h^2}+\sqrt{\lambda}}{\sqrt{1-h^2}-\sqrt{\lambda}}\right] - \frac{jh}{\sqrt{1-\lambda}}\ln\left[\frac{\sqrt{(1-\lambda)(1-h^2)}+h\sqrt{\lambda}}{\sqrt{(1-\lambda)(1-h^2)}-h\sqrt{\lambda}}\right], \tag{6.57}$$

$$\Lambda = \operatorname{Im} I - \frac{\pi}{2} = j\pi\left(1-\frac{h}{\sqrt{1-\lambda}}\right). \tag{6.58}$$

Our answer for Δ is identical to that found by means of the discrete WKB method in Ref. 34 [see Eqs. (5.1)–(5.5)]. Naturally, the points at the which the tunnel splitting vanishes are the same, too. In Fig. 1, we compare our result with a numerical evaluation of Δ. The error rises from $\sim 1.5\%$ at $h=0$ to $\sim 35\%$ at the largest values of h shown. However, given that our formula is only asymptotically valid as $j\to\infty$ for fixed h, and that it fits the overall behavior over five orders of magnitude, this is quite acceptable. The approximation is clearly not uniform in h. The energy barrier decreases with increasing h, and since semiclassical answers for splittings are generally more accurate the higher the barrier, the trend in the error is not surprising either.

The nontrivial aspect of this calculation is that there are $1/j$ corrections in the quenching condition. If we simply take the energy expectation $H(\overline{z},z)=\langle z|\hat{H}|z\rangle/\langle z|z\rangle$ in the Wess–Zumino

term, we have the problem that the anisotropy and field terms scale with j differently if $1/j$ corrections are included. This is how the quenching condition was found in Ref. 9, but the $1/j$ corrections were never considered, so it was somewhat serendipitous that the condition that was stated turned out to be rigorously correct. By including the SK correction, this deficiency is now repaired.

VII. DISCUSSION

We have shown in this article how to extend to the spin coherent-state path integrals, the methods used to calculate tunnel splittings from the Feynman path integral. Key to this extension is the inclusion of the extra phase of Solari and Kochetov. The examples we discuss show that with this inclusion, the spin coherent-state path integral is accurate and effective. It must therefore be possible to put the spin coherent-state path integral on the same sound mathematical footing as the conventional Feynman integral.

Our calculations also bear on the old question of the correct ''tunnelling action'' for spin. In their complex periodic orbit study of the rotational spectrum of the SF_6 molecule for example, Robbins *et al.*[13] take, without proof, the differential of the action to be

$$dS=\left(j+\frac{1}{2}\right)\cos\theta d\phi, \tag{7.1}$$

where θ and ϕ are the usual spherical polar coordinates. Harter and Patterson[12] use the quantity $[j(j+1)]^{1/2}$ instead of $(j+1/2)$. These are both attempts to include the first quantum corrections. From our perspective, these corrections are somewhat ambiguously defined, since they could equally well be absorbed into the prefactor P in the splitting. Even if we do regard Eq. (4.13) as the tunneling action, it is clear that there is no universal $j\to j+1/2$ rule. The Solari–Kochetov term must be included. This term makes no contribution when it is a constant (and therefore equal to ω_1). This happens in two very commonly studied cases: $\mathcal{H}=\mathbf{J}\cdot\mathbf{H}$ (Larmor precession), and $\mathcal{H}=g_{ik}J_iJ_k$, $i,k=x,y,z$ (a homogeneous second order polynomial in J_x, J_y, and J_z). Indeed, the special LMG model studied in Sec. V is of the second type. In general, however, the Solari–Kochetov phase will influence the first quantum corrections in any other semiclassical formula.

ACKNOWLEDGMENTS

We are indebted to C. L. Henley for his construcive critique and queries on an earlier version of this paper. Work at Urbana and Evanston was supported by the National Science Foundation under Grant Nos. DMR-98-17941 and DMR-9616749, respectively. EK thanks the Russian Foundation for Fundamental Research for supporting this work through Grant No. 00-01-00049.

APPENDIX: ZERO-POINT MOTION PROPAGATOR

Here we derive Eq. (4.6). We first apply an SU(2) rotation to

$$H_{\text{initial}}(\bar{z},z)=\frac{2j}{(1+z_i^*z_i)^2}\left[\omega_1(z-z_i)(\bar{z}-z_i^*)+\frac{1}{2}\omega_2(z-z_i)^2+\frac{1}{2}\omega_2^*(\bar{z}-z_i^*)^2\right] \tag{A1}$$

in order to place z_i, $\bar{z_i}$ at the origin, and to make the coefficient ω_2 real. The result is

$$H(\bar{z},z)=2j\left[\omega_1\bar{z}z+\frac{1}{2}\omega_2z^2+\frac{1}{2}\omega_2\bar{z}^2\right]. \tag{A2}$$

In the semiclassical limit, $2j\gg1$, we may ignore the curvature of the phase space and, after rescaling $\sqrt{2j}z\to z$ to account for the difference in the coefficient in the kinetic terms, identify $H(\bar{z},z)$ with the coherent state classical Hamiltonian for the squeezed harmonic oscillator

$$\hat{H} = \omega_1 a^\dagger a + \tfrac{1}{2}\omega_2 (a^{\dagger 2} + a^2). \tag{A3}$$

The Bogoliubov transformation

$$\begin{aligned} b &= \cosh\theta a + \sinh\theta a^\dagger, \\ b^\dagger &= \sinh\theta a + \cosh\theta a^\dagger, \end{aligned} \tag{A4}$$

reduces the Hamiltonian

$$\hat{H}_{\text{squeezed}} = \Omega \cosh 2\theta (a^\dagger a + \tfrac{1}{2}) + \tfrac{1}{2}\Omega \sinh 2\theta (a^{\dagger 2} + a^2) \tag{A5}$$

to

$$\hat{H}_{\text{squeezed}} = \Omega (b^\dagger b + \tfrac{1}{2}), \tag{A6}$$

and so we identify

$$\begin{aligned} \Omega = \omega &= \sqrt{\omega_1^2 - \omega_2^2}, \\ \Omega \cosh 2\theta &= \omega_1, \\ \Omega \sinh 2\theta &= \omega_2. \end{aligned} \tag{A7}$$

The eigenvalues of $\hat{H}$ are therefore

$$E_n = \omega(n + \tfrac{1}{2}) - \tfrac{1}{2}\omega_1. \tag{A8}$$

The operators $a^\dagger a$, a^2 and $a^{\dagger 2}$ generate the Lie algebra su(1,1). Therefore either the flat phase-space coherent state path integral or standard su(1,1) disentangling methods[35,36] can be used to derive

$$\langle \zeta_f | e^{-\hat{H}T} | \zeta_i \rangle = D^{-1/2} \exp\{D^{-1}(\overline{\zeta_f}\zeta_i - \tfrac{1}{2}\sinh 2\theta \sinh \omega T (\overline{\zeta_f^2} + \zeta_i^2))\} e^{-1/2\,\omega_1 T}, \tag{A9}$$

where

$$D = e^{\omega T}\cosh^2\theta - e^{-\omega T}\sinh^2\theta, \tag{A10}$$

and the harmonic oscillator coherent states $|\zeta\rangle$ are defined by

$$|\zeta\rangle = \exp \zeta a^\dagger |0\rangle, \quad a|0\rangle = 0. \tag{A11}$$

In the large-T limit, and with ζ_i and $\overline{\zeta_f}$ both at the origin, this reduces to

$$\langle 0 | e^{-\hat{H}T} | 0 \rangle \to (\cosh\theta)^{-1} e^{-(1/2)(\omega - \omega_1)T} = \sqrt{\frac{2\omega}{\omega + \omega_1}}\, e^{-(1/2)(\omega - \omega_1)T}. \tag{A12}$$

We now rotate back to the original z_i. Taking note of the transformation properties of the $|z\rangle$'s, we get

$$K_i = (1 + \overline{z_i} z_i)^{2j} \sqrt{\frac{2\omega}{\omega + \omega_1}}\, e^{-(1/2)(\omega - \omega_1)T}, \tag{A13}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

Central limit theorems for large graphs: Method of quantum decomposition

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(Received 13 February 2002; accepted 18 October 2002)

A new method is proposed for investigating spectral distribution of the combinatorial Laplacian (adjacency matrix) of a large regular graph on the basis of quantum decomposition and quantum central limit theorem. General results are proved for Cayley graphs of discrete groups and for distance-regular graphs. The Coxeter groups and the Johnson graphs are discussed in detail by way of illustration. In particular, the limit distributions obtained from the Johnson graphs are characterized by the Meixner polynomials which form a one-parameter deformation of the Laguerre polynomials. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1528275]

I. INTRODUCTION

Spectral analysis of the (combinatorial) Laplacian or the adjacency matrix of a graph has been studied from various aspects with many applications in geometry, combinatorics, physics and so forth. In this paper we focus on asymptotic spectral properties for a large regular graph and propose a new method based on algebraic probability theory. In fact, we consider a ''growing'' family of graphs $\{\mathcal{G}_\lambda=(V^{(\lambda)},E^{(\lambda)});\lambda\in\Lambda\}$ and study spectral properties of the limit

$$\lim_{\lambda\in\Lambda}\frac{A_\lambda}{Z_\lambda}, \tag{1.1}$$

where A_λ is the adjacency matrix of $\mathcal{G}_\lambda$ and Z_λ a normalizing constant. A standard strategy for obtaining spectral properties of the limit (1.1) would be to take the limit after computation of the spectrum of A_λ for each $\lambda\in\Lambda$ though tedious combinatorial arguments are often required. The aim of this paper is to show another route to solve the question.

The key steps are *quantum decomposition* of the adjacency matrix and *quantum central limit theorem* describing its asymptotic properties. We introduce a stratification: $V^{(\lambda)}=\cup_{n=0}^{\infty}V_n^{(\lambda)}$ on the basis of the natural distance function of $\mathcal{G}_\lambda$ and decompose the adjacency matrix A_λ into a sum of *quantum components*:

$$A_\lambda=A_\lambda^+ + A_\lambda^- . \tag{1.2}$$

The operators $A_\lambda^\pm$ act asymptotically in the Hilbert space $\Gamma(\mathcal{G}_\lambda)$ associated with the stratification of $V^{(\lambda)}$. Then we construct an interacting Fock space $(\Gamma,\{\lambda_n\},B^+,B^-)$ in which the limit

$$C^\pm=\lim_{\lambda\in\Lambda}\frac{A_\lambda^\pm}{Z_\lambda} \tag{1.3}$$

are described, where $C^{\pm}$ is a linear combination of $B^{\pm}$ and a function of the number operator N. In fact, the convergence (1.3) is formulated in the sense of matrix elements. Moreover, spectral properties of (1.1) can be obtained by using the direct relation between interacting Fock spaces and orthogonal polynomials. It is noteworthy that our approach does not require any combinatorial argument for A_λ which is often tedious. A combinatorial argument appears only after the limiting procedure and is much easier than that for A_λ. On the other hand, it is natural to think that the adjacency matrix A_λ grows as if it is added to new ''independent'' random variables when a graph $\mathcal{G}_\lambda$ grows up by adding new vertices and new edges. The limit theorem for (1.3) is thus called a quantum central limit theorem in algebraic probability theory.

The term of *quantum decomposition* was first introduced explicitly by Hashimoto[10] in a study of an adjacency matrix of a large Cayley graph. This idea was also successfully applied to a similar study for a large Hamming graph in Hashimoto *et al.*[11] Furthermore, from the viewpoint of quantum decomposition the singleton independence and the associated central limit theorem discussed in Accardi *et al.*[2,3] are understood naturally together with Gauss–Poisson deformation in Hashimoto.[10] It is plausible that our method of quantum decomposition can be applied to obtain scaled limit theorems with respect to such ''nonvacuum states'' as treated in Hashimoto[9] and Hora,[14] though the discussion in this paper is limited to the ''vacuum states.''

While, the idea of quantum decomposition is not very new for essentially the same idea has already emerged in many literatures. For example, the Brownian motion $\{B_t\}$, regarded as a family of multiplication operators acting on the L^2 functions on the Wiener space, is decomposed into a sum of noncommuting operators: $B_t = A_t + A_t^*$. The pair $\{A_t, A_t^*\}$, called a *quantum Brownian motion*, is a basis of the quantum Itô theory initiated by Hudson and Parthasarathy.[15] A Bernoulli random variable X admits an expression by 2×2 matrices:

$$X = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

which is often referred to as a *quantum coin-tossing*. A discrete Schrödinger operator $S+S^*$, where S is the one-sided shift operator on $\ell^2(\mathbf{N})$, is nothing but a quantum decomposition in our context. Operators of this kind are also widely utilized in representation theory of Lie algebras.

This paper is organized as follows: In Sec. II we assemble some fundamentals of an interacting Fock space first introduced by Accardi–Lu,[4] and explain general strategy to solve our question. In Sec. III we show a general result on asymptotic spectral properties of an adjacency matrix of a large Cayley graph with a concrete study of the Coxeter groups. We see that a result in Fendler[8] is reproduced from our quantum central limit theorem. In Sec. IV we discuss a quantum decomposition of an adjacency matrix of a general distance-regular graph. As a concrete example we prove the quantum central limit theorem associated with the Johnson graphs. Its classical reduction is sharper than the result obtained by Hora[12] with a classical method.

II. PRELIMINARIES

A. Interacting Fock space

Following Accardi–Lu–Volovich[5] and Accardi–Bożejko[1] we assemble some notion and notation. Let $\lambda_0 = 1, \lambda_1, \lambda_2, \ldots$ be a sequence of non-negative numbers and assume that if $\lambda_m = 0$ occurs for some $m \geqslant 1$ then $\lambda_n = 0$ for all $n \geqslant m$. Assume first that $\lambda_n > 0$ for all n. Let

$$\Gamma = \sum_{n=0}^{\infty} \oplus \mathbf{C}\Phi_n$$

be the Hilbert space with a complete orthonormal basis $\{\Phi_n\}$. We define linear operators $B^{\pm}$ by

$$B^+\Phi_n = \sqrt{\frac{\lambda_{n+1}}{\lambda_n}}\,\Phi_{n+1}, \quad n \geqslant 0, \tag{2.1}$$

$$B^-\Phi_n=\sqrt{\frac{\lambda_n}{\lambda_{n-1}}}\Phi_{n-1},\quad n\geqslant 1,\quad B^-\Phi_0=0. \tag{2.2}$$

Equipped with the natural domains, $B^{\pm}$ become closed operators which are mutually adjoint. When $\lambda_m=0$ occurs for some $m\geqslant 1$, the situation falls into a finite dimension. Take the last number m_0 such that $\lambda_{m_0}>0$ and define

$$\Gamma=\sum_{n=0}^{m_0}\oplus \mathbf{C}\Phi_n .$$

The linear operators $B^{\pm}$ are defined in a similar manner as in (2.1) and (2.2) with a tacit understanding that $B^+\Phi_{m_0}=0$. Then $\Gamma(\mathbf{C},\{\lambda_n\})=(\Gamma,\{\lambda_n\},B^+,B^-)$ is called an *interacting Fock space* associated with $\{\lambda_n\}$.

By a simple computation we have

$$B^+B^-\Phi_n=\frac{\lambda_n}{\lambda_{n-1}}\Phi_n,\quad n\geqslant 1;\quad B^+B^-\Phi_0=0, \tag{2.3}$$

$$B^-B^+\Phi_n=\frac{\lambda_{n+1}}{\lambda_n}\Phi_n,\quad n\geqslant 0, \tag{2.4}$$

$$B^{+n}\Phi_0=\sqrt{\lambda_n}\Phi_n,\quad n\geqslant 0. \tag{2.5}$$

The number operator N is defined as usual by

$$N\Phi_n=n\Phi_n,\quad n=0,1,2,\ldots .$$

The famous commutation relations are realized as follows:

(a) Boson commutation relation $B^-B^+-B^+B^-=1$ by $\lambda_n=n!$.
(b) Fermion commutation relation $B^-B^++B^+B^-=1$ by $\lambda_0=\lambda_1=1$ and $\lambda_n=0$ for $n\geqslant 2$.
(c) Free commutation relation $B^-B^+=1$ by $\lambda_n=1$ for all $n\geqslant 0$.

More generally, these are special cases of q-commutation relation: $B^-B^+-qB^+B^-=1$ with $-1\leqslant q\leqslant 1$. This is realized by

$$\lambda_n=[n]_q!=[n]_q[n-1]_q\cdots[1]_q,\quad [n]_q=1+q+q^2+\cdots+q^{n-1}.$$

For more details, see, e.g., van Leeuwen–Maassen.[18] Note that $N=B^+B^-$ occurs only for the Boson Fock space.

B. Orthogonal polynomials

An interacting Fock space is related to a system of orthogonal polynomials. Let μ be a probability measure with finite moments of all orders, i.e.,

$$\int_{\mathbf{R}}|x|^m\mu(dx)<\infty,\quad m=0,1,2,\ldots ,$$

and $\{P_n\}$ the associated orthogonal polynomials normalized as $P_n(x)=x^n+\cdots$. By orthogonality they satisfy the famous recurrence formula:

$$P_0(x)=1,$$

$$P_1(x)=x-\alpha_1,$$

$$(x-\alpha_{n+1})P_n(x)=P_{n+1}(x)+\omega_n P_{n-1}(x), \quad n\geqslant 1, \tag{2.6}$$

where $\alpha_1,\alpha_2,\ldots\in\mathbf{R}$ and $\omega_1,\omega_2,\ldots\geqslant 0$ are characteristic sequences for the orthogonal polynomials called the *Szegö–Jacobi parameter*. When the probability measure μ is supported by a finite set, the orthogonal polynomials $\{P_n\}$ terminates at a certain degree and the Szegö–Jacobi parameter is by definition a pair of finite sequences. Note also that μ is symmetric if and only if $\alpha_n=0$ for all $n\geqslant 1$.

Theorem 2.1: *Accardi–Bożejko:*[1] *Let $\{P_n\}$ be the orthogonal polynomials with respect to μ with Szegö–Jacobi parameters $\{\alpha_n\}$ and $\{\omega_n\}$. Let $\Gamma(\mathbf{C},\{\lambda_n\})$ be an interacting Fock space associated with*

$$\lambda_0=1, \quad \lambda_1=\omega_1, \quad \frac{\lambda_{n+1}}{\lambda_n}=\omega_{n+1}.$$

Then there exists an isometry U from $\Gamma(\mathbf{C},\{\lambda_n\})$ into $L^2(\mathbf{R},\mu)$ uniquely determined by

$$U\Phi_0=P_0, \quad UB^+U^*P_n=P_{n+1}, \quad Q=U(B^++B^-+\alpha_{N+1})U^*,$$

where Q is the multiplication operator by x densely defined in $L^2(\mathbf{R},\mu)$ and α_{N+1} is the operator defined by $\alpha_{N+1}\Phi_n=\alpha_{n+1}\Phi_n$. In particular,

$$\int_{\mathbf{R}} x^m\mu(dx)=\langle\Phi_0,(B^++B^-+\alpha_{N+1})^m\Phi_0\rangle_\Gamma, \quad m=0,1,2,\ldots. \tag{2.7}$$

The proof is straightforward. The isometry U is uniquely specified by

$$U:\sqrt{\lambda_n}\Phi_n=\sqrt{\omega_1\cdots\omega_n}\Phi_n\mapsto P_n.$$

A question of when U is a unitary, or equivalently when the polynomials span a dense subspace in $L^2(\mathbf{R},\mu)$ is related to the so-called determinate moment problem, see, e.g., Deift (Ref. 7, Sec. 2.4).

C. Quantum decomposition of a classical random variable

Let X be a classical random variable with probability distribution μ having moments of all orders. We keep the same notation as in Theorem 2.1. Define an algebraic probability space $(\mathcal{A},\phi)$, where $\mathcal{A}$ is the $*$-algebra generated by Q and ϕ is the state defined by

$$\phi(a)=\langle P_0,aP_0\rangle_{L^2(\mathbf{R},\mu)}, \quad a\in\mathcal{A}.$$

Then X and Q are stochastically equivalent by an obvious relation

$$\mathbf{E}(X^m)=\int_{\mathbf{R}} x^m\mu(dx)=\phi(Q^m), \quad m=0,1,2,\ldots. \tag{2.8}$$

On the other hand, consider an algebraic probability space canonically associated with the interacting Fock space $(\Gamma,\{\lambda_m\},B^+,B^-)$. Let $\mathcal{B}$ be the $*$-algebra generated by B^+,B^-,α_{N+1} and ψ the vacuum state defined by

$$\psi(b)=\langle\Phi_0,b\Phi_0\rangle_\Gamma, \quad b\in\mathcal{B}.$$

In view of (2.7) in Theorem 2.1 and (2.8) we see that X and $B^++B^-+\alpha_{N+1}$ are stochastically equivalent. In this sense we have

$$X = B^+ + B^- + \alpha_{N+1},$$

which is a prototype of the *quantum decomposition*. Note that the quantum components are no longer commuting each other. In other words, $(\mathcal{B}, \psi)$ is noncommutative though $(\mathcal{A}, \phi)$ is commutative (or classical).

D. General question and method

Let $\mathcal{G}=(V,E)$ be a graph, where V is the set of vertices and $E \subset \{\{x,y\}; x,y \in V, x \neq y\}$ the set of edges. If $\{x,y\} \in E$, we say that x and y are *adjacent* and write $x \sim y$. For a graph $\mathcal{G}$ the *adjacency matrix* $A=(A_{xy})_{x,y \in V}$ is defined by

$$A_{xy} = \begin{cases} 1, & x \sim y \\ 0 & \text{otherwise.} \end{cases} \tag{2.9}$$

Note that the (x,y)-component of A^n, $n \geqslant 1$, stands for the number of walks of length n from x to y.

The adjacency matrix acts on a Hilbert space $\ell^2(V)$ of all $\mathbf{C}$-valued functions f on V such that

$$\|f\|^2 = \sum_{x \in V} |f(x)|^2 < \infty$$

in such a way that

$$Af(x) = \sum_{y \in V} A_{xy} f(y) = \sum_{y \sim x} f(y), \quad f \in \ell^2(V).$$

The *degree* of $x \in V$ is defined by $\kappa(x) = |\{y \in V; y \sim x\}|$. The *graph Laplacian (combinatorial Laplacian)* is a slight modification of A:

$$\Delta f(x) = \kappa(x) f(x) - \sum_{y \sim x} f(y).$$

A graph is called *regular* if $\kappa(x) = \kappa < \infty$ is a finite constant independent of $x \in V$. For a regular graph there is no essential difference between the adjacency matrix and graph Laplacian. A graph is called *connected* if any pair of vertices $x,y \in V$ are connected by a path. Spectral properties of the adjacency matrix of a ''large'' regular connected graph is to be discussed. We shall briefly explain our method which consists of two steps: quantum decomposition and quantum central limit theorem.

Let $\mathcal{G}=(V,E)$ be a regular connected graph and consider the adjacency matrix A acting in the Hilbert space $\ell^2(V)$. Let $\mathcal{A}$ be the unital $*$-algebra generated by A. A state ϕ on $\mathcal{A}$ is chosen by a question. For example, for a fixed $x_0 \in V$ we often consider a vector state:

$$\phi(a) = \langle \delta_{x_0}, a\, \delta_{x_0} \rangle, \quad a \in \mathcal{A},$$

where δ_{x_0} denotes the indicator function of a singlet $\{x_0\}$. We thus consider A as an algebraic random variable of an algebraic probability space $(\mathcal{A}, \phi)$.

We fix $x_0 \in V$ as an origin and set

$$|x| = \partial(x, x_0), \quad x \in V,$$

where $\partial(x,y)$ denotes the distance of $x,y \in V$, namely, the length of the shortest path connecting x,y. Since $\mathcal{G}$ is connected, the graph is stratified

$$V=\bigcup_{n=0}^{\infty} V_n, \quad V_n=\{x\in V;|x|=n\}. \tag{2.10}$$

We see from the triangle inequality that if $x\in V_n$ and $\partial(x,y)=1$, then $y\in V_{n-1}\cup V_n\cup V_{n+1}$. In other words, there are no edges which connect strata beyond a stratum. Then the adjacency matrix is decomposed into a sum of quantum components

$$A=A^+ +A^-, \quad (A^+)^*=A^-, \tag{2.11}$$

which will be called the *quantum decomposition*.

In order to study the adjacency matrix of a "large" graph we consider a growing family of graphs $\{\mathcal{G}_\lambda=(V^{(\lambda)},E^{(\lambda)});\lambda\in\Lambda\}$, where Λ is an infinite directed set. The adjacency matrix A_λ of $\mathcal{G}_\lambda$ is decomposed into a sum of quantum components as in (2.11) Then we shall construct an interacting Fock space $(\Gamma,\{\lambda_n\},B^+,B^-)$ in which the limits

$$C^\pm=\lim_{\lambda\in\Lambda}\frac{A_\lambda^\pm}{Z_\lambda}, \tag{2.12}$$

are described, where $C^\pm$ is a linear combination of $B^\pm$ and a function of the number operator N on Γ. Finally, asymptotic spectral properties of A_λ follow from the probability distribution of $C^+ +C^-$ with the help of orthogonal polynomials and Theorem 2.1.

III. CAYLEY GRAPHS

A. Quantum decomposition

Consider a discrete group G with the identity e and a set of generators $\Sigma\subset G$ satisfying

(i) $\sigma\in\Sigma\Rightarrow\sigma^{-1}\in\Sigma$, i.e., $\Sigma^{-1}=\Sigma$;
(ii) $e\notin\Sigma$.

Then G becomes a graph, where a pair $x,y\in G$ satisfying $yx^{-1}\in\Sigma$ constitutes an edge, denoted by $x\sim y$. This is called a *Cayley graph* and denoted by (G,Σ). A Cayley graph is regular since the degree of $x\in G$ is a constant given by $\kappa(x)=|\Sigma|$.

Let (G,Σ) be a Cayley graph and $(\pi,\ell^2(G))$ the left regular representation of G defined by

$$\pi(g)f(x)=f(g^{-1}x), \quad g,x\in G, \quad f\in\ell^2(G).$$

The adjacency matrix is given by

$$A=\sum_{\sigma\in\Sigma}\pi(\sigma). \tag{3.1}$$

By definition each $g\in G$, $g\neq e$, is expressed in a finite product of generators:

$$g=\sigma_1\sigma_2\cdots\sigma_s, \quad \sigma_1,\ldots,\sigma_s\in\Sigma.$$

Let $|g|$ be the smallest number s among such expressions. We set $|e|=0$. Obviously, $|g|=1$ if and only if $g\in\Sigma$. Note also that $\partial(x,y)=|yx^{-1}|$. In particular, $|g|-1\leqslant|\sigma g|\leqslant|g|+1$ holds for any $g\in G$ and $\sigma\in\Sigma$. We assume

(A1) $|\sigma g|=|g|\pm1$ holds for any $\sigma\in\Sigma$ and $g\in G$.

Then, there exist no edges connecting two points in the same stratum. (In the next section, however, we shall deal with graphs allowing such edges.)

For quantum decomposition of A, we start with $\pi(\sigma)$. We define

$$\pi(\sigma)^+\delta_g=\begin{cases}\delta_{\sigma g} & \text{if } |\sigma g|=|g|+1\\ 0 & \text{otherwise,}\end{cases} \tag{3.2}$$

$$\pi(\sigma)^-\delta_g=\begin{cases}\delta_{\sigma g} & \text{if } |\sigma g|=|g|-1\\ 0 & \text{otherwise.}\end{cases} \tag{3.3}$$

Obviously, $\pi(\sigma)^{\pm}$ are bounded operators on $\ell^2(G)$ with $\|\pi(\sigma)^{\pm}\|=1$ and

$$\pi(\sigma)=\pi(\sigma)^+ + \pi(\sigma)^-, \quad (\pi(\sigma)^+)^*=\pi(\sigma^{-1})^-, \quad (\pi(\sigma)^-)^*=\pi(\sigma^{-1})^+.$$

Thus we come to the *quantum decomposition* of the adjacency matrix A in (3.1):

$$A=A^+ + A^-, \tag{3.4}$$

where

$$A^+=\sum_{\sigma\in\Sigma}\pi(\sigma)^+, \quad A^-=\sum_{\sigma\in\Sigma}\pi(\sigma)^-.$$

B. Quantum central limit theorem

Let $(G^{(N)},\Sigma^{(N)})$ be a sequence of Cayley graphs. As N increases, the Cayley graph grows by adding new vertices generated by new generators. Our aim is to study spectral property of the adjacency matrix A_N of $(G^{(N)},\Sigma^{(N)})$ as $N\to\infty$.

To state assumptions we set

$$\omega_-^{(N)}(g)=\{(\sigma,x)\in\Sigma^{(N)}\times G^{(N)};\pi(\sigma)^+\delta_x=\delta_g\}, \tag{3.5}$$

$$\omega_+^{(N)}(g)=\{(\sigma,x)\in\Sigma^{(N)}\times G^{(N)};\pi(\sigma)^-\delta_x=\delta_g\}. \tag{3.6}$$

Note that if $(\sigma,x)\in\omega_{\pm}^{(N)}(g)$, then $|x|=|g|\pm 1$ and

$$|\omega_+^{(N)}(g)|+|\omega_-^{(N)}(g)|=|\Sigma^{(N)}|.$$

We set the following two assumptions.

(A2) for each n there exist an integer $\omega_n\geqslant 1$ and a constant number $C_n\geqslant 0$ such that

$$|\{g\in G^{(N)};|g|=n,|\omega_-^{(N)}(g)|\neq\omega_n\}|\leqslant C_n|\Sigma^{(N)}|^{n-1}; \tag{3.7}$$

(A3) for each n,

$$\sup_N\sup\{|\omega_-^{(N)}(g)|;g\in G^{(N)},|g|=n\}\equiv W_n<\infty$$

and $\limsup_{n\to\infty}W_n^{1/n}<\infty$.

Roughly speaking, condition (A2) means that "almost every" $g\in G^{(N)}$ in the nth stratum is connected with ω_n vertices in the $(n-1)$th stratum. Obviously, $\omega_1=1$. By condition (A3), new edges added while the graph grows are mostly connected with vertices in the upper stratum.

For each $(G^{(N)},\Sigma^{(N)})$ we consider the regular representation $(\pi_N,\ell^2(G^{(N)}))$ and the adjacency matrix with quantum decomposition $A_N=A_N^+ + A_N^-$. According to the stratification of $G^{(N)}$ we set

$$\Phi_0^{(N)}=\delta_e, \quad \Phi_n^{(N)}=\sqrt{\frac{\omega_1\cdots\omega_n}{|\Sigma^{(N)}|^n}}\sum_{g\in G^{(N)},|g|=n}\delta_g, \quad n\geqslant 1.$$

Note that $\Phi_n^{(N)}$ is not exactly normalized:

$$\|\Phi_n^{(N)}\|^2 = 1 + O(|\Sigma^{(N)}|^{-1}).$$

While, obviously they are mutually orthogonal. Then the subspace of $\ell^2(G^{(N)})$ defined by

$$\Gamma^{(N)} = \sum_{n=0}^{\infty} \oplus \mathbf{C}\Phi_n^{(N)}$$

has a similar property of a Fock space. In fact, we see easily that

$$\frac{A_N^+}{\sqrt{|\Sigma^{(N)}|}}\Phi_n^{(N)} = \sqrt{\omega_{n+1}}\Phi_{n+1}^{(N)} + O(|\Sigma^{(N)}|^{-1/2}), \tag{3.8}$$

$$\frac{A_N^-}{\sqrt{|\Sigma^{(N)}|}}\Phi_{n+1}^{(N)} = \sqrt{\omega_{n+1}}\Phi_n^{(N)} + O(|\Sigma^{(N)}|^{-1}), \tag{3.9}$$

where $O(|\Sigma^{(N)}|^{\alpha})$ means that the norm of the error vector has this rate of decay. Setting $\lambda_n = \omega_1 \cdots \omega_n$, we consider an interacting Fock space $(\Gamma, \{\lambda_n\}, B^+, B^-)$. At a formal level we understand easily from (3.8) and (3.9) that

$$\lim_{N\to\infty} \frac{A_N^{\pm}}{\sqrt{|\Sigma^{(N)}|}} = B^{\pm}. \tag{3.10}$$

In other words, the expected interacting Fock space in the limit is completely determined by the constants $\{\omega_n\}$ in (A2), which are obtained from the Cayley graphs. To complete the discussion we need to show the convergence of (3.10) in the sense of algebraic probability theory. In fact, we have the following:

Theorem 3.1: *Let* $(G^{(N)}, \Sigma^{(N)})$ *be as above and* $(\Gamma, \{\lambda_n\}, B^+, B^-)$ *the interacting Fock space corresponding to the constants* $\{\omega_n\}$. *Let* $u = \Sigma_{n=0}^{\infty} u_n \Phi_n \in \Gamma$. *Then, whenever* $u^{(N)} = \Sigma_{n=0}^{\infty} u_n \Phi_n^{(N)} \in \Gamma^{(N)}$, *it holds that*

$$\lim_{N\to\infty} \left\langle u^{(N)}, \frac{A_N^{\epsilon_1}}{\sqrt{|\Sigma^{(N)}|}} \cdots \frac{A_N^{\epsilon_m}}{\sqrt{|\Sigma^{(N)}|}} \Phi_n^{(N)} \right\rangle = \langle u, B^{\epsilon_1} \cdots B^{\epsilon_m} \Phi_n \rangle$$

for any choice of $\epsilon_1, \ldots, \epsilon_m \in \{\pm\}$, $m \geqslant 1$.

The above statement is a slight generalization of the result by Hashimoto[10] though the proof is essentially the same and is omitted.

Example 3.2: For the lattice $(\mathbf{Z}^N, \{e_{\pm 1}, \ldots, e_{\pm N}\})$ we see easily that $\omega_n = n$. In fact, if $g \in \mathbf{Z}^N$ is in the nth stratum,

$$g = p_1 e_1 + \cdots + p_N e_N, \quad |p_1| + \cdots + |p_N| = n.$$

Then any element in the $(n-1)$th stratum connected with g is obtained by replacing p_i with $p_i - 1$ if $p_i > 0$, or p_i with $p_i + 1$ if $p_i < 0$. Therefore $1 \leqslant |\omega_-^{(N)}(g)| \leqslant n$ and for $N > n$ almost every g satisfies $|\omega_-^{(N)}(g)| = n$. Consequently, $\omega_n = n$, $\lambda_n = n!$. Moreover, $W_n = n$ is immediate. Then by Theorem 3.1, the quantum components of the adjacency matrix converge to the creation and annihilation operators on the Boson Fock space in the sense of algebraic probability theory:

$$\lim_{N\to\infty} \frac{A_N^{\pm}}{\sqrt{2N}} = B^{\pm}.$$

In particular, the spectral distribution of $A_N=A_N^+ + A_N^-$ in the vacuum state is asymptotically the normal distribution:

$$\lim_{N\to\infty}\left\langle \Phi_0^{(N)}, \left(\frac{A_N}{\sqrt{2N}}\right)^m \Phi_0^{(N)}\right\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} x^m e^{-x^2/2}\,dx, \quad m=0,1,2,\ldots.$$

Example 3.3: Consider a homogeneous tree $(F_N,\{g_{\pm 1},\ldots,g_{\pm N}\})$, where F_N is the free group on N generators. (For simplicity we write $g_{-i}=g_i^{-1}$.) It is obvious that for any $g\in F_N$ in the nth stratum there is just one element in the $(n-1)$th stratum which is adjacent to g. Thus, $\omega_n=1$ and $\lambda_n=1$ for all n. Moreover, $W_n=1$ is obvious. Consequently, the quantum components of the adjacency matrix converge to the creation and annihilation operators on the free Fock space. In particular, the spectral distribution in the vacuum state is asymptotically the Wigner semicircle law:

$$\lim_{N\to\infty}\left\langle \Phi_0^{(N)}, \left(\frac{A_N}{\sqrt{2N}}\right)^m \Phi_0^{(N)}\right\rangle = \frac{1}{2\pi}\int_{-2}^{+2} x^m \sqrt{4-x^2}\,dx, \quad m=0,1,2,\ldots.$$

C. Coxeter group

Let $S=\{g_1,g_2,\ldots\}$ be a countable infinite set and consider a function $m:S\times S\to\{1,2,\ldots,\infty\}$ such that $m(s,s)=1$ and $m(s,t)=m(t,s)\geqslant 2$ for $s\neq t$. For each $N\geqslant 1$ let G_N be a group generated by $S_N=\{g_1,g_2,\ldots,g_N\}$ subject only to the relations:

$$(st)^{m(s,t)}=1, \quad s,t\in S_N. \tag{3.11}$$

In case of $m(s,t)=\infty$ we understand that st is of infinite order. It is known that the inclusion $S_N\to S_{N+1}$ extends uniquely an injective homomorphism $G_N\to G_{N+1}$. Let G be the inductive limit.

By definition each $g\in G_N$, $g\neq e$, admits an expression of the form $g=s_1s_2\cdots s_r$, $s_i\in S_N$. If r is as small as possible, the expression is called a *reduced expression* and the number $r=|g|$ is called the *length* of g. The length function is well defined on G.

The next fact is known as the *deletion condition.*

Lemma 3.4: [Humphreys (Ref. 16, Sec. 5)]: Assume that $g\in G$ admits an expression $g=s_1s_2\cdots s_m$ with $s_i\in S$ such that $|g|<m$. Then there exist a pair of indices $1\leqslant i<j\leqslant m$ such that

$$g=s_1\cdots\hat{s}_i\cdots\hat{s}_j\cdots s_m,$$

where $\hat{s}$ stands for deletion. Thus, if $g=s_1s_2\cdots s_m$, $s_i\in S$, then a reduced expression of g is obtained by deleting even number of s_i appearing therein.

As an immediate consequence condition (A1) follows. To prove (A2) we start with the following.

Lemma 3.5: If $s_1,s_2,\ldots,s_n\in S$ are mutually distinct, $g=s_1s_2\cdots s_n$ is a reduced expression.

Proof: For $n=1$ the assertion is obvious since S is injectively contained in G. Let $n\geqslant 2$. Suppose that $g=s_1s_2\cdots s_n$ is not a reduced expression for mutually distinct $s_1,s_2,\ldots,s_n\in S$. Then by Lemma 3.4,

$$s_1\cdots s_n=s_1\cdots\hat{s}_i\cdots\hat{s}_j\cdots s_n$$

and hence

$$s_i=s_{i+1}\cdots s_{j-1}s_js_{j-1}\cdots s_{i+1}.$$

Since the right-hand side is of length 1, deleting an even number of elements from the right-hand side leads to a reduced expression. The obtained reduced expression should be one of $\{s_{i+1},\ldots,s_{j-1}\}$. This contradicts the assumption that $s_1,\ldots,s_n$ are mutually distinct. ■

Lemma 3.6: Assume that $m(s,t)\geqslant 3$ *whenever* $s\neq t$. *Let* $n\geqslant 1$ *and* $s_1,\ldots,s_n\in S$ *mutually distinct. If there exist* $s\in S$ *and* $x\in G$ *of length* $n-1$ *such that*

$$s_1\cdots s_n=sx,$$

then $s=s_1$.

Proof: For $n=1$ the assertion is obvious. Assume $n=2$ and $s_1s_2=sx$ where $|x|=1$. From $s=s_1s_2x$ we see easily that $s=s_1$ or $s=s_2$ or $s=x$. If $s=x$ we have $s_1=s_2$ which is contradiction. If $s=s_2$, $x=s_1$ and $(s_1s_2)^2=e$ which is again contradiction. Consequently, $s=s_1$ as desired.

Assume that the assertion is valid up to $n-1$, $n\geqslant 2$. Since

$$ss_1\cdots s_n=x \tag{3.12}$$

is of length $n-1$, deleting two elements from the left-hand side we obtain a reduced expression of x. If these two elements are chosen from $\{s_1,\ldots,s_n\}$, say, s_i,s_j $(i<j)$, we come back to

$$s_1\cdots\hat{s}_i\cdots\hat{s}_j\cdots s_n=sx=s_1\cdots s_n,$$

which is a reduced expression by Lemma 3.5. This is contradiction. Hence, to get a reduced expression of x in (3.12) we need to delete s and s_i for some $i=1,\ldots,n$. In that case we come to

$$s_1\cdots\hat{s}_i\cdots s_n=x,$$

and hence

$$ss_1\cdots s_{i-1}=s_1\cdots s_i. \tag{3.13}$$

If $1\leqslant i\leqslant n-1$, by the assumption of induction we have $s=s_1$. Suppose $i=n$, i.e.,

$$ss_1\cdots s_{n-1}=s_1\cdots s_n.$$

By a simple argument with the deletion condition we see that $s\in\{s_1,\ldots,s_n\}$. If $s=s_j$, $1\leqslant j\leqslant n-1$, then

$$s_n=s_{n-1}\cdots s_1s_js_1\cdots s_{n-1},$$

which implies that s_n coincides with some of $\{s_1,\ldots,s_{n-1}\}$. But this contradicts the assumption. Hence $s=s_n$, i.e.,

$$s_ns_1\cdots s_{n-1}=s_1\cdots s_n. \tag{3.14}$$

We shall prove that this does not occur. Note first that (3.14) is equivalent to the following:

$$(s_{n-2}\cdots s_1)s_n(s_1\cdots s_{n-2})s_{n-1}=s_{n-1}s_n.$$

Since this is of length 2, deleting an even number of elements from the left-hand side, we obtain a reduced expression of length 2, say, tt'. This is the case of $n=2$ so we know that $t=s_{n-1}$. But this is impossible. ■

Proposition 3.7: Assume that $m(s,t)\geqslant 3$ *for any pair* $s,t\in S$, $s\neq t$. *Then condition (A2) holds with* $\omega_n=1$.

Proof: It is sufficient to show that

$$|\{g\in G_N;|g|=n,|\omega_-^{(N)}(g)|\neq 1\}|\leqslant C_n|S_N|^{n-1}$$

with some constant $C_n \geqslant 0$. It follows from Lemma 3.6 that for $g \in G_N$ such that $g = s_{i_1} \cdots s_{i_n}$ with distinct $s_{i_1}, \ldots, s_{i_n} \in S_N$ we have $\omega_-^{(N)}(g) = 1$. The number of such g is $N(N-1)\cdots(N-n+1)$. Hence

$$|\{g \in G_N; |g| = n, |\omega_-^{(N)}(g)| \neq 1\}| \leqslant N^n - N(N-1)\cdots(N-n+1) = O(N^{n-1}).$$

This proves the assertion. ■

Condition (A3) is satisfied with $W_n = 2$, which follows again by repeated use of the deletion condition. This fact was also proved by Szwarc.[20] Appealing to Theorem 3.1, we have an algebraic central limit theorem for the quantum components of the adjacency matrix of the Coxter group with condition $m(s,t) \geqslant 3$ for any pair $s,t \in S$, $s \neq t$. The limit is described by the creation and annihilation operators on the free Fock space. Thus the situation is the same as in Example 3.3.

We remind that the semicircle law was also obtained by Fendler[8] with a totally different method.

Remark 3.8: Let $\mathfrak{S}_N$ be the group of permutations of the set $\{1,2,\ldots,N\}$ of N letters. It is known that $\mathfrak{S}_N$ is generated by the successive transpositions $(12),(23),\ldots,(N-1N)$. Then the situation falls into the case of Coxeter groups. If all the transpositions are taken to be the set of generators Σ_N, we see that conditions (A1)–(A3) are satisfied with $\omega_n = n$ and $W_n = n(n+1)/2$. Hence the quantum components $A_N^{\pm}$ converge to the creation and annihilation operators on the Boson Fock space and the situation is the same as in Example 3.2. The Gaussian limit for the spectral distribution of A_N was first obtained by Kerov[17] in the form of a central limit theorem for irreducible characters of $\mathfrak{S}_N$. See Hora[13] for extension of such a central limit theorem to arbitrary conjugacy classes.

IV. DISTANCE-REGULAR GRAPHS

A. Quantum decomposition

A finite connected graph $\mathcal{G} = (V,E)$ is called *distance-regular* if for any choice of $h,i,j \in \{0,1,\ldots,d\}$, d being the diameter of the graph,

$$|\{z \in V; \partial(x,z) = i, \partial(z,y) = j\}| \equiv p_{ij}^h$$

does not depend on the choice of $x,y \in V$ such that $\partial(x,y) = h$. We call $\{p_{ij}^h\}$ the *intersection numbers* of $\mathcal{G}$. For simplicity we set $\kappa_j = p_{jj}^0$ and $\kappa = \kappa_1 = p_{11}^0$. Obviously, the distance-regular graph is regular with degree κ.

As usual, consider the Hilbert space $\ell^2(V)$ with an orthonormal basis $\{\delta_x; x \in V\}$. We shall introduce a quantum decomposition of the adjancency matrix A acting on $\ell^2(V)$. The idea is modelled after Hashimoto *et al.*[11]

We first fix an arbitrary $x_0 \in V$ and introduce a stratification:

$$V = \bigcup_{j=0}^{d} V_j, \quad V_j = \{x \in V; |x| = \partial(x_0,x) = j\}. \tag{4.1}$$

Note that $|V_j| = \kappa_j$. We next introduce an orientation into the graph $\mathcal{G}$, namely give an orientation to each edge $x \sim y$, $x,y \in V$. If $x \in V_i$ and $y \in V_j$ with $i < j$ (in fact $j = i+1$), we set $x \to y$ naturally. In order to give an orientation for an edge $x \sim y$ with $x,y \in V_j$ we consider the subgraph $X^{(j)} = (V_j, E|_{V_j \times V_j})$ of (V,E). Note that $X^{(j)}$ is a regular graph with degree p_{1j}^j. We now assume the following.

(A4) for each j one of the two cases occurs

(Case 1) p_{1j}^j is even;

(Case 2) p_{1j}^j is odd and $X^{(j)}$ admits a perfect matching, i.e., there is a subset $M = \{e_1,\ldots,e_m\}$ of the edges of $X^{(j)}$ such that each $x \in V_j$ is an endpoint of just one edge of M.

When (case 1) occurs, there is an Euler path for $X^{(j)}$ along which each edge is given an orientation. When (case 2) occurs, deleting M from the subgraph $X^{(j)}$ we obtain another subgraph $\tilde{X}^{(j)}$ which is a regular graph with even degree. Taking an Euler path for $\tilde{X}^{(j)}$, we give an orientation to each edge of $\tilde{X}^{(j)}$. An edge of M is given an arbitrary orientation.

Thus, under assumption (A4) the distance-regular graph is equipped with an orientation. We then set

$$A^+\delta_x=\sum_{y:x\to y}\delta_y, \quad A^-\delta_x=\sum_{y:y\to x}\delta_y.$$

Obviously, $A=A^++A^-$, $(A^-)^*=A^+$. The action of the quantum components $A^\pm$ on particular vectors:

$$v_j=\sum_{x\in V_j}\delta_x$$

is of importance.

Lemma 4.1: Let $\mathcal{G}=(V,E)$ be a distance-regular graph satisfying condition (A4) and $A=A^++A^-$ the quantum decomposition of the adjacency matrix as above.

(1) If p_{1j}^j is even,

$$A^\pm v_j=p_{1j}^{j\pm1}v_{j\pm1}+\frac{p_{1j}^j}{2}v_j, \quad j\in\{0,1,\ldots,d\}. \tag{4.2}$$

(2) Assume p_{1j}^j is odd. Let V_j^- (respectively, V_j^+) be the set of all $x\in V_j$ which is the initial (terminal) vertex of an edge of M. Then $V_j=V_j^+\cup V_j^-$ and

$$A^\pm v_j=p_{1j}^{j\pm1}v_{j\pm1}+\frac{p_{1j}^j-1}{2}v_j+\sum_{y\in V_j^\pm}\delta_y, \quad j\in\{0,1,\ldots,d\}. \tag{4.3}$$

Proof: (1) By definition we have

$$\begin{aligned}
A^+v_j&=\sum_{x\in V_j}A^+\delta_x\\
&=\sum_{x\in V_j}\sum_{y:x\to y}\delta_y\\
&=\sum_{x\in V_j}\sum_{y\in V_{j+1},x\to y}\delta_y+\sum_{x\in V_j}\sum_{y\in V_j,x\to y}\delta_y\\
&=\sum_{y\in V_{j+1}}p_{1j}^{j+1}\delta_y+\sum_{y\in V_j}\frac{p_{1j}^j}{2}\delta_y\\
&=p_{1j}^{j+1}v_{j+1}+\frac{p_{1j}^j}{2}v_j.
\end{aligned}$$

A similar calulation proceeds for A^-.

(2) In a similar manner as above we come to

$$A^+v_j=\sum_{y\in V_{j+1}}p_{1j}^{j+1}\delta_y+\sum_{y\in V_j}\left\{\frac{p_{1j}^j-1}{2}+1_{V_j^+}(y)\right\}\delta_y$$
$$=p_{1j}^{j+1}v_{j+1}+\frac{p_{1j}^j-1}{2}v_j+\sum_{y\in V_j^+}\delta_y,$$

where $1_{V_j^+}(y)$ is the indicator function of V_j^+. A similar calulation proceeds for A^-. ■

B. Weak quantum decomposition and GNS representation

According to the stratification (4.1), we define

$$\Gamma(\mathcal{G})=\sum_{j=0}^{d}\oplus\mathbf{C}\Phi_j,\quad \Phi_j=\frac{1}{\sqrt{\kappa_j}}v_j.$$

Here we note that $\|\Phi_j\|=1$. In view of Lemma 4.1, the quantum components $A^\pm$ act on $\Gamma(\mathcal{G})$ if p_{1j}^j is even for all j. On the other hand, if p_{1j}^j is odd, these actions are not defined within $\Gamma(\mathcal{G})$. Nevertheless, regardless of the parity of p_{1j}^j we may define operators $A^\pm$ on $\Gamma(\mathcal{G})$ by

$$A^\pm v_j=p_{1j}^{j\pm1}v_{j\pm1}+\frac{p_{1j}^j}{2}v_j,\quad j\in\{0,1,\ldots,d\},\tag{4.4}$$

to have $A=A^++A^-$, $(A^+)^*=A^-$. This decomposition of the adjacency matrix A is meaningful for an arbitrary distance-regular graph. We call this the *weak quantum decomposition*.

The weak quantum decomposition is defined also in terms of the Bose–Mesner algebra. For a distance-regular graph $\mathcal{G}$, the ith adjacency matrix is defined by

$$(A_i)_{xy}=\begin{cases}1, & \partial(x,y)=i,\\ 0, & \text{otherwise,}\end{cases}\quad i\in\{0,1,\ldots,d\}.\tag{4.5}$$

By definition $A_1=A$. Then we have the following linearization formula:

$$A_iA_j=\sum_{h=0}^{d}p_{ij}^hA_h.\tag{4.6}$$

The unital $*$-algebra $\mathcal{A}$ generated by A is called the *Bose–Mesner algebra*. It is not difficult to see that $\mathcal{A}$ is the linear hull of $\{A_0=1,A_1,\ldots,A_d\}$, see, e.g., Bannai–Ito.[6]

The Bose–Mesner algebra becomes an algebraic probability space $(\mathcal{A},\mathrm{Tr})$, where Tr stands for the normalized trace. Then we consider the GNS representation of $\mathcal{A}$. Let $\mathcal{H}(\mathcal{A})$ be the Hilbert space obtained from $\mathcal{A}$ equipped with an inner product:

$$\langle Q_1,Q_2\rangle_{\mathcal{A}}=\mathrm{Tr}(Q_1^*Q_2),\quad Q_1,Q_2\in\mathcal{A}.$$

In view of an obvious relation

$$\langle A_i,A_j\rangle_{\mathcal{A}}=\delta_{ij}\kappa_i=\langle v_i,v_j\rangle_{\ell^2(V)},$$

the correspondence $A_i\leftrightarrow v_i$ yields a unitary isomorphism between $\mathcal{H}(\mathcal{A})$ and $\Gamma(\mathcal{G})$. Moreover, since

$$A_iv_j=\sum_{h=0}^{d}p_{ij}^hv_h,$$

which is easily verified by definition, we see from (4.6) that the above unitary isomorphism intertwines the action of the Bose–Mesner algebra $\mathcal{A}$. In particular, the action of the adjacency matrix A on $\Gamma(\mathcal{G})$ is unitarily equivalent to that induced from the GNS representation of $(\mathcal{A}, \mathrm{Tr})$.

By the triangle inequality we have

$$AA_j = p_{1j}^{j-1}A_{j-1} + p_{1j}^{j}A_j + p_{1j}^{j+1}A_{j+1}, \quad j \in \{0,1,\ldots,d\}.$$

The *weak quantum decomposition* of $A = A^+ + A^-$ is given by

$$A^{\pm}A_j = p_{1j}^{j\pm 1}A_{j\pm 1} + \frac{p_{1j}^{j}}{2}A_j, \quad j \in \{0,1,\ldots,d\},$$

which is equivalent to (4.4).

C. Quantum central limit theorem

We consider a growing family of distance-regular graphs $\{\mathcal{G}_\lambda\,;\,\lambda \in \Lambda\}$ such that $d(\lambda)\to\infty$ and $\kappa(\lambda)\to\infty$, where $d(\lambda)$ and $\kappa(\lambda)$ are the diameter and the degree of $\mathcal{G}_\lambda$, respectively. The adjacency matrix and the intersection numbers of $\mathcal{G}_\lambda$ are denoted by A_λ and $\{p(\lambda)_{ij}^h\}$, respectively. By definition

$$\Gamma(\mathcal{G}_\lambda) = \sum_{n=0}^{d(\lambda)} \oplus \mathbf{C}\Phi_n^{(\lambda)}.$$

Theorem 4.2: *Assume that every $\mathcal{G}_\lambda$ satisfies condition (A4) and let $A_\lambda = A_\lambda^+ + A_\lambda^-$ be the quantum decomposition of the adjacency matrix A_λ of $\mathcal{G}_\lambda$. Assume that the limits*

$$\lim_{\lambda\in\Lambda} p(\lambda)_{1j}^{j+1} = \omega_{j+1}, \quad \lim_{\lambda\in\Lambda} \frac{p(\lambda)_{1j}^{j}}{2\sqrt{\kappa(\lambda)}} = \psi_j, \tag{4.7}$$

exist for all $j \in \{0,1,2,\ldots\}$, and let $(\Gamma, \{\lambda_n\}, B^+, B^-)$ be the interacting Fock space, where $\lambda_0 = 1$, $\lambda_n = \omega_1\cdots\omega_n$ for $n \geqslant 1$. Define

$$C^{\pm} = B^{\pm} + \psi_N.$$

Then for any $m \geqslant 1$, $\epsilon_1,\ldots,\epsilon_m \in \{\pm\}$, $n \in \{0,1,2,\ldots\}$ and $u \in \Gamma$, it holds that

$$\lim_{\lambda\in\Lambda} \left\langle u^{(\lambda)}, \frac{A_\lambda^{\epsilon_1}}{\sqrt{\kappa(\lambda)}}\cdots\frac{A_\lambda^{\epsilon_m}}{\sqrt{\kappa(\lambda)}}\Phi_n^{(\lambda)} \right\rangle_{\ell^2(V^{(\lambda)})} = \langle u, C^{\epsilon_1}\cdots C^{\epsilon_m}\Phi_n\rangle_\Gamma, \tag{4.8}$$

where $u^{(\lambda)} \in \Gamma(\mathcal{G}_\lambda)$ is defined as $u^{(\lambda)} = \Sigma_{n=0}^{\infty} u_n \Phi_n^{(\lambda)}$ for $u = \Sigma_{n=0}^{\infty} u_n \Phi_n$, with understanding $\Phi_n^{(\lambda)} = 0$ for $n > d(\lambda)$.

Proof: (1°) To avoid notational bothersome we omit the suffix λ of the intersection numbers. We first show that

$$\frac{1}{\sqrt{\kappa}} p_{1j}^{j+1} \sqrt{\frac{\kappa_{j+1}}{\kappa_j}} \to \sqrt{\omega_{j+1}}, \quad j \geqslant 0. \tag{4.9}$$

It follows from (4.7) that $\omega_1 = 1$. Hence (4.9) holds for $j = 0$. Suppose $j \geqslant 1$. In view of $p_{1j}^{j} + p_{1,j-1}^{j} + p_{1,j+1}^{j} = \kappa$ and (4.7) we see that

$$\frac{p_{1,j+1}^{j}}{\kappa} \to 1.$$

Hence, combining $\kappa_j p^j_{1,j+1}=\kappa_{j+1}p^{j+1}_{1j}$, we obtain (4.9). We note also that

$$\frac{1}{\sqrt{\kappa}}p^{j-1}_{1j}\sqrt{\frac{\kappa_{j-1}}{\kappa_j}}=\frac{1}{\sqrt{\kappa}}p^{j}_{1,j-1}\sqrt{\frac{\kappa_j}{\kappa_{j-1}}}\to\sqrt{\omega_j},\quad j\geqslant 1. \tag{4.10}$$

(2°) We show the convergence of arbitrary matrix elements, i.e., for $u=\Sigma_{n=0}^{\infty}u_n\Phi_n\in\Gamma$ such that $u_n=1$ for only one n and $=0$ otherwise. By (4.2) and (4.3) we see that

$$\frac{1}{\sqrt{\kappa}}A^{\pm}_{\lambda}\Phi^{(\lambda)}_j=\frac{1}{\sqrt{\kappa}}p^{j\pm 1}_{1j}\sqrt{\frac{\kappa_{j\pm 1}}{\kappa_j}}\Phi^{(\lambda)}_{j\pm 1}+\frac{p^j_{1j}-1}{2\sqrt{\kappa}}\Phi^{(\lambda)}_j+\frac{1}{2\sqrt{\kappa}}w^{\pm}_j,$$

where

$$w^{\pm}_j=\begin{cases}\Phi^{(\lambda)}_j & (\text{Case } 1)\\ \dfrac{2}{\sqrt{\kappa_j}}\displaystyle\sum_{y\in V^{\pm}_j}\delta_y & (\text{Case } 2).\end{cases} \tag{4.11}$$

Then

$$w^+_j+w^-_j=2\Phi^{(\lambda)}_j,\quad |\langle\Phi^{(\lambda)}_n,w^{\pm}_j\rangle|\leqslant\sqrt{2}.$$

The proof proceeds by induction. Suppose that the assertion is valid up to m. Then, by virtue of (4.9) and (4.10), it suffices to prove

$$\delta^{\pm}\equiv\left\langle\Phi^{(\lambda)}_n,\frac{A^{\epsilon_1}_{\lambda}}{\sqrt{\kappa}}\frac{A^{\epsilon_2}_{\lambda}}{\sqrt{\kappa}}\cdots\frac{A^{\epsilon_m}_{\lambda}}{\sqrt{\kappa}}\frac{1}{2\sqrt{\kappa}}w^{\pm}_j\right\rangle\to 0.$$

This can be proved easily by use of $\delta^+ + \delta^-\to 0$ and $\delta^{\pm}\geqslant 0$.

(3°) For a general $u\in\Gamma$, the proof is completed by combination of (2°) and a standard argument of norm estimate (or Lebesgue's convergence theorem). ■

For a general distance-regular graph the above assertion remains true if we allow to use the weak quantum decomposition. The proof is essentially the same.

Theorem 4.3: *Let $A_\lambda=A^+_\lambda+A^-_\lambda$ be the weak quantum decomposition of the adjacency matrix A_λ of $\mathcal{G}_\lambda$. If the limits*

$$\lim_{\lambda\in\Lambda}p(\lambda)^{j+1}_{1j}=\omega_{j+1},\quad \lim_{\lambda\in\Lambda}\frac{p(\lambda)^j_{1j}}{2\sqrt{\kappa(\lambda)}}=\psi_j,$$

exist for all $j\in\{0,1,2,\dots\}$, the same assertion as in (4.8) holds.

D. Johnson graph

Let v, d be a pair of positive integers such that $d\leqslant v$. Set $S=\{1,2,\dots,v\}$ and $V=\{x\subset S;|x|=d\}$. We say that x, $y\in V$ are adjacent if $d-|x\cap y|=1$. Thus a graph structure is introduced in V, which is called a *Johnson graph* and denoted by $J(v,d)$. By symmetry we may assume that $2d\leqslant v$.

The Johnson graph $J(v,d)$ is distance regular with intersection numbers

$$\kappa=d(v-d),\quad p^j_{1j}=j(v-2j),\quad p^{j+1}_{1j}=(j+1)^2, \tag{4.12}$$

where $j\in\{0,1,\dots,d\}$. We fix the origin to be $x_0=\{1,2,\dots,d\}$. We start with the following.

Proposition 4.4: Every Johnson graph $J(v,d)$ fulfills condition (A4), and hence the adjacency matrix admits the quantum decomposition.

If v or j is even, p_{1j}^{j} becomes even by (4.12) and the situation falls into (case 1) of (A4). It is sufficient to prove that (case 2) occurs when both v,j are odd. We need the following.

Lemma 4.5: Assume that n is even, j is odd, and $j<n$. Then $J(n,j)$ admits a perfect matching (including the case of $j>n/2$).

Proof: Let us consider the Pascal triangle where the first row consists of (0,0), the second row consists of (1,0) and (1,1), etc. Then the vertex set of $J(n,j)$ is identified with the set of paths on the triangle passing from (0,0) to (n,j). We check by induction on even n that those paths to (n,j) (j is odd) admit a pair partition in which two paths making a pair pass through n common vertices. Among the set of paths to $(n+2,j)$, those paths passing through $(n,j-2)$ or (n,j) already admit such a pair partition by the assumption of induction. A path having reached $(n,j-1)$ can split in the $(n+1)$th row and produces two paths to $(n+2,j)$. Clearly two paths making such a pair correspond to two adjacent vertices of $J(n,j)$. ■

We complete the proof of Proposition 4.4 by the following.

Lemma 4.6: Assume that both v and j are odd. Then the subgraph $X^{(j)}$ obtained from the jth stratum of $J(v,d)$ admits a perfect matching.

Proof: Either d or $v-d$ is even. Assume $v-d$ is even. Every vertex of $X^{(j)}$ is made by removing j members from $x_0=\{1,2,\ldots,d\}$ and by getting j members of $\{d+1,\ldots,v\}$. Fix j members removed from $\{1,2,\ldots,d\}$. Applying Lemma 4.5 to $n=v-d$, we divide the totality of j-subsets of $\{d+1,\ldots.v\}$ into pairs consisting of two adjacent vertices in $J(v-d,j)$. Adding these two j-subsets to the fixed $(d-j)$-subset of $\{1,2,\ldots,d\}$, we get two adjacent vertices in $J(v,d)$, which is obviously adjacent in $X^{(j)}$ too. Taking all the choices of removed j members of $\{1,2,\ldots,d\}$ yields a perfect matching of $X^{(j)}$. A similar consideration proceeds in the case of even d if we first fix j members of $\{d+1,\ldots,v\}$ which should be added to the other side. ■

Consider the growing family of Johnson graphs $J(v,d)$, where $d\to\infty$ and $2d/v\to p\in(0,1]$. Condition (4.7) in Theorem 4.2 is satisfied with

$$\omega_{j+1}=(j+1)^2,\quad \psi_j=\frac{j}{\sqrt{p(2-p)}},\quad j\in\{0,1,\ldots,d\}.$$

Consequently, we come to the following.

Theorem 4.7: *Let $A_{(v,d)}=A^{+}_{(v,d)}+A^{-}_{(v,d)}$ be the quantum decomposition of the adjacency matrix of a Johnson graph $J(v,d)$. Then, in the limit as $d\to\infty$ and $2d/v\to p\in(0,1]$, the quantum central limit theorem holds and the limits are given by*

$$\lim_{d\to\infty,2d/v\to p}\frac{A^{\pm}_{(v,d)}}{\sqrt{d(v-d)}}=B^{\pm}+\frac{N}{\sqrt{p(2-p)}},$$

where B^{+}, B^{-}, N are, respectively, the creation operator, annihilation operator, and the number operator on the interacting Fock space $\Gamma=\Gamma(\mathbf{C},\{(n!)^2\})$.

E. Classical reduction

Let $p\in(0,1]$. It follows from Theorem 4.7 that

$$\lim_{d\to\infty,2d/v\to p}\left\langle \Phi_0^{(v,d)},\left(\frac{A_{(v,d)}}{\sqrt{\kappa(v,d)}}\right)^m\Phi_0^{(v,d)}\right\rangle=\left\langle \Phi_0,\left(B^{+}+B^{-}+\frac{2N}{\sqrt{p(2-p)}}\right)^m\Phi_0\right\rangle_{\Gamma}$$

for all $m=0,1,2,\ldots$. Let ν_p be the probability measure on $\mathbf{R}$ whose mth moment is given as above. We readily know from Theorem 2.1 that the Szegö–Jacobi parameters of the associated orthogonal polynomials are given by $\omega_n=n^2$, $\alpha_{n+1}=2n/\sqrt{p(2-p)}$.

We begin with the case of $p=1$. Recall that the Laguerre polynomials $L_n(x)=x^n+\cdots$ satisfies the recurrence formula

$$L_0(x)=1,$$

$$L_1(x)=x-1,$$

$$(x-(2n+1))L_n(x)=L_{n+1}(x)+n^2L_{n-1}(x),$$

and form the orthogonal polynomials with respect to the probability measure $e^{-x}\,dx$ on the half line $[0,\infty)$. Hence by Theorem 2.1

$$\int_0^\infty x^m e^{-x}\,dx=\langle\Phi_0,(B^+ + B^- + 2N+1)^m\Phi_0\rangle_\Gamma,$$

where $\Gamma=\Gamma(\mathbf{C},\{(n!)^2\})$. Since ν_1 is the spectral distribution of $B^+ + B^- + 2N$ in the vacuum state, it coincides with $e^{-(x+1)}\,dx$ on $[-1,\infty)$.

For $0<p<1$ we need the Meixner polynomials of the first kind. (We use this terminology to specify one among several kinds of Meixner polynomials.) These Meixner polynomials $\{y_n(x)\}$ with parameter $0<\mu<1$ satisfy the recurrence formula

$$y_0(x)=1,$$

$$y_1(x)=-\frac{1-\mu}{\mu}x+1,$$

$$-xy_n(x)=\frac{\mu(n+1)}{1-\mu}y_{n+1}(x)-\frac{n+\mu(n+1)}{1-\mu}y_n(x)+\frac{n}{1-\mu}y_{n-1}(x),$$

and form the orthogonal polynomials with respect to the geometric distribution

$$\sum_{x\in\{0,1,\dots\}}(1-\mu)\mu^x\delta_x.$$

See, e.g., Schoutens.[19] Set

$$\mu=\frac{p}{2-p},\quad M_n(x)=\left(\frac{p}{2-p}\right)^{n/2}(-1)^n n!\,y_n\left(\frac{\sqrt{p(2-p)}}{2(1-p)}x\right).$$

Then $\{M_n(x)\}$ forms the orthogonal polynomials with respect to the probability measure

$$\tilde{\nu}_p=\sum_{k=0}^\infty\frac{2(1-p)}{2-p}\left(\frac{p}{2-p}\right)^k\delta_{2(1-p)k/\sqrt{p(2-p)}},$$

and satisfies the recurrence formula

$$M_0(x)=1,$$

$$M_1(x)=x-\sqrt{\frac{p}{2-p}},$$

$$\left(x-\frac{2n+p}{\sqrt{p(2-p)}}\right)M_n(x)=M_{n+1}(x)+n^2M_{n-1}(x).$$

Then, applying Theorem 2.1, we have

$$\int_{\mathbf{R}} x^m \tilde{\nu}_p(dx) = \left\langle \Phi_0, \left(B^+ + B^- + \frac{2N+p}{\sqrt{p(2-p)}} \right)^m \Phi_0 \right\rangle_\Gamma ,$$

where $\Gamma = \Gamma(\mathbf{C}, \{(n!)^2\})$. Thus, by translation of $\tilde{\nu}_p$ we obtain

$$\nu_p = \sum_{k=0}^{\infty} \frac{2(1-p)}{2-p} \left(\frac{p}{2-p} \right)^k \delta_{-p+2(1-p)k/\sqrt{p(2-p)}} .$$

Remark 4.8: The above spectral distribution ν_p was first found by Hora[12] with a different method. Moreover, the result in Hora[12] for $p=1$ was obtained under an additional condition which is now removed.

ACKNOWLEDGMENTS

This work was supported by JSPS–PAN Joint Research Project ''Infinite Dimensional Harmonic Analysis.'' A. H. is supported partially by Grant-in-Aid for Scientific Research (C), JSPS (No. 13640175).

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The essential spectrum of Schrödinger operators with asymptotically constant magnetic fields on the Poincaré upper-half plane

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(Received 22 May 2002; accepted 11 October 2002)

We study the essential spectrum of the magnetic Schrödinger operators on the Poincaré upper-half plane and establish a hyperbolic analog of Iwatsuka's result [J. Math. Kyoto Univ. **23**(3), 475–480 (1983)] on the stability of the essential spectrum under perturbations from constant magnetic fields. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1527717]

I. INTRODUCTION AND RESULT

In this article, we study the essential spectrum of the magnetic Schrödinger operator on the Poincaré upper-half plane $\mathbf{H}=\{z=(x,y)|x\in\mathbf{R},y>0\}$ endowed with the standard metric

$$g=(g_{jk})_{j,k=1}^{2}=\begin{pmatrix} y^{-2} & 0 \\ 0 & y^{-2} \end{pmatrix}.$$

For a smooth one-form with real coefficients on $\mathbf{H}$, $\mathbf{a}(x,y)=a_1(x,y)dx+a_2(x,y)dy$, we consider the differential operator

$$\begin{aligned} H(\mathbf{a}) &= \frac{1}{\sqrt{\det g}}\sum_{j,k=1}^{2}\left(\frac{1}{i}\frac{\partial}{\partial x_j}-a_j(x,y)\right)g^{jk}\sqrt{\det g}\left(\frac{1}{i}\frac{\partial}{\partial x_k}-a_k(x,y)\right) \\ &= y^2\left(\frac{1}{i}\frac{\partial}{\partial x}-a_1(x,y)\right)^2+y^2\left(\frac{1}{i}\frac{\partial}{\partial y}-a_2(x,y)\right)^2, \end{aligned} \tag{1.1}$$

where we set $x_1=x$, $x_2=y$ and $g^{-1}=(g^{jk})_{j,k=1}^{2}$.

The operator (1.1) has a physical interpretation as the Hamiltonian which governs a charged particle moving on $\mathbf{H}$ under influence of *the magnetic field*

$$(d\mathbf{a})(x,y)=\left(\frac{\partial a_2}{\partial x}(x,y)-\frac{\partial a_1}{\partial y}(x,y)\right)dx\wedge dy. \tag{1.2}$$

The one-form $\mathbf{a}$ above is called *the magnetic vector potential*. In what follows, we say the magnetic field $d\mathbf{a}$ is *constant* if it is given, up to constant proportionality, by the volume form.

In the constant magnetic field case, the operator (1.1), which is sometimes called *the Maass Laplacian*, has been studied by many authors (see, e.g., Roelche, 1996; Elstrodt, 1973; Fay, 1977; Comtet, 1987; Grosche, 1988; Antane *et al.*, 1990; Avron and Pnueli, 1992; Ikeda and Matsumoto, 1999, and

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references therein). In particular, it is well-known that the spectrum of the Maass Laplacian consists of the absolutely continuous part and the point spectrum consisting of a finite number of eigenvalues of infinite multiplicity and the second part is absent for weak fields.

On the other hand, in the Euclidean case, the spectrum of the two-dimensional Schrödinger operator with nonzero constant magnetic field $B_0\,dx_1\wedge dx_2$ consists of the so-called Landau levels, i.e., the eigenvalues $\{(2n-1)B_0\}_{n=1}^{\infty}$ of infinite multiplicity. Iwatsuka (1993) has established the stability of the essential spectrum of the magnetic Schrödinger operators under the perturbation from the constant magnetic fields $(B_0+B_1(x_1,x_2))dx_1\wedge dx_2$, where B_1 is a real-valued, smooth function on $\mathbf{R}^2$ and decays at infinity. Moreover, the result needs no other decay properties of B_1 nor of the derivatives of B_1. The purpose of this article is to obtain an analog of Iwatsuka's result in the hyperbolic case.

In what follows, we identify a one-form a_1dx+a_2dy and a two-form $B\,dx\wedge dy$ with the vector-valued function (a_1,a_2) and the function B, respectively.

For a smooth manifold Ω, we denote the set of all complex-valued, smooth functions with compact support on Ω by $C_0^{\infty}(\Omega)$ and denote the set of all complex-valued, continuous funtions on Ω by $C(\Omega)$. We denote the set of all $\mathbf{R}^n$-valued, k-times continuously differentiable functions on Ω by $C^k(\Omega;\mathbf{R}^n)$ and denote the set of all $\mathbf{R}^n$-valued, continuous functions on Ω by $C(\Omega;\mathbf{R}^n)$. We denote $\partial/\partial x$, $(1/i)\partial/\partial x$ by ∂_x, D_x, respectively.

For a densely defined, closable linear operator A acting in a Hilbert space, we denote the domain of A by $D(A)$ and denote the operator closure of A by $\overline{A}$. For linear operators A_1,A_2, the notation $A_1\subset A_2$ means that $D(A_1)\subset D(A_2)$ and $A_1f=A_2f$ for all $f\in D(A_1)$. For any self-adjoint operator A we denote the spectrum of A by $\sigma(A)$ and denote the essential spectrum of A by $\sigma_{\mathrm{ess}}(A)$ (e.g., Reed and Simon, 1978, Vol. I). For simplicity, we denote by $\|\cdot\|$ both L^2-norms on any spaces and the operator norms for bounded linear operators on any Hilbert spaces when there is no fear of confusion.

In order to formulate the main result, we introduce the condition for the magnetic fields:

(B) The vector potential $\mathbf{a}\in C^{\infty}(\mathbf{H};\mathbf{R}^2)$ satisfies

$$d\mathbf{a}(x,y)=\frac{B_0+B_1(x,y)}{y^2}, \tag{1.3}$$

for some real constant B_0 and for some real-valued continuous function B_1. Moreover, the perturbation B_1 decays at infinity, i.e., for any $\varepsilon>0$, there exists a compact subset K of $\mathbf{H}$ such that $|B_1(x,y)|<\varepsilon$ holds for any $(x,y)\in K^c$. Here, we denote the complement of a subset K by K^c.

The next result is a special case of Theorem 1.1 in Shubin (2001).

Lemma 1.1: Assume that $\mathbf{a}\in C^1(\mathbf{H};\mathbf{R}^2)$. *Then the differential operator (1.1) is essentially self-adjoint on* $C_0^{\infty}(\mathbf{H})$.

In the sequel, we use the same symbol $H(\mathbf{a})$ also for the unique self-adjoint extension when there is no fear of confusion.

The main result of this article is the following:

Theorem 1.2: *Assume that* $\mathbf{a}$ *satisfies the condition (B). For each real number* B_0 *with* $|B_0|>\frac{1}{2}$, *we introduce the (discrete) Landau levels*

$$\sigma_L(B_0)=\bigcup_{l=0}^{N(B_0)}\{(2l+1)|B_0|-l(l+1)\}, \tag{1.4}$$

where the number $N(B_0)$ *is the largest integer less than* $|B_0|-\frac{1}{2}$.

Then we have

$$\sigma_{\mathrm{ess}}(H(\mathbf{a}))=\begin{cases}\sigma_L(B_0)\cup[\frac{1}{4}+B_0^2,\ \infty) & (|B_0|>\frac{1}{2}),\\ [\frac{1}{4}+B_0^2,\ \infty) & (|B_0|\leqslant\frac{1}{2}).\end{cases}$$

The rest of this article is organized as follows: In Sec. II, we recall some abstract results from the spectral theory and Sec. III contains some preliminary results for the operator $H(\mathbf{a})$. In Sec. IV, we study the continuous spectrum by constructing the so-called Weyl sequence, and we determine the location of $\sigma_{\mathrm{ess}}(H(\mathbf{a}))$ for the case of $|B_0| \leqslant \frac{1}{2}$ (Lemma 4.5 below). In Sec. V, we show that the bottom of $\sigma_{\mathrm{ess}}(H(\mathbf{a}))$ is the point B_0 for any $|B_0|>1$ (Lemma 5.3 below). In Sec. VI, we complete the proof of Theorem 1.2.

II. RESULTS FROM SPECTRAL THEORY

In this section, we collect the auxiliary results from the spectral theory for later use.

Lemma 2.1: Let A be a densely defined, closed operator acting as a separable Hilbert space. Then A^*A and AA^* have the same essential spectrum except perhaps at the point 0.

Proof: This is a basic result in spectral theory. However, for the sake of completeness, we give an outline of the proof.

Let $A=V|A|$ be the polar decomposition of A, where V is the unique partial isometry with the initial subspace $(\ker A)^{\perp}$ and the final subspace $(\ker A^*)^{\perp}$. Then the identity $A^*A=V^*(AA^*)V$ holds (see, e.g., Birman and Solomjak, 1987, Theorem 4, p. 186). Using the functional calculus, we have $P_{\Omega}(A^*A)=V^*P_{\Omega}(AA^*)V$ holds for each Borel subset $\Omega \subset (0,\infty)$, where $P_{\Omega}(T)$ is the spectral projections associated with the self-adjoint operators T on Ω. Since V, V^* are injective on the ranges of $P_{\Omega}(A^*A)$, $P_{\Omega}(AA^*)$, respectively, if Ω does not contain 0, it follows that dim Range $P_{\Omega}(A^*A)=$dim Range $P_{\Omega}(AA^*)$. This implies the lemma. ■

Lemma 2.2: Let λ be a real number and let A be a non-negative self-adjoint operator acting in a separable Hilbert space K. Assume that there is a sequence in K, $\{\varphi_n\}_{n=1}^{\infty}$ satisfying the conditions: $\|\varphi_n\|=1$ *for all n and $\varphi_n \to 0$ as $n\to\infty$ with respect to the weak topology on K, and $\|(A+1)^{-1}(A-\lambda)\varphi_n\| \to 0$ holds as $n\to\infty$. Then we have $\lambda \in \sigma_{\mathrm{ess}}(A)$.*

Proof: One can find a proof in Cycon *et al.* (1987), p. 117. ■

Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators acting in a Hilbert space. Then A_n is said to converge to A in the norm resolvent sense if

$$\|(A_n \pm i)^{-1} - (A \pm i)^{-1}\| \to 0 \quad \text{as} \quad n \to \infty,$$

respectively (see, e.g., Reed and Simon, 1978, Vol. I, p. 284).

Lemma 2.3: Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators and $A_n \to A$ in the norm resolvent sense. Then we have:

(i) Let $a,b \in \mathbf{R}$, $a<b$ and suppose that a and b belong to the resolvent set of A. Then

$$\|P_{(a,b)}(A_n) - P_{(a,b)}(A)\| \to 0 \quad \text{as} \quad n \to \infty,$$

where $P_{(a,b)}$ is the spectral projection on the open interval (a,b).

(ii) In addition, if $\sigma_{\mathrm{ess}}(A_n)=[\Sigma_n,\infty)$ for all n, then Σ_n converges as $n\to\infty$ to some Σ (possibly ∞) and $\sigma_{\mathrm{ess}}(A)=[\Sigma,\infty)$.

Proof: One can find proofs of the assertions (i) and (ii) in Reed and Simon (1978), Vol. I, Theorem VIII.23 (b) and Vol. IV, Corollary 2 of Theorem VIII.77, respectively. ■

III. PRELIMINARIES

To the end of the proof of Theorem 1.2, we always assume that **a** satisfies the condition (B), and we set

$$B(x,y)=y^2 d\mathbf{a}(x,y)=B_0+B_1(x,y).$$

Without loss of generality, we may assume that $B_0 \geqslant 0$, since if we consider, instead of $H(\mathbf{a})$, the operator

$$V^{-1}H(\mathbf{a})V=y^2(D_x+a_1(-x,y))^2+y^2(D_y-a_2(-x,y))^2$$

with $(Vf)(x,y)=f(-x,y)$, then we have

$$\partial_x(a_2(-x,y))-\partial_y(-a_1(-x,y))=-d\mathbf{a}(-x,y)=(-B_0-B_1(-x,y))/y^2.$$

We show the theorem for all non-negative B_0.

Throughout this article, B_1 is an arbitrary fixed function decaying at infinity in the sense of the condition (B). For any vector potential $\mathbf{b}(x,y)$ satisfying that $d\mathbf{b}(x,y)=d\mathbf{a}(x,y)=B(x,y)/y^2$, $H(\mathbf{a})$ and $H(\mathbf{b})$ are unitarily equivalent by the gauge transform. We often write $H_{B_0}(\mathbf{a})$ or H_{B_0} for $H(\mathbf{a})$ when there is no fear of confusion and we do not specify the dependence on B_1.

Let us introduce the following vector potential $\mathbf{b}$:

$$\mathbf{b}(x,y)=\left(\frac{B_0+B_1^{\natural}(x,y)}{y},\ 0\right), \tag{3.1}$$

where

$$B_1^{\natural}(x,y)=y\int_y^1\frac{B_1(x,t)}{t^2}dt. \tag{3.2}$$

It is easy to see that $d\mathbf{b}(x,y)=B(x,y)/y^2$. For this vector potential $\mathbf{b}$ we have

$$H_{B_0}(\mathbf{b})=y^2(D_x-b_1(x,y))^2+y^2D_y^2. \tag{3.3}$$

In the sequel we often assume that the vector potential is of the form as in (3.1) and the operator H_{B_0} is of the form as in (3.3).

Lemma 3.1: The operator inequality $H_{B_0}\geqslant\frac{1}{4}$ holds for any B_0.

Proof: For any $f,g\in C_0^\infty(\mathbf{H})$, an integration by parts yields

$$\begin{aligned}(D_yf,g)_{L^2(H)}&=\int_R dx\int_0^\infty\frac{dy}{y^2}\overline{D_yf(x,y)}g(x,y)\\&=\int_R dx\int_0^\infty\overline{f(x,y)}D_y(y^{-2}g(x,y))\\&=\int_R dx\int_0^\infty\overline{f(x,y)}(y^{-2}(D_yg)(x,y)+2iy^{-3}g(x,y))=\left(f,\left(D_y+\frac{2i}{y}\right)g\right)_{L^2(H)},\end{aligned}$$

from which we have

$$(yD_y)^*=(D_y+2i/y)y=D_yy+2i=yD_y+i. \tag{3.4}$$

Then we have, on $C_0^\infty(\mathbf{H})$,

$$\begin{aligned}0&\leqslant\left(y(D_y-a_2(x,y))+\frac{i}{2}\right)^*\left(y(D_y-a_2(x,y))+\frac{i}{2}\right)\\&=\left(y(D_y-a_2(x,y))+\frac{i}{2}\right)\left(y(D_y-a_2(x,y))+\frac{i}{2}\right)\\&=y(D_y-a_2(x,y))y(D_y-a_2(x,y))+iy(D_y-a_2(x,y))-\tfrac{1}{4}\\&=y^2(D_y-a_2(x,y))^2-\tfrac{1}{4},\end{aligned} \tag{3.5}$$

where we used (3.4) in the first equality, hence it follows that

$$y^2(D_y-a_2(x,y))\geqslant \tfrac{1}{4}.$$

Then, owing to Lemma 1.1, we have the conclusion since $y^2(D_x-a_1)^2\geqslant 0$. ■

We introduce the differential operators

$$A_{B_0}=y(D_x-a_1(x,y))+iy(D_y-a_2(x,y)), \tag{3.6}$$

$$A_{B_0}^{\dagger}=y(D_x-a_1(x,y))-iy(D_y-a_2(x,y))+1 \tag{3.7}$$

with domain $C_0^{\infty}(\mathbf{H})$.

Note that, using (3.4), we can find that

$$\begin{aligned} A_{B_0}^{*}&=(y(D_x-a_1)+iy(D_y-a_2))^{*}\\ &=y(D_x-a_1)-i(yD_y+i-ya_2)\\ &=y(D_x-a_1)-iy(D_y-a_2)+1=A_{B_0}^{\dagger} \end{aligned} \tag{3.8}$$

holds on $C_0^{\infty}(\mathbf{H})$.

Lemma 3.2: The following statements (i)–(iii) hold:

(i) The operator A_{B_0} maps $C_0^{\infty}(\mathbf{H})$ into $C(\mathbf{H})$ and A_{B_0} is closable on $C_0^{\infty}(\mathbf{H})$. Moreover, the adjoint $(\overline{A_{B_0}})^{*}$ coincides with $A_{B_0}^{\dagger}$ on $C_0^{\infty}(\mathbf{H})$.

(ii) The operator identity

$$H_{B_0}=(\overline{A_{B_0}})^{*}\overline{A_{B_0}}+B \tag{3.9}$$

holds, where the last term B on the rhs stands for the bounded multiplication operator by $B(x,y)$.

(iii) The operator identity

$$\overline{A_{B_0}}(\overline{A_{B_0}})^{*}+B=H_{B_0-1}(\mathbf{b})+2B-1 \tag{3.10}$$

holds for some $\mathbf{b}\in C^{\infty}(\mathbf{H};\mathbf{R}^2)$.

Proof: It follows from (3.8) that, for all $f,g\in C_0^{\infty}(\mathbf{H})$,

$$(A_{B_0}^{\dagger}f,\ g)=(f,\ A_{B_0}g). \tag{3.11}$$

The first part of the assertion (i) is obvious and the closability of A_{B_0} follows from the density of the domain of $A_{B_0}^{*}$. The rest of the statement follows also from (3.11).

Next we show (ii). If we set

$$\Pi_1=y(D_x-a_1),\quad \Pi_2=y(D_y-a_2),$$

then we have, on $C_0^{\infty}(\mathbf{H})$,

$$\Pi_1^2=y^2(D_x-a_1)^2,$$

$$\Pi_2^2=y(D_y-a_2)y(D_y-a_2)=y^2(D_y-a_1)-i\Pi_2,$$

$$\begin{aligned} \Pi_1\Pi_2&=y(D_x-a_1)y(D_y-a_2)\\ &=y^2(D_x-a_1)(D_y-a_2)\\ &=y^2(D_xD_y-a_1D_y-D_xa_2+a_1a_2)\\ &=y^2(D_xD_y-a_1D_y-a_2D_x+a_1a_2+i\partial_x a_2), \end{aligned}$$

$$\begin{aligned}\Pi_2\Pi_1 &= y(D_y-a_2)y(D_x-a_1)\\ &= y^2(D_y-a_2)(D_x-a_1)-i\Pi_1\\ &= y^2(D_xD_y-a_2D_x-a_1D_y+a_1a_2+i\partial_y a_1)-i\Pi_1,\\ \Pi_1\Pi_2-\Pi_2\Pi_1 &= iy^2(d\mathbf{a})+i\Pi_1 = iB+i\Pi_1.\end{aligned}$$

Then we have

$$\begin{aligned}A_{B_0}^{\dagger}A_{B_0}+B &= (\Pi_1-i\Pi_2+1)(\Pi_1+i\Pi_2)+B\\ &= \Pi_1^2+\Pi_2^2+i(\Pi_1\Pi_2-\Pi_2\Pi_1)+\Pi_1+i\Pi_2+B\\ &= H_{B_0}.\end{aligned}$$

From (i), it follows that both H_{B_0} and the operator on the rhs of (3.9) extends $A_{B_0}^{\dagger}A_{B_0}+B$ defined on $C_0^{\infty}(\mathbf{H})$. Then the essential self-adjointness of H_{B_0} implies the identity (3.9), since the rhs of (3.9) is self-adjoint (see, e.g., Reed and Simon, 1978, vol. II, Theorem X.25).

Finally we show the assertion (iii). We have

$$\begin{aligned}A_{B_0}A_{B_0}^{\dagger} &= (\Pi_1+i\Pi_2)(\Pi_1-i\Pi_2+1)\\ &= \Pi_1^2+\Pi_2^2-i(\Pi_1\Pi_2-\Pi_2\Pi_1)+\Pi_1+i\Pi_2\\ &= \Pi_1^2+2\Pi_1+y^2(D_y-a_2)^2+B\\ &= (\Pi_1+1)^2+y^2(D_y-a_2)^2+B-1\\ &= y^2\left(D_x-\left(a_1-\frac{1}{y}\right)\right)^2+y^2(D_y-a_2)^2+B-1 = H_{B_0-1}+B-1,\end{aligned}$$

from which the conclusion obeys as in the case of the assertion (ii). ■

The property like (3.10) above is often called *the (translation) shape invariance* in the study of the Morse-type Hamiltonian (see Molnár *et al.*, 2001; Benedict and Molnár, 1999, and references therein). The shape invariance plays an important role in Sec. V.

In the sequel, for simplicity, we use the symbols A_{B_0}, $A_{B_0}^*$ also for $\overline{A_{B_0}}$, $(\overline{A_{B_0}})^*$, respectively, when there is no fear of confusion.

Lemma 3.3: The operator $(H_{B_0}+1)^{-1}y(D_x-a_1)$ *defined on* $C_0^{\infty}(\mathbf{H})$ *extends to the unique bounded operator acting on* $L^2(\mathbf{H})$ *whose operator norm is less or equal to* 1.

Proof: Note that Lemma 3.1 ensures that -1 belongs to the resolvent set of H_{B_0}.

For any $f\in C_0^{\infty}(\mathbf{H})$, we have

$$\|y(D_x-a_1)f\|^2 = (f,\, y^2(D_x-a_1)^2 f)\leqslant (f,\, H_{B_0}f)+\|f\|^2\leqslant\|(H_{B_0}+1)^{1/2}f\|^2,$$

where we used the inequality $y^2(D_y-a_2)^2\geqslant 1/4$ in the first inequality. Then the operator domain of the closure of $y(D_x-a_1)$ contains $D(H_{B_0})$, and the operator $y(D_x-a_1)(H_{B_0}+1)^{-1/2}$ has the unique bounded extension, hence so $y(D_x-a_1)(H_{B_0}+1)^{-1}$. Finally the lemma follows from a simple duality argument via the inner product. ■

Lemma 3.4: Let z *belong to* $\mathbf{C}\backslash[0,\infty)$. *The family of operators* $\{(H_{B_0}-z)^{-1}\}$ $(B_0>0)$ *is continuous in* B_0 *with respect to the norm operator topology.*

Proof: Since

$$H_{B_0+\varepsilon}-H_{B_0} = y^2\left(D_x-\frac{B_0+\varepsilon+B_1^{\natural}}{y}\right)^2-y^2\left(D_x-\frac{B_0+B_1^{\natural}}{y}\right)^2 = -2\varepsilon y\left(D_x-\frac{B_0+B_1^{\natural}}{y}\right)+\varepsilon^2$$

holds for all $\varepsilon \in \mathbf{R}$ small enough, the resolvent equation yields

$$\|(H_{B_0+\varepsilon}-z)^{-1}-(H_{B_0}-z)^{-1}\| \leqslant 2\varepsilon \|(H_{B_0+\varepsilon}-z)^{-1} y\left(D_x - \frac{B_0+B_1^{\#}}{y}\right)(H_{B_0}-z)^{-1}\| + \varepsilon^2 \|(H_{B_0+\varepsilon}-z)^{-1}(H_{B_0}-z)^{-1}\| \leqslant C_z \varepsilon$$

for some $C_z > 0$ independent of ε, where we used Lemma 3.3 and the semi-boundedness of H_{B_0} in the last inequality. This proves the lemma. ■

Define the unitary operator U from $L^2(\mathbf{H})$ to $L^2(\mathbf{R}^2)$ endowed with the Lebesgue measure by

$$(Uf)(x,t) = f(x,e^t)e^{-t/2} \quad (f \in L^2(\mathbf{R}^2)). \tag{3.12}$$

It is easy to see that U maps $C_0^\infty(\mathbf{H})$ onto $C_0^\infty(\mathbf{R}^2)$ and the inverse U^{-1} is given by

$$(U^{-1}g)(x,y) = g(x,\log y)y^{1/2}$$

for each $g \in L^2(\mathbf{R}^2)$. By direct computations like

$$\begin{aligned}(UD_yU^{-1}g)(x,y) &= UD_y(g(x,\log y)\sqrt{y}) \\ &= U\left((D_tg)(x,\log y)y^{-1/2} - \frac{i}{2}g(x,\log y)y^{-1/2}\right) \\ &= \left((D_tg)(x,t)e^{-t/2} - \frac{i}{2}g(x,t)e^{-t/2}\right)e^{-t/2} \\ &= e^{-t}\left(D_t - \frac{i}{2}\right)g(x,t),\end{aligned}$$

we have the operator equalities

$$UD_xU^{-1} = D_x, \quad UD_yU^{-1} = e^{-t}\left(D_t - \frac{i}{2}\right), \quad Uf(x,y)U^{-1} = f(x,e^t), \tag{3.13}$$

where f stands for the multiplication by an arbitrary measurable function f on $\mathbf{H}$.

Lemma 3.5: Let L_{B_0} denote the operator $UH_{B_0}U^{-1}$ acting in $L^2(\mathbf{R}^2)$. Then we have

$$L_{B_0} = e^{2t}(D_x - a_1(x,e^t))^2 + D_t^2 + \tfrac{1}{4}. \tag{3.14}$$

Moreover, for each $t_0 \in \mathbf{R}$, there exists $g(\cdot\,;t_0) \in C^\infty(\mathbf{R}^2;\mathbf{R})$ such that

$$e^{-ig(\cdot\,;t_0)}L_{B_0}e^{ig(\cdot\,;t_0)} = e^{2t}\left(D_x - \frac{B_0+B_1^{\sharp}(x,t;t_0)}{e^t}\right)^2 + D_t^2 + \frac{1}{4}$$

holds on $C_0^\infty(\mathbf{R}^2)$, where

$$B_1^{\sharp}(x,t;t_0) = e^t\int_t^{t_0} e^{-s}B_1(x,e^s)ds.$$

Proof: We denote $\tilde{a}_1(x,t) = a_1(x,e^t)$. Then it follows from (3.13) that

$$L_{B_0} = UH_{B_0}U^{-1} = e^{2t}(D_x - \tilde{a}_1)^2 + e^{2t}\left(e^{-t}\left(D_t - \frac{i}{2}\right)\right)^2.$$

Then (3.14) follows since

$$\left(e^{-t}\left(D_t-\frac{i}{2}\right)\right)^2=\left(e^{-t}D_t-\frac{ie^{-t}}{2}\right)^2$$
$$=e^{-t}D_te^{-t}D_t-\frac{ie^{-t}D_te^{-t}}{2}-\frac{ie^{-2t}D_t}{2}-\frac{e^{-2t}}{4}$$
$$=e^{-2t}D_t^2+ie^{-2t}D_t-\frac{ie^{-2t}D_t}{2}+\frac{e^{-2t}}{2}-\frac{ie^{-2t}D_t}{2}-\frac{e^{-2t}}{4}$$
$$=e^{-2t}(D_t^2+\tfrac{1}{4}).$$

The second part follows immediately from a simple argument using the gauge transform since

$$\partial_t(a_1(x,e^t))=\partial_t\left(\frac{B_0+B_1^\sharp(x,t;t_0)}{e^t}\right)=-(B_0+B_1)e^{-t}.$$

■

Lemma 3.6: For the self-adjoint operator $-\Delta_H=-y^2(\partial_x^2+\partial_y^2)$, *the following statements (i) and (ii) hold:*

(i) For each $s>0$, *the operator* $e^{s\Delta_H}$ *has a positive integral kernel.*

(ii) For any continuous function on $\mathbf{H}$, V, *decaying at infinity in the same sense as in* (B), *the operator* $V(-\Delta_H+1)^{-1}$ *is compact.*

Proof: It is well-known (see, e.g., Terras, 1985) that the heat kernel is given explicitly by

$$\frac{\sqrt{2}e^{-s/8}}{(2\pi s)^{3/2}}\int_{d(z_1,z_2)}^{\infty}\frac{be^{-b^2/2s}}{\sqrt{\cosh b-\cosh d(z_1,z_2)}}db,$$

hence the statement (i) follows.

It follows from Elstrodt (1973), Part II, Satz 7.2 with $k=0$, that the resolvent $(-\Delta_H+1)^{-1}$ has the integral kernel $G(x,y;x',y')$ such that $\|G(x,y;\cdot)\|_{L^2(H)}$ is uniformly bounded in $(x,y)\in\mathbf{H}$. Then we can find that, for $V\in L^2(\mathbf{H})$, the operator $V(-\Delta_H+1)^{-1}$ belongs to the Hilbert–Schmidt class. Then, by approximating V by functions with compact support, we see the validity of (ii) for general V's. ■

Since $\mathbf{H}$ is a separable measure space, the next result follows immediately from the well-known Pitt theorem (Pitt, 1979, Theorem 1):

Lemma 3.7: Let P, Q *be bounded operators acting on* $L^2(\mathbf{H})$. *Assume that, for any* $g\in L^2(\mathbf{H})$, $|(Pg)(z)|\leqslant(Q|g|)(z)$ *for a.e.* $z\in\mathbf{H}$, *and assume* Q *is compact. Then* P *is compact.*

The next result is the strong version of the Trotter product formula (Reed and Simon, 1978, vol. I, Theorem VIII.31; see also Chernoff, 1968):

Lemma 3.8: Let X_1 *and* X_2 *be semi-bounded, self-adjoint operators. Assume that the operator sum* $Y=X_1+X_2$ *with domain* $D(Y)=D(X_1)\cap D(X_2)$ *is essentially self-adjoint. Then we have the Trotter product formula*

$$e^{-sY}=\mathrm{s}-\lim_{n\to\infty}(e^{-sX_1/n}e^{-sX_2/n})^n$$

for each $s>0$. *Here "*s-lim*" stands for the limit with respect to the strong operator topology.*

Lemma 3.9: For each $g\in L^2(\mathbf{H})$ *and for each* $s\in\mathbf{R}$, *we have the dia-magnetic inequality*

$$|(e^{-sH_{B_0}}g)(x,y)|\leqslant(e^{s\Delta_H}|g|)(x,y)\quad\text{a.e.}\tag{3.15}$$

Proof: We prove the lemma using Lemma 3.8. For each densely defined, semi-bounded, symmetric operator A, we denote the Friedrichs extension of A by A^F (e.g., Reed and Simon, 1978, Vol. II, Theorem X.23). Note that A^F is self-adjoint.

First, let A_1 and A_2 be the semi-bounded, symmetric, differential operators $A_1=y^2(D_x-a_1)^2$ and $A_2=y^2(D_y-a_2)^2$ defined on $C_0^\infty(\mathbf{H})$, respectively, and set $C=A_1^F+A_2^F$ with domain $D(A_1^F)\cap D(A_2^F)$ which contains $C_0^\infty(\mathbf{H})$, hence it is dense. Due to the essential self-adjointness of H_{B_0} on $C_0^\infty(\mathbf{H})$, we can deduce that H_{B_0} coincides with C^F and that $H_{B_0}=\overline{A_1+A_2}\subset\overline{C}$. On the other hand, we have $\overline{C}\subset C^F$ since C^F is closed and extends H_{B_0}. Hence, $\overline{C}$ coincides with H_{B_0}, so $C=A_1^F+A_2^F$ is essentially self-adjoint on $D(A_1^F)\cap D(A_2^F)$.

Second, let U be the unitary operator as in (3.12) and set

$$\Phi_1(x,t)=\int_0^x a_1(l,e^t)dl,\quad \Phi_2(x,t)=\int_0^t e^l a_2(x,e^l)dl.$$

Then we can find that $e^{-i\Phi_1}UA_1^FU^{-1}e^{i\Phi_1}$ and $e^{-i\Phi_2}UA_2^FU^{-1}e^{i\Phi_2}$ extend $e^{2t}D_x^2$ and $D_t^2+\frac{1}{4}$ on $C_0^\infty(\mathbf{R}^2)$, respectively. We denote the closures of $e^{2t}D_x^2$ and $D_t^2+\frac{1}{4}$ by X and Y, respectively. Applying Lemma 3.8 with $A_1=A_1^F$, $A_2=A_2^F$ and $C=C$, we have

$$\begin{aligned} Ue^{-sH_{B_0}}U^{-1}&=\mathrm{s}-\lim_{n\to\infty}(Ue^{-sA_1^F/n}U^{-1}Ue^{-sA_2^F/n}U^{-1})^n\\ &=\mathrm{s}-\lim_{n\to\infty}(e^{i\Phi_1}e^{-sX/n}e^{-i\Phi_1}e^{i\Phi_2}e^{-sY/n}e^{-i\Phi_2})^n. \end{aligned}\tag{3.16}$$

where we used the essential self-adjointness of X and Y on $C_0^\infty(\mathbf{R}^2)$ in the last equality.

Third, both X and Y possess the positivity preserving property (Reed and Simon, 1978, Vol. IV, p. 201), since they have the integral representations

$$(e^{-sX}f)(x,t)=\int_{-\infty}^{\infty}k_{se^{2t}}(x-x')f(x',t)dx',$$

$$(e^{-sY}f)(x,t)=\int_{-\infty}^{\infty}e^{-s/4}k_s(t-t')f(x,t')dt'$$

with the Gaussian kernel $k_s(w)=(4\pi s)^{-1/2}e^{-|w|^2/(4s)}$. Then we can deduce from (3.16) and Lemma 3.6 (i) that

$$|Ue^{-sH_{B_0}}U^{-1}f(x,y)|\leqslant\lim_{n\to\infty}U(e^{-sX/n}e^{-sY/n})^nU^{-1}|f|(x,y)\quad\text{a.e.}\tag{3.17}$$

holds for each $f\in L^2(\mathbf{H})$ and for each $s>0$. Using the essential self-adjointness of $-\Delta_H$ on $C_0^\infty(\mathbf{H})$, we can deduce from the argument similar to the first step that

$$\text{the rhs of (3.17)}=Ue^{-sH_0(0)}U^{-1}|f|(x,y).$$

Finally, setting $f=Ug$, we have the claim (3.15) since $|Ug|=U|g|$. ■

Lemma 3.10: For any $V\in C(\mathbf{H};\mathbf{R})$ decaying at infinity in the same sense of the condition (B), the multiplication operator V is relatively compact with respect to H_{B_0}. In particular, we have $\sigma_{\mathrm{ess}}(H_{B_0}+V)=\sigma_{\mathrm{ess}}(H_{B_0})$.

Proof: Applying the well-known formula

$$(A+1)^{-1}=\int_0^\infty e^{-sA}e^{-s}ds,$$

we deduce from Lemma 3.9 that

$$|V((H_{B_0}+1)^{-1}g)(x,y)| \leqslant (|V|(-\Delta_H+1)^{-1}|g|)(x,y) \quad \text{a.e.}$$

if $V \in C^\infty(\mathbf{H})$ decays at infinity. Then the lemma follows from Lemmas 3.6 (ii) and 3.7. ■

IV. THE CONTINUOUS SPECTRUM

In this section, we show that $\sigma_{\mathrm{ess}}(H_{B_0})$ consists of only the continuous spectrum $[B_0^2+\frac{1}{4},\infty)$ if $|B_0| \leqslant \frac{1}{2}$ (Lemma 4.5 below). Following the same line of argument in the Euclidean case (Cycon *et al.*, 1987, Theorem 6.1), we give an analytic proof using Weyl's criterion. The authors do not know whether the location of the continuous spectrum is determined only from some appropriate algebraic structures (e.g., the shape invariance).

In what follows, we use the symbols $C, C', \ldots$ (with indices) to denote various positive constants, whose values may change from line to line when there is no fear of confusion.

Take and fix $\chi_0 \in C^\infty(\mathbf{R})$ satisfying the following conditions: $0 \leqslant \chi_0(\lambda) \leqslant 1$ for all $\lambda \in \mathbf{R}$, and $\chi_0(\lambda)=1$ if $\lambda \leqslant 1$, $\chi_0(\lambda)=0$ if $\lambda \geqslant 4$, moreover, for each multi-index α, $|\partial_\lambda^\alpha \chi_0(\lambda)| \leqslant C_\alpha$ for some $C_\alpha > 0$, independent of λ. For each positive integer n, set

$$\chi_n(x,t) = \chi_0(\xi_n(x,t))$$

where

$$\xi_n(x,t) = \frac{x^2+(t+n^2)^2}{n^2}.$$

Note that $\operatorname{supp} \chi_n \cap \operatorname{supp} \chi_{n+3} = \varnothing$ for all $n \geqslant 1$.

Lemma 4.1: Let χ_n be as above. We have the estimate

$$\|D_t\chi_n\| + \|D_t^2\chi_n\| + \|e^t(D_x\chi_n)\| + \|e^{2t}(D_x^2\chi_n)\| \leqslant C$$

for some $C>0$ independent of $n \geqslant 1$.

Proof: By a direct computation, we have

$$\begin{aligned}
\partial_x\chi_n(x,t) &= \frac{2x}{n^2}\chi_0^{(1)}(\xi_n(x,t)),\\
\partial_x^2\chi_n(x,t) &= \frac{2}{n^2}\chi_0^{(1)}(\xi_n(x,t)) + 4\left(\frac{x}{n^2}\right)^2\chi_0^{(2)}(\xi_n(x,t)),\\
\partial_t\chi_n(x,t) &= \frac{2(t+n^2)}{n^2}\chi_0^{(1)}(\xi_n(x,t)),\\
\partial_t^2\chi_n(x,t) &= \frac{2}{n^2}\chi_0^{(1)}(\xi_n(x,t)) + 4\left(\frac{t+n^2}{n^2}\right)^2\chi_0^{(2)}(\xi_n(x,t)),
\end{aligned} \tag{4.1}$$

where $\chi^{(k)}$ denotes the derivative $(d^k/d\lambda^k)\chi_0$.

For each integer $k \geqslant 0$, we have

$$\|\chi_0^{(k)}(\xi_n(\cdot,\cdot))\|^2 = \int\int \left|\chi_0^{(k)}\left(\frac{x^2+(t+n^2)^2}{n^2}\right)\right|^2 dxdt = n^2\int\int |\chi_0^{(k)}(u^2+v^2)|^2 dudv \leqslant C_k n^2, \tag{4.2}$$

where we changed the variables $u=x/n$ and $v=(t+n^2)/n$ in the second equality, and the constant $C_k>0$ is independent of n.

Since $x^2+(t+n^2)^2\leqslant(2n)^2$ holds on supp $\partial^\alpha\chi_n$ for $|\alpha|\geqslant 1$, we observe that

$$|x|/n^2\leqslant\frac{2}{n},\quad |t+n^2|/n^2\leqslant\frac{2}{n} \tag{4.3}$$

on the region.

Then it follows from (4.1)–(4.3) that

$$\|D_t\chi_n\|\leqslant\frac{C}{n}\|\chi_0^{(1)}(\xi_n(\cdot,\cdot))\|\leqslant C,$$

$$\|D_t^2\chi_n\|\leqslant\frac{C}{n^2}(\|\chi_0^{(1)}(\xi_n(\cdot,\cdot))\|+\|\chi_0^{(2)}(\xi_n(\cdot,\cdot))\|)\leqslant C/n,$$

$$\|e^t(D_x\chi_n)\|\leqslant\frac{C}{n}\left(\sup_{|t+n^2|\leqslant 2n}e^t\right)\|\chi_0^{(1)}(\xi_n(\cdot,\cdot))\|\leqslant Ce^{2n-n^2}\leqslant C,$$

$$\|e^{2t}(D_x^2\chi_n)\|\leqslant\frac{C}{n^2}\left(\sup_{|t+n^2|\leqslant 2n}e^{2t}\right)(\|\chi_0^{(1)}(\xi_n(\cdot,\cdot))\|+\|\chi_0^{(2)}(\xi_n(\cdot,\cdot))\|)\leqslant\frac{C}{n}e^{2(2n-n^2)}\leqslant C.$$

This shows the lemma. ■

Lemma 4.2: Let $B_1^\sharp$ be as in Lemma 3.5 and let χ_n be as above. We have

$$\lim_{n\to\infty}\sup_{(x,t)\in\operatorname{supp}\chi_n}|B_1^\sharp(x,t;2n-n^2)|=0.$$

Proof: Due to (B), for each $\varepsilon>0$, we can find $y_0>0$ such that

$$\sup_{x\in R,0<y<y_0}|B_1(x,y)|<\frac{\varepsilon}{2}. \tag{4.4}$$

If we choose n so large that $2n-n^2<\log y_0$, then we have

$$\begin{aligned}
\sup_{\operatorname{supp}\chi_n}|B_1^\sharp(x,t;2n-n^2)| &\leqslant\sup_{x\in R}\sup_{|t+n^2|\leqslant 2n}\left|e^t\int_t^{2n-n^2}e^{-s}B_1(x,e^s)ds\right|\\
&\leqslant\sup_{x\in R}\sup_{|t+n^2|\leqslant 2n}\left|\sup_{|t'+n^2|\leqslant 2n}B_1(x,e^{t'})e^t\int_t^{2n-n^2}e^{-s}ds\right|\\
&\leqslant\sup_{x\in R}\left(\sup_{t'\leqslant 2n-n^2}B_1(x,e^{t'})\right)\sup_{t\leqslant 2n-n^2}e^t|e^{-t}-e^{-2n+n^2}|\\
&<\left(\frac{\varepsilon}{2}\right)\times 2=\varepsilon,
\end{aligned}$$

where we used (4.4) in the last inequality. ■

Lemma 4.3: We have the inclusion $[B_0^2+\frac{1}{4},\infty)\subset\sigma_{\mathrm{ess}}(H_{B_0})$.

Proof: Let $g(\cdot;t_0)$ be as in Lemma 3.5 and let χ_n be as above. For each $n\geqslant 1$ and for each $\kappa\in\mathbf{R}$, set $\psi_n(x,t)=g(x,t;2n-n^2)e^{i\kappa t}\chi_n(x,t)$. Without loss of generality, we may assume that the sequence $\{\psi_n/\|\psi_n\|\}_n$ is orthonormal, for the original sequence contains an orthonormal subsequence by the definition of χ_n's. We show that the sequence satisfies the assumption in Lemma 2.2. We have from (4.2) that

$$\|\psi_n\| = \|\chi_n\| = n\left(\int \int |\chi_0(u^2+v^2)|^2 du dv \right)^{1/2} \geqslant Cn \tag{4.5}$$

for some $C>0$.

In this proof, we denote the functions $B_1^\sharp(\cdot;2n-n^2)$ and $g(x,t;2n-n^2)$ simply by $B_1^\sharp$ and g, respectively. It follows from Lemma 3.5 that

$$e^{-g} L_{B_0} \psi_n = e^{2t}\left(D_x - \frac{B_0+B_1^\sharp}{e^t} \right)^2 (e^{i\kappa t}\chi_n) + \left(D_t^2 + \frac{1}{4} \right)(e^{i\kappa t}\chi_n). \tag{4.6}$$

On the other hand, we have

$$(D_t^2+\tfrac{1}{4})(e^{i\kappa t}\chi_n) = (\kappa^2+\tfrac{1}{4})(e^{i\kappa t}\chi_n) + \kappa e^{i\kappa t}(D_t\chi_n) + e^{i\kappa t}(D_t^2\chi_n), \tag{4.7}$$

and since

$$\begin{aligned} e^{2t}\left(D_x - \frac{B_0+B_1^\sharp}{e^t} \right)^2 &= (e^t D_x - (B_0+B_1^\sharp))^2 \\ &= (e^t D_x - (B_0+B_1^\sharp))((e^t D_x - B_0) - B_1^\sharp) \\ &= e^{2t} D_x^2 - (2B_0+B_1^\sharp) e^t D_x - B_0(B_0+B_1^\sharp) - (e^t D_x - (B_0+B_1^\sharp)) B_1^\sharp, \end{aligned}$$

we have

$$\begin{aligned} e^{2t}\left(D_x - \frac{B_0+B_1^\sharp}{e^t} \right)^2 (e^{i\kappa t}\chi_n) &= e^{i\kappa t} e^{2t}(D_x^2\chi_n) - (2B_0+B_1^\sharp) e^{i\kappa t} e^t (D_x\chi_n) - (B_0^2 + B_0 B_1^\sharp)(e^{i\kappa t}\chi_n) \\ &\quad - (e^t D_x - (B_0+B_1^\sharp)) B_1^\sharp (e^{i\kappa t}\chi_n). \end{aligned} \tag{4.8}$$

Then it follows from (4.6)–(4.8) that

$$\begin{aligned} e^{-ig}(L_{B_0} - (B_0^2 + \tfrac{1}{4} + \kappa^2))\psi_n &= e^{i\kappa t} e^{2t}(D_x^2\chi_n) - 2B_0 e^{i\kappa t} e^t (D_x\chi_n) + \kappa e^{i\kappa t}(D_t\chi_n) + e^{i\kappa t}(D_t^2\chi_n) \\ &\quad - e^{i\kappa t} B_1^\sharp e^t (D_x\chi_n) + B_0 B_1^\sharp (e^{i\kappa t}\chi_n) \\ &\quad - (e^t D_x - (B_0+B_1^\sharp)) B_1^\sharp (e^{i\kappa t}\chi_n), \end{aligned}$$

from which we have

$$\begin{aligned} \|(L_{B_0}+1)^{-1}(L_{B_0} - (B_0^2+\tfrac{1}{4}+\kappa^2))\psi_n\| &= \|e^{-ig}(L_{B_0}+1)^{-1} e^{ig} e^{-ig}(L_{B_0} - (B_0^2+\tfrac{1}{4}+\kappa^2)) e^{ig}(e^{i\kappa t}\chi_n)\| \\ &\leqslant \|e^{2t}(D_x^2\chi_n)\| + 2B_0\|e^t(D_x\chi_n)\| + |\kappa|\|D_t\chi_n\| + \|D_t^2\chi_n\| \\ &\quad + \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| \|e^t(D_x\chi_n)\| + B_0 \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| \|\psi_n\| \\ &\quad + \|(L_{B_0}+1)^{-1}(e^t D_x - (B_0+B_1^\sharp))\| \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| \|\psi_n\| \\ &\leqslant C + C \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| + C \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| \|\psi_n\| \end{aligned} \tag{4.9}$$

holds for some $C>0$ independent of n, where we used Lemma 3.3 in the second inequality.

Then we can deduce from (4.5), (4.9) and Lemma 4.2 that

$$\|(L_{B_0}+1)^{-1}(L_{B_0}-(B_0^2+\tfrac{1}{4}+\kappa^2))\psi_n\|/\|\psi_n\| \leqslant C/n + C \sup_{\operatorname{supp}\chi_n} |B_1^\sharp| \to 0$$

as $n\to\infty$. This proves the lemma. ■

Lemma 4.4: Let $B_1^\natural$ be as in (3.2). We have, on $C_0^\infty(\mathbf{H})$,

$$-(1-2B_0)y(D_x - B_1^\natural/y) \geqslant -H_{B_0} + B_0^2 + \tfrac{1}{4} + B_1.$$

Proof: We have, on $C_0^\infty(\mathbf{H})$,

$$\begin{aligned}
0 &\leqslant (A_{B_0}+B_0-\tfrac{1}{2})^*(A_{B_0}+B_0-\tfrac{1}{2}) \\
&= A_{B_0}^* A_{B_0} + (B_0-\tfrac{1}{2})(A_{B_0}^* + A_{B_0}) + (B_0-\tfrac{1}{2})^2 \\
&= A_{B_0}^* A_{B_0} + \left(B_0-\frac{1}{2}\right)\left(2y\left(D_x - \frac{B_0+B_1^\natural}{y}\right)+1\right) + \left(B_0-\frac{1}{2}\right)^2 \\
&= A_{B_0}^* A_{B_0} + \left(B_0-\frac{1}{2}\right)\left(2y\left(D_x - \frac{B_1^\natural}{y}\right)-(2B_0-1)\right) + \left(B_0-\frac{1}{2}\right)^2 \\
&= A_{B_0}^* A_{B_0} + (2B_0-1)y\left(D_x - \frac{B_1^\natural}{y}\right) - 2\left(B_0-\frac{1}{2}\right)^2 + \left(B_0-\frac{1}{2}\right)^2 \\
&= H_{B_0} - (B_0+B_1) + (2B_0-1)y\left(D_x - \frac{B_1^\natural}{y}\right) - \left(B_0-\frac{1}{2}\right)^2 \\
&= H_{B_0} - B_0^2 - \tfrac{1}{4} - B_1 + (2B_0-1)y(D_x - B_1^\natural/y).
\end{aligned}$$

This implies the lemma. ■

Lemma 4.5: Let $0\leqslant B_0 < \frac{1}{2}$. We have, on $C_0^\infty(\mathbf{H})$,

$$H_{B_0} - 2B_0B_1 \geqslant B_0^2 + \tfrac{1}{4}. \tag{4.10}$$

In particular, we have $\sigma_{\mathrm{ess}}(H_{B_0}) = [B_0^2+\frac{1}{4}, \infty)$ in case $0\leqslant B_0 \leqslant \frac{1}{2}$.

Proof: If $0\leqslant B_0 < \frac{1}{2}$, we have

$$\begin{aligned}
H_{B_0} &= y^2(D_x - (B_0+B_1^\natural)/y)^2 + y^2D_y^2 \\
&= y^2(D_x - B_1^\natural/y)^2 - 2B_0y(D_x - B_1^\natural/y) + B_0^2 + (yD_y + i/2)^*(yD_y+i/2) + \tfrac{1}{4} \\
&\geqslant -2B_0y(D_x - B_1^\natural/y) + B_0^2 + \tfrac{1}{4} \\
&\geqslant \frac{2B_0}{1-2B_0}\left(-H_{B_0} + B_0^2 + \frac{1}{4} + B_1\right) + B_0^2 + \frac{1}{4},
\end{aligned}$$

where we used (3.5) in the second equality and used Lemma 4.4 in the second inequality. Hence we have

$$\frac{1}{1-2B_0}H_{B_0} \geqslant \frac{2B_0}{1-2B_0}\left(B_0^2+\frac{1}{4}\right) + B_0^2 + \frac{1}{4} + \frac{2B_0}{1-2B_0}B_1,$$

from which (4.10) follows.

If $0\leqslant B_0 < \frac{1}{2}$, it follows from (4.10) and Lemma 3.10 that

$$\sigma_{\mathrm{ess}}(H_{B_0}) = \sigma_{\mathrm{ess}}(H_{B_0} - 2B_0B_1) \subset \sigma(H_{B_0} - 2B_0B_1) \subset [B_0^2+\tfrac{1}{4}, \infty).$$

For the case $B_0=\frac{1}{2}$, it follows from Lemma 3.2 that

$$H_{B_0}=A_{B_0}^{*}A_{B_0}+B\geqslant B=\tfrac{1}{2}+B_1.$$

Then, again by Lemma 3.10 we have

$$\sigma_{\mathrm{ess}}(H_{B_0})=\sigma_{\mathrm{ess}}(H_{B_0}-B_1)\subset\sigma(H_{B_0}-B_1)\subset[\tfrac{1}{2},\ \infty)=[(\tfrac{1}{2})^2+\tfrac{1}{4},\ \infty).$$

The converse inclusion holds for an arbitrary B_0 by Lemma 4.3. ■

V. THE BOTTOM OF $\sigma_{\mathrm{ess}}(H_{B_0})$ IF $B_0>1$

In this section, we assume that $B_0>1$ and show that the bottom of $\sigma_{\mathrm{ess}}(H_{B_0})$ is the point B_0. We follow the same line of argument as in Sec. 3 in Shigekawa (1991).

We decompose B as $B=B^{(1)}+B^{(2)}$ so that both $B^{(1)}$ and $B^{(2)}$ are real-valued smooth functions on $\mathbf{H}$, $\inf B^{(1)}>1$ and the support of $B^{(2)}$ is compact. For $j=1,2$, let $W^{(j)}$ be a real-valued, C^2-solution to the equation

$$y^2(\partial_x^2+\partial_y^2)W^{(j)}=B^{(j)}\quad\text{on }\mathbf{H}. \tag{5.1}$$

Such solutions do exist since the global solvability of elliptic partial differential equation guarantees distributional ones (See, Hörmander, 1963, Theorem 3.6.4 and Corolary 3.7.1) and then the elliptic regularity yields smoothness. In addition, we may assume that $W^{(2)}$ is bounded function on $\mathbf{H}$ because of the compactness of support of $B^{(2)}$.

We set

$$W=W^{(1)}+W^{(2)}$$

and introduce the space

$$\mathcal{A}_W=\{h\,|\,h\text{ is holomorphic in }\mathbf{H}\text{ and }he^{-W}\in L^2(H)\}.$$

Lemma 5.1: Let W be as above. Set $\mathbf{c}=(c_1,c_2)=(-\partial_y W,\partial_x W)$. Then we have

$$y^2 d\mathbf{c}=y^2(\partial_x^2+\partial_y^2)W=B,\quad \overline{\partial}_z W=-\frac{i}{2}(c_1+ic_2),$$

where $\overline{\partial}_z=\frac{1}{2}(\partial_x+i\partial_y)$.

Proof: The lemma follows easily from the definitions and the usual gauge transform gives the unitary equivalence. ■

The lemma above implies that H_{B_0} is unitarily equivalent to the operator $H(\mathbf{c})$ of the form (1.1), since both $\mathbf{a}$ and $\mathbf{c}$ give the same magnetic field. Then we may assume that $\mathbf{a}=\mathbf{c}$ without loss of generality.

Lemma 5.2: Let $\mathcal{A}_W$ be as above. Then dim $\mathcal{A}_W=\infty$ if $B_0>1$.

Proof: We transfer the problem to the one on the Poincaré disc $\mathbf{D}=\{w=(u,v)=re^{i\theta}|\ |w|=r<1,\ 0\leqslant\theta<2\pi\}$ endowed with the standard measure

$$d\mu_D=\frac{4rdrd\theta}{(1-r^2)^2}$$

and let $Ez=(z-i)(z+i)^{-1}$ denote the Cayley transform, which defines an isometric isomorphism from $\mathbf{H}$ to $\mathbf{D}$. In the end of this proof, for any function f on $\mathbf{H}$, we denote the function $f(E^{-1}\cdot)$ on $\mathbf{D}$ by $\tilde{f}$ for simplicity.

Then the Laplace equation (5.1) is equivalent to

$$\tfrac{1}{4}(1-r^2)^2(\partial_u^2+\partial_v^2)\widetilde{W^{(j)}}=\widetilde{B^{(j)}} \quad \text{on } \mathbf{D}.$$

Set

$$\varphi=2\widetilde{W^{(1)}}+2\log(1-r^2)$$

and introduce the function space

$$\tilde{\mathcal{A}}=\{\tilde{h}\mid \ \tilde{h} \text{ is holomorphic in } \mathbf{D} \text{ and } \tilde{h}e^{-\varphi/2}(1+r^2)^{3/2}\in L^2(\mathbf{D})\}$$

and set $\mathcal{A}=\{h\mid \tilde{h}\in\tilde{\mathcal{A}}\}$. Clearly the space $\mathcal{A}$ is isomorphic to $\tilde{\mathcal{A}}$ via the Cayley transform E.

Using the assumption $B_0>1$, we have

$$(\partial_u^2+\partial_v^2)\varphi=\frac{8\widetilde{B^{(1)}}}{(1-r^2)^2}+2\left(\partial_r+\frac{1}{r}\right)\partial_r(\log(1-r^2))=\frac{8}{(1-r^2)^2}(\widetilde{B^{(1)}}-1)>0.$$

This shows that φ is a subharmonic function, from which we conclude that the space $\tilde{\mathcal{A}}$ has infinite dimension by Hörmander (1966), Theorem 4.4.4.

On the other hand, the inequality

$$\int_D|\tilde{h}(w)|^2e^{-2\tilde{W}(w)}d\mu_D(w)=\int_D|\tilde{h}(w)|^2e^{-\varphi(w)}(1+r^2)^{-3}(1+r^2)^3e^{-2\widetilde{W^{(2)}}}dudv$$

$$\leqslant\int_D|\tilde{h}(w)|^2e^{-\varphi(w)}(1+r^2)^{-3}dudv$$

holds for all $\tilde{h}\in\tilde{\mathcal{A}}$, where we used the boundedness of $W^{(2)}$ and of $\mathbf{D}$. Thus we can deduce that the inclusion $\mathcal{A}\subset\mathcal{A}_W$ holds, from which the lemma follows. ■

Lemma 5.3: For $B_0>1$, we have $B_0\in\sigma_{\text{ess}}(H_{B_0})$.

Proof: We denote by H_{dist}, A_{dist} and $A_{\text{dist}}^{\dagger}$ the differential operators of the forms (1.1), (3.6) and (3.7) acting on the space of distributions, respectively.

Let $\{h_n\}_{n=1}^{\infty}$ be an orthogonal family of elements in the space $\mathcal{A}_W$ and set $\varphi_n=e^{-W}h_n$. Then it follows from Lemma 5.1 that

$$A_{\text{dist}}\varphi_n=0,$$

since

$$A_{B_0}=-2iy\overline{\partial_z}-y(a_1+ia_2)$$

and h_n is holomorphic and satisfies $\overline{\partial_z}h_n=0$.

The integration by parts yields that, for any $\psi\in C_0^{\infty}(\mathbf{H})$,

$$(\varphi_n,\ (H_{B_0}-B)\psi)=((H_{\text{dist}}-B)\varphi_n,\ \psi)=(A_{\text{dist}}^{\dagger}A_{\text{dist}}\varphi_n,\ \psi)=0. \tag{5.2}$$

Due to Lemma 1.1, the relation (5.2) holds also for all $\psi\in D(H_{B_0})$, from which we deduce that $\varphi_n\in D(H_{B_0})$ and

$$(H_{B_0}-B_1)\varphi_n=B_0\varphi_n. \tag{5.3}$$

Thus $B_0\in\sigma_e(H_{B_0}-B_1)$.

On the other hand, it follows from Lemma 3.10 that

$$\sigma_e(H_{B_0})=\sigma_e(H_{B_0}-B_1).$$

This completes the proof. ■

VI. PROOF OF THEOREM 1.2

We first show that the theorem holds when B_0 is contained in some subset of $\mathbf{R}$ by combining the shape invariance and the results obtained in the previous sections. Then, using the norm resolvent continuity of H_{B_0} with respect to B_0, we extend the validity to the case of general B_0.

In what follows, for any $k\in\mathbf{R}$ and for any $S\subset\mathbf{R}$, we denote the set $\{s+k|s\in S\}$ by $S+k$.

Lemma 6.1: Let $\sigma_L(B_0)$ be the set as in (4). Then we have

$$\sigma_L(B_0)+2(B_0+1)-1=\sigma_L(B_0+1)\backslash\{B_0+1\}.$$

Proof: By the definition (1.4), we have

$$\begin{aligned}\sigma_L(B_0)+2(B_0+1)-1&=\bigcup_{l=0}^{N(B_0)}\{(2l+1)B_0-l(l+1)+2(B_0+1)-1\}\\&=\bigcup_{l=0}^{N(B_0)}\{(2l+3)(B_0+1)-l^2-3l-2\}\\&=\bigcup_{m=1}^{N(B_0)+1}\{(2m+1)(B_0+1)-m(m+1)\}=\sigma_L(B_0+1)\backslash\{B_0+1\},\end{aligned}$$

where we used the fact that $N(B_0)+1=N(B_0+1)$ if $B_0>0$ and changed the variable $m=l+1$ in the third equality. ■

Lemma 6.2: If $B_0>1$, we have

$$\sigma_{\mathrm{ess}}(H_{B_0})=\sigma_{\mathrm{ess}}(H_{B_0-1}+(2B_0-1))\cup\{B_0\}$$

and, if $\frac{1}{2}<B_0\leqslant 1$, we have

$$\sigma_{\mathrm{ess}}(H_{B_0})\backslash\{B_0\}=[B_0^2+\tfrac{1}{4},\ \infty).$$

Proof: From Lemma 3.2 (i) and Lemma 3.10, we have

$$\sigma_{\mathrm{ess}}(H_{B_0})=\sigma_{\mathrm{ess}}(H_{B_0}-B_1)=\sigma_{\mathrm{ess}}(A_{B_0}^*A_{B_0}+B_0). \tag{6.1}$$

It follows from Lemmas 3.2 (ii) and 2.1 that the set (6.1) coincides, except perhaps at B_0, with the set

$$\sigma_{\mathrm{ess}}(A_{B_0}A_{B_0}^*+B_{\hat{0}})=\sigma_{\mathrm{ess}}(H_{B-1}(\mathbf{b})+(2B_0-1)).$$

Then the lemma follows from Lemmas 4.5 and 6.2. ■

Lemma 6.3: For each positive integer k, set

$$I_k=\{x\in\mathbf{R}|\ \ k<x\leqslant k+\tfrac{1}{2}\}.$$

Then, the conclusion of Theorem 1.2 is valid if $B_0\in\cup_{k\geqslant 0}I_k$.

Proof: By mathematical induction on k, we show the following propositions $P(k)$:

$$\sigma_{\mathrm{ess}}(H_{B_0})=[B_0^2+\tfrac{1}{4},\ \infty)\cup\sigma_L(B_0)\quad\text{holds if}\ B_0\in I_k.$$

When $k=1$, we have, from Lemma 6.2,

$$\begin{aligned}\sigma_{\mathrm{ess}}(H_{B_0})&=\sigma_{\mathrm{ess}}(H_{B_0-1}+2B_0-1)\cup\{B_0\}\\&=[(B_0-1)^2+\tfrac{1}{4}+2B_0-1,\ \infty)\cup\{B_0\}\\&=[B_0^2+\tfrac{1}{4},\ \infty)\cup\{B_0\}=[B_0^2+\tfrac{1}{4},\ \infty)\cup\sigma_L(B_0),\end{aligned}$$

where we used the fact that $|B_0-1|<\frac{1}{2}$ in the second equality.

Assume that $P(k)$ holds. By Lemma 6.1, we have

$$\begin{aligned}\sigma_{\mathrm{ess}}(H_{B_0+1})&=\sigma_{\mathrm{ess}}(H_{B_0}+2(B_0+1)-1)\cup\{B_0+1\}\\&=[B_0^2+\tfrac{1}{4}+2(B_0+1)-1,\ \infty)\cup(\sigma_L(B_0)+2(B_0+1)-1)\cup\{B_0+1\}\\&=[(B_0+1)^2+\tfrac{1}{4},\ \infty)\cup\sigma_L(B_0+1),\end{aligned}$$

where we used $P(k)$ in the second equality and used Lemma 6.2 in the last. This shows the validity of $P(k+1)$, hence the proof is completed. ■

Let I denote the open interval $(\frac{1}{2},\frac{3}{2})$ which is equipped with the usual relative topology induced from $\mathbf{R}$. We introduce the set

$$S=\{B_0\in I\,|\,B_0\in\sigma_{\mathrm{ess}}(H_{B_0})\}$$

and denote the complement set of S in I by S^c.

Lemma 6.4: Let S be as above. Then we have

(i) S is a closed set in I.

(ii) For any $x\in S$ and any $\varepsilon>0$, there exists $y\in S$ such that $x-\varepsilon<y<x$.

Proof: Assume that $x_n\in S$, $x\in I$ and $x_n\to x$ as $n\to\infty$. Then, owing to Lemma 3.4, we can apply Lemma 2.3 to $A=H_x$, $A_n=H_{x_n}$ and deduce that

$$\|P_{(x-\delta,\,x+\delta)}(H_x)-P_{(x-\delta,\,x+\delta)}(H_{x_n})\|\to 0$$

as $n\to\infty$ for any $\delta>0$ satisfying $x\pm\delta\in\mathbf{R}\backslash\sigma(H_x)$. Taking the fact that the dimension of range of $P_{(x-\delta,\,x+\delta)}(H_{x_n})$ is infinite for large n into account, we have the same conclusion for $P_{(x-\delta,\,x+\delta)}(H_{x_n})$, since the ranges of two orthogonal projections P, Q have same dimension if $\|P-Q\|<1$. Then the assertion (i) follows from the definition of the essential spectrum (Reed and Simon, 1978, Vol. I, p. 236).

We show (ii) by contradiction. Assume that there exists $x\in S$ and $\varepsilon>0$ such that $[x-\varepsilon,\,x)\subset S^c$. Applying Lemma 2.3 to $A_n=H_{x-\varepsilon/n}$, $A=H_x$ and $\Sigma_n=(x-\varepsilon/n)^2+\frac{1}{4}$, we have $\sigma_{\mathrm{ess}}(H_x)=[x^2+\frac{1}{4},\infty)$. This contradicts the assumption $x\in S$, for $x<x^2+\frac{1}{4}$ if $x\in I$. ■

First we claim that S^c is an empty set. We show this by contradiction. Assume that S^c is not empty. Note that the fact that $(1,\frac{3}{2})\subset S$. The set S^c contains a connected component (α,β) with $\alpha<\beta\leqslant 1$, since S^c is open in I by Lemma 6.4 (i). Then the maximality of (α,β) implies that $\beta\in S$. By Lemma 6.4 (ii), this contradicts the connectedness of (α,β). This proves the claim.

Then, if $\frac{1}{2}<B_0\leqslant 1$, we can deduce that

$$\sigma_{\mathrm{ess}}(H_{B_0})=\{B_0\}\cup[B_0^2+\tfrac{1}{4},\infty),\tag{6.2}$$

since Lemma 6.2 ensures that the possible point of $\sigma_{\mathrm{ess}}(B_0)$ below the continuous spectrum is the point B_0.

Finally, repeating the same argument as in Lemma 6.3, we can deduce from Lemma 5.3 and (6.2) that Theorem 1.2 is true for all B_0.

ACKNOWLEDGMENT

The authors would like to thank Professor Hiroyuki Matsumoto for bringing this problem to their attention and for his helpful advice.

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Noncommutative geometry of angular momentum space $U(\mathfrak{su}(2))$

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(Received 13 August 2002; accepted 3 September 2002)

We study the standard angular momentum algebra $[x_i,x_j]=\imath\lambda\epsilon_{ijk}x_k$ as a noncommutative manifold $\mathbb{R}^3_\lambda$. We show that there is a natural 4D differential calculus and obtain its cohomology and Hodge $*$ operator. We solve the spin 0 wave equation and some aspects of the Maxwell or electromagnetic theory including solutions for a uniform electric current density, and we find a natural Dirac operator $\partial\!\!\!/$. We embed $\mathbb{R}^3_\lambda$ inside a 4D noncommutative space–time which is the limit $q\to 1$ of q-Minkowski space and show that $\mathbb{R}^3_\lambda$ has a natural quantum isometry group given by the quantum double $\mathbb{C}(\mathrm{SU}(2))\bowtie \mathrm{U}(\mathfrak{su}(2))$ which is a singular limit of the q-Lorentz group. We view $\mathbb{R}^3_\lambda$ as a collection of all fuzzy spheres taken together. We also analyze the semiclassical limit via minimum uncertainty states $|j,\theta,\phi\rangle$ approximating classical positions in polar coordinates. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1517395]

I. INTRODUCTION

There has been much interest in recent years in the possibility that classical space or space–time itself (not only phase space) is in fact noncommutative and not a classical manifold. One simple model where

$$[x_i,t]=\imath\lambda x_i \tag{1}$$

has already been shown[3] to have physically measurable effects even if $\lambda\sim 10^{-44}$ s (the Planck time). So such a conjecture is not out of reach of experiment *even if* the noncommutativity is due to quantum gravity effects. Such noncommutativity of space–time, if verified, would amount to a new physical effect which could be called ''cogravity'' because it corresponds under non Abelian Fourier transform to curvature in momentum space.[17] We are usually familiar with this correspondence the other way around, i.e., on a curved space such as a sphere the canonical momenta (angular momentum) form a noncommutative algebra

$$[J_a,J_b]=\imath\epsilon_{abc}J_c,\quad a,b,c=1,2,3, \tag{2}$$

where ϵ_{abc} denotes the totally antisymmetric tensor; if one believes in Born reciprocity, then one should also allow the theoretical possibility of a sphere in momentum space, which would correspond to the algebra

$$[x_a,x_b]=\imath\lambda\epsilon_{abc}x_c. \tag{3}$$

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This is the algebra $\mathbb{R}^3_\lambda$ which we study in this article from the point of view of the x_i as coordinates of a noncommutative position space. We insert here a parameter λ of length dimension. The physical relevance of this algebra hardly needs to be justified, but we note some specific applications in string theory and quantum gravity in the discussion below. There are also possible other contexts where a noncommutative space–time might be a good effective model, not necessarily connected with gravity and indeed this is an entirely independent (dual) effect.

Also from a mathematical point of view, the algebra (3) is a standard example of a formal deformation quantization, namely of the Kirillov–Kostant Poisson bracket on $\mathfrak{su}_2^*$ in the coadjoint orbit method.[12] We identify $\mathfrak{su}(2)^*$ as the vector space $\mathbb{R}^3$ with basis J_a^*, say, dual to the J_a. Then among the algebra of suitable (polynomial) functions $\mathbb{C}(\mathbb{R}^3)$ on it we identify the J_a themselves with the ''coordinate functions'' $J_a(v)=v_a$ for any $v\in\mathfrak{su}(2)^*$ with component v_a in the J_a^* direction. These generate the whole coordinate algebra and their Poisson bracket is defined by

$$\{J_a,J_b\}(v)=v([J_a,J_b]),\quad \forall v\in\mathfrak{su}(2)^*.$$

Hence when viewed as functions on $\mathbb{R}^3$, the Lie algebra generators have a Poisson bracket given by the Lie bracket. Their standard ''quantization'' is evidently provided by (3) with deformation parameter λ.

Our goal in the present work is to use modern quantum group methods to take this further by developing the noncommutative differential geometry of this quantum space at the level of scaler fields, forms, and spinors, i.e., classical field theory. We will solve wave equations, etc., and generally show that physics is fully possible on $\mathbb{R}^3_\lambda$. Note that the earlier example (1) above was also of ''dual Lie'' type but there the Lie algebra was solvable whereas the $\mathfrak{su}(2)$ case that we address here is at the other extreme and very much harder to work with. We expect our methods to extend also to $\mathrm{U}(g)$ for other simple g.

The article begins in Sec. II with some mathematical preliminaries on quantum group methods and noncommutative geometry. As a quantum group, $\mathbb{R}^3_\lambda\cong\mathrm{U}(\mathfrak{su}(2))$ (the enveloping Hopf algebra) which means that at the end of the day all computations can be reduced to the level of $\mathfrak{su}(2)$ and Pauli matrices. One of the first things implied by quantum group theory is that $\mathbb{R}^3_\lambda$ has an isometry quantum group given by the Drinfeld quantum double $D(\mathrm{U}(\mathfrak{su}(2)))$ and we describe this first, in Sec. III. A suitable Casimir of this induces a scalar wave operator $\Box$ and we also describe spherical harmonics Y_l^m dictated by action of rotations. This theory could be called the ''level 0'' noncommutative geometry where we think of the space through its symmetries rather than its differential structure.

In Sec. IV we start the noncommutative differential geometry, introducing a natural differential calculus on $\mathbb{R}^3_\lambda$. The cotangent directions or basic forms are given literally by Pauli matrices plus an additional generator θ:

$$\mathrm{d}x_a=\tfrac{1}{2}\sigma_a,\quad \theta=\sigma_0, \tag{4}$$

where $\sigma_0=\mathrm{id}$ (the identity matrix). There are also noncommutation relations between functions and one-forms:

$$x_a\mathrm{d}x_b=(\mathrm{d}x_b)x_a+\frac{\imath\lambda}{2}\epsilon_{abc}\mathrm{d}x_c+\frac{\lambda}{4}\delta_{ab}\theta,\quad x_a\theta=\theta x_a+\lambda\,\mathrm{d}x_a. \tag{5}$$

Some other calculi are mentioned in the Appendix for comparison, but in fact this four-dimensional one appears to be the most reasonable one. The extra θ direction turns out to generate the cohomology, i.e., is not d of anything in $\mathbb{R}^3_\lambda$. We interpret it as a local time direction in the same spirit as in a different model.[9]

In Sec. V we introduce a Hodge * operator and solve the resulting wave equations for spin 0 and spin 1 (the Maxwell equations). We also find a natural Dirac operator for spin $\frac{1}{2}$. Among the solutions of interest are plane waves obeying

$$\Box e^{\imath k\cdot x}=-\frac{1}{\lambda^2}\left\{4\sin^2\left(\frac{\lambda|k|}{2}\right)+\left(\cos\left(\frac{\lambda|k|}{2}\right)-1\right)^2\right\}e^{\imath k\cdot x},$$

for momentum $k\in\mathbb{R}^3$. Among spin 1 solutions is a uniform electric current density in some direction and magnetic field increasing with normal distance. This is computationally the easiest case; we expect that the theory should similarly allow more conventional decaying solutions. In Sec. VI we briefly consider quantum spheres S^2_λ inside $\mathbb{R}^3_\lambda$ by setting $\Sigma_i x_i^2=1$. These are then the usual quantization of coadjoint orbits in $\mathfrak{su}(2)^*$ [as opposed to all of $\mathfrak{su}(2)^*$ as described above] and we show that they inherit a three-dimensional differential geometry. This case could be viewed as a slightly different approach to fuzzy spheres[14,5,11,20,21] that is more adapted to their classical limit $\lambda\to 0$. Fuzzy spheres also arise as world volume algebras in string theory,[2] hence it would be interesting to develop this point of contact further. In our case we obtain a 3D differential calculus on S^2_λ.

In Sec. VII we explain the origin of the θ direction as the remnant of the time direction dt of a standard four-dimensional noncommutative space–time $\mathbb{R}^{1,3}_q$ in a certain scaling limit as $q\to 1$. In the $q\neq 1$ setting the theory is much more nonsingular and there is a full q-Lorentz symmetry already covered in the q-deformation literature.[6,16,15] On the other hand, as $q\to 1$ we obtain either usual commutative Minkowski space or we can make a scaling limit and obtain the algebra

$$[x_a,x_b]=\imath ct\,\epsilon_{abc}x_c,\quad [x_a,t]=0, \tag{6}$$

where the parameter c has dimensions of velocity. Mathematically this is homogenized $\widetilde{\mathrm{U}(\mathfrak{su}(2))}$ and we see that it projects onto our above algebra (3) by sending $ct\to\lambda$. This algebra (6) is not itself a good noncommutative Minkowski space because the q-Lorentz group action becomes singular as $q\to 1$ and degenerates into an action of the above quantum double isometry group. On the other hand, it is the boundary point $q=1$ of a good and well-studied noncommutative Minkowski space.

The article concludes in Sec. VIII with a proposal for the interpretation which is needed before the noncommutative geometry can be compared with experiment. In addition to a normal ordering postulate [i.e., noncommutative $f(x)$ are compared with classical ones only when normal ordered] along the lines of Ref. 3, we also propose a simple quantum mechanical point of view inspired by Penrose's spin network theorem.[19] In our case we construct minimum uncertainty states $|j,\theta,\phi\rangle$ for each spin j in which expectations $\langle f(x)\rangle$ behave approximately like classical functions in polar coordinates r,θ,ϕ with $r=\lambda j$. In effect we view $\mathbb{R}^3_\lambda$ as a collection of fuzzy spheres for all spins j taken together. There are some similarities also with the star product and coherent states discussed recently in Ref. 11.

Finally, whereas the above includes electromagnetic theory on $\mathbb{R}^3_\lambda$, we explain now that exactly this noncommutative space is needed for a geometric picture underlying the approach to $2+1$ quantum gravity of Refs. 4 and 22. When a Euclidean signature and vanishing cosmological constant are assumed, the gauge group of the classical gravitational action (as a Chern–Simons field theory) is the group ISO(3).[23] Considering the three-dimensional space as the direct product $\Sigma\times\mathbb{R}$, where Σ is Riemann surface of genus g, one can find the space of solutions of the gravitational field in terms of the topology of Σ.[1,8] The simplest case is to consider Σ as a sphere with a puncture, which represents the topological theory of one particle coupled to gravity. It is known that the quantum states of this kind of theory correspond to irreducible representations of the quantum double $D(\mathrm{U}(\mathfrak{su}(2)))$.[4] A more detailed explanation, based on representation theory, of how the quantum double is a deformation ''quantization'' of the Euclidean group in three dimensions can be found in Ref. 22. However, the direct geometrical role of the quantum double has been missing except as an 'approximate' isometry of $\mathbb{R}^3$. Our present results therefore provide a new point of view, namely of the quantum double symmetry as an *exact* symmetry but of the noncommutative space $\mathbb{R}^3_\lambda$ on which we should build a noncommutative Chern–Simons action, etc. This fits with the discussion above that noncommutative space–time could be used as a better

effective description of corrections to geometry coming out of quantum gravity. Details of the required noncommutative Chern–Simons theory as well as gravity in the frame bundle approach of Ref. 18 will be presented in a sequel.

II. MATHEMATICAL PRELIMINARIES

Here we outline some notions from quantum group theory into which our example fits. For Hopf algebras (i.e., quantum groups) we use the conventions of Ref. 15. It means an algebra H equipped with a coproduct $\Delta: H\to H\otimes H$, counit $\epsilon: H\to\mathbb{C}$ and antipode $S: H\to H$. We will sometimes use the formal sum notation $\Delta(h)=\Sigma h_{(1)}\otimes h_{(2)}$, for any $h\in H$. The usual universal enveloping algebra algebra $\mathrm{U}(\mathfrak{su}(2))$ has a structure of cocommutative Hopf algebra generated by 1 and J_a, $a=1,2,3$ with relations (2) and

$$\Delta(J_a)=J_a\otimes 1+1\otimes J_a,\quad \epsilon(J_a)=0,\quad S(J_a)=-J_a. \tag{7}$$

We also recall that as for Abelian groups, for each Hopf algebra there is a dual one where the product of one is adjoint to the coproduct of the other. $\mathrm{U}(\mathfrak{su}(2))$ is dually paired with the commutative Hopf algebra $\mathbb{C}(\mathrm{SU}(2))$ generated by coordinate functions $t^i{}_j$, for $i,j=1,2$ on SU(2) satisfying the determinant relation $t^1{}_1t^2{}_2-t^1{}_2t^2{}_1=1$ and with

$$\Delta(t^i{}_j)=\sum_{k=1}^{2} t^i{}_k\otimes t^k{}_j,\quad \epsilon(t^i{}_j)=\delta^i{}_j,\quad St^i{}_j=t^{-1}{}^i{}_j, \tag{8}$$

where inversion is as an algebra-valued matrix. The pairing between the algebras $\mathrm{U}(\mathfrak{su}(2))$ and $\mathbb{C}(\mathrm{SU}(2))$ is defined by

$$\langle\xi,f\rangle=\frac{d}{dt}f(e^{t\xi})|_{t=0},$$

where $\xi\in\mathfrak{su}(2)$ and $f\in\mathbb{C}(\mathrm{SU}(2))$ which results in particular in

$$\langle J_a,t^i{}_j\rangle=\tfrac{1}{2}\sigma_a{}^i{}_j, \tag{9}$$

where $\sigma_a{}^i{}_j$ are the i, j entries of the Pauli matrices for $a=1,...,3$. We omit here a discussion of unitarity, but this is implicit and achieved by making the above into Hopf $*$-algebras (see Ref. 15 for further details).

We also need standard notions of actions and coactions. A left coaction of a Hopf algebra H on a space V means a map $V\to H\otimes V$ obeying axioms like those of an action but reversing all maps. So a coaction of $\mathbb{C}(\mathrm{SU}(2))$ essentially corresponds to an action of $\mathrm{U}(\mathfrak{su}(2))$ via the pairing. Examples are

$$\mathrm{Ad}_L(h)(g)=h\triangleright g=\sum h_{(1)}gS(h_{(2)}), \tag{10}$$

the left adjoint action $\mathrm{Ad}_L: H\otimes H\to H$. Its arrow-reversal is the left adjoint coaction $\mathrm{Ad}^L: H\to H\otimes H$,

$$\mathrm{Ad}^L(h)=\sum h_{(1)}S(h_{(3)})\otimes h_{(2)}. \tag{11}$$

There are also the regular action (given by the product), regular coaction (given by $\Delta: H\to H\otimes H$), and coadjoint actions and coregular actions of the dual, given via the pairing from the adjoint and regular coactions, etc.[15] We will need the left coadjoint action of H on a dual quantum group A:

$$\mathrm{Ad}_L^*(h)(\phi)=h\triangleright\phi=\sum \phi_{(2)}\langle(S\phi_{(1)})\phi_{(3)},h\rangle,\quad \forall h\in H,\quad \phi\in A, \tag{12}$$

and the right coregular action of A on H which we will view as a left action of the opposite algebra A^{op}:

$$\phi\triangleright h=\sum \langle\phi,h_{(1)}\rangle h_{(2)},\quad \forall h\in H,\quad \phi\in A. \tag{13}$$

Given a quantum group H dual to a quantum group A, there is a quantum double written loosely as $D(H)$ and containing H, A as sub-Hopf algebras. More precisely it is a double cross product $A^{\mathrm{op}}\bowtie H$ where there are cross relations given by mutual coadjoint actions.[15] Also, $D(H)$ is formally quasitriangular in the sense of a formal "universal R matrix" $\mathcal{R}$ with terms in $D(H)\otimes D(H)$. The detailed structure of $D(\mathrm{U}(\mathfrak{su}(2)))$ is covered in Sec. III and in this case is more simply a semidirect product $\mathbb{C}(\mathrm{SU}(2))\rtimes\mathrm{U}(\mathfrak{su}(2))$ by the coadjoint action.

We will also need the quantum double $D(H)$ when H is some other quasitriangular quantum group such as $\mathrm{U}_q(\mathfrak{su}(2))$. This is a standard deformation of (2) and the coproduct, etc., with a parameter q. In this case there is a second "braided" or covariantized version of $A=\mathbb{C}_q(\mathrm{SU}(2))$ which we denote by $\mathrm{BSU}_q(2)$. Then

$$D(\mathrm{U}_q(\mathfrak{su}(2)))\cong\mathrm{BSU}_q(2)\rtimes\mathrm{U}_q(\mathfrak{su}(2)), \tag{14}$$

where the product is a semidirect one by the adjoint action of $\mathrm{U}_q(\mathfrak{su}(2))$ and the coproduct is also a semidirect one. We will use this nonstandard "bosonization" version of $D(H)$ when H is quasitriangular. Also when H is quasitriangular with $\mathcal{R}_{21}\mathcal{R}$ nondegenerate, there is a third "twisting" version of the quantum double:

$$D(\mathrm{U}_q(\mathfrak{su}(2)))\cong\mathrm{U}_q(\mathfrak{su}(2))\blacktriangleright\!\!\blacktriangleleft_{\mathcal{R}}\mathrm{U}_q(\mathfrak{su}(2)), \tag{15}$$

where the algebra is a tensor product and the coproduct is

$$\Delta(h\otimes g)=\mathcal{R}_{23}^{-1}\Delta_{H\otimes H}(h\otimes g)\mathcal{R}_{23}.$$

We will use both versions in Sec. VII. Note that both isomorphisms are formal but the right hand sides are well defined and we take them as definitions. Especially, the isomorphism (15) is highly singular as $q\to 1$. In that limit the twisted version tends to U(so(1,3)) while the bosonization version tends to U(iso(3)).

Finally, we will need the notion of differential calculus on an algebra H. This is common to several approaches to noncommutative geometry including that of Connes.[7] A first order calculus means to specify (Ω^1,d), where Ω^1 is an $H-H$-bimodule, $\mathrm{d}:H\to\Omega^1$ obeys the Leibniz rule,

$$\mathrm{d}(hg)=(\mathrm{d}h)g+h(\mathrm{d}g), \tag{16}$$

and Ω^1 is spanned by elements of the form $(\mathrm{d}h)g$. A bimodule just means that one can multiply "one-forms" in Ω^1 by "functions" in H from the left or the right without caring about brackets.

When we have a Hopf algebra H, a differential calculus can be asked to be "bicovariant,"[25] which means that there are left and right coactions of H in Ω^1 (a bicomodule) which are themselves bimodule homomorphisms, and d intertwines the coactions with the regular coactions of H on itself. Given a bicovariant calculus one can find invariant forms

$$\omega(h)=\sum (\mathrm{d}h_{(1)})Sh_{(2)} \tag{17}$$

for any $h\in H$. The span of such invariant forms is a space Λ^1 and all of Ω^1 can be reconstructed from them via

$$\mathrm{d}h=\sum \omega(h_{(1)})h_{(2)}. \tag{18}$$

As a result, the construction of a differential structure on a quantum group rests on that of Λ^1, with $\Omega^1=\Lambda^1.H$. They in turn can be constructed in the form

$$\Lambda^1=\ker\ \epsilon/\mathcal{I},$$

where $\mathcal{I}\subset\ker\epsilon$ is some left ideal in H that is Ad^L-stable.[25] We will use this method in Sec. IV to introduce a reasonable calculus on $\mathrm{U}(\mathfrak{su}(2))$. Some general remarks (but not our calculus, which seems to be new) appeared in Ref. 18.

Any bicovariant calculus has a ''minimal'' extension to an entire exterior algebra.[25] One uses the universal R-matrix of the quantum double to define a braiding operator on $\Lambda^1\otimes\Lambda^1$ and uses it to ''antisymmetrize'' the formal algebra generated by the invariant forms. These and elements of H define Ω in each degree. In our case of $\mathrm{U}(\mathfrak{su}(2))$, because it is cocommutative, the braiding is the usual flip. Hence we have the usual anticommutation relations among invariant forms. We also extend $\mathrm{d}:\Omega^k\to\Omega^{k+1}$ as a (right-handed) super-derivation by

$$\mathrm{d}(\omega\wedge\eta)=\omega\wedge\mathrm{d}\eta+(-1)^{\deg\eta}\mathrm{d}\omega\wedge\eta.$$

A differential calculus is said to be inner if the exterior differentiation in Ω^1 (and hence in all degrees) is given by the (graded) commutator with an invariant one-form $\theta\in\Lambda^1$, that is,

$$\mathrm{d}\omega=\omega\wedge\theta-(-1)^{\deg\omega}\theta\wedge\omega.$$

Almost all noncommutative geometries that one encounters are inner, which is the fundamental reason that they are in many ways better behaved than the classical case.

III. THE QUANTUM DOUBLE AS EXACT ISOMETRIES OF $\mathbb{R}^3_\lambda$

In this section we first of all recall the structure of the quantum double $D(\mathrm{U}(\mathfrak{su}(2)))$ in the context of Hopf algebra theory. We will then explain its canonical action on a second copy $\mathbb{R}^3_\lambda\cong\mathrm{U}(\mathfrak{su}(2))$ arising from the general Hopf algebra theory, thereby presenting it explicitly as an exact quantum symmetry group of that. Here $x_a=\lambda J_a$ is the isomorphism valid for $\lambda\neq0$. By an exact quantum symmetry we mean that the quantum group acts on $\mathbb{R}^3_\lambda$ with the product of $\mathbb{R}^3_\lambda$ an intertwiner (i.e. the algebra is covariant).

Because $\mathrm{U}(\mathfrak{su}(2))$ is cocommutative, its quantum double $D(\mathrm{U}(\mathfrak{su}(2)))$ is a usual crossed product[15]

$$D(\mathrm{U}(\mathfrak{su}(2)))=\mathbb{C}(\mathrm{SU}(2))_{\mathrm{Ad}^*_L}\rtimes\mathrm{U}(\mathfrak{su}(2)),$$

where the action is induced by the adjoint action [it is the coadjoint action on $\mathbb{C}(\mathrm{SU}(2))$]. This crossed product is isomorphic as a vector space with $\mathbb{C}(\mathrm{SU}(2))\otimes\mathrm{U}(\mathfrak{su}(2))$ but with algebra structure given by

$$(a\otimes h)(b\otimes g)=\sum a\,\mathrm{Ad}^*_{L\,h_{(1)}}(b)\otimes h_{(2)}g,$$

for $a,b\in\mathbb{C}(\mathrm{SU}(2))$ and $h,g\in\mathrm{U}(\mathfrak{su}(2))$. In terms of the generators, the left coadjoint action (12) takes the form

$$\mathrm{Ad}^*_{L\,J_a}(t^i{}_j)=\sum t^k{}_l\langle J_a,S(t^i{}_k)t^l{}_j\rangle=\frac{1}{2}(t^i{}_k\sigma_a{}^k{}_j-\sigma_a{}^j{}_k t^k{}_j). \tag{19}$$

As a result we find that $D(\mathrm{U}(\mathfrak{su}(2)))$ is generated by $\mathrm{U}(\mathfrak{su}(2))$ and $\mathbb{C}(\mathrm{SU}(2))$ with cross relations

$$[J_a, t^i{}_j] = \tfrac{1}{2}(t^i{}_k \sigma_a{}^k{}_j - \sigma_a{}^j{}_k t^k{}_j). \tag{20}$$

Meanwhile the coproducts are the same as those of $\mathrm{U}(\mathfrak{su}(2))$ and $\mathbb{C}(\mathrm{SU}(2))$.

Next, a general feature of any quantum double is a canonical or "Schrödinger" representation, where $\mathrm{U}(\mathfrak{su}(2)) \subset D(\mathrm{U}(\mathfrak{su}(2)))$ acts on $\mathrm{U}(\mathfrak{su}(2))$ by the left adjoint action (10) and $\mathbb{C}(\mathrm{SU}(2)) \subset D(\mathrm{U}(\mathfrak{su}(2)))$ acts by the coregular one (13), see Ref. 15. We denote the acted-upon copy by $\mathbb{R}^3_\lambda$. Then J_a simply act by

$$J_a \triangleright f(x) = \lambda^{-1} \sum x_{a(1)} f(x) S(x_{a(2)}) = \lambda^{-1}[x_a, f(x)], \quad \forall f(x) \in \mathbb{R}^3_\lambda, \tag{21}$$

e.g.,

$$J_a \triangleright x_b = \imath \epsilon_{abc} x_c,$$

while the co-regular action reads

$$t^i{}_j \triangleright f(x) = \langle t^i{}_j, f(x)_{(1)} \rangle f(x)_{(2)}, \quad \text{e.g.,} \quad t^i{}_j \triangleright x_a = \frac{\lambda}{2} \sigma_a{}^i{}_j 1 + \delta^i{}_j x_a.$$

The general expression is given by a shuffle product (see Sec. IV). *With this action,* $\mathbb{R}^3_\lambda$ *turns into a left* $D(\mathrm{U}(\mathfrak{su}(2)))$*-covariant algebra.*

In order to analyze the classical limit of this action, let us consider the role of the numerical parameter λ used to define the algebra $\mathbb{R}^3_\lambda$. Considering the relations (3), we have already explained that $\mathbb{R}^3_\lambda$ becomes the usual algebra of functions on $\mathbb{R}^3$ as $\lambda \to 0$. The same parameter λ can be introduced into the quantum double by means of a redefinition of the generators of $\mathbb{C}(\mathrm{SU}(2))$ to

$$M^i{}_j = \frac{1}{\lambda}(t^i{}_j - \delta^i{}_j), \tag{22}$$

so that $t^i{}_j = \delta^i{}_j + \lambda M^i{}_j$. We stress that we are dealing with the same Hopf Algebra $D(\mathrm{U}(\mathfrak{su}(2)))$, but written in terms of new generators, it is only a change of variables. The homomorphism property of Δ gives

$$\Delta M^i{}_j = \sum_{k=1}^{2} (\delta^i{}_k \otimes M^k{}_j + M^i{}_k \otimes \delta^k{}_j + \lambda M^i{}_k \otimes M^k{}_j),$$

while the condition on the determinant, $t^1{}_1 t^2{}_2 - t^1{}_2 t^2{}_1 = 1$, implies that

$$\mathrm{Tr}(M) = M^1{}_1 + M^2{}_2 = -\lambda \det(M).$$

This means that in the limit $\lambda \to 0$, the elements $M^i{}_j$ have to obey $M^1{}_1 = -M^2{}_2$ and $\mathbb{C}(\mathrm{SU}(2))$ becomes the commutative Hopf algebra $\mathrm{U}(\mathbb{R}^3)$. To make this explicit, we can define the momentum generators

$$P_1 = -\imath(M^1{}_2 + M^2{}_1), \quad P_2 = M^1{}_2 - M^2{}_1, \quad P_3 = -\imath(M^1{}_1 - M^2{}_2), \tag{23}$$

or

$$P_a = -\imath \sigma_a{}^i{}_j M^j{}_i, \quad a = 1,2,3 \tag{24}$$

(sum over i,j). The inverse of this relationship is

$$M^i{}_j = \frac{\imath}{2} \sigma_a{}^i{}_j P_a + \delta^i{}_j P_0, \quad P_0 = \frac{1}{2}\mathrm{Tr}(M) = -\frac{1}{\lambda}\left(1 - \sqrt{1 - \frac{\lambda^2}{4} P^2}\right). \tag{25}$$

The other square root is also allowed, but then P_0 is not $\mathcal{O}(\lambda)$, i.e., this is not the "patch" of $\mathbb{C}(\mathrm{SU}(2))$ that concerns us. Note also that there are unitarity conditions that we do not explicitly discuss (if we put them in then the P_a are Hermitian). In these terms we have

$$\Delta P_a = P_a \otimes 1 + 1 \otimes P_a + \mathcal{O}(\lambda),$$

so that we have the usual additive coproduct in the $\lambda \to 0$ limit. Meanwhile, the left coadjoint action (19) and the resulting cross relations in the double become

$$\mathrm{Ad}^*_{L\,J_a}(P_b) = \imath \epsilon_{abc} P_c, \quad [J_a, P_b] = \imath \epsilon_{abc} P_c,$$

i.e., $D(\mathrm{U}(\mathfrak{su}(2)))$ in the limit $\lambda \to 0$ with these generators becomes the usual U(iso(3)). This part is essentially known.[4,22]

Moreover, our action of these scaled generators on $\mathbb{R}^3_\lambda$ is

$$M^i{}_j \triangleright f(x) = \partial^i{}_j(f(x)), \quad \text{e.g.,} \quad M^i{}_j \triangleright x_a = \langle J_a, t^i{}_j \rangle 1 = \tfrac{1}{2} \sigma_a{}^i{}_j 1, \tag{26}$$

where the operators $\partial^i{}_j$ are the same as those in the next section. We can also write the action of P_a as partial derivatives defined there [in (35)] by

$$P_a \triangleright f(x) = -\imath \partial^a f(x), \quad P_0 \triangleright f(x) = \frac{1}{c} \partial^0 f(x),$$

where the constant c is put in order to make the equations have the same form as the classical ones, interpreting roughly the zero-direction as a "time" direction. This relation will become clearer in Sec. VII.

In the limit $\lambda \to 0$, the action of J_a becomes usual rotations in three-dimensional Euclidean space while the action of P_a becomes the action of translation operators of the algebra $\mathrm{U}(\mathbb{R}^3)$, so we indeed recover the classical action of U(iso(3)) on $\mathbb{R}^3$. In three-dimensional gravity, considering the dimension of the gravitational constant G_3 and the speed of light to be equal to 1, we have that λ must be proportional to the Planck constant.[22]

Next, there are several applications of the action of the double based on the above point of view. First and foremost, we could look for a wave operator from a Fourier transform point of view as in Ref. 3 (we give a different point of view later). Namely we look for a Casimir of $D(\mathrm{U}(\mathfrak{su}(2)))$ lying in momentum space $\mathbb{C}(\mathrm{SU}(2))$, and define the wave operator as its action. The possible such Casimirs are the $\mathrm{U}(\mathfrak{su}(2))$-invariant functions, which means basically the class functions on SU(2). In our case this just means any function of the trace function $\tau = t^1{}_1 + t^2{}_2$. The one suggested by the noncommutative geometry in the next sections is

$$\mathcal{E} \equiv -P^2 - \frac{4}{\lambda^2}\left(1 - \sqrt{1 - \frac{\lambda^2}{4} P^2}\right)^2 = \frac{4}{\lambda^2}(\tau - 2) \tag{27}$$

and its action on $\mathbb{R}^3_\lambda$ is then the wave operator $\Box$ on degree zero in Sec. V, but with metric -4 in the time direction. Note that $S\tau = \tau$ for $\mathbb{C}(\mathrm{SU}(2))$ so any such wave operator is invariant under group inversion, which appears as the antipode $SP_a = -P_a$.

A different question we can also ask is about the noncommutative analogs of spherical harmonics as functions in $\mathbb{R}^3_\lambda$ in the sense of irreducible representations $Y_l{}^m$ under the above action (21) of the rotation group. We find the (unnormalized) lowest ones for $l \in \mathbb{Z}_+$ and $m = -l, -l+1, \ldots, l$ as

$$Y_0{}^0 = 1,$$

$$Y_1{}^{\pm 1} = \mp \frac{1}{\sqrt{2}}(x_1 \pm \imath x_2), \quad Y_1{}^0 = x_3,$$

$$Y_2{}^{\pm 2}=(x_1\pm \imath x_2)^2, \quad Y_2{}^{\pm 1}=\mp((x_1\pm \imath x_2)x_3+x_3(x_1\pm \imath x_2)),$$

$$Y_2{}^0=\frac{1}{\sqrt{6}}(4x_3^2-(x_1+\imath x_2)(x_1-\imath x_2)-(x_1-\imath x_2)(x_1+\imath x_2)).$$

Let us note that such spherical harmonics can have many applications beyond their usual role in physics. For example, they classify the possible noncommutative differential calculi on the classical coordinate algebra $\mathbb{C}(\mathrm{SU}(2))$ which is dual to the space we study here.

IV. THE FOUR-DIMENSIONAL CALCULUS ON $\mathbb{R}^3_\lambda$

The purpose of this section is to construct a bicovariant calculus on the algebra $\mathbb{R}^3_\lambda$ following the steps outlined in Sec. II, the calculus we obtain being that on the algebra $\mathrm{U}(\mathfrak{su}(2))$ on setting $\lambda=1$. We write $\mathbb{R}^3_\lambda$ as generated by x_+, x_- and h, say, and with the Hopf algebra structure given explicitly in terms of the generators as

$$[h,x_\pm]=\pm 2\lambda x_\pm; \quad [x_+,x_-]=\lambda h, \tag{28}$$

and the additive coproduct as before. The particular form of the coproduct, the relations and (17) show that $\mathrm{d}\xi=\omega(\xi)$ for all $\xi\in\mathfrak{su}(2)$. Because of the cocommutativity, all ideals in $\mathbb{R}^3_\lambda$ are invariant under adjoint coactions (11) so that first order differential calculi Ω^1 on $\mathbb{R}^3_\lambda$ are classified simply by the ideals $\mathcal{I}\subset\ker\epsilon$. In order to construct an ideal of $\ker\epsilon$, consider a two-dimensional representation $\rho:\mathbb{R}^3_\lambda\to\mathrm{End}\mathbb{C}^2$, which in the basis $\{e_1,e_2\}$ of $\mathbb{C}^2$ is given by

$$\rho(x_+)e_1=0, \quad \rho(x_+)e_2=\lambda e_1,$$

$$\rho(x_-)e_1=\lambda e_2, \quad \rho(x_-)e_2=0,$$

$$\rho(h)e_1=\lambda e_1, \quad \rho(h)e_2=-\lambda e_2.$$

The representation ρ is a surjective map onto $M_2(\mathbb{C})$, even when restricted to $\ker\epsilon$. The kernel of $\rho|_{\ker\epsilon}$ is a two-sided ideal in $\ker\epsilon$. Then we have

$$M_2(\mathbb{C})\equiv\ker\ \epsilon/\ker\ \rho. \tag{29}$$

This isomorphism allows us to identify the basic one-forms with 2×2 matrices, $\{e_{ij}\}$, for $i,j=1,2$, where e_{ij} is the matrix with 1 in the (i,j) entry and 0 otherwise. Then the first order differential calculus is

$$\Omega^1(\mathbb{R}^3_\lambda)=M_2(\mathbb{C})\otimes\mathbb{R}^3_\lambda.$$

The exterior derivative operator is

$$\mathrm{d}f(x)=\lambda^{-1}\sum\ \rho(f(x)_{(1)}-\epsilon(f(x)_{(1)})1)f(x)_{(2)}=e_{ij}\partial^i{}_j(f),$$

where the last equality is a definition of the partial derivatives $\partial^i{}_j:\mathbb{R}^3_\lambda\to\mathbb{R}^3_\lambda$. In particular, we have

$$\mathrm{d}\xi=\lambda^{-1}\rho(\xi), \quad \forall\,\xi\in\mathfrak{su}(2),$$

which, along with id, span the whole space $\mathrm{M}_2(\mathbb{C})$ of invariant one-forms. For a general monomial $\xi_1\cdots\xi_n$, the expression of the derivative is

$$\mathrm{d}(\xi_1\cdots\xi_n)=\lambda^{-1}\sum_{k=1}^{n}\sum_{\sigma\in S_{(n,k)}}\rho(\xi_{\sigma(1)}\cdots\xi_{\sigma(k)})\xi_{\sigma(k+1)}\cdots\xi_{\sigma(n)},$$

where σ is a permutation of 1,...,n, such that $\sigma(1)<\cdots<\sigma(k)$ and $\sigma(k+1)<\cdots<\sigma(n)$. This kind of permutation is called a (n,k)-shuffle. And finally, for a (formal power series) grouplike element g (where $\Delta g=g\otimes g$), the derivative is

$$\mathrm{d}g=\lambda^{-1}(\rho(g)-\theta)g.$$

On our basis we have

$$\mathrm{d}x_+=e_{12},\quad \mathrm{d}x_-=e_{21},\quad \mathrm{d}h=e_{11}-e_{22},\quad \theta=e_{11}+e_{22}.$$

The compatibility conditions of this definition of the derivative with the Leibniz rule is due to the following commutation relations between the generators of the algebra and the basic one-forms:

$$\begin{aligned}
x_\pm \mathrm{d}x_\pm &= (\mathrm{d}x_\pm)x_\pm,\\
x_\pm \mathrm{d}x_\mp &= (\mathrm{d}x_\mp)x_\pm+\frac{\lambda}{2}(\theta\pm\mathrm{d}h),\\
x_\pm \mathrm{d}h &= (\mathrm{d}h)x_\pm\mp\lambda\,\mathrm{d}x_\pm,\\
h\,\mathrm{d}x_\pm &= (\mathrm{d}x_\pm)h\pm\lambda\,\mathrm{d}x_\pm,\\
h\,\mathrm{d}h &= (\mathrm{d}h)h+\lambda\theta,\\
x_\pm\theta &= \theta x_\pm+\lambda\,\mathrm{d}x_\pm,\\
h\theta &= \theta h+\lambda\,\mathrm{d}h.
\end{aligned}\tag{30}$$

From these commutation relations, we can see that this calculus is inner, that is, the derivatives of any element of the algebra can be basically obtained by the commutator with the one-form θ. In the classical limit, this calculus turns out to be the commutative calculus on usual three-dimensional Euclidean space. The explicit expression for the derivative of a general monomial $x_-^a h^b x_+^c$ is given by

$$\begin{aligned}
\mathrm{d}(x_-^a h^b x_+^c)=\mathrm{d}h&\left(\sum_{i=0}^{[(b-1)/2]}\binom{b}{2i+1}\lambda^{2i}x_-^a h^{b-2i-1}x_+^c\right)+\theta\left(\sum_{i=1}^{[b/2]}\binom{b}{2i}\lambda^{2i-1}x_-^a h^{b-2i}x_+^c\right)\\
&+\mathrm{d}x_+\left(\sum_{i=0}^{b}\binom{b}{i}\lambda^i c x_-^a h^{b-i}x_+^{c-1}\right)+\mathrm{d}x_-\left(\sum_{i=0}^{b}\binom{b}{i}\lambda^i a x_-^{a-1}h^{b-i}x_+^c\right)+\frac{1}{2}(\theta-\mathrm{d}h)\\
&\times\left(\sum_{i=0}^{b}\binom{b}{i}\lambda^{i+1}acx_-^{a-1}h^{b-i}x_+^{c-1}\right),
\end{aligned}\tag{31}$$

where the symbol $[z]$ denotes the greatest integer less than z and only terms with $\geqslant 0$ powers of the generators are included. Note that this expression becomes in the limit $\lambda\to 0$ the usual expression for the derivative of a monomial in three commuting coordinates.

In terms of the generators x_a, $a=1,2,3$, which are related to the previous generators by

$$x_1=\frac{1}{2}(x_++x_-),\quad x_2=\frac{\imath}{2}(x_--x_+),\quad x_3=\frac{1}{2}h,$$

we have

$$\mathrm{d}x_a=\tfrac{1}{2}\sigma_a,\quad \theta=\sigma_0,\tag{32}$$

i.e., the Pauli matrices are nothing other than three of our basic one-forms, and together with $\sigma_0 = \mathrm{id}$ form a basis of the invariant one-forms. The commutation relations (30) have a simple expression:

$$\begin{aligned} x_a \mathrm{d}x_b &= (\mathrm{d}x_b)x_a + \frac{\imath\lambda}{2}\epsilon_{abc}\mathrm{d}x_c + \frac{\lambda}{4}\delta_{ab}\theta, \\ x_a\theta &= \theta x_a + \lambda\,\mathrm{d}x_a\,. \end{aligned} \tag{33}$$

In this basis the partial derivatives defined by

$$\mathrm{d}f(x) = (\mathrm{d}x_a)\partial^a f(x) + \theta\frac{1}{c}\partial^0 f(x) \tag{34}$$

are related to the previous ones by

$$\partial^i{}_j = \frac{1}{2}\sigma_a{}^i{}_j\partial^a + \frac{1}{c}\sigma_0{}^i{}_j\partial^0 \tag{35}$$

as in (25). The exterior derivative of a general monomial $x_1^a x_2^b x_3^c$ is quite complicated to write down explicitly, but we find it as

$$\begin{aligned} \mathrm{d}(x_1^a x_2^b x_3^c) = &\sum_{i=0}^{[a/2]}\sum_{j=0}^{[b/2]}\sum_{k=0}^{[c/2]} \theta\frac{\lambda^{2(i+j+k)-1}}{2^{2(i+j+k)}}\binom{a}{2i}\binom{b}{2j}\binom{c}{2k}x_1^{a-2i}x_2^{b-2j}x_3^{c-2k} \\ &+\sum_{i=0}^{[a/2]}\sum_{j=0}^{[b/2]}\sum_{k=0}^{[(c-1)/2]} \mathrm{d}x_3\frac{\lambda^{2(i+j+k)}}{2^{2(i+j+k)}}\binom{a}{2i}\binom{b}{2j}\binom{c}{2k+1}x_1^{a-2i}x_2^{b-2j}x_3^{c-2k-1} \\ &+\sum_{i=0}^{[a/2]}\sum_{j=0}^{[(b-1)/2]}\sum_{k=0}^{[c/2]} \mathrm{d}x_2\frac{\lambda^{2(i+j+k)}}{2^{2(i+j+k)}}\binom{a}{2i}\binom{b}{2j+1}\binom{c}{2k}x_1^{a-2i}x_2^{b-2j-1}x_3^{c-2k} \\ &+\sum_{i=0}^{[a/2]}\sum_{j=0}^{[(b-1)/2]}\sum_{k=0}^{[(c-1)/2]} \imath\mathrm{d}x_1\frac{\lambda^{2(i+j+k)+1}}{2^{2(i+j+k)+1}}\binom{a}{2i}\binom{b}{2j+1} \\ &\times\binom{c}{2k+1}x_1^{a-2i}x_2^{b-2j-1}x_3^{c-2k-1} + \sum_{i=0}^{[(a-1)/2]}\sum_{j=0}^{[b/2]}\sum_{k=0}^{[c/2]} \mathrm{d}x_1\frac{\lambda^{2(i+j+k)}}{2^{2(i+j+k)}}\binom{a}{2i+1}\binom{b}{2j} \\ &\times\binom{c}{2k}x_1^{a-2i-1}x_2^{b-2j}x_3^{c-2k} - \sum_{i=0}^{[(a-1)/2]}\sum_{j=0}^{[b/2]}\sum_{k=0}^{[(c-1)/2]} \imath\mathrm{d}x_2\frac{\lambda^{2(i+j+k)+1}}{2^{2(i+j+k)+1}}\binom{a}{2i+1}\binom{b}{2j} \\ &\times\binom{c}{2k+1}x_1^{a-2i-1}x_2^{b-2j}x_3^{c-2k-1} + \sum_{i=0}^{[(a-1)/2]}\sum_{j=0}^{[(b-1)/2]}\sum_{k=0}^{[c/2]} \imath\mathrm{d}x_3\frac{\lambda^{2(i+j+k)+1}}{2^{2(i+j+k)+1}}\binom{a}{2i+1} \\ &\times\binom{b}{2j+1}\binom{c}{2k}x_1^{a-2i-1}x_2^{b-2j-1}x_3^{c-2k} \\ &+\sum_{i=0}^{[(a-1)/2]}\sum_{j=0}^{[(b-1)/2]}\sum_{k=0}^{[(c-1)/2]} \theta\frac{\lambda^{2(i+j+k)+2}}{2^{2(i+j+k)+3}}\binom{a}{2i+1}\binom{b}{2j+1} \\ &\times\binom{c}{2k+1}x_1^{a-2i-1}x_2^{b-2j-1}x_3^{c-2k-1} - \frac{\theta}{\lambda}x_1^a x_2^b x_3^c. \end{aligned} \tag{36}$$

In both cases the expression for the derivatives of plane waves is very simple. In terms of generators x_a, the derivative of the plane wave $e^{\imath\Sigma_a k^a x_a}=e^{ik\cdot x}$ is given by

$$\mathrm{d}e^{\imath k\cdot x}=\left\{\frac{\theta}{\lambda}\left(\cos\left(\frac{\lambda|k|}{2}\right)-1\right)+\frac{2\imath\sin(\lambda|k|/2)}{\lambda|k|}k\cdot\mathrm{d}x\right\}e^{\imath k\cdot x}. \tag{37}$$

One can see that the limit $\lambda\to 0$ gives the correct formula for the derivative of plane waves, that is,

$$\lim_{\lambda\to 0}\mathrm{d}e^{\imath k\cdot x}=\left(\sum_{a=1}^{3}\imath k_a\mathrm{d}\overline{x_a}\right)e^{\imath k\cdot\overline{x}}=\imath k\cdot(\mathrm{d}\overline{x})e^{\imath k\cdot\overline{x}},$$

where at $\lambda=0$ on the right hand side we have the classical coordinates and the classical one-forms in usual three-dimensional commutative calculus. In terms of the generators $x_\pm$, h, the plane wave $e^{\imath(k_+x_++k_-x_-+k_0h)}=e^{\imath k\cdot x}$ is given by

$$\mathrm{d}e^{\imath k\cdot x}=\left\{\frac{\theta}{\lambda}(\cos(\lambda\sqrt{k_0^2+k_+k_-})-1)+\frac{\imath(k_+\mathrm{d}x_++k_-\mathrm{d}x_-+k_0\mathrm{d}h)}{\lambda\sqrt{k_0^2+k_+k_-}}\sin(\lambda\sqrt{k_0^2+k_+k_-})\right\}e^{ik\cdot x}. \tag{38}$$

This calculus is four-dimensional, in the sense that one has four basic one-forms, but these dimensions are entangled in a nontrivial way. For example, note that they satisfy the relation

$$\epsilon_{abc}x_a(\mathrm{d}x_b)x_c=0.$$

We can see that in the classical limit $\lambda\to 0$, the calculus turns out to be commutative and the extra dimension, namely the one-dimensional subspace generated by the one-form θ, decouples totally from the calculus generated by the other three one-forms. The relation between this extra dimension and quantization can also be perceived by considering the derivative of the Casimir operator

$$C=\sum_{a=1}^{3}(x_a)^2,$$

which implies

$$\mathrm{d}C=2\sum_{a=1}^{3}(\mathrm{d}x_a)x_a+\frac{3\lambda}{4}\theta.$$

The coefficient of the term in θ is exactly the eigenvalue of the Casimir in the spin $\frac{1}{2}$ representation, the same used to construct the differential calculus, and also vanishes when $\lambda\to 0$. We shall see later that this extra dimension can also be seen as a remnant of the time coordinate in the q-Minkowski space $\mathbb{R}_q^{1,3}$ when the limit $q\to 1$ is taken. A semi-classical analysis on this calculus can also be made in order to recover an interpretation of time in the three-dimensional noncommutative space.

We can also construct the full exterior algebra $\Omega^\cdot(\mathbb{R}_\lambda^3)=\oplus_{n=0}^{\infty}\Omega^n(\mathbb{R}_\lambda^3)$. In our case the general braiding[25] becomes the trivial flip homomorphism because the right invariant basic one-forms are also left invariant. Hence our basic one-forms in $\mathrm{M}_2(\mathbb{C})$ are totally anticommutative and their usual antisymmetric wedge product generates the usual exterior algebra on the vector space $\mathrm{M}_2(\mathbb{C})$. The full $\Omega^\cdot(\mathbb{R}_\lambda^3)$ is generated by these and elements of $\mathbb{R}_\lambda^3$ with the relations (30). The exterior differentiation in $\Omega^\cdot(\mathbb{R}_\lambda^3)$ is given by the graded commutator with the basic one-form θ, that is,

$$\mathrm{d}\omega=\omega\wedge\theta-(-1)^{\deg\omega}\theta\wedge\omega.$$

In particular, the basic one-forms $M_2(\mathbb{C})$ are all closed, among which θ is not exact. The cohomologies of this calculus were also calculated giving the following results:

Theorem 4.1: *The noncommutative de Rham cohomology of* $\mathbb{R}^3_\lambda$ *is*

$$H^0=\mathbb{C}.1, \quad H^1=\mathbb{C}.\theta, \quad H^2=H^3=H^4=\{0\}.$$

Proof: This is by direct (and rather long) computation of the closed forms and the exact ones in each degree using the explicit formula (31) on general monomials. To give an example of the procedure, we will do it in some detail for the case of one-forms of the particular type

$$\omega=\alpha(\mathrm{d}x_+)x_-^a h^b x_+^c+\beta(\mathrm{d}x_-)x_-^m h^n x_+^p+\gamma(\mathrm{d}h)x_-^r h^s x_+^t+\delta\theta x_-^u h^v x_+^w,$$

and impose $\mathrm{d}\omega=0$. We start analyzing the simplest cases, and then going to more complex ones.

Taking $\beta=\gamma=\delta=0$, then

$$\omega=\alpha(\mathrm{d}x_+)x_-^a h^b x_+^c.$$

The term in $dx_-\wedge dx_+$ leads to the conclusion that $c=0$. Similarly, the term in $\mathrm{d}h\wedge\mathrm{d}x_+$ leads to $b=0$ so that

$$\omega=\alpha(\mathrm{d}x_+)x_+^c=\mathrm{d}\left(\frac{1}{c+1}x_+^{c+1}\right),$$

which is an exact form, hence belonging to the null cohomology class. The cases $\alpha=\gamma=\delta=0$ and $\alpha=\beta=\delta=0$ also lead to exact forms. The case $\alpha=\beta=\gamma=0$ leads to the one-form

$$\omega=\delta\theta x_-^u h^v x_+^w.$$

The vanishing of the term in $\mathrm{d}x_+\wedge\theta$ implies that $w=0$, the term in $\mathrm{d}x_-\wedge\theta$ vanishes if and only if $u=0$ and the term in $\mathrm{d}h\wedge\theta$ has its vanishing subject to the condition $v=0$. Hence we have only the closed, nonexact form θ from this case.

Let us now analyze the case with two nonzero terms:

$$\omega=\alpha(\mathrm{d}x_+)x_-^a h^b x_+^c+\beta(\mathrm{d}x_-)x_-^m h^n x_+^p.$$

The vanishing condition in the term on $\mathrm{d}x_-\wedge\mathrm{d}x_+$ reads

$$\alpha\sum_{i=0}^{b}\binom{b}{i}\lambda^i a x_-^{a-1}h^{b-i}x_+^c=\beta\sum_{i=0}^{n}\binom{n}{i}\lambda^i p x_-^m h^{n-i}x_+^{p-1}.$$

Then we conclude that $b=n$, $a-1=m$, $c=p-1$ and $\alpha a=\beta(c+1)$. The vanishing of the term in $\mathrm{d}h\wedge\mathrm{d}x_+$ reads

$$\sum_{i=0}^{[(b-1)/2]}\binom{b}{2i+1}\lambda^{2i}x_-^a h^{b-2i-1}x_+^c=\frac{1}{2}\sum_{i=0}^{b}\binom{b}{i}\lambda^{i+1}acx_-^{a-1}h^{b-i}x_+^{c-1}.$$

The terms in odd powers of λ vanish if and only if $ac=0$. Then the left hand side vanishes if and only if $b=0$. The case $a=0$ implies that $\beta=0$, which reduces to the previous case already mentioned. For the case $c=0$ we have $\beta=\alpha a$ so that

$$\omega=\alpha((\mathrm{d}x_+)x_-^a+a(\mathrm{d}x_-)x_-^{a-1}x_+).$$

It is easy to see that ω is closed if and only if $a=1$. But

$$(\mathrm{d}x_+)x_- + (\mathrm{d}x_-)x_+ = \mathrm{d}\left(x_-x_+ + \frac{\lambda}{2}h\right) - \frac{\lambda}{2}\theta,$$

which is a form homologous to θ. It is a long, but straightforward, calculation to prove that all the other cases of closed one-forms of the type above rely on these cases. The general case is still more complicated.

The proof that all higher cohomologies are trivial is also an exhaustive analysis of all the possible cases and inductions on powers of h, as exemplified here for the four-forms: It is clear that all four-forms

$$\omega = \mathrm{d}x_- \wedge \mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^m h^n x_+^p$$

are closed. We use induction on n to prove that there exists a three-form η such that $\omega = d\eta$. For $n=0$, we have

$$\mathrm{d}x_- \wedge \mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^m x_+^p = \mathrm{d}\left(-\frac{1}{m+1}\mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^{m+1}x_+^p\right).$$

Suppose that there exist three-forms η_k, for $0 \leqslant k < n$, such that

$$\mathrm{d}x_- \wedge \mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^m h^k x_+^p = \mathrm{d}\eta_k.$$

Then

$$\begin{aligned}\mathrm{d}x_- \wedge \mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^m h^n x_+^p &= \mathrm{d}\left(-\frac{1}{m+1}\mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^{m+1}h^n x_+^p\right) \\ &\quad - \mathrm{d}x_- \wedge \mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta \sum_{i=1}^{n} \binom{n}{i} \lambda^i x_-^m h^{n-i} x_+^p \\ &= \mathrm{d}\left(-\frac{1}{m+1}\mathrm{d}h \wedge \mathrm{d}x_+ \wedge \theta x_-^{m+1}h^n x_+^p - \sum_{i=1}^{n}\binom{n}{i}\lambda^i \eta_{n-i}\right).\end{aligned}$$

Hence all four-forms are exact. The same procedure is used to show the triviality of the other cohomologies. ◇

For $\mathbb{R}^3_\lambda$ we should expect the cohomology to be trivial, since this corresponds to Stokes theorem and many other aspects taken for granted in physics. We find almost this except for the generator θ which generates the calculus and which has no three-dimensional classical analogs. We will see in Sec. VII that θ is a remnant of a time direction even though from the point of view of $\mathbb{R}^3_\lambda$ there is no time coordinate. The cohomology result says exactly that θ is an allowed direction but not d of anything.

V. HODGE ∗-OPERATOR AND ELECTROMAGNETIC THEORY

The above geometry also admits a metric structure. It is known that any nondegenerate bilinear form $\eta \in \Lambda^1 \otimes \Lambda^1$ defines an invariant metric on the Hopf algebra H.[18] For the case of $\mathbb{R}^3_\lambda$ we can define the metric

$$\eta = \mathrm{d}x_1 \otimes \mathrm{d}x_1 + \mathrm{d}x_2 \otimes \mathrm{d}x_2 + \mathrm{d}x_3 \otimes \mathrm{d}x_3 + \mu\,\theta \otimes \theta \tag{39}$$

for a parameter μ. This bilinear form is nondegenerate, invariant by left and right coactions and symmetric in the sense that $\wedge(\eta) = 0$. With this metric structure, it is possible to define a Hodge ∗-operator and then explore the properties of the Laplacian and find some physical consequences. Our picture is similar to Ref. 9 where the manifold is similarly three-dimensional but there is an extra time direction θ in the local cotangent space.

The Hodge $*$-operator on an n-dimensional calculus (for which the top form is of order n), over a Hopf algebra H with metric η is a map $*:\Omega^k\to\Omega^{n-k}$ given by the expression

$$*(\omega_{i_1}\cdots\omega_{i_k})=\frac{1}{(n-k)!}\epsilon_{i_1\cdots i_k i_{k+1}\cdots i_n}\eta^{i_{k+1}j_1}\cdots\eta^{i_n j_{n-k}}\omega_{j_1}\cdots\omega_{j_{n-k}}.$$

In the case of the algebra $\mathbb{R}^3_\lambda$, we have a four-dimensional calculus with $\omega_1=\mathrm{d}x_1$, $\omega_2=\mathrm{d}x_2$, $\omega_3=\mathrm{d}x_3$, $\omega_4=\theta$. The components of the metric inverse, as we can see from (39), are $\eta^{11}=\eta^{22}=\eta^{33}=1$, and $\eta^{44}=1/\mu$. The arbitrary factor μ in the metric can be set by imposing conditions on the map $*^2$. Then we have two possible choices for the constant μ: The first is $\mu=1$ making a four-dimensional Euclidean geometry; then for a k-form ω we have the constraint $**(\omega)=(-1)^{k(4-k)}\omega$. The second possibility is $\mu=-1$; then the metric is Minkowskian and the constraint on a k-form ω is $**(\omega)=(-1)^{1+k(4-k)}\omega$. In what follows, we will be using the Minkowskian convention on the grounds that this geometry on $\mathbb{R}^3_\lambda$ is a remnant of a noncommutative geometry on a q-deformed version of the Minkowski space, as we shall explain in Sec. VII. The expressions for the Hodge $*$-operator are summarized as follows:

$$\begin{aligned}
*1&=-\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3\wedge\theta,\\
*\mathrm{d}x_1&=-\mathrm{d}x_2\wedge\mathrm{d}x_3\wedge\theta,\\
*\mathrm{d}x_2&=\mathrm{d}x_1\wedge\mathrm{d}x_3\wedge\theta,\\
*\mathrm{d}x_3&=-\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\theta,\\
*\theta&=-\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_2)&=-\mathrm{d}x_3\wedge\theta,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_3)&=\mathrm{d}x_2\wedge\theta,\\
*(\mathrm{d}x_1\wedge\theta)&=\mathrm{d}x_2\wedge\mathrm{d}x_3,\\
*(\mathrm{d}x_2\wedge\mathrm{d}x_3)&=-\mathrm{d}x_1\wedge\theta,\\
*(\mathrm{d}x_2\wedge\theta)&=-\mathrm{d}x_1\wedge\mathrm{d}x_3,\\
*(\mathrm{d}x_3\wedge\theta)&=\mathrm{d}x_1\wedge\mathrm{d}x_2,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3)&=-\theta,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\theta)&=-\mathrm{d}x_3,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_3\wedge\theta)&=\mathrm{d}x_2,\\
*(\mathrm{d}x_2\wedge\mathrm{d}x_3\wedge\theta)&=-\mathrm{d}x_1,\\
*(\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3\wedge\theta)&=1.
\end{aligned}\tag{40}$$

Given the Hodge $*$-operator, one can write, for example, the coderivative $\delta=*\mathrm{d}*$ and the Laplacian operator $\Delta=\delta\mathrm{d}+\mathrm{d}\delta$. Note that the Laplacian maps to forms of the same degree. We prefer to work actually with the ''Maxwell-type'' wave operator

$$\Box=\delta\mathrm{d}=*\mathrm{d}*\mathrm{d},\tag{41}$$

which is just the same in degree 0 and the same in degree 1 if we work in a gauge where $\delta=0$. In the rest of this section, we are going to describe some features of the electromagnetic theory arising in this noncommutative context. The electromagnetic theory is the analysis of solutions $A\in\Omega^1(\mathbb{R}^3_\lambda)$ of the equation $\Box A=\mathrm{J}$ where J is a one-form which can be interpreted as a ''physical'' source. We demonstrate the theory on two natural choices of sources, namely an electrostatic and a magnetic one. We start with spin 0 and we limit ourselves to algebraic plus plane wave solutions.

A. Spin 0 modes

The wave operator on $\Omega^0(\mathbb{R}^3_\lambda)=\mathbb{R}^3_\lambda$ is computed from the definitions above as

$$\Box=*\mathrm{d}*\mathrm{d}=(\partial^a)^2-\frac{1}{c^2}(\partial^0)^2,$$

where the partials are defined by (34). The algebraic massless modes $\ker\Box$ are given by

(i) polynomials of degree one: $f(x)=\alpha+\beta_a x_a$,
(ii) linear combinations of polynomials of the type $f(x)=x_a^2-x_b^2$,
(iii) linear combinations of quadratic monomials of the type, $f(x)=\alpha_{ab}x_a x_b$, with $a\neq b$, and
(iv) The three particular combinations $f(x)=x_1x_2x_3-(\imath\lambda/4)\,x_a^2$, for $a=1,2,3$.

General eigenfunctions of $\Box$ in degree 0 are the plane waves; the expression for their derivatives can be seen in (37). Hence

$$\Box e^{\imath k\cdot x}=-\frac{1}{\lambda^2}\left\{4\sin^2\left(\frac{\lambda|k|}{2}\right)+\left(\cos\left(\frac{\lambda|k|}{2}\right)-1\right)^2\right\}e^{\imath k\cdot x}.$$

It is easy to see that this eigenvalue goes in the limit $\lambda\to 1$ to the usual eigenvalue of the Laplacian in three-dimensional commutative space acting on plane waves.

B. Spin 1 electromagnetic modes

On $\Omega^1(\mathbb{R}^3_\lambda)$, the Maxwell operator $\Box_1=*\mathrm{d}*\mathrm{d}$ can likewise be computed explicitly. If we write $A=(\mathrm{d}x_a)A^a+\theta A^0$ for functions A^μ, then

$$F=\mathrm{d}A=\mathrm{d}x_a\wedge\mathrm{d}x_b\partial^b A^a+\mathrm{d}x_a\wedge\theta\frac{1}{c}\partial^0A^a+\theta\wedge\mathrm{d}x_a\partial^aA^0.$$

If we break this up into electric and magnetic parts in the usual way, then

$$B_a=\epsilon_{abc}\partial^bA^c,\quad E_a=\frac{1}{c}\partial^0A^a-\partial^aA^0.$$

These computations have just the same form as for usual space–time. The algebraic zero modes $\ker\Box_1$ are given by

(i) forms of the type $A=\mathrm{d}x_a(\alpha+\beta_a x_a+\gamma_a x_a^2)$ with curvature

$$F=\frac{\lambda}{4}\gamma_a\mathrm{d}x_a\wedge\theta,$$

(ii) forms of the type $A=\beta_{ab}(\mathrm{d}x_a)x_b$, with $a\neq b$ and curvature

$$F=\beta_{ab}\mathrm{d}x_a\wedge\mathrm{d}x_b,$$

(iii) forms of the type $A=\theta f$ with $f\in\ker\Box$. The curvatures for the latter three $f(x)$ shown above are

$$F=-2(\mathrm{d}x_a\wedge\theta x_a-\mathrm{d}x_b\wedge\theta x_b),$$

$$F=\alpha_{ab}\left(\theta\wedge(\mathrm{d}x_a)x_b+\theta\wedge(\mathrm{d}x_b)x_a+\frac{\imath\lambda}{2}\epsilon_{abc}\theta\wedge\mathrm{d}x_c\right)$$

$$F=-\mathrm{d}x_1\wedge\theta\left(x_2x_3+\frac{\imath\lambda}{2}x_1\right)-\mathrm{d}x_2\wedge\theta\left(x_1x_3-\frac{\imath\lambda}{2}x_2\right)-\mathrm{d}x_3\wedge\theta\left(x_1x_2+\frac{\imath\lambda}{2}x_3\right)-\frac{\imath\lambda}{2}\mathrm{d}x_a\wedge\theta x_a.$$

These are ''self-propagating'' electromagnetic modes or solutions of the sourceless Maxwell equations for a one-form or ''gauge potential'' A.

C. Electrostatic solution

Here we take a uniform source in the ''purely time'' direction $\mathrm{J}=\theta$. In this case the solution of the gauge potential is

$$A=\tfrac{1}{6}\theta C,$$

where $C=\Sigma_a x_a^2$ is the Casimir operator. The curvature operator, which in this case can be interpreted as an electric field, is given by

$$F=\mathrm{d}A=\tfrac{1}{3}(\theta\wedge(\mathrm{d}x_1)x_1+\theta\wedge(\mathrm{d}x_2)x_2+\theta\wedge(\mathrm{d}x_3)x_3).$$

If θ is viewed as a time direction, then this curvature is a radial electric field. It has field strength increasing with the radius, which is a kind of solution exhibiting a confinement behavior. This is the correct physical solution for a uniform electric charge density throughout all space provided this is understood with the correct boundary conditions; if one builds the uniform charge density by a series of concentric shells about the origin, then, at radius r, all shells of greater radius produce no electric field and all shells of smaller radius total a charge proportional to r^3 and hence a radial electric field of strength proportional to r.

D. Magnetic solution

Here we take a uniform electric current density along a direction vector $k\in\mathbb{R}^3$, i.e., $\mathrm{J}=k\cdot\mathrm{d}x=\Sigma_a k^a\mathrm{d}x_a$. In this case, the gauge potential can be written as

$$A=\frac{1}{4}\left\{\left(\sum_{a=1}^{3}k_a\mathrm{d}x_a\right)C+\frac{\theta}{2}\left(\sum_{a=1}^{3}k_ax_a\right)-\sum_{a=1}^{3}k_a(\mathrm{d}x_a)x_a^2\right\}.$$

The field strength is

$$F=\mathrm{d}A=\tfrac{1}{2}\{\mathrm{d}x_1\wedge\mathrm{d}x_2(k_1x_2-k_2x_1)+\mathrm{d}x_1\wedge\mathrm{d}x_3(k_1x_3-k_3x_1)+\mathrm{d}x_2\wedge\mathrm{d}x_3(k_2x_3-k_3x_2)\}. \quad (42)$$

If we decompose the curvature in the usual way, then this is a magnetic field in a direction $k\times x$ (the vector cross product). This is a ''confining'' (in the sense of increasing with normal distance) version of the field due to a uniform current density in direction k, taken with cylindrical boundary conditions at infinity.

We have considered for the electromagnetic solutions only uniform sources J; we can clearly put in a functional dependence for the coefficients of the source to similarly obtain other solutions of both the electric and magnetic types. Solutions more similar to the usual decaying ones,

however, will not be polynomial (one would need the inverse of $\Sigma_a x_a^2$) and are therefore well outside our present scope; even at a formal level the problem of computing $\mathrm{d}(\Sigma_a x_a^2)^{-1}$ in a closed form appears to be formidable. On the other hand, these matters could probably be addressed by completing to C^*-algebras and using the functional calculus for such algebras.

E. Spin $\frac{1}{2}$ equation

For completeness, let us mention here also a natural spin $\frac{1}{2}$ wave operator, namely the Dirac operator. We consider the simplest (Weyl) spinors as two components $\psi^i \in \mathbb{R}^3_\lambda$. In view of the fact that the partial derivatives $\partial^i{}_j$ already form a matrix, and following the similar phenomenon as for quantum groups,[18] we are led to define

$$(\not\partial\psi)^i = \partial^i{}_j \psi^j. \tag{43}$$

According to (35) this could also be written as

$$\not\partial = \frac{1}{2}\sigma_a \partial^a + \frac{1}{c}\partial^0,$$

where the second term is suggested by the geometry over and above what we might also guess. This term is optional in the same way as $(\partial^0)^2$ in $\Box$ is not forced by covariance, and is $\mathcal{O}(\lambda)$ for bounded spatial derivatives.

Here $\not\partial$ is covariant under the quantum double action in Sec. III as follows (the same applies without the ∂^0 term). The action of J_a on $\mathbb{R}^3_\lambda$ is that of orbital angular momentum and we have checked already that $\Box$ on degree 0 is covariant. For spin $\frac{1}{2}$ the total spin should be

$$S_a = \tfrac{1}{2}\sigma_a + J_a, \tag{44}$$

and we check that this commutes with $\not\partial$:

$$\begin{aligned}(S_a \not\partial\psi)^i &= \tfrac{1}{2}\sigma_a{}^i{}_j \partial^j{}_k \psi^k + J_a M^i{}_j \triangleright \psi^j = \tfrac{1}{2}\sigma_a{}^i{}_j M^j{}_k \triangleright \psi^k + [J_a, M^i{}_j] \triangleright \psi^j + M^i{}_j J_a \triangleright \psi^j \\ &= \tfrac{1}{2} M^i{}_j \triangleright \sigma_a{}^j{}_k \psi^k + M^i{}_j J_a \triangleright \psi^j = M^i{}_j \triangleright (S_a\psi)^j = (\not\partial S_a \psi)^i,\end{aligned}$$

where we used the relations (20) (those with $M^i{}_j$ have the same form) and the action (26). The operator $\not\partial$ is clearly also translation invariant under $\mathbb{C}(\mathrm{SU}(2))$ since the $\partial^i{}_j$ mutually commute. The operators σ_a and $\partial^i{}_j$ also commute since one acts on the spinor indices and the other on $\mathbb{R}^3_\lambda$, so S_a in place of J_a still gives a representation of $D(\mathrm{U}(\mathfrak{su}(2)))$ on spinors, under which $\not\partial$ is covariant.

F. Yang–Mills U(1) fields

Finally, also for completeness, we mention that there is a different U(1) theory which behaves more like Yang–Mills. Namely instead of $F = \mathrm{d}A$ as in the Maxwell theory, we define $F = \mathrm{d}A + A \wedge A$ for a one-form A. This transforms by conjugation as $A \mapsto gAg^{-1} + g\mathrm{d}g^{-1}$ and is a nonlinear version of the above, where $g \in \mathbb{R}^3_\lambda$ is any invertible element, e.g., a plane wave. In this context one would expect to be able to solve for zero-curvature, i.e., A such that $F(A) = 0$ and thereby demonstrate the Bohm–Aharanov effect, etc. This is part of the nonlinear theory, however, and beyond our present scope.

VI. DIFFERENTIAL CALCULUS ON THE QUANTUM SPHERE

In this section we briefly analyze what happens if we try to set the ''length'' function given by the Casimir C of $\mathbb{R}^3_\lambda$ to a fixed number, i.e., a sphere. We take this at unit radius, i.e., we define S^2_λ as the algebra $\mathbb{R}^3_\lambda$ with the additional relation

$$C \equiv \sum_{a=1}^{3} (x_a)^2 = 1. \tag{45}$$

This immediately gives a ''quantization condition'' for the constant λ if the algebra is to have an irreducible representation, namely $\lambda = 1/\sqrt{j(j+1)}$ for some $j \in \frac{1}{2}\mathbb{Z}_+$. The image of S^2_λ in such a spin j representation is a $(2j+1)\times(2j+1)$-matrix algebra which can be identified with the class of noncommutative spaces known as ''fuzzy spheres.'' [14,2,5,20,21] In these works one does elements of noncommutative differential geometry directly on matrix algebras motivated by thinking about them as a projection of $\mathrm{U}(su(2))$ in the spin j representation, and the greater the spin $j \to \infty$, the greater the resemblance with a classical sphere. The role of this in our case is played by $\lambda \to 0$ according to the above formula. On the other hand, note that we are working directly on S^2_λ and are not required to look in one or any irreducible representation, i.e., this is a slightly more geometrical approach to ''fuzzy spheres'' where we deform the conventional geometry of S^2 by a parameter λ and do not work with matrix algebras.

Specifically, when we make the constraint (45), the four-dimensional calculus given by relations (33) is reduced to a three-dimensional calculus on the sphere because

$$\mathrm{d}C = \sum_{a=1}^{3} 2(\mathrm{d}x_a)x_a + \frac{3\lambda}{4}\theta = 0,$$

which means that θ can be written as an expression on $\mathrm{d}x_a$. The remaining relations are given by

$$\begin{aligned} x_a \mathrm{d}x_b &= (\mathrm{d}x_b)x_a + \frac{i}{2}\lambda \epsilon_{abc}\mathrm{d}x_c - \frac{2}{3}\delta_{ab}\sum_{d=1}^{3} (\mathrm{d}x_d)x_d, \\ \lambda^2 \mathrm{d}x_a &= \frac{4i}{3}\lambda \epsilon_{abc}(\mathrm{d}x_b)x_c - \frac{16}{9}\sum_{d=1}^{3} (\mathrm{d}x_d)x_d x_a. \end{aligned} \tag{46}$$

In the limit $\lambda \to 0$ we recover the ordinary two-dimensional calculus on the sphere, given in terms of the classical variables $\overline{x_a} = \lim_{\lambda\to 0} x_a$. This can be seen by the relation

$$\sum_{a=1}^{3} (\mathrm{d}\overline{x_a})\overline{x_a} = 0,$$

allowing us to write one of the three one-forms in terms of the other two. For example, in the region where $\overline{x_3} = \sqrt{1-\overline{x_1}^2-\overline{x_2}^2}$ is invertible, one can write

$$\mathrm{d}\overline{x_3} = -\frac{\overline{x_1}}{\sqrt{1-\overline{x_1}^2-\overline{x_2}^2}}\mathrm{d}\overline{x_1} - \frac{\overline{x_2}}{\sqrt{1-\overline{x_1}^2-\overline{x_2}^2}}\mathrm{d}\overline{x_2}.$$

VII. THE SPACE $\mathbb{R}^3_\lambda$ AS A LIMIT OF q-MINKOWSKI SPACE

In this section, we will express the noncommutative space $\mathbb{R}^3_\lambda$ as a spacelike surface of constant time in a certain scaling limit of the standard q-deformed Minkowski space $\mathbb{R}^{1,3}_q$ in Refs. 6, 16, and 15. This is defined in Ref. 15 as the algebra of 2×2 braided (Hermitian) matrices $\mathrm{BM}_q(2)$ generated by 1 and

$$\mathbf{u} = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

with the commutation relations

$$
\begin{aligned}
ba &= q^2 ab,\\
ca &= q^{-2} ac,\\
da &= ad,\\
bc &= cb + (1-q^{-2}) a(d-a),\\
db &= bd + (1-q^{-2}) ab,\\
cd &= dc + (1-q^{-2}) ca.
\end{aligned}
\tag{47}
$$

If we choose a suitable set of generators, namely,

$$
\tilde{t} = \frac{qd + q^{-1}a}{2}, \quad \tilde{x} = \frac{b+c}{2}, \quad \tilde{y} = \frac{b-c}{2i}, \quad \tilde{z} = \frac{d-a}{2},
$$

then the braided determinant

$$
\underline{\det}(\mathbf{u}) = ad - q^2 cb \tag{48}
$$

can be written as

$$
\underline{\det}(\mathbf{u}) = \frac{4q^2}{(q^2+1)^2}\tilde{t}^2 - q^2\tilde{x}^2 - q^2\tilde{y}^2 - \frac{2(q^4+1)q^2}{(q^2+1)^2}\tilde{z}^2 + 2q\left(\frac{q^2-1}{q^2+1}\right)^2 \tilde{t}\tilde{z}.
$$

This expression, in the limit $q \to 1$, becomes the usual Minkowskian metric on $\mathbb{R}^{1,3}$. Here we will consider a different scaled limit related to the role of this algebra as braided enveloping algebra of a braided Lie algebra $\widetilde{\mathfrak{su}_q(2)}$ (see Ref. 10 for a recent treatment). This is such that we can still have a noncommutative space even when $q \to 1$. Defining new generators

$$
x_+ = \frac{c}{(q-q^{-1})}, \quad x_- = \frac{b}{(q-q^{-1})}, \quad h = \frac{a-d}{(q-q^{-1})}, \quad t = \frac{qd + q^{-1}a}{c(q+q^{-1})}, \tag{49}
$$

and considering the commutation relations (47), we have

$$
\begin{aligned}
[x_+, x_-] &= q^{-1} cth + q^{-1}\frac{(q-q^{-1})}{(q+q^{-1})}h^2,\\
q^{-2} h x_+ &= x_+ h + q^{-2}(q+q^{-1}) c x_+ t,\\
q^2 h x_- &= x_- h - (q+q^{-1}) c x_- t,\\
t x_\pm &= x_\pm t,\\
th &= ht.
\end{aligned}
\tag{50}
$$

In the limit $q \to 1$, we obtain the commutation relations

$$
[x_a, x_b] = \imath ct \epsilon_{abc} x_c, \quad [x_a, t] = 0, \tag{51}
$$

of the so-called homogenized universal enveloping algebra $\widetilde{\mathrm{U}(\mathfrak{su}(2))}$, which we will denote by $\mathbb{R}^{1,3}_c$. Here c is a parameter required by dimensional analysis (of dimension ms^{-1}). When $ct = \lambda$ we recover exactly the relations (28) of $\mathbb{R}^3_\lambda$. So the noncommutative space that we have studied in previous sections is the "slice" at a certain time of $\mathbb{R}^{1,3}_c$, which in turn is a contraction

of $\mathbb{R}_q^{1,3}$. The possibility of these two $q\to 1$ limits where one gives a classical coordinate algebra and the other gives essentially its dual (an enveloping algebra) is called a ''quantum-geometry duality transformation.''

We now go further and also obtain the differential structure on $\mathbb{R}^3_\lambda$ via this scaling limit. Thus, the algebra $\mathbb{R}_q^{1,3}=\mathrm{BM}_q(2)$ has a standard $\mathrm{U}_q(\mathfrak{su}(2))$-covariant noncommutative differential calculus whose commutation relations between basic one-forms and the generators of the algebra are given by[15]

$$
\begin{aligned}
a\,\mathrm{d}a&=q^2(\mathrm{d}a)a,\\
a\,\mathrm{d}b&=(\mathrm{d}b)a,\\
a\,\mathrm{d}c&=q^2(\mathrm{d}c)a+(q^2-1)(\mathrm{d}a)c,\\
a\,\mathrm{d}d&=(\mathrm{d}d)a+(q^2-1)(\mathrm{d}b)c+(q-q^{-1})^2(\mathrm{d}a)a,\\
b\,\mathrm{d}a&=q^2(\mathrm{d}a)b+(q^2-1)(\mathrm{d}b)a,\\
b\,\mathrm{d}b&=q^2(\mathrm{d}b)b,\\
b\,\mathrm{d}c&=(\mathrm{d}c)b+(1-q^{-2})((\mathrm{d}d)a+(\mathrm{d}a)d)+(q-q^{-1})^2(\mathrm{d}b)c-(2-3q^{-2}+q^{-4})(\mathrm{d}a)a,\\
b\,\mathrm{d}d&=(\mathrm{d}d)b+(q^2-1)(\mathrm{d}b)d+(q^{-2}-1)(\mathrm{d}b)a+(q-q^{-1})^2(\mathrm{d}a)b,\\
c\,\mathrm{d}a&=(\mathrm{d}a)c,\\
c\,\mathrm{d}b&=(\mathrm{d}b)c+(1-q^{-2})(\mathrm{d}a)a,\\
c\,\mathrm{d}c&=q^2(\mathrm{d}c)c,\\
c\,\mathrm{d}d&=q^2(\mathrm{d}d)c+(q^2-1)(\mathrm{d}c)a,\\
d\,\mathrm{d}a&=(\mathrm{d}a)d+(q^2-1)(\mathrm{d}b)c+(q-q^{-1})^2(\mathrm{d}a)a,\\
d\,\mathrm{d}b&=q^2(\mathrm{d}b)d+(q^2-1)(\mathrm{d}a)b,\\
d\,\mathrm{d}c&=(\mathrm{d}c)d+(q^2-1)(\mathrm{d}d)c+(q-q^{-1})^2(\mathrm{d}c)a+(q^{-2}-1)(\mathrm{d}a)c,\\
d\,\mathrm{d}d&=q^2(\mathrm{d}d)d+(q^2-1)(\mathrm{d}c)b+(q^{-2}-1)(\mathrm{d}b)c-(1-q^{-2})^2(\mathrm{d}a)a.
\end{aligned}
\tag{52}
$$

This is designed in the $q\to 1$ limit to give the usual commutative calculus on classical $\mathbb{R}^{1,3}$. In order to obtain a noncommutative calculus in our noncommutative scaled limit $q\to 1$, we have to also redefine the derivative operator by a scale factor

$$\mathbf{d}=(q-q^{-1})\mathrm{d}.$$

This scaled derivative gives the following expressions for the basic one-forms:

$$\mathbf{d}x_+=\mathrm{d}c=(q-q^{-1})\mathrm{d}x_+,$$

$$\mathbf{d}x_-=\mathrm{d}b=(q-q^{-1})\mathrm{d}x_-,$$

$$\mathbf{d}h=\mathrm{d}a-\mathrm{d}d=(q-q^{-1})\mathrm{d}h.$$

Define also the basic one-form

$$\theta = q\,\mathrm{d}d + q^{-1}\mathrm{d}a,$$

which allows us to write

$$\mathbf{d}t = \frac{(q-q^{-1})}{c(q+q^{-1})}\,\theta. \tag{53}$$

This new set of generators and basic one-forms satisfy the following relations:

$$\begin{gathered}
x_+\mathbf{d}x_+ = q^2(\mathbf{d}x_+)x_+,\\
x_+\mathbf{d}x_- = (\mathbf{d}x_-)x_+ + \frac{q^{-1}}{(q+q^{-1})}\,\theta ct + \frac{1}{(q+q^{-1})}(\mathbf{d}h)ct + \mathcal{O}(q-q^{-1}),\\
x_+\mathbf{d}h = (\mathbf{d}h)x_+ - q\mathbf{d}x_+ + \mathcal{O}(q-q^{-1}),\\
x_-\mathbf{d}x_+ = (\mathbf{d}x_+)x_- + \frac{q^{-3}}{(q+q^{-1})}\,\theta ct - \frac{(2-q^{-2})}{(q+q^{-1})}(\mathbf{d}h)ct + \mathcal{O}(q-q^{-1}),\\
x_-\mathbf{d}x_- = q^2(\mathbf{d}x_-)x_-,\\
x_-\mathbf{d}h = q^2(\mathbf{d}h)x_- + q^{-1}(\mathbf{d}x_-)ct + \mathcal{O}(q-q^{-1}),\\
h\mathbf{d}x_+ = (\mathbf{d}x_+)h + q(\mathbf{d}x_+)ct + \mathcal{O}(q-q^{-1}),\\
h\mathbf{d}x_- = (\mathbf{d}x_-h) - q(\mathbf{d}x_-)ct + \mathcal{O}(q-q^{-1}),\\
h\mathbf{d}h = (\mathbf{d}h)h + \frac{2q}{(q+q^{-1})}\,\theta ct + \mathcal{O}(q-q^{-1}),\\
x_+\theta = \theta x_+ + q^2(\mathbf{d}x_+)ct + \mathcal{O}(q-q^{-1}),\\
x_-\theta = \theta x_- + q^2(\mathbf{d}x_-)ct + \mathcal{O}(q-q^{-1}),\\
h\theta = \theta h + \frac{2q}{(q+q^{-1})}(\mathbf{d}h)ct + \mathcal{O}(q-q^{-1}),\\
t\mathbf{d}x_+ = (\mathbf{d}x_+)t + \mathcal{O}(q-q^{-1}),\\
t\mathbf{d}x_- = (\mathbf{d}x_-)t + \mathcal{O}(q-q^{-1}),\\
t\mathbf{d}h = (\mathbf{d}h)t + \mathcal{O}(q-q^{-1}),\\
t\theta = \theta t + \mathcal{O}(q-q^{-1}).
\end{gathered} \tag{54}$$

In the limit $q\to 1$ we recover the relations (30) by setting $ct=\lambda$. Then the calculus on $\mathbb{R}^3_\lambda$ can be seen as the pull-back to the time slice of the scaled limit of the calculus on q-deformed Minkowski space. Unlike for usual $\mathbb{R}^3$, the dt direction in our noncommutative case does not "decouple" and has remnant θ. In other words, *the geometry of* $\mathbb{R}^3_\lambda$ *remembers that it is the pull-back of a relativistic theory*.

Finally, let us recall the action of the q-Lorentz group on the $\mathbb{R}^{1,3}_q$ and analyze its scaled limit when $q\to 1$. The appropriate q-Lorentz group can be written as the double cross coproduct $\mathrm{U}_q(\mathfrak{su}(2))\bowtie\mathrm{U}_q(\mathfrak{su}(2))$. The Hopf algebra $\mathrm{U}_q(\mathfrak{su}(2))$ is the standard q-deformed Hopf algebra which we write explicitly as generated by 1, X_+, X_- and $q^{\pm H/2}$ with

$$q^{\pm H/2}X_{\pm q}{}^{\mp H/2}=q^{\pm 1}X_{\pm},\quad [X_+,X_-]=\frac{q^H-q^{-H}}{q-q^{-1}},$$

$$\Delta(X_\pm)=X_\pm\otimes q^{H/2}+q^{-H/2}\otimes X_\pm,\quad \Delta(q^{\pm H/2})=q^{\pm H/2}\otimes q^{\pm H/2},$$

$$\epsilon(X_\pm)=0,\quad \epsilon(q^{\pm H/2})=1,$$

$$S(X_\pm)=-q^{\pm 1}X_\pm,\quad S(q^{\pm H/2})=q^{\mp H/2}. \tag{55}$$

It is well known that one may also work with these generators in an R-matrix form

$$\mathbf{l}^+=\begin{pmatrix} q^{H/2} & 0\\ q^{-1/2}(q-q^{-1})X_+ & q^{-H/2}\end{pmatrix},\quad \mathbf{l}^-=\begin{pmatrix} q^{-H/2} & q^{1/2}(q^{-1}-q)X_-\\ 0 & q^{H/2}\end{pmatrix}, \tag{56}$$

and most formulas are usually expressed in terms of these matrices of generators. In particular, the q-Lorentz group has two mutually commuting copies of $\mathrm{U}_q(\mathfrak{su}(2))$, so let us denote the generators of the first copy by $\mathbf{m}^\pm$ or $Y_\pm, G$ [related as for $\mathbf{l}^\pm$ and $X_\pm, H$ in (56)] and the generators of the second copy of $\mathrm{U}_q(\mathfrak{su}(2))$ by $\mathbf{n}^\pm$ or $Z_\pm, T$ (similarly related). The actions on $\mathbb{R}_q^{1,3}$ are given in Ref. 15 in an R-matrix form

$$\mathbf{n}^{\pm k}{}_l\triangleright\mathbf{u}^i{}_j=\langle\mathbf{n}^{\pm k}{}_l,t^m{}_j\rangle\mathbf{u}^i{}_m,\quad \mathbf{m}^{\pm k}{}_l\triangleright\mathbf{u}^i{}_j=\langle S\mathbf{m}^{\pm k}{}_l,t^i{}_m\rangle\mathbf{u}^m{}_j. \tag{57}$$

Here $\langle S\mathbf{m}^{\pm k}{}_l,t^i{}_j\rangle$ and $\langle\mathbf{n}^{\pm k}{}_l,t^i{}_j\rangle$ are the i,j matrix entries of the relevant functions of $Y_\pm, G$ and $Z_\pm, T$, respectively, in the Pauli matrix representation [as in (9) in other generators]. We need the resulting actions more explicitly, and compute them as

$$\frac{q^G-q^{-G}}{q-q^{-1}}\triangleright\begin{pmatrix} h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix} -\dfrac{2ct}{q-q^{-1}}-\dfrac{q-q^{-1}}{q+q^{-1}}h & -x_-\\ x_+ & \dfrac{q-q^{-1}}{q+q^{-1}}t-\dfrac{q-q^{-1}}{c(q+q^{-1})^2}h\end{pmatrix},$$

$$Y_+\triangleright\begin{pmatrix} h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix} -qx_+ & -\dfrac{qct}{q-q^{-1}}+\dfrac{h}{q+q^{-1}}\\ 0 & -\dfrac{q-q^{-1}}{c(q+q^{-1})}x_+\end{pmatrix}, \tag{58}$$

$$Y_-\triangleright\begin{pmatrix} h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix} q^{-1}x_- & 0\\ -\dfrac{q^{-1}ct}{q-q^{-1}}-\dfrac{h}{q+q^{-1}} & -\dfrac{q-q^{-1}}{c(q+q^{-1})}x_-\end{pmatrix},$$

$$\frac{q^T-q^{-T}}{q-q^{-1}}\triangleright\begin{pmatrix} h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix} \dfrac{2ct}{q-q^{-1}}+\dfrac{q-q^{-1}}{q+q^{-1}}h & -x_-\\ x_+ & -\dfrac{q-q^{-1}}{q+q^{-1}}t+\dfrac{q-q^{-1}}{c(q+q^{-1})^2}h\end{pmatrix},$$

$$Z_+\triangleright\begin{pmatrix} h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix} -x_+ & \dfrac{ct}{q-q^{-1}}+\dfrac{qh}{q+q^{-1}}\\ 0 & \dfrac{q(q-q^{-1})}{c(q+q^{-1})}x_+\end{pmatrix}, \tag{59}$$

$$Z_-\triangleright\begin{pmatrix} h & x_- \\ x_+ & t \end{pmatrix}=\begin{pmatrix} x_- & 0 \\ \dfrac{ct}{q-q^{-1}}-\dfrac{q^{-1}h}{q+q^{-1}} & \dfrac{q^{-1}(q-q^{-1})}{c(q+q^{-1})}x_- \end{pmatrix}.$$

We are now able to see that these actions (58) and (59) blow up in the limit $q\to 1$ because of some singular terms appearing in their expressions. Hence the scaling limit $\mathbb{R}_c^{1,3}$ is no longer Lorentz invariant.

On the other hand, we also have the same quantum group symmetry in an isomorphic form $\mathrm{BSU}_q(2)\rtimes \mathrm{U}_q(\mathfrak{su}(2))$ for $q\neq 1$, and this version survives. The braided algebra $\mathrm{BSU}_q(2)$ here is simply the braided matrices $\mathrm{BM}_q(2)$ with the additional condition $\det(\mathbf{u})=1$ (i.e., geometrically, it is the mass-hyperboloid in q-Minkowski space). To be clear, the generators of $\mathrm{BSU}_q(2)$ in this crossed product will be denoted by $\overline{\mathbf{u}}$ and the generators of $\mathrm{U}_q(\mathfrak{su}(2))$ in this cross product will be denoted by $\mathbf{l}^{\pm}$ or $X_{\pm}, H$ as before. The isomorphism with the q-Lorentz group in the form above is given by the assignments[15]

$$\overline{\mathbf{u}}\otimes 1\mapsto \mathbf{m}^+ S(\mathbf{m}^-)\otimes 1,\quad 1\otimes \mathbf{l}^{\pm}\mapsto \mathbf{m}^{\pm}\otimes \mathbf{n}^{\pm}. \tag{60}$$

Under the isomorphism (60), the expressions (58) and (59) become the action of $\mathrm{BSU}_q(2)\rtimes \mathrm{U}_q(\mathfrak{su}(2))$ on $\mathrm{BM}_q(2)$ given by

$$\overline{\mathbf{u}}\triangleright\mathbf{u}=\mathbf{m}^+ S(\mathbf{m}^-)\triangleright\mathbf{u},\quad \mathbf{l}^{\pm}\triangleright\mathbf{u}=\mathbf{m}^{\pm}\triangleright(\mathbf{n}^{\pm}\triangleright\mathbf{u}).$$

On the generators (49) the action of $\mathrm{BSU}_q(2)$ reads

$$\begin{aligned}
\overline{\mathbf{u}}_1^1\triangleright h&=-ct+qh-\frac{q(q-q^{-1})}{q+q^{-1}}h,\\
\overline{\mathbf{u}}_1^1\triangleright x_+&=qx_+,\\
\overline{\mathbf{u}}_1^1\triangleright x_-&=q^{-1}x_-,\\
\overline{\mathbf{u}}_1^1\triangleright t&=\frac{q^2+q^{-2}}{q+q^{-1}}t-\frac{(q-q^{-1})^2}{c(q+q^{-1})^2}h,\\
\overline{\mathbf{u}}_2^1\triangleright h&=q^{-2}(q-q^{-1})x_-\\
\overline{\mathbf{u}}_2^1\triangleright x_+&=-q^{-2}ct-\frac{q^{-1}(q-q^{-1})}{q+q^{-1}}h,\\
\overline{\mathbf{u}}_2^1\triangleright x_-&=0,\\
\overline{\mathbf{u}}_2^1\triangleright t&=-\frac{q-q^{-1}}{q+q^{-1}}t+\frac{q^{-1}(q-q^{-1})^2}{c(q+q^{-1})^2}h,\\
\overline{\mathbf{u}}_1^2\triangleright h&=-(q-q^{-1})x_+,\\
\overline{\mathbf{u}}_1^2\triangleright x_+&=0,\\
\overline{\mathbf{u}}_1^2\triangleright x_-&=-ct+\frac{q(q-q^{-1})}{q+q^{-1}}h,
\end{aligned} \tag{61}$$

$$\overline{\mathbf{u}}_1^2\triangleright t=-\frac{q(q-q^{-1})}{q+q^{-1}}t+\frac{(q-q^{-1})^2}{c(q+q^{-1})^2}h,$$

$$\overline{\mathbf{u}}_2^2\triangleright h=ct+qh-q^{-1}(q-q^{-1})ct-\frac{q^{-1}(q-q^{-1})-q^{-2}(q-q^{-1})^2}{q+q^{-1}}h,$$

$$\overline{\mathbf{u}}_2^2\triangleright x_+=q^{-1}x_++q^{-1}(q-q^{-1})^2x_+,$$

$$\overline{\mathbf{u}}_2^2\triangleright x_-=qx_-,$$

$$\overline{\mathbf{u}}_2^2\triangleright t=\frac{2t}{q+q^{-1}}+\frac{(q-q^{-1})^2}{q+q^{-1}}t\frac{(q-q^{-1})^2-q^{-1}(q-q^{-1})^3}{c(q+q^{-1})^2}h. \tag{62}$$

The action of $\mathrm{U}_q(\mathfrak{su}(2))$ is given by

$$\frac{q^H-q^{-H}}{q-q^{-1}}\triangleright\begin{pmatrix}h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix}0 & -(q+q^{-1})x_-\\ (q+q^{-1})x_+ & 0\end{pmatrix},$$

$$X_+\triangleright\begin{pmatrix}h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix}-q(q^{1/2}+q^{-1/2})x_+ & q^{1/2}h\\ 0 & 0\end{pmatrix}, \tag{63}$$

$$X_-\triangleright\begin{pmatrix}h & x_-\\ x_+ & t\end{pmatrix}=\begin{pmatrix}q^{-1/2}(q+q^{-1})x_- & 0\\ -q^{-1/2}h & 0\end{pmatrix}.$$

In the limit $q\to 1$, the crossed product $\mathrm{BSU}_q(2)\rtimes\mathrm{U}_q(\mathfrak{su}(2))$ becomes the double $D(\mathrm{U}(\mathfrak{su}(2)))=\mathbb{C}(\mathrm{SU}(2))\rtimes\mathrm{U}(\mathfrak{su}(2))$ as studied in Sec. III. The elements $\overline{\mathbf{u}}_j^i$ become in the limit the t_j^i, and $X_\pm$ and H become the usual $\mathfrak{su}(2)$ generators equivalent to the J_a there. (More precisely, we should map $\overline{u}_j^i$ to St_j^i for the action to become the right coregular one which we viewed in Sec. III as a left coaction.) Finally, this action of the double on $\mathrm{BM}_q(2)$ thus becomes in the scaling limit $q\to 1$ an action of $D(\mathrm{U}(\mathfrak{su}(2)))$ on $\mathbb{R}^{1,3}_c$ in the form

$$[x_+,x_-]=2cth,\quad [h,x_\pm]=\pm ctx_\pm,$$

with the same change of variables to x_a as in Sec. IV. The result is

$$M^i{}_j\triangleright t=0,\quad M^i{}_j\triangleright x_a=\frac{ct}{2\lambda}\sigma_a{}^i{}_j,\quad J_a\triangleright t=0,\quad J_a\triangleright x_a=\imath\epsilon_{abc}x_c.$$

This is consistent with the time slice $ct=\lambda$ and gives the action of the quantum double in Sec. III as in fact the nonsingular version of scaled limit of the q-Lorentz symmetry on the q-Minkowski space.

One can also analyze a different time slice of $\mathbb{R}^{1,3}_q$, namely, the quotient obtained by imposing the condition $ct=q^2+q^{-2}-1$. This algebra is the reduced braided algebra $\mathrm{BM}_q(2)^{\mathrm{red}}$, see Ref. 10, with commutation relations

$$x_+x_-=x_-x_++q^{-1}(q^2+q^{-2}-1)h+\frac{(q-q^{-1})}{(q+q^{-1})}h^2,$$

$$q^{-2}hx_+=x_+h+q^{-2}(q^2+q^{-2}-1)(q+q^{-1})x_+,$$

$$q^2hx_-=x_-h-(q^2+q^{-2}-1)(q+q^{-1})x_-.$$

This is also known in the literature as the "Witten algebra" [13,23] and in a scaled limit $q\to 1$ it likewise turns into the universal enveloping algebra $\mathrm{U}(\mathfrak{su}(2))$. A calculus on this reduced algebra, however, is not obtained from the calculus given by relations (52); consistency conditions result in the vanishing of all derivatives da, db and dc (note that the constraint on t allows one to write d in terms of the other generators).

VIII. QUANTUM MECHANICAL INTERPRETATION AND SEMICLASSICAL LIMIT OF $\mathbb{R}^3_\lambda$

Finally, we turn to the important question of how to relate expressions in the above noncommutative geometry to ordinary numbers in order to compare with experiment. We will first explain why a normal ordering postulate as proposed in Ref. 3 is not fully satisfactory and then turn to a quantum mechanical approach. Thus, one idea is to write elements of $\mathbb{R}^3_\lambda$ as: $f(x)$: where $f(x_1,x_2,x_3)$ is a classical function defined by a powerseries and : : denotes normal ordering when we use noncommutative variables x_i. If one sticks to this normal ordering, one can use it to compare classical with quantum expressions and express the latter as a strict deformation of the former controlled by the parameter λ governing the noncommutativity in (28). This will extend to the rest of the geometry and allows an order-by-order analysis. For example, the noncommutative partial derivatives ∂_a defined in (34) have the expressions to lowest order

$$\begin{aligned}
\partial_1{:}f(x){:} &= {:}\overline{\partial}_1 f(x){:}+\frac{\imath\lambda}{2}\overline{\partial}_2\overline{\partial}_3 f(x),\\
\partial_2{:}f(x){:} &= {:}\overline{\partial}_2 f(x){:}-\frac{\imath\lambda}{2}\overline{\partial}_1\overline{\partial}_3 f(x),\\
\partial_3{:}f(x){:} &= {:}\overline{\partial}_3 f(x){:}+\frac{\imath\lambda}{2}\overline{\partial}_2\overline{\partial}_2 f(x),\\
\frac{1}{c}\partial_0{:}f(x){:} &= \frac{\lambda}{4}((\overline{\partial}_1)^2 f(x)+(\overline{\partial}_2)^2 f(x)+(\overline{\partial}_3)^2 f(x)),
\end{aligned}\tag{64}$$

where $\overline{\partial}_a$ are the usual partial derivatives in classical variables and we do not write the normal ordering on expressions already $O(\lambda)$ since the error is higher order. Note that the expression for $(1/c)\,\partial_0$ is one order of λ higher than the other partial derivatives, which is another way to see that this direction is an anomalous dimension originating in the quantization process. The physical problem here is that the normal ordering is somewhat arbitrary; for algebras such as (1) or for usual phase space, putting all t to one side makes a degree of sense physically, as well as mathematically because the algebra is solvable. But in the simple case such as $\mathbb{R}^3_\lambda$, each of the x_1, x_2, x_3 should be treated equally. Or one could use other coordinates such as x_-, h, x_+ in keeping with the Lie algebra structure, etc.; all different ordering schemes giving a different form of the lowest order corrections and hence different predictions. Choosing a natural ordering is certainly possible but evidently would require further input into the model.

On the other hand, we can take a more quantum mechanical line and consider our algebra $\mathbb{R}^3_\lambda$ as, after all, a spin system. The main result of this section is to introduce "approximately classical" states' $|j,\theta,\phi\rangle$ for this system inspired in part by the theorem of Penrose[19] for spin networks, although not directly related to that. Penrose considered networks labeled by spins and showed how to assign probabilities to them and conditions for when the network corresponds approximately to spin measurements oriented with relative angles θ,ϕ. In a similar spirit we consider the problem of reconstructing classical angles from the noncommutative geometry.

We let $V^{(j)}$ be the vector space which carries a unitary irreducible representation of spin $j\in\frac{1}{2}\mathbb{Z}_+$, generated by states $|j,m\rangle$, with $m=-j,\ldots,j$ such that

$$x_\pm|j,m\rangle=\lambda\sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm 1\rangle,$$

$$h|j,m\rangle = 2\lambda m|j,m\rangle.$$

The projection of $\mathbb{R}^3_\lambda$ to an irreducible representation of spin j is geometrically equivalent to a restriction to a fuzzy sphere,[5,14] because the value of the Casimir $x\cdot x$ is $\lambda^2 j(j+1)$ in this representation. We have discussed this in Sec. VI, where we set $x\cdot x=1$ and considered the algebra geometrically as such a fuzzy sphere under a quantization condition for λ. By contrast in this section we leave $x\cdot x$ unconstrained and consider the geometry of our noncommutative three-dimensional space $\mathbb{R}^3_\lambda$ as the sum of geometries on all fuzzy spheres with the $V^{(j)}$ representation picking out the one of radius $\sim\lambda j$. Thus we use the Peter–Weyl decomposition of $\mathbb{C}(\mathrm{SU}_2)$ into matrix elements of irreducible representations regarded as functions on SU_2, which gives (up to some technical issues about completions) a similar decomposition for its dual as $\mathbb{R}^3_\lambda = \oplus_j \mathrm{End}(V^{(j)})$. This also underlies the spherical harmonics in Sec. III.

Next, for each fixed spin j representation we look for normalized states $|j,\theta,\phi\rangle$ parametrized by $0\leqslant\theta\leqslant\pi$ and $0\leqslant\varphi\leqslant 2\pi$, such that

$$\begin{aligned}\langle j,\theta,\varphi|x_1|j,\theta,\varphi\rangle &= r\sin\theta\cos\varphi,\\ \langle j,\theta,\varphi|x_2|j,\theta,\varphi\rangle &= r\sin\theta\sin\varphi,\\ \langle j,\theta,\varphi|x_3|j,\theta,\varphi\rangle &= r\cos\theta,\end{aligned} \tag{65}$$

where r is some constant (independent of θ,ϕ) which we do not fix. Rather, in the space of such states and possible $r\geqslant 0$, we seek to minimize the normalized variance

$$\delta = \frac{\langle x\cdot x\rangle - \langle x\rangle\cdot\langle x\rangle}{\langle x\rangle\cdot\langle x\rangle}, \tag{66}$$

where $\langle\ \rangle = \langle j,\theta,\phi|\ |j,\theta,\phi\rangle$ is the expectation value in our state and we regard $\langle x_a\rangle$ as a classical vector in the dot product. Thus we seek states which are ''closest to classical.'' This is a constrained problem and leads us to the following states:

$$|j,\theta,\varphi\rangle = \sum_{k=1}^{2j+1} 2^{-j}\sqrt{\binom{2j}{k-1}}(1+\cos\theta)^{(j-k+1)/2}(1-\cos\theta)^{(k-1)/2}e^{\imath(k-1)\varphi}|j,j-k+1\rangle. \tag{67}$$

These obey $\langle j,\theta,\phi|j,\theta,\phi\rangle = 1$ and (65)–(66) with

$$r = \sqrt{\langle x\rangle\cdot\langle x\rangle} = \lambda j, \quad \delta = \frac{1}{j}. \tag{68}$$

We see that in these states the ''true radius'' $|\langle x\rangle|$ is λj. The square root of the Casimir does not give this true radius since it contains also the uncertainty expressed in the variance of the position operators, but the error δ vanishes as $j\to\infty$. Thus the larger the representation, the more the geometry resembles to the classical.

We can therefore use these states $|j,\theta,\phi\rangle$ to convert noncommutative geometric functions $f(x)$ into classical ones in spherical polar coordinates defined by

$$\langle f\rangle(r,\theta,\phi) \equiv \langle j,\theta,\phi|f(x)|j,\theta,\phi\rangle, \tag{69}$$

where $r=\lambda j$ is the effective radius. If we start with a classical function f and insert noncommutative variables in some order, then $\langle f(x)\rangle$ (which depends on the ordering) looks more and more like $f(\langle x\rangle)$ as $j\to\infty$ and $\lambda\to 0$ with the product fixed to an arbitrary r. As an example, the noncommutative spherical harmonics Y_l^m in Sec. III are already ordered in such a way that replacing the noncommutative variables by the expectation values $\langle x_a\rangle$ gives something propor-

tional to the classical spherical harmonics. On the other hand, $\langle Y_l^m \rangle$ vanish for $l>2j$ and only approximate the classical ones for lower l. Moreover, in view of the above, we expect

$$\langle \partial_i f \rangle = \overline{\partial_i} \langle f \rangle + O\left(\lambda, \frac{1}{j}\right), \tag{70}$$

where $r=j\lambda$ and $\overline{\partial_i}$ are the classical derivatives in the polar form

$$\overline{\partial_1} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{1}{r}\sin\theta\sin\varphi\frac{\partial}{\partial\varphi},$$

$$\overline{\partial_2} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{1}{r}\sin\theta\cos\varphi\frac{\partial}{\partial\varphi},$$

$$\overline{\partial_3} = \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta},$$

where we understand $\partial/\partial r = (1/\lambda)(\partial/\partial j)$ on expectation values computed as functions of j. More precisely, one should speak in terms of the joint limit as explained above with $\lambda j = r$ a continuous variable in the limit. We note finally that the star product for $\mathbb{R}^3_\lambda$ as in Ref. 11 suggests that it should be possible to extend such a semiclassical analysis to all orders.

ACKNOWLEDGMENT

E.B. was supported by CAPES, proc. BEX0259/01-2. S.M. is a Royal Society University Research Fellow.

APPENDIX: 2-D AND 3-D CALCULI ON $\mathbb{R}^3_\lambda$

It might be asked why we need to take a four-dimensional calculus on $\mathbb{R}^3_\lambda$ and not a smaller one. In fact, bicovariant differential calculi on enveloping algebras $U(\mathfrak{g})$ such as $\mathbb{R}^3_\lambda \cong U(\mathfrak{su}(2))$ have been essentially classified[18] and in this appendix we look at some of the other possibilities for our model. In general the co-irreducible calculi (i.e., having no proper quotients) are labeled by pairs (V_ρ, Λ), with $\rho: U(\mathfrak{g}) \to \mathrm{End}V_\rho$ an irreducible representation of $U(\mathfrak{g})$ and Λ a ray in V_ρ. In order to construct an ideal in $\ker \epsilon$, take the map

$$\rho_\Lambda : U(\mathfrak{g}) \to V_\rho, \quad h \mapsto \rho(h)\cdot\Lambda.$$

It is easy to see that $\ker \rho_\Lambda$ is a left ideal in $\ker \epsilon$. Then, if ρ_Λ is surjective, the space of one-forms can be identified with $V_\rho = \ker\epsilon/\ker\rho_\Lambda$. The general commutation relations are

$$av = va + \rho(a)\cdot v, \tag{A1}$$

and the derivative for a general monomial $\xi_1\cdots\xi_n$ is given by the expression

$$\mathrm{d}(\xi_1\cdots\xi_n) = \sum_{k=1}^{n} \sum_{\sigma\in S_{(n,k)}} \rho_\Lambda(\xi_{\sigma(1)}\cdots\xi_{\sigma(k)})\xi_{\sigma(k+1)}\cdots\xi_{\sigma(n)},$$

the sum being over all (n,k) shuffles.

We explore some examples of co-irreducible calculi for the universal enveloping algebra $\mathbb{R}^3_\lambda$, generated by $x_\pm$ and h satisfying the commutation relations (28). First, let us analyze the three-dimensional, co-irreducible calculus on $\mathbb{R}^3_\lambda$ by taking $V_\rho = \mathbb{C}^3$, with basis

$$e_+ = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_- = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

In this basis, the representation ρ takes the form

$$\rho(x_+)=\lambda\begin{pmatrix}0&2&0\\0&0&1\\0&0&0\end{pmatrix},\quad \rho(x_-)=\lambda\begin{pmatrix}0&0&0\\1&0&0\\0&2&0\end{pmatrix},\quad \rho(h)=\lambda\begin{pmatrix}2&0&0\\0&0&0\\0&0&-2\end{pmatrix}.$$

We choose, for example, $\Lambda=e_0$. The space of one-forms will be generated by the vectors e_+, e_- and e_0. The derivatives of the generators of the algebra are given by

$$\mathrm{d}x_+=\lambda^{-1}\rho(x_+)\cdot e_0=2e_+,\quad \mathrm{d}x_-=\lambda^{-1}\rho(x_-)\cdot e_0=2e_-,\quad \mathrm{d}h=\lambda^{-1}\rho(h)\cdot e_0=0.$$

The commutation relations between the basic one-forms and the generators can be deduced from (A1) giving

$$\begin{gathered}x_+e_+=e_+x_+,\\ x_+e_0=e_0x_++2\lambda e_+,\\ x_+e_-=e_-x_++\lambda e_0,\\ x_-e_+=e_+x_-+\lambda e_0,\\ x_-e_0=e_0x_-+2\lambda e_-,\\ x_-e_-=e_-x_-,\\ he_+=e_+h+2\lambda e_+,\\ he_0=e_0h,\\ he_-=e_-h-2\lambda e_-.\end{gathered}\tag{A2}$$

The expression for the derivative of a general monomial $x_+^a x_-^b h^c$ is

$$\begin{aligned}\mathrm{d}(x_+^a x_-^b h^c)=&2ae_+x_+^{a-1}x_-^b h^c+2be_-x_+^a x_-^{b-1}h^c+2\lambda abe_0x_+^{a-1}x_-^{b-1}h^c\\&+4\lambda^2a(a-1)be_+x_+^{a-2}x_-^{b-1}h^c.\end{aligned}\tag{A3}$$

We define the exterior algebra by skew-symmetrizing and, using similar methods as in Sec. IV, we compute the cohomologies as

$$H^0=\mathbb{C}[h],\quad H^1=e_0\mathbb{C}[h],\quad H^2=H^3=\{0\}.$$

This calculus is a three-dimensional calculus but we have introduced an isotropy by choosing Λ, and related to this all functions of h are killed by d, which is why the cohomology is large. This is why we do not take this calculus even though it has the ''obvious'' dimension. There is the same problem if we choose any other direction Λ.

We can also have a two-dimensional coirreducible calculus on $\mathrm{U}(su(2))$ using then $V_\rho=\mathbb{C}^2$, with basis

$$e_1=\begin{pmatrix}1\\0\end{pmatrix},\quad e_2=\begin{pmatrix}0\\1\end{pmatrix}.$$

In this basis, the representation ρ takes the form

$$\rho(x_+)=\lambda\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad \rho(x_-)=\lambda\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad \rho(h)=\lambda\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Choosing $\Lambda=e_1$, the space of one-forms will be generated by e_1 and e_2 and the derivatives of the generators of the algebra are given by

$$\mathrm{d}x_+=\lambda^{-1}\rho(x_+)\cdot e_1=0,\quad \mathrm{d}x_-=\lambda^{-1}\rho(x_-)\cdot e_1=e_2,\quad \mathrm{d}h=\lambda^{-1}\rho(h)\cdot e_1=e_1.$$

The commutation relations between the basic one-forms and the generators are then

$$\begin{aligned}
x_+e_1&=e_1x_+,\\
x_+e_2&=e_2x_++\lambda e_1,\\
x_-e_1&=e_1x_-+\lambda e_2,\\
x_-e_2&=e_2x_-,\\
he_1&=e_1h+\lambda e_1,\\
he_2&=e_2h-\lambda e_2.
\end{aligned}\tag{A4}$$

And the derivative of a monomial $x_-^a h^b x_+^c$ is given by

$$\mathrm{d}(x_-^a h^b x_+^c)=e_1\left(\sum_{i=0}^{b}\binom{b}{i}\lambda^{i-1}x_-^a h^{b-i}x_+^c\right)+e_2\left(\sum_{i=0}^{b}(-1)^i\binom{b}{i}\lambda^i a x_-^{a-1}h^{b-i}x_+^c\right).\tag{A5}$$

The cohomology of this calculus comes out as

$$H^0=\mathbb{C}[x_+],\quad H^1=H^2=\{0\}.$$

Here again d vanishes on all functions of x_+, which is related to our choice of Λ. On the other hand, this calculus motivates us similarly to take for ρ the tensor product of the spin $\frac{1}{2}$ representations and its dual. In this tensor product representation there is a canonical choice of Λ, namely the 2×2 identity matrix. This solves the anisotropy and kernel problems and this is the calculus that we have used on $\mathbb{R}^3_\lambda$ as the natural choice in our situation. The above spinorial ones are coirreducible quotients of it.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

Chern–Simons field theories with non-semisimple gauge group of symmetry

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(Received 13 March 2002; accepted 18 September 2002)

The subject of this work is a class of Chern–Simons field theories with non-semisimple gauge group, which may well be considered as the most straightforward generalization of an Abelian Chern–Simons field theory. As a matter of fact, these theories, which are characterized by a non-semisimple group of gauge symmetry, have cubic interactions like those of non-Abelian Chern–Simons field theories, but are free from radiative corrections. Moreover, at the tree level in the perturbative expansion, there are only two connected tree diagrams, corresponding to the propagator and to the three vertex originating from the cubic interaction terms. For such theories it is derived here a set of BRST invariant observables, which lead to metric independent amplitudes. The vacuum expectation values of these observables can be computed exactly. From their expressions it is possible to isolate the Gauss linking number and an invariant of the Milnor type, which describes the topological relations among three or more closed curves. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1525049]

I. FOREWORD

In several situations it has been experimentally observed that the topological properties of certain physical systems may influence their behavior to a relevant extent. This is, for instance, the case of vortex structures in nematic liquid crystals[1] and in ^{3}He superfluids.[2] Other examples are provided by polymers[3] or by the lowest lying excitations of two-dimensional electron gases, which have topological nontrivial configurations at some filling fractions.[4] In the investigation of phenomena related to the presence of topological constraints in physical systems, the use of quantum or statistical mechanical models coupled to Abelian Chern–Simons (C-S) field theories[5] has been particularly successful. One reason of this success is the fact that Abelian models do not require a complex mathematical treatment as their non-Abelian counterparts do, and thus their physical meaning is more transparent.

Motivated by applications in polymer physics[6–8] the aim of this work is the construction of topological field theories with nontrivial cubic interactions similar to those of non-Abelian C-S field theories, but which still retain the simplicity of the Abelian case. For this purpose, suitable candidates are C-S field theories with non-semisimple group of gauge symmetry. Roughly speaking, Lie algebras associated to non-semisimple groups contain nontrivial Abelian ideals, so that one could expect on this ground that at least part of the observables of these theories should have ''Abelian'' characteristics.

Chern–Simons field theories and, more in general, gauge field theories with non-semisimple groups of symmetry have been already proposed in Refs. 9 and 10. Here it is picked up a particular class of such theories with the main property of being free from radiative corrections. Also at the tree level in the perturbative expansion several simplifications occur and it is possible to show that there are only two connected diagrams, the propagators and the three vertices corresponding to the fields' self-interactions. This situation is reminiscent of that of an Abelian field theory, in which there is just one connected diagram, namely the propagator. Most interestingly, the theories dis-

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cussed in this work admit a set of observables which resemble Abelian Wilson loops and lead to metric independent amplitudes. With respect to standard Wilson loops, these observables contain extra terms, which are required to enforce BRST invariance. From their vacuum expectation values, which are computed exactly, it is possible to isolate a topological invariant, which describes the topological properties of three or more closed loops.

The material presented in this article is divided as follows. In Sec. II a class of C-S field theories with non-semisimple group of symmetry is introduced, which consists in a set of Abelian BF models[11] coupled together by cubic interaction terms. The BRST quantization of these theories is discussed using the covariant gauge of Lorentz in order to fix gauge invariance. Further, it is shown that radiative corrections are absent and that there are only two connected Feynman diagrams at the tree level. The case of manifolds with nontrivial topology, in which zero modes may appear, is discussed in Sec. III. It is shown that zero modes generate large gauge transformations which leave invariant the action and the equations of motion of the theories under consideration. In this way, it becomes possible to treat zero modes as gauge degrees of freedom and to gauge them away, as advocated in Ref. 12. In Sec. IV a set of BRST invariant observables is derived and their vacuum expectation values are computed. Finally, the conclusions and a possible physical application of the results contained in this work are presented in Sec. V.

II. CHERN–SIMONS FIELD THEORIES WITH NON-SEMISIMPLE GROUP OF SYMMETRY

Let us consider a class of Chern–Simons field theories with action:

$$S=\int_M \Omega_{iI}\epsilon^{\mu\nu\rho}\left(B^I_\mu\partial_\nu A^i_\rho+\frac{\lambda}{6}f^I_{jk}A^i_\mu A^j_\nu A^k_\rho\right), \tag{1}$$

where i, $I=1,...,N$ and Ω_{Ii} denotes a nondegenerate bilinear form. Summation over repeated indices is everywhere understood. The theory is defined on a three-dimensional manifold M without boundary and equipped with a Euclidean metric. For simplicity, we assume for the moment that all the de Rham cohomology groups $H^n(M)$ are trivial, so that the problem of harmonic zero modes does not appear. We will discuss zero modes in the next section.

The action (1) is invariant under the following gauge transformations:

$$A^i_\mu\to A^i_\mu+\partial_\mu\eta^i, \tag{2}$$

$$B^I_\mu\to B^I_\mu+\partial_\mu\theta^I-\lambda f^I_{ij}\left(\frac{\eta^i\partial_\mu\eta^j}{2}+\eta^i A^i_\mu\right) \tag{3}$$

for arbitrary functions η^i and θ^I. The above transformations correspond to a non-semisimple group of symmetry. The related generators X_i and H_I satisfy the following non-semisimple Lie algebra:

$$[H_I,H_J]=[H_I,X_j]=0,\quad [X_i,X_j]=f^I_{ij}H_I \tag{4}$$

with structure constants f^I_{ij}. This Lie algebra consists in an Abelian Lie algebra $\mathfrak{g}$ with a central extension by an Abelian group $\mathfrak{h}$. The generators of $\mathfrak{g}$ and $\mathfrak{h}$ are the X_i and H_I's, respectively. Let us denote with the symbols $\mathfrak{G}$ and $\mathfrak{H}$ respectively the associated Abelian Lie groups. The matrix Ω_{Ii} appearing in (1) is the generalization of the Killing form to the case of non-semisimple groups. Theories such as those discussed here have been already proposed in Refs. 9 and 10. Other applications of non-semisimple Lie algebras can be found in Refs. 13 and 14.

To eliminate the gauge freedom of the action (1), we introduce the covariant gauge conditions:

$$\partial^\mu A^i_\mu=\partial^\mu B^I_\mu=0. \tag{5}$$

The theory can now be quantized using the procedure of BRST quantization. The BRST transformations associated to the gauge transformations (2) and (3) are given by

$$\delta A^i_\mu = \partial_\mu c^i, \tag{6}$$

$$\delta B^I_\mu = \partial_\mu \xi^I + \lambda f^I_{ij} A^i_\mu c^j, \tag{7}$$

$$\delta \xi^I = \frac{\lambda}{2} f^I_{ij} c^i c^j, \tag{8}$$

$$\delta c^i = 0, \tag{9}$$

$$\delta \overline{c_i} = i a_i, \quad \delta a_i = 0, \tag{10}$$

$$\delta \overline{\xi_I} = i b_I, \quad \delta b_I = 0, \tag{11}$$

where c^i, ξ^I and $\overline{c_i}$, $\overline{\xi_I}$ are anticommuting ghosts, while a_i, b_I are scalar fields. It is possible to verify that the transformations (6)–(11) are nilpotent, i.e., $\delta^2 = 0$.

At this point, one can write the expression of the gauge fixed BRST invariant action:

$$S_{\rm BRST} = S + S_{gf} + S_{\rm FP}, \tag{12}$$

where S is given by Eq. (1), while the gauge fixing and Fadeev–Popov terms are respectively

$$S_{gf} = i \int_M d^3x \, [a_i \partial^\mu A^i_\mu + b_I \partial^\mu B^I_\mu], \tag{13}$$

$$S_{\rm FP} = \int_M d^3x \, [\partial_\mu \overline{c_i} \partial^\mu c^i + \partial^\mu \overline{\xi_I} (\partial_\mu \xi^I + \lambda f^I_{ij} A^i_\mu c^j)]. \tag{14}$$

The combination $S_{gf} + S_{\rm FP}$ amounts to a BRST exact variation as expected:

$$S_{gf} + S_{\rm FP} = -\delta \int_M [\overline{c_i} \partial^\mu A^i_\mu + \overline{\xi_I} \partial^\mu B^I_\mu]. \tag{15}$$

Thus, the gauge fixing and Faddeev–Popov terms do not spoil the topological properties of the original action (1).

Let us note that the fields B^I_μ and ξ^I play in (12) the role of pure Lagrange multipliers, which constrain the fields A^i_μ and $\overline{\xi_I}$ in such a way that all possible radiative corrections vanish identically. In particular, the interaction term in the ghost action (14) disappears after an integration over the fields ξ^I, which gives as a result the constraints

$$\partial_\mu \partial^\mu \overline{\xi_I} = 0. \tag{16}$$

Choosing suitable boundary conditions for which the $\overline{\xi_I}$'s do not diverge at infinity, the above equation is satisfied only for constant fields $\overline{\xi_I}$. The integration over the fields B^I_μ leads instead to the flatness conditions:

$$\Omega_{Ii} \epsilon^{\mu\nu\rho} \partial_\nu A^i_\rho = 0. \tag{17}$$

The above equations determine the transverse components of the fields A^i_ρ, while the longitudinal components are fixed by the gauge fixing (13).

Since radiative corrections are absent, the theory (12) is purely classical. Thus, contrarily to what happens for instance in the case of Chern–Simons theories with gauge group SU(N), there

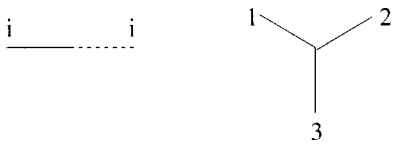

FIG. 1. Feynman rules corresponding to the action (12). Dashed lines propagate B^I_μ fields while solid lines are associated to A^i_μ fields.

is no rescaling of the Chern–Simons coupling constants, which here have been set equal to one. Also at the classical level several simplifications occur and in practice the theory admits only the two connected Feynman diagrams shown in Fig. 1. These diagrams correspond to the field propagators and to the three-vertex associated to the cubic interaction term present in Eq. (12). Higher order tree diagrams, which could in principle be constructed by contracting together the legs of many three-vertices, are actually ruled out due to the off-diagonal structure of the propagators, which forbids any self-interaction among the fields A^i_μ.

Due to the fact that the theory is purely classical, its partition function can be exactly derived once the classical solutions of the field equations are known. With a simple integration it is possible to eliminate the fields B^I_μ and the ghosts. As an upshot, one obtains the constraints (16) and (17). These constraints and the gauge fixing relations are enough to determine uniquely the remaining fields. If the theory is defined for instance on a manifold with flat metric, the solutions of the constraints (17) are simply $A^i_\mu = 0$, so that the partition function is the trivial one.

III. THE ZERO MODE PROBLEM

In this section we consider the case in which the fields admit nontrivial classical configurations, the so-called harmonic zero modes. We can ignore possible zero modes in the sectors of the ghost fields and of the Lagrange multipliers a_i, b_I, because these zero modes are not used in the gauge fixing procedure. We are thus left only with the zero modes of the fields A^i_μ, B^I_μ, which we denote with the symbols α^i_μ and β^I_μ, respectively. From the action (1) one finds the relevant equations of motion which define α^i_μ and β^I_μ:

$$\epsilon^{\mu\nu\rho}\partial_\nu A^i_\rho = 0, \tag{18}$$

$$\epsilon^{\mu\nu\rho}\partial_\nu B^I_\rho + \frac{\lambda}{2}\,\epsilon^{\mu\nu\rho} f^I_{jk} A^j_\nu A^k_\rho = 0. \tag{19}$$

The general solution of Eq. (18) is

$$A^i_\mu = \alpha^i_\mu + \partial_\mu \eta^i, \tag{20}$$

where $\partial_\mu \eta^i$ is an exact differential, while α^i_μ is a nontrivial Abelian flat connection corresponding to the Abelian subgroup of the underlying gauge group. Let us consider now Eq. (19). This relation can be rewritten as follows:

$$\epsilon^{\mu\nu\rho}\partial_\nu B^I_\rho = J^{I\mu} \tag{21}$$

with the current $J^{I\mu}$ given by

$$J^{I\mu} = -\frac{\lambda}{2}\,\epsilon^{\mu\nu\rho} f^I_{jk} A^j_\nu A^k_\rho. \tag{22}$$

Equation (18) implies that $J^{I\mu}$ is purely transverse, i.e., $\partial_\mu J^{I\mu} = 0$. Using this fact, it is possible to show that Eq. (19) is solved by

$$B^I_\mu = \int_M d^3y G_{\mu\nu}(x,y) J^{I\nu}(y) + \beta^I_\mu + \partial_\mu \eta^I, \tag{23}$$

where $G_{\mu\nu}(x,y)$ is the propagator of the theory in the Lorentz gauge (5) and β^I_μ is a nontrivial flat connection satisfying the flatness condition $\epsilon^{\mu\nu\rho}\partial_\nu \beta^I_\rho = 0$. We remember that the fields B^I_μ are pure Lagrange multipliers imposing the constraints (18) on the fields A^i_μ. It is easy to check that the presence or not of the term β^I_ρ does not affect these constraints nor the other equations of motion, so that one can put $\beta^I_\mu = 0$ without any loss of generality.

A possible strategy to treat harmonic zero modes is to consider them as gauge degrees of freedom and to gauge them away using BRST techniques. This approach has been proposed by Polyakov in Ref. 12 and further developed in Ref. 15. An application to the BF-systems can be found in Ref. 16. In order to check if it is possible to translate the zero mode problem in a gauge fixing problem also in the present case, the crucial point is to verify the invariance of the theory (1) under large gauge transformations. As a matter of fact, the α^i_μ's generate large gauge transformations, consisting in multivalued mapping of the manifold M onto the elements of the Abelian group which corresponds to the Lie algebra $\mathfrak{G}$ defined after Eq. (4).

To express the large gauge transformations acting on the fields in a closed form, it is convenient to introduce potentials Λ^i such that

$$\partial_\mu \Lambda^i = \alpha^i_\mu. \tag{24}$$

These potentials, which will be in general multivalued on the manifold M, are the analogous of the functions η^i appearing in the gauge transformations (2) and (3). In terms of the Λ^i's, the large gauge transformations induced by the harmonic modes α^i_μ are given by

$$A^i_\mu \to A^i_\mu + \partial_\mu \Lambda^i, \tag{25}$$

$$B^I_\mu \to B^I_\mu - \lambda f^I_{ij}\left(\frac{\Lambda^i \partial_\mu \Lambda^j}{2} + \Lambda^i A^j_\mu\right). \tag{26}$$

Actually, the full transformations of the fields B^I_μ are not necessary in order to discuss the gauge invariance of the action S and of the equations of motion. As a matter of fact, apart from a total derivative, the action (1) can be rewritten as follows:

$$S = \int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} A^i_\mu \left[\partial_\nu B^I_\rho + \frac{\lambda}{6} f^I_{jk} A^j_\nu A^k_\rho\right]. \tag{27}$$

Thus, only the transformations of the pseudo-tensors $\epsilon^{\mu\nu\rho}\partial_\nu B^I_\rho$ are needed:

$$\epsilon^{\mu\nu\rho}\partial_\nu B^I_\rho \to \epsilon^{\mu\nu\rho}\partial_\nu B^I_\rho - \frac{\lambda}{2}\epsilon^{\mu\nu\rho} f^I_{jk}(\partial_\nu \Lambda^j \partial_\rho \Lambda^k + 2\Lambda^j \partial_\nu A^k_\rho + 2\partial_\nu \Lambda^j A^k_\rho). \tag{28}$$

At this point we are ready to perform a large gauge transformation of the kind (25)–(28) in the action S. Since the right-hand side of Eq. (28) has an explicit dependence on the potentials Λ^i, the gauge transformed action will contain multivalued contributions. However, it is easy to prove that all these contributions vanish identically due to the following identities, valid up to total derivative terms which are irrelevant on a manifold without boundary:

$$\int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} A^i_\mu \partial_\rho A^j_\nu \Lambda^k = -\frac{1}{2}\int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} A^i_\mu A^j_\nu \alpha^k_\rho, \tag{29}$$

$$\int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} \alpha^i_\mu \partial_\rho A^j_\nu \Lambda^k = -\int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} \alpha^i_\mu A^j_\nu \alpha^k_\rho. \tag{30}$$

Another important identity, which follows from the fact that the α_μ^i's satisfy the classical equations of motion (18), is

$$\int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} \alpha^i_\mu \alpha^j_\nu \alpha^k_\rho = \int_M d^3x\, \Omega_{Ii} \epsilon^{\mu\nu\rho} f^I_{jk} \partial_\mu \Lambda^i \partial_\nu \Lambda^j \partial_\rho \Lambda^k = 0. \tag{31}$$

With the help of the relations (29)–(31) it is possible to verify the invariance of the action S under large gauge transformations as desired.

One can also check that the gauge transformations (25) and (28) preserve the form of the equations of motion (18) and (19). After a gauge transformation, in fact, one obtains the following result:

$$\epsilon^{\mu\nu\rho} \partial_\nu A^i_\rho = 0, \tag{32}$$

$$\epsilon^{\mu\nu\rho} \partial_\nu B^I_\rho + \frac{\lambda}{2} \epsilon^{\mu\nu\rho} f^I_{jk} (A^j_\nu A^k_\rho - 2 \partial_\nu A^k_\rho \Lambda^j) = 0. \tag{33}$$

The spurious term proportional to Λ^j in Eq. (33) vanishes identically due to Eq. (32).

IV. OBSERVABLES AND WILSON-LOOP-LIKE AMPLITUDES

Good observables of a topological field theory should be BRST invariant and lead to vacuum expectation values which are metric independent.

To derive a set of observables for the theory under consideration, we first observe that the following quantity is invariant under the BRST transformations (6)–(11):

$$\begin{aligned} T^I(\Gamma) = & \oint_\Gamma dx^\mu B^I_\mu + \frac{\lambda}{4\pi} f^I_{ij} \oint_\Gamma dx^\mu A^i_\mu \int d^3y \frac{1}{|x-y|} \partial^\rho_y A^j_\rho(y) \\ & + \frac{\lambda}{2(4\pi)^2} f^I_{ij} \oint_\Gamma dx^\mu \int d^3y \left(\partial^x_\mu \frac{1}{|x-y|} \right) \partial^\rho_y A^i_\rho(y) \int d^3z \frac{1}{|x-z|} \partial^\sigma_z A^j_\sigma(z). \end{aligned} \tag{34}$$

In the above formula as well as in the rest of this article, it has been assumed for simplicity that the manifold M coincides with the three-dimensional Euclidean space $\mathbf{R}^3$. The form of $T^I(\Gamma)$ has been obtained starting from the line integral $\oint_\Gamma dx^\mu B^I_\mu$ and adding suitable terms in order to make it gauge and BRST invariant. At this point, for M loops Γ^a, $a = 1,...,M$, it is possible to write down analogs of the holonomic connections as follows:

$$W(\overline{C}) = e^{iC_{aI} T^I(\Gamma^a)}, \tag{35}$$

where $\overline{C}$ is a matrix having as elements constant parameters C_{aI}.

We note that $W(\overline{C})$ is of the form

$$W(\overline{C}) = \exp\left[iC^{aI} \oint_{\Gamma_a} dx^\mu B^I_\mu + \int d^3x \chi_i(x) \partial^\mu A^i_\mu(x) \right]. \tag{36}$$

All contributions coming from the various line integrals which are present on the right-hand side of Eq. (34) are now contained in the scalars $\chi_i(x)$. As a consequence of Eq. (36), even if $W(\overline{C})$ is manifestly metric dependent, a metric variation of this observable can always be compensated by a shift of the Lagrange multipliers a_i which impose the gauge condition in the action (12). Thus, the vacuum expectation values of the operators $W(\overline{C})$ lead to metric independent amplitudes as required.

When computing the vacuum expectation value $\langle W(\overline{C})\rangle$ of the operator (34), several simplifications occur. One reason is that the fields A^i_μ are unaffected by the cubic interactions present in the action (12), because they can be contracted only with the fields B^I_μ due to the off-diagonal form of the kinetic terms. On the other hand, as already mentioned, the fields B^I_μ behave as Abelian fields and act as Lagrange multipliers, which impose the conditions

$$\Omega_{Ii}\epsilon^{\mu\nu\rho}\partial_\nu A^i_\rho(x)+\sum_{a=1}^{M} C_{Ia}\oint_{\Gamma^a} dy^\mu\,\delta(x-y)=0. \tag{37}$$

The solution of the above equation is given by

$$A^{(cl)i}_\mu(x)=(\Omega^{-1})^{iI}C_{Ia}\mathcal{B}^a_\mu(x) \tag{38}$$

with

$$\mathcal{B}^a_\mu(x)=-\frac{\epsilon_{\mu\sigma\tau}}{4\pi}\oint_{\Gamma^a} dx^\sigma\partial^\tau\frac{1}{|x-y|}. \tag{39}$$

Let us note that $A^{(cl)i}_\mu(x)$ is a purely transverse vector field because the longitudinal components have been fixed to zero by the gauge condition (5). At this point, it is possible to evaluate the explicit expression of $\langle W(\overline{C})\rangle$ using the saddle point evaluation method. After some calculations one finds

$$\langle W(\overline{C})\rangle=\exp\left[\frac{i\lambda}{6}\int d^3x\, l_{abc}\epsilon^{\mu\nu\rho}\mathcal{B}^a_\mu(x)\mathcal{B}^b_\nu(x)\mathcal{B}^c_\rho(x)\right], \tag{40}$$

where

$$l_{abc}=(\Omega^{-1})^{jJ}(\Omega^{-1})^{kK}C_{Ia}C_{Jb}C_{Kc}f^I_{jk}. \tag{41}$$

From Eq. (40) it turns out that the vacuum expectation values of the operators $W(\overline{C})$ deliver essentially a single topological invariant which is given by

$$\mathcal{H}=\int d^3x\, l_{abc}\epsilon^{\mu\nu\rho}\mathcal{B}^a_\mu(x)\mathcal{B}^b_\nu(x)\mathcal{B}^c_\rho(x). \tag{42}$$

Another topological invariant, namely the Gauss linking number, can be obtained by considering also amplitudes containing Abelian holonomic connections of the A^i_μ fields. Abelian connections are sufficient to grant BRST invariance in this case due to the simplicity of the BRST transformations (6) of the fields A^i_μ.

V. CONCLUSIONS

In this work we have investigated a class of topological field theories having the property that its perturbative series contains only the finite set of Feynman diagrams given in Fig. 1. These theories are exactly solvable and, besides the Gauss link invariant which is typical of Abelian C-S field theories, produce the topological invariant $\mathcal{H}$ of Eq. (42). The fact that a non-Abelian Chern–Simons field theory can sustain Abelian observables like the $W(\overline{C})$ of Eq. (34) is related to the presence of a nontrivial Abelian ideal in the gauge group of symmetry.

It is interesting to consider the above results from the point of view of possible applications to the statistical mechanics of random walks. Let $\Gamma^1,\ldots,\Gamma^M$ be a set of M closed random walks, interacting together via the topological potential (42). The partition function of this system coincides with the sum over all possible configurations of the trajectories $\Gamma^1,\ldots,\Gamma^M$:

$$Z=\int \mathcal{D}\mathbf{r}_1(s_1)\cdots\mathcal{D}\mathbf{r}_M(s_M)\exp\left[\sum_{a=1}^{M}\ \oint_{\Gamma^a}\dot{\mathbf{r}}_a^2+\mathcal{H}(\mathbf{r}_1,\ldots,\mathbf{r}_M)\right], \tag{43}$$

where $\mathbf{r}_a(s_a)$, $a=1,...,M$, are curves described in the space by the paths Γ^a and parametrized by means of their arc-lengths s_a. At this point the relation (40) may be interpreted as the analog of a Hubbard–Stratonovich transformation,[6] which decouples the trajectories Γ^a in the partition function Z. Such transformation simplifies the task of performing the path integration in Eq. (43), which is otherwise very complicated due to the presence of the topological term $\mathcal{H}(\mathbf{r}_1,\ldots,\mathbf{r}_M)$. Other applications can be in the study of the fractional quantum Hall effect.[17,18]

To conclude, one should mention that the idea of constructing a topological field theory with a finite number of Feynman diagrams has already been realized following a different route. This is the so-called Rozansky–Witten topological sigma model, which delivers topological invariants of the Milnor type of its hyper-Kähler target space.[19] Interesting new developments in this direction have been presented in Refs. 20 and 21.

ACKNOWLEDGMENTS

I wish to thank heartily the referee of this paper, G. Thompson, whose contribution has led to considerable improvements with respect to the original version. In particular, I am grateful to G. Thompson for pointing out that the theory in Eq. (1) is related to a Chern–Simons field theory with non-semisimple group of gauge symmetry and for suggesting Eqs. (2) and (3), which provide the full set of gauge transformations of the theory. I am also grateful to G. Thompson for having written a very enlightening referee report on this article and for his interest in my work. Finally, I wish to thank him for drawing my attention to the stimulating problem of the treatment of harmonic zero modes.

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Path integrals evaluation in two-dimensional de Sitter space

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(Received 8 June 2002; accepted 2 October 2002)

The propagator in de Sitter space is calculated based on the path integrals. The method of evaluation of path integrals for particles with spin is proposed. The calculations are compared with the quantum mechanical ones. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1526452]

I. INTRODUCTION

de Sitter space–time plays a special role in the general relativity theory (GRT): first, this space is curved, and, second, it possesses a maximal symmetry group.[1] Therefore, there is a possibility to investigate the gravitational effect on quantum processes on the basis of exact analytical expressions.

The propagator is one of the major objects of a quantum field theory. By means of the propagator one can obtain a vacuum expectation value of stress-energy tensor, pair creation intensity, etc. Moreover, propagator plays a central role in the renormalization procedure in curved space–time.[2]

In this article it is offered to use the Feynman path integrals and proper time formalism[3] for calculation of a propagator. Such an approach gives clear and simple interpretation of the process of a quantum particle interaction with an external gravitational field. In Ref. 4 the methods of a perturbation theory were used. However, in symmetric spaces the exact solution might be expected. Recent developments of the path integration technique actually enable one to solve this problem for a scalar particle.[5]

The Feynman integral for a particle with spin requires the operator of parallel transport, considerably complicating calculation of a propagator. In Refs. 6 and 7 the computational method suitable for two-dimensional spaces was proposed. In this case parallel transport is expressed through a phase factor, because the rotation group in two-dimensional space is Abelian. At the same time these methods fail in higher dimensional spaces. Moreover, we are unable to use directly the formalism developed in Refs. 5 and 8 because GRT deals with a wider class of manifolds than nonrelativistic quantum mechanics.

II. DESCRIPTION OF THE METHOD

A. Propagator for spinning particle

If the particle is described by Klein–Gordon equation (hereafter $c=\hbar=1$)

$$\nabla_\mu \nabla^\mu \phi + m^2 \phi = 0, \tag{1}$$

then the equation for Feynman propagator has the form

$$\nabla_\mu \nabla^\mu G(x,x_0) + m^2 G(x,x_0) = \delta(x,x_0). \tag{2}$$

The following substitution makes possible going to the path integral formulation:[9]

$$G(x,x_0) = \frac{i}{2}\int_0^\infty d\tau e^{-im^2\tau/2}\langle x,\tau|x_0,0\rangle, \tag{3}$$

$$i\frac{\partial}{\partial\tau}\langle x,\tau|x_0,0\rangle=-\frac{1}{2}\nabla_\mu\nabla^\mu\langle x,\tau|x_0,0\rangle, \tag{4}$$

$$\langle x,0|x_0,0\rangle=\delta(x,x_0), \tag{5}$$

because we obtain the Schrödinger-type equation

$$K(x,x_0;\tau)=\langle x,\tau|x_0,0\rangle=\int \mathcal{D}x(\tau)\exp\left\{-\frac{i}{2}\int\left(g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu+\frac{R}{3}\right)d\tau\right\}. \tag{6}$$

The appearance and the role of an additional term $\sim R/3$ is discussed in Refs. 4 and 9. Another way to obtain path integral formulation is based on the following operator identity:[9]

$$\begin{aligned}\frac{1}{\hat{H}}=i\int_0^\infty e^{-i\hat{H}\tau}d\tau\Rightarrow G(x,x_0)&=\langle x|\frac{1}{\nabla_\mu\nabla^\mu+m^2}|x_0\rangle\\&=\frac{1}{2}\langle x|\frac{1}{\frac{1}{2}(\nabla_\mu\nabla^\mu+m^2)}|x_0\rangle\\&=\frac{i}{2}\int_0^\infty d\tau e^{-im^2\tau/2}\langle x,\tau|x_0,0\rangle.\end{aligned} \tag{7}$$

This formalism allows us to obtain the generalization of (7):

$$\frac{1}{\hat{H}}=\hat{f}\frac{1}{\hat{f}\hat{H}\hat{f}}\hat{f}=i\hat{f}\int_0^\infty e^{-i\hat{f}\hat{H}\hat{f}\tau}d\tau\hat{f}. \tag{8}$$

Further, we will use this transformation with $\hat{f}=f(t)=\alpha/t$.

By analogy, for the particle with spin we have

$$(\nabla_\mu\nabla^\mu+m^2)\psi^A=0, \tag{9}$$

$$i\frac{\partial}{\partial\tau}K^A{}_{B_0}(x,x_0;\tau)=-\frac{1}{2}\nabla_\mu\nabla^\mu K^A{}_{B_0}(x,x_0;\tau), \tag{10}$$

$$K^A{}_{B_0}(x,x_0;0)=\delta(x,x_0)\,\delta^A_B, \tag{11}$$

but the Feynman propagator assumes the form

$$G^{A''}{}_{B'}(x'',x')=\int_0^\infty d\tau e^{-im^2\tau/2}\int\mathcal{D}x(\tau)\exp\left\{-\frac{i}{2}\int\left(g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu+\frac{R}{3}\right)d\tau\right\}P^{A''}{}_{B'}(x(\tau)), \tag{12}$$

where $P^{A''}{}_{B'}(x(\tau))$ is an operator of parallel transport.[7,10] The integral of such type has a more complicated structure than the ordinary one. This fact is caused by the difficulties connected with calculations of $P^{A''}{}_{B'}(x(\tau))$. Fortunately, fast development of the path integration technique gives us possibility to solve a wide range of problems.[8] The two-dimensional case is a good demonstration of these difficulties and also shows the possible way to overcome them.

B. Generation of an additional term by spin

Let us start with the consideration of parallel transport on pseudosphere. Then the metric in horicyclic coordinates has the form (the case $\alpha=1$ is considered in Refs. 11 and 12)

$$ds^2=\left(\frac{\alpha}{t}\right)^2(dt^2+dx^2), \tag{13}$$

where parameter α is closely related to the curvature scalar R:

$$R=-\frac{2}{\alpha^2}, \quad \alpha=\text{const}.$$

It is convenient to go from the natural basis

$$e_t=\frac{\partial}{\partial t}, \quad e_x=\frac{\partial}{\partial x} \tag{14}$$

to orthonormal one

$$e_t=\frac{t}{\alpha}\frac{\partial}{\partial t}, \quad e_x=\frac{t}{\alpha}\frac{\partial}{\partial x}, \tag{15}$$

and correspondingly

$$\mathbf{d}t,\mathbf{d}x\rightarrow e^t=\left(\frac{\alpha}{t}\right)\mathbf{d}t, e^x=\left(\frac{\alpha}{t}\right)\mathbf{d}x. \tag{16}$$

From (16) one can easily calculate the connection

$$\omega^t{}_x=-\omega^t{}_x=-\frac{1}{t}\mathbf{d}x. \tag{17}$$

Then

$$\nabla_x e^t=\frac{1}{t}e^x, \quad \nabla_x e^x=-\frac{1}{t}e^t. \tag{18}$$

It is convenient to use the following complex combination of basis vectors (isotropic basis):

$$\epsilon^{+1}=\frac{1}{\sqrt{2}}(e^t+ie^x), \quad \epsilon^{-1}=\frac{1}{\sqrt{2}}(e^t-ie^x), \tag{19}$$

in this basis

$$\begin{aligned}\nabla_x\epsilon^{+1}&=\nabla_x\frac{1}{\sqrt{2}}(e^t+ie^x)=\frac{1}{t}\frac{1}{\sqrt{2}}(e^x-ie^t)=-i\frac{1}{t}\epsilon^{+1}\\ \nabla_x\epsilon^{-1}&=\qquad\qquad\qquad\qquad\qquad\qquad=i\frac{1}{t}\epsilon^{-1}.\end{aligned} \tag{20}$$

Similarly,

$$\epsilon_{+1}=\frac{1}{\sqrt{2}}\left(\frac{t}{\alpha}\frac{\partial}{\partial t}-i\frac{t}{\alpha}\frac{\partial}{\partial x}\right), \quad \epsilon_{-1}=\frac{1}{\sqrt{2}}\left(\frac{t}{\alpha}\frac{\partial}{\partial t}+i\frac{t}{\alpha}\frac{\partial}{\partial x}\right). \tag{21}$$

Hence parallel transport reduces to the rotation; the angle of rotation is given by

$$\chi = -\int \frac{1}{t} dx. \tag{22}$$

Then it is possible to obtain explicitly the rotation associated with a loop Γ,

$$\chi(\Gamma) = -\oint_{\Gamma} \frac{1}{t} dx = \int \frac{1}{t^2} dS, \tag{23}$$

with $dS = dt\ dx$ as an element of spanned surface.

In the general case a two-dimensional manifold has the only "degree of freedom": in a tangent Euclidean space $e_i^2 = 1$, $de_{1,2} \sim e_{2,1}\ dx$-rotation in a single plane. Any geometrical object can be expanded into the sum of proper vectors of the operator of rotation:

$$i\hat{\mathbf{L}}\boldsymbol{\epsilon}^s = s\boldsymbol{\epsilon}^s, \quad s = 0, \quad \pm\tfrac{1}{2}, \quad \pm 1, \ldots . \tag{24}$$

Then the law of parallel transports acquires the simplest form

$$\hat{\mathrm{P}}\boldsymbol{\epsilon}^s = e^{is\chi}\boldsymbol{\epsilon}^s = e^{-is\int (1/t)dx}\boldsymbol{\epsilon}^s, \quad \nabla_x \boldsymbol{\epsilon}^s = -is\frac{1}{t}\boldsymbol{\epsilon}^s. \tag{25}$$

Hence the path integral will have the form

$$K(x, x_0; \tau) = \sum_s \boldsymbol{\epsilon}^s(x) \otimes \boldsymbol{\epsilon}_s(x_0) \int \mathcal{D}\{x(\tau)\} e^{iS(x(\tau)) + is\chi(x(\tau))}. \tag{26}$$

When the metric is pseudo-Euclidean, the isotropic basis looks like

$$\boldsymbol{\epsilon}^{\pm 1} = \frac{1}{\sqrt{2}}(\vec{e}_0 \pm \vec{e}_1), \tag{27}$$

and parallel transport can be described by a real phase factor:

$$\hat{\mathrm{P}}\boldsymbol{\epsilon}^s = e^{s\chi}\boldsymbol{\epsilon}^s.$$

Then

$$e^{iS(x(t))} \to e^{iS(x(t)) + is\chi(x(t))}$$

and additional term will be incorporated into Lagrangian in the following manner:

$$\mathcal{L} \to \mathcal{L}_{\text{eff}} = \mathcal{L} - is\omega_i \dot{x}^i.$$

III. PARTICLE WITH SPIN ON PSEUDOSPHERE

In the isotropic basis the calculation of the operator of parallel transport is reduced to calculation of a phase factor, and additional term arises in the effective Lagrangian:

$$L_{\text{eff}} = \frac{1}{2}\left(\frac{\alpha^2}{t^2}(\dot{t}^2 + \dot{x}^2) - \frac{s}{t}\dot{x} \right), \tag{28}$$

where s is the spin weight.[7] The problem is reduced to the quantum mechanical one with a Hamiltonian of the form

$$H = \frac{t}{\alpha}\left(\frac{p_t^2 + p_x^2}{2} - \frac{p_x}{t}s + \frac{s^2 - m^2\alpha^2}{2t^2} \right)\frac{t}{\alpha}.$$

Integration over x is quite simple, because neither L_{eff} nor H depends on $x(t)$ explicitly, but only on $\dot{x}(t)$ and p_x. In this case

$$\int \mathcal{D}(x(\tau))\mathcal{D}(p_x(\tau))e^{i\int p_x\dot{x}d\tau - i\int f(p_x(\tau))d\tau} = \int dp_x e^{ip_x(x-x_0)-if(p_x)\tau}. \tag{29}$$

Using (7) one obtains

$$\begin{aligned}\frac{1}{H} &= \langle t'',x''|\frac{\alpha}{t''}\frac{1}{(p_t^2+p_x^2)/2-(p_x/t)\,s+[(s^2-m^2\alpha^2)/2t^2]}\frac{\alpha}{t'}|t',x'\rangle \\ &= \frac{i}{2}\frac{\alpha^2}{t''t'}\int_0^\infty d\tau\int dp_x \exp(ip_x^2\tau/2)\exp(ip(x''-x')) \\ &\quad\times\int \mathcal{D}t(\tau)\exp i\int d\tau\left(\frac{\dot{t}^2}{2}-\frac{p_x}{t}s+\frac{s^2-m^2\alpha^2}{2t^2}\right).\end{aligned} \tag{30}$$

When integrating over t, one deals with a radial Coulomb problem. Its solution by means of continual integration can be found in Ref. 13. The propagator can be written as decomposition by eigenfunctions:

$$K(t'',x'';t',x';\tau)=\frac{\alpha^2}{t''t'}\sum_s \epsilon^s(x)\otimes\epsilon_s(x_0)\int dp_t dp_x e^{i\tau(p_t^2+p_x^2)/2}e^{ip_x(x''-x')}\,{}_s\psi(p_t,t'')\,{}_s\psi^*(p_t,t'), \tag{31}$$

where

$${}_s\psi(p_t,t)=\frac{\Gamma(\frac{1}{2}+\nu-isp_x/p_t)}{\sqrt{2\pi}\Gamma(2\nu+2)}M_{isp_x/p_t,\nu}(-2ip_t t),$$

$${}_s\psi^*(p_t,t)=\frac{\Gamma(\frac{1}{2}+\nu+isp_x/p_t)}{\sqrt{2\pi}\Gamma(2\nu+2)}M_{-isp_x/p_t,\nu}(2ip_t t),$$

$$\nu=\sqrt{s^2-m^2\alpha^2+1/4},$$

and $M_{s,\nu}(x)$ is the Whittaker function.

IV. TRANSITION TO de SITTER SPACE

The above decompositions of the propagator (31) were obtained as solutions of quantum mechanical problems in polar coordinates. In order to go from the space with the metric

$$ds^2=\left(\frac{\alpha}{t}\right)^2(dt^2+dx^2),\quad \text{with}\ \ t\geqslant 0,\quad -\infty\leqslant x\leqslant\infty,$$

to

$$ds^2=\left(\frac{\alpha}{t}\right)^2(dt^2-dx^2),\quad \text{with}\ \ -\infty\leqslant t,x\leqslant\infty,$$

one has to take into account the change of the variable t range and the change of the sign of the term dx^2.

The following limitation has been implicitly used in a radial Coulomb problem: radial coordinate varies in the range $(0,\infty)$. This means the use of the mirror principle (see discussion of boundary conditions in Refs. 5 and 8):

$$\psi(r)\to\psi(r)-\psi(-r).$$

In de Sitter space the appropriate coordinate varies from $-\infty$ to ∞. Therefore, it is necessary to discard the reflected part of a wave. It seems to be convenient to consider asymptotics of eigenfunctions, as at $t\to\infty$ the effective potential $(-i(p_x/t)s+(s^2-m^2\alpha^2)/2t^2)$ tends to zero, and eigenfunctions tends to $e^{\pm ip_t t}$. For a scalar particle with

$$s=0,$$

$$M_{0,\nu}(2iz)=i^{\nu+1/2}2^{2\nu+1/2}\sqrt{z}\Gamma(1+\nu)J_\nu(z),$$

the decomposition by cylindrical Bessel functions with the asymptotic

$$J_n(x)\sim\sqrt{\frac{2}{\pi x}}\sin\left(x-\frac{n\pi}{2}+\frac{\pi}{4}\right)=\sqrt{\frac{2}{\pi x}}\frac{1}{2i}(e^{i(x-n\pi/2+\pi/4)}-e^{-i(x-n\pi/2+\pi/4)})$$

can be obtained.

Cylindrical Hankel functions have the required asymptotic:

$$H_n^{(1)}(pt)\sim\sqrt{\frac{1}{pt}}e^{ipt},\quad H_n^{(2)}(pt)\sim\sqrt{\frac{1}{pt}}e^{-ipt}.$$

The Bessel function represents their linear combination. Then for a temporal part of the propagator we receive decomposition

$$K(t'',t';\ s)=\int p_t dp_t\sqrt{t''t'}H_\nu^{(1)}(p_t t'')H_\nu^{(1)*}(p_t t')e^{-isp_t^2/2},\quad \nu=\sqrt{-m^2\alpha^2+1/4}. \tag{32}$$

Similarly, for a particle with spin we should proceed from the Whittaker function of the first kind $M_{k,m}(x)$ to the Whittaker function of the second kind $W_{k,m}(x)$:

$$W_{k,m}(x)=\frac{\Gamma(-2m)}{\Gamma(\frac{1}{2}-m-k)}x^{m+1/2}e^{-x/2}{}_1F_1(m+\tfrac{1}{2}-k;\ 2m+1;\ x)$$
$$+\frac{\Gamma(2m)}{\Gamma(\frac{1}{2}+m-k)}x^{-m+1/2}e^{-x/2}{}_1F_1(-m+\tfrac{1}{2}-k;\ -2m+1;\ x), \tag{33}$$

possessing the asymptotics

$$W_{k,m}(x)\sim x^k e^{-x/2},\quad x\to\pm\infty.$$

The functions $M_{k,m}(x)$ represent a linear combination of $W_{k,m}(x)$ and $W_{-k,m}(-x)$.

The outcome can be again represented as decomposition by eigenfunctions:

$$K(t'',x'';\ t',x';\tau)=\frac{\alpha^2}{t''t'}\sum_s\ \epsilon^s(x)\otimes\epsilon_s(x_0)\int dp_t dp_x e^{i\tau(p_t^2+p_x^2)/2}e^{ip_x(x''-x')}\,{}_s\psi(p_t,t'')\,{}_s\psi^*(p_t,t'), \tag{34}$$

$${}_s\psi(t'')=e^{-ip_x\pi s/2p_t}W_{isp_x/p_t,\nu}(-2ip_t t),\quad \nu=\sqrt{s^2-m^2\alpha^2+\tfrac{1}{4}}.$$

The second problem to be solved is the transition from pseudosphere metric

$$ds^2=\frac{\alpha^2}{t^2}(dt^2+dx^2)$$

to the de Sitter space one

$$ds^2=\frac{\alpha^2}{t^2}(dt^2-dx^2).$$

It is convenient to rotate the x axis: $x\to ix$, and correspondingly

$$\begin{gathered}
p_x\to -ip_x,\\
\epsilon^{\pm 1}=\frac{\alpha}{t}\frac{1}{\sqrt{2}}(e^t\mp e^x),\quad \epsilon_{\pm 1}=\frac{1}{\sqrt{2}}\left(\frac{t}{\alpha}\frac{\partial}{\partial t}\pm\frac{t}{\alpha}\frac{\partial}{\partial x}\right),\\
\hat{P}\epsilon^s=e^{s\chi}\epsilon^s=e^{-s\int(1/t)dx}\epsilon^s,\quad \nabla_x\epsilon^s=-s\frac{1}{t}\epsilon^s,\\
L_{\text{eff}}=\frac{1}{2}\left(\frac{\alpha^2}{t^2}(\dot{t}^2-\dot{x}^2)-i\frac{s}{t}\dot{x}\right).
\end{gathered}\tag{35}$$

So, that propagator looks like

$$\begin{aligned}
K(t'',x'';\ t',x';\tau)=\frac{\alpha^2}{t''t'}\sum_s\ \epsilon^s\otimes\epsilon_s e^{i\tau(p_t^2-p_x^2)/2}\int dp_t dp_x e^{ip_x x''}e^{\pi p_x s/p_t}W_{p_x s/p_t,\nu}(2ip_t t'')\\
\times e^{-ip_x x'}e^{\pi p_x s/p_t}W_{-p_x s/p_t,\nu}(-2ip_t t'),
\end{aligned}\tag{36}$$

and

$$G(t'',x'';\ t',x')=\frac{i}{2}\int_0^\infty K(t'',x'';t',x';\tau)d\tau.\tag{37}$$

In order to make sure that this expression is a required propagator, one needs to analyze a short-time kernel. It is possible to use asymptotical expansion of Whittaker function

$$\begin{aligned}
W_{a,c}(x)&\approx e^{-x/2}\left(1-\frac{(\frac{1}{2}-a-c)(\frac{1}{2}-a+c)}{x}\right)x^a\\
&\approx\exp\left(-\left(\frac{(\frac{1}{2}-a-c)(\frac{1}{2}-a+c)}{x}\right)-\frac{x}{2}+a\ln(x)\right).
\end{aligned}\tag{38}$$

Substituting (38) into (36), one can ensure that

$$\begin{aligned}
\int\frac{dp_t}{2\pi}e^{\pi p_x s/p_t}W_{p_x s/p_t,\nu}(2ip_t t'')e^{\pi p_x s/p_t}W_{-p_x s/p_t,\nu}(-2ip_t t')\\
\to\frac{1}{\sqrt{2\pi i\tau}}\exp\left(i\frac{(t''-t')^2}{2\tau}-\frac{p_x s}{t'}\tau+i\frac{\alpha^2m^2-s^2}{2t''t'}\tau\right),
\end{aligned}\tag{39}$$

and this result actually leads to the initial effective Lagrangian (see the Appendix).

Propagator (36) has two important features:

(1) It satisfies the boundary conditions (11). Actually, if $\tau\to 0$, then

$$\frac{1}{\sqrt{2\pi i\tau}}\exp\left(i\frac{(t''-t')^2}{2\tau}-\frac{p_x s}{t'}\tau+i\frac{\alpha^2m^2-s^2}{2t''t'}\tau\right)\to\delta(t''-t'). \tag{40}$$

(2) This propagator satisfies Eq. (10) because eigenfunctions are the solutions of the equation

$$-\frac{1}{2}(\nabla_\mu\nabla^\mu+m^2)\left(\epsilon^s e^{ip_x x''}\frac{\alpha}{t}W_{p_x s/p_t,\nu}(2ip_t t'')\right)=\frac{p_t^2-p_x^2}{2}\left(\epsilon^s e^{ip_x x''}\frac{\alpha}{t}W_{p_x s/p_t,\nu}(2ip_t t'')\right). \tag{41}$$

With (35) one can obtain

$$-\frac{d^2}{dt^2}W_{p_x s/p_t,\nu}(2ip_t t'')-\left(\left(p_x+i\frac{s}{t}\right)^2+\frac{m^2\alpha^2}{t^2}\right)W_{p_x s/p_t,\nu}(2ip_t t'')=(p_t^2-p_x^2)W_{p_x s/p_t,\nu}(2ip_t t''),$$

$$-\frac{d^2}{dt^2}W_{p_x s/p_t,\nu}(2ip_t t'')-\left(2\frac{isp_x}{t}+\frac{m^2\alpha^2-s^2}{t^2}\right)W_{p_x s/p_t,\nu}(2ip_t t'')=p_t^2W_{p_x s/p_t,\nu}(2ip_t t'').$$

The Whittaker function actually satisfies this equation.

It is interesting to analyze a special case of this solution. The vector particle propagator is expanded into wavefunctions of the form $\epsilon^{-1}W_{-1,\nu}(2ikx)$ and $\epsilon^{+1}W_{1,\nu}(2ikx)$, since after final integration only point $p_t^2-p_x^2=0$ will be taken into account and $sp_x/p_t=\pm1$. It is common practice to solve equations for the vector field by separation into the transverse and longitudinal parts. Using the connection between Hankel and Whittaker functions,

$$H_\nu^{(1)}(-kt)=\sqrt{\frac{\pi}{2ikt}}W_{0,\nu}(2ikt)=-\frac{1}{2(ikt)^{3/2}}\sqrt{\frac{2}{\pi}}\left(\left(\nu^2-\frac{1}{4}\right)W_{-1,\nu}(2ikt)-W_{1,\nu}(2ikt)\right), \tag{42}$$

$$H_{\nu+1}^{(1)}(-kt)+H_{\nu-1}^{(1)}(-kt)=\frac{1}{2(ikt)^{3/2}}\sqrt{\frac{2}{\pi}}\left(\left(\nu^2-\frac{1}{4}\right)W_{-1,\nu}(2ikt)+(W_{0,\nu}(2ikt)+W_{1,\nu}(2ikt))\right), \tag{43}$$

and the following relation

$$\frac{d}{dt}H_\nu^{(1)}(-kt)=-\frac{ik}{2}(H_{\nu+1}^{(1)}(-kt)+H_{\nu-1}^{(1)}(-kt)), \tag{44}$$

one can ensure that these parts represent a linear combination of the above solutions. Actually, the longitudinal one is

$$\nabla\left(\sqrt{\frac{2ikt}{\pi}}H_\nu^{(1)}(-kt)e^{ikx}\right)=\epsilon^{+1}\left(\nu^2-\frac{1}{4}\right)W_{-1,\nu}(2ikt)e^{ikx}+\epsilon^{-1}W_{1,\nu}(2ikt)e^{ikx}. \tag{45}$$

The transverse part is proportional to

$$\epsilon^{+1}(\nu^2-\tfrac{1}{4})W_{-1,\nu}(2ikt)-\epsilon^{-1}W_{1,\nu}(2ikt). \tag{46}$$

V. CONCLUSION

The path integral for particles with spin includes an additional factor—the operator of parallel transport. The use of parallel transport requires the development of new calculation methods for functional integrals. In contrast to the differential equations approach, the path integral formalism

deals with a global object—the propagator. It has more general analytical properties, and gives the possibility to distinguish connections between compact and noncompact spaces, and continuous and discrete spectrum.

Two-dimensional solutions have similar forms for arbitrary spin. A similar situation occurs also in some four-dimensional problems. Note the Teukolsky equation[14] describing massless particles of spin 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, 2 in Kerr geometry.

Our interest in path integration is stimulated by the possibility of simple and clear description of a spinning quantum particle interaction with the curvature.[15] This approach may be useful when obtaining common features of the fields of different spins in curved space and in quantization of the gravitational field itself.

APPENDIX: PROOF OF EQ. (39)

We will consider (39) with $\tau\to 0$. In this case

$$p_t\to \frac{t''-t'^{\,\tau\to 0}}{\tau}\to\infty$$

and one has to take into account terms up to $(t''-t')^2$. After the substitution of expansion

$$W_{a,c}(x)\overset{x\to\infty}{\to} e^{-x/2}\left(1-\frac{\left(\frac{1}{2}-a-c\right)\left(\frac{1}{2}-a+c\right)}{x}+O\left(\frac{1}{x^2}\right)\right)x^a$$

$$\approx\exp\left(-\left(\frac{\left(\frac{1}{2}-a-c\right)\left(\frac{1}{2}-a+c\right)}{x}\right)-\frac{x}{2}+a\ln(x)\right)$$

to

$$e^{-ip_t^2\tau}e^{\pi p_x s/p_t}(2p_t)^{sp_x/p_t}W_{p_x s/p_t,\nu}(2ip_t t'')e^{\pi p_x s/p_t}(2p_t)^{-sp_x/p_t}W_{-p_x s/p_t,\nu}(-2ip_t t'), \quad \text{(A1)}$$

one has up to the accuracy of $1/p_t^2$

$$\exp\left(\frac{1}{p_t}\left(-\frac{is^2}{2t''}+\frac{iM^2\alpha^2}{2t''}+p_x s\ln(2ip_t t'')\right)-\frac{1}{p_t}\left(-\frac{is^2}{2t'}+\frac{iM^2\alpha^2}{2t'}+p_x s\ln(2ip_t t')\right)\right)e^{ip(t''-t')}$$

$$=e^{ip(t''-t')}\exp\left(\frac{1}{p_t}\left(i(s^2+M^2\alpha^2)\left(\frac{1}{t''}-\frac{1}{t'}\right)+sp_x(\ln(t'')-\ln(t'))\right)\right). \quad \text{(A2)}$$

After the use of

$$\frac{f(t'')-f(t')}{p_t}\approx\tau\frac{f'(t')(t''-t')+f''(t')(t''-t')^2+\cdots}{t''-t'}=\tau f'(t)+o(\tau), \quad \text{(A3)}$$

the following result can be obtained:

$$\exp\left(ip_t(t''-t')-i\tau\left(p_t^2+is\frac{p_x}{t'}+\frac{s^2-M^2\alpha^2}{t'^2}\right)\right). \quad \text{(A4)}$$

Finally, integration over p_t can be made:

$$\int_{-\infty}^{\infty} \exp\left(ip_t(t''-t') - i\tau\left(p_t^2 + is\frac{p_x}{t'} + \frac{s^2 - M^2\alpha^2}{t'^2}\right)\right)\frac{dp_t}{2\pi}$$

$$= \frac{1}{\sqrt{2\pi i\tau}}\exp\left(i\frac{(t''-t')^2}{2\tau} - \frac{p_x s}{t'}\tau + i\frac{\alpha^2 m^2 - s^2}{2t''t'}\tau\right).$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

Towards vacuum superstring field theory: The supersliver

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(Received 3 September 2002; accepted 13 September 2002)

We extend some aspects of vacuum string field theory to superstring field theory in Berkovits' formulation, and we study the star algebra in the fermionic matter sector. After clarifying the structure of the interaction vertex in the operator formalism of Gross and Jevicki, we provide an algebraic construction of the supersliver state in terms of infinite–dimensional matrices. This state is an idempotent string field and solves the matter part of the equation of motion of superstring field theory with a pure ghost BRST operator. We determine the spectrum of eigenvalues and eigenvectors of the infinite–dimensional matrices of Neumann coefficients in the fermionic matter sector. We then analyze coherent states based on the supersliver and use them in order to construct higher–rank projector solutions, as well as to construct closed subalgebras of the star algebra in the fermionic matter sector. Finally, we show that the geometric supersliver is a solution to the superstring field theory equations of motion, including the (super)ghost sector, with the canonical choice of vacuum BRST operator recently proposed by Gaiotto, Rastelli, Sen and Zwiebach. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1523149]

I. INTRODUCTION AND SUMMARY

In the last two years, the search for nonperturbative information in string field theory[1,2] has experienced a renewed interest mainly due to a series of conjectures by Sen[3–5] (also see Ref. 6 for a review and a list of references). These conjectures have been tested numerically to a high degree of precision in level truncated cubic string field theory, and some of them have been proven in boundary string field theory (see, e.g., Ref. 7 for a review and a list of references). In the meantime, the elegant construction of Berkovits[8–11] has emerged as a promising candidate for an open superstring field theory describing the NS sector: in here, Sen's conjectures about the fate of the tachyon in the non-BPS $D9$-brane have been successfully tested by level truncation to a high level of accuracy,[12–15] and kink solutions have been found that describe lower–dimensional D-branes[16] (see, e.g., Ref. 17 for a review and a more complete list of references).

So far, most of our understanding about tachyon condensation in both cubic string field theory and Berkovits' superstring field theory is based on level-truncated computations and it would be of course desirable to have an analytical control over the problem. For the bosonic string, Rastelli, Sen and Zwiebach have proposed in a series of papers[18–22] a new approach to this problem called vacuum string field theory (VSFT). In VSFT, the form of the cubic string field theory action around the tachyonic vacuum is postulated by exploiting some of the expected properties it should have (like the absence of open string states). Then one can show that this theory has solutions that describe the perturbative vacuum and the various D-branes. In particular, the matter sector of the maximal $D25$-brane is described by a special state called the sliver. This state was first constructed geometrically by Rastelli and Zwiebach[23] and then algebraically by Kostelecky and Potting,[24] and it is an idempotent state of the string field star algebra, in the matter sector. The construction of VSFT has been recently completed in Ref. 25, where Gaiotto, Rastelli, Sen, and Zwiebach have proposed a canonical choice of the ghost BRST operator around the vacuum, with which they identified closed string states; and also in Ref. 26, where Rastelli, Sen, and Zwiebach have found

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the eigenvalue and eigenvector spectrum of the Neumann matrices, which could allow for a proper definition of the string field space. The study of VSFT has also unveiled beautiful algebraic structures in cubic string field theory (for example, projectors of arbitrary rank in the star algebra have been constructed in detail in Refs. 20, 27, and 28).

The main purpose of this paper is to give the first steps towards the construction of vacuum superstring field theory around the tachyonic vacua of the non-BPS maximal $D9$-brane in type IIA superstring theory, and to explore the algebraic structure of the star algebra in the fermionic part of the matter sector. In Sec. II, we begin with a review of Berkovits' open superstring field theory for the NS sector and discuss the general features of vacuum superstring field theory. We shall show in detail that, assuming a pure ghost BRST operator around the vacuum as in VSFT, Berkovits' equation of motion for the superstring field admits factorized solutions whose matter part is an idempotent state of the star algebra. In a sense, idempotency is even more useful in Berkovits' theory since it drastically reduces the nonlinearity of the equation of motion. Idempotent string field solutions can be constructed in the GSO$(+)$ sector or in both GSO$(\pm)$ sectors.

In order to construct idempotent states in superstring field theory, one first has to understand in detail the structure of the star algebra in the fermionic matter sector. To do that, we use the operator construction of the interaction vertex for the superstring due to Gross and Jevicki,[29] which extends their previous work on the bosonic string[30,31] to the NSR superstring. In Sec. III we review some of the relevant results and we further clarify the structure of the vertex. This allows us to write the Neumann coefficients in terms of two simple infinite–dimensional matrices which shall play a key rôle in the constructions of this paper.

Given any boundary conformal field theory (BCFT) one can construct geometrically a special state which is an idempotent of the star algebra.[21] When the BCFT is that of a $D25$-brane, this state is called the sliver.[23,18] (Strictly speaking, the construction of the sliver state is purely geometric and is thus valid for arbitrary BCFT's. However, in this paper, we shall use the denotation of ''sliver'' for the particular BCFT associated to the maximal brane in flat space.) This geometric construction extends in a very natural way to the BCFT given by the NS sector of the open superstring which describes the unstable $D9$-brane. This yields an idempotent state that we call the supersliver. The matter part of the supersliver is a product of two squeezed states: one made of bosonic oscillators (the bosonic sliver previously considered in Refs. 24 and 19) and the other made of fermionic oscillators, that we shall call the fermionic sliver. Although the geometric construction gives a precise determination of the fermionic sliver, it is important for many purposes to have an algebraic construction as well. In Sec. IV, and making use the results of Sec. III for the interaction vertex, we find a simple expression for the fermionic sliver in terms of infinite-dimensional matrices, as in Refs. 24, 19, and we compare the result to the geometric construction. We also briefly address the supersliver conservation laws. In Sec. V we use the techniques recently introduced in Ref. 26 to determine the eigenvalue spectrum and the eigenvectors of the various infinite-dimensional matrices involved in the fermionic star algebra, including the matrices of Neumann coefficients.

Once the fermionic sliver has been constructed algebraically, one can take it as a sort of ''vacuum state'' in order to build fermionic coherent states. This we do in Sec. VI, where after constructing these fermionic coherent states on the fermionic sliver, we study their star algebras. As in Ref. 20, one can use these coherent states to construct higher-rank projectors of the fermionic star algebra. We shall show that one can also construct closed fermionic star subalgebras. These star subalgebras provide new idempotent states which yield new solutions to the vacuum superstring field theory equation of motion. However, some of them turn out to be related to the fermionic sliver by gauge transformations.

In Sec. VII we consider the ghost/superghost sector, and we show that if one chooses the vacuum BRST operator to be the recent canonical choice of Gaiotto, Rastelli, Sen and Zwiebach,[25] then the geometrical sliver is a solution to Berkovits' superstring field theory equations of motion, i.e., we solve the equations of motion in the (super)ghost sector.

Finally, in Sec. VIII we state some conclusions and open problems for the future. In the Appendix we give some of the details needed in the proof that the structure of the vertex found in

Sec. III agrees with the explicit expressions found by Gross and Jevicki in Ref. 29 using conformal mapping techniques.

II. BERKOVITS' SUPERSTRING FIELD THEORY

A. A Short review of Berkovits' superstring field theory

In this paper, we shall study the non-GSO projected open superstring in the NS sector. In the matter sector, there are two fermions $\psi^{\pm}(\sigma)$ with the mode expansion

$$\psi^{\mu}_{\pm}(\sigma)=\sum_{r\in \mathbf{Z}+1/2} e^{\pm ir\sigma}\psi^{\mu}_{r}, \tag{1}$$

where the modes satisfy the anticommutation relations

$$\{\psi^{\mu}_{r},\psi^{\nu}_{s}\}=\eta^{\mu\nu}\delta_{r+s,0}. \tag{2}$$

We will therefore write $\psi^{\dagger}_{r}=\psi_{-r}$ for $r>0$. The ghost/superghost sector includes the b,c, and the β,γ, system and we bosonize the last one in the standard way,[32]

$$\beta=\partial\xi e^{-\phi},\quad \gamma=\eta e^{\phi}. \tag{3}$$

A superstring field theory describing the GSO-projected NS sector of the open superstring was proposed by Berkovits in Ref. 8 (recent reviews can be found in, e.g., Refs. 10 and 17). In this theory, the string field Φ is Grassmann even, has zero ghost number and zero picture number. The action has the structure of a WZW model:

$$S[\Phi]=\frac{1}{2}\int\left((e^{-\Phi}Q_{B}e^{\Phi})(e^{-\Phi}\eta_{0}e^{\Phi})-\int_{0}^{1}dt(e^{-t\Phi}\partial_{t}e^{t\Phi})\{(e^{-t\Phi}Q_{B}e^{t\Phi}),(e^{-t\Phi}\eta_{0}e^{t\Phi})\}\right), \tag{4}$$

where Q_B is the BRST operator of the superstring and η_0 the zero-mode of η (the bosonized superconformal ghost).[32] In a WZW interpretation of this model, these operators play the role of a holomorphic and an antiholomorphic derivatives, respectively. In this action, the integral and the star products are evaluated with Witten's string field theory interaction.[1] The exponentiation of the string field Φ is defined by a series expansion with star products: $e^{\Phi}=\mathcal{I}+\Phi+\frac{1}{2}\Phi\star\Phi+\cdots$, where $\mathcal{I}$ is the identity string field. As usual, we refer to the first term in (4) as the kinetic term and to the second one as the Wess–Zumino term. It can be shown that the equation of motion derived from this action is:[8]

$$\eta_{0}(e^{-\Phi}Q_{B}e^{\Phi})=0. \tag{5}$$

The action (4) has a gauge symmetry given by

$$\delta e^{\Phi}=\Xi_{L}e^{\Phi}+e^{\Phi}\Xi_{R}, \tag{6}$$

where the gauge parameters $\Xi_{L,R}$ satisfy

$$Q_{B}\Xi_{L}=0,\quad \eta_{0}\Xi_{R}=0. \tag{7}$$

One can include GSO($-$) states by introducing Chan–Paton-type degrees of freedom.[12,13] The string field then reads,

$$\Phi=\Phi_{+}\otimes\mathbf{1}+\Phi_{-}\otimes\sigma_{1}, \tag{8}$$

where $\Phi_{\pm}$ are, respectively, in the GSO($\pm$) sectors, and σ_1 is one of the Pauli matrices. The Q_B and η_0 operators also have to be tensored with the appropriate matrices

$$\hat{Q}_B = Q_B \otimes \sigma_3, \quad \hat{\eta}_0 = \eta_0 \otimes \sigma_3. \tag{9}$$

The action is again given by one-half times (4), where the bracket now includes a trace over the Chan–Paton-type matrices (the 1/2 factor is included to compensate for the trace over the matrices). The gauge symmetry is given again by (6), where $\Xi_{L,R}$ take values in both sectors as in (8). It has been shown that Berkovits superstring field theory correctly reproduces the four–point tree amplitude in Ref. 11, and it can be used to computed the NS tachyon potential in level truncation (see Ref. 17 for a review), giving results which are compatible with Sen's conjectures.

B. Superstring field theory around a classical solution

In the cubic theory of Witten, one can consider a particular solution of the classical equations of motion, Φ_0, and study fluctuations around it: $\Phi = \Phi_0 + \tilde{\Phi}$. It is easy to see that the action governing the fluctuations $\tilde{\Phi}$ has the structure of the original action for Φ, but with a different BRST operator, $\mathcal{Q}$. Bosonic VSFT, as formulated in the series of papers,[18–22] is based on two assumptions:

(1) First, it is assumed that, when one expands around the tachyonic vacuum, the new BRST operator $\mathcal{Q}$ has vanishing cohomology and is made purely of ghost operators.

(2) Second, it is assumed that all Dp-brane solutions of VSFT have the factorized form

$$\Phi = \Phi_g \otimes \Phi_m, \tag{10}$$

where $\Phi_{g,m}$ denote states containing only ghost and only matter modes, respectively. Since the star product factorizes into the ghost and the matter sector, and since we have assumed that $\mathcal{Q}$ is pure ghost, the equations of motion split into

$$\mathcal{Q}\Phi_g + \Phi_g \star \Phi_g = 0 \tag{11}$$

and

$$\Phi_m \star \Phi_m = \Phi_m. \tag{12}$$

The second equation says that the matter part is an idempotent of the star algebra (where the star product is now restricted to the matter sector). If these assumptions hold, the string field action evaluated at a solution of the form (10) is simply proportional to the BPZ norm of $|\Phi_m\rangle$, and this allows one to compare in a simple way ratios of tensions of different D-branes.[19,21]

An interesting question is to which extent are these assumptions valid in Berkovits' superstring field theory. In order to answer this question, the first step is to analyze the fluctuations around a solution to the equations of motion. This was first addressed by Kluson in Ref. 33, where it was shown that with an appropriate parametrization of the fluctuations, the equation of motion is identical to (5), albeit with a deformed Q operator. It was thus concluded (without proof) in Ref. 33 that the action for the fluctuation should have the form (4) with the deformed operator. We shall now derive the equation of motion in a slightly different way from the one presented in Ref. 33, and this will allow us to show that the action is indeed of the required form by direct computation.

Let us define $G = e^{\Phi}$, the exponential of the string field that appears in Berkovits' action. Let Φ_0 be a solution to the classical equations of motion (5) and let us consider a fluctuation around this solution parameterized as follows:[33]

$$G = G_0 \star h, \quad G_0 = e^{\Phi_0}, \quad h = e^{\phi}. \tag{13}$$

Since Berkovits' action has the structure of a WZW theory, one should expect an analog of the Polyakov–Wiegmann equation[34] to be valid. In fact, it is easy to show (by using, for example, the geometric formulation of Refs. 33 and 35) that the action (4) satisfies

$$S[G_0\star h]=S[G_0]+S[h]-\int (G_0^{-1}Q_BG_0)(h\eta_0h^{-1}), \tag{14}$$

for arbitrary G_0 and h. The effective action for the fluctuations is then

$$S_{\text{eff}}[h]=S[h]-\int (G_0^{-1}Q_BG_0)(h\eta_0h^{-1}). \tag{15}$$

Let us now obtain the equation of motion satisfied by h. Varying $S[h]$, one obtains

$$\int h^{-1}\delta h\,\eta_0(h^{-1}Q_Bh),$$

and from the extra term in $S_{\text{eff}}[h]$ one gets

$$\int h^{-1}\delta h\,\eta_0(h^{-1}Ah),$$

where we denoted $A=G_0^{-1}Q_BG_0$ and we have used the equation of motion $\eta_0(A)=0$. Putting both pieces together, one finds that

$$\eta_0(h^{-1}Q_Bh+h^{-1}Ah-A)=0. \tag{16}$$

Therefore, the equation of motion is identical to (5) but with the deformed Q operator:

$$Q_A(X)=Q_B(X)+AX-(-1)^XXA. \tag{17}$$

One can moreover easily prove[33] that the new operator satisfies all the axioms of superstring field theory (it is a nilpotent derivation and it anticommutes with η_0).

We shall now show that $S_{\text{eff}}[h]$ has in fact the structure of (4) but with the operator Q_A. For that, we simply need to notice that

$$\int A(h\eta_0h^{-1})=\frac{1}{2}\int\left((h^{-1}Ah-A)(h^{-1}\eta_0h)-\int_0^1 dt\,A\partial_t(\hat{h}\eta_0\hat{h}^{-1}-\hat{h}^{-1}\eta_0\hat{h})\right), \tag{18}$$

where we have used integration by parts with respect to η_0, and the fact that Φ_0 satisfies its equation of motion. We have also denoted $\hat{h}=e^{t\phi}$. The first term in the RHS of (18) when added to the kinetic term in $S[h]$ gives a kinetic term with the Q_A operator, while the second term when added to the Wess–Zumino term in $S[h]$ gives a Wess–Zumino term with Q_A. The conclusion of this computation is that the action for the fluctuations is simply

$$S_{\text{eff}}[h]=\frac{1}{2}\int\left((e^{-\phi}Q_Ae^{\phi})(e^{-\phi}\eta_0e^{\phi})-\int_0^1 dt(e^{-t\phi}\partial_te^{t\phi})\{(e^{-t\phi}Q_Ae^{t\phi}),(e^{-t\phi}\eta_0e^{t\phi})\}\right), \tag{19}$$

as anticipated in Ref. 33.

Let us now consider the superstring field theory describing the non-BPS $D9$-brane, i.e., Berkovits' superstring field theory including both the GSO($\pm$) sectors. It has been shown in level truncation that this theory has two symmetric vacua where the tachyon condenses. According to Sen's conjectures, at any of these two vacua there are no open superstring degrees of freedom. Let us then choose one of these vacua and study the action for fluctuations around it. As we have seen, the action for the fluctuations has the same form as the original one, but with a different BRST operator, that we shall now denote by $\mathcal{Q}$. According to Sen's conjectures, at this chosen vacuum there are no open string degrees of freedom and it is thus natural to assume, as in the VSFT for the

bosonic string, that the new BRST operator has vanishing cohomology and is made purely of (super)ghost operators. In addition we will also assume that this operator annihilates the identity,

$$\mathcal{Q}\mathcal{I}=0. \tag{20}$$

This condition, although very natural, is strictly not necessary in order to preserve some of the basic features of bosonic VSFT. In the superstring case however, it is crucial. It was noticed in Ref. 18 that operators of the form $\mathcal{Q}=c_0+\Sigma_n u_n c_n$ also have vanishing cohomology in the superstring case. In particular, the $\mathcal{Q}$ operator recently proposed in Ref. 25 for the bosonic VSFT is of this form and annihilates the identity after some proper regularization, so that in principle it is a possible candidate for the superstring as well (where the superconformal ghost sector would be handled separately). We shall come back to this question in Sec. VII.

With these assumptions at hand, and given the fact that the action around the vacuum has the same form as the original one but with a pure (super)ghost operator $\mathcal{Q}$, it is now easy to show that the ansatz (10) solves the superstring field theory equations of motion if Φ_m is idempotent and Φ_g satisfies

$$\eta_0(e^{-\Phi_g}\mathcal{Q}e^{\Phi_g})=0. \tag{21}$$

In order to see this, notice that idempotency of Φ_m and factorization of the star product in matter and ghost parts yields

$$e^{\Phi}=e^{\Phi_g}\otimes\Phi_m+\mathcal{I}-\Phi_m, \tag{22}$$

and, since $\mathcal{Q}$ kills the identity and is pure ghost, one has

$$\mathcal{Q}e^{\Phi}=(\mathcal{Q}e^{\Phi_g})\otimes\Phi_m. \tag{23}$$

Using again idempotency of Φ_m, the equation of motion becomes

$$(\eta_0(e^{-\Phi_g}\mathcal{Q}e^{\Phi_g}))\otimes\Phi_m=0. \tag{24}$$

Therefore, the above conditions are sufficient to solve the equations of motion. In the same way, one can show that in these circumstances the action factorizes as

$$S=K\langle\Phi_m|\Phi_m\rangle, \tag{25}$$

where

$$K=S[\Phi_g]. \tag{26}$$

Let us now look at the gauge symmetry of the new action around the tachyon vacuum. We are particularly interested in transformations that preserve the structure of (22). Since both $\mathcal{Q}$ and η_0 annihilate the identity, it is easy to see that the gauge transformation (6) with

$$\Xi_L=\Xi_m\otimes\mathcal{I}_g, \quad \Xi_R=-\Xi_m\otimes\mathcal{I}_g, \tag{27}$$

preserves (22). This gauge transformation leaves Φ_g invariant and changes Φ_m as follows:

$$\delta\Phi_m=[\Xi_m,\Phi_m]_\star, \tag{28}$$

where $[A,B]_\star=A\star B-B\star A$ is the commutator in the star algebra. Notice that this transformation preserves idempotency of Φ_m at linear order. The gauge symmetry (28) is precisely the one that appears in bosonic VSFT when $\mathcal{Q}$ annihilates the identity.[19,21,25]

The condition of idempotency of Φ_m in the non-GSO projected theory involves in fact two different conditions. In general, a matter string field Φ_m has components in both GSO($\pm$) sectors,

$$\Phi_m = \Phi_m^+ \otimes 1 + \Phi_m^- \otimes \sigma_1 . \tag{29}$$

In this equation, $\Phi_m^\pm$ is Grassmann even (odd), and idempotency of Φ_m is equivalent to the following equations:

$$\begin{aligned} \Phi_m^+ \star \Phi_m^+ + \Phi_m^- \star \Phi_m^- &= \Phi_m^+ , \\ \Phi_m^+ \star \Phi_m^- + \Phi_m^- \star \Phi_m^+ &= \Phi_m^- . \end{aligned} \tag{30}$$

One particular solution is of course to take Φ_m^+ as an idempotent state and $\Phi_m^- = 0$. The matter supersliver state that we will discuss later is an example of such a solution. Another possibility is to take Φ_m^+ an idempotent and Φ_m^- a nilpotent state satisfying the second equation in (30). In Sec. VI we will construct solutions with these characteristics, although we will also show that they are related to the supersliver solution by gauge transformations at the vacuum.

III. NEUMANN COEFFICIENTS AND OVERLAP EQUATIONS

In this section we review some of the results of Ref. 29 and we explain in detail the structure of the overlap equations involving the matter part of the fermionic sector.

A. The identity

As in bosonic string field theory, the simplest vertex in superstring field theory is the integration, which corresponds to folding the string and identifying the two halves[1] thus defining the identity string field $|I\rangle$,

$$\int \Phi = \langle I | \Phi \rangle . \tag{31}$$

In the bosonic case, the overlap condition defining the identity is simply $x(\pi - \sigma) = x(\sigma)$. In the fermionic case, and due to the conformal weight $h = 1/2$, the precise conditions are as follows:

$$\begin{aligned} (\psi_+(\sigma) - i\psi_+(\pi - \sigma))|I\rangle = 0, \quad 0 \leqslant \sigma \leqslant \frac{\pi}{2}, \\ (\psi_-(\sigma) + i\psi_-(\pi - \sigma))|I\rangle = 0, \quad 0 \leqslant \sigma \leqslant \frac{\pi}{2}. \end{aligned} \tag{32}$$

The different sign in the second equation is due to the NS boundary conditions $\psi_-(0) = \psi_+(0)$, $\psi_-(\pi) = -\psi_+(\pi)$. As usual, we can define a single antiperiodic fermion field $\psi(\sigma)$ in the interval $[-\pi, \pi]$ by declaring that $\psi(\sigma) = \psi_+(\sigma)$ for $0 \leqslant \sigma \leqslant \pi$, and $\psi(\sigma) = \psi_-(-\sigma)$ for $-\pi \leqslant \sigma \leqslant 0$. In terms of this single field, the overlap conditions (32) read

$$\psi(\sigma) = \begin{cases} i\psi(\pi - \sigma), & 0 \leqslant |\sigma| \leqslant \dfrac{\pi}{2}, \\ -i\psi(\pi - \sigma), & \dfrac{\pi}{2} \leqslant |\sigma| \leqslant \pi. \end{cases} \tag{33}$$

This condition leads to the following relation for the modes:

$$\begin{pmatrix} \psi_r \\ \psi_{-r} \end{pmatrix} = \begin{pmatrix} M_{rs} & \tilde{M}_{rs} \\ -\tilde{M}_{rs} & -M_{rs} \end{pmatrix} \begin{pmatrix} \psi_r \\ \psi_{-r} \end{pmatrix}, \tag{34}$$

where the matrices M, $\tilde{M}$, are defined by

$$M_{rs}=-\frac{2}{\pi}\frac{i^{r-s}}{r+s},\quad r=s\pmod 2, \tag{35}$$

$$\tilde{M}_{rs}=\frac{2}{\pi}\frac{i^{r+s}}{s-r},\quad r=s+1\pmod 2. \tag{36}$$

These matrices will play an important role in this paper. They satisfy the following properties:

$$M^2-\tilde{M}^2=1,\quad [M,\tilde{M}]=0, \tag{37}$$

$$\overline{M}=M^T=M,\quad \overline{\tilde{M}}=-\tilde{M}^T=\tilde{M}. \tag{38}$$

From (34) one obtains the following relation between positive and negative modes for the fermion fields that annihilate the identity:

$$\psi_r=\left(\frac{\tilde{M}}{1-M}\right)_{rs}\psi_{-s}. \tag{39}$$

Using this relation, one can then show that the identity is a squeezed state,

$$|I\rangle=\mathcal{N}_I\exp\left[\frac{1}{2}\eta_{\mu\nu}\sum_{r,s\geqslant 1/2}\psi^\mu_{-r}I_{rs}\psi^\nu_{-s}\right]|0\rangle, \tag{40}$$

where

$$I=\frac{\tilde{M}}{1-M}. \tag{41}$$

This equation can be obtained acting with ψ^μ_r on $|I\rangle$ and using (39). In (40), $\mathcal{N}_I$ is a normalization constant that we shall determine later, when we discuss the supersliver. One can also determine the coefficients I_{rs} explicitly by using conformal mapping techniques. The result, derived in Ref. 29, is the following. Defining the coefficients

$$\hat{u}_{2n}=\hat{u}_{2n+1}=\binom{-1/2}{n}=\frac{(-1)^n(2n-1)!!}{2^n n!}, \tag{42}$$

one has

$$I_{rs}=i^{r+s}\left(\frac{I^+_{nm}}{r+s}-\frac{I^-_{nm}}{r-s}\right),\quad r=n+1/2,\quad s=m+1/2, \tag{43}$$

where

$$I^\pm_{nm}=\begin{cases}-m\hat{u}_n\hat{u}_m, & n=\text{even},\ m=\text{odd},\\ \pm n\hat{u}_n\hat{u}_m, & n=\text{odd},\ m=\text{even},\\ 0, & \text{otherwise}.\end{cases} \tag{44}$$

One can check that this explicit expression satisfies the equation (41) (see the Appendix).

B. Interaction vertex and overlap equations

The interaction vertex, $|V_3\rangle$, involves the gluing of three strings and determines the star algebra multiplication rule,

$$|\Phi\star\Psi\rangle_{(3)}={}_{(1)}\langle\Phi|_{(2)}\langle\Psi||V_3\rangle_{(123)}\,. \tag{45}$$

In the operator formulation, this vertex involves a set of infinite-dimensional matrices whose entries are called Neumann coefficients. Usually, in order to find an explicit expression for these coefficients, one uses conformal mapping techniques. On the other hand, in order to understand the structural properties of these matrices, it turns out to be very convenient to analyze the overlap equations as well. In this section we shall deduce an expression for the Neumann coefficients in terms of the matrices M, $\widetilde{M}$, which will be very useful in the following. The starting point is the overlap equation for the three string interaction vertex. This overlap equation simply states that the interaction is obtained by gluing the halves of the three strings in the usual way.[1] In the fermionic case the equation reads:[29]

$$(\psi^a(\sigma)-i\psi^{a-1}(\pi-\sigma))|V_3\rangle=0,\quad 0\leqslant\sigma\leqslant\frac{\pi}{2},\quad a=1,2,3. \tag{46}$$

The index a labels each of the three strings. As in Ref. 30, it is convenient to diagonalize this condition by introducing the following discrete Fourier transforms:

$$q=\frac{1}{\sqrt{3}}(\psi^1+\omega\psi^2+\overline{\omega}\psi^3), \tag{47}$$

$$q_3=\frac{1}{\sqrt{3}}(\psi^1+\psi^2+\psi^3), \tag{48}$$

together with their adjoints,

$$\overline{q}^\dagger=\frac{1}{\sqrt{3}}((\psi^1)^\dagger+\omega(\psi^2)^\dagger+\overline{\omega}(\psi^3)^\dagger), \tag{49}$$

$$q_3^\dagger=\frac{1}{\sqrt{3}}((\psi^1)^\dagger+(\psi^2)^\dagger+(\psi^3)^\dagger), \tag{50}$$

where $\omega=e^{2\pi i/3}$ is a cubic root of unity. The overlap conditions give the following condition for q_3:

$$q_3(\sigma)=iq_3(\pi-\sigma),\quad 0\leqslant\sigma\leqslant\frac{\pi}{2}, \tag{51}$$

which is identical in structure to (33). On the other hand, for $q(\sigma)$ we find

$$q(\sigma)=\begin{cases} i\omega q(\pi-\sigma), & 0\leqslant\sigma\leqslant\dfrac{\pi}{2},\\[2ex] -i\overline{\omega}q(\pi-\sigma), & \dfrac{\pi}{2}\leqslant\sigma\leqslant\pi. \end{cases} \tag{52}$$

The overlap conditions for q then yield the following relation between the modes,

$$\begin{pmatrix} q_r \\ \overline{q}_r^\dagger \end{pmatrix}=\left\{-\frac{1}{2}\begin{pmatrix} M_{rs} & \widetilde{M}_{rs} \\ -\widetilde{M}_{rs} & -M_{rs} \end{pmatrix}+\frac{\sqrt{3}}{2}\begin{pmatrix} 0 & iC_{rs} \\ -iC_{rs} & 0 \end{pmatrix}\right\}\begin{pmatrix} q_r \\ \overline{q}_r^\dagger \end{pmatrix}, \tag{53}$$

where the matrix C is defined by

$$C_{rs}=(-1)^{r+1/2}\delta_{rs}\,. \tag{54}$$

This matrix implements BPZ conjugation and satisfies the following conditions:

$$C^2=1,\quad C^T=\overline{C}=C, \tag{55}$$

$$CMC=M,\quad C\tilde{M}C=-\tilde{M}, \tag{56}$$

$$CIC=-I, \tag{57}$$

which guarantee the consistency of (53).

We now write the three string vertex as

$$|V_3\rangle=\exp[\tfrac{1}{2}q_3^\dagger\cdot I\cdot q_3+q^\dagger\cdot U\cdot\overline{q}^\dagger]|0\rangle_{(123)}\,, \tag{58}$$

where I is the matrix (41). This is of course a consequence of (51). Since $q|V_3\rangle=U\overline{q}^\dagger|V_3\rangle$, by using (53) we obtain an explicit expression for U in terms of M, $\tilde{M}$, and C:

$$U=-\frac{1}{2+M}\cdot(\tilde{M}-i\sqrt{3}C). \tag{59}$$

Using the above properties of M, $\tilde{M}$, and C, it is easy to show that U satisfies

$$\overline{U}=-U^T=-CUC,\quad IU=\overline{U}I,\quad I\overline{U}=UI. \tag{60}$$

The following formulas will also be useful:

$$\begin{aligned} I^2&=\frac{M+1}{M-1},\\ U^2=\overline{U}^2&=\frac{M-2}{M+2},\\ U+\overline{U}&=-\frac{2\tilde{M}}{M+2},\\ U-\overline{U}&=\frac{2\sqrt{3}iC}{M+2}. \end{aligned} \tag{61}$$

Let us now find the structure of the Neumann coefficients for the three string vertex. These coefficients are defined through

$$|V_3\rangle=\exp\left[\frac{1}{2}\,\eta_{\mu\nu}\sum\ \psi_{-r}^{(a)\mu}K_{rs}^{ab}\psi_{-s}^{(b)\nu}\right]|0\rangle_{(123)}\,, \tag{62}$$

and satisfy the condition

$$K_{rs}^{ab}=-K_{sr}^{ba}\,. \tag{63}$$

Using the above results, one finds that

$$K^{ab}=\tfrac{1}{3}(I+\omega^{b-a}U+\omega^{a-b}\overline{U}), \tag{64}$$

which has the same structure as the Neumann coefficients in the bosonic sector. We also have the cyclicity property, $K^{a+1,b+1}=K^{ab}$. We shall frequently use the matrices K^{11}, K^{12}, and K^{21}, which are given by

$$K^{11}=\frac{1}{3}(I+U+\overline{U}),$$

$$K^{12}=\frac{1}{3}I-\frac{1}{6}(U+\overline{U})+\frac{i\sqrt{3}}{6}(U-\overline{U}), \tag{65}$$

$$K^{21}=\frac{1}{3}I-\frac{1}{6}(U+\overline{U})-\frac{i\sqrt{3}}{6}(U-\overline{U}).$$

Again, one can use conformal mapping techniques to write explicit expressions for the Neumann coefficients.[29] The result is the following. Define the coefficients g_n through the expansion

$$\left(\frac{1+x}{1-x}\right)^{1/6}=\sum_{n=0}^{\infty} g_n x^n. \tag{66}$$

Next, define the following quantities:

$$\begin{aligned}
M^{+}_{nm}&=-[(-1)^n-(-1)^m][(n+1)g_{n+1}(m+1)g_{m+1}-ng_n mg_m],\\
M^{-}_{nm}&=-[(-1)^n-(-1)^m][ng_n(m+1)g_{m+1}-(n+1)g_{n+1}mg_m],\\
\overline{M}^{+}_{nm}&=[(-1)^n+(-1)^m][(n+1)g_{n+1}(m+1)g_{m+1}-ng_n mg_m],\\
\overline{M}^{-}_{nm}&=[(-1)^n+(-1)^m][ng_n(m+1)g_{m+1}-(n+1)g_{n+1}mg_m].
\end{aligned} \tag{67}$$

The Neumann coefficients are then given by,

$$\begin{aligned}
K^{aa}_{rs}&=\frac{1}{3}I_{rs}+i^{r+s}\left[\frac{M^{+}_{r-1/2,s-1/2}}{r+s}+\frac{M^{-}_{r-1/2,s-1/2}}{r-s}\right],\\
K^{aa+1}_{rs}&=\frac{1}{2}I_{rs}-\frac{1}{2}K^{aa}_{rs}-\frac{1}{2}\sqrt{3}i^{r+s-1}\left[\frac{\overline{M}^{+}_{r-1/2,s-1/2}}{r+s}+\frac{\overline{M}^{-}_{r-1/2,s-1/2}}{r-s}\right],\\
K^{aa-1}_{rs}&=\frac{1}{2}I_{rs}-\frac{1}{2}K^{aa}_{rs}+\frac{1}{2}\sqrt{3}i^{r+s-1}\left[\frac{\overline{M}^{+}_{r-1/2,s-1/2}}{r+s}+\frac{\overline{M}^{-}_{r-1/2,s-1/2}}{r-s}\right].
\end{aligned} \tag{68}$$

Using (64) and (68), one can find explicit expressions for the matrices $U+\overline{U}$ and $U-\overline{U}$:

$$\begin{aligned}
(U+\overline{U})_{rs}&=3i^{r+s}\left[\frac{M^{+}_{r-1/2,s-1/2}}{r+s}+\frac{M^{-}_{r-1/2,s-1/2}}{r-s}\right],\\
(U-\overline{U})_{rs}&=3i^{r+s}\left[\frac{\overline{M}^{+}_{r-1/2,s-1/2}}{r+s}+\frac{\overline{M}^{-}_{r-1/2,s-1/2}}{r-s}\right].
\end{aligned} \tag{69}$$

Notice that the matrix $U-\overline{U}$ has nonzero diagonal terms. Using the results of Ref. 29, one finds

$$(U-\overline{U})_{rr}=6i\left[\frac{(n+1)^2g_{n+1}^2-n^2g_n^2}{2n+1}+\frac{1}{3}\sum_{l=0}^{n}(-1)^l g_{n-l}^2\right]. \tag{70}$$

In the Appendix we show that these explicit expressions indeed agree with (59).

For the calculations in the next section, it will be useful to define the following matrices:

$$M^{ab}=CK^{ab}. \tag{71}$$

Using (64) and the relations (60), it is easy to see that these matrices satisfy the following properties:

$$[M^{ab},M^{a'b'}]=0, \quad [CI,M^{ab}]=0. \tag{72}$$

These properties are of course similar to the properties of the matrices M^{ab} in the bosonic case.[24,19]

IV. THE SUPERSLIVER

As we discussed in Sec. II, a factorized string field satisfies the equations of motion of vacuum superstring field theory, with a pure ghost BRST operator, $\mathcal{Q}$, if the ghost part satisfies (21) and the matter part is idempotent. We shall now consider idempotent matter states with the factorized form

$$|\Psi\rangle=|\Psi_b\rangle\otimes|\Psi_f\rangle, \tag{73}$$

where $|\Psi_{b,f}\rangle$ denote states which are obtained from the vacuum by acting with bosonic and fermionic oscillators, respectively, and which are idempotent with respect to the star product in their respective matter sectors. In this section we will look for idempotent states in the fermionic sector. First, we provide an algebraic construction, in the spirit of Ref. 24. Then we compare the solution to the geometric construction of the sliver given in Ref. 23.

A. Algebraic construction

Our purpose here is to find a state in the fermionic part of the matter sector that star squares to itself. Our ansatz is a squeezed state of the form

$$|\Psi_F\rangle=\mathcal{N}_F\exp\left[-\frac{1}{2}\eta_{\mu\nu}\sum_{r,s\geqslant 1/2}\psi^{\mu}_{-r}F_{rs}\psi^{\nu}_{-s}\right]|0\rangle, \tag{74}$$

where F_{rs} is an antisymmetric matrix. Recall that the star product of two states, $|\Psi\rangle$, $|\Phi\rangle$, defined as

$$|\Psi\star\Phi\rangle_{(3)}={}_{(1)}\langle\Psi|_{(2)}\langle\Phi||V_3\rangle_{(123)}, \tag{75}$$

involves the BPZ conjugate of the string field states. To obtain the BPZ conjugate of $|\Psi_F\rangle$, one has to take into account that

$$\mathrm{bpz}(\psi^{\mu}_r)=(-1)^{r+1/2}\psi^{\mu}_{-r}. \tag{76}$$

Therefore, the matrix that implements BPZ conjugation is C. It will be useful in the following to define:

$$H=CF. \tag{77}$$

In order to evaluate the star product, one still needs the following formula. Let b_i, $b_i^\dagger$ be fermionic oscillators with anticommutation relations $\{b_i,b_j^\dagger\}=\delta_{ij}$, let λ_i,μ_i be a set of Grassmann variables, and let S_{ij},T_{ij} be antisymmetric matrices. One then has

$$\langle 0|\exp(\lambda^T\cdot b+\tfrac{1}{2}b\cdot S\cdot b)\exp(\mu^T\cdot b^\dagger+\tfrac{1}{2}b^\dagger\cdot T\cdot b^\dagger)|0\rangle$$
$$=[\det(1+ST)]^{1/2}\ \exp[\mu^T(1+ST)^{-1}\lambda+\tfrac{1}{2}\lambda^T T(1+ST)^{-1}\lambda+\tfrac{1}{2}\mu^T(1+ST)^{-1}S\mu]. \tag{78}$$

Similar expressions for bosonic oscillators and for the ghost bc system were presented in Refs. 24 and 19. Using this formula, one obtains the following expression:

$$|\Psi_F\star\Psi_F\rangle_{(3)}=\mathcal{N}_F^2[\det(1+\Phi\mathcal{K})]^5\exp[\tfrac{1}{2}\eta_{\mu\nu}\{\chi^{\mu T}(1+\Phi\mathcal{K})^{-1}\Phi\chi^\nu+\tfrac{1}{2}\psi^{3\mu}_{-r}K^{33}_{rs}\psi^{3\nu}_{-s}\}]|0\rangle_{(3)}, \tag{79}$$

where

$$\Phi=\begin{pmatrix}-HC & 0\\ 0 & -HC\end{pmatrix},\quad \mathcal{K}=\begin{pmatrix}K^{11} & K^{12}\\ K^{21} & K^{22}\end{pmatrix},\quad \chi^\mu=\begin{pmatrix}K^{13}\psi^{3\mu\dagger}\\ K^{23}\psi^{3\mu\dagger}\end{pmatrix}. \tag{80}$$

Using (63) and the cyclicity property, one further obtains the following equation for H:

$$H=-M^{11}-(M^{12}\quad M^{21})\begin{pmatrix}1-HM^{11} & -HM^{12}\\ -HM^{21} & 1-HM^{22}\end{pmatrix}^{-1}\begin{pmatrix}HM^{21}\\ HM^{12}\end{pmatrix}, \tag{81}$$

and the following value for the normalization constant:

$$\mathcal{N}_F=[\det(1+\Phi\mathcal{K})]^{-5}. \tag{82}$$

Since the matrices M^{ab} commute, one can assume that $[H,M^{ab}]=0$ and proceed as if we were dealing with commuting variables. After some simple algebra, one finds the following cubic equation for H:

$$A_3H^3+A_2H^2+A_1H+A_0=0, \tag{83}$$

where

$$A_3=M^{12}M^{21}-(M^{11})^2,$$
$$A_2=3M^{11}M^{12}M^{21}-(M^{11})^3-(M^{12})^3-(M^{21})^3,$$
$$A_1=-1-2A_3, \tag{84}$$
$$A_0=-M^{11}.$$

In the bosonic case analyzed in Refs. 24 and 19, the coefficients of the cubic equation for the bosonic piece of the sliver could be simplified by using relations among the matrices of Neumann coefficients. Here, it is convenient to express (84) in terms of the matrices U, $\overline{U}$, and I, which in turn can be expressed in terms of C, M, and $\tilde{M}$. After some simple algebra, one finds the following:

$$A_3=\frac{1}{3}(U+\overline{U})I+\frac{1}{6}(U^2+\overline{U}^2)=\frac{M}{M+2},$$

$$A_2=\frac{1}{2}C(U^2+\overline{U}^2)I+\frac{2}{3}C(I+U+\overline{U})=-C\tilde{M}\frac{3M-2}{(M-1)(M+2)},$$

$$A_1 = -\frac{3M+2}{M+2}, \tag{85}$$

$$A_0 = C\tilde{M}\frac{M}{(M-1)(M+2)}.$$

Since $|I\star I\rangle = |I\rangle$, an important check of the above is whether $H=-CI$ is a solution of (83). In fact, one can further write (83) as

$$(H+CI)(MH^2 - 2C\tilde{M}H - M) = 0. \tag{86}$$

In order to solve the quadratic equation, one has to be careful when extracting the square root. Since F must be antisymmetric, and remembering that $F=CH$, one finds the two solutions,

$$F^{\pm} = \frac{\tilde{M}}{M}\left(1 \pm \frac{1}{\sqrt{1-M^2}}\right). \tag{87}$$

Notice that $CF^{\pm}C = -F^{\pm}$. It is also easy to check that H commutes with M^{ab}, as assumed in our initial ansatz. Using the above result for $F^{\pm}$, one can compute

$$(1+\Phi\mathcal{K})^{-1} = -\frac{1}{4}(M-1)(M+2)\left(1 \mp \frac{M+1}{\sqrt{1-M^2}}\right), \tag{88}$$

which determines the normalization constant $\mathcal{N}_{F^{\pm}}$ through (82). Using again (78), one can further compute the norm of $|\Psi^{F_{\pm}}\rangle$ and find, for both signs,

$$\langle \Psi^{F_{\pm}} | \Psi^{F_{\pm}} \rangle = [\det((1-M)(1+M/2)^2)]^5. \tag{89}$$

Finally, notice that in order for the identity to star square to itself, one needs

$$\mathcal{N}_I = [\det((1-M)(1+M/2))]^5, \tag{90}$$

and its BPZ norm turns out to be

$$\langle I|I\rangle = [\det(2(1-M)(1+M/2)^2)]^5. \tag{91}$$

B. Numerical results and comparison to the geometric sliver

The above results involve infinite-dimensional matrices. They can however be analyzed numerically by restricting the matrix rank to $L<\infty$ and then using suitable numerics in order to study the limit $L\to\infty$, as in Ref. 19. The first thing to notice is that the determinant of M converges to zero very rapidly. As a consequence, the solution F^+, which behaves like $2\tilde{M}M^{-1}$, has diverging eigenvalues. The other solution, which behaves like $\tilde{M}M/2$, has a better behavior. This is the solution that we will discuss in the rest of the paper, and we shall henceforth simply denote it by $F=F^-$.

It turns out that F is the matrix that appears in the fermionic part of the geometric sliver constructed by Rastelli and Zwiebach in Ref. 23. Since the sliver can be defined purely in geometric terms, one can construct a supersliver in the CFT given by the NS sector of the superstring. Recall that the (super)sliver is defined by

$$\langle \Xi| = \langle 0| U_f, \tag{92}$$

where U_f is the operator associated to the conformal transformation given by

$$f(z)=\arctan(z). \tag{93}$$

The structure of the operator U_f was found in Ref. 23. It is given by

$$U_f=\exp\sum_{n=1}^{\infty} a_n L_{-2n}, \tag{94}$$

where the coefficients a_n can be computed explicitly. The Virasoro operators split as $L=L_b+L_f+L_g$, where b, f, g refer, respectively, to the bosonic matter, fermionic matter and ghost/superghost sectors. As a consequence, the supersliver will factorize as

$$|\Xi\rangle=|\Xi_b\rangle\otimes|\Xi_f\rangle\otimes|\Xi_g\rangle. \tag{95}$$

The bosonic matter part is the one constructed algebraically in Ref. 24. In the following, we will present evidence that the fermionic matter part is the idempotent state constructed above and corresponding to F, i.e.,

$$|\Xi_f\rangle=|\Psi_F\rangle. \tag{96}$$

The first step is, as in Ref. 19, to write $|\Xi_f\rangle$ as a squeezed state

$$|\Xi_f\rangle=\mathcal{N}\exp\left[-\frac{1}{2}\eta_{\mu\nu}\sum_{r,s}\psi^{\mu}_{-r}\hat{F}_{rs}\psi^{\nu}_{-s}\right]|0\rangle. \tag{97}$$

Using the CFT techniques of Refs. 36, 37, and 38, one finds for the matrix $\hat{F}$:

$$\hat{F}_{rs}=-\oint_0\frac{dw}{2\pi i}\oint_0\frac{dz}{2\pi i}\frac{z^{-r-1/2}w^{-s-1/2}}{(1+z^2)^{1/2}(1+w^2)^{1/2}(\tan^{-1}(z)-\tan^{-1}(w))}. \tag{98}$$

One can see that $\hat{F}_{rs}=0$ if $r+s=$odd, i.e., $C\hat{F}C=-\hat{F}$, as follows from the algebraic description. Evaluating the residues, one finds for the first nonzero entries:

$$\hat{F}_{1/2,3/2}=-\tfrac{1}{6}\simeq-0.1666,\quad \hat{F}_{1/2,7/2}=\tfrac{43}{60}\simeq 0.1194,\quad \hat{F}_{1/2,11/2}=-\tfrac{1459}{15120}\simeq-0.0964,$$

$$\hat{F}_{3/2,5/2}=-\tfrac{1}{40}\simeq-0.0250,\quad \hat{F}_{3/2,9/2}=\tfrac{71}{15120}\simeq 0.0046,\quad \hat{F}_{5/2,7/2}=-\tfrac{239}{7560}\simeq-0.0316. \tag{99}$$

On the other hand, we can evaluate numerically the first few coefficients F_{rs}. Since $M,\tilde{M}$ do not commute at finite rank, we can approximate the matrix F in two ways: multiplying $\tilde{M}$ on the right, or on the left. The results are shown, respectively, in the following tables:

L	$F_{1/2,3/2}$	$F_{1/2,7/2}$	$F_{1/2,11/2}$	$F_{3/2,5/2}$	$F_{3/2,9/2}$	$F_{5/2,7/2}$
20	−0.1929	0.1427	−0.1186	0.0033	−0.0178	−0.0448
100	−0.1876	0.1347	−0.1102	−0.0058	−0.0099	−0.0398
150	−0.1847	0.1335	−0.1091	−0.0074	−0.0087	−0.0391
∞	−0.1676	0.1235	−0.1098	−0.0268	0.0036	−0.0347

L	$F_{1/2,3/2}$	$F_{1/2,7/2}$	$F_{1/2,11/2}$	$F_{3/2,5/2}$	$F_{3/2,9/2}$	$F_{5/2,7/2}$
20	−0.1140	0.0752	−0.0570	−0.0397	0.0163	−0.0076
100	−0.1299	0.0886	−0.0683	−0.0346	0.0122	−0.0155
150	−0.1328	0.0910	−0.0710	−0.0338	0.0115	−0.0168
∞	−0.1726	0.1251	−0.1020	−0.0250	0.0045	−0.0335

The last entry shows an extrapolation to $L=\infty$ by fitting fifteen points $L=10,20,\ldots,150$ to $a_0+a_1/(\log L)+a_2(\log L)^2$. We see that there is good agreement with the exact result (99), and this provides good numerical evidence that the matrix F is indeed given by the double residue (98).

It is also interesting to consider the behavior of the BPZ norms of the fermionic identity and the fermionic part of the sliver. The fermionic identity turns out not to be normalizable: the determinant in (90) grows very quickly as we increase the rank. On the other hand, the norm of $|\Xi_f\rangle$, given in (89), behaves like the norm of $|\Xi_b\rangle$ analyzed in Ref. 19: an extrapolation to infinite rank, by fitting one hundred points $L=10,20,\ldots,1000$, gives $\langle\Xi_f|\Xi_f\rangle^{1/5}=-0.0075$. This seems to indicate that the norm of the fermionic part of the supersliver is zero.

C. Conservation laws

In this subsection we wish to derive conservation laws satisfied by the supersliver, involving the superconformal generators, G_r, and following Refs. 23 and 19. We shall be schematic, as the procedure is by now well known. Observe that due to its purely geometrical construction (92) the supersliver will clearly satisfy all the Virasoro conservation laws outlined in the Appendix of Ref. 19, involving the L_n generators of the conformal algebra which now will have a fermionic matter piece as well as a bosonic and ghost pieces. Let us then outline how can one derive the conservation laws associated to the rest of the superconformal algebra, i.e., the ones depending on the G_r generators.

The sliver surface state is defined in the upper half plane by the conformal map,

$$f_{\mathrm{H}}(z)=\arctan(z), \tag{100}$$

while in the unit disk (coordinates that we will use in the following), it is given by

$$f_{\mathrm{U}}(z)=\frac{1+i\arctan(z)}{1-i\arctan(z)}. \tag{101}$$

The usual contour deformation argument yields the expected conservation law,

$$\langle\Xi|\oint dz\,\varphi(z)G(z)=0, \tag{102}$$

where $G(z)$ is the super stress tensor, $G(z)=\Sigma G_r/z^{r+\frac{3}{2}}$, and the conformal densities $\varphi(z)$ now have weight $-1/2$. Precisely because of this non-integer weight, one has to be careful when taking the conformal transformation,

$$\varphi(z)=\tilde{\varphi}(f(z))\left(\frac{df(z)}{dz}\right)^{-1/2}, \tag{103}$$

so that we shall adopt the standard conventions.[17]

With the choice of conformal density,

$$\varphi(z)=-\frac{4}{3}\sqrt{\frac{2}{3}}(1-i)\left(1+\frac{1}{z-1}\right), \tag{104}$$

one obtains the following conservation law:

$$\langle\Xi|(G_{-3/2}+\tfrac{11}{6}G_{1/2}+\tfrac{43}{360}G_{5/2}-\tfrac{1039}{15120}G_{9/2}+\cdots)=0. \tag{105}$$

If instead one chooses the conformal density,

$$\varphi(z)=-\frac{4}{3}\sqrt{\frac{2}{3}}(1-i)\left(\frac{1}{2}+i\frac{\sqrt{3}}{2}-\frac{1}{z-e^{2\pi i/3}}\right), \tag{106}$$

one obtains the conservation law

$$\langle\Xi|\left(G_{-1/2}+\frac{1}{\sqrt{3}}G_{1/2}+\frac{11}{6}G_{3/2}+\frac{3}{2\sqrt{3}}G_{5/2}+\frac{7}{72}G_{7/2}+\cdots\right)=0. \tag{107}$$

Other conservation laws can be obtained in similar fashions.

V. FERMIONIC STAR ALGEBRA SPECTROSCOPY

In this section we follow the methods of Ref. 26, in order to find the eigenvalue spectrum of the various infinite-dimensional matrices involved in the star algebra for the matter fermionic sector, as well as the corresponding eigenvectors. We first find by inspection an eigenvector of M and $\tilde{M}$, and we then adapt the methods of Ref. 26 to find the rest of the spectrum. The star algebra spectroscopy has also been studied in Refs. 39 and 40.

A. An eigenvector of M and $\tilde{M}$

In this section we want to show that the matrices M and $\tilde{M}$ have a common eigenvector with eigenvalues -1 and 0, respectively. First define

$$\nu_{n-1/2}=\begin{cases}\binom{-1/2}{k}, & n=2k+1,\\ 0, & n=2k.\end{cases} \tag{108}$$

Using (A1), and setting $r=n+1/2$, one easily finds

$$\sum_s M_{rs}\nu_s=-\frac{2}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^{n-m}}{2m+2n+1}\binom{-1/2}{m}=-\binom{-1/2}{n}=-\nu_r,$$

$$\sum_s \tilde{M}_{rs}\nu_s=\frac{2}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^{n+m}}{2m-2n-1}\binom{-1/2}{m}=\frac{(-1)^n}{\pi}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(-n-\frac{1}{2}\right)}{\Gamma(-n)}=0. \tag{109}$$

Therefore, ν_r is a common eigenvector to M and $\tilde{M}$ with eigenvalues -1 and 0, respectively. This vector can be understood geometrically as follows. Notice that its components are the negative modes in the Fourier expansion of the function

$$f(\sigma)=\frac{e^{-i\sigma/2}}{\sqrt{1+e^{-2i\sigma}}}. \tag{110}$$

This function is antiperiodic in $[-\pi,\pi]$ and satisfies the overlap equation $f(\sigma)=if(\pi-\sigma)$. Therefore, its modes satisfy the equation (34). Since the positive modes are set to zero, it follows from (34) that the coefficients of the Fourier expansion give an eigenvector of M and $\tilde{M}$ with the required eigenvalues. Finally, notice that the vector ν is BPZ odd, since $C\nu=-\nu$. A related discussion of the geometric meaning of the eigenvectors in the bosonic case can be found in Ref. 40.

B. Diagonalizing K_1

To find the rest of the spectrum, we generalize the considerations of Ref. 26 to the fermionic sector. The derivation of the star algebra,

$$K_1 = L_1 + L_{-1}, \tag{111}$$

has a fermionic part which is a sum of bilinears in the modes $\psi_{\pm r}$. This allows for a definition of an infinite-dimensional matrix as follows. Let $\{v_r\}_{r \geqslant 1/2}$ be an infinite-dimensional vector. Define then the matrix K_1 through

$$[K_1, v \cdot \psi] = (K_1 v) \cdot \psi, \tag{112}$$

where $v \cdot \psi = \Sigma_{r=1/2}^{\infty} v_r \psi_r$. In what follows, it will be quite useful to label the positive half-integer indices with integer numbers by setting $r = n - 1/2$, $n = 1,2,\ldots$. Using the explicit expression for the Virasoro generators, we then find

$$(K_1)_{nm} = -(n-1)\,\delta_{n-1,m} - n\,\delta_{n+1,m}. \tag{113}$$

This is a symmetric matrix that anticommutes with C, $\{K_1, C\} = 0$. To find its spectrum, one associates to every vector w a function $f_w(z)$ as follows:

$$f_w(z) = \sum_{n=1}^{\infty} w_n z^n. \tag{114}$$

The infinite-dimensional matrix K_1 is then represented in the space of functions by the differential operator

$$\mathcal{K}_1 = -(1+z^2)\frac{d}{dz} + \frac{1}{z}, \tag{115}$$

and the problem of finding eigenvectors of K_1 now becomes the problem of finding eigenfunctions for this differential operator. The solution is immediate: for any $-\infty < \kappa < \infty$ there is an eigenfunction of $\mathcal{K}_1$ given by

$$f_{w^{(\kappa)}}(z) = \frac{z}{\sqrt{1+z^2}}\,\exp(-\kappa \arctan(z)), \tag{116}$$

with eigenvalue κ. The normalization of this function has been chosen so that $w_1^{(\kappa)} = 1$. One then concludes that K_1 has a nondegenerate, continuous spectrum, similar to the bosonic case studied in Ref. 26. Also notice that

$$f_{Cw}(z) = -f_w(-z), \tag{117}$$

so that the BPZ matrix acts as

$$Cw^{(\kappa)} = -w^{(-\kappa)}. \tag{118}$$

C. Diagonalizing M and $\tilde{M}$

We can now use this information in order to find the spectrum of M and $\tilde{M}$. First, observe the following properties:

$$\begin{aligned} [K_1, CI] &= 0, \\ [K_1, M^{ab}] &= 0. \end{aligned} \tag{119}$$

The first equation follows from the fact that K_1 kills the identity, and the second one from the fact that K_1 is a derivation of the star algebra, and then $(K_1^{(1)}+K_1^{(2)}+K_1^{(3)})|V_3\rangle=0$.[41] To derive (119), we have also used the fact that K_1 anticommutes with C. Making use of (64), it follows that

$$[K_1,M]=[K_1,C\tilde{M}]=0. \tag{120}$$

Therefore, and since the spectrum of K_1 is nondegenerate, an eigenvector of K_1 has to be an eigenvector of M and $C\tilde{M}$ as well. Notice that this makes sense since M and $C\tilde{M}$ are symmetric, real matrices, and so they have real eigenvalues.

We have then shown that the eigenvectors $w^{(\kappa)}$ given implicitly in (116) are also eigenvectors of M and $C\tilde{M}$. Now, we have to find out which are the corresponding eigenvalues. This can be done with a trick from Sec. V B of Ref. 26. The eigenvalue equations are

$$\begin{aligned} M_{n-1/2,m-1/2}w_m^{(\kappa)}&=m(\kappa)w_n^{(\kappa)},\\ (C\tilde{M})_{n-1/2,m-1/2}w_m^{(\kappa)}&=\tilde{m}(\kappa)w_n^{(\kappa)}. \end{aligned} \tag{121}$$

Since we chose the normalization $w_1^{(\kappa)}=1$, one can consider the above equations with $n=1$ and obtain for the eigenvalues:

$$\begin{aligned} m(\kappa)&=\frac{2}{\pi}\sum_{q=1}^{\infty}\frac{(-1)^q}{2q-1}w_{2q-1}^{(\kappa)},\\ \tilde{m}(\kappa)&=-\frac{2}{\pi}\sum_{q=1}^{\infty}\frac{(-1)^q}{2q-1}w_{2q}^{(\kappa)}. \end{aligned} \tag{122}$$

Define now the functions

$$\begin{aligned} \mu(z)&=\sum_{q=1}^{\infty}\frac{(-1)^q}{2q-1}w_{2q-1}^{(\kappa)}z^{2q-1},\\ \tilde{\mu}(z)&=\sum_{q=1}^{\infty}\frac{(-1)^q}{2q-1}w_{2q}^{(\kappa)}z^{2q-1}, \end{aligned} \tag{123}$$

which can be found to satisfy

$$\begin{aligned} \frac{d\mu(z)}{dz}&=\frac{i}{2z}(f_{w^{(\kappa)}}(iz)-f_{w^{(\kappa)}}(-iz)),\\ \frac{d\tilde{\mu}(z)}{dz}&=\frac{i}{2z^2}(f_{w^{(\kappa)}}(iz)+f_{w^{(\kappa)}}(-iz)). \end{aligned} \tag{124}$$

Using the explicit expression for $f_{w^{(\kappa)}}(z)$, the fact that $\mu(0)=\tilde{\mu}(0)=0$, and integrating, one finally finds

$$\begin{aligned} \mu(1)&=-\frac{\pi}{2}\operatorname{sech}(\kappa\pi/2),\\ \tilde{\mu}(1)&=\frac{\pi}{2}\tanh(\kappa\pi/2). \end{aligned} \tag{125}$$

This determines the eigenvalues of M and $C\tilde{M}$ for the eigenvectors $w^{(\kappa)}$:

$$m(\kappa) = -\operatorname{sech}(\kappa\pi/2),$$
$$\tilde{m}(\kappa) = -\tanh(\kappa\pi/2). \tag{126}$$

The spectrum of M lies in the interval $[-1,0)$, while that of $C\tilde{M}$ lies in $(-1,1)$. The above results are of course compatible with the relation $M^2-\tilde{M}^2=1$. Notice finally that, for $\kappa=0$, we recover the results of the preceding section, since

$$f_{w^{(0)}}(z) = \frac{z}{\sqrt{1+z^2}} = \sum_{n=0}^{\infty} \binom{-1/2}{n} z^{2n+1}, \tag{127}$$

so $w^{(0)}=\nu$ and from (126) we read that the eigenvalues with respect to M and $\tilde{M}$ are in fact -1 and 0, respectively, in agreement with the explicit computations of the preceding section.

We can now diagonalize the symmetric matrix $H=CF$ that defines the fermionic sliver. Since the derivation K_1 kills the supersliver,[19] one has that

$$[K_1, H] = 0, \tag{128}$$

and by the same argument one has that $w^{(\kappa)}$ are eigenvectors of H. The corresponding eigenvalues will be denoted by $h(\kappa)$. In order to determine them first notice that, since H anticommutes with C, one has

$$h(\kappa) = -h(-\kappa). \tag{129}$$

We can determine $h(\kappa)$ from the explicit expression given in (87). However, one has to be careful when doing this. The reason is that $\tilde{M}/(1-M^2)^{1/2}$ gives an indeterminacy of the type 0/0 when acting on $w^{(0)}$. If one naively substitutes the eigenvalues in (87), one seems to find that $h(0)=0$, which contradicts (129). Of course the appropriate way to regularize this indeterminacy is by expanding $(1-M^2)^{-1/2}$ in powers of M, and if this is done then at every order in the expansion one indeed finds the right value of the eigenvalue, which is $h(0)=0$ (and can also be checked by computing $Hw^{(0)}$ in level truncation). Related issues associated to the appearance of inverses of singular matrices have been considered in the bosonic case in Ref. 39. Another subtlety (also present in the bosonic case analyzed in Ref. 26) is that the quadratic equation determining H gives two branches for the eigenvalues, and in fact there is a jump from one branch to the other at $\kappa=0$. Since the numerical analysis of the spectrum shows that the eigenvalues of H are in the interval $[-1,1]$, one finally finds that the spectrum of H is given by

$$h(\kappa) = \begin{cases} -\dfrac{\kappa}{|\kappa|} e^{-|\kappa|\pi/2}, & \kappa \neq 0, \\ 0, & \kappa = 0, \end{cases} \tag{130}$$

in agreement with (129).

Using all these results, one can also diagonalize the rest of the matrices that we have encountered so far. For example, the eigenvalues of the real symmetric matrices M^{11}, M^{12}, M^{21} are, respectively,

$$m^{11}(\kappa) = -\frac{\sinh(\kappa\pi/2)}{(1+\cosh(\kappa\pi/2))(1-2\cosh(\kappa\pi/2))},$$
$$m^{12}(\kappa) = \frac{\cosh(\kappa\pi/2)(1+\cosh(\kappa\pi/2)+\sinh(\kappa\pi/2))}{(1+\cosh(\kappa\pi/2))(1-2\cosh(\kappa\pi/2))}, \tag{131}$$

$$m^{21}(\kappa)=-\frac{\cosh(\kappa\pi/2)(1+\cosh(\kappa\pi/2)-\sinh(\kappa\pi/2))}{(1+\cosh(\kappa\pi/2))(1-2\cosh(\kappa\pi/2))}.$$

Of course there is still the possibility that all of these matrices have other eigenvectors which are not eigenvectors of K_1. We have not performed a systematic numerical search, but we are led to believe that, just as in the bosonic case, the above results determine the complete spectrum of eigenvectors and eigenvalues of the various infinite-dimensional matrices involved in the fermionic matter sector.

It is also interesting to observe that, again just as in the bosonic case,[40,26] the eigenvectors that we have found are not normalizable. This can be seen in detail as follows. Given two infinite-dimensional vectors v and w, their inner product is given by

$$v\cdot w\equiv\sum_{n=1}^{\infty}v_n w_n=\int_0^{2\pi}\frac{d\theta}{2\pi}f_v^*(e^{i\theta})f_w(e^{i\theta}). \tag{132}$$

The norm of a vector v is defined as usual by $\|v\|^2\equiv v\cdot v$. Using (116) and (132), one can find an explicit expression for the norm of $w^{(\kappa)}$,

$$\|w^{(\kappa)}\|^2=\cosh(\kappa\pi/2)\|\nu\|^2, \tag{133}$$

where

$$\|\nu\|^2=4\int_0^{\pi/2}\frac{d\theta}{2\pi}\frac{1}{\sqrt{2+2\cos(2\theta)}}. \tag{134}$$

This integral is logarithmically divergent, so the norm of ν (and therefore of all $w^{(\kappa)}$) is infinite. Another way to see this is to compute directly the sum:

$$\|\nu\|^2=\sum_{n=0}^{\infty}\binom{-1/2}{n}^2. \tag{135}$$

By using zeta-function regularization, we find that this series diverges as

$$\lim_{\epsilon\to 0}\frac{2}{\pi}K(e^{-\epsilon}), \tag{136}$$

where $K(x)$ is the elliptic K function, which indeed diverges logarithmically as $x\to 1$.

VI. COHERENT STATES AND HIGHER-RANK PROJECTORS

Once the fermionic sliver has been constructed, it is natural to consider fermionic coherent states based on it, in analogy to the bosonic case.[24,20] In this section we shall construct coherent states and determine their star products. This will be useful in order to construct higher-rank projectors of the fermionic star algebra—idempotent states that should represent multiple D-brane configurations.[20]

A. Coherent states on the supersliver

We define fermionic coherent states as follows. Let $\beta=\{\beta\}_r$, $r\geqslant 1/2$, be a Grassmannian vector. Then, the coherent state on the fermionic sliver associated to β, that we shall denote by $|\Xi_\beta\rangle$, is given by

$$|\Xi_\beta\rangle=\exp[(-C\beta)^T\cdot\psi^\dagger]|\Xi_f\rangle. \tag{137}$$

This definition guarantees that the BPZ conjugate of (137) has a simple expression,

$$\langle \Xi_\beta| = \langle \Xi_f| \exp[\beta^T \cdot \psi]. \tag{138}$$

The star product of two coherent states can be computed very easily by using (78), and one finds

$$|\Xi_{\beta_1}\rangle \star |\Xi_{\beta_2}\rangle = \exp(\chi^T (1+\Phi\mathcal{K})^{-1}\beta + \tfrac{1}{2}\beta^T \mathcal{K}(1+\Phi\mathcal{K})^{-1}\beta)|\Xi_f\rangle, \tag{139}$$

where Φ, $\mathcal{K}$ and χ are given in (80), and β denotes here the vector

$$\beta = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}. \tag{140}$$

An explicit computation yields

$$|\Xi_{\beta_1}\rangle \star |\Xi_{\beta_2}\rangle = \exp[N(\beta_1, \beta_2)]|\Xi_{\rho_1\beta_1 - \rho_2\beta_2}\rangle, \tag{141}$$

where

$$\rho_1 = -\frac{1}{1+\Phi\mathcal{K}}(H(M^{21})^2 + M^{12}(1-HM^{11})) = \frac{1}{2}(1+MH-C\tilde{M}),$$

$$\rho_2 = \frac{1}{1+\Phi\mathcal{K}}(H(M^{12})^2 + M^{21}(1-HM^{11})) = \frac{1}{2}(1-MH+C\tilde{M}), \tag{142}$$

and

$$\begin{aligned} N(\beta_1,\beta_2) &= \frac{1}{2}(\beta_1 \ \ \beta_2)\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{A} \end{pmatrix}\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \\ &= -\frac{1}{2}(\beta_1 \ \ \beta_2)\frac{C}{2(1-CIH)}\begin{pmatrix} HM+(M+2)M^{11} & (M+2)M^{12} \\ (M+2)M^{21} & HM+(M+2)M^{11} \end{pmatrix}\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}. \end{aligned} \tag{143}$$

The matrices ρ_1 and ρ_2 are real symmetric, and they have the following properties:

$$\begin{aligned} &\rho_1 + \rho_2 = 1, \quad \rho_1\rho_2 = 0, \\ &\rho_1^2 = \rho_1, \quad \rho_2^2 = \rho_2, \end{aligned} \tag{144}$$

just as in the bosonic case studied in Ref. 20. This means that ρ_1, ρ_2 are orthogonal projectors on complementary subspaces. We also have

$$C\rho_1 C = \rho_2.$$

Notice that the vectors $w^{(\kappa)}$ that we described in the previous section are eigenvectors of $\rho_{1,2}$. Let us denote by $\sigma_1(\kappa)$ and $\sigma_2(\kappa)$ the corresponding eigenvalues. By using (126) and (130), we find that

$$\sigma_1(\kappa) = \begin{cases} 1, & \kappa > 0, \\ 0, & \kappa < 0, \end{cases} \tag{145}$$

with $\sigma_2(\kappa) = 1 - \sigma_1(\kappa)$. Notice that the eigenvalues associated to the vector ν are $\sigma_1(\kappa) = \sigma_2(\kappa) = \frac{1}{2}$. This contradicts in principle the statement that $\rho_1\rho_2 = 0$, and it gives yet another example of a fact noticed in Ref. 39: formal computations involving inverses of matrices like $1 - M^2$ become ambiguous when acting on special eigenvectors.

B. Higher-rank projectors

It is obvious from (141) that the star multiplication law for coherent states becomes particularly simple when $\beta_{1,2}$ are eigenvectors of the projectors $\rho_{1,2}$ or combinations thereof. In this subsection, we will show that with this choice one finds states that form closed subalgebras of the fermionic star algebra. These states can be used to obtain new idempotent states that lead to higher-rank projectors, as in the bosonic situation.[20] The construction is indeed a direct generalization of section 5.2 of Ref. 20. Let v be an eigenvector of ρ_2,

$$\rho_1 v = 0, \quad \rho_2 v = v, \tag{146}$$

and define $w = -Cv$. Therefore, $\|v\| = \|w\|$, and it follows from $C\rho_1 C = \rho_2$ that one will have

$$\rho_1 w = w, \quad \rho_2 w = 0. \tag{147}$$

In addition, one has that $v \cdot w = v^T(\rho_1 + \rho_2)w = 0$, as in Ref. 20. Using the explicit expressions for $\rho_{1,2}$, one can also show that

$$\begin{aligned} v^T \mathcal{A} w &= v^T \mathcal{C} w = \tfrac{1}{2} v^T M v, \\ v^T \mathcal{B} w &= \tfrac{1}{2} v^T (1 + C\tilde{M}) v, \end{aligned} \tag{148}$$

where the matrices $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are the ones appearing in (143).

Consider now the following states, obtained by acting with fermionic creation operators on the fermionic sliver Ξ_f (we suppress the brackets for notational convenience):

$$\begin{aligned} \Sigma_v &= \left(\frac{v}{\|v\|} \cdot \psi^\dagger \right) \Xi_f, \\ \Sigma_w &= \left(\frac{w}{\|w\|} \cdot \psi^\dagger \right) \Xi_f, \\ \Xi_{v,w} &= \left(\frac{v}{\|v\|} \cdot \psi^\dagger \right) \left(\frac{w}{\|w\|} \cdot \psi^\dagger \right) \Xi_f. \end{aligned} \tag{149}$$

Observe that the state $\Xi_{v,w}$ is Grassmann even, since fermions only appear via bilinears, while the $\Sigma_{v,w}$ states are Grassmann odd. Consider now the coherent states Ξ_{β_1}, Ξ_{β_2}, where $\beta_1 = \theta_1 v + \theta_2 w$, $\beta_2 = \hat{\theta}_1 v + \hat{\theta}_2 w$, and $\theta_{1,2}$, $\hat{\theta}_{1,2}$ are arbitrary Grassmann variables. It is simple to show, by computing the star product $\Xi_{\beta_1} \star \Xi_{\beta_2}$, that the states defined in (149) satisfy the following subalgebra of the star product, in the fermionic matter sector:

$$\begin{aligned} &\Xi_f \star \Sigma_v = 0, \quad \Xi_f \star \Sigma_w = -\Sigma_w, \\ &\Sigma_v \star \Xi_f = \Sigma_v, \quad \Sigma_w \star \Xi_f = 0, \\ &\Sigma_v \star \Sigma_v = 0, \quad \Sigma_w \star \Sigma_w = 0, \\ &\Sigma_v \star \Sigma_w = \mathcal{A}_v \Xi_f - \Xi_{v,w}, \quad \Sigma_w \star \Sigma_v = -\mathcal{B}_v \Xi_f, \\ &\Xi_f \star \Xi_{v,w} = \mathcal{A}_v \Xi_f, \quad \Xi_{v,w} \star \Xi_f = \mathcal{A}_v \Xi_f, \\ &\Sigma_v \star \Xi_{v,w} = \mathcal{A}_v \Sigma_v, \quad \Sigma_w \star \Xi_{v,w} = \mathcal{B}_v \Sigma_w, \\ &\Xi_{v,w} \star \Sigma_v = -\mathcal{B}_v \Sigma_w, \quad \Xi_{v,w} \star \Sigma_w = -\mathcal{A}_v \Sigma_w, \end{aligned} \tag{150}$$

and finally

$$\Xi_{v,w}\star\Xi_{v,w}=\mathcal{A}_v(\mathcal{A}_v-\mathcal{B}_v)\Xi_f+\mathcal{B}_v\Xi_{v,w}\,. \tag{151}$$

In these equations we have introduced the notation

$$\mathcal{A}_v=\frac{v^T\mathcal{A}w}{\|v\|^2},\quad \mathcal{B}_v=\frac{v^T\mathcal{B}w}{\|v\|^2}. \tag{152}$$

One can also find the BPZ norm of these states by computing $\langle\Xi_\beta|\Xi_\beta\rangle$, with $\beta=\theta_1 v+\theta_2 w$. In this computation one has to evaluate the inner products

$$\begin{aligned} v^T\frac{F}{1-F^2}w&=-\|v\|^2\mathcal{A}_v\,,\\ v^T\frac{1}{1-F^2}v=w^T\frac{1}{1-F^2}w&=\|v\|^2\mathcal{B}_v\,, \end{aligned} \tag{153}$$

as it can be checked by using the explicit expression for F and the fact that v, w are eigenvectors of $\rho_{1,2}$. One obtains in the end:

$$\begin{aligned} \langle\Sigma_v|\Sigma_v\rangle&=\mathcal{B}_v\langle\Xi_f|\Xi_f\rangle,\\ \langle\Sigma_v|\Sigma_w\rangle&=0,\\ \langle\Xi_f|\Xi_{v,w}\rangle&=-\mathcal{A}_v\langle\Xi_f|\Xi_f\rangle,\\ \langle\Xi_{v,w}|\Xi_{v,w}\rangle&=-(\mathcal{A}_v^2+\mathcal{B}_v^2)\langle\Xi_f|\Xi_f\rangle, \end{aligned} \tag{154}$$

together with their BPZ conjugates (notice that that BPZ conjugation exchanges $v\leftrightarrow w$).

One can now use this subalgebra in order to generate new solutions to the idempotency condition, and thus new solutions to the vacuum superstring field theory equations of motion. This one can do by taking the most general combination of the four states, Ξ_f, $\Xi_{v,w}$, Σ_v and Σ_w, (and with the appropriate Chan–Paton factors, since the Σ's are Grassmann odd). One finds in this way two types of new solutions:

(1) There is one new solution, which is Grassmann even. It is given by

$$\chi_f=\alpha\Xi_f+\beta\Xi_{v,w}\,, \tag{155}$$

where $\chi_f\star\chi_f=\chi_f$ provided one chooses

$$\alpha=-\frac{\mathcal{A}_v}{\mathcal{B}_v},\quad \beta=\frac{1}{\mathcal{B}_v}. \tag{156}$$

One has that

$$\chi_f\star\Xi_f=\Xi_f\star\chi_f=0, \tag{157}$$

and also

$$\langle\chi_f|\chi_f\rangle=\langle\Xi_f|\Xi_f\rangle,\quad \langle\chi_f|\Xi_f\rangle=0. \tag{158}$$

Therefore, we see that if one interprets the fermionic sliver as a projector in the space of string fields, the string field χ_f is a projector on an orthogonal subspace and their sum is then a higher rank projector, as in Ref. 20. Indeed, the fermionic sliver is a rank-one projector on the fermionic sector of the space of half-string functionals. The best way to see this would be of course to

construct a half-string formalism for the fermion fields. Unfortunately we have not been able to do that, as we have not found good boundary conditions for the split fermions. However, one can still bosonize the fermions and reduce the problem to the case already analyzed in Ref. 20, 27, and 28. In fact, bosonization was used in Ref. 28 to show that the ghost part of the bosonic sliver is also a rank-one projector on the ghost sector of the space of half-functionals. (For a discussion on the bosonization of the interaction vertex of the superstring in the operator formalism, see Ref. 42.)

(2) There are two families of new solutions, which have both a Grassmann even and a Grassmann odd piece. The first one is

$$\Xi_\ell = \Xi_f \otimes 1 + \ell \Sigma_v \otimes \sigma_1, \quad \ell \in \mathbf{R}, \tag{159}$$

while the second one is

$$\chi_\ell = \chi_f \otimes 1 + \ell \Sigma_w \otimes \sigma_1, \quad \ell \in \mathbf{R}. \tag{160}$$

These string fields are idempotent for arbitrary real ℓ, since the Grassmann odd piece is a nilpotent state, and they have the same norm for any ℓ, which is the norm of the fermionic sliver. Moreover, one can show that Ξ_ℓ and χ_ℓ are related to Ξ and χ by gauge transformations at the vacuum. Indeed, using nilpotency of $\Sigma_{v,w}$ and the fact that

$$[\Sigma_v, \Xi_f]_\star = \Xi_f, \quad [\Sigma_w, \chi_f]_\star = \chi_f, \tag{161}$$

one finds

$$\begin{aligned} \Xi_\ell &= e^{\ell \Sigma_v \otimes \sigma_1} \star \Xi_f \star e^{-\ell \Sigma_v \otimes \sigma_1}, \\ \chi_\ell &= e^{\ell \Sigma_w \otimes \sigma_1} \star \chi_f \star e^{-\ell \Sigma_w \otimes \sigma_1}, \end{aligned} \tag{162}$$

i.e., in the terminology of Ref. 20 Ξ_ℓ and χ_ℓ are star rotations of Ξ_f and χ_f. But on the other hand, star rotations are indeed gauge transformations at the vacuum as it follows from (28). In the case we are considering, the gauge parameter is simply given by $\Xi_m = \ell\ \Sigma_{v,w} \otimes \sigma_1$.

In order to construct higher-rank projectors, we have used simultaneous eigenvectors of the projectors ρ_1 and ρ_2. These are precisely the $w^{(\kappa)}$ that we have found in Sec. V, if one assumes that all the eigenvectors of these matrices are the eigenvectors of K_1. In this case, one can take for v any vector $w^{(-\kappa)}$ with $\kappa > 0$, and then $w = w^{(\kappa)}$. The states defined in (149) give a family of fermionic subalgebras parametrized by $\kappa > 0$, with coefficients

$$\mathcal{A}_v = -\frac{e^{-\kappa\pi/2}}{1+e^{-\kappa\pi/2}}, \quad \mathcal{B}_v = \frac{1}{1+e^{-\kappa\pi/2}}. \tag{163}$$

Notice that we have normalized these states by introducing a factor $1/\|v\|$. In this way, the norms of v, w do not appear in the star subalgebra nor in the BPZ products. Since the vectors $w^{(\kappa)}$ have infinite norm, this normalization factor actually vanishes. Observe, however, that the norm of the (super)sliver is also strictly zero since it contains a positive power of $(\det(1+X))$, and the matrix X is known to have an eigenvalue $-1/3$.[39,40,26] In that respect, the states we have constructed are not essentially different. We should add that the same thing happens to the higher rank projectors constructed in Ref. 20: they are constructed from eigenvectors of the bosonic projectors, which have infinite norm,[40,26] and the construction involves dividing by this norm. This is yet another manifestation of the rather singular structure of the idempotents of the string field star algebra.

Some remarks are now in order. It is simple to see from (141) and the fermionic subalgebra (150), that associativity of the star product does not hold in the fermionic sector. The breakdown of associativity is however rather mild, as it holds up to signs. It is known that in order to have associativity of the string star product both the three vertex and the four vertex need to be cyclic (see for example, Ref. 36). Although the three vertex analyzed in Sec. III is indeed cyclic, it has

been shown by Bogojević, Jevicki, and Meng[43] that in the fermionic matter sector the four vertex is not cyclic. Cyclicity is however expected to hold once we restrict ourselves to the GSO(+) sector, and this is in agreement with the algebra (150).

VII. THE GEOMETRIC SUPERSLIVER AND THE (SUPER)GHOST SECTOR

So far, we have restricted ourselves to the matter sector. In order to have a complete picture, we still have to make a proposal for the the vacuum BRST $\mathcal{Q}$ operator, and one has to solve the equations of motion in the ghost sector (21). In this section we will show that the ghost/superghost part of the geometric supersliver satisfies (21) if we take $\mathcal{Q}$ to be the canonical BRST operator recently proposed by Gaiotto, Rastelli, Sen, and Zwiebach[25] for the bosonic string, and that we shall denote in the following by $\mathcal{Q}_{\mathrm{GRSZ}}$. Observe that this implies that the full geometric supersliver is a solution to the full superstring field theory equations of motion. Therefore, a natural proposal for vacuum superstring field theory is to take $\mathcal{Q}=\mathcal{Q}_{\mathrm{GRSZ}}$, and postulate that the maximal $D9$-brane is described by the full geometric supersliver.

Notice that the string field in Berkovits' theory has ghost and picture number zero, and therefore the geometric supersliver is a good string field. This is in contrast to bosonic string theory, where the string field has ghost number one and therefore the sliver is not an acceptable string field. Indeed, the $D25$-brane is conjecturally described by the twisted sliver, whose algebraic construction was presented in Ref. 44 and has later been constructed in BCFT in Ref. 25. The twisted sliver has in fact ghost number one, as required by cubic bosonic string field theory.

Let us then analyze the equation (21). We have seen in Sec. II that idempotency of the string field seems to be even more useful in superstring field theory, where it reduces drastically the nonlinearity of the equation of motion. In fact, it is easy to see that an idempotent ghost/superghost state satisfying $\Phi_g \star \Phi_g = \Phi_g$ reduces the WZW equation of motion (21) to a simpler form. If Φ_g is idempotent, the exponential is linearized as

$$e^{\Phi_g} = \mathcal{I} + (e-1)\Phi_g, \tag{164}$$

and so the equation of motion becomes

$$\eta_0 \left\{ \left(\mathcal{I} + \left(\frac{1}{e} - 1 \right) \Phi_g \right) \mathcal{Q} \Phi_g \right\} = 0. \tag{165}$$

It is clear that this equation of motion is solved if

$$\mathcal{Q}\Phi_g = 0. \tag{166}$$

Let us then assume that the vacuum BRST operator is the one chosen recently by Gaiotto, Rastelli, Sen, and Zwiebach[25] for the bosonic string,

$$\mathcal{Q}_{\mathrm{GRSZ}} = \frac{1}{2i}(c(i) - c(-i)). \tag{167}$$

In terms of oscillators, this operator is given by

$$\mathcal{Q}_{\mathrm{GRSZ}} = \sum_{n=0}^{\infty} (-1)^n \mathcal{C}_{2n}, \tag{168}$$

where

$$\begin{aligned} \mathcal{C}_n &= c_n + (-1)^n c_{-n}, \quad n \neq 0, \\ \mathcal{C}_0 &= c_0. \end{aligned} \tag{169}$$

We can now show that the ghost part of the supersliver is annihilated by $\mathcal{Q}_{\mathrm{GRSZ}}$, and therefore solves the equations of motion. (We thank L. Rastelli for pointing this out to us.) First of all, notice that the ghost part of the supersliver factorizes into bc and $\beta\gamma$ pieces,

$$|\Xi_g\rangle = |\Xi_{bc}\rangle \otimes |\Xi_{\beta\gamma}\rangle. \tag{170}$$

Since the choice $\mathcal{Q}_{\mathrm{GRSZ}}$ does not involve the superghosts, it is enough to show that

$$\mathcal{Q}_{\mathrm{GRSZ}}|\Xi_{bc}\rangle = 0. \tag{171}$$

We shall do this in two distinct ways. First, we use a geometric argument akin to that in Ref. 25. Second, we shall prove it by using oscillator methods.

The geometric argument goes as follows. The supersliver is defined by the following relation:

$$\langle \Xi | \phi \rangle = \langle f \circ \phi \rangle, \tag{172}$$

where $f(z) = \arctan(z)$, and $|\phi\rangle$ is any Fock state. If one now acts with the arbitrary Fock state $\langle\phi|$ on (171), one finds

$$\langle \phi \mathcal{Q}_{\mathrm{GRSZ}}|\Xi\rangle = \frac{1}{2i}\langle f\circ\phi(0)((f'(i))^{-1}c(i\infty) - (f'(-i))^{-1}c(-i\infty))\rangle. \tag{173}$$

But $(f'(\pm i))^{-1} = 0$, and therefore the above correlator is zero.

Let us now give an oscillator proof. Using the methods of Ref. 36, it is not too hard to show that the bc part of the (super)sliver is given by a squeezed state of the form

$$|\Xi_{bc}\rangle = \exp\left(\sum_{s,i} c_{-s} S_{si} b_{-i}\right)|0\rangle, \tag{174}$$

where $s = -1,0,1,\ldots$, $i = 2,3,\ldots$, and S_{si} is given by the double residue:

$$S_{si} = \oint_0 \frac{dz}{2\pi i}\frac{1}{z^{s-1}} \oint_0 \frac{dw}{2\pi i}\frac{1}{w^{i+2}} \frac{(f'(z))^2 (f'(w))^{-1}}{f(z)-f(w)} \left(\frac{f(w)}{f(z)}\right)^3. \tag{175}$$

A different expression for this matrix has been given in Ref. 45. If we now define $U = \Sigma_{s,i} c_{-s} S_{si} b_{-i}$, one has that for $n \geqslant 2$,

$$c_n U = U c_n - \sum_s c_{-s} S_{si}. \tag{176}$$

Using this result one can easily show that (171) holds if and only if the matrix S satisfies

$$\sum_{n=1}^{\infty} S_{2k,2n}(-1)^n = (-1)^k, \tag{177}$$

where we have also used that, due to twist invariance, $S_{si} = 0$ if $s + i = \text{odd}$. The above equation says essentially that S has an eigenvector with eigenvalue 1. One can check that (177) is true by using the explicit representation of S as a double residue and the techniques of Ref. 26. Indeed, since

$$\sum_{n=1}^{\infty} (-1)^n w^{-2n-2} = \frac{w^{-2}}{1+w^2}, \tag{178}$$

we have to deform the w contour to pick the residue at $w = z$, and this yields

$$\sum_{n=1}^{\infty} S_{2k,2n}(-1)^n = \oint_0 \frac{dz}{2\pi i} \frac{1}{z^{2k-1}} \frac{1}{1+z^2} = (-1)^k, \tag{179}$$

as we wanted to show. This gives yet another proof of (171), and also establishes a property of S that may be relevant in future investigations.

Notice that in order to annihilate the identity the BRST operator of Ref. 25 has to be regularized in an appropriate way. It is also immediate to observe that this regularization does not affect the above computations.

VIII. CONCLUSIONS AND FUTURE DIRECTIONS

In this paper we have taken the first steps towards the construction of vacuum superstring field theory. More concretely, we have shown that idempotent states play a distinctive role in Berkovits' string field theory, and after clarifying the structure of the fermionic vertex in the NS sector we have given an explicit algebraic construction of the fermionic sliver. We have also explored some aspects of the star algebra. In particular, we have computed the spectrum of the fermionic Neumann matrices and we have constructed higher-rank projectors by using closed star subalgebras obtained from coherent states. Finally, we have shown that the geometric sliver is a solution to the superstring field theory equations of motion including both matter and ghost sectors.

Clearly, many things remain to be done. There are some obvious open problems that one should address to put this construction on a firmer ground, which we now list as directions for future research.

The most pressing problem is to construct solutions describing the various BPS and non-BPS D-branes of type IIA superstring theory. It is natural to conjecture that the supersliver describes the tachyonic vacuum of the $D9$-brane, but a necessary test is to verify that one can construct other D-branes with the right ratio of tensions. In Ref. 19, lower dimensional D-branes were constructed in the bosonic case by first identifying the sliver state with the maximal $D25$-brane and then exploiting the spacetime dependence of the vertex. A more general construction was later described in Ref. 21 and implemented in detail in Ref. 46. It should be possible to adapt this construction to the supersymmetric case, although there might be some subtle points that need to be addressed. For example, it is not obvious to us how one would reproduce the mod two behavior of the D-brane descent relations in the superstring case, i.e., the fact that in the IIA theory Dp-branes with odd p are unstable while Dp-branes with even p are stable, and in particular the fact that unstable and stable D-brane tensions differ with an extra $\sqrt{2}$ factor. One possibility is that this question of ''BPS versus non-BPS'' brane solutions could also be associated to the construction of solutions to vacuum superstring field theory only in the GSO(+) sector or in both the GSO(±) sectors. Another possibility may have to do with the introduction of the Grassmann odd state $G_{-1/2}|\Xi\rangle$ in the game. But surely the most straightforward way to proceed would be to follow the methods of Refs. 21 and 46.

One should also understand the structure of the ghost and superghost components of the sliver. Notice that in Berkovits' theory the correlation functions that enter into the star product are defined in the large Hilbert space and, therefore, one should have a construction of the superghost vertex in terms of the bosonized superconformal ghosts. The full analysis of the ghost/superghost sector will be probably necessary in order to identify the closed superstrings at the nonperturbative vacuum, perhaps along the lines of Ref. 25.

It would be interesting to develop a half-string formalism[47] in the fermionic sector. This would make clear some of the properties of the fermionic sliver, like the fact that it is a rank-one projector. As we pointed out in Sec. VI, a way to see this is to bosonize the fermions, but it would be more convenient to have an explicit representation in terms of fermionic oscillators.

Although in this paper we have focused on Berkovits' superstring field theory, there exists another proposal for superstring field theory of the NS sector, which is cubic and has been also used to test Sen's conjectures (see, e.g., the recent review[48]). In this cubic superstring field theory, where the string field has picture number zero and ghost number one, one can immediately extend

all of the results of bosonic VSFT: assuming a pure ghost/superghost BRST operator, and factorization of the solution, the equation of motion in the matter part again reduces to idempotency of the string field. Since the star product is kept the same, all the results of this paper, concerning the fermionic matter sector, are as well valid for the cubic superstring field theory. The ghost sector, however, will probably require some sort of twisted ghost sliver as in Ref. 25.

Note added in proof: After this paper was completed, Ref. 49 appeared, which has some overlap with Secs. III and IV in this paper and constructs the fermionic sliver in the context of the cubic superstring field theory.

ACKNOWLEDGMENTS

We would like to thank N. Berkovits, A. Jevicki and especially L. Rastelli for very useful discussions and correspondence. M.M. is supported by the grant NSF-PHY/98-02709. R.S. is supported in part by funds provided by the Fundação para a Ciência e Tecnologia, under the grant Praxis XXI BPD-17225/98 (Portugal).

APPENDIX

In this appendix, we show that the explicit expressions given in (43) and (68) satisfy equations (41) and (59), respectively. Since this is very similar to the bosonic case analyzed in Ref. 30, we shall only give a few details. In the case of the identity, we are required to prove that $(1-M)I=\tilde{M}$. The only thing we actually need is the following result:

$$\sum_{\ell=0}^{\infty}\frac{(-1)^{\ell}}{\ell+a}\binom{-1/2}{\ell}=\frac{\Gamma\left(\frac{1}{2}\right)\Gamma(a)}{\Gamma\left(a+\frac{1}{2}\right)}. \tag{A1}$$

From this, one deduces that

$$\sum_{\ell=0}^{\infty}\frac{\hat{u}_{2\ell}}{2\ell+a+1}=\begin{cases}\dfrac{\pi}{2}\hat{u}_a, & a \text{ even},\\[2ex] \dfrac{1}{a\hat{u}_a}, & a \text{ odd},\end{cases} \tag{A2}$$

and this is enough to prove (41). For the interaction vertex, one has to prove the following equations:

$$\begin{aligned}(M+2)(U+\overline{U})&=-2\tilde{M}-2(U+\overline{U}),\\ (M+2)(U-\overline{U})&=2\sqrt{3}iC,\end{aligned} \tag{A3}$$

where the matrices $U+\overline{U}$, $U-\overline{U}$ are given in (69). The necessary ingredients to prove (A3) are the following. First, one can show that the coefficients g_n defined in (66) satisfy the recursion relation:

$$\tfrac{1}{3}g_n=(n+1)g_{n+1}-(n-1)g_{n-1}. \tag{A4}$$

Next, define as in Ref. 30 the following sums:

$$O_n=\sum_{m=2\ell+1}\frac{g_m}{n+m},$$
$$E_n=\sum_{m=2\ell}\frac{g_m}{n+m}. \tag{A5}$$

These sums can be written as integrals,

$$O_n=\frac{1}{2}\int_1^\infty\frac{dt}{t^{n+1}}\left[\left(\frac{t+1}{t-1}\right)^{1/6}-\left(\frac{t+1}{t-1}\right)^{1/6}\right],$$
$$E_n=\frac{1}{2}\int_1^\infty\frac{dt}{t^{n+1}}\left[\left(\frac{t+1}{t-1}\right)^{1/6}+\left(\frac{t+1}{t-1}\right)^{1/6}\right], \tag{A6}$$

and using this representation one can show that they satisfy the recursion relations:

$$(n+1)E_{n+1}=\tfrac{1}{3}O_n+(n-1)E_n,$$
$$(n+1)O_{n+1}=\tfrac{1}{3}E_n+(n-1)O_n. \tag{A7}$$

To evaluate these sums, we proceed as in Ref. 30. On the one hand, we have

$$g_{2\ell}=\frac{1}{2\pi i}\oint\frac{dz}{z^{2\ell+1}}\frac{1}{2}\left[\left(\frac{z+1}{z-1}\right)^{1/6}-\left(\frac{z+1}{z-1}\right)^{1/6}\right], \tag{A8}$$

where the contour is around the origin. On the other hand, when ℓ is greater than zero, one can deform the contour in the above integral to the real axis and obtain

$$O_{2\ell}=\pi g_{2\ell},\quad \ell\geqslant 1. \tag{A9}$$

Similarly, one proves that

$$E_{2\ell+1}=\pi g_{2\ell+1},\quad \ell\geqslant 0. \tag{A10}$$

The value of O_0 can be evaluated by direct integration. After performing the change of variables $x=\tanh((\log t)/2)$, one finds

$$O_0=\int_0^1\frac{dx}{1-x^2}(x^{-1/6}-x^{1/6})=\frac{1}{2}\left(\psi\left(\frac{7}{12}\right)-\psi\left(\frac{5}{12}\right)\right). \tag{A11}$$

We then find

$$O_0=\pi-\frac{\sqrt{3}}{2}. \tag{A12}$$

Using this value and the recursion relations, one can obtain $O_{-2\ell}$, $E_{-2\ell-1}$ as well. To evaluate the other sums, we follow the procedure in the Appendix of Ref. 30. First, define the series

$$S_n=\begin{cases}E_n, & n=2k,\\ O_n, & n=2k+1.\end{cases} \tag{A13}$$

Since the sums satisfy the recursion relation (A7), S_n satisfies the recursion relation of the coefficients g_n (A4). There is another solution to this relation which is given by

$$S_n = 3S_1 g_n + 3\sum_{m=0}^{n-1} (-1)^m \frac{g_m g_{n-m}}{m+1}. \tag{A14}$$

To derive this, one first writes a differential equation for the function $S(x)=\Sigma_{n=1}^{\infty} S_n x^n$ by using the recursion relation. The details are exactly like the ones in Ref. 30. To have the complete solution to the problem, we then just have to evaluate S_1,

$$S_1 = 1 + \frac{1}{\sqrt{3}} \log\left(\frac{\sqrt{3}-1}{\sqrt{3}+1}\right). \tag{A15}$$

Notice that $S_m \sim 1/m$, and one has $mS_m \to 1$ as $m \to 0$. The recursion relation also implies that S_{-m} diverges for $m=-1,-2,\ldots$, but mS_{-m-n} with $n>0$ has a finite limit as m goes to zero that can be evaluated using the recursion relations.

With these ingredients, we can already prove very easily the first equation in (A3). For example, in this proof one has to evaluate the quantity

$$A_m = (-1)^m m(m+1)(g_{m+1}S_m - S_{m+1}g_m). \tag{A16}$$

Using the recursion relations, one can see that A_m does not depend on m, therefore $A_m = A_1 = 1/3$. In order to prove the second equation in (A3), one needs some extra ingredients to deal with the diagonal terms, since these involve the sums

$$\begin{aligned} \widetilde{O}_n &= \sum_{m=2\ell 1} \frac{g_m}{(n+m)^2}, \\ \widetilde{E}_n &= \sum_{m=2\ell} \frac{g_m}{(n+m)^2}. \end{aligned} \tag{A17}$$

These sums have the integral representation

$$\begin{aligned} \widetilde{O}_n &= \frac{1}{2}\int_1^{\infty} dt \frac{\log t}{t^{n+1}} \left[\left(\frac{t+1}{t-1}\right)^{1/6} - \left(\frac{t+1}{t-1}\right)^{1/6} \right], \\ \widetilde{E}_n &= \frac{1}{2}\int_1^{\infty} dt \frac{\log t}{t^{n+1}} \left[\left(\frac{t+1}{t-1}\right)^{1/6} + \left(\frac{t+1}{t-1}\right)^{1/6} \right], \end{aligned} \tag{A18}$$

and using them one can prove the recursion relations:

$$\begin{aligned} (n+1)\widetilde{E}_{n+1} &= \tfrac{1}{3}\widetilde{O}_n + (n-1)\widetilde{E}_n + E_{n+1} - E_{n-1}, \\ (n+1)\widetilde{O}_{n+1} &= \tfrac{1}{3}\widetilde{E}_n + (n-1)\widetilde{O}_n + O_{n+1} - O_{n-1}. \end{aligned} \tag{A19}$$

These can be solved as in Ref. 30, but we shall not need their explicit expression, and in the evaluation of the relevant quantities it suffices to use the recursion relations they satisfy. For example, in the proof of the second equation in (A3) one has to compute

$$C_m = m(m+1)(g_{m+1}\widetilde{S}_m - \widetilde{S}_{m+1}g_m), \tag{A20}$$

where $\widetilde{S}_n$ is defined as follows:

$$\widetilde{S}_n = \begin{cases} \widetilde{O}_n, & n=2k, \\ \widetilde{E}_n, & n=2k+1. \end{cases} \tag{A21}$$

Using the recursion relations (A4) and (A19), as well as (A12), one can show that

$$C_m=\frac{\pi}{3}\sum_{l=0}^{m}(-1)^l g_{m-l}^2-\pi g_m g_{m+1}-\frac{\pi\sqrt{3}}{6}. \tag{A22}$$

Taking into account these results, the proof of the second equation in (A3) is immediate.

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An exact fluid model for relativistic electron beams

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(Received 17 October 2001; accepted 16 October 2002)

An interesting and satisfactory fluid model has been proposed in the literature for the description of relativistic electron beams. It is obtained by imposing the entropy principle up to a certain order with respect to a smallness parameter ϵ measuring the dispersion of the velocity about the mean. Here the general exact solution is found, satisfying the entropy principle and the relativity principle up to whatever order. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1527716]

I. INTRODUCTION

The following system of quasi-linear partial differential equations has been proposed by Amendt and Weitzner[1,2] to describe the behavior of relativistic electron beams,

$$\partial_\alpha V^\alpha = 0, \quad \partial_\alpha T^{\alpha\beta} = eF^{\beta\alpha}V_\alpha, \quad \partial_\alpha A^{\alpha\beta\gamma} = 2eT_\alpha^{(\beta}F^{\gamma)\alpha}, \tag{1}$$

where $F^{\alpha\beta}$ is the electromagnetic field tensor and e is the electron charge. V^α (particle number-particle flux vector) and $T^{\alpha\beta}$ (stress-energy-momentum tensor) are assumed as independent variables, while $A^{\alpha\beta\gamma}$ is a constitutive function whose determination is also called the ''closure problem.'' Restrictions on its generality can be obtained by considering the counterparts of the above variables in statistical mechanics. They are defined there as moments of the distribution function $f(x^\alpha, p^\alpha)$,

$$V^\alpha = \int fp^\alpha dP, \; T^{\alpha\beta} = \int fp^\alpha p^\beta dP, \quad A^{\alpha\beta\gamma} = \int fp^\alpha p^\beta p^\gamma dP, \tag{2}$$

where p^α is the four-momentum of the particle so that we have $p^\alpha p_\alpha = -m^2$ and $dP = \sqrt{-g}dp^1dp^2dp^3/p^0$ is the invariant element of momentum space; m is the particle mass.

Equations (2) show that $T^{\alpha\beta}$ and $A^{\alpha\beta\gamma}$ are symmetric with respect to all pairs of indices and that the following ''trace condition'' holds:

$$A^{\alpha\beta}_\beta = -m^2V^\alpha. \tag{3}$$

In Refs. 1 and 2, Amendt and Weitzner have proposed the following closure,

$$A^{\alpha\beta\gamma} = -3m^2(T^\mu_\mu)^{-1}V^{(\alpha}T^{\beta\gamma)} - 2m^{-1}(T^\mu_\mu)^{-2}V^\alpha V^\beta V^\gamma,$$

and a detailed study of the linear wave modes in this model has been made in Ref. 3. This model constitutes a great improvement of those previously known in literature, because it is fully covariant and complete; moreover the resulting system (1) is hyperbolic. However, it satisfies the condition (3) only approximately. In Refs. 4 and 5 a closure has been found satisfying exactly Eq. (3); it has also been imposed that this closure is such that the entropy principle is satisfied up to a certain order with respect to a smallness parameter ϵ measuring the dispersion of the velocity about the mean. The hyperbolicity of this model has been studied in Ref. 6. This new closure is more satisfactory also from a mathematical viewpoint; in fact, the resulting system is equivalent to a symmetric hyperbolic one, a fact which guarantees the existence, uniqueness, well-posedness

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and stability of the solution of the initial values problem. A particular ordering in terms of ϵ, which characterizes warm plasmas, is also satisfied. Here the exact general solution is found, satisfying all these conditions up to whatever order. Before showing it, let us recall that the entropy principle for the balance equations (1), exploited via Liu' s theorem,[7] amounts to assuming the existence of the Lagrange multipliers ξ, λ_β, $\Sigma_{\beta\gamma}$ and of a four-vectorial function h'^α (related to the entropy–entropy flux) such that

$$V^\alpha = \frac{\partial h'^\alpha}{\partial \xi}, \tag{4a}$$

$$T^{\alpha\beta} = \frac{\partial h'^\alpha}{\partial \lambda_\beta}, \tag{4b}$$

$$\left(A^{\alpha\mu\nu} - \frac{\partial h'^\alpha}{\partial \Sigma_{\mu\nu}} \right) \left(g^\beta_\mu g^\gamma_\nu - \frac{1}{4} g_{\mu\nu} g^{\beta\gamma} \right) = 0, \tag{4c}$$

$$V_{[\alpha}\lambda_{\beta]} + 2T^\gamma_{[\alpha}\Sigma_{\beta]\gamma} = 0, \tag{4d}$$

where the Lagrange multipliers have been taken as independent variables and it has been taken into account that $\Sigma_{\beta\gamma}$ is symmetric and traceless.

Usually, at this point, the representation of h'^α up to a certain order is introduced; from Eqs. (4) one obtains the representations of V^α, $T^{\alpha\beta}$, and $A^{\alpha\beta\gamma}$. The symmetry conditions on $T^{\alpha\beta}$ and $A^{\alpha\beta\gamma}$, and the trace condition (3), give restrictions on the above mentioned expression of h'^α; these restrictions have been imposed in the last papers, in a neighborhood of thermodynamic equilibrium and, consequently, of the state with $\epsilon = 0$.

In the present article, an exact solution is found and is

$$h'^\alpha_1 = \int F(\xi + \Sigma_{\mu\nu} p^\mu p^\nu, \lambda_\mu p^\mu) p^\alpha dP, \tag{5}$$

where the function $F(X,Y)$ is related to the distribution function at equilibrium by

$$\frac{\partial}{\partial X} F(X,Y) = f_{\text{eq}}(X,Y).$$

However, this solution of the above conditions is not unique; it will be shown below that the general one is $h'^\alpha = h'^\alpha_1 + h'^\alpha_2$ with

$$h'^\alpha_2 = \sum_{n=0}^{\infty} \frac{1}{n!} B^{\alpha\nu_1\sigma_1\nu_2\sigma_2\cdots\nu_n\sigma_n} \Sigma_{\nu_1\sigma_1} \Sigma_{\nu_2\sigma_2} \cdots \Sigma_{\nu_n\sigma_n}, \tag{6}$$

which is expressed in terms of the tensors

$$U^\alpha = (-\lambda^\mu \lambda_\mu)^{-1/2} \lambda^\alpha, \quad h^{\alpha\beta} = g^{\alpha\beta} + U^\alpha U^\beta, \tag{7}$$

$$B^{\alpha_1\alpha_2\cdots\alpha_{2h+1}} = \sum_{s=0}^{h} \binom{2h+1}{2s} \gamma^{-2h-3} g_{h,2s}(\xi,\gamma) \cdot \frac{1}{2s+1} h^{(\alpha_1\alpha_2} \cdots h^{\alpha_{2s-1}\alpha_{2s}} U^{\alpha_{2s+1}} \cdots U^{\alpha_{2h+1})}.$$

Moreover, we have

$$g_{h,2s-2} = \frac{-\gamma}{2s+1} \frac{\partial g_{h,2s}}{\partial \gamma} + g_{h,2s} \quad \text{for } s = 0,\ldots,h, \tag{8a}$$

$$\frac{\partial}{\partial\gamma}g_{h+1,2h+2}=-m^2\gamma(2h+3)\frac{\partial}{\partial\xi}g_{h,2h}, \tag{8b}$$

the last one which can be written, by using Eq. (8a) also as

$$-m^2\gamma^2\frac{\partial}{\partial\xi}g_{h,2h}=g_{h+1,2h+2}-g_{h+1,2h}. \tag{9}$$

The equations (8) have the following meaning: Among the functions $g_{h,2s}$ let us call $g_{h,2h}$ the ''leading function of order h.'' Equation (8a) is a recurrence formula which gives $g_{h,2s}$ in terms of this leading function, while (8b) gives the leading function of order $h+1$ in terms of the corresponding one of order h, except for a constant arising from integration; it is constant with respect to γ, but it may depend on ξ. We note that also the expansion of $h_1'^{\alpha}$ around equilibrium has the form (6) and (7) with

$$g_{h,2s}=-4\pi m^{2h+3}\gamma^{2h+3}\int_0^\infty\frac{\partial^h F(\xi,k\gamma\cosh\rho)}{\partial\xi^h}\cosh^{2h-2s+1}\rho\sinh^{2s+2}\rho\,d\rho, \tag{10}$$

and it is easy to see that this expression satisfies exactly Eqs. (8a) and (9). It is clear that $h_1'^{\alpha}$ is only a particular solution; in fact, it does not depend on the arbitrary functions of the single-variable ξ arising from integrating (8b). If one wants that $h_1'^{\alpha}+h_2'^{\alpha}$ yields for V^α, $T^{\alpha\beta}$, $A^{\alpha\beta\gamma}$ at equilibrium the same expressions which originate from $h_1'^{\alpha}$, it is sufficient that $g_{0,0}=g_{1,2}=0$. In this case Eqs. (8) yield polynomial expressions for $g_{h,2s}$ in the variable γ.

It is easy to see that if $h'^{\alpha}=h_1'^{\alpha}$, then the symmetry condition on $T^{\alpha\beta}$ and $A^{\alpha\beta\gamma}$ and the trace condition (3) are surely satisfied. There remains to prove this same result for the general exact solution $h'^{\alpha}=h_2'^{\alpha}$ and this will be the subject of the next section. The last condition (4d) will be exploited in Sec. III.

Before leaving the present section, it has to be noted that it is too much restrictive to take only $h'^{\alpha}=h_1'^{\alpha}$, when the function F depends on X and Y only through their sum, i.e., $F=F(X+Y)$. To understand better this point, let us substitute to h'^{α} in Eqs. (4a) and (4b) the arbitrary expression of $h_2'^{\alpha}$; one obtains at equilibrium

$$h_2'^{\alpha}=\gamma^{-3}g_{0,0}(\xi,\gamma)U^\alpha,\quad V^\alpha=\gamma^{-3}\frac{\partial g_{0,0}}{\partial\xi}U^\alpha,$$

$$T^{\alpha\beta}=-\frac{m}{k}\frac{\partial}{\partial\gamma}(\gamma^{-3}g_{0,0})U^\alpha U^\beta+\gamma^{-4}g_{0,0}\frac{m}{k}h^{\alpha\beta},$$

which yields

$$h^\alpha=-nsU^\alpha,\quad V^\alpha=nU^\alpha,\quad T^{\alpha\beta}=eU^\alpha U^\beta+ph^{\alpha\beta},$$

with n (particle density), p (pressure), e (energy density) and s (entropy density), given by

$$n=\gamma^{-3}\frac{\partial g_{0,0}}{\partial\xi}, \tag{11a}$$

$$p=\frac{m}{k}\gamma^{-4}g_{0,0}, \tag{11b}$$

$$e=-\frac{m}{k}\frac{\partial}{\partial\gamma}(\gamma^{-3}g_{0,0}), \tag{11c}$$

$$s=\left(\frac{\partial g_{0,0}}{\partial \xi}\right)^{-1}\left[g_{0,0}-\xi\frac{\partial g_{0,0}}{\partial \xi}-\gamma^4\frac{\partial}{\partial \gamma}(\gamma^{-3}g_{0,0})\right]. \tag{11d}$$

From (11d) and the Gibbs relation, it is evident that γ can be identified as m/kT, with T the absolute temperature. If the particular material is characterized by the state functions $n=n(p,\gamma)$ and $e=e(p,\gamma)$, then (11b) simply defines ξ in terms of p and γ, while (11a) and (11c) are equations from which to obtain $g_{0,0}$ in terms of $n(p,\gamma)$ and $e(p,\gamma)$; in fact, they are equivalent to

$$\frac{\partial}{\partial \xi}(\gamma^{-3}g_{0,0})=n\left(\frac{m}{k}\gamma^{-4}g_{0,0},\,\gamma\right),$$

$$\frac{\partial}{\partial \gamma}(\gamma^{-3}g_{0,0})=-\frac{k}{m}e\left(\frac{m}{k}\gamma^{-4}g_{0,0},\,\gamma\right).$$

These equations give $g_{0,0}$ iff the following integrability condition is satisfied,

$$(e+p)n_p+\gamma n_\gamma=ne_p, \tag{12}$$

where (11b) has been used. Equation (12) is not a new condition on the state functions because it is the same integrability condition for the equations

$$\frac{\partial s}{\partial p}=\frac{m}{k\gamma}\left[\frac{\partial}{\partial p}\left(\frac{e}{n}\right)+p\frac{\partial}{\partial p}\left(\frac{1}{n}\right)\right],$$

$$\frac{\partial s}{\partial \gamma}=\frac{m}{k\gamma}\left[\frac{\partial}{\partial \gamma}\left(\frac{e}{n}\right)+p\frac{\partial}{\partial \gamma}\left(\frac{1}{n}\right)\right],$$

which are equivalent to the Gibbs relation

$$Tds=d\left(\frac{e}{n}\right)+pd\left(\frac{1}{n}\right).$$

These considerations show that the most general state functions can be written as (11a)–(11c) with $g_{0,0}$ an arbitrary function of the two variables ξ and γ; this generality is not maintained if only $h_1'^{\alpha}$ is used and $F=F(X+Y)$, because in this case Eq. (10) yields

$$g_{0,0}=-4\pi m^3\gamma^3\int_0^\infty F(\xi+k\gamma\cosh\rho)\cosh\rho\sinh^2\rho d\rho,$$

which is expressed in terms of the single-variable function F.

This fact does not mean that this solution is wrong, but that it can be applied only to some materials. Examples of these applications can be found in Refs. 8–14, together with the guidelines which led to find this particular exact solution.

An example of the case $F=F(X+Y)$ is furnished by

$$f_{\mathrm{eq}}(X,Y)=\frac{y}{e^{(X+Y)/k}\pm 1},$$

i.e., the Jüttner[15,16] distribution function at equilibrium, where k is the Boltzmann constant, the upper and the lower signs refer to Fermions and Bosons, respectively, y is equal to w/h^3 with h the Planck' s constant, and w is equal to $2s+1$ for particles with spin $sh/2\pi$. In this case Eq. (10) becomes

$$g_{h,2s}=-4\pi y m^{2h+3}\gamma^{2h+3}\frac{\partial^{h-1}}{\partial\xi^{h-1}}J_{2s+2,2h-2s+1}$$

and

$$\frac{\partial^{-1}}{\partial\xi^{-1}}J,\quad \frac{\partial^{0}}{\partial\xi^{0}}J$$

can be considered symbols standing for

$$\int J d\xi,\quad J$$

respectively.

Let us conclude reporting the expression of $g_{0,0}$ in the general case $F=F(X,Y)$; Eq. (10) shows that it is

$$g_{0,0}=-4\pi m^3\gamma^3\int_0^\infty F(\xi,k\gamma\cosh\rho)\cosh\rho\sinh^2\rho d\rho.$$

II. EXISTENCE AND UNIQUENESS OF THE SOLUTION OF OUR CONDITIONS AND EXPRESSED BY $h'^{\alpha}=h_2'^{\alpha}$

Let us start with Eq. (6) which is the most general expansion of $h_2'^{\alpha}$ with respect to the state with $\Sigma_{\mu\nu}=0$, and substitute $B^{\alpha\nu_1\sigma_1\cdots\nu_n\sigma_n}$ with

$$B^{\alpha\mu_1\delta_1\cdots\mu_n\delta_n}(g_{\mu_1}^{(\nu_1}g_{\delta_1}^{\sigma_1)}-\tfrac{1}{4}g_{\mu_1\delta_1}g^{\nu_1\sigma_1})\cdots(g_{\mu_n}^{(\nu_n}g_{\delta_n}^{\sigma_n)}-\tfrac{1}{4}g_{\mu_n\delta_n}g^{\nu_n\sigma_n}),$$

because $\Sigma_{\mu\nu}$ is traceless; in this way an expression like (6) is obtained, but with $B^{\alpha\cdots\nu_i\sigma_i\cdots\nu_n\sigma_n}g_{\nu_i\sigma_i}=0$. Let us now write Eq. (6) as

$$h_2'^{\alpha}=\sum_{n=0}^{\infty}\frac{1}{n!}B^{\alpha A_1\cdots A_n}\Sigma_{A_1}\cdots\Sigma_{A_n},\tag{13}$$

where A_i stands for the couple $\nu_i\sigma_i$ and let us act on it as it is a single index. Moreover, the expression (13) of $h_2'^{\alpha}$ does not change if we replace $B^{\alpha A_1\cdots A_n}$ with

$$D^{\alpha A_1\cdots A_n}=B^{\alpha(A_1\cdots A_n)}+\sum_{s=0}^{n-1}C^{\alpha(A_1\cdots A_s}g^{A_{s+1}}\cdots g^{A_n)},$$

and this is true for whatever tensors $C^{\alpha A_1\cdots A_s}$; in particular, these last tensors may be chosen as defined by

$$C^{\alpha A_1\cdots A_s}=-\frac{1}{4}\frac{s+1}{n-s}C^{\alpha A A_1\cdots A_s}g_A\quad\text{for } s=0,\ldots,n-2$$

$$C^{\alpha A_1\cdots A_{n-1}}=-\frac{m^2}{4}n\frac{\partial}{\partial\xi}D^{\alpha A_1\cdots A_{n-1}}.$$

The first of these relations defines the tensor $C^{\alpha A_1\cdots A_s}$, of order $s+1$, in terms of the corresponding one of order $s+2$; the second one defines the tensor with the higher order. In this way, $D^{\alpha A_1\cdots A_n}$ is defined once $D^{\alpha A_1\cdots A_{n-1}}$ is known. As a consequence of these definitions, it can be seen that

$$D^{\alpha A_1 A_2 \cdots A_n} g_{A_1} = -m^2 \frac{\partial}{\partial \xi} D^{\alpha A_2 \cdots A_n}.$$

These considerations show that it is not restrictive to maintain Eq. (13) and impose that $B^{\alpha A_1 \cdots A_n}$ is symmetric with respect to all couples of indices A_i and A_j and, moreover, that

$$B^{\alpha A_1 A_2 \cdots A_n} g_{A_1} = -m^2 \frac{\partial}{\partial \xi} B^{\alpha A_2 \cdots A_n}. \tag{14}$$

In this way Eq. (4c), by using Eq. (4a), becomes

$$\begin{aligned} A^{\alpha\beta\gamma} = & -\frac{1}{4} m^2 \sum_{n=0}^{\infty} \frac{1}{n!} g^{\beta\gamma} \frac{\partial}{\partial \xi} B^{\alpha A_1 \cdots A_n} \Sigma_{A_1} \cdots \Sigma_{A_n} \\ & + \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(B^{\alpha\beta\gamma A_2 \cdots A_n} - \frac{1}{4} B^{\alpha A_1 A_2 \cdots A_n} g_{A_1} g^{\beta\gamma} \right) \Sigma_{A_2} \cdots \Sigma_{A_n} \\ = & \sum_{n=1}^{\infty} \frac{1}{(n-1)!} B^{\alpha\beta\gamma A_2 \cdots A_n} \Sigma_{A_2} \cdots \Sigma_{A_n}, \end{aligned} \tag{15}$$

because the first and third terms are opposite for Eq. (14).

From Eq. (15) it can be seen that the symmetry condition on $A^{\alpha\beta\gamma}$ holds iff $B^{\alpha\beta\gamma A_2 \cdots A_n}$ is symmetric with respect to $\alpha\beta\gamma$. More than that, it is symmetric with respect to every couple of indices; in fact, one has

$$B^{\alpha \nu_1 \sigma_1 \cdots \nu_i \sigma_i \cdots \nu_n \sigma_n} = B^{\alpha \nu_i \sigma_i \cdots \nu_1 \sigma_1 \cdots \nu_n \sigma_n} = B^{\nu_i \alpha \sigma_i \cdots \nu_1 \sigma_1 \cdots \nu_n \sigma_n} = B^{\nu_i \nu_1 \sigma_1 \cdots \alpha \sigma_i \cdots \nu_n \sigma_n},$$

$$B^{\alpha \cdots \nu_i \sigma_i \cdots \nu_n \sigma_n} = B^{\alpha \cdots \sigma_i \nu_i \cdots \nu_n \sigma_n} = B^{\sigma_i \cdots \alpha \nu_i \cdots \nu_n \sigma_n} = B^{\sigma_i \cdots \nu_i \alpha \cdots \nu_n \sigma_n},$$

$$B^{\alpha \cdots \alpha_j \cdots \alpha_k \cdots \alpha_n} = B^{\alpha_j \cdots \alpha \cdots \alpha_k \cdots \alpha_n} = B^{\alpha_k \cdots \alpha \cdots \alpha_j \cdots \alpha_n} = B^{\alpha \cdots \alpha_k \cdots \alpha_j \cdots \alpha_n}.$$

The first one of these relations shows that α can be exchanged with ν_i; in the second one α is exchanged with σ_i; in the third one, it is exchanged with a generic couple of indices α_j and α_k.

By using the representation theorems it can be seen that Eq. (7) is the most general expression for $B^{\alpha_1 \cdots \alpha_{2h+1}}$, which takes into account that it is symmetric and depends only on ξ and λ^{α}. The factor near $g_{h,2s}$ has been introduced for later convenience.

Let us now impose the symmetry condition on $T^{\alpha\beta}$ as defined by Eq. (4b); with some calculations, it can be seen that it is equivalent to Eq. (8a) and there remains

$$\begin{aligned} T^{\alpha_1 \alpha_2} = & \frac{m}{k} \sum_{h=0}^{\infty} \frac{1}{h!} \Bigg[-\sum_{s=0}^{h} \binom{2h+2}{2s} \frac{1}{2s+1} h^{(\alpha_1 \alpha_2} \cdots h^{\alpha_{2s-1} \alpha_{2s}} U^{\alpha_{2s+1}} \cdots U^{\alpha_{2h+2})} \cdot \frac{\partial}{\partial \gamma} (\gamma^{-2h-3} g_{h,2s}) \\ & + \gamma^{-2h-4} g_{h,2h} h^{(\alpha_1 \alpha_2} \cdots h^{\alpha_{2h+1} \alpha_{2h+2})} \Bigg] \cdot \Sigma_{\alpha_3 \alpha_4} \cdots \Sigma_{\alpha_{2h+1} \alpha_{2h+2}}. \end{aligned} \tag{16}$$

The symmetry condition on $A^{\alpha\beta\gamma}$ and the trace condition (3) are already satisfied; it remains to impose Eq. (14). With some calculations, it can be seen that it is equivalent to

$$g_{h,2s+2} - g_{h,2s} = -m^2 \gamma^2 \frac{\partial}{\partial \xi} g_{h-1,2s},$$

which, by use of (8a), becomes

$$\frac{\partial}{\partial\gamma}g_{h,2s+2}=-(2s+3)m^2\gamma\frac{\partial}{\partial\xi}g_{h-1,2s},$$

or, with $s-1$ instead of s,

$$\frac{\partial}{\partial\gamma}g_{h,2s}=-(2s+1)m^2\gamma\frac{\partial}{\partial\xi}g_{h-1,2s-2}. \tag{17}$$

Now, by using Eqs. (8a) and (17), one has also that

$$-(2s-1)m^2\gamma\frac{\partial}{\partial\xi}g_{h-1,2s-4}=-(2s-1)m^2\gamma\frac{\partial}{\partial\xi}\left(\frac{-\gamma}{2s-1}\frac{\partial g_{h-1,2s-2}}{\partial\gamma}+g_{h-1,2s-2}\right)=\frac{\partial}{\partial\gamma}g_{h,2s-2},$$

i.e., Eq. (17) with $s-1$ instead of s. Therefore, it is sufficient to impose Eq. (17) only for the higher value of s, that is, $s=h$:

$$\frac{\partial}{\partial\gamma}g_{h,2h}=-(2h+1)m^2\gamma\frac{\partial}{\partial\xi}g_{h-1,2h-2},$$

which proves (8b).

III. PROOF OF THE PROPERTY (4d)

Let us start by proving that a scalar function f^* exists, such that

$$h'^{\alpha}=\frac{\partial f^*}{\partial\lambda_\alpha}, \tag{18}$$

and it can be expressed in the form

$$f^*=\sum_{n=0}^{\infty}\frac{1}{n!}P^{\nu_1\sigma_1\cdots\nu_n\sigma_n}\Sigma_{\nu_1\sigma_1}\cdots\Sigma_{\nu_n\sigma_n},$$

with

$$P^{\nu_1\cdots\nu_{2n}}=\sum_{s=0}^{n}\binom{2n}{2s}\frac{1}{2s+1}\phi_{n,2s}(\xi,\gamma)h^{(\nu_1\nu_2}\cdots h^{\nu_{2s-1}\nu_{2s}}U^{\nu_{2s+1}}\cdots U^{\nu_{2n})}.$$

One obtains that (18) is satisfied iff

$$\phi_{n,2s}=-\frac{2n-2s-1}{2s+3}\phi_{n,2s+2}+\frac{k}{m}\frac{\gamma^{-2n-2}}{2s+3}g_{n,2s+2}\quad\text{for } s=0,\ldots,n-1, \tag{19a}$$

$$\frac{\partial}{\partial\gamma}\phi_{n,2s}=-\frac{k}{m}\gamma^{-2n-3}g_{n,2s}\quad\text{for } s=0,\ldots,n. \tag{19b}$$

This last one for $s=n$ reads

$$\frac{\partial}{\partial\gamma}\phi_{n,2n}=-\frac{k}{m}\gamma^{-2n-3}g_{n,2n}, \tag{20}$$

and it can be seen that (19b) is a consequence of (19a) and (20). Let us prove this by the recurrence method. It is true for $s=n$; let us assume that (19b) holds and prove that it is satisfied also when $s-1$ replaces s. We have

$$\frac{\partial}{\partial\gamma}\phi_{n,2s-2}=\frac{\partial}{\partial\gamma}\left(-\frac{2n-2s+1}{2s+1}\phi_{n,2s}+\frac{k}{m}\frac{\gamma^{-2n-2}}{2s+1}g_{n,2s}\right)$$
$$=-\frac{k}{m}\gamma^{-2n-3}g_{n,2s}+\frac{k}{m}\frac{\gamma^{-2n-2}}{2s+1}\frac{\partial}{\partial\gamma}g_{n,2s}=-\frac{k}{m}\gamma^{-2n-3}g_{n,2s-2},$$

where (19a), (19b) and (8a) have been used in this order. This completes the proof. Therefore, the function f^* exists and $\phi_{n,2s}$ are determined by (19a) and (20).

The condition (18) has already been found by Geroch and Lindblom[17] in a more general context; see also Ref. 18. Here the proof has been given that it is satisfied by the present exact solution; moreover, it helps in proving Eq. (4d) because it allows us to write it as

$$\frac{\partial^2 f^*}{\partial\xi\partial\lambda_{[\alpha}}\lambda_{\beta]}+2\frac{\partial^2 f^*}{\partial\lambda_\gamma\partial\lambda_{[\alpha}}\Sigma_{\beta]\gamma}=0. \tag{21}$$

Now the following identity holds, as a consequence only of the representation theorems,

$$\frac{\partial^2 f^*}{\partial\xi\partial\lambda_{[\alpha}}\lambda_{\beta]}+2\frac{\partial^2 f^*}{\partial\xi\partial\Sigma_{\gamma[\alpha}}\Sigma_{\beta]\gamma}=0. \tag{22}$$

It is simply a consequence of the fact that f^* depends on ξ, λ_α, and $\Sigma_{\gamma\alpha}$ through ξ, $G_0=\lambda_\alpha\lambda^\alpha$, $G_1=\lambda_\gamma\Sigma^{\gamma\alpha}\lambda_\alpha$, $G_2=\lambda_\gamma\Sigma^{\gamma\beta}\Sigma_{\beta\alpha}\lambda^\alpha$, $G_3=\lambda_\gamma\Sigma^{\gamma\beta}\Sigma_{\beta\delta}\Sigma^{\delta\alpha}\lambda_\alpha$, $Q_2=\Sigma^{\gamma\beta}\Sigma_{\beta\gamma}$, $Q_3=\Sigma^{\gamma\beta}\Sigma_{\beta\delta}\Sigma^{\delta}_{\gamma}$, and $Q_4=\Sigma^{\gamma\beta}\Sigma_{\beta\delta}\Sigma^{\delta\epsilon}\Sigma_{\epsilon\gamma}$.

The identity (22) allows us to write the condition (21) as

$$\left(\frac{\partial^2 f^*}{\partial\lambda_\gamma\partial\lambda_{[\alpha}}-\frac{\partial^2 f^*}{\partial\xi\partial\Sigma_{\gamma[\alpha}}\right)\Sigma^{\beta]}_{\gamma}=0 \tag{23}$$

or

$$\left(T^{\gamma[\alpha}-\frac{\partial^2 f^*}{\partial\xi\partial\Sigma_{\gamma[\alpha}}\right)\Sigma^{\beta]}_{\gamma}=0.$$

By using also (16), one obtains

$$\frac{\partial}{\partial\xi}\phi_{n,2s}=-\frac{m}{k}\frac{\partial}{\partial\gamma}(\gamma^{-2n-1}g_{n-1,2s}),\quad \text{for } s=0,\ldots,n-1, \tag{24a}$$

$$\frac{\partial}{\partial\xi}\phi_{n,2n}=\frac{m}{k}(2n+1)\gamma^{-2n-2}g_{n-1,2n-2}. \tag{24b}$$

Note that Eq. (20) gives $\phi_{n,2n}$ except for an arbitrary function of the single variable ξ; now Eqs. (20) and (24b) give $\phi_{n,2n}$ except for a constant, but there is an integrability condition which reads

$$-\frac{k^2}{m^2}\frac{\partial}{\partial\xi}(\gamma^{-2n-3}g_{n,2n})=(2n+1)\frac{\partial}{\partial\gamma}(\gamma^{-2n-2}g_{n-1,2n-2}),$$

or, equivalently,

$$\frac{\partial}{\partial\xi}g_{h+1,2h+2}=\frac{m^2}{k^2}(2h+3)\left[(2h+4)g_{h,2h}-\gamma\frac{\partial}{\partial\gamma}g_{h,2h}\right]. \tag{25}$$

Also in this case, note that (8b) gives $g_{h+1,2h+2}$ except for an arbitrary function of the single variable ξ, while Eqs. (25) and (8b) give it except for a constant arising from integration; the integrability condition is

$$k^2 \frac{\partial^2}{\partial \xi^2} g_{h,2h} - \frac{\partial^2}{\partial \gamma^2} g_{h,2h} + \frac{2h+3}{\gamma} \frac{\partial}{\partial \gamma} g_{h,2h} = 0. \tag{26}$$

Now, the first member of this relation written with $h+1$ instead of h, can be exploited by means of (8b) and (25), and becomes zero. Therefore, it is sufficient to impose Eq. (26) only for $h=0$, i.e.,

$$k^2 \frac{\partial^2}{\partial \xi^2} g_{0,0} - \frac{\partial^2}{\partial \gamma^2} g_{0,0} + \frac{3}{\gamma} \frac{\partial}{\partial \gamma} g_{0,0} = 0, \tag{27}$$

because for the other values of h it is surely satisfied.

It remains now to impose Eq. (24b); when $s=n-1$ it is an identity, as consequence of (19a), (24a) and (25). For the other values of s, let us impose it with the recurrence method. Let it be true when $s+1$ replaces s; by using this new relation and (19a), we see that (24a) is satisfied iff

$$\frac{\partial}{\partial \gamma}\left[\left(\frac{2n-2s-1}{2s+3} g_{n-1,2s+2} + g_{n-1,2s}\right)\gamma^{-2n-2}\right] + \frac{k^2}{m^2} \frac{\gamma^{-2n-2}}{2s+3} \frac{\partial}{\partial \xi} g_{n,2s+2} = 0 \quad \text{for } s=0,\ldots,n-2. \tag{28}$$

It can be seen that this relation holds also for $s=n-1$ as a consequence of (25) and of (8a). Let us write the first member of Eq. (28) with $s-1$ instead of s, and substitute in this expression the functions $g_{n-1,2s}$, $g_{n-1,2s-2}$, and $g_{n,2s}$ which can be obtained from (8a) in terms of $g_{n-1,2s+2}$, $g_{n-1,2s}$, and $g_{n,2s+2}$, respectively. In the result, let us substitute the expression of $(\partial/\partial\xi)\, g_{n,2s+2}$ which can be obtained from Eq. (28); after that, $g_{n-1,2s}$ can be expressed in terms of $g_{n-1,2s+2}$ from (8a) and the result is identically zero. Therefore, Eq. (28) is satisfied because it already holds for the higher value of s.

IV. CONCLUSIONS

The present results are very satisfactory, because the closure which is found constitutes a consistent improvement of the previous ones appearing in the literature. Not only does it satisfy the constraints exactly, still obeying the warm plasma ordering, but it satisfies exactly also the supplementary conservation law related to the entropy principle, not only in a neighborhood of equilibrium as in the previous versions. This fact guarantees the existence and uniqueness, well-posedness and stability of the solution of the initial values problem.

It allows also further deepening investigations, which may be the subject of future works.

ACKNOWLEDGMENT

This work has been partially supported by the G.N.F.M.

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On two dimensional coupled bosons and fermions

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(Received 8 July 2002; accepted 24 August 2002)

We study complex bosons and fermions coupled through a generalized Yukawa type coupling in the large-N_c limit following ideas of Rajeev [Int. J. Mod. Phys. A **9**, 5583 (1994)]. We study a linear approximation to this model. We show that in this approximation we do not have boson–antiboson and fermion–antifermion bound states occuring together. There is a possibility of having only fermion–antifermion bound states. We support this claim by finding distributional solutions with energies lower than the two mass treshold in the fermion sector. This has implications from the point of view of scattering theory to this model. We discuss some aspects of the scattering above the two mass treshold of boson pairs and fermion pairs. We also briefly present a gauged version of the same model and write down the linearized equations of motion. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1516846]

I. INTRODUCTION

Quantum field theories are both fundamental and challenging. Despite the fact that our description of the world of elementary particles is based on quantum field theory, we still do not have a complete understanding of interacting field theories, especially their bound state structure. For this reason it is interesting to study simple examples where one can actually make more progress. There are various such models in two dimensions and they have been a valuable source for new ideas and testing ground for many years (see Ref. 1 for a comprehensive selection of topics).

In this article we study a two dimensional model which could be another possible toy model for understanding Yukawa coupled field theories in four dimensions. The physically important one is the gauged Yukawa theory, as we know from the present day version of the standard model. In this work we will also study some aspects of the gauge coupled interacting bosons and fermions. We will actually present the linearized equations of the gauged version at the end of our article, but our main emphasis is to understand the simpler case without the gauge potentials (of course it is not so clear if this is really a simpler theory). A more complicated version of the model we discuss is investigated in Ref. 2 using path integral techniques. The results of the present article are somewhat different since we follow a Hamiltonian approach (and we are not taking the most complicated possible version).

Let us comment on some fundamental work in the literature that we are aware of: the literature on Yukawa theory is vast, we will mention only a few of them, a rigorous construction of two dimensional model is given in Refs. 3 and 4, and the construction of the probability measure within the Euclidean formalism is done in Ref. 5. The most recent rigorous analysis was given in Ref. 6 by following a renormalization group type idea essentially inspired from Ref. 7. It will be interesting to attempt such a rigorous approach for the model we discuss below. The standart Yukawa coupling in two dimensions in the light-cone approach is discussed in Refs. 8 and 9. A further analysis using the Tamm–Dancoff approximation in the light-cone is pursued in Ref. 10. A very interesting discussion of the Yukawa model in four dimensions is presented in Ref. 11, clearly a four dimensional model has many more interesting features. A more recent analysis of the

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fermion bound states of the same model is discussed in Ref. 12. The equivalence between the light-cone and covariant perturbation theory is analyzed in Ref. 13. (Good reviews of field theories in the light cone are given in Ref. 14 and renormalization of light cone Hamiltonians in Ref. 15.)

In this work, we introduce a color degree of freedom for the purpose of reaching a Hartree–Fock type approximation. Following the ideas suggested by Rajeev in Ref. 16 we reformulate the problem in terms of color invariant bilinears (see also Ref. 17 for some similar ideas). The details of this refromulation are explained in our previous work[18] within the context of gauge theories, therefore in this work we will use the results of the cited article directly. In some sense the present article is a natural continuation. The reader should consult Ref. 18 for more information on the geometry of the resulting classical phase space. We also recommend the lectures notes of Rajeev on two dimensional QCD.[19] In Ref. 16, it is shown that the $1+1$ dimensional QCD in the large-N_c limit can be reformulated as a classical field theory with an infinite dimensional phase space, which is identified to be the restricted Grassmanian. The study of two dimensional QCD in the large-N_c limit is given by 't Hooft in his well-known paper,[20] its generalization to scalar fields is done in Ref. 21 and in Ref. 22 using Hamiltonian methods. The two dimensional combined fermions and bosons QCD is given by Aoki in Refs. 23 and 24 and also discussed by Cavicchi.[2] Within Rajeev's approach one can reach the same results by using a linear approximation to the full theory. One can further study baryons by using a variational ansatz which does not correspond to small fluctuations of the fields, and therefore cannot be seen by the linear approximation. Here we obtain the general Hamitonian in the large-N_c limit for gauge coupled bosons and fermions which are also interacting through a generalized Yukawa type interaction. The meson equations are given for the linearized theory. Our presentation is incomplete since we do not study beyond the linear approximation and we plan to come to a more detailed analysis in the future.

In the simpler model we can actually solve the integral equations, ending up with some eigenvalue or scattering solutions. These equations require a simple renormalization to be meaningful (which at the end amounts to defining the singular integrals as the Hadamard principal value). We warn the reader that the form of the resulting Hamiltonian suggests that a physically more relevant approximation in the nongauged models could be given by a variational ansatz. This is due to the fact that the interactions in the linear approximation are all multiplied by the fermion mass. For heavy fermions we expect that the linear approximation gives valuable results, but, for example, in the case of massless fermions all the information is contained in the higher order terms, which cannot be accessed by the method we use.

II. COUPLING BETWEEN COMPLEX BOSONS AND FERMIONS

We start with the action of our model with two Yukawa type couplings,

$$S=\int d^2x\Big(i\overline{\psi}^{\alpha}\gamma^{\mu}\partial_{\mu}\psi_{\alpha}-\overline{\psi}^{\alpha}(\mu_{1Y}\phi^{*\beta}\phi_{\alpha}+\mu_{2Y}\phi^{*\lambda}\phi_{\lambda}\delta^{\alpha}_{\beta}+m_F\delta^{\beta}_{\alpha})\psi_{\beta}$$
$$+\partial^{\mu}\phi^{*\alpha}\partial_{\mu}\phi_{\alpha}-m^2_{B0}\phi^{*\alpha}\phi_{\alpha}-\frac{\lambda^2_{B0}}{4}(\phi^{*\alpha}\phi_{\alpha})^2\Big). \tag{1}$$

Here α refers to a common flavor index and it goes from 1 to N_c (we continue to write it as color symmetry, since at the end we will also talk about the gauged model). It is more natural to set $\mu_{1Y}=\mu_{2Y}$ when there are no gauge fields, since we will use the color degrees to arrive a mean-field description (but we will continue to use two different couplings). We rewrite the action in the light-cone coordinate system, and *we choose* x^+ *as our "time" coordinate*,

$$S=\int dx^+dx^-\Big(i\sqrt{2}\psi^{*\alpha}_L\partial_-\psi_{L\alpha}+i\sqrt{2}\psi^{*\alpha}_R\partial_+\psi_{R\alpha}+\phi^{*\alpha}(-2\partial_-)\partial_+\phi_{\alpha}-m^2_{0B}\phi^{*\alpha}\phi_{\alpha}$$
$$-(\psi^{*\alpha}_L\psi_{R\beta}+\psi^{*\alpha}_R\psi_{L\beta})(\mu_{1Y}\phi^{*\beta}\phi_{\alpha}+\mu_{2Y}\phi^{*\lambda}\phi_{\lambda}\delta^{\alpha}_{\beta}+m_F\delta^{\beta}_{\alpha})-\frac{\lambda^2_{B0}}{4}(\phi^{*\alpha}\phi_{\alpha})^2\Big).$$

There are many good introductions to the light-cone field theory; we refer the reader to Refs. 25–27. We note that the left-handed components of the fermion field are nondynamical, therefore we will remove $\psi_{L\alpha}$ and its complex conjugate through the equations of motion in the quantum theory (we refer to Ref. 18 for our conventions in quantizing this theory, below we summarize the results),

$$\hat{\psi}_{L\alpha}=\frac{\sqrt{2}}{2i\partial_-}[\mu_{1Y}:\hat{\phi}_\alpha\hat{\phi}^{\dagger\beta}\hat{\psi}_{R\beta}:+\mu_{2Y}:\hat{\phi}^{\dagger\beta}\hat{\phi}_\beta\hat{\psi}_{R\alpha}:+m_F\hat{\psi}_{R\alpha}]. \tag{2}$$

We do not really need to worry about the normal ordering in the first factor, since in the large-N_c limit these corrections will be of smaller order; we wrote it to emphasize that the reduction should be performed at the quantum level. At the second term we have a normal ordering for the color contracted bosons only. The second thing we notice from the light-cone action is that we are already in the Hamiltonian formalism. Therefore we can read off the Hamiltonian directly from the action when we insert the solution of the nondynamical field back into the action. Thus we arrive at the following Hamiltonian (*from now on we write ψ for ψ_R since this is the only fermionic field we have*),

$$\begin{aligned}\hat{H}=\int dx^-\Bigg(&\frac{\sqrt{2}m_F^2}{2}:\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha:+m_{B0}^2:\hat{\phi}^{\dagger\alpha}\hat{\phi}_\alpha:+\frac{\lambda_{B0}^2}{4}(:\hat{\phi}^{\dagger\alpha}\hat{\phi}_\alpha:)^2\\
&+\frac{\sqrt{2}}{2}\mu_{1Y}m_F\left[\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\phi}_\alpha\hat{\phi}^{\dagger\beta}\hat{\psi}_\beta+\hat{\psi}^{\dagger\beta}\hat{\phi}_\beta\hat{\phi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha\right]+\frac{\sqrt{2}}{2}\mu_{1Y}^2\hat{\psi}^{\dagger\beta}\hat{\phi}_\beta\hat{\phi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\phi}_\alpha\hat{\phi}^{\dagger\lambda}\hat{\psi}_\lambda\\
&+\frac{\sqrt{2}}{2}\mu_{1Y}\mu_{2Y}\left[\hat{\psi}^{\dagger\lambda}\hat{\phi}_\lambda\hat{\phi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha:\hat{\phi}^{\dagger\beta}\hat{\phi}_\beta:+:\hat{\phi}^{\dagger\lambda}\hat{\phi}_\lambda:\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\phi}_\alpha\hat{\phi}^{\dagger\beta}\hat{\psi}_\beta\right]\\
&+\frac{\sqrt{2}}{2}m_F\mu_{2Y}\left[\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha:\hat{\phi}^{\dagger\sigma}\phi_\sigma:+:\hat{\phi}^{\dagger\sigma}\hat{\phi}_\sigma:\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha\right]\\
&+\frac{\sqrt{2}}{2}\mu_{2Y}^2:\hat{\phi}^{\dagger\sigma}\hat{\phi}_\sigma:\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha:\hat{\phi}^{\dagger\beta}\hat{\phi}_\beta:\Bigg).\end{aligned} \tag{3}$$

This Hamiltonian as it stands is not normal ordered; to define it properly we need to normal order the color singlet products of bosons in the sixth term and the products of fermions in the last three terms. All these terms except one will give some divergences which can be cancelled by redefinitions of m_{B0} and λ_{B0}^2 in the original Hamiltonian as we will see. One of them cannot be removed by the original terms in the action and we will add a counter term which cannot be put into the original action. This Hamiltonian could be a better two dimensional representative of the four dimensional Yukawa theory, since in four dimensions phi-four coupling is necessary to renormalize the Yukawa interaction.

Let us recall the quantization of this system in the light-cone coordinates. The Fourier mode expansions read

$$\phi_\alpha(x^-)=\int a_\alpha(p)e^{-ipx^-}\frac{[dp]}{(2|p|)^{1/2}},\quad \psi_{L\alpha}(x^-)=\int \chi_\alpha(p)e^{-ipx^-}\frac{[dp]}{2^{1/4}}.$$

The normalization factors are chosen to reproduce the correct classical limits. To precisely define these expansions, we assume that the momenta range between $(-\infty,-\epsilon_0]$ and $[\epsilon_0,\infty)$, and at the end of our calculations we set $\epsilon_0\to 0$. This is physically meaningful due to charge conjugation invariance, and amounts to the principal value prescription (see Refs. 18 and 19 for details)

$$[\chi_\alpha(p),\chi^{\dagger\beta}(q)]_+=\delta_\alpha^\beta\delta[p-q],\quad [a_\alpha(p),a^{\dagger\beta}(q)]=\mathrm{sgn}(p)\,\delta_\alpha^\beta\delta[p-q]. \tag{4}$$

One defines a Fock vacuum state $|0\rangle$ by the conditions

$$a_\alpha(p)|0\rangle=\chi_\alpha(p)|0\rangle=0 \quad \text{for} \quad p>0 \qquad a^{\dagger\alpha}(p)|0\rangle=\chi^{\dagger\alpha}(p)|0\rangle=0 \quad \text{for} \quad p<0. \tag{5}$$

(Recall that we are assuming that there is an infinitesimal hole around $p=0$ to be taken to zero at the end of the calculations.) The corresponding normal orderings are defined in Ref. 18. It is useful to keep in mind the normal ordering rules of the bilinears,

$$:a^{\alpha\dagger}(p)a_\beta(q):=a^{\alpha\dagger}(p)a_\beta(q)-\tfrac{1}{2}\delta^\alpha_\beta(1-\mathrm{sgn}(p))\,\delta[p-q] \tag{6}$$

and

$$:\chi^{\dagger\alpha}(p)\chi_\beta(q):=\chi^{\dagger\alpha}(p)\chi_\beta(q)-\tfrac{1}{2}\delta^\alpha_\beta(1-\mathrm{sgn}(p))\,\delta[p-q]. \tag{7}$$

We provide some of the details of the reorganization of the Hamiltonian into normal ordered bilinears in the Appendix. We formulate the theory in terms of the color invariant bilinears following the idea proposed by Rajeev[16] and use our results in Ref. 18. For the convenience of the reader we recollect some of the essential points: to define the large-N_c limit we introduce

$$\begin{aligned}\hat{M}(p,q)&=\frac{2}{N_c}:\chi^{\dagger\alpha}(p)\chi_\alpha(q):,\\ \hat{N}(p,q)&=\frac{2}{N_c}:a^{\dagger\alpha}(p)a_\alpha(q):,\end{aligned} \tag{8}$$

and their odd counterparts,

$$\hat{Q}(p,q)=\frac{2}{N_c}\chi^{\dagger\alpha}(p)a_\alpha(q), \quad \hat{\bar{Q}}(r,s)=\frac{2}{N_c}a^{\dagger\alpha}(r)\chi_\alpha(s). \tag{9}$$

In the large-N_c limit these bilinears become classical variables,[28] and we postulate the super Poisson brackets satisfied by these variables, which defines the kinematics of our theory:

$$\begin{aligned}\{M(p,q),M(r,s)\}&=-2i[M(p,s)\,\delta[q-r]-M(r,q)\,\delta[p-s]\\ &\quad-\delta[p-s]\,\delta[q-r](\mathrm{sgn}(p)-\mathrm{sgn}(q))],\\ \{N(p,q),N(r,s)\}&=-2i[N(p,s)\mathrm{sgn}(q)\,\delta[q-r]-N(r,q)\mathrm{sgn}(p)\,\delta[p-s]\\ &\quad-\delta[q-r]\,\delta[p-s](\mathrm{sgn}(p)-\mathrm{sgn}(q))],\\ \{Q(p,q),\bar{Q}(r,s)\}_+&=-2i[M(p,s)\mathrm{sgn}(q)\,\delta[q-r]+N(r,q)\,\delta[p-s]\\ &\quad+\delta[p-s]\,\delta[q-r](1-\mathrm{sgn}(p)\mathrm{sgn}(q))],\\ \{M(p,q),Q(r,s)\}&=-2i\,\delta[q-r]Q(r,q),\\ \{N(p,q),Q(r,s)\}&=2i\,\delta[q-s]\mathrm{sgn}(p)Q(r,q),\\ \{M(p,q),\bar{Q}(r,s)\}&=2i\,\delta[p,s]\bar{Q}(r,q),\\ \{N(p,q),\bar{Q}(r,s)\}&=-2i\,\delta[p-s]\mathrm{sgn}(q)\bar{Q}(p,s).\end{aligned} \tag{10}$$

These classical variables now satisfy,

$$M(p,q)=M^*(q,p),\quad N(p,q)=N^*(q,p),\quad \overline{Q}(p,q)=Q^*(q,p). \tag{11}$$

There are also constraints satisfied by these variables when we restrict ourselves to the subspace of the color invariant states. For our problem, *this is an approximation, since there is no reason to expect that all the physical states are color singlets*. Furthermore, when there are no gauge fields, there are scattering states of our linearized equations. We write explicitly the constraints for the basic variables,

$$\begin{gathered}(M+\epsilon)^2+Q\epsilon Q^\dagger=1,\\ \epsilon Q^\dagger M+\epsilon Q^\dagger\epsilon+\epsilon N\epsilon Q^\dagger+Q^\dagger=0,\\ MQ+\epsilon Q+Q\epsilon N+Q\epsilon=0,\\ (\epsilon N+\epsilon)^2+\epsilon Q^\dagger Q=1.\end{gathered} \tag{12}$$

Above we use an operator notation, $\epsilon(p,q)=-\mathrm{sgn}(p)\delta[p-q]$, and $(AB)(p,q)=\int dsA(p,s)B(s,q)$. The phase space of the resulting restricted theory is shown to be a super-Grassmannian in Ref. 18, with its natural symplectic structure generalizing the results in Ref. 16.

We can reexpress our Hamiltonian in terms of the above mentioned basic variables. After a somewhat long but straightforward computation, the large-N_c limit Hamiltonian becomes

$$H=H_0+H_Y, \tag{13}$$

where

$$H_0=\frac{1}{4}m_F^2\int\frac{[dp]}{p}M(p,p)+\frac{1}{4}m_{BR}^2\int\frac{[dp]}{|p|}N(p,p), \tag{14}$$

$$\begin{aligned}H_Y=&\int\frac{[dpdqdsdt]}{\sqrt{|sq|}}\delta[p-q+s-t]\left(\frac{1}{16}\mu_{1Y}m_F\left[\frac{1}{p}+\frac{1}{t}\right]+\kappa\frac{1}{s-t}\right)Q(p,q)\overline{Q}(s,t)-\frac{\mu_{2Y}m_F}{16}\\ &\times\int\frac{[dpdqdsdt]}{\sqrt{|st|}}\delta[p-q+s-t]\left[\frac{1}{p}+\frac{1}{q}\right]M(p,q)N(s,t)+\frac{1}{64}\int\frac{[dpdqdkdl]}{\sqrt{|pqkl|}}\\ &\times\lambda_R^2\delta[p-q+k-l]N(p,q)N(k,l)-\int\frac{[dpdqdsdtdkdl]}{\sqrt{|qskl|}}\delta[p-q+s-t+k-l]\\ &\times\left[\frac{\mu_{1Y}\mu_{2Y}}{64}\left(\frac{1}{k-l-t}+\frac{1}{s-t-q}\right)+\frac{\mu_{1Y}^2}{64}\left(\frac{1}{s-t-l}\right)\right]Q(p,q)\overline{Q}(s,t)N(k,l)\\ &+\frac{\mu_{2Y}^2}{64}\int\frac{[dpdqdsdtdkdl]}{\sqrt{|pqkl|}}\delta[p-q+k-l+s-t]\frac{1}{t+l-k}N(p,q)N(k,l)M(s,t).\end{aligned} \tag{15}$$

Note that we have rescaled the coupling constants as $\mu_{1Y}N_c\mapsto\mu_{1Y}$, $\mu_{2Y}N_c\mapsto\mu_{2Y}$ and $\lambda_R^2N_c\mapsto\lambda_R^2$.

As we discussed in the Appendix, there are two possible renormalizations. In the first case we allow for the nonlocal counter terms and remove the divergent parts finding a local Hamiltonian–thus κ and λ_R are just constants. If we only allow for the local counter terms, then we find

$$\kappa=\kappa_R(\mu_R)-\frac{\mu_{1Y}^2}{64\pi}\ln\left|\frac{s-t}{\mu_R}\right|,$$

$$\lambda_R^2=\lambda_{RB}^2(\mu_R)+\frac{\mu_{2Y}^2}{\pi}\ln\left|\frac{k-l}{\mu_R}\right|.$$

We introduce a renormalization scale μ_R, and assume that the renormalized values of the couplings $\kappa_R(\mu_R)$, $\lambda_{RB}^2(\mu_R)$ vary with the scale μ_R such that the Hamiltonian does not really depend on this scale. This means we should impose

$$\begin{aligned}\kappa_R(\mu_R)&=\kappa_R(\tilde{\mu}_R)-\frac{\mu_{1Y}^2}{64\pi}\ln\left|\frac{\mu_R}{\tilde{\mu}_R}\right|,\\ \lambda_{RB}^2(\mu_R)&=\lambda_{RB}^2(\tilde{\mu}_R)+\frac{\mu_{2Y}^2}{\pi}\ln\left|\frac{\mu_R}{\tilde{\mu}_R}\right|.\end{aligned}\tag{16}$$

The sign of the new coupling κ_R should not be fixed since it does not exist in the original action, and *it has dimensions of mass square*.

For the rest of this work we will take the simpler Hamiltonian, that is we assume that all the renormalized couplings are ordinary numbers. From a more conservative point of view the local counter terms should be the general class of models we should investigate. We hope to return to a more detailed analysis allowing momenta dependent couplings in the future. *However, the Lorentz invariance is not clear in such a renormalization scheme. This may be a more serious objection, perhaps one can find a better suited approach to cure all the problems at the same time.*

This Hamiltonian along with the Poisson brackets and the contraint define our model completely. As it stands this is a complicated system. We plan to study a variational approach to this model in a future work. We will study a linear approximation to this model in the next section.

III. THE LINEAR APPROXIMATION

We assume that all the basic variables deviate from the vacuum by small amounts, therefore we keep everything to first order. This means the linearization of the constraint and the linearization of the equations of motion. The constraint implies that

$$M(u,v)=0,\quad N(u,v)=0,\quad Q(u,v)=0\quad \text{if } uv>0.\tag{17}$$

The equations of motion for $u>0$, $v<0$, found from

$$\frac{\partial O(u,v)}{\partial x^+}=\{O(u,v),H\},\tag{18}$$

where O refers to any one of our variables, could be linearized. Let us write these linearized equations of motion for all the variables,

$$\frac{\partial M(u,v)}{\partial x^+}=i\frac{m_F^2}{2}\left[\frac{1}{u}-\frac{1}{v}\right]M(u,v)-i\frac{\mu_{2Y}m_F}{4}\left[\frac{1}{u}+\frac{1}{v}\right]\int\frac{N(s,s-(u-v))}{\sqrt{|s((u-v)-s)|}}[ds],\tag{19}$$

$$\begin{aligned}\frac{\partial N(k,l)}{\partial x^+}&=i\frac{m_{BR}^2}{2}\left[\frac{1}{k}-\frac{1}{l}\right]N(k,l)-i\frac{\mu_{2Y}m_F}{4\sqrt{|kl|}}\int[ds]\left[\frac{1}{s}+\frac{1}{s-(k-l)}\right]M(s,s-(k-l))\\&\quad+\frac{i}{8}\lambda_R^2\int\frac{[ds]}{\sqrt{|skl((k-l)-s)|}}N(s,s-(k-l)),\end{aligned}\tag{20}$$

and

$$\frac{\partial Q(u,v)}{\partial x^+}=\frac{i}{2}\left[\frac{m_F^2}{u}-\frac{m_{RB}^2}{v}\right]Q(u,v)-\kappa\frac{4i}{u-v}\int\frac{Q(p,p-(u-v))}{\sqrt{|v(p-(u-v))|}}[dp]$$

$$+i\frac{\mu_{1Y}m_F}{4}\int\frac{[dp]}{\sqrt{|(p-(u-v))v|}}\left[\frac{1}{p}+\frac{1}{u}\right]Q(p,p-(u-v)). \tag{21}$$

The equation of motion for $\overline{Q}$ can be found by complex conjugation and does not carry new information. We note that the equations of motion for M and N are coupled, but the equations of motion for Q within the linear approximation are decoupled from the rest.

So we will start with this one and make an ansatz as in Refs. 16 and 19. Let us assume that the solution can be written as $Q(u,v;x^+)=c_Q(x)e^{iP_+x^+}$, where $x=u/P_-$, $P_-=u-v$ and define an invariant mass $\Lambda_Q^2=2P_-P_+$. [Strictly speaking we could take the solution of the form $c_Q(x)f_Q(P_-)e^{iP_+x^+}$, the arbitrary function f_Q factors out in the equations.] Then we find

$$\Lambda_Q^2c_Q(x)=\left[\frac{m_F^2}{x}+\frac{m_{BR}^2}{1-x}\right]c_Q(x)-8\kappa\int_0^1\frac{dy}{\sqrt{(1-y)(1-x)}}c_Q(y)$$

$$+\frac{1}{4}\mu_{1Y}m_F\int_0^1\frac{dy}{\sqrt{(1-y)(1-x)}}\left(\frac{1}{x}+\frac{1}{y}\right)c_Q(y).$$

This innocent looking equation actually requires a renormalization, as we will see shortly.

Let

$$\int_0^1\frac{dy}{\sqrt{(1-y)}}c_Q(y)=A\quad\int_0^1\frac{dy}{y\sqrt{(1-y)}}c_Q(y)=B. \tag{22}$$

Then we solve for $c_Q(x)$,

$$c_Q(x)=\sqrt{(1-x)}\frac{(aA+bB)x+bA}{\Lambda_Q^2x(1-x)-m_F^2(1-x)-m_B^2x}, \tag{23}$$

where

$$a=-8\kappa,\quad b=\tfrac{1}{4}\mu_{1Y}m_F. \tag{24}$$

A straightforward solution will actually produce a divergence, the integration defining B is divergent. To find a finite result we need a renormalization prescription. Let us assume that the phase is given by $e^{i(P_++\delta P_+(\epsilon_0))x^+}$, where $\delta P_+(\epsilon_0)$ denotes a divergent phase of the solution that we remove from the equations, and ϵ_0 denotes a low momentum cut-off. The time derivative will drop a factor of $\delta P_+(\epsilon_0)$, and multiplying by $2P_-$ we denote it as $\delta\Lambda_Q(\epsilon_0)$ and rewrite the same equation as

$$\left[\Lambda_Q^2+\delta\Lambda_Q(\epsilon_0)-\frac{m_F^2}{x}-\frac{m_{BR}^2}{1-x}\right]c_Q(x)=\frac{aA}{\sqrt{1-x}}+\frac{bA}{x\sqrt{1-x}}+\frac{bB(\epsilon_0)}{\sqrt{1-x}}. \tag{25}$$

Since the divergent part comes from the B term we expect that $\delta\Lambda_Q(\epsilon_0)c_Q(x)$ can be taken as a counter-term on the other side of the equality with the leading form $-\alpha_c(\epsilon_0)/\sqrt{1-x}$. The unknown function now is given by the same formula with a shifted coefficient of x,

$$c_Q(x)=\sqrt{(1-x)}\frac{(aA+bB(\epsilon_0)-\alpha_c(\epsilon_0))x+bA}{\Lambda_Q^2x(1-x)-m_F^2(1-x)-m_B^2x}. \tag{26}$$

Let us insert this back into (22) and find the constants $A, B(\epsilon_0)$. After some algebra, we reach

$$A = -F_2 \frac{aA + bB(\epsilon_0) - \alpha_c(\epsilon_0)}{2\Lambda_Q^2} - \left[\left(\frac{aA + bB(\epsilon_0) - \alpha_c(\epsilon_0)}{2\Lambda_Q^2} \right) (\Lambda_Q^2 - m_{RB}^2 + m_F^2) + bA \right] F_1(\Lambda_Q), \tag{27}$$

$$B(\epsilon_0) = \frac{bA}{m_F^2} \ln(\epsilon_0) + \frac{bA}{2m_F^2} F_2 - \left[\frac{bA}{2m_F^2} (\Lambda_Q^2 - m_{RB}^2 + m_F^2) + (aA + bB(\epsilon_0) - \alpha_c(\epsilon_0)) \right] F_1(\Lambda_Q), \tag{28}$$

where

$$F_2 = \int_0^1 dx \frac{2\Lambda_Q^2 x - (\Lambda_Q^2 - m_{RB}^2 + m_F^2)}{\Lambda_Q^2 x^2 - (\Lambda_Q^2 - m_{RB}^2 + m_F^2)x + m_F^2} = \ln\left[\frac{m_{RB}^2}{m_F^2} \right],$$
$$F_1(\Lambda_Q) = \int_0^1 \frac{dx}{\Lambda_Q^2 x^2 - (\Lambda_Q^2 - m_{RB}^2 + m_F^2)x + m_F^2}. \tag{29}$$

If we are looking for a bound state of a boson and a fermion, this requires

$$|m_{RB} - m_F| < \Lambda_Q < m_{RB} + m_F. \tag{30}$$

Then the last integral gives

$$F_1(\Lambda_Q) = \frac{2}{u} \left(\arctan\left[\frac{\Lambda_Q^2 + m_{BR}^2 - m_F^2}{u} \right] - \arctan\left[\frac{m_{BR}^2 - m_F^2 - \Lambda_Q^2}{u} \right] \right), \tag{31}$$

where

$$u = \sqrt{(\Lambda_Q^2 - (m_{RB} - m_F)^2)((m_{RB} + m_F)^2 - \Lambda_Q^2)}. \tag{32}$$

Let us impose the two conditions

$$B_* = B(\epsilon_0) - \frac{bA}{m_F^2} \ln(\epsilon_0), \quad bB(\epsilon_0) - \alpha_c(\epsilon_0) = bB_*. \tag{33}$$

Then we see that if we set

$$\alpha_c(\epsilon_0) = \frac{b^2 A}{m_F^2} \ln(\epsilon_0), \tag{34}$$

we can take $\epsilon_0 \to 0^+$ limit, and keep B_*, A finite. The renormalized equations become

$$A = -F_2 \frac{aA + bB_*}{2\Lambda_Q^2} - \left[\left(\frac{aA + bB_*}{2\Lambda_Q^2} \right) (\Lambda_Q^2 - m_{RB}^2 + m_F^2) + bA \right] F_1(\Lambda_Q), \tag{35}$$

$$B_* = \frac{bA}{2m_F^2} F_2 - \left[\frac{bA}{2m_F^2} (\Lambda_Q^2 - m_{RB}^2 + m_F^2) + (aA + bB_*) \right] F_1(\Lambda_Q). \tag{36}$$

If we solve for the ratio A/B_*, after some algebra, this gives us a consistency condition for the excitation energy Λ_Q^2,

$$\left[F_2-s(\Lambda_Q)F_1(\Lambda_Q)-\frac{2am_F^2}{b}F_1(\Lambda_Q)\right][F_2+s(\Lambda_Q)F_1(\Lambda_Q)]$$
$$=-[1+bF_1(\Lambda_Q)]\left[F_2+\left(s(\Lambda_Q)+\frac{2b\Lambda_Q^2}{a}\right)F_1(\Lambda_Q)+\frac{2\Lambda_Q^2}{a}\right]\frac{2m_F^2a}{b^2}, \tag{37}$$

or, equivalently,

$$\left[\ln\left|\frac{m_{RB}^2}{m_F^2}\right|-s(\Lambda_Q)F_1(\Lambda_Q)+\frac{64\kappa m_F}{\mu_{1Y}}F_1(\Lambda_Q)\right]\left[\ln\left|\frac{m_{RB}^2}{m_F^2}\right|+s(\Lambda_Q)F_1(\Lambda_Q)\right]$$
$$=\left[1+\frac{1}{4}\mu_{1Y}m_FF_1(\Lambda_Q)\right]\left[\ln\left|\frac{m_{RB}^2}{m_F^2}\right|+\left(s(\Lambda_Q)-\frac{\mu_{1Y}m_F\Lambda_Q^2}{16\kappa}\right)F_1(\Lambda_Q)+\frac{\Lambda_Q^2}{4\kappa}\right]\frac{128\kappa}{\mu_{1Y}^2}, \tag{38}$$

where $s(\Lambda_Q)=\Lambda_Q^2-m_{RB}^2+m_F^2$. This equation is written in terms of dimensionless ratios of the variables, and it should be investigated numerically under the conditions we have stated before for Λ_Q. Instead of numerically solving these equations we will look at one extreme case, when $\Lambda_Q \approx m_{BR}+m_F$ (weak coupling). (It is interesting to investigate the opposite limit $\Lambda_Q\approx|m_F-m_{BR}|$, but the result is not so simple to interpret.) It is better to use a different variable to study such limiting cases; we define Δ, via $\Lambda_Q^2=m_{BR}^2+m_F^2+2m_{BR}m_F\Delta$. Note that we have $-1<\Delta<1$. Our function $F_1(\Lambda_Q)$ becomes

$$F_1(\Delta)=\frac{1}{m_Fm_{BR}}\frac{1}{\sqrt{1-\Delta^2}}\left(\arctan\left[\frac{\omega+\Delta}{\sqrt{1-\Delta^2}}\right]+\arctan\left[\frac{1/\omega+\Delta}{\sqrt{1-\Delta^2}}\right]\right). \tag{39}$$

Here $\omega=m_{BR}/m_F$, and if we take $\Delta\to1^-$, that means $\Lambda_Q\to(m_{BR}+m_F)^-$ and $\Delta\to-1^+$ corresponds to $\Lambda_Q\to|m_F-m_{BR}|^+$. There is nothing subtle about the first limit; keeping everything to first order gives us

$$\Delta=1-\left[1-\left(2-\frac{\mu_{1Y}}{\kappa}(m_F+m_{BR})\right)^{-1}\frac{\mu_{1Y}}{m_F+m_{BR}}\ln\left|\frac{m_{BR}^2}{m_F^2}\right|\right]^{-2}\frac{\pi^2\mu_{1Y}^2}{m_B^2}. \tag{40}$$

We assumed all the way $\Delta\approx1$. This could be consistent if for example we choose the coupling constant μ_{1Y} such that $\mu_{1Y}\ll m_B$ when the ratio m_F/m_{BR} is not too large and if $\kappa<0$. There are other possibilities, but this simple one shows that there are solutions with the expected behavior. If we assume $\Delta\to-1^+$, the function $F_1(\Delta)\to1/m_Fm_{BR}$, and the calculations are more complex. If we set $\Delta=-1+\delta^2$, we have $F_1(-1+\delta^2)\approx(1/m_Fm_{BR})(1-3/2\,\delta^2)$. This can be used to study the opposite limit, but due to its algebraic complexity we leave it out, and only state that for various possible cases to be consistent, we find that $m_F\gg m_{BR}$ is a necessary condition.

Following the same strategy, we look for stationary solutions for the coupled equations: we start with the following ansatz for M,N: $M(u,v)=\xi_M(x)e^{iP_+x^+}$ and $N(k,l)=\xi_N(y)e^{iP_+x^+}$, where $x=u/P_M$, $P_M=u-v$ and similarly for N. If we now substitute these into the coupled equations of motion, we see that the oscillations in time cancel out (since we select the same P_+) and we end up with

$$\Lambda_M^2\xi_M(x)=m_F^2\left[\frac{1}{x}+\frac{1}{1-x}\right]\xi_M(x)-\frac{\mu_{2Y}m_F}{4\pi}\left[\frac{1}{x}-\frac{1}{1-x}\right]\int_0^1\frac{\xi_N(y)}{\sqrt{y(1-y)}}dy, \tag{41}$$

$$\Lambda_N^2 \xi_N(x) = m_{BR}^2 \left[\frac{1}{x} + \frac{1}{1-x} \right] \xi_N(x) - \frac{\mu_{2Y} m_F}{4\pi \sqrt{(1-x)x}} \int_0^1 dy \left(\frac{1}{y} - \frac{1}{1-y} \right) \xi_M(y)$$

$$+ \frac{\lambda_R^2}{8\pi} \int_0^1 \frac{dy}{\sqrt{x(1-x)y(1-y)}} \xi_N(y), \tag{42}$$

where we set $\Lambda_M^2 = 2P_M P_+$ and $\Lambda_N^2 = 2P_N P_+$ for the invariant masses of the excitations of M and N, respectively. We notice that the desired decoupling of the total momentum variables would not have happened in the above equations if we had used the more general Hamiltonians.

Before we plunge into the standard way to solve these equations we will talk about an interesting possibility, if we admit distributional solutions for these equations (this of course has a meaning in terms of scattering theory as we will elaborate at the end of this section).

Let us introduce

$$D = \int_0^1 dy \frac{\xi_N(y)}{\sqrt{y(1-y)}}. \tag{43}$$

Then we can rewrite the equation of motion for M as

$$\Lambda_M^2 \xi_M(x) = m_F^2 \left[\frac{1-dD}{x} + \frac{1+dD}{1-x} \right] \xi_M(x), \quad \text{where } d = \frac{\mu_{2Y}}{4\pi m_F}. \tag{44}$$

For the solution we have in mind we need to impose

$$dD < 1, \tag{45}$$

otherwise the energy will be unbounded from below. Let us assume that the last two terms in the ξ_N equation cancel against each other. This condition implies that

$$\frac{\mu_{2Y} m_F}{4\pi} \int_0^1 dy \left(\frac{1}{y} - \frac{1}{1-y} \right) \xi_M(y) = \frac{\lambda_R^2}{8\pi} \int_0^1 \frac{dy}{\sqrt{y(1-y)}} \xi_N(y), \tag{46}$$

or, equivalently,

$$\frac{\mu_{2Y} m_F}{4\pi} \int_0^1 dy \left(\frac{1}{y} - \frac{1}{1-y} \right) \xi_M(y) = \frac{\lambda_R^2}{8\pi} D. \tag{47}$$

Thus we have to consistently choose everything to satisfy these conditions. The equation for M and N can be solved by using $\xi_M(x) = \delta(x - x_F)$ and $\xi_N(x) = \delta(x - x_B)$. What should we take as x_F and x_B? One way is to minimize the excitation energy for fermions, and then fix the bosonic parameter to have the cancellation. The eigenvalue for M becomes, after the minimizing choice is made,

$$\Lambda_M^2 = m_F^2 [(1+dD)^{1/2} + (1-dD)^{1/2}]^2 < 4m_F^2. \tag{48}$$

The last inequality is interesting since it implies that the fermions actually form a bound state at this energy. Now the condition we should have for the cancellation reads

$$\left(\frac{1+dD}{1-dD} \right)^{1/2} - \left(\frac{1-dD}{1+dD} \right)^{1/2} = fD, \tag{49}$$

where

$$f=\frac{\lambda_R^2}{2\mu_{2Y}m_F}. \tag{50}$$

From here we can solve for D,

$$D^2=\frac{1}{d^2}-\frac{4}{f^2}. \tag{51}$$

We should have $D^2>0$. This puts a condition on our couplings and the fermion mass. But there is a stronger condition; once we have the solution for the value of D, we can find the parameter x_B to choose for the bosons from the definition of D,

$$D=\int_0^1\frac{dy}{\sqrt{y(1-y)}}\xi_N(y)=\frac{1}{\sqrt{x_B(1-x_B)}}. \tag{52}$$

It is possible to find x_B if $D\geqslant 2$, since the minimum of the function on the right is 2, thus we need $D^2\geqslant 4$. This implies a condition on our couplings,

$$\frac{1}{\pi}\left(\frac{\mu_{2Y}^2}{m_F^2}\right)\left[1-\frac{\mu_{2Y}^2}{4\pi^2m_F^2}\right]^{-1/2}<\frac{\lambda_R^2}{m_F^2}, \tag{53}$$

where we used dimensionless variables to express this inequality.

We have the other condition about D, which says $dD<1$. This is actually satisfied by our solution, so we need

$$2\leqslant D<1/d. \tag{54}$$

From these we have a condition on the strength of the Yukawa coupling constant,

$$\mu_{2Y}<2\pi m_F. \tag{55}$$

Now we can go back and find the actual value of the fermion bound state and the mass of the boson pair. The boson pair mass is simply given by

$$\Lambda_N^2=\frac{m_{RB}^2}{x_B(1-x_B)}=m_{RB}^2D^2=m_{RB}^2\left[\frac{1}{d^2}-\frac{4}{f^2}\right]=16m_{RB}^2\left[\frac{\pi^2m_F^2}{\mu_{2Y}^2}-\frac{\mu_{2Y}^2m_F^2}{\lambda_R^4}\right]>4m_{RB}^2. \tag{56}$$

Similarly we have for the fermion pair,

$$\begin{aligned}\Lambda_M^2&=m_F^2\left[\left(1+\left[1-\frac{4d^2}{f^2}\right]^{1/2}\right)^{1/2}+\left(1-\left[1-\frac{4d^2}{f^2}\right]^{1/2}\right)^{1/2}\right]^2\\&=m_F^2\left[\left(1+\left[1-\frac{\mu_{2Y}^4}{\pi^2\lambda_R^4}\right]^{1/2}\right)^{1/2}+\left(1-\left[1-\frac{\mu_{2Y}^4}{\pi^2\lambda_R^4}\right]^{1/2}\right)^{1/2}\right]^2.\end{aligned}$$

We note that the above solution is quite interesting: we assume that the relative strength of the Yukawa coupling is small, i.e., $\mu_{2Y}\ll\lambda_R$, and expand the square roots,

$$\Lambda_M^2\approx 2m_F^2\left(1+\frac{2d^2}{f^2}\right)=2m_F^2\left[1+\frac{1}{\pi}\frac{\mu_{2Y}^4}{\lambda_R^4}\right]. \tag{57}$$

This is not the result one should expect from a perturbative point of view.

Furthermore, the boson pair becomes in this approximation,

$$\Lambda_N^2 \approx 16\pi^2 \left(\frac{\mu_{2Y}}{m_F}\right)^{-2} m_{BR}^2 > 16 m_{RB}^2. \tag{58}$$

If we further assume that $\mu_{2Y} \ll m_F$, this implies that the boson pair mass becomes very large.

Actually, there is a whole range of solutions with $\xi_M(x) = \delta(x - x_F)$ and $\xi_N(x) = \delta(x - x_B)$. We are free to choose one of them, say x_F. Then the other one will be determined by the same consistency relation as above. We see that the boson pair excitation will always be bigger than $2m_{BR}$, since the minimum is given by $x_B = \frac{1}{2}$. For the fermion pair we choose the consistent x_F's such that the mass is less than the two mass threshold. Let us briefly present our findings using the same notation as above.

Let us search for a solution of the equation

$$m_F^2 \left[\frac{1 - dD}{x} + \frac{1 + dD}{1 - x}\right] \xi_M(x) = \Lambda_M^2 \xi_M(x) \quad \text{with} \quad \Lambda_M^2 < 4 m_F^2. \tag{59}$$

We assume again that $dD < 1$. Then the equality is satisfied if we set $\xi_M(x) = \delta(x - x_F)$, $x_F = 1/2(1 - \alpha dD)$ for $0 < \alpha < 1$. We require the same delta function solution for ξ_N. This means we should solve for the equation

$$\frac{1}{x_F} - \frac{1}{1 - x_F} = fD. \tag{60}$$

If we solve for D now, we find

$$D^2 = \left[1 - \frac{4\alpha d}{f}\right] \frac{1}{\alpha^2 d^2}. \tag{61}$$

This implies that the first factor in the big paratheses should be positive. This is true if $\lambda_R^2 > (2/\pi)\, \alpha \mu_{2Y}^2$. Again, to have a solution for x_B we need $4 \leqslant D^2$. This means

$$4\alpha^2 d^2 + \frac{4\alpha d}{f} - 1 \geqslant 0, \tag{62}$$

which can be satisfied if the quadratic form for d has real roots and we choose d in between—assuming α is chosen. This implies an inequality for λ_R,

$$\frac{2\alpha}{\pi} \left(\frac{\mu_{2Y}}{m_F}\right)^2 \left[1 - \left(\frac{\alpha \mu_{2Y}}{2\pi m_F}\right)^2\right]^{-1} < \frac{\lambda_R^2}{m_F^2}. \tag{63}$$

This means that we should choose λ_R above a certain value, and this condition is stronger than the first one we found above. A uniform bound for various values of α can be chosen,

$$\frac{2}{\pi} \left(\frac{\mu_{2Y}}{m_F}\right)^2 \left[1 - \left(\frac{\mu_{2Y}}{2\pi m_F}\right)^2\right]^{-1} < \frac{\lambda_R^2}{m_F^2}. \tag{64}$$

Incidentally this requires $\mu_{2Y} < 2\pi m_F$. We still have $dD < 1$ to satisfy. If we simply use this condition assuming α as given, we arrive at the positivity of a quadratic expression in α:

$$\alpha^2 + \frac{2\alpha}{\pi} \frac{\mu_{2Y}^2}{\lambda_R^2} - 1 > 0. \tag{65}$$

Notice that the range of allowed α will be bigger if we take μ_{2Y}/λ_R ratio as large as possible. If we use the uniform lower bound for λ_R, we will find the largest region, and if we denote the deviation from this value by a multiplicative factor $k>1$, we can insert this ratio into the quadratic expression,

$$\alpha^2+\frac{1}{k}\left[1-\left(\frac{\mu_{2Y}}{2\pi m_F}\right)^2\right]\alpha-1>0. \tag{66}$$

The positivity is guaranteed if we choose α outside of the region between the two roots. The choice consistent with $0<\alpha<1$ gives us

$$\frac{1}{2k}\left(\sqrt{\left[1-\frac{\mu_{2Y}^2}{4\pi^2 m_F^2}\right]^2+4k^2}-\left[1-\frac{\mu_{2Y}^2}{4\pi^2 m_F^2}\right]\right)<\alpha<1. \tag{67}$$

The lower bound is a decreasing function of k, so the stronger relative values of λ_R will have a smaller domain of α's. Since for these choices we have a continuous range of α's, the spectrum of the problem is rather different. Such distributional solutions are not eigenvalues, but they typically refer to the continuous part of the spectrum. In some sense these are still scattering states. This means we cannot use the free parts of the original Hamiltonian to study the scattering theory below the two mass thresholds. Above these values we will see that the scattering theory can be studied by conventional methods. Perhaps below this we need to use the minimum value of the spectrum to define new effective pair mass for the fermionic sector. The continuum of bound states suggest that the free parts we start with should not be used to define the vacuum of the theory, and we should go beyond the linear approximation. The correct minimum found for the classical variables in the fully interacting theory may then be used to study a better linear approximation. We are not able to resolve this issue at the moment.

If we now go back to the standard approach, again as in the case of boson–fermion pair, we will need to renormalize our equations, by assuming a divergent common phase $\delta P_+(\epsilon_0)$, $M=\xi_M e^{i(\delta P_+(\epsilon_0)+P_+)x^+}$, and similarly for N. The derivative will bring terms of the form $\delta\Lambda_N(\epsilon_0)=2P_N\delta P_+(\epsilon_0)$ and $\delta\Lambda_M(\epsilon_0)=2P_M\delta P_+(\epsilon_0)$. An inspection of the resulting equations shows that we have the leading behavior

$$\delta\Lambda_M(\epsilon_0)\xi_M(x)\sim\frac{\alpha_c(\epsilon_0)(1-2x)}{x(1-x)},\quad \delta\Lambda_N(\epsilon_0)\xi_N(x)\sim\frac{\beta_c(\epsilon_0)}{\sqrt{x(1-x)}}. \tag{68}$$

In general, $\beta_c(\epsilon_0)=\sigma\alpha_c(\epsilon_0)$, as we will see the precise value of σ is not important. Now we can solve for the unknown functions,

$$\begin{aligned}\xi_M(x)&=\frac{(1-2x)(aA(\epsilon_0)-\alpha_c(\epsilon_0))}{\Lambda_M^2 x(1-x)-m_F^2},\\ \xi_N(x)&=\sqrt{x(1-x)}\frac{2aB(\epsilon_0)+bA(\epsilon_0)-\sigma\alpha_c(\epsilon_0)}{\Lambda_N^2 x(1-x)-m_{BR}^2},\end{aligned} \tag{69}$$

where

$$A(\epsilon_0)=\int_{\epsilon_0}^1 dy\,\frac{\xi_N(y)}{\sqrt{y(1-y)}},\quad B(\epsilon_0)=\int_{\epsilon_0}^1 dy\,\frac{\xi_M(y)}{y}, \tag{70}$$

and

$$a=-\frac{\mu_{2Y}m_F}{4\pi},\quad b=\frac{\lambda_R^2}{8\pi}. \tag{71}$$

If we introduce

$$F(\Lambda,m)=\mathcal{P}\int_0^1 \frac{dy}{\Lambda^2 y(1-y)-m^2}, \tag{72}$$

we find from the defining conditions of $A(\epsilon_0)$, $B(\epsilon_0)$,

$$\begin{aligned} B(\epsilon_0)&=(aA(\epsilon_0)-\alpha_c(\epsilon_0))\frac{1}{m_F^2}\ln\epsilon_0+(aA(\epsilon_0)-\alpha_c(\epsilon_0))\left(\frac{\Lambda_M^2}{2m_F^2}-2\right)F(\Lambda_M,m_F),\\ A(\epsilon_0)&=[2aB(\epsilon_0)+bA(\epsilon_0)-\sigma\alpha_c(\epsilon_0)]F(\Lambda_N^2,m_{RB}). \end{aligned} \tag{73}$$

We now define $aA_*=aA(\epsilon_0)-\alpha_c(\epsilon_0)$, and $B_*=B(\epsilon_0)-(a/m_F^2)A_*\ln\epsilon_0$, and insert these back into our equations,

$$\begin{aligned} B_*&=A_* a\left(\frac{\Lambda_M^2}{2m_F^2}-2\right)F(\Lambda_M,m_F)\\ A_*&=\left[2aB_*+bA_*+\frac{2a^2}{m_F^2}A_*\ln\epsilon_0+\left[\frac{b}{a}-\sigma-\frac{1}{aF(\Lambda_N,m_{RB})}\right]\alpha_c(\epsilon_0)\right]F(\Lambda_N,m_{RB}). \end{aligned} \tag{74}$$

If we set

$$\alpha_c(\epsilon_0)=-\left[\frac{b}{a}-\sigma-\frac{1}{aF(\Lambda_N,m_{RB})}\right]^{-1}\frac{2a^2}{m_F^2}A_*\ln\epsilon_0, \tag{75}$$

we can take $\epsilon_0\to 0^+$ limit while keeping A_*, B_* finite. These will be our renormalized equations,

$$B_*=aA_*\left(\frac{\Lambda_M^2}{2m_F^2}-2\right)F(\Lambda_M,m_F),\quad A_*=[2aB_*+bA_*]F(\Lambda_N,m_{BR}). \tag{76}$$

Incidentally we note that this physical prescription implies that the proper way we should define these integral equations is to use the Hadamard finite value (see the similar issue in Refs. 19 and 29 for a recent discussion of the renormalization and distribution theory).

Let us assume that we are looking for bound state solutions. The principal value integral in $F(\Lambda,m)$ then becomes an ordinary integral. Now we have two different expressions for the ratio B_*/A_*, which give us the desired eigenvalues when we require square integrable solutions. If we assume that both of the eigenvalues are bound states, we find

$$\left[\frac{\mu_{2Y}^2}{4\pi^2}\frac{\sqrt{\Lambda_M^2-4m_F^2}}{\Lambda_M}\arctan\left[\frac{\Lambda_M}{\sqrt{4m_F^2-\Lambda_M^2}}\right]+\frac{\Lambda_R^2}{8\pi}\right]\frac{2}{\Lambda_N\sqrt{4m_{BR}^2-\Lambda_N^2}}\arctan\left[\frac{\Lambda_N}{\sqrt{4m_{BR}^2-\Lambda_N^2}}\right]=-1. \tag{77}$$

Since the left-hand side is positive and the right one is negative this has no solution! *If we demand both boson–antiboson and fermion–antifermion pairs to form bound states, there is no solution.* Another possibility is to demand a resonance for the bosonic sector. Then

$$\left[\frac{\mu_{2Y}^2}{4\pi^2}\frac{\sqrt{\Lambda_M^2-4m_F^2}}{\Lambda_M}\arctan\left[\frac{\Lambda_M}{\sqrt{4m_F^2-\Lambda_M^2}}\right]+\frac{\Lambda_R^2}{8\pi}\right]\frac{2}{\Lambda_N\sqrt{\Lambda_N^2-4m_{BR}^2}}\ln\left|\frac{\Lambda_N+\sqrt{\Lambda_N^2-4m_{BR}^2}}{\Lambda_N-\sqrt{\Lambda_N^2-4m_{BR}^2}}\right|=1, \tag{78}$$

and this has solutions in general. The resonance case seems to be special to $1+1$ dimensions; the other possibility is to require bosons to have scattering states and fermions to be bound. This can

be studied by analyzing the pole structure of the analytic continuation of the scattering amplitudes that will be worked out below. Due to the algebraic complexity of the resulting formulas, we will not be able to answer it in this work.

We study the scattering states when we are beyond the two mass threshold. Let us make a digression for the moment and study a simpler problem, the lambda-phi-four coupling. It is easy to see from our equations for $N(u,v)$ that the same ansatz for the solution leads to

$$\Lambda^2\xi(x)=\frac{m^2}{x(1-x)}\xi(x)+\frac{\lambda_B^2}{8\pi}\frac{1}{\sqrt{x(1-x)}}\int_0^1\frac{\xi(y)}{\sqrt{y(1-y)}}. \tag{79}$$

We assume that the operator on the right is acting on $L^2([0,1])$, with vanishing at the end points boundary conditions. The free part,

$$H_0=\frac{m^2}{x(1-x)}, \tag{80}$$

is an unbounded operator with a continuous spectrum $[4m^2,\infty)$. This is easy to understand by studying a particle and an antiparticle in the center of momentum frame.

If the added term is not a ''too strong'' perturbation, then the absolutely continuous part of the spectrum of the full operator on the right is the same as the spectrum of the free part and we can study the scattering states using the free part. (There are various conditions we can state so that ''too strong'' becomes a precise statement, we recommend Ref. 30 for a thorough mathematical discussion of these issues, and Ref. 31 with more physical emphasis.) The kind of scattering problem we want to study is analyzed in a recent valuable book by Albeverio and Kurasov.[32] The interaction term is called a rank one perturbation. The Hamiltonian

$$H=\frac{m^2}{x(1-x)}+\frac{\lambda_B^2}{8\pi}\frac{1}{\sqrt{x(1-x)}}\int_0^1 dy\,\frac{1}{\sqrt{y(1-y)}}, \tag{81}$$

where everything acts on functions in $L^2([0,1])$, can be written as

$$H=H_0+\frac{\lambda_B^2}{8\pi}|f\rangle\langle f|, \tag{82}$$

with $\langle x|f\rangle=f(x)=1/\sqrt{x(1-x)}$. If such a perturbation is relatively form bounded, then the scattering states are given by the scattering states of the free part. To verify this condition it is enough to show that the added term satisfies

$$\|f\|_{-1}=\|(|H_0|+1)^{-1/2}f\|<\infty, \tag{83}$$

where $\|.\|$ denotes the usual L^2 norm. It is now simple to check that

$$\|f\|_{-1}^2<\int_0^1 dx\left(\frac{m^2}{x(1-x)}\right)^{-1}\left(\frac{1}{\sqrt{x(1-x)}}\right)^2<\infty. \tag{84}$$

In fact, in the above problem we can find the resolvent of our integral operator (see Ref. 32):

$$(R_H(Z)f)(x)=[(H-Z)^{-1}f](x)=\left(\frac{m^2}{x(1-x)}-Z\right)^{-1}f(x)$$
$$+\frac{\lambda_B^2}{8\pi}\tilde{A}(Z)\frac{\sqrt{x(1-x)}}{Zx(1-x)-m^2}\int_0^1\frac{\sqrt{y(1-y)}dyf(y)}{Zy(1-y)-m^2},$$

for Z outside of the spectrum (and complex in general), and here we use the analytic continuation of $\tilde{A}(\lambda)$ to complex numbers and its explicit form is given below. The knowledge of the resolvent gives everything about the operator; for example, we can find the spectral density function $\rho(\Lambda)$ (which heuristically corresponds to the density of states in the ''eigenfunction'' expansion) by using the well-known Stone's identity,

$$\rho(\Lambda)=\frac{1}{\pi i}\lim_{\epsilon_0\to 0^+}\left(\frac{1}{H-\Lambda+i\epsilon_0}-\frac{1}{H-\Lambda-i\epsilon_0}\right). \tag{85}$$

In Ref. 32 the scattering theory of finite rank perturbations has been worked out by using rigorous methods. We will only contend with the result that the scattering theory makes sense *beyond the bound state thresholds for both particles*, and we can find the resolvents explicitly. For simplicity of our presentation we study the scattering theory by the standard methods in physics, and only find the wave operators. One can see that for a given value of $\Lambda^2=m^2/\lambda(1-\lambda)$ we have two roots,

$$\lambda_{\pm}=\frac{1}{2}\pm\left[\frac{1}{4}-\frac{m^2}{\Lambda^2}\right]^{1/2}. \tag{86}$$

In physics we typically think of two particles approaching and then scattering off to infinity. An inspection of the kinematics of a particle and an antiparticle pair in the center of momentum frame reveals that λ_+ corresponds to the particle moving in the positive x^1 direction (which we may take as ''incoming'' states), and λ_- corresponds to the particle moving in the negative x^1 direction. From a physical point of view, the scattering data should give us the information about transmission and reflection of the pair. An equivalent description would be to find the wave operator, Ω, which maps (in general the projection to the absolutely continuous part of the spectrum of the original operator) the Hilbert space to the scattering states (if we take the absolutely continuous part of the spectrum and use the spectral projections corresponding to these values) of the interacting Hamiltonian:

$$\xi=\Omega f. \tag{87}$$

(In physics one typically uses Ω_+ which takes the wave functions at time zero and evolves them to positive infinity. This requires the $+i\epsilon$ prescriptions in the integrals, and we will see that for our problem it is more suitable to define the principal value one. This is why we use Ω.)

To find the scattering amplitudes we rewrite the eigenvalue equation in the Lippmann–Schwinger form,

$$\xi_\lambda(x)=\delta(x-\lambda)+\frac{\lambda_B^2}{8\pi}\left[\Lambda^2-\frac{m^2}{x(1-x)}\right]^{-1}\frac{1}{\sqrt{x(1-x)}}\int_0^1 dy\,\frac{\xi_\lambda(y)}{\sqrt{y(1-y)}}. \tag{88}$$

We formally use the eigenvalue $\delta_\lambda(x)=\delta(x-\lambda)$ of the free Hamiltonian. We can now solve for $A(\lambda)=\int_0^1[\xi_\lambda(y)/\sqrt{y(1-y)}]$,

$$A(\lambda)=\left[1+\frac{\lambda_B^2}{4\pi\Lambda\sqrt{(\Lambda^2-4m^2)}}\ln\left|\frac{\Lambda-\sqrt{\Lambda^2-4m^2}}{\Lambda+\sqrt{\Lambda^2-4m^2}}\right|\right]^{-1}\frac{1}{\sqrt{\lambda(1-\lambda)}}, \tag{89}$$

where $\Lambda^2=m^2/\lambda(1-\lambda)$. Thus the wave operator acting on the (formal) eigenfunctions of the free Hamiltonian can be written as

$$\xi_\lambda(x)=(\Omega\delta_\lambda)(x)=\int_0^1 dy\left(\delta(x-y)+\frac{\lambda_B^2}{8\pi}\mathcal{P}\left[\frac{m^2}{y(1-y)}-\frac{m^2}{x(1-x)}\right]^{-1}\frac{\tilde{A}(y)}{\sqrt{x(1-x)y(1-y)}}\right)\delta(y-\lambda),$$

with $\tilde{A}(\lambda)=\sqrt{\lambda(1-\lambda)}A(\lambda)$. The left side of the expression gives the distributional kernel of the wave operator. (If we are interested in an incoming pair, we could restrict ourselves to λ_+ values.) We can expand an arbitrary vector into a series of the form $f=\int_0^1 d\lambda f(\lambda)\delta_\lambda(x)$, and we find

$$\xi(x)=\left[\Omega\left(\int_0^1 f(\lambda)\delta_\lambda\right)\right](x)=\int_0^1 d\lambda\,\Omega(x,\lambda)f(\lambda), \tag{90}$$

and this makes sense in general. Note that this result is exact (within the linearized large-N_c limit) and we have a complete charaterization of the set of scattering states once $A(\lambda)$ is given.

We will study the scattering states of the coupled equations beyond the bound state tresholds, that is, when the energies are larger than both $2m_F$ and $2m_{BR}$. The preceeding discussion indicates that the free part and the interacting coupled equations may not have the same scattering states (recall the distributional solutions we present). We follow the same idea as in the above problem and restrict ourselves to the heuristic Lippmann–Schwinger type approach. One should be able to find the resolvent exactly and verify the formulas below by more careful analysis.

We solve for the scattering amplitude by using a renormalized Lipmann–Schwinger equation: thus we have for the scattering

$$\xi_M(x;\Lambda)=\delta(x-\lambda_M)+\mathcal{P}\frac{1}{\Lambda^2x(1-x)-m_F^2}(1-2x)aA_*(\Lambda),$$

$$\xi_N(x;\Lambda)=\delta(x-\lambda_N)+\mathcal{P}\frac{1}{\Lambda_N^2x(1-x)-m_{BR}^2}\sqrt{x(1-x)}(aB_*(\Lambda)+bA_*(\Lambda)),$$

where $A_*(\Lambda),B_*(\Lambda)$ satisfy

$$A_*(\Lambda)=\frac{1}{\sqrt{\lambda_N(1-\lambda_N)}}+(aB_*(\Lambda)+A_*(\Lambda))F(\Lambda,m_{BR}),$$

$$B_*(\Lambda)=\frac{1}{\lambda_M}-\frac{1}{1-\lambda_M}+aA_*(\Lambda)\left(\frac{\Lambda^2}{m_F^2}-4\right)F(\Lambda,m_F),$$

and $F(\Lambda,m)$ is the same function as before and we choose $\mathrm{Max}(4m_{BR}^2,4m_F^2)<\Lambda^2$, with $\Lambda^2=m_F^2/\lambda_M(1-\lambda_M)=m_{BR}^2/\lambda_N(1-\lambda_N)$. *We can use λ_M as the only parameter and call it simply λ.* If we solve for the scattering amplitudes,

$$\begin{aligned}A_*(\lambda)=&\left[1-\left(\frac{\lambda_R^2}{4\pi m_F^2}+\frac{\mu_{2Y}^2}{4\pi^2m_F^2}\sqrt{(1-4\lambda(1-\lambda))}\ln\left|\frac{1-\sqrt{1-4\lambda(1-\lambda)}}{1+\sqrt{1-4\lambda(1-\lambda)}}\right|\right)\right.\\&\left.\times\frac{\lambda(1-\lambda)}{\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}\ln\left|\frac{1-\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}{1+\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}\right|\right]^{-1}\left[\frac{m_F}{m_{BR}}\frac{1}{\sqrt{\lambda(1-\lambda)}}\right.\\&\left.-\frac{\mu_{2Y}}{4\pi m_F}\frac{1-2\lambda}{\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}\ln\left|\frac{1-\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}{1+\sqrt{1-4(m_{BR}^2/m_F^2)\lambda(1-\lambda)}}\right|\right].\end{aligned}$$

Note that this result is written in terms of dimensionless variables. We can read off $B_*(\lambda)$ as well,

$$B_*(\lambda)=\frac{1-2\lambda}{\lambda(1-\lambda)}-\frac{\mu_{2Y}}{2\pi m_F}\sqrt{1-4\lambda(1-\lambda)}\,\ln\left|\frac{1-\sqrt{1-4\lambda(1-\lambda)}}{1+\sqrt{1-4\lambda(1-\lambda)}}\right|A_*(\lambda). \tag{91}$$

The reader can check that the above results actually reduce to the phi-four theory results we have found if we set $\mu_{2Y}=0$.

For the sake of completeness we will also present the scattering solutions for $c_Q(x)$ variables. Below, we use the same shorthand symbols $A(\lambda)$ and $B_*(\lambda)$ as in the bound state equation for c_Q: The renormalized scattering equations become

$$c_Q(x;\lambda)=\delta(x-\lambda)-\mathcal{P}\frac{1}{\Lambda^2x^2-(\Lambda^2-m_{BR}^2+m_F^2)x+m_F^2}\sqrt{1-x}[(aA(\lambda)+bB_*(\lambda))x+bA(\lambda)]. \tag{92}$$

We should set

$$\Lambda^2=\frac{m_F^2}{\lambda}+\frac{m_{BR}^2}{1-\lambda}. \tag{93}$$

Not surprisingly, $m_F+m_{BR}\leqslant\Lambda<\infty$, and $A(\lambda),B_*(\lambda)$ found from their definitions. When we simplify the result it becomes

$$A(\lambda)=\left[1-\frac{4\kappa}{\Lambda^2}F_2+\left(F_2\frac{\mu_{1Y}^2}{64\Lambda^2}-\frac{\mu_{1Y}^2}{64\Lambda^2}(\Lambda^2-m_{RB}^2+m_F^2)F_1+\frac{\mu_{1Y}m_F\kappa}{\Lambda^2}F_1\right)\right.$$
$$\left.\times\left(1+\frac{\mu_{1Y}m_F}{4}F_1\right)^{-1}F_2\right]^{-1}\frac{1}{\sqrt{1-\lambda}}\left[1+\frac{1}{\lambda}\frac{\mu_{1Y}^2m_F^2}{32\Lambda^2}\left(1+\frac{\mu_{1Y}m_F}{4}F_1\right)^{-1}F_2\right]$$

$$B_*(\lambda)=\left(1+\frac{\mu_{1Y}m_F}{4}F_1\right)^{-1}\left[\frac{1}{\lambda\sqrt{1-\lambda}}+\left(8\kappa F_1-\frac{\mu_{1Y}}{8m_F}(\Lambda^2-m_{RB}^2+m_F^2)F_1+\frac{\mu_{1Y}}{8m_F}F_2\right)A(\lambda)\right],$$

where

$$F_2=\ln\left|\frac{m_{BR}^2}{m_F^2}\right|,\quad F_1=\frac{1}{u}\ln\left|\frac{\Lambda^2+m_{BR}^2-m_F^2+u}{\Lambda^2+m_{BR}^2-m_F^2-u}\right|. \tag{94}$$

Here $u=\sqrt{(\Lambda^2-(m_F-m_{BR})^2)(\Lambda^2-(m_F+m_{BR})^2)}$.

These define the wave operators of our model, as discussed in the simpler model of phi-four coupling. We see that the results are fairly complex expressions. One should study various approximate forms of these equations, and a numerical investigation of the poles of the amplitudes should give information about the bound states.

Our present approach has one more weakness, our results are nontrivial since the fermions have nonzero mass. The results are also sensitive to the sign of the Yukawa type couplings—we treated them as positive, but they are valid if we simply assume them to be negative. A physically more interesting case would be to study the massless fermions. If we set $m_F=0$, all the interesting information we have is lost, and we should go beyond the linear approximation. This observation suggests that it is necessary to study some kind of variational approach to understand the system better. We plan to investigate this in the future.

IV. GAUGED MODEL

We will assume in this part that the model is gauged by introducing SU(N_c) Lie algebra valued gauge potentials A_μ and refer for our conventions to Ref. 18. In the light-cone coordinates, and setting $A_-=0$, the action becomes

$$S_Y=\int dx^+dx^-\Big[-\frac{1}{2}\mathrm{Tr}F_{+-}F^{+-}+i\sqrt{2}\psi_L^{*\alpha}\partial_-\psi_{L\alpha}+i\sqrt{2}\psi_R^{*\alpha}(\partial_++igA_+)^\beta_\alpha\psi_{R\beta}-2\phi^{*\alpha}\partial_-\partial_+\phi_\alpha$$
$$+ig(\partial_-\phi^{*\alpha}A^\beta_{+\alpha}\phi_\beta-\phi^{*\alpha}A^\beta_{+\alpha}\partial_-\phi_\beta)-m_{B0}^2\phi^{*\alpha}\phi_\alpha-\frac{\lambda_{B0}^2}{4}(\phi^{*\alpha})^2-(\psi_L^{*\alpha}\psi_{R\beta}+\psi_R^{*\alpha}\psi_{L\beta})$$
$$\times(\mu_{1Y}\phi^{*\beta}\phi_\alpha+\mu_{2Y}\phi^{*\lambda}\phi_\lambda\delta^\alpha_\beta+m_F\delta^\beta_\alpha)\Big]. \tag{95}$$

The restriction to the color invariant states in the gauge theory is actually necessary to make the Hamiltonian finite. For this theory the large-N_c limit should be a better approximation. Furthermore, one expects baryons in this theory; the geometry of the large-N_c phase space should be useful to find a variational ansatz (see Ref. 19 for a nice discussion of these ideas). Following the same reduction process, the Hamiltonian becomes

$$H=H_0+H_Y+H_G, \tag{96}$$

where

$$H_0=\frac{1}{4}\left(m_F^2-\frac{g^2}{\pi}\right)\int\frac{[dp]}{p}M(p,p)+\frac{1}{4}\left(m_{BR}^2-\frac{g^2}{\pi}\right)\int\frac{[dp]}{|p|}N(p,p), \tag{97}$$

H_Y is as given in Eq. (15), and the gauge contribution is exactly given in Ref. 18,

$$H_G=-\frac{g^2}{16}\int[dpdqdsdt]\left(\frac{1}{(p-t)^2}+\frac{1}{(q-s)^2}\right)\delta[p+s-t-q]M(p,q)M(s,t)$$
$$+\frac{g^2}{64}\int[dpdqdsdt]\left(\frac{1}{(p-t)^2}+\frac{1}{(q-s)^2}\right)\delta[p+s-t-q]\frac{qt+ps+st+pq}{\sqrt{|pqst|}}N(p,q)N(s,t)$$
$$+\frac{g^2}{8}\int[dpdqdsdt]\frac{q+s}{(q-s)^2}\frac{\delta[p+s-t-q]}{\sqrt{|qs|}}Q(p,q)\overline{Q}(s,t).$$

Above we rescaled our coupling constants by a factor of N_c as before and $g^2N_c\mapsto g^2$. Let us use exactly the same substitutions as before for the basic variables we have, and simplify the resulting equations into

$$\Lambda_M^2\xi_M(x)=\left(m_F^2-\frac{g^2}{\pi}\right)\left(\frac{1}{x}+\frac{1}{1-x}\right)\xi_M(x)-\frac{g^2}{\pi}\int_0^1\frac{dy}{(y-x)^2}\xi_M(y)$$
$$-\frac{\mu_{2Y}m_F}{4\pi}\left[\frac{1}{x}-\frac{1}{1-x}\right]\int_0^1\frac{\xi_N(y)}{\sqrt{y(1-y)}}dy$$

and

$$\Lambda_N^2\xi_N(x)=\left(m_{RB}^2-\frac{g^2}{\pi}\right)\left(\frac{1}{x}+\frac{1}{1-x}\right)\xi_N(x)-\frac{g^2}{4\pi}\int_0^1\frac{dy}{(y-x)^2}\frac{(x+y)(2-x-y)}{\sqrt{x(1-x)y(1-y)}}\xi_N(y)$$
$$-\frac{\mu_{2Y}m_F}{4\pi\sqrt{(1-x)x}}\int_0^1dy\left(\frac{1}{y}-\frac{1}{1-y}\right)\xi_M(y)+\frac{\lambda_R^2}{8\pi}\int_0^1dy\frac{\xi_N(y)}{\sqrt{x(1-x)y(1-y)}}. \tag{98}$$

Again we see that the equations for ξ_M and ξ_N are coupled and they should be solved together:

$$\Lambda_Q^2 c_Q(x)=\left[\left(m_F^2-\frac{g^2}{\pi}\right)\frac{1}{x}+\left(m_{BR}^2-\frac{g^2}{\pi}\right)\frac{1}{1-x}\right]c_Q(x)-\frac{g^2}{2\pi}\int_0^1\frac{dy}{(y-x)^2}\frac{2-x-y}{\sqrt{(1-x)(1-y)}}c_Q(y)$$
$$-8\kappa\int_0^1\frac{dy}{\sqrt{(1-y)(1-x)}}c_Q(y)+\frac{1}{4}\mu_{1Y}m_F\int_0^1\frac{dy}{\sqrt{(1-y)(1-x)}}\left(\frac{1}{x}+\frac{1}{y}\right)c_Q(y). \quad (99)$$

These singular integral equations can perhaps be investigated numerically. The linear approximation could be a better one for the gauged model, since the effect of the gauge interaction is to bring a more singular operator. The nongauged models require renormalizations; it is possible that the above equations will behave better due to the singular operators in them. Another important application is to find a variational ansatz for the baryonic solutions and have a linear expansion around these solutions. We plan to study these issues in more depth in the future.

ACKNOWLEDGMENTS

First of all the author would like to thank S. G. Rajeev for various discussions about large-N limit field theories. We also would like to thank M. Arik, J. Gracia-Bondia, A. Konechny, E. Langmann, J. Mickelsson, T. Rador, and C. Saclioglu for discussions. The author's stay in Stockholm is made possible by the G. Gustafsson fellowship, and we are grateful to J. Mickelsson for this great experience. Our work is also partially supported by the Young Investigator Award of Turkish Academy of Sciences (TUBA-GEBIP).

APPENDIX: REDUCTION OF THE HAMILTONIAN

In this appendix we will give some of the details of the reduction of the Hamiltonian to the desired color invariant products. Let us recall that the Hamiltonian is given in Eq. (15). Let us start with the term

$$\frac{\sqrt{2}}{2}\mu_{1Y}^2\int dx^-\hat{\psi}^{\dagger\beta}\hat{\phi}_\beta\hat{\phi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\phi}_\alpha\hat{\phi}^{\dagger\lambda}\hat{\psi}_\lambda. \quad (A1)$$

When we write this in terms of the Fourier mode expansions, it becomes

$$-\frac{\mu_{1Y}^2}{8}\int\frac{[dkdldtdpdqds]}{\sqrt{|stkq|}}\frac{\delta[k-l+t-s+q-p]}{t-k+l}\chi^{\dagger\alpha}(p)a_\alpha(q):a^{\dagger\beta}(s)a_\beta(t):a^{\dagger\lambda}(k)\chi_\lambda(l)$$
$$-\frac{\mu_{1Y}^2N_c}{16}\int\frac{[dkdldqds]}{\sqrt{|qk|}}\chi^{\dagger\alpha}(p)a_\alpha(q)a^{\dagger\lambda}(k)\chi_\lambda(l)\delta[k-l+q-s]\left(\int[ds]\frac{\mathrm{sgn}(s)-1}{s(k-l-s)}\right).$$

Notice that the divergent integral is isolated and a principal value regularization calculation shows that

$$\mathcal{P}\int[ds]\frac{\mathrm{sgn}(s)-1}{s(k-l-s)}=\frac{1}{\pi(k-l)}\ln\left|\frac{k-l}{\epsilon_R}\right|, \quad (A2)$$

where ϵ_R is an infrared cut-off. If we are only allowed to introduce local counter terms *in the original action*, we should introduce a momentum scale μ_R so that we can separate the momentum dependent part and purely divergent part of these type expressions (this point is somewhat difficult to decide for this particular term since it is not possible to write such a term in the original action):

$$\mathcal{P}\int[ds]\frac{\mathrm{sgn}(s)-1}{s(k-l-s)}=\frac{1}{\pi(k-l)}\ln\left|\frac{k-l}{\epsilon_R}\right|=\frac{1}{\pi(k-l)}\left(\ln\left|\frac{k-l}{\mu_R}\right|+\ln\left|\frac{\mu_R}{\epsilon_R}\right|\right). \quad (A3)$$

If we remove the divergent part by a counter term of the form

$$\left(\frac{\mu_{1Y}^2 N_c}{16\pi}\ln\left|\frac{\mu_R}{\epsilon_R}\right|+8\kappa_R(\mu_R)\right)\int\frac{[dpdqdkdl]}{\sqrt{qk}}\frac{1}{k-l}\delta[p-q+k-l]\chi^{\dagger\alpha}(p)a_\alpha(q)a^{\dagger\beta}(k)\chi_\beta(l), \tag{A4}$$

the finite term comes out to be

$$\int\frac{[dkdldqds]}{\sqrt{|lq|}}\left[8\kappa_R(\mu_R)-\frac{\mu_{1Y}^2}{8\pi}\ln\left|\frac{k-l}{\mu_R}\right|\right]\frac{1}{q-s}\chi^{\dagger\alpha}(k)a_\alpha(l)a^{\dagger\beta}(q)\chi_\beta(s)\delta[k-l+q-s]. \tag{A5}$$

If we require the theory not to have a dependence on the arbitrary scale we introduced, it is natural to demand that the residual coupling vary under a change of scale according to

$$\kappa_R(\mu_R)=\kappa_R(\tilde{\mu}_R)-\frac{\mu_{1Y}^2}{64\pi}\ln\left|\frac{\mu_R}{\tilde{\mu}_R}\right|. \tag{A6}$$

The reader may be alarmed by the nonlocal expression in the interaction, but if we actually go back to the position space, the inverse Fourier transform gives a term, up to some constants,

$$\int dxdy(a\,\mathrm{sgn}(x-y)-\ln|\mu_R(x-y)|\mathrm{sgn}(x-y))\hat{\psi}^{\dagger\alpha}(x)\hat{\phi}_\alpha(y)\hat{\phi}^{\dagger\beta}(y)\hat{\psi}_\beta(x), \tag{A7}$$

which has a logarithmic correction to the sign function. [This behaves worse for the short distance than the coulomb potential $|x-y|$, but we should interpret $\mathrm{sgn}(x-y)=0$ if $x=y$, so there is no real singularity at the short distance.] In the text we will only consider the cases where these nonlocal terms are dropped, or removed by taking them as part of the counter terms in the action. From a more conventional point of view we should only add local terms in the original action. We plan to study the more general case as a perturbation of the simplified models. (Notice that this is the interaction one finds if we use a parity broken model as in Ref. 18. The sign of the remaining interaction term is not determined. Since it is not in the original action, it should be left as an arbitrary parameter.)

As another example we will discuss the term

$$\frac{\sqrt{2}}{2}m_F\mu_{2Y}\int dx^-\hat{\psi}^{\dagger\alpha}\frac{1}{i\partial_-}\hat{\psi}_\alpha:\hat{\phi}^\sigma\hat{\phi}_\sigma:, \tag{A8}$$

a Fourier expansion and removing the vacuum expectation value gives us a term

$$-\frac{\mu_{2Y}m_F}{4}\int\frac{[dpdqdsdt]}{\sqrt{|st|}}\frac{\delta[p-q+s-t]}{s-t-q}:\chi^{\dagger\alpha}(p)\chi_\alpha(q)::a^{\dagger\beta}(s)a_\beta(t):$$
$$+\frac{\mu_{2Y}N_cm_F}{8}\int\frac{[ds]}{|s|}:a^{\dagger\beta}(s)a_\beta(s):\int[dp]\frac{1-\mathrm{sgn}(p)}{p},$$

and

$$\mathcal{P}\int[dp]\frac{1-\mathrm{sgn}(p)}{p}=-2\ln\left|\frac{\Lambda_R}{\epsilon_R}\right|, \tag{A9}$$

where we have ϵ_R and Λ_R as the infrared and ultraviolet cut-offs, respectively. If we introduce a boson mass counter-term of the form

$$\frac{\mu_{2Y} N_c m_F}{4} \ln\left|\frac{\Lambda_R}{\epsilon_R}\right| \int \frac{[ds]}{|s|} :a^{\dagger\beta}(s) a_\beta(s):, \tag{A10}$$

this divergence will be cancelled.

The other terms are also done in the same way, and the rest is to collect all of them to find the Hamiltonian in terms of large-N_c bilinears.

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Magnetoencephalography in ellipsoidal geometry

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(Received 20 June 2002; accepted 20 June 2002)

An exact analytic solution for the forward problem in the theory of biomagnetics of the human brain is known only for the (1D) case of a sphere and the (2D) case of a spheroid, where the excitation field is due to an electric dipole within the corresponding homogeneous conductor. In the present work the corresponding problem for the more realistic ellipsoidal brain model is solved and the leading quadrupole approximation for the exterior magnetic field is obtained in a form that exhibits the anisotropic character of the ellipsoidal geometry. The results are obtained in a straightforward manner through the evaluation of the interior electric potential and a subsequent calculation of the surface integral over the ellipsoid, using Lamé functions and ellipsoidal harmonics. The basic formulas are expressed in terms of the standard elliptic integrals that enter the expressions for the exterior Lamé functions. The laborious task of reducing the results to the spherical geometry is also included. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1522135]

I. INTRODUCTION

Biomagnetics is by now a well-established interdisciplinary field extending from mathematics to electrical engineering, computer sciences, physics, and of course medicine. References 1, 3, 14, 19, 22 provide an excellent exposure of the different models, methods, and techniques in biomagnetics available today.

The actual size of the human organs such as the brain, the heart, or the lungs[14,19] justifies the use of the quasistatic approximation of the Maxwell system,[17] where the time derivative of the induction field in Faraday's law and the time derivative of the displacement field in the Biot–Savart–Maxwell's law are considered to be negligible. As it is well known,[1,14,19] a chemically stimulated electric source gives rise to an electric current within the conductive tissues, which in turn generates a weak magnetic field in the surroundings of the organ. The direct biomagnetic problem consists of the evaluation of the magnetic field caused by a given current distribution. The inverse biomagnetic problem then seeks the current distribution which generates a given (through measurements) magnetic field. When the human organ under investigation is the brain, then we refer to the above problems as the direct MEG (MagnetoEncephaloGraphy) and the inverse MEG problem.[14,19]

The inverse MEG problem is not uniquely solvable in the sense that an exteriously measured magnetic field does not specify uniquely the current that generates it. Fokas, Gelfand, and Kurylev[9] have specified the extent of nonuniqueness for the case of a spherical brain model, which includes an arbitrary current density function.

The basic mathematics governing the MEG problem were developed by Geselowitz[10,11] in the late 60's, while the complete solution for spherical geometry was given by Ilmoniemi, Hämäläinen, and Knuutila[16] as well as by Sarvas.[23] For related results in the case of spheroidal volume conductors we refer to Refs. 4 and 8. A systematic analysis of the dipole singularity in the Geselowitz formula reveals that, as far as the magnetic field is concerned, one third of the contribution from the volume current is canceled by one third of the contribution from the primary source current.[7] Sarvas' solution for the sphere is based on the radial component of the primary dipole field, and it is calculated via the use of a magnetic potential representing the irrotational

magnetic field in the space exterior to the brain. For some closely related work we refer to Refs. 4, 8, 12, 13, 18, 20, 21.

The actual geometry of the human brain is that of an ellipsoid with semiaxes equal to 6, 6.5, and 9 cm.[24] In contrast to the complete isotropy that is represented by the sphere, the triaxial ellipsoid embodies the complete anisotropy of the three-dimensional space. As a consequence, the much more complicated theory of ellipsoidal harmonics, as opposed to the theory of spherical harmonics, is necessary to solve the direct MEG problem for a realistic brain model. This program is realized in the work at hand. The analysis is based on Lamé functions and ellipsoidal harmonics. In fact, only harmonics of degree less than or equal to 2 are needed to obtain the quadrupole term for the magnetic field. Besides the purely ellipsoidal expressions, the results are also given in the more tractable form where Cartesian coordinates are used for the interior harmonics plus the standard elliptic integrals that appear in the exterior Lamé products. The particular way these elliptic integrals are interconnected is provided in Appendix D.

Section II states the mathematical theory of the MEG problem. The solution of the interior boundary value problem that offers the electric potential within an ellipsoid due to an electric dipole is obtained in Sec. III, while Sec. IV involves the evaluation of the magnetic induction field in the exterior of the ellipsoid. The exact analytic form of the quadrupole term is given explicitly, while as it is expected, the dipole term vanishes. As it is well known,[5,6,15] the reduction of general results from the ellipsoidal to the spherical geometry is not a straightforward task because of the complicated indeterminacies that occur as the three semifocal distances of the ellipsoidal system approach zero. The only way to deal with these indeterminacies is to group appropriately the terms of the solution and to perform the algebraic manipulations that eliminate the indeterminacies before the limiting process is applied. In some cases this procedure is not much easier than the generation of the ellipsoidal solution itself. Section V is dedicated to this task and the corresponding result for the spherical case is recovered. The necessary material from the theory of ellipsoidal harmonics as well as some useful formulas associated with ellipsoidal functions are collected in the Appendices.

II. STATEMENT OF THE PROBLEM

In order to avoid technical complications and additional terminology, we will restrict attention to the single component model, which is actually what we need in the present work.

Let S denotes the triaxial ellipsoid

$$\frac{x_1^2}{\alpha_1^2}+\frac{x_2^2}{\alpha_2^2}+\frac{x_3^2}{\alpha_3^2}=1, \tag{1}$$

where $0<\alpha_3<\alpha_2<\alpha_1<+\infty$ are its semiaxes. The basic ellipsoid (1) specifies an ellipsoidal system[15] with coordinates $(\rho,\ \mu,\ \nu)$ which springs out of the focal ellipse

$$\frac{x_1^2}{h_2^2}+\frac{x_2^2}{h_1^2}=1, \tag{2}$$

with semifocal distance

$$h_3=\sqrt{h_2^2-h_1^2}, \tag{3}$$

where

$$\left.\begin{aligned} h_1&=\sqrt{\alpha_2^2-\alpha_3^2}\\ h_2&=\sqrt{\alpha_1^2-\alpha_3^2}\\ h_3&=\sqrt{\alpha_1^2-\alpha_2^2}\end{aligned}\right\} \tag{4}$$

are the semifocal distances of the principal ellipses of (1). The ellipsoidal coordinates (ρ, μ, ν), given in Appendix A, involve the ellipsoidal variable $\rho \in [h_2, +\infty)$ and the hyperboloidal variables $\mu \in [h_3, h_2]$ and $\nu \in [-h_3, h_3]$. The coordinate ρ plays the role of the radial variable r, while μ and ν correspond to the angular variable θ and φ in spherical coordinates. In particular, the value $\rho = h_2$ specifies the focal ellipse (2), the value $\rho = \alpha_1$ specifies the basic ellipsoid (1), and as $\rho \to +\infty$, the corresponding ellipsoid approaches a sphere of infinite radius. In what follows the $\rho = \alpha_1$ ellipsoid, given by (1), will represent the boundary of the ellipsoid representing the brain. Then, the brain fills the interior space $\rho \in [h_2, \alpha_1)$ while the exterior space is described by $\rho \in (\alpha_1, +\infty)$.

Having described the geometrical background, we turn now to the physics of our problem. Since the dielectric constant of the brain tissue is by five orders of magnitude higher than the dielectric constant of vacuum and its electric conductivity is approximately $0.3\ \Omega^{-1}\,\mathrm{m}^{-1}$,[14,19] a simple arithmetic shows that the physical realm of bioelectromagnetics is that of the quasistatic approximation of Maxwell's equations.[17] Hence, the set of governing equations, in the absence of electric charge, is taken to be

$$\nabla \times \mathbf{E} = \mathbf{0}, \tag{5}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}, \tag{6}$$

$$\nabla \cdot \mathbf{E} = 0, \tag{7}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{8}$$

where $\mathbf{E}$ is the electric field, $\mathbf{B}$ is the magnetic induction field, μ_0 is the magnetic permeability, which is assumed to be the same inside as well as outside the brain, while the expression

$$\mathbf{J} = \mathbf{J}^P + \sigma \mathbf{E}, \tag{9}$$

specifies the current density, with $\mathbf{J}^P$ the primarily imposed equivalent current and σ the conductivity of the brain tissue. The conductivity outside the brain is considered to be zero.

Since $\mathbf{E}$ is irrotational, there exist an electric potential u such that

$$\mathbf{E}(\mathbf{r}) = -\nabla u(\mathbf{r}). \tag{10}$$

In particular, we denote the electric potential in the interior of the ellipsoid $\rho = \alpha_1$ by u^- and in the exterior of $\rho = \alpha_1$ by u^+.

Equation (6) implies that $\mathbf{J}$ is solenoidal, and consequently (9) and (10) force the electric potential to solve Poisson's equation

$$\Delta u^-(\mathbf{r}) = \frac{1}{\sigma} \nabla \cdot \mathbf{J}^P(\mathbf{r}), \tag{11}$$

in the space V^- interior to the ellipsoid $\rho = \alpha_1$ and the Laplace's equation

$$\Delta u^+(\mathbf{r}) = 0, \tag{12}$$

in the space V^+ exterior to the ellipsoid $\rho = \alpha_1$.

It is easily shown[10,11,23] that in an unbounded, electrically homogeneous space with compactly supported primary current, the scalar field σu and the vector field $\mu_0^{-1}\mathbf{B}$ are the scalar and the vector invariants, respectively, of the dyadic field

$$\tilde{\mathbf{D}}(\mathbf{r}) = \frac{1}{4\pi} \int_\Omega \mathbf{J}^p(\mathbf{r}') \otimes \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3}\, dv(\mathbf{r}'), \tag{13}$$

where Ω denotes the support of $\mathbf{J}^p$.

Indeed, the electric field is given by

$$u(\mathbf{r})=\frac{1}{4\pi\sigma}\int_{\Omega}\mathbf{J}^p(\mathbf{r}')\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}d\upsilon(\mathbf{r}'), \tag{14}$$

while the magnetic field is given by

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\int_{\Omega}\mathbf{J}^p(\mathbf{r}')\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}d\upsilon(\mathbf{r}'). \tag{15}$$

In general, for a single component model the electric potential solves the following transmission problem:

$$\Delta u^-(\mathbf{r})=\frac{1}{\sigma}\nabla\cdot\mathbf{J}^p(\mathbf{r}),\qquad \mathbf{r}\in V^- \tag{16}$$

$$\Delta u^+(\mathbf{r})=0,\qquad \mathbf{r}\in V^+ \tag{17}$$

$$u^-(\mathbf{r})=u^+(\mathbf{r}),\qquad \mathbf{r}\in S \tag{18}$$

$$\sigma^-\frac{\partial u^-(\mathbf{r})}{\partial n}=\sigma^+\frac{\partial u^+(\mathbf{r})}{\partial n},\quad \mathbf{r}\in S \tag{19}$$

$$u^+(\mathbf{r})=O\left(\frac{1}{r}\right),\qquad r\to\infty \tag{20}$$

where the "$-$" and the "$+$" characterize the interior region V^- and the exterior region V^+, respectively. In the case of $\sigma^-=\sigma$, $\sigma^+=0$, as it is assumed in MEG, the above transmission problem splits into the interior Neumann problem

$$\Delta u^-(\mathbf{r})=\frac{1}{\sigma}\nabla\cdot\mathbf{J}^p(\mathbf{r}),\qquad \mathbf{r}\in V^- \tag{21}$$

$$\frac{\partial u^-(\mathbf{r})}{\partial n}=0,\qquad \mathbf{r}\in S \tag{22}$$

which can be solved independently, and the exterior Dirichlet problem

$$\Delta u^+(\mathbf{r})=0,\qquad \mathbf{r}\in V^+ \tag{23}$$

$$u^+(\mathbf{r})=u^-(\mathbf{r}),\qquad \mathbf{r}\in S \tag{24}$$

$$u^+(\mathbf{r})=O\left(\frac{1}{r}\right),\qquad r\to\infty \tag{25}$$

which is postulated via the trace of u^- on S.

Note that the interior problem (21), (22) involves an inhomogeneous equation with a homogeneous boundary condition, while the exterior problem (23)–(25) involves a homogeneous equation with an inhomogeneous boundary condition. In physical terms, the primary current $\mathbf{J}^p$ generates an electric field in V^- and the value of this field on S establishes the electric field in V^+. The asymptotic order of u^+ at infinity is dictated by (14).

The plan now is as follows: solve (21), (22) and then calculate the magnetic field from the integral form of the Biot–Savart–Maxwell law

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\int_{V^-}[\mathbf{J}^p(\mathbf{r}')-\sigma\nabla u^-(\mathbf{r}')]\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}dv(\mathbf{r}'). \tag{26}$$

Following magnetoencephalographic practice[1,14,19,23] we represent the actual localized electromagnetic activity of the brain tissue by an equivalent electric dipole current, at a fixed point $\mathbf{r}_0$, with a dipole moment equal to $\mathbf{Q}$. In other words, the primary current is given by

$$\mathbf{J}^P(\mathbf{r})=\mathbf{Q}\delta(\mathbf{r}-\mathbf{r}_0), \tag{27}$$

where δ stands for the Dirac measure at $\mathbf{r}_0$.

Introducing (27) in (14) and (15), it is obvious that this point current (27) furnishes the electric field

$$u_0(\mathbf{r})=\frac{1}{4\pi\sigma}\mathbf{Q}\cdot\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}, \tag{28}$$

and the magnetic field

$$\mathbf{B}_0(\mathbf{r})=\frac{\mu_0}{4\pi}\mathbf{Q}\times\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}. \tag{29}$$

Furthermore, in view of (27), Eq. (26) implies

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\mathbf{Q}\times\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}-\frac{\mu_0\sigma}{4\pi}\int_{V^-}\nabla u^-(\mathbf{r}')\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}dv(\mathbf{r}'). \tag{30}$$

The volume integral in (30) can be transformed to a surface integral,[2,7,11] providing the formula

$$\int_{V^-}\nabla u^-(\mathbf{r}')\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}dv(\mathbf{r}')=\int_S u^-(\mathbf{r}')\hat{\mathbf{n}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}ds(\mathbf{r}'), \tag{31}$$

where $\mathbf{r}\in\mathbb{R}^3-S$ and $\hat{\mathbf{n}}$ stands for the outward unit normal on S at $\mathbf{r}'$. Formula (31) shows that the volume distribution of dipoles, with moments proportional to ∇u^-, can be replaced by a surface distribution of dipoles, with moments proportional to $u^-\hat{\mathbf{n}}'$. Its proof demands a careful treatment of the singularity at $\mathbf{r}_0$.[7]

In terms of the transformation (31), the magnetic field (30) is expressed as

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\mathbf{Q}\times\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}-\frac{\mu_0\sigma}{4\pi}\int_S u^-(\mathbf{r}')\hat{\mathbf{n}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}ds(\mathbf{r}'). \tag{32}$$

The following section provides the evaluation of the interior electric field u^- when S is the ellipsoid (1).

III. THE INTERIOR ELECTRIC POTENTIAL

The goal of this section is to solve the interior problem (21), (22) where $\mathbf{J}^p$ is given by (27). Straightforward arguments conclude that the solution u^- assumes the form

$$u^-(\mathbf{r})=\Phi(\mathbf{r})+\frac{1}{4\pi\sigma}\mathbf{Q}\cdot\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}=\Phi(\mathbf{r})+\frac{1}{4\pi\sigma}\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\frac{1}{|\mathbf{r}-\mathbf{r}_0|}, \tag{33}$$

where Φ is an interior harmonic function inside the ellipsoid $h_2\leqslant\rho<\alpha_1$ which satisfies the Neumann boundary condition

$$\frac{\partial}{\partial\rho}\Phi(\mathbf{r})=-\frac{1}{4\pi\sigma}\frac{\partial}{\partial\rho}\mathbf{Q}\cdot\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}, \tag{34}$$

on the ellipsoid $\rho=\alpha_1$.

The completeness of the ellipsoidal harmonics[15] secures the existence of a sequence $\{b_n^m\}$, $n=0,1,2,...$, and $m=1,2,...,2n+1$ such that

$$\Phi(\mathbf{r})=\sum_{n=0}^{\infty}\sum_{m=1}^{2n+1}b_n^m\mathbb{E}_n^m(\rho,\mu,\nu), \tag{35}$$

for $\rho\in[h_2,\alpha_1)$, where $\mathbb{E}_n^m(\rho,\mu,\nu)$ denotes the interior solid ellipsoidal harmonic of degree n and order m (see Appendix B). The vector $\mathbf{r}$ is always assumed to be represented by the ellipsoidal triplet (ρ,μ,ν). In order to be able to use the orthogonality properties of the ellipsoidal eigenfunctions we need to express the particular solution of (21), which is the singular part of (33), in terms of surface ellipsoidal harmonics. To this end, we use the ellipsoidal expansion of the fundamental solution for the Laplace's operator[6] in the form

$$\frac{1}{|\mathbf{r}-\mathbf{r}_0|}=\sum_{n=0}^{\infty}\sum_{m=1}^{2n+1}\frac{4\pi}{2n+1}\frac{1}{\gamma_n^m}\mathbb{E}_n^m(\rho_0,\mu_0,\nu_0)\mathbb{F}_n^m(\rho,\mu,\nu), \tag{36}$$

where (ρ_0,μ_0,ν_0) represents the position $\mathbf{r}_0$ of the dipole expressed in ellipsoidal coordinates, $\mathbb{F}_n^m$ are the exterior solid ellipsoidal harmonics (see Appendix B) and γ_n^m are the ellipsoidal normalization constants given by

$$\gamma_n^m=\int_{\rho=\alpha_1}[E_n^m(\mu)E_n^m(\nu)]^2\frac{1}{\sqrt{\alpha_1^2-\mu^2}\sqrt{\alpha_1^2-\nu^2}}ds. \tag{37}$$

Actually, the constant γ_n^m is the square of the L^2 norm of the surface ellipsoidal harmonic $E_n^m(\mu)E_n^m(\nu)$ with respect to the weighting function

$$l(\mu,\nu)=[(\alpha_1^2-\mu^2)(\alpha_1^2-\nu^2)]^{-1/2}, \tag{38}$$

which depends on the ellipsoidal surface $\rho=\alpha_1$.

Expansion (36) holds for $\rho>\rho_0$ and provides the appropriate form for the application of the boundary condition (34). In view of (33), (35), and (36), the field u^- is written as

$$u^-(\rho,\mu,\nu)=\sum_{n=0}^{\infty}\sum_{m=1}^{2n+1}\left[b_n^m\mathbb{E}_n^m(\rho,\mu,\nu)+\frac{1}{\sigma(2n+1)\gamma_n^m}(\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0))\mathbb{F}_n^m(\rho,\mu,\nu)\right]. \tag{39}$$

Using the form of $\mathbb{F}_n^m$, as it is given by (B6) as well as the fact the $\mathbb{E}_0^1(\rho,\mu,\nu)=1$, Eq. (39) is written as

$$u^-(\rho,\mu,\nu)=b_0^1+\sum_{n=1}^{\infty}\sum_{m=1}^{2n+1}\left[b_n^m+\frac{1}{\sigma\gamma_n^m}(\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0))I_n^m(\rho)\right]\mathbb{E}_n^m(\rho,\mu,\nu), \tag{40}$$

where $I_n^m(\rho)$ is given by (B4).

Applying the boundary condition (34) to (39) and using the orthogonality properties of the surface ellipsoidal harmonics[15] we are led to

$$b_n^m=\frac{1}{\sigma\gamma_n^m}(\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0))\left[\frac{1}{\alpha_2\alpha_3E_n^m(\alpha_1)E_n^{m\prime}(\alpha_1)}-I_n^m(\alpha_1)\right], \tag{41}$$

for each $n=0,1,2,...$ and $m=1,2,...,2n+1$, where E_n^m denote the Lamé functions of the first kind (see Appendix B) and the prime denotes differentiation with respect to the argument.

Using expression (41) for the coefficients the electric potential within the ellipsoid, $\rho=\alpha_1$ is then written as

$$u^-(\mathbf{r})=b_0^1+\frac{1}{4\pi\sigma}\mathbf{Q}\cdot\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}-\sum_{n=1}^{\infty}\sum_{m=1}^{2n+1}\frac{1}{(2n+1)\sigma\gamma_n^m}(\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0))\frac{F_n^{m\prime}(\alpha_1)}{E_n^{m\prime}(\alpha_1)}\mathbb{E}_n^m(\mathbf{r}), \tag{42}$$

where F_n^m are the Lamé functions of the second kind (see Appendix B).

We observe that u^- is uniquely specified up to the additive constant b_0^1, a fact that is compatible with the wellposedness of the Neumann problem (21), (22).

In order to express the interior electric field u^- in a more tractable and useful form we use formulas (B16)–(B27) and restrict consideration to the leading two terms in the multipole ellipsoidal expansion of (42). Along these lines we introduce the following notation where the single wiggle on the top denotes a dyadic and the double wiggle on the top denotes a tetradic[2]

$$\tilde{\mathbf{M}}(\rho)=\sum_{m=1}^{3}(\rho^2-\alpha_1^2+\alpha_m^2)\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m, \tag{43}$$

$$\tilde{\mathbf{\Lambda}}=\sum_{m=1}^{3}\frac{\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m}{\Lambda-\alpha_m^2}, \tag{44}$$

$$\tilde{\mathbf{\Lambda}}'=\sum_{m=1}^{3}\frac{\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m}{\Lambda'-\alpha_m^2}, \tag{45}$$

$$\tilde{\mathbf{H}}_1(\rho)=\sum_{m=1}^{3}I_1^m(\rho)\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m, \tag{46}$$

$$\tilde{\tilde{\mathbf{H}}}_2(\rho)=\sum_{\substack{i,j=1\\ i\neq j}}^{3}I_2^{i+j}(\rho)\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j, \tag{47}$$

$$\tilde{\mathbf{N}}_1=\sum_{m=1}^{3}\frac{\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m}{\alpha_1^2+\alpha_2^2+\alpha_3^2-\alpha_m^2}, \tag{48}$$

$$\tilde{\tilde{\mathbf{N}}}_2=\sum_{\substack{i,j=1\\ i\neq j}}^{3}\frac{\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j}{\alpha_i^2+\alpha_j^2}, \tag{49}$$

where the constants Λ, Λ' are given by (B14) and the elliptic integrals that appear in (46)–(47) are given by (B4). The unit vectors $\hat{\mathbf{x}}_i$, $i=1,2,3$ stand for the Cartesian basis. The characteristic of the quantities (43)–(49) is that they are all modifications of the identity dyadic or the identity tetradic. If the (anisotropic) ellipsoid is replaced by the (isotropic) sphere all quantities (43)–(49) are reduced to multiples of the identity, while as they stand they incorporate the particular standards of each principal direction of the ellipsoid.

Furthermore, we define the dyadic functions

$$\tilde{\mathbf{A}}(\rho)=\frac{3}{4\pi\sigma}(\tilde{\mathbf{H}}_1(\rho)-\tilde{\mathbf{H}}_1(\alpha_1))+\frac{1}{\sigma V}\tilde{\mathbf{I}}, \tag{50}$$

$$\tilde{\mathbf{B}}(\mathbf{r})=-\frac{5}{4\pi\sigma(\Lambda-\Lambda')}\left[\left(I_2^1(\rho)-I_2^1(\alpha_1)+\frac{2\pi}{3V\Lambda}\right)\tilde{\mathbf{\Lambda}}\mathbb{E}_2^1(\mathbf{r})\right.$$
$$\left.-\left(I_2^2(\rho)-I_2^2(\alpha_1)+\frac{2\pi}{3V\Lambda'}\right)\tilde{\mathbf{\Lambda}}'\mathbb{E}_2^2(\mathbf{r})\right], \tag{51}$$

where V denotes the volume of the ellipsoid ($3V=4\pi\alpha_1\alpha_2\alpha_3$) and the tetradic function

$$\tilde{\tilde{\mathbf{\Gamma}}}(\rho)=\frac{15}{4\pi\sigma}(\tilde{\tilde{\mathbf{H}}}_2(\rho)-\tilde{\tilde{\mathbf{H}}}_2(\alpha_1))+\frac{5}{\sigma V}\tilde{\tilde{\mathbf{N}}}_2, \tag{52}$$

in terms of which the interior electric field within the shell $\rho_0<\rho<\alpha_1$ assumes the compact form

$$u^-(\mathbf{r})=b_0^1+\mathbf{Q}\cdot\tilde{\mathbf{A}}(\rho)\cdot\mathbf{r}+\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\mathbf{B}}(\mathbf{r})+\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\tilde{\mathbf{\Gamma}}}(\rho):\mathbf{r}\otimes\mathbf{r}+O(el_3), \tag{53}$$

where the notation $O(el_3)$ denotes terms in the multipole expansion that are of order greater or equal to 3 (octapole or higher terms) and the double contraction is defined as

$$\mathbf{a}\otimes\mathbf{b}:\mathbf{c}\otimes\mathbf{d}=(\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}). \tag{54}$$

In obtaining expression (53) for u^-, we have also used the multipole expansion

$$\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}=3\tilde{\mathbf{H}}_1(\rho)\cdot\mathbf{r}-\frac{5}{\Lambda-\Lambda'}\mathbf{r}_0\cdot[\tilde{\mathbf{\Lambda}}\mathbb{E}_2^1(\mathbf{r})I_2^1(\rho)$$
$$-\tilde{\mathbf{\Lambda}}'\mathbb{E}_2^2(\mathbf{r})I_2^2(\rho)]+15\mathbf{r}_0\cdot\tilde{\tilde{\mathbf{H}}}_2(\rho):\mathbf{r}\otimes\mathbf{r}+O(el_3). \tag{55}$$

Expressions (53) and (55) combine both the Cartesian coordinates of $\mathbf{r}$ and the elliptic integrals $I_n^m(\rho)$ that depend on the ellipsoidal variable ρ. This combination leads to the most compact way of expressing (53) and (55), and at the same time it minimizes the indeterminacies as the ellipsoid reduces to the sphere.

An equivalent expression for u^- which avoids the polyadic notation is furnished by

$$u^-(\rho,\mu,\nu)=b_0^1+\frac{3}{4\pi\sigma}\sum_{m=1}^{3}Q_m x_m\left[I_1^m(\rho)-I_1^m(\alpha_1)+\frac{1}{\alpha_1\alpha_2\alpha_3}\right]$$
$$-\frac{5}{4\pi\sigma(\Lambda-\Lambda')}\sum_{m=1}^{3}Q_m x_{0m}\left[\left(I_2^1(\rho)-I_2^1(\alpha_1)+\frac{1}{2\alpha_1\alpha_2\alpha_3\Lambda}\right)\frac{\mathbb{E}_2^1(\mathbf{r})}{(\Lambda-\alpha_m^2)}\right.$$
$$\left.-\left(I_2^2(\rho)-I_2^2(\alpha_1)+\frac{1}{2\alpha_1\alpha_2\alpha_3\Lambda'}\right)\frac{\mathbb{E}_2^2(\mathbf{r})}{(\Lambda'-\alpha_m^2)}\right]$$
$$+\frac{15}{4\pi\sigma}\sum_{\substack{i,j=1\\ i\neq j}}^{3}Q_i x_{0j}x_i x_j\left(I_2^{i+j}(\rho)-I_2^{i+j}(\alpha_1)+\frac{1}{\alpha_1\alpha_2\alpha_3(\alpha_i^2+\alpha_j^2)}\right)+O(el_3). \tag{56}$$

IV. THE EXTERIOR MAGNETIC FIELD

The magnetic induction field $\mathbf{B}$ is obtained from (32) after we insert the values of u^- on the surface $\rho=\alpha_1$ and perform the indicated integration. Our plan is to focus on the dipole and the quadrupole terms, which provide the leading two approximations of u^-. To this end, we rewrite the integral in (32) in such a way as to be able to use orthogonality of the surface ellipsoidal harmonics.

First, we observe that

$$\frac{1}{|\mathbf{r}-\mathbf{r}_0|}=\frac{4\pi}{\gamma_0^1}I_0^1(\rho)+\frac{4\pi}{3}\sum_{m=1}^{3}\frac{1}{\gamma_1^m}\mathbb{E}_1^m(\mathbf{r}_0)\mathbb{F}_1^m(\mathbf{r})+\frac{4\pi}{5}\sum_{m=1}^{5}\frac{1}{\gamma_2^m}\mathbb{E}_2^m(\mathbf{r}_0)\mathbb{F}_2^m(\mathbf{r})+O(el_3). \quad (57)$$

Taking the gradient of (57) and using (B17)–(B27), we obtain the following key formula in our work:

$$\begin{aligned}\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}=&\frac{3}{h_1h_2h_3}\sum_{m=1}^{3}h_mI_1^m(\rho)\hat{\mathbf{x}}_m\mathbb{E}_1^m(\mathbf{r})-\frac{5}{(\Lambda-\Lambda')h_1h_2h_3}\sum_{m=1}^{3}\frac{h_m}{\Lambda-\alpha_m^2}\mathbb{E}_1^m(\mathbf{r}_0)\hat{\mathbf{x}}_m\mathbb{E}_2^1(\mathbf{r})I_2^1(\rho)\\&+\frac{5}{(\Lambda-\Lambda')h_1h_2h_3}\sum_{m=1}^{3}\frac{h_m}{\Lambda'-\alpha_m^2}\mathbb{E}_1^m(\mathbf{r}_0)\hat{\mathbf{x}}_m\mathbb{E}_2^2(\mathbf{r})I_2^2(\rho)\\&+\frac{15}{h_1h_2h_3^3}\left[\frac{1}{h_1}\mathbb{E}_1^2(\mathbf{r}_0)\hat{\mathbf{x}}_1+\frac{1}{h_2}\mathbb{E}_1^1(\mathbf{r}_0)\hat{\mathbf{x}}_2\right]\mathbb{E}_2^3(\mathbf{r})I_2^3(\rho)\\&+\frac{15}{h_1h_2^3h_3}\left[\frac{1}{h_1}\mathbb{E}_1^3(\mathbf{r}_0)\hat{\mathbf{x}}_1+\frac{1}{h_3}\mathbb{E}_1^1(\mathbf{r}_0)\hat{\mathbf{x}}_3\right]\mathbb{E}_2^4(\mathbf{r})I_2^4(\rho)\\&+\frac{15}{h_1^3h_2h_3}\left[\frac{1}{h_2}\mathbb{E}_1^3(\mathbf{r}_0)\hat{\mathbf{x}}_2+\frac{1}{h_3}\mathbb{E}_1^2(\mathbf{r}_0)\hat{\mathbf{x}}_3\right]\mathbb{E}_2^5(\mathbf{r})I_2^5(\rho)+O(el_3). \quad (58)\end{aligned}$$

Obviously, expansion (58) is valid for $\rho>\rho_0$ and it can be used in (32) and in (42) to obtain the three dipole terms and the five quadrupole terms for the multipole expansion of the primary dipole field at $\mathbf{r}_0$, as well as for the induced dipole fields at the surface points $\mathbf{r}'$.

In order to be able to evaluate the surface integral in (32) we need to express the interior electric potential $u^-(\mathbf{r}')$, the outward unit normal $\hat{\boldsymbol{\rho}}'$, and the basic dipole field $|\mathbf{r}-\mathbf{r}'|^{-3}(\mathbf{r}-\mathbf{r}')$ in terms of surface ellipsoidal harmonics in the variable of integration $\mathbf{r}'$ on the surface $\rho=\alpha_1$. This is a long and tedious task which is developed in the following steps. First, we expand the interior electric field (53) to obtain

$$u^-(\alpha_1,\mu',\nu')=b_0^1+\sum_{m=1}^{3}\zeta_mE_1^m(\mu')E_1^m(\nu')+\sum_{m=1}^{5}\theta_mE_2^m(\mu')E_2^m(\nu')+O(el_3'), \quad (59)$$

where

$$\zeta_m=\frac{\alpha_mh_m}{\sigma Vh_1h_2h_3}(\mathbf{Q}\cdot\hat{\mathbf{x}}_m),\quad m=1,2,3 \quad (60)$$

and

$$\theta_1=-\frac{5}{6\sigma V(\Lambda-\Lambda')}(\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\boldsymbol{\Lambda}}), \quad (61)$$

$$\theta_2=\frac{5}{6\sigma V(\Lambda-\Lambda')}(\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\boldsymbol{\Lambda}}'), \quad (62)$$

$$\theta_3=\frac{5\alpha_1\alpha_2\alpha_3}{\sigma Vh_1h_2h_3}\frac{\mathbf{Q}\otimes\mathbf{r}_0:(\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_2+\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_1)}{\alpha_3h_3(\alpha_1^2+\alpha_2^2)}, \quad (63)$$

$$\theta_4=\frac{5\alpha_1\alpha_2\alpha_3}{\sigma Vh_1h_2h_3}\frac{\mathbf{Q}\otimes\mathbf{r}_0:(\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_3+\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_1)}{\alpha_2h_2(\alpha_1^2+\alpha_3^2)}, \quad (64)$$

$$\theta_5=\frac{5\alpha_1\alpha_2\alpha_3}{\sigma V h_1 h_2 h_3}\,\frac{\mathbf{Q}\otimes\mathbf{r}_0:(\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_3+\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_2)}{\alpha_1 h_1(\alpha_2^2+\alpha_3^2)}. \tag{65}$$

The outward unit normal is written as[5]

$$\hat{\boldsymbol{\rho}}'=\alpha_1\alpha_2\alpha_3 l(\mu',\nu')\tilde{\mathbf{M}}^{-1}(\alpha_1)\cdot\mathbf{r}', \tag{66}$$

and if the basic dipole field is expanded for $\rho>\rho'$ it provides the form

$$\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}=3\mathbf{r}\cdot\tilde{\mathbf{H}}_1(\rho)+\tilde{\mathbf{F}}(\mathbf{r})\cdot\mathbf{r}'+O(el_2'), \tag{67}$$

where

$$\tilde{\mathbf{F}}(\mathbf{r})=-\frac{\mathbb{F}_2^1(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\boldsymbol{\Lambda}}+\frac{\mathbb{F}_2^2(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\boldsymbol{\Lambda}}'+15\mathbf{r}\otimes\mathbf{r}:\tilde{\tilde{\mathbf{H}}}_2(\rho). \tag{68}$$

Then, we calculate the expression

$$\begin{aligned}\hat{\boldsymbol{\rho}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}&=\alpha_1\alpha_2\alpha_3 l(\mu',\nu')[3\mathbf{r}'\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{H}}_1(\rho)\cdot\mathbf{r}+\mathbf{r}'\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\mathbf{r}']+O(el_3')\\&=\alpha_1\alpha_2\alpha_3 l(\mu',\nu')\Bigg[3\sum_{m=1}^{3}(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{H}}_1(\rho)\cdot\mathbf{r})x_m'\\&\quad+\sum_{i,j=1}^{3}(\hat{\mathbf{x}}_i\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_j)x_i'x_j'\Bigg]+O(el_3').\end{aligned} \tag{69}$$

Expression (69) contains the variable of integration $\mathbf{r}'$ of (32) in Cartesian form. Since we want to use orthogonality properties over the ellipsoid $\rho'=\alpha_1$, we need to transform (69) to ellipsoidal coordinates. To end we use formulas (C7)–(C9) and perform some extensive algebraic manipulations that lead to the expression

$$\begin{aligned}\hat{\boldsymbol{\rho}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\Bigg|_{\rho'=\alpha_1}&=\alpha_1\alpha_2\alpha_3 l(\mu',\nu')\Bigg\{\frac{1}{3}\sum_{m=1}^{3}\alpha_m^2(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_m)\\&\quad+\frac{3}{h_1h_2h_3}\sum_{m=1}^{3}\alpha_m h_m(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{H}}_1(\rho)\cdot\mathbf{r})E_1^m(\mu')E_1^m(\nu')\\&\quad-\frac{1}{3(\Lambda-\Lambda')}\sum_{m=1}^{3}\frac{\alpha_m^2}{\Lambda-\alpha_m^2}(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_m)E_2^1(\mu')E_2^1(\nu')\\&\quad+\frac{1}{3(\Lambda-\Lambda')}\sum_{m=1}^{3}\frac{\alpha_m^2}{\Lambda'-\alpha_m^2}(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_m)E_2^2(\mu')E_2^2(\nu')\\&\quad+\frac{1}{h_1h_2h_3}\sum_{\substack{i,j=1\\i\neq j}}^{3}\frac{\alpha_i\alpha_j}{h_{6-(i+j)}}(\hat{\mathbf{x}}_i\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_j)E_2^{i+j}(\mu')E_2^{i+j}(\nu')\Bigg\}\\&\quad+O(el_3').\end{aligned} \tag{70}$$

At this stage we observe that the monopole term in (70) vanishes. Indeed, from (43)–(45), (47), and (68) we observe that

$$\sum_{m=1}^{3}\alpha_m^2(\hat{\mathbf{x}}_m\cdot\tilde{\mathbf{M}}^{-1}(\alpha_1)\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_m)$$

$$=\sum_{m=1}^{3}\hat{\mathbf{x}}_m\times\tilde{\mathbf{F}}(\mathbf{r})\cdot\hat{\mathbf{x}}_m$$

$$=-\frac{\mathbb{F}_2^1(\mathbf{r})}{\Lambda-\Lambda'}\sum_{m=1}^{3}\frac{\hat{\mathbf{x}}_m\times\hat{\mathbf{x}}_m}{\Lambda-\alpha_m^2}+\frac{\mathbb{F}_2^2(\mathbf{r})}{\Lambda-\Lambda'}\sum_{m=1}^{3}\frac{\hat{\mathbf{x}}_m\times\hat{\mathbf{x}}_m}{\Lambda'-\alpha_m^2}+15\sum_{m=1}^{3}\hat{\mathbf{x}}_m\times(\mathbf{r}\otimes\mathbf{r}:\tilde{\tilde{\mathbf{H}}}_2(\rho))\cdot\hat{\mathbf{x}}_m$$

$$=15\sum_{\substack{i,j=1\\ i\neq j}}^{3}x_ix_jI_2^{i+j}(\rho)\hat{\mathbf{x}}_j\times\hat{\mathbf{x}}_i=\mathbf{0}. \tag{71}$$

Then (70) is written as

$$\hat{\boldsymbol{\rho}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\bigg|_{\rho'=\alpha_1}=l(\mu',\nu')\left[\sum_{m=1}^{3}\boldsymbol{\beta}_mE_1^m(\mu')E_1^m(\nu')+\sum_{m=1}^{5}\boldsymbol{\delta}_mE_2^m(\mu')E_2^m(\nu')\right]+O(el_3'), \tag{72}$$

where

$$\boldsymbol{\beta}_m=3\frac{\alpha_1\alpha_2\alpha_3}{h_1h_2h_3}\frac{h_m}{\alpha_m}\hat{\mathbf{x}}_m\otimes\mathbf{r}\dot{\times}\tilde{\mathbf{H}}_1(\rho),\qquad m=1,2,3 \tag{73}$$

$$\boldsymbol{\delta}_1=-\frac{\alpha_1\alpha_2\alpha_3}{3(\Lambda-\Lambda')}\tilde{\boldsymbol{\Lambda}}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r}), \tag{74}$$

$$\boldsymbol{\delta}_2=\frac{\alpha_1\alpha_2\alpha_3}{3(\Lambda-\Lambda')}\tilde{\boldsymbol{\Lambda}}'\dot{\times}\tilde{\mathbf{F}}(\mathbf{r}), \tag{75}$$

$$\boldsymbol{\delta}_3=\frac{\alpha_1\alpha_2\alpha_3}{h_1h_2h_3^2}\left[\frac{\alpha_2}{\alpha_1}\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_2+\frac{\alpha_1}{\alpha_2}\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_1\right]\dot{\times}\tilde{\mathbf{F}}(\mathbf{r}), \tag{76}$$

$$\boldsymbol{\delta}_4=\frac{\alpha_1\alpha_2\alpha_3}{h_1h_2^2h_3}\left[\frac{\alpha_3}{\alpha_1}\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_3+\frac{\alpha_1}{\alpha_3}\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_1\right]\dot{\times}\tilde{\mathbf{F}}(\mathbf{r}), \tag{77}$$

$$\boldsymbol{\delta}_5=\frac{\alpha_1\alpha_2\alpha_3}{h_1^2h_2h_3}\left[\frac{\alpha_3}{\alpha_2}\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_3+\frac{\alpha_2}{\alpha_3}\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_2\right]\dot{\times}\tilde{\mathbf{F}}(\mathbf{r}), \tag{78}$$

and the cross-dot product is defined as

$$(\mathbf{a}\otimes\mathbf{b})\dot{\times}(\mathbf{c}\otimes\mathbf{d})=(\mathbf{a}\times\mathbf{c})(\mathbf{b}\cdot\mathbf{d}). \tag{79}$$

Finally, the surface integral in (32) can be evaluated after (37), (59), (72), and (B8) are appropriately used to conclude

$$\int_s u^-(\mathbf{r}')\hat{\boldsymbol{\rho}}'\times\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}ds(\mathbf{r}')=\sum_{m=1}^{3}\zeta_m\boldsymbol{\beta}_m\gamma_1^m+\sum_{m=1}^{5}\theta_m\boldsymbol{\delta}_m\gamma_2^m+O(el_3), \tag{80}$$

where the constants γ_n^m are given by (B17)–(B20).

Next, we analyze the dipole terms in (80), which in view of (60), (73), and (B17) provide

$$\sum_{m=1}^{3}\zeta_m\boldsymbol{\beta}_m\gamma_1^m=\frac{3}{\sigma}\sum_{m=1}^{3}(\mathbf{Q}\cdot\hat{\mathbf{x}}_m)\hat{\mathbf{x}}_m\otimes\mathbf{r}\dot{\times}\tilde{\mathbf{H}}_1(\rho)=\frac{3}{\sigma}\mathbf{Q}\otimes\mathbf{r}\dot{\times}\tilde{\mathbf{H}}_1(\rho). \tag{81}$$

If we substitute the dipole contribution (81) into (32) and use expansion (55), we immediately see that the dipole contribution to the exterior magnetic field vanishes, a conclusion that is compatible with the theory of magnetostatics.[7,17]

In the sequel we investigate further the form of the leading (quadrupole) contribution to the exterior magnetic field as it is given by (32) and (80). Indeed, formulas (55)–(65), (68), (74)–(78), (80), and (B18)–(B20) yield

$$\begin{aligned}\mathbf{B}(\mathbf{r})=&\frac{\mu_0}{4\pi}\mathbf{Q}\otimes\mathbf{r}_0\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})+\frac{\mu_0}{12\pi}\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{\Lambda-\Lambda'}\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\mathbf{\Lambda}}\otimes\tilde{\mathbf{\Lambda}}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})\\&-\frac{\mu_0}{12\pi}\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{\Lambda-\Lambda'}\mathbf{Q}\otimes\mathbf{r}_0:\tilde{\mathbf{\Lambda}}'\otimes\tilde{\mathbf{\Lambda}}'\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})\\&-\frac{\mu_0}{4\pi}\mathbf{Q}\otimes\mathbf{r}_0:\frac{(\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_2+\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_1)\otimes(\alpha_2^2\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_2+\alpha_1^2\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_1)}{\alpha_1^2+\alpha_2^2}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})\\&-\frac{\mu_0}{4\pi}\mathbf{Q}\otimes\mathbf{r}_0:\frac{(\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_3+\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_1)\otimes(\alpha_3^2\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_3+\alpha_1^2\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_1)}{\alpha_1^2+\alpha_3^2}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})\\&-\frac{\mu_0}{4\pi}\mathbf{Q}\otimes\mathbf{r}_0:\frac{(\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_3+\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_2)\otimes(\alpha_3^2\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_3+\alpha_2^2\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_2)}{\alpha_2^2+\alpha_3^2}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})+O(el_3).\end{aligned} \tag{82}$$

By means of the scalar identities

$$\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{(\Lambda-\alpha_i^2)^2}=(\Lambda-\alpha_i^2)-\sum_{m=1}^{3}(\Lambda-\alpha_m^2),\quad i=1,2,3 \tag{83}$$

and

$$\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{(\Lambda'-\alpha_i^2)^2}=(\Lambda'-\alpha_i^2)-\sum_{m=1}^{3}(\Lambda'-\alpha_m^2),\quad i=1,2,3 \tag{84}$$

we can easily prove the tetradic formula

$$\begin{aligned}&\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{3(\Lambda-\Lambda')}\tilde{\mathbf{\Lambda}}\otimes\tilde{\mathbf{\Lambda}}-\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{3(\Lambda-\Lambda')}\tilde{\mathbf{\Lambda}}'\otimes\tilde{\mathbf{\Lambda}}'\\&=\frac{1}{3}\tilde{\mathbf{I}}\otimes\tilde{\mathbf{I}}-\sum_{i=1}^{3}\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_i.\end{aligned} \tag{85}$$

Furthermore, the identities

$$\begin{aligned}&\frac{(\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i)\otimes(\alpha_j^2\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\alpha_i^2\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i)}{\alpha_i^2+\alpha_j^2}\\&=\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i+\frac{(\alpha_i^2\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j-\alpha_j^2\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i)\otimes(\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i-\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j)}{\alpha_i^2+\alpha_j^2},\quad i\neq j\end{aligned} \tag{86}$$

and

$$\hat{\mathbf{x}}_1\times\tilde{\mathbf{I}}=\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_2-\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_3, \tag{87}$$

$$\hat{\mathbf{x}}_2\times\tilde{\mathbf{I}}=\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_3-\hat{\mathbf{x}}_3\otimes\hat{\mathbf{x}}_1, \tag{88}$$

$$\hat{\mathbf{x}}_3\times\tilde{\mathbf{I}}=\hat{\mathbf{x}}_2\otimes\hat{\mathbf{x}}_1-\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_2, \tag{89}$$

can be used to reduce (82) to

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{12\pi}(\mathbf{Q}\cdot\mathbf{r}_0)\hat{\mathbf{I}}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})-\frac{\mu_0}{4\pi}(\mathbf{d}\times\tilde{\mathbf{I}})\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})+O(el_3), \tag{90}$$

where

$$\mathbf{d}=(\mathbf{Q}\cdot\tilde{\mathbf{M}}(\alpha_1)\times\mathbf{r}_0)\cdot\tilde{\mathbf{N}}_1. \tag{91}$$

Some further algebra reveals that

$$\tilde{\mathbf{I}}\dot{\times}\tilde{\mathbf{\Lambda}}=\tilde{\mathbf{I}}\dot{\times}\tilde{\mathbf{\Lambda}}'=\mathbf{0}, \tag{92}$$

and

$$\tilde{\mathbf{I}}\dot{\times}(\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i)=\mathbf{0} \tag{93}$$

for every pair i, j with $i\neq j$ which in view of (68) implies that

$$\tilde{\mathbf{I}}\dot{\times}\tilde{\mathbf{F}}(\mathbf{r})=\mathbf{0}. \tag{94}$$

Finally, relation (B15) confirms that

$$(\mathbf{d}\times\tilde{\mathbf{I}})\dot{\times}\tilde{\mathbf{\Lambda}}=\mathbf{d}\cdot\tilde{\mathbf{\Lambda}}, \tag{95}$$

$$(\mathbf{d}\times\tilde{\mathbf{I}})\dot{\times}\tilde{\mathbf{\Lambda}}'=\mathbf{d}\cdot\tilde{\mathbf{\Lambda}}', \tag{96}$$

and since for $i\neq j$

$$(\mathbf{d}\times\tilde{\mathbf{I}})\dot{\times}(\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i)=\mathbf{d}\cdot(\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+\hat{\mathbf{x}}_j\otimes\hat{\mathbf{x}}_i), \tag{97}$$

we arrive at the expression

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\mathbf{d}\cdot\left[\frac{\mathbb{F}_2^1(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\mathbf{\Lambda}}-\frac{\mathbb{F}_2^2(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\mathbf{\Lambda}}'-\frac{3}{h_1^2h_2^2h_3^2}\sum_{\substack{i,j=1\\ i\neq j}}^{3}h_ih_j\mathbb{F}_2^{i+j}(\mathbf{r})\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j\right]+O(el_3), \tag{98}$$

which provides the quadrupole approximation of the magnetic field exterior to the ellipsoid (1). Note that **B** is a harmonic function, a property that follows from the fact that **B** is both irrotational and solenoidal in the exterior to the ellipsoid space.

The vector

$$\mathbf{Q}\cdot\tilde{\mathbf{M}}(\alpha_1)=\sum_{i=1}^{3}\alpha_i^2Q_i\hat{\mathbf{x}}_i, \tag{99}$$

represents the dipole moment as it is modified by the spatial effects of the anisotropy imposed by the ellipsoid. It actually incorporates the effects of the geometry on the physics of the problem.

Relations (C3)–(C5) can be invoked to rewrite (98) in Cartesian form as follows:

$$\mathbf{B}(\mathbf{r})=\frac{5\mu_0}{4\pi}\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{\Lambda-\Lambda'}(\mathbf{d}\cdot\tilde{\mathbf{\Lambda}})(\tilde{\mathbf{\Lambda}}:\mathbf{r}\otimes\mathbf{r}+1)I_2^1(\rho)$$
$$-\frac{5\mu_0}{4\pi}\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{\Lambda-\Lambda'}(\mathbf{d}\cdot\tilde{\mathbf{\Lambda}}')(\tilde{\mathbf{\Lambda}}':\mathbf{r}\otimes\mathbf{r}+1)I_2^2(\rho)$$
$$-\frac{15\mu_0}{4\pi}\mathbf{d}\cdot\sum_{\substack{i,j=1\\ i\neq j}}^{3}x_ix_jI_2^{i+j}(\rho)\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j+O(el_3), \tag{100}$$

where the elliptic integrals $I_n^m(\rho)$ are given by (B4) and

$$\frac{3}{h_1^2h_2^2h_3^2}\sum_{\substack{i,j=1\\ i\neq j}}^{3}h_ih_j\mathbb{F}_2^{i+j}(\mathbf{r})\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j=15\sum_{\substack{i,j=1\\ i\neq j}}^{3}x_ix_jI_2^{i+j}(\rho)\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j=15\tilde{\tilde{\mathbf{H}}}_2(\rho):\mathbf{r}\otimes\mathbf{r}. \tag{101}$$

As in the case of the electric potential, we also provide an expression of the magnetic field which avoids the use of polyadics. Indeed, if

$$\mathbf{d}=\frac{\alpha_2^2Q_2x_{03}-\alpha_3^2Q_3x_{02}}{\alpha_2^2+\alpha_3^2}\hat{\mathbf{x}}_1+\frac{\alpha_3^2Q_3x_{01}-\alpha_1^2Q_1x_{03}}{\alpha_1^2+\alpha_3^2}\hat{\mathbf{x}}_2+\frac{\alpha_1^2Q_1x_{02}-\alpha_2^2Q_2x_{01}}{\alpha_1^2+\alpha_2^2}\hat{\mathbf{x}}_3, \tag{102}$$

then

$$\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}\frac{\mathbb{F}_2^1(\rho,\mu,\nu)}{\Lambda-\Lambda'}\sum_{i=1}^{3}\frac{d_i}{\Lambda-\alpha_i^2}\hat{\mathbf{x}}_i-\frac{\mu_0}{4\pi}\frac{\mathbb{F}_2^2(\rho,\mu,\nu)}{\Lambda-\Lambda'}\sum_{i=1}^{3}\frac{d_i}{\Lambda'-\alpha_i^2}\hat{\mathbf{x}}_i$$
$$-\frac{15\mu_0}{4\pi}\sum_{\substack{i,j=1\\ i\neq j}}^{3}d_ix_ix_jI_2^{i+j}(\rho)\hat{\mathbf{x}}_j+O\left(\frac{1}{\rho^4}\right). \tag{103}$$

V. REDUCTION TO THE SPHERE

The magnetic field outside a spherical conductor[23] is given by

$$\mathbf{B}_s(\mathbf{r})=\frac{\mu_0}{4\pi}\mathbf{Q}\times\mathbf{r}_0\cdot[\tilde{\mathbf{I}}+\mathbf{r}\otimes\nabla]\frac{1}{F(\mathbf{r})}, \tag{104}$$

where

$$F(\mathbf{r})=r|\mathbf{r}-\mathbf{r}_0|^2+\mathbf{r}\cdot(\mathbf{r}-\mathbf{r}_0)|\mathbf{r}-\mathbf{r}_0|. \tag{105}$$

In the interest of obtaining the quadrupole term of (104) we have to expand asymptotically (104) and calculate the leading terms of this expansion. This program furnishes

$$\frac{1}{F(\mathbf{r})}=\frac{1}{2r^3}+\frac{\mathbf{r}_0\cdot\hat{\mathbf{r}}}{r^4}+O\left(\frac{1}{r^5}\right), \tag{106}$$

$$\nabla\frac{1}{F(\mathbf{r})}=-\frac{3\hat{\mathbf{r}}}{2r^4}+\frac{\mathbf{r}_0}{r^5}\cdot(\tilde{\mathbf{I}}-5\hat{\mathbf{r}}\otimes\hat{\mathbf{r}})+O\left(\frac{1}{r^6}\right), \tag{107}$$

and finally

$$\mathbf{B}_s(\mathbf{r})=\frac{\mu_0}{8\pi}\mathbf{Q}\times\mathbf{r}_0\cdot\frac{\tilde{\mathbf{I}}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{r^3}+\frac{\mu_0}{4\pi}\mathbf{Q}\times\mathbf{r}_0\cdot\frac{\tilde{\mathbf{I}}\otimes\hat{\mathbf{r}}+\hat{\mathbf{r}}\otimes\tilde{\mathbf{I}}-5\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{r^4}\cdot\mathbf{r}_0+O\left(\frac{1}{r^5}\right). \tag{108}$$

We turn now to our ellipsoidal result (98) or (100) and we consider the limit as

$$(\alpha_1,\alpha_2,\alpha_3)\underset{e\to s}{\to}(\alpha,\alpha,\alpha), \tag{109}$$

where $e\to s$ indicates the limit as the ellipsoid becomes a sphere of radius α.

It is easily shown that

$$\lim_{e\to s}\Lambda=\lim_{e\to s}\Lambda'=\alpha^2, \tag{110}$$

$$\lim_{e\to s}h_i=0,\quad i=1,2,3 \tag{111}$$

$$\lim_{e\to s}\mu=\lim_{e\to s}\nu=0, \tag{112}$$

and

$$\lim_{e\to s}\rho=r, \tag{113}$$

where r denotes the spherical radial variable.

Furthermore

$$\lim_{e\to s}I_2^m(\rho)=\frac{1}{5r^5},\quad m=1,2,3,4,5. \tag{114}$$

The last term on the right-hand side of (100) is continuous in the spherical limit, and it provides the limit

$$\lim_{e\to s}\sum_{\substack{i,j=1\\ i\neq j}}^{3}x_ix_jI_2^{i+j}(\rho)\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j=\frac{1}{5r^5}\sum_{\substack{i,j=1\\ i\neq j}}^{3}x_ix_j\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_j=\frac{\mathbf{r}\otimes\mathbf{r}}{5r^5}-\frac{1}{5r^5}\sum_{i=1}^{3}x_i^2\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_i\,. \tag{115}$$

On the other hand, the corresponding limit of the first two terms on the right-hand side of (100) exhibit an indeterminant behavior and they need to be handled in the following special way.

Long but straightforward calculations are needed to prove the identities

$$\frac{\mathbb{E}_2^1(\rho,\mu,\nu)}{(\Lambda-\Lambda')(\Lambda-\alpha_m^2)}-\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{(\Lambda-\Lambda')(\Lambda'-\alpha_m^2)}=r^2-3x_m^2+\alpha_m^2-\frac{\alpha_1^2+\alpha_2^2+\alpha_3^2}{3}, \tag{116}$$

and

$$\frac{I_2^1(\rho)-I_2^2(\rho)}{\Lambda-\Lambda'}=\frac{3}{2}I_3^7(\rho)-\frac{1}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)}, \tag{117}$$

where

$$I_3^7(\rho)=\int_\rho^{+\infty}\frac{dt}{t^2(t^2-h_2^2)^{3/2}(t^2-h_3^2)^{3/2}}. \tag{118}$$

Then (116) and (117) are used to show that

$$\frac{\mathbb{E}_2^1(\rho,\mu,\nu)I_2^1(\rho)}{(\Lambda-\Lambda')(\Lambda-\alpha_m^2)}-\frac{\mathbb{E}_2^2(\rho,\mu,\nu)I_2^2(\rho)}{(\Lambda-\Lambda')(\Lambda'-\alpha_m^2)}$$
$$=\left(r^2-3x_m^2+\alpha_m^2-\frac{\alpha_1^2+\alpha_2^2+\alpha_3^2}{3}\right)I_2^1(\rho)$$
$$+\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{\Lambda'-\alpha_m^2}\left[\frac{3}{2}I_2^7(\rho)-\frac{1}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)}\right]. \tag{119}$$

Furthermore

$$\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{\Lambda'-\alpha_1^2}=(\Lambda'-\alpha_2^2)(x_3^2-x_1^2)+(\Lambda'-\alpha_3^2)(x_2^2-x_1^2)+(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2), \tag{120}$$

$$\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{\Lambda'-\alpha_2^2}=(\Lambda'-\alpha_1^2)(x_3^2-x_2^2)+(\Lambda'-\alpha_3^2)(x_1^2-x_2^2)+(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_3^2), \tag{121}$$

$$\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{\Lambda'-\alpha_3^2}=(\Lambda'-\alpha_1^2)(x_2^2-x_3^2)+(\Lambda'-\alpha_2^2)(x_1^2-x_3^2)+(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2), \tag{122}$$

which imply that

$$\lim_{e\to s}\frac{\mathbb{E}_2^2(\rho,\mu,\nu)}{\Lambda'-\alpha_m^2}=0,\quad m=1,2,3. \tag{123}$$

Consequently

$$\lim_{e\to s}\left[\frac{\mathbb{E}_2^1(\rho,\mu,\nu)I_2^1(\rho)}{(\Lambda-\Lambda')(\Lambda-\alpha_m^2)}-\frac{\mathbb{E}_2^2(\rho,\mu,\nu)I_2^2(\rho)}{(\Lambda-\Lambda')(\Lambda'-\alpha_m^2)}\right]=\frac{r^2-3x_m^2}{5r^5}, \tag{124}$$

and

$$\lim_{e\to s}\left[\frac{\mathbb{F}_2^1(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\mathbf{\Lambda}}-\frac{\mathbb{F}_2^2(\mathbf{r})}{\Lambda-\Lambda'}\tilde{\mathbf{\Lambda}}'\right]=5\sum_{m=1}^{3}\frac{r^2-3x_m^2}{5r^5}\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m=\frac{\tilde{\mathbf{I}}}{r^3}-\frac{3}{r^5}\sum_{m=1}^{3}x_m^2\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m\,. \tag{125}$$

By virtue of the reduction formulas (115) and (125), expression (98) provides the limit

$$\lim_{e\to s}\mathbf{B}(\mathbf{r})=\frac{\mu_0}{4\pi}(\lim_{e\to s}\mathbf{d})\cdot\left[\frac{\tilde{\mathbf{I}}}{r^3}-\frac{3}{r^5}\sum_{m=1}^{3}x_m^2\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m\right]-\frac{\mu_0}{4\pi}(\lim_{e\to s}\mathbf{d})\cdot\left[3\frac{\mathbf{r}\otimes\mathbf{r}}{r^5}-\frac{3}{r^5}\sum_{m=1}^{3}x_m^2\hat{\mathbf{x}}_m\otimes\hat{\mathbf{x}}_m\right]$$
$$=\frac{\mu_0}{8\pi}\mathbf{Q}\times\mathbf{r}_0\cdot\frac{\tilde{\mathbf{I}}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{r^3}+O\left(\frac{1}{r^4}\right)=\mathbf{B}_s(\mathbf{r}), \tag{126}$$

where $\mathbf{B}_s$ is the sphere solution given by (108).

APPENDIX A: THE ELLIPSOIDAL SYSTEM

The ellipsoidal coordinates (ρ,μ,ν) are connected to the Cartesian coordinates (x_1,x_2,x_3) via the expressions

$$x_1=\frac{\rho\mu\nu}{h_2h_3}, \tag{A1}$$

$$x_2=\frac{\sqrt{\rho^2-h_3^2}\sqrt{\mu^2-h_3^2}\sqrt{h_3^2-\nu^2}}{h_1h_3}, \tag{A2}$$

$$x_3=\frac{\sqrt{\rho^2-h_2^2}\sqrt{h_2^2-\mu^2}\sqrt{h_2^2-\nu^2}}{h_1h_2}, \tag{A3}$$

where the variable $\rho\in[h_2,+\infty)$ specifies the ellipsoid

$$\frac{x_1^2}{\rho^2}+\frac{x_2^2}{\rho^2-h_3^2}+\frac{x_3^2}{\rho^2-h_2^2}=1, \tag{A4}$$

the variable $\mu\in[h_3,h_2]$ specifies the hyperboloid of one sheet

$$\frac{x_1^2}{\mu^2}+\frac{x_2^2}{\mu^2-h_3^2}-\frac{x_3^2}{h_2^2-\mu^2}=1, \tag{A5}$$

and the variable $\nu\in[-h_3,h_3]$ specifies the hyperboloid of two sheets

$$\frac{x_1^2}{\nu^2}-\frac{x_2^2}{h_3^2-\nu^2}-\frac{x_3^2}{h_2^2-\nu^2}=1. \tag{A6}$$

The three families of second-degree surfaces (A4), (A5), (A6) share the same set of foci at the points $\pm h_1$, $\pm h_2$, $\pm h_3$. The outward unit normal on the ellipsoid $\rho=\alpha_1$ is given by

$$\frac{\partial}{\partial n}=\hat{\boldsymbol{\rho}}\cdot\nabla=\frac{\alpha_2\alpha_3}{\sqrt{\alpha_1^2-\mu^2}\sqrt{\alpha_1^2-\nu^2}}\frac{\partial}{\partial\rho}. \tag{A7}$$

APPENDIX B: ELLIPSOIDAL HARMONICS

Separation of variables for the Laplace's equation in the ellipsoidal coordinate system leads to the Lamé equation[15]

$$(x^2-h_2^2)(x^2-h_3^2)E''(x)+x(2x^2-h_2^2-h_3^2)E'(x)+(Ax^2+B)E(x)=0, \tag{B1}$$

for each one of the factors $E(\rho)$, $E(\mu)$, and $E(\nu)$ that form the harmonic function

$$\mathbb{E}(\rho,\mu,\nu)=E(\rho)E(\mu)E(\nu), \tag{B2}$$

where A and B are constants.

The only difference between these functions is that $E(\rho)$ satisfies (B1) in the interval $[h_2,+\infty)$, $E(\mu)$ in the interval $[h_2,h_3]$, and $E(\nu)$ in the interval $[-h_3,h_3]$.

Lamé equation (B1) has a long history that dominated differential equations the whole of the 19th century.[15] A complicated analysis shows that the constants A and B are appropriately associated with two integers n and m, where just like the spherical harmonics, n specifies the degree, and m specifies the order, of the different Lamé functions of the same degree. For each $n=0,1,2,...$ and each $m=1,2,...,2n+1$ Eq. (B1) has two linearly independent solutions, one regular at the origin and one regular at infinity. For fixed values of n and m, a solution of Eq. (B1) is called a Lamé function of degree n and order m. In particular, the solution E_n^m that is regular at the

origin is the Lamé function of the first kind (interior solution), while the solution F_n^m that is regular at infinity is the Lamé function of the second kind (exterior solution). The interior solutions $E_n^m(\rho)$ are connected to the exterior solutions $F_n^m(\rho)$ via the expression

$$F_n^m(\rho)=(2n+1)E_n^m(\rho)I_n^m(\rho), \tag{B3}$$

where the elliptic integrals $I_n^m(\rho)$ are given by

$$I_n^m(\rho)=\int_\rho^{+\infty}\frac{dt}{[E_n^m(t)]^2\sqrt{t^2-h_2^2}\sqrt{t^2-h_3^2}}=\frac{1}{2}\int_{\rho^2-\alpha_1^2}^{+\infty}\frac{dx}{[E_n^m(\sqrt{x+\alpha_1^2})]^2\sqrt{x+\alpha_1^2}\sqrt{x+\alpha_2^2}\sqrt{x+\alpha_3^2}}. \tag{B4}$$

The Lamé products

$$\mathbb{E}_n^m(\rho,\mu,\nu)=E_n^m(\rho)E_n^m(\mu)E_n^m(\nu), \tag{B5}$$

define the interior solid ellipsoidal harmonics and the Lamé products

$$\mathbb{F}_n^m(\rho,\mu,\nu)=F_n^m(\rho)E_n^m(\mu)E_n^m(\nu)=(2n+1)\mathbb{E}_n^m(\rho,\mu,\nu)I_n^m(\rho), \tag{B6}$$

define the exterior solid ellipsoidal harmonics. The surface ellipsoidal harmonics are defined by the product $E_n^m(\mu)E_n^m(\nu)$ and they form a complete orthogonal set of ''angular'' eigenfunctions on the surface of any ellipsoid from the confocal family (A4). In fact, the orthogonality is defined via the weighting function

$$l(\mu,\nu)=[(\rho_0^2-\mu^2)(\rho_0^2-\nu^2)]^{-1/2}, \tag{B7}$$

on the ellipsoid $\rho=\rho_0$ and provides the relations

$$\int\int_{\rho=\rho_0}E_n^m(\mu)E_n^m(\nu)E_{n'}^{m'}(\mu)E_{n'}^{m'}(\nu)l(\mu,\nu)ds=0, \tag{B8}$$

unless $n=n'$ and $m=m'$, in which case the normalization constants γ_n^m are given by (37).

Although the form of the ellipsoidal harmonics is known, the exact values of the parameters they involve are not expressed in terms of the semiaxes $\alpha_1,\alpha_2,\alpha_3$ when the degree n is higher than 3. This difficulty restricts the analytical solutions of related boundary value problems to the 16th-dimensional harmonic subspace spanned by the harmonics of degree less than or equal to 3.[15] The needs of the present work are restricted to the ellipsoidal harmonics of degree less than or equal to 2 which are given explicitly below. These harmonics are enough to obtain an analytic expression for the dipole as well as for the quadrupole term for the exterior magnetic field.

The interior Lamé functions of degree less than or equal to 2 are given by

$$E_0^1(x)=1, \tag{B9}$$

$$E_1^m(x)=\sqrt{|x^2-\alpha_1^2+\alpha_m^2|}, \qquad m=1,2,3 \tag{B10}$$

$$E_2^1(x)=x^2-\alpha_1^2+\Lambda, \tag{B11}$$

$$E_2^2(x)=x^2-\alpha_1^2+\Lambda' \tag{B12}$$

$$E_2^{6-m}(x)=\frac{E_1^1(x)E_1^2(x)E_1^3(x)}{E_1^m(x)}, \qquad m=1,2,3 \tag{B13}$$

where the constants

$$\left.\begin{matrix}\Lambda\\ \Lambda'\end{matrix}\right\}=\frac{1}{3}\sum_{n=1}^{3}\alpha_n^2\pm\frac{1}{3}\sqrt{\sum_{n=1}^{3}\left(\alpha_n^4-\frac{\alpha_1^2\alpha_2^2\alpha_3^2}{\alpha_n^2}\right)}, \tag{B14}$$

are the two roots of the quadradic equation

$$\sum_{n=1}^{3}\frac{1}{\Lambda-\alpha_n^2}=0. \tag{B15}$$

Once the interior Lamé functions are known, the corresponding exterior ones are obtained via formulas (B3), (B4). Interior and exterior solid ellipsoidal harmonics are then constructed via (B5) and (B6), respectively. Finally, the normalization constants used in the present work are the following:

$$\gamma_0^1=4\pi, \tag{B16}$$

$$\gamma_1^m=\frac{4\pi}{3}\frac{h_1^2h_2^2h_3^2}{h_m^2},\qquad m=1,2,3 \tag{B17}$$

$$\gamma_2^1=-\frac{8\pi}{5}(\Lambda-\Lambda')(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2), \tag{B18}$$

$$\gamma_2^2=\frac{8\pi}{5}(\Lambda-\Lambda')(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2), \tag{B19}$$

and

$$\gamma_2^{6-m}=\frac{4\pi}{15}h_1^2h_2^2h_3^2h_m^2,\qquad m=1,2,3. \tag{B20}$$

It can be shown that all γ_n^m's are positive as formula (36) demands. The following relations express the gradients of ellipsoidal harmonics in terms of ellipsoidal harmonics as well:

$$\nabla\mathbb{E}_0^1(\rho,\mu,\nu)=0, \tag{B21}$$

$$\nabla\mathbb{E}_1^m(\rho,\mu,\nu)=\frac{h_1h_2h_3}{h_m}\hat{\mathbf{x}}_m,\qquad m=1,2,3 \tag{B22}$$

where $\hat{\mathbf{x}}_m$ stand for the Cartesian orthonormal basis, and

$$\nabla\mathbb{E}_2^1(\rho,\mu,\nu)=2\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{h_1h_2h_3}\sum_{m=1}^{3}\frac{h_m}{\Lambda-\alpha_m^2}\mathbb{E}_1^m(\rho,\mu,\nu)\hat{\mathbf{x}}_m, \tag{B23}$$

$$\nabla\mathbb{E}_2^2(\rho,\mu,\nu)=2\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{h_1h_2h_3}\sum_{m=1}^{3}\frac{h_m}{\Lambda'-\alpha_m^2}\mathbb{E}_1^m(\rho,\mu,\nu)\hat{\mathbf{x}}_m, \tag{B24}$$

$$\nabla\mathbb{E}_2^3(\rho,\mu,\nu)=h_1h_2h_3\left[\frac{1}{h_1}\mathbb{E}_1^2(\rho,\mu,\nu)\hat{\mathbf{x}}_1+\frac{1}{h_2}\mathbb{E}_1^1(\rho,\mu,\nu)\hat{\mathbf{x}}_2\right], \tag{B25}$$

$$\nabla\mathbb{E}_2^4(\rho,\mu,\nu)=h_1h_2h_3\left[\frac{1}{h_1}\mathbb{E}_1^3(\rho,\mu,\nu)\hat{\mathbf{x}}_1+\frac{1}{h_3}\mathbb{E}_1^1(\rho,\mu,\nu)\hat{\mathbf{x}}_3\right], \tag{B26}$$

$$\nabla \mathbb{E}_2^5(\rho,\mu,\nu)=h_1h_2h_3\left[\frac{1}{h_2}\mathbb{E}_1^3(\rho,\mu,\nu)\hat{\mathbf{x}}_2+\frac{1}{h_3}\mathbb{E}_1^2(\rho,\mu,\nu)\hat{\mathbf{x}}_3\right]. \tag{B27}$$

APPENDIX C: CONNECTION FORMULAS

The solid ellipsoidal harmonics are expressed in terms of Cartesian coordinates as follows:[5]

$$\mathbb{E}_0^1(\rho,\mu,\nu)=1, \tag{C1}$$

$$\mathbb{E}_1^m(\rho,\mu,\nu)=\frac{h_1h_2h_3}{h_m}x_m, \qquad m=1,2,3 \tag{C2}$$

$$\mathbb{E}_2^1(\rho,\mu,\nu)=(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)\left(\sum_{n=1}^{3}\frac{x_n^2}{\Lambda-\alpha_n^2}+1\right), \tag{C3}$$

$$\mathbb{E}_2^2(\rho,\mu,\nu)=(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)\left(\sum_{n=1}^{3}\frac{x_n^2}{\Lambda'-\alpha_n^2}+1\right), \tag{C4}$$

$$\mathbb{E}_2^{6-m}(\rho,\mu,\nu)=h_1h_2h_3h_m\frac{x_1x_2x_3}{x_m}, \quad m=1,2,3. \tag{C5}$$

Furthermore, the Cartesian monomials of degree less than or equal to 2 are expressed in terms of surface ellipsoidal harmonics as follows:

$$1=\mathbb{E}_0^1(\rho,\mu,\nu), \tag{C6}$$

$$x_m=\frac{h_m}{h_1h_2h_3}\mathbb{E}_1^m(\rho,\mu,\nu), \quad m=1,2,3 \tag{C7}$$

$$x_m^2=\frac{\rho^2-\alpha_1^2+\alpha_m^2}{3}\left[1-\frac{E_2^1(\mu)E_2^1(\nu)}{(\Lambda-\Lambda')(\Lambda-\alpha_m^2)}+\frac{E_2^2(\mu)E_2^2(\nu)}{(\Lambda-\Lambda')(\Lambda'-\alpha_m^2)}\right], \quad m=1,2,3 \tag{C8}$$

$$\frac{x_1x_2x_3}{x_m}=\frac{1}{h_1h_2h_3h_m}\mathbb{E}_2^{6-m}(\rho,\mu,\nu), \quad m=1,2,3. \tag{C9}$$

APPENDIX D: USEFUL RELATIONS

The constants Λ, Λ' given in (B14), the semifocal distances h_1, h_2, h_3 given by (4), and the semiaxes $\alpha_1,\alpha_2,\alpha_3$, satisfy the following useful expressions:

$$3(\Lambda+\Lambda')=2(\alpha_1^2+\alpha_2^2+\alpha_3^2), \tag{D1}$$

$$3\Lambda\Lambda'=\alpha_1^2\alpha_2^2+\alpha_2^2\alpha_3^2+\alpha_3^2\alpha_1^2, \tag{D2}$$

$$\sum_{n=1}^{3}(-1)^n(\Lambda-\alpha_n^2)h_n^2=\sum_{n=1}^{3}(-1)^n(\Lambda'-\alpha_n^2)h_n^2=0, \tag{D3}$$

$$\sum_{n=1}^{3}(-1)^n(\Lambda-\alpha_n^2)h_n^2\alpha_n^2=\sum_{n=1}^{3}(-1)^n(\Lambda'-\alpha_n^2)h_n^2\alpha_n^2=h_1^2h_2^2h_3^2, \tag{D4}$$

$$\sum_{n=1}^{3}\frac{\alpha_n^2}{\alpha_n^2-\Lambda}=\sum_{n=1}^{3}\frac{\alpha_n^2}{\alpha_n^2-\Lambda'}=3, \tag{D5}$$

$$3h_n^2(\Lambda-\alpha_n^2)(\Lambda'-\alpha_n^2)=(-1)^{n+1}h_1^2h_2^2h_3^2, \tag{D6}$$

for each $n=1,2,3$.

The elliptic integrals that enter the exterior ellipsoidal harmonics $\mathbb{F}_n^m$, $n\leqslant 2$ are connected via the following relations:

$$I_1^1(\rho)+I_1^2(\rho)+I_1^3(\rho)=\frac{1}{\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}, \tag{D7}$$

$$\alpha_1^2I_1^1(\rho)+\alpha_2^2I_1^2(\rho)+\alpha_3^2I_1^3(\rho)=I_0^1(\rho)-\frac{\rho^2-\alpha_1^2}{\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}, \tag{D8}$$

$$I_2^1(\rho)=\frac{1}{2(\Lambda-\alpha_1^2+\rho^2)\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}-\frac{1}{2}\left(\frac{I_1^1(\rho)}{\Lambda-\alpha_1^2}+\frac{I_1^2(\rho)}{\Lambda-\alpha_2^2}+\frac{I_1^3(\rho)}{\Lambda-\alpha_3^2}\right), \tag{D9}$$

$$I_2^2(\rho)=\frac{1}{2(\Lambda'-\alpha_1^2+\rho^2)\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}-\frac{1}{2}\left(\frac{I_1^1(\rho)}{\Lambda'-\alpha_1^2}+\frac{I_1^2(\rho)}{\Lambda'-\alpha_2^2}+\frac{I_1^3(\rho)}{\Lambda'-\alpha_3^2}\right), \tag{D10}$$

$$I_2^3(\rho)=\frac{1}{h_3^2}(I_1^2(\rho)-I_1^1(\rho)), \tag{D11}$$

$$I_2^4(\rho)=\frac{1}{h_2^2}(I_1^3(\rho)-I_1^1(\rho)), \tag{D12}$$

$$I_2^5(\rho)=\frac{1}{h_1^2}(I_1^3(\rho)-I_1^2(\rho)). \tag{D13}$$

The expressions can be established through long and tedious manipulations and they actually show that among the nine integrals $I_n^m(\rho)$ with $n\leqslant 2$, only two are independent. For instance, if $I_0^1(\rho)$ and $I_1^1(\rho)$ are known the other seven integrals can be expressed, via (D7)–(D13), in terms of these two.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

The investigation into new integrable systems of equations in 2+1-dimensions

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(Received 9 July 2001; accepted 10 October 2002)

A new integrable class of systems of nonlinear partial differential equations (NPDEs) in $2+1$ dimensions is derived from the matrix Nizhnik–Novikov–Veselov (NVV) equation by means of an asymptotically exact nonlinear reduction method based on Fourier expansion and spatio-temporal rescaling. The integrability by the inverse scattering method is explicitly demonstrated, by applying the reduction technique also to the Lax pair of the starting matrix equation and thereby obtaining the Lax pair for the new class of systems of equations. A reduction to a system of two interacting complex fields is briefly described. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1525405]

I. INTRODUCTION

New classes of evolution nonlinear partial differential equations (NPDEs) integrable by the inverse scattering method (S-integrable) have been found in recent years. These equations are known to be applicable to various branches of physics such as fluid dynamics, nonlinear optics, condensed matter physics and so on. The most famous examples are the Korteweg–de Vries and the nonlinear Schrödinger equations in $1+1$ dimensions and the Kadomtsev–Petviashvili and the Davey–Stewartson equations in $2+1$ dimensions.[1]

A simple explanation of this coincidence (integrability and applicative relevance) is based on the observation that very large classes of evolution NPDEs in $1+1$ and $2+1$ dimensions, with a dispersive linear part, can be reduced, by a limiting procedure involving the wave modulation induced by weak nonlinear effects, to a very limited number of ''universal'' evolution NPDEs. Moreover, the same model equations obtained in this way appear in many applicative situations (for instance, in plasma physics, nonlinear optics, hydrodynamics, etc.), where weakly nonlinear effects are important.[2–4]

The reduction method preserves integrability and therefore the model equations are likely to be integrable; it is sufficient that the very large class of equations from which they are obtainable contains just one integrable equation, provided the limiting procedure preserves integrability so that the property of integrability is inherited through this limiting technique. Obviously, the last statement about the integrability is based on heuristic considerations and could not be characterized as a rigorous theorem, because no precise definition of integrability is available for evolution NPDEs.

In particular, the derivation of the Lax pair of the reduced equation from that of the original equation was first done, for a certain number of soliton equations in $1+1$ and $2+1$ dimensions, by Zakharov and Kuznetsov.[5]

The above mentioned approach, besides explaining why certain model equations are integrable and applicable, provides a powerful tool to investigate the relation among different integrable equations, to test the integrability of nonlinear evolution PDEs and, most importantly, to identify integrable evolution equations that are likely to be of applicative relevance.[6]

In previous papers, we applied this method to certain integrable equations in $2+1$ dimen-

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sions. The most interesting results are that the Davey–Stewarston equation[7,8] is the typical model equation in $2+1$ dimensions, while new integrable NPDEs can be obtained together with their Lax pair.[9–12] Moreover, we used the reduction method to derive two equations of applicative relevance in plasma physics.[13,14]

The basic idea of the reduction method is to consider a nonlinear evolution PDE whose linear part is dispersive; as it is well known the linear evolution is most appropriately described in terms of Fourier modes and each Fourier mode evolves with constant amplitude and an associated group velocity, that represents the speed with which a wave packet peaked at the Fourier mode would move in configuration space. To evaluate the weak nonlinear effects it is convenient to consider a specific Fourier mode and follow it by going over to a frame of reference that moves with its group velocity. The weak nonlinear effects may yield a non-negligible contribution, because they give rise to a modulation of the amplitude of that Fourier mode (that would remain constant in the absence of nonlinear effects). The modulation is best described in terms of rescaled ''coarse-grained'' and ''slow'' variables, that display the weak nonlinear effects on larger space and time scales; indeed, the first step of the reduction method is to use a moving frame of reference with the introduction of the slow variables:

$$\xi=\varepsilon^p(x-V_1t),\ \eta=\varepsilon^p(y-V_2t),\ \tau=\varepsilon^q t,$$
$$p>0,\quad q>0, \tag{1.1}$$

where $V_1=V_1(K_1,K_2)$, $V_2=V_2(K_1,K_2)$ are the components of the group velocity $\underline{V}(\underline{K})\equiv(V_1(K_1,K_2),V_2(K_1,K_2))$ of the linearized equation, i.e., of the equation obtained by neglecting all the nonlinear terms, and ε is a ''small'' expansion parameter.

It is thereby seen that the function that represents the amplitude modulation satisfies, in terms of the rescaled, slow, variables, evolution equations having a universal character; since the coarse-grained nature of the new variables implies that only certain general features of the nonlinear interaction are important.

In this paper we expose an interesting extension of this approach and consider the matrix Nizhnik–Novikov–Veselov (NVV) equation[15,16]

$$U_t+U_{xxx}+U_{yyy}-3(VU)_x-3(WU)_y=0, \tag{1.2a}$$

$$W_x=U_y,\quad V_y=U_x, \tag{1.2b}$$

where $U=U(x,y,t)$, $V=V(x,y,t)$, $W=W(x,y,t)$ are $N\otimes N$ complex matrices, the subscripts denote partial differentiation and $[U,V]=UV-VU=0$, $[U,W]=UW-WU=0$.

By applying the reduction method, a new class of integrable matrix systems of evolution NPDEs is obtained,

$$i\Psi_\tau+L\Psi+\Delta\Psi=0, \tag{1.3a}$$

$$\Delta_{\xi\eta}=-L(|\Psi|^2), \tag{1.3b}$$

where $[\Psi,\Psi^*]=\Psi\Psi^*-\Psi^*\Psi=0$, the linear differential operator L is given by

$$L=-\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}, \tag{1.4}$$

and $\Psi=\Psi(\xi,\eta,\tau)$ is an $N\otimes N$ complex matrix, while $\Delta=\Delta(\xi,\eta,\tau)$ is an $N\otimes N$ real matrix. For $N=1$ the matrix equation (1.3) reduces to the well-known scalar Davey–Stewartson I equation,[7,8] but for $N>1$ yields new integrable Davey–Stewartson type systems of equations.

The article is organized as follows. In the next section we apply the reduction method to the starting equation (1.2) and obtain the new system of matrix equations (1.3) and (1.4). Moreover, we reduce the matrix system of equations to a new integrable two-component complex fields

system of nonlinear equations, which, in the one-component case, reduces to the scalar Davey–Stewartson equation. In Sec. III we discuss in some detail how the reduction method can be applied to the Lax pair of the equation (1.2) and we derive the Lax pair of the system of matrix equations (1.3) and (1.4). Finally, in the last section we recapitulate the most important results and indicate some possible extensions.

II. A NEW INTEGRABLE MATRIX SYSTEM IN 2+1 DIMENSIONS

The linear dispersive part of the starting equation (1.2) admits as a solution a Fourier mode, with a group velocity $\underline{V}(\underline{K})=(V_1(K_1,K_2),V_2(K_1,K_2))$,

$$V_1(K_1,K_2)=-3K_1^2, \quad V_2(K_1,K_2)=-3K_2^2, \tag{2.1}$$

where

$$\underline{V}(\underline{K})=\frac{\partial\omega}{\partial\underline{K}}, \tag{2.2}$$

and

$$\omega=\omega(K_1,K_2)=-K_1^3-K_2^3 \tag{2.3}$$

is the dispersion relation.

We use the transformation (1.1) and introduce the following formal asymptotic Fourier expansion

$$U(x,y,t)=\sum_{n=-\infty}^{+\infty}\varepsilon^{\gamma_n}\psi_n(\xi,\eta,\tau;\varepsilon)\exp\{i(nz)\}, \tag{2.4}$$

where $z=K_1x+K_2y-\omega t$, $\gamma_n=|n|$ for $n\neq 0$, and $\gamma_0=r$ is a non-negative rational number which will be fixed later. The unknown functions ψ_n's depend on ε and it is supposed that their limit for $\varepsilon\to 0$ exists and is finite; in the following this limit will be denoted with $\psi_n(\xi,\eta,\tau)$. Moreover, we suppose that they can be expanded in power series of ε, i.e.,

$$\psi_n(\xi,\eta,\tau;\varepsilon)=\sum_{i=0}^{\infty}\varepsilon^i\psi_n^{(i)}(\xi,\eta,\tau), \quad \psi_n(\xi,\eta,\tau)=\psi_n^{(0)}(\xi,\eta,\tau). \tag{2.5}$$

We now introduce two analogous Fourier expansions

$$V(x,y,t)=\sum_{n=-\infty}^{+\infty}\varepsilon^{\tilde{\gamma}_n}\varphi_n(\xi,\eta,\tau;\varepsilon)\exp\{i(nz)\}, \tag{2.6a}$$

$$W(x,y,t)=\sum_{n=-\infty}^{+\infty}\varepsilon^{\tilde{\gamma}_n}\chi_n(\xi,\eta,\tau;\varepsilon)\exp\{i(nz)\}, \tag{2.6b}$$

and in the following for simplicity we use the abbreviations $\psi_1^{(0)}=\Psi$, $\psi_0^{(0)}=\Phi$ (and $\phi_n^{(0)}=\phi_n$, $\phi_0^{(0)}=\Lambda$, $\chi_n^{(0)}=\chi_n$, $\chi_0^{(0)}=\Omega$).

We obtain

$$\varphi_n=(K_1)(K_2)^{-1}\psi_n+O(\varepsilon^p), \quad \chi_n=(K_2)(K_1)^{-1}\psi_n+O(\varepsilon^p). \tag{2.7}$$

The final goal is to obtain the evolution equation satisfied by the modulation amplitudes $\Psi = \Psi(\xi, \eta, \tau)$ and to understand how it is modified by choosing different wave numbers. We insert the expansions (2.4) and (2.6) into the equation (1.2) and consider the different equations obtained by considering the coefficients of the Fourier modes.

It is convenient to separate the contributions of the linear and nonlinear parts by writing

$$\varepsilon^{\gamma_n} D_n \psi_n = \varepsilon^2 F_n, \tag{2.8}$$

where D_n is a linear differential operator acting on $\psi_n(\xi, \eta, \tau)$ and F_n is the contribution of the nonlinear part. The operator D_n is

$$D_n = (-in\omega + \varepsilon^q \partial_\tau - V_1 \varepsilon^p \partial_\xi - V_2 \varepsilon^p \partial_\eta) + (inK_1 + \varepsilon^p \partial_\xi)^3 + (inK_2 + \varepsilon^p \partial_\eta)^3. \tag{2.9}$$

F_n can be derived, by assessing the importance of the different terms, which originate from the nonlinear interaction of the Fourier amplitudes $\psi_n(\xi, \eta, \tau)$:

$$F_2 = 6i \frac{K_1^2}{K_2} \Psi^2 + O(\varepsilon^p), \tag{2.10a}$$

$$F_0 = 6\varepsilon^p \left(\frac{K_1}{K_2} (|\Psi|^2)_\xi + \frac{K_2}{K_1} (|\Psi|^2)_\eta \right) + O(\varepsilon^{2p}, \varepsilon^q, \varepsilon^2), \tag{2.10b}$$

$$F_1 = 3\varepsilon^{r-1} \left(-K_1 \Lambda \Psi - K_2 \Omega \Psi - \left(\frac{K_1^2}{K_2} + \frac{K_2^2}{K_1} \right) \Psi \Phi + 2 \left(\frac{K_1}{K_2^2} + \frac{K_2}{K_1^2} \right) |\Psi|^2 \Psi \right) + O(\varepsilon^{r+p-1}, \varepsilon^3), \tag{2.10c}$$

and so on.

By setting $q=2$, $p=1$, $r=2$ for the proper balance of terms, we obtain the equations for the Fourier modes at the lowest order for $n=2$:

$$\psi_2 = -\frac{1}{K_1^2} \Psi^2, \tag{2.11}$$

and after the cosmetic rescaling

$$\frac{3(K_1^3 + K_2^3)}{K_2 \sqrt{K_1 K_2}} \Lambda \to \Lambda, \quad \frac{3(K_1^3 + K_2^3)}{K_1 \sqrt{K_1 K_2}} \Omega \to \Omega, \tag{2.12a}$$

$$\frac{\sqrt{6(K_1^3 + K_1^3)}}{K_1 K_2} \Psi \to \Psi, \quad \frac{3(K_1^3 + K_2^3)}{K_1 K_2} \Phi \to \Phi, \tag{2.12b}$$

$$\lambda = \left(\frac{K_1}{K_2} \right)^{3/2}, \quad \xi' = \frac{\xi}{\sqrt{3K_1}}, \quad \eta' = \frac{\eta}{\sqrt{3K_2}}, \tag{2.12c}$$

and

$$\tau' = -\tau, \quad \Delta = |\Psi|^2 - \Phi - \frac{\lambda}{\lambda^2 + 1} (\Lambda + \Phi), \quad \sqrt{\frac{\lambda}{\lambda^2 + 1}} \Psi \to \Psi, \tag{2.13}$$

we arrive at the matrix system of nonlinear evolution equations (1.3) and (1.4).

This matrix system must be integrable by the spectral transform, because it has been derived from an S-integrable equation. This is explicitly demonstrated in the next section.

Let us now look in more detail at the integrable NPDEs implied these results. If we take $N=1$, we obtain obviously the scalar Davey–Stewartson I equation.

In the case $N=2$, we get a nonlinear system for four interacting fields. However, an interesting reduction is possible. If we set

$$\Psi=\begin{pmatrix}\psi_1 & \psi_2\\ \psi_2 & \psi_1\end{pmatrix},\quad \Phi=\begin{pmatrix}\varphi_1 & \varphi_2\\ \varphi_2 & \varphi_1\end{pmatrix},\quad \Lambda=\begin{pmatrix}\Lambda_1 & \Lambda_2\\ \Lambda_2 & \Lambda_1\end{pmatrix},\quad \Omega=\begin{pmatrix}\Omega_1 & \Omega_2\\ \Omega_2 & \Omega_1\end{pmatrix}, \tag{2.14}$$

we arrive at the matrix system of nonlinear evolution equations:

$$i\psi_{1,\tau}-L\psi_1+\frac{\lambda}{\lambda^2+1}(\Lambda_1\psi_1+\Lambda_2\psi_2+\Omega_1\psi_1+\Omega_2\psi_2)$$
$$+(\varphi_1\psi_1+\varphi_2\psi_2)-(|\psi_1|^2\psi_1+\psi_1^*\psi_2^2+2\psi_1|\psi_2|^2)=0, \tag{2.15a}$$

$$i\psi_{2,\tau}-L\psi_2+\frac{\lambda}{\lambda^2+1}(\Lambda_1\psi_2+\Lambda_2\psi_1+\Omega_1\psi_2+\Omega_2\psi_1)$$
$$+(\varphi_1\psi_2+\varphi_2\psi_1)-(|\psi_1|^2\psi_2+\psi_1^2\psi_2^*+2\psi_2|\psi_1|^2)=0, \tag{2.15b}$$

$$\lambda\Phi_{1,\xi}+\Phi_{1,\eta}-\lambda(|\psi_1|^2+|\psi_2|^2)_\xi-(|\psi_1|^2+|\psi_2|^2)_\eta=0, \tag{2.15c}$$

$$\lambda\Phi_{2,\xi}+\Phi_{2,\eta}-\lambda(\psi_1\psi_2^*+\psi_2\psi_1^*)_\xi-(\psi_1\psi_2^*+\psi_2\psi_1^*)_\eta=0, \tag{2.15d}$$

$$\Lambda_{1,\eta}=\Phi_{1,\xi},\Lambda_{2,\eta}=\Phi_{2,\xi}\Omega_{1,\xi}=\Phi_{1,\eta}\Omega_{2,\xi}=\Phi_{1,\eta}, \tag{2.15e}$$

where

$$L=\partial_\xi^2+\partial_\eta^2. \tag{2.15f}$$

Integrable nonlinear equations and system of equations in $2+1$ dimensions have been extensively investigated by many authors.[17–21] A detailed list of systems and equations integrable by the inverse scattering method has been recently given.[22] The system of equations (2.15) does not appear in these papers. We expect that this new system is integrable by the inverse scattering method, because it has been obtained from an integrable equation and the property of integrability is expected to be maintained through the application of the reduction method. The integrability of the system of equations (1.3) and (1.4) and of the system (2.15), which is a particular case, is demonstrated in the next section.

III. THE LAX PAIR FOR THE INTEGRABLE SYSTEM OF EQUATIONS

In this section we apply the reduction method also to the Lax pair of the starting matrix equation (1.2), to demonstrate explicitly the integrability by the spectral transform of the matrix system (1.3) and (1.4), and we thereby identify the Lax pair for the system of equations (1.3) and (1.4).

Let us apply the reduction method to the Lax pair of equation (1.2). The Lax operators are

$$L=\frac{\partial^2}{\partial x\partial y}-U(x,y,t),\quad L\phi(x,y,t)=0, \tag{3.1}$$

$$A=\frac{\partial^3}{\partial x^3}+\frac{\partial^3}{\partial y^3}-3V\frac{\partial}{\partial x}-3W\frac{\partial}{\partial y}, \tag{3.2}$$

with

$$\phi_t(x,y,t)+A\phi(x,y,t)=0. \tag{3.3}$$

It can be verified by direct substitution that the operator relation

$$L_t=i[L,A]=i(LA-AL) \tag{3.4}$$

reproduces Eq. (1.2).

The components $\phi_j(x,y,t)$, $j=1,...,N$, of the column vector $\phi(x,y,t)$ can be expanded in Fourier modes as follows:

$$\phi_j(x,y,t)=\sum_{n=-\infty}^{+\infty}\varepsilon^{\gamma_n}\phi_{j,n}(\xi,\eta,\tau;\varepsilon)\exp\left[i\left((\lambda_1 x+\lambda_2 y+\lambda_3 t)+\frac{n}{2}z\right)\right], \tag{3.5}$$

where $z=K_1x+K_2y-\omega t$, the $\phi_{j,n}(\xi,\eta,\tau;\varepsilon)$'s depend parametrically on ε and remain finite when $\varepsilon\to 0$, the γ_n's are non-negative rational numbers and λ_m, $m=1,...,3$, are real constants to be determined.

Inserting now the expression for $\phi_j(x,y,t)$ in (3.1), we derive a series of relations which are generated by the coefficients of the Fourier modes. Each relation must be valid for a given order of approximation in ε.

In particular, for the fundamental harmonics $n=\pm 1$, considering terms $O(\varepsilon^0)$ in (3.1) and (3.3), we obtain

$$\left(\pm\frac{iK_2}{2}+i\lambda_2\right)\left(\pm\frac{iK_1}{2}+i\lambda_1\right)=0, \tag{3.6a}$$

$$\left(\mp\frac{i\omega}{2}+i\lambda_3\right)+\left(\pm\frac{iK_1}{2}+i\lambda_1\right)^3+\left(\pm\frac{iK_2}{2}+i\lambda_{2\,1}\right)^3=0, \tag{3.6b}$$

and then

$$\lambda_1=\frac{K_1}{2},\quad \lambda_2=-\frac{K_2}{2},\quad \lambda_3=-\frac{K_2^3}{4}-\frac{K_1^3}{4}. \tag{3.7}$$

We thereby understand that the harmonics

$$\phi_{j,1},\phi_{j,-1},\quad j=1,...,N, \tag{3.8}$$

are fundamental, i.e., for them γ_n assumes the smallest value, $\gamma_n=0$.

The successive order ε for the equation (3.1) allows us to obtain the new spectral problem, because all the $\phi_{j,n}$'s may be expressed by means of the fundamental harmonics (3.8), which are connected through the relations:

$$iK_1\phi_{+,\eta}-\Psi\phi_-=0, \tag{3.9}$$

$$-iK_2\phi_{-,\xi}-\Psi^*\phi_+=0, \tag{3.10}$$

where we set $(\phi_{j,1};j=1,...,N)=\phi_+$, $(\phi_{j,-1};j=1,...,N)=\phi_-$.

By means of the variable rescaling (2.12), and by introducing the $2N\otimes 2N$ matrix operator L, we arrive at the final form

$$L\hat{\phi}=0, \tag{3.11}$$

where

$$L=\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}, \tag{3.12a}$$

$$L_{11}=iI\partial_\eta, \quad L_{12}=-\frac{1}{\sqrt{2(\lambda^2+1)}}\Psi, \tag{3.12b}$$

$$L_{21}=\frac{\lambda}{\sqrt{2(\lambda^2+1)}}\Psi^*, \quad L_{22}=iI\partial_\xi, \tag{3.12c}$$

$$\hat{\phi}=\begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}, \tag{3.12d}$$

and I is the $N\otimes N$ unit matrix.

To calculate the temporal evolution, we must insert the expression (3.5) in (3.3) and consider the relation obtained for the different harmonics n and for a given order of approximation in ε. If we consider the first order in ε, we obtain again the spectral problem (3.11) and (3.12). Only if we take into account the next orders of approximation of Eq. (3.3), i.e., the order ε^2, the temporal evolution can be determined. However, new quantities, the corrections $\tilde{\phi}_\pm(\xi,\eta,\tau)$ of order ε to the fundamental harmonics $\phi_\pm(\xi,\eta,\tau)$, appear. These unknown quantities can be eliminated in Eq. (3.3) by taking advantage of the relation obtained from Eq. (3.1), considering terms of order ε^2. This elimination is possible only because Eqs. (3.1) and (3.3) are identical at the order ε. In particular, if we consider (3.3) calculated to the order ε^2 for $n=\pm 1$, we get

$$\phi_{+,\tau}+3iK_1\phi_{+,\xi\xi}-3\frac{K_1}{K_2}\Psi\phi_{-,\xi}-3\frac{K_2}{K_1}\Psi\phi_{-,\eta_-}-3\frac{K_2}{K_1}\left(\frac{K_2}{K_1}\Psi_\xi-\Psi_\eta\right)\phi_- -3iK_1\Lambda\phi_+$$
$$-3\left(\frac{2iK_1^2}{K_2}+\frac{iK_2^2}{K_1}\right)\Psi^*\phi_{+3}+\frac{3K_2^2}{iK_1}(iK_1\tilde{\phi}_{+,\eta}-\Psi\tilde{\phi}_-)=0, \tag{3.13a}$$

and

$$\phi_{-,\tau}-3iK_2\phi_{-,\eta\eta}-3\frac{K_1}{K_2}\Psi^*\phi_{+,\xi}-3\frac{K_2}{K_1}\Psi^*\phi_{+,\eta}-3\frac{K_1}{K_2}\left(\frac{K_1}{K_2}\Psi^*_\eta-\Psi^*_\xi\right)\phi_+ +3iK_2\Omega\phi_-$$
$$+3\left(\frac{2iK_2^2}{K_1}+\frac{iK_1^2}{K_2}\right)\Psi\phi_{-3}-\frac{3K_1^2}{iK_2}(iK_2\tilde{\phi}_{-,\xi}-\Psi^*\tilde{\phi}_+)=0. \tag{3.13b}$$

To evaluate this expression we took advantage of the fact that $\phi_{\pm 3}$ are connected with the fundamental harmonics [these relations are obtained from (3.1) for $n=\pm 3$ at the lower order in ε]:

$$\phi_{+3}=\left(\frac{-1}{2K_1K_2}\right)\Psi\phi_+, \quad \phi_{-3}=\left(\frac{-1}{2K_1K_2}\right)\Psi^*\phi_-. \tag{3.14}$$

We now consider Eq. (3.1) at the order ε^2 for $n=\pm 1$, which provides the corrections $\tilde{\phi}_+(\xi,\eta,\tau)$, $\tilde{\phi}_-(\xi,\eta,\tau)$. Via the transformation (2.12) and after a lengthy calculation we arrive at the final form for the $2N\otimes 2N$ matrix operator A, which satisfies the equation

$$\hat{\phi}_\tau+A\hat{\phi}=0, \tag{3.15}$$

and is given by

$$A=\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \tag{3.16a}$$

where

$$A_{11}=i\partial_\xi^2 I-i\frac{\lambda\Lambda}{1+\lambda^2}-i\frac{\Phi}{1+\lambda^2}+i\frac{1}{(1+\lambda^2)}\Psi^*\Psi, \tag{3.16b}$$

$$A_{12}=\frac{1}{\sqrt{2(1+\lambda^2)}}(\Psi_\eta-\Psi\partial_\eta), \tag{3.16c}$$

$$A_{22}=-i\partial_\eta^2 I+i\frac{\lambda\Omega}{(1+\lambda^2)}+i\frac{\lambda^2\Phi}{1+\lambda^2}-i\frac{\lambda^2}{(1+\lambda^2)}\Psi\Psi^*, \tag{3.16d}$$

$$A_{21}=\frac{\lambda}{\sqrt{2(1+\lambda^2)}}(\Psi_\xi^*-\Psi^*\partial_\xi). \tag{3.16e}$$

The determination of the Lax pair (3.12) and (3.16), which satisfies Eqs. (3.11) and (3.15), demonstrates the S-integrability of the system (1.3) and (1.4).

IV. CONCLUSION

We have derived a new, integrable, and presumably of applicative interest, nonlinear matrix system of evolution equations from the integrable matrix NVV equation (1.2), by means of an extension of the reduction method based on Fourier expansion and space–time rescalings. It reduces to a known integrable equation in the single mode case and to a new integrable system of two interacting fields in the $N=2$ case. Moreover, we have applied the reduction method to the Lax pair (3.1)–(3.3) of the original equation and have demonstrated the integrability property of the new matrix system of equations, by exhibiting the corresponding Lax pair (3.11) and (3.12) and (3.15) and (3.16).

We have outlined the approach that permits us to obtain such a system of equations and the next steps will be the explicit resolution of the spectral problem and the possible identification of localized or asymptotically finite solutions.

It is also convenient to push the approach beyond its ''leading order'' application by looking at special cases when some key parameters vanish or considering different rescalings in the two spatial variables, in analogy to the case of the model equations treated in Refs. 9 and 10.

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Deformations of the Monge/Riemann hierarchy and approximately integrable systems

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(Received 27 May 2002; accepted 23 September 2002)

Dispersive deformations of the Monge equation $u_t = uu_x$ are studied using ideas originating from topological quantum field theory and the deformation quantization program. It is shown that, to a high order, the symmetries of the Monge equation may also be appropriately deformed, and that, if they exist at all orders, they are uniquely determined by the original deformation. This leads to either a new class of integrable systems or to a rigorous notion of an approximate integrable system. Quasi-Miura transformations are also constructed for such deformed equations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1522134]

I. INTRODUCTION

Consider a general scalar evolution equation

$$u_t = K(u), \tag{1.1}$$

where $K(u)$ is a smooth function depending on u and the x derivatives of u, but not explicitly on the independent variable x. A characteristic feature of an integrable system is the existence of an infinite hierarchy of compatible, commuting flows, these being the generalized symmetries of the original equation (1.1). Such symmetries have the form

$$u_\tau = Q(u)$$

(where again Q is a smooth function of u and the x derivatives of u, but not explicitly on the independent variable x), and must satisfy the equation

$$K'Q - Q'K = 0,$$

where the prime denotes the Fréchet derivative

$$K'(u)Q = \frac{\partial}{\partial \epsilon} K(u + \epsilon Q)\bigg|_{\epsilon=0}.$$

The paradigm for such constructions is the Korteweg–deVries equation

$$u_t = uu_x + u_{xxx}. \tag{1.2}$$

For this equation, the hierarchy of symmetries may be constructed by exploiting the bi-Hamiltonian structure of the KdV equation. Given the Hamiltonians

$$\mathcal{H}_1 = \partial, \quad \mathcal{H}_2 = \partial^3 + \tfrac{2}{3}u\partial + \tfrac{1}{3}u_x,$$

one may form the recursion operator $\mathcal{R} = \mathcal{H}_2\mathcal{H}_1^{-1}$, with which the symmetries take the form

$$u_{\tau_n} = \mathcal{R}^n u_x \tag{1.3}$$

(for more details see, for example, Ref. 8). Such flows constitute the KdV hierarchy.

There has been much interest recently in the properties of the dispersionless limits of integrable systems, these being examples of equations of hydrodynamic type. As well as being interesting integrable systems in their own right, they play an important role in topological quantum field theories and the construction of higher-genus Gromov–Witten invariants.[1,2] Under the scalings

$$t \mapsto \hbar^{-1} t,$$

$$x \mapsto \hbar^{-1} x,$$

$$u \mapsto u,$$

the KdV equation scales to

$$u_t = u u_x + \hbar^2 u_{xxx},$$

and under the classical limit $\hbar \to 0$ one obtains the Monge equation

$$u_t = u u_x. \tag{1.4}$$

This singular limit has a drastic effect on the solution space of the KdV equation, for example soliton solutions do not survive, but many properties do survive, notably the form of conservation laws and the existence of a bi-Hamiltonian hierarchy. Thus, a hierarchy of symmetries of the Monge equation may be obtained by scaling the KdV hierarchy and taking the $\hbar \to 0$ limit. This results in the Monge hierarchy (also called in Ref. 2 the Riemann hierarchy)

$$u_{\tau_n} = u^n u_x.$$

However, the Monge equation has many more symmetries; given any suitably differentiable function $f(u)$, then

$$u_\tau = f(u) u_x \tag{1.5}$$

is a symmetry, labeled not by a discrete integer, but by a $C^2(\mathbb{R})$ function.

The purpose of this paper is to study not the dispersionless limit but the reverse, regarding the KdV equation as a deformation of the Monge equation and constructing, term-by-term, the corresponding deformation of the general symmetry (1.5). In fact, a slightly more general equation than the KdV equation will be studied, namely the equation

$$u_t = u u_x + (a(u) u_{xxx} + b(u) u_{xx} u_x + c(u) u_x^3),$$

where a, b, c are arbitrary functions. The motivation for this comes from the work of Eguchi *et al.*,[3] Dubrovin and Zhang,[1,2] and, in particular, Lorenzoni.[6] Their approaches utilize the bi-Hamiltonian structure of their systems. No such assumption will be made here and, as a result, certain of Lorenzoni's results will appear as a special case of the constructions that will appear in the subsequent sections.

II. NOTATION AND THE FORM OF THE GENERAL PROBLEM

Let $\mathcal{D}$ denote the linear vector space/ring of differential polynomials in $\{u_1, u_2, \ldots\}$ where $u_1 = u_x, u_2 = u_{xx}$, etc., with coefficients in the space $C^\infty(\mathbb{R})$ of infinitely differentiable functions

$$\mathcal{D} = C^\infty(\mathbb{R})[u_1, u_2, \ldots],$$

so an arbitrary element $F \in \mathcal{D}$ takes the form

$$F=\sum_{|I|<\infty} a_I(u)u^I,$$

where

$$u^I=\prod_{k=1}^{\infty} u_k^{I_k},$$

$a_I(u)\in C^\infty(\mathbb{R})$, and I is a multi-index. To each monomial one may assign a scaling degree by counting the number of x-derivatives it contains, so

$$\deg(u_k)=k, \quad k\geqslant 1,$$

$$\deg(AB)=\deg(A)+\deg(B), \quad A,B\in\mathcal{D}$$

and no degree is assigned to the coefficient functions (this is very similar to the ideas used in the theory of normal forms,[4,5] but a different grading is used there). With this, $\mathcal{D}$ decomposes into a sum of subspaces/rings consisting of terms of the same degree

$$\mathcal{D}=\bigoplus_{k=0}^{\infty}\mathcal{D}_k.$$

Thus, for example

$$\mathcal{D}_3=\text{span}\{u_{xxx},u_{xx}u_x,u_x^3\}.$$

Clearly, dim $\mathcal{D}_k=$number of partitions of k, denoted by $\#(k)$. With this notation it is easy to describe the problem to be studied.

Consider the evolution equation

$$u_t=K_1, \tag{2.1}$$

where $K_1=uu_x\in\mathcal{D}_1$, and corresponding symmetry

$$u_\tau=Q_1, \tag{2.2}$$

where $Q_1=f(u)u_x\in\mathcal{D}_1$. Suppose the equation (2.1) is deformed by an arbitrary element $K_3\in\mathcal{D}_3$

$$u_t=K[\hbar],$$

$$=K_1+\hbar^2K_3.$$

Can one construct a corresponding deformation of the symmetry (2.2)

$$u_\tau=Q[\hbar],$$

$$=\sum_{n=0}^{\infty}\hbar^{2n}Q_{2n+1}$$

with $Q_i\in\mathcal{D}_i$ and Q_1 as above? The deformation parameter $\hbar$ should be regarded as a formal parameter, labeling the scaling dimensions of the terms it precedes, rather than a small parameter. One may, at the end of all calculations, set $\hbar=1$.

By definition, the symmetry $Q[\hbar]$ must satisfy the governing equation

$$K[\hbar]'Q[\hbar]-Q[\hbar]'K[\hbar]=0,$$

and equating powers of $\hbar$ give the basic equation

$$K_1'Q_{2n+1}-Q_{2n+1}'K_1=Q_{2n-1}'K_3-K_3'Q_{2n-1}, \quad n\in\mathbb{N}. \tag{2.3}$$

By construction the equation for the lowest power $\hbar^0$ is automatically satisfied. This equation (2.3) looks complicated but, since all the elements lie in various spaces with fixed scaling dimension, it reduces to an overdetermined linear system.

III. INTEGRABLE DEFORMATIONS OF THE MONGE EQUATION

In this section equation (2.3) will be studied in more detail, with

$$K_1=uu_x,$$

$$K_3=a(u)u_{xxx}+b(u)u_{xx}u_x+c(u)u_x^3, \quad a,b,c\in C^\infty(\mathbb{R}),$$

$$Q_1=f(u)u_x,$$

so

$$u_t=uu_x+\hbar^2(a(u)u_{xxx}+b(u)u_{xx}u_x+c(u)u_x^3). \tag{3.1}$$

With these (2.3) becomes

$$\left[\sum_{r=1}^{2n+1}[(uu_1)_r-uu_{r+1}]\frac{\partial}{\partial u_r}-u_1\right]Q_{2n+1}=\begin{bmatrix}(a'u_3+b'u_2u_1+c'u_1^3)+\\(a\partial^3+bu_1\partial^2+bu_2\partial+3u_1^2\partial)-\\\sum_{r=0}^{2n-1}\partial^r(au_3+bu_2u_1+cu_1^3)\frac{\partial}{\partial u_r}\end{bmatrix}Q_{2n-1}, \tag{3.2}$$

or schematically as

$$\mathcal{R}(Q_{2n+1})=\mathcal{S}(Q_{2n-1}), \tag{3.3}$$

where

$$\mathcal{R}:\mathcal{D}_n\to\mathcal{D}_{n+1},$$

$$\mathcal{S}:\mathcal{D}_n\to\mathcal{D}_{n+3}.$$

One may regard this equation in a number of ways.

(i) as a first-order quasilinear equation in the independent variables u_1,u_2 etc., and solve it using the method of characteristics. However, one requires, for the purposes of this paper, the solution to lie in $\mathcal{D}_{2n+1}$, which is hard to guarantee using this method;
(ii) as a problem in differential Galois theory—one requires the solution to this linear equation with coefficients in a particular ring to lie in that ring and not in some extension; and
(iii) as an overdetermined linear system.

This third approach is the one that we will be using here. This interpretation holds because ∂_u does not appear in the operator $\mathcal{R}$, so no derivatives of the unknown coefficients appear. By introducing a basis for $\mathcal{D}_{2n+3}$ one obtains $\#(2n+3)$ linear equations for $\#(2n+1)$ unknowns.

In the next section it will be shown that the rank of $\mathcal{R}$ (viewed as a matrix) is maximal, and hence the solution to this linear problem, if it exists, is unique. Existence is more problematic.

While the form of the matrix $\mathcal{R}$ is easy to understand, the "source" vector $\mathcal{S}(Q_{2n-1})$ is complicated, depending on all lower-order solutions, and so it would be extremely difficult to compute, in general, the rank of the extended matrix. By direct calculation (using MATHEMATICA) explicit solutions up to $O(\hbar^6)$ have been calculated. This suggests the conjecture that a solution exists for all n, so a formal symmetry of Eq. (3.1) of the form $\Sigma\hbar^{2n}Q_{2n+1}\in\mathcal{D}$ exists.

IV. UNIQUENESS

One way to prove that the equation (3.3) has a unique solution is to introduce an ordered basis for each subspace $\mathcal{D}_k$ of monomials u^I—the reverse lexiographic ordering—so, for example

$$\mathcal{D}_5=\text{span}\{u_5,u_4u_1,u_3u_2,u_3u_1^2,u_2^2u_1,u_2u_1^3,u_1^5\},$$

and this basis may be ordered

$$u_5\succ u_4u_1\succ u_3u_2\succ u_3u_1^2\succ u_2^2u_1\succ u_2u_1^3\succ u_1^5.$$

The symbol $\max\{v\}$ will denote the highest basis vector in the expansion of v in this ordered basis.

Lemma 1: In the reverse lexiographic ordered basis the operator $\mathcal{R}:\mathcal{D}_n\to D_{n+1}$ is lower-triangular.

It then follows that the equation $\mathcal{R}v=0$ has the unique solution $v=0$ and hence that the solution to (3.3), if it exists, is unique.

Proof: Let u^I be a monomial in $\mathcal{D}_n$, I being a multi-index. From the explicit form of $\mathcal{R}$ it follows that

$$\max\{\mathcal{R}u^I\}=u^Iu_1.$$

Suppose that $u^I\succ u^J$. Then

$$\max\{\mathcal{R}u^I\}=u^Iu_1\succ u^Ju_1=\max\{\mathcal{R}u^J\}.$$

Hence, in this basis, the matrix $\mathcal{R}$ is lower-triangular. □

For example

$$\mathcal{R}[g_1u_{xxx}+g_2u_{xx}u_x+g_3u_x^3]=3g_1u_{xxx}u_x+3g_1u_{xx}^2+3g_2u_{xx}u_x^2+2g_3u_x^4,$$

so in the reverse lexiographic basis, $\mathcal{R}$ may be represented as the 3×5 matrix

$$\mathcal{R}=\begin{pmatrix}0&0&0\\3&0&0\\3&0&0\\0&3&0\\0&0&2\end{pmatrix},$$

which clearly is of maximal rank.

V. EXISTENCE

Recall that the given data are K_1,K_3, and Q_1. Writing

$$Q_3=g_1u_{xxx}+g_2u_{xx}u_x+g_3u_x^3,$$

and solving the overdetermined linear system yields

$$g_1=af',$$

$$g_2 = bf' + 2af'',$$

$$g_3 = cf' + \tfrac{1}{2}bf'' + \tfrac{1}{2}af'''.$$

Thus, a solution exists. This gives an approximate symmetry, valid to $O(\hbar^2)$. Recycling this solution gives

$$Q_5 = h_1u_5 + h_2u_4u_1 + h_3u_3u_2 + h_4u_3u_1^2 + h_5u_2^2u_1 + h_6u_2u_1^3 + h_7u_1^5, \tag{5.1}$$

where the h_i are explicit functions of a, b, c, and f and their derivatives. These are given in Appendix A. The $O(\hbar^6)$ have also been calculated, again using MATHEMATICA, but little purpose is served by presenting them here—it suffices to say that they exist. Thus, for arbitrary functions a,b,c a unique symmetry, labeled by a suitably differentiable function f exists up to $O(\hbar^6)$. The existence of solutions up to this order of the over-determined linear system suggests the following.

Conjecture 1: A unique formal symmetry to the generalized KdV equation (3.1) *exists, labeled by a* $C^\infty(\mathbb{R})$-function.

If the conjecture is false, then this would raise the questions:

Conjecture 1′: At what order does the above conjecture fail? Is there a way to determine this order a priori?

Note that if the conjecture is true then one obtains an entirely new integrable hierarchy, depending on three arbitrary functions and with flows labeled by another arbitrary function. If it is false, then one may obtain the notion of an *approximately* integrable system, which has an infinite number of formal symmetries up to some fixed order (an example where obstructions do exist is given in Appendix B). Either outcome is of interest. In a particular case, Lorenzoni[6] has numerically observed elastic soliton scattering indicative of integrability. It would be interesting to see if basic integrability results such as inverse scattering could be modified (by, say, only including terms up to a given order) to include such approximate integrable systems.

A. Formal symmetries of the KdV equation

In this approach, the KdV equation itself is recovered as the special case $a=1$, $b=c=0$, and the symmetry takes the form

$$u_\tau = f(u)u_x + \hbar^2[f'u_{xx} + \tfrac{1}{2}u_x^2f'']_x + \hbar^4[\tfrac{1}{8}f^{(5)}u_x^4 + \tfrac{11}{10}f^{(4)}u_x^2u_{xx} + \tfrac{9}{10}f^{(3)}u_{xx}^2 + \tfrac{6}{5}f^{(3)}u_xu_{xxx} + \tfrac{3}{5}f^{(2)}u_{xxxx}]_x + O(\hbar^6).$$

[again, the $O(\hbar^6)$ terms have been calculated explicitly, though not displayed here]. One may prove from the now simplifier version of (2.3) that for the series to terminate the function f must be a polynomial, say $f=\Sigma_{r=0}^N\alpha_ru^r$, and one recovers a linear combination of the flows obtained via the recursion operator (1.3)

$$u_{t_N} = \left(\sum_{r=0}^{N}\alpha_r\mathcal{R}^r\right)u_x.$$

It would be of interest to see if the general flow generated from an arbitrary f could be written as $u_\tau = F(\mathcal{R})u_x$ for some suitable F.

Much has been written about the symmetries of the KdV equation. However, in such approaches the order of the symmetry is fixed, and the lower-order terms are determined from the higher ones. Here the approach is opposite—determine the higher-order terms from lower ones. The symmetries obtained in this way will turn out to be formal—infinite series. This approach is motivated, as was mentioned in the Introduction, by ideas originating in topological quantum field theories, where the deformation is known as a genus expansion, and from the deformation quantization program, where in both areas one constructs higher-order terms from lower-order ones.

B. Local Hamiltonian systems

An important subclass of systems in this class are those that are Hamiltonian with respect to the local Hamiltonian operator $\mathcal{H}_1=\partial$, so the generalized KdV equation (3.1) takes the form

$$u_t=\mathcal{H}_1\frac{\delta}{\delta u}H,$$

for some Hamiltonian H. This places the following restriction on the arbitrary functions a,b,c:

$$a(u)=s(u),$$

$$b(u)=2s'(u),$$

$$c(u)=\tfrac{1}{2}s''(u),$$

where s is an arbitrary function. With these (3.1) may be written in Hamiltonian form

$$\begin{aligned}u_t&=uu_x+\hbar^2[s(u)u_{xxx}+2s'(u)u_{xx}u_x+\tfrac{1}{2}s''(u)u_x^3],\\&=\frac{d}{dx}\frac{\delta}{\delta u}\left[\frac{u^3}{6}-\hbar^2\frac{1}{2}s(u)u_x^2\right].\end{aligned}$$

The formal symmetries are also Hamiltonian

$$u_\tau=\frac{d}{dx}\frac{\delta}{\delta u}\left[f^{(-2)}-\hbar^2\left\{\frac{1}{2}sf''\right\}u_x^2+\hbar^4\left\{\frac{3}{10}s^2f''u_{xx}^2-\frac{1}{4!}\left[\frac{3}{2}(s^2)''f''+s^2f^{(6)}\right]u_x^4\right\}\right]+O(\hbar^6)$$

(where $\partial^2 f^{(-2)}=f$). Again, the $O(\hbar^6)$ terms have been calculated, and are also Hamiltonian, which suggests the following.

Conjecture 2. The formal system in Conjecture 1 is Hamiltonian to all orders.

This system has been extensively studied, for $f(u)=u^n$, by Lorenzoni.[6] He showed that the system is, up to $O(\hbar^4)$, bi-Hamiltonian, with the second Hamiltonian structure being a deformation of the second Hamiltonian structure of the Monge/Riemann hierarchy. The existence of such terms in this deformation is controlled by a certain cohomology group.

C. Deformation of conservation laws and asymptotic integrability

Consider the special case of (3.1), where a,b and c are constants, so

$$u_t=uu_x+\hbar^2(au_{xxx}+bu_{xx}u_x+cu_x^3). \tag{5.2}$$

This equation coincides with an example obtained from the theory of asymptotic integrability.[4,5] With a scaling based on the dimensions $[u]=2,[\partial_x]=1$, the above equation may be written as

$$u_t=[uu_x+\hbar^2au_{xxx}]+\varepsilon[\hbar^2bu_{xx}u_x]+\varepsilon^2[\hbar^2cu_x^3],$$

and viewed as a deformation of the KdV equation (rather than of the dispersionless KdV equation). The method of asymptotic integrability considers deformations of the conservation laws of the KdV hierarchy. For the energy and momentum integrals

$$I_0=\int_{\mathrm{R}}u\,dx,\quad I_1=\int_{\mathrm{R}}u^2dx,$$

to be conserved integrals for (5.2) implies $b=c=0$, i.e., only the KdV equation itself belongs to the class. Thus, the existence of (physically reasonable) conservation laws places far stronger

conditions on the system that the existence of formal symmetries (at least at low order). Understanding the relationship between these two methods, based on different scaling, clearly deserves further study.

VI. TRIVIAL AND QUASI-TRIVIAL MIURA TRANSFORMATIONS

In Ref. 2, transformation of the form

$$u \mapsto v = u + \sum_{k=1}^{\infty} \hbar^k \tilde{F}_k(u; u_x, \ldots, u^{(n_k)}),$$

where $\tilde{F}_k$ are quasihomogeneous rational functions, was considered together with the corresponding action on bi-Hamiltonian pencils. Such transformations were called quasi-Miura transformations. In particular, the notion of trivial and quasitrivial transformations was given. In the context of this paper, where local bi-Hamiltonian structures are not considered, an evolution equation $u_t = uu_x + \Sigma_r \hbar^r K_r[u]$ will be said to be quasitrivial if it transforms under a quasi-Miura transformation to the Monge equation $v_t = vv_x$, and trivial if the further condition that the functions F_k are polynomial is satisfied.

With the ansatz

$$v = u + \sum_{r=1}^{\infty} \frac{\hbar^{2r}}{u_x^{4r-2}} F_r[u, u_1, \ldots, u_{6r-2}], \quad F_r \in \mathcal{D}_{6r-2}$$

one may easily obtain recursion relations for the F_r which take the form

$$\tilde{\mathcal{R}}(F_n) = \text{function of } F_1, \ldots, F_{n-1}$$

where

$$\tilde{\mathcal{R}}: \mathcal{D}_n \to \mathcal{D}_{n+2}$$

is given by

$$\tilde{\mathcal{R}} = u_1 \mathcal{R} + (2-4n) u_1^2$$

with $\mathcal{R}$ being the previously introduced recursion operator. It follows immediately from a repetition of the argument in Sec. IV that this quasi-Miura transformation, if it exists, is unique, since the operator $\tilde{\mathcal{R}}$ is lower-triangular in the reverse lexiographic ordered basis.

Lemma 2: The generalized KdV equation (3.1) is, up to $O(\hbar^4)$, quasitrivial.

This may be proved by direct calculation. The quasi-Miura transformation is

$$v = u + \frac{\hbar^2}{u_x^2}\left(\frac{1}{2}a(u)(u_{xxx}u_x - u_{xx}^2) + \frac{1}{2}b(u)u_{xx}u_x^2 + c(u)u_x^4\right) + \frac{\hbar^4}{u_x^6} f(u, u_x, \ldots, u_{10x}),$$

where $f \in \mathcal{D}_{10}$ has been explicitly calculated, though not displayed here. In Ref. 2 it was shown that the KdV equation is quasitrivial to all orders, this proof using the existing machinery for the KdV equation. Conjecturally the generalized KdV equation studied here will be quasitrivial to all orders, though to prove it would first involve the development of a lot of associated machinery which, for the KdV equation, already exists in the literature.

One immediate question is whether the quasitrivial equation (3.1) can, for suitable choice of functions a, b, c be trivial. From the above form of the quasi-Miura transformation, it follows that at $O(\hbar^2)$ one requires $a(u) = 0$ and at $O(\hbar^4)$ one requires, in addition, $b(u) = 0$. After this no new constraints appear, at least to $O(\hbar^{10})$, the explicit quasi-Miura map being

$$v=u-\hbar^2 c u_1^2+\hbar^4\left(\frac{4}{3}cc'u_1^4+2c^2u_1^2u_2\right)+\hbar^6\left(\frac{-28cc'^2u_1^6}{15}-\frac{14c^2c''u_1^6}{15}-\frac{26c^2c'u_1^4u_2}{3}-4c^3u_1^2u_2^2\right.$$
$$\left.-\frac{4c^3u_1^3u_3}{3}\right)+\hbar^8\left(\frac{836cc'^3u_1^8}{315}+\frac{1268c^2c'c''u_1^8}{315}+\frac{16c^3c^{(3)}u_1^8}{35}+\frac{1138c^2c'^2u_1^6u_2}{45}\right.$$
$$\left.+\frac{128c^3c''u_1^6u_2}{15}+\frac{112c^3c'u_1^4u_2^2}{3}+8c^4u_1^2u_2^3+8c^3c'u_1^5u_3+8c^4u_1^3u_2u_3+\frac{2c^4u_1^4u_4}{3}\right)+O(\hbar^{10}).$$

Thus, the first-order, third-degree evolution equation

$$u_t=uu_x+\hbar^2c(u)u_x^3,$$

is trivial to $O(\hbar^8)$ and conjecturally to all orders. Further properties of this system are outlined in the next section.

VII. FIRST-ORDER DEFORMATION OF ARBITRARY DEGREE

Exact results to all orders may be obtained in the above special case $a=b=0, c(u)=\alpha(u)$. The basic equation (3.1) simplifies to

$$u_t=uu_x+\hbar^2\alpha(u)u_x^3, \quad \alpha\in C^\infty(\mathbb{R}) \tag{7.1}$$

and the governing equation (2.3) simplifies drastically. With the ansatz

$$Q_{2n+1}=\beta_n(u)u_x^{2n+1},$$

one obtains the recursion relation

$$n\beta_n=(1-n)\alpha'\beta_{n-1}+\alpha\beta_{n-1}', \quad n\geqslant 1,$$

and hence, since $\beta=\beta_0$ is arbitrary, the solution

$$\beta_n=\frac{1}{n!}\alpha^n\beta^{(n)}.$$

Thus, the general symmetry of the first-order, third-degree equation (7.1) is

$$u_{\tau_\beta}=\sum_{n=0}^{\infty}\hbar^{2n}\frac{\alpha^n\beta^{(n)}}{n!}u_x^{2n+1}.$$

Thus, the space of commuting flows for Eq. (7.1) is labeled by an arbitrary function $\beta\in C^\infty(\mathbb{R})$. This series truncates if and only if β is a polynomial. This symmetry is, within the constraints of this paper, unique. It can easily be checked that all the symmetries commute amongst themselves, i.e.,

$$(u_{\tau_\beta})_{\tau_\gamma}=(u_{\tau_\gamma})_{\tau_\beta},$$

for arbitrary C^∞-functions α,β,γ.

The equation (7.1) is Hamiltonian with respect to the nonlocal Hamiltonian operator

$$\mathcal{H}=u_x\partial^{-1}u_x,$$

so

$$u_t=\left(\mathcal{H}\frac{\delta}{\delta u}\right)\int (u-\hbar^2\alpha(u)u_x^2)dx.$$

The symmetry itself is also Hamiltonian

$$u_{\tau_\beta}=\mathcal{H}\frac{\delta H_\beta}{\delta u},$$

where the Hamiltonian is

$$H_\beta=\int \sum_{r=0}^{\infty}\frac{\hbar^{2r}}{(1-2r)}\alpha^r\beta^{(r)}u_x^{2r}dx,$$

and these are all conserved with respect to all the symmetries, as one would expect for an integrable system. Owing to the arbitrariness in the functions α and β, it is unlikely that (7.1) will possess the Painlevé property.

VIII. CONCLUSIONS

The central philosophy behind this paper is that the dispersionless limits of integrable systems should not been seen as some limit, but as the kernel of the dispersive hierarchy itself, encapsulating its integrability. To describe the full dispersive hierarchy one just has to specify a suitable ''deformation vector'' in some space of possible first-order deformations, from which the dispersive hierarchy, if it exists, may be uniquely reconstructed. In this paper this vector is K_3, living in the space of possible first-order deformations $\mathcal{D}_3$. If the above conjecture is true, then this specifies the hierarchy at all orders. For equations of hydrodynamic type constructed from semisimple Frobenius manifolds this choice is automatic[2,3]—elliptic Gromov–Witten invariants may be constructed from the genus-zero data. See also Ref. 3, where examples are given where higher-order deformations do not exist.

As a multidimensional example, consider the system

$$\mathbf{U}_t=\mathbf{U}\circ\mathbf{U}_x,$$

where $\circ$ is the product is some N-dimensional, commutative N- dimensional algebra. With ceratin simple additional conditions on this algebra one may show that a hierarchy exists if and only if the algebra is a Jordan algebra.[9] It then may be shown that the deformed system

$$\mathbf{U}_t=\mathbf{U}\circ\mathbf{U}_x+\hbar^2\mathbf{U}_{xxx}$$

(corresponding to the deformation vector

$$\mathbf{U}_{xxx}\in\mathcal{D}_3^N=\text{span}\{u^i_{xxx},u^i_{xx}u^j_x,u^i_xu^j_xu^k_x,i,j,k=1,\ldots,N\},$$

where $\mathbf{U}=u^ie_i$ and the e_i form a basis for the algebra) defines a full dispersive hierarchy with no extra conditions required. It would be interesting to repeat these calculations for a more general vector in $\mathcal{D}_3^N$—the results in this paper being for $N=1$ only.

It may also be of interest to generalize the construction, in particular the quasitriviality property, to include K_5 terms in (2.3)

$$u_t=K_1+\hbar^2K_3+\hbar^4K_5.$$

A number of known systems fall into this class (with $K_1=u^2u_x$), including the higher flow of the KdV equation, KdV_5, the Sawada/Kotera equation, the Caudrey/Dodd/Gibbons/Kaup equation, and the Kaup/Kupershmidt equation. This paper suggests a possible classification of such fifth-

order systems. Also, little mention has been made of bi-Hamiltonian structures in this paper. Such structures may be generated from the known bi-Hamiltonian pencil of the Monge equation

$$\{u(x),u(y)\}_\lambda=(u-\lambda)\delta'(x-y)+\tfrac{1}{2}u_x\delta(x-y),$$

via the appropriate quasi-Miura transformation. These, however, are unlikely to truncate.

The results outlined here have been computational; to obtain rigorous results at all orders in the expansion new techniques will have to be developed. In particular, a better understanding of the overdetermined linear systems from which results of this paper were obtained will be required.

APPENDIX A: THE $O(\hbar^4)$ ORDER TERMS

The explicit form of the h_i in Eq. (5.1) are

$$h_1=(3a^2f'')/5,$$

$$h_2=abf''+(8aa'f'')/5+(9a^2f^{(3)})/5,$$

$$h_3=2abf''+2aa'f''+3a^2f^{(3)},$$

$$h_4=(2b^2f'')/5+(11acf'')/5+ba'f''+(13ab'f'')/10+(7af''a'')/5+(5abf^{(3)})/2 +(37aa'f^{(3)})/10+(23a^2f^{(4)})/10,$$

$$h_5=(8b^2f''+5b(a'f''+7af^{(3)})+a(14cf''+26b'f''+13f''a''+44a'f^{(3)}+31af^{(4)}))/10,$$

$$h_6=(9b^2f^{(3)}+b(18cf''+9b'f''+4f''a''+15a'f^{(3)}+25af^{(4)})+2(4ca'f''+10ac'f''+7af''b'' +16acf^{(3)}+14ab'f^{(3)}+12aa''f^{(3)}+2af''a^{(3)}+18aa'f^{(4)}+8a^2f^{(5)}))/10,$$

$$h_7=(4c^2f''+b^2f^{(4)}+2c(b'f''+2bf^{(3)}+a'f^{(3)}+2af^{(4)})+b(2c'f''+f''b''+2b'f^{(3)}+a''f^{(3)} +2a'f^{(4)}+2af^{(5)})+a(2f''c''+4c'f^{(3)}+3b''f^{(3)}+f^{(3)}a^{(3)}+f''b^{(3)}+3b'f^{(4)}+3a''f^{(4)} +3a'f^{(5)}+af^{(6)}))/8.$$

The 15 coefficients in the next-order term have been calculated, but are not presented here.

APPENDIX B: THE KURAMUTO–SIVASHINSKY EQUATION

Consider the Kuramoto–Sivashinsky equation (suitably scaled)

$$u_t=uu_x+\hbar u_{xx}+\hbar^3u_{xxxx}.$$

The dispersionless limit of this equation is just the Monge equation, and hence the methods developed in the main body of this paper may be applied to seek, term-by-term, a formal symmetry

$$u_\tau=f(u)u_x+\hbar Q_1+\hbar^2Q_2+\hbar_3Q_3+\hbar^4Q_4+O(\hbar^5).$$

By direct calculation, one obtains

$$Q_1=f'u_{xx}+f''u_x^2,$$

$$Q_2=\tfrac{2}{3}f''u_{xxx}+\tfrac{5}{3}f''u_{xx}u_x+\tfrac{1}{2}f^{(4)}u_x^3,$$

$$Q_3=(f'+\tfrac{1}{3})u_{xxxx}+(\tfrac{5}{2}f''+f^{(4)})u_{xxx}u_x+(\tfrac{3}{2}f''+\tfrac{2}{3}f^{(4)})u_{xx}^2+(\tfrac{5}{2}f^{(3)}+\tfrac{7}{6}f^{(5)})u_{xx}u_x^2 + (\tfrac{1}{2}f^{(4)}+\tfrac{1}{6}f^{(6)})u_x^4.$$

However, at the next order an obstruction appears, and hence Q_4 does not exist (interestingly, if the term u_{xxxx} is replaced by αu_{xxxx} an obstruction appear for Q_3; this vanishes if and only if $\alpha=1$). Thus, the Kuramoto–Sivashinsky equation does not possess a hierarchy of formal symmetries, thus indicating its nonintegrability (a result that may also be obtained via Painlevé analysis[7]). It does, however, possess an infinite number of formal symmetries up to $O(\hbar^3)$. Thus, this method may be used as a test of integrability (though, as with all such test, with care, as one is only looking for expansions in some given, *a priori*, ring of functions).

ACKNOWLEDGMENTS

I would like to thank the referee for his/her comments. Financial support was provided by the EPSRC Grant No. GR/R05093.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

Constructing solutions of Hamilton–Jacobi equations for 2D fields with one component by means of Bäcklund transformations

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(Received 14 March 1995; accepted 27 November 1995)

The Hamilton–Jacobi formalism generalized to two-dimensional field theories according to Lepage's canonical framework is applied to several relativistic real scalar fields, e.g., massless and massive Klein–Gordon, Sinh and Sine–Gordon, Liouville and ϕ^4 theories. The relations between the Euler–Lagrange and the Hamilton–Jacobi equations are discussed in DeDonder and Weyl's and the corresponding wave fronts are calculated in Carathéodory's formulation. Unlike mechanics one has to impose certain integrability conditions on the velocity fields to guarantee the transversality relations and especially the dynamical equivalence between Hamilton–Jacobi wave fronts and fields of extremals embedded therein. Bäcklund transformations play a crucial role in solving the resulting system of coupled nonlinear PDEs. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1526451]

I. INTRODUCTION

Varying a relativistically invariant action integral leads to covariant Euler–Lagrange equations. However, if one wants to reformulate the theory in terms of the conventional canonical Hamiltonian framework, one has to break the manifest covariance by distinguishing a time variable and regarding the other ''spatial'' coordinates as ''indices'' representing an infinite number of degrees of freedom. The method is widely known from elementary particle physics, canonical gravity, and other field theories. This approach, however, can obscure a part of the rich geometrical structure contained in a generally covariant framework, at least on the classical level.[1]

Utilizing Cartan's theory of alternating forms Lepage and others showed that a large variety of algebraically inequivalent covariant Hamiltonian formulations, including Hamilton–Jacobi equations, exists, e.g., that of DeDonder and Weyl[2,3] and that of Carathéodory,[4] where only the latter one provides a Hamilton–Jacobi equation the associated wave fronts which have the same nice transversality properties with respect to the extremals as one has in mechanics. All this has been discussed in detail in Ref. 1 where many references to previous work on the subject are given. Newer and additional papers can be found in Refs. 5–10, where the formalism is discussed in the framework of fibered Jet manifolds.

In mechanics one can construct solutions of the canonical equations of motion if one has an appropriate solution of the corresponding Hamilton–Jacobi equation, the solutions of which describe wave fronts which are transversal to a ''field'' of extremals and which contain the same dynamical information as the extremals themselves.

For field theories this is no longer true:[1] Solutions of the Hamilton–Jacobi equation (HJE) associated with one of the canonical frameworks mentioned above provide ''velocity'' fields which in general do not obey the necessary integrability conditions (ICs). The latter have to be postulated

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separately and give rise to an additional set of partial differential equations. However, if these equations and the associated Hamilton–Jacobi equation are satisfied, then combined they contain the same dynamical content as the Euler–Lagrange equations.[1] Thus, it is possible to construct solutions of the Euler–Lagrange field equations (ELEs) by solving a Hamilton–Jacobi equation and a set of integrability conditions.

The aims of the present article are the following ones:

(1) All the different canonical formalisms just mentioned coincide if the field has just one real component,[1] especially for fields in two space–time or Euclidean dimensions. In this case one can use the simpler DeDonder and Weyl HJE in order to solve it simultaneously with one integrability condition. Here we do not construct completely new solutions of the ELE but find one-parameter extensions of a given solution φ_0. The method is applied to the following one-component models in two dimensions: massive and massless Klein–Gordon, sinh–, sine–Gordon, Liouville and ϕ^4 theory. The solutions of the HJE plus IC are constructed by expanding the solutions of these equations in powers of the field variables. This leads to a hierarchy of nonlinear partial differential equations (PDEs) that can be transformed into linear PDEs with nonconstant coefficients. By applying integrable Bäcklund transformations these PDEs can be reduced further to free (massive or massless) Klein–Gordon equations. Remarkably, it is only necessary to solve just two linear PDEs in order to obtain the general solution for *every* order of the hierarchy!

(2) The solutions of the DeDonder and Weyl HJE do not have the appropriate transversality properties required to construct the wave fronts associated with a given one-parameter set of extremals. Those have to be given in terms of the solutions of the more complicated HJE of Carathéodory. As we are dealing with one-component fields here only, the two canonical frameworks are equivalent and one can construct the one-dimensional Carathéodory wave fronts from the solutions of the DeDonder and Weyl HJE. This procedure will be outlined and applied to given solutions (e.g., solitons) of the models mentioned above.

The article is organized as follows:

In Sec. II we very briefly summarize Lepage's reformulation of canonical mechanics and its generalization to field theories with one component in two dimensions and especially the HJEs of DeDonder and Weyl and of Carathéodory, respectively. All the details are contained in Ref. 1.

In Sec. III we study the hierarchy of equations derived within the Hamilton–Jacobi framework of DeDonder and Weyl and the associated integrability condition for the velocity fields by expanding the wave fronts in powers of the field variable φ in the neighborhood of φ_0.

In Sec. IV we determine the Bäcklund transformations which reduce this hierarchy of linear PDEs with nonconstant coefficients to free field equations.

In Sec. V we apply the general results to several well-known models and point out some relations to stability problems of solitons.

In Sec. VI we discuss the relations between the hierarchies of PDEs derived from expanding the HJE and the IC and a corresponding expansion of the Euler–Lagrange equations. Solutions of the equations of motions are determined from those of the HJE and the IC perturbatively. The kink solution of the sine–Gordon equations is treated in considerable detail here.

In Sec. VII we calculate the wave fronts by means of Carathéodory's formulation, especially for the kink solution just mentioned.

II. HAMILTON–JACOBI THEORIES FOR FIELDS

In the present chapter we very briefly recapitulate the main features of Lepage's approach to a geometrical canonical framework for field theories, especially its associated Hamilton–Jacobi equation. The details are discussed in Ref. 1. As we are interested mainly in local properties of the various partial differential equations and their solutions, we do not employ the more sophisticated formalism of fibered Jet manifolds, which can be found in Refs. 5–10 and which is more useful for the discussion of global and certain structural problems not investigated in the following. Furthermore, this formalism has been applied to the DeDonder and Weyl case only.

We begin by very briefly recalling Lepage's main idea[1,11] of introducing the canonical formalism in mechanics for one configuration variable q.

A. Lepage's canonical formulation of mechanics

The starting point of the canonical theory for Lagrangian canonical systems is an action functional. In mechanics it is given by a Lagrangian one-form ω integrated along a path $\mathcal{C} := \{t, q = q(t), t \in I_{1,2} = [t_1, t_2]\}$ in the extended configuration space $\mathcal{M}_{1+1} := \{(t,q)\}$:

$$\mathcal{A}[\mathcal{C}] = \int_{\mathcal{C}} \omega = \int_{I_{1,2}} L(t,q,\dot{q})\, dt.$$

As to the variational principle it is preferable to consider the generalized velocity v as an independent variable, which coincides with $\dot{q}$ on the extremals $\mathcal{C} = \mathcal{C}_0 := \{(t, q = q_0(t)), t \in I_{1,2}\}$. Normally this extension in the number of variables is performed by using Lagrangian multipliers. Lepage's reformulation of the variational principle is similar in spirit.[11]

The initial canonical Lagrangian form $\omega = L(t,q,\dot{q})\mathrm{d}t$ is extended by the product of a Lagrangian multiplier $h(t,q,v)$ and the Pfaffian form $\varrho = \mathrm{d}q - v\,\mathrm{d}t$ vanishing on the tangent vectors of the extremals, which ensures the identification of $v(t)$ with $\dot{q}(t)$ on the solutions of the equation of motion. Then the action integral $\mathcal{A}[\mathcal{C}]$ over the path $\mathcal{C} := \{(t, q(t)), t \in I_{1,2}\}$ can be modified

$$\mathcal{A}[\mathcal{C}] \to \tilde{\mathcal{A}}[\mathcal{C}] = \int_{\mathcal{C}} \Omega = \int_{I_{1,2}} [L(t,q,v)\,\mathrm{d}t + h(t,q,v)\varrho], \tag{2.1}$$

without changing the Euler–Lagrange equations and their solutions $\mathcal{C} = \mathcal{C}_0$.

The form ϱ generates an ideal $I[\varrho]$ in the algebra Λ of forms of the cotangent bundle of the extended configuration space $\mathcal{M}_{1+1} := \{(t,q)\}$: if $\alpha \in \Lambda$ and $\beta \in I[\varrho]$, then $\alpha \wedge \beta$ is also an element of the ideal $I[\varrho]$.

The Lagrangian multiplier $h(t,q,v)$ can be fixed by varying the action integral (2.1) with respect to q, v independently. This leads to the standard definition of the canonical momentum: $h \overset{!}{=} \partial_v L =: p$.

We obtain the same results by requiring $\mathrm{d}\Omega$ to be an element of the ideal $I[\varrho]$:

$$\mathrm{d}\Omega = (\partial_v L - h)\mathrm{d}v \wedge \mathrm{d}t + (\mathrm{d}h - \partial_q L\,\mathrm{d}t) \wedge \varrho = \underbrace{(\partial_v L - h)\mathrm{d}v \wedge \mathrm{d}t}_{=0!} + 0 (\mathrm{mod} I[\varrho]).$$

Hence Ω is a closed two-form on fields of extremals covering the extended configuration space $\mathcal{M}_{1+1} = \{(t,q)\}$—or correspondingly—a (Lagrangian) submanifold $\mathcal{Q} := \{t, q, p = \psi(t,q) | (t,q) \in M\}$ of the extended phase space $\mathcal{P}_{2+1} := \{(t,q,p)\}$.

Following Poincaré's lemma Ω is locally (at least) exact $\Omega = \mathrm{d}S(t,q)$ on $\mathcal{Q}$.

According to Lepage[11] the Legendre transformation $L \to H$, $v \to p$ can be implemented as a change of basis in the cotangent bundle $\mathcal{T}^*(\mathcal{M}_{1+1})$, $\varrho \to \mathrm{d}q$, $\mathrm{d}t \to \mathrm{d}t$:

$$\Omega = L\,\mathrm{d}t + p\varrho = L\,\mathrm{d}t + p(\mathrm{d}q - v\,\mathrm{d}t) = -(pv - L)\mathrm{d}t + p\,\mathrm{d}q = -H\mathrm{d}t + p\mathrm{d}q.$$

H denotes the usual Hamiltonian $H = pv - L = H(p,q,t)$.

The existence of a potential $S(t,q)$ for the basic differential form $\Omega = \mathrm{d}S$ yields the familiar Hamilton–Jacobi equation for $S(t,q)$ and the corresponding condition for the momentum:

$$\Omega = -H(t,q,p = \psi(t,q))\mathrm{d}t + \psi(t,q)\mathrm{d}q \overset{!}{=} \mathrm{d}S(t,q) = \partial_t S(t,q)\mathrm{d}t + \partial_q S(t,q)\mathrm{d}q.$$

Comparing the coefficients of $\mathrm{d}t$, $\mathrm{d}q$ yields

$$\partial_t S(t,q) + H(t,q,p = \psi(t,q)) = 0, \quad p = \psi(t,q) = \partial_q S(t,q).$$

The extremals can be determined, if a complete integral of the Hamilton–Jacobi equation is found. Dealing with one independent variable q this integral depends on one constant c_0. The solution of the equation of motion can be calculated by solving the algebraic relation $\partial_{c_0} S(t,q,c_0)=c_1$ with a second constant c_1.

In mechanics there exists a special relation between the wavefront $S(t,q)=\sigma=\text{const}$, $\sigma\in\mathcal{R}$ and the extremals $q=q_0(t)$ called "*transversality*:" the union of their respective tangent spaces $\text{span}\{e_t=\partial_t+\dot{q}(t)\partial_q\}$ and $\text{span}\{w=p\partial_t+H\partial_q\}$, span the whole tangent space $\mathcal{T}_P(\mathcal{M}_{1+1})$ at any point $P\in\mathcal{M}_{1+1}$, if the Lagrangian L does not vanish in the field of extremals, because of

$$\det(e_t,w)=\det\left|\begin{pmatrix}1 & p\\ v & H\end{pmatrix}\right|=(H-\dot{q}p)=-L.$$

This concept of the Hamilton–Jacobi framework developed for mechanics can easily be generalized to field theories. We confine our discussion to those theories depending on *one* real scalar field $\varphi=\varphi(z,\overline{z})$ in a 1+1 dimensions. Here $z,\overline{z}$ play the role of lightcone variables. For details see Refs. 1–3.

B. The Hamilton–Jacobi theories of DeDonder and Weyl and of Carathéodory

As in mechanics a canonical theory for fields is based on an action functional $\mathcal{A}[\Sigma]$ defined on a two-dimensional surface $\Sigma:=\{(z,\overline{z},\varphi(z,\overline{z})),z,\overline{z}\in\mathcal{G}\}$, where $\mathcal{G}\in\mathcal{R}^2$ is compact, in the extended configuration space $\mathcal{M}_{2+1}:=\{(z,\overline{z},\varphi)\}$:

$$\mathcal{A}[\Sigma]=\int_\Sigma\omega=\int_{\mathcal{G}}\mathcal{L}(z,\overline{z},\varphi(z,\overline{z}),\quad v=\partial_z\varphi,\quad \overline{v}=\partial_{\overline{z}}\varphi)\,\mathrm{d}z\wedge\mathrm{d}\overline{z}.$$

Only on the extremals $\varphi=\varphi_0(z,\overline{z})$ the generalized velocities v, $\overline{v}$ coincide with the derivatives of the fields: $v=\partial_z\varphi_0$, $\overline{v}=\partial_{\overline{z}}\varphi_0$.

The canonical two-form $\omega=\mathcal{L}\mathrm{d}z\wedge\mathrm{d}\overline{z}$ is extended by means of two Lagrangian parameters $h(z,\overline{z},\varphi)$, $\overline{h}(z,\overline{z},\varphi)$ and a one-form $\varrho=\mathrm{d}\varphi-v\,\mathrm{d}z-\overline{v}\,\mathrm{d}\overline{z}$ that vanishes on the two-dimensional extremals $\varphi=\varphi_0(z,\overline{z})$:

$$\Omega=\mathcal{L}\mathrm{d}z\wedge\mathrm{d}\overline{z}+\overline{h}\mathrm{d}z\wedge\varrho+h\varrho\wedge\mathrm{d}\overline{z}. \tag{2.2}$$

The Lagrangian multipliers $h,\overline{h}$ are determined by requiring $\mathrm{d}\Omega\in I[\varrho]$:

$$\mathrm{d}\Omega=(\partial_v\mathcal{L}-h)\mathrm{d}v\wedge\mathrm{d}z\wedge\mathrm{d}\overline{z}+(\partial_{\overline{v}}\mathcal{L}-\overline{h})\mathrm{d}\overline{v}\wedge\mathrm{d}z\wedge\mathrm{d}\overline{z}+0(\mathrm{mod}I[\varrho])\overset{!}{=}0(\mathrm{mod}I[\varrho]),$$

yielding

$$h\overset{!}{=}\partial_v\mathcal{L}=:p,\quad \overline{h}\overset{!}{=}\partial_{\overline{v}}\mathcal{L}=:\overline{p}.$$

The Legendre transformation $\mathcal{L}\to\mathcal{H}$, $\{v,\overline{v}\}\to\{p,\overline{p}\}$ can be implemented as a change of the basis in the cotangent bundle $\mathcal{T}^*(\mathcal{M}_{2+1})$, $\varrho\to\mathrm{d}\varphi$, $\mathrm{d}z\to\mathrm{d}z$, $\mathrm{d}\overline{z}\to\mathrm{d}\overline{z}$:

$$\Omega=-\mathcal{H}\mathrm{d}z\wedge\mathrm{d}\overline{z}+\overline{p}\mathrm{d}z\wedge\mathrm{d}\varphi+p\,\mathrm{d}\varphi\wedge\mathrm{d}\overline{z}\quad\text{with}\quad\mathcal{H}:=pv+\overline{pv}-\mathcal{L}. \tag{2.3}$$

Because $\mathrm{d}\Omega=0(\mathrm{mod}I[\varrho])$ it is locally exact $\Omega=\mathrm{d}\mathcal{S}$, $\mathcal{S}\in\mathcal{T}^*(\mathcal{M}_{2+1})$ on fields of extremals. However, contrary to mechanics Ω as an exact two-form can be represented in different ways by means of a Pfaffian form $\mathcal{S}$. In the case of DeDonder and Weyl,[2,3]

$$\mathcal{S}_{DW}=S(z,\overline{z},\varphi)\mathrm{d}z-\overline{S}(z,\overline{z},\varphi)\mathrm{d}\overline{z},$$

and in the case of Carathéodory[4]

$$\mathcal{S}_C = S^z(z,\bar{z},\varphi)\mathrm{d}S^{\bar{z}}(z,\bar{z},\varphi).$$

Comparing the exterior derivatives of these expressions with Eq. (2.3),

$$\Omega = -\mathcal{H}\mathrm{d}z\wedge\mathrm{d}\bar{z} + \bar{p}\mathrm{d}z\wedge\mathrm{d}\varphi + p\,\mathrm{d}\varphi\wedge\mathrm{d}\bar{z} \overset{!}{=} \mathrm{d}\bar{S}\wedge\mathrm{d}z - \mathrm{d}S\wedge\mathrm{d}\bar{z},$$

we obtain the Hamilton–Jacobi equations and the transversality conditions for a one-component field theory in DeDonder and Weyl's formulation,

$$\partial_z S + \partial_{\bar{z}}\bar{S} = -\mathcal{H}, \quad p = \partial_\varphi S, \quad \bar{p} = \partial_\varphi \bar{S}, \tag{2.4}$$

and in Carathéodory's case,

$$\Omega = -\mathcal{H}\mathrm{d}z\wedge\mathrm{d}\bar{z} + \bar{p}\mathrm{d}z\wedge\mathrm{d}\varphi + p\,\mathrm{d}\varphi\wedge\mathrm{d}\bar{z} \overset{!}{=} \mathrm{d}S^z\wedge\mathrm{d}S^{\bar{z}}, \tag{2.5}$$

we get

$$\partial_z S^z \partial_{\bar{z}}\bar{S}^{\bar{z}} - \partial_z S^{\bar{z}}\partial_{\bar{z}} S^z = -\mathcal{H}, \quad \begin{aligned} p &= \partial_{\bar{z}}\bar{S}^{\bar{z}}\partial_\varphi S^z - \partial_{\bar{z}}S^z\partial_\varphi \bar{S}^{\bar{z}}, \\ \bar{p} &= \partial_z S^z \partial_\varphi \bar{S}^{\bar{z}} - \partial_z S^{\bar{z}}\partial_\varphi S^z. \end{aligned} \tag{2.6}$$

The two theories here are equivalent because an n-form in a space of $n+1$ variables has always[12] the rank n. Due to this algebraic equivalence of covariant canonical formulations for one-component field theories we may choose DeDonder and Weyl's description to embed the extremals of interest in a system of solutions of the Hamilton–Jacobi equation. We use Carathéodory's theory for the explicit calculation of the wave fronts $S^z = \text{const}$, $S^{\bar{z}} = \text{const}$.

In two-dimensional field theories involving one field variable the basic two-form Ω has always the rank two, i.e., it can be constructed from two independent one-forms by linear combination of exterior products. Because Ω is closed its rank is equal to its class, which gives the codimension of the integral submanifold determined by Ω. To calculate this integral manifold—the wavefronts in our case—we can use a corollary of Frobenius' integrability theorem:[1] there exist two functions $S^z(z,\bar{z},\varphi)$, $S^{\bar{z}}(z,\bar{z},\varphi)$ in such a manner that the exterior product of their differentials equals Ω. The corresponding one-dimensional wave fronts are just the submanifolds determined by the conditions $S^z(z,\bar{z},\varphi) = \text{const}$, $S^{\bar{z}}(z,\bar{z},\varphi) = \text{const}$.

Thus the wave fronts are equipotential surfaces of the solutions of the Hamilton–Jacobi equation formulated in Carathéodory's framework. For simplicity we first solve the HJE of DeDonder and Weyl and the associated IC and afterwards we return to Carathéodory's equation in order to obtain an explicit expression for the wave fronts.

In mechanics for one variable q it is possible to construct wave fronts for one-parametric fields of extremals that cover a certain region of the extended configuration space $\mathcal{M}_{1+1}$ *and* vice versa. Provided a solution $S(t,q)$ of the Hamilton–Jacobi equation (HJE) is given, the corresponding velocity field, the so-called ''slope function,''

$$\Phi(t,q) = \partial_p H(t,q,p = \partial_q S(t,q)),$$

determines the corresponding one-parametric extremals by means of the ordinary first-order differential equation: $\dot{q}(t) = \Phi(t,q(t))$.

In general this is *not* true for field theories; the ability to embed extremals $\varphi_0(z,\bar{z})$ in a given wave front can be maintained only if the slope functions (velocity fields) $v = \Phi(\varphi,z,\bar{z})$, $\bar{v} = \bar{\Phi}(\varphi,z,\bar{z})$ obtained from the inverse Legendre transformation,

$$\partial_z\varphi(z,\bar{z}) = v(p = \partial_\varphi S, \bar{p} = \partial_\varphi \bar{S}, z, \bar{z}, \varphi) = \Phi(\varphi,z,\bar{z}), \tag{2.7}$$

$$\partial_{\bar z}\varphi(z,\bar z)=\bar v(p=\partial_\varphi S,\bar p=\partial_\varphi \bar S,z,\bar z,\varphi)=\bar\Phi(\varphi,z,\bar z),$$

satisfy the integrability condition $\partial_z\partial_{\bar z}\varphi(z,\bar z)\overset{!}{=}\partial_{\bar z}\partial_z\varphi(z,\bar z)$, which results in the requirement

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}\bar z}\Phi(z,\bar z,\varphi(z,\bar z)):=\partial_{\bar z}\Phi+\bar\Phi\cdot\partial_\varphi\Phi=\frac{\mathrm{d}}{\mathrm{d}z}\bar\Phi(z,\bar z,\varphi(z,\bar z)):=\partial_z\bar\Phi+\Phi\cdot\partial_\varphi\bar\Phi} \tag{2.8}$$

on Φ and $\bar\Phi$.

Provided the Hamilton–Jacobi equation and the integrability condition are fulfilled, the Euler–Lagrange equation is satisfied automatically. This can be seen as follows:

Differentiating the Hamilton–Jacobi equation (2.4) with respect to the field variable φ one obtains

$$\partial_z p+\partial_{\bar z}\bar p=-\partial_\varphi\mathcal{H}-\partial_p\mathcal{H}\partial_\varphi p-\partial_{\bar p}\mathcal{H}\partial_\varphi\bar p.$$

Because $\partial_\varphi\mathcal{H}=-\partial_\varphi\mathcal{L}$, $\partial_p\mathcal{H}=\Phi$ and $\partial_{\bar p}\mathcal{H}=\bar\Phi$ (see Ref. 1) we get

$$\frac{\mathrm{d}}{\mathrm{d}z}p+\frac{\mathrm{d}}{\mathrm{d}\bar z}\bar p=\frac{\mathrm{d}}{\mathrm{d}z}\frac{\partial\mathcal{L}}{\partial v}+\frac{\mathrm{d}}{\mathrm{d}\bar z}\frac{\partial\mathcal{L}}{\partial\bar v}=\partial_\varphi\mathcal{L}. \tag{2.9}$$

The momenta $p(z,\bar z,\varphi)$ and $\bar p(z,\bar z,\varphi)$ are defined on the extended configuration space $\mathcal{M}_{2+1}$ and are considered to be associated with a field of extremals $\varphi=\tilde\varphi(z,\bar z,u)$ parametrized by u. The Euler–Lagrange equation has to be fulfilled for every single extremal $\varphi=\tilde\varphi(z,\bar z,u=\text{const})$. Hence if we insert p and $\bar p$ into this equation of motion, we have to be aware of their implicit dependence of $z,\bar z$ via the field variable φ. Taking the defining equations (2.7) for the slope functions into account, the total derivatives in the PDEs (2.8) and (2.9) are defined as

$$\frac{\mathrm{d}}{\mathrm{d}z}:=\frac{\partial}{\partial z}\bigg|_{\bar z,\varphi=\text{const}}+\Phi\,\frac{\partial}{\partial\varphi}\bigg|_{\bar z,z=\text{const}},\qquad \frac{\mathrm{d}}{\mathrm{d}\bar z}:=\frac{\partial}{\partial\bar z}\bigg|_{z,\varphi=\text{const}}+\bar\Phi\,\frac{\partial}{\partial\varphi}\bigg|_{z,\bar z=\text{const}}.$$

Therefore the total derivatives are nothing but derivatives with respect to the independent variables $z,\bar z$ regarding u to be a constant.

Due to the extent to which the integrability condition is taken into account, there exist two different methods of using a Hamilton–Jacobi theory: the weak and the strong embedding of extremals in fields of wave fronts.

1. Weak embedding

This method is used to embed a given single extremal $\hat\varphi_0(z,\bar z)$ in fields of wave fronts. In order to obtain a weak embedding it is sufficient to take only the Hamilton–Jacobi equation and the transversality conditions (2.7) on $\hat\varphi_0(z,\bar z)$ into account. In this case usually one chooses a linear ansatz in the field variable for one of the functions S or $\bar S$. However, this approach in general will not provide new extremals, because the IC are fulfilled on the given extremal only. For details see Ref. 13.

2. Strong embedding:

Here one requires the IC not only to hold on the given extremal but in a whole neighborhood of it. If this is the case, then one is able to generate new extremals from a given one by integrating the slope functions (2.7).

In the following we study the strong embedding of a single given extremal into a field of wave fronts.

Like in mechanics there exists a transversality relation between extremals $\varphi(z,\bar z)$ and wave fronts $S^z(z,\bar z,\varphi)=\text{const}$, $S^{\bar z}(z,\bar z,\varphi)=\text{const}$, which holds if in every point $P\in\mathcal{M}_{1+2}$ the basis of tangent space $\mathcal{TM}_{1+2}$ is given by a union of the basis of the two-dimensional tangent space of the

extremals $e_z=\partial_z+v\partial_\varphi$, $e_{\bar z}=\partial_{\bar z}+\bar v\partial_\varphi$ and a basis vector $w=p\partial_z+\bar p\partial_{\bar z}+\mathcal{H}\partial_\varphi$ of the one-dimensional tangent space of the wave fronts, i.e., iff the Lagrangian density $\mathcal{L}$ does not vanish in the field of extremals:

$$\det(e_z,e_{\bar z},w)=\det\left|\begin{pmatrix}1&0&p\\0&1&\bar p\\v&\bar v&\mathcal{H}\end{pmatrix}\right|=(\mathcal{H}-pv-\overline{pv})=-\mathcal{L}\neq 0. \tag{2.10}$$

Notice that in theories with more than one real field ($d\geqslant 2$) both $\mathcal{L}$ and $\mathcal{H}$ have to be nonvanishing quantities to guarantee the transversality relation.[1]

III. HAMILTON–JACOBI THEORY FOR ONE REAL FIELD IN DEDONDER AND WEYL'S FORMULATION

We here restrict ourselves to Lagrangian densities of the following type: $\mathcal{L}=\partial_z\varphi\partial_{\bar z}\varphi-V(\varphi)$. The potential $V(\varphi)$ is an analytic function. Here we have the canonical momenta $p=\bar v$, $\bar p=v$, the Hamiltonian density $\mathcal{H}=p\bar p+V$, and the slope functions $\Phi=\partial_\varphi S$, $\bar\Phi=\partial_\varphi\bar S$. We have the (DeDonder and Weyl) Hamilton–Jacobi equation

$$\partial_z S+\partial_{\bar z}\bar S=\partial_\varphi S\partial_\varphi\bar S+V(\varphi) \tag{3.1}$$

and the related integrability condition

$$\partial_z\partial_\varphi S-\partial_{\bar z}\partial_\varphi\bar S=\partial_\varphi S\partial_\varphi^2\bar S-\partial_\varphi\bar S\partial_\varphi^2 S. \tag{3.2}$$

Knowing solutions S and $\bar S$ of the equations (3.1) and (3.2) a field of embedded extremals $\varphi=\tilde\varphi(z,\bar z)$ is determined by a system of first-order PDEs:

$$\partial_z\tilde\varphi(z,\bar z)=\Phi=\partial_\varphi\bar S(z,\bar z,\varphi=\tilde\varphi), \tag{3.3}$$

$$\partial_{\bar z}\tilde\varphi(z,\bar z)=\bar\Phi=\partial_\varphi S(z,\bar z,\varphi=\tilde\varphi). \tag{3.4}$$

A solution is obtained by expanding $S(z,\bar z,\varphi)$ and $\bar S(z,\bar z,\varphi)$ in powers of the difference $y=\varphi-\varphi_0$ between φ and a known extremal $\varphi_0(z,\bar z)$:

$$S(z,\bar z,\varphi)=\sum_{n=0}^{\infty}\frac{1}{n!}A_n(z,\bar z)y^n,\quad \bar S(z,\bar z,\varphi)=\sum_{n=0}^{\infty}\frac{1}{n!}\bar A_n(z,\bar z)y^n. \tag{3.5}$$

This method of expanding about a given solution of the equations of motion is commonly employed, e.g., with stability investigations or determining (quantum) fluctuations around c-number fields in self-interacting theories.[14,15]

Naturally φ_0 has to satisfy the transversality relations (3.4), which fix only the functions $A_1=\partial_{\bar z}\varphi_0$ and $\bar A_1=\partial_z\varphi_0$, without influencing the remaining coefficients. Inserting the expressions (3.5) into the HJE (3.1) and expanding the potential V in powers of y we see that the equation is automatically fulfilled up to the order y^1, whereas the IC (3.2) is fulfilled on the extremals up to the order y^0.

A_0 and $\bar A_0$ are only affected by the HJE of zeroth order in y:

$$\partial_z A_0+\partial_{\bar z}\bar A_0=\mathcal{L}|_{\varphi=\varphi_0}=\partial_z\varphi_0\partial_{\bar z}\varphi_0-V(\varphi_0). \tag{3.6}$$

The general solution of the homogeneous equation $\partial_z A_0^{\mathrm{hom}} + \partial_{\bar{z}} \overline{A_0^{\mathrm{hom}}} = 0$ is given—at least locally—by $A_0^{\mathrm{hom}} = \partial_{\bar{z}} \chi_0(z,\bar{z})$ and $\overline{A_0^{\mathrm{hom}}} = -\partial_z \chi_0(z,\bar{z})$. One special solution of the inhomogeneous PDE (3.6) can be obtained by integration: $\overline{A_0^{\mathrm{inh}}} = \int \mathcal{L}|_{\varphi=\varphi_0} d\bar{z}/2$ and $A_0^{\mathrm{inh}} = \int \mathcal{L}|_{\varphi=\varphi_0} dz/2$. This yields the general solution (locally):

$$A_0(z,\bar{z}) = \frac{1}{2} \int \left[\partial_z \varphi_0 \partial_{\bar{z}} \varphi_0 - V(\varphi_0) \right] dz + \partial_{\bar{z}} \chi_0(z,\bar{z}), \tag{3.7}$$

$$\overline{A_0}(z,\bar{z}) = \frac{1}{2} \int \left[\partial_z \varphi_0 \partial_{\bar{z}} \varphi_0 - V(\varphi_0) \right] d\bar{z} - \partial_z \chi_0(z,\bar{z}). \tag{3.8}$$

In order to determine the coefficients A_2 and $\overline{A_2}$, we insert $A_1 = \partial_{\bar{z}} \varphi_0$ and $\overline{A_1} = \partial_z \varphi_0$ into the IC of order y:

$$\partial_z A_2 - A_3 \partial_z \varphi_0 + \overline{A_1} A_3 + \overline{A_2} A_2 = \partial_{\bar{z}} \overline{A_2} - \overline{A_3} \partial_{\bar{z}} \varphi_0 + A_1 \overline{A_3} + A_2 \overline{A_2}. \tag{3.9}$$

Since y is a function of $z,\bar{z}$, its derivative with respect to z or $\bar{z}$ yields $\partial_z y = -\partial_z \varphi_0$ and $\partial_{\bar{z}} y = -\partial_{\bar{z}} \varphi_0$, respectively. Thus we infer from Eq. (3.9) that $\partial_z A_2 = \partial_{\bar{z}} \overline{A_2}$, which permits us to express these two functions at least locally by one generating potential function: $A_2 = \partial_{\bar{z}} \zeta_2(z,\bar{z})$ and $\overline{A_2} = \partial_z \zeta_2(z,\bar{z})$. ζ_2 has to fulfill the PDE

$$\partial_{\bar{z}} \partial_z \zeta_2(z,\bar{z}) + \partial_z \zeta_2(z,\bar{z}) \partial_{\bar{z}} \zeta_2(z,\bar{z}) + \tfrac{1}{2} \left[\partial_\varphi^2 V(\varphi = \varphi_0(z,\bar{z})) \right] = 0.$$

The ansatz

$$\zeta_2 = \ln \theta(z,\bar{z}) \Rightarrow A_2 = \partial_{\bar{z}} \ln \theta, \quad \overline{A_2} = \partial_z \ln \theta$$

linearizes the HJE of second order in y:

$$\boxed{\partial_{\bar{z}} \partial_z \theta(z,\bar{z}) + \tfrac{1}{2} \left[\partial_\varphi^2 V(\varphi = \varphi_0(z,\bar{z})) \right] \theta(z,\bar{z}) = 0.} \tag{3.10}$$

In order to obtain the expressions for A_n and $\overline{A_n}$ one has to substitute the power series (3.5) into the IC and the HJE and to compare the coefficients of the powers y^{n-1} and y^n, respectively. Starting with the IC in $(n-1)$th order

$$\partial_z A_n - A_{n+1} \partial_z \varphi_0 + \sum_{p=0}^{n-1} \binom{n-1}{p} \overline{A}_{p+1} A_{n-p+1} = \partial_{\bar{z}} \overline{A_n} - \overline{A}_{n+1} \partial_{\bar{z}} \varphi_0 + \sum_{p=0}^{n-1} \binom{n-1}{p} A_{p+1} \overline{A}_{n-p+1},$$

we draw our attention to the coefficients A_{n+1} and $\overline{A_{n+1}}$ of highest order. Fortunately they disappear from this equation as well as from the HJE due to the relations $A_1 = \partial_{\bar{z}} \varphi_0$ and $\overline{A_1} = \partial_z \varphi_0$. Provided the coefficients $A_0,\ldots,A_{n-1}$ and $\overline{A_0},\ldots,\overline{A_{n-1}}$ have already been determined recursively, one gets an equation for the functions $A_n(z,\bar{z})$ and $\overline{A_n}(z,\bar{z})$:

$$\begin{aligned} \partial_z(\theta^{n-2} A_n) - \partial_{\bar{z}}(\theta^{n-2} \overline{A_n}) &= \theta^{n-2} \sum_{p=2}^{n-2} \left[\binom{n-1}{p} - \binom{n-1}{p-1} \right] A_{p+1} \overline{A}_{n-p+1} \\ &=: \mathrm{Inh}(A_0,\ldots,A_{n-1};\overline{A_0},\ldots,\overline{A_{n-1}}). \end{aligned} \tag{3.11}$$

The inhomogeneity $\mathrm{Inh}(A_0,\ldots,A_{n-1};\overline{A_0},\ldots,\overline{A_{n-1}})$ vanishes for $n \leqslant 4$. Similarly to (3.8) this hierarchy of equations is solved by splitting the solution in two parts: a general solution of the homogeneous part $\partial_z(\theta^{n-2} A_n^{\mathrm{hom}}) - \partial_{\bar{z}}(\theta^{n-2} \overline{A_n^{\mathrm{hom}}}) = 0$, that is obtained—at least locally—by

$$A_n^{\mathrm{hom}} = \theta^{2-n}\partial_{\bar{z}}\zeta_n(z,\bar{z}) \quad \text{and} \quad \bar{A}_n^{\mathrm{hom}} = \theta^{2-n}\partial_z\zeta_n(z,\bar{z})$$

with an arbitrary smooth function $\zeta_n(z,\bar{z})$. The second part is a special solution of the inhomogeneous equation (3.11):

$$A_n^{\mathrm{inh}} = \theta^{2-n}\partial_{\bar{z}}\bar{\chi}_n(z,\bar{z}) \quad \text{and} \quad \bar{A}_n^{\mathrm{inh}} = -\theta^{2-n}\partial_z\bar{\chi}_n(z,\bar{z}) \tag{3.12}$$

with

$$\bar{\chi}_n(z,\bar{z}) = \frac{1}{2}\int^z\int^{\bar{z}} \mathrm{Inh}(A_0,\ldots,A_{n-1};\bar{A}_0,\ldots,\bar{A}_{n-1})\,dz'\,d\bar{z}'. \tag{3.13}$$

The general solution

$$A_n = \theta^{2-n}\partial_{\bar{z}}[\zeta_n(z,\bar{z}) + \bar{\chi}_n(z,\bar{z})] \quad \text{and} \quad \bar{A}_n = \theta^{2-n}\partial_z[\zeta_n(z,\bar{z}) - \bar{\chi}_n(z,\bar{z})]$$

has to satisfy the HJE (3.1) to nth order in y, in which, remarkably, the coefficients of highest order A_{n+1} and $\bar{A}_{n+1}$ vanish as well as in the IC, due to the relations $A_1 = \partial_{\bar{z}}\varphi_0$ and $\bar{A}_1 = \partial_z\varphi_0$. Separating the functions of the remaining highest order A_n, $\bar{A}_n$ leads to the equation

$$\partial_z(\theta^n A_n) + \partial_{\bar{z}}(\theta^n\bar{A}_n) = -\theta^n\sum_{p=2}^{n-2}\binom{n}{p}\bar{A}_{p+1}A_{n-p+1} - \theta^n\frac{d^n}{d\varphi^n}V(\varphi)\bigg|_{\varphi=\varphi_0}. \tag{3.14}$$

It is convenient to set $\zeta_n(z,\bar{z}) = \theta^{-1}\chi_n$ before inserting into expression (3.14). Using the relation (3.10) the HJE of nth order in y yields an equation, which is nothing but the inhomogeneous extension of the linear PDE (3.10):

$$\boxed{\partial_z\partial_{\bar{z}}\chi_n + \tfrac{1}{2}[\partial_\varphi^2 V(\varphi_0)]\chi_n = \widetilde{\mathrm{Inh}}(\chi_0,\ldots,\chi_{n-1}),} \tag{3.15}$$

with the inhomogeneity

$$\widetilde{\mathrm{Inh}}(\chi_0,\ldots,\chi_{n-1}) = \partial_{\bar{z}}\theta\partial_z\bar{\chi}_n - \partial_z\theta\partial_{\bar{z}}\bar{\chi}_n - \frac{1}{2}\theta^{n-1}\sum_{p=2}^{n-2}\binom{n}{p}\bar{A}_{p+1}A_{n-p+1} - \frac{1}{2}\theta^{n-1}\partial_\varphi^n V(\varphi_0).$$

In general the coefficients A_n, $\bar{A}_n$ are determined by the nth order of the HJE and the $(n-1)$th order of the IC for $n \geqslant 3$:

$$A_n = \theta^{2-n}\partial_{\bar{z}}\left[\frac{\chi_n(z,\bar{z})}{\theta} - \bar{\chi}_n(z,\bar{z})\right], \quad \bar{A}_n = \theta^{2-n}\partial_z\left[\frac{\chi_n(z,\bar{z})}{\theta} + \bar{\chi}_n(z,\bar{z})\right]. \tag{3.16}$$

Notably the infinite hierarchy of functions $\chi_n(z,\bar{z})$ has to fulfill *only* one PDE of second order: the equation (3.15). Its integral can be obtained by determining the general solution of the homogeneous PDE (3.10), *which is the same for all orders* $n \geqslant 2$ and *one* special solution of the inhomogeneous equation (3.15). It is given by using a Green function that can be chosen to be the same for all orders n without any loss of generality. The solutions of (3.10) can be obtained by employing Bäcklund transformations.

IV. BÄCKLUND TRANSFORMATIONS

Bäcklund transformations (BTs) are maps between the tangent bundles of integral submanifolds associated with PDEs. If we are able to find a BT from the PDE which we wish to solve and

to another one the general integral of which is known, we can obtain the general solution of the first one by integrating the BT. This treatment of a single PDE can be generalized to systems of partial differential equations.[16]

By applying BTs we want to reduce the linear PDEs of second order with *nonconstant* coefficients of type (3.10) to linear PDEs with *constant* coefficients. The inhomogeneous extension of Eq. (3.10) could be solved by BTs, too, but for sake of simplicity we construct a special solution of the inhomogeneous equation (3.10) by using a Green function and Fourier transformation. Like other authors[17] the general form of a BT we are starting from is given by two functions F_1, F_2:

$$\partial_z \hat{\theta}(z,\overline{z}) = F_1[z,\overline{z},\theta(z,\overline{z}),\hat{\theta}(z,\overline{z}),\partial_z\theta(z,\overline{z})],$$

$$\partial_{\overline{z}} \hat{\theta}(z,\overline{z}) = F_2[z,\overline{z},\theta(z,\overline{z}),\hat{\theta}(z,\overline{z}),\partial_{\overline{z}}\theta(z,\overline{z})].$$

θ has to fulfill the relation (3.10), whereas $\hat{\theta}$ denotes the transformed function which is supposed to obey a linear PDE with a constant coefficient m^2: $\partial_z\partial_{\overline{z}}\hat{\theta} - m^2\hat{\theta} = 0$. Of course m^2 can be equal to zero which would yield the wave equation. Obviously F_1 and F_2 have to fulfill the integrability condition $\partial_z\partial_{\overline{z}}\hat{\theta} = \partial_{\overline{z}}\partial_z\hat{\theta} \Rightarrow \mathrm{d}F_1/\mathrm{d}\overline{z} = \mathrm{d}F_2/\mathrm{d}z$. This integrability condition does not lead to a restriction on the solutions of the PDE (3.10), if such a BT is found. Thus F_1 and F_2 have to fulfill the two equations

$$\mathrm{d}F_1/\mathrm{d}\overline{z} = \mathrm{d}F_2/\mathrm{d}z, \quad \mathrm{d}F_1/\mathrm{d}\overline{z} = m^2\hat{\theta}. \tag{4.1}$$

We would like to point out that the more general ansatz $\partial_z\partial_{\overline{z}}\hat{\theta} = K(z,\overline{z})\hat{\theta}$ leads to the same BTs (4.4) below at least for the models discussed here.[18]

Differentiating Eqs. (4.1) with respect to $\partial_z\theta$ and $\partial_{\overline{z}}\theta$ leads to

$$\partial^2_{\theta_z} F_1 = 0 \Rightarrow F_1 = f_1(\theta,\hat{\theta},z,\overline{z})\partial_z\theta + m_1(\theta,\hat{\theta},z,\overline{z}),$$

$$\partial^2_{\theta_{\overline{z}}} F_2 = 0 \Rightarrow F_2 = f_2(\theta,\hat{\theta},z,\overline{z})\partial_{\overline{z}}\theta + m_2(\theta,\hat{\theta},z,\overline{z}).$$

Substituting these expressions into Eqs. (4.1), comparing the coefficients of $\partial_{\overline{z}}\theta$ and $\partial_z\theta$, and differentiating with respect to $\theta,\hat{\theta}$, we conclude by lengthy but straightforward calculations that

$$f_1 = -f_2 = c_0, \quad c_0 \in \mathcal{R}, \quad c_0 \neq 0,$$

$$0 = \partial_\theta m_1 - f_1\partial_{\hat{\theta}} m_1 \Rightarrow m_1 = g_1(f_1\theta + \hat{\theta},z,\overline{z}),$$

$$0 = \partial_\theta m_2 + f_1\partial_{\hat{\theta}} m_2 \Rightarrow m_2 = g_2(f_1\theta - \hat{\theta},z,\overline{z}).$$

Inserting these results into relations (4.1) and differentiating with respect to $f_1\theta + \hat{\theta} = \eta_1$ and $f_1\theta - \hat{\theta} = \eta_2$ we obtain $\partial^2_{\eta_1} m_1 = 0$, $\partial^2_{\eta_2} m_2 = 0$. Substituting $f_1\hat{\theta} \to \hat{\theta}$, $f_1\partial_z\hat{\theta} \to \partial_z\hat{\theta}$, and $f_1\partial_{\overline{z}}\hat{\theta} \to \partial_{\overline{z}}\hat{\theta}$ we get

$$\partial_z\hat{\theta} = \partial_z\theta + \alpha_1(z,\overline{z})[\theta + \hat{\theta}] + \beta_1(z,\overline{z}), \tag{4.2}$$

$$\partial_{\overline{z}}\hat{\theta} = -\partial_{\overline{z}}\theta + \alpha_2(z,\overline{z})[\hat{\theta} - \theta] + \beta_2(z,\overline{z}). \tag{4.3}$$

Considering the two functions β_1, β_2 is only necessary for transformations between *inhomogeneous* PDEs. Thus, we here can choose $\beta_1 = 0 = \beta_2$. Inserting our results (4.2) and (4.3) into Eqs. (4.1) and comparing the coefficients of $\theta,\hat{\theta}$ we finally obtain the linear BT

$$\boxed{\partial_z\hat{\theta} = \partial_z\theta + \{\theta + \hat{\theta}\}\partial_z\psi,} \quad \boxed{\partial_{\overline{z}}\hat{\theta} = -\partial_{\overline{z}}\theta + \{\hat{\theta} - \theta\}\partial_{\overline{z}}\psi,} \tag{4.4}$$

with the BT generating function $\psi=\psi(z,\bar{z})$ which is a *special* solution of

$$\partial_z\partial_{\bar{z}}\psi-(\partial_z\psi)(\partial_{\bar{z}}\psi)-\tfrac{1}{2}\partial_\varphi^2 V(\varphi_0)=0,\quad \partial_z\partial_{\bar{z}}\psi+(\partial_z\psi)(\partial_{\bar{z}}\psi)-m^2=0. \tag{4.5}$$

Substituting $\psi=-\ln(\tilde{\psi})$ in these equations we conclude

$$\partial_z\partial_{\bar{z}}\tilde{\psi}+\frac{1}{2}\partial_\varphi^2 V(\varphi_0)\tilde{\psi}=0,\quad \partial_z\partial_{\bar{z}}\left(\frac{1}{\tilde{\psi}}\right)-m^2\left(\frac{1}{\tilde{\psi}}\right)=0. \tag{4.6}$$

We therefore have to solve the following problem:

We have to find a solution of the equation (3.10)*, the inverse of which has to fulfill a Klein–Gordon or a wave equation. Then we can integrate the linear BT and obtain the general solution of* (3.10).

Another method of solving Eqs. (4.5) is based on their linear combinations:

$$\partial_z\partial_{\bar{z}}\psi=\tfrac{1}{4}(2m^2+\partial_\varphi^2 V(\varphi_0)),\quad (\partial_z\psi)(\partial_{\bar{z}}\psi)=\tfrac{1}{4}(2m^2-\partial_\varphi^2 V(\varphi_0)). \tag{4.7}$$

Integrating the first equation and inserting this solution into the second expression imposes a restriction on $\partial_\varphi^2 V(\varphi_0)$. We make use of Eqs. (4.7) when we study the ϕ^4-model.

V. APPLICATIONS

After solving the homogeneous equation (3.10), we calculate a special solution of their inhomogeneous extension (3.15) by determining a Green function—without need of specifying the inhomogeneity $\widetilde{\mathrm{Inh}}$. To obtain a solution of Eq. (3.15) specific for the models under consideration we have to fold the Green function with the inhomogeneity in every order y^n.

The Hamilton–Jacobi theory for the non-self-interacting scalar field theories $\mathcal{L}_0=\partial_z\varphi\partial_{\bar{z}}\varphi$ and $\mathcal{L}_1=\partial_z\varphi\partial_{\bar{z}}\varphi-1/2m^2\varphi^2$ with the light cone variables $z=(x+t)/2$ and $\bar{z}=(x-t)/2$ leads to the wave or the Klein–Gordon equation (3.10) without need for a Bäcklund transformation or specifying an extremal $\varphi_0(z,\bar{z})$:

$$\mathcal{L}_0:\partial_z\partial_{\bar{z}}\chi_n=\widetilde{\mathrm{Inh}}(\chi_0,\ldots,\chi_{n-1}),\quad \mathcal{L}_1:\partial_z\partial_{\bar{z}}\chi_n+m^2\chi_n=\widetilde{\mathrm{Inh}}(\chi_0,\ldots,\chi_{n-1}).$$

The general solutions of these relations are known. Therefore we draw our attention to the more interesting case of self-interacting theories:

A. The homogeneous equations

1. Liouville model

Applying our formalism to Liouville's theory $\mathcal{L}=\partial_z\varphi\partial_{\bar{z}}\varphi+2\exp(\varphi)$, using an arbitrary solution of the equation of motion for which the general expression is known,[17]

$$\varphi_0=\ln\left\{2\frac{(\partial_z s(z))(\partial_{\bar{z}}\bar{s}(\bar{z}))}{(s+\bar{s})^2}\right\},$$

with arbitrary smooth functions $s(z)$ and $\bar{s}(\bar{z})$, the relation (3.10) yields

$$\partial_z\partial_{\bar{z}}\theta^L-2\frac{(\partial_z s)(\partial_{\bar{z}}\bar{s})}{(s+\bar{s})^2}\theta^L=0\Rightarrow\partial_s\partial_{\bar{s}}\theta^L(s,\bar{s})-2\frac{1}{(s+\bar{s})^2}\theta^L(s,\bar{s})=0 \tag{5.1}$$

by employing a transformation of variables $z\to s(z),\bar{z}\to\bar{s}(\bar{z})$. Obviously *one* special solution of this equation is $\theta_0^L=1/(s+\bar{s})$. Its inverse fulfills the wave equation $\partial_s\partial_{\bar{s}}\hat{\theta}^L=0$. Thus we know that there exists at least one BT which connects the integral submanifolds of (5.1) and of the wave equation. Returning to the equation (4.6) we conclude that $\psi^L=\ln(s+\bar{s})$. So we can determine the BT by integrating the relation (4.4) and obtain the general solution of the equation (5.1):

$$\theta^L(s,\overline{s})=\partial_s C(s)-\partial_{\overline{s}}\overline{C}(\overline{s})+\frac{2}{(s+\overline{s})^2}\{\overline{C}(\overline{s})-C(s)\} \tag{5.2}$$

with two arbitrary smooth functions $C(s)$ and $\overline{C}(\overline{s})$.

2. Sine and sinh–Gordon model

In two-dimensional space–time two types of solitons exist: the "bell" with the same asymptotic value at $x=-\infty$ and $x=\infty$ and a "kink" soliton with different asymptotic values. Moreover, there exists a topological conserved quantum number associated with the asymptotic behavior of these solitons. The corresponding conserved current is given by $J^\mu=\epsilon^{\mu\nu}\partial_\nu\varphi$ with the antisymmetric tensor $\epsilon^{\mu\nu}=-\epsilon^{\nu\mu}$, μ, $\nu=0$, 1. Thus the charge associated with this current is: $N=\int_{-\infty}^{\infty}J^0\,dx=\varphi|_{x=\infty}-\varphi|_{x=-\infty}$, which vanishes obviously in the case of the bell solitons. For kinks it is a nontrivial quantum number.

The sine–Gordon theory possesses an infinite hierarchy of multikink solutions, which can be constructed by auto-Bäcklund transformations. In this model the conserved quantity is associated with a particle number. For details as to solitons, see, e.g., Refs. 14, 15, 19, and 20.

We want to embed for the sine–Gordon model $\mathcal{L}_2=\partial_z\varphi\partial_{\overline{z}}\varphi+2[1-\cos(\varphi)]$ the (anti) kink solution $\varphi_0=\pm 4\arctan[\exp(z+\overline{z})]$ and in the case of the sinh–Gordon model $\mathcal{L}_3=\partial_z\varphi\partial_{\overline{z}}\varphi-2[1-\cosh(\varphi)]$ the bell solution $\varphi_0=\pm 4\,\mathrm{arctanh}[\exp(z+\overline{z})]$, which is only defined for $z+\overline{z}<0$. We then obtain for Eq. (3.10)

$$\text{sine–Gordon:}\quad \partial_z\partial_{\overline{z}}\theta^{\mathrm{SG}}-\{2\tanh^2(z+\overline{z})-1\}\theta^{\mathrm{SG}}=0, \tag{5.3}$$

$$\text{sinh–Gordon:}\quad \partial_z\partial_{\overline{z}}\theta^{\mathrm{Sh}}-\{2\coth^2(z+\overline{z})-1\}\theta^{\mathrm{Sh}}=0. \tag{5.4}$$

Following the discussion of Liouville's theory we are able to solve these two equations by one BT. For this it is sufficient to realize that the inverses of the two solutions $\theta_0^{\mathrm{SG}}=1/\cosh(z+\overline{z})$ and $\theta_0^{\mathrm{Sh}}=1/\sinh(z+\overline{z})$ solve the Klein–Gordon equation $\partial_z\partial_{\overline{z}}\hat{\theta}=\hat{\theta}$. The functions $\theta_0^{\mathrm{SG}}=\tilde{\psi}^{\mathrm{SG}}$ and $\theta_0^{\mathrm{Sh}}=\tilde{\psi}^{\mathrm{Sh}}$ can be calculated by using the relations $\tilde{\psi}=\exp(-\psi)$ and (A7) and (A1) shown in the Appendix. Thus the two generating functions are $\psi^{\mathrm{SG}}=\ln(\cosh(z+\overline{z}))$ and $\psi^{\mathrm{Sh}}=\ln(\sinh(z+\overline{z}))$ which determine the BTs (4.4) between the Klein–Gordon equation and Eqs. (5.3) and (5.4). Their general solutions can be calculated by integration of the linear BTs (4.4):

$$\begin{aligned}\theta^{\mathrm{SG}}=&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[-i(qz+\overline{qz})]\,\delta(q\overline{q}+1)\,\Upsilon^{\mathrm{SG}}(q,\overline{q})\\&\times\left\{1-\frac{2}{q^2+1}-\frac{2iq}{q^2+1}\tanh(z+\overline{z})\right\}dq\,d\overline{q}+c_0\cosh^{-1}(z+\overline{z}),\end{aligned} \tag{5.5}$$

$$\begin{aligned}\theta^{\mathrm{Sh}}=&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[-i(kz+\overline{kz})]\,\delta(k\overline{k}+1)\,\Upsilon^{\mathrm{Sh}}(k,\overline{k})\\&\times\left\{\frac{i(k+\overline{k})}{2}-\coth(z+\overline{z})\right\}dk\,d\overline{k}+c_1\sinh^{-1}(z+\overline{z}),\end{aligned} \tag{5.6}$$

with arbitrary constants c_0, $c_1\in\mathcal{R}$ and two arbitrary functions $\Upsilon^{\mathrm{SG}}(q,\overline{q})$, $\Upsilon^{\mathrm{Sh}}(k,\overline{k})$ which have to be chosen in such a way that the integrals exist. A property of this BT is that the solution which was used for the transformation is multiplied with a constant and added to the modified solution of the Klein–Gordon or the wave equation.

This static kink $\varphi_0=\pm 4\arctan[\exp(x)]$ can be transformed by a Lorentz boost into time-dependent solutions of the relativistic invariant Euler–Lagrange equation φ_0

$=\pm 4\arctan[\exp(\gamma(x-vt)+\delta)]$, $\gamma^2=1/(1-v^2)$, parametrized by the velocity v and the phase shift δ. We are able to include the embedding of these solutions in our discussion, making use of the transformation of variables

$$z\to w=z\gamma(1-v)+\delta/2, \quad \overline{z}\to\overline{w}=\overline{z}\gamma(1+v)+\delta/2. \tag{5.7}$$

The same holds for the static solitons of the relativistic covariant sinh- and ϕ^4-models.

3. ϕ4-model

Contrary to the three previous models, the following ones can only be solved by at least two BTs: the ϕ^4-theories

$$\text{(I)}\quad \mathcal{L}=\partial_z\varphi\partial_{\overline{z}}\varphi-4\varphi^2+2\varphi^4 \quad \text{and} \quad \text{(II)}\quad \mathcal{L}=\partial_z\varphi\partial_{\overline{z}}\varphi+2\varphi^2-2\varphi^4.$$

Both theories have soliton solutions. We choose the (anti-) kink $\varphi_0^{\mathrm{I}}=\pm\tanh(z+\overline{z})$ and in case II the bell solution $\varphi_0^{\mathrm{II}}=\pm\cosh^{-1}(z+\overline{z})$. Then we get the two relation (3.10) for θ^I and θ^{II}:

$$\text{(I)}\quad \partial_z\partial_{\overline{z}}\theta^{\mathrm{I}}-\{6\tanh^2(z+\overline{z})-2\}\theta^{\mathrm{I}}=0, \tag{5.8}$$

$$\text{(II)}\quad \partial_z\partial_{\overline{z}}\theta^{\mathrm{II}}-\{6\tanh^2(z+\overline{z})-5\}\theta^{\mathrm{II}}=0. \tag{5.9}$$

Except for the special values of same of the constants they are the same PDEs as that of the sine–Gordon model, but they cannot be solved by *one* BT only (see the Appendix). Therefore we employ two BTs for each model: the first BTs leads to two equations in which the coefficient in front of $\tanh^2(z+\overline{z})$ is reduced to 2, the same as the one in the sine–Gordon theory. This allows us to obtain two Klein–Gordon equations which differ by the choice of m^2 after a second BT for each model.

Inserting the function $\partial_\varphi^2 V(\varphi_0)=v(z+\overline{z})$ in the results (A.12) and (A.1) of the Appendix we are able to calculate the functions ψ^{I}, ψ^{II} and the two solutions of the equations (5.8) and (5.9) which are necessary for the transformations:

$$\text{(I)}\quad \theta_0^{\mathrm{I}}=\cosh^{-2}(z+\overline{z}), \quad \text{(II)}\quad \theta_0^{\mathrm{II}}=\exp[d_0(z-\overline{z})]\cosh^{-2}(z+\overline{z}), \quad d_0^2=3.$$

Thus, with $\psi^{\mathrm{I}}=2\ln\{\cosh(z+\overline{z})\}$ and $\psi^{\mathrm{II}}=d_0(\overline{z}-z)+2\ln\{\cosh(z+\overline{z})\}$ we obtain after one BT and denoting the function $\hat{\theta}$ of Eq. (4.4) by $\tilde{\theta}$

$$\text{(I)}\quad \partial_z\partial_{\overline{z}}\tilde{\theta}^{\mathrm{I}}-\{2\tanh^2(z+\overline{z})+2\}\tilde{\theta}^{\mathrm{I}}=0,$$

$$\text{(II)}\quad \partial_z\partial_{\overline{z}}\tilde{\theta}^{\mathrm{II}}-\{2\tanh^2(z+\overline{z})-1\}\tilde{\theta}^{\mathrm{II}}=0.$$

The second relation is the same as in the sine–Gordon theory. Thus we only have to treat the first case here. This PDE has the special solution $\tilde{\theta}_0^{\mathrm{I}}=1/\cosh(z+\overline{z})\exp[id_1(z-\overline{z})]$, $d_1^2=3$ the inverse of which fulfills a Klein–Gordon equation, namely $\partial_z\partial_{\overline{z}}(1/\tilde{\theta}_0^{\mathrm{I}})=4/\tilde{\theta}_0^{\mathrm{I}}$. The solution $\tilde{\theta}_0^{\mathrm{I}}$ was found according to the method discussed in the Appendix. The generating function for this BT is $\psi_2^{\mathrm{I}}=\ln\{\cosh(z+\overline{z})\}+id_1(\overline{z}-z)=-\ln(\tilde{\theta}_0^{\mathrm{I}})$. Hence the resulting solutions of Eqs. (5.8) and (5.9) are

$$\theta^{\mathrm{I}}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Upsilon^{\mathrm{I}}(q,\overline{q})\,\delta(q\overline{q}+4)\exp[-i(qz+\overline{qz})]\{q^4+16-4q^2-(6iq^3-24iq)\tanh(z+\overline{z})$$
$$-12q^2\tanh^2(z+\overline{z})\}\,dq\,d\overline{q}+c_0\cosh^{-2}(z+\overline{z})+c_1\cosh^{-1}(z+\overline{z})\tanh(z+\overline{z})\exp[id_1(z-\overline{z})], \tag{5.10}$$

$$\theta^{\mathrm{II}}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Upsilon^{\mathrm{II}}(k,\overline{k})\,\delta(k\overline{k}+1)\exp[-i(kz+\overline{k}\overline{z})]\{-(k^2+1)^2-6ik(1-k^2)\tanh(z+\overline{z})$$
$$+12k^2\tanh^2(z+\overline{z})\}\,\mathrm{d}k\,\mathrm{d}\overline{k}+c_2\cosh^{-2}(z+\overline{z})\exp[d_0(z-\overline{z})]+c_3\cosh^{-1}(z+\overline{z})\tanh(z+\overline{z}) \tag{5.11}$$

with $d_0^2=d_1^2=3$, c_0, c_1, c_2, $c_3\in\mathcal{R}$, and two arbitrary functions $\Upsilon^{\mathrm{I}}(q,\overline{q})$, $\Upsilon^{\mathrm{II}}(k,\overline{k})$.

Expressions like (5.3) and (5.8) also occur, e.g., in stability investigations or in discussion small fluctuations around the known soliton solutions φ_0 of these theories.[14,15] Carrying out the second variation of the action functional in the case of the sine–Gordon and the ϕ^4-theory employing the soliton solutions given above—or equivalently inserting $\varphi=\varphi_0+\varphi_c$, $|\varphi_c|\ll|\varphi_0|$, into the Euler–Lagrange equation of the sine–Gordon or the ϕ^4-theory—yields

$$[-\partial_x^2+n(n+1)\tanh^2(x)+c_0]u(x)=\omega^2u(x), \tag{5.12}$$

where $\varphi_c(x,t)=\exp(i\omega t)u(x)$. We have $n=1$, $c_0=2$ for the sine–Gordon and $n=2$, $c_0=-2$ for the ϕ^4-model. Stability of the soliton solutions requires that all eigenvalues ω^2 of this Schrödinger-like equation should be non-negative, so that small perturbations about φ_0 do not grow exponentially in time. The lowest eigenvalue is $\omega^2=0$ and the corresponding solution $\hat{\varphi}_c$ is the translation mode. It must be present, because of the translation invariance of our models under consideration. Remarkably we have used it for both models to construct the Bäcklund transformations: $\hat{\varphi}_c^{\mathrm{SG}}=1/\cosh(x=z+\overline{z})$ and $\hat{\varphi}_c^{\mathrm{I}}=1/\cosh^2(x)$.

The equations (5.3) and (5.8) are reduced to Eq. (5.12) if one sets $x=z+\overline{z}$, $t=z-\overline{z}$ and $\exp(i\omega t)u(x)$. The equation (5.12) are solvable by transforming them into hypergeometric differential equations, the solutions of which can be given by *finite* series in powers of $\tanh(x)$ functions:[21]

$$\underline{\mathrm{SG}}:\quad \omega_k^2=k^2+1:\ u(x)=\exp(ikx)\{k+i\tanh(x)\},$$

$$\underline{\phi_1^4}:\quad \omega^2=3:\ u(x)=\tanh(x)/\cosh(x),$$

$$\omega_k^2=k^2+4:\ u(x)=\exp(ikx)\{-1-k^2-3ki\tanh(x)+3\tanh^2(x)\}.$$

These solutions are contained in our more general results (5.5) and (5.10).

4. A mathematical remark

As discussed in the Appendix our results can be generalized in order to reduce the hierarchy of linear PDEs:

$$\partial_z\partial_{\overline{z}}\theta=\{n(n+1)\,\eta^2+a\}\,\theta,\quad a\in\mathcal{R},\quad n=0,1,2,..., \tag{5.13}$$

by n BTs to a Klein–Gordon or a wave equation successively. One BT can raise or lower the coefficient n to $n+1$ or $n-1$. We have to assume that the smooth function $\eta(l)$ fulfills the nonlinear differential equation, $\partial_l\eta=\overline{b}\,\eta^2+\overline{c}$ with $\overline{c}\in\mathcal{R}$, $\overline{b}=\pm1$ and $l=z+\overline{z}$:

$$\frac{\overline{b}}{\overline{c}}>0:\ \eta=\sqrt{|\overline{c}|}\tan[\sqrt{|\overline{c}|}(l+l_0)],\quad \overline{c}\in\mathcal{R},\quad l_0\in\mathcal{C}, \tag{5.14}$$

$$\frac{\overline{b}}{\overline{c}}<0:\ \eta=-\sqrt{|\overline{c}|}\tanh[\sqrt{|\overline{c}|}(l+l_0)],\quad \overline{c}=0:\quad \eta=\frac{1}{l_0-bl}. \tag{5.15}$$

The PDEs (5.13) and (5.15) are solvable without need of specifying the constants a or $\overline{c}$.

Obviously the PDEs (5.8), (5.9), (5.3), and (5.4) correspond to special choices of a, $\bar{b}$, $\bar{c}$, and n: $\bar{b}=-1$, $\bar{c}=1$, $a=-1$, and $n=1$ give the sinh and the sine–Gordon models, whereas $n=2$, $\bar{b}=-1$, $\bar{c}=1$ give the ϕ^4-theory with $a=-2$ (case I) and $a=-1$ (case II).

B. The inhomogeneous equation

A special solution of the inhomogeneous equation (3.15) can be obtained for the sinh and sine–Gordon theories and both cases of the ϕ^4-theory by employing Fourier transformations. We discuss these theories first and return to the Liouville model later.

1. Sinh and sine–Gordon, ϕ4 equations

We introduce the Green function $\mathrm{G}(z,\bar{z},\hat{z},\hat{\bar{z}})$ for the inhomogeneous equation (3.15):

$$\partial_z\partial_{\bar{z}}\mathrm{G}+\tfrac{1}{2}\{\partial_\varphi^2 V(\varphi_0)\}\mathrm{G}=\delta(z-\hat{z})\,\delta(\bar{z}-\hat{\bar{z}}). \tag{5.16}$$

If a Green function is found, we can calculate the solutions χ_n of Eq. (3.15) to all orders of y^n:

$$\chi_n=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\widetilde{\mathrm{Inh}}\{\chi_0(\hat{z},\hat{\bar{z}}),\ldots,\chi_{n-1}(\hat{z},\hat{\bar{z}})\}\mathrm{G}(z,\bar{z},\hat{z},\hat{\bar{z}})\,\mathrm{d}\hat{z}\,\mathrm{d}\hat{\bar{z}}.$$

We introduce the Fourier transform $\tilde{\mathrm{G}}$ by

$$\mathrm{G}(z,\bar{z},\hat{z},\hat{\bar{z}})=\frac{1}{4\pi^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp\{i[q(\hat{z}-z)+\bar{q}(\hat{\bar{z}}-\bar{z})]\}\tilde{\mathrm{G}}(z,\bar{z},q,\bar{q})\,\mathrm{d}q\,\mathrm{d}\bar{q}. \tag{5.17}$$

As we need only a special G we try for $\tilde{\mathrm{G}}$ the ansatz that depends on q, $\bar{q}$, and $l=z+\bar{z}$ only. We then obtain

$$1=\partial_l^2\tilde{\mathrm{G}}-i(q+\bar{q})\partial_l\tilde{\mathrm{G}}-\tfrac{1}{2}\partial_\varphi^2 V\tilde{\mathrm{G}}. \tag{5.18}$$

In our cases the potential term is only a function of l: $\partial_\varphi^2 V=2a_0+2n[n+1]f^2(l)$, $a_0\in\mathcal{R}$, $n=1$, 2, and f denotes a $\tanh(l)$ [see (5.3), (5.9), and (5.8)] or $\coth(l)$ [see (5.4)]. In order to obtain one solution of Eq. (5.18) it is sufficient to assume any f that solves $\partial_l f=1-f^2$. Since (5.18) is only a linear differential equation we are able to calculate a special inhomogeneous solution, if we know a homogeneous one:

$$\tilde{\mathrm{G}}_{\mathrm{inh}}(q,\bar{q},l)=\int^{l}\tilde{\mathrm{G}}_{\mathrm{hom}}(q,\bar{q},\hat{l})^{-2}\exp(i[q+\bar{q}]\hat{l})\int^{\hat{l}}\tilde{\mathrm{G}}_{\mathrm{hom}}(q,\bar{q},\tilde{l})\exp(-i[q+\bar{q}]\tilde{l})\,\mathrm{d}\tilde{l}\,\mathrm{d}\hat{l}.$$

Substituting $\tilde{\mathrm{G}}_{\mathrm{hom}}(q,\bar{q},l)=\exp[i(q+\bar{q})l/2]\hat{\mathrm{G}}(q,\bar{q},l)$ leads to

$$\partial_l^2\hat{\mathrm{G}}-\left\{a_0-\frac{(q-\bar{q})^2}{4}+n(n+1)f^2\right\}\hat{\mathrm{G}}=0. \tag{5.19}$$

Choosing the special ansatz $\hat{\mathrm{G}}=(c_0+c_1 f)\exp(c_3 l)$, and comparing the coefficients of powers of f, we get for $n=1$ with $a=a_0-(q-\bar{q})^2/4$

$$a\neq-2:\quad c_3=\pm\sqrt{a+2},\quad c_0=-c_1c_3,\quad c_1\in\mathcal{R},\quad c_1\neq0, \tag{5.20}$$

$$a=-2:\quad c_3=0=c_0,\quad c_1\in\mathcal{R},\quad c_1\neq0. \tag{5.21}$$

This choice of parameters provides the Green function for the sinh and sine–Gordon theories (5.4) and (5.3). The case $n=2$ is of interest within the ϕ^4-models (5.8) and (5.9). Here we have to add the term $c_2 f^2\exp(c_3 l)$ to $\hat{\mathrm{G}}$. This yields finally

$$a\neq -6:\quad 3c_0=c_2(5+a),\quad c_2=-\frac{c_1}{c_3},\quad c_3=\pm\sqrt{a+6},\quad c_1\in\mathcal{R},\quad c_1\neq 0,$$

$$a=-6:\quad c_1=c_3=0,\quad 3c_0=-2c_2,\quad c_2\in\mathcal{R},\quad c_2\neq 0.$$

The sign of c_3 has to be chosen in such a way that the Fourier integral for the Green function $\tilde{\mathrm{G}}(z,\overline{z},q,\overline{q})$ exists.

Inserting these results into the expression for $\tilde{\mathrm{G}}_{\mathrm{inh}}$ and inverting the Fourier transformation we are able to obtain—in principle—the solution of Eq. (3.15) for every order of y^n by integration.

2. Liouville theory

For the Liouville model we start with Eq. (5.16), too, and obtain instead of Eq. (5.19), where $l=s(z)+\overline{s(z)}$

$$\partial_l^2\hat{\mathrm{G}}-\left\{-\frac{(q-\overline{q})^2}{4}+\frac{2}{l^2}\right\}\hat{\mathrm{G}}=0.$$

The solution is

$$\hat{\mathrm{G}}=c_0\left\{\frac{1}{l}a\sin(al)-a^2\cos(al)\right\}+c_1\left\{\frac{1}{l}a\cos(al)+a^2\sin(al)\right\},\quad a=\pm\frac{(q-\overline{q})}{2}.$$

Obviously we can not integrate $\tilde{\mathrm{G}}_{\mathrm{inh}}$ explicitly, if we use this solution. However, the Green function G can be obtained for the Liouville model. We return to Eq. (5.16) and choose the ansatz $\mathrm{G}(s(z),\hat{s},\overline{s(z)},\hat{\bar{s}})=\mathrm{H}(s(z)-\hat{s})\mathrm{H}(\overline{s(z)}-\hat{\bar{s}})\overline{\mathrm{G}}(s(z),\hat{s},\overline{s(z)},\hat{\bar{s}})$, where H is the usual Heaviside step function. We insert the ansatz into Eq. (5.19) and obtain

$$\begin{aligned}0=&\,\mathrm{H}(s-\hat{s})\mathrm{H}(\overline{s}-\hat{\bar{s}})\left\{\partial_s\partial_{\bar{s}}-\frac{2}{(s+\overline{s})^2}\right\}\overline{\mathrm{G}}+\delta(s-\hat{s})\,\delta(\overline{s}-\hat{\bar{s}})[\overline{\mathrm{G}}-1]\\&+\mathrm{H}(s-\hat{s})\,\delta(\overline{s}-\hat{\bar{s}})\partial_s\overline{\mathrm{G}}+\mathrm{H}(\overline{s}-\hat{\bar{s}})\,\delta(s-\hat{s})\partial_{\bar{s}}\overline{\mathrm{G}}.\end{aligned}$$

In order to solve this equation we have to find one solution $\overline{\mathrm{G}}$ of the homogeneous equation (5.1) with the following properties: $\overline{\mathrm{G}}(s=\hat{s},\overline{s}=\hat{\bar{s}})=1$, $\partial_{\bar{s}}\overline{\mathrm{G}}|_{s=\hat{s}}=0$, and $\partial_s\overline{\mathrm{G}}|_{\bar{s}=\hat{\bar{s}}}=0$. It can easily be verified that a solution is given by

$$\overline{\mathrm{G}}=\frac{1}{\hat{s}+\hat{\bar{s}}}\left\{2s(z)-\hat{s}+\hat{\bar{s}}-\frac{2}{s(z)+\overline{s(z)}}[s(z)+\hat{\bar{s}}][s(z)-\hat{s}]\right\}.\tag{5.22}$$

Thus we have determined an explicit expression for the Green function $\mathrm{G}=\mathrm{H}(z-\hat{z})\mathrm{H}(\overline{z}-\hat{\bar{z}})\overline{\mathrm{G}}$.

VI. RELATED EXTREMALS

Having determined solutions of the HJE (3.1) combined with the IC (3.2) associated with a given extremal in terms of power series we now want to indicate how new extremals can be generated from a given one.

In order to connect the functions χ_n from Eq. (3.15), with a one-parameter field of extremals $\tilde{\varphi}(z,\overline{z},u)$ embedded, we expand $\tilde{y}=(\tilde{\varphi}-\varphi_0(z,\overline{z}))$ in the parameter u of the solutions of the equation of motion. Therefore we have to consider the two-dimensional submanifold $\Sigma:=\{(z,\overline{z},\tilde{\varphi}(z,\overline{z}))\}$ of the extended configuration space $\mathcal{M}_{2+1}=\{(z,\overline{z},\varphi)\}$. The starting points of this calculation are the slope functions (3.4):

$$\partial_z\tilde{\varphi}(z,\bar{z})=\partial_\varphi\bar{S}|_{\varphi=\tilde{\varphi}}=\bar{A}_1+\sum_{i=2}^{\infty}\frac{1}{(i-1)!}\bar{A}_i\tilde{y}^i\Rightarrow\partial_z\tilde{y}=\sum_{i=1}^{\infty}\frac{1}{i!}\bar{A}_{i+1}\tilde{y}^{i+1},\tag{6.1}$$

$$\partial_{\bar{z}}\tilde{\varphi}(z,\bar{z})=\partial_\varphi S|_{\varphi=\tilde{\varphi}}=A_1+\sum_{i=2}^{\infty}\frac{1}{(i-1)!}A_i\tilde{y}^i\Rightarrow\partial_{\bar{z}}\tilde{y}=\sum_{i=1}^{\infty}\frac{1}{i!}A_{i+1}\tilde{y}^{i+1}\tag{6.2}$$

with $\tilde{y}=\tilde{\varphi}-\varphi_0$, $A_1=\partial_{\bar{z}}\varphi_0$, and $\bar{A}_1=\partial_z\varphi_0$. Expanding $\tilde{y}$ in a power series of u,

$$\tilde{y}(z,\bar{z},u)=\tilde{\varphi}(z,\bar{z},u)-\varphi_0(z,\bar{z})=u\sum_{k=0}^{\infty}\Lambda_k(z,\bar{z})\frac{u^k}{k!},\tag{6.3}$$

yields

$$\partial_{\bar{z}}\sum_{k=0}^{\infty}\frac{1}{k!}\Lambda_k u^{k+1}=\sum_{i=1}^{\infty}\frac{1}{i!}A_{i+1}\left\{\sum_{j=0}^{\infty}\frac{1}{j!}\Lambda_j u^{j+1}\right\}^i,\tag{6.4}$$

$$\partial_z\sum_{k=0}^{\infty}\frac{1}{k!}\Lambda_k u^{k+1}=\sum_{i=1}^{\infty}\frac{1}{i!}\bar{A}_{i+1}\left\{\sum_{j=0}^{\infty}\frac{1}{j!}\Lambda_j u^{j+1}\right\}^i.\tag{6.5}$$

Comparing the coefficients in $(l+1)$th order leads to

$$\partial_{\bar{z}}\Lambda_l=A_2\Lambda_l+\mathrm{Inh}(A_2,\ldots,A_{l+1};\Lambda_0,\ldots,\Lambda_{l-1}),$$
$$\partial_z\Lambda_l=\bar{A}_2\Lambda_l+\mathrm{Inh}(\bar{A}_2,\ldots,\bar{A}_{l+1};\Lambda_0,\ldots,\Lambda_{l-1}),$$

with the inhomogeneities Inh which depend on A_i, $\bar{A}_i$ calculated above and the functions of lower order Λ_j, $j<l$. Making use of $A_2=\partial_{\bar{z}}\ln(\theta)$ and $\bar{A}_2=\partial_z\ln(\theta)$ we get

$$\boxed{\begin{aligned}\Lambda_l&=\theta\left\{\int^z\frac{1}{\theta}\mathrm{Inh}(\bar{A}_2,\ldots,\bar{A}_{l+1};\Lambda_0,\ldots,\Lambda_{l-1})\,\mathrm{d}\hat{z}+\mathrm{const}\right\}\\&=\theta\left\{\int^{\bar{z}}\frac{1}{\theta}\mathrm{Inh}(A_2,\ldots,A_{l+1};\Lambda_0,\ldots,\Lambda_{l-1})\,\mathrm{d}\hat{\bar{z}}+\mathrm{const}\right\}.\end{aligned}}\tag{6.6}$$

So the solutions of the Euler–Lagrange equations $\tilde{\varphi}=\varphi_0+\Sigma_{k=0}^{\infty}\Lambda_k u^{k+1}/k!$ can be obtained by successive integration of the coefficients Λ_l. Regarding the lowest order $(l=0)$ $\partial_z\Lambda_0=\bar{A}_2\Lambda_0$, $\partial_{\bar{z}}\Lambda_0=A_2\Lambda_0$ leads to

$$\Lambda_0=c_0\theta,\quad c_0\in\mathcal{R}\Rightarrow\tilde{y}=uc_0\theta+\cdots.$$

Since θ obeys the linear PDE (3.10), c_0 can always be absorbed into it. θ is discussed in Sec. V. For applications, see (5.5), (5.6), (5.10), and (5.11).

Thus the one-parametric field of extremals in the vicinity $(u\ll 1)$ of the original solution of the equation of motion $\varphi_0(z,\bar{z})$ is determined by

$$\boxed{\tilde{\varphi}(z,\bar{z},u)=\varphi_0(z,\bar{z})+u\,\theta(z,\bar{z}).}\tag{6.7}$$

We compare our considerations with an expansion of the field variable $\tilde{\varphi}$ within the Euler–Lagrange equation. $\tilde{\varphi}$ is expanded in the parameter of the fields of the extremals denoted as u:

$$\tilde{\varphi}(z,\bar{z},u)=\tilde{\varphi}_0(z,\bar{z})+y(z,\bar{z},u)=\tilde{\varphi}_0(z,\bar{z})+u\sum_{n=0}^{\infty}\frac{1}{n!}\Lambda_n(z,\bar{z})u^n.$$

$\tilde{\varphi}_0(z,\bar{z})$ is an arbitrary extremal. The potential is assumed to be an analytic function of $\tilde{\varphi}$:

$$V(\tilde{\varphi}) = \sum_{m=0}^{\infty} \frac{1}{m!} \partial_{\varphi}^{m} V(\tilde{\varphi})|_{\tilde{\varphi}=\tilde{\varphi}_0} (\tilde{\varphi}-\tilde{\varphi}_0)^m$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!} \partial_{\varphi}^{m} V(\tilde{\varphi})|_{\tilde{\varphi}=\tilde{\varphi}_0} u^m$$

$$= \left\{ \sum_{n=0}^{\infty} \frac{1}{n!} \Lambda_n(z,\bar{z}) u^n \right\}^m .$$

Similar to the results of Sec. II, where we study the Hamilton–Jacobi theory, we obtain by comparing the coefficients of equal order of u^n:

$$u^0: \quad \partial_z \partial_{\bar{z}} \tilde{\varphi}_0(z,\bar{z}) + \tfrac{1}{2} \partial_{\tilde{\varphi}} V(\tilde{\varphi})|_{\tilde{\varphi}=\tilde{\varphi}_0} = 0,$$

which is fulfilled due to assumption and

$$u^1: \quad \partial_z \partial_{\bar{z}} \Lambda_0 + \tfrac{1}{2} \partial_{\tilde{\varphi}}^2 V(\tilde{\varphi}_0) \Lambda_0 = 0, \tag{6.8}$$

$$u^{n+1}: \quad \partial_z \partial_{\bar{z}} \Lambda_n + \tfrac{1}{2} \partial_{\tilde{\varphi}}^2 V(\tilde{\varphi}_0) \Lambda_n = \mathrm{Inh}(\Lambda_0 \cdots \Lambda_{n-1}, \partial_{\tilde{\varphi}}^2 V(\tilde{\varphi}_0) \cdots \partial_{\tilde{\varphi}}^{n+1} V(\tilde{\varphi}_0)). \tag{6.9}$$

The first one of these PDEs yields

$$\tilde{\varphi} = \tilde{\varphi}_0 + u \Lambda_0 .$$

Because Λ_0 has to fulfill the same linear equation as θ, which we introduced in the Hamilton–Jacobi theory (3.10), we are able to identify Λ_0 and θ with each other. Thus our result (6.7) is *equivalent* to a second variation of the action functional, which is commonly employed, e.g., with semiclassical considerations[14] and stability investigations.[15]

The PDE (6.9) is analogous to the equation (3.15), which we obtained in the Hamilton–Jacobi framework. Both can be used to determine the fluctuations in a neighborhood of a given extremal $\tilde{\varphi}_0$ in every order of u.

If one is able to find the general integral of the Hamilton–Jacobi equation and the integrability condition, the general solution of the Euler–Lagrange equation can be obtained.

A. An example

Here we would like to calculate the Hamilton–Jacobi functions $S(z,\bar{z},\varphi)$ and $\bar{S}(z,\bar{z},\varphi)$ and a related field of extremals $\tilde{\varphi}(z,\bar{z},u)$ according to the formalism developed in Secs. III, V, and VI. For this we choose the sine–Gordon model with the one-kink solution $\varphi_0 = 4 \arctan(\exp(z+\bar{z}))$. Though the functions S and $\bar{S}$ and the related extremals are determined perturbatively, the corresponding formal series (3.5) and (6.3) can be obtained explicitly.

1. The Hamilton–Jacobi potentials S and $\bar{S}$

The coefficients $A_n(z,\bar{z})$ and $\bar{A}_n(z,\bar{z})$ of (3.5) are determined by calculating the functions $\chi_n(z,\bar{z})$ and $\tilde{\chi}_n(z,\bar{z})$ as solutions of the PDEs (3.15) in every order $n = 0,1,2,\ldots$.

The coefficients $A_0(z,\bar{z})$ and $\bar{A}_0(z,\bar{z})$ can be calculated from (3.7) and (3.8) where the Lagrangian $\mathcal{L}_0$ is given by

$$\mathcal{L}_0 := \partial_z \varphi_0 \partial_{\bar{z}} \varphi_0 - V(\varphi_0) = 32 \left(\frac{e^{z+\bar{z}}}{1+e^{2(z+\bar{z})}} \right)^2 = 8 \frac{1}{(\cosh(z+\bar{z}))^2}$$

on the single extremal φ_0. Then we obtain

$$A_0(z,\overline{z}) = -4\cos\left(\frac{\varphi_0}{2}\right) + \partial_{\overline{z}}\chi_0(z,\overline{z}) = 4\tanh(z+\overline{z}) + \partial_{\overline{z}}\chi_0(z,\overline{z}), \tag{6.10}$$

$$\overline{A}_0(z,\overline{z}) = -4\cos\left(\frac{\varphi_0}{2}\right) - \partial_z\chi_0(z,\overline{z}) = 4\tanh(z+\overline{z}) - \partial_z\chi_0(z,\overline{z}). \tag{6.11}$$

The coefficients of first order are determined by the embedding conditions:

$$A_1(z,\overline{z}) = \partial_{\overline{z}}\varphi_0 = \frac{2}{\cosh l}, \quad \overline{A}_1(z,\overline{z}) = \partial_z\varphi_0 = \frac{2}{\cosh l}, \tag{6.12}$$

with the substitution $l = z + \overline{z}$. Obviously these expressions for the coefficients A_0, $\overline{A}_0$, A_1, and $\overline{A}_1$ obtained are the general solutions of these equations (6.10)–(6.12) in contrast to the following coefficients of higher orders of (3.5).

For the coefficients of the second order $A_2(z,\overline{z})$ and $\overline{A}_2(z,\overline{z})$ we choose the translation mode $\theta = 1/\cosh(l)$ of (5.5):

$$A_2(z,\overline{z}) = \partial_{\overline{z}}\ln(\theta) = -\tanh(l), \quad \overline{A}_2(z,\overline{z}) = \partial_z \ln(\theta) = -\tanh(l).$$

The inhomogeneity of the equation for $\overline{\chi}_3$ [see (3.13) and (3.16)] always vanishes. Therefore, according to (3.11), (3.13), and the discussion, thereby we can choose $\overline{\chi}_3(z,\overline{z}) \equiv 0$ without any loss of generality. Hence the coefficients A_3 and $\overline{A}_3$ are only determined by the function $\chi_3(z,\overline{z})$, which fulfill the inhomogeneous PDE (3.15):

$$\partial_z\partial_{\overline{z}}\chi_3 - \{2\tanh^2(z+\overline{z}) - 1\}\chi_3 = -\frac{1}{2}\partial_\varphi^3 V(\varphi)\big|_{\varphi=\varphi_0}\theta^2 = 2\frac{\tanh(l)}{\cosh^3(l)}.$$

A special solution is given by $\chi_3 = -\tanh(l)/(2\cosh(l))$, which yields

$$A_3(z,\overline{z}) = \frac{1}{\theta}\partial_{\overline{z}}\left(\frac{\chi_3}{\theta}\right) = -\frac{1}{2\cosh(l)}, \quad \overline{A}_3(z,\overline{z}) = \frac{1}{\theta}\partial_z\left(\frac{\chi_3}{\theta}\right) = -\frac{1}{2\cosh(l)}.$$

For $n = 4$ the inhomogeneity of the wave equation (3.11) for the coefficient $\overline{\chi}_4$ of (3.13) vanishes. Thus without any loss of generality we may set $\overline{\chi}_4 = 0$. The inhomogeneity of the equation (3.11) for the function χ_4 also vanishes. So we may choose the translation mode again:

$$A_4(z,\overline{z}) = \frac{1}{\theta^2}\partial_{\overline{z}}\left(\frac{\chi_4}{\theta}\right) = \frac{1}{4}\tanh(l), \quad \overline{A}_4(z,\overline{z}) = \frac{1}{\theta^2}\partial_z\left(\frac{\chi_4}{\theta}\right) = \frac{1}{4}\tanh(l).$$

Regarding the series of coefficients, we see that those for odd and even indices contain the same functions $1/\cosh(l)$ and $\tanh(l)$, respectively. So we assume the same for the higher orders:

$$A_{2n} = \overline{A}_{2n} = \frac{(-1)^n}{2^{2n-4}}\tanh(l) \quad \text{and} \quad A_{2n+1} = \overline{A}_{2n+1} = \frac{(-1)^n}{2^{2n-3}}\frac{1}{\cosh(l)}, \quad n = 0,1,2,3,\ldots.$$

Inserting these expressions into the formal expansion (3.5) we obtain

$$S(z,\bar{z},\varphi)=4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n}}{n!2^{2n}}\right)\tanh(l)+4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n+1}}{n!2^{2n+1}}\right)\frac{1}{\cosh(l)}+\partial_{\bar{z}}\chi_0(z,\bar{z})$$
$$=4\cos\left(\frac{y}{2}\right)\tanh(l)+4\sin\left(\frac{y}{2}\right)\frac{1}{\cosh(l)}+\partial_{\bar{z}}\chi_0(z,\bar{z})$$
$$=-4\cos\left(\frac{y+\varphi_0}{2}\right)+\partial_z\chi_0(z,\bar{z})$$
$$=-4\cos\left(\frac{\varphi}{2}\right)+\partial_z\chi_0(z,\bar{z}), \tag{6.13}$$

$$\bar{S}(z,\bar{z},y)=4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n}}{n!2^{2n}}\right)\tanh(l)+4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n+1}}{n!2^{2n+1}}\right)\frac{1}{\cosh(l)}-\partial_{\bar{z}}\chi_0(z,\bar{z})$$
$$=4\cos\left(\frac{y}{2}\right)\tanh(l)+4\sin\left(\frac{y}{2}\right)\frac{1}{\cosh(l)}-\partial_{\bar{z}}\chi_0(z,\bar{z})$$
$$=-4\cos\left(\frac{y+\varphi_0}{2}\right)-\partial_{\bar{z}}\chi_0(z,\bar{z})$$
$$=-4\cos\left(\frac{\varphi}{2}\right)-\partial_{\bar{z}}\chi_0(z,\bar{z}). \tag{6.14}$$

These solutions satisfy the HJE (3.1) and the IC (3.2). The embedding condition (3.4) is fulfilled on the single extremal φ_0 by construction.

2. Embedded extremals

The embedded extremals $\tilde{\varphi}(z,\bar{z},u)$ can be determined by a straightforward integration of the equations

$$\partial_z\tilde{\varphi}(z,\bar{z},u)=\Phi=\partial_{\varphi}\bar{S}(z,\bar{z},\varphi=\tilde{\varphi}(z,\bar{z},u))=2\sin\left(\frac{\tilde{\varphi}}{2}\right), \tag{6.15}$$

$$\partial_{\bar{z}}\tilde{\varphi}(z,\bar{z},u)=\bar{\Phi}=\partial_{\varphi}S(z,\bar{z},\varphi=\tilde{\varphi}(z,\bar{z},u))=2\sin\left(\frac{\tilde{\varphi}}{2}\right), \tag{6.16}$$

which leads to

$$\int^{\tilde{\varphi}}\frac{\mathrm{d}w}{2\sin(w/2)}=\ln\tan\left(\frac{\tilde{\varphi}}{4}\right)=z+\bar{f}(\bar{z}),$$

$$\int^{\tilde{\varphi}}\frac{\mathrm{d}w}{2\sin(w/2)}=\ln\tan\left(\frac{\tilde{\varphi}}{4}\right)=\bar{z}+f(z).$$

Obviously this system of algebraic equations can only be satisfied by the functions $f(z)=z+u$ and $\bar{f}(\bar{z})=\bar{z}+u$, $u=\text{const}$, which gives the field of extremals:

$$\tilde{\varphi}(z,\bar{z},u)=4\arctan(\exp(z+\bar{z}+u)),$$

parametrized by one parameter u.

However, here we would like to show how the embedded extremals can be calculated by the recursive formalism developed above, which is necessary if we are not able to determine the DeDonder and Weyl Hamilton–Jacobi functions or the corresponding family of extremals explicitly.

First we calculate the first three orders $(\Lambda_0,\Lambda_1,\Lambda_2)$ of the expansion (6.3) of $\tilde{y}(z,\bar{z},u)$ in u which will turn out to be sufficient to guess the general result for the embedded extremals $\tilde{y}$. From Eqs. (6.1)–(6.3) we get

$$\partial_z\tilde{y}=\bar{A}_2\tilde{y}+\frac{1}{2!}\bar{A}_3\tilde{y}^2+\frac{1}{3!}\bar{A}_4\tilde{y}^3+O(u^4),$$

$$\partial_{\bar{z}}\tilde{y}=A_2\tilde{y}+\frac{1}{2!}A_3\tilde{y}^2+\frac{1}{3!}A_4\tilde{y}^3+O(u^4),$$

in which the formal expansion

$$\tilde{y}(z,\bar{z},u)=\tilde{\varphi}(z,\bar{z},u)-\varphi_0(z,\bar{z})=u\sum_{k=0}^{\infty}\Lambda_k(z,\bar{z})\frac{u^k}{k!}$$

has to be inserted. For the first orders we obtain

$$\begin{aligned}
u^1:\quad & \partial_z\Lambda_0=\frac{1}{\theta}\partial_z(\theta)\Lambda_0,\\
& \partial_{\bar{z}}\Lambda_0=\frac{1}{\theta}\partial_{\bar{z}}(\theta)\Lambda_0,\\
u^2:\quad & \partial_z\Lambda_1=\frac{1}{\theta}\partial_z(\theta)\Lambda_1+\frac{1}{2!\,\theta}\partial_z\left(\frac{\chi_3}{\theta}\right)\Lambda_0^2,\\
& \partial_{\bar{z}}\Lambda_1=\frac{1}{\theta}\partial_{\bar{z}}(\theta)\Lambda_1+\frac{1}{2!\,\theta}\partial_{\bar{z}}\left(\frac{\chi_3}{\theta}\right)\Lambda_0^2,\\
u^3:\quad & \partial_z\Lambda_2=2\,\frac{1}{2!\,\theta}\partial_z(\theta)\Lambda_2+2\,\frac{1}{3!\,\theta^2}\partial_z\left(\frac{\chi_4}{\theta}\right)\Lambda_0^3+4\,\frac{1}{2!\,\theta}\partial_z\left(\frac{\chi_3}{\theta}\right)\Lambda_0\Lambda_1,\\
& \partial_{\bar{z}}\Lambda_2=2\,\frac{1}{2!\,\theta}\partial_{\bar{z}}(\theta)\Lambda_2+2\,\frac{1}{3!\,\theta^2}\partial_{\bar{z}}\left(\frac{\chi_4}{\theta}\right)\Lambda_0^3+4\,\frac{1}{2!\,\theta}\partial_{\bar{z}}\left(\frac{\chi_3}{\theta}\right)\Lambda_0\Lambda_1.
\end{aligned}$$

The solutions of these equations are determined up to a constant which may be absorbed by a redefinition of the parameter u:

$$\Lambda_0=2\,\theta=\frac{2}{\cosh(l)},\quad \Lambda_1=2\chi_3=-\frac{\tanh(l)}{\cosh(l)}=\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{1}{\cosh(l)}\right),$$

$$\Lambda_2=\frac{8}{3}\chi_4+4\,\frac{\chi_3^2}{\theta}-\frac{1}{3}\,\theta=\frac{4}{3\cosh^2(l)}\left(\sinh^2(l)-\frac{1}{2}\cosh^2(l)\right)=\frac{\mathrm{d}^2}{\mathrm{d}l^2}\left(\frac{2}{3\cosh(l)}\right).$$

From these coefficients we can already guess the form of the coefficients of the higher orders

$$\Lambda_k=\frac{1}{k+1}\,\frac{\mathrm{d}^k}{\mathrm{d}l^k}\left(\frac{2}{\cosh(l)}\right),$$

from which we obtain the embedded extremals:

$$\begin{aligned}\tilde{\varphi} &= \varphi_0 + u\sum_{k=0}^{\infty}\frac{u^k}{(k+1)!}\frac{\mathrm{d}^k}{\mathrm{d}l^k}\left(\frac{2}{\cosh(l)}\right)\\ &= \varphi_0 + \int^{l}\sum_{k=0}^{\infty}\frac{u^{k+1}}{(k+1)!}\frac{\mathrm{d}^{k+1}}{\mathrm{d}l'^{k+1}}\left(\frac{2}{\cosh(l')}\right)\mathrm{d}l'\\ &= \varphi_0 + \int^{l}\frac{2}{\cosh(l'+u)}\mathrm{d}l' - \int^{l}\frac{2}{\cosh(l')}\mathrm{d}l'\\ &= 4\arctan(\exp(l+u)).\end{aligned} \tag{6.17}$$

Obviously we get a one-parametric field of extremals satisfying the EL equations, as well as the equations (6.15) and (6.16). It covers a strip of the extended configuration space: $0<\varphi<2\pi$, $z,\overline{z} \in \mathcal{R}$. By translations $\varphi\to\varphi+2\pi$ the whole $\mathcal{R}^3$ parametrized by $z,\overline{z}$, $\varphi\in\mathcal{R}$ can be covered by fields of these extremals with the exception of the parallel planes $\varphi=2k\pi$, $k=0,\pm1,\pm2,...$, which are solutions of the equations of motion, too. These are the so-called ''vacuum'' solutions in the sine–Gordon theory. So this set of fields of extremals, counted by the integer number k can be completed by these planes $\varphi=2k\pi$, $k=0,\pm1,\pm2,...$, so that the whole space $\mathcal{R}^3$ is covered by extremals.

VII. WAVE FRONTS

In order to determine the wave fronts we have to turn to Carathéodory's framework, i.e., it is necessary to transform the DeDonder and Weyl Hamilton–Jacobi functions $S(z,\overline{z},\varphi)$ and $\overline{S}(z,\overline{z},\varphi)$ appearing in the expansion (3.5) and by the series (3.16) into those of Carathéodory $S^z(z,\overline{z},\varphi)$, $S^{\overline{z}}(z,\overline{z},\varphi)$, namely S^z and $S^{\overline{z}}$ of Eq. (2.6).

A. Carathéodory's Hamilton–Jacobi functions

As stated in Sec. II, the two Hamiltonian formulations are algebraically equivalent for fields with only one field component. Thus the Hamiltonian density $\mathcal{H}$ and the momenta p and $\overline{p}$ are the same in both formalisms. Therefore we can use the equality of the momenta in order to determine S^z and $S^{\overline{z}}$ from the functions S and $\overline{S}$ calculated above.

We therefore return to the transversality conditions in (2.4) and (2.6) and obtain

$$\partial_{\overline{z}}S^{\overline{z}}\partial_\varphi S^z - \partial_{\overline{z}}S^z\partial_\varphi S^{\overline{z}} = p = \partial_\varphi S = \sum_{i=0}^{\infty}\frac{1}{i!}A_{i+1}y^i, \tag{7.1}$$

$$\partial_z S^z\partial_\varphi S^{\overline{z}} - \partial_z S^{\overline{z}}\partial_\varphi S^z = \overline{p} = \partial_\varphi \overline{S} = \sum_{i=0}^{\infty}\frac{1}{i!}\overline{A}_{i+1}y^i. \tag{7.2}$$

Inserting the functions S^z and $S^{\overline{z}}$ expanded in powers of $y=\varphi-\varphi_0(z,\overline{z})$, like S and $\overline{S}$,

$$S^z(z,\overline{z},\varphi)=\sum_{i=0}^{\infty}\frac{1}{i!}A_i^z(z,\overline{z})y^i, \quad S^{\overline{z}}(z,\overline{z},\varphi)=\sum_{i=0}^{\infty}\frac{1}{i!}A_i^{\overline{z}}(z,\overline{z})y^i, \tag{7.3}$$

and comparing powers of y^n yields

$$\overline{A}_{n+1}-\sum_{i=0}^{n}\binom{n}{i}\{[\partial_z A_i^z - A_{i+1}^z\partial_z\varphi_0]A_{n-i+1}^{\overline{z}} - [\partial_z A_i^{\overline{z}} - A_{i+1}^{\overline{z}}\partial_z\varphi_0]A_{n-i+1}^z\}=0,$$

$$A_{n+1}+\sum_{i=0}^{n}\binom{n}{i}\{[\partial_{\overline{z}} A_i^z - A_{i+1}^z\partial_{\overline{z}}\varphi_0]A_{n-i+1}^{\overline{z}} - [\partial_{\overline{z}} A_i^{\overline{z}} - A_{i+1}^{\overline{z}}\partial_{\overline{z}}\varphi_0]A_{n-i+1}^z\}=0.$$

These equations determine the coefficients $A^z_{n+1}(z,\bar{z})$ and $A^{\bar{z}}_{n+1}(z,\bar{z})$ recursively:

$$(\partial_z A^z_0)A^{\bar{z}}_{n+1}-(\partial_z A^{\bar{z}}_0)A^z_{n+1}=\overline{A}_{n+1}+\mathrm{Inh}^{n+1}_1(A^z_0,A^{\bar{z}}_0,\ldots,A^z_n,A^{\bar{z}}_n), \tag{7.4}$$

$$(\partial_{\bar{z}} A^{\bar{z}}_0)A^z_{n+1}-(\partial_{\bar{z}} A^z_0)A^{\bar{z}}_{n+1}=A_{n+1}+\mathrm{Inh}^{n+1}_2(A^z_0,A^{\bar{z}}_0,\ldots,A^z_n,A^{\bar{z}}_n). \tag{7.5}$$

The functions Inh^{n+1}_1 and Inh^{n+1}_2 depend only on the coefficients of lower powers of y, namely A^z_0, $A^{\bar{z}}_0,\ldots,A^z_n$, $A^{\bar{z}}_n$. They vanish for $n=0$: $\mathrm{Inh}^1_1=\mathrm{Inh}^1_2=0$. For $n=1$ we get

$$\mathrm{Inh}^2_1=A^{\bar{z}}_1\partial_z A^z_1-A^z_1\partial_z A^{\bar{z}}_1 \quad \text{and} \quad \mathrm{Inh}^2_2=-A^{\bar{z}}_1\partial_{\bar{z}}A^z_1+A^z_1\partial_{\bar{z}}A^{\bar{z}}_1,$$

and for arbitrary orders $n>1$

$$\mathrm{Inh}^{n+1}_1=-\sum_{i=1}^{n-1}\binom{n}{i}\{[\partial_z A^z_i-A^z_{i+1}\partial_z\varphi_0]A^{\bar{z}}_{n-i+1}-[\partial_z A^{\bar{z}}_i-A^{\bar{z}}_{i+1}\partial_z\varphi_0]A^z_{n-i+1}\}+A^{\bar{z}}_1\partial_z A^z_n-A^z_1\partial_z A^{\bar{z}}_n, \tag{7.6}$$

$$\mathrm{Inh}^{n+1}_2=+\sum_{i=1}^{n-1}\binom{n}{i}\{[\partial_{\bar{z}} A^z_i-A^z_{i+1}\partial_{\bar{z}}\varphi_0]A^{\bar{z}}_{n-i+1}-[\partial_{\bar{z}} A^{\bar{z}}_i-A^{\bar{z}}_{i+1}\partial_{\bar{z}}\varphi_0]A^z_{n-i+1}\}-A^{\bar{z}}_1\partial_{\bar{z}}A^z_n+A^z_1\partial_{\bar{z}}A^{\bar{z}}_n. \tag{7.7}$$

The determinant

$$\Delta=(\partial_{\bar{z}}A^{\bar{z}}_0)(\partial_z A^z_0)-(\partial_z A^{\bar{z}}_0)(\partial_{\bar{z}}A^z_0)=\mathcal{L}|_{\varphi=\varphi_0}=\mathcal{L}_0=\partial_z\varphi_0\partial_{\bar{z}}\varphi_0-V(\varphi_0)$$

of this linear system of *algebraic* equations is assumed to be not zero. We consider only those extremals φ_0 and regions in the Minkowski space where the Lagrange density $\mathcal{L}|_{\varphi=\varphi_0}$ does not vanish. It makes sense to exclude those focal points and caustics, where $\mathcal{L}|_{\varphi=\varphi_0}=0$, because the transversality relations of the wave fronts and extremals are violated otherwise.[1]

To obtain the functions $A^{\bar{z}}_0$ and A^z_0 we have to consider the zeroth order of the Hamilton–Jacobi equation in (2.6):

$$(\partial_{\bar{z}}A^{\bar{z}}_0)(\partial_z A^z_0)-(\partial_z A^{\bar{z}}_0)(\partial_{\bar{z}}A^z_0)=\partial_z\varphi_0\partial_{\bar{z}}\varphi_0-V(\varphi_0)=\mathcal{L}_0. \tag{7.8}$$

If $\mathcal{L}_0\neq 0$, then one of the functions A^z_0 and $A^{\bar{z}}_0$ can be chosen arbitrarily and the other one has to be calculated according to this PDE. For example, we may choose $A^{\bar{z}}_0=\bar{z}$ and $A^z_0=\int\mathcal{L}_0\,\mathrm{d}z$. In the case of the kink solution $\varphi_0=\pm 4\arctan(\exp(z+\bar{z}))$ for the sine–Gordon theory we get $A^z_0=8\tanh(z+\bar{z})$.

The Hamilton–Jacobi equation of Carathéodory is satisfied automatically in any order of y^n, $n\geqslant 1$, because the corresponding equation of DeDonder and Weyl is fulfilled:

$$\partial_\varphi\{\partial_z S^z\partial_{\bar{z}}S^{\bar{z}}-\partial_z S^{\bar{z}}\partial_{\bar{z}}S^z+\mathcal{H}\}=\partial_z p+\partial_{\bar{z}}\bar{p}+\partial_\varphi\mathcal{H}=\partial_\varphi\{\partial_z S+\partial_{\bar{z}}\bar{S}+\mathcal{H}\}=0.$$

The integrability condition holds, too, because it imposes a constraint on the slope functions which are independent of the special Hamiltonian description for one component field theories.

The linear system of equations for $A^z(z,\bar{z})$ and $A^{\bar{z}}(z,\bar{z})$ can be solved easily:

$$A^z_{n+1}=\frac{1}{\mathcal{L}_0}[(\partial_z A^z_0)A_{n+1}+(\partial_{\bar{z}}A^z_0)\overline{A}_{n+1}]+\widetilde{\mathrm{Inh}}^{n+1}_1(A^z_0,A^{\bar{z}}_0,\ldots,A^z_n,A^{\bar{z}}_n), \tag{7.9}$$

$$A^{\bar{z}}_{n+1}=\frac{1}{\mathcal{L}_0}[(\partial_z A^{\bar{z}}_0)A_{n+1}+(\partial_{\bar{z}}A^{\bar{z}}_0)\overline{A}_{n+1}]+\widetilde{\mathrm{Inh}}^{n+1}_2(A^z_0,A^{\bar{z}}_0,\ldots,A^z_n,A^{\bar{z}}_n). \tag{7.10}$$

The functions $\widetilde{\mathrm{Inh}}_1^{n+1}$ and $\widetilde{\mathrm{Inh}}_2^{n+1}$ are linear combinations of the inhomogeneities (7.6), and (7.7) may easily be determined. So we get, e.g., for the coefficients A_1^z, $A_1^{\bar z}$ and A_2^z, $A_2^{\bar z}$ the expressions:

$$A_1^z=\frac{1}{\mathcal{L}_0}[(\partial_z A_0^z)A_1+(\partial_{\bar z}A_0^z)\overline{A_1}]=\frac{[(\partial_z A_0^z)\partial_{\bar z}\varphi_0+(\partial_{\bar z}A_0^z)\partial_z\varphi_0]}{\partial_z\varphi_0\partial_{\bar z}\varphi_0-V(\varphi_0)}, \tag{7.11}$$

$$A_1^{\bar z}=\frac{1}{\mathcal{L}_0}[(\partial_z A_0^{\bar z})A_1+(\partial_{\bar z}A_0^{\bar z})\overline{A_1}]=\frac{[(\partial_z A_0^{\bar z})\partial_{\bar z}\varphi_0+(\partial_{\bar z}A_0^{\bar z})\partial_z\varphi_0]}{\partial_z\varphi_0\partial_{\bar z}\varphi_0-V(\varphi_0)}, \tag{7.12}$$

and

$$A_2^z=\frac{1}{\mathcal{L}_0}[(\partial_z A_0^z)(A_2-A_1^{\bar z}\partial_{\bar z}A_1^z+A_1^z\partial_{\bar z}A_1^{\bar z})+(\partial_{\bar z}A_0^z)(\overline{A_2}+A_1^{\bar z}\partial_z A_1^z-A_1^z\partial_z A_1^{\bar z})], \tag{7.13}$$

$$A_2^{\bar z}=\frac{1}{\mathcal{L}_0}[(\partial_z A_0^{\bar z})(A_2-A_1^{\bar z}\partial_{\bar z}A_1^z+A_1^z\partial_{\bar z}A_1^{\bar z})+(\partial_{\bar z}A_0^{\bar z})(\overline{A_2}+A_1^{\bar z}\partial_z A_1^z-A_1^z\partial_z A_1^{\bar z})]. \tag{7.14}$$

The two coefficients A_0^z and $\overline{A_0^z}$ have to fulfill only one equation (7.8), because the closed two-form $\Omega=\mathrm{d}S^z\wedge\mathrm{d}S^{\bar z}$ is invariant under transformations $S^z\to\hat S^z(S^z,S^{\bar z})$ and $S^{\bar z}\to\hat S^{\bar z}(S^z,S^{\bar z})$ with a Jacobi determinant that equals one. A field of wave fronts given by

$$S^z(z,\bar z,\varphi)=\sum_{i=0}^{\infty}\frac{1}{i!}A_i^z(z,\bar z)(\varphi-\varphi_0(z,\bar z))^i=\sigma=\mathrm{const}, \tag{7.15}$$

$$S^{\bar z}(z,\bar z,\varphi)=\sum_{i=0}^{\infty}\frac{1}{i!}A_i^{\bar z}(z,\bar z)(\varphi-\varphi_0(z,\bar z))^i=\bar\sigma=\mathrm{const} \tag{7.16}$$

is not changed by this transformation, but only reparametrized,[22] $\sigma\to\hat\sigma=\hat S^z(\sigma,\bar\sigma)$ and $\bar\sigma\to\hat{\bar\sigma}=\hat S^{\bar z}(\sigma,\bar\sigma)$.

B. An explicit representation for the wave fronts

In order to obtain an explicit expression for the *one-dimensional* wave fronts $z(\sigma,\bar\sigma,\varphi)$ and $\bar z(\sigma,\bar\sigma,\varphi)$—$\sigma,\bar\sigma$ fixed—we have to invert the relations (7.16) which can be regarded as the defining equations for these functions $z(\varphi)$ and $\bar z(\varphi)$. Here they are assumed to be analytic functions of φ:

$$z=\sum_{i=0}^{\infty}\frac{1}{i!}\alpha_i(\sigma,\bar\sigma)(\hat y=\varphi-\hat\varphi_0(\sigma,\bar\sigma))^i,\quad \bar z=\sum_{i=0}^{\infty}\frac{1}{i!}\bar\alpha_i(\sigma,\bar\sigma)(\hat y=\varphi-\hat\varphi_0(\sigma,\bar\sigma))^i,$$

i.e., they can be expanded in powers of the difference $\hat y=\varphi-\hat\varphi_0(\sigma,\bar\sigma)$, where $\hat\varphi_0(\sigma,\bar\sigma)=\varphi_0(z(\sigma,\bar\sigma),\bar z(\sigma,\bar\sigma))$ denotes the extremal in terms of the variables $\sigma,\bar\sigma$. Obviously there is a difference between the quantities $y=\varphi-\varphi_0(z,\bar z)$ and $\hat y=\varphi-\hat\varphi_0(\sigma,\bar\sigma)$. Thus in order to determine the coefficients α_n, $\bar\alpha_n$ we have to insert this series into the defining equations for the wave fronts (7.15) and (7.16):

$$\sigma=\sum_{i=0}^{\infty}\frac{y^i}{i!}A_i^z\left(z=\alpha_0(\sigma,\bar\sigma)+\sum_{n=1}^{\infty}\frac{\hat y^n}{n!}\alpha_n(\sigma,\bar\sigma),\bar z=\bar\alpha_0(\sigma,\bar\sigma)+\sum_{m=1}^{\infty}\frac{\hat y^m}{m!}\bar\alpha_m(\sigma,\bar\sigma)\right), \tag{7.17}$$

$$\bar\sigma=\sum_{i=0}^{\infty}\frac{y^i}{i!}A_i^{\bar z}\left(z=\alpha_0(\sigma,\bar\sigma)+\sum_{n=1}^{\infty}\frac{\hat y^n}{n!}\alpha_n(\sigma,\bar\sigma),\bar z=\bar\alpha_0(\sigma,\bar\sigma)+\sum_{m=1}^{\infty}\frac{\hat y^m}{m!}\bar\alpha_m(\sigma,\bar\sigma)\right), \tag{7.18}$$

where the variables y have to be expanded in powers of $\hat{y}$, too:

$$y=\varphi-\varphi_0\left(z=\alpha_0(\sigma,\bar{\sigma})+\sum_{n=1}^{\infty}\frac{\hat{y}^n}{n!}\alpha_n(\sigma,\bar{\sigma}),\bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma})+\sum_{m=1}^{\infty}\frac{\hat{y}^m}{m!}\bar{\alpha}_m(\sigma,\bar{\sigma})\right). \tag{7.19}$$

The wave fronts on the extremals $\alpha_0(\sigma,\bar{\sigma})$ and $\bar{\alpha}_0(\sigma,\bar{\sigma})$ are determined by the zeroth-order of Eqs. (7.17)–(7.19):

$$\sigma=A_0^z(z=\alpha_0(\sigma,\bar{\sigma}),\bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma})) \quad \text{and} \quad \bar{\sigma}=A_0^{\bar{z}}(z=\alpha_0(\sigma,\bar{\sigma}),\bar{z}=\bar{\alpha}_0(\sigma,\bar{\alpha})). \tag{7.20}$$

For the sine–Gordon theory we obtain from the choice we have made for the functions A_0^z and $A_0^{\bar{z}}$ $\bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma})=\sigma$ and $z=\alpha_0(\sigma,\bar{\sigma})=\operatorname{artanh}(\bar{\sigma})-\sigma$.

Locally the functions $\alpha_0(\sigma,\bar{\sigma})$ and $\bar{\alpha}_0(\sigma,\bar{\sigma})$ are determined uniquely, because the Jacobi determinant $\Delta=(\partial_{\bar{z}}A_0^{\bar{z}})(\partial_z A_0^z)-(\partial_z A_0^{\bar{z}})(\partial_{\bar{z}}A_0^z)=\mathcal{L}|_{\varphi=\hat{\varphi}_0}$ of this transformation $z,\bar{z}\to\sigma,\bar{\sigma}$ does not vanish, as assumed.

Expanding the expressions (7.17) in $\hat{y}^n$, inserting the series (7.19), and separating the coefficients $\alpha_n(\sigma,\bar{\sigma})$ and $\bar{\alpha}_n(\sigma,\bar{\sigma})$ we obtain a pair of linear algebraic equations for these coefficients, which can be solved like the system (7.4) and (7.5). After inserting the coefficients A_1, $\bar{A}_1,\ldots,A_n$, $\bar{A}_n$ of the DeDonder and Weyl Hamilton–Jacobi theory we get the final result for $n\geqslant 2$:

$$\alpha_n=\frac{(-\mathcal{L}_0)^{n-1}}{\mathcal{H}_0^{n+1}}(V(\varphi_0)A_n-(\partial_{\bar{z}}\varphi_0)^2\bar{A}_n)+\mathrm{Inh}(A_1,\bar{A}_1,\ldots,A_{n-1},\bar{A}_{n-1},\mathrm{deriv.}), \tag{7.21}$$

$$\bar{\alpha}_n=\frac{(-\mathcal{L}_0)^{n-1}}{\mathcal{H}_0^{n+1}}(V(\varphi_0)\bar{A}_n-(\partial_{z}\varphi_0)^2A_n)+\mathrm{Inh}(A_1,\bar{A}_1,\ldots,A_{n-1},\bar{A}_{n-1},\mathrm{deriv.}). \tag{7.22}$$

The term ''deriv'' in the inhomogeneities denotes the derivatives of A_i^z and $A_i^{\bar{z}}$, $i=1,\ldots,n-1$ with respect to z and $\bar{z}$. The functions A_n^z and $A_n^{\bar{z}}$ and their derivatives are short-cuts of, e.g., $\partial_z A_n^z=\partial_z A_n^z|_{z=\alpha_0(\sigma,\bar{\sigma}),\bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma})}$ and thus depend on $\sigma,\bar{\sigma}$ only.

Obviously a not degenerated transformation $z,\bar{z}\to\sigma=S^z$, $\bar{\sigma}=S^{\bar{z}}$ only exists if the Lagrangian $\mathcal{L}_0$ and the Hamiltonian densities $\mathcal{H}_0$ on the extremals do not vanish.

The coefficients of zeroth order are given in (7.20); those of the next two powers in $\hat{y}$ are

$$\alpha_1(\sigma,\bar{\sigma})=\frac{\partial_{\bar{z}}\varphi_0}{\mathcal{H}_0}=\frac{\partial_{\bar{z}}\varphi_0}{\partial_z\varphi_0\partial_{\bar{z}}\varphi_0+V(\varphi_0)}, \quad \bar{\alpha}_1(\sigma,\bar{\sigma})=\frac{\partial_z\varphi_0}{\mathcal{H}_0}=\frac{\partial_z\varphi_0}{\partial_z\varphi_0\partial_{\bar{z}}\varphi_0+V(\varphi_0)}, \tag{7.23}$$

and

$$\begin{aligned}\alpha_2(\sigma,\bar{\sigma})=&\frac{V(\varphi_0)}{\mathcal{H}_0^3}[-\mathcal{L}_0\partial_{\bar{z}}\ln(\theta)+\partial_{\bar{z}}(\partial_z\varphi_0\partial_{\bar{z}}\varphi_0)]\\&-\frac{\partial_{\bar{z}}\varphi_0\partial_{\bar{z}}\varphi_0}{\mathcal{H}_0^3}[-\mathcal{L}_0\partial_z\ln(\theta)+\partial_z(\partial_z\varphi_0\partial_{\bar{z}}\varphi_0)]+\frac{\partial_{\bar{z}}\varphi_0}{\mathcal{H}_0^2}\partial_\varphi V(\varphi_0),\end{aligned} \tag{7.24}$$

$$\begin{aligned}\bar{\alpha}_2(\sigma,\bar{\sigma})=&\frac{V(\varphi_0)}{\mathcal{H}_0^3}[-\mathcal{L}_0\partial_z\ln(\theta)+\partial_z(\partial_z\varphi_0\partial_{\bar{z}}\varphi_0)]\\&-\frac{\partial_z\varphi_0\partial_z\varphi_0}{\mathcal{H}_0^3}[-\mathcal{L}_0\partial_{\bar{z}}\ln(\theta)+\partial_{\bar{z}}(\partial_z\varphi_0\partial_{\bar{z}}\varphi_0)]+\frac{\partial_z\varphi_0}{\mathcal{H}_0^2}\partial_\varphi V(\varphi_0).\end{aligned} \tag{7.25}$$

Thus the wave fronts $z(\sigma,\overline{\sigma},\varphi)$ and $\overline{z}(\sigma,\overline{\sigma},\varphi)$ can be calculated from the coefficients A_n and $\overline{A}_n$ of DeDonder and Weyl's Hamilton–Jacobi framework and the coefficients A_0^z and $A_0^{\overline{z}}$ of Carathéodory's one. Carathéodory's coefficients A_n^z and $A_n^{\overline{z}}$, $n\geqslant 1$, are not necessarily involved in the final expressions (7.21) and (7.22), since they can be substituted by those of DeDonder and Weyl—determined by Bäcklund transformations.

C. An alternative way to determine the wave fronts

If one is not interested in obtaining an explicit representation of Carathéodory's Hamilton–Jacobi functions $S^z(z,\overline{z},\varphi)$ and $S^{\overline{z}}(z,\overline{z},\varphi)$, it is possible to get the coefficients α_n and $\hat{\alpha}_n$ of the last paragraph much more easily. However, this method can only be applied if the Hamiltonian density $\mathcal{H}$ does not vanish! If $\mathcal{H}=0$, we have to calculate Carathéodory's Hamilton–Jacobi functions $S^z(z,\overline{z},\varphi)$ and $S^{\overline{z}}(z,\overline{z},\varphi)$ as described above.

For nonvanishing Hamiltonian densities $\mathcal{H}$ we may change the independent variables z and $\overline{z}$ to $\sigma=S^z(z,\overline{z},\varphi)$ and $\overline{\sigma}=S^{\overline{z}}(z,\overline{z},\varphi)$, while the field φ remains unchanged. The functional determinant of this transformation is just $\mathcal{H}$ according to Carathéodory's Hamilton–Jacobi equation (2.6). Then the wave fronts $z=z(\varphi,\sigma,\overline{\sigma})$ and $\overline{z}=\overline{z}(\varphi,\sigma,\overline{\sigma})$ can be determined explicitly from the equations

$$\partial_\varphi z(\varphi,\sigma,\overline{\sigma})=\frac{p}{\mathcal{H}},\quad \partial_\varphi \overline{z}(\varphi,\sigma,\overline{\sigma})=\frac{\overline{p}}{\mathcal{H}}.$$

These equations are obtained by comparing the coefficients of the wedge products $\mathrm{d}\varphi\wedge\mathrm{d}\sigma$ and $\mathrm{d}\varphi\wedge\mathrm{d}\overline{\sigma}$ in the equation (2.6), if the variables $\sigma=S^z$ and $\overline{\sigma}=S^{\overline{z}}$ and φ are regarded as the independent ones.[23] So we can, e.g., immediately determine the coefficients of the first-order α_1 and $\overline{\alpha}_1$ in (7.23). The remaining coefficients α_n and $\overline{\alpha}_n$ in (7.22) and (7.21) can be determined by expanding the DeDonder and Weyl momenta p and $\overline{p}$ and the Hamiltonian density $\mathcal{H}$ in powers of $\hat{y}$.

D. An example: The sine–Gordon theory

We return to our example in Sec. VI in order to illustrate the formalism discussed above.

1. Carathéodory's Hamilton–Jacobi functions

To obtain Carathéodory's Hamilton–Jacobi functions $S^z(z,\overline{z},\varphi)$ and $S^{\overline{z}}(z,\overline{z},\varphi)$ from those of DeDonder and Weyl, (6.13) and (6.14), we first have to solve the equation (7.8) in order to get the coefficients $A_0^z(z,\overline{z})$ and $A_0^{\overline{z}}(z,\overline{z})$ of order y^0. Because in our example the Lagrangian density depends only on $l=z+\overline{z}$ on the extremals, it is useful to transform the independent variables z and $\overline{z}$ into $l=z+\overline{z}$ and $\overline{l}=z-\overline{z}$:

$$(\partial_{\overline{l}}A_0^z)(\partial_l A_0^{\overline{z}})-(\partial_{\overline{l}}A_0^{\overline{z}})(\partial_l A_0^z)=\frac{1}{2}\mathcal{L}_0=\frac{4}{\cosh^2(l)}.$$

Due to the invariance of the two-form $\Omega=\mathrm{d}S^z\wedge\mathrm{d}S^{\overline{z}}$, with respect to the transformations $S^z\to\hat{S}^z(S^z,S^{\overline{z}})$ and $S^{\overline{z}}\to\hat{S}^{\overline{z}}(S^z,S^{\overline{z}})$ with a Jacobi determinant equal to one we can choose any single solution of this equation without any loss of generality, e.g.,

$$A_0^z=A_0^z(l)=4\tanh(z+\overline{z}),\quad A_0^{\overline{z}}=A_0^{\overline{z}}=-\overline{l}=\overline{z}-z.$$

Inserting this result into the equations (7.11) and (7.12) we get the coefficients of first order,

$$A_1^z=A_1^z(l)=\frac{2}{\cosh(l)},\quad A_1^{\overline{z}}=0,$$

which leads, using Eqs. (7.9), (7.10), (7.13), and (7.14), to the coefficients of second and third order in y:

$$A_2^z = A_2^z(l) = -\tanh(l), \quad A_3^z = A_3^z(l) = -\frac{1}{2\cosh(l)}, \quad A_2^{\bar{z}} = A_3^{\bar{z}} = 0. \tag{7.26}$$

Inspecting the series of these coefficients we get an ansatz for those of all orders y^n, $n \geqslant 1$,

$$A_{2n}^z = A_{2n}^z(l) = 4\frac{(-1)^n}{2^{2n}}\tanh(l), \quad A_{2n-1}^z = A_{2n-1}^z(l) = 4\frac{(-1)^n}{2^{2n-1}}\frac{1}{\cosh(l)}, \quad A_n^{\bar{z}} = 0,$$

from which we obtain Carathéodory's Hamilton–Jacobi functions $S^z(z,\bar{z},\varphi)$ and $S^{\bar{z}}(z,\bar{z},\varphi)$ by determining the sum (7.3):

$$\begin{aligned} S(z,\bar{z},\varphi) &= 4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n}}{n!2^{2n}}\right)\tanh(l) + 4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n+1}}{n!2^{2n+1}}\right)\frac{1}{\cosh(l)} \\ &= 4\cos\left(\frac{y}{2}\right)\tanh(l) + 4\sin\left(\frac{y}{2}\right)\frac{1}{\cosh(l)} = -4\cos\left(\frac{\varphi}{2}\right), \end{aligned} \tag{7.27}$$

$$S^{\bar{z}}(z,\bar{z},\varphi) = \bar{z} - z. \tag{7.28}$$

These functions satisfy Carathéodory's Hamilton–Jacobi equation (3.1) and the integrability condition (3.2) as well as the embedding conditions (3.3) and (3.4). The solutions (7.27) and (7.28) for S^z and $S^{\bar{z}}$ are the only ones provided that we have fixed the coefficients A_0^z and $A_0^{\bar{z}}$, because Eqs. (7.9), (7.10), (7.13), and (7.14) lead to unique solutions. The general solution of the system of PDEs (2.6), (3.2), and (3.4) is obtained by applying arbitrary smooth transformations $S^z \to \Sigma(S^z, S^{\bar{z}})$ and $S^{\bar{z}} \to \bar{\Sigma}(S^z, S^{\bar{z}})$ to the functions (7.27) and (7.28) with a Jacobi determinant $\partial_1\Sigma\,\partial_2\bar{\Sigma} - \partial_2\Sigma\,\partial_1\bar{\Sigma} = 1$:

$$S^z(z,\bar{z},\varphi) = \Sigma(\bar{z} - z, -4\cos(\varphi/2)) \quad \text{and} \quad S^{\bar{z}}(z,\bar{z},\varphi) = \bar{\Sigma}(\bar{z} - z, -4\cos(\varphi/2)). \tag{7.29}$$

2. An explicit representation of the wave fronts—the singular case

Carathéodory's Hamilton–Jacobi functions S^z and $S^{\bar{z}}$ are given now by the equations (7.29). If we would like to have them in the explicit form $z(\sigma,\bar{\sigma},\varphi)$ and $\bar{z}(\sigma,\bar{\sigma},\varphi)$, we have to invert the equations (7.15) and (7.16). Doing this we get only the zeroth-order coefficients,

$$\alpha_0(\sigma,\bar{\sigma}) = \frac{1}{2}\left(\operatorname{artanh}\frac{\sigma}{4} + \bar{\sigma}\right) \quad \text{and} \quad \bar{\alpha}_0(\sigma,\bar{\sigma}) = \frac{1}{2}\left(\operatorname{artanh}\frac{\sigma}{4} - \bar{\sigma}\right),$$

without any difficulties. All the other coefficients α_n and $\bar{\alpha}_n$, $n \geqslant 1$, *do not exist*, because the Hamiltonian density $\mathcal{H}_0 = p_0\bar{p}_0 + V(\varphi_0)$ with $V_0 = 2(\cos(\varphi) - 1)$ vanishes on the given extremals φ_0 [see (7.21) and (7.22)]!

From the results (7.27) and (7.28) it becomes obvious why this happens. The function (7.28) depends only on the difference $z - \bar{z}$ whereas (7.27) does not depend on the variables z and $\bar{z}$ at all! Therefore it is impossible to invert the equations (7.15) and (7.16) to get the functions $z(\sigma,\bar{\sigma},\varphi)$ and $\bar{z}(\sigma,\bar{\sigma},\varphi)$ at every point $(\sigma,\bar{\sigma})$ of the parameter space $\Upsilon = \{(\sigma,\bar{\sigma})\}$. Hence the wave fronts are only defined at points $(\sigma,\bar{\sigma},\varphi)$ for which

$$\varphi \overset{!}{=} g(\sigma) = 2\arccos(\sigma/4), \quad -4 \leqslant \sigma \leqslant 4,$$

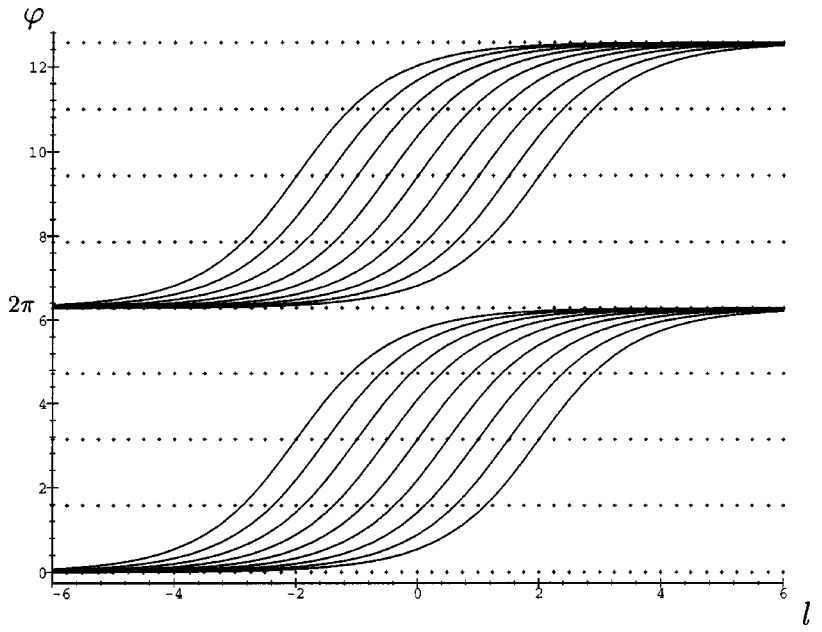

FIG. 1. Shown is the "singular" case (7.30). The extremals are plotted by solid line and the wave fronts by dotted lines. The axes are the field variable φ and the independent variable $l=\gamma(x-vt)$ which parametrizes the kink solution [see Eq. (5.7)].

holds. The real parameter $\overline{\sigma}$ remains arbitrary. Nevertheless the wave fronts are one dimensional straight lines parallel to each other: $z-\overline{z}=\overline{\sigma}=\text{const}$. They cover the extended configuration space $\mathcal{M}_{2+1}=\{z,\overline{z},\varphi\}$ as required, but the wave fronts cannot be given as functions $z(\sigma,\overline{\sigma},\varphi)$ and $\overline{z}(\sigma,\overline{\sigma},\varphi)$ because they are parallel to the surfaces $\varphi=\text{const}$.

Due to the transversality condition (2.10), the two-parametric field of 1D wave fronts (see Fig. 1),

$$z-\overline{z}=\overline{\sigma}=\text{const}, \quad \varphi=g(\sigma)=\text{const}, \tag{7.30}$$

and the one-parametric set of the 2D extremals $\tilde{\varphi}=4\arctan(\exp(l+u))$ intersect each other transversally everywhere in $\mathcal{M}_{2+1}=\{z,\overline{z},\varphi\}$, because the Lagrangian density $\mathcal{L}$ differs from zero in $\mathcal{M}_{2+1}$ contrary to the Hamiltonian density which vanishes everywhere in $\mathcal{M}_{2+1}$. The angle $\angle(w,e)$ between the basis vector W of the tangent space $\mathcal{T}_{\mathcal{P}}\mathcal{W}$ of the wave front

$$w=2\sin(\varphi/2)(\partial_z+\partial_{\overline{z}})$$

and an arbitrary nonvanishing vector e in the tangent space $\mathcal{T}_{\mathcal{P}}\mathcal{E}$ of the extremal parametrized by the variables λ and $\overline{\lambda}$,

$$e=\lambda\partial_z+\overline{\lambda}\partial_{\overline{z}}+2(\lambda+\overline{\lambda})\sin(\varphi/2)\partial_\varphi, \quad \text{with} \quad |\lambda|+|\overline{\lambda}|>0,$$

at the point $P=(z,\overline{z},\varphi)$ is given by

$$\angle(w,e)=\arccos\left(\frac{(w,e)}{|w||e|}\right)=\arccos\left(\frac{\lambda+\overline{\lambda}}{\sqrt{2}\sqrt{\lambda^2+\overline{\lambda}^2+4(\lambda+\overline{\lambda})^2\sin^2(\varphi/2)}}\right),$$

the minimum of which with respect to a variation of the parameters λ and $\overline{\lambda}$ gives the angle under which the wavefront intersects the extremal at P:

$$\angle(\mathcal{W},\mathcal{E})=\min\angle(w,e)=\arccos\left(\frac{1}{\sqrt{1+8\sin^2(\varphi/2)}}\right)=\arccos\left(\frac{1}{\sqrt{9-\sigma^2/2}}\right),$$

$\angle(\mathcal{W},\mathcal{E})$ is constant on a given wave front $\sigma=\text{const}$ and $\bar{\sigma}=\text{const}$. This angle $\angle(\mathcal{W},\mathcal{E})$ takes its minimum $\angle(\mathcal{W},\mathcal{E})=0$ for the values $\varphi=\varphi_k=2k\pi$, $k=0,\pm1,\pm2,\ldots$. So in the limit $z+\bar{z}=l\to\pm\infty$ the transversality condition is violated, since the wave fronts and extremals (6.17) are asymptotically parallel at all points P in the planes $\{z,\bar{z}\in\mathcal{R},\varphi=2k\pi\}\in\mathcal{M}_{2+1}$ parametrized by the integer number $k=0,\pm1,\pm2,\ldots$. Any of these planes separates the two one-parameter fields $\tilde{\varphi}=\arctan(\exp(l+u))+2(k-1)\pi$ and $\tilde{\varphi}=\arctan(\exp(l+u))+2k\pi$. Every extremal of these fields "touches" the plane $\varphi=2k\pi$ in the limits $l\to-\infty$ or $l\to\infty$. The maximum value for $\angle(\mathcal{W},\mathcal{E})=\arccos(\frac{1}{3})$ indicates that the wave fronts and the extremals are never perpendicular to each other.

Notice that the singular situation discussed above is essentially a coordinate singularity resulting from the singular change of variables z and $\bar{z}$ to $\sigma=S^z(z,\bar{z},\varphi)$ and $\bar{\sigma}=S^{\bar{z}}(z,\bar{z},\varphi)$. It shows that we cannot choose the parameters σ, $\bar{\sigma}$, and φ as independent variables to represent the wave fronts. The wave fronts are not degenerated at all.

However, the transversality between the wave fronts and extremals is violated in this case on the boundaries of the regions $\mathcal{M}_k=\{2k\pi<\varphi<2(k+1)\pi,z,\bar{z}\in\mathcal{R}\}$, where the fields of extremals (6.17) are defined—a singularity that cannot be circumvented by a coordinate transformation.

These results can be obtained in a straightforward manner by using the DeDonder–Weyl Hamilton–Jacobi functions $S(z,\bar{z},\varphi)$ and $\bar{S}(z,\bar{z},\varphi)$ from (6.13) and (6.14).

The Hamiltonian density $\mathcal{H}$ vanishes on the extremals $\tilde{\varphi}(z,\bar{z},u)$ of (6.17):

$$\mathcal{H}=\partial_\varphi S\,\partial_\varphi\bar{S}+V(\varphi)=(2\sin(\varphi/2))^2-2(1-\cos(\varphi))=0.$$

Notice that the "usual" canonical Hamiltonian density,

$$\mathcal{H}_{\text{can}}(x,t)=\frac{1}{2}\pi^2+\frac{1}{2}(\partial_x\varphi)^2+(1-\cos(\varphi))\quad\text{with}\quad\pi=\frac{\partial\mathcal{L}}{\partial(\partial_t\varphi)},$$

does not vanish on the kink solution φ_0, because the Legendre transformation is applied only with respect to the time derivatives $\partial_t\varphi$ of the field φ and does not affect its spatial derivative $\partial_x\varphi$. This underlines again that the energy density $\mathcal{H}_{\text{can}}$ is different from the "covariant" Hamiltonian density $\mathcal{H}$ in (2.3), which we use in this article.

Carathéodory's Hamilton–Jacobi equation (2.6) on the field of extremals (6.17),

$$\partial_z S^z\partial_{\bar{z}}S^{\bar{z}}-\partial_z S^{\bar{z}}\partial_{\bar{z}}S^z=-\mathcal{H}=0, \tag{7.31}$$

the solutions of which determine the wave fronts transversal to the extremals we are interested in, shows that the change of the variables z and $\bar{z}$ to $\sigma=S^z(z,\bar{z},\varphi)$ and $\bar{\sigma}=S^{\bar{z}}(z,\bar{z},\varphi)$ is *not* a regular one, because $\mathcal{H}$ is nothing but the functional determinant of this transformation.

The general solution of Eq. (7.31) is

$$S^z=\sum^{z}(f(z,\bar{z}),\varphi),\quad S^{\bar{z}}=\sum^{\bar{z}}(f(z,\bar{z}),\varphi),$$

with an arbitrary smooth function $f(z,\bar{z})$. Inserting this result into the conditions on the momenta (2.6),

$$p=2\sin(\varphi/2)=\partial_{\bar{z}}S^{\bar{z}}\partial_\varphi S^z-\partial_{\bar{z}}S^z\partial_\varphi S^{\bar{z}}=+(\partial_z f)\left(\partial_f\sum^{z}\partial_\varphi\sum^{\bar{z}}-\partial_\varphi\sum^{z}\partial_f\sum^{\bar{z}}\right),$$

$$\overline{p}=2\sin(\varphi/2)=\partial_z S^z\partial_\varphi S^{\overline{z}}-\partial_z S^{\overline{z}}\partial_\varphi S^z=-(\partial_{\overline{z}}f)\left(\partial_f\sum^{z}\partial_\varphi\sum^{\overline{z}}-\partial_\varphi\sum^{z}\partial_f\sum^{\overline{z}}\right),$$

shows, after subtracting these PDEs from each other, that the function f depends on the difference $\overline{l}=z-\overline{z}$ only: $f=f(z-\overline{z})$. Due to the invariance of the basic two-form (2.5) with respect to symplectic transformations we may choose $f=z-\overline{z}$, $\Sigma^z=-4\cos(\varphi/2)$, and $\Sigma^{\overline{z}}=\overline{z}-z$ without any loss of generality. This result coincides with (7.27) and (7.28).

3. An explicit representation of the wave fronts—the regular case

If we would like to circumvent the spurious singularity discussed above, we have to ensure that the Hamiltonian density does not vanish in $\mathcal{M}_{2+1}$, e.g., by adding a global constant c_0 to the Lagrangian density:

$$\mathcal{L}\Rightarrow\mathcal{L}=\partial_z\varphi\partial_{\overline{z}}\varphi+2(1-\cos(\varphi))+c_0, \tag{7.32}$$

which does not influence the equation of motion. More generally, we can add any exact two-form $\Gamma=\mathrm{d}(f(z,\overline{z})\mathrm{d}z+\overline{f}(z,\overline{z})\mathrm{d}\overline{z})$ to the basic form (2.2), $\Omega\to\Omega+\Gamma$, without affecting the momenta p and $\overline{p}$, the slope functions v and $\overline{v}$ and the equation of motion, but modifying the Hamiltonian and the Lagrangian densities $\mathcal{H}$, $\mathcal{L}$:

$$\mathcal{H}\to\mathcal{H}+\partial_{\overline{z}}f-\partial_z\overline{f},\quad \mathcal{L}\to\mathcal{L}-\partial_{\overline{z}}f+\partial_z\overline{f}.$$

We see that the form of the wave fronts is influenced by adding such a term Γ while the field of extremals (6.17) remains unchanged—a property which is known in mechanics, too. For the sake of simplicity we choose $f=0$ and $\overline{f}=c_0 z$, which shifts $\mathcal{L}$ and $\mathcal{H}$ merely by a constant c_0.

With the exception of the coefficients A_0 and $\overline{A}_0$ of zeroth order, which are of no interest in determing the embedded extremals and the corresponding wave fronts, the DeDonder and Weyl Hamilton–Jacobi functions $S(z,\overline{z},\varphi)$ and $\overline{S}(z,\overline{z},\varphi)$ and the resulting momenta $p=\partial_\varphi S$ and $\overline{p}=\partial_\varphi\overline{S}$ are not affected by this shift contrary to the wave fronts.

Using Carathéodory's Hamilton–Jacobi equation (2.6),

$$\partial_z S^z\partial_{\overline{z}}S^{\overline{z}}-\partial_z S^{\overline{z}}\partial_{\overline{z}}S^z=-\mathcal{H}\equiv c_0,$$

which represents nothing but the determinant of the linear system of equations [see (2.6)]

$$p=2\sin(\varphi/2)=\partial_{\overline{z}}S^{\overline{z}}\partial_\varphi S^z-\partial_{\overline{z}}S^z\partial_\varphi S^{\overline{z}}, \tag{7.33}$$

$$\overline{p}=2\sin(\varphi/2)=\partial_z S^z\partial_\varphi S^{\overline{z}}-\partial_z S^{\overline{z}}\partial_\varphi S^z. \tag{7.34}$$

For the functions $\partial_\varphi S^z$ and $\partial_\varphi S^{\overline{z}}$ we get a system of decoupled linear PDEs for the functions S^z and $S^{\overline{z}}$

$$(\mathcal{H}\partial_\varphi+p\partial_z+\overline{p}\partial_{\overline{z}})S^z=(-c_0\partial_\varphi+2\sin(\varphi/2)[\partial_z+\partial_{\overline{z}}])S^z=0,$$

$$(\mathcal{H}\partial_\varphi+p\partial_z+\overline{p}\partial_{\overline{z}})S^{\overline{z}}=(-c_0\partial_\varphi+2\sin(\varphi/2)[\partial_z+\partial_{\overline{z}}])S^{\overline{z}}=0.$$

The general solution

$$S^z=\sum(-c_0 z/2+2\cos(\varphi/2),-c_0\overline{z}/2+2\cos(\varphi/2)),$$

$$S^{\overline{z}}=\overline{\sum}(-c_0 z/2+2\cos(\varphi/2),-c_0\overline{z}/2+2\cos(\varphi/2))$$

of this system PDEs is obtained by the method of characteristics. The functions Σ and $\overline{\Sigma}$ have only to satisfy Carathéodory's Hamilton–Jacobi equation (2.6). Taking the invariance with respect to symplectic transformations into account we may choose the functions

$$S^z=\sqrt{2}[\overline{z}-(4/c_0)\cos(\varphi/2)] \quad \text{and} \quad S^{\overline{z}}=\sqrt{2}[-c_0 z/2+2\cos(\varphi/2)] \tag{7.35}$$

without any loss of generality.

Obviously the transformation

$$(z,\overline{z})\rightarrow(\sigma=S^z(z,\overline{z},\varphi),\overline{\sigma}=S^{\overline{z}}(z,\overline{z},\varphi))$$

exists now, leading to an explicit representation of the wave fronts:

$$z(\sigma,\overline{\sigma},\varphi)=-\frac{\sqrt{2}\overline{\sigma}}{c_0}+\frac{4}{c_0}\cos(\varphi/2), \quad \overline{z}(\sigma,\overline{\sigma},\varphi)=\frac{\sigma}{\sqrt{2}}+\frac{4}{c_0}\cos(\varphi/2) \tag{7.36}$$

with some properties different from those obtained in the ''singular'' case: the 1D wave fronts are not straight lines in the extended configuration space. Subtracting Eqs. (7.36) from each other shows that they lie in planes parallel to the *l*-axis like in the singular case.

Similar to the ''singular'' case, the angle $\angle(w,e)$ between the basis vector of the tangent space $\mathcal{T}_{\mathcal{P}}\mathcal{W}$ of the wave front

$$w=2\sin(\varphi/2)(\partial_z+\partial_{\overline{z}})-c_0\partial_\varphi$$

and an arbitrary nonvanishing vector in the tangent space $\mathcal{T}_{\mathcal{P}}\mathcal{E}$ of the extremal

$$e=\lambda\partial_z+\overline{\lambda}\partial_{\overline{z}}+2(\lambda+\overline{\lambda})\sin(\varphi/2)\partial_\varphi, \quad \text{with} \quad |\lambda|+|\overline{\lambda}|>0$$

at the point $(z,\overline{z},\varphi)$ is given by

$$\angle(w,e)=\arccos\left(\frac{(w,e)}{|w||e|}\right)=\arccos\left(\frac{2(1-c_0)(\lambda+\overline{\lambda})\sin(\varphi/2)}{\sqrt{c_0^2+8\sin^2(\varphi/2)}\sqrt{\lambda^2+\overline{\lambda}^2+4(\lambda+\overline{\lambda})^2\sin^2(\varphi/2)}}\right),$$

the minimum of which with respect to a variation of the parameters $\lambda,\overline{\lambda}$ gives the angle $\angle(\mathcal{W},\mathcal{E})$ in which the one-dimensional wavefront intersects the two-dimensional extremal at *P*:

$$\angle(\mathcal{W},\mathcal{E})=\min\angle(w,x)=\arccos\left(\frac{2\sqrt{2}|1-c_0||\sin(\varphi/2)|}{\sqrt{c_0^2+8\sin^2(\varphi/2)}\sqrt{1+8\sin^2(\varphi/2)}}\right).$$

Obviously in the case $c_0=1$ the wave fronts cross the extremals always *perpendicularly*, because $\angle(\mathcal{W},\mathcal{E})=\pi/2$ holds *everywhere* in $\mathcal{M}_{2+1}$ (see Fig. 2).

For $c_0\neq 0,1$ the maximum value $\angle(\mathcal{W},\mathcal{E})=\pi/2$ is taken only for $\varphi_k=2k\pi$, $k=0,\pm1,\pm2,...$, *contrary* to the singular case $c_0=0$, where for these values of the field variable the minimum of the angle $\angle(\mathcal{W},\mathcal{E})$ vanishes, indicating that the transversality relation between the wave fronts and extremals is violated there. The angle $\angle(\mathcal{W},\mathcal{E})$ has a local minimum at those points where $|\cos(\angle(\mathcal{W},\mathcal{E}))|$ becomes maximal:

$$|\cos(\angle(\mathcal{W},\mathcal{E})_{\min 1})|=\frac{2\sqrt{2}|1-c_0|}{3\sqrt{c_0^2+8}}, \quad |\cos(\angle(\mathcal{W},\mathcal{E})_{\min 2})|=\frac{|1-c_0|}{1+|c_0|}. \tag{7.37}$$

We find the first minima $\angle(\mathcal{W},\mathcal{E})_{\min 1}$ on planes $\varphi=(2k+1)\pi$, $k=0,\pm1,\pm2,...$, where the cosine of the field variable vanishes. They do exist for all values of the parameter $c_0\in\mathcal{R}\backslash\{0\}$. For c_0

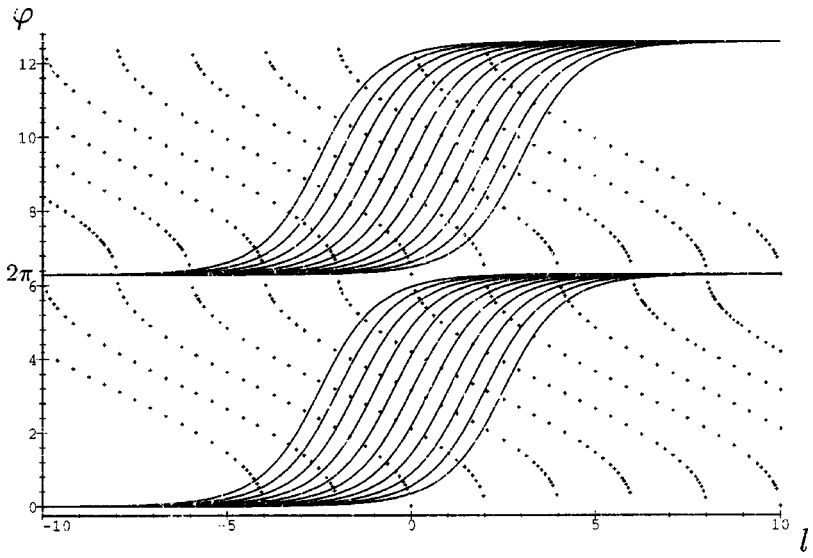

FIG. 2. Shown is the regular case for $c_0=1$ [see Eq. (7.32)]. Here the wave fronts intersect the extremals *everywhere* perpendicularly.

$\neq -8$ the angle $\angle(\mathcal{W},\mathcal{E})_{\min 1}$ differs from zero, i.e., the transversality relation is fulfilled. If $c_0=-8$, both minima (7.37) coincide, therefore this case is discussed below.

The second minima $\angle(\mathcal{W},\mathcal{E})_{\min 2}$ exist only in the range $|c_0|\leqslant 8$, $c_0\neq 0$. These minima lie at values of the field variable: $\varphi=2k\pi\pm 2\arcsin(\sqrt{|c_0|/8})$, $k=0,\pm 1,\pm 2,\ldots$. If $c_0<0$, this angle vanishes, whereas it differs from zero for all $c_0>0$.

It results that in the case $c_0>0$ or $c_0<-8$ the wave fronts and extremals are never parallel to each other ($\angle(\mathcal{W},\mathcal{E})_{\min 1,2}\neq 0$). This guarantees the transversality relations everywhere in the extended configuration space $\mathcal{M}_{2+1}$—even on the planes $\varphi_k=2k\pi$, $k=0,\pm 1,\pm 2,\ldots$ that separate the one parameter fields of extremals—contrary to the singular case. This result coincides with the fact that both the Lagrangian and the Hamiltonian densities do not vanish in $\mathcal{M}_{2+1}$ for $c_0>0$ or $c_0<-8$.

For $-8\leqslant c_0<0$ the minimum $\angle(\mathcal{W},\mathcal{E})_{\min 2}$ is equal to zero. This happens just for the points on the plane

$$\varphi=2k\pi\pm 2\arcsin(\sqrt{-c_0/8}),\quad k=0,\pm 1,\pm 2,\ldots, \tag{7.38}$$

where the shifted Lagrangian density (7.32) vanishes, as expected from the transversality relation (2.10) (see Fig. 3). The case $c_0=-8$ is a special one: here the two planes (7.38) that exist in every region $2k\pi<\varphi<2(k+1)\pi$, $z,\bar{z}\in\mathcal{R}$, $k=0,\pm 1,\pm 2,\ldots$, coincide. Hence we get only one plane, $\varphi=2k\pi+\pi$ in the range $2k\pi<\varphi<2(k+1)\pi$, where the transversality relations are violated due to a vanishing shifted Lagrangian density.

The dependence of the angle $\angle(\mathcal{W},\mathcal{E})$ on the constant c_0 shows that the geometrical properties of the wave fronts and even the transversality relation may be affected by changes of the Lagrangian density that do not influence the equation of motions and the corresponding extremals at all.

Now we would like to show how these results can be obtained using the recursion formulas given in Secs. VII A and VII B. We first calculate Carathéodory's Hamilton–Jacobi functions $S^z(z,\bar{z},\varphi)$, $S^{\bar{z}}(z,\bar{z},\varphi)$ from those of DeDonder and Weyl, (6.13) and (6.14). For the sake of simplicity we choose the shift $c_0=-2$ in order to eliminate the constant 2 in the Lagrangian of the sine–Gordon model $\mathcal{L}=\partial_z\varphi\partial_{\bar{z}}\varphi+2(1-\cos(\varphi))$.

The coefficients $A_0^z(z,\bar{z})$ and $A_0^{\bar{z}}(z,\bar{z})$ can be chosen as special solutions,

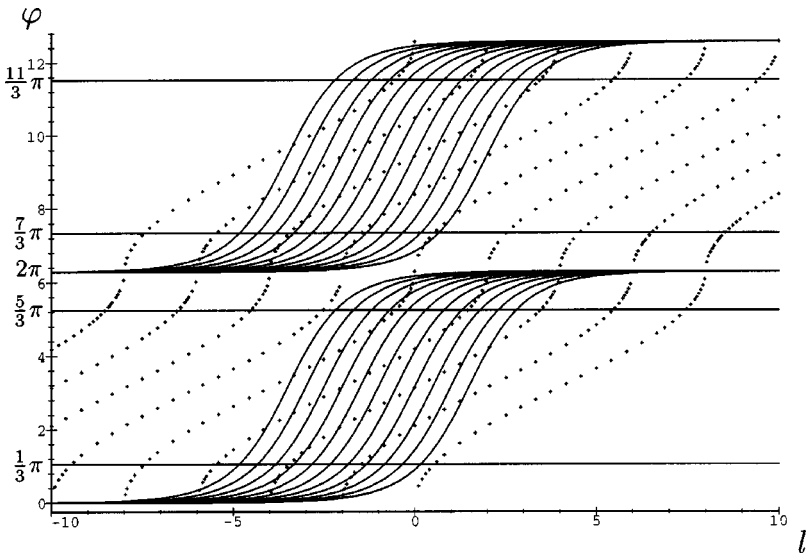

FIG. 3. Shown is the regular case for $c_0=-2$ [see Eq. (7.32)]. Here the transversality relations are fulfilled outside the planes $\varphi=2k\pi\pm\pi/3$, $k=0,\pm1,\pm2,...$, where the extremals and wave fronts are parallel since the Lagrangian density vanishes there. Notice that the transversality relations are fulfilled on the boundaries of the regions $\mathcal{M}_k=\{2k\pi<\varphi<2(k+1)\pi, z, \overline{z}\in\mathcal{R}\}$, where the fields of extremals (6.17) are defined. Therefore the wave fronts can be continued from one of these regions to the next smoothly, contrary to the extremals.

$$A_0^z=A_0^z(l)=4\tanh(l)-l, \quad A_0^{\overline{z}}=A_0^{\overline{z}}=-\overline{l}, \tag{7.39}$$

of the equation (7.8) written in terms of the variables $l=z+\overline{z}$ and $\overline{l}=z-\overline{z}$:

$$(\partial_{\overline{l}}A_0^z)(\partial_l A_0^{\overline{z}})-(\partial_{\overline{l}}A_0^{\overline{z}})(\partial_l A_0^z)=\frac{\mathcal{L}_0}{2}=\frac{4}{\cosh(l)^2}-1.$$

The equations (7.11) and (7.12) yield the coefficients of first order,

$$A_1^z=A_1^z(l)=\frac{2}{\cosh(l)}, \quad A_1^{\overline{z}}=0,$$

and the relations (7.9), (7.10), (7.13), and (7.14) lead to those of second and third order in y. They coincide with those of the singular case (7.26) since the ratios $(\partial_z A_0^z)/\mathcal{L}$ and $(\partial_{\overline{z}}A_0^z)/\mathcal{L}$ are the same in the regular and in the singular case. The same holds for the coefficients $A_n^z(z,\overline{z})$ and $A_n^{\overline{z}}(z,\overline{z})$ of higher orders in y. So we get for $n>0$

$$A_{2n}^z=A_{2n}^z(l)=4\frac{(-1)^n}{2^{2n}}\tanh(l), \quad A_{2n-1}^z=A_{2n-1}^z(l)=4\frac{(-1)^n}{2^{2n-1}}\frac{1}{\cosh(l)}, \quad A_n^{\overline{z}}=0,$$

which combine the expressions (7.39) and yield the Hamilton–Jacobi functions $S^z(z,\overline{z},\varphi)$ and $S^{\overline{z}}(z,\overline{z},\varphi)$:

$$S(z,\bar{z},\varphi)=4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n}}{n!\,2^{2n}}\right)\tanh(l)+4\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n+1}}{n!\,2^{2n+1}}\right)\frac{1}{\cosh(l)}-l$$

$$=4\cos\left(\frac{y}{2}\right)\tanh(l)+4\sin\left(\frac{y}{2}\right)\frac{1}{\cosh(l)}-l$$

$$=-4\cos\left(\frac{\varphi}{2}\right)-z-\bar{z}, \tag{7.40}$$

$$S^{\bar{z}}(z,\bar{z},\varphi)=\bar{z}-z. \tag{7.41}$$

Both functions S^z and $S^{\bar{z}}$ satisfy Carathéodory's Hamilton–Jacobi equation (3.1), the integrability criterion (3.2), and the embedding conditions (3.4). They are related to the solutions (7.35) by the transformation

$$S^z\to\tilde{S}^z=-\frac{1}{\sqrt{2}}(S^z+S^{\bar{z}}),\quad S^{\bar{z}}\to\tilde{S}^{\bar{z}}=\frac{1}{\sqrt{2}}(S^{\bar{z}}-S^z). \tag{7.42}$$

The wave fronts $z(\sigma,\bar{\sigma},\varphi)$ and $\bar{z}(\sigma,\bar{\sigma},\varphi)$ can be determined recursively following the ideas discussed Sec. VII A.

The coefficients $\alpha_0(\sigma,\bar{\sigma})$ and $\bar{\alpha}_0(\sigma,\bar{\sigma})$ of zeroth order in $\hat{y}$ are given by inverting Eqs. (7.20):

$$\sigma=A_0^z(z=\alpha_0(\sigma,\bar{\sigma}),\quad \bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma}))=4\tanh(\alpha_0+\bar{\alpha}_0)-(\alpha_0+\bar{\alpha}_0),$$

$$\bar{\sigma}=A_0^{\bar{z}}(z=\alpha_0(\sigma,\bar{\sigma}),\quad \bar{z}=\bar{\alpha}_0(\sigma,\bar{\sigma}))=-\alpha_0+\bar{\alpha}_0,$$

which yields:

$$\alpha_0=\tfrac{1}{2}(f^{-1}(\sigma)-\bar{\sigma})\quad\text{and}\quad\bar{\alpha}_0=\tfrac{1}{2}(f^{-1}(\sigma)+\bar{\sigma}),$$

where the symbol f^{-1} denotes the inverse of the function $f(x):=\tanh(x)-x$. The coefficients of $\hat{y}$, $\hat{y}^2$, and $\hat{y}^3$ are given by (7.22)–(7.25):

$$\alpha_1(\sigma)=\frac{\partial_{\bar{z}}\varphi_0}{\mathcal{H}_0}=\frac{1}{\cosh(f^{-1}(\sigma))},\quad \bar{\alpha}_1(\sigma)=\frac{\partial_z\varphi_0}{\mathcal{H}_0}=\frac{1}{\cosh(f^{-1}(\sigma))},$$

$$\alpha_2(\sigma)=-\tfrac{1}{2}\tanh(f^{-1}(\sigma)),\quad \bar{\alpha}_2(\sigma)=-\tfrac{1}{2}\tanh(f^{-1}(\sigma)),$$

$$\alpha_3(\sigma)=-\frac{1}{4\cosh(f^{-1}(\sigma))},\quad \bar{\alpha}_3(\sigma)=-\frac{1}{4\cosh(f^{-1}(\sigma))}.$$

This leads to a general ansatz for the coefficients α_n and $\bar{\alpha}_n$, $n\geqslant 1$:

$$\alpha_{2n}=\bar{\alpha}_{2n}=2\frac{(-1)^n}{2^{2n}}\tanh(f^{-1}(\sigma)),\quad \alpha_{2n-1}=\bar{\alpha}_{2n-1}=2\frac{(-1)^n}{2^{2n-1}}\frac{1}{\cosh(f^{-1}(\sigma))},$$

which give the wave fronts

$$z(\sigma,\bar{\sigma},\varphi)=2\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n}}{n!\,2^{2n}}\right)\tanh(f^{-1}(\sigma))+2\left(\sum_{n=0}^{\infty}\frac{(-1)^n y^{2n+1}}{n!\,2^{2n+1}}\right)\frac{1}{\cosh(f^{-1}(\sigma))}$$

$$-2\tanh(f^{-1}(\sigma))+\frac{1}{2}(f^{-1}(\sigma)-\bar{\sigma})=-2\cos\left(\frac{\varphi}{2}\right)-\frac{1}{2}(\sigma+\bar{\sigma}),$$

$$\bar{z}(\sigma,\bar{\sigma},\varphi)=-2\cos\left(\frac{\varphi}{2}\right)-\frac{1}{2}(\sigma-\bar{\sigma}),$$

which are related to the representation (7.36) by the transformation (7.42) applied to $S^z=\sigma$ and $S^{\bar z}=\bar\sigma$, which reparametrizes the field of wave fronts only.

VIII. CONCLUSIONS

Within the manifest covariant Hamilton–Jacobi canonical frameworks of DeDonder and Weyl and of Carathéodory we have investigated relations between fields of extremals and Hamilton–Jacobi wave fronts for two 2-dimensional one-component field theories. This is of interest, since the dynamics of fields can be described either by the Euler–Lagrange or the Hamilton–Jacobi equations supplemented by the integrability conditions.

We developed a formalism to solve the DeDonder and Weyl Hamilton–Jacobi equation and the integrability condition perturbatively by expanding the Hamilton–Jacobi functions in powers of the field variable. Starting from a single given extremal it is then possible to calculate new ones from it by using the two DeDonder and Weyl Hamilton–Jacobi functions.

This formalism is useful especially for investigating extremals in the neighborhood of known extremals in several two-dimensional field theories: the massless and massive Klein–Gordon, the sine– and Sinh–Gordon, the Liouville as well as the ϕ^4-theory. In the Sine–, sinh–Gordon and ϕ^4-theory we have studied the embedding of topologically nontrivial soliton solutions. This approach is related to the usual stability investigations of solitons where perturbations are considered which are a product of functions depending on the time and the space variables separately. We determined the *general* solutions of the equations of the second variation by using Bäcklund transformations. In this manner we have obtained all the extremals in the vicinity of a given one.

Calculating proper Hamilton–Jacobi wave fronts makes the use of Carathéodory's Hamilton–Jacobi functions $S^z(z,\bar z,\varphi)$ and $S^{\bar z}(z,\bar z,\varphi)$ necessary. Solving Carathéodory's Hamilton–Jacobi equation is considerably simplified by using the corresponding DeDonder–Weyl Hamilton–Jacobi functions. One first obtains the wave fronts as equipotential surfaces $S^z=\sigma=\text{const}$ and $S^{\bar z}=\bar\sigma=\text{const}$ in an implicit form. If the transformation of variables $(z,\bar z,\varphi)\to(\sigma,\bar\sigma,\varphi)$ is a regular one, i.e., if Carathéodory's Hamilton density does not vanish on the field of extremals under consideration, we get an explicit representation $z=z(\varphi,\sigma,\bar\sigma)$ and $\bar z=\bar z(\varphi,\sigma,\bar\sigma)$ for the wave fronts.

These general results have been applied in detail to a special single kink solution of the sine–Gordon equation. After calculating the DeDonder and Weyl Hamilton–Jacobi potentials S and $\bar S$ we obtained a corresponding one-parameter field of embedded extremals: a field of kink solutions of constant energy covering the extended configuration space. From the functions S and $\bar S$ we have determined Carathéodory's Hamilton–Jacobi functions S^z and $S^{\bar z}$ explicitly. The wave fronts have been determined for the singular ($\mathcal{H}=0$) as well as for the regular case ($\mathcal{H}\neq0$). In addition the transversality conditions between the wave fronts and the embedded extremals have been analyzed.

APPENDIX: SOME PROPERTIES OF THE EMPLOYED BÄCKLUND TRANSFORMATIONS

Bäcklund transformations are employed to map the integral submanifolds of the PDE (3.10) to those of the Klein–Gordon or wave equation, the *general* solutions of which are known. In this chapter we determine all the functions $\partial_l^2 V(\varphi_0(l))$ with $l=z+\bar z$ that allow this map by *one* BT. But unfortunately it turns out that the nonconstant coefficients $\partial_l^2 V(\varphi_0(l))$ in (5.8) and (5.9) for the ϕ^4 models do not belong to this class. Thus, we need at least two BTs to connect these two equations to one PDE with constant coefficients. Moreover, we have to discuss which relations of type (3.10) can be reduced to free field equations by one or a *finite* number of BTs at all.

We show that there is no BT which relates the PDEs (5.8) and (5.9) and $\partial_z\partial_{\bar z}\hat\theta=m^2\hat\theta$, $m^2\in\mathcal{R}$. Even if we make the more general assumption that the transformed function $\hat\theta$ obeys the equation $\partial_z\partial_{\bar z}\hat\theta=m^2(z,\bar z)\hat\theta$ with a nonconstant but separable coefficient m^2: $m^2=B(z)\bar B(\bar z)$, the equations (5.8) and (5.9) for the ϕ^4-theories cannot be reduced by *one* BT to such an equation for $\hat\theta$ and thus not solved like the PDEs (5.1), (5.3), and (5.4) for the Liouville, the sine–and the sinh–Gordon models. The reason is that the equation $\partial_z\partial_{\bar z}\hat\theta=m^2(z,\bar z)\hat\theta$ can be reduced to a

Klein–Gordon one by a suitable transformation[18] of the independent variables $z \to B(z)$ and $\bar{z} \to \bar{B}(\bar{z})$. The equations (5.8) and (5.9) *can* be transformed by *two* BTs to Klein–Gordon equations. This result can be generalized to PDEs of the following type:

$$\partial_z \partial_{\bar{z}} \theta = \{n[n+1]\eta^2(l = z+\bar{z}) + a\}\theta, \quad n = 1,2,..., \quad a \in \mathcal{R},$$

if η is a solution of $\partial_l \eta = \bar{b}\eta^2 + \bar{c}$ with $\bar{b}^2 = \pm 1$ and $\bar{c} \in \mathcal{R}$ by n BTs. Especially the PDEs (5.8) and (5.9) can be obtained by choosing $b = -1$, $\bar{c} = 1$, and $n = 2$. We start from Eqs. (4.7), assuming $m^2 \to m^2(l)$ to be a function of $l = z + \bar{z}$ and rename $\partial_\varphi^2 V(\varphi_0(l))$ as $2v(l)$. From the equations (4.7) we infer

$$\psi = \psi_0 + A(z) + \bar{A}(\bar{z}), \quad \psi_0(l) = \frac{1}{2}\int^l dl' \int^{l'} dl''(m^2(l'') + v(l'')), \tag{A1}$$

$$\Rightarrow 0 = \partial_l^2 \psi_0 + (\partial_l \psi_0 + \partial_z A)(\partial_l \psi_0 + \partial_{\bar{z}} \bar{A}) - m^2(l) \tag{A2}$$

with two arbitrary functions A and $\bar{A}$. We are interested in the relation between $m^2(l)$ and $v(l)$. First we have to determine the functions A and $\bar{A}$, which depend only on z and $\bar{z}$, respectively. Differentiating the PDE (A2) with respect to $\bar{l} = z - \bar{z}$ leads to

$$\partial_l \psi_0 [\partial_z^2 A - \partial_{\bar{z}}^2 \bar{A}] = \partial_{\bar{z}}^2 \bar{A} \partial_z A - \partial_z^2 A \partial_{\bar{z}} \bar{A}, \tag{A3}$$

because ψ_0 depends on l only. Now, if $\partial_{\bar{z}}^2 \bar{A} = 0$ or $\partial_z^2 A = 0$, we obtain from Eq. (A3) that either $\partial_{\bar{z}}^2 \bar{A} = 0$ and $\partial_z^2 A = 0$ (case I) or $\partial_l \psi_0 = -a_0$ (case II). The case II leads to $\partial_l^2 \psi_0 = 0$ and using relation (A2) gives $m^2(l) = 0$. The definition of ψ_0 finally yields $v = 0$, which is of no interest for us. Without any loss of generality we have chosen $\partial_z^2 A = 0 \Rightarrow \partial_z A = a_0$, $a_0 \in \mathcal{R}$.

If $0 = \partial_z^2 A - \partial_{\bar{z}}^2 \bar{A}$ (case III), then it follows that either $\partial_z^2 A = \partial_{\bar{z}}^2 \bar{A} = 0$ or $\partial_z A = \partial_{\bar{z}} \bar{A} = a = \text{const}$, the second case being a special case of the first one. So we have $\partial_z A = a_1$ and $\partial_{\bar{z}} \bar{A} = \bar{a}_1$ with a_1, $\bar{a}_1 \in \mathcal{R}$. Thus case III is contained in the first one.

If $\partial_z^2 A - \partial_{\bar{z}}^2 \bar{A} \neq 0$ (case IV), we are able to divide the relation (A2) by it and to apply the operator $\partial_{\bar{l}}$ once more:

$$0 = (\partial_z^3 A \partial_{\bar{z}}^2 \bar{A} + \partial_z^2 A \partial_{\bar{z}}^3 \bar{A})(\partial_z A - \partial_{\bar{z}} \bar{A}) - 2\partial_z^2 A \partial_{\bar{z}}^2 \bar{A}(\partial_z^2 A - \partial_{\bar{z}}^2 \bar{A}), \tag{A4}$$

$$\Rightarrow 0 = \partial_z \left\{ \frac{\partial_z^3 A}{\partial_z^2 A} \right\} - 2\partial_z \left\{ \frac{\partial_z^2 A - \partial_{\bar{z}}^2 \bar{A}}{\partial_z A - \partial_{\bar{z}} \bar{A}} \right\}. \tag{A5}$$

Differentiating this equation with respect to $\bar{z}$, dividing the result by $\partial_{\bar{z}}^2 \bar{A}$, and applying $\partial_{\bar{z}}$ leads to

$$\partial_{\bar{z}}^3 \bar{A} = \partial_{\bar{z}}^2 \bar{A}[e_0 \partial_{\bar{z}} \bar{A} + e_1], \quad \partial_z^3 A = \partial_z^2 A[e_2 \partial_z A + e_3], \quad e_0, e_1, e_2, e_3 \in \mathcal{R}. \tag{A6}$$

Substituting these results into the equation (A4) yields for $A(z)$ and $\bar{A}(\bar{z})$ the differential equations

$$\partial_{\bar{z}}^2 \bar{A} = \tfrac{1}{2}(\partial_{\bar{z}} \bar{A})^2 e_0 + e_4 \partial_{\bar{z}} \bar{A} + e_5, \quad \partial_z^2 A = \tfrac{1}{2}(\partial_z A)^2 e_0 + e_4 \partial_z A + e_5,$$

with the same constants e_0, e_4, and e_5 for both functions. Inserting these expressions into relation (A3) we get for $\partial_l^2 \psi_0 = (m^2 + v)/2$:

$$\partial_l^2 \psi_0 = -\frac{e_0 \partial_z^2 A \partial_{\bar{z}}^2 \bar{A}}{2[(e_0/2)(\partial_z A + \partial_{\bar{z}} \bar{A}) + e_4]^2}.$$

From Eq. (A2) it follows that

$$m^2(l)=\left(1-\frac{e_0}{2}\right)\partial_z^2 A\,\partial_{\bar z}^2\bar A\left[\frac{e_0}{2}(\partial_z A+\partial_{\bar z}\bar A)+e_4\right]^{-2},$$

$$v(l)=-\left(1+\frac{e_0}{2}\right)\partial_z^2 A\,\partial_{\bar z}^2\bar A\left[\frac{e_0}{2}(\partial_z A+\partial_{\bar z}\bar A)+e_4\right]^{-2}.$$

Thus we have to solve the differential equations (A6) for $\partial_z A$ and $\partial_{\bar z}\bar A$ with different choices of the constants e_0, e_4, and e_5. Depending on the sign of $\Delta=2e_0e_5-e_4^2$ there exist three different cases:

$$\text{IV.1: } \Delta=0:\partial_z A=-\frac{e_4}{e_0}-\frac{2}{c(z-z_0)},\quad \partial_{\bar z}\bar A=-\frac{e_4}{e_0}-\frac{2}{c(\bar z-\bar z_0)},\quad z_0,\bar z_0\in\mathcal{C}$$

$$\text{IV.2: } \Delta<0:\partial_z A=\frac{\sqrt{\Delta}}{e_0}\tan\left(\frac{\sqrt{\Delta}}{2}(z-z_0)\right)-\frac{e_4}{e_0},$$

$$\partial_{\bar z}\bar A=\frac{\sqrt{\Delta}}{e_0}\tan\left(\frac{\sqrt{\Delta}}{2}(\bar z-\bar z_0)\right)-\frac{e_4}{e_0},$$

$$\text{IV.3: } \Delta>0:\partial_z A=-\frac{\sqrt{-\Delta}}{e_0}\tanh\left(\frac{\sqrt{-\Delta}}{2}(z-z_0)\right)-\frac{e_4}{e_0},$$

$$\partial_{\bar z}\bar A=-\frac{\sqrt{-\Delta}}{e_0}\tanh\left(\frac{\sqrt{\Delta}}{2}(\bar z-\bar z_0)\right)-\frac{e_4}{e_0}.$$

For the case IV.1 we obtain

$$m^2(l)=\frac{4}{e_0^2}\left(1-\frac{e_0}{2}\right)[l-l_0]^{-2},\quad v=-\frac{4}{e_0^2}\left(1+\frac{e_0}{2}\right)[l-l_0]^{-2},\quad l_0=z_0+\bar z_0.$$

If we choose $e_0=2$, then $m^2(l)$ vanishes and $v=-2[l-l_0]^{-2}$ is for $l_0=0$ identical with $\partial_\varphi^2 V(\varphi_0)$ in Liouville's model and, on the other hand, if one would like to obtain the PDE (5.1) only (this means $m^2(l)=-2[l-l_0]^{-2}$), one has to calculate e_0 from the equation $-2=4(1-e_0/2)/e_0^2$ yielding $e_{0_{1,2}}=-1,2$. Therefore one obtains the wave equation or once again Liouville's model. The last case represents only a map of (5.1) onto itself (for details of auto-BTs, see e.g., Ref. 24).

The case IV.2 yields

$$m^2(l)=\frac{\Delta}{e_0^2}\left(1-\frac{e_0}{2}\right)\sin^{-2}\left[\frac{\sqrt{\Delta}}{2}(l-l_0)\right],\quad v=-\frac{\Delta}{e_0^2}\left(1+\frac{e_0}{2}\right)\sin^{-2}\left[\frac{\sqrt{\Delta}}{2}(l-l_0)\right].$$

This is of no interest for our special models. Notice, however, that the special choice $v=-\Delta 2^{-1}\sin^{-2}(\sqrt{\Delta}[l-l_0]/2)$ leads to the wave equation.

The case IV.3 is obviously similar to IV.2. The resulting functions $m^2(l)$ and $v(l)$ are

$$m^2(l)=\frac{\Delta}{e_0^2}\left(1-\frac{e_0}{2}\right)\sinh^{-2}\left[\frac{\sqrt{-\Delta}}{2}(l-l_0)\right],\quad v=\frac{\Delta}{e_0^2}\left(1+\frac{e_0}{2}\right)\sinh^{-2}\left[\frac{\sqrt{-\Delta}}{2}(l-l_0)\right].$$

As the equations (5.8) and (5.9) for the ϕ^4 models are not contained in the cases discussed up to now, we return to case I: $\partial_z A=a_1$ and $\partial_{\bar z}\bar A=\bar a_1$. Assuming m^2 to be independent of l Eq. (A2) then gives

$$\partial_l^2\psi_0+(\partial_l\psi_0)^2+(a_1+\bar a_1)\partial_l\psi_0+a_1\bar a_1-m^2=0.$$

Substituting $\xi=\partial_l\psi_0+(a_1+\overline{a_1})/2$ and $\tilde{\Delta}=m^2+(a_1-\overline{a_1})^2/4$ leads to

$$\text{I.1: } \tilde{\Delta}>0:\xi=\tilde{\Delta}\tanh(\tilde{\Delta}(l-l_0)),\quad \Rightarrow v=2\tilde{\Delta}^2(1-\tanh^2[\tilde{\Delta}(l-l_0)])-m^2, \tag{A7}$$

$$\text{I.2: } \tilde{\Delta}<0:\xi=-\tilde{\Delta}\tan(\tilde{\Delta}(l-l_0)),\quad \Rightarrow v=-2\tilde{\Delta}^2(1+\tan^2[\tilde{\Delta}(l-l_0)])-m^2, \tag{A8}$$

$$\text{I.3: } \tilde{\Delta}=0:\xi=\frac{1}{l-l_0},\quad \Rightarrow v=-2\frac{1}{(l-l_0)^2}-m^2. \tag{A9}$$

The case I.1 is the essential one for us. Because of the special type of Eqs. (5.8) and (5.9), we are able to eliminate Δ by a transformation of variables $z\to\Delta z$ and $\bar{z}\to\Delta\bar{z}$. Thus only the class of PDEs with a coefficient 2 in front of their $\tanh^2(l)$,

$$\partial_z\partial_{\bar{z}}\theta=\{n_0\tanh^2(l)+\overline{n_0}\}\theta,\quad n_0=2,\quad \overline{n_0}\in\mathcal{R}, \tag{A10}$$

can be reduced by *one* BT to a Klein–Gordon or wave equation, like the relations we obtain in the sine–Gordon (5.3) and the sinh–Gordon (5.4) theory. For the ϕ^4-models with $n_0=6$ we need at least two BTs.

Substituting $m^2(l)=2\psi_0(l)-v(l)$ in Eq. (A2) leads to

$$\partial_l^2\psi_0-(\partial_l\psi_0+a_1)(\partial_l\psi_0+\overline{a_1})-v=0. \tag{A11}$$

Choosing v to be equal to $-b\eta^2(l)-c$ where the function η has to obey the equation $\partial_l\eta=\overline{b}\eta^2+\overline{c}$ with $\overline{b}$, $\overline{c}\in\mathcal{R}$, making the special ansatz $\partial_l\psi_0=d_0+d_1\eta$ with two constants d_0, d_1, inserting all this into Eq. (A11), and comparing the coefficients in front of the powers of η yields

$$\underline{\eta^2}:d_1\overline{b}+b-d_1^2=0,\quad \Rightarrow d_{1_{1,2}}=\frac{\overline{b}}{2}\pm\sqrt{\left(\frac{b}{2}\right)^2+b},$$

$$\underline{\eta^1}:2d_0+a_1+\overline{a_1}=0,\quad \Rightarrow 2d_0=-a_1-\overline{a_1},$$

$$\underline{\eta^0}:d_1\overline{c}+c-(d_0+a_1)(d_0+\overline{a_1})=0,\quad \Rightarrow\overline{a_1}=\pm2\sqrt{-d_1\overline{c}-c}+a_1.$$

For $m^2(l)$ we obtains

$$m^2(l)=2\partial_l^2\psi_0-v=c+2d_1\overline{c}+(2d_1\overline{b}+b)\eta^2. \tag{A12}$$

Of special interest is the coefficient in front of η^2. Inserting d_1 into eq. (A12) we get

$$2d_1\overline{b}+b=\overline{b^2}+b\pm\overline{b}\sqrt{\overline{b^2}+4b},$$

with $b=n(n+1)$, and choosing $\overline{b}$ to be equal to ±1 we obtain

$$2d_1\overline{b}+b=n(n+1)+1\pm\sqrt{1+4n(n+1)}=\begin{cases}n(n-1),\\(n+1)(n+2).\end{cases}$$

Thus starting with a coefficient $n(n+1)$ one BT can raise or lower n by 1. Choosing $n=1,2,...$, we are able to calculate the functions ψ_i, which are essential in order to determine the ith BT of the hierarchy of n BTs, using the equation (A1). Moreover, the solutions $\tilde{\psi}_i=\exp(-\psi_i)$ of the ith PDE $\partial_z\partial_{\bar{z}}\theta+v_i\theta=0$, whose reciprocal fulfills $\partial_z\partial_{\bar{z}}\hat{\theta}+m_i^2(l)\hat{\theta}=0$ [see (4.4)], can be calculated. Obviously the special case $\overline{b}=-1$ and $\overline{c}=1$ leads to

$$\partial_z\partial_{\bar{z}}\theta=[n(n+1)\tanh^2(z+\overline{z})+a]\theta.$$

For $n=2$ and special choices of a this relation yields the PDEs (5.8) and (5.9) for the ϕ^4-theories. So they can be solved by $n=2$ BTs.

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R-matrix presentation for super-Yangians $Y(\mathrm{osp}(m|2n))$

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(Received 3 April 2002; accepted 27 September 2002)

We give a RTT presentation of super-Yangians $Y(\mathfrak{g})$ for $\mathfrak{g}=\mathrm{osp}(m|2n)$, thereby unifying the formalism with the cases of $\mathfrak{g}=\mathrm{so}(n)$ and $\mathfrak{g}=\mathrm{sp}(2n)$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1525406]

I. INTRODUCTION

The Yangian $Y(\mathfrak{a})$ based on a simple Lie algebra $\mathfrak{a}$ is defined[1,2] as the homogeneous quantization of the algebra $\mathfrak{a}[u]=\mathfrak{a}\otimes\mathbb{C}[u]$ endowed with its standard bialgebra structure, where $\mathbb{C}[u]$ is the ring of polynomials in the indeterminate u. There exists for the Yangian $Y(\mathfrak{a})$ three different realizations, due to Drinfel'd.[1–3] In the first realization the Yangian is generated by the elements J_0^a of the Lie algebra and a second set of generators J_1^a in one-to-one correspondence with J_0^a realizing a representation space thereof. The second realization is given in terms of generators and relations similar to the description of a loop algebra as a space of maps. However, in this realization no explicit formula for the comultiplication is known in general, except in the sl(2) case.[4] The third realization uses the Faddeev–Reshetikhin–Takhtajan (FRT) formalism,[5] but it is only established in the cases of classical Lie algebras.

The FRT formalism is also used as the original definition of the super Yangian $Y(\mathrm{gl}(M|N))$.[6,7] The purpose of this article is to define the Yangian for the orthosymplectic Lie superalgebras via the FRT formalism. As a by-product, we exhibit a unified construction which encompasses the three cases $\mathfrak{g}=\mathrm{so}(M)$, $\mathfrak{g}=\mathrm{sp}(N)$ and $\mathfrak{g}=\mathrm{osp}(M|N)$. A key feature in this procedure is the explicit expression of a ''quantum determinant''-like central element which coincides with that given by Drinfel'd in the $\mathfrak{g}=\mathrm{so}(M)$ case.[1]

Note that a first attempt for a FRT formulation of Yangians based on so(M) and sp(N) was done by Olshanski *et al.*[8,9] However, it led to the notion of twisted Yangians, which indeed are deformations of loop algebras on so(M) and sp(N), but appear as Hopf coideals rather than Hopf algebras. The same feature holds for twisted super Yangians, corresponding to osp($M|N$) superalgebras.[10]

Known rational solutions of the Yang–Baxter equation involve R-matrices of the form (i) $R(u)=\mathbb{I}+P/u$ and (ii) $R(u)=\mathbb{I}+P/u-K/(u+\kappa)$.[11–13] The first case, where P is defined as the (super)-permutation map, is known to define the Yangians $Y(\mathrm{sl}(N))$ and $Y(\mathrm{sl}(M|N))$ via the FRT formalism.[5,14] In the case (ii), K is a partial (super)-transposition of P. Some R-matrices of this type occur as factorized S-matrices of quantum field models in two dimensions exhibiting the so(M) symmetry.[11]

We will show that the R-matrix $R(u)=\mathbb{I}+P/u-K/(u+\kappa)$ can be used to define the Yangian

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$Y(\mathfrak{g})$ within the RTT formalism, for $\mathfrak{g}=\mathrm{osp}(M|N)$ (N even) as well as for the known cases of $\mathfrak{g}=\mathrm{so}(M)$ or $\mathfrak{g}=\mathrm{sp}(N)$ (N even). We prove that the algebra defined this way is indeed a quantization of $\mathfrak{g}[u]$ endowed with its canonical bialgebra structure.

The letter is organized as follows. In Sec. II, after some definitions, we introduce for each $\mathfrak{g}$ a rational R-matrix expressed in terms of the (super)-permutation and of its partial transposition. We check that it satisfies the (super) Yang–Baxter equation in all cases. In Sec. III we define a (super)-algebra through the RTT formalism. We establish that the quotient of this algebra by the quantum-determinant-like central element is the Yangian $Y(\mathfrak{g})$, as defined in Refs. 1 and 2.

II. GENERAL SETTING

Let $gl(M|N)$ be the $\mathbb{Z}_2$-graded algebra of $(M+N)\times(M+N)$ matrices X_{ij}. Let $\theta_0=\pm 1$. The $\mathbb{Z}_2$-gradation is defined by $(-1)^{[i]}=\theta_0$ if $1\leqslant i\leqslant M$ and $(-1)^{[i]}=-\theta_0$ if $M+1\leqslant i\leqslant M+N$. We will always assume that N is even. The following construction yields the osp($M|N$) Yangian, and it will lead to the *non-super-Yangians* by taking $N=0$, $\theta_0=1$ (orthogonal case) or $M=0$, $\theta_0=-1$ (symplectic case).

Definition 2.1: For each index i, we introduce a sign θ_i,

$$\theta_i=\begin{cases} +1 \quad \textit{for} \;\; 1\leqslant i\leqslant M+\dfrac{N}{2}, \\ -1 \quad \textit{for} \;\; M+\dfrac{N}{2}+1\leqslant i\leqslant M+N, \end{cases} \tag{2.1}$$

and a conjugate index $\overline{i}$,

$$\overline{i}=\begin{cases} M+1-i \quad \textit{for} \;\; 1\leqslant i\leqslant M, \\ 2M+N+1-i \quad \textit{for} \;\; M+1\leqslant i\leqslant M+N. \end{cases} \tag{2.2}$$

In particular $\theta_i\theta_{\overline{i}}=\theta_0(-1)^{[i]}$.

As usual E_{ij} denotes the elementary matrix with entry 1 in row i and column j and zero elsewhere.

Definition 2.2: For $A=\Sigma_{ij}A^{ij}E_{ij}$, we define the transposition t by

$$A^t=\sum_{ij}\,(-1)^{[i][j]+[j]}\theta_i\theta_j A^{ij}E_{\overline{j}\overline{i}}=\sum_{ij}\,(A^{ij})^tE_{ij}\,. \tag{2.3}$$

It satisfies $(A^t)^t=A$ and, for $\mathbb{C}$-valued matrices, $(AB)^t=B^tA^t$.

We shall use a graded tensor product, i.e., such that, for a, b, c and d with definite gradings, $(a\otimes b)(c\otimes d)=(-1)^{[b][c]}ac\otimes bd$.

Definition 2.3: Let P be the (super)permutation operator (i.e., $X_{21}\equiv PX_{12}P$)

$$P=\sum_{i,j=1}^{M+N}(-1)^{[j]}E_{ij}\otimes E_{ji} \tag{2.4}$$

and

$$K\equiv P^{t_1}=\sum_{i,j=1}^{M+N}(-1)^{[i][j]}\theta_i\theta_j E_{\overline{j}\overline{i}}\otimes E_{ji}\,, \tag{2.5}$$

where t_1 is the transposition in the first space of the tensor product. In particular $P_{21}=P_{12}$ and $K_{21}=K_{12}$.

We define the R-matrix

$$R(u)=\mathbb{I}+\frac{P}{u}-\frac{K}{u+\kappa}. \tag{2.6}$$

Proposition 2.4: The matrix $R(u)$ satisfies

$$R_{12}^{t_1}(-u-\kappa)=R_{12}(u) \quad (\textit{crossing symmetry}), \tag{2.7}$$

$$R_{12}(u)R_{12}(-u)=(1-1/u^2)\mathbb{I} \quad (\textit{unitarity}), \tag{2.8}$$

provided that $2\kappa=(M-N-2)\theta_0=(\alpha_0+2\rho,\alpha_0)/2$, where ρ is the super Weyl vector and α_0 the longest root.

Proof: We use the fact that the operators P and K satisfy

$$P^2=\mathbb{I}, \quad PK=KP=\theta_0 K, \quad \text{and} \quad K^2=\theta_0(M-N)K. \tag{2.9}$$

■

Theorem 2.5: *The R-matrix (26) satisfies the super Yang–Baxter equation*

$$R_{12}(u)R_{13}(u+v)R_{23}(v)=R_{23}(v)R_{13}(u+v)R_{12}(u) \tag{2.10}$$

for $2\kappa=(M-N-2)\theta_0$, where the graded tensor product is understood.

Proof: We use the following relations obeyed by the matrices P and K:

$$\begin{gathered} P_{13}K_{23}=K_{12}P_{13}, \quad K_{13}K_{12}=P_{23}K_{12}, \\ P_{12}P_{23}K_{12}=\theta_0 P_{13}K_{12}, \quad P_{12}K_{23}K_{12}=\theta_0 K_{13}K_{12}, \\ K_{12}K_{13}K_{23}=\theta_0 P_{13}K_{23}, \quad K_{12}P_{23}K_{12}=K_{12}. \end{gathered} \tag{2.11}$$

These relations are obtained by direct computation using the definition of the matrices P and K. ■

In the case related to so(N), this solution of the Yang–Baxter equation with spectral parameter was found in Ref. 11. It is also one of the cases explored in Ref. 12.

III. YANGIANS

We consider the Hopf (super)algebra $\mathcal{U}(R)$ generated by the operators $T_{(n)}^{ij}$, for $1\leqslant i, j\leqslant M+N$, $n\in\mathbb{Z}_{\geqslant 0}$, encapsulated into an $(M+N)\times(M+N)$ matrix,

$$T(u)=\sum_{n\in\mathbb{Z}_{\geqslant 0}} T_{(n)}u^{-n}=\sum_{i,j=1}^{M+N}\sum_{n\in\mathbb{Z}_{\geqslant 0}} T_{(n)}^{ij}u^{-n}E_{ij}=\sum_{i,j=1}^{M+N} T^{ij}(u)E_{ij}, \tag{3.1}$$

and $T_{(0)}^{ij}=\delta_{ij}$. One defines $\mathcal{U}(R)$ by imposing the following constraints on $T(u)$,

$$R_{12}(u-v)T_1(u)T_2(v)=T_2(v)T_1(u)R_{12}(u-v), \tag{3.2}$$

with the matrix $R(u)$ defined in (2.6).

The explicit commutation relations between the generating operators $T^{ij}(u)$ read

$$\begin{aligned} [T^{ij}(u),T^{kl}(v)]=&\frac{(-1)^{[k][i]+[k][j]+[i][j]}}{u-v}(T^{kj}(v)T^{il}(u)-T^{kj}(u)T^{il}(v)) \\ &+\frac{1}{u-v+\kappa}\sum_p (\delta_{i\bar{k}}(-1)^{[p]+[j][i]+[j][p]}\theta_{\bar{i}}\theta_{\bar{p}}T^{pj}(u)T^{\bar{p}\bar{l}}(v) \\ &-\delta_{j\bar{l}}(-1)^{[k][j]+[i][k]+[i][p]}\theta_{\bar{p}}\theta_{\bar{j}}T^{k\bar{p}}(v)T^{ip}(u)), \end{aligned} \tag{3.3}$$

that is, in terms of the generators $T^{ij}_{(n)}$,

$$
\begin{aligned}
&[T^{ij}_{(r+2)},T^{kl}_{(s)}]+[T^{ij}_{(r)},T^{kl}_{(s+2)}]\\
&\quad=2[T^{ij}_{(r+1)},T^{kl}_{(s+1)}]-\kappa[T^{ij}_{(r+1)},T^{kl}_{(s)}]+\kappa[T^{ij}_{(r)},T^{kl}_{(s+1)}]+(-1)^{[k][i]+[k][j]+[i][j]}\\
&\qquad\times(T^{kj}_{(s)}T^{il}_{(r+1)}-T^{kj}_{(r+1)}T^{il}_{(s)}-T^{kj}_{(s+1)}T^{il}_{(r)}+T^{kj}_{(r)}T^{il}_{(s+1)}+\kappa T^{kj}_{(s)}T^{il}_{(r)}-\kappa T^{kj}_{(r)}T^{il}_{(s)})\\
&\qquad+\sum_{p}\,(\delta_{ik}(-1)^{[p]+[j][i]+[j][p]}\theta_{\bar{i}}\theta_{\bar{p}}(T^{pj}_{(r+1)}T^{\bar{p}\bar{l}}_{(s)}-T^{pj}_{(r)}T^{\bar{p}\bar{l}}_{(s+1)})\\
&\qquad-\delta_{j\bar{l}}(-1)^{[k][j]+[i][k]+[i][p]}\theta_{\bar{p}}\theta_{\bar{j}}(T^{k\bar{p}}_{(s)}T^{ip}_{(r+1)}-T^{k\bar{p}}_{(s+1)}T^{ip}_{(r)})),
\end{aligned}
\tag{3.4}
$$

where $r,\ s\geqslant -2$ with, by convention, $T^{ij}_{(n)}=0$ for $n<0$.

The Hopf algebra structure of $\mathcal{U}(R)$ is given by[5]

$$
\Delta(T(u))=T(u)\dot{\otimes}T(u),\quad \text{i.e.,}\quad \Delta(T^{ij}(u))=\sum_{k=1}^{M+N}T^{ik}(u)\otimes T^{kj}(u),
\tag{3.5}
$$

$$
S(T(u))=T(u)^{-1};\quad \epsilon(T(u))=\mathbb{I}_{M+N}.
\tag{3.6}
$$

Theorem 3.1: *The operators generated by* $C(u)=T^{t}(u-\kappa)\,T(u)$ *lie in the center of the algebra* $\mathcal{U}(R)$ *and* $C(u)=c(u)\mathbb{I}$. *Furthermore,* $\Delta(c(u))=c(u)\otimes c(u)$ *and the two-sided ideal* $\mathcal{I}$ *generated by* $C(u)-\mathbb{I}$ *is also a coideal. The quotient* $\mathcal{U}/\mathcal{I}$ is then a Hopf algebra.

Proof: We first prove that $C(u)$ is diagonal. Indeed, the relation (3.2) implies

$$
K_{12}T_1(u-\kappa)T_2(u)=T_2(u)T_1(u-\kappa)K_{12}
\tag{3.7}
$$

from which it follows, after having transposed in space 1,

$$
\sum_{ijkl}(-1)^{[k]}T^{t}(u-\kappa)^{ij}T(u)^{jl}E_{ik}\otimes E_{kl}=\sum_{pqsr}(-1)^{[p][s]+[p][r]+[s][r]}T(u)^{pq}T^{t}(u-\kappa)^{qr}E_{sr}\otimes E_{ps}.
\tag{3.8}
$$

Therefore, one has

$$
\sum_{j}T^{t}(u-\kappa)^{ij}T(u)^{jl}=\delta_{il}c(u)\quad\text{or}\quad C(u)=c(u)\mathbb{I}.
\tag{3.9}
$$

Let us prove that $c(u)$ is a central element. One gets

$$
C(u)T_2(v)=T^{t}_1(u-\kappa)T_1(u)T_2(v)=T^{t}_1(u-\kappa)R^{-1}_{12}(u-v)T_2(v)T_1(u)R_{12}(u-v),
\tag{3.10}
$$

where we have used the unitarity and crossing properties (2.8) and (2.7) of $R(u)$. Now using the transposition of the relation (3.2) in space 1 and the crossing property of $R(u)$, one can derive the following exchange relation:

$$
T^{t}_1(u-\kappa)R^{-1}_{12}(u-v)T_2(v)=T_2(v)R^{-1}_{12}(u-v)T^{t}_1(u-\kappa).
\tag{3.11}
$$

Hence

$$
C(u)T_2(v)=T_2(v)R^{-1}_{12}(u-v)T^{t}_1(u-\kappa)T_1(u)R_{12}(u-v)=T_2(v)R^{-1}_{12}(u-v)C(u)R_{12}(u-v).
\tag{3.12}
$$

Since $C(u)=c(u)\mathbb{I}$, one obtains easily $C(u)T_2(v)=T_2(v)C(u)$.

From the defining relations of $C(u)$ the coproduct of $c(u)$ is straightforwardly obtained as $\Delta(c(u))=c(u)\otimes c(u)$ which shows that $\mathcal{I}$ is a coideal. It is interesting to note that this is precisely the structure of the coproduct of the quantum determinant whenever such an object has been constructed. ■

At order u^{-1} the equation $C(u)=\mathbb{I}$ yields the relation $T^t_{(1)}+T_{(1)}=0$. Note that those linear relations $T^{ij^t}_{(1)}+T^{ij}_{(1)}=0$ for which $i\neq j$ were already implied by the commutation relations (3.4). At higher orders, $C(u)=\mathbb{I}$ induces relations with the generic form $T^t_{(n)}+T_{(n)}=\mathcal{F}(T_{(m)},m<n)$ where $\mathcal{F}$ is a quadratic function.

In particular, once the exchange relations (3.4) (for $r=s=0$) are taken into account, the generators $T^{ij}_{(1)}$ exhibit the structure of the Lie (super) algebra $\mathfrak{g}$.

Definition 3.2: Let $\mathfrak{g}$ be a finite dimensional complex simple Lie (super) algebra. We define the bialgebra $\mathfrak{g}[u]$ as $\mathfrak{g}\otimes_{\mathbb{C}}\mathbb{C}[u]$ endowed with the Poisson cobracket δ defined by

$$\delta f(u,v)=2\left[\mathbb{I}\otimes f(v)+f(u)\otimes\mathbb{I},\frac{\mathfrak{C}}{u-v}\right], \tag{3.13}$$

where $\mathfrak{C}$ is the tensorial Casimir element of $\mathfrak{g}$ associated with a given nondegenerate invariant bilinear form $\mathfrak{B}$, and $f:\mathbb{C}\to\mathfrak{g}$ is a polynomial map, i.e., an element of $\mathfrak{g}[u]$.

Theorem 3.3: *Let $\mathfrak{g}$ be a finite dimensional complex simple Lie (super) algebra of type* so(M), sp(N), osp$(M|N)$. *Let $\mathcal{U}(R)$ be the Hopf algebra with generators $T(u)$ subject to the relations (3.2) and Hopf structure (3.5) and (3.6). The quotient of the algebra $\mathcal{U}(R)$ by the two-sided ideal $\mathcal{I}$ generated by $C(u)=T^t(u-\kappa)T(u)=\mathbb{I}$* [i.e., $c(u)=1$] *is a homogeneous quantization of $(\mathfrak{g}[u],\delta)$.*

Proof: We define $\mathcal{U}_\hbar$ as the algebra generated by the generating functional $\tilde{t}(u)$,

$$\tilde{t}(u)=\frac{1}{\hbar}(T(u/\hbar)-1), \tag{3.14}$$

and the identity, the relations being derived from those of $\mathcal{U}(R)$, i.e.,

$$[\tilde{t}_1(u),\tilde{t}_2(v)]=\left[\tilde{t}_1(u)+\tilde{t}_2(v),\frac{P}{u-v}\right]-\frac{\hbar}{u-v}(P\tilde{t}_1(u)\tilde{t}_2(v)-\tilde{t}_1(u)\tilde{t}_2(v)P)-\left[\tilde{t}_1(u)+\tilde{t}_2(v),\frac{K}{u-v+\hbar\kappa}\right]+\frac{\hbar}{u-v+\hbar\kappa}(K\tilde{t}_1(u)\tilde{t}_2(v)-\tilde{t}_1(u)\tilde{t}_2(v)K). \tag{3.15}$$

Thus the relations in $\mathcal{U}_\hbar/(\hbar\mathcal{U}_\hbar)$ are

$$[\tilde{t}_1(u),\tilde{t}_2(v)]=\left[\tilde{t}_1(u)+\tilde{t}_2(v),\frac{P-K}{u-v}\right]. \tag{3.16}$$

The equation $C(u)=\mathbb{I}$ expressed in $\mathcal{U}_\hbar$ generates a two-sided ideal $\mathcal{I}_\hbar$, which now induces relations with the generic form $\tilde{t}^t_{(n)}+\tilde{t}_{(n)}=\hbar\mathcal{F}(\tilde{t}_{(m)},m<n)$ where $\mathcal{F}$ is a quadratic function. In the quotient algebra $\mathcal{U}_\hbar/(\hbar\mathcal{U}_\hbar)$ this becomes equivalent to the standard linear symmetrization relation $J^t_{(n)}+J_{(n)}=0$ for the generators of the loop algebra $\mathfrak{g}[u]$, so that $\mathcal{U}'_\hbar/(\hbar\mathcal{U}'_\hbar)\simeq\mathcal{U}(\mathfrak{g}[u])$ as algebras, for $\mathcal{U}'_\hbar\equiv\mathcal{U}_\hbar/\mathcal{I}_\hbar$. This characterizes $\mathcal{U}'_\hbar$ as a quantization of the algebra $\mathcal{U}(\mathfrak{g}[u])$.

We now examine the coproduct structure in order to recognize it as a quantization of the cocommutator δ, namely,

$$\left.\frac{\Delta-\Delta^{op}}{\hbar}(\tilde{t}(u))\right|_{\text{mod }\hbar}=\delta(\tilde{t}(u)|_{\text{mod }\hbar}). \tag{3.17}$$

From (3.5), the order u^{-m} of the (i,j) entry of the left hand side of this formula reads

$$\frac{\Delta-\Delta^{op}}{\hbar}\tilde{t}_{(m)}\Big|_{\text{mod }\hbar}=\sum_{r=0}^{m}\left(\tilde{t}_{(r)}\dot{\otimes}\tilde{t}_{(m-r)}-\tilde{t}_{(r)}\dot{\otimes}\tilde{t}_{(m-r)}\right)\Big|_{\text{mod }\hbar}. \tag{3.18}$$

Now, denoting generically $\tilde{t}^a=\tilde{t}^{ij}-(\tilde{t}^{ij})^t$ and $E_a=E_{ij}-(E_{ij})^t$, and using $\tilde{t}=\tilde{t}^t$ mod $\hbar$, we can symmetrize and get

$$\begin{aligned}\sum_c\frac{\Delta-\Delta^{op}}{\hbar}\tilde{t}^c_{(m)}E_c\Big|_{\text{mod }\hbar}&=\sum_{a,b}\sum_{r=0}^{m}\tilde{t}^a_{(r)}\otimes\tilde{t}^b_{(m-r)}[E_a,E_b]\Big|_{\text{mod }\hbar}\\&=\sum_{a,b}\sum_{r=0}^{m}\tilde{t}^a_{(r)}\otimes\tilde{t}^b_{(m-r)}f_{ab}{}^cE_c\Big|_{\text{mod }\hbar}.\end{aligned} \tag{3.19}$$

The right hand side of the formula (3.17) can be computed once one recalls that $\mathfrak{C}=\Sigma_{ab}\mathfrak{B}_{ab}t^a\otimes t^b$. One obtains

$$\delta(t^a_{(m)})=\sum_{a,b}\sum_{r=0}^{m}t^a_{(r)}\otimes t^b_{(m-r)}f^c{}_{ab}, \tag{3.20}$$

where the $t^a_{(m)}$ denote the generators of the loop algebra $\mathfrak{g}[u]$. Since the modes of $(\tilde{t}(u)|_{\text{mod }\hbar})$ coincide with the $t^a_{(m)}$ and the structure constants $f_{ab}{}^c$ and $f^c{}_{ab}$ are identified through the bilinear form $\mathfrak{B}$, one gets the desired result (3.17).

Therefore the Hopf algebra $\mathcal{U}(R)/\mathcal{I}\equiv\mathcal{U}'_{\hbar=1}$ is a quantization of $\mathcal{U}(\mathfrak{g}[u])$ and Δ is a quantization of δ. ■

From the above theorem, we are naturally led to the following definition:

Definition 3.4: We define the Yangian of osp$(M|N)$ *as* $Y(\mathfrak{g})\equiv\mathcal{U}(R)/\mathcal{I}$. *Explicitly, its defining relations are given by*

$$R_{12}(u-v)T_1(u)T_2(v)=T_2(v)T_1(u)R_{12}(u-v),$$

$$C(u)=T^t(u-\kappa)T(u)=\mathbb{I},$$

where $R_{12}(u)=\mathbb{I}+P/u-K/(u+\kappa)$.

For $N=0$ or $M=0$, this definition is consistent with the one of Drinfel'd[1,2] for the so(M) and sp(N) cases, respectively.

Remark: The explicit R-matrices for the Yangians $Y(\text{so}(N))$ and $Y(\text{sp}(N))$ can be obtained by taking the scaling limit $q\to1$, $z=q^u\to1$ keeping u fixed, of the evaluated trigonometric R-matrices of $\mathcal{U}_q(\widehat{\text{so}(N)})$ and $\mathcal{U}_q(\widehat{\text{sp}(N)})$ computed in Ref. 15. Similarly, one can show that the R-matrix of $Y(\text{osp}(1|2))$ is the scaling limit of the evaluated trigonometric R-matrix of $\mathcal{U}_q(\widehat{\text{osp}(1|2)})$.[16]

IV. TWISTED YANGIANS AND REFLECTION ALGEBRAS

We would finally like to comment upon a possible connection between the notions of twisted Yangians and reflection algebras within the framework of this Yangian construction.

Following the lines of Refs. 8 and 9 (see also Ref. 10 for the supersymmetric case), we define on $\mathcal{U}(R)$

$$\tau[T(u)]=T^t(-u-\kappa), \tag{4.1}$$

which reads for the super-Yangian generators

$$\tau(T^{ab}(u))=(-1)^{[a]([b]+1)}\theta_a\theta_bT^{\bar{b}\bar{a}}(-u-\kappa). \tag{4.2}$$

Here τ is an algebra automorphism, as a direct consequence of unitarity, crossing symmetry and the property $R^{t_1 t_2}(u)=R(u)$ which itself comes from $P^{t_1 t_2}=P$.

The twisted super-Yangian $\mathcal{U}(R)^{tw}$ is the subalgebra generated by $S(u)=\tau[T(u)]T(u)$, with τ given in (4.2). $S(u)$ obeys the following relation:

$$R_{12}(u-v)S_1(u)R_{12}(u+v)S_2(v)=S_2(v)R_{12}(u+v)S_1(u)R_{12}(u-v). \tag{4.3}$$

It is easy to show that $\mathcal{U}(R)^{tw}$ is a coideal in $\mathcal{U}(R)$.

Similarly, one introduces the notion of reflection algebras $\mathcal{S}(R)$, generated by

$$B(u)=T^{-1}(-u)T(u), \tag{4.4}$$

which obeys the same relation (4.3), interpreted here as a reflection equation. $\mathcal{S}(R)$ is also a coideal of $\mathcal{U}(R)$. This type of algebra was originally introduced in Ref. 17 for the Yangian $Y(N)$, based on gl(N), and plays an important role in integrable systems with boundaries (see, e.g., Ref. 18).

However, in the coset $\mathcal{U}(R)/\mathcal{I}$, one has $B(u)=S(u)$, so that $\mathcal{S}(R)$ and $\mathcal{U}(R)^{tw}$ are two versions of the same Hopf coideal in $\mathcal{U}(R)$. The situation is here different from the case of the Yangian $Y(N)$. Indeed the twisted Yangians $Y^{\pm}(N)$ and the boundary algebras $B(N,\ell)$ are known to be different for $N>2$, while for $N=2$ one has $B(2,0)=Y^{-}(2)$ and $B(2,1)=Y^{+}(2)$.[19]

ACKNOWLEDGMENTS

We would like to thank A. Molev and V. Tolstoy for discussions and comments.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 1 JANUARY 2003

On powers of Bessel functions

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(Received 16 August 2002; accepted 3 October 2002)

A formula for the Taylor series expansion of the rth power of the modified Bessel function $[I_\nu(z)]^r$ is derived for arbitrary r. The result is expressed in terms of a recursive formula for a class of polynomials, which facilitates the systematic construction of the expansion of $[I_\nu(z)]^r$. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1526940]

I. INTRODUCTION

Bessel functions are important special functions that appear widely in science and engineering. Bessel functions of the first kind $J_\nu(x)$ are oscillatory and may be regarded as generalizations of trigonometric functions. Indeed, for large argument ($x \gg 1$) the function $\sqrt{\pi x/2}J_\nu(x)$ is well approximated by the trigonometric function $\cos(x-\pi\nu/2-\pi/4)$. Similarly, modified Bessel functions of the first kind $I_\nu(x)$, which are Bessel functions of imaginary argument, may be regarded as generalizations of exponentials. Exponential functions have the unique and special property that they are particularly easy to multiply and to raise to powers: $e^{ax}e^{bx}=e^{(a+b)x}$ and $(e^x)^r=e^{rx}$. This raises the following question: How does one multiply modified Bessel functions and raise them to powers? This article shows that there are relatively elementary formulas for the powers of Besel functions in terms of ascending Taylor series.

While many of the mathematical properties of Bessel functions are well understood,[1,2] surprisingly little is known about the products of Bessel functions. Yet, powers and sums of powers of Bessel functions are of importance in many applications. For example, the expression for the sum of products of pairs of Bessel functions have applications in the study of a beam of charged particles in a plasma.[3] Sums of products of Bessel functions typically arise in any statics or dynamics problem in which there is a spherical symmetry. An interesting case is that of the Casimir effect for a sphere.[4]

In the area of statistical mechanics, modified Bessel functions appear in the study of the XY model. In particular, an application of the group theoretic method for lattice spin models, introduced in Ref. 5, to the two-dimensional XY model shows that the partition function can be expressed as a sum of products of modified Bessel functions. Given the importance of products of Bessel functions in physical applications, it is desirable to have explicit representations for products and powers of these functions.

The purpose of this article is to derive an explicit formula for arbitrary powers of the modified Bessel function $I_\nu(z)$. Specifically, we use the Taylor series for $I_\nu(z)$,

$$I_\nu(z)=\sum_{k=0}^{\infty}\frac{1}{k!\Gamma(k+\nu+1)}\left(\frac{z}{2}\right)^{2k+\nu}, \tag{1}$$

to construct a formula for the coefficients $A_k(r)$ of the Taylor series in powers of z of the rth power of $I_\nu(z)$,

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$$[I_\nu(z)]^r=\sum_{k=0}^{\infty} A_k(r)z^k, \tag{2}$$

where r is not necessarily an integer.

In Sec. II we consider the special case $\nu=0$ and derive the recursion formula for the coefficients of z^k in the power series for $[I_0(z)]^r$. These results are extended in Sec. III to the case $[I_\nu(z)]^r$, where ν is arbitrary.

II. POWERS OF I_0

We begin by considering the special case $\nu=0$. The Taylor expansion for the modified Bessel function $I_0(z)$ is

$$I_0(z)=\sum_{k=0}^{\infty}\frac{1}{(k!)^2}\left(\frac{z}{2}\right)^{2k}. \tag{3}$$

There is a simple formula for the Taylor series of the square $I_0^2(z)$ of this Bessel function:

$$I_0^2(z)=1+\frac{1}{2}z^2+\frac{3}{32}z^4+\frac{5}{576}z^6+\frac{35}{73728}z^8+\cdots=\sum_{k=0}^{\infty}\frac{(2k-1)!!}{2^k(k!)^3}z^{2k}. \tag{4}$$

More generally, there is also a simple formula for the square of $I_\nu(z)$,

$$I_\nu^2(z)=\sum_{k=0}^{\infty}\frac{1}{[(n+\nu)!]^2}\binom{2n+2\nu}{n}\left(\frac{z}{2}\right)^{2n+2\nu}. \tag{5}$$

[The derivation of (5) follows from the identity $\Sigma_{k=0}^{n}\binom{n+\nu}{n-k}\binom{n+\nu}{k}=\binom{2n+2\nu}{n}$. The referee of this article has pointed out that this identity has a combinatorial interpretation. It comes from asking how many ways there are to choose n people from among $n+\nu$ physicists and $n+\nu$ mathematicians, k being the number of mathematicians chosen. Most of the results given in this article can be presented in combinatorial terms. However, we prefer to use the generating function approach that is used in this article.] However, if the Bessel function is raised to a power other than 2, the Taylor series coefficients are rather complicated, even for integer powers. For example, when $r=4$ we have

$$I_0^4(z)=1+z^2+\frac{7}{16}z^4+\frac{1}{9}z^6+\frac{679}{36864}z^8+\cdots. \tag{6}$$

Because $679=7\times 97$ and 97 is a large prime number, it appears that there is no simple formula like that in (4) for the Taylor coefficients.

If we raise the Taylor series (3) to the power r, where r is any number, possibly complex, we obtain the series

$$[I_0(z)]^r=1+\frac{r}{4}z^2+\frac{r}{64}(2r-1)z^4+\frac{r}{2304}(6r^2-9r+4)z^6+\cdots\equiv 1+\sum_{k=0}^{\infty}c_k r P_k(r)z^{2(k+1)}, \tag{7}$$

where the combinatoric factors

$$c_k=\frac{1}{2^{2(k+1)}[(k+1)!]^2} \tag{8}$$

are independent of r, and $P_k(r)$ are polynomials in r having integer coefficients. The first seven of these polynomials are

$$P_0(r)=1,$$

$$P_1(r)=2r-1,$$

$$P_2(r)=6r^2-9r+4,$$

$$P_3(r)=24r^3-72r^2+82r-33, \tag{9}$$

$$P_4(r)=120r^4-600r^3+1250r^2-1225r+456,$$

$$P_5(r)=720r^5-5400r^4+17700r^3-30\,600r^2+27\,041r-9460,$$

$$P_6(r)=5040r^6-52\,920r^5+249\,900r^4-661\,500r^3+1\,011\,017r^2-826\,336r+274\,800.$$

These polynomials satisfy the condition $P_k(1)=1$, which follows from comparing equations (7) and (3), and they obey the recursion relation

$$P_k(r)=rkP_{k-1}(r)+\sum_{j=1}^{k-1} M_j(-1)^k\frac{k-j}{k(j+1)}\binom{k}{j}^2 P_{k-j}(r), \tag{10}$$

where the numbers M_j are positive integers. The first nine of the M_j are 1, 1, 3, 16, 130, 1485, 22 645, 444 136, 10 889 676.

The advantage of the recursion relation (10) is that it reduces the problem of determining the polynomials $P_k(r)$ to the much simpler problem of identifying the integer sequence M_j ($j=1,2,3,\ldots$). If we now set $b_j\equiv(-1)^jM_j$, we find that the integers b_j obey the inhomogeneous linear difference equation

$$b_n=(n-1)-\sum_{m=2}^{n-1} b_m\frac{n!(n-1)!}{m!(m-1)!(n-m)!(n-m+1)!}. \tag{11}$$

This equation is derived from (10) by setting $r=1$ and recalling that $P_k(1)=1$.

We solve this difference equation by introducing the generating functions $f(x)$ and $g(x)$ as follows:

$$f(x)=\sum_{m=1}^{\infty}\frac{x^m b_m}{m!(m-1)!} \quad \text{and} \quad g(x)=\sum_{m=0}^{\infty}\frac{x^m}{m!(m+1)!}=\frac{1}{\sqrt{x}}I_1(2\sqrt{x}). \tag{12}$$

Multiplying the difference equation (11) by x^n and dividing by $n!(n-1)!$ gives

$$\frac{b_n x^n}{n!(n-1)!}=\frac{(n-1)x^n}{n!(n-1)!}-\sum_{m=2}^{n-1}\frac{x^m b_m}{m!(m-1)!}\cdot\frac{x^{n-m}}{(n-m)!(n-m+1)!}, \tag{13}$$

which is precisely the coefficient of x^n in the equation

$$f(x)g(x)=\sum_{n=1}^{\infty}\frac{(n-2)x^n}{n!(n-1)!}=xI_0(2\sqrt{x})-2\sqrt{x}I_1(2\sqrt{x}). \tag{14}$$

Finally, dividing both sides of (14) by $g(x)$ gives

$$\sum_{m=0}^{\infty} \frac{x^m b_m}{m!(m-1)!} = x\left(\frac{\sqrt{x} I_0(2\sqrt{x})}{I_1(2\sqrt{x})} - 2 \right), \tag{15}$$

where we have used the Taylor series in (1) for the modified Bessel functions.

The power series expansion of the right side of (15) is

$$x\left(\frac{\sqrt{x} I_0(2\sqrt{x})}{I_1(2\sqrt{x})} - 2 \right) = -x + \frac{1}{2}x^2 - \frac{1}{12}x^3 + \frac{1}{48}x^4 - \frac{1}{180}x^5 + \frac{13}{8640}x^6 - \cdots. \tag{16}$$

If we let a_k denote the coefficient of x^k on the right-hand side of (16), it is easy to see that the sequence defined by $k!(k-1)!a_k$ takes the values -1, 1, -1, 3, -16, 130, -1485, 22 645, and so on. In other words, the formula for the integers M_k is given by

$$M_k = (-1)^k (k+1)!k!a_{k+1} \tag{17}$$

for $k = 1,2,\ldots$.

We are able to determine the integer sequence M_j by using the key fact that $P_k(1) = 1$. However, because we also have an explicit power series expression (4) for the square of $I_0(z)$, by comparing this formula with (7) and setting $r = 2$, we obtain

$$P_k(2) = \frac{2^k (2k+1)!!}{(k+1)!}. \tag{18}$$

This expression allows us to obtain an alternative method of determining the sequence M_j. Specifically, if we set $r = 2$ in (10) and substitute (18) in the resulting expression, we deduce the identity

$$\sum_{j=0}^{k-1} M_j \left[\frac{(k-j)(2k-2j+1)!!}{2^j (j+1)(k-j+1)!} \binom{k}{j}^2 \right] = \frac{k(2k-1)!!}{(k+1)!}(1+k-k^2) \tag{19}$$

satisfied by the sequence M_j. Therefore, along with $M_1 = 1$ we can determine values of the integer sequence M_j iteratively from (19).

III. POWERS OF MODIFIED BESSEL FUNCTIONS

Having obtained the recursive formula that allows us to generate the power series expansion of $[I_0(z)]^r$, we now develop the corresponding formula for the powers of general modified Bessel functions: $[I_\nu(z)]^r$. Our method follows very closely the approach of the previous section.

In order to simplify the computation, we define $\tilde{I}_\nu$ by[2]

$$\tilde{I}_\nu(z) = 2^\nu \nu! z^{-\nu} I_\nu(z) = \sum_{k=0}^{\infty} \frac{\nu!}{k!(k+\nu)!} \left(\frac{z}{2} \right)^{2k}, \tag{20}$$

so that the Taylor series representation for $\tilde{I}_\nu(z)$ begins with 1. [In this section we use the notation $\nu!$ to mean $\Gamma(\nu+1)$ when ν is not a positive integer.] We write the series expansion of an arbitrary power of $\tilde{I}_\nu$ as

$$[\tilde{I}_\nu(z)]^r = \sum_{k=0}^{\infty} \frac{\nu!}{2^{2k} k!(\nu+k)!} B_k^\nu(r) z^{2k}. \tag{21}$$

The polynomial $B_k^\nu(r)$ indexed by ν is the generalization of the polynomial $P_k(r)$ considered in the previous section. That is, $P_k(r) = B_k^0(r)$. We observe that, analogous to the polynomial $P_k(r)$,

if we set $r=1$ in (21), we find that the polynomials $B_k^\nu(r)$ satisfy $B_k^\nu(1)=1$ for arbitrary k and ν. However, unlike the case for $\nu=0$, there is no simple formula for $[\tilde{I}_\nu(z)]^2$ which allows us to determine an elementary expression for $B_k^\nu(2)$.

The first five of the polynomials $B_k^\nu(r)$ are

$$B_0^\nu(r)=1,$$

$$B_1^\nu(r)=r,$$

$$B_2^\nu(r)=\frac{\nu+2}{\nu+1}r^2-\frac{1}{\nu+1}r, \tag{22}$$

$$B_3^\nu(r)=\frac{(\nu+2)(\nu+3)}{(\nu+1)^2}r^3-3\frac{\nu+3}{(\nu+1)^2}r^2+4\frac{1}{(\nu+1)^2}r,$$

$$B_4^\nu(r)=\frac{(\nu+2)(\nu+3)(\nu+4)}{(\nu+1)^3}r^4-6\frac{(\nu+3)(\nu+4)}{(\nu+1)^3}r^3+\frac{(\nu+4)(19\nu+41)}{(\nu+1)^3(\nu+2)}r^2$$
$$-6\frac{5\nu+11}{(\nu+1)^3(\nu+2)}r.$$

from which we obtain the recursion relation for the polynomials $B_k^\nu(r)$. This is given by

$$B_k^\nu(r)=\frac{r(\nu+k)}{\nu+1}B_{k-1}^\nu(r)+\sum_{j=1}^{k}(-1)^j W_j(\nu)\frac{(k-j)!(\nu+k-j+1)!}{k!(\nu+k-1)!}B_{k-j}^\nu(r), \tag{23}$$

where

$$W_1(\nu)=\frac{1}{(\nu+1)(\nu+2)},$$

$$W_2(\nu)=\frac{1}{(\nu+1)(\nu+2)^2(\nu+3)},$$

$$W_3(\nu)=\frac{2}{(\nu+1)(\nu+2)^3(\nu+3)(\nu+4)},$$

$$W_4(\nu)=\frac{5\nu+16}{(\nu+1)(\nu+2)^4(\nu+3)^2(\nu+4)(\nu+5)},$$

$$W_5(\nu)=\frac{2(7\nu+26)}{(\nu+1)(\nu+2)^5(\nu+3)^2(\nu+4)(\nu+5)(\nu+6)},$$

and so on.

If we further define $W_{jk}(\nu)$ by

$$W_{jk}(\nu)=\frac{(\nu+k-j+1)!}{(\nu+k-1)!}W_j(\nu) \tag{24}$$

for $k\geqslant j$, then the recursion relation (23) for $B_k^\nu(r)$ now reads

$$B_k^{\nu}(r)=\frac{r(\nu+k)}{\nu+1}B_{k-1}^{\nu}(r)+\sum_{j=1}^{k}(-1)^j W_{jk}(\nu)\frac{(k-j)!}{k!}B_{k-j}^{\nu}(r). \tag{25}$$

Thus, if we define $b_j(\nu)=(-1)^j W_{jj}(\nu)$, then by setting $r=1$ in (25) we obtain the difference equation

$$\frac{\nu+k}{\nu+1}-2=\sum_{j=0}^{k} b_j(\nu)\frac{(k-1)!(\nu+1)!(\nu+k)!}{(k-j)!(\nu+k-j+1)!(\nu+j)!(j-1)!}, \tag{26}$$

which is analogous to (11). Equation (26) may be rewritten as

$$\sum_{k=1}^{\infty}\frac{k-\nu-2}{(k-1)!(\nu+k)!}\frac{x^k}{(\nu+1)(\nu+1)!}=\sum_{k=1}^{\infty}\frac{x^k b_j(\nu)}{(\nu+j)!(j-1)!}\frac{1}{(k-j)!(\nu+k-j+1)!}. \tag{27}$$

As in (12) we introduce a pair of generating functions as follows:

$$f(x)=\sum_{k=1}^{\infty}\frac{x^k b_k(\nu)}{(\nu+k)!(k-1)!}\quad\text{and}\quad g(x)=\sum_{k=0}^{\infty}\frac{x^k}{k!(\nu+k+1)!}. \tag{28}$$

Then the product of these two functions gives

$$f(x)g(x)=-\frac{2}{(\nu+1)!}\sum_{k=0}^{\infty}\frac{x^{k+1}}{k!(\nu+k+1)!}+\frac{1}{(\nu+1)(\nu+1)!}\sum_{k=0}^{\infty}\frac{x^{k+1}}{k!(\nu+k)!}. \tag{29}$$

Dividing both sides of (29) by $g(x)$ we finally deduce that

$$\sum_{k=1}^{\infty}\frac{x^k b_k(\nu)}{(\nu+k)!(k-1)!}=\frac{x}{(\nu+1)!}\left(\frac{\sqrt{x}}{(\nu+1)}\frac{I_{\nu}(2\sqrt{x})}{I_{\nu+1}(2\sqrt{x})}-2\right), \tag{30}$$

where we have again used the Taylor series in (1) for the modified Bessel functions.

In summary, we have derived an explicit recursive formula that determines the coefficients in the Taylor series expansion of powers of modified Bessel functions. Specifically, we have

$$[I_{\nu}(z)]^r=\sum_{k=0}^{\infty}\frac{1}{k!(\nu+k)!(\nu!)^{r-1}}B_k^{\nu}(r)\left(\frac{z}{2}\right)^{2k+r\nu}, \tag{31}$$

where the polynomials $B_k^{\nu}(r)$ are determined recursively by

$$B_k^{\nu}(r)=r\frac{\nu+k}{\nu+1}B_{k-1}^{\nu}(r)+\sum_{j=0}^{k} b_j(\nu)\frac{1}{k}\frac{(\nu+1)!}{(\nu+1+j)!}\binom{\nu+k}{j}B_{k-1}^{\nu}(r), \tag{32}$$

and the integer sequence $b_j(\nu)$ is identified by expanding the right-hand side of (30).

ACKNOWLEDGMENTS

D.C.B. gratefully acknowledges financial support from The Royal Society. This work was supported in part by the U.S. Department of Energy.

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A Poincaré–Birkhoff–Witt commutator lemma for $U_q[\mathrm{gl}(m|n)]$

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(Received 6 April 2002; accepted 29 July 2002)

We present and prove in detail a Poincaré–Birkhoff–Witt commutator lemma for the quantum superalgebra $U_q[\mathrm{gl}(m|n)]$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1511828]

I. INTRODUCTION

This paper presents and proves in detail a Poincaré–Birkhoff–Witt (PBW) commutator lemma for the quantum superalgebra $U_q[\mathrm{gl}(m|n)]$. The lemma itself is not new; it dates from a 1993 paper of Rui Bin Zhang[3] on the representation theory of $U_q[\mathrm{gl}(m|n)]$. However, its previous incarnation contained several typographical and other minor errors in its details; and in any case an explicit proof was not supplied. Here, we correct those errors, and supply detailed proofs for our claims.

We mention that we use the phrase ''PBW commutator lemma'' to indicate a result showing commutations sufficient to render any expression within an algebra into a normal form in a PBW basis; for more details for our specific case $U_q[\mathrm{gl}(m|n)]$, we again refer the reader to the original work by Zhang.

II. THE STRUCTURE OF $U_q[\mathrm{gl}(m|n)]$

Following Zhang (Ref. 3, pp. 1237–1238), we provide a full description of $U_q[\mathrm{gl}(m|n)]$ in terms of simple generators and relations. We do so after first introducing the generators and various divers notations.

First, we define a $\mathbb{Z}_2$ grading $[\cdot]$ on the set of $\mathrm{gl}(m|n)$ indices $\{1,\ldots,m+n\}$:

$$[a]\triangleq\begin{cases}0, & a\leqslant m, \quad \text{even indices},\\ 1, & a>m, \quad \text{odd indices},\end{cases}$$

where we use the symbol ''$\triangleq$'' to mean ''is defined as being.'' Throughout, we shall use dummy indices a,b, etc., where meaningful.

A set of generators for the associative superalgebra $U_q[\mathrm{gl}(m|n)]$ is then

$$\{K_a^{\pm};E_b^a|1\leqslant a,b\leqslant m+n,a\neq b\},$$

where the $K_a^{\pm}$ are called ''Cartan generators'' (and of course we intend ''± 1'' where we write ''$\pm$''), and E_b^a is called a ''raising generator'' if $a<b$ and a ''lowering generator'' if $a>b$. We indeed intend that K_a and K_a^{-1} are inverses, that is, that we have relations $K_aK_a^{-1}=K_a^{-1}K_a=\mathrm{Id}$, where Id is the $U_q[\mathrm{gl}(m|n)]$ identity element.

Elements of $U_q[\mathrm{gl}(m|n)]$ are then in general weighted sums of noncommuting products of these generators, where each weight is in general a rational expression of integer-coefficient Laurent polynomials in the polynomial variable q. Under the phrase ''products of generators,'' we include powers of the K_a (see below).

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For various invertible X, we will repeatedly use the notation $\overline{X}\triangleq X^{-1}$; in particular, we set $\overline{q}\triangleq q^{-1}$. Next, for any index a we shall write

$$q_a\triangleq q^{(-)^{[a]}},$$

where we have invoked the shorthand "$(-)$" for "(-1)." For any power N, replacing q with q^N immediately shows that $(q_a)^N=(q^N)_a$, so we may write q_a^N with impunity; in particular, we will write $\overline{q}_a\equiv q_a^{-1}$. Further, we will use the following notation:

$$\Delta\triangleq q-\overline{q},\quad \Delta_a\triangleq q_a-\overline{q}_a=(-)^{[a]}(q-\overline{q})=(-)^{[a]}\Delta,$$

$$\overline{\Delta}\triangleq(\Delta)^{-1},\quad \overline{\Delta}_a\triangleq(\Delta_a)^{-1}=(-)^{[a]}\overline{\Delta}.$$

Now, in terms of q, an equivalent notation for K_a is $q_a^{E_a^a}$. (Here, the exponentiation may be understood in terms of a power series expansion of the $U[\mathrm{gl}(m|n)]$ Cartan generators E_a^a. Strictly speaking, we *could* define these E_a^a as the $U_q[\mathrm{gl}(m|n)]$ Cartan generators, allowing them to appear in infinite sums as exponents of q, but the K_a notation is more convenient.) Thus, powers K_a^N are meaningful, although we will only deal with $N\in\frac{1}{2}\mathbb{Z}$ (that is, integer and half-integer powers). So, we may write $\overline{K}_a\triangleq K_a^{-1}$; indeed the mapping $q\mapsto\overline{q}$ sends K_a^N to $\overline{K}_a^N$, and as expected, for arbitrary powers M,N:

$$K_a^MK_a^N=K_a^{M+N},\quad \text{where}\ \ K_a^0\equiv\mathrm{Id}.$$

Apart from $N\in\mathbb{N}$, powers (i.e., products) of the non-Cartan generators $(E_b^a)^N$ for $a\neq b$, are not meaningful.

The generators inherit a $\mathbb{Z}_2$ grading from the indices

$$[K_a]\triangleq 0\quad\text{and}\ [E_b^a]\triangleq[a]+[b]\ \ (\mathrm{mod}\,2),$$

so we may also use the terms "even" and "odd" for generators. Elements of $U_q[\mathrm{gl}(m|n)]$ are said to be *homogeneous* if they are linear combinations of generators of the same grading or products of other homogeneous elements; the product XY of homogeneous X,Y has grading $[XY]\triangleq[X]+[Y](\mathrm{mod}\,2)$.

Now, the full set of generators includes some redundancy; in that its elements may be expressed in terms of a subset of them, that is the following $U_q[\mathrm{gl}(m|n)]$ *simple generators*:

$$\{K_a^{\pm};E_a^{a+1},E_{a+1}^a|1\leqslant a,a+1\leqslant m+n\};$$

note that there are only two *odd* simple generators: E_m^{m+1} (lowering) and E_{m+1}^m (raising). In the $\mathrm{gl}(m|n)$ case, the remaining *nonsimple* (non-Cartan) generators satisfy the same commutation relations as the simple generators. However, for $U_q[\mathrm{gl}(m|n)]$, the nonsimple generators are instead recursively defined in terms of weighted sums of products of simple generators [Ref. 2, p. 1971, (3)] and [Ref. 3, p. 1238, (2)]. Writing $S_b^a\triangleq\mathrm{sign}(a-b)$, the elements of the set of nonsimple generators $\{E_b^a|\ |a-b|>1\}$ may be defined by

$$E_b^a\triangleq E_c^aE_b^c-q_c^{S_b^a}E_b^cE_c^a,\tag{1}$$

where we intend c to be an *arbitrary* index strictly between a and b; we do *not* intend a sum here.

Last, the *graded commutator* $[\cdot,\cdot]$ is defined for homogeneous X,Y by

$$[X,Y]\triangleq XY-(-)^{[X][Y]}YX,\tag{2}$$

and extended by linearity. As $U_q[\mathrm{gl}(m|n)]$ is an *associative* superalgebra, we have the following useful identities involving homogeneous elements:

$$\begin{aligned} &\text{(a)} \quad [XY,Z]=X[Y,Z]+(-)^{[Y][Z]}[X,Z]Y, \\ &\text{(b)} \quad [X,YZ]=[X,Y]Z+(-)^{[X][Y]}Y[X,Z]. \end{aligned} \tag{3}$$

A. $U_q[\mathrm{gl}(m|n)]$ relations

In terms of the set of simple generators, that is

$$\{K_a^{\pm};E_a^{a+1},E_{a+1}^a|1\leqslant a,a+1\leqslant m+n\},$$

our algebra $U_q[\mathrm{gl}(m|n)]$ satisfies the following relations.

(1) The Cartan generators commute, that is for $M,N\in\{\pm 1\}$,

$$K_a^M K_b^N=K_b^N K_a^M. \tag{4}$$

(2) The Cartan generators commute with the simple raising and lowering generators in the following manner:

$$K_a E_{b\pm 1}^b=q_a^{(\delta_b^a-\delta_{b\pm 1}^a)}E_{b\pm 1}^b K_a. \tag{5}$$

(3) The non-Cartan simple generators satisfy

$$[E_{a+1}^a,E_b^{b+1}]=\delta_b^a\overline{\Delta}_a(K_a\overline{K}_{a+1}-\overline{K}_a K_{a+1}). \tag{6}$$

and, for $|a-b|>1$, we have the commutations

$$E_a^{a+1}E_b^{b+1}=E_b^{b+1}E_a^{a+1} \quad \text{and} \quad E_{a+1}^a E_{b+1}^b=E_{b+1}^b E_{a+1}^a. \tag{7}$$

(4) The squares of the odd simple generators are zero

$$(E_{m+1}^m)^2=(E_m^{m+1})^2=0. \tag{8}$$

(5) If neither m nor n is 1, we have the $U_q[\mathrm{gl}(m|n)]$ *Serre relations* (else if either m or n is 1, omit them). Most succinctly expressed in terms of the nonsimple generators, for $a\neq m$, we have

$$\begin{aligned} &\text{(a)} \quad E_a^{a+1}E_a^{a+2}=q_a E_a^{a+2}E_a^{a+1}, \\ &\text{(b)} \quad E_{a+1}^a E_{a+2}^a=q_a E_{a+2}^a E_{a+1}^a, \\ &\text{(c)} \quad E_{a-1}^{a+1}E_a^{a+1}=q_a E_a^{a+1}E_{a-1}^{a+1}, \\ &\text{(d)} \quad E_{a+1}^{a-1}E_{a+1}^a=q_a E_{a+1}^a E_{a+1}^{a-1}, \end{aligned} \tag{9}$$

and also

$$[E_m^{m+1},E_{m-1}^{m+2}]=[E_{m+1}^m,E_{m+2}^{m-1}]=0.$$

The interested reader may use (1) to expand these into expressions involving only the simple generators; however the results are cumbersome and unedifying.

B. Useful results from the $U_q[\mathrm{gl}(m|n)]$ relations

(1) From (4), it immediately follows that all powers of the Cartan generators commute; that is, for any powers $M,N\in\frac{1}{2}\mathbb{Z}$:

$$K_a^M K_b^N=K_b^N K_a^M. \tag{10}$$

(2) Lemma 2 of Ref. 1 shows that (5) may be much strengthened to cover all non-Cartan generators and all powers of Cartan generators:

$$K_a^N E_c^b=q_a^{N(\delta_b^a-\delta_c^a)}E_c^b K_a^N, \tag{11}$$

that is, where b,c are *any* meaningful indices (i.e., even including the case $b=c$), and $N\in\frac{1}{2}\mathbb{Z}$ is any power.

The proof of our PBW commutator lemma uses these results, and also calls on Lemma 1 of Ref. 3, which we now cite, with some slight notational changes and simplifications:

Lemma 1: Where $a<b$, we have the following two results.

First, if $a,b\neq c,c+1$, then

$$\begin{aligned}&\text{(a)}\quad [E_b^a,E_{c+1}^c]=0,\\ &\text{(b)}\quad [E_a^b,E_c^{c+1}]=0.\end{aligned}\tag{12}$$

Second, if $a\neq c$ or $b\neq c+1$, then

$$\begin{aligned}&\text{(a)}\quad [E_b^a,E_c^{c+1}]=\delta_b^{c+1}K_c\overline{K}_{c+1}E_c^a-\delta_c^a(-)^{[E_c^{c+1}]}E_b^{c+1}\overline{K}_cK_{c+1},\\ &\text{(b)}\quad [E_a^b,E_{c+1}^c]=\delta_a^cK_c\overline{K}_{c+1}E_{c+1}^b-\delta_{c+1}^b(-)^{[E_{c+1}^c]}E_a^c\overline{K}_cK_{c+1}.\end{aligned}\tag{13}$$

C. The algebra antiautomorphism ω

Again following Zhang,[3] we introduce an *ungraded* $U_q[\mathrm{gl}(m|n)]$ algebra antiautomorphism ω, defined for *simple* generators E_b^a by

$$\omega(E_b^a)\triangleq E_a^b,\quad \omega(K_a)\triangleq\overline{K}_a,\quad \omega(q)\triangleq\overline{q},\tag{14}$$

where by $\omega(q)=\overline{q}$, we intend the more intelligible $\omega(q\,\mathrm{Id})=\overline{q}\,\mathrm{Id}$. Declaring ω to be an ungraded antiautomorphism means that we intend

$$\omega(XY)=\omega(Y)\omega(X)\quad\text{and}\quad\omega(X+Y)=\omega(X)+\omega(Y);\tag{15}$$

observe that ω does indeed preserve grading, that is for homogeneous X, we have $[\omega(X)]=[X]$. Then, for homogeneous X,Y, we have, using (2),

$$\omega([X,Y])=[\omega(Y),\omega(X)].\tag{16}$$

The expression $\omega(E_b^a)=E_a^b$ in fact holds for *all* E_b^a; the generalization to nonsimple generators follows from the application of ω to their definition in (1). Moreover, we have immediately from (14) the following useful results:

$$\omega(K_a^N)=\overline{K}_a^N,\quad \omega(q^N)=\overline{q}^N,\quad \omega(q_a^N)=\overline{q}_a^N,\quad \omega(\Delta_a)=-\Delta_a.$$

Zhang goes on to define a set of ''generalized Lusztig automorphisms,'' but we do not require these. In fact, it appears to be impossible to define them consistently for superalgebras (as claimed in Ref. 3), hence invalidating their use in the proof of the PBW commutator lemma.

III. THE PBW COMMUTATOR LEMMA

Using the above machinery, we are now ready to state and prove the $U_q[\mathrm{gl}(m|n)]$ PBW commutator lemma. To whit, we will prove the following, which is slightly different from the original (Lemma 2 of Ref. 3).

Lemma 2: We have the following commutations.

First, (6) *generalizes to the case of nonsimple generators, that is*

$$[E_b^a,E_a^b]=\overline{\Delta}_a(K_a\overline{K}_b-\overline{K}_aK_b)\quad\text{all}\quad a,b.\tag{17}$$

Second, where there are three distinct indices, we have

$$[E_c^a,E_b^c]=\begin{cases}(\mathrm{a}) & \overline{K}_b K_c E_b^a, \quad c<b<a,\\ (\mathrm{b}) & E_b^a K_a \overline{K}_c, \quad c<a<b,\\ (\mathrm{c}) & E_b^a \overline{K}_a K_c, \quad b<a<c,\\ (\mathrm{d}) & K_b \overline{K}_c E_b^a, \quad a<b<c,\end{cases} \tag{18}$$

$$[E_a^c,E_b^c]=[E_c^a,E_c^b]=0, \quad a<c<b \ \text{ or } \ b<c<a, \tag{19}$$

$$[E_a^c,E_b^c]=\begin{cases}(\mathrm{a}) & (-)^{[E_b^c]} q_c E_b^c E_a^c, \quad a<b<c,\\ (\mathrm{b}) & (-)^{[E_a^c]} q_c E_b^c E_a^c, \quad c<a<b,\end{cases}$$
$$E_c^a E_c^b=\begin{cases}(\mathrm{c}) & (-)^{[E_c^b]} q_c E_c^b E_c^a, \quad a<b<c,\\ (\mathrm{d}) & (-)^{[E_c^a]} q_c E_c^b E_c^a, \quad c<a<b.\end{cases} \tag{20}$$

Third, we describe the situation where there are no common indices, where we have $a<b$ *and* $c<d$. *For* $i,j\in\mathbb{N}$, *let* $S(i,j)$ *denote the set* $\{i,i+1,\ldots,j\}$. *Then, if* $S(a,b)$ *and* $S(c,d)$ *are either disjoint or one is totally contained within the other, that is if* $a<c<d<b$. $a<b<c<d$. $c<a<b<d$ *or* $c<d<a<b$, *we have a total of 16 cases*:

$$[E_b^a,E_d^c]=[E_b^a,E_c^d]=[E_a^b,E_d^c]=[E_a^b,E_c^d]=0. \tag{21}$$

More interestingly, if there is some other overlap between the sets $S(a,b)$ *and* $S(c,d)$, *that is if* $a<c<b<d$ *or* $c<a<d<b$, *then we have the eight cases*

$$[E_b^a,E_d^c]=\begin{cases}(\mathrm{a}) & +\Delta_b E_d^a E_b^c, \quad a<c<b<d,\\ (\mathrm{b}) & -\Delta_d E_d^a E_b^c, \quad c<a<d<b,\end{cases}$$
$$[E_a^b,E_c^d]=\begin{cases}(\mathrm{c}) & +\Delta_b E_a^d E_c^b, \quad a<c<b<d,\\ (\mathrm{d}) & -\Delta_d E_a^d E_c^b, \quad c<a<d<b,\end{cases} \tag{22}$$

$$[E_b^a,E_c^d]=\begin{cases}(\mathrm{a}) & -\Delta_b \overline{K}_b K_c E_c^a E_b^d, \quad a<c<b<d,\\ (\mathrm{b}) & +\Delta_d E_b^d E_c^a \overline{K}_a K_d, \quad c<a<d<b,\end{cases}$$
$$[E_a^b,E_d^c]=\begin{cases}(\mathrm{c}) & -\Delta_c E_d^b E_a^c \overline{K}_c K_b, \quad a<c<b<d,\\ (\mathrm{d}) & +\Delta_a \overline{K}_d K_a E_a^c E_d^b, \quad c<a<d<b.\end{cases} \tag{23}$$

In the above, we disagree with the results published in Ref. 3 in several places. First (11) shows that (18a) and (18d) are actually equivalent to the published results

$$[E_c^a,E_b^c]=\begin{cases}(\mathrm{a}) & q_b E_b^a K_c \overline{K}_b, \quad c<b<a,\\ (\mathrm{d}) & \overline{q}_b E_b^a K_b \overline{K}_c, \quad a<b<c.\end{cases}$$

However, for all the commutators involving no common indices, we differ in substance. The published results for (22) are

$$[E_b^a,E_d^c]=+\Delta_b E_d^a E_b^c, \quad a<c<b<d, \quad c<a<d<b,$$

$$[E_a^b,E_c^d]=-\Delta_b E_c^b E_a^d, \quad a<c<b<d, \quad c<a<d<b,$$

and for (23) are

$$[E_b^a,E_c^d]=\begin{cases}\text{(a)} & +\Delta_b E_b^d E_c^a \overline{K}_b K_a, \quad a<c<b<d,\\ \text{(b)} & +\Delta_a E_c^a E_b^d \overline{K}_a K_d, \quad c<a<d<b,\end{cases}$$

$$[E_a^b,E_d^c]=\begin{cases}\text{(c)} & -\Delta_b \overline{K}_a K_b E_a^c E_d^b, \quad a<c<b<d,\\ \text{(d)} & -\Delta_a K_a \overline{K}_d E_d^b E_a^c, \quad c<a<d<b.\end{cases}$$

We mention that it was the discovery of errors in *computations* while working on material described in Ref. 1 that led us to check and correct these PBW results, and consequently rediscover and debug the proof.

Proof of Lemma 2: We prove the components of the lemma in a different order to that in which we state them. This is to ensure consistency as later parts of the proof recycle results previously shown.

(21) These are the 16 commutators involving $a<b$ and $c<d$, with no overlap betwen $S(a,b)$ and $S(c,d)$.

First, in the cases $a<b<c<d$ and $a<c<d<b$, in evaluating $[E_b^a,E_d^c]$, we may use (1) to recursively expand the raising generator E_d^c into a sum of products of simple raising generators, and then apply (3b) until we have a weighted sum of terms all involving commutators of the form $[E_b^a,E_{e+1}^e]$, where $a,b\neq e,e+1$, all of which are necessarily 0 by (12a), thus $[E_b^a,E_d^c]=0$ for these two cases.

Second, swapping $a\leftrightarrow c$ and $b\leftrightarrow d$ in these two cases, and rearranging then yields $[E_b^a,E_d^c]=0$ for the cases $c<d<a<b$ and $c<a<b<d$.

Third, the four cases $[E_b^a,E_c^d]=0$ follow by a similar argument, calling on (13a) rather than (12a).

Last, the remaining eight cases $[E_a^b,E_d^c]=0$ and $[E_a^b,E_c^d]=0$ follow by the application of ω to the first eight cases, and reversing the commutators.

(19) Initially, we show (19a), that is for the case $a<c<b$ we show $[E_a^c,E_b^c]=0$. If in fact $a=c-1$, then the result is already known from (13a), so we assume otherwise, that is we consider the case $a<c-1<c<b$,

$$\begin{aligned}[E_a^c,E_b^c]&\overset{(1)}{=}[E_{c-1}^c E_a^{c-1},E_b^c]-q_{c-1}[E_a^{c-1}E_{c-1}^c,E_b^c]\\ &\overset{(3a)}{=}E_{c-1}^c[E_a^{c-1},E_b^c]+(-)^{[E_a^{c-1}][E_b^c]}[E_{c-1}^c,E_b^c]E_a^{c-1}\\ &\quad -q_{c-1}(E_a^{c-1}[E_{c-1}^c,E_b^c]+(-)^{[E_{c-1}^c][E_b^c]}[E_a^{c-1},E_b^c]E_{c-1}^c)\\ &\overset{(21)}{=}(-)^{[E_a^{c-1}][E_b^c]}[E_{c-1}^c,E_b^c]E_a^{c-1}-q_{c-1}E_a^{c-1}[E_{c-1}^c,E_b^c]\overset{(13a)}{=}0.\end{aligned}$$

Swapping $a\leftrightarrow b$ and reversing the commutator then yields $[E_a^c,E_b^c]=0$ for the case $b<c<a$. Taking ω of these two cases yields $[E_c^a,E_c^b]=0$ for the cases $a<c<b$ and $b<c<a$.

(17) We show the result for $a<b$ using strong mathematical induction, that is, we assume it true for all a',b' such that $|a'-b'|<|a-b|$, and use this to show that it is then necessarily true for our a,b. To this end, we already know from (6) that it is true for $|a-b|=1$. (If $|a-b|\leqslant 1$, the result is already true, indeed trivially so if $a=b$.) To whit, where $a<b$, and $b-a>1$, that is $a<b-1<b$, we have

$$[E_b^a,E_a^b]\overset{(1)}{=}[E_b^a,E_{b-1}^bE_a^{b-1}-q_{b-1}E_a^{b-1}E_{b-1}^b]$$

$$\overset{(3b)}{=}[E_b^a,E_{b-1}^b]E_a^{b-1}+(-)^{[E_b^a][E_{b-1}^b]}E_{b-1}^b[E_b^a,E_a^{b-1}]$$
$$-q_{b-1}[E_b^a,E_a^{b-1}]E_{b-1}^b-(-)^{[E_b^a][E_{b-1}^a]}q_{b-1}E_a^{b-1}[E_b^a,E_{b-1}^b], \tag{24}$$

where the factors $[E_b^a]\equiv[a]+[b]$ within the parity factors are redundant. In (24), we thus require the evaluation of the commutators $[E_b^a,E_{b-1}^b]$ and $[E_b^a,E_a^{b-1}]$. To this end, we have first

$$[E_b^a,E_{b-1}^b]\overset{(13a)}{=}K_{b-1}\overline{K}_bE_{b-1}^a, \tag{25}$$

and second

$$[E_b^a,E_a^{b-1}]\overset{(1)}{=}[E_{b-1}^aE_b^{b-1}-\overline{q}_{b-1}E_b^{b-1}E_{b-1}^a,E_a^{b-1}]$$

$$\overset{(3a)}{=}E_{b-1}^a[E_b^{b-1},E_a^{b-1}]+(-)^{[E_b^{b-1}][E_a^{b-1}]}[E_{b-1}^a,E_a^{b-1}]E_b^{b-1}$$
$$-\overline{q}_{b-1}E_b^{b-1}[E_{b-1}^a,E_a^{b-1}]-\overline{q}_{b-1}(-)^{[E_a^{b-1}]}[E_b^{b-1},E_a^{b-1}]E_{b-1}^a$$

$$\overset{(19)}{=}[E_{b-1}^a,E_a^{b-1}]E_b^{b-1}-\overline{q}_{b-1}E_b^{b-1}[E_{b-1}^a,E_a^{b-1}].$$

Using the strong inductive assumption, we then have

$$[E_b^a,E_a^{b-1}]=\overline{\Delta}_a\begin{pmatrix}(K_a\overline{K}_{b-1}-\overline{K}_aK_{b-1})E_b^{b-1}\\-\overline{q}_{b-1}E_b^{b-1}(K_a\overline{K}_{b-1}-\overline{K}_aK_{b-1})\end{pmatrix}$$
$$\overset{(11)}{=}\overline{\Delta}_aE_b^{b-1}\begin{pmatrix}\overline{q}_{b-1}K_a\overline{K}_{b-1}-q_{b-1}\overline{K}_aK_{b-1}\\-\overline{q}_{b-1}K_a\overline{K}_{b-1}+\overline{q}_{b-1}\overline{K}_aK_{b-1}\end{pmatrix}$$
$$=-\overline{\Delta}_aE_b^{b-1}\overline{K}_aK_{b-1}(q_{b-1}-\overline{q}_{b-1})$$
$$=-\overline{\Delta}(-)^{[a]}\Delta(-)^{[b-1]}E_b^{b-1}\overline{K}_aK_{b-1}$$
$$=-(-)^{[E_a^{b-1}]}E_b^{b-1}\overline{K}_aK_{b-1}. \tag{26}$$

Now substitute (25) and (26) into (24),

$$[E_b^a,E_a^b]=K_{b-1}\overline{K}_bE_{b-1}^aE_a^{b-1}-(-)^{[E_{b-1}^b]}(-)^{[E_a^{b-1}]}E_{b-1}^bE_b^{b-1}K_{b-1}\overline{K}_a$$
$$+(-)^{[E_a^{b-1}]}q_{b-1}E_b^{b-1}K_{b-1}\overline{K}_aE_{b-1}^b-(-)^{[E_a^{b-1}]}q_{b-1}E_a^{b-1}K_{b-1}\overline{K}_bE_{b-1}^a$$
$$=(E_{b-1}^aE_a^{b-1}-(-)^{[E_a^{b-1}]}E_a^{b-1}E_{b-1}^a)K_{b-1}\overline{K}_b-(-)^{[E_b^a]}(E_{b-1}^bE_b^{b-1}$$
$$-(-)^{[E_b^{b-1}]}E_b^{b-1}E_{b-1}^b)K_{b-1}\overline{K}_a$$
$$\overset{(2)}{=}[E_{b-1}^a,E_a^{b-1}]K_{b-1}\overline{K}_b-(-)^{[E_b^a]}[E_{b-1}^b,E_b^{b-1}]K_{b-1}\overline{K}_a$$
$$=\overline{\Delta}_a(K_a\overline{K}_{b-1}-\overline{K}_aK_{b-1})K_{b-1}\overline{K}_b-(-)^{[E_b^a]}\overline{\Delta}_b(K_b\overline{K}_{b-1}-\overline{K}_bK_{b-1})K_{b-1}\overline{K}_a$$

$$= \overline{\Delta}_a(K_a\overline{K}_b - \overline{K}_a K_{b-1}^2\overline{K}_b - K_b\overline{K}_a + \overline{K}_b K_{b-1}^2\overline{K}_a)$$
$$= \overline{\Delta}_a(K_a\overline{K}_b - \overline{K}_a K_b).$$

Thus, we have shown (17) for general $a<b$. The case $a>b$ then follows by swapping $a\leftrightarrow b$ in the above, and rearranging.

(**18**) We first show (18a), that is for the case $c<b<a$,

$$[E_c^a, E_b^c] \overset{(1)}{=} [E_b^a E_c^b, E_b^c] - q_b[E_c^b E_b^a, E_b^c]$$

$$\overset{(3a)}{=} E_b^a[E_c^b, E_b^c] + (-)^{[E_c^b]}[E_b^a, E_b^c]E_c^b - q_b E_c^b[E_b^a, E_b^c] - (-)^{[E_b^a][E_b^c]}q_b[E_c^b, E_b^c]E_b^a$$

$$\overset{(19)}{=} E_b^a[E_c^b, E_b^c] - q_b[E_c^b, E_b^c]E_b^a$$

$$\overset{(17)}{=} \overline{\Delta}_b(E_b^a(K_b\overline{K}_c - \overline{K}_b K_c) - q_b(K_b\overline{K}_c - \overline{K}_b K_c)E_b^a) \overset{(11)}{=} \overline{\Delta}_b(q_b K_b\overline{K}_c - \overline{q}_b\overline{K}_b K_c - q_b K_b\overline{K}_c$$
$$+ q_b\overline{K}_b K_c)E_b^a$$
$$= \overline{K}_b K_c E_b^a.$$

A parallel proof yields (18c) for the case $b<a<c$,

$$[E_c^a, E_b^c] \overset{(1)}{=} [E_c^a, E_a^c E_b^a] - q_a[E_c^a, E_b^a E_a^c]$$

$$\overset{(3b)}{=} [E_c^a, E_a^c]E_b^a + (-)^{[E_c^a]}E_a^c[E_c^a, E_b^a] - q_a[E_c^a, E_b^a]E_a^c - (-)^{[E_c^a][E_b^a]}q_a E_b^a[E_c^a, E_a^c]$$

$$\overset{(19)}{=} [E_c^a, E_a^c]E_b^a - q_a E_b^a[E_c^a, E_a^c]$$

$$\overset{(17)}{=} \overline{\Delta}_a((K_a\overline{K}_c - \overline{K}_a K_c)E_b^a - q_a E_b^a(K_a\overline{K}_c - \overline{K}_a K_c))$$

$$\overset{(11)}{=} \overline{\Delta}_a E_b^a(q_a K_a\overline{K}_c - \overline{q}_a\overline{K}_a K_c - q_a K_a\overline{K}_c + q_a\overline{K}_a K_c) = E_b^a\overline{K}_a K_c.$$

Taking ω of (18a) yields

$$[E_c^b, E_a^c] \overset{(15,16)}{=} E_a^b K_b\overline{K}_c, \quad c<b<a,$$

and swapping $a\leftrightarrow b$ then yields (18b),

$$[E_c^a, E_b^c] = E_b^a K_a\overline{K}_c, \quad c<a<b.$$

Similarly, taking ω of (18c) yields

$$[E_c^b, E_a^c] \overset{(15,16)}{=} K_a\overline{K}_c E_a^b, \quad b<a<c,$$

and swapping $a \leftrightarrow b$ then yields (18d),

$$[E_c^a, E_b^c] = K_b \overline{K}_c E_b^a \quad a < b < c.$$

(**20**) In a sense, these results are really glorified Serre relations. We first prove (20a), that is for the case $a<b<c$. Initially assume that $b \neq c-1$ that is $a<b<c-1<c$. Then we have

$$E_a^c E_b^c \overset{(1)}{=} E_a^c (E_{c-1}^c E_b^{c-1} - q_{c-1} E_b^{c-1} E_{c-1}^c) \overset{(21)}{=} E_a^c E_{c-1}^c E_b^{c-1} - (-)^{[E_b^{c-1}]} q_{c-1} E_b^{c-1} E_a^c E_{c-1}^c. \tag{27}$$

Thus, we must investigate $E_a^c E_{c-1}^c$. To this end, observe that our assumption that $b \neq c-1$ means that we have already assumed that $a \neq c-2$, that is, that we safely have $a<c-2<c-1<c$, hence

$$E_a^c E_{c-1}^c \overset{(1)}{=} (E_{c-2}^c E_a^{c-2} - q_{c-2} E_a^{c-2} E_{c-2}^c) E_{c-1}^c \overset{(21)}{=} E_{c-2}^c E_{c-1}^c E_a^{c-2} - q_{c-2} E_a^{c-2} E_{c-2}^c E_{c-1}^c. \tag{28}$$

So now, we must investigate $E_{c-2}^c E_{c-1}^c$, and this falls into two cases. In the general case, if $c \neq m+1$, the Serre relation of (9c) gives us $E_{c-2}^c E_{c-1}^c = q_{c-1} E_{c-1}^c E_{c-2}^c$. On the other hand, if $c = m+1$, then we have

$$E_{m-1}^{m+1} E_m^{m+1} \overset{(1)}{=} (E_m^{m+1} E_{m-1}^m - q_m E_{m-1}^m E_m^{m+1}) E_m^{m+1} \overset{(8)}{=} E_m^{m+1} E_{m-1}^m E_m^{m+1},$$

$$E_m^{m+1} E_{m-1}^{m+1} \overset{(1)}{=} E_m^{m+1} (E_m^{m+1} E_{m-1}^m - q_m E_{m-1}^m E_m^{m+1}) \overset{(8)}{=} -q_m E_m^{m+1} E_{m-1}^m E_m^{m+1},$$

hence $E_{m-1}^{m+1} E_m^{m+1} = -\overline{q}_m E_m^{m+1} E_{m-1}^{m+1}$. Taken together, we have for *any* c,

$$E_{c-2}^c E_{c-1}^c = (-)^{[E_{c-1}^c]} q_c E_{c-1}^c E_{c-2}^c. \tag{29}$$

Installing (29) into (28), we have

$$\begin{aligned} E_a^c E_{c-1}^c &= (-)^{[E_{c-1}^c]} q_c (E_{c-1}^c E_{c-2}^c E_a^{c-2} - q_{c-2} E_a^{c-2} E_{c-1}^c E_{c-2}^c) \\ &\overset{(21)}{=} (-)^{[E_{c-1}^c]} q_c E_{c-1}^c (E_{c-2}^c E_a^{c-2} - q_{c-2} E_a^{c-2} E_{c-2}^c) \\ &\overset{(1)}{=} (-)^{[E_{c-1}^c]} q_c E_{c-1}^c E_a^c. \end{aligned} \tag{30}$$

Installing (30) into (27), we obtain the required (20a) for the special case $a<b<c-1<c$,

$$\begin{aligned} E_a^c E_b^c &= (-)^{[E_{c-1}^c]} q_c (E_{c-1}^c E_a^c E_b^{c-1} - (-)^{[E_b^{c-1}]} q_{c-1} E_b^{c-1} E_{c-1}^c E_a^c) \\ &\overset{(21)}{=} (-)^{[E_{c-1}^c]} (-)^{[E_b^{c-1}]} q_c (E_{c-1}^c E_b^{c-1} - q_{c-1} E_b^{c-1} E_{c-1}^c) E_a^c \\ &\overset{(1)}{=} (-)^{[E_b^c]} q_c E_b^c E_a^c. \end{aligned}$$

If in fact $b=c-1$, then if also $a \neq c-2$, then (30) covers our result, and if $a=c-2$, then (29) covers it. Together, we have (20a) for all $a<b<c$. A parallel proof covers (20b), that is, the case $c<a<b$; but we omit this. Before proceeding, we condense our notation. We have

$$E^c_a E^c_b = \begin{cases} (-)^{[E^c_b]} q_c E^c_b E^c_a, & a<b<c, \\ (-)^{[E^c_a]} q_c E^c_b E^c_a, & c<a<b. \end{cases}$$

Combining these two results, we may write, for $a<b$,

$$E^c_a E^c_b = (-)^{[E^c_{z(a,b,c)}]} q_c E^c_b E^c_a \quad \text{if } z(a,b,c)\neq c, \tag{31}$$

where $z(a,b,c)$ is a little function which picks out the median element of the set of natural numbers $\{a,b,c\}$. Applying ω to (31) and cross multiplying yields

$$E^a_c E^b_c \overset{(15)}{=} (-)^{[E^{z(a,b,c)}_c]} q_c E^b_c E^a_c \quad \text{if } z(a,b,c)\neq c,$$

which is immediately seen to cover (20c) and (20d),

$$E^a_c E^b_c = \begin{cases} (-)^{[E^b_c]} q_c E^b_c E^a_c, & a<b<c, \\ (-)^{[E^a_c]} q_c E^b_c E^a_c, & c<a<b. \end{cases}$$

(**22**) Beginning with the case $a<c<b<d$, we have

$$[E^a_b, E^c_d] \overset{(2)}{=} E^a_b E^c_d - (-)^{[E^a_b][E^c_d]} E^c_d E^a_b$$

$$\overset{(1)}{=} E^a_b (E^c_b E^b_d - \overline{q}_b E^b_d E^c_b) - (-)^{[E^c_b]} (E^c_b E^b_d - \overline{q}_b E^b_d E^c_b) E^a_b$$

$$= (E^a_b E^c_b E^b_d - (-)^{[E^c_b]} E^c_b E^b_d E^a_b) - \overline{q}_b (E^a_b E^b_d E^c_b - (-)^{[E^c_b]} E^b_d E^c_b E^a_b).$$

Now, for $a<c<b$, by (20c), we have $E^a_b E^c_b = (-)^{[E^c_b]} q_b E^c_b E^a_b$. Installing this, we quickly obtain (22a),

$$[E^a_b, E^c_d] = (-)^{[E^c_b]} E^c_b (q_b E^a_b E^b_d - E^b_d E^a_b) - \overline{q}_b (E^a_b E^b_d - \overline{q}_b E^b_d E^a_b) E^c_b$$

$$\overset{(1)}{=} (-)^{[E^c_b]} q_b E^c_b E^a_d - \overline{q}_b E^a_d E^c_b \overset{(21)}{=} E^a_d E^c_b (q_b - \overline{q}_b) = \Delta_b E^a_d E^c_b.$$

Swapping $a \leftrightarrow c$ and $b \leftrightarrow d$ in (22a) then yields

$$[E^c_d, E^a_b] = \Delta_d E^c_b E^a_d, \quad c<a<d<b. \tag{32}$$

Reversing both the commutator and the RHS product yields

$$-(-)^{[E^c_d][E^a_b]} [E^a_b, E^c_d] \overset{(21)}{=} (-)^{[E^c_b][E^a_d]} \Delta_d E^a_d E^c_b,$$

but for $c<a<d<b$, in fact $[E^c_d][E^a_b] = [E^c_b][E^a_d] = [E^a_d]$, yielding (22b),

$$[E^a_b, E^c_d] = -\Delta_d E^a_d E^c_b, \quad c<a<d<b.$$

Next, applying ω to (22a) yields

$$[E^d_c, E^b_a] \overset{(15,16)}{=} -\Delta_b E^b_c E^d_a, \quad a<c<b<d.$$

Reversing both the commutator and the RHS product yields (22c),

$$[E_a^b,E_c^d] \overset{(21)}{=} \Delta_b E_a^d E_c^b, \quad a<c<b<d.$$

Last, applying ω to (32) yields (22d),

$$[E_a^b,E_c^d] \overset{(15,16)}{=} -\Delta_d E_a^d E_c^b, \quad c<a<d<b.$$

(**23**) We first show (23a), that is for the case $a<c<b<d$. We have

$$\begin{aligned}
[E_b^a,E_c^d] &\overset{(1)}{=} [E_b^a,E_b^d E_c^b] - q_b[E_b^a,E_c^b E_b^d] \\
&\overset{(3b)}{=} [E_b^a,E_b^d]E_c^b + (-)^{[E_b^d][E_b^a]} E_b^d [E_b^a,E_c^b] - q_b([E_b^a,E_c^b]E_b^d + (-)^{[E_b^a][E_c^b]} E_c^b [E_b^a,E_b^d]) \\
&\overset{(19)}{=} E_b^d [E_b^a,E_c^b] - q_b [E_b^a,E_c^b] E_b^d \\
&\overset{(18d)}{=} E_b^d K_c \overline{K}_b E_c^a - q_b K_c \overline{K}_b E_c^a E_b^d \\
&\overset{(11,21)}{=} -\Delta_b \overline{K}_b K_c E_c^a E_b^d .
\end{aligned}$$

Applying ω to (23a) yields

$$[E_d^c,E_a^b] \overset{(15,16)}{=} \Delta_b E_d^b E_a^c \overline{K}_c K_b, \quad a<c<b<d, \tag{33}$$

and swapping $a \leftrightarrow c$ and $b \leftrightarrow d$ then yields (23b),

$$[E_b^a,E_c^d] = \Delta_d E_b^d E_c^a \overline{K}_a K_d, \quad c<a<d<b.$$

Next, reversing the commutator in (33) yields

$$[E_a^b,E_d^c] \overset{(16)}{=} -(-)^{[E_a^b][E_d^c]} \Delta_b E_d^b E_a^c \overline{K}_c K_b .$$

However, for the case $a<c<b<d$, we have $[E_a^b][E_d^c]=[E_c^b]$, thus, $(-)^{[E_a^b][E_d^c]}\Delta_b = (-)^{[E_c^b]}(-)^{[b]}\Delta = (-)^{[c]}\Delta = \Delta_c$, yielding (23c),

$$[E_a^b,E_d^c] = -\Delta_c E_d^b E_a^c \overline{K}_c K_b, \quad a<c<b<d.$$

Last, applying ω to (23c) yields

$$[E_c^d,E_b^a] \overset{(15,16)}{=} \Delta_c \overline{K}_b K_c E_c^a E_b^d, \quad a<c<b<d,$$

and then swapping $a \leftrightarrow c$ and $b \leftrightarrow d$ yields (23d),

$$[E_a^b,E_d^c] = \Delta_a \overline{K}_d K_a E_a^c E_d^b, \quad c<a<d<b.$$

□

IV. DISCUSSION

Of some interest is that we may use our PBW commutator lemma to show that (8) in fact generalizes to the nonsimple odd generators, that is

$$(E_b^a)^2=0,$$

for any indices a, b such that $[a]\neq[b]$. The proof of this statement is left as an (easy) exercise involving (20).

Now that it is established, we may concentrate the notation of our lemma—this is useful for encoding purposes.

The entirety of (19) and (20) may be summarized by

$$E_c^a E_c^b=\kappa E_c^b E_c^a \quad \text{and} \quad E_a^c E_b^c=\kappa E_b^c E_a^c, \quad \text{any} \quad a\neq b\neq c,$$

where

$$\kappa \triangleq \begin{cases} 1 & \text{if } z(a,b,c)=c, \\ (-)^{[E_c^{z(a,b,c)}]}\overline{q}_c^{s_b^a} & \text{otherwise} \end{cases}$$

and where $z(a,b,c)$ is our little function which picks out the median element of the set of three distinct natural numbers $\{a,b,c\}$. (The 1 factor follows as $[E_c^a][E_c^b]=0$ for c strictly between a and b.)

The entirety of (21) to (23) may be summarized by

$$[E_b^a,E_d^c]=\begin{cases} +\Delta_b E_d^a E_b^c, & a<c<b<d, \\ -\Delta_d E_d^a E_b^c, & c<a<d<b, \\ +\Delta_a E_b^c E_d^a, & b<d<a<c, \\ -\Delta_c E_b^c E_d^a, & d<b<c<a, \\ -\Delta_b \overline{K}_b K_d E_d^a E_b^c, & a<d<b<c, \\ +\Delta_c E_b^c E_d^a \overline{K}_a K_c, & d<a<c<b, \\ -\Delta_c E_d^a E_b^c \overline{K}_c K_a, & b<c<a<d, \\ +\Delta_b \overline{K}_d K_b E_b^c E_d^a, & c<b<d<a, \\ 0, & a\neq b\neq c\neq d \ \text{otherwise.} \end{cases}$$

Finally, we mention that the consistency (if not the veracity) of our lemma is also supported by extensive computer tests using MATHEMATICA. By this, we mean that we confirm that

$$\texttt{NormalOrder}(XY)=\texttt{NormalOrder}(\texttt{ExpandNS}(XY)), \tag{34}$$

for a range of $U_q[\mathrm{gl}(m|n)]$ nonsimple generators X, Y, where $\texttt{NormalOrder}(X)$ is a function which renders X in a normal form, and $\texttt{ExpandNS}(X)$ is a function which recursively expands all nonsimple generators in X, using (1).

To be more specific, let the *height* of generator $X\equiv E_b^a$ be $|a-b|$; this is a measure of its distance from simplicity. For $U_q[\mathrm{gl}(m|n)]$, it varies from 0 (for Cartan generators), to 1 (for simple non-Cartan generators); and then for the nonsimple generators from a minimum of 2 to a maximum of $m+n-1$ for the maximally nonsimple E_1^{m+n} and E_{m+n}^1.

Then, we confirm that our code satisfies (37), for all $U_q[\mathrm{gl}(m|n)]$ generators X,Y of height at most $m+n-1$ for all m,n such that $m+n\leqslant 5$; at most 3 for $m+n\leqslant 10$; and at most 2 for $m+n\leqslant 18$. The computational expense in performing these checks rises at least exponentially with

height, so we have to abandon our calculations at this point. However, our results do amount to a complete consistency check of our lemma, for all $U_q[\mathrm{gl}(m|n)]$ such that $m+n\leqslant 5$.

ACKNOWLEDGMENTS

I am grateful to Rui Bin Zhang and David McAnally for advice on issues related to this proof. The bulk of the work for this paper was carried out in the year 2000, while I was a Postdoctoral Fellow at Kyoto University in Japan (funded by a Postdoctoral Fellowship for Foreign Researchers # P99703, provided by the Japan Society for the Promotion of Science). Domo arigato gozaimashita! The last algebraic details were worked out in October 2001, while my mind was pacified somewhat by doing Hatha Yoga at Sri Ved Niketan Ashram at Rishikesh, India. Dhanyabad! Editing was later performed in March 2002, while I was a guest of Ebadollah Mahmoodian of Sharif University of Technology in Tehran, Iran. Motashakkeram! Last-minute edits were made in July 2002, while I was a guest of Karin van Dijk in Deventer, The Netherlands. Dank u wel!

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On certain geometric aspects of CP^N harmonic maps

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(Received 25 September 2002; accepted 10 October 2002)

A Weierstrass-type system of equations corresponding to CP^N harmonic maps is presented. It constitutes a generalization of the previously constructed systems for CP^1 and CP^2 fields. From the linear spectral problem for the CP^N model a set of conserved quantities is derived and used for a construction of a generalized Weierstrass representation for conformally parametrized surfaces immersed in multidimensional Euclidean spaces. Based on this representation a possible geometrical interpretation of CP^N harmonic maps is discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1528272]

I. INTRODUCTION

Recently many studies have been performed of various σ models in low dimensions. Of these, σ models in two spatial dimensions have, perhaps, been the most commonly studied as, on one hand, they lead to interesting generalizations of harmonic maps and on the other, they can be treated as analogs, with many properties in common, of four-dimensional non-Abelian gauge theories.

Among two-dimensional σ models perhaps the most interesting ones, from the topological point of view, are the so-called CP^N sigma models. Their classical solutions are examples of topological solitons, i.e., extended structures whose stability is partially guaranteed by topological considerations.

The CP^N models are, in fact, a generalization of the, perhaps the s mplest, sigma model, namely the S^2 model—also called the vector $O(3)$ model. The CP^N models involve maps from R^2, or S^2 if one wants to have a nontrivial topology, to CP^N, i.e.,

$$CP^N: C \supset \Omega \ni \zeta = \zeta_1 + i\zeta_2 \mapsto z = (z^1, \ldots, z^N) \in S^{2N} \cong \mathrm{SU}(N)/\mathrm{SU}(N-1), \tag{1}$$

where the homogeneous coordinates $z = (z^1, \ldots, z^N)$ have the following properties

$$z \sim z' = \lambda z \quad \text{for } \lambda \neq 0.$$

Exploiting projective invariance we can require that

$$z^\dagger \cdot z = 1, \tag{2}$$

holds, where † denotes the Hermitian conjugation, and we are still left with gauge symmetry

$$z \sim z' = z e^{i\phi}, \tag{3}$$

where ϕ is the real-valued function.

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It is easiest to define CP^N models in terms of the Lagrangian density[1]

$$L=\tfrac{1}{4}(D_\mu z)^\dagger\cdot D_\mu z,\quad z^\dagger\cdot z=1, \tag{4}$$

where the covariant derivatives D_μ act on $z:S^2\to CP^N$ according to the formula

$$D_\mu z=\partial_\mu z-(z^\dagger\cdot\partial_\mu z)z. \tag{5}$$

Here the index $\mu=1,2$ denotes ζ_1 and ζ_2. Note that the covariant derivatives $D_\mu z$ transform under gauge (3)

$$D_\mu z\to D_\mu z'=(D_\mu z)e^{i\phi}, \tag{6}$$

so that the dependence on phase ϕ drops out of Lagrangian density (4) and hence the model is really based on CP^N. The total Lagrangian is given by

$$\mathcal{L}=\int L\,d\zeta\,d\overline{\zeta} \tag{7}$$

and if the CP^N model is defined over S^2 we require that $\mathcal{L}$ is finite.

For the CP^N sigma model it is convenient to define

$$z=\frac{f}{|f|}, \tag{8}$$

where we have used the following notation $|f|=(f^\dagger\cdot f)^{1/2}$. In terms of f the Lagrangian (7) becomes

$$\mathcal{L}=\int\frac{|\overline{\partial}f|^2+|\partial f|^2}{|f|^4}d\zeta\,d\overline{\zeta}, \tag{9}$$

where $|\partial f|^2=(\partial f)^\dagger\cdot(\partial f)$ and $|\overline{\partial}f|^2=(\overline{\partial}f)^\dagger\cdot\overline{\partial}f$. The Euler Lagrange equations for f take the form

$$\left(1-\frac{f\otimes f^\dagger}{|f|^2}\right)\left[\partial\overline{\partial}f-\partial f\frac{(f^\dagger\cdot\overline{\partial}f)}{|f|^2}-\overline{\partial}f\frac{(f^\dagger\cdot\partial f)}{|f|^2}\right]=0, \tag{10}$$

where we have introduced holomorphic and antiholomorphic derivatives

$$\partial=\frac{\partial}{\partial(\zeta_1+i\zeta_2)}=\frac{\partial}{\partial\zeta},\quad \overline{\partial}=\frac{\partial}{\partial(\zeta_1-i\zeta_2)}=\frac{\partial}{\partial\overline{\zeta}} \tag{11}$$

and a bar denotes the complex conjugation.

As is well known[2] equation (10) can be written as a compatibility condition for a set of two linear spectral equations for a N component auxiliary vector Ψ

$$\begin{aligned}\partial\Psi&=\frac{2}{1+\lambda}[\partial P,P]\Psi,\\ \overline{\partial}\Psi&=\frac{2}{1-\lambda}[\overline{\partial}P,P]\Psi,\end{aligned} \tag{12}$$

where λ is a spectral parameter and the N by N matrix P is the projector given by

$$P=\frac{1}{|f|^2}f\otimes f^\dagger,\quad P^\dagger=P,\quad P^2=P. \tag{13}$$

The compatibility conditions for (12) are,

$$[\partial\overline{\partial}P, P]=0 \tag{14}$$

which, as can be easily checked, are equivalent to equations (10). Note that (14) can be written in the form of a conservation law

$$\partial[\overline{\partial}P, P]+\overline{\partial}[\partial P, P]=0 \tag{15}$$

or, equivalently, using the tracelessness of matrix K

$$\partial K-\overline{\partial}K^{\dagger}=0, \tag{16}$$

where the matrices K and $K^{\dagger}$ are given by

$$K=[\overline{\partial}P, P]=\frac{\overline{\partial}f\otimes f^{\dagger}-f\otimes\overline{\partial}f^{\dagger}}{|f|^2}+\frac{f\otimes f^{\dagger}}{|f|^4}[(\overline{\partial}f^{\dagger}\cdot f)-(f^{\dagger}\cdot\overline{\partial}f)], \quad \operatorname{tr}K=0, \tag{17}$$

and consequently

$$K^{\dagger}=-[\partial P, P]=-\frac{\partial f\otimes f^{\dagger}-f\otimes\partial f^{\dagger}}{|f|^2}+\frac{f\otimes f^{\dagger}}{|f|^4}[(\partial f^{\dagger}\cdot f)-(f^{\dagger}\cdot\partial f)].$$

Note that due to the invariance of the Lagrangian (4) under gauge (3), without loss of generality, we can set one of the components of the vector field f, say f_1, to 1. Then, in the CP^1 case, all quantities are expressible through one variable

$$w=\frac{f_2}{f_1}=f_2 \tag{18}$$

and the Euler Lagrange equations (10) take the form

$$\partial\overline{\partial}w-\frac{2\overline{w}}{(1+|w|^2)}\partial w\overline{\partial}w=0. \tag{19}$$

Recently, a lot of effort has been put into relating CP^1 maps to the solutions of the Weierstrass problem.[3,6] In this case one considers a system of first order equations (of Dirac type) for two complex fields φ and ψ of the form

$$\partial\psi=p\varphi, \quad \overline{\partial}\varphi=-p\psi, \quad p=|\varphi|^2+|\psi|^2. \tag{20}$$

In Ref. 7 it was shown that solutions of the Weierstrass system (20) are in a one to one correspondence with the solutions of the CP^1 sigma eqution (19). If ψ and φ are solutions of the Weierstrass system (20), then the function w, defined by

$$w=\frac{\psi}{\overline{\varphi}}, \tag{21}$$

is a solution of the CP^1 equations (19). The converse is also true.[6] Thus, if w is a solution of (19), then the functions φ and ψ of the Weierstrass system (20) have the form (up to an overall multiplication of φ and ψ by -1)

$$\psi=w\frac{(\overline{\partial}\overline{w})^{1/2}}{1+|w|^2}, \quad \varphi=\frac{(\partial w)^{1/2}}{1+|w|^2}, \quad p=\frac{|\partial w|}{1+|w|^2}. \tag{22}$$

From the Weierstrass system (20) one can construct three conservation laws (15). These, in turn, allow us to determine four real valued quantities $X_i(\zeta,\overline{\zeta})$, three of which are linearly independent (due to the tracelessness of the matrix K). X_i are constructed by taking diagonal and off-diagonal entries of matrix K and are given by[3]

$$X_1=\int_\gamma(\psi_1^2-\psi_2^2)d\zeta'+(\overline{\psi}_1^2-\overline{\psi}_2^2)d\overline{\zeta}',$$

$$X_2=\int_\gamma(\psi_1^2+\psi_2^2)d\zeta'-(\overline{\psi}_1^2+\overline{\psi}_2^2)d\overline{\zeta}', \tag{23}$$

$$X_3=-\int_\gamma\psi_1\psi_2\,d\zeta'+\overline{\psi}_1\overline{\psi}_2\,d\overline{\zeta}',$$

respectively, where γ is any curve from a fixed point to ζ.

The geometrical aspects of surfaces obtained from representation (23), where functions ψ and φ obey the Weierstrass system (20), are described in detail in Ref. 4. In two recent papers[8,9] we have generalized this construction to the case of the CP^2 sigma model.[5] The aim of this paper is to present a generalization to the CP^N case.

The paper is organized as follows. In Sec. II, we derive the explicit form of conservation laws corresponding to the CP^N model. Section III deals with CP^N maps and the corresponding Weierstrass representation for conformally parametrized two-dimensional surfaces immersed in multidimensional Euclidean space. In Sec. IV we discuss some geometric aspects of CP^N maps and present some geometric characteristics of surfaces. The last section presents further remarks, discusses some possible developments and mentions some more ambitious objectives.

II. THE CP^N MODEL

Here we derive explicit conservation laws (15) which are equivalent to the Euler Lagrange equations (10). In order to construct them we look first at the general form of the elements of the matrices K and $K^\dagger$ in terms of f, given by (17). Thus we have

$$K_{ij}=\frac{1}{A^2}[\overline{f}_k f_k\,\overline{\partial}f_i\,\overline{f}_j-\overline{f}_k f_k f_i\,\overline{\partial f_j}+f_i\,\overline{f}_j\,\overline{\partial f_k}\,f_k-f_i\,\overline{f}_j\,\overline{f}_k\,\overline{\partial}f_k], \tag{24}$$

and consequently

$$K^\dagger_{ij}=\frac{-1}{A^2}[\overline{f}_k f_k\,\partial f_i\,\overline{f}_j-\overline{f}_k f_k f_i\,\partial\overline{f}_j+f_i\,\overline{f}_j\,\partial\overline{f}_k\,f_k-f_i\,\overline{f}_j\,\overline{f}_k\,\partial f_k],$$

where $A=f^\dagger\cdot f$ and the summation convention over the repeated indices from now on, is assumed throughout this paper.

Let us define

$$F_{ij}=f_i\,\partial f_j-f_j\partial f_i,$$

and

$$G_{ij}=f_i\,\overline{\partial}f_j-f_j\overline{\partial}f_i. \tag{25}$$

Then, using expressions (25), the matrices K and $K^\dagger$ take, equivalently, a simple form

$$K_{ij}=\overline{f}_j\overline{\Phi}_i^2-f_i\overline{\varphi}_j^2, \tag{26}$$

and

$$K_{ij}^{\dagger}=-\overline{f}_j\varphi_i^2-f_i\Phi_j^2, \tag{27}$$

where we have introduced

$$\varphi_i^2=\frac{1}{A^2}\overline{f}_k F_{ki}, \tag{28}$$

and

$$\Phi_i^2=\frac{1}{A^2}f_k\overline{G_{ki}}. \tag{29}$$

Note that from equations (25), (28), and (29) we have two algebraic constraints, namely

$$\overline{f}_k\,\varphi_k^2=0, \quad f_k\,\Phi_k^2=0, \tag{30}$$

which imply that only $(N-1)$ functions φ_i^2 are linearly independent. So in our further discussion it is convenient to take as indepedent functions $\varphi_2^2,\ldots,\varphi_N^2$. Analogous situation holds for functions Φ_i^2. Making use of the symmetry (3) we can set, without loss of generality, say, $f_1=1$, and so we end up with the expressions [for (28) and (29)]

$$\varphi_i^2=\frac{1}{A^2}[(1+f_k\overline{f}_k)\,\partial f_i-f_i(\overline{f}_k\,\partial f_k)],$$

$$\Phi_i^2=\frac{1}{A^2}[(1+f_k\overline{f}_k)\,\overline{\partial} f_i-f_i(\overline{f}_k\,\overline{\partial} f_k)], \quad i=2,\ldots,N, \tag{31}$$

where

$$A=1+|f_2|^2+|f_3|^2\ldots+|f_N|^2,$$

and all the sums over repeated indices run over $k=2,\ldots,N$. Note that in (31) the terms $k=i$ in the sum cancel leaving just term ∂f_i. For instance if $k=i=2$ then we have

$$\varphi_2^2=\frac{1}{A^2}[(1+f_l\overline{f}_l)\,\partial f_2-f_2(\overline{f}_l\,\partial f_l)],$$

where the sums over the repeated indices run over $l=3,\ldots,N$. This fact allows us to invert expressions (31) and so express all derivatives ∂f_i in terms of φ_i^2's and f_i. This way we find

$$\partial f_i=A\,[\varphi_i^2+f_i\,\overline{f}_k\varphi_k^2]. \tag{32}$$

Thus, in particular, for the CP^1 case, equation (32) becomes

$$\partial f_2=A^2\varphi_2^2, \quad A=1+|f_2|^2,$$

and f_2 is often denoted in Ref. 1 by w, while in the CP^2 case we have

$$\partial f_2=A[(1+|f_2|^2)\varphi_2^2+f_2\overline{f}_3\,\varphi_3^2],$$

$$\partial f_3=A[(1+|f_3|^2)\varphi_3^2+f_3\overline{f}_2\,\varphi_2^2], \tag{33}$$

$$A=1+|f_2|^2+|f_3|^2.$$

Note that in Refs. 8 and 9 the functions f_2 and f_3 are denoted by w_1 and w_2, respectively. Similarly, all this discussion can be repeated for Φ_i^2's in the same way but using $\overline{\partial}$ instead of ∂, $\overline{f}$ instead of f, and $\overline{G}_{ij}$ instead of F_{ij}.

III. THE GENERALIZED WEIERSTRASS REPRESENTATION IN R^M

To introduce a generalized Weierstrass system in multidimensional spaces we need a set of φ_i and ψ_i which generalize the φ and ψ of the CP^1 case and φ_i and ψ_i, $i=1,2$ of the CP^2 case.

Note that the quantities φ_i^2, $i=2,...,N$, defined in (28) provide such a choice as (32) agrees with the definition of the function φ in expression (22). Next we address the question of what should we use for the function ψ_i? Clearly, relation (21) suggests that we put

$$\psi_i = f_i\,\overline{\varphi}_i \tag{34}$$

with no summation over the indices $i=2,\ldots,N$. Then to complete the generalization of the Weierstrass system in multidimensional spaces we need analogs of relations (20). We need to prescribe the first derivatives $\overline{\partial}\varphi_i$ and $\partial\psi_i$ in terms of φ_i and ψ_i. Note that from (34) we get

$$\partial\psi_i = \partial(f_i\,\overline{\varphi}_i) = \partial f_i\,\overline{\varphi}_i + f_i\,\overline{(\overline{\partial}\varphi_i)}. \tag{35}$$

So we need to specify $\overline{\partial}\varphi_i$ in terms of φ_i, f_i and their derivatives. To do this we note that from (32) we get

$$\varphi_i^2 = \frac{1}{A}\,\partial f_i - f_i\frac{f^\dagger\cdot\partial f}{A^2}, \quad A=(f^\dagger\cdot f+1). \tag{36}$$

So we have

$$\overline{\partial}\varphi_i^2 = 2\,\frac{f_i(\overline{f_l}\,\partial f_l)}{A^3}(\overline{f_k}\,\overline{\partial}f_k + f_k\,\overline{\partial f_k}) + \frac{1}{A^2}[(1+|f|^2)\partial\overline{\partial}f_i - (\overline{f_k}\overline{\partial}f_k)\partial f_i - (f_k\overline{\partial f_k})\partial f_i - \overline{\partial}f_i(\overline{f_k}\partial f_k)$$
$$- f_i(\overline{\partial f_k}\partial f_k) - f_i(\overline{f_k}\,\partial\overline{\partial}f_k)]. \tag{37}$$

However, equation (10) gives us

$$\partial\overline{\partial}f_i = f_i\frac{(\overline{f_k}\,\partial\overline{\partial}f_k)}{A} + \partial f_i\frac{(\overline{f_k}\,\overline{\partial}f_k)}{A} + \overline{\partial}f_i\frac{(\overline{f_k}\,\partial f_k)}{A} - 2\,f_i\frac{(\overline{f_k}\,\partial f_k)(\overline{f_l}\,\overline{\partial}f_l)}{A^2}. \tag{38}$$

Eliminating the second derivatives $\partial\overline{\partial}f_i$ from equations (37) and (38) we note that all the terms involving the first derivatives $\overline{\partial}f$ and $\partial\overline{f}$ in (37) cancel and we end up with a simple expression

$$\overline{\partial}\varphi_i = -\frac{\varphi_i}{2A}(f_k\,\overline{\partial f_k}) - \frac{f_i}{2\varphi_i A^2}(\overline{\partial f_k}\partial f_k) + \frac{f_i}{2\varphi_i A^3}(\overline{\partial f_k}f_k)(\overline{f_l}\partial f_l). \tag{39}$$

Moreover, taking the complex conjugation of (32),

$$\overline{\partial f_k} = A\,[\overline{\varphi}_k^2 + \overline{f_k}\,f_l\overline{\varphi}_l^2] \tag{40}$$

and so by the virtue of (40) we have

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\} \tag{41}$$

(no summation over i). The second pair of equations for ψ_i then follows from (35)

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)] \tag{42}$$

(no summation over i).

To summarize: the modified Weierstrass system in multidimensional space is a set of $(2N-2)$ complex functions φ_i and ψ_i, $i=2,3,\ldots,N$ which obey the following system of equations (no summation over i):

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\}$$

and

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)], \tag{43}$$

where

$$A = 1 + \sum_{k=2}^{N}\frac{|\psi_k|^2}{|\varphi_k|^2}.$$

From our construction it is clear that the above system of equations is equivalent to the equations of the CP^N sigma model (10). Moreover, it is easy to check that the system of equations (43), for $N=1$ reduces to the equations (20), and for $N=2$ to the equations which were studied in Refs. 8 and 9.

Note that under the requirement of finiteness of the action all solutions of the CP^N sigma model (10) are well known[1] and they split into three separate cases: analytic, antianalytic and the mixed ones. Hence based on this result we can construct large classes of solutions of the modified Weierstrass system (43).

IV. GEOMETRICAL ASPECTS

Here we address the question of the existence of real variables Z_i, of ζ and $\overline{\zeta}$, which are constructed out of our ψ_i's and φ_i's determined by the system of equations (43). Here we treat $Z_i(\zeta,\overline{\zeta})$ as a map of C into R^M

$$Z = (Z_1,\ldots,Z_M): D\subset C\to R^M, \tag{44}$$

where D is a region in the complex plane C. For some values of M we can give a geometrical interpretation of two-dimensional surfaces immersed in R^M. This discussion will generalize the result obtained by Konopelchenko and colaborators.[3,4,10] Moreover, we will find that the surface is immersed in $M=(N^2-1)$-dimensional Euclidean space. To construct real valued functions $Z_i(\zeta,\overline{\zeta})$ it is convenient to exploit the conservation laws for the system of equations (43). To derive these conservation laws we look at (16) and we note that we can exploit the matrices K and $K^\dagger$ given by (26) and (27). However, we note that we can drop the terms Φ_j^2 in expressions (26) and (27) and we still have the conservation laws associated with (10). Namely, we can define

$$K'_{ij} = -f_i\,\overline{\varphi}_j^2 \tag{45}$$

and

$$(K'_{ij})^\dagger = \varphi_i^2\,\overline{f}_j, \tag{46}$$

and we still have the conservation laws of the form

$$\partial K' + \overline{\partial}(K')^{\dagger} = 0. \tag{47}$$

It is easy to check the validity of (47) by making use of the equations (40) and (41).

Note that as our conservation laws do not involve terms containing Φ_i then they can be written entirely in terms of Weierstrass variables φ_i and ψ_i. As a result of so obtained conservation laws we can introduce real valued functions

$$Z_{ll} = \int_\gamma \overline{f}_l \varphi_l^2 \, d\zeta + \int_\gamma f_l \, \overline{\varphi}_l^2 \, d\overline{\zeta} = \int_\gamma \overline{\psi}_l \varphi_l \, d\zeta + \int_\gamma \psi_l \, \overline{\varphi}_l \, d\overline{\zeta} \tag{48}$$

(no summation over index $l=1,\ldots,N$). These quantities have been constructed from the diagonal entries of matrices K' and $(K')^{\dagger}$. From the off-diagonal entries of matrices K' and $(K')^{\dagger}$ we can construct

$$Z_{lk} = X_{lk} + iY_{lk} = \int_\gamma (\alpha \overline{f}_l \varphi_k^2 + \overline{\alpha} \overline{f}_k \varphi_l^2) d\zeta + \int_\gamma (\overline{\alpha} f_l \, \overline{\varphi}_k^2 + \alpha f_k \, \overline{\varphi}_l^2) d\overline{\zeta}, \quad \alpha \in C. \tag{49}$$

The transposition of the indices lk to kl in Eq. (49) corresponds to the interchange α to $\overline{\alpha}$ and vice versa. In our expression we take all $l,k=1,\ldots,N$ and for $k=1$ or $l=1$ we can use our algebraic constraints (30) to rewrite all our expressions in terms of independent functions φ_i and ψ_i, $i=2,\ldots,N$. For our real variables Z_i we take Z_{ii}, X_{lk} and Y_{lk}.

Note that the conservation laws (47) guarantee that Z_{ll} and Z_{lk} do not depend on the choice of the contour γ but only on its endpoints in C. This fact takes place because all Z's can be written in the form

$$Z = \int_\Gamma F(\zeta,\overline{\zeta}) \, d\zeta + \overline{F}(\zeta,\overline{\zeta}) \, d\overline{\zeta},$$

where F and $\overline{F}$ satisfy the conserved quantity

$$\overline{\partial} F = \partial \overline{F},$$

which shows that the integrands are total derivatives.

Looking at the diagonal terms in (48) we note that

$$\sum_l Z_{ll} = 0. \tag{50}$$

This follows from the tracelessness of matrices K' and $(K')^{\dagger}$.

Note that all our expressions for Z_{ll} and Z_{lk} are quadratic in terms of φ_i and $\overline{\psi_i}$ and their complex conjugates. They formally include φ_1 and ψ_1, with $\psi_1 = f_1 \overline{\varphi_1}$. However, both these quantities (ψ_1 and φ_1) should be eliminated using the algebraic constraint [i.e., the first expression in (30)] and $f_1=1$. It is easy to check that this process of elimination, in the CP^1 case leads to

$$Z_{11} = -2 \int_\gamma \overline{\psi}\varphi \, d\zeta' + \psi\overline{\varphi} \, d\overline{\zeta}',$$

$$X_{12} = \int_\gamma (\overline{\psi}_2^2 - \varphi_2^2) \, d\zeta' + (\psi_2^2 - \overline{\varphi}_2^2) \, d\overline{\zeta}', \tag{51}$$

$$Y_{12} = i \int_\gamma (\overline{\psi}_2^2 + \varphi_2^2) \, d\zeta' - (\psi_2^2 + \overline{\varphi}_2^2) \, d\overline{\zeta}',$$

which appeared in Ref. 3.

Next, following Ref. 11 we can calculate some geometric characteristics of a surface immersed in multidimensional space. We treat the functions Z_{ll}, X_{lk}, and Y_{lk}, as the coordinates of a surface. We introduce the components of the induced metric

$$g_{\alpha\beta}=\sum_{lk}\frac{\partial Z_{lk}}{\partial\alpha}\frac{\partial\overline{Z}_{lk}}{\partial\beta}, \tag{52}$$

where α and β are ζ or $\overline{\zeta}$. For conformally parametrized surfaces we have to make a choice for the normalization of the off-diagonal entries of coordinates X_{kl} and Y_{kl}. We make the natural choice $\alpha=(1+i)/2$. We find that

$$g_{\zeta\zeta}=\left(\sum_{i=1}^{N}\overline{f}_i\,\varphi_i^2\right)^2=0 \tag{53}$$

which coincides with the first algebraic contraint (30). Similarly, its respective complex conjugate equation is

$$g_{\overline{\zeta}\overline{\zeta}}=0. \tag{54}$$

The only nonzero term of the induced metric is

$$g_{\zeta\overline{\zeta}}=(1+|f_2|^2+|f_3|^2+\cdots+|f_N|^2)\left[\left|\sum_{k=2}^{N}\overline{f}_k\varphi_k^2\right|^2+|\varphi_2|^4+|\varphi_3|^4+\cdots+|\varphi_N|^4\right]. \tag{55}$$

Of course, we can rewrite this expression to involve Weierstrass data φ_i and ψ_i by using expressions (34) but the expressions become very complicated. Note, however, that writing all quantities in terms of f_i and ∂f_i, through (31), our expressions simplify considerably and we obtain

$$g_{\zeta\overline{\zeta}}=|Dz|^2, \tag{56}$$

where $D=\frac{1}{2}(D_1-iD_2)$ and D_1, D_2 are the covariant derivatives given by (5) involving ∂ (i.e., evaluated with respect to ζ).

In the special case of the CP^1 maps the component of the induced metric $g_{\zeta\overline{\zeta}}$ takes a particularly simple form; it is given by

$$g_{\zeta\overline{\zeta}}=\left(1+\frac{|\psi_2|^2}{|\varphi_2|^2}\right)[|\varphi_2|^4+|\psi_2|^2|\varphi_2|^2]=[|\psi_2|^2+|\varphi_2|^2]^2=\frac{|\partial f_2|^2}{(|f_2|^2+1)^2} \tag{57}$$

which is exactly, of course $|Dz|^2$; while in the CP^2 case we have

$$g_{\zeta\overline{\zeta}}=\frac{|\partial f_2|^2+|\partial f_3|^2+|f_2\partial f_3-f_3\partial f_2|^2}{(1+|f_2|^2+|f_3)^2|} \tag{58}$$

which also is $|Dz|^2$.

Thus we have proved that the conformal immersion of surfaces in R^{N^2-1} are determined by the generalized Weierstrass representation (48) and (49), where the functions φ_l and ψ_l, or equivalently φ_l and f_l, have to obey system (43) of first order equations. Note that formulas (48) and (49) define a surface on SU(N) and then using expressions in Ref. 12 we can calculate, in a closed form, all geometric characteristics of this surface.

V. SUMMARY AND CONCLUDING REMARKS

The main aim of this paper has been to derive a generalization of the Weierstrass system to the CP^N case. Thus we have found a set of $2N$ complex functions ψ_i and φ_i which satisfy a system of first order equations (43) that are equivalent to the full system of equations of the CP^N model (10).

We have also introduced a set of (N^2-1) real quantities Z's, which can be treated as coordinates of a surface immersed in R^{N^2-1} and we have shown that the induced metric of our map is given by

$$ds^2 = 2|Dz|^2\, d\zeta\, d\overline{\zeta}. \tag{59}$$

The study of the generalized Weierstrass representations for surfaces immersed in multidimensional spaces was initiated by Konopelchenko *et al.*[10] Our work here, in which we adopted an alternative approach based on CP^N sigma models, provides a generalization of their results.

A question arises whether our approach can be extended to Weierstrass systems describing surfaces immersed in multidimensional pseudo-Riemannian spaces. Further, can it provide new classes of solutions which will describe types of surfaces more diverse than those found in multidimensional Euclidean spaces.

ACKNOWLEDGMENTS

One of the authors, A.M.G., would like to thank the University of Durham and the Grey College for the award of Alan Richards fellowship that allowed him to spend two terms in Durham during the academic years 2001 and 2002. Partial support for the work of A.M.G. was provided by a research grant from NSERC of Canada and Fonds FCAR du Gouvernement du Quebec.

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The extended Lotka–Volterra lattice and affine Jacobi varieties of spectral curves

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(Received 6 September 2002; accepted 7 October 2002)

Based on the work by Smirnov and Zeitlin, we study a simple realization of the matrix construction of the affine Jacobi varieties. We find that the realization is given by a classical integrable model, the extended Lotka–Volterra lattice. We investigate the integrable structure of the representative for the gauge equivalence class of matrices, which is isomorphic to the affine Jacobi variety, and make use of it to discuss the solvability of the model. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1527224]

I. INTRODUCTION

Consider an N by N matrix whose matrix elements are polynomials of z of degree $M \in \mathbb{Z}_{>0}$. We write the characteristic equation of the matrix as

$$F(z,w) \equiv w^N - f_1(z)w^{N-1} + f_2(z)w^{N-2} - \cdots + (-1)^N f_N(z) = 0, \tag{1.1}$$

then each $f_i(z)$ satisfies $\deg f_i(z) \leqslant iM$. We assume that the algebraic curve X defined by (1.1) is smooth. The genus of the curve X is $g = \frac{1}{2}(N-1)(MN-2)$.

For the matrix and the curve X, Beauville introduced an isomorphism,[1]

$$\mathcal{M}_F \simeq X(g) - D.$$

Here the left-hand side is the gauge equivalence class $\mathcal{M}_F$ defined as

$$\mathcal{M}_F = \{\mathbf{M}(z) \,|\, \deg(\mathbf{M}(z)_{i,j}) \leqslant M \quad \text{for all } i,j,$$

$$\mathrm{Det}|w\mathbb{1} - \mathbf{M}(z)| = F(z,w)\}/\mathbf{GL}_N(\mathbb{C}),$$

and on the right-hand side we have the set of nontrivial divisors $X(g) = X^g/\mathfrak{S}_g \subset \mathrm{Div}(X)$ where $\mathfrak{S}_g$ is the symmetric group. The last term D is a subset of $X(g)$, where by the Abel transformation D is mapped to a $(g-1)$-dimensional subvariety of the Jacobi variety $J(X)$, which is called the theta divisor Θ. The Abel transformation induces an isomorphism,

$$X(g) - D \simeq J(X) - \Theta,$$

and we call $J(X) - \Theta$ the affine Jacobi variety. In other words, the gauge equivalence class $\mathcal{M}_F$ gives a matrix construction of the affine Jacobi variety. Before Beauville's work, Mumford studied the case that the curve X is a hyperelliptic curve (the $N=2$ case), and introduced a unique representative of the gauge equivalence class.[2]

As discussed in Refs. 1–3, the above correspondence of matrices and Jacobi varieties closely relates to the study of finite dimensional integrable systems. The coefficients of the characteristic equation (1.1) correspond to commuting integrals of motion which generate g independent vector fields on the affine Jacobi variety. These fields determine the time evolution of the divisors in

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$X(g)-D$, which is linearized on the Jacobi variety $J(X)$. Recently Nakayashiki and Smirnov studied Mumford's representative of a 2×2 matrix from the view point of the affine ring for the affine Jacobi variety.[4] They investigated how the commuting integrals act on the polynomial ring generated by the matrix elements, by calculating the cohomology group. The extension of their work to that for integrable $N\times N$ matrices is studied by Smirnov and Zeitlin.[5,6] Starting with an $N\times N$ integrable monodromy matrix, they introduced a unique representative for the gauge equivalence class $\boldsymbol{\mathcal{M}}_F$ which is isomorphic to a divisor in $X(g)-D$. The generalization of Mumford's representative appears in Refs. 6 and 7. We should remark that the way of constructing the divisor from the monodromy matrix is nothing but the separation of variables (SoV) invented by Sklyanin.[8]

The aim of this paper is to study a simple realization of the representative for $\boldsymbol{\mathcal{M}}_F$, based on Ref. 5. For the characteristic equation (1.1) we have assumed

$$f_k(z)=f_k^{(0)}z^{kM}+f_k^{(1)}z^{kM-1}+\cdots+f_k^{(kM)} \quad \text{for } k=1,\ldots,N,$$

and we add a condition

$$f_N^{(0)}=0. \tag{1.2}$$

The realization of the representative is given by the extended Lotka–Volterra lattice (In some papers we call it the Bogoyavlensky lattice.) This is a classical integrable dynamical model defined by $(1+1)$-dimensional differential-difference equation,[9–11]

$$\frac{\mathrm{d}V_n}{\mathrm{d}t}=2V_n\sum_{k=1}^{N-1}(V_{n+k}-V_{n-k}), \tag{1.3}$$

where $V_n\equiv V_n(t)$, $n\in\mathbb{Z}$. In this article we denote this model using LV(N). The integrable structure of LV(N) is based on the Poisson algebra $\mathcal{A}_{\mathrm{LV}}$ generated by V_n, and on the N by N Lax matrix given by[9,11]

$$\tilde{\mathbf{L}}_n(z)=(V_n)^{-1/N}\left(z^{1/N}\mathbf{E}_{1,1}+(-1)^{N-1}V_n\mathbf{E}_{1,N}+\sum_{k=1}^{N-1}\mathbf{E}_{k+1,k}\right). \tag{1.4}$$

Here $z\in\mathbb{C}$ is a spectral parameter and $(\mathbf{E}_{i,j})_{m,n}=\delta_{m,i}\delta_{n,j}$. The Lax matrix composes the monodromy matrix which generates a family of commuting integrals of motion. This proves the integrability of the model in Liouville's sense.[11] It is remarkable that the model has an integrable quantization which can be applied to construct the vertex model linked on the crystal base theory.[12] In this paper, we study LV(N) of a periodic boundary condition, which gives a realization of the representative of $\boldsymbol{\mathcal{M}}_F$ introduced in Ref. 5. For the case of $N=2$ our realization is essentially the same as that introduced in Ref. 13, and the previous article gives what corresponds to its generalization. Based on some special properties of the correspondence of LV(N) and the representative, we try to solve LV(N) by describing the dynamical variables V_n (1.3) in terms of the divisor in $X(g)-D$.

The plan of this paper is as follows; in Sec. II, starting with LV(N) we construct a monodromy matrix $\overline{\mathbf{T}}(z)$ whose matrix elements have a special form of polynomials of z, and whose characteristic equation is (1.1) with (1.2). By applying the method SoV we obtain a divisor in $X(g)-D$. In Sec. III, following Ref. 5 we review the gauge transformation which derives the representative of $\boldsymbol{\mathcal{M}}_F$, $\mathbf{M}_F(z)$, from $\overline{\mathbf{T}}(z)$. We let $\mathcal{A}_{M_F}$ be the Poisson algebra for the polynomial ring generated by the coefficients of the matrix elements of the representative $\mathbf{M}_F(z)$. Next we investigate some nice properties of this gauge transformation; the transformation does not change the zeros of the separating equation (2.16), and erases the zero mode B_0. These assure the injection from a divisor to the representative. After eliminating the center of $\mathcal{A}_{M_F}$, a family of nontrivial integrals for $\mathcal{A}_{M_F}$ is composed of g independent variables. These integrals govern the

evolution of the divisor, which is linearized on $J(X)$. In Sec. IV, we investigate LV(N) by making use of the results in Sec. III. We show that the center of $\mathcal{A}_{M_F}$ is a subset of the center for $\mathcal{A}_{\mathrm{LV}}$, and the nontrivial integrals of motion of both algebras coincide. Our claims are that the representative $\mathbf{M}_F(z)$ can be written in terms of the dynamical variable V_n, and that the structure of $\mathbf{M}_F(z)$ has a close relationship with the solvability of LV(N). The last section, Sec. V, is devoted to summary and remarks. We mention the quantization of LV(N) and propose some future problems.

II. SPECTRAL CURVE OF LV(N) AND DIVISOR

A. Derivation of a proper monodromy matrix

We study the integrable structure of LV(N), and derive a monodromy matrix of a special form which fits to the construction in Ref. 5.

We consider the dynamical system (1.3) with a periodic boundary condition $V_{n+L}=V_n$, and set $L=N(N-1)M$, $M\in\mathbb{Z}_{>0}$ for later convenience. The Hamiltonian structure of LV(N) is defined by the Poisson brackets

$$\{V_n,V_m\}=2V_mV_n\sum_{k=1}^{N-1}(\delta_{m,n+k}-\delta_{m,n-k}), \tag{2.1}$$

and the Hamiltonian $H_1=\Sigma_{n=1}^{L}V_n$.[9] We let $\mathcal{A}_{\mathrm{LV}}$ be the Poisson algebra for $\mathbb{C}[V_n,V_n^{-1};n\in\mathbb{Z}]$, whose defining relations are given by (2.1). After a variable transformation[12]

$$V_n=(P_nP_{n+1}\cdots P_{n+N-1})^{-1}Q_n^{-1}Q_{n+N-1}, \tag{2.2}$$

(2.1) is transformed into the Poisson brackets

$$\{P_n,\ Q_m\}=\delta_{n,m}P_nQ_n,\quad \{P_n,\ P_m\}=\{Q_n,\ Q_m\}=0, \tag{2.3}$$

where P_n and Q_n are canonical variables. Using these variables we apply a gauge transformation to the Lax matrix (1.4), $\mathbf{L}_n(z)=\mathbf{\Omega}_{n+1}(z)\tilde{\mathbf{L}}_n(z)\mathbf{\Omega}_n(z)^{-1}$, and obtain the following *local* Lax matrix:

$$\mathbf{L}_n(z)=z^{1/N}\left(P_n\mathbf{E}_{1,1}+Q_n\mathbf{E}_{1,2}+\frac{1}{z}(-1)^{N-1}Q_n^{-1}\mathbf{E}_{N,1}+\sum_{k=2}^{N-1}\mathbf{E}_{k,k+1}\right). \tag{2.4}$$

See Appendix A for the concrete description of the gauge matrix $\mathbf{\Omega}_n(z)$. We introduce another Lax matrix,

$$\overline{\mathbf{L}}_n(z)=(\mathbf{L}_n^{-1}(z))^T=\frac{1}{z^{1/N}}\left(Q_n^{-1}\mathbf{E}_{1,2}+\sum_{k=2}^{N-1}\mathbf{E}_{k,k+1}+z(-1)^{N-1}Q_n\mathbf{E}_{N,1}+z(-1)^{N-2}P_n\mathbf{E}_{N,2}\right), \tag{2.5}$$

where the superscript T denotes a transposition of the matrices. Note that $\mathrm{Det}\,\mathbf{L}_n(z)=\mathrm{Det}\,\overline{\mathbf{L}}_n(z)=1$. These Lax matrices satisfy the Poisson relations as

$$\begin{aligned}
\{\mathbf{L}_n(z)\overset{\otimes}{,}\mathbf{L}_m(z')\}&=\delta_{n,m}[\mathbf{r}(z/z'),\ \mathbf{L}_n(z)\otimes\mathbf{L}_n(z')],\\
\{\overline{\mathbf{L}}_n(z)\overset{\otimes}{,}\overline{\mathbf{L}}_m(z')\}&=\delta_{n,m}[-\mathbf{r}(z'/z),\ \overline{\mathbf{L}}_n(z)\otimes\overline{\mathbf{L}}_n(z')],\\
\{\mathbf{L}_n(z)\overset{\otimes}{,}\overline{\mathbf{L}}_m(z')\}&=\delta_{n,m}[-\mathbf{r}^{T_2}(z/z'),\ \mathbf{L}_n(z)\otimes\overline{\mathbf{L}}_n(z')],
\end{aligned} \tag{2.6}$$

where $\mathbf{r}(z)$ is a classical r-matrix,

$$\mathbf{r}(z)=\frac{z+1}{z-1}\sum_{k=1}^{N}\mathbf{E}_{k,k}\otimes\mathbf{E}_{k,k}+\frac{2}{z-1}\sum_{1\leqslant j<k\leqslant N}(\mathbf{E}_{k,j}\otimes\mathbf{E}_{j,k}+z\mathbf{E}_{j,k}\otimes\mathbf{E}_{k,j}).$$

In deriving the second Poisson relation in (2.6), we have used $\mathbf{r}(z/z')^{T_1T_2}=-\mathbf{r}(z'/z)$, where T_i denotes a transposition in the ith space. Now the meaning of the *local* Lax matrix becomes clear that the Lax matrices (2.4) and (2.5) satisfy the Poisson relations with $\delta_{n,m}$.

We define two monodromy matrices,

$$\mathbf{T}(z)=\overset{\curvearrowleft}{\prod_{k=1}^{L}}\mathbf{L}_k(z),\quad \overline{\mathbf{T}}(z)=\overset{\curvearrowleft}{\prod_{k=1}^{L}}\overline{\mathbf{L}}_k(z).$$

Due to (2.6) the monodromy matrices satisfy the following Poisson relations:

$$\{\mathbf{T}(z)\overset{\otimes}{,}\mathbf{T}(z')\}=[\mathbf{r}(z/z'),\ \mathbf{T}(z)\otimes\mathbf{T}(z')], \tag{2.7}$$

$$\{\overline{\mathbf{T}}(z)\overset{\otimes}{,}\overline{\mathbf{T}}(z')\}=[-\mathbf{r}(z'/z),\ \overline{\mathbf{T}}(z)\otimes\overline{\mathbf{T}}(z')], \tag{2.8}$$

$$\{\mathbf{T}(z)\overset{\otimes}{,}\overline{\mathbf{T}}(z')\}=[-\mathbf{r}^{T_2}(z/z'),\ \mathbf{T}(z)\otimes\overline{\mathbf{T}}(z')]. \tag{2.9}$$

The first relation denotes that the commuting integrals of motion for LV(N) are generated by Tr $\mathbf{T}(z)$, since the Hamiltonian H_1 is obtained by expanding Tr $\mathbf{T}(z)$ by z. Latter two denote that the matrix $\overline{\mathbf{T}}(z)$ also generate the commuting integrals of motion for LV(N).

The matrix elements of $\mathbf{T}(z)$ and $\overline{\mathbf{T}}(z)$ turn out to be polynomials of z, and these matrices have forms as

$$\mathbf{T}(z)=\mathbf{T}_-(z)+\mathbf{T}_0(z)+z\mathbf{T}_+(z), \tag{2.10}$$

$$\overline{\mathbf{T}}(z)=z\overline{\mathbf{T}}_-(z)+\overline{\mathbf{T}}_0(z)+\overline{\mathbf{T}}_+(z). \tag{2.11}$$

Here $\mathbf{T}_\pm(z)$, $\overline{\mathbf{T}}_\pm(z)$ are upper/lower triangular matrices without diagonal terms, and $\mathbf{T}_0(z)$, $\overline{\mathbf{T}}_0(z)$ are diagonal matrices. All matrix elements of $\mathbf{T}_\pm(z)$ and $\mathbf{T}_0(z)$ are polynomials of degree $M(N-1)-1$ but $(\mathbf{T}_0(z))_{1,1}$ which has a polynomial of degree $M(N-1)$. On the other hand, elements of $\overline{\mathbf{T}}_0(z)$ are degree M except for $(\overline{\mathbf{T}}_0(z))_{1,1}$ which is degree $M-1$, and $\overline{\mathbf{T}}_\pm(z)$ has polynomials of degree $M-1$.

We find that the matrix $\overline{\mathbf{T}}(z)$ has the characteristic equation, $\mathrm{Det}|w\mathbb{1}-\overline{\mathbf{T}}(z)|=0$, which coincides with (1.1) of (1.2) and satisfies $f_N(z)=1$. Moreover, the construction of the matrix $\overline{\mathbf{T}}(z)$ (2.11) and its Poisson relation (2.8) are exactly the same as those discussed in Ref. 5 where the Poisson relation (2.8) defines what is called *the classical algebra of observables* generated by the coefficients of polynomials which compose the matrix. Therefore we conclude that LV(N) gives a realization of the algebra of observables. In the following, unless we give a notification, we let $\overline{\mathbf{T}}(z)$ be a matrix of a special form (2.11) whose Poisson structure is given by (2.8) and forget about the model LV(N).

B. Separation of variables and divisor

We apply SoV method to obtain the eigenvalues of the monodromy matrix $\overline{\mathbf{T}}(z)$ algebraically, following Refs. 6, 14, and 15. This method gives a surjective map from the monodromy matrix $\overline{\mathbf{T}}(z)$ to a divisor on the curve X.

Divide the matrix $\overline{\mathbf{T}}(z)$ into parts as

$$\overline{\mathbf{T}}(z)=\begin{pmatrix} a(z) & \vec{b}(z) \\ \vec{c}(z)^T & \mathbf{d}(z) \end{pmatrix}, \tag{2.12}$$

where $a(z)=(\overline{\mathbf{T}}(z))_{1,1}$, $\vec{b}(z)$, and $\vec{c}(z)$ are low vectors of $N-1$ entries, and $\mathbf{d}(z)$ is an $N-1$ by $N-1$ matrix. We transform $\overline{\mathbf{T}}(z)$ as

$$\mathbf{U}(z)=\mathbf{K}\overline{\mathbf{T}}(z)\mathbf{K}^{-1}, \quad \mathbf{K}=\mathbb{1}+\sum_{j=1}^{N-2} k_i \mathbf{E}_{i+1,N},$$

where $k_i \in \mathbb{C}$. On the matrix $\mathbf{U}(z)$ we impose some conditions,

$$(\mathbf{U}(z))_{i,N}=0 \quad \text{for } i=1,\ldots,N-1. \tag{2.13}$$

One sees that these conditions reduce to

$$\vec{b}(z)\cdot\vec{x}^T=0, \quad \vec{x}_i\mathbf{d}(z)\cdot\vec{x}^T=0 \quad \text{for } i=1,\ldots,N-2, \tag{2.14}$$

where $\vec{x}$, $\vec{x}_i \in \mathbb{C}^{N-1}$ are low vectors,

$$\vec{x}_i=(0,\ldots,0,1,0,\ldots,0,k_i), \quad \vec{x}=(-k_1,-k_2,\ldots,-k_{N-2},1).$$

These vectors satisfy $\vec{x}_i \perp \vec{x}$ for all i, then the vectors $\vec{x}_i$ compose basis of the plane normal to $\vec{x}$. Since the vector $\vec{b}(z)$ is also orthogonal to $\vec{x}$, it can be uniquely written as

$$\vec{b}(z)=\sum_{i=1}^{N-2} \lambda_i \vec{x}_i, \quad \lambda_i \in \mathbb{C}.$$

By using (2.14), we have $\vec{b}(z)\mathbf{d}(z)\cdot\vec{x}^T=0$ which enables to write $\vec{b}(z)\mathbf{d}(z)$ as a linear combination of $\vec{x}_i$ again. By repeating this procedure, we obtain $\vec{b}(z)\mathbf{d}^k\cdot\vec{x}^T=0$ for $k\in\mathbb{Z}_{\geqslant 0}$. Since $\vec{x}$ is not a zero vector, the condition (2.14) finally reduces to[6]

$$B(z)\equiv \mathrm{Det}\begin{pmatrix} \vec{b}(z) \\ \vec{b}(z)\mathbf{d}(z) \\ \vec{b}(z)\mathbf{d}(z)^2 \\ \vdots \\ \vec{b}(z)\mathbf{d}(z)^{N-2} \end{pmatrix}=0. \tag{2.15}$$

By the construction of $\overline{\mathbf{T}}(z)$, $B(z)$ becomes a polynomial of z of degree g,

$$B(z)=B_0\prod_{i=1}^{g}(z-z_i). \tag{2.16}$$

The Poisson relation (2.8) ensures that all z_i and B_0 are Poisson commutative to each other. For each z_i the eigenvalue of the matrix $\mathbf{U}(z)$, $w_i\equiv(\mathbf{U}(z_i))_{N,N}$, is obtained as

$$w_i = \mathrm{Det}\begin{pmatrix} b(z_i) \\ b(z_i)\mathbf{d}(z_i) \\ \vdots \\ b(z_i)\mathbf{d}(z_i)^{N-3} \\ \vec{\xi}\mathbf{d}(z_i) \end{pmatrix} \mathrm{Det}\begin{pmatrix} b(z_i) \\ b(z_i)\mathbf{d}(z_i) \\ \vdots \\ b(z_i)\mathbf{d}(z_i)^{N-3} \\ \vec{\xi} \end{pmatrix}^{-1},$$

where $\vec{\xi}$ is a low vector of $N-1$ entries, $\vec{\xi}=(0,\ldots,0,1)$. The Poisson relation (2.8) shows that the separated variables, w_i and z_i $(i=1,\ldots,g)$, satisfy the canonical Poisson brackets,

$$\{z_i,z_j\}=\{w_i,w_j\}=0, \quad \{z_i,w_j\}=2\delta_{i,j}z_i w_i,$$

and B_0 is a zero mode,

$$\{B_0,z_i\}=0, \quad \{B_0,w_i\}=-B_0 w_i.$$

We conclude that via SoV we get the map from the matrix $\overline{\mathbf{T}}(z)$ to a divisor over X, $P=\Sigma_{i=1}^{g}[(w_i,z_i)]$, as each pair of separated variables (w_i,z_i) is a point on the curve X. We assume that (2.16) has different zeros, $z_i \neq z_j$ for all $i \neq j$, and that no point (w_i,z_i) coincides with the ramification points of the map from X to $\mathbb{P}^1$. These assumptions assure $P \in X(g)-D$.

III. INTEGRABLE MONODROMY MATRIX AND AFFINE JACOBI VARIETY

A. Representative of $\mathcal{M}_F$

Let $\{\overline{\mathbf{T}}(z)\}_F$ be a set of matrices with a form (2.11) and whose characteristic equations coincide with (1.1). In the preceding section SoV defines a surjective map from the set $\{\overline{\mathbf{T}}(z)\}_F$ to a certain set of divisors $P \in X(g)-D$, but it is not an injective map. One easily sees the reason by comparing their dimensions, namely $\{\overline{\mathbf{T}}(z)\}_F$ and $X(g)-D$, respectively, have $(g+N-1)$-dimension and g-dimension as affine spaces. Smirnov and Zeitlin introduced a representative of $\mathcal{M}_F$ by setting a gauge transformation which eliminate the excessive dimension $N-1$ of $\{\overline{\mathbf{T}}(z)\}_F$. Following Ref. 5, we review the way to introduce the representative of $\mathcal{M}_F$.

For the matrix $\overline{\mathbf{T}}(z)$ we set

$$\overline{\mathbf{T}}(z)=\boldsymbol{\mu}_0 z^M+\boldsymbol{\mu}_1 z^{M-1}+\cdots+\boldsymbol{\mu}_M, \tag{3.1}$$

and define $\vec{\nu}=\vec{e}_1\cdot\boldsymbol{\mu}_1$ where $\vec{e}_i$ is a N-dimensional low vector whose entries are zero but ith is 1. The gauge transformation from the monodromy matrix $\overline{\mathbf{T}}(z)$ to the representative of $\mathcal{M}_F$, $\mathbf{M}_F(z)$, is

$$\mathbf{M}_F(z)=\mathbf{S}\overline{\mathbf{T}}(z)\mathbf{S}^{-1}, \quad \text{where } \mathbf{S}=\begin{pmatrix} \vec{e}_1 \\ \vec{\nu}\boldsymbol{\mu}_0^{N-2} \\ \vdots \\ \vec{\nu}\boldsymbol{\mu}_0 \\ \vec{\nu} \end{pmatrix}. \tag{3.2}$$

Then we obtain $\mathbf{M}_F(z)$ as

$$\mathbf{M}_F(z)=\mathbf{U}z^M+O(z^{M-1}), \quad \mathbf{U}=\sum_{k=1}^{N} m^{(k)}\mathbf{E}_{2,k}+\sum_{k=3}^{N}\mathbf{E}_{k,k-1}, \tag{3.3}$$

where $m^{(k)}$ are given by

$$m^{(1)}=(-1)^N \mathrm{Det}\begin{pmatrix} \vec{\nu} \\ \vec{e}_2\boldsymbol{\mu}_0 \\ \vec{e}_3\boldsymbol{\mu}_0 \\ \vdots \\ \vec{e}_N\boldsymbol{\mu}_0 \end{pmatrix}, \quad z^{N-1}-\sum_{k=2}^{N} m^{(k)}z^{N-k}=\prod_{k=2}^{N}(z-(\boldsymbol{\mu}_0)_{k,k})).$$

Especially we have

$$(\mathbf{M}_F(z))_{1,N}=z^{N-1}+O(z^{N-2}), \quad (\mathbf{M}_F(z))_{1,i}=O(z^{N-2}), \quad \text{for } i=1,\ldots,N-1.$$

The set $\{\overline{\mathbf{T}}(z)\}_F$ is transformed to $\{\mathbf{M}_F(z)\}$, and one sees that $\{\mathbf{M}_F(z)\}$ is a g-dimensional affine space.

Under the gauge transformation (3.2), the zeros of $B(z)$ (2.16) are invariant and the zero mode B_0 is canceled (see Appendix B for the proof);

$$B(z)\mapsto B_F(z)=(-)^{1/2(N-1)(N-2)}\prod_{k=1}^{g}(z-z_k).$$

Therefore a divisor $P=\Sigma_{i=1}^{g}[(w_i,z_i)]$ determines $B_F(z)$ uniquely. In conclusion, we get the isomorphism, $\boldsymbol{\mathcal{M}}_F\simeq X(g)-D$, where the representative $\mathbf{M}_F(z)$ concretely gives the matrix construction of the affine Jacobi variety.

B. Integrable system on the Jacobi variety

Let us see how the integrable structure of the monodromy matrix $\overline{\mathbf{T}}(z)$ is translated to that of the matrix $\mathbf{M}_F(z)$. Via (3.2), the Poisson structure of the matrix elements of $\overline{\mathbf{T}}(z)$ (2.8) induces the Poisson algebra $\mathcal{A}_{M_F}$ generated by the matrix elements of $\mathbf{M}_F(z)$. For the defining relation of $\mathcal{A}_{M_F}$, see the last part of Sec. II in Ref. 5 and take its classical limit. We study a commuting family of integrals of motion for $\mathcal{A}_{M_F}$ without referring to the defining relation of $\mathcal{A}_{M_F}$.

From (2.8), one obtains

$$\{\mathrm{Det}\,\overline{\mathbf{T}}(z)\overset{\otimes}{,}\overline{\mathbf{T}}(z')\}=0, \tag{3.4}$$

$$\{\mathrm{Det}(w\mathbb{1}-\overline{\mathbf{T}}(z)),\mathrm{Det}(w'\mathbb{1}-\overline{\mathbf{T}}(z'))\}=0. \tag{3.5}$$

Equation (3.4) denotes that $\mathrm{Det}\,\overline{\mathbf{T}}(z)$ is Poisson commutative with all elements of $\overline{\mathbf{T}}(z')$, namely $\mathrm{Det}\,\overline{\mathbf{T}}(z)$ belongs to the center of $\mathcal{A}_{M_F}$, $\mathcal{A}^0_{M_F}$. Equation (3.5) assures that the variables $f_k^{(j)}$ compose a commutative subalgebra of $\mathcal{A}_{M_F}$, $\{f_k^{(j)},f_{k'}^{(j')}\}=0$. Therefore, the dynamical system in $\mathcal{A}_{M_F}$ has a family of integrals of motion, $\{f_k^{(j)}|k=1,\ldots,N-1,\ j=0,\ldots,kM\}$, whose number is $g+2(N-1)$. In the following we show that $2(N-1)$ integrals, $f_k^{(0)}$ and $f_k^{(kM)}$, $k=1,\ldots,N-1$, belong to $\mathcal{A}^0_{M_F}$, namely the number of nontrivial integrals of motion is g. What we should show is

$$\{f_k^{(j)}\overset{\otimes}{,}\mathbf{M}_F(z)\}=0, \quad \text{for } k=1,\ldots,N-1 \quad \text{and } j=0,kM. \tag{3.6}$$

One sees that since $f_k(z)$ can be written in terms of $t_k(z)\equiv\mathrm{Tr}(\overline{\mathbf{T}}(z))^k$,

$$f_1(z)=t_1(z), \quad f_2(z)=\tfrac{1}{2}(t_1(z)^2-t_2(z)), \quad \text{etc.},$$

(3.6) are reduced to

$$\{t_k^{(j)\otimes}, \mathbf{M}_F(z)\} = 0, \quad \text{for } j = 0, kM. \tag{3.7}$$

Here we denote the dominant terms of $\mathrm{Tr}(\overline{\mathbf{T}}(z))^k$ in the $z \to 0, \infty$ limits using $t_k^{(kM)}$, $t_k^{(0)}$, respectively. The Poisson relation (2.8) reduces to

$$\{t_k(z)^{\otimes}, \overline{\mathbf{T}}(z')\} = \mathrm{Tr}_1\{(\overline{\mathbf{T}}(z))^{k\otimes}, \overline{\mathbf{T}}(z')\} = k\,\mathrm{Tr}_1[\mathbf{r}(z/z'), (\overline{\mathbf{T}}(z))^k \otimes \overline{\mathbf{T}}(z')],$$

which derives

$$\{t_k^{(j)\otimes}, \overline{\mathbf{T}}(z')\} = k[(\mathbf{K}^{(j)})^k, \overline{\mathbf{T}}(z')],$$

$$\{t_k^{(j)\otimes}, \vec{\nu}\} = -k\vec{\nu}(\mathbf{K}^{(j)})^k, \tag{3.8}$$

$$\{t_k^{(j)\otimes}, \boldsymbol{\mu}_0\} = k[(\mathbf{K}^{(j)})^k, \boldsymbol{\mu}_0],$$

for $j = 0, kM$. Here we use the matrices $\boldsymbol{\mu}_k$ (3.1) and

$$\mathbf{K}^{(0)} = \mathrm{diag}[0, (\boldsymbol{\mu}_0)_{2,2}, \ldots, (\boldsymbol{\mu}_0)_{N,N}],$$

$$\mathbf{K}^{(kM)} = -\mathrm{diag}[0, (\boldsymbol{\mu}_M)_{2,2}, \ldots, (\boldsymbol{\mu}_M)_{N,N}].$$

Due to the relations (3.8) we get

$$\{t_k^{(i)\otimes}, \mathbf{S}\} = -k(\mathbf{S} - \mathbf{E}_{1,1})(\mathbf{K}^{(i)})^k, \quad \text{for } i = 0, kM, \tag{3.9}$$

and (3.7) is proved.

We arrange the nontrivial integrals as

$$f_1^{(1)}, \ldots, f_1^{(M-1)}, f_2^{(1)}, \ldots, f_2^{(2M-1)}, \ldots, f_{N-1}^{(1)}, \ldots, f_{N-1}^{(M(N-1)-1)},$$

and number them in order,

$$\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_g. \tag{3.10}$$

In conclusion, we obtain the integrable structure of $\mathcal{A}_{M_F}$ that the g commuting integrals $\mathcal{H}_i$ describe the time evolution for $\mathcal{O} \in \mathcal{A}_{M_F}$;

$$\frac{\partial \mathcal{O}}{\partial \tau_i} \equiv \{\mathcal{H}_i, \mathcal{O}\} \quad \text{for } i = 1, \ldots, g. \tag{3.11}$$

On the Jacobi variety $J(X)$, $\mathcal{H}_i$ generate the invariant vector field where the time evolution of the image of the divisor P is linearized. By the inverse map of the Abel transformation, we get z_i as functions of times τ_i, $z_i = z_i(\tau_1, \ldots, \tau_g)$ once the initial values $z_i(0, \ldots, 0) = z_i^0$ is given. Note that the curve X is determined by the eigenvalues of $\mathcal{H}_i$.

IV. DESCRIPTION OF THE LV(N)

Now we study the realization of $\mathbf{M}_F(z)$ given by LV(N). Since the characteristic equation (1.1) is invariant under the gauge transformation, the commuting family can be written in terms of the dynamical variables of LV(N) by making use of the Lax matrix $\tilde{\mathbf{L}}_n(z)$ (1.4). We introduce variables $\mathcal{P}_k$ and $\mathcal{P}'_k$,

$$\mathcal{P}_0=\prod_{n=1}^{L}(V_n)^{-1/N},$$

$$\mathcal{P}_k=\prod_{n=1}^{NM}(V_{(N-1)n+k}) \quad \text{for } k=1,\ldots,N-1,$$

$$\mathcal{P}'_k=\prod_{n=1}^{(N-1)M}(V_{Nn+k}) \quad \text{for } k=1,\ldots,N.$$

These variables constitute the center of $\mathcal{A}_{\mathrm{LV}}$, $\mathcal{A}^0_{\mathrm{LV}}$. Note that not all of them are independent, and the generators of $\mathcal{A}^0_{\mathrm{LV}}$ are obtained by choosing any $2(N-1)$ variables from $\{\mathcal{P}_{k\geqslant 1},\mathcal{P}'_k\}$. The direct calculations show that the elements of $\mathcal{A}^0_{M_F}$ are written in terms of these variables as

$$f_N(z)=\mathrm{Det}\,\overline{\mathbf{T}}(z)=1,$$

$$f^{(0)}_{N-1}=\mathcal{P}_0,$$

$$f^{(0)}_1=\mathcal{P}_0^{-1}(\mathcal{P}_1^{-1}+\cdots+\mathcal{P}_{N-1}^{-1}),$$

$$f^{(N-1)M}_{N-1}=\mathcal{P}_0(\mathcal{P}'_1+\cdots+\mathcal{P}'_N),$$

$$f^{(N-1)M}_1=\mathcal{P}_0^{-1}(\mathcal{P}_1'^{-1}+\cdots+\mathcal{P}_N'^{-1}),$$

and that other elements, $f^{(0)}_k$, $f^{(kM)}_k$ for $k=2,\ldots,N-2$, are obtained from the above. Therefore we see $\mathcal{A}^0_{M_F}\subset\mathcal{A}^0_{\mathrm{LV}}$, and the nontrivial integrals of motion for LV(N) have one-to-one correspondence to $\mathcal{H}_i$.

Based on the above observation, we conjecture that

(i) the matrix $\mathbf{M}_F(z)$ can be written in terms of V_n, namely $\mathcal{A}_{M_F}\subset\mathcal{A}_{\mathrm{LV}}$,

(ii) then all zeros of $B_F(z)$ are given by $V_n, z_i=z_i(\{V_n\})$, and we can *solve* LV(N) as

$$V_n=V_n(\mathcal{P}_k,\mathcal{P}'_k,\mathcal{H}_i;z_i).$$

To discuss the conjecture, using (A1) and (3.2) we rewrite $\mathbf{M}_F(z)$ as

$$\mathbf{M}_F(z)=\mathbf{S}(\mathbf{\Omega}_1(z)^{-1})^T((\tilde{\mathbf{L}}_L(z)\cdots\tilde{\mathbf{L}}_1(z))^{-1})^T\mathbf{\Omega}_1(z)^T\mathbf{S}^{-1}. \tag{4.1}$$

Due to the construction of the gauge matrix $\mathbf{\Omega}_1(z)$ (A2), we reduce (4.1) to

$$\mathbf{M}_F(z)=\tilde{\mathbf{S}}\mathbf{X}(z)^{-1}((\tilde{\mathbf{L}}_L(z)\cdots\tilde{\mathbf{L}}_1(z))^{-1})^T\mathbf{X}(z)\tilde{\mathbf{S}}^{-1}. \tag{4.2}$$

We have conjectured by (i) that the matrix $\tilde{\mathbf{S}}$ is written in terms of V_n. Remember that LV(N) has $N(N-1)M$ dynamical variables V_n. Once we accept (i), (ii) follows (i) since we have enough number of relations to describe V_n in terms of $\mathcal{P}_k$, $\mathcal{P}'_k$, $\mathcal{H}_i$, and z_i. Actually we have g relation equations between z_i and V_n, g nontrivial integrals of motion $\mathcal{H}_i$, and $2(N-1)$ independent

generators of $\mathcal{A}^0_{\mathrm{LV}}$, whose summation coincides with $N(N-1)M$. It should be remarked that due to the periodic boundary condition of the system, we essentially have the translation invariance such as $\mathcal{P}_1=\cdots=\mathcal{P}_{N-1}$ and $\mathcal{P}'_1=\cdots=\mathcal{P}'_N$.

In the following, we study the cases of $N=2,3$ which illustrate the correspondence of LV(N) and the integrable structure on the affine Jacobi variety. We prove the conjecture in the $N=2$ case, and the simplest case of $N=3$. For general N, it seems to be very complicated even to show (i).

$N=2$ case: We have $L=2M$, $g=M-1$, the integrals of motion $\mathcal{H}_i$, $i=1,\ldots,M-1$, and the elements of $\mathcal{A}^0_{\mathrm{LV}}$,

$$\mathcal{P}_1=(\mathcal{P}_0)^{-2}=\prod_{k=1}^{2M} V_k, \quad \mathcal{P}'_1=\prod_{k=1}^{M} V_{2k-1}, \quad \mathcal{P}'_2=\prod_{k=1}^{M} V_{2k}.$$

By definition, we have

$$\mathbf{S}=\begin{pmatrix} 1 & 0 \\ -P_2\cdots P_{L-1}Q_1Q_L^{-1} & P_1\cdots P_{L-1}Q_L^{-1} \end{pmatrix}$$
$$=\begin{pmatrix} 1 & 0 \\ -\mathcal{P}_0V_L & \mathcal{P}_0P_L^{-1}Q_L^{-1} \end{pmatrix},$$

$$\mathbf{B}_1^{-1}=P_1^{1/2}Q_1^{-1/2}\begin{pmatrix} 1 & 0 \\ 0 & P_1^{-1}Q_1 \end{pmatrix},$$

where P_n, Q_n are canonical variables (2.3), and $V_n=(P_nP_{n+1})^{-1}Q_n^{-1}Q_{n+1}$ (2.2). Then (4.1) reduces to (4.2) where the matrix $\tilde{\mathbf{S}}$ is

$$\tilde{\mathbf{S}}=\begin{pmatrix} 1 & 1 \\ 0 & -\mathcal{P}_0V_L \end{pmatrix},$$

which justifies (i).

Let us consider the case of $M=2$, $L=4$, and $g=1$. Now (1.1) becomes

$$w^2-\mathcal{P}_0(z^2-H_1z+\mathcal{P}'_1+\mathcal{P}'_2)w+1=0,$$

where we have three independent integrals of motion,

$$H_1=\sum_{k=1}^{4} V_k, \quad \mathcal{P}'_1=V_1V_3, \quad \mathcal{P}'_2=V_2V_4. \tag{4.3}$$

Due to the translation invariance we set $\mathcal{P}\equiv\mathcal{P}'_1=\mathcal{P}'_2$ which yields $\mathcal{P}_0^2=\mathcal{P}^{-2}$. The polynomial $B_F(z)$ has a zero z_1,

$$z_1=V_1+V_2. \tag{4.4}$$

Here z_1 is a function of τ_1 defined by (3.11) with $\mathcal{H}_1=\mathcal{P}_0H_1$. Finally, the dynamical variables $V_n=V_n(\mathcal{P},\mathcal{H}_1;z_1(\tau_1))$ for $n=1,2,3,4$ are obtained from (4.3) and (4.4).

$N=3$ case: We consider the $L=6$, $M=1$, and $g=1$ case. Now the characteristic equation is

$$w^3+\mathcal{P}_0^2(z(\mathcal{P}_1+\mathcal{P}_2)-(\mathcal{P}'_1\mathcal{P}'_2+\mathcal{P}'_1\mathcal{P}'_3+\mathcal{P}'_2\mathcal{P}'_3))w^2+\mathcal{P}_0(z^2+zH_1+\mathcal{P}'_1+\mathcal{P}'_2+\mathcal{P}'_3)w-1=0,$$

where

$$\mathcal{P}_i = V_i V_{i+2} V_{i+4}, \quad \text{for } i=1,2, \quad \mathcal{P}'_i = V_i V_{i+3} \quad \text{for } i=1,2,3, \quad H_1 = \sum_{k=1}^{6} V_k. \tag{4.5}$$

We set $\mathcal{P}'_i \equiv \mathcal{P}$, and for simplicity consider the case of $\mathcal{P}_i \equiv \mathcal{P}^{3/2}$ and $\mathcal{P}_0 \equiv \mathcal{P}^{-1}$. Then the matrix $\mathbf{M}(z)$ reduces to (4.2) where the gauge matrix $\tilde{\mathbf{S}}$ is written in terms of V_n,

$$\tilde{\mathbf{S}} = \begin{pmatrix} 0 & 1 & 1 \\ \mathcal{P}^{-1}(V_5+V_6)+2\mathcal{P}^{-1/2} & \mathcal{P}^{-1}V_6 & -\mathcal{P}^{-1}(V_5+V_6)-2\mathcal{P}^{-1/2} \\ -1 & -\mathcal{P}^{-1/2}V_6 & 1 \end{pmatrix}.$$

The polynomial $B_F(z)$ has a zero z_1,

$$z_1 = -(V_1+V_2)\left(\frac{V_3 V_4}{\mathcal{P}^{1/2}(V_3+V_4)+\mathcal{P}}+1\right). \tag{4.6}$$

As the same as in the $N=2$ case, we obtain $V_n = V_n(\mathcal{P}, \mathcal{H}_1; z_1(\tau_1))$ by using (4.5) and (4.6).

For the general N cases we support (i) and (ii), and the dynamical variables of LV(N) should be solved as

$$V_n = V_n(\mathcal{P}, \mathcal{H}_1, \ldots, \mathcal{H}_g; z_1, \ldots, z_g),$$

where $z_i = z_i(\tau_1, \ldots, \tau_g)$.

V. SUMMARY AND REMARKS

In this paper, we have studied the realization of the representative of the gauge equivalence class $\boldsymbol{\mathcal{M}}_F$, which is given by the classical integrable model, the extended Lotka–Volterra lattice.

The gauge equivalence class $\boldsymbol{\mathcal{M}}_F$ have the elements whose characteristic equation (1.1) is common, and the coefficients of (1.1) correspond to a set of commuting integrals of motion. There is the isomorphism from $\boldsymbol{\mathcal{M}}_F$ to a set of divisors $X(g)-D$, and the time evolution of the divisor is linearized on the Jacobi variety $J(X)$. In Ref. 5, it was introduced that the way to construct the representative of $\boldsymbol{\mathcal{M}}_F$ by starting with the integrable monodromy matrix $\overline{\mathbf{T}}(z)$ (2.11). Based on the integrable Poisson structure of the monodromy matrix, the divisor is determined via SoV.

We have found that LV(N) gives the realizations not only for the monodromy matrix $\overline{\mathbf{T}}(z)$ but also for the representative $\mathbf{M}_F(z)$. We have studied the correspondence of LV(N) and the representative and their Poisson algebras in detail. Then we have shown that the family of nontrivial integrals of motion for the representative coincides with that of LV(N), and that the number of these integrals are necessary and sufficient to describe the model. Especially our claim is that $\mathbf{M}_F(z)$ can be written in terms of the dynamical variables of LV(N). These make possible to solve the model, and the time evolutions of the dynamical variables V_n are obtained as

$$V_n = V_n(\mathcal{P}, \mathcal{H}_1, \ldots, \mathcal{H}_g; z_1(\{\tau_i\}), \ldots, z_g(\{\tau_i\})).$$

Here $\mathcal{P}$ and $\mathcal{H}_i$ are the integrals of motion, where each $\mathcal{H}_i$ generates the independent time τ_i.

In closing, we would like to mention the quantization of LV(N). By replacing the canonical variables (2.3) in the Lax matrices $\mathbf{L}_n(z)$ (2.4) and $\overline{\mathbf{L}}_n(z)$ (2.5) with the Weyl operators,

$$[\hat{P}_n, \hat{Q}_m] = \delta_{n,m}\hat{P}_n\hat{Q}_n, \quad [\hat{P}_n, \hat{P}_m] = [\hat{Q}_n, \hat{Q}_m] = 0,$$

we get the quantum integrable model.[11,12] As is the same as the classical case we note the Lax matrix $\overline{\mathbf{L}}_n(z)$ (2.5). Now this matrix with Weyl operators satisfies the fundamental commuting relation

$$\mathbf{R}(z/z';q)(\overline{\mathbf{L}}_n(z)\otimes 1)(1\otimes\overline{\mathbf{L}}_n(z'))=(1\otimes\overline{\mathbf{L}}_n(z'))(\overline{\mathbf{L}}_n(z)\otimes 1)\mathbf{R}(z/z';q),$$

where R-matrix is

$$\mathbf{R}(z;q)=\sum_{k=1}^{N}(z-q^2)\mathbf{E}_{k,k}\otimes\mathbf{E}_{k,k}+\sum_{j=1}^{N}\sum_{k=1}^{N-1}q(z-1)\mathbf{E}_{j,j}\otimes\mathbf{E}_{j+k,j+k}$$

$$+\sum_{1\leqslant j<k\leqslant N}(1-q^2)(\mathbf{E}_{j,k}\otimes\mathbf{E}_{k,j}+z\mathbf{E}_{k,j}\otimes\mathbf{E}_{j,k}).$$

Especially in the $N=2$ case the Lax matrix becomes

$$\overline{\mathbf{L}}_n(z)=\frac{1}{z^{1/2}}\begin{pmatrix}0 & \hat{Q}_n^{-1}\\ -z\hat{Q}_n & z\hat{P}_n\end{pmatrix}. \tag{5.1}$$

Taking into account the canonical transformation, this is essentially the same as what is discussed in Ref. 13. In the general N case, the monodromy matrix $\overline{\mathbf{T}}(z)$ is written as

$$\overline{\mathbf{T}}(z)=\prod_{k=1}^{\overleftarrow{MN}}\mathbb{L}_k(z),$$

where $\mathbb{L}_k(z)=(\overline{\mathbf{L}}_{k(N-1)}(z)\overline{\mathbf{L}}_{k(N-1)-1}(z)\cdots\overline{\mathbf{L}}_{(k-1)(N-1)+1}(z))$ is

$$\frac{1}{z^{(N-1)/N}}\begin{pmatrix}0 & 0 & \cdots & 0 & \hat{Q}_{N-1}^{-1}\\ z(-)^{N-1}\hat{Q}_1 & z(-)^{N-2}\hat{P}_1 & 0 & \cdots & 0\\ 0 & z(-)^{N-1}\hat{Q}_2\hat{Q}_1^{-1} & z(-)^{N-2}\hat{P}_2 & 0 & \vdots\\ \vdots & 0 & \ddots & \ddots & 0\\ 0 & \cdots & 0 & z(-)^{N-1}\hat{Q}_{N-1}\hat{Q}_{N-2}^{-1} & z(-)^{N-2}\hat{P}_{N-1}\end{pmatrix}_{[k-1]}.$$

Here in the matrix with the subscript $[k-1]$ the operators $\hat{P}_i$ and $\hat{Q}_i$ are regarded as $\hat{P}_{i+(k-1)(N-1)}$ and $\hat{Q}_{i+(k-1)(N-1)}$, respectively. We expect that the matrix $\mathbb{L}_n(z)$ gives a key to generalize the Baxter equations and their dual structure in the sense of Ref. 13, which is a future problem. The matrix $\mathbb{L}_k(z)$ may link to the relatives or the extension to sl_N of the Toda lattice. It seems to be interesting to study this matrix in both the classical and quantum cases from this point of view.

ACKNOWLEDGMENTS

The author thanks Professor A. Nakayashiki for helpful comments, and Professor A. Kuniba for kind encouragement. She appreciates discussions with T. Yamazaki. She is grateful to Professor B. de Wit and members of ITP and Spinoza Institute in Utrecht University for their hospitality. A part of this work was done during her stay at Spinoza Institute. R. I. is a Research Fellow of the Japan Society for the Promotion of Science.

APPENDIX A: LOCAL LAX MATRIX FOR LV(N)

We define a gauge transformation of $\tilde{\mathbf{L}}_n(x)$ (1.4) as follows:

$$\mathbf{L}_n(z)=\mathbf{\Omega}_{n+1}(z)\tilde{\mathbf{L}}_n(z)\mathbf{\Omega}_n(z)^{-1}, \tag{A1}$$

Here the gauge matrix $\mathbf{\Omega}_n(z)$ is

$$\mathbf{\Omega}_n(z)=\mathbf{B}_n\mathbf{A}\mathbf{X}(z), \tag{A2}$$

where

$$\mathbf{A}=\left(\sum_{k=1}^{N}\mathbf{E}_{k,N+1-k}\right)\left(\mathbb{1}-\sum_{k=1}^{N-1}\mathbf{E}_{k,k+1}\right),$$

$$\mathbf{B}_n=\prod_{k=0}^{N-2}(P_{n+k})^{-\Sigma_{j=k+2}^{N}\mathbf{D}^{(j)}}(Q_{n+k})^{\mathbf{D}^{(k+2)}},$$

$$\mathbf{X}(z)=\sum_{k=1}^{N}z^{(k-1)/N}\mathbf{E}_{k,k},$$

and we use

$$\mathbf{D}^{(j)}=\frac{1}{N}\mathbb{1}-\mathbf{E}_{j,j},\quad (P_n)^{\mathbf{D}^{(j)}}=\sum_{k=1}^{N}P_n^{(\mathbf{D}^{(j)})_{k,k}}\mathbf{E}_{k,k}.$$

In the above we have used a notation,

$$P_n^{\mathbf{D}}=\mathrm{diag}[P_n^{d_1},P_n^{d_2},\ldots,P_n^{d_N}],\quad \text{where } \mathbf{D}=\mathrm{diag}[d_1,\ldots,d_N].$$

Finally we obtain the local Lax matrix (2.5),

$$\mathbf{L}_n(z)=z^{1/N}\left(P_n\mathbf{E}_{1,1}+Q_n\mathbf{E}_{1,2}+\frac{1}{z}(-1)^{N-1}Q_n^{-1}\mathbf{E}_{N,1}+\sum_{k=2}^{N-1}\mathbf{E}_{k,k+1}\right).$$

Note that the gauge matrix $\mathbf{\Omega}_n(z)$ is different from that introduced in Ref. 12.

APPENDIX B: GAUGE TRANSFORMATION OF $B(z)$

We divide the matrix $\mathbf{S}$ (3.2) in the same way as (2.12),

$$\mathbf{S}=\begin{pmatrix}1 & \vec{0}\\ \vec{s}_1^{\,T} & \mathbf{s}_2\end{pmatrix},$$

where we use

$$\vec{s}_1=\vec{c}_0(\mathbf{d}_0^{N-1-i})^T,\quad \mathbf{s}_2=\begin{pmatrix}\vec{b}_0\mathbf{d}_0^{N-2}\\ \vdots\\ \vec{b}_0\mathbf{d}_0\\ \vec{b}_0\end{pmatrix},$$

and $\vec{c}_0$, $\vec{b}_0$, and $\mathbf{d}_0$ are dominant parts of $\vec{c}(z)$, $\vec{b}(z)$, and $\mathbf{d}(z)$ in $z\to\infty$. The matrix $\mathbf{S}$ transforms the monodromy matrix $\overline{\mathbf{T}}(z)$ to

$$\mathbf{M}_F(z)=\mathbf{S}\overline{\mathbf{T}}(z)\mathbf{S}^{-1}=\begin{pmatrix}\sharp & \vec{b}(z)\mathbf{s}_2^{-1}\\ \flat & (\vec{s}_1^{\,T}\vec{b}(z)+\mathbf{s}_2\mathbf{d}(z))\mathbf{s}_2^{-1}\end{pmatrix},$$

where the parts indicated by $\sharp$ and $\flat$ are not important now. Following this transformation, the polynomial $B(z)$ (2.16) becomes $B_F(z)$ as

$$B_F(z)=\mathrm{Det}\begin{pmatrix}\vec{b}(z)\mathbf{s}_2^{-1}\\ \vec{b}(z)\mathbf{s}_2^{-1}(\vec{s}_1^{T}\vec{b}(z)\mathbf{s}_2^{-1}+\mathbf{s}_2\mathbf{d}(z)\mathbf{s}_2^{-1})\\ \vdots\\ \vec{b}(z)\mathbf{s}_2^{-1}(\vec{s}_1^{T}\vec{b}(z)\mathbf{s}_2^{-1}+\mathbf{s}_2\mathbf{d}(z)\mathbf{s}_2^{-1})^{N-2}\end{pmatrix}$$

$$=\mathrm{Det}\begin{pmatrix}\vec{b}(z)\\ \vec{b}(z)\mathbf{d}(z)\\ \vdots\\ \vec{b}(z)\mathbf{d}(z)^{N-2}\end{pmatrix}\mathrm{Det}(\mathbf{s}_2^{-1})$$

$$=(-)^{1/2(N-1)(N-2)}B(z)B_0^{-1}.$$

The second equality is due to

$$\vec{b}(z)\mathbf{s}_2^{-1}\vec{s}_1^{T}\vec{b}(z)\propto\vec{b}(z),$$

and the third one follows (2.15) and

$$\mathrm{Det}\,\mathbf{s}_2=(-)^{1/2(N-1)(N-2)}B_0,$$

where B_0 is the zero mode of $B(z)$. Finally we obtain $B_F(z)$ which do not have the zero mode.

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Fourier transforms of Lorentz invariant functions

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(Received 22 December 2000; accepted 30 August 2002)

Fourier transforms of Lorentz invariant functions in Minkowski space, with support on both the timelike and the spacelike domains are performed by means of direct integration. The cases of $1+1$ and $1+2$ dimensions are worked out in detail, and the results for $1+n$ dimensions are given. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1522817]

I. INTRODUCTION

The main goal of this paper is to perform spherical averages over the hyperbolic coordinates in Minkowski space–time by means of direct integration. We work with Lorentz invariant (or "radial") functions, defined on $\mathbb{R}^{1,n}$, which depend only on the distance to the light-cone $s^2=(x^0)^2-(\vec{x})^2$. (x^0 is the time coordinate and $\vec{x}$ stands for the spatial coordinates). In particular, we will compute their Fourier transforms:

$$F(k):=\int_{\mathbb{R}^{1,n}} dx^{n+1}\, f(\eta_{\mu\nu}x^\mu x^\nu)\exp(-2\pi i k_\mu x^\mu), \tag{1}$$

where the metric $\eta_{\mu\nu}$ is of the form

$$\eta_{\mu\nu}=\mathrm{diag}(1,-1,\ldots,-1). \tag{2}$$

(We set the 2π in the exponential to avoid factors of 2π appearing in front of the integral. Here it is just for convenience but this strategy becomes crucial when integrating over infinite-dimensional spaces.[1])

This type of integral is ubiquitous in quantum field theory (QFT), since the fields can be decomposed in terms of their Fourier components, and the correlation functions depend only on the radial distance s^2. Although QFT is defined in Minkowski space, a common procedure is to perform a Wick rotation at an early stage (this procedure can be found in standard textbooks, e.g., Ref. 2) in which all integrals over space–time are reduced to Euclidean integrals.

There are several obvious disadvantages to relying on the Wick rotation procedure, in which the time coordinate t is rotated to imaginary values $t\to -it$, and Minkowski space–time is transformed into Euclidean space. First, the special structure of Minkowski space–time in which there is a preferred direction (i.e., time direction) is lost. Second, Wick rotation might not be a valid procedure in all circumstances, e.g., in cases where the arc at infinity does not vanish.

The motivation for this work is to provide tools for performing calculations in QFT while working directly in Minkowski space.

In analogy with Euclidean space, we introduce a (pseudo-) spherical coordinate atlas, i.e., one of the angles is hyperbolic. Integrating over all the angular variables leaves us with a one-

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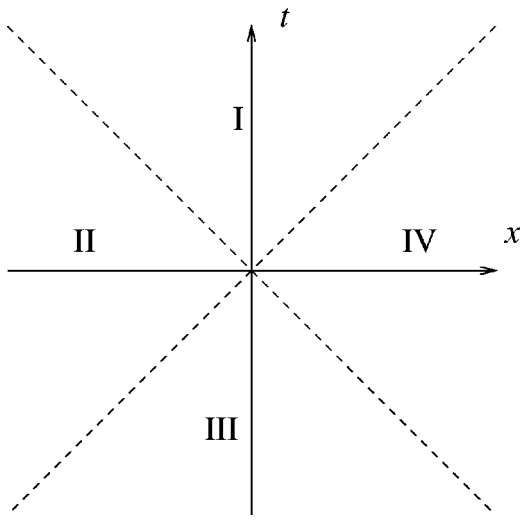

FIG. 1. Standard division of $\mathbb{R}^{1,1}$. I is the forward light-cone, III the backward light-cone, and II and IV the spacelike domains.

dimensional radial integral. The advantage of this procedure is that any possible light-cone singularities of the integrand are mapped to point singularities in the radial variable and therefore easier to deal with.

In this paper we will not specify the function space for which the integrals are convergent. We will assume that only such functions have been chosen.

Below, we will discuss the cases $n=1$ and $n=2$ in detail. For the case of general n we only quote the results.

After preparing an earlier version of this paper we found an article by Codelupi[3] which seems to be largely unknown. Codelupi studied Fourier transforms of Lorentz invariant functions $f(s)$, using related methods, and found the same results. To find the case of arbitrary n he proved a recursion relation, that relates Fourier transform of $n+2$ spatial dimensions to the Fourier transform of n spatial dimensions. In Sec. IV we adapt Codelupi's elegant method to our case.

II. CASE $\mathbb{R}^{1,1}$

A. Pseudospherical coordinate atlas for $\mathbb{R}^{1,1}$

A characteristic feature of manifolds with an indefinite metric is that a global spherical coordinate system does not exist.[4] To cover $\mathbb{R}^{1,1}$ we use four patches and four different parametrizations. The parametrizations coincide on the boundary between the domains, i.e., on the light-cone. (See Fig. 1).

Denote by t,x the global Cartesian coordinate system with distance $s^2=t^2-x^2$. We parametrize the different patches as follows.

Patch I:

$$t=s\cosh\psi, \quad x=s\sinh\psi,$$

where $s\in[0,+\infty[$ and $\psi\in]-\infty,+\infty[$.

Volume element: $dt\wedge dx=s\,ds\wedge d\psi$.

Line element: $s^2=t^2-x^2$.

Patch II:

$$t = is \sinh\psi, \quad x = is \cosh\psi,$$

where $s \in]i\infty, i0]$ and $\psi \in]-\infty, +\infty[$.
Volume element: $dt \wedge dx = s\, ds \wedge d\psi$.
Line element: $s^2 = t^2 - x^2$.

Patch III:

$$t = s \cosh\psi, \quad x = s \sinh\psi,$$

where $s \in [0, -\infty[$ and $\psi \in]-\infty, +\infty[$.
Volume element: $dt \wedge dx = s\, ds \wedge d\psi$.
Line element: $s^2 = t^2 - x^2$.

Patch IV:

$$t = is \sinh\psi, \quad x = is \cosh\psi,$$

where $s \in]-i\infty, i0]$ and $\psi \in]-\infty, +\infty[$.
Volume element: $dt \wedge dx = s\, ds \wedge d\psi$.
Line element: $s^2 = t^2 - x^2$.

The limits of integration in each patch are chosen to yield a positive result when the volume element is integrated over a small, finite volume.

B. Fourier transform of radial functions

We integrate the function $f(s^2)$ separately in the timelike and spacelike domain for the cases of timelike and spacelike momenta. To simplify the calculation, we set $k_x = 0$ when the momentum is timelike, and $k_t = 0$ when the momentum is spacelike. This can always be achieved with a Lorentz transformation and is not a restriction on the results.

Patch I+III:

(i) Timelike momentum: $k_x = 0$,

$$\begin{aligned} I_{\mathrm{I+III}}(k_t) &= \int_{\mathrm{I+III}} dt\, dx\, f(t^2 - x^2) \exp(-2\pi i k_t t) \\ &= \int_0^{\infty} ds\, s f(s^2) \int_{-\infty}^{+\infty} d\psi\, \exp(-2\pi i k_t s \cosh\psi) \\ &\quad + \int_0^{-\infty} ds\, s f(s^2) \int_{-\infty}^{+\infty} d\psi\, \exp(-2\pi i k_t s \cosh\psi) \\ &= 2 \int_0^{\infty} ds_0\, s_0\, f(s_0^2) \int_{-\infty}^{+\infty} d\psi \cos(2\pi k_t s_0 \cosh\psi) \\ &= -2\pi \int_0^{\infty} ds_0\, s_0\, f(s_0^2) N_0(2\pi k_t s_0), \end{aligned} \tag{3}$$

where N_0 is a Bessel function of zeroth order and

$$s_0 = \sqrt{t^2 - x^2}. \tag{4}$$

In the last line we have used formula 3.868(2) from Ref. 5, after a change of variable to $x = e^{\psi}$.

(iii) Spacelike momentum: $k_t=0$,

$$I_{\mathrm{I+III}}(k_x)=\int_{\mathrm{I+III}} dt\,dx\, f(t^2-x^2)\exp(-2\pi i k_x x)$$

$$=\int_0^{\infty} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi \exp(-2\pi i k_x s\sinh\psi)$$

$$+\int_0^{-\infty} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi \exp(-2\pi i k_x s\sinh\psi)$$

$$=\int_0^{\infty} ds_0\, s_0\, f(s_0^2)\int_{-\infty}^{+\infty} d\psi \cos(2\pi k_x s_0\sinh\psi)=4\int_0^{\infty} ds_0\, s_0\, f(s_0^2)K_0(2\pi k_x s_0), \qquad (5)$$

where K_0 is a Bessel function of zeroth order and s_0 as before. In the last line we have used formula 3.868(4) from Ref. 5, after a change of variable to $x=e^{\psi}$.

Patch II+IV:

(i) Timelike momentum: $k_x=0$,

$$I_{\mathrm{II+IV}}(k_t)=\int_{\mathrm{II+IV}} dt\,dx\, f(t^2-x^2)\exp(-2\pi i k_t t)$$

$$=\int_{i\infty}^{i0} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi\, \exp(2\pi k_t s\sinh\psi)$$

$$+\int_{-i\infty}^{i0} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi\, \exp(2\pi k_t s\sinh\psi)$$

$$=\int_0^{\infty} ds_1\, s_1\, f(s_1^2)\int_{-\infty}^{+\infty} d\psi \cos(2\pi k_t s_1\sinh\psi)$$

$$=4\int_0^{\infty} ds_1\, s_1\, f(s_1^2)K_0(2\pi k_t s_1), \qquad (6)$$

where K_0 is a Bessel function of zeroth order and

$$s_1=\sqrt{x^2-t^2}. \qquad (7)$$

In the last line we have used formula 3.868(4) from Ref. 5, after a change of variable $x=e^{\psi}$.

(ii) Spacelike momentum: $k_t=0$,

$$I_{\mathrm{II+IV}}(k_x)=\int_{\mathrm{II+IV}} dt\,dx\, f(t^2-x^2)\exp(-2\pi i k_x x)$$

$$=\int_{i\infty}^{i0} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi\, \exp(2\pi k_x s\cosh\psi)$$

$$+\int_{-i\infty}^{i0} ds\, sf(s^2)\int_{-\infty}^{+\infty} d\psi\, \exp(2\pi k_x s\cosh\psi)$$

$$=2\int_0^{\infty} ds_1\, s_1\, f(s_1^2)\int_{-\infty}^{+\infty} d\psi \cos(2\pi k_x s_1\cosh\psi)$$

$$=-2\pi\int_0^{\infty} ds_1\, s_1\, f(s_1^2)N_0(2\pi k_x s_1), \qquad (8)$$

where N_0 is a Bessel function of zeroth order and s_1 as before. In the last line we have used formula 3.868(2) from Ref. 5, after a change of variable to $x=e^{\psi}$.

In summary

$$I(k_t)=-2\pi\int_0^\infty ds_0\, s_0 f(s_0^2)N_0(2\pi k_t s_0)+4\int_0^\infty ds_1\, s_1 f(s_1^2)K_0(2\pi k_t s_1),$$

$$I(k_x)=4\int_0^\infty ds_0\, s_0 f(s_0^2)K_0(2\pi k_x s_0)-2\pi\int_0^\infty ds_1\, s_1 f(s_1^2)N_0(2\pi k_x s_1).$$

C. Example: Fourier transform of a Gaussian

In this section we apply the results from above to a specific test function and show that the correct answer is obtained. Whenever necessary, we define the integral $\int_0^\infty dx\, f(x)$ as $\lim_{\epsilon\to 0}\int_0^\infty dx\, e^{-\epsilon x^2} f(x)$. With this proviso, we can directly compute the Fourier transform of a ''Gaussian'' (where the quotation marks remind us that the exponential is imaginary),

$$\int dt\, dx\, e^{i(t^2-x^2)} e^{-2\pi i k_t t}=\pi e^{-i\pi^2 k_t^2}.$$

We can now check that our Fourier transform integrals give the same result,

$$I_1(k_t)=4\int_0^\infty dr\, r e^{-(\epsilon+i)r^2}K_\nu(2\pi r k_t)$$

$$=\frac{1}{\pi k_t}\frac{1}{\sqrt{\epsilon+i}}\Gamma\left(1+\frac{\nu}{2}\right)\Gamma\left(1-\frac{\nu}{2}\right)e^{\pi^2 k_t^2/2(\epsilon+i)}W_{-1/2,\,\nu/2}\left(\frac{\pi^2 k_t^2}{2(\epsilon+i)}\right),$$

$$I_2(k_t)=-2\pi\int_0^\infty dr\, r e^{-(\epsilon-i)r^2}N_\nu(2\pi r k_t)$$

$$=-\frac{1}{k_t}\frac{1}{\sqrt{\epsilon-i}}\frac{1}{\sin\left(\frac{\pi\nu}{2}\right)}e^{-\pi^2 k_t^2/2(\epsilon-i)}\left[W_{1/2,\,\nu/2}\left(\frac{\pi^2 k_t^2}{2(\epsilon-i)}\right)\right.$$

$$\left.-\cos\left(\frac{\nu\pi}{2}\right)\frac{\Gamma\left(1+\frac{\nu}{2}\right)}{\Gamma(1+\nu)}M_{1/2,\,\nu/2}\left(\frac{\pi^2 k_t^2}{2(\epsilon-i)}\right)\right],$$

where we have used 6.631(2,3) from Ref. 5. Each integral has a pole as $\nu\to 0$; the W function with negative first argument has a simple pole in ν, and there is an inverse sine in ν in the second integral. However, as we will see, this singularity exactly cancels between the two integrals. Thus we may, in fact, take $\nu\to 0$ in the sum. First we convert the M function to W functions,

$$M_{1/2,\,\nu/2}(z)=i\frac{\Gamma(1+\nu)}{\Gamma\left(\frac{\nu}{2}\right)}W_{-1/2,\,\nu/2}(z)+\frac{\Gamma(1+\nu)}{\Gamma\left(1+\frac{\nu}{2}\right)}e^{-i\pi\nu/2}W_{1/2,\,\nu/2}(z)$$

using formula 9.233(1) in Ref. 5. Then we make use of the following identities [9.234(1,2) and 9.235 in Ref. 5]:

$$W_{1/2,\,\nu/2}(z)=\frac{\sqrt{z}}{2}W_{0,(1+\nu)/2}(z)+\frac{\sqrt{z}}{2}W_{0,(1-\nu)/2}(z),$$

$$W_{-1/2,\,\nu/2}(z)=\frac{2\sqrt{z}}{\nu}W_{0,(1+\nu)/2}(z),$$

$$W_{0,1/2}(z)=e^{-z/2}.$$

Expanding the Γ functions and $1/\sin z=1/z+z/6+\mathcal{O}(z^2)$, we can explicitly verify that the singularity cancels:

$$I_1+I_2=-\frac{2i}{\nu}+\frac{2i}{\nu}+\mathcal{O}(1)=0+\mathcal{O}(1).$$

We have verified numerically that the constant term is, in fact,

$$I_1+I_2=\pi e^{-i\pi^2k^2}.$$

III. CASE $\mathbb{R}^{1,2}$

A. Pseudospherical coordinate atlas for $\mathbb{R}^{1,2}$

Global coordinate system: t,x,y, distance $s^2=t^2-x^2-y^2$.

Patch I:

$$t=s\cosh\psi,\quad x=s\sinh\psi\cos\theta,\quad y=s\sinh\psi\sin\theta,$$

where $s\in[0,+\infty[$, $\psi\in]-\infty,+\infty[$ and $\theta\in[-\pi/2,\pi/2]$.

To avoid problems when $\sinh\psi$ switches sign at 0, the integral over ψ needs to be split up into two integrals: $\psi\in[0,+\infty]$ and $\psi\in[0,-\infty]$.

Volume element: $dt\wedge dx\wedge dy=s^2\sinh\psi\,ds\wedge d\psi\wedge d\theta$.

Line element: $s^2=t^2-x^2-y^2$.

Patch II:

$$t=is\sinh\psi,\quad x=is\cosh\psi\cos\theta,\quad y=is\cosh\psi\sin\theta,$$

where $s\in[i0,i\infty[$, $\psi\in]-\infty,+\infty[$, and $\theta\in[-\pi/2,\pi/2]$.

Volume element: $dt\wedge dx\wedge dy=is^2\cosh\psi\,ds\wedge d\psi\wedge d\theta$.

Line element: $s^2=t^2-x^2-y^2$.

Patch III:

$$t=s\cosh\psi,\quad x=s\sinh\psi\cos\theta,\quad y=s\sinh\psi\sin\theta,$$

where $s\in[0,-\infty[$, $\psi\in]-\infty,+\infty[$, and $\theta\in[-\pi/2,\pi/2]$.

To avoid problems when $\sinh\psi$ switches sign at 0, the integral over ψ needs to be split up into two integrals: $\psi\in]+\infty,0]$ and $\psi\in]-\infty,0]$.

Volume element: $dt\wedge dx\wedge dy=s^2\sinh\psi\,ds\wedge d\psi\wedge d\theta$.

Line element: $s^2=t^2-x^2-y^2$.

Patch IV:

$$t=is\sinh\psi,\quad x=is\cosh\psi\cos\theta,\quad y=is\cosh\psi\sin\theta,$$

where $s\in]-i\infty,i0]$, $\psi\in]-\infty,+\infty[$, and $\theta\in[-\pi/2,\pi/2]$.

Volume element: $dt\wedge dx\wedge dy=is^2\cosh\psi\,ds\wedge d\psi\wedge d\theta$.

Line element: $s^2=t^2-x^2-y^2$.

The limits of integration in each patch are chosen to yield a positive result when the volume element is integrated over a small, finite volume.

B. Fourier transform of radial functions

As before, we integrate the function $f(s^2)$ separately in the timelike and spacelike domain for the cases of timelike and spacelike momenta. To simplify the calculation, we set $k_x=k_y=0$ when the momentum is timelike, and $k_t=k_y=0$ when the momentum is spacelike. This can always be achieved with a Lorentz transformation and is not a restriction on the results.

Patch I+III:

(i) Timelike momentum: $k_x=k_y=0$,

$$
\begin{aligned}
I_{\mathrm{I+III}}(k_t) &= \int_{\mathrm{I+III}} dt\,dx\,dy\; f(t^2-x^2-y^2)\exp(-2\pi i k_t t)\\
&= \pi\int_0^\infty ds\, s^2 f(s^2)\left[\int_0^\infty d\psi \sinh\psi \exp(-2\pi i k_t s\cosh\psi)\right.\\
&\quad \left.+\int_0^{-\infty} d\psi \sinh\psi \exp(-2\pi i k_t s\cosh\psi)\right]\\
&\quad +\pi\int_0^{-\infty} ds\, s^2 f(s^2)\left[\int_\infty^0 d\psi \sinh\psi \exp(-2\pi i k_t s\cosh\psi)\right.\\
&\quad \left.+\int_{-\infty}^0 d\psi \sinh\psi \exp(-2\pi i k_t s\cosh\psi)\right]\\
&= \int_0^\infty ds\, s^2 f(s^2)\frac{\exp(-2\pi i k_t s)}{i k_t s}-\int_0^{-\infty} ds\, s^2 f(s^2)\frac{\exp(-2\pi i k_t s)}{i k_t s}\\
&= -\frac{2}{k_t}\int_0^\infty ds_0\, s_0\, f(s_0^2)\sin(2\pi k_t s_0), \qquad (9)
\end{aligned}
$$

where

$$
s_0=\sqrt{t^2-x^2-y^2}. \qquad (10)
$$

The angular integrals have been computed as follows:

$$
\begin{aligned}
&\int_0^\infty d\psi \sinh\psi\exp(-ia\cosh\psi)+\int_0^{-\infty} d\psi\sinh\psi\exp(-ia\cosh\psi)\\
&\quad=\lim_{\epsilon\to 0} 2\int_{0-i\epsilon}^{+\infty-i\epsilon} d\psi\sinh\psi\exp(-ia\cosh\psi)\\
&\quad=\lim_{\epsilon\to 0}\frac{2}{ia}[-\exp(-ia\cosh(\infty-i\epsilon))+\exp(-ia\cosh(0-i\epsilon))]=\frac{2}{ia}\exp(-ia),
\end{aligned}
$$

where $a=2\pi k_t s$, and in the last line $\cosh(\psi\pm i\epsilon)=\cosh\psi\pm i\epsilon\sinh\psi$ has been used.

(ii) Spacelike momentum: $k_t = k_y = 0$,

$$
\begin{aligned}
I_{\mathrm{I+III}}(k_x) &= \int_{\mathrm{I+III}} dt\, dx\, dy\, f(t^2-x^2-y^2)\exp(-2\pi i k_x x) \\
&= \int_0^\infty ds\, s^2 f(s^2) \int_{-\pi/2}^{\pi/2} d\theta \Bigg[\int_0^\infty d\psi \sinh\psi \exp(-2\pi i k_x s \sinh\psi\cos\theta) \\
&\quad + \int_0^{-\infty} d\psi \sinh\psi \exp(-2\pi i k_x s \sinh\psi\cos\theta) \Bigg] \\
&\quad + \int_0^{-\infty} ds\, s^2 f(s^2) \int_{-\pi/2}^{\pi/2} d\theta \Bigg[\int_\infty^0 d\psi \sinh\psi \exp(-2\pi i k_x s \sinh\psi\cos\theta) \\
&\quad + \int_{-\infty}^0 d\psi \sinh\psi \exp(-2\pi i k_x s \sinh\psi\cos\theta) \Bigg] \\
&= \int_0^\infty ds\, s^2 f(s^2) \frac{\exp(-2\pi k_x s)}{k_x s} + \int_0^{-\infty} ds\, s^2 f(s^2) \frac{\exp(-2\pi k_x s)}{i k_x s} \\
&= \frac{2}{k_x} \int_0^\infty ds_0\, s_0\, f(s_0^2) \exp(-2\pi k_x s_0). \qquad (11)
\end{aligned}
$$

The angular integrals have been computed as follows ($a = 2\pi k_x s$):

$$
\begin{aligned}
&\int_{-\pi/2}^{\pi/2} d\theta \Bigg[\int_0^\infty d\psi \sinh\psi \exp(-ia \sinh\psi\cos\theta) + \int_0^{-\infty} d\psi \sinh\psi \exp(-ia \sinh\psi\cos\theta) \Bigg] \\
&\quad = 4 \int_0^\infty d\psi \sinh\psi \int_0^{\pi/2} d\theta \cos(a \sinh\psi\cos\theta) \\
&\quad = 2\pi \int_0^\infty d\psi \sinh\psi J_0(a \sinh\psi) \\
&\quad = \frac{2\pi}{a} \exp(-a).
\end{aligned}
$$

To get to the third line we have used formula 3.753(2) from Ref. 5, after a change of variable to $x = \cos\theta$. The last line is obtained using 6.554(1) from Ref. 5, after a change of variable to $y = \sinh\psi$.

Patch II+IV:

(i) Timelike momentum: $k_x = k_y = 0$,

$$
\begin{aligned}
I_{\mathrm{II+IV}}(k_t) &= \int_{\mathrm{II+IV}} dt\, dx\, dy f(t^2-x^2-y^2)\exp(-2\pi i k_t t) \\
&= i \int_{i0}^{i\infty} ds\, s^2 f(s^2) \int_{-\pi/2}^{\pi/2} d\theta \int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(2\pi k_t s \sinh\psi) \\
&\quad + i \int_{-i\infty}^{i0} ds\, s^2 f(s^2) \int_{-\pi/2}^{\pi/2} d\theta \int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(2\pi k_t s \sinh\psi) \\
&= -\pi \int_0^{-\infty} ds'\, s'^2 f(-s'^2) \int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(-2\pi i k_t s' \sinh\psi) \\
&\quad - \pi \int_\infty^0 ds'\, s'^2 f(-s'^2) \int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(-2\pi i k_t s' \sinh\psi) = 0. \qquad (12)
\end{aligned}
$$

The angular integrals have been computed as follows (with $a=2\pi k_t s'$):

$$\int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(-ia\sinh\psi) = \lim_{\epsilon\to 0} \int_{-\infty-i\epsilon}^{+\infty-i\epsilon} d\psi \cosh\psi \exp(-ia\sinh\psi)$$

$$= \lim_{\epsilon\to 0} \frac{i}{a}[\exp(-ia\sinh\psi)]_{-\infty-i\epsilon}^{+\infty-i\epsilon}$$

$$= \lim_{\epsilon\to 0} \frac{i}{a}[\exp(-ia\infty)\exp(-\epsilon a\infty) - \exp(ia\infty)\exp(-\epsilon a\infty)] = 0.$$

(ii) Spacelike momentum: $k_t = 0$,

$$I_{\mathrm{II+IV}} = \int_{\mathrm{II+IV}} dt\, dx\, dy f(t^2-x^2-y^2)\exp(-2\pi i k_x x)$$

$$= i\int_{i0}^{i\infty} ds\, s^2 f(s^2) \int_{-\pi/2}^{\pi/2} d\theta \int_{-\infty}^{+\infty} d\psi \cosh\psi \exp(2\pi k_x s \cosh\psi\cos\theta)$$

$$+ i\int_{-i\infty}^{i0} ds\, s^2 f(s^2) \int_{-\infty}^{+\infty} d\psi \cosh\psi \int_{-\pi/2}^{\pi/2} d\theta \exp(2\pi k_x s\cosh\psi\cos\theta)$$

$$= 4\int_0^{\infty} ds_1 s_1^2 f(-s_1^2) \int_0^{\pi/2} d\theta \int_0^{\infty} d\psi \cosh\psi \exp(2\pi i k_x s_1 \cosh\psi\cos\theta)$$

$$+ 4\int_0^{\infty} ds_1 s_1^2 f(s_1^2) \int_0^{\pi/2} d\theta \int_0^{\infty} d\psi \cosh\psi \exp(-2\pi i k_x s_1 \cosh\psi\cos\theta)$$

$$= 8\int_0^{\infty} ds_1 s_1^2 f(s_1^2) \int_0^{\pi/2} d\theta \int_0^{\infty} d\psi \cosh\psi \cos(2\pi k_x s_1)$$

$$= \frac{2}{k_x}\int_0^{\infty} ds_1 s_1 f(s_1^2)\cos(2\pi k_x s_1), \tag{13}$$

where

$$s_1 = \sqrt{x^2+y^2-t^2}.$$

The angular integral has been computed as follows (with $a=2\pi k_x s_1$):

$$\int_0^{\infty} d\psi \cosh\psi \int_0^{\pi/2} d\theta \cos(a\cosh\psi\cos\theta) = \frac{\pi}{2}\int_0^{\infty} d\psi \cosh\psi J_0(a\cosh\psi) = \frac{\pi}{a}\cos(a),$$

where in the second line, formula 3.715(19) from Ref. 5, and in the last line formula 6.554(3) from Ref. 5 have been used, after a change of variable to $x=\cosh\psi$.

In summary

$$I(k_t) = -\frac{2}{k_t}\int_0^{\infty} ds_0\, s_0 f(s_0^2)\sin(2\pi k_t s_0),$$

$$I(k_x) = \frac{2}{k_x}\int_0^{\infty} ds_0\, s_0 f(s_0^2)\exp(-2\pi k_x s_0) + \frac{2}{k_x}\int_0^{\infty} ds_1\, s_1 f(s_1^2)\cos(2\pi k_x s_1).$$

IV. CASE $\mathbb{R}^{1,n}$

In this section we follow Codelupi's derivation[3] of the $1+n$ dimensional case. The idea is to derive a recursion relation between the Fourier transform in n and $n+2$ spatial dimensions, and then use the explicit expressions found before to construct the general case.

A. Recursion relation

Define the radius in n spatial dimensions as follows:

$$r^2=\sum_{i=1}^{n} x_i^2 .$$

Formally, the function $f(s)=f(\sqrt{t^2-r^2})$ always looks the same, independent of the number of spatial dimensions. Suppose we have spaces with spatial dimensions $n=1$ to $n=m$. For each of these spaces exists a transform

$$F^{(n)}(k,k_0)=\int_0^\infty dr\, \chi_n(r,k)G(r,k_0), \tag{14}$$

where (proof given in the appendix)

$$\chi_n(r,k)=2\pi\frac{r^{n/2}}{k^{n/2-1}}J_{n/2-1}(2\pi rk) \tag{15}$$

and

$$G(r,k_0)=\int_{-\infty}^{+\infty} dt\, f(\sqrt{t^2-r^2})\exp(-2\pi ik_0t). \tag{16}$$

But formally, $G(r,k_0)$ looks the same for all cases, for example,

$$G(r,k_0)=\int_0^\infty dk\, \chi_m(k,r)F^{(m)}(k,k_0), \tag{17}$$

assuming that in the inverse Fourier transform, the angular contribution can also be integrated out.

Substitute in the line before,

$$\begin{aligned} F^{(n)}(k,k_0)&=\int_0^\infty dr\, \chi_n(r,k)\int_0^\infty du\, \chi_m(u,r)F^{(m)}(u,k_0)\\ &=\int_0^\infty du\, F^{(m)}(u,k_0)\int_0^\infty dr\, \chi_n(r,k)\chi_m(u,r). \end{aligned} \tag{18}$$

We can explicitly evaluate the second integral using formula 6.575(1) from Ref. 5. The result is

$$\int_0^\infty dr\, \chi_n(r,k)\chi_m(u,r)=\frac{2\pi^h}{\Gamma(h)}u(u^2-k^2)^{h-1}\Theta(u-k), \tag{19}$$

where $h=(m-n)/2$, $\Gamma(x)$ Euler's gamma function and Θ the step function. Equation (18) now takes on the form

$$F^{(n)}(k,k_0)=\frac{2\pi^h}{\Gamma(h)}\int_k^\infty du\, F^{(n+2h)}(u,k_0)u(u^2-k^2)^{h-1}. \tag{20}$$

Considering the special case $h=1$, i.e., $m=n+2$, and taking the derivative with respect to k of both sides of this equation leads to the recursion formula

$$F^{(n+2)}(k,k_0)=-\frac{1}{2\pi k}\frac{\partial}{\partial k}F^{(n)}(k,k_0). \tag{21}$$

So the problem is solved, at least in principle, once we find the explicit expressions for $n=1$ and $n=2$. But as we will show in the next section (again following Codelupi[3]), the recursion relation above will also allow us to find explicit formulas for the case of general n.

B. Explicit expressions for $\mathbb{R}^{1,n}$

Let us define

$$l_0=\sqrt{k_0^2-k^2},$$

$$l_1=\sqrt{k^2-k_0^2}.$$

The recursion relation Eq. (21) can be rewritten in terms of l_0 and l_1,

$$F^{(n+2)}(l_0)=-\frac{1}{2\pi k}\frac{\partial}{\partial k}F^{(n)}(l_0)=\frac{1}{2\pi l_0}\frac{d}{dl_0}F^{(n)}(l_0), \tag{22}$$

$$F^{(n+2)}(l_1)=-\frac{1}{2\pi k}\frac{\partial}{\partial k}F^{(n)}(l_1)=-\frac{1}{2\pi l_1}\frac{d}{dl_1}F^{(n)}(l_1). \tag{23}$$

To find expressions for general n consider the following two cases:

(a) n-even,

$$F^{(n)}(l_0)=\left(\frac{1}{2\pi l_0}\frac{d}{dl_0}\right)^{n/2-1}F^{(2)}(l_0)=(-1)^{n/2}2\pi\int_0^\infty ds_0\, f(s_0)\frac{s_0^{(n+1)/2}}{l_0^{(n-1)/2}}J_{(n-1)/2}(2\pi s_0 l_0). \tag{24}$$

The last equation is proved be iteratively applying the derivative to $F^{(2)}(l_0)$ (result of Sec. III B) and using formula 8.472(2) from Ref. 5. Similarly, we find

$$F^{(n)}(l_1)=4\int_0^\infty ds_0\, f(s_0)\frac{s_0^{(n+1)/2}}{l_1^{(n-1)/2}}K_{(n-1)/2}(2\pi s_0 l_1)-2\pi\int_0^\infty ds_1\, f(s_1)\frac{s_1^{(n+1)/2}}{l_1^{(n-1)/2}}N_{(n-1)/2}(2\pi s_1 l_1), \tag{25}$$

where the formulas 8.472(2) and 8.486(13) from Ref. 5 have been used.

(b) n-odd,

$$\begin{aligned}F^{(n)}(l_0)&=\left(\frac{1}{2\pi l_0}\right)^{(n-1)/2}F^{(1)}(l_0)\\&=(-1)^{(n+1)/2}2\pi\int_0^\infty ds_0\, f(s_0)\frac{s_0^{(n+1)/2}}{l_0^{(n-1)/2}}N_{(n-1)/2}(2\pi s_0 l_0)+(-1)^{(n-1)/2}4\\&\quad\times\int_0^\infty ds_1\, f(s_1)\frac{s_1^{(n+1)/2}}{l_0^{(n-1)/2}}K_{(n-1)/2}(2\pi s_1 l_0)\end{aligned} \tag{26}$$

and

$$F^{(n)}(l_1)=4\int_0^\infty ds_0\, f(s_0)\frac{s_0^{(n+1)/2}}{l_1^{(n-1)/2}}K_{(n-1)/2}(2\pi s_0 l_1)-2\pi\int_0^\infty ds_1\, f(s_1)\frac{s_1^{(n+1)/2}}{l_1^{(n-1)/2}}N_{(n-1)/2}(2\pi s_1 l_1), \tag{27}$$

using the results of Sec. II B, and, again, formulas 8.472(2) and 8.486(13) from Ref. 5.

For even n, the Fourier transform with a timelike momentum has no contribution from the spacelike region of space–time.

We can summarize both cases in the following formulas, now valid for arbitrary n:

$$F^{(n)}(l_0)=-2\pi\int_0^\infty ds_0 f(s_0)\frac{s_0^{(n+1)/2}}{l_0^{(n-1)/2}}\left[N_{(n-1)/2}(2\pi s_0 l_0)\cos\left(\pi\frac{n-1}{2}\right)\right.$$
$$\left.+J_{(n-1)/2}(2\pi s_0 l_0)\sin\left(\pi\frac{n-1}{2}\right)\right]$$
$$+4\int_0^\infty ds_1 f(s_1)\frac{s_1^{(n+1)/2}}{l_0^{(n-1)/2}}K_{(n-1)/2}(2\pi s_1 l_0)\cos\left(\pi\frac{n-1}{2}\right),$$

$$F^{(n)}(l_1)=4\int_0^\infty ds_0 f(s_0)\frac{s_0^{(n+1)/2}}{l_1^{(n-1)/2}}K_{(n-1)/2}(2\pi s_0 l_1)-2\pi\int_0^\infty ds_1 f(s_1)\frac{s_1^{(n+1)/2}}{l_1^{(n-1)/2}}N_{(n-1)/2}(2\pi s_1 l_1).$$

APPENDIX: DERIVATION OF EQ. (15)

Equation (15) can be derived in several different ways. For direct integration see, e.g., Ref. 6, Chap. 4. We follow here a derivation presented in Ref. 7.

We define the Fourier transform on $\mathbb{R}^n$ by

$$F(k_1,\ldots,k_n)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}dx_1\cdots dx_n\, f(x_1,\ldots,x_2)\exp(-2\pi i(k_1x_1+\cdots+k_nx_n)), \quad \text{(A1)}$$

or short

$$F(\vec{k})=\int_{\mathbb{R}^n}d^nx\, f(\vec{r})\exp(-2\pi i\vec{k}\cdot\vec{r}) \quad \text{(A2)}$$

and the inverse Fourier transform by

$$f(\vec{r})=\int_{\mathbb{R}^n}d^nk\, F(\vec{k})\exp(2\pi i\vec{k}\cdot\vec{r}). \quad \text{(A3)}$$

One property we will need is

$$\Delta^2 f(\vec{r})=\sum_m\frac{\partial^2 f}{\partial x_m^2}=-4\pi^2\int_{\mathbb{R}^n}d^nk\, k^2F(\vec{k})\exp(2\pi i\vec{k}\cdot\vec{r}). \quad \text{(A4)}$$

Now assume we have a radial function, and we work in spherical coordinates. We would like to write the Fourier transformation as

$$F(k)=\int_0^\infty dr\, f(r)\chi_n(r,k) \quad \text{(A5)}$$

and the inverse Fourier transform as

$$f(r)=\int_0^\infty dk\,F(k)\chi_n(k,r), \tag{A6}$$

where the χ's contain the integration over the compact $n-1$ angular coordinates. From Eq. (A4) we also know

$$\Delta^2 f(r)=-4\pi^2\int_0^\infty dk\,k^2\chi_n(k,r)F(k). \tag{A7}$$

Calculating $\Delta^2 f(r)$ [now starting with Eq. (A6)],

$$\frac{\partial^2 f(r)}{\partial x_m^2}=\int_0^\infty dk\,F(k)\,\frac{\partial^2}{\partial x_m^2}\chi_n(k,r),$$

where

$$\frac{\partial^2}{\partial x_m^2}\chi_n(k,r)=\left(\frac{1}{r}-\frac{x_m^2}{r^3}\right)\frac{\partial}{\partial r}\chi_n(k,r)+\frac{x_m^2}{r^2}\,\frac{\partial^2}{\partial r^2}\chi_n(k,r)$$

yields

$$\Delta^2 f(r)=\sum_m\,\frac{\partial^2 f(r)}{\partial x_m^2}=\int_0^\infty dk\,F(k)\left(\frac{n-1}{r}\,\frac{\partial}{\partial r}\chi_n(k,r)+\frac{\partial^2}{\partial r^2}\chi_n\right). \tag{A8}$$

But with Eq. (A7),

$$\int_0^\infty dk\,F(k)\left[\frac{\partial^2}{\partial r^2}\chi_n(k,r)+\frac{n-1}{r}\,\frac{\partial}{\partial r}\chi_n(k,r)+4\pi^2k^2\chi_n(k,r)\right]=0. \tag{A9}$$

This equation is valid for arbitrary $F(k)$, so the expression in brackets has to be zero. This ODE (in r) has the general solution (see Ref. 8, p. 146)

$$\chi_n(k,r)=A_n(k)r^{1-n/2}Z_p(2\pi kr), \tag{A10}$$

where $A_n(k)$ is determined by the initial conditions, Z is a Bessel function of order p, and $p=\pm(1-n/2)$. Computing the inverse Fourier transform explicitly in the cases of $n=1$ and $n=2$, determines p to be $n/2-1$.

To find A_n, consider $f(r)$ at $r=0$,

$$f(0)=\int_0^\infty dk\,F(k)\chi_n(k,0).$$

From Eq. (A10) we have

$$\begin{aligned}\chi_n(k,0)&=\lim_{r\to 0}A_n(k)r^{1-n/2}J_{n/2-1}(2\pi rk)\\&=A_n(k)\,\frac{r^{1-n/2}(\pi rk)^{n/2-1}}{\Gamma(n/2)}\\&=A_n(k)\,\frac{(\pi k)^{n/2-1}}{\Gamma(n/2)},\end{aligned}$$

where 9.1.7 from Ref. 9 has been used.

But according to the definition of the inverse Fourier transform

$$f(0)=\int_{\mathbb{R}^n} dk^n\, F(k)=\frac{\pi^{n/2}n}{\Gamma(1+n/2)}\int_0^\infty dk\, k^{n-1}F(k).$$

The factor in front of the integral is the volume of the unit $n-1$-sphere. Equating both expressions for $f(0)$, which are valid for arbitrary $F(k)$, yields

$$A_n(k)=2\pi k^{n/2},$$

and therefore as the final result

$$\chi_n(k,r)=2\pi k^{n/2}r^{1-n/2}J_{n/2-1}(2\pi rk). \tag{A11}$$

Because of the symmetry of the transformation

$$\chi_n(r,k)=2\pi r^{n/2}k^{1-n/2}J_{n/2-1}(2\pi rk). \tag{A12}$$

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Erratum: "Contact metric 5-manifolds, CR twistor spaces and integrability," [J. Math. Phys. 43, 3783 (2002)]

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[DOI: 10.1063/1.1521523]

The scalar curvature conditions in Theorem 1.1, Corollary 1.1 and in Theorem 1.3 are not necessary. These theorems must be changed as follows.

Theorem 1.1: Let (M,η,ξ,ϕ,g) be a K-contact 5-manifold and $\mathcal{Z}=\mathbf{U}(\Lambda^2_-(\mathbf{E}^*))$ its CR twistor space.

Then, $\mathcal{J}$ on $\mathcal{Z}$ is integrable if and only if (M,g) is self-dual contact metric, in other words, $\mathcal{W}^-_-$ vanishes.

Corollary 1.1: Let (M,η,ξ,ϕ,g) be a K-contact 5-manifold. The almost complex manifold $(\mathcal{Z}\times\mathbf{R},\mathcal{I})$ is integrable if

$$\mathcal{W}^-_-=0 \quad \text{and} \quad \mathcal{R}^-_o=\mathcal{W}^-_o+\mathcal{B}^-_o=0.$$

Theorem 1.3: Let (M,η,ξ,ϕ,g) be a K-contact 5-manifold which is an S^1-principal bundle over a 4-manifold N with a connection form η. Then the CR twistor space $\mathcal{Z}$ of M is integrable if and only if N is self-dual, i.e., $\mathcal{W}^-_N=0$.

The proof of Corollary 1.1 and Theorem 1.3 is based on Theorem 1.1. So, we will recover the proof of Theorem 1.1 to correct its parts 3 and 4, pages 3795–3796.

3. Take another local section e' of $P_{\mathbf{E}}$; $e':U\to P_{\mathbf{E}}$, $e'=(e'_1,\cdots,e'_4)$. e' is then written as

$$e'=e\ \ a$$

for a mapping $a:U\to\mathrm{SO}(4)$.

The almost complex structure $J'=J^{\Phi_u(e')}$ of $\mathbf{E}_y$ at $y\in U$, defined in terms of u and e', satisfies

$$J'(e'_1)=e'_2,\quad J'(e'_3)=-e'_4.$$

To see this, define a linear transformation of $\mathbf{E}_y$ by

$$A=A_a\ :\ \mathbf{E}_y\to\mathbf{E}_y;X=\sum\ x^ie_i\mapsto A(X)=\sum\ x^ie'_i$$

and observe that one writes

$$J'=AJA^{-1}$$

in terms of the $J=J^{\Phi_u(e)}$. This is from the definition of J';

$$(e')^{-1}(J'X)\cdot u=\sqrt{-1}((e')^{-1}(X)\cdot u),X\in\mathbf{E}_y$$

where we regard the sections e and e' in $P_{\mathbf{E}}$ at y as linear mappings $:\mathbf{R}^4\to\mathbf{E}_y$.

By using the section e' of $P_{\mathbf{E}}$ we identify

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$$P_{\mathbf{E}}|_U = U \times SO(4); \quad e'(y)a \leftrightarrow (y,a).$$

So the horizontal lift of e'_i, $i=1,\cdots,4$, is

$$Z'_i = e'_i - (\omega^{\mathbf{E}}(e'_i))^*.$$

Here $\omega^{\mathbf{E}}(\cdot)$ is the connection matrix of $\nabla^{\mathbf{E}}$ relative to the orthonormal frame field $e' = (e'_1, \cdots, e'_4)$;

$$\omega^{\mathbf{E}}(X) = \sum_{j,k=1}^{4} \omega^{\mathbf{E}}_{j'k'}(X) E_{j'k'}, \quad \nabla^{\mathbf{E}}_X e'_i = \sum_{j=1}^{4} \omega^{\mathbf{E}}_{j'k'}(X) e'_j.$$

We have then from the definition of $\hat{\mathcal{J}}$

$$\hat{\mathcal{J}}(Z'_1) = Z'_2, \quad \hat{\mathcal{J}}(Z'_3) = -Z'_4.$$

So, the relation (ii″) in **A** is in this case that at a point $e'(x) \in P_{\mathbf{E}}$, $x \in U$

$$\hat{\mathcal{J}}^{q'}(\Omega^{\mathbf{E}}_{e'}(Z'_1 - \sqrt{-1}Z'_2, Z'_3 + \sqrt{-1}Z'_4))^* - \sqrt{-1}(\Omega^{\mathbf{E}}_{e'}(Z'_1 - \sqrt{-1}Z'_2, Z'_3 + \sqrt{-1}Z'_4))^*$$

is spanned by $\mathfrak{h}$. This means that the Y_5- and Y_6-components must vanish.

Without loss of generality we assume $\omega^{\mathbf{E}}$ vanishes at the point x of U.

Denote by $\theta'_1, \cdots, \theta'_4$ the dual frame of e'. Then, by calculating similarly as in **A** and **B** we have

$$\mathcal{W}(\theta'_1 \wedge \theta'_4 - \theta'_2 \wedge \theta'_3, \theta'_1 \wedge \theta'_4 - \theta'_2 \wedge \theta'_3) = \mathcal{W}(\theta'_1 \wedge \theta_3 + \theta'_2 \wedge \theta'_4, \theta'_1 \wedge \theta'_3 + \theta'_2 \wedge \theta'_4), \tag{21′}$$

$$\mathcal{W}(\theta'_1 \wedge \theta'_4 - \theta'_2 \wedge \theta'_3, \theta'_1 \wedge \theta'_3 + \theta'_2 \wedge \theta'_4) = 0. \tag{22′}$$

We now choose a particular $a \in \mathrm{SO}(4)$ such that at $x \in U$

$$\theta'_1 \wedge \theta'_4 - \theta'_2 \wedge \theta'_3 = \theta_1 \wedge \theta_2 - \theta_3 \wedge \theta_4,$$

$$\theta'_1 \wedge \theta'_3 + \theta'_2 \wedge \theta'_4 = \theta_1 \wedge \theta_3 + \theta_2 \wedge \theta_4$$

which we denote by σ_1 and σ_2, respectively. So, we have from (21′)

$$\mathcal{W}(\sigma_1, \sigma_1) = \mathcal{W}(\sigma_2, \sigma_2).$$

By a similar argument

$$\mathcal{W}(\sigma_1, \sigma_1) = \mathcal{W}(\sigma_3, \sigma_3),$$

where we set $\sigma_3 = \theta_1 \wedge \theta_4 - \theta_2 \wedge \theta_3$.

Moreover, we choose a suitable $a \in \mathrm{SO}(4)$ so that from (22′)

$$\mathcal{W}(\sigma_i, \sigma_j) = 0, \quad i \neq j$$

from which it follows

$$\mathcal{W}^- = 0.$$

As a concrete example of CR twistor space, we take a standard 5-sphere S^5 which is K-contact and also conformally flat and consider a subspace $\mathcal{Z}^- \subset S^5 \times (\mathbf{C}P^2)^*$, more precisely

$$\mathcal{Z}^- = \left\{ (z,[w]) \middle| z \in S^5, \quad [w]=[w_1:w_2:w_3] \in (\mathbf{C}P^2)^*, \quad \sum_i z_i w_i = 0 \right\}.$$

This space turns out by Theorem 1.3 to be the CR twistor space over S^5, since the Hopf fibration $\pi: S^5 \to \mathbf{C}P^2$ is the Boothby-Wang fibration and the Penrose twistor space of $\mathbf{C}P^2$ is the flag manifold F_3 in $\mathbf{C}^3$. Thus the canonical projection π yields the S^1 fibration: $\mathcal{Z}^- \to F_3$ between the CR twistor space and the Penrose twistor space.

The author is thankful to Dr. D. Kobayashi for pointing him to the erratum.

Scattering on compact manifolds with infinitely thin horns

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(Received 19 September 2002; accepted 1 November 2002)

The quantum-mechanical scattering on a compact manifold with semi-axes attached to the manifold (''hedgehog-shaped manifold'') is considered. The complete description of the spectral structure of Schrödinger operators on such a manifold is done, the proof of existence and uniqueness of scattering states is presented, an explicit form for the scattering matrix is obtained and unitarity of this matrix is proven. It is shown that the positive part of the spectrum of the Schrödinger operator on the initial compact manifold as well as the spectrum of a point perturbation of such an operator may be recovered from the scattering amplitude for one attached half-line. Moreover, the positive part of the spectrum of the initial Schrödinger operator is fully determined by the conductance properties of an ''electronic device'' consisting of the initial manifold and two ''wires'' attached to it. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1534893]

I. INTRODUCTION

In the paper of Ref. 1, Faddeev initiated the investigation of the quantum mechanical scattering on manifolds of constant negative curvature with cusps (sometimes also called ''horns[2];'' further developments of this theory are presented, e.g., in Refs. 3–6. It is interesting to note that an explicit expression for the reflection coefficient in the case of one horn was obtained earlier by Godement.[7] Note also that Gutzwiller has revealed a relation between the scattering theory on manifolds with horns and the description of chaotic behavior of quantum systems.[2,8,9]

If we imagine the width of the horns tending to zero, then we obtain a so-called hedgehog-shaped topological space (or ''horned manifold''). Strictly speaking, we consider the limit of a family of horned spaces in the sense of the Hausdorff–Gromov distance.[10] The simplest specimen of such a manifold is the Euclidean plane with an attached half-line. The quantum mechanical scattering in this system has been investigated for the first time by Exner and Šeba;[11] in Ref. 12 these authors consider a compact plane domain with a half-line glued to it. A series of significant physical applications of the corresponding results as well as an intensive bibliography related to the subject in question may be found in the paper of Ref. 13; we may add that the considered problem is also connected with the scattering on graphs.[14–19] An explicit expression for the transmission coefficient in the case of two half-lines (''wires'') attached to a compact Riemannian manifold of dimension two or three with some special boundary conditions at the points of gluing has been obtained by Kiselev.[20] A general method of solving the transmission problem through an arbitrary quantum device was proposed in Ref. 21, this method is based on an approach to the modeling of quantum systems developed by Pavlov;[22] some of its applications are given, e.g., in Refs. 23–27. Many-terminal problems for a bounded domain in $\mathbb{R}^d$ ($d=2$ or 3) with wires attached to the boundary of the domain are considered recently in Refs. 28 and 29.

In this paper we consider the quantum mechanical scattering in a hedgehog-shaped space which is constructed by gluing a finite number of half-lines to distinct points of a compact Riemannian manifold of dimension less than four. The Hamiltonian of a quantum particle in such

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a system coincides with a Schrödinger operator on the punctured manifold (the points of gluing are removed) and with the free Schrödinger operator on each half-line. At the gluing points, some boundary conditions are imposed. In particular, the Schrödinger operator in a magnetic field is included in our scheme. The approach we use is based on the Krein resolvent formula from operator extension theory,[30] therefore in Sec. II we give a very brief sketch of results needed from this theory. Section III is devoted to the construction of Schrödinger operators on the hedgehog-shaped space; we use the theory of boundary value spaces[31] to describe all possible kinds of boundary conditions defining the Schrödinger operators. We distinguish among them operators of ''Dirichlet'' and of ''Neumann'' type. It is worth noting that the results of Sec. III are valid for all Riemannian manifolds of dimension less than four, not only for the compact ones. In principle, the definition of the Schrödinger operator on a hedgehog-shaped space may be given in the framework of pseudo-differential operator theory on such a space,[32] but our approach is more convenient for investigating the scattering parameters and connected with the approach to spectral problems for point perturbations on Riemannian manifolds.[33,34]

The main results of the paper are contained in Secs. IV and V. Here we get a complete description of the spectral structure of Schrödinger operators on hedgehog-shaped spaces (Theorem 4), the proof of existence and uniqueness of scattering states (Theorem 5), and the proof of the unitary nature of the scattering matrix (Theorem 6). An explicit form for the scattering matrix is given in the cases of arbitrary Schrödinger operator on the hedgehog-shaped space [Formula (67)]. In the particular case of the boundary conditions of Neumann types our formulas contain the main result of Kiselev[20] as a very special case. Theorem 7 from Sec. V shows that the positive part of the spectrum of the initial Schrödinger operator on the compact manifold as well as the spectrum of a point perturbation of such an operator may be recovered from the scattering amplitude for one attached half-line (so, an ''infinitely thin horn'' may be considered as a kind of ''quantum stethoscope''). Moreover, the positive part of the spectrum of the initial Schrödinger operator is fully determined by the conductance properties of an ''electronic device'' consisting of the initial manifold and two ''wires'' attached to it (Propositions 8 and 9). We can choose the boundary conditions in such a way, that in the limiting case when wires are attached at the same point, the scattering matrix coincides with that for the δ'-interaction on the line. This fact is related to a conjecture from Ref. 35: the scattering on the ''δ'-potential'' may be realized geometrically. Finally, in Sec. VI we give a series of examples in which the Krein $\mathcal{Q}$-function entering our expressions for the scattering matrix may be obtained in an explicit form. Note that some applications of the results of this paper to the conductance of the quantum sphere were considered recently in Ref. 36. Some aspects of the geometric scattering on noncompact Riemannian manifolds within the framework of the approach presented here are discussed in Ref. 37.

II. PRELIMINARIES

Here we rephrase some results of operator extension theory using the language of boundary value spaces and linear symplectic geometry (see, e.g., Refs. 22, 31, 38–41 for details).

Let V be a complex vector space with a skew-Hermitian sesquilinear form $[x|y]$; this form can be degenerate, moreover, it is degenerate in the case of nontrivial problems of the symplectic geometry. The orthogonality with respect to this form will be denoted by $[\perp]$: $x[\perp]y$ means that $[x|y]=0$; the orthogonal complement of a set $X\subset V$ is denoted as $X^{[\perp]}$. A subspace $\Lambda\subset V$ is called *isotropic* (respectively, *Lagrangian*) if $\Lambda\subset\Lambda^{[\perp]}$ (respectively, $\Lambda=\Lambda^{[\perp]}$). If $\mathcal{H}$ is a Hilbert space with the scalar product $\langle x|y\rangle$,[1] then the Hilbert space $\mathcal{H}\oplus\mathcal{H}$ is endowed with the *standard* skew-Hermitian form

$$[x|y]=\langle x_1|y_2\rangle-\langle x_2|y_1\rangle\,,$$

i.e., $[x|y]=\langle x|Jy\rangle$, where $J:\mathcal{H}\oplus\mathcal{H}\to\mathcal{H}\oplus\mathcal{H}$ is a unitary operator of the form $J(x_1,x_2)=(x_2,-x_1)$. (Throughout this paper, we assume that the scalar product is linear with respect to the *second* argument.) It is clear that $[x|y]$ is a continuous sesquilinear form on the Hilbert space $\mathcal{H}\oplus\mathcal{H}$, hence, every Lagrangian subspace in $\mathcal{H}\oplus\mathcal{H}$ is closed. Moreover, for every subset $X\subset\mathcal{H}$

$\oplus\mathcal{H}$ we have $X^{[\perp]}=(JX)^{\perp}=J(X^{\perp})$, where $X^{\perp}$ is the orthogonal complement with respect to the standard scalar product $\langle x|y\rangle$ in $\mathcal{H}\oplus\mathcal{H}$: $\langle x|y\rangle=\langle x_1|y_1\rangle+\langle x_2|y_2\rangle$. Therefore, a subspace $\Lambda\subset\mathcal{H}\oplus\mathcal{H}$ is isotropic (respectively, Lagrangian) iff $J\Lambda\subset\Lambda^{\perp}$ (respectively, $J\Lambda=\Lambda^{\perp}$).

For every skew-Hermitian sesquilinear form $[x|y]$ the form $i[x|y]$ is Hermitian (generally speaking, degenerate); therefore the geometry of a skew-Hermitian sesquilinear form does not differ from that of a Hermitian form. Nevertheless, the symplectic language is very useful in operator extension theory. For example, let $A:\mathcal{D}(A)\to\mathcal{H}$ be a densely defined linear operator in $\mathcal{H}$ with the graph $\mathrm{Gr}(A)$, $\mathrm{Gr}(A)\subset\mathcal{H}\oplus\mathcal{H}$. Then it is easy to check the following statements:

(1) *A is symmetric if and only if* $\mathrm{Gr}(A)$ *is an isotropic subspace of* $\mathcal{H}\oplus\mathcal{H}$.
(2) *A is self-adjoint if and only if* $\mathrm{Gr}(A)$ *is a Lagrangian subspace of* $\mathcal{H}\oplus\mathcal{H}$.

Remark 1: It is clear that every Lagrangian subspace is a maximal isotropic subspace, the converse is not true even in the one-dimensional case. On the other hand, if V is a finite-dimensional complex space having at least one Lagrangian subspace, then according to the Witt theorem,[42] every maximal isotropic subspace is Lagrangian. Therefore, in the finite-dimensional space $V=\mathcal{H}\oplus\mathcal{H}$ every maximal isotropic subspace is Lagrangian. On the contrary, let $\mathcal{H}$ be an infinite-dimensional Hilbert space, and let A be a maximal symmetric operator in $\mathcal{H}$ which is not self-adjoint. Then $\mathrm{Gr}(A)$ is a maximal isotropic subspace of $\mathcal{H}\oplus\mathcal{H}$ which is not Lagrangian.

A linear mapping $u:V_1\to V_2$ of complex vector spaces V_1, V_2 with skew-Hermitian forms $[\,\cdot\,|\,\cdot\,]_1$, $[\,\cdot\,|\,\cdot\,]_2$, respectively, is called *skew-unitary* if $[u(x)|u(y)]_2=[x|y]_1\ \forall\, x,y\in V_1$. Now let S be a symmetric operator in $\mathcal{H}$; in the graph $\mathrm{Gr}(S^*)$ of S^* we shall consider the skew-Hermitian form induced by the standard form from $\mathcal{H}\oplus\mathcal{H}$. A pair $(\mathcal{G},\Gamma)$, where $\mathcal{G}$ is a Hilbert space and Γ is a surjective skew-unitary mapping from $\mathrm{Gr}(S^*)$ onto $\mathcal{G}\oplus\mathcal{G}$ is called *a boundary value space* for S. It is known that a boundary value space for S exists if and only if the deficiency indices $n_+(S)$ and $n_-(S)$ for S coincide, i.e., if and only if S has a self-adjoint extension. If this is the case and $(\mathcal{G},\Gamma)$ is a boundary value space for S, then $\dim\mathcal{G}=n_+(S)(=n_-(S))$ and Γ is a continuous operator with respect to the standard Hilbert space topologies in $\mathrm{Gr}(S^*)$ and $\mathcal{G}\oplus\mathcal{G}$. Let $\hat{\Gamma}:\mathcal{D}(S^*)\to\mathcal{G}\oplus\mathcal{G}$ be the composition of the canonical bijection $\mathcal{D}(S^*)\to\mathrm{Gr}(S^*)$ $(x\mapsto(x,S^*x))$ and Γ; it is clear that $\hat{\Gamma}$ is surjective. Moreover, if $\mathcal{D}(S^*)$ is endowed with the graph scalar product $\langle x|y\rangle_S=\langle x|y\rangle+\langle S^*x|S^*y\rangle$, then $\hat{\Gamma}$ is continuous. Denote by P_1 and P_2 the canonical projections of $\mathcal{G}\oplus\mathcal{G}$ onto $\mathcal{G}\oplus\{0\}$ and $\{0\}\oplus\mathcal{G}$, respectively, and by $\Gamma^{(1)}$, $\Gamma^{(2)}$ the operators $P_1\hat{\Gamma}$ and $P_2\hat{\Gamma}$, respectively. Then for all $x,y\in\mathcal{D}(S^*)$ the following relation is valid:

$$\langle x|S^*y\rangle-\langle S^*x|y\rangle=\langle\Gamma^{(1)}x|\Gamma^{(2)}y\rangle-\langle\Gamma^{(2)}x|\Gamma^{(1)}y\rangle\,. \tag{1}$$

Conversely, a triple $(\mathcal{G},\Gamma^{(1)},\Gamma^{(2)})$, where $\mathcal{G}$ is a Hilbert space and $\Gamma^{(j)}:\mathcal{D}(S^*)\to\mathcal{G}$ $(j=1,2)$ are linear operators, uniquely defines a boundary value space, if the mapping $\mathcal{D}(S^*)$ $\ni x\mapsto(\Gamma^{(1)}x,\Gamma^{(2)}x)\in\mathcal{G}\oplus\mathcal{G}$ is surjective and the condition (1) holds. Indeed, it is sufficient to define Γ by the rule $\Gamma(x,S^*x)=(\Gamma^{(1)}x,\Gamma^{(2)}x)$. The triple $(\mathcal{G},\Gamma^{(1)},\Gamma^{(2)})$ is also called a boundary value space for S.

The following theorem describes all self-adjoint extensions of S with help of the boundary value space.

Theorem A: *Let S be a symmetric operator in a Hilbert space $\mathcal{H}$ with equal deficiency indices, and let $(\mathcal{G},\Gamma)$ be a boundary value space for S. Then for every Lagrangian subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ the set $\Gamma^{-1}(\Lambda)$ is the graph of a self-adjoint operator H^{Λ} that is a self-adjoint extension of S. Moreover, the correspondence $\Lambda\mapsto H^{\Lambda}$ is a bijection between all Lagrangian subspaces of $\mathcal{G}\oplus\mathcal{G}$ and all self-adjoint extensions of S.* ■

In other words, the self-adjoint extension H^{Λ} is defined by the boundary condition

$$(\Gamma^{(1)}x,\Gamma^{(2)}x)\in\Lambda\,. \tag{2}$$

More precisely, the domain of H^Λ is the subspace of $\mathcal{D}(S^*)$ given by $\mathcal{D}(H^\Lambda)=\{x \in \mathcal{D}(S^*)\colon (\Gamma^{(1)}x,\Gamma^{(2)}x)\in\Lambda\}$, and H^Λ is the restriction of S^* to $\mathcal{D}(H^\Lambda)$. Condition (2) can be written in a more convenient "operator" form. Namely, for every Lagrangian subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ there exists a uniquely defined unitary operator U_Λ acting in $\mathcal{G}$ such that the relations $(x_1,x_2)\in\Lambda$ and $i(I+U_\Lambda)x_1=(I-U_\Lambda)x_2$ are equivalent; U_Λ is called the *Cayley transform* for Λ. (If Λ is the graph of a self-adjoint operator L in $\mathcal{G}$, then U_Λ is just the Cayley transform for L.) Moreover, the correspondence $\Lambda\mapsto U_\Lambda$ is a bijection between the sets of all Lagrangian subspaces of $\mathcal{G}\oplus\mathcal{G}$ and all unitary operators in $\mathcal{G}$. Using the notations above we can rewrite condition (2) in the desired operator form:

$$(I-U_\Lambda)\Gamma^{(2)}x=i(I+U_\Lambda)\Gamma^{(1)}x\,.$$

It is clear that a given Lagrangian subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ has different equations of the form $Lx_1=Mx_2$, where L and M are bounded linear operators in $\mathcal{G}$. Hence, a given boundary condition $(\Gamma^{(1)}x,\Gamma^{(2)}x)\in\Lambda$ may be represented in the operator form

$$L\Gamma^{(1)}x=M\Gamma^{(2)}x, \tag{3}$$

in many ways. Denote by $A(L,M)$ the bounded operator from $\mathcal{G}\oplus\mathcal{G}$ to $\mathcal{G}$ taking $x=(x_1,x_2)\in\mathcal{G}\oplus\mathcal{G}$ to $Lx_1-Mx_2\in\mathcal{G}$.

Proposition B: Let $L,M\colon\mathcal{G}\to\mathcal{G}$ be bounded linear operators. The subspace Λ of $\mathcal{G}\oplus\mathcal{G}$ determined by the equation $Lx_1=Mx_2$ is Lagrangian if and only if the following conditions are satisfied: (a) $LM^*=ML^*$; (b) the restriction of $A(L,M)$ to the subspace $J(\Lambda)$ is injective.

Proof: First of all we prove the equivalence of the following assertions:

(1) $\Lambda\supset\Lambda^{[\perp]}$; (2) $LM^*=ML^*$.

Indeed, by definition $\Lambda=\mathrm{Ker}\,A(L,M)$; on the other hand we have the well-known relation $\mathrm{Ker}\,A(L,M)^\perp=\overline{\mathrm{Ran}\,A(L,M)^*}$. Since $\mathrm{Ker}\,A(L,M)$ is closed, condition (1) is equivalent to the condition (3) $J(\mathrm{Ker}A(L,M))\supset\mathrm{Ran}A(L,M)^*$. Because $A(L,M)^*x=(L^*x,-M^*x)$ for every $x\in\mathcal{G}$, the equivalence of (2) and (3) follows immediately.

Now let Λ be a Lagrangian subspace, then $J(\Lambda)=\mathrm{Ker}\,A(L,M)^\perp$; therefore, the restriction of $A(L,M)$ to $J(\Lambda)$ is obviously injective. On the other hand, if conditions (a) and (b) are satisfied, then $J(\Lambda)\supset\Lambda^\perp$. Moreover, if $J(\Lambda)\neq\Lambda^\perp$, then $J(\Lambda)$ contains a nonzero element from $\mathrm{Ker}\,A(L,M)$, and we have a contradiction with (b). ∎

Note that a finite-dimensional version of Proposition B has been given in Ref. 17, based on different arguments.

The self-adjoint extensions of S defined by the conditions $\Gamma^{(1)}x=0$ and $\Gamma^{(2)}x=0$ will be denoted by $H^{(1)}$ and $H^{(2)}$, respectively; they correspond to the Lagrangian subspaces $\{0\}\oplus\mathcal{G}$ and $\mathcal{G}\oplus\{0\}$, respectively. If Λ is the graph of a self-adjoint operator L in $\mathcal{G}$ [i.e., if Λ is transversal to $\{0\}\oplus\mathcal{G}$: $\Lambda\cap(\{0\}\oplus\mathcal{G})=\{0\}$], then the condition (2) takes the simpler form

$$\Gamma^{(2)}x=L\Gamma^{(1)}x\,. \tag{4}$$

The self-adjoint extension H^Λ of S is defined by a boundary condition of the form (4) with a self-adjoint L, if and only if H^Λ is disjoint from $H^{(1)}$ [this means that $\mathcal{D}(H^{(1)})\cap\mathcal{D}(H^\Lambda)=\mathcal{D}(S)$].

On the other hand, at least in the case of a finite-dimensional $\mathcal{G}$ we can always define a given extension H^Λ by a condition of the form (4). This may be done with the help of the above mentioned Witt theorem, but a more useful way is to use the complex version of the Arnold Lemma.[43] To state this lemma we need some auxiliary notations. Let $\mathbf{e}_1,\ldots,\mathbf{e}_n$ be a fixed orthonormal basis in $\mathcal{G}$, then the vectors $\mathbf{a}_j=(\mathbf{e}_j,0)$ and $\mathbf{b}_j=(0,\mathbf{e}_j)$ $(j=1,\ldots,n)$ form a symplectic basis in $\mathcal{G}\oplus\mathcal{G}$:

$$[\mathbf{a}_j|\mathbf{a}_k]=[\mathbf{b}_j|\mathbf{b}_k]=0\,,\quad [\mathbf{a}_j|\mathbf{b}_k]=-[\mathbf{b}_k|\mathbf{a}_j]=\delta_{jk}\,. \tag{5}$$

Let η be a subset of $\{1,\ldots,n\}$, $\eta'=\{1,\ldots,n\}\setminus\eta$; by virtue of (5) the linear hull of the set $\{\mathbf{a}_j : j \in \eta\}\cup\{\mathbf{b}_j : j\in\eta'\}$, is a Lagrangian subspace of $\mathcal{G}\oplus\mathcal{G}$ which is called a *coordinate subspace* and denoted by $\mathcal{G}_\eta$. It is clear that if $\eta=\{1,\ldots,n\}$, then $\mathcal{G}\oplus\{0\}=\mathcal{G}_\eta$, $\{0\}\oplus\mathcal{G}=\mathcal{G}_{\eta'}$.

Proposition C (Arnold's Lemma): Let $\mathcal{G}$ be finite-dimensional. Then every Lagrangian subspace of $\mathcal{G}\oplus\mathcal{G}$ is transversal to some coordinate subspace. ■

Moreover, $\mathcal{G}\oplus\mathcal{G}=\mathcal{G}_\eta\oplus\mathcal{G}_{\eta'}$ where the sums are orthogonal with respect to the standard scalar product $\langle x|y\rangle$ in $\mathcal{G}\oplus\mathcal{G}$. Denote the orthoprojection of $\mathcal{G}\oplus\mathcal{G}$ onto $\mathcal{G}_\eta$ by P_η; by $J_\eta^{(1)}$ we shall denote the isomorphism of $\mathcal{G}_\eta$ onto $\mathcal{G}$ which takes the elements from $\mathcal{G}_\eta$ of the form $\mathbf{a}_j$ or $\mathbf{b}_j$ to $\mathbf{e}_j$, by $J_\eta^{(2)}$ we denote the isomorphism of $\mathcal{G}_{\eta'}$ onto $\mathcal{G}$ which takes the elements from $\mathcal{G}_\eta$ of the form $\mathbf{a}_j$ to $-\mathbf{e}_j$ and of the form $\mathbf{b}_j$ into $\mathbf{e}_j$. Let now $(\mathcal{G},\Gamma)$ be a boundary value space for a symmetric operator S; denote $\Gamma_\eta^{(1)}=J_\eta^{(1)}P_\eta\Gamma$, $\Gamma_\eta^{(2)}=J_\eta^{(2)}P_\eta\Gamma$. Then the triple $(\mathcal{G},\Gamma_\eta^{(1)},\Gamma_\eta^{(2)})$ is a boundary value space for S as well. For example, if $\eta=\{1,\ldots,n\}$, then $\Gamma_\eta^{(j)}=\Gamma^{(j)}$; on the other hand, $\Gamma_\varnothing^{(1)}=\Gamma^{(2)}$, $\Gamma_\varnothing^{(2)}=-\Gamma^{(1)}$.

By virtue of the Arnold lemma, for every Lagrangian subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ there exists $\eta\subset\{1,\ldots,n\}$ such that the self-adjoint extension H^Λ is given by the boundary condition of the form $\Gamma_\eta^{(2)}x=L\Gamma_\eta^{(1)}x$ where L is a self-adjoint operator in $\mathcal{G}$. We shall denote this extension by $H^{L,\eta}$; the representation of H^Λ in the form $H^{L,\eta}$ is, clearly, not unique. The extensions of S defined by the conditions $\Gamma_\eta^{(j)}x=0$ $(j=1,2)$ will be defined by $H_\eta^{(j)}$.

There exists a very convenient expression for the resolvent $R^\Lambda(z)=(H^\Lambda-z)^{-1}$ of the operator H^Λ which is given by the so-called Krein resolvent formula. To give this formula, we need some preliminary notions (details may be found in Refs. 38 and 44. Let $z\in\mathbb{C}\setminus\mathbb{R}$, denote by $\mathcal{N}_z$ the deficiency subspace for S: $\mathcal{N}_z=\mathrm{Ker}\,(S^*-z)$. It may be proven that the restrictions of both the operators $\Gamma^{(j)}$ $(j=1,2)$ to $\mathcal{N}_z$ are linear-topological isomorphisms of $\mathcal{N}_z$ onto $\mathcal{G}$; we denote these restrictions as $\Gamma^{(j)}(z)$. Moreover, the operators $\gamma(z)=(\Gamma^{(1)}(z))^{-1}$ form a holomorphic family of elements from the Banach space $\mathcal{L}(\mathcal{G},\mathcal{H})$ of all linear continuous operators from $\mathcal{G}$ to $\mathcal{H}$. Further, the operators $Q(z)=\Gamma^{(2)}\gamma(z)$ form a holomorphic family in the Banach space $\mathcal{L}(\mathcal{G},\mathcal{G})$. The holomorphic operator-valued functions $z\mapsto\gamma(z)$ and $z\mapsto Q(z)$ have analytic continuations on the set $\rho(H^{(1)})$ of the regular values of $H^{(1)}$: $\rho(H^{(1)})=\mathbb{C}\setminus\sigma(H^{(1)})$. This assertion follows from the relations below, which are valid for every $z,\zeta\in\mathbb{C}\setminus\mathbb{R}$:

$$\gamma(z)=\gamma(\zeta)+(z-\zeta)(H^{(1)}-z)^{-1}\gamma(\zeta);$$

$$Q(z)-Q(\zeta)=(z-\zeta)\,\gamma^*(\overline{\zeta})\,\gamma(z).$$

The functions $\gamma:\rho(H^{(1)})\to\mathcal{L}(\mathcal{G},\mathcal{H})$ and $Q:\rho(H^{(1)})\to\mathcal{L}(\mathcal{G},\mathcal{G})$ are called Krein Γ-field and Krein $\mathcal{Q}$-function of the operator S associated with the boundary value space $(\mathcal{G},\Gamma)$.

Further, we shall consider a subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ as the graph of a multi-valued linear operator M_Λ with the domain $\mathcal{D}(M_\Lambda)=P_1(\Lambda)$. The operator M_Λ takes each $x\in\mathcal{D}(M_\Lambda)$ to an affine subspace $\{y\in\mathcal{G}:(x,y)\in\Lambda\}$ of $\mathcal{G}$. For every subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$ we denote by Λ^{-1} the "inverse" subspace $\Lambda^{-1}=\{(x,y)\in\mathcal{G}\oplus\mathcal{G}:(y,x)\in\Lambda\}$. In particular, if Λ is the graph of an invertible operator $L:\mathcal{D}(L)\to\mathcal{G}$, then Λ^{-1} is the graph of the inverse operator L^{-1}. In the following we shall identify mappings and their graphs if this does not lead to ambiguities.

Theorem D: *Let S be a symmetric operator in a Hilbert space $\mathcal{H}$ with boundary value space $(\mathcal{G},\Gamma)$, and let γ and Q be the corresponding Γ-field and $\mathcal{Q}$-function for S, respectively. Suppose that H^Λ is a self-adjoint extension of S associated with a Lagrangian subspace Λ of $\mathcal{G}\oplus\mathcal{G}$. Then for every $z\in\rho(H^{(1)})\cap\rho(H^\Lambda)$ the subspace $[Q(z)-\Lambda]^{-1}$ is the graph of a bounded (single-valued) operator in $\mathcal{G}$ and the resolvent of $R^\Lambda(z)=(H^\Lambda-z)^{-1}$ has the form*

$$R^\Lambda(z)=R^{(1)}(z)-\gamma(z)[Q(z)-\Lambda]^{-1}\gamma^*(\overline{z}), \tag{6}$$

where $R^{(1)}(z)=(H^{(1)}-z)^{-1}$ is the resolvent of $H^{(1)}$. ■

If H^Λ and $H^{(1)}$ are not disjoint, then the Krein formula (6) contains a multi-valued operator Λ. To avoid the use of such operators we can proceed as follows (see Ref. 44). Let Λ be a Lagrangian subspace of $\mathcal{G}\oplus\mathcal{G}$ and U_Λ be its Cayley transform. Denote by P_Λ the orthogonal projection of $\mathcal{G}$

onto subspace $\mathcal{G}_\Lambda = \overline{\mathrm{Ran}\,(U_\Lambda - I)}$, by J_Λ the canonical embedding of $\mathcal{G}_\Lambda$ into $\mathcal{G}$, and by I_Λ the identity operator in $\mathcal{G}_\Lambda$. Then $V_\Lambda = P_\Lambda U_\Lambda J_\Lambda$ is a unitary operator in $\mathcal{G}_\Lambda$, and 1 is not an eigenvalue of this operator. Therefore, $L = i(I_\Lambda + V_\Lambda)(I_\Lambda - V_\Lambda)^{-1}$ is a self-adjoint operator in $\mathcal{G}_\Lambda$, and

$$[Q(z) - \Lambda]^{-1} = J_\Lambda [P_\Lambda Q(z) J_\Lambda - L]^{-1} P_\Lambda . \tag{7}$$

Moreover, the following proposition holds.[44]

Proposition E: Let L_n be a self-adjoint operator in $\mathcal{G}$ of the form $L_n = J_\Lambda L P_\Lambda + n(I - P_\Lambda)$. Then for every $z \in \rho(H^{(1)}) \cap \rho(H^\Lambda)$,

$$\lim_{n\to\infty} [Q(z) - L_n]^{-1} = J_\Lambda [P_\Lambda Q(z) J_\Lambda - L]^{-1} P_\Lambda$$

in the strong operator topology. ■

If $\mathcal{G}$ is finite-dimensional, then we can adapt the Arnold Lemma to avoid the use of multivalued mappings in the Krein formula. Namely, denote the Krein Γ-field and $\mathcal{Q}$-function for the boundary value space $(\mathcal{G}, \Gamma_\eta^{(1)}, \Gamma_\eta^{(2)})$ by $\gamma_\eta(z)$ and $Q_\eta(z)$, respectively. Since H^Λ coincides with some operator of the form $H^{L,\eta}$; then (6) may be rewritten in the form

$$R^\Lambda(z) \equiv R^{L,\eta}(z) = R_\eta^{(1)}(z) - \gamma_\eta(z)[Q_\eta(z) - L]^{-1} \gamma_\eta^*(\overline{z}) , \tag{8}$$

where $R_\eta^{(1)}(z) = (H_\eta^{(1)} - z)^{-1}$.

III. SCHRÖDINGER OPERATOR ON A "HEDGEHOG-SHAPED" SPACE

Consider a complete (not necessarily connected) Riemannian manifold X of dimension d, with metric $g_{\mu\nu}$. We shall denote by g the determinant $\det(g_{\mu\nu})$, by $d\lambda$ the Riemannian measure, and by $r(x,y)$ the geodesic distance on X. Fix a nonempty finite subset $\{q_1, \ldots, q_n\}$ of X, and let $\mathbb{R}_+^{(j)}$ $(j = 1, \ldots, n)$ be copies of the half-line $\mathbb{R}_+ = \{x \in \mathbb{R}: x \geqslant 0\}$. Let $\hat{X}$ be the topological space obtained from the disjoint union $X \sqcup \mathbb{R}_+^{(1)} \sqcup \cdots \sqcup \mathbb{R}_+^{(n)}$ by gluing the point $0 \in \mathbb{R}_+^{(j)}$ to the point q_j. The "hedgehog-shaped" topological space $\hat{X}$ may be considered as a limit of manifolds with n horns as the widths of the horns tend to zero. Let $\mathcal{H}_0 := L^2(X, d\lambda)$, $\mathcal{H}_j := L^2(\mathbb{R}_+^{(j)}, dx)$. The sum of the Riemannian measure $d\lambda$ on X and the Lebesgue measures dx on $\mathbb{R}_+^{(j)}$ is a natural measure $d\mu$ on $\hat{X}$; the space $L^2(\hat{X}, d\mu)$ will be identified with the space $\mathcal{H} := \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_n$.

To define a Schrödinger operator on $\hat{X}$ we proceed as follows. Consider the symmetric operator τ in $\mathcal{H}_0$, with domain $C_0^\infty(X)$, defined by the differential expression

$$\tau = -g^{-1/2}(x)(\partial_\mu + i\mathcal{A}_\mu(x)) g^{1/2}(x) g^{\mu\nu}(x)(\partial_\nu + i\mathcal{A}_\nu(x)) + p(x) ,$$

where $\mathcal{A}_\mu$ $(\mu = 1, \ldots, d)$ and p are real-valued smooth functions on X. The functions $\mathcal{A}_\mu$ are the components of a vector potential $\mathcal{A}$, giving rise to a magnetic field on X. Similarly p may be viewed as the scalar potential whose gradient is an electric field. We denote the closure of τ in $\mathcal{H}_0$ by H_0, and suppose that the potentials $\mathcal{A}$ and p are chosen in such a way that H_0 is a self-adjoint operator in $\mathcal{H}_0$, i.e., we assume that τ is essentially self-adjoint. Note that this is the case, if $\mathcal{A}_\mu$ and p have compact supports, in particular, if X is compact. If $\mathcal{A} = 0$ and $p = 0$ we get the Laplace–Beltrami operator $-\Delta_X$ on X. To use the techniques of the operator extension theory we need the condition (C) $\mathcal{D}(H_0)$ *imbeds in* $C(X)$.

By virtue of the well-known Sobolev embedding theorems, this condition is satisfied if and only if $d \leqslant 3$. Therefore, *from this point on we suppose that* $0 < d \leqslant 3$.

Let now S_0 be the operator in $\mathcal{H}_0$ that is the restriction of H_0 to the domain

$$\mathcal{D}(S_0) = \{f \in \mathcal{D}(H_0): f(q_j) = 0, \quad \forall\, j = 1, \ldots, n\} .$$

It is clear that S_0 is symmetric in $\mathcal{H}_0$, and Lemma 4 below shows that the deficiency indices of S_0 are (n, n). Denote next by S_j $(j = 1, \ldots, n)$ the closure in $\mathcal{H}_j$ of the operator $-d^2/dx^2$ defined on

$C_0^\infty(0,\infty)$; S_j is a symmetric operator in $\mathcal{H}_j$ with the deficiency indices (1,1). Finally, we set $S := S_0 \oplus S_1 \oplus \cdots \oplus S_n$; it is evident that S is a symmetric operator in $\mathcal{H}$ with deficiency indices $(2n, 2n)$.

Definition: Any self-adjoint extension H of the operator S we shall call a *Schrödinger operator on* $\hat{X}$ with vector potential $\mathcal{A}$ and scalar potential p.

According to the theory presented in Sec. II to describe all the Schrödinger operators on $\hat{X}$ with given vector and scalar potentials we must construct a boundary value space for S. For this purpose we construct boundary value spaces for the operators $S_0, S_1, \ldots, S_n$ and take the direct sum of these spaces. Let us start with a simple case of the operators S_j $(j=1,\ldots,n)$.

Lemma 1: Set $\mathcal{G}_j=\mathbb{C}$ *and define the operators* $\Gamma_j^{(1)}, \Gamma_j^{(2)} \in \mathcal{L}(\mathcal{D}(S_j^*),\mathcal{G}_j)$, $j=1,\ldots,n$, *by the rule*

$$\Gamma_j^{(1)}(f) = -f'(0), \quad \Gamma_j^{(2)}(f) = f(0). \tag{9}$$

Then the triple $(\mathcal{G}_j,\Gamma_j^{(1)},\Gamma_j^{(2)})$ *is a boundary value space for* S_j.
We omit the simple proof.

It is clear that $H_j^{\mathrm{N}} := H_j^{(1)}$ and $H_j^{\mathrm{D}} := H_j^{(2)}$ is the free Schrödinger operator on the semi-axis $\mathbb{R}_+^{(j)}$ with the Neumann and Dirichlet boundary condition at the point $x=0$, respectively. Since the space $\mathcal{G}_j$ is one-dimensional, the corresponding Γ-field $\gamma_j(z)$ may be considered as a holomorphic function on $\mathbb{C}\backslash\mathbb{R}_+ = \rho(H_j^{(1)})$ with values in $\mathcal{H}_j = L^2(\mathbb{R}_+)$, and the corresponding $\mathcal{Q}$-function $Q_j(z)$ as a holomorphic function in $\mathbb{C}\backslash\mathbb{R}_+$. It is clear that γ_j and Q_j are independent of j.

Lemma 2: The Γ*-field and the* $\mathcal{Q}$*-function for* S_j *associated with the boundary value space* $(\mathcal{G}_j,\Gamma_j^{(1)},\Gamma_j^{(2)})$ *are given by*

$$\gamma_j(z)(x) = \frac{1}{\sqrt{-z}}\exp(-\sqrt{-z}\,x), \qquad Q_j(z) = \frac{1}{\sqrt{-z}}. \tag{10}$$

Remark 2: Throughout the paper, the continuous branch of the square root is chosen in $\mathbb{C}\backslash(-\infty,0)$, such that $\mathrm{Re}\,\sqrt{z}>0$ if $z\neq 0$.

Proof: It is clear that S_j is the restriction of H_j^{N} to the domain $\{f\in\mathcal{D}(H_j^{\mathrm{N}}) : f(0)=0\}$. On the other hand, it is easy to check that the Green's function $G_j^{\mathrm{N}}(x,y;z)$ of the Neumann operator H_j^{N} is given as

$$G_j^{\mathrm{N}}(x,y;z) = \frac{1}{2\sqrt{-z}}[\exp(-\sqrt{-z}\,|x-y|) + \exp(-\sqrt{-z}\,(x+y))]. \tag{11}$$

Hence, the function $g(x)=G_j^{\mathrm{N}}(x,0;z)$ is a nonzero element of $\mathrm{Ker}(S_j^*-z)$. Since $-g'(0)=1$, the operator $\Gamma_j^{(1)}\gamma_j(z)$ is the identity on $\mathcal{G}_j$. Therefore, $\gamma_j(z)$ is the Γ-field. The equation $Q_j(z) = \Gamma_j^{(2)}\gamma(z)$ is trivial, so $Q_j(z)$ is the $\mathcal{Q}$-function. ∎

Sometimes it is more convenient to use the boundary value space $(\mathcal{G}_j,\Gamma_{\varnothing,j}^{(1)},\Gamma_{\varnothing,j}^{(2)})$ (see notations in the preceding section). It is clear that $\Gamma_{\varnothing,j}^{(1)}f = f(0)$, and $\Gamma_{\varnothing,j}^{(2)}f = f'(0)$; thus $H_{\varnothing,j}^{(1)} = H_j^{\mathrm{D}}$, $H_{\varnothing,j}^{(2)} = H_j^{\mathrm{N}}$. Using the definitions and Lemma 2, we get the following.

Lemma 3: The Γ*-field* γ_j^{D} *and* $\mathcal{Q}$*-function* Q_j^{D} *for* S_j *associated with the boundary value space* $(\mathcal{G}_j,\Gamma_{\varnothing,j}^{(1)},\Gamma_{\varnothing,j}^{(2)})$ *have the following form:*

$$\gamma_j^{\mathrm{D}}(z)(x) \equiv \gamma_{\varnothing,j}(z)(x) = \exp(-\sqrt{-z}\,x), \qquad Q_j^{\mathrm{D}}(z) \equiv Q_{\varnothing,j}(z) = -\sqrt{-z}. \tag{12}$$

Now we turn to the operator S_0. First of all, denote by $R_0(z)$ the resolvent for H_0, $R_0(z)=(H_0-z)^{-1}$; by $G_0(x,y;z)$ we shall denote the Green's function for H_0 [the integral kernel of $R_0(z)$ in the space $L^2(X, d\lambda)$]. Fix $q\in X$ and $z\in\rho(H_0)$, then near q the function $G_0(x,q;z)$ has the expansion[45–47]

$$G_0(x,q;z)=F_0(x,q)+F_1(x,q;z)+R(x,q;z)\,, \tag{13}$$

where F_0 is independent of the spectral parameter z and has the following form:

$$F_0(x,q)=\begin{cases} -\dfrac{c_1(x,q)}{2}r(x,q)\,, & \text{if } d=1;\\ -\dfrac{c_2(x,q)}{2\pi}\ln r(x,q)\,, & \text{if } d=2;\\ \dfrac{c_3(x,q)}{4\pi}[r(x,q)]^{-1}\,, & \text{if } d=3. \end{cases} \tag{14}$$

Here $c_j(x,q)$ $(j=1,2,3)$ does not depend on z, is a continuous functions of x, and $c_j(q,q)=1$; moreover, c_1 is a smooth function of x. Further, the function F_1 is continuous with respect to x; as for the remainder term R, it has the following behavior near q as $x\to q$:

$$R(x,q;z)=\begin{cases} o(r(x,q))\,, & \text{if } d=1;\\ o\,(1)\,, & \text{if } d=2 \text{ or } d=3\,. \end{cases} \tag{15}$$

Finally, F_1 and R are analytic functions of z in the domain $\rho(H_0)=\mathbb{C}\setminus\sigma(H_0)$.

For $z\in\rho(H_0)$ define a matrix $Q_0(z)$ by the relations

$$[Q_0(z)]_{lm}:=\begin{cases} G_0(q_l,q_m;z)\,, & \text{if } l\neq m;\\ F_1(q_l,q_l;z)\,, & \text{if } l=m \end{cases} \tag{16}$$

(note that $[Q_0(z)]_{lm}=G_0(q_l,q_m;z)$ for all l and m, if $d=1$). Clearly, $Q_0(z)$ is a holomorphic matrix-valued function in the domain $\rho(H_0)$ obeying the condition

$$\overline{[Q_0(z)]}_{lm}=[Q_0(\overline{z})]_{ml}\,. \tag{17}$$

The following assertion supplies a basis in the deficiency subspace $\mathcal{N}_z=\mathrm{Ker}(S_0^*-z)$.

Lemma 4: If $z\in\mathbb{C}\setminus\mathbb{R}$, then the functions $G_0(\cdot\,,q_j;z)$, $j=1,\ldots,n$, form a vector basis in $\mathcal{N}_z$.

The lemma is proved in Ref. 48 for an operator H_0 with the resolvent having the Carleman integral kernel G_0 [i.e., $\int_{X_0}|G_0(x,y;z)|^2\,dx<\infty$ for all $z\in\rho(H_0)$ and almost all $y\in X_0$]. More restrictive conditions have been considered previously in Refs. 49, 50.

Fix $z\in\mathbb{C}\setminus\mathbb{R}$, then $\mathcal{D}(S_0^*)=\mathcal{D}(\overline{S_0})\dot{+}\mathcal{N}_z\dot{+}\mathcal{N}_{\overline{z}}$ (there is an algebraic direct sum here; if $z=i$, then this sum is orthogonal with respect to the scalar product $\langle x|y\rangle_S$). By Lemma 4 each function f from $\mathcal{D}(S_0^*)$ has the following asymptotic expansion near the point q_j:

$$f(x)=a_j(f)F_0(x,q_j)+b_j(f)+R(x)\,, \tag{18}$$

where $a_j(f), b_j(f)\in\mathbb{C}$, and the behavior of the remainder term $R(x)$ is given by (15) as $x\to q_j$.

Lemma 5: Set $\mathcal{G}_0=\mathbb{C}^n$ and define operators $\Gamma_0^{(1)}, \Gamma_0^{(2)}\in\mathcal{L}(\mathcal{D}(S_0^*),\mathcal{G}_0)$ by

$$\Gamma_0^{(1)}(f):=(a_j(f))_{1\leqslant j\leqslant n}\,,$$

$$\Gamma_0^{(2)}(f):=(b_j(f))_{1\leqslant j\leqslant n}\,,$$

where $a_j(f)$ and $b_j(f)$ are the constants from (18). Then the triple $(\mathcal{G}_0,\Gamma_0^{(1)},\Gamma_0^{(2)})$ is a space of boundary values for S_0.

Proof: Since $C_0^\infty(X)\subset\mathcal{D}(H_0)$ it is easy to conclude that the mapping $f\mapsto(\Gamma_0^{(1)}f,\Gamma_0^{(2)}f)$ is surjective. It remains to prove the condition (1).

Consider the sesquilinear forms B_1, B_2 defined as follows:

$$B_1(f,g):=\langle f|S_0^*g\rangle-\langle S_0^*f|g\rangle,$$

$$B_2(f,g):=\langle\Gamma_0^{(1)}f|\Gamma_0^{(2)}g\rangle-\langle\Gamma_0^{(2)}f|\Gamma_0^{(1)}g\rangle=\sum_{j=1}^{n}[\overline{a_j(f)}b_j(g)-\overline{b_j(f)}a_j(g)],$$

and set

$$g_j^{\pm}(x)=G_0(x,q_j;\pm i),\quad j=1,\ldots,n.$$

It is easy to check the following properties of the functions $g_j^{\pm}$:

$$\text{(i)}\quad S_0^*g_j^{\pm}=\pm ig_j^{\pm};\quad \text{(ii)}\quad a_j(g_k^{\pm})=\delta_{jk};\quad \text{(iii)}\quad b_j(g_k^{\pm})=Q_0^{jk}(\pm i). \tag{19}$$

To prove the lemma, it is enough to verify that $B_1(f,g)=B_2(f,g)$ for $f,g\in\mathcal{D}(S_0^*)$. Since $\mathcal{D}(S_0^*)=\mathcal{D}(\overline{S_0})\oplus\mathcal{N}_i\oplus\mathcal{N}_{-i}$, it is enough to check the equality $B_1(f,g)=B_2(f,g)$ for all functions $f,g\in\mathcal{D}(S_0)\cup\{g_j^{\pm}:j=1,\ldots,n\}$. It is clear that $a_j(f)=b_j(f)=0$ if $f\in\mathcal{D}(S_0)$; therefore $B_1(f,g)=0=B_2(f,g)$ if $f\in\mathcal{D}(S_0)$ or $g\in\mathcal{D}(S_0)$. By (i) from (19), $B_1(g_j^+,g_k^-)=0\ \forall\, j,k\in\{1,\ldots,n\}$. On the other hand, Eqs. (ii) and (iii) from (19) and (17) imply that

$$B_2(g_j^+,g_k^-)=b_j(g_k^-)-\overline{b_k(g_j^+)}=[Q_0(-i)]_{jk}-\overline{[Q_0(i)]}_{kj}=0. \tag{20}$$

Hence, $B_1(g_j^+,g_k^-)=B_2(g_j^+,g_k^-)\ \forall\, j,k\in\{1,\ldots,n\}$. Since $B_l(f,g)=-\overline{B_l(g,f)}$ $(l=1,2)$, we have $B_1(g_j^-,g_k^+)=B_2(g_j^-,g_k^+)\ \forall\, j,k\in\{1,\ldots,n\}$. Similarly, we get

$$B_2(g_j^+,g_k^+)=b_j(g_k^+)-\overline{b_k(g_j^+)}=[Q(i)]_{jk}-\overline{[Q(i)]}_{kj}=[Q(i)]_{jk}-[Q(-i)]_{jk}.$$

Further,

$$\begin{aligned}B_1(g_j^+,g_k^+)&=2i\langle g_j^+|g_k^+\rangle=2i\int_X\overline{G_0(x,q_j;i)}G_0(x,q_k;i)\,d\lambda(x)\\&=2i\int_X G_0(q_j,x;-i)G_0(x,q_k;i)\,d\lambda(x).\end{aligned} \tag{21}$$

Using the Hilbert resolvent identity we obtain from (21) in case $j\neq k$:

$$B_1(g_j^+,g_k^+)=G_0(q_j,q_k;i)-G_0(q_j,q_k;-i)=B_2(g_j^+,g_k^+).$$

If $j=k$, then using the Hilbert identity again we get

$$\begin{aligned}B_1(g_j^+,g_j^+)&=2i\lim_{q\to q_j}\int_X G_0(q,x;-i)G_0(x,q_j;i)\,d\lambda(x)\\&=\lim_{q\to q_j}[G_0(q,q_j;i)-G_0(q,q_j;-i)]\\&=[Q(i)]_{jj}-[Q(-i)]_{jj}=B_2(g_j^+,g_j^+)\end{aligned}$$

(of course, in the case $d=1$ we can omit the limiting procedure). The proof of the equalities $B_1(g_j^-,g_k^-)=B_2(g_j^-,g_k^-)$ is similar. ∎

Remark 3: It is clear that in the case $d=1$ we have $b_j(f)=f(q_j)$. Moreover, we can get a simple expression for $a_j(f)$ in this case. Namely, choose a chart $U\subset X$ such that $q_j\in U\ \forall\ j=1,\ldots,n$ and U is isometric to an interval $(a,b)\subset\mathbb{R}$. Using the Cartesian coordinates in U we obtain from (18) that every function $f\in\mathcal{D}(S_0^*)$ has the following expansion near each point q_j:

$$f(x)=-\tfrac{1}{2}a_j(f)|x-q_j|+f(q_j)+o(|x-q_j|); \tag{22}$$

thus it follows from (22) that

$$a_j(f)=f'(q_j-0)-f'(q_j+0),$$

where the derivative is taken with respect to the Cartesian coordinate in U.

Now we describe the Krein Γ-field and $\mathcal{Q}$-function for S_0 associated with the boundary value space $(\mathcal{G}_0,\Gamma_0^{(1)},\Gamma_0^{(2)})$.

Lemma 6: The Krein Γ-field for S_0 associated with the boundary value space $(\mathcal{G}_0,\Gamma_0^{(1)},\Gamma_0^{(2)})$ is an operator valued family $\gamma_0(z)\in\mathcal{L}(\mathcal{G}_0,\mathcal{H}_0)$ defined for an element $\zeta=(\zeta_j)_{1\leqslant j\leqslant n}$ from $\mathcal{G}_0=\mathbb{C}^n$ by

$$\gamma_0(z)(\zeta)=\sum_{j=1}^{n}\zeta_j G_0(\cdot,q_j;z). \tag{23}$$

The corresponding $\mathcal{Q}$-function coincides with the matrix-valued function $Q_0(z)$.

Proof: To prove the first part of the lemma, it is enough to check that $\Gamma_0^{(1)}\gamma_0(z)$ is the identity operator on $\mathcal{G}_0$, but this follows immediately from the definition of $\Gamma_0^{(1)}$ and from (13) and (14).

Let $g_k(x)=G_0(x,q_k;z)$, then $b_j(g_k)=[Q_0(z)]_{jk}$ by definition. Thus for $\zeta\in\mathcal{G}_0$ we have

$$[\Gamma_0^{(2)}\gamma_0(z)\zeta]_j=\sum_{k=1}^{n}[Q_0(z)]_{jk}\zeta_k;$$

therefore, $Q_0(z)$ is the $\mathcal{Q}$-function. ∎

Now we set

$$\begin{gathered}\mathcal{G}:=\mathcal{G}_0\oplus\mathcal{G}_1\oplus\cdots\oplus\mathcal{G}_n\ (=\mathbb{C}^{2n});\\ \Gamma^{(j)}:=\Gamma_0^{(j)}\oplus\Gamma_1^{(j)}\oplus\cdots\oplus\Gamma_n^{(j)}\quad(j=1,2);\\ \gamma(z):=\gamma_0(z)\oplus\gamma_1(z)\oplus\cdots\oplus\gamma_n(z)\quad(z\in\mathbb{C}\setminus\mathbb{R});\\ Q(z):=Q_0(z)\oplus Q_1(z)\oplus\cdots\oplus Q_n(z)\quad(z\in\mathbb{C}\setminus\mathbb{R}).\end{gathered} \tag{24}$$

Then the following theorem is an evident consequence of the preceding lemmas.

Theorem 1: *The triple $(\mathcal{G},\Gamma^{(1)},\Gamma^{(2)})$ is a boundary value space for the operator S. The corresponding Krein Γ-field and $\mathcal{Q}$-function coincide with $\gamma(z)$ and $Q(z)$, respectively. The operator $H=H^{(1)}$ given by the boundary condition $\Gamma^{(1)}f=0$ coincides with the direct sum $H=H_0\oplus H_1^{\mathrm{N}}\oplus\cdots\oplus H_n^{\mathrm{N}}$ (we shall denote this operator by H_{N}).* ∎

Remark 4: It is convenient to describe explicitly the boundary value space $(\mathcal{G},\Gamma_\eta^{(1)},\Gamma_\eta^{(2)})$ for an arbitrary set $\eta\subset\{1,\ldots,2n\}$. Denote

$$\begin{gathered}\theta=\eta\cap\{1,\ldots,n\},\quad \omega=\eta\cap\{n+1,\ldots,2n\};\\ \theta'=\{1,\ldots,n\}\setminus\eta,\quad \omega'=\{n+1,\ldots,2n\}\setminus\eta.\end{gathered} \tag{25}$$

Then

$$\Gamma_\eta^{(l)}=\Gamma_{\theta,0}^{(l)}\oplus\tilde{\Gamma}_1^{(l)}\oplus\cdots\oplus\tilde{\Gamma}_n^{(l)}\quad(l=1,2);$$

$$\gamma_\eta(z)=\gamma_{\theta,0}(z)\oplus\tilde{\gamma}_1(z)\oplus\cdots\oplus\tilde{\gamma}_n(z)\quad(z\in\mathbb{C}\backslash\mathbb{R}); \tag{26}$$

$$Q_\eta(z)=Q_{\theta,0}(z)\oplus\tilde{Q}_1(z)\oplus\cdots\oplus\tilde{Q}_n(z)\quad(z\in\mathbb{C}\backslash\mathbb{R}).$$

Here for $j=1,\ldots,n$,

$$\tilde{\Gamma}_j^{(l)}=\begin{cases}\Gamma_j^{(l)}, & \text{if } j+n\in\omega,\\ \Gamma_{\varnothing,j}^{(l)}, & \text{if } j+n\in\omega';\end{cases}$$

and similarly for $\tilde{\gamma}_\eta(z)$ and $\tilde{Q}_\eta(z)$. In particular, if $\eta=\{1,\ldots,n\}$, then we denote $\Gamma_\eta^{(l)}=\Gamma_{\mathrm{D}}^{(l)}$, $\gamma_\eta=\gamma_{\mathrm{D}}$, $Q_\eta=Q_{\mathrm{D}}$. The operator $H=H_{\mathrm{D}}^{(1)}$ given by the boundary condition $\Gamma_{\mathrm{D}}^{(1)}f=0$ coincides with the direct sum $H=H_0\oplus H_1^{\mathrm{D}}\oplus\cdots\oplus H_n^{\mathrm{D}}$ and will be denoted by H_{D}.

Now we can describe all Schrödinger operators on $\hat{X}$ with given vector and scalar potentials in terms of boundary conditions at the points $q_1,\ldots,q_n$. First of all, we describe the elements of $\mathcal{D}(S^*)$ as functions on $\hat{X}$. For $f\in L^2(\hat{X})=\mathcal{H}$ we denote by $f_0,f_1,\ldots,f_n$ the components of f in $L^2(X)=\mathcal{H}_0$, $L^2(\mathbb{R}_+^{(1)})=\mathcal{H}_1,\ldots,L^2(\mathbb{R}_+^{(n)})=\mathcal{H}_n$, respectively. It is clear that $f\in\mathcal{D}(S^*)$ if and only if $f_j\in H^2(\mathbb{R}_+)$ $(j=1,\ldots,n)$ whereas $f_0\in H^2_{\mathrm{loc}}(X\backslash\{q_1,\ldots,q_n\})$ and has the asymptotics (18) near each point q_j.

Theorem 2: *The Schrödinger operators on $\hat{X}$ with a given vector potential $\mathcal{A}$ and a given scalar potential p are in bijective correspondence with the Lagrangian subspaces of $\mathcal{G}\oplus\mathcal{G}$. More precisely, if Λ is such a subspace and U_Λ is the Cayley transform of Λ having the matrix (u_{jk}) in the standard basis of $\mathcal{G}$, then the corresponding Schrödinger operator $H=H^\Lambda$ is defined on those functions $f\in\mathcal{D}(S^*)$ the components of which obey the boundary conditions*

$$\sum_{k=1}^{n}\left[(\delta_{jk}-u_{jk})b_k(f_0)+(\delta_{j,k+n}-u_{j,k+n})f_k(0)\right]$$

$$=i\sum_{k=1}^{n}\left[(\delta_{jk}+u_{jk})a_k(f_0)-(\delta_{j,k+n}+u_{j,k+n})f_k'(0)\right],\quad j=1,\ldots,2n. \tag{27}$$

If Λ is the graph of a self-adjoint operator L in $\mathcal{G}$ with a Hermitian $2n\times2n$-matrix (λ_{jk}) then conditions (27) take a simpler form:

$$b_j(f_0)=\sum_{k=1}^{n}\left[\lambda_{j,k}a_k(f_0)-\lambda_{j,k+n}f_k'(0)\right],$$

$$f_j(0)=\sum_{k=1}^{n}\left[\lambda_{j+n,k}a_k(f_0)-\lambda_{j+n,k+n}f_k'(0)\right],\quad j=1,\ldots,n. \tag{28}$$

In the general case there are a finite subset $\eta\subset\{1,\ldots,2n\}$ and a Hermitian $2n\times2n$-matrix $L=(\lambda_{jk})$ such that the conditions (27) take the following equivalent form:

$$b_j(f_0)=\sum_{k\in\theta}\lambda_{jk}a_k(f_0)-\sum_{k\in\theta'}\lambda_{jk}b_k(f_0)-\sum_{k\in\omega}\lambda_{jk}f_{k-n}'(0)+\sum_{k\in\omega'}\lambda_{jk}f_{k-n}(0),\quad j\in\theta;$$

$$a_j(f_0)=\sum_{k\in\theta}\lambda_{jk}a_k(f_0)-\sum_{k\in\theta'}\lambda_{jk}b_k(f_0)-\sum_{k\in\omega}\lambda_{jk}f_{k-n}'(0)+\sum_{k\in\omega'}\lambda_{jk}f_{k-n}(0),\quad j\in\theta';$$

$$f_j(0)=\sum_{k\in\theta}\lambda_{j+n,k}a_k(f_0)-\sum_{k\in\theta'}\lambda_{j+n,k}b_k(f_0)-\sum_{k\in\omega}\lambda_{j+n,k}f'_{k-n}(0)+\sum_{k\in\omega'}\lambda_{j+n,k}f_{k-n}(0),$$
$$j+n\in\omega;$$

$$f'_j(0)=\sum_{k\in\theta}\lambda_{j+n,k}a_k(f_0)-\sum_{k\in\theta'}\lambda_{j+n,k}b_k(f_0)-\sum_{k\in\omega}\lambda_{j+n,k}f'_{k-n}(0)+\sum_{k\in\omega'}\lambda_{j+n,k}f_{k-n}(0),$$
$$j+n\in\omega'; \tag{29}$$

where the sets θ, θ', ω, and ω' are defined in Remark 4.

Proof: The result follows immediately from Theorem A, Theorem 1, and Proposition C. ■

Below we collect the most interesting particular cases of Schrödinger operators on $\hat{X}$ with given potentials. For this purpose we need some notions concerning point perturbations of Schrödinger operators on the manifold X. Let $B=(\beta_{jk})$ be a Hermitian $n\times n$-matrix, θ a subset of $\{1,\ldots,n\}$, and $\theta'=\{1,\ldots,n\}\setminus\theta$. Then the conditions

$$f_0\in\mathcal{D}(S_0^*);$$

$$b_j(f_0)=\sum_{k\in\theta}\beta_{jk}a_k(f_0)-\sum_{k\in\theta'}\beta_{jk}b_k(f_0),\quad j\in\theta; \tag{30}$$

$$a_j(f_0)=\sum_{k\in\theta}\beta_{jk}a_k(f_0)-\sum_{k\in\theta'}\beta_{jk}b_k(f_0),\quad j\in\theta';$$

define a generic self-adjoint extension $H_0^{B,\theta}$ of the operator S_0. In particular, if $B=0$ and $\theta=\varnothing$, then $H_0^{B,\theta}$ is the Schrödinger operator H_0. If $\theta=\{1,\ldots,n\}$, then the operator $H_0^B=H_0^{B,\theta}$ is called a *point perturbation* of H_0 supported by the points $q_1,\ldots,q_n$ (see, e.g., Ref. 51). Generally speaking, this perturbation is nonlocal in the sense of Ref. 52. If B is a diagonal matrix, $\beta_{jk}=\beta_j\delta_{jk}$, $\beta_j\in\mathbb{R}$, then H_0^B is called a *local* point perturbation of H_0.

In what follows we shall represent **an arbitrary Hermitian $2n\times 2n$-matrix $L=(\lambda_{jk})$ in block form**:

$$L=\begin{bmatrix}B & A\\ A^* & C\end{bmatrix}, \tag{31}$$

where $B=(\beta_{jk})$ and $C=(\gamma_{jk})$ are Hermitian $n\times n$-matrices whereas $A=(\alpha_{jk})$ is an arbitrary complex $n\times n$-matrix.

Examples: We list four important particular cases of the Schrödinger operator H.

(1) Let $\eta=\varnothing$. Then the conditions (29) take the following simpler form:

$$a_j(f_0)=-\sum_{k=1}^{n}\beta_{jk}b_k(f_0)+\sum_{k=1}^{n}\alpha_{jk}f_k(0),$$

$$f'_j(0)=-\sum_{k=1}^{n}\overline{\alpha_{kj}}b_k(f_0)+\sum_{k=1}^{n}\gamma_{jk}f_k(0),\quad j=1,\ldots,n.$$

If $A=C=0$, then $H=H_0^{B,\varnothing}\oplus H_1^{\mathrm{N}}\oplus\cdots\oplus H_n^{\mathrm{N}}$. If, in addition, $B=0$, then

$$a_j(f_0)=0,\quad f'_j(0)=0,\quad j=1,\ldots,n,$$

hence H coincides with H_{N}.

(2) Let $\eta=\{1,\ldots,2n\}$, then the conditions (29) take the form

$$b_j(f_0)=\sum_{k=1}^{n}\beta_{jk}a_k(f_0)-\sum_{k=1}^{n}\alpha_{jk}f_k'(0)\,,$$

$$f_j(0)=\sum_{k=1}^{n}\overline{\alpha}_{kj}a_k(f_0)-\sum_{k=1}^{n}\gamma_{jk}f_k'(0)\,,\quad j=1,\ldots,n\,,$$

and we return to the conditions (28). We shall denote this operator by H_{D}^{L} and call it a *Schrödinger operator of the Dirichlet type*. It is clear that this operator is disjoint from H_{N}. If $A=C=0$, then $H_{\mathrm{D}}^{L}=S_0^B\oplus H_1^{\mathrm{D}}\oplus\cdots\oplus H_n^{\mathrm{D}}$.

(3) Let $\eta=\{n+1,\ldots,2n\}$. Then the conditions (29) become

$$a_j(f_0)=-\sum_{k=1}^{n}\beta_{jk}b_k(f_0)-\sum_{k=1}^{n}\alpha_{jk}f_k'(0)\,,$$

$$f_j(0)=-\sum_{k=1}^{n}\overline{\alpha}_{kj}b_k(f_0)-\sum_{k=1}^{n}\gamma_{jk}f_k'(0)\,,\quad j=1,\ldots,n\,.$$

If $A=C=0$, then we get an operator $H=H_0^{B,\varnothing}\oplus H_1^{\mathrm{D}}\oplus\cdots\oplus H_n^{\mathrm{D}}$. If, in addition, $B=0$, then

$$a_j(f_0)=0\,,\quad f_j(0)=0\,,\quad j=1,\ldots,n\,,$$

i.e., H coincides with H_{D}.

(4) Let $\eta=\{1,\ldots,n\}$. Then the conditions (29) take the form

$$b_j(f_0)=\sum_{k=1}^{n}\beta_{jk}a_k(f_0)+\sum_{k=1}^{n}\alpha_{jk}f_k(0)\,,$$

$$f_j'(0)=\sum_{k=1}^{n}\overline{\alpha}_{kj}a_k(f_0)+\sum_{k=1}^{n}\gamma_{jk}f_k(0)\,,\quad j=1,\ldots,n\,.$$

We shall denote this operator by H_{N}^{L} and call it a *Schrödinger operator of the Neumann type*. It is clear that this operator is disjoint from H_{D}. If $A=C=0$, then $H_{\mathrm{N}}^{L}=H_0^B\oplus H_1^{\mathrm{N}}\oplus\cdots\oplus H_n^{\mathrm{N}}$. In the case $n=2$, the operator H_{N}^{L} has been considered in Refs. 13 and 20.

Theorem 1 implies the following description of the resolvents of Schrödinger operators.

Theorem 3: *Let Λ be a Lagrangian subspace of $\mathcal{G}\oplus\mathcal{G}$ and $H=H^{\Lambda}$ the Schrödinger operator defined by the boundary condition $\Gamma f\in\Lambda$. Then the resolvent $R(z)=(H-z)^{-1}$ of H is given by the Krein formula*

$$R(z)=R_{\mathrm{N}}(z)-\gamma(z)[Q(z)-\Lambda]^{-1}\gamma^{*}(\overline{z})\,, \tag{32}$$

where $R_{\mathrm{N}}(z)=(H_{\mathrm{N}}-z)^{-1}$.

Similarly, if H is defined by the boundary condition $\Gamma_{\mathrm{D}}f\in\Lambda$, then the resolvent $R(z)=(H-z)^{-1}$ is given by the expression

$$R(z)=R_{\mathrm{D}}(z)-\gamma_{\mathrm{D}}(z)[Q_{\mathrm{D}}(z)-\Lambda]^{-1}\gamma_{\mathrm{D}}^{*}(\overline{z})\,, \tag{33}$$

where $R_{\mathrm{D}}(z)=(H_{\mathrm{D}}-z)^{-1}$. In particular, if $H=H_{\mathrm{D}}^{L}$ (respectively, $H=H_{\mathrm{N}}^{L}$), then (32) [respectively, (33)] contains a single-valued operator Λ with matrix L. In any case, using (8), we can rewrite (32) [or (33)] in the form

$$R^{L,\eta}(z)=R_{\eta}(z)-\gamma_{\eta}(z)[Q_{\eta}(z)-L]^{-1}\gamma_{\eta}^{*}(\overline{z})\,,$$

where L is a Hermitian operator in $\mathcal{G}$. ■

IV. SPECTRAL AND SCATTERING PROPERTIES OF THE SCHRÖDINGER OPERATORS ON A "HEDGEHOG-SHAPED" SPACE

From this section on we, *suppose that the manifold X is compact*. Therefore, the spectrum $\sigma(H_0)$ is discrete; let $\mu_0<\mu_1<\cdots<\mu_m<\cdots$ be the complete set of eigenvalues of H_0. We shall denote the eigenspace of H_0 corresponding to μ_m by $\mathcal{H}_0(\mu_m)$; in each $\mathcal{H}_0(\mu_m)$ we fix an orthonormal basis $\psi_m^{(1)},\ldots,\psi_m^{(l_m)}$. Denote by $\sigma^p(H_0)$ the following subset of $\sigma(H_0)$:

$$\sigma^p(H_0):=\{\mu_m\in\sigma(H_0):\exists j\in\{1,\ldots,n\},\ \exists\psi\in\mathcal{H}_0(\mu_m)\ \text{s.t.}\ \psi(q_j)\neq 0\}\,.$$

Proposition 1: $Q_0(z)$ is a meromorphic matrix-valued function on the complex plain $\mathbb{C}$. The set of poles of Q_0 is infinite and coincides with $\sigma^p(H_0)$.

Proof: Using Mercer's Theorem it is not hard to derive the equality

$$\frac{\partial[Q_0(z)]_{jk}}{\partial z}=\sum_{m=0}^{\infty}(\mu_m-z)^{-2}\sum_{s=1}^{l_m}\overline{\psi_m^{(s)}(q_j)}\psi_m^{(s)}(q_k)\,, \tag{34}$$

where the series converges absolutely and locally uniformly with respect to z, $z\in\mathbb{C}\backslash\sigma(H_0)$. It is hence clear that Q_0 is meromorphic and $\sigma^p(H_0)$ is the set of poles for Q_0. Suppose that this set is finite; then there exists m_0 such that $\mu_m\notin\sigma^p(H_0)\ \forall m>m_0$. Consider the linear hull $\mathcal{L}$ of all the eigenfunctions $\psi_m^{(s)}$; then $\mathcal{L}\subset C(X)$. Fix $j\in\{1,\ldots,n\}$ and set $q=q_j$. If $\varphi\in\mathcal{L}$, then the relations $\langle\psi_m^{(s)}|\varphi\rangle=0\ \forall m\leqslant m_0$, $s=1,\ldots,l_m$, imply $\delta_q(\varphi):=\varphi(q)=0$. Therefore the linear functional δ_q on $\mathcal{L}$ is a linear combination of the linear functionals $\langle\psi_m^{(s)}|$ $(m\leqslant m_0, s=1,\ldots,l_m)$. Since $\mathcal{L}$ is dense in $C(X)$ with respect to both the Hilbert and Chebyshev norms, we conclude that δ_q is a continuous functional on $C(X)$ with respect to the topology induced from $L^2(X)$. This contradiction concludes the proof. ∎

Remark 5: Generally speaking, the set $\sigma^p(H_0)$ depends on the tuple $(q_1,\ldots,q_n)$ but the set $Y=\{(q_1,\ldots,q_n)\in X^n:\sigma^p(H_0)=\sigma(H_0)\}$ is generic both in the sense of measure and category (i.e., the set $X^n\backslash Y$ is a zero-measure set of the first Baire class). Moreover, if X is a homogeneous manifold, then $X=Y$ independently of the tuple $(q_1,\ldots,q_n)$.

The structure of the spectrum for an arbitrary self-adjoint extension of the operator S_0 (in particular, for the point perturbation of H_0) is very simple. Namely, the following proposition is an evident consequence of Theorems 14.9 and 14.10 from Ref. 53.

Proposition 2: Let $\tilde{H}_0$ be a self-adjoint extension of S_0. Then $\tilde{H}_0$ is bounded from below and the spectrum of $\tilde{H}_0$ is purely discrete: $\sigma(\tilde{H}_0)=\sigma_{\text{dis}}(\tilde{H}_0)$.

The spectral properties of a Schrödinger operator on $\hat{X}$ are rather rich. Before we describe them, we settle the following notations. For the rest of this section H will denote the Schrödinger operator on $\hat{X}$ defined by a Schrödinger operator H_0 on X and a Lagrangian subspace $\Lambda\subset\mathcal{G}\oplus\mathcal{G}$. The next theorem describes the spectral properties of H.

Theorem 4: *The following assertions hold.*

(i) $\sigma_{\text{ess}}(H)=\sigma_{\text{ac}}(H)=[0,+\infty)$;
(ii) $\sigma_{\text{sc}}(H)=\varnothing$;
(iii) $\sigma_{\text{dis}}(H)$ *is a finite (possibly, empty) subset of* $(-\infty,0)$;
(iv) $\sigma_{\text{pp}}(H)\cap[0,+\infty)\subset\sigma(\tilde{H}_0)$, *where* $\tilde{H}_0$ *is a self-adjoint extension of* S_0 *[therefore,* $\sigma_{\text{pp}}(H)$ *has no accumulation points];*
(v) the multiplicity of an eigenvalue $E_0\in\sigma_{\text{pp}}(H)$ *does not exceed* $2n+m$, *where* m *is the multiplicity of* E_0 *in the spectrum of* H_0. *Moreover, let* N *be the number of eigenvalues* E *of* H *(counting multiplicity) obeying the inequality* $E<\min(0,\inf\sigma(H_0))$; *then* $0\leqslant N\leqslant 2n$.

Proof: Clearly, the spectrum of H_N possesses all the properties (i)–(v). Therefore, general theorems about self-adjoint extensions with finite deficiency indices (Theorems 14.9 and 14.10 from Ref. 53, and Theorem 18 from Ref. 30) imply properties (iii) and (v) for the operator H.

Furthermore, taking into account (32) we see that the equality $\sigma_{\mathrm{ess}}(H)=[0,+\infty)$ follows from the Weyl theorem (see Ref. 54, Theorem XII.14) and that the equality $\sigma_{\mathrm{ac}}(H)=[0,+\infty)$ is a consequence of the Birman–Kuroda theorem (Ref. 54, Theorem XI.9).

Let us prove property (iv). Fix a representation of H in the form $H^{L,\eta}$, where $\eta\subset\{1,\ldots,2n\}$ and L is a Hermitian $2n\times 2n$-matrix. Let E_0, $E_0\geqslant 0$, be an eigenvalue of H with an eigenvector $f=(f_0,f_1,\ldots,f_n)$. For every $j=1,\ldots,n$ the function f_j belongs to $L^2(\mathbb{R}_+)$ and obeys the equation $-f_j''=E_0 f_j$; hence, $f_j=0$. Using the first two equations from (29) we show that E_0 is an eigenvalue of $\widetilde{H}_0=H_0^{B,\theta}$, where $\theta=\{1,\ldots,n\}\cap\eta$ and B is related to L by Eq. (31).

It remains to prove property (ii). Denote by $\mathcal{L}$ the dense subspace of all elements $f=(f_0,f_1,\ldots,f_n)$ from $\mathcal{H}$ such that $f_0\in C(X)$, $f_j\in C_0^\infty(0,+\infty)$, $j=1,\ldots,n$. Let $\mathcal{F}$ be a family of functions which are analytic in the upper half-plane $\mathbb{C}^+=\{z\in\mathbb{C}:\mathrm{Im}\,z>0\}$; we say that the family $\mathcal{F}$ is bounded near a point E, $E\in\mathbb{R}$, if there exists a neighborhood V of E such that every function from $\mathcal{F}$ is bounded in $V\cap\mathbb{C}^+$. According to Theorem XIII.20 from Ref. 54 it is enough to prove that for some countable subset Z of $\mathbb{R}$ the family of the functions $z\mapsto\langle f|R(z)g\rangle$, where f and g run through $\mathcal{L}$, is bounded near every point E, $E\in(0,+\infty)\backslash Z$. It is clear that for $H=H_{\mathrm{N}}$ this family is bounded near the points from $(0,+\infty)\backslash\sigma(H_0)$. Moreover, let $\mathcal{F}$ be the family of functions of the form

$$z\mapsto\int_X G_0(x,q_j;z)f_0(x)d\lambda(x),$$

or

$$z\mapsto\int_0^\infty G_j(x,0;z)f_j(x)dx,$$

where $j=1,\ldots,n$ and $f=(f_0,f_1,\ldots,f_n)\in\mathcal{L}$. Then the family $\mathcal{F}$ is bounded near every point from $(0,+\infty)\backslash\sigma(H_0)$. According to (32) it remains to show that there exists a discrete subset $Z_0\subset\mathbb{R}\backslash\sigma(H_0)$ such that the elements of the matrix $[Q(z)-\Lambda]^{-1}$ form a bounded family near every point from $(0,+\infty)\backslash Z_0$. Rewrite $[Q(z)-\Lambda]^{-1}$ in the form $J_\Lambda[P_\Lambda Q(z)J_\Lambda-L]^{-1}P_\Lambda$ [see (7)]. The elements of the matrix $Q(z)$ have analytic continuations from the half-plane $\mathbb{C}_+$ to a neighborhood of the set $(0,+\infty)\backslash\sigma(H_0)$; moreover, $\det[P_\Lambda Q(z)J_\Lambda-L]\neq 0$, if $\mathrm{Im}\,z>0$. Therefore, we obtain the required property from standard analyticity arguments. ■

Now we are going to define the scattering matrix for the Schrödinger operator H on $\hat{X}$ following the ideas of geometric scattering theory (see, e.g., Ref. 55). First of all we note that there exists a natural extension of H to a domain of functions not belonging to $L^2(\hat{X})$. Namely, Lemma 1 defines the boundary value operators $\Gamma_j^{(1)}$ and $\Gamma_j^{(2)}$ for every function from $H^2_{\mathrm{loc}}(\mathbb{R}_+^{(j)})$. Therefore, (24) defines the operators $\Gamma_j^{(1)}$ and $\Gamma_j(2)$ for every function $f=(f_0,f_1,\ldots,f_n)$ from $\mathcal{D}(S_0^*)\oplus H^2_{\mathrm{loc}}(\mathbb{R}_+^{(1)})\oplus\cdots\oplus H^2_{\mathrm{loc}}(\mathbb{R}_+^{(n)})$. Hence, we can consider the operator H to be defined on the domain, $\mathcal{D}_{\mathrm{loc}}(H)$, consisting of all functions f from $\mathcal{D}(S_0^*)\oplus H^2_{\mathrm{loc}}(\mathbb{R}_+^{(1)})\oplus\cdots\oplus H^2_{\mathrm{loc}}(\mathbb{R}_+^{(n)})$ obeying the boundary condition $(\Gamma^{(1)}f,\Gamma^{(2)}f)\in\Lambda$ [this operator takes values in the space $L^2_{\mathrm{loc}}(\hat{X})=L^2(X)\oplus L^2_{\mathrm{loc}}(\mathbb{R}_+^{(1)})\oplus\cdots\oplus L^2_{\mathrm{loc}}(\mathbb{R}_+^{(n)})$]. If H is represented in the form $H=H^{L,\eta}$, then the last condition may be replaced by condition (29). To define the scattering matrix we need solutions to the Schrödinger equation,

$$Hf=k^2f, \tag{35}$$

$f\in\mathcal{D}_{\mathrm{loc}}(H)$, $k\geqslant 0$, the so-called *scattering states*, which have a special behavior in the channels $\mathbb{R}_+^{(j)}$. The following theorem provides us with such solutions.

Theorem 5: (Existence and uniqueness of scattering states.) *For every Schrödinger operator $H=H^\Lambda$ on $\hat{X}$ there exists a discrete subset Z_H of $\mathbb{R}$ such that the following assertion is valid.*

For a given $j\in\{1,\ldots,n\}$ and every $k>0$, $k^2\notin Z_H$, the Schrödinger equation (35) has a unique solution $f=(f_0,f_1,\ldots,f_n)$ satisfying the following conditions:

(i) $f_j(x)=\exp(-ikx)+r_j(k)\exp(ikx)$,
(ii) *if* $l\in\{1,\dots,n\}$ *and* $l\neq j$, *then* $f_l(x)=t_{lj}(k)\exp(ikx)$,
where $r_j(k)$, $t_{lj}(k)\in\mathbb{C}$.

Proof: We define Z_H as the union of the following sets: (1) $\sigma(H_0)$; (2) $\sigma(H_0^{B,\theta})$ if H may be represented in the form $H=H^{L,\eta}$ and (B,θ) is related to (L,η) with (25), (31); (3) the set of all solutions to the equation $\det[P_\Lambda Q(E)J_\Lambda-L]=0$ where $Q(E)$ is the analytic continuation of $Q(z)$ from the upper half-plane $\mathbb{C}^+$ to $\mathbb{R}^+$ (see the proof of Theorem 4). Clearly, Z_H is discrete.

Further we note that for every $\zeta=(\zeta_l)_{1\leqslant l\leqslant 2n}\in\mathbb{C}^{2n}=\mathcal{G}$ the function $\gamma(z)\zeta=(\varphi_0,\varphi_1,\dots,\varphi_n)$ has the form

$$\varphi_0(x)=\sum_{m=1}^{n}\zeta_m G_0(x,q_m;z), \tag{36}$$

$$\varphi_l(x)=\frac{\zeta_{l+n}}{\sqrt{-z}}\exp(-\sqrt{-z}x),\quad 0<l\leqslant n, \tag{37}$$

[see (10)), (23), and (24)]. Therefore, for any $\varphi\in\mathcal{H}$,

$$\gamma^*(\overline{z})\varphi=(\zeta_l)_{1\leqslant l\leqslant 2n},$$

where

$$\zeta_l=\int_X G_0(q_l,x;z)\varphi_0(x)d\lambda(x),\quad 1\leqslant l\leqslant n; \tag{38}$$

$$\zeta_l=\frac{1}{\sqrt{-z}}\int_0^\infty \exp(-\sqrt{-z}x)\varphi_{l-n}(x)dx,\quad n+1\leqslant l\leqslant 2n. \tag{39}$$

Fix now $k>0$, $k^2\notin Z_H$, and put $z=k^2+i\varepsilon$, where $0<\varepsilon\leqslant\varepsilon_0$, with some $\varepsilon_0>0$. It is clear that an element g from $\mathcal{H}$ belongs to $\mathcal{D}(H)$ if and only if $g=R(z)h$, where h is an element from $\mathcal{H}$ (which depends on z). Set $\psi=R_{\mathrm{N}}(z)h$, then $\psi\in\mathcal{D}(H_{\mathrm{N}})$ and from (32),

$$g=\psi-\gamma(z)[Q(z)-\Lambda]^{-1}\gamma^*(\overline{z})(H_{\mathrm{N}}-z)\psi, \tag{40}$$

and

$$(H-z)g=(H_{\mathrm{N}}-z)\psi. \tag{41}$$

Conversely, every function $\psi\in\mathcal{D}(H_{\mathrm{N}})$ defines, by (40), an element g from $\mathcal{D}(H)$ in such a way that (41) holds. Note that according to (38) and (39), the vector $\xi=\gamma^*(\overline{z})(H_{\mathrm{N}}-z)\psi$ has the form

$$\xi_l=\begin{cases}\psi_0(q_l), & \text{if } 1\leqslant l\leqslant n;\\ \psi_{l-n}(0), & \text{if } n+1\leqslant l\leqslant 2n.\end{cases}$$

Therefore, we can rewrite (40) as

$$g=\psi-\gamma(z)\zeta(\psi),$$

with

$$\zeta_l(\psi)=\sum_{m=1}^{n}[Q(z)-\Lambda]^{-1}_{lm}\psi_0(q_m)+\sum_{m=n+1}^{2n}[Q(z)-\Lambda]^{-1}_{lm}\psi_{m-n}(0). \tag{42}$$

Now fix $j\in\{1,\ldots,n\}$ and define $\psi=(\psi_0,\psi_1,\ldots,\psi_n)$ from $L^2_{\mathrm{loc}}(\hat{X})$ by

$$\psi_l(x)=\begin{cases}\exp(ikx)+\exp(-ikx), & \text{if } l=j,\\ 0, & \text{otherwise.}\end{cases} \tag{43}$$

It is clear that $\psi\in\mathcal{D}_{\mathrm{loc}}(H_{\mathrm{N}})$ but $\psi\notin\mathcal{D}(H_{\mathrm{N}})$. To obtain a function from $\mathcal{D}(H)$ we choose for $a>0$ a cut-off function $\chi_a\in C_0^\infty(\mathbb{R}_+)$ such that $\chi_a(x)=1$ if $0\leqslant x\leqslant a$, $\chi_a(x)=0$ if $x>a+1$, and $0\leqslant\chi_a(x)\leqslant 1$, $\forall x\in\mathbb{R}_+$. Set $\tilde{\chi}_a:=(1,\chi_a,\ldots,\chi_a)$, it is clear that the product $\tilde{\chi}_a\psi=(\psi_0,\chi_a\psi_1,\ldots,\chi_a\psi_n)$ is in $\mathcal{D}(H_{\mathrm{N}})$, and hence defines a function,

$$g^{(a)}:=\tilde{\chi}_a\psi-\gamma(z)\zeta(\tilde{\chi}_a\psi), \tag{44}$$

in $\mathcal{D}(H)$ such that

$$(H-z)g^{(a)}=(H_{\mathrm{N}}-z)\tilde{\chi}_a\psi. \tag{45}$$

We write the matrix $[Q(z)-\Lambda]^{-1}$ in block form,

$$[Q(z)-\Lambda]^{-1}=\begin{bmatrix}N(z) & W(z)\\ M(z) & V(z)\end{bmatrix}; \tag{46}$$

where $W(z)=(w_{lm}(z))$ and $V(z)=(v_{lm}(z))$ are $n\times n$-matrices. From (42) we have

$$\zeta_l(\tilde{\chi}_a\psi)=\sum_{m=n+1}^{2n}[Q(z)-\Lambda]^{-1}_{l,m}\psi_{m-n}(0)=2\sum_{m=1}^{n}[Q(z)-\Lambda]^{-1}_{l,m+n}\delta_{jm}=2[Q(z)-\Lambda]^{-1}_{l,j+n}.$$

In other words,

$$\zeta_l(\tilde{\chi}_a\psi)=\begin{cases}2w_{lj}(z), & \text{if } 1\leqslant l\leqslant n,\\ 2v_{lj}(z), & \text{if } n+1\leqslant l\leqslant 2n.\end{cases}$$

Hence, from (36), (37), and (44) we get

$$g_0^{(a)}(x)=-2\sum_{m=1}^{n}w_{mj}(z)G_0(x,q_m;z), \tag{47}$$

$$g_l^{(a)}(x)=\delta_{lj}\chi_a(x)\psi_j(x)-\frac{2v_{lj}(z)}{\sqrt{-z}}\exp(-\sqrt{-z}x), \quad 0<l\leqslant n. \tag{48}$$

Passing to the limit $a\to\infty$ in (47) and (48), we obtain $g=(g_0,g_1,\ldots,g_n)\in L^2_{\mathrm{loc}}(\hat{X})$ with

$$g_0(x)=-2\sum_{m=1}^{n}w_{mj}(z)G_0(x,q_m;z),$$

$$g_l(x)=\delta_{lj}\psi_j(x)-\frac{2v_{lj}(z)}{\sqrt{-z}}\exp(-\sqrt{-z}x), \quad 0<l\leqslant n.$$

Moreover, since $\Gamma^{(1)}g^{(a)}$ and $\Gamma^{(2)}g^{(a)}$ are independent of a, g satisfies the boundary condition $(\Gamma^{(1)}g,\Gamma^{(2)}g)\in\Lambda$, and from (45) we have

$$(H-z)g=(H_{\mathrm{N}}-z)\psi.$$

In the limit $\varepsilon\to 0$ we have $\sqrt{-z}\to -ik$, whereas g has a limit f in $L^2_{\mathrm{loc}}(\hat{X})$ such that

$$f_0(x)=-2\sum_{m=1}^{n} w_{mj}(k^2)G_0(x,q_m;k^2),$$
$$f_l(x)=\delta_{lj}\psi_j(x)+\frac{2v_{lj}(k^2)}{ik}\exp(ikx),\quad 0<l\leqslant n, \tag{49}$$

since $k^2\notin\sigma(H_0)$. Moreover, in the sense of distributions,

$$(H-z)g\to(H-k^2)f,$$
$$(H_{\mathrm{N}}-z)\psi\to(H_{\mathrm{N}}-k^2)\psi=0.$$

Hence, $(H-k^2)f=0$. Further, f satisfies the boundary condition $(\Gamma^{(1)}f,\Gamma^{(2)}f)\in\Lambda$. Indeed, since $k^2\notin\sigma(H_0)$ we have

$$a_m(G_0(\cdot,q_l;z))\to\delta_{lm},\quad b_m(G_0(\cdot,q_l;z))\to Q_0^{ml}(k^2),$$

as $z\to k^2$ [see (14) and (16)]. On the other hand, direct calculations show that $\Gamma_l^{(1)}g_l\to\Gamma_l^{(1)}f_l$ and $\Gamma_l^{(2)}g_l\to\Gamma_l^{(2)}f_l$ as $z\to k^2$ $(l=1,\ldots,n;)$. Finally, from (49) we get the properties (i) and (ii) with

$$r_j(k)=1-2ik^{-1}v_{jj}(k^2),$$
$$t_{lj}(k)=-2ik^{-1}v_{lj}(k^2). \tag{50}$$

The proof is completed by establishing the uniqueness of f which follows from Lemma 7 below. ■

Lemma 7: Let f be a solution to the Schrödinger equation (35) for some $k^2\notin Z_H$, with the property that for all l, $1\leqslant l\leqslant n$,

$$f_l(x)=\alpha_l\exp(ikx), \tag{51}$$

for some $\alpha_l\in\mathbb{C}$. Then $f=0$.

Proof: Take $z_\varepsilon=k^2+i\varepsilon$ and $a>0$ as in the proof of the theorem. It is evident that $\tilde{\chi}_a f\in\mathcal{D}(H)$; denote

$$\psi^{(\varepsilon)}=R_{\mathrm{N}}(z_\varepsilon)(H-z_\varepsilon)\tilde{\chi}_a f.$$

Then

$$(H_{\mathrm{N}}-z_\varepsilon)\psi^{(\varepsilon)}=(H-z_\varepsilon)\tilde{\chi}_a f, \tag{52}$$

and

$$\tilde{\chi}_a f=\psi^{(\varepsilon)}-\gamma(z_\varepsilon)\zeta(\psi^{(\varepsilon)}). \tag{53}$$

Consider the integral kernel $G_l^{\mathrm{N}}(x,y;z)$ of the operator $R_l^{\mathrm{N}}(z)=(H_l^{\mathrm{N}}-z)^{-1}$; then

$$G_l^{\mathrm{N}}(x,y;z_\varepsilon)\to\frac{i}{2k}[\exp(ik|x-y|)+\exp(ik(x+y))]\equiv G_l^{\mathrm{N}}(x,y;k^2),$$

as $\varepsilon\to 0$ [see (11)]. Denote by $\mathcal{H}_l^{(a)}$ the following subspace of $\mathcal{H}_l=L^2(\mathbb{R}_+^{(l)})$:

$$\mathcal{H}_l^{(a)}:=\{\varphi\in L^2(\mathbb{R}_+^{(l)}):\mathrm{supp}\,\varphi\subset[0,a+1]\};$$

then $G_l^{\mathrm{N}}(x,y;z)$ is the kernel of a continuous linear operator from $\mathcal{H}_l^{(a)}$ to $L^2_{\mathrm{loc}}(\mathbb{R}_+^{(l)})$ [recall that $L^2_{\mathrm{loc}}(\mathbb{R}_+^{(l)})$ is endowed with the topology of L^2-convergence on compact subsets of $\mathbb{R}_+^{(l)}$]. Set $\mathcal{H}^{(a)}:=\mathcal{H}_0\oplus\mathcal{H}_1^{(a)}\oplus\cdots\oplus\mathcal{H}_n^{(a)}$; then

$$R_{\mathrm{N}}(k^2):=R_0(k^2)\oplus R_1^{\mathrm{N}}(k^2)\oplus\cdots\oplus R_n^{\mathrm{N}}(k^2)$$

is a continuous linear operator from $\mathcal{H}^{(a)}$ to $L^2_{\mathrm{loc}}(\hat{X})$. Moreover, if $h\in\mathcal{H}^{(a)}$ then $R_{\mathrm{N}}(z_\varepsilon)h\to R_{\mathrm{N}}(k^2)h$ as $\varepsilon\to 0$; in particular $\psi^{(\varepsilon)}\to R_{\mathrm{N}}(k^2)(H-k^2)\tilde{\chi}_a f=:\psi^{(0)}$. Hence, $\tilde{\chi}_a\psi^{(\varepsilon)}\to\tilde{\chi}_a\psi^{(0)}$ in $L^2(\hat{X})$ as $\varepsilon\to 0$, too. Fix $\varepsilon_0>0$ and put $z_0=k^2+i\varepsilon_0$; then

$$(H_{\mathrm{N}}-z_0)\psi^{(\varepsilon)}=(H_{\mathrm{N}}-z_\varepsilon)\psi^{(\varepsilon)}+(z_\varepsilon-z_0)\psi^{(\varepsilon)}=(H-z_\varepsilon)\tilde{\chi}_a f+(z_\varepsilon-z_0)\psi^{(\varepsilon)}.$$

Therefore, $(H_{\mathrm{N}}-z_0)\psi^{(\varepsilon)}$ has a limit in $L^2_{\mathrm{loc}}(\hat{X})$ as $\varepsilon\to 0$. Consequently,

$$\psi_l^{(\varepsilon)}(x)\to\psi_l^{(0)}(x),\quad \frac{d}{dx}\psi_l^{(\varepsilon)}(x)\to\frac{d}{dx}\psi_l^{(0)},$$

locally uniformly on $\mathbb{R}_+^{(l)}$ for each l, $1\leqslant l\leqslant n$. Now we have

$$(H_{\mathrm{N}}-z_0)\tilde{\chi}_a\psi^{(\varepsilon)}=\tilde{\chi}_a(H_{\mathrm{N}}-z_0)\psi^{(\varepsilon)}-2(0,\chi_a'(\psi_1^{(\varepsilon)})',\ldots,\chi_a'(\psi_n^{(\varepsilon)})')-(0,\chi_a''\psi_1^{(\varepsilon)},\ldots,\chi_a''\psi_n^{(\varepsilon)}). \tag{54}$$

It follows from (54) that also $(H_{\mathrm{N}}-z_0)\tilde{\chi}_a\psi^{(\varepsilon)}$ has a limit in $L^2(\hat{X})$, and therefore, $\tilde{\chi}_a\psi^{(\varepsilon)}$ has a limit in the graph topology of $\mathcal{D}(H_{\mathrm{N}})$ as $\varepsilon\to 0$. Thus, $\tilde{\chi}_a\psi^{(0)}\in\mathcal{D}(H_{\mathrm{N}})$ and $(H_{\mathrm{N}}-z_0)\tilde{\chi}_a\psi^{(\varepsilon)}\to(H_{\mathrm{N}}-z_0)\tilde{\chi}_a\psi^{(0)}$ in $L^2(\hat{X})$.

Now (52) implies that

$$(H_{\mathrm{N}}-z_\varepsilon)\tilde{\chi}_a\psi^{(\varepsilon)}=\tilde{\chi}_a(H-z_\varepsilon)\tilde{\chi}_a f-2(0,\chi_a'(\psi_1^{(\varepsilon)})',\ldots,\chi_a'(\psi_n^{(\varepsilon)})')-(0,\chi_a''\psi_1^{(\varepsilon)},\ldots,\chi_a''\psi_n^{(\varepsilon)}). \tag{55}$$

Since $(\tilde{\chi}_a(H-k^2)\tilde{\chi}_a f)(x)=0$ if $x\in\mathbb{R}_+^{(l)}$ and $0\leqslant x\leqslant a$, we get from (55) by passing to the limit $\varepsilon\to 0$,

$$(H_{\mathrm{N}}-\lambda)\hat{\chi}_a\psi^{(0)}(x)=0,\quad \text{if} x\in\mathbb{R}_+^{(l)},\ 0\leqslant x\leqslant a.$$

Because $\tilde{\chi}_a\psi^{(0)}\in\mathcal{D}(H_{\mathrm{N}})$, we have for every $l\geqslant 1$:

$$\psi_l^{(0)}(x)=c_l(\exp(ikx)+\exp(-ikx)),\quad \text{if } x\in[0,a].$$

Now, we turn to (53); for $l\geqslant 1$ this equality reads as

$$\chi_a(x)f_l(x)=\psi_l^{(\varepsilon)}(x)-\frac{\zeta_{l+n}(\psi^{(\varepsilon)})}{\sqrt{-z}}\exp(-\sqrt{-z}x), \tag{56}$$

where

$$\zeta_{l+n}(\psi^{(\varepsilon)})=\sum_{m=1}^{n}[Q(z)-\Lambda]^{-1}_{l+n,m}\psi_0^{(\varepsilon)}(q_m)+\sum_{m=n+1}^{2n}[Q(z)-\Lambda]^{-1}_{l+n,m}\psi^{(\varepsilon)}_{m-n}(0)$$

[see (37) and (42)]. By definition of $\psi^{(\varepsilon)}$ we have $\psi_0^{(\varepsilon)}=R_0(k^2+i\varepsilon)(S_0^*-k^2-i\varepsilon)f_0$. Moreover $R_0(z)$ is a continuous mapping from $L^2(X)$ to $\mathcal{D}(H_0)$ endowed with the graph topology and, hence, a continuous mapping from $L^2(X)$ to $C(X)$ which continuously depends on $\varepsilon\in[0,\varepsilon_0]$. Therefore, $\psi_0^{(\varepsilon)}(q_m)\to\psi_0^{(0)}(q_m)$ as $\varepsilon\to 0$. Hence, we obtain from (56) that for $l\geqslant 1$,

$$\chi_a(x)f_l(x)=\psi_l^{(0)}(x)+\frac{\zeta_{l+n}(\psi^{(0)})}{ik}\exp(ikx), \tag{57}$$

where the coefficients

$$\zeta_{l+n}(\psi^{(0)})=\sum_{m=1}^{n}[Q(k^2)-\Lambda]^{-1}_{l+n,m}\psi_0^{(0)}(q_m)+\sum_{m=n+1}^{2n}[Q(k^2)-\Lambda]^{-1}_{l+n,m}\psi^{(0)}_{m-n}(0) \tag{58}$$

are well defined because $k^2\notin Z_H$. Moreover, $\psi_0^{(0)}(q)=0$, since $k^2\notin\sigma(H_0)$, and (57) implies that for $x\in[0,a]$ and $l\geqslant 1$ the functions f_l have the form

$$f_l(x)=c_l\exp(-ikx)+c_l'\exp(ikx).$$

Comparing with (51), we get $c_l=0$ and, hence, $\psi_l^{(0)}(x)=0$ for $x\in[0,a]$. Returning to (57) and (58) we obtain that $f_l(x)=0$ for $x\in[0,a]$. Since a is arbitrary, $f_l=0$, $\forall l=1,\ldots,n$.

Using (29) we see that f_0 satisfies the boundary conditions (30). Moreover, by the hypothesis of the lemma, f_0 is a solution to the equation $(S_0^*-k^2)f_0=0$. Since $k^2\notin\sigma(H_0^{B,\theta})$, we get $f_0=0$. Thus, the lemma is proven, and the proof of Theorem 5 is completed. ■

Property (i) of Theorem 5 means that the function $f_j(x)$ represents a superposition of an incoming wave $\exp(-ikx)$ and a reflected wave $r_j(k)\exp(ikx)$ in the channel $\mathbb{R}_+^{(j)}$.

Definition: $r_j(k)$ is called *the reflection amplitude* for H in the channel $\mathbb{R}_+^{(j))}$ at energy $E=k^2$. The quantity $R_j(k)=|r_j(k)|^2$ is called *the reflection coefficient* (*or the reflection probability*) in the channel $\mathbb{R}_+^{(j)}$.

Condition (ii) in Theorem 5 means that the function $f_l(x)$ $(l\neq j)$ represents an outgoing wave $t_{lj}(k)\exp(ikx)$ in the channel $\mathbb{R}_+^{(l)}$.

Definition: $t_{lj}(k)$ is called *the transmission amplitude* for H from the channel $\mathbb{R}_+^{(j)}$ to the channel $\mathbb{R}_+^{(l)}$ at energy $E=k^2$. The quantity $T_{lj}(k)=|t_{lj}(k)|^2$ is called *the transmission coefficient* (*or the transmission probability*) from $\mathbb{R}_+^{(j)}$ to $\mathbb{R}_+^{(l)}$.

Set

$$s_{lj}(k)=\begin{cases} r_j(k), & \text{if } l=j;\\ t_{lj}(k), & \text{otherwise.}\end{cases}$$

The matrix $\Sigma(k)=(s_{lj}(k))_{1\leqslant l,j\leqslant n}$ is called the *scattering matrix* for H. We stress that $\Sigma(k)$ is defined for all $k>0$ with the exception of such values of k that k^2 belongs to a discrete subset Z_H of $\mathbb{R}$.

Theorem 6: *The scattering matrix $\Sigma(k)$ is unitary for all $k>0$ such that $k^2\notin Z_H$. If the matrix $[Q(k^2)-\Lambda]^{-1}$ is represented in the form (46), then*

$$\Sigma(k)=I-2ik^{-1}V(k^2). \tag{59}$$

If Λ is the graph of a Hermitian operator L in $\mathcal{G}$ and the matrix L is represented in the form (31), *then*

$$\Sigma(k)=[C+A^*(Q_0(k^2)-B)^{-1}A+ik^{-1}I][C+A^*(Q_0(k^2)-B)^{-1}A-ik^{-1}I]^{-1}. \tag{60}$$

In particular, if the matrix A is invertible, and C is a scalar matrix (*i.e.*, $C=\gamma I$, $\gamma\in\mathbb{R}$), *then*

$$\begin{aligned}\Sigma(k)&=[ikI+(ik\gamma-1)A^{-1}(Q_0(k^2)-B)A^{*-1}][ikI+(ik\gamma+1)A^{-1}(Q_0(k^2)-B)A^{*-1}]^{-1}\\&=A^{-1}[ikAA^*+(ik\gamma-1)(Q_0(k^2)-B)][ikAA^*+(ik\gamma+1)(Q_0(k^2)-B)]^{-1}A.\end{aligned} \tag{61}$$

Proof: (59) follows immediately from (50) as obtained in the proof of Theorem 5. To get (60) we use the Frobenius formula for the inverse of a block-matrix:[56]

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} = \begin{bmatrix} [A_{11}-A_{12}A_{22}^{-1}A_{21}]^{-1} & A_{11}^{-1}A_{12}[A_{21}A_{11}^{-1}A_{12}-A_{22}]^{-1} \\ [A_{21}A_{11}^{-1}A_{12}-A_{22}]^{-1}A_{21}A_{11}^{-1} & [A_{22}-A_{21}A_{11}^{-1}A_{12}]^{-1} \end{bmatrix}. \tag{62}$$

Since

$$Q(z)-L=\begin{bmatrix} Q_0(z)-B & -A \\ -A^* & ik^{-1}I-C \end{bmatrix},$$

then

$$V(k^2)=[ik^{-1}I-C-A^*(Q_0(k^2)-B)^{-1}A]^{-1},$$

and hence

$$\Sigma(k)=I-2[I+ik(C+A^*(Q_0(k^2)-B)^{-1}A)]^{-1}. \tag{63}$$

Now we get (60) from (63) after some elementary algebra; (61) is an evident consequence of (60).

In particular, (60) shows that $\Sigma(k)$ is the Cayley transform of the Hermitian matrix $C+A^*(Q_0(k^2)-B)^{-1}A$. Hence, in case Λ is the graph of a Hermitian operator in $\mathcal{G}$; $\Sigma(k)$ is a unitary matrix. To prove the general case we use Proposition E. ■

In the notation of Example (2) from Sec. III, (60) gives the scattering matrix for the Schrödinger operator of Dirichlet type, H_{D}^{L}. We now derive an explicit expression for the scattering matrix in case of an arbitrary Schrödinger operator H^{Λ}. It is convenient to write the boundary conditions in the form (3) where the $(2n\times 2n)$-matrices L and M have a block structure,

$$L=\begin{bmatrix} B & A_1 \\ A_2 & C \end{bmatrix}, \quad M=\begin{bmatrix} Y & X_1 \\ X_2 & Z \end{bmatrix}, \tag{64}$$

and satisfy conditions (a) and (b) from Proposition B. In particular, condition (a) is equivalent to the relations

$$\begin{aligned} BY^*+A_1X_1^*&=YB^*+X_1A_1^*, \\ BX_2^*+A_1Z^*&=YA_2^*+X_1C^*, \\ A_2X_2^*+CZ^*&=X_2A_2^*+ZC^*. \end{aligned} \tag{65}$$

Suppose for the moment that M is invertible, then condition (3) reads as $\Gamma^{(2)}x=\Lambda\Gamma^{(1)}x$ where $\Lambda=M^{-1}L$. Therefore, using the Frobenius formula (62) we obtain the following expression for the matrix V from (46):

$$\begin{aligned} V=&[ik^{-1}Z-C-(X_2Q_0-A_2)(YQ_0-B)^{-1}(ik^{-1}X_1-A_1)]^{-1} \\ &\cdot[Z-(X_2Q_0-A_2)(YQ_0-B)^{-1}X_1]. \end{aligned} \tag{66}$$

Substituting (66) in (59), we finally obtain

$$\begin{aligned} \Sigma(k)=&[ikC+Z-(X_2Q_0(k^2)-A_2)(YQ_0(k^2)-B)^{-1}(ikA_1+X_1)]^{-1} \\ &\cdot[ikC-Z-(X_2Q_0(k^2)-A_2)(YQ_0(k^2)-B)^{-1}(ikA_1-X_1)]. \end{aligned} \tag{67}$$

Since invertible matrices are dense in the space of all $(2n\times 2n)$-matrices, expression (67) is valid for all boundary conditions of the form (3). In particular, if $M=I$ then we recover (60).

Next we consider some particular cases of (67) and determine the scattering matrices for the Schrödinger operators from Examples (1), (3), and (4) of Sec. III [Example (2) contains operators of the Dirichlet type which are covered by (60)].

(1) Consider Example (1) from Sec. III. Using the notations there we have

$$L=\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \quad M=\begin{bmatrix} -B & A \\ A^* & -C \end{bmatrix}.$$

Therefore,

$$\Sigma(k)=[ik+C-A^*(Q_0^{-1}(k^2)+B)^{-1}A][ik-C+A^*(Q_0^{-1}(k^2)+B)^{-1}A]^{-1}. \tag{68}$$

In particular, if $A=B=C=0$ (i.e., if $H=H_{\mathrm{N}}$), then $\Sigma(k)=I$ for all $k>0$. In this case the thin horns are decoupled from the manifold; therefore, the transmission coefficients vanish.

(2) Now we turn to Example (3) from Sec. III. In this case

$$L=\begin{bmatrix} -I & A \\ 0 & C \end{bmatrix}, \quad M=\begin{bmatrix} B & 0 \\ A^* & I \end{bmatrix}.$$

Hence

$$\Sigma(k)=[C+ik^{-1}-A^*(Q_0^{-1}(k^2)+B)^{-1}A][C-ik^{-1}-A^*(Q_0^{-1}(k^2)+B)^{-1}A]^{-1}. \tag{69}$$

In particular, if $A=B=C=0$ (i.e., if $H=H_{\mathrm{D}}$), then $\Sigma(k)=-I$ for all $k>0$. As in the case of the operator H_{N}, the transmission coefficients vanish, since the horns are decoupled from the manifold X_0.

(3) Finally, let us consider an operator of Neumann type H_{N}^L [as in Example (4) of Sec. III]. Now

$$L=\begin{bmatrix} B & 0 \\ -A^* & -I \end{bmatrix}, \quad M=\begin{bmatrix} I & -A \\ 0 & C \end{bmatrix},$$

and we get a simple expression for $\Sigma(k)$, which is similar to (60):

$$\Sigma(k)=[ikI+C+A^*(Q_0(k^2)-B)^{-1}A][ikI-C-A^*(Q_0(k^2)-B)^{-1}A]^{-1}. \tag{70}$$

In particular, if the matrix A is invertible and C is a Hermitian scalar matrix ($C=\gamma I$), then

$$\begin{aligned}\Sigma(k)&=[(ik+\gamma)A^{-1}(Q_0(k^2)-B)A^{*-1}+I][(ik-\gamma)A^{-1}(Q_0(k^2)-B)A^{*-1}-I]^{-1}\\ &=A^{-1}[(ik+\gamma)(Q_0(k^2)-B)+AA^*][(ik-\gamma)(Q_0(k^2)-B)-AA^*]^{-1}A.\end{aligned} \tag{71}$$

Remark 6: There is another way to get (70) which is similar to the derivation of (60). Namely, if we use (33) to express the resolvent of H_{N}^L and start with the function

$$\psi_j(x)=\exp(ikx)-\exp(-ikx)$$

in the channel $\mathbb{R}_+^{(j)}$ [instead of the function (43)], then we get, arguing as in the proof of Theorem 5,

$$\Sigma(k)=2ikV_{\mathrm{D}}(k^2)-1, \tag{72}$$

where V_{D} is the $n\times n$-matrix in the block representation of $[Q_{\mathrm{D}}(z)-\Lambda]^{-1}$:

$$[Q_{\mathrm{D}}(z)-\Lambda]^{-1}=\begin{bmatrix} N_{\mathrm{D}}(z) & W_{\mathrm{D}}(z) \\ M_{\mathrm{D}}(z) & V_{\mathrm{D}}(z) \end{bmatrix}. \tag{73}$$

[Note that Q_D and γ_D in (33) are given by (12), (16), (26)]. From (72) and (73) we get (70) again.

It is interesting to note that for the Schrödinger operator $H=H_0^{B,\theta}\oplus H_1^N\oplus\cdots\oplus H_n^N$ (see Example 1 from Sec. III), we have $\Sigma(k)=I$ independently of k, i.e., we have in each channel a complete reflection without phase shift. On the other hand, if $H=H_0^{B,\theta}\oplus H_1^D\oplus\cdots\oplus H_n^D$ (see Example 3 from Sec. III), then $\Sigma(k)=-I$ independently of k, i.e., there is complete reflection in each channel with a phase shift of magnitude π.

Remark 7: With obvious modifications, the results of this section are valid for the case $d=0$ (X is a finite set of isolated points). This case is not as empty as it seems at first sight. For example, if we put in (67) $A_1=A_2=X_1=X_2=0$, then

$$\Sigma(k)=[ikC+Z]^{-1}[ikC-Z]. \tag{74}$$

This is the scattering matrix for a system of quantum wires with a single common vertex derived in Ref. 17.

V. THE CASES OF ONE AND TWO "HORNS"

We consider now the most interesting particular cases. For $n=1$ we denote q_1 as q and r_1 as r for simplicity. If H is an operator of Dirichlet type, i.e., if $H=H_D^L$ (see Example 2 of Sec. III), then

$$Q(k^2)-L=\begin{bmatrix} Q_0(k^2)-\beta & \alpha \\ \overline{\alpha} & ik^{-1}-\gamma \end{bmatrix},$$

where $\alpha\in\mathbb{C}$, $\beta,\gamma\in\mathbb{R}$ are arbitrary. In this case $\Sigma(k)$ coincides with the reflection amplitude $r(k)$. Using (61), we get

$$\Sigma(k)=\frac{(i\gamma k-1)(Q_0(k^2)-\beta)+i|\alpha|^2k}{(i\gamma k+1)(Q_0(k^2)-\beta)+i|\alpha|^2k}. \tag{75}$$

Obviously, we have $R(k)\equiv 1$ for the reflection coefficient.

Similarly, for the operator of Neumann type $H=H_N^L$ (see Example 4 of Sec. III) we obtain

$$\Sigma(k)=\frac{(ik+\gamma)(Q_0(k^2)-\beta)+|\alpha|^2}{(ik-\gamma)(Q_0(k^2)-\beta)-|\alpha|^2}. \tag{76}$$

It is convenient to write

$$\Sigma(k)=e^{i\Phi(k)},$$

where $\Phi(k)$ is the so-called *scattering phase*.

Equations (75) and (76) have interesting consequences. First we recall that a point $E\in\mathbb{R}$ is called a *point level* of the operator $\tilde{H}_0=H_0^B\equiv H_0^\beta$, if $Q(E)-\beta=0$. The spectrum of $\tilde{H}_0$ (recall that $\tilde{H}_0$ is a point perturbation of H_0) consists of all point levels and all multiple eigenvalues of the unperturbed operator H_0.

Theorem 7: *1. Let $n=1$ and H be a Schrödinger operator of Dirichlet type: $H=H_D^L$. Then the following assertions hold.*

(1a) $\Sigma(k)=1$ [i.e., $\Phi(k)\equiv 0 \bmod 2\pi$] if and only if k^2 is an energy level for the point perturbation H_0^β of H_0.

(1b) Let, in addition, $\gamma=0$. Then $\Sigma(k)=-1$ [i.e., $\Phi(k)\equiv\pi \bmod 2\pi$] if and only if $k^2\in\sigma^p(H_0)$. Therefore, for a generic point $q\in X$, $\Sigma(k)=-1$ if and only if $k^2\in\sigma(H_0)$.

2. Let $n=1$ and H be a Schrödinger operator of Neumann type: $H=H_N^L$. Then the following assertions hold.

(2a) $\Sigma(k)=-1$ *[i.e.,* $\Phi(k)\equiv\pi \bmod 2\pi$*] if and only if* k^2 *is an energy level for the point perturbation* H_0^β *of* H_0.

(2b) Let, in addition, $\gamma=0$. *Then* $\Sigma(k)=1$ *[i.e.,* $\Phi(k)\equiv 0 \bmod 2\pi$*] if and only if* $k^2 \in \sigma^p(H_0)$. *Therefore, for a generic point* $q\in X$, $\Sigma(k)=1$ *if and only if* $k^2\in\sigma(H_0)$.

Proof: The theorem is an immediate consequence of (75) and (76). ■

Theorem 7 shows that by means of an infinitely thin horn $\mathbb{R}_+$ attached to the manifold X at a point q we can "hear" the positive point levels of a point perturbation of H_0 at the point q. Moreover, if q is a generic point, we can hear the positive part of the spectrum of the Schrödinger operator H_0 on X. Therefore, we can think of the horn $\mathbb{R}_+$ *as a kind of quantum stethoscope.*

Next we consider the case of two horns $(n=2)$ in some detail. For simplicity we shall write

$$\tilde{Q}(k^2)=Q_0(k^2)-B,$$

where B is a given Hermitian 2×2-matrix. We start with the Schrödinger operator H of Dirichlet type, $H=H_{\mathrm{D}}^L$. Let $A=(\alpha_{jl})$ be an invertible 2×2-matrix, $C=\gamma I$ $(\gamma\in\mathbb{R})$ a scalar 2×2-matrix. We shall denote the matrix AA^* by N:

$$N\equiv\begin{bmatrix}\nu_{11} & \nu_{12}\\ \nu_{21} & \nu_{22}\end{bmatrix}=\begin{bmatrix}|\alpha_{11}|^2+|\alpha_{12}|^2 & \alpha_{11}\overline{\alpha}_{21}+\alpha_{12}\overline{\alpha}_{22}\\ \alpha_{21}\overline{\alpha}_{11}+\alpha_{22}\overline{\alpha}_{12} & |\alpha_{22}|^2+|\alpha_{21}|^2\end{bmatrix}.$$

Further we set

$$\begin{aligned}\Delta(k)&=(k^2\gamma-ik)(\nu_{12}\tilde{Q}_{21}(k^2)+\nu_{21}\tilde{Q}_{12}(k^2)-\nu_{11}\tilde{Q}_{22}(k^2)-\nu_{22}\tilde{Q}_{11}(k^2))\\&\quad+(ik\gamma+1)^2\det\tilde{Q}(k^2)-k^2|\det A|^2,\end{aligned}$$

$$\begin{aligned}M_{11}(k)&=(k^2\gamma+ik)(\nu_{21}\tilde{Q}_{12}(k^2)-\nu_{22}\tilde{Q}_{11}(k^2))+(k^2\gamma-ik)\\&\quad\times(\nu_{12}\tilde{Q}_{21}(k^2)-\nu_{11}\tilde{Q}_{22}(k^2))-(k^2\gamma^2+1)\det\tilde{Q}(k^2)-k^2|\det A|^2,\end{aligned}$$

$$\begin{aligned}M_{22}(k)&=(k^2\gamma+ik)(\nu_{12}\tilde{Q}_{21}(k^2)-\nu_{11}\tilde{Q}_{22}(k^2))+(k^2\gamma-ik)(\nu_{21}\tilde{Q}_{12}(k^2)\\&\quad-\nu_{22}\tilde{Q}_{11}(k^2))-(k^2\gamma^2+1)\det\tilde{Q}(k^2)-k^2|\det A|^2,\end{aligned}$$

$$M_{12}(k)=2ik(\nu_{12}\tilde{Q}_{11}(k^2)-\nu_{11}\tilde{Q}_{12}(k^2)),$$

$$M_{21}(k)=2ik(\nu_{21}\tilde{Q}_{22}(k^2)-\nu_{22}\tilde{Q}_{21}(k^2)).$$

Then we have for the elements of the scattering matrix $\Sigma(k)$:

$$s_{11}(k)=\frac{\alpha_{11}\alpha_{22}M_{11}(k)-\alpha_{12}\alpha_{21}M_{22}(k)+\alpha_{21}\alpha_{22}M_{12}(k)-\alpha_{11}\alpha_{12}M_{21}(k)}{\det A\ \ \Delta(k)},\tag{77}$$

$$s_{22}(k)=\frac{\alpha_{11}\alpha_{22}M_{22}(k)-\alpha_{12}\alpha_{21}M_{11}(k)+\alpha_{11}\alpha_{12}M_{21}(k)-\alpha_{22}\alpha_{21}M_{12}(k)}{\det A\ \ \Delta(k)},\tag{78}$$

$$s_{12}(k)=\frac{\alpha_{12}\alpha_{22}(M_{11}(k)-M_{22}(k))+\alpha_{22}^2M_{12}(k)-\alpha_{12}^2M_{21}(k)}{\det A\ \ \Delta(k)},\tag{79}$$

$$s_{21}(k)=\frac{\alpha_{11}\alpha_{21}(M_{22}(k)-M_{11}(k))+\alpha_{11}^2M_{21}(k)-\alpha_{21}^2M_{12}(k)}{\det A\ \ \Delta(k)}.\tag{80}$$

Shortly, we have

$$\Sigma(k)=\Delta^{-1}(k)A^{-1}M(k)A\,, \tag{81}$$

where $M=(M_{jl})_{j,l=1,2}$.

Similarly we can obtain the scattering matrix for an operator of Neumann type, $H=H^L_{\mathrm{N}}$. We assume for simplicity that the matrix A is diagonal: $A=(\alpha_j\delta_{jl})_{1\leqslant j,l\leqslant n}$ with real numbers α_j, and that C is a scalar matrix, $C=\gamma I$, $\gamma\in\mathbb{R}$. In this case we set

$$\Delta_{\mathrm{N}}(k):=-|\alpha_1\alpha_2|^2+(ik-\gamma)(|\alpha_2|^2\widetilde{Q}_{11}(k^2)+|\alpha_1|^2\widetilde{Q}_{22}(k^2))-(ik-\gamma)^2\det\widetilde{Q}(k^2)\,.$$

Then (71) yields

$$s_{11}(k)=[|\alpha_1\alpha_2|^2+(ik+\gamma)|\alpha_2|^2\widetilde{Q}_{11}(k^2)-(ik-\gamma)|\alpha_1|^2\widetilde{Q}_{22}(k^2)+(k^2+\gamma^2)\det\widetilde{Q}(k^2)]\Delta_{\mathrm{N}}^{-1}(k)\,,$$

$$s_{22}(k)=[|\alpha_1\alpha_2|^2+(ik+\gamma)|\alpha_1|^2\widetilde{Q}_{22}(k^2)-(ik-\gamma)|\alpha_2|^2\widetilde{Q}_{11}(k^2)+(k^2+\gamma^2)\det\widetilde{Q}(k^2)]\Delta_{\mathrm{N}}^{-1}(k)\,,$$

$$s_{12}(k)=2ik\overline{\alpha_1}\alpha_2\widetilde{Q}_{12}(k^2)\Delta_{\mathrm{N}}^{-1}(k)\,, \tag{82}$$

$$s_{21}(k)=2ik\alpha_1\overline{\alpha_2}\widetilde{Q}_{21}(k^2)\Delta_{\mathrm{N}}^{-1}(k)\,.$$

Remark 8: If $-H^0$ is the Laplace–Beltrami operator, then the scattering matrix (82) coincides (up to notation) with the one derived in Ref. 13. Moreover, if we put in (82) $B=C=0$ and $\alpha_1=\alpha_2=\alpha$, then we get

$$s_{21}(k)=\frac{2ik|\alpha|^2[Q_0(k^2)]_{12}}{k^2\det Q_0(k^2)+ik|\alpha|^2([Q_0(k^2)]_{11}+[Q_0(k^2)]_{22})-|\alpha|^4}\,.$$

This result was obtained by Kiselev.[20]

Let us list some interesting consequences of (77)–(80). First consider the following permutation of the matrix elements of A: $\alpha_{11}\leftrightarrow\alpha_{12}$, $\alpha_{21}\leftrightarrow\alpha_{22}$. Then the elements of $\Sigma(k)$ undergo the permutation $s_{11}\leftrightarrow s_{22}$, $s_{12}\leftrightarrow s_{21}$. The reason for this effect is intuitively clear: the permutation $\alpha_{11}\leftrightarrow\alpha_{12}$, $\alpha_{21}\leftrightarrow\alpha_{22}$ means that we attach the semi-axis $\mathbb{R}^+_1$ to the point q_2 in place of q_1, whereas the semi-axis $\mathbb{R}^+_2$ is attached to q_1.

Another interesting consequence is related to the conducting properties of a quantum-mechanical system with the configuration space $\hat{X}$. Namely, at zero temperature the ballistic conductance $\sigma(k)$ of an electric chain consisting of two one-dimensional wires $\mathbb{R}^{(1)}_+$ and $\mathbb{R}^{(2)}_+$ attached to a mesoscopic device X is given by the Landauer–Büttiker formula,

$$\sigma(k)=\frac{e^2}{\pi\hbar}\,\frac{T_{12}(k)}{R_1(k)}\,,$$

where e is the electron charge, $\hbar$ is the Planck constant, and k^2 is the Fermi energy.[57,58] For a generic point $(q_1,q_2)\in X\times X$, $q_1\neq q_2$ and for fixed $z_0\in\sigma(H_0)$, the function $z\mapsto\det\widetilde{Q}_0(z)$ has a pole of the second order at z_0. On the other hand, the functions $z\mapsto\widetilde{Q}_{jl}(z)$ have poles at most of the first order at the same point. Therefore, for $T_{12}(k)=T_{21}(k)=|s_{12}(k)|^2$ we have at a generic point $(q_1,q_2)\in X\times X$, $q_1\neq q_2$, that $T_{12}(k)=0$ if $k^2\in\sigma(H_0)$. In other words, if $k^2\in\sigma(H_0)$, then $\sigma(k)=0$. The converse is true, e.g., for a real operator H_0 (i.e., for the operator H_0 commuting with the operator J of complex conjugation: $Jf=\overline{f}$) at least if the following conditions are satisfied: (1) the matrix A is diagonal and $\alpha_{11}\alpha_{22}\neq0$; (2) $\operatorname{Im}\beta_{12}\neq0$. In this case $[Q_0(k^2)]_{12}$ is a real number if $k^2\notin\sigma(H_0)$, and thus we have the following proposition.

Proposition 8: Let $\sigma(k)$ be the conductance of an electric chain consisting of the "wires" $\mathbb{R}^{(1)}_+$ and $\mathbb{R}^{(2)}_+$ attached to the "device" X at some generic points. Suppose that the Hamiltonian of the device X is a real Schrödinger operator H_0 of the Dirichlet type. If the conditions (1) and (2) above are satisfied, then $\sigma(k)$ vanishes if and only if k^2 is an eigenvalue of H_0. ■

Assume now that $\dim X \geqslant 2$. If the geodesic distance $r(q_1,q_2)$ between q_1 and q_2 tends to zero, then at a fixed value of the energy k^2, $k^2 \notin \sigma(H_0)$, the numbers $\tilde{Q}_{11}(k^2)$ and $\tilde{Q}_{22}(k^2)$ remain bounded, whereas $\tilde{Q}_{12}(k^2)$ and $\tilde{Q}_{21}(k^2)$ tend to infinity. Therefore, the conductance $\sigma(k)$ tends to zero [see (79) and (80)]. This paradoxical result is intimately related to an unusual behavior of the point perturbations of the Schrödinger operators in dimensions 2 or 3. Namely, consider a point perturbation H_0^B of H_0 supported on a two-point set $\{q_1,q_2\}$. Then in the sense of the norm-resolvent convergence, H_0^B tends to the unperturbed operator H_0 as $r(q_1,q_2)\to 0$. Indeed, the above considerations imply the following assertion: *If z is an arbitrary element of $\rho(H_0)$, then*

$$[Q_0(z)-B]^{-1}\to 0, \quad \text{as} \quad r(q_1,q_2)\to 0\,. \tag{83}$$

A discussion of such a property of point perturbations may be found in Ref. 59. To overcome the difficulties arising in the limit $r(q_1,q_2)\to 0$, a renormalization procedure for boundary conditions has been used.[60] It is not our intention to discuss here this subject in detail; we restrict our consideration to some consequences of (83) for the limiting behavior of the Schrödinger operator H on $\hat{X}$.

Applying (62) to the matrix $[Q(z)-L]^{-1}$, we get

$$[Q(z)-L]^{-1}=\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

where

$$A_{11}=[I-\tilde{Q}_0^{-1}(z)A((-z)^{-1/2}I-C)^{-1}A^*]^{-1}\tilde{Q}_0^{-1}(z)\,,$$

$$A_{12}=\tilde{Q}_0^{-1}(z)A[A^*\tilde{Q}_0^{-1}(z)A-(-z)^{-1/2}I+C]^{-1}\,,$$

$$A_{21}=[A^*\tilde{Q}_0^{-1}(z)A-(-z)^{-1/2}I+C]^{-1}A^*\tilde{Q}_0^{-1}(z)\,,$$

$$A_{22}=[(-z)^{-1/2}I-C-A^*\tilde{Q}_0^{-1}(z)A]^{-1}\,. \tag{84}$$

Now using (83) we show that as $r(q_1,q_2)\to 0$, the operator H tends in the norm-resolvent sense to the direct sum $H_0\oplus H'$ where H' is a point perturbation (supported in 0) of the free Hamiltonian $-d^2/dx^2$ on the line $\mathbb{R}$. It follows from Arnold's Lemma that in the limit $r(q_1,q_2)\to 0$, we can obtain any operator of the form $H_0\oplus H'$ where H' is an *arbitrary* point perturbation of $-d^2/dx^2$ supported on the point 0. In the case of the operator $H=H_{\mathrm{D}}^L$, the limiting scattering matrix can be obtained from (60); it has the form

$$\Sigma_{\mathrm{D}}^{\lim}(k)=(ikC-I)(ikC+I)^{-1}\,.$$

Similarly, if $H=H_{\mathrm{N}}^L$, then for the limiting form of the scattering matrix we obtain from (70),

$$\Sigma_{\mathrm{N}}^{\lim}(k)=(ik+C)(ik-C)^{-1}\,.$$

We note that in both cases $\Sigma^{\lim}(k)$ depends on the block C of the matrix L only.

In particular, the matrix elements of $\Sigma_{\mathrm{N}}^{\lim}$ have the form

$$s_{jl}^{\lim}(k)=\frac{-2ik\gamma_{jl}}{k^2+ik\operatorname{Tr}C-\det C}, \quad j\neq l\,; \tag{85}$$

$$s_{jj}^{\lim}(k)=\frac{k^2-ik(\gamma_{jj}-\gamma_{ll})+\det C}{k^2+ik\,\mathrm{Tr}\,C-\det C},\quad j=1,2,\quad l\neq j\,. \tag{86}$$

Moreover, if $A=I$, then the elements of the scattering matrix $\Sigma_{\mathrm{N}}(k)$ of the initial operator H_{N}^{L} are the following:

$$s_{11}(k)=\frac{(k^2-ik(\gamma_{11}-\gamma_{22})+\det C)\det\tilde{Q}(k^2)+ik(\tilde{Q}_{11}(k^2)-\tilde{Q}_{22}(k^2))+\mathrm{Tr}\,(C\tilde{Q}(k^2))+1}{\Delta_1(k)},$$

$$s_{22}(k)=\frac{(k^2-ik(\gamma_{22}-\gamma_{11})+\det C)\det\tilde{Q}(k^2)+ik(\tilde{Q}_{22}(k^2)-\tilde{Q}_{11}(k^2))+\mathrm{Tr}\,(C\tilde{Q}(k^2))+1}{\Delta_1(k)},$$

$$s_{12}(k)=\frac{2ik(\tilde{Q}_{12}(k^2)-\gamma_{12}\det\tilde{Q}(k^2))}{\Delta_1(k)},$$

$$s_{21}(k)=\frac{2ik(\tilde{Q}_{21}(k^2)-\gamma_{21}\det\tilde{Q}(k^2))}{\Delta_1(k)},$$

where

$$\Delta_1(k):=(k^2+ik\,\mathrm{Tr}\,C-\det C)\det\tilde{Q}(k^2)+ik\,\mathrm{Tr}\,\tilde{Q}(k^2)-\mathrm{Tr}\,(C\tilde{Q}(k^2))-1\,.$$

It is interesting to compare these elements with those for the scattering matrix of H_{N}^{L} in the case of an arbitrary diagonal matrix A and a scalar matrix C [see (82)].

An important particular case of (85) and (86) arises if we choose the matrix C in the form

$$C=\begin{bmatrix}\gamma & -\gamma\\ -\gamma & \gamma\end{bmatrix},$$

where $\gamma\in\mathbb{R}$, $\gamma\neq 0$. In this case,

$$s_{11}^{\lim}(k)=s_{22}^{\lim}(k)=\frac{-ik\gamma^{-1}}{2-ik\gamma^{-1}},$$

$$s_{12}^{\lim}(k)=s_{21}^{\lim}(k)=\frac{2}{2-ik\gamma^{-1}}.$$

Therefore, the limiting matrix $\Sigma^{\lim}(k)$ coincides with the scattering matrix for the δ'-perturbation of the free Schrödinger operator on the line $\mathbb{R}$.[51] There is a conjecture that the scattering on the δ'-potential can be realized geometrically.[35] Our result shows that *the scattering on the δ'-perturbation can be realized with an arbitrary accuracy by means of a nontrivial geometric scattering on an arbitrary compact manifold of dimension 2 or 3.*

Now we give an example of nontrivial boundary conditions such that the scattering matrix of the corresponding Schrödinger operator H^{Λ} in the limit $r(q_1,q_2)\to 0$ (for generic points) has the form

$$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},$$

i.e., in this limit we obtain a system with zero ballistic resistance (the condition $\dim X\geqslant 2$ is kept). Namely, let us consider the boundary conditions of the form (3), where L and M have the following 2×2-blocks [see (64) for notation]: $X_1=X_2=0$, $Y=I$,

$$Z=\begin{bmatrix}0 & 0\\ \zeta & -\zeta\end{bmatrix},\quad A_1=\begin{bmatrix}\alpha_1 & 0\\ \alpha_2 & 0\end{bmatrix},\quad A_2=\begin{bmatrix}0 & 0\\ \hat{\alpha}_1 & \hat{\alpha}_2\end{bmatrix},\quad C=\begin{bmatrix}\gamma & \gamma\\ 0 & 0\end{bmatrix},$$

and B is an arbitrary Hermitian 2×2-matrix. It is easy to prove that conditions (65) are satisfied iff $\hat{\alpha}_j=\zeta\overline{\alpha}_j$. In this case the scattering matrix $\Sigma(k)$ is independent of Z, A_2, and C; its elements have the form

$$s_{11}(k)=s_{22}(k)$$
$$=\frac{|\alpha_1|^2\,\tilde{Q}_{11}(k^2)+|\alpha_2|^2\,\tilde{Q}_{22}(k^2)-\overline{\alpha_1}\alpha_2\tilde{Q}_{12}(k^2)-\overline{\alpha_2}\alpha_1\tilde{Q}_{21}(k^2)}{|\alpha_1|^2\,\tilde{Q}_{11}(k^2)+|\alpha_2|^2\,\tilde{Q}_{22}(k^2)-\overline{\alpha_1}\alpha_2\tilde{Q}_{12}(k^2)-\overline{\alpha_2}\alpha_1\tilde{Q}_{21}(k^2)-2ik^{-1}\det\tilde{Q}(k^2)},\tag{87}$$

$$s_{12}(k)=s_{21}(k)$$
$$=\frac{2ik^{-1}\det\tilde{Q}(k^2)}{2ik^{-1}\det\tilde{Q}(k^2)-|\alpha_1|^2\,\tilde{Q}_{11}(k^2)-|\alpha_2|^2\,\tilde{Q}_{22}(k^2)+\overline{\alpha_1}\alpha_2\tilde{Q}_{12}(k^2)+\overline{\alpha_2}\alpha_1\tilde{Q}_{21}(k^2)}.\tag{88}$$

It is curious that the conductance of a system with the Hamiltonian H^Λ is in some sense reciprocal to the one described in Proposition 8. In fact, (87) and (88) show immediately that the following proposition is true.

Proposition 9: Suppose that the semi-axes $\mathbb{R}_+^{(1)}$ and $\mathbb{R}_+^{(2)}$ are attached to X in generic points and that the Schrödinger operator H^Λ on $\hat{X}$ is given as above. Then $\sigma(k)=\infty$ (i.e., the system $\hat{X}$ is a superconductor at the energy level k^2) if and only if $k^2\in\sigma(H_0)$. Moreover, $\sigma(k)=0$ if and only if k^2 is an energy level for the point perturbation H_0^B of H_0.

VI. A FEW EXAMPLES

Here some examples of Schrödinger operators H_0 on a compact manifold X of constant curvature are collected for which we can give an explicit form of the Q-matrix Q_0 and, hence, get an explicit expression for the scattering matrix $\Sigma(k)$ via (60) or (70). Recall that for $j\neq l$,

$$[Q_0(z)]_{jl}=G_0(q_j,q_l;z),\tag{89}$$

where $G_0(x,y;z)$ is the Green's function of H_0. Therefore, as a rule, only the diagonal terms $Q_0(z)]_{jj}$ are written explicitly below.

A. Ring $\mathbb{S}_a$

Let X be a ring $\mathbb{S}_a$ (i.e., a circle) of radius a. It is easy to show that the Green's function for the Schrödinger operator of a free charged particle,

$$H_0=-\frac{1}{a^2}\frac{d^2}{d\varphi^2}$$

($\varphi\in[0,2\pi)$ being the polar coordinate on $\mathbb{S}_a$) has the form

$$G_0(\varphi,\varphi';z)=-\frac{1}{2\sqrt{z}}\frac{\cos a\sqrt{z}(\varphi'-\varphi\pm\pi)}{\sin\pi a\sqrt{z}},$$

where the sign "plus" is taken if $\varphi\geqslant\varphi'$, otherwise we take "minus." The diagonal elements of the matrix Q_0 have the form

$$[Q_0(z)]_{jj}=G_0(q_j,q_j;z)\,. \tag{90}$$

B. Aharonov–Bohm ring

Consider a ring $\mathbb{S}_a$ of radius a located in an axially symmetric magnetic field perpendicular to the plane of the ring. Let Φ be the total magnetic flux through the ring. Put $\vartheta=\Phi/\Phi_0$, where Φ_0 is the quantum of the magnetic flux: $\Phi_0=2\pi\hbar c/|e|$. Then the Schrödinger operator for a charged particle in the system considered has the form

$$H_0=\frac{1}{a^2}\left(-i\frac{d}{d\varphi}+\vartheta\right)^2.$$

For the Green's function we have:[61]

$$G_0(\varphi,\varphi';z)=\frac{1}{4\sqrt{z}}\left[\frac{\exp(i(\varphi'-\varphi\pm\pi)(\vartheta-a\sqrt{z}))}{\sin\pi(\vartheta-a\sqrt{z})}-\frac{\exp(i(\varphi'-\varphi\pm\pi)(\vartheta+a\sqrt{z}))}{\sin\pi(\vartheta+a\sqrt{z})}\right]$$

(the choice of the signs is as in the previous example). In the considered case the matrix Q_0 is given by (89) and (90) again.

C. Flat torus $\mathbb{T}^d$ ($d=2$ or 3)

Let Λ_d be a lattice in $\mathbb{R}^d$ with generators $\vec{a}_1,\ldots,\vec{a}_d$:

$$\Lambda_d=\{n_1\vec{a}_1+\cdots+n_d\vec{a}_d: n_j\in\mathbb{Z}, j=1,\ldots,d\}\,,$$

and let Γ_d be the dual lattice for Λ_d, i.e. Γ_d be the lattice with generators $\vec{b}_1,\ldots,\vec{b}_d$ obeying the condition $\vec{a}_j\vec{b}_k=2\pi\delta_{jk}$. Denote by F_d the elementary cell for Λ_d:

$$F_d=\{x_1\vec{a}_1+\cdots+x_d\vec{a}_d: -\tfrac{1}{2}\leqslant x_j<\tfrac{1}{2}\}\,,$$

and fix points $q_1,\ldots,q_n$ from F_d. Let $H_0=-\Delta_X$ where X is the the torus $\mathbb{T}^d=\mathbb{R}^d/\Lambda_d$. Choosing points $q_1,\ldots,q_n\in\mathbb{T}^d$, we have[51]

$$[Q_0(z)]_{jl}=\begin{cases}v_d^{-1}\lim\limits_{\omega\to\infty}\sum\limits_{\gamma\in\Gamma_d,\,|\gamma|\leqslant\omega}\dfrac{e^{i\gamma(q_j-q_l)}}{|\gamma|^2-z}, & \text{if}\quad j\neq l;\\[2ex] (2\pi)^{-d}\lim\limits_{\omega\to\infty}\left[\sum\limits_{\gamma\in\Gamma_d,\,|\gamma|\leqslant\omega}\dfrac{\hat{v}_d}{|\gamma|^2-z}-\xi_d(\omega)\right], & \text{if}\quad j=l\,.\end{cases} \tag{91}$$

Here v_d and $\hat{v}_d$ are the volumes of the tori $\mathbb{R}^d/\Lambda^d$ and $\mathbb{R}^d/\Gamma^d$, respectively; the functions ξ_d ($d=2,3$) have the form

$$\xi_d(\omega)=\begin{cases}2\pi\ln\omega\,, & \text{if}\quad d=2;\\ 4\pi\omega\,, & \text{if}\quad d=3\,.\end{cases}$$

Using either the eigenfunction expansion for the Laplace operator on $\mathbb{T}^d$ or the Poisson summation formula we can get a convergent absolutely series expansion for $Q_0(k^2)_{jl}$ (see Ref. 62 for the case $d=3$):

$$[Q_0(k^2)]_{jl}=(1+z)v_d^{-1}\sum_{\gamma\in\Gamma_d}\frac{e^{i\gamma(q_j-q_l)}}{(|\gamma|^2-z)(|\gamma|^2+1)}+\kappa_d(q_j-q_l)\,. \tag{92}$$

Here the functions κ_d are defined as follows: If $d=2$, then

$$\kappa_2(x)=\begin{cases}\dfrac{1}{2\pi}\displaystyle\sum_{\lambda\in\Lambda_d} K_0(|x+\lambda|)\,, & \text{if} \quad x\notin\Lambda_d\,;\\ \dfrac{1}{2\pi}\left[\displaystyle\sum_{\lambda\in\Lambda_d,\,\lambda\neq 0} K_0(|\lambda|)+\ln 2-C_{\mathrm{E}}\right], & \text{if} \quad x\in\Lambda_d\,,\end{cases}$$

where K_0 is the Macdonald function (i.e., the modified Bessel function of the third kind) and C_{E} is the Euler constant. In the case $d=3$ we have

$$\kappa_3(x)=\begin{cases}\dfrac{1}{4\pi}\displaystyle\sum_{\lambda\in\Lambda_d}\frac{e^{-|x+\lambda|}}{|x+\lambda|}, & \text{if} \quad x\notin\Lambda_d\,;\\ \dfrac{1}{4\pi}\left[\displaystyle\sum_{\lambda\in\Lambda_d,\,\lambda\neq 0}\frac{e^{-|\lambda|}}{|\lambda|}-1\right], & \text{if} \quad x\in\Lambda_d\,.\end{cases}$$

D. Flat torus with Aharonov–Bohm fluxes

Consider the torus $\mathbb{T}^d$ as the product of d Aharonov–Bohm rings $\mathbb{S}_{a_j}$ with fluxes ϑ_j ($j=1,\ldots,d$). Let

$$H_j=\frac{1}{a_j^2}\left(-i\frac{d}{d\varphi}+\vartheta_j\right)^2,$$

and

$$H_0=\begin{cases}H_1\otimes I_2+I_1\otimes H_2\,, & \text{if} \quad d=2\,;\\ H_1\otimes I_2\otimes I_3+I_1\otimes H_2\otimes I_3+I_1\otimes I_2\otimes H_3\,, & \text{if} \quad d=3\,.\end{cases}$$

The operator H_0 may be considered as the Schrödinger operator on a torus $\mathbb{T}^d$ with a nonuniform magnetic field. Denote by ϑ the vector $(\vartheta_1,\ldots,\vartheta_d)$; then the $\mathcal{Q}$-function Q_0 now takes the form

$$[Q_0(z)]_{jl}=\begin{cases}v_d^{-1}\displaystyle\lim_{\omega\to\infty}\sum_{\gamma\in\Gamma_d,\,|\gamma+\theta|\leqslant\omega}\frac{e^{i(\gamma+\vartheta)(q_j-q_l)}}{|\gamma+\vartheta|^2-z}, & \text{if} \quad j\neq l;\\ (2\pi)^{-d}\displaystyle\lim_{\omega\to\infty}\left[\sum_{\gamma\in\Gamma_d,\,|\gamma+\theta|\leqslant\omega}\frac{\hat{v}_d}{|\gamma+\vartheta|^2-z}-\xi_d(\omega)\right], & \text{if} \quad j=l\,,\end{cases}$$

or

$$[Q_0(z)]_{jl}=(1+z)v_d^{-1}\sum_{\gamma\in\Gamma_d}\frac{e^{i(\gamma+\vartheta)(q_j-q_l)}}{(|\gamma+\vartheta|^2-z)(|\gamma+\vartheta|^2+1)}+\kappa_{d,\vartheta}(q_j-q_l)\,.$$

Now the functions $\kappa_{d,\vartheta}$ ($d=2,3$) are defined as follows:

$$\kappa_{2,\vartheta}(x)=\begin{cases}\dfrac{1}{2\pi}\displaystyle\sum_{\lambda\in\Lambda_d}K_0(|x+\lambda|)e^{-i\vartheta\lambda}, & \text{if} \quad x\notin\Lambda_d\,;\\ \dfrac{1}{2\pi}\left[\displaystyle\sum_{\lambda\in\Lambda_d,\,\lambda\neq 0}K_0(|\lambda|)e^{-i\vartheta\lambda}+\ln 2-C_{\mathrm{E}}\right], & \text{if} \quad x\in\Lambda_d\,;\end{cases}$$

$$\kappa_{3,\vartheta}(x)=\begin{cases}\dfrac{1}{4\pi}\displaystyle\sum_{\lambda\in\Lambda_d}\frac{e^{-|x+\lambda|-i\vartheta\lambda}}{|x+\lambda|}, & \text{if} \quad x\notin\Lambda_d\,;\\ \dfrac{1}{4\pi}\left[\displaystyle\sum_{\lambda\in\Lambda_d,\,\lambda\neq 0}\frac{e^{-|\lambda|-i\vartheta\lambda}}{|\lambda|}-1\right], & \text{if} \quad x\in\Lambda_d\,.\end{cases}$$

E. Flat torus $\mathbb{T}^2$ with a perpendicular uniform magnetic field

Consider the Euclidean plane $\mathbb{R}^2$ with the lattice Λ_2 and let **B** be a uniform magnetic field that is perpendicular to the plane and has the strength B. Denote by ϑ the number of the magnetic flux quanta through the elementary cell F_2: $\vartheta = Bv_d/\Phi_0$. The Green's function G^0 for the Schrödinger operator of a charged particle on the plane $\mathbb{R}^2$ with the field **B** has the form

$$G^0(x,y;z) = \frac{1}{4\pi}\Gamma\left(\frac{1}{2} - \frac{v_d z}{4\pi|\vartheta|}\right) \times \exp\left[-i\pi\vartheta v_d^{-1} x\wedge y - \frac{\pi|\vartheta|}{2v_d}(x-y)^2\right]$$
$$\times \Psi\left(\frac{1}{2} - \frac{v_d z}{4\pi|\vartheta|}, 1; \frac{\pi|\vartheta|}{v_d}(x-y)^2\right),$$

where $\Gamma(z)$ is the Euler Γ-function, $\Psi(a,c;z)$ is the Tricomi function (the confluent hypergeometric function), and $x\wedge y = x_1y_2 - x_2y_1$ is the standard symplectic product in $\mathbb{R}^2$. Let the following quantization condition be satisfied: *the number $\vartheta = Bv_d/\Phi_0$ of the flux quanta through the cell F_2 is an integer*. Then we can consider the corresponding magnetic Schrödinger operator on the torus $\mathbb{T}^2$. Using results from Ref. 63 we obtain for the Krein $\mathcal{Q}$-matrix,

$$[Q_0(z)]_{jl} = \sum_{\lambda\in\Lambda_2,\,\lambda\neq 0} G^0(\lambda + q_j, q_l; z)\exp[\pi i\vartheta v_d^{-1}(q_j\wedge\lambda) - \pi i\vartheta\lambda_1\lambda_2] + \xi_{jl}(z). \qquad (93)$$

Here

$$\xi_{jl}(z) = \begin{cases} G^0(q_j, q_l; z), & \text{if } j\neq l; \\ -\dfrac{1}{4\pi}\left[\psi\left(\dfrac{1}{2} - \dfrac{v_d z}{4\pi|\vartheta|}\right) + \ln(\pi|\vartheta|v_d^{-1}) + 2C_{\mathrm{E}}\right], & \text{if } j = l, \end{cases}$$

where $\psi(z)$ is the digamma function (the logarithmic derivative of the Γ-function). Note that in (93), λ_1, λ_2 are the coordinates of λ in the basis $\vec{a}_1$, $\vec{a}_2$ of Λ_2: $\lambda = \lambda_1\vec{a}_1 + \lambda_2\vec{a}_2$.

F. Sphere $\mathbb{S}^2_a$

Let X be a two-dimensional sphere $\mathbb{S}^2_a$ of radius a; then the Green's function for the Schrödinger operator H_0 of a free particle on X, $H_0 = -\Delta_X$, has the form[64]

$$G_0(x,y;z) = -\frac{1}{4\cos(\pi t(z))}\,\mathcal{P}_{-1/2+t(z)}\left(-\cos\frac{r(x,y)}{a}\right),$$

where $\mathcal{P}_a(z)$ is the Legendre function and

$$t(z) = \frac{1}{2}\sqrt{1+4a^2 z}.$$

Therefore, for every j,

$$[Q_0(z)]_{jj} = -\frac{1}{4\pi}\left[\psi\left(\frac{1}{2} + t(z)\right) + \psi\left(\frac{1}{2} - t(z)\right) - 2\ln(2a) + 2C_{\mathrm{E}}\right]$$
$$= -\frac{1}{2\pi}\left[\psi\left(\frac{1}{2} + t(z)\right) - \frac{\pi}{2}\,\mathrm{tg}\,(\pi t(z)) - \ln(2a) + C_{\mathrm{E}}\right].$$

G. Sphere $\mathbb{S}^3_a$

Consider now a three-dimensional sphere $X=\mathbb{S}^3_a$ of radius a. Then the Green's function for the Schrödinger operator H_0 of a free particle on X, $H_0=-\Delta_X$, reads[64] as

$$G_0(x,y;z)=\frac{1}{4\pi a\sin\dfrac{r(x,y)}{a}}\left[\cos\frac{r(x,y)\sqrt{a^2z+1}}{a}-\sin\frac{r(x,y)\sqrt{a^2z+1}}{a}\operatorname{ctg}\pi\sqrt{a^2z+1}\right].$$

Therefore, for every j,

$$[Q_0(z)]_{jj}=-\frac{\sqrt{a^2z+1}}{4\pi a}\operatorname{cotan}\pi\sqrt{a^2z+1}\,.$$

H. Compact manifold of constant negative curvature

Let now X be a compact d-dimensional manifold of constant negative curvature (with sectional curvature $-a^{-2}$ for some $a>0$). We shall consider X as a quotient $\mathbf{H}^d/\Gamma$, where $\mathbf{H}^d$ is the d-dimensional Lobachevsky space (i.e., the complete simply connected d-dimensional Riemannian manifold of constant negative curvature) and Γ is a cocompact discontinuous group of motions in $\mathbf{H}^d$. Denote by G^0_d the Green's function for the Laplace–Beltrami operator on $\mathbf{H}^d$. Recall that

$$G^0_d(x,y;z)=\begin{cases}\dfrac{\Gamma^2(s_2(z))}{4\pi\Gamma(2s_2(z))}\left[\cosh\dfrac{r(x,y)}{2a}\right]^{-2s_2(z)}F\left(s_2(z),s_2(z);2s_2(z);\cosh^{-2}\dfrac{r(x,y)}{2a}\right), & \text{if } d=2;\\ \dfrac{\exp[a^{-1}r(x,y)(1-s_3(z))]}{4\pi a\sinh(a^{-1}r(x,y))}, & \text{if } d=3\end{cases}$$

(see Refs. 3 and 65). Here $F(a,b;c;z)$ is the Gauss hypergeometric function and

$$s_d(z)=\frac{d-1+\sqrt{(d-1)^2-4a^2z}}{2},\quad d=2\,,3\,. \tag{94}$$

Let H_0 be a Schrödinger operator on X of the form $H_0=-\Delta_X$. If $\operatorname{Re}s_d(z)$ is sufficiently large, then there is an expansion of the Green's function $G_0(x,y;z)$ for $x\neq y$ into an absolutely convergent series:[3,65]

$$G_0(x,y;z)=\sum_{\gamma\in\Gamma}G^0_d(x,\gamma y;z)\,. \tag{95}$$

To find $G_0(x,y;z)$ for an arbitrary $z\in\mathbb{C}\setminus\sigma(H_0)$ we choose a number $z'=\operatorname{Re}z+ik$, where $k\in\mathbb{R}$ is so large that the series (95) absolutely converges at $z=z'$. Then the Neumann series,

$$R_0(z)=\sum_{n=0}^{\infty}(z-z')^nR_0^{n+1}(z')\,,$$

gives the desired value $R_0(z)$ and $G_0(x,y;z)$ may be found as an infinite sum of iterated integral kernels $G_0(x,y;z')$.

To find the Krein $\mathcal{Q}$-function we use (95) again. If $\operatorname{Re}s_d(z)$ is sufficiently large, then

$$[Q_0(z)]_{jj}=\sum_{\gamma\in\Gamma,\ \gamma\neq1}G^0_d(q_j,\gamma q_j;z)+\kappa_d(z)\,, \tag{96}$$

where

$$\kappa_d(z)=\begin{cases} -\dfrac{1}{2\pi}[\psi(s_2(z))-\ln 2a+C_{\mathrm{E}}], & \text{if } d=2; \\ -\dfrac{1}{4\pi a}\sqrt{1-a^2z}, & \text{if } d=3. \end{cases}$$

To find $[Q_0(z)]_{jj}$ at an arbitrary point z, $z\notin\sigma(H_0)$, we fix $z_0\in\mathbb{R}$, $z_0<0$ such that $[Q_0(z_0)]_{jj}$ is given by (96). Using the Hilbert resolvent identity and taking into consideration that the integral kernel for $R_0(z)R_0(z_0)$ is continuous,[3,65] we get

$$[Q_0(z)]_{jj}=[Q_0(z_0)]_{jj}+(z-z_0)\int_X G_d^0(q_j,x;z)G_d^0(x,q_j;z_0)\,d\lambda(x).$$

Remark 9: In some sense (96) is an analog of (91) for the space of constant negative curvature. Let us consider for simplicity the case of one horn ($n=1$, $q_1=q$) and try to transform (96) to an equality similar to (92) hoping to get a more convenient expression. First note that in general $Q_0(z)$ depends on q: $Q_0(z)=Q_0(z,q)$. But the Poisson summation formula gives us an averaged value $Q_0^{\mathrm{av}}(z)$ of $Q_0(z,q)$:

$$Q_0^{\mathrm{av}}(z):=(\mathrm{vol}\,X)^{-1}\int_X Q_0(z,q)\,dq.$$

If X is a homogeneous manifold, then $Q_0^{\mathrm{av}}(z)$ is independent of q and $Q_0(z)=Q_0^{\mathrm{av}}(z)$. Therefore, in the case of the torus $\mathbb{T}^d$, $Q_0(z)$ is given by (92). Let now X be a compact surface of constant negative curvature. In this case the role of the Poisson summation formula is played by the Selberg trace formula. Using the Selberg formula in the form obtained by Cartier and Voros[66] we get an explicit expression for $Q_0^{\mathrm{av}}(z)$ up to an additive constant c:

$$Q_0^{\mathrm{av}}(z)=(2-2g)\psi(s_2(z))+\frac{1}{\sqrt{1-4a^2z}}\frac{\mathcal{Z}_X'(s_2(z))}{\mathcal{Z}_X(s_2(z))}+c,$$

where g is the genus of X, $\mathcal{Z}_X(s)$ is the Selberg zeta function for X (see Refs. 67 and 68), and $s_2(z)$ is given by (94). Note that without loss of generality we can put $c=0$, otherwise we add c to the parameter β in (75) and (76).

I. Compact Riemann surface of constant negative curvature with a uniform magnetic field

Consider the Lobachevsky plane $\mathbf{H}^2$ with a uniform magnetic field $\mathbf{B}$ of strength B perpendicular to the plane.[69] Using the Poincaré half-plane realization for $\mathbf{H}^2$ ($\mathbf{H}^2=\{x\in\mathbb{R}^2: x_2>0\}$ with the metric $r(x,y)=a\cosh^{-1}(1+(2x_2y_2)^{-1}|x-y|^2)$), we have the following representation for the Green's function $G^0(x,y;z)$ of the magnetic Schrödinger operator on $\mathbf{H}^2$ (see Refs. 65 and 69):

$$G^0(x,y;z)=\frac{\exp(ib\varphi)}{4\pi}\frac{\Gamma(t(z)+b)\Gamma(t(z)-b)}{\Gamma(2t(z))}\times\left[\cosh\frac{r(x,y)}{2a}\right]^{-2t(z)}$$
$$\times F\left(t(z)+b,\,t(z)-b;\,2t(z);\,\cosh^{-2}\frac{r(x,y)}{2a}\right),$$

where

$$\varphi = 2 \arctan \frac{x_1 - y_1}{x_2 + y_2},$$

$$t(z) = \tfrac{1}{2}\left(1 + \sqrt{1 - 4(a^2 z - b^2)}\right),$$

$$b = Ba^2/\Phi_0 .$$

Let S_Γ be the area of a fundamental domain for Γ and suppose that BS_Γ/Φ_0 is an integer. Then one can define the magnetic Schrödinger operator H_0 on the manifold $X = \mathbf{H}^2/\Gamma$, and its Green's function has the form (95) for sufficiently large $\mathrm{Re}\, t(z)$ (Ref. 65). For this $t(z)$ we obtain, using a result from Ref. 33,

$$[Q_0(z)]_{jl} = \sum_{\gamma \in \Gamma,\ \gamma \neq 1} G^0(q_j, \gamma q_l; z) + \xi_{jl}(z),$$

where

$$\xi_{jl}(z) = \begin{cases} G^0(q_j, q_l; z), & \text{if} \quad j \neq l; \\ -\dfrac{1}{4\pi}\left[\psi(t(z)+b) - \psi(t(z)-b) - 2\ln 2a + 2C_{\mathrm{E}}\right], & \text{if} \quad j = l. \end{cases}$$

To define the $\mathcal{Q}$-matrix at other points of $\mathbb{C}\backslash\sigma(H_0)$ it is sufficient to apply the method presented in Example 7.

ACKNOWLEDGMENTS

The authors are grateful to P. Exner for useful discussions and for the possibility to get acquainted with the results of Ref. 13 before publication. We gratefully acknowledge grants of DFG (No. 436 RUS 113/572/1) and INTAS (No. 00-257). The second named author is also very grateful to RFBR (Grant No. 02-01-00804) and to the SFB 288 for financial support, and to Humboldt University of Berlin for warm hospitality during the preparation of this paper.

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Bound states in one and two spatial dimensions

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(Received 25 September 2002; accepted 18 October 2002)

In this article we study the number of bound states for potentials in one and two spatial dimensions. We first show that in addition to the well-known fact that an arbitrarily weak attractive potential has a bound state, it is easy to construct examples where weak potentials have an infinite number of bound states. These examples have potentials which decrease at infinity faster than expected. Using somewhat stronger conditions, we derive explicit bounds on the number of bound states in one dimension, using known results for the three-dimensional zero angular momentum. A change of variables which allows us to go from the one-dimensional case to that of two dimensions results in a bound for the zero angular momentum case. Finally, we obtain a bound on the total number of bound states in two dimensions, first for the radial case and then, under stronger conditions, for the noncentral case. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1532538]

I. INTRODUCTION

In recent years, it has become apparent that studying physics in two spatial dimensions is not just an academic exercise, especially for condensed matter physics where there are bound states due to impurities on the surface of a semiconductor or at a junction.[1] In addition, we have established a remarkable universality property for low energy scattering in two dimensions. Namely, excluding some well-defined and rare exceptional cases, the $m=0$ phase shift for a radial potential behaves like $(\pi/2)(\ln k)^{-1}$ as $k\to 0$.[2] This result has been recently generalized to nonradial and even nonlocal potentials.[3]

We believe that relatively little is known about bound states in one and two dimensions. For any dimension, including one and two, we know that if the potential is sufficiently smooth and sufficiently rapidly decreasing at large distances, there is a semi-classical asymptotic estimate of the number of bound states for a potential gV, $g\to\infty$, which was first established for the radial case in Ref. 4, then generalized in Ref. 5 to arbitrary dimensions.

However, concerning strict bounds on the number of bound states the situation is radically different for one and two dimensions from that in higher dimensions (including three dimensions). Lieb,[6] Cwikel[7] and Rozenblum[8] have shown that for $n\geqslant 3$, n being the number of spatial dimensions, there is a bound

$$N\leqslant B_n\int |V|^{n/2}\,\mathrm{d}^n x, \tag{1}$$

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where B_n is definitely *larger*, even for very large dimensions, contrary to earlier belief,[9] than the semi-classical constant C_n appearing in the asymptotic estimate[5]

$$N(g)\sim C_n\ g^{n/2}\int (V^-)^{n/2}\,\mathrm{d}^n x,\quad g\to\infty,\ C_n=\frac{2^{-n}\pi^{-n/2}}{\Gamma(1+n/2)}, \tag{2}$$

for a potential gV where $-V^-$ is the negative part of the potential: $V=V^+-V^-$, $V^\pm\geqslant 0$. For central potentials, $B_n/C_n\to 1$ for $n\to\infty$.[9] Other proofs have been obtained.[9,10] Furthermore, it is well known that for one and two dimensions a potential globally attractive, arbitrarily weak, such that

$$\int d^n x V(x)<0,\ n=1,2, \tag{3}$$

has a bound state. The proof is trivial for $n=1$ by using a Gaussian trial function. For $n=2$, there is a proof by Simon, for instance.[11] The simplest one is by Yang and De Llano[12] who use a trial function $\exp-(r+r_0)^\alpha$, α sufficiently small.

However, this bound state has an incredibly small binding energy in absolute value, for a potential gV, which behaves like $\exp-(c/g)$ for small g, as shown in Appendix A.

In addition to the above, we note that for the s-state $(m=0)$, and $n=2$, there is an old bound on the number of bound states due to Newton[13] and Setô.[14] However, this bound is bilinear in V and does not behave like the semi-classical result for large g.

It was noticed in Ref. 9 that the number of bound states in two dimensions is certainly larger than $-1/4\int rV(r)\mathrm{d}r$, in the central case.

In this article we first find examples of potentials in one dimension for which the number of bound states is infinite. Using a transformation which is systematically studied, one can find more refined potentials for which the number of bound states is infinite.

This same transformation allows us also to find radial potentials in two dimensions for which the zero angular momentum bound states are infinite in number. Examples with nonradial potentials are also constructed. All these examples possess the property, $\int \mathrm{d}^2x|V(\vec{x})|<\infty$, and in addition $\int \mathrm{d}^2x|V(\vec{x})|\ln(2+|\vec{x}|)^{1-\varepsilon}<\infty$.

In Sec. III we find explicit bounds on the number of bound states in one dimension by using well-known bounds for the three-dimensional radial case with zero angular momentum. In addition, using the above noted change of variables, we also obtain bounds on the number of zero angular momentum bound states in two dimensions.

Finally, in Sec. IV, we get bounds on the *total* number of bound states in two dimensions. This bound has the property that it is linear in g for a potential gV and is thus similar to the semi-classical estimate.

In Appendix A we give upper and lower bounds on the ground state energy in two dimensions.

Next, in Appendix B, we present a system of transformations which first allow us to derive more and more refined examples of limit potentials with a finite or infinite number of bound states. Second, these transformations allow us to convert results obtained in a given dimension to results for another dimension for zero angular momentum.

In Appendix C we compare one of our two dimensional bounds with the Newton–Setô bound. Finally, in Appendix D, we sketch the proof that bound states are on real analytic Regge trajectories.[15]

A preliminary account of these results was presented at a workshop in Les Houches.[16]

II. EXAMPLES WHERE THE NUMBER OF BOUND STATES IS INFINITE

We begin by using the well-known result that in one dimension, and for the radial case in two and three dimensions, the number of negative energy bound states is equal to the number of nodes of the zero energy wave-function.[17]

For any two potentials $V_1(x)\leqslant 0$, and $V_2(x)\leqslant 0$ in one dimension, one can easily show that, if $V_1(x)>V_2(x)$, then for any interval $a\leqslant x\leqslant b$, we have

$$n_2(a,b)\geqslant n_1(a,b)-1, \tag{4}$$

where $n(a,b)$ is the number of nodes in the interval (a,b). Thus if $n_1(x,\infty)$ is infinite, $n_2(x,\infty)$ is also infinite.

We write the zero energy one-dimensional Schrödinger equation for an attractive potential $V=-\lambda/x^2$, $x>x_0>0$, $\lambda>0$:

$$\left(-\frac{d^2}{dx^2}-\frac{\lambda}{x^2}\right)\phi(x)=0. \tag{5}$$

Because of the homogeneity of Eq. (5), $\phi=x^s$, where s is given by the two roots $s_\pm$ of the equation

$$s(s-1)=-\lambda,$$

or

$$s_\pm=\tfrac{1}{2}\pm\sqrt{\tfrac{1}{4}-\lambda}. \tag{6}$$

For $\lambda>\frac{1}{4}$, both s_+ and s_- are complex, and the solution ϕ can be constructed by taking a linear combination of x^{s_+} and x^{s_-}. We have

$$\phi(x)=\sqrt{x}\cos(\sqrt{\lambda-1/4}\ln x+\delta). \tag{7}$$

Obviously, this ϕ has an infinite number of nodes for any $X\leqslant x<\infty$, $X>0$.

We can now use the theorem summarized in Eq. (4) to get the following general result: the number of one-dimensional bound states is infinite if there exists an $X>0$ such that

$$\begin{aligned}&\text{either}\quad x^2V(x)<L<-1/4,\ \text{ for }\ x>X,\\ &\text{and/or}\quad x^2V(x)<L<-1/4,\ \text{ for }\ x<-X.\end{aligned} \tag{8}$$

On the other hand, if V is bounded from below and if $x^2V(x)>-\frac{1}{4}$ for $|x|>|X|$, then the number of bound states is finite.

Using the series of transformation described in Appendix B it is possible to approach the limiting case in a more refined way. For example, if

$$V(x)<-\frac{1}{4x^2}-\frac{\mu_1}{4x^2(\ln x)^2},\quad x>X,\ \ \mu_1>1,$$

or

$$V(x)<-\frac{1}{4x^2}-\frac{1}{4x^2(\ln x)^2}\left[1+\frac{\mu_2}{(\ln\ln x)^2}\right],\quad x>X,\ \ \mu_2>1, \tag{9}$$

the number of bound states is *infinite*. Notice that this is true for X arbitrarily large, i.e., in a way, V arbitrarily small.

These two examples are such that $\int dx|V(x)|^{1/2}\to\infty$. This is not surprising since in the three-dimensional radial case we have for a monotonic potential the Cohn–Calogero[18] bound,

$$n<\frac{2}{\pi}\int_0^\infty dr|V|^{1/2}. \tag{10}$$

However, we can have nonmonotonic potentials such that the above integral converges but the number of bound states is infinite. For example, one can set

$$V=-\sum_{0}^{+\infty}\delta(x-2n). \tag{11}$$

For this potential $\int|V|^{1/2}\,dx=0$ since the δ-function can be effectively replaced by suitably chosen square wells of decreasing widths ε_n and depth $1/\varepsilon_n$ with $\Sigma\sqrt{\varepsilon_n}$ convergent, and ε_o arbitrarily small.

Next we consider the two-dimensional case. In this case we introduce a simple transformation which converts the *one*-dimensional zero energy Schrödinger equation to the $m=0$, *two*-dimensional radial Schrödinger equation. In one dimension $-\infty<x<+\infty$ we have

$$\left[-\frac{d^2}{dx^2}+U(x)\right]\phi(x)=0. \tag{12}$$

Our change of variables is given by

$$\begin{gathered} x\equiv\ln r/R,\quad 0\leqslant r<\infty;\\ U(x)\equiv r^2\ \ V(r);\\ \phi(x)=\psi(r). \end{gathered} \tag{13}$$

This transformation is a particular case of the Liouville transformation.[19] Equation (12) now becomes

$$\left(-\frac{d^2}{dr^2}-\frac{1}{r}\ \frac{d}{dr}+V(r)\right)\phi(r)=0. \tag{14}$$

But this equation is precisely the $m=0$ *two*-dimensional radial Schrödinger equation.

Using Eq. (8) we now see that for a radial potential $V(r)$, the number of bound states is infinite if

$$r^2\left(\ln\frac{r}{R}\right)^2 V(r)<L<-\frac{1}{4},\quad r>R_0>R. \tag{15}$$

This time we see that the integral appearing in the semi-classical estimate, $\int_0^\infty r|V(r)|dr$ is convergent and yet the number of bound states is infinite. Furthermore, the integral $\int_0^\infty r\,dr|V(r)|[\ln(2+r)]^{1-\varepsilon}$ is also convergent for $\varepsilon>0$, and the integral can be made arbitrarily small by taking R_0 arbitrarily large.

Our limit potentials in the two-dimensional case are given by

$$\begin{gathered} V(r)=-\frac{\mu}{4}\ \frac{1}{r^2(\ln r/R)^2},\quad r\geqslant R_0\geqslant 1;\\ V(r)=0,\quad r<R_0, \end{gathered} \tag{16}$$

with $\mu>1$.

In addition we can also solve the Schrödinger equation exactly for the class

$$V(r)=\begin{cases} 0,\ \ r<R,\ \ \text{with } R>1,\\ -g/r^2(\ln r)^\alpha,\ r>R,\ 1<\alpha<2, \end{cases} \tag{17}$$

with $g>0$. The solution is given by

$$\psi(r)=a+b\ln r, \quad r<R,$$
$$\psi(r)=(\ln r)^{1/2}[AJ_\nu(2\nu\sqrt{g}(\ln r)^{1/2\nu})+BY_\nu(2\nu\sqrt{g}(\ln r)^{1/1/2\nu})], \quad r\geqslant R, \tag{18}$$

where $\nu\equiv(2-\alpha)^{-1}$, and J_ν and Y_ν are Bessel functions. This last solution has an infinite number of nodes for $r>R$ and hence the potential (17) has an infinite number of bound states, and this is true for arbitrarily small g.

A completely different approach to get infinitely many bound states abandons radial symmetry and considers scattering by circular ''delta shell'' potentials in the plane. Indeed a very simple example where $\int V\mathrm{d}^2x$ is finite, arbitrarily small, and where one sees that has a bound state has been invented by Richard.[20] It is a delta shell potential:

$$V=-g\,\delta(r-1). \tag{19}$$

Here $\int \mathrm{d}^2x V=-2\pi g$ is finite. The zero-energy Schrödinger equation

$$\left(-\frac{d^2}{dr^2}-\frac{1}{r}\,\frac{d}{dr}+V\right)\psi=0$$

has a solution, finite at the origin, which is

$$\psi=1 \quad \text{for } r<1,$$
$$\psi=1-g\ln r \quad \text{for } r\geqslant 1. \tag{20}$$

Hence the zero-energy radial solution has a node at

$$r_0=\exp\frac{1}{g}, \tag{21}$$

and therefore this potential has a bound state for arbitrarily small g.

If, in addition, we now impose a Dirichlet boundary condition at $r=\exp(1/g)$ and set ψ to be identically zero for $r>\exp(1/g)$, i.e., physically, having an infinitely repulsive wall, we will still have a solution with a node at $r=\exp(1/g)$, and hence a zero-energy bound state.

Take now a sequence of potentials

$$V_n=-g_n\,\delta(|\vec{x}-\vec{x}_n|-1), \tag{22}$$

$g_n>0$, such that $\Sigma\, g_n$ converges, $\vec{x}_n$ on the positive x axis. For simplicity, g_n will be chosen a decreasing sequence. It is always possible to choose the $\vec{x}_n$'s in such a way that the disks

$$|\vec{x}-\vec{x}_n|\leqslant \exp\frac{1}{g_n}=r_n \tag{23}$$

do not overlap.

The number of bound states of $V=\Sigma_{n=0}^{n_0}V_n$ is certainly larger than n_0, the result one gets when one imposes Dirichlet boundary conditions on the border of each disk (this strategy was already used in Ref. 5). Letting n_0 go to infinity, we see that we have infinitely many bound states, and yet the integral $\int|V|\mathrm{d}^2x=2\pi\Sigma g_n$ is finite and can be arbitrarily small.

We can, however, do better than that, i.e., try to build an example in which

$$\int |V|[\ln(2+|\vec{x}|)]^\alpha\,\mathrm{d}^2x$$

is finite, where α is to be determined. We take the centers of the circles on a line, and since the g_n's are decreasing, we have

$$|\vec{x}_n| + r_n < (2n+1)\exp\frac{1}{g_n},$$

and hence

$$\int |V_n| \ |\ln(2+|\vec{x}|)|^\alpha \, \mathrm{d}^2x < g_n \ln\left[2+(2n+1)\exp\frac{1}{g_n}\right]^\alpha.$$

However,

$$\ln\left(2+(2n+1)\exp\frac{1}{g_n}\right) < \frac{\ln 3}{\ln 2}\left[\ln(2n+1)+\frac{1}{g_n}\right],$$

and hence

$$\sum_{n=1}^{\infty} \int |V_n| \ |\ln(2+|\vec{x}|)|^\alpha \, \mathrm{d}^2x < 2\pi\left(\frac{\ln 3}{\ln 2}\right)^\alpha \left[\Sigma g_n\left[\ln(2n+1)+\frac{1}{g_n}\right]^\alpha\right].$$

Since we want the series on the right-hand side to converge, α is chosen to be less than 1.

With the choice

$$g_n = g_0 \exp(-\lambda n),$$

this series will converge for any $\alpha < 1$.

III. BOUNDS ON THE NUMBER OF BOUND STATES IN ONE AND TWO DIMENSIONS

We start by considering the one-dimensional case, and write always, in obvious notations, $V = V^+ - V^-$ where V^+ and V^- are both $\geqslant 0$.

The zero-energy one-dimensional Schrödinger equation is

$$\left(-\frac{d^2}{dx^2}+V(x)\right)\psi(x)=0, \quad x\in(-\infty,+\infty). \tag{24}$$

Except for the fact that one is restricted to the half line, the above equation is the same as the reduced $\ell = 0$, three-dimensional Schrödinger equation

$$\left(-\frac{d^2}{dr^2}+V(r)\right)u(r)=0, \quad r\in[0,\infty). \tag{25}$$

Now if, in the one-dimensional case, $V(x)$ has N bound states, then $\psi(x)$ has N nodes, x_p, $p=1,\ldots,N$. Let k be such that

$$x_k < 0 < x_{k+1}.$$

Then the three-dimensional potential, $V_1(r) = V(x)$ with $r \equiv x - x_{k+1}$, has $(N-k-1)$ $\ell = 0$ bound states. Also the potential, $V_2(r) \equiv V(x)$ with $r = -(x - x_k)$ has k bound states with $\ell = 0$. Hence any three-dimensional bound gives a one-dimensional bound.

Starting with the well-known Bargmann[21] bound for angular momentum ℓ, we write

$$N(\ell) < \frac{1}{2\ell+1}\int_0^\infty r\, V^-(r)\, \mathrm{d}r. \tag{26}$$

Using $\ell=0$, we get, for the one-dimensional case,

$$N(1D)-1<\int_{-\infty}^{x_\kappa}|x-x_\kappa|\,V^-(x)\,dx+\int_{x_{\kappa+1}}^{\infty}|x-x_{\kappa+1}|\,V^-(x)\,dx,$$

and hence

$$N(1D)<1+\int_{-\infty}^{+\infty}|x|\,V^-(x)\,dx. \tag{27}$$

Similarly, we can use the bound obtained by one of us[22] in the radial three-dimensional case:

$$N(3D,\ell=0)<\left[\int_0^\infty r^2V^-(r)\,dr\int_0^\infty V^-(r)\,dr\right]^{1/4} \tag{28}$$

to get, in the one-dimensional case, after some manipulations,

$$N(1D)<1+\sqrt{2}\left[\int_{-\infty}^{+\infty}x^2\,V^-(x)\,dx\int_{-\infty}^{+\infty}V^-(x)\,dx\right]^{1/4}, \tag{29}$$

which behaves like $\sqrt{g}$ if $V=gV$, like the semi-classical estimate.

Now to get bounds in two dimensions for the $m=0$ case is very simple. The change of variables given in Eq. (13) allows us to go from Eq. (27) to a bound for the 2D case:

$$N(2\mathrm{D},m=0)<1+\int_0^\infty r\left|\ln\left(\frac{r}{R}\right)\right|\;\;V^-(r)\,dr. \tag{30}$$

In this bound R is arbitrary. We can minimize with respect to R. $R_{\min}$ is given by

$$\int_0^{R_{\min}}x|V(x)|dx=\int_{R_{\min}}^\infty x|V(x)|dx. \tag{31}$$

The bound (30) with $R=R_{\min}$ should be compared with the bound previously obtained by Newton[13] and Setô[14] which is

$$N(m=0)<1+\frac{\frac{1}{2}\int r\,dr\,r'\;\;dr'V^-(r)V^-(r')|\ln(r/r')|}{\int r\;\;dr\;\;V^-(r)}=1+J. \tag{32}$$

It turns out that

$$J<I(R_{\min})<2J. \tag{33}$$

This is demonstrated in Appendix C. So the Newton–Setô bound is slightly better but has a more complex structure. Both bounds are ''optimal'' in the sense that multiplying factors in them cannot be improved. This is because the Bargmann bound is itself known to be optimal.

Applying the same change of variable in Eqs. (13) and (29) gives

$$N(m=0,2\mathrm{D})<1+\sqrt{2}\left[\int_0^\infty(\ln r)^2r\,dr\,V^-(r)\int_0^\infty r\,dr\,V(r)\right]. \tag{34}$$

For large coupling this behaves like $\sqrt{g}$ for a potential gV. The integrals appearing in Eq. (34) are those which were required to converge in our original paper on low energy scattering in two dimensions.

IV. A BOUND ON THE TOTAL NUMBER OF BOUND STATES IN TWO DIMENSIONS

In this section, we study the total number of bound states in two dimensions, mostly for a rotationally symmetrical potential. The bound for this rotationally symmetrical case gives also some information for the general case, as discussed near the end of this section.

For the radial case, the easiest thing to do is to notice that the radial reduced equation (11) can be viewed as a radial three-dimensional equation with noninteger angular momentum $\ell = m - \frac{1}{2}$. Therefore the Bargmann bound[18] is valid:

$$N_m < \frac{1}{2m} \int_0^\infty r\, V^-(r)\, \mathrm{d}r. \tag{35}$$

To get the total number of bound states, we must remember that for $m \neq 0$ we have a multiplicity 2 and for $m = 0$ multiplicity 1. Hence

$$N_{\text{total}} < N_0 + \sum_{m=1}^{m=2\int r V^-(r) dr} \frac{1}{m} \int r\, V^-(r)\, \mathrm{d}r$$

$$N_{\text{total}} < N_0 + \left[\int r\, V^-(r)\, \mathrm{d}r \right] \ln\left[2 + 2 \int r\, V^-(r)\, \mathrm{d}r \right], \tag{36}$$

where N_0 is for instance given by (30).

However, the logarithm is spurious. This has already happened in the past, for instance in the three-dimensional bound obtained by Glaser, Grosse, Martin and Thirring.[21]

To show this, we use a technique due to Glaser, Grosse and Martin,[9] in which the counting of bound states for a radial potential is reduced to the calculation of a bound on the moment of the eigenvalues of a one-dimensional problem.

The reduced radial Schrödinger equation for bound states,

$$\left[-\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2} + V(r) - E_i(m) \right] u_i(r) = 0, \tag{37}$$

where i designates the number of nodes of the solution (ith eigenfunction starting from the ground state designated by $i = 0$), has been generalized by Regge[23] to noninteger and even complex angular momentum. What can be shown, under the weak condition

$$\int r|V(r)|\mathrm{d}r < \infty, \tag{38}$$

is that each $E_i(m)$, $i = 0,1,\ldots$, is the restriction to m integer (physical) of a real analytic, monotonically increasing function of m, $0 < m < m_i$, where m_i is such that $E_i(m_i) = 0$. That m_i exist follows from the Bargmann bound and condition (38). (Notice that $m_0 > m_1 > \cdots$.) This is what is called a ''Regge trajectory.'' Different trajectories with different m_i's do not intersect, due to general Sturm–Liouville theory. In Appendix D, we sketch the proof of these statements.

The number of bound states on a given trajectory, with $m \geqslant 1$, will be $[m_i]$, where $[x]$ is the integer part of x. Each of those bound states with $m \neq 0$ has a multiplicity 2. So the total number of bound states with $m \neq 0$ is

$$2 \sum_{i,[m_i] \geqslant 1} [m_i].$$

On the other hand, by using the change of variables (13) already employed in Secs. II and III the zero-energy reduced Schrödinger equation

$$\left(-\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2} + V(r) \right) \quad u(r) = 0 \tag{39}$$

becomes

$$\left(-\frac{d^2}{dz^2} + U(x) \right) \phi(x) = -\left(m^2 - \frac{1}{4} \right) \phi(x). \tag{40}$$

The eigenvalues of (39) are just the $m_i^2 - \frac{1}{4}$, m_i defined previously. The sum $\Sigma[m_i]$ is very similar to the sum of moments of power $\frac{1}{2}$ of the eigenvalues of (38):

$$\sum_{[m_i]>1} [m_i] < \frac{2}{\sqrt{3}} \sum \left(m_i^2 - \frac{1}{4} \right)^{1/2}. \tag{41}$$

It happens that this moment satisfies a bound proposed by Lieb and Thirring[24]

$$\sum |e_i|^{1/2} < L_{1/2,1} \int_{-\infty}^{+\infty} \mathrm{d}x \, U^-(x) = L_{1/2,1} \int_0^{\infty} r \, V^-(r) \, \mathrm{d}r, \tag{42}$$

where the e_i's are the eigenvalues of the one-dimensional Schrödinger equation with a potential U. $L_{1/2,1}$ has been shown to be finite by Weidel[25] and less than 1.005. More recently Hundertmark, Lieb and Thomas[26] have found the optimal value for $L_{1/2,1}$, namely, $\frac{1}{2}$:

$$\sum |e_i|^{1/2} < \frac{1}{2} \int_{-\infty}^{+\infty} U^-(x) \, \mathrm{d}x, \tag{43}$$

which is obtained in the one-bound-state case with a delta function potential.

Therefore, using (30), (41) and (43) we get a bound on the total number of bound states in two space dimensions for a central potential

$$N < 1 + \int_0^{\infty} r \, V^-(r) \quad \left| \ln\left(\frac{r}{R} \right) \right| \mathrm{d}r + \frac{2}{\sqrt{3}} \int_0^{\infty} r \, V^-(r) \, \mathrm{d}r. \tag{44}$$

We notice that for a potential gV the bound is *linear* in g, similar to the semi-classical estimate for large g. It is probably almost optimal, in the sense that it is optimal for $m = 0$ and that for $m \neq 0$ the only foreseeable improvement is to remove the multiplicative factor $2/\sqrt{3}$.

It is trivial, but not very elegant, to obtain also a bound on the total number of bound states for a noncentral potential. Let

$$B(r) = \sup_{0<\theta<2\pi} V^-(r, \theta). \tag{45}$$

Then replacing $V(r)$ by $B(r)$ in (44) we get a bound on the total number of bound states in a nonradial potential because of the monotonicity of the bound-state energies with respect to the potential.

For a potential with a single singular point the replacement of V^- by $B(r)$ is not too bad. However, if V has several singular points the replacement will be catastrophic since B will be infinite on successive circles corresponding to these singular points. It is certainly desirable to find a better bound.

Our conjecture is

$$N < 1 + 2 \int \frac{\mathrm{d}^2 x}{2\pi} V_R(|x|) \ln^-\left(\frac{|x|}{R} \right) + \int \frac{\mathrm{d}^2 x}{2\pi} V^-(x) \ln\left(\frac{|x|}{R} \right) + \frac{2}{\sqrt{3}} \int \frac{\mathrm{d}^2 x}{2\pi} V^-(x), \tag{46}$$

where $V_R(|x|)$ is the decreasing rearrangement of $V^-(x)$ (see Appendix A). The reasons for which we propose this are the following.

(i) For a central decreasing potential, (46) coincides with (44).
(ii) For a central potential not necessarily decreasing, the rhs of (46) is larger than the rhs of (44).
(iii) If we take a shifted central with a center outside the origin, the first and the last integrals in (46) are, of course, invariant. The second integral, because of the harmonic properties of $\ln r$ in two dimensions, is larger than the one corresponding to a central potential centred at the origin.

Proving (46) or something similar might be rather difficult but, seeing what has been achieved for higher dimensions, not impossible.

Notice that the integrals in (44) and (46) will certainly converge under the conditions of Ref. 1, and we can announce that they do converge in Ref. 2 also.

ACKNOWLEDGMENTS

We would like to thank J. M. Richard and W. Thirring for crucial information. Two of us, N.N.K. and T.T.W., are grateful to the CERN Theory Division for its kind hospitality. This work was supported in part by the U.S. Department of Energy under Grant No. DE-FG02-91ER40651, Task B, and under Grant No. DE-FG02-84ER40158.

Note added in proof: Dr. P. Blanchard drew our attention to a paper by A. Laptev[28] in which he finds a bound on the number of bound states for a potential $b|x|^{-2}-|V(|x|)|$, which is

$$N<\frac{A(b)}{4\pi}\int |V(x)|\mathrm{d}^2x,$$

when $A(b)\to\infty$ for $b\to 0$. With methods developed in the present article, using the Bargmann bound for the $m=0$ contribution and (42) for the rest, we get

$$A(b)<\frac{1}{\sqrt{b}}+\frac{4}{\sqrt{3}}.$$

APPENDIX A: UPPER AND LOWER BOUNDS ON THE GROUND STATE ENERGY IN TWO DIMENSIONS

We use the Schrödinger equation in integral form, for a potential gV:

$$\psi(x)=-\frac{g}{2\pi}\int K_0(\kappa|x-y|)V(y)\psi(y)\mathrm{d}^2y, \tag{A1}$$

for an energy $E=-\kappa^2$.

First we shall get an algebraic lower bound. Then V can be replaced by $-V^-$, the attractive part of the potential. We have

$$|\psi(x)|<\frac{g}{2\pi}\int K_0(\kappa|x-y|)V^-(y)\mathrm{d}^2y\ \sup|\psi|. \tag{A2}$$

Since $K_0(t)$ is a decreasing function of t and given the rearrangement inequality,

$$\int AB\ \mathrm{d}^2x<\int A_R\ B_R\ \mathrm{d}^2x,$$

where A and B are positive, going to zero at infinity, and A_R and B_R are their decreasing circular rearrangements, we have

$$|\psi(x)| < \frac{g}{2\pi} \int K_0(\kappa|y|) V_R(|y|) \mathrm{d}^2 y \sup|\psi|, \tag{A3}$$

where V_R is the rearrangement of V^-. (A_R is a decreasing function of $|x|$ such that $\forall\ t$, $\mu(A_R > t) = \mu(A > t)$, where μ is the Lesbègue measure.) Hence, if we take the supremum of the left-hand side over x, we can divide by $\sup|\psi|$ and obtain

$$1 < \frac{g}{2\pi} \int K_0(\kappa|y|) V_R(|y|) \mathrm{d}^2 y.$$

From the property

$$K_0(ab) < \ln^+\left(\frac{1}{a}\right) + K_0(b), \tag{A4}$$

where $\ln^+(t) = \ln t$ for $t > 1$, $= 0$ for $t < 1$, which is proved at the end of this appendix, we get

$$K_0(\kappa) > \frac{1}{g} \frac{1 - (g/2\pi) \int \ln^+(1/|y|) V_R(y) \mathrm{d}^2 y}{(1/2\pi) \int V_-(y) \mathrm{d}^2 y} = X. \tag{A5}$$

As long as X is positive, this gives a lower bound on $K_0(\kappa)$ and hence an upper bound on κ and an upper bound on κ^2, the absolute value of the binding energy.

If $X > K_0(1) = 0.42,\ldots$, we can again use the inequality (A4) and get

$$\kappa^2 < \exp 2\left(-\frac{1}{g} \frac{1 - (1/2\pi) \int \ln^+\left(1/y\right) V_R(y) \mathrm{d}^2 y}{(1/2\pi) \int V_-(y) \mathrm{d}^2 y} + K_0(1) \right), \tag{A6}$$

which demonstrates that the absolute value of the binding energy is bounded by $\exp -C/g$, $C > 0$ for $g \to 0$.

In the special case of a *purely attractive* potential we can get an inequality going in the opposite direction. We start again from (A1) and use the fact that the ground-state wave function is positive. We have

$$\psi(x) > \frac{g}{2\pi} \int_{|y| < R} K_0(\kappa|x-y|) |V(y)| \mathrm{d}^2 y \times \mathrm{Inf}_{|y| < R} |\psi(y)|$$

and, taking also $|x| < R$, and using the fact that K_0 is decreasing,

$$\mathrm{Inf}|\psi(y)|_{|x| < R} > \frac{g}{2\pi} K_0(2\kappa R) \int_{|y| < R} |V(y)| \mathrm{d}^2 y \quad \mathrm{Inf}|\psi(y)|_{|x| < R}. \tag{A7}$$

However, $\mathrm{Inf}|\psi(y)|_{|x| < R}$ cannot vanish in the ground state and hence we can divide (A7) by $\mathrm{Inf}|\psi(x)|$. From

$$K_0(t) > \ln\frac{1}{t} + \ln 2 - \gamma, \tag{A8}$$

when γ is the Euler constant $= 0.577\ldots$ we get

$$\kappa^2 > \frac{e^{-2\gamma}}{R^2}\exp - \frac{2}{gMi_{|x|<R}|V(\kappa)|\mathrm{d}^2x}, \tag{A9}$$

which goes in the opposite direction to (A6), but again has the form $\exp-(C/g)$ for small g. Both upper and lower bounds on κ^2 have the same qualitative behavior for small g. The lower bound on κ^2 can be optimized with respect to R. Of course we cannot do that for a potential which is not strictly attractive but only globally attractive. Nevertheless, we believe that the same qualitative result will hold.

In a recent paper[27] Nieto has given an explicit example in which he shows that the binding energy in absolute value is incredibly small. A square well with unit radius and strength 0.1 in natural units produces a bound state with energy -10^{-18}.

Finally we give a proof of (A4) and (A8): consider the quantity

$$Z = K_0(x) - \ln\left(\frac{x_0}{x}\right),$$

$$Z' = -K_1(x) + \frac{1}{x}.$$

From

$$K_1(x) = \int_1^\infty \frac{t\,dt}{\sqrt{t^2-1}}\exp - tx < \int_1^\infty \frac{t\,dt}{\sqrt{t^2-1}}\exp - x\sqrt{t^2-1},$$

we get $K_1(x) < 1/x$, and hence

$$Z' > 0.$$

So, for $x < x_0$ $Z(x) < Z(x_0) = K_0(x_0)$, which proves (A4). On the other hand, we have $\lim_{x\to 0} Z(x) = \ln 2 - \gamma$, and so

$$K_0(x) > \ln 2 - \gamma + \ln\left(\frac{1}{x}\right).$$

APPENDIX B: TRANSFORMATIONS OF THE SCHRÖDINGER EQUATION FROM ONE TO TWO DIMENSIONS, THE CONVERSE, LIMIT POTENTIALS, AND GENERALIZATION

In Sec. II we presented a transformation of the one-dimensional zero energy Schrödinger equation,

$$\left(-\frac{d^2}{dx^2} + U(x)\right)\phi(\kappa) = 0, \quad x \in (-\infty, +\infty), \tag{B1}$$

into the two-dimensional, zero angular momentum, Schrödinger equation,

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r}\,\frac{d}{dr} + V(r)\right)\phi(r) = 0, \quad r \in [0,\infty). \tag{B2}$$

The transformation is given by

$$x \equiv \ln\left(\frac{r}{R}\right), \quad x \in (-\infty, +\infty), \quad r \in [0,\infty),$$

$$U(x) \equiv r^2 \; V(r), \tag{B3}$$

$$\phi(x) \equiv \psi(r), \qquad x \geqslant 0.$$

This enables us to prove that since a potential, $U(x)$, given by

$$U(x) = 0, \quad x < X,$$

$$U(x) = -\frac{\mu}{4x^2}, \quad \mu > 1, \; x \geqslant X, \tag{B4}$$

has infinitely many bound states in one dimension, the potential

$$V(r) = 0, \quad r < R_0;$$

$$V(r) = -\frac{\mu}{r^2(\ln(r/R))^2}, \quad r \geqslant R_0 > R, \; \mu > 1, \tag{B5}$$

will also have infinitely many bound states in two dimensions for the $m = 0$, radial case.

This procedure can be continued further. Restricting ourselves now to $x > 0$, we can retransform (B1) to make it look like a two-dimensional equation by defining $\chi(x)$ as

$$\phi(x) \equiv x^{1/2} \; \chi(x). \tag{B6}$$

The κ satisfies the equation

$$\left(-\frac{d^2}{dx^2} - \frac{1}{x} \; \frac{d}{dx} + W(x) \right) \chi(x) = 0,$$

with

$$W(x) = U(x) - \frac{1}{4x^2}. \tag{B7}$$

Relabeling x as r we have

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r} \; \frac{d}{dr} + W(r) \right) \chi(r) = 0. \tag{B8}$$

This last equation is for $r \geqslant 0$ exactly the two-dimensional radial equation.

From the chain,

$$V(r) \to U(x) \to W(r),$$

we obtain

$$W(r) = -\frac{1}{4r^2(\ln r)^2} + \frac{1}{r^2} V(\ln r). \tag{B9}$$

Thus if for $x > x_0$ we set

$$U(x) = -\frac{\mu}{4x^2},$$

or

$$V(r) = -\frac{\mu}{4r^2(\ln r)^2},$$

we get

$$W(r) = -\frac{1}{4r^2(\ln r)^2} - \frac{\mu}{4r^2(\ln r)^2(\ln\ln r)^2}, \tag{B10}$$

with $r > R_0 > 0$.

This potential has infinitely many bound states if $\mu > 1$. Our procedure can be repeatedly iterated producing potentials which are closer to the limit, and with wave functions which can be expressed explicitly in terms of elementary functions.

Finally we stress that this procedure is not restricted to the connection between one and two dimensions, and the construction of limit potentials in one or two dimensions. It also applies in N dimensions.

In N dimensions the radial Schrödinger equation becomes

$$\left(-\frac{d^2}{dr^2} - \frac{N-1}{r}\frac{d}{dr} + V(r)\right)\psi(r) = 0.$$

We set

$$\psi(r) = r^{1-N/2}\ \tilde{\psi}(r);$$

and obtain

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{(1-N/2)^2}{r^2} + V(r)\right)\tilde{\psi}(r) = 0.$$

We can define $\tilde{V}(r) \equiv V(r) + (1-N/2)^2/r^2$, and hence again obtain the 2D form.

The conclusion is, using (B5), that in N dimensions, the potential

$$\begin{aligned} V(r) &= -\frac{(N-2)^2}{4r^2} - \frac{\mu}{r^2(\ln r)^2}, \quad r > R > 1, \\ &= 0, \quad r \leqslant R, \end{aligned} \tag{B11}$$

has infinitely many bound states if $\mu > 1$, and a finite number if $\mu < 1$.

This procedure can be further iterated to get more refined results.

APPENDIX C: COMPARISON OF OUR BOUND ON THE NUMBER OF $m=0$ BOUND STATES AND OF THE NEWTON-SETÔ BOUND

We wish to compare our bound

$$\begin{aligned} N(m=0) &< 1 + I(R), \\ I(R) &= \int_0^\infty r\, dr\, V^-(r) \left|\ln\left(\frac{R}{r}\right)\right| \end{aligned} \tag{C1}$$

and $I(R_{\min})$ given by

$$\int_0^{R_{\min}} r\ \ V^-(r)\mathrm{d}r = \int_{R_{\min}}^{\infty} r\ \ V^-(r)\mathrm{d}r, \tag{C2}$$

with the Newton–Setô bound

$$N(m=0) < 1+J,$$

where

$$J = \frac{\frac{1}{2}\int\int r\ \mathrm{d}r\ r'\mathrm{d}r'\,|\ln(r/r')|V^-(r)\ \ V^-(r')}{\int r\ \mathrm{d}r\ V^-(r)}. \tag{C3}$$

Here J can be rewritten as

$$J = \frac{\frac{1}{2}\int r\ \mathrm{d}r\ V^-(r)\ \ I^-(r)}{\int r\ \mathrm{d}r\ V^-(r)}. \tag{C4}$$

Hence, from the mean value theorem,

$$J \geqslant \tfrac{1}{2}\ \ I(R_{\min}). \tag{C5}$$

On the other hand, taking into account (C2), one has, with $R > R_{\min}$,

$$I(R) = I(R_{\min}) + 2\int_{R_{\min}}^{R} r\ \mathrm{d}r\ V^-(r)\ \ \ln\left(\frac{R}{r}\right). \tag{C6}$$

One gets

$$I(R) < I(R_{\min}) + 2\ln\left(\frac{R}{R_{\min}}\right)\int_{R_{\min}}^{\infty} r\ \mathrm{d}r\ V^-(r) = I(R_{\min}) + \ln\left(\frac{R}{R_{\min}}\right)\int_0^{\infty} r\ \mathrm{d}r\ V^-(r).$$

The case $R < R_{\min}$ can be treated in the same way and one gets

$$I(R) < I(R_{\min}) + \left|\ln\left(\frac{R}{R_{\min}}\right)\right|\int_0^{\infty} r\ \mathrm{d}r\ V^-(r). \tag{C7}$$

Inserting in (C4) leads to

$$J < I(R_{\min}). \tag{C8}$$

APPENDIX D: REGGE TRAJECTORIES FOR BOUND STATES

What follows here is somewhat implicit in the work of Regge.[23] We give here some details for the sake of completeness.

To find bound state energies $E = -\kappa^2$ for a given m (real >0), but not necessarily integer, we must find a solution of

$$\left[-\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2} + V(r) + \kappa^2\right]u = 0, \tag{D1}$$

such that $u \to 0$ for $r \to 0$ and $r \to \infty$. For general m and κ, $\mathrm{Re}\, m > 0$, $\mathrm{Re}\, \kappa > 0$, if

$$\int\ r|V(r)|\mathrm{d}r < \infty, \tag{D2}$$

(D1) has in general two independent solutions y and z such that

$$y \sim r^m, \quad r \to 0,$$
$$z \sim \exp(-\kappa r), \quad r \to \infty. \tag{D3}$$

It is then shown that both $y(m,\kappa;r)$ and $z(m,\kappa;r)$ are analytic in m and κ in $\{\mathrm{Re}\, m>0 \otimes \mathrm{Re}\, \kappa >0\}$. The Wronskian of y and z is given by

$$W(y,z) \equiv yz' - y'z = F(m,\kappa),$$

where F is analytic in the same domain. The bound state energies are given by

$$F(m,\kappa)=0. \tag{D4}$$

This defines the bound state energies as implicit functions of m. If $F(\tilde{m}_i,\tilde{\kappa}_i)=0$, $\tilde{m}_i$ and $\tilde{\kappa}_i>0$, and $(\partial/\partial\kappa)^p F=0$, $p=1,2,...,q-1$, and $(\partial/\partial\kappa)^q F \neq 0$ at that point, we have q different solutions in the neighborhood of $\tilde{m}_i$, $\tilde{\kappa}_i$. However, this is impossible for $q \geqslant 2$ because there cannot be any degeneracy as a general consequence of Sturm–Liouville theory. Hence, κ is analytic in m in the neighborhood of $\tilde{m}_i$, $\tilde{\kappa}_i$, and κ_i is a real analytic function of m for $0<m<m_i$, where m_i is such that $E_i(m_i)=0$. In addition, κ_i is a decreasing function of m since, from the Feynman–Hellmann theorem,

$$\frac{dE_i}{dm} = 2m \int \frac{u_i^2}{r^2}\, \mathrm{d}r. \tag{D5}$$

Let us remark here that the condition (D2) is certainly too strong. It is needed to ensure that y and z have the properties given by (D3). But if V has strong repulsive singularities, one could approach it by $V_M, V_M=V$ if $V<M$, $V_M=M$ if $V \geqslant M$, and use a limiting procedure.

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Flux-across-surfaces theorem for a Dirac particle

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(Received 6 June 2002; accepted 18 October 2002)

We consider the asymptotic evolution of a relativistic spin-$\frac{1}{2}$ particle, i.e., a particle whose wave function satisfies the Dirac equation with external static potential. We prove that the probability for the particle crossing a (detector) surface converges to the probability, that the direction of the momentum of the particle lies within the solid angle defined by the (detector) surface, as the distance of the surface goes to infinity. This generalizes earlier nonrelativistic results, known as flux across surfaces theorems, to the relativistic regime. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1528276]

I. INTRODUCTION

In scattering experiments the scattered particles are measured at a macroscopic distance, but the computations of scattering cross sections are based on the distribution of the wave function in momentum space. Therefore a relationship between the crossing probability through a far distant detector surface and the shape of the wave function in momentum space is needed.

This relationship is given by the flux-across-surfaces theorem, which—as a problem in mathematical physics—has been formulated by Combes, Newton, and Shtokhamer,[3] see also Refs. 5 and 8. For scattering states (material on scattering states for the Dirac equation is in Ref. 14) the theorem asserts that the probability of crossing a far distant surface (physical interaction with the detector is neglected) subtended by a solid angle is equal to the probability that the scattered particle will, in the distant future, have a momentum, whose direction lies in that same solid angle. Moreover, the probability, that the particle will cross the detector within a certain area is given by the integral of the flux over that area and time. This has been proven for Schrödinger evolutions in great generality, see for instance, Refs. 15, 2, 1, 16, 12, and 6.

We consider here wave functions $\psi_t \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ which satisfy the Dirac equation (conveniently setting $c=\hbar=1$),

$$i\frac{\partial\psi_t}{\partial t} = -i\sum_{l=1}^{3}\alpha_l\partial_l\psi_t + \not{A}\psi_t + \beta m\psi_t \equiv H\psi_t, \tag{1}$$

where

$$\alpha_l = \begin{pmatrix} 0 & \sigma_l \\ \sigma_l & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}, \quad l=1,2,3, \tag{2}$$

σ_l being the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$\mathbf{1}$ the 2×2-unit matrix and $\not{A}$ the four-potential in the form

$$\not{A} := A_0 + \mathbf{A}\cdot\boldsymbol{\alpha}$$

with $\boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3)$. In the following we will always denote solutions of the Dirac equation by ψ_t and by ψ_0 the "time zero" wave function.

$\mathcal{A}$ is an external static four-potential, which satisfies condition A [see (3)], which concerns smoothness and is for the sake of simplicity taken stronger than needed.

Condition A:

$$\mathcal{A}(\mathbf{x}) \in C^\infty \quad \exists M, \xi > 0: \quad |\mathcal{A}(\mathbf{x})| \leqslant M \langle x \rangle^{-(4+\xi)}, \tag{3}$$

where $\langle x \rangle = |x| + 1$ and the norm $|\cdot|$ is defined as

$$|B| := \sup_{\|\varphi\|_s = 1} \|B\varphi\|_s ,$$

where

$$\|\varphi\|_s := \langle \varphi, \varphi \rangle^{1/2}$$

with the inner product in spin space

$$\langle \cdot, \cdot \rangle : \mathbb{C}^4 \otimes \mathbb{C}^4 \to \mathbb{C} \quad \langle \varphi, \chi \rangle := \sum_{l=1}^{4} \overline{\varphi_l} \chi_l .$$

Often we have spinors depending on $\mathbf{x}$, in that case we have $\|\varphi\|_s(\mathbf{x})$.

The continuity equation involving the quantum flux of a relativistic spin-$\frac{1}{2}$ particle reads

$$\frac{\partial}{\partial t} \overline{\psi_t} \psi_t = \nabla \cdot \mathbf{j}, \tag{4}$$

whereas the 4-flux is defined for any $\varphi \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ by

$$\underline{j} = \begin{pmatrix} j_0 \\ \mathbf{j} \end{pmatrix} = \langle \varphi, \underline{\alpha} \varphi \rangle, \tag{5}$$

with $\underline{\alpha} = \left| \begin{smallmatrix} 1 \\ \boldsymbol{\alpha} \end{smallmatrix} \right|$.

For notational convenience we sometimes omit the dependence on $\mathbf{x}$. Furthermore, we have the usual L^2-Norm on the space of 4-spinors given by

$$\|\varphi\| = \left(\int \|\varphi\|_s^2 \, d^3x \right)^{1/2}.$$

We introduce the Fourier transform of $\varphi(\mathbf{x})$ as representation in the generalized basis (13) of the free Hamiltonian, i.e.,

$$\hat{\varphi}_s(\mathbf{k}) = \int (2\pi)^{-3/2} \langle \varphi_{\mathbf{k}}^s(\mathbf{x}), \varphi(\mathbf{x}) \rangle d^3x, \quad \hat{\varphi}(\mathbf{k}) := \sum_{s=1}^{2} s_{\mathbf{k}}^s \hat{\varphi}_s(\mathbf{k}). \tag{6}$$

We denote by x the Euclidian length of $\mathbf{x}$.

We assume that asymptotic completeness holds, i.e., that the wave operators exist on the spectral subspace $\mathcal{H}_{ac}$ of the continuous positive spectrum ("scattering state") of the Dirac Hamiltonian: Let ψ_{out} denote the wave function of the free asymptotic of a scattering state ψ then

$$\lim_{t \to \infty} \| e^{-iH_0 t} \psi_{\text{out}} - e^{-iHt} \psi \| = 0,$$

ψ_{out} is given by the wave operator

$$\Omega_+ = \lim_{t\to\infty} e^{iHt} e^{-iH_0 t}, \quad \psi = \Omega_+ \psi_{\text{out}}.$$

The existence of the wave operators and asymptotic completeness has been proven for short range potentials. See, e.g., Thaller.[14]

We remark [see Lemma 3.4(d)] (41), that the Fourier transform $\hat{\psi}_{\text{out},s}(\mathbf{k})$ of ψ_{out} equals the generalized Fourier transform $\psi_s^{\pm}$ of ψ in the generalized eigenbasis of the Dirac Hamiltonian with potential.

In general, we do not have much information about scattering states. One can prove the flux across surface theorem with conditions merely on the "out"-states, where the corresponding properties of the scattering states are hidden in the mapping properties of the wave operators, or, better, in the smoothness properties of the generalized eigenfunctions. On the other hand, one would like to be sure, that such conditions are not too restrictive on the set of scattering states.

We introduce the set $\mathcal{G}$ of functions $\hat{\psi}_{\text{out}}$, for which the flux across surfaces can naturally be proven,

$$f(\mathbf{k}) \in \mathcal{G} \Leftrightarrow \begin{cases} \exists M \in \mathbb{R}: & \|\partial_k^j f(\mathbf{k})\|_s \leqslant M \langle k \rangle^{-n} \quad \text{for } j = 0,1,2; n \in \mathbb{N} \\ \forall \mathbf{k} \neq 0: & \|k^{|\gamma|-1} D_{\mathbf{k}}^{\gamma} f(\mathbf{k})\|_s \leqslant M \langle k \rangle^{-n} \quad \text{for } n \in \mathbb{N}, \end{cases} \tag{7}$$

where $\gamma = (\gamma_1; \gamma_2; \gamma_3)$ is a multi-index with $|\gamma| \leqslant 2$, $D_{\mathbf{k}}^{\gamma} := \partial_{k_1}^{\gamma_1} \partial_{k_2}^{\gamma_2} \partial_{k_3}^{\gamma_3}$ and ∂_k is the partial derivative with respect to the radial coordinate k.

This set maps under the wave operator to a dense set in the set of scattering states. After the theorem we shall give under more restrictive conditions more detailed information on the set of scattering states for which the theorem holds.

The paper is organized as follows: In the next section we shall state the theorem. We shall also give its formulation in covariant form, but we shall prove the theorem using the rest frame of the dectector and the potential.

The following sections contain the proof of the theorem. We first prove the statement for the free case ($\not{A} = 0$) and then for the case of nonzero potential. Both are done in Section 3. The proof relies almost entirely on the stationary phase method, which we need to adapt to our purposes. The main lemma is lemma (3.1), whose lengthy technical proof is put in the Appendix.

The difficulty we have to face and which makes this paper not a simple generalization of the results in the Schrödinger situation is, that the time evolution with the Dirac Hamiltonian is not of a "nice" form for the stationary phase method to be easily applied to. The Schrödinger case is easier. On the other hand, the expression for the flux needs no differentiability of the wave function and one might be lead to believe, that to describe scattering in the relativistic regime is simpler—in particular less restrictive theorems should result. One may even get the idea, that asymptotic completeness and the flux across surfaces theorem become more or less equivalent statements in the relativistic regime. But we are far from that. Nevertheless, that we require smoothness and good decay on the potential may well be due to our method of proof.

We also need information about the generalized eigenfunctions of the Dirac Hamiltonian with external potential, see Lemma 3.4, whose proof is also set in the Appendix. The Appendix, which in fact is almost half of this paper, contains other tedious technical details.

II. THE THEOREM

The flux-across-surfaces theorem deals with the flux **j** integrated over a spherical surface at a far distance and asserts the following:

(1) the absolute value of the flux and the flux itself yield the same asymptotics, allowing to interpret the flux integral as crossing probability;[5,4]
(2) the crossing probability equals the probability for the momentum to lie within the cone defined by the surface.

Theorem 2.3: *Let ψ be a scattering state with outgoing free asymptotic $\hat{\psi}_{\text{out}}$, whose Fourier transform $\hat{\psi}_{\text{out}}$ lies in $\mathcal{G}$ [cf. (7)]. Let $R^2\,d\Omega$ be the surface element at distance R with solid angle differential $d\Omega$ and let* $\mathbf{n}$ *denote the outward normal of the surface element. Furthermore let S be a subset of the unit sphere. Then for all $t_i \in R$:*

$$\lim_{R\to\infty}\int_S\int_{t_i}^{\infty} j(\mathbf{R},t)\,dt\,R^2\,d\Omega = \lim_{R\to\infty}\int_S\int_{t_i}^{\infty}\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega = \int_S\int_0^{\infty}\langle\hat{\psi}_{\text{out}}(\mathbf{k}),\hat{\psi}_{\text{out}}(\mathbf{k})\rangle k^2\,dk\,d\Omega. \tag{8}$$

Observing that $\|\hat{\psi}_{\text{out}}\|(\mathbf{k})$ does not depend on time, we can choose a coordinate system $t' = t - t_i$, so that we may for definiteness always set $t_i = 0$ in (8).

The conditions on ψ_{out} can be translated into more detailed conditions on the scattering states under more restrictive conditions on the potential. Let

Condition B: $|\partial_x^n \mathbb{A}(\mathbf{x})| \in L^2(\mathbb{R}^3)\ \forall n \in \{0,1,2,\dots\} \quad \exists M |\mathbb{A}(\mathbf{x})| \leqslant M\langle x\rangle^{-6}$.

Then (for the proof see the Appendix).

Lemma 2.2:

$$\hat{\psi}_{\text{out}}(\mathbf{k}) \in \mathcal{G} \Leftrightarrow \psi(\mathbf{x}) \in \hat{\mathcal{G}}, \tag{9}$$

where $\hat{\mathcal{G}}$ is the space of functions $\psi(\mathbf{x}) \in \mathcal{H}_{ac}$ with $x^j \nabla^n \psi(\mathbf{x}) \in L^2$ for all $j = 0,1,2$; $n \in \mathbb{N}_0$, where $\nabla := -i\Sigma_{l=1}^3 \alpha_l \partial_l$.

Covariant form of the theorem: As we deal with a relativistic regime, it might be of interest to have also a covariant formulation of the theorem. As $\langle\hat{\psi}_{\text{out}},\hat{\psi}_{\text{out}}\rangle$ is not conserved under Lorentz function we use

$$\hat{\psi}_{\text{out}}^{LI}(\underline{k}) = (k^2 + m^2)^{1/4}\hat{\psi}_{\text{out}}(\underline{k}),$$

of which it is known that $\langle\hat{\psi}_{\text{out}}^{LI},\hat{\psi}_{\text{out}}^{LI}\rangle$ is a Lorentz-scalar (see, for instance, Ref. 9). Then the flux-across-surfaces theorem reads in a general and covariant way.

Theorem 2.3: *Let the conditions of Theorem 2.1 be satisfied. Let*

$$\underline{x} \diamond \underline{y} := x_0 y_0 - \sum_{j=1}^{3} x_j y_j$$

be the Minkowski scalar product. Then for any subspace $Z \subseteq \{\underline{x} | \underline{x} \diamond \underline{x} = m^2\} \subset \mathbb{R}^4$ and any smooth scalar function $\eta(\underline{x})$, nonequal to zero for all $\mathbf{x}$*:*

$$\lim_{\lambda\to\infty}\int_{\tilde{Z}(\lambda)} \underline{j}(\mathbf{x}) \diamond \underline{n}\,\widetilde{d\sigma} = \int_Z \langle\hat{\psi}_{\text{out}}^{LI}(\underline{k}),\hat{\psi}_{\text{out}}^{LI}(\underline{k})\rangle d\sigma, \tag{10}$$

where

$$\tilde{Z}(\lambda) := \{\underline{y} | \exists \underline{x} \in Z : \underline{y} = \lambda\,\eta(\underline{x})\underline{x}\} \subset \mathbb{R}^4$$

and $d\sigma$ is the invariant measure on Z, $\widetilde{d\sigma}$ the invariant measure on $\tilde{Z}$ and $\underline{n}$ is the vector orthogonal on $\tilde{Z}$ with Lorentz length one.

This formulation may perhaps not be directly guessed, but once one understands its basics like (19), this formulation becomes clear: The arbitrariness of the scalar function η follows directly from (19), observing that

$$\lim_{\lambda\to\infty}\psi(\lambda\underline{k}) = \lim_{\lambda\to\infty}\psi(\lambda\,\eta(\underline{k})\underline{k}).$$

Physically this is related to the fact, that (on big scales) it is possible to ''catch'' any part of the wave function in different ways (for example, by using a detector which is ''close'' and catches the wave function at an ''early'' time or one uses a far detector at a later time interval).

Let us explain how (8) follows from (10). We choose a set Z whose projection on the $t=0$-subspace is a cone with angular distribution S:

$$Z=\left\{ \underline{k} \,\middle|\, \frac{\mathbf{k}}{k} \in S \right\} \cap \{\underline{k} \diamond \underline{k} = m^2\}.$$

The invariant measure on the mass hyperboloid $d\sigma = d^3k/\sqrt{k^2+m^2}$ we get for the right-hand side of (10)

$$\int_Z \langle \hat{\psi}^{LI}_{\text{out}}(\underline{k}), \hat{\psi}^{LI}_{\text{out}}(\underline{k}) \rangle d\sigma = \int_S \int_0^\infty \langle \hat{\psi}_{\text{out}}(\mathbf{k}), \hat{\psi}_{\text{out}}(\mathbf{k}) \rangle k^2 \, dk \, d\Omega. \tag{11}$$

For the left-hand side of (10) we take

$$\eta(\underline{x}) := \frac{1}{x}, \quad x \neq 0.$$

As both integrands in (10) are bounded, a small neighborhood of $\mathbf{x}=0$ can be neglected. For constant λ, $\tilde{Z}$ represents a radial surface with arbitrary time $t \geqslant 0$. So we have

$$\lim_{\lambda \to \infty} \int_{\tilde{Z}(\lambda)} \underline{j}(\mathbf{x}) \diamond \underline{n} \, \widetilde{d\sigma} = \lim_{R \to \infty} \int_S \int_{t_i}^\infty j(\mathbf{R}, t) dt \, R^2 \, d\Omega. \tag{12}$$

III. THE PROOF

A. Scattering into cones heuristics

The flux-across-surfaces theorem is based on an asymptotic connection between the shape of the wave function in momentum space and in ordinary space. This is often referred to as the scattering into cones theorem, which has been proven for nonrelativistic particles by Dollard.[7] For that one chooses a certain parametrization of $\mathbb{R}^4$ and evaluates the wave function, as the parameter of the parametrizations goes to infinity. In the nonrelativistic case, it is easiest to choose time as the parameter of the parametrization. In the relativistic case it is simplest to have Lorentz-invariant three-dimensional subspaces of the timelike part of $\mathbb{R}^4$ as leaves of the parametrization. (We only parametrize the timelike region, as for big time scales the main part of our wave function will be in this region.) This can easily be done, by choosing a Lorentz-vector as an argument of ψ, i.e., a vector $\underline{x}$ with $\underline{x} \diamond \underline{x} = x_0^2 - \mathbf{x}\cdot\mathbf{x} = \lambda m^2$. Set $\psi(\lambda \underline{k}) = \psi(\mathbf{x} = \lambda \mathbf{k}, t = \lambda \sqrt{k^2+m^2})$. We denote the two different eigenstates of momentum $\mathbf{k}$ of the free Hamiltonian with positive energy by $\varphi^s_{\mathbf{k}}$, whereas the s labels the two different spins our electron may have. In the standard representation these eigenstates can be written as

$$\varphi^s_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{x}} s^s_{\mathbf{k}}, \tag{13}$$

where the $s^s_{\mathbf{k}}$ are

$$s^1_{\mathbf{k}} = (2E_k \hat{E}_k)^{-1/2} \begin{pmatrix} \hat{E}_k \\ 0 \\ k_1 \\ k^+ \end{pmatrix}, \quad s^2_{\mathbf{k}} = (2E_k \hat{E}_k)^{-1/2} \begin{pmatrix} 0 \\ \hat{E}_k \\ k^- \\ -k_1 \end{pmatrix},$$

where

$$k^{\pm}=k_2\pm ik_3,\quad \hat{E}_k=E_k+m,\quad E_k=\sqrt{k^2+m^2}.$$

(For a detailed calculation of these spinors see Ref. 14.)

The asymptotics result from a stationary phase analysis:

$$\begin{aligned}\psi(\lambda\underline{k})&=U(t=\lambda\sqrt{k^2+m^2})\psi(\lambda\mathbf{k},0)\\&=\sum_{s=1}^{2}e^{-iH\lambda\sqrt{k^2+m^2}}\int(2\pi)^{-3/2}\varphi^s_{\mathbf{k}'}(\lambda\mathbf{k})\hat{\psi}_s(\mathbf{k}')d^3k'\\&=\sum_{s=1}^{2}e^{-iH\lambda\sqrt{k^2+m^2}}\int(2\pi)^{-3/2}e^{i\mathbf{k}'\cdot\lambda\mathbf{k}}s^s_{\mathbf{k}'}\hat{\psi}_s(\mathbf{k}')d^3k'.\end{aligned}$$

For convenience we define

$$\hat{\psi}(\mathbf{k}')=\sum_{s=1}^{2}s^s_{\mathbf{k}'}\hat{\psi}_s(\mathbf{k}').$$

This leads to

$$\begin{aligned}\psi(\lambda\underline{k})&=e^{-iH\lambda\sqrt{k^2+m^2}}\int(2\pi)^{-3/2}e^{i\mathbf{k}'\cdot\lambda\mathbf{k}}\hat{\psi}(\mathbf{k}')d^3k'\\&=\int(2\pi)^{-3/2}e^{-i\lambda(\sqrt{k'^2+m^2}\sqrt{k^2+m^2}-\mathbf{k}'\cdot\mathbf{k})}\hat{\psi}(\mathbf{k}')d^3k'.\end{aligned}\tag{14}$$

In view of the stationary phase method, in the limit $\lambda\to\infty$ only a small neighborhood of the stationary point of the phase function

$$h(\mathbf{k}'):=(\sqrt{k'^2+m^2}\sqrt{k^2+m^2}-\mathbf{k}'\cdot\mathbf{k})$$

will be relevant for the integral. The stationary point is given by

$$\nabla_{\mathbf{k}'}h(\mathbf{k}_{\text{stat}})=0\Rightarrow\mathbf{k}_{\text{stat}}=\mathbf{k}.\tag{15}$$

Without loss of generality we can set $k_2=k_3=0$. Near the stationary point the phase is to second order

$$-i\lambda(\sqrt{k'^2+m^2}\sqrt{k^2+m^2}-\mathbf{k}'\cdot\mathbf{k})\approx-i\lambda\left(m^2+\frac{m^2}{2(k^2+m^2)}(k_1'-k)^2+\frac{1}{2}(k_2'^2+k_3'^2)\right).$$

This in Eq. (14) leads to

$$\psi(\lambda\underline{k})\approx\int(2\pi)^{-3/2}e^{-i\lambda(m^2+m^2/2(k^2+m^2)(k_1'-k)^2+1/2(k_2'^2+k_3'^2))}\hat{\psi}(\mathbf{k}')d^3k',$$

and replacing $\hat{\psi}(\mathbf{k}')$ by $\hat{\psi}(\mathbf{k})$ we obtain by integrating the Gaussian

$$\psi(\lambda\underline{k})\approx\frac{e^{-i\lambda m^2}}{(i\lambda)^{3/2}}\hat{\psi}(\mathbf{k})\sqrt{\frac{k^2}{m^2}+1}.$$

We shall state now the stationary phase result in a somewhat more general setting, to cover also applications to the potential case considered later.

B. The stationary phase

Lemma 3.1: Let $\tilde{\chi}$ *be in* $\mathcal{G}$ *[see (7)] and let the "phase function"* g *be*

$$g(\mathbf{k}')=\sqrt{k'^2+m^2}+a|k'|-\mathbf{y}\cdot\mathbf{k}'.$$

Let $\mathbf{k}_{\text{stat}}$ *be the stationary point of the phase function*

$$\nabla g(\mathbf{k}_{\text{stat}})=0.$$

Then there exist $C_1\in\mathbb{C},C_2,C_3\in\mathbb{R}$ *so, that for all* χ *with* $\|\partial_k^j\chi\|_s\leqslant\|\partial_k^j\tilde{\chi}\|_s$ *for* $j=0,1,2$ *and* $\mathbf{y}\in\mathbb{R}^3$.
(a) For $a=0$,

$$\left\|\int e^{-i\mu g(\mathbf{k}')}\chi(\mathbf{k}')d^3k'-C_1\mu^{-3/2}\chi(\mathbf{k}_{\text{stat}})\right\|_s<C_2\mu^{-2}. \tag{16}$$

For phase functions without stationary point $C_1=0$, *otherwise we can choose*

$$C_1=(-2\pi i)^{3/2}e^{-i\mu g(\mathbf{k}_{\text{stat}})}\frac{(k_{\text{stat}}^2+m^2)^{5/4}}{m}.$$

(b) For $a>0$,

$$\left\|\int e^{-i\mu g(\mathbf{k}')}\chi(\mathbf{k}')d^3k'\right\|_s<C_3\left(\frac{k_{\text{stat}}}{\mu}\right)^{1/2}\|\chi(\mathbf{k}_{\text{stat}})\|_s+|C_1|\mu^{-3/2}\|\chi(\mathbf{k}_{\text{stat}})\|_s+C_2\mu^{-2}. \tag{17}$$

For phase functions without stationary point $C_1=C_3=0$.
Moreover the C_j *are uniformly bounded for all* χ, a *and* $\mathbf{y}$.

In our application in the case $a\neq 0$, k_{stat} will be of order μ^{-1} so that the $|C_1|$-term and the C_3-term are of the same order.

This statement is a slight adaptation to our situation of a theorem of Hörmander,[10] and its proof is in the Appendix.

C. Scattering into cones for a free particle

Applying Lemma 3.1 to (14) we choose

$$\mu=\lambda\sqrt{k^2+m^2},\quad a=0,\quad \mathbf{y}=\frac{\mathbf{k}}{\sqrt{k^2+m^2}},\quad \chi(\mathbf{k}')=(2\pi)^{-3/2}\hat{\psi}(\mathbf{k}')$$

and calculate the stationary point k_{stat},

$$\frac{\mathbf{k}_{\text{stat}}}{\sqrt{k_{\text{stat}}^2+m^2}}-\mathbf{y}=0,$$

$$k_{\text{stat}}^2=y^2(k_{\text{stat}}^2+m^2),$$

$$k_{\text{stat}}=\frac{ym}{\sqrt{1-y^2}},$$

obtaining the following.

Corollary 3.2 ("Scattering into cones"): There exists a constant $C<\infty$ *so that for all* $\mathbf{k}\in\mathbb{R}^3$,

$$\left\| \psi(\lambda \underline{k}) - \frac{e^{-i\lambda m^2}}{(i\lambda)^{3/2}} \hat{\psi}(\mathbf{k}) \sqrt{\frac{k^2}{m^2}+1} \right\|_s \leqslant C\lambda^{-2}.$$

Note, that this implies

$$\lim_{\lambda\to\infty} \sup_{\mathbf{k}} \left(\|\sqrt{\lambda}^3 \psi(\lambda \underline{k})\|_s - \left\| \hat{\psi}(\mathbf{k}) \sqrt{\frac{k^2}{m^2}+1} \right\|_s \right) = 0. \tag{18}$$

For the flux-across-surfaces theorem we need the asymptotics of the relativistic quantum flux (5) of the particle. Since all the α_l are bounded matrices and $\hat{\psi} \in \mathcal{G}$, we obtain from (5) and (18) for the flux

$$\lim_{\lambda\to\infty} \sup_{\mathbf{k}} \left| \lambda^3 j_l(\lambda \underline{k}) - \langle \hat{\psi}(\mathbf{k}), \alpha_l \hat{\psi}(\mathbf{k}) \rangle \left(\frac{k^2}{m^2}+1 \right) \right| = 0. \tag{19}$$

Next observe (see the Appendix) that

$$\langle \hat{\psi}(\mathbf{k}), \boldsymbol{\alpha} \hat{\psi}(\mathbf{k}) \rangle = \frac{\mathbf{k}}{\sqrt{k^2+m^2}} \langle \hat{\psi}(\mathbf{k}), \hat{\psi}(\mathbf{k}) \rangle. \tag{20}$$

Thus we get the uniform bound.

Corollary 3.3:

$$\forall \varepsilon > 0 \quad \exists \lambda \in \mathbb{R}:$$

$$\sup_{\mathbf{k}} \left| \lambda^3 \mathbf{j}(\lambda \underline{k}) - \langle \hat{\psi}(\mathbf{k}), \hat{\psi}(\mathbf{k}) \rangle \frac{\mathbf{k}}{m^2} \sqrt{k^2+m^2} \right| < \varepsilon. \tag{21}$$

Observe, that after a long time of propagation, the flux at $\mathbf{x} = \lambda \mathbf{k}$ will always be parallel to $\mathbf{k}$. So in the limit $t \to \infty$ it will always point away from the origin of the coordinate system.

D. Flux across surfaces for a free particle

Theorem 2.1 reads in this case

$$\lim_{R\to\infty} \int_S \int_0^\infty \mathbf{j}(\mathbf{R},t) \cdot \mathbf{n}\, dt\, R^2\, d\Omega - \int_S \int_0^\infty \langle \hat{\psi}(\mathbf{k}), \hat{\psi}(\mathbf{k}) \rangle k^2\, dk\, d\Omega = 0 \tag{22}$$

and

$$\lim_{R\to\infty} \int_S \int_0^\infty j(\mathbf{R},t) dt\, R^2\, d\Omega - \int_S \int_0^\infty \langle \hat{\psi}(\mathbf{k}), \hat{\psi}(\mathbf{k}) \rangle k^2\, dk\, d\Omega = 0. \tag{23}$$

In the following, we will prove (22) by inserting the longtime asymptotic (21) for $\mathbf{j}$ and showing, that the integral of the error we get by this approximation tends to zero in the limit $R \to \infty$.

Now, the longtime asymptotic of $\mathbf{j}$ is parallel to the normal $\mathbf{n}$ of the radial surface. Therefore the longtime asymptotic of j is equal to the longtime asymptotic of $\mathbf{j} \cdot \mathbf{n}$. More detailed, one sees that using the approximation (21) for $\mathbf{j}$ in (22) and (23), the bound on the error terms in (22) and (23) arising from (21) are equal.

So the proof of (23) is essentially the same as for (22) and we shall concentrate only on showing (22).

The left-hand side of (22) includes an integral over t, whereas the right-hand side is integrated over k. We therefore substitute for t in the first term, to get integration over k, too. Since λ plays the role of a time parameter it is natural to substitute

$$\mathbf{k}=\frac{R\mathbf{n}}{\lambda}$$

with

$$\lambda=\frac{\sqrt{t^2-R^2}}{m}.$$

But this substitution is only possible in the timelike region ($t\geqslant R$). So we first handle the integral starting at $t=R$, later we deal with the spacelike part of the integral. Then, substituting t by k, we obtain

$$\int_S\int_R^\infty \mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega=\int_S\int_0^\infty \mathbf{j}\left(\mathbf{R},\frac{R}{k}\sqrt{k^2+m^2}\right)\cdot\mathbf{n}\frac{m^2}{\sqrt{k^2+m^2}}\frac{R^3}{k^2}dk\,d\Omega$$

$$=\int_S\int_0^\infty \mathbf{j}(\lambda(k)k,\lambda(k)\sqrt{k^2+m^2})\cdot\mathbf{n}\frac{m^2}{\sqrt{k^2+m^2}}k\lambda(k)^3\,dk\,d\Omega.$$

The integrand is now in the form that we can replace it by the asymptotic in (21).

It turns out however, that the error in the integrand will be $\sim k/\sqrt{k^2+m^2}$ which is not integrable, therefore the replacement is not straightforward. We separate large momenta $k>X$ and small momenta $k<X$. In the following we choose $X>m$. Given X and $R_0=\lambda_0 X$,

$$k\leqslant X\Leftrightarrow\frac{R_0}{k}=\lambda(k)\geqslant\lambda_0=\frac{R_0}{X}.$$

Then by (21) for small momenta $[k\leqslant X\Leftrightarrow t\geqslant R\sqrt{1+(m^2/X^2)}]$,

$$\forall\varepsilon>0\quad\exists R_0\in R\quad\forall R\geqslant R_0,$$

$$\left|\int_S\int_{R\sqrt{1+(m^2/X^2)}}^\infty\left(\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2-\int_0^X\langle\hat{\psi}(\mathbf{k}),\hat{\psi}(\mathbf{k})\rangle k^2\right)dk\,d\Omega\right|$$

$$=\left|\int_S\int_0^X\mathbf{j}(\lambda k,\lambda\sqrt{k^2+m^2})\cdot\mathbf{n}\frac{m^2}{\sqrt{k^2+m^2}}k\lambda^3-\langle\hat{\psi}(\mathbf{k}),\hat{\psi}(\mathbf{k})\rangle k^2\,dk\,d\Omega\right|$$

$$\leqslant\int_S\int_0^X\frac{km^2\varepsilon}{\sqrt{k^2+m^2}}dk\,d\Omega=:\chi(X)\varepsilon,\tag{24}$$

where

$$\chi(X):=4\pi\int_0^X\frac{km^2}{\sqrt{k^2+m^2}}dk.$$

Given X we can take ε arbitrarily small, choosing R_0 large enough, so that the rhs of (24) goes to zero. Thus

$$\lim_{X\to\infty}\lim_{R\to\infty}\left|\int_S\int_{R\sqrt{1+(m^2/X^2)}}^{\infty}\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega-\int_S\int_0^X\langle\hat{\psi}(\mathbf{k}),\hat{\psi}(\mathbf{k})\rangle k^2\,dk\,d\Omega\right|=0. \tag{25}$$

For the large momenta note that by virtue of $\hat{\psi}\in\mathcal{G}$:

$$\lim_{X\to\infty}\int_S\int_X^{\infty}\langle\hat{\psi}(\mathbf{k}),\hat{\psi}(\mathbf{k})\rangle k^2\,dk\,d\Omega=0 \tag{26}$$

and all it remains to show is that

$$\lim_{X\to\infty}\lim_{R\to\infty}\int_S\int_0^{R\sqrt{1+(m^2/X^2)}}\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega=0, \tag{27}$$

where we also included the time integration outside the light cone, which we excluded in the substitution.

We first estimate the part of the integral (27) that lies in the spacelike region (more precisely, $t\in[0,R]$) then we estimate the timelike part near the light cone ($t\in[R,R\sqrt{1+(m^2/X^2)}]$). That is, we first show that

$$\lim_{R\to\infty}\int\int_0^R\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega=0. \tag{28}$$

That this holds is physically related to the fact, that a particle moves slower than light, so for big time and space scales the main part of the wave function will be inside the light cone. This follows from a straightforward application of the stationary phase method, outside of the stationary point, choosing a special coordinate system, where the k_1 coordinate is along the direction $\mathbf{x}$. Two partial integrations lead to

$$\begin{aligned}\|\psi(\mathbf{x},\eta x)\|_s&=\left\|\int(2\pi)^{-3/2}e^{-ix(\sqrt{k^2+m^2}\eta-k_1)}\hat{\psi}(\mathbf{k})d^3k\right\|_s\\&=\left\|\int(2\pi)^{-3/2}e^{-ixg}\hat{\psi}(\mathbf{k})d^3k\right\|_s\\&\leqslant\frac{1}{x^2}\int\left\|(2\pi)^{-3/2}\left(\frac{\hat{\psi}''}{g'^2}-\frac{3\hat{\psi}'g''}{g'^3}+\frac{3\hat{\psi}g''^2}{g'^4}-\frac{\hat{\psi}g'''}{g'^3}\right)\right\|_s d^3k,\end{aligned}$$

where

$$g:=(\sqrt{k^2+m^2}\,\eta-k_1),\quad f':=\partial_{k_1}f.$$

Since

$$-g'=1-\frac{k_1\eta}{\sqrt{k^2+m^2}}\geqslant 1-\frac{|k_1|}{\sqrt{k^2+m^2}}>0$$

it follows

$$\|\psi(\mathbf{x},\eta x)\|_s\leqslant(2\pi)^{-3/2}\frac{C_2}{x^2} \tag{29}$$

uniform in $\eta\leqslant 1$. Hence

$$\lim_{R\to\infty}\int\int_0^R \mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega \leqslant 4\pi\lim_{R\to\infty}\int_0^R \|\psi(\mathbf{x},t)\|_s^2\,dt\,R^2 \leqslant \frac{1}{2\pi^2}C_2^2\lim_{R\to\infty}R^3\frac{1}{R^4}=0.$$

It is left to prove that the second part of the integral in (27) goes to zero, i.e., that

$$\lim_{X\to\infty}\lim_{R\to\infty}\int_S\int_R^{R\sqrt{1+(m^2/X^2)}}\mathbf{j}(R,t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega=0.$$

The scalar norm of $\psi(\mathbf{x},t)$ is

$$\|\psi(\mathbf{x},t)\|_s=\left\|\int(2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t+i\mathbf{k}\cdot\mathbf{x}}\hat{\psi}\,d^3k\right\|_s \tag{30}$$

$$=\left\|\int(2\pi)^{-3/2}e^{-i(\sqrt{k^2+m^2}-\mathbf{k}\cdot\mathbf{r})t}\hat{\psi}\,d^3k\right\|_s. \tag{31}$$

Applying Lemma 3.1 with

$$\mu=t,\quad a=0,\quad \mathbf{y}=\mathbf{r},\quad \chi(\mathbf{k}')=(2\pi)^{-3/2}\hat{\psi}(\mathbf{k}'),$$

we have by (16), that

$$\left\|\int e^{-iE_kt+i\mathbf{k}\cdot\mathbf{x}}\hat{\psi}(\mathbf{k})d^3k-C_1t^{-3/2}\hat{\psi}(k_{\text{stat}})\right\|_s<C_2t^{-2}.$$

As $\hat{\psi}$ is bounded, we have

$$\exists M\in\mathbb{R}:\forall t>R\quad \|\psi(\mathbf{x},t)\|_s=\left\|\int e^{-iE_kt+i\mathbf{k}\cdot\mathbf{x}}\hat{\psi}(\mathbf{k})d^3k\right\|_s\leqslant Mt^{-3/2}.$$

So

$$\left|\int_S\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}R^2\,d\Omega\right|\leqslant 4\pi\frac{MR^2}{t^3}.$$

So we can write

$$\left|\int_S\int_R^{R\sqrt{1+m^2/X^2}}\mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\,dt\,R^2\,d\Omega\right|$$

$$\leqslant 2\pi MR^2\left(R^{-2}-R^{-2}\left(1+\frac{m^2}{X^2}\right)^{-1}\right)=2\pi M\left(1-\left(1+\frac{m^2}{X^2}\right)^{-1}\right).$$

This term goes to zero as $X\to\infty$.

E. The flux-across-surfaces theorem with potential

1. Generalized eigenfunctions for the Dirac equation with potential

For the proof of the free flux-across-surfaces theorem we used the $\varphi_{\mathbf{k}}^s$ as basis of the Hilbert space. In the potential case we adopt a new basis for doing calculations.

Like in the free case, we again get four linear independent eigenfunctions for each $\mathbf{k}$, two of them have positive energy-eigenvalue $E_k^{\text{eig}}=E_k=\sqrt{k^2+m^2}$, two of them have negative energy-eigenvalue $E_k^{\text{eig}}=-E_k$. We denote by $\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x})$ the eigenfunctions with $s\in\{1,2\}$:

$$E_k\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})=(H_0+\mathcal{A})\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}). \tag{32}$$

The corresponding Lipmann Schwinger equation reads

$$\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})=\varphi^s_{\mathbf{k}}(\mathbf{x})+(E_k-H_0)^{-1}\mathcal{A}\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}). \tag{33}$$

We replace the formal expression $(E_k-H_0)^{-1}$ by the integral kernel G^+_k:

$$(E_k-H_0)G^+_k(\mathbf{x}-\mathbf{x}')=\delta(\mathbf{x}-\mathbf{x}'). \tag{34}$$

The explicit form for $G^+_k(\mathbf{x}-\mathbf{x}')$ can be found in Ref. 14

$$G^+_k(\mathbf{x})=\frac{1}{4\pi}e^{ikx}\left(-x^{-1}\left(E_k+\sum_{j=1}^3\alpha_j k\frac{x_j}{x}+\beta m\right)+x^{-2}\sum_{j=1}^3\alpha_j\frac{x_j}{x}\right)=:\frac{e^{ikx}}{x}S^+_k(\mathbf{x}). \tag{35}$$

Thus

$$\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})=\varphi^s_{\mathbf{k}}(\mathbf{x})-\int\mathcal{A}(\mathbf{x}')G^+_k(\mathbf{x}-\mathbf{x}')\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x'. \tag{36}$$

For $S^+_{\mathbf{k}}$, defined in (35), we have

$$\begin{aligned}|\partial^j_k S^+_{\mathbf{k}}|&=\left|\frac{1}{4\pi}\partial^j_k\left(-E_k-\sum_{j=1}^3\alpha_j k\frac{x_j}{x}-\beta m+x^{-1}\sum_{j=1}^3\alpha_j\frac{x_j}{x}\right)\right|\\&=\left|\frac{1}{4\pi}\partial^j_k\left(E_k+\sum_{j=1}^3\alpha_j\left(k\frac{x_j}{x}-\frac{x_j}{x^2}\right)+\beta m\right)\right|\end{aligned}$$

for $j=0,1,2$. For $x\geqslant 1$ we have

$$\left|\frac{x_j}{x}\right|\leqslant 1,\quad \left|\frac{x_j}{x^2}\right|\leqslant 1$$

and for such x, observing, that $\partial^j_k E_k\geqslant 0$ and k enters linearly in the second term, it follows, that

$$|\partial^j_k S^+_{\mathbf{k}}|\leqslant\left|\frac{1}{4\pi}\partial^j_k\left(E_k+\sum_{j=1}^3\alpha_j(k+1)+\beta m\right)\right|.$$

Thus with

$$\tilde{S}^+_{\mathbf{k}}:=\frac{1}{4\pi}\left(E_k+\sum_{j=1}^3\alpha_j(k+1)+\beta m\right), \tag{37}$$

we have

$$|\partial^j_k S^+_{\mathbf{k}}|\leqslant|\partial^j_k\tilde{S}^+_{\mathbf{k}}| \tag{38}$$

for $j=0,1,2$, $x\geqslant 1$.

For the next steps we need some properties of the generalized eigenfunctions. We summarize these properties in the following Lemma which is proven in the Appendix.

Lemma 3.4: Let $\mathcal{A}$ satisfy Condition A (3). Then there exist unique solutions $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ of (36) for all $k\in\mathbb{R}^3$, such that

(a) For any $\mathbf{k}\in\mathbb{R}^3$, $s=1,2$ *the functions* $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ *are Hölder continuous of degree 1 in* $\mathbf{x}$.
(b) Any $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ *which is a solution of (36) automatically satisfies (32).*
(c) The functions

$$\zeta^s_{\mathbf{k}}(\mathbf{x}) := \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}) - \varphi^s_{\mathbf{k}}(\mathbf{x}) \tag{39}$$

are infinitely often continuously differentiable with respect to k, *furthermore we have for* $j\in\mathbb{N}$ *and any multi-index* γ *with* $|\gamma|\leqslant 2$*:*

$$\text{(i)} \quad \sup_{\mathbf{x}\in\mathbb{R}^3} \|x\zeta^s_{\mathbf{k}}(\mathbf{x})\|_s < \infty,$$

$$\text{(ii)} \quad \sup_{\mathbf{x}\in\mathbb{R}^3} \left\| \partial^j_k \frac{\zeta^s_{\mathbf{k}}(\mathbf{x})}{|x+1|^{j-1}} \right\|_s < \infty,$$

$$\text{(iii)} \quad \sup_{\mathbf{x}\in\mathbb{R}^3} \left\| k^{|\gamma|-1} D^\gamma_{\mathbf{k}} \frac{\zeta^s_{\mathbf{k}}(\mathbf{x})}{|x+1|^{j-1}} \right\|_s < \infty.$$

The $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ *form a basis of the space of scattering states, i.e., for scattering states* $\psi(\mathbf{x},t)$*:*

$$\psi(\mathbf{x},t) = \sum_{s=1}^{2} \int (2\pi)^{-3/2} e^{-i\sqrt{k^2+m^2}t} \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})\, \hat{\psi}_{\text{out},s}(\mathbf{k}) d^3k, \tag{40}$$

$$\hat{\psi}_{\text{out},s}(\mathbf{k}) = \int (2\pi)^{-3/2} \langle \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}), \psi(\mathbf{x})\rangle d^3x, \tag{41}$$

where $\hat{\psi}_{out,s}(\mathbf{k})$ *is the Fourier transform of* $\psi_{out} = \Omega_+ \psi$.

2. Flux-across-surfaces for the Dirac equation with potential

We prove now Theorem 2.1. As in the free case only the equality of the second and third integral is shown. From the nature of the estimates in the proof it will become evident, that essentially by the same argument as in the free case, the first equality can be established, and we do not say anything more to that.

We again split our flux integral into two parts, one inside the light-cone (from R to ∞) and one outside the light-cone (from 0 to R), where the main contribution comes from the times $t>R$, i.e., we prove that

$$\begin{aligned} &\text{(i)} \quad \lim_{R\to\infty} \left| \int_S \int_R^\infty \mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\, dt\, R^2\, d\Omega - \int_S \int_0^\infty \langle \hat{\psi}_{\text{out}}(\mathbf{k}), \hat{\psi}_{\text{out}}(\mathbf{k})\rangle k^2\, dk\, d\Omega \right| = 0, \\ &\text{(ii)} \quad \lim_{R\to\infty} \int \int_0^R \mathbf{j}(\mathbf{R},t)\cdot\mathbf{n}\, dt\, R^2\, d\Omega = 0. \end{aligned} \tag{42}$$

We start with (i).

According to (40),

$$\psi(\mathbf{x},t) = \sum_{s=1}^{2} \int (2\pi)^{-3/2} e^{-i\sqrt{k^2+m^2}t} \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})\, \hat{\psi}_{\text{out},s}(\mathbf{k}) d^3k.$$

Setting

$$\hat{\psi}_{\text{out}}(\mathbf{k}') = \sum_{s=1}^{2} s^s_{\mathbf{k}'} \hat{\psi}_{\text{out},s}(\mathbf{k}')$$

and using (36) with (39) we get

$$\psi(\mathbf{x},t)=\int (2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}e^{i\mathbf{k}\cdot\mathbf{x}}\hat{\psi}_{\text{out}}(\mathbf{k})d^3k$$
$$-\int (2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}\int \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}S_k^+(\mathbf{x}-\mathbf{x}')\mathcal{A}(\mathbf{x}')e^{i\mathbf{k}\cdot\mathbf{x}'}\,d^3x'\,\hat{\psi}_{\text{out}}(\mathbf{k})d^3k$$
$$-\sum_{s=1}^{2}\int (2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}\int \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}S_k^+(\mathbf{x}-\mathbf{x}')\mathcal{A}(\mathbf{x}')\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'\,\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k$$
$$=:S_0+S_1+S_2. \tag{43}$$

S_0 is the propagation of the free outgoing state. The free flux-across-surfaces theorem yields therefore,

$$\lim_{R\to\infty}\left|\int_S\int_R^\infty\langle S_0,\boldsymbol{\alpha}S_0\rangle\cdot\mathbf{n}\,dt\,R^2\,d\Omega-\int_S\int_0^\infty\langle\hat{\psi}_{\text{out}}(\mathbf{k}),\hat{\psi}_{\text{out}}(\mathbf{k})\rangle k^2\,dk\,d\Omega\right|=0.$$

Hence for (42)(i) it remains to show, that [using (5)]

$$\lim_{R\to\infty}\int_S\int_R^\infty(\mathbf{j}(R,t)-\langle S_0,\boldsymbol{\alpha}S_0\rangle)\cdot\mathbf{n}\,dt\,R^2\,d\Omega$$
$$=\lim_{R\to\infty}\int_S\int_R^\infty\left(\left\langle\sum_{j=0}^{2}S_j,\boldsymbol{\alpha}\sum_{j=0}^{2}S_j\right\rangle-\langle S_0,\boldsymbol{\alpha}S_0\rangle\right)\cdot\mathbf{n}\,dt\,R^2\,d\Omega$$
$$=\lim_{R\to\infty}\int_S\int_R^\infty\left(\left\langle\psi,\boldsymbol{\alpha}\sum_{j=1}^{2}S_j\right\rangle+\left\langle\sum_{j=1}^{2}S_j,\boldsymbol{\alpha}\psi\right\rangle\right)\cdot\mathbf{n}\,dt\,R^2\,d\Omega=0.$$

By Schwartz inequality we need only show

$$\lim_{R\to\infty}\int_S\int_R^\infty\|\psi\|_s\sum_{j=1}^{2}\|S_j\|_s\,dt\,R^2\,d\Omega=0. \tag{44}$$

We first want to estimate $\|S_1\|_s$. Recalling (43) we get by Fubinis theorem

$$S_1=-\int(2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}\int\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}S_k^+(\mathbf{x}-\mathbf{x}')\mathcal{A}(\mathbf{x}')e^{i\mathbf{k}\cdot\mathbf{x}'}\,d^3x'\,\hat{\psi}_{\text{out}}(\mathbf{k})d^3k$$
$$=-\int\int(2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}S_k^+(\mathbf{x}-\mathbf{x}')\mathcal{A}(\mathbf{x}')e^{i\mathbf{k}\cdot\mathbf{x}'}\,d^3x'\,\hat{\psi}_{\text{out}}(\mathbf{k})d^3k$$
$$=:-\int(2\pi)^{-3/2}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\tilde{S}_1(\mathbf{x},\mathbf{x}')\mathcal{A}(\mathbf{x}')d^3x',$$

where

$$\tilde{S}_1(\mathbf{x},\mathbf{x}')=\int(2\pi)^{-3/2}e^{-i\sqrt{k^2+m^2}t}e^{ik|\mathbf{x}-\mathbf{x}'|}S_k^+(\mathbf{x}-\mathbf{x}')e^{i\mathbf{k}\cdot\mathbf{x}'}\,d^3x'\,\hat{\psi}_{\text{out}}(\mathbf{k})d^3k. \tag{45}$$

Next we use Lemma 3.1, setting

$$\mu=t,\quad a=t^{-1}|\mathbf{x}-\mathbf{x}'|,\quad \mathbf{y}=t^{-1}\mathbf{x}',\quad k'=k,\quad \chi(\mathbf{k}')=(2\pi)^{-3/2}S_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{k}').$$

With regard to (38), the function

$$\tilde{\chi}(\mathbf{k}) = (2\pi)^{-3/2} \tilde{S}^{+}_{\mathbf{k}} \hat{\psi}(\mathbf{k}')$$

satisfies the properties we need in (17). Furthermore we observe that for the stationary point

$$\frac{k_{\text{stat}}}{\sqrt{k^2_{\text{stat}} + m^2}} + a - y = 0,$$

$$k_{\text{stat}} = \sqrt{k^2_{\text{stat}} + m^2}(y - a).$$

So we can estimate k_{stat} by

$$k_{\text{stat}} = \sqrt{k^2_{\text{stat}} + m^2} t^{-1}(x' - |\mathbf{x} - \mathbf{x}'|) \leqslant \sqrt{k^2_{\text{stat}} + m^2} x t^{-1}. \tag{46}$$

Hence by (17) we obtain for (45) that there exists $M_1 < \infty$, bounding in particular $\sqrt{k^2_{\text{stat}} + m^2}\hat{\chi}(\mathbf{k}_{\text{stat}})$, which is bounded by the choice of $\hat{\psi}_{\text{out}} \in \mathcal{G}$ and incorporating also the constants C_1 and C_2, uniformly in $\mathbf{y}$ and a so that

$$\|S_1\|_s \leqslant \left\| M_1 t^{-3/2}(1 + x^{1/2}) \int \frac{1}{|\mathbf{x} - \mathbf{x}'|} \not{A}(\mathbf{x}') d^3x' \right\|_s = M_1 t^{-3/2} P_1(\mathbf{x}) \to_{x \to \infty} 0. \tag{47}$$

That the function P_1 goes to zero in the limit $x \to \infty$ may be seen as follows: For any function $f(\mathbf{x}) \in L^1$ with $\limsup_{x \to \infty} |x^3 f(\mathbf{x})| < \infty$, we have

$$\begin{aligned}
&\lim_{x \to \infty} x \left| \int \frac{1}{|\mathbf{x} - \mathbf{x}'|} f(\mathbf{x}') d^3x' \right| \\
&\leqslant \lim_{x \to \infty} x \int \left| \frac{1}{x'} f(\mathbf{x} - \mathbf{x}') \right| d^3x' \\
&= \lim_{x \to \infty} x \left(\int_{B(0,x/2)} \left| \frac{1}{x'} f(\mathbf{x} - \mathbf{x}') \right| d^3x' + \int_{\mathbb{R}^3 \setminus B(0,x/2)} \left| \frac{1}{x'} f(\mathbf{x} - \mathbf{x}') \right| d^3x' \right) \\
&\leqslant \lim_{x \to \infty} x \left(\sup_{\tilde{x} \geqslant x/2} \{|f(\tilde{\mathbf{x}})|\} \int_{B(0,x/2)} \frac{1}{x'} d^3x' + \frac{2}{x} \int_{\mathbb{R}^3 \setminus B(0,x/2)} |f(\mathbf{x} - \mathbf{x}')| d^3x' \right) \\
&\leqslant \lim_{x \to \infty} \frac{1}{8} x^3 \sup_{\tilde{x} \geqslant x/2} \{|f(\tilde{\mathbf{x}})|\} + \lim_{x \to \infty} 2 \int_{\mathbb{R}^3 \setminus B(0,x/2)} |f(\mathbf{x} - \mathbf{x}')| d^3x' < \infty,
\end{aligned} \tag{48}$$

where $B(\mathbf{a}, r)$ means the ball with center $\mathbf{a}$ and radius r.

Next we estimate $\|S_2\|_s$. According to (43) we can write it as

$$S_2 = -\sum_{s=1}^{2} \int (2\pi)^{-3/2} e^{-i\sqrt{k^2 + m^2} t} \int \frac{e^{ik|\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} S^{+}_{k}(\mathbf{x} - \mathbf{x}')(x' + 1) \not{A}(\mathbf{x}') \frac{\zeta^s_{\mathbf{k}}(\mathbf{x}')}{x' + 1} d^3x' \, \hat{\psi}_{\text{out},s}(\mathbf{k}) d^3k.$$

Therefore we again use Lemma 3.1, setting

$$\mu = t, \quad a = t^{-1}(|\mathbf{x} - \mathbf{x}'|), \quad \mathbf{y} = 0, \quad k' = k, \quad \chi(\mathbf{k}') = (2\pi)^{-3/2} \sum_{s=1}^{2} \frac{\zeta^s_{\mathbf{k}}(\mathbf{x}')}{x' + 1} S^{+}_{\mathbf{k}}(\mathbf{x} - \mathbf{x}') \hat{\psi}_{\text{out},s}(\mathbf{k}').$$

With regard to (38) and Lemma 3.4(c) there exists a $M_2 < \infty$, so that the function

$$\tilde{\chi} = (2\pi)^{-3/2} M_2 \tilde{S}^+_{\mathbf{k}} \hat{\psi}(\mathbf{k}')$$

satisfies the properties we need in Lemma 3.1.

Since our phase function has no stationary point we get with (17),

$$\|S_2\|_s \leqslant M_2 t^{-2} \left| \int \frac{1}{|\mathbf{x}-\mathbf{x}'|} (x'+1) \mathcal{A}(\mathbf{x}') d^3x' \right| = M_2 t^{-2} P_2(\mathbf{x}) \underset{x\to\infty}{\to} 0.$$

Choosing $(x'+1)\mathcal{A}(\mathbf{x}')$ for f on the most left-hand side of (48), one can see, that $xP_2(\mathbf{x})$ is bounded, so P_2 goes to zero in the limit $x\to\infty$. Since S_0 is the analogue of the freely evolving wave function, we have by Corollary 3.2,

$$\|S_0\|_s \leqslant M_0 t^{-3/2}. \tag{49}$$

We use the estimates (49), (47), and (49) on the right-hand side of (44) and get, defining $M := M_0 + M_1 + M_2$:

$$\begin{aligned} \lim_{R\to\infty} \left| \int_S \int_R^\infty \left(\|\psi\|_s \left\| \sum_{j=1}^2 S_j \right\|_s \right) dt\, R^2\, d\Omega \right| &\leqslant \lim_{R\to\infty} \int_R^\infty M^2 (P_1(\mathbf{R}) + P_2(\mathbf{R})) t^{-3}\, dt\, R^2 \\ &\leqslant \lim_{R\to\infty} 3M^2 (P_1(\mathbf{R}) + P_2(\mathbf{R})) = 0 \end{aligned}$$

and (44) is proved.

Like in the free case, (42)(ii) follows directly from an analogous argument which used Eq. (29), thus we prove (29) for the case at hand. Since in (42)(ii) we need only estimates of the wave function for times $t \leqslant x$ we have in view of (43), setting $t = \eta x$ with $0 \leqslant \eta \leqslant 1$ and using Fubinis theorem:

$$\begin{aligned} \psi(\mathbf{x}, \eta x) = &\int (2\pi)^{-3/2} e^{-i\sqrt{k^2+m^2}\eta x + i\mathbf{k}\cdot\mathbf{x}} \hat{\psi}_{\text{out}}(\mathbf{k}) d^3k \\ &- \int\int e^{-i\sqrt{k^2+m^2}\eta x + ik|\mathbf{x}-\mathbf{x}'| + i\mathbf{k}\cdot\mathbf{x}'} \frac{\mathcal{A}(\mathbf{x}') S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}') \hat{\psi}_{\text{out}}(\mathbf{k})}{(2\pi)^{3/2}|\mathbf{x}-\mathbf{x}'|} d^3k\, d^3x' \\ &- \sum_{s=1}^2 \int\int e^{-i\sqrt{k^2+m^2}\eta x + ik|\mathbf{x}-\mathbf{x}'|} \frac{\mathcal{A}(\mathbf{x}') \zeta^s_{\mathbf{k}}(\mathbf{x}') S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}') \hat{\psi}_{\text{out},s}(\mathbf{k})}{(2\pi)^{3/2}|\mathbf{x}-\mathbf{x}'|} d^3k\, d^3x' \\ =: &S_0 + S_1 + S_2. \end{aligned}$$

For S_0 we have (29), for the other summands we define

$$\tilde{S}_1 := \int (2\pi)^{-3/2} e^{-i\sqrt{k^2+m^2}\eta x + ik|\mathbf{x}-\mathbf{x}'| + i\mathbf{k}\cdot\mathbf{x}'} S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}') \hat{\psi}_{\text{out}}(\mathbf{k}) d^3$$

$$\tilde{S}_2 := \sum_{s=1}^2 \int (2\pi)^{-3/2} e^{-i\sqrt{k^2+m^2}\eta x + ik|\mathbf{x}-\mathbf{x}'| + i\mathbf{k}\cdot\mathbf{x}'} e^{-i\mathbf{k}\cdot\mathbf{x}'} \zeta^s_{\mathbf{k}}(\mathbf{x}') S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}') \hat{\psi}_{\text{out},s}(\mathbf{k}) d^3k.$$

So we have for S_j, $j = 1;2$,

$$S_j = -\int \tilde{S}_j \frac{\mathcal{A}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d^3x'.$$

We can estimate the $\tilde{S}_j$ by two partial integrations. One can easily see, that the phase functions of $\tilde{S}_j$ have no stationary point. This leads to

$$\begin{aligned}\|\tilde{S}_j\|_s &= \left\| \int (2\pi)^{-3/2} e^{-ixg(\mathbf{k})} \chi_j(\mathbf{x},\mathbf{x}',\mathbf{k}) d^3k \right\|_s \\ &= \frac{1}{x^2} \left\| \int (2\pi)^{-3/2} e^{-ixg(\mathbf{k})} \partial_{k_1} \left(\frac{1}{g'} \partial_{k_1} \frac{\chi_j}{g'} \right) d^3k \right\|_s \\ &= \frac{1}{x^2} \left\| \int (2\pi)^{-3/2} \left(\frac{\chi_j''}{g'^2} - \frac{3\chi_j' g''}{g'^3} + \frac{3\chi_j g''^2}{g'^4} \right) d^3k \right\|_s ,\end{aligned}$$

where

$$g(\mathbf{k}) := \sqrt{k^2+m^2}\,\eta - k\frac{|\mathbf{x}-\mathbf{x}'|}{x} - \mathbf{k}\cdot\frac{\mathbf{x}'}{x},$$

$$\chi_1(\mathbf{x},\mathbf{x}',\mathbf{k}) := S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}')\hat{\psi}_{\text{out}}(\mathbf{k}),$$

$$\chi_2(\mathbf{x},\mathbf{x}',\mathbf{k}) := \sum_{s=1}^{2} e^{-i\mathbf{k}\cdot\mathbf{x}'} \zeta^s_{\mathbf{k}}(\mathbf{x}') S^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}') \hat{\psi}_{\text{out},s}(\mathbf{k}),$$

$$g' := \partial_{k_1} g.$$

Since

$$\begin{aligned}|g'| &= \frac{x'}{x} + \frac{k_1|\mathbf{x}-\mathbf{x}'|}{kx} - \frac{k_1\eta}{\sqrt{k^2+m^2}} \\ &\geqslant \frac{k_1}{k}\left(\frac{x'}{x} + \frac{|\mathbf{x}-\mathbf{x}'|}{x} - \frac{k}{\sqrt{k^2+m^2}} \right) \\ &\geqslant \frac{k_1}{k}\left(1 - \frac{k}{\sqrt{k^2+m^2}} \right) > 0.\end{aligned}$$

g'' is bounded and due to Lemma 3.4 the χ_j are bounded, we can find $C_2 < \infty$ with

$$\sum_{j=1}^{2} \tilde{S}_j \leqslant \frac{C_2}{x^2}.$$

So $x^2 \Sigma_{j=1}^2 S_j$ is bounded [see (48)] and the analogue of (29) is proved.

ACKNOWLEDGEMENT

Very helpful discussions with Stefan Teufel are gratefully acknowledged.

APPENDIX

Proof of Lemma 3.1

We consider for a family of phase functions g, which we should think of being indexed by $a \geqslant 0, \mathbf{y}$:

$$g(\mathbf{k}) = \sqrt{k^2+m^2} + a|k| - \mathbf{y}\cdot\mathbf{k}$$

the integral

$$I := \int e^{-i\mu g(\mathbf{k})} \chi(\mathbf{k}) d^3k,$$

where $\chi \in \mathcal{G}$ [see (7)].

We shall find its asymptotic behavior as a function of μ. In major parts we will recall the proof of theorem 7.7.5 in the book of Hörmander,[10] which unfortunately is formulated for compactly supported χ and which moreover does not give uniformity over the family, i.e., uniformity in $a,\mathbf{y}$ which we need. The compactness can easily be handled but for the uniformity we must invoke the special form of the family of phase functions g and we shall give the argument here.

The stationary points of the phase functions are given by

$$g'(\mathbf{k}_{\text{stat}}) = \frac{\mathbf{k}_{\text{stat}}}{\sqrt{k_{\text{stat}}^2 + m^2}} + a\frac{\mathbf{k}_{\text{stat}}}{k_{\text{stat}}} - \mathbf{y} = 0,$$

$$k_{\text{stat}}^2 = (k_{\text{stat}}^2 + m^2)(y-a)^2,$$

$$k_{\text{stat}} = \frac{m(y-a)}{\sqrt{1-(y-a)^2}},$$

$$\mathbf{k}_{\text{stat}} \| \mathbf{y}. \tag{A1}$$

Since k_{stat} is a function of a and $\mathbf{y}$, we sometimes use the phrase: uniform in k_{stat} to express uniformity in a and $\mathbf{y}$. (I) For $y \geqslant a+1$ there is no stationary point and for $y = a$ the stationary point is at $k_{\text{stat}} = 0$.

First we handle the family where $y \in [a+\frac{1}{2}; a+1[$. These phase-functions do exactly have one stationary point bounded away from zero,

$$k_{\text{stat}} = \frac{m(y-a)}{\sqrt{1-(y-a)^2}} \geqslant \frac{m}{\sqrt{3}}. \tag{A2}$$

Later we will handle phase functions, where the stationary point is close to zero and phase functions without stationary point.

We choose a coordinate system, where the k_1 direction is parallel to $\mathbf{y}$. So the stationary points will have the coordinates $(k_{\text{stat}},0,0)$. To estimate the integral, we separate from the integral the contribution coming from near the stationary point. This part of integral includes the leading term. Therefore we define a smooth function $\rho_{k_{\text{stat}}}$ which is one near the stationary points and zero away from the stationary point. (We shall omit further on for ease of notation the index k_{stat}).

More precisely we define the compact set Q by

$$\mathbf{k} \in Q \Leftrightarrow k_1 \in \left[\frac{k_{\text{stat}}}{2}, 2k_{\text{stat}}\right] \wedge k_2, k_3 \in [-1,1]$$

and choose

$$\rho(\mathbf{k}) := 1 \quad \forall \mathbf{k} \in Q$$

falling quickly off to zero outside of Q, let's say

$$\rho(\mathbf{k}) := 0 \quad \forall k \notin Q_\varepsilon, \tag{A3}$$

where Q_ε is some ε-neighborhood of Q for some $\varepsilon>0$. With the help of ρ we can split $\chi=\chi_1+\chi_2$ by defining

$$\chi_1 := \rho\chi, \qquad \chi_2 := (1-\rho)\chi,$$

$$I_1 := \int e^{-i\mu g(\mathbf{k})}\chi_1(\mathbf{k})d^3k, \quad I_2 := \int e^{-i\mu g(\mathbf{k})}\chi_2(\mathbf{k})d^3k. \tag{A4}$$

This split has the following advantages:

The compactly supported χ_1 includes the stationary point, so I_1 can be estimated the same way as in Hörmanders theorem, but with focus on the uniformity of the estimates. χ_2 is zero near the stationary point, so I_2 can be easily estimated by partial integrations. ρ has been defined in such a way, that we may estimate the terms we get by the partial integrations uniform in k_{stat}.

We start with I_1. We move the stationary point to the center of our coordinate system setting $\mathbf{k}' := \mathbf{k}-\mathbf{k}_{\text{stat}}$, i.e., $g(\mathbf{k})$ becomes $\tilde{g}(\mathbf{k}')=g(\mathbf{k}'+\mathbf{k}_{\text{stat}})$. Slightly abusing notation we simply write $g(\mathbf{k}')$ for $\tilde{g}$. By Taylor's formula we obtain a function f:

$$g(\mathbf{k}')=g(\mathbf{k}'=0)+\sum_{|\gamma|=2}\frac{D^\gamma_{\mathbf{k}'}g(\mathbf{k}'=0)\mathbf{k}'^\gamma}{\gamma!}+f(\mathbf{k}'), \tag{A5}$$

where $f(\mathbf{k}')/k'^3$ bounded.

Computing the second-order terms of $g(\mathbf{k}')$ we find that only diagonal terms survive at $(k_{\text{stat}},0,0)$ and

$$\partial^2_{k_j'}g(\mathbf{k}'=0)=\partial^2_{k_j}g(\mathbf{k}=\mathbf{k}_{\text{stat}})=\left(\partial_{k_j}\left(\frac{k_j}{\sqrt{k^2+m^2}}+a\frac{k_j}{k}-y_l\right)\right)\Bigg|_{\mathbf{k}=\mathbf{k}_{\text{stat}}}$$

$$=\left(\frac{k^2-k_j^2+m^2}{\sqrt{k^2+m^2}^3}+a\frac{k^2-k_j^2}{k^3}\right)\Bigg|_{\mathbf{k}=\mathbf{k}_{\text{stat}}},$$

so that

$$\partial^2_{k_j'}g(\mathbf{k}'=0)=\frac{k_{\text{stat}}^2+m^2}{\sqrt{k_{\text{stat}}^2+m^2}^3}+a\frac{1}{k_{\text{stat}}} \quad \text{for } j=2,3,$$

$$\partial^2_{k_1'}g(\mathbf{k}'=0)=\frac{m^2}{\sqrt{k_{\text{stat}}^2+m^2}^3}. \tag{A6}$$

We define

$$g_2(\vartheta,\theta) := \frac{\Sigma_{j=1}^3\partial^2_{k_j'}g(\mathbf{k}'=0)k_j'^2}{k'^2}. \tag{A7}$$

By this definition, g_2 does only depend on the angular, not on the radial coordinate of $\mathbf{k}'$. Using (A7) in (A5), we may write

$$g(\mathbf{k}')=g(0)+\tfrac{1}{2}k'^2g_2(\vartheta,\theta)+f(\mathbf{k}'). \tag{A8}$$

Furthermore for $s\in[0,1]$ set

$$g_s := g(0)+\tfrac{1}{2}k'^2g_2(\vartheta,\theta)+sf(\mathbf{k}') \tag{A9}$$

and

$$I(s)=\int e^{-i\mu g_s(\mathbf{k}')}\chi_1(\mathbf{k}')d^3k'.$$

Note that $g=g_1$, $I_1=I(1)$. By Taylor's formula there exits $\xi\leqslant 1$ so that

$$I_1=I(1)=I(0)+\partial_s I(s)\big|_\xi. \tag{A10}$$

We begin with $I(0)$, introducing spherical coordinates. With slight abuse of notation: (leaving the notation for the functions unchanged)

$$I(0)=\int e^{-i\mu(g(0)+1/2\,k'^2 g_2(\vartheta,\theta))}\chi_1(k',\vartheta,\theta)k'^2\,dk'\,d\Omega.$$

Writing $\chi_1=\chi(k'=0)+\tilde{\chi}$ the integral splits into

$$\begin{aligned}I(0)=&\int e^{-i\mu(g(0)+1/2\,k'^2 g_2(\vartheta,\theta))}\chi(k'=0)k'^2\,dk'\,d\Omega\\&+\int e^{-i\mu(g(0)+1/2\,k'^2 g_2(\vartheta,\theta))}\tilde{\chi}(k',\vartheta,\theta)k'^2\,dk'\,d\Omega=:I_1^1+I_1^2.\end{aligned} \tag{A11}$$

The integral I_1^1 is a Gaussian integral, which includes the leading term

$$\begin{aligned}I_1^1=&\int e^{-i\mu(g(0)+1/2\,k'^2 g_2(\vartheta,\theta))}\chi(k'=0)k'^2\,dk'\,d\Omega\\=&\int e^{-i\mu\Sigma_{j=1}^3 1/2\,\partial_{k_j'}^2 g(\mathbf{k}'=0))k_j^2}e^{-i\mu g(0)}\chi(\mathbf{k}'=0)k'^2\,d^3k'\\=&(2\pi)\frac{3}{2}\mu^{-3/2}e^{-i\mu g(0)}\left(\prod_{j=1}^3\partial_{k_j'}^2 g(\mathbf{k}'=0)\right)^{-1/2}\chi(\mathbf{k}_{\text{stat}}).\end{aligned} \tag{A12}$$

For $a=0$ the $\partial_{k_j'^2}g(\mathbf{k}'=0)$ terms can be easily calculated. We get

$$\partial_{k_j'}^2 g(\mathbf{k}'=0)=\partial_{k_j'}^2 g(\mathbf{k}=\mathbf{k}_{\text{stat}})=\partial_{k_j'}\frac{k_j}{\sqrt{k^2+m^2}}\bigg|_{\mathbf{k}=\mathbf{k}_{\text{stat}}}=\frac{k^2+m^2-k_j^2}{\sqrt{k^2+m^2}^3}\bigg|_{\mathbf{k}=\mathbf{k}_{\text{stat}}}.$$

So we get

$$\prod_{j=1}^3\partial_{k_j'}^2 g(\mathbf{k}'=0)=\frac{m^2(k_{\text{stat}}^2+m^2)^2}{\sqrt{k_{\text{stat}}^2+m^2}^9}=\frac{m^2}{\sqrt{k_{\text{stat}}^2+m^2}^5}.$$

I_1^1 is the leading term of our integral. For $a=0$ we get the desired value for C_1 (Lemma 3.1).

For I_1^2 set

$$\phi(k',\vartheta,\theta):=\tilde{\chi}(k',\vartheta,\theta)k'^{-1}$$

which is bounded and smooth,

$$I_1^2=\int e^{-i\mu(g(0)+1/2\,k'^2 g_2(\vartheta,\theta))}\phi(k',\vartheta,\theta)k'^3\,dk'\,d\Omega. \tag{A13}$$

One partial integration leads to

$$\|I_1^2\|_s = \mu^{-1}\left\| \int e^{-i\mu\, 1/2\, k'^2 g_2(\vartheta,\theta)} \partial_{k'} \frac{\phi(k',\vartheta,\theta)k'^3}{k' g_2(\vartheta,\theta)} dk'\, d\Omega \right\|_s$$
$$= \mu^{-1}\left\| \int e^{-i\mu\, 1/2\, k'^2 g_2(\vartheta,\theta)} \frac{\partial_{k'}\phi(k',\vartheta,\theta)k'^2 + 2\phi(k',\vartheta,\theta)k'}{g_2(\vartheta,\theta)} dk'\, d\Omega \right\|_s .$$

So another partial integration is possible

$$\|I_1^2\|_s = \mu^{-2}\left\| \int e^{-i\mu\, 1/2\, k'^2 g_2(\vartheta,\theta)} \partial_{k'}\left(\frac{\partial_{k'}\phi(k',\vartheta,\theta)k'^2 + 2\phi(k',\vartheta,\theta)k'}{k'(g_2(\vartheta,\theta))^2} \right) dk'\, d\Omega \right\|_s$$
$$= \mu^{-2}\left\| \int e^{-i\mu\, 1/2\, k'^2 g_2(\vartheta,\theta)} \partial_{k'}\left(\frac{\partial_{k'}\phi(k',\vartheta,\theta)k' + 2\phi(k',\vartheta,\theta)}{(g_2(\vartheta,\theta))^2} \right) dk'\, d\Omega \right\|_s$$
$$\leqslant \mu^{-2}\left\| \int \partial_{k'}\left(\frac{\partial_{k'}\phi(k',\vartheta,\theta)k' + 2\phi(k',\vartheta,\theta)}{(g_2(\vartheta,\theta))^2} \right) dk'\, d\Omega \right\|_s . \tag{A14}$$

With our definition of Q, the support of the integrand increases and $g_2(\vartheta,\theta)$ decreases polynomially with k_{stat} [see (A6) and (A7)]. While the support moves away from the center of our coordinate system. But $\tilde{\chi} = \chi - \chi(\mathbf{k}_{\text{stat}})$ and its derivatives decay faster in k_{stat} than any power, so we get a constant C uniform in k_{stat} with

$$I_1^2 \leqslant \mu^{-2} C.$$

For I_1 it is left to estimate $\partial_s I(s)|_\xi$:

$$\partial_s I(s)|_\xi = \int -i\mu f(k',\vartheta,\theta) e^{-i\mu g_\xi(k',\vartheta,\theta)} \chi_1(k',\vartheta,\theta) k'^2\, dk'\, d\Omega. \tag{A15}$$

By Taylor's formula we can define

$$\tilde{f}(k',\vartheta,\theta) := f(k',\vartheta,\theta)k'^{-3}, \quad \tilde{g}(k',\vartheta,\theta) := k'^{-1}\partial_{k'} g_\xi(k',\vartheta,\theta)$$

and thus

$$\partial_s I(s)|_\xi = \int -i\mu \tilde{f}(k',\vartheta,\theta) e^{-i\mu g_\xi(k',\vartheta,\theta)} \chi_1(k',\vartheta,\theta) k'^5\, dk'\, d\Omega. \tag{A16}$$

On Q_ε [see below (A3)], g is infinitely often differentiable. So these functions are well defined and bounded on Q_ε.

To estimate the integral by partial integrations we have to assure, that g_ξ has only one stationary point, which is $k_{\text{stat}} = 0$ as one easily sees from (A17).

By (A9),

$$g_\xi = g(k'=0) + \tfrac{1}{2}k'^2 g_2(\vartheta,\theta) + \xi f(\mathbf{k}') = \xi g + (1-\xi)(g(k'=0) + \tfrac{1}{2}k'^2 g_2(\vartheta,\theta)). \tag{A17}$$

Looking at

$$\partial_{k'}^2 g_\xi = \xi \partial_{k'}^2 g + (1-\xi)\partial_{k'}^2 \tfrac{1}{2}k'^2 g_2$$

we observe, that

$$\partial_{k'}^2 g = \partial_{k'}^2 \left(\sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2 + m^2} + a \sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2} - \mathbf{y}\cdot\mathbf{k}' \right)$$

$$= \partial_{k'} \left(\frac{k' - k_{\text{stat}} \cos(\vartheta)}{\sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2 + m^2}} + a \frac{k' - k_{\text{stat}} \cos(\vartheta)}{\sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2}} \right)$$

$$= \frac{(1 - \cos(\vartheta)^2) k_{\text{stat}}^2 + m^2}{\sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2 + m^2}^3} + a \frac{(1 - \cos(\vartheta)^2) k_{\text{stat}}^2}{\sqrt{k'^2 - 2k' k_{\text{stat}} \cos(\vartheta) + k_{\text{stat}}^2}^3} > 0.$$

And for $\mathbf{k} \in Q_\varepsilon$, k_1 is positive, so the angular component $\vartheta \in]-\pi/2, \pi/2[$, we also have, that on Q_ε also g_2 is positive. Since $\xi \in [0;1]$ it follows, that $\partial_{k'}^2 g_\xi$ is positive, so $\partial_{k'} g_\xi$ is strictly monotonous on Q_ε and has only one stationary point. Recalling the definition of $\tilde{g}$ [see (A16)] we see, that $\tilde{g}$ is bounded away from zero.

Now we can estimate the integral (A16). By partial integration

$$\partial_s I(s)|_\xi = \int e^{-i\mu g_\xi(k',\vartheta,\theta)} \partial_{k'} \frac{\tilde{f}(k',\vartheta,\theta)\chi_1(k',\vartheta,\theta) k'^4}{\tilde{g}(k',\vartheta,\theta)} dk'\, d\Omega$$

$$= \int e^{-i\mu g_\xi(k',\vartheta,\theta)} \left(\partial_{k'} \frac{\tilde{f}(k',\vartheta,\theta)\chi_1(k',\vartheta,\theta)}{\tilde{g}(k',\vartheta,\theta)} k'^4 + 4 \frac{\tilde{f}(k',\vartheta,\theta)\chi_1(k',\vartheta,\theta)}{\tilde{g}(k',\vartheta,\theta)} \right) k'^3\, dk'\, d\Omega.$$

Setting

$$\tilde{\psi}(k',\vartheta,\theta) := \partial_{k'} \frac{\tilde{f}(k',\vartheta,\theta)\chi_1(k',\vartheta,\theta)}{\tilde{g}(k',\vartheta,\theta)} k' + 4 \frac{\tilde{f}(k',\vartheta,\theta)\chi_1(k',\vartheta,\theta)}{\tilde{g}(k',\vartheta,\theta)}. \tag{A18}$$

Hence

$$\partial_s I(s)|_\xi = \int e^{-i\mu g_\xi(k',\vartheta,\theta)} \tilde{\psi}(k',\vartheta,\theta) k'^3\, dk'\, d\Omega.$$

This term is similar to (A13). The only differences are, that we have $\tilde{\psi}$ instead of ϕ and g_ξ instead of g_0.

So with the same estimate as in (A13) we get:

$$\| \partial_s I(s)|_\xi \|_s \leq \mu^{-2} \left\| \int \partial_{k'} \frac{\partial_{k'} \tilde{\psi}(k',\vartheta,\theta) k' + 2\tilde{\psi}(k',\vartheta,\theta)}{(\tilde{g}(\mathbf{k}',\vartheta,\theta))^2} dk'\, d\Omega \right\|_s. \tag{A19}$$

This term again has uniform bound in k_{stat}, as its support moves away from the center of the coordinate system. So we get a constant C uniform in k_{stat} with

$$\| \partial_s I(s)|_\xi \|_s \leq \mu^{-2} C.$$

Now we estimate I_2 (A4). As this integral includes no stationary point, two partial integrations are possible without any problem, but we have to assure, that we can estimate the factors we get by these partial integrations uniform in k_{stat}. To be able to find an uniform estimate, we estimate the areas of χ separately.

So we again split our integral

$$I_2=\int_{k_1<k_{\mathrm{stat}}/2} e^{-i\mu g(\mathbf{k})}\chi_2(\mathbf{k})d^3k+\int_{k_1>2k_{\mathrm{stat}}} e^{-i\mu g(\mathbf{k})}\chi_2(\mathbf{k})d^3k+\int_{k_1\in B;|k_2|>1} e^{-i\mu g(\mathbf{k})}\chi_2(\mathbf{k})d^3k$$
$$+\int_{k_1\in B;|k_2|<1;|k_3|>1} e^{-i\mu g(\mathbf{k})}\chi_2(\mathbf{k})d^3k=:I_2^1+I_2^2+I_2^3+I_2^4,$$

where

$$B:=\left[\frac{k_{\mathrm{stat}}}{2};2k_{\mathrm{stat}}\right].$$

The integrals I_2^1 and I_2^2 we estimate by two partial integrations under the k_1 integral. This leads to

$$\begin{aligned}\|I_2^1\|_s&\leqslant\mu^{-2}\int_{k_1<k_{\mathrm{stat}}/2}\left\|\partial_{k_1}\left(\frac{1}{\dot g(\mathbf{k})}\partial_{k_1}\frac{\chi_2(\mathbf{k})}{\dot g(\mathbf{k})}\right)\right\|_s d^3k\\&=\mu^{-2}\int_{k_1<k_{\mathrm{stat}}/2}\left\|3\frac{\ddot\chi_2}{\dot g^2}+3\frac{\chi_2\ddot g^2}{\dot g^4}-3\frac{\dot\chi_2\ddot g}{\dot g^3}\right\|_s d^3k,\\\|I_2^2\|_s&\leqslant\mu^{-2}\int_{k_1>2k_{\mathrm{stat}}}\left\|\partial_{k}\left(\frac{1}{g'(\mathbf{k})}\partial_{k}\frac{\chi_2(\mathbf{k})}{g'(\mathbf{k})}\right)\right\|_s d^3k\\&=\mu^{-2}\int_{k_1>2k_{\mathrm{stat}}}\left\|3\frac{\chi_2''}{g'^2}+3\frac{\chi_2 g''^2}{g'^4}-3\frac{\chi_2' g''}{g'^3}\right\|_s d^3k,\end{aligned}\tag{A20}$$

where $\dot g(\mathbf{k}):=\partial_{k_1}g(\mathbf{k})$; $g'(\mathbf{k}):=\partial_k g(\mathbf{k})$.

At first sight these estimates do not seem to be uniform in a and $\mathbf{y}$. In fact

$$\ddot g(\mathbf{k})=\frac{m^2}{\sqrt{k^2+m^2}^3}+a\frac{k_2^{2\prime}+k_3^2}{k^3}$$

and

$$g''(\mathbf{k})=\frac{m^2}{\sqrt{k^2+m^2}^3}$$

are bounded on the area of integration. So it is left to show, that we can find functions h_j with $j=1;2$, which do not depend on a and $\mathbf{y}$ and which is bounded away from zero on $\mathbb{R}^3\backslash Q$ with

$$h_1(\mathbf{k})\leqslant g'(\mathbf{k}),\quad h_2(\mathbf{k})\leqslant\dot g(\mathbf{k})$$

for all a, $\mathbf{y}$, $\mathbf{k}$.

For this we estimate $\dot g$ for $k_1\leqslant k_{\mathrm{stat}}/2$. As $\ddot g>0$, it follows, that [see (A11)]

$$|\dot g(\mathbf{k})|=y-\frac{k_1}{\sqrt{k^2+m^2}}-a\frac{k_1}{k}\geqslant\frac{1}{2}.$$

For $k_1<0$ and by virtue $y\geqslant a+\frac{1}{2}\geqslant\frac{1}{2}$.

For $k_1>0$ we estimate, using that $y-a-k_{\mathrm{stat}}/\sqrt{k_{\mathrm{stat}}^2+m^2}=0$,

$$
\begin{aligned}
|\dot g(\mathbf{k})| &= y - \frac{k_1}{\sqrt{k^2+m^2}} - a\frac{k_1}{k} \\
&\geqslant y - a - \frac{k_1}{\sqrt{k^2+m^2}} \\
&\geqslant y - a - \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} + \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} - \frac{k_1}{\sqrt{k^2+m^2}} = \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} - \frac{k_1}{\sqrt{k^2+m^2}} \\
&\geqslant \frac{k_{\mathrm{stat}}\sqrt{k^2+m^2} - k_1\sqrt{k_{\mathrm{stat}}^2+m^2}}{\sqrt{k^2+m^2}\sqrt{k_{\mathrm{stat}}^2+m^2}} \\
&= \frac{k_{\mathrm{stat}}^2(k^2+m^2) - k_1^2(k_{\mathrm{stat}}^2+m^2)}{(k_{\mathrm{stat}}\sqrt{k^2+m^2} + k_1\sqrt{k_{\mathrm{stat}}^2+m^2})\sqrt{k_1^2+m^2}\sqrt{k_{\mathrm{stat}}^2+m^2}}.
\end{aligned}
$$

Recalling $k \in [0; k_{\mathrm{stat}}/2]$,

$$
\begin{aligned}
|\dot g(\mathbf{k})| &\geqslant \frac{\frac{3}{4}k_{\mathrm{stat}}^2 m^2}{(k_{\mathrm{stat}}\sqrt{k^2+m^2} + k_1\sqrt{k_{\mathrm{stat}}^2+m^2})\sqrt{k_1^2+m^2}\sqrt{k_{\mathrm{stat}}^2+m^2}} \\
&= \frac{3m^2}{4(\sqrt{k^2+m^2} + k_1\sqrt{1+(m/k_{\mathrm{stat}})^2})\sqrt{k_1^2+m^2}\sqrt{1+(m/k_{\mathrm{stat}})^2}}.
\end{aligned}
$$

As $k_{\mathrm{stat}} \geqslant m/\sqrt{3}$ [see (A2)] it follows:

$$
|\dot g(\mathbf{k})| \geqslant \frac{3m^2}{8(\sqrt{k^2+m^2} + 2k_1)\sqrt{k_1^2+m^2}} =: h_1.
$$

For $k_1 \geqslant 2k_{\mathrm{stat}}$, g' is positive. Therefore similar as before

$$
\begin{aligned}
|g'(\mathbf{k})| &= \frac{k}{\sqrt{k^2+m^2}} + a - y\cos(\vartheta) \\
&\geqslant \frac{k}{\sqrt{k^2+m^2}} - \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} + \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} + a - y \\
&= \frac{k}{\sqrt{k^2+m^2}} - \frac{k_{\mathrm{stat}}}{\sqrt{k_{\mathrm{stat}}^2+m^2}} \\
&= \frac{k\sqrt{k_{\mathrm{stat}}^2+m^2} - k_{\mathrm{stat}}\sqrt{k^2+m^2}}{\sqrt{k^2+m^2}\sqrt{k_{\mathrm{stat}}^2+m^2}} \\
&= \frac{k^2(k_{\mathrm{stat}}^2+m^2) - k_{\mathrm{stat}}^2(k^2+m^2)}{(k^2+m^2)(k_{\mathrm{stat}}^2+m^2)} \geqslant \frac{\frac{1}{4}k^2m^2}{(k^2+m^2)^2} =: h_2(\mathbf{k}).
\end{aligned}
$$

Note, that h_1 and h_2 do not depend on a and $\mathbf{y}$.

We can use this estimate in (A20). As g'' and $\ddot g$ have uniform bounds in a and $\mathbf{y}$ we get uniform estimates for I_2^1 and I_2^2,

$$\|I_2^1\|_s \leqslant \mu^{-2} \int_{k_1<k_{\text{stat}}/2} \left\| 3\frac{\ddot{\chi}_2}{h_1^2} + 3\frac{\chi_2 \ddot{g}^2}{h_1^4} + 3\frac{\dot{\chi}_2 \ddot{g}}{h_1^3} \right\|_s d^3k$$

$$\leqslant \mu^{-2} \int_{\mathbb{R}^3} \left\| 3\frac{\dddot{\tilde{\chi}}_2}{h_1^2} + 3\frac{\tilde{\chi}_2 \ddot{g}^2}{h_1^4} + 3\frac{\dot{\tilde{\chi}}_2 \ddot{g}}{h_1^3} \right\|_s d^3k$$

$$\|I_2^2\|_s \leqslant \mu^{-2} \int_{k_1>2k_{\text{stat}}} \left\| 3\frac{\chi_2''}{h_2^2} + 3\frac{\chi_2 g''^2}{h_2^4} + 3\frac{\chi_2' g''}{h_2^3} \right\|_s d^3k$$

$$\leqslant \mu^{-2} \int_{k_1 \geqslant m/\sqrt{3}} \left\| 3\frac{\tilde{\chi}_2''}{h_2^2} + 3\frac{\tilde{\chi}_2 g''^2}{h_2^4} + 3\frac{\tilde{\chi}_2' g''}{h_2^3} \right\|_s d^3k.$$

Hence

$$\|I_2^1\|_s + \|I_2^2\|_s \leqslant \mu^{-2} C$$

with a constant C uniform in k_{stat}.

The integrals I_2^3 and I_2^4 can be estimated in a similar way, partial integration now be done with k_2 and k_3

$$|\partial_{k_j} g(\mathbf{k})| = \frac{1}{\sqrt{k^2+m^2}} + \frac{a k_j}{k^2} \leqslant \frac{1}{\sqrt{k^2+m^2}} + \frac{a}{k} \quad \text{for } j=1;2$$

which is uniformly bounded away from zero on the area of integration.

So we have a uniform constant C with

$$I_2 \leqslant \mu^{-2} C,$$

and the lemma is proven for $y \in [a+\frac{1}{2}, a+1]$.

(II) Next we prove the Lemma for $y < a+1/2$.

We again have to assure, that all estimates are uniform in a and $\mathbf{y}$. In the last section the main difficulty we had to solve was, that g' near the stationary point was increasing with k_{stat} (recall that $\lim_{y \to a+1} k_{\text{stat}} = \infty$).

So on the first view it seems to be simple to have uniform estimates for $y < a+1/2$ just by setting $Q = \mathbb{R}^3$. But we have to face a new problem, which is, that the stationary point may be very close to zero. This is problematical in the differentiation of k appearing in our estimates.

For $a=0$ this problem does not appear and the lemma is also proven for $y < \frac{1}{2}$ with $a=0$.

As the divergence only appears for small k_{stat} we can set $k_{\text{stat}} < \frac{1}{2}$ [For $k_{\text{stat}} \geqslant \frac{1}{2}$ the estimates can be done very closely to the ones of (I), setting $Q = \mathbb{R}^3$.]

We solve the problem by first ''cutting out'' the stationary point. We split our integral

$$I = \int_{B(0,\sqrt{k_{\text{stat}}})} e^{-i\mu g(\mathbf{k})} \chi(\mathbf{k}) d^3k + \int_{\mathbb{R}^3 \setminus B(0,\sqrt{k_{\text{stat}}})} e^{-i\mu g(\mathbf{k})} \chi(\mathbf{k}) d^3k =: I_1 + I_2.$$

As $k_{\text{stat}} < \frac{1}{2}$, the stationary point is inside the ball.

We estimate I_1, writing it in spherical coordinates ''centered'' around the stationary point, by one partial integration,

$$\|I_1\|_s \leqslant \left\| \int_{B(0,\sqrt{k_{\text{stat}}})} e^{-i\mu g(\mathbf{k}')} \chi(\mathbf{k}') k'^2 \, dk' \, d\Omega \right\|_s$$
$$\leqslant \left\| \mu^{-1} \int_{B(0,\sqrt{k_{\text{stat}}})} \left(\frac{\chi' k'^2}{g'} + \frac{2\chi k'}{g'} + \frac{\chi g'' k'^2}{g'^2} \right) dk' \, d\Omega \right\|_s .$$

As $\chi \in \mathcal{G}$ all these terms are bounded, we have

$$\|I_1\|_s \leqslant M \mu^{-1} \sqrt{k_{\text{stat}}}.$$

We now estimate I_2.

The first idea is to estimate this integral by two partial integrations. But the integrand still comes "very close" to the stationary point, where $(g')^{-1}$ is not bounded. So this procedure will not yield uniform bound in a and $\mathbf{y}$.

The trick to get uniform bound is to redo the split (A10), (A11) of (I) into the integral for $a + \frac{1}{2} < y < a + 1$.

$$I_2 = I_1^1 + I_1^2 + \partial_s I(s)|_{s=\xi}$$

now using $k = 0$ as the center for our Taylor expansion. So we get

$$I_1^1 = \int_{\mathbb{R}^3 \setminus B(0,\sqrt{k_{\text{stat}}})} e^{i(g'(0)k + \frac{1}{2} g''(0) k^2)} \chi(0) d^3k$$

$$I_1^2 = \int_{\mathbb{R}^3 \setminus B(0,\sqrt{k_{\text{stat}}})} e^{i(g'(0)k + \frac{1}{2} g''(0) k^2)} (\chi(\mathbf{k}) - \chi(0)) k^2 \, dk \, d\Omega$$

$$\partial_s I(s)|_{s=\xi} = \int_{\mathbb{R}^3 \setminus B(0,\sqrt{k_{\text{stat}}})} \lambda k^3 \tilde{f}(\mathbf{k}) e^{g_\xi(\mathbf{k})} \chi(k) k^2 \, dk \, d\Omega,$$

where

$$g'(0) = \frac{k}{\sqrt{k^2 + m^2}} + a - y \cos(\vartheta)|_{k=0} = a - y \cos(\vartheta),$$

$$g''(0) = \partial_k^2 g = \left. \frac{m^2}{\sqrt{k^2 + m^2}^3} \right|_{k=0} = \frac{1}{m},$$

$$\tilde{f}(\mathbf{k}) = (g(\mathbf{k}) - g(0) - g'(0)k - \tfrac{1}{2} g''(0) k^2) k^{-3}, \tag{A21}$$

$$g_\xi(\mathbf{k}) = g(0) + g'(0)k + \tfrac{1}{2} g''(0) k^2 + \xi \tilde{f}(\mathbf{k}).$$

As by similar argument concerning (A17) g_ξ has only one stationary point $\tilde{\mathbf{k}}_{\text{stat}}$. One can easily see, that

$$g'(0) + g''(0)k = a - y \cos(\vartheta) + \frac{k}{m} \geqslant a - y \cos(\vartheta) + \frac{k}{\sqrt{k^2 + m^2}} = g'(\mathbf{k}).$$

Furthermore we have, that

$$g'_\xi(\mathbf{k}) = (1 - \xi)(g'(0) + g''(0)k) + \xi g'(\mathbf{k}).$$

It follows, that

$$g'(0)+g''(0)k \geqslant g'_\xi \geqslant g'.$$

Therefore at $\mathbf{k}=\tilde{\mathbf{k}}_{\text{stat}}$ [where by definition $g'_\xi(\tilde{\mathbf{k}}_{\text{stat}})=0$] the g' has to be negative. It follows (recalling, that g' increases monotonously on the k_1 axis), that

$$0 \leqslant \tilde{k}_{\text{stat}} \leqslant k_{\text{stat}}.$$

For the same reasons we have the zero point $\overline{\mathbf{k}}_{\text{stat}}$ of $g'(0)+g''(0)k$ (i.e., $\overline{\mathbf{k}}_{\text{stat}}=-g'(0)/g''(0)$):

$$0 \leqslant \overline{k}_{\text{stat}} \leqslant k_{\text{stat}}.$$

As the second derivative of $g''_\xi(\tilde{k}_{\text{stat}})$ is not equal to zero, we can define a function $\tilde{g}_\xi$ with

$$0 < M \leqslant \tilde{g}_\xi := |\mathbf{k}-\tilde{\mathbf{k}}_{\text{stat}}|^{-1} g_\xi. \tag{A22}$$

The integral I_1^1 includes the leading term. It can be estimated like (A12). The other terms can be estimated again by partial integrations. For that we define

$$\zeta_1 := (\chi(\mathbf{k})-\chi(0))k^2 =: \tilde{\zeta}_1 k^3, \quad \zeta_2 := \tilde{f}(\mathbf{k})\chi(k)k^5 =: \tilde{\zeta}_2 k^5,$$

where $\tilde{\zeta}_{1,2}$ are bounded C^∞ functions.

We now make two partial integrations in I_1^2 and three partial integrations in $\partial_s I(s)$ to get the estimates

$$\begin{aligned}
\|I_1^2\|_s &\leqslant \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k \left(\frac{1}{g'(0)+g''(0)k} \partial_k \left(\frac{\zeta_1}{g'(0)+g''(0)k} \right) \right) dk\, d\Omega \right\|_s \\
&= \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k \left(\frac{\zeta_1'}{(g'(0)+g''(0)k)^2} - \frac{\zeta_1 g''(0)}{(g'(0)+g''(0)k)^3} \right) dk\, d\Omega \right\|_s,
\end{aligned}$$

$$\begin{aligned}
\|\partial_s I(s)|_{s=\xi}\|_s &\leqslant \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k \left(\frac{1}{g'_\xi} \partial_k \left(\frac{1}{g'_\xi} \partial_k \frac{\zeta_2}{g'_\xi} \right) \right) dk d\Omega \right\|_s \\
&= \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k \left(\frac{1}{g'_\xi} \partial_k \left(\frac{\zeta_2'}{g'^2_\xi} - \frac{\zeta_2 g''_\xi}{g'^3_\xi} \right) \right) dk\, d\Omega \right\|_s \\
&= \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k \left(\frac{\zeta_2''}{g'^3_\xi} - 3\frac{\zeta_2' g''_\xi}{g'^4_\xi} - \frac{\zeta_2 g'''_\xi}{g'^3_\xi} + 3\frac{\zeta_2 g''^2_\xi}{g'^5_\xi} \right) dk d\Omega \right\|_s.
\end{aligned}$$

So we can define functions f_j, $j=1;\ldots;5$ which are bounded, with

$$\|I_1^2\|_s \leqslant \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k (f_1 q_1^2 + f_2 q_1^3) dk d\Omega \right\|_s,$$

$$\|\partial_s I(s)|_{s=\xi}\|_s \leqslant \mu^{-2} \left\| \int_{\mathbb{R}^3\setminus B(0,\sqrt{k_{\text{stat}}})} \partial_k (f_3 q_2^3 + f_4 q_2^4 + f_5 q_2^5) dk\, d\Omega \right\|_s,$$

where

$$q_1 := \frac{k}{|\mathbf{k}-\overline{\mathbf{k}}_{\text{stat}}|}, \quad q_2 := \frac{k}{|\mathbf{k}-\tilde{\mathbf{k}}_{\text{stat}}|}.$$

So it is only left to show, that $\partial_k q_1$ and $\partial_k q_2$ are bounded on $\mathbb{R}^3 \backslash B(0, \sqrt{k_{\text{stat}}})$. But this is easy

$$\partial_k q_1 = \partial_k \frac{1}{\sqrt{1-2\dfrac{k_{\text{stat}}\cos(\vartheta)}{k}+\dfrac{k_{\text{stat}}^2}{k^2}}} = \frac{1}{\sqrt{1-2\dfrac{k_{\text{stat}}\cos(\vartheta)}{k}+\dfrac{k_{\text{stat}}^2}{k^2}}^3}\left(\frac{k_{\text{stat}}^2}{k^3}-\frac{k_{\text{stat}}\cos(\vartheta)}{k^2}\right)$$

for $k \geqslant \sqrt{k_{\text{stat}}}$ this term has obviously uniform bound.

The derivative of q_2 can be estimated in the same way. We only have to replace $\tilde{k}_{\text{stat}}$ by $\overline{k}_{\text{stat}}$.

(III) For $y > a+1$ we have no stationary point any more. So two partial integrations are possible without any problem. We again choose k_1 parallel to $\mathbf{y}$

$$\begin{aligned}\|I_2\|_s &\leqslant \mu^{-2}\int \left\| \partial_k\left(\frac{1}{g'(\mathbf{k})}\partial_k \frac{\chi_2(\mathbf{k})}{g'(\mathbf{k})}\right)\right\|_s d^3k \\ &= \mu^{-2}\int \left\| \partial_k\left(\frac{\chi'}{g'^2}-\frac{\chi g''}{g'^3}\right)\right\|_s d^3k \\ &= \mu^{-2}\int \left\| \frac{\chi''}{g'^2}-2\frac{\chi' g''}{g'^3}-\frac{\chi' g''}{g'^3}-\frac{\chi g'''}{g'^3}+3\frac{\chi g''^2}{g'^4}\right\|_s d^3k\end{aligned}$$

(f' means $\partial_{k_1} f$).

This integral still depends on k_{stat}. To get an estimate uniform in k_{stat} we use

$$|g'(\mathbf{k})| = y - \frac{k_1}{\sqrt{k^2+m^2}} - a\frac{k_1}{k} \geqslant 1 - \frac{k_1}{\sqrt{k^2+m^2}} =: h(\mathbf{k}).$$

It follows

$$\|I_2\|_s \leqslant \mu^{-2}\int \left\| \frac{\chi''}{h^2}+3\frac{\chi' g''}{h^3}+3\frac{\chi g''^2}{h^4}+\frac{\chi g'''}{h^3}\right\|_s d^3k =: \mu^{-2} C.$$

Proof of Eq. (20)

For each $\mathbf{k}$ we have two eigenstates for electrons. These two eigenstates span the two dimensional spinor subspace for electrons. In the standard representation of the Dirac matrices these two spinors (the spinors here are not normalized) are

$$s^1_{\mathbf{k}} = \begin{pmatrix} \hat{E}_k \\ 0 \\ k_1 \\ k^+ \end{pmatrix}, \quad s^2_{\mathbf{k}} = \begin{pmatrix} 0 \\ \hat{E}_k \\ k^- \\ -k_1 \end{pmatrix},$$

where

$$k^{\pm} = k_2 \pm i k_3, \quad \hat{E}_k = E_k + m, \quad E_k = \sqrt{k^2+m^2}.$$

If we now take any linear combination of these spinors $s_{\mathbf{k}} = a_{\mathbf{k}} s^1(\mathbf{k}) + b(\mathbf{k}) s^2_{\mathbf{k}}$ and compute, for example, $\langle s^*_{\mathbf{k}}, \alpha_1 s_{\mathbf{k}}\rangle$, we get [see (2)],

$$\langle s^*_{\mathbf{k}}, \alpha_1 s_{\mathbf{k}}\rangle = \langle (a^*(\mathbf{k}) s^{1*}_{\mathbf{k}} + b^*(\mathbf{k}) s^{2*}_{\mathbf{k}}), \alpha_1 (a(\mathbf{k}) s^1_{\mathbf{k}} + b(\mathbf{k}) s^2_{\mathbf{k}})\rangle$$

$$= \left(a^*(\mathbf{k}) \begin{pmatrix} \hat{E}_k \\ 0 \\ k_1 \\ k^- \end{pmatrix} + b^*(\mathbf{k}) \begin{pmatrix} 0 \\ \hat{E}_k \\ k^+ \\ -k_1 \end{pmatrix} \right),$$

$$\left(a(\mathbf{k}) \begin{pmatrix} k_1 \\ -k^+ \\ \hat{E}_k \\ 0 \end{pmatrix} + b(\mathbf{k}) \begin{pmatrix} k^- \\ k_1 \\ 0 \\ -\hat{E}_k \end{pmatrix} \right) = (a^2(\mathbf{k}) + b^2(\mathbf{k})) 2 \hat{E}_k k_1 .$$

With the normalization factor

$$\begin{aligned} \langle s^*_{\mathbf{k}}, s_{\mathbf{k}}\rangle &= (a^2(\mathbf{k}) + b^2(\mathbf{k}))(\hat{E}_k^2 + k^2) \\ &= (a^2(\mathbf{k}) + b^2(\mathbf{k}))(E_k^2 + 2E_k m + m^2 + k^2) \\ &= (a^2(\mathbf{k}) + b^2(\mathbf{k}))(2E_k(E_k + m)) \\ &= (a^2(\mathbf{k}) + b^2(\mathbf{k}))(2E_k \hat{E}_k), \end{aligned}$$

we get

$$\langle s^*_{\mathbf{k}}, \alpha_1 s_{\mathbf{k}}\rangle = \frac{k_1}{\sqrt{k^2 + m^2}} \langle s^*_{\mathbf{k}}, s_{\mathbf{k}}\rangle.$$

Analogously we get

$$\langle s^*_{\mathbf{k}}, \alpha s_{\mathbf{k}}\rangle = \frac{\mathbf{k}}{\sqrt{k^2 + m^2}} \langle s^*_{\mathbf{k}}, s_{\mathbf{k}}\rangle.$$

By linearity (20) follows.

Proof of Lemma 3.4

(a) To begin with, we consider the integral

$$I(\mathbf{x}) = \int \frac{1}{|\mathbf{x} - \mathbf{x}'|^j} f(\mathbf{x}') d^3x' \tag{A23}$$

for bounded, integrable $\|f\|_s$ and j=1;2.

For $j=1$ it has been proven by Ikebe,[11] that I is Hölder continuous. We extend this to $j=2$. Therefore we need to estimate

$$I(\mathbf{x} + \mathbf{h}) - I(\mathbf{x} - \mathbf{h})$$

for arbitrary $\mathbf{h}$ with $h \leqslant \frac{1}{4}$. [We do not need to focus on $h > \frac{1}{4}$, as $I(\mathbf{x})$ is bounded.] We split the integral into

$$I(\mathbf{x} + \mathbf{h}) - I(\mathbf{x} - \mathbf{h}) \tag{A24}$$

$$
\begin{aligned}
&= \int_{B(\mathbf{x},\sqrt{h})} \left(\frac{1}{|\mathbf{x}+\mathbf{h}-\mathbf{x}'|^2} - \frac{1}{|\mathbf{x}-\mathbf{h}-\mathbf{x}'|^2} \right) f(\mathbf{x}')\, d^3x' \\
&\quad + \int_{B(\mathbf{x},1)\setminus B(\mathbf{x},\sqrt{h})} \left(\frac{1}{|\mathbf{x}+\mathbf{h}-\mathbf{x}'|^2} - \frac{1}{|\mathbf{x}-\mathbf{h}-\mathbf{x}'|^2} \right) f(\mathbf{x}')\, d^3x' \\
&\quad + \int_{\mathbb{R}^3\setminus B(\mathbf{x},1)} \left(\frac{1}{|\mathbf{x}+\mathbf{h}-\mathbf{x}'|^2} - \frac{1}{|\mathbf{x}-\mathbf{h}-\mathbf{x}'|^2} \right) f(\mathbf{x}')\, d^3x' \\
&=: I_1 + I_2 + I_3 . \qquad \text{(A25)}
\end{aligned}
$$

For I_1 we have

$$
\|I_1\|_s \leqslant 2 \sup_{x\in\mathbb{R}^3} \{\|f(\mathbf{x})\|_s\} \int_{B(\mathbf{x},\sqrt{h})} \frac{1}{|\mathbf{x}-\mathbf{x}'|^2}\, d^3x' .
$$

So we can find a constant $M<\infty$, so that

$$
\|I_1(\mathbf{x},\mathbf{h})\|_s \leqslant M\sqrt{h}, \quad \forall \mathbf{h}\in\mathbb{R}^3. \qquad \text{(A26)}
$$

For I_2 we have, using $|\sqrt{h}-h| \leqslant \frac{1}{2}\sqrt{h}$:

$$
\begin{aligned}
\|I_2\|_s &= \left\| \int_{B(\mathbf{x},1)\setminus B(0,\sqrt{h})} \left(\frac{1}{|\mathbf{x}'+\mathbf{h}|^2} - \frac{1}{|\mathbf{x}'-\mathbf{h}|^2} \right) f(\mathbf{x}-\mathbf{x}')\, d^3x' \right\|_s \\
&\leqslant \sup_{x\in\mathbb{R}^3} \{\|f(\mathbf{x})\|_s\} \int_{B(\mathbf{x},1)\setminus B(0,\sqrt{h})} \frac{\big||\mathbf{x}'-\mathbf{h}|^2-|\mathbf{x}'+\mathbf{h}|^2\big|}{|\mathbf{x}'+\mathbf{h}|^2|\mathbf{x}'-\mathbf{h}|^2}\, d^3x' \\
&\leqslant \sup_{x\in\mathbb{R}^3} \{\|f(\mathbf{x}\|_s)\} \int_{B(\mathbf{x},1)\setminus B(0,\sqrt{h})} \frac{4hx'}{|\mathbf{x}'+\mathbf{h}|^2|\mathbf{x}-\mathbf{h}|^2}\, d^3x' \\
&\leqslant \sup_{x\in\mathbb{R}^3} \{\|f(\mathbf{x})\|_s\} \int_{B(\mathbf{x},1)\setminus B(0,\sqrt{h})} \frac{8h}{x'^3}\, d^3x' .
\end{aligned}
$$

So we can find a constant $M<\infty$, so that

$$
\|I_2(\mathbf{x},\mathbf{h})\|_s \leqslant M\sqrt{h}, \quad \forall \mathbf{h}\in\mathbb{R}^3. \qquad \text{(A27)}
$$

For I_3 we have, using similar reasoning as above,

$$
\|I_3\|_s \leqslant \int_{\mathbb{R}^3\setminus B(\mathbf{0},1)} \frac{8h}{x'^3} \|f(\mathbf{x}-\mathbf{x}')\|_s\, d^3x' \leqslant 8h \int \|f(\mathbf{x}-\mathbf{x}')\|_s\, d^3x' .
$$

Since f is absolutely integrable, we can find a constant $M<\infty$, so that

$$
\|I_3(\mathbf{x},\mathbf{h})\|_s \leqslant Mh \quad \forall \mathbf{h}\in\mathbb{R}^3. \qquad \text{(A28)}
$$

We use this estimate on (36), observing, that $G^+_{\mathbf{k}}$ multiplied by $\mathcal{A}\tilde{\varphi}^s_{\mathbf{k}}$ is essentially of the form of the integrals in (A23). Therfore,

$$
\|\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}+\mathbf{h}) - \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})\|_s \leqslant M\sqrt{h} \quad \forall \mathbf{h}\in\mathbb{R}^3. \qquad \text{(A29)}
$$

Now we want to focus on integrals of the form (A23) for $j=2$ where $f(\mathbf{x})$ satisfies

$$
\|f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x})\|_s \leqslant M\sqrt{h}. \qquad \text{(A30)}
$$

We do a similar splitting as in (A24). Now we have for I_1, using (A30):

$$\|I_1\|_s \leqslant \left\| \int_{B(\mathbf{x},\sqrt{\hbar})} \frac{1}{|\mathbf{x}-\mathbf{x}'|^2} (f(\mathbf{x}'+\mathbf{h})-f(\mathbf{x}'-\mathbf{h}))d^3x' \right\|_s \leqslant \left| \int_{B(\mathbf{x},\sqrt{\hbar})} \frac{1}{|\mathbf{x}-\mathbf{x}'|^2} M\sqrt{h}d^3x' \right|.$$

Thus with an appropriate $\tilde{M}<\infty$:

$$\|I_1(\mathbf{x},\mathbf{h})\|_s \leqslant Mh \quad \forall \mathbf{h}\in\mathbb{R}^3. \tag{A31}$$

For I^2 we have

$$\begin{aligned}\|I_2^2\|_s &= \left\| \int_{B(0,1)\setminus B(0,\sqrt{\hbar})} \left(\frac{1}{|\mathbf{x}'+\mathbf{h}|^2} - \frac{1}{|\mathbf{x}'-\mathbf{h}|^2} \right) f(\mathbf{x}-\mathbf{x}')d^3x' \right\|_s \\ &= \left\| \int_{B(0,1)\setminus B(0,\sqrt{\hbar})} \frac{|\mathbf{x}'-\mathbf{h}|^2-|\mathbf{x}'+\mathbf{h}|^2}{|\mathbf{x}'-\mathbf{h}|^2|\mathbf{x}'+\mathbf{h}|^2} f(\mathbf{x}-\mathbf{x}')d^3x' \right\|_s .\end{aligned}$$

Since the fraction under this integral is point-symmetric to zero, we can estimate the integral by

$$\begin{aligned}\|I_2^2\|_s &\leqslant \left\| \int_{B(0,1)\setminus B(0,\sqrt{\hbar})} \left| \frac{|\mathbf{x}'-\mathbf{h}|^2-|\mathbf{x}'+\mathbf{h}|^2}{|\mathbf{x}'-\mathbf{h}|^2|\mathbf{x}'+\mathbf{h}|^2} \right| (f(\mathbf{x}-\mathbf{x}')-f(\mathbf{x}+\mathbf{x}'))d^3x' \right\|_s \\ &\leqslant \left\| \int_{B(0,1)\setminus B(0,\sqrt{\hbar})} \left| \frac{|\mathbf{x}'-\mathbf{h}|^2-|\mathbf{x}'+\mathbf{h}|^2}{|\mathbf{x}'-\mathbf{h}|^2|\mathbf{x}'+\mathbf{h}|^2} \right| M\sqrt{2x'}\, d^3x' \right\|_s \\ &\leqslant \left\| \int_{B(0,1)\setminus B(0,\sqrt{\hbar})} 4\left| \frac{2h}{x'^3} \right| M\sqrt{2x'}\, d^3x' \right| \\ &\leqslant \left\| 16\pi M\sqrt{2} \int_{\sqrt{\hbar}}^1 \left| \frac{2h}{x'^{-1/2}} \right| d^3x' \right\|_s .\end{aligned}$$

So we can find a $\tilde{M}<\infty$ with

$$\|I_2^2(\mathbf{x},\mathbf{h})\|_s \leqslant \tilde{M}h \quad \forall \mathbf{h}\in\mathbb{R}^3. \tag{A32}$$

For I_3 we do the same estimations as before.

Applying this to (36) we obtain the Hölder continuity of degree 1 for $\tilde{\varphi}^s_{\mathbf{k}}$.

(b) Assume that $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ satisfies (36) and is Hölder continuous of degree 1. Inserting $\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$ in the right-hand side of (32) leads to

$$\begin{aligned}H\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}) &= (H_0+\mathcal{A}(\mathbf{x}))\left(\varphi^s_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}')G_k^+(\mathbf{x}-\mathbf{x}')\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x' \right) \\ &= (E_k+\mathcal{A}(\mathbf{x}))\varphi^s_{\mathbf{k}}(\mathbf{x}) - (H_0+\mathcal{A}(\mathbf{x}))\int \mathcal{A}(\mathbf{x}')G_k^+(\mathbf{x}-\mathbf{x}')\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x'.\end{aligned}$$

For (32) this term has to be equal to $E_k\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})$. So we have to prove, that

$$(H_0-E_k)\int G_k^+(\mathbf{x}-\mathbf{x}')\mathcal{A}(\mathbf{x}')\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x' = \mathcal{A}(\mathbf{x})\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}).$$

In other words we have to prove, that with f Hölder continuous of degree 1,

$$(H_0-E_k)\int G_k^+(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'=f(\mathbf{x}'). \tag{A33}$$

G_k^+ can be written as[14]

$$G_k^+(\mathbf{x})=(H_0+E_k)\frac{e^{ikx}}{4\pi x}=:(H_0+E_k)G_k^{KG}$$

with

$$(H_0-E_k)(H_0+E_k)G_k^{KG}=(\Delta-k^2)G_k^{KG}=\delta. \tag{A34}$$

So for (A33) we need to show that

$$(H_0-E_k)(H_0+E_k)\int G_k^{KG}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'=(\Delta-k^2)\int G_k^{KG}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'=f(\mathbf{x}). \tag{A35}$$

We define for $\varepsilon>0$ the following function G_k^ε:

$$G_k^\varepsilon(\mathbf{x}):=G_{\mathbf{k}}^{KG}(\mathbf{x}) \quad \text{for } x\geqslant\varepsilon, \quad G_k^\varepsilon(\mathbf{x})=G_{\mathbf{k}}^{KG}(\mathbf{x})(1-e^{x/(\varepsilon-x)}) \quad \text{for } x<\varepsilon. \tag{A36}$$

We denote

$$G_k'(\mathbf{x})=\nabla G_k^{KG}=\frac{ik\mathbf{x}e^{ikx}}{4\pi x^2}+\frac{\mathbf{x}e^{ikx}}{x^3}. \tag{A37}$$

We split the right-hand side of (A35) into

$$(\Delta-k^2)\int (G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^\varepsilon(\mathbf{x}))f(\mathbf{x}')d^3x'+(\Delta-k^2)\int G_k^\varepsilon(\mathbf{x})f(\mathbf{x}')d^3x'. \tag{A38}$$

By definition of G_k^{KG} (A34) we have outside the ball $B(0,\varepsilon)$:

$$(\Delta-k^2)G_k^\varepsilon(\mathbf{x})=(\triangle-k^2)G_k^{KG}(\mathbf{x})=0. \tag{A39}$$

So for the first summand we have

$$
\begin{aligned}
&\lim_{\varepsilon\to 0}\left\|(\Delta-k^2)\int (G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))f(\mathbf{x}')d^3x'\right\|_s\\
&\quad=\lim_{\varepsilon\to 0}\left\|\Delta\int_{B(\mathbf{x},\varepsilon)}(G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))f(\mathbf{x}')d^3x'\right\|_s\\
&\quad=\lim_{\varepsilon\to 0}\left\|\nabla\int_{B(\mathbf{x},\varepsilon)}\nabla(G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))f(\mathbf{x}')d^3x'\right\|_s\\
&\quad=\lim_{\varepsilon\to 0}\left\|\nabla\int_{B(\mathbf{x},\varepsilon)}(\nabla_{x'}(G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')))f(\mathbf{x}')d^3x'\right\|_s\\
&\quad=\lim_{\varepsilon\to 0}\left\|\nabla\int_{B(\mathbf{x},\varepsilon)}(\nabla_{x'}(G_k^{KG}(\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}')))f(\mathbf{x}-\mathbf{x}')d^3x'\right\|_s\\
&\quad\leqslant\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}\left\|(\nabla_{x'}(G_k^{KG}(\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}')))\frac{f(\mathbf{x}-\mathbf{x}')-f(\mathbf{x}+\mathbf{h}-\mathbf{x}')}{h}\right\|_s d^rx'.
\end{aligned}
$$

As f is Hölder continuous, the last term can be estimated by

$$
\begin{aligned}
&\lim_{\varepsilon\to 0}\left\|(\Delta-k^2)\int (G_k^{KG}(\mathbf{x}-\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))f(\mathbf{x}')d^3x'\right\|_s\\
&\quad\leqslant\lim_{\varepsilon\to 0}\int_{B(0,\varepsilon)}|\nabla_{x'}(G_k^{KG}(\mathbf{x}')-G_k^{\varepsilon}(\mathbf{x}'))M|d^3x'\\
&\quad\leqslant\lim_{\varepsilon\to 0}\int_{B(0,\varepsilon)}\left|\left(G_k'(\mathbf{x}')-G_k'(\mathbf{x}')(1-e^{x^2/(\varepsilon-x)})-G_k^{\varepsilon}(\mathbf{x}')\frac{-\varepsilon}{(x-\varepsilon)^2}\right)M\right|d^3x'=0.
\end{aligned}
$$

For the second summand, we use (A39) and the mean value theorem

$$
\begin{aligned}
&\lim_{\varepsilon\to 0}(\Delta-k^2)\int G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}(\Delta-k^2)\int_{B(\mathbf{x},\varepsilon)}G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}(\Delta-k^2)G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}(\Delta-k^2)(e^{-ik|\mathbf{x}-\mathbf{x}'|}G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')e^{ik|\mathbf{x}-\mathbf{x}'|})f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}(\Delta-k^2)(e^{-ik|\mathbf{x}-\mathbf{x}'|}G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}')e^{ik|\mathbf{x}-\mathbf{x}'|})f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}(\Delta+2ik\nabla)(e^{-ik|\mathbf{x}-\mathbf{x}'|}G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))e^{ik|\mathbf{x}-\mathbf{x}'|}f(\mathbf{x}')d^3x'\\
&\quad=\lim_{\varepsilon\to 0}\int_{B(\mathbf{x},\varepsilon)}\Delta(e^{-ik|\mathbf{x}-\mathbf{x}'|}G_k^{\varepsilon}(\mathbf{x}-\mathbf{x}'))e^{ik|\mathbf{x}-\mathbf{x}'|}f(\mathbf{x}')d^3x'
\end{aligned}
$$

$$= \lim_{\varepsilon\to 0} e^{ik|\mathbf{x}-\mathbf{x}_\varepsilon|} f(\mathbf{x}_\varepsilon) \int_{B(\mathbf{x},\varepsilon)} \Delta(e^{-ik|\mathbf{x}-\mathbf{x}'|} G_k^\varepsilon(\mathbf{x}-\mathbf{x}'))\, d^3x',$$

where $\mathbf{x}_\varepsilon \in B(\mathbf{x},\varepsilon)$ using the positivity of

$$\Delta(e^{-ik|\mathbf{x}-\mathbf{x}'|} G_k^\varepsilon(\mathbf{x}-\mathbf{x}')) = 2\frac{1-e^{x/(\varepsilon-x)}}{4\pi x^3} + 2\frac{\varepsilon e^{x/(g-x)}}{(x-\varepsilon)^2 4\pi x^2} + \frac{(\varepsilon^2+2x\varepsilon)e^{x/(\varepsilon-x)}}{(x-\varepsilon)^4 4\pi x} \geqslant 0.$$

Hence with Gauss' theorem and (A37)

$$\begin{aligned}
\lim_{\varepsilon\to 0}(\Delta-k^2)\int G_k^\varepsilon(\mathbf{x}-\mathbf{x}') f(\mathbf{x}')\, d^3x' &= f(\mathbf{x}) \lim_{\varepsilon\to 0} \int_{B(\mathbf{x},\varepsilon)} \Delta(e^{-ik|\mathbf{x}-\mathbf{x}'|} G_k^\varepsilon(\mathbf{x}-\mathbf{x}'))\, d^3x' \\
&= f(\mathbf{x}) \lim_{\varepsilon\to 0} \int_{\partial B(\mathbf{x},\varepsilon)} \nabla(e^{-ik|\mathbf{x}-\mathbf{x}'|} G_k^\varepsilon(\mathbf{x}-\mathbf{x}'))\cdot \mathbf{n}\, d\Omega \\
&= f(\mathbf{x}) \lim_{\varepsilon\to 0} \int_{\partial B(\mathbf{x},\varepsilon)} \nabla(e^{-ik|\mathbf{x}-\mathbf{x}'|} G_k^{KG}(\mathbf{x}-\mathbf{x}'))\cdot \mathbf{n}|\mathbf{x}-\mathbf{x}'|'^2\, d\Omega \\
&= f(\mathbf{x}) \lim_{\varepsilon\to 0} \int_{\partial B(\mathbf{x},\varepsilon)} \frac{\mathbf{x}-\mathbf{x}'}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\cdot \mathbf{n}|\mathbf{x}-\mathbf{x}'|^2 d\Omega = f(\mathbf{x})
\end{aligned}$$

and (b) is proved.

We show now, that for any $\mathbf{k}\in\mathbb{R}^3$ there exists a unique solution $\tilde{\varphi}_\mathbf{k}^s(\mathbf{x})$ of (36).

Using the definition of the $\zeta_\mathbf{k}^s(\mathbf{x})$ [see (39)] in (36) yields

$$\zeta_\mathbf{k}^s(\mathbf{x}) = v_\mathbf{k}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') G_\mathbf{k}^+(\mathbf{x}-\mathbf{x}') \zeta_\mathbf{k}^s(\mathbf{x}')\, d^3x', \tag{A40}$$

where

$$v_\mathbf{k}(\mathbf{x}) := -\int \mathcal{A}(\mathbf{x}') G_\mathbf{k}^+(\mathbf{x}-\mathbf{x}') \varphi_\mathbf{k}^s(\mathbf{x}')\, d^3x'. \tag{A41}$$

It suffices to prove, that (A40) has a unique solution for any $\mathbf{k}\in\mathbb{R}^3$. For the Schrödinger Greens function, this has already been proven by Ikebe.[11] We want to proceed in the same way.

Let $\mathcal{B}$ be the Banach space of all continuous functions tending uniformly to zero as $x\to\infty$. Due to (48) $v(\mathbf{x})\in\mathcal{B}$. Ikebe uses the Riesz–Schauder theory of completely continuous operators in a Banach space.[13]

If T is a completely continuous operator in $\mathcal{B}$, then for any given $g\in\mathcal{B}$ the equation

$$f = g + Tf \tag{A42}$$

has a unique solution in $\mathcal{B}$ if $\tilde{f}=T\tilde{f}$ implies that $\tilde{f}=0$.

Defining the integral operator T by

$$Tf(\mathbf{x}) := -\int \mathcal{A}(\mathbf{x}') G_\mathbf{k}^+(\mathbf{x}-\mathbf{x}') f(\mathbf{x}')\, d^3x'$$

and using v for g, (A42) is equivalent to (A40). Note, that this operator is completely continuous by the proof of Lemma 3.4(a) following a similar argumentation as in Ref. 11 Lemma 4.2. So it is left to show, that the integral equation

$$\tilde{f}(\mathbf{x}) = -\int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')\tilde{f}(\mathbf{x}')d^3x' \tag{A43}$$

has the unique solution $\tilde{f}\equiv 0$.

Obviously $\tilde{f}\equiv 0$ is a solution of (A43). By virtue of (48) any solution of (A43) has to be of order x^{-1}. Furthermore $\tilde{f}$ satisfies

$$(-\Delta - k^2 + \mathcal{A})\tilde{f} = 0 \tag{A44}$$

which can be shown by direct calculation.

Following Ikebe, $\tilde{f}\equiv 0$ is the only solution of (A43).

(c) (i) follows directly from (48). For (c) (ii) we need to work more. We prove (c) (ii) for $j=1,2$.

Heuristically deriving (A40) with respect to k will yield $\partial_k \zeta$. We denote the function we get by this formal method by $\zeta_{\mathbf{k}}'^{s}$. Then

$$\zeta_{\mathbf{k}}'^{s}(\mathbf{x}) = \partial_k v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}')\partial_k G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}^{s}(\mathbf{x}')d^3x' - \int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}'^{s}(\mathbf{x}')d^3x'. \tag{A45}$$

We will now show, that this integral equation has a unique solution. We define

$$p(\mathbf{x}) := \partial_k v_{\mathbf{k}}(\mathbf{x}) + \int \mathcal{A}(\mathbf{x}')\partial_k G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}^{s}(\mathbf{x}')d^3x' \tag{A46}$$

$$\overline{\zeta_{\mathbf{k}}^{s}}(\mathbf{x}) := \zeta_{\mathbf{k}}'^{s}(\mathbf{x}) - p(\mathbf{x}) \tag{A47}$$

so $\overline{\zeta_{\mathbf{k}}^{s}}$ satisfies

$$\overline{\zeta_{\mathbf{k}}^{s}}(\mathbf{x}) = -\int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')p(\mathbf{x}')d^3x' - \int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')\overline{\zeta_{\mathbf{k}}'^{s}}(\mathbf{x}')d^3x'.$$

Since

$$v'(\mathbf{x}) := -\int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}}^{+}(\mathbf{x}-\mathbf{x}')v'(\mathbf{x}')d^3x' \in \mathcal{B}$$

this integral equation again has a unique solution, so does (A46).

We will now show, that $\zeta' = \partial_k \zeta$.

We define the integral of ζ',

$$\tilde{\zeta}_{k,\vartheta,\varphi}^{s}(\mathbf{x}) := \zeta_0^{s}(\mathbf{x}) + \int_0^k \zeta_{k',\vartheta,\varphi}'^{s}(\mathbf{x})dk'. \tag{A48}$$

Obviously $\partial_k \tilde{\zeta}_{\mathbf{k}}^{s} = \zeta_{\mathbf{k}}^{s'}$ and $\tilde{\zeta}_0^{s} = \zeta_0^{s}$. Using (A40) and (A46) in (A48) leads to

$$\begin{aligned}
\tilde{\zeta}_{\mathbf{k}}^{s}(\mathbf{x}) &= \zeta_0^{s}(\mathbf{x}) + \int_0^k \zeta_{k',\vartheta,\varphi}'^{s}(\mathbf{x})dk' \\
&= v_0(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}')G_0^{+}(\mathbf{x}-\mathbf{x}')\zeta_0^{s}(\mathbf{x}')d^3x' + \int_0^k \partial_{k'} v_{\mathbf{k}'}(\mathbf{x})dk' \\
&\quad - \int\int \mathcal{A}(\mathbf{x}')\partial_{k'}G_{\mathbf{k}'}^{+}(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}'}^{s}(\mathbf{x}')d^3x' + \int \mathcal{A}(\mathbf{x}')G_{\mathbf{k}'}^{+}(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}'}'^{s}(\mathbf{x}')d^3x'\,dk'
\end{aligned}$$

$$
\begin{aligned}
&= v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') G_0^+(\mathbf{x}-\mathbf{x}') \tilde{\zeta}_0^s(\mathbf{x}') d^3x' \\
&\quad - \int \int \mathcal{A}(\mathbf{x}') \partial_{k'} G_{\mathbf{k}'}^+(\mathbf{x}-\mathbf{x}') \tilde{\zeta}_{\mathbf{k}'}^s(\mathbf{x}') d^3x' + \int \mathcal{A}(\mathbf{x}') G_{\mathbf{k}'}^+(\mathbf{x}-\mathbf{x}') \zeta_{\mathbf{k}'}'^s(\mathbf{x}') d^3x'\, dk' \\
&\quad - \int \int \mathcal{A}(\mathbf{x}') \partial_{k'} (G_{\mathbf{k}'}^+(\mathbf{x}-\mathbf{x}') \tilde{\zeta}_{\mathbf{k}'}^s(\mathbf{x}')) d^3x'\, dk' \\
&= v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}') \tilde{\zeta}_{\mathbf{k}}^s(\mathbf{x}') d^3x'.
\end{aligned}
$$

So $\tilde{\zeta}_{\mathbf{k}}^s$ satisfies (A40). As the solution is unique, it follows, that $\tilde{\zeta}_{\mathbf{k}}^s = \zeta_{\mathbf{k}}^s$, hence

$$\partial_k \zeta_{\mathbf{k}}^s = \zeta_{\mathbf{k}}^{s'}.$$

By (48) $\tilde{\zeta}_{\mathbf{k}}^s$ and $p(\mathbf{x})$ have uniform bound, so

$$\sup_{\mathbf{x}\in\mathbb{R}^3} \|\partial_k \zeta_{\mathbf{k}}^s(\mathbf{x})\|_s < \infty.$$

For the second derivative we have

$$\partial_k^2 \frac{\zeta^s}{x+1} = \partial_k \frac{\overline{\zeta^s}}{x+1} + \partial_k \frac{p}{x+1}.$$

The proof of the existence and uniqueness of $\partial_k(\overline{\zeta^s}/x)$ is the same as for $\partial_k \zeta^s$, furthermore $\partial_k \overline{\zeta^s}$ is bounded uniformly in x.

For $\partial_k[p/(x+1)]$ we have

$$
\begin{aligned}
\left\| \partial_k \frac{p}{x+1} \right\|_s &= \left\| \frac{1}{x+1} \partial_k \left(\partial_k v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') \partial_k G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}') \tilde{\zeta}_{\mathbf{k}}^s(\mathbf{x}') d^3x' \right) \right\|_s \\
&= \left\| \frac{1}{x+1} \left(\partial_k^2 v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') \partial_k^2 G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}') \zeta_{\mathbf{k}}^s(\mathbf{x}') d^3x' \right.\right. \\
&\quad \left.\left. - \int \mathcal{A}(\mathbf{x}') \partial_k G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}') \partial_k \zeta_{\mathbf{k}}^s(\mathbf{x}') d^3x' \right) \right\|_s . \qquad \text{(A49)}
\end{aligned}
$$

Note, that

$$|\partial_k^2 G_{\mathbf{k}}^+(\mathbf{x})| = |x^2 S_{\mathbf{k}}^+(\mathbf{x}) + x \partial_k S_{\mathbf{k}}^+(\mathbf{x}) + \partial_k^2 S_{\mathbf{k}}^+(\mathbf{x})| \leq M\left(xk + \frac{k}{x^2} \right). \qquad \text{(A50)}$$

Observing (A50) and (35) $\partial_k^2 G_{\mathbf{k}}^+/x+1$ and $\partial_k \zeta_{\mathbf{k}}^s$ are bounded uniformly in $\mathbf{x}$, we have also, that

$$\frac{1}{x+1} \left(\partial_k^2 v_{\mathbf{k}}(\mathbf{x}) - \int \mathcal{A}(\mathbf{x}') \partial_k G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}') \partial_k \zeta_{\mathbf{k}}^s(\mathbf{x}') d^3x' \right)$$

is uniformly bounded in $\mathbf{x}$.

For the other summand we get

$$\sup_{x,k\in\mathbb{R}^3}\left\|\frac{1}{x+1}\int \mathcal{A}(\mathbf{x}')\partial_k^2 G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'\right\|_s$$
$$\leqslant \sup_{x\in\mathbb{R}^3}\left\|\frac{1}{x+1}\int \mathcal{A}(\mathbf{x}')(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'\right\|_s$$
$$\leqslant \sup_{x\in\mathbb{R}^3}\left\|\int \mathcal{A}(\mathbf{x}')\frac{M(\mathbf{x}-\mathbf{x}')}{(x+1)(x'+1)}(x'+1)\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'\right\|_s$$
$$\leqslant \sup_{x\in\mathbb{R}^3}\left\|\int \mathcal{A}(\mathbf{x}')M(x'+1)\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'\right\|_s<\infty.$$

This proves (c)(ii).

(c)(iii) The proof of (c)(iii) is very similar to the proof of (c)(ii). The only difference is, that we get new functions $p(\mathbf{x})$.

$$p(\mathbf{x})=k^{|\gamma|-1}D_{\mathbf{k}}^{\gamma}v_{\mathbf{k}}(\mathbf{x})+\int \mathcal{A}(\mathbf{x}')k^{|\gamma|-1}D_{\mathbf{k}}^{\gamma}G_{\mathbf{k}}^+(\mathbf{x}-\mathbf{x}')\zeta_{\mathbf{k}}^s(\mathbf{x}')d^3x'.$$

To have $p(\mathbf{x})$ in $\mathcal{B}$ one only has to assure, that $k^{|\gamma|-1}D_{\mathbf{k}}^{\gamma}k$ is bounded for $|\gamma|\leqslant 2$, which follows by direct calculation.

(d) For potentials satisfying condition A (3) the scattering system (H,H_0) is asymptotically complete (see Ref. 14), i.e., for any scattering state ψ there exists a free outgoing asymptotic ψ_{out} with

$$\lim_{t\to\infty}\|\psi(\mathbf{x},t)-\psi_{\text{out}}(\mathbf{x},t)\|=0. \tag{A51}$$

We write this, using the Fourier transform $\hat{\psi}_{\text{out}}^s$ of ψ_{out},

$$\lim_{t\to\infty}\left\|\psi(\mathbf{x},t)-\sum_{s=1}^{2}\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\varphi_{\mathbf{k}}^s(\mathbf{x},t)d^3k\right\|=0.$$

We shall show that

$$\lim_{t\to\infty}\left\|\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})(\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x},t)-\varphi_{\mathbf{k}}^s(\mathbf{x},t))d^3k\right\|=0. \tag{A52}$$

With that

$$\lim_{t\to\infty}\left\|\psi(\mathbf{x},t)-\sum_{s=1}^{2}\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x},t)d^3k\right\|$$
$$=\lim_{t\to\infty}\left\|e^{-iHt}\left(\psi(\mathbf{x})-\sum_{s=1}^{2}\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x})d^3k\right)\right\|$$
$$=\left\|\psi(\mathbf{x})-\sum_{s=1}^{2}\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x})d^3k\right\|=0$$

which establishes (40). For (A52) we consider

$$\int (2\pi)^{-3/2}\hat{\psi}_{\mathrm{out},s}(\mathbf{k})(\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x},t)-\varphi^s_{\mathbf{k}}(\mathbf{x},t))d^3k$$
$$=\int (2\pi)^{-3/2}e^{iE_kt}\hat{\psi}_{\mathrm{out},s}(\mathbf{k})\zeta^s_{\mathbf{k}}(\mathbf{x})d^3k$$
$$=\int (2\pi)^{-3/2}e^{iE_kt}\hat{\psi}_{\mathrm{out},s}(\mathbf{k})v^s_{\mathbf{k}}(\mathbf{x})d^3k$$
$$-\int (2\pi)^{-3/2}e^{iE_kt}\hat{\psi}_{\mathrm{out},s}(\mathbf{k})\int \mathcal{A}(\mathbf{x}')G^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}')\zeta^s_{\mathbf{k}}(\mathbf{x}')d^3x'\,d^3k=:\xi_1(\mathbf{x})+\xi_2(\mathbf{x}). \tag{A53}$$

For the k-integration of ξ_1 we introduce (A41) and (35) and then use Lemma 3.1, setting

$$\mu=t,\quad a=t^{-1}|\mathbf{x}-\mathbf{x}'|,\quad \mathbf{y}=t^{-1}\mathbf{x}',\quad k'=k,\quad \chi(\mathbf{k}')=(2\pi)^{-3/2}\hat{\psi}_{\mathrm{out},s}(\mathbf{k}').$$

Furthermore we recall that

$$\frac{k_{\mathrm{stat}}}{\sqrt{k^2_{\mathrm{stat}}+m^2}}+a-y=0$$
$$k^2_{\mathrm{stat}}=(k^2_{\mathrm{stat}}+m^2)(y-a)^2$$
$$k_{\mathrm{stat}}=m(y-a)\sqrt{k^2_{\mathrm{stat}}+m^2}=m\frac{x'}{t}\sqrt{k^2_{\mathrm{stat}}+m^2}.$$

For ξ_2 we set

$$\mu=t,\quad a=t^{-1}|\mathbf{x}-\mathbf{x}'|,\quad \mathbf{y}=0,\quad k'=k,\quad \chi(\mathbf{k}')=(2\pi)^{-3/2}\zeta^s_{\mathbf{k}}(\mathbf{k}')\hat{\psi}_{\mathrm{out},s}(\mathbf{k}').$$

Hence by (17) we obtain for (A53) that there exists $M<\infty$ uniform in $\mathbf{y}$ and a, such that

$$\|\xi_1(\mathbf{x})+\xi_2(\mathbf{x})\|_s\leqslant Mt^{-3/2}\left|\int \mathcal{A}(\mathbf{x}')G^+_{\mathbf{k}}(\mathbf{x}-\mathbf{x}')(1+x')d^3x'\right|=:Mt^{-3/2}G(\mathbf{x}). \tag{A54}$$

The integral $G(\mathbf{x})$ is bounded and goes to zero in the limit $x\to\infty$ [see (48)]. This we shall use in the following estimate. For (A52) we need to control

$$\lim_{t\to\infty}\|\xi_1+\xi_2\|=\lim_{t\to\infty}\left(\int \left\|\xi_1+\xi_2\right\|^2_s d^3x\right)^{1/2}.$$

We split this integral into three parts, which are time dependent by introducing for all $\varepsilon>0$,

$$\rho_\varepsilon(\mathbf{x})=\mathbb{I}_{B(0,\varepsilon t)},\ \text{the indicator function of the set } B(0,\varepsilon t),$$
$$\tilde{\rho}_\varepsilon(\mathbf{x})=\mathbb{I}_{B(0,t)\setminus B(0,\varepsilon t)},$$
$$\rho_{\mathrm{out}}(\mathbf{x})=\mathbb{I}_{\mathbb{R}^3\setminus B(0,t)},$$

thus splitting our integral into

$$\lim_{t\to\infty}\int \|\xi_1+\xi_2\|_s^2\, d^3x=\lim_{t\to\infty}\int \rho_\varepsilon(\mathbf{x})\|\xi_1+\xi_2\|_s^2\, d^3x+\lim_{t\to\infty}\int \tilde{\rho}_\varepsilon(\mathbf{x})\|\xi_1+\xi_2\|_s^2\, d^3x$$

$$+\lim_{t\to\infty}\int \rho_{\text{out}}(\mathbf{x})\|\xi_1+\xi_2\|_s^2\, d^3x=:I_1+I_2+I_3. \tag{A55}$$

The last part of this integral is the part, that lies outside the light cone. For large times, all wave functions which are solutions of the free or full Dirac equation will lie inside the light cone. By virtue of (29),

$$\lim_{t\to\infty}\|\rho_{\text{out}}(\mathbf{x})\,\psi_{\text{out},s}(\mathbf{x})\|=0,$$

$$\lim_{t\to\infty}\left\|\rho_{\text{out}}(\mathbf{x})\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\varphi_{\mathbf{k}}^s(\mathbf{x})d^3k\right\|=0,$$

or by (A51),

$$\lim_{t\to\infty}\left\|\rho_{\text{out}}(\mathbf{x})\int (2\pi)^{-3/2}\hat{\psi}_{\text{out},s}(\mathbf{k})\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x})d^3k\right\|=0.$$

By (A53) it follows, that:

$$I_3=\lim_{t\to\infty}\left\|\rho_{\text{out}}(\mathbf{x})\int \hat{\psi}_{\text{out},s}(\mathbf{k})(\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x})-\varphi_{\mathbf{k}}^s(\mathbf{x}))d^3k\right\|=0.$$

Now we use (A54) on:

$$I_1\leqslant M^2\lim_{t\to\infty}(\sup_{x\leqslant\varepsilon t}\{G(x)\})^2 t^{-3}\frac{4\pi}{3}(\varepsilon t)^3=C\varepsilon^3.$$

Since ε is arbitrary, $I_1=0$.

For I_2 we have

$$I_2=\lim_{t\to\infty}\left|\int \tilde{\rho}_\varepsilon(\mathbf{x})\|\xi_1+\xi_2\|_s^2\, d^3x\right|=\lim_{t\to\infty}\left|M^2\int t^{-3}\tilde{\rho}_\varepsilon(\mathbf{x})G(\mathbf{x})^2\, d^3x\right|\leqslant\limsup_{t\to\infty x\geqslant\varepsilon t}|G(\mathbf{x})^2|=0$$

and (40) is proved.

We first prove (41) for wave functions, where ψ_{out} is in $L^1\cap L^2$. The general result can then be obtained by density arguments.

Therefore we again use the unitarity of the time propagator

$$\int (2\pi)^{-3/2}\langle\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}),\psi(\mathbf{x})\rangle d^3x=\lim_{t\to\infty}\int (2\pi)^{-3/2}e^{iHt}\langle\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}),e^{-iHt}\psi(\mathbf{x})\rangle d^3x$$

$$=\lim_{t\to\infty}e^{iEt}\int (2\pi)^{-3/2}\langle\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}),\psi(\mathbf{x},t)\rangle d^3x$$

$$=\lim_{t\to\infty}e^{iEt}\int_{B(0,R)}(2\pi)^{-3/2}\langle\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}),\psi(\mathbf{x},t)\rangle d^3x$$

$$+\lim_{t\to\infty}e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}),\psi(\mathbf{x},t)\rangle d^3x.$$

By asymptotical completeness (A51) we obtain therefore

$$\int (2\pi)^{-3/2}\langle\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}),\psi(\mathbf{x})\rangle d^3x = \lim_{t\to\infty} e^{iEt}\int_{B(0,R)}(2\pi)^{-3/2}\langle\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x + \lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x.$$

By the free scattering into cones theorem, the first integral of the right-hand side goes to zero because any freely evolving wave function leaves any bounded region. For the second integral we write for all $R>0$,

$$\int (2\pi)^{-3/2}\langle\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}),\psi(\mathbf{x})\rangle d^3x = \lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\varphi^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x + \lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\zeta^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x.$$

Using Lemma 3.4(c)(i), the second integral on the right-hand side becomes

$$\begin{aligned}&\left|\lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\zeta^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x\right|\\ &\leqslant \lim_{R\to\infty}\frac{M}{R}\left\|\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\psi_{\text{out}}(\mathbf{x},t)d^3x\right\|\\ &= \lim_{R\to\infty}\frac{M}{R}\left\|\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\psi_{\text{out}}(\mathbf{x},0)d^3x\right\| = 0.\end{aligned}$$

Therefore,

$$\begin{aligned}\int (2\pi)^{-3/2}\langle\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}),\psi(\mathbf{x})\rangle d^3x &= \lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\varphi^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x\\ &= \lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int_{\mathbb{R}^3\setminus B(0,R)}(2\pi)^{-3/2}\langle\varphi^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x\\ &= \lim_{R\to\infty}\lim_{t\to\infty} e^{iEt}\int (2\pi)^{-3/2}\langle\varphi^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},t)\rangle d^3x\\ &= \lim_{R\to\infty}\int (2\pi)^{-3/2}\langle\varphi^s_{\mathbf{k}}(\mathbf{x}),\psi_{\text{out}}(\mathbf{x},0)\rangle d^3x = \hat{\psi}_{\text{out},s}(\mathbf{k}).\end{aligned}$$

and (41) is proved.

Proof of Lemma 2.2

First we want to prove $\Rightarrow$.

Let $\hat{\psi}_{\text{out}}(\mathbf{k})\in\mathcal{G}$. According to (40) we have for any $n\in\mathbb{N}_0$:

$$H^n\psi(\mathbf{x}) = \sum_{s=1}^{2}\int (2\pi)^{-3/2}H^n\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k = \sum_{s=1}^{2}\int (2\pi)^{-3/2}E_k^n\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k.$$

Since $\hat{\psi}_{\text{out}}(\mathbf{k})$ decays faster than any polynom, this term is bounded and in $L^2\otimes\mathbb{C}^4$ for all $n \in \mathbb{N}_0$. As the potential $\mathcal{A}\in C^\infty$, also

$$(H-\mathcal{A}-\beta m)^n\psi(\mathbf{x})=\nabla^n\psi(\mathbf{x})$$

is bounded and in $L^2\otimes\mathbb{C}^4$ for all $n\in\mathbb{N}_0$.

Furthermore we have, using (36) in (40):

$$\begin{aligned}H^n\psi(\mathbf{x})&=\sum_{s=1}^{2}\int(2\pi)^{-3/2}\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x})E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k\\&=\sum_{s=1}^{2}\int(2\pi)^{-3/2}\varphi^s_{\mathbf{k}}(\mathbf{x})E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k\\&\quad-\sum_{s=1}^{2}\int(2\pi)^{-3/2}\int\mathcal{A}(\mathbf{x}')G_k^+(\mathbf{x}-\mathbf{x}')\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x'\,E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k=:I_1+I_2.\end{aligned}$$

I_1 is the Fourier transform of $E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})$. As $E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})\in\mathcal{G}$, I_1 lies in $\hat{G}$.

Next we write for I_2,

$$\begin{aligned}I_2&=-\sum_{s=1}^{2}\int(2\pi)^{-3/2}\int\mathcal{A}(\mathbf{x}')e^{ikx+ik(|\mathbf{x}-\mathbf{x}'|-x)}\frac{S_k^+(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}')d^3x'\,E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})d^3k\,d\Omega\\&=-\sum_{s=1}^{2}\int\int_0^\infty(2\pi)^{-3/2}\int\mathcal{A}(\mathbf{x}')e^{ikx}F(\mathbf{k},\mathbf{x},\mathbf{x}')d^3x'E_k^n\hat{\psi}_{\text{out},s}(\mathbf{k})k^2\,dk\,d\Omega,\end{aligned}$$

where

$$F(\mathbf{k},\mathbf{x},\mathbf{x}'):=e^{ik(|\mathbf{x}-\mathbf{x}'|-x)}\frac{S_k^+(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}'). \tag{A56}$$

We make now two partial integrations under the k integral, which is possible by Fubinis theorem,

$$\begin{aligned}I_2&=-\sum_{s=1}^{2}\int(2\pi)^{-3/2}\int_0^\infty\int\mathcal{A}(\mathbf{x}')e^{ikx}F(\mathbf{k},\mathbf{x},\mathbf{x}')d^3x'\,E_k^nk^2\hat{\psi}_{\text{out},s}(\mathbf{k})dk\,d\Omega\\&=-\sum_{s=1}^{2}\frac{1}{x^2}\int(2\pi)^{-3/2}\int_0^\infty\int\mathcal{A}(\mathbf{x}')e^{ikx}\partial_k^2(F(\mathbf{k},\mathbf{x},\mathbf{x}')d^3x'\,E_k^nk^2\hat{\psi}_{\text{out},s}(\mathbf{k}))dk\,d\Omega\\&=-\sum_{s=1}^{2}\frac{1}{x^2}\int\int_0^\infty\int(2\pi)^{-3/2}\mathcal{A}(\mathbf{x}')e^{ikx}\partial_k^2F(\mathbf{k},\mathbf{x},\mathbf{x}')E_k^nk^2\hat{\psi}_{\text{out},s}(\mathbf{k})\\&\quad+2\partial_kF(\mathbf{k},\mathbf{x},\mathbf{x}')\partial_k(E_k^nk^2\hat{\psi}_{\text{out},s}(\mathbf{k}))dk\,d\Omega\,d^3x'\\&\quad-\sum_{s=1}^{2}\frac{1}{x^2}\int_0^\infty\int(2\pi)^{-3/2}\int\mathcal{A}(\mathbf{x}')e^{ikx}F(\mathbf{k},\mathbf{x},\mathbf{x}')d^3x',s(\mathbf{k}))dk\,d\Omega=:I_3+I_4.\end{aligned}$$

For I_4 we can write, using the definition of F (A56) and (36)

$$x^2 I_4 = \sum_{s=1}^{2} \int (2\pi)^{-3/2} \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}) \partial_k^2 (E_k^n k^2 \hat{\psi}_{\mathrm{out},s}(\mathbf{k})) \frac{1}{k^2} d^3k$$
$$- \sum_{s=1}^{2} \int (2\pi)^{-3/2} \varphi^s_{\mathbf{k}}(\mathbf{x}) \partial_k^2 (E_k^n k^2 \hat{\psi}_{\mathrm{out},s}(\mathbf{k})) \frac{1}{k^2} d^3k.$$

As $\hat{\psi}_{\mathrm{out}} \in \mathcal{G}$, $\partial_k^2 (E_k^n k^2 \hat{\psi}_{\mathrm{out},s}(\mathbf{k}))\,(1/k^2)$ lies in L^2 and so does $x^2 \partial_x^n I_4$ for $n \in \mathbb{N}_0$.

Under the k integral in I_3 one more partial integration is possible,

$$I_3 = -\sum_{s=1}^{2} \frac{1}{x^3} \int (2\pi)^{-3/2} \int \mathcal{A}(\mathbf{x}') \tilde{F}(\mathbf{k},\mathbf{x},\mathbf{x}') d^3x,$$

where

$$\tilde{F}(\mathbf{k},\mathbf{x},\mathbf{x}') := \partial_k (\partial_k^2 F(\mathbf{k},\mathbf{x},\mathbf{x}') E_k^n k^2 \hat{\psi}_{\mathrm{out},s}(\mathbf{k}) + 2\partial_k F(\mathbf{k},\mathbf{x},\mathbf{x}') \partial_k (E_k^n k^2 \hat{\psi}_{\mathrm{out},s}(\mathbf{k}))).$$

Due to Lemma 3.4 (c) $\partial_k^n \tilde{\varphi}_{\mathbf{k}}(\mathbf{x}') \leqslant M x'$. Furthermore we have, that

$$|\partial_k e^{ik(|\mathbf{x}-\mathbf{x}'|-x)}| = |(|\mathbf{x}-\mathbf{x}'|-x) e^{ik(|\mathbf{x}-\mathbf{x}'|-x)}| \leqslant x' |e^{ik(|\mathbf{x}-\mathbf{x}'|-x)}|.$$

It follows, that [remember the definition of F (A56)]

$$\|\tilde{F}(\mathbf{x},\mathbf{x})\|_s \leqslant M_2 \frac{x'^3}{|\mathbf{x}-\mathbf{x}'|}.$$

So due to (48), with condition B (9) on the potential, the integral

$$\int \mathcal{A}(\mathbf{x}') \tilde{F}(\mathbf{k},\mathbf{x},\mathbf{x}') d^3x'$$

decays as fast as or faster than x^{-1}, so $x^4 I_3$ is bounded. It follows, that $x^2 I_3$ lies in L^2 for $n \in \mathbb{N}_0$.

The proof, that $x \partial_x^n \psi \in L^2$ is similar as above, just with one partial integration less. It follows, that $\psi \in \hat{\mathcal{G}}$.

It is left to prove $\Leftarrow$.

By Lemma 3.4(b) it follows, that

$$E_k \hat{\psi}_{\mathrm{out},s}(\mathbf{k}) = H \hat{\psi}_{\mathrm{out},s}(\mathbf{k})$$
$$= \int (2\pi)^{-3/2} \langle \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}), H\psi(\mathbf{x}) \rangle d^3x$$
$$= \int (2\pi)^{-3/2} \langle \tilde{\varphi}^s_{\mathbf{k}}(\mathbf{x}), (H_0 + \mathcal{A})\psi(\mathbf{x}) \rangle d^3x.$$

For $\psi \in \hat{\mathcal{G}}$, the right-hand side is integrable, so $E_k \hat{\psi}_{\mathrm{out},s}(\mathbf{k})$ is bounded. As $\mathcal{A} \in C^\infty$, this can be repeated, so $E_k^n \hat{\psi}_{\mathrm{out},s}(\mathbf{k})$ is bounded for any $n \in \mathbb{N}$.

Since $E_k = \sqrt{k^2 + m^2} \geqslant k$, it follows, that

$$k^n \hat{\psi}_{\mathrm{out},s}(\mathbf{k}) < \infty.$$

Equivalently we get

$$E_k^n \partial_k^j \hat{\psi}_{\mathrm{out},s}(\mathbf{k}) = \int (2\pi)^{-3/2} \langle \partial_k^j \tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}), H^n \psi(\mathbf{x}) \rangle d^3x,$$

$$E_k^n k^{|\gamma|-1} D_{\mathbf{k}}^\gamma \hat{\psi}_{\mathrm{out},s}(\mathbf{k}) = \int (2\pi)^{-3/2} \langle k^{|\gamma|-1} D_{\mathbf{k}}^\gamma \tilde{\varphi}_{\mathbf{k}}^s(\mathbf{x}), H^n \psi(\mathbf{x}) \rangle d^3x.$$

With (c) of Lemma 3.4 it follows, that for $\psi \in \hat{\mathcal{G}}$ these terms are bounded for $j=1,2$, $n \in \mathbb{N}_0$ and $|\gamma| \leqslant 2$. So $\hat{\psi}_{\mathrm{out},s}(\mathbf{k}) \in \mathcal{G}$.

ACKNOWLEDGEMENT

Very helpful discussions with Stefan Teufel are gratefully acknowledged.

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Covariant phase difference observables in quantum mechanics

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(Received 17 September 2002; accepted 1 November 2002)

Covariant phase difference observables are determined in two different ways, by a direct computation and by a group theoretical method. A characterization of phase difference observables which can be expressed as the difference of two phase observables is given. The classical limits of such phase difference observables are determined and the Pegg-Barnett phase difference distribution is obtained from the phase difference representation. The relation of Ban's theory to the covariant phase theories is exhibited. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1534383]

I. INTRODUCTION

In quantum optical phase measurements like heterodyne and eight-port homodyne detections one can measure the phase difference between two single-mode input fields. However, if the second field, the reference field, can be considered as a classical field with well-known phase and (high) amplitude, then the theory reduces to a single-mode theory with one input beam. Under such conditions the heterodyne[1,2] and the eight-port homodyne[3–5] detection schemes measure the single-mode phase observable

$$X \mapsto E_{|0\rangle}(X) := \frac{1}{\pi} \int_X \int_0^\infty |z\rangle\langle z| \, |z| \, \mathrm{d}|z| \, \mathrm{d}(\arg z)$$

defined in terms of the coherent states $|z\rangle := e^{-|z|^2/2} \Sigma_{n=0}^\infty z^n / \sqrt{n!} \, |n\rangle$. Here $|z\rangle\langle z|$ denotes the projection on the one-dimensional subspace spanned by $|z\rangle$ and $z = |z| \arg z$ is a complex number. The phase observable $E_{|0\rangle}$ is covariant with respect to the shifts generated by the single-mode number operator $N := \Sigma_{n=0}^\infty n |n\rangle\langle n|$, that is,

$$e^{i\theta N} E_{|0\rangle}(X) e^{-i\theta N} = E_{|0\rangle}(X \dot{+} \theta)$$

for all (Borel) sets $X \subseteq [0, 2\pi)$ and $\theta \in \mathbb{R}$, with $\dot{+}$ denoting the addition modulo 2π. This condition is a natural covariance condition for observables describing coherent state phase measurements, and one may define a (single-mode) phase observable as a phase shift covariant normalized positive operator measure.[6–9] The structure of such observables is completely known and they can be characterized in at least four different ways in terms of phase matrices, sequences of unit vectors, sequences of generalized vectors, or using covariant trace-preserving operations, see, e.g., Refs. 6, 8, 10, and 11.

In this article we consider the difference of two (single-mode) phase observables and we notice that it satisfies a natural covariance condition. We take this condition as the defining

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condition of (two-mode) phase difference observables. We give both a direct (Sec. III) and a group theoretical (Sec. IV) characterization of such observables whereas in Sec. V we obtain a characterization of the phase difference observables which can be expressed as a difference of two phase observables. Section VI puts the phase difference distribution of Barnett and Pegg[12,13] in the present context. Section VII studies the classical limit of the two-mode theory whereas Sec. VIII discusses the relation of Ban's theory[14–16] to the covariant phase and phase difference theories. In the final section of the article some historical remarks are due and the question of measurability of the phase difference is briefly reviewed.

II. PHASE DIFFERENCE OBSERVABLES

Two phase observables can be joined in a natural way into a phase difference observable. Indeed, suppose that $E_1:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ and $E_2:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ are phase observables, where $\mathcal{B}([0,2\pi))$ is the Borel σ-algebra of the phase interval $[0,2\pi)$, $\mathcal{H}$ is a separable Hilbert space spanned by the number states $|n\rangle$, $n\in\mathbb{N}$, and $\mathcal{L}(\mathcal{H})$ is the set of bounded operators on $\mathcal{H}$. The product map $(X,Y)\mapsto E_1(X)\otimes E_2(Y)$ determines through a continuous linear extension a unique operator measure

$$\widetilde{E}:\mathcal{B}([0,2\pi)\times[0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H}),$$

with the property

$$\widetilde{E}(X\times Y)=E_1(X)\otimes E_2(Y).$$

Using the function

$$f:[0,2\pi)\times[0,2\pi)\to[0,2\pi),\quad (x,y)\mapsto x-y(\mathrm{mod}\,2\pi)$$

one gets from $\widetilde{E}$ the observable which is the difference of the observables E_1 and E_2:

$$E^{\mathrm{diff}}:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H}),\quad E^{\mathrm{diff}}(X):=\widetilde{E}(f^{-1}(X)).$$

Using the explicit form[10] of a phase observable $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$,

$$E(X)=\sum_{n,m=0}^{\infty}\langle\varphi_n|\varphi_m\rangle\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\mathrm{d}\theta\;|n\rangle\langle m|, \tag{1}$$

where $(\varphi_n)_{n\in\mathbb{N}}\subset\mathcal{H}$ is a sequence of unit vectors, one easily computes that the difference of E_1 and E_2 is

$$E^{\mathrm{diff}}(X)=\sum_{n,m,k,l\in\mathbb{N}}\delta_{n-m,l-k}\langle\varphi_n^1|\varphi_m^1\rangle\langle\varphi_k^2|\varphi_l^2\rangle\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\mathrm{d}\theta\;\;|n,k\rangle\langle m,l|. \tag{2}$$

Here δ is the Kronecker delta, $|n,k\rangle\langle m,l|$ stands for the rank one operator $\mathcal{H}\otimes\mathcal{H}\ni\psi\mapsto\langle m,l|\psi\rangle|n,k\rangle\in\mathcal{H}\otimes\mathcal{H}$, and, for instance, $|n,k\rangle$ is the short-hand notation for the tensor product vector $|n\rangle\otimes|k\rangle$.

Let

$$\Sigma N:=N\otimes I+I\otimes N,$$

$$\Delta N:=N\otimes I-I\otimes N$$

denote the sum and the difference of the number operators of the two modes, and let $\Sigma N=\Sigma_{k\in\mathbb{N}}kP_k^{\Sigma}$ and $\Delta N=\Sigma_{k\in\mathbb{Z}}kP_k^{\Delta}$ be their respective spectral decompositions, with the spectral projections

$$P_k^{\Sigma}=\sum_{n=0}^{k}|k-n,n\rangle\langle k-n,n|,\quad k\in\mathbb{N},$$

$$P_k^{\Delta}=\sum_{n\geqslant\max\{0,-k\}}|k+n,n\rangle\langle k+n,n|,\quad k\in\mathbb{Z}.$$

Consider the unitary operators

$$V_{\Sigma}(\alpha)=e^{i\alpha\Sigma N},\quad \alpha\in\mathbb{R},$$

$$V_{\Delta}(\beta)=e^{i\beta\Delta N},\quad \beta\in\mathbb{R}.$$

The difference E^{diff} of the phase observables E_1 and E_2 is *invariant* under V_{Σ},

$$V_{\Sigma}(\alpha)E^{\mathrm{diff}}(X)V_{\Sigma}(\alpha)^*=E^{\mathrm{diff}}(X),\tag{3}$$

for all $\alpha\in\mathbb{R},X\in\mathcal{B}([0,2\pi))$. This condition is equivalent to the commutativity of ΣN and E^{diff}, that is,

$$P_k^{\Sigma}E^{\mathrm{diff}}(X)=E^{\mathrm{diff}}(X)P_k^{\Sigma}$$

for all $k\in\mathbb{N},X\in\mathcal{B}([0,2\pi))$. Since the number sum is a projection valued observable $k\mapsto P_k^{\Sigma}$, the commutativity of ΣN and E^{diff} equals with their being (functionally) coexistent, that is, they have a joint observable, see, for instance, Ref. 17. It is another immediate observation that E^{diff} satisfies the following *covariance* condition under V_{Δ}:

$$V_{\Delta}(\beta)E^{\mathrm{diff}}(X)V_{\Delta}(\beta)^*=E^{\mathrm{diff}}(X\dot{+}2\beta),\tag{4}$$

for all $\beta\in\mathbb{R},X\in\mathcal{B}([0,2\pi))$.

Let

$$\Theta(\alpha,\beta)=e^{i\alpha N\otimes I+i\beta I\otimes N},\ \alpha,\beta\in\mathbb{R}.$$

Since

$$\Theta(\alpha,\beta)=V_{\Sigma}\left(\frac{\alpha}{2}\right)V_{\Delta}\left(\frac{\alpha}{2}\right)V_{\Sigma}\left(\frac{\beta}{2}\right)V_{\Delta}\left(-\frac{\beta}{2}\right),$$

we observe that the invariance and covariance conditions (3) and (4) are equivalent with the condition

$$\Theta(\alpha,\beta)E^{\mathrm{diff}}(X)\Theta(\alpha,\beta)^*=E^{\mathrm{diff}}(X\dot{+}(\alpha-\beta))\tag{5}$$

for all $X\in\mathcal{B}([0,2\pi))$ and $\alpha,\beta\in\mathbb{R}$.

These observations lead us to the following definition.

Definition 1: A *phase difference observable* is a normalized positive operator measure $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ which satisfies the covariance condition

$$\Theta(\alpha,\beta)E(X)\Theta(\alpha,\beta)^*=E(X\dot{+}(\alpha-\beta))\tag{6}$$

for all $X\in\mathcal{B}([0,2\pi))$ and $\alpha,\beta\in\mathbb{R}$.

In the next sections we characterize all phase difference observables and we also give a necessary and sufficient condition for a phase difference observable to be a difference of two (one-mode) phase observables.

III. DIRECT METHOD

The following lemma simplifies the proof of the Theorem 1 below.

Lemma 1: Let $q\in\mathbb{Z}$ *and let* $\nu_q:\mathcal{B}([0,2\pi))\to\mathbb{C}$ *be a* σ*-additive set function. Then* $\nu_q(X\dot{+}\theta)=e^{iq\theta}\nu_q(X)$ *for all* $X\in\mathcal{B}([0,2\pi))$ *and* $\theta\in[0,2\pi)$ *if and only if* $\nu_q(X)=c_q(1/2\pi)\int_X e^{iq\theta}\mathrm{d}\theta$ *for all* $X\in\mathcal{B}([0,2\pi))$, *where* $c_q\in\mathbb{C}$.

Proof: The "if" part of the lemma is clear, so we have to prove "only if"statement. Assume that $\nu_q(X\dot{+}\theta)=e^{iq\theta}\nu_q(X)$ for all $X\in\mathcal{B}([0,2\pi))$ and $\theta\in[0,2\pi)$. Since $[0,2\pi)\dot{+}\theta=[0,2\pi)$ it follows that

$$\nu_q([0,2\pi))=\nu_q([0,2\pi)\dot{+}\theta)=e^{iq\theta}\nu_q([0,2\pi)),$$

and thus $\nu_q([0,2\pi))=c_0\delta_{0,q}$, where c_0 is a complex constant. The rest of the proof is same as the proof of Lemma 1 in Ref. 10. □

Let $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ be an arbitrary operator measure, that is, an $\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$-valued map defined on $\mathcal{B}([0,2\pi))$ which is σ-additive with respect to the weak operator topology.

Theorem 1: *(a) If the operator measure* $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ *satisfies the covariance condition (6), then for all* $X\in\mathcal{B}([0,2\pi))$,

$$E(X)=\sum_{n,m,k,l=0}^{\infty}c_{n,m,k,l}\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\mathrm{d}\theta|n,k\rangle\langle m,l|, \tag{7}$$

where $c_{n,m,k,l}\in\mathbb{C}$, *and* $c_{n,m,k,l}=0$ *if* $n-m\neq l-k$, *for all* $n,m,k,l\in\mathbb{N}$.

(b) If, in addition, E is positive, that is, $E(X)\geqslant O$ *for all* $X\in\mathcal{B}([0,2\pi))$, *then* $\Sigma_{n,m,k,l=0}^{N}c_{n,m,k,l}|n,k\rangle\langle m,l|\geqslant O$ *for all* $N\in\mathbb{N}$, *and*

(c) if E is normalized, that is, $E([0,2\pi))=I$, *then* $c_{n,n,k,k}=1$ *for all* $n,k\in\mathbb{N}$.

Proof: (a) Using the covariance condition we get

$$\langle n,k|E(X\dot{+}(\alpha-\beta))|m,l\rangle=e^{i\alpha(n-m)+i\beta(k-l)}\langle n,k|E(X)|m,l\rangle$$

for all $n,m,k,l\in\mathbb{N}$, $\alpha,\beta\in\mathbb{R}$ and $X\in\mathcal{B}([0,2\pi))$. Choosing $\alpha=\beta$ it follows that $\langle n,k|E(X)|m,l\rangle=0$ if $n-m\neq l-k$. Denote

$$\nu_{n,m,k}(X):=\langle n,k|E(X)|m,k+n-m\rangle.$$

We get

$$\begin{aligned}\nu_{n,m,k}(X\dot{+}(\alpha-\beta))&=\langle n,k|E(X\dot{+}(\alpha-\beta))|m,k+n-m\rangle\\&=e^{i(\alpha(n-m)+\beta(m-n))}\langle n,k|E(X)|m,k+n-m\rangle\\&=e^{i(\alpha-\beta)(n-m)}\nu_{n,m,k}(X).\end{aligned}$$

Taking $q=n-m$, Lemma 1 now gives Eq. (7).

(b) If $\Sigma_{n,m,k,l=0}^{N}c_{n,m,k,l}\langle\psi|n,k\rangle\langle m,l|\psi\rangle<0$ for some $N\in\mathbb{N}$ and $\psi\in\mathcal{H}\otimes\mathcal{H}$, then, due to the continuity of the density function, one may choose an $\epsilon>0$ such that $\langle P_N\psi|E([0,\epsilon))P_N\psi\rangle<0$, where $P_N:=\Sigma_{n,k=0}^{N}|n,k\rangle\langle n,k|$. This is a contradiction.

(c) This is a direct check. □

To prove the converse of the above theorem, consider a positive normalized operator measure $\tilde{E}:\mathcal{B}([0,2\pi)\times[0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ and a set of complex numbers $\tilde{\mathbf{c}}:=(\tilde{c}_{n,m,k,l})_{n,m,k,l\in\mathbb{N}}$. We say that $\tilde{E}$ is Θ-*covariant* if

$$\Theta(\alpha,\beta)\tilde{E}(Z)\Theta(\alpha,\beta)^*=\tilde{E}(Z\dot{+}(\alpha,\beta))$$

for all $Z\in\mathcal{B}([0,2\pi)\times[0,2\pi))$, $\alpha,\beta\in\mathbb{R}$, with $\dot{+}$ meaning (componentwise) addition mod 2π, and we say that $\tilde{\mathbf{c}}$ is *normalized positive semidefinite* if

$$\tilde{c}_{n,n,m,m}=1,$$

$$\sum_{n,m,k,l=0}^{N} \tilde{c}_{n,m,k,l}|n,k\rangle\langle m,l| \geqslant O,$$

for all $n,m,N \in \mathbb{N}$.

With the above notations the following theorem is then obtained. Its proof is essentially the same as in the one-dimensional case[8] so that we omit it here.

Theorem 2: *(a) If $\tilde{E}$ is Θ-covariant, then there is a normalized positive semidefinite $\tilde{\mathbf{c}}$ such that for any $Z \in \mathcal{B}([0,2\pi)\times[0,2\pi))$,*

$$\tilde{E}(Z)=\sum_{n,m,k,l=0}^{\infty} \tilde{c}_{n,m,k,l}\int_Z e^{i[(n-m)x+(k-l)y]}\frac{dx}{2\pi}\,\frac{dy}{2\pi}|n,k\rangle\langle m,l|. \tag{8}$$

(b) If $\tilde{\mathbf{c}}$ is normalized positive semidefinite, then formula (8) defines (weakly) a Θ-covariant normalized positive operator measure $\tilde{E}:\mathcal{B}([0,2\pi)\times[0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$.

By the above theorem, given a normalized positive semidefinite set of complex numbers $\tilde{\mathbf{c}}$ we get a Θ-covariant normalized positive operator measure $\tilde{E}$. Consider again the function $f(x,y)=x-y(\mathrm{mod}\,2\pi)$, defined on the rectangle $[0,2\pi)\times[0,2\pi)$. Then the map $\mathcal{B}([0,2\pi)) \ni X\mapsto\tilde{E}^f(X):=\tilde{E}(f^{-1}(X))\in\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ is a phase difference observable with the structure given in Eq. (7), where now

$$c_{n,m,k,l}=\tilde{c}_{n,m,k,l}\delta_{n-m,l-k}. \tag{9}$$

Remark 1: Let $(\psi_{n,k})_{n,k\in\mathbb{N}}$ be a set of unit vectors in $\mathcal{H}$. It is clear that defining

$$\tilde{c}_{n,m,k,l}=\langle\psi_{n,k}|\psi_{m,l}\rangle, \tag{10}$$

$\tilde{\mathbf{c}}$ is normalized positive semidefinite. Also the converse is true, any normalized positive semidefinite set of complex numbers is of the form (10). Construction of a set of unit vectors $\{\psi_{n,k}\}_{n,k\in\mathbb{N}}$ for a given $\tilde{\mathbf{c}}$ is similar than the one given in Ref. 10, Sec. II.B. We note also that if $\tilde{\mathbf{c}}$ is positive semidefinite defined by unit vectors $(\psi_{n,k})_{n,k\in\mathbb{N}}$, then $\mathbf{c}$ defined as in Eq. (9) is positive semidefinite since one may choose a sequence $(\psi_{n,k}\otimes|n+k\rangle)_{n,k\in\mathbb{N}}$ of unit vectors to construct $\mathbf{c}$.

Remark 2: Equation (9) shows that Θ-covariant observables $\tilde{E}$ form a ''wider'' class of observables than phase difference observables of Definition 1 in the sense that there are many Θ-covariant observables which give the same phase difference observable, and any phase difference observable with $\mathbf{c}$ defines a Θ-covariant observable which has, for instance, the same $\mathbf{c}$ as its structure unit. One may define an equivalence relation between Θ-covariant observables as follows: two Θ-covariant observables with $\tilde{\mathbf{c}}$ and $\tilde{\mathbf{d}}$ are equivalent if $\tilde{c}_{n,m,k,l}=\tilde{d}_{n,m,k,l}$ for all $n,m,k,l\in\mathbb{N}$, $n-m=l-k$, that is, if they define the same phase difference observable.

Remark 3: Using (7), it easy to see that any phase difference observable E has a uniform distribution in states where one mode is in a number state. For example, if $\psi:=\varphi\otimes|s\rangle$, $\varphi\in\mathcal{H}$, $\|\psi\|=1$, $s\in\mathbb{N}$, then

$$\langle\psi|E(X)|\psi\rangle=\frac{1}{2\pi}\int_X \mathrm{d}\theta, \quad n,k\in\mathbb{N}, \quad X\in\mathcal{B}([0,2\pi)).$$

Moreover, one may also witness that there is no projection valued phase difference observable. For example,

$$\langle 0,0|E(X)^2|0,0\rangle=\left|\frac{1}{2\pi}\int_X \mathrm{d}\theta\right|^2,$$

and choosing $X=[0,\pi)$ we get $\langle 0,0|E([0,\pi))^2|0,0\rangle=\frac{1}{4}$. Compared to $\langle 0,0|E([0,\pi))|0,0\rangle=\frac{1}{2}$, this shows that a phase difference observable cannot be a spectral measure.

IV. GROUP THEORETICAL SOLUTION

In Ref. 10 all phase observables were calculated using a generalized imprimitivity theorem. Here we follow the same method to give an alternative way to derive the structure of phase difference observables. In using group theoretical methods, it is convenient to work in the torus $\mathbb{T}:=\{z\in\mathbb{C}:|z|=1\}$, instead of phase interval $[0,2\pi)$ where addition is to be taken modulo 2π. We regard $\mathbb{T}$ as a compact (second countable) Abelian group and we let μ denote its Haar measure. The product group $\mathbb{T}\times\mathbb{T}$ has a unitary representation U on $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, defined by

$$[U(a,b)f](z_1,z_2)=f(az_1,bz_2). \tag{11}$$

To solve the covariance condition (6), we will first characterize all positive normalized operator measures $F:\mathcal{B}(\mathbb{T})\to\mathcal{L}(L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu))$ that satisfy

$$U(a,b)F(X)U(a,b)^*=F(ab^{-1}X) \tag{12}$$

for all $X\in\mathcal{B}(\mathbb{T})$, $a,b\in\mathbb{T}$. The canonical spectral measure F_{can} satisfying this condition is of the form

$$[F_{\mathrm{can}}(X)f](z_1,z_2)=\chi_X(z_1^{-1}z_2)f(z_1,z_2), \tag{13}$$

where χ_X is the characteristic function of the set X.

Notice that $U(a,b)=U(a,1)U(1,b)$, so that the covariance conditions

$$U(a,1)F(X)U(a,1)^*=F(aX),\quad a\in\mathbb{T},X\in\mathcal{B}(\mathbb{T}), \tag{14}$$

and

$$U(1,b^{-1})F(X)U(1,b^{-1})^*=F(bX),\quad b\in\mathbb{T},X\in\mathcal{B}(\mathbb{T}), \tag{15}$$

taken together are equivalent with the condition (12). We will denote the representation $a\mapsto U(a,1)$ as U_1 and the representation $a\mapsto U(1,a^{-1})$ as U_2.

Covariance condition (12) can be solved by looking at the action $z\mapsto ab^{-1}z$ of $\mathbb{T}\times\mathbb{T}$ on $\mathbb{T}$ and noting that the stability subgroup is $\mathbb{T}$.[18] Here we proceed in a different way. We characterize the normalized positive operator measures satisfying separately conditions (14) and (15). Then we combine the results to obtain operator measures satisfying condition (12). Finally, we go back to the original Hilbert space $\mathcal{H}$ and to the phase interval $[0,2\pi)$ to get all the phase difference observables.

Let F be a normalized positive operator measure satisfying condition (14). Since the action $z\mapsto az$ of $\mathbb{T}$ on itself is transitive, (U_1,F) is a transitive system of covariance based on $\mathbb{T}$ and, hence, (U_1,F) is described by Ref. 19, Proposition 2. In order to apply the cited result, let us notice the following facts. The stability subgroup of any point of $\mathbb{T}$ is the trivial subgroup $\{1\}$. The trivial representation σ of $\{1\}$ acting on $L_2(\mathbb{T},\mu)$ contains all the (trivial) representations of $\{1\}$ and the corresponding imprimitivity system (R,P) for $\mathbb{T}$ based on $\mathbb{T}$ induced by σ acts on $L^2(\mathbb{T},\mu,L_2(\mathbb{T},\mu))\simeq L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ as

$$(R(a)\varphi)(z_1,z_2)=\varphi(a^{-1}z_1,z_2), \tag{16}$$

$$(P(X)\varphi)(z_1,z_2)=\chi_X(z_1)\varphi(z_1,z_2), \tag{17}$$

where $\varphi\in L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, $a\in\mathbb{T},X\in\mathcal{B}(\mathbb{T})$ and z_1, $z_2\in\mathbb{T}$.

Proposition 2 of Ref. 19 shows that, given a normalized covariant positive operator measure F, there exists an isometry

$$W_1:L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)\to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu),$$

which intertwines the action U_1 with R and such that

$$F(X)=W_1^*P(X)W_1, \qquad X\in\mathcal{B}(\mathbb{T}). \tag{18}$$

Conversely, given an intertwining isometry W_1 from $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ to $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, Eq. (18) defines a positive normalized operator measure F satisfying Eq. (14).

Hence, to classify all normalized positive operator measures satisfying condition (14), one has to determine all the isometric mappings W_1 such that

$$W_1U_1(a)=R(a)W_1, \qquad a\in\mathbb{T}. \tag{19}$$

To perform this task, observe that the monomials e_n, $n\in\mathbb{Z}$, $e_n(z)=z^n$, $z\in\mathbb{T}$, form an orthonormal basis of $L_2(\mathbb{T},\mu)$. Similarly, the product vectors

$$(e_ne_k)(z_1,z_2)=e_n(z_1)e_k(z_2)=z_1^nz_2^k,\ n,k\in\mathbb{Z},$$

form an orthonormal basis of $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$.

The action of U_1 in this base is

$$U_1(a)(e_ne_k)=a^n(e_ne_k)$$

and the action of R is simply

$$R(a)(e_ne_k)=a^{-n}(e_ne_k).$$

From Eq. (19) we get

$$R(a)W_1(e_ne_k)=W_1U_1(a)(e_ne_k)=a^nW_1(e_ne_k)$$

for all $n,k\in\mathbb{Z}$. It follows that $W_1(e_ne_k)$ must be in the vector space $\overline{\text{span}}\{(e_{-n}e_j)\}_{j\in\mathbb{Z}}\simeq L_2(\mathbb{T},\mu)$. This means that $W_1(e_ne_k)=(e_{-n}\psi_{n,k})$, where $\psi_{n,k}$ is some unit vector in $L_2(\mathbb{T},\mu)$.

The matrix elements of F in the basis $\{(e_ne_k)\}_{n,k\in\mathbb{N}}$ are thus

$$\begin{aligned}\langle(e_ne_k)|F(X)(e_me_l)\rangle&=\langle(e_ne_k)|W_1^*P(X)W_1(e_me_l)\rangle\\&=\langle W_1(e_ne_k)|P(X)W_1(e_me_l)\rangle\\&=\langle(e_{-n}\psi_{n,k})|P(X)(e_{-m}\psi_{m,l})\rangle\\&=\langle\psi_{n,k}|\psi_{m,l}\rangle\int_X z^{n-m}\,\mathrm{d}\mu(z).\end{aligned} \tag{20}$$

We consider next condition (15). Like in the previous case, U_2 and a normalized positive operator measure F satisfying (15) form a transitive system of covariance based on $\mathbb{T}$. The corresponding imprimitivity system is the same pair (R,P), defined in Eqs. (16) and (17). The action of U_2 in the basis $\{(e_ne_k)\}_{n,k\in\mathbb{N}}$ is

$$U_2(a)(e_ne_k)=a^{-k}(e_ne_k).$$

If W_2 is an isometry intertwining representations U_2 and R, then

$$R(a)W_2(e_ne_k)=W_2U_2(a)(e_ne_k)=a^{-k}W_2(e_ne_k). \tag{21}$$

Thus $W_2(e_ne_k)$ must be in the vector space $\overline{\text{span}}\{(e_ke_j)\}_{j\in\mathbb{Z}}\simeq L_2(\mathbb{T},\mu)$ and $W_2(e_ne_k)=e_k\varphi_{n,k}$ for some unit vector $\varphi_{n,k}\in L_2(\mathbb{T},\mu)$.

Matrix elements are now

$$\begin{aligned}\langle (e_n e_k)|F(X)(e_m e_l)\rangle &= \langle (e_n e_k)|W_2^* P(X) W_2(e_m e_l)\rangle \\ &= \langle W_2(e_n e_k)|P(X)W_2(e_m e_l)\rangle = \langle (e_k\varphi_{n,k})|P(X)(e_l\varphi_{m,l})\rangle \\ &= \langle \varphi_{n,k}|\varphi_{m,l}\rangle \int_X z^{l-k}\,\mathrm{d}\mu(z). \end{aligned} \tag{22}$$

Assume now that F is a normalized positive operator measure that satisfies condition (12), or, equivalently, conditions (14) and (15). This means that the matrix elements (20) and (22) are the same:

$$\langle \psi_{n,k}|\psi_{m,l}\rangle \int_X z^{n-m}\,\mathrm{d}\mu(z) = \langle \varphi_{n,k}|\varphi_{m,l}\rangle \int_X z^{l-k}\,\mathrm{d}\mu(z) \tag{23}$$

for all $n,m,k,l\in\mathbb{Z}$ and $X\in\mathcal{B}(\mathbb{T})$. From this we get $n-m=l-k$ and $\langle \psi_{n,k}|\psi_{m,l}\rangle = \langle \varphi_{n,k}|\varphi_{m,l}\rangle$.

We summarize the above construction in the following theorem.

Theorem 3: *Any normalized positive operator measure $F:\mathcal{B}(\mathbb{T})\to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ satisfying covariance condition (12) is of the form*

$$F(X) = \sum_{n,m,k,l\in\mathbb{Z}} \delta_{n-m,l-k}\langle \psi_{n,k}|\psi_{m,l}\rangle \int_X z^{n-m}\mathrm{d}\mu(z)\ \ |e_n e_k\rangle\langle e_m e_l| \tag{24}$$

for some set $(\psi_{n,k})_{n,k\in\mathbb{Z}}\subset L_2(\mathbb{T},\mu)$ of unit vectors.

We note that in (24) only the inner products of the vectors $\psi_{n,k}$ are relevant. Thus two sets of unit vectors $(\psi_{n,k})_{n,k\in\mathbb{Z}}$ and $(\eta_{n,k})_{n,k\in\mathbb{Z}}$ define the same positive operator measure exactly when

$$\delta_{n-m,l-k}\langle \psi_{n,k}|\psi_{m,l}\rangle = \delta_{n-m,l-k}\langle \eta_{n,k}|\eta_{m,l}\rangle$$

for all $n,m,k,l\in\mathbb{Z}$.

Example 1: The canonical spectral measure F_{can} of Eq. (13) written in the above form is simply

$$F_{\mathrm{can}}(X) = \sum_{n,m,k,l\in\mathbb{Z}} \delta_{n-m,l-k}\int_X z^{n-m}\mathrm{d}\mu(z)\ \ |e_n e_k\rangle\langle e_m e_l|,$$

showing that F_{can} can be defined by a set $(\psi_{n,k})_{n,k\in\mathbb{Z}}$, where $\psi_{n,k}=\psi$ for all $n,k\in\mathbb{Z}$ and ψ is any unit vector.

We are now ready to solve the covariance condition (6). Let $\mathcal{H}$ be a complex separable Hilbert space with an orthonormal basis $\{|n\rangle\}_{n\in\mathbb{N}}$, and $T:\mathcal{H}\otimes\mathcal{H}\to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ be a linear isometry with the property

$$T|n,m\rangle = e_n e_m, \ \text{ for all } \ n,m\in\mathbb{N}.$$

If $[0,2\pi)$ is identified with $\mathbb{T}$ by the mapping $\alpha\mapsto e^{i\alpha}$, then Θ can be regarded as a unitary representation of $\mathbb{T}\times\mathbb{T}$. Clearly, T intertwines representations Θ and U, $T\Theta=UT$. If $\widetilde{F}:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ satisfies the equation

$$\Theta(a,b)\widetilde{F}(X)\Theta(a,b)^* = \widetilde{F}(ab^{-1}X) \tag{25}$$

for all $a,b\in\mathbb{T}$, $X\in\mathcal{B}(\mathbb{T})$, then $F(X):=T\widetilde{F}(X)T^*$ is a normalized positive operator measure having property (12). Moreover, if $F:\mathcal{B}(\mathbb{T})\to\mathcal{L}(L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu))$ satisfies condition (12), then $X\to T^*F(X)T$ is a normalized positive operator measure acting in $\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ and satisfying (25). Using Theorem 3, one thus has the following result.

Theorem 4: *A normalized positive operator measure $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ is a phase difference observable if and only if*

$$E(X)=\sum_{n,m,k,l\in\mathbb{N}}\delta_{n-m,l-k}\langle\xi_{n,k}|\xi_{m,l}\rangle\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\mathrm{d}\theta\ \ |n,k\rangle\langle m,l|, \tag{26}$$

for some set of unit vectors $(\xi_{n,k})_{n,k\in\mathbb{N}}$ *of* $\mathcal{H}$.

In view of Remark 1, this result is the same as the one obtained in Sec. III. Since $T:\mathcal{H}\otimes\mathcal{H}\to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ is not surjective, there is no projection valued phase difference observable.

Remark 4: The moment operators $E^{(r)}, r\in\mathbb{N}$, of the phase difference observable E are defined as

$$E^{(r)}:=\int_0^{2\pi}\theta^r\mathrm{d}E(\theta)$$

and they are bounded self-adjoint operators. By direct calculation we get

$$\langle n,k|E^{(1)}|m,l\rangle=\delta_{n-m,l-k}\langle\xi_{n,k}|\xi_{m,l}\rangle\frac{i}{m-n},$$

when $n\neq m$. For $n=m$ one gets

$$\langle n,k|E^{(1)}|n,l\rangle=\pi\delta_{k,l}.$$

Thus the phase difference observable E is uniquely determined by its first moment operator $E^{(1)}$. This is notable since E is not projection valued. The same result holds also for phase observables; see Ref. 20 for a further discussion of this conundrum.

Similarly, the rth cyclic moment operator of E is defined as the operator $C_E^{(r)}$,

$$C_E^{(r)}:=\int_0^{2\pi}e^{ir\theta}\mathrm{d}E(\theta),\quad r\in\mathbb{N}.$$

They are easily determined to be

$$C_E^{(r)}=\sum_{n,l=0}^{\infty}\langle\xi_{n,l+r}|\xi_{n+r,l}\rangle|n,l+r\rangle\langle n+r,l|.$$

Since $C_E^{(1)}|0,0\rangle=0$, the first cyclic moment is not unitary. This is another way to see the already mentioned fact that there is no projection valued phase difference observable.

V. PHASE DIFFERENCE OBSERVABLE VERSUS DIFFERENCE OF PHASE OBSERVABLES

Till now we have characterized in two different ways the phase difference observables, and we have also constructed explicitly the difference of two phase observables. The following proposition characterizes those phase difference observables which are, that is, can be expressed as, the difference of two phase observables. Its proof is a direct comparison of formulas (2) and (26).

Proposition 1: Let $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H}\otimes\mathcal{H})$ *be a phase difference observable, characterized by a set* $(\xi_{n,k})_{n,k\in\mathbb{N}}$. *Observable* E *is a difference of two phase observables if and only if there are sequences* $(\varphi_n^1)_{n\in\mathbb{N}}$ *and* $(\varphi_n^2)_{n\in\mathbb{N}}$ *of unit vectors in* $\mathcal{H}$ *such that*

$$\delta_{n-m,l-k}\langle\xi_{n,k}|\xi_{m,l}\rangle=\delta_{n-m,l-k}\langle\varphi_n^1|\varphi_m^1\rangle\langle\varphi_k^2|\varphi_l^2\rangle \tag{27}$$

for all $n,k,m,l\in\mathbb{N}$.

The next example shows that there are phase difference observables that are not the difference of two phase observables. It also opens the question of finding physically meaningful conditions for Proposition 1.

Example 2: Fix an arbitrary unit vector $\psi\in\mathcal{H}$ and let $\theta_j, j=1,2,3,4$, be real numbers. Define $\xi_{0,2}=e^{i\theta_1}\psi$, $\xi_{2,2}=e^{i\theta_2}\psi$, $\xi_{0,4}=e^{i\theta_3}\psi$, $\xi_{2,4}=e^{i\theta_4}\psi$ and $\xi_{n,k}=\psi$ otherwise. Assume now that there are sequences $(\varphi_n^1)_{n\in\mathbb{N}}$ and $(\varphi_n^2)_{n\in\mathbb{N}}$ such that Eq. (27) holds. Then

$$e^{i\theta_4}=\langle\xi_{3,3}|\xi_{2,4}\rangle=\langle\varphi_3^1|\varphi_2^1\rangle\langle\varphi_3^2|\varphi_4^2\rangle=\frac{\langle\varphi_3^1|\varphi_2^1\rangle\langle\varphi_1^2|\varphi_2^2\rangle\langle\varphi_1^1|\varphi_0^1\rangle\langle\varphi_3^2|\varphi_4^2\rangle}{\langle\varphi_1^1|\varphi_0^1\rangle\langle\varphi_1^2|\varphi_2^2\rangle}$$
$$=\frac{\langle\xi_{3,1}|\xi_{2,2}\rangle\langle\xi_{1,3}|\xi_{0,4}\rangle}{\langle\xi_{1,1}|\xi_{0,2}\rangle}=e^{i(\theta_2+\theta_3-\theta_1)}.$$

Choosing the numbers θ_j in such a way that $e^{i\theta_4}\neq e^{i(\theta_2+\theta_3-\theta_1)}$ we thus get a contradiction.

From Eq. (27) it is also clear that two different pairs of phase observables may define the same phase difference observable.

We close this section with a terminological choice. We say that a phase difference observable is *canonical* if it is the difference of two canonical phase observables and we denote it by $E_{\mathrm{can}}^{\mathrm{diff}}$. Since the canonical phase observable E_{can} has the structure

$$E_{\mathrm{can}}(X)=\sum_{n\in\mathbb{N}}\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\mathrm{d}\theta|n\rangle\langle m|,$$

the explicit form of $E_{\mathrm{can}}^{\mathrm{diff}}$ can be read from both (2) and (24) with the involved inner products equal to one in each case. Some properties of the canonical phase difference observable are discussed in Secs. VI and VIII.

VI. RADON-NIKODÝM DERIVATIVES AND THE PHASE DIFFERENCE REPRESENTATION

Let T be a state (positive trace-one operator) on $\mathcal{H}\otimes\mathcal{H}$, let E be a phase difference observable with $\mathbf{c}$, and let $\widetilde{E}$ be a Θ-covariant observable with $\widetilde{\mathfrak{c}}$. Using similar methods as in Ref. 11, Sec. V, one can show that

$$\mathrm{tr}(TE(X))=\frac{1}{2\pi}\int_X g_T^E(\theta)\,\mathrm{d}\theta,\qquad X\in\mathcal{B}([0,2\pi)),$$

$$\mathrm{tr}(T\widetilde{E}(Z))=\frac{1}{(2\pi)^2}\int_Z\tilde{g}_T^{\widetilde{E}}(x,y)\,\mathrm{d}x\,\mathrm{d}y,\qquad Z\in\mathcal{B}([0,2\pi)\times[0,2\pi)),$$

where

$$g_T^E(\theta)=\sum_{n,m,k,l=0}^{\infty}c_{n,m,k,l}e^{i(n-m)\theta}\langle m,l|T|n,k\rangle,$$

$$\tilde{g}_T^{\widetilde{E}}(x,y)=\sum_{n,m,k,l=0}^{\infty}\tilde{c}_{n,m,k,l}e^{i(n-m)x+i(k-l)y}\langle m,l|T|n,k\rangle;$$

for $\mathrm{d}\theta$—almost all $\theta\in\mathbb{R}$, and for $\mathrm{d}x\mathrm{d}y$—almost all $(x,y)\in\mathbb{R}^2$. The above notations $\Sigma_{n,m,k,l=0}^{\infty}$ mean that for some increasing subsequences $(s_t)_{t\in\mathbb{N}}\subseteq\mathbb{N}$, $\Sigma_{n,m,k,l=0}^{\infty}=\lim_{t\to\infty}\Sigma_{n,m,k,l=0}^{s_t}$. It is easy to see that if E is constructed from $\widetilde{E}$ [that is, Eq. (9) holds], then

$$g_T^E(\theta)=\frac{1}{2\pi}\int_0^{2\pi}\tilde{g}_T^{\widetilde{E}}(x+\theta,x)\mathrm{d}x.$$

Since $\mathcal{H}$ is isomorphic with the Hardy space H^2 of the unit circle spanned by the vectors e_n, $n \in \mathbb{N}$, one can consider any $\psi \in \mathcal{H}$ as an element of H^2, that is, as a function (or equivalence class of functions). Using this interpretation, for any $\varphi, \psi \in \mathcal{H}$ and $X \in \mathcal{B}([0,2\pi))$, one may write

$$\langle \varphi \otimes \psi | E^{\mathrm{diff}}_{\mathrm{can}}(X) \varphi \otimes \psi \rangle = \frac{1}{2\pi} \int_X \frac{1}{2\pi} \int_0^{2\pi} |\varphi(x+\theta)|^2 |\psi(x)|^2 \mathrm{d}x \mathrm{d}\theta. \tag{28}$$

This phase difference distribution was first suggested by Barnett and Pegg.[12,13]

VII. CLASSICAL LIMIT

Like in the one-mode case,[9] it is easy to show that for any operator measure $E: \mathcal{B}([0,2\pi)) \to \mathcal{L}(\mathcal{H} \otimes \mathcal{H})$ the condition

$$\langle z_1 e^{i\alpha}, z_2 e^{i\beta} | E(X) | z_1 e^{i\alpha}, z_2 e^{i\beta} \rangle = \langle z_1, z_2 | E(X \dotplus (\alpha - \beta)) | z_1, z_2 \rangle,$$

$z_1, z_2 \in \mathbb{C}$, $\alpha, \beta \in \mathbb{R}$, $X \in \mathcal{B}([0,2\pi))$, equals the covariance condition (6) where $|z_1, z_2\rangle := |z_1\rangle \otimes |z_2\rangle$ is a two-mode coherent state.

Suppose that E^{diff} is the difference of phase observables E_1 and E_2 with $(c^1_{n,m})$ and $(c^2_{n,m})$, respectively. If, for example, $\lim_{n\to\infty} c^2_{n,n+k} = e^{ik\alpha}$ for all $k \geqslant 1$, $\alpha \in [0,2\pi)$, then for any continuous function $g: [0,2\pi] \to \mathbb{C}$

$$\lim_{\substack{|z|\to\infty \\ \arg z \ \text{fixed}}} \int_0^{2\pi} g(x) \mathrm{d}\langle z | E_2(x) | z \rangle = g(\arg z - \alpha)$$

(see Ref. 21, Th. 7.1). Let $g^{E_n}_{|z\rangle}: [0,2\pi] \to [0,\infty)$ be a continuous Radon-Nikodým derivative of the probability measure $X \mapsto \langle z | E_n(X) | z \rangle$, $n = 1,2$. Then

$$\lim_{\substack{|z_2|\to\infty \\ \arg z_2 \ \text{fixed}}} \frac{1}{2\pi} \int_0^{2\pi} g^{E_1}_{|z_1\rangle}(x+\theta) g^{E_2}_{|z_2\rangle}(x) \mathrm{d}x = g^{E_1}_{|z_1\rangle}(\theta + \arg z_2 - \alpha),$$

which implies the following proposition:

Proposition 2: For any $X \in \mathcal{B}([0,2\pi))$,

$$\lim_{\substack{|z_2|\to\infty \\ \arg z_2 \ \text{fixed}}} \langle z_1, z_2 | E^{\mathrm{diff}}(X) | z_1, z_2 \rangle = \langle z_1 | E_1(X + \arg z_2 - \alpha) | z_1 \rangle.$$

This means that, in the classical limit $|z_2| \to \infty$ of the second mode, the two-mode theory reduces to a single-mode theory. Moreover, if also $\lim_{n\to\infty} c^1_{n,n+k} = e^{ik\alpha'}$ for all $k \geqslant 1$, then

$$\lim_{\substack{|z_1|,|z_2|\to\infty \\ \arg z_1, \arg z_2 \ \text{fixed}}} \langle z_1, z_2 | E^{\mathrm{diff}}(X) | z_1, z_2 \rangle = \delta_{\arg z_1 - \arg z_2 - \alpha' + \alpha}(X),$$

where δ_p is a Dirac measure concentrated on the point p. This is the classical limit of the two-mode system.

Remark 5: It is known from the theory of homodyne detection[22,23] that when the reference mode is in a large amplitude coherent state $|z\rangle$, $|z| \gg 0$, the lowering operator a of the reference mode can be replaced with the "classical" observable $z\,I$ in practical calculations. This means that the energy and the phase of the reference field are well known and fixed. A similar result also holds for the difference of phase observables, as well.

Let $\alpha \in [0,2\pi)$ and define a *fixed-phase observable*

$$F_\alpha : \mathcal{B}([0,2\pi)) \to \mathcal{L}(\mathcal{H}), \quad X \mapsto \delta_\alpha(X)\, I$$

where δ_α is the Dirac measure concentrated on α. The fixed-phase observable F_α is the spectral measure of a self-adjoint operator αI and, thus, it is not a phase observable. If we choose the phase observable E_2 to be the fixed-phase observable F_α (this can be done similarly as in the case of two phase observables although F_α is not covariant), then $E^{\mathrm{diff}}(X) = E_1(X \dot{+} \alpha) \otimes I$, that is, the "phase difference" E^{diff} and the single-mode phase E_1 are practically the same observables (up to unitary equivalence or the choice of the reference phase α).

VIII. BAN'S THEORY

In a series of papers[14–16] Ban has proposed a unitary two-mode phase operator in relation to the number difference. To discuss Ban's theory in the present context, consider the number difference $\Delta N = \Sigma_{k\in\mathbb{Z}} k P_k^\Delta$ defined in Sec. II. All the eigenspaces $\mathcal{H}_k := P_k^\Delta(\mathcal{H}\otimes\mathcal{H})$ are infinite dimensional and the vectors $\{|k+n,n\rangle\}_{n\geqslant \max\{0,-k\}}$ constitute an orthonormal basis of $\mathcal{H}_k$. One may thus define a unitary operator D on $\mathcal{H}\otimes\mathcal{H}$ so that, for each $k\in\mathbb{Z}$, $D(\mathcal{H}_k) = \mathcal{H}_{k-1}$. To exhibit such an operator we rename the basis vectors using the notation of Ban:

$$|k,n\rangle\!\rangle := \begin{cases} |n+k,n\rangle, & k \geqslant 0, \\ |n,n-k\rangle, & k < 0. \end{cases}$$

Then, for any $k\in\mathbb{Z}$, the spectral projection P_k^Δ can be expressed as $P_k^\Delta = \Sigma_{n\in\mathbb{N}} |k,n\rangle\!\rangle\langle\!\langle k,n|$, and one may choose, for instance,

$$D = \sum_{k\in\mathbb{Z}} \sum_{n\in\mathbb{N}} |k-1,n\rangle\!\rangle\langle\!\langle k,n|.$$

This is Ban's proposal for a phase operator. Writing

$$D = \int_0^{2\pi} e^{i\theta}\ \mathrm{d}B(\theta), \tag{29}$$

the spectral measure B of D has the form

$$B(X) = \sum_{k,l\in\mathbb{Z}} \sum_{n\in\mathbb{N}} \frac{1}{2\pi} \int_X e^{i(k-l)\theta} \mathrm{d}\theta\ |k,n\rangle\!\rangle\langle\!\langle l,n|.$$

Clearly, B is not phase shift covariant so that it is not a phase observable in the sense of Ref. 6 or 7. However, the spectral measure B fulfills the covariance condition

$$V_\Delta(\beta) B(X) V_\Delta(\beta)^* = B(X \dot{+} \beta)$$

for all $\beta\in\mathbb{R}, X\in\mathcal{B}([0,2\pi))$. This differs from the covariance condition (4) by the factor 2. Thus B is not a phase difference observable in the sense of Definition 1. The difference by the factor 2 in the covariance conditions satisfied by B and $E_{\mathrm{can}}^{\mathrm{diff}}$ is also reflected in the commutation properties of D and $C^{(1)}_{E_{\mathrm{can}}^{\mathrm{diff}}}$ with ΔN. Indeed, for all $k\in\mathbb{Z}$ and $n\in\mathbb{N}$,

$$[D,\Delta N]|k,n\rangle\!\rangle = D|k,n\rangle\!\rangle \tag{30}$$

whereas

$$[C^{(1)}_{E_{\mathrm{can}}^{\mathrm{diff}}}, \Delta N]|k,n\rangle\!\rangle = 2C^{(1)}_{E_{\mathrm{can}}^{\mathrm{diff}}}|k,n\rangle\!\rangle. \tag{31}$$

Notice also that the first cyclic moment $C^{(1)}_{E_{\mathrm{can}}}$ of the canonical phase observable E_{can} satisfies

$$[C_{E_{\mathrm{can}}}^{(1)}, N]|n\rangle = C_{E_{\mathrm{can}}}^{(1)}|n\rangle$$

for all $n \in \mathbb{N}$. The factor 2 in the covariance condition (4) and the commutation relation (31) is natural for a phase difference observable. It is also worthwhile to note that condition (4) has a projection valued solution.[18] The corresponding unitary operator is

$$\sum_{k\in\mathbb{Z}} \sum_{n\in\mathbb{N}} |k-2,n\rangle\rangle\langle\langle k,n|.$$

Compared to (29), here is again 2 instead of 1.

Although spectral measure B is neither a phase observable nor a phase difference observable, it has the following relation to canonical phase observable. When the second mode is in the vacuum state and the first mode is in an arbitrary state T, then

$$\mathrm{tr}(T\otimes|0\rangle\langle 0|\, B(X)) = \mathrm{tr}(TE_{\mathrm{can}}(X)), \qquad X \in \mathcal{B}([0,2\pi)).$$

IX. DISCUSSION

The first phase difference operators studied in the literature were suggested by Susskind and Glogower[24] (see also Refs. 25 and 26). Their operators were the so-called cosine and sine phase difference operators which can be represented as $C_{12} = \int_0^{2\pi} \cos\theta \, \mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)$ and $S_{12} = \int_0^{2\pi} \sin\theta \, \mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)$, respectively. The operators C_{12} and S_{12} do not commute, and their spectra are the interval $[-1,1]$, including a countable dense set of eigenvalues.[24–26]

Lévy-Leblond[27] defined the relative exponential phase operator $\int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}(\theta) \otimes \int_0^{2\pi} e^{-i\theta}\mathrm{d}E_{\mathrm{can}}(\theta) = \int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)$ by analogy with the classical expression $e^{i(\theta_1-\theta_2)} = e^{i\theta_1}e^{-i\theta_2}$. The operator $\int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)$ is not unitary but it is associated with the polar decomposition of $a\otimes a^*$ in the following way: using $|a\otimes a^*| = \sqrt{N\otimes(N+I)}$,

$$a\otimes a^* = \int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)\, \sqrt{N\otimes(N+I)}.$$

We can add an extra operator $T := \Sigma_{n=0}^{\infty}|n\rangle\langle 0|\otimes|0\rangle\langle n|$ to $\int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta)$ and it still satisfies the polar decomposition relation of $a\otimes a^*$. When doing this we get a unitary operator $\mathcal{E}_{12} := \int_0^{2\pi} e^{i\theta}\mathrm{d}E_{\mathrm{can}}^{\mathrm{diff}}(\theta) + T$ and, thus, a self-adjoint operator Φ_{12} such that $\mathcal{E}_{12} = e^{i\Phi_{12}}$. Obviously, the operator Φ_{12} is not the first moment operator of a covariant phase difference observable. Luis and Sánchez-Soto have shown[28] that the point spectrum of Φ_{12} consists of eigenvalues $\{2\pi r/(n+1) | n \in \mathbb{N},\ r = 0,1,\ldots,n\} \subset [0,2\pi)$, the closure of this set being $[0,2\pi]$. When the second mode is in a large amplitude coherent state $|z\rangle$, the spectral measure of Φ_{12} gives essentially the same results as E_{can} (or the difference of E_{can} and $F_{\arg z}$).[28,29]

Finally, we note that in eight-port homodyne detection the measurement data is always discrete. Only in the limit of large intensity of the known fixed-phase reference oscillator the data becomes (essentially) ''continuous,'' giving rise to the phase observable $E_{|0\rangle}$. Thus, strictly speaking eight-port homodyne detection cannot be described as a measurement of the phase difference observable in *two* arbitrary signal fields. However, using two eight-port homodyne detectors with the same large amplitude fixed-phase reference field one can measure the difference of the two phase observables $E_{|0\rangle}$ and $E_{|0\rangle}$.[30]

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Some integrable systems in nonlinear quantum optics

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(Received 30 August 2002; accepted 17 October 2002)

In the paper we investigate the theory of quantum optical systems. As an application we integrate and describe the quantum optical systems which are generically related to the classical orthogonal polynomials. The family of coherent states related to these systems is constructed and described. Some applications are also presented. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1530756]

I. INTRODUCTION

Quantum optics affords a large amount of very interesting physical phenomena having important application at the same time. Our aim is to formulate the theory of these phenomena and elucidate their connection with the theory of orthogonal polynomials. This allows us to use the last one for the rigorous integration of some nonlinear quantum optical models describing the interaction of the finite number of modes of electromagnetic field with nonlinear medium. Let us mention that, in quantum optical literature (see, e.g., Refs. 3, 5, and 13–15), the solutions of the models of this type are usually approached by approximative or semiclassical methods.

In Sec. II we deduce from natural and not restrictive assumptions, the general form [see (2.35)] of the Hamiltonian $\mathbf{H}_I$ describing the interaction of the finite number of modes of electric field with the matter. Later on, in Sec. III, we investigate the quantum reduction method which allows us to describe the quantum optical systems by the use of the theory of orthogonal polynomials (see Refs. 1, 2, and 22). We also show that the reduced system is related to some quantum algebras, [see relations (3.27)]. These algebras were investigated in Ref. 20, where their relations to the theory of special and q-special functions were shown.

Having the spectral measure of the interaction Hamiltonian, which is, for example, the case if the model under consideration is related to the classical orthogonal polynomials or their q-deformation, see Refs. 22 and 12, we can introduce spectral coherent states. They are direct generalizations of Glauber coherent states (corresponding to the Hermite polynomials) and squeezed states. In Sec. IV, we show that spectral coherent states admit the holomorphic representation for the Hamiltonians under consideration which supplements the spectral and Fock representations. This simplifies remarkably the calculation of many important physical characteristics of the described system.

The spectral coherent states should have some physical meaning which needs deeper understanding. In any case, they give the link of quantum optical systems with complex analytic and symplectic geometry. This opens the application of coherent states method, investigated in Refs. 20 and 21, to the problems of the theory of quantum optics.

In Sec. V, we give complete solution of the quantum systems [see (5.1)] related to the classical orthogonal polynomials.

Finally, in Sec. VI, we present the physical interpretation of the Hamiltonian given by (2.37) as the parametric modulator, which includes as special cases such quantum optical systems as nondegenerate parametric amplifier and the frequency up-converter (see Ref. 26).

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At the end we express our conviction that the proposed method will be helpful in better understanding of quantum optical problems.

II. QUANTUM ELECTROMAGNETIC FIELD IN NONLINEAR MEDIUM

Nonlinear optics deals with phenomena that occur as a consequence of the modification of the optical properties of a material system in the presence of light. Practically, only laser light is sufficiently intense to produce the measurable effects. By an optical nonlinearity we mean that the dipole moment per unit volume, or polarization $\vec{P}$, of a material system depends in a nonlinear way upon the strength of the applied electromagnetic field. As many authors do,[5,23] we assume that $\vec{P}$ depends only on the electric part $\vec{E}$ of the electromagnetic field $(\vec{E},\vec{B})$ i.e., $\vec{P}\equiv\vec{P}[\vec{E}]$. We assume moreover that this dependence is a functional one. Thus, in the most general case we can write

$$\vec{P}[\vec{E}](t,\vec{r})=\varepsilon_0\sum_{N=0}^{\infty}\int \mathrm{d}t_1\ \ \mathrm{d}^3\vec{r}_1\cdots\mathrm{d}t_N\ \ \mathrm{d}^3\vec{r}_N\vec{T}_{(N)}(t,\vec{r},t_1,\vec{r}_1,\ldots,t_N,\vec{r}_N)(\vec{E}(t_1,\vec{r}_1),\ldots,\vec{E}(t_N,\vec{r}_N)), \tag{2.1}$$

where the vector valued N-linear map $\vec{T}_{(N)}$ is called in optical literature Nth response tensor of the medium.[5]

The time-invariance principle, which says that the dynamical properties of the system are assumed to be unchanged by a translation of the time origin, leads to

$$\vec{T}_{(N)}(t,\vec{r},t_1,\vec{r}_1,\ldots,t_N,\vec{r}_N)=:\vec{R}_{(N)}(\vec{r},t_1-t,\vec{r}_1,t_2-t,\vec{r}_2,\ldots,t_N-t,\vec{r}_N). \tag{2.2}$$

The interaction of the electromagnetic field $(\vec{E},\vec{B})$ with a nonlinear medium characterized by polarization $\vec{P}$ can be described by the source-free Maxwell equations

$$\begin{aligned}\nabla\times\vec{E}&=-\ \frac{\partial}{\partial t}\vec{B},\\ \nabla\times\vec{B}&=\mu_0\frac{\partial}{\partial t}(\varepsilon_0\vec{E}+\vec{P}[\vec{E}]),\\ \nabla\cdot(\varepsilon_0\vec{E}+\vec{P}[\vec{E}])&=0,\\ \nabla\cdot\vec{B}&=0.\end{aligned} \tag{2.3}$$

Therefore the divergence of the Poynting vector $(1/\mu_0)\,\vec{E}\times\vec{B}$ takes the form

$$\frac{1}{\mu_0}\nabla\cdot(\vec{E}\times\vec{B})=-\frac{\partial}{\partial t}\left(\frac{1}{2\mu_0}\vec{B}^2+\frac{\varepsilon_0}{2}\vec{E}^2\right)-\vec{E}\cdot\frac{\partial\vec{P}}{\partial t}[\vec{E}], \tag{2.4}$$

where the quantity

$$u_0:=\frac{1}{2\mu_0}\vec{B}^2+\frac{\varepsilon_0}{2}\vec{E}^2 \tag{2.5}$$

is the energy density of the free electromagnetic field. Analogously, we define the interaction energy density u_1 by the equation

$$\frac{\partial u_I}{\partial t}:=\vec{E}\cdot\frac{\partial\vec{P}}{\partial t}[\vec{E}]. \tag{2.6}$$

The energy density

$$u(t,\vec{r}) := u_0(t,\vec{r}) + u_1(t,\vec{r}) \tag{2.7}$$

determines the Hamiltonian H of our system

$$H = H_0 + H_1, \tag{2.8}$$

where

$$H_0 = \int u_0(t,\vec{r})\, \mathrm{d}^3\vec{r} \tag{2.9}$$

is the Hamiltonian of the free electromagnetic field and the Hamiltonian

$$H_1 = \int u_1(t,\vec{r})\, \mathrm{d}^3\vec{r} \tag{2.10}$$

describes the interaction of electric field $\vec{E}$ with the medium under consideration.

In order to obtain an explicit formula for u_1 let us consider the electromagnetic field potential $\vec{A}$,

$$\vec{A}(t,\vec{r}) = \sum_{\lambda} \int \mathrm{d}^3\vec{k}[\vec{e}_{k,\lambda} A_\lambda(\vec{k}) e^{i(\omega_k t - \vec{k}\cdot\vec{r})} + \vec{e}^{\,*}_{k,\lambda} A^*_\lambda(\vec{k}) e^{-i(\omega_k t - \vec{k}\cdot\vec{r})}], \tag{2.11}$$

expressed in terms of Fourier modes, where the index $\lambda \in \{1,2\}$ labels the polarization of the field, which is described by the pair of unit vectors $\vec{e}_{k,1}$ and $\vec{e}_{k,2}$ orthogonal to the wave vector $\vec{k}$ (we choose the Coulomb gauge $\nabla\cdot\vec{A}=0$). Here we do not specify the form of the dispersion relation, so we assume that ω_k is any function of $|\vec{k}|$. In this gauge we have

$$\vec{E} = -\frac{\partial}{\partial t}\vec{A}, \qquad\qquad \vec{B} = \nabla\times\vec{A}. \tag{2.12}$$

Let us introduce the following simplifying notation:

$$\vec{e}^{\,\sigma}_{k,\lambda} := \begin{cases} -i\omega_k\, \vec{e}_{\,k,\lambda} & \text{for} \quad \sigma = 1, \\ i\omega_k\, \vec{e}^{\,*}_{\,k,\lambda} & \text{for} \quad \sigma = -1, \end{cases} \tag{2.13}$$

$$A^\sigma_\lambda(\vec{k}) := \begin{cases} A_\lambda(\vec{k}) & \text{for} \quad \sigma = 1, \\ A^*_\lambda(\vec{k}) & \text{for} \quad \sigma = -1. \end{cases} \tag{2.14}$$

We have now

$$\vec{E}(t,\vec{r}) = \sum_{\lambda,\sigma} \int \vec{e}^{\,\sigma}_{k,\lambda}\ A^\sigma_\lambda(\vec{k})\ e^{\sigma i(\omega_k t - \vec{k}\cdot\vec{r})}\, \mathrm{d}^3\vec{k} \tag{2.15}$$

and, therefore, (2.1) becomes

$$\vec{P}[\vec{E}](t,\vec{r}) = \sum_{N=0}^{\infty} \sum_{\sigma_1,\lambda_1} \cdots \sum_{\sigma_N,\lambda_N} \int \mathrm{d}^3\vec{k}_1 \cdots \mathrm{d}^3\vec{k}_N \quad e^{it\Sigma_{r=1}^N \sigma_r \omega_{k_r}} A^{\sigma_1}_{\lambda_1}(\vec{k}_1) \cdots A^{\sigma_N}_{\lambda_N}(\vec{k}_N)$$
$$\times \vec{\chi}_{(N)}(\vec{r},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N})(\vec{e}^{\,\sigma_1}_{k_1,\lambda_1},\ldots,\vec{e}^{\,\sigma_N}_{k_N,\lambda_N}), \tag{2.16}$$

where $\vec{\chi}_{(N)}(\vec{r},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N})$, is the Nth susceptibility tensor[5] defined by

$$\vec{\chi}_{(N)}(\vec{r},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N}) := \int \vec{R}_{(N)}(\vec{r},\tau_1,\vec{r}_1,\ldots,\tau_N,\vec{r}_N)e^{i\Sigma_{s=1}^N\sigma_s\omega_{ks}\tau_s}e^{-i\Sigma_{s=1}^N\sigma_s\vec{k}_s\cdot\vec{r}_s}\,\mathrm{d}\tau_1\,\mathrm{d}^3\vec{r}_1\cdots\mathrm{d}\tau_n\,\mathrm{d}^3\vec{r}_N. \tag{2.17}$$

Inserting (2.16) into (2.6) we find up to an additive constant that

$$\begin{aligned} u_1(t,\vec{r}) = \sum_{N=0}^{\infty} \sum_{\sigma_0,\lambda_0} \sum_{\sigma_1,\lambda_1} \cdots \sum_{\sigma_N,\lambda_N} \int \mathrm{d}^3\vec{k}_1\cdots\mathrm{d}^3\vec{k}_N \\ \times \vec{e}^{\sigma_0}_{k_0,\lambda_0}\cdot\vec{\chi}_{(N)}(\vec{r},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N})(\vec{e}^{\sigma_1}_{k_1,\lambda_1},\ldots,\vec{e}^{\sigma_N}_{k_N,\lambda_N}) \\ \times \frac{\Sigma_{r=1}^N\sigma_r\omega_{k_r}}{\Sigma_{s=0}^N\sigma_s\omega_{k_s}}e^{it\Sigma_{s=0}^N\sigma_s\omega_{k_s}}e^{-i\sigma_0\vec{k}_0\cdot\vec{r}}\; A^{\sigma_0}_{\lambda_0}(\vec{k}_0)A^{\sigma_1}_{\lambda_1}(\vec{k}_1)\cdots A^{\sigma_N}_{\lambda_N}(\vec{k}_N). \end{aligned} \tag{2.18}$$

In the quantization procedure the classical quantities $A^{\sigma}_{\lambda}(\vec{k})$ in (2.11) are replaced by the operators

$$\mathbf{a}^{\sigma}_{k,\lambda} := \begin{cases} \mathbf{a}_{k,\lambda} & \text{for} \quad \sigma=1, \\ \mathbf{a}^*_{k,\lambda} & \text{for} \quad \sigma=-1, \end{cases} \tag{2.19}$$

which satisfy the commutation relations of a free quantum field:

$$[\mathbf{a}^{\sigma}_{\lambda,k},\mathbf{a}^{\sigma'}_{\lambda',k'}] = \delta_{\lambda\lambda'}\delta(k-k')\frac{\sigma}{2}(1-\sigma\sigma'). \tag{2.20}$$

The products $A^{\sigma_0}_{\lambda_0}(\vec{k}_0)\cdots A^{\sigma_N}_{\lambda_N}(\vec{k}_N)$ in (2.16) and (2.18) are, moreover, replaced by the normally ordered products of corresponding operators, i.e., by $:\mathbf{a}^{\sigma_0}_{k_0,\lambda_0}\cdots\mathbf{a}^{\sigma_N}_{k_N,\lambda_N}:$.

In order to obtain the Hamiltonian it is enough to insert (2.19) into (2.18) and then (2.18) into (2.10). With the Hamiltonian of the free electromagnetic field,

$$\mathbf{H}_0 = \sum_{\lambda}\int \mathrm{d}^3\vec{k}\,\omega_k\mathbf{a}^*_{k,\lambda}\mathbf{a}_{k,\lambda}, \tag{2.21}$$

we obtain

$$\begin{aligned} \mathbf{H} = \mathbf{H}_0 + \sum_{N=0}^{\infty}\sum_{\sigma_0,\lambda_0}\cdots\sum_{\sigma_N,\lambda_N}\int \mathrm{d}^3\vec{k}_0\cdots\mathrm{d}^3\vec{k}_N e^{it\Sigma_{s=0}^N\sigma_s\omega_{k_s}}:\mathbf{a}^{\sigma_0}_{k_0,\lambda_0}\cdots\mathbf{a}^{\sigma_N}_{k_N,\lambda_N}: \\ \times\vec{e}^{\sigma_0}_{k_0,\lambda_0}\cdot\vec{\Theta}_{(N)}(\sigma_0,\vec{k}_0,\omega_{k_0},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N})(\vec{e}^{\sigma_1}_{k_1,\lambda_1},\cdots,\vec{e}^{\sigma_N}_{k_N,\lambda_N}), \end{aligned} \tag{2.22}$$

where

$$\vec{\Theta}_{(N)}(\sigma_0,\vec{k}_0,\omega_{k_0},\sigma_1,\vec{k}_1,\omega_{k_1}\cdots,\sigma_N,\vec{k}_N,\omega_{k_N}) := \frac{\Sigma_{r=1}^N\sigma_r\omega_{k_r}}{\Sigma_{s=0}^N\sigma_s\omega_{k_s}}\int \vec{\chi}_{(N)}(\vec{r},\sigma_1,\vec{k}_1,\omega_{k_1},\ldots,\sigma_N,\vec{k}_N,\omega_{k_N})e^{-i\sigma_0\vec{k}_0\cdot\vec{r}}\;\mathrm{d}^3\vec{r}. \tag{2.23}$$

Using the commutation relations (2.20) one can prove that

$$e^{-i\mathbf{H}_0 t}\mathbf{a}^{\sigma}_{k,\lambda}e^{i\mathbf{H}_0 t}=e^{i\sigma\omega_k t}\mathbf{a}^{\sigma}_{k,\lambda}. \tag{2.24}$$

Hence the Hamiltonian (2.8) becomes

$$\mathbf{H}=\mathbf{H}_0+e^{-i\mathbf{H}_0 t}\mathbf{H}_I e^{i\mathbf{H}_0 t}, \tag{2.25}$$

where due to (2.22)

$$\begin{aligned}\mathbf{H}_I=\sum_{N=0}^{\infty}\sum_{\sigma_0,\lambda_0}\cdots\sum_{\sigma_N,\lambda_N}\int \mathrm{d}^3\vec{k}_0\cdots\mathrm{d}^3\vec{k}_N :\mathbf{a}^{\sigma_0}_{k_0,\lambda_0}\cdots\mathbf{a}^{\sigma_N}_{k_N,\lambda_N}:\\ \times\vec{e}\ ^{\sigma_0}_{k_0,\lambda_0}\cdot\vec{\Theta}_{(N)}(\sigma_0,\vec{k}_0,\omega_{k_0},\sigma_1,\vec{k}_1,\omega_{k_1},\cdots,\sigma_N,\vec{k}_N,\omega_{k_N})(\vec{e}^{\sigma_1}_{k_1,\lambda_1},\cdots,\vec{e}^{\sigma_N}_{k_N,\lambda_N})\end{aligned} \tag{2.26}$$

does not depend on time, and therefore the solution of the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle=\mathbf{H}|\psi(t)\rangle \tag{2.27}$$

is given by

$$|\psi(t)\rangle=e^{-i\mathbf{H}_0 t}e^{-i\mathbf{H}_I t}|\psi(0)\rangle. \tag{2.28}$$

The operator

$$\mathbf{U}_0(t):=e^{-i\mathbf{H}_0 t} \tag{2.29}$$

is the free electromagnetic field evolution operator. The operator

$$\mathbf{U}_I(t):=e^{-i\mathbf{H}_I t} \tag{2.30}$$

is the evolution operator of the system in the interaction picture.

For the real models in quantum optics one assumes that the system under consideration contains a finite number of modes of electric field (see Refs. 3, 13, 14, and 23). This means that the label $(\vec{k},\lambda)$ in (2.26) and (2.21) takes a finite number of values

$$(\vec{k},\lambda)\equiv j\in\{0,1,\ldots,M\}, \tag{2.31}$$

and the integrals are reduced to finite sums over j:

$$\mathbf{H}_0=\sum_j \omega_j\mathbf{a}^*_j\mathbf{a}_j, \tag{2.32}$$

$$\mathbf{H}_I=\sum_{N=0}^{\infty}\sum_{\sigma_0,j_0}\cdots\sum_{\sigma_N,j_N}:\mathbf{a}^{\sigma_0}_{j_0}\cdots\mathbf{a}^{\sigma_N}_{j_N}:\vec{e}^{\sigma_0}_{j_0}\cdot\vec{\Theta}_{(N)}(\sigma_0,\omega_{j_0},\ldots,\sigma_N,\omega_{j_N})(\vec{e}^{\sigma_1}_{j_1},\ldots,\vec{e}^{\sigma_N}_{j_N}). \tag{2.33}$$

In this case the Hamiltonian (2.33) can be transformed into the form which is more useful for our aims. It is defined by the exchange of the normal ordering of the annihilation and creation operators into the one which we will call boson-number ordering in the sequel.

In order to define the **boson-number ordering** let us introduce the following notation for creation and annihilation operators.

$$\mathbf{a}^l := \begin{cases} \mathbf{a}^l & \text{for } l=1,2,\ldots, \\ 1 & \text{for } l=0, \\ (\mathbf{a}^*)^{-l} & \text{for } l=-1,-2,\ldots . \end{cases} \tag{2.34}$$

A product of m annihilation and n creation operators being in the same mode is said to be boson-number ordered if it is of the form $P(\mathbf{a}^*\mathbf{a})\mathbf{a}^{m-n}$, where P is a polynomial.

Changing the normal ordering in each term of the Hamiltonian (2.33) to the boson-number ordering $P(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\ \mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M}$ where P is a polynomial of $M+1$ variables and collecting the terms with the same factor $\mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M}$ we obtain

$$\mathbf{H}_I = \sum_{l_0,\ldots,l_M \in \mathbb{Z}} g_{l_0,\ldots,l_M}(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M}, \tag{2.35}$$

where $g_{l_0,\ldots,l_M}$ are functions of $(M+1)$-variables dependent on $\vec{\Theta}_{(N)}$. The Hamiltonian $\mathbf{H}_I$ is a symmetric operator if

$$[g_{l_0,\ldots,l_M}(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)]^* = g^*_{-l_0,\ldots,-l_M}(\mathbf{a}_0^*\mathbf{a}_0-l_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M-l_M). \tag{2.36}$$

In the next sections we restrict our considerations to the Hamiltonians of the form

$$\mathbf{H}_I = h(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M) + (g(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M} + \text{h.c.}). \tag{2.37}$$

Such form of the Hamiltonian is strictly related to the theory of orthogonal polynomials. The physical interpretation of this Hamiltonian is given in Sec. VI A.

III. REDUCTION OF THE HAMILTONIAN

In this section, we briefly describe the decomposition of the Hilbert space $\mathcal{H}$ spanned by elements of the orthonormal Fock basis

$$\mathcal{B}_F = \left\{ |n_0,\ldots,n_M\rangle := \frac{1}{\sqrt{n_0!\ldots n_M!}}(\mathbf{a}_0^*)^{n_0}\cdots(\mathbf{a}_M^*)^{n_M}|0\rangle : \quad n_0,\ldots,n_M \in \mathbb{N}\cup\{0\} \right\} \tag{3.1}$$

into invariant subspaces of the operators $\mathbf{H}_0$ and $\mathbf{H}_I$. The method of this decomposition is presented in details in Ref. 22. In such a way we obtain the reduction of the Hamiltonian $\mathbf{H}$.

The invariant subspaces of $\mathbf{H}_I$ are obtained in two steps. The first step is related to some family of integrals of motion; the second one is related to a family of pseudo-vacuum vectors.

Let us start with a few definitions:

$$\mathbf{A} := g(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\mathbf{a}_0^{l_0}\cdots\mathbf{a}_M^{l_M} \tag{3.2}$$

and

$$\mathbf{A}_i = \mathbf{A}_i^* := \sum_{j=0}^{M} \alpha_{ij}\ \mathbf{a}_j^*\mathbf{a}_j, \quad =0,1,\ldots,M, \tag{3.3}$$

where $\alpha=(\alpha_{ij})$ is a real $(M+1)\times(M+1)$-matrix satisfying the conditions

$$\det\alpha \neq 0, \tag{3.4}$$

$$\sum_{j=0}^{M} \alpha_{ij}l_j = \delta_{0i}. \tag{3.5}$$

The invertibility of the matrix α allows one to express the boson-number operators $\mathbf{a}_i^*\mathbf{a}_i$ by $\mathbf{A}_j$, which gives

$$\mathbf{H}_0=\sum_{j=0}^{M}\gamma_j\mathbf{A}_j \tag{3.6}$$

with real constants γ_j determined by the matrix α. In particular we have

$$\gamma_0=\sum_{i=0}^{M}\omega_j l_j. \tag{3.7}$$

Additionally

$$\mathbf{H}_I=\mathbf{H}_d(\mathbf{A}_0,\mathbf{A}_1,\ldots,\mathbf{A}_M)+\mathbf{A}+\mathbf{A}^* \tag{3.8}$$

with $\mathbf{H}_d$ uniquely determined by the function h and the matrix α. Using the canonical commutation relations for creation and annihilation operators one obtains

$$\mathbf{A}\mathbf{A}^*=\mathcal{G}(\mathbf{A}_0,\mathbf{A}_1,\ldots,\mathbf{A}_M), \tag{3.9}$$

$$\mathbf{A}^*\mathbf{A}=\mathcal{G}(\mathbf{A}_0-1,\mathbf{A}_1,\ldots,\mathbf{A}_M), \tag{3.10}$$

$$[\mathbf{A}_0,\mathbf{A}]=-\mathbf{A},\quad [\mathbf{A}_0,\mathbf{A}^*]=\mathbf{A}^*, \tag{3.11}$$

$$[\mathbf{A}_j,\mathbf{A}]=0,\quad j=1,\ldots,M, \tag{3.12}$$

$$[\mathbf{A}_i,\mathbf{A}_j]=0,\quad i,j=0,\ldots,M, \tag{3.13}$$

with the non-negative function $\mathcal{G}$ uniquely determined by g and α.

Direct calculations gives

$$[\mathbf{A}_j,\mathbf{H}_0]=[\mathbf{A}_j,\mathbf{H}_I]=0,\quad j=1,2,\ldots,M, \tag{3.14}$$

which means that operators $\mathbf{A}_1,\mathbf{A}_2,\ldots,\mathbf{A}_M$ are integrals of motion.

In order to reduce $\mathbf{H}_0$ and $\mathbf{H}_I$ to the common eigenspace of integrals of motion let us notice that the operators $\mathbf{A}^*\mathbf{A}$, $\mathbf{A}\mathbf{A}^*$, $\mathbf{A}_0,\ldots,\mathbf{A}_M$ are diagonal in the Fock basis $\mathcal{B}_F$. This, in particular, means that each vector $|n_0,\ldots,n_M\rangle\in\mathcal{B}_F$ is the eigenvector of the operators $\mathbf{A}_j$, $j=0,\ldots,M$, with eigenvalues given by

$$\lambda_j=\sum_{i=0}^{M}\alpha_{ji}n_i. \tag{3.15}$$

Moreover, the operators $\mathbf{A}_0,\ldots,\mathbf{A}_M$ form a system of commuting independent observables. In such a way we can use the sequences of eigenvalues $(\lambda_0,\lambda_1,\ldots,\lambda_M)$ as a new parametrization $\{|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle\}$ of the Fock basis elements. So we obtain

$$\mathbf{A}_j|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle=\lambda_j|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle,\quad j=0,\ldots,M. \tag{3.16}$$

Since $[\mathbf{A}_0,\mathbf{A}]=-\mathbf{A}$, then, from (3.10) and (3.9), we have

$$\mathbf{A}|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle=\sqrt{\mathcal{G}(\lambda_0-1,\lambda_1,\ldots,\lambda_M)}|\lambda_0-1,\lambda_1,\ldots,\lambda_M\rangle, \tag{3.17}$$

$$\mathbf{A}^*|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle=\sqrt{\mathcal{G}(\lambda_0,\lambda_1,\ldots,\lambda_M)}|\lambda_0+1,\lambda_1,\ldots,\lambda_M\rangle. \tag{3.18}$$

It is clear that the subspace $\mathcal{H}_{\lambda_1\ldots\lambda_M}$ of the Fock space $\mathcal{H}$ spanned by the eigenvectors $|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle$ with fixed $\lambda_1,\ldots,\lambda_M$ is $\mathbf{H}_0$ and $\mathbf{H}_I$-invariant and $\dim\mathcal{H}_{\lambda_1\ldots\lambda_M}=\infty$ if and only if all l_j in (3.2) are non-negative. The problem of integration of the system (2.25) is reduced to integration of the system described by the reduced Hamiltonian

$$\mathbf{H}_{0,\mathrm{red}}:=\gamma_0\mathbf{A}_0+\sum_{j=1}^{M}\gamma_j\lambda_j, \tag{3.19}$$

$$\mathbf{H}_{I,\mathrm{red}}:=\mathbf{H}_d(\mathbf{A}_0,\lambda_1,\ldots,\lambda_M)+\mathbf{A}+\mathbf{A}^*, \tag{3.20}$$

and therefore (up to additive constant)

$$\mathbf{H}_{\mathrm{red}}=\gamma_0\mathbf{A}_0+e^{-i\gamma_0\mathbf{A}_0t}\mathbf{H}_{I,\mathrm{red}}e^{i\gamma_0\mathbf{A}_0t}. \tag{3.21}$$

Now we go to the next step of the reduction. In order to make it let us define the pseudo-vacuum vector as such vector $|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle$ from the Fock basis in $\mathcal{H}_{\lambda_1,\ldots,\lambda_M}$ which is annihilated by the operator $\mathbf{A}$, i.e.,

$$\mathbf{A}|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle=0 \tag{3.22}$$

or equivalently

$$\mathcal{G}(\lambda_0-1,\lambda_1,\ldots,\lambda_M)=0. \tag{3.23}$$

In Ref. 22 it was shown that the set $\{\lambda_{0,l}\}_{l=1}^{K}:=\{\lambda_0:\ \mathbf{A}|\lambda_0,\lambda_1,\ldots,\lambda_M\rangle=0\}$ of the solutions of (3.22) is nonempty if in the definition (3.2) any l_i, $i=0,1,\ldots,M$, is greater then zero.

Now, if for simplicity, we introduce the notation

$$\begin{gathered}|n\rangle:=|\lambda_{0,l}+n,\lambda_1,\ldots,\lambda_M\rangle,\\ b(n):=\sqrt{\mathcal{G}(\lambda_{0,l}+n-1,\lambda_1,\ldots,\lambda_M)},\\ \mathbf{N}:=\mathbf{A}_0-\lambda_{0,l},\end{gathered} \tag{3.24}$$

then

$$\begin{gathered}\mathbf{N}|n\rangle=n|n\rangle,\\ \mathbf{A}|n\rangle=b(n)|n-1\rangle,\\ \mathbf{A}^*|n\rangle=b(n+1)|n+1\rangle.\end{gathered} \tag{3.25}$$

Thus we obtain that the space

$$\mathcal{F}:=\mathrm{span}\{|n\rangle,\ \ n=0,1,\ldots\} \tag{3.26}$$

is the irreducible representation space for the algebra $\mathcal{A}_{\mathrm{red}}$ generated by the operators $\mathbf{N},\mathbf{A}$, and $\mathbf{A}^*$, which satisfy the relations:

$$\begin{gathered}[\mathbf{N},\mathbf{A}]=-\mathbf{A},\quad [\mathbf{N},\mathbf{A}^*]=\mathbf{A}^*,\\ \mathbf{A}^*\mathbf{A}=b^2(\mathbf{N}),\\ \mathbf{A}\mathbf{A}^*=b^2(\mathbf{N}+1).\end{gathered} \tag{3.27}$$

These algebras were investigated in Ref. 21. The question when the dimension of $\mathcal{F}$ is finite or infinite was discussed in detail in Ref. 22. Here we assume that $\dim \mathcal{F}=\infty$. After restriction to $\mathcal{F}$, the Hamiltonians (3.19) and (3.20) belongs to $\mathcal{A}_{\mathrm{red}}$ and take the form (up to additive constant)

$$\mathbf{H}_{0,\mathrm{red}}=\gamma_0\mathbf{N}, \tag{3.28}$$

$$\mathbf{H}_{I,\mathrm{red}}=h(\mathbf{N})+\mathbf{A}+\mathbf{A}^*, \tag{3.29}$$

where $h(\mathbf{N}):=\mathbf{H}_d(\mathbf{N}+\lambda_{0,I},\lambda_1,\ldots,\lambda_M)$. Thus the operators $\mathbf{H}_{0,\mathrm{red}}$, $\mathbf{H}_{I,\mathrm{red}}$ and consequently $\mathbf{H}_{\mathrm{red}}$ belong to the algebra $\mathcal{A}_{\mathrm{red}}$. In the Fock basis $\{|n\rangle,\ n=0,1,\ldots\}$ the operator $\mathbf{H}_{I,\mathrm{red}}$ assumes the three diagonal (Jacobi) form:

$$\mathbf{H}_{I,\mathrm{red}}|n\rangle=h(n)|n\rangle+b(n)|n-1\rangle+b(n+1)|n+1\rangle, \tag{3.30}$$

whereas $\mathbf{H}_{0,\mathrm{red}}$ is diagonal,

$$\mathbf{H}_{0,\mathrm{red}}|n\rangle=\gamma_0 n|n\rangle. \tag{3.31}$$

From now on we restrict our consideration to the space $\mathcal{F}$. In particular we restrict all operators discussed above to $\mathcal{F}$ and omit the index red for simplicity.

The evolution of the system given by (2.28) now takes the form

$$|\psi(t)\rangle=e^{-i\gamma_0\mathbf{N}t}e^{-i\mathbf{H}_I t}|\psi(0)\rangle, \tag{3.32}$$

and therefore for any operator $\mathbf{F}$ we have

$$\langle\psi(t)|\mathbf{F}\psi(t)\rangle=\langle\psi(0)|e^{i\mathbf{H}_I t}e^{i\gamma_0\mathbf{N}t}\mathbf{F}e^{-i\gamma_0\mathbf{N}t}e^{-i\mathbf{H}_I t}|\psi(0)\rangle. \tag{3.33}$$

For a special but interesting case this formula simplifies. Namely,

$$\langle\psi(t)|f(\mathbf{N})\ \psi(t)\rangle=\langle\psi(0)|\ e^{i\mathbf{H}_I t}f(\mathbf{N})e^{-i\mathbf{H}_I t}|\psi(0)\rangle, \tag{3.34}$$

$$\langle\psi(t)|f(\mathbf{A})\ \psi(t)\rangle=f(e^{-i\gamma_0 t})\langle\psi(0)|\ e^{i\mathbf{H}_I t}f(\mathbf{A})e^{-i\mathbf{H}_I t}|\psi(0)\rangle, \tag{3.35}$$

$$\langle\psi(t)|\ \mathbf{H}\ \psi(t)\rangle=\gamma_0\langle\psi(0)|\ e^{i\mathbf{H}_I t}\mathbf{N}e^{-i\mathbf{H}_I t}|\psi(0)\rangle+\langle\psi(0)|\ \mathbf{H}_I\psi(0)\rangle, \tag{3.36}$$

where f is an analytic function.

The next section is devoted to the detailed study of the operator $\mathbf{H}_I$ and one-parameter group $e^{-i\mathbf{H}_I t}$ generated by it.

IV. SPECTRAL AND COHERENT STATES REPRESENTATIONS

The operators $\mathbf{H}_I$ of the type (3.29) are very well known in the theory of orthogonal polynomials.[1,2,7] They are symmetric in $\mathcal{F}$ and, by (3.30), have a dense domain which consists of finite linear combinations of elements of the Fock basis. The deficiency indices of $\mathbf{H}_I$ are (0,0) or (1,1). One can prove that if $\Sigma_{n=1}^{\infty}1/b(n)=\infty$, then the operator $\mathbf{H}_I$ has deficiency indices (0,0), which is equivalent to its essential self-adjointness.

From now on we will assume that the deficiency indices of $\mathbf{H}_I$ are (0,0). Hence $\mathbf{H}_I$ admits a unique self-adjoint extension, which will be denoted by the same symbol. Moreover, $\mathbf{H}_I$ has simple spectrum. This fact allows us to identify the Fock space $\mathcal{F}$ with the Hilbert space of square integrable functions $L^2(\mathbb{R},d\sigma)$ of real variable $\omega\in\mathbb{R}$. The measure $d\sigma$ is determined by the spectral measure $\mathbf{d}E$ of the Hamiltonian $\mathbf{H}_I$ and is defined by the formula

$$d\sigma(\omega):=\langle 0|\mathbf{d}E(\omega)0\rangle. \tag{4.1}$$

Additionally one can prove that polynomials $\{\omega^n\}_{n=0}^{\infty}$ form a linearly dense subset in $L^2(\mathbb{R}, d\sigma)$. After the Gram–Schmidt orthonormalization of the basis $\{\omega^n\}_{n=0}^{\infty}$ we obtain an orthonormal set $\{P_n\}_{n=0}^{\infty}$ in $L^2(\mathbb{R}, d\sigma)$ called the orthonormal polynomial system. Notice that deg $P_n = n$.

The unitary isomorphism $\mathbf{U}: \mathcal{F} \to L^2(\mathbb{R}, d\sigma)$ of Hilbert spaces is given by

$$\mathbf{U}|\psi\rangle := \sum_{n=0}^{\infty} \langle n|\psi\rangle P_n . \tag{4.2}$$

According to the spectral theorem and (4.2) one has

$$(\mathbf{U} \circ f(\mathbf{H}_I) \circ \mathbf{U}^{-1})\, \psi(\omega) = f(\omega)\, \psi(\omega) \tag{4.3}$$

for $\psi \in L^2(\mathbb{R}, d\sigma)$ and any measurable function f. By (4.2) and (4.3) the expression (3.30) converts into the three-term recurrence formula

$$\omega P_n(\omega) = h(n) P_n(\omega) + b(n) P_{n-1}(\omega) + b(n+1) P_{n+1}(\omega) \tag{4.4}$$

for the system of orthonormal polynomials $\{P_n\}_{n=0}^{\infty}$. So by the spectral theorem in the notion of this orthonormal system, we have

$$\langle m|f(\mathbf{H}_I)\, n\rangle = \int f(\omega) P_m(\omega) P_n(\omega)\, \mathrm{d}\sigma(\omega). \tag{4.5}$$

In particular, for $f(\mathbf{H}_I) = (1/P_0^2)\, \mathbf{H}_I^k$ we obtain the moments μ_k of the measure (4.1):

$$\mu_k := \int \omega^k \mathrm{d}\sigma(\omega) = \frac{1}{P_0^2} \langle 0|\ \ \mathbf{H}_I^k\, |0\rangle. \tag{4.6}$$

Similarly, for $f(\mathbf{H}_I) = (1/P_0^2)\, |\mathbf{H}_I|^k$ we obtain the absolute moments $|\mu_k|$ of (4.1):

$$|\mu_k| := \int |\omega|^k\, \mathrm{d}\sigma(\omega) = \frac{1}{P_0^2} \langle 0|\ \ |\mathbf{H}_I|^k\ \ |0\rangle. \tag{4.7}$$

For the case under consideration the moments $\{\mu_k\}_{k=0}^{\infty}$ determine $\mathrm{d}\sigma$ in the unique way.[1]

From (4.3) and (4.5) one obtains that the evolution operator $e^{-i\mathbf{H}_I t}$, $t \in \mathbb{R}$, in the Hilbert space $L^2(\mathbb{R}, d\sigma)$ is given by

$$(\mathbf{U} \circ e^{-i\mathbf{H}_I t} \circ \mathbf{U}^{-1})\, \psi(\omega) = e^{-i\omega t} \psi(\omega) \tag{4.8}$$

and its mean value in the vacuum is realized by the characteristic function

$$\hat{\sigma}(t) := \int e^{-i\omega t} \mathrm{d}\sigma(\omega) = \frac{1}{P_0^2} \langle 0|e^{-i\mathbf{H}_I t}|0\rangle \tag{4.9}$$

of the measure $\mathrm{d}\sigma$ (compare with Ref. 10).

After these preliminary remarks we will show that apart from realizations of the Hamiltonian $\mathbf{H}_I$ in the Fock space $\mathcal{F}$ and in the Hilbert space $L^2(\mathbb{R}, \mathrm{d}\sigma)$ it is useful and natural to consider its realization in some Hilbert space which consists of square integrable holomorphic functions defined on an open subset of complex plane. To do it let us first prove the following:

Lemma 4.1: Let us assume that absolute moments $|\mu|_n$ are finite for all $n \in \mathbb{N} \cup \{0\}$ and they satisfy the condition

$$\overline{\lim_{n\to\infty}} \frac{\sqrt[n]{|\mu|_n}}{n} =: \frac{1}{eR} < +\infty. \tag{4.10}$$

Then there exists a maximal strip in $\mathbb{C}$*, which is open, connected and invariant under the one-parameter group of translations*

$$T_t z := z + t, \quad t \in \mathbb{R}, \tag{4.11}$$

such that the characteristic function $\hat{\sigma}(t)$ *can be holomorphically extended to it.*

The maximality of the strip means that $\hat{\sigma}(t)$ *cannot be extended to a larger set with the same properties.*

Proof: We prove firstly that characteristic function $\hat{\sigma}$ is analytic on the strip $|\mathrm{Im}\, z| < R$. One has

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}\hat{\sigma}(t) = (-i)^n \int e^{-it\omega}\omega^n \mathrm{d}\sigma(\omega) \tag{4.12}$$

for $n = 0,1,\ldots$. In order to prove (4.12) one proceeds by induction. The equality (4.12) is valid for $n = 0$. Let us assume that it is true for n. Then

$$\begin{aligned}\frac{\mathrm{d}^{(n+1)}}{\mathrm{d}t^{(n+1)}}\hat{\sigma}(t) &= \lim_{h\to\infty}\int \frac{e^{-i(t+h)\omega} - e^{-it\omega}}{h}\omega^n \ \mathrm{d}\sigma(\omega) \\ &= \int \lim_{h\to\infty}\frac{e^{-ih\omega}-1}{h}e^{-it\omega}\omega^n \ \mathrm{d}\sigma(\omega) = -i\int e^{-it\omega}\omega^{n+1}\mathrm{d}\sigma(\omega). \end{aligned} \tag{4.13}$$

Since

$$\left|\frac{e^{-ih\omega}-1}{h}\omega^n\right| \leqslant |\omega|^{n+1} \tag{4.14}$$

and $|\mu|_n$ is finite for $n = 0,1,\ldots$, we were able to use Lebesgue theorem in (4.13). For $h \in \mathbb{R}$ we have the estimate

$$\begin{aligned}\left|\hat{\sigma}(t+h) - \sum_{k=0}^{n-1}\frac{h^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}t^k}\hat{\sigma}(t)\right| &= \left|\hat{\sigma}(t+h) - \int \sum_{k=0}^{n-1}\frac{(-ih\omega)^k}{k!}e^{-it\omega}\,\mathrm{d}\sigma(\omega)\right| \\ &= \left|\int\left(e^{-i(t+h)\omega} - \sum_{k=0}^{n-1} e^{-it\omega}\frac{(-ih)^k}{k!}\omega^k\right)\mathrm{d}\sigma(\omega)\right| \\ &\leqslant \frac{1}{n!}\int |h\omega|^n \,\mathrm{d}\sigma(\omega) = \frac{|h|^n}{n!}|\mu|_n, \end{aligned} \tag{4.15}$$

where for the last inequality we used

$$\left|e^{-ih} - \sum_{k=0}^{n-1}\frac{(-ih)^k}{k!}\right| \leqslant \frac{|h|^n}{n!}. \tag{4.16}$$

By the Cauchy criterion and the Stirling formula,

$$n! = \sqrt{2\pi n}\, n^n e^{-n} e^{\Theta(n)}, \tag{4.17}$$

where $\Theta(n) < 1/12\, n$, the series $\Sigma_{n=0}^{\infty}|h|^n/n!\,|\mu|_n$ is convergent for $|h| < R$. This and (4.15) imply that Taylor expansion

$$\hat{\sigma}(t+z) = \sum_{k=0}^{\infty}\frac{z^k}{k!}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\hat{\sigma}(t) \tag{4.18}$$

is convergent for $|z|<R$. We have proved the analyticity of $\hat{\sigma}$ on the strip $|\mathrm{Im}\, z|<R$. So there exist a nonempty, maximal strip $\{z\in\mathbb{C}: 2r<\mathrm{Im}\, z<2s\}$, such that the characteristic function $\hat{\sigma}(t)$ can be holomorphically extended to it. We have shown, moreover, that this strip contains the real axis, i.e., $-\infty\leqslant 2r<0<2s\leqslant+\infty$. Q.E.D.

Let us consider a "half" of the strip $\{z\in\mathbb{C}: 2r<\mathrm{Im}\, z<2s\}$, i.e.,

$$\Sigma := \{z\in\mathbb{C}: r<\mathrm{Im}\, z<s\}. \tag{4.19}$$

As a consequence of Lemma 1 we can formulate the following.

Proposition 4.1: Under the assumptions of Lemma 4.1 the map

$$\widetilde{K}: \Sigma \ni z \mapsto e^{-iz\cdot} \in L^2(\mathbb{R}, d\sigma) \tag{4.20}$$

is holomorphic and its image $\widetilde{K}(\Sigma)$ is linearly dense in $L^2(\mathbb{R}, d\sigma)$.

Proof: In order to see that the function $e^{-iz\cdot}$ belongs to $L^2(\mathbb{R}, d\sigma)$ let us notice that

$$\int |e^{-iz\omega}|^2\, \mathrm{d}\sigma(\omega) = \int e^{-i(z-\overline{z})\omega}\, \mathrm{d}\sigma(\omega) = \hat{\sigma}(z-\overline{z}) < +\infty \tag{4.21}$$

for $(z-\overline{z})\in\{z\in\mathbb{C}: 2r<\mathrm{Im}\, z<2s\}$. Thus in the basis $\{P_n\}_{n=0}^{\infty}$ we have

$$\widetilde{K}(z) = e^{-iz\cdot} = \sum_{n=0}^{\infty} \hat{\sigma}_n(z) P_n(\cdot), \tag{4.22}$$

where the coefficients functions $\hat{\sigma}_n$ are holomorphic extensions of

$$\hat{\sigma}_n(t) := \int e^{-it\omega} P_n(\omega)\, \mathrm{d}\sigma(\omega) \tag{4.23}$$

onto the whole strip Σ. Thus the map $\widetilde{K}$ is a complex analytic map of the strip Σ into Hilbert space $L^2(\mathbb{R}, d\sigma)$.

In order to show that $\widetilde{K}(\Sigma)$ is linearly dense in $L^2(\mathbb{R}, d\sigma)$ let us notice that the monomials

$$\omega^n = i^n \frac{\mathrm{d}^n}{\mathrm{d}z^n} \widetilde{K}(z)(\omega)\big|_{z=0}, \tag{4.24}$$

where $n=0,1,\ldots$, belong to the linear closure of $\widetilde{K}(\Sigma)$. Therefore, they form a linearly dense subset of $L^2(\mathbb{R}, d\sigma)$ and the same property is shared by $\widetilde{K}(\Sigma)$. Q.E.D.

Combining (4.2) with (4.22) we obtain a holomorphic map

$$K := \mathbf{U}^{-1} \circ \widetilde{K}: \Sigma \ni z \mapsto |z\rangle := \sum_{n=0}^{\infty} \hat{\sigma}_n(z) |n\rangle \in \mathcal{F} \tag{4.25}$$

of Σ into Fock space $\mathcal{F}$. Following Refs. 20 and 21 we shall call $K: \Sigma \to \mathcal{F}$ the coherent states map related to the quantum system described by the Hamiltonian $\mathbf{H}_I$. The states $|z\rangle$, where $z\in\Sigma$, will be called **spectral coherent states**. The coherent states map has nice physical properties and, as we will show later, it is useful for the calculations of physical characteristics of the system.

By the formulas

$$\Omega := i \frac{\partial^2}{\partial\overline{z}\partial z} (\log \hat{\sigma}(z-\overline{z}))\ \ \mathrm{d}\overline{z}\wedge\mathrm{d}z = -\frac{1}{2}\frac{d^2}{dy^2}(\log\hat{\sigma}(2iy))\, \mathrm{d}x\wedge\mathrm{d}y, \tag{4.26}$$

where $z=x+iy$, we will define the symplectic form Ω on Σ. Using the mean value function

$$\langle \mathbf{H}_I \rangle_z := \frac{\langle z|\mathbf{H}_I|z\rangle}{\langle z|z\rangle} = -\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}y}\log \hat{\sigma}(2iy) \tag{4.27}$$

of the Hamiltonian in spectral coherent states $|z\rangle$, $z \in \Sigma$, we define the classical Hamiltonian system

$$X_{\langle \mathbf{H}_I \rangle_z} \lrcorner \Omega = d\langle \mathbf{H}_I \rangle_z \tag{4.28}$$

on the symplectic manifold (Σ,Ω). The Hamiltonian flow, tangent to the vector field $X_{\langle \mathbf{H}_I \rangle_z}$ is given by (4.11). Let us denote by $\mathbb{C}P(\mathcal{F})$ the complex projective Hilbert space modeled on the Fock space $\mathcal{F}$. Let Ω_{FS} denote Fubini-Study (1,1)-form on $\mathbb{C}P(\mathcal{F})$, (for the definition of Ω_{FS} consult, for example, Ref. 11). The form Ω_{FS} is closed and nonsingular. So, $(\mathbb{C}P(\mathcal{F}),\Omega_{FS})$ can be considered as a symplectic manifold which can be interpreted as the quantum phase space of the system described by the Hamiltonian $\mathbf{H}_I$.

Proposition 4.2: The projectivization $\mathcal{K}:\Sigma \to \mathbb{C}P(\mathcal{F})$, $\mathcal{K}(z) := \mathbb{C}|z\rangle$ of the coherent states map (4.25) is the holomorphic symplectic map, i.e.,

$$\mathcal{K}^* \Omega_{FS} = \Omega \tag{4.29}$$

and the diagram

$$\begin{array}{ccc} & \overset{\mathcal{K}}{} & \\ \Sigma & \to & \mathbb{C}P(\mathcal{F}) \\ T_t \uparrow & & \uparrow e^{-i\mathbf{H}_I t} \\ & \overset{\mathcal{K}}{} & \\ \Sigma & \to & \mathbb{C}P(\mathcal{F}) \end{array} \tag{4.30}$$

is commutative for any $t \in \mathbb{R}$.

Proof: The equality (4.29) can be checked by direct calculation. The commutativity of the diagram (4.30) follows from (4.22) by the use of the formulas for quantum (4.8) and classical (4.11) evolution of the system. Q.E.D.

Recapitulating: we see that the coherent states map maps symplectically the classical phase space Σ of the system $(\Sigma,\Omega,\langle \mathbf{H}_I \rangle_z)$ into the quantum phase space $\mathbb{C}P(\mathcal{F})$ of the system $(\mathbb{C}P(\mathcal{F}),\Omega_{FS},\mathbf{H}_I)$. It is equivariant with respect to the classical and the quantum flows. The mean value function $\langle \mathbf{H}_I \rangle_z$ of the quantum Hamiltonian $\mathbf{H}_I$ give the classical Hamiltonian of the system. So, the above picture is analogous to the one related to the harmonic oscillator (see Ref. 24). For the general theory of quantization and description of physical systems in terms of the coherent states map see Ref. 20. The model of the physical system considered here gives an important and interesting example illustrating the theory which was developed in Ref. 21.

Let us define **spectral annihilation operator** $\boldsymbol{\alpha}$ by the condition

$$\boldsymbol{\alpha}|z\rangle = z|z\rangle, \tag{4.31}$$

which means that $\boldsymbol{\alpha}$ has the spectral coherent states $|z\rangle$ as eigenvectors with eigenvalues $z \in \Sigma$. It is defined on the dense linear domain, spanned by spectral coherent states. The representation in $L^2(\mathbb{R},d\sigma)$ is given by

$$(\mathbf{U} \circ \boldsymbol{\alpha} \circ \mathbf{U}^{-1}\psi)(\omega) \equiv i\,\frac{d}{d\omega}\,\psi(\omega). \tag{4.32}$$

The domain $D(\mathbf{U} \circ \boldsymbol{\alpha} \circ \mathbf{U}^{-1})$ is given as a vector space of all polynomials.

According to Proposition 4.1, the spectral coherent states form a linearly dense subset in $\mathcal{F}$. Hence one can define antilinear monomorphism $\overline{\mathbf{U}}$,

$$\mathcal{F}\ni|\psi\rangle\mapsto\overline{\mathbf{U}}|\psi\rangle:=\langle\psi|K(\cdot)\rangle\in\mathcal{O}(\Sigma), \tag{4.33}$$

of the Fock space $\mathcal{F}$ into vector space $\mathcal{O}(\Sigma)$ of holomorphic functions on Σ. In such a way we obtain the third realization of Hilbert space of states, this time as the space of holomorphic functions $\overline{\mathbf{U}}(\mathcal{F})\subset\mathcal{O}(\Sigma)$ with the scalar product defined by

$$\langle\Phi|\Psi\rangle\equiv\langle\overline{\mathbf{U}}(|\phi\rangle),\overline{\mathbf{U}}(|\psi\rangle)\rangle:=\langle\psi|\phi\rangle, \tag{4.34}$$

where $\Psi=\overline{\mathbf{U}}|\psi\rangle$, $\Phi=\overline{\mathbf{U}}|\phi\rangle$.

Proposition 4.3: Let the measure

$$d\mu(\overline{z},z)=\mu(y)dxdy, \tag{4.35}$$

on Σ, $(z=x+iy)$ *be such that the weight function* μ *satisfies*

$$\frac{d\sigma}{d\omega}(\omega)\int_r^s dy\,\mu(y)e^{2y\omega}=1 \tag{4.36}$$

for $\omega\in supp\ d\sigma$.

Then the scalar product (4.34) can be expressed by the integral

$$\langle\psi|\phi\rangle=\int_\Sigma\overline{\Psi}(z)\Phi(z)\,d\mu(\overline{z},z). \tag{4.37}$$

Moreover, the kernel function

$$\langle z|v\rangle=\hat{\sigma}(v-\overline{z}) \tag{4.38}$$

is a reproducing kernel function with respect to the measure (4.35), i.e.

$$\Psi(v)=\int_\Sigma\hat{\sigma}(v-\overline{z})\Psi(z)\,d\mu(\overline{z},z) \tag{4.39}$$

for any $\Psi\in\overline{\mathbf{U}}(\mathcal{F})$.

Proof: In order to prove that (4.37) and (4.39) are valid for $d\mu(\overline{z},z)$ given by (4.35) and (4.36) let us observe that $d\mu(\overline{z},z)$ has the form (4.35) since the kernel $\hat{\sigma}(\cdot-\overline{z})$ is invariant with respect to the one-parameter group of translation (4.11). Hence we have

$$\begin{aligned}
&\int_\Sigma\hat{\sigma}(v-\overline{z})\hat{\sigma}(z-\overline{w})\,\mathrm{d}\mu(\overline{z},z)\\
&\quad=\int\mathrm{d}\sigma(\omega)\int\mathrm{d}\sigma(\omega')\int_{-\infty}^{\infty}\mathrm{d}x\int_r^s\mu(y)\mathrm{d}y e^{-iv\omega+i\overline{w}\omega'}e^{-ix(\omega'-\omega)}e^{y(\omega+\omega')}\\
&\quad=\int\mathrm{d}\sigma(\omega)\int\mathrm{d}\sigma(\omega')\,\delta(\omega-\omega')\int_r^s\mathrm{d}y\,\mu(y)e^{y(\omega+\omega')}e^{-iv\omega+i\overline{w}\omega'}\\
&\quad=\int\mathrm{d}\sigma(\omega)\int\frac{\mathrm{d}\sigma}{\mathrm{d}\omega}(\omega+\tau)\,\delta(\tau)\ \ \mathrm{d}\tau\int_r^s\mathrm{d}y\,\mu(y)e^{y(2\omega+\tau)}e^{-i(v-\overline{w})\omega}e^{i\overline{w}\tau}\\
&\quad=\int\mathrm{d}\sigma(\omega)\frac{\mathrm{d}\sigma}{\mathrm{d}\omega}(\omega)\int_r^s\mathrm{d}y\,\mu(y)e^{2y\omega}e^{-i(v-\overline{w})\omega}.
\end{aligned} \tag{4.40}$$

If μ satisfies (4.36), then (4.40) takes the form

$$\int \hat{\sigma}(v-\overline{z})\hat{\sigma}(z-\overline{w})\,\mathrm{d}\mu(\overline{z},z)=\hat{\sigma}(v-\overline{w}), \tag{4.41}$$

which the reproducing property. Q.E.D.

In the sequel, let us assume that $\overline{\mathbf{U}}(\mathcal{F})=L^2\mathcal{O}(\Sigma,d\mu)$, where $L^2\mathcal{O}(\Sigma,d\mu)$ denotes the Hilbert space of holomorphic functions which are square-integrable with respect to $d\mu$ on Σ. Due to this assumption $\overline{\mathbf{U}}$ is an anti-unitary map and the holomorphic functions

$$\overline{\mathbf{U}}|n\rangle=\langle n|z\rangle=\hat{\sigma}_n(z), \quad n=0,1,\ldots, \tag{4.42}$$

form an orthonormal basis in $L^2\mathcal{O}(\Sigma,d\mu)$.

One has the commutative diagram

$$\begin{array}{ccc} & \mathcal{F} & \\ \mathbf{U}\swarrow & & \searrow\overline{\mathbf{U}} \\ L^2(\mathbb{R},d\sigma) & \xrightarrow{\overline{\mathbf{U}}\circ\mathbf{U}^{-1}} & L^2\mathcal{O}(\Sigma,d\mu) \end{array} \tag{4.43}$$

where the anti-unitary map $\overline{\mathbf{U}}\circ\mathbf{U}^{-1}$ is given by

$$(\overline{\mathbf{U}}\circ\mathbf{U}^{-1}\psi)(z)=\int e^{-iz\omega}\overline{\psi}(\omega)\,\mathrm{d}\sigma(\omega), \tag{4.44}$$

where $\psi\in L^2(\mathbb{R},d\sigma)$. Thus the Hamiltonian is given by

$$(\overline{\mathbf{U}}\circ\mathbf{H}_I\circ\overline{\mathbf{U}}^{-1}\Psi)(z)\equiv i\frac{d}{dz}\Psi(z) \tag{4.45}$$

and is defined on the domain $D(\overline{\mathbf{U}}\circ\mathbf{H}_I\circ\overline{\mathbf{U}}^{-1})=\{\Psi\in L^2\mathcal{O}(\Sigma,d\mu)\colon (d/dz)\,\Psi\in L^2\mathcal{O}(\Sigma,d\mu)\}$.

In terms of the Hilbert space $L^2\mathcal{O}(\Sigma,d\mu)$ it is possible to find an explicit form of the creation operator $\boldsymbol{\alpha}^*$, i.e., Hermitian conjugate of the spectral annihilation operator $\boldsymbol{\alpha}$ defined by (4.31). We will call $\boldsymbol{\alpha}^*$ the **spectral creation operator**. Using (4.31) and (4.33), we obtain

$$(\overline{\mathbf{U}}\circ\boldsymbol{\alpha}^*\circ\overline{\mathbf{U}}^{-1}\Psi)(z)\equiv z\Psi(z). \tag{4.46}$$

Thus we see that the domain of $\overline{\mathbf{U}}\circ\boldsymbol{\alpha}^*\circ\overline{\mathbf{U}}^{-1}$ is given by

$$D(\overline{\mathbf{U}}\circ\boldsymbol{\alpha}^*\circ\overline{\mathbf{U}}^{-1})=\{\Psi\in L^2\mathcal{O}(\Sigma,d\mu)\colon z\Psi\in L^2\mathcal{O}(\Sigma,d\mu)\}. \tag{4.47}$$

Taking into the account the above considerations let us notice that the operator $\boldsymbol{\alpha}^*$ is described explicitly in the $L^2\mathcal{O}(\Sigma,d\mu)$-realization and the operator $\boldsymbol{\alpha}$ is explicitly given in $L^2(\mathbb{R},d\sigma)$-realization. They satisfy the canonical commutation relations

$$[\mathbf{H}_I,\boldsymbol{\alpha}]=[\mathbf{H}_I,\boldsymbol{\alpha}^*]=i \tag{4.48}$$

with the Hamiltonian $\mathbf{H}_I$, giving

$$[\mathbf{H}_I,\boldsymbol{\alpha}-\boldsymbol{\alpha}^*]=0, \tag{4.49}$$

i.e., the operator $\boldsymbol{\alpha}-\boldsymbol{\alpha}^*$ is an integral of motion for the system under consideration.

From a physical point of view [see (3.34)–(3.36)] it is important to describe the time evolution in interaction picture of the system, i.e., $e^{-i\mathbf{H}_I t}|\psi(0)\rangle$. To do this let us introduce the following notation for the matrix elements of $e^{-i\mathbf{H}_I t}$

$$\hat{\sigma}_{m,n}(t) := \langle m|e^{-i\mathbf{H}_I t}n\rangle = \int e^{-i\omega t}P_m(\omega)P_n(\omega)\,\mathrm{d}\sigma(\omega). \tag{4.50}$$

Note that

$$\hat{\sigma}_{m,n}(t) = P_m\left(i\frac{d}{dt}\right)\hat{\sigma}_n(t), \tag{4.51}$$

where $\hat{\sigma}_n(t)$ are given by (4.23) and they satisfy

$$\hat{\sigma}_n(t) = \frac{1}{P_0}\langle n|e^{-i\mathbf{H}_I t}0\rangle = P_n\left(i\frac{d}{dt}\right)\hat{\sigma}(t). \tag{4.52}$$

The interaction evolution in the space $\mathcal{F}$ is thus given by

$$e^{-i\mathbf{H}_I t}|\psi\rangle = \sum_{m,n=0}^{\infty}\langle m|\psi\rangle\hat{\sigma}_{m,n}(t)|n\rangle, \tag{4.53}$$

while in the space $L^2(\mathbb{R},d\sigma)$ the evolution is described by (4.8). In $L^2\mathcal{O}(\Sigma,d\mu)$-realization we have

$$(\overline{\mathbf{U}}\circ e^{-i\mathbf{H}_I t}\circ\overline{\mathbf{U}}^{-1})\Psi(z) = \Psi(z+t). \tag{4.54}$$

As a consequence of (4.50) and (4.54) we obtain the relation

$$\hat{\sigma}_{m,n}(z_1+z_2) = \sum_k \hat{\sigma}_{m,k}(z_1)\hat{\sigma}_{k,n}(z_2), \tag{4.55}$$

which for $m=0$ can be expressed in the form

$$\hat{\sigma}_n(z_1+z_2) = \sum_k \hat{\sigma}_{k,n}(z_1)\hat{\sigma}_k(z_2). \tag{4.56}$$

Moreover, putting $m=n=0$ in (4.55) we obtain the formulas (4.38) for the reproducing kernel.

At the end of Sec. III it was shown [see (3.34)–(3.36)] that the quantities

$$\langle\psi(0)|\,e^{i\mathbf{H}_I t}\,\mathbf{F}\,e^{-i\mathbf{H}_I t}\psi(0)\rangle \tag{4.57}$$

plays an important role if we consider the expectation values of the operator $\mathbf{F}$ on the time evolving state $|\psi(t)\rangle$ [see (2.28)].

The variety of the realizations of our model, namely, the $\mathcal{F}$, $L^2(\mathbb{R},d\sigma)$ and $L^2\mathcal{O}(\Sigma,d\mu)$ representations, allow us to give three equivalent formulas on (4.57)

$$\begin{aligned}\langle\psi(0)|e^{i\mathbf{H}_I t}\mathbf{F}e^{-i\mathbf{H}_I t}\,\psi(0)\rangle &= \sum_{m,n,k,l}\langle\psi(0)|m\rangle\hat{\sigma}^*_{m,n}(t)\langle n|\mathbf{F}\,k\rangle\hat{\sigma}_{k,l}(t)\langle l|\psi(0)\rangle\\ &= \int e^{-i\omega t}\overline{\psi(\omega)}(\mathbf{U}\circ\mathbf{F}\circ\mathbf{U}^{-1})(e^{i\omega t}\psi(\omega))\,d\sigma(\omega)\\ &= \int_{\Sigma}\overline{\Psi}(z+t)(\overline{\mathbf{U}}\circ\mathbf{F}\circ\overline{\mathbf{U}}^{-1})(\Psi(z+t))\,d\mu(z,\overline{z}),\end{aligned} \tag{4.58}$$

where $\psi=\mathbf{U}|\psi(0)\rangle$ and $\Psi=\overline{\mathbf{U}}|\psi(0)\rangle$. In this way we have a very strong instrument for calculations of many physical characteristics of the system under consideration.

In particular we have

$$e^{i\mathbf{H}_I t}\boldsymbol{\alpha}e^{-i\mathbf{H}_I t}=\boldsymbol{\alpha}+t \tag{4.59}$$

and therefore

$$\langle\psi(0)|e^{i\mathbf{H}_I t}\boldsymbol{\alpha}e^{-i\mathbf{H}_I t}\,\psi(0)\rangle=\langle\psi(0)|\boldsymbol{\alpha}\psi(0)\rangle+t\langle\psi(0)|\psi(0)\rangle. \tag{4.60}$$

V. INTEGRABLE SYSTEMS RELATED TO CLASSICAL ORTHOGONAL POLYNOMIALS

Here we shall investigate the classes of the physical systems with Hamiltonians of the form (3.30) with the coefficients $b(n)$ and $h(n)$ given in Table III in the Appendix. The three classes of Hamiltonian operators are related to Hermite, Laguerre and Jacobi polynomials. We choose one mode case for simplicity and the circumstances which make the reduction not necessary. Then the Hamiltonians are expressed in terms of usual creation and annihilation operators in the following form:

$$\mathbf{H}_I^{\mathrm{Her}}:=-\frac{a_0}{a_1}+\sqrt{-\frac{b_0}{a_1}}\;(\mathbf{a}+\mathbf{a}^*), \tag{5.1a}$$

$$\mathbf{H}_I^{\mathrm{Lag}}:=-\frac{b_1}{a_1}\mu-\frac{b_0}{b_1}-\frac{2b_1}{a_1}\mathbf{a}^*\mathbf{a}-\frac{b_1}{a_1}\sqrt{\mathbf{a}^*\mathbf{a}+\mu}\;\;\mathbf{a}-\frac{b_1}{a_1}\sqrt{\mathbf{a}^*\mathbf{a}+\mu+1}\;\;\mathbf{a}^*, \tag{5.1b}$$

$$\begin{aligned}\mathbf{H}_I^{\mathrm{Jac}}:=&\frac{2\mathbf{a}^*\mathbf{a}(a+b)(\mu+\nu-1)+2(\mathbf{a}^*\mathbf{a})^2(a+b)-2b\mu-2a\nu+\mu\nu(a+b)+b\mu^2+a\nu^2}{(\mu+\nu-2+2\mathbf{a}^*\mathbf{a})(\mu+\nu+2\mathbf{a}^*\mathbf{a})}\\&+(b-a)\sqrt{\frac{(\mu+\mathbf{a}^*\mathbf{a})(\nu+\mathbf{a}^*\mathbf{a})(\mu+\nu+\mathbf{a}^*\mathbf{a}-1)}{(\mu+\nu+2\mathbf{a}^*\mathbf{a}-1)(\mu+\nu+2\mathbf{a}^*\mathbf{a})^2(\mu+\nu+2\mathbf{a}^*\mathbf{a}+1)}}\;\;\mathbf{a}\\&+(b-a)\sqrt{\frac{(\mu+\mathbf{a}^*\mathbf{a}+1)(\nu+\mathbf{a}^*\mathbf{a}+1)(\mu+\nu+\mathbf{a}^*\mathbf{a})}{(\mu+\nu+2\mathbf{a}^*\mathbf{a}+1)(\mu+\nu+2\mathbf{a}^*\mathbf{a}+2)^2(\mu+\nu+2\mathbf{a}^*\mathbf{a}+3)}}\;\;\mathbf{a}^*.\end{aligned} \tag{5.1c}$$

The ranges of the parameters μ, ν, b_0, and a_1 are chosen such that the operators are well defined and are essentially self-adjoint. In $L^2(\mathbb{R},d\sigma)$ (i.e., spectral) representation the formulas (3.30) lead to three-term recurrence relation (4.4) [see also (A10)].

From Pearson equation [see (A5) and Table I in the Appendix] we obtain the expressions for measures:

$$d\sigma^{\mathrm{Her}}(\omega)=Ce^{(a_1/2b_0)(\omega+a_0/a_1)^2}\;\;d\omega\qquad\text{for}\qquad\omega\in\mathbb{R}, \tag{5.2a}$$

$$d\sigma^{\mathrm{Lag}}(\omega)=C\left(\omega+\frac{b_0}{b_1}\right)^{\mu-1}e^{(a_1/b_1)\,\omega}\;\;d\omega\qquad\text{for}\qquad\omega\in\left(-\frac{b_0}{b_1},\infty\right), \tag{5.2b}$$

$$d\sigma^{\mathrm{Jac}}(\omega)=C(\omega-a)^{\mu-1}(b-\omega)^{\nu-1}\;\;d\omega\qquad\text{for}\qquad\omega\in(a,b). \tag{5.2c}$$

In the holomorphic representation $L^2\mathcal{O}(\Sigma,d\mu)$ all Hamiltonians act as derivations: id/dz [see formulas (4.45)], but the difference between the systems is hidden in the reproducing measures $d\mu(\overline{z},z)=\mu(y)\,dxdy$, $(z=x+iy)$, and the choice of the domain Σ. The general case is described in Proposition 4.3. Here we solve Eq. (4.36) for $\mu(y)$ in the special class, namely, continuous functions except possibly finite number of points in every compact subset. The discontinuity points are assumed to be of first kind. Let us summarize the results in the following:
(**H**) **Hermite case:** $\Sigma=\mathbb{C}$ and

$$\mu^{\mathrm{Her}}(y)=\frac{1}{C}e^{-a_0^2/2b_0a_1}\sqrt{-\frac{a_1}{2b_0\pi}}\,e^{(2b_0/a_1)(y+a_0/2b_0)^2}, \tag{5.3a}$$

(**L**) **Laguerre case:** $\Sigma=\{z=x+iy\in\mathbb{C}: y<-a_1/2b_1\}$ and for $\mu>1$

$$\mu^{\mathrm{Lag}}(y)=\frac{2}{C\,\Gamma(\mu-1)}\,e^{b_0a_1/b_1^2}\left(-2y-\frac{a_1}{b_1}\right)^{\mu-2}e^{(2b_0/b_1)y}. \tag{5.3b}$$

For $\mu=1$ we obtain an isomorphism of $L^2\mathcal{O}(\Sigma,d\mu)$ with $H^2(D,d\lambda)$—the Hardy class of functions on the unit disc $D\subset\mathbb{C}$ with the measure $d\lambda$ supported on the circle $\partial D=\{e^{i\varphi}:\varphi\in[0,2\pi]\}$ and given by

$$d\lambda=\frac{1}{1-\sin\varphi}\,d\varphi. \tag{5.4}$$

(**J**) **Jacobi case:** $\Sigma=\mathbb{C}$ and for $\mu+\nu>3$

$$\mu^{\mathrm{Jac}}(y)=\begin{cases}\dfrac{2}{C}\,\dfrac{(b-a)^{1-(\mu+\nu)/2}}{\Gamma(\mu-1)}\,e^{-(b+a)y}(2y)^{(\mu+\nu)/2-2}\,W_{(\nu-\mu)/2,\,3/2-(\mu+\nu)/2}[2(b-a)y] & \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{for}\quad y>0, & \\ \dfrac{2}{C}\,\dfrac{(b-a)^{1-(\mu+\nu)/2}}{\Gamma(\nu-1)}\,e^{-(b+a)y}(-2y)^{(\mu+\nu)/2-2}\,W_{(\mu-\nu)/2,\,3/2-(\mu+\nu)/2}[-2(b-a)y] & \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{for}\quad y<0, & \end{cases} \tag{5.3c}$$

where $W_{\kappa,\lambda}(z)$ are confluent hypergeometric Whittaker's functions (for definition, see Ref. 4). This formula simplifies in the case $\mu=\nu$ corresponding to the Gegenbauer polynomials. The following statement is true for a larger domain of parameter μ, namely for $\mu>1$,

$$\mu^{\mathrm{Geg}}(y)=\frac{2}{C}\left(\frac{-2y}{b-a}\right)^{\mu-3/2}\quad e^{-(b+a)y}\,\frac{1}{\Gamma(\mu-1)\sqrt{\pi}}K_{\mu-3/2}((a-b)y) \tag{5.5}$$

with $K_\alpha(z)$ being the modified Bessel functions (for definition, see Ref. 4).

For all three cases one can find the explicit form of matrix elements of propagator (4.50). Because of the relations (4.52) and (4.51), we should display the characteristic functions (4.9) first:

$$\hat\sigma^{\mathrm{Her}}(z)=C\,\sqrt{-\pi\frac{2b_0}{a_1}}\,e^{a_0^2/2a_1b_0}\,e^{(b_0/2a_1)(z+i\,a_0/b_0)^2}, \tag{5.6a}$$

$$\hat\sigma^{\mathrm{Lag}}(z)=C\Gamma(\mu)\,e^{-b_0a_1/b_1^2}\left(-\frac{z}{i}-\frac{a_1}{b_1}\right)^{-\mu}e^{(b_0/b_1)iz}, \tag{5.6b}$$

$$\hat\sigma^{\mathrm{Jac}}(z)\equiv\hat\sigma_J(z;\mu,\nu)=C\,\frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)}(b-a)^{\mu+\nu-1}e^{-iaz}\,{}_1F_1\left(\begin{matrix}\mu\\ \mu+\nu\end{matrix};(a-b)iz\right). \tag{5.6c}$$

The symbols $\hat\sigma^{\mathrm{Jac}}(z;\mu,\nu)$ are introduced in order to simplify the next formulas. Using the Rodrigues formula [see (A8)] we obtain the explicit form of $\hat\sigma_n(z)$:

$$\hat\sigma_n^{\mathrm{Her}}(z)=c_n^{\mathrm{Her}}(ib_0z)^n\,\hat\sigma^{\mathrm{Her}}(z), \tag{5.7a}$$

$$\hat\sigma_n^{\mathrm{Lag}}(z)=c_n^{\mathrm{Lag}}\left(\frac{b_1z}{z+i\,a_1/b_1}\right)^n\frac{\Gamma(\mu+n)}{\Gamma(\mu)}\,\hat\sigma^{\mathrm{Lag}}(z), \tag{5.7b}$$

$$\hat{\sigma}_n^{\mathrm{Jac}}(z)=c_n^{\mathrm{Jac}}(ib_2z)^n\,\hat{\sigma}^{\mathrm{Jac}}(z;\mu+n,\nu+n). \tag{5.7c}$$

After a simple but tedious calculation we find

$$\hat{\sigma}_{m,n}^{\mathrm{Her}}(z)=e^{(b_0/2a_1)(z+i\,a_0/b_0)^2}e^{a_0^2/2a_1b_0}(iz)^{m+n}\sqrt{\left(-\frac{b_0}{a_1}\right)^{m+n}}\sqrt{m!n!}\sum_{k=0}^{min\{m,n\}}\frac{(a_1/b_0)^kz^{-2k}}{(m-k)!(n-k)!k!}, \tag{5.8a}$$

$$\hat{\sigma}_{m,n}^{\mathrm{Lag}}(z)=c_m^{\mathrm{Lag}}c_n^{\mathrm{Lag}}b_1^{m+n}\frac{\Gamma(\mu+m)\Gamma(\mu+n)}{\Gamma^2(\mu)}\,\hat{\sigma}^{\mathrm{Lag}}(z)$$
$$\times\sum_{k=0}^{m}\binom{m}{k}\left(\frac{ia_1}{b_1z+ia_1}\right)^k{}_2F_1\left(\begin{matrix}\mu+k,-n\\ \mu\end{matrix};\frac{ia_1}{ia_1+b_1z}\right), \tag{5.8b}$$

$$\hat{\sigma}_{m,n}^{\mathrm{Jac}}(z)=c_m^{\mathrm{Jac}}c_n^{\mathrm{Jac}}(-b_2)^{m+n}\sum_{k=0}^{m}\sum_{l=0}^{n}\binom{m}{k}\binom{n}{l}(-1)^{k+l}\frac{\Gamma(\mu+m)\Gamma(\mu+n)}{\Gamma(\mu+m-k)\Gamma(\mu+n-l)}$$
$$\times\frac{\Gamma(\nu+m)\Gamma(\nu+n)}{\Gamma(\nu+k)\Gamma(\nu+l)}\,\hat{\sigma}^{\mathrm{Jac}}(z;\mu+m+n-k-l,\nu+k+l). \tag{5.8c}$$

The physical quantities which are of great importance are the Hamiltonians $\mathbf{H}$ and $\mathbf{H}_I$, the creation $\mathbf{a}^*$ and annihilation $\mathbf{a}$ operators, and the occupation number operator $\mathbf{N}=\mathbf{a}^*\mathbf{a}$. In our case the operators $\mathbf{A}$, $\mathbf{A}^*$ are also important. They can be interpreted as the cluster annihilation and cluster creation operators. Similarly, the operators $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}^*$ which are related to the spectral coherent states map (4.25) are interesting, too. Their physical meaning is partially explained by the commutation relations (4.48). They are related to $\mathbf{H}_I$, $\mathbf{a}$ and $\mathbf{a}^*$ in the following way:

$$\boldsymbol{\alpha}^{\mathrm{Her}}=\frac{-i\,a_1}{\sqrt{-a_1b_0}}\mathbf{a}, \tag{5.9a}$$

$$(b_0+b_1\,\mathbf{H}^{\mathrm{Lag}})\boldsymbol{\alpha}^{\mathrm{Lag}}=-i\,b_1\,\mathbf{a}^*\mathbf{a}+i\sqrt{b_1^2(\mathbf{a}^*\mathbf{a}+\mu)}\;\;\mathbf{a}, \tag{5.9b}$$

$$(a-\mathbf{H}^{\mathrm{Jac}})(b-\mathbf{H}^{\mathrm{Jac}})\boldsymbol{\alpha}^{\mathrm{Jac}}=i\,\mathbf{a}^*\mathbf{a}\frac{b(2\mu-\nu+\mathbf{a}^*\mathbf{a}-1)+a(2\nu-\mu+\mathbf{a}^*\mathbf{a}-1)}{\mu+\nu+2\,\mathbf{a}^*\mathbf{a}-2}$$
$$-i\,\mathbf{H}^{\mathrm{Jac}}\mathbf{a}^*\mathbf{a}-i\frac{(b-a)(-\mu-\nu+\mathbf{a}^*\mathbf{a}-1)(\mu+\mathbf{a}^*\mathbf{a})(\nu+\mathbf{a}^*\mathbf{a})}{|b_2|(\mu+\nu+2\,\mathbf{a}^*\mathbf{a}-1)^2(\mu+\nu+2\,\mathbf{a}^*\mathbf{a})^3}$$
$$\times\sqrt{\frac{\mu+\nu+2\,\mathbf{a}^*\mathbf{a}+1}{(\mu+\nu+\mathbf{a}^*\mathbf{a}-1)}}\;\;\mathbf{a}. \tag{5.9c}$$

In the spectral representation of $\mathbf{H}_I$ the operator $\boldsymbol{\alpha}$ is given for all the cases by $id/d\omega$ but the conjugates are given by different formulas:

$$(\boldsymbol{\alpha}^{\mathrm{Her}})^*=-i\left(\frac{a_1}{b_0}\omega+\frac{a_0}{b_0}+\frac{d}{d\omega}\right), \tag{5.10a}$$

$$(\boldsymbol{\alpha}^{\mathrm{Lag}})^*=-i\left(\frac{a_1\omega+a_0-b_1}{b_1\omega+b_0}+\frac{d}{d\omega}\right)\qquad\text{for}\;\;\mu>1, \tag{5.10b}$$

$$(\boldsymbol{\alpha}^{\mathrm{Jac}})^*=-i\left(\frac{(a_1+2b_2)\omega+a_0-b_2(a+b)}{b_2(\omega-a)(b-\omega)}+\frac{d}{d\omega}\right)\qquad\text{for}\;\;\mu,\,\nu>1. \tag{5.10c}$$

In the holomorphic representation the operator $\boldsymbol{\alpha}^*$ is given by (4.46), i.e., as the operator of multiplication by the argument z. The operators $\boldsymbol{\alpha}^{\mathrm{Her}}$, $\boldsymbol{\alpha}^{\mathrm{Lag}}$ and $\boldsymbol{\alpha}^{\mathrm{Jac}}$ are pseudodifferential ones and we shall not express them explicitly here.

The occupation number operators $\mathbf{N}$ defined by (3.25) take in the spectral representation the following form:

$$\mathbf{N}^{\mathrm{Her}}=\left(\omega+\frac{a_0}{a_1}\right)\frac{d}{d\omega}+\frac{b_0}{a_1}\frac{d^2}{d\omega^2}, \tag{5.11a}$$

$$\mathbf{N}^{\mathrm{Lag}}=\left(\omega+\frac{a_0}{a_1}\right)\frac{d}{d\omega}+\left(\frac{b_1}{a_1}\omega+\frac{b_0}{a_1}\right)\frac{d^2}{d\omega^2}. \tag{5.11b}$$

For the Jacobi case $\mathbf{N}^{\mathrm{Jac}}$ we are able to write down only the relation

$$\mathbf{N}^{\mathrm{Jac}}(\mathbf{N}^{\mathrm{Jac}}-\mu-\nu-1)=(\omega-a)(b-\omega)\frac{d^2}{d\omega^2}+[(-\mu-\nu)\omega+\mu b+\nu a]\frac{d}{d\omega}. \tag{5.11c}$$

In the holomorphic representation $\mathbf{N}$ can be expressed as

$$\mathbf{N}^{\mathrm{Her}}=-\frac{b_0}{a_1}\left(z-i\frac{a_0}{b_0}\right)z+z\frac{d}{dz}, \tag{5.12a}$$

$$\mathbf{N}^{\mathrm{Lag}}=i\left(\frac{b_1}{a_1}\mu+\frac{b_0}{b_1}+i\frac{b_0}{a_1}z\right)z+\left(1+\frac{b_1}{a_1}i\,z\right)z\frac{d}{dz}. \tag{5.12b}$$

Now, we will present the expectation values on the following states, interesting from the physical point of view:

(i) occupation number states $|n\rangle$, $n\in\mathbb{N}\cup\{0\}$, i.e., the eigenstates of $\mathbf{N}$, $\mathbf{N}|n\rangle=n|n\rangle$;
(ii) Gaussian coherent states $|\zeta\rangle$, $\zeta\in\mathbb{C}$, i.e., the eigenstates of $\mathbf{a}$, $\mathbf{a}|\zeta\rangle=\zeta|\zeta\rangle$;
(iii) spectral coherent states $|z\rangle$, $z\in\Sigma$, i.e., the eigenstates of $\boldsymbol{\alpha}$, $\boldsymbol{\alpha}|z\rangle=z|z\rangle$.

Using the operators U and $\overline{U}$ one can realize these states in spectral or holomorphic representation, too [see (4.2), (4.20), (4.33), and (4.42)].

Of course the Hamiltonian $\mathbf{H}_I$ does not depend on time t and its mean values are given by

$$\langle\mathbf{H}_I\rangle_n=h(n), \tag{5.13}$$

$$\langle\mathbf{H}_I\rangle_\zeta=e^{-|\zeta|^2}\sum_{n=0}^{\infty}\frac{|\zeta|^{2n}}{n!}\left[h(n)+\frac{b(n+1)}{\sqrt{n+1}}(\overline{\zeta}+\zeta)\right], \tag{5.14}$$

$$\langle\mathbf{H}_I\rangle_z=-\frac{1}{2}\frac{d}{dy}\ln\hat{\sigma}(2iy),\quad y=\frac{z-\overline{z}}{2i}. \tag{5.15}$$

The indices n, ζ, z are related to the occupation number eigenstates, Gaussian coherent states, and spectral coherent states, respectively. The function $b(n)$ and $h(n)$ are given in Table III in the Appendix and $\hat{\sigma}(z)$ is presented in (5.7).

The mean values of the powers of the occupation number operator are given as follows:

$$\langle\mathbf{N}^l(t)\rangle_n=\sum_{k=0}^{\infty}|\hat{\sigma}_{n,k}(t)|^2n^l, \tag{5.16}$$

$$\langle \mathbf{N}^l(t)\rangle_\zeta = e^{-|\zeta|^2}\sum_{m,k,n}^{\infty}\frac{\zeta^n\overline{\zeta}^m}{\sqrt{m!n!}}k^l\overline{\hat{\sigma}_{m,k}(t)}\hat{\sigma}_{n,k}(t), \tag{5.17}$$

$$\langle \mathbf{N}^l(t)\rangle_z = \frac{1}{\hat{\sigma}(z-\overline{z})}\sum_{n=0}^{\infty}|\hat{\sigma}_n(z+t)|^2 n^l, \tag{5.18}$$

where $l\in\mathbb{N}$. It is interesting to rewrite the last formula for every polynomial class separately

$$\langle(\mathbf{N}^{\mathrm{Her}}(t))^l\rangle_z = e^{(b_0/a_1)|z+t|^2}\left(-\frac{b_0}{a_1}\right)|z+t|^2{}_{l-1}F_{l-1}\left(\begin{matrix}2,\ldots,2\\1,\ldots,1\end{matrix};-\frac{b_0}{a_1}|z+t|^2\right), \tag{5.19a}$$

$$\langle(\mathbf{N}^{\mathrm{Lag}}(t))^l\rangle_z = \frac{(-2(a_1/b_1)(z-\overline{z}/2i)+(a_1^2/b_1^2))^\mu|z+t|^2\mu}{|z+t-i(a_1/b_1)|^{2\mu+2}}{}_lF_{l-1}$$
$$\times\left(\begin{matrix}\mu+1,2\ldots,2\\1,\ldots,1\end{matrix};\left|\frac{z+t}{z+t-i(a_1/b_1)}\right|^2\right), \tag{5.19b}$$

$$\langle(\mathbf{N}^{\mathrm{Jac}}(t))^l\rangle_z = \frac{1}{\hat{\sigma}^{\mathrm{Jac}}(z-\overline{z})}\sum_{n=0}^{\infty}c_n^{\mathrm{Jac}^2}|b_2(z+t)|^{2n}|\hat{\sigma}^{\mathrm{Jac}}(z+t;\mu+n,\nu+n)|^2 n^l. \tag{5.19c}$$

We give now the formulas for the correlation functions:

$$\langle \mathbf{a}^{*\,r}(t)\mathbf{a}^s(t)\rangle_n = \sum_{m=0}^{\infty}\overline{\hat{\sigma}_{n,m+r}(t)}\hat{\sigma}_{n,m+s}(t)\frac{\sqrt{(m+r)!(m+s)!}}{m!}, \tag{5.20}$$

$$\langle \mathbf{a}^{*\,r}(t)\mathbf{a}^s(t)\rangle_\zeta = e^{-|\zeta|^2}\sum_{k,m,n=0}^{\infty}\frac{\overline{\zeta}^m\zeta^k}{\sqrt{m!k!}}\overline{\hat{\sigma}_{m,n+r}(t)}\hat{\sigma}_{n+s,k}(t)\frac{\sqrt{(n+r)!(n+s)!}}{n!}, \tag{5.21}$$

$$\langle \mathbf{a}^{*\,r}(t)\mathbf{a}^s(t)\rangle_z = \frac{1}{\hat{\sigma}(z-\overline{z})}\sum_{n=0}^{\infty}\overline{\hat{\sigma}_{n+r}(z+t)}\hat{\sigma}_{n+s}(z+t)\frac{\sqrt{(n+r)!(n+s)!}}{n!}. \tag{5.22}$$

Replacing the creation and annihilation operators $\mathbf{a}^*$, $\mathbf{a}$ by the cluster creation and the cluster annihilation operators $\mathbf{A}^*$ and $\mathbf{A}$ we obtain the functions which by analogy will be called the cluster correlation functions:

$$\langle \mathbf{A}^{*\,r}(t)\mathbf{A}^s(t)\rangle_n = \sum_{k,l=0}^{\infty}b(k+r)\ldots b(k+1)b(k+s)\cdots b(k+1)\overline{\hat{\sigma}_{n,k+r}(t)}\hat{\sigma}_{k+s,l}(t), \tag{5.23}$$

$$\langle \mathbf{A}^{*\,r}(t)\mathbf{A}^s(t)\rangle_\zeta = e^{-|\zeta|^2}\sum_{k,m,l=0}^{\infty}\frac{\overline{\zeta}^m\zeta^l}{\sqrt{m!l!}}b(k+r)\ldots b(k+1)$$
$$\times b(k+s)\cdots b(k+1)\overline{\hat{\sigma}_{m,k+r}(t)}\hat{\sigma}_{k+s,l}(t), \tag{5.24}$$

$$\langle \mathbf{A}^{*\,r}(t)\mathbf{A}^l(t)\rangle_z = \frac{1}{\hat{\sigma}(z-\overline{z})}\sum_{k=0}^{\infty}b(k+r)\ldots b(k+1)b(k+s)\cdots b(k+1)\overline{\hat{\sigma}_{k+r}(z+t)}\hat{\sigma}_{k+s}(z+t). \tag{5.25}$$

The time evolution of $\boldsymbol{\alpha}$ is given by (4.59). This allows us to express the time dependence of $\langle\boldsymbol{\alpha}^l(t)\rangle_\psi$, (where $|\psi\rangle$ is an arbitrary state and $l\in\mathbb{N}$), in terms of the mean values of some powers $\boldsymbol{\alpha}\equiv\boldsymbol{\alpha}(0)$ acting on the state $|\psi\rangle$:

$$\langle \boldsymbol{\alpha}^l(t)\rangle_\psi = \sum_{k=0}^{l} \binom{l}{k} t^k \langle \boldsymbol{\alpha}^{l-k}\rangle_\psi . \tag{5.26}$$

As a consequence we conclude that the dispersion $(\Delta\boldsymbol{\alpha}(t))_\psi = \sqrt{\langle\psi|[\boldsymbol{\alpha}^2(t) - \langle\psi|\boldsymbol{\alpha}(t)\psi\rangle^2]\psi\rangle}$ of the operator $\boldsymbol{\alpha}(t)$ in an arbitrary state $|\psi\rangle$ does not depend on time,

$$(\Delta\boldsymbol{\alpha}(t))_\psi \equiv (\Delta\boldsymbol{\alpha})_\psi . \tag{5.27}$$

The following expectations take especially simple form:

$$\langle \boldsymbol{\alpha}^l(t)\rangle_n = t^l, \tag{5.28}$$

$$\langle \boldsymbol{\alpha}^l(t)\rangle_z = (z+t)^l. \tag{5.29}$$

Let us now see what will happen when the intensity of electromagnetic field is sufficiently large (the light of a strong laser). This corresponds to the limit of the large n in the Hamiltonian (3.30) (see Table III in the Appendix, too). We get the following strong-field Hamiltonians $\mathbf{H}_s$:

$$\mathbf{H}_s^{\mathrm{Her}} = \sqrt{-\frac{b_0}{a_1}}(\mathbf{a}+\mathbf{a}^*), \tag{5.30a}$$

$$\mathbf{H}_s^{\mathrm{Lag}} = -2\frac{b_1}{a_1}\mathbf{a}^*\mathbf{a} - \frac{b_1}{a_1}(\sqrt{\mathbf{a}^*\mathbf{a}+1}\,\mathbf{a} + \sqrt{\mathbf{a}^*\mathbf{a}+2}\,\mathbf{a}^*), \tag{5.30b}$$

$$\mathbf{H}_s^{\mathrm{Jac}} = \frac{a+b}{2} + \frac{b-a}{4}\left(\frac{1}{\sqrt{\mathbf{a}^*\mathbf{a}+1}}\mathbf{a} + \frac{1}{\sqrt{\mathbf{a}^*\mathbf{a}+2}}\mathbf{a}^*\right). \tag{5.30c}$$

These Hamiltonians belong to the respective families given by (5.1). They are obtained in the Hermite case by putting $a_0 = 0$ in (5.1a), in the Laguerre case by putting $\mu = 1$ and $b_0 = -b_1^2/a_1$ in (5.1b), and in the Jacobi case by putting $\mu = \nu = \frac{3}{2}$ in (5.1c).

Let us recall the definition of the phase operator $\hat{\phi}$:[23]

$$\exp(i\hat{\phi}) := (\mathbf{a}^*\mathbf{a}+1)^{-1/2}\mathbf{a}, \tag{5.31}$$

$$\exp(-i\hat{\phi}) := \mathbf{a}^*(\mathbf{a}^*\mathbf{a}+1)^{-1/2}, \tag{5.32}$$

$$\cos(\hat{\phi}) := \tfrac{1}{2}(\exp(i\hat{\phi}) + \exp(-i\hat{\phi})). \tag{5.33}$$

We can now rewrite (5.30b) and (5.30c):

$$\mathbf{H}_s^{\mathrm{Lag}} = -\frac{b_1}{a_1}(2\mathbf{a}^*\mathbf{a} + 2\mathbf{a}^*\mathbf{a}\cos(\hat{\phi}) + \exp(i\hat{\phi})), \tag{5.34}$$

$$\mathbf{H}_s^{\mathrm{Jac}} = \frac{a+b}{2} + \frac{b-a}{2}\cos(\hat{\phi}). \tag{5.35}$$

So, in the Jacobi case in the strong-field limit, the Hamiltonian tends, up to a constant, to the cosine of the phase operator. This subcase does not depend on the choice of the ranges of the parameters μ, ν.

VI. A PHYSICAL REMARKS

A. Parametric modulator

In order to present some physical interpretations of the Hamiltonian (2.25) with $\mathbf{H}_I$ given by (2.37), let us rewrite it in the following form

$$\mathbf{H}_I=\sum_{j=0}^{M}\omega_j\mathbf{a}_j^*\mathbf{a}_j+h(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)+(e^{it\Sigma_{j=0}^{M}\omega_j\mathbf{a}_j^*\mathbf{a}_j}g(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M}$$
$$+[e^{it\Sigma_{j=0}^{M}\omega_j\mathbf{a}_j^*\mathbf{a}_j}g(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)\mathbf{a}_0^{l_0}\ldots\mathbf{a}_M^{l_M}]^*). \tag{6.1}$$

The first term, which is linear in photon number operators, describes the free field. The second term, which is an arbitrary function of these operators, may be treated as a generalization of the Kerr medium description, where $\mathbf{H}_I=(\chi/2)\,((\mathbf{a}^*\mathbf{a})^2-\mathbf{a}^*\mathbf{a})$, where χ is proportional to the third-order nonlinear susceptibility.[23] The terms of the type $h(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)$, after the appropriate choice of the function h, play an important role in the theory of the nondemolition measurement[26,19] and in the description of many other phenomena, e.g., the optical bistability effect.[9]

The last term in (6.1) one can interpret as a general form of the parametric modulator Hamiltonian. To motivate this interpretation let us recall the form of the Hamiltonian of nondegenerate parametric amplifier,[17,18]

$$\mathbf{H}=\omega_0\mathbf{a}_0^*\mathbf{a}_0+\omega_1\mathbf{a}_1^*\mathbf{a}_1+ig(e^{2i\omega t}\mathbf{a}_0\mathbf{a}_1-(e^{2i\omega t}\mathbf{a}_0\mathbf{a}_1)^*). \tag{6.2}$$

This Hamiltonian describes the case when the classical pump mode at frequency 2ω interacts in a nonlinear optical medium with two modes at frequency ω_0 and ω_1, such that $\omega_0+\omega_1=2\omega$. If the system starts in an initial Gaussian two-photon coherent state $|\zeta_0\zeta_1\rangle$, the mean photon number in 0-mode after time t is

$$\langle\mathbf{a}_0^*(t)\mathbf{a}_0(t)\rangle=|\zeta_0\cosh gt+\zeta_1^*\sinh gt|^2+\sinh^2 gt, \tag{6.3}$$

hence this mode is amplified. The next example is the Hamiltonian for the frequency up-converter,[26]

$$\mathbf{H}=\omega_0\mathbf{a}_0^*\mathbf{a}_0+\omega_1\mathbf{a}_1^*\mathbf{a}_1+\kappa(e^{i\omega t}\mathbf{a}_0^*\mathbf{a}_1+e^{-i\omega t}\mathbf{a}_0\mathbf{a}_1^*), \tag{6.4}$$

where $\omega=\omega_1-\omega_0$.

It is easy to compare (6.1) with (6.2) and with (6.4) and conclude that our Hamiltonian is a natural generalization of that describing parametric amplification. In order to understand that in general (6.1) describes not only amplification but also modulation, let us notice that due to (3.3) we can express the mean values $\langle\mathbf{a}_j^*(t)\mathbf{a}_j(t)\rangle$, $j=0,\ldots,M$, in terms of the mean values of the operators $\mathbf{A}_0(t),\ldots,\mathbf{A}_M(t)$. But $\mathbf{A}_1(t),\ldots,\mathbf{A}_M(t)$ are the integrals of the motion, so if our system starts at the initial state from the reduced subspace $\mathcal{F}$ [see (3.26)] we obtain

$$\langle\mathbf{a}_j^*(t)\mathbf{a}_j(t)\rangle=l_j\langle\mathbf{A}_0(t)\rangle+\beta_j, \tag{6.5}$$

where the constant β_j are uniquely determined by $\lambda_1,\ldots,\lambda_M$ and the matrix α. This means that the mean photon number in each mode is a linear function of $\langle\mathbf{A}_0(t)\rangle$ or, in other words, the strength of the light in each mode is modulated by the function $\langle\mathbf{A}_0(t)\rangle$. The modulation of the jth mode depends on the exponent l_j. The shape of the function $\langle\mathbf{A}_0(t)\rangle$ depends on the choice of the coupling function $g(\mathbf{a}_0^*\mathbf{a}_0,\ldots,\mathbf{a}_M^*\mathbf{a}_M)$ in (6.1) and the initial state of the system.

As an example of the modulation function $\langle\mathbf{A}_0(t)\rangle$ let us consider the situation when, after reduction, we obtain the case corresponding to Laguerre polynomials and the initial state is the spectral coherent state $|z\rangle$. From (5.19b) we obtain

$$\langle \mathbf{A}_0(t)\rangle_z = E|z+t|^2 + F, \tag{6.6}$$

where the real constants E,F depend on μ, a_1, b_1 and $\lambda_{0,l}$. In this example the modulation function is of parabolic shape. This means that in some interval of time we have the amplification and dumping of the light signal in others.

B. Generalized squeezed states

The special cases of the interaction evolution operators $e^{-i\mathbf{H}_I t}$ are the unitary displacement operators[16]

$$\mathbf{D}(\zeta) = \exp(\zeta \mathbf{a}^* - \overline{\zeta}\mathbf{a}), \quad \zeta \in \mathbb{C}, \tag{6.7}$$

the unitary squeeze operators[6]

$$\mathbf{S}(z) = \exp(\overline{z}\mathbf{a}^2 - z\mathbf{a}^{*2}), \quad z \in \mathbb{C}, \tag{6.8}$$

and the unitary two-mode squeeze operators[8]

$$\mathbf{T}(\xi) = \exp(\overline{\xi}\mathbf{a}_0\mathbf{a}_1 - \xi\mathbf{a}_0^*\mathbf{a}_1^*), \quad \xi \in \mathbb{C}. \tag{6.9}$$

This means that the Glauber coherent states and the squeezed states are special cases of the spectral coherent states defined in Sec. IV. In such a way, the two concepts of the notion of the coherent states meet each other in our framework. The first one, presented in Refs. 24, 16, 6, and 8, is related to the minimalization of the suitable uncertainty relations. The second one, presented in Refs. 20 and 21, is based on the symplectic embedding of the classical phase space of the system into the quantum phase space (equipped with the Fubini–Study symplectic form).

ACKNOWLEDGMENTS

We would like to thank Professor J. Tolar and Dr. Z. Hasiewicz for careful reading and suggestions that made our paper better. This work was supported in part by KBN Grant No. 2 PO3 A 012 19.

APPENDIX: CLASSICAL POLYNOMIALS

Here we present some facts from the theory of classical polynomials.[25]

Let us consider a pair of real polynomials $(A(\omega),B(\omega))$ of degree not greater than one and two, respectively

$$A(\omega) := a_1\omega + a_0, \qquad a_i \in \mathbb{R}, \tag{A1}$$

$$B(\omega) := b_2\omega^2 + b_1\omega + b_0, \qquad b_i \in \mathbb{R}. \tag{A2}$$

The Pearson equation associated with $(A(\omega),B(\omega))$ on the interval $(a,b)\subset\mathbb{R}$ $(-\infty \leqslant a < b \leqslant +\infty)$ is the differential equation for the weight function ϱ:

$$\frac{d}{d\omega}(\varrho B) = \varrho A \tag{A3}$$

with the boundary conditions

$$\varrho(a)B(a) = 0 = \varrho(b)B(b). \tag{A4}$$

Each family of classical orthogonal polynomials $\{\tilde{P}_n\}$ can be obtained by the Gram–Schmidt orthogonalization of the basis $\{\omega^n\}_{n=0}^{\infty}$ in $L^2(\mathbb{R},d\sigma)$, where

TABLE I. Pearson data and solutions of Pearson equation.

Pearson data $(A(\omega),\ B(\omega))$	(a,b)	Weight function $\varrho(\omega)$
$A^{\mathrm{Her}}(\omega)=a_1\omega+a_0$ $B^{\mathrm{Her}}(\omega)=b_0$	$(-\infty,\infty)$	$\varrho^{\mathrm{Her}}(\omega)=Ce^{a_1/2b_0(\omega+\ a_0/a_1)^2}$ where $C>0,\quad \frac{a_1}{b_0}<0$
$A^{\mathrm{Lag}}(\omega)=a_1\omega+a_0$ $B^{\mathrm{Lag}}(\omega)=b_1\omega+b_0$	$\left(-\frac{b_0}{b_1},\infty\right)$	$\varrho^{\mathrm{Lag}}(\omega)=C\left(\omega+\frac{b_0}{b_1}\right)^{\mu-1}e^{a_1/b_1\,\omega}$ where $C>0,\quad \frac{a_1}{b_1}<0,$ $\mu:=\frac{a_0b_1-b_0a_1}{b_1^2}>0$
$A^{\mathrm{Jac}}(\omega)=a_1\omega+a_0$ $B^{\mathrm{Jac}}(\omega)=b_2(\omega-a)(b-\omega)$	(a,b)	$\varrho^{\mathrm{Jac}}(\omega)=C(\omega-a)^{\mu-1}(b-\omega)^{\nu-1}$ where $C>0,\ a<b,\ b_2>0$ $\mu:=\frac{aa_1+a_0}{b_2(b-a)}>0,\quad \nu:=\frac{ba_1+a_0}{b_2(a-b)}>0$

$$d\sigma(\omega):=\begin{cases}0, & \omega<a,\\ \varrho(\omega)\,d\omega, & a\leqslant\omega\leqslant b,\\ 0, & \omega>b,\end{cases} \tag{A5}$$

and ϱ satisfies the Pearson equation with appropriately chosen polynomials $(A(\omega),B(\omega))$. Namely if $\deg B(\omega)=0$ (i.e., $b_2=b_1=0$), then we obtain the Hermite polynomials; if $\deg B(\omega)=1$ (i.e., $b_2=0,\ b_1\neq 0$), we obtain the Laguerre polynomials and if $\deg B(\omega)=2$ (i.e., $b_2\neq 0$), we obtain the Jacobi polynomials. In the last case the boundary conditions (A4) hold if and only if a and b are roots of $B(\omega)$. For solution of the Pearson equation in these cases, see Table I. Additional conditions enforced on $A(\omega)$ by (A4) are presented in this table, too.

By straightforward calculation one can prove that the family of polynomials $\{(d^k/d\omega^k)\,P_n(\omega)\}_{n=k}^{\infty},\ k\in\mathbb{N}$, is orthogonal in the space $L^2(\mathbb{R},d\sigma^{(k)})$, where

$$d\sigma^{(k)}(\omega):=B^k(\omega)\,d\sigma(\omega). \tag{A6}$$

The weight function $\varrho^{(k)}$ satisfies the Pearson equation on the interval (a,b) associated with $(A^{(k)}(\omega),B(\omega))$, where

TABLE II. Normalizing factor in Rodrigue's formulae (A8).

c_n—in Rodrigues' formula
$c_n^{\mathrm{Her}}=\left(Cn!\,(-a_1b_0)^n\sqrt{-\pi\frac{2b_0}{a_1}}\right)^{-1/2}$
$c_n^{\mathrm{Lag}}=\left(Cn!\,(-a_1b_1)^n\left(-\frac{b_1}{a_1}\right)^{\mu+n}\Gamma(\mu+n)e^{-a_1b_0/b_1^2}\right)^{-1/2}$
$c_n^{\mathrm{Jac}}=\left(Cn!\,b_2^{2n}(b-a)^{\mu+\nu+2n-1}\times\frac{\Gamma(\mu+n)\Gamma(\nu+n)}{(\mu+\nu+2n-1)\Gamma(\mu+\nu+n-1)}\right)^{-1/2}$

TABLE III. Coefficients in recurrence formula (A10).

$b(n),\ h(n)$
$b^{\mathrm{Her}}(n)=\sqrt{-\frac{b_0}{a_1}n}$
$h^{\mathrm{Her}}(n)=-\frac{a_0}{a_1}$
$b^{\mathrm{Lag}}(n)=-\frac{b_1}{a_1}\sqrt{n(n+\mu-1)}$
$h^{\mathrm{Lag}}(n)=-\frac{b_1}{a_1}(2n+\mu)-\frac{b_0}{b_1}$
$b^{\mathrm{Jac}}(n)=(b-a)\sqrt{\frac{n(\mu+n-1)(\nu+n-1)(\mu+\nu+n-2)}{(\mu+\nu+2n-3)(\mu+\nu+2n-2)^2(\mu+\nu+2n-1)}}$
$h^{\mathrm{Jac}}(n)=\frac{2n(a+b)(\mu+\nu-1)+2n^2(a+b)-2b\mu-2a\nu+\mu\nu(a+b)+b\mu^2+a\nu^2}{(\mu+\nu+2n-2)(\mu+\nu+2n)}$

Attention: The necessary condition $b(0)=0$ is automatically satisfied with the exception of the Jacobi case for $\mu=\nu=1/2$ and $\mu=\nu=3/2$ where we must put it additionally.

$$A^{(k)}(\omega):=A(\omega)+k\frac{dB(\omega)}{d\omega}. \tag{A7}$$

Proposition A1: For a given Pearson data, i.e., a pair $(A(\omega),B(\omega))$ *on* $(a,b)\subset\mathbb{R}$, *the following statements are equivalent:*

(A) $\{P_n(\omega)\}_{n=0}^{\infty}$ *form an orthonormal system in* $L^2(\mathbb{R},d\sigma)$.

(B) The polynomials are given by Rodrigues' formula

$$P_n(\omega)=c_n\frac{1}{\varrho(\omega)}\cdot\frac{d^n}{d\omega^n}(\varrho(\omega)B^n(\omega)), \tag{A8}$$

where c_n *is the normalizing constant (see Table II).*

(C) The polynomials $\{P_n(\omega)\}_{n=0}^{\infty}$ *satisfy the differential equation*

$$\left(A(\omega)\frac{d}{d\omega}+B(\omega)\frac{d^2}{d\omega^2}\right)P_n(\omega)=\lambda_nP_n(\omega), \tag{A9}$$

where $\lambda_n=a_1n+b_2n(n-1)$.

(D) The polynomials $\{P_n(\omega)\}_{n=0}^{\infty}$ *are related by the three-term recurrence formula [for* $h(n)$ *and* $b(n)$ *see Table III]*

$$\omega P_n(\omega)=h(n)P_n(\omega)+b(n)P_{n-1}(\omega)+b(n+1)P_{n+1}(\omega) \tag{A10}$$

with the initial condition

$$P_0(\omega)\equiv\mathrm{const}=\left[\int d\sigma(\omega)\right]^{-1/2}. \tag{A11}$$

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Wigner measures and codimension two crossings

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(Received 23 April 2002; accepted 4 October 2002)

This article gives a semiclassical description of nucleonic propagation through codimension two crossings of electronic energy levels. Codimension two crossings are the simplest energy level crossings, which affect the Born–Oppenheimer approximation in the zeroth order term. The model we study is a two-level Schrödinger equation with a Laplacian as kinetic operator and a matrix-valued linear potential, whose eigenvalues cross, if the two nucleonic coordinates equal zero. We discuss the case of well-localized initial data and obtain a description of the wavefunction's two-scaled Wigner measure and of the weak limit of its position density, which is valid globally in time. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1527221]

I. INTRODUCTION

The quantum-mechanical description of molecular dynamics is given by the time-dependent Schrödinger equation

$$ih\,\partial_t\phi^h = H^h_{mol}\,\phi^h, \quad \phi^h(0)=\phi^h_0. \tag{1}$$

Ignoring spin degrees of freedom, we assume initial data $\phi^h_0 \in L^2(\mathbb{R}^{3N},\mathbb{C})$, $N \geqslant 1$, and a self-adjoint molecular Hamiltonian H^h_{mol} to have a unique solution

$$\phi^h(t) \in \mathcal{C}(\mathbb{R},L^2(\mathbb{R}^{3N},\mathbb{C})).$$

If the molecule consists of k_e electrons and k_n nuclei with $k_e+k_n=N$, the molecular Hamiltonian H^h_{mol} can be written as

$$H^h_{mol} = -\frac{h^2}{2}\Delta_{x_n} + H_e(x_n),$$

where Δ_{x_n} denotes the Laplacian acting on the $3k_n$ nucleonic coordinates, while $H_e(x_n)$ is the electronic Hamiltonian acting on the $3k_e$ electronic coordinates. $H_e(x_n)$ depends parametrically on the nucleonic coordinates x_n and comprises the electrons' kinetics as well as the interaction between electrons and nuclei. The scale-parameter $h>0$ is given by $h=\sqrt{m_e/M}$, where m_e is the electronic mass and M is the average mass of the molecule's nuclei. In the following, we will study the limit

$$h \to 0, \quad \text{i.e.,} \quad M \to \infty.$$

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We will concentrate on a closed subset $\sigma_*(x_n)$ of the electronic spectrum $\sigma(H_e(x_n))$, which is the union of two eigenvalues $\lambda_{1,2}(x_n)$ with the same multiplicity k and which is uniformly isolated from the rest of the electronic spectrum. That is, there is a constant $d>0$, such that

$$\text{dist}(\,\sigma_*(x_n),\sigma(H_e(x_n))\backslash\sigma_*(x_n)\,)\geqslant d \quad \text{for all} \quad x_n\in\mathbb{R}^{3k_n}.$$

We denote the spectral projection of $H_e(x_n)$ associated with $\sigma_*(x_n)$ by $P_e(x_n)$ and the extension to $L^2(\mathbb{R}^{3N},\mathbb{C})$ by $P_*=\int^{\oplus}_{\mathbb{R}^{3k_n}}P_e(x_n)\,dx_n$. If $\{\chi_j(x_n)(\cdot)\}_{j=1}^{2k}$ is a family of normalized eigenfunctions of $H_e(x_n)$ for the eigenvalues $\lambda_{1,2}(x_n)$, then we can write

$$\text{Ran}\,P_*=\left\{\sum_{j=1}^{2k}\int^{\oplus}_{\mathbb{R}^{3k_n}}\phi_j(x_n)\chi_j(x_n)\,dx_n:\phi=(\phi_j)_{j=1}^{2k}\in L^2(\mathbb{R}^{3k_n},\mathbb{C}^{2k})\right\}.$$

This description of Ran P_* induces an isometry $\mathcal{U}$:Ran $P_*\to L^2(\mathbb{R}^{3k_n},\mathbb{C}^{2k})$. Now, time-dependent Born–Oppenheimer theory, as carried out by H. Spohn and S. Teufel in Ref. 20, gives the following: If we choose initial data $\phi_0^h\in\text{Ran}\,P_*$ with $\|\phi_0^h\|_{L^2}=1$, such that $(\|h^2\Delta\phi_0^h\|_{L^2})_{h>0}$ is a bounded sequence, then the solution ϕ^h of the molecular Schrödinger equation (1) can be approximated by a Born–Oppenheimer solution modulo an error of order h. That is, there exists a constant $C>0$, such that

$$\|\phi^h(t)-\phi^h_{BO}(t)\|_{L^2}\leqslant C(1+|t|)\,h,$$

for all times $t\in\mathbb{R}$, where $\phi^h_{BO}(t)=\mathcal{U}^*\exp(-i\,(t/h)\,H^h_{BO})\,\mathcal{U}\,\phi^h_0$. If the eigenfunctions $\chi_j(x_n)(\cdot)$ can be chosen real-valued, then the Born–Oppenheimer Hamiltonian is given by

$$H^h_{BO}=-\frac{h^2}{2}\Delta_{x_n}+V(x_n), \tag{2}$$

where $V(x_n)$ is a potential, whose values are $2k\times 2k$ matrices. In this framework, Ran P_* is referred to as an adiabatically protected subspace (*adiabatos*~impassable). We also note that this type of observation dates back to the late 1920s and is originally assigned to M. Born, V. Fock, and R. Oppenheimer.

If the eigenvalues λ_1 and λ_2 also satisfy the gap-condition, that is, if

$$|\lambda_1(x_n)-\lambda_2(x_n)|\geqslant d \quad \text{for all} \quad x_n\in\mathbb{R}^{3k_n},$$

then Born–Oppenheimer theory shows again adiabatic decoupling between the subspaces associated with λ_1 and λ_2, and the two-level Hamiltonian (2) splits into two scalar Born–Oppenheimer Hamiltonians, modulo an error of order h. If the preceding gap-condition is violated, we have to consider two cases: either the eigenvalues cross, i.e.,

$$\exists\,\tilde{x}_n\in\mathbb{R}^{3k_n}:\lambda_1(\tilde{x}_n)=\lambda_2(\tilde{x}_n) \quad \text{(crossing)},$$

or they do not cross, but cannot be separated uniformly (avoided crossing). For generic crossings with mimimal multiplicity k, general symmetry considerations, as carried out in G. Hagedorn's monograph,[12] restrict the codimension of the crossing manifold to be one, two, three, or five:

$$\text{codim}_{\,\mathbb{R}^{3k_n}}\{x_n\in\mathbb{R}^{3k_n}:\lambda_1(x_n)=\lambda_2(x_n)\}=1,2,3, \quad \text{or} \quad 5.$$

Codimension two, three, and five crossings affect the Born–Oppenheimer approximation in the zeroth order term. This means that there is leading order exchange between the eigenspaces associated to λ_1 and λ_2. In the following, we will turn to the simplest model system showing a codimension two crossing and study the Wigner measure associated with its solution. Reducing the nucleonic configuration space $\mathbb{R}^{3k_n}$ to $\mathbb{R}^2$, we study

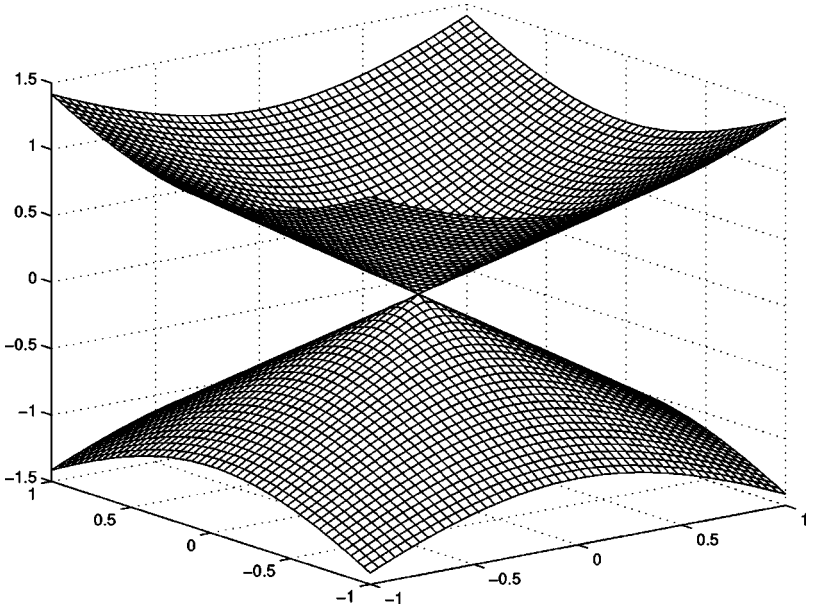

FIG. 1. The eigenvalues.

$$ih\,\partial_t\psi^h = -\frac{h^2}{2}\Delta_x\,\psi^h + V(x)\psi^h, \quad \psi^h(0) = \psi_0^h, \tag{3}$$

with $(\psi_0^h)_{h>0}$ a bounded family in $L^2(\mathbb{R}^2,\mathbb{C}^2)$, and V a matrix-valued potential of the form

$$V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}, \quad x \in \mathbb{R}^2.$$

The Hamiltonian $-(h^2/2)\Delta_x + V(x)$ is an essentially self-adjoint operator on $L^2(\mathbb{R}^2,\mathbb{C}^2)$, and we have a unique solution $\psi^h \in \mathcal{C}(\mathbb{R},L^2(\mathbb{R}^2,\mathbb{C}^2))$. The potential's eigenvalues $\pm|x|$ cross for $x=0$ as depicted in Fig. 1 below, which plots $\pm|x|$ versus x_1 and x_2.

The mathematical analysis of the above model system has been initiated by G. Hagedorn in Ref. 12. His result describes the evolution of the solution ψ^h itself, given special initial data, so called semi-classical wave packets. Recently, the first author and P. Gérard[6] have studied codimension two crossings from a Wigner measures' point of view. Their method applies to general initial data and covers Hamiltonians of the form $H^W(x,hD_x)$ with symbol $H(x,\xi)=K(\xi)+V(x)$, $K\in\mathcal{C}^\infty(\mathbb{R}^2,\mathbb{R})$.

Here, we aim at applying their result to well-localized initial data and the case where the kinetics is given by a Laplacian, i.e., for $K(\xi)=|\xi|^2/2$. For this special situation, we will obtain an asymptotic description of the solution $\psi^h(t)$, which is valid *globally in time*.

Actually, we consider for a family of solutions $(\psi^h(t))_{h>0}$ of (3) the Wigner transforms

$$(W^h\psi^h)(t,x,\xi) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \exp(iy\cdot\xi)\,\psi^h\left(t,x-\frac{h}{2}y\right)\otimes\overline{\psi^h}\left(t,x+\frac{h}{2}y\right)\mathrm{d}y,$$

where $t\in\mathbb{R}$ and $(x,\xi)\in T^*\mathbb{R}^2=\mathbb{R}^2\times\mathbb{R}^2$. Since $\psi^h(t,x)$ is a vector in $\mathbb{C}^2$, the Wigner transform is a Hermitian matrix in $\mathbb{C}^{2,2}$. The families $(\psi^h(t))_{h>0}$ inherit uniform boundedness in $L^2(\mathbb{R}^2,\mathbb{C}^2)$ for all times $t\in\mathbb{R}$ from the initial data. Therefore, the family $(W^h\psi^h)_{h>0}$ is bounded in $L^\infty(\mathbb{R},\mathcal{S}'(T^*\mathbb{R}^2,\mathbb{C}^{2,2}))$, which means

$$\left| \int_{T^*\mathbb{R}^2} (W^h \psi^h)(t,x,\xi)\, a(x,\xi)\, dx d\xi \right| \leqslant C$$

for all $t \in \mathbb{R}$ and all $a \in \mathcal{S}(T^*\mathbb{R}^2, \mathbb{C}^{2,2})$. Thus, there exist weak *-limit points of $(W^h \psi^h)_{h>0}$ in $L^\infty(\mathbb{R}, \mathcal{S}'(T^*\mathbb{R}^2, \mathbb{C}^{2,2}))$. These limit points are called *Wigner measures*, since for fixed times t they are positive matrix-valued Radon measures on the phase space $T^*\mathbb{R}^2$. We refer to Refs. 7, 8, 17, and to Ref. 10 for a complete treatment of these measures.

One important property of the Wigner measures $\mu(t,\cdot)$ is their relation to the position density $|\psi^h(t,x)|^2$. Let us consider some fixed time $t \in \mathbb{R}$. If the family of initial data $(\psi_0^h)_{h>0}$ is *h-oscillating*, that is, if

$$\limsup_{h\to 0} \quad \int_{|\xi| \geqslant R/h} |\widehat{\psi_0^h}(\xi)|^2 \, \mathrm{d}\xi \xrightarrow[R\to+\infty]{} 0,$$

then $(\psi^h(t))_{h>0}$ inherits this property as well (see the proof of Corollary 1 in Sec. IV). Roughly speaking, h-oscillating families have frequencies of oscillations, which are of order less or equal than $1/h$. Furthermore, as in Ref. 9, given h-oscillation, the weak limit points of $(|\psi^h(t,x)|^2)_{h>0}$ in $L^1(\mathbb{R}^2, \mathbb{C}^2)$ can be described by Wigner measures $\mu(t,\cdot)$ of $(\psi^h(t))_{h>0}$ via

$$w - \lim_{h\to 0} |\psi^h(t,x)|^2 = \int_{\mathbb{R}^2_\xi} tr(\mu(t,x,\mathrm{d}\xi)). \tag{4}$$

In the following, we will perform a *complete* study of the evolution of Wigner measures associated with solutions to (3), assuming specific initial data. The reader will find precise assumptions and statements in Sec. IV, Theorem 2. For example, our result applies to initial data microlocally localized on a set Σ_0 of the form

$$\Sigma_0 = \{(x,\xi) \in T^*\mathbb{R}^2 : |x| = R, x = \xi\}$$

with radius $R > 0$, which means

$$\forall a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^2 \backslash \Sigma_0, \mathbb{C}^{2,2}) : \int_{T^*\mathbb{R}^2} (W^h \psi_0^h)(x,\xi)\, a(x,\xi)\, dx d\xi \xrightarrow[h\to 0]{} 0.$$

Thus, $(\psi_0^h)_{h>0}$ concentrates asymptotically on a circle in position space and has asymptotically equal position and momentum. Moreover, we assume that $(\psi_0^h)_{h>0}$ is h-oscillating and localized on the eigenspace associated, say, with the eigenvalue $+|x|$ of $V(x)$. For example, we suppose

$$\Pi^-(x)\psi_0^h(x) \xrightarrow[h\to 0]{} 0$$

strongly in $L^2(\mathbb{R}^2, \mathbb{C}^2)$, where $\Pi^\pm(x) = 1/2\,(\mathrm{Id} \pm V(x)/|x|)$ denote the spectral projectors of $V(x)$ associated with $\pm|x|$. Assuming these initial data, the solution $(\psi^h(t))_{h>0}$ stays localized on the mode plus until it hits the crossing manifold $\{x = 0\}$. At the crossing, we observe a Landau–Zener exchange between the eigenspaces, and $(\psi^h(t))_{h>0}$ will be localized on both modes. Our analysis, which is summarized later on in Sec. IV, Theorem 2, results in the following description of the weak limit of the position density for all times.

Theorem 1: *Let $(\psi_0^h)_{h>0}$ be bounded in $L^2(\mathbb{R}^2, \mathbb{C}^2)$, h-oscillating, microlocally localized on Σ_0, and localized on the mode plus. Let $(\psi^h(t))_{h>0}$ be a family of solutions of (3) given the initial data $(\psi_0^h)_{h>0}$. We denote $C = R^2/2 + R$ and choose a smooth, compactly supported function $\phi \in \mathcal{C}_0^\infty(\{x \in \mathbb{R}^2 : |x| > C\}, \mathbb{C})$. Then we have*

$$\lim_{h\to 0}\int_{\mathbb{R}^2}\phi(x)|\Pi^+(x)\psi^h(t,x)|^2\,\mathrm{d}x=0$$

for all times $t\in\mathbb{R}$. *Moreover, there exists a positive, increasing sequence* $(t_j)_{j\geqslant 0}$ *with* $t_j\to+\infty$ *as* $j\to+\infty$, *a sequence* $(\alpha_j)_{j\geqslant 0}$ *of positive Radon measures on* $\mathbf{S}^1$, *and a sequence* $(x_j)_{j\geqslant 0}$ *in* $\mathcal{C}(\mathbb{R},\mathbb{R}^2)$, *such that*

$$\lim_{h\to 0}\int_{\mathbb{R}^2}\phi(x)|\Pi^-(x)\psi^h(t,x)|^2\mathrm{d}x=\sum_{0\leqslant k\leqslant j}\int_{\mathbf{S}^1}\phi(x_k(t)\omega)\alpha_k(\mathrm{d}\omega)$$

for $t\in(t_{j-1},t_j)$, $j\in\mathbb{N}_0$, *where* $t_{-1}=0$.

Thus, on the mode plus the solution asymptotically stays inside the ball of radius C. On the mode minus, points outside the ball are charged recurrently in time. Explicit formulas for the α_j, t_j and x_j are given in Sec. IV.

We will proceed as follows: In Sec. II, we discuss propagation of Wigner measures and study the classical trajectories associated with the Schrödinger equation (3). Section III introduces two-scaled Wigner measures and gives some examples for well-localized data. In Sec. IV, we discuss Landau–Zener transitions between the two eigenspaces at points, where classical trajectories hit the crossing manifold $\{x=0\}$ recurrently in time, and obtain an asymptotic description of the solution's position density, which is valid globally in time.

II. PROPAGATION OF WIGNER MEASURES

Let $(\psi_0^h)_{h>0}$ be a family of initial data, which is bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$, $(\psi^h(t))_{h>0}$ be a family of solutions of (3), and $\mu(t,\cdot)$ be an associated Wigner measure. The evolution of Wigner measures associated with solutions of a system, whose principal symbol admits eigenvalues of constant multiplicity (and thus no crossings), has been studied in Ref. 10. These results apply to system (3) *outside* the crossing manifold

$$S=\{(x,\xi)\in T^*\mathbb{R}^2: x=0\}.$$

We consider initial data $(\psi_0^h)_{h>0}$, such that the associated Wigner measures μ_0 have support outside the singular set S. By the results of Ref. 10, outside S the Wigner measure $\mu(t,\cdot)$ commutes with the projectors $\Pi^\pm$ and thus can be decomposed as

$$\mu(t,\cdot)=\Pi^+\mu(t,\cdot)\Pi^+ +\Pi^-\mu(t,\cdot)\Pi^-$$

in $\mathcal{D}'(\mathbb{R},\mathcal{S}'(T^*\mathbb{R}^2,\mathbb{C}^{2,2}))$. Since the eigenspaces are one-dimensional, the decomposition simplifies to

$$\mu(t,\cdot)=\mu^+(t,\cdot)\Pi^+ +\mu^-(t,\cdot)\Pi^-,$$

where $\mu^\pm(t,\cdot)=tr(\Pi^\pm\mu(t,\cdot))$ are scalar positive Radon measures satisfying the transport equations

$$\partial_t\mu^\pm+\xi\cdot\nabla_x\mu^\pm\mp\frac{x}{|x|}\cdot\nabla_\xi\mu^\pm=0,\quad \mu^\pm(0)=tr(\Pi^\pm\mu_0). \tag{5}$$

These transport equations give continuity of the maps $t\mapsto\mu^\pm(t,\cdot)$ and thus a description of $\mu^\pm(t,\cdot)$ on any given time interval, provided that the supports of $\mu^\pm(t,\cdot)$ do not intersect the crossing manifold S. We consider the flows of the associated Hamiltonian systems

$$\dot{x}^\pm(t)=\xi^\pm(t),\quad \dot{\xi}^\pm(t)=\mp\frac{x^\pm(t)}{|x^\pm(t)|}, \tag{6}$$

which describe the classical motion corresponding to the quantum-mechanical motion issued by the Schrödinger equation (3). Therefore, their solutions are called *classical trajectories*. The following proposition characterizes the trajectories, which touch the singular set S. For this, we will use the symplectic product

$$x \wedge \xi = x^{\perp} \cdot \xi = x_1 \xi_2 - x_2 \xi_1$$

for $(x,\xi) \in T^*\mathbb{R}^2$.

Proposition 1: We consider classical trajectories with initial data $x^{\pm}(0)=x_0$, $\xi^{\pm}(0)=\xi_0$, $(x_0,\xi_0) \in T^*\mathbb{R}^2 \backslash \{(0,0)\}$.

1. *If* $x_0 \wedge \xi_0 \neq 0$, *then* $x^{\pm}(t) \wedge \xi^{\pm}(t) \neq 0$ *for all* $t \in \mathbb{R}$, *and the classical trajectories do not reach* $S=\{x=0\}$.
2. *If* $x_0 \wedge \xi_0 = 0$, *then* $x^{\pm}(t) \wedge \xi^{\pm}(t) = 0$ *for all* $t \in \mathbb{R}$, *and the trajectory associated with the mode* $+|x|$ *is the first classical trajectory to hit S for a positive time* t_0,

$$t_0 = \xi_0 \cdot \omega + \sqrt{|\xi_0|^2 + 2|x_0|},$$

where $\omega = x_0/|x_0|$ *for* $x_0 \neq 0$ *and* $\omega = \xi_0/|\xi_0|$ *for* $x_0 = 0$. *Moreover we have for* $t \in (0,t_0)$

$$x^{\pm}(t) = \mp \frac{t^2}{2}\omega + t\,\xi_0 + x_0, \quad \xi^{\pm}(t) = \mp\, t\omega + \xi_0. \tag{7}$$

Proof: Omitting the plus-minus superscripts for $x(t)$ and $\xi(t)$ unless the context requires, we start with the observation that the Hamiltonian systems (6) are equivalent to the Newtonian equations

$$\ddot{x}(t) = -\nabla U^{\pm}(x(t)), \quad \dot{x}(0)=\xi_0, \quad x(0)=x_0,$$

with central field $U^{\pm}(y) = \pm|y|$. Motion in a central field conserves the angular momentum. Thus, we have

$$x(t) \wedge \dot{x}(t) = x_0 \wedge \xi_0, \quad \text{i.e.,} \quad x(t) \wedge \xi(t) = x_0 \wedge \xi_0 \quad \text{for all} \quad t \in \mathbb{R},$$

and the first assertion follows.

We turn to the case $x_0 \wedge \xi_0 = 0$. Inserting a Taylor expansion of $x(t)$ into (6), we get

$$\frac{x(t)}{|x(t)|} \xrightarrow[t \to 0^+]{} \omega = \begin{cases} \dfrac{x_0}{|x_0|} & \text{if} \quad x_0 \neq 0, \\ \dfrac{\xi_0}{|\xi_0|} & \text{if} \quad x_0 = 0. \end{cases}$$

We rewrite $x(t), \xi(t)$ for small $t>0$ as $x(t)=k(t)\omega$, $\xi(t)=l(t)\omega$ with $k(t), l(t) \in \mathbb{R}$, and are left with

$$\dot{k}^{\pm}(t) = l^{\pm}(t), \quad \dot{l}^{\pm}(t) = \mp\, 1, \quad k(0)=k_0, \quad l(0)=l_0.$$

Thus, we have $l^{\pm}(t) = \mp t + l_0$, $k^{\pm}(t) = \mp t^2/2 + l_0 t + k_0$ for small $t>0$. Since $x(t) = x_0 + t\xi_0 + o(t)$, we have $k_0 = |x_0|$. Moreover, $l_0 = \operatorname{sgn}(x_0 \cdot \xi_0)|\xi_0|$ if $x_0 \neq 0$ and $l_0 = |\xi_0|$ if $x_0 = 0$.

The determinant for the zeros of $k^{\pm}(t)$ is $l_0^2 \pm 2k_0$. We distinguish different cases.

If $l_0^2 < 2k_0$, then only the plus-trajectory hits S for some positive time t_0, i.e., for $t_0 = l_0 + \sqrt{l_0^2 + 2k_0}$.

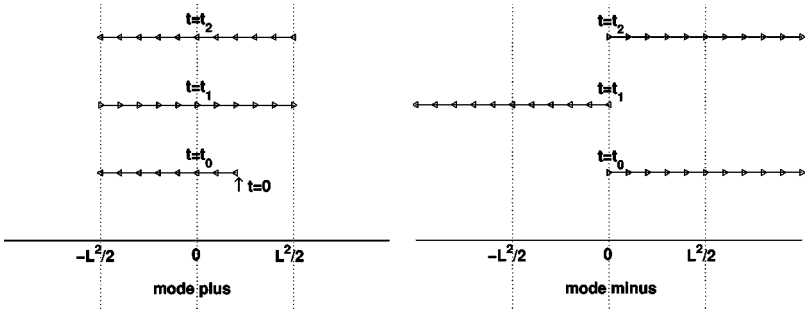

FIG. 2. The classical trajectories.

If $l_0^2 \geqslant 2k_0$, then $l_0 \neq 0$ and we have to distinguish two cases. If $\mathrm{sgn}(l_0)>0$, then only the plus-trajectory has a positive hitting time t_0, and we get again $t_0 = l_0 + \sqrt{l_0^2 + 2k_0}$. If $\mathrm{sgn}(l_0)<0$, then the minus-trajectory also has a positive hitting time $s_0 = |l_0| - \sqrt{l_0^2 - 2k_0}$. However, an easy calculation gives $t_0 < s_0$, and we are done.

The preceding proof contains the following easy observation concerning the trajectory associated with the mode $-|x|$, which will be useful later on.

Remark 1: The minus-trajectory with initial data $x^-(0)=0$, $\xi^-(0)=\xi_0$ with $\xi_0 \neq 0$ is given for positive times $t \in \mathbb{R}^+$ by

$$x^-(t) = \left(\frac{t^2}{2|\xi_0|} + t \right) \xi_0, \quad \xi^-(t) = \left(\frac{t}{|\xi_0|} + 1 \right) \xi_0.$$

This trajectory does not hit S for times $t \in \mathbb{R}^+$.

Next, we consider the plus-trajectory with initial data (x_0, ξ_0), $x_0 \wedge \xi_0 = 0$, $x_0 \neq 0$. By Proposition 1, we can also calculate the plus-trajectory after the first hitting time t_0. For this, we set again $\omega = x_0/|x_0|$ and

$$L = \sqrt{|\xi_0|^2 + 2|x_0|}, \quad t_j = \xi_0 \cdot \omega + (2j+1)L \quad (j \in \mathbb{N}_0).$$

Remark 2: The positive times, at which the plus-trajectory hits S, are given by t_j, $j \in \mathbb{N}_0$, and we have for $t \in (t_j, t_{j+1})$, $j \in \mathbb{N}_0$,

$$x^+(t) = (-1)^j \left(\frac{(t-t_j)^2}{2} - L(t-t_j) \right) \omega, \quad \xi^+(t) = (-1)^j (t - t_j - L)\, \omega.$$

We point out, that at any hitting time t_j we have $\xi^+(t_j) = (-1)^{j+1} L\omega \neq 0$. Thus, the preceeding remark is an immediate consequence of Proposition 1, using the change of sign of the fraction $x^{\pm}(t)/|x^{\pm}(t)|$ at the hitting times $t = t_j$.

Figure 2 summarizes our discussion, depicting the trajectories' x-component: Classical trajectories touching the singular set S are contained in the hypersurface

$$I = \{(x,\xi) \in T^*\mathbb{R}^2 : x \wedge \xi = 0\}.$$

Starting a plus-trajectory with initial data $(x_0, \xi_0) \in I \backslash S$, its x-component runs along the straight line given by ω. It hits S at time $t = t_0$ for the first time, and we start a minus-trajectory going off in the opposite direction. The plus-trajectory hits S again at time $t = t_1$, and the mode minus goes off in the opposite direction, and so on.

If we consider initial data $(\psi_0^h)_{h>0}$ for the Schrödinger equation (3), such that the associated Wigner measures μ_0 are supported in $\{(x_0, \xi_0)\}$ with $(x_0, \xi_0) \in I \backslash S$, then the transport equations (5) describe the evolution of the measures $\mu^{\pm}(t, \cdot)$ until the hitting time t_0. When arriving on S, we will observe some exchange between the plus and the minus mode, a Landau–Zener phe-

nomenon. This quantum-mechanical effect has been described quantitatively for the first time by L. Landau in Ref. 16 and C. Zener in Ref. 21, independently from each other. The work of the first author and P. Gérard[6] shows that this transfer does not depend on microlocal, i.e., phase space, information only, but that a second level of observation, which can be called "two-microlocal," must be taken into account as well. Their Landau–Zener type formula relies on some two-scaled variant of Wigner measures, which we will focus on in the following, such that we can continue the evolution of $\mu^{\pm}(t,\cdot)$ for times $t>t_0$ in the manner described for the classical trajectories above.

These two-scaled Wigner measures, which have first been introduced in Ref. 19 in another context, quantify the way a wave packet concentrates on the hypersurface I by introducing a new variable $\eta\in\overline{\mathbb{R}}$, which, roughly speaking, describes the position of the core of a wave packet with respect to I versus the scale $\sqrt{h}$, that is,

$$\eta=\frac{x\wedge\xi}{\sqrt{h}}.$$

We note that, for all types of crossings, avoided and real crossings, the scale $\sqrt{h}$ is known to play an important role (see the work of Y. Colin de Verdière, M. Lombardi, and J. Pollet,[1] G. Hagedorn,[11,12] G. Hagedorn and A. Joye,[13,14] A. Joye,[15] P. Exner and A. Joye,[3] or P. Martin and G. Nenciu.[18]

III. TWO-SCALED WIGNER MEASURES

The critical hypersurface $I=\{x\wedge\xi=0\}$ is an involutive (or coisotropic) submanifold of $T^*\mathbb{R}^2\setminus\{0,0\}$, i.e., we have $(T_zI)^{\perp}\subset T_zI$ for all $z\in I$, where $(T_zI)^{\perp}$ denotes the symplectic complement of the tangent space T_zI in $T_z\mathbb{R}^2$. This is an immediate consequence of the obvious fact that $(T_zI)^{\perp}$ is the linear span of the Hamiltonian vector field associated with the function

$$g:T^*\mathbb{R}^2\to\mathbb{R},\quad (x,\xi)\mapsto x\wedge\xi.$$

We now define a two-scaled Wigner transform of $(\psi^h)_{h>0}$ for $I=\{x\wedge\xi=0\}$ with scale $\sqrt{h}$ by

$$W_2^h\psi^h(x,\xi,\eta)=W^h\psi^h(x,\xi)\otimes\delta\left(\eta-\frac{x\wedge\xi}{\sqrt{h}}\right),\quad (x,\xi,\eta)\in T^*\mathbb{R}^2\times\mathbb{R},$$

which acts on the following class of test functions

$$\mathcal{A}=\{a\in\mathcal{C}^{\infty}(T^*\mathbb{R}^2\times\mathbb{R},\mathbb{C}^{2,2}):\operatorname{supp}(a)\subset K\times\mathbb{R}\ \text{ for compact }\ K\subset T^*\mathbb{R}^2\setminus\{(0,0)\},$$

$$\exists a_{\infty}\in\mathcal{C}^{\infty}(T^*\mathbb{R}^2\times\{\pm1\},\mathbb{C}^{2,2}),\ \ \exists R=R(a)\in[0,+\infty),\forall x,\xi\in\mathbb{R}^2,\forall|\eta|>R:$$

$$a(x,\xi,\eta)=a_{\infty}(x,\xi,\operatorname{sgn}(\eta))\}.$$

These test functions differ from standard matrix-valued test functions in two ways: first, as functions of (x,ξ) alone they are compactly supported outside $\{(0,0)\}$. This restriction assures that we are working in regions of the phase space $T^*\mathbb{R}^2$, where the gradient of the function g chosen to describe I does not vanish. Second, there is an additional coordinate $\eta\in\mathbb{R}$, which is used for measuring the position of points in $T^*\mathbb{R}^2$ with respect to the hypersurface I versus the scale $\sqrt{h}$. We denote by $\overline{\mathbb{R}}$ the one point compactification of $\mathbb{R}$ and continue $a(x,\xi,\cdot)$ continuously on $\overline{\mathbb{R}}$.

Let $(\psi^h)_{h>0}$ be a bounded family in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Theorem 1 in Ref. 6 shows that there exists a subsequence $(h_k)_{k>0}$ with $h_k\to0$ and a positive matrix-valued Radon measure ν on $I\times\overline{\mathbb{R}}$, such that for all $a\in\mathcal{A}$

$$\int_{T^*\mathbb{R}^2\times\mathbb{R}} tr(W_2^h\psi^h(x,\xi,\eta)a(x,\xi,\eta))\mathrm{d}x\mathrm{d}\xi\mathrm{d}\eta$$

$$= \int_{T^*\mathbb{R}^2} tr\left(W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\right)\mathrm{d}x\mathrm{d}\xi \overset{h_k\to 0}{\to} \int_{T^*\mathbb{R}^2\setminus I} tr(a(x,\xi,\mathrm{sgn}(x\wedge\xi)\infty)\mu(\mathrm{d}x,\mathrm{d}\xi))$$

$$+ \int_{I\times\mathbb{R}} tr(a(x,\xi,\eta)\nu(\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta)), \tag{8}$$

where μ is a Wigner measure of $(\psi^h)_{h>0}$.

Definition 1: Let $(\psi^h)_{h>0}$ be a bounded family in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Then we call the Radon measures ν, which are associated via (8) to the weak*-*limit points of $(W_2^h\psi^h)_{h>0}$ in $\mathcal{A}'$, two-scaled Wigner measures of $(\psi^h)_{h>0}$ for $I=\{x\wedge\xi=0\}$ with scale $\sqrt{h}$.*

We note that a two-scaled Wigner measure ν depends on the function g chosen to describe the hypersurface I; we consider another function $\tilde{g}=fg$ with $f(x,\xi)\neq 0$ for all $x,\xi\in\mathbb{R}^2$ to describe the hypersurface I and a two-scaled Wigner measure $\tilde{\nu}$ associated with $\tilde{g}$ via (8). Then, we have for $a\in\mathcal{A}$

$$\int_{I\times\mathbb{R}} a(x,\xi,\eta)\,\tilde{\nu}(\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta) = \int_{I\times\mathbb{R}} a(x,\xi,f(x,\xi)\,\eta)\,\nu(\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta). \tag{9}$$

This relation allows a geometrical interpretation of ν, see Sec. 1.3 in Ref. 6. For our purpose, however, it will be enough to have relation (9). The key property of two-scaled Wigner measures is

$$\mathbb{1}_I(x,\xi)\,\mu(x,\xi) = \int_{\mathbb{R}}\nu(x,\xi,\mathrm{d}\eta).$$

That is, we can recover a Wigner measure's μ restriction to I by projecting a two-scaled measure ν onto I. Indeed, if we consider $a\in\mathcal{C}_0^\infty(T^*\mathbb{R}^2,\mathbb{C}^{2,2})$ with support outside (0,0), then we obviously have

$$\int_{T^*\mathbb{R}^2\times\mathbb{R}} tr(W_2^h\psi^h(x,\xi,\eta)\,a(x,\xi))\,\mathrm{d}x\mathrm{d}\xi\mathrm{d}\eta = \int_{T^*\mathbb{R}^2} tr(W^h\psi^h(x,\xi)\,a(x,\xi))\,\mathrm{d}x\mathrm{d}\xi\,,$$

and passing to the limit, we obtain $\mathbb{1}_{T^*\mathbb{R}^2\setminus I}\ \mu+\mathbb{1}_I\int_{\mathbb{R}}\nu(d\eta)=\mu$ outside (0,0).

In Ref. 12, G. Hagedorn has also studied molecular propagation through codimension three and five crossings. For those systems, the codimension of the associated critical submanifold I is greater than one, but the submanifolds I are still involutive, and two-scaled Wigner measures of the same type as here can be applied. We refer to Ref. 6 for a definition of two-scaled Wigner measures associated with general involutive submanifolds. Notice that two-scaled measures can also be associated with symplectic subspaces (see Ref. 5); the measures obtained are then more complicated and close to those of Ref. 4.

In the following, we discuss some examples for two-scaled Wigner measures associated with $I=\{x\wedge\xi=0\}$. For simplicity, the considered functions are all scalar-valued.

A. Some coherent states

We start with some coherent states of the form

$$\psi^h(x)=h^{-\beta}\Phi\left(\frac{x-x_0-h^\gamma\eta_0}{h^\beta}\right)\exp\left(\frac{i}{h}\,\xi_0\cdot x\right)$$

with $\Phi\in L^2(\mathbb{R}^2,\mathbb{C})$, $0<\beta\leqslant 1$, $0<\gamma<\beta$, and $x_0,\xi_0,\eta_0\in\mathbb{R}^2$ with $x_0\wedge\xi_0=0$.

If we choose $\beta=1/2$, $\eta_0=0$, and $\Phi(x)=\exp((x\cdot BA^{-1}x)/2)$ with $A,B\in\mathbb{C}^{2,2}$ invertible, then ψ^h is a semiclassical wave packet as considered by G. Hagedorn in Ref. 12. Moreover, $(\psi^h)_{h>0}$ is h-oscillating, and we have for scalar-valued test functions $a\in\mathcal{A}$

$$\int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\,\mathrm{d}x\mathrm{d}\xi=(2\pi)^{-2}\int_{T^*\mathbb{R}^2\times\mathbb{R}^2}\exp(iy\cdot\xi)\Phi(x-y/2)\overline{\Phi}\,(x+y/2)\times a(x_0 + h^\beta x+h^\gamma\eta_0,\xi_0+h^{1-\beta}\xi,h^{-1/2}d(x,\xi))\,\mathrm{d}y\mathrm{d}x\mathrm{d}\xi,$$

where $d(x,\xi)=hx\wedge\xi+h^\beta x\wedge\xi_0+h^{1-\beta}x_0\wedge\xi+h^{1+\gamma-\beta}\eta_0\wedge\xi+h^\gamma\eta_0\wedge\xi_0$, so that

$$\frac{d(x,\xi)}{\sqrt{h}}=h^{\beta-1/2}x\wedge\xi_0+h^{1/2-\beta}x_0\wedge\xi+h^{\gamma-1/2}\,\eta_0\wedge\xi_0+o(h^{1/2-\beta})+o(1). \tag{10}$$

Ignoring the η-component of a, we obtain the Wigner measure of (ψ^h),

$$\mu(x,\xi)=\|\Phi\|_{L^2}^2\quad\delta(x-x_0)\otimes\delta(\xi-\xi_0),$$

which shows that (ψ^h) concentrates on $I=\{x\wedge\xi=0\}$.

However, the two-scaled measure for I with scale $\sqrt{h}$ depends on η_0 and γ. If $\beta=1/2$ and $\eta_0\wedge\xi_0=0$, then the concentration of (ψ^h) on I is issued from finite distance. Otherwise, the concentration occurs from infinite distance (versus $\sqrt{h}$). Below, we discuss some significant cases. For simplicity, we assume $|x_0|=|\xi_0|=1$.

$\beta=1/2$ and $\eta_0\wedge\xi_0=0$: The dominating term in (10) is $x\wedge\xi_0+x_0\wedge\xi$. For $t\in\mathbb{R}$ and $z\in\mathbb{R}^2$, we set $\Psi(x)=\exp(-(i/2)\,|x|^2\mathrm{sgn}(x_0\cdot\xi_0))\Phi(x)$. Then,

$$\nu(x,\xi,\eta)=\delta(x-x_0)\otimes\delta(\xi-\xi_0)\otimes(2\pi)^{-2}\left(\int_{\mathbb{R}}|\hat{\Psi}(tx_0+\eta x_0^\perp)|^2\,\mathrm{d}t\right)\mathrm{d}\eta.$$

$\gamma<\beta=1/2$ and $\eta_0\wedge\xi_0\neq0$: The dominating term in (10) is $h^{\gamma-1/2}\eta_0\wedge\xi_0$ and

$$\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta-\mathrm{sgn}(\eta_0\wedge\xi_0)\,\infty).$$

$\gamma<\beta<1/2$: The dominating term in (10) is $h^{\gamma-1/2}\eta_0\wedge\xi_0$ if $\eta_0\wedge\xi_0\neq0$ and $h^{\beta-1/2}x\wedge\xi_0$ if $\eta_0\wedge\xi_0=0$. In the first case we obtain as before

$$\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta-\mathrm{sgn}(\eta_0\wedge\xi_0)\,\infty).$$

In the second case we have to consider

$$\int_{\mathbb{R}^2}|\Phi(x)|^2a(x_0,\xi_0,\mathrm{sgn}(x\wedge\xi_0)\infty)\,\mathrm{d}x=\int_{\mathbb{R}^2}|\Phi(t\xi_0+\eta\xi_0^\perp)|^2a(x_0,\xi_0,-\mathrm{sgn}(\eta)\infty)\,\mathrm{d}t\mathrm{d}\eta.$$

Therefore,

$$\nu(x,\xi,\eta)=\delta(x-x_0)\otimes\delta(\xi-\xi_0)\otimes\left[\left(\int_{x\cdot\xi_0^\perp>0}|\Phi(x)|^2\,\mathrm{d}x\right)\delta(\eta+\infty)+\left(\int_{x\cdot\xi_0^\perp<0}|\Phi(x)|^2\,\mathrm{d}x\right)\delta(\eta-\infty)\right].$$

The case $\beta>1/2$ leads to a similar discussion with results depending on the sign of $\gamma-(1-\beta)$.

B. Arbitrary phase

Replacing the linear phase by an arbitrary one, we now consider families of the form

$$\psi^h(x)=h^{-\beta}\Phi\left(\frac{x-x_0}{h^\beta}\right)\exp\left(\frac{i}{2h}f(|x|^2)\right)$$

with $\Phi \in L^2(\mathbb{R}^2,\mathbb{C})$, $f \in \mathcal{C}^1(\mathbb{R},\mathbb{R})$, $0<\beta<1$, and $x_0 \in \mathbb{R}^2\backslash\{0\}$. Again, this family is h-oscillating. Writing

$$\begin{aligned} &f(|x_0+h^\beta z|^2)-f(|x_0+h^\beta z'|^2)\\ &\quad=2h^\beta(z-z')\cdot\left(x_0+h^\beta\frac{z+z'}{2}\right)\int_0^1 f'(t|x_0+h^\beta z|^2+(1-t)|x_0+h^\beta z'|^2)\,\mathrm{d}t\\ &\quad=:2h^\beta(z-z')\cdot\left(x_0+h^\beta\frac{z+z'}{2}\right)l_h(x_0,z,z'), \end{aligned}$$

for $z,z' \in \mathbb{R}^2$, we calculate for scalar-valued $a \in \mathcal{A}$

$$\begin{aligned} &\int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\mathrm{d}x\mathrm{d}\xi\\ &\quad=(2\pi)^{-2}\int_{T^*\mathbb{R}^2\times\mathbb{R}^2}\exp(iy\cdot\xi)\Phi(x-y/2)\overline{\Phi}(x+y/2)\\ &\qquad\times a\left(x_0+h^\beta x,l_h\left(x_0,x+\frac{y}{2},x-\frac{y}{2}\right)(x_0+h^\beta x)+h^{1-\beta}\xi,\frac{d(x,\xi)}{\sqrt{h}}\right)\mathrm{d}y\mathrm{d}x\mathrm{d}\xi, \end{aligned}$$

with

$$\frac{d(x,\xi)}{\sqrt{h}}=h^{(1/2)-\beta}(x_0+h^\beta x)\wedge\xi=h^{(1/2)-\beta}x_0\wedge\xi+o(1). \tag{11}$$

Since $\lim_{h-0} l_h(x_0,z,z')=f'(|x_0|^2)$, we obtain the Wigner measure

$$\mu(x,\xi)=\|\Phi\|_{L^2}^2\delta(x-x_0)\otimes\delta(\xi-f'(|x_0|^2)\,x_0),$$

and have again concentration on $I=\{x\wedge\xi=0\}$. However, $\sqrt{h}$-concentration is issued from finite distance if and only if $\beta\leqslant 1/2$. We distinguish three different cases, assuming $|x_0|=1$.

$\beta<1/2$:

$$\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta).$$

$\beta=1/2$:

$$\nu(x,\xi,\eta)=\delta(x-x_0)\otimes\delta(\xi-f'(1)\,x_0)\otimes(2\pi)^{-2}\left(\int_{\mathbb{R}}|\hat{\Phi}(tx_0+\eta x_0^\perp)|^2\,dt\right)\mathrm{d}\eta.$$

$\beta>1/2$:

$$\begin{aligned} \nu(x,\xi,\eta)=\delta(x-x_0)\otimes\delta(\xi-f'(1)\,x_0)\otimes(2\pi)^{-2}\Bigg[&\left(\int_{x_0\wedge\xi>0}|\hat{\Phi}(\xi)|^2\,\mathrm{d}\xi\right)\delta(\eta-\infty)\\ &+\left(\int_{x_0\wedge\xi<0}|\hat{\Phi}(\xi)|^2\,\mathrm{d}\xi\right)\delta(\eta+\infty)\Bigg]. \end{aligned}$$

Of course, the above discussion easily extends to families

$$\psi^h(x)=h^{-\beta}\Phi\left(\frac{x-x_0-h^\gamma\eta_0}{h^\beta}\right)\exp\left(\frac{i}{2h}f(|x|^2)\right)$$

with $0<\gamma<\beta$ and $\eta_0 \in \mathbb{R}^2$.

C. Concentration on a circle

Finally, we consider families of the form

$$\psi^h(x)=h^{-1/4}\Phi\left(\frac{|x|^2-R^2}{\sqrt{h}}\right)\exp\left(\frac{i}{2h}|x-h^\gamma x_0|^2\right),$$

where $\Phi \in \mathcal{C}_0^\infty(\mathbb{R},\mathbb{C})$, $x_0 \in \mathbb{R}^2$, $R>0$ and $0<\gamma<1$. Once again, such families are h-oscillating. We have for scalar-valued $a \in \mathcal{A}$

$$\begin{aligned} I_h &:= \int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\mathrm{d}x\mathrm{d}\xi \\ &= \int_{T^*\mathbb{R}^2\times\mathbb{R}^2} \exp(iy\cdot\xi)\Phi\left(\frac{|x-y/2|^2-R^2}{\sqrt{h}}\right)\overline{\Phi}\left(\frac{|x+y/2|^2-R^2}{\sqrt{h}}\right) \\ &\quad \times a(x,x-h^\gamma x_0+h\xi,\sqrt{h}x\wedge\xi+h^{\gamma-1/2}x_0\wedge x)\,\frac{\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^2\sqrt{h}}, \end{aligned}$$

and thus by the Fourier inversion formula

$$\begin{aligned} I_h &= \int a(x,x-h^\gamma x_0+h\xi,\sqrt{h}x\wedge\xi+h^{\gamma-(1/2)}x_0\wedge x)\hat{\Phi}(\mu-v/2)\overline{\hat{\Phi}}(\mu+v/2) \\ &\quad \times\exp(iy\cdot\xi)\exp\left(-\frac{2i}{\sqrt{h}}\mu\, x\cdot y-\frac{i}{\sqrt{h}}v\left(|x|^2+\frac{|y|^2}{4}-R^2\right)\right)\frac{\mathrm{d}\mu\,\mathrm{d}v\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^4\sqrt{h}}. \end{aligned}$$

Substituting ξ by $2h^{-1/2}\mu x+h^{-1/4}\zeta$ and y by $h^{1/4}z$, we obtain

$$\begin{aligned} I_h &= \int a(x,x-h^\gamma x_0+2\sqrt{h}\,\mu\quad x+h^{3/4}\zeta,h^{1/4}x\wedge\zeta+h^{\gamma-(1/2)}x_0\wedge x)\hat{\Phi}(\mu-v/2) \\ &\quad \times\overline{\hat{\Phi}}(\mu+2/v)\exp\left(iz\cdot\zeta-\frac{i}{4}v|z|^2\right)\exp\left(-\frac{i}{\sqrt{h}}v(|x|^2-R^2)\right)\frac{\mathrm{d}\mu\,\mathrm{d}v\,\mathrm{d}z\,\mathrm{d}x\,\mathrm{d}\zeta}{(2\pi)^4\sqrt{h}}. \end{aligned}$$

Then, the stationary phase method in the variables v and $\rho=|x|$ yields that

$$I_h \underset{h-0}{\sim} (2\pi)^{-2}\|\Phi\|_{L^2}^2\int_{|x|=R} a(x,x,h^{\gamma-(1/2)}x_0\wedge x)\,\mathrm{d}x.$$

Therefore, we obtain the Wigner measure

$$\mu(x,\xi)=(2\pi)^{-2}\|\Phi\|_{L^2}^2\,\mathbb{1}_{\{|x|=R\}}(x)\,\mathrm{d}x\otimes\delta(\xi-x),$$

and observe again concentration on $I=\{x\wedge\xi=0\}$. The two-scaled measure provides additional information concerning the exponent γ and the direction x_0. There are three different cases.

$\gamma<1/2$: $\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta-\mathrm{sgn}(x_0\wedge x)\infty)$,
$\gamma=1/2$: $\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta-x_0\wedge x)$,
$\gamma>1/2$: $\nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta)$.

IV. LANDAU–ZENER TRANSITIONS AT HITTING POINTS

A. Propagation outside the crossing

Next, we discuss the propagation of two-scaled Wigner measures outside the singular set S. As before, $\Pi^{\pm}(x)$ denote the orthogonal projectors of $V(x)$ corresponding to the eigenvalues $\pm|x|$. The weak*-limit points in $L^{\infty}(\mathbb{R},\mathcal{A}')$ of $(W_2^h\psi^h(t))_{h>0}$, which are associated via (8) with solutions $(\psi^h(t))_{h>0}$ of the Schrödinger equation (3), are referred to as two-scaled Wigner measures $\nu(t,\cdot)$ of the family $(\psi^h(t))_{h>0}$.

Proposition 2: Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3) with given initial data $(\psi_0^h)_{h>0}$, which are bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Let $\nu(t,\cdot)$ and ν_0 be two-scaled Wigner measures of $(\psi^h(t))_{h>0}$ and $(\psi_0^h)_{h>0}$ for the hypersurface $I=\{x\wedge\xi=0\}$ and the second scale $\sqrt{h}$. If $\operatorname{supp}(\nu_0)\cap S=\varnothing$, *then $\nu(t,\cdot)$ can be decomposed in $\mathcal{D}'(\mathbb{R},\mathcal{A}')$ as*

$$\nu(t,\cdot)=\nu^+(t,\cdot)\Pi^+ + \nu^-(t,\cdot)\Pi^- \quad \textit{outside} \quad S\,, \tag{12}$$

where $\nu^{\pm}(t,\cdot)$ are scalar-valued positive Radon measures supported on $I\times\overline{\mathbb{R}}$,

$$\partial_t\nu^{\pm} + \xi\cdot\nabla_x\nu^{\pm} \mp \frac{x}{|x|}\cdot\nabla_\xi\nu^{\pm}=0 \quad \textit{outside} \quad S\,. \tag{13}$$

Proposition 2 is a consequence of Theorem 2′ in Ref. 6. We note, however, that Theorem 2′ shows transport terms in η-direction, which vanish in our case. This is due to the fact that $\{|\xi|^2/2\pm|x|,x\wedge\xi\}=0$, where $\{f,g\}=\nabla_\xi f\cdot\nabla_x g-\nabla_x g\cdot\nabla_\xi$ denotes the Poisson bracket of two functions f and g on phase space $T^*\mathbb{R}^2$. For the convenience of the reader, we give a proof of Proposition 2 in the Appendix.

From the above transport equations (13) we deduce the continuity of the map $t\mapsto\nu^{\pm}$ on any given time interval, provided the support of $\nu^{\pm}$ does not intersect the singular set S. To obtain $\nu^{\pm}$ on S and to restart the tranport equations every time when hitting S, the work in Ref. 6 provides us with a local result describing the branching of $\nu^{\pm}$ near some point $(0,\xi_0)\in S\backslash\{(0,0)\}$, which we shall explain next.

B. A local Landau–Zener formula

We consider some hitting point $(0,\xi_0)\in S$ with $\xi_0\neq 0$ and some neighborhood W of $(0,\xi_0)$ with $(0,0)\notin W$, such that any classical trajectory included in W crosses S at most once for some given bounded time interval. Such an open set W exists due to the geometry of the trajectories described in Sec. III. We denote by $J^{\pm,p}$ ($p\sim$ past) the sets of classical trajectories, which go into $S\cap W$,

$$J^{\pm,p}=\{(x,\xi)\in T^*\mathbb{R}^2:\exists(0,\zeta_0)\in S\cap W,\exists s\in(-\infty,0),x=x_{\zeta_0}^{\pm}(s),\xi=\xi_{\zeta_0}^{\pm}(s)\},$$

where $(x_{\zeta_0}^{\pm}(s),\xi_{\zeta_0}^{\pm}(s))$ are the plus-minus trajectories with initial datum $(0,\zeta_0)$. Similarly, we define the sets $J^{\pm,f}$ ($f\sim$ future) of classical trajectories, which go out of $S\cap W$,

$$J^{\pm,f}=\{(x,\xi)\in T^*\mathbb{R}^2:\exists(0,\zeta_0)\in S\cap W,\exists s\in(0,+\infty),x=x_{\zeta_0}^{\pm}(s),\xi=\xi_{\zeta_0}^{\pm}(s)\}.$$

Measures $\nu^{\pm}$ with support in W are supported in $(J^{\pm,p}\cup J^{\pm,f})\cap W$ and propagate along the classical trajectories of the corresponding mode. For any $(0,\zeta_0)\in J^{\pm,p}\cap W\cap S$ the tangential space $T_{(0,\zeta_0)}(J^{\pm,p}\cap W)$ is spanned by (ζ_0,e_1) and (ζ_0,e_2), where the e_j denote the canonical unit vectors of $\mathbb{R}^2$. Since $T_{(0,\zeta_0)}(S)$ is spanned by $(0,e_1)$ and $(0,e_2)$, and since $\zeta_0\neq 0$, $J^{\pm,p}\cap W$ and S intersect transversally, and the restriction of $\nu^{\pm}$ to $J^{\pm,p}\cap W\cap S$ is a well-defined distribution, which we denote by $\nu^{\pm,p}$. Analogously, we define $\nu^{\pm,f}$.

If $\nu^{+,p}$ and $\nu^{-,p}$ are mutually singular on $\{|\eta|<+\infty\}$, then according to Theorem 3 in Ref. 6

$$\begin{pmatrix} \nu^{+,f} \\ \nu^{-,f} \end{pmatrix} = \begin{pmatrix} 1-T & T \\ T & 1-T \end{pmatrix} \begin{pmatrix} \nu^{+,p} \\ \nu^{-,p} \end{pmatrix} \quad \text{in} \quad S \cap W \tag{14}$$

with $T=T(\xi,\eta)=\exp(-\pi\eta^2/|\xi|^3)$. We point out that we have described I by the function $g(x,\xi)=x\wedge\xi$, while in the framework of Ref. 6 the hypersurface I is specified by the equation $\tilde{g}(x,\xi)=|\xi|^{-1}(x\wedge\xi)$. Thus, our transfer coefficient T is different from the one in Ref. 6. It is obtained using relation (9).

The proof[6] of the above Landau–Zener formula reduces the Schrödinger equation (3) to a scattering problem, which is close to the original system studied by Landau[16] and Zener[21] in the early 1930s and can be solved explicitly; see the Appendix of Ref. 6. The reduction is achieved by a change of symplectic time-space coordinates $(t,x,\tau,\xi)\mapsto(s,z,\sigma,\zeta)$, such that in the new coordinates

$$J^{\pm,p}=\{\sigma\pm s=0,\zeta_2=0,s<0\},$$

$$J^{\pm,f}=\{\sigma\mp s=0,\ \zeta_2=0,s>0\},$$

$$I=\{\zeta_2=0\},S=\{\sigma=s=\zeta_2=0\}.$$

The system (3) reduces to

$$\frac{h}{i}\partial_s v^h = Q^W(s,z,hD_s,hD_z)v^h$$

with

$$Q=\begin{pmatrix} s & \alpha(\sigma,z)\zeta_2 \\ \alpha(\sigma,z)\zeta_2 & -s \end{pmatrix},$$

$\alpha(z,\sigma)\neq 0$ for all $z\in\mathbb{R}^2$, $\sigma\in\mathbb{R}$, and $v^h=U\psi^h$, where U is a suitably chosen unitary, matrix-valued Fourier integral operator. Of course, most of the work in Ref. 6 deals with the σ-dependence of the function α.

Roughly speaking, the singularity condition on the incident measures $\nu^{+,p}$ and $\nu^{-,p}$ excludes $\sqrt{h}$-interferences between $\Pi^+\psi^h$ and $\Pi^-\psi^h$ at the crossing. One might expect that after one hitting time this seemingly restrictive condition does not hold any more. However, the following result shows that for several interesting cases the singularity condition is indeed satisfied for all hitting times. Thus, the local result (14) can be used to describe the evolution of two-scaled Wigner measures *globally in time*. Recovering the Wigner measure from the two-scaled measure, we also obtain a global description of the weak limit of the position density via relation (4).

C. A global result

We consider a family of initial data $(\psi_0^h)_{h>0}$ bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$ and we suppose that its two-scaled Wigner measure ν_0 is supported in some set $\Sigma\subset I$ such that

$$\Sigma=\{(k(\omega)\omega,l(\omega)\omega):\omega\in\Omega\}$$

with $\Omega\subseteq\mathbf{S}^1$ and measurable functions $k:\Omega\to(0,+\infty)$ and $l:\Omega\to\mathbb{R}$. Such families can be easily built provided the examples of Section 3. If we also assume localization on the mode plus, we have an associated two-scaled Wigner measure ν_0 of the form

$$\nu_0(x,\xi,\eta)=\nu_0^+(x,\xi,\eta)\Pi^+(x).$$

Using the one-to-one mapping between Σ and Ω, we rewrite ν_0 as

$$\nu_0^+(x,\xi,\eta)=\left(\int_\Omega \rho_0(\eta,d\omega)\otimes\delta(x-k(\omega)\omega)\otimes\delta(\xi-l(\omega)\omega)\right)\Pi^+(x), \tag{15}$$

where ρ_0 is a positive Radon measure on $\overline{\mathbb{R}}\times\Omega$.

In this situation there are two types of classical trajectories, which carry the energy. The first type are plus-trajectories with initial data (x_0,ξ_0) for $x_0=k(\omega_0)\omega_0$, $\xi_0=l(\omega_0)\omega_0$ with $\omega_0\in\Omega$. The second type consists of minus-trajectories, which are issued by plus-trajectories hitting S. By Remarks 1 and 2, there are two important facts:

(i) At any of the hitting points $(t,0,\xi,\eta)$, the incident energy is only carried into S by the plus-trajectories, so that the required singularity assumption holds.
(ii) At any of the hitting points $(t,0,\xi,\eta)$ we have $\xi\neq 0$, so that we can use the Landau–Zener formula (14).

We denote by $(x^+(t,\omega),\xi^+(t,\omega))$ the plus-trajectory described in Remark 2 with initial data $(k(\omega)\omega,l(\omega)\omega)$, $\omega\in\Omega$, and we set

$$L(\omega)=\sqrt{|l(\omega)|^2+2|k(\omega)|},\quad t_j(\omega)=l(\omega)+2(j+1)L(\omega),\quad j\in\mathbb{N}_0.$$

Moreover, for $t\geqslant t_j(\omega)$ we denote by $(x_j^-(t,\omega),\xi_j^-(t,\omega))$ the minus-trajectory, which has initial data $(0,\xi^+(t_j(\omega),\omega))$ at time $t=t_j(\omega)$. By Remark 1, we have for $t\geqslant t_j(\omega)$

$$x_j^-(t,\omega)=(-1)^j((t-t_j(\omega))^2/2-L(\omega)(t-t_j(\omega)))\omega,$$

$$\xi_j^-(t,\omega)=(-1)^j(t-t_j(\omega)-L(\omega))\omega.$$

Now, we can describe the evolution of a two-scaled Wigner measure $\nu(t,\cdot)$ for the solutions $(\psi^h(t))_{h>0}$ of the Schrödinger equation (3) as follows.

Theorem 2: *Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3) with initial data $(\psi_0^h)_{h>0}$, which are bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Let $(\psi_0^h)_{h>0}$ have a two-scaled Wigner measure ν_0 for $I=\{x\wedge\xi=0\}$ and scale $\sqrt{h}$, which is of the form (15). If we decompose a two-scaled Wigner measure $\nu(t,\cdot)$ of $(\psi^h(t))_{h>0}$ for I and scale $\sqrt{h}$ as $\nu(t,\cdot)=\nu^+(t,\cdot)\Pi^+ +\nu^-(t,\cdot)\Pi^-$ in $\mathcal{D}'(\mathbb{R},\mathcal{A}')$, then we have for all $t\geqslant 0$*

$$\nu^+(t,x,\xi,\eta)=\int_\Omega \rho^+(t,\eta,\mathrm{d}\omega)\otimes\delta(x-x^+(t,\omega))\otimes\delta(\xi-\xi^+(t,\omega)),$$

$$\nu^-(t,x,\xi,\eta)=\sum_{j\geqslant 0}\ \int_\Omega \rho_j^-(t,\eta,\mathrm{d}\omega)\otimes\ \delta(x-x_j^-(t,\omega))\otimes\delta(\xi-\xi_j^-(t,\omega)),$$

where ρ^+ and ρ_j^-, $j\geqslant 0$, are time-dependent positive scalar-valued Radon measures on $\overline{\mathbb{R}}\times\Omega$ given by

$$\rho^+(t,\eta,\omega)=\sum_{j\geqslant 0}\ \mathbb{1}_{(t_{j-1}(\omega),t_j(\omega))}(t)\,(1-T(\eta,\omega))^j\,\rho_0(\eta,\omega),$$

$$\rho_j^-(t,\eta,\omega)=\mathbb{1}_{(t_j(\omega),+\infty)}(t)\ \ T(\eta,\omega)\,(1-T(\eta,\omega))^j\,\rho_0(\eta,\omega)$$

with $T(\eta,\omega)=\exp(-\pi\eta^2/L(\omega)^3)$ and $t_{-1}(\omega)=0$ for all $\eta\in\overline{\mathbb{R}}$, $\omega\in\Omega$.

Proof: We consider first some ν_0 of the form

$$\nu_0(x,\xi,\eta)=(\delta(x-x_0)\otimes\delta(\xi-\xi_0)\otimes\tilde{\rho}_0(\eta))\Pi^+(x).$$

As mentioned before, we just have to use the description of the classical trajectories issued from the point $(x_0,\xi_0)=(k_0\omega_0,l_0\omega_0)$, $\omega_0\in\Omega$, which is contained in Remarks 1 and 2. We know that for all $t\in(0,t_0(\omega_0))$ the measure ν^+ propagates along the trajectory $(x^+(t,\omega_0),\xi^+(t,\omega_0))$. Thus, we have

$$\nu(t,x,\xi,\eta)=(\delta(x-x^+(t,\omega_0))\otimes\delta(\xi-\xi^+(t,\omega_0))\otimes\tilde{\rho}_0(\eta))\Pi^+(x),$$

when testing against functions $\phi\in\mathcal{C}_0^\infty(\mathbb{R},\mathcal{A})$ with $\mathrm{supp}(\phi)\subset(0,t_0(\omega_0))$. At time $t=t_0(\omega_0)$, there occurs some Landau–Zener partition of energy. Using (14), we obtain

$$\nu(t,x,\xi,\eta)=\nu^+(t,x,\xi,\eta)\,\Pi^+(x)+\nu^-(t,x,\xi,\eta)\Pi^-(x),$$

when testing on $(t_0(\omega_0),t_1(\omega_0))$, where

$$\nu^+(t,x,\xi,\eta)=(1-T(\eta,\omega_0))\tilde{\rho}_0(\eta)\otimes\delta(x-x^+(t,\omega_0))\otimes\delta(\xi-\xi^+(t,\omega_0)),$$

$$\nu^-(t,x,\xi,\eta)=T(\eta,\omega_0)\,\tilde{\rho}_0(\eta)\otimes\delta(x-x_0^-(t,\omega_0))\otimes\delta(\xi-\xi_0^-(t,\omega_0)).$$

The measure ν^- propagates along $(x_1^-(t,\omega_0),\xi_1^-(t,\omega_0))$ for $t\in(t_0(\omega_0),t_1(\omega_0))$, while for ν^+ there happens a new Landau–Zener phenomenon at time $t=t_1(\omega_0)$ at the point $(0,L(\omega_0)\omega_0)$, which opens another trajectory on the mode minus. Now, that is, for $t\in(t_1(\omega_0),t_2(\omega_0))$, the measure ν^- propagates along the two trajectories $(x_j^-(t,\omega_0),\xi_j^-(t,\omega_0))$, $j=1,2$. The same arguments apply recurrently for any of the hitting points

$$t=t_j(\omega_0),\quad x=0,\quad \xi=(-1)^{j+1}L(\omega_0)\omega_0.$$

This proves Theorem 2 for a measure $\rho_0(\eta,\omega)$ of the form $\tilde{\rho}_0(\eta)\otimes\delta(\omega-\omega_0)$. By linearity, the above arguments directly extend to $\rho_0(\eta,\omega)$, which is a discrete Radon measure with respect to ω. Since discrete Radon measures are dense in the set of positive Radon measures, this observation also closes our proof.

Remark 3: If $\nu_0(\{|\eta|=+\infty\})=0$, *then* $(1-T(\eta,\omega))^j$ *goes to zero for* $(\eta,\omega)\in\mathrm{supp}(\rho_0)$ *as* $j\to+\infty$, *and*

$$\int_{\mathbb{R}\times\Omega}\rho^+(t,\mathrm{d}\eta,\mathrm{d}\omega)\xrightarrow[t\to+\infty]{}0.$$

Thus, as t goes to $+\infty$ *all the energy is transferred from the mode plus to the mode minus.*

Remark 4: Since the singularity assumption guaranteeing (14) concerns only the parts of the two-scaled measure supported in $\{|\eta|<+\infty\}$, *the result of Theorem 2 easily extends to initial data* ν_0, *which are also localized on the mode minus with* $\mathrm{supp}(\nu_0^-)\subseteq\{|\eta|=+\infty\}$.

Remark 5: We note that for the linear codimension three and five crossings considered by G. Hagedorn in Ref. 12, again the classical trajectories are the Hamiltonian curves of the functions $|\xi|^2/2\pm|x|$. *Therefore, provided the expected generalization of Ref. 6 to these crossings, the same result as in Theorem 2 will hold for them as well.*

We close by a corollary concerning the weak $L^1(\mathbb{R}^2,\mathbb{C})$-limit of the position density, which implies Theorem 1 of the Introduction when applied to $\Sigma=\Sigma_0$.

Corollary 1: Let us suppose initial data $(\psi_0^h)_{h>0}$, *which are bounded in* $L^2(\mathbb{R}^2,\mathbb{C}^2)$, *which are h-oscillating, and which have a Wigner measure* μ_0 *with* $supp(\mu_0)\subseteq\Sigma$ *and* $\mu_0=\mu_0^+\,\Pi^+$. *If we denote*

$$C=\sup\{|k(\omega)|+\tfrac{1}{2}|l(\omega)|^2:\omega\in\Omega\},$$

then we have for the solutions $(\psi^h(t))_{h>0}$ *of the Schrödinger equation (3) for all times* $t\geqslant 0$ *and for all* $\phi\in\mathcal{C}_0^\infty(\{x\in\mathbb{R}^2:|x|>C\},\mathbb{C})$

$$\lim_{h-0}\int_{\mathbb{R}^2}\phi(x)|\Pi^+(x)\psi^h(t,x)|^2\,\mathrm{d}x=0,$$

$$\lim_{h-0}\int_{\mathbb{R}^2}\phi(x)|\Pi^-(x)\psi^h(t,x)|^2\,\mathrm{d}x=\int_\Omega\sum_{j\geqslant 0}\mathbb{1}_{(t_j(\omega),+\infty)}(t)\;\phi(x_j^-(t,\omega))\;\alpha_j(\mathrm{d}\omega),$$

where $\alpha_j(\omega)=\int_{\overline{\mathbb{R}}}T(\eta,\omega)(1-T(\eta,\omega))^j\rho_0(\mathrm{d}\eta,\omega)$.

Proof: First we prove that for all times $t\geqslant 0$ the family of solutions $(\psi^h(t))_{h>0}$ inherits the property of h-oscillation from the initial data $(\psi_0^h)_{h>0}$. We consider some function $\chi\in\mathcal{C}^\infty(\mathbb{R}^2,\mathbb{R})$ with $\chi(u)=1$ for $|u|>1$ and $\chi(u)=0$ for $|u|<\frac{1}{2}$. We study

$$w^h(t,x)=\chi^W\left(\frac{hD_x}{R}\right)\psi^h(t,x)$$

for $h,R>0$. We have

$$0\;\leqslant\int_{h|\xi|\geqslant R}|\hat{\psi}^h(t,\xi)|^2\,\mathrm{d}\xi\leqslant\|w_R^h(t)\|^2_{L^2(\mathbb{R}^2)}.$$

Moreover, if we denote $H(x,\xi)=(|\xi|^2/2)+V(x)$, then we have

$$ih\,\partial_t w_R^h=H^W(x,hD_x)w_R^h+\frac{h}{R}M_R^h\,\psi^h$$

with $M_R^h=(R/h)\,[\chi^W(hD_x/R),V(x)]$. Analyzing M_R^h, the linear growth of $V(x)$, prevents a direct application of semiclassical Weyl calculus. However, since M_R^h is a linear polynomial in x, the standard arguments still apply—see the proof of Proposition 7.7 in Ref. 2 for example—and we have

$$M_R^h=\frac{1}{2i}(\{\chi,V\}-\{V,\chi\})^W(x,hD_x).$$

Thus, M_R^h is a bounded operator, whose norm is independent from h,R, and will be denoted by $\|M\|$. Since $H^W(x,hD_x)$ is symmetric, we have for all times t

$$\frac{d}{dt}\|w_R^h(t)\|^2_{L^2(\mathbb{R}^2)}\;\leqslant\;\frac{\|M\|}{R}\;\|\psi^h(t)\|_{L^2(\mathbb{R}^2)}\;\|w_R^h(t)\|_{L^2(\mathbb{R}^2)}.$$

Since $(\psi^h(t))_{h>0}$ is bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$ uniformly for all times $t\geqslant 0$, we obtain

$$\|w_R^h(t)\|_{L^2(\mathbb{R}^2)}\leqslant\|w_R^h(0)\|_{L^2(\mathbb{R}^2)}+\frac{C\|M\|\,t}{2R}.$$

Passing to the limits $h\to 0$ and $R\to\infty$, we get the h-oscillation of $(\psi^h(t))_{h>0}$ for all times t. Finally, integrating over the distance η and the momentum ξ in the formulas of Theorem 2, we conclude our corollary's proof.

Observe that $|k(\omega)|+\frac{1}{2}|l(\omega)|^2=L(\omega)^2/2$ describes the boundaries of the strip in the $\mathbb{R}^2_x$-plane, between which the plus-trajectory oscillates. In other words, Corollary 1 means that if we consider $\overline{x}=\varepsilon r\omega$ with $\omega\in\Omega,\varepsilon\in\{\pm 1\},r>|k(\omega)|+1/2\,|l(\omega)|^2$, then the weak limit of $(|\Pi^-(x)\psi^h(t,x)|^2)_{h>0}$ charges $\overline{x}$ recurrently at times

$$t=t_k(\omega)+L(\omega)+\sqrt{L(\omega)^2+2|\overline{x}|},$$

for $k\in\mathbb{N}$ such that $(-1)^k=\varepsilon$. Moreover, the mass above $\overline{x}$ is $\alpha_k(\omega)$.

Remark 6: Theorem 2 and thus Corollary 1 rely on the special features of the Hamiltonian curves of the functions $|\xi|^2/2\pm|x|$. We emphasize that the special form of the initial data has been assumed, such that explicit calculations can easily be performed. However, as long as we choose initial data, which have a Wigner measure μ_0 with support outside S and a two-scaled Wigner measure ν_0 with $\mathrm{supp}(\nu_0^-)\subseteq\{|\eta|=+\infty\}$, the assumption for applying (14) is fulfilled for each hitting time at the crossing. Thus, the evolution of the weak-limit of the position density is utterly described by the transport equations (13) and the Landau–Zener formula (14).

APPENDIX: PROPAGATION OUTSIDE THE CROSSING

Proof: Proposition 2 gives a description of the two-scaled Wigner measure ν outside the singular set $S=\{x=0\}$. Thus, all the test functions $a\in\mathcal{A}$ used in the following have $\mathrm{supp}(a)\cap S=\varnothing$, assuring that in the region under investigation the projectors $\Pi^{\pm}(x)$ depend smoothly on x. There are two steps:

(1) First, we show $[\nu(t,\cdot),\Pi^{\pm}]=0$ in $\mathcal{D}'(\mathbb{R},\mathcal{A}')$ by analyzing

$$L_1^h(t)=\int_{T^*\mathbb{R}^2} tr\left((W^h\psi^h)(t,x,\xi)\,a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\right)\mathrm{d}x\mathrm{d}\xi$$

for matrix-valued test functions $a\in\mathcal{A}$. Due to this commutativity, we can then decompose $\nu(t,\cdot)$ as $\nu(t,\cdot)=\nu^+(t,\cdot)\Pi^+ +\nu^-(t,\cdot)\Pi^-$ with $\nu^{\pm}(t,\cdot)=tr(\nu(t,\cdot)\Pi^{\pm})$.

(2) Second, we show the transport equations for the scalar-valued measures $\nu^{\pm}(t,\cdot)$. Thus, we study the evolution of

$$L_2^h(t)=\int_{T^*\mathbb{R}^2} tr\left((W^h\psi^h)(t,x,\xi)\,\Pi^{\pm}(x)\,a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\right)\mathrm{d}x\mathrm{d}\xi,$$

for scalar-valued test functions $a\in\mathcal{A}$.

First step: Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3), whose Hamiltonian's symbol will be denoted by $H(x,\xi)=(|\xi|^2/2)+V(x)$. Testing against functions $a\in\mathcal{A}$, we will use the notation $a_h(x,\xi)=a(x,\xi,(x\wedge\xi/\sqrt{h}))$. In the distributional sense, we have by the duality of Wigner transformation and Weyl quantization

$$\begin{aligned} ih\frac{d}{dt}L_1^h(t)&=\langle\psi^h(t)|a_h^W(x,hD)\,H^W(x,hD)\,\psi^h(t)\rangle_{L^2(\mathbb{R}^2)}\\ &\quad-\langle H^W(x,hD)\,\psi^h(t)|a_h^W(x,hD)\,\psi^h(t)\rangle_{L^2(\mathbb{R}^2)}\\ &=\langle\psi^h(t)|[a_h^W(x,hD),H^W(x,hD)]\,\psi^h(t)\rangle_{L^2(\mathbb{R}^2)}, \end{aligned}\tag{A1}$$

where the last equation is due to the symmetry of $H^W(x,hD)$. Analyzing this commutator by semiclassical Weyl calculus—see for example Proposition 7.7 in Ref. 2—we apply a cut-off function $\chi\in\mathcal{C}_0^{\infty}(\mathbb{R}^2,\mathbb{R})$ compensating the linear growth in x of $H(x,\xi)$. We choose χ with support outside $\{x=0\}$, such that $\chi(x)=1$ for all $x\in\mathbb{R}^2$, which lie in the projection of $\mathrm{supp}(a)$ onto position space. Since $\chi a=a$ and $a(\nabla_x\chi)=0$, we have

$$a_h^W(x,hD)=a_h^W(x,hD)\,\chi=\chi\,a_h^W(x,hD)$$

and therefore

$$[a_h^W(x,hD),V]=[a_h^W(x,hD),\chi V]=[a_h,\chi V]^W(x,hD)+\frac{h}{2i}(\{a_h,\chi V\}-\{\chi V,a_h\})^W(x,hD).$$

Moreover,

$$\left[a_h^W(x,hD),-\frac{h^2}{2}\Delta\right]=\frac{h}{i}\left\{a_h,\frac{|\xi|^2}{2}\right\}^W(x,hD)+h^2R^h,$$

where $(R^h)_{h>0}$ is a sequence of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$ built with second order derivatives of a_h. We note, that L^2-continuity here and in the following is always implied by the Theorem of Calderon-Vaillancourt; see for example, Theorem 7.11 in Ref. 2. Since every derivative of a_h produces an extra factor $1/\sqrt{h}$, we have

$$[a_h^W(x,hD),H^W(x,hD)]=[a_h,V]^W(x,hD)+\sqrt{h}\,Q^h \tag{A2}$$

with $(Q^h)_{h>0}$ a bounded sequence of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Since we also have $\|\psi^h(t)\|_{L^2}=\|\psi_0^h\|_{L^2}$ for all $t\in\mathbb{R}$, we obtain

$$ih\frac{d}{dt}L_1^h(t)=\int_{T^*\mathbb{R}^2}tr([(W^h\psi^h)(t,x,\xi),V(x,\xi)]\,a_h(x,\xi))\mathrm{d}x\mathrm{d}\xi+\sqrt{h}\,q^h(t)$$

with $(q^h)_{h>0}$ a bounded sequence in $L^\infty(\mathbb{R},\mathbb{C})$. Obviously, we have for all $\phi\in\mathcal{C}_0^\infty(\mathbb{R},\mathcal{A})$

$$ih\int_{\mathbb{R}}\frac{d}{\mathrm{d}t}L_1^h(t)\,\phi(t)\,dt=ih\int_{\mathbb{R}}L_1^h(t)\frac{d}{dt}\phi(t)\,\mathrm{d}t\xrightarrow[h-0]{}0,$$

since $(L_1^h)_{h>0}$ is bounded in $L^\infty(\mathbb{R},\mathbb{C})$. Therefore, in view of (A2), passing to the limit in (A1), we obtain $[\nu,V]=0$ and thus $[\nu,\Pi^\pm]=0$. Since the $\Pi^\pm$ are rank one projectors, we can simplify the decomposition $\nu=\Pi^+\nu\Pi^++\Pi^-\nu\Pi^-$ to $\nu=\nu^+\Pi^++\nu^-\Pi^-$, where $\nu^\pm=tr(\nu\Pi^\pm)$.

Second step: Now, we consider scalar-valued test functions $a\in\mathcal{A}$. We have

$$\frac{d}{dt}L_2^h(t)=\frac{i}{h}\langle[\Pi^\pm a_h^W(x,hD)\Pi^\pm,H^W(x,hD)]\,\psi^h(t)|\psi^h(t)\rangle_{L^2(\mathbb{R}^2)}.$$

We denote $\lambda_\pm(x,\xi)=(|\xi|^2/2)\pm|x|$. Obviously,

$$[\Pi^\pm a_h^W(x,hD)\Pi^\pm,H^W(x,hD)]=[\Pi^\pm a_h^W(x,hD)\Pi^\pm,\lambda_\pm^W(x,hD)].$$

We reuse the cut-off function χ and obtain

$$\chi\,\Pi^\pm\lambda_\pm^W(x,hD)=\lambda_\pm^W(x,hD)\,\chi\,\Pi^\pm+\frac{h}{2i}r^W(x,hD)+o(h),$$

$$\lambda_\pm^W(x,hD)\,\chi\,\Pi^\pm=\chi\Pi^\pm\lambda_\pm^W(x,hD)-\frac{h}{2i}r^W(x,hD)+o(h),$$

where $r(x,\xi)=\{\chi\Pi^\pm,|\xi|^2/2\}$. Here and in the following, the o-notation refers to the space of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Therefore,

$$\begin{aligned}&\frac{i}{h}[\Pi^\pm a_h^W(x,hD)\Pi^\pm,\lambda_\pm^W(x,hD)]\\&\quad=\frac{i}{h}\chi\,\Pi^\pm[a_h^W(x,hD),\lambda_\pm^W(x,hD)]\,\chi\,\Pi^\pm+\frac{1}{2}(\chi\,\Pi^\pm a_h^W(x,hD)r^W(x,hD)\\&\quad+r^W(x,hD)a_h^W(x,hD)\chi\,\Pi^\pm)+o(1).\end{aligned}$$

Since $\chi a=a$ and $a(\nabla_x\chi)=0$, we obtain

$$\begin{aligned}\chi\,\Pi^{\pm}\,a_h^W(x,hD)r^W(x,hD)+r^W(x,hD)a_h^W(x,hD)\chi\,\Pi^{\pm}\\ =\Pi^{\pm}\,a_h^W(x,hD)r^W(x,hD)+r^W(x,hD)a_h^W(x,hD)\Pi^{\pm}\\ =q_h^W(x,hD)+o(1)\end{aligned}$$

with $q=q(x,\xi,\eta)$,

$$q=a(\Pi^{\pm}r+r\Pi^{\pm})=a(\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}+\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}).$$

Moreover, using $\{x\wedge\xi,\lambda_{\pm}(x,\xi)\}=0$, we have

$$\frac{i}{h}\chi[a_h^W(x,hD),\,\lambda_{\pm}^W(x,hD)]\chi=b_h^W(x,hD)+o(1),$$

with $b(x,\xi,\eta)=-\xi\cdot\nabla_x a\pm(x/|x|)\cdot\nabla_\xi a$. Thus, the η-dependance drops, and we obtain

$$\begin{aligned}\lim_{h-0}\frac{d}{dt}L_2^h(t)&=\int_{T^*\mathbb{R}^2}tr((\Pi(x)^{\pm}b(x,\xi,\eta)\Pi^{\pm}(x)+q(x,\xi,\eta))\,\nu(t,\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta))\\ &=\int_{T^*\mathbb{R}^2}b(x,\xi,\eta)\;\nu^{\pm}(t,\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta)+\int_{T^*\mathbb{R}^2}tr(q(x,\xi,\eta)\;\nu(t,\mathrm{d}x,\mathrm{d}\xi,\mathrm{d}\eta)).\end{aligned}$$

For concluding the proof, it remains to show that $tr(q\;\nu(t,\cdot))=0$. Using $(\Pi^{\pm})^2=\Pi^{\pm}$, we get $\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}=\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}+\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}=0$. Since traces are invariant under cyclic permutations, and since $[\,\nu(t,\cdot),\Pi^{\pm}]=0$, we finally have

$$tr(q\;\nu(t,\cdot))=tr(a\;\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}\nu(t,\cdot)+a\;\Pi^{\pm}\{\Pi^{\pm},|\xi|^2/2\}\Pi^{\pm}\nu(t,\cdot))=0.$$

ACKNOWLEDGMENTS

The authors wish to thank A. Joye, who brought their attention to this problem, and P. Gérard and S. Teufel for various discussions.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Choi's proof as a recipe for quantum process tomography

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(Received 5 February 2002; accepted 16 August 2002)

Quantum process tomography is a procedure by which an unknown quantum operation can be fully experimentally characterized. We reinterpret Choi's proof [Linear Algebr. Appl. **10**, 285 (1975)] of the fact that any completely positive linear map has a Kraus representation as a method for quantum process tomography. The analysis for obtaining the Kraus operators is extremely simple. We discuss the systems in which this tomography method is particularly suitable. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1518554]

I. INTRODUCTION

The formalism of quantum operation can be used to describe a very large class of dynamical evolution of quantum systems, including quantum algorithms, quantum channels, noise processes, and measurements. The task to fully characterize an unknown quantum operation $\mathcal{E}$ by applying it to carefully chosen input state(s) and analyzing the output is called quantum process tomography. The parameters characterizing the quantum operation are contained in the density matrices of the output states, which can be measured using quantum state tomography.[1] Recipes for quantum process tomography have been proposed.[2–6] In earlier methods,[2–4] $\mathcal{E}$ is applied to different input states each of exactly the input dimension of $\mathcal{E}$. In Refs. 5 and 6, $\mathcal{E}$ is applied to part of a fixed bipartite entangled state. In other words, the input to $\mathcal{E}$ is entangled with a reference system, and the joint output state is analyzed.

Quantum processing tomography is an essential tool in reliable quantum information processing, allowing error processes and possibly imperfect quantum devices such as gates and channels to be characterized. The method in Ref. 3 has been experimentally demonstrated and used to benchmark the fidelities of teleportation[7] and the controlled-NOT gate,[8] and to verify a core assumption in fault tolerant quantum computation.[8]

The minimum experimental resource for quantum process tomography is determined by the number of parameters characterizing a quantum operation $\mathcal{E}$, and is fixed by the input and output dimensions of $\mathcal{E}$. However, different methods that consume the same quantity of resource can require different types of resources, and be suitable for different physical systems. Furthermore, each method defines a procedure to convert the measured output density matrices to a desired representation of $\mathcal{E}$, and a simpler procedure will enhance the necessary error analysis.

In this paper, we describe in detail the method initially reported in Ref. 6, which is derived as a simple corollary of a mathematical proof reported in Ref. 9. Our goal is twofold. We hope to make this interesting proof more accessible to the quantum information community, as well as to provide a simple recipe for obtaining the Kraus operators of an unknown quantum operation. In the rest of the paper, we review the different approaches of quantum operations, describe Choi's proof and the recipe for quantum process tomography in Secs. II, III, and IV. We discuss the relative merits of various tomography methods in Sec. V.

II. EQUIVALENT APPROACHES FOR QUANTUM OPERATIONS

A quantum state is usually described by a density matrix ρ that is positive semidefinite ($\rho \geqslant 0$, i.e., all eigenvalues are non-negative) with $\mathrm{tr}(\rho)=1$. A quantum operation $\mathcal{E}$ describes the evolution of one state ρ to another $\rho' = \mathcal{E}(\rho)$.

More generally, let $\mathcal{H}_1$ and $\mathcal{H}_2$ denote the input and output Hilbert spaces of $\mathcal{E}$. A density matrix can be regarded as an operator acting on the Hilbert space (but it evolves as a state rather than as an operator). Let $\mathcal{B}(\mathcal{H}_i)$ denote the set of all bounded linear operators acting on $\mathcal{H}_i$ for $i=1,2$. We can consider $\mathcal{E}(M)$ for any $M\in\mathcal{B}(\mathcal{H}_1)$ without restricting the domain to density matrices. A map $\mathcal{E}$ from $\mathcal{B}(\mathcal{H}_1)$ to $\mathcal{B}(\mathcal{H}_2)$ is a quantum operation if it satisfies the following equivalent sets of conditions:

(1) $\mathcal{E}$ is (i) linear, (ii) trace nonincreasing for all $M\geqslant 0$ ($\mathrm{tr}(\mathcal{E}(M))\leqslant\mathrm{tr}(M)$), and (iii) *completely positive*.[10] The map $\mathcal{E}$ is *positive* if $M\geqslant 0$ in $\mathcal{B}(\mathcal{H}_1)$ implies $\mathcal{E}(M)\geqslant 0$ in $\mathcal{B}(\mathcal{H}_2)$. It is completely positive if, for any auxiliary Hilbert space $\mathcal{H}_a$, $\tilde{M}\geqslant 0$ in $\mathcal{B}(\mathcal{H}_1\otimes\mathcal{H}_a)$ implies $(\mathcal{E}\otimes\mathcal{I})(\tilde{M})\geqslant 0$ in $\mathcal{B}(\mathcal{H}_2\otimes\mathcal{H}_a)$ where $\mathcal{I}_a$ is the identity operation on $\mathcal{B}(\mathcal{H}_a)$.

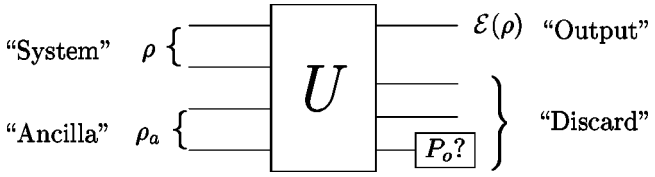
(2) $\mathcal{E}$ has a *Kraus representation* or an *operator sum representation*:[11,9,12]

$$\mathcal{E}(M)=\sum_k A_k M A_k^\dagger, \tag{1}$$

where $\Sigma_k A_k^\dagger A_k\leqslant I$, and I is the identity operator in $\mathcal{B}(\mathcal{H}_1)$. The A_k operators are called the Kraus operators or the operation elements of $\mathcal{E}$.

(3) $\mathcal{E}(M)=\mathrm{Tr}_0[U(M\otimes\rho_a)U^\dagger(I\otimes P_0)]$ for some unitary U in $\mathcal{B}(\mathcal{H}_1\otimes\mathcal{H}_a)$. Here, $\rho_a\in\mathcal{B}(\mathcal{H}_a)$ is a density matrix of the initial state of the ancilla, I is the identity operator in $\mathcal{B}(\mathcal{H}_2)$, $\mathcal{H}_2\otimes\mathcal{H}_0=\mathcal{H}_1\otimes\mathcal{H}_a$, $P_0\in\mathcal{B}(\mathcal{H}_0)$ is a projector, and Tr_0 is a partial trace over $\mathcal{H}_0$.

Each set of conditions represents an approach to quantum operation when the input is a density matrix ($M=\rho$). The first approach puts down three axioms any quantum operation should satisfy. Completely positivity requires that if the input is entangled with some other system (described by the Hilbert space $\mathcal{H}_a$), the output after $\mathcal{E}$ acts on $\mathcal{H}_1$ should still be a valid state. The second approach describes a noise process in which A_k is applied to the state at random, which is particularly convenient in quantum information theory (see Ref. 13 for a review). The third approach describes system-ancilla (or system-environment) interaction. Each evolution results from a unitary interaction of the system with a fixed ancilla state ρ_a, followed by a measurement on a subsystem $\mathcal{H}_0$ with measurement operators $\{P_0, I-P_0\}$, post-selection of the first outcome, and removal of $\mathcal{H}_0$ [see (2)].



(2)

The fact that the third approach is equivalent to the first is nontrivial—the operations in the third approach are actually all that satisfy the three basic axioms.

The earliest proof of the equivalence of the three approaches is due to Ref. 11. Summaries and simplified proofs can be found in Refs. 6, 14, and 15. There are four major steps, showing that the first set of conditions implies the second set and vice versa, and similarly for the second and third sets of conditions. The most nontrivial step is to show that every linear and completely positive map has a Kraus representation. We will describe a proof due to Choi,[9] which is independent of Ref. 11 and is much simpler and elementary.

III. CHOI'S PROOF

The precise statement to be proved is that, if $\mathcal{E}$ is a completely positive linear map from $\mathcal{B}(\mathcal{H}_1)$ to $\mathcal{B}(\mathcal{H}_2)$, then $\mathcal{E}(M)=\Sigma_k A_k M A_k^\dagger$ for some $n_2\times n_1$ matrices A_k, where n_i is the dimension of $\mathcal{H}_i$. Let $|\Phi\rangle=(1/\sqrt{n_1})\,\Sigma_i|i\rangle\otimes|i\rangle$ be a maximally entangled state in $\mathcal{H}_1\otimes\mathcal{H}_1$. Here, $\{|i\rangle\}_{i=1,\cdots,n_1}$ is a basis for $\mathcal{H}_1$. Consider $(\mathcal{I}\otimes\mathcal{E})(\tilde{M})$ where

$$\tilde{M} = n_1 |\Phi\rangle\langle\Phi| = \sum_{i,j=1}^{n_1} |i\rangle\langle j| \otimes |i\rangle\langle j|. \tag{3}$$

$\tilde{M}$ is an $n_1 \times n_1$ array of $n_1 \times n_1$ matrices. The (i,j) block is exactly $|i\rangle\langle j|$:

$$\tilde{M} = \left[\begin{array}{cccc|cccc|cccc|cccc}
1 & 0 & \cdot & 0 & 0 & 1 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 1 \\
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
\hline
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
1 & 0 & \cdot & 0 & 0 & 1 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
\hline
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\hline
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
0 & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 0 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
1 & 0 & \cdot & 0 & 0 & 1 & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & \cdot & 1
\end{array}\right] \tag{4}$$

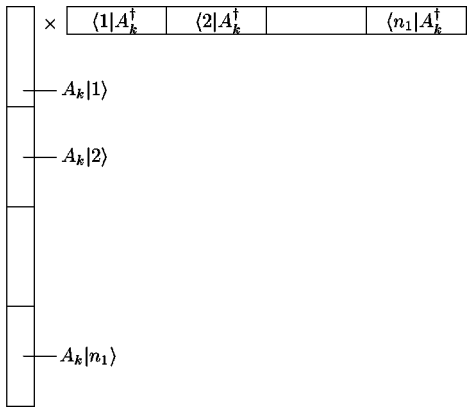
When $\mathcal{I} \otimes \mathcal{E}$ is applied to $\tilde{M}$, the (i,j) block becomes $\mathcal{E}(|i\rangle\langle j|)$, and

$$(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \left[\begin{array}{c|c|c|c}
\mathcal{E}\begin{pmatrix} 1 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} &
\mathcal{E}\begin{pmatrix} 0 & 1 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 1 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} \\
\hline
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} &
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 1 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} \\
\hline
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} \\
\hline
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & 0 \end{pmatrix} &
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & 0 \end{pmatrix} &
\begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} &
\mathcal{E}\begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 1 \end{pmatrix}
\end{array}\right] \tag{5}$$

which is an $n_1 \times n_1$ array of $n_2 \times n_2$ matrices.

We now express $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ in a manner completely independent of Eq. (5). Since $\tilde{M}$ is positive and $\mathcal{E}$ is completely positive, $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ is positive, and can be expressed as $(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \Sigma_k |a_k\rangle\langle a_k|$, where $|a_k\rangle$ for $k = 1, \cdots, n_1 n_2$ are the eigenvectors of $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$, normalized to the respective eigenvalues. One can represent each $|a_k\rangle$ as a column vector and each $\langle a_k|$ as a row vector. We can divide the column vector $|a_k\rangle$ into n_1 segments each of length n_2, and define a matrix A_k with the ith column being the ith segment, so that the ith segment is exactly $A_k|i\rangle$. Then

$$(\mathcal{I}\otimes\mathcal{E})(\tilde{M})=\sum_k$$



(6)

$$(\mathcal{I}\otimes\mathcal{E})(\tilde{M})=\sum_k\begin{bmatrix} A_k|1\rangle\langle 1|A_k^\dagger & A_k|1\rangle\langle 2|A_k^\dagger & \cdots & A_k|1\rangle\langle n_1|A_k^\dagger \\ A_k|2\rangle\langle 1|A_k^\dagger & A_k|2\rangle\langle 2|A_k^\dagger & \cdots & A_k|2\rangle\langle n_1|A_k^\dagger \\ \cdots & \cdots & \cdots & \cdots \\ A_k|n_1\rangle\langle 1|A_k^\dagger & A_k|n_1\rangle\langle 2|A_k^\dagger & \cdots & A_k|n_1\rangle\langle n_1|A_k^\dagger \end{bmatrix} \tag{7}$$

Comparing Eqs. (5) and (7) block by block $\mathcal{E}(M)=\Sigma_k A_k M A_k^\dagger$ for $\forall M=|i\rangle\langle j|$, and thus $\forall M \in \mathcal{B}(\mathcal{H}_1)$ by linearity.

IV. RECIPE FOR QUANTUM PROCESS TOMOGRAPHY

The basic assumptions in quantum process tomography are as follows. The unknown quantum operation $\mathcal{E}$ is available as an ''oracle'' or a ''blackbox'' without information about its internal mechanism. One prepares certain input states and *measures* the corresponding output density matrices to learn about $\mathcal{E}$ systematically. The task to measure the density matrix of a quantum system is called quantum state tomography.[1] To obtain a Kraus representation for $\mathcal{E}$, one needs an experimental procedure that specifies the input states to be prepared, and a numerical method for obtaining the Kraus operators from the measured output density matrices.

A method follows immediately from the proof in Sec. III. We retain all the previously defined notation. The crucial observation is that $(1/n_1)\tilde{M}$ and $(1/n_1)(\mathcal{I}\otimes\mathcal{E})(\tilde{M})$ correspond to the input and output physical states $|\Phi\rangle\langle\Phi|$ and $(\mathcal{I}\otimes\mathcal{E})(|\Phi\rangle\langle\Phi|)$ which can be prepared and measured. Therefore, the procedure is as follows.

(1) Prepare a maximally entangled state $|\Phi\rangle$ in $\mathcal{H}_1\otimes\mathcal{H}_1$.
(2) Subject one system to the action of $\mathcal{E}$, keeping the other system from evolving.
(3) Measure the joint output density matrix $(\mathcal{I}\otimes\mathcal{E})(|\Phi\rangle\langle\Phi|)=(1/n_1)(\mathcal{I}\otimes\mathcal{E})(\tilde{M})$, multiply by n_1, obtain the eigen-decomposition $\Sigma_k|a_k\rangle\langle a_k|$. Divide $|a_k\rangle$ (of length n_1n_2) into n_1 equal segments each of length n_2. A_k is the $n_2\times n_1$ matrix having the ith segment as its ith column.

The maximally entangled state in the above procedure can be replaced by any pure state with maximum Schmidt number, $|\phi\rangle=\Sigma_i\alpha_i(U|i\rangle)\otimes(V|i\rangle)$ where $\alpha_i>0$ are real and $\Sigma_i\alpha_i^2=1$. The output density matrix ρ_{out} is equal to $(\mathcal{I}\otimes\mathcal{E})(|\phi\rangle\langle\phi|)=\Sigma_{i,j}\alpha_i\alpha_j(U|i\rangle\langle j|U^\dagger)\otimes\mathcal{E}(V|i\rangle\langle j|V^\dagger)$. One computes $(U^\dagger\otimes I)\rho_{\text{out}}(U\otimes I)$, divides the (i,j) block by $\alpha_i\alpha_j$, and performs eigen-decomposition to obtain a set of A_k operators. The Kraus operators of $\mathcal{E}$ are given by $A_kV^\dagger$.

V. DISCUSSION

We have provided an experimental and analytic procedure for obtaining a set of Kraus operators A_k for an unknown quantum operation $\mathcal{E}$. The set of A_k is called ''canonical'' in Ref. 9, meaning that the A_k are linearly independent. We remark that any other Kraus representation can be obtained from A_k using the fact that $\mathcal{E}(\rho)=\Sigma_k A_k \rho A_k^\dagger = \Sigma_k B_k \rho B_k^\dagger$ if and only if $A_k = \Sigma_j u_{kj} B_k$ when u_{kj} are the entries of an isometry.[9] Alternatively, one can replace the eigen-decomposition of $(\mathcal{I}\otimes\mathcal{E})(|\Phi\rangle\langle\Phi|)$ by any decomposition into a positive sum to obtain other valid sets of Kraus operators.

Previous methods of quantum process tomography[2–4] involve preparing a set of physical input states ρ_i that form a basis of $\mathcal{B}(\mathcal{H}_1)$, and measuring $\mathcal{E}(\rho_i)$ to determine $\mathcal{E}$. Since the input ρ_i are physical states, they are not trace orthonormal, causing complications in the analysis. [A set of $n\times n$ matrices $\{O_i\}$ is trace orthonormal if $\mathrm{tr}(O_i^\dagger O_j)=\delta_{ij}$.] In contrast, the output state in the current method automatically contains complete information on $\mathcal{E}(|i\rangle\langle j|)$ for the unphysical orthonormal basis for operators $|i\rangle\langle j|$ [see Eq. (5)], which greatly simplifies the analysis to obtain the Kraus operators.

Both previous and current methods require state tomography. The current method requires the preparation of an entangled input state and the ability to stop the evolution of the reference system while $\mathcal{E}$ is being applied. In systems such as the optical system, these requirements are all straightforward, and process tomography can be realized with current experimental techniques. In solution NMR,[16,17] the method still applies to an effective pure maximally entangled input state,[16] if the evolution of the reference system can be stopped. This is possible using decoupling techniques though at the risk of increased error rates due to the decoupling procedure. In general, the current method is suitable for any system in which a maximally entangled can be easily prepared with a controllable reference system (such as one physically separated from the original system).

Any efficient quantum process tomography procedure consumes approximately the same amount of resources, which is determined by the number of degrees of freedom in the quantum operation. In general, to measure an $n\times n$ density matrix, n^2 *ensemble* measurements are needed, requiring $\approx\mathcal{O}(n^2)$ steps. The previous methods require the determination of n_1^2 density matrices each $n_2\times n_2$ and take $\approx\mathcal{O}(n_1^2 n_2^2)$ steps. The current method requires the determination of one $n_1 n_2 \times n_1 n_2$ density matrix which also requires $\approx\mathcal{O}(n_1^2 n_2^2)$ steps. In both cases, the number of steps is of the same order as the number of degrees of freedom in the quantum operation and are optimal in some sense.

ACKNOWLEDGMENTS

We thank Isaac Chuang for suggesting the application of Choi's proof in quantum process tomography. After the initial report of the current result in Ref. 6, G. D'Ariano and P. Presti independently reported a related tomography method.[5] This work is supported in part by the NSA and ARDA under the US Army Research Office, Grant No. DAAG55-98-C-0041.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Robust procedures for converting among Lindblad, Kraus and matrix representations of quantum dynamical semigroups

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(Received 22 January 2002; accepted 1 September 2002)

Given a quantum dynamical semigroup expressed as an exponential superoperator acting on a space of N-dimensional density operators, eigenvalue methods are presented by which canonical Kraus and Lindblad operator sum representations can be computed. These methods provide a mathematical basis on which to develop novel algorithms for quantum process tomography—the statistical estimation of superoperators and their generators—from a wide variety of experimental data. Theoretical arguments and numerical simulations are presented which imply that these algorithms will be quite robust in the presence of random errors in the data. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1518555]

I. INTRODUCTION

The statistical estimation of superoperators from experimental data is variously known as ''quantum channel identification'' [1] or ''quantum process tomography'' (QPT).[2] While this task is important throughout experimental quantum physics, it is an essential component of on-going efforts to develop devices capable of reliable quantum information processing and transmission. At the same time, it is only through these efforts that it is now becoming possible to observe and control quantum systems with the precision needed to collect sufficient data for QPT. At the time of writing, however, very few experimental efforts to systematically determine the complete superoperators of natural or engineered quantum processes have been carried out. An instructive example may be found in Ref. 3, where the QPT procedure detailed in Ref. 2 was applied to NMR data on the two-qubit molecule chloroform. This was followed by fitting a specific decoherence model to the superoperators thereby obtained at multiple time points, in order to estimate the decoherence rates in the model.

The goal of the present paper is to give a reasonably complete and self-contained account of the mathematics needed for *robust* QPT, assuming for the most part that the quantum dynamics may be aptly modelled as a quantum dynamical semigroup (QDS). A QDS describes the evolution of a general open quantum system under the Born–Markov approximations,[4–6] and as such is sufficient to cover most of the systems currently being used or developed for quantum information processing and transmission. By ''robust,'' we mean that the QPT results will not be sensitive to random errors in the data, which is critical since these data are often difficult to obtain and significantly contaminated by noise and other errors. In addition, it is desirable to avoid model fitting and instead to determine the complete superoperator making no prior assumptions about it, although this significantly increases the number of parameters to be estimated.

The robustness of our approach is obtained primarily by using the orthogonal projection of an arbitrary Hermiticity-preserving superoperator or QDS generator onto the convex cone of completely positive superoperators and their generators.[4–6] Of necessity, therefore, this account will rederive much that is already known about quantum dynamical semigroups as well as more general completely positive superoperators, using a consistent notation, fixed operator basis, and a standard set of matrix tools.[7,8] These derivations do not involve qualitative physical arguments (coarse-graining, separation of time scales, etc.), but only the mathematical definitions of the objects involved, and extend much of our earlier work on the ''Hadamard'' representation, which

exists for any ''diagonal'' superoperator, to more general completely positive superoperators and QDS generators.[9]

The main results will be eigenvalue methods by which the projection of an arbitrary Hermiticity-preserving superoperator or QDS generator onto the convex cone of completely positive superoperators can be computed. These projections will be shown to yield certain canonical Kraus and Lindblad representations of completely positive superoperators and QDS generators, respectively, which may be novel and are certainly not well known. The explicit form of the involution which identifies a Hermiticity-preserving superoperator with a quadratic form (or Hermitian supermatrix), herein denoted by ''*Choi*,'' also appears to be new (see Corollary 2 ff.). It is not the intention of this paper to give a single fixed recipe for QPT, because any such recipe must depend to some extent on the nature of the data to be analyzed. Nevertheless, a simple example will be given using simulated data plus added random noise, which should make it clear how such recipes can be derived from these results and further demonstrates that such recipes may be expected to be robust.

II. BACKGROUND ON QUANTUM DYNAMICAL SEMIGROUPS AND THEIR REPRESENTATIONS

This section provides the essential background on quantum dynamical semigroups needed in the remainder of the paper, and in addition defines the basic mathematical operations and notation to be used throughout the paper. A quantum dynamical semigroup (QDS)[4–6] constitutes a bounded one-parameter family of ''superoperators'' $\mathcal{S} = \mathcal{S}(t;\cdot)$ acting linearly on a space of self-adjoint ''density'' operators ρ, and satisfying $\mathcal{S}(t+t';\ \rho) = S(t;\ \rho)S(t';\ \rho)$ for all ρ and $t,\ t' \geqslant 0$. Assuming that ρ acts in turn on a complex Hilbert space of dimension $N<\infty$, a general means of representing a QDS is as a *Kraus operator sum*,[10] namely

$$\rho(t) \equiv \mathcal{S}(t;\rho) = \sum_{m=0}^{M} S_m(t)\rho\, S_m^{\dagger}(t), \tag{1}$$

where one may take $M < N^2$, the S_m act on the same Hilbert space as $\rho = \rho(0)$, and the dagger (†) denotes the adjoint. This ensures not merely that $\mathcal{S}$ preserves the positive semidefiniteness of the density operator ρ, but moreover that it is *completely positive*, meaning that the trace over any other quantum system on which $\mathcal{S}$ acts trivially is again a positive semidefinite operator, as expected for any physically realizable process [*loc. cit.*].

On identifying the Kraus operators S_m with a matrix representation thereof $\mathbf{S}_m$, a well-known result regarding Kronecker matrix (or tensor) products[7,8] implies

$$\mathrm{col}(\boldsymbol{\rho}(t)) = \boldsymbol{\mathcal{S}}(t)\,\mathrm{col}(\boldsymbol{\rho}) \equiv \sum_{m=0}^{M} (\overline{\mathbf{S}}_m(t)\otimes\mathbf{S}_m(t))\,\mathrm{col}(\boldsymbol{\rho}), \tag{2}$$

where $\mathrm{col}(\boldsymbol{\rho})$ denotes the result of stacking the columns of the corresponding density matrix $\boldsymbol{\rho}$ in left-to-right order on top of one another to get a single column vector of dimension N^2, the overline denotes the complex conjugate, ''$\otimes$'' the Kronecker product and juxtaposition denotes matrix multiplication. Although this result (which can be proved by straightforward index gymnastics) is often neglected in theoretical treatises on open quantum systems, it is extremely useful for computational purposes. In particular, it converts the two-sided operations in the Kraus operator sum to one-sided matrix operations, thereby providing a matrix representation of the one-parameter semigroup $\mathcal{S}$. It further makes clear that a completely general linear transformation $\mathcal{T}$ of the ''Liouville'' (matrix) space $\mathbb{C}^{N\times N}$ can also be written in operator sum form as

$$\mathbf{X}' \equiv \mathcal{T}(\mathbf{X}) = \sum_{m,n=0}^{N^2-1} \tau_{mn}\mathbf{T}_m\,\mathbf{X}\,\mathbf{T}_n^{\dagger}, \tag{3}$$

where $\mathbf{X}\in\mathbb{C}^{N\times N}$, the $\mathbf{T}_m$ are a matrix basis thereof, and $\tau_{mn}\in\mathbb{C}$ are coefficients, since

$$\mathrm{col}(\mathbf{X}') \;=\; \left(\sum_{m,n=0}^{N^2-1} \tau_{mn}\;\overline{\mathbf{T}}_n\otimes\mathbf{T}_m\right)\mathrm{col}(\mathbf{X}) \;\equiv\; \mathcal{T}\,\mathrm{col}(\mathbf{X}), \tag{4}$$

and $[\overline{\mathbf{T}}_n\otimes\mathbf{T}_m|0\leqslant m,\;\; n\leqslant N^2-1]$ constitutes an induced basis for the space of ''supermatrices'' $\mathbb{C}^{N^2\times N^2}$. It is easily shown that $\mathcal{T}$ preserves Hermiticity if and only if the matrix of coefficients $[\tau_{mn}]_{m,n=0}^{N^2-1}$ is Hermitian, and that Eq. (3) can be reduced to a Kraus operator sum as in Eq. (1) if and only if the matrix of coefficients is positive semidefinite.[2,4]

The semigroup property $\mathcal{S}(t+t';\rho) \;=\; S(t;\rho)S(t';\rho)$ is of course not assured by the existence of a Kraus operator sum representation, but it is equivalent to the existence of a constant superoperator $\mathcal{G}\in\mathbb{C}^{N^2\times N^2}$ such that $\mathcal{S}(t) = Exp(-\mathcal{G}t)$ for all $t\geqslant 0$, where $Exp(-\mathcal{G}t) = \mathcal{I} -\mathcal{G}t+\frac{1}{2}\mathcal{G}^2t^2+\cdots$ is the corresponding exponential superoperator (see Ref. 11 and citations therein). In general, however, such an exponential will not possess a Kraus operator sum representation, even if the real parts of the eigenvalues of $\mathcal{G}$ are non-negative (ensuring that the evolution is bounded). General necessary and sufficient conditions for a bounded one-parameter family of superoperators to be a QDS were first derived independently by Lindblad[12] and by Gorini, Kossakowski, and Sudarshan,[13] and require that the derivative $\dot\rho$ can be written in the so-called *Lindblad form*,

$$\dot\rho(t) \;=\; \mathcal{L}(\rho(t)) \;\equiv\; \imath[\rho(t),\;H] + \sum_{m=0}^{M}\left(L_m\,\rho(t)\,L_m^\dagger - \frac{1}{2}L_m^\dagger L_m\,\rho(t) - \frac{1}{2}\rho(t)\,L_m^\dagger L_m\right), \tag{5}$$

where $M< N^2$ as above, and both the Hamiltonian H and Lindblad operators L_m are time independent. The superoperator $\mathcal{L}$ itself is called the *Lindbladian*. Translated into matrices, this implies that the decoherent part of the Lindbladian $\mathcal{G}(\cdot)=\mathcal{L}(\cdot)-\imath[\,\cdot\,,H]$ can be written as

$$-\mathcal{G} \;=\; \sum_{m=0}^{M}\left(\overline{\mathbf{L}}_m\otimes\mathbf{L}_m - \frac{1}{2}\mathbf{I}\otimes(\mathbf{L}_m^\dagger\mathbf{L}_m) - \frac{1}{2}(\overline{\mathbf{L}}_m^\dagger\overline{\mathbf{L}}_m)\otimes\mathbf{I}\right), \tag{6}$$

where $\mathbf{I}$ is the $N\times N$ identity matrix.

III. A CANONICAL KRAUS OPERATOR SUM REPRESENTATION

Although superoperators on Liouville space can be represented with respect to an arbitrary matrix basis, as in Eq. (4), any Liouville space basis induced by an arbitrary Hilbert space basis can be regarded as the basis of elementary matrices $\mathbf{E}_{ij}$ (with a ''1'' in the ijth position and zeros elsewhere), which has the advantage identifying the coefficients and the supermatrix elements. For example, one can write the transpose of an arbitrary $N\times N$ matrix in operator sum form as

$$\mathbf{X}^\mathsf{T} \;=\; \sum_{i,j=0}^{N-1}\mathbf{E}_{ij}\,\mathbf{X}\,\mathbf{E}_{ji}^\dagger \;=\; \sum_{i,j=0}^{N-1}\mathbf{E}_{ij}\,\mathbf{X}\,\mathbf{E}_{ij}\,, \tag{7}$$

or equivalently, as

$$\mathrm{col}(\mathbf{X}^\mathsf{T}) \;=\; \left(\sum_{i,j=0}^{N-1}\mathbf{E}_{ji}\otimes\mathbf{E}_{ij}\right)\mathrm{col}(\mathbf{X}) \;\equiv\; \mathcal{K}\,\mathrm{col}(\mathbf{X}). \tag{8}$$

It should be clear that the existence of this operator sum representation of the transpose does not imply that it is a completely positive superoperator (which it is not), since the left and right operators here are identical rather than adjoints of one another as in Eq. (3).

The above supermatrix $\mathcal{K}$ plays a important role in what follows. It is easily seen to be both symmetric and orthogonal, i.e. involutory. Using the relation $\mathbf{E}_{ij} = \mathbf{e}_i \mathbf{e}_j^{\mathsf{T}}$ (where $\mathbf{e}_i, \mathbf{e}_j$ are the elementary unit column vectors) together with the mixed product formula $(\mathbf{A}\otimes\mathbf{B})(\mathbf{C}\otimes\mathbf{D}) = \mathbf{AC}\otimes\mathbf{BD}$,[7] we can also show that it has the interesting property of swapping the order of the factors in a Kronecker product, since

$$\begin{aligned}
\mathcal{K}(\mathbf{X}\otimes\mathbf{Y})\mathcal{K} &= \left(\sum_{i,j=0}^{N-1} \mathbf{E}_{ji}\otimes\mathbf{E}_{ij}\right)(\mathbf{X}\otimes\mathbf{Y})\left(\sum_{k,\ell=0}^{N-1} \mathbf{E}_{\ell k}\otimes\mathbf{E}_{k\ell}\right) \\
&= \sum_{i,j,k,\ell=0}^{N-1} (\mathbf{E}_{ji}\,\mathbf{X}\,\mathbf{E}_{\ell k})\otimes(\mathbf{E}_{ij}\,\mathbf{Y}\,\mathbf{E}_{k\ell}) \\
&= \sum_{i,j,k,\ell=0}^{N-1} (\mathbf{e}_j(\mathbf{e}_i^{\mathsf{T}}\mathbf{X}\,\mathbf{e}_\ell)\,\mathbf{e}_k^{\mathsf{T}})\otimes(\mathbf{e}_i(\mathbf{e}_j^{\mathsf{T}}\mathbf{Y}\,\mathbf{e}_k)\,\mathbf{e}_\ell^{\mathsf{T}}) \\
&= \left(\sum_{j,k=0}^{N-1} Y_{jk}\mathbf{E}_{jk}\right)\otimes\left(\sum_{i,\ell=0}^{N-1} X_{i\ell}\,\mathbf{E}_{i\ell}\right) = \mathbf{Y}\otimes\mathbf{X}, \qquad (9)
\end{aligned}$$

where the matrix elements have been denoted by $X_{i\ell} \equiv \mathbf{e}_i^{\mathsf{T}}\mathbf{X}\,\mathbf{e}_\ell$ and $Y_{jk} \equiv \mathbf{e}_j^{\mathsf{T}}\mathbf{Y}\,\mathbf{e}_k$.

We now use the relation $\mathrm{col}(\mathbf{xy}^{\mathsf{T}}) = \mathbf{y}\otimes\mathbf{x}$ for arbitrary column vectors $\mathbf{x}$, $\mathbf{y}$ to show how the matrix $\mathcal{K}$ also gives us the col of a Kronecker product of matrices as a Kronecker product of their respective cols.

Lemma 1: Given any two $N\times N$ matrices $\mathbf{X}$, $\mathbf{Y}$, *we have*

$$\mathrm{col}(\mathbf{X})\otimes\mathrm{col}(\mathbf{Y}) = (\mathbf{I}\otimes\mathcal{K}\otimes\mathbf{I})\,col(\mathbf{X}\otimes\mathbf{Y}), \qquad (10)$$

where $\mathcal{K}$ is defined as in Eq. (8).

Proof: Applying the definitions, we obtain

$$\begin{aligned}
(\mathbf{I}\otimes\mathcal{K}\otimes\mathbf{I})\,col(\mathbf{X}\otimes\mathbf{Y}) &= \sum_{i,j=0}^{N-1} ((\mathbf{I}\otimes\mathbf{E}_{ji})\otimes(\mathbf{E}_{ij}\otimes\mathbf{I}))\,col(\mathbf{X}\otimes\mathbf{Y}) \\
&= col\left(\sum_{i,j=0}^{N-1} (\mathbf{E}_{ij}\otimes\mathbf{I})(\mathbf{X}\otimes\mathbf{Y})(\mathbf{I}\otimes\mathbf{E}_{ij})\right) \\
&= col\left(\sum_{i,j=0}^{N-1} ((\mathbf{E}_{ij}\,\mathbf{X})\otimes(\mathbf{Y}\,\mathbf{E}_{ij}))\right) \\
&= col\left(\sum_{i,j=0}^{N-1} ((\mathbf{e}_i(\mathbf{e}_j^{\mathsf{T}}\mathbf{X}))\otimes((\mathbf{Y}\,\mathbf{e}_i)\,\mathbf{e}_j^{\mathsf{T}}))\right) \\
&= col\left(\left(\sum_{i=0}^{N-1} (\mathbf{e}_i\otimes(\mathbf{Y}\,\mathbf{e}_i))\right)\left(\sum_{j=0}^{N-1} ((\mathbf{e}_j^{\mathsf{T}}\mathbf{X})\otimes\mathbf{e}_j^{\mathsf{T}})\right)\right) \\
&= col(\mathrm{col}(\mathbf{Y})\,\mathrm{col}^{\mathsf{T}}(\mathbf{X})) = \mathrm{col}(\mathbf{X})\otimes\mathrm{col}(\mathbf{Y}). \qquad (11)
\end{aligned}$$

Q.E.D.

Corollary 2: With everything defined as in the Lemma,

$$\mathrm{col}(\mathbf{Y})\,\mathrm{col}^{\dagger}(\mathbf{X}) \;=\; \sum_{i,j=0}^{N-1} (\mathbf{E}_{ij}\otimes\mathbf{I})(\overline{\mathbf{X}}\otimes\mathbf{Y})(\mathbf{I}\otimes\mathbf{E}_{ij}). \tag{12}$$

Proof: Just apply the inverse of the col operation to the second and last lines of the proof of the Lemma, and add a complex conjugation to account for our use of "†" instead of "T."

Q.E.D.

The "super-superoperator" on the right-hand side of Eq. (12) maps any $N^2\times N^2$ supermatrix $\boldsymbol{\mathcal{S}}$, acting on $N \times N$ matrices $\mathbf{X}$ as $\boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{X})$, to a new supermatrix $\boldsymbol{\mathcal{T}} = \Sigma_{i,j=0}^{N-1}(\mathbf{E}_{ij}\otimes\mathbf{I})\,\boldsymbol{\mathcal{S}}\,(\mathbf{I}\otimes\mathbf{E}_{ij})$, the elements of which are a permutation of those of $\boldsymbol{\mathcal{S}}$. The Corollary shows that if $\boldsymbol{\mathcal{S}}$ is a sum of Kronecker products, as in Eq. (2), then $\boldsymbol{\mathcal{T}}$ is a sum of the corresponding rank one dyadic products, as in Eq. (12). Thus, while Eq. (4) allows us to construct a supermatrix representation from an operator sum, we are now able to give a procedure for going in the other direction.

Proposition 3: Let $\boldsymbol{\mathcal{S}},\boldsymbol{\mathcal{T}}\in\mathbb{C}^{N^2\times N^2}$ *with* $\boldsymbol{\mathcal{T}} = \Sigma_{i,j=0}^{N-1}(\mathbf{E}_{ij}\otimes\mathbf{I})\boldsymbol{\mathcal{S}}(\mathbf{I}\otimes\mathbf{E}_{ij})$, *and let*

$$\boldsymbol{\mathcal{T}} \;\equiv\; \boldsymbol{\mathcal{V}}\,\boldsymbol{\Omega}\,\boldsymbol{\mathcal{W}}^{\dagger} \;=\; \sum_{k=0}^{N^2-1} \omega_k\,\mathbf{v}_k\,\mathbf{w}_k^{\dagger}, \tag{13}$$

be the singular value decomposition of $\boldsymbol{\mathcal{T}}$ (*where* $\mathbf{v}_k$, $\mathbf{w}_k$ *are the columns of the unitary supermatrices* $\boldsymbol{\mathcal{V}}$, $\boldsymbol{\mathcal{W}}$, *respectively, and* $\omega_k\geqslant 0$ *are the singular values). Then for any* $\mathbf{X}\in\mathbb{C}^{N\times N}$,

$$\boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{X}) \;=\; \mathrm{col}(\boldsymbol{\mathcal{T}}\triangleright\mathbf{X}) \;\equiv\; \mathrm{col}\left(\sum_{k=0}^{N^2-1} \omega_k\,\mathbf{V}_k\,\mathbf{X}\,\mathbf{W}_k^{\dagger}\right), \tag{14}$$

where $\mathrm{col}(\mathbf{V}_k) \;=\; \mathbf{v}_k$, $\mathrm{col}(\mathbf{W}_k) \;=\; \mathbf{w}_k$ *and the symbol "*$\triangleright$*" should be read as "applied to."*

Proof: This follows immediately from our foregoing observations, together with the fact that the super-superoperator is involutory, since

$$\begin{aligned}
&\sum_{k,\ell=0}^{N-1} (\mathbf{E}_{k\ell}\otimes\mathbf{I})\left(\sum_{i,j=0}^{N-1} (\mathbf{E}_{ij}\otimes\mathbf{I})\,\boldsymbol{\mathcal{S}}\,(\mathbf{I}\otimes\mathbf{E}_{ij})\right)(\mathbf{I}\otimes\mathbf{E}_{k\ell}) \\
&\quad= \sum_{i,j,k,\ell=0}^{N-1} \delta_{i\ell}\,\delta_{jk}\,(\mathbf{E}_{kj}\otimes\mathbf{I})\,\boldsymbol{\mathcal{S}}\,(\mathbf{I}\otimes\mathbf{E}_{i\ell}) \\
&\quad= \left(\sum_{j=0}^{N-1} \mathbf{E}_{jj}\otimes\mathbf{I}\right)\boldsymbol{\mathcal{S}}\left(\mathbf{I}\otimes\sum_{i=0}^{N-1} \mathbf{E}_{ii}\right) \;=\; \boldsymbol{\mathcal{S}}.
\end{aligned} \tag{15}$$

Q.E.D.

The matrices $\{\mathbf{V}_k\}$ and $\{\mathbf{W}_k\}$ are not generally unitary, but each of these two sets forms a basis for $\mathbb{C}^{N\times N}$, and each is orthonormal with respect to the Hilbert–Schmidt (or Frobenius) inner product $\langle\mathbf{X},\mathbf{Y}\rangle \;\equiv\; \mathrm{tr}(\mathbf{X}^{\dagger}\mathbf{Y})$. By expanding the right-matrices $\mathbf{W}_k$ as linear combinations of the left $\mathbf{V}_k$, one can rewrite the action of $\boldsymbol{\mathcal{T}}$ on $\mathbf{X}$ in the more symmetric form given in Eq. (3). Thus we have obtained a general means of converting a supermatrix $\boldsymbol{\mathcal{S}}$ acting on columnized matrices $\mathrm{col}(\mathbf{X})$ to operator sum form. Much of the foregoing can of course be extended to nonsquare matrices $\mathbb{C}^{M\times N}$, but we shall have no need of that here.

In the case that $\boldsymbol{\mathcal{S}}$ is an elementary (super)matrix representation of a quantum dynamical semigroup, the matrix $\boldsymbol{\mathcal{T}}$ derived from it has considerably more structure, as we shall now show.

Proposition 4: With everything defined as in Proposition 3, the derived supermatrix $\boldsymbol{\mathcal{T}}$ *can be written as*

$$\boldsymbol{\mathcal{T}} = \sum_{i,j=0}^{N-1} \mathrm{col}(\mathbf{S}_{ij})\,\mathrm{col}^{\mathsf{T}}(\mathbf{E}_{ij}) = [\mathcal{S}(\mathbf{E}_{ij})]_{i,j=0}^{N-1} \equiv \begin{bmatrix} \mathcal{S}(\mathbf{E}_{11}) & \mathcal{S}(\mathbf{E}_{12}) & \cdots \\ \mathcal{S}(\mathbf{E}_{21}) & \mathcal{S}(\mathbf{E}_{22}) & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}, \tag{16}$$

where $\mathcal{S}(\mathbf{E}_{ij}) \in \mathbb{C}^{N\times N}$ *is defined by* $\mathrm{col}(\mathcal{S}(\mathbf{E}_{ij})) = \boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{E}_{ij})$, *and* $\mathbf{S}_{ij}$ *is the* ijth $N\times N$ *block of the supermatrix* $\boldsymbol{\mathcal{S}}$.

Proof: The first equality in Eq. (16) follows immediately from Corollary 2 together with the obvious fact that $\boldsymbol{\mathcal{S}} = \Sigma_{i,j=0}^{N-1} \mathbf{E}_{ij}\otimes\mathbf{S}_{ij}$. To prove the second, we first note that for any $0 \leqslant k,\ \ell < N$,

$$\boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{E}_{k\ell}) = \left(\sum_{i,j=0}^{N-1} \mathbf{E}_{ij}\otimes\mathbf{S}_{ij}\right)\mathrm{col}(\mathbf{E}_{k\ell}) = \mathrm{col}\left(\sum_{i,j=0}^{N-1} \mathbf{S}_{ij}\,\mathbf{E}_{k\ell}\,\mathbf{E}_{ji}\right) = \mathrm{col}\left(\sum_{i=0}^{N-1} \mathbf{S}_{i\ell}\,\mathbf{E}_{ki}\right). \tag{17}$$

It follows that

$$\begin{aligned} [\mathcal{S}(\mathbf{E}_{k\ell})]_{k,\ell=0}^{N-1} &= \sum_{k,\ell=0}^{N-1} \mathbf{E}_{k\ell}\otimes\mathcal{S}(\mathbf{E}_{k\ell}) \\ &= \sum_{k,\ell=0}^{N-1} \mathbf{E}_{k\ell}\otimes\left(\sum_{i=0}^{N-1} \mathbf{S}_{i\ell}\mathbf{E}_{ki}\right) \\ &= \sum_{i,k,\ell=0}^{N-1} (\mathbf{I}\otimes\mathbf{S}_{i\ell})(\mathbf{E}_{k\ell}\otimes\mathbf{E}_{ki}). \end{aligned} \tag{18}$$

On the other hand,

$$\begin{aligned} \boldsymbol{\mathcal{T}} = \sum_{i,\ell=0}^{N-1} \mathrm{col}(\mathbf{S}_{i\ell})\,\mathrm{col}^{\mathsf{T}}(\mathbf{E}_{i\ell}) &= \sum_{i,\ell=0}^{N-1} (\mathbf{I}\otimes\mathbf{S}_{i\ell})\,\mathrm{col}(\mathbf{I})\,\mathrm{col}^{\mathsf{T}}(\mathbf{E}_{i\ell}) \\ &= \sum_{i,\ell=0}^{N-1} (\mathbf{I}\otimes\mathbf{S}_{i\ell})\left(\sum_{k=0}^{N-1} \mathbf{e}_k\otimes\mathbf{e}_k\right)(\mathbf{e}_\ell^{\mathsf{T}}\otimes\mathbf{e}_i^{\mathsf{T}}) \\ &= \sum_{i,\ell,k=0}^{N-1} (\mathbf{I}\otimes\mathbf{S}_{i\ell})(\mathbf{E}_{k\ell}\otimes\mathbf{E}_{ki}). \end{aligned} \tag{19}$$

Q.E.D.

In the form $\Sigma_{k,l}\,\mathrm{col}(\mathbf{S}_{k\ell})\mathrm{col}^{\mathsf{T}}(\mathbf{E}_{k\ell})$ the derived supermatrix $\boldsymbol{\mathcal{T}}$ appears to have first been studied in connection with superoperators by Jordan and Sudarshan,[14] whereas the form $[\mathcal{S}(\mathbf{E}_{ij}]_{i,j=0}^{N-1}$ was first used to give an intrinsic characterization of completely positive superoperators by Choi.[15] For this reason we shall henceforth denote it by $Choi(\boldsymbol{\mathcal{S}}) \equiv \Sigma_{i,j=0}^{N-1}(\mathbf{E}_{ij}\otimes\mathbf{I})\boldsymbol{\mathcal{S}}(\mathbf{I}\otimes\mathbf{E}_{ij})$. The next Lemma will enable us to show that in the cases of interest here, it is a Hermitian matrix.

Lemma 5: A superoperator $\mathcal{S}$ *commutes with the operation of taking its adjoint, i.e.,* $\mathcal{S}(Z^\dagger) = (\mathcal{S}(Z))^\dagger$ *for all operators* Z *in its domain, if and only if it maps self-adjoint operators to self-adjoint operators, and if and only if for any elementary matrix representation* $\boldsymbol{\mathcal{S}}$ *of* $\mathcal{S}$,

$$\bar{\boldsymbol{\mathcal{S}}} = \boldsymbol{\mathcal{K}}\,\boldsymbol{\mathcal{S}}\,\boldsymbol{\mathcal{K}}, \tag{20}$$

where the overbar denotes the complex conjugate and $\boldsymbol{\mathcal{K}}$ *is defined as in Eq. (8).*

Proof: Clearly if $\mathcal{S}$ commutes with the adjoint, it maps self-adjoint operators to the same. Now suppose that $\boldsymbol{\mathcal{S}}$ is a matrix representation of $\mathcal{S}$, and let $\mathbf{X} \in \mathbb{C}^{N\times N}$ satisfy $\mathbf{X} = \mathbf{X}^\dagger$; then

$$\mathrm{col}(\mathbf{X}) = \boldsymbol{\mathcal{K}}\,\mathrm{col}(\mathbf{X}^\mathsf{T}) = \boldsymbol{\mathcal{K}}\,\mathrm{col}(\overline{\mathbf{X}}) \tag{21}$$

and hence if $\boldsymbol{\mathcal{S}}$ preserves Hermiticity,

$$\boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{X}) \equiv \mathrm{col}(\mathbf{Y}) = \boldsymbol{\mathcal{K}}\,\mathrm{col}(\overline{\mathbf{Y}}) \equiv \boldsymbol{\mathcal{K}}\bar{\boldsymbol{\mathcal{S}}}\,\mathrm{col}(\overline{\mathbf{X}}) = \boldsymbol{\mathcal{K}}\bar{\boldsymbol{\mathcal{S}}}\boldsymbol{\mathcal{K}}\,\mathrm{col}(\mathbf{X}). \tag{22}$$

Letting $\mathbf{X}$ range over any Hermitian basis of $\mathbb{C}^{N\times N}$ now proves Eq. (20). And finally, if $\mathbf{Z} \in \mathbb{C}^{N\times N}$ is any (not necessarily Hermitian) matrix and $\boldsymbol{\mathcal{S}}$ satisfies Eq. (20), we have

$$\mathrm{col}(\mathcal{S}(\mathbf{Z}^\dagger)) \equiv \boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{Z}^\dagger) = \boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{K}}\,\mathrm{col}(\overline{\mathbf{Z}}) = \boldsymbol{\mathcal{K}}\bar{\boldsymbol{\mathcal{S}}}\,\mathrm{col}(\overline{\mathbf{Z}}) \equiv \mathrm{col}((\mathcal{S}(\mathbf{Z}))^\dagger) \tag{23}$$

which, since it holds for any representation $\boldsymbol{\mathcal{S}}$ and matrix $\mathbf{Z}$, proves $\mathcal{S}(Z^\dagger) = (\mathcal{S}(Z))^\dagger$.

Q.E.D.

Corollary 6: If a superoperator $\mathcal{S}$ commutes with the adjoint operation on its domain, then any Choi matrix for it is Hermitian.

Proof: Clearly a Choi matrix $[\mathcal{S}(\mathbf{E}_{ij})]_{i,j=0}^{N-1}$ is Hermitian if and only if $\mathcal{S}(\mathbf{E}_{ij}) = (\mathcal{S}(\mathbf{E}_{ji}))^\dagger$ for all $0 \leqslant i, j < N$, and if $\boldsymbol{\mathcal{S}}$ is the corresponding matrix representation of $\mathcal{S}$, Lemma 5 implies

$$\begin{aligned}\mathrm{col}((\mathcal{S}(\mathbf{E}_{ji}))^\dagger) &= \boldsymbol{\mathcal{K}}\,\mathrm{col}(\,\overline{\mathcal{S}}(\mathbf{E}_{ji})) = \boldsymbol{\mathcal{K}}\bar{\boldsymbol{\mathcal{S}}}\,\mathrm{col}(\mathbf{E}_{ji}) = (\boldsymbol{\mathcal{K}}\bar{\boldsymbol{\mathcal{S}}}\boldsymbol{\mathcal{K}})\,\mathrm{col}(\mathbf{E}_{ij}) = \boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{E}_{ij}) \\ &= \mathrm{col}(\mathcal{S}(\mathbf{E}_{ij})).\end{aligned} \tag{24}$$

Q.E.D.

Theorem 7 (Choi[15]): *Let $\mathcal{S}$ be a superoperator which commutes with the adjoint operation on its domain. Then $\mathcal{S}$ is completely positive if and only if the Choi matrix associated with any matrix representation of $\mathcal{S}$ is positive semidefinite.*

Proof: Let $\boldsymbol{\mathcal{S}}$ be an elementary matrix representation of $\mathcal{S}$ and $\boldsymbol{\mathcal{T}} = \mathit{Choi}(\boldsymbol{\mathcal{S}})$ be its Choi matrix. This is Hermitian by Corollary 6, and accordingly, we let

$$\boldsymbol{\mathcal{T}} = \boldsymbol{\mathcal{U}}\boldsymbol{\Xi}\boldsymbol{\mathcal{U}}^\dagger = \sum_{n=0}^{N^2-1} \xi_n\,\mathbf{u}_n\,\mathbf{u}_n^\dagger \tag{25}$$

be its eigenvector decomposition, where $\boldsymbol{\mathcal{U}}$ is unitary and the eigenvalues ξ_n are real. Then if $\xi_n \geqslant 0$ for $0 \leqslant n < N^2$, we let $\mathbf{T}_n$ be the sequence of $N \times N$ matrices such that $\mathrm{col}(\mathbf{T}_n) = \sqrt{\xi_n}\ \mathbf{u}_n$. It now follows from Proposition 3 that

$$\boldsymbol{\mathcal{S}}\,\mathrm{col}(\boldsymbol{\rho}) = \left(\sum_{n=0}^{N^2-1} \overline{\mathbf{T}}_n \otimes \mathbf{T}_n\right)\mathrm{col}(\boldsymbol{\rho}) = \mathrm{col}\left(\sum_{n=0}^{N^2-1} \mathbf{T}_n\,\boldsymbol{\rho}\,\mathbf{T}_n^\dagger\right). \tag{26}$$

The right-hand side provides a Kraus operator sum representation for $\mathcal{S}$, which by the previously mentioned work of Kraus[10] proves that $\mathcal{S}$ is completely positive, as claimed.

Conversely, if $\mathcal{S}$ is completely positive, it may be expressed in Kraus operator sum form as

$$\mathcal{S}(\rho) = \sum_{m=0}^{M} S_m\,\rho\,S_m^\dagger, \tag{27}$$

and it follows from Eq. (2) that any elementary matrix representation $\boldsymbol{\mathcal{S}}$ thereof satisfies

$$\boldsymbol{\mathcal{S}} = \sum_{m=0}^{M} \overline{\mathbf{S}}_m \otimes \mathbf{S}_m \tag{28}$$

for suitable $\mathbf{S}_m \in \mathbb{C}^{N\times N}$. By Proposition 3, therefore, corresponding Choi matrix $\boldsymbol{\mathcal{T}} = Choi(\boldsymbol{\mathcal{S}})$ is a sum of dyads, that is

$$\boldsymbol{\mathcal{T}} = \sum_{m=0}^{M} \mathrm{col}(\mathbf{S}_m)\,\mathrm{col}^{\dagger}(\mathbf{S}_m), \tag{29}$$

which is necessarily positive semidefinite.

Q.E.D.

Corollary 8: Any Kraus operator sum $\mathcal{S}(\rho) = \Sigma_{m=0}^{M} S_m \rho S_m^{\dagger}$ *can be written in canonical operator sum form as*

$$\mathcal{S}(\rho) = \sum_{n=0}^{N^2-1} T_n \rho T_n^{\dagger}, \tag{30}$$

with $\langle T_n, T_{n'}\rangle = \mathrm{tr}(T_n^{\dagger} T_{n'}) = 0$ *for all* $0 \leqslant n \neq n' < N^2$ *and* $\|T_n\|^2 = \langle T_n, T_n\rangle = 0$ *for all* $n > M$. *Subject to these conditions, the canonical form is unique up to the overall phase of the operators* T_n *unless the Hilbert–Schmidt norms satisfy* $\|T_n\| = \|T_{n'}\|$ *for some* $n' \neq n$, *in which case it is only unique up to unitary linear combinations of the operators in such degenerate subspaces.*

Proof: Implicit in the proof of Theorem 7.

Q.E.D.

IV. A CANONICAL LINDBLAD REPRESENTATION

We now turn our attention specifically to quantum dynamical semigroups, which (as mentioned in the Introduction) may be assumed to be given in the form of a superoperator exponential $\mathcal{S} = Exp(-\mathcal{F}t)$. The time-independent generator will usually be of the form $\mathcal{F} = \mathcal{G} + \imath\mathcal{H}$ for superoperators $\mathcal{G}$ and $\mathcal{H}$, where $\imath^2 = -1$, $\mathcal{H}(\rho) \equiv [H, \rho]$ for the Hamiltonian H of the system in question, and $\mathcal{G}$ is often called the *relaxation superoperator*.[16] Although $\mathcal{G}$ may often be self-adjoint, this is not necessarily the case.

An important property of physically meaningful operations on density operators ρ, which we have neglected up to now, is that they preserve the trace $\mathrm{tr}(\rho) = 1$. Given an operator sum representation $\mathcal{S}(\rho) = \Sigma_{m,n=0}^{N^2-1} \tau_{mn} T_m \rho T_n^{\dagger}$, this is easily seen to be equivalent to $\Sigma_{m,n=0}^{N^2-1} \tau_{mn} T_n^{\dagger} T_m = I$, the identity. We seek an equivalent condition in terms of an elementary matrix representation $\boldsymbol{\mathcal{S}}$. To this end we expand $\boldsymbol{\mathcal{S}}$ versus the basis of elementary matrices as

$$\boldsymbol{\mathcal{S}} \equiv \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij} \ (\mathbf{E}_{\ell j} \otimes \mathbf{E}_{ki}) = \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij} \ (\mathbf{e}_{\ell} \otimes \mathbf{e}_k)(\mathbf{e}_j \otimes \mathbf{e}_i)^{\dagger}, \tag{31}$$

where

$$s_{k\ell}^{ij} \equiv \mathrm{tr}((\mathbf{E}_{\ell j} \otimes \mathbf{E}_{ki})^{\dagger} \boldsymbol{\mathcal{S}}) = (\mathbf{e}_{\ell} \otimes \mathbf{e}_k)^{\dagger} \boldsymbol{\mathcal{S}} (\mathbf{e}_j \otimes \mathbf{e}_i), \tag{32}$$

so that the corresponding operator sum representation becomes

$$\boldsymbol{\mathcal{S}}\,\mathrm{col}(\boldsymbol{\rho}) = \mathrm{col}\left(\sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij} \ \mathbf{E}_{ki} \boldsymbol{\rho} \mathbf{E}_{j\ell} \right). \tag{33}$$

For future reference, we note further that the associated Choi matrix is given by

$$\begin{aligned} Choi(\boldsymbol{\mathcal{S}}) &\equiv \sum_{i,j,k,\ell=0}^{N-1} \sum_{m,n=0}^{N-1} s_{k\ell}^{ij} \ (\mathbf{E}_{mn}\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki}\mathbf{E}_{mn}) \\ &= \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij} \ (\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell}) \\ &= \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij} \ (\mathbf{e}_i\otimes\mathbf{e}_k)\,(\mathbf{e}_j\otimes\mathbf{e}_\ell)^\dagger. \end{aligned} \tag{34}$$

This shows that while the representative supermatrix $\boldsymbol{\mathcal{S}}$ in this basis is formed by identically ordering the upper and lower index pairs of $s_{k\ell}^{ij}$ and using the resulting list as the row and column indices, the Choi matrix is obtained by ordering the right and left index pairs and using the result as the row and column indices, respectively.

Lemma 9: A superoperator $\mathcal{S}$ with representative matrix $\boldsymbol{\mathcal{S}} = [s_{k\ell}^{ij}]_{k,\ell;i,j=0}^{N-1}$ versus a Hilbert space basis $\{\mathbf{e}_i\}_{i=0}^{N-1}$ preserves the trace of its operands if and only if

$$\mathrm{col}^\dagger(\mathbf{I})\,\boldsymbol{\mathcal{S}}\,(\mathbf{e}_i\otimes\mathbf{e}_j) = \sum_{k=0}^{N-1} s_{kk}^{ij} = \delta^{ij} \quad \text{for } 0 \leqslant i,\ j < N, \tag{35}$$

where δ^{ij} is a Kronecker delta.

Proof: The usual trace-preservation condition can be written as

$$\begin{aligned} \mathbf{I} = \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij}\ \mathbf{E}_{j\ell}\mathbf{E}_{ki} = \sum_{i,j,k=0}^{N-1} s_{kk}^{ij}\ \mathbf{E}_{ji} &= \sum_{i,j=0}^{N-1} \left(\sum_{k=0}^{N-1} (\mathbf{e}_k\otimes\mathbf{e}_k)^\dagger\,\boldsymbol{\mathcal{S}}\,(\mathbf{e}_j\otimes\mathbf{e}_i) \right) \mathbf{E}_{ji} \\ &= \sum_{i,j=0}^{N-1} (\mathrm{col}^\dagger(\mathbf{I})\,\boldsymbol{\mathcal{S}}\,(\mathbf{e}_i\otimes\mathbf{e}_j))\mathbf{E}_{ij}, \end{aligned} \tag{36}$$

which is equivalent to the stated conditions.

Q.E.D.

The Lemma can be stated more succinctly by saying that $\mathrm{col}(\mathbf{I})$ is a left-eigenvector of $\boldsymbol{\mathcal{S}}$ with eigenvalue 1. We note that for another important class of superoperators, namely the identity preserving or *unital* superoperators, the operator sum representations of which satisfy $I = \mathcal{S}(I) = \sum_{m,n=0}^{N^2-1} \tau_{mn} T_m T_n^\dagger$, may also be characterized in terms of their supermatrix representations by $\sum_{i=0}^{N-1} s_{k\ell}^{ii} = (\mathbf{e}_k\otimes\mathbf{e}_\ell)^\dagger \boldsymbol{\mathcal{S}}\,\mathrm{col}(\mathbf{I}) = \delta_{k\ell}$, i.e., $\mathrm{col}(\mathbf{I})$ is a right-eigenvector of $\boldsymbol{\mathcal{S}}$ with eigenvalue 1. It is easily seen that if the Lindblad operators are normal (or commute with the adjoints), then $\mathcal{S} = \mathcal{S}(t)$ is a unital QDS.

Returning now to the problem of deriving a Lindblad representation for a QDS $\boldsymbol{\mathcal{S}}(t)$ from a matrix exponential representation $\boldsymbol{\mathcal{S}}(t) = Exp(-\boldsymbol{\mathcal{F}}t)$ thereof, the obvious way to proceed, given the results of the preceding section, is to simply differentiate it,

$$\begin{aligned} \partial_t\, Exp(-\boldsymbol{\mathcal{F}}t)\big|_{t=0} = -\boldsymbol{\mathcal{F}} &\equiv -\sum_{i,j,k,\ell=0}^{N-1} f_{k\ell}^{ij}\ (\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki}) \\ &= \partial_t \sum_{i,j,k,\ell=0}^{N-1} s_{k\ell}^{ij}\ (\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki})\Big|_{t=0} \\ &\equiv \sum_{i,j,k,\ell=0}^{N-1} \dot{s}_{k\ell}^{ij}\ (\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki}) \end{aligned} \tag{37}$$

(note that the generator is actually time independent). Differentiation of our trace-preservation condition similarly yields $\sum_{k=0}^{N-1} \dot{s}_{kk}^{ij} = -\sum_{k=0}^{N-1} f_{kk}^{ij} = 0$ for all $0 \leqslant i,\ j < N$, and hence

$$\dot{\boldsymbol{\rho}}(t) = \sum_{i,j,k,\ell=0}^{N-1} \dot{s}^{ij}_{k\ell} \ \mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} = -\sum_{i,j,k,\ell=0}^{N-1} f^{ij}_{k\ell} \ \mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell}$$

$$= \dot{\boldsymbol{\rho}}(t) - \frac{1}{2}\sum_{i,j,k=0}^{N-1} \dot{s}^{ij}_{kk}(\mathbf{E}_{ji}\,\boldsymbol{\rho} + \boldsymbol{\rho}\,\mathbf{E}_{ji})$$

$$= \sum_{i,j,k,\ell=0}^{N-1} \dot{s}^{ij}_{k\ell} \ \left(\mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} - \frac{1}{2}(\mathbf{E}_{j\ell}\,\mathbf{E}_{ki}\,\boldsymbol{\rho} + \boldsymbol{\rho}\,\mathbf{E}_{j\ell}\,\mathbf{E}_{ki})\right). \tag{38}$$

Thus we could in principle obtain a canonical Lindblad representation for $\dot{\boldsymbol{\rho}}(t)$ simply by diagonalizing the (time-independent) Choi matrix of the generator $[\dot{s}^{ij}_{k\ell}]^{N-1}_{i,k;j,\ell=0} = [\Sigma^{N-1}_{m,n=0} \ \varphi^m_n \ u^{im}_{kn} \ \overline{u}^{jm}_{\ell n}]^{N-1}_{i,k;j,\ell=0}$, and letting the Lindblad operators be defined by the matrices

$$\mathbf{L}^m_n \equiv \sqrt{\varphi^m_n}\sum_{i,k=0}^{N-1} u^{im}_{kn}\,\mathbf{E}_{ik} \tag{39}$$

—*providing* that the eigenvalues $\varphi^m_n \geqslant 0$ for all $0 \leqslant m, n < N$. But then our trace-preservation condition for $\dot{\boldsymbol{\rho}}$ implies

$$\sum_{m,n=0}^{N-1} \mathbf{L}^m_n(\mathbf{L}^m_n)^\dagger = \sum_{m,n=0}^{N-1} \varphi^m_n \sum_{i,j,k,\ell=0}^{N-1} u^{im}_{kn}\,\overline{u}^{jm}_{\ell n}\,\mathbf{E}_{ik}\,\mathbf{E}_{\ell j}$$

$$= \sum_{i,j,k=0}^{N-1}\sum_{m,n=0}^{N-1} (\varphi^m_n\, u^{im}_{kn}\overline{u}^{jm}_{kn})\mathbf{E}_{ij}$$

$$= \sum_{i,j,k=0}^{N-1} \dot{s}^{ij}_{kk}\ \mathbf{E}_{ji} = \mathbf{0}, \tag{40}$$

which contradicts the fact that a nontrivial sum of positive semidefinite matrices cannot vanish. This result is easily shown to be independent of the choice of matrix basis.

It follows that there must be some redundance in our choice of coefficients in any nondiagonal Lindblad-type equation of the form given in Eq. (38). Moreover, such an equation, by its very form, is assured of preserving the trace ($\partial_t \operatorname{tr}(\boldsymbol{\rho}(t)) = \operatorname{tr}(\dot{\boldsymbol{\rho}}(t)) = 0$), so that the trace-preservation condition satisfied by the derivatives of the coefficients in an operator sum representation is not needed. Our problem is to find a way to modify the matrix of coefficients $[\dot{s}^{ij}_{k\ell}]^{N-1}_{m,n=0}$, while preserving the underlying mapping $\boldsymbol{\rho} \mapsto \dot{\boldsymbol{\rho}}$, such that the result is positive semidefinite and so can be diagonalized to obtain a canonical Lindbladian. Because any Lindblad operator of the form $\mathbf{L} = \alpha\mathbf{I}$ with $\alpha \in \mathbb{C}$ adds nothing to $\dot{\boldsymbol{\rho}}$, we shall seek to eliminate the corresponding degree of freedom from the coefficients.

Lemma 10: In any quantum dynamical semigroup with exponential representation $\mathcal{S}(t) = \mathit{Exp}(-\mathcal{F}t)$, *the generator's matrix* $\boldsymbol{\mathcal{F}}$ *versus a Hilbert space basis satisfies*

$$\operatorname{col}^\dagger(\mathbf{I})\ \mathit{Choi}(-\boldsymbol{\mathcal{F}})\ \operatorname{col}(\mathbf{I}) < 0. \tag{41}$$

If the generator is of the form $\mathcal{F} = \mathcal{G} + \imath\mathcal{H}$ *where* $\mathcal{H}$ *is a commutation superoperator and* $\langle \mathcal{G}, \mathcal{C}\rangle \equiv \operatorname{tr}(\mathcal{G}^\dagger\mathcal{C}) = 0$ *for any commutation superoperator* $\mathcal{C}$, *then the corresponding matrix projection satisfies*

$$\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,\mathit{Choi}(\boldsymbol{\mathcal{G}})\,\boldsymbol{\mathcal{P}}^{\mathbf{I}} = \boldsymbol{\mathcal{P}}^{\mathbf{I}}\,\mathit{Choi}(\boldsymbol{\mathcal{F}})\,\boldsymbol{\mathcal{P}}^{\mathbf{I}} \quad (\boldsymbol{\mathcal{P}}^{\mathbf{I}} \equiv \mathbf{I}\otimes\mathbf{I} - \operatorname{col}(\mathbf{I})\operatorname{col}^\dagger(\mathbf{I})/N). \tag{42}$$

Proof: To prove Eq. (41), we first observe that

$$\begin{aligned}\mathrm{col}^\dagger(\mathbf{I})\, \mathit{Choi}(-\boldsymbol{\mathcal{F}})\, \mathrm{col}(\mathbf{I}) &= -\sum_{m,n=0}^{N-1} (\mathbf{e}_m\otimes\mathbf{e}_m)^\dagger \left(\sum_{i,j,k,\ell=0}^{N-1} f_{k\ell}^{ij}\, (\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell}) \right) (\mathbf{e}_n\otimes\mathbf{e}_n) \\ &= -\sum_{m,n=0}^{N-1} \left(\sum_{i,j,k,\ell=0}^{N-1} (f_{k\ell}^{ij}\, ((\mathbf{e}_m^\dagger \mathbf{E}_{ij}\, \mathbf{e}_n)\otimes(\mathbf{e}_m^\dagger \mathbf{E}_{k\ell}\, \mathbf{e}_n))) \right) \\ &= -\sum_{m,n=0}^{N-1} f_{mn}^{mn} = -\mathrm{tr}(\boldsymbol{\mathcal{F}}). \end{aligned} \tag{43}$$

Since $\mathit{Choi}(-\boldsymbol{\mathcal{F}})$ is Hermitian, this quantity is real, and since $\mathcal{S}(t)$ is bounded, the eigenvalues of $-\boldsymbol{\mathcal{F}}$ must all have negative real parts, so that $-\mathrm{tr}(\boldsymbol{\mathcal{F}}) < 0$.

To prove Eq. (42), we first note that it is sufficient to prove this for the commutation superoperator of an arbitrary elementary matrix $\mathbf{E}_{ij}$, and transform its generating supermatrix to the corresponding Choi matrix:

$$\begin{aligned}\mathit{Choi}(\mathbf{E}_{ij}\otimes\mathbf{I} - \mathbf{I}\otimes\mathbf{E}_{ji}) &= \sum_{k,\ell=0}^{N-1} ((\mathbf{E}_{k\ell}\, \mathbf{E}_{ij})\otimes\mathbf{E}_{k\ell} - \mathbf{E}_{k\ell}\otimes(\mathbf{E}_{ji}\mathbf{E}_{k\ell})) \\ &= \sum_{k=0}^{N-1} (\mathbf{E}_{kj}\otimes\mathbf{E}_{ki} - \mathbf{E}_{ik}\otimes\mathbf{E}_{jk}). \end{aligned} \tag{44}$$

Plugging the second term into the projection now yields

$$\begin{aligned}\boldsymbol{\mathcal{P}}^{\mathbf{I}} \left(\sum_{k=0}^{N-1} \mathbf{E}_{ik}\otimes\mathbf{E}_{jk} \right) \boldsymbol{\mathcal{P}}^{\mathbf{I}} &= \sum_{k=0}^{N-1} \mathbf{E}_{ik}\otimes\mathbf{E}_{jk} - \frac{\delta_{ij}}{N}\mathrm{col}(\mathbf{I}) \sum_{k=0}^{N-1} (\mathbf{e}_k\otimes\mathbf{e}_k)^\dagger \\ &\quad - (\mathbf{e}_i\otimes\mathbf{e}_j)\, \mathrm{col}^\dagger(\mathbf{I}) + \frac{\delta_{ij}}{N}\mathrm{col}(\mathbf{I})\, \mathrm{col}^\dagger(\mathbf{I}). \end{aligned} \tag{45}$$

Since the first and third terms as well as the second and fourth terms on the right-hand side differ only in sign, this projection vanishes identically. A similar calculation shows that the projection of the first term on the right-hand side of Eq. (44) likewise vanishes, establishing the Lemma.

Q.E.D.

Henceforth, we take $\mathcal{G} = \mathcal{F} - \imath\mathcal{H}$ where $\mathcal{H}$ is the commutator part of $\mathcal{F}$, and let $g_{k\ell}^{ij}$ be the corresponding array of coefficients. A final technical Lemma will be needed to prove the first real result in this section.

Lemma 11: If $\langle \mathcal{G},\mathcal{C}\rangle \equiv \mathrm{tr}(\mathcal{G}^\dagger\mathcal{C}) = 0$ *for every commutation superoperator* $\mathcal{C}$ *as above, then the coefficients* $g_{k\ell}^{ij}$ *of any supermatrix representation* $\boldsymbol{\mathcal{G}}$ *satisfy*

$$\sum_{k=0}^{N-1} g_{km}^{kn} = \sum_{\ell=0}^{N-1} g_{n\ell}^{m\ell} \tag{46}$$

for all $0 \leqslant m, n < N$.

Proof: The proof is by direct computation:

$$
\begin{aligned}
0 &= \mathrm{tr}\left((\mathbf{E}_{nm}\otimes\mathbf{I} - \mathbf{I}\otimes\mathbf{E}_{mn}) \sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\, (\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki}) \right) \\
&= \mathrm{tr}\left(\sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\, ((\mathbf{E}_{nm}\,\mathbf{E}_{\ell j})\otimes\mathbf{E}_{ki} - \mathbf{E}_{\ell j}\otimes(\mathbf{E}_{mn}\,\mathbf{E}_{ki})) \right) \\
\Rightarrow \quad \mathrm{tr}\left(\sum_{i,j,k=0}^{N-1} g^{ij}_{km}\, (\mathbf{E}_{nj}\otimes\mathbf{E}_{ki}) \right) &= \mathrm{tr}\left(\sum_{i,j,\ell=0}^{N-1} g^{ij}_{n\ell}\, (\mathbf{E}_{\ell j}\otimes\mathbf{E}_{mi}) \right) \\
\Rightarrow \quad \sum_{i,j,k=0}^{N-1} g^{ij}_{km}\ \mathrm{tr}(\mathbf{E}_{nj})\,\mathrm{tr}(\mathbf{E}_{ki}) &= \sum_{i,j,\ell=0}^{N-1} g^{ij}_{n\ell}\ \mathrm{tr}(\mathbf{E}_{\ell j})\,\mathrm{tr}(\mathbf{E}_{mi}) \\
\Rightarrow \quad \sum_{i,j,k=0}^{N-1} g^{ij}_{km}\ \delta_{nj}\,\delta_{ki} &= \sum_{i,j,\ell=0}^{N-1} g^{ij}_{n\ell}\ \delta_{\ell j}\,\delta_{mi}\,. \qquad (47)
\end{aligned}
$$

Q.E.D.

This Lemma may be paraphrased by saying that the ''partial trace'' (or contraction by $\mathbf{I}$) of $\boldsymbol{\mathcal{G}}$ with respect to either its left or right Kronecker factors are the transposes of one another.

Proposition 12: Let $\mathcal{S}(t) = Exp(-\mathcal{F}t)$ *be a quantum dynamical semigroup with* $\mathcal{F} = \mathcal{G} + \imath\mathcal{H}$ *as above. Then if their supermatrices versus a Hilbert space basis are* $\boldsymbol{\mathcal{F}} = [f^{ij}_{k\ell}]^{N-1}_{k,\ell;i,j=0}$, $\boldsymbol{\mathcal{G}} = [g^{ij}_{k\ell}]^{N-1}_{k,\ell;i,j=0}$ *and* $\boldsymbol{\mathcal{H}} = \mathbf{I}\otimes\mathbf{H} - \overline{\mathbf{H}}\otimes\mathbf{I}$, *we have*

$$
\begin{aligned}
\dot{\boldsymbol{\rho}}(t) &\equiv -\sum_{i,j,k,\ell=0}^{N-1} f^{ij}_{k\ell}\ \mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} \equiv \imath[\boldsymbol{\rho}(t),\mathbf{H}] - \sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\ \mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} \\
&= \imath[\boldsymbol{\rho}(t),\mathbf{H}] - \frac{1}{2}\sum_{i,j,k,\ell=0}^{N-1} \breve{g}^{ij}_{k\ell}\,(2\,\mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} - \mathbf{E}_{j\ell}\,\mathbf{E}_{ki}\,\boldsymbol{\rho}(t) - \boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell}\,\mathbf{E}_{ki}) \\
&= \imath[\boldsymbol{\rho}(t),\mathbf{H}] - \sum_{i,j=0}^{N-1}\left(\sum_{k,\ell=0}^{N-1} \breve{g}^{ij}_{k\ell}\,\mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} - \frac{1}{2}\sum_{k=0}^{N-1} \breve{g}^{ij}_{kk}\,(\mathbf{E}_{ji}\,\boldsymbol{\rho}(t) + \boldsymbol{\rho}(t)\,\mathbf{E}_{ji}) \right),
\end{aligned}
\qquad (48)
$$

where $[\breve{g}^{ij}_{k\ell}]^{N-1}_{k,\ell;i,j=0}$ *are the coefficients of the supermatrix*

$$
\breve{\boldsymbol{\mathcal{G}}} \equiv Choi(\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,Choi(\boldsymbol{\mathcal{G}})\,\boldsymbol{\mathcal{P}}^{\mathbf{I}}) = Choi(\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,Choi(\boldsymbol{\mathcal{F}})\,\boldsymbol{\mathcal{P}}^{\mathbf{I}}). \qquad (49)
$$

Proof: Note that $\mathcal{H}$ occurs on both sides of Eq. (48), so we can just ignore it (i.e., set $\mathbf{H} = 0$) in the proof. Since $\mathrm{col}(\mathbf{I})\mathrm{col}^{\dagger}(\mathbf{I}) = \Sigma^{N-1}_{m,n=0}\,\mathbf{E}_{mn}\otimes\mathbf{E}_{mn}$, we find that

$$
\begin{aligned}
\boldsymbol{\mathcal{P}}^{\mathbf{I}}\ Choi(\boldsymbol{\mathcal{G}})\boldsymbol{\mathcal{P}}^{\mathbf{I}} &= \sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\left(\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell} - \frac{1}{N}\sum_{m,n=0}^{N-1} (\mathbf{E}_{mn}\mathbf{E}_{ij}\otimes\mathbf{E}_{mn}\mathbf{E}_{k\ell} + \mathbf{E}_{ij}\mathbf{E}_{mn}\otimes\mathbf{E}_{k\ell}\mathbf{E}_{mn}) \right. \\
&\qquad \left. + \frac{1}{N^2}\sum_{m,n,p,q=0}^{N-1} \mathbf{E}_{mn}\mathbf{E}_{ij}\mathbf{E}_{pq}\otimes\mathbf{E}_{mn}\mathbf{E}_{k\ell}\mathbf{E}_{pq} \right) \\
&= \sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\left(\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell} - \frac{1}{N}\left(\delta^i_k \sum_{m=0}^{N-1} \mathbf{E}_{mj}\otimes\mathbf{E}_{m\ell} + \delta^j_{\ell}\sum_{n=0}^{N-1} \mathbf{E}_{in}\otimes\mathbf{E}_{kn} \right) \right.
\end{aligned}
$$

$$
\begin{aligned}
&\quad + \frac{1}{N^2}\,\delta^i_k\,\delta^j_\ell \sum_{m,n=0}^{N-1} \mathbf{E}_{mn}\otimes\mathbf{E}_{mn}\Bigg) \\
&= \sum_{i,j,k,\ell=0}^{N-1} \Bigg(g^{ij}_{k\ell} - \frac{\delta^i_k}{N}\sum_{m=0}^{N-1} g^{mj}_{m\ell} - \frac{\delta^j_\ell}{N}\sum_{n=0}^{N-1} g^{in}_{kn} \\
&\qquad + \frac{\delta^i_k\delta^j_\ell}{N^2}\sum_{m,n=0}^{N-1} g^{mn}_{mn}\Bigg)\,\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell} \\
&\equiv \sum_{i,j,k,\ell=0}^{N-1} \check{g}^{ij}_{k\ell}\;\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell}\,. \qquad (50)
\end{aligned}
$$

Equation (50) thus determines the projected coefficients $\check{g}^{ij}_{k\ell}$ in terms of the original coefficients, and if we compute the Lindbladian versus a Hilbert space basis using the projected coefficients as in the last line of Eq. (48), we get

$$
\mathcal{L}(\boldsymbol{\rho}(t)) \equiv \sum_{i,j=0}^{N-1}\Bigg(\sum_{k,\ell=0}^{N-1}\check{g}^{ij}_{k\ell}\,\mathbf{E}_{ki}\,\boldsymbol{\rho}(t)\,\mathbf{E}_{j\ell} - \frac{1}{2}\sum_{k=0}^{N-1}\check{g}^{ij}_{kk}\,(\mathbf{E}_{ji}\,\boldsymbol{\rho}(t) + \boldsymbol{\rho}(t)\,\mathbf{E}_{ji})\Bigg). \qquad (51)
$$

The supermatrix representation of the first operator sum in this equation can be further simplified as follows:

$$
\begin{aligned}
\sum_{i,j,k,\ell=0}^{N-1}\check{g}^{ij}_{k\ell}\;\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki} &= \sum_{i,j,k,\ell=0}^{N-1} g^{ij}_{k\ell}\,\mathbf{E}_{\ell j}\otimes\mathbf{E}_{ki} - \sum_{j,\ell=0}^{N-1}\Bigg(\frac{1}{N}\sum_{m=0}^{N-1} g^{mj}_{m\ell}\Bigg)\mathbf{E}_{\ell j}\otimes\mathbf{I} \\
&\quad - \sum_{i,k=0}^{N-1}\Bigg(\frac{1}{N}\sum_{n=0}^{N-1} g^{in}_{kn}\Bigg)\mathbf{I}\otimes\mathbf{E}_{ki} + \Bigg(\frac{1}{N^2}\sum_{m,n=0}^{N-1} g^{mn}_{mn}\Bigg)\mathbf{I}\otimes\mathbf{I}. \qquad (52)
\end{aligned}
$$

Similarly, by Eq. (50) the supermatrix representation of the second operator sum in Eq. (51) simplifies to

$$
\begin{aligned}
&\frac{1}{2}\sum_{i,j,k,\ell=0}^{N-1}\delta_{k\ell}\;\check{g}^{ij}_{k\ell}\,(\mathbf{E}_{ji}\otimes\mathbf{I} + \mathbf{I}\otimes\mathbf{E}_{ij}) \\
&\quad = \frac{1}{2}\sum_{i,j=0}^{N-1}\Bigg(\sum_{k=0}^{N-1} g^{ij}_{kk} - \frac{1}{N}\sum_{m=0}^{N-1} g^{mj}_{mi} - \frac{1}{N}\sum_{n=0}^{N-1} g^{in}_{jn}\Bigg)(\mathbf{E}_{ij}\otimes\mathbf{I} + \mathbf{I}\otimes\mathbf{E}_{ji}) \\
&\qquad + \Bigg(\frac{1}{N^2}\sum_{m,n=0}^{N-1} g^{mn}_{mn}\Bigg)\mathbf{I}\otimes\mathbf{I}. \qquad (53)
\end{aligned}
$$

Taking into account the difference in the signs of the operator sums in Eq. (51), the last terms on the right-hand sides of Eqs. (52) and (53) clearly cancel, while the first summation on the right-hand side of Eq. (53) vanishes by our trace preservation condition (cf. Lemma 9). The remaining terms on the right-hand side of Eq. (53) can be rearranged using the symmetries of the summations proved in Lemma 11, as follows:

$$
\begin{aligned}
&-\frac{1}{2N}\sum_{i,j=0}^{N-1}\left(\sum_{m=0}^{N-1} g_{mi}^{mj} + \sum_{n=0}^{N-1} g_{jn}^{in}\right)(\mathbf{E}_{ij}\otimes\mathbf{I} + \mathbf{I}\otimes\mathbf{E}_{ji}) \\
&\quad = -\frac{1}{2N}\sum_{i,j=0}^{N-1}\left(\left(\sum_{m=0}^{N-1} g_{mi}^{mj}\right)\mathbf{E}_{ij}\otimes\mathbf{I} + \left(\sum_{m=0}^{N-1} g_{jm}^{im}\right)\mathbf{I}\otimes\mathbf{E}_{ji}\right. \\
&\qquad\qquad \left. + \left(\sum_{n=0}^{N-1} g_{ni}^{nj}\right)\mathbf{E}_{ij}\otimes\mathbf{I} + \left(\sum_{n=0}^{N-1} g_{jn}^{in}\right)\mathbf{I}\otimes\mathbf{E}_{ji}\right) \\
&\quad = -\frac{1}{N}\sum_{i,j=0}^{N-1}\left(\left(\sum_{m=0}^{N-1} g_{mi}^{mj}\right)\mathbf{E}_{ij}\otimes\mathbf{I} + \left(\sum_{n=0}^{N-1} g_{jn}^{in}\right)\mathbf{I}\otimes\mathbf{E}_{ji}\right). \qquad (54)
\end{aligned}
$$

It is now apparent that these terms cancel with the second and third terms in Eq. (52) after a change of dummy indices, leaving only its first term behind.

Q.E.D.

It is easily shown that applying the projection $\boldsymbol{\mathcal{P}}^{\mathbf{I}}$ to the Choi matrix obtained from the Lindbladian of any one Lindblad, $L\rho L^{\dagger} - (L^{\dagger}L\rho + \rho L^{\dagger}L)/2$, annihilates the last two terms while removing the trace from the Lindblad L in the first. Removing the trace from L does not affect the action of the (Hermiticity-preserving) Lindbladian on ρ, but it can also be shown that it is equivalent to projecting the Lindbladian onto the orthogonal complement of the subspace of commutation superoperators. The above superoperator derivation has the advantage, however, of not assuming that the derivative of the superoperator $\dot{\mathcal{S}}|_{t=0}$ can be placed in Lindbland form. It remains to be shown that the Choi matrix of the operator sum is positive semidefinite if and only if the projection of the Choi matrix of its derivative is positive semidefinite. For the sake of completeness, we first prove the following (well-known) result, using only the techniques developed above.

Lemma 13: The composition of two completely positive superoperators $\mathcal{A}\circ\mathcal{B}$ is again completely positive.

Proof: Let $\boldsymbol{\mathcal{U}}\,Diag(\boldsymbol{\alpha})\boldsymbol{\mathcal{U}}^{\dagger}$ and $\boldsymbol{\mathcal{V}}\,Diag(\boldsymbol{\beta})\,\boldsymbol{\mathcal{V}}^{\dagger}$ be the eigenvalue decompositions of the supermatrices $Choi(\boldsymbol{\mathcal{A}})$ and $Choi(\boldsymbol{\mathcal{B}})$, respectively, and consider the Choi matrix of their product, namely

$$
\begin{aligned}
Choi(\boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{B}}) &= \sum_{i,j,k,\ell=0}^{N-1}\left(\sum_{m,n=0}^{N-1} a_{k\ell}^{mn} b_{mn}^{ij}\right)\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell} \\
&= \sum_{i,j,k,\ell=0}^{N-1}\left(\sum_{m,n=0}^{N-1}\left(\sum_{p,q=0}^{N-1} u_{kq}^{mp}\overline{u}_{\ell q}^{np}\alpha_q^p\right)\left(\sum_{r,s=0}^{N-1} v_{ms}^{ir}\overline{v}_{ns}^{jr}\beta_s^r\right)\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell}\right) \\
&= \sum_{i,j,k,\ell=0}^{N-1}\left(\sum_{p,q,r,s=0}^{N-1}\alpha_q^p\,\beta_s^r\left(\sum_{m=0}^{N-1} u_{kq}^{mp}v_{ms}^{ir}\right)\left(\sum_{n=0}^{N-1}\overline{u}_{\ell q}^{np}\overline{v}_{ns}^{jr}\right)\mathbf{E}_{ij}\otimes\mathbf{E}_{k\ell}\right) \\
&= \sum_{p,q,r,s=0}^{N-1}\alpha_q^p\,\beta_s^r\left(\sum_{i,k=0}^{N-1}(\mathbf{e}_i\otimes\mathbf{e}_k)\left(\sum_{m=0}^{N-1} u_{kq}^{mp}v_{ms}^{ir}\right)\right) \\
&\qquad \cdots\left(\sum_{j,\ell=0}^{N-1}(\mathbf{e}_j\otimes\mathbf{e}_\ell)^{\dagger}\left(\sum_{n=0}^{N-1}\overline{u}_{\ell q}^{np}\overline{v}_{ns}^{jr}\right)\right) \\
&\equiv \sum_{p,q,r,s=0}^{N-1}\alpha_q^p\,\beta_s^r\,\mathbf{x}_{qs}^{pr}(\mathbf{x}_{qs}^{pr})^{\dagger}. \qquad (55)
\end{aligned}
$$

Such a sum of positive semidefinite matrices (Hermitian dyads, in this case) is always again positive semidefinite, proving the Lemma.

Q.E.D.

Theorem 14: *The integral of a Lindbladian yields a quantum dynamical semigroup, and conversely, and the derivative of any quantum dynamical semigroup can be placed in canonical Lindblad form.*

Proof: Given any Kraus operator sum for a quantum dynamical semigroup $\mathcal{S}(t)$, we know that its time derivative will be equal to the result of applying a fixed generator $-\mathcal{F}$ to the density operator $\rho(t)$ at any given $t \geqslant 0$. Integration of a matrix representation thus yields $\boldsymbol{\mathcal{S}}(t) = Exp(-\boldsymbol{\mathcal{F}}t)$, and for a sufficiently small $\delta t > 0$ this exponential may be approximated arbitrarily closely by

$$Exp(-\boldsymbol{\mathcal{F}}t) \approx \boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{F}}\,\delta t + O((\delta t)^2) = \boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{G}}\,\delta t - \imath\boldsymbol{\mathcal{H}}\,\delta t + O((\delta t)^2), \tag{56}$$

where $\boldsymbol{\mathcal{I}} \equiv \mathbf{I}\otimes\mathbf{I}$ and $\imath\boldsymbol{\mathcal{H}}$ denotes the commutator part of $\boldsymbol{\mathcal{F}}$. Since $\mathcal{S}(t)$ is completely positive, any Choi matrix for it must be positive semidefinite, and so must any projection thereof, in particular,

$$\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,Choi(\boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{F}}\,\delta t)\,\boldsymbol{\mathcal{P}}^{\mathbf{I}} = -\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,Choi(\boldsymbol{\mathcal{G}})\,\boldsymbol{\mathcal{P}}^{\mathbf{I}}\,\delta t \equiv -Choi(\check{\boldsymbol{\mathcal{G}}})\,\delta t. \tag{57}$$

This allows $-\check{\mathcal{G}}$ and hence also its sum with $-\imath\mathcal{H}$ to be placed in canonical Lindblad form, which by Proposition 12 must have the same action on any ρ as the differential superoperator $-\mathcal{F}$.

Conversely, suppose that a given superoperator $\mathcal{F} = \mathcal{G} + \imath\mathcal{H}$ can be placed in canonical Lindblad form,

$$-\mathcal{F}(\rho) = \mathcal{L}(\rho) \equiv -\imath\mathcal{H}(\rho) + \sum_{m=1}^{M}\left(L_m\,\rho\,L_m^\dagger - \frac{1}{2}L_m^\dagger L_m\,\rho - \frac{1}{2}\rho\,L_m^\dagger L_m\right), \tag{58}$$

where $\mathcal{H}(\rho) \equiv [H,\rho]$ for the commutator part of $\mathcal{F}$. In terms of a matrix representation $\mathbf{H}$, $\mathbf{L}_m$ of these operators, this is equivalent to

$$-\boldsymbol{\mathcal{F}} = -\boldsymbol{\mathcal{G}} - \imath\boldsymbol{\mathcal{H}} \equiv \sum_{m=1}^{M}\left(\overline{\mathbf{L}}_m\otimes\mathbf{L}_m - \frac{1}{2}\mathbf{I}\otimes\mathbf{L}_m^\dagger\mathbf{L}_m - \frac{1}{2}\overline{\mathbf{L}}_m^\dagger\overline{\mathbf{L}}_m\otimes\mathbf{I}\right) + \imath(\overline{\mathbf{H}}\otimes\mathbf{I} - \mathbf{I}\otimes\mathbf{H}). \tag{59}$$

Then over a sufficiently small time interval δt, the exponential (integral) can be approximated arbitrarily closely by the product of the exponentials

$$\begin{aligned} Exp(-\delta t\,\boldsymbol{\mathcal{F}}) &\approx Exp\left(-\frac{1}{2}\delta t\sum_{m=1}^{M}(\mathbf{I}\otimes\mathbf{L}_m^\dagger\mathbf{L}_m + \overline{\mathbf{L}}_m^\dagger\overline{\mathbf{L}}_m\otimes\mathbf{I})\right)\cdots \\ &\quad \cdots Exp\left(\delta t\sum_{m=1}^{M}\overline{\mathbf{L}}_m\otimes\mathbf{L}\right)Exp(-\delta t\,\imath\boldsymbol{\mathcal{H}}) + O((\delta t)^2) \\ &\equiv \boldsymbol{\mathcal{A}}(\delta t)\,\boldsymbol{\mathcal{B}}(\delta t)\,\boldsymbol{\mathcal{C}}(\delta t) + O((\delta t)^2). \end{aligned} \tag{60}$$

Since the two types of terms in the argument to the first exponential commute, it evaluates to a Kronecker product, namely

$$\begin{aligned} \boldsymbol{\mathcal{A}}(\delta t) &\equiv Exp\left(-\frac{1}{2}\delta t\sum_{m=1}^{M}(\mathbf{I}\otimes\mathbf{L}_m^\dagger\mathbf{L}_m + \overline{\mathbf{L}}_m^\dagger\overline{\mathbf{L}}_m\otimes\mathbf{I})\right) \\ &= Exp\left(-\frac{1}{2}\delta t\sum_{m=1}^{M}\mathbf{L}_m^\dagger\mathbf{L}_m\right)\otimes Exp\left(-\frac{1}{2}\delta t\sum_{m=1}^{M}\overline{\mathbf{L}}_m^\dagger\overline{\mathbf{L}}_m\right) \end{aligned} \tag{61}$$

Thus by Lemma 2, the corresponding Choi matrix is the dyad

$$Choi(\boldsymbol{\mathcal{A}}(\delta t)) \;=\; \mathrm{col}\left(Exp\left(-\frac{1}{2}\delta t \sum_{m=1}^{M} \mathbf{L}_m^\dagger \mathbf{L}_m \right) \right) \; \mathrm{col}^\dagger\left(Exp\left(-\frac{1}{2}\delta t \sum_{m=1}^{M} \mathbf{L}_m^\dagger \mathbf{L}_m \right) \right), \quad (62)$$

which is necessarily positive semidefinite, proving that $\mathcal{A}(t)$ is completely positive for all t. As for the second factor in Eq. (60), we may expand it as

$$\boldsymbol{\mathcal{B}}(\delta t) \;\equiv\; Exp\left(\delta t \sum_{m=1}^{M} \overline{\mathbf{L}}_m \otimes \mathbf{L}_m \right) \;\approx\; \boldsymbol{\mathcal{I}} \;+\; \delta t \sum_{m=1}^{M} \overline{\mathbf{L}}_m \otimes \mathbf{L}_m \;+\; O((\delta t)^2). \quad (63)$$

Because $\boldsymbol{\mathcal{P}}^{\mathbf{I}} Choi(\mathbf{X}\otimes\mathbf{I})\boldsymbol{\mathcal{P}}^{\mathbf{I}} = \boldsymbol{\mathcal{P}}^{\mathbf{I}} Choi(\mathbf{I}\otimes\mathbf{X})\boldsymbol{\mathcal{P}}^{\mathbf{I}} = \mathbf{0}$ for all $\mathbf{X}\in\mathbb{C}^{N\times N}$, the Choi matrix of the summation on the right-hand side is easily seen to be $Choi(\check{\boldsymbol{\mathcal{G}}}) \equiv \boldsymbol{\mathcal{P}}^{\mathbf{I}} Choi(\boldsymbol{\mathcal{G}})\boldsymbol{\mathcal{P}}^{\mathbf{I}}$, so that

$$Choi(\boldsymbol{\mathcal{B}}(\delta t)) \approx \mathrm{col}(\mathbf{I})\,\mathrm{col}^\dagger(\mathbf{I}) \;+\; \delta t\, Choi(\check{\boldsymbol{\mathcal{G}}}) \;+\; O((\delta t)^2). \quad (64)$$

The Choi matrix $Choi(\check{\boldsymbol{\mathcal{G}}}) = \Sigma_{m=1}^{M} \mathrm{col}(\mathbf{L}_m)\mathrm{col}^\dagger(\mathbf{L}_m)$ is of course positive semidefinite, and [since $\check{\boldsymbol{\mathcal{G}}} = \Sigma_{n=1}^{N} \check{\gamma}_n(\overline{\mathbf{U}}_n\otimes\mathbf{U}_n)$ where $\check{\gamma}_n$, $\mathrm{col}(\mathbf{U}_n)$ are the eigenvalues and eigenvectors of $Choi(\check{\boldsymbol{\mathcal{G}}})$] so are the Choi matrices of all higher terms in the Taylor expansion of $Choi(\boldsymbol{\mathcal{B}}(\delta t))$, thus showing that $\mathcal{B}(t)$ is also completely positive for all $t \geqslant 0$. Finally, the last factor of Eq. (60),

$$\boldsymbol{\mathcal{C}}(\delta t) \equiv Exp(-\delta t\, \imath \boldsymbol{\mathcal{H}}), \quad (65)$$

is unitary and hence likewise corresponds to a completely positive superoperator for all time.

It now follows from Lemma 13 that for $\delta t \ll \|\mathcal{G}\|^{-1}$, the product of all three factors $\boldsymbol{\mathcal{A}}(\delta t)$, $\boldsymbol{\mathcal{B}}(\delta t)$, $\vec{\boldsymbol{\mathcal{C}}}(\delta t)$ in Eq. (60) will be completely positive, and hence for any given $t \geqslant 0$ the telescoping product

$$Exp(-t\boldsymbol{\mathcal{F}}) \approx \underbrace{(\boldsymbol{\mathcal{A}}(t/n)\boldsymbol{\mathcal{B}}(t/n)\boldsymbol{\mathcal{C}}(t/n)\cdots\boldsymbol{\mathcal{A}}(t/n)\boldsymbol{\mathcal{B}}(t/n)\boldsymbol{\mathcal{C}}(t/n))}_{n \text{ times}}{}^{1/n} \;+\; O((t/n)^2) \quad (66)$$

will also be completely positive for all $n > t/\delta t$. The Theorem now follows by noting that the set of completely positive superoperators is closed, and taking the limit as $n \to \infty$.

Q.E.D.

V. APPLICATION TO QUANTUM PROCESS TOMOGRAPHY

The applicability of the foregoing results to QPT derives from the following theorem, whose origins can be traced back to work by Eckart, Young, and Householder,[17,18] and has since given rise to a field of statistical data analysis widely known as "principal component analysis." [19] The present author has proven it several times in the course of his career,[20–22] and regards the following proof as the simplest.

Theorem 15: *Let $\mathbf{M}\in\mathbb{C}^{N\times N}$ be a Hermitian matrix with eigenvalue decomposition*

$$\mathbf{M} \;=\; \mathbf{U}^\dagger \boldsymbol{\Lambda}\, \mathbf{U} \;=\; \sum_{\ell=0}^{N-1} \lambda_\ell\, \mathbf{u}_\ell\, \mathbf{u}_\ell^\dagger, \quad (67)$$

where the eigenvalues have been sorted in nonincreasing order $\lambda_\ell \geqslant \lambda_{\ell+1}$ for $0 \leqslant \ell \leqslant N-2$. Also let $\mathbb{P}$ denote the convex cone of positive semidefinite matrices in $\mathbb{C}^{N\times N}$ and $\boldsymbol{\mathcal{P}}_{\mathbb{P}}(\mathbf{M})$ be the orthogonal projection of $\mathbf{M}$ onto $\mathbb{P}$ with respect to the Hilbert–Schmidt (or Frobenius) matrix norm $\|\cdot\|$, which satisfies the "least-squares" criterion[23]

$$\| \mathbf{M} - \boldsymbol{\mathcal{P}}_{\mathbb{P}}(\mathbf{M}) \|^2 = \min_{\mathbf{M}' \in \mathbb{P}} \| \mathbf{M} - \mathbf{M}' \|^2. \tag{68}$$

Then we have

$$\boldsymbol{\mathcal{P}}_{\mathbb{P}}(\mathbf{M}) = \mathbf{M}^\star \equiv \mathbf{U}^\dagger \boldsymbol{\Lambda}^\star \mathbf{U} = \sum_{\ell=0}^{N^\star-1} \lambda^\star_\ell \mathbf{u}_\ell \mathbf{u}_\ell^\dagger, \tag{69}$$

where $\boldsymbol{\Lambda}^\star$ *is the diagonal matrix of eigenvalues* $\boldsymbol{\Lambda}$ *with all of its* $N-N^\star$ *nonpositive eigenvalues set to zero.*

Proof: Any positive semidefinite $N\times N$ matrix can be written as $\mathbf{X}\mathbf{X}^\dagger$, where $\mathbf{X}\in\mathbb{C}^{N\times N'}$ and N' is its rank. It follows that the minimum in Eq. (68) can also be written as

$$\min_{\mathbf{X}\in\mathbb{C}^{N\times N'}} \zeta(\mathbf{X}) \equiv \min_{\mathbf{X}\in\mathbb{C}^{N\times N'}} \| \mathbf{X}\mathbf{X}^\dagger - \mathbf{M} \|^2. \tag{70}$$

It is easily seen that the gradient matrix of $\zeta(\mathbf{X})$ is

$$\frac{\mathrm{d}\zeta}{\mathrm{d}\mathbf{X}} = \frac{\mathrm{d}}{\mathrm{d}\mathbf{X}} \mathrm{tr}((\mathbf{X}\mathbf{X}^\dagger - \mathbf{M})^2) = 2\,(\mathbf{X}\mathbf{X}^\dagger - \mathbf{M})\,\mathbf{X}. \tag{71}$$

On setting this to the zero matrix, we obtain the nonlinear matrix equation

$$\mathbf{M}\,\mathbf{X} = \mathbf{X}(\mathbf{X}^\dagger\mathbf{X}), \tag{72}$$

wherein $\mathbf{X}^\dagger\mathbf{X}$ is an $N'\times N'$ Hermitian matrix which, for $N' = 3$ and $\mathbf{X}\in\mathbb{R}^{N\times 3}$, is essentially the inertial tensor (plus a multiple of the identity) of a system of unit mass points with coordinates $\mathbf{e}_i^\mathsf{T}\mathbf{X}$ $(0 \leqslant i < N)$. Since the Hilbert–Schmidt norm is unitarily invariant, we may assume that these ''coordinates'' have been chosen so that $\mathbf{X}^\dagger\mathbf{X} = \mathit{Diag}(\xi_1,\ldots,\xi_{N'})$ is diagonal, in which case Eq. (72) becomes

$$\mathbf{M}\,\mathbf{x}_j = \xi_j\,\mathbf{x}_j \quad (j=0,\ldots,N-1), \tag{73}$$

where $\mathbf{x}_j \equiv \mathbf{X}\mathbf{e}_j$ are the columns of $\mathbf{X}$. It follows that the $\mathbf{x}_j$ are proportional to the eigenvectors $\mathbf{u}_j$ associated with certain nonnegative eigenvalues $\lambda_j = \xi_j$ of $\mathbf{M}$ where, since $\|\mathbf{x}_j\|^2 = \xi_j$, the constant of proportionality is $\sqrt{\lambda_j}$. On expanding the trace in the function $\zeta(\mathbf{X})$, we now obtain

$$\zeta(\mathbf{X}) = \mathrm{tr}(\,\mathbf{M}^2 - 2\,\mathbf{X}\mathbf{X}^\dagger\,\mathbf{M} + (\mathbf{X}\mathbf{X}^\dagger)^2\,) = \mathrm{tr}(\,\mathbf{M}^2\,) - \mathrm{tr}(\,2\,\mathbf{X}^\dagger\mathbf{M}\,\mathbf{X} - (\mathbf{X}^\dagger\mathbf{X})^2\,). \tag{74}$$

By Eq. (72), however, the matrix $\mathbf{X}'\in\mathbb{C}^{N\times N'}$ that minimizes $\zeta(\mathbf{X})$ satisfies

$$(\mathbf{X}')^\dagger\,\mathbf{M}\,\mathbf{X}'^\dagger = (\,(\mathbf{X}')^\dagger\mathbf{X}'\,)^2 = \mathit{Diag}(\,\lambda_0^2,\ldots,\lambda_{N'-1}^2\,), \tag{75}$$

so that

$$\zeta(\mathbf{X}) = \mathrm{tr}(\,\mathbf{M}^2\,) - \sum_{j=0}^{N'-1} \lambda_j^2. \tag{76}$$

From this we see that, for any integer N'' with $0 \leqslant N'' \leqslant N'$ and $\lambda_j \geqslant 0$ for $0 \leqslant j < N''$, the minimizing $\mathbf{X}''\in\mathbb{C}^{N\times N''}$ is obtained by setting $\mathbf{X}'' \equiv [\,\sqrt{\lambda_j}\mathbf{u}_j]_{j=0}^{N''-1}$. It follows that the minimizing positive semidefinite matrix $\mathbf{X}^\star(\mathbf{X}^\star)^\dagger$ is obtained by setting N'' to the number $N^\star$ of positive eigenvalues of $\mathbf{M}$.

Q.E.D.

This theorem can be used to "filter" statistical estimates of either superoperators or their generators so as to obtain a completely positive estimate. In the case of an estimate $\boldsymbol{\mathcal{S}}'$ of a matrix representing an unknown superoperator $\mathcal{S}$, one simply sets any negative eigenvalues of the associated Choi matrix $\boldsymbol{\mathcal{T}}' = \mathit{Choi}(\boldsymbol{\mathcal{S}}')$ to zero, reconstructs the improved estimate $\boldsymbol{\mathcal{T}}^\star$ from these modified eigenvalues and the original eigenvectors as in the theorem, and converts the result back into a new estimate $\boldsymbol{\mathcal{S}}^\star = \mathit{Choi}(\boldsymbol{\mathcal{T}}^\star)$ of the superoperator via the same involutory mapping Choi. The theorem assures us that this procedure makes the smallest possible change in $\boldsymbol{\mathcal{T}}'$, with respect to the Hilbert–Schmidt norm, so as to render it positive semidefinite and so ensure that $\boldsymbol{\mathcal{S}}^\star$ represents a completely positive superoperator. Because the mapping Choi simply permutes the elements of its argument, we can be sure that this procedure also minimizes the change $\|\boldsymbol{\mathcal{S}}' - \boldsymbol{\mathcal{S}}^\star\|$ in $\boldsymbol{\mathcal{S}}'$. We now show that $\boldsymbol{\mathcal{S}}^\star$ is assured of being an improved estimate of the corresponding matrix of the true superoperator $\boldsymbol{\mathcal{S}}$, again in the least-squares sense.

Corollary 16: For $\boldsymbol{\mathcal{S}}$, $\boldsymbol{\mathcal{S}}'$, and $\boldsymbol{\mathcal{S}}^\star$ defined as above, we have

$$\|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}\| \leqslant \|\boldsymbol{\mathcal{S}}' - \boldsymbol{\mathcal{S}}\|. \tag{77}$$

Proof: Since $\boldsymbol{\mathcal{S}}^\star$ is the orthogonal projection of $\boldsymbol{\mathcal{S}}'$ onto the convex cone $\mathit{Choi}(\mathbb{P})$ of matrices representing completely positive superoperators, $\boldsymbol{\mathcal{S}}' - \boldsymbol{\mathcal{S}}^\star$ is orthogonal to a supporting hyperplane at $\boldsymbol{\mathcal{S}}^\star$, while by its definition $\boldsymbol{\mathcal{S}} \in \mathit{Choi}(\mathbb{P})$ must be on the opposite side of this hyperplane from $\boldsymbol{\mathcal{S}}'$. This in turn implies that the angle θ between $\boldsymbol{\mathcal{S}}$ and $\boldsymbol{\mathcal{S}}'$ at $\boldsymbol{\mathcal{S}}^\star$ satisfies $\theta \geqslant \pi/2$, and hence by the law of cosines

$$0 \geqslant \cos(\theta) = \frac{1}{2}(\|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}'\|^2 + \|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}\|^2 - \|\boldsymbol{\mathcal{S}}' - \boldsymbol{\mathcal{S}}\|^2), \tag{78}$$

i.e., $\|\boldsymbol{\mathcal{S}}' - \boldsymbol{\mathcal{S}}\|^2 \geqslant \|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}'\|^2 + \|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}\|^2 \geqslant \|\boldsymbol{\mathcal{S}}^\star - \boldsymbol{\mathcal{S}}\|^2$.

Q.E.D.

The procedure in the case of a QDS generator $\mathcal{F} = \mathcal{G} + \iota\mathcal{H}$ is a bit more involved, since one needs to compute the projection of the Choi matrix $\boldsymbol{\mathcal{E}}' \equiv \boldsymbol{\mathcal{P}}^{\mathbf{I}} \mathit{Choi}(\boldsymbol{\mathcal{F}}') \boldsymbol{\mathcal{P}}^{\mathbf{I}}$ of the estimate $\boldsymbol{\mathcal{F}}'$ before diagonalizing it. This of course will remove the Hamiltonian superoperator component, which must then be obtained by some other means. In addition, one cannot reconstruct a matrix $\boldsymbol{\mathcal{G}}^\star$ for the decoherent component $\mathcal{G}$ of $\mathcal{F}$ from the matrix $\boldsymbol{\mathcal{E}}^\star$ obtained by setting any negative eigenvalues ε_m of $\boldsymbol{\mathcal{E}}'$ to zero simply by applying the Choi mapping, since the other terms needed to preserve the trace will also have been lost in the projection (if indeed the estimate $\boldsymbol{\mathcal{F}}'$ itself were trace preserving). Instead, one has to construct all the Lindblad operators $\mathbf{L}_m$ such that $\mathrm{col}(\mathbf{L}_m) = \sqrt{\varepsilon_m}\mathbf{v}_m$, where $\varepsilon_m > 0$, $\mathbf{v}_m$ are eigenvalue, eigenvector pairs of $\boldsymbol{\mathcal{E}}'$, and compute $\boldsymbol{\mathcal{G}}^\star$ as indicated in Eq. (6). As a result, there is no guarantee that $\boldsymbol{\mathcal{G}}^\star$ will be closer to its true value $\boldsymbol{\mathcal{G}}$ versus the Hilbert–Schmidt norm, although we expect that this will usually be the case. Further discussion regarding how one might go about solving these problems must take the exact experimental situation at hand into account, and as such is outside the scope of this paper.

In the remainder of this section we will illustrate how the above results may be applied to a simple example, namely the *Bloch equations* for a single spin-1/2 qubit in a frame rotating at its Larmour frequency in an applied magnetic field.[16] As is well-known,[24] these can be expressed in canonical Lindblad form as

$$\begin{aligned}\dot{\boldsymbol{\rho}} = \boldsymbol{\mathcal{L}}(\boldsymbol{\rho}) \equiv{}& \frac{1+\Delta}{4T_1}(2\,\mathbf{E}_{01}\boldsymbol{\rho}\mathbf{E}_{10} - \mathbf{E}_{00}\boldsymbol{\rho} - \boldsymbol{\rho}\mathbf{E}_{00}) \\ &+ \frac{1-\Delta}{4T_1}(2\,\mathbf{E}_{10}\boldsymbol{\rho}\mathbf{E}_{01} - \mathbf{E}_{11}\boldsymbol{\rho} - \boldsymbol{\rho}\mathbf{E}_{11}) \\ &+ \left(\frac{1}{2T_2} - \frac{1}{4T_1}\right)((\mathbf{E}_{00} - \mathbf{E}_{11})\,\boldsymbol{\rho}\,(\mathbf{E}_{00} - \mathbf{E}_{11}) - \boldsymbol{\rho}),\end{aligned} \tag{79}$$

where T_1 and T_2 are the characteristic relaxation and decoherence times and $\Delta = p_0 - p_1$ is the excess probability in the ground state $\mathbf{E}_{00}$ at equilibrium. The supermatrix of the generator versus a Hilbert space basis in the ordering $\mathbf{E}_{00}$, $\mathbf{E}_{10}$, $\mathbf{E}_{01}$, $\mathbf{E}_{11}$ induced by the "col" operator is

$$\begin{aligned}
&\frac{1+\Delta}{4T_1}(2\,\mathbf{E}_{01}\otimes\mathbf{E}_{01}-\mathbf{I}\otimes\mathbf{E}_{00}-\mathbf{E}_{00}\otimes\mathbf{I})\\
&\quad+\frac{1-\Delta}{4T_1}(2\,\mathbf{E}_{10}\otimes\mathbf{E}_{10}-\mathbf{I}\otimes\mathbf{E}_{11}-\mathbf{E}_{11}\otimes\mathbf{I})\\
&\quad+\left(\frac{1}{2T_2}-\frac{1}{4T_1}\right)((\mathbf{E}_{00}-\mathbf{E}_{11})\otimes(\mathbf{E}_{00}-\mathbf{E}_{11})-\mathbf{I}\otimes\mathbf{I})\\
&=\begin{bmatrix}
-\frac{1-\Delta}{2T_1} & 0 & 0 & \frac{1+\Delta}{2T_1}\\
0 & -\frac{1}{T_2} & 0 & 0\\
0 & 0 & -\frac{1}{T_2} & 0\\
\frac{1-\Delta}{2T_1} & 0 & 0 & -\frac{1+\Delta}{2T_1}
\end{bmatrix}\equiv\mathcal{L}.
\end{aligned}\tag{80}$$

The time-dependent exponential of this matrix may be shown to be

$$\begin{aligned}
&Exp(-\mathcal{L}\,t)\\
&=\frac{1}{2}\begin{bmatrix}
(1+e^{-t/T_1})+\Delta(1-e^{-t/T_1}) & 0 & 0 & (1-e^{-t/T_1})+\Delta(1-e^{-t/T_1})\\
0 & 2\,e^{-t/T_2} & 0 & 0\\
0 & 0 & 2\,e^{-t/T_2} & 0\\
(1-e^{-t/T_1})-\Delta(1-e^{-t/T_1}) & 0 & 0 & (1+e^{-t/T_1})-\Delta(1-e^{-t/T_1})
\end{bmatrix},
\end{aligned}\tag{81}$$

which in turn corresponds to the Choi matrix

$$\begin{aligned}
&\mathcal{M}(t)\\
&\equiv\frac{1}{2}\begin{bmatrix}
(1+e^{-t/T_1})+\Delta\,(1-e^{-t/T_1}) & 0 & 0 & 2\,e^{-t/T_2}\\
0 & (1-e^{-t/T_1})(1-\Delta) & 0 & 0\\
0 & 0 & (1-e^{-t/T_1})(1+\Delta) & 0\\
2\,e^{-t/T_2} & 0 & 0 & (1+e^{-t/T_1})-\Delta\,(1-e^{-t/T_1})
\end{bmatrix}.
\end{aligned}\tag{82}$$

This in turn is readily shown to be positive semidefinite for all $t \geqslant 0$ if $2T_1 \geqslant T_2$. Its derivative at $t = 0$, however, is

$$\dot{\boldsymbol{\mathcal{M}}}(0) = -Choi(\boldsymbol{\mathcal{L}}) = \frac{1}{2}\begin{bmatrix} -\frac{1-\Delta}{2T_1} & 0 & 0 & -\frac{1}{T_2} \\ 0 & \frac{1-\Delta}{2T_1} & 0 & 0 \\ 0 & 0 & \frac{1+\Delta}{2T_1} & 0 \\ -\frac{1}{T_2} & 0 & 0 & -\frac{1+\Delta}{2T_1} \end{bmatrix}, \tag{83}$$

and the outermost 2×2 block of this matrix is positive semidefinite *only* if $2T_1 \leqslant T_2$. Applying the projection $\boldsymbol{\mathcal{P}}^{\mathbf{I}} \equiv \boldsymbol{\mathcal{I}} - \mathrm{col}(\mathbf{I})\mathrm{col}^{\dagger}(\mathbf{I})/2$ converts it to

$$-\boldsymbol{\mathcal{P}}^{\mathbf{I}} Choi(\boldsymbol{\mathcal{L}})\, \boldsymbol{\mathcal{P}}^{\mathbf{I}} = \begin{bmatrix} \frac{1}{2T_2} - \frac{1}{4T_1} & 0 & 0 & \frac{1}{4T_1} - \frac{1}{2T_2} \\ 0 & \frac{1-\Delta}{2T_1} & 0 & 0 \\ 0 & 0 & \frac{1+\Delta}{2T_1} & 0 \\ \frac{1}{4T_1} - \frac{1}{2T_2} & 0 & 0 & \frac{1}{2T_2} - \frac{1}{4T_1} \end{bmatrix}, \tag{84}$$

which is now positive semidefinite with eigenvalue, eigenvector pairs:

$$\left(0, \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}\right), \quad \left(\frac{1}{2T_2} - \frac{1}{4T_1}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix}\right), \quad \left(\frac{1+\Delta}{2T_1}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}\right), \quad \left(\frac{1-\Delta}{2T_1}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}\right). \tag{85}$$

The eigenvectors are easily seen to be obtained by applying the ''col'' operator to the matrices $\mathbf{I} = \mathbf{E}_{00} + \mathbf{E}_{11}$, $\mathbf{E}_{00} - \mathbf{E}_{11}$, $\mathbf{E}_{10}$, and $\mathbf{E}_{01}$, returning us to the canonical Lindblad form in Eq. (79).

We will now use this example to illustrate how the matrix formulas obtained in this paper can be applied to QPT, by numerically simulating the ''data'' needed for QPT from the above solution to the Bloch equations. These data correspond to an experimental scenario in which a set of precisely known input states $\{\boldsymbol{\rho}_k^{\mathrm{in}}\}_{k=1}^K$ were allowed to evolve under the propagator in Eq. (81) for varying periods of time, and the results $\{\boldsymbol{\rho}_k^{\mathrm{out}}\}_{k=1}^K$ determined by *state* tomography.[2,3,25–27] Assuming that the input states span the space of single-qubit Hermitian operators, this allows us to determine the propagators at each time point according to

$$\begin{aligned} Exp(-\boldsymbol{\mathcal{L}}\,t)[\mathrm{col}(\boldsymbol{\rho}_1^{\mathrm{in}}),\ldots,\mathrm{col}(\boldsymbol{\rho}_K^{\mathrm{in}})] &= [\mathrm{col}(\boldsymbol{\rho}_1^{\mathrm{out}}),\ldots,\mathrm{col}(\boldsymbol{\rho}_K^{\mathrm{out}})] \;\Leftrightarrow\; Exp(-\boldsymbol{\mathcal{L}}\,t) \\ &= [\mathrm{col}(\boldsymbol{\rho}_1^{\mathrm{out}}),\ldots,\mathrm{col}(\boldsymbol{\rho}_K^{\mathrm{out}})][\mathrm{col}(\boldsymbol{\rho}_1^{\mathrm{in}}),\ldots,\mathrm{col}(\boldsymbol{\rho}_K^{\mathrm{in}})]^{-1}. \end{aligned} \tag{86}$$

Although this relation is exact when the output states are known precisely, in actual practice experimental errors would result in only an approximate estimate $\boldsymbol{\mathcal{S}}'(t)$ of the actual propagator $\boldsymbol{\mathcal{S}}(t) \equiv Exp(-\boldsymbol{\mathcal{L}}\,t)$. If one obtains such estimates at an arithmetic sequence of time points $0 = t_0, t_1, \ldots, t_J = Jt_1$, however, one may solve a linear least-squares problem to obtain an improved estimate of the propagator $\boldsymbol{\mathcal{S}}_1 \equiv \boldsymbol{\mathcal{S}}(t_1)$ at the first nonzero time point,[28] namely

TABLE I. Average over 100 runs of Hilbert–Schmidt norms of the changes in the propagators on symmetrizing and filtering the eigenvalues $\{\psi\}$ of their Choi matrices, divided by the norm of the actual propagator $\|\boldsymbol{\mathcal{S}}\|$ (see text); the last column shows the average number $|\{\psi < 0\}|$ of negative eigenvalues of that were set to zero.

	t_1	t_2	t_3	t_4	$\lvert\{\psi < 0\}\rvert$
Ω_1	0.0108	0.0121	0.0116	0.0127	0.000
Ω_2	0.0581	0.0601	0.0644	0.0605	0.000
Ω_3	0.3062	0.3038	0.3074	0.3098	0.290

$$\min_{\boldsymbol{\mathcal{T}}}(\chi(\boldsymbol{\mathcal{T}})) \quad \text{where} \quad \chi(\boldsymbol{\mathcal{T}}) \equiv \sum_{j=0}^{J-1} \|\boldsymbol{\mathcal{T}}\boldsymbol{\mathcal{S}}'_j - \boldsymbol{\mathcal{S}}'_{j+1}\|^2. \tag{87}$$

One may of course set $\boldsymbol{\mathcal{S}}'_0 = \boldsymbol{\mathcal{S}}(t_0) = \mathbf{I}\otimes\mathbf{I}$, the 4×4 identity, and one should also filter the remaining estimates by symmetrizing their Choi matrices (i.e., by adding them to their adjoints and dividing by 2), setting any negative eigenvalues $\psi = 0$ and transforming back to a new estimate (as described previously). The minimizing solution to this least-squares problem is easily shown to be

$$\boldsymbol{\mathcal{S}}''_1 \equiv \left(\sum_{j=1}^{J-1} \boldsymbol{\mathcal{S}}'_j\,(\boldsymbol{\mathcal{S}}'_{j-1})^\dagger\right)\left(\sum_{j=1}^{J-1} \boldsymbol{\mathcal{S}}'_j\,(\boldsymbol{\mathcal{S}}'_j)^\dagger\right)^\ddagger, \tag{88}$$

where in most cases the Moore–Penrose inverse (‡) may be replaced by the usual matrix inverse.[23]

Finally, $\boldsymbol{\mathcal{S}}''_1$ may be converted into an estimate of the generator via the matrix "pseudologarithm," Plog. This is computed by diagonalizing $\boldsymbol{\mathcal{S}}''_1 = \boldsymbol{\mathcal{W}}\boldsymbol{\Phi}\boldsymbol{\mathcal{W}}^{-1}$, setting any eigenvalues $\phi_i \leqslant 0$ or $\phi_i \geqslant 1$ to zero while taking the usual logarithm of the rest, then performing the inverse similarity transformation and dividing by t_1, i.e.,

$$t_1\,\boldsymbol{\mathcal{L}}'' = \mathit{Plog}(\boldsymbol{\mathcal{S}}''_1) \equiv \boldsymbol{\mathcal{W}}\,\mathit{Plog}(\boldsymbol{\Phi})\,\boldsymbol{\mathcal{W}}^{-1} = \sum_{i=0}^{3} \mathrm{plog}(\phi_i)\,(\boldsymbol{\mathcal{W}}\mathbf{e}_i)(\boldsymbol{\mathcal{W}}^{-1}\mathbf{e}_i)^\dagger, \tag{89}$$

where

$$\mathrm{plog}(\phi_i) \equiv \begin{cases} \log(\phi_i) & \text{if } 0 < \phi_i < 1, \\ 0 & \text{otherwise.} \end{cases} \tag{90}$$

The eigenvalues will be real since no Hamiltonian was assumed in the simulations, and arguments similar to those involved in Theorem 15 can be used to show that the pseudo-logarithm will then yield a generator $\boldsymbol{\mathcal{L}}''$ that minimizes $\|\boldsymbol{\mathcal{S}}''_1 - \mathit{Exp}(-\boldsymbol{\mathcal{L}}''t_1)\|$. Last, the estimate $\boldsymbol{\mathcal{L}}''$ is filtered by projecting its symmetrized Choi matrix by $\boldsymbol{\mathcal{P}}^{\mathbf{I}}$, setting any eigenvalues $\varepsilon = 0$, and reconstructing to obtain the optimum estimate $\boldsymbol{\mathcal{L}}^\star$, as described above.

The specific values of the parameters used for the simulations were $T_1 = 0.5$, $T_2 = 0.1$, and $\Delta = 0.1$; the relaxation times T_1 and T_2 are typical of liquid-state NMR samples, while the polarization Δ was deliberately made larger to render it visible despite the noise. In accord with Eq. (80), these gave rise to the generator

$$\boldsymbol{\mathcal{L}} \equiv \begin{bmatrix} -0.9 & 0 & 0 & 1.1 \\ 0 & -10.0 & 0 & 0 \\ 0 & 0 & -10.0 & 0 \\ 0.9 & 0 & 0 & -1.1 \end{bmatrix} \tag{91}$$

TABLE II. Average Hilbert–Schmidt distances (columns 1–3) among the estimates of the generators divided by the norm of the actual generator $\|\mathcal{L}\|$, and (columns 4–5) average numbers of eigenvalues set to zero in obtaining these estimates (see text).

	$\|\mathcal{L}''-\mathcal{L}^{\star}\|$	$\|\mathcal{L}''-\mathcal{L}\|$	$\|\mathcal{L}^{\star}-\mathcal{L}\|$	$\|\{\phi < 0\}\|$	$\|\{\varepsilon < 0\}\|$
Ω_1	0.0077	0.0305	0.0300	0.000	0.000
Ω_2	0.0634	0.1720	0.1676	0.010	0.420
Ω_3	0.2971	0.6355	0.5553	0.580	0.840

The input states were taken to be $\mathbf{E}_{00}$, $\mathbf{E}_{11}$, $(\mathbf{e}_0+\mathbf{e}_1)(\mathbf{e}_0+\mathbf{e}_1)/2$, and $(\mathbf{e}_0-\imath\mathbf{e}_1)(\mathbf{e}_0+\imath\mathbf{e}_1)/2$, while the times used were set to $t_j \equiv j/4$ ($j = 0,\ldots,4$). Finally, the noise levels evaluated were $\Omega_1 = 0.01$, $\Omega_2 = 0.05$ and $\Omega_3 = 0.25$, where the noise was simply added to the output states $\{\boldsymbol{\rho}_k^{\mathrm{out}}\}$ with a Gaussian distribution, zero mean, and variances $\sigma_j^2\Omega_k^2$ proportional to the mean-square size σ_j^2 of the elements of $\boldsymbol{\mathcal{S}}(t_j)$ ($j = 0,\ldots,J$; $k = 1, 2, 3$). The results below were averaged over 100 independent estimations of the propagators at each time point, using different random noise for each estimation and time point, followed by filtering and fitting to obtain estimates of the generator, all at each of the three specified noise levels.

Table I shows the average changes made to the propagator estimates upon symmetrizing and filtering the eigenvalues of their Choi matrices, as measured by the Hilbert–Schmidt norm of the difference divided by that of the true propagator, together with the average number $|\{\psi < 0\}|$ of eigenvalues set to zero in the process. It may be seen that the changes in the estimated propagators upon filtering became significant as the noise level increased, but were generally little more than the added noise. Negative eigenvalues were frequently encountered only at the highest noise level $\Omega_3 = 0.25$, however, so in fact most of these changes were due to the symmetrization needed to make the estimated Choi matrices Hermitian.

Table II shows the average changes made to the various generator estimates computed (this time normalized by the norm of the true generator), together with the average numbers of eigenvalues set to zero in computing the pseudologarithm ($|\{\phi < 0\}|$) and in filtering ($|\{\varepsilon < 0\}|$). Again, few eigenvalues with incorrect signs were encountered either in computing the pseudologarithm, or in symmetrizing and filtering the resulting generators. This means that, once again, most of the improvement was obtained via the projection $\boldsymbol{\mathcal{P}}^{\mathbf{I}}$ and subsequent reconstruction, forcing the estimated generators $\boldsymbol{\mathcal{L}}^{\star}$ to preserve the trace (which the unfiltered estimates $\boldsymbol{\mathcal{L}}''$ did not). Finally, it should be noted that the filtered generators $\boldsymbol{\mathcal{L}}^{\star}$ usually came out closer to the actual solution than the unfiltered, although this was not invariably so. Together, these numerical results strongly support our claim that the formulas derived in this paper provide a powerful set of tools with which to tackle quantum process tomography on systems that may be aptly modeled as a quantum dynamical semigroup.

VI. CONCLUSIONS

In this paper we have presented formulas by which the supergenerators and superpropagators of quantum dynamical semigroups may be manipulated, placed in canonical Lindblad and Kraus form, and all these forms interconverted. These formulas constitute a set of tools that should be particularly valuable in developing robust procedures for quantum process tomography[2] and quantum channel identification,[1] using diverse forms of experimental data. We have illustrated one such application using data simulated from the well-known Bloch relaxation equations on a single spin-1/2 qubit,[16] which assumed that full state tomography versus a basis of input states could be performed. This example demonstrated the anticipated robustness of the procedures employed, which was the result of combining the eigenvalue characterizations of completely positive supergenerators and superpropagators derived in this paper with powerful matrix approximation methods derived from the field of principal component analysis.[19]

It should be clearly understood, nevertheless, that the procedures given above were intended primarily to provide a concrete example of how the mathematical results derived in this paper can be applied to quantum process tomography, and not as a prescriptive recipe that is in all cases optimal—or even applicable. For example, the system of interest will often evolve coherently as it relaxes towards equilibrium, and at a rate far larger than the relaxation processes themselves. In this case the relaxation generator itself will be averaged, significantly complicating its physical interpretation, and the superpropagators determined from full state tomography versus an input basis set will usually have complex eigenvalues. Even assuming its matrix can be fully diagonalized, the well-known ambiguity of the matrix logarithm with respect to the addition of arbitrary multiples of $2\pi\imath$ onto its eigenvalues will render our ''pseudologarithm'' technique inapplicable. Particularly in such cases, better results can be expected from nonlinear fits of the supergenerator to the superpropagators,[11,28] but the question of whether these problems are best solved by computational means, experimental means, or some combination thereof, will clearly depend upon the circumstances.

There are further many other ways to represent a quantum state besides a density matrix, for example by a Wigner distribution,[25] or it may even be desirable to forgo state tomography altogether and to base quantum process tomography on a sequence of time-dependent observations which, although individually insufficient to fully determine the superoperator or even the system's quantum state, nevertheless do so in aggregate. Alternatively, one might utilize a form of indirect measurement via qubits outside of, but interacting with, the system of interest.[1,16,29] We anticipate that many creative applications and extensions of the techniques introduced in this paper will be developed in the years ahead, as quantum information processing technologies progress towards experimental reality.

ACKNOWLEDGMENTS

This work was supported by ARO Grants Nos. DAAD19-01-1-0678 and DAAD19-01-1-0519, and by DARPA Grant No. MDA972-01-1-0003. The author thanks David G. Cory, Nicolas Boulant and Lorenza Viola for helpful conversations, and Mary-Beth Ruskai for pointing out the connection of this work to that of Choi.[15] After this paper was submitted, a paper by D. W. Leung[29] came to our attention, which also proposes using some of the results in Sec. III for quantum process tomography.

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Non-Abelian braid statistics versus projective permutation statistics

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(Received 29 January 2002; accepted 10 October 2002)

Recent papers by Finkelstein, Galiautdinov, and co-workers [J. Math. Phys. **42**, 1489 (2001); **42**, 3299 (2001)] discuss a suggestion by Wilczek that non-Abelian projective representations of the permutation group can be used as a new type of particle statistics, valid in any dimension. Wilczek's suggestion was based in part on an analysis by Nayak and Wilczek (NW) of the non-Abelian representation of the braid group in a quantum Hall system. We point out that projective permutation statistics is not possible in a local quantum field theory as it violates locality, and show that the NW braid group representation is not equivalent to a projective representation of the permutation group. The structure of the finite image of the braid group in a $2^{n/2-1}$-dimensional representation is obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1530369]

Moore and Read[1] showed that a physical realization of non-Abelian statistics (as a non-Abelian representation of the braid group) was a possibility in a quantum Hall effect system. The Moore–Read state now seems likely to be the ground state in the $\nu=5/2$ quantum Hall effect (for a review, see Ref. 2). The non-Abelian statistics was analyzed further,[3–5] and in particular Nayak and Wilczek (NW)[3] showed that exchange of the quasiparticles by braiding can be represented using a subgroup of the rotation group $\mathrm{SO}(n)$, acting in the spinor (projective) representation, using Clifford algebra methods. Wilczek[6] then proposed a connection with the projective representations of the permutation group, and suggested that such ''projective permutation statistics'' are a possibility in any space dimension. This was explored extensively in Refs. 7–9, where it was termed ''Clifford statistics.'' In view of the interest in non-Abelian statistics also in connection with quantum computation,[10] it seems worthwhile to correct the confusion that has arisen.

To begin, consider n indistinguishable point objects in a two-dimensional plane. For generic positions, they can be projected onto a generic line in such a way that they do not coincide, and can then be labeled 1,..., n in sequence from left to right. The permutation (or symmetric) group acting on the objects is generated by the set of s_j, $j=1,\ldots,n-1$, that exchange objects j, $j+1$. The generators obey relations

$$s_j^2=1, \tag{1}$$

$$(s_j s_k)^3=1 \quad (|j-k|=1), \tag{2}$$

$$s_j s_k=s_k s_j \quad (|j-k|>1) \tag{3}$$

(where 1 denotes the identity element of the group), and this set of generators and relations defines the symmetric group on n objects S_n. It has $n!$ elements.

Similarly, the braid group B_n is generated by nearest-neighbor transpositions t_j, but now they do not square to the identity. The braid group can be defined by the relations (see, e.g., Ref. 11)

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$$t_j t_k t_j = t_k t_j t_k \quad (|j-k|=1), \tag{4}$$

$$t_j t_k = t_k t_j \quad (|j-k|>1). \tag{5}$$

The braid group is an infinite discrete group.

The projective representations of the symmetric group S_n can be viewed as ordinary linear representations of a covering group, that is a nontrivial central extension of S_n by U(1) (or by a subgroup thereof). The central extensions of S_n by U(1) are classified up to isomorphism by the cohomology group $H^2(S_n, \mathrm{U}(1))$ which for $n \geqslant 4$ is $\cong \mathbf{Z}_2$.[12–14] Hence for $n \geqslant 4$ (we consider only this range from here on) there are nontrivial extensions of S_n by $\mathbf{Z}_2$, which have $2 \cdot n!$ elements, and we denote one of these by $\tilde{S}_n$. $\tilde{S}_n$ can be defined by n generators σ_j $(j=1,..., n-1)$, z and relations[14,15]

$$z^2 = 1, \tag{6}$$

$$z\sigma_j = \sigma_j z, \tag{7}$$

$$\sigma_j^2 = z, \tag{8}$$

$$\sigma_j \sigma_k \sigma_j = \sigma_k \sigma_j \sigma_k \quad (|j-k|=1), \tag{9}$$

$$\sigma_j \sigma_k = z\sigma_k \sigma_j \quad (|j-k|>1). \tag{10}$$

Thus z is a central element that commutes with all elements, and can be set to either $+1$ or -1 in any irreducible representation (note that we do not distinguish between the abstract generators z, s_j, t_j, σ_j, etc., and their matrix representatives in a particular representation). The relations are the same as for the symmetric group, modulo factors of z. Representations in which $z=1$ descend to linear representations of the quotient group, $\tilde{S}_n/\{1,z\} \cong S_n$, while representations in which $z=-1$ are projective representations of S_n. (The only other nontrivial double cover $\hat{S}_n$, not isomorphic to $\tilde{S}_n$ except for $n=6$,[14] is obtained by using instead generators σ_j' which obey similar relations but with 1 in place of z in Eq. (8).[14,15] In a representation in which $z=-1$, this results from setting $\sigma_j' = i\sigma_j$ for all j. These were the relations used in Ref. 6.)

The proposal for projective permutation statistics[6] was that, as quantum mechanics welcomes the use of projective representations of symmetries, identical particles might be described by projective representations of the permutation group. Since the permutations do not refer to the topology of space (unlike the braiding operations), this proposal, if correct, could be used in any dimension (the ordering of the particles along the line is then arbitrary). Then the operation of exchange of nearest neighbors would be represented by an element T_j acting on Hilbert space, and in the projective permutation statistics proposal, each T_j must be either σ_j or $-\sigma_j$, since these are the elements that project to transpositions s_j in the quotient group S_n. In particular, there is a representation of $\tilde{S}_n$ of dimension $2^{[(n-1)/2]}$ (where $[x]$ denotes the largest integer $\leqslant x$). This coincides with the dimension of the representation of the braid group identified[1,3,4] in the Moore–Read quantum Hall state, and Wilczek[6] claimed that this representation of $\tilde{S}_n$ is equivalent to the representation of the braid group obtained in Ref. 3, up to some phase factors that we will discuss in a moment. Note that the complex Clifford algebra on m generators γ_j, with relations $\gamma_j^2 = 1$, $\gamma_j \gamma_k = -\gamma_k \gamma_j$ $(j \neq k)$, has dimension 2^m. For m even, the Clifford algebra is isomorphic to the algebra of matrices on a vector space of dimension $2^{m/2}$. This applies here with $m = 2[(n-1)/2]$.

The difficulty with the general proposal is that statistics of particles in quantum field theory or many-body theory must obey locality. That is, the underlying physics is presumed to be given by a local Hamiltonian containing local interactions between local fields (for example, the electrons in the quantum Hall system). The locality assumption plays a crucial role in the general rigorous analysis of particle statistics; see, e.g., Refs. 16–21. In particular, it appears that projective rep-

resentations of the permutation group are explicitly ruled out (see, e.g., Theorem. 2.2.3c in Chap. IV of Ref. 21 for the case of relativistic theories in space dimension $\geqslant 3$ under some technical assumptions that are relaxed by the end of Sec. IV.3.3, and Sec. IV.5 of Ref. 21 for some discussion of space dimension 2 where the braid group enters). The central step of the analysis is to move particles around *continuously* in space–time, and the results depend only on the homotopy class of the path taken in configuration space. In particular, exchanges of disjoint well-separated pairs of particles must commute as the two orderings of the exchanges are homotopically equivalent, so in particular $T_j T_k = T_k T_j$ for $|j-k|>1$, or in other words the group-theoretic commutator $T_j T_k T_j^{-1} T_k^{-1} = 1$. In the projective representations of the symmetric group, the commutator is instead -1 (whatever the choice of the lift, $T_j = \sigma_j$ or $-\sigma_j$, of each s_j), and so *projective statistics violates locality*. On the other hand, locality is not violated by braid statistics, where $T_j = t_j$ in some representation of B_n, and it is known that non-Abelian braid statistics can be realized in a local theory in $2+1$ dimensions,[19,18] for example in pure Chern–Simons gauge theory.

Independent of the physical requirement of locality, the difference between the commutators of generators in B_n (5) and in $\tilde{S}_n$ (10) implies that a projective representation of S_n (in which $z = -1$) *cannot* also be a representation of the braid group B_n, in contradiction to Wilczek's claim.[6] Put another way, the image of the braid group in $\mathrm{U}(2^{[(n-1)/2]})$ given by the representation matrices (the existence of which will be checked later) and that of $\tilde{S}_n$ are not isomorphic as groups (given the way that both project to the symmetric group). (Later we will see that these two groups, though both finite, are actually of different orders.)

No escape from these conclusions can be found in a remark by Wilczek[6] that in the quantum Hall example, the projective statistics is combined with anyonic phase factors, $e^{2\pi i/8}$ in a T_j. If this is taken to mean that the physical exchanges T_j act in a tensor product of the $2^{[(n-1)/2]}$ dimensional representation of $\tilde{S}_n$ as above, with an Abelian representation of the braid group $t_j = e^{i\theta}$ for some real θ, so $T_j = \sigma_j \otimes t_j$, then it is clear that this does not affect the noncommutation of disjoint exchanges, $T_j T_k T_j^{-1} T_k^{-1} = -1$. (A special case is $e^{i\theta} = i$, discussed earlier.) These generators clearly obey the relations (reintroducing z for convenience)

$$z^2 = 1, \tag{11}$$

$$z\tau_j = \tau_j z, \tag{12}$$

$$\tau_j \tau_k \tau_j = \tau_k \tau_j \tau_k \quad (|j-k|=1), \tag{13}$$

$$\tau_j \tau_k = z\tau_k \tau_j \quad (|j-k|>1). \tag{14}$$

The existence of representations $T_j = \tau_j$ of these relations implies their consistency, and hence the existence of a nontrivial central extension $\tilde{B}_n$ of the braid group, defined abstractly by the generators z, τ_j and the above-given relations. Any of the four groups mentioned earlier, $\tilde{S}_n$, B_n, S_n, or $\hat{S}_n$ can be obtained from $\tilde{B}_n$ by imposing additional relations $\tau_j^2 = z$, $z=1$, both of these, or $\tau_j^2 = 1$, respectively. Similarly, if $t_j^{(1)}$ and $t_j^{(2)}$, $j = 1,\ldots, n-1$, are two representations of the braid group B_n, then $t_j = t_j^{(1)} \otimes t_j^{(2)}$ gives another one. In particular, $t_j^{(2)} = e^{i\theta}$ (for all j) is a one-dimensional representation, and so a continuum of distinct representations of the same dimension can be found for each choice of $t_j^{(1)}$'s. In quantum Hall effect systems, such Abelian tensor factors are common, as there is a contribution to T_j from the charge degrees of freedom, which produces a θ that depends on the filling factor.

If one considers representations modulo phase factors, then this distinction between the commutators (5), (10) cannot be made. This is the notion of isomorphism of groups modulo scalars, in contrast to the usual isomorphism we have been invoking so far. Isomorphism modulo scalars amounts to isomorphism of the images of the group(s) in the projective linear group $\mathrm{PGL}(N) \cong \mathrm{GL}(N)/\mathrm{GL}(1)$, or since we are considering unitary representations, $\mathrm{PU}(N) \cong \mathrm{U}(N)/\mathrm{U}(1)$. However, isomorphism modulo scalars is generally too weak a property to use in quantum phys-

ics. That is because we must keep track of interference between processes that correspond to distinct group operations, and the phases involved may be relative phases that affect such interference. That is, we are interested in more than just the representation of a group. For example, S_n has two one-dimensional representations, one in which $s_j=+1$, one in which $s_j=-1$, corresponding to Bose and Fermi statistics, respectively. Modulo scalars, these are isomorphic, but linearly (and physically) they are not.

We now examine the construction of NW[3] to find the structure of their braid group representation of dimension $2^{[(n-1)/2]}=2^{n/2-1}$ (we consider only n even from here on; there are similar results for n odd). Essentially the same construction, based on the Temperley–Lieb (TL) algebra specialized to the Ising model, was obtained much earlier by Jones.[22] See also Ref. 23. NW deduce most of its properties from the properties of conformal blocks of spin fields in the Ising model, as in Ref. 1. The central idea is that each object corresponds to an orthogonal direction in real n-dimensional Euclidean space $\mathbf{R}^n$, and the elementary transpositions T_j correspond to a rotation v_j by $\pi/2$ in the plane spanned by objects j, $j+1$, acting in one of the two inequivalent spinor representations of dimension $2^{n/2-1}$ of the covering group Spin(n) of SO(n), up to a j-independent phase factor as just discussed: $T_j=e^{i\theta}v_j$. Clearly these operations have the effect of permuting the n axes (if we ignore the direction along each axis), and thus do project to the action of the permutation group as desired. Each rotation can be defined as $v_j=\exp[i(\pi/2)e_{j,j+1}]$, where $e_{j,k}$ $(j<k)$ is the element of the Lie algebra so(n) that generates a rotation in the jk plane, acting here in the chosen spinor representation. Since the generators $e_{j,k}$ for disjoint pairs j_1k_1, j_2k_2 commute, and this remains true in any representation including the spinors (there are no nontrivial central extensions of any semisimple Lie algebra!), the v_j's commute, $v_jv_kv_j^{-1}v_k^{-1}=1$ for $|j-k|>1$. Hence there is no difficulty with locality of the proposal of Ref. 3, and so far it is consistent with the claim that the v_j's form a linear representation of the braid group, with $t_j=v_j$. It remains to check the other relation (4).

To understand the structure of the representation of the braid group of dimension $2^{n/2-1}$ given by $t_j=v_j$, it is useful first to consider the geometry of the group of rotations by $\pi/2$ about the axes in $\mathbf{R}^n$ in more detail. This amounts to studying the group generated by elements $u_j=\exp[i(\pi/2)e_{j,j+1}]$, where this time $e_{j,k}$ act in the defining n-dimensional representation of SO(n). The operation u_1, for example, sends the point with coordinates $(x_1,\ldots,x_n)$ to $(-x_2,x_1,x_3,\ldots,x_n)$. The group generated by the u_j's can be seen to be the set of all permutations of $x_1,\ldots,x_n$, together with sign changes, but with the condition that an even permutation is combined with an even number of sign changes, and an odd permutation with an odd number of sign changes. If the latter condition is dropped, we obtain the group of all permutations and sign changes, which is generated by all reflections in the diagonals $x_j=x_k$ $(1\leqslant j<k\leqslant n)$ and in the coordinate planes $x_j=0$, $j=1,\ldots n$. This is therefore a Coxeter group, denoted $\mathcal{B}_n$ (Ref. 24) [it is the Weyl group of so$(2n+1)$ and sp$(2n)$]. It can be described by generators and relations, but we will not need these here. There is a subgroup of index 2, which we denote $\mathcal{B}_n^+$, consisting of the elements that are proper rotations, and it is exactly the group generated by the u_j's. $\mathcal{B}_n$ is a semidirect product of S_n with the group of sign changes $(\mathbf{Z}_2)^n$, and has order $2^n\cdot n!$. Its rotation subgroup $\mathcal{B}_n^+$ has order $2^{n-1}\cdot n!$, and is an extension of S_n by $(\mathbf{Z}_2)^{n-1}$, but not a semidirect product (that is, there is no S_n subgroup of $\mathcal{B}_n^+$ that projects onto S_n under the quotient map $\mathcal{B}_n^+\to\mathcal{B}_n^+/(\mathbf{Z}_2)^{n-1}\cong S_n$). Finally, the cover Spin(n) of SO(n), and the inclusion of $\mathcal{B}_n^+$ in SO(n), induce a double cover $\tilde{\mathcal{B}}_n^+$ (there is a similar double cover $\tilde{\mathcal{B}}_n$ of $\mathcal{B}_n$). $\tilde{\mathcal{B}}_n^+$, which has order $2^n\cdot n!$, is almost the group we need. It is generated by the lifts of the u_j's, and the irreducible representations of dimension $2^{n/2-1}$ of Spin(n) induce representations of the same dimension of $\tilde{\mathcal{B}}_n^+$, which can also be viewed as projective representations of $\mathcal{B}_n^+$. To find the order of the image of $\tilde{\mathcal{B}}_n^+$ in the irreducible spinor representations, we note that, for $n\geqslant 6$, the only normal subgroups of Spin(n) are contained in its center, which is $\mathbf{Z}_4$ ($n/2$ odd), $\mathbf{Z}_2\times\mathbf{Z}_2$ ($n/2$ even), so the kernel of the map $\tilde{\mathcal{B}}_n^+\to\mathrm{U}(2^{n/2-1})$ must also be contained in the center of Spin(n). Hence the order of the image of $\tilde{\mathcal{B}}_n^+$ is the same as the order of $\tilde{\mathcal{B}}_n^+$, within a factor of 2 or 4. For $n=4$, Spin(4)

$\cong \mathrm{SU}(2)\times\mathrm{SU}(2)$, and the irreducible spinor representations do not faithfully represent the Lie algebra so(4), so the factor could be larger.

For $\mathcal{B}_n^+$, it is easy to show that setting $t_j = u_j$ does satisfy relation (4) defining the braid group B_n. To study the other groups explicitly, we resort to Clifford algebra methods. The reducible spinor representation of so(n), of dimension $2^{n/2}$, can be naturally constructed as a representation of the even part of a complex Clifford algebra on n generators by setting $e_{j,k} = -i\gamma_j\gamma_k/2$. The representation splits into two irreducibles of dimension $2^{n/2-1}$ (this is also the structure of the Temperley–Lieb algebra in the Ising model,[22] and of a full Clifford algebra on only $n-1$ generators, which Jones constructs[22]). Spin(n) and its center (and hence $\tilde{\mathcal{B}}_n^+$, by a similar argument to that in the previous paragraph) act faithfully in the $2^{n/2}$-dimensional representation. We find $v_j = (1+\gamma_j\gamma_{j+1})/\sqrt{2}$.[23] It is then easy to verify that setting $t_j = v_j$, relation (4) is satisfied. The center of Spin(n) is contained in $\tilde{\mathcal{B}}_n^+$. It includes the elements $U = v_1^2 v_3^2 \cdots v_{n-1}^2 = \gamma_1\gamma_2\cdots\gamma_n$ and $v_j^4 = -1$. For $n/2$ odd, $U^2 = -1$, and U generates the center $\cong \mathbf{Z}_4$ of Spin(n). The two irreducible components are distinguished by the values $U = i, -i$. In these cases, $\mathbf{Z}_4$ and hence the whole of $\tilde{\mathcal{B}}_n^+$ are represented faithfully in the $2^{n/2-1}$-dimensional representations, and hence the image of B_n has order $2^n \cdot n!$. For $n/2$ even, $U^2 = 1$, and the center of Spin(n) is $\{1, U, -U, -1\}$. $U = 1$ in one irreducible component, $U = -1$ in the other, and the reverse for $-U$. Hence for $n \geqslant 8$ the image of $\tilde{\mathcal{B}}_n^+$ (and of B_n) is $\cong \tilde{\mathcal{B}}_n^+/\mathbf{Z}_2$ for some $\mathbf{Z}_2$ in either component, and has order $2^{n-1}\cdot n!$. For $n = 4$, one finds[22] that $v_3 = v_1^{-1}$, v_1 in the two components, and the image of $\tilde{\mathcal{B}}_4^+$ and B_4 is isomorphic to $\tilde{\mathcal{B}}_3^+$ ($\tilde{\mathcal{B}}_n^+$ for n odd is defined the same way as for n even) of order $2^3 \cdot 3! = 48$. Finally, for all even $n \geqslant 4$, the center of the even part of the Clifford algebra is generated by U, and the center of $\tilde{\mathcal{B}}_n^+$ is the same as that of Spin(n).

Our conclusion for the order of the finite group generated by the images v_j of the t_j's in these irreducible representations agrees with the analysis by Jones, who showed that the image of B_n in $\mathrm{PU}(2^{n/2-1})$ has order $2^{n-2}\cdot n!$ for $n \geqslant 6$, and 24 for $n = 4$ (see Theorem. 5.2 in Ref. 22). This is consistent with our results since passing to the projective group involves division by the center (the center of $\tilde{\mathcal{B}}_3^+$ is $\mathbf{Z}_2$).

For comparison, the symmetric group S_n can be viewed as the Coxeter group $\mathcal{A}_{n-1}$ (Ref. 24) [the Weyl group of su(n)]. As such it is generated by reflections (representing the s_j's) in the hyperplanes $x_j = x_{j+1}$ in $\mathbf{R}^n$, and this represents it as a subgroup of O(n). As all the generators leave the points on the line $x_1 = x_2 = \cdots x_n$ fixed, the reflections can be restricted to the orthogonal hypersurface $\Sigma_j x_j = 0$, and so generate a subgroup of O($n-1$). O($n-1$) has an irreducible projective spinor representation [or linear representation of its double cover Pin($n-1$)] of dimension $2^{n/2-1}$, in which the lift of a reflection in any hyperplane is represented by a linear combination of generators of a Clifford algebra on $n-1$ generators. The lifts σ_j', $z\sigma_j'$ to Pin($n-1$) of s_j ($j = 1,\ldots, n-1$) then generate $\hat{S}_n$. In terms of the Clifford algebra (for convenience we will continue to use the Clifford algebra associated with $\mathbf{R}^n$), the explicit expressions are $\sigma_j' = (\gamma_j - \gamma_{j+1})/\sqrt{2}$ (these elements generate a full Clifford algebra on $n-1$ generators), and the anticommutation of σ_j', σ_k' for $|j-k| > 1$ follows.[14] This is *not* the construction proposed in Ref. 3 for the braiding operations. If an Abelian factor $e^{i\theta}$ is tensored into each σ_j', then the image of $\tilde{B}_n$ in $\mathrm{U}(2^{n/2-1})$ is again a finite group if $\theta/2\pi$ is rational. Even if this finite group happens to have the same order as $\tilde{\mathcal{B}}_n^+$, it has a different structure, as we have already shown.

We should mention that the statistics described by representations of the group $\tilde{\mathcal{B}}_n^+$ discussed here cannot describe particles in more than two space dimensions, because the exchanges T_j do not obey (even up to a phase) the well-known conditions $T_j^2 = 1$ that are required[16,21] in higher dimensions.

There are also other examples of quantum Hall systems with non-Abelian braid statistics, with no obvious relation to Clifford algebras. In the sequence of quantum Hall states, labeled by $k = 1, 2,\ldots$, constructed in Ref. 25, the braiding of the quasiparticles is the same as that of Wilson lines in SU(2) Chern–Simons gauge theory of level k, up to tensoring by an Abelian representation. It is known that the image of the braid group in U(N) (for certain N) in these cases is finite

for $k=1$, 2, 4 (Abelian for $k=1$), and dense in SU(N) for all other k.[26] Therefore in general, study of the statistics involves the braid group, and not a finite group.

To conclude, we have pointed out that the image of the braid group in any $2^{[(n-1)/2]}$-dimensional representation is not isomorphic to the nontrivial double cover of the symmetric group, even if an Abelian representation of the braid group is tensored with the latter. Projective permutation statistics is not consistent with locality, but the physical examples in quantum Hall states are described by the braid group and are consistent with locality. In the case of the quasiparticles in the Moore–Read state, the statistics is nonetheless related to Clifford algebras.

ACKNOWLEDGMENTS

I am grateful to Zhenghan Wang and Jürg Fröhlich for helpful communications. This work was supported by the NSF under Grant no. DMR-98-18259.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

A connection between distributivity and locality in compound P-lattices

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(Received 6 June 2002; accepted 16 October 2002)

A P-lattice is a σ-complete, orthomodular atomic lattice $\mathcal{L}$ which is formed by the set of propositions of a physical system. A composition of physical systems is considered, and some concept of locality in a compound physical system is represented in terms of P-lattices. We give a remark toward necessary and sufficient conditions for it to hold, which have been provided implicitly in antecedent studies, and we show that it can be provided under weaker conditions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1532537]

I. INTRODUCTION

For the realist, the main motivation to tackle an interpretative problem of quantum theory is that it seems impossible to apply some concepts of physical reality to this new theory consistently. As a result of analyses for problems to be called ''the hidden variable problem,'' this kind of gap between classical and quantum concepts is becoming clear gradually. On the one hand, by the algebraic analyses,[1] it is known that (noncontextual) definite value assignments to every observable in quantum system are impossible. On the other hand, according to the stochastic arguments for compound systems,[2] we must admit that there exists some sort of nonlocality in quantum systems. Then, do the new features have any logical connection such that the one implies the other?[3] Or, do they merely show how far the distance between classical and quantum pictures is?

To deal with the problems of (non-)locality, we must consider compound physical systems. Now, we would like to regard the combination of two physical systems S_1, S_2 as a single one S. In the context of lattice-theoretical description, there have been various discussions about the problem of the representation of the compound system S in terms of S_1 and S_2.[4–10] Aerts and Daubechies[5] proposed some natural requirements to describe a compound system based on the recognition of subsystems. In the line of them, we would like to deal with the relation between the problem of locality and algebraic structures of physical systems. In antecedent studies concerning it, some authors explicitly or implicitly have provided some important results. However, these results were given under somewhat strong conditions. We shall show similar results under weaker conditions, and give a remark toward a necessary and sufficient condition for some concept of locality to hold, and show logical connections between (non-)locality in a compound system and structures of its components.

Remark: For lattice-theoretical construction of so-called ''tensor product,'' there is the well-known open question about its uniqueness in quantum case.[4–10] However, our purposes are not to deal with this problem but to consider some property in a compound system if such construction is possible.

II. PROPOSITIONAL STRUCTURE OF PHYSICAL SYSTEMS

A *P-lattice* is a σ-complete, orthomodular atomic lattice $\mathcal{L}$ which is formed by the set of propositions of a physical system.[11]

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A distributive P-lattice is called *classical*, which is isomorphic to the Borel σ-field of some phase space in classical mechanics. An irreducible P-lattice is called *quantum*, which is isomorphic to the lattice of all closed subspaces of some Hilbert space.

Let $\mathcal{L}$ and $\mathcal{L}'$ be P-lattices. A map $h:\mathcal{L}\to\mathcal{L}'$ is called an *injective σ-orthohomomorphism* if it is one-to-one and it preserves σ-meets, orthocomplements and the minimal element (consequently, it preserves σ-joins and the maximal element as well). If an injective σ-orthohomomorphism h preserves all existing meets, including meets (if they exist) for families which are not necessarily countable, then it is called an *injective strong orthohomomorphism*.

Let $\mathcal{L}_1$, $\mathcal{L}_2$ be σ-complete lattices, and $\mathcal{L}_1 \uplus \mathcal{L}_2$ be the direct sum[12] of $\mathcal{L}_1$ and $\mathcal{L}_2$. If $\mathcal{L}_1$ and $\mathcal{L}_2$ are P-lattices, then it is easy to show that $\mathcal{L}_1 \uplus \mathcal{L}_2$ is also a P-lattice.

For notation, $(a,b)\,\mathsf{C}$ denotes that elements $a, b \in \mathcal{L}$ commute with each other, $\mathcal{C}(\mathcal{L})$ stands for the center of $\mathcal{L}$, and $\mathcal{A}(\mathcal{L})$ for the set of all atoms of $\mathcal{L}$.

III. SOME THEOREMS ABOUT P-LATTICES

Let $\mathcal{L}$ be a lattice. Recall that $\mathcal{L}$ is called *atomic* when every nonzero element majorizes at least one atom, and is called *atomistic* when every element is the join of the atoms it contains.

Lemma (A): If an orthomodular lattice is atomic, then it is also atomistic.

Proof: Let $\mathcal{L}$ be an orthomodular atomic lattice. Put $\mathcal{S}=\{p\in\mathcal{A}(\mathcal{L})|p\leqslant a\}$ for nonzero $a \in \mathcal{L}$. Let b be an upper bound of $\mathcal{S}$ such that $b\leqslant a$. Suppose that $a\wedge b^{\perp}\neq 0$. By atomicity, there is $q\in\mathcal{A}(\mathcal{L})$ such that $q\leqslant a\wedge b^{\perp}$. We have $q\leqslant a$, so $q\in\mathcal{S}$. Therefore we get $q\leqslant b$, then $q\leqslant b\wedge b^{\perp}=0$, a contradiction.

Now, let c be any upper bound of $\mathcal{S}$. Then $a\wedge c$ is so, and $a\wedge c\leqslant a$. From above results, we have $a\wedge(a\wedge c)^{\perp}=0$. Due to orthomodularity of $\mathcal{L}$, we get $a=(a\wedge c)\vee[a\wedge(a\wedge c)^{\perp}]=a\wedge c$, which means $a\leqslant c$. Therefore a is the least upper bound of $\mathcal{S}$, i.e., $a=\vee\mathcal{S}$, which shows $\mathcal{L}$ is also atomistic. □

Lemma (B): Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be P-lattices, and a map $h:\mathcal{L}_1\to\mathcal{L}_2$ be an injective σ-orthohomomorphism. Let a be any nonzero element in $\mathcal{L}_1$. Then,

$$h(a)=\vee\{h(p)\in\mathcal{L}_2|p\in\mathcal{A}(\mathcal{L}_1),p\leqslant a\}.$$

In particular, $I_2=h(I_1)=\vee\{h(p)\in\mathcal{L}_2|p\in\mathcal{A}(\mathcal{L}_1)\}$.

Proof: It is obvious that image $h(\mathcal{L}_1)\subseteq\mathcal{L}_2$ is isomorphic to $\mathcal{L}_1$ and is also a P-lattice. It is also obvious that $\mathcal{A}(h(\mathcal{L}_1))=\{h(p)\in\mathcal{L}_2|p\in\mathcal{A}(\mathcal{L}_1)\}$. Since $h(\mathcal{L}_1)$ is atomistic by virtue of Lemma (A), for any nonzero element $h(a)$ in $h(\mathcal{L}_1)$ we have

$$h(a)=\vee\{h(p)\in\mathcal{L}_2|p\in\mathcal{A}(\mathcal{L}_1),p\leqslant a\}.$$

In the case of $a=I_1$, the last statement in the lemma immediately follows. □

In the following sections, we prove some theorems. For their proofs, we shall appeal frequently to the following two theorems:

Theorem (Foulis-Holland): *If, in an orthomodular lattice, one of the elements a,b,c commutes with the other two, then triple (a,b,c) is distributive.*

Theorem (direct sum decomposition): *Let $\mathcal{L}$ be a lattice. If $\mathcal{L}$ has a nontrivial central element c, then $\mathcal{L}=[0,c]\uplus[0,c^{\perp}]$, where $[\bullet,\bullet]$ denotes a segment.*

IV. THE REQUIREMENTS FOR COMPOUND SYSTEM

We shall be almost exclusively concerned with a compound system S consisting of the subsystems S_1 and S_2. In this case, it is natural to require at least the following;

(1) Structures of S_1 and S_2 must be preserved if they are considered as subsystems of S.
(2) Maximum information about S_1 and S_2 implies maximum information about S.
(3) Propositions (or properties) on S that refer only to subsystem S_1 have to be compatible with propositions on S that refer only to subsystem S_2.

(4) Compound system S contains only S_1 and S_2 as the subsystems.

These requirements seem to represent very minimal and natural assumptions.[5,6] Mathematical formulation is the following: Let $\mathcal{L}_1$, $\mathcal{L}_2$ and $\mathcal{L}$ be P-lattices associated with S_1, S_2 and S, respectively. $\mathcal{L}$ is called the *compound P-lattice* of $\mathcal{L}_1$, $\mathcal{L}_2$ if

(i) there exist two injective σ-orthohomomorphisms $h_i:\mathcal{L}_i\to\mathcal{L}$ $(i=1,2)$,
(ii) $h_1(p)\wedge h_2(q)\in\mathcal{A}(\mathcal{L})$ for every $p\in\mathcal{A}(\mathcal{L}_1)$, $q\in\mathcal{A}(\mathcal{L}_2)$,
(iii) $(h_1(a),h_2(b))$ C for every $a\in\mathcal{L}_1$, $b\in\mathcal{L}_2$, and
(iv) $h_1(\mathcal{L}_1)\cup h_2(\mathcal{L}_2)$ generates $\mathcal{L}$, that is the smallest P-lattice containing both $h_1(\mathcal{L}_1)$ and $h_2(\mathcal{L}_2)$ is $\mathcal{L}$.

Remark that it is not required that maximum information about S is merely the sum of maximum information about S_1 and S_2. That is, it is not assumed that a compound P-lattice $\mathcal{L}$ always has the property such that

$$\mathcal{A}(\mathcal{L})=\{h_1(x)\wedge h_2(y)|x\in\mathcal{A}(\mathcal{L}_1),\, y\in\mathcal{A}(\mathcal{L}_2)\}.$$

If every atom in a P-lattice corresponds to some pure state of the system, we can regard this property as expressing some sort of locality, i.e., the separability of states of the compound system. So we will call this property *SEPARABILITY*.

V. NECESSARY CONDITION FOR SEPARABILITY IN COMPOUND P-LATTICES

In antecedent studies, some authors have provided necessary conditions for SEPARABILITY in their schemes. For example, Pulmannová (Ref. 8, Theorem 2) provided a necessary condition for SEPARABILITY in the free orthodistributive product of *complete* atomistic orthomodular lattices, in which injective maps $h_i:\mathcal{L}_i\to\mathcal{L}$ $(i=1,2)$ are not only σ-orthohomomorphisms but also *strong* orthohomomorphisms. It is easy to show that a similar result applies to our compound P-lattice as follows:

Theorem 1: Let $\mathcal{L}_1$, $\mathcal{L}_2$ *be P-lattices and* $\mathcal{L}$ *be the compound P-lattice of* $\mathcal{L}_1$ *and* $\mathcal{L}_2$. *If* $\mathcal{A}(\mathcal{L})=\{h_1(x)\wedge h_2(y)|x\in\mathcal{A}(\mathcal{L}_1),\, y\in\mathcal{A}(\mathcal{L}_2)\}$, *then at least one of* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *is classical.*

In the proof by Pulmannová (Ref. 8, Theorem 2), three lemmas (Lemma 1, 3, and 4) are used, and only one of them (Lemma 4) is proved by using strong conditions which is not supposed in our compound P-lattice. Therefore only what we need is to prove Pulmannová's Lemma 4 under our conditions. In this lemma, we say that the elements $b,c\in\mathcal{L}$ are separated by a superselection rule if for any atom $a\leqslant b\vee c$ we have $a\leqslant b$ or $a\leqslant c$.

Lemma 1.1 [Pulmannová (Ref. 8, Lemma 4)]: Let $\mathcal{L}$ *be a P-lattice. If* $a,b\in\mathcal{L}$ *are two different atoms which are separated by a superselection rule, then* $a\perp b$.

Proof: Let $a,b\in\mathcal{L}$ be two different atoms which are separated by a superselection rule. Put $x:=(a\vee b)\wedge a^{\perp}$. Now, we will show $x\neq 0$. Suppose $x=0$. Since $a\leqslant a\vee b$ and $\mathcal{L}$ is orthomodular, we have

$$a\vee b=a\vee[(a\vee b)\wedge a^{\perp}]=a\vee x=a,$$

so we have $b\leqslant a$, which contradicts the supposition that a,b are two different atoms. Therefore we see $x\neq 0$. By atomicity, there exists an atom p such that $p\leqslant x\leqslant a\vee b$. It is obvious that $p\leqslant x\leqslant a^{\perp}$, so $p\neq a$. If $a^{\perp}\wedge b=0$, then we have

$$p\wedge b\leqslant x\wedge b=(a\vee b)\wedge a^{\perp}\wedge b=0,$$

so $p\neq b$, which contradicts to the supposition that a,b are separated by a superselection rule. Therefore we see $a^{\perp}\wedge b\neq 0$. Since $a^{\perp}\wedge b\leqslant b$ and $b\in\mathcal{A}(\mathcal{L})$, we obtain $b=a^{\perp}\wedge b$, which means $a\perp b$. □

VI. SUFFICIENT CONDITION FOR SEPARABILITY IN COMPOUND P-LATTICES

There have been many important results concerning compositions of a quantum and a classical system,[6,8,9,13] derived from somewhat strong conditions as mentioned in previous section. It might be unnoticed that some of them can be provided under weaker conditions. In particular, we can show a similar result, which provides a sufficient condition for SEPARABILITY, as follows:

Theorem 2: *Let $\mathcal{L}_1$, $\mathcal{L}_2$ be P-lattices and $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$. If at least one of $\mathcal{L}_1$ and $\mathcal{L}_2$ is classical, then $\mathcal{A}(\mathcal{L})=\{h_1(x)\wedge h_2(y)|x\in\mathcal{A}(\mathcal{L}_1), y\in\mathcal{A}(\mathcal{L}_2)\}$.*

Proof: Let $\mathcal{L}_1$ be a classical P-lattice and $\mathcal{L}_2$ be an arbitrary P-lattice. As a first step, we need the following lemma:

Lemma 2.1: Let $\mathcal{L}_1$ be a classical P-lattice and $\mathcal{L}_2$ be an arbitrary P-lattice. Let $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$. Then $h_1(a)\in\mathcal{C}(\mathcal{L})$ for every $a\in\mathcal{A}(\mathcal{L}_1)$.

Proof of Lemma 2.1: Put $\mathcal{S}:=\{x\in\mathcal{L}|(x,h_1(a))\ \mathsf{C}\}$. First, we will show that $\mathcal{S}$ is a P-lattice whose order-relation is due to $\mathcal{L}$.

(1) By supposition, it is obvious that $\mathcal{S}$ is a partially ordered set.
(2) Due to σ-completeness of $\mathcal{L}$, there exist $\vee_i x_i$ and $\wedge_i x_i$ in $\mathcal{L}$ for $\{x_i\}_{i\in\mathbb{N}}\subseteq\mathcal{S}$. Then, it follows that $(\vee_i x_i, h_1(a))\ \mathsf{C}$ and $(\wedge_i x_i, h_1(a))\ \mathsf{C}$ (see Ref. 12, Lemma 36.4). So $\vee_i x_i\in\mathcal{S}$ and $\wedge_i x_i\in\mathcal{S}$. Therefore $\mathcal{S}$ is a σ-complete lattice. Further, it is evident that $0,I\in\mathcal{S}$.
(3) Since $(x^\perp, h_1(a))\ \mathsf{C}$ for every $x\in\mathcal{S}$, we have $x^\perp\in\mathcal{S}$, which means that $\mathcal{S}$ is orthocomplemented.
(4) Due to orthomodularity of $\mathcal{L}$, $[x\leqslant y\Rightarrow y=x\vee(y\wedge x^\perp)]$ holds for every $x,y\in\mathcal{S}$. Therefore $\mathcal{S}$ is orthomodular.
(5) We can write $x=(x\wedge h_1(a))\vee(x\wedge h_1(a)^\perp)$ for nontrivial $x\in\mathcal{S}$. Suppose that $x\wedge h_1(a)\neq 0$. Since $\mathcal{L}$ is atomic and $x\wedge h_1(a)\in\mathcal{L}$, there exists an atom p in $\mathcal{L}$ such that $p\leqslant x\wedge h_1(a)$. Then, we have $h_1(a)\geqslant p$, which means that p belongs to $\mathcal{S}$. After all, we have $x\geqslant p$, which shows $\mathcal{S}$ is atomic. Similar steps are applied to $x\wedge h_1(a)^\perp\neq 0$ if $x\wedge h_1(a)=0$.

Second, we will show that $\mathcal{S}=\mathcal{L}$. By the definition of $\mathcal{S}$, we have $\mathcal{S}\subseteq\mathcal{L}$. Since $h_1(\mathcal{L}_1)\subseteq\mathcal{S}$ and $h_2(\mathcal{L}_2)\subseteq\mathcal{S}$ by the requirement (iii), we have $h_1(\mathcal{L}_1)\cup h_2(\mathcal{L}_2)\subseteq\mathcal{S}$. From the result above, we can see that $\mathcal{S}$ is a P-lattice and contains $h_1(\mathcal{L}_1)\cup h_2(\mathcal{L}_2)$. On the other hand, $\mathcal{L}$ is the smallest P-lattice containing the set because of the requirement(iv). Therefore we obtain $\mathcal{S}=\mathcal{L}$, which means $h_1(a)\in\mathcal{C}(\mathcal{L})$. This completes the proof of Lemma 2.1.

Let $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$. Suppose that there exists an atom p such that $p\notin\{h_1(x)\wedge h_2(y)|x\in\mathcal{A}(\mathcal{L}_1), y\in\mathcal{A}(\mathcal{L}_2)\}$. Hence, there must exist at least one atom $\alpha\in\mathcal{A}(\mathcal{L}_1)$ such that $p\leqslant h_1(\alpha)$ for the atom p. (Otherwise, we have $p\wedge h_1(a)=0$ for every $a\in\mathcal{A}(\mathcal{L}_1)$. By using Lemmas (B) and 2.1, it follows that $0=\vee\{p\wedge h_1(a)|a\in\mathcal{A}(\mathcal{L}_1)\}=p\wedge(\vee\{h_1(a)|a\in\mathcal{A}(\mathcal{L}_1)\})=p\wedge h_1(I_1)=p$, a contradiction). By using the direct sum theorem for the $h_1(\alpha)$, $\mathcal{L}$ is represented by $\mathcal{L}=[0, h_1(\alpha)]\uplus[0, h_1(\alpha)^\perp]$.

Let us consider the mapping from $\mathcal{L}_2$ into the segment $[0, h_1(\alpha)]$ defined as

$$u_{2,\alpha}: y\mapsto h_1(\alpha)\wedge h_2(y) \quad \text{for every } y\in\mathcal{L}_2.$$

It is obvious that the image $u_{2,\alpha}(\mathcal{L}_2)$ does not contain the atom p above. Further, if we define

$$\mathcal{L}^*:=u_{2,\alpha}(\mathcal{L}_2)\uplus[0, h_1(\alpha)^\perp],$$

then we can show the following:

Lemma 2.2: $\mathcal{L}^*$ defined above is a P-lattice such that $\mathcal{L}^*\subsetneq\mathcal{L}$.

Proof of Lemma 2.2: First, we will show that the segment $[0, h_1(\alpha)^\perp]\subset\mathcal{L}$ is a P-lattice in which orthocomplement is defined as the relative orthocomplement in $\mathcal{L}$ mod $h_1(\alpha)^\perp$.

(1) By supposition, it is obvious that the $[0, h_1(\alpha)^\perp]$ is a partially ordered set.

(2) Due to σ-completeness of $\mathcal{L}$, there exist $\vee_i x_i$ and $\wedge_i x_i$ in $\mathcal{L}$ for $\{x_i\}_{i\in\mathbb{N}}\subseteq[0, h_1(\alpha)^\perp]$. Obviously, $\vee_i x_i \leqslant h_1(\alpha)^\perp$ and $\wedge_i x_i \leqslant h_1(\alpha)^\perp$. So we have $\vee_i x_i \in [0, h_1(\alpha)^\perp]$ and $\wedge_i x_i \in [0, h_1(\alpha)^\perp]$, which mean $[0, h_1(\alpha)^\perp]$ is σ-complete. The maximal element is $h_1(\alpha)^\perp$ and the minimal element is 0.

(3) By supposition, $x^r := h_1(\alpha)^\perp \wedge x^\perp \leqslant h_1(\alpha)^\perp$ for all $x\in[0, h_1(\alpha)^\perp]$. Then we have $x^r \in [0, h_1(\alpha)^\perp]$. It shows that $[0, h_1(\alpha)^\perp]$ is orthocomplemented.

(4) Due to orthomodularity of $\mathcal{L}$, for all $x,y\in[0, h_1(\alpha)^\perp]$

$$x\leqslant y \Rightarrow y = x\vee(y\wedge x^\perp)$$

$$= x\vee(y\wedge h_1(\alpha)^\perp\wedge x^\perp).$$

Therefore $[0, h_1(\alpha)^\perp]$ is orthomodular.

(5) Since $\mathcal{L}$ is atomic and $x\in\mathcal{L}$ for nontrivial $x\in[0, h_1(\alpha)^\perp]$, there exists an atom q such that $h_1(\alpha)^\perp \geqslant x \geqslant q$. It shows that $[0, h_1(\alpha)^\perp]$ is atomic.

Second, because the image $u_{2,\alpha}(\mathcal{L}_2)$ is isomorphic to $\mathcal{L}_2$ by definition, we can see that $u_{2,\alpha}(\mathcal{L}_2)$ is also a P-lattice in which orthocomplement is defined as relative orthocomplement in $\mathcal{L}$ mod $h_1(\alpha)$. Remark that, for all $y\in\mathcal{L}_2$,

$$\begin{aligned} u_{2,\alpha}(y)^r &:= h_1(\alpha)\wedge u_{2,\alpha}(y)^\perp \\ &= h_1(\alpha)\wedge(h_1(\alpha)\wedge h_2(y))^\perp \\ &= h_1(\alpha)\wedge h_2(y^\perp) = u_{2,\alpha}(y^\perp). \end{aligned}$$

Then the $\mathcal{L}^*$ is a direct sum of P-lattices, which is also a P-lattice. Because $u_{2,\alpha}(\mathcal{L}_2)$ does not contain the atom p above, it is obvious that $\mathcal{L}^*\subsetneq\mathcal{L}$. This completes the proof of Lemma 2.2.

Now, since $h_1(\alpha)\in\mathcal{C}(\mathcal{L})$, we have, for $y\in\mathcal{L}_2$,

$$h_2(y) = (h_1(\alpha)\wedge h_2(y))\vee(h_1(\alpha)^\perp\wedge h_2(y)).$$

Further, since $h_1(\alpha)\wedge h_2(y)\in u_{2,\alpha}(\mathcal{L}_2)$ and $h_1(\alpha)^\perp\wedge h_2(y)\in[0, h_1(\alpha)^\perp]$, we have also $h_2(y)\in\mathcal{L}^*$. Therefore, $h_2(\mathcal{L}_2)\subset\mathcal{L}^*$.

Moreover, it follows that, for $x\in\mathcal{L}_1$, we have the following.

(i) In the case of $\alpha\leqslant x$:
Let $\mathcal{P}$ be a set of atoms $\{b\in\mathcal{A}(\mathcal{L}_1)\,|\,b\leqslant x, b\neq\alpha\}$. Then we have $x=\alpha\vee(\vee\mathcal{P})$ because of atomicity of $\mathcal{L}_1$. Since $b\perp\alpha$ for all b, we have $h_1(b)\leqslant h_1(\alpha)^\perp$. As a consequence, we obtain $h_1(x)=h_1(\alpha)\vee(\vee h_1(\mathcal{P}))$, which belongs to $\mathcal{L}^*$ because of $h_1(\alpha)\in u_{2,\alpha}(\mathcal{L}_2)$ and $\vee h_1(\mathcal{P})\in[0, h_1(\alpha)^\perp]$.

(ii) In the case of $\alpha\not\leqslant x$:
Let $\mathcal{Q}$ be a set of atoms $\{b\in\mathcal{A}(\mathcal{L}_1)\,|\,b\leqslant x\}$. Then we have $x=\vee\mathcal{Q}$ and $b\perp\alpha$ for all b. Therefore, we have $h_1(x)=0\vee(\vee h_1(\mathcal{Q}))$, which belongs to $\mathcal{L}^*$ because of $0\in u_{2,\alpha}(\mathcal{L}_2)$ and $\vee h_1(\mathcal{Q})\in[0, h_1(\alpha)^\perp]$.

Thus we obtain $h_1(\mathcal{L}_1)\subset\mathcal{L}^*$, therefore, $h_1(\mathcal{L}_1)\cup h_2(\mathcal{L}_2)\subset\mathcal{L}^*$.

From these results and the requirement (iv), it must be $\mathcal{L}=\mathcal{L}^*$. However, $p\in\mathcal{L}$ and $p\notin\mathcal{L}^*$, which show a contradiction. Therefore, we have $\mathcal{A}(\mathcal{L})=\{h_1(x)\wedge h_2(y)\,|\,x\in\mathcal{A}(\mathcal{L}_1), y\in\mathcal{A}(\mathcal{L}_2)\}$. This completes the proof of Theorem 2. □

VII. CONCLUDING REMARKS

From the previous two sections, we have just obtained a necessary and sufficient condition for the SEPARABILITY in compound P-lattice: Let $\mathcal{L}_1$, $\mathcal{L}_2$ be P-lattices and $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$.

Corollary: The SEPARABILITY holds in $\mathcal{L}$ if and only if at least one of $\mathcal{L}_1$ and $\mathcal{L}_2$ is classical.

Or, equivalently, we have the following.

TABLE I. $\mathcal{L}_1$ and $\mathcal{L}_2$ are P-lattices respectively associated with subsystems S_1 and S_2 of a compound physical system S. $\mathcal{L}$ is the compound P-lattice of them. This table shows connections between properties of $\mathcal{L}$ and those of $\mathcal{L}_1$ and $\mathcal{L}_2$.

$\mathcal{L}_1$	$\mathcal{L}_2$	Properties of $\mathcal{L}$
Distributive	Distributive	Distributive and separable
Either Distributive		Nondistributive and separable
Nondistributive	Nondistributive	Nondistributive and nonseparable

Corollary: The SEPARABILITY violates in $\mathcal{L}$ if and only if both $\mathcal{L}_1$ and $\mathcal{L}_2$ are not classical.

For discussions, we need to add some to the results above. It is easy to show the following two theorems:

Theorem: *Let $\mathcal{L}_1$, $\mathcal{L}_2$ be P-lattices and $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$. If both $\mathcal{L}_1$ and $\mathcal{L}_2$ are classical, then $\mathcal{L}$ is also classical.*

Remark that the compound P-lattice in this case is a *Boolean product*.[14]

Theorem: *Let $\mathcal{L}_1$, $\mathcal{L}_2$ be P-lattices and $\mathcal{L}$ be the compound P-lattice of $\mathcal{L}_1$ and $\mathcal{L}_2$. If either $\mathcal{L}_1$ or $\mathcal{L}_2$ is not classical, then $\mathcal{L}$ is not classical.*

From all the results above, we can summarize a connection between the distributivity of P-lattices and the separability of atoms in a compound P-lattice in Table I.

We should state that there can be compound systems, nonclassical and separable. Therefore, if one recognizes our requirements for compound P-lattice, nonclassicality of the system does not necessarily mean nonlocality of it. When we explain some property of a quantum system in the logico-algebraic approach, it is incomplete only to show that distributive law does not hold in the system. We must show the way of construction of the compound system if we would like to know the nonseparable properties of quantum systems.

ACKNOWLEDGMENTS

I would like to express my gratitude to Professor T. Ishigaki for many helpful discussions and valuable suggestions. The research of the author is supported by JSPS Research Fellowships for Young Scientists.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

On dimensional regularization of sums

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(Received 24 January 2002; accepted 23 October 2002)

We discuss a systematic way to dimensionally regularize divergent sums arising in field theories with an arbitrary number of physical compact dimensions or finite temperature. The method preserves the same symmetries of the action as the conventional dimensional regularization and allows an easy separation of the regulated divergence from the finite term that depends on the compactification radius (temperature). © *2003 American Institute of Physics.* [DOI: 10.1063/1.1531215]

I. THE PROBLEM

In a variety of problems one has to deal with formally divergent sums, usually related to Feynman diagrams with one or more discrete momenta, as in the case of theories with compact extra-dimension, finite-size scaling theory in critical phenomena, thermal field theory. It is crucial to find a regulator that preserves the symmetries of the problem and leads to a simple computational procedure. When the momenta are not discrete but continuous, such a procedure exists and it is the well-known dimensional regularization (DR) of integrals.[1,2] In this article we discuss a systematic way to obtain the dimensional regularization of an important class of sums, following closely the analogy with the case of a continuous variable.[3] Even if practical recipes to deal with particular examples have been given in the past and the use of special functions to this purpose is not new,[4–9] our aim is to provide a general method, which extends and in a sense justifies the analysis of Ref. 10, where the idea of dimensionally regularized series was applied to a number of different loop sums. In Ref. 11 the approach to dimensional continuation was adopted and combined with complex analysis techniques to delineate a general procedure, restricting, however, to the case of only one physical compact dimension. In Ref. 12 the use of the Mellin transform, together with dimensional regularization, was introduced to deal with asymptotic expansion of series in thermal field theory, formally the same problem as discussed in Ref. 11.

We propose to *define* sums in complex dimension using the analytic properties of a generalized zeta function, resulting in a simple method where the regulated divergence can be easily separated from the finite part. Our technique has some common points with the well-known zeta-function regularization,[8] which leads to quite similar calculations but is well distant from the spirit of analytical continuation in the number of dimensions.

We hope that this work may contribute to clarify some debated aspects of regularization in extra-dimensional models, where it is crucial to preserve the symmetries of the action.[13–16] In Ref. 14 it was suggested that the finite result obtained by Barbieri, Hall and Nomura[13] for the radiative correction to the Higgs mass coming from the Yukawa sector of their model was a regularization artifact. Unfortunately, the authors of Ref. 14 made use of a sharp cut-off on the series, which explicitly breaks the supersymmetry of the model of Ref. 13 and invalidates their argument. The result of Ref. 13 was reobtained in Ref. 15 by using a thick brane as a regulator for the series and in Ref. 16 in two different ways, with a Pauli–Villars and by using dimensional regularization. In this work we give a formal procedure to introduce the dimensional regularization of a series and

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demonstrate in detail some important properties. In particular, we show that there is *no ambiguity* in exchanging the series and the integral over loop momenta if both are properly regularized.

The article is organized as follows. In Sec. II we briefly review standard dimensional regularization of integrals and give our rules for extending it to the case of a series by using a generalized zeta function. We discuss the infinite radius limit in Sec. III, showing that the (regulated) divergence equals that of the corresponding integral and as such does not depend on the radius. A representation using ϑ-functions is also given in Sec. III B, which is useful to perform explicit computations of sums in a class of physical problems. In Sec. IV we show how the method works on an explicit example, computing the Casimir energy of a massive scalar field. In Sec. V we draw our conclusions.

Finally, in the appendices we briefly recall the definition of the Mellin transform (Appendix A), present the analytic continuation of the generalized zeta function, together with its asymptotic behavior (Appendix B), and discuss some important properties of the dimensionally regularized series (Appendix C).

II. DIMENSIONALLY REGULARIZED SERIES

Dimensional regularization of integrals was introduced in Ref. 1 as a simple tool to manage the divergences that arise in (perturbative) field theory, preserving the gauge symmetry. It was later derived as an axiomatic procedure by Wilson[2] (see Ref. 3 for a detailed discussion). The problem is to give a meaning to the integration of a function $f(p^2)$ over a space of complex dimension d, getting the usual result whenever d is an integer and the integral exists in the ordinary sense. Without going into too much detail, one can *define* the integral through the formula

$$\int \mathrm{d}^d p\, f(p^2) = \Omega_d \int_0^\infty \mathrm{d}p\, p^{d-1} f(p^2) \quad ; \quad \Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}, \tag{1}$$

for all (complex) values of d for which the integral converges and then analytically continue the result to the desired value. Typically one has to cope with ultraviolet (UV) divergences, which are cured by considering a sufficiently small (real part of) d and appear as poles in the final expression for the integral. It may happen that the value of d that makes (1) UV-convergent is so small that the integral diverges in the infrared (IR): in this case one defines the integral subtracting the leading behavior of the function f for $p^2 \to 0$. Let us suppose that $f(t)$ has the following asymptotic expansion for $t \to 0$:

$$\begin{gathered} f(t) = a_0\, t^{\alpha_0} + a_1\, t^{\alpha_1} + a_2\, t^{\alpha_2} + \cdots, \\ \alpha_0 < \alpha_1 < \alpha_2 < \cdots, \end{gathered} \tag{2}$$

and $f(t) \sim t^{-\rho}$ for $t \to \infty$. Then, for $-\alpha_q < \mathrm{Re}\, d/2 < \min(-\alpha_{q-1}, \rho)$, q a positive integer, the integral is defined by

$$\int \mathrm{d}^d p\, f(p^2) = \Omega_d \int_0^\infty \mathrm{d}p\, p^{d-1} \left[f(p^2) - \sum_{k=0}^{q-1} a_k (p^2)^{\alpha_k} \right]. \tag{3}$$

If $-\alpha_0 < \rho$, subtractions are not really needed and the integral on the r.h.s. of Eq. (1) converges for $-\alpha_0 < \mathrm{Re}\, d/2 < \rho$; in this case Eq. (3) is simply the correct analytic extension to the interval $-\alpha_q < \mathrm{Re}\, d/2 < -\alpha_{q-1}$, $q > 0$. On the contrary, when $-\alpha_0 > \rho$, there is no value of d that makes (1) both UV- and IR-convergent and (3) becomes a definition.

This general procedure does not work in the case of sums, given that there is no closed form for what corresponds to the "solid angle" Ω_d in the case of a hypercubic lattice and one cannot directly take advantage of the spherical symmetry of the function f. We then proceed as described below, following closely the analysis of Ref. 3 for the integrals.

We want to give a meaning to the expression

$$\sum_{n\in\mathbb{Z}^d}{}' \; f(n), \tag{4}$$

where the prime means that $n=0$ is omitted in the sum and f is assumed to be continuous. We restrict for simplicity to the case of a scalar function (the case of tensorial functions can be addressed in the same way as for standard DR of integrals) and require covariance of our result under (discrete) rotations of the hypercubic lattice. In the case of only one variable, this implies that the function f depends only on the norm of the vector n and not on its direction. The general case in which f depends also on external momenta is considered below.

An operation of summation in arbitrary complex dimension is uniquely determined by requiring the following basic properties, valid for standard summation: [Except for an arbitrary normalization, which can be fixed on a set of basis functions.[2,3] We require the usual result of integer dimensions

$$\sum_{n\in\mathbb{Z}^d} e^{-\pi s n^2} = \vartheta^d(s),$$

to hold for all $d\in\mathbb{C}$ (see Appendix B for the definition of the ϑ-function).]

(1) *Linearity:* for any complex numbers a, b

$$\sum_{n\in\mathbb{Z}^d}{}' \; [a\;\; f(n)+b\;\; g(n)] = a\sum_{n\in\mathbb{Z}^d}{}' \; f(n)+b\sum_{n\in\mathbb{Z}^d}{}' \; g(n). \tag{5}$$

(2) *Invariance under lattice translations:* for any vector q in $\mathbb{Z}^d$

$$\sum_{n\in\mathbb{Z}^d} f(n+q) = \sum_{n\in\mathbb{Z}^d} f(n). \tag{6}$$

Notice that the scaling axiom required for dimensionally regularized integrals does not hold for the series. (It states that $\forall\, s>0$,

$$\int \mathrm{d}^d p\, f(s^2 p^2) = s^{-d}\int \mathrm{d}^d p\, f(p^2).$$

See Ref. 3.) As for the standard case of integrals, vectors are thought to lie in an infinite dimensional space, with the difference that now each component of the vector has an integer value. The dimensionality d is introduced by the sum operation with the requirement that if d is a positive integer, all vectors collapse in a d-dimensional subspace. When the function f depends also on some external momenta q_i [actually only through the scalar products $(n\cdot q_i)$, $(q_i\cdot q_j)$ being a scalar function], one can proceed again in complete analogy with Ref. 3: it is always possible to find an N-dimensional sublattice $\mathbb{Z}^N$ (with N finite being the external vectors in finite number), which contains all the external vectors. Let us decompose n into a longitudinal and a transverse part with respect to $\mathbb{Z}^N$: $n=n_\parallel+n_\perp$, so that

$$\sum_{n\in\mathbb{Z}^d} f(n,q_i) = \sum_{n_\parallel\in\mathbb{Z}^N}\; \sum_{n_\perp\in\mathbb{Z}^{d-N}} f(n_\perp^2+n_\parallel^2, n_\parallel q_i, q_i\cdot q_j). \tag{7}$$

The outer sum in the r.h.s. of (7) is a standard series on the lattice $\mathbb{Z}^N$, while the inner one can be defined through (4), f now being independent of the direction of $n_\perp$. Then there is no loss of generality in reducing to the case in which f is a function of only the dummy variable.

Let us now describe an explicit procedure for summing in complex dimensions. Given a function $f(t)$ continuous for $t\in\mathbb{R}^+$, let us assume that $\theta(t-a)f(t)$ (where θ is the step function) is Mellin-transformable with fixed $0<a<1$ (see Appendix A and Refs. 17 and 18 for details on the Mellin transform), i.e., $\exists\ \ \rho\in\mathbb{R}$ such that

$$\int_a^\infty \mathrm{d}t\ \ |f(t)|\ \ t^{\sigma-1}<\infty \quad \forall\ \sigma<\rho.$$

Then the Mellin transform

$$\mathcal{M}_a[f,s]\equiv\mathcal{M}[\,\theta(t-a)f(t),s]=\int_a^\infty \mathrm{d}t\ \ f(t)\ \ t^{s-1} \tag{8}$$

is an analytic function for $s\in\mathbb{C}$ if $\mathrm{Re}\,s<\rho$. In particular, the assumption of the existence of the Mellin transform excludes from our discussion those functions $f(t)$ growing exponentially for $t\to+\infty$. The inversion theorem guarantees that

$$\theta(t-a)f(t)\ =\ \frac{1}{2\pi i}\int_{c-i\infty,\ \ c<\rho}^{c+i\infty}\mathrm{d}s\mathcal{M}_a[f,s]\ t^{-s}. \tag{9}$$

Usually, the Mellin transform of the function f is defined in the strip $-\alpha_0<\mathrm{Re}\,s<\rho$, if $f(t)\sim t^{\alpha_0}$ for $t\to 0$; choosing the parameter $a>0$ allows the lower limit $-\alpha_0$ to be sent to $-\infty$. Let us now assume that there exists an integer value of d such that (4) exists in the ordinary sense. It is easy to realize that if it is the case, then $d/2<\rho$ and

$$\sum_{n\in\mathbb{Z}^d}{}'\ \ f(n^2)=\frac{1}{2\pi i}\int_{c-i\infty,\ \ c<\rho}^{c+i\infty}\mathrm{d}s\mathcal{M}_a[f,s]\sum_{n\in\mathbb{Z}^d}{}'\ \ \frac{1}{(n^2)^s}, \tag{10}$$

where exchanging the series with the integral is allowed in the domain of uniform convergence (see below). We define a generalized ζ-function (a particular Epstein's zeta function, see Refs. 8 and 19)

$$\zeta(s,d)\equiv\sum_{n\in\mathbb{Z}^d}{}'\ \ \frac{1}{(n^2)^s}, \tag{11}$$

whose properties are discussed in Appendix B. This series converges uniformly in any closed subset of the line $\mathrm{Re}\,s>d/2$, i.e., the function $\zeta(s,d)$ is analytic in the half-plane $\mathrm{Re}\,s>d/2$. Thus we may give the following representation of our original sum:

$$\sum_{n\in\mathbb{Z}^d}{}'\ \ f(n^2)=\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\ \ \zeta(s,d)\mathcal{M}_a[f,s];\quad \Gamma=\{\mathrm{Re}\,s=c;d/2<c<\rho\}. \tag{12}$$

Let us observe that both $\mathcal{M}_a[f,s]$ and $\zeta(s,d)$ can be analytically continued outside their definition domains. Their analytic continuations will generally have singularities in the complex plane. Now the recipe to define the sum (4) even for $d/2\geqslant\rho$ is clear: it is simply the continuation of integral (12), where we consider the analytic continuation of $\mathcal{M}_a[f,s]$ and $\zeta(s,d)$ in the integrand. In the same way we can *define* (4) by using the representation (12) even if there is no integer value of d such that $d/2<\rho$ (for example, if $f(x)\sim x^\alpha$ for $x\to\infty$ and $\alpha\geqslant -1$) and the same considerations apply for complex d if one considers $\mathrm{Re}\,d$ instead of d in previous relations.

When $\mathrm{Re}\,d$ is increased towards values greater than ρ, the integral (12) gets a residue contribution from the pole of $\zeta(s,d)$ in $s=d/2$: as we will show below, this term is divergent for $\mathrm{Re}\,d/2>\rho$ and coincides with the infinite radius limit. [If the physical value of d is less than 2ρ, the series is convergent and there is no need to (dimensionally) regularize it; in this case the

representation (12) is still useful for an explicit evaluation.] The remaining complex integral along the contour $\Gamma=\{\mathrm{Re}\, s=c; c<\rho<d/2\}$ corresponds to the finite radius-dependent part; in the following section we give a practical recipe to evaluate it using the ϑ-function. Note that the operation (12) respects the required properties: linearity follows from linearity of the Mellin transform; translational invariance follows from translational invariance of the usual sum over the transverse subspace, if this is taken sufficiently large to contain the vector q in Eq. (6). In Appendix C we prove some remarkable properties which hold for the sum over complex dimensions.

Finally, a comment on (12) is in order to clarify the meaning of the parameter a: as already said after Eq. (1), going to too small d without performing an appropriate subtraction in the case of the integral would introduce a spurious IR divergence which has no physical meaning. In the same way, had we not introduced the parameter $a>0$, the Mellin transform

$$\int_0^\infty \mathrm{d}t\ f(t)\ t^{s-1}$$

would have been divergent (for any s) in all cases in which the integral corresponding to the series needs IR subtraction to be defined in dimensional regularization. Setting $a>0$ is a simple way of avoiding IR subtractions for the series. We prove below that the final result does not depend on a, as one expects having the initial series (4) no IR problems at all.

III. AN ALTERNATIVE REPRESENTATION

Once given the definition of a series in complex dimensions, we present an alternative representation of (12) to show that

(i) the result is independent of the actual value of $0<a<1$;
(ii) the UV dimensional poles are the same as those of the corresponding integral;
(iii) the property (analogous to that for ordinary sums)

$$\lim_{R\to\infty}\frac{1}{R^d}{\sum_{n\in\mathbb{Z}^d}}'\ f(n^2/R^2)=\int \mathrm{d}^d p\ f(p^2) \tag{13}$$

is formally valid.

The final formula will be easier to handle for a numerical evaluation or an expansion in the parameters.

A. The infinite radius limit

Our strategy is to obtain first a compact expression for $\mathrm{Re}\, d/2<\rho$ and then analytically continue this result to the case $\mathrm{Re}\, d/2>\rho$. Introducing the radius R explicitly, definition (12) becomes $(0<a<1)$

$$S(d,R)\equiv\frac{1}{R^d}{\sum_{n\in\mathbb{Z}^d}}'\ f(n^2/R^2)=\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\ \zeta(s,d)\ R^{2s-d}\mathcal{M}_{a/R^2}[f,s], \tag{14}$$

where the contour Γ has to be fixed according to (12). Let us assume that $f(t)$ has the asymptotic expansion (2) for $t\to 0$ and $f(t)\sim t^{-\rho}$ for $t\to\infty$, even if the derivation goes the same way for more general expansions. We can take

$$\Gamma=\{\mathrm{Re}\, s=c\ ;\ -\alpha_q<\mathrm{Re}\, d/2<c<\min(-\alpha_{q-1},\rho)\},$$

q being the smallest integer such that $-\alpha_q<\mathrm{Re}\, d/2<\rho$ (see Fig. 1). [For $q=0$ the subtraction terms are omitted and we mean $\min(-\alpha_{-1},\rho)\equiv\rho$.] Defining

$$f_{\mathrm{sub}}(t)=f(t)-\sum_{k=0}^{q-1} a_k\ t^{\alpha_k}, \tag{15}$$

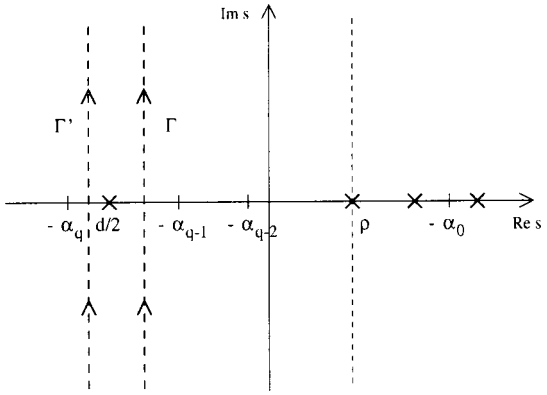

FIG. 1. Position of the contour Γ and Γ': the poles for $\mathrm{Re}\, s \geqslant \rho$ are those of the continuation of $\mathcal{M}_a[f,s]$.

it follows, for $-\alpha_q < \mathrm{Re}\, s < \min(-\alpha_{q-1}, \rho)$,

$$\mathcal{M}_{a/R^2}[f,s] = \mathcal{M}[f_{\mathrm{sub}},s] - \int_0^{a/R^2} \mathrm{d}t\, f_{\mathrm{sub}}(t)\, t^{s-1} - \sum_{k=0}^{q-1} \frac{a_k}{s+\alpha_k} \left(\frac{a}{R^2}\right)^{s+\alpha_k}. \tag{16}$$

Note that the Mellin transform in the first term is IR-convergent thanks to the subtraction made on f and the second term is analytic for $\mathrm{Re}\, s > -\alpha_q$. Using the asymptotic limit $\zeta(s,d) \to 2d$ for $\mathrm{Re}\, s \to +\infty$ (see Appendix B), and moving the contour Γ at infinity in the positive half-plane, one easily finds that the integral in the complex variable s of the second term vanishes, since $a < 1$. Integrating the third term along Γ, again closing the contour in the positive half-plane, one gets instead a residue contribution from the poles $s = -\alpha_k$, $k = 0, \ldots, (q-1)$. We end up with

$$S(d,R) = \frac{1}{2\pi i} \int_\Gamma \mathrm{d}s\ \zeta(s,d)\ R^{2s-d} \mathcal{M}[f_{\mathrm{sub}},s] + \sum_{k=0}^{q-1} \frac{a_k}{R^{2\alpha_k+d}} \zeta(-\alpha_k,d). \tag{17}$$

This expression represents a definition of the series for $-\alpha_q < \mathrm{Re}\, d/2 < \min(-\alpha_{q-1}, \rho)$ alternative to (12), where the use of the IR cut-off a has been replaced by an appropriate subtraction of the initial function, much in the same way as one does in standard DR.

If $-\alpha_0 < \rho$ the IR subtractions are not really required to define the series: choosing d in the strip $-\alpha_0 < \mathrm{Re}\, d/2 < \rho$ $(q = 0)$, Eq. (17) coincides with (12) with $a = 0$. In this case Eq. (17) with $q > 0$ represents the correct analytical extension of the series to the interval $-\alpha_q < \mathrm{Re}\, d/2 < -\alpha_{q-1}$, but it becomes nontrivial when $-\alpha_0 > \rho$ and the subtractions are really necessary to give a meaning to the expression. It is interesting to notice that $\mathcal{M}[f_{\mathrm{sub}},s]$ in the first term is nothing but the dimensionally regularized integral of f in $d = 2s$ dimensions, up to a solid-angle factor.

The limit $R \to \infty$ cannot be extracted immediately from (17), as one must first extrapolate the result to values of $\mathrm{Re}\, d/2$ greater than $-\alpha_0$. To analytically continue (17) to $\mathrm{Re}\, d/2 > \min(-\alpha_{q-1}, \rho)$ we have to take into account that increasing $\mathrm{Re}\, d/2$, the pole $s = d/2$ of $\zeta(s,d)$ crosses the contour Γ and gives a residue term. To simplify the analytic continuation, we can rewrite (17) in a suitable form, evaluating this residue term from the very beginning, i.e., moving the contour Γ into a new one (see Fig. 1),

$$\Gamma' = \{\mathrm{Re}\, s = c\ ;\ -\alpha_q < c < \mathrm{Re}\, d/2 < \min(-\alpha_{q-1}, \rho)\},$$

so that

$$S(d,R)=\frac{\pi^{d/2}}{\Gamma(d/2)}\mathcal{M}[f_{\rm sub},d/2]+\frac{1}{2\pi i}\int_{\Gamma'}\mathrm{d}s\ \zeta(s,d)\ R^{2s-d}\mathcal{M}[f_{\rm sub},s]$$
$$+\sum_{k=0}^{q-1}\frac{a_k}{R^{2\alpha_k+d}}\zeta(-\alpha_k,d). \tag{18}$$

The continuation of this expression can be easily found by considering those of $\mathcal{M}[f_{\rm sub},d/2]$ in the first term and of $\zeta(s,d)$ in the second and third ones, while the contour is always given by $\Gamma'=\{\mathrm{Re}\,s=c;-\alpha_q<c<\min(-\alpha_{q-1},\rho,\mathrm{Re}\,d/2)\}$.

Dimensional poles of this expression may arise from the first and third terms on the r.h.s.: the former is R-independent and exactly corresponds to the integral (3) defined in dimensional regularization with the proper subtraction. Its possible IR divergences are cancelled by the poles of the last term for $d=-2\alpha_k$, $k=0,\ldots,(q-1)$, which may be ''physically'' accessible, i.e., be positive, if some α_k is negative. The final result is thus IR-finite, as it should be, the series being free from IR divergences. From (18) it is evident that the UV divergences are the same for the series and the corresponding integral. Finally, when $\mathrm{Re}\,d>-2\alpha_0$ the infinite radius limit can be safely extracted from (18), leading to Eq. (13) as stated.

B. Evaluating the finite part with a ϑ-function

A general formula for the complex integral in (18) can be obtained under particular assumptions. Performing the appropriate IR subtraction, one always reduces oneself to the computation of the integral

$$\frac{1}{2\pi i}\int_{\Gamma}\mathrm{d}s\ \zeta(s,d)R^{2s-d}\mathcal{M}[f,s], \tag{19}$$

where, if the function f has the usual asymptotic expansion (2) and $f(t)\sim t^{-\rho}$ for $t\to\infty$, then $\Gamma=\{\mathrm{Re}\,s=c\,;-\alpha_0<c<\min(\rho,\mathrm{Re}\,d/2)\}$. Let us suppose that

(1) $f(s)$ is analytical in the half-plane $\mathrm{Re}\,s>\overline{c}$, $\overline{c}\leqslant 0$,

(2) $\lim_{\mathrm{Re}\,s\to+\infty} f(s)=0$, i.e., $\rho>0$, and

(3) $\frac{1}{2\pi i}\int_{c-i\infty,\ c>\overline{c}}^{c+i\infty}\mathrm{d}s f(s)\ e^{ts}<\infty$ for $t>0$.

Under these hypotheses the inversion theorem (see Ref. 17) guarantees that the Laplace antitransform

$$\mathcal{L}^{-1}[f,t]=\frac{1}{2\pi i}\int_{c-i\infty,\ c>\overline{c}}^{c+i\infty}\mathrm{d}s f(s)\ e^{ts}, \tag{20}$$

exists for $t>0$ and

$$f(s)=\int_0^\infty \mathrm{d}t\ \mathcal{L}^{-1}[f,t]\ \ e^{-st},\quad \mathrm{Re}\,s>\overline{c}. \tag{21}$$

Using these results, the Mellin transform can be expressed as follows:

$$\mathcal{M}[f,s]=\int_0^\infty \mathrm{d}t\, t^{s-1}f(t)=\int_0^\infty \mathrm{d}t\, t^{s-1}\int_0^\infty \mathrm{d}y\, e^{-ty}\mathcal{L}^{-1}[f,y]$$

$$=\Gamma(s)\int_0^\infty \mathrm{d}y\, \mathcal{L}^{-1}[f,y]\,y^{-s}. \tag{22}$$

This relation holds when $-\alpha_0<\mathrm{Re}\,s<\rho$ and it is therefore valid along the contour Γ of Eq. (19). If $\alpha_0>0$, $\mathrm{Re}\,s$ can be negative and $f^{(k)}(0)=0$, for $k=0,\ldots,\lfloor\alpha_0\rfloor$, $\lfloor x\rfloor\equiv\max\{n\in\mathbb{N}\,|\,n<x\}$. Then the simple poles in $s=0,-1,-2,\ldots,-\lfloor\alpha_0\rfloor$ of $\Gamma(s)$ in (22) are cancelled by corresponding first order zeros of the integral of the Laplace antitransform

$$\int_0^\infty \mathrm{d}y\, \mathcal{L}^{-1}[f,y]\,y^k=(-1)^k f^{(k)}(0)=0 \quad \text{for} \quad k=0,1,\ldots,\lfloor\alpha_0\rfloor \quad \text{if} \quad \alpha_0>0,$$

resulting in a Mellin transform well defined in the whole interval $-\alpha_0<\mathrm{Re}\,s<\rho$. Using (22) and the analytic extension of $\zeta(s,d)$ in terms of the ϑ-function (see Appendix B),

$$\zeta(s,d)=\frac{\pi^s}{\Gamma(s)}\left\{\frac{1}{s-d/2}-\frac{1}{s}+\int_1^\infty \mathrm{d}y\,(y^{s-1}+y^{d/2-s-1})\,[\,\vartheta^d(y)-1\,]\right\},$$

it is not difficult to compute the complex integral in (19) by applying standard residue techniques. The result is

$$\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\,\zeta(s,d)R^{2s-d}\mathcal{M}[f,s]$$

$$=-\frac{\pi}{R^{d-2}}\int_1^\infty \mathrm{d}y\;\;(\mathcal{L}^{-1}[f,y\pi R^2]\,y^{-d/2}+\mathcal{L}^{-1}[f,\pi R^2/y]\,y^{-2})$$

$$+\frac{\pi}{R^{d-2}}\int_1^\infty \mathrm{d}y\;\;[\,\vartheta^d(y)-1\,](\mathcal{L}^{-1}[f,\pi R^2 y]+y^{d/2-2}\mathcal{L}^{-1}[f,\pi R^2/y]). \tag{23}$$

The two integrals converge under the assumed hypotheses. [This is easily understood from the asymptotic behavior of the Laplace antitransform (see Ref. 17):

$$\mathcal{L}^{-1}[f,t]\sim\begin{cases}t^{\rho-1}, & t\to 0,\\ t^{-(\alpha_0+1)}, & t\to\infty,\end{cases} \quad \text{which follows if} \quad f(t)\sim\begin{cases}t^{-\rho}, & t\to\infty,\\ t^{\alpha_0}, & t\to 0.\end{cases}]$$

Equation (23) is a useful representation for the complex integral in (18), which allows an expansion of the result in terms of the parameters in f or even to perform a numerical integration. The results of Ref. 10 are easily obtained as particular applications of (23). It is worth noting that one could have derived the same result by giving a definition of the series directly in terms of the ϑ-function, never using ζ-functions, and this is exactly the procedure adopted in Ref. 10. Of course, to define the series using ϑ-functions one has to assume the same hypotheses we imposed on the function f to guarantee the existence of the Laplace antitransform. In this respect, our definition seems more general and more suitable to isolate the divergent from the finite term.

IV. A SAMPLE COMPUTATION: THE CASIMIR ENERGY

To give an explicit example of our procedure, we compute the Casimir energy $\mathcal{E}(R)$ for a scalar field with mass m and periodicity conditions in a space geometry $\mathbb{T}^d\times\mathbb{R}^D$, corresponding to

$\bar{d}$ compactified dimensions with radius R. This is defined as the R-dependent part of the zero point energy $V(R)$ of the $(\bar{D}+\bar{d})$-dimensional theory multiplied by the volume $(2\pi R)^{\bar{d}}$ of the compact space:

$$\mathcal{E}(R)=(2\pi R)^{\bar{d}}\ [V(R)-V(\infty)]. \tag{24}$$

Continuing the physical dimensions $\bar{D}$, $\bar{d}$ to generic values

$$D=\bar{D}-\epsilon\,;\quad d=\bar{d}-\eta, \tag{25}$$

the one-loop contribution to the zero point energy is given by

$$V(R)=\frac{1}{2}\frac{\mu^{\epsilon+\eta}}{(2\pi R)^d}\sum_{n\in\mathbb{Z}^d}\int\frac{\mathrm{d}^D p}{(2\pi)^D}\log(p^2+n^2/R^2+m^2). \tag{26}$$

To extract $\mathcal{E}(R)$ we first compute $V(R)$, then extract the limit $\epsilon\to 0$, $\eta\to 0$ and finally multiply by the volume factor.

For convenience let us call $V_0(R)$ the zero mode contribution in (26). We will show explicitly that performing first the series and then the integral or vice versa leads to the same result (see Property 2 in Appendix C) and there is no ambiguity. Let us perform the integral first. The function $f(x)=\log(x+c)$ has the asymptotic behavior $f(x)\sim\log x$ for $x\to\infty$ and $f(x)\sim$ const for $x\to 0$; this means that the dimensionally regulated integral needs subtractions to be defined. Performing one subtraction, i.e., considering $f_{\mathrm{sub}}(x)=\log(x/c+1)$, we can fix $-2<D<-1$, obtaining

$$V(R)-V_0(R)=-\frac{1}{2}\mu^{\epsilon+\eta}\frac{\pi^{D/2}}{(2\pi)^D}\Gamma(-D/2)\frac{1}{(2\pi R)^d}\sum_{n\in\mathbb{Z}^d}{}'\ (n^2/R^2+m^2)^{D/2}. \tag{27}$$

Because D is negative and the function $g(x)=(x+m^2)^{D/2}$ has the asymptotic behavior $g(x)\sim x^{D/2}$ for $x\to\infty$ and $g(x)\sim$ const for $x\to 0$, the series is defined by (17) with $\Gamma=\{\mathrm{Re}\,s=c;0<d/2<c<-D/2<1\}$ and without any subtraction:

$$V(R)-V_0(R)=-\frac{1}{2}\mu^{\epsilon+\eta}\frac{\pi^{D/2}}{(2\pi)^D}\Gamma(-D/2)\frac{1}{(2\pi R)^d}\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\ \ \zeta(s,d)\ \ R^{2s}\mathcal{M}[g,s]. \tag{28}$$

Even if the Mellin transform is easy to derive,

$$\mathcal{M}[g,s]=\frac{\Gamma(s)\Gamma(-D/2-s)}{\Gamma(-D/2)}(m^2)^{D/2+s},$$

the complex integral along the contour Γ cannot be solved with simple residue techniques because of the nontrivial behavior of the integrand at infinity. However, $g(s)$ is analytic in the half-plane $\mathrm{Re}\,s>-m^2$ and the requirements needed to apply the representation in terms of the ϑ-function are fulfilled. From Eqs. (18) and (23) with a Laplace antitransform

$$\mathcal{L}^{-1}[g,y]=\frac{e^{-m^2 y}}{\Gamma(-D/2)}y^{-D/2-1},$$

we obtain

$$V(R)-V_0(R)=-\frac{1}{2}\mu^{\epsilon+\eta}\frac{\pi^{(D+d)/2}}{(2\pi)^{D+d}}\Gamma\left(-\frac{D+d}{2}\right)(m^2)^{(D+d)/2}$$
$$+\frac{1}{2}\frac{\mu^{\epsilon+\eta}}{(2\pi R)^{D+d}}\left\{\int_1^\infty dy\ \ (e^{-\pi y(mR)^2}y^{-(D+d)/2-1}+e^{-\pi(mR)^2/y}y^{D/2-1})\right.$$
$$\left.-\int_1^\infty dy\ \ [\vartheta^d(y)-1](e^{-\pi y(mR)^2}y^{-D/2-1}+e^{-\pi(mR)^2/y}y^{(D+d)/2-1})\right\}. \quad (29)$$

We recognize the infinite radius contribution in the first R-independent term, while the remaining terms are finite. More exactly, the integral in the second line is convergent when $\mathrm{Re}\,D<0$ as supposed from the beginning to regularize the dimensional integral. Therefore, when $\mathrm{Re}\,D$ is increased to (physical) values $\mathrm{Re}\,D>0$ a divergence appears which, however, depends only on D but not on the value of d. This means that in some way this must be a ''zero mode'' divergence and this becomes evident by rewriting

$$\int_1^\infty dy\, e^{-\pi(mR)^2/y}y^{D/2-1}=[\pi(mR)^2]^{D/2}\Gamma(-D/2)-\int_1^\infty dy\, e^{-\pi y(mR)^2}y^{-D/2-1}. \quad (30)$$

The first term on the r.h.s. of (30) exactly cancels the zero mode contribution $V_0(R)$ in (29) and we get the final result

$$V(R)=-\frac{1}{2}\mu^{\epsilon+\eta}\frac{\pi^{(D+d)/2}}{(2\pi)^{D+d}}\Gamma\left(-\frac{D+d}{2}\right)(m^2)^{(D+d)/2}+\frac{1}{2}\frac{\mu^{\epsilon+\eta}}{(2\pi R)^{D+d}}$$
$$\times\left\{\int_1^\infty dy\ \ e^{-\pi y(mR)^2}(y^{-(D+d)/2-1}+y^{-D/2-1})\right.$$
$$\left.-\int_1^\infty dy\ \ [\vartheta^d(y)-1](e^{-\pi y(mR)^2}y^{-D/2-1}+e^{-\pi(mR)^2/y}y^{(D+d)/2-1})\right\}. \quad (31)$$

The first term is the ordinary divergent renormalization of the cosmological constant, which can be put to zero with a suitable counterterm if we accept the usual fine tuning. Whatever scheme of renormalization one chooses, the radius dependent part $V(R)-V(\infty)$ of the zero point energy is nonambiguous and finite. We can therefore safely extract the limit $\epsilon\to 0$, $\eta\to 0$ and insert the result for $V(R)-V(\infty)$ in Eq. (24) to extract the Casimir energy

$$\mathcal{E}(R)=\frac{1}{2}\frac{1}{(2\pi R)^{\bar{D}}}\left\{\int_1^\infty dy\ \ e^{-\pi y(mR)^2}(y^{-(\bar{D}+\bar{d})/2-1}+y^{-\bar{D}/2-1})-\int_1^\infty dy\ \ [\vartheta^{\bar{d}}(y)-1]\right.$$
$$\left.\times(e^{-\pi y(mR)^2}y^{-\bar{D}/2-1}+e^{-\pi(mR)^2/y}y^{(\bar{D}+\bar{d})/2-1})\right\}. \quad (32)$$

The same result can be obtained by performing first the series. Again, subtractions are necessary if one does not introduce an IR cut-off in the Mellin transform. The function $f(x)=\log(x+p^2+m^2)$ has an expansion around $x=0$ as in (2) with $\alpha_0=0$, $\alpha_1=1$; we can therefore apply definition (17) with one subtraction and, choosing the contour $\Gamma=\{\mathrm{Re}\,s=c;-1<d/2<c<-\frac{1}{2}\}$, we obtain

$$V(R)-V_0(R)=\frac{1}{2}\frac{\mu^{\epsilon+\eta}}{(2\pi R)^d}\int\frac{d^Dp}{(2\pi)^D}\zeta(0,d)\log(p^2+m^2)$$
$$+\frac{1}{2}\frac{\mu^{\epsilon+\eta}}{(2\pi R)^d}\int\frac{d^Dp}{(2\pi)^D}\frac{1}{2\pi i}\int_\Gamma ds\ \ \zeta(s,d)\ \ R^{2s}\mathcal{M}[f_{\mathrm{sub}},s], \quad (33)$$

with

$$\mathcal{M}[f_{\rm sub},s]=-[p^2+m^2]^s\Gamma(s)\Gamma(-s).$$

The complex integral along the contour Γ cannot be solved with simple residue techniques nor we can apply the ϑ-function representation ($f_{\rm sub}$ diverges at infinity), but we can make use of a standard trick. Namely, defining

$$S(p^2+m^2)=\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\ \ \zeta(s,d)\ \ R^{2s}\mathcal{M}[f_{\rm sub},s],$$

we know how to sum the series $dS(p^2+m^2)/dp^2$ because $df_{\rm sub}/dp^2=1/(x+p^2+m^2)$ goes to zero for $x\to\infty$. Then we can deduce the expression of $S(p^2+m^2)$ except for an unknown function independent of p^2, which, however, is irrelevant as its dimensional integral in p gives zero. In particular, we have

$$\begin{aligned}\frac{d}{dp^2}S(p^2+m^2)&=\frac{1}{2\pi i}\int_\Gamma \mathrm{d}s\ \ \zeta(s,d)\ \ R^{2s}\frac{d}{dp^2}\mathcal{M}[f_{\rm sub},s]\\&=\frac{1}{2\pi i}\int_{\Gamma'} \mathrm{d}s\ \ \zeta(s,d)\ \ R^{2s}\frac{d}{dp^2}\mathcal{M}[f_{\rm sub},s]-\zeta(0,d)\frac{1}{p^2+m^2},\end{aligned}\tag{34}$$

where the contour Γ has been moved into a new one, $\Gamma'=\{\mathrm{Re}\,s=c;d/2<0<c<1\}$, and a residue contribution in $s=0$ has been isolated. The first term corresponds to the (dimensionally regularized) series of the function $d\log(p^2+n^2/R^2+m^2)/dp^2$, defined without subtractions by choosing the contour Γ', and it can be easily computed using the ϑ-function representation (23). We do not show the details of this calculation but we only notice that using (34) to extract $S(p^2+m^2)$ and, finally plugging the result into (33), the residue term in the former equation cancels the subtraction term of the latter and we end up with

$$\begin{aligned}V(R)-V_0(R)=\frac{1}{2}\mu^{\epsilon+\eta}\int\frac{\mathrm{d}^Dp}{(2\pi)^D}\Bigg\{&-\frac{\pi^{D/2}}{(2\pi)^d}\Gamma(-D/2)[p^2+m^2]^{d/2}\\&+\frac{1}{(2\pi R)^d}\Bigg[\int_1^\infty \mathrm{d}y\ \ (e^{-\pi y(m^2+p^2)R^2}y^{-d/2-1}+e^{-\pi(m^2+p^2)R^2/y}y^{-1})\\&+\int_1^\infty \mathrm{d}y\ \ [\vartheta^d(y)-1](e^{-\pi y(m^2+p^2)R^2}y^{-1}+e^{-\pi(m^2+p^2)R^2/y}y^{d/2-1})\Bigg]\Bigg\}.\end{aligned}\tag{35}$$

The result of the dimensional integration over p coincides with Eq. (29), from which the final expression (31) follows.

V. CONCLUSIONS

We discussed in detail a general procedure to dimensionally regularize divergent series. The novelty of the method consists in using a suitable combination of two well-known tools, i.e., Mellin transform and analytic extension of special functions, to provide a continuation of the series in the number of dimensions.

The virtue of conventional dimensional regularization is to preserve all the symmetries of the action that do not depend on the dimensionality, in particular gauge invariance and supersymmetry (if the dimensional reduction scheme is used). The same happens with dimensional regularization of sums, making this technique a natural choice to handle divergences of field theory. In this respect, our analysis should contribute to clarify some controversial aspects about the computation of quantum corrections in supersymmetric theories with extra dimensions.[13–16] In particular, we

have shown that there is no ambiguity in exchanging the series and the integral over loop momenta if both are consistently regularized with dimensional regularization (see Property 2 in Appendix C and the example in Sec. IV). The same is not true, for instance, if the sum over Kaluza–Klein modes is truncated by a raw cut-off.

Our definition of sums in complex dimensions by using a generalized zeta function is particularly suited to isolate the divergence from the finite part and applies to a large class of functions. Moreover, it leads to simple computations and it is valid for an arbitrary number of physical compact dimensions. The idea of dimensionally regularized series was applied in Ref. 10 to compute a number of loop sums by using a representation in terms of ϑ-functions. We obtain the results of Ref. 10 as particular cases of our general formulas. A different method was proposed in Ref. 11, which however applies only to the case of one physical compact dimension. Our procedure has no such limitation and it is therefore more general; in the case of only one physical compact dimension it gives the same result as Ref. 11, as we have explicitly checked for particular examples.

Although the class of functions we considered is not the most general one, the basic idea may be applied to more complicated cases by using suitable zeta functions. In particular, our formulas are specific to series that appear in theories with toroidal compact dimensions and scalar fields with simple periodical conditions. In the case of twisted periodic conditions or theories with fermions, our method should be easily extended introducing the following zeta function

$$\zeta(s,d\,|\,a)\equiv{\sum_{n\in\mathbb{Z}^d}}'\,\frac{1}{[(n+a)^2]^s},\quad -\frac{1}{2}<a\leqslant\frac{1}{2},$$

whose properties are sketched in Appendix B. The way to treat spinors in the dimensional continuation is similar as in conventional DR (see Refs. 3 and 11).

Even when the compact manifold is not toroidal (see, for example, Ref. 20) or the single dimensions have different radii, we see no obstacle in principle to apply the approach of dimensional regularization, maybe taking advantage of more general special functions such as those introduced in Ref. 8. In these cases, however, computations may become involved and particular recipes specific to the case may be simpler to use.

ACKNOWLEDGMENTS

We thank S. Caracciolo, A. Pelissetto and R. Rattazzi for a critical reading of the manuscript. R.C. acknowledges in a special way R. Rattazzi for many useful discussions and suggestions. This work is partially supported by the EC under TMR Contract No. HPRN-CT-2000-00148.

APPENDIX A: MELLIN TRANSFORM

Let us briefly recall the definition of the Mellin transform.[17,18] Given a function f, if $\alpha,\beta\in\mathbb{R}$, $\alpha<\beta$ exist such that

$$\int_0^\infty \mathrm{d}t|f(t)|t^{\rho-1}\ <\ \infty;\quad \forall\rho:\ \alpha<\rho<\beta,$$

then one can define the Mellin transform of $f(t)$,

$$\mathcal{M}[f,s]=\int_0^\infty \mathrm{d}t f(t)t^{s-1}, \tag{A1}$$

which is an analytic function of $s\in\mathbb{C}$ in the strip $\alpha<\mathrm{Re}\,s<\beta$. This inversion formula holds:

$$f(t)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\mathrm{d}s\,\mathcal{M}[f,s]\,t^{-s};\ \ \alpha<c<\beta. \tag{A2}$$

Obviously it is a linear integral transformation. It has very useful applications and remarkable properties (see, for instance, Ref. 17).

APPENDIX B: PROPERTIES OF $\zeta(s,d)$

We define, for integer d,

$$\zeta(s,d) \equiv {\sum_{n \in \mathbb{Z}^d}}' \frac{1}{(n^2)^s}, \tag{B1}$$

which is absolutely convergent for $\mathrm{Re}\, s > d/2$. This function is a particular case of the more general zeta functions (see, for example, Ref. 8 and 19). Let us write an explicit expression for the analytic continuation of $\zeta(s,d)$ to the whole complex plane in s and, eventually, extend its definition also for all complex d. The function (related to Jacobi's ϑ_3),[18]

$$\vartheta(t) \equiv \sum_{n=-\infty}^{+\infty} e^{-\pi t n^2} \tag{B2}$$

has the following modular property, which is easily derived from Poisson's resummation formula:[17]

$$\vartheta(t) = \frac{1}{t^{1/2}} \vartheta(1/t). \tag{B3}$$

By means of

$$\frac{1}{(n^2)^s} = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t \;\; t^{s-1} \;\; e^{-t n^2}, \tag{B4}$$

we may write

$$\zeta(s,d) = \frac{\pi^s}{\Gamma(s)} \int_0^\infty \mathrm{d}t \;\; t^{s-1} \;\; [\vartheta^d(t) - 1]; \tag{B5}$$

incidentally, this tells us that the Mellin transform of $[\vartheta^d(t) - 1]$ is $\pi^{-s}\Gamma(s)\zeta(s,d)$.

For $\mathrm{Re}\, s > 0$, $\mathrm{Re}\, s > d/2$, it follows from (B3) that

$$\int_0^1 \mathrm{d}t\, t^{s-1} [\vartheta^d(t) - 1] = \int_1^\infty \mathrm{d}t\, t^{d/2-s-1} [\vartheta^d(t) - 1] + \frac{1}{s - d/2} - \frac{1}{s},$$

which gives

$$\zeta(s,d) = \frac{\pi^s}{\Gamma(s)} \left\{ \frac{1}{s - d/2} - \frac{1}{s} + \int_1^\infty \mathrm{d}t\, (t^{s-1} + t^{d/2-s-1}) [\vartheta^d(t) - 1] \right\}. \tag{B6}$$

This expression represents the analytic continuation of $\zeta(s,d)$ in both s and d. It is easy to demonstrate the following properties:

(1) $\zeta(s,d)$ is a meromorphic function, having a simple pole for $s = d/2$, $d \neq 0$, with residue

$$\mathrm{Res}\{\zeta(s,d); s = d/2\} = \frac{\pi^{d/2}}{\Gamma(d/2)};$$

(2) $\zeta(s,0) = 0$, $\forall s \in \mathbb{C}$;

(3) $\zeta(0,d) = -1$, for $d \neq 0$;

(4) $\zeta(-n,-2n)=(-1)^n\,n!/\pi^n$, for $n\in\mathbb{N}$, $n\neq 0$;
(5) $\zeta(-n,d)=0$, for $d\neq -2n$ and $n\in\mathbb{N}$, $n\neq 0$;
(6) Given the symmetry $s\to d/2-s$ of the terms inside the brackets in (B6), we have

$$\frac{\Gamma(s)\,\zeta(s,d)}{\pi^s}=\frac{\Gamma(d/2-s)\,\zeta(d/2-s,d)}{\pi^{d/2-s}}.$$

This is the so-called *reflection formula*, which is also valid in the more general case of Epstein zeta functions.[8]

We now derive a "convolution" property of $\zeta(s,d)$, used in Appendix C, Eq. (C3). For $p,q>0$ and $\mathrm{Re}\,s>(p+q)/2$,

$$\begin{aligned}\zeta(s,p+q)&=\sum_{m\in\mathbb{Z}^p}{}'\ \sum_{n\in\mathbb{Z}^q}{}'\ \frac{1}{(m^2+n^2)^s}+\sum_{m\in\mathbb{Z}^p}{}'\ \frac{1}{(m^2)^s}+\sum_{n\in\mathbb{Z}^q}{}'\ \frac{1}{(n^2)^s}\\&=\sum_{m\in\mathbb{Z}^p}{}'\ \sum_{n\in\mathbb{Z}^q}{}'\ \frac{1}{(m^2+n^2)^s}+\zeta(s,p)+\zeta(s,q).\end{aligned}\tag{B7}$$

We can write the argument of the double sum using (B4) and then introduce the Mellin representation for one of the two exponential factors, getting the result

$$\begin{aligned}&\sum_{m\in\mathbb{Z}^p}{}'\ \sum_{n\in\mathbb{Z}^q}{}'\ \frac{1}{(m^2+n^2)^s}\\&\quad=\frac{1}{\Gamma(s)}\int_0^\infty \mathrm{d}t\ \ t^{s-1}\sum_{n\in\mathbb{Z}^q}{}'\ e^{-t\,n^2}\sum_{m\in\mathbb{Z}^p}{}'\ \frac{1}{2\pi i}\int_{c-i\infty,c>0}^{c+i\infty}\mathrm{d}w\ \ \Gamma(w)\ \ (m^2\,t)^{-w}\\&\quad=\frac{1}{\Gamma(s)}\,\frac{1}{2\pi\,i}\int_{c-i\infty}^{c+i\infty}\mathrm{d}w\ \ \Gamma(w)\,\zeta(w,p)\,\Gamma(s-w)\,\zeta(s-w,q),\end{aligned}\tag{B8}$$

where, in the last line, $p/2<c<\mathrm{Re}\,s-q/2$. Taking into account relation (B7), we have

$$\begin{aligned}&\frac{1}{2\pi\,i}\int_{c-i\infty}^{c+i\infty}\mathrm{d}w\ \ \Gamma(w)\,\zeta(w,p)\,\Gamma(s-w)\,\zeta(s-w,q)\\&\qquad=\Gamma(s)\,\zeta(s,p+q)-\Gamma(s)\,\zeta(s,p)-\Gamma(s)\,\zeta(s,q).\end{aligned}\tag{B9}$$

This relation is still valid if one considers the analytic extensions of the functions involved. (Note that it is not possible to close the contour of integration at infinity, given the asymptotic behavior of the integrand.)

Next, we determine the asymptotic behavior of $\zeta(s,d)$ for large $\mathrm{Re}\,s$ and $d>0$. Let us observe that we may write

$$\vartheta^d(t)=1+2d\,e^{-\pi\,t}+\sum_{k=0}^{\infty}\ \mathcal{N}_k(d)\,e^{-\alpha_k\,\pi\,t},\tag{B10}$$

where $\mathcal{N}_k(d)$ are real coefficients and $4\leqslant\alpha_0<\alpha_1<\cdots$. For large k, the series is asymptotic to the one with $\alpha_k=k^2$ and $\mathcal{N}_k(d)$ is the number of points in $\mathbb{Z}^d$ with a distance from the origin bounded between k and $(k+1)$. So $\mathcal{N}_k(d)\sim\Omega_d\,k^{d-1}$ (for $k\gg 1$). For $\mathrm{Re}\,s>d/2$ we may insert (B10) into (B5), obtaining

$$\zeta(s,d)=2d+\sum_{k=0}^{\infty}\ \mathcal{N}_k(d)\ \alpha_k^{-s},$$

so that

$$|\zeta(s,d)-2d| \leqslant \alpha_0^{-\mathrm{Re}\, s} \sum_{k=0}^{\infty} \mathcal{N}_k(d)\, (\alpha_k/\alpha_0)^{-\mathrm{Re}\, s}. \tag{B11}$$

The series on the r.h.s. is always convergent for $\mathrm{Re}\, s > d/2$, and therefore $\zeta(s,d)-2d \sim \alpha_0^{-\mathrm{Re}\, s}$ for $\mathrm{Re}\, s \to +\infty$. Using the reflection formula we immediately obtain the asymptotic behavior for $\mathrm{Re}\, s \to -\infty$: in this case the function is unbounded:

$$\zeta(-x,d) = (-1)^{\lfloor x \rfloor} \frac{2d(x/\pi)^{2x+d/2}\, e^{-2x}}{\Gamma(x-\lfloor x \rfloor+1)\, \Gamma(\lfloor x \rfloor - x)} (1+O(x^{-1})), \quad x \in \mathbb{R}^+. \tag{B12}$$

[We use the fact that for $x \in \mathbb{R}^+$, $m \equiv \lfloor x \rfloor$, $q \equiv x - \lfloor x \rfloor$, one has

$$\Gamma(-x) = (-1)^m \frac{\Gamma(q+1)\, \Gamma(-q)}{\Gamma(x+1)},$$

$$\Gamma(-x) = (-1)^m \Gamma(q+1)\, \Gamma(-q) \frac{x^{-x} e^x}{\sqrt{2\pi x}} (1+O(x^{-1})).]$$

1. A useful generalization

In some cases of interest (such as in theories with fermions) it is useful to introduce the following generalization of our zeta function. Given a constant $-\frac{1}{2} < a \leqslant \frac{1}{2}$, we define

$$\zeta(s,d \mid a) \equiv {\sum_{n \in \mathbb{Z}^d}}' \frac{1}{[(n+a)^2]^s}, \tag{B13}$$

where now Σ' means that for $a=0$ we omit the term $n=0$ in the sum. This series converges for $\mathrm{Re}\, s > d/2$. Obviously $\zeta(s,d \mid 0) = \zeta(s,d)$. To get the analytic continuation of this function one proceeds as in the case of $\zeta(s,d)$. Introducing the ϑ-function [It has the asymptotic behavior:

$$\vartheta(t|a) \sim e^{-\pi t a^2} \quad \text{for} \quad t \to \infty; \quad \vartheta(t|a) \sim t^{-1/2} \quad \text{for} \quad t \to 0.] \tag{B14}$$

$$\vartheta(t \mid a) \equiv \sum_{n=-\infty}^{+\infty} e^{-\pi t (n+a)^2}, \tag{B15}$$

from the Poisson resummation formula easily follows the modular property

$$\vartheta(t|a) = \frac{e^{-\pi a^2 t}}{t^{1/2}}\, \vartheta(1/t \mid i\, a\, t). \tag{B16}$$

The analogs of Eqs. (B5) and (B6) are

$$\zeta(s,d \mid a) = \frac{\pi^s}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} [\, \vartheta^d(t \mid a) - \delta_{a,0}], \tag{B17}$$

$$\zeta(s,d\,|\,a)=\frac{\pi^s}{\Gamma(s)}\left\{\frac{1}{s-d/2}-\frac{1}{s}\,\delta_{a,0}+\int_1^\infty \mathrm{d}t\, t^{s-1}[\,\vartheta^d(t\,|\,a)-\delta_{a,0}]\right.$$
$$\left.+\int_1^\infty \mathrm{d}t\, t^{d/2-s-1}\,[e^{-\pi a^2\, d/t}\vartheta^d(t\,|\,ia/t)-1]\right\}, \tag{B18}$$

where the last expression has a meromorphic extension with the same general properties as those of $\zeta(s,d)$. We remark that the reflection formula does not hold in the general case $a\neq 0$.

APPENDIX C: PROPERTIES OF DIMENSIONAL CONTINUATION OF SUMS

We present here some basic properties of the dimensionally regularized series as defined by (12). They are the analogs of those discussed in Ref. 3, valid for dimensionally regularized integrals.

Property 1:

$$\sum_{n\in\mathbb{Z}^p}\sum_{m\in\mathbb{Z}^q} f(n^2+m^2)=\sum_{n\in\mathbb{Z}^{p+q}} f(n^2). \tag{C1}$$

Proof: Consider a Mellin-transformable function $f(x)$, assuming for simplicity that $f(x)\to 0$ for $x\to 0$ and $f(x)\sim x^{-\rho}$, $\rho>0$ for $x\to\infty$, such that its series can be defined without IR subtractions, which are irrelevant to this discussion. Let us denote by $\mathcal{M}[f,s;y]$ the Mellin transform of $f(x+y)$ with respect to the variable x:

$$\mathcal{M}[f,s;y]\equiv\int_0^\infty \mathrm{d}x\, f(x+y)\, x^{s-1}.$$

Transforming also on y and performing a change of variables we get

$$\mathcal{M}[f,s;w]\equiv\int_0^\infty \mathrm{d}y\, \mathcal{M}[f,s;y]\, y^{w-1}$$
$$=\int_0^\infty \mathrm{d}t\, f(t)\, t^{s+w-1}\int_0^1 \mathrm{d}v\, v^{s-1}(1-v)^{w-1}$$
$$=\frac{\Gamma(s)\Gamma(w)}{\Gamma(s+w)}\,\mathcal{M}[f,s+w], \tag{C2}$$

with $\mathrm{Re}\,s$, $\mathrm{Re}\,w>0$, $\mathrm{Re}\,s+\mathrm{Re}\,w<\rho$ for these expressions to make sense. Applying the definition of regularized sums and using (C2), it follows that

$$\sum_{m\in\mathbb{Z}^p}{}'\ \sum_{n\in\mathbb{Z}^q}{}'\ f(n^2+m^2)=\frac{1}{(2\pi i)^2}\int_{\Gamma_w}\mathrm{d}w\ \int_{\Gamma_s}\mathrm{d}s\ \ \zeta(w,p)\zeta(s,q)\,\frac{\Gamma(s)\Gamma(w)}{\Gamma(s+w)}\,\mathcal{M}[f,s+w].$$

By making a change of variable in the double complex integral and taking into account Eqs. (B8) and (B9), we get

$$\sum_{m\in\mathbb{Z}^p}{}' \sum_{n\in\mathbb{Z}^q}{}' f(n^2+m^2) = \frac{1}{(2\pi i)^2}\int_{\Gamma_u} du\, \frac{\mathcal{M}[f,u]}{\Gamma(u)} \int_{\Gamma_w} dw\ \Gamma(w)\zeta(w,p)\Gamma(u-w)\zeta(u-w,q)$$

$$= \frac{1}{2\pi i}\int_{\Gamma_u} du\, \mathcal{M}[f,u]\,[-\zeta(u,p)-\zeta(u,q)+\zeta(u,p+q)]$$

$$= -\sum_{m\in\mathbb{Z}^p}{}' f(m^2) - \sum_{n\in\mathbb{Z}^q}{}' f(n^2) + \sum_{n\in\mathbb{Z}^{p+q}}{}' f(n^2), \tag{C3}$$

where Γ_u is a contour laying in the half-plane $\mathrm{Re}\, w<\rho$. This is exactly the equality we are looking for.

Property 2:

$$\int d^D p \sum_{n\in\mathbb{Z}^d}{}' f(p^2,n^2) = \sum_{n\in\mathbb{Z}^d}{}' \int d^D p\ f(p^2,n^2). \tag{C4}$$

Proof: It is convenient to introduce an auxiliary function

$$f(a,p^2,n^2) = f(p^2,n^2)\ e^{-a(p^2+n^2)},$$

for which the right- and left-hand sides of (C4) become

$$\text{l.h.s.:}\quad \frac{\Omega_D}{2}\int_0^\infty dx\ x^{D/2-1}\frac{1}{2\pi i}\int_\Gamma ds\ \zeta(s,d)\ \int_0^\infty dy\ y^{s-1}\ f(a,x,y), \tag{C5L}$$

$$\text{r.h.s.:}\quad \frac{\Omega_D}{2}\frac{1}{2\pi i}\int_\Gamma ds\ \zeta(s,d)\ \int_0^\infty dy\ y^{s-1}\ \int_0^\infty dx\ x^{D/2-1}\ f(a,x,y). \tag{C5R}$$

Thanks to the exponential factor, the series and the integral in both expressions have been defined without recourse to subtractions, by simply choosing a large enough value for (the real part of) D and d to have IR convergence. Also, the contour $\Gamma=\{\mathrm{Re}\, s=c\,;c>d/2\}$ can be defined to be the same in (C5L) and (C5R) by fixing c sufficiently large. Then, Property 2 for the auxiliary function follows trivially from exchanging the integrals over x and y and (C5L) and (C5R) are both equal to the same function $I(D,d,a)$ analytic in its variables. The analytical continuation of $I(D,d,a)$ down to smaller D and d is still given by (C5L) and (C5R), but now with subtractions made. If we take (the real part of) D and d small enough to have UV convergence even without the exponential factor, we can put $a=0$ and (C4) follows.

Property 3:

$$\sum_{n\in\mathbb{Z}^p}{}' \sum_{m\in\mathbb{Z}^q}{}' f(n,m) = \sum_{m\in\mathbb{Z}^q}{}' \sum_{n\in\mathbb{Z}^p}{}' f(n,m). \tag{C6}$$

Proof: We give the proof only for the simpler case in which the function $f(n^2,m^2)$ does not depend on the product $(m\cdot n)$. Proceeding as in the previous case, one can introduce the auxiliary function

$$f(a,n^2,m^2) = f(n^2,m^2)\ e^{-a(n^2+m^2)},$$

for which the right- and left-hand sides of (C6) become

$$\text{l.h.s.:}\quad \frac{1}{(2\pi i)^2}\int_{\Gamma_s} ds\ \zeta(s,p)\int_0^\infty dx\ x^{s-1}\int_{\Gamma_u} du\ \zeta(u,q)\int_0^\infty dy\ y^{u-1}\ f(a,x,y), \tag{C7L}$$

$$\text{r.h.s.:}\quad \frac{1}{(2\pi i)^2}\int_{\Gamma_u} du\ \ \zeta(u,q)\int_0^\infty dy\ \ y^{u-1}\int_{\Gamma_s} ds\ \ \zeta(s,p)\int_0^\infty dx\ \ x^{s-1}\ \ f(a,x,y). \quad \text{(C7R)}$$

Again, both series have been defined without recourse to subtraction, by choosing a large enough value for $\mathrm{Re}\, s$ and $\mathrm{Re}\, u$ along the contours $\Gamma_s=\{\mathrm{Re}\, s=c;c>p/2\}$, $\Gamma_s=\{\mathrm{Re}\, u=c;c>q/2\}$. Property 3 follows trivially for the auxiliary function by simply exchanging the various integrals and we recover (C6) by continuing both sides (C7L) and (C7R) analytically to $a=0$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Interacting fermions and domain wall defects in 2+1 dimensions

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(Received 30 May 2002; accepted 11 October 2002)

We consider a Dirac field in $2+1$ dimensions with a domain wall like defect in its mass, minimally coupled to a dynamical Abelian vector field. The mass of the fermionic field is assumed to have just one linear domain wall, which is externally fixed and unaffected by the dynamics. We show that, under some general conditions on the parameters, the localized zero modes predicted by the Callan and Harvey mechanism are stable under the electromagnetic interaction of the fermions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1528270]

I. INTRODUCTION

It is a well-known fact that, in an odd dimensional space–time, a domain wall defect in the mass term of a Dirac field induces a fermionic zero mode localized on the defect.[1] This effect is known to occur even in the presence of an external gauge field, if the corresponding electromagnetic field is contained in the defect hyperplane. Different aspects of this kind of system have been studied both for static,[2,3] and dynamical[4] defects. As far as we know, however, possible effects due to interactions between the fermions have not been considered for this system. In this article, we shall study the stability of this kind of configuration when the electromagnetic interaction between the fermions is turned on. That the localization phenomenon should survive this interaction is not *a priori* evident. For example, for a static configuration, the Coulomb repulsion between the localized charges could be so important as to spread the charge density out over a large region, since the charge density due to the zero mode shall induce an electromagnetic field normal to the defect hypersurface. On the other hand, we note that our study may be thought of as a domain-wall analog of the consideration of the self-consistent vacuum currents in the presence of vortices.[5]

This paper is organized as follows: In Sec. II, we introduce the model and derive a self-consistent equation based in some approximations. This equation is solved for two different mass profiles in Sec. III. Finally, in Sec. IV we discuss the effects of the nonzero modes and present our conclusions.

II. THE MODEL

The Euclidean action S, for the system we shall consider, is given by

$$S = S_F + S_G, \tag{1}$$

where

$$S_F = \int d^3x \, \bar{\psi}(x)[\not{\partial} + ie\not{A}(x) + M(x)]\psi(x), \tag{2}$$

is the fermionic action, and

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$$S_G = \int d^3x \tfrac{1}{4} F_{\mu\nu} F_{\mu\nu}, \tag{3}$$

the Maxwell action, which defines the gauge field dynamics. $x=(x_0,x_1,x_2)$ denote the Euclidean coordinates, and the Hermitian γ matrices are assumed to be in an irreducible 2×2 representation of the Dirac algebra, verifying the anticommutation relations $\{\gamma_\mu,\gamma_\nu\}=2\delta_{\mu\nu}$. The complete Green's functions can be derived from the generating functional

$$\mathcal{Z}[j_\mu;\overline{\eta},\eta] = \int \mathcal{D}A_\mu \mathcal{D}\overline{\psi}\mathcal{D}\psi \exp\left\{ -S[\overline{\psi},\psi;A] + \int d^3x [j_\mu(x)A_\mu(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x)\right\}, \tag{4}$$

where we included source terms for the gauge and fermionic fields. The fermion mass is regarded as an external classical "field," dependent on the x_2 coordinate only. We also fix the number of defects to one, by requiring $M(x)$ to cross 0 once, at $x_2=0$, say.

By applying the property that the functional integral of a (functional) derivative vanishes to Eq. (4), we derive the "quantum equations of motion"

$$0 = \int \mathcal{D}A_\mu \mathcal{D}\overline{\psi}\mathcal{D}\psi \left[\frac{\delta S}{\delta A_\mu(x)} - j_\mu(x) \right] \times \exp\left\{ -S[\overline{\psi},\psi;A_\mu] + \int d^3x [j_\mu(x)A_\mu(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x)] \right\}, \tag{5}$$

for A_μ, and

$$0 = \int \mathcal{D}A_\mu \mathcal{D}\overline{\psi}\mathcal{D}\psi \left[\frac{\delta S}{\delta \overline{\psi}(x)} - \eta(x) \right] \times \exp\left\{ -S[\overline{\psi},\psi;A_\mu] + \int d^3x [j_\mu(x)A_\mu(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x)] \right\}, \tag{6}$$

for $\overline{\psi}$ (the adjoint equation is trivially obtained). Taking the functional derivative with respect to $\eta(y)$ in (6), and putting all the external sources equal to zero afterwards, we find that Eqs. (5) and (6) reduce to

$$\partial_\mu F_{\mu\nu}(x) = J_\nu(x) \tag{7}$$

and

$$\langle [\not{\partial} + ie\not{A}(x) + M(x)]\psi(x)\overline{\psi}(y)\rangle = \delta(x-y), \tag{8}$$

where

$$J_\nu(x) = ie\langle \overline{\psi}(x)\gamma_\nu\psi(x)\rangle \tag{9}$$

and

$$F_{\mu\nu} = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu, \quad \mathcal{A}_\mu = \langle A_\mu \rangle. \tag{10}$$

Equation (7) is an inhomogeneous "classical" Maxwell equation, with the average gauge field $\mathcal{A}_\mu=\langle A_\mu\rangle$ playing the role of the classical gauge field, and the average (vacuum) fermionic current J_μ as its source. Equation (8) involves the expectation values $\langle \psi\overline{\psi}\rangle$ and $\langle A\psi\overline{\psi}\rangle$. Of

course, an exact treatment would require the use of an infinite set of coupled equations involving all the different Green's functions of the system. In order to find a simpler and closed system of equations, we make the following approximation:

$$\langle A_\mu(x)\psi(x)\overline{\psi}(y)\rangle \simeq \langle A_\mu(x)\rangle\langle \psi(x)\overline{\psi}(y)\rangle = \mathcal{A}_\mu(x)S_{\mathcal{A}}(x,y), \tag{11}$$

where we introduced $S_{\mathcal{A}}(x,y)$, which denotes the fermionic propagator in the presence of an "external field" $\mathcal{A}(x)$, which corresponds to the average gauge field. This amounts to a sort of mean-field approximation, where the gauge field is treated classically. To make the approximation involved more explicit, we note that the (exact) three point function appearing in (11) can be written in the equivalent form

$$\langle A_\mu(x)\psi(x)\overline{\psi}(y)\rangle = \int \mathcal{D}A \;\; A_\mu(x)\langle x|(\not\partial + ie\not A + M)^{-1}|y\rangle e^{-S_G[A]-\Gamma_F[A]}, \tag{12}$$

where

$$\Gamma_F[A] = -\log\det[\not\partial + ie\not A + M]. \tag{13}$$

The approximation (11) is obtained from (12) by replacing A by its saddle point value. Namely, the approximation amounts to using the (leading) saddle point approximation, where the "action" which is minimized at the saddle point is the bare Maxwell action plus an effective contribution $\Gamma_F[A]$ coming from the fermionic determinant.

Equation (11) is sufficient to close the system of equations, since then (8) becomes

$$[\not\partial + ie\not{\mathcal{A}}(x) + M(x)]S_{\mathcal{A}} = \delta(x-y). \tag{14}$$

It is now important to realize that the average current can be expressed as a functional of $\mathcal{A}$, as follows:

$$J_\mu(x) = ie\,\mathrm{tr}[\gamma_\mu\langle\psi(x)\overline{\psi}(x)\rangle] = -ie\,\mathrm{tr}[\gamma_\mu S_{\mathcal{A}}(x,x)]. \tag{15}$$

Equation (7), together with (15), define a closed system of equations, which allows us to find the average gauge field $\mathcal{A}$, and then the current density induced in that background. The equation that determines $\mathcal{A}$ is obtained by replacing J_μ by its expression (15) into (7)

$$\partial_\mu F_{\mu\nu}(x) = -ie\,\mathrm{tr}[\gamma_\mu S_{\mathcal{A}}(x,x)], \tag{16}$$

which, in general, and depending on the approximation used to evaluate $S_{\mathcal{A}}$, will be a nonlinear integro-differential equation. The nonlinearity comes from the fermionic propagator $S_{\mathcal{A}}$, which is defined as

$$S_{\alpha\beta}(x,y) = \langle x,\alpha|\mathcal{D}^{-1}|y,\beta\rangle, \tag{17}$$

where $\mathcal{D} = (\not\partial + ie\not A + M)$.

We shall now look for particular solutions of the coupled set of equations, under some restrictions and simplifying approximations. We shall restrict ourselves to *static*, purely electric solutions, with no electric current (hence, no magnetic field). In the Coulomb gauge, the only remaining component for the (average) gauge field is $\mathcal{A}_0$, which is determined by the equation

$$\nabla^2 V = -ie\,\mathrm{tr}[\gamma_0 S_V(x,x)], \tag{18}$$

where $V = \mathcal{A}_0$. It should be noted that this equation involves the fermion propagator evaluated at coincident points, thus introducing the danger of a possible ambiguity (infinity). In a homogeneous system, the corresponding ambiguity is related to the infinite charge of the Dirac sea, and one usually regards as neutral the states where the Dirac sea is filled. The ambiguity is just a constant

density for a homogeneous system but may have a spatial dependence when there are inhomogeneities. Indeed, this will appear later as the need to fix the charge at the defect.

It is perhaps worth remarking that, for this particular kind of situation, the problem we consider amounts to solving a Poisson equation for the potential, combined with a Dirac equation for the fermion field. The latter determines the gauge field through its associated density, and the fermions move in the gauge field background. The charge density is gauge invariant, as well as the Gauss law. The only point were a gauge has been chosen is in the Coulomb gauge choice, which is the most sensible choice for an static situation such as this.

Our approach to solve the system of equations shall be to first evaluate the fermionic propagator in the external potential V. Then, we shall find the corresponding vacuum charge density as a functional of V, and insert it into the Gauss law (18) to determine V. The resulting V can then be used to fix the precise form of the charge density. We will be able to say that there are localized modes if the system admits solutions where the charge density is confined to a small region around the defect. Of course, we shall have to make some assumptions also on the allowed boundary conditions for the fields. The choice of these conditions is also part of the kind of ansatz used, and also on the amount of generality one wants to introduce into the treatment.

To find the fermion propagator in the presence of the external field V, we shall use the perturbative expansion of $\mathcal{D}^{-1}$ in powers of V, namely, we decompose $\mathcal{D}$ as follows:

$$\mathcal{D}=\mathcal{D}_0+\mathcal{V}, \tag{19}$$

where

$$\mathcal{D}_0=\not{\partial}+M(x) \tag{20}$$

and

$$\mathcal{V}=ie\gamma_0 V(x). \tag{21}$$

Thus, $\mathcal{D}^{-1}$ is naturally expanded as

$$\mathcal{D}^{-1}=\mathcal{D}_0^{-1}-\mathcal{D}_0^{-1}\mathcal{V}\mathcal{D}_0^{-1}+\mathcal{D}_0^{-1}\mathcal{V}\mathcal{D}_0^{-1}\mathcal{V}\mathcal{D}_0^{-1}-\cdots. \tag{22}$$

We note that the ''free'' propagator $\mathcal{D}_0^{-1}$ includes the mass field and its space dependence exactly. This must be so, since the defect changes the spectrum of the Dirac field, an effect that cannot be described perturbatively. To find the inverse of $\mathcal{D}_0$, we use the equivalent expression

$$\mathcal{D}_0^{-1}=(\mathcal{D}_0^{\dagger}\mathcal{D}_0)^{-1}\mathcal{D}_0^{\dagger}. \tag{23}$$

which requires finding the inverse of the Hermitian operator

$$\mathcal{H}_0=\mathcal{D}_0^{\dagger}\mathcal{D}_0. \tag{24}$$

This is a much simpler task than inverting $\mathcal{D}_0$, and it allows one to dimensionally reduce the problem. To see this, we follow the procedure of Ref. 2, of which we give a lightning review here. First we write

$$\mathcal{D}_0=(a+\hat{\not{\partial}})P_L+(a^{\dagger}+\hat{\not{\partial}})P_R, \tag{25}$$

where $\hat{\not{\partial}}=\gamma_0\partial_0+\gamma_1\partial_1$. We define the operators $a^{\dagger}$ and a, that act on functions of the x_2 coordinate as

$$a=\partial_2+M \quad a^{\dagger}=-\partial_2+M, \tag{26}$$

and the projectors P_L, P_R

$$P_L=\frac{1+\gamma_2}{2}, \quad P_R=\frac{1-\gamma_2}{2}. \tag{27}$$

These projectors behave like chirality projectors from the point of view of the $1+1$ dimensional theory which describes the chiral zero mode. This decomposition makes it possible to disentangle the dynamics corresponding to the x_2 coordinate from the coordinates $\hat{x}=(x_0,x_1)$. The ''dimensional reduction'' can be seen to arise at the level of the operator $\mathcal{H}_0$

$$\mathcal{H}_0=(h-\hat{\partial}^2)P_L+(\tilde{h}-\hat{\partial}^2)P_R, \tag{28}$$

where

$$h=a^\dagger a \quad \tilde{h}=aa^\dagger. \tag{29}$$

To expand the fermionic fields, we define ϕ_n and $\tilde{\phi}_n$, eigenstates of the operators h and $\tilde{h}$, respectively. We denote by λ_n^2 their (common) eigenvalues

$$h\phi_n=\lambda_n^2\phi_n, \quad \tilde{h}\tilde{\phi}_n=\lambda_n^2\tilde{\phi}_n, \tag{30}$$

$$\langle\phi_n|\phi_m\rangle=\delta_{nm}, \quad \langle\tilde{\phi}_n|\tilde{\phi}_m\rangle=\delta_{nm}, \tag{31}$$

since the spectra coincide, except for $\lambda_n=0$, and the eigenvalues are of course positive. The $\lambda_n=0$ eigenvalue will, by assumption, be present only for h. This will depend of course on the mass profile near the defect, i.e., the zero of the mass. Since the sign of λ_n is arbitrary, we take it positive by convention.

Thus, the fermionic fields can be expanded as

$$\psi(\hat{x},x_2)=\sum_n\ [\phi_n(x_2)\psi_L^{(n)}(\hat{x})+\tilde{\phi}_n(x_2)\psi_R^{(n)}(\hat{x})], \tag{32}$$

$$\overline{\psi}(\hat{x},x_2)=\sum_n\ [\overline{\psi}_L^{(n)}(\hat{x})\phi_n^\dagger(x_2)+\overline{\psi}_R^{(n)}(\hat{x})\tilde{\phi}_n^\dagger(x_2)]. \tag{33}$$

The spinors that carry the dependence on $\hat{x}$ are defined by

$$\psi_{L,R}^{(n)}(\hat{x})=P_{L,R}\psi^{(n)}(\hat{x}), \quad \overline{\psi}_{L,R}^{(n)}(\hat{x})=\overline{\psi}^{(n)}(\hat{x})P_{R,L}, \tag{34}$$

where $\psi_{L,R}^{(n)}$ denotes a general bidimensional fermionic field (one for each value of the index n). In terms of this expansion, the fermionic action becomes

$$S=S_L^{(0)}+\sum_n\ S^{(n)}, \tag{35}$$

where $S_L^{(0)}$ denotes the action for a chiral left-handed fermion in $1+1$ dimensions, while $S^{(n)}$ is a massive Dirac action, also in $1+1$ dimensions, with a mass equal to λ_n (the sign of the mass is irrelevant in $1+1$ dimensions).

Since

$$\mathcal{H}_0^{-1}=(h-\hat{\partial}^2)^{-1}P_L+(\tilde{h}-\hat{\partial}^2)^{-1}P_R, \tag{36}$$

the free propagator becomes

$$\mathcal{D}_0^{-1}=(h-\hat{\partial}^2)^{-1}P_L(a^\dagger-\hat{\partial})+(\tilde{h}-\widehat{*\partial}^2)^{-1}P_R(a-\hat{\partial}). \tag{37}$$

Translation invariance along the x_0 and x_1 coordinates suggests the use of a potential depending only on x_2, $\mathcal{V}=\mathcal{V}(x_2)$. To find the propagator in configuration space, we need to evaluate the following expression:

$$S_{\alpha\beta}(x,y)=(\mathcal{D}_0^{-1})_{\alpha\beta}(x,y)-(\mathcal{D}_0^{-1}\mathcal{V}\mathcal{D}_0^{-1})_{\alpha\beta}(x,y)+\cdots\ , \tag{38}$$

with $\mathcal{V}=\mathcal{V}(x_2)$. In the perturbative expansion for the propagator, we insert expansions of the identity constructed with intermediate states corresponding to eigenstates of the operator $\mathcal{H}_0$. Using the fact that each eigenvalue λ_n corresponds to the effective mass of a two-dimensional mode, and that the lowest mode is massless (the zero mode), it is natural to keep only the zero mode in the intermediate states as a first approximation. Note that the mass λ_n of the nonzero modes is separated from the zero mode by a finite gap whose magnitude is controlled by the profile of the mass near the defect (see Ref. 2). With this in mind, we shall first use the leading approximation of keeping just the zero mode, and then make a quantitative evaluation of the error involved in this procedure, by including the correction corresponding to the lowest massive mode. On the other hand, we shall keep the full dependence in the potential, namely, we shall use no truncation for the perturbative series in $\mathcal{V}$. To implement this approximation, we introduce projectors P_0 along the zero mode. They are explicitly given by

$$P_0=\phi_0\phi_0^{\dagger}\sum_n\ \psi_L^{(n)}\overline{\psi}_L^{(n)}. \tag{39}$$

Taking this into account, after some algebra one can show that, in this approximation, the propagator is given by

$$S_{\alpha\beta}(x,y)\simeq\phi_0^{\dagger}(x_2)\,\phi_0(y_2)\langle x_0,x_1,\alpha|\,\frac{\hat{\partial}+ie\gamma_0V_{0,0}P_L}{(\hat{\partial}+ie\gamma_0V_{0,0})^2}|y_0,y_1,\beta\rangle. \tag{40}$$

In this expression there appears the average of V in the zero mode which is denoted by

$$V_{0,0}=\langle\phi_0|V|\phi_0\rangle. \tag{41}$$

It is worth noting that this result is approximate in the sense that only the zero mode has been included, but all the powers of A_μ have been added, as it is evident from the nonlinear dependence of the propagator on A_μ. The charge density is evaluated by multiplying by γ_0, taking the Dirac trace, and finally calculating the coincidence limit $x\to y$. Inserting the result so obtained for the charge density as a functional of the potential into (18) yields

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\phi_0(x_2)\,\phi_0^{\dagger}(x_2)\int\frac{d^2k}{2\pi}\,\frac{-ik_0+ieV_{0,0}}{(-ik_0+ie\gamma_0V_{0,0})^2}. \tag{42}$$

The momentum space integral has both linear and logarithmic divergences. We make sense out of it by applying a symmetric limit kind of regularization. Specifically, the momentum integrals are evaluated by first defining the integrals over a symmetric interval around zero, and then taking the limit of an infinite interval. Namely,

$$\int\ d^2k\cdots\equiv\lim_{\Lambda_1\to\infty}\lim_{\Lambda_2\to\infty}\int_{-\Lambda_1}^{+\Lambda_1}\int_{-\Lambda_2}^{+\Lambda_2}\cdots. \tag{43}$$

By an application of this regularization, we see that (42) can be expressed as

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\phi_0(x_2)\,\phi_0^{\dagger}(x_2)\,\frac{e^2V_{0,0}}{2}. \tag{44}$$

It is remarkable that, as a consequence of the fact that we are only keeping the zero mode, the expression for the charge density becomes linear in the potential. This happens in spite of the fact that we have kept all the powers of the potential in the fermionic propagator, since the result is a consequence of the fact that massless two-dimensional QED is exactly solvable,[6] with the exact fermionic determinant being quadratic in the gauge field.

Now we come back to the arbitrariness in the coincidence limit for the propagator. This limit is not, of course, the only possible choice, since one may modify its value according to the total charge in the system. Indeed, if the system is neutral, something we shall assume, one may allow for the addition of a constant to the density. This constant reflects the charge of the Dirac sea at the defect, and as such it is concentrated on $x_2=0$. Thus, the form of (44) for a neutral system is

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\frac{e^2V_{0,0}}{2}\phi_0(x_2)\phi_0^\dagger(x_2)-\frac{e^2}{2}V_{0,0}\delta(x_2), \tag{45}$$

where the constant multiplying the δ function has been chosen in order to have zero total charge.

We have obtained an integro-differential equation involving derivatives of V and its average on the lowest energy mode. To solve it self-consistently, we first derive from (44) (by integration) an equation for V, depending also the average of the potential. Then, as a second step, we shall insert this average into (44) in order to obtain the explicit profile of the potential as a function of x_2. At this point, it is clear that the existence of a self-consistent solution depends on the particular form of the zero modes appearing in Eq. (44). This differential equation will have a solution only if the charge density is localized in such a way that the integrals involved are well defined. In particular, the zero modes need to be localized around the defect. It was shown in Ref. 1 that in $2n+1$ dimensions the zero mode has the form

$$\eta e^{-\int_a^{x_2}dyM(y)}, \tag{46}$$

where η is an spinor independent of x_2.

III. EXAMPLES

In what follows we will discuss the possible solutions of Eq. (44) for two different kinds of mass profiles.

• Step-like defect.

Given a mass of the form:

$$M(x_2)=\Lambda(2\Theta(x_2)-1), \tag{47}$$

where Λ is a constant with the dimensions of a mass, and Θ is the Heaviside function, there is only one zero mode,[2] which can be explicitly written as

$$\phi_0(x_2)=\Lambda^{1/2}e^{-\Lambda|x_2|}. \tag{48}$$

In this case, the differential equation becomes

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\frac{1}{2}\Lambda e^2V_{0,0}e^{-2\Lambda|x_2|}-\frac{e^2}{2}V_{0,0}\delta(x_2), \tag{49}$$

and integrating it twice we obtain for the potential V

$$V(x_2)=a+\frac{1}{8\Lambda}e^2V_{0,0}e^{-2\Lambda|x_2|}, \tag{50}$$

where a is a constant, akin to a chemical potential for the charge of the zero mode. In this expression, the neutrality implies the decay in the potential for large values of x_2. Of course, we

might have wanted to consider a charged system; the resulting potential would then be the superposition of (50) and the potential due to the δ function, which is linearly rising.

In order to find a self-consistent solution for the potential we evaluate the expectation value of V, which is expressed by (50), in the zero mode

$$V_{0,0}=a+\frac{1}{8\Lambda}e^2V_{0,0}\int_{-\infty}^{\infty}dx|\phi_0(x)|^2e^{-2\Lambda|x|}. \tag{51}$$

Thus, $V_{0,0}$ is easily seen to be given by

$$V_{0,0}=\frac{a}{1-\dfrac{e^2}{16\Lambda}}. \tag{52}$$

Therefore, the potential written in terms of the zero modes results

$$V(x_2)=|\phi_0(x)|^2\frac{2ae^2}{16\Lambda^2-\Lambda e^2}. \tag{53}$$

Notice that the solution is only stable if the electromagnetic coupling constant and the mass coupling constant satisfy the bound: $e^2<16\Lambda$, which means that the strength of the interaction (repulsion) between the electrons cannot be larger than the scale given by the height of the defect. We note that ''stability'' refers here to the property of having a confining potential. We see that in this case, i.e., for an step-like mass and keeping only the zero energy mode, there exist a self-consistent solution for the fermionic interaction potential. In other words, even in the case of interacting electrons, the fermions are localized in the x_2 direction and can only move along the defect.

The interpretation of a as a chemical potential proceeds from the fact that the Gauss law (49), combined with (52), means that the charge density of the configuration is

$$\rho(x_2)=a\frac{\Lambda e^2}{2\left(1-\dfrac{e^2}{16\Lambda}\right)}e^{-2\Lambda|x_2|}, \tag{54}$$

and (by integrating over x_2) one sees that the total charge is proportional to the constant a. Of course, the *total* charge is zero, but it may be decomposed into the contributions from the zero mode (which is fixed by a) and the ''neutralizing'' charge density, which is proportional to $\delta(x_2)$.

• Linear defect.

Assuming than the mass can be expanded as a power series in x_2, for small enough x_2 we only keep the first-order term

$$M(x_2)=M'(0)x_2, \tag{55}$$

where we assume $M'(0)\neq 0$ being M' the first derivative of the mass. For this mass profile we can still find the zero mode by defining[2]

$$h=-\partial_2^2-M'+M^2x_2^2. \tag{56}$$

which is an harmonic oscillator Hamiltonian. The lowest energy mode is

$$\phi_0(x_2)=\left(\frac{|M'|}{\pi}\right)^{1/4}e^{-|M'|/2\,x_2^2}. \tag{57}$$

Following the same steps as in the previous example we find that the potential can be written in terms of the zero mode as

$$V(x_2)=a+\int_B^{x_2}dy\int_A^y dz|\phi_0(z)|^2\left(\frac{e^2a}{2-e^2C}\right), \tag{58}$$

where

$$C=\int_{-\infty}^{\infty}dx_2|\phi_0(x_2)|^2\int_B^{x_2}dy\int_A^y dz|\phi_0(z)|^2. \tag{59}$$

Thus we see that also in this case there exists a self-consistent solution for the Gauss law, for a charge density localized around the defect. However there is a necessary condition for the existence of this localized mode. The wave function of the zero mode has to vanish rapidly outside the region of the space where the mass can be approximated linearly. A quantitative criterion for the validity of this condition can be found in Ref. 2.

In summary, up to know we have shown the existence of localized solutions if we keep only the lowest energy modes in the expansion of the fermionic propagator. This solution depends on the mass profile, and it is nonperturbative in the electromagnetic interaction between the fermions. We have neglected the (more energetic) massive modes based on the fact that the terms on the action that come from these modes go as $1/\lambda_n^2$, where λ_n is the mass of the mode.[2] Therefore, for a large and steep enough mass, our approximation will be valid. In particular, for a linear defect, the mass of the modes is proportional to the slope of the mass profile. Therefore, by changing this slope we could make λ_n arbitrarily large.

IV. EFFECT OF THE MASSIVE MODES

We shall now study the problem of including one massive mode in our calculation in order to check whether there still exist localized solutions or not. It will provide also a quantitative idea about the error involved in considering only the lowest energy modes.

We proceed as follows: In the perturbative expansion for the fermion propagator (22), we consider only the projection of the operators $\mathcal{D}_0^{-1}$ and $\mathcal{V}$ onto the two lowest energy modes. Then each factor $\mathcal{D}_0^{-1}$ contributes with

$$\mathcal{D}_0^{-1}\simeq\tilde{\phi}_1\phi_1^\dagger\lambda_1P_L-\tilde{\phi}_1\tilde{\phi}_1^\dagger\hat{\theta}P_R+\phi_1\tilde{\phi}_1^\dagger\lambda_1P_R-\phi_1\phi_1^\dagger\hat{\theta}P_L-\phi_0\phi_0^\dagger\hat{\theta}P_L. \tag{60}$$

For an even $V(x_2)$, selection rules imply the vanishing of the matrix elements $V_{n,m}$, $V_{n,\tilde{m}}$, and $V_{\tilde{n},\tilde{m}}$.

Replacing (60) into (22), and keeping only the nonvanishing matrix elements of V, the first-order correction in $\mathcal{V}$ to the fermion propagator [i.e., correction to (60)] is

$$\begin{aligned}\mathcal{D}_0^{-1}\mathcal{V}\mathcal{D}_0^{-1}\simeq{}&\frac{ie\tilde{\phi}_1\phi_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[-\hat{\theta}\lambda_1\gamma^0V^0_{\tilde{1},\tilde{1}}-\lambda_1\gamma^0V_{1,1}\hat{\theta}]P_L+\frac{ie\tilde{\phi}_1\phi_0^\dagger}{(\lambda_1^2-\hat{\partial}^2)\hat{\partial}^2}[-\lambda_1\gamma^0V_{1,0}\hat{\theta}]P_L\\&+\frac{ie\tilde{\phi}_1\tilde{\phi}_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[\lambda_1^2\gamma^0V_{1,1}+\hat{\theta}\gamma^0V_{\tilde{1},\tilde{1}}\hat{\theta}]P_R+\frac{ie\phi_1\tilde{\phi}_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[-\hat{\theta}\lambda_1\gamma^0V_{1,1}-\lambda_1\gamma^0V_{\tilde{1},\tilde{1}}\hat{\theta}]P_R\\&+\frac{ie\phi_0\tilde{\phi}_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)\hat{\partial}^2}[-\hat{\theta}\lambda_1\gamma^0V_{1,1}]P_R+\frac{ie\phi_1\phi_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[\lambda_1^2\gamma^0V_{\tilde{1},\tilde{1}}+\hat{\theta}\gamma^0V_{1,1}\hat{\theta}]P_L\end{aligned}$$

$$+\frac{ie\phi_1\phi_0^\dagger}{(\lambda_1^2-\hat{\partial}^2)\hat{\partial}^2}[\hat{\not{\partial}}\gamma^0 V_{1,0}\not{\partial}P_L+\frac{ie\phi_0\phi_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)\hat{\partial}^2}[\hat{\not{\partial}}\gamma^0 V_{0,1}\hat{\not{\partial}}]P_L+\frac{ie\phi_0\phi_0^\dagger}{(\hat{\partial}^2)^2}[\hat{\not{\partial}}\gamma^0 V_{0,0}\hat{\not{\partial}}]P_L. \tag{61}$$

Notice that in this case it is not possible to obtain a nonperturbative expression for the fermion propagator due to the fact that we are taking into account massive modes as well as the massless one. In order to write the Gauss law we need to compute

$$\begin{aligned}\mathrm{tr}(\gamma_0\mathcal{D}^{-1})\simeq&-\frac{ie(\tilde{\phi}_1\tilde{\phi}_1^\dagger+\phi_1\phi_1^\dagger)}{(\lambda_1^2-\hat{\partial}^2)}\partial_0+\frac{ie\phi_0\phi_0^\dagger}{(\hat{\partial}^2)}\partial_0+\frac{ie\tilde{\phi}_1\tilde{\phi}_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[\lambda_1^2 V_{1,1}+(2\partial_0^2-\hat{\partial}^2)V_{\tilde{1},\tilde{1}}]\\&+\frac{ie\phi_1\phi_1^\dagger}{(\lambda_1^2-\hat{\partial}^2)^2}[\lambda_1^2 V_{\tilde{1},\tilde{1}}+(2\partial_0^2-\hat{\partial}^2)V_{1,1}]+\frac{ie(\phi_1\phi_0^\dagger+\phi_0\phi_1^\dagger)}{(\lambda_1^2-\hat{\partial}^2)\hat{\partial}^2}[(2\partial_0^2-\hat{\partial}^2)V_{0,1}]\\&+\frac{ie\phi_0\phi_0^\dagger}{(\hat{\partial}^2)^2}[(2\partial_0^2-\hat{\partial}^2)V_{0,0}].\end{aligned} \tag{62}$$

Taking the Fourier transform in the above expression and regularizing the integrals by a symmetric limit, the Gauss law becomes

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\tilde{\phi}_1(x_2)\tilde{\phi}_1^\dagger(x_2)\frac{e^2V_{1,1}}{2}+\phi_1(x_2)\phi_1^\dagger(x_2)\frac{e^2V_{\tilde{1},\tilde{1}}}{2}. \tag{63}$$

Thus we have obtained a differential equation whose solution will depend on the localization properties of the fermionic modes around the defect.

In the case of a mass that can be approximated by a linear function of x_2 near the defect, it is simple to check that[2]

$$\phi_n=\tilde{\phi}_{n+1}, \tag{64}$$

therefore, there is only one zero mode, and the Gauss equation becomes

$$\frac{\partial^2}{\partial x_2^2}V(x_2)=\phi_0(x_2)\phi_0^\dagger(x_2)\frac{e^2V_{1,1}}{2}+\phi_1(x_2)\phi_1^\dagger(x_2)\frac{e^2V_{0,0}}{2}. \tag{65}$$

Integrating this expression we find

$$V(x_2)=a+\left(\frac{e^2V_{1,1}}{2}\right)\int_B^{x_2}dy\int_A^y dz|\phi_0(z)|^2+\left(\frac{e^2V_{0,0}}{2}\right)\int_B^{x_2}dy\int_A^y dz|\phi_1(z)|^2. \tag{66}$$

Once again, we look for the self-consistent solutions for the expectation values of the potential. When computed on the two lowest energy modes, they are given by the solution of the equations

$$V_{i,i}=a+\left(\frac{e^2V_{1,1}}{2}\right)D_{i0}+\left(\frac{e^2V_{0,0}}{2}\right)D_{i1}, \tag{67}$$

where $i=0,1$ and D_{ij} are

$$2D_{ij}=\int_{-\infty}^{\infty}dx_2|\phi_i(x_2)|^2\int_B^{x_2}dy\int_A^y dz|\phi_j(z)|^2. \tag{68}$$

Solving (67) we obtain

$$V_{0,0}=a\,\frac{1-e^2D_{10}+e^2D_{00}}{(1-e^2D_{01})(1-e^2D_{10})-e^4D_{11}D_{00}}, \tag{69}$$

$$V_{1,1}=a\,\frac{1-e^2D_{01}+e^2D_{11}}{(1-e^2D_{01})(1-e^2D_{10})-e^4D_{11}D_{00}}. \tag{70}$$

We have found that, in the case of a linear mass, there exist a self-consistent solution of the Gauss equation to first order in the interaction potential, if we include apart from the zero mode, one massive mode. Notice that, for a linear mass around the defect, ϕ_n and $\tilde{\phi}_n$ are harmonic oscillator eigenstates. Far enough from the defect, the eigenstates decay exponentially (as a Gaussian function), ensuring that the charge density is localized around the defect in such a way that there is a solution for the Gauss equation. Obviously all the caveats regarding the range of validity of approximating the mass by a linear function, that we mention in the previous case, must be taken into account here.

Summarizing, we have considered a Dirac field in $2+1$ dimensions with a domain wall like defect in its mass, minimally coupled to a dynamical Abelian vector field. The mass of the fermionic field is assumed to have just one linear domain wall, externally fixed and unaffected by the dynamics. In the absence of electromagnetic interactions among the fermions, it is a well-known fact that localized zero modes exist on the defect.[1] We have studied here the effect of the fermionic interactions on these modes showing that, under some general conditions on the parameters, the localized zero modes stable under the electromagnetic interactions of the fermions.

There are of course many interesting direction around which one could extend this result, by extending the family of field configurations entering into the coupled equations. An interesting possibility is perhaps the consideration of a system with a nonvanishing current on the defect; this would of course require the introduction of extra fields into the game: Magnetic fields generated by the current and fermionic states with energies just above the ground state.

ACKNOWLEDGMENTS

This work is partially supported by CONICET (Argentina), by ANPCyT through Grant No. 03-03924 (AL), and by Fundación Antorchas (Argentina).

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Casimir energy of a relativistic perfect fluid confined to a *D*-dimensional hypercube

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(Received 23 August 2002; accepted 18 October 2002)

Compact formulas are obtained for the Casimir energy of a relativistic perfect fluid confined to a D-dimensional hypercube with von Neumann or Dirichlet boundary conditions. The formulas are conveniently expressed as a finite sum of the well-known gamma and Riemann zeta functions. Emphasis is placed on the mathematical technique used to extract the Casimir energy from a D-dimensional infinite sum regularized with an exponential cutoff. Numerical calculations show that initially the Dirichlet energy decreases rapidly in magnitude and oscillates in sign, being positive for even D and negative for odd D. This oscillating pattern stops abruptly at the critical dimension of $D=36$ after which the energy remains negative and the magnitude increases. We show that numerical calculations performed with 16-digit precision are inaccurate at higher values of D. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1531822]

I. INTRODUCTION

If a system has boundary conditions, the infinite vacuum energy is slightly altered compared to the free continuum case; this leads to a force on the boundaries called the Casimir force. In 1948, Casimir[1] calculated the attractive force between two conducting plane-parallel plates in vacuum due to the zero-point fluctuations of the electromagnetic field. There has been an enormous amount of theoretical work on the subject since the pioneering work of Casimir (for a general review up to 1997 we refer the reader to Refs. 2 and 3). The earliest experiment to test Casimir's calculation was carried out by Sparnaay[4] in 1958. The results were inconclusive due to large systematic errors and uncontrollable electrostatic forces leading to a 100% uncertainty in the results. In 1997, a landmark experiment[5,6] using a torsion pendulum improved significantly on previous results. The most recent experiments using atomic force microscopes[7] and high precision capacitance bridges[8] are now in agreement with theoretical calculations to within 1%, eliminating any doubt as to the reality of the Casimir force.

In this work, we calculate the Casimir energy for phonons in a relativistic perfect fluid confined to a D-dimensional hypercube using the cut-off method. The Casimir energy of a scalar field in a rectangular cavity with p sides of lengths $a_1, a_2, \ldots a_p$ and $D-p$ sides of characteristic length $L \gg a_i$ was calculated in Ref. 10 using the Epstein zeta function regularization scheme. It was shown that Neumann and periodic boundary conditions yield a negative Casimir energy. Determining the sign for Dirichlet boundary conditions turned out to be more complicated and was studied in detail in Refs. 11 and 12 where Epstein zeta function regularization was again employed. In Ref. 11 it was shown that in a rectangular cavity with p sides of equal length L and $D-p$ sides of length $\gg L$, the sign of the Dirichlet energy depends on whether p is even or odd. For even values of p, the energy is positive when D is less than a critical value D_c and negative when D is above D_c. For odd values of p the sign is always negative and no critical dimension exists. It was later shown[12] that it is possible for the Dirichlet energy to be positive for odd values of p if the sides have unequal lengths.

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One alternative to zeta function regularization is the exponential cutoff. The cut-off method was employed in Ref. 13 to calculate the Casimir energy of scalar fields confined to parallel plates in higher dimensions. In our article, we apply the cutoff method to a perfect fluid confined to a D-dimensional hypercube. We develop a mathematical technique that enables us to extract the relevant Casimir term from a D-dimensional infinite sum: one that contains the square root of a sum of D squares modified by an exponential cut-off term. This technique makes repeated use of the Euler–Maclaurin integration formula and a series expansion for the infinite sum of modified Bessel functions. For both von Neumann and Dirichlet boundary conditions we obtain convenient formulas for the Casimir energy as a function of D. The formulas are expressed as a single sum of D terms containing the Riemann zeta and gamma functions. Numerical calculations show that the Dirichlet energy exhibits a clear oscillating pattern up to $D=35$: it is positive for even D, negative for odd D and its magnitude decreases rapidly. However, this oscillating pattern stops abruptly at the critical dimension of $D=36$; for $D\geqslant 36$, the sign remains negative and the magnitude increases. In contrast to the Dirichlet energy, the Neumann energy is negative for all values of D.

It is instructive to compare the Casimir calculation of a perfect fluid to that of the open bosonic string. A string embedded in D spatial dimensions supports transverse vibrations in $D-1$ orthogonal directions. The boundary conditions at the two ends of the string, responsible for the Casimir effect, is independent of the dimension D. Therefore, the number of dimensions does not complicate the Casimir calculation: the quantity $D-1$ contributes only a multiplicative factor (see Ref. 9 for details). A fluid confined to a D-dimensional hypercube supports longitudinal vibrations in D orthogonal directions. In contrast to the string, it has boundary conditions in all D directions leading to a Casimir energy with a non-trivial dependence on D. Simply put, for the open bosonic string one needs to calculate a single infinite sum which is multiplied $D-1$ times whereas for the fluid one needs to calculate a D- dimensional infinite sum. This reflects the fact that the perfect fluid is described by one scalar field which is a function of $D+1$ spacetime dimensions whereas the string is described by $D+1$ scalar fields each a function of two spacetime dimensions.

II. THE ACOUSTIC MODES IN A RELATIVISTIC PERFECT FLUID

A perfect fluid is defined as having at each point a velocity $\mathbf{v}$ such that an observer moving with this velocity observes the fluid as being isotropic. This occurs when the mean free path between collisions is small compared to the wavelength. In a frame where the fluid is at rest at some particular position and time the energy-momentum tensor $T^{\mu\ \nu}$ has spherical symmetry and is given by[14]

$$T^{ij}=P\,\delta^{ij}\,,\quad T^{i0}=0\,,\quad T^{00}=\rho\,, \tag{1}$$

where ρ is defined as the proper energy density and P the pressure. In the same frame the current four-vector N^{μ} is given by

$$N^{i}=0\,,\quad N^{0}=n \tag{2}$$

where n is defined as the particle number density. The motion of the fluid is governed by conservation of energy momentum and particle number, i.e.,

$$\partial_{\alpha}T^{\alpha\beta}=0\,,\quad \partial_{\alpha}N^{\alpha}=0\,. \tag{3}$$

Small perturbations from equilibrium ($\rho=\rho_0$, $P=P_0$, and $n=n_0$) lead to sound waves with the following scalar equation:

$$\frac{\partial^2\rho(x)}{\partial^2 t}-v^2\nabla^2\rho(x)=0, \tag{4}$$

where $\rho(x)$ is a scalar field, v is the speed of the sound waves given by $v=\sqrt{P_0/\rho_0}$ and $x=(\mathbf{x},t)$. Consider the fluid confined to a D-dimensional hypercube with sides of length L. The von Neumann (N) and Dirichlet (Di) boundary conditions at $x^i=0$ and $x^i=L$ are $\partial^i\rho(x)=0$ and $\rho(x)=0$ respectively (where $i=1,2,\ldots,D$). The solution to the wave equation (4) for the von Neumann and Dirichlet boundary conditions are respectively,

$$\rho(x)=\sum_{\{n_i\}=0}^{\infty}(\alpha^{\dagger}_{\{n_i\}}e^{i\omega t}+\alpha_{\{n_i\}}e^{-i\omega t})\prod_{i=1}^{D}\cos\left(\frac{n_i\pi x^i}{L}\right)+at+b \tag{5}$$

and

$$\rho(x)=\sum_{\{n_i\}=1}^{\infty}(\alpha^{\dagger}_{\{n_i\}}e^{i\omega t}+\alpha_{\{n_i\}}e^{-i\omega t})\prod_{i=1}^{D}\sin\left(\frac{n_i\pi x^i}{L}\right) \tag{6}$$

where ω is given by

$$\omega=\frac{\pi v}{L}(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}=\pi\beta(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}. \tag{7}$$

The parameter $\beta\equiv v/L$ is dependent on the physical and geometrical properties of the fluid: the pressure P_0, the proper density ρ_0 and the proper length L of the sides of the hypercube.

III. QUANTIZATION AND CASIMIR ENERGY

After imposing equal time commutation relations on the scalar field $\rho(x)$, i.e.,

$$[\rho(\mathbf{x},t),\dot{\rho}(\mathbf{x}',t)]=i\delta^D(\mathbf{x}-\mathbf{x}') \tag{8}$$

one obtains the well-known form for the vacuum energy $E=\frac{1}{2}\Sigma\omega$ (where $\hbar=1$). For the D-dimensional perfect fluid in consideration, ω is given by (7) and the vacuum energy in the Neumann (N) and Dirichlet (Di) cases are

$$E=\frac{\pi\beta}{2}\sum_{\{n_i\}=0(N)\atop\{n_i\}=1(Di)}^{\infty}(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}. \tag{9}$$

The multiple sum corresponds to the vacuum energy of the fluid with boundary conditions and is divergent due to the high-frequency modes. The vacuum energy with no boundaries, i.e., of the continuum, is given by multiple integrals and is also divergent. It is the difference between these two energies that is of interest and leads to the finite quantity we call the Casimir energy (the energy needed to set up the boundaries starting from the continuum). To extract the relevant constant from the infinite sum (9), one regularizes the sum to isolate the infinite contribution of the continuum from the finite contribution stemming from the boundary conditions. There are many ways to regularize a sum. In this article we choose an exponential cutoff term $e^{-a(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}}$ where the parameter a is a positive real number. The regularized vacuum energy E_{Di} in the Dirichlet case is then

$$\begin{aligned}E_{\mathrm{Di}}&=\left(\frac{\pi\beta}{2}\right)\sum_{n_D=1}^{\infty}\cdots\sum_{n_1=1}^{\infty}(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}\,e^{-a(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}}\\&=\left(\frac{\pi\beta}{2}\right)(-\partial_a)\sum_{n_D=1}^{\infty}\cdots\sum_{n_1=1}^{\infty}e^{-a(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}}.\end{aligned} \tag{10}$$

In the Neumann case the sums start at $n_i=0$ instead of $n_i=1$. The regularized vacuum energy (10) is finite and is a function of the parameter a. Our goal is to obtain the leading terms in this sum as $a\to 0$ and extract the constant Casimir term as a function of the dimension D. To accomplish this task we make repeated use of the Euler–Maclaurin integration formula: a formula that relates an infinite sum of a function to its integral, i.e.,

$$\sum_{i=1}^{\infty} f(i)=\int_0^{\infty} f(x)\,dx-\frac{1}{2}f(0)-\sum_{p=1}^{\infty}\frac{1}{(2p)!}B_{2p}\,f^{(2p-1)}(0), \tag{11}$$

where $f^{(2p-1)}(0)$ are odd derivatives of f evaluated at zero. There are D sums in (10) to evaluate and we apply the Euler–Maclaurin formula to each sum except the last one. In Appendix A we show that for the exponential function f in (10), the value of $f^{2p-1}(0)$ is always zero except for the last sum. At the last sum, the value of $f^{2p-1}(0)$ can diverge and oscillate between positive and negative infinity (depending on the value of p) and we therefore use a different method of calculation. To summarize, we convert $D-1$ sums in (10) into multiple integrals by repeated application of the Euler–Maclaurin formula and then evaluate separately the last sum. We see from (11) that each sum (except the last one) gets replaced by an integral of the function minus half of the function at zero. This can be expressed by a simple and useful prescription

$$\sum \to \int -\frac{1}{2}. \tag{12}$$

The prescription (12) can be applied repeatedly to convert multiple sums to multiple integrals. The case $D=3$ is illustrated below where two of the three sums are replaced by (12):

$$\begin{aligned}\sum_{n_3=1}^{\infty}\sum_{n_2=1}^{\infty}\sum_{n_1=1}^{\infty} e^{-a(n_1^2+n_2^2+n_3^2)^{1/2}} &\to \sum_{n_3=1}^{\infty}\left(\int -\frac{1}{2}\right)^2\\ &=\sum_{n_3=1}^{\infty}\left(\int^2-\int+\frac{1}{4}\right)\\ &=\sum_{n_3=1}^{\infty}\int_0^{\infty} e^{-a(n_1^2+n_2^2+n_3^2)^{1/2}}\,dn_1\,dn_2\\ &\quad-\sum_{n_3=1}^{\infty}\int_0^{\infty} e^{-a(n_2^2+n_3^2)^{1/2}}\,dn_2+\frac{1}{4}\sum_{n_3=1}^{\infty} e^{-a n_3}\,.\end{aligned}$$

To evaluate (10), we apply $D-1$ times the prescription given in (12). This yields

$$\begin{aligned}E_{\mathrm{Di}} &= -(\pi\beta/2)\,\partial_a\sum_{n_D=1}^{\infty}\left(\int -\frac{1}{2}\right)^{D-1}\\ &=\pi\beta(-1)^D 2^{-D}\,\partial_a\sum_{n_D=1}^{\infty}\left(1-2\int\right)^{D-1}\\ &=\pi\beta(-1)^D 2^{-D}\sum_{p=0}^{D-1}\binom{D-1}{p}(-2)^p\,\partial_a\sum_{n_D=1}^{\infty}\int^p\\ &=\pi\beta(-1)^D 2^{-D}\sum_{p=0}^{D-1}\binom{D-1}{p}(-2)^p\,\partial_a I(p,a),\end{aligned} \tag{13}$$

where $I(p,a)$ is defined by

$$I(p,a)\equiv\sum_{n=1}^{\infty}\int^{p}=\sum_{n=1}^{\infty}\int_{0}^{\infty}e^{-a\,(n^2+x_1^2+\ldots+x_p^2)^{1/2}}dx_1\cdots dx_p. \tag{14}$$

To determine (13) we need to evaluate $\partial_a I(p,a)$. The p-dimensional integral in $I(p,a)$ can be expressed in terms of the derivative of the modified Bessel function $K_{(p-1)/2}(a\,n)$[15]

$$\int_{0}^{\infty}e^{-a\,(n^2+x_1^2+\ldots+x_p^2)^{1/2}}dx_1\cdots dx_p=-2^{(1-p)/2}\,\pi^{(p-1)/2}\partial_a\left(K_{(p-1)/2}(a\,n)\left(\frac{n}{a}\right)^{(p-1)/2}\right). \tag{15}$$

Using the identity

$$\left(\frac{d}{z\,dz}\right)^{m}\{z^{-\nu}K_{\nu}(Z)\}=(-1)^{m}\,Z^{-\nu-m}\,K_{\nu+m}(Z) \tag{16}$$

with $\nu=0$, $m=(p-1)/2$, $Z=a\,n$ yields

$$(-1)^{(1-p)/2}\left(\frac{d}{a\,da}\right)^{(p-1)/2}K_0(a\,n)=K_{(p-1)/2}(a\,n)\left(\frac{n}{a}\right)^{(p-1)/2}. \tag{17}$$

By substituting (17) and (15) into (14) one obtains

$$\partial_a I(p,a)=2^{(1-p)/2}\pi^{(p-1)/2}(-1)^{(3-p)/2}(\partial_a)^2\left(\frac{d}{a\,da}\right)^{(p-1)/2}\sum_{n=1}^{\infty}K_0(a\,n). \tag{18}$$

We are interested in obtaining a series expansion of (18) and isolating the relevant constant from the infinite continuum in the limit as $a\to 0$. We therefore replace the infinite sum of $K_0(a\,n)$ by the following series expansion:[15]

$$\sum_{n=1}^{\infty}K_0(a\,n)=\frac{1}{2}(C+\ln(a/4\,\pi))+\frac{\pi}{2\,a}+\pi\sum_{m=1}^{\infty}\left\{\frac{1}{\sqrt{a^2+4\,m^2\,\pi^2}}-\frac{1}{2\,m\,\pi}\right\}. \tag{19}$$

Consider the terms $\ln(a/4\,\pi)/2$ and $\pi/(2\,a)$ in (19). They yield terms proportional to $1/a^{p+1}$ and $1/a^{p+2}$, respectively, in the series expansion of (18). These two terms correspond to the infinite continuum as $a\to 0$. The relevant constant related to the Casimir energy stems from the infinite sum in (19), i.e.,

$$\begin{aligned}&\lim_{a\to 0}(\partial_a)^2\left(\frac{d}{a\,da}\right)^{(p-1)/2}\sum_{m=1}^{\infty}\frac{\pi}{\sqrt{a^2+4\,m^2\pi^2}}\\&\quad=\lim_{a\to 0}\frac{(-1)^{(p+1)/2}\Gamma(p+1)}{\Gamma\left(\frac{p+1}{2}\right)2^{(p-1)/2}}\sum_{m=1}^{\infty}\frac{\pi}{(a^2+4m^2\pi^2)^{(p+2)/2}}+O(a)\\&\quad=\frac{(-1)^{(p+1)/2}\Gamma\left(\frac{p+2}{2}\right)}{\pi^{(2p+3)/2}2^{(p+3)/2)}}\sum_{m=1}^{\infty}\frac{1}{m^{p+2}}=\frac{(-1)^{(p+1)/2}\Gamma\left(\frac{p+2}{2}\right)\zeta(p+2)}{\pi^{(2p+3)/2}2^{(p+3)/2}}.\end{aligned} \tag{20}$$

Inserting (20) into (18) one obtains

$$\partial_a I(p,a)=\frac{\Gamma\left(\frac{p+2}{2}\right)\zeta(p+2)}{2^{p+1}\pi^{(p+4)/2}}. \tag{21}$$

TABLE I. Dirichlet and Neumann Casimir energies in units of β.

	$D=1$	$D=2$	$D=3$	$D=4$	$D=5$	$D=6$
E_{Di}	-0.131	0.0415	-0.0157	0.00625	-0.00261	0.00112
E_N	-0.131	-0.220	-0.284	-0.331	-0.367	-0.396

We finally obtain the Casimir energy for the Dirichlet case by substituting (21) into (13),

$$E_{\mathrm{Di}}=\beta\, 2^{(-D-1)}\sum_{p=0}^{D-1}\binom{D-1}{p}(-1)^{p+D}\pi^{(-p-2)/2}\Gamma\left(\frac{p+2}{2}\right)\zeta(p+2). \tag{22}$$

Equation (22) is our final formula for the Casimir energy of a relativistic perfect fluid confined to a hypercube with Dirichlet boundary conditions. It is conveniently expressed as a finite sum of D terms involving the gamma and Riemann zeta functions; this makes it well-suited for numerical calculations. The parameter β encompasses the physical and geometrical properties of the relativistic perfect fluid: its proper energy density, pressure and length L. It plays the same role for the fluid as the string tension does for the bosonic string; both β and the string tension appear in the Casimir energy as dimensionful free parameters.

Having solved the Dirichlet case it is now relatively straightforward to obtain the Neumann case. The regularized vacuum sum in the Neumann case, labeled E_N, has its sums starting at $n_i=0$ instead of $n_i=1$, i.e.,

$$E_N=\left(\frac{\pi\beta}{2}\right)(-\partial_a)\sum_{n_D=0}^{\infty}\cdots\sum_{n_1=0}^{\infty}e^{-a(n_1^2+n_2^2+\cdots+n_D^2)^{1/2}}. \tag{23}$$

The above D-dimensional sum can be expressed as a series of k-dimensional sums that start at $n_i=1$ instead of $n_i=0$, i.e., k-dimensional Dirichlet sums. The procedure is as follows: we choose k out of the D sums and let these k sums start at 1 instead of zero (while the remaining $D-k$ variables are not summed and set to zero). One is left with a k-dimensional Dirichlet sum $E_{\mathrm{Di}}^{(k)}$. There are $\binom{D}{k}$ ways to choose k among D sums so that the Neumann Casimir energy is given by

$$E_N=\sum_{k=1}^{D}\binom{D}{k}E_{\mathrm{Di}}^{(k)}, \tag{24}$$

where $E_{\mathrm{Di}}^{(k)}$ is the k-dimensional Dirichlet Casimir energy obtained by replacing D by k in (22). Equations (22) and (24) are our final expressions for the Dirichlet and Neumann Casimir energies, respectively.

In Table I we quote values of the Dirichlet and Neumann Casimir energies for D up to 6 calculated using (22) and (24). Note that the Neumann Casimir energy is negative. In Appendix B, we prove that it is negative for all values of D. The Neumann energy, plotted in Fig. 1, has a magnitude which increases with D. The Dirichlet case is considerably more complicated. Table I shows that the sign of the Dirichlet energy is negative for odd values of D, positive for even values of D and that its magnitude decreases rapidly. These features of the Dirichlet energy are valid for low values of D and are plotted in Fig. 2. The values quoted in Table I are in agreement with those calculated using the Epstein zeta function in Ref. 10 (values in Ref. 10 are quoted up to $D=5$). It is important that the numerical values agree because the Casimir force should be independent of the regularization scheme employed.

Calculations of the Dirichlet energy at higher values of D reveal that the oscillation of the sign and the rapid decrease in magnitude stops at the critical dimension of $D=36$. The Dirichlet energy decreases by 12 orders of magnitude from $D=1$ to $D=36$. To view a plot over such a large span requires the energy to be scaled. The magnitude of the Dirichlet energy E is less than 1 for the range we consider so that the function $-E/(|E|\log(|E|))$ is well-suited for plotting; it preserves the

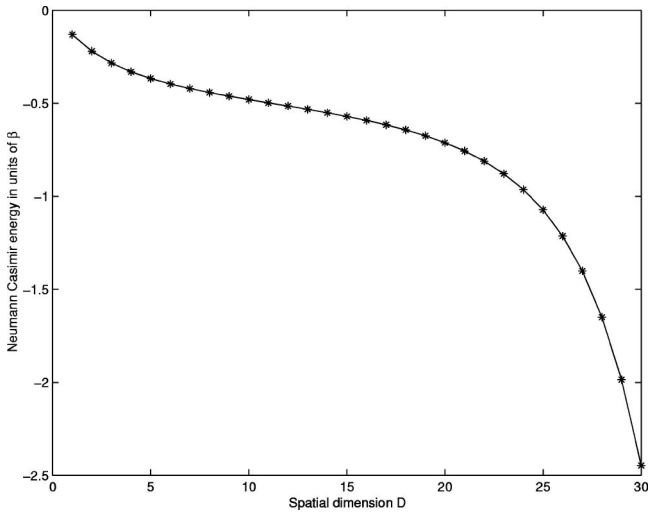

FIG. 1. Neumann Casimir energy as a function of the dimension D.

sign and scales the magnitude appropriately. A plot of this function up to $D=110$ is shown in Fig. 3. The distinctive features of Fig. 3 are the oscillating pattern which stops abruptly at the critical dimension of $D=36$ and the plateau region which emerges immediately afterwards. For $D\geqslant 36$, the energy remains negative and the magnitude increases, though slowly in the plateau region extending to approximately $D=80$. To obtain accurate values of the Casimir energy at higher values of D, numerical calculations must be performed with greater precision than 16-digit precision. We quote in Table II the Dirichlet energy from $D=10$ to $D=80$ for calculations performed using 16-digit, 24-digit and 50-digit precision. With 16-digit precision, numbers begin to show errors in the first significant digit at $D=42$ and the sign is wrong for the first time at $D=49$ (yields a positive instead of a negative sign). Note that in 16-digit precision oscillations in the sign resume in the region $D>49$. This is incorrect; higher-precision calculations show that the sign remains negative starting at $D=35$. The plot in Fig. 3 corresponds to numerical calculations done with 50-digit precision; for our plot up to $D=110$ this is more than enough precision. Note that the 24-digit and 50-digit precision calculations yield identical results for values quoted up to $D=80$ with four significant digits.

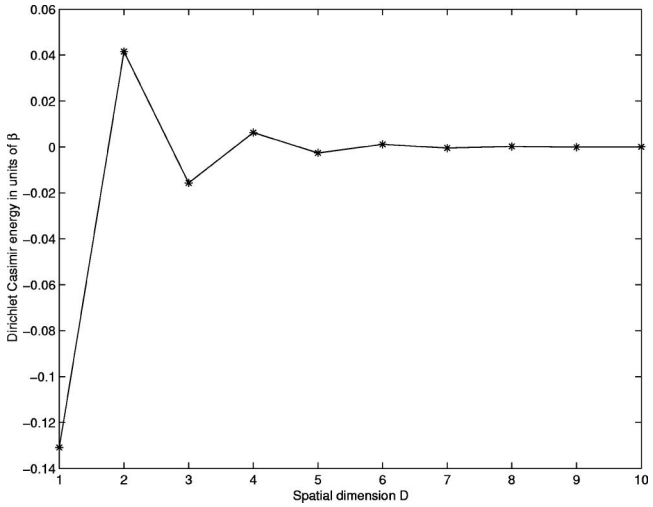

FIG. 2. Dirichlet Casimir energy at low values of D.

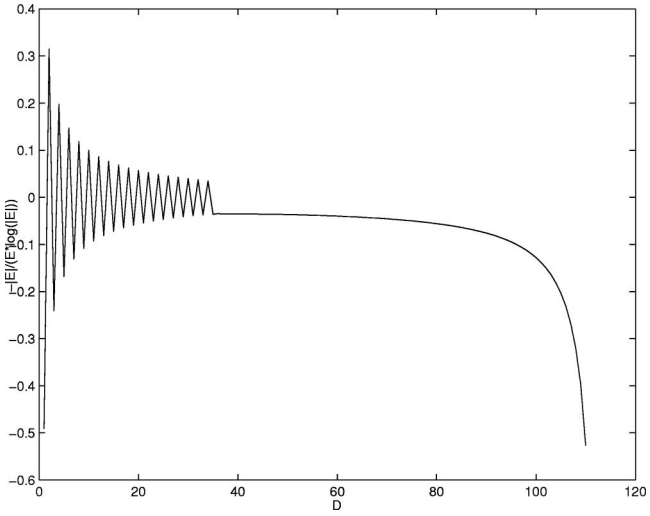

FIG. 3. Scaled Value of the Dirichlet Casimir energy E.

We now summarize our results in light of previous work on the Casimir energy of scalar fields confined to rectangular boundaries. One of our goals was mathematical: to develop a procedure for calculating (10), a multidimensional infinite sum regularized with an exponential cutoff. By repeated use of the Euler–Maclaurin formula and a series expansion for the infinite sum of the modified Bessel function $K_0(a\,n)$, we were able to isolate the divergent terms and extract the finite Casimir energy. In effect, we reduced (10) to a finite sum containing only the gamma and Riemann zeta functions, i.e., formula (22). Numerical calculations show that $D=36$ is a critical dimension, being the first even dimension with negative Dirichlet energy. Our work focused on the simple geometry of the hypercube whereas previous work[10–12] considered the more general rectangular case and employed Epstein zeta function regularization. Results for the rectangular case are expressed in terms of asymptotic formulas. In Ref. 11, the Dirichlet energy for a D-dimensional rectangle with p equal sides is conveniently expressed by a single integral with limits running from zero to infinity and integrand containing the elliptic θ function. In Refs. 10 and 11, numerical values are quoted for low values of D for the hypercube case and they are in agreement with our values. However, the finite formula (22) was not derived in Refs. 10 and 11 for the special case when all sides of the rectangle are equal.

It is worth noting that the original sum (9) is mathematically a special case of a more general class of multiple sums involving arbitrary exponents, i.e.,

$$M(s;a_1,\ldots,a_D;\alpha_1,\ldots,\alpha_D;c)=\sum_{n_1,\ldots,n_D=1}^{\infty}(a_1n_1^{\alpha_1}+\ldots+a_Dn_D^{\alpha_D}+c)^{-s}. \tag{25}$$

Using zeta function regularization, Elizalde[16] obtained explicit formulas for (25) expressed as an asymptotic expansion containing the Riemann and Hurwitz zeta functions. In contrast to the exponential cutoff method, zeta function regularization does not require the introduction of new terms like exponentials for convergence; one starts with a convergent sum like (25) valid for $\mathrm{Re}\,s>0$ big enough and then one makes an analytical (usually meromorphic) continuation to other values of s. For a detailed mathematical treatment of the zeta function regularization theorem and its applications to the Casimir energy, the reader is referred to Ref. 17.

TABLE II. Dirichlet Energy (in units of β) for Different Precision Calculations.

D	16-digit precision	24-digit precision	50-digit precision
10	4.438e−05	4.438e−05	4.438e−05
11	−2.035e−05	−2.035e−05	−2.035e−05
12	9.389e−06	9.389e−06	9.389e−06
13	−4.360e−06	−4.360e−06	−4.360e−06
14	2.034e−06	2.034e−06	2.034e−06
15	−9.538e−07	−9.538e−07	−9.538e−07
16	4.487e−07	4.487e−07	4.487e−07
17	−2.120e−07	−2.120e−07	−2.120e−07
18	1.004e−07	1.004e−07	1.004e−07
19	−4.770e−08	−4.770e−08	−4.770e−08
20	2.269e−08	2.269e−08	2.269e−08
21	−1.085e−08	−1.085e−08	−1.085e−08
22	5.177e−09	5.177e−09	5.177e−09
23	−2.488e−09	−2.488e−09	−2.488e−09
24	1.189e−09	1.189e−09	1.189e−09
25	−5.754e−10	−5.754e−10	−5.754e−10
26	2.741e−10	2.741e−10	2.741e−10
27	−1.345e−10	−1.345e−10	−1.345e−10
28	6.303e−11	6.303e−11	6.303e−11
29	−3.205e−11	−3.205e−11	−3.205e−11
30	1.416e−11	1.416e−11	1.416e−11
31	−8.027e−12	−8.028e−12	−8.028e−12
32	2.855e−12	2.856e−12	2.856e−12
33	−2.322e−12	−2.323e−12	−2.323e−12
34	2.635e−13	2.651e−13	2.651e−13
35	−9.364e−13	−9.389e−13	−9.389e−13
36	−3.207e−13	−3.169e−13	−3.169e−13
37	−5.916e−13	−5.975e−13	−5.975e−13
38	−4.621e−13	−4.516e−13	−4.516e−13
39	−5.104e−13	−5.255e−13	−5.255e−13
40	−5.293e−13	−5.041e−13	−5.041e−13
41	−5.079e−13	−5.414e−13	−5.414e−13
42	−6.230e−13	−5.631e−13	−5.631e−13
43	−5.106e−13	−6.071e−13	−6.071e−13
44	−7.900e−13	−6.572e−13	−6.572e−13
45	−4.473e−13	−7.244e−13	−7.244e−13
46	−1.239e−12	−8.075e−13	−8.075e−13
47	−1.927e−13	−9.126e−13	−9.126e−13
48	−2.230e−12	−1.044e−12	−1.044e−12
49	7.406e−13	−1.210e−12	−1.210e−12
50	−4.455e−12	−1.418e−12	−1.418e−12
51	4.079e−12	−1.683e−12	−1.683e−12
52	−1.250e−11	−2.020e−12	−2.020e−12
53	1.403e−11	−2.452e−12	−2.452e−12
54	−3.676e−11	−3.010e−12	−3.010e−12
55	5.400e−11	−3.735e−12	−3.735e−12
56	−1.040e−10	−4.685e−12	−4.685e−12
57	1.560e−10	−5.937e−12	−5.937e−12
58	−3.040e−10	−7.603e−12	−7.603e−12
59	5.219e−10	−9.834e−12	−9.834e−12
60	−9.100e−10	−1.285e−11	−1.285e−11
61	1.702e−09	−1.694e−11	−1.694e−11
62	−2.655e−09	−2.256e−11	−2.256e−11
63	4.438e−09	−3.033e−11	−3.033e−11
64	−7.300e−09	−4.115e−11	−4.115e−11
65	1.000e−08	−5.634e−11	−5.634e−11
66	−1.600e−08	−7.782e−11	−7.782e−11

TABLE II. (*Continued*.)

D	16-digit precision	24-digit precision	50-digit precision
67	1.300e−08	−1.084e−10	−1.084e−10
68	−3.700e−08	−1.524e−10	−1.524e−10
69	7.062e−08	−2.161e−10	−2.161e−10
70	−9.500e−08	−3.088e−10	−3.088e−10
71	1.100e−07	−4.451e−10	−4.451e−10
72	−7.000e−08	−6.467e−10	−6.467e−10
73	2.000e−07	−9.472e−10	−9.472e−10
74	−1.213e−07	−1.398e−09	−1.398e−09
75	−1.000e−06	−2.080e−09	−2.080e−09
76	5.000e−07	−3.119e−09	−3.119e−09
77	0.000e−01	−4.710e−09	−4.710e−09
78	0.000e−01	−7.168e−09	−7.168e−09
79	−2.000e−05	−1.099e−08	−1.099e−08
80	4.000e−05	−1.697e−08	−1.697e−08

ACKNOWLEDGMENTS

I wish to thank Professor Manu Paranjape and the Particle Physics group of the University of Montreal for their invitation to present a talk on this subject at the Montreal Joint High Energy Physics Seminars on March 28, 2002. I also wish to thank Dr. Paranjape for his useful comments and suggestions on the paper.

APPENDIX A

In applying the Euler–Maclaurin formula (11) to the sums in (10), we show that $f^{2p-1}(0)=0$ [except when applied to the last sum in (10)]. The most general form for the function f is a k-dimensional integral

$$f\equiv\int_0^\infty e^{-a(n_1^2+\cdots+n_q^2+x_1^2+\cdots+x_k^2)^{1/2}}dx_1\cdots dx_k=\int_0^\infty G\,dx_1\cdots dx_k, \tag{A1}$$

where $G\equiv e^{-a(n_1^2+\cdots+n_q^2+x_1^2+\cdots+x_k^2)^{1/2}}$. In f there are k continuous variables $x_1,\ldots,x_k$ which run from zero to infinity and there are q discrete variables $n_1,\ldots,n_q$ which run from one to infinity, i.e., f is being summed q times. Our goal is to show that the odd derivatives of G with respect to one of the discrete variables, say n_1, evaluated at $n_1=0$ is zero, i.e., that $G^{2p-1}(0)=0$. The first derivative of G with respect to n_1 is $G'=-a\,n_1\,G\,(n_1^2+\cdots+n_q^2+x_1^2+\cdots+x_k^2)^{-1/2}=-a\,n_1 G\,H$ where $H\equiv(n_1^2+\cdots+n_q^2+x_1^2+\cdots+x_k^2)^{-1/2}$. The derivative of H with respect to n_1 is $H'=-n_1 H^3$. Note that G' and H' are expressed in terms of G, H, a, and n_1. Any subsequent derivatives of G' will therefore contain terms of the form

$$a^i n_1^j H^l G, \tag{A2}$$

where i, j, and l are non-negative integers. Every additional derivative of G either increases or decreases j by one. Two consecutive derivatives will therefore produce an *even* change in j. The first derivative of G, G', has $j=1$ so that an additional even number of derivatives applied to G' leads to j being odd and positive. Therefore, odd derivatives of G cannot produce terms with $j=0$. As long as G and H^m do not diverge at $n_1=0$, the terms (A2) are zero at $n_1=0$. Clearly, G does not diverge at $n_1=0$. H^m does not diverge at $n_1=0$ as long as $q\geqslant 2$, i.e., after n_1 is set to zero the denominator in H^m is never zero if there exists at least one other discrete variable besides n_1. Therefore, if $q\geqslant 2$, the odd derivatives of G evaluated at $n_1=0$ are zero (and hence the odd derivatives of f evaluated at $n_1=0$ are zero).

If n_1 is the last discrete variable, i.e., $q=1$, then H^m evaluated at $n_1=0$ diverges at the point where the limits of integration are zero. The last sum is therefore calculated using a different method.

APPENDIX B

In this Appendix we show that the Neumann Casimir energy is negative for all values of D. The Neumann Casimir energy is given by (24), i.e.,

$$E_N=\sum_{k=1}^{D}\binom{D}{k}E_{\mathrm{Di}}^{(k)}, \tag{B1}$$

where $E_{\mathrm{Di}}^{(k)}$ is the k-dimensional Dirichlet Casimir energy obtained by replacing D by k in (22), i.e.,

$$E_{\mathrm{Di}}^{(k)}=\beta(-1)^k 2^{-k}\sum_{i=1}^{k}\binom{k-1}{i-1}\frac{(-2)^{i-1}\Gamma(i)\zeta(i+1)}{2^{2i-1}\pi^{i/2}\Gamma\left(\frac{i}{2}\right)}. \tag{B2}$$

Substituting (B2) into (B1) one obtains

$$\begin{aligned}E_N&=\beta\sum_{k=1}^{D}\sum_{i=1}^{k}\binom{D}{k}\binom{k-1}{i-1}(-1)^{k+i-1}2^{-i-k}\pi^{-i/2}\zeta(i+1)\frac{\Gamma(i)}{\Gamma\left(\frac{i}{2}\right)}\\&=-\beta\sum_{i=1}^{D}\pi^{-i/2}\zeta(i+1)\frac{\Gamma(i)2^{-2i}}{\Gamma\left(\frac{i}{2}\right)(i-1)!}\sum_{k=i}^{D}\binom{D}{k}(k-1)\cdots(k-i+1)\left(\frac{-1}{2}\right)^{k-i}\end{aligned} \tag{B3}$$

where we used the equality $(-1)^{k+i-1}=-(-1)^{k-i}$. Note the change in the limits of the double sum, i.e., k runs now from i to D and i runs now from 1 to D. This change does not affect the double sum because one obtains the same pairs (k,i). To show that E_N is negative all we need to show is that the sum over k in (B3) is positive. The sum over k is

$$\begin{aligned}&\sum_{k=i}^{D}\binom{D}{k}(k-1)\cdots(k-i+1)\left(\frac{-1}{2}\right)^{k-i}\\&\quad=\left(\frac{d}{dx}\right)^{i-1}\sum_{k=1}^{D}\binom{D}{k}x^{k-1}\Bigg|_{x=-1/2}\\&\quad=\left(\frac{d}{dx}\right)^{i-1}\left(\frac{(x+1)^D-1}{x}\right)\Bigg|_{x=-1/2}\\&\quad=\left(\frac{d}{dy}\right)^{i-1}\left(\frac{y^D-1}{y-1}\right)\Bigg|_{y=1/2}=\left(\frac{d}{dy}\right)^{i-1}(y^{D-1}+y^{D-2}+\cdots+1)\Bigg|_{y=1/2},\end{aligned} \tag{B4}$$

where $y=x+1$. Clearly derivatives of the polynomial $y^{D-1}+y^{D-2}+\cdots+1$ evaluated at $y=1/2$ are positive. We therefore have shown that the Neumann Casimir energy is negative for all values of D (assuming the dimension D are positive integers).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Proof of a mass singularity free property in high temperature QCD

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(Received 8 October 2002; accepted 12 November 2002)

It is shown that three series of diagrams entering the calculation of some hot QCD process, are mass (or collinear) singularity free, indeed. This generalizes a result which was recently established up to the third nontrivial order of (thermal) perturbation theory. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1536255]

I. INTRODUCTION

During the past 14 years, a considerable amount of work has been devoted to the study of quantized fields at high temperature and/or chemical potential[1] (high temperature, e.g, means higher than any bare or renormalized mass involved in the theory). The inherent non perturbative character of thermal quantum field theories has been recognized,[2] and naive perturbation theories accordingly reorganized. This is achieved by means of a resummation program (RP),[3] which, in the high temperature limit, must be used whenever one is calculating processes involving Green's functions with soft external/internal lines. The soft scale is defined to be on the order of gT where T is the temperature and g some relevant and small enough coupling constant, so as to *decide*, at least formally,[4] of two separate hard (on the order of T) and soft energy scales. The RP is given by effective Feynman rules, consisting of effective field propagators and n-points proper vertices, all at a given leading order of approximation which turns out to be g^2T^2, and is referred to as HTL (*hard thermal loops*). While HTL vertices are purely perturbative objects, effective propagators are not, as they give rise to pole residues and dispersion laws that do not admit perturbative series expansions in the coupling constant. In the course of practical calculations, effective propagators are easily handled, relying on analyticity properties and Cauchy's theorem.

Endowed with most beautiful symmetries, the RP is an effective theory that has led to a number of satisfying results,[1] but has also met two serious obstructions, emanating both from the infrared (IR) sector.[5,6]

Now, resummations can in general be defined a number of consistent, still different ways. In this article, we take advantage of a so-called perturbative resummation scheme, hereafter denoted PR for short, previously introduced[7] in the context of the first obstruction,[5] to address the problem of the soft real photon emission rate of thermal QCD.[6] This problem is the following. When use is made of the resummation program to calculate the soft real photon emission rate, out of a quark–gluon plasma in thermal equilibrium, the answer comes out affected with a collinear singularity. In the context of massless quantum field theories, it may be worth recalling that collinear singularities[8] manifest themselves as singularities of the angular integration, or equivalently, of the integration on the virtuality, $P^2=p_0^2-p^2$, and are thus also called mass singularities. Though of a different nature, mass/collinear singularities are regrouped with singularities of the integration on three-momenta $|\vec{p}|$, under the common spell of infrared singularities.

Several attempts to cure that IR disease have been proposed ever since,[9] which, though consistent at one loop order, encounter further important difficulties when extended to higher number of loop calculations.[10] Our present work is motivated by a recent study of the problem, projected out on a toy model, with the conclusion that things come out very different according to

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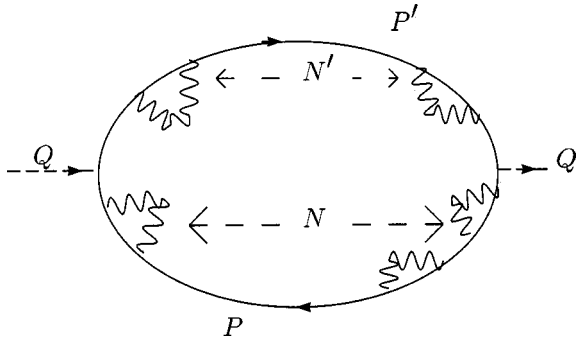

FIG. 1. A graph denoted by $(N,N';0)$, with $N(N')$ insertions of HTL self-energy along the $P(P')$-line, and two bare vertices $-ie\gamma_\mu$ of (2.4).

the resummation scheme in use, RP or PR.[11] Then, the case of interest, that is hot QCD, has been studied in its first three nontrivial perturbative orders: Again, no collinear singularity did show up in a PR resummation scheme. Moreover, both the questionable nature of that singularity,[12] and the very mechanism through which it comes about in an RP scheme, have been discovered thanks to an original comparison with the PR scheme.[13]

However encouraging, this first analysis of the QCD case has only been performed up to three loop order. In order to see if a PR resummation scheme has any chance to avoid that serious problem, it is crucial to extend the proofs of Ref. 13 to any loop order, and this sets in, we think, the strategical interest of the present analysis. By the same token, we note that the quite as much important collinear enhancement problem,[10] which comes out of the latter if one tries to solve the difficulty by introducing a so-called asymptotic thermal mass, m_∞,[9] is circumvented also.

The paper is organized as follows. Section II is a reminder of the collinear singularity problem under consideration, while introducing elements and notations necessary to the next sections. In Sec. III, topologies involving only bare vertices, with $N(N')$ HTL self-energy insertions along the $P(P')$ internal fermionic lines, denoted by $(N,N';0)$, are investigated in details. To do so, the matter of Ref. 7 is exploited so as to show that any $(N,N';0)$ imaginary part is mass singularity free, or msf for short. The same property can be established concerning the contributions attached to $(N,N';1)$ topologies, with one HTL-vertex correction included, and this is Sec. IV. The results of both preceding sections are obtained on the basis of purely technical calculations, but it seems almost impossible to proceed further along this line of approach: For contributions of type $(N,N';2)$, involving two HTL-vertex corrections, functions at play are so complicated that they preclude any control of the ensuing integrals. Remarkably enough, though, Sec. III is able to provide enough information so as to initiate an efficient, global and conclusive approach by induction. On the other hand, used right from the onset, an induction procedure does not appear to be, by itself, fully conclusive. This efficient articulation of Sec. III calculational approach, to an induction process is the matter of Sec. V. All three series of diagrams are definitely shown to possess mass/collinear singularity free imaginary parts, in the end.

Our conclusions are gathered in Sec. VI, whereas an Appendix displays the technical complexities encountered by a calculational approach to $(N,N';2)$-type diagrams.

Throughout the article, we work in the R/A real time formalism, which is based on retarded/advanced free field functions.[14] Also, we will be using the convention of upper case letters for quadrimomenta and lower case ones for their components, writing, for example, $P=(p_0,\vec{p})$. Our conventions for labeling internal and external momenta can be read off Fig. 1.

II. THE SOFT REAL PHOTON EMISSION RATE OF HOT QCD

It is convenient to work in the real time formalism with retarded/advanced (R/A) field functions, where a concise and elegant derivation of the famous collinear singularity can be achieved.[15] The soft real photon emission rate is essentially related to the imaginary part of the quantity

$\Pi_{RR^{\mu}_{\mu}}(Q)$, trace of the soft real photon polarization tensor, hereafter written as $\Pi_R(Q)$. At pure one loop order, this imaginary part is zero. However, when the photon is soft, this result is incomplete and the resummation program must be used instead of bare thermal perturbation theory. This amounts to keep the one loop diagram of ordinary perturbation theory, while replacing bare vertices and propagators by their HTL-dressed counterparts. In Feynman gauge, the resulting expression reads (with n_F, the Fermi–Dirac statistical factor, defined without absolute value),

$$\Pi_R(Q)=i\int \frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\ \ \mathrm{disc}$$
$$\times \mathrm{Tr}\{{}^{\star}S_R(P){}^{\star}\Gamma_{\mu}(P_R,Q_R,-P'_A){}^{\star}S_R(P')\ \ {}^{\star}\Gamma^{\mu}(P_R,Q_R,-P'_A)\}. \tag{2.1}$$

The discontinuity is to be taken in the energy variable p_0, by forming the difference of R and A-indiced P-dependent quantities. Within standard notations, the fermionic HTL self-energies, effective propagators and vertices are, respectively, given by

$$\Sigma_{\alpha}(P)=m^2\int \frac{\mathrm{d}\hat{K}}{4\pi}\frac{\not{\hat{K}}}{\hat{K}\cdot P+i\epsilon_{\alpha}},\qquad m^2=C_F\frac{g^2T^2}{8},\quad \alpha=R,A, \tag{2.2}$$

$${}^{\star}S_{\alpha}(P)=\frac{i}{\not{P}-\Sigma_{\alpha}(P)}, \tag{2.3}$$

$${}^{\star}\Gamma_{\mu}(P_{\alpha},Q_{\beta},P'_{\delta})=-ie(\gamma_{\mu}+\Gamma^{\mathrm{HTL}}_{\mu}(P_{\alpha},Q_{\beta},P'_{\delta})), \tag{2.4}$$

$$\Gamma^{\mathrm{HTL}}_{\mu}(P_{\alpha},Q_{\beta},P'_{\delta})=m^2\int \frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}_{\mu}\not{\hat{K}}}{(\hat{K}\cdot P+i\epsilon_{\alpha})(\hat{K}\cdot P'+i\epsilon_{\delta})}, \tag{2.5}$$

where $\hat{K}$ is the lightlike four vector $(1,\hat{k})$. In the sequel, it will reveal extremely useful to introduce a ''self-energy four vector'' (of course, not a genuine Lorentz-4-vector), by writing, instead of standard expression (2.2),

$$\Sigma_{\alpha}(P)\overset{(\mathrm{def})}{=}\mathbf{\Sigma}_{\alpha}(P)=\gamma\cdot\Sigma_{\alpha}(P)=\gamma_{\mu}\,m^2\int \frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}^{\mu}}{\hat{K}\cdot P+i\epsilon_{\alpha}}. \tag{2.6}$$

The RP basic steps entering the soft real photon emission rate calculation of thermal QCD are as follows. In view of (2.1) and (2.4), one gets three types of terms: A term with two bare vertices $\Gamma^{(0)}_{\mu}$, two terms with one bare vertex $\Gamma^{(0)}_{\mu}$ and the other $\Gamma^{\mathrm{HTL}}_{\mu}$, and a term with two HTL vertices $\Gamma^{\mathrm{HTL}}_{\mu}$. In QCD, the first three terms pose no problem: Terms of second type entail a collinear singularity which, thanks to a $U(1)$-Ward identity, cancels out with a similar singularity coming from the last term. A residual collinear singularity remains though, induced by the latter, and we therefore focus on that particular contribution including two vertices $\Gamma^{\mathrm{HTL}}_{\mu}$. One gets

$$\Pi_R(Q)=i\int \frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\ \mathrm{disc}$$
$$\times \mathrm{Tr}\{{}^{\star}S_R(P)\Gamma^{\mathrm{HTL}}{}_{\mu}(P_R,Q_R,-P'_A){}^{\star}S_R(P')\Gamma^{\mathrm{HTL}\mu}(P_R,Q_R,-P'_A)\}. \tag{2.7}$$

Then substituing the relevant QCD expressions, (2.2)–(2.5), one can write, with the convention $\epsilon_R=+\epsilon$,

$$\Pi_R(Q)=-ie^2m^4\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))$$
$$\times\int\frac{\mathrm{d}\hat{K}}{4\pi}\int\frac{\mathrm{d}\hat{K}'}{4\pi}\mathrm{disc}\frac{\hat{K}\cdot\hat{K}'\,\mathrm{Tr}(^\star S_R(P)\hat{\not{K}}^\star S_R(P')\hat{\not{K}}')}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}. \tag{2.8}$$

Because of the factor $\hat{K}\cdot\hat{K}'$ appearing in the numerator, there is no double pole but a simple collinear one at $\hat{K}=\hat{Q}$, whose residue just involes the $U(1)$ Ward identity alluded to above, that is,

$$m^2\int\frac{\mathrm{d}\hat{K}'}{4\pi}\frac{[\hat{Q}\cdot\hat{K}']\hat{\not{K}}'}{(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}=\frac{1}{q}[\Sigma_R(P)-\Sigma_R(P')] \tag{2.9}$$

and yields for $\Pi_R(Q)$ the expression

$$-i\frac{e^2m^2}{q}\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\mathrm{disc}\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{1}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}$$
$$\times\mathrm{Tr}(^\star S_R(P)\hat{\not{Q}}^\star S_R(P')[\Sigma_R(P)-\Sigma_R(P')]). \tag{2.10}$$

The discontinuity in p_0 can be taken, and an appropriate choice of the integration contour in the p_0-complex plane allows to write

$$\Pi_R(Q)=-2\frac{e^2m^2}{q}\int\frac{\mathrm{d}^4P}{(2\pi)^3}(1-2n_F(p_0))\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\delta(\hat{K}\cdot P)}{\hat{K}\cdot Q+i\epsilon}$$
$$\times\mathrm{Tr}(^\star S_A(P)\hat{\not{Q}}^\star S_R(P')[\Sigma_A(P)-\Sigma_R(P')]), \tag{2.11}$$

where a factor of 2 accounts for the two possibilities $\hat{K}=\hat{Q}$ and $\hat{K}'=\hat{Q}$, and where the relation $P'=P+Q$ has been used. The angular integration develops a collinear singularity at $\hat{K}=\hat{Q}$, and is responsible for that singular part of $\Pi_R(Q)$ which can be expressed as

$$-2\frac{e^2m^2}{q}\left(\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{1}{Q\cdot\hat{K}+i\epsilon}\right)\int\frac{\mathrm{d}^4P}{(2\pi)^3}\delta(P\cdot\hat{Q})(1-2n_F(p_0))$$
$$\times\mathrm{Tr}(^\star S_A(P)\hat{\not{Q}}^\star S_R(P')[\Sigma_A(P)-\Sigma_R(P')]). \tag{2.12}$$

The two terms involving one bare vertex γ_μ and a one loop HTL correction $\Gamma_\mu^{\mathrm{HTL}}$, entail a similar singularity which, when combined with (2.12), leave uncancelled the $\Pi_R(Q)$ singular contribution

$$-2i\frac{e^2m^2}{q^2}\left(\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{1}{\hat{Q}\cdot\hat{K}+i\epsilon}\right)\int\frac{\mathrm{d}^4P}{(2\pi)^3}\delta(P\cdot\hat{Q})(1-2n_F(p_0))$$
$$\times[\mathrm{Tr}(^\star S_A(P)\hat{\not{Q}})-\mathrm{Tr}(^\star S_R(P')\hat{\not{Q}})]. \tag{2.13}$$

It is this result which, in the literature[6] is most usually written in the form

$$\frac{C^{st}}{\varepsilon}\int \frac{d^4P}{(2\pi)^4}\delta(\hat{Q}\cdot P)(1-2n_F(p_0))\sum_{s=\pm 1,V=P,P'}\pi\left(1-s\frac{v_0}{v}\right)\beta_s(V), \tag{2.14}$$

where the overall $1/\varepsilon$ results of a dimensionally regularized evaluation of the factored out angular integration of (2.13), and where $\beta_s(V)$ is related to the effective fermionic propagator usual parametrization,[16]

$$^{\star}S_{R,A}(P)=i\sum_{s=\pm 1}\frac{\hat{\not{P}}_s}{D^s_{R,A}(p_0,\vec{p})} \tag{2.15}$$

with $\widehat{P_s}=(1,s\hat{p})$, the label s referring to the two dressed fermion propagating modes. Then one has

$$\frac{1}{D^s_{R,A}(V)}=\alpha_s(V)\mp i\pi\beta_s(V). \tag{2.16}$$

III. SELF-ENERGY DIAGRAMS, OF TYPE (N, N'; 0)

The imaginary part of a general term of type (N, N'; 0), depicted in Fig. 1, can be written

$$2e^2\int \frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\mathrm{Tr}\not{P}\,\mathrm{disc}_P\left(\frac{(\not{\Sigma}_R(P)\not{P})^N}{(P^2)^{N+1}}\right)\not{P}'\,\mathrm{disc}_{P'}\left(\frac{(\not{\Sigma}_R(P')\not{P}')^{N'}}{(P'^2)^{N'+1}}\right), \tag{3.1}$$

where the "self-energy four-vector" (2.2) has components,

$$\Sigma^0_\alpha(P)=\frac{m^2}{2p}\ln\left(\frac{p_0+p}{p_0-p}\right),\quad \Sigma^i_\alpha(P)=\left(\frac{\vec{p}^{\,i}}{p}\equiv\hat{p}^i\right)\frac{m^2}{p}Q_1\left(\frac{p_0}{p}\right) \tag{3.2}$$

with Q_1 standing for the Legendre function of the second kind

$$Q_1(x)=xQ_0(x)-1,\quad Q_0(x)=\frac{1}{2}\ln\left(\frac{x+1}{x-1}\right). \tag{3.3}$$

The label $\alpha=\{R,A\}$ denoting one of the two retarded or advanced specifications of the real time formalism being used, in the right-hand sides of (3.2) these specifications are encoded in the logarithmic determinations.

It is elementary to prove that one has

$$(\not{\Sigma}_R\not{P})^N=a_N\not{\Sigma}_R\not{P}+b_N\mathbb{I}_4, \tag{3.4}$$

where $\mathbb{I}_4$ is the 4×4 identity matrix, and the coefficients a_N and b_N are polynomials in the variables $P\cdot\Sigma_R(P)=m^2$ and $-P^2\Sigma_R^2$ whose formation laws can be found to be given by

$$a_N=(m^2)^{N-1}\sum_{j=0}^{j_M(N)}C_N^{2k+1}\left(1-\frac{P^2\Sigma^2}{m^4}\right)^k, \tag{3.5}$$

$$b_N=(m^2)^N\left(-\frac{P^2\Sigma^2}{m^4}\right)\sum_{j=0}^{j_M(N-1)}C_{N-1}^{2k+1}\left(1-\frac{P^2\Sigma^2}{m^4}\right)^k. \tag{3.6}$$

The C_N^{2k+1} are the binomial coefficients, and j_M, the maximal value of j can be expressed as

$$j_M(N)=\frac{(N-1-\Theta((-1)^N))}{2}, \tag{3.7}$$

where $\Theta(x)$ is the usual Heaviside step function.

Because of the decomposition law (3.4), four types of trace factors are found, that are

$$4P\cdot P', \tag{3.8}$$

$$8m^2P\cdot P'-4P^2P'\cdot\Sigma_R(P) \quad + \quad (P\leftrightarrow P'), \tag{3.9}$$

$$(3.9)(P\leftrightarrow P'), \tag{3.9'}$$

$$(2m^2)^2 4P\cdot P'-(8m^2P'^2P\cdot\Sigma_R(P')+(P\leftrightarrow P'))+4P^2P'^2\Sigma_R(P)\cdot\Sigma_R(P'). \tag{3.10}$$

We will therefore begin with proving that integrals of the generic type

$$\int \frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\mathrm{disc}_P\left(\frac{(-P^2\Sigma_R^2(P))^n}{(P^2+i\epsilon p_0)^{N+1}}\right)\mathrm{disc}_{P'}\left(\frac{(-P'^2\Sigma_R^2(P'))^{n'}}{(P'^2+i\epsilon p_0')^{N'+1}}\right) \tag{3.11}$$

are mass singularity free, or msf, for short. Then, since all of the trace factors (3.8)–(3.10) come into play as multiplicative functions of the integrands appearing in (3.11), we will check that they leave unaltered its msf character.

Integrals of generic type (3.11): With $y=\hat{q}\cdot\hat{p}$, where $\hat{q}$ and $\hat{p}$ are the unit three vectors in the directions of $\vec{q}$ and $\vec{p}$, respectively, integration on y can be traded for an integration on the virtuality $P'^2=-x'p'^2(y)$ by writing

$$\int_{[(P^2+2qp_0/2qp)]}^{1}\mathrm{d}y=\frac{(p_0+q)^2}{2qp}\int_0^{1-[(p_0+q)^2/(p+q)^2]}\frac{\mathrm{d}x'}{(1-x')^2}, \tag{3.12}$$

where the restrictions on y and x' come from the $\Theta(-P'^2)$ support of the distribution to be folded in (3.11). Now, particular to the thermal context,[17] so-called Lebesgue nonintegrable mass (and/or IR) singularities do arise, which cannot be taken care of by means of a standard dimensional regularization procedure, and require that an extra IR regulator be introduced.[18] This is achieved by proceeding to the following replacement:

$$\frac{1}{(P'^2+i\epsilon p_0')^{N'+1}}\mapsto\frac{1}{(P'^2-\mu^2+i\epsilon p_0')^{N'+1}} \tag{3.13}$$

that is also,

$$\delta^{(N')}(P'^2)\mapsto\delta^{(N')}(P'^2-\mu^2), \quad \frac{\mathbf{P}}{(P'^2)^{N'+1}}\mapsto\frac{\mathbf{P}}{(P'^2-\mu^2)^{N'+1}}, \tag{3.14}$$

where, as shown in Ref. 7, Appendix B, the auxiliary IR regulator μ^2, is chosen to be a small, negative parameter, to be taken to zero in the end. Gathering pieces, integration on y can eventually be written as

$$\frac{(m^4)^{n'}}{(-\mu^2+(p_0+q)^2)^{N'+1}}(-1)^{N'+1}\frac{(p_0+q)^2}{2qp}\int_0^{1-[(p_0+q)^2/(p+q)^2]}\frac{dx'}{(1-x')^2}$$
$$\times(1-x')^{N'+1}\,(x')^{n'}\Bigg\{\frac{\mathbf{P}}{(x'-\lambda')^{N'+1}}\mathrm{Im}\Bigg(-1+\frac{x'}{4}[\epsilon(p_0')\ln X']^2+\sqrt{1-x'}\;\;[\epsilon(p_0')\ln X']\Bigg)^{n'}$$
$$+\pi\epsilon(p_0')\frac{(-1)^{N'}}{N'!}\delta^{(N')}(x'-\lambda')\mathrm{Re}\Bigg(-1+\frac{x'}{4}[\epsilon(p_0')\ln X']^2+\sqrt{1-x'}\;\;[\epsilon(p_0')\ln X']\Bigg)^{n'}\Bigg\}, \tag{3.15}$$

where we have defined

$$\lambda' \overset{\text{def}}{=}\frac{-\mu^2}{-\mu^2+(p_0+q)^2},\quad X' \overset{\text{def}}{=}\frac{\epsilon(p_0')\sqrt{1-x'}+1}{\epsilon(p_0')\sqrt{1-x'}-1}, \tag{3.16}$$

and where $\epsilon(p_0')$ is the distribution "sign of p_0'." The remaining two integrations are on $p=|\vec{p}|$, and p_0, and the latter can be translated into an integration on the virtuality variable $x=-P^2/p^2$.

Now, if we consider the integral,

$$\int_{-p}^{+p}dp_0\;(1-2n_F(p_0))\mathrm{disc}_P\Bigg(\frac{(-P^2\Sigma_R^2(P))^n}{(P^2+i\epsilon p_0)^{N+1}}\Bigg) \tag{3.17}$$

which enters (3.11) as a building block:

$$(3.11)=\int\frac{p^2\,dp}{(2\pi)^3}\int_{-p}^{+p}dp_0(1-2n_F(p_0))\mathrm{disc}_P\Bigg(\frac{(-P^2\Sigma_R^2(P))^n}{(P^2+i\epsilon p_0)^{N+1}}\Bigg)\times(3.15), \tag{3.18}$$

we get for (3.17) the expression

$$\frac{1}{2}p\Bigg(\frac{-1}{p^2}\Bigg)^{N+1}(m^4)^n\sum_{\epsilon(p_0)=\pm1}\int_0^1\frac{dx}{\sqrt{1-x}}(1-2n_F(\epsilon(p_0)p\sqrt{1-x}))\;\;x^n\Bigg\{\frac{\mathbf{P}}{(x-\lambda)^{N+1}}$$
$$\times\mathrm{Im}\Bigg(-1+\frac{x}{4}[\epsilon(p_0)\ln X]^2+\sqrt{1-x}[\epsilon(p_0)\ln X]\Bigg)^n+\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)$$
$$\times\mathrm{Re}\Bigg(-1+\frac{x}{4}[\epsilon(p_0)\ln X]^2+\sqrt{1-x}[\epsilon(p_0)\ln X]\Bigg)^n\Bigg\} \tag{3.19}$$

with the definitions,

$$\lambda\;\overset{\text{def}}{=}\frac{-\mu^2}{p^2}\;,\quad X\overset{\text{def}}{=}\frac{\epsilon(p_0)\sqrt{1-x}+1}{\epsilon(p_0)\sqrt{1-x}-1}. \tag{3.20}$$

Eventually, an integration on p must be performed, which can symbolically be written as

$$\int_{p_m}^{p^\star}\frac{p^2\,dp}{(2\pi)^3}\;\times G(p,q,m). \tag{3.21}$$

An upper bound of integration on p is introduced so as to avoid the hard region $p=\mathcal{O}(T)$ (a customary choice consists in taking $p^\star$ on the order of an intermediate scale, say, on the order of $\sqrt{g}T$), whereas the lower boundary, p_m, not relevant to our concern here, will be discussed

elsewhere.[19] Note that in (3.15) and (3.19), we have written between brackets expressions of the form $[\epsilon(p_0)\ln X]$. This is because, irrespective of the sign of p_0, these expressions can be written with the help of a most efficient representation[7,11,13]

$$\epsilon(p_0)\ln X(p_0)=\epsilon(-p_0)\ln X(-p_0)=\lim_{\varepsilon=0}\frac{1}{\varepsilon}\left(1-\frac{x^{\varepsilon}e^{i\pi\varepsilon}}{(1+\sqrt{1-x})^{2\varepsilon}}\right). \tag{3.22}$$

Thanks to the x^{ε} factor, this representation is able to provide mass/collinear singularities with the same regularization as a dimensional one would operate, while being far simpler. It is also endowed with interesting regularity properties, since, in particular, the limit $\varepsilon=0$, commutes with both the sum over N and integral on p_0.[7]

Using (3.22), one obtains an expansion

$$\begin{aligned}&\left(-1+\frac{x}{4}[\epsilon(p_0)\ln X]^2+\sqrt{1-x}[\epsilon(p_0)\ln X]\right)^n\\&\quad=\sum_{i=0}^{n}C_n^i(-1)^i\left(\frac{x}{4}\right)^{n-i}\sum_{k=0}^{i}C_i^k(-1)^k\sqrt{1-x}^k\times\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C_{2(n-i)+k}^m\\&\quad\times(-1)^m\frac{e^{i\pi m\varepsilon}x^{m\varepsilon}}{(1+\sqrt{1-x})^{2m\varepsilon}}\end{aligned} \tag{3.23}$$

which can be put back into (3.19). Introducing the following family of functions:

$$\mathcal{F}_{k-1,m}(m\varepsilon,x)=\frac{\sqrt{1-x}^{k-1}}{(1+\sqrt{1-x})^{2m\varepsilon}}(1-2n_F(\epsilon(p_0)p\sqrt{1-x})) \tag{3.24}$$

we note that it is convenient to proceed as for the moving fermion damping rate problem,[7] keeping the leading order term of the statistical weight high temperature expansion

$$\mathcal{F}_{k-1,m}(m\varepsilon,x)=\frac{p\epsilon(p_0)}{2T}\frac{\sqrt{1-x}^k}{(1+\sqrt{1-x})^{2m\varepsilon}}(1+\mathcal{O}(g^2))\ \stackrel{\text{def}}{=}\frac{p\epsilon(p_0)}{2T}F_{km}(m\varepsilon,x)\ \ (1+\mathcal{O}(g^2)). \tag{3.25}$$

Though no way mandatory (the same results being obtained otherwise), this simplification is consistent with the leading order calculation we are concerned with, preserves the correct parity in p_0, and allows to recognize in F_{km} the same expression as defined in Ref. 7, Eq. (7.2). Whereof we know that (3.19) is rigorously integrable and nonintegrable mass singularity free: The expression (3.19) can effectively be written as

$$\begin{aligned}&\frac{1}{4T}p^2\left(\frac{-1}{p^2}\right)^{N+1}(m^4)^n\sum_{\epsilon(p_0)=\pm1}\sum_{i=0}^{n}C_n^i(-1)^i\left(\frac{1}{4}\right)^{n-i}\sum_{k=0}^{i}C_i^k(-1)^k\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C_{2(n-i)+k}^m\\&\quad\times(-1)^m\int_0^1\mathrm{d}x\ \ \left\{\mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon})}{(x-\lambda)^{N+1}}+\mathcal{R}e(e^{i\pi m\varepsilon})\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\right\}\\&\quad\times x^{2n-i+m\varepsilon}F_{km}(m\varepsilon,x)\end{aligned} \tag{3.26}$$

which is Eq. (D.3) of Ref. 7. Mass singularities of the *nonintegrable* type, $\mathcal{O}(1/\lambda)^k$, cancel out

$$\int_0^1 \mathrm{d}x \left\{ \mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon})}{(x-\lambda)^{N+1}} + \mathcal{R}e(e^{i\pi m\varepsilon})\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\right\} x^{2n-i+l+m\varepsilon}$$
$$= \frac{\sin(\pi m\varepsilon)}{2n-i+l-N+m\varepsilon} + \mathcal{O}(\lambda), \tag{3.27}$$

whereas *integrable* mass singularities obey arithmetical cancellation patterns thanks to the identities

$$\left\{\frac{\varepsilon^p}{\varepsilon^j}\right\} \times \sum_{m=0}^{j} C_j^m (-1)^m \ m^p = 0, \quad 1 \leqslant p \leqslant j-1, \tag{3.28}$$

$$\sum_{m=0}^{j} C_j^m (-1)^m m^j = (-1)^j j! \tag{3.29}$$

It can even be shown (Appendix D of Ref. 7) that (3.26) defines a mapping of $C\times C$ into C which is analytic for (ε, λ) choosen in the product of discs $D(0,1/2N)\times D(0,\frac{1}{2})$. The limit $\varepsilon=0,\lambda=0$ therefore exists and is independent of the sequence along which it is taken.

The entirely new feature is of course that the integrand appearing in (3.19), gets supplied, now, with the extra function (3.15). Considered as a function of x, the properties of (3.15) are therefore crucial in order to address the ensuing behavior of generic type (3.11) integrals, and this is what we now turn to examine in the particular case of positive energies, $p_0>0$, for the sake of a simpler illustration.

As made obvious by inspection, (3.15) is essentially relevant of the same structure as displayed by (3.19): Up to an overall multiplicative function of p_0,

$$\frac{(m^4)^{n'}}{(-\mu^2+(p_0+q)^2)^{N'+1}}\frac{(p_0+q)^2}{2qp} \tag{3.30}$$

the difference is entirely in the integration range

$$0 \leqslant x' \leqslant x'_M(x) \ \overset{\text{def}}{=} 1 - \frac{(p_0(x)+q)^2}{(p+q)^2} \tag{3.31}$$

instead of $0\leqslant x\leqslant 1$. Using the representation (3.22) for the expression $[\epsilon(p_0')\ln X']$, and the binomial expansion (3.23), the same functions as in (3.25) can effectively be identified, with accordingly, the same properties

$$F_{2(N'-1)+k',\, m'}(m'\varepsilon', x') = \frac{\sqrt{1-x'}^{2(N'-1)+k'}}{(1+\sqrt{1-x'})^{2m'\varepsilon'}}. \tag{3.32}$$

In the limit of $\lambda'=0$, we learn out of Ref. 7, that *Lebesgue non-integrable* mass singularities cancel out: Up to the overall multiplicative factor (3.30), one is left for the full expression (3.15), with an expression which still displays a finite series of Lebesgue integrable mass singularities:

$$\sum_{l'=0}^{\infty}\frac{1}{l'!}\sum_{i'=0}^{n'}C_{n'}^{i'}(-1)^{i'}\sum_{k'=0}^{i'}C_{i'}^{k'}(-1)^{k'}\left(g(p_0)\frac{(q+p)^2}{-P^2}\right)^{N'-(2n'-i'+l')}$$
$$\times\frac{1}{\varepsilon'^{2(n'-i')+k'}}\sum_{m'=0}^{m'=2(n'-i')+k'}C_{2(n'-i')+k'}^{m'}(-1)^{m'}\frac{\sin(\pi m'\varepsilon')}{N'-(2n'-i'+l')-m'\varepsilon'}$$
$$\times\left(g(p_0)\frac{(q+p)^2}{-P^2}\right)^{-m'\varepsilon'}F^{(l')}_{2(N'-1)+k',\,m'}(m'\varepsilon',0), \tag{3.33}$$

where we have defined the function,

$$g(p_0)\overset{\text{def}}{=}\frac{p+p_0}{p+p_0+2q}=1-\frac{2q}{2q+p}\left(1+\frac{p}{2q+p}\sqrt{1-x}\right)^{-1}. \tag{3.34}$$

Type $\mathcal{O}(\varepsilon'^{-r})$-mass singularities are thus controlled by the finite sum,

$$\frac{1}{\varepsilon'^{2(n'-i')+k'}}\sum_{m'=0}^{m'=2(n'-i')+k'}C_{2(n'-i')+k'}^{m'}(-1)^{m'}\left(\frac{x}{g(p_0)}\right)^{m'\varepsilon'}$$
$$\times\frac{\sin(\pi m'\varepsilon')}{N'-(2n'-i'+l')-m'\varepsilon'}\times\left(\left(\frac{p}{p+q}\right)^2\right)^{m'\varepsilon'}\times F^{(l')}_{2(N'-1)+k',m'}(m'\varepsilon',0), \tag{3.35}$$

where the last term appearing in the right-hand side of (3.35), stands for the l'th-order derivative of the function (3.32), taken at $x'=0$. This means that, in deriving (3.35), we have interchanged the sum on l', in the Taylor expansion of (3.32),

$$F_{2(N'-1)+k',\,m'}(m'\varepsilon',x')=\sum_{l'=0}^{\infty}\frac{(x')^{l'}}{l'!}F^{(l')}_{2(N'-1)+k',\,m'}(m'\varepsilon',0) \tag{3.36}$$

with the integration on x'. Such a permutation is proven to be licit in Ref. 7, Appendix C (note that in the present situation, this permutation is the more licit, as the integration range (3.31) lies within the unit convergence radius of the series expansion for the functions $F_{2(N'-1)+k',\,m'}(m'\varepsilon',x')$). Likewise, it is demonstrated [Eqs. (C.7)–(C.9), (C.12) of Ref. 7] that each of the coefficients $F^{(l')}_{2(N'-1)+k',\,m'}(m'\varepsilon',0)$ admits a Taylor series expansion in the parameter $m'\varepsilon'$. Now, whatever N' and $2n'-i'+l'$, the same property holds clearly true, for any of the other three factors of (3.35) which, with $F^{(l')}_{2(N'-1)+k',\,m'}(m'\varepsilon',0)$, enter the sum over m'.

Then, forming the Cauchy's product of their $m'\varepsilon'$-Taylor series expansions, and relying on the set of arithmetical identities (3.28) and (3.29), we conclude that the $\varepsilon'=0$ limit of (3.35) is msf, and reduces to a polynomial of degree $2(n'-i')+k'$ in the variable $\ln(x/g(p_0))$,

$$\lim_{\varepsilon'=0}(3.35)=(-1)^{2(n'-i')+k'}\sum_{j'=0}^{2(n'-i')+k'}C^{j'}_{2(n'-i')+k'}H^{(2(n'-i')+k'-j')}(0)\,\ln^{j'}\left(\frac{x}{g(p_0)}\right), \tag{3.37}$$

where $H^{(2(n'-i')+k'-j')}(0)$, a pure (real) number, is a shorthand notation for the derivative of order $(2(n'-i')+k'-j')$, taken at $m'\varepsilon'=0$, of the product

$$\frac{\sin(\pi m'\varepsilon')}{N'-(2n'-i'+l')-m'\varepsilon'}\times\left(\left(\frac{p}{p+q}\right)^2\right)^{m'\varepsilon'}\times F^{(l')}_{2(N'-1)+k',m'}(m'\varepsilon',0). \tag{3.38}$$

Gathering all pieces, the whole expression (3.15) can eventually be written as

$$-\frac{(m^4)^{n'}}{(-\mu^2+(p_0+q)^2)^{N'+1}}\frac{(p_0+q)^2}{2qp}\times\sum_{l'=0}^{\infty}\frac{(-1)^{l'}}{l'!}\sum_{i'=0}^{n'}C_{n'}^{i'}\left(g(p_0)\frac{(q+p)^2}{+P^2}\right)^{N'-(2n'-i'+l')}$$
$$\times\sum_{k'=0}^{i'}C_{i'}^{k'}\sum_{j'=0}^{2(n'-i')+k'}H^{(2(n'-i')+k'-j')}(0)\ \ln^{j'}\left(\frac{x}{g(p_0)}\right). \tag{3.39}$$

Getting back to (3.18), one is now in a position so as to estimate the incidence on (3.19) of any of the extra x-dependences which are introduced by (3.39).

For positive (as well as negative) energies, the auxiliary IR regulator $-\mu^2$ can safely be taken to zero in the prefactor of (3.39), and the latter expanded as

$$\frac{-(m^4)^{n'}}{(-\mu^2+(p_0+q)^2)^{N'+1}}\ \frac{(p_0+q)^2}{2qp}=-\frac{(m^4)^{n'}}{2pq}\sum_{r=0}^{\infty}\mathcal{C}_k(N',p,q)\ \left(\sqrt{1-x}\right)^r, \tag{3.40}$$

where it is easy to check that the existence of (3.40) does not depend on the relative magnitude of p and q, contrarily, of course, to the explicit form of the coefficients $\mathcal{C}_k(N',p,q)$. The same property is obviously shared by the function

$$g(p_0)^{N'-(2n'-i'+l')}=\left(1-\left(\frac{2q}{2q+p}\right)\frac{1}{1+\dfrac{p}{2q+p}\sqrt{1-x}}\right)^{N'-(2n'-i'+l')}. \tag{3.41}$$

Eventually, such is also the case of factors like

$$\left(\ln\frac{1}{g(p_0)}\right)^{r'}=(-1)^{r'}\ln^{r'}\left(1-\left(\frac{2q}{2q+p}\right)\frac{1}{1+\dfrac{p}{2q+p}\sqrt{1-x}}\right). \tag{3.42}$$

The product of terms (3.40)–(3.42) can therefore be written as a series in the variable $\sqrt{1-x}$, whose general term, no matters how complicated, just redefines the integer power k of the function $F_{km}(m\varepsilon,x)$ introduced in (3.25). The properties of (3.25) are thus left the same, and the extra x-dependences introduced through (3.40)–(3.42) preserve the msf character of (3.19).

The extra factors of (3.39),

$$\left(\frac{(q+p)^2}{P^2}\right)^{N'-(2n'-i'+l')} \tag{3.43}$$

redefine the power $N+1$ of the scalar propagator appearing in (3.11), according to the replacement

$$\frac{1}{(P^2-\mu^2+i\epsilon p_0)^{N+1}}\ \mapsto\ \frac{1}{(P^2-\mu^2+i\epsilon p_0)^{N+1+N'-(2n'-i'+l')}}.$$

This splits into the distributions

$$\delta^{(N+N'-(2n'-i'+l'))}(P^2-\mu^2)\ ,\quad\frac{\mathbf{P}}{(P^2-\mu^2)^{N+1+N'-(2n'-i'+l')}}$$

which, with respect to the previous power of $N+1$, require extra differentiability of the x dependences they act upon. Now, this condition is clearly met thanks both to a full identification of the new x dependences brought about by (3.39), and to the introduction of the auxiliary IR regulator

$\lambda=-\mu^2/p^2$ of (3.20). Since, at $N\geqslant 2n-i+l+1$ (which is just the condition for the occurrence of mass singularities), the overall compensation of mass singularities does not depend on the relative magnitude of the integers $N+1$ and $2n-i+l$, in mass singularity compensation patterns of the generic type,[7]

$$\lim_{\varepsilon,\lambda=0}\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C^m_{2(n-i)+k}(-1)^m F^{(l)}_{km}(m\varepsilon,0)\int_0^1 dx\ \left\{\mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon})}{(x-\lambda)^{N+1}}\right.$$
$$\left.+\mathcal{R}e(e^{i\pi m\varepsilon})\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\right\}x^{2n-i+l+m\varepsilon}\ =\mathcal{O}(1) \tag{3.44}$$

we deduce that the same mass singularity compensations hold true of (3.44), with $N+1+N'-(2n'-i'+l')$ replacing $N+1$, and that extra factors of type (3.43) are msf preserving.

Eventually, the last extra x-dependences introduced into (3.18) by (3.39), are the functions

$$\ln^{r'}x\ ,\quad r'\in\mathbb{N}\ ,\quad 0\leqslant r'\leqslant 2(n'-i')+k'. \tag{3.45}$$

Previous patterns (3.44) are now taken to the form

$$\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C^m_{2(n-i)+k}(-1)^m F^{(l)}_{km}(m\varepsilon,0)\int_0^1 dx\quad\left\{\mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon})}{(x-\lambda)^{N+1}}\right.$$
$$\left.+\mathcal{R}e(e^{i\pi m\varepsilon})\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\right\}x^{2n-i+l+m\varepsilon}\ln^{r'}x. \tag{3.46}$$

As in (3.22), we introduce the representation

$$\ln^{r'}x=\lim_{\hat\varepsilon=0}\frac{(-1)^{r'}}{\hat\varepsilon^{r'}}\sum_{s'=0}^{r'}C^{s'}_{r'}(-1)^{s'}(x)^{s'\hat\varepsilon} \tag{3.47}$$

and interchange the sum on s', which is finite, with the integration on x. In the limit $\lambda=0$, we get first the expression,[7]

$$\frac{(-1)^{r'}}{\hat\varepsilon^{r'}}\sum_{s'=0}^{r'}C^{s'}_{r'}(-1)^{s'}\frac{-\sin(\pi m\varepsilon)}{N-(2n-i+l)+m\varepsilon+s'\hat\varepsilon}\ +\mathcal{O}(\lambda). \tag{3.48}$$

At $N\geqslant 2n-i+l+1$, such a factor admits an $s'\hat\varepsilon$-Taylor series expansion, so that relying on arithmetical identities (3.28) and (3.29), the $\hat\varepsilon=0$-limit of (3.48) is readily obtained to be given by

$$\left(\frac{\sin(\pi m\varepsilon)}{N-(2n-i+l)+m\varepsilon+s'\hat\varepsilon}\right)^{(r')}_{|_{s'\hat\varepsilon\ =0}}=(-1)^{r'}r'!\,\frac{\sin(\pi m\varepsilon)}{(N-(2n-i+l)+m\varepsilon)^{r'+1}}. \tag{3.49}$$

At its turn, (3.49) admits itself a Taylor series expansion in the variable $m\varepsilon$. Since the whole expression (3.46) factors out a global factor of

$$\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C^m_{2(n-i)+k}\,(-1)^m F^{(l)}_{km}(m\varepsilon,0) \tag{3.50}$$

the $\varepsilon=0$-limit of (3.46) is finite in view, again, of arithmetical identities (3.28) and (3.29), and extra factors of type (3.45) are msf-preserving too.

We thus reach the conclusion that generic type (3.11) integrals are msf. Now, getting back to the mass singularity issue of $(N,N';0)$ self-energy diagrams, it is immediate to realize that all of

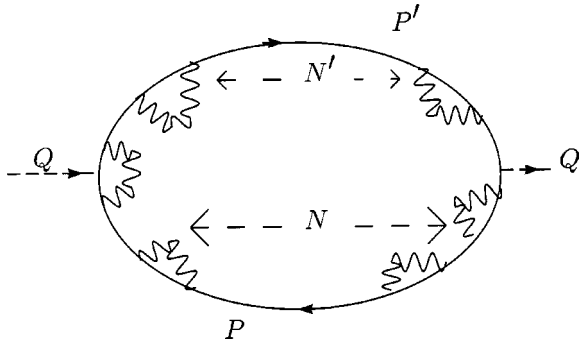

FIG. 2. A graph denoted by $(N,N';1)$, with $N(N')$ insertions of HTL self-energy along the $P(P')$-line, one bare vertex $-ie\gamma_\mu$, and one HTL vertex correction (2.5).

the trace factors (3.8)–(3.10) only involve $x(x')$, $\sqrt{1-x}(\sqrt{1-x'})$, and $[\epsilon(p_0)\ln X]([\epsilon(p_0')\ln X'])$ msf-preserving dependences (some of them will be treated in full details in next Sec. V), as, for example, the most involved piece of (3.10),

$$4P^2P'^2\Sigma_R(P)\cdot\Sigma_R(P')=4p(p_0+q)\frac{xx'}{1-x'}(m^2)^2Q_0\left(\frac{p_0}{p}\right)\ \sqrt{1-x'}\ Q_0\left(\frac{p_0'}{p'}\right)$$
$$-4p\frac{xx'}{1-x'}(m^2)^2Q_1\left(\frac{p_0}{p}\right)$$
$$\times Q_1\left(\frac{p_0'}{p'}\right)\left\{p(1-x')+\frac{q}{2}\left(\frac{p}{q}+\frac{q}{p}\right)x'+\left(q\sqrt{1-x}-\frac{p}{2}x\right)\right\}.$$

Since the same analysis can be carried through in the case of negative energies, we can conclude that $(N,N';0)$ self-energy diagrams have collinear singularity free imaginary parts.

IV. DIAGRAMS OF TYPE $(N, N'; 1)$, WITH ONE EFFECTIVE VERTEX

Using (3.4), the trace factors associated with diagrams of type $(N,\ N';\ 1)$, depicted in Fig. 2, are easily obtained to be

$$8\,(\hat{K}\cdot P)(\hat{K}\cdot P'), \tag{4.1}$$

$$16m^2\ \ (\hat{K}\cdot P)(\hat{K}\cdot P')-8P^2\hat{K}\cdot P'\hat{K}\cdot\Sigma_R(P), \tag{4.2}$$

$$(4.2)(P\leftrightarrow P'), \tag{4.2'}$$

$$8(2m^2)^2\ \ (\hat{K}\cdot P)(\hat{K}\cdot P')-8(2m^2)(P^2\hat{K}\cdot P'\hat{K}\cdot\Sigma_R(P)+(P\leftrightarrow P'))$$
$$+8P^2P'^2\hat{K}\cdot\Sigma_R(P)\hat{K}\cdot\Sigma_R(P'). \tag{4.3}$$

In $(N,\ N';1)$-type diagrams, each of the trace factors (4.1)–(4.3) must be integrated over $\hat{K}$ with the "measure,"

$$m^2\int\frac{d\hat{K}}{4\pi}\frac{1}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}. \tag{4.4}$$

Then the above trace factors yield, respectively,

$$8m^2, \tag{4.5}$$

$$16m^4 - 8P^2\Sigma_R^2(P), \tag{4.6}$$

$$(4.6)(P \leftrightarrow P'), \tag{4.6'}$$

$$8m^2\left((2m^2)^2 - 2(P^2\Sigma_R^2(P) + (P \to P')) + P^2P'^2 \int \frac{d\hat{K}}{4\pi} \frac{\hat{K}\cdot\Sigma_R(P)}{\hat{K}\cdot P + i\epsilon} \frac{\hat{K}\cdot\Sigma_R(P')}{\hat{K}\cdot P' + i\epsilon} \right). \tag{4.7}$$

One may observe that the trace factors of $(N,N';0)$ diagrams are more involved than those attached to diagrams of type $(N,\ N';\ 1)$. In particular, it should be clear that at the exception of the last term of (4.7), all of the factors appearing in (4.5)–(4.7) will preserve the msf character of type (3.11) integrals.

That is, the whole mass singularity issue of $(N,\ N';1)$ contributions is entirely in the incidence, upon generic type (3.11) integrals, of the very function

$$\int \frac{d\hat{K}}{4\pi} \frac{\hat{K}\cdot\Sigma_R(P)}{\hat{K}\cdot P + i\epsilon} \frac{\hat{K}\cdot\Sigma_R(P')}{\hat{K}\cdot P' + i\epsilon}. \tag{4.8}$$

As it stands, (4.8) can be calculated with the help of the three angular identities,

$$\int \frac{d\hat{K}}{4\pi} \frac{\hat{K}^0\hat{K}^0}{(\hat{K}\cdot R + i\epsilon)^2} = \frac{1}{R^2 + i\epsilon r_0}, \tag{4.9}$$

$$\int \frac{d\hat{K}}{4\pi} \frac{\hat{K}^0\hat{K}^i}{(\hat{K}\cdot R + i\epsilon)^2} = \hat{r}^i\left(\frac{-1}{2r^2} \ln\left(\frac{r_0 + r}{r_0 - r} \right) + \frac{r_0}{r} \frac{1}{R^2 + i\epsilon r_0} \right), \tag{4.10}$$

$$\int \frac{d\hat{K}}{4\pi} \frac{\hat{K}^i\hat{K}^j}{(\hat{K}\cdot R + i\epsilon)^2} = -\frac{g^{ij}}{r^2} Q_1\left(\frac{r_0}{r} \right) - \hat{r}^i\hat{r}^j\left(\frac{3}{r^2} Q_1\left(\frac{r_0}{r} \right) - \frac{1}{R^2 + i\epsilon r_0} \right), \tag{4.11}$$

where a Feynman parameter, s, has been introduced so as to rewrite (4.8) as

$$\Sigma_\mu(P)\Sigma(P')_\nu \int_0^1 ds \int \frac{d\hat{K}}{4\pi} \frac{\hat{K}^\mu\hat{K}^\nu}{(\hat{K}\cdot R(s) + i\epsilon)^2} \tag{4.12}$$

with

$$R(s) = P + sQ. \tag{4.13}$$

At this point, and though not immediately relevant to our concern, the following remark may be in order.

Some years ago, the use of a Feynman parametrization in thermal quantum field theories has been questioned.[20] Feynman parametrization was suspected delicate, using, for example, bare propagator determinations different from the usual $+i\epsilon$-Feynman's one. Of course, passing from (4.8) to (4.12), this situation is not encountered, but the difficulty may come about, in particular in a real time formalism using retarded/advanced propagator prescriptions. The solution to this difficulty has been given in Ref. 21. Later on, it has even been suggested that using a Feynman parametrization in a hot quantum field context could lead to nongauge invariant results.[22] This latter statement however was erroneous, based on incorrect calculations, and indeed, taking the

modification of Ref. 21 into account, it must be stated that there is definitely no problem in dealing with Feynman parametrizations in nonzero temperature quantum field theories.

Getting back to (4.8), a shortcut to its calculation consists in writing,

$$\frac{\hat{K}\cdot\Sigma_R(P)}{\hat{K}\cdot P+i\epsilon}=\frac{m^2}{p^2}Q_1\left(\frac{p_0}{p}\right)+\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\frac{1}{\hat{K}\cdot P+i\epsilon} \tag{4.14}$$

from which a remarkable relation may be deduced,

$$m^2\int\frac{d\hat{K}}{4\pi}\quad\frac{\hat{K}\cdot\Sigma_R(P)}{\hat{K}\cdot P+i\epsilon}=\Sigma_R^2(P) \tag{4.15}$$

and likewise, in obvious notations,

$$\begin{aligned}(4.8)=&\frac{m^2}{p^2}Q_1\frac{m^2}{p'^2}Q_1'+\left(\frac{m^2}{p^2}Q_1\frac{m^2}{p'}\left(\frac{p_0'}{p'}-\frac{1}{2}\frac{P'^2}{p'^2}\ln X'\right)\frac{1}{2p'}\ln X'++(P\leftrightarrow P')\right)\\&+\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\ \frac{m^2}{p'}\left(\frac{p_0'}{p'}-\frac{1}{2}\frac{P'^2}{p'^2}\ln X'\right)\ \frac{1}{2Q\cdot P+i\epsilon q_0}\ln\frac{P'^2+i\epsilon p_0'}{P^2+i\epsilon p_0},\end{aligned} \tag{4.16}$$

where identity (4.9) only, has been used. Noting that $2Q\cdot P=P'^2-P^2$, one recovers in (4.16) the full original symmetry of (4.8) under the exchange $P\leftrightarrow P'$. Since the terms appearing in (4.16) just redefine the integer numbers $k(k')$, $n(n')$ and $2(n-i)+k$ $(2(n'-i')+k')$, they leave totally unaffected the msf structures of Sec. III. The only new feature is the factor $(2Q\cdot P)^{-1}\ln P'^2/P^2$. As observed in Ref. 13 for the topology (1, 1; 1), this factor is reminiscent of the collinear singularity plaguing $(N,N';1)$ diagrams at the light cone, when an RP treatment of the problem is adopted.

In the end, recalling that (4.8) comes out affected with a multiplicative factor of $8m^2P^2P'^2$, this means that expressions

$$\begin{aligned}\int\frac{d^4P}{(2\pi)^4}(1-2n_F(p_0))&\left(\frac{(-P'^2\Sigma_R^2(P'))^{n'}}{(P'^2+i\epsilon p_0')^{N'}}\right)\\&\times\mathrm{disc}\left(\frac{(-P^2\Sigma_R^2(P))^n}{(P^2+i\epsilon p_0)^N}\right)\quad\int\frac{d\hat{K}}{4\pi}\ \frac{\hat{K}\cdot\Sigma_R(P)}{\hat{K}\cdot P+i\epsilon}\ \frac{\hat{K}\cdot\Sigma_R(P')}{\hat{K}\cdot P'+i\epsilon}\end{aligned} \tag{4.17}$$

do have msf imaginary parts, if integrals

$$\int\frac{d^4P}{(2\pi)^4}(1-2n_F(p_0))\frac{(-P'^2\Sigma_R^2(P'))^{n'}}{(P'^2+i\epsilon p_0')^{N'}}\mathrm{disc}\frac{(-P^2\Sigma_R^2(P))^n}{(P^2+i\epsilon p_0)^N}\ \frac{1}{2Q\cdot P+i\epsilon q_0}\ln\frac{P'^2+i\epsilon p_0'}{P^2+i\epsilon p_0} \tag{4.18}$$

have msf imaginary parts either. That it is so can be demonstrated quite easily. However, a byproduct of the next section will provide this statement with a systematic derivation, so that we can here content ourselves with a heuristic, still instructive argument.

The potential collinear singularity due to the HTL vertex comes from the factor $(1/2Q\cdot P)$, as $Q\cdot P$ reaches zero. For example, in the RP calculation of Sec. II, we learn out of Eqs. (2.12)–(2.14), that the collinear singularity expression effectively involves a $\delta(P\cdot Q)$ constraint. Now, as $Q\cdot P$ tends to zero, one has indeed

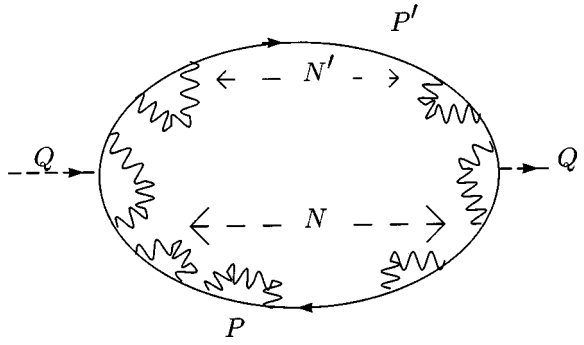

FIG. 3. A graph denoted by $(N,N';2)$, with $N(N')$ insertions of HTL self-energy along the $P(P')$-line, and two HTL vertex corrections (2.5).

$$\frac{1}{2Q\cdot P+i\epsilon q_0}\ln\frac{P^2+2Q\cdot P+i\epsilon p_0'}{P^2+i\epsilon p_0}\simeq\frac{1}{P^2+i\epsilon p_0} \tag{4.19}$$

and this light cone potentially singular behavior obviously gets mixed with partial effective propagator $S_R^{(N)}(P)$ own light cone potentially singular behavior,

$$P^2S_R^{(N)}(P)=P^2\frac{i\not{P}(\Sigma_R(P)\not{P})^N}{(P^2+i\epsilon p_0)^{N+1}} \tag{4.20}$$

the whole just boiling down to a simple shift of power,

$$P^2\frac{1}{(P^2+i\epsilon p_0)^{N+1}}\ \mapsto\ P^2\frac{1}{(P^2+i\epsilon p_0)^{N+2}}.$$

From Sec. III, Eqs. (3.43)–(3.44), we know that the overall detailed balance compensation of mass singularities is preserved by such a shift, and this is how we can see that $(N,N';1)$ contributions to the soft real photon emission rate are msf.

This generalizes to any $(N,N';1)$ contribution, the observation first made in Ref. 13, Sec. 5, for the diagram (1, 1; 1), and simply enforces the conclusion we drew then, that HTL vertex collinear singularities should not be desentangled from partial effective propagator mass singularities, as they all mix up into structural patterns which grant their overall compensations. In an RP resummation scheme, unfortunately, a dissociation of Eqs. (4.19) and (4.20) potentially singular behaviors is achieved right from the onset. There, in effect, the sum over N being performed before the integration on p_0, partial effective propagators $S_R^{(N)}(P)$, get replaced by full effective ones, ${}^\star S_R(P)$, whose poles, contrarily to $S_R^{(N)}(P)$-poles, are no longer lightlike at $P^2\simeq 0$, but timelike, at $p_0=\pm\omega_s(p)$[1]. It results that the light cone singular behavior of (4.19) remains isolated, with no other singular behavior to cancel with.

V. TWO EFFECTIVE VERTEX DIAGRAMS $(N, N'; 2)$

We now turn to the analysis of $(N, N';2)$ topologies depicted in Fig. 3, which are the most important to consider, the famous collinear problem of hot QCD being induced by these double effective vertex insertions.

In Ref. 13, it was shown that (1, 0; 2) is singularity free. While an encouraging result, it would certainly be preposterous to take it for granted that the property trivially extends to any $(N, N';2)$ diagram, and in our opinion, this is why the present analysis had to be undertaken.

The contribution to $\Pi_R(Q)$ of a diagram $(N, N';2)$ reads

$$\Pi_R^{(N,N';2)}(Q)=ie^2m^4\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\int\frac{\mathrm{d}\hat{K}}{4\pi}\int\frac{\mathrm{d}\hat{K}'}{4\pi}\ \hat{K}\cdot\hat{K}'$$
$$\times\,\mathrm{disc}\quad\mathrm{Tr}\left(\not{P}\frac{(\Sigma_R(P)\not{P})^N}{(P^2+i\epsilon p_0)^{N+1}}\hat{\not{K}}\not{P}'\frac{(\Sigma_R(P')\not{P}')^{N'}}{(P'^2+i\epsilon p_0')^{N'+1}}\hat{\not{K}}'\right)$$
$$\times\frac{1}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}. \tag{5.1}$$

Expanding the $(\Sigma_R(P)\not{P})^N$ factors as in (3.4), four types of traces come about,

$$4(2\hat{K}\cdot P\hat{K}'\cdot P'-\hat{K}\cdot\hat{K}'P\cdot P'), \tag{5.2}$$

$$8m^2(2\hat{K}\cdot P\hat{K}'\cdot P'-\hat{K}\cdot\hat{K}'P\cdot P')-4P^2(2\hat{K}\cdot\Sigma\hat{K}'\cdot P'-\hat{K}\cdot\hat{K}'P'\cdot\Sigma), \tag{5.3}$$

$$8m^2(2\hat{K}\cdot P\hat{K}'\cdot P'-\hat{K}\cdot\hat{K}'P\cdot P')-4P'^2(2\hat{K}\cdot\Sigma'\hat{K}'\cdot P-\hat{K}\cdot\hat{K}'P\cdot\Sigma'), \tag{5.4}$$

$$(2m^2)^2(8\hat{K}\cdot P\hat{K}'\cdot P'-4\hat{K}\cdot\hat{K}'P\cdot P')-8m^2P'^2(2\hat{K}\cdot\Sigma'\hat{K}'\cdot P-\hat{K}\cdot\hat{K}'P\cdot\Sigma')$$
$$-8m^2P^2(2\hat{K}\cdot\Sigma\hat{K}'\cdot P'-\hat{K}\cdot\hat{K}'P'\cdot\Sigma)+4P^2P'^2(2\hat{K}\cdot\Sigma\hat{K}'\cdot\Sigma'-\hat{K}\cdot\hat{K}'\Sigma\cdot\Sigma'). \tag{5.5}$$

Integrated on both lightlike vectors $\hat{K},\hat{K}'$, the first trace (5.2) yields the expression

$$\frac{8}{m^4}\Sigma\cdot\Sigma'-4P\cdot P'W_2(P,P'), \tag{5.6}$$

where $W_2(P,P')$ is the double vertex function met in Ref. 13,

$$W_2(P,P')=\int\frac{\mathrm{d}\hat{K}}{4\pi}\int\frac{\mathrm{d}\hat{K}'}{4\pi}\ \frac{(\hat{K}\cdot\hat{K}')^2}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}. \tag{5.7}$$

The second trace (5.3) gives

$$2m^2\times(5.6)-4P^2\left\{\frac{2}{m^2}\int\frac{\mathrm{d}\hat{K}}{4\pi}\ \frac{(\hat{K}\cdot\Sigma)^2}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}-P'\cdot\Sigma\ \ W_2(P,P')\right\}. \tag{5.8}$$

The third trace (5.4) gives the same as (5.8) with P and P' interchanged,

$$2m^2\times(5.6)-4P'^2\left\{\frac{2}{m^2}\int\frac{\mathrm{d}\hat{K}}{4\pi}\ \frac{(\hat{K}\cdot\Sigma')^2}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}-P\cdot\Sigma'\ \ W_2(P,P')\right\}. \tag{5.9}$$

Eventually, the fourth trace (5.5) yields

$$-(2m^2)^2\times(5.6)+2m^2\times(5.8)+2m^2\times(5.9)-4P^2P'^2\ \ \Sigma\cdot\Sigma'W_2(P,P')$$
$$+8P^2P'^2\int\frac{\mathrm{d}\hat{K}}{4\pi}\int\frac{\mathrm{d}\hat{K}'}{4\pi}\ \frac{(\hat{K}\cdot\hat{K}')(\hat{K}\cdot\Sigma)(\hat{K}'\cdot\Sigma')}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}. \tag{5.10}$$

To summarize, the whole expression (5.1) reads

$$\Pi_R^{(N,N';2)}(Q)=ie^2m^4\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))\,\frac{1}{(P'^2+i\epsilon p_0')^{N'+1}}\times\mathrm{disc}\,\frac{1}{(P^2+i\epsilon p_0)^{N+1}}$$
$$\times\{b_Nb_{N'}\times(5.6)+a_Nb_{N'}\times(5.8)+b_Na_{N'}\times(5.9)+a_Na_{N'}\times(5.10)\},\tag{5.11}$$

where the coefficients a_N,b_N, polynomials of degree $j_M(N)$ and $j_M(N)+1$ in the variable $-P^2\Sigma^2/m^4$, respectively, are given in (3.5) and (3.6). That is, one must again investigate the incidence upon generic type (3.11) integrals, of the new multiplicative functions appearing through (5.6)–(5.10). For example, we quote that an expression like (5.6) will contribute $(N,N';2)$ a quantity,

$$(m^2)^{N+N'}\sum_{j=0}^{j_M}C_{N-1}^{2j+1}\sum_{j'=0}^{j'_M}C_{N'-1}^{2j'+1}\sum_{n=0}^{j}C_j^{n-1}\sum_{n'=0}^{j'}C_{j'}^{n'-1}\;\times\;ie^2m^4\int\frac{\mathrm{d}^4P}{(2\pi)^4}(1-2n_F(p_0))$$
$$\times\frac{1}{(m^4)^{n+n'}}\,\frac{(-P'^2\Sigma'^2)^{n'}}{(P'^2+i\epsilon p_0')^{N'+1}}\,\mathrm{disc}\,\frac{(-P^2\Sigma^2)^n}{(P^2+i\epsilon p_0)^{N+1}}\left(\frac{8}{m^4}\Sigma\cdot\Sigma'-4P\cdot P'W_2(P,P')\right),\tag{5.12}$$

where the sums over j and n, which are finite, have been interchanged with the integral on P.

Actually, things may be further reduced, and this helps identify the new mutiplicative functions that come out to be specific to the double effective vertex diagrams. To do so, we can make use of the relation

$$\int\frac{\mathrm{d}\hat K}{4\pi}\,\frac{(\hat K\cdot\Sigma)^2}{(\hat K\cdot P+i\epsilon)(\hat K\cdot P'+i\epsilon)}$$
$$=\frac{1}{p^2}Q_1\left(\frac{p_0}{p}\right)\Sigma\cdot\Sigma'+\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\frac{m^2}{p^2}Q_1\left(\frac{p_0}{p}\right)\frac{1}{2p'}\ln X'$$
$$+\left(\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\right)^2\;\frac{1}{2Q\cdot P+i\epsilon q_0}\ln\frac{P^2+2Q\cdot P+i\epsilon p_0'}{P^2+i\epsilon p_0}\tag{5.13}$$

and of a similar one, with P' and P interchanged, and likewise,

$$\int\frac{\mathrm{d}\hat K}{4\pi}\int\frac{\mathrm{d}\hat K'}{4\pi}\,\frac{(\hat K\cdot\hat K')(\hat K\cdot\Sigma)(\hat K'\cdot\Sigma')}{(\hat K\cdot P+i\epsilon)(\hat K\cdot P'+i\epsilon)(\hat K'\cdot P+i\epsilon)(\hat K'\cdot P'+i\epsilon)}$$
$$=\frac{1}{p^2}Q_1\left(\frac{p_0}{p}\right)\frac{1}{p'^2}Q_1\left(\frac{p_0'}{p'}\right)\Sigma\cdot\Sigma'+\frac{m^2}{p^2}Q_1\left(\frac{p_0}{p}\right)\frac{m^2}{p'^2}Q_1\left(\frac{p_0'}{p'}\right)$$
$$\times\left(\frac{1}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\frac{1}{2p'}\ln X'+(P\leftrightarrow P')\right)$$
$$+\left(\frac{1}{p'^2}Q_1\left(\frac{p_0'}{p'}\right)\left(\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\right)^2\frac{1}{2Q\cdot P+i\epsilon q_0}\ln\frac{P^2+2Q\cdot P+i\epsilon p_0'}{P^2+i\epsilon p_0}+(P\leftrightarrow P')\right)$$
$$+\left(\frac{m^2}{p}\left(\frac{p_0}{p}-\frac{1}{2}\frac{P^2}{p^2}\ln X\right)\right)\left(\frac{m^2}{p'}\left(\frac{p_0'}{p'}-\frac{1}{2}\frac{P'^2}{p'^2}\ln X'\right)\right)W_1(P,P'),\tag{5.14}$$

where $W_1(P,P')$ is another double effective vertex function, not encountered in Ref. 13,

$$W_1(P,P')=\int \frac{d\hat{K}}{4\pi}\int \frac{d\hat{K}'}{4\pi}\ \frac{(\hat{K}\cdot\hat{K}')^1}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}. \tag{5.15}$$

Deriving (5.13) and (5.14), identities (4.9) and (4.14) only, have been used. As expected on the basis of general gauge invariance arguments,[15] (5.13) and (5.14) entail some potential collinear structures similar to those found in the case of one effective vertex diagrams (4.16). Now, a comparison with the previous cases of $(N,\ N';0)$ and $(N,\ N';1)$, also allows to identify with W_1 and W_2, the new extra mutiplicative functions that come out to be specific to the double effective vertex diagrams, $(N,\ N';2)$.

But it seems difficult to proceed further : As shown in the Appendix, an explicit calculation of functions W_1 and W_2 is able, relying this time, on the full set of angular identities (4.9)–(4.11). Results, however, come out so cumbersome that controlling the ensuing integrals on x' and on x, is rendered extremely hazardous. In order to prove that (5.11) does have an msf imaginary part, we must therefore proceed differently, and construct a proof by induction.

We consider the contribution to $\Pi_R(Q)$ of the diagram $(N+2,N';2)$. It is,

$$\Pi_R^{(N+2,N';2)}(Q)=8ie^2m^4\int \frac{p^2\,dp}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{dx}{2\pi}\,\frac{p_0(x)}{2T}\,\mathrm{disc}\,\frac{1}{(P^2)_R^{N+3}}$$
$$\times\int_0^{x'_M}\frac{dx'}{(P'^2)_R^{N'+1}}\int_{\hat{K},\hat{K}'}\ \hat{K}\cdot\hat{K}'\,\frac{\mathrm{Tr}(\not{P}(\Sigma_R\not{P})^{N+2}\ \not{\hat{K}}\not{P}'(\Sigma'_R\not{P}')^{N'}\not{\hat{K}}')}{(\hat{K}\cdot P)_R(\hat{K}\cdot P')_R(\hat{K}'\cdot P)_R(\hat{K}'\cdot P')_R}, \tag{5.16}$$

where some obvious shorthand notations have been introduced so as to alleviate too large expressions,

$$\int\frac{d\hat{K}}{4\pi}\int\frac{d\hat{K}'}{4\pi}\equiv\int_{\hat{K},\hat{K}'}\ ,\qquad \frac{1}{P^2+i\epsilon p_0}\equiv\frac{1}{(P^2)_R}\ ,\quad \Sigma_R(P)\equiv\Sigma_R\ ,\quad \Sigma_R(P)'$$
$$\equiv\Sigma'_R,\ \frac{1}{P'^2+i\epsilon p'_0}\equiv\frac{1}{(P'^2)_R}\ ,\quad \frac{1}{\hat{K}\cdot P+i\epsilon p_0}\equiv\frac{1}{(\hat{K}\cdot P)_R}\ . \tag{5.17}$$

Having,

$$(\Sigma_R\not{P})^2=2m^2\Sigma_R\not{P}-P^2\Sigma_R^2\mathbb{I}_4, \tag{5.18}$$

Eq. (5.16) may be written as

$$8ie^2m^4\int\frac{p^2\,dp}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{dx}{2\pi}\,\frac{p_0(x)}{2T}\Bigg\{\mathrm{disc}\ \frac{2m^2}{(P^2)_R^{N+3}}$$
$$\times\int_0^{x'_M}\frac{dx'}{(P'^2)_R^{N'+1}}\int_{\hat{K},\hat{K}'}\ \hat{K}\cdot\hat{K}'\frac{\mathrm{Tr}(\cdots(\Sigma_R\not{P})^{N+1}\ \cdots)}{(\hat{K}\cdot P)_R\ \cdots(\hat{K}'\cdot P')_R}-\mathrm{disc}\ \frac{\Sigma_R^2}{(P^2)_R^{N+2}}\int_0^{x'_M}\frac{dx'}{(P'^2)_R^{N'+1}}$$
$$\times\int_{\hat{K},\hat{K}'}\ \hat{K}\cdot\hat{K}'\ \frac{\mathrm{Tr}(\cdots(\Sigma_R\not{P})^N\ \cdots)}{(\hat{K}\cdot P)_R\ \cdots(\hat{K}'\cdot P')_R}\Bigg\}, \tag{5.19}$$

where the dots stand for all of those factors which are left the same as in (5.16). Next, we can form the difference of (5.16) with the first term of (5.19), obtaining

$$8ie^2m^4\int\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\;\mathrm{disc}\;\frac{1}{(P^2)_R^{N+3}}$$
$$\times\int_0^{x'_M}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\int_{\hat{K},\hat{K}'}\quad\hat{K}\cdot\hat{K}'\;\frac{\mathrm{Tr}(\cdots\{(\Sigma_R\not{P})^{N+2}-2m^2(\Sigma_R\not{P})^{N+1}\}\;\cdots)}{(\hat{K}\cdot P)_R\;\cdots\;(\hat{K}'\cdot P')_R}. \tag{5.20}$$

This difference is, of course, also given by

$$-8ie^2m^4\int\;\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\;\mathrm{disc}\;\frac{\Sigma^2}{(P^2)_R^{N+2}}$$
$$\times\int_0^{x'_M}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\int_{\hat{K},\hat{K}'}\quad\hat{K}\cdot\hat{K}'\frac{\mathrm{Tr}(\cdots(\Sigma_R\not{P})^{N}\;\cdots)}{(\hat{K}\cdot P)_R\;\cdots(\hat{K}'\cdot P')_R}. \tag{5.21}$$

Our induction hypothesis is that $(N+1,N';2)$ is endowed with an msf imaginary part, that is, the expression

$$8ie^2m^4\int\;\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\;\mathrm{disc}\;\frac{1}{(P^2)_R^{N+2}}$$
$$\times\int_0^{x'_M}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\int_{\hat{K},\hat{K}'}\quad\hat{K}\cdot\hat{K}'\frac{\mathrm{Tr}(\cdots(\Sigma_R\not{P})^{N+1}\;\cdots)}{(\hat{K}\cdot P)_R\;\cdots(\hat{K}'\cdot P')_R}. \tag{5.22}$$

We will need the following result: Let there be $S^{(2)}(q,p;p_0)$ some function, such that, for all integers k and l, and all integers i and n, with $0\leqslant n-i$, the following finite sum of integrals,

$$\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C^m_{2(n-i)+k}(-1)^mF^{(l)}_{km}(m\varepsilon,0)\int_0^1\mathrm{d}x\left\{\mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon}S^{(2)}(q,p;p_0))}{(x-\lambda)^{N+1}}\right.$$
$$\left.+\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\;\;\mathcal{R}e(e^{i\pi m\varepsilon}S^{(2)}(q,p;p_0))\right\}x^{2n-i+l+m\varepsilon} \tag{5.23}$$

has msf imaginary part in the limits $\lambda=0$ and $\varepsilon=0$, with no further specifications required.[7] Then we claim that so is the case of the finite sum of integrals,

$$\frac{1}{\varepsilon^{2(n-i)+k}}\sum_{m=0}^{2(n-i)+k}C^m_{2(n-i)+k}(-1)^mF^{(l)}_{km}(m\varepsilon,0)\int_0^1\mathrm{d}x\left\{\mathbf{P}\frac{\mathcal{I}m(e^{i\pi m\varepsilon}\;S^{(2)}(q,p;p_0)\times\Sigma^2_R(P))}{(x-\lambda)^{N+1}}\right.$$
$$\left.+\pi\epsilon(p_0)\frac{(-1)^N}{N!}\delta^{(N)}(x-\lambda)\;\;\mathcal{R}e(e^{i\pi m\varepsilon}S^{(2)}(q,p;p_0)\times\Sigma^2_R(P))\right\}x^{2n-i+l+m\varepsilon} \tag{5.24}$$

with

$$\Sigma^2_R(P)=\frac{m^4}{p^2}\left(-1+\frac{x}{4}[\,\epsilon(p_0)\ln X]^2+\sqrt{1-x}[\,\epsilon(p_0)\ln X]\right). \tag{5.25}$$

Before we proceed further, the relation of structural patterns (5.23) [and (5.24)], with a general term $(N,\,N';2)$ is worth making explicit. This is achieved by noting that the imaginary part of $(N,\,N';2)$ can be written as

$$8e^2m^4\int\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)=\pm1}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\,\mathrm{disc}_P\,\frac{a_NS_a^{(2)}+b_NS_b^{(2)}}{(P^2)_R^{N+1}} \tag{5.26}$$

with $p_0(x)=\epsilon(p_0)p\sqrt{1-x}$, and $S^{(2)}(q,p;p_0)$ the distributions,

$$S_a^{(2)}(q,p;p_0)=\frac{1}{2}\,\mathrm{disc}_{P'}\int_0^{x'_M(x)}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\int_{\hat K,\hat K'}\quad\hat K\cdot\hat K'\;\frac{\mathrm{Tr}(\not P\{\Sigma_R\not P\}\;\not K\not P'(\Sigma'_R\not P')^{N'}\not K')}{(\hat K\cdot P)_R\;\cdots\;(\hat K'\cdot P')_R}, \tag{5.27}$$

$$S_b^{(2)}(q,p;p_0)=\frac{1}{2}\,\mathrm{disc}_{P'}\int_0^{x'_M(x)}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\int_{\hat K,\hat K'}\quad\hat K\cdot\hat K'\;\frac{\mathrm{Tr}(\not P\{\mathbb{I}_4\}\not K\not P'(\Sigma'_R\not P')^{N'}\not K')}{(\hat K\cdot P)_R\;\cdots\;(\hat K'\cdot P')_R}. \tag{5.28}$$

In the R/A real time formalism we are using, the imaginary part of $(N,N';2)$ is effectively obtained out of (5.1), by forming the difference (divided by a factor of 2) of retarded and advanced P'-lines. Whereof results (after integrating on x') functions of P which exhibit the features of distributions rather than of ordinary functions. As displayed, for example, by (3.43) in the $(N,N';0)$ case, the discontinuities in p_0 of the $S^{(2)}(q,p;p_0)$ may develop imaginary parts, and this is why they appear inside the discontinuity prescription of (5.26), and not simply factored out, as would be the overall real valued multiplicative functions.

The connection with patterns (5.23) and (5.24) is made complete by recalling that, in virtue of (3.5) and (3.6), the coefficients a_N and b_N are polynomials of degree $j_M(N)$ in the variable $(-P^2\Sigma_R^2/m^4)$. We have then, for all n, $0\leqslant n\leqslant j_M(N)$,

$$\int_0^1\mathrm{d}x\;\mathrm{disc}_P\left(\frac{(-P^2\Sigma_R^2)^n\;S^{(2)}}{(P^2)_R^{N+1}}\right)=\sum_{l=0}^{\infty}\frac{1}{l!}\sum_{i=0}^{n}C_n^i(-1)^i\left(\frac{1}{4}\right)^{n-i}\sum_{k=0}^{i}C_i^k(-1)^k\times(5.23). \tag{5.29}$$

Now, the statement (5.23)–(5.24) is rather obvious indeed, because expression (5.25) is nothing but a linear combination of terms whose general form reads

$$x^a\left(\sqrt{1-x}\right)^b[\,\epsilon(p_0)\ln X]^c\;,\qquad 0\leqslant a,b\leqslant1\;,\qquad 0\leqslant c\leqslant2. \tag{5.30}$$

The first contribution of (5.25) to (5.24), is at $a=b=c=0$, and up to an overall multiplicative factor of $-m^4/p^2$, leaves (5.23) the same as it is. The second contribution, is at $a=1,b=0,c=2$. Up to an overall multiplicative factor of $m^4/4p^2$, this contribution leaves (5.23) unchanged, but for the only modification brought about by the shift of integer number $n-i$,

$$(n-i)\;\mapsto\;(n-i)+1. \tag{5.31}$$

The third contribution is at $a=0,b=1,c=1$, and up to an overall multiplicative factor of m^4/p^2, it is entirely contained in the shift of integer number k, with

$$k\;\mapsto\;k+1. \tag{5.32}$$

It results that, if (5.23) has an msf imaginary part, then, so does (5.24). Somehow conversely, the very structure of mass singularity compensation patterns (5.23), makes it clear that if (5.29) is msf, then so is the case of the same whole expression, but taken at $n-1$ instead of n.

Next we need to proof that if (5.22) has an msf imaginary part, then, so does

$$-8ie^2m^4\int\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\;\mathrm{disc}\;\frac{1}{(P^2)_R^{N+2}}\times\int_0^{x'_M}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}$$
$$\times\int_{\hat K,\hat K'}\quad\hat K\cdot\hat K'\;\frac{\mathrm{Tr}(\cdots(\Sigma_R\not P)^N\;\cdots)}{(\hat K\cdot P)_R\;\cdots(\hat K'\cdot P')_R},\tag{5.33}$$

where the difference with (5.22) is that, inside the trace, we have now a power of N instead of $N+1$. This statement is again rather obvious if one considers that the only change is in the substitution of the couple of polynomials (a_{N+1},b_{N+1}) by the couple (a_N,b_N). However, the proof of the above statement can be obtained by induction either, assuming first that the involvement holds true at $(N+1,N';2)$, that is between (5.22) and (5.33). At next order, $(N+2,N';2)$ is given by (5.16), which decomposes into the sum (5.19). Now, it has just been assumed that (5.22), and hence (5.33) have msf imaginary parts. In view of statement (5.23)–(5.24), the same is therefore true of the second term in (5.19), which only differs (5.33) a multiplicative function of Σ_R^2. It results that if $(N+2,N';2)$ has an msf imaginary part, then so does the expression

$$8ie^2m^4\int\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\;\mathrm{disc}\,\frac{1}{(P^2)_R^{N+3}}\times\int_0^{x'_M}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}$$
$$\times\int_{\hat K,\hat K'}\quad\hat K\cdot\hat K'\frac{\mathrm{Tr}\,(\not P(\Sigma_R\not P)^{N+1}\;\not{\hat K}\not P'(\Sigma'_R\not P')^{N'}\not{\hat K}')}{(\hat K\cdot P)_R(\hat K\cdot P')_R(\hat K'\cdot P)_R(\hat K'\cdot P')_R}.\tag{5.34}$$

That is, the involvement extends from $(N+1,N';2)$ to $(N+2,N';2)$. Eventually, we learn out of Ref. 13, that (0,0;2) and (1,0;2) have msf imaginary parts. Whereas it is immediate to check that the property of involvement under consideration is verified at $N=1$; and thus, at all N.

Getting back to our central induction hypothesis that $(N+1,N';2)$ has an msf imaginary part, the above two statements allow to conclude that (5.21) does have an msf imaginary part, and this establishes that the imaginary part of the difference (5.20) is msf.

Two possibilities have to be considered whereupon: Either mass singular behaviors of both members compensate for each others in the difference (5.20), or both members of (5.20) have, separately, msf imaginary parts.

Let us suppose that a compensation of singularities is at the origin of the difference msf imaginary part. The trace of (5.20) can be written as

$$\mathrm{Tr}(\not P(\Sigma_R\not P)^{N+1}\{\Sigma_R\not P-2m^2\}\not{\hat K}\not P'(\Sigma'_R\not P')^{N'}\not{\hat K}').\tag{5.35}$$

As (5.35) stands, however, inspection shows that nothing conclusive can be derived. Relying again on (3.4)–(3.6), it is interesting to decompose (5.35) into a sum of terms

$$(\Delta a)a_{N'}\,\mathrm{Tr}(\not P(\Sigma_R\not P)\not{\hat K}\not P'(\Sigma'_R\not P')\not{\hat K}')+(\Delta a)b_{N'}\,\mathrm{Tr}(\not P(\Sigma_R\not P)\not{\hat K}\not P\not{\hat K}')$$
$$+(\Delta b)a_{N'}\,\mathrm{Tr}(\not P\not{\hat K}\not P'(\Sigma'_R\not P')\not{\hat K}')+(\Delta b)b_{N'}\,\mathrm{Tr}(\not P\not{\hat K}\not P'\not{\hat K}'),\tag{5.36}$$

where we have defined

$$\Delta a=a_{N+2}-2m^2a_{N+1}\;,\qquad\Delta b=b_{N+2}-2m^2b_{N+1}.\tag{5.37}$$

At its turn, the first trace of (5.36), decomposes into a sum of terms,

$$\mathrm{Tr}(\not P(\Sigma_R\not P)\not{\hat K}\not P'(\Sigma'_R\not P')\not{\hat K}')=m^2\,\mathrm{Tr}(\not P(\Sigma_R\not P)\not{\hat K}\not P'\not{\hat K}')+m^2\,\mathrm{Tr}(\not P\not{\hat K}\not P'(\Sigma'_R\not P')\not{\hat K}')\;+\;\cdots,\tag{5.38}$$

where the two traces of the right-hand side are the second and third traces of (5.36), respectively, whereas the dots stand for terms which belong, in proper, to the trace under consideration. If the latter induce further singular imaginary parts, the imaginary part msf character of (5.20) indicates that mass singularity compensations are taking place, that is,

$$\Delta a = 0. \tag{5.39}$$

If N is an even number, then, $j_M(N+1) = j_M(N+2) = N/2$, and one has

$$\Delta a = (m^2)^{N+1} \sum_{j=0}^{N/2} (C_{N+2}^{2j+1} - 2C_{N+1}^{2j+1}) \sum_{n=0}^{j} C_j^n \left(-\frac{P^2 \Sigma_R^2}{m^4} \right)^n. \tag{5.40}$$

For some given powers n to induce singular integrations to be further compensated in the difference, the following condition must therefore be satisfied:

$$\sum_{j=n}^{N/2} C_j^n (C_{N+2}^{2j+1} - 2C_{N+1}^{2j+1}) = 0. \tag{5.41}$$

Binomial coefficients are positive definite, and if $n > N/4$, then, the terms in the sum (5.41) are positive definite either, precluding any compensations of possible singular contributions. That is, contributions attached to the range of powers $N/4 < n \leqslant N/2$ are necessarily msf in imaginary parts, separately. Now, so are also all of the other powers, $1 \leqslant n \leqslant N/2$, in virtue of the statement ''somehow reciprocal'' to (5.24). Since a similar argument can be developed in case of an odd number N, it results that the dots of (5.38) induce, in both members of the difference (5.20), contributions whose imaginary parts are msf, separately.

We consider the second trace, and note that in view of (5.36) and (5.38), it has coefficient

$$(b_{N'} + m^2 a_{N'}) \Delta a. \tag{5.42}$$

If, when plugged into (5.20), the second trace of (5.36) generates non-msf imaginary parts, then the latter have to compensate each others in the difference. Now, selecting a power of n' in the variable $(-P'^2 \Sigma_R'^2 / m^4)$, its coefficient reads

$$\sum_{j'=n'}^{N'/2} (C_{j'}^{n'-1} C_{N'-1}^{2j'+1} + C_{j'}^{n'} C_{N'}^{2j'+1}), \tag{5.43}$$

where an even value of N' is choosen, for the sake of illustration. It is clear that for all $n' \in \{1,2,...,N'/2\}$, (5.43) is a never vanishing quantity. A compensation of possible singular subsequent integrations on x, can only come from (5.39), with the conclusion that for this second trace of (5.36), both members of the difference (5.20) have, separately, msf imaginary parts.

The third trace of (5.36) comes into play with a coefficient of

$$a_{N'} (\Delta b + m^2 \Delta a) \tag{5.44}$$

which may be wtitten as

$$a_{N'} (m^2)^{N+2} \left\{ \sum_{j=0}^{N/2} (C_{N+2}^{2j+1} - 2C_{N+1}^{2j+1}) \left(1 - \frac{P^2 \Sigma_R^2}{m^4} \right)^j + \left(-\frac{P^2 \Sigma_R^2}{m^4} \right) \right.$$
$$\left. \times \sum_{j=0}^{N/2-1} (C_{N+1}^{2j+1} - 2C_N^{2j+1}) \left(1 - \frac{P^2 \Sigma_R^2}{m^4} \right)^j + \left(-\frac{P^2 \Sigma_R^2}{m^4} \right) \left(1 - \frac{P^2 \Sigma_R^2}{m^4} \right)^{N/2} \right\}. \tag{5.45}$$

The higher power in the variable $-P^2 \Sigma_R^2 / m^4$ is a power of $N/2+1$, with coefficient 1. There is no available compensation for this isolated term of (5.45) which must accordingly yield a regular

subsequent integration on x. So is therefore the case of all of the powers $n \in \{1,2,...,N/2+1\}$, because of the statement reciprocal to (5.24). Whereas results that, irrespective of possible compensations among the other (regular) terms of (5.45), both members of the difference (5.20) have msf imaginary parts attached to the third trace of (5.36).

The fourth trace of (5.36) has coefficient,

$$(m^2)^2 a_{N'} \Delta a + m^2 (a_{N'} \Delta b + b_{N'} \Delta a) + b_{N'} \Delta b = (b_{N'} + m^2 a_{N'})(\Delta b + m^2 \Delta a). \tag{5.46}$$

If this trace generates any singular subsequent integration on x, when put back into both members of (5.20), the msf character of the imaginary part of (5.20) requires that $\Delta b + m^2 \Delta a$ vanishes. This condition turns out to be the one just dealt with, and it results that, when put into both members of the difference (5.20), the fourth trace of (5.36) induce subsequent x integrations that have, separately, msf imaginary parts.

To summarize, both (0,0;2) and (1,0;2) diagrams, have been shown to possess msf imaginary parts in Ref. 13. Then, assuming that a diagram $(N+1,N';2)$ has msf imaginary part, we have been able to prove that the next diagram $(N+2,N';2)$, with one more HTL self-energy insertion, has an msf imaginary part either. We can therefore conclude that any of the two effective vertex diagrams contribute msf imaginary parts to the soft real photon emission rate.

The power and simplicity of the proof just developed appears to be more clear as one realizes that the distributions $S^{(2)}(q,p;p_0)$ introduced in full generality in (5.23), entail the double vertex function $W_2(P,P')$ and $W_1(P,P')$ defined in (5.7) and (5.15), respectively. We have in effect, for the $S^{(2)}(q,p;p_0)$, the expressions

$$\frac{1}{2}\mathrm{disc}_{P'} \int_0^{x'_M(x)} \mathrm{d}x' \frac{a_{N'}(-P'^2\Sigma'^2/m^4)}{(P'^2)_R^{N'+1}} \int_{\hat{K},\hat{K}'} \hat{K}\cdot\hat{K}' \frac{\mathrm{Tr}(\not{P}\{\not{\Sigma}_R \not{P}, \mathbb{I}_4\}\hat{\not{K}}\not{P}'\{\not{\Sigma}'_R \not{P}'\}\hat{\not{K}}')}{(\hat{K}\cdot P)_R..(\hat{K}'\cdot P')_R}$$

$$\frac{1}{2}\mathrm{disc}_{P'} \int_0^{x'_M(x)} \mathrm{d}x' \frac{b_{N'}(-P'^2\Sigma'^2/m^4)}{(P'^2)_R^{N'+1}} \int_{\hat{K},\hat{K}'} \hat{K}\cdot\hat{K}' \frac{\mathrm{Tr}(\not{P}\{\not{\Sigma}_R \not{P}, \mathbb{I}_4\}\hat{\not{K}}\not{P}'\{\mathbb{I}_4\}\hat{\not{K}}')}{(\hat{K}\cdot P)_R..(\hat{K}'\cdot P')_R} \tag{5.47}$$

and whereas the second term entails $W_2(P,P')$, the first one entails both $W_2(P,P')$ and $W_1(P,P')$ which are so complicated functions of P,P', that they practically exclude any control of the ensuing integrations on x', and *a posteriori* on x, contrarily to what could be achieved in Secs. III and IV, for the topologies $(N,N';0)$ and $(N,N';1)$.

An interesting byproduct of this analysis is obtained by writing

$$S_a^1(q,p;p_0) = \frac{1}{2}\,\mathrm{disc}_{P'} \int_0^{x'_M(x)} \frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}} \int \frac{\mathrm{d}\hat{K}}{4\pi} \frac{\mathrm{Tr}(\not{P}\{\not{\Sigma}_R \not{P}\}\hat{\not{K}}\not{P}'(\not{\Sigma}'_R \not{P}')^{N'}\hat{\not{K}})}{(\hat{K}\cdot P)_R(\hat{K}\cdot P')_R}, \tag{5.48}$$

$$S_b^1(q,p;p_0) = \frac{1}{2}\,\mathrm{disc}_{P'} \int_0^{x'_M(x)} \frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}} \int \frac{\mathrm{d}\hat{K}}{4\pi} \frac{\mathrm{Tr}(\not{P}\{\mathbb{I}_4\}\hat{\not{K}}\not{P}'(\not{\Sigma}'_R \not{P}')^{N'}\hat{\not{K}})}{(\hat{K}\cdot P)_R(\hat{K}\cdot P')_R}, \tag{5.49}$$

and by recognizing that the imaginary part of a diagram $(N,N';1)$ is hereby expressed as

$$8e^2m^2 \int \frac{p^2\,\mathrm{d}p}{(2\pi)^2} \sum_{\epsilon(p_0)=\pm 1} \int_0^1 \frac{\mathrm{d}x}{2\pi} \frac{p_0(x)}{2T} \mathrm{disc}_P \frac{a_N S_a^1 + b_N S_b^1}{(P^2)_R^{N+1}}. \tag{5.50}$$

Then, knowing from Ref. 13 that (0,0;1), (1,0;1), and (1,1;1) have msf imaginary parts, the same steps as followed throughout this section can be taken, and allow to conclude by induction that $(N,N';1)$ diagrams contribute msf parts to the soft photon emission rate. This is the more systematic derivation which was advertised in the end of Sec. IV: It encompasses all of the terms (4.5)–(4.7) of the $(N,N';1)$ situation, and not solely the peculiar one, (4.8), which was treated there.

Likewise, identifying now $S_a^0(q,p;p_0)$ and $S_b^0(q,p;p_0)$, the distributions

$$S_a^0(q,p;p_0)=\frac{1}{2}\,\mathrm{disc}_{P'}\int_0^{x'_M(x)}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\,\mathrm{Tr}(\not P\{\Sigma_R\not P\}\not P'(\Sigma'_R\not P')^{N'}),$$

$$S_b^0(q,p;p_0)=\frac{1}{2}\,\mathrm{disc}_{P'}\int_0^{x'_M(x)}\frac{\mathrm{d}x'}{(P'^2)_R^{N'+1}}\,\mathrm{Tr}(\not P\{\mathbb{I}_4\}\not P'(\Sigma'_R\not P')^{N'}),$$

and observing that the imaginary part of a diagram $(N,N';0)$ can be expressed as

$$8e^2\int\frac{p^2\,\mathrm{d}p}{(2\pi)^2}\sum_{\epsilon(p_0)=\pm1}\int_0^1\frac{\mathrm{d}x}{2\pi}\,\frac{p_0(x)}{2T}\,\mathrm{disc}_P\frac{a_N S_a^0+b_N S_b^0}{(P^2)_R^{N+1}},$$

we can make use of the msf character of (1,0;0) and (2,0;0) imaginary parts as established in Ref. 13 so as to follow the same steps as taken throughout this section and conclude, in agreement with the calculational approach of Sec. III, that $(N,N';0)$ diagrams contribute msf parts to the soft photon emission rate.

VI. CONCLUSION

Some years ago,[23] we had suggested that the collinear problem met in hot QCD when the resummation program (RP) is used, could be traced back to the particular perturbative series rearrangement the RP amounts to. Strictly speaking though (and contrarily to what can be read off the existing literature) the RP should not be mistaken for any Feynman diagrams resummation, possibly infinite. This happens to be so, simply because of the effective propagators nonperturbative character: Pole residues and dispersion relations, in effect, cannot be derived out of pure thermal perturbation theory.

This suggestion has motivated our construction of a coherent perturbative resummation scheme (PR) of the leading thermal effects (the so-called hard thermal loops, HTL) enjoying by construction the same symmetry properties as the usual RP, with the hope that things could come out at variance with the troublesome (undefined) RP results.

In the case of the so-called rapid fermion damping rate problem of both QED and QCD, a first obstruction met by the RP,[5] this hope revealed itself nondeceptive indeed,[6,7] whereas the collinear problem under consideration was subsequently projected out on a simpler toy model, with promising results.[11]

In a recent publication,[13] the physically interesting case of hot QCD has been analyzed through its first nontrivial perturbative orders, with very instructive new insights. As stated in the introduction, not only did the PR analysis allow to elucidate the so far questionable nature[12] of the collinear singularity encountered in hot QCD, when the RP is used, but a tight and original comparison of both RP and PR calculations made it possible to understand how the collinear singularity unavoidably shows up in an RP treatment.

Now, a PR calculation of the soft real photon emission rate, involves the infinite resummations on N and N', of any perturbative contribution of type $(N,N';0)$, $(N,N';1)$, and $(N,N';2)$, describing one loop photonic self-energy diagrams at $N(N')$ HTL self-energy insertions along the $P(P')$ -fermionic line, respectively, endowed with zero, one and two HTL effective vertex corrections. In order to set our PR calculation a sound, significant result, in contradistinction to the yet confused RP situation, it was therefore crucial to check that the properties that could be

derived for the perturbative orders of m^2, m^4, and m^6, extended indeed to any contribution of order m^{2n}, and this is the task which has been achieved throughout the present article.

However tedious the calculational developments of Sec. III, they eventually revealed extremely useful so as to provide a proof by induction with sound enough a basis. In other words, a proof by induction is not reliable until enough information is gained concerning the mass singularity cancellation patterns, and not before.

Physically, a salient aspect comes out to be the one of propagator's pole migration. This migration in effect, from the lightlike to the timelike region, appears to be at the very origin of the RP dramatic consequence under consideration, and in contrast to the $T=0$ situation, is really peculiar to the thermal context.[7] This is because pole displacements involve a decoupling of partial effective propagators (potential) mass singularities, from effective vertices collinear ones: Whereas all singularities mix up into patterns which grant their overall compensations in a PR calculation, effective vertices mass/collinear singularities remain isolated in an RP calculation, with no singular counterpart to cancel against. This mechanism, first guessed in Ref. 11, then discovered in Ref. 13 for the perturbative orders of m^2, m^4, and m^6, is easily seen here to spread to any perturbative orders, $(m^2)^n$.

As we have long been suspecting,[23] the collinear singularity plaguing the soft real photon emission rate RP calculation is likely to be nothing but an artefact, peculiar to the RP resummation scheme itself. Here may be the place to recall a part of our conclusion in Ref. 13: *After all, whenever resummation is required by the context, a guiding principle could very well be that it be conceived and taken out of finite, well-defined elements, and in particular, of mass singularity free terms. In this respect, it is instructive to come back to the original article where the RP was mostly founded, and to realize that the authors were conscious of difficulties that could be inherited from the fact that the RP did not necessarily comply with this requirement.*[24]

ACKNOWLEDGMENT

It is a pleasure to thank B. Candelpergher for encouraging discussions.

APPENDIX: CALCULATING THE $W_i(P,P')$

In this appendix account is given of the difficulty inherent to the explicit calculations of the double effective vertex functions $W_i(P,P')$, $i=1,2$. The first function, $W_1(P,P')$ is given in (5.15). It is given by the integration on a Feynman parameter s, of the squared norm of a *would be* four-vector with components on the right-hand sides of (4.9) and (4.10),

$$m^2\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}^\mu}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}m^2\int\frac{\mathrm{d}\hat{K}'}{4\pi}\frac{\hat{K}'_\mu}{(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}$$
$$=m^4\int_0^1\mathrm{d}s\left(\frac{r_0}{r^3}\frac{\ln X_r}{R^2+i\epsilon r_0}-\frac{1}{4r^4}\ln^2 X_r-\frac{1}{r^2(R^2+i\epsilon r_0)}\right). \tag{A1}$$

As it stands however, the remaining integration on s is not very easy. A more economic way to proceed consists in writing

$$m^4\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}^\mu}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}\int\frac{\mathrm{d}\hat{K}'}{4\pi}\frac{\hat{K}'_\mu}{(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}$$
$$=\int_0^1\mathrm{d}s\int_0^1\mathrm{d}s'm^2\int\frac{\mathrm{d}\hat{K}}{4\pi}\frac{\hat{K}^\mu}{(\hat{K}\cdot R(s)+i\epsilon)^2}m^2\int\frac{\mathrm{d}\hat{K}'}{4\pi}\frac{\hat{K}'_\mu}{(\hat{K}'\cdot R(s')+i\epsilon')^2}. \tag{A2}$$

This allows to write (A1) as,

$$\left(-\frac{\mathrm{d}}{\mathrm{d}i\epsilon}\right)\left(-\frac{\mathrm{d}}{\mathrm{d}i\epsilon'}\right)\int_0^1 \mathrm{d}s\int_0^1 \mathrm{d}s'\,\Sigma(R(s))\cdot\Sigma(R(s'))$$
$$=\int_0^1 \mathrm{d}s\int_0^1 \mathrm{d}s'\frac{m^2}{R^2(s)+i\epsilon r_0(s)}\,\frac{m^2}{R^2(s')+i\epsilon r_0(s')}\left(1-\frac{r_0}{r}(s)\frac{r_0}{r}(s')\hat{r}\cdot\hat{r}'\right). \quad \text{(A3)}$$

The term $+1$ in the right hand side last parenthesis yields simply,

$$\int_0^1 \mathrm{d}s\int_0^1 \mathrm{d}s'\frac{m^2}{R^2(s)+i\epsilon r_0(s)}\,\frac{m^2}{R^2(s')+i\epsilon r_0(s')}=\left(\frac{m^2}{2P\cdot Q}\ln\frac{P'^2}{P^2}\right)^2. \quad \text{(A4)}$$

The contribution of the term involving the cosine $\hat{r}\cdot\hat{r}'$ is of course more involved. It is

$$-\int_0^1 \mathrm{d}s\,\frac{m^2}{R^2(s)+i\epsilon r_0(s)}\,\frac{p_0+qs}{r^2(s)}$$
$$\times\int_0^1 \mathrm{d}s'\frac{m^2}{R^2(s')+i\epsilon r_0(s')}\,\frac{p_0+qs'}{r^2(s')}\,(p(p+qys)+q(py+qs)s'), \quad \text{(A5)}$$

where

$$r^2(s)=p^2+2pqys+q^2s^2,\quad R^2(s)=P^2+2P\cdot Qs. \quad \text{(A6)}$$

Introducing the three functions

$$F_1(P,Q)=\frac{1}{2Q\cdot P}\ln\frac{P'^2}{P^2}, \quad \text{(A7)}$$

$$F_2(P,Q)=\frac{1}{qp\sqrt{1-y^2}}\arctan\frac{q\sqrt{1-y^2}}{p+qy}, \quad \text{(A8)}$$

$$F_3(P,Q)=\frac{1}{(P^2\vec{p}'-\vec{p}P'^2)^2}$$
$$\times\{\tfrac{1}{2}(2Q\cdot P)^2F_1(P,Q)-(q^2P^2-qp_0(2Q\cdot P)+\tfrac{1}{2}(2Q\cdot P)^2)F_2(P,Q)\} \quad \text{(A9)}$$

one verifies that (A4) cancels out, and that the integration of (A1) can be given by the interesting following form:

$$m^2\int\frac{\mathrm{d}\hat{K}}{4\pi}\,\frac{\hat{K}^\mu}{(\hat{K}\cdot P+i\epsilon)(\hat{K}\cdot P'+i\epsilon)}\,m^2\int\frac{\mathrm{d}\hat{K}'}{4\pi}\,\frac{\hat{K}'_\mu}{(\hat{K}'\cdot P+i\epsilon)(\hat{K}'\cdot P'+i\epsilon)}$$
$$=-m^4\sum_{i,j=1}^{3}\left(\sum_{k=-2}^{+1}a_{ij}^k(2Q\cdot P)^k\right)F_iF_j, \quad \text{(A10)}$$

where the nonvanishing a_{ij}^k coefficients are given by

$$a_{22}^{-2}=-q^2P^2,\quad a_{22}^{-1}=qp_0, \quad \text{(A11)}$$

$$a_{33}^{-2}=-q^2(P^2)^3,\quad a_{33}^{-1}=\frac{5}{2}qp_0(P^2)^2,\quad a_{33}^{0}=-\frac{9}{4}(P^2)^2-\frac{5}{2}p^2P^2,\quad a_{33}^{1}=\frac{p_0(3P^2+4p^2)}{4q}, \quad \text{(A12)}$$

$$a_{12}^{0}=1, \tag{A13}$$

$$a_{13}^{-1}=-qp_0P^2, \quad a_{13}^{0}=\frac{3}{2}P^2, \quad a_{13}^{1}=-\frac{p_0}{q}, \tag{A14}$$

$$a_{23}^{-2}=2q^2(P^2)^2, \quad a_{23}^{-1}=-4qp_0P^2, \quad a_{23}^{0}=\frac{11}{4}P^2+\frac{3}{2}p^2, \quad a_{23}^{1}=-\frac{p_0}{q}. \tag{A15}$$

Calculating $W_2(P,P')$, given in (5.7), is the most tedious angular integration to be coped with, ''an order of magnitude'' more difficult than the latter. One has

$$W_2(P,P')=\int_0^1 \mathrm{d}s \int_0^1 \mathrm{d}s' \int \frac{\mathrm{d}\hat{K}}{4\pi} \int \frac{\mathrm{d}\hat{K}'}{4\pi} \frac{1-2\hat{K}^i\hat{K}'_i+\hat{K}^i\hat{K}^j\hat{K}'_i\hat{K}'_j}{(\hat{K}\cdot R(s)+i\epsilon)^2(\hat{K}'\cdot R(s')+i\epsilon)^2}. \tag{A16}$$

The full set of angular identities (4.9)–(4.11) must be used, but since the first two terms in the numerator of (A16) are those which have just been dealt with in the calculation of $W_1(P,P')$, we may focus on the contribution due to the third term, $\{\hat{K}^i\hat{K}^j\hat{K}'_i\hat{K}'_j\}$. Relying on the angular identity (4.11), one finds, with Q_1 as defined in (3.3),

$$\begin{aligned}
&-3\left(\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}\right)^2+6\left(\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}\right)\left(\int_0^1 \frac{\mathrm{d}s'}{R^2(s')+i\epsilon r_0(s')}\right)\\
&\quad+9\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}\int_0^1 \mathrm{d}s'[\hat{r}(s)\cdot\hat{r}(s')]^2\frac{Q_1(R(s'))}{r^2(s')}-6\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}\\
&\quad\times\int_0^1 \mathrm{d}s' \frac{[\hat{r}(s)\cdot\hat{r}(s')]^2}{R^2(s')+i\epsilon r_0(s')}+\int_0^1 \frac{\mathrm{d}s}{(R^2(s)+i\epsilon r_0(s))}\int_0^1 \mathrm{d}s' \frac{[\hat{r}(s)\cdot\hat{r}(s')]^2}{(R^2(s')+i\epsilon r_0(s'))}.
\end{aligned} \tag{A17}$$

The second term gives

$$6F_1\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}=\frac{3F_1}{pq(1-y^2)}\left(\left(p_0y-p+\frac{Z}{2p}\right)\frac{\ln X'}{p'}-(p_0y-p)\frac{\ln X}{p}\right)-\frac{3}{2}\frac{(ZF_1)^2}{p^2q^2(1-y^2)}, \tag{A18}$$

where the shorthand notation $Z=2Q\cdot P$ has been introduced. The first term of (A17) gives

$$-3\left(\int_0^1 \mathrm{d}s \frac{Q_1(R(s))}{r^2(s)}\right)^2=\frac{-3}{4p^2q^2(1-y^2)^2}\left(-\frac{1}{2}\frac{Z^2F_1}{pq}+\left(p_0y-p+\frac{Z}{2p}\right)\frac{\ln X'}{p'}-(p_0y-p)\frac{\ln X}{p}\right)^2. \tag{A19}$$

The fifth term of (A17) gives

$$\sum_{i,j=1}^{3}\left(\sum_{k=-2}^{+1}c_{ij}^{k}Z^k\right)F_iF_j, \tag{A20}$$

where the nonvanishing c_{ij}^{k} are given by

$$c_{11}^{0}=1, \tag{A21}$$

$$c_{22}^{-2}=2q^2p^2(1-y^2), \tag{A22}$$

$$c_{33}^{-2}=-2q^2p^4(1-y^2)^2P^2, \quad c_{33}^{-1}=-2qp_0p^2(1-y^2)P^2, \quad c_{33}^{0}=\frac{p^2+3p_0^2}{2}, \tag{A23}$$

$$c_{13}^{0}=-2p^2(1-y^2), \tag{A24}$$

$$c_{23}^{-2}=2q^2p^2(1-y^2)(-P^2+p^2(1-y^2)), \quad c_{23}^{-1}=2qp_0p^2(1-y^2), \quad c_{23}^{0}=-\frac{3p^2(1-y^2)}{2}. \tag{A25}$$

The fourth term of (A17) can first be expressed as

$$-6(F_1-p^2(1-y^2)F_3)\left(\int_0^1 \mathrm{d}s\,\frac{Q_1(R(s))}{r^2(s)}\right)+6p^2(1-y^2)(F_1-2p^2F_3)\left(\int_0^1 \mathrm{d}s\,\frac{Q_1(R(s))}{r^4(s)}\right)$$
$$-12qp^3y(1-y^2)F_3\left(\int_0^1 \mathrm{d}s\,s\,\frac{Q_1(R(s))}{r^4(s)}\right) \tag{A26}$$

allowing to see that the second term contribution, (A18), cancels out with an identical part in (A26). In terms of more elementary integrals, the remaining parts of (A26) may be written

$$6F_1F_2-6F_1p^2(1-y^2)\int_0^1\frac{\mathrm{d}s}{r^4(s)}-6F_1\left(\frac{1}{2}\int_0^1\frac{\mathrm{d}s}{r^3(s)}r_0\ln X_{R(s)}\right)+6p^2(1-y^2)(F_1-F_3)$$
$$\times\left(\frac{1}{2}\int_0^1\frac{\mathrm{d}s}{r^5(s)}r_0\ln X_{R(s)}\right)-6F_3p^2(1-y^2)\left(F_2-2p^2\int_0^1\frac{\mathrm{d}s}{r^4(s)}-2qpy\int_0^1\mathrm{d}s\,\frac{s}{r^4(s)}\right)$$
$$+12q(1-y^2)\frac{F_2-P^2F_3}{Z}\left(p^3y\int_0^1\frac{\mathrm{d}s}{r^4(s)}+qP^2\int_0^1\mathrm{d}s\,\frac{s}{r^4(s)}\right)-6qp^2(1$$
$$-y^2)\frac{F_2-P^2F_3}{Z}\left\{\int_0^1\mathrm{d}s\,\frac{\ln X_{R(s)}}{r^3}+p(yp_0-p)\int_0^1\mathrm{d}s\,\frac{\ln X_{R(s)}}{r^5}+\frac{Z}{2}\int_0^1\mathrm{d}s\,\frac{s\ln X_{R(s)}}{r^5}\right\}. \tag{A27}$$

The third term of (A17) is the more involved one, and may be written as

$$9\left(\int_0^1\mathrm{d}s\,\frac{Q_1(R(s))}{r^2(s)}\right)^2-18p^2(1-y^2)\left(\int_0^1\mathrm{d}s\,\frac{Q_1(R(s))}{r^2(s)}\right)\left(\int_0^1\mathrm{d}s\,\frac{Q_1(R(s))}{r^4(s)}\right)$$
$$+18p^4(1-y^2)\left(\int_0^1\mathrm{d}s\,\frac{Q_1(R(s))}{r^4(s)}\right)^2+36qp^3y(1-y^2)\left(\int_0^1\mathrm{d}s\,\frac{Q_1(R(s))}{r^4(s)}\right)\left(\int_0^1\mathrm{d}s\,s\,\frac{Q_1(R(s))}{r^4(s)}\right)$$
$$+18q^2p^2(1-y^2)\left(\int_0^1\mathrm{d}s\,s\,\frac{Q_1(R(s))}{r^4(s)}\right)^2. \tag{A28}$$

To summarize, the last piece of $W_2(P,P')$ can eventually be expressed in the form

$$\sum_{i,j=1}^{3}\left(\sum_{k=-2}^{+1}c_{ij}^{k}Z^{k}\right)F_iF_j+6p^2(1-y^2)\left\{F_3\left(\int_0^1 ds\,\frac{Q_1}{r^2}\right)+(F_1-2p^2F_3)\left(\int_0^1 ds\,\frac{Q_1}{r^4}\right)\right\}$$
$$+12qp^3y(1-y^2)\left(\int_0^1 ds\,s\,\frac{Q_1}{r^4}\right)\left(-F_3+3\int_0^1 ds\,\frac{Q_1}{r^4}\right)+6\left(\int_0^1 ds\,\frac{Q_1}{r^2}\right)^2$$
$$-18p^2(1-y^2)\left(\int_0^1 ds\,\frac{Q_1}{r^2}\right)\left(\int_0^1 ds\,\frac{Q_1}{r^4}\right)+18p^4(1-y^2)\left(\int_0^1 ds\,\frac{Q_1}{r^4}\right)^2$$
$$+18q^2p^2(1-y^2)\left(\int_0^1 ds\,s\,\frac{Q_1}{r^4}\right)^2. \tag{A29}$$

We will not proceed further, giving, for example, the more elementary integrals displayed in (A27) and (A29), as it should already appear clear that the statement concerning "*so cumbersome calculations that they practically preclude any peer control of ensuing integrations on x' and then on x…*" is not exaggerated.

Before concluding this appendix we may stress that the calculation of $W_1(P,P')$ and $W_2(P,P')$ does not display singularities other than (potentially) collinear ones, showing up by the light cone boundary, at $P^2\simeq 0$. For the function F_3 of (A9), this property may be not so easy to see. However, it is straightforward to check that the denominator of (A9) reads as

$$(P^2\vec{p}\,'-\vec{p}P'^2)^2=4q^2p^2p_0^2\left(y-\frac{p_0^2+p^2}{2p_0p}\right)^2. \tag{A30}$$

It vanishes at the light cone only, at $p_0=\pm p$, and this corresponds effectively to a collinear singularity, at $y=\pm 1$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Geometry of crossing null shells

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(Received 8 May 2002; accepted 11 July 2002)

New geometric objects on null thin layers are introduced and their importance for crossing null-like shells are discussed. The Barrabès–Israel equations are represented in a new geometric form and they split into a decoupled system of equations for two different geometric objects: tensor density $\mathbf{G}_b^a$ and vector field I. Continuity properties of these objects through a crossing sphere are proved. In the case of spherical symmetry Dray–t'Hooft–Redmount formula results from continuity property of the corresponding object. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1512973]

I. INTRODUCTION

Self-gravitating matter shell (see Refs. 15 and 18) became an important laboratory for testing global properties of gravitational field interacting with matter. Models of a thin matter layer allow us to construct useful mini-superspace examples. Toy models of quantum gravity, started by Dirac,[5] may give us a deeper insight into a possible future shape of the quantum theory of gravity (see Refs. 7 and 14). Especially interesting are null-like shells, carrying a self-gravitating light-like matter (see Refs. 10–13). Classical equations of motion of such a shell have been derived by Barrabès and Israel in their seminal paper.[3] Junction conditions for general hypersurfaces in space–time are also given in Ref. 22.

A complete Lagrangian and Hamiltonian description of the theory of self-gravitating light-like matter shell, which is no longer spherically symmetric, was given (in terms of gauge-independent geometric quantities) in Ref. 17. For this purpose the notion of an extrinsic curvature for a null-like hypersurface was discussed and the corresponding Gauss–Codazzi equations were proved. These equations imply Bianchi identities for space–times with null-like, singular curvature. Energy-momentum tensor density of a light-like matter shell is unambiguously defined in terms of an invariant matter Lagrangian density. Noether identity and Belinfante–Rosenfeld theorem for such a tensor density was also proved. Finally, the Hamiltonian dynamics of the interacting system: ''gravity+matter'' was derived from the total Lagrangian, the latter being an invariant scalar density.[1,19,26]

Starting from the action functional for a single spherical shell due to Louko, Whiting, and Friedman,[21] Hájíček and Kouletsis generalized it for any number of spherically symmetric null shells, including the cases, when the shells intersect.[12]

In this paper we consider a general nonsymmetric case of two crossing null shells. It occurs that the geometric objects on the null shells are continuous through an intersecting sphere due to the observation that ''jump of the jump'' vanishes (see Lemma 2). This implies that the dynamics of the crossing shells is described by the equations for a single shell plus continuity property across an intersecting sphere.

We also discuss a special case of spherical symmetry. In particular, we give a simple argument (in the case of spherical symmetry) for triviality of the whole ''ADM-momentum'' tensor density $\mathbf{G}_b^a$ which implies that the corresponding energy-momentum tensor density τ_b^a of a light-like matter shell is vanishing.

Geometry of a single shell introduced in Ref. 17 is completed by an extra object—a null

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vector field I, which is always well defined on a null shell and does not vanish in the case of spherical symmetry. Roughly speaking, in the case of a null shell the ''ADM-momentum'' tensor density $\mathbf{G}^{ab}$ (which is well defined for any nondegenerate surface S) splits into two geometric objects: a tensor density $\mathbf{G}^a_b$ and a null vector I^a. They contain a similar information as the jump of a ''transverse'' extrinsic curvature $\mathcal{K}_{ab}$ in Barrabès–Israel approach.

The dynamical system constituted of two spherically symmetric null shells has been studied in Ref. 11. The shells at intersection sphere $S_\times$ exchange energy according to the Dray–t'Hooft–Redmount formula.[6,25] We show that the continuity of the metric (around intersection sphere) implies the continuity of the vector field I through $S_\times$ on both shells. Moreover, in the case of spherical symmetry we show that the continuity of I gives the Dray–t'Hooft–Redmount formula. This means that our new object should be useful in generalizations of the Dray–t'Hooft–Redmount formula for the case of crossing two null shells without any symmetry.

II. GEOMETRY OF A SINGLE NULL SHELL

A. Geometry of a null hypersurface and Gauss–Codazzi constraints

A null hypersurface in a Lorentzian spacetime M is a three-dimensional submanifold $S\subset M$ such that the restriction g_{ab} of the spacetime metric $g_{\mu\nu}$ to S is degenerate.

We shall often use adapted coordinates, where coordinate x^3 is constant on S. Space coordinates will be labeled by k, $l=1, 2, 3$; coordinates on S will be labeled by a, $b=0, 1, 2$; finally, coordinates on $S_t:=V_t\cap S$ (where V_t is a Cauchy surface corresponding to constant value of the ''time-like'' coordinate $x^0=t$) will be labeled by A, $B=1, 2$. Space–time coordinates will be labeled by Greek characters α, β, μ, ν.

The nondegeneracy of the space–time metric implies that the metric g_{ab} induced on S from the space–time metric $g_{\mu\nu}$ has signature $(0, +, +)$. This means that there is a nonvanishing null-like vector field X^a on S, such that its four-dimensional embedding X^μ to M (in adapted coordinates $X^3=0$) is orthogonal to S. Hence, the covector $X_\nu=X^\mu g_{\mu\nu}=X^a g_{a\nu}$ vanishes on vectors tangent to S and, therefore, the following identity holds:

$$X^a g_{ab}\equiv 0. \tag{2.1}$$

It is easy to prove (cf. Ref. 16) that integral curves of X^a, after a suitable reparameterization, are geodesic curves of the space–time metric $g_{\mu\nu}$. Moreover, any null hypersurface S may always be embedded in a one-parameter congruence of null hypersurfaces.

We assume that topologically we have $S=\mathbb{R}^1\times S^2$. Since our considerations are purely local, we fix the orientation of the $\mathbb{R}^1$ component and assume that null-like vectors X describing degeneracy of the metric g_{ab} of S will be always compatible with this orientation. Moreover, we shall always use coordinates such that the coordinate x^0 increases in the direction of X, i.e., inequality $X(x^0)=X^0>0$ holds. In these coordinates degeneracy fields are of the form $X=f(\partial_0-n^A\partial_A)$, where $f>0$, $n_A=g_{0A}$ and we rise indices with the help of the two-dimensional matrix $\tilde{g}^{AB}$, inverse to g_{AB}.

If by λ we denote the two-dimensional volume form on each surface $x^0=\text{const}$:

$$\lambda:=\sqrt{\det g_{AB}}, \tag{2.2}$$

then for any degeneracy field X of g_{ab} the following object

$$v_X:=\frac{\lambda}{X(x^0)}$$

is a well-defined scalar density on S according to Ref. 17. This means that $\mathbf{v}_X:=v_X\,dx^0\wedge dx^1\wedge dx^2$ is a coordinate-independent differential three-form on S. However, v_X depends upon the choice of the field X.

It follows immediately from the above definition that the following object:

$$\Lambda = v_X X$$

is a well defined (i.e., coordinate-independent) vector density on S. Obviously, it *does not depend* upon any choice of the field X:

$$\Lambda = \lambda(\partial_0 - n^A \partial_A). \tag{2.3}$$

Hence, it is an intrinsic property of the internal geometry g_{ab} of S. The same is true for the divergence $\partial_a \Lambda^a$, which is, therefore, an invariant, X-independent, scalar density on S. Mathematically (in terms of differential forms), the quantity Λ represents the two-form

$$\mathbf{L} := \Lambda^a (\partial_a \rfloor dx^0 \wedge dx^1 \wedge dx^2),$$

whereas the divergence represents its exterior derivative (a three-from): $d\mathbf{L} := (\partial_a \Lambda^a) dx^0 \wedge dx^1 \wedge dx^2$. In particular, a null surface with vanishing $d\mathbf{L}$ is called a *nonexpanding horizon* (see Ref. 2).

Both objects $\mathbf{L}$ and $\mathbf{v}_X$ may be defined geometrically, without any use of coordinates. For this purpose we note that at each point $x \in S$, the tangent space $T_x S$ may be quotiented with respect to the degeneracy subspace spanned by X. The quotient space carries a nondegenerate Riemannian metric and, therefore, is equipped with a volume form ω (its coordinate expression would be $\omega = \lambda\, dx^1 \wedge dx^2$). The two-form $\mathbf{L}$ is equal to the pull-back of ω from the quotient space to $T_x S$. The three-form $\mathbf{v}_X$ may be defined as a product: $\mathbf{v}_X = \alpha \wedge \mathbf{L}$, where α is *any* one-form on S, such that $\langle X, \alpha \rangle \equiv 1$.

The degenerate metric g_{ab} on S does not allow to define *via* the compatibility condition $\nabla g = 0$, any natural connection, which could be applied to generic tensor fields on S. Nevertheless, there is one exception: it was shown in Ref. 17 that the degenerate metric defines *uniquely* a certain covariant, first order differential operator. The operator may be applied only to mixed (contravariant-covariant) tensor density fields $\mathbf{H}^a_b$, satisfying the following algebraic identities:

$$\mathbf{H}^a_b X^b = 0, \tag{2.4}$$

$$\mathbf{H}_{ab} = \mathbf{H}_{ba}, \tag{2.5}$$

where $\mathbf{H}_{ab} := g_{ac} \mathbf{H}^c_b$. Its definition cannot be extended to other tensorial fields on S. Fortunately, the extrinsic curvature of a null-like surface and the energy-momentum tensor of a null-like shell are described by tensor densities of this type.

The operator, which we denote by $\overline{\nabla}_a$, is defined by means of the four-dimensional metric connection in the ambient space–time M in the following way: Given $\mathbf{H}^a_b$, take any its extension $\mathbf{H}^{\mu\nu}$ to a four-dimensional, symmetric tensor density, "orthogonal" to S, i.e., satisfying $\mathbf{H}^{\perp\nu} = 0$ ("$\perp$" denotes the component transversal to S). Define $\overline{\nabla}_a \mathbf{H}^a_b$ as the restriction to S of the four-dimensional covariant divergence $\nabla_\mu \mathbf{H}^\mu_\nu$. It was shown in Ref. 17 that ambiguities which arise when extending three-dimensional object $\mathbf{H}^a_b$ living on S to the four-dimensional one, cancel finally and the result is unambiguously defined as a covector density on S. It turns out, however, that this result does not depend upon the space–time geometry and may be defined intrinsically on S as follows:

$$\overline{\nabla}_a \mathbf{H}^a_b = \partial_a \mathbf{H}^a_b - \tfrac{1}{2} \mathbf{H}^{ac} g_{ac,b},$$

where $g_{ac,b} := \partial_b g_{ac}$, a tensor density $\mathbf{H}^a_b$ satisfies identities (2.4) and (2.5), and moreover, $\mathbf{H}^{ac}$ is *any* symmetric tensor density, which reproduces $\mathbf{H}^a_b$ when lowering an index:

$$\mathbf{H}^a_b = \mathbf{H}^{ac} g_{cb}. \tag{2.6}$$

It is easily seen, that such a tensor density always exists due to identities (2.4) and (2.5), but the reconstruction of $\mathbf{H}^{ac}$ from $\mathbf{H}^{a}_{b}$ is not unique, because $\mathbf{H}^{ac}+CX^{a}X^{c}$ also satisfies (2.6) if $\mathbf{H}^{ac}$ does. Conversely, two such symmetric tensors $\mathbf{H}^{ac}$ satisfying (2.6) may differ only by $CX^{a}X^{c}$. Fortunately, this nonuniqueness does not influence the value of (2.6). Hence, the following definition makes sense:

$$\overline{\nabla}_{a}\mathbf{H}^{a}_{b}:=\partial_{a}\mathbf{H}^{a}_{b}-\tfrac{1}{2}\mathbf{H}^{ac}g_{ac,b}\,. \tag{2.7}$$

The right-hand side does not depend upon any choice of coordinates (i.e., transforms like a genuine covector density under change of coordinates).

To express directly the result in terms of the original tensor density $\mathbf{H}^{a}_{b}$, we observe that it has five independent components and may be uniquely reconstructed from $\mathbf{H}^{0}_{A}$ (two independent components) and the symmetric two-dimensional matrix $\mathbf{H}_{AB}$ (three independent components). Indeed, identities (2.4) and (2.5) may be rewritten as follows:

$$\mathbf{H}^{A}_{B}=\tilde{g}^{AC}\mathbf{H}_{CB}-n^{A}\mathbf{H}^{0}_{B}, \tag{2.8}$$

$$\mathbf{H}^{0}_{0}=\mathbf{H}^{0}_{A}n^{A}, \tag{2.9}$$

$$\mathbf{H}^{B}_{0}=(\tilde{g}^{BC}\mathbf{H}_{CA}-n^{B}\mathbf{H}^{0}_{A})n^{A}. \tag{2.10}$$

The correspondence between $\mathbf{H}^{a}_{b}$ and $(\mathbf{H}^{0}_{A},\mathbf{H}_{AB})$ is one-to-one.

To reconstruct $\mathbf{H}^{ab}$ from $\mathbf{H}^{a}_{b}$ up to an arbitrary additive term $CX^{a}X^{b}$, take the following, coordinate dependent, symmetric quantity:

$$\mathbf{F}^{AB}:=\tilde{g}^{AC}\mathbf{H}_{CD}\tilde{g}^{DB}-n^{A}\mathbf{H}^{0}_{C}\tilde{g}^{CB}-n^{B}\mathbf{H}^{0}_{C}\tilde{g}^{CA}, \tag{2.11}$$

$$\mathbf{F}^{0A}:=\mathbf{H}^{0}_{C}\tilde{g}^{CA}=:\mathbf{F}^{A0}, \tag{2.12}$$

$$\mathbf{F}^{00}:=0. \tag{2.13}$$

It is easy to observe that any $\mathbf{H}^{ab}$ satisfying (2.6) must be of the following form:

$$\mathbf{H}^{ab}=\mathbf{F}^{ab}+\mathbf{H}^{00}X^{a}X^{b}. \tag{2.14}$$

The nonuniqueness in the reconstruction of $\mathbf{H}^{ab}$ is, therefore, completely described by the arbitrariness in the choice of the value of $\mathbf{H}^{00}$. Using these results, we finally obtain

$$\overline{\nabla}_{a}\mathbf{H}^{a}_{b}:=\partial_{a}\mathbf{H}^{a}_{b}-\tfrac{1}{2}\mathbf{H}^{ac}g_{ac,b}=\partial_{a}\mathbf{H}^{a}_{b}-\tfrac{1}{2}\mathbf{F}^{ac}g_{ac,b}=\partial_{a}\mathbf{H}^{a}_{b}-\tfrac{1}{2}(2\mathbf{H}^{0}_{A}n^{A}_{,b}-\mathbf{H}_{AC}\tilde{g}^{AC}_{,b}). \tag{2.15}$$

The operator on the right-hand side of (2.15) is called the (three-dimensional) covariant derivative of $\mathbf{H}^{a}_{b}$ on S with respect to its degenerate metric g_{ab}. It was proved in Ref. 17 that it is well defined (i.e., coordinate-independent) for a tensor density $\mathbf{H}^{a}_{b}$ fulfilling conditions (2.4) and (2.5). It was also shown that the above definition coincides with the one given in terms of the four-dimensional metric connection and due to (2.6), it equals

$$\nabla_{\mu}\mathbf{H}^{\mu}_{b}=\partial_{\mu}\mathbf{H}^{\mu}_{b}-\tfrac{1}{2}\mathbf{H}^{\mu\lambda}g_{\mu\lambda,b}=\partial_{a}\mathbf{H}^{a}_{b}-\tfrac{1}{2}\mathbf{H}^{ac}g_{ac,b}\,, \tag{2.16}$$

and, whence, coincides with $\overline{\nabla}_{a}\mathbf{H}^{a}_{b}$ defined intrinsically on S.

To describe exterior geometry of S we begin with covariant derivatives *along* S of the ''orthogonal vector X.'' Consider the tensor $\nabla_{a}X^{\mu}$. Unlike in the nondegenerate case, there is no unique ''normalization'' of X and, therefore, such an object does depend upon a choice of the field X. The length of X vanishes. Hence, the tensor is again orthogonal to S, i.e., the components

corresponding to $\mu=3$ vanish identically in adapted coordinates. This means that $\nabla_a X^b$ is a purely three-dimensional tensor living on S. For our purposes it is useful to use the "ADM-momentum" version of this object, defined in the following way:

$$Q^a_b(X) := -s\{v_X(\nabla_b X^a - \delta^a_b \nabla_c X^c) + \delta^a_b \partial_c \Lambda^c\}, \tag{2.17}$$

where $s := \operatorname{sgn} g^{03} = \pm 1$. Due to above convention, the object $Q^a_b(X)$ feels only *external orientation* of S and does not feel any internal orientation of the field X.

Remark: If S is a *nonexpanding horizon*, the last term in the above definition vanishes.

The last term in (2.17) is X independent. It has been introduced in order to correct algebraic properties of the quantity $v_X(\nabla_b X^a - \delta^a_b \nabla_c X^c)$: it was shown in Ref. 17 that Q^a_b satisfies identities (2.4) and (2.5) and, therefore, its covariant divergence with respect to the degenerate metric g_{ab} on S is uniquely defined. This divergence enters into the Gauss–Codazzi equations, which relate the divergence of Q with the transversal component $\mathcal{G}^\perp_b$ of the Einstein tensor density $\mathcal{G}^\mu_\nu = \sqrt{|\det g|}(R^\mu_\nu - \delta^\mu_\nu \frac{1}{2} R)$. The transversal component of such a tensor density is a well-defined three-dimensional object living on S. In coordinate system adapted to S, i.e., such that the coordinate x^3 is constant on S, we have $\mathcal{G}^\perp_b = \mathcal{G}^3_b$. Due to the fact that $\mathcal{G}$ is a tensor density, components $\mathcal{G}^3_b$ *do not change* with changes of the coordinate x^3, provided it remains constant on S. These components describe, therefore, an intrinsic covector density living on S.

Proposition 1: The following null-like-surface version of the Gauss–Codazzi equation is true:

$$\overline{\nabla}_a Q^a_b(X) + s v_X \partial_b \left(\frac{\partial_c \Lambda^c}{v_X} \right) \equiv - \mathcal{G}^\perp_b \,. \tag{2.18}$$

We remind the reader that the ratio between two scalar densities: $\partial_c \Lambda^c$ and v_X, is a scalar function. Its gradient is a covector field. Finally, multiplied by the density v_X, it produces an intrinsic covector density on S. This proves that also the left-hand side is a well-defined geometric object living on S: The Eq. (2.18) is closely related to Raychaudhuri[24] equation for the congruence of null geodesics generated by the vector field X.

B. Bianchi identities for space–times with distribution valued curvature

In this paper we consider a space–time M with distribution valued curvature tensor in the sense of Taub.[27] This means that the metric tensor, although continuous, is not necessarily C^1-smooth across S: we assume that the connection coefficients $\Gamma^\lambda_{\mu\nu}$ may have only step discontinuities (jumps) across S. Formally, we may calculate the Riemann curvature tensor of such a space–time, but derivatives of these discontinuities with respect to the variable x^3 produce a δ-like, singular part of R:

$$\operatorname{sing}(R)^\lambda_{\mu\nu\kappa} = (\delta^3_\nu [\Gamma^\lambda_{\mu\kappa}] - \delta^3_\kappa [\Gamma^\lambda_{\mu\nu}])\, \boldsymbol{\delta}(x^3), \tag{2.19}$$

where by $\boldsymbol{\delta}$ we denote the Dirac distribution (in order to distinguish it from the Kronecker symbol δ) and by $[f]$ we denote the jump of a discontinuous quantity f between the two sides of S. The above formula is invariant under *smooth* transformations of coordinates. There is, however, no sense to impose such a smoothness across S. In fact, the smoothness of space–time is an independent condition on both sides of S. The only reasonable assumption imposed on the differentiable structure of M is that the metric tensor—which is smooth separately on both sides of S—remains continuous across S. Admitting coordinate transformations preserving the above condition, we lose a part of the information contained in quantity (2.19), which becomes now coordinate-dependent. It turns out, however, that another part, namely the Einstein tensor density calculated from (2.19), preserves its geometric, intrinsic (i.e., coordinate-independent) meaning. In case of a nondegenerate geometry of S, the following formula was used by many authors (see Refs. 7–9, 15 and 18):

$$\mathrm{sing}(\mathcal{G})^{\mu\nu}=\mathbf{G}^{\mu\nu}\boldsymbol{\delta}(x^3), \tag{2.20}$$

where the "transversal-to-S" part of $\mathbf{G}^{\mu\nu}$ vanishes identically,

$$\mathbf{G}^{\perp\nu}\equiv 0, \tag{2.21}$$

and the "tangent-to-S" part $\mathbf{G}^{ab}$ equals to the jump of the ADM-momentum Q^{ab} of S [$Q^{ab}=\sqrt{|\det g_{cd}|}(g^{ab}\mathrm{tr}K-K^{ab})$, where g^{ab} is the inverse three-metric and K^{ab} is an extrinsic curvature] between the two sides of the surface:

$$\mathbf{G}^{ab}=[Q^{ab}]. \tag{2.22}$$

This quantity is a purely *three-dimensional*, symmetric tensor density living on S. When multiplied by the *one-dimensional density* $\boldsymbol{\delta}(x^3)$ in the transversal direction, it produces the *four-dimensional* tensor density $\mathcal{G}$ according to formula (2.20).

In the case of our degenerate surface S it was shown in Ref. 17 that formulas (2.20) and (2.21) remain valid also in this case. In particular, the latter formula means that the four-dimensional quantity $\mathcal{G}^{\mu\nu}$ reduces in fact to an intrinsic, three-dimensional quantity living on S. However, formula (2.22) cannot be true, because—as we have seen—there is no way to define uniquely the object Q^{ab} for the degenerate metric on S. Instead, we are able to prove the following formula:

$$\mathbf{G}^{a}_{b}=[Q^{a}_{b}(X)], \tag{2.23}$$

where the bracket denotes the jump of $Q^{a}_{b}(X)$ between the two sides of the singular surface. This quantity *does not depend* upon any choice of X and the singular part $\mathrm{sing}(\mathcal{G})^{a}_{b}$ of the Einstein tensor is well defined. We will show in the sequel that the missing component $\mathbf{G}^{00}$ can be recovered in another geometric object, which is presented in the next section.

Remark: Otherwise as in the nondegenerate case, the contravariant components $\mathbf{G}^{ab}$ in formula (2.20) do not transform as a tensor density on S. Hence, the quantity defined by these components would be coordinate-dependent. According to (2.23), $\mathbf{G}$ becomes an intrinsic three-dimensional tensor density on S only after lowering an index, i.e., in the version of $\mathbf{G}^{a}_{b}$. This proves that $\mathbf{G}^{\mu\nu}$ may be reconstructed from $\mathbf{G}^{a}_{b}$ up to an additive term $CX^{\mu}X^{\nu}$ only. We stress that the dynamics of the shell is unambiguously expressed in terms of the gauge-invariant, intrinsic quantity $\mathbf{G}^{a}_{b}$.

We conclude that the total Einstein tensor of our space–time is a sum of the regular part [the regular part is a smooth tensor density on both sides of the surface S (calculated for the metric g separately) with possible step discontinuity across S] $\mathrm{reg}(\mathcal{G})$ and the above singular part $\mathrm{sing}(\mathcal{G})$ living on the singularity surface S. Thus

$$\mathcal{G}^{\mu}_{\nu}=\mathrm{reg}(\mathcal{G})^{\mu}_{\nu}+\mathrm{sing}(\mathcal{G})^{\mu}_{\nu}, \tag{2.24}$$

and the singular part is given *up to an additive term* $CX^{\mu}X_{\nu}\boldsymbol{\delta}(x^3)$. The following *four-dimensional* covariant divergence is unambiguously defined:

$$0=\nabla_{\mu}\mathcal{G}^{\mu}_{c}=\partial_{\mu}\mathcal{G}^{\mu}_{c}-\mathcal{G}^{\mu}_{\alpha}\Gamma^{\alpha}_{\mu c}=\partial_{\mu}\mathcal{G}^{\mu}_{c}-\tfrac{1}{2}\mathcal{G}^{\mu\lambda}g_{\mu\lambda,c}. \tag{2.25}$$

It is proved in Ref. 17 that this quantity vanishes identically and the total singular part of the Bianchi identities reads

$$\mathrm{sing}(\nabla_{\mu}\mathcal{G}^{\mu}_{c})=([\mathrm{reg}(\mathcal{G})^{\perp}_{c}]+\overline{\nabla}_{a}\mathbf{G}^{a}_{b})\boldsymbol{\delta}(x^3)\equiv 0, \tag{2.26}$$

and vanishes identically due to the Gauss–Codazzi equation (2.18), when we calculate its jump across S. Hence, the Bianchi identity $\nabla_{\mu}\mathcal{G}^{\mu}_{c}\equiv 0$ holds universally (in the sense of distributions) for space–times with singular, light-like curvature.

It is worthwhile to notice that the last term in definition (2.17) of the tensor density Q of S is identical on its both sides. Hence, its jump across S vanishes identically. This way the singular part of the Einstein tensor density (2.23) reduces to

$$\mathbf{G}^a_b = [Q^a_b] = -s v_X([\nabla_b X^a] - \delta^a_b[\nabla_c X^c]). \tag{2.27}$$

C. Energy-momentum tensor of a light-like matter. Belinfante–Rosenfeld identity

The interaction between a thin light-like matter-shell and the gravitational field is described in Ref. 17. In particular, all the properties of such a matter are derived from its Lagrangian density L, which depends upon (nonspecified) matter fields z^K living on a null-like surface S, together with their first derivatives $z^K_a := \partial_a z^K$ and, of course, the (degenerate) metric tensor g_{ab} of S,

$$L = L(z^K; z^K_a; g_{ab}). \tag{2.28}$$

We assume that L is an invariant scalar density on S. Similarly as in the standard case of canonical field theory, invariance of the Lagrangian with respect to reparametrizations of S implies important properties of the theory: the Belinfante–Rosenfeld identity and the Noether theorem, which will be discussed in this section. To get rid of some technicalities, we assume in this paper that the matter fields z^K are ''space–time scalars,'' like, e.g., material variables of any thermomechanical theory of continuous media (see, e.g., Refs. 8 and 20). This means that the Lie derivative $\mathcal{L}_Y z$ of these fields with respect to a vector field Y on S coincides with the partial derivative:

$$(\mathcal{L}_Y z)^K = z^K_a Y^a.$$

The following Lemma characterizes Lagrangians which fulfill the invariance condition:

Lemma 1: Lagrangian density (2.28) concentrated on a null hypersurface S is invariant if and only if it is of the following form:

$$L = v_X f(z; \mathcal{L}_X z; g), \tag{2.29}$$

where X is any degeneracy field of the metric g_{ab} on S and $f(\cdot;\cdot;\cdot)$ is a scalar function, homogeneous of degree 1 with respect to its second variable.

Remark: Because of the homogeneity of f with respect to $\mathcal{L}_X z$, the above quantity does not depend upon a choice of the degeneracy field X.

Dynamical properties of such a matter are described by its canonical energy-momentum tensor density, defined in a standard way:

$$T^a_b := \frac{\partial L}{\partial z^K_a} z^K_b - \delta^a_b L. \tag{2.30}$$

It is ''symmetric'' in the following sense.

Proposition 2: Canonical energy-momentum tensor density T^a_b constructed from an invariant Lagrangian density fulfills identities (2.4) and (2.5), i.e., the following holds:

$$T^a_b X^b = 0 \quad \text{and} \quad T_{ab} = T_{ba}. \tag{2.31}$$

In the case of a nondegenerate geometry of S, one considers also the ''symmetric energy-momentum tensor density'' τ^{ab}, defined as follows:

$$\tau^{ab} := 2\frac{\partial L}{\partial g_{ab}}. \tag{2.32}$$

In our case the degenerate metric fulfills the constraint: $\det g_{ab} \equiv 0$. Hence, the above quantity *is not* uniquely defined. However, we may define it, but only *up to an additive term* equal to the

annihilator of this constraint. It is easy to see that the annihilator is of the form CX^aX^b. Hence, the ambiguity in the definition of the symmetric energy-momentum tensor is precisely equal to the ambiguity in the definition of T^{ab}, if we want to reconstruct it from the well-defined object T^a_b. This ambiguity is cancelled, when we lower an index. The next theorem says that for field configurations satisfying field equations, both the canonical and the symmetric tensors coincide. [In our convention, the energy is described by formula: $H=T^0_0=p^0_K\dot{z}^K-L\geqslant 0$, analogous to $H=p\dot{q}-L$ in mechanics and well adapted for Hamiltonian purposes. This convention differs from the one used in Ref. 23, where the energy is given by T_{00}. To keep standard conventions for Einstein equations, we take standard definition of the *symmetric* energy-momentum tensor τ^a_b. This is why Belinfante–Rosenfeld theorem takes form $\tau^a_b=-T^a_b$.] This is an analog of the standard Belinfante–Rosenfeld identity (see Ref. 4). Moreover, Noether theorem (vanishing of the divergence of T) is true. We summarize these facts in the following:

Proposition 3: If L is an invariant Lagrangian and if the field configuration z^K satisfies Euler–Lagrange equations derived from L:

$$\frac{\partial L}{\partial z^K}-\partial_a\frac{\partial L}{\partial z^K_a}=0, \tag{2.33}$$

then the following statements are true:

(1) Belinfante–Rosenfeld identity: canonical energy-momentum tensor T^a_b coincides with (minus—because of the convention used) symmetric energy-momentum tensor τ^{ab}:

$$T^a_b=-\tau^{ac}g_{cb}, \tag{2.34}$$

(2) Noether theorem:

$$\overline{\nabla}_a T^a_b=0. \tag{2.35}$$

It is shown in Ref. 17 that the Einstein equations for the singular part

$$\mathbf{G}^a_b=8\pi\tau^a_b \tag{2.36}$$

can be derived from an action principle and they contain an intrinsic part of the Barrabès–Israel equations in mixed (contravariant–covariant) tensor density representation. Let us notice that if we assume vacuum Einstein equations outside surface S then, in particular, they imply $\mathrm{reg}(\mathcal{G})^\perp_c=0$ which gives compatibility of (2.26) with (2.35).

Remark: We may also include a regular matter part into the action and we obtain that the regular part of the energy momentum tensor density is no longer vanishing. In that case our null singular matter fulfills the following equation:

$$\mathrm{sing}(\nabla_\mu\mathcal{T}^\mu_c)=([\mathrm{reg}(\mathcal{T})^\perp_c]+\overline{\nabla}_a\tau^a_b)\boldsymbol{\delta}(x^3)=0, \tag{2.37}$$

where $\mathcal{T}_{\mu\nu}$ is the symmetric energy-momentum tensor density of the whole matter surrounding our shell S. If $\mathrm{reg}(\mathcal{T})^{\mu\nu}$ is derived form the (regular part of) Lagrangian then Eq. (2.36) may be also considered as a generalized Noether theorem for the full (regular+singular) Lagrangian of matter.

III. CANONICAL NULL VECTOR ON A SINGLE SHELL

Let us rewrite the Ricci tensor:

$$R_{\mu\nu}=\partial_\lambda\Gamma^\lambda_{\mu\nu}-\partial_{(\mu}\Gamma^\lambda_{\nu)\lambda}+\Gamma^\lambda_{\sigma\lambda}\Gamma^\sigma_{\mu\nu}-\Gamma^\lambda_{\mu\sigma}\Gamma^\sigma_{\nu\lambda}, \tag{3.1}$$

in terms of the following combinations of Christoffel symbols:

$$A^\lambda_{\mu\nu}:=\Gamma^\lambda_{\mu\nu}-\delta^\lambda_{(\mu}\Gamma^\kappa_{\nu)\kappa}. \tag{3.2}$$

We have

$$R_{\mu\nu}=\partial_\lambda A^\lambda_{\mu\nu}-A^\lambda_{\mu\sigma}A^\sigma_{\nu\lambda}+\tfrac{1}{3}A^\lambda_{\mu\lambda}A^\sigma_{\nu\sigma}. \tag{3.3}$$

The terms quadratic in A's may have only step-like discontinuities. The derivatives along S are thus bounded and belong to the regular part of the Ricci tensor. The singular part of the Ricci tensor is obtained from the transversal derivatives only. In our adapted coordinate system, where x^3 is constant on S, we obtain

$$\mathrm{sing}(R_{\mu\nu})=\partial_3 A^3_{\mu\nu}=\boldsymbol{\delta}(x^3)[A^3_{\mu\nu}], \tag{3.4}$$

where by $\boldsymbol{\delta}$ we denote the Dirac delta-distribution and by square brackets we denote the jump of the value of the corresponding expression between the two sides of S. Consequently, the singular part of Einstein tensor density reads

$$\mathrm{sing}(\mathcal{G}^\mu_\nu):=\sqrt{|g|}\,\mathrm{sing}(R^\mu_\nu-\tfrac{1}{2}R)=\boldsymbol{\delta}(x^3)\mathbf{G}^\mu_\nu, \tag{3.5}$$

where

$$\mathbf{G}^\mu_\nu:=\sqrt{|g|}(\,\delta^\beta_\nu g^{\mu\alpha}-\tfrac{1}{2}\delta^\mu_\nu g^{\alpha\beta})[A^3_{\alpha\beta}]=[\tilde{Q}^\mu_\nu], \tag{3.6}$$

$$\tilde{Q}^{\mu\nu}:=\sqrt{|g|}(g^{\mu\alpha}g^{\nu\beta}-\tfrac{1}{2}g^{\mu\nu}g^{\alpha\beta})A^3_{\alpha\beta}, \tag{3.7}$$

and explicit formulas for $\tilde{Q}^\mu_\nu$ are given in Appendix B. It was also shown in Ref. 17 that the contravariant version of this quantity:

$$\mathrm{sing}(\mathcal{G})^{\mu\nu}=[\tilde{Q}^{\mu\nu}]\boldsymbol{\delta}(x^3),$$

is coordinate-dependent and, therefore, does not define any geometric object. Let us observe that $\mathbf{G}^{ab}:=[\tilde{Q}^{ab}]$ is not well-defined intrinsic tensor density on S in contrast to $\mathbf{G}^a_b=[\tilde{Q}^a_b]$, as was shown in Appendix A of Ref. 17. However, one can extract the following object:

$$I^a:=sX^a\frac{\mathbf{G}^{00}}{X^0\Lambda^0}, \tag{3.8}$$

which is well defined because of the following.

Proposition 4: The vector field I defined by (3.8) does not depend on the choice of the field X and coordinate x^0, hence it is a well-defined intrinsic object on the null surface S.

Proof: Let us express the component $\mathbf{G}^{00}$ in terms of the objects which arise in $(1+2+1)$-decomposition of space–time (see Appendix B):

$$\begin{aligned}\mathbf{G}^{00}&=[\tilde{Q}^{00}]=g^{03}[\tilde{Q}^0_3]+g^{0b}[\tilde{Q}^0_b]\\&=\frac{\lambda}{M}(-[\partial_3\ln\lambda]+m^b[w_b])-s\left(\frac{1}{N^2}X^b+\frac{s}{M}m^b\right)\lambda[w_b]\\&=-\frac{1}{M}[\partial_3\lambda]=-sY^\mu[\partial_\mu\lambda],\end{aligned} \tag{3.9}$$

where the last equality holds because tangent to S derivatives $\partial_a\lambda$ are continuous, hence $[\partial_a\lambda]=0$. The transformation laws, introduced in Ref. 16 and given in Appendix A, imply that

$$sX^a\frac{\mathbf{G}^{00}}{X^0\Lambda^0}=-Y^\mu[\partial_\mu\ln\lambda]X^a$$

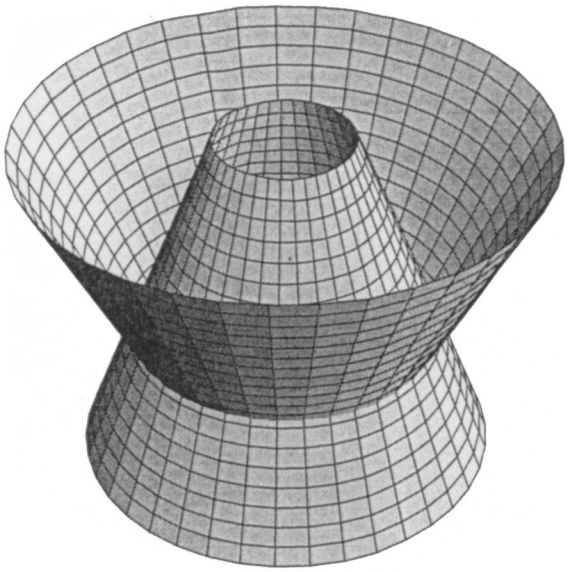

FIG. 1. Crossing shells.

is not dependent on the choice of the basis X, ∂_A, Y at the point $x \in S$. More precisely, for any two tetrads X, ∂_A, Y and $\tilde{X}$, $\partial_{\tilde{B}}$, $\tilde{Y}$ related by (A1), (A2), and (A14) we get $[Y(\ln \lambda)]X=[\tilde{Y}(\ln \tilde{\lambda})]\tilde{X}$.

We also have $\mathbf{G}_{\mu\nu}Y^\mu Y^\nu=\mathbf{G}^{00}$ because $\mathbf{G}_{\mu\nu}X^\mu=0$ [cf. (2.21) and Appendix B].

□

Remark: One can define a symmetric tensor density $W:=I\otimes\Lambda=\Lambda\otimes I$ on S. However, there is no possibility to include object W^{ab} into $\mathbf{G}^{ab}$ unless $\mathbf{G}^a_b=0$. Moreover, if $\mathbf{G}^a_b$ is vanishing (which happens for spherical symmetry cf. Prop. 5), one can check from Bianchi identities $\nabla_\mu \mathcal{G}^\mu_\nu=0$ that

$$\nabla_\mu I^\mu|_S=0$$

for any extension I^μ which is tangent to S. Unfortunately, this equation is not intrinsic on S.

The Eq. (2.36) cannot be completed by the equality $\mathbf{G}^{00}=8\pi\tau^{00}$ on the tensor density level because nor $\mathbf{G}^{ab}$ neither τ^{ab} are geometric objects (in the nondegenerate case both tensor densities are well defined) on S. On the other hand, the definition (3.8) allows to complete singular Einstein equations (2.36) in the following form:

$$I^a=8\pi P^a, \tag{3.10}$$

where the vector field P^a defined as follows:

$$P^a:=sX^a\frac{\tau^{00}}{X^0\Lambda^0} \tag{3.11}$$

contains missing information about singular energy-momentum tensor density $\tau^{\mu\nu}$.

Let us finish this section with the following observation: for nondegenerate surface S the tensor density $\mathbf{G}^{ab}$ [given by (2.22)] is well defined. For the null shell S it splits into two objects: the tensor density $\mathbf{G}^a_b$ defined by (2.23) and the null vector I^a given by (3.8). This means that the information about the jump of a "transverse" extrinsic curvature $\mathcal{K}_{ab}$ (in Barrabès–Israel approach) is contained in two different geometric objects $-\mathbf{G}^a_b$ and I^a.

IV. CROSSING SHELLS

Let us consider two shells intersecting each other along surface $S_\times$ which is a sphere. One can imagine this situation with the help of Fig. 1, where one spherical coordinate is suppressed and the

spheres are drawn as one-dimensional circles.

Let us introduce a local coordinate system (v,x^A,u) around $S_\times$, such that $N_u := \{u=u_0\}$ is the first shell and $N_v := \{v=v_0\}$ is a second one. Hence $S_\times = N_u \cap N_v$. The metric takes the form similar to (B1) but now both (transversal to $S_\times$) coordinates u and v are null, i.e., corresponding level three-surfaces are degenerate. More precisely,

$$g_{\mu\nu} = \begin{bmatrix} n^A n_A & n_A & sM + m^A n_A \\ n_A & g_{AB} & m_A \\ sM + m^A n_A & m_A & m^A m_A \end{bmatrix} \tag{4.1}$$

which gives $\sqrt{|\det g_{\mu\nu}|} = \lambda M$, and the contravariant four-metric takes the form

$$g^{\mu\nu} = \begin{bmatrix} 0 & -s\dfrac{m^A}{M} & \dfrac{s}{M} \\ -s\dfrac{m^A}{M} & \tilde{g}^{AB} + s\dfrac{n^A m^B + m^A n^B}{M} & -s\dfrac{n^A}{M} \\ \dfrac{s}{M} & -s\dfrac{n^A}{M} & 0 \end{bmatrix}, \tag{4.2}$$

where $M>0$, $s := \operatorname{sgn} g^{uv} = \pm 1$, g_{AB} is the induced two-metric on surfaces $\{u=\text{const}, v=\text{const}\}$ and $\tilde{g}^{AB}$ is its inverse (contravariant) metric. Both $\tilde{g}^{AB}$ and g_{AB} are used to rise and lower indices $A,B=1,2$ of the two-vectors n^A and m^A.

Let us choose the null vector fields

$$K := \partial_v - n^A \partial_A \quad \text{and} \quad L := \partial_u - m^A \partial_A$$

which are tangent to N_u or N_v, respectively, and $g(K,L) = sM$. We can use the coordinates (v,x^A) on the first shell N_u. On the second shell N_v we have the coordinate system (x^A,u). The canonical vector field I is well defined on both shells:

$$I(K) = -\frac{K}{M}[L(\ln\lambda)]_u, \quad I(L) = -\frac{L}{M}[K(\ln\lambda)]_v, \tag{4.3}$$

where the index u or v corresponds to jump across first or second shell, respectively.

Several continuity properties of discontinuities across $S_\times$ are implied by the observation that *jump of the jump vanishes* which we explain below on the example of a real function of two variables.

Let f be a function on an open set $U \subset \mathbb{R}^2$ containing point (0,0) such that f is smooth outside axes (corresponding to our crossing shells), i.e., $f \in C^k(U')$ for sufficiently large $k \geqslant 2$ and

$$U' := U \setminus (\{(x,y) \in \mathbb{R}^2 | x=0\} \cup \{(x,y) \in \mathbb{R}^2 | y=0\}).$$

Moreover, we assume that f is continuous across the axes with finite jumps of first normal derivatives. More precisely, the jump

$$\left[\frac{\partial f}{\partial x}\right]_x := \lim_{x \to 0^+} \frac{\partial f}{\partial x}(x,y) - \lim_{x \to 0^-} \frac{\partial f}{\partial x}(x,y)$$

is well defined for $y \neq 0$ and splits into upper (positive y) and lower (negative y) parts. Under the above assumptions we get the following.

Lemma 2: The jump $[\partial f/\partial x]_x$ *is continuous across* (0,0), *i.e.*,

$$\lim_{y\to 0^+}\left[\frac{\partial f}{\partial x}\right]_x(y)=\lim_{y\to 0^-}\left[\frac{\partial f}{\partial x}\right]_x(y)$$

and the similar property holds on the x axis.

Proof: Let us enumerate the quadrants of the plane: I, II, III, IV, i.e., $\mathrm{I}\to\{(x,y)\in\mathbb{R}^2|x>0,y>0\}$, $\mathrm{II}\to\{(x,y)\in\mathbb{R}^2|x<0,y>0\}$, $\mathrm{III}\to\{(x,y)\in\mathbb{R}^2|x<0,y<0\}$, $\mathrm{IV}\to\{(x,y)\in\mathbb{R}^2|x>0,y<0\}$, and the corresponding restrictions of the function f we denote by index, e.g., the function f in the second quadrant we denote by f^{II}. Continuity of f and its tangent derivatives across positive y-half-axis implies $f^{\mathrm{I}}(0,y)=f^{\mathrm{II}}(0,y)$ and $(\partial^n f^{\mathrm{I}}/\partial y)(0,y)=(\partial^n f^{\mathrm{II}}/\partial y)(0,y), n=1,2,...,k$, where the boundary values of f and its derivatives are defined in an obvious way, e.g., $f^{\mathrm{I}}(0,y)=\lim_{x\to 0^+} f^{\mathrm{I}}(x,y)$. In particular, we have

$$\frac{\partial f^{\mathrm{I}}}{\partial y}(0,y)=\frac{\partial f^{\mathrm{II}}}{\partial y}(0,y)\quad \text{for } y>0,$$

$$\frac{\partial f^{\mathrm{IV}}}{\partial y}(0,y)=\frac{\partial f^{\mathrm{III}}}{\partial y}(0,y)\quad \text{for } y<0.$$

Passing to the limit at $(0,0)$, we get

$$\frac{\partial f^{\mathrm{I}}}{\partial y}(0,0):=\lim_{y\to 0^+}\frac{\partial f^{\mathrm{I}}}{\partial y}(0,y)=\lim_{y\to 0^+}\frac{\partial f^{\mathrm{II}}}{\partial y}(0,y)=:\frac{\partial f^{\mathrm{II}}}{\partial y}(0,0)$$

and similarly

$$\frac{\partial f^{\mathrm{IV}}}{\partial y}(0,0):=\lim_{y\to 0^-}\frac{\partial f^{\mathrm{IV}}}{\partial y}(0,y)=\lim_{y\to 0^-}\frac{\partial f^{\mathrm{III}}}{\partial y}(0,y)=:\frac{\partial f^{\mathrm{III}}}{\partial y}(0,0).$$

Finally, from the last two equations we get

$$\frac{\partial f^{\mathrm{I}}}{\partial y}(0,0)-\frac{\partial f^{\mathrm{IV}}}{\partial y}(0,0)=\frac{\partial f^{\mathrm{II}}}{\partial y}(0,0)-\frac{\partial f^{\mathrm{III}}}{\partial y}(0,0),$$

which implies continuity of jump $[\partial f/\partial x]_x$ across $y=0$. □

We can denote symbolically the results as $[[\partial f/\partial x]_x]_y=0$, i.e., jump of the jump at the crossing point vanishes.

Using Lemma 2 one can show the following:

Theorem 1: *The continuity of the metric across null shells implies that the vector fields $I(K)$ and $I(L)$ are continuous across $S_\times$.*

Moreover, from Lemma 2 we get that $\mathbf{G}^a_b(K)$ on N_u and $\mathbf{G}^a_b(L)$ on N_v are also continuous [although $\mathbf{G}^a_b(K)$ does not depend on the choice of the null field K, we keep this argument to distinguish the shells; moreover, we should remember that the coordinates x^a depend on the shell, i.e., $(x^a)=(v,x^A)$ for N_u but $(x^a)=(u,x^A)$ for N_v] across $S_\times$.

Proof: From definition (4.3) of the null field K and (4.1) we have

$$I(K)=-\frac{K}{M\lambda}[\partial_u\lambda]_u,$$

hence we apply Lemma 2 for the function λ. More precisely, we take

$$f(x,y):=\lambda(u=x+u_0,v=y+v_0,x^A)$$

with fixed coordinates x^A, hence the point $x=0$, $y=0$ corresponds to the fixed point on $S_\times$ with coordinates x^A.

For $\mathbf{G}^a_b(K)$ we observe that

$$\mathbf{G}^a_b(K)=s\Lambda^a[w_b]=\frac{\lambda}{2M}K^aK^c[\partial_u g_{cb}]_u$$

which is implied by (B11), and (B14) and (B15). Moreover, from (B15) we get $[w_v]=n^A[w_A]$, hence it is enough to consider

$$[w_A]=\frac{s}{2M}g_{AB}[\partial_u n^B]_u$$

implied by (B14), and using Lemma 2 for the function $f:=n^B$ we obtain the result. □

The above theorem and the considerations from Sec. II imply that *the dynamics of crossing shells is described by Eqs. (2.36) and (2.37) which hold on both shells plus continuity property across* $S_\times$.

A. Spherically symmetric shells

Proposition 5: For spherically symmetric null shell the tensor density $\mathbf{G}^a_b$ *is vanishing.*

This implies that the dynamics of the spherical shell is very simple, i.e., $\tau^a_b=0$, hence Eqs. (2.36) and (2.37) are trivially satisfied but vector field I is not vanishing as we show in the sequel.

Proof: From (2.27), (B11), and (B15) we get

$$\mathbf{G}^a_b=[Q^a_b]=\Lambda^a[w_b] \tag{4.4}$$

but spherical symmetry gives $[w_A]=0$ and, moreover, (B15) implies $[w_0]=0$. □

Let us check the value of I for the spherical null shell which arises from matching two Schwarzschild metrics along spherically symmetric null surface,

$$g_i=-\left(1-\frac{2m_i}{r_i}\right)\mathrm{d}u^2-2\,\mathrm{d}u\,\mathrm{d}r_i+r_i^2\,\mathrm{d}\Omega,\quad i=1,2, \tag{4.5}$$

where

$$\mathrm{d}\Omega:=\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\varphi^2.$$

We take $u\geqslant 0$ for g_1 and $u\leqslant 0$ for g_2, and $r_i(R,u):=R+(m_i/r)u$. This implies that the full metric is continuous in coordinates (u,R) across the shell $u=0$. More precisely,

$$\begin{aligned}g_1|_{u=0}&=-\left(1-\frac{2m_1}{R}\right)\mathrm{d}u^2-2\,\mathrm{d}u\left(\mathrm{d}R+\frac{m_1}{R}\mathrm{d}u\right)+R^2\,\mathrm{d}\Omega\\&=-\mathrm{d}u^2-2\,\mathrm{d}u\,\mathrm{d}R+R^2\mathrm{d}\Omega\\&=-\left(1-\frac{2m_2}{R}\right)\mathrm{d}u^2-2\,\mathrm{d}u\left(\mathrm{d}R+\frac{m_2}{R}\mathrm{d}u\right)+R^2\,\mathrm{d}\Omega=g_2|_{u=0}.\end{aligned}$$

Moreover, if we choose null field $X=\partial/\partial R$ then the transversal field may be chosen as $Y=-\partial/\partial u$ and $\lambda=r_i^2\sin\theta$, hence

$$Y(\ln\lambda)|_{u=0}=-2\frac{\partial}{\partial u}\ln\left(R+\frac{m_i}{R}u\right)\Big|_{u=0}=-\frac{2m_i}{R^2}$$

and finally

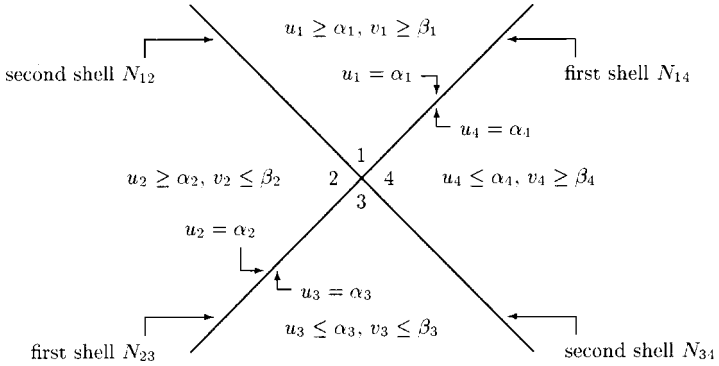

FIG. 2. Matching domains.

$$I = 2\,\frac{m_1 - m_2}{R^2}\,X. \tag{4.6}$$

Next, for crossing two spherical null shells we may check the Dray–t'Hooft–Redmount formula[6,25] as follows: first we apply Theorem 1 which from continuity of the metric implies continuity of the vector field *I*, second we check that the vector field *I* is continuous through the crossing sphere if and only if the Dray–t'Hooft–Redmount formula is true.

Theorem 2: *If the shells are spherically symmetric than continuity of the vector field I gives the Dray–t'Hooft–Redmount formula* (4.13).

Proof: Let us consider the full description of crossing spherically symmetric null shells which can be nicely given in Kruskal–Szekeres coordinates [instead of Eddington–Finkelstein used in (4.5)]. We assume four domains (cf. Fig. 2) equipped with the Schwarzschild metrics

$$g_i = -\,\frac{32m_i^3}{r_i}\exp\!\left(-\frac{r}{2m_i}\right)\mathrm{d}u_i\,\mathrm{d}v_i + r_i^2\,\mathrm{d}\Omega, \quad i = 1,2,3,4, \tag{4.7}$$

where $r_i = 2m_i\kappa(-u_iv_i)$ and the Kruskal function κ is defined by its inverse $\kappa^{-1}(x) = (x-1)e^x$ on the interval $(0,\infty)\subset\mathbb{R}$. One can easily check the following identity for the first derivative of κ:

$$\kappa' = \frac{\exp(-\kappa)}{\kappa}. \tag{4.8}$$

The four domains M_i $(i = 1,2,3,4)$ are matched together along null surfaces $\{x \in M_i |\ u_i = \alpha_i\} \subset M_i$ and $\{x \in M_i |\ v_i = \beta_i\} \subset M_i$, as is shown in Fig. 2.

The coordinates v_1, v_4 on the shell N_{14} do not match but

$$r = 2m_1\kappa(-\alpha_1 v_1) = 2m_4\kappa(-\alpha_4 v_4) \tag{4.9}$$

is the same on both sides and can be chosen as a coordinate on the surface N_{14}. This equality also means that λ is continuous across this shell. On the other hand, the continuity of the term $(32m_i^3/r_i)\exp(-r/2m_i)\ \mathrm{d}u_i\,\mathrm{d}v_i$ across N_{14} implies

$$\frac{m_1^3}{r}\exp\!\left(-\frac{r}{2m_1}\right)\mathrm{d}u_1\,\mathrm{d}v_1\big|_{u_1=\alpha_1} = \frac{m_4^3}{r}\exp\!\left(-\frac{r}{2m_4}\right)\mathrm{d}u_4\,\mathrm{d}v_4\big|_{u_4=\alpha_4},$$

hence using (4.8) and (4.9) we obtain the transformation law between first derivatives of coordinates u_1 and u_4,

$$\frac{du_4}{du_1}=\left(\frac{m_1}{m_4}\right)^3 \exp\left(-\frac{r}{2m_1}\right)\exp\left(\frac{r}{2m_4}\right)\frac{dv_1}{dv_4}=\frac{m_1\alpha_4}{m_4\alpha_1}. \tag{4.10}$$

Moreover, the null vector field X tangent to the first shell can be represented in M_1 as follows:

$$X=\frac{\partial}{\partial r}=\left(\frac{dr}{dv_1}\right)^{-1}\frac{\partial}{\partial v_1},$$

and using (4.8) we have

$$\frac{dr}{dv_1}=-2m_1\alpha_1\kappa'(-\alpha_1 v_1)=-2m_1\alpha_1(\kappa(-\alpha_1 v_1)\exp[\kappa(-\alpha_1 v_1)])^{-1},$$

hence

$$X=-\frac{\kappa(-\alpha_1 v_1)\exp(\kappa(-\alpha_1 v_1))}{2\alpha_1 m_1}\frac{\partial}{\partial v_1}.$$

The transversal vector field

$$Y=\frac{\alpha_1}{4m_1}\frac{\partial}{\partial u_1}$$

fulfills normalization condition $g_1(X,Y)=1$. Moreover, using equality

$$Y(\ln\lambda)=\frac{\alpha_1}{2m_1 r_1}\frac{\partial r_1}{\partial u_1}=\frac{r_1-2m_1}{r_1^2}$$

and the similar one in M_4 we can check the formula (4.6) in new coordinate representation

$$I_{14}=-[Y(\ln\lambda)]X=\frac{2m_1-2m_4}{r^2}X.$$

Similar considerations for the first shell N_{23} give the following expression for the vector field (3.8):

$$I_{23}=\frac{2m_2-2m_3}{r^2}X,$$

where now $r=2m_2\kappa(-\alpha_2 v_2)=2m_3\kappa(-\alpha_3 v_3)$ and

$$X=\frac{\partial}{\partial r}=-\frac{\kappa(-\alpha_2 v_2)\exp(\kappa(-\alpha_2 v_2))}{2\alpha_2 m_2}\frac{\partial}{\partial v_2}=-\frac{\kappa(-\alpha_3 v_3)\exp(\kappa(-\alpha_3 v_3))}{2\alpha_3 m_3}\frac{\partial}{\partial v_3}.$$

We can compare I_{14} with I_{23} across $S_\times$ by using the transformation law [cf. (4.10)] between v_4 and v_3,

$$\frac{dv_4}{dv_3}=\frac{\beta_4 m_3}{\beta_3 m_4}, \tag{4.11}$$

which is implied by continuity of the metrics g_3 and g_4 across second shell N_{34} ($v_3=\beta_3$ and $v_4=\beta_4$). Finally, we obtain

$$I_{23}(v_3=\beta_3)=-\frac{2(m_2-m_3)}{r^2}\,\frac{\kappa(-\alpha_3\beta_3)\exp(\kappa(-\alpha_3\beta_3))}{2\alpha_3 m_3}\,\frac{\partial}{\partial v_3}$$

$$=-\frac{2(m_2-m_3)}{r^2}\,\frac{\frac{r}{2m_3}\exp\left(\frac{r}{2m_3}\right)}{2\alpha_3 m_3}\,\frac{\beta_4 m_3}{\beta_3 m_4}\,\frac{\partial}{\partial v_4}$$

$$=-\frac{(m_2-m_3)\beta_4\exp\left(\frac{r}{2m_3}\right)}{2r\alpha_3\beta_3 m_4 m_3}\,\frac{\partial}{\partial v_4}$$

and

$$I_{14}(v_4=\beta_4)=-\frac{2(m_1-m_4)}{r^2}\,\frac{\frac{r}{2m_4}\exp\left(\frac{r}{2m_4}\right)}{2\alpha_4 m_4}\,\frac{\partial}{\partial v_4},$$

hence $I_{23}=I_{14}$ on $S_\times$ implies

$$\frac{(m_1-m_4)\exp\left(\frac{r}{2m_4}\right)}{2r\alpha_4 m_4}=\frac{(m_2-m_3)\beta_4\exp\left(\frac{r}{2m_3}\right)}{2r\alpha_3\beta_3 m_3},$$

or

$$(m_1-m_4)\alpha_3\beta_3 m_3\exp\left(-\frac{r}{2m_3}\right)=(m_2-m_3)\alpha_4\beta_4 m_4\exp\left(-\frac{r}{2m_4}\right). \tag{4.12}$$

Moreover, on $S_\times$,

$$\alpha_i\beta_i\exp\left(-\frac{r}{2m_i}\right)=1-\kappa(-\alpha_i\beta_i)=1-\frac{r}{2m_i}$$

which applied to (4.12) gives

$$(m_1-m_4)(r-2m_3)=(m_2-m_3)(r-2m_4),$$

which is equivalent to Dray–t'Hooft–Redmount formula

$$(r-2m_1)(r-2m_3)=(r-2m_2)(r-2m_4). \tag{4.13}$$

□

In the above proof we have restricted ourselves to the case of positive masses m_i and to the matching null surfaces which are not horizons. The analysis of possible special cases one can find in Ref. 11 but obviously the formula (4.13) remains valid for any special case.

ACKNOWLEDGMENTS

The author is much indebted to Petr Hájíček for inspiring discussions. This work was partially supported by Swiss National Funds.

APPENDIX A: TRANSFORMATION RULES

The triad (X,∂_A) on S depends upon a particular $(2+1)$-decomposition of S, given by the choice of the time coordinate x^0 on S. However, several objects constructed by means of the triad do not depend upon this choice and describe the geometry of S. To prove this independence, observe that we have the following transformation law:

$$\tilde{X}=cX, \tag{A1}$$

$$\tilde{\partial}_{\tilde{B}}=C^{A}_{\tilde{B}}\partial_A+f_{\tilde{B}}X, \tag{A2}$$

where $(\tilde{X},\tilde{\partial}_{\tilde{B}})$ is the new triad, corresponding to the new coordinate system $(\tilde{x}^{\tilde{a}})$ on S. The coefficient c may be obtained from the following equation:

$$1=\langle d\tilde{x}^0,\tilde{X}\rangle=\left\langle \frac{\partial\tilde{x}^0}{\partial x^A}dx^A+\frac{\partial\tilde{x}^0}{\partial x^0}dx^0,cX\right\rangle=c\left(-\frac{\partial\tilde{x}^0}{\partial x^A}n^A+\frac{\partial\tilde{x}^0}{\partial x^0}\right), \tag{A3}$$

hence,

$$c=\left(\frac{\partial\tilde{x}^0}{\partial x^0}-\frac{\partial\tilde{x}^0}{\partial x^A}n^A\right)^{-1}. \tag{A4}$$

On the other hand, we have

$$\partial_{\tilde{B}}=\frac{\partial x^A}{\partial\tilde{x}^{\tilde{B}}}\partial_A+\frac{\partial x^0}{\partial\tilde{x}^{\tilde{B}}}(X+n^A\partial_A)=\left(\frac{\partial x^A}{\partial\tilde{x}^{\tilde{B}}}+\frac{\partial x^0}{\partial\tilde{x}^{\tilde{B}}}n^A\right)\partial_A+\frac{\partial x^0}{\partial\tilde{x}^{\tilde{B}}}X, \tag{A5}$$

hence,

$$C^{A}_{\tilde{B}}=\frac{\partial x^A}{\partial\tilde{x}^{\tilde{B}}}+\frac{\partial x^0}{\partial\tilde{x}^{\tilde{B}}}n^A, \tag{A6}$$

$$f_{\tilde{B}}=\frac{\partial x^0}{\partial\tilde{x}^{\tilde{B}}}. \tag{A7}$$

The transformation law for g_{AB}

$$g_{\tilde{A}\tilde{B}}=C^{A}_{\tilde{A}}C^{B}_{\tilde{B}}g(\partial_A+f_AX,\partial_B+f_BX)=C^{A}_{\tilde{A}}C^{B}_{\tilde{B}}g_{AB} \tag{A8}$$

implies

$$\tilde{\lambda}=\lambda\ \det C^{B}_{\tilde{A}}. \tag{A9}$$

In order to complete the triad (X,∂_A) on S to a tetrad in M it is useful to choose a transverse field Y fulfilling the following ''normalization conditions:''

$$g(Y,X)=1, \tag{A10}$$

$$g(Y,\partial_A)=0. \tag{A11}$$

These equations *do not* determine Y uniquely, but *modulo* an additive term proportional to X: a ''gauge transformation''

$$Y \to Y + hX, \tag{A12}$$

with an arbitrary scalar field h is always possible. Extending coordinate x^0 from S to a neighborhood of S, we may choose the following transverse field:

$$Y = \frac{s}{M}(\partial_3 - m^A \partial_A). \tag{A13}$$

We stress, however, that this particular choice of Y depends not only upon a $(2+1)$-decomposition of S, but also on a $(3+1)$-decomposition of M in a neighborhood of S. Because of (A11), the vectors X and Y span the bundle of vectors normal to S.

The transformation law for Y, when passing from one to another $(2+1)$-decomposition of S, reads

$$\tilde{Y} = c^{-1}(Y - k^A \partial_A) + hX, \tag{A14}$$

where the scalar field h is arbitrary [it is determined by the extension of the $(2+1)$-decomposition of S to a $(3+1)$-decomposition of M], and the coefficients k^A are uniquely determined by equation

$$f_{\tilde{B}} = C^A_{\tilde{B}} g_{AC} k^C, \tag{A15}$$

with $f_{\tilde{B}}$ given by (A7). Despite of the freedom in choice of Y, some geometric objects constructed with help of the tetrad (X, ∂_A, Y) do not depend upon this choice and characterize only the geometry of $S \subset M$.

APPENDIX B: STRUCTURE OF THE SINGULAR EINSTEIN TENSOR

We are going to relate the coordinate-dependent quantity $\tilde{Q}^{\mu\nu}$ with the external curvature Q^a_b of S. We use the form of the metric introduced in Ref. 16,

$$g_{\mu\nu} = \begin{bmatrix} n^A n_A & n_A & sM + m^A n_A \\ n_A & g_{AB} & m_A \\ sM + m^A n_A & m_A & \left(\frac{M}{N}\right)^2 + m^A m_A \end{bmatrix}, \tag{B1}$$

and

$$g^{\mu\nu} = \begin{bmatrix} -\left(\frac{1}{N}\right)^2 & \frac{n^A}{N^2} - s\frac{m^A}{M} & \frac{s}{M} \\ \frac{n^A}{N^2} - s\frac{m^A}{M} & \tilde{g}^{AB} - \frac{n^A n^B}{N^2} + s\frac{n^A m^B + m^A n^B}{M} & -s\frac{n^A}{M} \\ \frac{s}{M} & -s\frac{n^A}{M} & 0 \end{bmatrix}, \tag{B2}$$

where $M > 0$, $s := \operatorname{sgn} g^{03} = \pm 1$, g_{AB} is the induced two-metric on surfaces $\{x^0 = \text{const}, x^3 = \text{const}\}$ and $\tilde{g}^{AB}$ is its inverse (contravariant) metric. Both $\tilde{g}^{AB}$ and g_{AB} are used to rise and lower indices $A, B = 1, 2$ of the two-vectors n^A and m^A.

Formula (B1) implies $\sqrt{|\det g_{\mu\nu}|} = \lambda M$. Moreover, the object Λ^a defined by formula (2.3), takes the form $\Lambda^a = \lambda X^a$, where λ is given by formula (2.2) and $X := \partial_0 - n^A \partial_A$. This means that we have chosen the following degeneracy field: $X^\mu = (1, -n^A, 0)$.

For calculational purposes it is useful to rewrite the two-dimensional inverse metric $\tilde{g}^{AB}$ in three-dimensional notation, setting $\tilde{g}^{0a} := 0$. This object satisfies the obvious identity

$$\tilde{g}^{ac}g_{cb}=\delta^a_b-X^a\delta^0_b.$$

Hence, the contravariant metric (B2) may be rewritten as follows:

$$g^{ab}=\tilde{g}^{ab}-\frac{1}{N^2}X^aX^b-\frac{s}{M}(m^aX^b+m^bX^a), \tag{B3}$$

where $m^a:=\tilde{g}^{aB}m_B$, so that $m^0:=0$, and

$$g^{3\mu}=\frac{s}{M}X^\mu.$$

It may be easily checked (see, e.g., Ref. 16, p. 406) that covariant derivatives of the field X *along* S are equal to

$$\nabla_aX=-w_aX-l_{ab}\tilde{g}^{bc}\partial_c, \tag{B4}$$

where

$$w_a:=-X^\mu\Gamma^0_{\mu a} \tag{B5}$$

and

$$l_{ab}:=-g(\partial_b,\nabla_aX)=g(\nabla_a\partial_b,X)=X_\mu\Gamma^\mu_{ab}. \tag{B6}$$

Moreover,

$$\partial_c\Lambda^c=-\lambda g^{ab}l_{ab}=-\lambda\tilde{g}^{ab}l_{ab}=-\lambda l, \tag{B7}$$

where $l=\tilde{g}^{ab}l_{ab}$.

The following lemma was proved in Ref. 17.

Lemma 3. *The object* $\tilde{Q}^a_b$ *is related to* Q^a_b *as follows:*

$$s\tilde{Q}^b_a=sQ^a_b-\tfrac{1}{2}\lambda l\delta^a_b+\Lambda^a\chi_b-\delta^a_b\Lambda^c\chi_c, \tag{B8}$$

where $\chi_c:=\frac{1}{2}\partial_c\ln(M/\lambda)$.

Moreover, from definition (2.17) and property (B4) one can check that

$$\begin{aligned}sQ^a_b&=\lambda\delta^a_b\nabla_cX^c-\lambda\nabla_bX^a-\delta^a_b\partial_c\Lambda^c\\&=-\lambda\delta^a_b(w_cX^c+l)+\lambda(w_bX^a+\tilde{g}^{ac}l_{cb})+\delta^a_b\lambda l\\&=\lambda\tilde{g}^{ac}l_{cb}+\Lambda^aw_b-\delta^a_b\Lambda^cw_c.\end{aligned} \tag{B9}$$

Remark: Formula (B9), together with $l_{ab}X^b=0=g_{ab}X^b$, gives us the orthogonality condition $Q^a_bX^b=0$ and symmetry of the tensor $Q_{ab}:=g_{ac}Q^c_b$.

Now, we would like to examine the properties of $\mathbf{G}^{\mu\nu}=[\tilde{Q}^{\mu\nu}]$. From continuity of the metric across S we obtain

$$[l_{ab}]=sM[A^3_{ab}]=sM[\Gamma^3_{ab}]=X^c[\Gamma_{cab}]=0, \tag{B10}$$

$$s[\tilde{Q}^a_b]=\Lambda^a[A^3_{3b}]-\delta^a_b\Lambda^c[A^3_{3c}]=\Lambda^a[w_b]-\delta^a_b\Lambda^c[w_c]=s[Q^a_b], \tag{B11}$$

and

$$[\tilde{Q}^3_\mu]=0 \tag{B12}$$

because $s\tilde{Q}^3_3=-\frac{1}{2}\lambda l$ and $s\tilde{Q}^3_a=0$.

Finally, the missing component $[\tilde{Q}^a_3]$ has the following form:

$$[\tilde{Q}^a_3]=s\Lambda^a\{-[\partial_3 \ln\lambda]+m^b[w_b]\}+M\lambda\tilde{\tilde{g}}^{ab}[w_b]. \tag{B13}$$

We also have from

$$[w_a]=-X^b g^{03}[\Gamma_{3\ ba}]=\frac{s}{2M}X^b[g_{ab,3}] \tag{B14}$$

that

$$X^a[w_a]=\frac{s}{2M}[X^aX^bg_{ab,3}]=0. \tag{B15}$$

Using these results from (B12) one can easily check the property (2.21),

$$\mathbf{G}^{33}=[\tilde{Q}^{33}]=g^{33}[\tilde{Q}^3_3]+g^{3b}[\tilde{Q}^3_b]=0,$$

$$\mathbf{G}^{3a}=[\tilde{Q}^{3a}]=g^{33}[\tilde{Q}^a_3]+g^{3b}[\tilde{Q}^a_b]=-\frac{s}{M}[X^bQ^a_b]=0,$$

where we used the equality $[\tilde{Q}^a_b]=[Q^a_b]$ which is crucial to admit that the object $\mathbf{G}^a_b$ is a well defined geometric object on S.

APPENDIX C: GAUSS–CODAZZI EQUATIONS

It was shown in Ref. 17 that

$$s\mathcal{G}^3_a=-s\partial_bQ^b_a+\tfrac{1}{2}sQ^{bc}g_{bc,a}+\lambda\partial_a l, \tag{C1}$$

where we have used the formula

$$sQ^{ab}=\lambda\tilde{\tilde{g}}^{ac}\tilde{\tilde{g}}^{bd}l_{cd}+(\Lambda^a\tilde{\tilde{g}}^{bc}+\Lambda^b\tilde{\tilde{g}}^{ac}-\tilde{\tilde{g}}^{ab}\Lambda^c)w_c\,.$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Scalar and spin-$\frac{1}{2}$ particle creation in gravitational and constant electric field backgrounds

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(Received 31 January 2002; accepted 22 April 2002)

By considering the quantum vacuum states in the asymptotic regions of the gravitational background, the production rates of scalar and spin-$\frac{1}{2}$ particles created by gravitational fields in specific geometries are computed, with energy distributions shown to be of the Bose–Einstein and Fermi–Dirac types. The analysis is extended in the case of scalar particles to include a constant electric field. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1500793]

I. INTRODUCTION

Particle creation in time dependent cosmologies[1–7] is a most exciting problem in contemporary theoretical physics. Following the pioneer works[5,6] performed in this area, a new approach was suggested by Hawking[7] and further by a series of authors who have given the relation between thermal distribution and thermodynamics. Recently, Villalba[2] used the semiclassical approximation in which the gravitational field was treated classically and analyzed quantized elementary particles propagating on the classical background. The idea behind this approach is to study quantum effects in gravitational backgrounds in the neighborhood of the timelike singularity, concentrating in particular on the vacuum solutions.

In this article, some specific classes of Friedman–Robertson–Walker (FRW) geometries with timelike singularities are analyzed from that point of view, in order to identify the vacuum states in the asymptotic regions.

The rates of scalar and spin-$\frac{1}{2}$ particle creation may be computed through Bogoliubov transformations,[8] which, however, requires first to identify the ''in'' and ''out'' vacuum states. Since, for our choices of geometries, the gravitational background does not possess a timelike Killing vector, the standard interpretation of positive and negative frequency solutions is absent. This difficulty is circumvented by identifying such modes through a comparison of their asymptotic behavior to that of the solutions to the relativistic Hamilton–Jacobi Eq. (1).

The organization of this article is as follows. In Sec. II we introduce the natural criterion for identifying the initial and final states based on the asymptotic behavior of the quasiclassical modes solving the Hamilton–Jacobi equation. In Secs. III and IV, the Klein–Gordon and Dirac equations are solved, whose results are compared to the previous quasiclassical solutions. After identification of the positive and negative frequency states, the distributions of scalar and spin-$\frac{1}{2}$ particle productions by the considered gravitational fields is computed. In Sec. V, some particular cases of Kantowiski–Sacks, Bianchi I, and Bianchi III backgrounds in the presence of a constant electric field are analyzed, and the rate of thermal distribution of scalar particle production is given.

II. SOLUTION OF THE HAMILTON–JACOBI EQUATION

The relativistic Hamilton–Jacobi equation is

$$g^{\alpha\beta}\partial_\alpha S\partial_\beta S+m^2=0, \tag{1}$$

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where we adopt the convention $c=1$, $\hbar=1$. Since the metric[15]

$$ds^2=-dt^2+a^2(t)(dx^2+b^2(x)[dy^2+c^2(y)dz^2]) \tag{2}$$

depends on t, x and y, the solution of Eq. (1) can be written as a sum

$$S=F(t)+G(x)+H(y)-k_z z. \tag{3}$$

Let us analyze two special models for expansion.

(i) $a(t)=a_0 t$, where a_0 is an arbitrary constant: The line element (2) becomes

$$ds^2=-dt^2+a_0^2t^2(dx^2+b^2(x)[dy^2+c^2(y)dz^2]). \tag{4}$$

Substituting (3) into (1) and taking into account (4), we obtain

$$-F_{.t}^2+\frac{1}{a_0^2t^2}G_{.x}^2+\frac{1}{b^2a_0^2t^2}H_{.y}^2+\frac{1}{b^2c^2a_0^2t^2}k_z^2+m^2=0, \tag{5}$$

where by the dot we denote a derivative with respect to t, x, and y.

Then the quasiclassical behavior of the solution of the Klein–Gordon and Dirac equations in the metric (4) is

$$\begin{aligned}\phi(t,x,y,z)=e^{iS}&\rightarrow C(x,y,z)\exp\left(\pm i\int\sqrt{m^2+\frac{\lambda^2}{a_0^2t^2}}\,dt\right)\\&=C(x,y,z)\frac{\exp(\pm im\sqrt{t^2+\lambda^2/m^2a_0^2})t^{\pm i\lambda/a_0}}{(\lambda/ma_0+\sqrt{t^2+\lambda^2/m^2a_0^2})^{i\lambda/a_0}}.\end{aligned} \tag{6}$$

Then as $t\rightarrow\infty$ we find

$$\phi_\infty\rightarrow C(x,y,z)\exp(\mp imt), \tag{7}$$

and as $t\rightarrow 0$

$$\phi_0\rightarrow C(x,y,z)\left(\frac{2\lambda}{ma_0}\right)^{-i\lambda/a_0}t^{\mp i\lambda/a_0}, \tag{8}$$

where the upper and the lower signs in (7) and (8) correspond respectively to the positive and the negative frequency modes. The results (7) and (8) give the quasiclassical asymptotic behaviors of the relativistic wave equations.

(ii) $a(t)=e^{Ht}$: The line element (2) becomes

$$ds^2=-dt^2+e^{2Ht}(dx^2+b^2(x)[dy^2+c^2(y)dz^2]). \tag{9}$$

Substituting (3) into Hamilton Jacobi equation (1) and taking into account (9), we arrive at

$$-F_{.t}^2+\frac{1}{e^{2Ht}}G_{.x}^2+\frac{1}{b^2e^{2Ht}}H_{.y}^2+\frac{1}{b^2c^2e^{2Ht}}k_z^2+m^2=0. \tag{10}$$

The solution of Eq. (10) has the form

$$S(t,x,y,z)=-k_z z\pm i\int\sqrt{\lambda^2+\frac{k^2}{b^2}}\,dx\pm\int\sqrt{k^2-\frac{k_z^2}{c^2}}\,dy\pm\int\sqrt{m^2+\lambda^2e^{-2Ht}}dt, \tag{11}$$

which in $t\rightarrow-\infty$ reduces to

$$S(t,x,y,z)=-k_z z\pm i\int \sqrt{\lambda^2+\frac{k^2}{b^2}}\,dx\pm\int \sqrt{k^2-\frac{k_z^2}{c^2}}\,dy\mp\frac{\lambda}{H}e^{-Ht}. \tag{12}$$

The quasiclassical behavior of the solution of the Klein–Gordon and Dirac equations in the metric (9) is

$$\phi_{-\infty}=e^{iS}\to C(x,y,z)\exp\left(\mp\frac{i\lambda}{H}e^{-Ht}\right). \tag{13}$$

Analogously, we have that as $t\to\infty$ reduces to

$$S(t,x,y,z)=-k_z z\pm i\int \sqrt{\lambda^2+\frac{k^2}{b^2}}\,dx\pm\int \sqrt{k^2-\frac{k_z^2}{c^2}}\,dy\pm mt\mp\frac{\lambda^2 e^{-2Ht}}{4Hm}, \tag{14}$$

and, consequently,

$$\phi_{\infty}=e^{iS}\to C(x,y,z)e^{\mp imt}\exp\left(\mp i\frac{\lambda^2 e^{-2Ht}}{4Hm}\right), \tag{15}$$

where the upper and the lower signs in (13) and (15) correspond respectively to the positive frequency modes and to the negative frequency modes. After making this identification, we can analyze the solution of the Klein–Gordon and Dirac equations in the background field (2).

III. SOLUTION OF THE KLEIN–GORDON EQUATION

The covariant generalization of the Klein–Gordon equation takes the form

$$g^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi-(m^2+\xi R)\phi=0, \tag{16}$$

where ∇_α is the covariant derivative and R the scalar curvature. We consider a scalar field interacting only with the space–time geometry, with the mass m and minimal coupling $\xi=0$.

We can write (16) in the form

$$\left(\partial_t^2-\frac{1}{a^2}\partial_x^2-\frac{1}{a^2b^2}\partial_y^2-\frac{1}{a^2b^2c^2}\partial_z^2+m^2\right)\psi=0. \tag{17}$$

Since (17) commutes with the operator $-i\partial_z$ we can look at a solution of the form $\psi=e^{ik_z z}\phi$ which reduces Eq. (18) to

$$\left(\partial_t^2-\frac{1}{a^2}\left(\partial_x^2+\frac{1}{b^2}\partial_y^2-\frac{1}{b^2c^2}k_z^2\right)+m^2\right)\phi=0. \tag{18}$$

Equation (18) can be solved by using separation of variables. Therefore,

$$\left(\frac{d^2}{dt^2}+\frac{\lambda^2}{a^2}+m^2\right)\phi_1=0, \tag{19}$$

$$\left(\frac{d^2}{dx^2}+\frac{k^2}{b^2}-\lambda^2\right)\phi_2=0, \tag{20}$$

$$\left(\frac{d^2}{dy^2}-\frac{k_z^2}{c^2}-k^2\right)\phi_3=0, \tag{21}$$

where λ and k are constants of separation and $\phi(t,x,y)=\phi_1(t)\phi_2(x)\phi_3(y)$. To solve Eqs. (19), (20) and (21) we set the following for a FRW space–time

(a) $b(x)=\sinh x$: Equation (20) becomes

$$\left(\frac{d^2}{dx^2}+\frac{k^2}{\sinh^2 x}-\lambda^2\right)\phi_2=0, \tag{22}$$

and the solution is given by

$$\phi_2=A\sinh^q x F(\tfrac{1}{2}(q+\lambda),\tfrac{1}{2}(q-\lambda),q+\tfrac{1}{2},-\sinh^2 x), \tag{23}$$

with $q=\frac{1}{2}+i(k^2-\frac{1}{4})^{1/2}$.

(b) $c(y)=\sin y$: Equation (21) becomes

$$\left(\frac{d^2}{dy^2}-\frac{k_z^2}{\sin^2 y}-k^2\right)\phi_3=0, \tag{24}$$

and the solution takes the form

$$\phi_3=B\sin^q y F(\tfrac{1}{2}(q+ik),\tfrac{1}{2}(q-ik),q+\tfrac{1}{2},\sin^2 y), \tag{25}$$

with $q=\frac{1}{2}+(k_z^2+\frac{1}{4})^{1/2}$.

(i) $a(t)=a_0 t$, a curvature-dominated model of FRW space–time: Equation (19) can be written as follows:

$$\left(\frac{d^2}{dt^2}+m^2+\frac{\lambda^2}{a_0^2 t^2}\right)\phi_1=0. \tag{26}$$

Making the change of variables $z=2imt$, we obtain the Whittaker equation

$$\left(\frac{d^2}{dz^2}+\frac{\lambda^2-\frac{1}{4}}{a_0^2 z^2}\right)\phi_1=0, \tag{27}$$

the solution of which is

$$\phi_1=C_1 W_{k,\mu}(z)+C_2 M_{k,\mu}(z), \tag{28}$$

where $k=0$ and $\mu=(i/4)(4\lambda^2/a_0^2-1)^{1/2}$.

Looking at the asymptotic behavior for $|z|\to\infty$, (Ref. 9)

$$W_{k,\mu}(z)\to e^{-z/2}z^k, \tag{29}$$

and, for $z\to 0$,

$$M_{k,\mu}(z)\to z^{\mu+1/2}. \tag{30}$$

We have that the solution of Eq. (27), having an asymptotic behavior of the form (7), is

$$\phi_\infty=C_\infty^+ W_{k,\mu}(z)+C_\infty^- W_{-k,\mu}(-z), \tag{31}$$

where C_∞^+ and C_∞^- are normalization constants.

Analogously, referring at the quasiclassical solution $t=0$, Eq. (8), the corresponding negative $(-)$ and positive $(+)$ frequency solutions take the form

$$\phi_0=C_0^- M_{k,\mu}(z)+C_0^+ M_{k,-\mu}(z), \tag{32}$$

where C_0^- and C_0^+ are normalization constants.

Then, using the relation between $M_{k,\mu}(z)$ and $W_{k,\mu}(z)$, Ref. 9

$$M_{k,\mu}(z)=\Gamma(2\mu+1)e^{-i\pi k}\left[\frac{W_{-k,\mu}(-z)}{\Gamma(\frac{1}{2}+\mu-k)},+e^{i\pi(\mu+1/2)}\frac{W_{k,\mu}(z)}{\Gamma(\frac{1}{2}+\mu+k)}\right], \tag{33}$$

with $(-\pi/2<\arg z<3\pi/2;\ 2\mu\neq -1,-2,\dots)$, we have that the negative frequency solution ϕ_0^- can be written in terms of ϕ_∞^- and $(\phi_\infty^-)^*$ as follows:

$$\phi_0^-=\Gamma(2\mu+1)e^{-i\pi k}\left[\frac{\phi_\infty^-}{\Gamma(\frac{1}{2}+\mu-k)}+e^{i\pi(\mu+1/2)}\frac{(\phi_\infty^-)^*}{\Gamma(\frac{1}{2}+\mu+k)}\right], \tag{34}$$

where we have used the property $(W_{k,\mu}(z))^*=W_{-k,\mu}(-z)$.

Since we have been able to obtain single-particle states in the vicinity of $t=0$ as well as in the asymptote $t\to\infty$, we can compute the density of particles created by gravitational field.

From (34), and using the Bogoliubov coefficients,[8] we can write

$$\phi_0^-=\alpha\phi_\infty^-+\beta(\phi_\infty^-)^*. \tag{35}$$

From the normalization of the wave function, $|\alpha|^2-|\beta|^2=1$ and, taking into account (34), we obtain

$$\frac{|\beta|^2}{|\alpha|^2}=\exp-2\pi\sqrt{\lambda^2/a_0^2-\tfrac{1}{4}}, \tag{36}$$

that the density of scalar particles created is thermal.

(ii) $a(t)=e^{Ht}$, an inflationary universe: The basic idea of inflation is that the vacuum energy is the dominant component of the energy density of the universe, so the scale factor $a(t)$ grows exponentially. When that occurs the universe begins a de Sitter phase, expanding exponentially.

Substituting the above expression into (19), we obtain

$$\left(\frac{d^2}{dt^2}+\lambda^2e^{-2Ht}+m^2\right)\phi_1=0. \tag{37}$$

Introducing the new coordinate $z=(\lambda/H)\,e^{-Ht}$, Eq. (37) becomes the Bessel equation

$$\left(z^2\frac{d^2}{dz^2}+z\frac{d}{dz}+z^2+\frac{m^2}{H^2}\right)\phi_1=0, \tag{38}$$

whose solution can be expressed in terms of the Hankel functions[9] $H_\nu^{(1)}$ and $H_\nu^{(2)}$,

$$\phi_1=C_1H_{i\nu}^{(1)}\left(\frac{\lambda}{H}e^{-Ht}\right)+C_2H_{i\nu}^{(2)}\left(\frac{\lambda}{H}e^{-Ht}\right), \tag{39}$$

where C_1 and C_2 are arbitrary constants and $\nu=m/H$.

Let us analyze the behavior of the solution of Eq. (38). As $t\to-\infty$, we find that

$$\phi_{1,-\infty}=C_{1,-\infty}H_{i\nu}^{(1)}\left(\frac{\lambda}{H}e^{-Ht}\right)+C_{2,-\infty}H_{i\nu}^{(2)}\left(\frac{\lambda}{H}e^{-Ht}\right)=C'_{1,-\infty}e^{i(\lambda/H)\,e^{-Ht}}+C'_{2,-\infty}e^{-i\,(\lambda/H)\,e^{-Ht}}, \tag{40}$$

and when $t\to\infty$ we obtain

$$\phi_{1,\infty}=C_{1,\infty}J_{i\nu}\left(\frac{\lambda}{H}e^{-Ht}\right)+C_{2,\infty}J_{-i\nu}\left(\frac{\lambda}{H}e^{-Ht}\right)=C'_{1,\infty}(e^{-Ht})^{i\nu}+C'_{2,\infty}(e^{-Ht})^{-i\nu}$$
$$=C'_{1,\infty}e^{-imt}+C'_{2,\infty}e^{imt}. \tag{41}$$

We can identify the first and the second right hand side terms as positive and negative frequency modes, respectively, by comparing (40) and (41) with (13) and (15).

The recurrence relation between $H^{(1)}_{i\nu}(z)$ and $J_{i\nu}(z)$,

$$H^{(1)}_{i\nu}(z)=\frac{1}{\sinh(\pi\nu)}(e^{\pi\nu}J_{i\nu}(z)-J_{-i\nu}(z)), \tag{42}$$

permits one to express

$$\phi^{+}_{1,-\infty}=\frac{1}{\sinh(\pi\nu)}(e^{\pi\nu}\phi^{+}_{1,\infty}-(\phi^{+}_{1,\infty})^{*}). \tag{43}$$

Since $\phi^{+}_{1,-\infty}$ and $\phi^{+}_{1,\infty}$ are related via Bogoliubov coefficients, Eq. (43) gives

$$\phi^{+}_{1,-\infty}=\alpha\phi^{+}_{1,\infty}+\beta(\phi^{+}_{1,\infty})^{*}. \tag{44}$$

From $|\alpha|^2-|\beta|^2=1$, we obtain

$$\frac{|\beta|^2}{|\alpha|^2}=e^{-2\pi\nu}=e^{-2\pi m/H}. \tag{45}$$

The density of scalar particles created is thermal, and we get the Bose–Einstein distribution of scalar particles as follows:

$$|\beta|^2=\frac{1}{e^{2\pi m/H}-1}. \tag{46}$$

IV. SOLUTION OF THE DIRAC EQUATION

Now, we proceed to discuss the process of creation of spin-$\frac{1}{2}$ particles in the cosmological background (2). The covariant generalization of the Dirac equation in curved-space–time is

$$\{\overline{\gamma}^{\alpha}(\partial_{\alpha}-\Gamma_{\alpha})+m\}\Psi=0, \tag{47}$$

where Γ_{α} are the spinor connections, and $\overline{\gamma}^{\alpha}$ are the curvilinear Dirac matrices satisfying the anticommutation relations $\{\overline{\gamma}^{\alpha},\overline{\gamma}^{\beta}\}=2g^{\alpha\beta}$. The matrices $\overline{\gamma}^{\alpha}$ are related to the γ^{i}-standard flat Dirac matrices as follows:

$$\overline{\gamma}^{\alpha}=h^{\alpha}_{i}\gamma^{i}, \tag{48}$$

with $\{\gamma^{i},\gamma^{j}\}_{+}=2\eta^{ij}$. In the diagonal tetrad gauge h^{α}_{i} takes the form

$$h^{\alpha}_{i}=\mathrm{diag}\left(1,\frac{1}{a},\frac{1}{ab},\frac{1}{abc}\right), \tag{49}$$

and we can verify that $g^{\alpha\beta}=h^{\alpha}_{i}h^{\beta}_{j}\eta^{ij}$.

The connection spinor is defined by the relation

$$\Gamma_{\alpha}=-\tfrac{1}{4}(\partial_{\alpha}h^{\rho}_{i}+\Gamma^{\rho}_{\sigma\alpha}h^{\sigma}_{i})g_{\beta\rho}h^{\beta}_{j}\gamma^{j}\gamma^{i}, \tag{50}$$

and Γ_{α} take the form

$$\Gamma_0=0,\ \Gamma_1=\tfrac{1}{2}a_{.t}\gamma^0\gamma^1,\ \Gamma_2=\tfrac{1}{2}ba_{.t}\gamma^0\gamma^2+\tfrac{1}{2}b_{.x}\gamma^1\gamma^2,$$
$$\Gamma_3=\tfrac{1}{2}bca_{.t}\gamma^0\gamma^3+\tfrac{1}{2}cb_{.x}\gamma^1\gamma^3+\tfrac{1}{2}c_{.y}\gamma^2\gamma^3. \tag{51}$$

Substituting Eqs. (48), (49) and (51) into (47), we obtain

$$\left\{\gamma^0\partial_t+\frac{1}{a}\gamma^1\partial_x+\frac{1}{ab}\gamma^2\partial_y+\frac{1}{abc}\gamma^3\partial_z+m\right\}\psi=0, \tag{52}$$

where Ψ is related to ψ by

$$\Psi=a^{-3/2}b^{-1}c^{-1/2}\psi. \tag{53}$$

Since Eq. (52) commutes with $-i\partial_z$, we can write

$$\psi=\psi(t,x,y)e^{ik_zz}. \tag{54}$$

Applying the algebraic method of separation of variables,[14] it is possible to write Eq. (52) as a sum of two first-order differential operators commuting between them as follows:

$$[\hat{K}_1,\ \hat{K}_2]_-=0,\ (\hat{K}_1+\hat{K}_2)\Phi=0;\ \hat{K}_1\Phi=-k\Phi,\ \hat{K}_2\Phi=k\Phi, \tag{55}$$

where k is a constant of separation, and

$$\hat{K}_1=-i(ab\gamma^0\partial_t+b\gamma^1\partial_x+abm)\gamma^1\gamma^0,\ \hat{K}_2=-i\left(\gamma^2\partial_y+\frac{1}{c}\gamma^3\partial_z\right)\gamma^1\gamma^0, \tag{56}$$

$$\psi=\gamma^1\gamma^0\Phi. \tag{57}$$

Adopting a suitable representation of Dirac matrices,[13] we can apply the transformation $\Phi=S\phi$ defined by (Ref. 12)

$$S=\tfrac{1}{2}(I+\gamma^1\gamma^2+\gamma^2\gamma^3+\gamma^3\gamma^1), \tag{58}$$

and Eq. (55) reduces to the form

$$(ab\gamma^3\partial_t+b\gamma^0\partial_x+abm\gamma^3\gamma^0+ik)\phi=0, \tag{59}$$

$$\left(\gamma^1\gamma^3\gamma^0\partial_y+\frac{1}{c}\gamma^2\gamma^3\gamma^0\partial_z-ik\right)\phi=0. \tag{60}$$

Now, we proceed to solve Eq. (60), where the spinor ϕ has the following structure:[12]

$$\phi=\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}=\begin{pmatrix}\alpha(t,x)\chi_1(y)\\ \alpha(t,x)\chi_2(y)\\ \beta(t,x)\chi_1(y)\\ -\beta(t,x)\chi_2(y)\end{pmatrix}e^{ik_zz}. \tag{61}$$

Let us put the following as above.

(a) $c(y)=\sin y$: Substituting (61) into (60), we obtain

$$\left(\frac{d}{dy}+\frac{k_z}{\sin y}\right)\chi_1-k\chi_2=0,\quad \left(\frac{d}{dy}-\frac{k_z}{\sin y}\right)\chi_2+k\chi_1=0, \tag{62}$$

and the solutions take the form

$$\chi_1 = d_1(\sin y)^{k_z} \sin(y/2) P_n^{(k_z+1/2,k_z-1/2)}(\cos y), \tag{63}$$

$$\chi_2 = d_2(\sin y)^{k_z} \cos(y/2) P_n^{(k_z-1/2,k_z+1/2)}(\cos y), \tag{64}$$

where n reads as $n = ik - k_z - \frac{1}{2}$. To solve Eq. (59), it is convenient to introduce the auxiliary function ζ defined by

$$\phi = \left[(a\gamma^0\partial_t + am)\gamma^3\gamma^0 + \left(\gamma^0\partial_x - \frac{ik}{b} \right) \right] \zeta. \tag{65}$$

Substituting Eq. (65) into Eq. (59) we obtain two first-order differential operators commuting between them,

$$[\hat{K}_3,\ \hat{K}_4]_- = 0,\ (\hat{K}_3 + \hat{K}_4)\zeta = 0, \tag{66}$$

with

$$\hat{K}_3 = (a\gamma^0\partial_t + am)(-a\gamma^0\partial_t + am),\ \hat{K}_4 = \left(\gamma^0\partial_x + \frac{ik}{b} \right)\left(\gamma^0\partial_x - \frac{ik}{b} \right), \tag{67}$$

$$\hat{K}_3\zeta = -\lambda^2\zeta,\ \hat{K}_4\zeta = \lambda^2\zeta, \tag{68}$$

and λ is a constant of separation. From Eqs. (65), (67) and (68) the spinor ϕ can be written as follows:

$$\phi = C_0 \begin{pmatrix} f_1(t)g_1(x)\chi_1(y) \\ f_1(t)g_1(x)\chi_2(y) \\ f_3(t)g_3(x)\chi_1(y) \\ -f_3(t)g_3(x)\chi_2(y) \end{pmatrix} e^{ik_z z}, \tag{69}$$

where $f_1(t)$, $f_3(t)$, $g_1(x)$ and $g_3(x)$ satisfy

$$\left(\partial_x + \frac{k}{b} \right) g_1 = \lambda g_3, \quad \left(\partial_x - \frac{k}{b} \right) g_3 = -\lambda g_1, \tag{70}$$

$$(a\partial_t + iam) f_3 = -i\lambda f_1, \quad (a\partial_t - iam) f_1 = -i\lambda f_3. \tag{71}$$

(b) $b(x) = \sinh x$: Equation (70) becomes

$$\left(\frac{d}{dx} + \frac{k}{\sinh x} \right) g_1 - \lambda g_3 = 0, \quad \left(\frac{d}{dx} - \frac{k}{\sinh x} \right) g_3 + \lambda g_1 = 0, \tag{72}$$

the solutions of which are given by

$$g_1 = c_1(\sinh x)^k \sinh(x/2) P_n^{(k-1/2,k+1/2)}(-\cosh x), \tag{73}$$

$$g_3 = c_2(\sinh x)^k \cosh(x/2) P_n^{(k+1/2,k-1/2)}(-\cosh x), \tag{74}$$

where n is given by $n = i\lambda - k - \frac{1}{2}$.

When n is not an integer value, we have to express the Jacobi polynomials in terms of the Gauss hypergeometric functions by means of the relation[11]

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)} F\left(-n, n+\alpha+\beta+1, \alpha+1, \frac{1-x}{2} \right). \tag{75}$$

Now we proceed to analyze the asymptotic limit as $t\to 0$ and $t\to\infty$ of the spinor solution (69). We consider these two special models for expansion:

(i) $a(t)=a_0 t$: From Eq. (71), we obtain

$$\left(\frac{d^2}{dt^2}+\frac{\lambda^2/a_0^2+1/4}{t^2}\mp\frac{im}{t}+m^2\right)h_{1,3}=0, \tag{76}$$

where $f_{1,3}=t^{-1/2}h_{1,3}$. This Whittaker equation has as a solution the expression

$$C_1 W_{k,\mu}(2imt)+C_2 M_{k,\mu}(2imt), \tag{77}$$

where $k=\frac{1}{2}$, $\mu=i\lambda/a_0$ and the type of Whittaker function to be considered depends on the value of t.

For large values in time ($t\to\infty$) the positive and negative frequency modes are solutions

$$\begin{gathered} f^{+}_{1,\infty}=C^{+}_{\infty}t^{-1/2}W_{k,\mu}(2imt),\quad f^{-}_{1,\infty}=C^{-}_{\infty}t^{-1/2}W_{-k,\mu}(-2imt),\\ f^{+}_{3,\infty}=-\frac{ia_0{}^{1/2}}{\lambda}C^{+}_{\infty}t^{-1/2}W_{-k,\mu}(2imt),\quad f^{-}_{3,\infty}=\frac{i\lambda}{a_0^{3/2}}C^{-}_{\infty}t^{-1/2}W_{k,\mu}(-2imt), \end{gathered} \tag{78}$$

where C^{+}_{∞}, C^{-}_{∞} are normalization constants, and we have the Whittaker identity[9] with $k=+\frac{1}{2}$ to the first identity and $k=-\frac{1}{2}$ to the second identity:

$$\begin{gathered} z\frac{d}{dz}W_{k,\mu}(z)=\left(\frac{1}{2}+\mu-k\right)\left(\frac{1}{2}-\mu-k\right)W_{k-1,\mu}(z)+\left(k-\frac{z}{2}\right)W_{k,\mu}(z),\\ z\frac{d}{dz}W_{k,\mu}(z)=\left(\frac{z}{2}-k\right)W_{k,\mu}(z)-W_{k+1,\mu}(z). \end{gathered} \tag{79}$$

Analogously for small values of t ($t\to 0$) we have

$$\begin{gathered} f^{+}_{1,0}=C^{+}_{0}t^{-1/2}M_{k,-\mu}(2imt),\quad f^{-}_{1,0}=C^{-}_{0}t^{-1/2}M_{k,\mu}(2imt),\\ f^{+}_{3,0}=C^{+}_{0}t^{-1/2}M_{-k,-\mu}(2imt),\quad f^{-}_{3,0}=-C^{-}_{0}t^{-1/2}M_{-k,\mu}(2imt), \end{gathered} \tag{80}$$

where C^{+}_{0}, C^{-}_{0} are normalization constants, and we have used the following relation:[11]

$$z\frac{d}{dz}M_{k,\mu}(z)=\left(\frac{z}{2}-k\right)M_{k,\mu}(z)+\left(\frac{1}{2}+\mu+k\right)M_{k+1,\mu}(z). \tag{81}$$

In both cases, the choice of the modes was based on a comparison with the quasiclassical behavior given by Eqs. (7) and (8). In the asymptotes, we obtain a time dependent term multiplied by a factor depending on space variables.

Considering Eq. (33), we can express the negative frequency mode solution $\phi^{-}_{1,0}$ in terms of $\phi^{-}_{1,\infty}$ and $\phi^{+}_{1,\infty}$ as follows:

$$\phi^{-}_{1,0}=\Gamma(2\mu+1)e^{-i\pi k}\left[\frac{\phi^{-}_{1,\infty}}{\Gamma\left(\frac{1}{2}+\mu-k\right)}+e^{i\pi(\mu+1/2)}\frac{\phi^{+}_{1,\infty}}{\Gamma\left(\frac{1}{2}+\mu+k\right)}\right], \tag{82}$$

and using the Bogoliubov coefficients we obtain

$$\phi^{-}_{1,0}=\alpha\phi^{-}_{1,\infty}+\beta\phi^{+}_{1,\infty}. \tag{83}$$

Considering the normalization condition of the wave function $|\alpha|^2+|\beta|^2=1$, we arrive at

$$\frac{|\beta|^2}{|\alpha|^2}=e^{-2\pi\lambda/a_0}, \tag{84}$$

and we compute the density of particles created by the gravitational field

$$n=|\beta|^2=\frac{1}{e^{2\pi\lambda/a_0}+1}, \tag{85}$$

a result that can be identified as a Fermi–Dirac distribution of particles. We can already establish that the spectrum of particles created is a thermal one with the temperature $T=a_0/2\pi$.

(ii) $a(t)=e^{Ht}$: From Eq. (71) we have

$$\left(\frac{d^2}{dt^2}-\frac{H^2}{4}\mp imH+\lambda^2e^{-2Ht}+m^2\right)h_{1,3}=0, \tag{86}$$

where $f_{1,3}=e^{-Ht/2}h_{1,3}$. Introducing the change of variables $z=(\lambda/H)\,e^{-Ht}$ into (86), we get the Bessel equation

$$\left(z^2\frac{d^2}{dz^2}+z\frac{d}{dz}+z^2-\nu^2\right)h_{1,3}=0, \tag{87}$$

the solution of which has the form

$$h_{1,3}=CZ_{1/2\pm im/H}(z). \tag{88}$$

Then, looking at the asymptotic behavior of the Hankel function as $z\to\infty$ $(t\to-\infty)$, (Ref. 9)

$$H_\nu^{(2)}(z)\sim\sqrt{\frac{2}{\pi z}}e^{-i(z-\nu\pi/2-\pi/4)}, \tag{89}$$

and the behavior of the Bessel function at $z\to0$ $(t\to\infty)$,

$$J_\nu(z)\sim\frac{z^\nu}{2^\nu\Gamma(\nu+1)}, \tag{90}$$

we have for $z\to\infty$ $(t\to-\infty)$ that the positive and negative frequency modes are solutions

$$\begin{gathered}f_{1,\infty}^{+}=C_\infty^{+}z^{1/2}H_{1/2+im/H}^{(2)}(z),\quad f_{1,\infty}^{-}=C_\infty^{-}z^{1/2}H_{-1/2-im/H}^{(2)}(z),\\ f_{3,\infty}^{+}=-iC_\infty^{+}z^{1/2}H_{-1/2+im/H}^{(2)}(z),\quad f_{3,\infty}^{-}=iC_\infty^{-}z^{1/2}H_{1/2-im/H}^{(2)}(z),\end{gathered} \tag{91}$$

where C_∞^{+}, C_∞^{-} are constants of normalization, and we have used the Bessel functions identities[11]

$$\begin{aligned}\frac{d}{dz}J_\nu(z)&=J_{\nu-1}(z)-\frac{\nu}{z}J_\nu(z),\\ \frac{d}{dz}J_\nu(z)&=-J_{\nu+1}(z)+\frac{\nu}{z}J_\nu(z).\end{aligned} \tag{92}$$

Analogously for $z\to0$ $(t\to\infty)$ we obtain

$$f^{+}_{1,0}=C^{+}_{0}z^{1/2}J_{1/2+im/H}(z),\quad f^{-}_{1,0}=C^{-}_{0}z^{1/2}J_{-1/2-im/H}(z),$$
$$f^{+}_{3,0}=-iC^{+}_{0}z^{1/2}J_{-1/2+im/H}(z),\quad f^{-}_{3,0}=iC^{-}_{0}z^{1/2}J_{1/2-im/H}(z), \tag{93}$$

where C^{+}_{∞}, C^{-}_{∞} are constants of normalization.

From the relation existing between the Hankel and the Bessel functions,[11]

$$H^{(2)}_{\nu}(z)=\frac{e^{i\pi\nu}J_{\nu}(z)-J_{-\nu}(z)}{i\sin\pi\nu}, \tag{94}$$

we have that the positive frequency mode solution $\phi^{+}_{1,\infty}$ can be expressed in terms of $\phi^{+}_{1,0}$ and $\phi^{-}_{1,0}$ as

$$\phi^{+}_{1,\infty}=\mathcal{D}(\phi^{+}_{1,0}-e^{i\pi\nu}\phi^{-}_{1,0})=\alpha\phi^{+}_{1,0}+\beta\phi^{-}_{1,0}, \tag{95}$$

where $\mathcal{D}$ is a constant. Since $|\alpha|^2+|\beta|^2=1$, we obtain

$$\frac{|\beta|^2}{|\alpha|^2}=e^{-2\pi m/H}, \tag{96}$$

and the rate of particles created is

$$n=|\beta|^2=\frac{1}{e^{2\pi m/H}+1}. \tag{97}$$

We obtain the thermal Fermi–Dirac distribution for $|\beta|^2$ and the exponential has the form of a Boltzmann factor with temperature $T=H/2\pi$.

V. SCALAR PARTICLES IN THE PRESENCE OF A CONSTANT ELECTRIC FIELD

Now, we consider the scalar particles when a constant electric field minimally coupled to the spinor field is present. Then the Hamilton–Jacobi equation coupled to an electromagnetic field can be written as

$$g^{\alpha\beta}(\partial_{\alpha}S-eA_{\alpha})(\partial_{\beta}S-eA_{\beta})+m^2=0. \tag{98}$$

Reducing b at unit, the line element (2) takes the following form,

$$ds^2=-dt^2+e^{2Ht}(dx^2+dy^2+c^2(y)dz^2), \tag{99}$$

where $a(t)=e^{Ht}$ for an inflationary universe and we obtain some particular cases

$$c(y)=\begin{cases}\sin y & \text{Kantowiski–Sacks models,}\\ y & \text{Bianchi I,}\\ \sinh y & \text{Bianchi III.}\end{cases} \tag{100}$$

The solution of Eq. (98) can be separated as

$$S=F(t)-k_x x+H(y)-k_z z. \tag{101}$$

The vector potenial A_{μ} associated with a constant field E_0 is

$$A_{\mu}=\left(0,\ -\frac{E_0}{H}e^{Ht},\ 0,\ 0\right). \tag{102}$$

Substituting (99) and (101) into (98) we obtain

$$-F_{.t}^2+\frac{1}{e^{2Ht}}\left(-k_x+\frac{eE_0}{H}e^{Ht}\right)^2+\frac{1}{e^{2Ht}}H_{.y}^2+\frac{1}{c^2e^{2Ht}}k_z^2+m^2=0. \tag{103}$$

Then the solution of Eq. (103) presents the following asymptotic behavior. For $t\to-\infty$,

$$S(t,x,y,z)=-k_xx-k_zz\pm\int\sqrt{\lambda^2-\frac{k_z^2}{c^2}}dy\mp\frac{\sqrt{\lambda^2+k_x^2}}{H}e^{-Ht}, \tag{104}$$

$$\phi_{-\infty}=e^{iS}\to C(x,y,z)\exp\left(\mp i\frac{\sqrt{\lambda^2+k_x^2}}{H}e^{-Ht}\right), \tag{105}$$

and for $t\to\infty$

$$S(t,x,y,z)=-k_xx-k_zz\pm\int\sqrt{\lambda^2-\frac{k_z^2}{c^2}}dy\pm\sqrt{m^2+\frac{e^2E_0^2}{H^2}}t, \tag{106}$$

$$\phi_{\infty}=e^{iS}\to C(x,y,z)\exp\left(\mp i\sqrt{m^2+\frac{e^2E_0^2}{H^2}}t\right). \tag{107}$$

For scalar particles, the Klein–Gordon equation in minimal coupling is written as

$$g^{\alpha\beta}(\nabla_\alpha-ieA_\alpha)(\nabla_\beta-ieA_\beta)\phi-m^2\phi=0. \tag{108}$$

Equation (108) becomes

$$\left(\partial_t^2-\frac{1}{a^2}\left((\partial_x-ieA_1)^2+\partial_y^2+\frac{1}{c^2}\partial_z^2\right)+m^2\right)\psi=0. \tag{109}$$

Since Eq. (109) commutes with the operators $-i\partial_x$ and $-i\partial_z$, we can look at a solution of the form $\psi=e^{ik_xx+ik_zz}\phi$, which reduces Eq. (109) after separation of variables to

$$\left(\partial_t^2-\frac{1}{a^2}\left(ik_x+ie\frac{E_0e^{Ht}}{H}\right)^2+\frac{1}{a^2}\lambda^2+m^2\right)\phi_1=0, \tag{110}$$

$$\left(\partial_y^2-\frac{1}{c^2}k_z^2+\lambda^2\right)\phi_2=0, \tag{111}$$

where λ is a constant of separation and $\phi(t,y)=\phi_1(t)\phi_2(y)$.

For the Kantowiski–Sacks model $c(y)=\sin y$, and we obtain the solution by

$$\phi_2=A\sin^qyF(\tfrac{1}{2}(q+\lambda),\tfrac{1}{2}(q-\lambda),q+\tfrac{1}{2},\sin^2y), \tag{112}$$

where $q=\frac{1}{2}+(k_z^2+\frac{1}{4})^{1/2}$.

For the Bianchi I model $c(y)=y$, we arrive at

$$\phi_2=By^{1/2}Z_\nu(\lambda y), \tag{113}$$

where Z_ν is the general solution of the cylindrical Bessel equation and $\nu=(k_z^2+\frac{1}{4})^{1/2}$.

For the Bianchi III model $c(y)=\sinh y$, the solution takes the form

$$\phi_2=C\sinh^qyF(\tfrac{1}{2}(q+i\lambda),\tfrac{1}{2}(q-i\lambda),q+\tfrac{1}{2},-\sinh^2y), \tag{114}$$

where $q=\frac{1}{2}+(k_z^2+\frac{1}{4})^{1/2}$.

We analyze the inflationary universe case $a(t)=e^{Ht}$, and Eq. (101) can be written as follows,

$$\left(\frac{d^2}{dz^2}+\frac{1}{z}\frac{d}{dz}+\frac{2eE_0k_x}{H^2z}+\frac{e^2E_0^2}{H^2z^2}+\frac{m^2}{H^2z^2}+k_x^2+\lambda^2\right)\phi_1=0, \tag{115}$$

where $z=(1/H)\,e^{-Ht}$. Therefore, we can reduce Eq. (115) to

$$\left(\frac{d^2}{dz^2}+\frac{\frac{1}{4}+e^2E_0^2/H^4+m^2/H^2}{z^2}+\frac{2eE_0k_x}{H^2z}+k_x^2+\lambda^2\right)f=0, \tag{116}$$

with $\phi_1=z^{-1/2}f$. Making a change of variables $u=2i\epsilon(k_x^2+\lambda^2)^{1/2}z$, with $\text{sign}(\epsilon)=\pm1$, we get as a solution for $\text{sign}(\epsilon)=-1$

$$C_1W_{k,\mu}(2i\sqrt{k_x^2+\lambda^2}z)+C_2M_{k,\mu}(2i\sqrt{k_x^2+\lambda^2}z), \tag{117}$$

where

$$\mu=\frac{i}{H^2}\sqrt{m^2H^2+e^2E_0^2}=i|\mu|,\quad k=\frac{ieE_0k_x}{H^2\sqrt{k_x^2+\lambda^2}}. \tag{118}$$

For $z\to\infty$ $(t\to-\infty)$, we get the negative and the positive frequency mode solutions in the form

$$\begin{aligned}\phi_{1,\infty}^{+}&=C_\infty^{+}z^{-1/2}W_{k,\mu}(2i\sqrt{k_x^2+\lambda^2}z),\\ \phi_{1,\infty}^{-}&=C_\infty^{-}z^{-1/2}W_{-k,\mu}(-2i\sqrt{k_x^2+\lambda^2}z),\end{aligned} \tag{119}$$

and for $z\to0$ $(t\to\infty)$ we have

$$\begin{aligned}\phi_{1,0}^{+}&=C_0^{+}z^{-1/2}M_{k,-\mu}(2i\sqrt{k_x^2+\lambda^2}z),\\ \phi_{1,0}^{-}&=C_0^{-}z^{-1/2}M_{k,\mu}(-2i\sqrt{k_x^2+\lambda^2}z),\end{aligned} \tag{120}$$

where C_∞^{+}, C_∞^{-}, C_0^{+} and C_0^{-} are constants of normalization.

Then, using the relation[9]

$$M_{k,\mu}(z)=\Gamma(2\mu+1)e^{i\pi\lambda}\left[\frac{W_{-k,\mu}(e^{i\pi}z)}{\Gamma(\mu-k+\frac{1}{2})}+e^{-i\pi(\mu+1/2)}\frac{W_{k,\mu}(z)}{\Gamma(\mu+k+\frac{1}{2})}\right], \tag{121}$$

with $(-3\pi/2<\arg z<\pi/2;\ 2\mu\neq-1,-2,\ldots)$, and the following relation[9]

$$|\Gamma(\tfrac{1}{2}+iy)|^2=\frac{\pi}{\cosh\pi y}, \tag{122}$$

we arrive at

$$\frac{|\alpha|^2}{|\beta|^2}=\frac{\cosh(\pi|\mu|+\pi eE_0k_x/H^2\sqrt{k_x^2+\lambda^2})}{\cosh(\pi|\mu|-\pi eE_0k_x/H^2\sqrt{k_x^2+\lambda^2})}e^{-2\pi|\mu|}. \tag{123}$$

For $|\mu\pm eE_0k_x/H^2\sqrt{k_x^2+\lambda^2}|\gg1$, Eq. (123) becomes

$$\frac{|\alpha|^2}{|\beta|^2}=\exp\left(-2\pi\left[|\mu|-\frac{eE_0k_x}{H^2\sqrt{k_x^2+\lambda^2}}\right]\right). \tag{124}$$

Considering the normalization condition $|\alpha|^2+|\beta|^2=1$, we obtain the thermal distribution

$$|\beta|^2=\frac{1}{1+\exp(2\pi[|\mu|-eE_0k_x/H^2\sqrt{k_x^2+\lambda^2}])}\approx\exp\left(-\frac{2\pi}{H^2}\left[(m^2H^2+e^2E_0^2)^{1/2}-\frac{eE_0k_x}{H^2\sqrt{k_x^2+\lambda^2}}\right]\right). \tag{125}$$

It points out that the temperature depends on the intensity of the electric field E_0 and on the impulsion k_x of the particle. Moreover, we have that $|\beta|^2$ changes according to the sign of ϵ; the result for $\text{sign}(\epsilon)=+1$ is obtained by replacing e by $-e$ in Eq. (125).

In $(1+1)$ dimension,[2,4] we have $\lambda=0$ and Eq. (125) becomes

$$|\beta|^2\approx\exp\left(-\frac{2\pi}{H^2}[(m^2H^2+e^2E_0^2)^{1/2}-eE_0]\right). \tag{126}$$

In the limit $H\to 0$, we obtain a Minkowski (flat) metric, and the exponent of $|\beta|^2$ in Eq. (126) takes the form

$$\lim_{H\to 0}\left(-\frac{2\pi eE_0}{H^2}\left[\left(\frac{m^2H^2}{e^2E_0^2}+1\right)^{1/2}-1\right]\right)\to-\frac{\pi m^2}{eE_0}, \tag{127}$$

which reduces the flat limit of the density of particles created to

$$|\beta|^2_{\text{flat}}=\lim_{H\to 0}|\beta|^2=e^{-\pi m^2/eE_0}. \tag{128}$$

This result is obtained by Villalba[2] in the study of particle creation by a strong constant electric field in de Sitter space, and it is proportional to the probability, per unit time, per unit volume of pair created by a constant electric field obtained by Schwinger.[10]

VI. CONCLUSION

After solving the relativistic Hamilton–Jacobi, Klein–Gordon and Dirac equations in the gravitational background (2) by separation of variables, we identify the relativistic solutions of negative and positive frequency modes and make comparison with the quasiclassical one obtained by the Hamilton–Jacobi equation to compute the density of scalar and spin-$\frac{1}{2}$ particles.

We also study some special cases of background when a constant electric field is present and calculate the thermal distribution of the density of particles created. We recover the result found in de Sitter space[2,4] in $(1+1)$ dimensions.

ACKNOWLEDGMENTS

It is a pleasure to thank J. Govaerts for useful discussions. My thanks also go to M. N. Hounkonnou and J. Tossa for many conversations.

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Trigonometric osp(1|2) Gaudin model

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(Received 10 July 2002; accepted 22 October 2002)

The problems connected with Gaudin models are reviewed by analyzing model related to the trigonometric osp(1|2) classical r-matrix. The eigenvectors of the trigonometric osp(1|2) Gaudin Hamiltonians are found using explicitly constructed creation operators. The commutation relations between the creation operators and the generators of the trigonometric loop superalgebra are calculated. The coordinate representation of the Bethe states is presented. The relation between the Bethe vectors and solutions to the Knizhnik–Zamolodchikov equation yields the norm of the eigenvectors. The generalized Knizhnik–Zamolodchikov system is discussed both in the rational and in the trigonometric case. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1531250]

I. INTRODUCTION

Classifying integrable systems solvable in the framework of the quantum inverse scattering method[1–3] by underlying dynamical symmetry algebras, one could say that the Gaudin models are the simplest ones being based on loop algebras and classical r-matrices. More sophisticated solvable models correspond to more complicated algebras: Yangians, quantum affine algebras, elliptic quantum groups, dynamical quantum groups, etc.

Gaudin models[4,5] are related to classical r-matrices, and the density of Gaudin Hamiltonians

$$H^{(a)}=\sum_{b\neq a}^{N} r_{ab}(z_a-z_b) \tag{1.1}$$

coincides with the r-matrix. The condition of their commutativity $[H^{(a)},H^{(b)}]=0$ is nothing else but the classical Yang–Baxter equation (YBE)

$$[r_{ab}(z_a-z_b),r_{ac}(z_a-z_c)+r_{bc}(z_b-z_c)]+[r_{ac}(z_a-z_c),r_{bc}(z_b-z_c)]=0, \tag{1.2}$$

where r is antisymmetric and belongs to the tensor product $\mathfrak{g}\otimes\mathfrak{g}$ of a Lie algebra $\mathfrak{g}$, or its representations and the indices fix the corresponding factors in the N-fold tensor product of this algebra (see Sec. II).

The Gaudin models (GMs) related to classical r-matrices of simple Lie algebras were studied intensively (see Refs. 5–14 and references therein). The spectrum and eigenfunctions were found using different methods (coordinate and algebraic Bethe ansatz,[5,6] separated variables,[6] etc.). The correlation functions were evaluated for $\mathfrak{g}=\mathrm{sl}(2)$ by the Gauss factorization approach.[7] A relation to the Knizhnik–Zamolodchikov (KZ) equation of conformal filed theory was established.[11–13]

There exists a variety of classical r-matrices with trigonometric dependence on spectral parameter. Although algebraic construction of integrals of motion is straightforward, the calculation

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of the spectrum and the corresponding eigenstates, by means of algebraic Bethe ansatz, still depends on the underlining Lie algebra and r-matrix. Moreover, many trigonometric r-matrices are invariant under diagonal action of the Cartan subalgebra only,

$$[h_a+h_b \ , \ r_{ab}(z_a-z_b)]=0\,, \tag{1.3}$$

as opposed to the rational case where the classical r-matrix is invariant under the action of the whole Lie algebra $\mathfrak{g}$. Hence, one can modify the Gaudin Hamiltonian (1.1) by adding a local generator of the Cartan subalgebra

$$H_a \to \tilde{H}^{(a)}=g\,h_a+H^{(a)}\,. \tag{1.4}$$

This modification does not change the creation operators, but the Bethe equations and solutions to the KZ system. However, the dependence on the parameter g (a magnetic field) will be described by a difference equation.[15,16]

The aim of this article is to review problems connected with Gaudin models by analyzing the model related to the trigonometric osp(1|2) classical r-matrix. Results obtained here are in many respects similar to the ones we obtained in the case of osp(1|2)-invariant rational r-matrix.[17] However, connection of Gaudin model with magnetic field and KZ equations requires modification of the latter by adding a dynamical difference equation.[15,16]

There are additional peculiarities of Gaudin models related to classical r-matrices based on Lie superalgebras due to Z_2-grading of representation spaces and operators. The study of the osp(1|2)-invariant Gaudin model corresponding to the simplest nontrivial super-case of the osp(1|2) invariant r-matrix[18] started in Ref. 19. The spectrum of the osp(1|2) invariant Gaudin Hamiltonians $H^{(a)}$ was given, an antisymmetry property of their eigenstates was claimed, and a two site model was connected with some physically interesting one (a Dicke model). Let us also point out that recently rational and trigonometric sl(2) Gaudin models were used to describe different physical phenomena in metallic grains[20] and a condensate fragmentation of confined bosons.[21] Connection with perturbed WZNW models of conformal field theory was found in Ref. 22.

The creation operators used in the sl(2) Gaudin model [and similarly for sl(n) case] coincide with one of the L-matrix entry.[5,6] However, in the osp(1|2) case, as it was shown for rational r-matrix,[17] the creation operators are complicated polynomials of the two generators $X^+(\lambda)$ and $v^+(\mu)$ of the loop superalgebra. We introduce B-operators belonging to the Borel subalgebra of the trigonometric loop superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$ by a recurrence relation. Acting on the lowest spin vector (bare vacuum) $B_M(\mu_1,\ldots,\mu_M)\Omega_-$ the B-operators generate exact eigenstates of the Gaudin Hamiltonians $H^{(a)}$, provided Bethe equations are imposed on parameters $\{\mu_j\}$ of the states. For this reason the B-operators are sometimes referred to as the creation operators and the eigenstates as the Bethe vectors, or simply B-vectors. Furthermore, the recurrence relation is solved explicitly and the commutation relations between the B-operators and the generators of the loop superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$ as well as the generators of the global superalgebra $\mathrm{osp}(1|2)\subset\mathcal{L}_t(\mathrm{osp}(1|2))$ are calculated. We prove that the constructed states are eigenvectors of the generator of the global Cartan subalgebra h_{gl}, but the B-vectors are not the lowest spin vectors anymore, as it was the case for the invariant model.[23,17] Analogously to the rational case,[17] a striking coincidence between the spectrum of the osp(1|2) invariant Gaudin Hamiltonians of spin s and the spectrum of the Hamiltonians of the sl(2) Gaudin model of the integer spin $2s$ is also confirmed in the trigonometric case.

A connection between the B-states, when the Bethe equations are not imposed on their parameters (''off-shell Bethe states''), of the Gaudin models for simple Lie algebras to the solutions of the Knizhnik–Zamolodchikov equation was established in Refs. 11 and 12. An explanation of this connection based on Wakimoto modules at critical level of the underlying affine algebra was given in Ref. 12. An explicit form of the Bethe vectors in the coordinate representation was given in both Refs. 11 and 12. The coordinate Bethe ansatz for the B-states of the osp(1|2) Gaudin model is obtained in our article as well. Using commutation relations between the B-operators and the

transfer matrix $t(\lambda)$, as well as the Hamiltonians $H^{(a)}$, we give an algebraic proof of the fact that explicitly constructed B-states yield a solution to the Knizhnik–Zamolodchikov equation corresponding to a conformal field theory. This connection permits us to calculate the norm of the eigenstates of the Gaudin Hamiltonians. An analogous connection is expected between quantum osp(1|2) spin system related to the graded Yang–Baxter equation[18,24–26] and quantum Knizhnik–Zamolodchikov equation following the lines of Ref. 27. We point out possible modifications of the Gaudin Hamiltonians and corresponding modifications of the Knizhnik–Zamolodchikov equation, similar to the case of the sl(2) Gaudin model which was interpreted in Refs. 28 and 29 as a quantization of the Schlesinger system for isomonodromy deformation.

The norm and correlation functions of the sl(2) invariant Gaudin model were evaluated in Ref. 7 using Gauss factorization of a group element and the Riemann–Hilbert problem. The study of this problem for the trigonometric Gaudin model based on the osp(1|2) Lie superalgebra is in progress. However, we propose a formula for the scalar products of the Bethe states which is analogous to the sl(2) case.

The article is organized as follows. In Sec. II we review the main data of the quantum trigonometric osp(1|2) spin system: the osp(1|2) solution to the graded Yang–Baxter equation (R-matrix), monodromy matrix $T(\lambda)$, the transfer matrix $t(\lambda)=\mathrm{str}T(\lambda)$, its eigenvalues and the Bethe equations. The eigenvectors of this quantum integrable spin system can be constructed only by a complicated recurrence procedure[30] which is not given here. Nevertheless, it is useful to remind the main data of the quantum integrable spin system because some characteristics of the corresponding Gaudin model can be obtained easily as a quasi-classical limit of these data. The trigonometric osp(1|2) Gaudin model and its creation operators B_M are discussed thoroughly in Sec. III. Some of the most important properties of these operators are formulated and demonstrated pure algebraically: antisymmetry with respect to their arguments, commutation relations with the trigonometric loop superalgebra generators, commutation relations with the generating function $t(\lambda)$ of the Gaudin Hamiltonians, and a differential identity, valid in the case of the Gaudin realization of the loop superalgebra. Using these properties of the B-operators we prove in Sec. IV that, acting on the lowest spin vector Ω_-, these operators generate eigenvectors of the generating function of integrals of motion, provided the Bethe equations are imposed on the arguments of the B-operators. Possible modifications of the Gaudin Hamiltonians are pointed out, also. In particular, one of them yields Ricardson type Hamiltonian. An algebraic proof is given in Sec. V that constructed Bethe vectors are entering into solutions of the Knizhnik–Zamolodchikov equation of conformal field theory. A quasi-classical asymptotic with respect to a parameter of the Knizhnik–Zamolodchikov equation permits us to calculate the norm of the eigenstates of the Gaudin Hamiltonian. We pointed out that modification of Gaudin Hamiltonians by adding a Cartan element requires a more complicated change of KZ system, as opposed to the rational case. Further development on possible evaluation of correlation functions is discussed in Sec. VI. Finally, some definitions of the orthosymplectic Lie superalgebra osp(1|2) are given in the Appendix.

II. QUANTUM osp(1|2) SUPERALGEBRA AND CORRESPONDING SPIN SYSTEM

The quantum superalgebra $\mathcal{U}_q(\mathrm{osp}(1|2))$ as a deformation of the universal enveloping algebra of the Lie superalgebra osp(1|2) (see Appendix) is generated by three elements h, v^+, v^-.[31,32] The q-deformed commutation relations between the generators are

$$[h,v^{\pm}]_-=\pm v^{\pm}, \quad [v^+,v^-]_+=-\frac{q^h-q^{-h}}{q-q^{-1}}:=-[h]_q. \tag{2.1}$$

Its center is spanned by the q-deformed Casimir element

$$c_2(q)=A(q)([h]_q)^2+B(q)-\frac{(q^{1/2}+q^{-1/2})^2}{2}[v^{+2},v^{-2}]_+ +\frac{(q+q^{-1})}{4}(q^h+q^{-h})[v^+,v^-]_- \tag{2.2}$$

with $2A(q)=q+q^{-1}+\frac{1}{2}(q-q^{-1})^2$ and $B(q)=(q^{1/2}+q^{-1/2})^{-2}$. The q-deformed Casimir element can be written also in the form

$$c_2(q)=([h-\tfrac{1}{2}]_q)^2-(q^{1/2}+q^{-1/2})^2 v^+{}^2 v^-{}^2+(q^{h-1}+q^{-h+1})v^+v^-. \tag{2.3}$$

Like in the case of the Lie superalgbra osp(1|2) (see the Appendix), there exists an element

$$c_1(q)=([h-\tfrac{1}{2}]_q+(q^{1/2}+q^{-1/2})v^+v^-), \quad (c_1(q))^2=c_2(q), \tag{2.4}$$

with a grading property $[c_1,h]=0$ and $c_1v^{\pm}=-v^{\pm}c_1$. In the quasi-classical limit $q\to 1$ the relations (2.1)–(2.4) are reduced to the Lie superalgebra osp(1|2) ones.[33] There is a coproduct map $\Delta:\mathcal{U}_q\to\mathcal{U}_q\otimes\mathcal{U}_q$ consistent with the commutation relations (2.1) and a universal R-matrix $\mathcal{R}$ as an element of $\mathcal{U}_q\otimes\mathcal{U}_q$.[31,32] Let us write its matrix form $R(q)=(\rho\otimes\rho)\mathcal{R}$ in the basis $e_1\otimes e_1, e_1\otimes e_2, e_1\otimes e_3,\ldots,e_3\otimes e_3$ of the tensor product of two copies of the fundamental representation $V^{(1)}\otimes V^{(1)}$, $\rho:\mathcal{U}_q\to\mathrm{End}(V^{(1)})$,

$$R(q)=\begin{pmatrix} q & & & & & & & & \\ & 1 & & a & & & & & \\ & & q^{-1} & & b & & c & & \\ & & & 1 & & & & & \\ & & & & 1 & & b & & \\ & & & & & 1 & & a & \\ & & & & & & q^{-1} & & \\ & & & & & & & 1 & \\ & & & & & & & & q \end{pmatrix}, \tag{2.5}$$

here $a=q-q^{-1}$, $b=q^{-3/2}-q^{1/2}$ and $c=(1+q^{-1})(q-q^{-1})$. Multiplying $R(q)$ by the graded permutation $\mathcal{P}$ of $V^{(1)}\otimes V^{(1)}$: $(\mathcal{P})_{ab;cd}=(-1)^{p(a)p(b)}\delta_{ad}\delta_{bc}$, one gets the braid group form of the R-matrix $\check{R}(q)=R(q)\mathcal{P}$ which has a spectral decomposition. Using the projectors on the irreducible representation components in the Clebsch–Gordan decomposition $V^{(1)}\otimes V^{(1)}=V^{(2)}\oplus V^{(1)}\oplus V^{(0)}$, one can represent this R-matrix in the form[31,32]

$$\check{R}(q)=-q^{-2}P_0(q)-q^{-1}P_1(q)+qP_2(q), \tag{2.6}$$

where projectors are

$$P_0(q)=\frac{q^{1/2}+q^{-1/2}}{q^{3/2}+q^{-3/2}}\begin{pmatrix} 0 & & & & & & & & \\ & 0 & & & & & & & \\ & & q^{-1} & & q^{-1/2} & & -1 & & \\ & & & 0 & & & & & \\ & & -q^{-1/2} & & -1 & & q^{1/2} & & \\ & & & & & 0 & & & \\ & & -1 & & -q^{1/2} & & q & & \\ & & & & & & & 0 & \\ & & & & & & & & 0 \end{pmatrix}, \tag{2.7}$$

$$P_1(q)=\frac{1}{q+q^{-1}}\begin{pmatrix} 0 & & & & & & & & \\ & q^{-1} & & -1 & & & & & \\ & & -1 & & -\nu & & 1 & & \\ & -1 & & q & & & & & \\ & & \nu & & \nu^2 & & -\nu & & \\ & & & & & q^{-1} & & -1 & \\ & & 1 & & \nu & & -1 & & \\ & & & & & -1 & & q & \\ & & & & & & & & 0 \end{pmatrix}, \tag{2.8}$$

here $\nu=q^{1/2}+q^{-1/2}$, and $P_2(q)=I-P_0(q)-P_1(q)$. By the Baxterization procedure, or simply changing functions $(\lambda-a)/(\lambda+a)$ to the trigonometric ones $\sinh(\lambda-a)/\sinh(\lambda+a)$ in the osp(1|2)-invariant R-matrix,[18,17] one gets the trigonometric R-matrix related to the quantum affine algebra $\mathcal{U}_q(\widehat{\mathrm{osp}(1|2)})$

$$\check{R}(\lambda,\eta)=P_2-\frac{\sinh(\lambda-2\eta)}{\sinh(\lambda+2\eta)}P_1-\frac{\sinh(\lambda-3\eta)}{\sinh(\lambda+3\eta)}P_0. \tag{2.9}$$

Here $q=e^{2\eta}$ (normalized to $\lambda=0$ $\check{R}=\mathbf{1}$). The L-operator of the quantum spin system on a one-dimensional lattice with N sites coincides with R-matrix acting on a tensor product $V_0\otimes V_a$ of auxiliary space V_0 and the space of states at site $a=1,2,\ldots N$,

$$L_{0a}(\lambda-z_a)=R_{0a}(\lambda-z_a), \tag{2.10}$$

where z_a is a parameter of inhomogeneity (site dependence) and $R_{0a}(\lambda,\eta)=\mathcal{P}\check{R}(\lambda,\eta)$ is the usual R-matrix. Corresponding monodromy matrix T is an ordered product of the L-operators

$$T(\lambda;\{z_a\}_1^N)=L_{0N}(\lambda-z_N)\cdots L_{01}(\lambda-z_1)=\prod_{\substack{a=1\\ \leftarrow}}^{N} L_{0a}(\lambda-z_a). \tag{2.11}$$

The commutation relations of the T-matrix entries follow from the (Z_2-graded) FRT-relation[2]

$$R_{12}(\lambda-\mu)T_1(\lambda)T_2(\mu)=T_2(\mu)T_1(\lambda)R_{12}(\lambda-\mu). \tag{2.12}$$

Multiplying (2.12) by R_{12}^{-1} and taking the super-trace over $V_1\otimes V_2$, one gets commutativity of the transfer matrix

$$t(\lambda)=\mathrm{str}\ \ T(\lambda)=\sum_j (-1)^{j+1}T_{jj}(\lambda;\{z_a\}_1^N)=T_{11}-T_{22}+T_{33} \tag{2.13}$$

for different values of the spectral parameter $t(\lambda)t(\mu)=t(\mu)t(\lambda)$.

The choice of the L-operators (2.10) corresponds to the following space of states of the osp(1|2)-spin system

$$\mathcal{H}=\bigotimes_{a=1}^{N} V_a^{(1)}.$$

The eigenvalues of the transfer matrix $t(\lambda)$ in this space are[18,24,25]

$$\Lambda(\lambda;\{\mu_j\}_1^M)=\alpha_1^{(N)}(\lambda;\{z_a\}_1^N)\prod_{j=1}^{M} S_1(\lambda-\mu_j)-\alpha_2^{(N)}(\lambda;\{z_a\}_1^N)$$
$$\times\prod_{j=1}^{M} S_1(\lambda-\mu_j+\eta)S_{-1}(\lambda-\mu_j+2\eta)$$
$$+\alpha_3^{(N)}(\lambda;\{z_a\}_1^N)\prod_{j=1}^{M} S_{-1}(\lambda-\mu_j+3\eta), \tag{2.14}$$

where $\alpha_j^{(N)}(\lambda;\{z_a\}_1^N)=\Pi_{b=1}^N\alpha_j(\lambda-z_b)$; $j=1,2,3$,

$$\alpha_1(\lambda)=\sinh(\lambda+2\eta)\sinh(\lambda+3\eta),\quad \alpha_2(\lambda)=\sinh(\lambda)\sinh(\lambda+3\eta),$$
$$\alpha_3(\lambda)=\sinh(\lambda)\sinh(\lambda+\eta),\quad S_n(\mu)=\frac{\sinh(\mu-n\eta)}{\sinh(\mu+n\eta)}. \tag{2.15}$$

Although according to (2.14) the eigenvalue has formally two sets of poles at $\lambda=\mu_j-\eta$ and $\lambda=\mu_j-2\eta$, the corresponding residues are zero due to the Bethe equations on the parameters $\{\mu_j\}$ of the eigenstate[18,24,25]

$$\prod_{a=1}^{N}\frac{\sinh(\mu_j-z_a+\eta)}{\sinh(\mu_j-z_a-\eta)}=\prod_{k=1}^{M} S_1(\mu_j-\mu_k)S_{-2}(\mu_j-\mu_k). \tag{2.16}$$

If we take different spins l_a at different sites of the lattice and the following space of states

$$\mathcal{H}=\bigotimes_{a=1}^{N} V_a^{(l_a)},$$

then the factors on the left hand side of (2.16) will be spin dependent, too.

Due to the more complicated structure of the R-matrix (2.9) [see (2.7) and (2.8)], than the $gl(n)$, or $gl(m|n)$ trigonometric R-matrices, the commutation relations of the entries $T_{ij}(\lambda)$ of the T-matrix (2.11) have more terms and construction of the eigenstates of the transfer matrix $t(\lambda)$ by the algebraic Bethe ansatz can be done only using a complicated recurrence relation expressed in terms of $T_{ij}(\mu_k)$.[30] It will be shown below that due to a simplification of this recurrence relation in the quasi-classical limit $\eta\to 0$ one can solve it and find the creation operators for the trigonometric osp(1|2) Gaudin model explicitly. Furthermore, the commutation relations between the creation operators and the generators of the trigonometric loop superalgebra as well as the generating function $t(\lambda)$ of the Gaudin Hamiltonians will be given explicitly, yielding the solution to the eigenvalue problem.

III. osp(1|2) TRIGONOMETRIC GAUDIN MODEL

As in the case of any simple Lie algebra, the trigonometric classical r-matrix of the orthosymplectic Lie superalgebra osp(1|2) can be expressed in a pure algebraic form as an element in the tensor product $\mathrm{osp}(1|2)\otimes\mathrm{osp}(1|2)$

$$\hat{r}(\lambda)=\coth(\lambda)\,h\otimes h+\frac{2}{\sinh(\lambda)}(e^{-\lambda}X^+\otimes X^-+e^{\lambda}X^-\otimes X^+)$$
$$+\frac{1}{\sinh(\lambda)}(e^{-\lambda}v^+\otimes v^-+e^{\lambda}v^-\otimes v^+), \tag{3.1}$$

and it is a solution of the Z_2-graded classical YBE (1.2).[2] This r-matrix can be decomposed naturally into positive and negative parts,[34]

$$\hat{r}(\lambda)=\frac{1}{\sinh\lambda}(e^{\lambda}r^{(-)}+e^{-\lambda}r^{(+)})$$
$$=\frac{e^{\lambda}}{\sinh\lambda}\left(\frac{1}{2}h\otimes h+2X^{-}\otimes X^{+}-v^{-}\otimes v^{+}\right)$$
$$+\frac{e^{-\lambda}}{\sinh\lambda}\left(\frac{1}{2}h\otimes h+2X^{+}\otimes X^{-}+v^{+}\otimes v^{-}\right). \tag{3.2}$$

It can also be represented in another form useful for modifications,

$$\hat{r}(\lambda)=\coth(\lambda)\quad c_2^{\otimes}+2(X^{-}\otimes X^{+}-X^{+}\otimes X^{-})-(v^{-}\otimes v^{+}+v^{+}\otimes v^{-}); \tag{3.3}$$

here

$$c_2^{\otimes}=h\otimes h+2(X^{+}\otimes X^{-}+X^{-}\otimes X^{+})+(v^{+}\otimes v^{-}-v^{-}\otimes v^{+}). \tag{3.4}$$

The matrix form of $\hat{r}$ in the fundamental representation of osp(1|2) follows from (3.1) by substituting appropriate 3×3 matrices instead of the osp(1|2) generators and taking into account the Z_2-graded tensor product of even and odd matrices. One can get it also as the quasi-classical limit $\eta\to0$ from the R-matrix (2.9). Let us write explicitly the matrix form of $\hat{r}$ in the basis of the tensor product of two copies of the fundamental representation $V^{(1)}\otimes V^{(1)}$ (see the Appendix):

$$r(\lambda)=\frac{1}{\sinh(\lambda)}\begin{pmatrix}\cosh(\lambda)&&&&&&&&\\&0&&e^{-\lambda}&&&&&\\&&-\cosh(\lambda)&&-e^{-\lambda}&&2e^{-\lambda}&&\\&e^{\lambda}&&0&&&&&\\&&e^{\lambda}&&0&&-e^{-\lambda}&&\\&&&&&0&&e^{-\lambda}&\\&&2e^{\lambda}&&e^{\lambda}&&-\cosh(\lambda)&&\\&&&&&e^{\lambda}&&0&\\&&&&&&&&\cosh(\lambda)\end{pmatrix} \tag{3.5}$$

with all the other entries of this 9×9 matrix being identically equal to zero.

A quasi-classical limit $\eta\to0$ of the FRT-relations (2.12) $[R(\lambda;\eta)=I+\eta r(\lambda)+\mathcal{O}(\eta^2)$ and $T(\lambda;\eta)=I+\eta L(\lambda)+\mathcal{O}(\eta^2)]$ results in a matrix form of the loop superalgebra relation, the so-called Sklyanin linear bracket,

$$[\underset{1}{L}(\lambda),\underset{2}{L}(\mu)]=-[r_{12}(\lambda-\mu),\underset{1}{L}(\lambda)+\underset{2}{L}(\mu)]. \tag{3.6}$$

Both sides of this relation have the usual commutators of even 9×9 matrices $\underset{1}{L}(\lambda)=L(\lambda)\otimes I_3$, $\underset{2}{L}(\mu)=I_3\otimes L(\mu)$ and $r_{12}(\lambda-\mu)$, where I_3 is 3×3 unit matrix and $L(\lambda)$ has loop superalgebra valued entries:

$$L(\lambda)=\begin{pmatrix}h(\lambda)&-v^{-}(\lambda)&2X^{-}(\lambda)\\v^{+}(\lambda)&0&v^{-}(\lambda)\\2X^{+}(\lambda)&v^{+}(\lambda)&-h(\lambda)\end{pmatrix}. \tag{3.7}$$

From the expression (3.2) of the classical r-matrix it is natural to assume that the L-operator has a triangular decomposition $L_\pm$ as $\lambda \to \pm\infty$,

$$L_+ = h\otimes h_{gl} + 4X^-\otimes X^+_{gl} - 2v^-\otimes v^+_{gl}, \tag{3.8}$$

$$L_- = h\otimes h_{gl} + 4X^+\otimes X^-_{gl} + 2v^+\otimes v^-_{gl}. \tag{3.9}$$

Here the first factors are generators in the fundamental representation $V^{(1)}$ (see the Appendix) and the second factors are generators of a finite dimensional osp(1|2) Lie superagebra.

The relation (3.6) is a compact matrix form of the following commutation relations between the generators $h(\lambda)$, $v^\pm(\mu)$, $X^\pm(\nu)$ of the trigonometric loop superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$:

$$\begin{aligned}
&[h(\lambda),\ h(\mu)]_- = 0\,,\\
&[h(\lambda),\ X^\pm(\mu)]_- = \frac{\pm 2}{\sinh(\lambda-\mu)}\left(\cosh(\lambda-\mu)X^\pm(\mu) - e^{\mp(\lambda-\mu)}X^\pm(\lambda)\right),\\
&[X^+(\lambda),\ X^-(\mu)]_- = \frac{-e^{(\lambda-\mu)}}{\sinh(\lambda-\mu)}\left(h(\lambda)-h(\mu)\right),\\
&[h(\lambda),\ v^\pm(\mu)]_- = \frac{\pm 1}{\sinh(\lambda-\mu)}\left(\cosh(\lambda-\mu)v^\pm(\mu) - e^{\mp(\lambda-\mu)}v^\pm(\lambda)\right),\\
&[v^+(\lambda),\ v^-(\mu)]_+ = \frac{e^{(\lambda-\mu)}}{\sinh(\lambda-\mu)}\left(h(\lambda)-h(\mu)\right),\\
&[v^\pm(\lambda),\ v^\pm(\mu)]_+ = \frac{\pm 2}{\sinh(\lambda-\mu)}\left(e^{\pm(\lambda-\mu)}X^\pm(\mu) - e^{\mp(\lambda-\mu)}X^\pm(\lambda)\right),\\
&[X^\pm(\lambda),\ v^\mp(\mu)]_- = \frac{e^{\pm(\lambda-\mu)}}{\sinh(\lambda-\mu)}\left(v^\pm(\mu)-v^\pm(\lambda)\right),\\
&[X^\pm(\lambda),\ v^\pm(\mu)]_- = [X^\pm(\lambda),\ X^\pm(\mu)]_- = 0.
\end{aligned} \tag{3.10}$$

In order to define a dynamical system besides the algebra of observables we need to specify a Hamiltonian. Due to the r-matrix relation (3.6) the elements

$$\begin{aligned}
t(\lambda) &= \tfrac{1}{2}\ \mathrm{str}\ L^2(\lambda) = h^2(\lambda) + 2[X^+(\lambda), X^-(\lambda)]_+ + [v^+(\lambda), v^-(\lambda)]_-\\
&= h^2(\lambda) + h'(\lambda) + 4X^+(\lambda)X^-(\lambda) + 2v^+(\lambda)v^-(\lambda)
\end{aligned} \tag{3.11}$$

commute for different values of the spectral parameter

$$t(\lambda)t(\mu) = t(\mu)t(\lambda)\,. \tag{3.12}$$

Thus, $t(\lambda)$ can be considered as a generating function of integrals of motion. The supertrace in (3.11) for an even matrix $\{A_{ij}\}$ means $\mathrm{str}A = \Sigma_{i=1}^3(-1)^{p(i)}A_{ii}$, and we use the grading $p(1) = p(3) = 0$, $p(2) = 1$ (see the Appendix).

One way to show (3.12) is to notice that the commutation relation between $t(\lambda)$ and $L(\mu)$ can be written in the form

$$[t(\lambda)\,, L(\mu)] = [M(\lambda,\mu)\,, L(\mu)]\,, \tag{3.13}$$

where

$$M(\lambda,\mu)=-\operatorname*{str}_1(r_{12}(\lambda-\mu)L_1(\lambda))-\tfrac{1}{2}\operatorname*{str}_1(r_{12}^2(\lambda-\mu)), \tag{3.14}$$

and the second term is a quantum correction, which is absent if we consider the left hand side of (3.6) and (3.10) as Poisson brackets.[35] Also, in the sl(n) case this term does not contribute since it is proportional to the unit matrix. Using (3.5) and (3.7) it is straightforward to calculate $M(\lambda,\mu)$ explicitly:

$$M(\lambda,\mu)=\frac{-2}{\sinh(\lambda-\mu)}\begin{pmatrix}\cosh(\lambda-\mu)\,h(\mu) & -e^{\lambda-\mu}v^-(\mu) & 2e^{\lambda-\mu}X^-(\mu)\\ e^{-(\lambda-\mu)}v^+(\mu) & 0 & e^{\lambda-\mu}v^-(\mu)\\ 2e^{-(\lambda-\mu)}X^+(\mu) & e^{-(\lambda-\mu)}v^+(\mu) & -\cosh(\lambda-\mu)\,h(\mu)\end{pmatrix}$$
$$-\frac{1}{\sinh^2(\lambda-\mu)}\begin{pmatrix}\cosh^2(\lambda-\mu)+1 & 0 & 0\\ 0 & -2 & 0\\ 0 & 0 & \cosh^2(\lambda-\mu)+1\end{pmatrix}. \tag{3.15}$$

Substituting (3.15) into the equation (3.13) we obtain the commutation relations between $t(\lambda)$ and the generators of the superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$. In particular,

$$[t(\lambda),\ X^+(\mu)]_-=4\coth(\lambda-\mu)\,X^+(\mu)h(\lambda)-\frac{4e^{-(\lambda-\mu)}}{\sinh(\lambda-\mu)}X^+(\lambda)h(\mu)+4X^+(\mu)$$
$$-\frac{2e^{-(\lambda-\mu)}}{\sinh(\lambda-\mu)}(v^+(\lambda)v^+(\mu)-v^+(\mu)v^+(\lambda)), \tag{3.16}$$

$$[t(\lambda),\ v^+(\mu)]_-=2\coth(\lambda-\mu)\,v^+(\mu)h(\lambda)-\frac{2e^{-(\lambda-\mu)}}{\sinh(\lambda-\mu)}v^+(\lambda)h(\mu)+v^+(\mu)$$
$$+\frac{4}{\sinh(\lambda-\mu)}(e^{-(\lambda-\mu)}X^+(\lambda)v^-(\mu)-e^{-(\mu-\lambda)}X^+(\mu)v^-(\lambda)). \tag{3.17}$$

Preserving some generality we can consider the representation space $\mathcal{H}$ of the dynamical algebra to be a lowest spin $\rho(\lambda)$ representation of the loop superalgebra with the lowest spin vector Ω_-,

$$h(\lambda)\Omega_-=\rho(\lambda)\Omega_-,\quad v^-(\lambda)\Omega_-=0\,. \tag{3.18}$$

One can study spectrum and eigenstates of $t(\lambda)$ in this general representation $\mathcal{H}$. However, to have a physical interpretation we will use a local realization of the trigonometric superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$ with

$$\mathcal{H}=\bigotimes_{a=1}^{N}V_a,$$

as a tensor product of osp(1|2) representations. Then,

$$h(\lambda)=\sum_{a=1}^{N}\coth(\lambda-z_a)\,h_a\,, \tag{3.19}$$

$$v^+(\lambda)=\sum_{a=1}^{N}\frac{e^{\lambda-z_a}}{\sinh(\lambda-z_a)}v_a^+\,,\quad v^-(\lambda)=\sum_{a=1}^{N}\frac{e^{-\lambda+z_a}}{\sinh(\lambda-z_a)}v_a^-\,, \tag{3.20}$$

$$X^+(\lambda)=\sum_{a=1}^{N}\frac{e^{\lambda-z_a}}{\sinh(\lambda-z_a)}X_a^+,\quad X^-(\lambda)=\sum_{a=1}^{N}\frac{e^{-\lambda+z_a}}{\sinh(\lambda-z_a)}X_a^-, \tag{3.21}$$

where h_a, $v_a^{\pm}$, $X_a^{\pm}\in \mathrm{End}\,(V_a)$ are osp(1|2) generators in a representation V_a associated with each site a. If in this realization one considers the limits $\lambda\to\pm\infty$, then one finds the expressions of the generators of the global Lie superalgebra $\mathrm{osp}(1|2)\subset\mathcal{L}_t(\mathrm{osp}(1|2))$ in terms of the local generators

$$Y_{gl}=\sum_{a=1}^{N} Y_a; \tag{3.22}$$

here $Y=(h,X^{\pm},v^{\pm})$.

In particular, a representation of the Gaudin realization can be obtained by considering at each site a an irreducible representations $V_a^{(l_a)}$ of the Lie superalgebra osp(1|2) defined by a spin l_a and a lowest spin vector ω_a such that $v_a^-\omega_a=0$ and $h_a\omega_a=-l_a\omega_a$. Thus,

$$\Omega_-=\bigotimes_{a=1}^{N}\omega_a,\quad \text{and}\quad \rho(\lambda)=\sum_{a=1}^{N}(-l_a)\coth(\lambda-z_a). \tag{3.23}$$

It is a well-known fact in the theory of Gaudin models[5,6] that the Gaudin Hamiltonian is related to the classical r-matrix (1.1) and (3.2),

$$\begin{aligned}H^{(a)}&=\sum_{b\neq a} r_{ab}(z_a-z_b)\\&=\sum_{b\neq a}\frac{1}{\sinh(z_a-z_b)}(e^{(z_a-z_b)}r_{ab}^{(-)}+e^{(z_b-z_a)}r_{ab}^{(+)})\\&=\sum_{b\neq a}\coth(z_a-z_b)h_ah_b+\frac{2}{\sinh(z_a-z_b)}(e^{-(z_a-z_b)}X_a^+X_b^-+e^{(z_a-z_b)}X_a^-X_b^+)\\&\quad+\frac{1}{\sinh(z_a-z_b)}(e^{-(z_a-z_b)}v_a^+v_b^--e^{(z_a-z_b)}v_a^-v_b^+),\end{aligned} \tag{3.24}$$

and can be obtained as the residue of the operator $t(\lambda)$ at the point $\lambda=z_a$ using the expansion

$$t(\lambda)=h_{gl}^2+\sum_{a=1}^{N}\left(\frac{c_2(a)}{\sinh^2(\lambda-z_a)}+2\frac{e^{\lambda-z_a}}{\sinh(\lambda-z_a)}H^{(a)}\right), \tag{3.25}$$

$c_2(a)=h_a^2+2(X_a^+X_a^-+X_a^-X_a^+)+v_a^+v_a^--v_a^-v_a^+$. As opposed to the rational osp(1|2)-invariant case,[17] the generating function (3.25) commutes only with one generator h_{gl} of the global superalgebra osp(1|2):

$$[t(\lambda),h_{gl}]=0. \tag{3.26}$$

To construct the set of eigenstates of the generating function of integrals of motion $t(\lambda)$ we have to define appropriate creation operators. The creation operators used in the sl(2) Gaudin model coincide with one of the L-matrix entry.[5,6] However, in the osp(1|2) case the creation operators are complicated functions of the two generators of the loop superalgebra $X^+(\lambda)$ and $v^+(\mu)$.

Definition 3.1: Let $B_M(\mu_1,\ldots,\mu_M)$ *belong to the Borel subalgebra of the* osp(1|2) *loop super algebra* $\mathcal{L}_t(\mathrm{osp}(1|2))$ *such that*

$$\begin{aligned}B_M(\mu_1,\ldots,\mu_M)&=v^+(\mu_1)B_{M-1}(\mu_2,\ldots,\mu_M)\\&\quad+2X^+(\mu_1)\sum_{j=2}^{M}(-1)^j\frac{e^{-(\mu_1-\mu_j)}}{\sinh(\mu_1-\mu_j)}B_{M-2}^{(j)}(\mu_2,\ldots,\mu_M)\end{aligned} \tag{3.27}$$

with $B_0=1$, $B_1(\mu)=v^+(\mu)$ *and* $B_M=0$ *for* $M<0$. *The notation* $B^{(j)}_{M-2}(\mu_2,\ldots,\mu_M)$ *means that the argument* μ_j *is omitted.*

As we will show below, the B-operators are such that the Bethe vectors are generated by their action on the lowest spin vector Ω_- (3.18). To prove this result we will need some important properties of the B-operators. All the properties of the creation operators $B_M(\mu_1,\ldots,\mu_M)$ listed below can be demonstrated by induction method. Since the proofs are lengthy and quite technical we will present only two of them.

Lemma 3.1: The creation operators $B_M(\mu_1,\ldots,\mu_M)$ *are antisymmetric functions of their arguments*

$$B_M(\mu_1,\ldots,\mu_k,\mu_{k+1},\ldots,\mu_M)=-B_M(\mu_1,\ldots,\mu_{k+1},\mu_k,\ldots,\mu_M), \tag{3.28}$$

here $1\leqslant k<M$ *and* $M\geqslant 2$.

Lemma 3.2: The commutation relations between the creation operator B_M *and the generators* $v^+(\lambda)$, $h(\lambda)$, $v^-(\lambda)$ *of the loop superalgebra are given by*

$$v^+(\lambda)B_M=(-1)^M B_M v^+(\lambda)+2\sum_{j=1}^{M}\frac{(-1)^j}{\sinh(\lambda-\mu_j)}\times(e^{-(\lambda-\mu_j)}X^+(\lambda)-e^{-(\mu_j-\lambda)}X^+(\mu_j))B^{(j)}_{M-1}, \tag{3.29}$$

$$\begin{aligned}h(\lambda)B_M=B_M\Bigg(h(\lambda)+\sum_{i=1}^{M}\coth(\lambda-\mu_i)\Bigg)+\sum_{i=1}^{M}(-1)^i\frac{e^{-(\lambda-\mu_i)}}{\sinh(\lambda-\mu_i)}\\ \times\Bigg(v^+(\lambda)B^{(i)}_{M-1}+2X^+(\lambda)\sum_{j\neq i}^{M}(-1)^{j+\Theta(i-j)}\frac{e^{-(\mu_i-\mu_j)}}{\sinh(\mu_i-\mu_j)}B^{(i,j)}_{M-2}\Bigg),\end{aligned} \tag{3.30}$$

$$\begin{aligned}v^-(\lambda)B_M=(-1)^M B_M v^-(\lambda)+\sum_{j=1}^{M}(-1)^{j-1}B^{(j)}_{M-1}\Bigg(\frac{e^{-(\lambda-\mu_j)}}{\sinh(\lambda-\mu_j)}(h(\lambda)-h(\mu_j))\\ +\sum_{k\neq j}^{M}\frac{e^{-(\lambda-\mu_k)}}{\sinh(\lambda-\mu_k)}\frac{e^{-(\mu_k-\mu_j)}}{\sinh(\mu_k-\mu_j)}\Bigg)+v^+(\lambda)\sum_{i<j}^{M}(-1)^{i-j-1}\\ \times\frac{e^{-(\mu_i-\mu_j)}}{\sinh(\mu_i-\mu_j)}B^{(i,j)}_{M-2}\Bigg(\frac{e^{-(\lambda-\mu_i)}}{\sinh(\lambda-\mu_i)}+\frac{e^{-(\lambda-\mu_j)}}{\sinh(\lambda-\mu_j)}\Bigg).\end{aligned} \tag{3.31}$$

Here the upper index of $B^{(j)}_{M-1}$ *means that the argument* μ_j *is omitted, the upper index of* $B^{(i,j)}_{M-2}$ *means that the parameters* μ_i,μ_j *are omitted and* $\Theta(j)$ *is Heaviside function*

$$\Theta(j)=\begin{cases}1 & \text{if } j>0,\\ 0 & \text{if } j\leqslant 0.\end{cases}$$

It is useful to have explicit formulas for the commutators between the global generators and the B-operators.

Remark 3.1: The commutation relations between the generators of the global osp(1|2) *(3.22) and the* B_M *elements follow from the previous Lemma 3.2. To see this we take the appropriate limit* $\lambda\to\pm\infty$ *in (3.29)–(3.31). In this way we obtain*

$$v^+_{gl}B_M=(-1)^M B_M v^+_{gl}-2\sum_{j=1}^{M}(-1)^j X^+(\mu_j)B^{(j)}_{M-1}, \tag{3.32}$$

$$h_{gl}B_M=B_M(h_{gl}+M), \tag{3.33}$$

$$v_{gl}^{-}B_M=(-1)^M B_M v_{gl}^{-}+\sum_{j=1}^{M}(-1)^j B_{M-1}^{(j)}\left(h_{gl}+h(\mu_j)+\sum_{k\neq j}^{M}\frac{e^{(\mu_j-\mu_k)}}{\sinh(\mu_j-\mu_k)}\right). \tag{3.34}$$

Lemma 3.3: The generating function of integrals of motion $t(\lambda)$ (3.11) has the following commutation relation with the creation operator $B_M(\mu_1,\ldots,\mu_M)$,

$$\begin{aligned}t(\lambda)B_M=&B_M t(\lambda)+B_M\left(2h(\lambda)\sum_{i=1}^{M}\coth(\lambda-\mu_i)+2\sum_{i<j}^{M}\coth(\lambda-\mu_i)\coth(\lambda-\mu_j)+M\right)\\&+2\sum_{i=1}^{M}(-1)^i\frac{e^{-(\lambda-\mu_i)}}{\sinh(\lambda-\mu_i)}\left(v^{+}(\lambda)B_{M-1}^{(i)}+2X^{+}(\lambda)\sum_{j\neq i}^{M}(-1)^{j+\Theta(i-j)}\right.\\&\left.\times\frac{e^{-(\mu_i-\mu_j)}}{\sinh(\mu_i-\mu_j)}B_{M-2}^{(i,j)}\right)\hat{\beta}_M(\mu_i)+4\sum_{i=1}^{M}(-1)^{i+M}\frac{B_{M-1}^{(i)}}{\sinh(\lambda-\mu_i)}(e^{-(\lambda-\mu_i)}X^{+}(\lambda)v^{-}(\mu_i)\\&-e^{-(\mu_i-\lambda)}X^{+}(\mu_i)v^{-}(\lambda)).\end{aligned} \tag{3.35}$$

The notation used here for the operator $\hat{\beta}_M(\mu_i)$ is $\hat{\beta}_M(\mu_i)=h(\mu_i)+\Sigma_{j\neq i}^{M}\coth(\mu_i-\mu_j)$.

In the trigonometric Gaudin realization (3.17)–(3.19) the creation operators $B_M(\mu_1,\ldots,\mu_M)$ have some specific analytical properties.

Lemma 3.4: The B-operators in the Gaudin realization (3.17)–(3.19) satisfy an important differential identity

$$\begin{aligned}\frac{\partial}{\partial z_a}B_M=&\sum_{j=1}^{M}\frac{\partial}{\partial\mu_j}\left((-1)^j\frac{e^{\mu_j-z_a}}{\sinh(\mu_j-z_a)}\right.\\&\left.\times\left(v_a^{+}B_{M-1}^{(j)}+2X_a^{+}\sum_{k\neq j}^{M}(-1)^{k+\Theta(j-k)}\frac{e^{-(\mu_j-\mu_k)}}{\sinh(\mu_j-\mu_k)}B_{M-2}^{(j,k)}\right)\right).\end{aligned} \tag{3.36}$$

This identity will be a fundamental step in establishing a connection between the Bethe vectors and solutions to the KZ equation.

The proofs of the lemmas are based on the induction method. As illustrations, we prove explicitly Lemma 3.1 and the formula (3.29) in Lemma 3.2.

Proof of Lemma 3.1: Consider $M=2$:

$$B_2(\mu_1,\mu_2)=v^{+}(\mu_1)v^{+}(\mu_2)+\frac{2e^{-(\mu_1-\mu_2)}}{\sinh(\mu_1-\mu_2)}X^{+}(\mu_1).$$

Using the commutation relations (3.10) it is straightforward to check that $B_2(\mu_1,\mu_2)$ is antisymmetric:

$$B_2(\mu_1,\mu_2)=-B_2(\mu_2,\mu_1).$$

Assume $B_N(\mu_1,\ldots,\mu_N)$ is antisymmetric for $N\geqslant 2$ and for $N<M$. We have to prove that $B_M(\mu_1,\ldots,\mu_M)$ is antisymmetric also.

Consider $j\geqslant 2$, the antisymmetry of $B_M(\mu_1,\ldots,\mu_M)$ with respect to μ_j and μ_{j+1} follows directly form the recurrence relation (3.27) and our assumption. Namely, the terms $B_{M-2}^{(j)}(\mu_2,\ldots,\mu_M)e^{-(\mu_1-\mu_j)}/\sinh(\mu_1-\mu_j)$ and $B_{M-2}^{(j+1)}(\mu_2,\ldots,\mu_M)e^{-(\mu_1-\mu_{(j+1)})}/\sinh(\mu_1-\mu_{(j+1)})$ enter with the opposite sign.

Therefore we only have to show the antisymmetry of $B_M(\mu_1,\ldots,\mu_M)$ with respect to the interchange of μ_1 and μ_2. To see this we have to iterate the recurrence relation (3.27) twice and combine the appropriate terms

$$B_M(\mu_1,\ldots,\mu_M)=\left(v^+(\mu_1)v^+(\mu_2)+\frac{2e^{-(\mu_1-\mu_2)}}{\sinh(\mu_1-\mu_2)}X^+(\mu_1)\right)B_{M-2}(\mu_3,\ldots,\mu_M)$$
$$+2v^+(\mu_1)X^+(\mu_2)\sum_{j=3}^{M}(-1)^{j+1}\frac{e^{-(\mu_2-\mu_j)}}{\sinh(\mu_2-\mu_j)}\ B^{(j)}_{M-3}(\mu_3,\ldots,\mu_M)$$
$$+2v^+(\mu_2)X^+(\mu_1)\sum_{j=3}^{M}(-1)^{j}\frac{e^{-(\mu_1-\mu_j)}}{\sinh(\mu_1-\mu_j)}\ B^{(j)}_{M-3}(\mu_3,\ldots,\mu_M)$$
$$+4X^+(\mu_1)X^+(\mu_2)\sum_{j=3}^{M}(-1)^{j}\frac{e^{-(\mu_1-\mu_j)}}{\sinh(\mu_1-\mu_j)}\sum_{k=3}^{M}(-1)^{k+\Theta(j-k)}$$
$$\times\frac{e^{-(\mu_2-\mu_k)}}{\sinh(\mu_2-\mu_k)}B^{(j,k)}_{M-4}(\mu_3,\ldots,\mu_M),\tag{3.37}$$

where $B^{(j,k)}_{M-4}(\mu_3,\ldots,\mu_M)$ means that the arguments μ_j and μ_k are omitted. Since $v^+(\mu)$ commutes with $X^+(\nu)$, the antisymmetry of the right hand side of (3.37) with respect to μ_1 and μ_2 follows. Hence we have demonstrated the lemma. □

Proof of Lemma 3.2: Here we prove explicitly only formula (3.29). In particular, when $M=1$, the expression (3.29) is just the anticommutator between $v^+(\lambda)$ and $v^+(\mu)$. Using the recurrence relations (3.27) it is straightforward to check that the formula (3.29) holds for $M=2$:

$$v^+(\lambda)B_2(\mu_1,\mu_2)=B_2(\mu_1,\mu_2)v^+(\lambda)-\frac{2}{\sinh(\lambda-\mu_1)}(e^{-(\lambda-\mu_1)}X^+(\lambda)$$
$$-e^{\lambda-\mu_1}X^+(\mu_1))\ \ v^+(\mu_2)+\frac{2}{\sinh(\lambda-\mu_2)}(e^{-(\lambda-\mu_2)}X^+(\lambda)$$
$$-e^{\lambda-\mu_2}X^+(\mu_2))\ \ v^+(\mu_1).\tag{3.38}$$

Therefore we can proceed to demonstrate Lemma 3.3 by induction. Assume that the relation (3.29) holds for B_N, $M\geqslant N\geqslant 2$. Then we have to show the formula (3.29) is valid for $M+1$. We use the recurrence relations (3.27) to write

$$v^+(\lambda)B_{M+1}=v^+(\lambda)\left(v^+(\mu_1)B_M+2X^+(\mu_1)\sum_{j=2}^{M+1}\frac{e^{-(\mu_1-\mu_j)}}{\sinh(\mu_1-\mu_j)}B^{(j)}_{M-1}\right)$$
$$=-v^+(\mu_1)v^+(\lambda)B_M-\frac{2}{\sinh(\lambda-\mu_1)}(e^{-(\lambda-\mu_1)}X^+(\lambda)-e^{\lambda-\mu_1}X^+(\mu_1))B_M$$
$$+2X^+(\mu_1)\sum_{j=2}^{M+1}(-1)^{j}\frac{e^{-(\mu_1-\mu_j)}}{\sinh(\mu_1-\mu_j)}v^+(\lambda)B^{(j)}_{M-1}.\tag{3.39}$$

Now we can substitute the expressions for $v^+(\lambda)B_M$ and $v^+(\lambda)B^{(j)}_{M-1}$. After rearranging the terms in an appropriate way we have

$$v^+(\lambda)B_{M+1}=(-1)^{M+1}B_{M+1}v^+(\lambda)+2\sum_{j=1}^{M+1}\frac{(-1)^j}{\sinh(\lambda-\mu_j)}$$
$$\times(e^{-(\lambda-\mu_j)}X^+(\lambda)-e^{-(\mu_j-\lambda)}X^+(\mu_j))B^{(j)}_M\ \ .\tag{3.40}$$

This completes the proof of the lemma. □

The proofs of the other lemmas are analogous to the proofs we have illustrated above. They do not contain illuminating insights and are considerably longer than the two we have seen. Thus, we will omit them.

The recurrence relation (3.27) can be solved explicitly. To be able to express the solution in a compact form it is useful to introduce a contraction operator d.

Definition 3.2: Let d be a contraction operator whose action on an ordered product $\prod_{j=1}^{M}\overrightarrow{v^+(\mu_j)}$, $M\geqslant 2$, is given by

$$d(v^+(\mu_1)v^+(\mu_2)\cdots v^+(\mu_M))=2\sum_{j=1}^{M-1}X^+(\mu_j)\sum_{k=j+1}^{M}(-1)^{\sigma(jk)}\frac{e^{-(\mu_j-\mu_k)}}{\sinh(\mu_j-\mu_k)}\prod_{m\neq j,k}^{M}\overrightarrow{v^+(\mu_m)}, \tag{3.41}$$

where $\sigma(jk)$ is the parity of the permutation

$$\sigma:(1,2,\ldots,j,j+1,\ldots,k,\ldots,M)\to(1,2,\ldots,j,k,j+1,\ldots,M).$$

The d operator can be applied on an ordered product $\prod_{j=1}^{M}\overrightarrow{v^+(\mu_j)}$ consecutively several times, up to $[M/2]$, the integer part of $M/2$.

Theorem 3.1: *Explicit solution to the recurrence relation (3.27) is given by*

$$B_M(\mu_1,\ldots,\mu_M)=\prod_{j=1}^{M}\overrightarrow{v^+(\mu_j)}+\sum_{m=1}^{[M/2]}\frac{1}{m!}\,d^m\prod_{j=1}^{M}\overrightarrow{v^+(\mu_j)}=\exp d\prod_{j=1}^{M}\overrightarrow{v^+(\mu_j)}. \tag{3.42}$$

The properties of the creation operators B_M studied in the this section will be fundamental tools in determining characteristics of the trigonometric osp(1|2) Gaudin model. Our primary interest is to obtain the spectrum and the eigenvectors of the generating function of integrals of motion $t(\lambda)$ (3.11).

IV. SPECTRUM AND EIGENSTATES OF TRIGONOMETRIC osp(1|2) GAUDIN MODEL

With the help of the creation operators B_M it is possible to obtain the eigenvectors as well as the corresponding eigenvalues of the Hamiltonians of the trigonometric Gaudin model. This result is a direct consequence of the following theorem.

Theorem 4.1: *The lowest spin vector Ω_- (3.18) is an eigenvector of the generating function of integrals of motion $t(\lambda)$ (3.11) with the corresponding eigenvalue $\Lambda_0(\lambda)$:*

$$t(\lambda)\,\Omega_-=\Lambda_0(\lambda)\,\Omega_-,\quad \Lambda_0(\lambda)=\rho^2(\lambda)+\rho'(\lambda). \tag{4.1}$$

Furthermore, the action of the B-operators (3.27) on the lowest spin vector Ω_- yields the eigenvectors

$$\Psi(\mu_1,\ldots,\mu_M)=B_M(\mu_1,\ldots,\mu_M)\quad\Omega_- \tag{4.2}$$

of the $t(\lambda)$ operator

$$t(\lambda)\Psi(\mu_1,\ldots,\mu_M)=\Lambda(\lambda;\{\mu_j\}_{j=1}^{M})\,\Psi(\mu_1,\ldots,\mu_M), \tag{4.3}$$

with the eigenvalues

$$\Lambda(\lambda;\{\mu_j\}_{j=1}^{M})=y^2+\partial_\lambda y. \tag{4.4}$$

Here

$$y(\lambda;\{\mu_j\}_{j=1}^M)=\rho(\lambda)+\sum_{k=1}^{M}\coth(\lambda-\mu_k), \tag{4.5}$$

provided that the Bethe equations are imposed on the parameters $\{\mu_j\}_{j=1}^M$ *of the state (4.2):*

$$\beta_M(\mu_j)=\rho(\mu_j)+\sum_{k\neq j}^{M}\coth(\mu_j-\mu_k)=0. \tag{4.6}$$

Proof: The equation (4.1) can be checked by a direct substitution of the definitions of the operator $t(\lambda)$ and the lowest spin vector Ω_-, the equations (3.11) and (3.18), respectively.

To show the second part of the theorem, we use the equation (4.2) to express the Bethe vectors $\Psi(\mu_1,\ldots,\mu_M)$,

$$t(\lambda)\Psi(\mu_1,\ldots,\mu_M)=t(\lambda)\ \ B_M(\mu_1,\ldots,\mu_M)\ \ \Omega_-. \tag{4.7}$$

Our next step is to use the third property of the B-operators, the equation (3.3), and the definition of the lowest spin vector Ω_-, the equation (3.18), in order to calculate the action of the operator $t(\lambda)$ on the Bethe vectors when the Bethe equations (4.6) are imposed:

$$\begin{aligned} t(\lambda)B_M\Omega_- &= B_M t(\lambda)\Omega_- \\ &\quad+\left(2\rho(\lambda)\sum_{i=1}^{M}\coth(\lambda-\mu_i)+2\sum_{i<j}^{M}\coth(\lambda-\mu_i)\coth(\lambda-\mu_j)+M\right)B_M\Omega_-. \end{aligned} \tag{4.8}$$

We can express the first term on the right hand side since we know how the operator $t(\lambda)$ acts on the vector Ω_-, the equation (4.1). Thus we have

$$t(\lambda)\ \ B_M\Omega_-=\Lambda(\lambda;\{\mu_j\}_{j=1}^M)\ \ B_M\Omega_-, \tag{4.9}$$

with

$$\Lambda(\lambda;\{\mu_j\}_{j=1}^M)=\Lambda_0(\lambda)+2\rho(\lambda)\sum_{i=1}^{M}\coth(\lambda-\mu_i)+2\sum_{i<j}^{M}\coth(\lambda-\mu_i)\coth(\lambda-\mu_j)+M,$$

and we complete the proof by expressing the eigenvalue as

$$\Lambda(\lambda;\{\mu_j\}_{j=1}^M)=y^2+\partial_\lambda y,\quad \text{with}\quad y(\lambda;\{\mu_j\}_{j=1}^M)=\rho(\lambda)+\sum_{k=1}^{M}\coth(\lambda-\mu_k).$$

□

Corollary 4.1: In the trigonometric Gaudin realization given by the equations (3.19)–(3.21) and (3.23) the Bethe vectors $\Psi(\mu_1,\ldots,\mu_M)$ *(4.2) are the eigenvectors of the Gaudin Hamiltonians (3.24) (see also Ref. 36)*

$$H^{(a)}\Psi(\mu_1,\ldots,\mu_M)=E_M^{(a)}\Psi(\mu_1,\ldots,\mu_M), \tag{4.10}$$

with the eigenvalues

$$E_M^{(a)}=\sum_{\substack{b=1\\ b\neq a}}^{N} l_a\, l_b\coth(z_a-z_b)+\sum_{j=1}^{M} l_a\coth(\mu_j-z_a), \tag{4.11}$$

when the Bethe equations are imposed:

$$\beta_M(\mu_j)=\rho(\mu_j)+\sum_{k\neq j}^{M}\coth(\mu_j-\mu_k)=\sum_{a=1}^{N}(-l_a)\coth(\mu_j-z_a)+\sum_{k\neq j}^{M}\coth(\mu_j-\mu_k)=0. \tag{4.12}$$

Proof: The statement of the corollary follows from residue of the equation (4.3) at the point $\lambda=z_a$. The residue can be determined using (3.25), (4.4) and (4.1). □

Comparing the eigenvalues $E_M^{(a)}$ (4.11) of the Gaudin Hamiltonians and the Bethe equations (4.12) with the corresponding quantities of the sl(2) Gaudin model[5,6] we arrive at an interesting observation.

Remark 4.1: The spectrum of the osp(1|2) *trigonometric Gaudin model with the spins* l_a *coincides with the spectrum of the* sl(2) *trigonometric Gaudin system for the integer spins (see an analogous observation for partition functions of corresponding anisotropic vertex models in Ref. 32).*

Remark 4.2: The Bethe vectors are eigenstates of the global generator h_{gl}

$$h_{gl}\Psi(\mu_1,\ldots,\mu_M)=\left(-\sum_{a=1}^{N}l_a+M\right)\Psi(\mu_1,\ldots,\mu_M). \tag{4.13}$$

As opposed to the osp(1|2)-invariant model,[17] these Bethe vectors are not the lowest spin vectors of the global osp(1|2) since they are not annihilated by the generator v_{gl}^{-},

$$v_{gl}^{-}\Psi(\mu_1,\ldots,\mu_M)\neq 0, \tag{4.14}$$

once the Bethe equations are imposed, (4.12). These conclusions follow from Remark 3.1, in particular the equations (3.33) and (3.34), and the definition of the Bethe vectors (4.2).

As was pointed out already in Ref. 5 for the sl(2) case, there are several modifications of the Hamiltonians (3.24). One of them is the Richardson's pairing-force Hamiltonian.[37,38,5] These modifications can be formulated in the framework of the universal L-operator and r-matrix formalism (3.6).[6]

Due to invariance of the r-matrix (3.5) with respect to the Cartan element

$$[r(\lambda),h\otimes I+I\otimes h]=0,\quad h\in\mathrm{osp}(1|2), \tag{4.15}$$

one can add to the L-operator the element h,

$$L(\lambda)\to\tilde{L}(\lambda)=g\,h+L(\lambda), \tag{4.16}$$

preserving commutation relations (3.6). Then

$$\tilde{t}(\lambda)=\tfrac{1}{2}\,\mathrm{str}\,\tilde{L}^2(\lambda)=t(\lambda)+2g\,h(\lambda)+g^2 \tag{4.17}$$

will have the commutativity property, i.e., $\tilde{t}(\lambda)\tilde{t}(\mu)=\tilde{t}(\mu)\tilde{t}(\lambda)$. Hence we can take $\tilde{t}(\lambda)$ to be the generating function of the (modified) integrals of motion,

$$\tilde{t}(\lambda)=(h_{gl}-g)^2+\sum_{a=1}^{N}\left(\frac{c_2(a)}{\sinh^2(\lambda-z_a)}+2\,\frac{e^{\lambda-z_a}}{\sinh(\lambda-z_a)}\tilde{H}^{(a)}\right), \tag{4.18}$$

$$\tilde{H}^{(a)}=\operatorname*{res}_{\lambda=z_a}\tilde{t}(\lambda)=g\;\;h_a+H^{(a)}. \tag{4.19}$$

In this case the eigenstates Ψ_M are generated by the same B-operators. However, corresponding eigenvalues and Bethe equations are now given by

$$\tilde{\Lambda}(\lambda;\{\mu_j\}_{j=1}^{M})=(y+g)^2+\partial_\lambda y; \tag{4.20}$$

here as before $y(\lambda;\{\mu_j\}_{j=1}^{M})=\Sigma_{a=1}^{N}(-l_a)\coth(\lambda-z_a)+\Sigma_{k=1}^{M}\coth(\lambda-\mu_k)$,

$$\tilde{E}_M^{(a)}=E_M^{(a)}+g\,(-l_a), \tag{4.21}$$

$$\sum_{a=1}^{N}(-l_a)\coth(\mu_j-z_a)+\sum_{k\neq j}^{M}\coth(\mu_j-\mu_k)+g=0. \tag{4.22}$$

The crucial step in the proof of these equations is the observation that the commutation relations between the operator $\tilde{t}(\lambda)$ (4.17) and the creation operators B_M are equal to the commutation relations (3.3) but with modified operator $\hat{\beta}_M(\mu_j)\to\hat{\beta}_M(\mu_j)+g$. To see this notice the similarity between the terms with $v^+(\lambda)B_{M-1}^{(i)}$ operators and with $X^+(\lambda)B_{M-2}^{(i,j)}$ operators in Lemma 3.2, the equation (3.30), and in Lemma 3.3, the equation (3.3).

A Richardson-like Hamiltonian[37,38,5,20,21] can be obtained as a coefficient in the $\lambda\to+\infty$ expansion,[17]

$$\tilde{t}(\lambda)=(h_{gl}+g)^2+4e^{-2\lambda}\Big((h_{gl}-1+g)\Big(\sum_a e^{2z_a}h_a\Big)+4X_{gl}^{+}\Big(\sum_a e^{2z_a}X_a^{-}\Big)+2v_{gl}^{+}\Big(\sum_a e^{2z_a}v_a^{-}\Big)\Big)$$
$$+O(e^{-4\lambda}). \tag{4.23}$$

Let us denote the coefficient next to the factor $4e^{-2\lambda}$ by H_+:

$$H_+=(h_{gl}-1+g)\Big(\sum_i e^{2z_a}h_a\Big)+4X_{gl}^{+}\Big(\sum_a e^{2z_a}X_a^{-}\Big)+2v_{gl}^{+}\Big(\sum_a e^{2z_i}v_a^{-}\Big). \tag{4.24}$$

This Hamiltonian is obviously not symmetric. Similar Hamiltonian can be obtained as a coefficient in the $\lambda\to-\infty$ expansion

$$\tilde{t}(\lambda)=(h_{gl}-g)^2+4e^{2\lambda}\Big(\Big(\sum_a e^{-2z_a}h_a\Big)(h_{gl}-1-g)+4\Big(\sum_a e^{-2z_a}X_a^{+}\Big)X_{gl}^{-}$$
$$+2\Big(\sum_a e^{-2z_a}v_a^{+}\Big)v_{gl}^{-}\Big)+O(e^{4\lambda}). \tag{4.25}$$

Let us denote the coefficient next to the factor $4e^{2\lambda}$ by H_-, which is also not symmetric. Thus, we choose the following symmetric combination for a trigonometric generalization of the Richardson Hamiltonian:

$$H_R=\frac{1}{2}(H_++H_-)=(h_{gl}-1)\Big(\sum_a \cosh(2z_a)\;\;h_a\Big)+g\;\;\Big(\sum_a \sinh(2z_a)\;\;h_a\Big)$$
$$+2\Big(X_{gl}^{+}\Big(\sum_a e^{2z_a}X_a^{-}\Big)+\Big(\sum_a e^{-2z_a}X_a^{+}\Big)X_{gl}^{-}\Big)+v_{gl}^{+}\Big(\sum_i e^{2z_a}v_a^{-}\Big)+\Big(\sum_a e^{-2z_a}v_a^{+}\Big)v_{gl}^{-}. \tag{4.26}$$

The eigenvalues of H_R have different dependence on the quasi-momenta from the rational case,[37,17]

$$H_R\Psi_M(\mu_1,\ldots,\mu_M)=E_R(M)\Psi_M(\mu_1,\ldots,\mu_M), \tag{4.27}$$

with

$$E_R(M)=\left(\sum_{j=1}^{M}\cosh(2\mu_j)-\sum_{a=1}^{N}l_a\cosh(2z_a)\right)\left(M-\sum_{a=1}^{N}l_a-1\right)$$
$$+\left(\sum_{j=1}^{M}\sinh(2\mu_j)-\sum_{a=1}^{N}l_a\sinh(2z_a)\right)g. \tag{4.28}$$

More complicated modifications of Gaudin models can be obtained considering the quasiclassical limit of the quantum spin system with nonperiodic boundary conditions and corresponding reflection equation.[39,40] The L-operator can be expressed in terms of the original one (3.7) as

$$L^{(bGM)}(\lambda;\{z_j\})=L(\lambda;\{z_j\})-L(-\lambda;\{z_j\}), \tag{4.29}$$

in the case of the open chain, and it will satisfy more complicated liner brackets, defining a subalgebra of the loop algebra (3.6) (see also Ref. 41 and references therein).

Most of the trigonometric Gaudin model relations have their counterparts in the rational osp(1|2)-invariant case. To show this one takes a scaling limit $\lambda\to\varepsilon\lambda$, $z_a\to\varepsilon z_a$,

$$\lim_{\varepsilon\to 0}\varepsilon L_{\mathrm{trig}}(\varepsilon\lambda;\{\varepsilon z_a\})=L_{\mathrm{inv}}(\lambda;\{z_a\}), \tag{4.30}$$

and in this way one reproduces known results for the osp(1|2)-invariant model. However, as we shall see in the next section, some relations of the invariant GM have quite complicated analogs in the trigonometric case (a generalization of KZ system to include a ''magnetic field'' parameter g requires a difference dynamical equation[15,16]). Also the modified L-operator (4.16) requires to scale the parameter $g\to g/\varepsilon$.

Another modification can be obtained by performing the similarity transformation on the r-matrix (3.1) by the tensor square of the element $\exp(tX^+)$. Then the scaling limit $\lambda\to\varepsilon\lambda$, $t\to\xi/2\varepsilon$, results in a modified r-matrix:

$$\hat{r}(\lambda)=\frac{c_2^{\otimes}}{\lambda}+\xi(h\otimes X^+-X^+\otimes h-v^+\otimes v^+). \tag{4.31}$$

The loop superalgebra will be modified, as well as corresponding Hamiltonians (1.1). Similarly, the algebraic Bethe ansatz will require changes, although the Bethe equations and the spectrum will be the same as in the osp(1|2)-invariant case [see the sl(2) case in Ref. 42].

The expression of the eigenvectors of a solvable model in terms of local variables parametrized by sites of the chain or by space coordinates, is known as coordinate Bethe ansatz.[5] The coordinate representation of the Bethe vectors gives explicitly analytical dependence on the parameters $\{\mu_i\}_1^M$ and $\{z_a\}_1^N$ useful in a relation to the Knizhnik–Zamolodchikov equation (Sec. V). Using the Gaudin realization (3.19)–(3.21) of the generators

$$v^+(\mu)=\sum_{a=1}^{N}\frac{e^{\mu-z_a}}{\sinh(\mu-z_a)}v_a^+,\quad X^+(\mu)=\sum_{a=1}^{N}\frac{e^{\mu-z_a}}{\sinh(\mu-z_a)}X_a^+,$$

and the definition of the creation operators (3.42), one can get the coordinate representation of the B-operators:

$$B_M(\mu_1,\mu_2,\ldots,\mu_M)=\sum_{\pi}(v_{a_1}^+\cdots v_{a_M}^+)_{\pi}\prod_{a=1}^{N}\varphi(\{\mu_m^{(a)}\}_1^{|\mathcal{K}_a|};z_a), \tag{4.32}$$

where the first sum is taken over ordered partitions π of the set $(1,2,\ldots,M)$ into subsets $\mathcal{K}_a$, $a=1,2,\ldots,N$, including empty subsets with the constraints

$$\bigcup_a \mathcal{K}_a=(1,2,\ldots,M), \quad \mathcal{K}_a\cap\mathcal{K}_b=\varnothing \quad \text{for} \quad a\neq b.$$

The corresponding subset of quasimomenta

$$(\mu_1^{(a)}=\mu_{j_1},\mu_2^{(a)}=\mu_{j_2},\ldots,\mu_{|\mathcal{K}_a|}^{(a)}=\mu_{j_{|\mathcal{K}_a|}};j_m\in\mathcal{K}_a),$$

where $|\mathcal{K}_a|$ is the cardinality of the subset $\mathcal{K}_a$, and $j_k<j_{k+1}$, entering into the coordinate wave function

$$\varphi(\{\nu_m\}_1^{|\mathcal{K}|};z)=\sum_{\sigma\in\mathcal{S}_{|\mathcal{K}|}}(-1)^{p(\sigma)}\frac{e^{\nu_{\sigma(1)}-\nu_{\sigma(2)}}}{\sinh(\nu_{\sigma(1)}-\nu_{\sigma(2)})}\frac{e^{\nu_{\sigma(2)}-\nu_{\sigma(3)}}}{\sinh(\nu_{\sigma(2)}-\nu_{\sigma(3)})}\cdots\frac{e^{\nu_{\sigma(|\mathcal{K}|)}-z}}{\sinh(\nu_{\sigma(|\mathcal{K}|)}-z)}.$$

Due to the alternative sum over permutations $\sigma\in\mathcal{S}_{|\mathcal{K}|}$ this function is antisymmetric with respect to the quasi-momenta. Finally, the first factor in (4.32),

$$(v_{a_1}^+\cdots v_{a_M}^+)_\pi,$$

means that for $j_m\in\mathcal{K}_a$, corresponding indices of $v_{a_{j_m}}^+$ are equal to a so that $v_{a_{j_m}}^+=v_a^+$. One can collect these operators into product $\Pi_{a=1}^N(v_a^+)^{|\mathcal{K}_a|}$; consequently, we have an extra sign factor $(-1)^{p(\pi)}$.

This coordinate representation is similar to the representations obtained in Refs. 11–13 for the Gaudin models related to the simple Lie algebras (see also Ref. 43). The Z_2-grading of superalgebra results in extra signs, while the complicated structure of the B_M-operators [for the sl(2) Gaudin model they are just products of B_1-operators $B_1(\mu_j)=X^+(\mu_j)$] is connected with the fact that $(v_j^+)^2=X_j^+\neq 0$ while for $j\neq k$ v_j^+ and v_k^+ anticommute.

V. SOLUTIONS TO THE KNIZHNIK–ZAMOLODCHIKOV EQUATION

Correlation functions $\psi(z_1,\ldots,z_N)$ of a two dimensional conformal field theory satisfy the Knizhnik–Zamolodchikov equation[44]

$$\kappa\ \partial_{z_a}\ \psi(z_1,\ldots,z_N)=H^{(a)}\psi(z_1,\ldots,z_N), \tag{5.1}$$

where $H^{(a)}(a=1,\ldots,N)$ are the Gaudin Hamiltonians (3.24) and $\psi(z_1,\ldots,z_N)$ is a function of N complex variables with its values in a tensor product $\mathcal{H}=\otimes_{a=1}^N V_a^{(l_a)}$.

A relation between the Bethe vectors of the Gaudin model related to simple Lie algebras and the solutions to the Knizhnik–Zamolodchikov equation is well known for some time.[11,12] Approach used here to obtain solutions to the Knizhnik–Zamolodchikov equation corresponding to conformal field theory and Lie superalgebra osp(1|2) starting from B-vectors (4.2) is based on Ref. 11.

A solution in question is represented as a contour integral over the variables $\mu_1,\ldots,\mu_M$

$$\psi(z_1,\ldots,z_N)=\oint\cdots\oint\ \phi(\vec{\mu}|\vec{z})\Psi(\vec{\mu}|\vec{z})\ \ \mathrm{d}\mu_1\cdots\mathrm{d}\mu_M, \tag{5.2}$$

where an integrating factor $\phi(\vec{\mu}|\vec{z})$ is a scalar function

$$\phi(\vec{\mu}|\vec{z})=\prod_{i<j}^M\sinh(\mu_i-\mu_j)^{1/\kappa}\prod_{a<b}^N\sinh(z_a-z_b)^{l_al_b/\kappa}\left(\prod_{k=1}^M\prod_{c=1}^N\sinh(\mu_k-z_c)^{-l_c/\kappa}\right), \tag{5.3}$$

and $\Psi(\vec{\mu}|\vec{z})$ is a Bethe vector (4.2) where the corresponding Bethe equations are not imposed.

As a first step in the proof that $\psi(z_1,\ldots,z_N)$ given by (5.2) is a solution of (5.1) we differentiate the product $\phi\Psi$ with respect to z_a and obtain

$$\partial_{z_a}(\phi\Psi)=\partial_{z_a}(\phi)\Psi+\phi\partial_{z_a}(\Psi). \tag{5.4}$$

Using (5.3) the first term on the right hand side can be calculated explicitly:

$$\kappa\partial_{z_a}\phi=\left(\sum_{\substack{b=1\\ b\neq a}}^{N} l_a\, l_b\coth(z_a-z_b)-\sum_{j=1}^{M} l_a\coth(z_a-\mu_j)\right)\phi=E_M^{(a)}\phi. \tag{5.5}$$

Furthermore, taking a residue of (3.3) at $\lambda=z_a$ we have

$$H^{(a)}\Psi=E_M^{(a)}\Psi+\sum_{j=1}^{M}(-1)^j\frac{e^{-(z_a-\mu_j)}}{\sinh(z_a-\mu_j)}\beta_M(\mu_j)\tilde{\Psi}^{(j,a)}, \tag{5.6}$$

where

$$\tilde{\Psi}^{(j,a)}=\left(v_a^+ B_{M-1}^{(j)}+2X_a^+\sum_{k\neq j}^{M}(-1)^{k+\Theta(j-k)}\frac{e^{-(\mu_j-\mu_k)}}{\sinh(\mu_j-\mu_k)}B_{M-2}^{(j,k)}\right)\ \Omega_-. \tag{5.7}$$

Hence (5.4) can be written as

$$\kappa\partial_{z_a}(\phi\Psi)=H^{(a)}(\phi\Psi)+\phi\sum_{j=1}^{M}(-1)^j\frac{e^{\mu_j-z_a}}{\sinh(\mu_j-z_a)}\beta_M(\mu_j)\tilde{\Psi}^{(j,a)}+\kappa\phi\partial_{z_a}(\Psi). \tag{5.8}$$

Moreover, from (5.3) we also have

$$\kappa\partial_{\mu_j}\phi=\left(\sum_{a=1}^{N}(-l_a)\coth(\mu_j-z_a)+\sum_{\substack{k=1\\ j\neq k}}^{M}\coth(\mu_j-\mu_k)\right)\phi=\beta_M(\mu_j)\phi, \tag{5.9}$$

and from Lemma 3.4 follows

$$\partial_{z_a}\Psi=\sum_{j=1}^{M}(-1)^j\partial_{\mu_j}\left(\frac{e^{\mu_j-z_a}}{\sinh(\mu_j-z_a)}\tilde{\Psi}^{(j,a)}\right). \tag{5.10}$$

Thus, using (5.9) and (5.10), we can combine the last two terms in (5.8) into a sum of first order derivatives in μ_j:

$$\kappa\partial_{z_a}(\phi\Psi)=H^{(a)}(\phi\Psi)+\kappa\sum_{j=1}^{M}(-1)^j\partial_{\mu_j}\left(\frac{e^{\mu_j-z_a}}{\sinh(\mu_j-z_a)}\phi\,\tilde{\Psi}^{(j,a)}\right). \tag{5.11}$$

A closed contour integration of $\phi\Psi$ with respect to $\mu_1,\ldots,\mu_M$ will cancel the contribution from the terms under the sum in (5.11) and therefore $\psi(z_1,\ldots,z_N)$ given by (5.2) satisfies the Knizhnik–Zamolodchikov equation.

Conjugated Bethe vectors $(B_M\Omega_-)^*$ are entering into the solution $\tilde{\psi}(z_1,\ldots,z_N)$ of the dual Knizhnik–Zamolodchikov equation

$$-\kappa\frac{\partial}{\partial z_a}\tilde{\psi}(z_1,\ldots,z_N)=\tilde{\psi}(z_1,\ldots,z_N)\ \ H^{(a)}. \tag{5.12}$$

The scalar product $(\tilde{\psi}(z_1,\ldots,z_N),\ \psi(z_1,\ldots,z_N))$ does not depend on $\{z_j\}_1^N$ and its quasi-classical limit $\kappa\to 0$ gives the norm of the Bethe vectors due to the fact that the stationary points of the contour integrals for $\kappa\to 0$ are solutions to the Bethe equations[13]

$$\frac{\partial S}{\partial \mu_j}=\sum_{a=1}^{N}(-l_a)\coth(\mu_j-z_a)+\sum_{\substack{k=1\\ j\neq k}}^{M}\coth(\mu_j-\mu_k)=0, \tag{5.13}$$

$$S(\vec{\mu}|\vec{z})=\kappa\ln\phi=\sum_{a<b}^{N}l_a l_b\ln(\sinh(z_a-z_b))+\sum_{i<j}^{M}\ln(\sinh(\mu_i-\mu_j))$$
$$-\sum_{a=1}^{N}\sum_{j=1}^{M}l_a\ln(\sinh(z_a-\mu_j)). \tag{5.14}$$

According to the remark at the end of Sec. IV, analytical properties of the Bethe vectors of the trigonometric osp(1|2) Gaudin model coincide with the analytical properties of the trigonometric sl(2) Gaudin model. Thus, the expression for the norm of the Bethe vectors Ψ (4.2) obtained as the first term in the asymptotic expansion $\kappa\to 0$ coincides also

$$(\Psi,\Psi)=\det\left(\frac{\partial^2 S}{\partial\mu_j\ \partial\mu_k}\right), \tag{5.15}$$

$$\frac{\partial^2 S}{\partial\mu_j^2}=\sum_{a=1}^{N}\frac{l_a}{\sinh^2(\mu_j-z_a)}-\sum_{k\neq j}^{M}\frac{1}{\sinh^2(\mu_j-\mu_k)},\quad \frac{\partial^2 S}{\partial\mu_j\ \partial\mu_k}=\frac{1}{\sinh^2(\mu_j-\mu_k)}, \tag{5.16}$$

for $j\neq k$.

Finally we notice that the modification of the Gaudin Hamiltonians we discussed at the end of the previous section can be easily transfered to the corresponding modification of the Knizhnik–Zamolodchikov equations. The modification (4.16) for the sl(2)-invariant Gaudin model was studied in Ref. 29 as a quantization of the Schlesinger system (see also Ref. 28). This modification is related with extra factor in the integrating scalar function (5.3),

$$\phi_j=\exp\left(\frac{S_j}{\kappa}\right),\quad j=0,1, \tag{5.17}$$

where $S_0=S$ (5.14) and

$$S_1=S_0+g\sum_{j=1}^{M}\mu_j-g\sum_{a=1}^{N}l_a z_a \tag{5.18}$$

correspond to the modification (4.16).

Moreover, following the lines of Ref. 29, one can try to extend the connection between the KZ equation and the Guadin model based on the modified L-operator (4.16) by extending the KZ system to include an equation of the form

$$\left(\kappa\frac{\partial}{\partial g}-H_{\mathrm{Rich}}\right)\psi=0\ . \tag{5.19}$$

However, such a straightforward generalization has failed in the trigonometric case (see below). We can comment on the extension in the rational case[17] as a scaling limit of the trigonometric Gaudin model (4.30). The equations of original KZ system are defined by mutually commuting differential operators [see (3.4)]:

$$\nabla_a=\kappa\frac{\partial}{\partial z_a}-\tilde{H}^{(a)}=\kappa\frac{\partial}{\partial z_a}-gh_a-\sum_{b\neq a}\frac{c_2^{\otimes}(a,b)}{z_a-z_b}. \tag{5.20}$$

The operator

$$\nabla_g = \kappa \frac{\partial}{\partial g} - H_{\mathrm{Rich}} = \kappa \frac{\partial}{\partial g} - \sum_{a=1}^{N} z_a h_a - \frac{1}{2g}(c_2(gl) - h_{gl}(h_{gl}-1)) \tag{5.21}$$

is commuting pairwise with the operators ∇_a. Thus in the rational case the KZ system can be generalized to include the operator ∇_g.

To prove that the solution to the modified KZ system with ϕ_1 given by (5.17) and (5.18) is a solution to the generalized KZ system we have to extend the trigonometric KZ equations (5.1) with modified Hamiltonians $gh_a + H^{(a)}$ along the lines of Refs. 15 and 16. A difference equation must be introduced,

$$K(z_1,\ldots,z_N;g) \quad \psi(z_1,\ldots,z_N;g) = \psi(z_1,\ldots,z_N;g-2\kappa), \tag{5.22}$$

instead of (5.21). The operator K is defined on the space $\mathcal{H}$

$$K(z_1,\ldots,z_N;g) = \exp\left(-2\sum_{a=1}^{N} z_a h_a\right) P(g;h_{gl},v_{gl}^{+},v_{gl}^{-}), \tag{5.23}$$

where the operator P depends on the global generators of the subalgebra $\mathrm{osp}(1|2) \subset \mathcal{L}_t$, and is constructed form the extremal projector $p(h,v^{+},v^{-})$ by a shift of the Cartan generator (see the Appendix). We introduce only one K operator since the rank of osp(1|2) Lie superalgebra is one. In the general case of simple Lie superalgebra of rank r, one has to consider a set of K_k, $k=1,\ldots,r$ (see Refs. 15 and 16).

VI. CONCLUSION

By analyzing the model related to the trigonometric osp(1|2) classical r-matrix the algebraic Bethe ansatz approach to the Gaudin models is reviewed. The results presented in this article are in some sense analogous to the ones we obtained for the osp(1|2)-invariant model.[17] In particular, a striking similarity between some of the most fundamental characteristics of this system and the sl(2) trigonometric Gaudin model was confirmed. Although explicitly constructed creation operators B_M (3.42) of the Bethe vectors are complicated polynomials of the L-operator entries $v^{+}(\lambda)$ and $X^{+}(\lambda)$, the coordinate form of the eigenfunctions differs only in signs from the corresponding states in the case of sl(2) trigonometric model, being antisymmetric functions of the quasimomenta. Moreover, the eigenvalues and the Bethe equations coincide, provided that the sl(2) Gaudin model with integer spins is considered. Analogously, the KZ equations based on both trigonometric models and for the nontrivial magnetic field g require extension of the system of equations by the dynamical difference equation.

Let us point out that by the method presented in this article one can construct explicitly creation operators of the Gaudin models related to trigonometric Izergin-Korepin r-matrix[3,30] corresponding to the twisted affine algebra $A_2^{(2)}$. Similarly to the simple Lie algebra case, solutions to the Knizhnik–Zamolodchikov equation were constructed from the Bethe vectors using algebraic properties of the creation operators B_M and the Gaudin realization of the loop superalgebra $\mathcal{L}_t(\mathrm{osp}(1|2))$. This interplay between the Gaudin model and the Knizhnik–Zamolodchikov equation enabled us to determine the norm of eigenfunctions of the Gaudin Hamiltonians

$$\|\Psi(\mu_1,\ldots,\mu_M;\{z_a\}_1^N)\|^2 = \det\left(\frac{\partial^2 S}{\partial \mu_j \ \partial \mu_k}\right).$$

The difficult problem of correlation function calculation for general Bethe vectors

$$\mathcal{C}(\{\nu_j\}_1^M;\{\mu_i\}_1^M;\{\lambda_k\}_1^K) = \left(\Omega_-, \ B_M^{*}(\nu_1,\ldots,\nu_M)\prod_{k=1}^{K} h(\lambda_k)\, B_M(\mu_1,\ldots,\mu_M)\Omega_-\right)$$

was solved nicely for the sl(2)-invariant Gaudin model in Ref. 7 using the Gauss factorization of the loop algebra group element and the appropriate Riemann-Hilbert problem. Although the corresponding factorization is known even for the quantum superalgebra $\mathcal{U}_q(\mathrm{osp}(1|2))$,[45] the final expression of the correlation functions is difficult to obtain due to the complicated structure of the creation operators $B_M(\mu_1,\ldots,\mu_M)=\mathrm{Poly}(v^+,X^+)$ (3.42). The study of this problem is in progress and the following expression for the scalar product of the Bethe states is conjectured (see Ref. 7):

$$(\Omega_-,\ B_M^*(\nu_1,\ldots,\nu_M)B_M(\mu_1,\ldots,\mu_M)\Omega_-)=\sum_{\sigma\in\mathcal{S}_M}(-1)^{p(\sigma)}\det\mathcal{M}^{\sigma},$$

where the sum is over symmetric group $\mathcal{S}_M$ and $M\times M$ matrix $\mathcal{M}^{\sigma}$ is given by

$$\mathcal{M}^{\sigma}_{jj}=\frac{e^{\mu_j-\nu_{\sigma(j)}}}{\sinh(\mu_j-\nu_{\sigma(j)})}(\rho(\mu_j)-\rho(\nu_{\sigma(j)}))-\sum_{k\neq j}^{M}\frac{e^{\mu_j-\mu_k}e^{-(\nu_{\sigma(j)}-\nu_{\sigma(k)})}}{\sinh(\mu_j-\mu_k)\sinh(\nu_{\sigma(j)}-\nu_{\sigma(k)})},$$

$$\mathcal{M}^{\sigma}_{jk}=\frac{e^{\mu_j-\mu_k}e^{-(\nu_{\sigma(j)}-\nu_{\sigma(k)})}}{\sinh(\mu_j-\mu_k)\sinh(\nu_{\sigma(j)}-\nu_{\sigma(k)})},\quad \text{for } j,k=1,2,\ldots,M.$$

ACKNOWLEDGMENTS

We acknowledge useful discussions and communications with N. Yu. Reshetikhin, V. O. Tarasov and T. Takebe. This work was supported by Grant No. PRAXIS XXI/BCC/22204/99, INTAS Grant No. N 99-01459 and FCT Project No. POCTI/33858/MAT/2000.

APPENDIX: ORTHOSYMPLECTIC LIE SUPERALGEBRA osp(1|2)

The rank of the orthosymplectic Lie algebra osp(1|2) is one and its dimension is five.[33] The three even generators are h,X^+,X^- and the two odd generators are v^+,v^-. The (graded) commutation relations of the generators are

$$\begin{gathered}[h,X^{\pm}]_-=\pm 2X^{\pm},\quad [X^+,X^-]_-=h,\\ [h,v^{\pm}]_-=\pm v^{\pm},\quad [v^+,v^-]_+=-h,\\ [X^{\mp},v^{\pm}]_-=v^{\mp},\quad [v^{\pm},v^{\pm}]_+=\pm 2X^{\pm},\\ [X^{\pm},v^{\pm}]_-=0.\end{gathered}\tag{A1}$$

The Casimir element is

$$c_2=h^2+2(X^+X^-+X^-X^+)+(v^+v^--v^-v^+)=h^2-h+4X^+X^-+2v^+v^-.\tag{A2}$$

It is interesting to point out the existance of a ''square root'' of this element

$$c_1=h+2v^+v^--\tfrac{1}{2},\quad (c_1)^2=c_2+\tfrac{1}{4},\tag{A3}$$

with a grading property $[c_1,X^{\pm}]=0$, $[c_1,h]=0$ and $c_1v^{\pm}=-v^{\pm}c_1$. The finite dimensional irreducible representations $V^{(l)}$ of the osp(1|2) Lie superalgebra are parametrized by an integer l, so that their dimensions $2l+1$ and the values of the Casimir element (A2) $c_2=l(l+1)$ coincide with the same characteristics of the integer spin l irreducible representations of sl(2).

The fundamental irreducible representation $V^{(1)}$ of osp(1|2) is three dimensional. We choose a grading of the basis vectors e_j, $j=1,2,3$, to be (0,1,0). Explicitly we have

$$h=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$v_-=(v_+)^{st}=\begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

together with $X^{\pm}=\pm(v^{\pm})^2$. The matrix v^+ in the representation $V^{(l)}$ has $2l$ nonzero elements on the second upper diagonal only, and these elements are

$$\{(v^+)_{jj+1}\}=(\sqrt{l},\sqrt{1},\sqrt{l-1},\sqrt{2},\ldots,\sqrt{1},\sqrt{l}),\quad j=1,2,\ldots,2l. \tag{A4}$$

The extermal projector[46] for osp(1|2) (on the lowest weight vectors) is

$$\begin{aligned} p(h,v^+,v^-)&=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\left((v^+)^{2k}(v^-)^{2k}+(v^+)^{2k+1}(v^-)^{2k+1}\frac{1}{h-k-1}\right)\prod_{j=1}^{k}\frac{1}{h-j} \\ &=\left(1+v^+v^-\frac{1}{h-1}\right)\left(\sum_{k=0}^{\infty}(X^+)^k(X^-)^k\prod_{j=1}^{k}\frac{1}{j(h-j-1)}\right) \\ &=p_s(h,v^+,v^-)p_0(h,X^+,X^-); \end{aligned} \tag{A5}$$

here $p_0(h,X^+,X^-)$ is the usual sl(2) extermal projector. There is no such factorization property for the extermal projector of the quantum superalgebra $\mathcal{U}_q(\mathrm{osp}(1|2))$.[31]

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Category of nonlinear evolution equations, algebraic structure, and *r*-matrix

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(Received 5 December 2000; accepted 29 October 2002)

In this paper we deal with the category of nonlinear evolution equations (NLEEs) associated with the spectral problem and provide an approach for constructing their algebraic structure and *r*-matrix. First we introduce the category of NLEEs, which is composed of various positive order and negative order hierarchies of NLEEs both integrable and nonintegrable. The whole category of NLEEs possesses a generalized Lax representation. Next, we present two different Lie algebraic structures of the Lax operator: one of them is universal in the category, i.e., independent of the hierarchy, while the other one is nonuniversal in the hierarchy, i.e., dependent on the underlying hierarchy. Moreover, we find that two kinds of adjoint maps are *r*-matrices under the algebraic structures. In particular, the Virasoro algebraic structures without a central extension of isospectral and nonisospectral Lax operators can be viewed as reductions of our algebraic structure. Finally, we give several concrete examples to illustrate our methods. Particularly, the Burgers' category is linearized when the generator, which generates the category, is chosen to be independent of the potential function. Furthermore, an isospectral negative order hierarchy in the Burgers' category is solved with its general solution. Additionally, in the KdV category we find an interesting fact: the Harry–Dym hierarchy is contained in this category as well as the well-known Harry–Dym equation is included in a positive order KdV hierarchy.
[DOI: 10.1063/1.1532769]

I. INTRODUCTION

The integrability study of nonlinear evolution equations has been an attractive topic in soliton theory and nonlinear phenomenon. Calogero[1] proposed the *C*-integrable (namely, linearizable by an appropriate change of variables) and *S*-integrable (namely, integrable via some spectral transform technique) terminology for dealing with nonlinear partial diiferetial equations (PDEs). Many nonlinear PDEs were shown *C*-integrable and *S*-integrable.[2] Mikhailov, Shabat and Sokolov[3] discussed some classes of nonlinear *C*-integrable and *S*-integrable PDEs through using the symmetry approach. Flaschka, Newell and Tabor[4] considered in detail the Painleve analysis process for both ODEs and PDEs and investigated its test for integrable equations.

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On the other hand, the r-matrix method is also an important part in classical and quantum integrable systems.[5] The classical r-matrix has been first introduced by Sklyanin in Refs. 6 and 7 as the limit of its quantum counterpart. Subsequently, Drinfeld used this to introduce a new geometric notion, that of a Poisson Lie group.[8] Following Drinfeld's ideas[8] Semenov–Tian–Shansky showed that the concept of a classical r-matrix leads to an algebraic construction of integrable systems generalizing the AKS scheme. In terms of the r-matrix[9] an effective view of the multi-Hamiltonian property of such equations can be presented. In addition, it gives a general explanation of the dressing transformations used for obtaining solutions in terms of group factorizations.[10] In Ref. 11 Jimbo constructed explicit solutions of the quantum YB equation for the generalized Toda system and moreover obtained many beautiful results[12–14] by using the r-matrix method.

For the study of an algebraic structure of integrable evolution equations, there has also been a discussion in the literature. For example, the well-known W-algebra was constructed by Orlov and Schulman through using the vertex operator.[15] The KP system was also found to have this kind of W-algebraic structure by Dickey,[16] which includes the Virasoro algebra as its subalgebra. The W-algebra played an important role in the so-called second Poinsson structure.[16] For this, the most important thing is to find the generators of W-algebra. All these facts were only for the case of integrable hierarchies. How about the case for both integrable and nonintegrable hierarchies? In this paper we will deal with this problem through introducing the category of nonlinear evolution equations (NLEEs). The category of NLEEs develops the positive order to the negative order hierarchies for both the integrable and the nonintegrable cases. In particular, the positive and the negative order integrable hierarchies will be generated by the recursion operator, its inverse, and some kernel elements from the pair of Lenard's operators. Mikhailov, Shabat and Sokolov[3] extended the integrable equations by employing the symmetry procedure and discussed the classifications for the integrable hierarchies. All of their results were for C-integrable and S-integrable cases. In this paper, we will discuss the case for both integrable and nonintegrable hierarchies and will not interfere with the existence of symmetries. Here, we point out that throughout this paper: ''integrable'' means the sense of Lax, namely, the PDE admits isospectral (i.e., $\lambda_t=0$) or usual nonisospectral (i.e., $\lambda_t=a\lambda^n$, $n\in\mathbb{Z}$, $a\in\mathbb{R}/\mathbb{C}$) Lax form; otherwise, we say the PDE is nonintegrable in the sense of the Lax form.

Our purpose in the present paper is to give an approach to the category of nonlinear evolution equations directly from a spectral problem and to connect the r-matrix to the category of NLEEs. The whole paper is organized as follows. In the next section we first introduce the notation of the category of NLEEs, which is composed of various positive and negative order hierarchies of both integrable and nonintegrable NLEEs, and then we give the generalized Lax representation (GLR). In Secs. III and IV we, respectively, present two different Lie algebraic structures of the Lax operator. One structure is produced independently of the hierarchy in the category while the other holds only within one hierarchy. Moreover, by using these algebraic structures we find that two kinds of adjoint maps result in r-matrices for the NLEEs. In Sec. V, it is pointed out that the well known Virasoro algebraic structures (without the central extension) of isospectral and nonisospectral Lax operators are obtained as reductions of our algebraic structure. Finally, in Sec. VI the examples of several continuous spectral problems are given to illustrate our methods. Particularly, the Burgers' category is linearized when the generator, which generates the category, is chosen to be independent of the potential function. Furthermore, an isospectral negative order hierarchy in the Burgers' category is solved with its general solution. Additionally, in the KdV category we find an interesting fact: the Harry–Dym hierarchy is contained in this category as well as the well-known Harry-Dym equation is included in a positive order KdV hierarchy.

Before displaying our main results, let us first give some necessary notations:

$$x\in R^l,\ \ t\in R,\ \ u=(u_1,\ldots,u_m)^T\in S^m(R^l,R)=\overbrace{S(R^l,R)\times\cdots\times S(R^l,R)}^{m},$$

$$u_i=u_i(x,t)\in S(R^l,R),\ \ i=1,2,\ldots,m,$$

for arbitrarily fixed t, $S(R^l,R)$ stands for the Schwartz function space on R^l. $\mathcal{B}$ denotes all complex (or real) value functions $P(x,t,u)$ of the class C^∞ with respect to x, t, and of the class C^∞ in Gateaux's sense with respect to u. $\mathcal{B}^N=\{(P_1,\ldots,P_N)^T|P_i\in\mathcal{B}\}$, $\mathcal{V}^N$ stands for all linear operators $\phi=\phi(x,t,u)$: $\mathcal{B}^N\to\mathcal{B}^N$ which are of the class C^∞ with respect to x, t, and of the class C^∞ in Gateaux's sense with respect to u.

The Gateaux derivate of vector function $X\in\mathcal{B}^n$ in the direction $Y\in\mathcal{B}^m$ is defined by

$$X_*(Y)=\frac{d}{d\epsilon}\bigg|_{\epsilon=0} X(u+\epsilon Y). \tag{1.1}$$

For the two arbitrary vector fields X, $Y\in\mathcal{B}^m$, define the following operation:

$$[X,\ Y]=X_*(Y)-Y_*(X). \tag{1.2}$$

Then, $\mathcal{B}^m$ composes a Lie algebra about the above multiplication operation.[17] For the operator $\phi\in\mathcal{V}^N$, its Gateaux derivate operator $\phi_*:\mathcal{B}^m\to\mathcal{V}^N$ in the direction ξ is defined as follows:

$$\phi_*(\xi)=\frac{d}{d\epsilon}\bigg|_{\epsilon=0}\phi(u+\epsilon\xi),\quad \xi\in\mathcal{B}^m. \tag{1.3}$$

If not otherwise stated, the spectral operators $L=L(u)$ [or the spectral operators $L=L(u,\ \lambda)$ with the spectral parameter λ] considered in this paper are denoted by $L\in\mathcal{V}^N$, and we always assume that $L_*:\mathcal{B}^m\to\mathcal{V}^N$ is an injective homomorphism. An operator H acting on a function f is denoted by $H\cdot f$. I stands for the $N\times N$ unit operator.

II. CATEGORY OF NLEEs AND GENERALIZED LAX REPRESENTATION (GLR)

In this section, a procedure for constructing the category of NLEEs and generalized Lax representations are presented, and, moreover, it is shown how to construct the $L-A-B$ triple representation[18] for a given nonlinear quation.

Let us start from a general $N\times N$ spectral problem:

$$L\cdot\psi=\lambda\psi,\quad L\in\mathcal{V}^N, \tag{2.1}$$

where λ is a spectral parameter, $\psi\in\mathcal{B}^N$. Denote the functional gradient of spectral parameter λ with regard to the potential vector u by $\delta\lambda/\delta u=(\delta\lambda/\delta u_1,\cdots,\delta\lambda/\delta u_m)^T$. Tu and Cao, respectively, gave some discussions about the calculations of the functional gradient in Ref. 19 and Ref. 20. Strampp ever studied recursion operators, spectral problems, and Bäcklund transformations by introducing a relation between recursion operators and eigenvalue functions.[21,22] Thus, we define the Lenard operators as follows:

Definition 2.1: If there exists a pair of $m\times m$ operators $K=K(u)$, $J=J(u)$: $S^m(R^l,\ R)\to S^m(R^\cdot R)$ such that

$$K\cdot\frac{\delta\lambda}{\delta u}=\lambda^c J\cdot\frac{\delta\lambda}{\delta u}, \tag{2.2}$$

then K, J are called a pair of Lenard operators of (2.1), and (2.2) is called the Lenard spectral problem of (2.1). Here the constant c is definitely chosen by the concrete form of (2.1).

In many cases, there exist (but not unique) the pair of Lenard's operators satisfying (2.2), and frequently both of them are Hamiltonian operators. For instance, for the KdV–Schrödinger spectral problem $\psi_{xx}+u\psi=\lambda\psi$, $\delta\lambda/\delta u=\psi^2$, only choosing $K=-\frac{1}{4}\partial^3-\frac{1}{2}(u\partial+\partial u)$, $J=\partial=\partial/\partial x$, we have $K\cdot\delta\lambda/\delta u=\lambda J\cdot\delta\lambda/\delta u$. Eq. (2.2) plays an important role in the nonlinearization theory and the construction of completely integrable finite-dimensional systems.[23]

Let $M=(m_{ij})_{N\times N}$, $\tilde{M}=(\tilde{m}_{ij})_{N\times N}$ be the arbitrarily given $1+l$-dimensional [i.e., independent variables $(x,\ t)\in R^l\times R,\ l\geqslant 1$] linear $N\times N$ matrix operators. Then we have the following definitions.

Definition 2.2: $G_0\in S^m(R^l,\ R)$, $G_{-1}\in S^m(R^l,\ R)$ *are, respectively, called the positive order and the negative order generators, if they, respectively, satisfy the operator equations,*

$$L_*(J\cdot G_0)=M, \tag{2.3}$$

$$L_*(K\cdot G_{-1})=\tilde{M}. \tag{2.4}$$

Denote the solution sets of (2.3) and (2.4) by $\mathcal{N}_J(M)$ and $\mathcal{N}_K(\tilde{M})$, respectively. In general, they are not empty.

Definition 2.3: Let $\mathcal{N}_J(M)\neq\varnothing$, $\mathcal{N}_K(\tilde{M})\neq\varnothing$ *and choose* $G_0\in\mathcal{N}_J(M)$, $G_{-1}\in\mathcal{N}_K(\tilde{M})$. *Write the recursion operator* $\mathcal{L}=J^{-1}K$. *The sequence* $\{G_j\}_{j=-\infty}^{\infty}\subseteq S^m(R^l,R)$ *recursively determined by*

$$G_j=\begin{cases}\mathcal{L}^j\cdot G_0, & j\geqslant 0,\\ \mathcal{L}^{j+1}\cdot G_{-1}, & j<0,\end{cases} \tag{2.5}$$

is called the Lenard's sequence of (2.1); the set of the following nonlinear equations:

$$u_t=X_m(u,G_0,G_{-1}),\ \ m\in Z, \tag{2.6}$$

produced by the vector field

$$X_m(u,G_0,G_{-1})\triangleq J\cdot G_m,\ \ m\in Z, \tag{2.7}$$

is called the category of nonlinear evolution equations of (2.1). The subset of the equations (2.6) obtained for $m\geqslant 0$ *is called the positive order category while the subset obtained for* $m<0$ *is called the negative order category.*

Apparently, the positive and the negative order generators G_0, G_{-1} depend on the choice of matrix operators M, $\tilde{M}$, thus the category (2.6) is composed of various hierarchies (both integrable and nonintegrable) of NLEEs which are generated according to the choice of operators M, $\tilde{M}$.

For example, with $M\equiv 0$ (i.e., $G_0\in\mathrm{Ker}\ J$), the hierarchy in the positive order category of (2.6) just reads as the isospectral hierarchy of evolution equations;[24] with $\tilde{M}\equiv 0$ (i.e., $G_{-1}\in\mathrm{Ker}\,K$), the hierarchy in the negative order category of (2.6) is exactly the second isospectral hierarchy of evolution equations studied in Ref. 25. Additionally, the negative order generator G_{-1} can be considered to produce finite-dimensional constrained Hamiltonian systems.[26] Obviously, the negative order category of (2.6) is generated with the help of the inverse recursion operator $\mathcal{L}$. Strampp and Oevel gave the inverse recursion operator in an explicit form for the nonlinear derivative Schrödinger equation.[27] In 1991 we suggested the commutator representations for the negative order hierarchy of isospectral NLEEs.[28] Afterwards, we[29] further found that the same spectral problem can generate two different hierarchies of integrable NLEEs: one is the usual higher order (i.e., positive order) hierarchy of NLEEs, the other is the negative order hierarchy of NLEEs. All these equations have the Lax representations.[29] Here we study the generalized case, i.e., the category of NLEEs.

With $M=I$ or $\tilde{M}=I$, under the basic condition $\mathcal{N}_J(I)\neq\varnothing$ or $\mathcal{N}_K(I)\neq\varnothing$, Eq. (2.6) actually gives the positive and the negative order hierarchies of nonisospectral evolution equations, which can be obtained from the following, Theorem 2.2. Thus, by the arbitrariness of M and $\tilde{M}$, Eq. (2.6) unifies together all possible hierarchies of evolution equations associated with the spectral problem (2.1). Due to this fact, Eq. (2.6) is named ''the category of nonlinear evolution equations.''

Theorem 2.1: *Let* $M=(m_{ij})_{N\times N}$, $\tilde{M}=(\tilde{m}_{ij})_{N\times N}$ *be two arbitrarily given* $N\times N$ *linear matrix operators,* $\mathcal{N}_J(M)\neq\varnothing$, *and* $\mathcal{N}_K(\tilde{M})\neq\varnothing$. *Suppose that for* $G=(G^{[1]},\ldots,G^{[m]})^T\in S^m(R^l, R)$ *and* $\alpha,\beta\in Z$ *the operator equation,*

$$[V,L]=L_*(K\cdot G)L^{\beta}-L_*(J\cdot G)L^{\alpha}, \tag{2.8}$$

possesses a solution $V=V(G)$; *then the vector field* $X_m=X_m(u,G_0,G_{-1})$ *satisfy*

$$L_*(X_m)=[W_m,L]+\bar{M}L^{m\eta},\quad m\in Z,\quad \bar{M}=\begin{cases}M, & m\geqslant 0,\\ \tilde{M}, & m<0,\end{cases} \tag{2.9}$$

where $\eta=\alpha-\beta$ *and the operator* W_m *is given by*

$$W_m=\sum V(G_j)L^{(m-j)\eta-\alpha},\quad \sum=\begin{cases}\sum_{j=0}^{m-1}, & m>0,\\ 0, & m=0,\\ -\sum_{j=m}^{-1}, & m<0.\end{cases} \tag{2.10}$$

Here G_j *are determined by (2.5), and* L^{-1} *is the inverse of* L, *i.e.,* $LL^{-1}=L^{-1}L=I$, *and* $[\cdot,\cdot]$ *denotes the usual commutator.*

Proof: For $m=0$, it is obvious. For $m>0$,

$$\begin{aligned}[W_m,L]&=\sum_{j=0}^{m-1}[V(G_j),L]L^{(m-j)\eta-\alpha}\\ &=\sum_{j=0}^{m-1}\{L_*(K\cdot G_j)L^{(m-j-1)\eta}-L_*(J\cdot G_j)L^{(m-j)\eta}\}\\ &=\sum_{j=0}^{m-1}\{L_*(J\cdot G_{j+1})L^{(m-j-1)\eta}-L_*(J\cdot G_j)L^{(m-j)\eta}\}=L_*(X_m)-L_*(J\cdot G_0)L^{m\eta}\\ &=L_*(X_m)-ML^{m\eta}.\end{aligned}$$

For $m<0$, the proof is similar. ■

Remark 2.1: The structure equation (2.8) of commutator representations is a natural generalization of the structure equation $[V,L]=L_*(K\cdot G)-L_*(J\cdot G)L$ presented by Cao Cewen.[30]

Remark 2.2: The choice of constants $\alpha,\beta\in Z$ is determined by the concrete form of (2.1). In many cases,[29] $V=V(G)$ can be solved for the given L.

Theorem 2.2: *The category (2.6) of NLEEs has the following representation:*

$$L_t=[W_m,L]+\bar{M}L^{m\eta},\quad m\in Z,\quad \bar{M}=\begin{cases}M, & m>0,\\ \tilde{M}, & m<0.\end{cases} \tag{2.11}$$

Proof: For $m\geqslant 0$, because $L_*(u_t)=L_t$ and L_* is injective,

$$L_t=[W_m,L]+ML^{m\eta}\Leftrightarrow L_*(u_t-X_m)=0\Leftrightarrow u_t=X_m,$$

which completes the proof. ■

Definition 2.4: Equation (2.11) and W_m *are called the generalized Lax representations (GLR) and the generalized Lax-operator (GLO), respectively.*

Obviously, with $\overline{M}=0$ (i.e., $G_0 \in \mathrm{Ker}\, J$, $G_{-1} \in \mathrm{Ker}\, K$), Eq. (2.11) reduces the standard (i.e., isospectral case: $\lambda_t=0$) Lax representations, and with $\overline{M}=I$ [of course $\mathcal{N}_J(I)\neq\varnothing$ and $\mathcal{N}_K(I)\neq\varnothing$ are needed], Eq. (2.11) reduces the nonisospectral (i.e., $\lambda_t=\lambda^{m\eta}$, $m\in Z$) Lax representations. For two special cases: the isospectral case (i.e. $M=\tilde{M}=0$) and the nonisospectral case (i.e., $M=\tilde{M}=I$), Ma[31] discussed the Lax operator algebras of the positive order (i.e., $m>0$) hierarchy of NLEEs. But a general framework has not been obtained for all integer $m\in Z$ and all linear matrix operators $M,\tilde{M}$. In the following sections, we shall construct a general frame–generalized algebraic structure and furthermore present the r-matrix for the category of NLEEs.

Remark 2.3: Equation (2.11) admits the structure of $L-A-B$ representations of the category (2.6) in an explicit form. Thus, we give a constructive approach to the Manakov operator pair A, B in the $L-A-B$ triple representation.[18] In Ref. 32, we determined the range of the $L-A-B$ triple representation through defining the Lie quotient algebras.

Remark 2.4: Equation (2.11) contains both the integrable and the nonintegrable hierachies because of the multiple choices of $\overline{M}$. Therefore, our category of NLEEs are not included in the system of multi-component KP and its reduction.

Corollary 2.1: Assume that the potential vector function u is independent of t and the following condition holds:

$$\left[\sum_{i=-r}^{s} c_i W_i, L\right] = -\overline{M}\sum_{i=-r}^{s} c_i L^{i\eta},$$

with constants c_i $(-r\leqslant i\leqslant s)$. Then u will satisfy the stationary system of the category (2.6):

$$\sum_{i=-r}^{s} c_i X_i(u)=0,\ \forall r,s\in Z^+.$$

We shall give several concrete examples in Sec. VI.

III. UNIVERSAL ALGEBRAIC STRUCTURE AND *r*-MATRIX

From (2.9), we have seen that for various linear matrix operators $M,\tilde{M}$, the category (2.6) of NLEEs indeed yields different hierarchies of NLEEs. That means the hierarchy in the category (2.6) changes according to the choice of $M,\tilde{M}$. In this section, we shall construct the algebraic structure and r-matrix which holds for all hierarchies of NLEEs in the category (2.6). Let us start from the following definition.

Definition 3.1: Suppose that for a spectral operator $L\in\mathcal{V}^N$ and an integer $n\in Z$ there exist pairs (A,M) of vector fields $X\in\mathcal{B}^m$ and operators $A,M\in\mathcal{V}^N$ with the property

$$[A,L]=L_*(X)-ML^n. \tag{3.1}$$

Then (A,M) is called a Manakov operator pair of L. The set of all Manakov operator pairs is denoted by $\mathcal{M}_L^n$. X is called the vector field corresponding to (A,M). The set of all vector fields X is denoted by $V(\mathcal{M}_L^n)$. The set of all triples (A,M,X) is denoted by $\mathcal{P}_L^n$.

As long as Eq. (2.8) has an operator solution for a given $L\in\mathcal{V}^N$, then by theorem 2.1 and Eq. (2.9) there exists a triple $(A,M,X)\in\mathcal{P}_L^n$ satisfying (3.1).

It is easy to prove the following proposition.

Proposition 3.1:

(1) The vector field associated with each Manakov operator pair is unique;
(2) both $\mathcal{P}_L^n$ and $\mathcal{M}_L^n$ form linear spaces.

Apparently, if there is $A,\quad M\in\mathcal{V}^N$ for $X\in\mathcal{B}^m$ such that Eq. (3.1) holds, then $u_t=X$ possesses the GLR $L_t=[A,\ L]+ML^n$. It is not difficult to see that $\mathcal{P}_L^n$ and $\mathcal{P}_L^0$, $\mathcal{M}_L^n$ and $\mathcal{M}_L^0$ are equiva-

lent, respectively, under the bijective map $\Phi: \mathcal{P}_L^n \to \mathcal{P}_L^0$, defined by $(A, M, X) \mapsto (A, ML^n, X)$. So, in the following we simply consider $\mathcal{P}_L^0$, $\mathcal{M}_L^0$ and write $\mathcal{M}_L^0 = \mathcal{M}_L$, $\mathcal{P}_L^0 = \mathcal{P}_L$.

Definition 3.2: Let $(A, M, X), (B, N, Y) \in \mathcal{P}_L$. *In* $\mathcal{M}_L$, *define a binary operation as follows:*

$$(A, M) \odot (B, N) = (A \odot B, M \odot N), \tag{3.2}$$

where

$$A \odot B = A_*(Y) - B_*(X) + [A, B], \tag{3.3}$$

$$M \odot N = M_*(Y) - N_*(X) + [M, B] - [N, A]. \tag{3.4}$$

Obviously (3.2) is a skew-symmetric and bilinear operation.

Theorem 3.1: *Let* $(A, M, X), (B, N, Y) \in \mathcal{P}_L$, *then* $(A \odot B, M \odot N, [X, Y]) \in \mathcal{P}_L$, *and* $\mathcal{M}_L$ *form a Lie algebra under the operation (3.2).*

Proof: Since $(\mathcal{V}^N, [\cdot, \cdot])$ builds up a Lie algebra under the usual commutator operation, we have

$$\begin{aligned} [[A, B], L] &= [[L, B], A] - [[L, A], B] \\ &= [L_*(X) - M, B] - [L_*(Y) - N, A] \\ &= [L_*(X), B] - [L_*(Y), A] + [N, A] - [M, B]. \end{aligned}$$

For arbitrary $L \in \mathcal{V}^N$, $X, Y \in \mathcal{B}^m$, we also have

$$(L_*(X))_*(Y) - (L_*(Y))_*(X) = L_*([X, Y]).$$

Thus,

$$\begin{aligned} [A \odot B, L] &= [A_*(Y) - B_*(X) + [A, B], L] \\ &= [A_*(Y), L] - [B_*(X), L] + [L_*(X), B] - [L_*(Y), A] + [N, A] - [M, B] \\ &= ([A, L])_*(Y) - ([B, L])_*(X) + [N, A] - [M, B] \\ &= (L_*(X))_*(Y) - (L_*(Y))_*(X) - M_*(Y) + N_*(X) + [N, A] - [M, B] \\ &= L_*([X, Y]) - M \odot N. \end{aligned}$$

That means $(A \odot B, M \odot N, [X, Y]) \in \mathcal{P}_L$.

Now, we shall prove the Jacobi identity. Choosing any $(A_i, M_i, X_i) \in \mathcal{P}_L$, $i = 1, 2, c3$, then we have

$$\begin{aligned} (A_1 \odot A_2) \odot A_3 + c.p. &= (A_{1*}(X_2) - A_{2*}(X_1) + [A_1, A_2]) \odot A_3 + c.p. \\ &= [[A_1, A_2], A_3] + c.p. \\ &= 0. \end{aligned}$$

Similarly, we can show the following equality:

$$(M_1 \odot M_2) \odot M_3 + c.p. = 0, \tag{$*$}$$

which completes the proof. ■

Corollary 3.1: The set of all vector fields $V(\mathcal{M}_L)$ *forms a Lie subalgebra of* $\mathcal{B}^m$ *with regard to the operation (1.2).*

Denote the vector fields of (A, M) and (B, N) by X and Y, respectively, then $u_t=X$, $u_t=Y$ represent the two *different* hierarchies of NLEEs, respectively, determined by M,N. Theorem 3.1 shows that there is universal algebraic structure for the *different* hierarchies of NLEEs, and if both $u_t=X$, and $u_t=Y$ $(X, Y\in\mathcal{B}^m)$ have GLR, then so does the new hierarchy of equations $u_t=[X, Y]$ produced by X, Y.

For the given spectral operator $L\in\mathcal{V}^N$, we now consider the following adjoint map:

$$\mathrm{ad}_L: A\mapsto M=\mathrm{ad}_L A=[L, A],\ \forall A\in\mathcal{V}^N. \tag{3.5}$$

Then according to the original definition of an r-matrix,[9] we have the following theorem.

Theorem 3.2: *The adjoint map* ad_L *is an r-matrix.*

Proof: For any $A, B\in\mathcal{V}^N$, write $M=\mathrm{ad}_L A$, $N=\mathrm{ad}_L B$. Then we have

$$[A, B]_{\mathrm{ad}_L}\triangleq[\mathrm{ad}_L A, B]+[A, \mathrm{ad}_L B]=[M, B]+[A, N]=M\odot N.$$

The last equality holds because the associated vector fields are obviously zero. And Eq. $(*)$ implies that $[A,B]_{\mathrm{ad}_L}$ satisfies the Jacobi identity. Thus the adjoint map ad_L is an r-matrix. ■

In the last section we shall illustrate that through giving several examples.

IV. NONUNIVERSAL ALGEBRAIC STRUCTURE AND *r*-MATRIX

For a given spectral operator $L\in\mathcal{V}^N$ and integer $n\in Z$, in the above section we discussed the Manakov operator pair (A,M), the universal Lie algebraic structure and the r-matrix available for *different* hierarchies of NLEEs. Now, for a given $N\times N$ matrix operator M and a spectral operator $L\in\mathcal{V}^N$, we study the operator algebra and r-matrix which can be attached only to the *underlying* hierarchy of NLEEs.

Let us first give some conventions in this section: (i) M is invertible; (ii) For a given $L\in\mathcal{V}^N$, $\mathcal{V}_L^N$ stands for all matrix operators $S:\mathcal{B}^N\to\mathcal{B}^N$ possessing the following form $S=\Sigma_{\alpha\in Z}P_\alpha(u)L^\alpha$, $P_\alpha(u)\in\mathcal{B}$, where $\Sigma_{\alpha\in Z}$ is a finite sum. Next, we introduce the following definition.

Definition 4.1: Let $L\in\mathcal{V}^N$ *and* M *be a spectral operator and an* $N\times N$ *matrix operator, respectively. If there exist a vector field* $X\in\mathcal{B}^m$ *and operators* $A,P\in\mathcal{V}_L^N$ *such that*

$$[A, L]+MP=L_*(X), \tag{4.1}$$

then (A, P) *is said to be an* LM *operator pair of* L. *The set of all such pairs is denoted by* $\mathcal{L}_L^M$. X *is called the vector field of* (A, P) *associated with* LM. *The set of all associated vector fields is denoted by* $V(\mathcal{L}_L^M)$. *Furthermore, we denote the set of all triples* (A, P, X) *by* $\mathcal{R}_L^M$.

For a given $L\in\mathcal{V}^N$ and an $N\times N$ matrix operator M or $\tilde{M}$ theorem 2.1 and Eq. (2.8) assure that there exists a triple $(A, P, X)\in\mathcal{R}_L^M$ satisfying (4.1). Definition 4.1 directly leads to the following proposition.

Proposition 4.1:

(1) The vector field associated with each LM *operator pair is unique.*
(2) Both $\mathcal{L}_L^M$ *and* $\mathcal{R}_L^M$ *are linear spaces.*

If for given operators L, M there exist $A, P\in\mathcal{V}_L^N$ such that (4.1) holds, then obviously the evolution equation $u_t=X$ has the following representation [also called generalized Lax representation (GLR)]:

$$L_t=[A, L]+MP. \tag{4.2}$$

Now, we define a binary operation in $\mathcal{L}_L^M$.

Definition 4.2: Let $(A, P),(B, Q)\in\mathcal{L}_L^M, X,Y\in V(\mathcal{L}_L^M)$, *respectively, be the vector fields of* $(A, P),(B, Q)$. *Declare a binary operation,*

$$(A,P)\ominus(B,Q)=(A\ominus B,P\ominus Q), \tag{4.3}$$

through

$$A\ominus B=A_*(Y)-B_*(X)+[A,B], \tag{4.4}$$

$$\begin{aligned}P\ominus Q=&P_*(Y)-Q_*(X)+[A,Q]-[B,P]\\&+M^{-1}(M_*(Y)-[B,M])P-M^{-1}(M_*(X)-[A,M])Q.\end{aligned} \tag{4.5}$$

Proposition 4.2:

(1) Equation (4.3) is a skew-symmetric, bilinear binary operation.
(2) $\mathcal{V}_L^N$ is closed under the operations (4.4) and (4.5).

Proof: The proof follows directly from Definition 4.2. ■

Theorem 4.1: *Let $(A,\ P,\ X),(B,\ Q,\ Y)\in\mathcal{R}_L^M$, then $(A\ominus B,\ P\ominus Q,\ [X,Y])\in\mathcal{R}_L^M$, where $[X,\ Y]$ is defined by (1.2). Thus under the operation (4.3) $\mathcal{L}_L^M$ forms an algebra, and $(V(\mathcal{L}_L^M),\ [\cdot,\cdot])$ composes a Lie subalgebra of $\mathcal{B}^m$.*

Proof: Because $(A,\ P,\ X),(B,\ Q,\ Y)\in\mathcal{R}_L^M$, and

$$[[A,\ B],\ L]=[[L,\ B],\ A]-[[L,\ A],\ B]=[L_*(X),\ B]-[L_*(Y),\ A]+[MQ,\ A]-[MP,\ B],$$

we have

$$\begin{aligned}[A\ominus B,\ L]=&[A_*(Y),\ L]-[B_*(X),\ L]+[[A,\ B],\ L]\\=&(L_*(X))_*(Y)-(L_*(Y))_*(X)-(MP)_*(Y)+(MQ)_*(X)+[MQ,A]-[MP,\ B]\\=&L_*([X,\ Y])-M(P\ominus N),\end{aligned}$$

which completes the proof. ■

For a given spectral operator L and an $N\times N$ matrix operator M, denote the vector fields of $(A,\ P),(B,\ Q)$ by $X,\ Y$, respectively. Then from Sec. II we know $u_t=X,\ u_t=Y$ are the two different NLEEs in the *same* hierarchy. Theorem 4.1 reveals that there exists an algebraic structure available for all equations in the *same* hierarchy. And if $u_t=X,\ u_t=Y$ $(X,\ Y\in\mathcal{B}^m)$ have the GLR (4.2); then the evolution equation $u_t=[X,\ Y]$ is still in the same hierarchy, and possesses the GLR (4.2), too.

Remark 4.1: In general, $\mathcal{L}_L^M$ is not forming a Lie algebra under the operation (4.3), because the Jacobi identity cannot be guaranteed. Nevertheless, the subset $S_L^M\subset\mathcal{L}_L^M$, considered below, is an exception.

Set $S_L^M=\{(A,\ P)\in\mathcal{V}_L^N\times\mathcal{V}_L^N|\ P=M^{-1}\,\mathrm{ad}_L A\}$; then S_L^M is corresponding to the stationary system $X(u)=0$ of evolution equation $u_t=X(u)$.

Theorem 4.2: *For all $(A,\ P)\in S_L^M$, define a map r^M:$A\mapsto P=M^{-1}\,\mathrm{ad}_L A$. The map r^M is an r-matrix under the operation (4.5) iff $M=aI,\ a\neq 0,a\in R$.*

Proof: For any $(A,\ P),(B,\ Q)\in S_L^M$, define

$$[A,\ B]_{r^M}\triangleq[r^M(A),\ B]+[A,\ r^M(B)].$$

Then

$$[A,\ B]_{r^M}=[P,\ B]+[A,\ Q]=P\ominus Q\Leftrightarrow M=aI,\ \ a\neq 0,\ \ a\in R,$$

i.e., the map r^M is an r-matrix $\Leftrightarrow M=aI,\ a\neq 0,\ a\in R$. ■

Since M and $\tilde{M}$ can be fixed arbitrarily we have found two algebraic operator structures, namely a universal one being independent of the hierarchy in the category and a nonuniversal one depending on the underlying hierarchy. In addition, in this procedure we have found two kinds of adjoint maps being r-matrices.

The two algebraic structures are associated with the category of NLEEs (2.11) which includes both the integrable and the nonintegrable cases (see Remark 2.4). Therefore, here our algebraic structures are not contained in any W-algebras which are usually suitable for the integrable hierarchy such as the KP, etc.

In the next section, we shall give two reductions of the algebraic structure and the related r-matrix.

V. TWO REDUCTIONS: VIRASORO ALGEBRA AND r-MATRIX OF ISOSPECTRAL AND NONISOSPECTRAL LAX OPERATOR

If we choose $M=0$ in Definition 4.1, then we have $[A,L]=L_*(X)$. That means A is an isospectral ($\lambda_t=0$) Lax operator. Set $[B,L]=L_*(Y)$; then the operation $A\ominus B$ defined by (4.4) forms an algebraic structure of the isospectral Lax operator, which just coincides with the result described in Ref. 31. In this case, the r-matrix is zero, i.e., $\mathrm{ad}_L A=0$, $\forall A\in\mathcal{V}^N$.

In this section, we always choose $M=\tilde{M}=I$ and assume that the conditions of Theorem 2.1 hold. Then, by Theorem 2.1, we obtain

$$(W_m,\ L^{m\eta},\ \sigma_m)\in\mathcal{R}_L^I,\ m\in Z,$$

where W_m is expressed through (2.10), σ_m stands for the corresponding vector field. Therefore W_m is a sequence of nonisospectral ($\lambda_t=\lambda^{m\eta},m\in Z$) Lax operators and this matches with choosing $A=W_m$, $P=L^{m\eta}$ $(m\in Z)$, $X=\sigma_m$ in (4.1). By Theorem 4.1 $\{(W_m,L^{m\eta}),m\in Z\}$ represents an algebra under the operation (4.3), which is called the nonisospectral Lax operator algebra of the spectral operator L. In the stationary case where $\sigma_i=\sigma_j=0$ the following holds.

Theorem 5.1: *A realization of the operations (4.5) and (4.4) on pairs* $(W_i,L^{i\eta})$, $(W_j,L^{j\eta})\in S_L^I$ *is given by*

$$L^{i\eta}\ominus L^{j\eta}=(|i|-|j|)L^{(i+j-1)\eta},\quad \forall i,j\in Z, \tag{5.1}$$

$$W_i\ominus W_j=(|i|-|j|)W_{i+j-1},\quad \forall i,j\in Z, \tag{5.2}$$

respectively.

Proof: For $(W_i,\ L^{i\eta}),(W_j,\ L^{j\eta})\in S_L^I$, we have

$$[W_i,\ L]=-L^{i\eta},\quad [W_j,\ L]=-L^{j\eta}.$$

Thus, in the case $i,j\geqslant 0$,

$$\begin{aligned}L^{i\eta}\ominus L^{j\eta}&=[L^{i\eta},\ W_j]-[L^{j\eta},\ W_i]\\&=\sum_{k=0}^{i-1}L^{(i-1-k)\eta}IL^{(k+j)\eta}-\sum_{k=0}^{j-1}L^{(j-1-k)\eta}IL^{(k+i)\eta}\\&=iL^{(i+j-1)\eta}-jL^{(i+j-1)\eta}=(i-j)L^{(i+j-1)\eta}.\end{aligned}$$

Similarly, Eq. (5.1) holds for the other three cases $i\geqslant 0$, $j\leqslant 0$; $i\leqslant 0$, $j\leqslant 0$; $i\leqslant 0$, $j\geqslant 0$.

Equation (5.2) can be directly obtained by (5.1) and Theorem 4.1. ■

Corollary 5.1: If $M=\tilde{M}=I$, under the operation (5.1) the map $r^I:W_i\mapsto L^{i\eta}$ is an r-matrix.

Proof: This can be directly derived from Theorem 5.1 and Theorem 4.3. ■

Remark 5.1: Theorem 5.1 and Corollary 5.1 actually describe the Lie algebraic structure of the Lax operator for the stationary equation $\sigma_j=0$ $(j\in Z)$ and the r-matrix of a concrete form of an operation (4.5) and (4.4), respectively.

For the usual nonstationary vector field $\sigma_j\neq 0$ $(j\in Z)$ in the nonisospectral case, (5.1) and (5.2) do not hold. But, we have the following results.

Theorem 5.2: *Let* $(W_j,\ L^{j\eta})\in\mathcal{L}_L^I,\ j\in Z$; *then for any* $i,j\in Z$, L *satisfies the relation*

$$L^{i\eta}\ominus L^{j\eta}=(|i|-|j|)\,\eta L^{(i+j+1)\eta-1},\quad \forall i,\ j\in Z. \tag{5.3}$$

Proof: We give the proof only for the case of $i\geqslant 0$, $j\geqslant 0$. The other cases are shown analogously.

Let $(W_i,\ L^{i\eta},\ \sigma_i)$, $(W_j,\ L^{j\eta},\ \sigma_j)\in\mathcal{R}_L^I$; then we have

$$\begin{aligned}(L^{i\eta})_*(\sigma_j)&=\sum_{k=0}^{i-1}L^{(i-1-k)\eta}L_*^{\eta}(\sigma_j)L^{k\eta}\\&=\sum_{k=0}^{i-1}L^{(i-1-k)\eta}([W_j,\ L^{\eta}]+\eta L^{(j+1)\eta+\eta-1})L^{k\eta}\\&=[W_j,\ L^{i\eta}]+i\,\eta L^{(i+j+1)\eta-1},\end{aligned}$$

and

$$(L^{j\eta})_*(\sigma_i)=[W_i,\ L^{j\eta}]+j\,\eta L^{(i+j+1)\eta-1}.$$

So, by Eq. (4.5) and noticing $M=I$, we obtain

$$L^{i\eta}\ominus L^{j\eta}=(i-j)\,\eta L^{(i+j+1)\eta-1},\quad \forall i,\ j\in Z^+, \tag{5.4}$$

which is the desired result. ■

Equations (5.1), (5.2), and (5.3) are three special Virasoro algebras, namely, without a central extension. Because here we do calculations based on our definitions of binary operations (4.4) and (4.5), they have no central extensions.

Remark 5.2: For the usual nonstationary vector field $\sigma_j\neq 0$ $(j\in Z)$ in the nonisospectral case the operation (5.1) does not always satisfy the Jacobi identity, (see Remark 4.1). Thus Corollary 5.1 does not hold in general.

Remark 5.3: A particular case of Theorem 5.2 is $\eta=1$. Then Eq. (5.3) becomes

$$L^{i}\ominus L^{j}=(|i|-|j|)L^{i+j},\quad \forall i,\ j\in Z, \tag{5.5}$$

which implies the following equations:

$$W_i\ominus W_j=(|i|-|j|)\,W_{i+j},\quad \forall i,\ j\in Z, \tag{5.6}$$

and

$$[\sigma_i,\sigma_j]=(|i|-|j|)\sigma_{i+j},\quad \forall i,\ j\in Z. \tag{5.7}$$

Theorem 5.2 reveals that under Eq. (5.5) for the same nonisospectral hierarchy the following holds: if $u_t=\sigma_m$ and $u_t=\sigma_n$, respectively, possess the nonisospectral Lax operators W_m and W_n, then $u_t=\sigma_{m+n}$ still possesses the nonisospectral Lax operator $1/(|m|-|n|)\,W_m\ominus W_n$, $\forall m,n\in Z$. Thus, the Virasoro operator algebras (without the central extension) for the nonisospectral hierarchy of NLEEs is reflected by Eqs. (5.5)–(5.7).

Remark 5.4: If we choose $M=0$ and $M=I$, respectively, then under the algebraic operation (3.3) we can also have the Virasoro algebra of the Lax operator for the isospectral hierarchy and the nonisospectral hierarchy, which is actually a special case of universal algebraic structure.

VI. SOME EXAMPLES

Through taking several examples, we illustrate our methods. For our convenience, we make the following conventions:

$$f^{(m)}=\begin{cases}\dfrac{\partial^m}{\partial x^m}f=f_{mx}, & m\geqslant 0,\\ \underbrace{\int\cdots\int}_{-m} f\,dx, & m<0,\end{cases}\qquad \sum=\begin{cases}\displaystyle\sum_{j=0}^{m-1}, & m>0,\\ 0, & m=0,\\ \displaystyle-\sum_{j=m}^{-1}, & m<0,\end{cases}$$

$f_t=\partial f/\partial t$, $f_{mxt}=\partial^{m+1}f/\partial t\,\partial x^m\,(m\geqslant 0)$, $\partial=\partial/\partial x$, ∂^{-1} is the inverse of ∂, i.e., $\partial\partial^{-1}=\partial^{-1}\partial=1$, $\partial^m f$ means the operator $\partial^m f$ acts on some function g, i.e., $\partial^m f\cdot g=\partial^m(fg)$, $m\in Z$. C_m^k stands for the combinatorial constants: $C_m^k=m(m-1)\cdots(m-k+1)/k!$, i an imaginary unit satisfying $i^2=-1$, and $I_{2\times 2}$ the 2×2 unit matrix.

In the spectral problems (6.1), (6.32) and (6.74) the function u stands for the potential function, and the potential functions in spectral problems (6.43) and (6.56) are denoted by q, r. In those spectral problems, λ is always assumed to be a spectral parameter. The domain of the spatial variable x is Ω which becomes equal to $(-\infty, +\infty)$ or $(0, T)$, while the domain of the time variable t is the positive time axis $R^+=\{t|t\in R,\ t\geqslant 0\}$. In the case $\Omega=(-\infty, +\infty)$ the decaying condition at infinity and in the case $\Omega=(0, T)$ the periodicity condition for the potential function, is imposed.

6.1: Consider the Burger's spectral problem:[33]

$$L\cdot y=\lambda y,\quad L=L(u)=\partial+u. \tag{6.1}$$

Choosing the recursion operator $\mathcal{L}=\partial+\partial u\partial^{-1}$ leads to

$$\mathcal{L}\cdot y_x=\lambda y_x. \tag{6.2}$$

Obviously, $L_*(\xi)=\xi, \forall\,\xi\in\mathcal{B}$, i.e., L_* is an identity operator. In this case, the Lenard's operators pair is chosen as $J=1$, and $K=\mathcal{L}$.

The Lenard recursive sequence $\{G_j\}_{j=-\infty}^{\infty}$ $(G_j=\mathcal{L}^j\cdot M,\ j\in Z)$ gives the Burgers category of NLEEs:

$$u_t=\mathcal{L}^m\cdot M=(e^{-u^{(-1)}}(e^{u^{(-1)}}M^{(-1)})^{(m)})_x,\quad m\in Z, \tag{6.3}$$

where $M\in\mathcal{B}$ is an arbitrarily given function, and $\mathcal{L}=\partial e^{-u^{(-1)}}\partial e^{u^{(-1)}}\partial^{-1}$, $\mathcal{L}^{-1}=\partial e^{-u^{(-1)}}\partial^{-1}e^{u^{(-1)}}\partial^{-1}$ which implies $\mathcal{L}^j=\partial e^{-u^{(-1)}}\partial^j e^{u^{(-1)}}\partial^{-1}$, $j\in Z$.

For an arbitrary $G\in\mathcal{B}$, the operator equation $[V, L]=L_*(\mathcal{L}\cdot G)-L_*(G)L$, which matches with choosing $\beta=0$, $\alpha=1$ in (2.8), has the following solution:

$$V=V(G)=-G+G^{(-1)}\partial. \tag{6.4}$$

Thus the category (6.3) possesses the generalized Lax representation (GLR),

$$L_t=[W_m, L]+ML^m,\quad m\in Z, \tag{6.5}$$

with $W_m=M^{(-1)}L^m-L^m\cdot M^{(-1)}$, $L^m=e^{-u^{(-1)}}\partial^m e^{u^{(-1)}}$, $m\in Z$.

The transformation $u=(\ln v)_x$ yields a simple form of Eq. (6.3):

$$v_t=(vM^{(-1)})^{(m)},\quad m\in Z, \tag{6.6}$$

which has the GLR $L_t=[W_m, L]+ML^m$ with $L=\partial+(\ln v)_x$, $W_m=v^{-1}(M^{(-1)}\partial^m v - (vM^{(-1)})^{(m)})$.

Apparently, if M is chosen to be independent of v ($v=e^{u^{(-1)}}$), then the category (6.3) is linearized. Thus, (6.3) includes many linearized hierarchies. Now, let us discuss reductions of the category (6.3) or (6.6).

A. Positive case ($m=0, 1, 2,\ldots$)

In this case, the Lax operator W_m can be written as

$$W_m=v^{-1}\sum_{k=1}^{m} C_m^k v^{(m-k)}(M^{(-1)}\partial^k-M^{(k-1)}). \tag{6.7}$$

(i) With $M=0$, $0^{(-1)}=1$, the positive order category of (6.3) reads as the well-known Burgers' hierarchy,

$$u_t=((\partial+u)^m\cdot 1)_x. \tag{6.8}$$

Particularly, with $m=2$ it becomes the Burger's equation $u_t=u_{xx}+2uu_x$ whose Lax operator is $W_2=\partial^2+2u\partial$ in the standard Lax representation $L_t=[W_2,L]$. This corresponds to the isospectral case: $\lambda_t=0$. According to Eq. (6.6), a simple but quite interesting fact is that under the transformation $u=v_x/v$ the whole Burgers' hierarchy (6.8) is linearized as

$$v_t=v_{mx},\ m=0,1,2,\ldots. \tag{6.9}$$

Equation (6.9) can be solved very easily and have the standard Lax pair $W_m=v^{-1}\Sigma_{k=1}^m C_m{}^k v^{(m-k)}\partial^k$ and $L=\partial+v_x/v$. In this way, the solutions of all equations in the Burgers' hierarchy (6.8) can be worked out.

(ii) With $M=a$, $a^{(-1)}=ax+f(t)$, $a\in R$, $f(t)\in C^\infty(R)$, the positive order category of (6.3) becomes the nonisospectral ($\lambda_t=a\lambda^m$) Burgers' hierarchy,

$$u_t=((\partial+u)^m\cdot(ax+f(t)))_x. \tag{6.10}$$

A representative equation ($m=2$) of Eq. (6.10) is

$$u_t=(ax+f(t))(u_{xx}+2uu_x)+3au_x+au^2, \tag{6.11}$$

possessing the GLR $L_t=[W_2,L]+aL^2$ with $W_2=(ax+f(t))(\partial^2+2u\partial)-2au$ and $L=\partial+u$. By virtue of $M=a$ and $u=(\ln v)_x$, Eq. (6.10) is linearized as

$$v_t=(ax+f(t))v_{mx}+mav_{(m-1)x}, \tag{6.12}$$

which can be solved. Equation (6.12) has the generalized Lax operator (GLO) $W_m=(ax+f(t))v^{-1}\Sigma_{k=1}^m C_m^k v^{(m-k)}\partial^k-mav^{-1}v^{(m-1)}$. Particularly, Eq. (6.11) has a linearization equation ($m=2$),

$$v_t=(ax+f(t))v_{xx}+2av, \tag{6.13}$$

possessing the GLO $W_2=(ax+f(t))(\partial^2+2v^{-1}v_x\partial)-2av^{-1}v_x$. In a general case, M can be extended as $M=\Sigma_{j=0}^n c_j(t)x^j$, $c_j(t)\in C^\infty(R)$, which will be considered below.

(iii) With $M=\Sigma_{j=0}^n c_j(t)x^j$, $c_j(t)\in C^\infty(R)$, the positive order category of (6.3) reads as a nonisospectral ($\lambda_t=(\Sigma_{j=0}^n c_j(t)x^j)\lambda^m$) hierarchy,

$$u_t=\left((\partial+u)^m\cdot\left(f(t)+\sum_{j=0}^{n} c_j(t)\frac{x^{j+1}}{j+1}\right)\right)_x, \tag{6.14}$$

where an arbitrary $f(t)\in C^\infty(R)$ is attached by virtue of integration with respect to x. Of course, Eq. (6.14) is easily linearized as

$$v_t=\frac{\partial^m}{\partial x^m}\left(vf(t)+v\sum_{j=0}^{n}\frac{c_j(t)}{j+1}x^{j+1}\right), \tag{6.15}$$

via $u=(\ln v)_x$. Equation (6.15) has the generalized Lax operator,

$$W_m=v^{-1}\sum_{k=1}^{m} C_m^k v^{(m-k)}(M^{(-1)}\partial^k-M^{(k-1)}),$$

with

$$M^{(-1)}=f(t)+\sum_{j=0}^{n}\frac{c_j(t)}{j+1}x^{j+1}.$$

(iv) With $M=(u^{-1})_x$, $M^{(-1)}=u^{-1}$, the positive order category of (6.3) reads as the following hierarchy of NLEEs:

$$u_t=((\partial+u)^m\cdot u^{-1})_x,\quad m=0,1,2\ldots. \tag{6.16}$$

A representative equation of (6.16) is

$$u_t=\left(\frac{1}{u}\right)_{xx}, \tag{6.17}$$

with the GLO $W_0=-(u^{-1})_x+u^{-1}\partial$.

B. Negative case ($m=-1,-2,\ldots$)

(i) With $M=0$, the generator $G_{-1}=\partial e^{-u^{(-1)}}\partial^{-1}e^{u^{(-1)}}\partial^{-1}\cdot 0$ is determined by the following two seed functions:

$$\overline{G}_{-1}=f(t)(e^{-u^{(-1)}})_x \tag{6.18}$$

and

$$\tilde{G}_{-1}=g(t)(e^{-u^{(-1)}}(e^{u^{(-1)}})^{(-1)})_x, \tag{6.19}$$

where $f(t)$, $g(t)\in C^\infty(R)$ are two arbitrarily given functions. Apparently, the seed function (6.18) produces the following isospectral ($\lambda_t=0$) negative order hierarchy of (6.3),

$$u_t=f(t)(e^{-u^{(-1)}}1^{(m)})_x,\quad m<0,\ m\in Z, \tag{6.20}$$

i.e.,

$$u_t=f(t)e^{-u^{(-1)}}\sum_{k=0}^{-m-1} c_k\frac{x^{-m-k-2}(-m-k-1-xu)}{(-m-k-1)!},\quad c_0=1, \tag{6.21}$$

where $c_k=c_k(t)\in C^\infty(R)$ $(-m-1\geqslant k\geqslant 1)$ is arbitrarily given. Thus although Eq. (6.20) is nonlinear, we have its general solution:

$$u(x,t)=\frac{\Sigma_{k=0}^{-m-2}c_k(t)\dfrac{x^{-m-k-2}}{(-m-k-2)!}\partial_t^{-1}f(t)+h'(x)}{\Sigma_{k=0}^{-m-1}c_k(t)\dfrac{x^{-m-k-1}}{(-m-k-1)!}\partial_t^{-1}f(t)+h(x)},\quad \forall h(x),\ c_k(t)\in C^\infty(R), \tag{6.22}$$

where $\partial_t^{-1}f(t)=\int f(t)dt$, $c_0(t)=1$, $h'(x)=(d/dx)\,h(x)$. Of course, Eq. (6.21) has the standard Lax representation $L_t=[W_m,L]$ with $W_m=-f(t)e^{-u^{(-1)}}\Sigma_{k=0}^{-m-1}c_k(t)\ x^{-m-k-1}/(-m-k-1)!$.

On the other hand, the seed function (6.19) generates the following isospectral ($\lambda_t=0$) negative order hierarchy of (6.3):

$$u_t=g(t)(e^{-u^{(-1)}}(e^{u^{(-1)}})^{(m)})_x,\quad m<0,\ m\in Z, \tag{6.23}$$

which is a hierarchy of integro-differential equations and can be changed to the linear differential equations,

$$v_{-mxt}=g(t)v,\ \ m<0,\ \ m\in Z, \tag{6.24}$$

via the transformation $u=v^{-1}v_x$. The Lax operator W_m of (6.23) or (6.24) is $W_m=-g(t)e^{-u^{(-1)}}(e^{u^{(-1)}})^{(m)}$ or $W_m=-g(t)v^{-1}v^{(m)}$, $m<0$.

(ii) With $M=a$, $a^{(-1)}=ax+f(t)$, $a\in R$, $f(t)\in C^\infty(R)$, the negative order category of (6.3) through setting $u=v^{-1}v_x$ reads as the linear equations,

$$v_{-mxt}=(ax+f(t))v,\ \ m<0,\ \ m\in Z, \tag{6.25}$$

which corresponds to the nonisospectral case: $\lambda_t=a\lambda^m$, and has the GLO $W_m=v^{-1}(ax+f(t))\partial^m v-v^{-1}(v(ax+f(t)))^{(m)}$, $m<0$. For a general case, we have the following.

(iii) Setting $M=\Sigma_{j=0}^n c_j(t)x^j$ $(c_j(t)\in C^\infty(R))$ yields a negative order hierarchy of (6.3),

$$u_t=\left(e^{-u^{(-1)}}\partial^m e^{u^{(-1)}}\cdot\sum_{j=0}^n c_j(t)\frac{x^{j+1}}{j+1}\right)_x,\ \ m<0,\ \ m\in Z, \tag{6.26}$$

which corresponds to the nonisospectral case $\lambda_t=(\Sigma_{j=0}^n c_j(t)x^j)\lambda^m$, and can be linearized as

$$v_{-mxt}=v\sum_{j=0}^n c_j(t)\frac{x^{j+1}}{j+1},\ m<0,\ m\in Z, \tag{6.27}$$

via $u=v^{-1}v_x$. Equation (6.27) has the Lax operator

$$W_m=v^{-1}\sum_{j=0}^n\frac{c_j(t)}{j+1}(x^{j+1}\partial^m v-(vx^{j+1})^{(m)}),\quad m<0.$$

(iv) With $M=(v/v_x)_x$, $\partial^{-1}M=v/v_x$, the associated negative order hierarchy of (6.3) is

$$v_{-mxt}=\frac{v^2}{v_x},\ \ m<0,\ \ m\in Z, \tag{6.28}$$

which has a representative equation $(m=-1)$

$$v_xv_{xt}=v^2, \tag{6.29}$$

with the Lax operator $W_{-1}=(1/v_x)\partial^{-1}v-(1/v)(v^2/v_x)^{(-1)}$.

Through choosing different M, we still have other hierarchies of (6.3). Because of the arbitrariness of M, all results in Secs. III–V are valid for the Burgers' (B) spectral problem (6.1). Particularly, the r-matrix ad_L becomes

$$\mathrm{ad}_L^{\mathcal{B}}: W_m\mapsto ML^m,\ \ m\in Z, \tag{6.30}$$

where $W_m=M^{(-1)}L^m-L^m\cdot M^{(-1)}$, $L^m=e^{-u^{(-1)}}\partial^m e^{u^{(-1)}}$, $M\in\mathcal{B}$ is an arbitrarily given function. And the r-matrix r^M $(M=a\neq 0,\ a\in R)$ reads as

$$r_B^a: W_m\mapsto L^m,\ \ m\in Z, \tag{6.31}$$

where $W_m=(ax+f(t))L^m-L^m\cdot(ax+f(t))$. Equations (6.30) and (6.31) generate the stationary B-categorical systems $(L^m\cdot M^{(-1)})_x=0$ and $(L^m\cdot(ax+f(t)))_x=0$, respectively.

We can also apply the above procedure to other spectral problems. Now, we list some main results as follows.

6.2: KdV case. The KdV–Schrödinger spectral problem,[34]

$$L\cdot y=\lambda y,\ L=L(u)=\partial^2+u, \tag{6.32}$$

has the following Lenard operator pair:

$$K=\tfrac{1}{4}\partial^3+\tfrac{1}{2}(\partial u+u\partial),\quad J=\partial. \tag{6.33}$$

Apparently, $L_*(\xi)=\xi,\forall\,\xi\in\mathcal{B}$. Setting $u=-\phi_{xx}/\phi$ yields the product-form of K and its inverse,

$$\begin{aligned} K&=\tfrac{1}{4}\phi^{-2}\,\partial\phi^2\,\partial\phi^2\,\partial\phi^{-2},\\ K^{-1}&=4\phi^2\,\partial^{-1}\phi^{-2}\,\partial^{-1}\phi^{-2}\,\partial^{-1}\phi^2. \end{aligned} \tag{6.34}$$

Let $M,\ \tilde{M}\in\mathcal{B}$ be two arbitrarily given functions. Then the positive order and negative order generators,

$$G_0=M^{(-1)};\ \ G_{-1}=K^{-1}\cdot\tilde{M}=4\phi^2\,\partial^{-1}\phi^{-2}\,\partial^{-1}\phi^{-2}\,\partial^{-1}\cdot(\phi^2\tilde{M}), \tag{6.35}$$

leads to the KdV category of NLEEs

$$u_t=J\cdot G_m,\ \ m\in Z,\ \ G_m=\begin{cases}\mathcal{L}^m\cdot G_0, & m\geqslant 0,\\ \mathcal{L}^{m+1}\cdot G_{-1}, & m<0,\end{cases} \tag{6.36}$$

where the recursion operator $\mathcal{L}$ is given by

$$\mathcal{L}=J^{-1}K=\tfrac{1}{4}\partial^2+\tfrac{1}{2}(u+\partial^{-1}u\partial)=\tfrac{1}{4}\partial^{-1}\phi^{-2}\,\partial\phi^2\,\partial\phi^2\,\partial\phi^{-2},$$

and its inverse is

$$\mathcal{L}^{-1}=4\phi^2\,\partial^{-1}\phi^{-2}\,\partial^{-1}\phi^{-2}\,\partial^{-1}\phi^2\,\partial.$$

For an arbitrary $G\in\mathcal{B}$, the operator equation $[V,L]=L_*(K\cdot G)-L_*(J\cdot G)L$ has the following operator solution:

$$V=V(G)=-\tfrac{1}{4}G_x+\tfrac{1}{2}G\partial, \tag{6.37}$$

which implies that the KdV category (6.36) possesses the GLR,

$$L_t=[W_m,\,L]+\overline{M}L^m,\ \ m\in Z,\ \overline{M}=\begin{cases}M, & m\geqslant 0,\\ \tilde{M}, & m<0,\end{cases} \tag{6.38}$$

with the GLO

$$W_m=\sum V(G_j)L^{m-j-1}. \tag{6.39}$$

Here $V(G_j)$ is determined by (6.37) with $G=G_j=\mathcal{L}^j\cdot G_0,\ \ j\geqslant 0$ or $G=G_j=\mathcal{L}^{j+1}\cdot G_{-1},\ j<0$, $L=\partial^2+u=\phi^{-1}\,\partial\phi^{-2}\,\partial\phi^{-2}$, and $L^{-1}=\phi^2\,\partial^{-1}\phi^2\,\partial^{-1}\phi$.

In particular, we are concerned with the following reduction.

(i) With $M=4(u^{-1/2})_x$, $G_0=M^{(-1)}=4u^{-1/2}$, the positive order category of (6.36) reads as the well-known Harry–Dym hierarchy,

$$u_t=J\mathcal{L}^m\cdot 4u^{-1/2},\ \ m=0,1,2,\ldots. \tag{6.40}$$

With $m=1$, Eq. (6.40) yields the Harry–Dym equation,

$$u_t=\left(\frac{1}{\sqrt{u}}\right)_{xxx}, \tag{6.41}$$

which has now the GLR $L_t=[W_0,L]+4(u^{-1/2})_xL$ with $W_0=-(u^{-1/2})_x+2u^{-1/2}\partial$, and apparently belongs to the KdV category (6.36); with $m=2$, Eq. (6.40) yields a higher order Harry–Dym equation,

$$u_t=\tfrac{1}{4}\left(\frac{1}{\sqrt{u}}\right)_{4x}+u\left(\frac{1}{\sqrt{u}}\right)_{3x}+\tfrac{1}{2}u_x\left(\frac{1}{\sqrt{u}}\right)_{xx} \tag{6.42}$$

possessing the GLO $W_1=2u^{-1/2}\partial^3-(u^{-1/2})_x\partial^2+\frac{1}{2}((u^{-1/2})_{xx}+4u^{-1/2})\partial-\frac{1}{4}(u^{-1/2})_{xxx}+u^{-1/2}u_x$.

So, we have obtained an interesting fact: *the Harry–Dym equation (6.41) can be included in the KdV category (6.36) with the generalized Lax operator*. Similar to the process of the Burgers' case, we can also have many reduced hierarchies both positive and negative from Eq. (6.36).

6.3: AKNS case. The ZS-AKNS spectral problem,[35,36]

$$L\cdot y=\lambda y,\quad L=L(q,r)=i\begin{pmatrix}\partial & -q\\ r & -\partial\end{pmatrix},\quad y=\begin{pmatrix}y_1\\ y_2\end{pmatrix}, \tag{6.43}$$

has its Lenard's operators pair,

$$K=\begin{pmatrix}q\,\partial^{-1}q & \frac{1}{2}\partial-q\,\partial^{-1}r\\ \frac{1}{2}\partial-r\,\partial^{-1}q & r\,\partial^{-1}r\end{pmatrix},\quad J=i\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{6.44}$$

Apparently,

$$L_*(\xi)=\begin{pmatrix}0 & -i\xi_1\\ i\xi_2 & 0\end{pmatrix},\quad \xi=(\xi_1,\xi_2)^T\in\mathcal{B}^2, \tag{6.45}$$

is an injective homomorphism.

Equation (6.44) gives the recursion operator

$$\mathcal{L}=J^{-1}K=\frac{1}{2}i\begin{pmatrix}-\partial+2r\,\partial^{-1}q & -2r\,\partial^{-1}r\\ 2q\,\partial^{-1}q & \partial-2q\,\partial^{-1}r\end{pmatrix}. \tag{6.46}$$

Choosing two functions θ, $\sigma\in C^\infty(R)$ satisfying $\theta_x=\frac{1}{2}\theta^2+r^{-1}r_x\theta-2qr$, $\sigma_x=\frac{1}{2}\sigma^2+q^{-1}q_x\sigma-2qr$, leads to the inverse of $\mathcal{L}$,

$$\mathcal{L}^{-1}=K^{-1}J=-2i\begin{pmatrix}-\mathcal{E}(\partial r^{-1}\,\partial r^{-1}-2qr^{-1}) & -2\mathcal{E}\\ 2\mathcal{F} & \mathcal{F}(\partial q^{-1}\,\partial q^{-1}-2rq^{-1})\end{pmatrix}, \tag{6.47}$$

where $\mathcal{E}$, $\mathcal{F}$ denote the following two operators:

$$\mathcal{E}=e^{-\theta^{(-1)}}\partial^{-1}e^{\theta^{(-1)}}\,r\,\partial^{-1}r\,e^{\theta^{(-1)}}\partial^{-1}e^{-\theta^{(-1)}},\quad \mathcal{F}=e^{-\sigma^{(-1)}}\partial^{-1}e^{\sigma^{(-1)}}\,q\,\partial^{-1}q\,e^{\sigma^{(-1)}}\partial^{-1}e^{-\sigma^{(-1)}}. \tag{6.48}$$

Let $A,B,C,D\in\mathcal{B}$ be four arbitrarily given functions; then iff

$$M=\begin{pmatrix}0 & -B\\ -A & 0\end{pmatrix},\quad \tilde{M}=\begin{pmatrix}0 & -D\\ -C & 0\end{pmatrix}, \tag{6.49}$$

the operator equations $L_*(J\cdot G_0)=M$, $L_*(K\cdot G_{-1})=\tilde{M}$ give the positive order and negative order generators (function vectors),

$$G_0=\begin{pmatrix}A\\B\end{pmatrix},\quad G_{-1}=-2i\begin{pmatrix}-\mathcal{E}\cdot(\partial r^{-1}\cdot(r^{-1}C)_x-2qr^{-1}C+2D)\\ \mathcal{F}\cdot(\partial q^{-1}\cdot(q^{-1}D)_x-2rq^{-1}D+2C)\end{pmatrix}, \tag{6.50}$$

which directly leads to the AKNS category of NLEEs:

$$\begin{pmatrix}q\\r\end{pmatrix}_t=\begin{cases}J\mathcal{L}^m\cdot(A,B)^T, & m=0,1,2,...,\\ J\mathcal{L}^m\cdot(C,D)^T, & m=-1,-2,\ldots,\end{cases} \tag{6.51}$$

where J, $\mathcal{L}$ and $\mathcal{L}^{-1}$ are defined by (6.44), (6.46) and (6.47), respectively.

For an arbitrarily given $G=(G^{[1]},G^{[2]})^T\in\mathcal{B}^2$, the operator equation $[V,L]=L_*(K\cdot G)-L_*(J\cdot G)L$ has the solution

$$V=V(G)=\frac{1}{2}\begin{pmatrix}-(rG^{[2]}-qG^{[1]})^{(-1)} & G^{[2]}\\ G^{[1]} & (rG^{[2]}-qG^{[1]})^{(-1)}\end{pmatrix}, \tag{6.52}$$

which is obviously a function matrix. Thus, the AKNS category (6.51') has the GLR:

$$L_t=[W_m,L]+\bar{M}L^m,\quad m\in Z, \tag{6.53}$$

$$\bar{M}=\begin{cases}\begin{pmatrix}0 & B\\ A & 0\end{pmatrix}, & m\geqslant 0,\\ \begin{pmatrix}0 & D\\ C & 0\end{pmatrix}, & m<0,\end{cases}$$

with the GLO

$$W_m=\sum V(G_j)L^{m-j-1},\quad m\in Z. \tag{6.54}$$

Here $V(G_j)$ is given by (6.52) with $G=G_j=\mathcal{L}^j\cdot(A,B)^T$, $j\geqslant 0$ or $\mathcal{L}^j\cdot(C,D)^T$, $j<0$, L is defined by (6.43), and its inverse L^{-1} is determined by

$$L^{-1}=i\begin{pmatrix}\mathcal{S}\partial q^{-1} & -\mathcal{S}\\ -\mathcal{T} & \mathcal{T}\partial r^{-1}\end{pmatrix}, \tag{6.55}$$

with the operators $\mathcal{S}=e^{-\rho^{(-1)}}\partial^{-1}e^{2\rho^{(-1)}}q\,\partial^{-1}e^{-\rho^{(-1)}}$, $\mathcal{T}=e^{-\mu^{(-1)}}\partial^{-1}e^{2\mu^{(-1)}}r\,\partial^{-1}e^{-\mu^{(-1)}}$, where ρ and μ are two functions satisfying $\rho_x=\rho^2+q^{-1}q_x\rho-qr$, $\mu_x=\mu^2+r^{-1}r_x\mu-qr$.

Here, we omit the reductions and the r-matrix representation of the AKNS category (6.51).

6.4: WKI (Wadati–Konno–Ichikowa) case. The WKI spectral problem,[37]

$$L\cdot y=\lambda y,\ L=L(q,r)=\frac{1}{1-qr}\begin{pmatrix}i & -q\\ -r & -i\end{pmatrix}\partial,\ y=\begin{pmatrix}y_1\\y_2\end{pmatrix}, \tag{6.56}$$

has the following Lenard's operators pair:

$$K=\frac{1}{2i}\begin{pmatrix}-\frac{1}{2}\partial^2\frac{q}{p}\partial^{-1}\frac{q}{p}\partial^2 & \partial^3+\frac{1}{2}\partial^2\frac{q}{p}\partial^{-1}\frac{r}{p}\partial^2\\ \partial^3+\frac{1}{2}\partial^2\frac{r}{p}\partial^{-1}\frac{q}{p}\partial^2 & -\frac{1}{2}\partial^2\frac{r}{p}\partial^{-1}\frac{r}{p}\partial^2\end{pmatrix}, \tag{6.57}$$

$$J=\begin{pmatrix} 0 & -\partial^2 \\ \partial^2 & 0 \end{pmatrix}, \quad p=\sqrt{1-qr}, \tag{6.58}$$

which yields the recursion operator $\mathcal{L}=J^{-1}K$

$$\mathcal{L}=\frac{1}{2i}\begin{pmatrix} \partial+\frac{r}{2p}\partial^{-1}\frac{q}{p}\partial^2 & -\frac{r}{2p}\partial^{-1}\frac{r}{p}\partial^2 \\ \frac{q}{2p}\partial^{-1}\frac{q}{p}\partial^2 & -\partial-\frac{q}{2p}\partial^{-1}\frac{r}{p}\partial^2 \end{pmatrix}. \tag{6.59}$$

Apparently, the Gateaux derivative operator $L_*(\xi)$ of the spectral operator L in the direction $\xi=(\xi_1,\xi_2)^T\in\mathcal{B}^2$ is

$$L_*(\xi)=\frac{1}{1-qr}\begin{pmatrix} q\xi_2 & -i\xi_1 \\ i\xi_2 & r\xi_1 \end{pmatrix}L, \tag{6.60}$$

which is an injective homomorphism.

Through lengthy calculations, one can obtain the invertible operators of L, J, K and $\mathcal{L}$:

$$L^{-1}=\begin{pmatrix} -i\partial^{-1} & \partial^{-1}q \\ \partial^{-1}r & i\partial^{-1} \end{pmatrix}, \tag{6.61}$$

$$J^{-1}=\begin{pmatrix} 0 & \partial^{-2} \\ -\partial^{-2} & 0 \end{pmatrix}, \tag{6.62}$$

$$K^{-1}=2i\begin{pmatrix} \frac{1}{2}\partial^{-1}r\,\partial^{-1}r\,\partial^{-1} & \partial^{-3}-\frac{1}{2}\partial^{-1}r\,\partial^{-1}q\,\partial^{-1} \\ \partial^{-3}-\frac{1}{2}\partial^{-1}q\,\partial^{-1}r\,\partial^{-1} & \frac{1}{2}\partial^{-1}q\,\partial^{-1}q\,\partial^{-1} \end{pmatrix}, \tag{6.63}$$

$$\mathcal{L}^{-1}=2i\begin{pmatrix} \partial^{-1}-\frac{1}{2}\partial^{-1}r\,\partial^{-1}q\,\partial & -\frac{1}{2}\partial^{-1}r\,\partial^{-1}r\,\partial \\ \frac{1}{2}\partial^{-1}q\,\partial^{-1}q\,\partial & -\partial^{-1}+\frac{1}{2}\partial^{-1}q\,\partial^{-1}r\,\partial \end{pmatrix}. \tag{6.64}$$

Let A, B, C, D be four arbitrarily given C^∞-functions; then iff

$$M=\frac{1}{1-qr}\begin{pmatrix} qA & iB \\ iA & -rB \end{pmatrix}L, \quad \tilde{M}=\frac{1}{1-qr}\begin{pmatrix} qC & iD \\ iC & -rD \end{pmatrix}L, \tag{6.65}$$

the operator equations $L_*(J\cdot G_0)=M$, $L_*(K\cdot G_{-1})=\tilde{M}$ have the following solutions:

$$G_0=\begin{pmatrix} A^{(-2)} \\ B^{(-2)} \end{pmatrix}, \tag{6.66}$$

$$G_{-1}=\begin{pmatrix} 2iC^{(-3)}-i\,\partial^{-1}r\,\partial^{-1}\cdot(rD^{(-1)}+qC^{(-1)}) \\ -2iD^{(-3)}+i\,\partial^{-1}q\,\partial^{-1}\cdot(rD^{(-1)}+qC^{(-1)}) \end{pmatrix}, \tag{6.67}$$

which directly yields the WKI category of NLEEs:

$$\begin{pmatrix} q \\ r \end{pmatrix}_t = J \cdot G_m, \quad m \in Z, \tag{6.68}$$

$$G_m = \begin{cases} \mathcal{L}^m \cdot (A^{(-2)}, B^{(-2)})^T, & m = 0,1,2,..., \\ \mathcal{L}^m \cdot (C^{(-2)}, D^{(-2)})^T, & m = -1,-2,\ldots, \end{cases} \tag{6.69}$$

where J, $\mathcal{L}$ and $\mathcal{L}^{-1}$ are defined by (6.58), (6.59) and (6.64), respectively.

For any given $G = (G^{[1]}, G^{[2]})^T \in \mathcal{B}^2$, the equation $[V, L] = L_*(K \cdot G)L^{-1} - L_*(J \cdot G)$ has the following operator solution:

$$V = V(G) = \begin{pmatrix} 0 & \overline{B} \\ \overline{C} & 0 \end{pmatrix} + \overline{A} \begin{pmatrix} -i & q \\ r & i \end{pmatrix} L, \tag{6.70}$$

where $\overline{A}$, $\overline{B}$, $\overline{C}$ are the following three functions given by

$$\overline{A} = \overline{A}(G) = \frac{1}{2p}\left(\frac{q}{p}G_{xx}^{[1]} - \frac{r}{p}G_{xx}^{[2]}\right)^{(-1)}, \quad p = \sqrt{1-qr},$$

$$\overline{B} = \overline{B}(G) = \frac{1}{4i}\left(2G_{xx}^{[2]} - \partial\frac{q}{p} \cdot \left(\frac{q}{p}G_{xx}^{[1]} - \frac{r}{p}G_{xx}^{[2]}\right)^{(-1)}\right),$$

$$\overline{C} = \overline{C}(G) = \frac{1}{4i}\left(2G_{xx}^{[1]} + \partial\frac{r}{p} \cdot \left(\frac{q}{p}G_{xx}^{[1]} - \frac{r}{p}G_{xx}^{[2]}\right)^{(-1)}\right).$$

Thus, the WKI category (6.68) has the GLR:

$$L_t = [W_m, L] + \overline{M}L^{m+1}, \quad m \in Z, \tag{6.71}$$

$$\overline{M} = \begin{cases} \dfrac{1}{1-qr}\begin{pmatrix} qA & iB \\ iA & -rB \end{pmatrix}, & m \geqslant 0, \\ \dfrac{1}{1-qr}\begin{pmatrix} qC & iD \\ iC & -rD \end{pmatrix}, & m < 0, \end{cases} \tag{6.72}$$

with the GLO

$$W_m = \sum V(G_j)L^{m-j}, \quad m \in Z. \tag{6.73}$$

Here L, L^{-1} and $V(G_j)$ are given by (6.56), (6.61) and (6.70) with $G = G_j$ defined by (6.69), respectively.

6.5: The following spectral problem:

$$L \cdot y = \lambda y, \quad L = L(u) = \frac{1}{u}\begin{pmatrix} i & 1-u \\ 1 & -i \end{pmatrix}\partial, \quad y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \tag{6.74}$$

yields its Lenard operators pair,

$$K = \partial^3, \quad J = -2(\partial u + u\partial).$$

The Gateaux derivative operator $L_*(\xi)$ of the spectral operator L in the direction $\xi \in \mathcal{B}$ is

$$L_*(\xi)=\frac{\xi}{u^2}\begin{pmatrix}-i & -1\\ -1 & i\end{pmatrix}\partial=\frac{\xi}{u}\begin{pmatrix}0 & -i\\ 0 & -1\end{pmatrix}L. \tag{6.75}$$

Apparently, L_* is a homomorphism and $L_*(\xi)=0\Leftrightarrow\xi=0$.

In the category derived from Eq. (6.75), we can obtain the Harry–Dym hierarchy as well as some new integrable equations. For example, the following nonlinear equation:

$$v_{xt_{-2}}=2vv_{xx}+v_x^2 \tag{6.76}$$

is a new integrable equation with many unknown physical properties. In fact, this equation is included in an isospectral ($\lambda_{t_{-2}}=0$) negative order hierarchy of (6.74), and its standard Lax operator is

$$W_{-2}=-V(G_{-2})L^{-1}-V(G_{-1})L^{-3},$$

where $V(G_j)$ $(j=-2,-1)$ is given by

$$V=V(G)=G_{xx}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}+G_x\begin{pmatrix}1 & -2i\\ 0 & -1\end{pmatrix}L+2G\begin{pmatrix}-i & u-1\\ -1 & i\end{pmatrix}L^2, \tag{6.77}$$

with $G=G_{-2}=-v^{(-1)}$, $G_{-1}=\frac{1}{2}$, respectively, and L^{-1} is the inverse of L, given by

$$L^{-1}=\begin{pmatrix}-i\partial^{-1} & \partial^{-1}v_x-\partial^{-1}\\ -\partial^{-1} & i\partial^{-1}\end{pmatrix}. \tag{6.78}$$

We will give in detail some reductions for the latter four spectral problems in a later paper.

ACKNOWLEDGMENTS

The first author (Z.Q.) would like to express his sincere thanks to Professor Gu Chaohao and Professor Hu Hesheng for their enthusiastic encouragements and helps, to Professor Dr. Strampp for his warm invitation, and also to D. D. Holm, J. M. Hyman and L. G. Margolin for their friendly academic discussions. The authors are very grateful to the referees for mentioning the Refs. 1, 3, 15, 16 and their precious opinions. This work was supported by the U.S. Department of Energy under Contracts No. W-7405-ENG-36 and the Applied Mathematical Sciences Program KC-07-01-01; the Alexander von Humboldt Foundation, Germany; the Special Grant of National Excellent Doctorial Dissertation of China; and also the Doctoral Program Foundation of the Insitution of High Education of China.

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Dirichlet forms and symmetric Markovian semigroups on CCR algebras with respect to quasi-free states

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(Received 21 February 2001; accepted 4 November 2002)

Employing the construction method of Dirichlet forms on standard forms of von Neumann algebras developed in *Infinite Dimensional Analysis, Quantum Probability and Related Topics*, 2000, Vol. 3, No. 1, pp. 1–14 (Ref. 1), we construct Dirichlet forms and associated symmetric Markovian semigroups on CCR algebras with respect to quasi-free states. More precisely, let $\mathcal{A}(\mathfrak{h}_0)$ be the CCR algebra over a complex separable pre-Hilbert space $\mathfrak{h}_0$ and let ω be a quasi-free state on $\mathcal{A}(\mathfrak{h}_0)$. For any normalized admissible function f and complete orthonormal system (CONS) $\{g_n\}\subset\mathfrak{h}_0$, we construct a Dirichlet form and corresponding symmetric Markovian semigroup on the natural standard form associated to the GNS representation of $(\mathcal{A}(\mathfrak{h}_0),\omega)$. It turns out that the form is independent of admissible function f and CONS $\{g_n\}$ chosen. By analyzing the spectrum of the generator (Dirichlet operator) of the semigroup, we show that the semigroup is ergodic and tends to the equilibrium exponentially fast. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1532770]

I. INTRODUCTION

Our purpose in this paper is to construct Dirichlet forms and associated symmetric Markovian semigroups on CCR algebras with respect to gauge invariant quasi-free states, and then investigate detailed properties such as ergodicity of the semigroups. Let $\mathcal{A}(\mathfrak{h}_0)$ be the CCR algebra over a complex separable pre-Hilbert space $\mathfrak{h}_0$ and let ω be a gauge invariant quasi-free state on $\mathcal{A}(\mathfrak{h}_0)$.[2] For any normalized admissible function f and complete orthonormal system (CONS) $\{g_n\}\subset\mathfrak{h}_0$, we use the general construction method of Dirichlet forms developed in Ref. 1 to construct a Dirichlet form and corresponding symmetric Markovian semigroup on the natural standard form associated to the GNS representation of the pair $(\mathcal{A}(\mathfrak{h}_0),\omega)$. We show that the Dirichlet form we constructed is independent of the admissible function f and the CONS $\{g_n\}$ chosen. By establishing a (chaos) decomposition of the quasi-free Hilbert space (see Sec. V) and investigating the spectrum of the generator (Dirichlet operator) of the semigroup, we prove that the semigroup is ergodic and tends to the equilibrium exponentially fast.

The study of noncommutative Dirichlet forms was pioneered by Albeverio and Høegh-Krohn,[3] Sauvageot[4–6] and extensively developed by Davies and Lindsay,[7] and Guido, Isola, and Scarlatti.[8] All these authors considered Markovianity of forms and semigroups only with respect to a tracial state ϕ_0. Recently, the abstract theory has been extended to a faithful normal state ϕ_0 by Goldstein and Lindsay[9,10] in the setting of the Haagerup's standard forms and by Cipriani[11] in the context of general standard forms of von Neumann algebras, respectively.

The need to construct Markovian semigroups on von Neumann algebras, which are symmetric with respect to a nontracial state, is clear for various applications to open systems,[12] quantum

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statistical mechanics,[2] and quantum probability theory.[13–15] Although on an abstract level we have quite a well-developed theory as mentioned above, the progress in a concrete application is very slow. We would like to mention a few recent works in this direction. The completely positive Hamiltonian semigroup for quantum spin chains in the ground state representation has been considered in Refs. 16–18. In Refs. 19–20, Majewski and Zegarlinski used the generalized conditional expectation to construct generators of spin-flip type dynamics for quantum spin systems. In Ref. 1, one of the authors gave a general construction method of Dirichlet forms on standard forms of von Neumann algebras and applied the method to construct translation invariant Markovian semigroups for quantum spin systems. In Ref. 21, quantum Ornstein–Uhlenbeck semigroups were constructed by means of noncommutative Dirichlet forms. Extending the methods of Ref. 1 and the techniques developed in this paper, we construct symmetric Markovian semigroups on CAR algebras with respect to quasi-free states.[22]

Let us describe the content of this paper briefly. Let $\mathfrak{h}_0$ be a complex separable pre-Hilbert space and $\mathfrak{h}$ the completion of $\mathfrak{h}_0$. Denote by $\mathcal{A}(\mathfrak{h}_0)$ the C^*-algebra over $\mathfrak{h}_0$ generated by the Weyl operators $W(g)$, $g\in\mathfrak{h}_0$. Let A be a self-adjoint operator on $\mathfrak{h}$ satisfying

$$0<A\leqslant\alpha\mathbf{1}<\mathbf{1}, \tag{1.1}$$

for some $\alpha\in(0,1)$. The gauge invariant quasi-free state ω on $\mathcal{A}(\mathfrak{h}_0)$ is given by

$$\omega(W(f))=\exp\{-(f,\tfrac{1}{4}(\mathbf{1}+A)(\mathbf{1}-A)^{-1}f)\},\quad f\in\mathfrak{h}_0.$$

We assume that A^{-1} exists as a (unbounded) self-adjoint operator and that any vector in $\mathfrak{h}_0$ is an analytic vector for $A^{-1/2}$ (Assumption 3.1).

Let $(\mathcal{H}_\omega,\pi_\omega,\Omega_\omega)$ be the GNS representation of the pair $(\mathcal{A}(\mathfrak{h}_0),\omega)$ and $\mathcal{M}=\pi_\omega(\mathcal{A}(\mathfrak{h}_0))''$. We suppress ω and π_ω from the notation, i.e., $\mathcal{H}=\mathcal{H}_\omega$, $W(f)=\pi_\omega(W(f))$, etc. We also write $\xi_0=\Omega_\omega$. Let $\sigma_t:\mathcal{M}\to\mathcal{M}$ be the one parameter group of automorphisms defined by

$$\sigma_t(W(f))=W(A^{it}f),\quad f\in\mathfrak{h}_0,\ t\in\mathbb{R}.$$

Then ω satisfies σ-KMS conditions.[2] We use Δ and J to denote the modular operator and the modular conjugation, respectively. Then σ_t becomes the modular group : $\sigma_t(B)=\Delta^{it}B\Delta^{-it}$, $B\in\mathcal{M}$. Let $\mathcal{M}'$ be the commutant of $\mathcal{M}$. The map $j:\mathcal{M}\to\mathcal{M}'$ is the antilinear $*$-isomorphism defined by $j(B)=JBJ$, $B\in\mathcal{M}$. The natural positive cone $\mathcal{P}$ associated with $(\mathcal{M},\xi_0)$ is the closure of the set $\{Bj(B)\xi_0: B\in\mathcal{M}\}$. The form $(\mathcal{M},\mathcal{H},\mathcal{P},J)$ is the standard form associated with $(\mathcal{M},\xi_0)$.

For any $g\in\mathfrak{h}_0$, let $\Phi(g)$ be the infinitesimal generator of the unitary group $W(tg)$, $t\in\mathbb{R}$, and

$$a(g)=2^{-1/2}(\Phi(g)+i\Phi(ig)),$$

$$a^*(g)=2^{-1/2}(\Phi(g)-i\Phi(ig)).$$

For any $f,g\in\mathfrak{h}_0$, $a(f)$ and $a^*(g)$ are densely defined, closed and $a(f)^*=a^*(f)$, and satisfy the canonical commutation relations (CCRs).[2] Notice that $a^\#(g)$ and $j(a^\#(g))$, $g\in\mathfrak{h}_0$, are affiliated with $\mathcal{M}$ and $\mathcal{M}'$, respectively, where $a^\#(g)$ stands for either $a(g)$ or $a^*(g)$.

For any $B\in\mathcal{M}$ and $n\in\mathbb{N}$, we write

$$B_n=\left(\frac{n}{\pi}\right)^{1/2}\int\sigma_t(B)e^{-nt^2}dt.$$

Let $\mathcal{W}$ be the algebra generated by $W(f)$, $f\in\mathfrak{h}_0$. We set $W_n(f):=W(f)_n$, where $W(f)_n$ is defined in the above with $B=W(f)$. We use $\mathcal{W}_0$ and $\mathcal{M}_0$ to denote the algebras generated by $W_n(f)$, $f\in\mathfrak{h}_0$, $n\in\mathbb{N}$ and by B_n, $B\in\mathcal{M}$, $n\in\mathbb{N}$, respectively. We also use $\mathcal{H}_{\text{fin}}$ to denote the subspace of $\mathcal{H}$ spanned by the vectors of the form $(\Pi_{j=1}^n\Phi(g_j))\xi_0$, $g_j\in\mathfrak{h}_0$, $j=1,2,\ldots,n$. Obviously, $\mathcal{W}\xi_0$, $\mathcal{W}_0\xi_0$, $\mathcal{M}_0\xi_0$ and $\mathcal{H}_{\text{fin}}$ are dense in $\mathcal{H}$.

For any normalized admissible function f (Definition 2.1) and CONS $\{g_n\}\subset\mathfrak{h}_0$ for $\mathfrak{h}$, we define a sesquilinear form $\mathcal{E}:D(\mathcal{E})\times D(\mathcal{E})\to\mathbb{C}$ by

$$\begin{aligned} &D(\mathcal{E})=\mathcal{W}_0\xi_0\ (\text{ or } \mathcal{W}\xi_0,\ \mathcal{M}_0\xi_0),\\ &\mathcal{E}(\eta,\ \xi)=\sum_{n=1}^{\infty}\ \mathcal{E}^{(n)}(\eta,\ \xi),\quad \eta,\ \xi\in D(\mathcal{E}), \end{aligned} \tag{1.2}$$

where for each $n\in\mathbb{N}$, $\eta,\ \xi\in D(\mathcal{E}^{(n)})=\mathcal{W}_0\xi_0$ (or $\mathcal{W}\xi_0,\ \mathcal{M}_0\xi_0$)

$$\begin{aligned} \mathcal{E}^{(n)}(\eta,\ \xi)=&\int\langle(\sigma_{t-i/4}(a(g_n))-j(\sigma_{t-i/4}(a^*(g_n))))\eta,\\ &(\sigma_{t-i/4}(a(g_n))-j(\sigma_{t-i/4}(a^*(g_n))))\xi\rangle f(t)\,dt\\ &+\int\langle(\sigma_{t-i/4}(a^*(g_n))-j(\sigma_{t-i/4}(a(g_n))))\eta,\\ &(\sigma_{t-i/4}(a^*(g_n))-j(\sigma_{t-i/4}(a(g_n))))\xi\rangle f(t)\,dt. \end{aligned} \tag{1.3}$$

See Sec. III for the details.

It turns out that the forms $(\mathcal{E},\ \mathcal{W}\xi_0)$ and $(\mathcal{E},\ \mathcal{W}_0\xi_0)$ are closable and independent of the admissible function f and the CONS $\{g_n\}$ chosen (Proposition 3.1). For each $n\in\mathbb{N}$, the form $(\mathcal{E}^{(n)},\ \mathcal{M}_0\xi_0)$ is closable and its closure $(\overline{\mathcal{E}^{(n)}},\ D(\overline{\mathcal{E}^{(n)}}))$ is a Dirichlet form (Proposition 3.2). Let $\overline{\mathcal{E}}$ be the form defined by

$$\overline{\mathcal{E}}=\sum_{n=1}^{\infty}\ \overline{\mathcal{E}^{(n)}}.$$

Then $(\overline{\mathcal{E}},\ D(\overline{\mathcal{E}}))$ is a densely defined Dirichlet form (Theorem 3.1). As a Corollary of Theorem 3.2, the form $(\overline{\mathcal{E}},\ D(\overline{\mathcal{E}}))$ is also independent of the f and $\{g_n\}$ we have chosen.

Let H be the infinitesimal generator of the Markovian semigroup $\{T_t\}_{t\geqslant 0}$ associated to $(\overline{\mathcal{E}},\ D(\overline{\mathcal{E}}))$. In order to analyze the spectrum $\sigma(H)$ of H, we introduce a (chaos) decomposition of $\mathcal{H}$. Let B be the operator given by

$$B:=A^{-1/2}-A^{1/2}. \tag{1.4}$$

For any $g\in\mathfrak{h}_0$, let $D_1(g)$ and $D_2(g)$ be the operators on $\mathcal{H}$ defined by

$$\begin{aligned} &D_1(g):=\sigma_{-i/4}(a(B^{-1/2}g))-j(\sigma_{-i/4}(a^*(B^{-1/2}g))),\\ &D_2(g):=\sigma_{-i/4}(a^*(B^{-1/2}g))-j(\sigma_{-i/4}(a(B^{-1/2}g))). \end{aligned}$$

Then $D_i(f)\xi_0=0$, $i=1,2$, $f\in\mathfrak{h}_0$ (Lemma 5.1) and the following CCRs hold (Proposition 5.1) : for any $f,\ g\in\mathfrak{h}_0$,

$$\begin{aligned} &[D_1(f),\ D_1(g)^*]=(f,\ g)\mathbf{1},\\ &[D_2(f),\ D_2(g)^*]=(g,\ f)\mathbf{1},\\ &[D_i(f),\ D_i(g)]=0,\quad i=1,2,\\ &[D_1(f)^{\#},D_2(g)^{\#}]=0, \end{aligned}$$

where $D_i(f)^{\#}$ is either $D_i(f)$ or $D_i(f)^*$, $i=1,2$. Thus $D_i(f)$ and $D_i(g)^*$ can be considered as annihilation and creation operators, respectively, and ξ_0 is the vacuum vector. Thus $\mathcal{H}$ has the following decomposition (Theorem 5.1):

$$\mathcal{H}=\bigoplus_{m,n=0}^{\infty}\mathcal{H}^{(m,n)},$$

where for each $m,n\in\mathbb{N}\cup\{0\}$, $\mathcal{H}^{(m,n)}$ is the closure of the subspace spanned by vectors of the form

$$\left(\prod_{j=1}^{m}D_1(g_j)^*\right)\left(\prod_{l=1}^{n}D_2(h_l)^*\right)\xi_0,\quad g_j,h_l\in\mathfrak{h}_0.$$

It follows that $\mathcal{H}_{\text{fin}}\subset D(H)$ and for any CONS $\{g_n\}\subset\mathfrak{h}_0$,

$$H=\sum_{n=1}^{\infty}\{D_1(B^{1/2}g_n)^*D_1(B^{1/2}g_n)+D_2(B^{1/2}g_n)^*D_2(B^{1/2}g_n)\},$$

as a bilinear form on $\mathcal{H}_{\text{fin}}\times\mathcal{H}_{\text{fin}}$ [Lemma 5.4(b)]. Let $\mathcal{F}$ be the symmetric Fock space over $\mathfrak{h}$.[2] Then there is an anti-unitary operator $V:\mathcal{F}\to\mathcal{F}$ and a unitary operator $U:\mathcal{H}\to\mathcal{F}\otimes V\mathcal{F}(=\mathcal{F}\otimes\mathcal{F})$ (Proposition 5.2) such that

$$UHU^{-1}=d\Gamma(B)\otimes\mathbf{1}+\mathbf{1}\otimes d\Gamma(B),$$

where $d\Gamma(B)$ is the second quantization of B.[2] Thus H is essentially self-adjoint on $\mathcal{H}_{\text{fin}}$ and independent of the admissible function f and CONS $\{g_n\}\subset\mathfrak{h}_0$ chosen. Moreover the zero is a simple eigenvalue of H with eigenvector ξ_0 and $(0,\alpha^{-1/2}-\alpha^{1/2})\cap\sigma(H)=\varnothing$ (Theorem 3.2).

We should mention that the main results in this paper can be generalized. For instance, if one replaces g_n by $B^{\lambda}g_n$, $n\in\mathbb{N}$, $\lambda\in[-\frac{1}{2},\infty)$, in the definition of $\mathcal{E}(\eta,\xi)$ in (1.2) and (1.3), the results in Sec. III still hold with an appropriate modification on the spectral gap. See Remark 3.3.

We organize this paper as follows: In Sec. II we first introduce some terminologies in the theory of noncommutative Dirichlet forms[11] and then review the general construction method of Ref. 1. We extend the method of Ref. 1 slightly and produce its proof. In Sec. III, we give an explicit expression of a Dirichlet form for given normalized admissible function f and CONS $\{g_n\}\subset\mathfrak{h}_0$ for $\mathfrak{h}$, and then state main results in this paper. Section IV is devoted to the proofs of Proposition 3.1, Proposition 3.2 and Theorem 3.1. In Sec. V, we introduce a chaos decomposition of $\mathcal{H}$ and then prove the ergodicity of the semigroup and the existence of a spectral gap. In the Appendix, we give the proofs of technical lemmas (Lemma 4.3 and Lemma 5.4).

II. REVIEW ON CONSTRUCTION OF DIRICHLET FORMS ON STANDARD FORMS OF VON NEUMANN ALGEBRAS

In this section, we first introduce necessary terminologies in the theory of noncommutative Dirichlet forms in the sense of Cipriani,[11] and then describe the general construction method of Dirichlet forms on the standard form of von Neumann algebras developed in Ref. 1. We extend the result of Ref. 1 slightly and give its proof.

Let $\mathcal{M}$ be a σ-finite von Neumann algebra acting on a complex Hilbert space $\mathcal{H}$. A self-dual cone $\mathcal{P}$ in $\mathcal{H}$ is a subset satisfying the property

$$\{\xi\in\mathcal{H}:\langle\xi,\eta\rangle\geqslant 0,\quad\forall\,\eta\in\mathcal{P}\}=\mathcal{P}.$$

$\mathcal{P}$ is then a closed convex cone and $\mathcal{H}$ is the complexification of the real subspace $\mathcal{H}^J:=\{\xi\in\mathcal{H}:\langle\xi,\eta\rangle\in\mathbb{R},\ \forall\,\eta\in\mathcal{P}\}$, which elements are called *J-real*: $\mathcal{H}=\mathcal{H}^J+i\mathcal{H}^J$. Such a $\mathcal{P}$ gives rise to a structure of ordered Hilbert space on $\mathcal{H}^J$ (denoted by $\leqslant$) and to an anti-unitary involution J on

$\mathcal{H}$, which preserves $\mathcal{H}^J$: $J(\xi+i\eta):=\xi-i\eta$ for all $\xi,\eta\in\mathcal{H}^J$. Any J-real element $\xi\in\mathcal{H}^J$ can be decomposed uniquely as a difference, $\xi=\xi_+-\xi_-$, of two orthogonal, positive elements, called the positive and the negative part of ξ: ξ_+, $\xi_-\in\mathcal{P}$, $\langle\xi_+,\xi_-\rangle=0$.

A *standard form* $(\mathcal{M},\mathcal{H},\mathcal{P},J)$ of the von Neumann algebra $\mathcal{M}$ acting faithfully on the Hilbert space $\mathcal{H}$ consists of self-dual, closed, convex cone $\mathcal{P}$ in $\mathcal{H}$ and the anti-unitary involution J satisfying the following properties:

(a) $J\mathcal{M}J=\mathcal{M}'$
(b) $JxJ=x^*,\quad \forall x\in\mathcal{M}\cap\mathcal{M}'$
(c) $J\xi=\xi,\quad \forall\xi\in\mathcal{P}$
(d) $xJxJ(\mathcal{P})\subset\mathcal{P},\quad \forall x\in\mathcal{M}$,

where $\mathcal{M}'$ is the commutant of $\mathcal{M}$.

A bounded operator A on $\mathcal{H}$ is called *J-real* if $AJ=JA$ and *positive preserving* if $A\mathcal{P}\subset\mathcal{P}$. The semigroup $\{T_t\}_{t\geqslant 0}$ is said to be *J-real* if T_t is J-real for any $t\geqslant 0$ and it is called *positive preserving* if T_t is positive preserving for any $t\geqslant 0$.

Let us fix a cyclic and separating vector ξ_0 in $\mathcal{P}$. A bounded operator $A:\mathcal{H}\to\mathcal{H}$ is called *sub-Markovian* (with respect to ξ_0) if $0\leqslant\xi\leqslant\xi_0$ implies $0\leqslant A\xi\leqslant\xi_0$. A is called *Markovian* if it is sub-Markovian and also $A\xi_0=\xi_0$. A semigroup $\{T_t\}_{t\geqslant 0}$ is said to be *sub-Markovian* (with respect to ξ_0) if T_t is sub-Markovian for every $t\geqslant 0$. The semigroup $\{T_t\}_{t\geqslant 0}$ is called *Markovian* if T_t is Markovian for every $t\geqslant 0$.

Next, we consider a sesquilinear form on some linear manifold of $\mathcal{H}$: $\mathcal{E}(\cdot,\cdot):D(\mathcal{E})\times D(\mathcal{E})\to\mathbb{C}$. We also consider the associated quadratic form: $\mathcal{E}[\cdot]:D(\mathcal{E})\to\mathbb{C}$, $\mathcal{E}[\xi]:=\mathcal{E}(\xi,\xi)$. A real valued quadratic form $\mathcal{E}[\cdot]$ is said to be *semi-bounded* if $\inf\{\mathcal{E}[\xi]:\xi\in D(\mathcal{E}),\ \|\xi\|=1\}=-b>-\infty$. A quadratic form $(\mathcal{E},D(\mathcal{E}))$ is said to be *J-real* if $JD(\mathcal{E})\subset D(\mathcal{E})$ and $\mathcal{E}[J\xi]=\overline{\mathcal{E}[\xi]}$ for any $\xi\in D(\mathcal{E})$. For a given semi-bounded quadratic form $\mathcal{E}$, one consider the inner product given by $\langle\xi,\eta\rangle_\lambda:=\mathcal{E}(\xi,\eta)+\lambda\langle\xi,\eta\rangle$, for $\lambda>b$. The form $\mathcal{E}$ is *closed* if $D(\mathcal{E})$ is a Hilbert space for some of the above norms. The form $\mathcal{E}$ is called *closable* if it admits a closed extension.

Associated to a semi-bounded closed form $\mathcal{E}$, there are a self-adjoint operator $(H,\ D(H))$ and a strongly continuous, symmetric semigroup $\{T_t\}_{t\geqslant 0}$. Each of the above objects determines uniquely the others according to well known relations (see Section 3.1 of Ref. 2 and Section 1.3 of Ref. 23).

From now on we will consider only J-real, real-valued, semi-bounded, densely defined quadratic forms. It is easy to check that these forms satisfy the relation $\mathcal{E}[\xi+i\eta]=\mathcal{E}[\xi]+\mathcal{E}[\eta]$ for all $\xi+i\eta\in D(\mathcal{E})^J+iD(\mathcal{E})^J=D(\mathcal{E})$ where $D(\mathcal{E})^J:=D(\mathcal{E})\cap H^J$.

Let us denote by $\mathrm{Proj}\,(\xi,\mathcal{Q})$ the projection of the vector $\xi\in\mathcal{H}^J$ onto the closed, convex cone $\mathcal{Q}\subset\mathcal{H}^J$. For $\xi,\eta\in\mathcal{H}^J$, define

$$\xi\vee\eta:=\mathrm{Proj}\,(\xi,\eta+\mathcal{P}),$$

$$\xi\wedge\eta:=\mathrm{Proj}\,(\xi,\eta-\mathcal{P}).$$

A J-real, real-valued, densely defined quadratic form $(\mathcal{E},D(\mathcal{E}))$ is called *Markovian* with respect to $\xi_0\in\mathcal{P}$ if

$$\xi\in D(\mathcal{E})^J \text{ implies } \quad \xi\wedge\xi_0\in D(\mathcal{E}) \text{ and } \mathcal{E}[\xi\wedge\xi_0]\leqslant\mathcal{E}[\xi].$$

A closed Markovian form is called a *Dirichlet form*. Let $\{T_t\}_{t\geqslant 0}$ be the semigroup associated to a semi-bounded closed form $(\mathcal{E},D(\mathcal{E}))$. Then one of the main results in Ref. 11 is that $\{T_t\}_{t\geqslant 0}$ is sub-Markovian if and only if $(\mathcal{E},D(\mathcal{E}))$ is a Dirichlet form (Theorem 4.11 of Ref. 11).

Next, we describe a general construction method of Dirichlet forms on the natural standard forms of von Neumann algebras associated with the Tomita–Takesaki theory.[2,24] The method has been developed in Ref. 1. However we generalize the result of Ref. 1 slightly and produce the proof.

Let $\mathcal{M}$ be a σ-finite von Neumann algebra acting on a Hilbert space $\mathcal{H}$ and let $\xi_0 \in \mathcal{H}$ be a cyclic and separating vector for $\mathcal{M}$. We use Δ and J to denote, respectively, the modular operator and the modular conjugation associated with the pair $(\mathcal{M}, \xi_0)$.[2,25] The associated modular automorphism group is denoted by $\sigma_t : \sigma_t(A) = \Delta^{it} A \Delta^{-it}$, $A \in \mathcal{M}$. Finally, $j : \mathcal{M} \to \mathcal{M}'$ is the antilinear $*$-isomorphism defined by $j(A) = JAJ$, $A \in \mathcal{M}$. The natural positive cone $\mathcal{P}$ associated with $(\mathcal{M}, \xi_0)$ is the closure of the set

$$\{Aj(A)\xi_0 : A \in \mathcal{M}\}.$$

By a general result the cone $\mathcal{P}$ can be obtained by the closure of the set,

$$\{\Delta^{1/4} AA^* \xi_0 : A \in \mathcal{M}\}.$$

The natural cone $\mathcal{P}$ is self-dual.[2,25] For the detailed properties of $\mathcal{P}$, we refer to Section 2.5.4 of Ref. 2. The form $(\mathcal{M}, \mathcal{H}, \mathcal{P}, J)$ is the standard form associated with the pair $(\mathcal{M}, \xi_0)$.

In order to construct Dirichlet forms, let us introduce the notion of admissible functions:

Definition 2.1: An analytic function $f : D \to \mathbb{C}$ on a domain D containing the strip $\mathrm{Im}\, z \in [-1/4, 1/4]$ *is said to be admissible if the following properties hold:*

(a) $f(t) \geqslant 0$ *for* $\forall t \in \mathbb{R}$,
(b) $f(t + i/4) + f(t - i/4) \geqslant 0$, *for* $\forall t \in \mathbb{R}$,
(c) there exist $M > 0$ *and* $p > 1$ *such that the bound*

$$|f(t + is)| \leqslant M(1 + |t|)^{-p}$$

holds uniformly in $s \in [-1/4, 1/4]$.

Let us give an example of an admissible function. Using the residue integration method it is easy to check that

$$\int_{-\infty}^{\infty} (\cosh k)^{-1} e^{ikt}\, dk = 2\pi (e^{\pi/2\, t} + e^{-\pi/2\, t})^{-1}.$$

See also the expression in p. 94 of Ref. 2. Consider the following function:

$$f(t) = \frac{2}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (e^{k/4} + e^{-k/4})^{-1} e^{-1/2\, k^2} e^{-ikt}\, dk. \tag{2.1}$$

Clearly f has an analytic extension to a domain containing the strip. It can be checked that f is an admissible function such that the bound in Definition 2.1 (c) holds with any $p > 1$. See the proof of Lemma 3.1 of Ref. 1.

We are ready to give a construction of Dirichlet forms on the standard form $(\mathcal{M}, \mathcal{H}, \mathcal{P}, J)$ associated with the pair $(\mathcal{M}, \xi_0)$. Denote by $\mathcal{M}_{\mathrm{an}}$ the dense subset of $\mathcal{M}$ consisting of every σ_t-analytic element with a domain containing the strip $I_{1/2} := \{z : |\mathrm{Im}\, z| \leqslant \frac{1}{2}\}$.[2] By Prop. 2.5.21 of Ref. 2, any $A \in \mathcal{M}_{\mathrm{an}}$ is strongly analytic. In the following, the inner product $\langle \cdot, \cdot \rangle$ on $\mathcal{H}$ is conjugate linear in the first and linear in the second variable. For given admissible function f and $x \in \mathcal{M}_{\mathrm{an}}$, define a sesquilinear form $\mathcal{E} : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ by

$$\begin{aligned}
\mathcal{E}(\eta, \xi) = & \int \langle (\sigma_{t - i/4}(x) - j(\sigma_{t - i/4}(x^*)))\eta, (\sigma_{t - i/4}(x) - j(\sigma_{t - i/4}(x^*)))\xi \rangle f(t)\, dt \\
& + \int \langle (\sigma_{t - i/4}(x^*) - j(\sigma_{t - i/4}(x)))\eta, (\sigma_{t - i/4}(x^*) - j(\sigma_{t - i/4}(x)))\xi \rangle f(t)\, dt \\
\equiv & \mathcal{E}^{(1)}(\eta, \xi) + \mathcal{E}^{(2)}(\eta, \xi).
\end{aligned} \tag{2.2}$$

Then the associated quadratic form is given by

$$\mathcal{E}[\xi]=\int \|[\sigma_{t-i/4}(x)-j(\sigma_{t-i/4}(x^*))]\xi\|^2 f(t)\,dt+\int \|[\sigma_{t-i/4}(x^*)-j(\sigma_{t-i/4}(x))]\xi\|^2 f(t)\,dt$$
$$\equiv \mathcal{E}^{(1)}[\xi]+\mathcal{E}^{(2)}[\xi]. \tag{2.3}$$

In Ref. 1, we have considered the case $x=x^*\in\mathcal{M}_{\mathrm{an}}$. The following is the result corresponding to Theorem 3.1 of Ref. 1.

Theorem 2.1: *For a given admissible function f and $x\in\mathcal{M}_{\mathrm{an}}$, let $(\mathcal{E},\mathcal{H})$ be defined as in (2.2). Let H be the self-adjoint operator associated with $(\mathcal{E},\mathcal{H})$. Assume that there exists a constant $M>0$ such that the bound*

$$\sup_{s\in[-1/4,1/4]} \|\sigma_{t+is}(x)\|\leqslant M$$

holds uniformly in $t\in\mathbb{R}$. Then the following properties hold:

(a) $H\xi_0=0$,
(b) $\mathcal{E}$ *is J-real,*
(c) $\mathcal{E}(\xi_+,\xi_-)\leqslant 0 \quad \forall \xi\in\mathcal{H}^J$.

Furthermore the form $(\mathcal{E},\mathcal{H})$ is a Dirichlet form.

We will produce the proof of Theorem 2.1 at the end of this section. The following is a consequence of Theorem 2.1.

Theorem 2.2: *Let $\{T_t\}_{t\geqslant 0}$ be the semigroup generated by the form $(\mathcal{E},\mathcal{H})$ in Theorem 2.1. Then $\{T_t\}_{t\geqslant 0}$ is a J-real, strongly continuous, symmetric Markovian semigroup.*

Proof: It follows from Theorem 2.1 (a) that $T_t(\xi_0)=\xi_0$ for any $t\geqslant 0$. Thus the theorem follows from Theorem 4.11 of Ref. 11. □

Remark 2.1: Consider the symmetric embedding:

$$i_0:\mathcal{M}\to\mathcal{H},$$

$$i_0(A)=\Delta^{1/4}A\xi_0.$$

Define the maps S_t on $\mathcal{M}$ by

$$S_t:\mathcal{M}\to\mathcal{M},\quad i_0\circ S_t\equiv T_t\circ i_0.$$

It follows from Theorem 2.12 of Ref. 11 that $\{S_t\}_{t\geqslant 0}$ is a weakly continuous, Markovian semigroup on $\mathcal{M}$. The Markoviam semigroup $\{T_t\}$ extends also to a strongly continuous semigroup on its predual space and to a family of strongly continuous Markovian semigroups on their interpolation L^p-space. See Theorem 2.12 and Theorem 2.14 of Ref. 11.

We now produce the proof of Theorem 2.1.

Proof of Theorem 2.1: (a) Notice that $JA\xi_0=\Delta^{1/2}A^*\xi_0$ for any $A\in\mathcal{M}$. Thus we have that

$$(\sigma_{t-i/4}(x)-j(\sigma_{t-i/4}(x^*)))\,\xi_0=\Delta^{1/4}\sigma_t(x)\xi_0-J\Delta^{1/4}\sigma_t(x)^*\Delta^{-1/4}\xi_0$$
$$=\Delta^{1/4}\sigma_t(x)\xi_0-\Delta^{1/4}\sigma_t(x)\xi_0=0.$$

Replacing x by x^* in the above, we get

$$(\sigma_{t-i/4}(x^*)-j(\sigma_{t-i/4}(x)))\,\xi_0=0.$$

Thus (a) follows from (2.2) and the above facts.

(b) A direct estimate shows that

$$\|(\sigma_{t-i/4}(x)-j(\sigma_{t-i/4}(x^*)))J\xi\|^2 = \|-J(\sigma_{t-i/4}(x^*)-j(\sigma_{t-i/4}(x)))\xi\|^2$$
$$= \|(\sigma_{t-i/4}(x^*)-j(\sigma_{t-i/4}(x)))\xi\|^2,$$

which implies $\mathcal{E}^{(1)}[J\xi]=\mathcal{E}^{(2)}[\xi]$. The method used in the above also implies that $\mathcal{E}^{(2)}[J\xi]=\mathcal{E}^{(1)}[\xi]$.

(c) By the expression of $\mathcal{E}(\eta,\xi)$ in (2.2), $\mathcal{E}(\xi_+,\xi_-)$ can be written as

$$\mathcal{E}(\xi_+,\xi_-)=\mathcal{E}^{(1)}(\xi_+,\xi_-)+\mathcal{E}^{(2)}(\xi_+,\xi_-)=(\mathrm{I}^{(1)}+\mathrm{II}^{(1)})+(\mathrm{I}^{(2)}+\mathrm{II}^{(2)}), \tag{2.4}$$

where

$$\mathrm{I}^{(1)}=\int(\langle\sigma_{t-i/4}(x)\xi_+,\sigma_{t-i/4}(x)\xi_-\rangle+\langle\sigma_{t-i/4}(x^*)\xi_-,\sigma_{t-i/4}(x^*)\xi_+\rangle)f(t)\,dt, \tag{2.5}$$

$$\mathrm{II}^{(1)}=-\int(\langle\sigma_{t-i/4}(x)\xi_+,j(\sigma_{t-i/4}(x^*))\xi_-\rangle+\langle j(\sigma_{t-i/4}(x^*))\xi_+,\sigma_{t-i/4}(x)\xi_-\rangle)f(t)\,dt$$

and $\mathrm{I}^{(2)}$ and $\mathrm{II}^{(2)}$ are obtained from $\mathrm{I}^{(1)}$ and $\mathrm{II}^{(1)}$, respectively, replacing x by x^* in the above.

As a consequence of Theorem 4(7) of Ref. 25, $\mathcal{M}\xi_+\perp\mathcal{M}\xi_-$, which implies $\mathrm{I}^{(1)}=0$ and $\mathrm{I}^{(2)}=0$. See also the proof of Proposition 5.3 (ii) of Ref. 11. Next, we first consider $\mathrm{II}^{(1)}$. It can be checked that $\sigma_{t-is}(x)^*=\sigma_{t+is}(x^*)$, for any $x\in\mathcal{M}_{\mathrm{an}}$ and $s\in\mathbb{R}$, and so

$$\langle\sigma_{t-i/4}(x)\xi_+,j(\sigma_{t-i/4}(x^*))\xi_-\rangle=\langle\xi_+,\sigma_{t+i/4}(x^*)j(\sigma_{t+i/4}(x)^*)\xi_-\rangle \tag{2.6}$$

and

$$\langle j(\sigma_{t-i/4}(x^*))\xi_+,\sigma_{t-i/4}(x)\xi_-\rangle=\langle\xi_+,\sigma_{t-i/4}(x)j(\sigma_{t-i/4}(x^*)^*)\xi_-\rangle. \tag{2.7}$$

It follows from (2.5)–(2.7) that

$$\mathrm{II}^{(1)}=-\int\langle\xi_+,\sigma_{t+i/4}(x^*)j(\sigma_{t+i/4}(x)^*)\xi_-\rangle f(t)dt$$
$$-\int\langle\xi_+,\sigma_{t-i/4}(x)j(\sigma_{t-i/4}(x^*)^*)\xi_-\rangle f(t)dt.$$

Notice that the map $A\mapsto j(A^*)$ from $\mathcal{M}$ to $\mathcal{M}'$ is linear. It can be shown that for any $x\in\mathcal{M}_{\mathrm{an}}$ and $\xi\in\mathcal{H}$, the map

$$z\mapsto j(\sigma_z(x)^*)\xi$$

is analytic on a domain containing the strip $I_{1/2}$. In fact, the analyticity follows from the facts that $\langle\eta,j(\sigma_z(x)^*)\xi\rangle=P(\sigma_z(x)^*J\xi,J\eta\rangle=\langle J\xi,\sigma_z(x)J\eta\rangle$ for any $\eta,\xi\in\mathcal{H}$, and that weak analyticity implies strong analyticity (see Theorem VI.4 of Ref. 26).

Using the Cauchy integral theorem, the assumption in the theorem, the property (c) in the Definition 2.1 and $\sigma_t(x)^*=\sigma_t(x^*)$, we obtain that

$$\mathrm{II}^{(1)}=-\int\langle\xi_+,\sigma_t(x)^*j(\sigma_t(x)^*)\xi_-\rangle f(t-i/4)\,dt-\int\langle\xi_+,\sigma_t(x)j(\sigma_t(x))\xi_-\rangle f(t+i/4)\,dt.$$

Replacing x and x^* in the above, we obtain the expression of $\mathrm{II}^{(2)}$. Thus we get

$$\mathrm{II}=-\int\langle\xi_+,[\sigma_t(x)j(\sigma_t(x))+\sigma_t(x)^*j(\sigma_t(x)^*)]\xi_-\rangle\cdot(f(t-i/4)+f(t+i/4))\,dt.$$

Since $\sigma_t(x)j(\sigma_t(x))\xi_- \in \mathcal{P}$, $\langle \xi_+, [\sigma_t(x)j(\sigma_t(x))+\sigma_t(x)^*j(\sigma_t(x)^*)]\xi_- \rangle \geqslant 0$ for $t \in \mathbb{R}$. By the property (b) in the Definition 2.1, we conclude that II$\leqslant 0$. This proved the part (c) of the theorem.

Clearly $\mathcal{E}[\cdot] \geqslant 0$. Note that $\mathcal{E}(\xi_0, \xi)=0$, $\forall \xi \in \mathcal{H}$. By Theorem 2.1 (b)–(c), Proposition 4.5 (b) of Ref. 11 and Proposition 4.10 (ii) of Ref. 11, $(\mathcal{E}, \mathcal{H})$ is a Dirichlet form. □

III. DIRICHLET FORMS ON CCR ALGEBRAS WITH RESPECT TO QUASI-FREE STATES: PRELIMINARIES AND MAIN RESULTS

Let $\mathfrak{h}_0$ be a complex separable pre-Hilbert space. Denote by $\mathfrak{h}$ the completion of $\mathfrak{h}_0$. The inner product $(\cdot,\cdot)$ on $\mathfrak{h}$ is conjugate linear in the first and linear in the second variable. Let $\mathcal{A}(\mathfrak{h}_0)$ be the C^*-algebra generated by the Weyl operators $W(f)$, $f \in \mathfrak{h}_0$, satisfying

$$W(-f)=W(f)^*,$$

$$W(f)W(g)=e^{-(i/2)\,\mathrm{Im}(f,g)}W(f+g), \quad \forall f,g \in \mathfrak{h}_0. \tag{3.1}$$

For the abstract properties of $\mathcal{A}(\mathfrak{h}_0)$, see Theorem 5.2.8 of Ref. 2.

Next, we describe quasi-free states on $\mathcal{A}(\mathfrak{h}_0)$. Let A be a bounded and non-negative operator on $\mathfrak{h}$. Recall that $\varphi \in \mathfrak{h}$ is an analytic vector for an operator B on $\mathfrak{h}$ if $\varphi \in D(B^n)$, $n \in \mathbb{N}$, and if

$$\sum_{n=0}^{\infty} \frac{\|B^n\varphi\|}{n!}t^n < \infty,$$

for some $t>0$. In the rest of this paper, we assume that A satisfies the following properties.

Assumption 3.1: *(a) There exists* $\alpha \in (0,1)$ *such that*

$$0 < A \leqslant \alpha \mathbf{1} < \mathbf{1}.$$

(b) The inverse A^{-1} *of* A *exists as a (unbounded) self-adjoint and positive operator on* $\mathfrak{h}$.

(c) For any $z \in \mathbb{C}$, A^z *leaves* $\mathfrak{h}_0$ *invariant, i.e.,* $A^z\mathfrak{h}_0 \subset \mathfrak{h}_0$. *Moreover,* $z \mapsto A^z\varphi$ *is entire analytic for any* $\varphi \in \mathfrak{h}_0$.

(d) Any $\varphi \in \mathfrak{h}_0$ *is an analytic vector for* $A^{-1/2}$.

We remark that a dense submanifold $\mathfrak{h}_0$ of $\mathfrak{h}$ satisfying the assumption exists by the spectral theorem.

Example 3.1 (ideal Bose gases): Let $\mathfrak{h}$ *be* $L^2(\mathbb{R}^d, dx)$ *and* Δ *the Laplacian operator on* $L^2(\mathbb{R}^d, dx)$. *Let* A *be given by*

$$A=\exp\{-\beta(-\tfrac{1}{2}\Delta+\mu\mathbf{1})\},$$

where $\beta>0$ *and* $\mu>0$. *For* $f \in L^2(\mathbb{R}^d, dx)$, *denote by* $\hat{f}$ *the Fourier transform of* f. *Choose* $\mathfrak{h}_0 = \{f \in L^2(\mathbb{R}^d, dx) : \hat{f} \in C_c(\mathbb{R}^d)\}$. *Clearly Assumption 3.1 satisfied with* $\alpha = \exp(-\beta\mu)$.

For given $A \in \mathcal{L}(\mathfrak{h})$ satisfying Assumption 3.1, the gauge invariant quasi-free state ω on $\mathcal{A}(\mathfrak{h}_0)$ is defined by

$$\omega(W(f))=\exp\{-(f, \tfrac{1}{4}(\mathbf{1}+A)(\mathbf{1}-A)^{-1}f)\}, \quad f \in \mathfrak{h}_0. \tag{3.2}$$

Let $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ be the *GNS* representation[2] of $(\mathcal{A}(\mathfrak{h}_0), \omega)$, and let $\mathcal{M}=\pi_\omega(\mathcal{A}(\mathfrak{h}_0))''$. Notice that the representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of the CCR algebra $\mathcal{A}(\mathfrak{h}_0)$ is regular[2] in the sense that the unitary groups $t \in \mathbb{R} \mapsto \pi_\omega(W(tf))$ are strongly continuous for all $f \in \mathfrak{h}_0$. We use the notation $\Phi_\omega(f)$ to denote the infinitesimal generator of the unitary group $\pi_\omega(W(tf))$:

$$\pi_\omega(W(tf))=\exp(it\Phi_\omega(f)). \tag{3.3}$$

Notice that, since ω is an entire analytic state[2] by (3.2) and Assumption 3.1, the cyclic vector Ω_ω is an entire analytic vector for all $\Phi_\omega(f)$, $f\in\mathfrak{h}_0$. The annihilation and creation operators defined for each $f\in\mathfrak{h}_0$ by

$$D(a_\omega(f))=D(\Phi_\omega(f))\cap D(\Phi_\omega(if))=D(a_\omega^*(f))$$

and

$$\begin{aligned} a_\omega(f)&:=2^{-1/2}(\Phi_\omega(f)+i\Phi_\omega(if)),\\ a_\omega^*(f)&:=2^{-1/2}(\Phi_\omega(f)-i\Phi_\omega(if)), \end{aligned} \tag{3.4}$$

are densely defined, closed and $a_\omega(f)^*=a_\omega^*(f)$, and satisfy the canonical commutation relations (CCRs): for $\forall f,\ g\in\mathfrak{h}_0$,

$$\begin{aligned} [a_\omega(f),\ a_\omega(g)]&=0,\\ [a_\omega(f),\ a_\omega^*(g)]&=(f,g)\mathbf{1}. \end{aligned} \tag{3.5}$$

See Sec. 5.2.3 of Ref. 2 for the details.

In the rest of this paper, we suppress ω and π_ω from the notations. Thus $\mathcal{H}=\mathcal{H}_\omega$, $W(f)=\pi_\omega(W(f))$, $\Phi(f)=\Phi_\omega(f)$, $a(f)=a_\omega(f)$ and $a^*(f)=a_\omega^*(f)$ for any $f\in\mathfrak{h}_0$. We also use the notation $\xi_0=\Omega_\omega$. Let $\sigma_t:\mathcal{M}\to\mathcal{M}$ be the group of automorphisms on $\mathcal{M}$ defined by

$$\sigma_t(W(f))=W(A^{it}f),\quad f\in\mathfrak{h}_0.$$

It can be checked that the state ω defined by (3.2) is a σ-KMS state.[2] Thus σ_t, $t\in\mathbb{R}$, is the modular automorphism by Theorem 5.3.10 of Ref. 2. Let Δ and J be the modular operator and modular conjugation, respectively. Then $(\mathcal{M},\ \mathcal{H},\ \mathcal{P},\ J)$ is the natural standard form associated to $(\mathcal{M},\ \xi_0)$.

Next, we introduce several dense manifolds of $\mathcal{H}$. For any $B\in\mathcal{M}$, define

$$B_n=\left(\frac{n}{\pi}\right)^{1/2}\int\sigma_t(B)e^{-nt^2}dt,\quad n\in\mathbb{N}. \tag{3.6}$$

Then B_n is an entire analytic element for σ_t, $\|B_n\|\leqslant\|B\|$ for all $n\in\mathbb{N}$ and $B_n\to B$ strongly. See the proof of Proposition 2.5.22 of Ref. 2. In the rest of this paper, we write that $W_n(f):=W(f)_n$, $f\in\mathfrak{h}_0$, where $W(f)_n$ is defined as in (3.6) with $B=W(f)$. Put

$$\begin{aligned} \mathcal{M}_0&:=\text{the algebra generated by}\quad B_n,\quad B\in\mathcal{M},n\in\mathbb{N};\\ \mathcal{W}_0&:=\text{the algebra generated by}\quad W_n(f),\quad f\in\mathfrak{h}_0,n\in\mathbb{N};\\ \mathcal{W}&:=\text{the algebra generated by}\quad W(f),\quad f\in\mathfrak{h}_0. \end{aligned} \tag{3.7}$$

Denote by $\mathcal{H}_{\text{fin}}$ the subset of finite linear combinations of the vectors of the following type:

$$\psi_n=\left[\prod_{j=1}^{n}\Phi(f_j)\right]\xi_0,\quad \text{for } f_j\in\mathfrak{h}_0,\ j=1,\ldots,n,\ n\in\mathbb{N}.$$

Clearly $\mathcal{M}_0\xi_0$, $\mathcal{W}_0\xi_0$, $\mathcal{W}\xi_0$ and $\mathcal{H}_{\text{fin}}$ are dense in $\mathcal{H}$ (See Lemma 4.1).

We denote by $a^\#(f)$ either $a(f)$ or $a^*(f)$, for any $f\in\mathfrak{h}_0$. Notice that $a^\#(f)$ and $j(a^\#(f))$, $f\in\mathfrak{h}_0$, are affiliated with $\mathcal{M}$ and $\mathcal{M}'$, respectively. For any $f\in\mathfrak{h}_0$ and $z\in\mathbb{C}$, we write

$$\sigma_z(a(f)):=a(A^{i\bar{z}}f), \tag{3.8}$$

$$\sigma_z(a^*(f)) := a^*(A^{iz}f).$$

In fact, one may be able to show that for any $f \in \mathfrak{h}_0$ and $\xi \in \mathcal{M}_0\xi_0$ the function $t \mapsto \sigma_t(a^\#(f))\xi$ has an analytic extension on $\mathbb{C}$, which is denoted by $\sigma_z(a^\#(f))\xi$, and that $\sigma_z(a^\#(f))$ is equal to that on the right hand side of (3.8) on $\mathcal{M}_0\xi_0$. See the proof of Lemma 4.3.

We are ready to describe Dirichlet forms. An admissible function f is said to be *normalized* if $\int f(t)dt = 1$. For given normalized admissible function f and a complete orthonormal system-(CONS) $\{g_n\}_{n=1}^{\infty} \subset \mathfrak{h}_0$ of $\mathfrak{h}$, define a sesquilinear form $\mathcal{E}: D(\mathcal{E}) \times D(\mathcal{E}) \to \mathbb{C}$ as follows:

$$\begin{aligned} &D(\mathcal{E}) = \mathcal{W}_0\xi_0 \ (\text{or } \mathcal{W}\xi_0, \mathcal{M}_0\xi_0), \\ &\mathcal{E}(\eta, \xi) = \sum_{n=1}^{\infty} \mathcal{E}^{(n)}(\eta, \xi), \quad \eta, \xi \in D(\mathcal{E}), \end{aligned} \tag{3.9}$$

where for each $n \in \mathbb{N}$, $\eta, \xi \in D(\mathcal{E}^{(n)}) = \mathcal{W}_0\xi_0$ (or $\mathcal{W}\xi_0, \mathcal{M}_0\xi_0$):

$$\begin{aligned} \mathcal{E}^{(n)}(\eta, \xi) = &\int \langle (\sigma_{t-i/4}(a(g_n)) - j(\sigma_{t-i/4}(a^*(g_n))))\eta, \\ &(\sigma_{t-i/4}(a(g_n)) - j(\sigma_{t-i/4}(a^*(g_n))))\xi \rangle f(t)\, dt \\ &+ \int \langle (\sigma_{t-i/4}(a^*(g_n)) - j(\sigma_{t-i/4}(a(g_n))))\eta, \\ &(\sigma_{t-i/4}(a^*(g_n)) - j(\sigma_{t-i/4}(a(g_n))))\xi \rangle f(t)\, dt. \end{aligned} \tag{3.10}$$

We also define the associated quadratic forms by

$$\mathcal{E}^{(n)}[\xi] = \mathcal{E}^{(n)}(\xi, \xi), \quad \xi \in D(\mathcal{E}^{(n)}), \ n \in \mathbb{N};$$

$$\mathcal{E}[\xi] = \sum_{n=1}^{\infty} \mathcal{E}^{(n)}[\xi], \quad \xi \in D(\mathcal{E}).$$

We remark that the expression $\mathcal{E}^{(n)}(\eta, \xi)$ in (3.10) can be obtained from $\mathcal{E}(\eta, \xi)$ in (2.2) by replacing x by $a(g_n)$.

We state the main results. It turns out that the form defined in (3.9) and (3.10) is independent of the normalized admissible function f and the CONS $\{g_n\} \subset \mathfrak{h}_0$ we have chosen.

Proposition 3.1: Let $D(\mathcal{E})$ be either $\mathcal{W}_0\xi_0$ or else $\mathcal{W}\xi_0$ and let $(\mathcal{E}, D(\mathcal{E}))$ be defined as in (3.9) and (3.10). The form $(\mathcal{E}, D(\mathcal{E}))$ is closable. Moreover, $(\mathcal{E}, D(\mathcal{E}))$ is independent of the normalized admissible function f and the CONS $\{g_n\} \subset \mathfrak{h}_0$ we have chosen.

Proposition 3.2: For each $n \in \mathbb{N}$, $(\mathcal{E}^{(n)}, \mathcal{M}_0\xi_0)$ is closable. The closure $(\overline{\mathcal{E}^{(n)}}, D(\overline{\mathcal{E}^{(n)}}))$ is a Dirichlet form.

Theorem 3.1: *Let us consider the following form:*

$$D(\overline{\mathcal{E}}) = \left\{ \xi \in \bigcap_{n=1}^{\infty} D(\overline{\mathcal{E}^{(n)}}) : \sum_{n=1}^{\infty} \overline{\mathcal{E}^{(n)}}[\xi] < \infty \right\},$$

$$\overline{\mathcal{E}}[\xi] = \sum_{n=1}^{\infty} \overline{\mathcal{E}^{(n)}}[\xi],$$

where for each $n \in \mathbb{N}$, $(\overline{\mathcal{E}^{(n)}}, D(\overline{\mathcal{E}^{(n)}}))$ is the Dirichlet form obtained in Proposition 3.2. Then $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$ is a densely defined Dirichlet form.

Theorem 3.2: *Let $\{T_t\}$ be the symmetric Markovian semigroup associated to the Dirichlet form $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$, and let H be the Dirichlet operator, i.e., $T_t = e^{-tH}$, $t \geq 0$. Then the following results hold:*

(a) H is essentially self-adjoint on $\mathcal{H}_{\text{fin}}$.
(b) H is independent of the normalized admissible function f and the CONS $\{g_n\} \subset \mathfrak{h}_0$ we have chosen.
(c) The zero is a simple eigenvalue of H with eigenvector ξ_0. Moreover $(0, \alpha^{-1/2} - \alpha^{1/2}) \cap \sigma(H) = \varnothing$. Thus $\{T_t\}$ is ergodic in the sense of Cipriani.[27] See Remark 3.2.

By the spectral theorem, Theorem 3.2 (c) implies that for any $\xi \in \mathcal{H}$ and $t \geq 0$,

$$\|T_t \xi - \langle \xi_0, \xi \rangle \xi_0\|_{\mathcal{H}} \leq e^{-mt} \|\xi - \langle \xi_0, \xi \rangle \xi_0\|_{\mathcal{H}}, \tag{3.11}$$

where $m = \alpha^{-1/2} - \alpha^{1/2}$. Thus $\{T_t\}_{t \geq 0}$ converges to the equilibrium exponentially fast. Before closing this section, we would like to make the following remarks.

Remark 3.1: As a consquence of Theorem 2.12 of Ref. 11 and Theorem 3.1 in the above, the Markovian semigroup extends to a weakly continuous Markovian semi-group S_t on $\mathcal{M} = (\pi(\mathcal{A}(\mathfrak{h}_0)))''$. See Remark 2.1.

Remark 3.2: Theorem 3.2 (c) implies that the vector ξ_0 is a simple, strictly positive ground state for the generator H. In view of Ref. 27, T_t satisfies the indecomposability and the ergodicity (for each positive ξ, η, there exists $t > 0$ such that $\langle \xi, T_t \eta \rangle > 0$). See Theorem 4.3 of Ref. 27.

Remark 3.3: The main results in this paper can be generalized in several ways. For instance, let B be the operator on $\mathfrak{h}$ defined in (1.4). If one replaces g_n by $B^{\lambda} g_n$, $n \in \mathbb{N}$, for some $\lambda \in [-\frac{1}{2}, \infty)$ in the definition of $\mathcal{E}(\eta, \xi)$ in (3.9) and (3.10), and modify Assumption 3.1 (d) appropriately, then all of the results in this section still hold with a modified spectral gap in Theorem 3.2 (c), i.e., $(0, (\alpha^{-1/2} - \alpha^{1/2})^{1+2\lambda}) \cap \sigma(H) = \varnothing$.

IV. MARKOVIANITY OF FORMS: PROOFS OF PROPOSITION 3.1–THEOREM 3.1

In this section, we produce the proofs of Proposition 3.1, Proposition 3.2 and Theorem 3.1. The most difficult part is the proof of Proposition 3.2 which states the Dirichlet property of each component $\mathcal{E}^{(n)}$, $n \in \mathbb{N}$, of $\mathcal{E}$ in (3.10). In Theorem 2.1, we established the Dirichlet property for any σ_t-analytic element $x \in \mathcal{M}$. However $a(g_n)$ in the definition of $\mathcal{E}^{(n)}$ in (3.10) is an unbounded operator affiliated with $\mathcal{M}$ for any $g_n \in \mathfrak{h}_0$. Thus we have to employ several limiting processes which make the paper lengthy.

Recall the definitions of $\mathcal{W}$, $\mathcal{W}_0$, and $\mathcal{M}_0$ in (3.7) and $\mathcal{H}_{\text{fin}}$ in the below of (3.7). In the rest of this paper, we denote by $a^{\#}(f)$ either $a(f)$ or $a^*(f)$, $f \in \mathfrak{h}_0$. We first state elementary facts.

Lemma 4.1: (a) $\mathcal{W}\xi_0$, $\mathcal{W}_0\xi_0$, $\mathcal{M}_0\xi_0$ and $\mathcal{H}_{\text{fin}}$ are dense in $\mathcal{H}$.

(b) The inclusions

$$\mathcal{W}\xi_0 \subset D(a^{\#}(f)), \quad \mathcal{W}_0\xi_0 \subset D(a^{\#}(f)) \text{ and } \quad \mathcal{H}_{\text{fin}} \subset D(a^{\#}(f))$$

hold for any $f \in \mathfrak{h}_0$.

(c) The inclusion

$$\mathcal{M}_0\xi_0 \subset D(a^{\#}(f))$$

holds for any $f \in \mathfrak{h}_0$. Moreover the relation

$$a^{\#}(f) B \xi_0 = j(\sigma_{-i/2}(B^*)) a^{\#}(f) \xi_0$$

holds for any $f \in \mathfrak{h}_0$ and $B \in \mathcal{M}_0$.

Proof: (a) Since $\mathcal{W}$ is norm-dense in $\pi_\omega(\mathcal{A}(\mathfrak{h}_0))$, $\mathcal{W}\xi_0$ is dense in $\mathcal{H}$. Let $f \in \mathfrak{h}_0$ be given. Using (3.6) and (3.2) it is easy to show that the sequence $\{W_n(f)\xi_0\}$ converges to $W(f)\xi_0$. This implies that $\mathcal{W}_0\xi_0$ is dense in $\mathcal{H}$. Since $\mathcal{W}_0\xi_0 \subset \mathcal{M}_0\xi_0$, $\mathcal{M}_0\xi_0$ is dense in $\mathcal{H}$. It follows from (3.2)

and Assumption 3.1 that ω is an entire analytic state[2] and so the cyclic vector ξ_0 is an entire analytic vector for $\Phi(f)$, $f\in\mathfrak{h}_0$. Also see Sec. 5.2.3 of Ref. 2. Thus the sequence of the vectors,

$$\sum_{k=0}^{n}\frac{i^k}{k!}\Phi(f)^k\xi_0,$$

converge to $W(f)\xi_0$, which implies that $\mathcal{H}_{\text{fin}}$ is dense in $\mathcal{H}$.

(b) For any $f\in\mathfrak{h}_0$ and $n\in\mathbb{N}$, we write that

$$\Phi(f,n)=-in\left(W\left(\frac{1}{n}f\right)-1\right).$$

For given $g\in\mathfrak{h}_0$, consider the sequence $\{\Phi(f,n)W(g)\xi_0\}$. Using (3.1) and (3.2), it can be checked that the sequence is a Cauchy sequence. Thus $W(g)\xi_0\in D(\Phi(f))$ for any $f,g\in\mathfrak{h}_0$, and so $\mathcal{W}\xi_0\subset D(\Phi(f))$, $f\in\mathfrak{h}_0$. By (3.4), this implies that $\mathcal{W}\xi_0\subset D(a^{\#}(f))$, $f\in\mathfrak{h}_0$. The method similar to that used in the above implies that $\mathcal{W}_0\xi_0\subset D(a^{\#}(f))$, $f\in\mathfrak{h}_0$. Since ξ_0 is an entire analytic vector for $\Phi(f)$, $f\in\mathfrak{h}_0$, $\mathcal{H}_{\text{fin}}\subset D(a^{\#}(f))$, $f\in\mathfrak{h}_0$.

(c) Notice that for any $B\in\mathcal{M}_0$, $j(\sigma_{-i/2}(B^*))\xi_0=B\xi_0$. Thus we have that

$$\Phi(f,n)B\xi_0=\Phi(f,n)j(\sigma_{-i/2}(B^*))\xi_0=j(\sigma_{-i/2}(B^*))\Phi(f,n)\xi_0.$$

Since the sequence $\{\Phi(f,n)\xi_0\}$ converges to $\Phi(f)\xi_0$, it follows that $B\xi_0\in D(\Phi(f))$ and the relation

$$\Phi(f)B\xi_0=j(\sigma_{-i/2}(B^*))\Phi(f)\xi_0,$$

hold for any $f\in\mathfrak{h}_0$ and $B\in\mathcal{M}_0$. By (3.4), this proved the part (c). □

We next state a well-known formula (4.2) on quasi-free expectations which we will use repeatedly in the sequel.

Lemma 4.2: Let ω be the quasi-free state given in (3.2). The equalities

$$\omega(\Phi(f)\Phi(g))=\tfrac{1}{2}((f,(\mathbf{1}-A)^{-1}g)+(g,A(\mathbf{1}-A)^{-1}f)) \tag{4.1}$$

and

$$\begin{aligned}&\omega\left(\Phi(f)\left(\prod_{j=1}^{m}\Phi(g_j)\right)\left(\prod_{l=1}^{n}W(h_l)\right)\right)\\&\quad=\sum_{k=1}^{m}\omega(\Phi(f)\Phi(g_k))\omega\left(\left(\prod_{j=1}^{k-1}\Phi(g_j)\right)\left(\prod_{j=k+1}^{m}\Phi(g_j)\right)\left(\prod_{l=1}^{n}W(h_l)\right)\right)\\&\quad+i\sum_{k=1}^{n}\omega(\Phi(f)\Phi(h_k))\omega\left(\left(\prod_{j=1}^{m}\Phi(g_j)\right)\left(\prod_{l=1}^{n}W(h_l)\right)\right)\end{aligned} \tag{4.2}$$

hold for any $f,g,g_j,h_l\in\mathfrak{h}_0$, $j=1,\ldots,m$, $l=1,\ldots,n$.

Proof: The Weyl relations in (3.1) and the quasi-free expectation in (3.2) yield

$$\omega(W(f)W(g))=\exp\left\{-\frac{i}{2}\text{Im}(f,g)-\tfrac{1}{4}(f+g,D(f+g))\right\},$$

for any $f,g\in\mathfrak{h}_0$, where $D=(\mathbf{1}+A)(\mathbf{1}-A)^{-1}$. Replacing f and g by tf and sg, respectively, in the above, and differentiating both sides with respect to $t\in\mathbb{R}$ and $s\in\mathbb{R}$ at the zero, one obtains (4.1).

Again, replacing f by tf in the above relation and differentiating with respect to $t \in \mathbb{R}$ at the zero, one can deduce that

$$\omega(\Phi(f)W(g)) = i\omega(\Phi(f)\Phi(g))\omega(W(g)).$$

Setting $g = g_1 + \cdots + g_p$ in the above and using the relation in (3.1), one obtains

$$\omega\left(\Phi(f)\left(\prod_{j=1}^{p} W(g_j)\right)\right) = i\left(\sum_{k=1}^{p} \omega(\Phi(f)\Phi(g_k))\right)\omega\left(\prod_{j=1}^{p} W(g_j)\right).$$

Choose $p = m + n$. Replacing g_j by $t_j g_j$, $j = 1,\ldots,m$ and g_{m+l} by h_l, $l = 1,\ldots,n$, in the above, and differentiating with respect to t_j, $j = 1,\ldots,m$, at the zero, we obtain (4.2). □

We remark that $f \mapsto a(f)$ is conjugate linear and $f \mapsto a^*(f)$ is linear. See (3.4), (3.1) and (3.2). Recall the definitions of $\sigma_z(a^{\#}(f))$, $f \in \mathfrak{h}_0$, $z \in \mathbb{C}$ in (3.8), i.e.,

$$\sigma_z(a(f)) := a(A^{i\bar{z}}f),$$

$$\sigma_z(a^*(f)) := a^*(A^{iz}f).$$

We also write that

$$\sigma_z(\Phi(f)) := \frac{1}{\sqrt{2}}\{a(A^{i\bar{z}}f) + a^*(A^{iz}f)\}, \tag{4.3}$$

for any $z \in \mathbb{C}$ and $f \in \mathfrak{h}_0$. Using CCRs in (3.5), one can check that for any $f, g \in \mathfrak{h}_0$ the relations

$$\begin{aligned} [a(f),\ W(g)] &= \frac{i}{\sqrt{2}}(f,\ g)W(g), \\ [a^*(f),\ W(g)] &= -\frac{i}{\sqrt{2}}(g,\ f)W(g), \end{aligned} \tag{4.4}$$

hold on $\mathcal{W}\xi_0$ (also on $\mathcal{W}_0\xi_0$). See also the proof of Proposition 5.2.4.(1) of Ref. 2.

For any $f \in \mathfrak{h}_0$ and $m, n \in \mathbb{N}$, we write that

$$\begin{aligned} \Phi(f,n) &:= -in\left\{\exp\left(\frac{i}{n}\Phi(f)\right) - 1\right\}, \\ \Phi_m(f) &:= \sqrt{\frac{m}{\pi}}\int \sigma_t(\Phi(f))e^{-mt^2}\,dt, \\ \Phi_m(f,n) &:= \sqrt{\frac{m}{\pi}}\int \sigma_t(\Phi(f,n))e^{-mt^2}\,dt. \end{aligned} \tag{4.5}$$

Notice that for any $f \in \mathfrak{h}_0$ and $m,\ n \in \mathbb{N}$, $\Phi_m(f,\ n)$ is an entire analytic element for σ_t and $\sigma_z(\Phi_m(f,n))$ is given by

$$\sigma_z(\Phi_m(f,\ n)) = \sqrt{\frac{m}{\pi}}\int \sigma_t(\Phi(f,\ n))e^{-m(t-z)^2}\,dt, \tag{4.6}$$

for any $z \in \mathbb{C}$. See the proof of Proposition 2.5.22 of Ref. 2.

We establish technical lemmas which will be used later.

Lemma 4.3: (a) For any $f\in\mathfrak{h}_0$, $m,n\in\mathbb{N}$ *and* $z=t+is\in\mathbb{C}$, *there exist constants* $M_1(f,\ s)$ *and* $M_2(f,\ s)$ *depending only on* $f\in\mathfrak{h}_0$ *and* $s=\mathrm{Im}\,z$ *such that the bounds*

$$\|\sigma_z(\Phi_m(f,\ n))\xi_0\|\leqslant M_1(f,\ s),$$

$$\|\sigma_z(\Phi(f))\xi_0\|\leqslant M_2(f,\ s),$$

hold (*uniformly on* $m,\ n\in\mathbb{N}$).

(b) For any $f\in\mathfrak{h}_0$, $n\in\mathbb{N}$ *and* $z\in\mathbb{C}$, *the equality*

$$\sigma_z(\Phi(f))\xi_0=\lim_{n\to\infty}\sigma_z(\Phi_n(f,n))\xi_0$$

holds.

The proof of the above lemma will be given in the Appendix.

We define that for any $f\in\mathfrak{h}_0$ and $m,n\in\mathbb{N}$,

$$a_m(f,\ n):=\frac{1}{\sqrt{2}}\{\Phi_m(f,\ n)+i\Phi_m(if,\ n)\},\tag{4.7}$$

$$a_m^*(f,\ n):=\frac{1}{\sqrt{2}}\{-\Phi_m(-f,\ n)+i\Phi_m(-if,\ n)\}.$$

We denote by $a_m^{\#}(f,\ n)$ either $a_m(f,\ n)$ or $a_m^*(f,\ n)$. The following is a consequence of Lemma 4.3.

Corollary 4.1: (a) For any $f\in\mathfrak{h}_0$, $m,\ n\in\mathbb{N}$ *and* $z=t+is\in\mathbb{C}$, *there exist constants* $M_3(f,\ s)$ *and* $M_4(f,\ s)$ *depending only on* $f\in\mathfrak{h}_0$ *and* $s=\mathrm{Im}\,z$ *such that the bounds*

$$\|\sigma_z(a_m^{\#}(f,\ n))\xi_0\|\leqslant M_3(f,\ s),$$

$$\|\sigma_z(a^{\#}(f))\xi_0\|\leqslant M_4(f,\ s),$$

hold (*uniformly on* $m,n\in\mathbb{N}$).

(b) For any $f\in\mathfrak{h}_0$, $n\in\mathbb{N}$ *and* $z\in\mathbb{C}$, *the equality*

$$\sigma_z(a^{\#}(f))\xi_0=\lim_{n\to\infty}\sigma_z(a_n^{\#}(f,\ n))\xi_0$$

holds.

Proof: The corollary follows from Lemma 4.3 and the definition of $a_m^{\#}(f,\ n)$ in (4.7). □

Lemma 4.4: (a) For any $f\in\mathfrak{h}_0$, $m,n\in\mathbb{N}$, $z=t+is\in\mathbb{C}$ *and* $B\in\mathcal{M}_0$, *there exist constants* $M_5(B,\ f,\ s)$ *and* $M_6(B,\ f,\ s)$ *such that the bounds*

$$\|\sigma_z(a_m^{\#}(f,n))B\xi_0\|\leqslant M_5(B,\ f,\ s),$$

$$\|\sigma_z(a^{\#}(f))B\xi_0\|\leqslant M_6(B,\ f,\ s)$$

hold (*uniformly on* $m,\ n\in\mathbb{N}$).

(b) The equality

$$\sigma_z(a^{\#}(f))B\xi_0=\lim_{n\to\infty}\sigma_z(a_n^{\#}(f,\ n))B\xi_0$$

holds for any $f\in\mathfrak{h}_0$, $z\in\mathbb{C}$ *and* $B\in\mathcal{M}_0$.

Proof: (a) As in the proof of Lemma 4.1 (c), one has that for any m, $n\in\mathbb{N}$, $B\in\mathcal{M}_0$ and $z\in\mathbb{C}$,

$$\sigma_z(a_m^{\#}(f,\,n))B\xi_0=j(\sigma_{-i/2}(B^*))\sigma_z(a_m^{\#}(f,\,n))\xi_0. \tag{4.8}$$

Thus the bounds follow from Corollary 4.1 (a), Lemma 4.1 (c) and the above relations.

(b) This follows from Corollary 4.1 (b), (4.8) and Lemma 4.1 (c). □

In order to show the closability of the form $(\mathcal{E}^{(n)},\,\mathcal{M}_0\xi_0)$, $n\in\mathbb{N}$, in Proposition 3.2, we will use the proposition listed below. The proposition is probably well known to the experts.

Proposition 4.1: Let $(\Omega,\,\mu)$ be a probability space, $\mathcal{H}$ a separable Hilbert space and D a dense subset in $\mathcal{H}$. For any $t\in\Omega$, let $A(t)$ be an operator defined on D satisfying the following properties:

(a) $(A(t),\,D)$ is closable for each $t\in\Omega$,
(b) for any $\xi\in D$, $\Omega\ni t\mapsto\|A(t)\xi\|^2$ is an integrable function on Ω.

Then the quadratic form defined by

$$D(\mathcal{E})=D,$$

$$\mathcal{E}[\xi]=\int_\Omega\|A(t)\xi\|^2d\mu(t),\quad \xi\in D,$$

is closable.

Proof: Let $\{\xi_n\}$ be a sequence in D such that $\xi_n\to0$ as $n\to\infty$ and $\mathcal{E}[\xi_n-\xi_m]\to0$ as $n,\,m\to\infty$. One has to show that $\mathcal{E}[\xi_n]\to0$ as $n\to\infty$. Since $\{\xi_n\}$ is a $\mathcal{E}$-Cauchy sequence, one can choose a subsequence $\{\xi_{n_k}\}$ of $\{\xi_n\}$ such that $\mathcal{E}[\xi_{n_{k+1}}-\xi_{n_k}]<1/2^{2k}$ for any $k\in\mathbb{N}$, which implies that

$$\sum_{k=1}^{\infty}\mathcal{E}[\xi_{n_{k+1}}-\xi_{n_k}]^{1/2}<\infty.$$

It follows from the Schwarz inequality and the above bound that

$$\sum_{k=1}^{\infty}\int_\Omega\|A(t)(\xi_{n_{k+1}}-\xi_{n_k})\|\,d\mu(t)<\infty.$$

The monotone convergence theorem and the above bound imply that

$$\sum_{k=1}^{\infty}\|A(t)(\xi_{n_{k+1}}-\xi_{n_k})\|<\infty,\quad \mu-a.e.$$

This implies that $\{A(t)\xi_{n_k}\}$ is a Cauchy sequence $\mu-a.e.$ Since $A(t)$ is closable on D for any $t\in\Omega$, we conclude that

$$A(t)\xi_{n_k}\to0,\quad \text{as } k\to\infty,\ \mu-a.e.$$

Using Fatou's lemma and the above result, we obtain that

$$\mathcal{E}[\xi_n]=\int\underline{\lim}_{k\to\infty}\|A(t)(\xi_n-\xi_{n_k})\|^2\,d\mu(t)\leqslant\underline{\lim}_{k\to\infty}\mathcal{E}[\xi_n-\xi_{n_k}],$$

which implies that $\mathcal{E}[\xi_n]\to0$ as $n\to\infty$. This proved the proposition. □

We write that

$$\delta(a^{\#}(f)) := a^{\#}(f) - j(\sigma_{-i/2}((a^{\#}(f))^*)), \tag{4.9}$$

for $f \in \mathfrak{h}_0$. By Lemma 4.1, $\delta(a^{\#}(f))$ is well defined on $\mathcal{W}\xi_0$ and also on $\mathcal{M}_0\xi_0$ for any $f \in \mathfrak{h}_0$. Notice that for any $B \in \mathcal{M}_0$, $j(\sigma_{-i/2}(B^*))\xi_0 = B\xi_0$. Thus it follows from Lemma 4.1 (b) and Corollary 4.1 (b) that for any $f, h \in \mathfrak{h}_0$,

$$\delta(a^{\#}(f))W(h)\xi_0 = [a^{\#}(f), W(h)]\xi_0. \tag{4.10}$$

Since $(\sigma_{-i/4}(a^{\#}(f)))^* = \sigma_{i/4}((a^{\#}(f))^*)$ by (3.8), we have that

$$\delta(\sigma_{-i/4}(a^{\#}(f))) = \sigma_{-i/4}(a^{\#}(f)) - j(\sigma_{-i/4}((a^{\#}(f))^*)), \tag{4.11}$$

for any $f \in \mathfrak{h}_0$.

We are ready to prove Proposition 3.1, Proposition 3.2 and Theorem 3.1. We first produce the proof of Proposition 3.1.

Proof of Proposition 3.1: Let us first consider $(\mathcal{E}, \mathcal{W}\xi_0)$. Recall the definition of $\mathcal{E}(\eta, \xi)$ in (3.9)–(3.10). Let f be a normalized admissible function and let $\{g_n\} \subset \mathfrak{h}_0$ be a CONS for $\mathfrak{h}$. We first note that by (4.10) and (4.4),

$$\delta(\sigma_{t-i/4}(a(g_n)))W(h)\xi_0 = \delta(a(A^{it-1/4}g_n))W(h)\xi_0 = \frac{i}{\sqrt{2}}(A^{it-1/4}g_n,\ h)W(h)\xi_0,$$

$$\delta(\sigma_{t-i/4}(a^*(g_n)))W(h)\xi_0 = -\frac{i}{\sqrt{2}}(h,\ A^{it+1/4}g_n)W(h)\xi_0.$$

It follows from (3.9), the above relations, the dominated convergence theorem and the Parserval relations that for $g, h \in \mathfrak{h}_0$,

$$\begin{aligned}
\mathcal{E}(W(g)\xi_0,\ W(h)\xi_0) = &\left\{ \frac{1}{2}\sum_{n=1}^{\infty} \int (A^{-it-1/4}g,\ g_n)(g_n,\ A^{-it-1/4}h) f(t)\, dt \right\} \\
&\times \langle W(g)\xi_0, W(h)\xi_0 \rangle \\
&+ \left\{ \frac{1}{2}\sum_{n=1}^{\infty} \int (A^{-it+1/4}h,\ g_n)(g_n,\ A^{-it+1/4}g) f(t)\, dt \right\} \\
&\times \langle W(g)\xi_0,\ W(h)\xi_0 \rangle \\
= &\frac{1}{2}\{(g,\ A^{-1/2}h) + (h,\ A^{1/2}g)\}\langle W(g)\xi_0, W(h)\xi_0 \rangle.
\end{aligned} \tag{4.12}$$

Here we have used the fact that by the Schwarz inequality and the Bessel inequality,

$$\left| \sum_{n=1}^{m} (A^{-it}h_1,\ g_n)(g_n,\ A^{-it}h_2) \right| \leqslant \|h_1\|\|h_2\|,$$

for any $m \in \mathbb{N}$, $t \in \mathbb{R}$ and $h_1,\ h_2 \in \mathfrak{h}_0$. Thus $\mathcal{E}$ is well defined on $\mathcal{W}\xi_0$ and independent of the normalized admissible function f and the CONS $\{g_n\}$ chosen.

In order to show that the closability of $(\mathcal{E}, \mathcal{W}\xi_0)$, we introduce the operator $(H, \mathcal{W}\xi_0)$ defined by

$$D(H) = \mathcal{W}\xi_0,$$

$$HW(h)\xi_0=\frac{i}{\sqrt{2}}(\delta(a(A^{-1/2}h)))^*W(h)\xi_0-\frac{i}{\sqrt{2}}(\delta(a^*(A^{1/2}h)))^*W(h)\xi_0. \tag{4.13}$$

By (4.9) and Lemma 4.1 (b), H is well-defined on $\mathcal{W}\xi_0$. It follows from (4.10) and (4.4) that for any $g,h\in\mathfrak{h}_0$,

$$\begin{aligned}\langle W(g)\xi_0,HW(h)\xi_0\rangle&=\frac{i}{\sqrt{2}}\langle\delta(a(A^{-1/2}h))W(g)\xi_0,W(h)\xi_0\rangle\\&\quad-\frac{i}{\sqrt{2}}\langle\delta(a^*(A^{1/2}h))W(g)\xi_0,W(h)\xi_0\rangle\\&=\tfrac{1}{2}\{(g,A^{-1/2}h)+(h,A^{1/2}g)\}\langle W(g)\xi_0,W(h)\xi_0\rangle.\end{aligned} \tag{4.14}$$

By the method used in the above, we get that for any $g,h\in\mathfrak{h}_0$, $\langle HW(g)\xi_0,W(h)\xi_0\rangle$ is equal to the right hand side of (4.14). Thus H is symmetric on $\mathcal{W}\xi_0$. It follows from (4.12) and (4.14) that

$$\langle\eta,H\xi\rangle=\mathcal{E}(\eta,\xi),$$

for $\eta,\xi\in\mathcal{W}\xi_0$. Since $(H,\mathcal{W}\xi_0)$ is a positive symmetric operator, the form $(\mathcal{E},\mathcal{W}\xi_0)$ is closable (Theorem X.23 of Ref. 26).

Next, we consider $(\mathcal{E},\mathcal{W}_0\xi_0)$. Employing the method similar to that used to derive (4.12), one can check that $(\mathcal{E},\mathcal{W}_0\xi_0)$ is independent of admissible function f and the CONS $\{g_n\}\subset\mathfrak{h}_0$ chosen. To prove the closability, one may introduce the Dirichlet operator $(H,\mathcal{W}_0\xi_0)$ similar to that in (4.13) and then use the argument in the below of (4.13). We leave the details to the reader. □

Remark 4.1: For any CONS $\{g_n\}\subset\mathfrak{h}_0$, the relation

$$\begin{aligned}\mathcal{E}(\eta,\xi)&=\sum_{n=1}^{\infty}\langle\delta(\sigma_{-i/4}(a(g_n)))\eta,\ \delta(\sigma_{-i/4}(a(g_n)))\xi\rangle\\&\quad+\sum_{n=1}^{\infty}\langle\delta(\sigma_{-i/4}(a^*(g_n)))\eta,\ \delta(\sigma_{-i/4}(a^*(g_n)))\xi\rangle\end{aligned} \tag{4.15}$$

holds for any $\eta,\xi\in\mathcal{W}\xi_0$. In fact, the relation follows from the method used to derive (4.12).

In order to show Proposition 3.2, we introduce the following forms: For given normalized admissible function f and $g\in\mathfrak{h}_0$, let $(\tilde{\mathcal{E}},\mathcal{M}_0\xi_0)$ be a sesquilinear form defined by

$$D(\tilde{\mathcal{E}})=\mathcal{M}_0\xi_0,$$

$$\begin{aligned}\tilde{\mathcal{E}}(\eta,\xi)&=\int\langle\delta(\sigma_{t-i/4}(a(g)))\eta,\ \delta(\sigma_{t-i/4}(a(g)))\xi\rangle f(t)dt\\&\quad+\int\langle\delta(\sigma_{t-i/4}(a^*(g)))\eta,\ \delta(\sigma_{t-i/4}(a^*(g)))\xi\rangle f(t)dt,\end{aligned} \tag{4.16}$$

where for any $h\in\mathfrak{h}_0$, $\delta(a^{\#}(h))$ has been defined in (4.9). For any $n\in\mathbb{N}$, let $(\tilde{\mathcal{E}}_n,\mathcal{H})$ be the form given by

$$\begin{aligned}\tilde{\mathcal{E}}_n(\eta,\xi)&=\int\langle\delta(\sigma_{t-i/4}(a_n(g,n)))\eta,\ \delta(\sigma_{t-i/4}(a_n(g,n)))\xi\rangle f(t)dt\\&\quad+\int\langle\delta(\sigma_{t-i/4}(a_n^*(g,n)))\eta,\ \delta(\sigma_{t-i/4}(a_n^*(g,n)))\xi\rangle f(t)dt,\end{aligned} \tag{4.17}$$

where for $n \in \mathbb{N}$ and $g \in \mathfrak{h}_0$, $a_n^{\#}(g, n)$ has been defined in (4.7). Since $a_n^{\#}(g, n) \in \mathcal{M}_0$, it follows from Theorem 2.1 that $(\tilde{\mathcal{E}}_n, \mathcal{H})$ is a Dirichlet form for each $n \in \mathbb{N}$.

Lemma 4.5: For any $\eta, \xi \in \mathcal{M}_0\xi_0$,

$$\tilde{\mathcal{E}}(\eta, \xi) = \lim_{n\to\infty} \tilde{\mathcal{E}}_n(\eta, \xi).$$

Proof: The lemma follows from Lemma 4.4 and the dominated convergence theorem. □

Proposition 4.2: The form $(\tilde{\mathcal{E}}, \mathcal{M}_0\xi_0)$ *defined in (4.16) is closable. Denote by* $(\tilde{\mathcal{E}}, D(\tilde{\mathcal{E}}))$ *the closure of* $(\tilde{\mathcal{E}}, \mathcal{M}_0\xi_0)$ *and by* $\tilde{H}$ *the positive self-adjoint operator associated to* $(\tilde{\mathcal{E}}, D(\tilde{\mathcal{E}}))$. *Then the following properties hold:*

(a) $\xi_0 \in D(\tilde{H})$ *and* $\tilde{H}\xi_0 = 0$,

(b) $\tilde{\mathcal{E}}$ *is J-real,*

(c) $\tilde{\mathcal{E}}(\xi_+, \xi_-) \leqslant 0$ *for any* $\xi \in D(\tilde{\mathcal{E}})^J$.

Furthermore the form $(\tilde{\mathcal{E}}, D(\tilde{\mathcal{E}}))$ *is a Dirichlet form.*

Proof of Proposition 3.2: By setting $g = g_n$, $n \in \mathbb{N}$, the proposition follows from Proposition 4.2. □

Proof of Proposition 4.2: The closability of $(\tilde{\mathcal{E}}, \mathcal{M}_0\xi_0)$ follows from Lemma 4.1 (c), Lemma 4.4 and Proposition 4.1.

(a) It follows from (4.16) that for $m, n \in \mathbb{N}$ and $h_1, h_2 \in \mathfrak{h}_0$,

$$\tilde{\mathcal{E}}(W_m(h_1)\xi_0, W_n(h_2)\xi_0) = \langle W_m(h_1)\xi_0, \tilde{H}W_n(h_2)\xi_0\rangle,$$

where

$$\tilde{H} = \int (\delta(\sigma_{t-i/4}(a(g))))^* \delta(\sigma_{t-i/4}(a(g)))\, f(t)\, dt + \int (\delta(\sigma_{t-i/4}(a^*(g))))^* \delta(\sigma_{t-i/4}(a^*(g)))\, f(t)\, dt.$$

Using (4.10) and Lemma 4.4 (a), it is not hard to show that $\tilde{H}W_n(h_2)\xi_0$ is defined as a vector in $\mathcal{H}$. Since $\mathcal{W}_0\xi_0 \subset \mathcal{M}_0\xi_0$, we conclude that $\mathcal{W}_0\xi_0 \subset D(\tilde{H})$. By (4.10), we get that

$$\delta(\sigma_{t-i/4}(a^{\#}(g)))\xi_0 = 0,$$

for any $t \in \mathbb{R}$ and $g \in \mathfrak{h}_0$, and so $\tilde{H}\xi_0 = 0$.

(b) This follows from the method in the proof of the property (b) in Theorem 2.1 and the fact that $\mathcal{M}_0\xi_0$ is a form core.

(c) The proof of the property (c) is the hardest part in the proof. We have to employ several limiting processes. We assert that

$$\xi \in \mathcal{M}_0\xi_0 \cap \mathcal{H}^J \Rightarrow \xi_+, \xi_- \in D(\tilde{\mathcal{E}}) \quad \text{and} \quad \tilde{\mathcal{E}}[\xi_\pm] = \lim_{m\to\infty} \tilde{\mathcal{E}}_m[\xi_\pm]. \tag{4.18}$$

Let us prove our assertion. Let s_+ and s_- be the projections onto the closure of $\mathcal{M}'\xi_+$ and $\mathcal{M}'\xi_-$, where $s_+, s_- \in \mathcal{M}$. See Ref. 25. For $\xi = A\xi_0, A \in \mathcal{M}_0$, we write that

$$\xi_{n,\pm} = (s_\pm A)_n \xi_0,$$

where

$$(s_\pm A)_n = \sqrt{\frac{n}{\pi}} \int \sigma_t(s_\pm A) e^{-nt^2}\, dt.$$

Notice that $\|(s_\pm A)_n\| \leq \|A\|$, $n \in \mathbb{N}$, and that for any $\eta \in \mathcal{H}$, $(s_\pm A)_n \eta \to s_\pm A \eta$ as $n \to \infty$. See, i.e., the proof of Proposition 2.5.22 of Ref. 2. Since $\Delta^{it}\mathcal{P} \subset \mathcal{P}$ for $t \in \mathbb{R}$, $\xi_{n,\pm} = (s_\pm A)_n \xi_0 = j((s_\pm A)_n)\xi_0$, and so

$$\sigma_z(a^\#(g))\xi_{n,\pm} = j((s_\pm A)_n)\sigma_z(a^\#(g))\xi_0,$$

for any $z \in \mathbb{C}$. Since $\sigma_z(a^\#(g))$ is a closed operator for any $g \in \mathfrak{h}_0$, $z \in \mathbb{C}$, we take n to infinity to conclude that $\xi_\pm \in D(\sigma_z(a^\#(g)))$, and

$$\sigma_z(a^\#(g))\xi_\pm = j(s_\pm A)\sigma_z(a^\#(g))\xi_0,$$

and so

$$\delta(\sigma_z(a^\#(g)))\xi_\pm = j(s_\pm A)\sigma_z(a^\#(g))\xi_0 - (s_\pm A)j(\sigma_{-i/2}(\sigma_z(a^\#(g)))^*)\xi_0. \tag{4.19}$$

Thus, it follows from Corollary 4.1 (a) and the dominated convergence theorem that $\tilde{\mathcal{E}}[\xi_{m,\pm} - \xi_{n,\pm}] \to 0$ as $m,n \to \infty$. Since $(\tilde{\mathcal{E}}, D(\tilde{\mathcal{E}}))$ is closed, $\xi_\pm \in D(\tilde{\mathcal{E}})$. Next we will prove that $\tilde{\mathcal{E}}_n[\xi_\pm]$ converges to $\tilde{\mathcal{E}}[\xi_\pm]$ as n tends to infinity. Using (4.19), the analogous relation for $\sigma_z(a_n^\#(g,n))$, and Corollary 4.1 (a), we conclude that for $\xi = A\xi_0$, there exists a constant $M > 0$ such that the bounds

$$\|\delta(\sigma_{t-i/4}(a_n^\#(g,n)))\xi_\pm\| + \|\delta(\sigma_{t-i/4}(a^\#(g)))\xi_\pm\| \leq M$$

hold uniformly in $n \in \mathbb{N}$ and $t \in \mathbb{R}$. Using the above bounds, (4.19) and Corollary 4.1, we get that

$$\begin{aligned}|\tilde{\mathcal{E}}_n[\xi_\pm] - \tilde{\mathcal{E}}[\xi_\pm]| &\leq 2M \int \|\{\delta(\sigma_{t-i/4}(a_n^\#(g,\, n))) - \delta(\sigma_{t-i/4}(a^\#(g)))\}\xi_\pm\| f(t)dt \\ &\leq M' \int \|\sigma_{t-i/4}(a_n^\#(g,\, n))\xi_0 - \sigma_{t-i/4}(a^\#(g))\xi_0\| f(t)dt \to 0, \text{ as } n \to \infty.\end{aligned}$$

Here we have used Corollary 4.1 (b) and the dominated convergence theorem to obtain the last conclusion in the above. This completes the proof of our assertion.

We turn to the proof of the property (c). A direct computation shows that

$$\|\xi_\pm - \eta_\pm\| \leq \|\xi - \eta\|, \quad \forall \xi,\, \eta \in \mathcal{H}^J. \tag{4.20}$$

See also the proof of Proposition 1.2 of Ref. 7. Since $|\xi| = \xi_+ + \xi_-$, the assertion (4.18) implies that

$$\xi \in \mathcal{M}_0\xi_0 \cap \mathcal{H}^J \Rightarrow |\xi| \in D(\tilde{\mathcal{E}}) \quad \text{and} \quad \tilde{\mathcal{E}}[|\xi|] = \lim_{n\to\infty} \tilde{\mathcal{E}}_n[|\xi|]. \tag{4.21}$$

Let $\xi \in D(\tilde{\mathcal{E}}) \cap \mathcal{H}^J$ be given. Choose $\{\xi_k\}$ in $\mathcal{M}_0\xi_0 \cap \mathcal{H}^J$ such that $\xi_k \to \xi$ and $\tilde{\mathcal{E}}[\xi_k] \to \tilde{\mathcal{E}}[\xi]$ as $k \to \infty$. By (4.20), $|\xi_k| \to |\xi|$ as $k \to \infty$. Notice that $\tilde{\mathcal{E}}[|\xi|] \leq \tilde{\mathcal{E}}[\xi]$ is equivalent to $\tilde{\mathcal{E}}(\xi_+,\, \xi_-) \leq 0$ and that each $\tilde{\mathcal{E}}_m$, $m \in \mathbb{N}$, satisfies the property (c) by Theorem 2.1. By the lower semi-continuity of $\tilde{\mathcal{E}}$ and (4.21), we obtain that

$$\tilde{\mathcal{E}}[|\xi|] \leq \underline{\lim}_{k\to\infty} \tilde{\mathcal{E}}[|\xi_k|] = \underline{\lim}_{k\to\infty} \left(\lim_{n\to\infty} \tilde{\mathcal{E}}_n[|\xi_k|] \right) \leq \underline{\lim}_{k\to\infty} \left(\lim_{n\to\infty} \tilde{\mathcal{E}}_n[\xi_k] \right) = \underline{\lim}_{k\to\infty} \tilde{\mathcal{E}}[\xi_k] = \tilde{\mathcal{E}}[\xi].$$

Thus $|\xi| \in D(\tilde{\mathcal{E}})$ and $\tilde{\mathcal{E}}[|\xi|] \leq \tilde{\mathcal{E}}[\xi]$. This completes the proof of the property (c).

Since $\tilde{\mathcal{E}}(\xi, \xi_0) = 0$ for any $\xi \in D(\tilde{\mathcal{E}})$, the properties (b) and (c) imply that $\tilde{\mathcal{E}}$ is a Dirichlet form. □

Proof of Theorem 3.1: By Proposition 3.1, $\mathcal{W}_0\xi_0 \subset D(\overline{\mathcal{E}})$. Since each component $\overline{\mathcal{E}_n}$ is a Dirichlet form, it follows from Theorem 5.2 of Ref. 11 that $(\overline{\mathcal{E}}, D(\overline{\mathcal{E}}))$ is a Dirichlet form. □

V. DECOMPOSITION OF QUASI-FREE HILBERT SPACE: ERGODICITY

For given quasi-free state ω, we will decompose the Hilbert space $\mathcal{H}=\mathcal{H}_\omega$ into a direct sum of $\mathcal{H}^{(m,n)}$, $m, n \in \mathbb{N}\cup\{0\}$, where $\mathcal{H}^{(m,n)}$ is the Hilbert space of m quasi-particles and n anti-quasi-particles. We then use the result to show that the symmetric Markovian semigroup is ergodic.

Recall the definition of $\delta(a^{\#}(g))$, $g \in \mathfrak{h}_0$ in (4.9). Denote by B the operator given by

$$B = A^{-1/2} - A^{1/2}. \tag{5.1}$$

It follows from (4.9) that for $g \in \mathfrak{h}_0$,

$$\begin{aligned}\delta(a(B^{-1/2}A^{-1/4}g)) &= a(B^{-1/2}A^{-1/4}g) - j(\sigma_{-i/2}(a^*(B^{-1/2}A^{-1/4}g)))\\ &= a(B^{-1/2}A^{-1/4}g) - j(a^*(B^{-1/2}A^{1/4}g)),\end{aligned} \tag{5.2}$$

$$\begin{aligned}\delta(a^*(B^{-1/2}A^{1/4}g)) &= a^*(B^{-1/2}A^{1/4}g) - j(\sigma_{-i/2}(a(B^{-1/2}A^{1/4}g)))\\ &= a^*(B^{-1/2}A^{1/4}g) - j(a(B^{-1/2}A^{-1/4}g)).\end{aligned}$$

The above operators are well defined on $\mathcal{M}_0\xi_0$ and also on $\mathcal{H}_{\text{fin}}$. Since $(j(a(g)))^* = j(a^*(g))$, etc., a computation shows that

$$\begin{aligned}(\delta(a(B^{-1/2}A^{-1/4}g)))^* &= a^*(B^{-1/2}A^{-1/4}g) - j(a(B^{-1/2}A^{1/4}g))\\ &= a^*(B^{-1/2}A^{-1/4}g) - j(\sigma_{-i/2}(a(B^{-1/2}A^{3/4}g)))\\ &= a^*(B^{1/2}A^{1/4}g) + \delta(a^*(B^{-1/2}A^{3/4}g)).\end{aligned} \tag{5.3}$$

Here we have used the fact that $B^{-\frac{1}{2}}(A^{-\frac{1}{4}} - A^{\frac{3}{4}}) = B^{\frac{1}{2}}A^{\frac{1}{4}}$. Using the method similar to that used in the above, we get that

$$(\delta(a^*(B^{-1/2}A^{1/4}g)))^* = -a(B^{1/2}A^{-1/4}g) + \delta((a(B^{-1/2}A^{-3/4}g)). \tag{5.4}$$

From notational brevity, we write that for $g \in \mathfrak{h}_0$,

$$\begin{aligned}D_1(g) &:= \delta(a(B^{-1/2}A^{-1/4}g)),\\ D_2(g) &:= \delta(a^*(B^{-1/2}A^{1/4}g)).\end{aligned} \tag{5.5}$$

Then it follows from (5.3) and (5.4) that

$$D_1(g)^* = a^*(B^{1/2}A^{1/4}g) + D_2(A^{1/2}g), \tag{5.6}$$

$$D_2(g)^* = -a(B^{1/2}A^{-1/4}g) + D_1(A^{-1/2}g).$$

We first collect some properties of $D_i(g)$ for $g \in \mathfrak{h}_0$ and $i = 1, 2$.

Lemma 5.1: $D_i(g)\xi_0 = 0$ *for any* $g \in \mathfrak{h}_0$ *and* $i = 1, 2$.

Proof: This follows from (5.5) and (4.10). □

Lemma 5.2: As operators defined on $\mathcal{W}\xi_0$ *and* $\mathcal{W}_0\xi_0$, *the following relations hold for any* $g, h \in \mathfrak{h}_0$:

(a) $[D_i(g), {}_j(h)] = 0$, $i = 1, 2$, $j = 1, 2$,
(b) $[D_1(g), a(h)] = 0$,

(c) $[D_2(g),\ a^*(h)]=0$,

(d) $[D_1(g),\ a^*(B^{\frac{1}{2}}A^{\frac{1}{4}}h)]=(g,\ h)\mathbf{1}$,

(e) $[D_2(g),\ a(B^{\frac{1}{2}}A^{-\frac{1}{4}}h)]=-(h,\ g)\mathbf{1}$.

Proof: We first remark that each operator in the commutators in the lemma is defined on $\mathcal{W}\xi_0$ and also $\mathcal{W}_0\xi_0$. (a) This follows from (4.10), (4.4) and the definition of $D_i(g)$, $i=1, 2$, in (5.5). (b) and (c) follow from (5.5) and (4.9). (d) and (e) follow from (5.5), (4.9) and the CCRs in (3.5). □

Proposition 5.1: As operators defined on $\mathcal{W}\xi_0$, $\mathcal{W}\xi_0$ and also on $\mathcal{H}_{\text{fin}}$, the following canonical commutation relations (CCRs) hold for any $g, h\in\mathfrak{h}_0$:

(a) $[D_1(g),\ D_1(h)^*]=(g,\ h)\mathbf{1}$,
$[D_1(g),\ D_1(h)]=0$, $[D_1(g)^*,\ D_1(h)^*]=0$;

(b) $[D_2(g),\ D_2(h)^*]=(h,\ g)\mathbf{1}$,
$[D_2(g),\ D_2(h)]=0$, $[D_2(g)^*,\ D_2(h)^*]=0$;

(c) $[D_1(g),\ D_2(h)]=0$, $[D_1(g),\ D_2(h)^*]=0$,
$[D_1(g)^*,\ D_2(h)]=0$, $[D_1(g)^*,\ D_2(h)^*]=0$.

Proof: The commutation relations on $\mathcal{W}\xi_0$ and $\mathcal{W}_0\xi_0$ in the proposition follow from Lemma 5.2 and (5.6). Thus we need to extend the relations to $\mathcal{H}_{\text{fin}}$. Recall the definition of $\Phi(f,\ n)$, $f\in\mathfrak{h}_0$, $n\in\mathbb{N}$, in (4.5). Using Lemma 4.2 and (3.2), it is not hard to check that for any $g,\ h,\ f_j,\ \in\mathfrak{h}_0,\ n_j\in\mathbb{N},\ j=1,\ldots,m$,

$$\Phi(g)\Phi(h)\left(\prod_{j=1}^{m}\Phi(f_j,n_j)\right)\xi_0\to\Phi(g)\Phi(h)\left(\prod_{j=1}^{m}\Phi(f_j)\right)\xi_0, \tag{5.7}$$

as $n_j\to\infty$, $j=1,\ldots,m$. This implies that the relations in the proposition extend to $\mathcal{H}_{\text{fin}}$. □

We are ready to decompose the Hilbert space $\mathcal{H}=\mathcal{H}_\omega$, called quasi-free Hilbert space. According to Lemma 5.1 and the CCRs in Proposition 5.1, $D_i(g)$ and $D_i(h)^*$, $g,\ h\in\mathfrak{h}_0$, $i=1, 2$, can be thought of as annihilation and creation operators, respectively. We remark that $h\mapsto D_1(h)^*$ is linear, but $g\to D_2(g)^*$ is conjugate linear. With an abuse of terminology, we call $D_1(h)^*$ and $D_2(h)^*$ the creation operators for quasi-particles and anti-quasi-particles, respectively, for $h\in\mathfrak{h}_0$. The following is the decomposition of $\mathcal{H}$.

Theorem 5.1: *The following decomposition holds:*

$$\mathcal{H}=\bigoplus_{m,n=0}^{\infty}\mathcal{H}^{(m,n)},$$

where for each $m,n\in\mathbb{N}\cup\{0\}$, $\mathcal{H}^{(m,n)}$ is the closure of the subspace spanned by the vectors of the form

$$\left(\prod_{j=1}^{m}D_1(g_j)^*\right)\left(\prod_{l=1}^{n}D_2(h_l)^*\right)\xi_0,\ g_j,\ h_l\in\mathfrak{h}_0.$$

In the case in which $m=0$ $(n=0)$, we replace the operator in the first (second) parentheses in the above by the identity.

Proof: It follows from (5.6) that any $\Phi(g), g\in\mathfrak{h}_0$, can be written as the sum of four $D_i(h)^\#$, $h\in\mathfrak{h}_0$, $i=1, 2$. Thus any $(\Pi_{l=1}^{m}\Phi(g_l))\xi_0$, $g_l\in\mathfrak{h}_0$, $l=1,\ldots,m$, can be expressed as a finite linear combination of the vectors of the form

$$\left(\prod_{j=1}^{p}D_1(g_j')^\#\right)\left(\prod_{l=1}^{q}D_2(h_l')^\#\right)\xi_0,\ g_j',\ h_l'\in\mathfrak{h}_0,$$

where $D_i^{\#}(g)$ is either $D_i(g)$ or $D_i^*(g)$, $i=1,2$. As a consequence of Lemma 5.1 and the CCRs in Proposition 5.1, the above vector can be expressed as a finite linear combination of the vector of the form

$$\left(\prod_{j=1}^{m'} D_1(g_j')^*\right)\left(\prod_{l=1}^{n'} D_2(h_l')^*\right)\xi_0,\ g_j',\ h_l' \in \mathfrak{h}_0,\ m',\ n' \in \mathbb{N}\cup\{0\}.$$

Since $\mathcal{H}_{\text{fin}}$ is dense in $\mathcal{H}$, we conclude that the set of finite linear combinations of the vectors of the above form is dense in $\mathcal{H}$. Thus the decomposition follows from Lemma 5.1 and the CCRs in Proposition 5.1. □

Recall that $\mathfrak{h}_0$ is a dense subspace of a complex Hilbert space $\mathfrak{h}$. Let $\mathcal{F}=\mathcal{F}(\mathfrak{h})$ be the symmetric Fock space over $\mathfrak{h}$, and $a(g)$ and $a^*(g)$, $g\in\mathfrak{h}_0$, the annihilation and creation operator, respectively. Denote by Ω the vacuum vector in $\mathcal{F}$. Let $C:\mathfrak{h}\to\mathfrak{h}$ be an anti-unitary operator. If $\mathfrak{h}$ is a L^2-space, one may consider that C is the complex conjugation. Denote by $\Gamma(C)$ the second quantization of C. See Sec. 5.2.1 of Ref. 2. Let $\mathcal{F}_1$, Ω_1, $a_1(g)$ and $a_1^*(g)$, $g\in\mathfrak{h}_0$ be the identical copies of $\mathcal{F}$, Ω, $a(g)$ and $a^*(g)$, $g\in\mathfrak{h}_0$, respectively. Notice that $\Gamma(C)a^{\#}(g)\Gamma(C)^{-1}=a^{\#}(Cg)$. We write that $\mathcal{F}_2=\Gamma(C)\mathcal{F}(=\mathcal{F})$, $\Omega_2=\Omega$, $a_2(g)=a(Cg)$, and $a_2^*(g)=a^*(Cg)$, $g\in\mathfrak{h}_0$. Then the following commutation relations hold: for $g,h\in\mathfrak{h}_0$,

$$\begin{aligned}[a_2(g),\ a_2^*(h)]&=(h,\ g)\mathbf{1},\\ [a_2(g),\ a_2(h)]&=0.\end{aligned}\tag{5.8}$$

One may compare the above relations to those in Proposition 5.1 (b).

Proposition 5.2: Let U be the operator defined by

$$U:\mathcal{H}\to\mathcal{F}_1\otimes\mathcal{F}_2,\left(\prod_{j=1}^{m} D_1(g_j)^*\right)\left(\prod_{l=1}^{n} D_2(h_l)^*\right)\xi_0\mapsto\left(\prod_{j=1}^{m} a_1^*(g_j)\right)\Omega_1\otimes\left(\prod_{l=1}^{n} a_2^*(h_l)\right)\Omega_2,$$

for g_j, $h_l\in\mathfrak{h}_0$, $j=1,\ldots,m$, $l=1,\ldots,n$. Then U is unitary.

Proof: Since $D_1^{\#}(g)$ and $a_1^{\#}(g)$, and $D_2^{\#}(g)$ and $a_2^{\#}(g)$ for $g\in\mathfrak{h}_0$ satisfy the same commutation relations, respectively, by Proposition 5.1 and (5.8), the unitarity of U follows from the fact that $a(g)\Omega=0$ for any $g\in\mathfrak{h}_0$. □

We next turn to the spectral analysis of $\overline{H}$, where $\overline{H}$ is the generator of the symmetric Markovian semigroup $\{T_t\}_{t\geqslant 0}$ associated to the Dirichlet form $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$.

Let us first describe the basic idea of the proof Theorem 3.2. Recall the definitions of $D_1(g)$ and $D_2(g)$ in (5.5). Let $\{f_n\}\subset\mathfrak{h}_0$ *be a CONS for* $\mathfrak{h}$. By Remark 4.1 and (5.5), we have that for any $g,h\in\mathfrak{h}_0$,

$$\begin{aligned}\overline{\mathcal{E}}(W(g)\xi_0,W(h)\xi_0)&=\sum_{n=1}^{\infty}\langle D_1(B^{1/2}f_n)W(g)\xi_0,\ D_1(B^{1/2}f_n)W(h)\xi_0\rangle\\ &\quad+\sum_{n=1}^{\infty}\langle D_2(B^{1/2}f_n)W(g)\xi_0,\ D_2(B^{1/2}f_n)W(h)\xi_0\rangle\\ &=\langle W(g)\xi_0,HW(h)\xi_0\rangle,\end{aligned}$$

where

$$H=\sum_{n=1}^{\infty}\{D_1^*(B^{1/2}f_n)D_1(B^{1/2}f_n)+D_2^*(B^{1/2}f_n)D_2(B^{1/2}f_n)\},\tag{5.9}$$

as a bilinear form on $\mathcal{W}\xi_0\times\mathcal{W}\xi_0$. By Proposition 5.2, one can see that H is unitary equivalent to sum of two second quantizations of B. If one can show that $\mathcal{H}_{\text{fin}}\subset D(\overline{H})$, $\overline{H}=H$ on $\mathcal{H}_{\text{fin}}$, and that $\mathcal{H}_{\text{fin}}$ is a core for $\overline{H}$, then one expects that the spectrum of $\overline{H}$ can be analyzed completely.

We first establish technical lemmas. Recall that $\mathcal{W}_0\xi_0\subset D(\overline{\mathcal{E}})$.

Lemma 5.3: $\mathcal{W}\xi_0\subset D(\overline{\mathcal{E}})$

Proof: Since $(\overline{\mathcal{E}},D(\overline{\mathcal{E}}))$ is closed and $\mathcal{W}_0\xi_0\subset D(\mathcal{E})$, it is sufficient to show that for any $g\in\mathfrak{h}_0$,

$$\overline{\mathcal{E}}[W_n(g)\xi_0-W(g)\xi_0]\to 0,\quad \text{as}\quad n\to\infty.$$

Notice that by Remark 4.1,

$$\begin{aligned}\overline{\mathcal{E}}[(W_n(g)-W(g))\xi_0]&=\sum_{m=1}^{\infty}\int\|\delta(\sigma_{\tau-i/4}(a(g_m)))(W_n(g)-W(g))\xi_0\|^2 f(\tau)\,d\tau\\&\quad+\sum_{m=1}^{\infty}\int\|\delta(\sigma_{\tau-i/4}(a^*(g_m)))(W_n(g)-W(g))\xi_0\|^2 f(\tau)\,d\tau\\&\equiv A_n^{(1)}+A_n^{(2)}.\end{aligned}$$

Employing the method similar to that used to derive (4.12), it is easy to show that

$$A_n^{(1)}=\frac{n}{2\pi}\int\int K(t_1,t_2,g)e^{-nt_1^2}e^{-nt_2^2}\,dt_1\,dt_2,$$

where

$$\begin{aligned}K(t_1,t_2,g)&=(A^{it_1}g,\,(A^{it_2}-\mathbf{1})A^{-1/2}g)\langle W(A^{it_1}g)\xi_0,W(A^{it_2}g)\xi_0\rangle\\&\quad+(A^{it_1}g,\,A^{-1/2}g)\langle W(A^{it_1}g)\xi_0,(W(A^{it_2}g)-W(g))\xi_0\rangle\\&\quad+(g,\,A^{-1/2}A^{it_2}g)\langle W(g)\xi_0,(W(g)-W(A^{it_2}g))\xi_0\rangle\\&\quad+(g,\,A^{-1/2}(\mathbf{1}-A^{it_2})g)\langle W(g)\xi_0,W(g)\xi_0\rangle.\end{aligned}$$

Notice that $K(t_1,\,t_2,\,g)$ is bounded uniformly with respect to $(t_1,\,t_2)\in\mathbb{R}^2$. Changing the variables $(t_1'=n^{1/2}t_1,\,t_2'=n^{1/2}t_2)$ and using the dominated convergence theorem, we conclude that

$$A_n^{(1)}\to 0,\quad \text{as}\quad n\to\infty.$$

By the similar calculation, we get that

$$A_n^{(2)}\to 0,\quad \text{as}\quad n\to\infty.$$

This proved the lemma completely. □

Lemma 5.4: (a) $\mathcal{H}_{\text{fin}}\subset D(\overline{\mathcal{E}})$.

(b) Let $\{g_n\}\subset\mathfrak{h}_0$ *be a CONS for* $\mathfrak{h}$. *Then for* $\xi\in\mathcal{H}_{\text{fin}}$ *the equality*

$$\overline{\mathcal{E}}[\xi]=\sum_{n=1}^{\infty}\{\|D_1(B^{1/2}g_n)\xi\|^2+\|D_2(B^{1/2}g_n)\xi\|^2\}\tag{5.10}$$

holds.

The proof of the above lemma will be given in the Appendix.

The following theorem is one of the main results in this section.

Theorem 5.2: *(a) Let* $H:\mathcal{H}_{\text{fin}}\to\mathcal{H}$ *be the operator defined by*

$$H\prod_{p=1}^{m} D_1(g_p)^*\prod_{q=1}^{n} D_2(h_q)^*\xi_0=\sum_{k=1}^{m}\prod_{p=1}^{k-1} D_1(g_p)^*D_1(Bg_k)^*\prod_{p=k+1}^{m} D_1(g_p)^*\prod_{q=1}^{n} D_2(h_q)^*\xi_0$$
$$+\sum_{k=1}^{n}\prod_{p=1}^{m} D_1(g_p)^*\prod_{q=1}^{k-1} D_2(h_q)^*D_2(Bh_k)^*\prod_{q=k+1}^{n} D_2(h_q)^*\xi_0, \tag{5.11}$$

for any $m,\ n\in\mathbb{N}\cup\{0\}$ *and* $g_p,\ h_q\in\mathfrak{h}_0$, $p=1,\ldots,m, q=1,\ldots,n$. *Then the relation*

$$\overline{\mathcal{E}}(\eta,\xi)=\langle\eta,\ H\xi\rangle$$

holds for any $\eta,\ \xi\in\mathcal{H}_{\mathrm{fin}}$.

(b) H is essential self-adjoint and the self-adjoint extension denoted by H again is equal to the Dirichlet operator $\overline{H}$.

Proof: (a) Let $(\mathcal{E}_1,\ \mathcal{H}_{\mathrm{fin}})$ be the form given by

$$\mathcal{E}_1[\xi]=\sum_{k=1}^{\infty}\|D_1(B^{1/2}f_k)\xi\|^2,$$

where $\{f_k\}$, $f_k\in\mathfrak{h}_0$ is a CONS for $\mathfrak{h}$. We write $H=H_1+H_2$, where the image under H_1 (resp., H_2) is defined by the first (resp., second) vector on the right hand side of (5.11). The CCRs in Proposition 5.1 (a) and Lemma 5.1 imply that

$$\mathcal{E}_1\left[\left(\prod_{j=1}^{m} D_1(g_j)^*\right)\xi_0\right]=\sum_{k=1}^{\infty}\sum_{p=1}^{m}\sum_{q=1}^{m}(B^{1/2}g_p,\ f_k)(f_k,\ B^{1/2}g_q)G(g_1,\ldots,\ g_m;\ p,q),$$

where

$$G(g_1,\ldots,\ g_m;\ p,\ q):=\left\langle\prod_{\tau=1}^{p-1} D_1(g_\tau)^*\prod_{\tau=p+1}^{m} D_1(g_\tau)^*\xi_0,\ \prod_{\tau=1}^{q-1} D_1(g_\tau)^*\prod_{\tau=q+1}^{m} D_1(g_\tau)^*\xi_0\right\rangle.$$

Using the Parserval relations and the fact that

$$\sum_{p=1}^{m}(g_p,\ Bg_q)G(g_1,\ldots,\ g_m;\ p,q)$$
$$=\left\langle D_1(Bg_q)\prod_{k=1}^{m} D_1(g_k)^*\xi_0,\ \prod_{k=1}^{q-1} D_1(g_q)^*\prod_{k=q+1}^{m} D_1(g_k)^*\xi_0\right\rangle,$$

we have that

$$\mathcal{E}_1\left[\prod_{j=1}^{m} D_1(g_j)^*\xi_0\right]=\sum_{q=1}^{m}\left\langle\prod_{j=1}^{m} D_1(g_j)^*\xi_0,\prod_{j=1}^{q-1} D_1(g_j)^*D_1(Bg_q)^*\prod_{j=q+1}^{m} D_1(g_j)^*\xi_0\right\rangle$$
$$=\left\langle\prod_{j=1}^{m} D_1(g_j)^*\xi_0,\ H_1\prod_{j=1}^{m} D_1(g_j)^*\xi_0\right\rangle.$$

Notice that $H_2=H-H_1$ commutes with $D_1(g)^*$ for any $g\in\mathfrak{h}_0$ by (5.11). Thus by the polarization identity, we proved that

$$\mathcal{E}_1(\eta,\ \xi)=\langle\eta,\ H_1\xi\rangle,$$

for any $\eta, \xi \in \mathcal{H}_{\text{fin}}$. The method similar to that used in the above implies that

$$\mathcal{E}_2(\eta, \xi) = \langle \eta, H_2 \xi \rangle,$$

for any $\eta, \xi \in \mathcal{H}_{\text{fin}}$. This proved the part (a) of the theorem.

(b) By Proposition 5.2, we have that

$$UHU^{-1} = d\Gamma_1(B) \otimes \mathbf{1} + \mathbf{1} \otimes d\Gamma_2(B), \tag{5.12}$$

where each i, $i=1, 2$, $d\Gamma_i(B)$ is the second quantization of B on $\mathcal{F}_i$. We remark that $d\Gamma_2(B)$ is anti-unitary equivalent to $d\Gamma_1(B)$. By Assumption 3.1, any $g \in \mathfrak{h}_0$ is an analytic vector for B, and so it is easy to check that $(\Pi_{j=1}^m a^*(g_j))\Omega$ is an analytic vector for $d\Gamma(B)$ for any $g_j \in \mathfrak{h}_0$, $j = 1, \ldots, m$. Thus it follows that any $\xi \in \mathcal{H}_{\text{fin}}$ is an analytic vector for H. Since $H\mathcal{H}_{\text{fin}} \subset \mathcal{H}_{\text{fin}}$ by (5.11) and since $H = \overline{H}$ on $\mathcal{H}_{\text{fin}}$ by part (a) of the theorem, it follows from Corollary 2 of Theorem X. 39 in Ref. 26 that H and $\overline{H}$ are essentially self-adjoint on $\mathcal{H}_{\text{fin}}$, and so $H = \overline{H}$. □

Finally we are able to produce the proof of Theorem 3.2.

Proof of Theorem 3.2: (a) and (b) follow from Theorem 5.2.

To show (c), recall $0 < A \leqslant \alpha \mathbf{1}$, $0 < \alpha < 1$. Since $B = A^{-1/2} - A^{1/2}$,

$$\inf \sigma(B) \geqslant \alpha^{-1/2} - \alpha^{1/2}.$$

It follows from the above lower bound and (5.12) that zero is a simple eigenvalue with eigenvector ξ_0 and

$$\inf(\sigma(H) - \{0\}) \geqslant \alpha^{-1/2} - \alpha^{1/2}.$$

Thus the Markovian semigroup $\{T_t\}_{t \geqslant 0}$ is ergodic. This completes the proof of Theorem 3.2. □

ACKNOWLEDGMENTS

This work was supported in Part by Korea Research Foundation (99-005-D00010), Korean Ministry of Education.

APPENDIX: PROOFS OF LEMMA 4.3 AND LEMMA 5.4

Proof of Lemma 4.3: (a) Let us prove the first bound. Recall the definition of $\Phi(f, n)$, $f \in \mathfrak{h}_0$, $n \in \mathbb{N}$, in (4.5). Notice that

$$\Phi(f, n) = \int_0^1 W\left(\frac{s}{n} f\right) \Phi(f) \, ds. \tag{A1}$$

It follows from (4.6) and (A1) that

$$\|\sigma_z(\Phi_m(f, n))\xi_0\|^2 = \left(\frac{m}{\pi}\right) \int \int \left(\int_0^1 \int_0^1 F(t_1, t_2, s_1, s_2; f, n) \, ds_1 \, ds_2 \right) \cdot e^{-m(t_1 - \bar{z})^2} e^{-m(t_2 - z)^2} dt_1 \, dt_2,$$

where

$$F(t_1, t_2, s_1, s_2; f, n) := \omega\left(\sigma_{t_1}(\Phi(f)) \sigma_{t_1}\left(W\left(-\frac{s_1}{n} f \right) \right) \sigma_{t_2}\left(W\left(\frac{s_2}{n} f \right) \right) \sigma_{t_2}(\Phi(f)) \right).$$

We use (4.4) and the fact that $\sigma_t(\Phi(f)) = \Phi(A^{it} f)$, etc., to obtain that

$$F(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)=\omega\Big(\Phi(A^{it_1}f)\Phi(A^{it_2}f)W\Big(-\frac{s_1}{n}A^{it_1}f\Big)W\Big(\frac{s_2}{n}A^{it_2}f\Big)\Big)$$
$$+\frac{s_1}{n}\mathrm{Im}\,(A^{it_1}f,A^{it_2}f)\,\omega\Big(\Phi(A^{it_1}f)W\Big(-\frac{s_1}{n}A^{it_1}f\Big)W\Big(\frac{s_2}{n}A^{it_2}f\Big)\Big).$$

Iterating (4.2) and then using (4.1), (3.1) and (3.2), the above function can be calculated explicitly. More precisely, let us use (4.2) iteratively in the above to obtain that

$$F(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)=\sum_{k=1}^{7}F^{(k)}(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n),$$

where

$$F^{(1)}(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)=\omega(\Phi(A^{it_1}f)\Phi(A^{it_2}f))\omega\Big(W\Big(-\frac{s_1}{n}A^{it_1}f\Big)W\Big(\frac{s_2}{n}A^{it_2}f\Big)\Big),$$

and appropriate expressions for $F^{(k)}(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)$, $k=2,\ldots,7$. It follows from (4.1), (3.1) and (3.2) that

$$F^{(1)}(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)=\tfrac{1}{2}((f,\,(\mathbf{1}-A)^{-1}A^{-it_1}A^{it_2}f)+(f,\,A(\mathbf{1}-A)^{-1}A^{it_1}A^{-it_2}f))$$
$$\cdot\exp\Big\{\frac{i}{2}\mathrm{Im}\Big(f,\,\frac{s_1}{n}\frac{s_2}{n}A^{-it_1}A^{it_2}f\Big)\Big\}$$
$$\cdot\exp\Big\{-\frac{1}{4}\Big(\Big(\frac{s_2}{n}A^{it_2}-\frac{s_1}{n}A^{it_1}\Big)f,\,D\Big(\frac{s_2}{n}A^{it_2}-\frac{s_1}{n}A^{it_1}\Big)f\Big)\Big\},$$

where $D=(\mathbf{1}+A)(\mathbf{1}-A)^{-1}$. By Assumption 3.1, $F^{(1)}$ has an analytic extension on $\mathbb{C}\times\mathbb{C}$ in t_1 and t_2 variables. From the above expression, it is easy to see that there exists a constant $C_1(f,\mathrm{Im}\,z)$ independent of n such that

$$\sup_{s_1,s_2\in[0,1]}|F^{(1)}(t_1+\overline{z},\,t_2+z,\,s_1,\,s_2;\,f,\,n)|\leqslant C_1(f,\mathrm{Im}\,z),$$

for any $n\in\mathbb{N}$. Using the Cauchy integral theorem and the above bound, we conclude that the contribution of $F^{(1)}$ in F is bounded by $C_1(f,\mathrm{Im}\,z)$. Now, it is obvious that the function $F(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)$ has an analytic extension on $\mathbb{C}\times\mathbb{C}$ in t_1 and t_2 variables and there exists a constant $M_1(f,\mathrm{Im}\,z)$ depending only on $f\in\mathfrak{h}_0$ and $\mathrm{Im}\,z$ such that the bound similar to that in the above holds. We use the Cauchy integral theorem to conclude that

$$\|\sigma_z(\Phi_m(f,\,n))\xi_0\|^2=\Big(\frac{m}{\pi}\Big)\int\int\Big(\int_0^1\int_0^1F(t_1+\overline{z},\,t_2+z,\,s_1,\,s_2;\,f,\,n)ds_1\,ds_2\Big)$$
$$\cdot e^{-mt_1^2}e^{-mt_2^2}dt_1\,dt_2\leqslant M_1(f,\,\mathrm{Im}\;z)^2.$$

We leave the details to the reader.

We next consider the second bound. It follows from (4.1) that

$$\omega(a^*(f)a(g))=(g,\,A(\mathbf{1}-A)^{-1}f),\tag{A2}$$
$$\omega(a(g)a^*(f))=(g,\,(\mathbf{1}-A)^{-1}f).$$

A direct computation yields that

$$\|\sigma_z(\Phi(f))\xi_0\|^2 = \tfrac{1}{2}(\omega(a^*(A^{i\overline{z}}f)a(A^{i\overline{z}}f)) + \omega(a(A^{iz}f)a^*(A^{iz}f))).$$

Thus the bound follows from (A2) and the above result.

(b) Notice that

$$\begin{aligned}\|\sigma_z(\Phi_n(f,\,n))\xi_0 - \sigma_z(\Phi(f))\xi_0\| &\leqslant \|\sigma_z(\Phi_n(f,\,n))\xi_0 - \sigma_z(\Phi_n(f))\xi_0\| \\ &\quad + \|\sigma_z(\Phi_n(f))\xi_0 - \sigma_z(\Phi(f))\xi_0\| \\ &\equiv A_n^{(1)} + A_n^{(2)}. \end{aligned} \tag{A3}$$

It follows from (4.5) and (A1) that

$$(A_n^{(1)})^2 = \left(\frac{n}{\pi}\right)\int\int\left(\int_0^1\int_0^1 G(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)\,ds_1\,ds_2\right)\cdot e^{-n(t_1-\overline{z})^2}e^{-n(t_2-z)^2}\,dt_1\,dt_2,$$

where

$$G(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n) := \omega\left(\Phi(A^{it_1}f)\left(W\left(-\frac{s_1}{n}A^{it_1}f\right)-\mathbf{1}\right)\left(W\left(\frac{s_2}{n}A^{it_2}f\right)-\mathbf{1}\right)\Phi(A^{it_2}f)\right). \tag{A4}$$

Notice that for $s,\,t\in\mathbb{R}$,

$$W\left(\frac{s}{n}A^{it}f\right)-\mathbf{1} = i\frac{s}{n}\Phi(A^{it}f)\int_0^1 W\left(\frac{s\tau}{n}A^{it}f\right)d\tau. \tag{A5}$$

We substitute (A5) into (A4). Iterating (4.2), and then using (4.1) and (3.2), the function given in (A4) can be calculated explicitly. Using Assumption 3.1, it can be proved that $G(t_1,\,t_2,\,s_1,\,s_2;\,f,\,n)$ has an analytic extension on $\mathbb{C}\times\mathbb{C}$ in the t_1 and t_2 variables. By using the method similar to that used in the proof of the part (a) of the lemma, it is not hard to check that there exists constant $C_2(f,\,\mathrm{Im}\,z)$ such that

$$\sup_{s_1,s_2\in[0,1]}|G(t_1+\overline{z},\,t_2+z,\,s_1,\,s_2;\,f,\,n)| \leqslant \frac{1}{n^2}C_2(f,\,\mathrm{Im}\quad z).$$

It follows from the Cauchy integral theorem and the above bound that

$$(A_n^{(1)})^2 \to 0, \quad \text{as } n\to\infty.$$

We leave again the details to the reader.

Next, consider $A_n^{(2)}$ defined in (A3). Notice that

$$(A_n^{(2)})^2 = \left(\frac{n}{\pi}\right)\int\int\widetilde{G}(t_1,\,t_2;\,f)e^{-n(t_1-\overline{z})^2}e^{-n(t_2-z)^2}\,dt_1\,dt_2,$$

where

$$\widetilde{G}(t_1,\,t_2;\,f) = \omega((\Phi(A^{it_1}f)-\sigma_{\overline{z}}(\Phi(f)))(\Phi(A^{it_2}f)-\sigma_z(\Phi(f)))).$$

We use (A2) to obtain that

$$\begin{aligned}\tilde{G}(t_1,t_2;f) &= \tfrac{1}{2}\omega(\{a(A^{it_1}f)-a(A^{iz}f)\}\{a^*(A^{it_2}f)-a^*(A^{iz}f)\})\\ &\quad+\tfrac{1}{2}\omega(\{a^*(A^{it_1}f)-a^*(A^{i\bar{z}}f)\}\{a(A^{it_2}f)-a(A^{i\bar{z}}f)\})\\ &= \tfrac{1}{2}((A^{it_1}-A^{iz})f,\ (\mathbf{1}-A)^{-1}(A^{it_2}-A^{iz})f)\\ &\quad+\tfrac{1}{2}((A^{it_2}-A^{i\bar{z}})f,\ A(\mathbf{1}-A)^{-1}(A^{it_1}-A^{i\bar{z}})f).\end{aligned}$$

Thus $\tilde{G}(t_1,tt_2;\ f)$ has an analytic extension on $\mathbb{C}\times\mathbb{C}$ in the t_1 and t_2 variables and

$$\begin{aligned}\tilde{G}(t_1+\bar{z},\ t_2+z;\ f) &= \tfrac{1}{2}(f,\ (\mathbf{1}-A)^{-1}(A^{-it_1}-\mathbf{1})(A^{it_2}-\mathbf{1})A^{-i\bar{z}}A^{iz}f)\\ &\quad+\tfrac{1}{2}(f,\ A(\mathbf{1}-A)^{-1}(A^{it_1}-\mathbf{1})(A^{-it_2}-\mathbf{1})A^{-iz}A^{i\bar{z}}f).\end{aligned}\tag{A6}$$

We use the Cauchy integral theorem to get

$$(A_n^{(2)})^2=\left(\frac{n}{\pi}\right)\int\int \tilde{G}(t_1+\bar{z},\ t_2+z;\ f)e^{-nt_1^2}e^{-nt_2^2}\,dt_1dt_2.$$

By (A6), $\tilde{G}(t_1+\bar{z},\ t_2+z;\ f)$ is bounded uniformly with respect to $(t_1,\ t_2)\in\mathbb{R}^2$. Changing the variables ($t_1'=n^{1/2}t_1$ and $t_2'=n^{1/2}t_2$) and using the dominated convergence theorem, we conclude that

$$A_n^{(2)}\to 0,\quad \text{as}\ \ n\to\infty.$$

This proved the part (b) of the lemma completely. □

Proof of Lemma 5.4: (a) Recall the definition of $\Phi(f,\ n)$ in (4.5) for any $f\in\mathfrak{h}_0$ and $n\in\mathbb{N}$. For given (fixed) $m\in\mathbb{N}\cup\{0\}$ and $h_l\in\mathfrak{h}_0,\ l=1,\ldots,m$ we will use the following abbreviated notations:

$$\begin{gathered}\Phi_l(n):=\Phi(h_l,\ n),\ l=1,\ldots,m,\\ \Phi_l:=\Phi(h_l),\ l=1,\ldots,m,\\ \xi(n):=\left(\prod_{l=1}^{m}\Phi_l(n)\right)\xi_0,\ \text{and}\ \ \xi:=\left(\prod_{l=1}^{m}\Phi_l\right)\xi_0.\end{gathered}\tag{A7}$$

Notice that $\xi(n)\in\mathcal{W}\xi_0,\ n\in\mathbb{N}$ and $\xi\in\mathcal{H}_{\text{fin}}$. It is not hard to show that $\xi(n)\to\xi$ as $n\to\infty$. See the method used below. We will show that $\overline{\mathcal{E}}[\xi(n)-\xi]\to 0$ as $n\to\infty$. Since $\overline{\mathcal{E}}$ is closed, this implies that $\mathcal{H}_{\text{fin}}\subset D(\overline{\mathcal{E}})$ and

$$\overline{\mathcal{E}}[\xi]=\lim_{n\to\infty}\overline{\mathcal{E}}[\xi(n)].\tag{A8}$$

By Remark 4.1 and (5.5), the relation (5.10) holds for $\xi\in\mathcal{W}\xi_0$. Let ξ and $\xi(n),\ n\in\mathbb{N}$ be defined as in (A7). Notice that

$$\xi(n)-\xi=\sum_{p=1}^{m}\left(\prod_{l=1}^{p-1}\Phi_l(n)\right)(\Phi_p(n)-\Phi_p)\left(\prod_{l=p+1}^{m}\Phi_l\right)\xi_0.$$

We use the Schwarz inequality twice to obtain that

$$\|D_1(B^{1/2}g_k)(\xi(n)-\xi)\|^2 \leq m\sum_{p=1}^{m}\left\|D_1(B^{1/2}g_k)\left(\prod_{l=1}^{p-1}\Phi_l(n)\right)(\Phi_p(n)-\Phi_p)\left(\prod_{l=p+1}^{m}\Phi_l\right)\xi_0\right\|^2. \tag{A9}$$

Recall that $D_1(B^{1/2}g_k)=a(A^{-1/4}g_k)-j(\sigma_{-i/2}(a(A^{-1/4}g_k)))$. It follows from the CCRs and Lemma 5.1 that

$$D_1(B^{1/2}g_k)\left(\prod_{l=1}^{p-1}\Phi_l(n)\right)(\Phi_p(n)-\Phi_p)\left(\prod_{l=p+1}^{m}\Phi_l\right)\xi_0=\frac{1}{\sqrt{2}}\sum_{q=1}^{m}(g_k, A^{-1/4}h_q)\Psi^{(m)}(p, q; n), \tag{A10}$$

where

$$\Psi^{(m)}(p, q; n):=\left(\prod_{l=1}^{q-1}\Phi_l(n)\right)W\left(\frac{1}{n}h_q\right)\left(\prod_{l=q+1}^{p-1}\Phi_l(n)\right)\cdot(\Phi_p(n)-\Phi_p)\left(\prod_{l=p+1}^{m}\Phi_l\right)\xi_0,$$

$$1\leq q\leq p-1,$$

$$\Psi^{(m)}(p, q; n):=\left(\prod_{l=1}^{p-1}\Phi_l(n)\right)\left(W\left(\frac{1}{n}h_p\right)-\mathbf{1}\right)\left(\prod_{l=p+1}^{m}\Phi_l\right)\xi_0, \quad q=p,$$

$$\Psi^{(m)}(p, q; n):=\left(\prod_{l=1}^{p-1}\Phi_l(n)\right)(\Phi_p(n)-\Phi_p)\left(\prod_{l=p+1}^{q-1}\Phi_l(n)\right)\cdot\left(\prod_{l=q+1}^{m}\Phi_l\right)\xi_0, \quad p+1\leq q\leq m.$$

We use the Schwarz inequality twice again to (A10) and substitute the result into (A9) to conclude that

$$\|D_1(B^{1/2}g_k)(\xi(n)-\xi)\|^2\leq\frac{1}{2}m^2\sum_{p=1}^{m}\sum_{q=1}^{m}|(g_k, A^{-1/4}h_q)|^2\|\Psi^{(m)}(p, q; n)\|^2.$$

Using the Parserval relation, we obtain that

$$\sum_{k=1}^{\infty}\|D_1(B^{1/2}g_k)(\xi(n)-\xi)\|^2\leq\frac{1}{2}m^2\sum_{p=1}^{m}\sum_{q=1}^{m}\|A^{-1/4}h_q\|^2\|\Psi^{(m)}(p, q; n)\|^2. \tag{A11}$$

Iterating (4.2), $\|\Psi^{(m)}(p, q; n)\|^2$ can be calculated explicitly for any p, q and n. One notes that each $\Psi^{(m)}(p, q; n)$ contains either $(\Phi_p(n)-\Phi_p)$ or else $(W(1/n\,h_p)-\mathbf{1})$, which implies that

$$\|\Psi^{(m)}(p, q; n)\|^2\to 0, \text{ as } n\to\infty,$$

for any p, q. Thus it follows from (A11) that

$$\sum_{k=1}^{\infty}\|D_1(B^{1/2}g_k)(\xi(n)-\xi)\|^2\to 0, \text{ as } n\to\infty.$$

The method similar to that used in the above implies that

$$\sum_{k=1}^{\infty}\|D_2(B^{1/2}g_k)(\xi(n)-\xi)\|^2\to 0, \quad \text{as } n\to\infty.$$

This proved part (a) of this lemma.

(b) This follows from (5.9) and (A8). □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Finite growth representations of infinite Lie conformal algebras

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(Received 25 September 2002; accepted 28 October 2002)

We classify all finite growth representations of all infinite rank subalgebras of the Lie conformal algebra gc_1 that contain a Virasoro subalgebra. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1534890]

I. INTRODUCTION

In this paper we study representation theory of some infinite rank subalgebras of the Lie conformal algebra gc_1 associated to the Lie algebra $\mathcal{D}$ of differential operators on the circle. Recall that $gc_1=\mathbb{C}[\partial,x]$, with λ-bracket given by (see Refs. 3 and 7)

$$[a(\partial,x)_\lambda b(\partial,x)]=a(-\lambda,\lambda+\partial+x)b(\lambda+\partial,x)-b(\lambda+\partial,-\lambda+x)a(-\lambda,x).$$

Also recall that the *Virasoro conformal algebra* (which is particularly important in physics) is defined as the free $\mathbb{C}[\partial]$-module of rank 1 generated by an element L, with λ-bracket defined by

$$[L_\lambda L]=(2\lambda+\partial)L,$$

and extended to $\mathbb{C}[\partial]L$ using sesquilinearity. Observe that all Virasoro subalgebras of gc_1 are generated by

$$L=x+\alpha\partial, \quad \alpha\in\mathbb{C}.$$

The complete list of infinite rank proper subalgebras of gc_1 that contain a Virasoro subalgebra is (see Ref. 3 and Remark 3.10 in Ref. 5):

$$gc_{1,x}=x\,\mathbb{C}[\partial,x],$$

$$oc_1=\{a(\partial,x)-a(\partial,-\partial-x)\mid a(\partial,x)\in\mathbb{C}[\partial,x]\},$$

$$spc_1=\{x[a(\partial,x)+a(\partial,-\partial-x)]\mid a(\partial,x)\in\mathbb{C}[\partial,x]\},$$

where the Virasoro element is $x+\alpha\partial$, with $\alpha=0,\frac{1}{2},0$, respectively. They are the most important gc_1-subalgebras from the point of view of physics.

In the present paper we classify all finite growth representations of all infinite rank conformal subalgebras of gc_1 that contain a Virasoro subalgebra.

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This problem reduces to the study of finite growth representations on the corresponding extended annihilation algebras, which are certain subalgebras of $\mathcal{D}$ (see Ref. 7). The main tools used here are the recent results (Refs. 1, 4, 9–11) on the classification of quasifinite highest weight modules over the central extension of $\mathcal{D}$ and some of its important subalgebras.

The paper is organized as follows. In Sec. II, we describe the infinite rank Lie algebra $\widehat{g\ell}_{\infty}^{[m]}$ and its classical subalgebras, and discuss their representation theory that will be needed. In Secs. III–VI, we obtain the classification of all finite growth representations of gc_1, $gc_{1,x}$, oc_1, and spc_1 respectively.

II. LIE ALGEBRA $\widehat{g\ell}_{\infty}^{[m]}$ AND ITS CLASSICAL SUBALGEBRAS

A. Lie algebra $\widehat{g\ell}_{\infty}^{[m]}$

Denote by $\mathbb{C}^{+\infty}$ the set of all sequences $\lambda=(\lambda_1,\lambda_2,\ldots)$ for which all but a finite number of λ_i's are zero, and let $d(\lambda)$ denote the number of nonzero λ_i's and $|\lambda|$ denote their sum. Denote by Par^+ the subset of $\mathbb{C}^{+\infty}$ consisting of nonincreasing sequences of (non-negative) integers.

Denote by $g\ell_{+\infty}$ the Lie algebra of all matrices $(a_{ij})_{i,j=1}^{+\infty}$ with a finite number of nonzero entries $a_{ij}\in\mathbb{C}$. Given $\lambda\in\mathbb{C}^{+\infty}$, there exists a unique irreducible $g\ell_{+\infty}$-module $L^+(\lambda)$, also denoted by $L(g\ell_{+\infty};\lambda)$, which admits a nonzero vector v_λ such that

$$E_{ij}v_\lambda=0 \quad \text{for} \quad i<j \quad \text{and} \quad E_{ii}v_\lambda=\lambda_i v_\lambda\,. \tag{2.1}$$

Here and further E_{ij} denotes, as usual, the matrix whose (i,j)-entry is 1 and all other entries are 0. Each $L^+(\lambda)$ has a unique $\mathbb{Z}_+$-gradation. $L^+(\lambda)=\oplus_{j\in\mathbb{Z}_+}L^+(\lambda)_j$, called its *principal gradation*, which satisfies the properties

$$L^+(\lambda)_0=\mathbb{C}v_\lambda\,,\quad E_{ij}L^+(\lambda)_k\subset L^+(\lambda)_{k+i-j}\,.$$

Since $\lambda\in\mathbb{C}^{+\infty}$, it is easy to see that $\dim L^+(\lambda)_j<\infty$, hence we can define the q-character

$$\mathrm{ch}_q L^+(\lambda)=\sum_{j\in\mathbb{Z}_+}(\dim L^+(\lambda)_j)q^j\,.$$

For $\lambda\in\mathrm{Par}^+$, let $d=d(\lambda)$ and $\overline{\lambda}=(\lambda_1,\ldots,\lambda_d)$. Let $g\ell_d$ be the Lie algebra of all $d\times d$ matrices $(a_{ij})_{i,j=1}^d$; it may be viewed as a subalgebra of $g\ell_{+\infty}$ in a natural way. Denote by $\overline{L^+}(\overline{\lambda})$ the (irreducible) $g\ell_d$-submodule of $L^+(\lambda)$ generated by v_λ. It is, of course, isomorphic to the finite-dimensional irreducible $g\ell_d$-module associated to $\overline{\lambda}$, so that its q-character is a (well-known) polynomial in q.

Lemma 2.1: Let $\lambda\in\mathrm{Par}^+, d=d(\lambda)$. *Then*

$$\mathrm{ch}_q L^+(\lambda)=\mathrm{ch}_q\overline{L^+}(\overline{\lambda})\Big/\prod_{j=1}^{d}(1-q^j)_q^{\lambda_{d-j+1}}\,,$$

where $(1-a)_q^m=(1-a)(1-qa)\cdots(1-q^{m-1}a)$.

Proof: Recall the well-known formula (see Ref. 6):

$$\mathrm{ch}_q L^+(\lambda)=\prod_{\alpha>0}(1-q^{\langle\lambda+\rho,\alpha\rangle})/(1-q^{\langle\rho,\alpha\rangle})\,. \tag{2.2}$$

Here the product is taken over the set of all positive coroots of $g\ell_{+\infty}$, which are all elements $E_{ii}-E_{jj}$ with $i<j$, $\langle\lambda,E_{ii}\rangle=\lambda_i$ and $\langle\rho,E_{ii}\rangle=-i$. Of course, a similar formula holds for $\mathrm{ch}_q\overline{L^+}(\overline{\lambda})$; it is a part of the product (2.2) corresponding to $i<j\leqslant d$.

It is also clear that the factors of (2.2) corresponding to $d<i<j$ are equal to 1, and it is easy to see that the product over all pairs i, j with fixed $i\leqslant d$ and all $j>d$ is equal to $1/(1-q^{d-i+1})_q^{\lambda_i}$.

□

Recall that, given a vector space V with an increasing filtration by finite-dimensional subspaces $V_{[j]}$, the *growth* of V is defined by

$$\text{growth}\, V=\overline{\lim_{j\to+\infty}}\,(\log\dim V_{[j]})/\log j\,.$$

We define the growth of $L^+(\lambda)$ using its filtration $L^+(\lambda)_{[j]}=\oplus_{i\leqslant j}L^+(\lambda)_i$ associated to the principal gradation.

Theorem 2.2: (*a*) *If* $\lambda\in\text{Par}^+$, *then*

$$\text{growth}\, L^+(\lambda)=|\lambda|\,.$$

(*b*) *If* $\lambda\in\mathbb{C}^{+\infty}\backslash\text{Par}^+$, *then* growth$L^+(\lambda)=\infty$.

Proof: It follows from Lemma 2.1 that for $\lambda\in\text{Par}^+$, growth$L^+(\lambda)$ is equal to the growth of the polynomial algebra on generators of degree $1,2,\ldots,\lambda_s$; $2,3,\ldots,\lambda_{s-1}+1$; ...; $s,s+1,\ldots,\lambda_1+s-1$. The total number of these generators is $|\lambda|$, and since growth of a polynomial algebra is independent of the degrees of generators, (a) is proved.

Let now $\lambda\in\mathbb{C}^{+\infty}\backslash\text{Par}^+$. Then $\lambda_k-\lambda_{k+1}\notin\mathbb{Z}_+$ for some k. But then $E_{k+1,k}^N v_\lambda\neq 0$ for each $N\in\mathbb{Z}_+$. Looking at the subalgebra of $g\ell_{+\infty}$ spanned by all E_{ij} with $i,j\geqslant k+1$, we conclude from (a) that

$$\text{growth}\, L^+(\lambda)\geqslant N+\sum_{i\geqslant k+1}\lambda_i\,.$$

This proves (b). □

In a similar fashion one may consider the Lie algebra $g\ell_{-\infty}$ of all matrices $(a_{ij})_{i,j=0}^{-\infty}$ with a finite number of nonzero entries and the irreducible $g\ell_{-\infty}$-modules $L^-(\lambda)$, also denoted by $L(g\ell_{-\infty};\lambda)$, parametrized by the set $\mathbb{C}^{-\infty}$ of sequences $\mu=(\ldots,\mu_{-1},\mu_0)$ with finitely many nonzero members. Results similar to Lemma 2.1 and Theorem 2.2 hold for the subset $\text{Par}^-\subset\mathbb{C}^{-\infty}$ consisting of nonincreasing sequences of (nonpositive) integers.

Let $\widetilde{g\ell}_\infty$ denote the Lie algebra of all matrices $(a_{ij})_{i,j\in\mathbb{Z}}$ such that $a_{ij}=0$ if $|i-j|\gg 0$. Denote by $\widetilde{g\ell}_{+\infty}$ (respectively, $\widetilde{g\ell}_{-\infty}$) the subalgebra of $\widetilde{g\ell}_\infty$ consisting of matrices with $a_{ij}=0$ for i or $j\leqslant 0$ (respectively, i or $j>0$). Note that these two subalgebras commute and that $\widetilde{g\ell}_{\pm\infty}$ contains $g\ell_{\pm\infty}$ as a subalgebra. Note also that the $g\ell_{\pm\infty}$-modules $L^\pm(\lambda)$ extend uniquely to $\widetilde{g\ell}_{\pm\infty}$.

The Lie algebra $\widetilde{g\ell}_\infty$ has a well-known central extension $\widehat{g\ell}_\infty=\widetilde{g\ell}+\mathbb{C}C$ by $\mathbb{C}$ defined by the cocycle

$$\alpha(A,B)=\text{tr}[J,A]B\,,\quad\text{where}\quad J=\sum_{i\leqslant 0}E_{ii}\,.\tag{2.3}$$

The restriction of this cocycle to $\widetilde{g\ell}_{+\infty}$ and to $\widetilde{g\ell}_{-\infty}$ is zero.

We will also need briefly the Lie algebra $\widehat{g\ell}_\infty^{[m]}$ defined for each $m\in\mathbb{Z}_+$ by replacing $\mathbb{C}$ by $R_m=\mathbb{C}[u]/(u^{m+1})$. That is, $\widehat{g\ell}_\infty^{[m]}=\widetilde{g\ell}_\infty^{[m]}\oplus R_m$ is the central extension of $\widetilde{g\ell}_\infty^{[m]}$ by the 2-cocycle (2.3) with values in R_m, where $\widetilde{g\ell}_\infty^{[m]}$ is the Lie algebra of infinite matrices with finitely many nonzero diagonals with entries in R_m.

The principal $\mathbb{Z}$-gradation of all the above Lie algebras is defined by letting

$$\deg E_{ij}=i-j\tag{2.4}$$

(in the case of $\widehat{g\ell}_\infty^{[m]}$ we also let $\deg R_m=0$). This gives us a triangular decomposition

$$\widehat{g\ell}_\infty^{[m]}=(\widehat{g\ell}_\infty^{[m]})_+\oplus(\widehat{g\ell}_\infty^{[m]})_0\oplus(\widehat{g\ell}_\infty^{[m]})_-,$$

where

$$(\widehat{g\ell}_\infty^{[m]})_\pm=\oplus_{j\in\mathbb{N}}(\widehat{g\ell}_\infty^{[m]})_{\pm j}.$$

The Lie algebra $\widehat{g\ell}_\infty$ has a family of modules $L(\widehat{g\ell}_\infty;\lambda,c)$, parametrized by $\lambda\in\mathbb{C}^\infty=\{(\lambda_i)_{i\in\mathbb{Z}}|$ all but finitely many of λ_i are $0\}$ and $c\in\mathbb{C}$, defined by (2.1) and $Cv_\lambda=cv_\lambda$. Similarly, $\widehat{g\ell}_\infty^{[m]}$ has a family of modules $L(\widehat{g\ell}_\infty^{[m]};\vec{\lambda},\vec{c})$, where $\vec{\lambda}\in(\mathbb{C}^\infty)^{m+1}$, $\vec{c}\in\mathbb{C}^{m+1}$, defined in a similar fashion. That is, the highest weight $\widehat{g\ell}_\infty^{[m]}$-module $L(\widehat{g\ell}_\infty^{[m]};\Lambda)$, with highest weight $\Lambda\in(\widehat{g\ell}_\infty^{[m]})_0^*$ that is determined by its *labels* $\vec{\lambda}_i^{(j)}=\Lambda(u^jE_{ii})$ and the *central charges* $\vec{c}_j=\Lambda(u^j)$.

The gradation (2.4) is obviously consistent with the principal gradation of $L^\pm(\lambda)$ and of $L(\widehat{g\ell}_\infty;\lambda,c)$.

B. Lie algebras $b_\infty^{[m]}$ and $d_\infty^{[m]}$

The Lie algebra $\widetilde{g\ell}_\infty^{[m]}$ acts on the vector space $R_m[t,t^{-1}]$ via the usual formula

$$E_{ij}v_k=\delta_{j,k}v_i,$$

where $v_i=t^{-i}$, $i\in\mathbb{Z}$ is an R_m basis. Now consider the following $\mathbb{C}$-bilinear forms on this space:

$$B(u^mv_i,u^nv_j)=u^m(-u^n)\delta_{i,-j},$$

$$D(u^mv_i,u^nv_j)=u^m(-u^n)\delta_{i,1-j}.$$

Denote by $\overline{b}_\infty^{[m]}$ (respectively, $\overline{d}_\infty^{[m]}$) the Lie subalgebra of $\tilde{g}\ell_\infty^{[m]}$ which preserves the bilinear form B (respectively, D). We have

$$\overline{b}_\infty^{[m]}=\{(a_{ij}(u))_{i,j\in\mathbb{Z}}\in\widetilde{g\ell}_\infty^{[m]}\,|\,a_{ij}(u)=-a_{-j,-i}(-u)\},$$

$$\overline{d}_\infty^{[m]}=\{(a_{ij}(u))_{i,j\in\mathbb{Z}}\in\widetilde{g\ell}_\infty^{[m]}\,|\,a_{ij}(u)=-a_{1-j,1-i}(u)\}.$$

Denote by $b_\infty^{[m]}=\overline{b}_\infty^{[m]}\oplus R_m$ (respectively, $d_\infty^{[m]}=\overline{d}_\infty^{[m]}\oplus R_m$) the central extension of $\overline{b}_\infty^{[m]}$ (respectively, $\overline{d}_\infty^{[m]}$) given by the 2-cocycle defined in $\widetilde{g\ell}_\infty^{[m]}$. Both subalgebras inherit the form $\widehat{g\ell}_\infty^{[m]}$ the principal $\mathbb{Z}$-gradation and the triangular decomposition, (see Refs. 11 and 6 for notation)

$$b_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(b_\infty^{[m]})_j,\quad b_\infty^{[m]}=(b_\infty^{[m]})_+\oplus(b_\infty^{[m]})_0\oplus(b_\infty^{[m]})_-,$$

$$d_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(d_\infty^{[m]})_j,\quad d_\infty^{[m]}=(d_\infty^{[m]})_+\oplus(d_\infty^{[m]})_0\oplus(d_\infty^{[m]})_-.$$

In particular when $m=0$, we have the usual Lie subalgebras of $\widehat{g\ell}_\infty$, denoted by b_∞ (respectively, d_∞).

Denote by $L(b_\infty^{[m]};\lambda)$ [respectively, $L(d_\infty^{[m]};\lambda)$] the highest weight module over $b_\infty^{[m]}$ (respectively, $d_\infty^{[m]}$) with highest weight $\lambda\in(b_\infty^{[m]})_0^*$ [respectively $\lambda\in(d_\infty^{[m]})_0^*$] parametrized by ${}^b\vec{\lambda}\in(\mathbb{C}^\infty)^{m+1}$, $\vec{c}\in\mathbb{C}^{m+1}$, with

$$\vec{c}_i=\lambda(u^i),$$

$${}^b\vec{\lambda}_j^{(i)}=\lambda(u^iE_{j,j}-(-u)^iE_{-j,-j}),$$

[respectively, ${}^d\vec{\lambda}\in(\mathbb{C}^\infty)^{m+1}$, with ${}^d\vec{\lambda}_j^{(i)}=\lambda(u^iE_{j,j}-(-u)^iE_{1-j,1-j})$]. The superscripts b and d here mean B and D type, respectively. The ${}^b\vec{\lambda}_j^{(i)}$ (respectively, ${}^d\vec{\lambda}_j^{(i)}$) are called the labels and $\vec{c}_j$ the central charges of $L(b_\infty^{[m]};\lambda)$ [respectively, $L(d_\infty^{[m]};\lambda)$].

All these modules will appear in Sec. V. Now, we are interested in representation theory of b_∞.

The set of simple coroots of b_∞, can be described as follows [cf. Ref. 11]:

$$\Pi^\vee=\{\alpha_0{}^\vee=2(E_{-1,-1}-E_{1,1})+2C,$$

$$\alpha_i{}^\vee=E_{i,i}-E_{i+1,i+1}-E_{-i,-i}+E_{-1-i,-1-i},\ i\in\mathbb{N}\}.$$

The set of roots is

$$\Delta=\{\pm\varepsilon_0,\ \pm\varepsilon_i,\ \pm\varepsilon_i\pm\varepsilon_j,\ i\neq j,\ i,j\in\mathbb{N}\}.$$

The set of positive coroots is

$$\Delta_+{}^\vee=\{\alpha_i{}^\vee+\alpha_{i+1}{}^\vee+\cdots+\alpha_j{}^\vee,\ 0\leqslant i\leqslant j\}\cup\{\alpha_0{}^\vee+2\alpha_1{}^\vee+\cdots+2\alpha_i{}^\vee+\alpha_{i+1}{}^\vee+\cdots+\alpha_{j-1}{}^\vee,\ 1\leqslant i<j\}.$$

The set of simple roots

$$\Pi=\{\alpha_0=-\varepsilon_1,\ \alpha_i=\varepsilon_i-\varepsilon_{i+1},\ i\in\mathbb{N}\}.$$

Here ε_i are viewed restricted to the restricted dual of the Cartan subalgebra of b_∞, so that $\varepsilon_i=-\varepsilon_{-i}$. Given $\lambda\in(b_\infty)_0^*$, the labels and central charge are simply (in this case, we skip the superscript b)

$$\lambda_i=\lambda(E_{i,i}-E_{-i,-i}),\quad i>0,\quad c=\lambda(C).$$

So that $\lambda(\alpha_0{}^\vee)=2c-2\lambda_1$ and $\lambda(\alpha_i{}^\vee)=\lambda_i-\lambda_{i+1}$ for $i\in\mathbb{N}$. Denote by Λ_i the ith fundamental weight of b_∞, namely $\Lambda_i(\alpha_j{}^\vee)=\delta_{i,j}$.

Let $P_+=\{\lambda\in(b_\infty)_0^*\,|\,\langle\lambda,\alpha_i{}^\vee\rangle\in\mathbb{Z}_+$, for all $i\in\mathbb{Z}_+\}$ denote the set of dominant integral weights of b_∞. Given $\lambda\in P_+$, we have $\lambda=\Lambda_{n_1}+\Lambda_{n_2}+\cdots+\Lambda_{n_k}+h\Lambda_0$, $n_1\geqslant n_2\geqslant\cdots\geqslant n_k\geqslant 1$, $h\in\mathbb{Z}_+$, and the module $L(b_\infty;\lambda)$ has central charge $c=k+h/2$. Observe that the conjugate of the Young diagram corresponding to the partition $(n_1,n_2,\ldots,n_k)$ is $(\lambda_1,\ldots,\lambda_{n_1})$, and $\lambda_i=0$ for $i>n_1$. Note that $n_1=n_1(\lambda)=\max\{i\in\mathbb{N}\,|\,\langle\lambda,\alpha_i\rangle\neq 0\}$. Observe that $\mathfrak{so}(2n_1+1)$ may be viewed as a subalgebra of b_∞ in a natural way, whose set of simple roots is $\{-\varepsilon_1,\varepsilon_1-\varepsilon_2,\ldots,\varepsilon_{n_1-1}-\varepsilon_{n_1}\}$. Denote by $\overline{\lambda}$ the dominant integral weight of $\mathfrak{so}(2n_1+1)$ given by $\overline{\lambda}(2(E_{-1,-1}-E_{1,1}))=2(c-\lambda_1)$ and $\overline{\lambda}(E_{i,i}-E_{i+1,i+1}-E_{-i,-i}+E_{-1-i,-1-i})=\lambda_i-\lambda_{i+1}$ for $1\leqslant i<n_1$. Denote by $\overline{L(\lambda)}$ the (irreducible) $\mathfrak{so}(2n_1+1)$-submodule of $L(b_\infty;\lambda)$ generated by its highest weight vector. It is, of course, isomorphic to the finite-dimensional irreducible $\mathfrak{so}(2n_1+1)$-module associated to $\overline{\lambda}$, so that its q-character is a (well-known) polynomial in q.

Lemma 2.3: Let $\lambda\in P_+$, $n_1=n_1(\lambda)$. *Then*

$$\mathrm{ch}_q L(b_\infty;\lambda)=\mathrm{ch}_q\overline{L(\lambda)}\prod_{j=1}^{n_1}\frac{1}{(1-q^j)_q^{\lambda_{n_1-j+1}}}\prod_{i=1}^{n_1}\frac{1}{(1-q^{n_1+i})_q^{2c-\lambda_i}}\prod_{n_1\leqslant i}\frac{1}{(1-q^{2i+1})_q^{2c}},$$

where $(1-a)_q^m=(1-a)(1-qa)\cdots(1-q^{m-1}a)$.

Proof: The proof is completely similar to the one of Lemma 2.1, using the data introduced above (cf. proof of Proposition 1.1 in Ref. 11).

□

Theorem 2.4: *All nontrivial modules* $L(b_\infty^{[m]};\lambda)$ *have infinite growth.*

Proof: It is enough to consider the case $m=0$. Given $\lambda \in (b_\infty)_0^*$, we look at the subalgebra of b_∞ isomorphic to $g\ell_{+\infty}$ spanned by all $E_{i,j}-E_{-j,-i}$ with $i,j\geqslant 1$, and by Theorem 2.2, we conclude that $L(b_\infty;\lambda)$ has infinite growth if $\lambda_i-\lambda_{i+1}\notin \mathbb{Z}_+$ for some $i\geqslant 1$.

Let us assume $\lambda_i-\lambda_{i+1}\in\mathbb{Z}_+$ for all $i\geqslant 1$. If $2c-2\lambda_1\notin\mathbb{Z}_+$, then $(E_{1,0}-E_{0,-1})^N v_\lambda\neq 0$ for each $N\in\mathbb{Z}_+$. Looking at the subalgebra of b_∞ isomorphic to $g\ell_{+\infty}$ previously defined, we conclude from Theorem 2.2 that

$$\operatorname{growth} L(b_\infty;\lambda)\geqslant N+\sum_{i\geqslant 1}\lambda_i .$$

If $2c-2\lambda_1\in\mathbb{Z}_+$, then by the same argument in the proof of Theorem 2.2, and looking at the last factor in Lemma 2.3, we conclude that $L(b_\infty;\lambda)$ has the same growth as the polynomial algebra in infinitely many generators, finishing the proof.

□

C. Lie algebra $c_\infty^{[m]}$

As before, we consider the vector space $R_m[t,t^{-1}]$, and take the R_m-basis $v_i=t^{-i}$, $i\in\mathbb{Z}$. Denote by $\overline{c}_\infty^{[m]}$ the Lie subalgebra of $\widetilde{g\ell}_\infty^{[m]}$ which preserves the bilinear form

$$C(u^m v_i,u^n v_j)=u^m(-u^n)(-1)^i\,\delta_{i,1-j}. \tag{2.5}$$

We have

$$\overline{c}_\infty^{[m]}=\{(a_{ij}(u))_{i,j\in\mathbb{Z}}\in\widetilde{g\ell}_\infty^{[m]}\mid a_{ij}(u)=(-1)^{i+j+1}a_{1-j,1-i}(-u)\}.$$

Denote by $c_\infty^{[m]}=\overline{c}_\infty^{[m]}\oplus R_m$ the central extension of $\overline{c}_\infty^{[m]}$ given by the 2-cocycle defined in $\widetilde{g\ell}_\infty^{[m]}$. This subalgebra inherits the form $\widehat{g\ell}_\infty^{[m]}$ of the principal $\mathbb{Z}$-gradation and the triangular decomposition (see Refs. 11 and 6 for notation)

$$c_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(c_\infty^{[m]})_j,\quad c_\infty^{[m]}=(c_\infty^{[m]})_+\oplus(c_\infty^{[m]})_0\oplus(c_\infty^{[m]})_- .$$

In particular when $m=0$, we have the usual Lie subalgebra of $\widehat{g\ell}_\infty$, denoted by c_∞ (see Ref. 6).

Denote by $L(c_\infty^{[m]};\lambda)$ the highest weight module over $c_\infty^{[m]}$ with highest weight $\lambda\in(c_\infty^{[m]})_0^*$ parametrized by its labels ${}^c\vec{\lambda}\in(\mathbb{C}^\infty)^{m+1}$ and central charges $\vec{c}\in\mathbb{C}^{m+1}$, with

$$\vec{c}_i=\lambda(u^i),$$

$${}^c\vec{\lambda}_j^{(i)}=\lambda(u^i E_{j,j}-(-u)^i E_{1-j,1-j}).$$

Now, we are interested in representation theory of c_∞.

The set of simple coroots of c_∞, denoted by $\Pi^\vee$, can be described as follows (cf. Ref. 11):

$$\Pi^\vee=\{\alpha_0{}^\vee=E_{0,0}-E_{1,1}+C,$$

$$\alpha_i{}^\vee=E_{i,i}-E_{i+1,i+1}+E_{-i,-i}-E_{1-i,1-i},\ i\in\mathbb{N}\}.$$

The set of roots is

$$\Delta=\{\pm 2\varepsilon_i,\ \pm\varepsilon_i\pm\varepsilon_j,\ i\neq j,\ i,j\in\mathbb{N}\}.$$

The set of positive coroots is

$$\Delta_+{}^\vee=\{\alpha_i{}^\vee+\alpha_{i+1}{}^\vee+\cdots+\alpha_j{}^\vee,\ 0\leqslant i\leqslant j\}\cup\{2\alpha_0{}^\vee+2\alpha_1{}^\vee+\cdots+2\alpha_i{}^\vee+\alpha_{i+1}{}^\vee+\cdots+\alpha_j{}^\vee,\ 0\leqslant i<j\}.$$

The set of simple roots is

$$\Pi=\{\alpha_0=-2\varepsilon_1,\ \alpha_i=\varepsilon_i-\varepsilon_{i+1},\ i\in\mathbb{N}\}.$$

Here ε_i are viewed restricted to the restricted dual of the Cartan subalgebra of c_∞, so that $\varepsilon_i=-\varepsilon_{1-i}$. Given $\lambda\in(c_\infty)_0^*$, the labels and central charge are simply (in this case, we skip the superscript c):

$$\lambda_j=\lambda(E_{j,j}-E_{1-j,1-j}),\quad j\in\mathbb{N},\quad c=\lambda(C).$$

So that $\lambda(\alpha_0\hat{})=-\lambda_1+c$ and $\lambda(\alpha_i\hat{})=\lambda_i-\lambda_{i+1}$ for $i\in\mathbb{N}$. Denote by Λ_i the ith fundamental weight of b_∞, namely $\Lambda_i(\alpha_j\hat{})=\delta_{i,j}$.

Let $P_+=\{\lambda\in(c_\infty)_0^*\mid\langle\lambda,\alpha_i\hat{}\rangle\in\mathbb{Z}_+,\text{for all } i\in\mathbb{Z}_+\}$ denote the set of dominant integral weights of c_∞. Given $\lambda\in P_+$, we have $\lambda=\Lambda_{n_1}+\Lambda_{n_2}+\cdots+\Lambda_{n_k}+h\Lambda_0$, $n_1\geqslant n_2\geqslant\cdots\geqslant n_k\geqslant 1$, $h\in\mathbb{Z}_+$, and the module $L(c_\infty,\lambda)$ has central charge $c=k+h$. Observe that the conjugate of the Young diagram corresponding to the partition $(n_1,n_2,\ldots,n_k)$ is $(\lambda_1,\ldots,\lambda_{n_1})$, and $\lambda_i=0$ for $i>n_1$. Note that $n_1=n_1(\lambda)=\max\{i\in\mathbb{N}\mid\langle\lambda,\alpha_i\rangle\neq 0\}$. Observe that $\mathfrak{sp}(2n_1)$ may be viewed as a subalgebra of c_∞ in a natural way, whose set of simple roots is $\{-2\varepsilon_1,\varepsilon_1-\varepsilon_2,\ldots,\varepsilon_{n_1-1}-\varepsilon_{n_1}\}$. Denote by $\overline{\lambda}$ the dominant integral weight of $\mathfrak{sp}(2n_1)$ given by $\overline{\lambda}((E_{0,0}-E_{1,1}))=c-\lambda_1$ and $\overline{\lambda}(E_{i,i}-E_{i+1,i+1}+E_{-i,-i}-E_{1-i,1-i})=\lambda_i-\lambda_{i+1}$ for $1\leqslant i<n_1$. Denote by $\overline{L(\lambda)}$ the (irreducible) $\mathfrak{sp}(2n_1)$-submodule of $L(c_\infty,\lambda)$ generated by its highest weight vector. It is, of course, isomorphic to the finite-dimensional irreducible $\mathfrak{sp}(2n_1)$-module associated to $\overline{\lambda}$, so that its q-character is a (well-known) polynomial in q.

Lemma 2.5: Let $\lambda\in P_+$, $n_1=n_1(\lambda)$. *Then*

$$\mathrm{ch}_q L(c_\infty;\lambda)=\mathrm{ch}_q\overline{L(\lambda)}\prod_{i=1}^{n_1}\frac{1}{(1-q^j)_q^{\lambda_{n_1-j+1}}}\cdot\prod_{i=1}^{n_1}\frac{1}{(1-q^{n_1+i+3})_q^{2c-\lambda_{i+1}}}$$
$$\times\frac{1}{(1-q^{n_1+1})_q^{c}}\prod_{n_1\leqslant i}\frac{1}{(1-q^{2i+3})_q^{2c}},$$

where $(1-a)_q^m=(1-a)(1-qa)\cdots(1-q^{m-1}a)$.

Proof: The proof is completely similar to the one of Lemma 2.1, using the data introduced above (cf. proof of Proposition 1.1 in Ref. 11).

□

Theorem 2.6: *All nontrivial modules* $L(c_\infty^{[m]};\lambda)$ *have infinite growth.*

Proof: It is enough to consider the case $m=0$. Given $\lambda\in(c_\infty)_0^*$, we look at the subalgebra of c_∞ isomorphic to $g\ell_{+\infty}$ spanned by all $E_{i,j}-E_{1-j,1-i}$ with $i,j\geqslant 1$, and by Theorem 2.2, we conclude that $L(c_\infty,\lambda)$ has infinite growth if $\lambda_i-\lambda_{i+1}\notin\mathbb{Z}_+$ for some $i\geqslant 1$.

Let us assume $\lambda_i-\lambda_{i+1}\in\mathbb{Z}_+$ for all $i\geqslant 1$. If $c-\lambda_1\notin\mathbb{Z}_+$, then $(E_{1,0})^N v_\lambda\neq 0$ for each $N\in\mathbb{Z}_+$. Looking at the subalgebra of c_∞ isomorphic to $g\ell_{+\infty}$ previously defined, we conclude from Theorem 2.2 that

$$\mathrm{growth}\,L(c_\infty,\lambda)\geqslant N+\sum_{i\geqslant 1}\lambda_i.$$

If $c-\lambda_1\in\mathbb{Z}_+$, then by the same argument in the proof of Theorem 2.2, and looking at the last factor in Lemma 2.3, we conclude that $L(c_\infty,\lambda)$ has the same growth as the polynomial algebra in infinitely many generators, finishing the proof.

□

III. IRREDUCIBLE FINITE GROWTH gc_1-MODULES

We are interested in representation theory of the Lie algebra $\mathcal{D}^-$ of regular differential operators on $\mathbb{C}$. It consists of linear combinations of differential operators of the form $f(t)\times(d/dt)^m$, where f is a polynomial and $m\in\mathbb{Z}_+$. In particular, $D=t(d/dt)\in\mathcal{D}^-$. The principal $\mathbb{Z}$-gradation $\mathcal{D}^-=\oplus_{j\in\mathbb{Z}}\mathcal{D}^-_j$ is defined by letting

$$\deg t=-1 \quad \deg\frac{d}{dt}=1.$$

Given a sequence of complex numbers $\Delta=(\Delta_0,\Delta_1,\ldots)$ we define the highest weight module $L(\Delta;\mathcal{D}^-)$ over $\mathcal{D}^-$ as the (unique) irreducible module that has a nonzero vector v_Δ with the following properties:

$$\mathcal{D}^-_j v_\Delta=0 \quad \text{for } j<0, \quad D^n v_\Delta=\Delta_n v_\Delta \quad \text{for } n\in\mathbb{Z}_+.$$

The principal gradation of $\mathcal{D}^-$ induces the principal gradation $L(\Delta;\mathcal{D}^-)=\oplus_{j\in\mathbb{Z}_+}L_j$ such that $L_0=\mathbb{C}v_\Delta$. The module $L(\Delta;\mathcal{D}^-)$ is called *quasifinite* if $\dim L_j<\infty$ for all $j\in\mathbb{Z}_+$.

Quasifinite modules over $\mathcal{D}^-$ can be constructed as follows. Consider the natural action of $\mathcal{D}^-$ on $\mathbb{C}[t,t^{-1}]$ and choose the basis $v_j=t^{-j}(j\in\mathbb{Z})$ of $\mathbb{C}[t,t^{-1}]$. This gives an embedding of $\mathcal{D}^-$ in $\widetilde{g\ell}_\infty$. Since $\mathbb{C}[t]$ is $\mathcal{D}^-$-invariant, we get $\mathcal{D}^-$-modules $\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ and $\mathbb{C}[t]$, which gives us an embedding of $\mathcal{D}^-$ in $\widetilde{g\ell}_{+\infty}$ and $\widetilde{g\ell}_{-\infty}$, respectively, hence an embedding of $\mathcal{D}^-$ in $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$. All these embeddings respect the principal gradations. Now take $\lambda^\pm\in\mathbb{C}^{\pm\infty}$ and consider the $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$-module $L^+(\lambda^+)\otimes L^-(\lambda^-)$. The same argument as in Ref. 10, gives us the following.

Lemma 3.1: When restricted to $\mathcal{D}^-$, the module $L^+(\lambda^+)\otimes L^-(\lambda^-)$ remains irreducible.

It follows immediately that $L^+(\lambda^+)\otimes L^-(\lambda^-)$ is an irreducible highest weight module over $\mathcal{D}^-$, which is obviously quasifinite. It is easy to see that we have

$$\Delta_n=\sum_{j\geqslant 1}(-j)^n\lambda_j^+ +\sum_{j\leqslant 0}(-j)^n\lambda_j^-,$$

so that

$$\Delta(x):=\sum_{n\geqslant 0}\Delta_n x^n/n!=\sum_{j\geqslant 1}\lambda_j^+ e^{-jx}+\sum_{j\leqslant 0}\lambda_j^- e^{-jx}.$$

It is also clear that for $\lambda^\pm\in\mathrm{Par}^\pm$ we have (cf. Theorem 1a):

$$\mathrm{growth}\, L^+(\lambda^+)\otimes L^-(\lambda^-)=|\lambda^+|+|\lambda^-|.$$

We shall prove the following theorem.

Theorem 3.2: *The $\mathcal{D}^-$-modules $L^+(\lambda^+)\otimes L^-(\lambda^-)$, where $\lambda^\pm\in\mathrm{Par}^\pm$, exhaust all quasifinite irreducible highest weight $\mathcal{D}^-$-modules that have finite growth.*

Let $\mathcal{D}$ denote the Lie algebra of all regular differential operators on $\mathbb{C}^*$. The Lie algebra $\mathcal{D}$ is the linear span of differential operators $f(t)(d/dt)^k$, where $f(t)\in\mathbb{C}[t,t^{-1}]$ and $k\in\mathbb{Z}_+$, or, equivalently of operators $t^k f(D)$, where $f(D)\in\mathbb{C}[D]$ and $k\in\mathbb{Z}$. Obviously, $\mathcal{D}^-$ is a subalgebra of $\mathcal{D}$, and the principal gradation extends from $\mathcal{D}^-$ to $\mathcal{D}$ in the obvious way.

The basic idea of the proof of Theorem 3.2 is the same as in Ref. 10: to reduce the problem to the well developed (in Ref. 10) representation theory of the universal central extension $\hat{\mathcal{D}}$ of $\mathcal{D}$. Recall that the central extension $\hat{\mathcal{D}}=\mathcal{D}+\mathbb{C}C$ is defined by the cocycle[10]

$$\Psi\left(f(t)\left(\frac{d}{dt}\right)^m, g(t)\left(\frac{d}{dt}\right)^n\right)=\mathrm{Res}_0\, dt\, f^{(n+1)}(t)g^{(m)}(t). \tag{3.1}$$

The principal gradation of $\mathcal{D}$ lifts to $\hat{\mathcal{D}}$ by letting $\deg C=0$. Note also that the restriction of the cocycle Ψ to $\mathcal{D}^-$ is zero.

For each $s\in\mathbb{C}$ one defines a Lie algebra homomorphism $\varphi_s:\mathcal{D}\to\widetilde{g\ell}_\infty$ (via the action of $\mathcal{D}$ on $t^s\mathbb{C}[t,t^{-1}]$) by

$$\varphi_s(t^k f(D))=\sum_{j\in\mathbb{Z}} f(-j+s)E_{j-k,j}\,. \tag{3.2}$$

This homomorphism lifts to a homomorphism of central extension $\hat{\varphi}_s:\hat{\mathcal{D}}\to\widehat{g\ell}_\infty$ by

$$\begin{aligned}&\hat{\varphi}_s(t^k f(D))=\varphi_s(t^k f(D))\text{if}\quad k\neq 0\,,\\ &\hat{\varphi}_s(e^x D)=\varphi_s(e^{xD})-\frac{e^{sx}-1}{e^x-1},\hat{\varphi}_s(C)=C\,.\end{aligned} \tag{3.3}$$

More generally, for each $m\in\mathbb{Z}_+$ one defines a homomorphism $\varphi_s^{[m]}:\mathcal{D}\to\widetilde{g\ell}_\infty^{[m]}$ by

$$\varphi_s^{[m]}(t^k f(D))=\sum_{j\in\mathbb{Z}} f(-j+s+u)E_{j-k,j}=\sum_{i=0}^{m}\sum_{j\in\mathbb{Z}}\frac{f^{(i)}(-j+s)}{i}u^i E_{j-k,j}\,, \tag{3.4}$$

which lifts to $\hat{\varphi}_s^{[m]}:\hat{\mathcal{D}}\to\widehat{g\ell}_\infty^{[m]}$ in a similar way. One of the main results of Ref. 10 is the following.

Lemma 3.3: For each $i=1,\dots,r$, *pick a collection* $m_i\in\mathbb{Z}_+$, $s_i\in\mathbb{C}$, $\vec{\lambda}_i\in(\mathbb{C}^\infty)^{m_i+1}$, $\vec{c}_i\in\mathbb{C}^{m_i+1}$, *such that* $s_i-s_j\notin\mathbb{Z}$ *for* $i\neq j$. *Then the* $\oplus_{i=1}^r\widehat{g\ell}_\infty^{[m_i]}$*-module* $\otimes_{i=1}^r L^{[m_i]}(\vec{\lambda}_i,\vec{c}_i)$ *remains irreducible when restricted to* $\hat{\mathcal{D}}$ *via the embedding* $\oplus_{i=1}^r\hat{\varphi}_{s_i}^{[m_i]}:\hat{\mathcal{D}}\to\oplus_{i=1}^r\widehat{g\ell}_\infty^{[m_i]}$. *All irreducible quasifinite highest weight* $\hat{\mathcal{D}}$*-modules are obtained in this way.*

Proof of Theorem 3.2: Note that for $j\geqslant 1$ one has

$$\mathcal{D}_j^-=\{t^{-j}f(D)\,|\,f(0)=f(1)=\cdots=f(j-1)=0\}\,. \tag{3.5}$$

Hence $\mathcal{D}_j^-$ has finite codimension in $\mathcal{D}_j$ and therefore the quasifiniteness of a $\mathcal{D}^-$-module $L(\Delta;\mathcal{D}^-)$ implies the quasifiniteness of any of the $\hat{\mathcal{D}}$-modules $L(\Delta,c;\hat{\mathcal{D}})$. Due to Lemma 3.3, $L(\Delta,c;\hat{\mathcal{D}})$ is a tensor product of the $\widehat{g\ell}_\infty^{[m]}$-modules $L^{[m]}(\vec{\lambda},\vec{c})$ on which $\hat{\mathcal{D}}$ acts via the embedding $\hat{\varphi}_s^{[m]}$ defined by (3.2) and (3.3).

It is clear from Theorem 2.2 that all non-trivial modules $L^{[m]}(\vec{\lambda}_i,\vec{c}_i)$ have infinite growth (by choosing an appropriate subalgebra isomorphic to $g\ell_{+\infty}$ in $g\ell_\infty$).

Recall that for any quasifinite $\hat{\mathcal{D}}$-module one can extend the action of $\hat{\mathcal{D}}_j$ for $j\neq 0$ to $\hat{\mathcal{D}}_j^{\mathcal{O}}$, where $\mathcal{O}$ is the algebra of all holomorphic functions on $\mathbb{C}$,[10] in other words, in (3.2) and (3.3) one can take any $f\in\mathcal{O}$ if $j\neq 0$. The same holds for $\mathcal{D}^-$, except that for $j\geqslant 1$, f must obey conditions in (3.5). We apply this to the $\hat{\mathcal{D}}$-module $L(\widehat{g\ell}_\infty^{[m]};\vec{\lambda},\vec{c})$ on which $\hat{\mathcal{D}}$ acts via $\hat{\varphi}_s^{[m]}$.

Choosing $f\in\mathcal{O}$ such that for all $j\in\mathbb{Z}$:

$$f(-j+s)=\delta_{rj},\ f^{(i)}(-j+s)=0\quad\text{if}\quad i=1,\dots,m\,,$$

we see from (3.2) that all operators $E_{r+1,r}$ lie in the image of $\hat{\varphi}_s^{[m]}(\mathcal{D}^{-\mathcal{O}})$, except for $E_{1,0}$ when $s=0$ [here we use (3.5) for $j=1$]. Hence, when restricted to $\mathcal{D}^-$, the module $L^{[m]}(\vec{\lambda},\vec{c})$ remains irreducible, provided that $s\neq 0$. Thus, if $L(\Delta;\mathcal{D}^-)$ has finite growth, then $L(\Delta;\hat{\mathcal{D}})=L^{[m]}(\vec{\lambda},\vec{c})$ on which $\hat{\mathcal{D}}$ acts via the embedding $\hat{\varphi}_0^{[m]}$.

Choosing $f\in\mathcal{O}$ to vanish in all $j\in\mathbb{Z}$ up to mth derivative except for ith derivative ($0<i\leqslant m$) at $j=-r$, we see that all operators $u^i E_{r+1,r}$ with $0<i\leqslant m$ lie in the image of $\hat{\varphi}_s^{[m]}(\mathcal{D}^{-\mathcal{O}})$.

Suppose that the mth coordinate of $\vec{\lambda}_r$ is nonzero, and that $m>0$. Then $v:=(u^m E_{r+1,r})^N v_{\vec{\lambda}} \neq 0$ for all $N>0$. But

$$E_{rr}v=(-N+\lambda_r^0)v,\ E_{r+1,r+1}v=(N+\lambda_{r+1}^0)v.$$

Therefore, restricting to the subalgebra of $g\ell_\infty$ consisting of matrices $(a_{ij})_{i,j\leqslant r}$ or $(a_{ij})_{i,j\geqslant r+1}$ we conclude by Theorem 2.2, that $L(\widehat{g\ell_\infty^{[m]}};\vec{\lambda},\vec{c})$ is either trivial or is of infinite growth.

Thus, the only possibility that remains is $s=m=0$. As has been already shown, the image of $\hat{\varphi}_s(\mathcal{D}^{-\mathcal{O}})$ contains all $E_{r+1,r}$ except for $E_{1,0}$, hence it contains all operators from $g\ell_{-\infty} \oplus g\ell_{+\infty}$. Therefore, by Theorem 2.2, the highest weight of a finite growth $\mathcal{D}^-$-module must be the same as one of the $\mathcal{D}^-$-modules $L^+(\lambda^+)\otimes L^-(\lambda^-)$ with $\lambda^\pm \in \mathrm{Par}^\pm$.

□

Given two partitions $\lambda^\pm \in \mathrm{Par}^\pm$, we denote by $L(\lambda^+,\lambda^-)$ the $\mathcal{D}^-$-module, obtained by restriction via φ_0 from the $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$-module $L^+(\lambda^+)\otimes L^-(\lambda^-)$. Now we shall construct the $\mathcal{D}^-$-modules $L(\lambda^+,\lambda^-)$ explicitly.

Consider the $\mathcal{D}^-$-module $\mathbb{C}[t,t^{-1}]$. Then $\mathbb{C}[t]$ is its maximal submodule (which is irreducible). Hence the $\mathcal{D}^-$-module

$$V:=\mathbb{C}[t,t^{-1}]/\mathbb{C}[t] \tag{3.6}$$

is irreducible. It is clear that this is the highest weight $\mathcal{D}^-$-module of growth 1 with a highest weight vector $t^{-1}+\mathbb{C}[t]$. It is immediate to deduce that V is isomorphic to $L(\omega_1,0)$ where $\omega_1=(1,0,\ldots)\in \mathrm{Par}^+$.

Likewise, the $\mathcal{D}^-$-module $\mathbb{C}[t]^*=\oplus_{j\in\mathbb{Z}_+}(\mathbb{C}t^j)^*$ is an irreducible highest weight module of growth 1 with a highest weight vector 1^*, hence it is isomorphic to $L(0,\omega_{-1})$, where $\omega_{-1}=(\ldots,0,-1)\in \mathrm{Par}^-$. We denote this $\mathcal{D}^-$-module by V'.

As in the Schur–Weyl theory, the $\mathcal{D}^-$-module $T^M(V)\otimes T^N(V')$ has a natural decomposition as $(\mathcal{D}^-,S_M\times S_N)$-modules:

$$T^M(V)\otimes T^N(V')=\bigoplus_{\substack{\lambda^\pm\in \mathrm{Par}^\pm\\ |\lambda^+|=M\\ |\lambda^-|=N}} (V_{\lambda^+}\otimes V'_{\lambda^-})\otimes(U_{\lambda^+}\otimes U_{\lambda^-}),$$

where $U_{\lambda^+ \text{ (respectively, } \lambda^-)}$ denotes the irreducible $S_{M \text{ (respectively, } N)}$-module corresponding to the partition λ^+ (respectively, λ^-).

Lemma 3.4: The $\mathcal{D}^-$-modules $V_{\lambda^+}\otimes V'_{\lambda^-}$ are irreducible.

Proof: As in the proof of Theorem 3.2, we extend the action of $\mathcal{D}^-$ on $V_{\lambda^+}\otimes V'_{\lambda^-}$ to $\mathcal{D}_j^{-\mathcal{O}}$ for each $j\neq 0$, to obtain that any $\mathcal{D}^-$-submodule of $V_{\lambda^+}\otimes V'_{\lambda^-}$ is a submodule over $g\ell_{+\infty}\oplus g\ell_{-\infty}$. But, by Schur–Weyl theory, the $g\ell_{+\infty}\oplus g\ell_{-\infty}$-module $V_{\lambda^+}\otimes V'_{\lambda^-}$ is irreducible, which completes the proof. □

Thus, we have proved the following.

Theorem 3.5: *The $\mathcal{D}^-$-module $L(\lambda^+,\lambda^-)$ is isomorphic to $V_{\lambda^+}\otimes V'_{\lambda^-}$ for any pair $\lambda^\pm \in \mathrm{Par}^\pm$.*

Remark: Considering $\lambda=(\lambda^-,\lambda^+)\in\mathbb{C}^\infty$ we may say that irreducible highest weight $\mathcal{D}^-$-modules of finite growth are parametrized by nonincreasing sequences of integers $(\lambda_j)_{j\in\mathbb{Z}}\in\mathbb{C}^\infty$ with the exception that $\lambda_0\leqslant\lambda_1$. Equivalently, letting $m_i=\lambda_i-\lambda_{i+1}$ we may say that these modules are parametrized by sequences of non-negative integers $(m_i)_{i\in\mathbb{Z}\setminus\{0\}}$, all but finite numbers of which are zero.

Recall that the extended annihilation algebra $\mathrm{Lie}^-(gc_1)$ for gc_1 is isomorphic to the direct sum of the Lie algebra $\mathcal{D}^-$ and the one-dimensional Lie algebra $\mathbb{C}[\partial+(d/dt)]$ and that conformal modules for a Lie conformal algebra coincide with the conformal modules over the associated extended annihilation algebra.[7]

Given a module M over a Lie conformal algebra R and $\alpha\in\mathbb{C}$, we may construct the α-twisted module M_α by replacing ∂ by $\partial+\alpha$ in the formulas for action of R on M. Theorems 3.2 and 3.5 and the above remarks imply the following.

Theorem 3.6: *The gc_1-modules $L(\lambda^+,\lambda^-)_\alpha$, where $\lambda^\pm\in\mathrm{Par}^\pm$, $\alpha\in\mathbb{C}$, exhaust all irreducible conformal gc_1-modules of finite growth.*

Corollary: The gc_1-modules $\mathbb{C}[\partial]_\alpha$ and $\mathbb{C}[\partial]^*_\alpha$, where $\alpha\in\mathbb{C}$, exhaust all finite irreducible gc_1-modules.

Remark: It is straightforward to generalize Theorems 3.2 and 3.5 to the case of $N\times N$ matrix differential operators and hence Theorem 3.6 to the case of gc_N. In particular the gc_N-modules $\mathbb{C}[\partial]^N_\alpha$ and $(\mathbb{C}[\partial]^N*)_\alpha$, where $\alpha\in\mathbb{C}$, exhaust all finite irreducible gc_N-modules. This is a result of Kac, Radul, and Wakimoto. Moreover, these authors completely described all finite gc_N-modules, which amounted to prove a complete reducibility result for finite modules over the annihilation algebra (see Ref. 8). It is an open question whether a similar complete reducibility result holds in the case of finite growth modules.

IV. IRREDUCIBLE FINITE GROWTH $gc_{1,x}$-MODULES

The results of this section are almost the same as the preceding section as well as the proofs. Therefore, we will skip the details.

Let $\mathcal{D}_0$ (respectively, $\mathcal{D}_0^-$) be the Lie subalgebra of $\mathcal{D}$ (respectively, $\mathcal{D}^-$) of all regular differential operators on $\mathbb{C}^*$ (respectively, $\mathbb{C}$) that kill constants. That is, $\mathcal{D}_0$ consists of linear combinations of elements of the form $t^kDf(D)$, where f is a polynomial. Denote by $\hat{\mathcal{D}}_0$ the corresponding central extension. These algebras inherit the $\mathbb{Z}$-gradation from $\hat{\mathcal{D}}$.

In this section, we will need the representation theory of the Lie algebra $\mathcal{D}_0^-$.

Given a sequence of complex numbers $\Delta=(\Delta_1,\Delta_2,\ldots)$ we define the highest weight module $L(\Delta;\mathcal{D}_0^-)$ over $\mathcal{D}_0^-$ as the (unique) irreducible module that has a nonzero vector v_Δ with the following properties:

$$(\mathcal{D}_0^-)_j v_\Delta=0 \quad \text{for } j<0, \quad D^n v_\Delta=\Delta_n v_\Delta \quad \text{for } n\in\mathbb{N}.$$

The principal gradation of $\mathcal{D}_0^-$ induces the principal gradation $L(\Delta;\mathcal{D}_0^-)$.

Quasifinite modules over $\mathcal{D}_0^-$ can be constructed as follows. The $\mathcal{D}_0^-$-modules $\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ and $\mathbb{C}[t]/\mathbb{C}$, give us an embedding of $\mathcal{D}_0^-$ in $\widetilde{g\ell}_{+\infty}$ and $\widetilde{g\ell}_{-\infty}$, respectively, hence an embedding of $\mathcal{D}_0^-$ in $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$. All these embeddings respect the principal gradations. Now take $\lambda^\pm\in\mathbb{C}^{\pm\infty}$ and consider the $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$-module $L^+(\lambda^+)\otimes L^-(\lambda^-)$.

The same argument as in Ref. 10, gives us the following.

Lemma 4.1: When restricted to $\mathcal{D}_0^-$, the module $L^+(\lambda^+)\otimes L^-(\lambda^-)$ remains irreducible.

It follows immediately that $L^+(\lambda^+)\otimes L^-(\lambda^-)$ is an irreducible highest weight module over $\mathcal{D}_0^-$, which is obviously quasifinite.

We have the following theorem.

Theorem 4.2: *The $\mathcal{D}_0^-$-modules $L^+(\lambda^+)\otimes L^-(\lambda^-)$, where $\lambda^\pm\in\mathrm{Par}^\pm$, exhaust all quasifinite irreducible highest weight $\mathcal{D}_0^-$-modules that have finite growth.*

The proof of Theorem 4.2 is the same as Theorem 3.2, but in this case we reduce the problem to the representation theory of the universal central extension $\hat{\mathcal{D}}_0$ of $\mathcal{D}_0$ that was developed in Refs. 1 and 9.

Let $s\in\mathbb{Z}$ and denote by $\widehat{g\ell}^{[m]}_{\infty,s}$ the Lie subalgebra of $\widehat{g\ell}^{[m]}_\infty$ generated by C and $\{u^lE_{ij}|0\leqslant l\leqslant m, i\neq s \text{and } j\neq s\}$. Observe that $\widehat{g\ell}^{[m]}_{\infty,s}$ is naturally isomorphic to $\widehat{g\ell}^{[m]}_\infty$. Let $p_s:\widehat{g\ell}^{[m]}_\infty\to\widehat{g\ell}^{[m]}_{\infty,s}\to\widehat{g\ell}^{[m]}_\infty$ be the projection map composed with this isomorphism. If $s\notin\mathbb{Z}$, we also denote by $\hat{\varphi}^{[m]}_s$ the homomorphism (3.4) restricted to $\hat{\mathcal{D}}_0$. If $s\in\mathbb{Z}$, we redefine $\hat{\varphi}^{[m]}_s$ by the homomorphism $p_s\circ\hat{\varphi}^{[m]}_s:\hat{\mathcal{D}}_0\to\widehat{g\ell}^{[m]}_{\infty,s}$.

In this case, we should replace Lemma 3.3 by one of the results of Ref. 9 (see also Ref. 1):

Lemma 4.3: For each $i=1,\ldots,r$, *pick a collection* $m_i\in\mathbb{Z}_+$, $s_i\in\mathbb{C}$, $\vec{\lambda}_i\in(\mathbb{C}^\infty)^{m_i+1}$, $\vec{c}_i\in\mathbb{C}^{m_i+1}$, *such that* $s_i-s_j\notin\mathbb{Z}$ *for* $i\neq j$. *Then the* $\oplus_{i=1}^r\widehat{g\ell}_\infty^{[m_i]}$*-module* $\otimes_{i=1}^r L^{[m_i]}(\vec{\lambda}_i,\vec{c}_i)$ *remains irreducible when restricted to* $\hat{\mathcal{D}}_0$ *via the embedding* $\oplus_{i=1}^r\hat{\varphi}_{s_i}^{[m_i]}:\hat{\mathcal{D}}_0\to\oplus_{i=1}^r\widehat{g\ell}_\infty^{[m_i]}$. *All irreducible quasifinite highest weight* $\hat{\mathcal{D}}_0$*-modules are obtained in this way.*

Proof of Theorem 4.2: The proof is the same as Theorem 3.2 but use Lemma 4.3, and in the case $s=0$ one should use the redefined $\hat{\varphi}_0^{[m]}$.

□

Given two partitions $\lambda^\pm\in\mathrm{Par}^\pm$, the $\mathcal{D}^-$-module $L(\lambda^+,\lambda^-)$ that is obtained by restriction via φ_0 from the $\widetilde{g\ell}_{+\infty}\oplus\widetilde{g\ell}_{-\infty}$-module $L^+(\lambda^+)\otimes L^-(\lambda^-)$, remains irreducible as a $\mathcal{D}_0^-$-module. The construction of the $\mathcal{D}_0^-$-modules $L(\lambda^+,\lambda^-)$ is the same as before, and Lemma 3.4 and Theorem 3.5 holds for $\mathcal{D}_0^-$.

In this case, the extended annihilation algebra $\mathrm{Lie}^-(gc_{1,x})$ for $gc_{1,x}$ is isomorphic to the direct sum of the Lie algebra $\mathcal{D}_0^-$ and the one-dimensional Lie algebra $\mathbb{C}[\partial+(d/dt)]$. Theorems 4.2 and 3.5 and the above remarks imply the following.

Theorem 4.4: *The* $gc_{1,x}$*-modules* $L(\lambda^+,\lambda^-)_\alpha$, *where* $\lambda^\pm\in\mathrm{Par}^\pm$, $\alpha\in\mathbb{C}$, *exhaust all irreducible conformal* $gc_{1,x}$*-modules of finite growth.*

Corollary: The $gc_{1,x}$-modules $\mathbb{C}[\partial]_\alpha$ and $\mathbb{C}[\partial]_\alpha^*$, where $\alpha\in\mathbb{C}$, exhaust all finite irreducible $gc_{1,x}$-modules.

V. IRREDUCIBLE FINITE GROWTH oc_1-MODULES

Now, consider the anti-involution σ on $\mathcal{D}$ defined by (cf. Ref. 11)

$$\sigma(t)=t,\quad \sigma\left(\frac{d}{dt}\right)=-\frac{d}{dt}.$$

Denote by $\mathcal{D}_\sigma$ the fixed subalgebra of $\mathcal{D}$ by $-\sigma$, namely, $\mathcal{D}_\sigma=\{a\in\mathcal{D}\,|\,\sigma(a)=-a\}$. This subalgebra corresponds to the Lie algebra denoted by $\mathcal{D}^+$ in Ref. 11. Let $\hat{\mathcal{D}}_\sigma=\mathcal{D}_\sigma+\mathbb{C}C$ denote the central extension given by the restriction of the cocycle (3.1) on $\mathcal{D}$.

We are interested in representation theory of the Lie subalgebra $\mathcal{D}_\sigma^-=\mathcal{D}^-\cap\hat{\mathcal{D}}_\sigma$ of regular differential operators on $\mathbb{C}$ that are invariant by $-\sigma$. Both subalgebras inherit a $\mathbb{Z}$-gradation from $\mathcal{D}$, since σ preserve the principal $\mathbb{Z}$-gradation of $\mathcal{D}$, and we have $\mathcal{D}_\sigma=\oplus_{j\in\mathbb{Z}}(\mathcal{D}_\sigma)_j$, where

$$(\mathcal{D}_\sigma)_j=\{t^jg(D+(j+1)/2)\,|\,g(w)\in\mathbb{C}[w]\text{is odd}\}. \tag{5.1}$$

In the case of $(\mathcal{D}_\sigma^-)_j$, we need to add condition (3.5) for $j<0$.

Similarly, we have the corresponding subalgebras of $\mathcal{D}^{\mathcal{O}}$, denoted by $\mathcal{D}_\sigma^{\mathcal{O}}$ and $\mathcal{D}_\sigma^{-\mathcal{O}}$.

As in the case of $\mathcal{D}^-$, given a sequence of complex numbers $\Delta=\{\Delta_n\}_{n\in\mathbb{N}_{\mathrm{odd}}}$, we define the highest weight module $L(\Delta;\mathcal{D}_\sigma^-)$ over $\mathcal{D}_\sigma^-$ as the (unique) irreducible module that has a nonzero vector v_Δ with the following properties:

$$(\mathcal{D}_\sigma^-)_jv_\Delta=0\quad\text{for } j<0,\quad (D+1/2)^nv_\Delta=\Delta_nv_\Delta\quad\text{for } n\in\mathbb{N}_{\mathrm{odd}}.$$

The principal gradation of $\mathcal{D}_\sigma^-$ induces the principal gradation $L(\Delta;\mathcal{D}_\sigma^-)=\oplus_{j\in\mathbb{Z}_+}L_j$ such that $L_0=\mathbb{C}v_\Delta$. The module $L(\Delta;\mathcal{D}_\sigma^-)$ is called *quasifinite* if $\dim L_j<\infty$ for all $j\in\mathbb{Z}_+$.

Quasifinite modules over $\mathcal{D}_\sigma^-$ can be constructed as follows. The $\mathcal{D}_\sigma^-$-module $\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ gives us an embedding of $\mathcal{D}_\sigma^-$ in $\widetilde{g\ell}_{+\infty}$. This embedding respect the principal gradations. Now take $\lambda^+\in\mathbb{C}^{+\infty}$ and consider the $\widetilde{g\ell}_{+\infty}$-module $L^+(\lambda^+)$ introduced in (2.1). The same argument as in Ref. 10, gives us the following.

Lemma 5.1: When restricted to $\mathcal{D}_\sigma^-$, *the module* $L^+(\lambda^+)$ *remains irreducible.*

Therefore $L^+(\lambda^+)$ is an irreducible quasifinite highest weight module over $\mathcal{D}_\sigma^-$, and it is easy to see that we have

$$\Delta_n=\sum_{j\geqslant 1}(-j+1/2)^n\lambda_j^+\,,\quad n\in\mathbb{N}_{\text{odd}}\,,$$

so that

$$\Delta(x):=\sum_{n\in\mathbb{N}_{\text{odd}}}\Delta_n x^n/n!=\sum_{j\geqslant 1}\lambda_j^+\,2\sinh((-j+1/2)x)\,.$$

We shall prove the following theorem.

Theorem 5.2: *The $\mathcal{D}_\sigma^-$-modules $L^+(\lambda^+)$, where $\lambda^+\in\mathrm{Par}^+$, exhaust all quasifinite irreducible highest weight $\mathcal{D}_\sigma^-$-modules that have finite growth.*

The basic idea of the proof of Theorem 5.2 is the same as in Theorem 3.2: to reduce the problem to the well developed (in Ref. 11) representation theory of the universal central extension $\hat{\mathcal{D}}_\sigma$.

Recall that the homomorphism $\hat{\varphi}_s^{[m]}:\hat{\mathcal{D}}\to\widehat{g\ell}_\infty^{[m]}$ defined in (3.4) lift to a homomorphism $\hat{\varphi}_s^{[m]}:\hat{\mathcal{D}}^{\mathcal{O}}\to\widehat{g\ell}_\infty^{[m]}$. Now, the restriction $\hat{\varphi}_s^{[m]}:\hat{\mathcal{D}}_\sigma^{\mathcal{O}}\to\widehat{g\ell}_\infty^{[m]}$ to $\hat{\mathcal{D}}_\sigma^{\mathcal{O}}$ is surjective iff $s\notin\mathbb{Z}/2$, and in the other cases, using (5.1), we have that (see Ref. 11 for details)

$$\hat{\varphi}_0^{[m]}:\hat{\mathcal{D}}_\sigma^{\mathcal{O}}\to d_\infty^{[m]}\,,\quad \hat{\varphi}_{-1/2}^{[m]}:\hat{\mathcal{D}}_\sigma^{\mathcal{O}}\to b_\infty^{[m]}\tag{5.2}$$

are surjective homomorphisms. Now, let us consider the restriction to $\mathcal{D}_\sigma^{-\mathcal{O}}$. Since the constrains given by (3.5) do not affect the case $s\neq 0$, we still have that $\hat{\varphi}_s^{[m]}:\mathcal{D}_\sigma^{-\mathcal{O}}\to\widehat{g\ell}_\infty^{[m]}$ $(s\notin\mathbb{Z}/2)$ and $\hat{\varphi}_{-1/2}^{[m]}:\mathcal{D}_\sigma^{-\mathcal{O}}\to b_\infty^{[m]}$ are surjective.

One of the main results of Ref. 11 is the following.

Lemma 5.3: For each $i=1,\ldots,r$, pick a collection $m_i\in\mathbb{Z}_+$, $s_i\in\mathbb{C}$, $\vec{\lambda}_i\in(\mathbb{C}^\infty)^{m_i+1}$, $\vec{c}_i\in\mathbb{C}^{m_i+1}$, such that $s_i\in\mathbb{Z}$ implies $s_i=0$, $s_i\in\frac{1}{2}+\mathbb{Z}$ implies $s_i=-\frac{1}{2}$, and $s_i-s_j\notin\mathbb{Z}$ for $i\neq j$. Then the $\oplus_{i=1}^r\mathfrak{g}^{[m_i]}$-module $\otimes_{i=1}^r L(\mathfrak{g}^{[m_i]};\vec{\lambda}_i,\vec{c}_i)$ remains irreducible when restricted to $\hat{\mathcal{D}}_\sigma$ via the embedding $\oplus_{i=1}^r\hat{\varphi}_{s_i}^{[m_i]}:\hat{\mathcal{D}}_\sigma\to\oplus_{i=1}^r\mathfrak{g}^{[m_i]}$, where $\mathfrak{g}^{[m_i]}=\widehat{g\ell}_\infty^{[m_i]}$ (respectively, $b_\infty^{[m_i]}$ or $d_\infty^{[m_i]}$) if $s_i\notin\mathbb{Z}/2$ (respectively, $s_i=-\frac{1}{2}$ or si=0). All irreducible quasifinite highest weight $\hat{\mathcal{D}}_\sigma$-modules are obtained in this way.

Proof of Theorem 5.2: The proof is similar to that of Theorem 3.2. Due to Lemma 5.3, Theorem 2.4 and (5.2), it is easy to see that if $L(\Delta;\mathcal{D}_\sigma^-)$ has finite growth, then $L(\Delta;\hat{\mathcal{D}}_\sigma)=L(d_\infty^{[m]};\vec{\lambda},\vec{c})$ on which $\hat{\mathcal{D}}_\sigma$ acts via the embedding $\hat{\varphi}_0^{[m]}$.

Choosing $f\in\mathcal{O}_{\text{odd}}$ to vanish in all $j\in\mathbb{Z}$ up to mth derivative except for ith derivative $(0<i\leqslant m)$ at $j=-r$, we see that all operators $u^iE_{r+1,r}-(-u)^iE_{-r+1,-r}$ with $0<i\leqslant m$ lie in the image of $\hat{\varphi}_0^{[m]}(\mathcal{D}_\sigma^{-\mathcal{O}})$.

Suppose that the mth coordinate of $\vec{\lambda}_r$ is nonzero, and that $m>0$. Then $v:=(u^mE_{r+1,r}-(-u)^iE_{-r+1,-r})^Nv_{\vec{\lambda}}\neq 0$ for all $N>0$. But

$$E_{r+1,r+1}v=(N+\lambda_{r+1}^0)v\,.$$

As in Theorem 3.2, restricting to the subalgebra of $d_\infty^{[m]}$ isomorphic to $g\ell_{+\infty}$ consisting of matrices $(a_{i,j}-a_{1-j,1-i})_{i,j\geqslant r+1}$ we conclude by Theorem 2.2, that $L(d_\infty^{[m]};\vec{\lambda},\vec{c})$ is either trivial or is of infinite growth.

Thus, the only possibility that remains is $s=m=0$. As has been already shown, the image of $\hat{\varphi}_s(\mathcal{D}_\sigma^{-\mathcal{O}})$ contains all $E_{r+1,r}-E_{1-r,-r}$ for all $r\neq 0$, hence it contains all operators from $d_\infty\cap(g\ell_{-\infty}\oplus g\ell_{+\infty})\simeq g\ell_{+\infty}$. Therefore, by Theorem 2.2, the highest weight of a finite growth $\mathcal{D}_\sigma^-$-module must be the same as one of the $\mathcal{D}_\sigma^-$-modules $L^+(\lambda^+)$ with $\lambda^+\in\mathrm{Par}^+$.

□

Now we shall construct the $\mathcal{D}_\sigma^-$-modules $L^+(\lambda^+)$ explicitly. The $\mathcal{D}^-$-module $V=\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ defined in (3.6), viewed as a $\mathcal{D}_\sigma^-$-module, remains irreducible. This is the highest weight $\mathcal{D}_\sigma^-$-module of growth 1 isomorphic to $L^+(\omega_1)$ where $\omega_1=(1,0,\ldots)\in \mathrm{Par}^+$.

Observe that the $\mathcal{D}_\sigma^-$-module $\mathbb{C}[t]^*=\oplus_{j\in\mathbb{Z}_+}(\mathbb{C}t^j)^*$ is isomorphic to $L^+(\omega_1)$.

As in the Schur–Weyl theory, the $\mathcal{D}_\sigma^-$-module $T^M(V)$ has a natural decomposition as $(\mathcal{D}_\sigma^-,S_M)$-modules:

$$T^M(V)=\bigoplus_{\substack{\lambda^+\in \mathrm{Par}^+\\ |\lambda^+|=M}} V_{\lambda^+}\otimes U_{\lambda^+},$$

where U_{λ^+} denotes the irreducible S_M-module corresponding to the partition λ^+.

Lemma 5.4: The $\mathcal{D}_\sigma^-$-modules V_{λ^+} are irreducible.

Proof: As in the proof of Theorem 5.2, we extend the action of $\mathcal{D}_\sigma^-$ on V_{λ^+} to $(\mathcal{D}_\sigma^{-\mathcal{O}})_j$ for each $j\neq 0$, to obtain that any $\mathcal{D}_\sigma^-$-submodule of V_{λ^+} is a submodule over $g\ell_{+\infty}[\simeq d_\infty\cap(g\ell_{+\infty}\oplus g\ell_{-\infty})]$. But, by Schur–Weyl theory, the $g\ell_{+\infty}$-module V_{λ^+} is irreducible, which completes the proof. □

Thus, we have proved the following.

Theorem 5.5: *The $\mathcal{D}_\sigma^-$-module $T^M(V)$ has the following decomposition as $(\mathcal{D}_\sigma^-,S_M)$-modules:*

$$T^M(V)=\bigoplus_{\substack{\lambda^+\in \mathrm{Par}^+\\ |\lambda^+|=M}} L^+(\lambda^+)\otimes U_{\lambda^+},$$

where U_{λ^+} denotes the irreducible S_M-module corresponding to the partition λ^+.

Remark: Considering $\lambda^+\in\mathbb{C}^{+\infty}$ we may say that irreducible highest weight $\mathcal{D}_\sigma^-$-modules of finite growth are parametrized by nonincreasing sequences of integers $(\lambda_j)_{j\in\mathbb{N}}\in\mathbb{C}^{+\infty}$. Equivalently, letting $m_i=\lambda_i-\lambda_{i+1}$ we may say that these modules are parametrized by sequences of non-negative integers $(m_i)_{i\in\mathbb{N}}$, all but finite numbers of which are zero.

Recall that the extended annihilation algebra $\mathrm{Lie}^-(oc_1)$ for oc_1 is isomorphic to the direct sum of the Lie algebra $\mathcal{D}_\sigma^-$ and the one-dimensional Lie algebra $\mathbb{C}[\partial+d/dt]$ and that conformal modules for a Lie conformal algebra coincide with the conformal modules over the associated extended annihilation algebra.[7]

Theorems 5.2 and the above remarks imply the following.

Theorem 5.6: *The oc_1-modules $L^+(\lambda^+)_\alpha$, where $\lambda^+\in\mathrm{Par}^+$, $\alpha\in\mathbb{C}$, exhaust all irreducible conformal oc_1-modules of finite growth.*

Corollary: The gc_1-modules $L^+(\lambda^+)$, where $\lambda^+\in\mathrm{Par}^+$, remain irreducible when restricted to oc_1.

Corollary: The oc_1-modules $\mathbb{C}[\partial]_\alpha$, where $\alpha\in\mathbb{C}$, exhaust all finite irreducible oc_1-modules.

VI. IRREDUCIBLE FINITE GROWTH spc_1-MODULES

Now, consider the anti-involution $\overline{\sigma}$ on $\mathcal{D}_0$ defined by

$$\overline{\sigma}(t^kDf(D))=-t^kDf(-D-k).$$

This antiinvolution was studied by Bloch[2] in connection with the values of ζ-function.

Denote by $\mathcal{D}_{0,\overline{\sigma}}$ the Lie subalgebra of $\mathcal{D}_0$ fixed by $-\overline{\sigma}$. Let $\hat{\mathcal{D}}_{0,\overline{\sigma}}=\mathcal{D}_{0,\overline{\sigma}}+\mathbb{C}C$ denote the central extension given by the restriction of the cocycle on $\mathcal{D}$.

We are interested in representation theory of the Lie subalgebra $\mathcal{D}^-_{0,\overline{\sigma}}=\mathcal{D}^-\cap\hat{\mathcal{D}}_{0,\overline{\sigma}}$ of regular differential operators on $\mathbb{C}$ that kills constants and are invariant by $-\overline{\sigma}$. Both subalgebras inherit a $\mathbb{Z}$-gradation from $\mathcal{D}_0$, since $\overline{\sigma}$ preserve the principal $\mathbb{Z}$-gradation of $\mathcal{D}_0$: $\mathcal{D}_{0,\overline{\sigma}}=\oplus_{j\in\mathbb{Z}}(\mathcal{D}_{0,\overline{\sigma}})_j$, where

$$(\mathcal{D}_{0,\bar{\sigma}})_j=\left\{ t^j D\, g\left(D+\frac{j}{2}\right) \,\middle|\, g(w)\in\mathbb{C}[w]\text{is even} \right\}. \tag{6.1}$$

In the case of $(\mathcal{D}^-_{0,\bar{\sigma}})_j$, we need to add condition (3.5) for $j<0$.

Similarly, we have the corresponding subalgebras of $\mathcal{D}^{\mathcal{O}}$, denoted by $\mathcal{D}^{\mathcal{O}}_{0,\bar{\sigma}}$ and $\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}}$.

As in the case of $\mathcal{D}^-$, given a sequence of complex numbers $\Delta=\{\Delta_n\}_{n\in\mathbb{N}_{\text{odd}}}$, we define the highest weight module $L(\Delta;\mathcal{D}^-_{0,\bar{\sigma}})$ over $\mathcal{D}^-_{0,\bar{\sigma}}$ as the (unique) irreducible module that has a nonzero vector v_Δ with the following properties:

$$(\mathcal{D}^-_{0,\bar{\sigma}})_j v_\Delta=0 \quad \text{for } j<0, \quad D^n v_\Delta=\Delta_n v_\Delta \quad \text{for } n\in\mathbb{N}_{\text{odd}}.$$

The principal gradation of $\mathcal{D}^-_{0,\bar{\sigma}}$ induces the principal gradation $L(\Delta;\mathcal{D}^-_{0,\bar{\sigma}})=\oplus_{j\in\mathbb{Z}_+}L_j$ such that $L_0=\mathbb{C}v_\Delta$. The module $L(\Delta;\mathcal{D}^-_{0,\bar{\sigma}})$ is called *quasifinite* if $\dim L_j<\infty$ for all $j\in\mathbb{Z}_+$.

As in the preceding section, the $\mathcal{D}^-_{0,\bar{\sigma}}$-module $\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ gives us an embedding of $\mathcal{D}^-_{0,\bar{\sigma}}$ in $\widetilde{g\ell}_{+\infty}$. This embedding respects the principal gradations. Now take $\lambda^+\in\mathbb{C}^{+\infty}$ and consider the $\widetilde{g\ell}_{+\infty}$-module $L^+(\lambda^+)$ introduced in (2.1). The same argument as in Ref. 10, gives us the following.

Lemma 6.1: When restricted to $\mathcal{D}^-_{0,\bar{\sigma}}$, the quasifinite module $L^+(\lambda^+)$ remains irreducible.

We shall prove the following theorem.

Theorem 6.2: *The $\mathcal{D}^-_{0,\bar{\sigma}}$-modules $L^+(\lambda^+)$, where $\lambda^+\in\text{Par}^+$, exhaust all quasifinite irreducible highest weight $\mathcal{D}^-_{0,\bar{\sigma}}$-modules that have finite growth.*

The basic idea of the proof of Theorem 6.2 is the same as in Theorem 3.2: to reduce the problem to the recently developed (in Ref. 4) representation theory of the universal central extension $\hat{\mathcal{D}}_{0,\bar{\sigma}}$.

Recall that the homomorphism $\hat{\varphi}^{[m]}_s:\hat{\mathcal{D}}\to\widehat{g\ell}^{[m]}_\infty$ defined in (3.4) lift to a homomorphism $\hat{\varphi}^{[m]}_s:\hat{\mathcal{D}}^{\mathcal{O}}\to\widehat{g\ell}^{[m]}_\infty$. Now, the restriction $\hat{\varphi}^{[m]}_s:\hat{\mathcal{D}}^{\mathcal{O}}_{0,\bar{\sigma}}\to\widehat{g\ell}^{[m]}_\infty$ to $\hat{\mathcal{D}}^{\mathcal{O}}_{0,\bar{\sigma}}$ is surjective iff $s\notin\mathbb{Z}/2$, and in the other case, using (6.1), we have that (see Ref. 2 for details)

$$\hat{\varphi}^{[m]}_s:\hat{\mathcal{D}}^{\mathcal{O}}_{0,\bar{\sigma}}\to c^{[m]}_\infty, \qquad s\in\mathbb{Z}/2 \tag{6.2}$$

is a surjective homomorphism. Now, let us consider the restriction to $\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}}$. Since the constrains given by (3.5) do not affect the case $s\neq0$, we still have that $\hat{\varphi}^{[m]}_s:\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}}\to\widehat{g\ell}^{[m]}_\infty$ $(s\notin\mathbb{Z}/2)$ and $\hat{\varphi}^{[m]}_{-1/2}:\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}}\to c^{[m]}_\infty$ are surjective.

One of the main results of Ref. 4 is the following.

Lemma 6.3: For each $i=1,\ldots,r$, pick a collection $m_i\in\mathbb{Z}_+$, $s_i\in\mathbb{C}$, $\vec{\lambda}_i\in(\mathbb{C}^\infty)^{m_i+1}$, $\vec{c}_i\in\mathbb{C}^{m_i+1}$, such that $s_i\in\mathbb{Z}$ implies $s_i=0$, $s_i\in\frac{1}{2}+\mathbb{Z}$ implies $s_i=-\frac{1}{2}$, and $s_i-s_j\notin\mathbb{Z}$ for $i\neq j$. Then the $\oplus^r_{i=1}\mathfrak{g}^{[m_i]}$-module $\otimes^r_{i=1}L(\mathfrak{g}^{[m_i]};\vec{\lambda}_i,\vec{c}_i)$ remains irreducible when restricted to $\hat{\mathcal{D}}_{0,\bar{\sigma}}$ via the embedding $\oplus^r_{i=1}\hat{\varphi}^{[m_i]}_{s_i}:\hat{\mathcal{D}}_{0,\bar{\sigma}}\to\oplus^r_{i=1}\mathfrak{g}^{[m_i]}$, where $\mathfrak{g}^{[m_i]}=\widehat{g\ell}^{[m_i]}_\infty$ (respectively, $c^{[m_i]}_\infty$) if $s_i\notin\mathbb{Z}/2$ (respectively, $s_i=-\frac{1}{2}$ or $s_i=0$). All irreducible quasifinite highest weight $\hat{\mathcal{D}}_{0,\bar{\sigma}}$-modules are obtained in this way.

Proof of Theorem 6.2: The proof is similar to that of Theorem 3.2. Due to Lemma 6.3, Theorem 2.6 and (6.2), it is easy to see that if $L(\Delta;\mathcal{D}^-_{0,\bar{\sigma}})$ has finite growth, then $L(\Delta;\hat{\mathcal{D}}_{0,\bar{\sigma}})=L(c^{[m]}_\infty;\vec{\lambda},\vec{c})$ on which $\hat{\mathcal{D}}_{0,\bar{\sigma}}$ acts via the embedding $\hat{\varphi}^{[m]}_0$.

Choosing $f\in\mathcal{O}_{\text{odd}}$ to vanish in all $j\in\mathbb{Z}$ up to mth derivative except for ith derivative $(0<i\leqslant m)$ at $j=-r$, we see that all operators $u^iE_{r+1,r}+(-u)^iE_{-r+1,-r}$ with $0<i\leqslant m$ lie in the image of $\hat{\varphi}^{[m]}_0(\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}})$.

Suppose that the mth coordinate of $\vec{\lambda}_r$ is nonzero, and that $m>0$. Then $v:=(u^mE_{r+1,r}+(-u)^iE_{-r+1,-r})^Nv_{\vec{\lambda}}\neq0$ for all $N>0$. But

$$E_{r+1,r+1}v=(N+\lambda^0_{r+1})v.$$

As in Theorem 3.2, restricting to the subalgebra of $c_\infty^{[m]}$ isomorphic to $g\ell_{+\infty}$ consisting of matrices $(a_{i,j}-(-1)^{i+j}a_{1-j,1-i})_{i,j\geqslant r+1}$ we conclude by Theorem 2.2, that $L(c_\infty^{[m]};\vec{\lambda},\vec{c})$ is either trivial or is of infinite growth.

Thus, the only possibility that remains is $s=m=0$. As has been already shown, the image of $\hat{\varphi}_s(\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}})$ contains all $E_{r+1,r}+E_{1-r,-r}$ for all $r\neq 0$, hence it contains all operators from $c_\infty\cap(g\ell_{-\infty}\oplus g\ell_{+\infty})\simeq g\ell_{+\infty}$. Therefore, by Theorem 2.2, the highest weight of a finite growth $\mathcal{D}^-_{0,\bar{\sigma}}$-module must be the same as one of the $\mathcal{D}^-_{0,\bar{\sigma}}$-modules $L^+(\lambda^+)$ with $\lambda^+\in \mathrm{Par}^+$.

□

As in the preceding section, we can construct the $\mathcal{D}^-_{0,\bar{\sigma}}$-modules $L^+(\lambda^+)$ explicitly. The $\mathcal{D}^-$-module $V=\mathbb{C}[t,t^{-1}]/\mathbb{C}[t]$ defined in (3.6), viewed as a $\mathcal{D}^-_{0,\bar{\sigma}}$-module, remains irreducible. This is the highest weight $\mathcal{D}^-_{0,\bar{\sigma}}$-module of growth 1 isomorphic to $L^+(\omega_1)$ where $\omega_1=(1,0,\ldots)\in \mathrm{Par}^+$.

Observe that the $\mathcal{D}^-_{0,\bar{\sigma}}$-module $\mathbb{C}[t]^*=\oplus_{j\in\mathbb{Z}_+}(\mathbb{C}t^j)^*$ is isomorphic to $L^+(\omega_1)$.

As in the Schur–Weyl theory, the $\mathcal{D}^-_{0,\bar{\sigma}}$-module $T^M(V)$ has a natural decomposition as $(\mathcal{D}^-_{0,\bar{\sigma}},S_M)$-modules:

$$T^M(V)=\bigoplus_{\substack{\lambda^+\in \mathrm{Par}^+\\ |\lambda^+|=M}} V_{\lambda^+}\otimes U_{\lambda^+},$$

where U_{λ^+} denotes the irreducible S_M-module corresponding to the partition λ^+.

Lemma 6.4: The $\mathcal{D}^-_{0,\bar{\sigma}}$-modules V_{λ^+} are irreducible.

Proof: As in the proof of Theorem 5.2, we extend the action of $\mathcal{D}^-_{0,\bar{\sigma}}$ on V_{λ^+} to $(\mathcal{D}^{-\mathcal{O}}_{0,\bar{\sigma}})_j$ for each $j\neq 0$, to obtain that any $\mathcal{D}^-_{0,\bar{\sigma}}$-submodule of V_{λ^+} is a submodule over $g\ell_{+\infty}[\simeq c_\infty\cap(g\ell_{+\infty}\oplus g\ell_{-\infty})]$. But, by Schur–Weyl theory, the $g\ell_{+\infty}$-module V_{λ^+} is irreducible, which completes the proof. □

Thus, we have proved the following.

Theorem 6.5: *The $\mathcal{D}^-_{0,\bar{\sigma}}$-module $T^M(V)$ has the following decomposition as $(\mathcal{D}^-_{0,\bar{\sigma}},S_M)$-modules:*

$$T^M(V)=\bigoplus_{\substack{\lambda^+\in \mathrm{Par}^+\\ |\lambda^+|=M}} L^+(\lambda^+)\otimes U_{\lambda^+},$$

where U_{λ^+} denotes the irreducible S_M-module corresponding to the partition λ^+.

Recall that the extended annihilation algebra $\mathrm{Lie}^-(spc_1)$ for spc_1 is isomorphic to the direct sum of the Lie algebra $\mathcal{D}^-_{0,\bar{\sigma}}$ and the one-dimensional Lie algebra $\mathbb{C}[\partial+(d/dt)]$ and that conformal modules for a Lie conformal algebra coincide with the conformal modules over the associated extended annihilation algebra.[7]

Theorems 6.2 and the above remarks imply the following.

Theorem 6.6: *The spc_1-modules $L^+(\lambda^+)_\alpha$, where $\lambda^+\in \mathrm{Par}^+$, $\alpha\in\mathbb{C}$, exhaust all irreducible conformal spc_1-modules of finite growth.*

Corollary: The gc_1-modules $L^+(\lambda^+)$, where $\lambda^+\in \mathrm{Par}^+$, remain irreducible when restricted to spc_1.

Corollary: The spc_1-modules $\mathbb{C}[\partial]_\alpha$, where $\alpha\in\mathbb{C}$, exhaust all finite irreducible spc_1-modules.

ACKNOWLEDGMENTS

C. Boyallian and J. Liberati were supported in part by Conicet, ANPCyT, Agencia Cba Ciencia, Secyt-UNC and Fomec (Argentina). Special thanks go to MSRI (Berkeley) for the hospitality during our stay there, where part of this work was done.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

On the invariants of some solvable rigid Lie algebras

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(Received 5 April 2002; accepted 21 October 2002)

We determine fundamental systems of invariants for complex solvable rigid Lie algebras having nonsplit nilradicals of characteristic sequence (3,1,...,1), these algebras being the natural followers of solvable algebras having Heisenberg nilradicals. A special case of this allows us to obtain a criterion to determine the number of functionally independent invariants of rank one subalgebras of (real or complex) solvable Lie algebras. Finally, we give examples of the inverse procedure, obtaining fundamental systems of an algebra starting from rank one subalgebras, and a criterion for the nonexistence of nontrivial invariants. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1532536]

I. INTRODUCTION

An important problem arising in the theory of representations of Lie algebras and various physical applications is the determination of invariant functions for the coadjoint representation. These are useful for labeling irreducible representations or splitting arbitrary representations into irreducible ones. Reductions like the Levi decomposition theorem simplify the question to the classes of semi-simple and solvable Lie algebras. The invariants in the semi-simple case were determined in 1950 by Racah.[18] Here the invariants are polynomials, which correspond to classical Casimir operators (i.e., polynomials in the generators which are in the center of the universal enveloping algebra). Their number coincides with the rank of the algebra. The study of the non-semi-simple case is physically motivated by considerations like internal symmetries of particles or the invariant operators of symmetry groups of physical systems.[9,13] Important groups such as the Galilei and Poincaré groups have been deeply studied,[11–13,19] as well as the subgroups of the latter. These invariants allow us to characterize certain systems by giving their energy spectra, angular momenta, etc. For solvable Lie algebras, much less is known. These algebras have shown their interest in relation with the integrability problem of Hamiltonian systems. Their invariants have been determined up to dimension six.[15,17] The invariants found here need not be polynomials any more, which suggests calling them generalized invariants. The nonexistence of classifications of solvable algebras in dimension $n \geqslant 7$ forces us to restrict to more concrete classes. In this frame, the generalized Casimir invariants of solvable algebras having an Abelian or a Heisenberg Lie algebra as nilradical (i.e., as maximal nilpotent ideal) have recently been computed.[14,20] The choice of these maximal nilpotent ideals is not casual. The Heisenberg Lie algebra is the simplest nontrivial nilpotent Lie algebra, and has the lowest nilpotence index. Their deformations are of much interest in the study of Lie algebras of nilindex 2. However, for a solvable Lie algebra with arbitrary nilradical the invariants will not be inferrable in arbitrary dimension, either because the structure of the algebra depends on too many parameters or because of formidable computational obstructions.[20] However, if we restrict to the class of rigid (also called stable) Lie algebras, i.e., the algebras all of whose deformations lead to an equivalent structure, the number and form of the invariants can always be determined in arbitrary dimension, at least what concerns solvable algebras (the semi-simple being well known). This is a consequence of the structural properties of these algebras, which are determined, in some sense, by the action of semisimple elements on the

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maximal nilpotent ideal. The main advantage of studying rigid algebras lies in the fact that the analysis of the invariants in low dimension will always allow us to determine the number and the form of the invariants in arbitrary dimension.

Starting from this situation, we determine fundamental systems of invariants for all solvable rigid Lie algebras whose nilradical is a nonsplit of characteristic sequence (3,1,...,1). These algebras are the natural followers of those having Heisenberg nilradicals. It is shown that the number of functionally independent invariants is a linear function of their rank. As applications, we deduce a general result on the cardinal of fundamental systems of invariants of rank one subalgebras of a solvable Lie algebra. The converse of this procedure, whenever possible, is also of interest, since it allows us to calculate fundamental systems of an algebra analyzing certain rank one subalgebras. In particular, we can find a criterion to ensure that a solvable Lie algebras has no nontrivial invariants.

We convene that nonwritten brackets are either zero or obtained by antisymmetry. We also use Einstein's convention for sums. Unless otherwise stated, any Lie algebra is nonsplit (i.e., it is not a direct sum of ideals) and complex.

II. GENERALITIES

Let G be a connected Lie group and $\mathfrak{g}$ its Lie algebra. As known, the coadjoint representation is given by

$$\mathrm{ad}^*: \mathrm{G} \to \mathrm{GL}(\mathfrak{g}^*): \quad (\mathrm{ad}_g^* x)(y) = x(\mathrm{ad}_{g^{-1}} y), \quad x, y \in \mathfrak{g}^*, g \in \mathrm{G} \tag{2.1}$$

and a function $F \in C^\infty \mathfrak{g}^*$ is called invariant if $F(x) = F(\mathrm{ad}_g^* x)$. Clearly it suffices to find a maximal set of functionally independent invariants to obtain all of them. Such a family is usually called a fundamental set of invariants for the coadjoint representation. The most extended method in the physical literature to obtain the invariants of a Lie algebra is not the orbit method,[9] but its reduction to the problem of solving a system of linear first order partial differential equations.[1] Low dimensional Lie algebras and subalgebras of the Poincaré algebra have been studied using this procedure.[14–17] Let $\mathfrak{g}$ be an n-dimensional Lie algebra with structure constants $\{C_{ij}^k\}$ over the basis $\{X_1, \ldots, X_n\}$. Let $\{x_1, \ldots, x_n\}$ be the dual basis and consider the differential operators

$$\widehat{X}_i = -C_{ij}^k x_k \frac{\partial}{\partial x_j}, \quad 1 \leqslant i \leqslant n. \tag{2.2}$$

These operators act on differentiable functions $f(x_1, \ldots, x_n) \in C^\infty(\mathfrak{g}^*)$. It is a straightforward verification that these operators satisfy the brackets

$$[\hat{X}_i, \hat{X}_j] = C_{ij}^k \hat{X}_k,$$

and therefore define a representation of $\mathfrak{g}$. Now an invariant is a function $F(x_1, \ldots, x_n)$ such that

$$\hat{X}_i F(x_1, \ldots, x_n) = 0, \quad 1 \leqslant i \leqslant n. \tag{2.3}$$

This reduces the problem to solve the system of partial differential equations (PDEs):

$$-C_{ij}^k x_k \frac{\partial}{\partial x_j} F(x_1, \ldots, x_n) = 0, \ 1 \leqslant i \leqslant n. \tag{2.4}$$

Since the solutions of this system are not necessarily polynomials, it is reasonable to call the solutions generalized Casimir invariants. If F is a polynomial solution of (2.4), then we obtain a Casimir operator by symmetrizing the polynomial with respect to the variables x_i and then substituting them by the corresponding generator X_i of the algebra. The corresponding bracket in the enveloping algebra satisfies

$$[X_i, F(X_1,\ldots,X_n)]=0, \tag{2.5}$$

which is easily seen to be equivalent to requirement (2.4). For rational invariants an analogous procedure is possible, by symmetrizing numerator and denominator and substituting properly.

The number of functionally independent invariants $\mathcal{N}$ of the coadjoint representation ad* of a Lie algebra $\mathfrak{g}$ can be computed by elementary algebraic means, as shown Beltrametti and Blasi.[5] They proved that

$$\mathcal{N}(\mathfrak{g})=\dim(\mathfrak{g})-sup_{x_1,\ldots,x_n}\{\text{rank } (C_{ij}^k x_k)\}, \tag{2.6}$$

where $(C_{ij}^k x_k)$ is the matrix representing the commutator table of $\mathfrak{g}$ for the chosen basis. Since the matrix $(C_{ij}^k x_k)$ is skew-symmetric, its rank is even, which implies that dim $(\mathfrak{g})$ and $\mathcal{N}(\mathfrak{g})$ have the same parity. However, the preceding formula does not distinguish whether the solutions are polynomials or not. Thus we will have $p \leqslant \mathcal{N}(\mathfrak{g})$ Casimir operators (and possibly none, as happens for the algebra of dilatations and translations in the plane, which has one rational solution[1]) for the general case.

The following example illustrates the method and the application of the Beltrametti–Blasi formula: Consider the four dimensional Lie algebra given by the brackets

$$[X_0,X_1]=X_2,$$

$$[X_0,X_2]=X_3,$$

over the basis $\{X_0,X_1,X_2,X_3\}$ (the representations of this algebra are used in the theory of anharmonic oscillators). The matrix associated to the commutator table is

$$\begin{pmatrix} 0 & x_2 & x_3 & 0 \\ -x_2 & 0 & 0 & 0 \\ -x_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.7}$$

The rank of the matrix is two, so that this algebra has a fundamental set of invariants formed by two functions, which are solutions of the following system:

$$\hat{X}_0 F=(-x_2\partial_{x_2}-x_3\partial_{x_2})F=0, \tag{2.8}$$

$$\hat{X}_1 F=(x_2\partial_{x_0})F=0, \tag{2.9}$$

$$\hat{X}_2 F=(x_3\partial_{x_0})F=0, \tag{2.10}$$

$$\hat{X}_3 F=0. \tag{2.11}$$

The equations $\hat{X}_i F=0$ $(i=1,2)$ imply that F does not depend on x_0. From $\hat{X}_3 F=0$ we see that x_3 is a polynomial solution, while the equation $\hat{X}_1 F=0$ gives us the subsidiary equation

$$\frac{dx_1}{x_2}=\frac{dx_2}{x_3}, \tag{2.12}$$

which can be immediately integrated and gives the solution $x_2^2-2x_1x_3$. In this case both solutions are polynomials and correspond to classical Casimir operators.

As told before, invariants of solvable Lie algebras have been determined only in low dimensions, due to the impossibility of obtaining classifications in dimensions $n \geqslant 7$ (even the existing

classification of six dimensional solvable Lie algebras has been proven to contain mistakes). Two types of solvable algebras have been analyzed in some detail in arbitrary dimension: those having Abelian nilradical and those having it isomorphic to the Heisenberg Lie algebra $\mathfrak{h}_k$. An important class of solvable rigid Lie algebras consists of those algebras having a Heisenberg Lie algebra $\mathfrak{h}_k$ as nilradical. Since for rigid Lie algebras the torus determines almost completely the isomorphism class of the nilradical and these algebras decompose in a particular manner, in addition to the existing algorithms that allow (theoretically) a classification of solvable rigid Lie algebras,[4] it is reasonable to focus on this class and their invariants. We therefore recall the most elementary facts about rigidity:

The set $\mathcal{L}^n$ of all n-dimensional Lie algebras is well known to form an algebraic variety, on which the general linear group $\mathrm{GL}(n,\mathbb{C})$ acts as follows:

$$\phi*[X,Y]_{\mathfrak{g}}=\phi[\phi^{-1}X,\phi^{-1}Y]_{\mathfrak{g}},\quad x,y\in\mathfrak{g}, \tag{2.13}$$

where $[\_,\_]_{\mathfrak{g}}$ denotes the Lie bracket of $\mathfrak{g}$. The action is nothing more than the changes of basis, so that it is immediate that the orbit $\mathcal{O}(\mathfrak{g})$ of $\mathfrak{g}$ by this action consists of all Lie algebras isomorphic to $\mathfrak{g}$.

Definition 1: The algebra $\mathfrak{g}$ is called rigid if the orbit $\mathcal{O}(\mathfrak{g})$ is open in $\mathcal{L}^n$.

If an algebra $\mathfrak{g}$ does not admit nontrivial deformations, i.e., if it is rigid in the sense of Gerstenhaber, then its orbit is easily seen to be open. Indeed the classical definition of rigidity and Definition 1 are equivalent over $\mathbb{C}$. Rigidity imposes severe structural restrictions in the solvable case, which simplifies their description. Solvable rigid Lie algebras $\mathfrak{g}$ decompose as a semidirect product:

$$\mathfrak{g}=\mathfrak{n}\vec{\oplus}\mathfrak{t}, \tag{2.14}$$

where $\mathfrak{n}$ is the nilradical of $\mathfrak{g}$ and $\mathfrak{t}$ is an Abelian subalgebra consisting of ad-semisimple endomorphisms. Such an algebra will be called decomposable, and $\mathfrak{t}$ will called a torus of derivations. The similarity of this decomposition with the Cartan decomposition of classical algebras is suggested to consider a linear system of roots for solvable decomposable Lie algebras. These are formal linear systems for which the eigenvalues of the adjoint operators $\mathrm{ad}(X)$ for elements $X\in\mathfrak{t}$ are solutions. The rank of this system provides a useful criterion for the rigidity of a solvable Lie algebra.

Given a solvable rigid Lie algebra $\mathfrak{n}\vec{\oplus}\mathfrak{t}$, we say that $X\neq 0$ is a regular vector if the dimension of the kernel of the adjoint operator is minimal among the elements of $\mathfrak{t}$, i.e.,

$$\dim\ \mathrm{Ker}\,\mathrm{ad}(X)=\min\ \{\dim\ \mathrm{Ker}\,\mathrm{ad}(Y)\ \mid\ Y\in\mathfrak{t}\}. \tag{2.15}$$

If $q=\dim\ \mathrm{Ker}\,\mathrm{ad}(X)$, then we can find a basis formed by eigenvectors of the adjoint operator $(X_1,\ldots,X_n=X)$ such that $(X_1,\ldots,X_{p+q})$ is a basis of the nilradical $\mathfrak{n}$, $(X_{p+1+q},\ldots,X_n)$ is a basis of $\mathfrak{t}$ and $(X_{p+1},\ldots,X_n)$ is a basis of $\mathrm{Ker}\ \mathrm{ad}(X)$.

The linear system of roots associated to $(X_1,\ldots,X_n)$ is the linear system to $n-1$ variables x_i whose equations are

$$x_i+x_j=x_k \tag{2.16}$$

if the X_k-component of the bracket $[X_i,X_j]$ is nonzero. We will note this system by $S(X)$ or simply (S). The following result establishes a necessary condition for a Lie algebra to be rigid.[10]

Theorem 1: *(of the rank[10]) If the solvable, decomposable Lie algebra $\mathfrak{g}=\mathfrak{n}\vec{\oplus}\mathfrak{t}$ is rigid, then for all regular vectors X we have*

$$\mathrm{rank}\ \ S(X)=\dim\mathfrak{n}-1.$$

In particular the rank does not depend on the choice of the basis or the regular vector.

Corollary 1: If $\mathfrak{g}=\mathfrak{n}\vec{\oplus}\mathfrak{t}$ *is rigid, then* $\mathfrak{t}$ *is a maximal torus (for the inclusion relation).*

As an example of how the linear system is applied, let us consider the four dimensional subalgebra $P_{7,4}$ of the Poincaré algebra generated by $\{K_3, L_1-K_2, L_2+K_1, P_0-P_3\}$, where L_i denotes the rotation operators, K_i the boosts and P_j the translations.[1] $P_{7,4}$ is a solvable Lie algebra whose derived algebra $[P_{7,4}, P_{7,4}]$ is isomorphic to the three dimensional Abelian algebra $3A_1$. Therefore the system (S) associated to $P_{7,4}$ is zero (K_3 being a regular vector), and since $\dim(3A_1)-1\neq\operatorname{rank}(S)$, this algebra is not rigid. Indeed the minimal dimensional rigid Lie algebra which contains $P_{7,4}$ as subalgebra is $P_{7,2}$, which is generated by the above generators and $\{P_1, P_2\}$.[17]

For a decomposable algebra, we note the rank by $rg(\mathfrak{g})=\dim\ \mathfrak{t}$. If $\mathfrak{g}$ is rigid we can always find a regular vector such that the operator $\operatorname{ad}(X)$ is diagonalizable and its eigenvalues are integers.[10] The preceding results allow us to search for rigid laws either starting with a sequence of weights for a fixed regular vector X, or considering fixed nilpotent Lie algebras as nilradicals and analyzing their semisimple derivations. Since nilpotent Lie algebras are classified only for dimension $n\leqslant 7$, the latter method is valid in generic dimension only if we introduce a new invariant, called the characteristic sequence.[10] This invariant measures the dimension of successive Jordan blocks of the matrices of adjoint operators $\operatorname{ad}(X)$, and in particular it indicates the nilpotence index of the algebra. Let $\mathfrak{n}$ be a nilpotent Lie algebra and $X\in\mathfrak{n}-[\mathfrak{n},\mathfrak{n}]$ be a nonzero vector. We denote by $c(X)$ the ordered sequence of dimensions of the Jordan blocks for the adjoint operator $\operatorname{ad}(X)$. Considering the lexicographical order in the set of these sequences, i.e.,

$$(c_1,\ldots,c_t)\geqslant(c_1',\ldots,c_s')\Leftrightarrow\exists i \text{ such that } c_j=c_j' \text{ for } i>j \text{ and } c_i>c_i', \tag{2.17}$$

we define the characteristic sequence of $\mathfrak{g}$ as

$$c(\mathfrak{g})=\max_{X\in\mathfrak{g}-[\mathfrak{g},\mathfrak{g}]}\{c(X)\}. \tag{2.18}$$

A vector $X\neq 0$, $X\in\mathfrak{g}-[\mathfrak{g},\mathfrak{g}]$ satisfying $c(\mathfrak{g})=c(X)$ is called characteristic vector.

Example 1: Let $\mathfrak{n}$ *be a nilpotent Lie algebra.*

(i) *If* $c(\mathfrak{n})=(1,1,\ldots,1)$, *then for any element* $X\notin[\mathfrak{n},\mathfrak{n}]$ *the Jordan form of* $\operatorname{ad}(X)$ *is zero. This shows that* $\mathfrak{n}$ *is an Abelian Lie algebra.*

(ii) *If* $c(\mathfrak{n})=(2,1,\ldots,1)$, *then* $\mathfrak{n}$ *is an algebra of nilindex 2, i.e.,* $[X,[Y,Z]]=0$ *for any* $X,Y,Z\in\mathfrak{n}$. *We can find a basis* $\{X_1,\ldots,X_n\}$ *such that* X_1 *is a regular vector,* $[X_1,X_2]=X_3$ *and* $[X_1,X_i]=0$ *for* $i\geqslant 3$. *In particular the rank of the matrix of* $\operatorname{ad}(X_1)$ *is one. If there exists a vector* $Y=\Sigma_{i\geqslant 3}a_iX_i$ *such that* $[X_2,Y]\neq 0$, *then necessarily* $[X_2,Y]=\alpha X_3$, *since otherwise we can consider the vector* $X_1'=X_1+X_2$ *whose matrix of* $\operatorname{ad}(X_1')$ *has rank 2, contradicting the assumption that* X_1 *is regular. Therefore we can reorder the basis such that* $\mathfrak{g}\simeq\mathfrak{h}_k\oplus\mathbb{C}^{n-(2k+1)}$, *where* $\mathfrak{h}_k$ *is the* $(2k+1)$*-dimensional Heisenberg Lie algebra. If, moreover,* $\mathfrak{g}$ *is not a direct sum of ideals, then* $\dim(\mathfrak{g})$ *is odd and* $\mathfrak{g}=\mathfrak{h}_k$ *for some* $k\geqslant 1$.

Thus the characteristic sequence divides the nilpotent Lie algebras of nilindex k into more specific classes. It should be remarked that the classification of seven-dimensional nilpotent Lie algebras can be made by using only this invariant. The natural followers of Heisenberg Lie algebras are those of characteristic sequence $(3,1,\ldots,1)$. These are the simplest nilpotent Lie algebras of nilindex 3. Contrary to the previous case, where the Heisenberg is the only nonsplit algebra obtained, we will obtain two families of algebras having this property:[2]

Theorem 2: *Any solvable rigid law whose nilradical* $\mathfrak{n}$ *is of characteristic sequence* $(3,1,\ldots,1)$ *is isomorphic to one of the following algebras:*

(i) The Lie algebra $\mathfrak{d}_{2m}=\mathfrak{g}_{2m}\vec{\oplus}\mathfrak{t}(m\geqslant 2)$ *with basis* $(X_0,X_1,X_2,X_3,Y_1,\ldots,Y_{2m-4},V_1,\ldots,V_m)$ *and brackets*

$$[X_0,X_i]=X_{i+1},\quad i=1,2,$$

$$[Y_{2i-1},Y_{2i}]=X_3,\ \ 1\leqslant i\leqslant m-2,$$

$$[V_1,X_i]=X_i,\ \ i=0,2,$$

$$[V_1,X_3]=2Y_3,$$

$$[V_1,Y_{2i}]=2Y_{2i},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_2,X_i]=X_i,\ \ i=1,2,3,$$

$$[V_2,Y_{2i}]=Y_{2i},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_{i+2},Y_{2i-1}]=Y_{2i-1},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_{i+2},Y_{2i}]=-Y_{2i},\ \ 1\leqslant i\leqslant m-2.$$

(ii) The Lie algebra $\mathfrak{d}_{2m+1}=\mathfrak{g}_{2m+1}\vec{\oplus}\mathfrak{t}(m\geqslant 2)$ *with basis* $(X_0,\ldots,X_3,Y_1,\ldots,Y_{2m-3},V_1,\ldots,V_m)$ *and brackets*

$$[X_0,X_i]=X_{i+1},\ \ i=1,2,$$

$$[X_1,Y_{2m-3}]=X_3,$$

$$[Y_{2i-1},Y_{2i}]=X_3,\ \ 1\leqslant i\leqslant m-2,$$

$$[V_1,X_i]=X_i,\ \ i=0,2,$$

$$[V_1,X_3]=2X_3,$$

$$[V_1,Y_{2i}]=2Y_{2i},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_1,Y_{2m-3}]=2Y_{2m-3},$$

$$[V_2,X_i]=X_i,\ \ i=1,2,3,$$

$$[V_2,Y_{2i}]=Y_{2i},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_{i+2},Y_{2i-1}]=Y_{2i-1},\ \ 1\leqslant i\leqslant m-2,$$

$$[V_{i+2},Y_{2i}]=-Y_{2i},\ \ 1\leqslant i\leqslant m-3.$$

(iii) The seven dimensional Lie algebra $\mathfrak{d}_5'$ *with basis* $(X_0,\ldots,X_3,Y_1,V_1,V_2)$ *and brackets*

$$[X_0,X_i]=X_{i+1},\ \ i=1,2,$$

$$[X_1,X_2]=Y_1,$$

$$[V_1,X_i]=(i+1)X_i,\ \ i=0,1,2,3,$$

$$[V_1,Y_1]=5Y_1,$$

$$[V_2,X_i]=X_i,\ \ i=1,2,3,$$

$$[V_2,Y_1]=2Y_1.$$

Remark 1: Indeed more is true: any nonsplit nilpotent Lie algebra $\mathfrak{n}$ *of characteristic sequence* (3,1,...,1) *is isomorphic to the nilradical of one of the former solvable algebras.*[2]

III. THE INVARIANTS

In this section we determine the invariants of the preceding solvable Lie algebras. We claim that it suffices to analyze the lowest dimensional algebras to deduce both the number $\mathcal{N}$ and the explicit form of the invariants in arbitrary dimension. Table I presents the invariants of the algebras for the values $m=2,3,4,5$.

We observe that the algebras $\mathfrak{d}_4$, $\mathfrak{d}_6$, $\mathfrak{d}_8$ and $\mathfrak{d}_{10}$ admit the same invariant $I=(v_3x_3+y_1y_2)/x_3$, and that

$$\mathcal{N}(\mathfrak{d}_{10})=\mathcal{N}(\mathfrak{d}_8)+1=\mathcal{N}(\mathfrak{d}_6)+2=\mathcal{N}(\mathfrak{d}_4)+3. \tag{3.1}$$

We can thus expect that for the general case we will have $\mathcal{N}(\mathfrak{d}_{2m})=m-2$, and that a fundamental set of invariants is formed by the rational functions $I=(v_{i+2}x_3+y_{2i-1}y_{2i})/x_3$. For the algebras $\mathfrak{d}_{2m+1}$ the situation is similar: $\mathfrak{d}_{11}$ has four invariants, three invariants $(v_3x_3+y_1y_2)/x_3$, $(v_4x_3+y_3y_4)/x_3$, $(v_5x_3+y_5y_6)/x_3$, from which the first is an invariant of $\mathfrak{d}_7$ and $\mathfrak{d}_9$ and the second an invariant of $\mathfrak{d}_9$, and a function $(x_0x_2x_3+x_2^2y_7-2x_3^2v_2+v_1x_3^2-2x_1x_3y_7)/x_3^2$. This is also an invariant of $\mathfrak{d}_5$, $\mathfrak{d}_7$ and $\mathfrak{d}_9$ if we substitute y_7 by y_1, y_3 and y_5, respectively. We can thus expect that $\mathcal{N}(\mathfrak{d}_{2m+1})=m-1$ and that the invariants are of the preceding form.

Theorem 3: *Let* $\mathfrak{r}$ *be a solvable rigid Lie algebra whose nilradical is nonsplit of characteristic sequence* (3,1,...,1). *Then a fundamental set of invariants is given by*

(i) $\{y_{2k-1}y_{2k}+x_3v_{k+2}/x_3\}_{1\leqslant k\leqslant m-2}$ *if* $\mathfrak{r}\simeq\mathfrak{d}_{2m}$,

(ii) $\{x_0x_2x_3+x_2^2y_{2m-3}-2x_3^2v_2+v_1x_3^2-2x_1x_3y_{2m-3}/-2x_3^2, x_3v_{k+2}+y_{2k-1}y_{2k}/x_3\}_{1\leqslant k\leqslant m-2}$ *if* $\mathfrak{r}\simeq\mathfrak{d}_{2m+1}$,

(iii) $\{(2x_0y_1+x_2^2-2x_1x_3)^3/(x_3y_1)^2\}$ *if* $\mathfrak{r}\simeq\mathfrak{d}_5'$.

Proof:

(i) Let $\mathfrak{r}=\mathfrak{d}_{2m}$. The system (2.4) is in this case

$$\widehat{X_0}F=(-x_2\partial_{x_1}-x_3\partial_{x_2}+x_0\partial_{v_1})=0, \tag{3.2}$$

$$\widehat{X_1}F=(x_2\partial_{x_0}+x_1\partial_{v_2})F=0, \tag{3.3}$$

$$\widehat{X_2}F=(x_3\partial_{x_0}+x_2\partial_{v_1}+x_2\partial_{v_2})F=0, \tag{3.4}$$

$$\widehat{X_3}F=(2x_3\partial_{v_1}+x_3\partial_{v_2})F=0, \tag{3.5}$$

$$\hat{Y}_{2i-1}F=(-x_3\partial_{y_{2i}}+y_{2i-1}\partial_{v_{i+2}})F=0,\quad 1\leqslant i\leqslant m-2, \tag{3.6}$$

$$\widehat{Y_{2i}}F=(x_3\partial_{y_{2i-1}}-y_{2i}\partial_{v_{i+2}}+2y_{2i}\partial_{v_1}+y_{2i-1}\partial_{v_2})F=0,\quad 1\leqslant i\leqslant m-2, \tag{3.7}$$

$$\hat{V}_1F=\left(x_0\partial_{x_0}+x_2\partial_{x_2}+2x_3\partial_{x_3}+2\sum_{i=1}^{m-2}y_{2i}\partial_{y_{2i}}\right)F=0, \tag{3.8}$$

$$\hat{V}_2F=\left(x_1\partial_{x_1}+x_2\partial_{x_2}+x_3\partial_{x_3}+\sum_{i=1}^{m-2}y_{2i}\partial_{y_{2i}}\right)F=0, \tag{3.9}$$

$$\hat{V}_{i+1}F=(y_{2i-1}\partial_{y_{2i-1}}-y_{2i}\partial_{y_{2i}})F=0,\quad 1\leqslant i\leqslant m-2. \tag{3.10}$$

TABLE I. Invariants in low dimensions.

$\mathfrak{g}$	dim	Brackets		Invariants
$\mathfrak{d}_4$	6	$[X_0,X_i]=X_{i+1},\ i=1,2;$ $[V_1,X_i]=X_i,\ i=0,2;$	$[V_1,X_3]=2X_3$ $[V_2,X_i]=X_i, i=1,2,3$	none
$\mathfrak{d}_5$	7	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[V_1,X_i]=X_i\ (i=0,2);$ $[V_1,Y_1]=2Y_1;$	$[X_1,Y_1]=X_3$ $[V_1,X_3]=2X_3$ $[V_2,X_i]=X_i\ (i=1,2,3)$	$I_1=\frac{x_0x_2x_3+x_2^2y_1}{x_3^2}$ $+\frac{x_3^2(v_1-2v_2)-2x_1x_3y_1}{x_3^2}$
$\mathfrak{d}_6$	9	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[V_1,X_i]=X_i\ (i=0,2);$ $[V_1,Y_2]=2Y_2;$ $[V_2,Y_2]=Y_2;$ $[V_3,Y_2]=-Y_2;$	$[Y_1,Y_2]=X_3$ $[V_1,X_3]=2X_3$ $[V_2,X_i]=X_i\ (i=1,2,3)$ $[V_3,Y_1]=Y_1$	$I_1=\frac{v_3x_3+y_1y_2}{x_3}$
$\mathfrak{d}_7$	10	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[Y_1,Y_2]=X_3;$ $[V_1,X_3]=2X_3;$ $[V_2,X_i]=X_i\ (i=1,2,3);$ $[V_3,Y_1]=Y_1;$	$[X_1,Y_3]=X_3$ $[V_1,X_i]=X_i\ (i=0,2)$ $[V_1,Y_{2i}]=2Y_{2i}\ (i=1,\frac{3}{2})$ $[V_2,Y_2]=Y_2$ $[V_3,Y_2]=-Y_2$	$I_1=\frac{x_0x_2x_3+x_2^2y_3}{x_3^2}$ $+\frac{x_3^2(v_1-2v_2)-2x_1x_3y_3}{x_3^2}$ $I_2=\frac{v_3x_3+y_1y_2}{x_3}$
$\mathfrak{d}_8$	12	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[V_1,X_i]=X_i\ (i=0,2);$ $[V_1,Y_{2i}]=2Y_{2i}\ (i=1,2);$ $[V_2,Y_{2i}]=Y_{2i}\ (i=1,2);$ $[V_{i+2},Y_{2i}]=-Y_{2i}\ (i=1,2);$	$[Y_{2i-1},Y_{2i}]=X_3\ (i=1,2)$ $[V_1,X_3]=2X_3$ $[V_2,X_i]=X_i\ (i=1,2,3)$ $[V_{i+2},Y_{2i-1}]=Y_{2i-1}\ (i=1,2)$	$I_1=\frac{v_3x_3+y_1y_2}{x_3}$ $I_2=\frac{v_4x_3+y_3y_4}{x_3}$
$\mathfrak{d}_9$	13	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[Y_{2i-1},Y_{2i}]=X_3\ (i=1,2);$ $[V_1,X_3]=2X_3;$ $[V_2,X_i]=X_i\ (i=1,2,3);$ $[V_{i+2},Y_{2i-1}]=Y_{2i-1}\ (i=1,2);$	$[X_1,Y_5]=X_3$ $[V_1,X_i]=X_i\ (i=0,2)$ $[V_1,Y_{2i}]=2Y_{2i}\ (i=1,2,\frac{5}{2})$ $[V_2,Y_{2i}]=Y_{2i}\ (i=1,2)$ $[V_{i+2},Y_{2i}]=-Y_{2i}\ (i=1,2)$	$I_1=\frac{x_0x_2x_3+x_2^2y_5}{x_3^2}$ $+\frac{x_3^2(v_1-2v_2)-2x_1x_3y_5}{x_3^2}$ $I_2=\frac{v_3x_3+y_1y_2}{x_3}$ $I_3=\frac{v_4x_3+y_3y_4}{x_3}$
$\mathfrak{d}_{10}$	15	$[X_0,X_i]=X_{i+1}\ (i=1,2);$ $[V_1,X_i]=X_i\ (i=0,2);$ $[V_1,Y_{2i}]=2Y_{2i}\ (i=1,2,3);$ $[V_2,Y_{2i}]=Y_{2i}\ (i=1,2,3);$ $[V_{i+2},Y_{2i}]=-Y_{2i}\ (i=1,2,3)$	$[Y_{2i-1},Y_{2i}]=X_3\ (i=1,2,3);$ $[V_1,X_3]=2X_3$ $[V_2,X_i]=X_i\ (i=1,2,3)$ $[V_{i+2},Y_{2i-1}]=Y_{2i-1}\ (i=1,2,3)$	$I_1=\frac{v_3x_3+y_1y_2}{x_3}$ $I_2=\frac{v_4x_3+y_3y_4}{x_3}$ $I_3=\frac{v_5x_3+y_5y_6}{x_3}$

TABLE I. (*Continued.*)

$\mathfrak{g}$	dim	Brackets		Invariants
$\mathfrak{d}_{11}$	16	$[X_0,X_i]=X_{i+1}$ $(i=1,2)$;	$[X_1,Y_7]=X_3$	$I_1=\frac{x_0x_2x_3+x_2^2y_7}{x_3^2}$
		$[Y_{2i-1},Y_{2i}]=X_3$ $(i=1,2,3)$;	$[V_1,X_i]=X_i$ $(i=0,2)$	$+\frac{x_3^2(v_1-2v_2)-2x_1x_3y_7}{x_3^2}$
		$[V_1,X_3]=2X_3$;	$[V_1,Y_{2i}]=2Y_{2i}$ $(i=1,2,3,\frac{7}{2})$	$I_2=\frac{v_3x_3+y_1y_2}{x_3}$
		$[V_2,X_i]=X_i$ $(i=1,2,3)$;	$[V_2,Y_{2i}]=Y_{2i}$ $(i=1,2,3)$	$I_3=\frac{v_4x_3+y_3y_4}{x_3}$
		$[V_{i+2},Y_{2i-1}]=Y_{2i-1}$ $(i=1,2,3)$;	$[V_{i+2},Y_{2i}]=-Y_{2i}$ $(i=1,2,3)$	$I_4=\frac{v_5x_3+y_5y_6}{x_3}$
$\mathfrak{d}_5'$	7	$[X_0,X_i]=X_{i+1}$ $(i=1,2)$;	$[X_1,X_2]=Y_1$	$I_1=\frac{(2x_0y_1+x_2^2-2x_1x_3)^3}{x_3^2y_1^2}$
		$[V_1,X_i]=(i+1)X_i$ $(i=0,...,3)$;	$[V_1,Y_1]=5Y_1$	
		$[V_2,X_i]=X_i$ $(i=1,2,3)$;	$[V_2,Y_1]=2Y_1$	

Elementary manipulations of the equations $\widehat{X}_iF=0(0\leqslant i\leqslant 3)$ show that $\partial_{v_i}F=0(i=1,2)$ and $\partial_{x_0}F=0$. Moreover, from the equations $\hat{V}_iF=0(i=1,2)$ we easily deduce that $\partial_{x_i}F=0$ for $i=1,2$. This reduces the system to the following:

$$(-x_3\partial_{y_{2i}}+y_{2i-1}\partial_{v_{i+2}})F=0,\quad 1\leqslant i\leqslant m-2, \tag{3.11}$$

$$(x_3\partial_{y_{2i-1}}-y_{2i}\partial_{v_{i+2}})F=0,\quad 1\leqslant i\leqslant m-2, \tag{3.12}$$

$$\left(x_3\partial_{x_3}+\sum_{i=1}^{m-2}y_{2i}\partial_{y_{2i}}\right)F=0, \tag{3.13}$$

$$(y_{2i-1}\partial_{y_{2i-1}}-y_{2i}\partial_{y_{2i}})F=0. \tag{3.14}$$

Equations (3.11), (3.12) and (3.14) show that we can find invariants of the form $f(x_3,y_{2i-1},y_{2i},v_{i+2})$, which are clearly functionally independent for distinct values of i. Integration of Eq. (3.13) taking into account this observaion provides us with the following fundamental set of invariants:

$$\left\{f_i=\frac{y_{2i-1}y_{2i}+x_3v_{i+2}}{x_3}\right\}_{1\leqslant i\leqslant m-2}. \tag{3.15}$$

(ii) Let $\mathfrak{r}=\mathfrak{d}_{2m+1}$. The system of PDEs corresponding to this algebra has the following subsystem:

$$\widehat{X}_i.F=0,\ 0\leqslant i\leqslant 3, \tag{3.16}$$

$$\hat{Y}_{2m-3}.F=0. \tag{3.17}$$

This is the same system which we obtain for $m=2$, whose invariant has already been computed in Table I:

$$f_1=\frac{2x_3^2v_2-x_3^2v_1+2x_1x_3y_{2m-3}-x_0x_2x_3-x_2^2y_{2m-3}}{x_3^2}. \tag{3.18}$$

Therefore this function is an invariant of $\mathfrak{d}_{2m+1}$ for any $m\geqslant 2$. Now observe that, since $\widehat{X_3}.F=x_3(2\partial_{v_1}+\partial_{v_2})=0$, the equation $\widehat{Y_{2i}}.F=0$ can be reduced to

$$\widehat{Y'_{2i}}F=(x_3\partial_{y_{2i-1}}-y_{2i}\partial_{v_{i+2}})F=0. \tag{3.19}$$

As a consequence, the function f_1 is a solution of (3.16) and (3.17) for any $m\geqslant 3$, and the remaining fundamental solutions are obtained from the system

$$\hat{Y}_{2i-1}.F=(-x_3\partial_{y_{2i}}+y_{2i-1}\partial_{v_{i+2}})F=0, \tag{3.20}$$

$$\hat{Y}'_{2i}.F=0,\ 1\leqslant i\leqslant m-2,\quad \hat{V}_1.F=(x_3\partial_{y_{2i-1}}-y_{2i}\partial_{v_{i+2}})F=0, \tag{3.21}$$

$$\hat{V}_{i+2}.F=(y_{2i-1}\partial_{y_{2i-1}}-y_{2i}\partial_{y_{2i}})F=0,\quad i\geqslant 1, \tag{3.22}$$

for $1\leqslant i\leqslant m-2$. This system is equivalent to the one given by Eqs. (3.11)–(3.14), from which we deduce the solutions

$$f_{i+1}=\frac{x_3v_{i+2}+y_{2i-1}y_{2i}}{x_3}. \tag{3.23}$$

Thus a fundamental system of invariants for $\mathfrak{d}_{2m+1}$ is given by $\{f_1,f_{i+1}\}_{1\leqslant i\leqslant m-2}$.

(iii) It is easily verified that any invariant satisfies $\partial_{v_1}F=\partial_{v_2}F=0$. Elementary transformations of the corresponding system show that an invariant function F must be a solution of the following equation:

$$(-x_2^2+y_1x_0+2x_1x_3)\partial_{x_1}F+3y_1x_3\partial_{y_1}F=0. \tag{3.24}$$

This equation admits the rational solution

$$F_1=\frac{(2x_0y_1+x_2^2-2x_1x_3)^3}{x_3^2y_1^2} \tag{3.25}$$

and it can be easily verified that this function satisfies the system. Thus a set of invariants is given by $\{F_1\}$.

■

Since the fundamental sets of invariants of the algebras $\mathfrak{d}_m$ and $\mathfrak{d}'_5$ consist of rational functions, one can ask whether these invariants will confirm the observation that rational functions occur as ratio of two commuting polynomials.[15,17] For the algebras $\mathfrak{d}_{2m}$ we have $[X_3,Y]=0$ for any $Y\notin\mathbb{C}V_1\oplus\mathbb{C}V_2$. Thus, as polynomial operators, the following identity holds for any $k\in\{1,...,m-2\}$:

$$[X_3,Y_{2k-1}Y_{2k}+X_3V_{k+2}]=0, \tag{3.26}$$

which shows that the numerator and denominator of the invariants are commuting polynomials. For the algebras $\mathfrak{d}_{2m+1}$ we also have $[X_3,Y]=0$ whenever $Y\notin\mathbb{C}V_1\oplus\mathbb{C}V_2$. Therefore the invariants $(v_{k+2}x_3+y_{2k-1}y_{2k})/x_3$ are also the ratio of commuting polynomials. The remaining invariant $I=(x_0x_2x_3+x_2^2y_{2m-3}+x_3^2(v_1-2v_2)-2x_1x_3y_{2m-3})/x_3^2$ depends on both V_1 and V_2, but, since $[V_1,X_3]=2X_3$ and $[V_2,X_3]=X_3$, we again obtain that

$$[X_0X_2X_3+X_2^2Y_{2m-3}+X_3^2(V_1-2V_2)-2X_1X_3Y_{2m-3},X_3]=0. \tag{3.27}$$

Finally, for the special case $\mathfrak{d}_5'$ the center is spanned by X_3 and Y_1, and since the invariant does not depend on the variables v_1,v_2 associated to toral elements, the numerator and denominator of the invariant are commuting polynomials.

In terms of representation theory this fact is of importance, since it ensures us the existence of bases for irreducible representations in which the operators are all simultaneously diagonal, giving to the invariants a precise meaning which is useful to characterize the representations of these algebras.

IV. APPLICATIONS TO RANK ONE SUBALGEBRAS

The seven dimensional rigid Lie algebra $\mathfrak{d}_5'$ is a nice example to illustrate how, under certain assumptions, we can deduce the invariants of some subalgebras. Let us consider the rank one solvable (non-nilpotent) subalgebras $\mathfrak{d}_5^{a,b}$ of $\mathfrak{d}_5'$ having the following brackets:

$$[X_0,X_1]=X_2,\quad [X_0,X_2]=X_3,\quad [X_1,X_2]=Y_1,$$

$$[V,X_0]=aX_0,\quad [V,X_1]=bX_1,\quad [V,X_2]=(a+b)X_2,$$

$$[V,X_3]=(2a+b)X_3,\quad [V,Y_1]=(a+2b)Y_1;\quad a,b\in\mathbb{C}.$$

Clearly we have $V=aV_1+bV_2$. The system of PDEs giving the invariants of $\mathfrak{d}_5^{a,b}$ is

$$\widehat{X}_iF=0,\ 0\leqslant i\leqslant 3, \tag{4.1}$$

$$\hat{Y}_1F=0, \tag{4.2}$$

$$\hat{V}F=0, \tag{4.3}$$

where

$$\hat{V}=(ax_0\partial_{x_0}+bx_1\partial_{x_1}+(a+b)x_2\partial_{x_2}+(2a+b)x_3\partial_{x_3}+(a+2b)y_1\partial_{y_1}). \tag{4.4}$$

Now any invariant F satisfies $\partial_vF=0$, and we obtain that any invariant of $\mathfrak{d}_5'$ is also an invariant of $\mathfrak{d}_5^{a,b}$, since the five first equations coincide and the sixth is a linear combination of the toral equations of $\mathfrak{d}_5'$.

Lemma 1: For any $a,b\in\mathbb{C}$ not simultaneously zero we have $\mathcal{N}(\mathfrak{d}_5^{a,b})=2$.

Proof: Since F_1 satisfies the system, $\mathcal{N}\geqslant 1$. Now it can easily be seen that the matrix obtained from the commutation table has rank four, from which the assertion follows. ■

We make a distinction among the subalgebras $\mathfrak{d}_5^{a,b}$: those having trivial center and those not. It is a routine verification that $\mathfrak{d}_5^{a,b}$ has nontrivial center if and only if $a+2b=0$ or $2a+b=0$. Since solvable Lie algebras having nontrivial center admit at least a polynomial invariant, we obtain the following:

Lemma 2: Let $\mathfrak{d}_5^{a,b}$ have nontrivial center. Then a fundamental set of invariants is given by
(i) $\{F_1,x_3\}$ *if* $2a+b=0$,
(ii) $\{F_1,y_1\}$ *if* $a+2b=0$.

For the case of a nontrivial center, it is easy to verify that any invariant of $\mathfrak{d}_5^{a,b}$ is a function of F_1, x_3 and y_1. Specifically, we have the following.

Lemma 3: If $Z(\mathfrak{d}_5^{a,b})\neq 0$, a fundamental set of invariants for $\mathfrak{d}_5^{a,b}$ is given by $\{F_1,y_1^{2a+b}/x_3^{a+2b}\}$.

The interest of this example is that it provides us with a general result: Let $\mathfrak{r}=\mathfrak{n}\vec{\oplus}\mathfrak{t}$ be a solvable non-nilpotent Lie algebra over $\mathbb{K}=\{\mathbb{R},\mathbb{C}\}$ and $\mathfrak{t}$ a torus of derivations. Let $\{X_1,\ldots,X_n,V_1,\ldots,V_p\}$ be a basis such that the nilradical $\mathfrak{n}$ is generated by the X_i and the torus by the V_i. Suppose, moreover, that $\mathfrak{r}$ satisfies the following property:

$$\partial_{v_i}F=0, \quad 1\leqslant i\leqslant p \text{ for any invariant } F, \quad \forall v_i\in\mathfrak{t}. \tag{4.5}$$

Let $\mathfrak{t}'$ be a one dimensional subtorus of $\mathfrak{t}$ and $\mathfrak{r}'=\mathfrak{n}\vec{\oplus}\mathfrak{t}'$ such that $\mathfrak{t}'.Z(\mathfrak{n})\neq 0$, i.e., the action of the subtorus $\mathfrak{t}'$ on the center of the nilradical is nonzero.

Proposition 1: In the preceding conditions, any element F of a fundamental set of invariants for $\mathfrak{r}$ is an invariant of $\mathfrak{r}'$. Moreover, $\mathcal{N}(\mathfrak{r}')\geqslant\mathcal{N}(\mathfrak{r})$.

Proof: Let V generate $\mathfrak{t}'$. We can find coefficients $\alpha_1,\ldots,\alpha_p\in\mathbb{K}$ such that $V=\Sigma_{i=1}^{p}\alpha_iV_i$. Since $\mathfrak{n}$ is nilpotent, its center is nonzero, and by $\mathfrak{t}'.Z(\mathfrak{n})\neq 0$, we deduce that $\partial_vF=0$ for any invariant F of $\mathfrak{r}'$. The system of PDEs giving the invariants is

$$\widehat{X_i}.F=-[X_i,X_j]\partial_{x_j}.F=0, \quad 1\leqslant i\leqslant n, \tag{4.6}$$

$$\hat{V}.F=-[V,X_i]\partial_{x_i}.F=0. \tag{4.7}$$

Now $\hat{V}=\Sigma_{i=1}^{p}\alpha_i\hat{V}_i$. This shows that any invariant G of $\mathfrak{r}$ also satisfies the system (4.6) and (4.7), since the equations concerning the operators $\widehat{X_i}$ coincide, and the last equation is a linear combination of the equations $\{\hat{V}_i.F=0\}$ of $\mathfrak{r}$. Thus any fundamental set of invariants for $\mathfrak{r}$ is a set of functionally independent invariants for $\mathfrak{r}'$. As a consequence $\mathcal{N}(\mathfrak{r}')\geqslant\mathcal{N}(\mathfrak{r})$. ■

Remark 2: If p is even, by the Beltrametti–Blasi formula we deduce $\mathcal{N}(\mathfrak{r}')\geqslant\mathcal{N}(\mathfrak{r})+1$.

The main interest of this result is its application in the other direction (whenever it makes sense), i.e., starting from the invariants of a rank one subalgebra to find a fundamental set of the algebra $\mathfrak{r}$. We illustrate it by an example:

Example 2: Consider the solvable Lie algebra $\mathfrak{g}$ given by the brackets

$$[V_1,Y_i]=iY_i, \quad 1\leqslant i\leqslant 7,$$

$$[V_2,Y_i]=Y_i, \quad 2\leqslant i\leqslant 7,$$

$$[Y_1,Y_i]=Y_{i+1}, \quad 2\leqslant i\leqslant 6.$$

This algebra is of rank two, and a torus is generated by V_1 and V_2. From the corresponding system (2.4) it can be seen that for any invariant F of $\mathfrak{g}$ we have $\partial_{v_i}F=0, i=1,2$, thus we can apply the preceding proposition. Consider the one dimensional subtorus generated by V_2. The semidirect product of this torus and the nilradical is an eight dimensional Lie algebra $\mathfrak{g}'$ satisfying $\mathcal{N}(\mathfrak{g}')=2$. A fundamental set of invariants for this algebra is formed by the following functions:

$$g_1=\frac{6y_4y_6y_7^2-6y_3y_7^3+2y_6^4-8y_5y_6^2y_7+5y_5^2y_7^2}{3y_4y_7^3+y_6^3y_7-3y_5y_6y_7^2},$$

$$g_2=\frac{-5y_2y_7^4+5y_4y_5y_7^3+5y_5y_6^3y_7-5y_5^2y_6y7^2-y_6^5+5y_3y_6y_7^3-5y_4y_6^2y_7^2}{3y_4y_7^4+y_6^3y_7^2-3y_5y_6y_7^3}.$$

As the assumption of the proposition are satisfied, we know that there exists a function $F(g_1,g_2)$ that forms a fundamental system of invariants for the Lie algebra $\mathfrak{g}$. In this case it is not difficult to see that such a function is given by $F=g_2/g_1^2$. Since both g_1 and g_2 are ratios of commuting polynomials, we deduce that F is also a rational invariant of this kind (in the corresponding enveloping algebras).

Of course this inverse procedure is applicable only in quite concrete cases, since the algebra $\mathfrak{r}$ could have no invariants, while a rank one odd dimensional Lie subalgebra necessarily has solutions. Condition (4.5) provides us with another interesting fact: Let $\mathfrak{r}=\mathfrak{n}\vec{\oplus}\mathfrak{t}$ be an even dimensional solvable Lie algebra satisfying (4.5).

Proposition 2: If $\mathcal{N}(\mathfrak{n})=1$, *then* $\mathfrak{r}$ *has no nontrivial invariants.*

Proof: Since $\partial_v F=0$ for any invariant F and any $v\in\mathfrak{t}$, over an arbitrary basis $\{X_1,\ldots,X_{2p+1},V_1,\ldots,V_{2q+1}\}$ such that $\{X_1,\ldots,X_{2p+1}\}$ is a basis of $\mathfrak{n}$ and $\{V_1,\ldots,V_{2q+1}\}$ is a basis of $\mathfrak{t}$, the system of PDEs giving the invariants is

$$\hat{X}_i.F=0,\ 1\leqslant i\leqslant 2p+1, \tag{4.8}$$

$$\hat{V}_i.F=0,\ 1\leqslant i\leqslant 2q+1. \tag{4.9}$$

Since there is only one functionally independent invariant F_0 satisfying the equation (4.8), because it corresponds exactly to the system of $\mathfrak{n}$, we would obtain a fundamental set of invariants of $\mathfrak{r}$ generated by at most one invariant, namely some function of F_0. But this contradicts the fact that $\mathcal{N}(\mathfrak{r})$ has the same parity as dim $\mathfrak{r}$, which is even. Thus $\mathcal{N}(\mathfrak{r})=0$. ■

This property can be of interest for some physical applications. The six dimensional subalgebra $P_{5,2}$ of the Poincaré algebra generated by $\{\cos\alpha L_3+\sin\alpha K_3, L_2+K_1, L_1-K_2, P_0-P_3, P_1, P_2\}$ with $0\leqslant\alpha\leqslant\pi, \alpha\neq\pi/2$ satisfies the preceding conditions. Its nilradical $\mathfrak{n}$ is five dimensional, and the center of $\mathfrak{n}$ is generated by (P_0-P_3). This ensures that $\partial_t F=0$ for any invariant, where $t=\cos\alpha l_3+\sin\alpha k_3$. Since the invariants of $\mathfrak{n}$ are all functions of (p_0-p_3), the algebra $P_{5,2}$ has none invariants.

V. CONCLUDING REMARKS

The preceding results show that rigid Lie algebras are an adequate class for studying the generalized Casimir invariants. Since the torus determines the nilradical, the equations describing the action of the torus are of importance for the structure of the invariants, specifically if those invariants do not depend on the variables corresponding to toral elements. Since solvable rigid Lie algebras can theoretically be classified following the algorithm given in Ref. 4, the analysis of these algebras in relatively low dimension and their subalgebras can provide alternative criteria to attack the general case, as classifications in general are not possible. This in particular applies to the class of two-step solvable Lie algebras (the Heisenberg algebras being the most important examples), for which general constructions exist.[6] Observe further that, like in Proposition 1, the results do not depend on the field, which allows us to derive results for both real and complex Lie algebras. The reason to analyze the complex rigid laws lies in their decomposition: for real rigid Lie algebras no decomposition like (2.14) is known, and it is still an open question whether it can exist.[8]

Finally, the same analysis could be applied to any solvable Lie algebra whose nilradical has characteristic sequence $(p,1,...,1)$ for $p\geqslant 4$. These algebras, which are completely classified up to $p=5$,[3,7] consist of a low dimensional subalgebra $\mathfrak{m}$ generated by a characteristic vector, to which three dimensional Heisenberg Lie algebras having their derived subalgebras in the center of $\mathfrak{m}$ are glued. For the solvable Lie algebras having nilradicals of this type the determination of a fundamental set of invariants should also be possible from the analysis in low dimensions. This structure makes this class worthy of being analyzed to obtain alternative criteria for the generalized Casimir invariants of solvable Lie algebras.

Finally, the absence of invariants of an algebra is a very interesting property, because, whenever the algebra is related to some physical system, other solutions in more general spaces could also provide important information on the system (as happens with the sign of energy for the Poincaré algebra).[17] It is also of interest to find characterizations of these algebras.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 2 FEBRUARY 2003

Modified braid equations, Baxterizations and noncommutative spaces for the quantum groups $GL_q(N)$, $SO_q(N)$, and $Sp_q(N)$

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(Received 20 June 2002; accepted 15 October 2002)

Modified braid equations satisfied by generalized $\hat{R}$ matrices (for a *given* set of group relations obeyed by the elements of T matrices) are constructed for q-deformed quantum groups $GL_q(N)$, $SO_q(N)$, and $Sp_q(N)$ with arbitrary values of N. The Baxterization of $\hat{R}$ matrices, treated as an aspect complementary to the *modification* of the braid equation, is obtained for all these cases in particularly elegant forms. A new class of braid matrices is discovered for the quantum groups $SO_q(N)$ and $Sp_q(N)$. The $\hat{R}$ matrices of this class, while being distinct from the restrictions of the universal $\hat{\mathcal{R}}$ matrix to the corresponding vector representations, satisfy the *standard* braid equation. The modified braid equation and the Baxterization are obtained for this new class of $\hat{R}$ matrices. Diagonalization of the generalized $\hat{R}$ matrices is studied. The diagonalizers are obtained explicitly for some lower dimensional cases in a convenient way, giving directly the eigenvalues of the corresponding $\hat{R}$ matrices. Applications of such diagonalization are then studied in the context of associated covariantly quantized noncommutative spaces. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1530370]

I. INTRODUCTION

Previously one of us has studied the *modified* braid equation (MBE) in the context of the quantum groups $GL_{p,q}(2)$, $GL_{g,h}(2)$, and $GL_{q,h}(1|1)$ (biparametric unitary, nonstandard Jordanian and hybrid deformations respectively) in Ref. 1; and also the orthogonal quantum group $SO_q(3)$ in Ref. 2. The terminology is adopted from that of Gerstenhaber, Giaquinto, and Schack,[3,4] who have studied a generalized class of deformations leading to MBE, where unlike the standard Yang–Baxter equation there are also inhomogeneous terms linear in tensored $\hat{R}$ matrices. These authors indicate the significance of and the interest in this equation. In Refs. 1 and 2 the most general solutions of the quantum inverse scattering equation

$$\hat{R}\mathsf{T}_1\mathsf{T}_2-\mathsf{T}_1\mathsf{T}_2\hat{R}=0, \quad \mathsf{T}_1=\mathsf{T}\otimes\mathsf{I}, \quad \mathsf{T}_2=\mathsf{I}\otimes\mathsf{T} \tag{1.1}$$

for the relevant quantum groups were considered. Starting from a *given* set of group relations of the elements of the monodromy matrix T, the most general $\hat{R}$ matrix satisfying (1.1) was constructed. It was observed that the standard braid equation was modified for this generalized $\hat{R}$ matrix. In this procedure the *conservation of the group laws postulated for the elements of the* T *matrix was maintained*.

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Here we construct, systematically and explicitly, the MBE for the quantized groups $\mathrm{GL}_q(N)$, $\mathrm{SO}_q(N)$, and $\mathrm{Sp}_q(N)$, respectively. As explained in Sec. 1 of Ref. 2, we will methodically use the generalized spectral decomposition of the relevant $\hat{R}$ matrices in the vector representations. For an $\hat{R}$ matrix obeying the characteristic equation

$$(\hat{R}-k_1\mathsf{I})\ (\hat{R}-k_2\mathsf{I})\cdots(\hat{R}-k_p\mathsf{I})=0, \quad (k_i\neq k_j \ \text{ if } \ i\neq j|(i,j)=(1,2,\ldots,p)), \tag{1.2}$$

the projectors in the eigenspaces of this $\hat{R}$ matrix read

$$P_i=\prod_{j\neq i}\frac{(\hat{R}-k_j\mathsf{I})}{(k_i-k_j)}, \tag{1.3}$$

and satisfy the usual property

$$P_iP_j=P_i\delta_{ij}, \quad \sum_i P_i=\mathsf{I}. \tag{1.4}$$

This orthonormalized set then provides the spectral decomposition.

Following Refs. 5–7 we first review the situation for the standard braid equation. In our discussion concerning braiding matrices, projectors and so on, we draw on Refs. 5 and 6. In our study of the Baxterization of the $\hat{R}$ matrices the analysis in Ref. 7 is particularly relevant. A large number of sources are cited in Ref. 7, and we also refer to that list. The standard, i.e., nonmodified in our context, braid equation reads

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12}-\hat{R}_{23}\hat{R}_{12}\hat{R}_{23}=0. \tag{1.5}$$

The spectral decomposition of the braid matrix of the quantum group $\mathrm{GL}_q(N)$ with the conventional normalization[7] is given by

$$\hat{\mathsf{R}}=qP_{(+)}-q^{-1}P_{(-)}, \tag{1.6}$$

whereas braid matrices of the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ (where $N=2n$) in the usual normalization[7] may be written in a unified manner

$$\hat{\mathsf{R}}=qP_{(+)}-q^{-1}P_{(-)}+\varepsilon q^{\varepsilon-N}P_{(0)}. \tag{1.7}$$

In (1.7) we have $\varepsilon=1(-1)$ for the quantum group $\mathrm{SO}_q(N)$ $[\mathrm{Sp}_q(N)]$. The explicit expressions of the $\hat{R}$ matrices and the corresponding projectors for the above quantum groups are given in Refs. 5–7.

Now we proceed as follows. Maintaining the *same* projectors as in the standard braid equation, we generalize the $\hat{R}$ matrix of the quantum group $\mathrm{GL}_q(N)$ as

$$\hat{R}(v)=\mathsf{I}+vP_{(-)}=P_{(+)}+(1+v)P_{(-)}. \tag{1.8}$$

A similar parametrization in the context of the quantum group $\mathrm{GL}_q(2)$ was used in Ref. 8. The generalized $\hat{R}$ matrices for the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ read

$$\hat{R}(v,w)=\mathsf{I}+vP_{(-)}+wP_{(0)}=P_{(+)}+(1+v)P_{(-)}+(1+w)P_{(0)}. \tag{1.9}$$

Setting the braid values of the variables

$$v=-(1+q^{\mp 2}), \quad w=-(1-\varepsilon q^{\mp(N+1-\varepsilon)}) \tag{1.10}$$

in (1.8) and (1.9) we may recover the $\hat{R}^{\pm 1}$ matrices satisfying the braid equation (1.5). Here and henceforth we adopt the convention that for the braid matrices satisfying (1.5) we do not explicitly exhibit the corresponding values of the relevant spectral variables. We will throughout implement the normalizations used in (1.8) and (1.9). For the purpose of later use we enlist here the braid matrices and their inverses according to our normalization scheme. The $\hat{R}^{\pm 1}$ matrices of the quantum group $\mathrm{GL}_q(N)$ read

$$\hat{R}^{\pm 1} = \mathsf{I} - (1+q^{\mp 2})P_{(-)}, \tag{1.11}$$

whereas the $\hat{R}^{\pm 1}$ matrices of the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ are given by

$$\hat{R}^{\pm 1} = \mathsf{I} - (1+q^{\mp 2})P_{(-)} - (1-\varepsilon q^{\mp(N+1-\varepsilon)})P_{(0)}. \tag{1.12}$$

We observe that the braid matrices defined in (1.11) and (1.12) following our normalization scheme and the corresponding matrices given, respectively, by (1.6) and (1.7) as per the usual normalization prescriptions, differ by an overall multiplicative factor

$$\hat{\mathsf{R}} = q\hat{R}. \tag{1.13}$$

The $\hat{R}(v)$ and $\hat{R}(v,w)$, defined, respectively, in (1.8) and (1.9), satisfy the following characteristic equations:

$$(\hat{R}(v)-\mathsf{I})(\hat{R}(v)-(1+v)\mathsf{I}) = 0, \tag{1.14}$$

$$(\hat{R}(v,w)-\mathsf{I})(\hat{R}(v,w)-(1+v)\mathsf{I})(\hat{R}(v,w)-(1+w)\mathsf{I}) = 0. \tag{1.15}$$

Using (1.3) the relevant projectors can also be expressed directly as linear and quadratic functions of $\hat{R}(v)$ and $\hat{R}(v,w)$, respectively. We also note that any $\hat{R}$ matrix satisfying (1.1) also necessarily satisfies

$$f(\hat{R})\mathsf{T}_1\mathsf{T}_2 - \mathsf{T}_1\mathsf{T}_2 f(\hat{R}) = 0, \tag{1.16}$$

where $f(x)$ is any well-behaved function. Due to the relations (1.14) and (1.15) the operator $f(\hat{R})$ reduces to a linear and a quadratic expression in the matrix $\hat{R}$ in the respective cases. Thus for arbitrary values of the variables v and (v,w), our constructions in (1.8) and (1.9) provide the *most general solutions* in the relevant examples.

Now comes the crucial question. What modifications in the braid equation (1.5) are enacted as the variables v and (v,w) move away from the braid values given in (1.10)? We are thus lead to our MBE for each case considered. As shown later in Sec. II, the MBE for the quantum group $\mathrm{GL}_q(N)$ reads

$$\hat{R}_{12}(v)\hat{R}_{23}(v)\hat{R}_{12}(v) - \hat{R}_{23}(v)\hat{R}_{12}(v)\hat{R}_{23}(v) = c(\hat{R}_{12}(v) - \hat{R}_{23}(v)), \tag{1.17}$$

whereas in the examples of the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ these equations have the form

$$\begin{aligned}
&\hat{R}_{12}(v,w)\hat{R}_{23}(v,w)\hat{R}_{12}(v,w) - \hat{R}_{23}(v,w)\hat{R}_{12}(v,w)\hat{R}_{23}(v,w) \\
&\quad = c_1(\hat{R}_{12}(v,w) - \hat{R}_{23}(v,w)) + c_2(\hat{R}_{12}^{-1}(v,w) - \hat{R}_{23}^{-1}(v,w)) + c_3(\hat{R}_{12}(v,w)\hat{R}_{23}^{-1}(v,w) \\
&\qquad - \hat{R}_{23}(v,w)\hat{R}_{12}^{-1}(v,w)) - c_3(\hat{R}_{12}^{-1}(v,w)\hat{R}_{23}(v,w) - \hat{R}_{23}^{-1}(v,w)\hat{R}_{12}(v,w)).
\end{aligned} \tag{1.18}$$

The coefficients c and (c_1,c_2,c_3) are given explicitly in Secs. II and III, respectively. Inhomogeneous terms linearly depending on $\hat{R}$ matrix elements on the right hand side of the modified

braid equation, as in (1.17), were first considered[3,4] in the context of the quantum group $GL_q(N)$ with two projectors. There is, however, a sudden leap in complexity as the number of projectors increases by one as in the cases of quantum groups $SO_q(N)$ and $Sp_q(N)$. By restricting the parameters v and w, we also select special cases in Secs. III and IV, where, for instance, $c_3=0$ or $\{c_2=0,c_3=0\}$ holds.

There is another aspect of our analysis. In Refs. 1 and 2 (particularly in Sec. 4 of Ref. 2) it was pointed out that the *modification* of the braid equation and the Baxterization of the $\hat{R}$ matrix are two complimentary facets of the generalized spectral decompositions in (1.8) and (1.9). It is possible to proceed in one of the following two alternate directions.

(i) The variables v and w are held fixed in each factor of the left, as in (1.17) and (1.18), and the inhomogeneous terms on the right are computed. This yields the MBE.

(ii) The inhomogeneous terms on the right-hand side of the braid equation may be constrained to be zero. This fixes the variables v and w in the appropriate $\hat{R}$ matrices in a particular fashion to be shown below. This provides the Baxterization of the $\hat{R}$ matrices.

The final results for the first possibility were presented above. Similarly we enlist below the final results for the other possibility. In Sec. III C we study the additive form of Baxterization of the $\hat{R}$ matrices

$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\theta')\hat{R}_{12}(\theta')-\hat{R}_{23}(\theta')\hat{R}_{12}(\theta+\theta')\hat{R}_{23}(\theta)=0, \tag{1.19}$$

where $q=\exp(h)$. For this form of Baxterization the variable $v(\theta)$ reads

$$v(\theta)=\frac{\sinh(h-\theta)}{\sinh(h+\theta)}-1, \tag{1.20}$$

for all the quantum groups studied here, namely $GL_q(N)$, $SO_q(N)$, and $Sp_q(N)$. The variable $w(\theta)$, appearing for the quantum groups $SO_q(N)$ and $Sp_q(N)$, assumes two alternate forms. For the orthogonal quantum group $SO_q(N)$ it is given by

$$w(\theta)=\frac{\cosh\left(\frac{N}{2}h-\theta\right)}{\cosh\left(\frac{N}{2}h+\theta\right)}-1 \tag{1.21}$$

or

$$w(\theta)=\frac{\sinh\left(\left(\frac{N}{2}-1\right)h-\theta\right)\sinh(h-\theta)}{\sinh\left(\left(\frac{N}{2}-1\right)h+\theta\right)\sinh(h+\theta)}-1. \tag{1.22}$$

For the symplectic quantum group $Sp_q(N)$, where $N=2n$, the variable $w(\theta)$ assumes the form

$$w(\theta)=\frac{\sinh((n+1)h-\theta)}{\sinh((n+1)h+\theta)}-1 \tag{1.23}$$

or

$$w(\theta)=\frac{\cosh(nh-\theta)\sinh(h-\theta)}{\cosh(nh+\theta)\sinh(h+\theta)}-1. \tag{1.24}$$

In each case our parametrization and normalization assure the validity of the constraint

$$\hat{R}(\theta)\hat{R}(-\theta)=\mathrm{I}. \tag{1.25}$$

It has been implicitly assumed above that $v\neq 0, w\neq 0$. But the parametrization (1.9) insistently points at the following question. What happens for the special choices $(v\neq 0, w=0)$ and $(v=0, w\neq 0)$? Certain properties of the projectors $P_{(-)}$ and $P_{(0)}$ being different, there is no reciprocal symmetry concerning the two above choices. For the $w=0$ case there is no nontrivial solution. But for the $v=0$ case we discuss *a hitherto unnoticed new class of solutions* studied in detail in Sec. IV. Even in the limit $q=1$, this class of solutions *remains nontrivial*. For the purpose of comparison with the preceding results, here we just exhibit the Baxterized values of the spectral variables corresponding to these solutions for the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$:

$$v=0, \quad w(\theta)=\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}-1, \quad \text{where} \quad \tanh\eta=(1-4(1+\varepsilon[N-\varepsilon])^{-2})^{1/2}. \tag{1.26}$$

In (1.26) we have used the standard notation $[x]=(q^x-q^{-x})/(q-q^{-1})$. The quantity under the radical sign in (1.26) is positive for $N>2$, and hence its square root is real.

In Sec. V we construct matrices diagonalizing the generalized braid operators $\hat{R}(v)$ and $\hat{R}(v,w)$. Explicit results are presented for the quantum groups $\mathrm{GL}_q(2)$, $\mathrm{SO}_q(3)$, and $\mathrm{SO}_q(4)$. The key result valid for the cases studied is that the indefinite parameters in the diagonalizers may be chosen to ensure *the mutual orthogonality of their rows*. This remarkably helpful property allows us to effortlessly obtain the eigenvectors of the generalized braiding matrices $\hat{R}(v)$ and $\hat{R}(v,w)$. These can be of interest in related statistical models.

Also we show, in Sec. VI, how such diagonalizations may be exploited in the description of associated noncommutative spaces. One principal objective in introducing our generalized spectral decompositions has been[1,2] the exploration of the roles of the variables (v,w) in the instances, where the generalized braid matrices $\hat{R}(v)$ and $\hat{R}(v,w)$ are used to construct the relevant noncommutative spaces. The constraints due to Leibnitz rule and the covariance properties—discussed, for instance, in Refs. 9–11 and a large number of sources cited therein—are presented in Sec. VI after incorporating our spectral variables.

But in this paper our study remains essentially limited to showing how the the diagonalization of Sec. V can help in better understanding certain features of such spaces. We hope to develop other aspects elsewhere. Remarks on various features of the results obtained and other perspectives are presented in Sec. VII.

II. MODIFIED BRAID EQUATION AND BAXTERIZATION FOR THE QUANTUM GROUP $\mathrm{GL}_q(N)$

In the vector representation the braid matrix $\hat{R}$ of the quantum group $\mathrm{GL}_q(N)$ has two orthogonal projectors. The spectral decomposition of its generalized $\hat{R}(v)$ matrix has been defined in (1.8). Adopting the definitions

$$X_1=P_{(-)}\otimes\mathrm{I}, \quad X_2=\mathrm{I}\otimes P_{(-)}, \quad S_1=(X_1-X_2), \quad T_1=(X_1X_2X_1-X_2X_1X_2), \tag{2.1}$$

we write

$$\hat{R}_{12}(v)\hat{R}_{23}(v')\hat{R}_{12}(v'')-\hat{R}_{23}(v'')\hat{R}_{12}(v')\hat{R}_{23}(v)=(v+v''+vv''-v')S_1+vv'v''T_1. \tag{2.2}$$

Equating the variables to their braid values $v=v'=v''=-(1+q^{-2})$ the right-hand side of (2.2) vanishes as in this limit the braid matrix $\hat{R}$ in (1.11) satisfying the braid equation (1.5) is obtained. This restricts

$$T_1=\frac{S_1}{[2]^2}. \tag{2.3}$$

Hence the right-hand side of (2.2) reads

$$\left((v+v''+vv''-v')+\frac{vv'v''}{[2]^2}\right)S_1, \tag{2.4}$$

where following (1.8) and the related discussions we obtain

$$S_1=v^{-1}(\hat{R}_{12}(v)-\hat{R}_{23}(v))=-q[2]^{-1}(\hat{R}_{12}-\hat{R}_{23}). \tag{2.5}$$

Setting $v=v'=v''$ we obtain the MBE obeyed by the generalized braid matrix $\hat{R}(v)$ of the quantum group $\mathrm{GL}_q(N)$:

$$\hat{R}_{12}(v)\hat{R}_{23}(v)\hat{R}_{12}(v)-\hat{R}_{23}(v)\hat{R}_{12}(v)\hat{R}_{23}(v)=(1+v+[2]^{-2}v^2)(\hat{R}_{12}(v)-\hat{R}_{23}(v)). \tag{2.6}$$

Comparing the above MBE with (1.17) we obtain

$$c=1+v+[2]^{-2}v^2. \tag{2.7}$$

For the Baxterization of the $\hat{R}(v)$ matrix we set

$$v=v(x), \quad v''=v(y), \quad v'=v(xy) \tag{2.8}$$

and denote $\hat{R}(v)\equiv\hat{R}(x)$. Now for the right-hand side of (2.2) to vanish, we must have

$$v(xy)=\frac{v(x)+v(y)+v(x)v(y)}{1-[2]^{-2}v(x)v(y)}. \tag{2.9}$$

This functional relation is solved in a more general form in Sec. III. Here we present the final result concerning the function $v(x)$ as follows. The solution satisfying the constraint

$$\hat{R}(x)\hat{R}(x^{-1})=1 \tag{2.10}$$

reads

$$v(x)=\frac{qx^{-1}-q^{-1}x}{qx-q^{-1}x^{-1}}-1. \tag{2.11}$$

Setting $x=\exp(\theta)$ and $q=\exp(h)$ in (2.11), we obtain the functional structure in (1.20). For the choice $y=\exp(\theta')$ and the above value of $v(\theta)$ the braid equation takes the form given in (1.19). Combining (1.8), (1.11), and (2.11) we may express $\hat{R}(x)$ as

$$\hat{R}(x)=\frac{qx\hat{R}-q^{-1}x^{-1}\hat{R}^{-1}}{qx-q^{-1}x^{-1}}. \tag{2.12}$$

Suitably changing the normalizations, namely, observing (1.13) and setting

$$\hat{\mathsf{R}}(x)=(qx^{-1}-q^{-1}x)\hat{R}(x^{-1}), \tag{2.13}$$

we obtain

$$\hat{\mathsf{R}}(x)=x^{-1}\hat{\mathsf{R}}-x\hat{\mathsf{R}}^{-1}. \tag{2.14}$$

In this form the Baxterization of the $\hat{R}$ matrix of the quantum group $\mathrm{GL}_q(N)$ is often presented.[7] We have preferred (2.12) to achieve uniform utilization of the same functional equation in Secs. II, III, and IV. This also ensures *one uniform normalization prescription*, whether the $\hat{R}$ matrix is Baxterized or not, by fixing the top left element (row 1, column 1) to be unity. This condition is evidently satisfied by (2.12).

III. MODIFIED BRAID EQUATION AND BAXTERIZATION FOR THE QUANTUM GROUPS $\mathrm{SO}_q(N)$ AND $\mathrm{Sp}_q(N)$

A. Reduction of trilinear terms

For arbitrary parameters (v,w) the generalized $\hat{R}(v,w)$ matrix is given by (1.9). In addition to quantities already introduced in (2.1), here we further define the following objects:

$$Y_1=P_{(0)}\otimes \mathsf{I}, \quad Y_2=\mathsf{I}\otimes P_{(0)}, \quad S_2=(Y_1-Y_2),$$

$$J_1=(X_1Y_2-Y_1X_2), \quad J_2=(Y_2X_1-X_2Y_1),$$

$$K_1=(X_1X_2Y_1-Y_2X_1X_2), \quad K_2=(X_1Y_2X_1-X_2Y_1X_2), \quad K_3=(Y_1X_2X_1-X_2X_1Y_2),$$

$$L_1=(Y_1Y_2X_1-X_2Y_1Y_2), \quad L_2=(Y_1X_2Y_1-Y_2X_1Y_2), \quad L_3=(X_1Y_2Y_1-Y_2Y_1X_2),$$

$$S_3=(K_1+K_2+K_3), \quad S_4=(L_1+L_2+L_3), \quad T_2=(Y_1Y_2Y_1-Y_2Y_1Y_2). \tag{3.1}$$

In terms of these quantities we obtain

$$\begin{aligned}
&\hat{R}_{12}(v,w)\hat{R}_{23}(v',w')\hat{R}_{12}(v'',w'')-\hat{R}_{23}(v'',w'')\hat{R}_{12}(v',w')\hat{R}_{23}(v,w)\\
&\quad=(v+v''+vv''-v')S_1+(w+w''+ww''-w')S_2+(vw'-v'w)J_1+(w'v''-w''v')J_2\\
&\qquad+(vv'w'')K_1+(vw'v'')K_2+(wv'v'')K_3+(ww'v'')L_1+(wv'w'')L_2+(vw'w'')L_3\\
&\qquad+(vv'v'')T_1+(ww'w'')T_2.
\end{aligned} \tag{3.2}$$

We will discuss below how to express the trilinear combinations $(K_1,K_2,K_3,L_1,L_2,L_3,T_1,T_2)$ in terms of the linear (S_1,S_2) and the bilinear (J_1,J_2) constructs. For the braid values of the parameters

$$v=v'=v''=-(1+q^{-2}), \quad w=w'=w''=-(1-\varepsilon q^{-(N+1-\varepsilon)}) \tag{3.3}$$

the right-hand side of (3.2) vanishes. As noted before, when the spectral variables assume their braid values, the generalized braid matrix $\hat{R}(v,w)$, while satisfying (1.5), reduces to the $\hat{R}$ matrix given in (1.12). The characteristic equation (1.2) for the $\hat{R}$ matrix now reads

$$(\hat{R}-\mathsf{I})(\hat{R}+q^{-2}\mathsf{I})(\hat{R}-\varepsilon q^{-(N+1-\varepsilon)}\mathsf{I})=0. \tag{3.4}$$

The projectors may be extracted from (3.4) as quadratic expression in the matrix $\hat{R}$ *à la* (1.3). For the choice

$$v=v'=v''=-(1+q^{2}), \quad w=w'=w''=-(1-\varepsilon q^{N+1-\varepsilon}) \tag{3.5}$$

the inverse of the braiding matrix, namely $\hat{R}^{-1}$ is obtained. The braid matrix and its inverse $\hat{R}^{\pm 1}$ obtained following the choices (3.3) and (3.5) have been listed in (1.12). For these matrices, as mentioned before, we will suppress the particular values of the spectral variables. For future use here we note that the inverse of the generalized braid matrix (1.9) is given by

$$(\hat{R}(v,w))^{-1}=\mathrm{I}-v(1+v)^{-1}P_{(-)}-w(1+w)^{-1}P_{(0)}. \tag{3.6}$$

The braid equation (1.5) may be utilized to yield the well-known constraints

$$f(\hat{R}_{12}^{\pm 1})\hat{R}_{23}^{\pm 1}\hat{R}_{12}^{\pm 1}=\hat{R}_{23}^{\pm 1}\hat{R}_{12}^{\pm 1}f(\hat{R}_{23}^{\pm 1}),\quad \hat{R}_{12}^{\pm 1}\hat{R}_{23}^{\pm 1}\ \ f(\hat{R}_{12}^{\pm 1})=f(\hat{R}_{23}^{\pm 1})\ \ \hat{R}_{12}^{\pm 1}\hat{R}_{23}^{\pm 1}, \tag{3.7}$$

where $f(x)$ is any well-behaved function of x. The projectors $P_{(-)}$ and $P_{(0)}$ are quadratic functions of the matrix $\hat{R}$. Choosing these particular functions in the constraints (3.7), and utilizing the definitions (2.1) and (3.1) we obtain

$$X_1A_{(\pm)}=A_{(\pm)}X_2,\quad Y_1A_{(\pm)}=A_{(\pm)}Y_2,\quad B_{(\pm)}X_1=X_2B_{(\pm)},\quad B_{(\pm)}Y_1=Y_2B_{(\pm)}, \tag{3.8}$$

where the bilinear elements read

$$\begin{aligned}A_{(\pm)}=\hat{R}_{23}^{\pm 1}\hat{R}_{12}^{\pm 1}=&\mathrm{I}-(1+q^{\mp 2})(X_1+X_2)-(1-\varepsilon q^{\mp(N+1-\varepsilon)})(Y_1+Y_2)+(1+q^{\mp 2})^2X_2X_1\\&+(1+q^{\mp 2})(1-\varepsilon q^{\mp(N+1-\varepsilon)})(X_2Y_1+Y_2X_1)+(1-\varepsilon q^{\mp(N+1-\varepsilon)})^2Y_2Y_1,\end{aligned} \tag{3.9}$$

$$\begin{aligned}B_{(\pm)}=\hat{R}_{12}^{\pm 1}\hat{R}_{23}^{\pm 1}=&\mathrm{I}-(1+q^{\mp 2})(X_1+X_2)-(1-\varepsilon q^{\mp(N+1-\varepsilon)})(Y_1+Y_2)+(1+q^{\mp 2})^2X_1X_2\\&+(1+q^{\mp 2})(1-\varepsilon q^{\mp(N+1-\varepsilon)})(X_1Y_2+Y_1X_2)+(1-\varepsilon q^{\mp(N+1-\varepsilon)})^2Y_1Y_2.\end{aligned} \tag{3.10}$$

We also enlist other useful relations,

$$Y_iY_jY_i=(1+\varepsilon[N-\varepsilon])^{-2}Y_i, \tag{3.11}$$

$$Y_iX_jY_i=\frac{\varepsilon[N-\varepsilon]([2]+\varepsilon[N-1-\varepsilon])}{[2](1+\varepsilon[N-\varepsilon])^2}Y_i, \tag{3.12}$$

where $(i,j)=(1,2)$ or (2, 1). Employing the above constraints and defining the following quantities:

$$\begin{aligned}c=&\frac{\varepsilon[N-\varepsilon+1]}{[2](1+\varepsilon[N-\varepsilon])},\quad d=(1+\varepsilon[N-\varepsilon])^{-1},\\k=&(q-q^{-1})\frac{q^{(N+1-\varepsilon)/2}-\varepsilon q^{-(N+1-\varepsilon)/2}}{q^{(N-1-\varepsilon)/2}+\varepsilon q^{-(N-1-\varepsilon)/2}},\end{aligned} \tag{3.13}$$

we obtain the promised reduction

$$\begin{aligned}&K_1=-c(J_2+(1-c)S_2),\quad K_2=(1-c)(J_1+J_2+(1-c)S_2),\quad K_3=-c(J_1+(1-c)S_2),\\&L_1=-d(J_1+(1-c)S_2),\quad L_2=(1-c)(1-d)S_2,\quad L_3=-d(J_2+(1-c)S_2),\\&T_1=[2]^{-2}(S_1+k(J_1+J_2+(1-c)S_2)),\quad T_2=d^2S_2.\end{aligned} \tag{3.14}$$

It is useful to define the ratios of the spectral variables (w/v) for the $\hat{R}^{\pm 1}$ matrices as given in (1.12):

$$f_{\pm}=q^{\pm 1}[2]^{-1}(1-\varepsilon q^{\mp(N+1-\varepsilon)})=-\varepsilon q^{\mp(N+1-\varepsilon)}f_{\mp}. \tag{3.15}$$

Then it may be shown that

$$c=[2]^{-1}\left(\frac{q^{-1}f_+-qf_-}{f_+-f_-}\right),\quad d=\frac{q-q^{-1}}{[2](f_+-f_-)},$$
$$k=-(q^2-q^{-2})\left(\frac{f_+f_-}{f_+-f_-}\right)=-[2]^2df_+f_-. \tag{3.16}$$

For the special case of the quantum group $SO_q(3)$, where $\varepsilon=1$ and $N=3$, we obtain the parametric values

$$c=1-[2]^{-1},\quad d=(1+[2])^{-1},\quad k=-(1+[2])(2-[2]). \tag{3.17}$$

As a valuable consistency check we carried through the reduction starting directly with $\varepsilon=1$, $N=3$. Agreement for this special case was obtained as the reduction scheme (3.14) was reproduced with the appropriate values of the parameters (3.17).

B. Modified braid equation

For the choice of the variables $v=v'=v''$ and $w=w'=w''$, the result (3.2) reduces to

$$\hat{R}_{12}(v,w)\hat{R}_{23}(v,w)\hat{R}_{12}(v,w)-\hat{R}_{23}(v,w)\hat{R}_{12}(v,w)\hat{R}_{23}(v,w)$$
$$=v(1+v)S_1+w(1+w)S_2+v^2wS_3+vw^2S_4+v^3T_1+w^3T_2, \tag{3.18}$$

where, using (3.14) we obtain

$$S_3=K_1+K_2+K_3=(1-c)(1-3c)S_2+(1-2c)(J_1+J_2),$$
$$S_4=L_1+L_2+L_3=(1-c)(1-3d)S_2-d(J_1+J_2). \tag{3.19}$$

Using the reduction (3.14) for the trilinear constructs T_1 and T_2, we finally obtain the right-hand side of (3.18) as

$$a_1S_1+a_2S_2+b(J_1+J_2), \tag{3.20}$$

where the coefficients read

$$a_1=[2]^{-2}v(v+[2]q)(v+[2]q^{-1}),$$
$$a_2=w(1+w)+d^2w^3+(1-c)v^3\left([2]^{-2}k+(1-3c)\left(\frac{w}{v}\right)+(1-3d)\left(\frac{w}{v}\right)^2\right), \tag{3.21}$$
$$b=-dv^3\left(\frac{w}{v}-f_+\right)\left(\frac{w}{v}-f_-\right).$$

The choice of the 'braid values' for the variables $v=-[2]q^{\mp1}$, $w/v=f_\pm$ for the $\hat{R}^{\pm1}$ matrices readily reduces (3.21) to $a_1=0$, $a_2=0$, $b=0$. This is obvious for a_1 and b, whereas the result for a_2 provides a good consistency check.

To obtain the general MBE we now express (3.20) in terms of $(\hat{R}(v,w))^{\pm1}$. The projectors now read

$$P_{(-)}=\frac{1+v}{v(v-w)}((\hat{R}(v,w)-\mathrm{I})+(1+w)(\hat{R}^{-1}(v,w)-\mathrm{I})),$$
$$P_{(0)}=\frac{1+w}{w(w-v)}((\hat{R}(v,w)-\mathrm{I})+(1+v)(\hat{R}^{-1}(v,w)-\mathrm{I})). \tag{3.22}$$

In passing we mention that by implementing the braid values (1.10) of the variables (v,w) the projectors $P_{(+)}$ and $P_{(0)}$ may also be expressed in terms of the braid matrices $\hat{R}^{\pm 1}$. Now we can express the constructs S_1, S_2, J_1 and J_2 defined in (3.1) in terms of the generalized braid matrices $\hat{R}_{12}^{\pm 1}(v,w)$ and $\hat{R}_{23}^{\pm 1}(v,w)$. Substituting these results in (3.20) we obtain the general MBE stated in (1.18), where, with the values of (a_1,a_2,b) given in (3.21), the coefficients read

$$c_1=\frac{(1+v)(1+w)}{vw(v-w)}\left(\frac{w}{1+w}a_1-\frac{v}{1+v}a_2+2b\right),$$
$$c_2=\frac{(1+v)(1+w)}{vw(v-w)}(wa_1-va_2-2b),\quad c_3=-\frac{(1+v)(1+w)}{vw(v-w)}\,b. \tag{3.23}$$

For the braid values (1.10) of the variables v and w the coefficients (c_1,c_2,c_3) vanish.

We now discuss the following special cases depending on values of the parameters v and w.

(i) For an *arbitrary* nonzero value of v, and for the choices $w=f_{\pm}v$, we, *via* (3.21) and (3.23), obtain $c_3=0$. Hence the right hand side of the MBE (1.18) reduces to the first two terms. Using the characteristic equation (1.15) the right-hand side of the MBE may now be expressed in terms of the generalized braiding operators $(\hat{R}_{12}(v,w)-\hat{R}_{23}(v,w))$ and $(\hat{R}_{12}^2(v,w)-\hat{R}_{23}^2(v,w))$.

(ii) For $v=0$ and an arbitrary value of w we have an interesting case deserving a detailed treatment that is provided in Sec. IV. Here we just note that, for these parametric values, the operator $\hat{R}(0,w)$ satisfies a *quadratic* rather than a cubic characteristic equation; and the right-hand side of the MBE (1.18) is now proportional to $(\hat{R}_{12}(0,w)-\hat{R}_{23}(0,w))$.

C. Baxterization

As was noted in Sec. I, the MBE and the Baxterization are two complementary aspects of the generalized braid operator $\hat{R}(v,w)$ with its spectral decomposition given in (1.9). Having formulated the MBE, we now turn to Baxterization of the braid operator.

From (3.2) and (3.14) we obtain

$$\hat{R}_{12}(v,w)\hat{R}_{23}(v',w')\hat{R}_{12}(v'',w'')-\hat{R}_{23}(v'',w'')\hat{R}_{12}(v',w')\hat{R}_{23}(v,w)=\mathsf{a}_1S_1+\mathsf{a}_2S_2+\mathsf{b}_1J_1+\mathsf{b}_2J_2, \tag{3.24}$$

where, with the parameters c, d and k given by (3.13), the coefficients read

$$\begin{aligned}
\mathsf{a}_1&=(v+v''+vv'')-(1-[2]^{-2}vv'')v',\\
\mathsf{a}_2&=(w+w''+ww'')-(1-d^2ww'')w'+(1-c)((1-c)vv''w'-c(vw''+v''w)v')\\
&\quad+(1-c)((1-d)ww''v'-d(vw''+v''w)w')+(1-c)k[2]^{-2}vv''v',\\
\mathsf{b}_1&=(vw'-wv')-cwv''v'+(1-c)vv''w'-dwv''w'+k[2]^{-2}vv''v',\\
\mathsf{b}_2&=(v''w'-w''v')-cvw''v'+(1-c)vv''w'-dvw''w'+k[2]^{-2}vv''v'.
\end{aligned} \tag{3.25}$$

For Baxterization the variables (v,v'',v') and (w,w'',w') are re-expressed as $(v(x),v(y),v(xy))$ and $(w(x),w(y),w(xy))$, respectively; and then the functional equations

$$\mathsf{a}_i(x,y)=0,\quad \mathsf{b}_i(x,y)=0,\quad i=(1,2) \tag{3.26}$$

obtained *via* (3.25) are solved.

We start by noting a crucial constraint on the functional solutions to be implemented systematically. In (3.24) the $\hat{R}(v,w)$ matrix may be replaced with its inverse $\hat{R}^{-1}(v,w)$ given in (3.6). Hence for consistency our functional solutions must be such that

$$-\frac{v(x)}{1+v(x)}=v(x'),\quad -\frac{w(x)}{1+w(x)}=w(x'), \tag{3.27}$$

where x' is some suitable function of x. We have chosen the parametrization

$$x'=x^{-1} \tag{3.28}$$

such that the validity of the constraint

$$\hat{R}(x)\hat{R}(x^{-1})=\mathsf{I} \tag{3.29}$$

is assured. The functions $f(x)$ and $g(x)$ being suitably well-defined, the relations (3.27) and (3.28) now imply

$$v(x)=\frac{f(x)}{f(x^{-1})}-1,\quad w(x)=\frac{g(x)}{g(x^{-1})}-1. \tag{3.30}$$

It will, in fact, thus be necessary to solve only *two* functional equations from the set (3.26):

$$\mathsf{a}_1(x,y)=0,\quad \mathsf{b}_1(x,y)=0. \tag{3.31}$$

As for the function b_2 we note that the following exchange relation holds:

$$\mathsf{b}_2(x,y)=\mathsf{b}_1(y,x). \tag{3.32}$$

Moreover the solutions of the functional equations (3.31), along with (3.30), will be seen to fix the functions $v(x)$ and $w(x)$ *completely with all the parameters determined*. Then the much more complicated functional equation for $\mathsf{a}_2(x,y)$ does not have to be solved at all. The consistency of the scheme may be verified by checking that $\mathsf{a}_2(x,y)$ indeed vanishes by implementing $v(x)$ and $w(x)$ already available. So now we consider the equations in (3.31). The first equation in (3.31) implies (2.9). It will turn out to be quite useful to solve a more general function equation with arbitrary λ given by

$$u(xy)=\frac{u(x)+u(y)+u(x)u(y)}{1-\lambda^2u(x)u(y)}. \tag{3.33}$$

By direct substitution it may be verified that the general solution maintaining the structure (3.30), namely

$$u(x)=\frac{\alpha(x)}{\alpha(x^{-1})}-1 \tag{3.34}$$

is given by

$$\alpha(x)=-(x-x^{-1})\pm\sqrt{1-4\lambda^2}(x+x^{-1}). \tag{3.35}$$

For all cases of interest to us the square root will turn out to be real. The lower sign before the root in the right-hand side of (3.35) corresponds to $u(x^{-1})$ with the upper sign. So it is sufficient to consider only one, say, the upper sign before the root, since, more generally, replacing of x by x^p in (3.30) does not change the essential functional form. Now setting $\lambda=[2]^{-1}$, we obtain the solution of the first equation in (3.30) with the function $f(x)$ given by

$$f(x)=-(x-x^{-1})+(q-q^{-1})[2]^{-1}(x+x^{-1}). \tag{3.36}$$

Apart from the basic structures (3.34) and (3.35), the following form is also of interest:

$$u(x)=\beta\left(\frac{x^2-1}{x^2+\beta+1}\right), \quad \text{where} \quad \beta=-2(1+\sqrt{1-4\lambda^2})^{-1}. \tag{3.37}$$

Substituting $x=\exp(\theta)$, $\tanh\gamma=\sqrt{1-4\lambda^2}$ we obtain the elegant form of additive Baxterization, as seen in the context of (1.19):

$$u(x)\sim u(\theta)=\frac{\sinh(\gamma-\theta)}{\sinh(\gamma+\theta)}-1. \tag{3.38}$$

For the function $v(x)\sim v(\theta)$, we obtain, after setting $q=\exp(h)$, the solution (1.20).

Now to solve the second equation in (3.31) we proceed in successive steps as follows. Expressing the parameters (c,d,k) in terms of the ratios $f_\pm$ as given in (3.16), we define

$$\mathsf{b}_1\equiv-\frac{vv'v''}{[2](f_+-f_-)}F, \tag{3.39}$$

where

$$F=(q-q^{-1})\frac{w}{v}\frac{w'}{v'}+[2]\frac{f_+-f_-}{v''}\left(\frac{w}{v}-\frac{w'}{v'}\right)+(q^{-1}f_+-qf_-)\frac{w}{v}$$
$$-(qf_+-q^{-1}f_-)\frac{w'}{v'}+(q-q^{-1})f_+f_-. \tag{3.40}$$

In (3.40) we have assumed that the spectral function $v\neq 0$. Now defining

$$U=[2]d(wv^{-1}-f_+), \tag{3.41}$$

we obtain after simplification

$$F=(q-q^{-1})\frac{UU'}{([2]d)^2}\left(1+\left(q+\frac{[2]}{v''}\right)\frac{1}{U'}-\left(q^{-1}+\frac{[2]}{v''}\right)\frac{1}{U}\right). \tag{3.42}$$

In the context of (3.41) we note that by translating the ratio (w/v) by f_- the same functional solutions are finally obtained. Substituting for the function v the form corresponding to (3.37), i.e.,

$$v''=v(y)=-[2]q^{-1}(y^2-1)(y^2-q^{-2})^{-1}, \tag{3.43}$$

we find that the requirement for $F=0$ reads

$$U^{-1}(xy)+(q-q^{-1})^{-1}=(U^{-1}(x)+(q-q^{-1})^{-1})y^2. \tag{3.44}$$

Hence, with an as yet arbitrary parameter δ that is to be fixed immediately afterwards, we obtain the solution as

$$U^{-1}(x)+(q-q^{-1})^{-1}=\delta(q-q^{-1})^{-1}x^2. \tag{3.45}$$

Now the spectral function $w(x)$ may be solved in terms of the already known solution $v(x)$:

$$w(x)=(f_+\delta x^2-f_-)(\delta x^2-1)^{-1}v(x). \tag{3.46}$$

Using the crucial constraint (3.30) on $w(x)$ now it may be shown that there are *only two permitted values* of the parameter δ, which, in turn, generate the corresponding solutions of the spectral function $w(x)$:

$$\delta=-\varepsilon q^{(N+1-\varepsilon)}\Rightarrow w(x)=\frac{x+\varepsilon q^{(N+1-\varepsilon)}x^{-1}}{x^{-1}+\varepsilon q^{(N+1-\varepsilon)}x}-1, \tag{3.47}$$

$$\delta=\varepsilon q^{(N-1-\varepsilon)}\Rightarrow w(x)=\frac{(qx-\varepsilon q^{(N-\varepsilon)}x^{-1})(q^{-1}x-qx^{-1})}{(qx^{-1}-\varepsilon q^{(N-\varepsilon)}x)(q^{-1}x^{-1}-qx)}-1. \tag{3.48}$$

At this stage our procedure of Baxterization of the braid operator is complete. In view of the discussion following (3.32) we need not solve the functional equations corresponding to $\mathsf{a}_2(x,y)$ and $\mathsf{b}_2(x,y)$. The function $w(x)$ corresponding to the additive form of Baxterization may be obtained by setting $x=\exp(\theta),q=\exp(h)$ in the solutions (3.47) and (3.48). For the quantum group $\mathrm{SO}_q(N)$, with $\varepsilon=1$, these solutions assume the form (1.21) and (1.22), respectively. Similarly for the quantized symplectic group $\mathrm{Sp}_q(N)$, where $\varepsilon=-1$ and $N=2n$, they are given by (1.23) and (1.24), respectively.

Finally, expressing the projection operators $P_{(-)}$ and $P_{(0)}$ in terms of the braid matrices $\hat{R}^{\pm 1}$, as discussed following equation (3.22), we obtain

$$\hat{R}(x)=l_{(0)}(x)\mathsf{I}+l_{(+)}(x)\hat{R}+l_{(-)}(x)\hat{R}^{-1}. \tag{3.49}$$

Denoting the braid values (1.10) of the spectral variables corresponding to the $\hat{R}$ matrix by (v_0,w_0), respectively, the coefficients in (3.49) may be listed as

$$\begin{aligned}
l_{(0)}(x)&=1-(1+v_0)(2+w_0)v_0^{-1}(v_0-w_0)^{-1}\,v(x)-(2+v_0)(1+w_0)w_0^{-1}(w_0-v_0)^{-1}\,w(x),\\
l_{(+)}(x)&=(1+v_0)v_0^{-1}(v_0-w_0)^{-1}\,v(x)+(1+w_0)w_0^{-1}(w_0-v_0)^{-1}\,w(x),\\
l_{(-)}(x)&=(1+v_0)(1+w_0)(v_0^{-1}(v_0-w_0)^{-1}\,v(x)+w_0^{-1}(w_0-v_0)^{-1}w(x)).
\end{aligned} \tag{3.50}$$

Consistent with our normalization, the relation $l_{(0)}(x)+l_{(+)}(x)+l_{(-)}(x)=1$ is maintained.

IV. A NEW CLASS OF SOLUTIONS OF THE BRAID EQUATION

So far we have been studying the general case $(v\neq 0,w\neq 0)$ of the spectral variables. We note that for the choice $w=0$, there is no solution of the braid equation with nontrivial v as more than one functional constraints on the single spectral parameter, or the function $v(x)$ in the Baxterized case, need to be satisfied.

For the alternate choice $v=0$, it is, however, *possible* to obtain a remarkable class of generalized braid matrices $\hat{R}(w)$ depending on the single variable w. This was already studied in the context of the quantum group $\mathrm{SO}_q(3)$ in Ref. 2. Here we present this class for general quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$. Denoting the generalized braid matrix $\hat{R}(0,w)$ by $\hat{R}(w)$, we write

$$\hat{R}(w)=\mathsf{I}+wP_{(0)},\quad \hat{R}^{-1}(w)=\mathsf{I}-w(1+w)^{-1}P_{(0)}, \tag{4.1}$$

where the matrix $\hat{R}(w)$ satisfies a quadratic characteristic equation

$$(\hat{R}(w)-\mathsf{I})(\hat{R}(w)-(1+w)\,\mathsf{I})=0. \tag{4.2}$$

Instead of restricting our preceding general formulas to the special case $v=0$ it is much simpler to start again with (3.2) which, in conjunction with the last relation in (3.14), now gives

$$\hat{R}_{12}(w)\hat{R}_{23}(w)\hat{R}_{12}(w)-\hat{R}_{23}(w)\hat{R}_{12}(w)\hat{R}_{23}(w)$$
$$=(w(1+w)+d^2w^3)S_2=(1+w+d^2w^2)(\hat{R}_{12}(w)-\hat{R}_{23}(w)). \tag{4.3}$$

Thus we have already obtained the MBE with a simple linear structure in the generalized braid matrix on the right-hand side. But as the coefficient on the right-hand side of (4.3) may be factorized as

$$d^2w^2+w+1=d^2(w-w_+)(w-w_-), \quad w_\pm=2^{-1}d^{-2}(-1\pm\sqrt{1-4d^2}), \tag{4.4}$$

we obtain two nonmodified *new braid matrices*:

$$\hat{R}_{12}(w_\pm)\hat{R}_{23}(w_\pm)\hat{R}_{12}(w_\pm)-\hat{R}_{23}(w_\pm)\hat{R}_{12}(w_\pm)\hat{R}_{23}(w_\pm)=0. \tag{4.5}$$

But the constraint

$$\hat{R}(w_+)\hat{R}(w_-)=\mathsf{I}, \tag{4.6}$$

observed using (4.1) and (4.4) indicate the presence of only *one* braid matrix and its inverse. Following the expression of d in (3.13) we also note that the quantity under the radical sign in (4.4) satisfies $1>(1-4d^2)>0$ for all values of (N,ε) relevant to us. Hence the square root is real.

The prescription of Baxterization of this class of $\hat{R}(w)$ matrices is immediately obtained from (3.33)–(3.35). Only relevant functional equation $\mathsf{a}_2(x,y)=0$ in the set (3.26) now yields

$$w(xy)=\frac{w(x)+w(y)+w(x)w(y)}{1-d^2w(x)\,w(y)}, \tag{4.7}$$

whereas the other functional equations in the set (3.26) trivially vanishes for the case $v=0$. The solution of the equation (4.7) read

$$w(x)=\frac{-(x-x^{-1})+\sqrt{1-4d^2}(x+x^{-1})}{(x-x^{-1})+\sqrt{1-4d^2}(x+x^{-1})}-1. \tag{4.8}$$

Setting $x=\exp(\theta)$ and $\tanh\eta=\sqrt{1-4d^2}$, we, following (3.38), obtain

$$w(x)\sim w(\theta)=\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}-1. \tag{4.9}$$

For the quantum group $\mathrm{SO}_q(3)$ the generalized braid operator $\hat{R}(w)$ in the present class was explicitly presented before in Ref. 2. Here we present the general prescription regarding the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$. To this end we include the standard and well-known construction of the projectors for the sake of completeness. Let $(\rho_1,\rho_2,\ldots,\rho_N)$ denote the N-tuple with the following assignments for the respective quantum groups:

$$\left(n-\tfrac{1}{2},n-\tfrac{3}{2},\ldots,\tfrac{1}{2},0,-\tfrac{1}{2},\ldots,-n+\tfrac{1}{2}\right) \quad \text{for } \mathrm{SO}_q(2n+1),$$
$$(n-1,n-2,\ldots,1,0,0,-1,\ldots,-n+1) \quad \text{for } \mathrm{SO}_q(2n), \tag{4.10}$$
$$(n,n-1,\ldots,1,-1,\ldots,-n) \quad \text{for } \mathrm{Sp}_q(2n).$$

We also fix the values $\{\epsilon_i=1|i=1,\ldots,N\}$ for the quantum group $\mathrm{SO}_q(N)$; and $\{\epsilon_i=1$, if $i\leqslant n$, $\epsilon_i=-1$, if $i>n\}$ for the quantum group $\mathrm{Sp}_q(2n)$. As usual E_{ij} denotes the $N\times N$ matrix where the only nonzero element (i,j) equals unity. With these notations the projectors are given by

$$P_{(0)}=(1+[N-1])^{-1}\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}\ E_{i',j}\otimes E_{i,j'} \tag{4.11}$$

and

$$P_{(0)}=(1-[N+1])^{-1}\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}\ \epsilon_i\epsilon_j\ E_{i',j}\otimes E_{i,j'} \tag{4.12}$$

for the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$, (where $N=2n$), respectively. In the above equations we have used the notation $i'=N+1-i$. We have recapitulated the above standard prescription for the additional purpose of displaying the braid operators in the $q=1$ limit.

We enlist below the lowest dimensional cases as examples. The projector $P_{(0)}$ in the 9×9 vector representation for the quantum group $\mathrm{SO}_q(3)$ is given by

$$\begin{aligned}(1+[2])P_{(0)}=&q^{-1}E_{11}\otimes E_{33}+q^{-1/2}E_{12}\otimes E_{32}+E_{13}\otimes E_{31}+q^{-1/2}E_{21}\otimes E_{23}+E_{22}\otimes E_{22}+q^{1/2}E_{23}\\&\otimes E_{21}+E_{31}\otimes E_{13}+q^{1/2}E_{32}\otimes E_{12}+qE_{33}\otimes E_{11},\end{aligned} \tag{4.13}$$

whereas 16×16 vector representations for the quantum groups $\mathrm{SO}_q(4)$ and $\mathrm{Sp}_q(4)$ read as

$$\begin{aligned}(1+[3])P_{(0)}=&q^{-2}E_{11}\otimes E_{44}+q^{-1}E_{12}\otimes E_{43}+q^{-1}E_{13}\otimes E_{42}+E_{14}\otimes E_{41}+q^{-1}E_{21}\otimes E_{34}+E_{22}\otimes E_{33}\\&+E_{23}\otimes E_{32}+qE_{24}\otimes E_{31}+q^{-1}E_{31}\otimes E_{24}+E_{32}\otimes E_{23}+E_{33}\otimes E_{22}+qE_{34}\otimes E_{21}+E_{41}\\&\otimes E_{14}+qE_{42}\otimes E_{13}+qE_{43}\otimes E_{12}+q^2E_{44}\otimes E_{11}\end{aligned} \tag{4.14}$$

and

$$\begin{aligned}([5]-1)P_{(0)}=&q^{-4}E_{11}\otimes E_{44}+q^{-3}E_{12}\otimes E_{43}-q^{-1}E_{13}\otimes E_{42}-E_{14}\otimes E_{41}+q^{-3}E_{21}\otimes E_{34}+q^{-2}E_{22}\\&\otimes E_{33}-E_{23}\otimes E_{32}-qE_{24}\otimes E_{31}-q^{-1}E_{31}\otimes E_{24}-E_{32}\otimes E_{23}+q^2E_{33}\otimes E_{22}+q^3E_{34}\\&\otimes E_{21}-E_{41}\otimes E_{14}-qE_{42}\otimes E_{13}+q^3E_{43}\otimes E_{12}+q^4E_{44}\otimes E_{11},\end{aligned} \tag{4.15}$$

respectively.

For this class, directly setting $q=1$ we still get nontrivial braid matrices, the MBE satisfied by them, and also the Baxterized forms of these braid matrices. (We note that we are not considering the so-called quasiclassical limit obtained as the coefficients of the terms linear in h, while implementing series expansion in $h\equiv\ln q$. We simply set $q=1$ in the relevant quantities, and thus obtain the terms of zero order in h). The corresponding example for the quantum group $\mathrm{SO}_q(3)$ was discussed in Ref. 2.

In the classical $q=1$ limit, we denote the projectors by $\hat{P}$ to avoid confusion. Using (4.11) we now obtain the projector for the classical group $\mathrm{SO}(N)$ as

$$\hat{P}_{(0)}=N^{-1}\sum_{i,j=1}^{N} E_{i',j}\otimes E_{i,j'}, \tag{4.16}$$

while the projector for the classical symplectic group $\mathrm{Sp}(N)$ reads

$$\hat{P}_{(0)}=-N^{-1}\sum_{i,j=1}^{N} \epsilon_i\epsilon_j E_{i',j}\otimes E_{i,j'}. \tag{4.17}$$

Moreover the parameters, *via* (3.13), (4.4), and (4.9), are obtained in the limit $q=1$ as

$$d|_{(q=1)} \equiv \hat{d} = \varepsilon N^{-1}, \quad \eta|_{(q=1)} \equiv \hat{\eta} = \operatorname{arctanh}(N^{-1}\sqrt{N^2-4}),$$
$$w_{(\pm)}|_{(q=1)} \equiv \hat{w}_{(\pm)} = \frac{N}{2}(-N \pm \sqrt{N^2-4}). \tag{4.18}$$

Using the above value of $\hat{d}$ in (4.3) we may directly obtain the MBE in the $q=1$ case. In the Baxterized function (4.9) we now use the value of $\hat{\eta}$ given in (4.18), and thereby obtain the limiting structure

$$w(\theta)|_{(q=1)} = \hat{w}(\theta) = \frac{\sinh(\hat{\eta}-\theta)}{\sinh(\hat{\eta}+\theta)} - 1. \tag{4.19}$$

We now focus on the $q=1$ limiting case of the braid solution described in (4.5). The braid matrices in this limit has the structure

$$\hat{R}(\hat{w}_{(\pm)}) = \mathrm{I} + \hat{w}_{(\pm)}\hat{P}_{(0)}. \tag{4.20}$$

Even in the said $q=1$ limit, these matrices, on account of the characteristic equation (4.2), satisfy a nontrivial Hecke condition. These braid matrices are not of co-boundary type, which may be obtained by twisting the identity operator. The situation may be profitably contrasted with the $q=1$ limiting behavior of the general case ($v \neq 0$) of braid matrices satisfying (1.5). Setting the limit $q=1$ in the braid values (1.10) of the spectral variables we obtain

$$v|_{(q=1)} \equiv \hat{v} = -2, \quad w|_{(q=1)} \equiv \hat{w} = -(1-\varepsilon). \tag{4.21}$$

Incidentally, identical conditions in the said classical limit $h=0$ may be derived from the Baxterized version of the spectral variables given in (1.20)–(1.24). For the values of the spectral variables given in (4.21) the braid matrix for the quantum group $\mathrm{SO}_q(N)$ assumes the form

$$\hat{R}(\hat{v},\hat{w}) = \mathrm{I} - 2P_{(-)}, \tag{4.22}$$

whereas the the braid matrix for the quantum group $\mathrm{Sp}_q(N)$ reads

$$\hat{R}(\hat{v},\hat{w}) = \mathrm{I} - 2P_{(-)} - 2P_{(0)} = 2P_{(+)} - \mathrm{I}. \tag{4.23}$$

The above two braid matrices satisfy the condition $(\hat{R}(\hat{v},\hat{w}))^2 = \mathrm{I}$, typical of twisted identity matrices. Finally we note that here the result parallel to (2.12) is

$$\hat{R}(w) = \frac{(w-w_-)\hat{R}(w_+) - (w-w_+)\hat{R}(w_-)}{(w_+ - w_-)}, \tag{4.24}$$

where $w_\pm$, *via* (4.4), is given by $w_\pm = -(1+\exp(\mp 2\eta))$.

V. DIAGONALIZATION OF THE MODIFIED BRAID MATRICES AND THEIR CORRESPONDING EIGENVECTORS

We present below explicitly the 4×4, 9×9, and 16×16 matrices which, through similarity transformations, diagonalize respectively the matrices $\hat{R}(v)$ for the quantum group $\mathrm{GL}_q(2)$, and $\hat{R}(v,w)$ for the quantum groups $\mathrm{SO}_q(3)$ and $\mathrm{SO}_q(4)$. Explicit constructions for arbitrary dimensions $N\times N$ is beyond the scope of the present work. But we start by considering, for deeper understanding, certain aspect of the problem for the general quantized orthogonal group $\mathrm{SO}_q(N)$. The case for the general linear quantum group $\mathrm{GL}_q(N)$ is, as usual, much simpler. In the diago-

nalization process, as throughout the present work, the projectors involved in the spectral decomposition of the generalized braid matrices play essential roles. Interest in the results obtained will be discussed at the end.

Traces of the projectors satisfying the completeness property

$$P_{(+)}+P_{(-)}+P_{(0)}=\mathsf{I}_{N^2\times N^2}, \tag{5.1}$$

are given by

$$\mathrm{Tr}\,P_{(+)}=\tfrac{1}{2}N(N+1)-\tfrac{1}{2}(\varepsilon+1),\quad \mathrm{Tr}\,P_{(-)}=\tfrac{1}{2}N(N-1)+\tfrac{1}{2}(\varepsilon-1),\quad \mathrm{Tr}\,P_{(0)}=1. \tag{5.2}$$

The sum of the above three traces, consistent with (5.1), is N^2. We consider below only the examples of quantum orthogonal algebras corresponding to the choice $\varepsilon=1$. Moreover, in view of (5.1), we will only consider the projectors $P_{(-)}$ and $P_{(0)}$, thus continuing the methodology followed in the earlier sections.

A projector when diagonalized can have for each diagonal element *either zero or unity*. The number of unit elements are fixed by trace. The diagonal elements can be permuted by successive similarity transformations. So we can choose a suitable canonical ordering for them as follows. Denoting a diagonalized projector P by $P^{(\mathrm{d})}$, we choose the ordering presented below. For the quantum group $\mathrm{SO}_q(3)$ the diagonalized projectors read

$$\begin{aligned} P^{(\mathrm{d})}_{(0)}&=(1,0,0,0,0,0,0,0,0)_{(\mathrm{diagonal})},\\ P^{(\mathrm{d})}_{(-)}&=(0,1,1,1,0,0,0,0,0)_{(\mathrm{diagonal})}, \end{aligned} \tag{5.3}$$

whereas these diagonalized projectors for the quantum group $\mathrm{SO}_q(4)$ are given by

$$\begin{aligned} P^{(\mathrm{d})}_{(0)}&=(1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)_{(\mathrm{diagonal})},\\ P^{(\mathrm{d})}_{(-)}&=(0,1,1,1,1,1,1,0,0,0,0,0,0,0,0,0)_{(\mathrm{diagonal})}. \end{aligned} \tag{5.4}$$

The prescription for general quantized orthogonal group $\mathrm{SO}_q(N)$ is evident.

A transformation that diagonalizes the generalized braid matrix $\hat{R}(v,w)$ must diagonalize each projector *separately*, as these projectors are functions of the matrix $\hat{R}(v,w)$. Using the above form of the diagonalized projectors, we avoid introducing the inverse of the diagonalizing matrix M as follows. Assuming that a diagonalizing matrix of nonzero determinant exists, we have

$$MP_{(0)}=P^{(\mathrm{d})}_{(0)}M,\quad MP_{(-)}=P^{(\mathrm{d})}_{(-)}M, \tag{5.5}$$

where the diagonalized projectors $P^{(\mathrm{d})}$ have explicit forms given by (5.3) and (5.4), and their evident generalizations. The projectors $P_{(0)}$ and $P_{(-)}$ being known from the standard results, we avoid direct introduction of the matrix M^{-1}, which is nonlinear in elements of M.

The diagonalizing relations (5.5) generate a set of *linear* constraints on the elements of M. The coefficients in each equation are fully known. They will in general leave room for many arbitrary parameters in the matrix M, subject to the constraint that it has a nonzero determinant. This arbitrariness can be factored out as follows. Supposing that in the case of the the quantum group $\mathrm{SO}_q(3)$ we have found a convenient solution $\hat{M}$ for the diagonalizing matrix, the relation (5.5) in conjunction with (5.3) yield the structure

$$\hat{M}\hat{R}(v,w)\hat{M}^{-1}=\hat{M}(\mathsf{I}+vP_{(-)}+wP_{(0)})\hat{M}^{-1}=(1+w,1+v,1+v,1+v,1,1,1,1,1)_{(\mathrm{diagonal})}. \tag{5.6}$$

Keeping the above block structure in mind we now use a block diagonal matrix

$$\mathsf{M}=(\mathsf{M}_{(0)},\mathsf{M}_{(-)},\mathsf{M}_{(+)})_{(\text{block diagonal})}, \tag{5.7}$$

where $\mathsf{M}_{(0)}$, $\mathsf{M}_{(-)}$, and $\mathsf{M}_{(+)}$, respectively, are 1×1, 3×3, and 5×5 invertible matrices with nonzero determinant. Using the property (5.6) and the above structure of the matrix M, we obtain

$$(\mathsf{M}\hat{M})\hat{R}(v,w)(\mathsf{M}\hat{M})^{-1}=\hat{M}\hat{R}(v,w)\hat{M}^{-1}. \tag{5.8}$$

Thus the diagonalization is preserved exactly. The above matrix $\mathsf{M}_{(0)}$ is a nonzero constant, whereas the matrices $\mathsf{M}_{(\mp)}$, apart from the single constraint of invertibility have *arbitrary* elements. This is the source of arbitrariness in the diagonalization procedure. For the general case the dimensions of $\mathsf{M}_{(0)}$, $\mathsf{M}_{(-)}$, and $\mathsf{M}_{(+)}$ are given by the respective traces (5.2) of the corresponding projectors.

But how do we select $\hat{M}$? For the quantum groups $\mathrm{SO}_q(3)$ and $\mathrm{SO}_q(4)$ we present below the diagonalizing matrix $\hat{M}$ possessing a remarkably helpful feature: *the rows of $\hat{M}$ are mutually orthogonal*. It is presumably possible to choose the diagonalizing matrix $\hat{M}$ retaining this feature for all orthogonal quantum groups. But here we do not attempt to construct such a general solution for an arbitrary case.

For the quantum group $\mathrm{SO}_q(3)$ we define the parameters $s=-q^{-1/2}(1-q)$, $t=-q^{-3/2}(1+q)$, and obtain the relevant diagonalizing matrix:

$$\hat{M}=\begin{pmatrix} 0 & 0 & 1 & 0 & q^{1/2} & 0 & q & 0 & 0 \\ 0 & 1 & 0 & -q & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -q & 0 \\ 0 & 0 & 1 & 0 & s & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & q^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & t & 0 & q^{-2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & q^{-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.9}$$

Here we note the existence of the following orthogonal triplets:

$$(1,q^{1/2},q),(1,s,-1),(1,t,q^{-2}), \tag{5.10}$$

which, as will be seen later, play a role in the context of the noncommutative coordinates. For the quantum group $\mathrm{SO}_q(4)$, one possible choice of the ordering of the rows gives the following diagonalizing matrix:

$$\hat{M}=\begin{pmatrix}
0&0&0&1&0&0&q&0&0&q&0&0&q^2&0&0&0\\
0&0&0&1&0&0&q&0&0&-q^{-1}&0&0&-1&0&0&0\\
0&1&0&0&-q&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&-q&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0&0&-q&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&0&-q&0\\
0&0&0&1&0&0&-q^{-1}&0&0&q&0&0&-1&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&q^{-1}&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&q^{-1}&0&0&0&0&0&0&0\\
0&0&0&1&0&0&-q^{-1}&0&0&-q^{-1}&0&0&q^{-2}&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0&0&q^{-1}&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&0&q^{-1}&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1
\end{pmatrix}. \tag{5.11}$$

Here the relevant orthogonal quadruplets read

$$(1,q,q,q^2),(1,q,-q^{-1},-1),(1,-q^{-1},q,-1),(1,-q^{-1},-q^{-1},q^{-2}). \tag{5.12}$$

It may be noted that the orthogonality of the rows delivers the inverse of the diagonalizing matrix $\hat{M}^{-1}$ effortlessly. To this end, we take the transposed matrix $\hat{M}^{\mathsf{T}}$ and normalize each element of its column j by the same factor c_j so that the sum of squares of all elements of this column j multiplied with c_j equates to unity. For the diagonalizing matrix $\hat{M}$ in (5.9), these normalization constants are given by

$$\begin{aligned}q(1+[2])c_1=q[2]c_2=q[2]c_3=[2]c_4=c_5=q^{-1}[2]c_6,\\ =q^{-2}[2](1+[2])c_7=q^{-1}[2]c_8=c_9=1,\end{aligned} \tag{5.13}$$

whereas the corresponding normalization constants for the matrix in (5.11) read

$$\begin{aligned}q^2[2]^2c_1=[2]^2c_2=q[2]c_3=q[2]c_4=q[2]c_5=q[2]c_6=[2]^2c_7=c_8=q^{-1}[2]c_9=q^{-1}[2]c_{10}\\ =q^{-2}[2]^2c_{11}=q^{-1}[2]c_{12}=q^{-1}[2]c_{13}=c_{14}=c_{15}=c_{16}=1.\end{aligned} \tag{5.14}$$

Now we show that the orthogonality of the rows also directly leads to the eigenvectors of the generalized braid matrix $\hat{R}(v,w)$. We again choose the quantum group $\mathrm{SO}_q(3)$ as a typical example. Let $\{|V_k\rangle|(k=1,\ldots,9)\}$ be the eigenvectors of the $\hat{R}(v,w)$ matrix with the eigenvalues a_k:

$$\hat{R}(v,w)|V_k\rangle=a_k|V_k\rangle, \tag{5.15}$$

where no summation over the index k on the right is implied. Multiplying the equation (5.15) with the matrix $\hat{M}$ on both sides and employing diagonalization property (5.6) we obtain

$$(1+w,1+v,1+v,1+v,1,1,1,1,1)_{(\mathrm{diagonal})}|\hat{M}V_k\rangle=a_k|\hat{M}V_k\rangle. \tag{5.16}$$

Hence, apart from overall constant factors, we may choose the transposed vectors as follows:

$$|\hat{M}V_k\rangle^{\mathsf{T}}=\{(1,0,\ldots,0),(0,1,0,\ldots,0),\ldots,(0,\ldots,0,1)\}. \tag{5.17}$$

The eigenvalues are given by the diagonal elements of the matrix $\hat{M}\hat{R}(v,w)\hat{M}^{-1}$ as exhibited in (5.6). Hence the obvious construction $|V_k\rangle=\hat{M}^{-1}|\hat{M}V_k\rangle$, along with (5.17) furnishes the eigenvector $|V_k\rangle$ as the kth column of $\hat{M}^{-1}$. Now, in view of the construction of the inverse matrix $\hat{M}^{-1}$ previously discussed preceding (5.13), the eigenvector $|V_k\rangle$ *is finally given by the* kth *row of the matrix* $\hat{M}$. Replacing here the matrix $\hat{M}$ by its alternatives $\mathsf{M}\hat{M}$ amounts to, as given in (5.8), taking linear combinations of the above eigenvectors with the same eigenvalue. The eigenvectors and particularly the highest eigenvalue, dependent here on the choice of the spectral variables (v,w), of the generalized braid matrix $\hat{R}(v,w)$ are of interest in related models of statistical mechanics. Another, quite different, interest in the above diagonalization of the $\hat{R}(v,w)$ matrix will be pointed out in Sec. VI in the context of noncommutative spaces.

So far we have considered the orthogonal quantum group $\mathrm{SO}_q(N)$. A parallel, but much simpler, formalism may be developed for the linear quantum group $\mathrm{GL}_q(N)$, as only two projectors are present there. Instead of discussing the general case, we, for the purpose of illustration, consider a biparametric (p,q) deformation of the group GL(2) in the remaining part of the present section. In Ref. 1 one of us introduced the generalized braid matrix (for $p\neq 0$)

$$\hat{R}(K;p,q)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-K) & Kp^{-1} & 0 \\ 0 & Kq & (1-Kqp^{-1}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{5.18}$$

which satisfies the strict braid equation for the two parametric values $K=1,pq^{-1}$. Maintaining a specific parametrization of the spectral variable v, we write in conformity with the notations of the Sec. II:

$$\hat{R}(K;p,q)=\mathsf{I}-K(1+qp^{-1})P_{(-)}, \tag{5.19}$$

where the projector is

$$P_{(-)}=(1+qp^{-1})^{-1}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -p^{-1} & 0 \\ 0 & -q & qp^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5.20}$$

The projector $P_{(-)}$ may be diagonalized by

$$\hat{M}=\begin{pmatrix} 0 & -1 & p^{-1} & 0 \\ 0 & q & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \end{pmatrix} \tag{5.21}$$

giving $\hat{M}P_{(-)}\hat{M}^{-1}=(1,0,0,0)_{(\mathrm{diagonal})}$. This, following the spectral decomposition (5.19), provides the diagonalized $\hat{R}$ matrix. In this simple case the matrix $\hat{M}^{-1}$ may be easily computed for all values of deformation parameters (p,q). But except for the special case $pq=1$, the first two rows of the present diagonalizer $\hat{M}$ are not orthogonal to each other.

VI. GENERALIZED BRAID MATRICES AND CONSEQUENT NONCOMMUTATIVE SPACES

We first present the general prescription for covariant quantization of spaces implementing the generalized braid matrices $\hat{R}(v)$ and $\hat{R}(v,w)$. Our prescription follow the standard structure except for the presence of the arbitrary values of the spectral variables (v,w). Then we will display how the diagonalizations of the generalized braid matrices presented in Sec. V enable us to extract in a convenient fashion the contents of the above prescription using, as before, the quantum groups $\mathrm{GL}_q(2)$, $\mathrm{SO}_q(3)$, and $\mathrm{SO}_q(4)$ as examples. Generalization to higher dimensional quantum groups can then be easily carried out. Our study will thus be limited. We hope to present elsewhere a fuller exploration of the possible roles of the variables (v,w).

For the quantum group $\mathrm{GL}_q(2)$, we use the projector (5.20) with the restriction $p=q^{-1}$, and set the $\hat{R}(v)$ matrix as in (1.8) satisfying the characteristic equation (1.14). Using the standard notations with coordinates and differentials given, respectively, by $\{x_i,\xi_i\equiv dx_i|i=(1,2)\}$, we obtain

$$P_{(-)}x\otimes x=0 \tag{6.1}$$

and

$$x\otimes\xi=B\xi\otimes x, \tag{6.2}$$

whereas Leibnitz rule and covariance lead to

$$(B+\mathrm{I})\xi\otimes\xi=0. \tag{6.3}$$

The matrix B reads

$$B=-\mathrm{I}+\mu(\hat{R}(v)-(1+v)\mathrm{I}), \tag{6.4}$$

while the parameter μ is arbitrary. We also note that the above structure of B ensures the orthogonality: $(B+\mathrm{I})P_{(-)}=0$. Using the diagonalizer $\hat{M}$ given in (5.21), and adapting it to the parametric choice $p=q^{-1}$, we evaluate

$$\hat{M}x\otimes\xi=\hat{M}\begin{pmatrix}x_1\xi_1\\ x_1\xi_2\\ x_2\xi_1\\ x_2\xi_2\end{pmatrix}=\begin{pmatrix}-x_1\xi_2+qx_2\xi_1\\ qx_1\xi_2+x_2\xi_1\\ x_1\xi_1+x_2\xi_2\\ x_1\xi_1-x_2\xi_2\end{pmatrix}. \tag{6.5}$$

The analogous results for $\hat{M}x\otimes x$, $\hat{M}\xi\otimes\xi$, and $\hat{M}\xi\otimes x$ can be read off (6.5) readily. Using the previous explicit constructions we may now obtain the following diagonalized structures:

$$\begin{aligned}\hat{M}P_{(-)}\hat{M}^{-1}&=(1,0,0,0)_{(\mathrm{diagonal})},\\ \hat{M}\hat{R}(v)\hat{M}^{-1}&=(1+v,1,1,1)_{(\mathrm{diagonal})},\\ \hat{M}(B+\mathrm{I})\hat{M}^{-1}&=\mu(0,-v,-v,-v)_{(\mathrm{diagonal})},\\ \hat{M}B\hat{M}^{-1}&=-(1,1+\mu v,1+\mu v,1+\mu v)_{(\mathrm{diagonal})},\end{aligned} \tag{6.6}$$

which in conjunction with (6.5) allow us to immediately write down the relations

$$x_1x_2=qx_2x_1,\quad \xi_1\xi_2=-q^{-1}\xi_2\xi_1,\quad \xi_1^2=0,\quad \xi_2^2=0 \tag{6.7}$$

and

$$
\begin{aligned}
(-x_1\xi_2+qx_2\xi_1)&=-(-\xi_1x_2+q\xi_2x_1),\\
(qx_1\xi_2+x_2\xi_1)&=-(1+\mu v)(q\xi_1x_2+\xi_2x_1),\\
(x_1\xi_1+x_2\xi_2)&=-(1+\mu v)(\xi_1x_1+\xi_2x_2),\\
(x_1\xi_1-x_2\xi_2)&=-(1+\mu v)(\xi_1x_1-\xi_2x_2).
\end{aligned}
\tag{6.8}
$$

Adapting notations and parametrizations the corresponding results of Ref. 1 may be obtained. But the consequences of the diagonalization is particularly striking in the modular structure evident in (6.8). Linear combinations of $x_i\xi_j$ are picked out that are *proportional to the same combination* of ξ_ix_j on the right. This is, as will be seen, a general feature in all cases. It was shown in Ref. 1 that

$$\Phi^2=(\xi_1x_2-q\xi_2x_1)^2=0. \tag{6.9}$$

Here, using (6.8) it immediately follows that the combination $(x_1\xi_2-qx_2\xi_1)$ is also nilpotent. Our formalism also signals clearly special values of the parameters. It is evident from (6.8) that $\mu=-v^{-1}$ is a very special case. For the quantum group $\mathrm{GL}_q(N)$ for an arbitrary N the prescriptions (6.1) to (6.4) remain the same except that higher dimensional $N^2\times N^2$ matrices need to be considered.

Now we consider the noncommuting spaces associated with the generalized braid matrix $\hat{R}(v,w)$ of the orthogonal quantum group $\mathrm{SO}_q(N)$. This matrix has the structure (1.9) and it satisfies the characteristic equation (1.15). The braiding structure (6.1) of the noncommutative coordinates now may also be expressed as

$$(\hat{R}(v,w)-\mathrm{I})(\hat{R}(v,w)-(1+w)\mathrm{I})x\otimes x=0. \tag{6.10}$$

Leibnitz rule and covariance ensure equations (6.2) and (6.3) with the matrix B given by (6.4). As there are three projectors for the orthogonal quantum groups, the braiding relation (6.3) now reduces to

$$P_{(+)}\xi\otimes\xi=0,\quad P_{(0)}\xi\otimes\xi=0. \tag{6.11}$$

Now we will explicitly demonstrate the above structure for the quantum groups $\mathrm{SO}_q(3)$ and $\mathrm{SO}_q(4)$. For the quantum group $\mathrm{SO}_q(3)$ the diagonalizing matrix $\hat{M}$ is given in (5.9). The diagonalized operators now read

$$
\begin{aligned}
\hat{M}P_{(-)}\hat{M}^{-1}&=(0,1,1,1,0,0,0,0,0)_{(\mathrm{diagonal})},\\
\hat{M}\hat{R}(v,w)\hat{M}^{-1}&=(1+w,1+v,1+v,1+v,1,1,1,1,1)_{(\mathrm{diagonal})},\\
\hat{M}B\hat{M}^{-1}&=-(1+\mu(v-w),1,1,1,1+\mu v,1+\mu v,1+\mu v,1+\mu v,1+\mu v)_{(\mathrm{diagonal})}.
\end{aligned}
\tag{6.12}
$$

Here we choose, as in Ref. 2, the triplets (x_-,x_0,x_+) and (ξ_-,ξ_0,ξ_+) as the basis elements for the noncommuting coordinates and the differentials, respectively. Using the diagonalizing matrix $\hat{M}$ given in (5.9) we now compute

$$\hat{M}x\otimes\xi=\hat{M}\begin{pmatrix} x_-\xi_- \\ x_-\xi_0 \\ x_-\xi_+ \\ x_0\xi_- \\ x_0\xi_0 \\ x_0\xi_+ \\ x_+\xi_- \\ x_+\xi_0 \\ x_+\xi_+ \end{pmatrix}=\begin{pmatrix} x_-\xi_+ + q^{1/2}x_0\xi_0 + qx_+\xi_- \\ x_-\xi_0 - qx_0\xi_- \\ x_0\xi_+ - qx_+\xi_0 \\ x_-\xi_+ + sx_0\xi_0 - x_+\xi_- \\ x_-\xi_- \\ x_-\xi_0 + q^{-1}x_0\xi_- \\ x_-\xi_+ + tx_0\xi_0 + q^{-2}x_+\xi_- \\ x_0\xi_+ + q^{-1}x_+\xi_0 \\ x_+\xi_+ \end{pmatrix}. \tag{6.13}$$

The matrices $\hat{M}x\otimes x$, $\hat{M}\xi\otimes\xi$ and $\hat{M}\xi\otimes x$ have evident analogous forms. The parameters (μ,v,w) do not appear in the braiding structures (6.1) and (6.11). Therefore these braiding relations have the usual form, given, for example, in Eq. (3.48) of Ref. 2. For the sake of completeness we present them here

$$x_-x_0=qx_0x_-,\quad x_0x_+=qx_+x_0,\quad x_+x_- - x_-x_+=(q^{1/2}-q^{-1/2})x_0^2,$$

$$\xi_-^2=0,\quad \xi_+^2=0,\quad \xi_-\xi_+ + \xi_+\xi_-=0, \tag{6.14}$$

$$q\xi_-\xi_0+\xi_0\xi_-=0,\quad q\xi_0\xi_+ + \xi_+\xi_0=0,\quad \xi_0^2=(q^{1/2}-q^{-1/2})\xi_-\xi_+ .$$

The constraints due to (6.2) do involve the parameters (μ,v,w) and have been obtained in Eq. (3.48) of Ref. 2. Here we present them in the form directly given by (6.12) and (6.13). After implementing our diagonalization, we obtain

$$(x_-\xi_+ + q^{1/2}x_0\xi_0 + qx_+\xi_-)=-(1+\mu(v-w))(\xi_-x_+ + q^{1/2}\xi_0x_0 + q\xi_+x_-),$$

$$(x_-\xi_+ + sx_0\xi_0 - x_+\xi_-)=-(\xi_-x_+ + s\xi_0x_0 - \xi_+x_-),$$

$$(x_-\xi_+ + tx_0\xi_0 + q^{-2}x_+\xi_-)=-(1+\mu v)(\xi_-x_+ + t\xi_0x_0 + q^{-2}\xi_+x_-),$$

$$(x_-\xi_0 - qx_0\xi_-)=-(\xi_-x_0 - q\xi_0x_-),$$

$$(x_-\xi_0 + q^{-1}x_0\xi_-)=-(1+\mu v)(\xi_-x_0 + q^{-1}\xi_0x_-), \tag{6.15}$$

$$(x_0\xi_+ - qx_+\xi_0)=-(\xi_0x_+ - q\xi_+x_0),$$

$$(x_0\xi_+ + q^{-1}x_+\xi_0)=-(1+\mu v)(\xi_0x_+ + q^{-1}\xi_+x_0),$$

$$x_-\xi_-=-(1+\mu v)\xi_-x_-,$$

$$x_+\xi_+=-(1+\mu v)\xi_+x_+ .$$

Thus, as signaled before, the diagonalization selects out linear combinations, which are proportional under the operation $x_i\xi_j\rightarrow\xi_ix_j$. We note that the coefficients appearing in the triplets, namely: $(1,q^{1/2},q),(1,-q^{-1/2}(1-q),-1),(1,-q^{-3/2}(1+q),q^{-2})$ are mutually orthogonal. The same property is evident with the doublets: $(1,-q),(1,q^{-1})$. The parametric values $\mu=-v^{-1}$ again generate a special case. Using (6.15) each $x_i\xi_j$ may be written as linear combination of ξ_kx_l terms. This is provided in Ref. 2. Here we want to emphasize the modular structure of (6.15). In the preceding discussion regarding the quantum group $\mathrm{GL}_q(2)$ it was noted that a nilpotent bilinear structure, given in (6.9), arise directly out of the diagonalization process. Presence of such structures in (6.15) should be sought. A detailed study of our generalized spaces, arising as a consequence of generalized braid matrices, will be presented elsewhere.

To investigate our noncommutative spaces associated with the quantum group $SO_q(4)$, we proceed exactly as in the previous example. Now the diagonalizing matrix $\hat{M}$ is given by (5.11). The basis for the coordinates and the corresponding basis for the differentials are denoted by (x_1,x_2,x_3,x_4) and $(\xi_1,\xi_2,\xi_3,\xi_4)$, respectively. The braiding relations for the bilinears $x\otimes x$ and $\xi\otimes\xi$ are independent of the parameters (μ,v,w) introduced here; and, consequently, remain the standard noncommutativity constraints. We exhibit below, for brevity, only the relevant modular structure analogous to (6.15). Now we have the quadruplets, doublets and singlets with typically orthogonalized constraints as before:

$$\begin{gathered}(x_1\xi_4+qx_2\xi_3+qx_3\xi_2+q^2x_4\xi_1)=-(1+\mu(v-w))(\xi_1x_4+q\xi_2x_3+q\xi_3x_2+q^2\xi_4x_1),\\ (x_1\xi_4+qx_2\xi_3-q^{-1}x_3\xi_2-x_4\xi_1)=-(\xi_1x_4+q\xi_2x_3-q^{-1}\xi_3x_2-\xi_4x_1),\\ (x_1\xi_4-q^{-1}x_2\xi_3+qx_3\xi_2-x_4\xi_1)=-(\xi_1x_4-q^{-1}\xi_2x_3+q\xi_3x_2-\xi_4x_1),\\ (x_1\xi_4-q^{-1}x_2\xi_3-q^{-1}x_3\xi_2+q^{-2}x_4\xi_1)=-(1+\mu v)(\xi_1x_4-q^{-1}\xi_2x_3-q^{-1}\xi_3x_2+q^{-2}\xi_4x_1),\end{gathered} \tag{6.16}$$

$$\begin{gathered}(x_i\xi_j-qx_j\xi_i)=-(\xi_ix_j-q\xi_jx_i),\\ (x_i\xi_j+q^{-1}x_j\xi_i)=-(1+\mu v)(\xi_ix_j+q^{-1}\xi_jx_i),\\ x_k\xi_k=-(1+\mu v)\xi_kx_k,\end{gathered}$$

where $(i,j)=\{(1,2),(1,3),(2,4),(3,4)\}$, and $k=\{1,2,3,4\}$. No summation over the index k is meant in the last equation in (6.16). Comments parallel to those following (6.15) are relevant here.

Here we sum up the above procedure for the quantum group $SO_q(N)$ with an arbitrary value of N. The formalism described in equations (6.1)–(6.4), and also in (6.11) holds for an arbitrary value of N. We have emphasized on the modular structure and the parameter dependence of the braiding relations arising from (6.2) and our diagonalization of the generalized braid matrices. Setting the spectral variables (v,w) equal to their braid values (1.10), and also fixing the parameter $\mu=q^2$, we may recover the standard quantization prescriptions. So far we have implicitly assumed that the spectral variables are nonvanishing: $v\neq 0,w\neq 0$. When one of them vanishes, the characteristic equation obeyed by the generalized braid matrix becomes, as discussed for instance in (4.2), quadratic rather than cubic. The corresponding reformulation of the prescription for our noncommutative spaces is straightforward and will not be presented here.

VII. REMARKS

The following braid matrices,

$$\hat{R}=\begin{pmatrix}1&0&0&1\\0&1&-1&0\\0&1&1&0\\-1&0&0&1\end{pmatrix} \tag{7.1}$$

and

$$\hat{R}=\begin{pmatrix}0&0&0&q\\0&1&0&0\\0&0&1&0\\q&0&0&0\end{pmatrix}, \tag{7.2}$$

were studied in detail[12–14] in the context of exotic bialgebras. These authors investigated the spectral decomposition of these braid matrices and the Baxterization thereof. These respective cases were denominated as $S03$ and $S14$ in the classification scheme of 4×4 braid matrices presented in Ref. 15. The analogies and differences of the $\hat{R}$ matrix in (7.1) with the unitary case, and that in (7.2) with the orthogonal case have been discussed[12–14] earlier. Noncommutative spaces associated with these two and other exotic 4×4 $\hat{R}$ matrices have also been studied.[12–14] These 4×4 matrices classified in Ref. 15 are exotic in the sense that they are not obtained by restricting some universal $\hat{\mathcal{R}}$ matrix to this dimension. They represent distinct supplementary possibilities for the dimension 4×4.

How do we construct higher dimensional analogues of these matrices? In Sec. IV we have presented a canonical construction of a class of $N^2\times N^2$ braid matrices complete with the corresponding MBE and the Baxterized forms of these matrices. In fact for each even N we have *two* solutions: exotic orthogonal for the choice $\varepsilon=1$, and exotic symplectic for the parametric value $\varepsilon=-1$. But these class presumably does not exhaust such possibilities for each N. Our general reduction of trilinear terms in Sec. III insistently pointed out the class studied in Sec. IV. How do we investigate other possibilities? Generalization of Hietarinta's approach[15] to higher dimensional cases would be extremely laborious. Still a more thorough search may be worthwhile.

Several interesting aspects of our formalism have not been addressed in the present work. Quasiclassical limits, L operators and Yangians are relevant examples. Applications, particularly of our new class of solutions, to integrable models[16,17] would be worth exploring. Certain specific properties would be lost if the parameters (μ,υ,w) move away from their standard values. We wish to study new interesting features which may emerge for other values of the parameters (μ,υ,w). The present approach via diagonalization may be helpful.

Let us end by taking a closer look at the mutually orthogonal sets of triplets and quadruplets, appearing in (5.10) and (5.12) as a consequence of our diagonalizations. For the quantum group $\mathrm{SO}_q(3)$ the constraint (6.1) contain, corresponding to the set $(1,(q^{1/2}-q^{-1/2}),-1)$ in (5.10), the commutation relation, listed before in the set (6.14) but remodeled here for the purpose of convenience:

$$x_-x_+-x_+x_-+(q^{1/2}-q^{-1/2})x_0^2=0. \tag{7.3}$$

A constraint trivially true in the commutative limit $(q=1)$ is thus consistently maintained. The analogous expressions corresponding to the other two triplets in the set (5.10), selected out by the other two diagonalized projectors $P_{(0)}$ and $P_{(+)}$ are *not* constrained to be zero. Introducing the metric and the star operation (Ex. 4.1.22 in Ref. 10) as

$$(x_\pm)^*=q^{\mp1/2}(x_\mp),\quad x_0^*=x_0, \tag{7.4}$$

the other two triplets mentioned above lead to the surfaces with invariants k_1 and k_2:

$$\begin{aligned} x_-^*x_-+x_+^*x_++x_0^*x_0&=\mathsf{k}_1,\\ q^{-3/2}x_-^*x_-+q^{3/2}x_+^*x_+-(q^{1/2}+q^{-1/})x_0^*x_0&=\mathsf{k}_2, \end{aligned} \tag{7.5}$$

where k_1 is usually denoted as the distance squared, i.e., $\mathsf{k}_1\equiv\mathsf{r}^2\geqslant0$. The above two surfaces denote a q-deformed sphere and a q-deformed hyperboloid, respectively. In the context of our diagonalization scheme these two noncommutative surfaces enter in a parallel fashion.

For the quantum group $\mathrm{SO}_q(4)$ the second and the third quadruplets in the set (5.12) correspond to the constraints originating from (6.1), namely

$$\begin{aligned} x_1x_4+qx_2x_3-q^{-1}x_3x_2-x_4x_1&=0,\\ x_1x_4-q^{-1}x_2x_3+qx_3x_2-x_4x_1&=0. \end{aligned} \tag{7.6}$$

The consistency with the commutative limit is, therefore, maintained. The other two quadruplets in the list (5.12) correspond to the action of the diagonalized projectors $P_{(+)}$ and $P_{(0)}$ on the tensor product space $\hat{M}(x\otimes x)$, and thereby lead to the q-deformation of the surfaces

$$x_1x_4+x_2x_3=\mathsf{k}_1, \quad x_1x_4-x_2x_3=\mathsf{k}_2. \tag{7.7}$$

Changing the basis from (x_1,x_4) and (x_2,x_3) to $(x\pm it)$ and $(y\pm iz)$, respectively, we obtain a 3-sphere in the first case (with $\mathsf{k}_1\geqslant 0$) and a noncompact surface in the second case, as obtained before in the second equation in (7.5). Suitably implementing the q-dependent star operation we may obtain the corresponding noncommutative deformations related to the first and the last quadruplets in (5.12).

APPENDIX A

Here we briefly indicate the derivations of the relations (3.11) and (3.12). We demonstrate this in the case of the quantum group $\mathrm{SO}_q(N)$, where the parameter $\varepsilon=1$. To this end we define the operator

$$K\equiv(1+[N-1])P_{(0)}=\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}E_{i',j}\otimes E_{i,j'}, \tag{A1}$$

where $i'=N+1-i$. The relevant notations are explained in Sec. IV. Using the standard tensor structures

$$K_{12}=\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}E_{i',j}\otimes E_{i,j'}\otimes \mathsf{I}_{N\times N} \quad K_{23}=\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}\mathsf{I}_{N\times N}\otimes E_{i',j}\otimes E_{i,j'}, \tag{A2}$$

and the identity $E_{i,j'}E_{k',l}=\delta_{j,k}E_{i,l}$, we obtain

$$K_{12}K_{23}=\sum_{i,j,k=1}^{N} q^{(\rho_i-\rho_k)}E_{i',j}\otimes E_{i,k}\otimes E_{j,k'} \tag{A3}$$

and the following triple product rules:

$$K_{12}K_{23}K_{12}=\left(\sum_{i,j=1}^{N} q^{(\rho_i-\rho_j)}E_{i',j}\otimes E_{i,j'}\right)\otimes\sum_{k=1}^{N} E_{k,k}=K\otimes \mathsf{I}_{N\times N}\equiv K_{12},$$

$$K_{23}K_{12}K_{23}=\sum_{i=1}^{N} E_{i,i}\otimes\left(\sum_{j,k=1}^{N} q^{(\rho_j-\rho_k)}E_{j',k}\otimes E_{j,k'}\right)\mathsf{I}_{N\times N}\otimes K\equiv K_{23}. \tag{A4}$$

The triple product rules (A4) and the defining property (A1) ensure that the following identities hold:

$$P_{(0)12}P_{(0)23}P_{(0)12}=(1+[N-1])^{-2}P_{(0)12}, \quad P_{(0)23}P_{(0)12}P_{(0)23}=(1+[N-1])^{-2}P_{(0)23}. \tag{A5}$$

Using the definitions (4.10) and (4.12) we may proceed analogously for the quantum group $\mathrm{Sp}_q(N)$, where $N=2n$. The two cases can finally be unified after adopting the following definition:

$$K\equiv(1+\varepsilon[N-\varepsilon])P_{(0)} \tag{A6}$$

and then proceeding as before. The final results may be summarized as

$$P_{(0)12}P_{(0)23}P_{(0)12}=(1+\varepsilon[N-\varepsilon])^{-2}P_{(0)12},$$
$$P_{(0)23}P_{(0)12}P_{(0)23}=(1+\varepsilon[N-\varepsilon])^{-2}P_{(0)23}. \tag{A7}$$

Employing the definitions of (Y_1,Y_2) given in (3.1), we now obtain (3.11).

In order to prove the identity (3.12) we proceed as follows. Using the standard expressions for the braid generators $\hat{R}^{\pm 1}$ for the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$, and proceeding exactly analogously as before we obtain

$$P_{(0)12}\hat{R}^{\pm 1}_{23}P_{(0)12}=\frac{\varepsilon q^{\pm(N-1-\varepsilon)}}{1+\varepsilon[N-\varepsilon]}P_{(0)12}, \quad P_{(0)23}\hat{R}^{\pm 1}_{12}P_{(0)23}=\frac{\varepsilon q^{\pm(N-1-\varepsilon)}}{1+\varepsilon[N-\varepsilon]}P_{(0)23}. \tag{A8}$$

Expressing the braid matrices as in (1.12) we now use the relations (A7) and (A8) to obtain

$$P_{(0)12}P_{(-)23}P_{(0)12}=\frac{\varepsilon[N-\varepsilon]([2]+\varepsilon[N-1-\varepsilon])}{[2](1+\varepsilon[N-\varepsilon])^2}P_{(0)12}. \tag{A9}$$

The above result also holds after an exchange of the tensor indices: $(12)\rightleftharpoons(23)$. The equation (A9), in conjunction with the definitions (2.1) and (3.1), now produces the identity (3.12).

APPENDIX B

The correspondence between our result for Baxterization and that of Ref. 7 being quite simple in the context of the quantum group $\mathrm{GL}_q(N)$, we discuss below the results for the quantum groups $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$. In Sec. 3.9 of Ref. 7 Isaev starts Baxterization of the braid matrices with the parametrization

$$\hat{\mathsf{R}}(x)=c(x)(\mathsf{I}+a(x)\hat{\mathsf{R}}+b(x)K), \tag{B1}$$

where the matrices $\hat{\mathsf{R}}$ and K are given in (1.7) and (A6), respectively. Substituting these results we may rewrite

$$\hat{\mathsf{R}}=c(x)(1+qa(x))\hat{R}(x), \tag{B2}$$

where

$$\hat{R}(x)=\mathsf{I}-\frac{[2]a(x)}{1+qa(x)}P_{(-)}+\frac{(1+\varepsilon[N-\varepsilon])b(x)-q(1-\varepsilon q^{-(N+1-\varepsilon)})a(x)}{1+qa(x)}P_{(0)}. \tag{B3}$$

Comparing this with our starting point (1.9) we obtain the relations

$$a(x)=-\frac{v(x)}{[2]+qv(x)}, \quad b(x)=\frac{[2](w(x)-f_+v(x))}{([2]+qv(x))(1+\varepsilon[N-\varepsilon])}, \quad c(x)=[2]^{-1}([2]+qv(x)), \tag{B4}$$

where the parameter f_+ has been defined in (3.15). In the present work we have preferred the parametrization in (1.9) as it assigns the key roles to the two projectors $P_{(-)}$ and $P_{(0)}$, leading to the systematic reduction of the trilinear forms presented in (3.14). As emphasized earlier this permitted us to display MBE and Baxterization as complementary facets of the same generalized $\hat{R}(v,w)$ matrix. As for solutions of the braid equation obtained in the present work we note that the special case of the spectral variables $v=0, w\neq 0$ has not been discussed in Ref. 7. We have devoted Sec. IV to study this remarkable new class of solutions.

Our formalism led through (3.27) to the significant parallel structures of the Baxterized functions $v(x)$ and $w(x)$ given in (3.30). This enabled us to obtain the solutions *completely* by solving the two simplest equations, before verifying that the more complex functional equation [corre-

sponding to a_2 in (3.25)] is indeed consistent with them. In Ref. 7 the relatively complicated equation [Eq. (3.9.7) of Ref. 7] had to be used to fix the two possible values of a parameter [Eq. (3.9.15) of Ref. 7]. The attractive forms of additive Baxterization, as evident in (1.20) and (1.21)–(1.24) for the functions $v(\theta)$ and $w(\theta)$, respectively, are also direct consequences of our formalism.

ACKNOWLEDGMENTS

We thank C. de Calan, J. Lascoux, and J. Madore for discussions. One of us (R.C.) is partially supported by Grant No. DAE/2001/37/12/BRNS, Government of India.

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Note: *This article is a spurious duplicate copy of the original article, which was published in the January 2003 issue. AIP apologizes for this publication error. Proper citation of this article follows: A. M. Grundland and W. J. Zakrzewski, J. Math. Phys.* ***44****, 328 (2003).*

On certain geometric aspects of CP^N harmonic maps

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(Received 25 September 2002; accepted 10 October 2002; publisher error corrected 6 May 2003)

A Weierstrass-type system of equations corresponding to CP^N harmonic maps is presented. It constitutes a generalization of the previously constructed systems for CP^1 and CP^2 fields. From the linear spectral problem for the CP^N model a set of conserved quantities is derived and used for a construction of a generalized Weierstrass representation for conformally parametrized surfaces immersed in multidimensional Euclidean spaces. Based on this representation a possible geometrical interpretation of CP^N harmonic maps is discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1534384]

I. INTRODUCTION

Recently many studies have been performed of various σ models in low dimensions. Of these, σ models in two spatial dimensions have, perhaps, been the most commonly studied as, on one hand, they lead to interesting generalizations of harmonic maps and on the other, they can be treated as analogs, with many properties in common, of four-dimensional non-Abelian gauge theories.

Among two-dimensional σ models perhaps the most interesting ones, from the topological point of view, are the so-called CP^N sigma models. Their classical solutions are examples of topological solitons, i.e., extended structures whose stability is partially guaranteed by topological considerations.

The CP^N models are, in fact, a generalization of the, perhaps the s mplest, sigma model, namely the S^2 model—also called the vector $O(3)$ model. The CP^N models involve maps from R^2, or S^2 if one wants to have a nontrivial topology, to CP^N, i.e.,

$$CP^N: C \supset \Omega \ni \zeta = \zeta_1 + i\zeta_2 \mapsto z = (z^1, \ldots, z^N) \in S^{2N} \cong \mathrm{SU}(N)/\mathrm{SU}(N-1), \tag{1}$$

where the homogeneous coordinates $z = (z^1, \ldots, z^N)$ have the following properties

$$z \sim z' = \lambda z \quad \text{for } \lambda \neq 0.$$

Exploiting projective invariance we can require that

$$z^\dagger \cdot z = 1, \tag{2}$$

holds, where † denotes the Hermitian conjugation, and we are still left with gauge symmetry

$$z \sim z' = z e^{i\phi}, \tag{3}$$

where ϕ is the real-valued function.

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It is easiest to define CP^N models in terms of the Lagrangian density[1]

$$L=\tfrac{1}{4}(D_\mu z)^\dagger\cdot D_\mu z,\quad z^\dagger\cdot z=1, \tag{4}$$

where the covariant derivatives D_μ act on $z:S^2\to CP^N$ according to the formula

$$D_\mu z=\partial_\mu z-(z^\dagger\cdot\partial_\mu z)z. \tag{5}$$

Here the index $\mu=1,2$ denotes ζ_1 and ζ_2. Note that the covariant derivatives $D_\mu z$ transform under gauge (3)

$$D_\mu z\to D_\mu z'=(D_\mu z)e^{i\phi}, \tag{6}$$

so that the dependence on phase ϕ drops out of Lagrangian density (4) and hence the model is really based on CP^N. The total Lagrangian is given by

$$\mathcal{L}=\int L\,d\zeta\,d\overline{\zeta} \tag{7}$$

and if the CP^N model is defined over S^2 we require that $\mathcal{L}$ is finite.

For the CP^N sigma model it is convenient to define

$$z=\frac{f}{|f|}, \tag{8}$$

where we have used the following notation $|f|=(f^\dagger\cdot f)^{1/2}$. In terms of f the Lagrangian (7) becomes

$$\mathcal{L}=\int\frac{|\overline{\partial}f|^2+|\partial f|^2}{|f|^4}d\zeta\,d\overline{\zeta}, \tag{9}$$

where $|\partial f|^2=(\partial f)^\dagger\cdot(\partial f)$ and $|\overline{\partial}f|^2=(\overline{\partial}f)^\dagger\cdot\overline{\partial}f$. The Euler Lagrange equations for f take the form

$$\left(1-\frac{f\otimes f^\dagger}{|f|^2}\right)\left[\partial\overline{\partial}f-\partial f\frac{(f^\dagger\cdot\overline{\partial}f)}{|f|^2}-\overline{\partial}f\frac{(f^\dagger\cdot\partial f)}{|f|^2}\right]=0, \tag{10}$$

where we have introduced holomorphic and antiholomorphic derivatives

$$\partial=\frac{\partial}{\partial(\zeta_1+i\zeta_2)}=\frac{\partial}{\partial\zeta},\quad \overline{\partial}=\frac{\partial}{\partial(\zeta_1-i\zeta_2)}=\frac{\partial}{\partial\overline{\zeta}} \tag{11}$$

and a bar denotes the complex conjugation.

As is well known[2] equation (10) can be written as a compatibility condition for a set of two linear spectral equations for a N component auxiliary vector Ψ

$$\begin{aligned}\partial\Psi&=\frac{2}{1+\lambda}[\partial P,P]\Psi,\\ \overline{\partial}\Psi&=\frac{2}{1-\lambda}[\overline{\partial}P,P]\Psi,\end{aligned} \tag{12}$$

where λ is a spectral parameter and the N by N matrix P is the projector given by

$$P=\frac{1}{|f|^2}f\otimes f^\dagger,\quad P^\dagger=P,\quad P^2=P. \tag{13}$$

The compatibility conditions for (12) are,

$$[\partial\overline{\partial}P, P]=0 \tag{14}$$

which, as can be easily checked, are equivalent to equations (10). Note that (14) can be written in the form of a conservation law

$$\partial[\overline{\partial}P, P]+\overline{\partial}[\partial P, P]=0 \tag{15}$$

or, equivalently, using the tracelessness of matrix K

$$\partial K-\overline{\partial}K^{\dagger}=0, \tag{16}$$

where the matrices K and $K^{\dagger}$ are given by

$$K=[\overline{\partial}P, P]=\frac{\overline{\partial}f\otimes f^{\dagger}-f\otimes\overline{\partial}f^{\dagger}}{|f|^2}+\frac{f\otimes f^{\dagger}}{|f|^4}[(\overline{\partial}f^{\dagger}\cdot f)-(f^{\dagger}\cdot\overline{\partial}f)], \quad \operatorname{tr}K=0, \tag{17}$$

and consequently

$$K^{\dagger}=-[\partial P, P]=-\frac{\partial f\otimes f^{\dagger}-f\otimes\partial f^{\dagger}}{|f|^2}+\frac{f\otimes f^{\dagger}}{|f|^4}[(\partial f^{\dagger}\cdot f)-(f^{\dagger}\cdot\partial f)].$$

Note that due to the invariance of the Lagrangian (4) under gauge (3), without loss of generality, we can set one of the components of the vector field f, say f_1, to 1. Then, in the CP^1 case, all quantities are expressible through one variable

$$w=\frac{f_2}{f_1}=f_2 \tag{18}$$

and the Euler Lagrange equations (10) take the form

$$\partial\overline{\partial}w-\frac{2\overline{w}}{(1+|w|^2)}\partial w\overline{\partial}w=0. \tag{19}$$

Recently, a lot of effort has been put into relating CP^1 maps to the solutions of the Weierstrass problem.[3,6] In this case one considers a system of first order equations (of Dirac type) for two complex fields φ and ψ of the form

$$\partial\psi=p\varphi, \quad \overline{\partial}\varphi=-p\psi, \quad p=|\varphi|^2+|\psi|^2. \tag{20}$$

In Ref. 7 it was shown that solutions of the Weierstrass system (20) are in a one to one correspondence with the solutions of the CP^1 sigma eqution (19). If ψ and φ are solutions of the Weierstrass system (20), then the function w, defined by

$$w=\frac{\psi}{\overline{\varphi}}, \tag{21}$$

is a solution of the CP^1 equations (19). The converse is also true.[6] Thus, if w is a solution of (19), then the functions φ and ψ of the Weierstrass system (20) have the form (up to an overall multiplication of φ and ψ by -1)

$$\psi=w\frac{(\overline{\partial}\overline{w})^{1/2}}{1+|w|^2}, \quad \varphi=\frac{(\partial w)^{1/2}}{1+|w|^2}, \quad p=\frac{|\partial w|}{1+|w|^2}. \tag{22}$$

From the Weierstrass system (20) one can construct three conservation laws (15). These, in turn, allow us to determine four real valued quantities $X_i(\zeta,\overline{\zeta})$, three of which are linearly independent (due to the tracelessness of the matrix K). X_i are constructed by taking diagonal and off-diagonal entries of matrix K and are given by[3]

$$X_1=\int_\gamma(\psi_1^2-\psi_2^2)d\zeta'+(\overline{\psi}_1^2-\overline{\psi}_2^2)d\overline{\zeta}',$$

$$X_2=\int_\gamma(\psi_1^2+\psi_2^2)d\zeta'-(\overline{\psi}_1^2+\overline{\psi}_2^2)d\overline{\zeta}', \tag{23}$$

$$X_3=-\int_\gamma\psi_1\psi_2\,d\zeta'+\overline{\psi}_1\overline{\psi}_2\,d\overline{\zeta}',$$

respectively, where γ is any curve from a fixed point to ζ.

The geometrical aspects of surfaces obtained from representation (23), where functions ψ and φ obey the Weierstrass system (20), are described in detail in Ref. 4. In two recent papers[8,9] we have generalized this construction to the case of the CP^2 sigma model.[5] The aim of this paper is to present a generalization to the CP^N case.

The paper is organized as follows. In Sec. II, we derive the explicit form of conservation laws corresponding to the CP^N model. Section III deals with CP^N maps and the corresponding Weierstrass representation for conformally parametrized two-dimensional surfaces immersed in multidimensional Euclidean space. In Sec. IV we discuss some geometric aspects of CP^N maps and present some geometric characteristics of surfaces. The last section presents further remarks, discusses some possible developments and mentions some more ambitious objectives.

II. THE CP^N MODEL

Here we derive explicit conservation laws (15) which are equivalent to the Euler Lagrange equations (10). In order to construct them we look first at the general form of the elements of the matrices K and $K^\dagger$ in terms of f, given by (17). Thus we have

$$K_{ij}=\frac{1}{A^2}[\overline{f}_k f_k\,\overline{\partial}f_i\,\overline{f}_j-\overline{f}_k f_k f_i\,\overline{\partial f_j}+f_i\,\overline{f}_j\,\overline{\partial f_k}\,f_k-f_i\,\overline{f}_j\,\overline{f}_k\,\overline{\partial}f_k], \tag{24}$$

and consequently

$$K^\dagger_{ij}=\frac{-1}{A^2}[\overline{f}_k f_k\,\partial f_i\,\overline{f}_j-\overline{f}_k f_k f_i\,\partial\overline{f}_j+f_i\,\overline{f}_j\,\partial\overline{f}_k\,f_k-f_i\,\overline{f}_j\,\overline{f}_k\,\partial f_k],$$

where $A=f^\dagger\cdot f$ and the summation convention over the repeated indices from now on, is assumed throughout this paper.

Let us define

$$F_{ij}=f_i\,\partial f_j-f_j\partial f_i,$$

and

$$G_{ij}=f_i\,\overline{\partial}f_j-f_j\overline{\partial}f_i. \tag{25}$$

Then, using expressions (25), the matrices K and $K^\dagger$ take, equivalently, a simple form

$$K_{ij}=\overline{f}_j\overline{\Phi}_i^2-f_i\overline{\varphi}_j^2, \tag{26}$$

and

$$K_{ij}^{\dagger}=-\overline{f}_j\varphi_i^2-f_i\Phi_j^2, \tag{27}$$

where we have introduced

$$\varphi_i^2=\frac{1}{A^2}\overline{f}_k F_{ki}, \tag{28}$$

and

$$\Phi_i^2=\frac{1}{A^2}f_k\overline{G_{ki}}. \tag{29}$$

Note that from equations (25), (28), and (29) we have two algebraic constraints, namely

$$\overline{f}_k\,\varphi_k^2=0, \quad f_k\,\Phi_k^2=0, \tag{30}$$

which imply that only $(N-1)$ functions φ_i^2 are linearly independent. So in our further discussion it is convenient to take as indepedent functions $\varphi_2^2,\ldots,\varphi_N^2$. Analogous situation holds for functions Φ_i^2. Making use of the symmetry (3) we can set, without loss of generality, say, $f_1=1$, and so we end up with the expressions [for (28) and (29)]

$$\varphi_i^2=\frac{1}{A^2}[(1+f_k\overline{f}_k)\,\partial f_i-f_i(\overline{f}_k\,\partial f_k)],$$

$$\Phi_i^2=\frac{1}{A^2}[(1+f_k\overline{f}_k)\,\overline{\partial} f_i-f_i(\overline{f}_k\,\overline{\partial} f_k)], \quad i=2,\ldots,N, \tag{31}$$

where

$$A=1+|f_2|^2+|f_3|^2\ldots+|f_N|^2,$$

and all the sums over repeated indices run over $k=2,\ldots,N$. Note that in (31) the terms $k=i$ in the sum cancel leaving just term ∂f_i. For instance if $k=i=2$ then we have

$$\varphi_2^2=\frac{1}{A^2}[(1+f_l\overline{f}_l)\,\partial f_2-f_2(\overline{f}_l\,\partial f_l)],$$

where the sums over the repeated indices run over $l=3,\ldots,N$. This fact allows us to invert expressions (31) and so express all derivatives ∂f_i in terms of φ_i^2's and f_i. This way we find

$$\partial f_i=A\,[\varphi_i^2+f_i\,\overline{f}_k\varphi_k^2]. \tag{32}$$

Thus, in particular, for the CP^1 case, equation (32) becomes

$$\partial f_2=A^2\varphi_2^2, \quad A=1+|f_2|^2,$$

and f_2 is often denoted in Ref. 1 by w, while in the CP^2 case we have

$$\partial f_2=A[(1+|f_2|^2)\varphi_2^2+f_2\overline{f}_3\,\varphi_3^2],$$

$$\partial f_3=A[(1+|f_3|^2)\varphi_3^2+f_3\overline{f}_2\,\varphi_2^2], \tag{33}$$

$$A=1+|f_2|^2+|f_3|^2.$$

Note that in Refs. 8 and 9 the functions f_2 and f_3 are denoted by w_1 and w_2, respectively. Similarly, all this discussion can be repeated for Φ_i^2's in the same way but using $\overline{\partial}$ instead of ∂, $\overline{f}$ instead of f, and $\overline{G}_{ij}$ instead of F_{ij}.

III. THE GENERALIZED WEIERSTRASS REPRESENTATION IN R^M

To introduce a generalized Weierstrass system in multidimensional spaces we need a set of φ_i and ψ_i which generalize the φ and ψ of the CP^1 case and φ_i and ψ_i, $i=1,2$ of the CP^2 case.

Note that the quantities φ_i^2, $i=2,...,N$, defined in (28) provide such a choice as (32) agrees with the definition of the function φ in expression (22). Next we address the question of what should we use for the function ψ_i? Clearly, relation (21) suggests that we put

$$\psi_i = f_i \overline{\varphi}_i \tag{34}$$

with no summation over the indices $i=2,\ldots,N$. Then to complete the generalization of the Weierstrass system in multidimensional spaces we need analogs of relations (20). We need to prescribe the first derivatives $\overline{\partial}\varphi_i$ and $\partial\psi_i$ in terms of φ_i and ψ_i. Note that from (34) we get

$$\partial\psi_i = \partial(f_i \overline{\varphi}_i) = \partial f_i \overline{\varphi}_i + f_i \overline{(\overline{\partial}\varphi_i)}. \tag{35}$$

So we need to specify $\overline{\partial}\varphi_i$ in terms of φ_i, f_i and their derivatives. To do this we note that from (32) we get

$$\varphi_i^2 = \frac{1}{A}\partial f_i - f_i \frac{f^\dagger \cdot \partial f}{A^2}, \quad A = (f^\dagger \cdot f + 1). \tag{36}$$

So we have

$$\overline{\partial}\varphi_i^2 = 2\frac{f_i(\overline{f_l}\,\partial f_l)}{A^3}(\overline{f_k}\,\overline{\partial} f_k + f_k\,\overline{\partial f_k}) + \frac{1}{A^2}[(1+|f|^2)\partial\overline{\partial} f_i - (\overline{f_k}\overline{\partial} f_k)\partial f_i - (f_k\overline{\partial f_k})\partial f_i - \overline{\partial} f_i(\overline{f_k}\partial f_k)$$
$$- f_i(\overline{\partial f_k}\partial f_k) - f_i(\overline{f_k}\,\partial\overline{\partial} f_k)]. \tag{37}$$

However, equation (10) gives us

$$\partial\overline{\partial} f_i = f_i\frac{(\overline{f_k}\,\partial\overline{\partial} f_k)}{A} + \partial f_i\frac{(\overline{f_k}\,\overline{\partial} f_k)}{A} + \overline{\partial} f_i\frac{(\overline{f_k}\,\partial f_k)}{A} - 2\,f_i\frac{(\overline{f_k}\,\partial f_k)(\overline{f_l}\,\overline{\partial} f_l)}{A^2}. \tag{38}$$

Eliminating the second derivatives $\partial\overline{\partial} f_i$ from equations (37) and (38) we note that all the terms involving the first derivatives $\overline{\partial f}$ and $\overline{\partial f}$ in (37) cancel and we end up with a simple expression

$$\overline{\partial}\varphi_i = -\frac{\varphi_i}{2A}(f_k\,\overline{\partial f_k}) - \frac{f_i}{2\varphi_i A^2}(\overline{\partial f_k}\partial f_k) + \frac{f_i}{2\varphi_i A^3}(\overline{\partial f_k} f_k)(\overline{f_l}\partial f_l). \tag{39}$$

Moreover, taking the complex conjugation of (32),

$$\overline{\partial f_k} = A\,[\overline{\varphi}_k^2 + \overline{f_k}\,f_l\overline{\varphi}_l^2] \tag{40}$$

and so by the virtue of (40) we have

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\} \tag{41}$$

(no summation over i). The second pair of equations for ψ_i then follows from (35)

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)] \tag{42}$$

(no summation over i).

To summarize: the modified Weierstrass system in multidimensional space is a set of $(2N-2)$ complex functions φ_i and ψ_i, $i=2,3,\ldots,N$ which obey the following system of equations (no summation over i):

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\}$$

and

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)], \tag{43}$$

where

$$A = 1 + \sum_{k=2}^{N}\frac{|\psi_k|^2}{|\varphi_k|^2}.$$

From our construction it is clear that the above system of equations is equivalent to the equations of the CP^N sigma model (10). Moreover, it is easy to check that the system of equations (43), for $N=1$ reduces to the equations (20), and for $N=2$ to the equations which were studied in Refs. 8 and 9.

Note that under the requirement of finiteness of the action all solutions of the CP^N sigma model (10) are well known[1] and they split into three separate cases: analytic, antianalytic and the mixed ones. Hence based on this result we can construct large classes of solutions of the modified Weierstrass system (43).

IV. GEOMETRICAL ASPECTS

Here we address the question of the existence of real variables Z_i, of ζ and $\overline{\zeta}$, which are constructed out of our ψ_i's and φ_i's determined by the system of equations (43). Here we treat $Z_i(\zeta,\overline{\zeta})$ as a map of C into R^M

$$Z = (Z_1,\ldots,Z_M): D\subset C\to R^M, \tag{44}$$

where D is a region in the complex plane C. For some values of M we can give a geometrical interpretation of two-dimensional surfaces immersed in R^M. This discussion will generalize the result obtained by Konopelchenko and colaborators.[3,4,10] Moreover, we will find that the surface is immersed in $M=(N^2-1)$-dimensional Euclidean space. To construct real valued functions $Z_i(\zeta,\overline{\zeta})$ it is convenient to exploit the conservation laws for the system of equations (43). To derive these conservation laws we look at (16) and we note that we can exploit the matrices K and $K^\dagger$ given by (26) and (27). However, we note that we can drop the terms Φ_j^2 in expressions (26) and (27) and we still have the conservation laws associated with (10). Namely, we can define

$$K'_{ij} = -f_i\,\overline{\varphi}_j^2 \tag{45}$$

and

$$(K'_{ij})^\dagger = \varphi_i^2\,\overline{f}_j, \tag{46}$$

and we still have the conservation laws of the form

$$\partial K' + \overline{\partial}(K')^{\dagger} = 0. \tag{47}$$

It is easy to check the validity of (47) by making use of the equations (40) and (41).

Note that as our conservation laws do not involve terms containing Φ_i then they can be written entirely in terms of Weierstrass variables φ_i and ψ_i. As a result of so obtained conservation laws we can introduce real valued functions

$$Z_{ll} = \int_\gamma \overline{f}_l \varphi_l^2 \, d\zeta + \int_\gamma f_l \, \overline{\varphi}_l^2 \, d\overline{\zeta} = \int_\gamma \overline{\psi}_l \varphi_l \, d\zeta + \int_\gamma \psi_l \, \overline{\varphi}_l \, d\overline{\zeta} \tag{48}$$

(no summation over index $l = 1, \ldots, N$). These quantities have been constructed from the diagonal entries of matrices K' and $(K')^{\dagger}$. From the off-diagonal entries of matrices K' and $(K')^{\dagger}$ we can construct

$$Z_{lk} = X_{lk} + iY_{lk} = \int_\gamma (\alpha \overline{f}_l \varphi_k^2 + \overline{\alpha} \overline{f}_k \varphi_l^2) d\zeta + \int_\gamma (\overline{\alpha} f_l \, \overline{\varphi}_k^2 + \alpha f_k \, \overline{\varphi}_l^2) d\overline{\zeta}, \quad \alpha \in C. \tag{49}$$

The transposition of the indices lk to kl in Eq. (49) corresponds to the interchange α to $\overline{\alpha}$ and vice versa. In our expression we take all $l,k = 1,\ldots,N$ and for $k = 1$ or $l = 1$ we can use our algebraic constraints (30) to rewrite all our expressions in terms of independent functions φ_i and ψ_i, $i = 2,\ldots,N$. For our real variables Z_i we take Z_{ii}, X_{lk} and Y_{lk}.

Note that the conservation laws (47) guarantee that Z_{ll} and Z_{lk} do not depend on the choice of the contour γ but only on its endpoints in C. This fact takes place because all Z's can be written in the form

$$Z = \int_\Gamma F(\zeta, \overline{\zeta}) \, d\zeta + \overline{F}(\zeta, \overline{\zeta}) \, d\overline{\zeta},$$

where F and $\overline{F}$ satisfy the conserved quantity

$$\overline{\partial} F = \partial \overline{F},$$

which shows that the integrands are total derivatives.

Looking at the diagonal terms in (48) we note that

$$\sum_l Z_{ll} = 0. \tag{50}$$

This follows from the tracelessness of matrices K' and $(K')^{\dagger}$.

Note that all our expressions for Z_{ll} and Z_{lk} are quadratic in terms of φ_i and $\overline{\psi_i}$ and their complex conjugates. They formally include φ_1 and ψ_1, with $\psi_1 = f_1 \overline{\varphi_1}$. However, both these quantities (ψ_1 and φ_1) should be eliminated using the algebraic constraint [i.e., the first expression in (30)] and $f_1 = 1$. It is easy to check that this process of elimination, in the CP^1 case leads to

$$Z_{11} = -2 \int_\gamma \overline{\psi}\varphi \, d\zeta' + \psi\overline{\varphi} \, d\overline{\zeta}',$$

$$X_{12} = \int_\gamma (\overline{\psi}_2^2 - \varphi_2^2) \, d\zeta' + (\psi_2^2 - \overline{\varphi}_2^2) \, d\overline{\zeta}', \tag{51}$$

$$Y_{12} = i \int_\gamma (\overline{\psi}_2^2 + \varphi_2^2) \, d\zeta' - (\psi_2^2 + \overline{\varphi}_2^2) \, d\overline{\zeta}',$$

which appeared in Ref. 3.

Next, following Ref. 11 we can calculate some geometric characteristics of a surface immersed in multidimensional space. We treat the functions Z_{ll}, X_{lk}, and Y_{lk}, as the coordinates of a surface. We introduce the components of the induced metric

$$g_{\alpha\beta}=\sum_{lk}\frac{\partial Z_{lk}}{\partial\alpha}\frac{\partial\overline{Z}_{lk}}{\partial\beta}, \tag{52}$$

where α and β are ζ or $\overline{\zeta}$. For conformally parametrized surfaces we have to make a choice for the normalization of the off-diagonal entries of coordinates X_{kl} and Y_{kl}. We make the natural choice $\alpha=(1+i)/2$. We find that

$$g_{\zeta\zeta}=\left(\sum_{i=1}^{N}\overline{f}_i\,\varphi_i^2\right)^2=0 \tag{53}$$

which coincides with the first algebraic contraint (30). Similarly, its respective complex conjugate equation is

$$g_{\overline{\zeta}\overline{\zeta}}=0. \tag{54}$$

The only nonzero term of the induced metric is

$$g_{\zeta\overline{\zeta}}=(1+|f_2|^2+|f_3|^2+\cdots+|f_N|^2)\left[\left|\sum_{k=2}^{N}\overline{f}_k\varphi_k^2\right|^2+|\varphi_2|^4+|\varphi_3|^4+\cdots+|\varphi_N|^4\right]. \tag{55}$$

Of course, we can rewrite this expression to involve Weierstrass data φ_i and ψ_i by using expressions (34) but the expressions become very complicated. Note, however, that writing all quantities in terms of f_i and ∂f_i, through (31), our expressions simplify considerably and we obtain

$$g_{\zeta\overline{\zeta}}=|Dz|^2, \tag{56}$$

where $D=\frac{1}{2}(D_1-iD_2)$ and D_1, D_2 are the covariant derivatives given by (5) involving ∂ (i.e., evaluated with respect to ζ).

In the special case of the CP^1 maps the component of the induced metric $g_{\zeta\overline{\zeta}}$ takes a particularly simple form; it is given by

$$g_{\zeta\overline{\zeta}}=\left(1+\frac{|\psi_2|^2}{|\varphi_2|^2}\right)[|\varphi_2|^4+|\psi_2|^2|\varphi_2|^2]=[|\psi_2|^2+|\varphi_2|^2]^2=\frac{|\partial f_2|^2}{(|f_2|^2+1)^2} \tag{57}$$

which is exactly, of course $|Dz|^2$; while in the CP^2 case we have

$$g_{\zeta\overline{\zeta}}=\frac{|\partial f_2|^2+|\partial f_3|^2+|f_2\partial f_3-f_3\partial f_2|^2}{(1+|f_2|^2+|f_3)^2|} \tag{58}$$

which also is $|Dz|^2$.

Thus we have proved that the conformal immersion of surfaces in R^{N^2-1} are determined by the generalized Weierstrass representation (48) and (49), where the functions φ_l and ψ_l, or equivalently φ_l and f_l, have to obey system (43) of first order equations. Note that formulas (48) and (49) define a surface on SU(N) and then using expressions in Ref. 12 we can calculate, in a closed form, all geometric characteristics of this surface.

V. SUMMARY AND CONCLUDING REMARKS

The main aim of this paper has been to derive a generalization of the Weierstrass system to the CP^N case. Thus we have found a set of $2N$ complex functions ψ_i and φ_i which satisfy a system of first order equations (43) that are equivalent to the full system of equations of the CP^N model (10).

We have also introduced a set of (N^2-1) real quantities Z's, which can be treated as coordinates of a surface immersed in R^{N^2-1} and we have shown that the induced metric of our map is given by

$$ds^2 = 2|Dz|^2\, d\zeta\, d\overline{\zeta}. \tag{59}$$

The study of the generalized Weierstrass representations for surfaces immersed in multidimensional spaces was initiated by Konopelchenko *et al.*[10] Our work here, in which we adopted an alternative approach based on CP^N sigma models, provides a generalization of their results.

A question arises whether our approach can be extended to Weierstrass systems describing surfaces immersed in multidimensional pseudo-Riemannian spaces. Further, can it provide new classes of solutions which will describe types of surfaces more diverse than those found in multidimensional Euclidean spaces.

ACKNOWLEDGMENTS

One of the authors, A.M.G., would like to thank the University of Durham and the Grey College for the award of Alan Richards fellowship that allowed him to spend two terms in Durham during the academic years 2001 and 2002. Partial support for the work of A.M.G. was provided by a research grant from NSERC of Canada and Fonds FCAR du Gouvernement du Quebec.

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A Laplace operator and harmonics on the quantum complex vector space

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(Received 26 July 2002; accepted 28 October 2002)

The aim of this article is to study the q-Laplace operator and q-harmonic polynomials on the quantum complex vector space generated by elements z_i, w_i, $i=1,2,\ldots,n$, on which the quantum group $\mathrm{GL}_q(n)$ [or $\mathrm{U}_q(n)$] acts. The q-harmonic polynomials are defined as solutions of the equation $\Delta_q p=0$, where p is a polynomial in z_i, w_i, $i=1,2,\ldots,n$, and the q-Laplace operator Δ_q is determined in terms of q-derivatives. The q-Laplace operator Δ_q commutes with the action of $\mathrm{GL}_q(n)$. The projector $\mathsf{H}_{m,m'}:\mathcal{A}_{m,m'}\to\mathcal{H}_{m,m'}$ is constructed, where $\mathcal{A}_{m,m'}$ and $\mathcal{H}_{m,m'}$ are the spaces of homogeneous (of degree m in z_i and of degree m' in w_i) polynomials and homogeneous q-harmonic polynomials, respectively. By using these projectors, a q-analog of the classical zonal spherical and associated spherical harmonics are constructed. They constitute an orthogonal basis of $\mathcal{H}_{m,m'}$. A q-analog of separation of variables is given. The quantum algebra $\mathrm{U}_q(\mathrm{gl}_n)$, acting on $\mathcal{H}_{m,m'}$, determines an irreducible representation of $\mathrm{U}_q(\mathrm{gl}_n)$. This action is explicitly constructed. The results of the article lead to the dual pair $(\mathrm{U}_q(\mathrm{sl}_2),\mathrm{U}_q(\mathrm{gl}_n))$ of quantum algebras. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1532106]

I. INTRODUCTION

Laplace operators, harmonic polynomials, and related separations of variables of the classical analysis are of a great importance for mathematical and theoretical physics. They are closely related to the rotation groups $\mathrm{SO}(n)$ (if we deal with Euclidean space) and to the unitary groups $\mathrm{U}(n)$ (if we deal with the complex vector space) (see, for example, Ref. 1, Chaps. 10 and 11). In this article we are interested in a q-analog of Laplace operators, harmonic polynomials, and related separations of variables on complex spaces.

Harmonic polynomials on the n-dimensional complex vector space are defined by the equation $\Delta p=0$, where Δ is the Laplace operator $\sum_{i=1}^{n}\partial^2/\partial z_i\partial\overline{z_i}$ and p belongs to the space $\mathcal{R}$ of polynomials in $z_1,\ldots,z_n,\overline{z_1},\ldots,\overline{z_n}$ on the complex space $\mathbb{C}^n$. The space $\mathcal{H}$ of all harmonic polynomials on $\mathbb{C}^n$ decomposes as a direct sum of the subspaces $\mathcal{H}_{m,m'}$ of homogeneous harmonic polynomials of degree m in $z_1,\ldots,z_n$ and of degree m' in $\overline{z_1},\ldots,\overline{z_n}$: $\mathcal{H}=\oplus_{m,m'=0}^{\infty}\mathcal{H}_{m,m'}$. The Laplace operator Δ on $\mathbb{C}^n$ commutes with the natural action of the unitary group $\mathrm{U}(n)$ on the space $\mathbb{C}^n$. This means that the subspaces $\mathcal{H}_{m,m'}$ are invariant with respect to $\mathrm{U}(n)$. The irreducible representation $T_{m,m'}$ of the group $\mathrm{U}(n)$ with highest weight $(m,0,\ldots,0,-m')$ is realized on $\mathcal{H}_{m,m'}$.

The equation $\Delta p=0$ permits solutions in separated variables on the space $\mathcal{H}_{m,m'}$. In other words, there exist different coordinate systems (spherical, polyspherical, etc.) on $\mathbb{C}^n$ and for each of them it is possible to find the corresponding basis of the space of solutions of the equation $\Delta p=0$ consisting of products of functions depending on separated variables (see Ref. 2 for the general theory of separation of variables). To different coordinate systems there correspond different separations of variables. From the other side, to different coordinate systems there correspond different chains of subgroups of the group $\mathrm{U}(n)$ (see Ref. 1, Chap. 11, for details of this

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correspondence). The bases of the space $\mathcal{H}_{m,m'}$ in separated variables consist of products of Jacobi polynomials multipled by $r^{m+m'}$ (different sets of Jacobi polynomials for different separations of variables), where r is the radius. These polynomials (considered only on the unit sphere $S_{\mathbb{C}}^{n-1}$ in $\mathbb{C}^n$) are matrix elements of the class 1 [with respect to the subgroup $U(n-1)$] irreducible representations $T_{m,m'}$ of $U(n)$ belonging to zero column (see Ref. 1, Chap. 11).

Many new directions of mathematical physics are related to quantum group and noncommutative geometry. It is natural to generalize the above-described theory to noncommutative spaces. Such generalizations can be of a great importance for further development of some branches of mathematical and theoretical physics related to noncommutative geometry.

The aim of this article is to construct a q-deformation of the above-described classical theory. In the q-deformed case, instead of $\mathbb{C}^n$ we take the quantum complex vector space. It is defined by the associative algebra $\mathcal{A}$ generated by the elements $z_1,\ldots,z_n,w_1,\ldots,w_n$ satisfying a certain natural defining relations. The elements $z_1,\ldots,z_n$ play a role of Cartesian coordinates of $\mathbb{C}^n$ and $w_1,\ldots,w_n$ play a role of $\overline{z_1},\ldots,\overline{z_n}$.

The q-Laplace operator Δ_q on $\mathcal{A}$ is defined in terms of q-derivatives [see formula (17) below]. The quantum group $U_q(n)$ plays a role of the unitary group $U(n)$ in the q-deformed case. It will be convenient for us to use the quantum algebra (that is, the quantized universal enveloping algebra) $U_q(\mathrm{gl}_n)$ instead of the quantum group $U_q(n)$. The q-harmonic polynomials on the quantum complex vector space are defined as elements p of the algebra $\mathcal{A}$ (that is, polynomials in $z_1,\ldots,z_n,w_1,\ldots,w_n$) for which $\Delta_q p=0$. By using the quantum algebra $U_q(\mathrm{gl}_n)$ we construct for q-harmonic polynomials a theory similar to the theory for classical harmonic polynomials. We construct the projector $\mathsf{H}_{m,m'}:\mathcal{A}_{m,m'}\to\mathcal{H}_{m,m'}$, where $\mathcal{A}_{m,m'}$ and $\mathcal{H}_{m,m'}$ are the subspaces of homogeneous (of degree m in $z_1,\ldots,z_n$ and of degree m' in $w_1,\ldots,w_n$) polynomials in $\mathcal{A}$ and in the space $\mathcal{H}$ of all q-harmonic polynomials from $\mathcal{A}$, respectively. Using these projectors we can make different calculations in $\mathcal{H}_{m,m'}$. In this way, zonal spherical and associated spherical polynomials can be calculated. The associated spherical polynomials of $\mathcal{H}_{m,m'}$ constitute an orthogonal basis of this space. Here we obtain a q-analog of the spherical separation of coordinates. We show that the natural action of the algebra $U_q(\mathrm{gl}_n)$ on the quantum complex vector space realizes on the space $\mathcal{H}_{m,m'}$ the irreducible representation of this algebra with highest weight $(m,0,\ldots,0,-m')$. Note that restrictions of zonal spherical and associated spherical polynomials from $\mathcal{H}_{m,m'}$ to the quantum sphere in the quantum complex vector space coincide with matrix elements of irreducible representations $T_{m,m'}$ of the quantum group $U_q(n)$ corresponding to zero column (the latter matrix elements were calculated in Ref. 3; see also Ref. 4). Some our formulas coincide with formulas of Ref. 3. However, no Laplace operator and no q-harmonic polynomials are presented in Ref. 3.

Note that this article is an extension of the results of our previous paper (see Ref. 5) (where we studied q-Laplace operator and q-harmonic polynomials on the quantum real vector space) to the case of quantum complex vector space. It is well known that in the classical case, the theory of Laplace operators and harmonic polynomials on $\mathbb{C}^n$ can be reduced to the corresponding theory for the real space $\mathbb{R}^{2n}$ (see Ref. 1, Chap. 11). It is not the case for the quantum spaces. The reason is that the quantum complex vector space cannot be obtained from the quantum real vector space in the same way as in the classical case.

Everywhere below we suppose that q is not a root of unity. Under considering a scalar product on the spaces $\mathcal{A}$ and $\mathcal{H}$ we assume that q is a positive real number. By $[a]$, $a\in\mathbb{C}$, we denote the so called q-number defined as

$$[a]=\frac{q^a-q^{-a}}{q-q^{-1}}.$$

II. THE QUANTUM ALGEBRA $U_q(\mathrm{gl}_n)$ AND THE QUANTUM VECTOR SPACE

The Drinfeld-Jimbo quantum algebra $U_q(\mathrm{gl}_n)$ is generated by the elements $k_i^{1/2}\equiv q^{h_i/2}$, $k_i^{-1/2}\equiv q^{-h_i/2}$, $i=1,2,\ldots,n$, and e_j, f_j, $j=1,2,\ldots,n-1$, satisfying the relations

$$k_i k_i^{-1}=k_i^{-1}k_i=1,\quad k_i k_j=k_j k_i,\qquad k_i e_j k_i^{-1}=q^{a_{ij}}e_j,\quad k_i f_j k_i^{-1}=q^{-a_{ij}}f_j,$$

$$[e_i,f_j]\equiv e_i f_j-f_j e_i=\delta_{ij}\frac{k_i k_{i+1}^{-1}-k_i^{-1}k_{i+1}}{q-q^{-1}},$$

$$e_i^2 e_{i\pm1}-(q+q^{-1})e_i e_{i\pm1}e_i+e_{i\pm1}e_i^2=0,$$

$$f_i^2 f_{i\pm1}-(q+q^{-1})f_i f_{i\pm1}f_i+f_{i\pm1}f_i^2=0,$$

$$[e_i,e_j]=[f_i,f_j]=0,\qquad |i-j|>1,$$

where $a_{ii}=1$, $a_{i,i-1}=a_{i-1,i}=-1$ and $a_{ij}=0$ otherwise (see, for example, Ref. 6, Chap. 6).

The algebra $\mathrm{U}_q(\mathrm{gl}_n)$ is a Hopf algebra, and the Hopf algebra operations (comultiplication Δ, counit ε and antipode S) are given by the formulas

$$\Delta(k_i^{\pm1})=k_i^{\pm1}\otimes k_i^{\pm1},\qquad \Delta(e_i)=e_i\otimes k_i^{-1/2}k_{i+1}^{1/2}+k_i^{1/2}k_{i+1}^{-1/2}\otimes e_i,$$

$$\Delta(f_i)=f_i\otimes k_i^{-1/2}k_{i+1}^{1/2}+k_i^{1/2}k_{i+1}^{-1/2}\otimes f_i,\qquad \varepsilon(k_i)=1,\qquad \varepsilon(e_i)=\varepsilon(f_i)=0,$$

$$S(k_i)=k_i^{-1},\qquad S(e_i)=-q^{-1}e_i,\qquad S(f_i)=-qf_i.$$

The group $\mathrm{GL}(n,\mathbb{C})$ and its Lie algebra $\mathrm{gl}(n,\mathbb{C})$ act linearly on the n-dimensional complex vector space. Similarly, the quantum group $\mathrm{GL}_q(n,\mathbb{C})$ and the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ acts on the quantum (noncommutative) analog of the complex vector space. This quantum space is determined by the algebra of polynomials $\mathcal{A}\equiv\mathbb{C}_q[z_1,\ldots,z_n,\ w_1,\ldots,w_n]$ (see Ref. 7). This algebra is the associative algebra generated by elements $z_1,\ z_2,\ldots,z_n,\ w_1,\ w_2,\ldots,w_n$ satisfying the defining relations

$$z_i z_j=q z_j z_i,\qquad w_i w_j=q^{-1}w_j w_i,\qquad i<j, \tag{1}$$

$$w_j z_i=q z_i w_j,\qquad i\neq j,\quad i,j=1,2,\ldots,n, \tag{2}$$

$$w_k z_k=z_k w_k+(1-q^2)\sum_{s=1}^{k-1} z_s w_s. \tag{3}$$

The elements $w_1,\ldots,\ w_n$ play a role of $\overline{z_1},\ldots,\ \overline{z_n}$ in the classical analysis.

A $*$-operation can be defined on the algebra $\mathcal{A}$ turning it into a $*$-algebra. This $*$-operation is uniquely determined by the relations $z_i^*=w_i,\ w_i^*=z_i,\ i=1,2,\ldots,\ n$. The compact quantum group $\mathrm{U}_q(n)$ acts on this $*$-algebra. Note that the algebra $\mathcal{A}$ is similar to (and not coinciding with) the algebra considered by Pusz and Woronowicz.[8]

Note that the relations (3) are equivalent to the following ones:

$$z_k w_k=w_k z_k-(1-q^2)\sum_{s=1}^{k-1} q^{2(k-s-1)}w_s z_s. \tag{4}$$

The set of all monomials

$$z_1^{r_1}z_2^{r_2}\cdots z_n^{r_n}w_1^{s_1}w_2^{s_2}\cdots w_n^{s_n},\quad r_j,\ s_j=0,1,2,\ldots, \tag{5}$$

form a basis of the algebra $\mathcal{A}$ (see Ref. 9). The set

$$w_1^{r_1}w_2^{r_2}\cdots w_n^{r_n}z_1^{s_1}z_2^{s_2}\cdots z_n^{s_n},\quad r_j,\ s_j=0,1,2,\ldots, \tag{6}$$

also form a basis of this algebra.

The vector space of the algebra $\mathcal{A}$ can be represented as a direct sum of the vector subspaces $\mathcal{A}_{m,m'}$ consisting of homogeneous polynomials of homogeneity degree m in $z_1, z_2, \ldots, z_n$ and of homogeneity degree m' in $w_1, w_2, \ldots, w_n$, $m, m' = 0, 1, 2, \ldots$:

$$\mathcal{A} = \bigoplus_{m=0}^{\infty} \bigoplus_{m'=0}^{\infty} \mathcal{A}_{m,m'}. \tag{7}$$

We have the linear space isomorphism

$$\mathcal{A} \simeq \mathcal{A}_z \otimes \mathcal{A}_w,$$

where the associative algebra $\mathcal{A}_z$ (the associative algebra $\mathcal{A}_w$) is a subalgebra of $\mathcal{A}$ coinciding with $\oplus_{m=0}^{\infty} \mathcal{A}_{m,0}$ (respectively, with $\oplus_{m'=0}^{\infty} \mathcal{A}_{0,m'}$).

We can define an action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ on the vector space $\mathcal{A}$. To determine this action we give the action of $\mathrm{U}_q(\mathrm{gl}_n)$ on z_j and w_j by the formulas[9]

$$k_i \triangleright z_j = q^{\delta_{ij}} z_j, \qquad e_i \triangleright z_j = \delta_{j,i+1} z_{j-1}, \quad f_i \triangleright z_j = \delta_{j,i} z_{j+1}, \tag{8}$$

$$k_i \triangleright w_j = q^{-\delta_{ij}} w_j, \qquad e_i \triangleright w_j = -\delta_{j,i} q^{-1} w_{j+1}, \quad f_i \triangleright w_j = -\delta_{j,i+1} q w_{j-1}, \tag{9}$$

and extend it to $\mathcal{A}$ by using the comultiplication, that is, by means of the relation

$$X \triangleright (p_1 p_2) = \sum (X_{(1)} \triangleright p_1)(X_{(2)} \triangleright p_2),$$

where $\Delta(X) = \Sigma X_{(1)} \otimes X_{(2)}$ (in the Sweedler notation), and linearity.

This action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ on the vector space $\mathcal{A}$ determines a representation of $\mathrm{U}_q(\mathrm{gl}_n)$ on this space (we denote it by L). Evidently, the subspaces $\mathcal{A}_{m,m'}$ are invariant with respect to this action. Therefore, L determines representations of $\mathrm{U}_q(\mathrm{gl}_n)$ on these subspaces, which are denoted by $L_{m,m'}$. We have $L = \oplus_{m,m'=0}^{\infty} L_{m,m'}$.

III. OPERATORS ON THE ALGEBRA $\mathcal{A}$

In order to introduce the q-Laplace operator on $\mathcal{A}$ and to study q-harmonic polynomials we need some operators on the linear space of the algebra $\mathcal{A}$. By γ_i and $\overline{\gamma_i}$ we denote the linear operators acting on monomials as

$$\gamma_i(z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n}) = q^{r_i} z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n},$$

$$\overline{\gamma_i}(w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n}) = q^{r_i} w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n}.$$

Definition of the operators γ_i^{-1} and $\overline{\gamma_i}^{-1}$ is obvious.

By $\hat{z}_i$ and $\check{z}_i$ we denote the linear operators of multiplication by the element z_i:

$$\hat{z}_i(z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n}) = z_i z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n},$$

$$\check{z}_i(z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n}) = z_1^{r_1} z_2^{r_2} \cdots z_n^{r_n} z_i w_1^{s_1} w_2^{s_2} \cdots w_n^{s_n}.$$

The corresponding linear operators $\hat{w}_i$ and $\check{w}_i$ are defined as

$$\hat{w}_i(w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n}) = w_i w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n},$$

$$\check{w}_i(w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n}) = w_1^{r_1} w_2^{r_2} \cdots w_n^{r_n} w_i z_1^{s_1} z_2^{s_2} \cdots z_n^{s_n}.$$

We define on $\mathcal{A}$ the q-differentiations ∂_i and $\overline{\partial_i}$. The linear operators ∂_i act as $\partial_i p=0$ on monomials p of the form (5) not containing z_i and as

$$\partial_i=\check{z}_i^{-1}\frac{\gamma_i-\gamma_i^{-1}}{q-q^{-1}} \tag{10}$$

on monomials containing z_i. The q-differentiations $\overline{\partial_i}$ are linear operators acting as $\overline{\partial_i}p=0$ on monomials p of the form (6) not containing w_i and as

$$\overline{\partial_i}=\check{w}_i^{-1}\frac{\overline{\gamma_i}-\overline{\gamma_i}^{-1}}{q-q^{-1}} \tag{11}$$

on monomials containing w_i. In particular, we have

$$\partial_i(z_1^{r_1}\cdots z_n^{r_n}w_1^{s_1}\cdots w_n^{s_n})=[r_i]q^{r_{i+1}+\cdots+r_n}z_1^{r_1}\cdots z_i^{r_i-1}\cdots z_n^{r_n}w_1^{s_1}\cdots w_n^{s_n},$$

$$\overline{\partial_i}(w_1^{r_1}\cdots w_n^{r_n}z_1^{s_1}\cdots z_n^{s_n})=[r_i]q^{-(r_{i+1}+\cdots+r_n)}w_1^{r_1}\cdots w_i^{r_i-1}\cdots w_n^{r_n}z_1^{s_1}\cdots z_n^{s_n}.$$

The action formulas (8) and (9) mean that the multiplication operators $\hat{z}_j$, $j=1, 2,\ldots, n$, and $\hat{w}_j$, $j=1, 2,\ldots, n$, constitute tensor operators transforming under the vector representation and under the contragredient to the vector representation, respectively.

The actions (8) and (9) of $\mathrm{U}_q(\mathrm{gl}_n)$ on z_j and w_j determines its action on the operators ∂_j and $\overline{\partial_j}$:

$$k_i\triangleright\partial_j=q^{-\delta_{ij}}\partial_j,\qquad e_i\triangleright\partial_j=-\delta_{j,i}q^{-1}\partial_{j+1},\quad f_i\triangleright\partial_j=-\delta_{j,i+1}q\partial_{j-1}, \tag{12}$$

$$k_i\triangleright\overline{\partial_j}=q^{\delta_{ij}}\overline{\partial_j},\qquad e_i\triangleright\overline{\partial_j}=\delta_{j,i+1}q^{-2}\overline{\partial_{j-1}},\quad f_i\triangleright\overline{\partial_j}=\delta_{j,i}q^{2}\overline{\partial_{j+1}}. \tag{13}$$

That is, the set $\overline{\partial_j}$, $j=1, 2,\ldots, n$, (respectively, the set ∂_j, $j=1, 2,\ldots, n$) is a tensor operator transforming under vector (respectively, contragredient to vector) representation.

The operators ∂_i, $\overline{\partial_i}$, $\hat{z}_i$, $\hat{w}_i$ satisfy the relations, which will be presented by means of the quantum R-matrix R for the quantum algebra $\mathrm{U}_q(\mathrm{gl}_n)$ (see, for example, Ref. 6, Sec. 8.1, and Ref. 7 for definition of the R-matrix). Let $\mathbf{R}=PR$, where the matrix P permutes the spaces in the tensor product of two spaces on which R-matrix acts. Then

$$\mathbf{R}_{kl}^{ij}=q^{\delta_{ij}}\delta_{il}\delta_{jk}+(q-q^{-1})\,\delta_{ik}\delta_{jl}\theta(j-i),$$

where $\theta(k)=1$ if $k>0$ and $\theta(k)=0$ if $k\leqslant 0$. Its inverse matrix is

$$(\mathbf{R}^{-1})_{kl}^{ij}=q^{-\delta_{ij}}\delta_{il}\delta_{jk}-(q-q^{-1})\,\delta_{ik}\delta_{jl}\theta(i-j).$$

We also need the matrix $\Phi_{kl}^{ij}=\mathbf{R}_{lk}^{ji}q^{2(i-l)}$, which satisfies the relations

$$\sum_{j,l}\Phi_{pj}^{ul}(\mathbf{R}^{-1})_{lk}^{ji}=\sum_{j,l}(\mathbf{R}^{-1})_{pj}^{ul}\Phi_{lk}^{ji}=\delta_{up}\delta_{ik},$$

$$\sum_{l}\Phi_{lk}^{li}=\delta_{ik}q^{2(n-i)+1},\quad \sum_{k}\Phi_{lk}^{jk}=\delta_{jl}q^{2l-1}.$$

The relations (1)–(3) rewritten for operators $\hat{z}_i$ and $\hat{w}_i$ can be presented as

$$\hat{z}_i\hat{z}_j=q^{-1}\mathbf{R}_{ij}^{kl}\hat{z}_k\hat{z}_l,\quad \hat{w}_i\hat{w}_j=q^{-1}\mathbf{R}_{lk}^{ji}\hat{w}_k\hat{w}_l,\quad \hat{w}_i\hat{z}_j=q(\mathbf{R}^{-1})_{jl}^{ik}\hat{z}_k\hat{w}_l.$$

We also have the relations

$$\partial_i\partial_j = q^{-1}\mathbf{R}^{ji}_{lk}\partial_k\partial_l, \quad \overline{\partial_i\partial_j} = q^{-1}\mathbf{R}^{kl}_{ij}\overline{\partial_k}\,\overline{\partial_l}, \quad \partial_i\overline{\partial_j} = q^{-1}\Phi^{ki}_{lj}\overline{\partial_k}\partial_l,$$

$$\partial_i\hat{w}_j = q(\mathbf{R}^{-1})^{ji}_{lk}\hat{w}_k\partial_l, \quad \overline{\partial_i}\hat{z}_j = q\Phi^{lk}_{ji}\hat{z}_k\overline{\partial_l},$$

$$\partial_i\hat{z}_j = \gamma^{\mp 1}\delta_{ij} + (\mathbf{R}^{\pm 1})^{ik}_{jl}\hat{z}_k\partial_l, \quad \overline{\partial_i}\hat{w}_j = \overline{\gamma^{\mp 1}}\delta_{ij} + (\mathbf{R}^{\pm 1})^{lj}_{ki}\hat{w}_k\overline{\partial_l},$$

which can be represented in the form

$$\partial_i\partial_j = q^{-1}\partial_j\partial_i, \quad \overline{\partial_i\partial_j} = q\overline{\partial_j}\,\overline{\partial_i}, \quad i<j,$$

$$\overline{\partial_i}\partial_j = q\partial_j\overline{\partial_i}, \quad i\neq j, \quad \overline{\partial_i}\partial_i = \partial_i\overline{\partial_i} + (1-q^2)\sum_{k>i}\partial_k\overline{\partial_k},$$

$$\partial_i\overline{\partial_i} = \overline{\partial_i}\partial_i + (1-q^{-2})\sum_{k>i} q^{2(k-i)}\overline{\partial_k}\partial_k.$$

$$\partial_i\hat{w}_i = \hat{w}_i\partial_i, \quad \partial_i\hat{w}_j - q\hat{w}_j\partial_i = (1-q^2)\hat{w}_i\partial_j, \quad \partial_j\hat{w}_i = q\hat{w}_i\partial_j, \quad i<j,$$

$$\overline{\partial_i}\hat{z}_i = \hat{z}_i\overline{\partial_i}, \quad \overline{\partial_i}\hat{z}_j - q^{-1}\hat{z}_j\overline{\partial_i} = (1-q^{-2})q^{2(j-i)}\hat{z}_i\overline{\partial_j}, \quad \overline{\partial_j}\hat{z}_i = q^{-1}\hat{z}_i\overline{\partial_j}, \quad i<j,$$

$$\partial_i\hat{z}_j = \hat{z}_j\partial_i, \quad \overline{\partial_i}\hat{w}_j = \hat{w}_j\overline{\partial_i}, \quad i\neq j,$$

$$\partial_i\hat{z}_i = q\hat{z}_i\partial_i + (q-q^{-1})\sum_{k>i}\hat{z}_k\partial_k + \gamma^{-1} = q^{-1}\hat{z}_i\partial_i - (q-q^{-1})\sum_{k<i}\hat{z}_k\partial_k + \gamma,$$

$$\overline{\partial_i}\hat{w}_i = q\hat{w}_i\overline{\partial_i} + (q-q^{-1})\sum_{k<i}\hat{w}_k\overline{\partial_k} + \overline{\gamma}^{-1} = q^{-1}\hat{w}_i\overline{\partial_i} - (q-q^{-1})\sum_{k>i}\hat{w}_k\overline{\partial_k} + \overline{\gamma},$$

where $\gamma = \gamma_1\gamma_2\cdots\gamma_n$ and $\overline{\gamma} = \overline{\gamma_1}\,\overline{\gamma_2}\cdots\overline{\gamma_n}$. From last two lines, we obtain

$$\sum_{k=1}^{n}\hat{z}_k\partial_k = \{\gamma\} \equiv \frac{\gamma-\gamma^{-1}}{q-q^{-1}}, \quad \sum_{k=1}^{n}\hat{w}_k\overline{\partial_k} = \{\overline{\gamma}\} \equiv \frac{\overline{\gamma}-\overline{\gamma}^{-1}}{q-q^{-1}}.$$

We also have the relations

$$\gamma\hat{z}_i = q\hat{z}_i\gamma, \quad \gamma\hat{w}_i = \hat{w}_i\gamma, \quad \overline{\gamma}\hat{z}_i = \hat{z}_i\overline{\gamma}, \quad \overline{\gamma}\hat{w}_i = q\hat{w}_i\overline{\gamma},$$

$$\gamma\partial_i = q^{-1}\partial_i\gamma, \quad \gamma\overline{\partial_i} = \overline{\partial_i}\gamma, \quad \overline{\gamma}\partial_i = \partial_i\overline{\gamma}, \quad \overline{\gamma}\,\overline{\partial_i} = q^{-1}\overline{\partial_i}\,\overline{\gamma}.$$

Note that

$$\gamma p = q^m p, \quad \overline{\gamma}p = q^{m'}p, \quad p\in\mathcal{A}_{m,m'}. \tag{14}$$

To compare these relations with those known from literature, we introduce the operators $\partial_i' = \gamma\partial_i$, $\overline{\partial_i'} = \overline{\gamma}^{-1}\overline{\partial_i}$. Then the operators $\hat{z}_i$, $\hat{w}_i$, ∂_i', $\overline{\partial_i'}$, $i=1,\ldots,n$, satisfy the relations from Ref. 10 which are known to be covariant with respect to $\mathrm{U}_q(\mathrm{gl}_n)$. Note that the operators $\partial_i' = \gamma\partial_i$ coincide with the q-deformed differential operators of Pusz and Woronowicz[8] and of Wess and Zumino[11] if to restrict their action upon the subalgebra $\mathcal{A}_z$ generated by $z_1, z_2, \ldots, z_n$.

Note that the above elements $\hat{z}_1,\ldots,\hat{z}_n$, $\partial_1',\ldots,\partial_n'$ generate the q-Weyl algebra, that is, they satisfy the relations

$$\hat{z}_i\hat{z}_j = q\hat{z}_j\hat{z}_i, \quad \partial'_i\partial'_j = q^{-1}\partial'_j\partial'_i \quad i<j, \quad \partial'_i\hat{z}_j = q\hat{z}_j\partial'_i, \quad i\neq j,$$

$$\partial'_i\hat{z}_i - q^2\hat{z}_i\partial'_i = 1 + (q^2-1)\sum_{j>i}\hat{z}_j\partial'_j$$

(the definition of the q-Weyl algebra; see, for example, in Ref. 6, Chap. 12). Similarly, the elements $\hat{w}_1,\ldots,\hat{w}_n,\overline{\partial'_1},\ldots,\overline{\partial'_n}$ generate the q^{-1}-Weyl algebra.

The operators $D:=\Sigma_{k=1}^n\hat{z}_k\partial_k$ and $\overline{D}:=\Sigma_{k=1}^n\hat{w}_k\overline{\partial_k}$ are called the *q-Euler operators*. The formula (7) gives the decomposition of $\mathcal{A}$ into a direct sum of eigenspaces of the operators D and $\overline{D}$.

Let us show that the above relations for the operators $\partial_i,\overline{\partial_i},\hat{z}_i,\hat{w}_i$ determine uniquely the formulas (10) and (11) for $\partial_i,\overline{\partial_i}$. We use the action formulas $\partial_i 1=\overline{\partial_i}1=0$, take into account that $\hat{z}_i$, $\hat{w}_i$ act as the operators of left multiplication on the basis elements (5) and (6), respectively, and γ, $\overline{\gamma}$ are gradation operators on $\mathcal{A}$ [see (14)]. By means of commutation relations between ∂_i and $\hat{w}_j$, it is easy to obtain that $\partial_i w_1^{s_1}w_2^{s_2}\cdots w_n^{s_n}=0$. To calculate $\partial_i(z_i^{r_i}w_1^{s_1}w_2^{s_2}\cdots w_n^{s_n})$ with $r_i>0$, we use the relation

$$\partial_i\hat{z}_i = q\hat{z}_i\partial_i + (q-q^{-1})\sum_{k>i}\hat{z}_k\partial_k + \gamma^{-1}.$$

It gives $\partial_i(z_i^{r_i}w_1^{s_1}w_2^{s_2}\cdots w_n^{s_n}) = [r_i]z_i^{r_i-1}w_1^{s_1}w_2^{s_2}\cdots w_n^{s_n}$. Finally, we have the action formula

$$\begin{aligned}\partial_i(z_1^{r_1}\cdots z_i^{r_i}\cdots z_n^{r_n}w_1^{s_1}\cdots w_n^{s_n}) &= q^{r_i(r_{i+1}+\cdots+r_n)}\partial_i(z_1^{r_1}\cdots z_{i-1}^{r_{i-1}}z_{i+1}^{r_{i+1}}\cdots z_n^{r_n}z_i^{r_i}w_1^{s_1}\cdots w_n^{s_n})\\ &= q^{r_i(r_{i+1}+\cdots+r_n)}\hat{z}_1^{r_1}\cdots\hat{z}_{i-1}^{r_{i-1}}\hat{z}_{i+1}^{r_{i+1}}\cdots\hat{z}_n^{r_n}\partial_i(z_i^{r_i}w_1^{s_1}\cdots w_n^{s_n})\\ &= q^{r_{i+1}+\cdots+r_n}[r_i]z_1^{r_1}\cdots z_i^{r_i-1}\cdots z_n^{r_n}w_1^{s_1}\cdots w_n^{s_n},\end{aligned}$$

which exactly coincides with the action (10). The action formula for $\overline{\partial_i}$ is recovered in a similar way.

The action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ on $\mathcal{A}\simeq\mathcal{A}_z\otimes\mathcal{A}_w$, defined by formulas (8) and (9), can be determined in terms of the operators ∂_i and $\overline{\partial_j}$. We first note that the action of $\mathrm{U}_q(\mathrm{gl}_n)$ on $\mathcal{A}_z$ is given by the operators

$$L(k_i)=\gamma_i, \qquad L(e_i)=q^{-1/2}(\gamma_i\gamma_{i+1})^{1/2}\check{z}_i\partial_{i+1}, \qquad L(f_i)=q^{1/2}(\gamma_i\gamma_{i+1})^{-1/2}\check{z}_{i+1}\partial_i$$

and on $\mathcal{A}_w$ by the operators

$$L(k_i)=\overline{\gamma}_i^{-1}, \quad L(e_i)=-q^{-3/2}(\overline{\gamma}_i\overline{\gamma}_{i+1})^{1/2}\check{w}_{i+1}\overline{\partial}_i, \quad L(f_i)=-q^{3/2}(\overline{\gamma}_i\overline{\gamma}_{i+1})^{-1/2}\check{w}_i\overline{\partial}_{i+1}.$$

Taking into account the comultiplication on $\mathrm{U}_q(\mathrm{gl}_n)$ the action of $\mathrm{U}_q(\mathrm{gl}_n)$ on the linear space $\mathcal{A}\simeq\mathcal{A}_z\otimes\mathcal{A}_w$ can be written as $L(k_i)=\gamma_i\otimes\overline{\gamma}_i^{-1}$ and

$$L(e_i)=q^{-1/2}(\gamma_i\gamma_{i+1})^{1/2}\check{z}_i\partial_{i+1}\otimes(\overline{\gamma}_i\overline{\gamma}_{i+1}^{-1})^{1/2}-q^{-3/2}(\gamma_i\gamma_{i+1}^{-1})^{1/2}\otimes(\overline{\gamma}_i\overline{\gamma}_{i+1})^{1/2}\check{w}_{i+1}\overline{\partial}_i,$$

$$L(f_i)=q^{1/2}(\gamma_i\gamma_{i+1})^{-1/2}\check{z}_{i+1}\partial_i\otimes(\overline{\gamma}_i\overline{\gamma}_{i+1}^{-1})^{1/2}-q^{3/2}(\gamma_i\gamma_{i+1}^{-1})^{1/2}\otimes(\overline{\gamma}_i\overline{\gamma}_{i+1})^{-1/2}\check{w}_i\overline{\partial}_{i+1}.$$

IV. SQUARED *q*-RADIUS AND *q*-LAPLACE OPERATOR

The element

$$Q=\sum_{i=1}^n z_iw_i=\sum_{i=1}^n q^{2(n-i)}w_iz_i\in\mathcal{A}_{1,1} \tag{15}$$

of the algebra $\mathcal{A}$ is called the *squared q-radius* on the quantum complex vector space. It is an important element in $\mathcal{A}$. One can check by a direct computation that Q *is invariant with respect to the representation* $L_{1,1}$ (and hence with respect to the representation L), that is, $L(k_i^{\pm 1})Q=Q$, $L(e_j)Q=0$ and $L(f_j)Q=0$. Similarly, the element $Q^k \in \mathcal{A}_{k,k}$ is invariant with respect to the representation $L_{k,k}$.

The squared q-radius Q belongs to the center of the algebra $\mathcal{A}$, that is, $Qz_i=z_iQ$, $Qw_i=w_iQ$, $i=1, 2,\ldots, n$. We shall also use the elements

$$Q_j=\sum_{i=1}^{j} z_iw_i=\sum_{i=1}^{j} q^{2(j-i)}w_iz_i,$$

which are squared q-radii for the subalgebras $\mathbb{C}_q[z_1, w_1,\ldots, z_j, w_j]$. They satisfy the relations[9]

$$Q_jQ_i=Q_iQ_j, \qquad z_iw_i=Q_i-Q_{i-1}, \qquad w_iz_i=Q_i-q^2Q_{i-1},$$

$$z_iQ_j=q^{-2}Q_jz_i, \qquad w_iQ_j=q^2Q_jw_i \qquad \text{for} \qquad i>j,$$

$$z_iQ_j=Q_jz_i, \qquad w_iQ_j=Q_jw_i \qquad \text{for} \qquad i\leqslant j.$$

It can be checked[9] by direct computation that

$$z_i^kw_i^k=Q_i^k(Q_{i-1}/Q_i;q^{-2})_k, \quad w_i^kz_i^k=Q_i^k(q^2Q_{i-1}/Q_i;q^2)_k, \tag{16}$$

where

$$(a;q)_s=(1-a)(1-aq)\cdots(1-aq^{s-1}).$$

We consider on $\mathcal{A}$ the operator

$$\Delta_q=\partial_1\overline{\partial_1}+\partial_2\overline{\partial_2}+\cdots+\partial_n\overline{\partial_n}=\sum_{i=1}^{n} q^{2(i-1)}\overline{\partial_i}\partial_i, \tag{17}$$

which is called the *q-Laplace operator* on the quantum complex vector space. Since $\gamma\Delta_q=q^{-1}\Delta_q\gamma$ and $\overline{\gamma}\Delta_q=q^{-1}\Delta_q\overline{\gamma}$, then $\Delta_q:\mathcal{A}_{m,m'}\to\mathcal{A}_{m-1,m'-1}$.

To the element (15) there corresponds the operator $\hat{Q}$ on $\mathcal{A}$ defined as

$$\hat{Q}=\hat{z}_1\hat{w}_1+\hat{z}_2\hat{w}_2+\cdots+\hat{z}_n\hat{w}_n.$$

Proposition 1: The operators Δ_q *and* $\hat{Q}$ *satisfy the relations*

$$\Delta_q\hat{Q}^k-\hat{Q}^k\Delta_q=q^{n-1}\hat{Q}^{k-1}[k]\{q^{k+n-1}\gamma\overline{\gamma}\}, \tag{18}$$

$$\Delta_q(Q^k)=q^{n-1}Q^{k-1}[k][k+n-1], \tag{19}$$

where

$$\{a\}=\frac{a-a^{-1}}{q-q^{-1}}$$

and $[r]\equiv\{q^r\}$ *is a q-number.*

Proof: First we prove the relation $[\Delta_q,\hat{Q}]=q^{n-1}\{q^n\gamma\overline{\gamma}\}$. Using relations of Sec. III we derive

$$\Delta_q\hat{Q}=\sum_{k,l}\partial_k\overline{\partial}_k\hat{z}_l\hat{w}_l$$

$$=\sum_{k,l,i,j}\partial_k(q^{-1}\Phi^{ji}_{lk}\hat{z}_i\overline{\partial}_j)\hat{w}_l$$

$$=\sum_{k,l,i,j}q^{-1}\Phi^{ji}_{lk}\left(\delta_{ik}\gamma^{-1}+\sum_{r,s}\mathbf{R}^{kr}_{is}\hat{z}_r\partial_s\right)\overline{\partial}_j\hat{w}_l$$

$$=\sum_{k,l,j}q^{-1}\Phi^{jk}_{lk}\gamma^{-1}\overline{\partial}_j\hat{w}_l+\sum_{k,l,i,j,r,s}q^{-1}\Phi^{ji}_{lk}\mathbf{R}^{kr}_{is}\hat{z}_r\partial_s\left(\delta_{jl}\overline{\gamma}+\sum_{u,p}(\mathbf{R}^{-1})^{ul}_{pj}\hat{w}_p\overline{\partial}_u\right)$$

$$=\sum_l q^{2l-2}\gamma^{-1}\overline{\partial}_l\hat{w}_l+\sum_{i,r,s}q^{2(n-i)}\mathbf{R}^{ir}_{is}\hat{z}_r\partial_s\overline{\gamma}+\sum_{k,i,r,s}q^{-1}\mathbf{R}^{kr}_{is}\hat{z}_r\partial_s\hat{w}_i\overline{\partial}_k.$$

The third summand is equal to

$$\sum_{k,i,r,s}q^{-1}\mathbf{R}^{kr}_{is}\hat{z}_r\partial_s\hat{w}_i\overline{\partial}_k=\sum_{k,i,r,s}q^{-1}\mathbf{R}^{kr}_{is}\hat{z}_r\left(q\sum_{u,p}(\mathbf{R}^{-1})^{is}_{pu}\hat{w}_u\partial_p\right)\overline{\partial}_k=\hat{Q}\Delta_q.$$

Using explicit expressions for matrix elements of $\mathbf{R}$ and $\mathbf{R}^{-1}$ we have

$$\sum_i q^{2(n-i)}\mathbf{R}^{ir}_{is}=q^{2n-1}\delta_{rs},\qquad \sum_l q^{2l-2}(\mathbf{R}^{-1})^{ul}_{pl}=q^{-1}\delta_{pu},$$

$$\sum_l q^{2l-2}\overline{\partial}_l\hat{w}_l=\sum_l q^{2l-2}\left(\overline{\gamma}+\sum_{u,p}(\mathbf{R}^{-1})^{ul}_{pl}\hat{w}_p\overline{\partial}_u\right)$$

$$=q^{n-1}[n]\overline{\gamma}+q^{-1}\sum_p\hat{w}_p\overline{\partial}_p$$

$$=q^{n-1}[n]\overline{\gamma}+q^{-1}\{\overline{\gamma}\}$$

$$=q^{n-1}\{q^n\overline{\gamma}\}.$$

Thus, $[\Delta_q,\hat{Q}]=q^{n-1}\gamma^{-1}\{q^n\overline{\gamma}\}+q^{2n-1}\{\gamma\}\overline{\gamma}=q^{n-1}\{q^n\gamma\overline{\gamma}\}$. Now, it is easy to obtain (18) by induction if to use the relation $\{q^r\gamma\overline{\gamma}\}\hat{Q}=\hat{Q}\{q^{r+2}\gamma\overline{\gamma}\}$ and the explicit expression for $\{a\}$. Acting by both sides of (18) on 1 we obtain (19).

Proposition 2: The operators Δ_q and $\hat{Q}$ commute with the action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ on $\mathcal{A}$, that is, with all operators of the representation L of $\mathrm{U}_q(\mathrm{gl}_n)$.

Proof: It follows from (12) and (13) that $k_i\triangleright\Delta_q=\Delta_q$, $e_j\triangleright\Delta_q=0$ and $f_j\triangleright\Delta_q=0$. Now using the comultiplication for k_i, e_j and f_j, we obtain the proposition for the q-Laplace operator. For $\hat{Q}$ the proposition is proved similarly.

V. *q*-HARMONIC POLYNOMIALS

A polynomial $p\in\mathcal{A}$ is called *q-harmonic* if $\Delta_q p=0$. The linear subspace of $\mathcal{A}$ consisting of all q-harmonic polynomials is denoted by $\mathcal{H}$. Let

$$\mathcal{H}_{m,m'}=\mathcal{A}_{m,m'}\cap\mathcal{H}.$$

Proposition 3: The space $\mathcal{A}_{m,m'}$ can be represented as the direct sum

$$\mathcal{A}_{m,m'}=\mathcal{H}_{m,m'}\oplus Q\mathcal{A}_{m-1,m'-1}. \tag{20}$$

Proof: First we prove that $\mathcal{H}_{m,m'} \cap Q\mathcal{A}_{m-1,m'-1} = \{0\}$. If it is not true, then there exists nonzero element $p \in \mathcal{H}_{m,m'} \cap Q\mathcal{A}_{m-1,m'-1}$. Let k be a maximal integer such that $p = Q^k p'$ with some nonzero polynomial p'. Then it follows from $\Delta_q(p) = 0$ and (18) that

$$0 = \Delta_q(Q^k p') = Q^k \Delta_q(p') + Q^{k-1} q^{n-1} [k][k+n-1+m+m'-2k] p'.$$

Since $q^{n-1}[k][k+n-1+m+m'-2k] \neq 0$, then p' can be divided by Q. This is a contradiction. Thus, $\mathcal{H}_{m,m'} \cap Q\mathcal{A}_{m-1,m'-1} = \{0\}$. Using this fact and the equality $\ker \Delta_q = \mathcal{H}_{m,m'}$, where Δ_q is considered only on $\mathcal{A}_{m,m'}$, we obtain the chain of inequalities

$$\dim\ \mathcal{A}_{m,m'} - \dim\ \ker\ \Delta_q \geqslant \dim\ Q\mathcal{A}_{m-1,m'-1} = \dim\ \mathcal{A}_{m-1,m'-1} \geqslant \dim\ \mathrm{im}\ \Delta_q.$$

The last inequality follows from the fact that $\Delta_q : \mathcal{A}_{m,m'} \to \mathcal{A}_{m-1,m'-1}$. Now we take into account the relation $\dim \ker \Delta_q + \dim \mathrm{im}\, \Delta_q = \dim \mathcal{A}_{m,m'}$. Thus, in fact, the above inequalities are exact equalities, and $\mathcal{A}_{m,m'} = \mathcal{H}_{m,m'} \oplus Q\mathcal{A}_{m-1,m'-1}$. Proposition is proved.

Remark: If $n = 1$, then $\mathcal{A}$ consists of all polynomials in commuting elements z_1 and w_1. In this case, the space $\mathcal{H}$ of q-harmonic polynomials has a basis consisting of the polynomials

$$1, \quad z_1^k, \quad w_1^k, \qquad k = 1, 2, \ldots. \tag{21}$$

The decomposition (20) has also the following consequences:

Corollary 1: If $p \in \mathcal{H}_{m,m'}$, then p cannot be represented as $p = Q^k p'$, $k \neq 0$, with some polynomial p'.

Corollary 2: The space $\mathcal{A}_{m,m'}$ decomposes into the direct sum

$$\mathcal{A}_{m,m'} = \bigoplus_{j=0}^{\min(m,m')} Q^j \mathcal{H}_{m-j,m'-j}. \tag{22}$$

Corollary 3: For dimension of the space of q-harmonic polynomials $\mathcal{H}_{m,m'}$ we have the formula

$$\dim\ \mathcal{H}_{m,m'} = \frac{(m+n-2)!(m'+n-2)!(m+m'+n-1)}{(n-1)!(n-2)!m!m'!}.$$

Corollary 4: The space of q-harmonic polynomials $\mathcal{H}$ can be represented in the form of a direct sum

$$\mathcal{H} = \bigoplus_{m=0}^{\infty} \bigoplus_{m'=0}^{\infty} \mathcal{H}_{m,m'}.$$

Corollary 1 is a direct consequence of formula (20). Corollary 2 easily follows from repeated application of (20). Corollary 3 is proved in the same way as in the classical case (see, for example, Ref. 1, Chap. 10). For this we note that

$$\dim\ \mathcal{A}_{m,m'} = \frac{(n+m-1)!(n+m'-1)!}{(n-1)!^2 m!m'!}.$$

Hence, for $\dim \mathcal{H}_{m,m'} = \dim \mathcal{A}_{m,m'} - \dim \mathcal{A}_{m-1,m'-1}$ we obtain the expression stated in the corollary. In order to prove Corollary 4 we note that

$$\mathcal{A} = \bigoplus_{m \geqslant 0} \bigoplus_{m' \geqslant 0} \bigoplus_{j=0}^{p} Q^j \mathcal{H}_{m-j,m'-j} = \bigoplus_{m \geqslant 0} \bigoplus_{m' \geqslant 0} \left(\mathcal{H}_{m,m'} \oplus \left(\bigoplus_{j=1}^{p} Q^j \mathcal{H}_{m-j,m'-j} \right) \right),$$

where $p = \min(m,m')$. Now Corollary 4 follows from here and Corollary 1.

Theorem 1: *The linear space isomorphism* $\mathcal{A}\simeq\mathbb{C}[Q]\otimes\mathcal{H}$ *is true, where* $\mathbb{C}[Q]$ *is the space of all polynomials in* Q.

This theorem follows from Corollary 2.

The decomposition $\mathcal{A}\simeq\mathbb{C}[Q]\otimes\mathcal{H}$ is a q-analog of the theorem on separation of variables for Lie groups in an abstract form.[12] It follows from this decomposition that

$$\mathcal{A}\simeq\mathbb{C}[Q]\otimes\mathcal{H}\simeq\mathbb{C}[Q]\otimes\bigoplus_{m\geqslant 0}\bigoplus_{m'\geqslant 0}\mathcal{H}_{m,m'}=\bigoplus_{m\geqslant 0}\bigoplus_{m'\geqslant 0}(\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'}). \tag{23}$$

Since the subspaces $\mathcal{A}_{m,m'}$ are invariant with respect to the action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$, it follows from Proposition 2 for Δ_q that the subspace $\mathcal{H}_{m,m'}$ is invariant with respect to the representation $L_{m,m'}$ of $\mathrm{U}_q(\mathrm{gl}_n)$. We denote the restriction of this representation to $\mathcal{H}_{m,m'}$ by $T_{m,m'}$. It follows from Proposition 2 for Q and from (22) that

$$L_{m,m'}=\bigoplus_{j=0}^{\min(m,m')}T_{m-j,m'-j}. \tag{24}$$

Proposition 4: The representations $T_{m-j,m'-j}$ of $\mathrm{U}_q(\mathrm{gl}_n)$ *in (24) are irreducible with highest weights* $(m-j,0,\ldots,0,-m'+j)$, *respectively.*

Proof: Let us show that the representation $L_{m,0}=T_{m,0}$ in the space of holomorphic polynomials $\mathcal{A}_{m,0}$ is irreducible with highest weight $(m,0,\ldots,0)$. In fact, a direct calculation shows that the monomials $z_1^{m_1}\cdots z_n^{m_n}$, $m_1+\cdots+m_n=m$, are weight vectors of this representation. The highest weight vector coincides with z_1^m. Therefore, the irreducible representation with highest weight $(m,0,\ldots,0)$ is a subrepresentation of $L_{m,0}=T_{m,0}$. Since their dimensions coincide, $L_{m,0}=T_{m,0}$ is an irreducible representation with highest weight $(m,0,\ldots,0)$. It can be proved in the same way that the representation $L_{0,m'}=T_{0,m'}$ in the space of polynomials $\mathcal{A}_{0,m'}$ is irreducible with highest weight $(0,\ldots,0,-m')$.

Now we can prove the proposition by the induction. Assume that the proposition is true for the representations $T_{m-1-j,m'-1-j}$ which are contained in the decomposition

$$L_{m-1,m'-1}=\bigoplus_{j=0}^{\min(m-1,m'-1)}T_{m-1-j,m'-1-j}. \tag{25}$$

Note that since $\mathcal{A}_{m,m'}=\mathcal{H}_{m,m'}\oplus Q\mathcal{A}_{m-1,m'-1}$, then $L_{m-1,m'-1}$ is a subrepresentation in $L_{m,m'}$ and

$$\dim\mathcal{A}_{m-1,m'-1}=\dim L_{m-1,m'-1}=\sum_{j=0}^{\min(m-1,m'-1)}\dim T_{m-1-j,m'-1-j}.$$

The space $\mathcal{A}_{m,m'}$ contains the highest weight vector $z_1^m w_n^{m'}$ which is of the weight $(m,0,\ldots,0,-m')$. Therefore, $L_{m,m'}$ contains an irreducible representation $\hat{T}_{m,m'}$ of $\mathrm{U}_q(\mathrm{gl}_n)$ with highest weight $(m,0,\ldots,0,-m')$. This irreducible representation is absent in the decomposition (25). Hence, $\hat{T}_{m,m'}$ is a subrepresentation in $T_{m,m'}$. By the formula for dimensions of irreducible representations of $\mathrm{U}_q(\mathrm{gl}_n)$ and by Corollary 3 we have $\dim\hat{T}_{m,m'}=\dim\mathcal{H}_{m,m'}$. Therefore, $\hat{T}_{m,m'}$ is equivalent to $T_{m,m'}$. Proposition is proved.

Thus, we proved that the action of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$ on the space $\mathcal{A}$ realizes the irreducible representations $T_{m,m'}$ on the subspaces $\mathcal{H}_{m,m'}$ of homogeneous q-harmonic polynomials, respectively.

We denote by $\mathcal{A}^{U_q(\mathrm{gl}_n)}$ the space of elements of $\mathcal{A}$ consisting of invariant elements with respect to the action of $\mathrm{U}_q(\mathrm{gl}_n)$.

Proposition 5: We have $\mathcal{A}^{U_q(\mathrm{gl}_n)}=\mathbb{C}[Q]$ *and*

$$\mathcal{A}^{U_q(\mathrm{gl}_{n-1})} \simeq \bigoplus_{k,l} \mathbb{C}[Q_{n-1}] z_n^k w_n^l \simeq \bigoplus_{k,l} \mathbb{C}[Q] z_n^k w_n^l .$$

Proof: The formula (23) leads to the decomposition of the representation L on $\mathcal{A}$ into irreducible subrepresentations of $\mathrm{U}_q(\mathrm{gl}_n)$ (the representation multiple to the irreducible representation $T_{m,m'}$ is realized on $\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'}$). Since the trivial representation of $\mathrm{U}_q(\mathrm{gl}_n)$ is realized only on $\mathcal{H}_{0,0}$, then $\mathcal{A}^{U_q(\mathrm{gl}_n)}$ coincides with $\mathbb{C}[Q]\otimes\mathcal{H}_{0,0} \equiv \mathbb{C}[Q]\otimes\mathbb{C} \simeq \mathbb{C}[Q]$.

In order to prove the second equality we note that for $\mathrm{U}_q(\mathrm{gl}_{n-1})$-module $\mathcal{A}$ we have

$$\mathcal{A} = \mathbb{C}_q[z_1, w_1, \ldots, z_n, w_n] = \bigoplus_{k,l} \mathbb{C}_q[z_1, w_1, \ldots, z_{n-1}, w_{n-1}] z_n^k w_n^l .$$

The action of the subalgebra $\mathrm{U}_q(\mathrm{gl}_{n-1})$ on monomials $z_n^k w_n^l$ is trivial. Moreover, $\mathbb{C}[z_1, w_1, \ldots, z_{n-1}, w_{n-1}]^{U_q(\mathrm{gl}_{n-1})} = \mathbb{C}[Q_{n-1}]$, where $Q_{n-1} = z_1 w_1 + \cdots + z_{n-1} w_{n-1}$. Since $Q = Q_{n-1} + z_n w_n$, we have $\mathcal{A}^{U_q(\mathrm{gl}_{n-1})} \simeq \oplus_{k,l} \mathbb{C}[Q_{n-1}] z_n^k w_n^l \simeq \oplus_{k,l} \mathbb{C}[Q] z_n^k w_n^l$. Proposition is proved.

VI. THE DUAL PAIR $(\mathrm{U}_q(\mathrm{sl}_2), \mathrm{U}_q(\mathrm{gl}_n))$

The formulas

$$ke = q^2 ek, \qquad kf = q^{-2} fk, \qquad ef - fe = \frac{k - k^{-1}}{q - q^{-1}} \tag{26}$$

determine the quantum algebra $\mathrm{U}_q(\mathrm{sl}_2)$ generated by the elements k, k^{-1}, e, f. Let $\mathcal{L}(\mathcal{A})$ be the space of linear operators on the algebra $\mathcal{A}$. It is directly verified by means of formula (18) that the operators

$$\omega(k) = q^n \gamma\overline{\gamma}, \qquad \omega(e) = q^{-n+1}\hat{Q}, \qquad \omega(f) = -\Delta_q \tag{27}$$

satisfy relations (26). This means that the algebra homomorphism $\omega: \mathrm{U}_q(\mathrm{sl}_2) \to \mathcal{L}(\mathcal{A})$ uniquely determined by formulas (27) is a representation of $\mathrm{U}_q(\mathrm{sl}_2)$.

Since the operators $\omega(k)$, $\omega(e)$, $\omega(f')$ commute with the operators $L(X)$, $X \in \mathrm{U}_q(\mathrm{gl}_n)$ we can introduce the representation $\omega \times L$ of the algebra $\mathrm{U}_q(\mathrm{sl}_2) \times \mathrm{U}_q(\mathrm{gl}_n)$ on $\mathcal{A}$, where L is the above defined natural action of $\mathrm{U}_q(\mathrm{gl}_n)$ on $\mathcal{A}$. This representation is reducible. Let us decompose it into irreducible constituents.

By (23), we have $\mathcal{A} = \oplus_{m,m' \geqslant 0} (\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'})$. The subspaces $\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'}$ are invariant under $\mathrm{U}_q(\mathrm{sl}_2) \times \mathrm{U}_q(\mathrm{gl}_n)$, since the space $\mathbb{C}[Q]$ is elementwise invariant under $\mathrm{U}_q(\mathrm{gl}_n)$, and for $f \in \mathbb{C}[Q]$ and $h_{m,m'} \in \mathcal{H}_{m,m'}$ we have

$$\hat{Q}(f(Q)\otimes h_{m,m'}) = Qf(Q)\otimes h_{m,m'}, \tag{28}$$

$$\Delta_q(Q^r \otimes h_{m,m'}) = q^{n-1}[r][r+m+m'+n-1] Q^{r-1} \otimes h_{m,m'}, \tag{29}$$

$$\gamma\overline{\gamma}(Q^r \otimes h_{m,m'}) = q^{2r+m+m'}(Q^r \otimes h_{m,m'}). \tag{30}$$

These formulas show that $\mathrm{U}_q(\mathrm{sl}_2)$ acts on $\mathbb{C}[Q]$ and $\mathrm{U}_q(\mathrm{gl}_n)$ acts on $\mathcal{H}_{m,m'}$. However, this action of $\mathrm{U}_q(\mathrm{sl}_2)$ depends on the component $\mathcal{H}_{m,m'}$. Taking the basis

$$|r\rangle := q^{-r(n-1)}[r+m+m'+n-1]!^{-1} Q^r, \quad r = 0, 1, 2, \ldots,$$

in the space $\mathbb{C}[Q]$, we find from (28)–(30) that

$$\omega(k)|r\rangle = q^{2r+m+m'+n}|r\rangle, \qquad \omega(f)|r\rangle = -[r]|r-1\rangle,$$

$$\omega(e)|r\rangle = [r+m+m'+n]|r+1\rangle.$$

Comparing this representation with the known irreducible representations of $U_q(sl_2)$ (see, for example, Ref. 13) we derive that the irreducible representation of $U_q(sl_2)$ of the discrete series with lowest weight $m+m'+n$ is realized on the component $\mathbb{C}[Q]$ of the space $\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'}$. We denote this representation of $U_q(sl_2)$ by $D_{m+m'+n}$.

Thus, we have derived that on the subspace $\mathbb{C}[Q]\otimes\mathcal{H}_{m,m'}\subset\mathcal{A}$ the irreducible representation $D_{m+m'+n}\times T_{m,m'}$ of the algebra $U_q(sl_2)\times U_q(gl_n)$ acts. This means that for the reducible representation $\omega\otimes L$ we have the following decomposition into irreducible components:

$$\omega\times L=\bigoplus_{m,m'=0}^{\infty} D_{m+m'+n}\times T_{m,m'},$$

that is, each irreducible representation of $U_q(gl_n)$ in this decomposition determines uniquely the corresponding irreducible representation of $U_q(sl_2)$ and vise versa. This means that $U_q(sl_2)$ and $U_q(gl_n)$ constitute a *dual pair* under the action on $\mathcal{A}$.

VII. RESTRICTION OF *q*-HARMONIC POLYNOMIALS ONTO THE QUANTUM SPHERE

The associative algebra $\mathcal{F}(S^{\mathbb{C}}_{q,n-1})$ generated by the elements $z_1,\ldots,z_n,\ w_1,\ldots,\ w_n$ satisfying the relations (1)–(3) and the relation

$$z_1w_1+z_1w_1+\cdots+z_nw_n=1$$

is called *the algebra of functions on the quantum sphere* $S^{\mathbb{C}}_{q,n-1}$ (see Ref. 6, Chap. 11, and Ref. 7). It is clear that the following canonical algebra isomorphism has place:

$$\mathcal{F}(S^{\mathbb{C}}_{q,n-1})\simeq\mathcal{A}/\mathcal{I},$$

where $\mathcal{I}$ is the two-sided ideal of $\mathcal{A}$ generated by the element $Q-1\equiv\Sigma_i z_iw_i-1$. We denote by τ the canonical algebra homomorphism

$$\tau:\mathcal{A}\to\mathcal{A}/\mathcal{I}\simeq\mathcal{F}(S^{\mathbb{C}}_{q,n-1}).$$

This homomorphism is called the *restriction* of polynomials of $\mathcal{A}$ onto the quantum sphere $S^{\mathbb{C}}_{q,n-1}$.

Proposition 6: We have $\tau\mathcal{H}\simeq\mathcal{F}(S^{\mathbb{C}}_{q,n-1})$. *This means that* $\tau:\mathcal{H}\to\mathcal{F}(S^{\mathbb{C}}_{q,n-1})$ *is a one-to-one mapping, that is, the restriction of a q-harmonic polynomial to the sphere* $S^{\mathbb{C}}_{q,n-1}$ *determines this polynomial uniquely.*

Proof: By Theorem 1, we have $\mathcal{F}(S^{\mathbb{C}}_{q,n-1})=\tau\mathcal{A}=\tau(\mathbb{C}[Q]\otimes\mathcal{H})=\tau\mathcal{H}$. Since Q is invariant with respect to the action of the algebra $U_q(gl_n)$, then the ideal $\mathcal{I}$ is an invariant subspace under the action of $U_q(gl_n)$ on $\mathcal{A}$. Therefore, an action of $U_q(gl_n)$ on $\mathcal{A}/\mathcal{I}$ is defined. This action coincides with the action in Ref. 9. The homomorphism τ intertwines the action of $U_q(gl_n)$ on $\mathcal{A}$ and on $\mathcal{A}/\mathcal{I}$. Since $\tau\mathcal{H}_{m,m'}\neq\{0\}$, then the action of $U_q(gl_n)$ realizes the same irreducible representation on $\mathcal{H}_{m,m'}$ and on $\tau\mathcal{H}_{m,m'}$. This means that $\dim\mathcal{H}_{m,m'}=\dim\tau\mathcal{H}_{m,m'}$, that is, the mapping τ is one-to-one on $\mathcal{H}_{m,m'}$. Therefore, it is one-to-one on $\mathcal{H}$. Proposition is proved.

Proposition 6 allows us to determine a scalar product on $\mathcal{H}$. For this, we use the invariant functional h on the quantum sphere defined in Ref. 9, Sec. 4.2. This functional h is determined by introducing a linear gradation in $\tau\mathcal{A}$: $\tau\mathcal{A}=\Sigma_{\lambda\in\mathbb{Z}^n}(\tau\mathcal{A})^\lambda$, where $(\tau\mathcal{A})^\lambda=\{p\in\tau\mathcal{A}|p(\mathbf{tz},\mathbf{t}^{-1}\mathbf{w})=\mathbf{t}^\lambda p(\mathbf{z},\mathbf{w})\}$, $\mathbf{t}=(t_1,t_2,\ldots,t_n)$ are n indeterminates, and

$$\mathbf{tz}=(t_1z_1,\ldots,t_nz_n),\qquad \mathbf{t}^{-1}\mathbf{w}=(t_1^{-1}w_1,\ldots,t_n^{-1}w_n),\ [\backslash]n\quad \mathbf{t}^\lambda=t_1^{\lambda_1}\ldots t_n^{\lambda_n}.$$

The subalgebra $(\tau\mathcal{A})^0$ is spanned by the monomials $z_1^{\mu_1}\cdots z_n^{\mu_n}w_n^{\mu_n}\cdots w_1^{\mu_1}$ (or by the monomials $w_1^{\mu_1}\cdots w_n^{\mu_n}z_n^{\mu_n}\cdots z_1^{\mu_1}$), $\mu_i=0,1,2,\ldots$. The functional h is defined as a linear mapping $h:\tau\mathcal{A}\to\mathbb{C}$ such that $h(p)=0$ if $p\in((\tau\mathcal{A})^\lambda,\ \lambda\neq0$, and

$$h(w_1^{\mu_1}\cdots w_n^{\mu_n}z_n^{\mu_n}\cdots z_1^{\mu_1})=\frac{(q^2;\,q^2)_{\mu_1}\cdots(q^2;\,q^2)_{\mu_n}(q^2;\,q^2)_{n-1}}{(q^2;\,q^2)_{\mu_1+\cdots+\mu_n+n-1}}.$$

The following assertions are proved in Ref. 9:

(a) The subalgebra $(\tau\mathcal{A})^0$ is a commutative algebra generated by the elements Q_{n-1}, $Q_{n-2},\ldots,Q_1$.

(b) The algebra $(\tau\mathcal{A})^0$ is isomorphic to the polynomial algebra in $n-1$ commuting indeterminates.

(c) For any polynomial $p(\mathbf{z},\mathbf{w})=f(Q_1,\ldots,\,Q_{n-1})\in(\tau\mathcal{A})^0$ the value $h(p)$ is expressed in term of Jackson integral:

$$h(p)=\frac{(q^2;q^2)_{n-1}}{(1-q^2)^{n-1}}\int_0^1\int_0^{Q_{n-1}}\cdots\int_0^{Q_2}f(Q_1,\ldots,\,Q_{n-1})d_{q^2}Q_1\cdots d_{q^2}Q_{n-1}$$

(the definition of Jackson integral; see, for example, in Ref. 14, Chap. 1).

(d) Now we can introduce a scalar product $\langle\cdot,\cdot\rangle$ on $\mathcal{H}$:

$$\langle p_1,\,p_2\rangle=h((\tau p_1)(\tau p_2)^*),\tag{31}$$

where a^* determines an element conjugate to $a\in\mathcal{A}$ under action of the $*$-operation.

Proposition 7: We have $\mathcal{H}_{m,m'}\perp\mathcal{H}_{r,r'}$ *if* $(m,\,m')\neq(r,\,r')$.

Proof follows from the fact that $(\tau p_1)(\tau p_2)^*\notin(\tau\mathcal{A})^0$ if $p_1\in\mathcal{H}_{m,m'}$, $p_2\in\mathcal{H}_{r,r'}$, and $(m,\,m')\neq(r,\,r')$.

VIII. THE PROJECTION $\mathcal{A}_{m,m'}\to\mathcal{H}_{m,m'}$

Let us go back to the decomposition (20) and construct the projector

$$\mathsf{H}_{m,m'}:\mathcal{A}_{m,m'}=\mathcal{H}_{m,m'}\oplus Q\mathcal{A}_{m-1,m'-1}\to\mathcal{H}_{m,m'}.$$

We present this projector in the form

$$\mathsf{H}_{m,m'}p=\sum_{k=0}^{\min(m,m')}\alpha_k\hat{Q}^k\Delta_q^k p,\quad \alpha_k\in\mathbb{C},\qquad p\in\mathcal{A}_{m,m'}.\tag{32}$$

We have to calculate values of the coefficients α_k. In order to do this, we act by the operator Δ_q upon both parts of (32) and use the relation (18). Under this action, the left hand side vanishes. Equating the right hand side to 0, we derive a recurrence relation

$$q^{n-1}[k][m+m'+n-k-1]\alpha_k+\alpha_{k-1}=0$$

for α_k which gives

$$\alpha_k=(-1)^k q^{-(n-1)k}\frac{[m+m'+n-k-2]!}{[k]![m+m'+n-2]!},\tag{33}$$

where $[s]!=[s][s-1][s-2]\cdots[1]$ for $s\neq0$ and $[0]!=1$.

Note that the coefficients α_k are determined by the recurrence relation uniquely up to a constant. In (33) we have chosen this constant in such a way that $\mathsf{H}_{m,m'}p=p$ for $p\in\mathcal{H}_{m,m'}$. This means that $\mathsf{H}_{m,m'}^2=\mathsf{H}_{m,m'}$.

Proposition 8: The operator $\mathsf{H}_{m,m'}$ *commutes with the action of* $\mathrm{U}_q(\mathrm{gl}_n)$, *that is, with the operators of the representation* $L_{m,m'}$ *of* $\mathrm{U}_q(\mathrm{gl}_n)$.

Proof: This assertion follows from the fact that the operators $L_{m,m'}(X)$, $X\in\mathrm{U}_q(\mathrm{gl}_n)$, commute with $\hat{Q}$ and Δ_q (see Proposition 2). Proposition is proved.

A polynomial φ of the space $\mathcal{H}_{m,m'}$ is called *zonal* if it is invariant with respect to operators $L_{m,m'}(X)$, $X \in \mathrm{U}_q(\mathrm{gl}_{n-1})$. We shall show below that zonal polynomials can be expressed in terms of the basic hypergeometric function ${}_2\varphi_1$ which is defined by the formula

$$ {}_2\varphi_1(a,\ b;\ c;\ q,\ x) = \sum_{k=0}^{\infty} \frac{(a;\ q)_k (b;\ q)_k}{(c;\ q)_k (q;\ q)_k} x^k $$

(see Refs. 14 and 15 for properties of this function).

Proposition 9: (a) The subspace of zonal polynomials in $\mathcal{H}_{m,m'}$ is one-dimensional. (b) Up to a constant, a zonal polynomial of $\mathcal{H}_{m,m'}$ is given by the formula

$$ \varphi'_{m,m'} = z_n^{m-m'} Q^{m'} \sum_{s=0}^{m'} \frac{(q^{-2m'};q^2)_s (q^{2(m+n-1)};q^2)_s}{(q^{2(n-1)};q^2)_s (q^2;q^2)_s} \frac{Q_{n-1}^s}{Q^s} q^{2s} \tag{34} $$

if $m \geqslant m'$, and by the formula

$$ \varphi'_{m,m'} = Q^m \sum_{s=0}^{m} \frac{(q^{-2m};q^2)_s (q^{2(m'+n-1)};q^2)_s}{(q^{2(n-1)};q^2)_s (q^2;q^2)_s} \frac{Q_{n-1}^s}{Q^s} q^{2s} w_n^{m'-m} \tag{35} $$

if $m \leqslant m'$.

Proof: (a) As we have seen, the irreducible representation $T_{m,m'}$ of $\mathrm{U}_q(\mathrm{gl}_n)$ with highest weight $(m, 0, \ldots, 0, -m')$ is realized on $\mathcal{H}_{m,m'}$. It is known that this representation, under restriction to $\mathrm{U}_q(\mathrm{gl}_{n-1})$, contains trivial (one-dimensional) representation of this subalgebra with multiplicity 1. This proves the first assertion.

(b) We construct a zonal polynomial of $\mathcal{H}_{m,m'}$ by using the projection operator $\mathsf{H}_{m,m'}$. In order to do this, we have to take a polynomial $p \in \mathcal{A}_{m,m'}$ invariant with respect to $\mathrm{U}_q(\mathrm{gl}_{n-1})$ and to act upon it by the operator $\mathsf{H}_{m,m'}$. Since the projector $\mathsf{H}_{m,m'}$ commutes with the action of $\mathrm{U}_q(\mathrm{gl}_{n-1})$, a polynomial obtained in this way is a zonal polynomial. Clearly, the polynomial $p = z_n^m w_n^{m'}$ belongs to $\mathcal{A}_{m,m'}$ and is invariant under the action of $\mathrm{U}_q(\mathrm{gl}_{n-1})$. In order to find an expression for $\mathsf{H}_{mm'}(z_n^m w_n^{m'})$ we first assume that $m \geqslant m'$.

Using the second expression for Δ_q in (17) and relation $\overline{\partial}_n \hat{z}_n = \hat{z}_n \overline{\partial}_n$ we have

$$ \varphi_{m,m'} := \mathsf{H}_{m,m'}(z_n^m w_n^{m'}) = \sum_{s=0}^{m'} \alpha_s \hat{Q}^s \Delta_q^s z_n^m w_n^{m'} $$

$$ = z_n^{m-m'} \sum_{s=0}^{m'} \alpha_s q^{2(n-1)s} \hat{Q}^s \frac{[m]!}{[m-s]!} \frac{[m']!}{[m'-s]!} z_n^{m'-s} w_n^{m'-s}. $$

Taking into account the expression for the coefficients α_s and using the formulas

$$ [s]! = \frac{(q^2;q^2)_s (-1)^s}{(q-q^{-1})^s} q^{-s(s+1)/2}, \qquad \frac{[m]!}{[m-s]!} = \frac{(q^{-2m};q^2)_s}{(q-q^{-1})^s} q^{ms-s(s-1)/2}, $$

we obtain

$$ \varphi_{m,m'} = z_n^{m-m'} \sum_{s=0}^{m'} q^{2s} \frac{(q^{-2m};q^2)_s (q^{-2m'};q^2)_s}{(q^2;q^2)_s (q^{-2(m+m'+n-2)};q^2)_s} Q^s z_n^{m'-s} w_n^{m'-s}. \tag{36} $$

Using the first relation in (16) we obtain from (36) that

$$\varphi_{m,m'}=Q^{m'}z_n^{m-m'}\sum_{s=0}^{m'} q^{2s}\frac{(q^{-2m};q^2)_s(q^{-2m'};q^2)_s}{(q^2;q^2)_s(q^{-2(m+m'+n-2)};q^2)_s}(Q_{n-1}/Q;q^{-2})_{m'-s}.$$

Since [see relation (II.4) from Appendix II in Ref. 14]

$$(Q_{n-1}/Q;q^{-2})_{m'-s}=\sum_{\nu=0}^{m'-s} q^{2\nu}\frac{(q^{-2(m'-s)};q^2)_\nu}{(q^2;q^2)_\nu}Q_{n-1}^\nu/Q^\nu,$$

we have

$$\begin{aligned}\varphi_{m,m'}&=Q^{m'}z_n^{m-m'}\sum_{s=0}^{m'}\frac{q^{2s}(q^{-2m};\,q^2)_s(q^{-2m'};\,q^2)_s}{(q^2;\,q^2)_s(q^{-2(m+m'+n-2)};\,q^2)_s}\sum_{\nu=0}^{m'-s} q^{2\nu}\frac{(q^{-2(m'-s)};\,q^2)_\nu}{(q^2;\,q^2)_\nu}\frac{Q_{n-1}^\nu}{Q^\nu}\\&=Q^{m'}z_n^{m-m'}\sum_{\nu=0}^{m'}\frac{Q_{n-1}^\nu}{Q^\nu}q^{2\nu}\sum_{s=0}^{m'-\nu}\frac{(q^{-2(m'-s)};\,q^2)_\nu}{(q^2;\,q^2)_\nu}\frac{q^{2s}(q^{-2m};\,q^2)_s(q^{-2m'};\,q^2)_s}{(q^2;\,q^2)_s(q^{-2(m+m'+n-2)};\,q^2)_s}.\end{aligned}\tag{37}$$

Applying relation (I.7) and then relation (I.13) from Appendix I in Ref. 14 we find

$$(q^{-2(m'-s)};\,q^2)_\nu=(-1)^\nu q^{-2m'\nu}q^{\nu(\nu-1)}\frac{(q^{2m'-2\nu+2};\,q^2)_\nu(q^{-2m'+2\nu};\,q^2)_s}{(q^{-2m'};\,q^2)_s}.$$

Therefore, for the sum over s in (37) (which will be denoted by I_ν) we obtain the expression

$$I_\nu=(-1)^\nu q^{-2m'\nu}q^{\nu(\nu-1)}\frac{(q^{2m'-2\nu+2};\,q^2)_\nu}{(q^2;\,q^2)_\nu}\sum_{s=0}^{m'-\nu}\frac{(q^{-2m'+2\nu};\,q^2)_s(q^{-2m};\,q^2)_s q^{2s}}{(q^2;\,q^2)_s(q^{-2(m+m'+n-2)};\,q^2)_s}.$$

The sum over s here is the basic hypergeometric function

$${}_2\varphi_1(q^{-2m},\ q^{-2m'+2\nu};\ q^{-2(m+m'+n-2)};\,q^2,\ q^2)=\frac{q^{-2mm'+2m\nu}(q^{-2m'-2n+4};\,q^2)_{m'-\nu}}{(q^{-2(m+m'+n-2)};\,q^2)_{m'-\nu}},$$

where we used formula (II.6) from Appendix II in Ref. 14.

Therefore, for the function $\varphi_{m,m'}$ we have the expression

$$\begin{aligned}\varphi_{m,m'}=Q^{m'}z_n^{m-m'}\sum_{\nu=0}^{m'}\frac{Q_{n-1}^\nu}{Q^\nu}q^{2\nu}(-1)^\nu q^{-2m'\nu}q^{\nu(\nu-1)}q^{-2mm'+2m\nu}\\\times\frac{(q^{2m'-2\nu+2};\,q^2)_\nu}{(q^2;\,q^2)_\nu}\frac{(q^{-2m'-2n+4};\,q^2)_{m'-\nu}}{(q^{-2(m+m'+n-2)};\,q^2)_{m'-\nu}}.\end{aligned}$$

By formula (I.8) of Appendix I in Ref. 14 we have

$$(q^{2m'-2\nu+2};\,q^2)_\nu=(q^{-2m'};\,q^2)_\nu(-1)^\nu q^{2m'\nu}q^{-\nu(\nu-1)}$$

and by formula (I.11) from Appendix I in Ref. 14 we obtain

$$\frac{(q^{-2m'-2n+4};\,q^2)_{m'-\nu}}{(q^{-2(m+m'+n-2)};\,q^2)_{m'-\nu}}=q^{-2m\nu}\frac{(q^{-2m'-2n+4};\,q^2)_{m'}}{(q^{-2(m+m'+n-2)};\,q^2)_{m'}}\frac{(q^{2(m+n-1)};\,q^2)_\nu}{(q^{2n-2};\,q^2)_\nu}.$$

For this reason, we have

$$\mathsf{H}_{mm'}(z_n^m w_n^{m'}) = \varphi_{m,m'} = q^{-2mm'} \frac{(q^{-2m'-2n+4};\, q^2)_{m'}}{(q^{-2(m+m'+n-2)};q^2)_{m'}} Q^{m'} z_n^{m-m'}$$
$$\times \sum_{\nu=0}^{m'} \frac{(q^{-2m'};\, q^2)_\nu (q^{2(m+n-1)};\, q^2)_\nu}{(q^2;q^2)_\nu (q^{2(n-1)};q^2)_\nu} \frac{Q_{n-1}^\nu}{Q^\nu} q^{2\nu}$$
$$= \frac{(q^{2(n-1)};\, q^2)_{m'}}{(q^{2(m+n-1)};\, q^2)_{m'}} Q^{m'} z_n^{m-m'}\, {}_2\varphi_1(q^{-2m'},\, q^{2(m+n-1)};$$
$$\times q^{2(n-1)};\, q^2,\, q^2 Q_{n-1}/Q).$$

This proves the second assertion of the proposition for the case $m \geqslant m'$. The case $m < m'$ is proved in the same way. Proposition is proved.

The formula

$$P_k^{(\alpha,\beta)}(x;\ q) = {}_2\varphi_1(q^{-k},\ q^{\alpha+\beta+k+1};\ q^{\alpha+1};\ q,\ qx)$$

defines the so-called little q-Jacobi polynomials. The zonal polynomials from Proposition 9 can be written in term of these polynomials as

$$\varphi'_{m,m'} = Q^{m'} z_n^{m-m'} P_{m'}^{(n-2,m-m')}(Q_{n-1}/Q;\ q^2)$$

if $m \geqslant m'$ and as

$$\varphi'_{m,m'} = Q^m P_m^{(n-2,m'-m)}(Q_{n-1}/Q;\ q^2) w_n^{m'-m}$$

if $m \leqslant m'$. Restricting these polynomials onto the quantum sphere $S^{\mathbb{C}}_{q,n-1}$ we obtain

$$\tau\varphi'_{m,m'} = z_n^{m-m'} P_{m'}^{(n-2,m-m')}(Q_{n-1};q^2)$$

if $m \geqslant m'$ and

$$\tau\varphi'_{m,m'} = P_m^{(n-2,m'-m)}(Q_{n-1};\ q^2) w_n^{m'-m}$$

if $m \leqslant m'$. These polynomials are called *zonal spherical functions* on the quantum sphere $S^{\mathbb{C}}_{q,n-1}$ and were calculated in Ref. 9 (see also Refs. 3 and 4).

IX. q-ANALOG OF ASSOCIATED SPHERICAL HARMONICS WITH RESPECT TO $\mathsf{U}_q(\mathsf{gl}_{n-1})$

It is known (see Ref. 1, Chap. 11) that in the space of classical homogeneous harmonic polynomials on the unitary (complex Euclidean) space $E^{\mathbb{C}}_n$ there exist different orthonormal bases. They correspond to different separations of variables. Each separation of variables corresponds to a certain chain of subgroups of the unitary group $U(n)$. A similar picture has place for the spaces $\mathcal{H}_{m,m'}$ of homogeneous q-harmonic polynomials. We consider in this section a q-analog of separation of variables corresponding to spherical coordinates on the sphere $S^{\mathbb{C}}_{n-1}$ (see Ref. 1, Chap. 11).

In the classical case, the tree method distinguishes different separations of variables. Different separations of variables are in a one-to-one correspondence with different chains of subgroups of $\mathrm{U}(n)$. The same tree method can be used for q-harmonic polynomials, but instead of chains of subgroups of $\mathrm{U}(n)$ we have to take the corresponding chains of subalgebras of the algebra $\mathrm{U}_q(\mathrm{gl}_n)$. A certain orthogonal basis corresponds to such a chain of subalgebras.

The aim of this section is to construct an orthogonal basis of the space $\mathcal{H}_{m,m'}$ of homogeneous q-harmonic polynomials which corresponds to the chain

$$\mathrm{U}_q(\mathrm{gl}_n)\supset \mathrm{U}_q(\mathrm{gl}_{n-1})\supset\cdots\supset \mathrm{U}_q(\mathrm{gl}_3)\supset \mathrm{U}_q(\mathrm{gl}_2)\supset \mathrm{U}_q(\mathrm{gl}_1). \tag{38}$$

This basis is a q-analog of the set of associated spherical harmonics on the complex vector space which are products of certain Jacobi polynomials (see Ref. 1, Chap. 11). The basis elements give solutions of the equation $\Delta_q p=0$ in "separated coordinates." So, we obtain a q-analog of the classical separation of variables.

Lemma 1: Let $f_{k'}(\mathbf{z}')$ and $g_{l'}(\mathbf{w}')$ be homogeneous polynomials of degrees k' in $\mathbf{z}'\equiv(z_1, z_1,\ldots, z_{n-1})$ and of degrees l' in $\mathbf{w}'\equiv(w_1, w_1,\ldots, w_{n-1})$, respectively. Then for any non-negative integers k and l we have

$$\Delta_q(z_n^k w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'))=q^{l-k}z_n^k w_n^l\Delta_{n-1}(f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'))+q^{2(n-1)}q^{l'+k'}[k]\times[l]z_n^{k-1}w_n^{l-1}f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'),$$

where $\Delta_{n-1}=\Sigma_{i=1}^{n-1}q^{2i-2}\overline{\partial}_i\partial_i$ is the q-Laplace operator for the elements $\mathbf{z}'\equiv(z_1,\ldots, z_{n-1})$ and $\mathbf{w}'\equiv(w_1,\ldots,w_{n-1})$.

Proof: Using the relations for the operators from Sec. III we derive

$$\begin{aligned}
\overline{\partial}_n\partial_n z_n^k w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')&=q^{(l-k)k'}\overline{\partial}_n\partial_n f_{k'}(\mathbf{z}')z_n^k w_n^l g_{l'}(\mathbf{w}')\\
&=q^{(l-k)k'}[k]\overline{\partial}_n f_{k'}(\mathbf{z}')z_n^{k-1}w_n^l g_{l'}(\mathbf{w}')\\
&=q^{(l-1)k'}[k]\overline{\partial}_n z_n^{k-1}f_{k'}(\mathbf{z}')w_n^l g_{l'}(\mathbf{w}')\\
&=q^{(l-1)k'}[k]z_n^{k-1}\overline{\partial}_n f_{k'}(\mathbf{z}')w_n^l g_{l'}(\mathbf{w}')\\
&=q^{-2k'+l(k'+l')}[k]z_n^{k-1}f_{k'}(\mathbf{z}')\overline{\partial}_n g_{l'}(\mathbf{w}')w_n^l\\
&=q^{-2k'+lk'+l'}[k][l]z_n^{k-1}f_{k'}(\mathbf{z}')w_n^{l-1}g_{l'}(\mathbf{w}')\\
&=q^{-k'+l'}[k][l]z_n^{k-1}w_n^{l-1}f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}').
\end{aligned}$$

Since $\partial_i\hat{w}_n=q\hat{w}_n\partial_i+(1-q^2)\hat{w}_i\partial_n$, $i<n$, and $\partial_n(w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'))=0$, we have

$$\overline{\partial}_i\partial_i z_n^k w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=\overline{\partial}_i z_n^k\partial_i w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=q^l\overline{\partial}_i z_n^k w_n^l\partial_i f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}').$$

Using recurrently the relation $\overline{\partial}_i\hat{z}_n=q^{-1}\hat{z}_n\overline{\partial}_i+(1-q^{-2})q^{2(n-i)}\hat{z}_i\overline{\partial}_n$, we obtain

$$\overline{\partial}_i\partial_i z_n^k w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=q^{l-k}z_n^k w_n^l\overline{\partial}_i\partial_i f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')+q^{2(n-i)}(1-q^{-2})q^{l'+1}[k]\times[l]z_n^{k-1}w_n^{l-1}\hat{z}_i\partial_i f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}').$$

Thus, one has

$$\Delta_{n-1}(z_n^k w_n^l f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'))=q^{l-k}z_n^k w_n^l\Delta_{n-1}f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')+q^{2n-3}(q^2-1)q^{l'}[k][l]\times[k']z_n^{k-1}w_n^{l-1}f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}'),$$

where the relation

$$\sum_{i=1}^{n-1}\hat{z}_i\partial_i f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=\sum_{i=1}^{n}\hat{z}_i\partial_i f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=\{\gamma\}f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')=[k']f_{k'}(\mathbf{z}')g_{l'}(\mathbf{w}')$$

has been used. From the above results and from the equality $\Delta_q = q^{2(n-1)}\overline{\partial}_n \partial_n + \Delta_{n-1}$, the lemma follows.

Proposition 10: Let s and s' be integers such that $0 \leqslant s \leqslant m$ and $0 \leqslant s' \leqslant m'$. Let $h_{s,s'}(\mathbf{z}', \mathbf{w}')$ be a homogeneous harmonic polynomial of degree s in $\mathbf{z}' = (z_1, z_2, \ldots, z_{n-1})$ and of degree s' in $\mathbf{w}' = (w_1, w_2, \ldots, w_{n-1})$. Then for $z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}') \in \mathcal{A}_{m,m'}$ we have

$$\mathsf{H}_{m,m'}(z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}')) = z_n^{m-s-m'+s'} Q^{m'-s'} d_{ss'}^{mm'} h_{s,s'}(\mathbf{z}', \mathbf{w}'), \tag{39}$$

where $m - s \geqslant m' - s'$,

$$d_{ss'}^{mm'} = q^{-2(m-s)(m'-s')} \frac{(q^{-2m'-2s-2n+4}; q^2)_{m'-s'}}{(q^{-2m-2m'-2n+4}; q^2)_{m'-s'}} \times {}_2\varphi_1(q^{-2(m'-s')}, q^{2(m+s'+n-1)}; q^{2(s+s'+n-1)};\ q^2,\ q^2 Q_{n-1}/Q),$$

and

$$\mathsf{H}_{m,m'}(z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}')) = Q^{m-s} d_{ss'}^{mm'} w_n^{m'-s'-m+s} h_{s,s'}(\mathbf{z}', \mathbf{w}'), \tag{40}$$

where $m - s \leqslant m' - s'$,

$$d_{ss'}^{mm'} = q^{-2(m-s)(m'-s')} \frac{(q^{-2m-2s'-2n+4}; q^2)_{m-s}}{(q^{-2m-2m'-2n+4}; q^2)_{m-s}} \times {}_2\varphi_1(q^{-2(m-s)}, q^{2(m'+s+n-1)}; q^{2(s+s'+n-1)};\ q^2,\ q^2 Q_{n-1}/Q).$$

Proof: The proof of this proposition is similar to that of Proposition 6 and we shall omit details. Taking into account formula (32) for the projector $\mathsf{H}_{m,m'}$ and Lemma 1, we obtain

$$\begin{aligned}\mathsf{H}_{m,m'}(z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}')) &= \sum_{k=0}^{\min(m,m')} \alpha_k Q^k \Delta_q^k z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}') \\ &= \sum_{k=0}^{b} \alpha_k Q^k q^{2(n-1)k} q^{(s+s')k} \frac{[m-s]![m'-s']!}{[m-s-k]![m'-s'-k]!} \\ &\quad \times z_n^{m-s-k} w_n^{m'-s'-k} h_{s,s'}(\mathbf{z}', \mathbf{w}'),\end{aligned}$$

where $b = \min(m-s, m'-s')$. Let $m - s \geqslant m' - s'$, then

$$\mathsf{H}_{m,m'}(z_n^{m-s} w_n^{m'-s'} h_{s,s'}(\mathbf{z}', \mathbf{w}')) = z_n^{m-s-m'+s'} Q^{m'-s'} d_{ss'}^{mm'} h_{s,s'}(\mathbf{z}', \mathbf{w}'),$$

where

$$d_{ss'}^{mm'} = \sum_{k=0}^{m'-s'} q^{2k} \frac{(q^{-2(m-s)};\, q^2)_k (q^{-2(m'-s')};\, q^2)_k}{(q^2;\, q^2)_k (q^{-2(m+m'+n-2)};\, q^2)_k} \sum_{\nu=0}^{d} q^{2\nu} \frac{(q^{-2(m'-s'-k)};\, q^2)_\nu}{(q^2;\, q^2)_\nu} \frac{Q_{n-1}^\nu}{Q^\nu}.$$

Here $d = m' - s' - k$. Changing the order of summations in the last expression we have

$$d_{ss'}^{mm'} = \sum_{\nu=0}^{\sigma'} \frac{(Q_{n-1}/Q)^\nu q^{2\nu}}{(q^2;\, q^2)_\nu} \sum_{k=0}^{\sigma'-\nu} q^{2k} \frac{(q^{-2(m-s)};\, q^2)_k (q^{-2(m'-s'-k)};\, q^2)_\nu (q^{-2(m'-s')};\, q^2)_k}{(q^2;\, q^2)_k (q^{-2(m+m'+n-2)};\, q^2)_k}, \tag{41}$$

where $\sigma'=m'-s'$. Since

$$(q^{-2(m'-s'-k)};\,q^2)_\nu=q^{\nu(\nu-1)}(-q^{-2(m'-s'-k)})^\nu(q^{2m'-2s'-2k}q^{-2\nu+2};\,q^2)_\nu$$
$$=(-1)^\nu q^{\nu(\nu-1)}q^{-2(m'-s')\nu}\frac{(q^{2m'-2s'-2\nu+2};\,q^2)_\nu(q^{-2m'+2s'+2\nu};\,q^2)_k}{(q^{-2m'+2s'};\,q^2)_k},$$

for the sum over k in (41) we have

$$\frac{(-1)^\nu q^{\nu(\nu-1)}(q^{-2\nu}q^{2m'-2s'+2};\,q^2)_\nu}{q^{2(m'-s')\nu}}\sum_{k=0}^{\sigma'-\nu}\frac{(q^{-2m'+2s'+2\nu};\,q^2)_k(q^{-2(m-s)};\,q^2)_k}{(q^2;\,q^2)_k(q^{-2(m+m'+n-2)};q^2)_k}q^{2k}$$
$$=a_\nu(-1)^\nu q^{\nu(\nu-1)}q^{-2(m'-s')\nu}{}_2\varphi_1(q^{-2(m-s)},\,q^{-2(m'-s')+2\nu};\,q^{-2(m+m'+n-2)};\;q^2,\,q^2)$$
$$=a_\nu(-1)^\nu q^{\nu(\nu-1)}q^{-2(m'-s')\nu}\frac{(q^{-2m'-2s-2n+4};\,q^2)_{m'-s'-\nu}}{(q^{-2m-2m'-2n+4};\,q^2)_{m'-s'-\nu}}q^{-2(m-s)(m'-s'-\nu)}$$
$$=a_\nu\frac{(-1)^\nu q^{\nu(\nu-1)}}{q^{2(m'-s')\nu}}\frac{(q^{-2m'-2s-2n+4};\,q^2)_{m'-s'}}{(q^{-2m-2m'-2n+4};\,q^2)_{m'-s'}}\frac{(q^{2m+2s'+2n-2};\,q^2)_\nu}{(q^{2s+2s'+2n-2};\,q^2)_\nu}q^{-2(m-s)(m'-s')},$$

where $a_\nu=(q^{-2\nu}q^{2m'-2s'+2};\,q^2)_\nu$. Since

$$a_\nu\equiv(q^{-2\nu}q^{2m'-2s'+2};\,q^2)_\nu=(-1)^\nu q^{-\nu(\nu-1)}q^{2(m'-s')\nu}(q^{-2m'+2s'};\,q^2)_\nu,$$

for $d_{ss'}^{mm'}$ we have the expression

$$d_{ss'}^{mm'}=c_{ss'}^{mm'}{}_2\varphi_1(q^{-2(m'-s')},\,q^{2(m+s'+n-1)};\,q^{2(s+s'+n-1)};\;q^2,\;q^2Q_{n-1}/Q),$$

where

$$c_{ss'}^{mm'}=q^{-2(m-s)(m'-s')}\frac{(q^{-2m'-2s-2n+4};\,q^2)_{m'-s'}}{(q^{-2m-2m'-2n+4};\,q^2)_{m'-s'}}=\frac{(q^{2(s+n-1)};\,q^2)_{m'-s'}}{(q^{2(m+n-1)};\,q^2)_{m'-s'}}.$$

In the case when $m-s\leqslant m'-s'$, the proof is similar and we omit it. Proposition is proved.

Remark: If $n=2$, then polynomials $h_{s,s'}(z_1,\,w_1)$ in Proposition 10 are multiple to elements from (21), that is, we have $s=0$ or $s'=0$ or $s=s'=0$.

The expressions for $d_{ss'}^{mm'}$ from Proposition 10 can be represented in terms of little q-Jacobi polynomials $P_k^{(\alpha,\beta)}(x;\,q)$ as

$$d_{ss'}^{mm'}=c_{ss'}^{mm'}P_{m'-s'}^{(s+s'+n-2,m-s-m'+s')}(Q_{n-1}/Q),$$

if $m-s\geqslant m'-s'$, and as

$$d_{ss'}^{mm'}=c_{s's}^{m'm}P_{m-s}^{(s+s'+n-2,m'-s'-m+s)}(Q_{n-1}/Q),$$

if $m-s\leqslant m'-s'$.

We denote the expression $z_n^{m-s+m'+s'}Q^{m'-s'}d_{ss'}^{mm'}$ from formula (39) and the expression $Q^{m-s}d_{ss'}^{mm'}w_n^{m'-s'+m+s}$ from (40) by $t_{s,s'}^{n;m,m'}$. Then

$$\mathsf{H}_{m,m'}(z_n^{m-s}w_n^{m'-s'}h_{s,s'}(\mathbf{z}',\mathbf{w}'))=t_{s,s'}^{n;m,m'}h_{s,s'}(\mathbf{z}',\mathbf{w}'). \tag{42}$$

Moreover, the space $\mathcal{H}_{m,m'}$ can be represented as the direct sum

$$\mathcal{H}_{m,m'}=\bigoplus_{s=0}^{m}\bigoplus_{s'=0}^{m'} t_{s,s'}^{n;m,m'}\mathcal{H}_{s,s'}^{(n-1)}, \tag{43}$$

where $\mathcal{H}_{s,s'}^{(n-1)}$ are the corresponding spaces of homogeneous q-harmonic polynomials in z_i, w_i, $i=1, 2,\ldots, n-1$. To prove this, we note that the subspaces $t_{s,s'}^{n;m,m'}\mathcal{H}_{s,s'}^{(n-1)}$ pairwise do not intersect and $\oplus_{s=0}^{m}\oplus_{s'=0}^{m'}t_{s,s'}^{n;m,m'}\mathcal{H}_{s,s'}^{(n-1)}\subset\mathcal{H}_{mm'}$. Now the equality (43) follows from the fact that dimensions of the spaces on the right and on the left coincide.

To have a correspondence with the classical case, below we denote $t_{s,s'}^{2;m,m'}$ (in this case $s=0$ or $s'=0$) by $t_{s}^{2;m,m'}$ if $s'=0$ and by $t_{-s'}^{2;m,m'}$ if $s=0$.

Taking into account the orthogonality relation (7.3.3) in Ref. 14 for little q-Jacobi polynomials we obtain for the scalar product of $t_{s,s'}^{n;m,m'}h_{s,s'}^{(n-1)}$ and $t_{r,r'}^{n;m,m'}h_{r,r'}^{(n-1)}$, $h_{p,p'}^{(n-1)}\in\mathcal{H}_{p,p'}^{(n-1)}$, the expression

$$\langle t_{s,s'}^{n;m,m'}h_{s,s'}^{(n-1)},\ t_{r,r'}^{n;m,m'}h_{r,r'}^{(n-1)}\rangle=\delta_{sr}\delta_{s'r'}(c_{ss'}^{mm'})^{-2}b_{ss'}^{mm'}\langle h_{s,s'}^{(n-1)},\ h_{r,r'}^{(n-1)}\rangle_{(n-1)},$$

where $\langle\cdot,\cdot\rangle_{(n-1)}$ is the scalar product in the space $\mathcal{H}_{ss'}^{(n-1)}$ and

$$b_{ss'}^{mm'}=\frac{(1-q^{2(n+s+s'-1)})q^{2(m'-s')(n+s+s'-1)}(q^2;\,q^2)_{m-s}(q^2;\,q^2)_{m'-s'}}{(1-q^{2(2m+n-1)})(q^{2(n+s+s'-1)};\,q^2)_{m-s}(q^{2(n+s+s'-1)};\,q^2)_{m'-s'}}.$$

Note that a calculation of this scalar product reduces to q-integration (see Refs. 3 and 4 on calculation of q-integrals of this type).

Now we apply the decomposition (43) to the subspaces $\mathcal{H}_{s,s'}^{(n-1)}$ and obtain

$$\mathcal{H}_{m,m'}=\bigoplus_{s=0}^{m}\bigoplus_{s'=0}^{m'}\bigoplus_{r=0}^{s}\bigoplus_{r'=0}^{s'} t_{s,s'}^{n;m,m'}t_{r,r'}^{n-1;s,s'}\mathcal{H}_{r,r'}^{(n-2)},$$

where $\mathcal{H}_{r,r'}^{(n-2)}$ are the subspaces of homogeneous q-harmonic polynomials in z_i, w_i, $i=1, 2,\ldots, n-2$. Continuing such decompositions we obtain the decomposition

$$\mathcal{H}_{m,m'}=\bigoplus_{\mathbf{m},\mathbf{m}',m_1}\mathbb{C}\Xi_{\mathbf{m},\mathbf{m}',m_1}(\mathbf{z},\mathbf{w}),$$

where the polynomials $\Xi_{\mathbf{m},\mathbf{m}',m_1}$ are given by the formula

$$\Xi_{\mathbf{m},\mathbf{m}',m_1}(\mathbf{z},\mathbf{w})=t_{m_{n-1},m'_{n-1}}^{n;m,m'}\,t_{m_{n-2},m'_{n-2}}^{n-1;m_{n-1},m'_{n-1}}\cdots t_{m_2,m'_2}^{3;m_3,m'_3}t_{m_1}^{2;m_2,m'_2}t^{1;m_1}, \tag{44}$$

and the summation is over all sets of $2n-3$ integers $\mathbf{m}=(m_{n-1},\ldots, m_2)$, $\mathbf{m}'=(m'_{n-1},\ldots, m'_2)$, m_1 such that $m_i\geqslant 0$, $m'_i\geqslant 0$, $i=2, 3,\ldots, n-1$, $m_2\geqslant m_1\geqslant -m'_2$,

$$m\geqslant m_{n-1}\geqslant m_{n-2}\geqslant\cdots\geqslant m_2,\quad m'\geqslant m'_{n-1}\geqslant m'_{n-2}\geqslant\cdots\geqslant m'_2.$$

Here $t_{m_{p-1},m'_{p-1}}^{p;m_p,m'_p}$ and $t_{m_1}^{2;m_2,m'_2}$ are determined by formulas given above and

$$t^{1;m_1}=z_1^{m_1}\quad\text{for } m_1>0,\quad t^{1;0}=1,\quad t^{1;m_1}=w_1^{-m_1}\quad\text{for } m_1<0.$$

It is easy to show that the basis (44) is orthogonal with respect to the scalar product introduced above.

At $q=1$, polynomials (44) turn into the basis elements of the spaces of homogeneous harmonic polynomials on $\mathbb{C}^n$ in separated coordinates determined by formulas (2) of Sec. 11.1.4 in Ref. 1. These classical homogeneous harmonic polynomials, restricted to the sphere $S^{\mathbb{C}}_{n-1}$, coincide with associated spherical functions from Sec. 11.3 in Ref. 1. They are matrix elements of zero column of the corresponding irreducible representations of the group $\mathrm{U}(n)$.

The basis elements (44) give solutions of the equation $\Delta p=0$ in $\mathcal{H}_{m,m'}$. A representation of solutions in the form (44) can be considered as a q-analog of the corresponding classical separation of variables.

In order to have an orthonormal basis in $\mathcal{H}_{m,m'}$ we replace each $t^{n-i;m_{n-i},m'_{n-i}}_{m_{n-i-1},m'_{n-i-1}}$ in the expression (44) for $\Xi_{\mathbf{m},\mathbf{m}',m_1}(\mathbf{z},\mathbf{w})$ by

$$\hat{t}^{n-i;m_{n-i},m'_{n-i}}_{m_{n-i-1},m'_{n-i-1}}=c^{m_{n-i},m'_{n-i}}_{m_{n-i-1},m'_{n-i-1}}\,(b^{m_{n-i},m'_{n-i}}_{m_{n-i-1},m'_{n-i-1}})^{-1/2}t^{n-i;m_{n-i},m'_{n-i}}_{m_{n-i-1},m'_{n-i-1}}.$$

We denote the expression (44) with such the replacement by $\hat{\Xi}_{\mathbf{m},\mathbf{m}',m_1}(\mathbf{z},\mathbf{w})$. These polynomials constitute an orthonormal basis of $\mathcal{H}_{m,m'}$.

It was shown above that the irreducible representation $T_{m,m'}$ with highest weight $(m,0,\ldots,0,-m')$ acts on the space $\mathcal{H}_{m,m'}$. The following assertion is true.

Proposition 11: The operators $T_{m,m'}(e_j)$, $T_{m,m'}(f_j)$ and $T_{m,m'}(k_j)$, corresponding to the generating elements e_j,f_j,k_j of the algebra $\mathrm{U}_q(\mathrm{gl_n})$, act upon the basis elements $\hat{\Xi}_{\mathbf{m},\mathbf{m}',m_1}\equiv|\mathbf{m},\mathbf{m}',m_1\rangle$ as

$$T_{m,m'}(e_{j-1})|\mathbf{m},\mathbf{m}',m_1\rangle=A(\mathbf{m},\mathbf{m}')|\mathbf{m}^{+1}_{j-1},\mathbf{m}',m_1\rangle+B(\mathbf{m},\mathbf{m}')|\mathbf{m},\mathbf{m}'^{-1}_{j-1},m_1\rangle,$$

$$T_{m,m'}(f_{j-1})|\mathbf{m},\mathbf{m}',m_1\rangle=A(\mathbf{m}^{-1}_{j-1},\mathbf{m}')|\mathbf{m}^{-1}_{j-1},\mathbf{m}',m_1\rangle+B(\mathbf{m},\mathbf{m}'^{+1}_{j-1})|\mathbf{m},\mathbf{m}'^{+1}_{j-1},m_1\rangle,$$

$$T_{m,m'}(k_{j-1})|\mathbf{m},\mathbf{m}',m_1\rangle=q^{m'_j-m_j+m_{j-1}-m'_{j-1}}|\mathbf{m},\mathbf{m}',m_1\rangle,$$

where

$$A(\mathbf{m},\mathbf{m}')=\left(\frac{[m_j-m_{j-1}][m'_j+m_{j-1}+j-1][m_{j-1}-m_{j-2}+1][m_{j-1}+m'_{j-2}+j-2]}{[m_{j-1}+m'_{j-1}+j-2][m_{j-1}+m'_{j-1}+j-1]}\right)^{1/2},$$

$$B(\mathbf{m},\mathbf{m}')=\left(\frac{[m'_j-m'_{j-1}+1][m_j+m'_{j-1}+j-2][m'_{j-1}-m'_{j-2}][m'_{j-1}+m_{j-2}+j-3]}{[m_{j-1}+m'_{j-1}+j-2][m_{j-1}+m'_{j-1}+j-3]}\right)^{1/2},$$

$m_n\equiv m$, $m'_n\equiv m'$, and $\mathbf{m}^{\pm1}_j$ *denotes the set of the numbers* $\mathbf{m}_{j-1}$ *with* m_{j-1} *replaced by* $m_{j-1}\pm1$, *respectively*.

A proof of this proposition is awkward. Since it is similar to that of Theorem 1 in Ref. 5, we omit it.

X. q-ANALOG OF ASSOCIATED SPHERICAL HARMONICS WITH RESPECT TO $\mathrm{U}_q(\mathrm{gl}_p)\times\mathrm{U}_q(\mathrm{gl}_{n-p})$

In Sec. IX we found an orthogonal basis of the space $\mathcal{H}_{mm'}$ of homogeneous q-harmonic polynomials corresponding to the chain of subalgebras (38). In this section we shall find orthogonal bases of the same space corresponding to the reductions

$$\mathrm{U}_q(\mathrm{gl}_n)\supset\mathrm{U}_q(\mathrm{gl}_p)\times\mathrm{U}_q(\mathrm{gl}_{n-p})\supset\cdots. \tag{45}$$

In the classical case (see Ref. 1, Chap. 11), further reductions can be made taking any chain of subgroups of the groups $U(p)$ and $U(n-p)$. In particular, the usual tree method (see Ref. 1, Sec. 10.2) can be used to describe different chains of these groups corresponding to different orthogonal bases of $\mathcal{H}_{mm'}$. In our case, there are some difficulties with construction of orthogonal bases corresponding to any chain of subalgebras in (45). For this reason, we construct orthogonal bases corresponding to the case, when we take chains of the type (38) for the subalgebras $U_q(gl_p)$ and $U_q(gl_{n-p})$ in (45).

We represent the set $(\mathbf{z},\mathbf{w})=(z_1,\ldots,z_n;w_1,\ldots,w_n)$ as $(\mathbf{y},\mathbf{t})$, where $\mathbf{y}=(z_1,z_2,\ldots,z_p,w_1,w_2,\ldots,w_p)$ and $\mathbf{t}=(z_{p+1},\ldots,z_n,w_{p+1},\ldots,w_n)$. Then the q-Laplace operator Δ_q can be written as

$$\Delta_q=\Delta_{(\mathbf{y})}+\Delta_{(\mathbf{t})}, \tag{46}$$

where

$$\Delta_{(\mathbf{y})}=\partial_1\overline{\partial}_1+\cdots+\partial_p\overline{\partial}_p, \quad \Delta_{(\mathbf{t})}=\partial_{p+1}\overline{\partial}_{p+1}+\cdots+\partial_n\overline{\partial}_n=\sum_{i=1}^{n-p}q^{2(i-1)}\overline{\partial}_{p+i}\partial_{p+i}. \tag{47}$$

The operator Δ_q can be also represented as

$$\Delta_q=\hat{\Delta}_{(\mathbf{y})}+q^{2p}\Delta_{(\mathbf{t})},$$

where

$$\hat{\Delta}_{(\mathbf{y})}=\overline{\partial}_1\partial_1+q^2\overline{\partial}_2\partial_2+\cdots+q^{2(p-1)}\overline{\partial}_p\partial_p. \tag{48}$$

We have

$$\Delta_{(\mathbf{y})}-\hat{\Delta}_{(\mathbf{y})}=(1-q^{2p})\Delta_{(\mathbf{t})}. \tag{49}$$

In order to find bases of $\mathcal{H}_{m,m'}$ corresponding to the reduction (45) we take non-negative numbers r, r', s, s' such that

$$u:=m-r-s=m'-r'-s'\geqslant 0.$$

We wish to find a harmonic projection of the polynomials

$$Q_{\mathbf{y}}^u h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y})\in\mathcal{A}_{mm'}, \quad h_{s,s'}(\mathbf{t})\in\tilde{\mathcal{H}}_{ss'}^{(\mathbf{t})}, \quad h_{r,r'}(\mathbf{y})\in\mathcal{H}_{r,r'}^{(\mathbf{y})}, \tag{50}$$

where $Q_{\mathbf{y}}:=z_1w_1+\cdots+z_pw_p$, $\mathcal{H}_{r,r'}^{(\mathbf{y})}$ is the space of homogeneous q-harmonic polynomials in $\mathbf{y}=(z_1,z_2,\ldots,z_p,w_1,w_2,\ldots,w_p)$, and $\tilde{\mathcal{H}}_{s,s'}^{(\mathbf{t})}$ is the space obtained in the following way. We take the space $\mathcal{H}_{s,s'}^{(n-p)}$ of homogeneous q-harmonic polynomials in $(z_1,\ldots,z_{n-p},w_1,\ldots,w_{n-p})$ and, using the relations between z_i and w_j, represent each of its polynomial in such a form that in each of its summands (monomials) the elements $z_1,\ldots,z_{n-p}$ stand before the elements $w_1,\ldots,w_{n-p}$. Then we replace $z_1,\ldots,z_{n-p},w_1,\ldots,w_{n-p}$ by $z_{p+1},\ldots,z_n,w_{p+1},\ldots,w_n$, respectively, in each of these polynomials. The space of these polynomials in $z_{p+1},\ldots,z_n,w_{p+1},\ldots,w_n$ is denoted by $\tilde{\mathcal{H}}_{ss'}^{(\mathbf{t})}$.

Lemma 2: Polynomials P of $\tilde{\mathcal{H}}_{s,s'}^{(\mathbf{t})}$ satisfy the conditions $\partial_iP=0$, $\overline{\partial}_iP=0$, $i=1,2,\ldots,p$.

Proof: Fulfillment of the conditions $\partial_iP=0$, $i=1,2,\ldots,p$, follow from the construction of polynomials of the space $\tilde{\mathcal{H}}_{s,s'}^{(\mathbf{t})}$. In order to prove the fulfillment of the conditions $\overline{\partial}_iP=0$, $i=1,2,\ldots,p$, we note that according to formulas (8) and (9) the space $\tilde{\mathcal{H}}_{s,s'}^{(\mathbf{t})}$ is elementwise invariant with respect to the subalgebra $U_q(gl_p)$. Moreover, this space is invariant and irreducible with respect to the subalgebra $U_q(gl_{n-p})$ acting on $\mathbf{t}$.

Now we rearrange elements $z_{p+1},\dots,z_n,\ w_{p+1},\dots,w_n$ in each of polynomials of $\widetilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$ such that in each summand (monomial) elements $w_{p+1},\dots,w_n$ stand before the elements $z_{p+1},\dots,z_n$. We denote the space $\widetilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$ with this rearrangement in polynomials by $\mathcal{L}^{(\mathbf{t})}_{s,s'}$. Because of element-wise invariance with respect to $\mathrm{U}_q(\mathrm{gl}_p)$, the space $\mathcal{L}^{(\mathbf{t})}_{s,s'}$ can be represented as a direct sum

$$\mathcal{L}^{(\mathbf{t})}_{s,s'}=\mathcal{R}_{s,s'}\oplus Q_{\mathbf{y}}\mathcal{R}_{s-1,s'-1}\oplus Q^2_{\mathbf{y}}\mathcal{R}_{s-2,s'-2}\oplus\cdots, \tag{51}$$

where $\mathcal{R}_{s-j,s'-j}$ denote the space of homogeneous polynomials in which $w_{p+1},\dots,w_n$ stand before $z_{p+1},\dots,z_n$. Due to formulas (8) and (9), the spaces $\mathcal{R}_{s-j,s'-j}$ are invariant with respect to $\mathrm{U}_q(\mathrm{gl}_{n-p})$. However, the representation of $\mathrm{U}_q(\mathrm{gl}_{n-p})$ on $\mathcal{L}^{(\mathbf{t})}_{s,s'}$ is irreducible. Therefore, the decomposition (51) contains only one summand and $\mathcal{L}^{(\mathbf{t})}_{s,s'}=\mathcal{R}_{s,s'}$. It is clear that for elements of $\mathcal{R}_{s,s'}$ the conditions $\overline{\partial}_i P=0$, $i=1,2,\dots,p$, are fulfilled. Lemma is proved.

Corollary 1: Elements P of the space $\widetilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$, satisfy the relation $\Delta_{(\mathbf{t})}P=0$.

Corollary 2: Elements P of the space $\widetilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$, are q-harmonic, that is, $\Delta_q P=0$.

Corollary 1 follows from (47)–(49). Corollary 2 follows from Corollary 1 and formula (46).

Lemma 3: For polynomial $h_{s,s'}(\mathbf{t})\in\widetilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$, and arbitrary polynomial $f(\mathbf{y})$ we have

$$\hat{\Delta}_{(\mathbf{y})}h_{s,s'}(\mathbf{t})f(\mathbf{y})=q^{s-s'}h_{s,s'}(\mathbf{t})\hat{\Delta}_{(\mathbf{y})}f(\mathbf{y}).$$

Proof: We first prove the relations $\partial_i h_{s,s'}(\mathbf{t})f(\mathbf{y})=q^{s'}h_{s,s'}(\mathbf{t})\partial_i f(\mathbf{y})$, $i=1,\dots,p$. The polynomial $h_{s,s'}(\mathbf{t})$ can be represented in the form of a linear combination of monomials $z^{k_{p+1}}_{p+1}\cdots z^{k_n}_n w^{l_n}_n\cdots w^{l_{p+1}}_{p+1}$, where $k_{p+1}+\cdots+k_n=s$, $l_{p+1}+\cdots+l_n=s'$. We have

$$\begin{aligned}\partial_i z^{k_{p+1}}_{p+1}\cdots z^{k_n}_n w^{l_n}_n\cdots w^{l_{p+1}}_{p+1}f(\mathbf{y})&=z^{k_{p+1}}_{p+1}\cdots z^{k_n}_n(\partial_i w^{l_n}_n\cdots w^{l_{p+1}}_{p+1}f(\mathbf{y}))\\&=q^{s'}z^{k_{p+1}}_{p+1}\cdots z^{k_n}_n w^{l_n}_n\cdots w^{l_{p+1}}_{p+1}(\partial_i f(\mathbf{y})),\end{aligned}$$

where the relation $\partial_j f(\mathbf{y})=0$ and relations from Sec. III were used. It proves our relations. We analogously prove the relations $\overline{\partial}_i h_{s,s'}(\mathbf{t})f(\mathbf{y})=q^{-s}h_{s,s'}(\mathbf{t})\overline{\partial}_i f(\mathbf{y})$, $i=1,\dots,p$. In this case, it is useful to represent the polynomial $h_{s,s'}(\mathbf{t})$ in the form of a linear combination of monomials $w^{l_{p+1}}_{p+1}\cdots w^{l_n}_n z^{k_n}_n\cdots z^{k_{p+1}}_{p+1}$ (such representation is possible due to Lemma 2). Now the lemma follows from explicit formula for $\hat{\Delta}_{(\mathbf{y})}$. Lemma is proved.

Since $\Delta_{(\mathbf{t})}(Q^u_{\mathbf{y}}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))=0$, then using Lemma 3 and relation (18) with n replaced by p we have

$$\begin{aligned}\Delta_q(Q^u_{\mathbf{y}}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))&=\hat{\Delta}_{(\mathbf{y})}(Q^u_{\mathbf{y}}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))\\&=q^a h_{s,s'}(\mathbf{t})\Delta_{(\mathbf{y})}Q^u_{\mathbf{y}}h_{r,r'}(\mathbf{y})\\&=q^a[u][p+u+r+r'-1](Q^{u-1}_{\mathbf{y}}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y})),\end{aligned}$$

where $a=2(s-s')u+s'-s$.

Now we may find a harmonic projection of the polynomials (50). Denoting this projection by $h^{(r,r';s,s')}_{m,m'}(\mathbf{z},\mathbf{w})$ we have

$$\begin{aligned}h^{(r,r';s,s')}_{m,m'}(\mathbf{z},\mathbf{w})&=\sum_{k=0}^{\min(m,m')}\alpha_k Q^k\Delta^k_q(Q^u_{\mathbf{y}}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))\\&=\left(\sum_{k=0}^{u}\alpha_k Q^k q^{(s-s'+p-1)k}\frac{[u]![r+r'+p+u-1]!}{[u-k]![r+r'+p+u-k-1]!}Q^{u-k}_{\mathbf{y}}\right)h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}),\end{aligned}$$

where α_k is determined by formula (33). Denoting the expression in the parentheses by $t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},Q_{\mathbf{t}})$, we have

$$h^{(r,r';s,s')}_{m,m'}(\mathbf{z},\mathbf{w})=\mathsf{H}_{m,m'}(Q_{\mathbf{y}}^{m-r-s}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))=t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},Q_{\mathbf{t}})h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}). \quad (52)$$

After some simple transformations, we obtain for $t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},\ Q_{\mathbf{t}})$ the expression

$$t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},\ Q_{\mathbf{t}})=Q_{\mathbf{y}}^{u}\sum_{k=0}^{u}\frac{(q^{-2u};\ q^2)_k(q^{-2(r+r'+p+u-1)};\ q^2)_k}{(q^{-2(m+m'+n-2)};\ q^2)_k(q^2;\ q^2)_k}q^{k\sigma}Q^kQ_{\mathbf{y}}^{-k},$$

where $\sigma=-2n-2s'+2+2p$. Taking into account the definition of the basis hypergeometric function ${}_2\varphi_1$, we derive

$$t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},\ Q_{\mathbf{t}})=Q_{\mathbf{y}}^{u}\,{}_2\varphi_1(q^{-2u},\ q^{-2(r+r'+p+u-1)};\ q^{-2(m+m'+n-2)};\ q^2,\ QQ_{\mathbf{y}}^{-1}q^{\sigma}).$$

Applying the relation

$${}_2\varphi_1(q^{-n},\ b;\ c;\ q,\ z)=q^{-(n+1)n/2}(-z)^n\frac{(b;\ q)_n}{(c;\ q)_n}\,{}_2\varphi_1(q^{-n},\ q^{1-n}/c;\ q^{1-n}/b;\ q,\ cq^{n+1}/bz)$$

[see, for example, formula (2) of Sec. 14.1.8 in Ref. 16] we reduce this expression to

$$t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},\ Q_{\mathbf{t}})=(-q^{\sigma})^uq^{-(u+1)u}\frac{(q^{-2(r+r'+p+u-1)};\ q^2)_u}{(q^{-2(m+m'+n-2)};\ q^2)_u}Q^u$$
$$\times\,{}_2\varphi_1(q^{-2u},\ q^{2(m+m'+n-u-1)};\ q^{2(r+r'+p)};\ q^2,\ q^{-2s+2}Q_{\mathbf{y}}/Q).$$

Using the definition of the little q-Jacobi polynomials, we derive from here that

$$t^{n,p;m,m'}_{r,r';s,s'}(Q_{\mathbf{y}},Q_{\mathbf{t}})=(-q^{\sigma})^uq^{-(u+1)u}\frac{(q^{-2(r+r'+p+u-1)};\ q^2)_u}{(q^{-2(m+m'+n-2)};\ q^2)_u}Q^u$$
$$\times P_u^{(r+r'+p-1,s+s'+n-p-1)}(q^{-2s}Q_{\mathbf{y}}/Q;\ q^2). \quad (53)$$

Thus, we proved that *the projection* $\mathsf{H}_{m,m'}(Q_{\mathbf{y}}^{m-r-s}h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}))$ *is given by formula (52), where* $t^{n,p;m,m'}_{r,r';s,s'}$ *is determined by (53).* The restriction $\tau h^{(r,r';s,s')}_{m,m'}(\mathbf{z},\mathbf{w})$ of this projection onto the quantum sphere $S^{\mathbb{C}}_{q,n-1}$ is given by

$$\tau h^{(r,r';s,s')}_{m,m'}(\mathbf{z},\mathbf{w})=(\tau t^{n,p;m,m'}_{r,r';s,s'})(Q_{\mathbf{y}})h_{s,s'}(\mathbf{t})h_{r,r'}(\mathbf{y}),$$

where $(\tau t^{n,p;m,m'}_{r,r';s,s'})(Q_{\mathbf{y}})=cP_u^{(r+r'+p-1,s+s'+n-p-1)}(q^{-2s}Q_{\mathbf{y}}/Q;q^2)$ [c is the multiplier from the right hand side of (53)].

For the scalar product of polynomials of the form (52) we have

$$\langle h^{(r,r';s,s')}_{m,m'},h^{(r'',r''';s'',s''')}_{m,m'}\rangle=0 \quad \text{if} \quad (r,\ r',s,\ s')\neq(r'',\ r''',\ s'',\ s''')$$

(since the spaces $\mathcal{H}^{(\mathbf{y})}_{r,r'}$ and $\mathcal{H}^{(\mathbf{y})}_{r'',r'''}$ and the spaces $\tilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$ and $\tilde{\mathcal{H}}^{(\mathbf{t})}_{s'',s'''}$ are orthogonal). If $(r,\ r',\ s,\ s')=(r'',\ r''',\ s'',\ s''')$, then the norm of the polynomial (52) reduces to the orthogonality relation for q-Jacobi polynomials and to norms of $h_{s,s'}(\mathbf{t})$ and $h_{r,r'}(\mathbf{y})$.

In order to obtain a q-analog of separation of variables in this case we have to take bases of the spaces $\mathcal{H}^{(\mathbf{y})}_{r,r'}$ and $\tilde{\mathcal{H}}^{(\mathbf{t})}_{s,s'}$ in separated coordinates (as it was made in Sec. IX).

ACKNOWLEDGMENT

The research by the first author (N.Z.I.) was partially supported by INTAS Grant No. 2000-334.

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A sum rule for associated Legendre polynomials with spherical triangles

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(Received 14 September 2001; accepted 27 September 2002)

An explicit solution to the classical electrostatic problem of the electrostatic force between *N* conducting spheres requires the expansion of the electrostatic potential. The boundary conditions for the potentials are given by Gauss which requires an expansion of the inverse of the distance that encompasses six angles. A sum rule for this expansion is presented in terms of associated Legendre polynomials with complex exponentials. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1525048]

The expansion of the inverse of the distance in systems involving more than two objects requires a sum rule for associated Legendre polynomials on the sphere. A solution is presented that expresses the product of the associated Legendre polynomials and the complex exponentials in terms of the relations for oblique spherical triangles.

Consider *N* conducting spheres each held at constant potential. The boundary condition on the surface of the spheres is given by Gauss,[1]

$$V_i = K \sum_{j=1}^{N} \int \frac{dQ_j}{R_{ij}}, \tag{1}$$

where the geometry is shown in Fig. 1. For a system comprised of three conducting spheres. Equation (1) can be written terms of Legendre polynomials. Since V_2, V_3, etc. follow from obvious interchange of symbols we need only to consider the expression for V_1:

$$V_1 = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[P_\ell^m(\cos\beta) \frac{1}{a_1^{\ell+1}} e^{im\phi} A_{\ell,m}^1 + P_\ell^m(\cos\beta) e^{im\phi} \sum_{j=0}^{\infty} \frac{(\ell+j)!}{(\ell+m)!(j-m)!} \frac{a_1^\ell}{h_{12}^{j+\ell+1}} A_{j,m}^2 \right.$$
$$\left. + P_\ell^m(\cos\beta_{13}') e^{im\phi'} \sum_{j=0}^{\infty} \frac{(\ell+j)!}{(\ell+m)!(j-m)!} \frac{a_1^\ell}{h_{13}^{j+\ell+1}} A_{j,m}^3 \right], \tag{2}$$

where $A_{j,m}^n = (-1)^m a_n^{j+2} \int_0^\pi \int_0^{2\pi} \sigma_n(\theta,g) \sin\theta \, d\theta dg \, P_j^{-m}(\cos\theta) e^{img}$, and where $\sigma_n(\theta,g)$ is the electric charge density on the surface of the *n*th sphere and where the first, second, and third terms are the contributions stemming from charges on sphere 1, sphere 2, and sphere 3, respectively. To express the expansion of the inverse of the distance in *N*-body systems thus requires a sum rule for associated Legendre polynomials expressed as the product of the two basis—the associated Legendre polynomials and the complex exponentials, $P_\ell^m(\cos\beta_{13}') e^{im\phi'}$.

The derivation of a sum rule for associated Legendre polynomials proceeds as follows given that the six angles (Fig. 1) satisfy the relationships for oblique spherical triangles:[2]

$$\cos\beta_{13}' = \cos\lambda_{13}\cos\beta + \sin\lambda_{13}\sin\beta\cos(\phi - \phi_{\lambda 13}), \tag{3}$$

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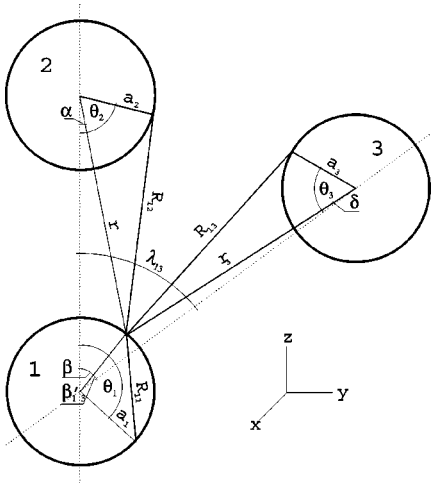

FIG. 1. Schematic representation of three spheres with radii a_1, a_2, and a_3 each having constant potential.

$$\frac{\sin\beta}{\sin(\phi_{\lambda 13}-\phi')}=\frac{\sin\beta'_{13}}{\sin(\phi-\phi_{\lambda 13})}.$$

From Eq. (3) it follows that

$$\cos\beta=\cos\lambda_{13}\cos\beta'_{13}+\sin\lambda_{13}\sin\beta'_{13}\cos(\phi_{\lambda 13}-\phi') \tag{4}$$

and, substitution of $\cos\beta'_{13}$ from Eq. (3) into Eq. (4) gives

$$-\sin\lambda_{13}\cos\beta+\cos\lambda_{13}\sin\beta\cos(\phi-\phi_{\lambda 13})+\sin\beta'_{13}\cos(\phi_{\lambda 13}-\phi')=0. \tag{5}$$

From Eqs. (3)–(5) the following relations [Eqs. (6) and (7)] are obtained when the partial derivatives are performed with β and ϕ constant (we have dropped the subscripts 13 in what follows):

$$\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)\cos\beta'=\sin\beta' e^{\pm i(\phi'-\phi_\lambda)}, \tag{6}$$

$$\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)\sin\beta' e^{\pm i(\phi'-\phi_\lambda)}=\frac{\cos\lambda}{\sin\lambda}\sin\beta' e^{\pm i(\phi-\phi_\lambda)}. \tag{7}$$

It follows that

$$\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)P_\ell(\cos\beta')=\left(\frac{e^{\pm i(\phi'-\phi_\lambda)}}{\sin\lambda}\right)P_\ell^1(\cos\beta'), \tag{8}$$

from which the recursive product to all orders follows:

$$\begin{aligned}\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)P_\ell(\cos\beta')&=\left(\frac{e^{\pm i(\phi'-\phi_\lambda)}}{\sin\lambda}\right)^2P_\ell^2(\cos\beta')\\ &\vdots\\ \left(\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}\pm\frac{i}{\sin\lambda}\frac{\partial}{\partial\phi_\lambda}\right)\right)^mP_\ell(\cos\beta')&=\left(\frac{e^{\pm i(\phi'-\phi_\lambda)}}{\sin\lambda}\right)^mP_\ell^m(\cos\beta'),\end{aligned} \tag{9}$$

which can also be written as

$$e^{im\phi'}P_\ell^m(\cos\beta')=\sin^m\lambda\, e^{im\phi_\lambda}\left[\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}+\frac{i}{\sin\lambda}\,\frac{\partial}{\partial\phi_\lambda}\right)\right]^m P_\ell(\cos\beta') \tag{10}$$

where $P_\ell(\cos\beta')=\Sigma_{n=-\ell}^{\ell}(-1)^m P_\ell^{-n}(\cos\beta)P_\ell^n(\cos\lambda)e^{in(g_\lambda-g)}$ and is the sought-after sum rule for the associated Legendre polynomial with complex exponentials. Noticeably, this result was obtained directly from the boundary conditions on the spheres given by Gauss without invoking any approximations or simplifications with respect to vectorial quantities of the electric field. For the sake of completeness we also give the relation:

$$\left[\frac{1}{\sin\lambda}\left(\frac{\partial}{\partial\lambda}+\frac{i}{\sin\lambda}\,\frac{\partial}{\partial\phi_\lambda}\right)\right]^m P_\ell^k(\cos\lambda)e^{-ik\phi_\lambda}$$
$$=e^{-ik\phi_\lambda}\sum_{j=k}^{\ell}(-1)^j\frac{(\ell+1)!(1+\cos\lambda)^{k/2}(1-\cos\lambda)^{j-k/2-m}}{2^j(\ell-j)!(j-k)!(j-m)!},$$

which may be verified directly using the definition[2] for associated Legendre polynomials $P_\ell^k(x)=\Sigma_{j=0}^{\ell}(-1)^j[(\ell+j)!/2^j j!(\ell-j)!(j-k)!](1+x)^{k/2}(1-x)^{j-k/2}$. Using the well-known orthogonality relations of Legendre polynomials and the new sum rule the boundary condition for sphere 1 can now be written as

$$V_1\delta_{k,0}\delta_{\ell',0}=(-1)^k\frac{1}{a_1^{\ell'+1}}A_{\ell',-k}^1+(-1)^k\sum_{j=0}^{\infty}\frac{(\ell'+j)!}{(\ell'-k)!(j+k)!}\,\frac{a_1^{\ell'}}{h_{12}^{j+\ell'+1}}A_{j,-k}^2$$
$$+\sum_{j=0}^{\infty}(\ell'+j)!\,\frac{a_1^{\ell'}}{h_{13}^{j+\ell'+1}}\sum_{m=-\ell'}^{\ell'}\frac{g_{\ell',k}^m(-\cos\lambda_{13})}{(\ell'+m)!(j-m)!}(-1)^{m+\ell+k}e^{i(m+k)\phi_{\lambda_{13}}}A_{j,m}^3$$

for $k\geqslant 0$, and

$$g_{\ell',k}^m(-\cos\lambda)=\sum_{n=0}^{\ell'}\frac{(-1)^n(\ell'+n)!}{2^n(n-m)!(n-k)!(\ell'-n)!}\,(1-\cos\lambda)^{(k+m)/2}(1+\cos\lambda)^{n-(k+m)/2} \tag{11}$$

and, importantly, be generalized to any number of spheres by cyclic permutation.

The sum rule for associated Legendre polynomials is an important result because it allows the expansion of the potential that is proportional to the inverse of the distance for any number of spheres that are finite in size. As a result, many-body interactions between spheres can now be accounted for in a true three-dimensional system by explicitly including the r, θ, and ϕ components of the potentials.

A consequence of the expansion [Eq. (10)] is an explicit definition of an operator, here called a ''rotor,'' to all orders in the from ($J'_{+,1}\equiv J_+$)

$$J'_{+,m}=(\sin\lambda\, e^{i\phi_\lambda})^m\left[\frac{1}{\sin\lambda\, e^{i\phi_\lambda}}J_+\right]^m, \tag{12}$$

where

$$J_+=e^{i\phi}\left(\frac{\partial}{\partial\lambda}+\frac{i}{\sin\lambda}\,\frac{\partial}{\partial\phi_\lambda}\right)=L_++S_+.$$

Examination of its structure exhibits the familiar characteristics of the angular momentum operator $J_+=L_++S_+$ where the complex angular momentum operator for space is

$$L_+ = e^{i\phi_\lambda}\left(\frac{\partial}{\partial\lambda} + i\cot\lambda\,\frac{\partial}{\partial\phi_\lambda}\right) \tag{13}$$

and the second term is identified as the first-order spin operator

$$S_+ = ie^{i\phi_\lambda}\tan\frac{\lambda}{2}\,\frac{\partial}{\partial\phi_\lambda}. \tag{14}$$

In this light,

$$e^{im\phi'}P_\ell^m(\cos\beta') = L_+^m(\beta',\phi')P_\ell(\cos\beta') = J'_{+,m}(\lambda,\phi_\lambda)P_\ell(\cos\beta'), \tag{15}$$

which states that $J'_{+,m}(\lambda,\phi_\lambda)$ is the eigenvalue of the space angular momentum $L_+^m(\beta',\phi')$ noting that no assumptions with respect to vectorial quantities of the electric field have been made.

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Probability density distribution of random line segments inside a convex body: Application to random media

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(Received 26 August 2002; accepted 11 November 2002)

We study the probability density distribution of random line segments entirely contained inside a convex body of $\mathbf{R}^n$. Relations between this distribution function and other distribution functions of importance in geometric probability are shown. The expression for the probability density distribution of random line segments is given for several simple geometric bodies in $\mathbf{R}^2$, $\mathbf{R}^3$, and $\mathbf{R}^n$, application to random media is then presented. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1536254]

I. INTRODUCTION

In his paper on random packing, Dixmier[1] introduces the probability distribution of radii for a convex body K in $\mathbf{R}^n$, where the radius of length r is defined by the distance of a point inside K to the frontier ∂K of K. Dixmier also considers sets of random lines which intersect K, measured with the uniform density M in the sense of the theory of geometric probability.[2–4] Let $P(l)=\Pr\{l(M)\leqslant l: M\cap K\neq\varnothing\}$ be the distribution function of l (the length of the chord) and $G(r)=\Pr\{|P_1P_2|\leqslant r:\ P_1\in K,\ P_2\in\partial K\}$ the distribution function of the radii. Moreover, let $p(l)=dP(l)/dl$ and $g(r)=dG(r)/dr$ be the corresponding density functions. Dixmier shows that since the radii are supported by the chords of length greater than r, the distribution of radii $g(r)$ is related to the distribution of random chords $p(l)$ by

$$g(r)=\frac{1}{\overline{l}}\int_r^{\delta} p(l)\,dl, \tag{1}$$

where $\delta=\max(l)$ and $\overline{l}$ is the mean value of the chord:

$$\overline{l}=\int_0^{\delta} l\,p(l)\,dl. \tag{2}$$

Dixmier found several interesting relations between kth moments of the chords and kth moments of the radii, in particular:

$$\overline{r}=\frac{\overline{l^2}}{2\overline{l}}, \tag{3}$$

Following Dixmier's approach we define the probability distribution function for a line segment of length z of being entirely inside K as $S(z)=\Pr\{S(M)\leqslant z:\ M\cap K\neq\varnothing,\ S\subset K\}$, and let $s(z)=dS(z)/dz$ be the corresponding density function. Considering that a line segment of length z belongs to a chord of length greater than z, the conditional density distribution function follows from the definition:

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$$s(z)=\frac{\int_{y\leqslant\delta}\Theta(y-z)(y-z)p(y)dy}{\int_{z\leqslant\delta}dz\int_{y\leqslant\delta}\Theta(y-z)(y-z)p(y)dy}, \tag{4}$$

where $\Theta(x)$ is the Heavyside step function.

The denominator is

$$\int_0^\delta dz\int_0^y(y-z)p(y)dy=\int_0^\delta dyp(y)\int_0^y dz(y-z)=\frac{\overline{l^2}}{2}, \tag{5}$$

where $\overline{l^2}$ is the second moment of the chord distribution:

$$\overline{l^2}=\int_0^\delta l^2\ \ p(l)dl. \tag{6}$$

Thus, the line segment distribution function is related to the chord distribution by

$$s(z)=\frac{2}{\overline{l^2}}\int_z^\delta(y-z)p(y)dy. \tag{7}$$

II. PROPERTIES OF THE PROBABILITY DENSITY OF RANDOM LINE SEGMENTS

Properties of the function $s(z)$ are easily obtained from Eq. (7). $s(z)$ is a concave function since

$$d^2s(z)/dz^2=2p(z)/\overline{l^2}\geqslant 0 \tag{8}$$

moreover $s(0)=2\overline{l}/\overline{l^2}$, and $s(0)'=-2/\overline{l^2}$.

More generally, the kth moment of the random line segment is given by

$$\overline{s^k}=\frac{2}{\overline{l^2}}\int_0^\delta dzz^k\int_0^y(y-z)p(y)dy=\frac{2}{\overline{l^2}}\int_0^\delta dyp(y)\int_0^y dzz^k(y-z)=\frac{2}{(k+1)(k+2)}\frac{\overline{l^{k+2}}}{\overline{l^2}}, \tag{9}$$

where $\overline{l^k}$ denotes the kth moment of the random chord.
In particular, the mean line segment is given by

$$\overline{s}=\frac{1}{3}\frac{\overline{l^3}}{\overline{l^2}}. \tag{10}$$

Except in the one-dimensional case, where $\overline{s^k}=L^k2/(k+1)(k+2)$ where L is the length of K, from Eq. (9), there is no simple relation between $\overline{s^k}$ and the surface and the volume of the body. However, by using (see Ref. 2 for instance)

$$\overline{l^{n+1}}=n(n+1)\frac{V^2}{F}\Gamma\left[\frac{n+1}{2}\right]\pi^{(1-n)/2}$$

where F is the surface area of K, $\overline{s^{n-1}}$ simplifies to

$$\overline{s^{n-1}}=2\frac{V^2}{F}\frac{\Gamma\left[\dfrac{n+1}{2}\right]}{\pi^{(n-1)/2}}\frac{1}{\overline{l^2}}. \tag{11}$$

Another distribution function of interest in geometric probability is the distribution function of the distance $|P_1P_2|$ between two random points P_1 and P_2 in K: $T(z)=\Pr\{|P_1P_2|\leqslant r\colon P_1,P_2 \in K\}$. $t(z)=dT(z)/dz$ is as usual the corresponding probability function. Piefke[5] proves that

$$t(z)=B_n z^{n-1}\int_z^\delta (y-z)p(y)dy \quad \text{with } n\geqslant 2 \tag{12}$$

where

$$B_n=F\pi^{(n-1)/2}\left[V^2\Gamma\left[\frac{n+1}{2}\right]\right]^{-1}.$$

So from Eqs. (7) and (12) the distribution function of line segments and the distribution function of the distance of two random points in K are related by

$$s(z)=\frac{2}{\overline{l^2}B_n}\frac{t(z)}{z^{n-1}}. \tag{13}$$

Normalizing Eq. (13) leads to

$$\overline{l^2}=\frac{2}{B_n}\int_0^\delta \frac{t(z)}{z^{n-1}}dz \tag{14}$$

and Eq. (13) can be rewritten only in terms of $t(z)$,

$$s(z)=\frac{\dfrac{t(z)}{z^{n-1}}}{\displaystyle\int_0^\delta \frac{t(z)}{z^{n-1}}dz}. \tag{15}$$

The last relation will be useful when $\overline{l^2}$ is unknown.

As a consequence of Eq. (13) there are also relations between the moments of the line segments distribution and the moments of the distance distribution. A simple calculation shows that

$$\overline{s^k}=\frac{2}{\overline{l^2}B_n}\overline{t^{k+1-n}} \quad \text{with} \quad k+1-n\geqslant 0 \quad \text{and} \quad n\geqslant 2. \tag{16}$$

By taking $k=n-1$ in Eq. (16) we recover Eq. (11). Equation (16) gives also the remarkable identity:

$$\overline{t}=\frac{\overline{s^n}}{\overline{s^{n-1}}}. \tag{17}$$

In Sec. III we shall derive an analytical expression for $s(z)$ and its moments for various simple geometric objects in two, three, and n dimensions and then extend our analysis to random media.

III. EXAMPLES

A. Sphere

The chord distribution function for a sphere of diameter D in arbitrary dimension has been derived by Dixmier:[1]

$$p(l)=\begin{cases}(n-1)D^{-2}\ \ l\left(1-\dfrac{l^2}{D^2}\right)^{(n-3)/2} & (l\leqslant D)\\ 0 \quad (l>D)\end{cases}. \tag{18}$$

The kth moment of the chord is given by

$$\overline{l^k}=D^k\,\frac{\Gamma\left(\dfrac{k}{2}+1\right)\Gamma\left(\dfrac{n+1}{2}\right)}{\Gamma\left(\dfrac{n+k+1}{2}\right)}. \tag{19}$$

Since the second moment of the chord is $\overline{l^2}=2D^2/(n+1)$, by using Eq. (9) we obtain

$$\overline{s^k}=D^k\,\frac{\Gamma\left(\dfrac{k}{2}+1\right)\Gamma\left(\dfrac{n+3}{2}\right)}{(k+1)\Gamma\left(\dfrac{n+k+3}{2}\right)} \tag{20}$$

and in particular the mean line segment is

$$\overline{s}=\frac{D}{4}\sqrt{\pi}\,\frac{\Gamma\left(\dfrac{n+3}{2}\right)}{\Gamma\left(\dfrac{n+4}{2}\right)}, \quad \overline{s}\underset{n\to\infty}{\sim}\frac{D}{2}\sqrt{\frac{\pi}{2n}}. \tag{21}$$

Using Dixmier's result,[1] namely

$$\overline{l}\underset{n\to\infty}{\sim}D\sqrt{\pi/2n},$$

yields:

$$\lim_{n\to\infty}\frac{\overline{s}}{\overline{l}}=\frac{1}{2}. \tag{22}$$

Analytical expressions for $s(z)$ in the two- and three-dimensional case are given in the following.

1. Two-dimensional case (disk)

The chord density distribution function for the disk is given by Eq. (18) (with $n=2$). A straightforward integration of Eq. (7) gives

$$s(z)=\frac{3}{4D^2}\left[\pi D-2z\sqrt{1-\frac{z^2}{D^2}}-2D\arcsin\left(\frac{z}{D}\right)\right] \tag{23}$$

in agreement with Santalo.[2]

This result can be achieved by a simple geometric argument as follows: Since the disk is invariant under rotations we can fix the direction Ω of the random line segments. Let $D(z,\Omega)$ be the translate of D by a distance z in the direction Ω. Line segments of length z that contribute to $s(z)$ have their right end lying inside $D\cap D(z,\Omega)\equiv A(z)$ (hatched area in Fig. 1). So the line segments distribution function is $A(z)$ averaged over all possible $A(z)$, i.e.,

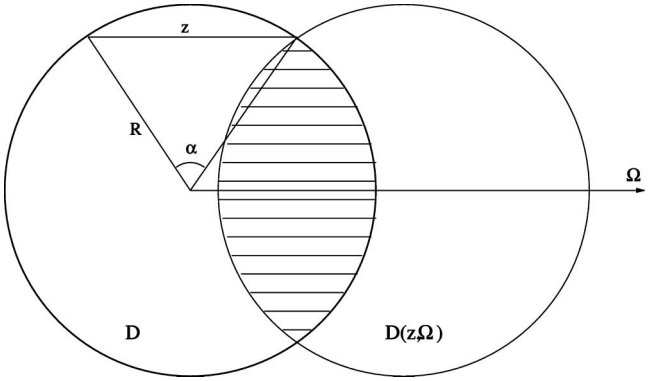

FIG. 1. Geometric interpretation of the distribution function of the random line segment for the disk.

$$s(z)=\frac{A(z)}{\int_0^D A(z)dz}. \tag{24}$$

Figure 1 yields

$$A(z)=\pi\left(\frac{D}{2}\right)^2-2z\frac{D}{2}\cos\left(\frac{\alpha}{2}\right)-\left(\frac{D}{2}\right)^2\frac{(\alpha-\sin\alpha)}{2}=\frac{D}{4}\left[\pi D-2z\sqrt{1-\frac{z^2}{D^2}}-2D\arcsin\left(\frac{z}{D}\right)\right]. \tag{25}$$

Since $\int_0^D A(z)dz=D^3/3$, by using Eq. (24) we recover Eq. (23). These geometric techniques have been recently used by Tu and Fischbach[6] for calculating the random distance between two uniform random points inside an N-dimensional spherical object. Several of their analytical results are similar to ours since the distance distribution is linked to the line segments distribution through Eq. (13). The authors of Ref. 6 also discussed the cases of nonuniform random point distributions (spherically symmetric density distributions and arbitrary density distributions).

2. Three-dimensional case (sphere)

This case is particularly simple since, with $n=3$, Eq. (18) reduces to $p(l)=2l/D^2$. We find:

$$s(z)=\frac{8}{D^4}\left[D^2\left(\frac{D}{3}-\frac{z}{2}\right)+\frac{z^3}{6}\right] \tag{26}$$

and $\overline{s^k}=8D^k/(k+1)(k+2)(k+4)$ in particular $\overline{s}=4D/15$, again in agreement with Santalo's results.[2]

B. Three-dimensional hemisphere

The chord density distribution for the three-dimensional unit hemisphere has been obtained by Dirac and co-workers,[7]

$$p(l)=\begin{cases}\dfrac{2}{3\pi}\left[\sqrt{1-\dfrac{l^2}{D^2}}\left(\dfrac{3}{D}+\dfrac{D}{2l^2}\right)+\dfrac{D^2}{2l^3}\arccos\left(\dfrac{l}{D}\right)-\dfrac{\pi}{4}\left(\dfrac{D^2}{l^3}-16\dfrac{l}{D^2}\right)\right] & \left(l\leqslant\dfrac{1}{2}\right)\\ \dfrac{2}{3\pi}\left[\sqrt{1-\dfrac{l^2}{D^2}}\left(\dfrac{3}{D}+\dfrac{D}{2l^2}\right)+\dfrac{D^2}{2l^3}\arccos\left(\dfrac{l}{D}\right)\right] & \left(l>\dfrac{1}{2}\right)\end{cases}. \tag{27}$$

From Eq. (27), we first calculate $\overline{l^2}=D^2/4$. Using Eq. (7) we thus obtain the probability density function of the random line segment:

$$s(z)=\begin{cases}\dfrac{2}{9\pi z}\left[6\dfrac{z}{D}\left(1+2\left(\dfrac{z}{D}\right)^2\right)\sqrt{1-\left(\dfrac{z}{D}\right)^2}+6\arccos\left(\dfrac{z}{D}\right)\right. & \\ \left.\quad+\pi\left(4\dfrac{z}{D}\left(4-9\dfrac{z}{D}+4\left(\dfrac{z}{D}\right)^3\right)-3\right)+24\left(\dfrac{z}{D}\right)^2\arcsin\left(\dfrac{z}{D}\right)\right] & \left(z\leqslant\dfrac{D}{2}\right) \\ \dfrac{4}{3\pi z}\left[\dfrac{z}{D}\left(1+2\left(\dfrac{z}{D}\right)^2\right)\sqrt{1-\left(\dfrac{z}{D}\right)^2}+\left(1-4\left(\dfrac{z}{D}\right)^2\right)\arccos\left(\dfrac{z}{D}\right)\right] & \left(z>\dfrac{D}{2}\right)\end{cases}. \tag{28}$$

The kth moment of the random line segment in the hemisphere is

$$\overline{s^k}=\frac{2}{(k+1)(k+2)}\left(\frac{D}{2}\right)^k\left[\frac{(k+1)\Gamma(5+k)-4(k+3)\Gamma\left(2+\dfrac{k}{2}\right)\Gamma\left(3+\dfrac{k}{2}\right)}{3k(k+3)\Gamma\left(3+\dfrac{k}{2}\right)^2}\right]. \tag{29}$$

In particular the mean random line segment is

$$\overline{s}=\frac{4(32-3\pi)}{135\pi}D. \tag{30}$$

C. Square

To the author's knowledge the chord length distribution function for the square has not been derived. However, Ghosh[8] found that the cumulative probability for the distance between two points randomly positioned in a unit square is

$$T(z)=\begin{cases}z^2\left(\dfrac{z^2}{2}-\dfrac{8z}{3}+\pi\right) & (0\leqslant z\leqslant 1) \\ \dfrac{4}{3}\sqrt{z^2-1}(2z^2+1)-\left(\dfrac{z^4}{2}+2z^2-\dfrac{1}{3}\right) & \\ \quad+2z^2\left(\arcsin\left(\dfrac{1}{z}\right)-\arccos\left(\dfrac{1}{z}\right)\right) & (1<z\leqslant\sqrt{2})\end{cases}. \tag{31}$$

Thus, the probability distribution of the distance is

$$t(z)=\begin{cases}2\pi z+2z^2(z-4) & (0\leqslant z\leqslant 1) \\ -4z-2z^2+\dfrac{16}{3}z\sqrt{z^2-1}-\dfrac{8}{3}\dfrac{z}{\sqrt{z^2-1}}+\dfrac{8}{3}\dfrac{z^3}{\sqrt{z^2-1}} & \\ \quad+4z\left(\arcsin\left(\dfrac{1}{z}\right)-\arccos\left(\dfrac{1}{z}\right)\right) & (1<z\leqslant\sqrt{2})\end{cases}. \tag{32}$$

Since $\overline{l^2}$ is unknown, we use Eq. (15) to compute $s(z)$; the denominator of Eq. (15) is

$$\int_0^{\sqrt{2}}\frac{t(z)}{z}dz=\frac{4}{3}[1-\sqrt{2}+3\log(1+\sqrt{2})]=C_0, \tag{33}$$

which is the mean value of the inverse of the distance for two random points inside the square. Finaly from Eqs. (15), (32), and (33) we get

$$s(z)=\frac{1}{C_0}\begin{cases} 2\pi z+2z^2(z-4) & (0\leqslant z\leqslant 1)\\ -4-2z+\dfrac{16}{3}\sqrt{z^2-1}-\dfrac{8}{3}\dfrac{1}{\sqrt{z^2-1}} & \\ +\dfrac{8}{3}\dfrac{z^2}{\sqrt{z^2-1}}+4\left(\arcsin\left(\dfrac{1}{z}\right)-\arccos\left(\dfrac{1}{z}\right)\right) & (1<z\leqslant\sqrt{2}) \end{cases}. \tag{34}$$

D. Cube

The chord density distribution for the three-dimensional unit cube has been obtained independently by several authors:[9,10]

$$p(l)=\frac{1}{3\pi}\begin{cases} 8-3l & (0\leqslant l\leqslant 1)\\ \dfrac{6\pi-1}{l^3}+6l-\dfrac{8}{l^3}(2l^2+1)\sqrt{l^2-1} & (1<l\leqslant\sqrt{2})\\ \dfrac{6\pi-5}{l^3}-3l+\dfrac{8}{l^3}(l^2+1)\sqrt{l^2-2} & \\ -\dfrac{24}{l^3}\arctan\sqrt{l^2-2} & (\sqrt{2}<l\leqslant\sqrt{3}) \end{cases}. \tag{35}$$

Unfortunately due to the term $\arctan(\sqrt{l^2-2})/l$, $\overline{l^2}$ cannot be simply evaluated. A numerical integration gives $\overline{l^2}=0.5978$. Using Eq. (13) with $B_3(\text{cube})=6\pi$ and another result due to Piefke[5] who found the density distribution of the distance inside the unit cube (see the Appendix for Piefke's result, where we calculate the interaction energy of two constant charge distributions inside a cube), we obtain

$$s(z)=\frac{1.673}{3\pi}\begin{cases} 4\pi-6\pi z+8z^2-z^3 & (0\leqslant z\leqslant 1)\\ \dfrac{6\pi-1}{z}-8\pi+6z+2z^3-\dfrac{8}{z}(2z^2+1)\sqrt{z^2-1} & \\ +24z\arccos\left(\dfrac{1}{z}\right) & (1<z\leqslant\sqrt{2})\\ \dfrac{6\pi-5}{z}+4\pi-6(1+\pi)z-z^3 & \\ +\dfrac{8}{z}(z^2+1)\sqrt{z^2-2}-\dfrac{24}{z}A(z) & (\sqrt{2}<z\leqslant\sqrt{3}) \end{cases} \tag{36}$$

with

$$A(z)=\arctan\sqrt{z^2-2}+2z\arctan(z^2-1-z\sqrt{z^2-2})-z^2\arctan\frac{1}{\sqrt{z^2-2}}.$$

Density distributions of random line segments inside a disk, a sphere, an hemisphere, a square, and a cube are plotted in Fig. 2.

E. Random media

In the last section we considered a two phase random media made of monosize hard spheres of radius R randomly placed in space. Under such conditions the system is statistically isotropic. Spheres fill the space with a volume fraction (or packing fraction) ϕ_2 and the void has the volume fraction $\phi_1=1-\phi_2$. Following Torquato[11] we define the chords as the line segments between the

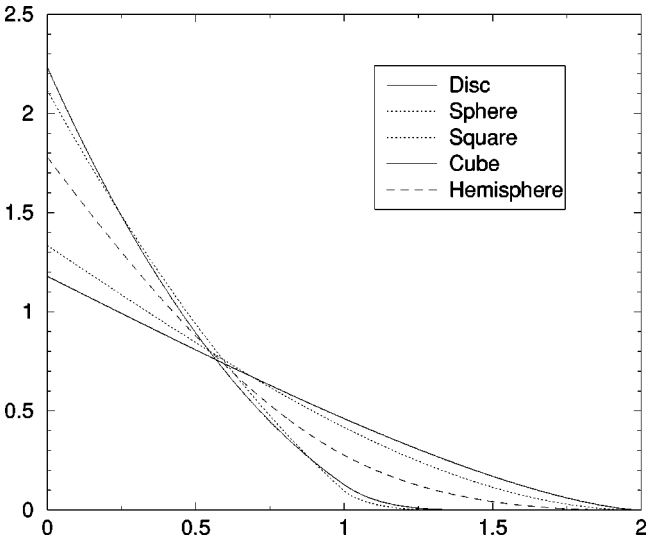

FIG. 2. Random line segment distribution functions for various geometric shapes.

intersections of an infinitely long line with the two-phase interface (these lines are measured as usual with the uniform density). The void is in general a nonconvex domain as shown in Fig. 3.

With these hypotheses, valid in any dimension, Torquato found that the density distribution function for the chords inside the void region is given by

$$p(l)=\frac{\phi_2\omega_{n-1}}{\phi_1\omega_n R}\exp\left[-\frac{\phi_2\omega_{n-1}}{\phi_1\omega_n}\frac{l}{R}\right], \tag{37}$$

where ω_n is the n-dimensional volume of the unit sphere, i.e., $\omega_n=\pi^{n/2}/\Gamma(1+n/2)$. Note that formula (37) is exact only in one dimension, in higher dimension formula (37) is an accurate approximation for isotropic equilibrium hard-sphere system Ref. 12. Since $\overline{l}=(\phi_1\omega_n R)/(\phi_2\omega_{n-1})$, we rewrite Eq. (37) as

$$p(l)=\frac{1}{\overline{l}}e^{-l/\overline{l}}. \tag{38}$$

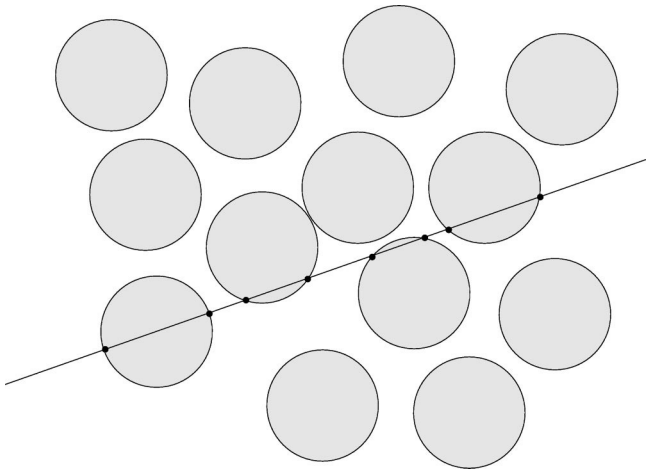

FIG. 3. Examples of chords for randomly placed disks in the plane.

From Eq. (38) we have immediately $\overline{l^2}=2\overline{l}^2$ and from Eq. (7):

$$s(z)=\frac{1}{\overline{l}}e^{-z/\overline{l}}. \tag{39}$$

So $p(l)$ and $s(z)$ have the same distribution function. As a matter of fact, in an infinite medium, if $p(l)$ and $s(z)$ are the same, they must be exponential distributions (38): In Eq. (8), with $s(z)=p(z)$ we have: $d^2s(z)/dz^2=2s(z)/\overline{l^2}$ whose solution with the condition $\int_0^\infty s(z)dz=1$ is:

$$s(z)=\sqrt{\frac{2}{\overline{l^2}}}\exp\left[-\sqrt{\frac{2}{\overline{l^2}}}z\right],$$

which is just Eq. (39).

Moreover, for asymptotically large n we have

$$\overline{s}\underset{n\to\infty}{\sim}\frac{\phi_1}{\phi_2}\sqrt{\frac{n}{2}}R. \tag{40}$$

Thus, as n gets large, the behavior of $\overline{s_{\text{void}}}$ is the inverse of $\overline{s_{\text{sphere}}}$ (see Eq. (21)). More precisely

$$\overline{s_{\text{void}}}\ \overline{s_{\text{sphere}}}=\frac{R^2}{2}\sqrt{\pi}\frac{\phi_1}{\phi_2}, \tag{41}$$

which is independent of n.

Lu and Torquato[13] also introduce a useful statistical measure $L^i(z)$ called the lineal-path-function, which is defined for statistically isotropic media as the probability that a line segment of length z lies wholly in phase i when randomly thrown into the sample.

Note that $L^i(z)$ is a probability and not a probability density. Using a simple probabilist argument these authors[12] show that $L^i(z)$ is related to the usual chord length probability density function in phase i, $p^i(z)$ by

$$L^i(z)=\frac{\phi_i}{\overline{l}}\int_0^\infty \Theta(y-z)(y-z)p(y)dy. \tag{42}$$

So we have immediately from Eqs. (42) and (7) the simple relation between $L^i(z)$ and $s^i(z)$:

$$L^i(z)=\phi_i\frac{\overline{l^2}}{2\overline{l}}s^i(z). \tag{43}$$

IV. CONCLUSION

As already noted by Santalo,[2] the problem of finding the measure of segments of a constant length that are contained in a convex body has no simple solution. The solution depends largely on the shape of the body through the $\overline{l^2}$ term. However this article shows that the links between the segment distribution function and other distribution functions thoroughly covered in the literature, allow us to find an analytical solution for several geometric shapes such as the square, the cube, or the hemisphere. Results can also be applied for certain types of random media where the chord distribution function is well defined. Moreover, in the Appendix, we have shown that geometric probability techniques are a powerful tool for calculating quantities that are extremely difficult to treat otherwise.

ACKNOWLEDGMENTS

It is a pleasure to thank Jean-Pierre Both, Cheikh Diop, Benoît Roesslinger, and David Gueron for reading the manuscript and their comments.

APPENDIX: INTERACTION ENERGY OF TWO CONSTANT CHARGE DISTRIBUTIONS IN A CUBE

In this Appendix, we show how Piefke's results regarding the random distribution of distance inside a cube, allow us to calculate the electrostatic energy of two constant charge distributions inside a cube. So far, this quantity, of interest in the theory of ionic crystals as well as in other areas of solid state theory (Ref. 14), has only been evaluated numerically (Ref. 15).

We consider two electrons of charge e in a cubic box of length L and we assume that both electrons have a constant charge density $\rho=e/L^3$ in this box. The Coulomb electrostatic interaction energy of such a charge distribution is:

$$\left[\int_{r_1\in\Omega_L^1}\left(\int_{r_2\in\Omega_L^2}\frac{d\mathbf{V}_2}{|\mathbf{r}_1-\mathbf{r}_2|}\right)d\mathbf{V}_1\right]\left(\frac{e}{L^3}\right)^2\equiv C_c\frac{e^2}{L^6}, \tag{A1}$$

where Ω_L^i $(i=1,2)$ denote the cubic regions over which the integration variables, $r_i=(x_i,y_i,z_i)$ take their values. If we introduce units so that $e=L=1$ these regions are then $\Omega^i=\{(x_i,y_i,z_i);\ 0\leqslant x_i\leqslant 1,\ 0\leqslant y_i\leqslant 1,\ 0\leqslant z_i\leqslant 1\}$ $(i=1,2)$ and the energy can simply be expressed as

$$C_c=\int_{\Omega^1}\int_{\Omega^2}\frac{d\mathbf{V}_1 d\mathbf{V}_2}{|\mathbf{r}_1-\mathbf{r}_2|} \tag{A2}$$

or alternatively in the form of a six-dimensional integral

$$C_c=\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\frac{dx_1dy_1dz_1dx_2dy_2dz_2}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}}. \tag{A3}$$

Essen and Nordmark have performed this integral numerically (five integrations are done analytically and the last integration is done numerically, see Ref. 15 for calculation details), they found:

$$C_c=1.882\ \ 312\ \ 645. \tag{A4}$$

In light of geometric probability, integral (A2) is reinterpreted as the average of the function $1/z$ taken with the probability density function $t(z)$ of finding two points separated by a distance z, randomly chosen in a uniform cube. So, C_c immediately appears as a one-dimensional integral:

$$C_c=\int_0^\delta dz\,\frac{t(z)}{z}. \tag{A5}$$

This approach has been applied with success for general radial potential Ref. 16 and the uniform ellipsoid Ref. 17. We used Piefke's formula Ref. 5 for the density distribution of the distance inside the unit cube

$$t(z)=\begin{cases}4\pi z^2-6\pi z^3+8z^4-z^5\equiv t_1(z) & (0\leqslant z\leqslant 1)\\ (6\pi-1)z-8\pi z^2+6z^3+2z^5-8z(2z^2+1)\sqrt{z^2-1} & \\ \quad+24z\arccos\left(\dfrac{1}{z}\right)\equiv t_2(z) & (1<z\leqslant\sqrt{2})\\ (6\pi-5)z+4\pi z^2-6(1+\pi)z^3-z^5 & \\ \quad+8z(z^2+1)\sqrt{z^2-2}-24zA(z)\equiv t_3(z) & (\sqrt{2}<z\leqslant\sqrt{3})\end{cases} \tag{A6}$$

with:

$$A(z)=\arctan\sqrt{z^2-2}+2z\arctan(z^2-1-z\sqrt{z^2-2})-z^2\arctan\frac{1}{\sqrt{z^2-2}}.$$

So C_c is

$$C_c=\int_0^1\frac{t_1(z)}{z}dz+\int_1^{\sqrt{2}}\frac{t_2(z)}{z}dz+\int_{\sqrt{2}}^{\sqrt{3}}\frac{t_3(z)}{z}dz. \tag{A7}$$

These three integrals can be evaluated analytically and we obtain

$$\int_0^1\frac{t_1(z)}{z}dz=\frac{9}{5},$$

$$\int_1^{\sqrt{2}}\frac{t_2(z)}{z}dz=-\frac{7}{5}-\frac{47\sqrt{2}}{5}+10(\sqrt{2}-1)\pi+2\log(1+\sqrt{2}), \tag{A8}$$

$$\int_{\sqrt{2}}^{\sqrt{3}}\frac{t_3(z)}{z}dz=\frac{49\sqrt{2}}{5}-\frac{4\sqrt{3}}{5}+\left(\frac{28}{3}-10\sqrt{2}\right)\pi-2\log 2+4\log(1+\sqrt{3}),$$

and eventually the constant C_c is

$$C_c=\frac{2}{5}+\frac{2\sqrt{2}}{5}-\frac{4\sqrt{3}}{5}-\frac{2\pi}{3}-2\log 2+2\log(1+\sqrt{2})+4\log(1+\sqrt{3}). \tag{A9}$$

The numerical value is $C_c=1.882\ 312\ 644\ 389$, which is very close to the approximate value of Eq. (A4) given by Essen and Nordmark.

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Induced representations of $U_q so(5)$

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(Received 15 February 2002; accepted 21 October 2002)

We study the reduction of the left regular representation of the quantum algebra $U_q so(5)$. This yields induced representations of $U_q so(5)$ on some quotient space of the matrix quantum group $SO_q(5)$. To facilitate the construction of a suitable basis the Gauss decomposition of $SO_q(5)$ is worked out explicitly. We then investigate the behavior of these representations for a generic q as well as when q is an Nth root of unity leading to some finite dimensional irreducible representations of $U_q so(5)$. Two basic intertwining operators are also constructed via the right action. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1531822]

I. INTRODUCTION

A canonical method for the construction of differential operators intertwining representations of semisimple Lie groups was proposed in Ref. 1. This rather algebraic procedure was generalized to the case of quantum groups also. The left regular representation, its reduction to infinite family of reducible and irreducible representaions and the q-difference intertwining operators were studied on many quantum algebras, namely, the Lorentz quantum algebra,[2] the Euclidean algebra $U_q e(2)$ (Ref. 3) [as a contraction of $U_q sl(2)$] and generalizations to $U_q sl(3)$ (Ref. 4) and $U_q sl(n)$.[5,6] Recently induced representations of the three dimensional quantum orthogonal algebra $U_q so(3)$ have also been obtained.[7]

In this article we investigate the case of $U_q so(5,\mathbb{C})$, a quantization of the five dimensional complex special orthogonal Lie algebra of rank two. For simplicity we shall prefer to call it just $U_q so(5)$ (and similarly for the dual group). Besides being computationally horrendous, it presents some interesting features which would facilitate generalization to the n-dimensional case and also help us to understand better the important relation between representation theory and the geometry of quantum groups. On the other hand, one of the real forms of this algebra obtained by conjugation is the noncompact quantum anti-de Sitter (AdS) algebra $U_q so(3,2)$ which happens to be the symmetry algebra of the noncommutative AdS space. This aroused a lot of interest especially after the AdS–conformal field theory duality conjecture was formulated (see, for example, Ref. 8 and references therein for physical applications). This connection motivates us further to look at $U_q so(5)$ in somewhat more detail but mainly from the point of view of representation theory.

We start out by defining the quantum matrix group $SO_q(5)$ and the quantum algebra $U_q so(5)$ in Sec. II. The duality pairings between these two Hopf algebras are explicitly given. In Secs. III and IV we present the left and right regular representations of $U_q so(5)$ on the matrix elements (generators) of the dual group $SO_q(5)$. Recall that the classical SO(5) group is defined by ten independent generators, whereas here our quantum group $SO_q(5)$ has 25 generators. We must therefore, redefine these generators to get only ten independent ones. The monomials in these would give us a suitable basis to extend the left and right action. This is achieved by Gauss decomposition of the quantum matrix belonging to $SO_q(5)$ and is explicitly worked out in Sec. V.

Next, in Sec. VI we carry out the procedure of reduction of the left regular representation. As in the classical case the left and right actions commute (due to associativity). Therefore, we use the right covariance to reduce the left regular representation, i.e., we select the eigenspaces of the right regular representation of some particular generators of the quantum algebra $U_q so(5)$. This basi-

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cally implies imposing the condition that the Cartan generators act as a multiplication by a constant and that some of the aforementioned generators act as a multiplication by zero. In this way we obtain an infinite family of induced representations of $U_q$so(5) realized on the noncommutative coset space of $SO_q(5)$. In Sec. VII we investigate the reducibility of these induced representaions when q is in general a complex number and also when q is an Nth root of unity. This leads to some finite dimensional irreducible representations under some restricted values of the labels which parametrize them. The right action of the remaining generators on the basis is presented in Sec. VIII. These remaining $U_q$so(5) generators yield (via the right action) interesting intertwining operators which we give in Sec. IX. The explicit commutation relations of the quantum group $SO_q(5)$ are contained in the Appendix. We conclude the article with some remarks.

II. $SO_q(5)$ AND THE DUAL $U_q$so(5)

We begin by defining the matrix quantum group $SO_q(5)$ and its corresponding quantum universal enveloping algebra $U_q$so(5) which can be recovered from the general formulas of Ref. 9.

$SO_q(5)$ is generated by I and elements $T=(t_{ij})$, $i,j=1,\ldots,5$, obeying the following commutation relations:

$$RT_1T_2 = T_2T_1R, \tag{2.1}$$

$$TCT^tC^{-1} = CT^tC^{-1}T = I, \tag{2.2}$$

where R is a quantum $5^2\times 5^2$ invertible matrix, $T_1=T\otimes I$, $T_2=I\otimes T$, I is the identity 5×5 matrix, and C is an (antidiagonal) 5×5 matrix. The coalgebra structure is given by the following co-product Δ, co-unit ε, and antipode S:

$$\Delta(t_{ij}) = \sum_{k=1}^{5} t_{ik}\otimes t_{kj}, \tag{2.3a}$$

$$\varepsilon(t_{ij}) = \delta_{ij}, \tag{2.3b}$$

$$S(T) = C\ T^t\ C^{-1}. \tag{2.3c}$$

Using this compact matrix form relations (2.2) can be rewritten in the general form:

$$T\ S(T) = S(T)\ T = I. \tag{2.4}$$

The quantum R-matrix is given by

$$\begin{aligned} R= & \ q\sum_{i\neq i'}^{5} e_{ii}\otimes e_{ii}+e_{3,3}\otimes e_{3,3}+\sum_{i\neq j,j'}^{5} e_{ii}\otimes e_{jj}+q^{-1}\sum_{i\neq i'}^{5} e_{i'i'}\otimes e_{ii} \\ & +\lambda\sum_{i>j}^{5} e_{ij}\otimes e_{ji}-\lambda\sum_{i>j}^{5} q^{\rho_i-\rho_j}e_{ij}\otimes e_{i'j'}, \end{aligned} \tag{2.5}$$

with $\lambda=q-q^{-1}$, $(\rho_1,\ldots,\rho_5)=(\frac{3}{2},\frac{1}{2},0,-\frac{1}{2},-\frac{3}{2})$ and $i'=5+1-i$. For $SO_q(5)$ the quantum R matrix is a lower triangular 25×25 matrix whose non zero elements are explicitly given below $(R_{ij}^{kl}=e_{ik}\otimes e_{jl})$:

$$R_{ii}^{ii}=q,\ i\neq 3, \qquad R_{ii'}^{ii'}=q^{-1},\ i\neq 3, \qquad R_{33}^{33}=1,$$

$$R_{ij}^{ij}=1,\ i\neq j,j', \qquad R_{ij}^{ji}=\lambda, \quad i>j, \quad i\neq j',$$

$$R^{24}_{33}=R^{33}_{42}=-\lambda q^{-1/2}=\alpha, \qquad R^{24}_{42}=-\lambda(q^{-1}-1)=\beta, \tag{2.6}$$

$$R^{15}_{42}=R^{24}_{51}=-\lambda q^{-2}=\gamma, \qquad R^{15}_{51}=-\lambda(q^{-3}-1)=\delta,$$

$$R^{15}_{33}=R^{33}_{51}=-\lambda q^{-3/2}=\eta, \qquad R^{15}_{24}=R^{42}_{51}=-\lambda q^{-1}=\xi.$$

The corresponding antidiagonal C-matrix is

$$C = \begin{pmatrix} 0 & 0 & 0 & 0 & q^{-3/2} \\ 0 & 0 & 0 & q^{-1/2} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & q^{1/2} & 0 & 0 & 0 \\ q^{3/2} & 0 & 0 & 0 & 0 \end{pmatrix}, \quad C^2 = I. \tag{2.7}$$

In order to derive the explicit commutation relations among the 25 generators t_{ij} of $\mathrm{SO}_q(5)$ we need to substitute the above R and C matrices in the defining relations (2.1) and (2.2).

By doing so we get an overwhelming number of relations ($\approx$400). These have been condensed to less than 40 in such a way that transparency is not lost. They are given in the Appendix as they would be essential for the Gauss decomposition in Sec. V.

The quantum universal enveloping algebra $\mathrm{U}_q\mathrm{so}(5)$ dual to $\mathrm{SO}_q(5)$ is generated by the unit 1 and the functionals l^+_{ij} with $i<j$; l^-_{ij} with $i>j$; l^+_{ii} and l^-_{ii}, where $i,j=1,\ldots,5$. When arranged in upper- and lower-triangular matrices $L^{\pm}$, respectively, they are defined by the duality conditions[9]

$$(L^{\pm},\ T_1 \ldots T_m)=R^{\pm}_1 \cdots R^{\pm}_m \ , \quad \text{for } m=1,2,\ldots, \tag{2.8}$$

where for $1\leqslant \ell \leqslant m$, $T^{\pm}_{\ell}$ act in the ℓth factor; $R^{\pm}_{\ell}$ act in the $(0,\ell)$th factor of $(\mathbb{C}^5)^{\otimes(m+1)}$; $R^+ = PRP$, $R^- = R^{-1}$ and $P \in \mathrm{Mat}(\mathbb{C}^5 \otimes \mathbb{C}^5)$ is the permutation matrix.

The commutation relations are written in a compact form

$$R^+ L^{\pm}_1 L^{\pm}_2 = L^{\pm}_2 L^{\pm}_1 R^+ \ , \quad R^+ L^+_1 L^-_2 = L^-_2 L^+_1 R^+. \tag{2.9}$$

Additional constraints are

$$l^+_{ii} l^-_{ii} = l^-_{ii} l^+_{ii} = 1, \ \ i=1,...,5 \ ; \tag{2.10}$$

$$l^+_{11} \cdots l^+_{55} = l^-_{11} \cdots l^-_{55} = 1 \ ; \tag{2.11}$$

$$L^{\pm} C^t (L^{\pm})^t (C^{-1})^t = C^t (L^{\pm})^t (C^{-1})^t L^{\pm} = I. \tag{2.12}$$

The complete Hopf algebra structure is given by

$$\Delta(l^{\pm}_{ij}) = \sum_{k=1}^{5} l^{\pm}_{ik} \otimes l^{\pm}_{kj}, \tag{2.13}$$

$$\varepsilon(l^{\pm}_{ij}) = \delta_{ij}, \tag{2.14}$$

$$S(L^{\pm}) = C^t (L^{\pm})^t (C^{-1})^t. \tag{2.15}$$

Since we shall be needing the explicit form of the antipode in defining the left action in the next section, we give it below:

$$S(L^+) = \begin{pmatrix} l_{55}^+ & q l_{45}^+ & q^{3/2} l_{35}^+ & q^2 l_{25}^+ & q^3 l_{15}^+ \\ 0 & l_{44}^+ & q^{1/2} l_{34}^+ & q l_{24}^+ & q^2 l_{14}^+ \\ 0 & 0 & l_{33}^+ & q^{1/2} l_{23}^+ & q^{3/2} l_{13}^+ \\ 0 & 0 & 0 & l_{22}^+ & q l_{12}^+ \\ 0 & 0 & 0 & 0 & l_{11}^+ \end{pmatrix}, \tag{2.16}$$

$$S(L^-) = \begin{pmatrix} l_{55}^- & 0 & 0 & 0 & 0 \\ q^{-1} l_{54}^- & l_{44}^- & 0 & 0 & 0 \\ q^{-3/2} l_{53}^- & q^{-1/2} l_{43}^- & l_{33}^- & 0 & 0 \\ q^{-2} l_{52}^- & q^{-1} l_{42}^- & q^{-1/2} l_{32}^- & l_{22}^- & 0 \\ q^{-3} l_{51}^- & q^{-2} l_{41}^- & q^{-3/2} l_{31}^- & q^{-1} l_{21}^- & l_{11}^- \end{pmatrix}. \tag{2.17}$$

The $l_{ij}^{\pm}$ can be expressed in terms of more popular generators $H_i, X_i^{\pm}$, $i=1,2$, via

$$\begin{gathered} q^{H_2} = l_{11}^+ (l_{22}^+)^{-1}, \quad q^{H_1} = (l_{22}^+)^2, \\ X_2^- = \lambda^{-1} q^{1/2} l_{12}^+ (l_{11}^+)^{-1/2} (l_{22}^+)^{-1/2}, \quad X_1^- = \lambda^{-1} \sqrt{[2]_q} q^{1/2} l_{23}^+ (l_{22}^+)^{-1/2}, \\ X_2^+ = -\lambda^{-1} q^{-1/2} l_{21}^- (l_{11}^+)^{1/2} (l_{22}^+)^{1/2}, \quad X_1^+ = -\lambda^{-1} \sqrt{[2]_q} l_{32}^- (l_{22}^+)^{1/2}. \end{gathered} \tag{2.18}$$

They satisfy the following commutation relations:

$$\begin{gathered} [H_i, H_j] = 0, \ [H_i, X_j^{\pm}] = \pm (a_{ij}) X_j^{\pm}, \ i,j = 1,2, \\ [X_i^+, X_j^-] = \delta_{ij} [H_i]_{q_i}, \ q_1 = q, \ q_2 = q^2, \\ (X_1^{\pm})^3 X_2^{\pm} - [3]_{q_1} (X_1^{\pm})^2 X_2^{\pm} X_1^{\pm} + [3]_{q_1} X_1^{\pm} X_2^{\pm} (X_1^{\pm})^2 - X_2^{\pm} (X_1^{\pm})^3 = 0, \\ (X_2^{\pm})^2 X_1^{\pm} - [2]_{q_2} X_2^{\pm} X_1^{\pm} X_2^{\pm} + X_1^{\pm} (X_2^{\pm})^2 = 0, \end{gathered} \tag{2.19}$$

where $[x]_{q_i} = (q_i^{x/2} - q_i^{-x/2})/(q_i^{1/2} - q_i^{-1/2})$ and $a_{ij} = \begin{pmatrix} 2 & -2 \\ -1 & 2 \end{pmatrix}$ is the Cartan matrix for so(5). The duality between $U_q so(5)$ and $SO_q(5)$ is given by the pairing (2.8) between the generators H_i, $X_i^{\pm}$ and the T matrix:

$$\langle H_1, T \rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \langle H_2, T \rangle = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\langle X_1^+, T \rangle = \sqrt{[2]_{q_1}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \langle X_1^-, T \rangle = \sqrt{[2]_{q_1}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{2.20}$$

$$\langle X_2^+, T\rangle = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \langle X_2^-, T\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \end{pmatrix}.$$

To complete the Hopf algebra structure, the other maps are given as ($i=1,2$)

$$\Delta(H_i) = 1\otimes H_i + H_i \otimes 1, \tag{2.21a}$$

$$\Delta(X_i^{\pm}) = q_i^{H_i/4}\otimes X_i^{\pm} + X_i^{\pm}\otimes q_i^{-H_i/4}, \tag{2.21b}$$

$$\varepsilon(H_i) = 0, \qquad \varepsilon(X_i^{\pm}) = 0, \tag{2.21c}$$

$$S(H_i) = -H_i, \qquad S(X_i^{\pm}) = -q_i^{-H_i/4} X_i^{\pm} q_i^{H_i/4}. \tag{2.21d}$$

III. LEFT REGULAR REPRESENTATION

The left regular representation of $U_q so(5)$ is defined in a standard way as

$$\pi_L(X)\ t_{ij} = \sum_{k=1}^{5} \langle S(X),\ t_{ik}\rangle\ t_{kj}, \qquad X \in U_q so(5), \tag{3.1}$$

which when $q=1$ can be seen as the infinitesimal version of

$$\pi_L(T')\ T = T'^{-1}\ T, \qquad T',\ T \in SO(5). \tag{3.2}$$

In the present case it is explicitly given as

$$\pi_L(H_1)T = 2 \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -t_{21} & -t_{22} & -t_{23} & -t_{24} & -t_{25} \\ 0 & 0 & 0 & 0 & 0 \\ t_{41} & t_{42} & t_{43} & t_{44} & t_{45} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\pi_L(H_2)T = \begin{pmatrix} -t_{11} & -t_{12} & -t_{13} & -t_{14} & -t_{15} \\ t_{21} & t_{22} & t_{23} & t_{24} & t_{25} \\ 0 & 0 & 0 & 0 & 0 \\ -t_{41} & -t_{42} & -t_{43} & -t_{44} & -t_{45} \\ t_{51} & t_{52} & t_{53} & t_{54} & t_{55} \end{pmatrix},$$

$$\pi_L(X_1^+)T = q_1^{-1/2}\sqrt{[2]}_{q_1} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -t_{31} & -t_{32} & -t_{33} & -t_{34} & -t_{35} \\ t_{41} & t_{42} & t_{43} & t_{44} & t_{45} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.3}$$

$$\pi_L(X_1^-)T = q_1^{1/2}\sqrt{[2]}_{q_1}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -t_{21} & -t_{22} & -t_{23} & -t_{24} & -t_{25} \\ t_{31} & t_{32} & t_{33} & t_{34} & t_{35} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\pi_L(X_2^+)T = q_2^{-1/2}\begin{pmatrix} -t_{21} & -t_{22} & -t_{23} & -t_{24} & -t_{25} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ t_{51} & t_{52} & t_{53} & t_{54} & t_{55} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\pi_L(X_2^-)T = q_2^{1/2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -t_{11} & -t_{12} & -t_{13} & -t_{14} & -t_{15} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ t_{41} & t_{42} & t_{43} & t_{44} & t_{45} \end{pmatrix},$$

supplemented by the following action on the unit element of $SO_q(5)$:

$$\pi_L(H_i)I=0, \qquad \pi_L(X_i^{\pm})I=0, \quad i=1,2. \tag{3.4}$$

The action π_L can be extended on arbitrary monomials by making use of the following twisted derivation rule consistent with the coproduct and the representation structure:

$$\pi_L(x)a\ \ b = m(\pi_L(\sigma\circ\Delta(x))(a\otimes b)), \tag{3.5}$$

where m is the multiplication map and σ is the permutation operator. Explicitly we obtain

$$\pi_L(H_i)a\ \ b = a\cdot\pi_L(H_i)\ \ b+\pi_L(H_i)\ \ a\cdot b, \tag{3.6a}$$

$$\pi_L(X_i^{\pm})a\ \ b = \pi_L(X_i^{\pm})\ \ a\cdot\pi_L(q_i^{H_i/4})\ \ b+\pi_L(q_i^{-H_i/4})\ \ a\cdot\pi_L(X_i^{\pm})\ \ b. \tag{3.6b}$$

Further, we have

$$\begin{aligned} \pi_L(xy) &= \pi_L(x)\cdot\pi_L(y), \\ \pi_L(\alpha x+\beta y) &= \alpha\pi_L(x) + \beta\pi_L(y), \quad \alpha,\beta\in\mathbb{C}, x,\ y\in U_q so(5). \end{aligned} \tag{3.7}$$

IV. RIGHT REGULAR REPRESENTATION

Analogous to the previous section we now introduce the right regular representation of $U_q so(5)$ on $SO_q(5)$ as

$$\pi_R(X)\ \ t_{ij} = \sum_{k=1}^{5} t_{ik}\ \langle X,\ t_{kj}\rangle, \qquad X\in U_q so(5), \tag{4.1}$$

which in the classical case is the infinitesimal counterpart of

$$\pi_R(T')T = TT', \quad T,\ T'\ \in SO(5). \tag{4.2}$$

The explicit expressions are given below in matrix form:

$$
\begin{aligned}
\pi_R(H_1)T &= 2\begin{pmatrix} 0 & t_{12} & 0 & -t_{14} & 0 \\ 0 & t_{22} & 0 & -t_{24} & 0 \\ 0 & t_{32} & 0 & -t_{34} & 0 \\ 0 & t_{42} & 0 & -t_{44} & 0 \\ 0 & t_{52} & 0 & -t_{54} & 0 \end{pmatrix}, \\
\pi_R(H_2)T &= \begin{pmatrix} t_{11} & -t_{12} & 0 & t_{14} & -t_{15} \\ t_{21} & -t_{22} & 0 & t_{24} & -t_{25} \\ t_{31} & -t_{32} & 0 & t_{34} & -t_{35} \\ t_{41} & -t_{42} & 0 & t_{44} & -t_{45} \\ t_{51} & -t_{52} & 0 & t_{54} & -t_{55} \end{pmatrix}, \\
\pi_R(X_1^+)T &= \sqrt{[2]}_{q_1}\begin{pmatrix} 0 & 0 & t_{12} & -t_{13} & 0 \\ 0 & 0 & t_{22} & -t_{23} & 0 \\ 0 & 0 & t_{32} & -t_{33} & 0 \\ 0 & 0 & t_{42} & -t_{43} & 0 \\ 0 & 0 & t_{52} & -t_{53} & 0 \end{pmatrix}, \\
\pi_R(X_1^-)T &= \sqrt{[2]}_{q_1}\begin{pmatrix} 0 & t_{13} & -t_{14} & 0 & 0 \\ 0 & t_{23} & -t_{24} & 0 & 0 \\ 0 & t_{33} & -t_{34} & 0 & 0 \\ 0 & t_{43} & -t_{44} & 0 & 0 \\ 0 & t_{53} & -t_{54} & 0 & 0 \end{pmatrix}, \\
\pi_R(X_2^+)T &= \begin{pmatrix} 0 & t_{11} & 0 & 0 & -t_{14} \\ 0 & t_{21} & 0 & 0 & -t_{24} \\ 0 & t_{31} & 0 & 0 & -t_{34} \\ 0 & t_{41} & 0 & 0 & -t_{44} \\ 0 & t_{51} & 0 & 0 & -t_{54} \end{pmatrix}, \\
\pi_R(X_2^-)T &= \begin{pmatrix} t_{12} & 0 & 0 & -t_{15} & 0 \\ t_{22} & 0 & 0 & -t_{25} & 0 \\ t_{32} & 0 & 0 & -t_{35} & 0 \\ t_{42} & 0 & 0 & -t_{45} & 0 \\ t_{52} & 0 & 0 & -t_{55} & 0 \end{pmatrix}.
\end{aligned}
\tag{4.3}
$$

Similar to the left action, the right action of the generators of $U_q so(5)$ on the unit element of $SO_q(5)$ is zero.

The twisted derivation rule is given by

$$
\pi_R(x)a \quad b = m(\pi_R(\Delta(x))(a\otimes b)), \tag{4.4}
$$

which in the present situation translates into

$$\pi_R(H_i)a\ \ b\ =\ a\cdot\pi_R(H_i)\ \ b+\pi_R(H_i)\ \ a\cdot\ \ b, \tag{4.5a}$$

$$\pi_R(X_i^{\pm})a\ \ b\ =\ \pi_R(X_i^{\pm})\ \ a\cdot\pi_R(q_i^{-H_i/4})\ \ b+\pi_R(q_i^{H_i/4})\ \ a\cdot\pi_R(X_i^{\pm})\ \ b. \tag{4.5b}$$

Note that since π_R is a representation, relations similar to (3.7) hold for the right action also.

V. GAUSS DECOMPOSITION OF $SO_q(5)$

We know that the classical SO(5) group is defined in terms of ten generators and the Poincare–Birkoff–Witt (PBW) basis is defined as monomials in these generators. We have seen in Sec. II that the quantum analog $SO_q(5)$ has 25 generators t_{ij} obeying hundreds of commutation relations among them, which gives us a lot of freedom to introduce the PBW basis. Here we shall adopt the method of Gauss decomposition to achieve it.

The Gauss decomposition for the quantum T matrix of the $SO_q(5)$ group is

$$T=T_LT_DT_U, \tag{5.1}$$

where $T_L=(l_{ij})$ is a strictly lower-triangular matrix with units on the main diagonal ($l_{ii}=1$), $T_D=\mathrm{diag}(A_{ii})$ and $T_U=(u_{ij})$ is a strictly upper-triangular matrix ($u_{ii}=1$). All these are 5×5 matrices, i.e., $i,\ j=1,\ldots,5$.

After very lengthy and cumbersome computations we find that the matrix elements can be described in terms of generators of which only ten are independent. The diagonal generators A_{ii} are assumed to be invertible:

$$A_{11}=t_{11},\qquad A_{22}=t_{22}-t_{21}{t_{11}}^{-1}t_{12}\ =\ t_{22}-l_{21}A_{11}u_{12},$$

$$A_{33}=t_{33}-l_{31}A_{11}u_{13}-l_{32}A_{22}u_{23}\ =1, \tag{5.2}$$

$$A_{44}={A_{22}}^{-1},\qquad A_{55}={A_{11}}^{-1},$$

$$u_{12}={t_{11}}^{-1}t_{12},\quad u_{13}={t_{11}}^{-1}t_{13},\quad u_{14}={t_{11}}^{-1}t_{14},$$

$$u_{15}={t_{11}}^{-1}t_{15}=-u_{12}u_{14}-q[2]^{-1}{u_{13}}^2,$$

$$u_{23}={A_{22}}^{-1}(t_{23}-t_{21}{t_{11}}^{-1}t_{13}),\quad u_{24}=-[2]^{-1}{u_{23}}^2, \tag{5.3}$$

$$u_{25}=-u_{24}u_{12}-q^{-1/2}u_{23}u_{13}-q^{-1}u_{14},\quad u_{34}=-q^{1/2}u_{23},$$

$$u_{35}=q^{1/2}u_{23}u_{12}-q^{-1/2}u_{13},\quad u_{45}=-u_{12},$$

$$l_{21}=t_{21}{t_{11}}^{-1},\quad l_{31}=t_{31}{t_{11}}^{-1},\quad l_{41}=t_{41}{t_{11}}^{-1},$$

$$l_{51}=t_{51}{t_{11}}^{-1}=-l_{21}l_{41}-q[2]^{-1}{l_{31}}^2,$$

$$l_{32}=(t_{32}-t_{31}{t_{11}}^{-1}t_{12}){A_{22}}^{-1},\quad l_{42}=-[2]^{-1}{l_{32}}^2, \tag{5.4}$$

$$l_{52}=-l_{21}l_{42}-q^{1/2}l_{31}l_{32}-ql_{41},\quad l_{43}=-q^{-1/2}l_{32},$$

$$l_{53}=q^{-1/2}l_{21}l_{32}-q^{1/2}l_{31},\quad l_{54}=-l_{21},$$

where $[2]=(q-q^{-1})/(q^{1/2}-q^{-1/2})$.

It turns out that A_{33} commutes with all the other generators, hence we have set it to 1. So the ten independent generators are A_{11}, A_{22}, u_{12}, u_{13}, u_{14}, u_{23}, l_{21}, l_{31}, l_{41} and l_{32}. Below we give the commutation relations among them ($i,j=2,3,4$) by making use of the relations between the t_{ij} from the Appendix:

$$
\begin{aligned}
A_{11}u_{1i} &= q u_{1i} A_{11}, \qquad & A_{11}l_{i1} &= q l_{i1} A_{11}, \\
A_{11}u_{23} &= u_{23} A_{11}, \qquad & A_{11}l_{32} &= l_{32} A_{11}, \\
[u_{ki}, l_{jl}] &= 0, \ k,l=1,2, \quad k<i, \quad j>l, \qquad & A_{11}A_{22} &= A_{22}A_{11}, \\
A_{22}u_{12} &= q^{-1} u_{12} A_{22}, \qquad & A_{22}l_{21} &= q^{-1} l_{21} A_{22}, \\
A_{22}u_{13} &= u_{13} A_{22}, \qquad & A_{22}l_{31} &= l_{31} A_{22}, \\
A_{22}u_{14} &= q u_{14} A_{22}, \qquad & A_{22}l_{41} &= q l_{41} A_{22}, \\
A_{22}u_{23} &= q u_{23} A_{22}, \qquad & A_{22}l_{32} &= q l_{32} A_{22}, \\
u_{12}u_{13} &= q u_{13} u_{12}, \qquad & l_{21}l_{31} &= q l_{31} l_{21}, \\
u_{12}u_{14} &= u_{14}u_{12} - \lambda [2]^{-1} u_{13}u_{13}, \qquad & l_{21}l_{41} &= l_{41}l_{21} - \lambda [2]^{-1} l_{31}l_{31}, \\
u_{12}u_{23} &= q^{-1} u_{23}u_{12} + q^{-1}\lambda u_{13}, \qquad & l_{21}l_{32} &= q^{-1} l_{32}l_{21} + \lambda l_{31}, \\
u_{13}u_{14} &= q u_{14}u_{13}, \quad & l_{31}l_{41} &= q l_{41}l_{31}, \\
u_{13}u_{23} &= u_{23}u_{13} - q^{-1/2}\lambda u_{14}, \qquad & l_{31}l_{32} &= l_{32}l_{31} - q^{1/2}\lambda l_{41}, \\
u_{14}u_{23} &= q u_{23}u_{14}, \qquad & l_{41}l_{32} &= q l_{32}l_{41}.
\end{aligned}
\tag{5.5}
$$

There is an inherent symmetry in the relations for u's and l's. Note that the diagonal generators A_{ii} form an Abelian subgroup while A_{22}, u_{23} and l_{32} generate the subgroup $\mathrm{SO}_q(3)$. The above commutation relations obtained by Gauss decomposition are much simpler in form and easier to handle and would thus result in a convenient basis for $\mathrm{SO}_q(5)$.

VI. INDUCED REPRESENTATIONS

In this section we shall use the right action to reduce the left regular representation (which is highly reducible). But before we do so we need to construct a basis from the above ten independent generators. Let us choose the following ordering. Then the representation space will have elements which are formal power series in the basis:

$$
\phi \ = \ \sum \ {l_{21}}^{n_1} {l_{31}}^{n_2} {l_{41}}^{n_3} {l_{32}}^{n_4} {A_{11}}^{n_5} {A_{22}}^{n_6} {u_{12}}^{n_7} {u_{13}}^{n_8} {u_{14}}^{n_9} {u_{23}}^{n_{10}}. \tag{6.1}
$$

Here the summation is over n_i, $i=1,2,\ldots,10$. They take values in the set of non-negative integers $\mathbb{Z}_+$, except n_5 and n_6 which belong to the set of integers $\mathbb{Z}$.

We shall now impose the condition of (infinitesimal) right covariance on this independent basis of $\mathrm{SO}_q(5)$. This essentially means annihilation by the raising operators X_i^+ and scalar multiplication by exponentials of the Cartan generators H_i (similar to a highest weight module). Therefore, the right covariance conditions for the holomorphic representations with respect to X_1^+, X_2^+, K_1 and K_2 where $K_1 = q_1^{H_1/2}$, $K_2 = q_2^{H_2/2}$ are given by

$$
\pi_R(X_i^+) \ \phi \ = \ 0, \qquad i=1,2, \tag{6.2a}
$$

$$
\pi_R(K_1) \ {l_{21}}^{n_1} \cdots {u_{23}}^{n_{10}} \ = \ q^{n_6+n_7-n_9-n_{10}} \ {l_{21}}^{n_1} \cdots {u_{23}}^{n_{10}}, \tag{6.2b}
$$

$$
\pi_R(K_2) \ {l_{21}}^{n_1} \cdots {u_{23}}^{n_{10}} \ = \ q^{n_5-n_6-2n_7-n_8+n_{10}} \ {l_{21}}^{n_1} \cdots {u_{23}}^{n_{10}}. \tag{6.2c}
$$

All the l's and A's are annihilated by the right action of X_1^+ and X_2^+ whereas we get nontrivial action on the u's. Thus (6.2) implies that the function ϕ does not depend on u's and hence it is reduced to

$$\phi = \sum_{\substack{n_1,\ldots,n_4\in\mathbb{Z}_+ \\ n_5,n_6\in\mathbb{Z}}} {l_{21}}^{n_1}{l_{31}}^{n_2}{l_{41}}^{n_3}{l_{32}}^{n_4}{A_{11}}^{n_5}{A_{22}}^{n_6}. \tag{6.3}$$

For convenience let us denote by Φ the above ordered monomial, i.e.,

$$\Phi =: {l_{21}}^{n_1}{l_{31}}^{n_2}{l_{41}}^{n_3}{l_{32}}^{n_4}{A_{11}}^{n_5}{A_{22}}^{n_6}. \tag{6.4}$$

Then the right covariance conditions on the reduced basis become

$$\pi_R(X_i^+)\ \Phi = 0, \tag{6.5a}$$

$$\pi_R(K_1)\ \Phi = q^{n_6}\ \Phi, \tag{6.5b}$$

$$\pi_R(K_2)\ \Phi = q^{n_5-n_6}\ \Phi. \tag{6.5c}$$

So the monomial Φ forms a basis in the space of common solutions of the equations (6.5). The above algebra with PBW basis Φ may be viewed as the q-deformation of the quotient manifold $\mathrm{SO}(5)/U$, where U is the subgroup of upper diagonal matrices with 1 on the diagonal.

Next, we shall reduce the left regular representation on the eigenspaces of the right regular representation obtained above. For this we need the left action of K_1 and K_2 on the reduced basis Φ. This turns out to be

$$\pi_L(K_1)\ \Phi = q^{-n_1+n_3+n_4-n_6}\ \Phi, \tag{6.6a}$$

$$\pi_L(K_2)\ \Phi = q^{2n_1+n_2-n_4-n_5+n_6}\ \Phi. \tag{6.6b}$$

In order to proceed for the calculation of the left action of X_i^+ and X_i^- on Φ, it would be convenient to first find the action on the powers of the individual generators. This is obtained by iterating the twisted derivation rule (3.6) which yields

$$\pi_L(X_1^+)\ {l_{21}}^{n_1} = -\sqrt{[2]}\ q^{-n_1/2}\ [n_1]_{q^2}\ {l_{21}}^{n_1-1}\ l_{31}, \tag{6.7a}$$

$$\pi_L(X_1^+)\ {l_{31}}^{n_2} = \sqrt{[2]}\ q^{-n_2/2}\ [n_2]_q\ {l_{31}}^{n_2-1}\ l_{41}, \tag{6.7b}$$

$$\pi_L(X_1^+)\ {l_{41}}^{n_3} = 0, \tag{6.7c}$$

$$\pi_L(X_1^+)\ {l_{32}}^{n_4} = \sqrt{[2]}^{-1}\ q^{-1}\ [n_4]_q\ {l_{32}}^{n_4+1}, \tag{6.7d}$$

$$\pi_L(X_1^+)\ {A_{11}}^{n_5} = 0, \tag{6.7e}$$

$$\pi_L(X_1^+)\ {A_{22}}^{n_6} = -\sqrt{[2]}\ q^{(n_6-2)/2}\ [n_6]_{q^2}\ l_{32}\ {A_{22}}^{n_6}, \tag{6.7f}$$

$$\pi_L(X_2^+)\ {l_{21}}^{n_1} = q^{-3/2}\ [n_1]_{q^2}\ {l_{21}}^{n_1+1}, \tag{6.8a}$$

$$\pi_L(X_2^+)\ {l_{31}}^{n_2} = q^{-(n_2+3)/2}\ [n_2]_{q^2}\ l_{21}\ {l_{31}}^{n_2}, \tag{6.8b}$$

$$\pi_L(X_2^+)\ {l_{41}}^{n_3} = -[2]^{-1}\ q^{-(2n_3+1)/2}\ [n_3]_{q^2}\ {l_{31}}^2\ {l_{41}}^{n_3-1}, \tag{6.8c}$$

$$\pi_L(X_2^+)\ l_{32}{}^{n_4} = -q^{(n_4-3)/2}\ [n_4]_{q^2}\ l_{21}\ l_{32}{}^{n_4} + q^{n_4-1}\ [n_4]_q\ l_{31}\ l_{32}{}^{n_4-1} + (q^{n_4}-1)[n_4-1]_q\ l_{41} l_{32}{}^{n_4-2}, \tag{6.8d}$$

$$\pi_L(X_2^+)\ A_{11}{}^{n_5} = -q^{(n_5-3)/2}\ [n_5]_{q^2}\ l_{21}\ A_{11}{}^{n_5}, \tag{6.8e}$$

$$\pi_L(X_2^+)\ A_{22}{}^{n_6} = q^{-(n_6+3)/2}\ [n_6]_{q^2}\ l_{21}\ A_{22}{}^{n_6}, \tag{6.8f}$$

$$\pi_L(X_1^-)\ l_{21}{}^{n_1} = 0, \tag{6.9a}$$

$$\pi_L(X_1^-)\ l_{31}{}^{n_2} = -\sqrt{[2]}\ q^{(2-n_2)/2}\ [n_2]_q\ l_{21}\ l_{31}{}^{n_2-1}, \tag{6.9b}$$

$$\pi_L(X_1^-)\ l_{41}{}^{n_3} = \sqrt{[2]}\ q^{(2-n_3)/2}\ [n_3]_{q^2}\ l_{31}\ l_{41}{}^{n_3-1}, \tag{6.9c}$$

$$\pi_L(X_1^-)\ l_{32}{}^{n_4} = -\sqrt{[2]}\ q\ [n_4]_q\ l_{32}{}^{n_4-1}, \tag{6.9d}$$

$$\pi_L(X_1^-)\ A_{11}{}^{n_5} = 0, \tag{6.9e}$$

$$\pi_L(X_1^-)\ A_{22}{}^{n_6} = 0, \tag{6.9f}$$

$$\pi_L(X_2^-)\ l_{21}{}^{n_1} = -q^{3/2}\ [n_1]_{q^2}\ l_{21}{}^{n_1-1}, \tag{6.10a}$$

$$\pi_L(X_2^-)\ l_{31}{}^{n_2} = 0, \tag{6.10b}$$

$$\pi_L(X_2^-)\ l_{41}{}^{n_3} = 0, \tag{6.10c}$$

$$\pi_L(X_2^-)\ l_{32}{}^{n_4} = 0, \tag{6.10d}$$

$$\pi_L(X_2^-)\ A_{11}{}^{n_5} = 0, \tag{6.10e}$$

$$\pi_L(X_2^-)\ A_{22}{}^{n_6} = 0. \tag{6.10f}$$

Using the above expressions and again using the twisted derivation rules (3.6) we obtain the left action of the generators on the entire monomial Φ:

$$\pi_L(X_1^+)\ \Phi = -q^{(-n_1+n_3+n_4-n_6)/2}\sqrt{[2]}[n_1]_{q^2}\ \Phi(n_1-1,\ n_2+2) + q^{(n_1-n_2+n_3+n_4-n_6)/2}\sqrt{[2]}[n_2]_q\ \Phi(n_2-1,\ n_3+1) + q^{(n_1-n_3+n_6-2)/2}\sqrt{[2]}[n_4/2-n_6]_{q^2}\ \Phi(n_4+1), \tag{6.11}$$

$$\pi_L(X_2^+)\ \Phi = q^{(-n_2+n_4+n_5-n_6-3)/2}[n_1+n_2-n_4-n_5+n_6]_{q^2}\ \Phi(n_1+1) - q^{(-2n_1-n_2-2n_3+3n_4+3n_5-3n_6-1)/2}[2]^{-1}[n_3]_{q^2}\ \Phi(n_2+2,\ n_3-1) + q^{(-2n_1-n_2-2n_3+2n_4+3n_5-3n_6-2)/2}[n_4]_q\ \Phi(n_2+1,\ n_4-1) + (q^{(-2n_1-n_2-n_5+n_6)/2}+q^{(-2n_1-n_2+n_4+n_5-n_6-2)/2}[n_5-n_6]_{q^2}\lambda) \times (q^{n_4}-1)[n_4-1]_q\ \Phi(n_3+1,\ n_4-2), \tag{6.12}$$

$$\pi_L(X_1^-)\ \Phi = q^{(n_1-n_2+n_3+n_4-n_6+2)/2}\sqrt{[2]}[n_2]_q\ \Phi(n_1+1,\ n_2-1) + q^{(n_1-n_3+n_4-n_6+2)/2}\sqrt{[2]}[n_3]_{q^2}\ \Phi(n_2+1,\ n_3-1) - q^{(n_1-n_3-n_6+2)/2}\sqrt{[2]}[n_4]_q\ \Phi(n_4-1), \tag{6.13}$$

$$\pi_L(X_2^-)\ \Phi = -q^{(n_2-n_4-n_5+n_6+3)/2}[n_1]_{q^2}\ \Phi(n_1-1). \tag{6.14}$$

Therefore, we have obtained induced representations of $U_q so(5)$ on the coset space of $SO_q(5)$ which are parametrized by the integers n_5 and n_6. The noncommutative representation space is spanned by functions Φ obeying the covariance conditions (6.5). Notice that the dependence of Φ on n_5 and n_6 remain constant under the above transformations. Hence it is appropriate to label our representaions by these two integers. For the remaining *n's* the left action induces an increase or decrease in some of these powers. For example, $\Phi(n_1-1, n_2+1)$ appearing on the r.h.s. means that the power of the generator l_{21} is lowered by one while that of l_{31} is raised by one, keeping the other powers constant. More explicitly,

$$\Phi(n_1-1,\ n_2+1)=l_{21}{}^{n_1-1}l_{31}{}^{n_2+1}l_{41}{}^{n_3}l_{32}{}^{n_4}A_{11}{}^{n_5}A_{22}{}^{n_6}.$$

VII. REDUCIBILITY FOR *q* GENERIC AND ROOT OF UNITY

The induced representations obtained above are in general irreducible for complex q and n_5, n_6. However, they become reducible for $q\in\mathbb{C}$ and some specific values of n_5 and n_6. The representation space decomposes into two invariant subspaces as we see below.

Setting $\pi_L(X_1^-)\ \Phi=0$ implies that $n_2=n_3=n_4=0$, which gives us the corresponding lowest weight vector, while setting $\pi_L(X_1^+)\ \Phi=0$ yields the highest weight vector under the condition $n_1=n_2=0$ and $n_4=2n_6$. We call this invariant subspace V_1. The parameter n_6 which up to now belonged to the set of integers, is restricted to only non-negative integers, i.e., $n_6\in\mathbb{Z}_+$.

Similarly for the second subspace V_2, by imposing $\pi_L(X_2^{\pm})\ \Phi=0$ we get the lowest weight vector when $n_1=0$ and the highest weight vector when $n_3=n_4=0$ and $n_1+n_2=n_5-n_6$. Since n_1 and n_2 are both non-negative integers, this restricts the values of $n_5-n_6\geqslant 0$. Thus we get finite dimensional irreducible representations of the quantum algebra $U_q so(5)$ obtained as subrepresentations of the elementary representations realized on the quotient group of $SO_q(5)$ and parametrized by n_5 and n_6.

Next, we wish to observe the behavior of our representations when q is a root of unity, i.e., $q^N=1$ for $N=3,4,5,\ldots$. For this we substitute $q=e^{2\pi i/N}$ and find conditions on the labels $n_1,\ldots,n_6$ for which the representations become reducible (i.e., r.h.s. becomes zero as was done above for the general q). One has to be careful here since we would be dealing with two different q-numbers $[n_j]_q$ and $[n_j]_{q^2}$. Hence we obtain

$$\pi_L(X_1^+)\ \Phi\ =\ 0,\quad n_1=k_1N',\quad n_2=k_2N,\qquad n_4/2-n_6=k'N', \tag{7.1}$$

where k_j $(j=1,2,3,4)$ $=0,1,2,3,\ldots$, $k'=0,\pm1,\pm2,\ldots$, $N'=N$ for odd N and $N/2$ for even N. Also $[2]=\sin(2\pi/N)/\sin(\pi/N)\neq 0$ since $N=3,4,\ldots$,

$$\pi_L(X_1^-)\ \Phi\ =\ 0,\quad n_2=k_2N,\quad n_3=k_3N',\quad n_4=k_4N, \tag{7.2}$$

$$\pi_L(X_2^+)\ \Phi\ =\ 0,\quad n_1+n_2-n_4-n_5+n_6=kN',\quad n_3=k_3N',\quad n_4=k_4N, \tag{7.3}$$

where $k=0,\pm1,\pm2,\ldots$,

$$\pi_L(X_2^-)\ \Phi\ =\ 0,\quad n_1=k_1N', \tag{7.4}$$

It is clear that in this case we have an enlarged center as elements of the form $(l_{ij})^N$ would belong to the center of the group. Analogously elements of the form $(X_i^{\pm})^N$ would lie in the center of the quantum algebra $U_q so(5)$.

Let us now analyze the non trivial conditions given above. The third condition in (7.1) can be written as $n_4=2(k'N'+n_6)$. We know that n_4 is a non-negative integer while n_6 is an integer. Hence two possibilities arise:

$$n_6\geqslant 0,\quad k'=0,1,2,\ \ldots\ , \tag{7.5a}$$

$$n_6<0,\quad k'N'\geqslant -n_6. \tag{7.5b}$$

The first condition in (7.3) can be written as $n_1+n_2=N+n_5-n_6+kN'$. Since the l.h.s. is always a non-negative number, there are three main possibilities:

(1) If $n_5-n_6>0$, then $k=0,1,2,\ldots$ (N and N' are positive valued). k can also have negative values provided $N+n_5-n_6\geqslant -KN'$.
(2) If $n_5-n_6=0$, then $k=0,1,2,\ldots$. No negative values are allowed here.
(3) If $n_5-n_6<0$, then $kN'+N\geqslant -(n_5-n_6)$.

There could be further many subcases of each of the three possibilities mentioned above:

(1) $n_5-n_6>0$ is possible when

$$n_5>0, \quad n_6>0, \quad n_5>n_6, \tag{7.6a}$$
$$n_5<0, \quad n_6<0, \quad n_5>n_6, \tag{7.6b}$$
$$n_5>0, \quad n_6<0, \tag{7.6c}$$
$$n_5>0, \quad n_6=0, \tag{7.6d}$$
$$n_5=0, \quad n_6<0. \tag{7.6e}$$

(2) $n_5-n_6=0$ is possible when

$$n_5=0, \quad n_6=0, \tag{7.7a}$$
$$n_5=n_6\neq 0. \tag{7.7b}$$

(3) $n_5-n_6<0$ is possible when

$$n_5>0, \quad n_6>0, \quad n_5<n_6, \tag{7.8a}$$
$$n_5<0, \quad n_6<0, \quad n_5<n_6, \tag{7.8b}$$
$$n_5<0, \quad n_6>0, \tag{7.8c}$$
$$n_5<0, \quad n_6=0, \tag{7.8d}$$
$$n_5=0, \quad n_6>0. \tag{7.8e}$$

In this way we obtain finite dimensional irreps under certain restrictions on the values of the parameters labeling them. As is clear from the above analysis, the representation theory which is quite similar to the classical case for a generic q changes drastically when q is taken to be a root of unity.

VIII. RIGHT "ACTION"

For the sake of completeness we evaluate the right action on the monomial Φ. The covariance condition (6.5a) implies that the right action of the raising generators X_i^+ on the monomial Φ is zero. Thus we need to compute it only for the remaining lowering generators.

Right action of X_1^- :

$$\pi_R(X_1^-)\ {l_{21}}^{n_1} = 0, \tag{8.1a}$$
$$\pi_R(X_1^-)\ {l_{31}}^{n_2} = 0, \tag{8.1b}$$
$$\pi_R(X_1^-)\ {l_{41}}^{n_3} = 0, \tag{8.1c}$$
$$\pi_R(X_1^-)\ {l_{32}}^{n_4} = \sqrt{[2]}\ q^{(2-n_4)/2}\ [n_4]_q\ {l_{32}}^{n_4-1}\ {A_{22}}^{-1}, \tag{8.1d}$$
$$\pi_R(X_1^-)\ {A_{11}}^{n_5} = 0, \tag{8.1e}$$
$$\pi_R(X_1^-)\ {A_{22}}^{n_6} = \sqrt{[2]}\ q^{(1-n_6)/2}\ [n_6]_{q^2} {A_{22}}^{n_6}\ u_{23}. \tag{8.1f}$$

Right action of X_2^- :

$$\pi_R(X_2^-)\ l_{21}{}^{n_1} = q^{(3-2n_1)/2}\ [n_1]_{q^2} l_{21}{}^{n_1-1}\ A_{11}{}^{-1}\ A_{22}, \tag{8.2a}$$

$$\pi_R(X_2^-)\ l_{31}{}^{n_2} = q^{(2-n_2)/2}([n_2]_q\ l_{31}{}^{n_2-1}\ l_{32}+(q-q^{1-n})[n_2-1]_q\ l_{31}{}^{n_2-2}\ l_{41}) \times A_{11}{}^{-1}\ A_{22}, \tag{8.2b}$$

$$\pi_R(X_2^-)\ l_{41}{}^{n_3} = -[2]^{-1}\ q^{(3-2n_3)/2}\ [n_3]_{q^2}\ l_{41}{}^{n_3-1}\ l_{32}{}^2\ A_{11}{}^{-1}\ A_{22}, \tag{8.2c}$$

$$\pi_R(X_2^-)\ l_{32}{}^{n_4} = 0, \tag{8.2d}$$

$$\pi_R(X_2^-)\ A_{11}{}^{n_5} = q^{(1-n_5)/2}\ [n_5]_{q^2}\ A_{11}{}^{n_5}\ u_{12}, \tag{8.2e}$$

$$\pi_R(X_2^-)\ A_{22}{}^{n_6} = -q^{(1+n_6)/2}\ [n_6]_{q^2}\ A_{22}{}^{n_6}\ u_{12}. \tag{8.2f}$$

So the action on the entire monomial becomes

$$\pi_R(X_1^-)\ \Phi = \sqrt{[2]}\ q^{(2-n_4-n_6)/2}\ [n_4]_q\ \Phi(n_4-1,n_6-1) + \sqrt{[2]}\ q^{(1-n_6)/2}\ [n_6]_{q^2}\ \Phi\ u_{23}, \tag{8.3}$$

$$\begin{aligned}\pi_R(X_2^-)\ \Phi = {} & q^{(-2n_1-2n_2+2n_4-n_5+n_6+3)/2}\ [n_1]_{q^2}\ \Phi(n_1-1,n_5-1,n_6+1)\\ & +q^{(-n_2-2n_3+2n_4-n_5+n_6+2)/2}\ [n_2]_q\Phi(n_2-1,n_4+1,n_5-1,n_6+1)\\ & +q^{(2n_4-n_5+n_6)/2}(q-q^{1-n_2})[n_2-1]_q\ \Phi(n_2-2,n_3+1,n_5-1,n_6+1)\\ & -q^{(-2n_3+2n_4-n_5+n_6+3)/2}\ [2]^{-1}\ [n_3]_{q^2}\ \Phi(n_3-1,n_4+2,n_5-1,n_6+1)\\ & +\ q^{(-n_5+n_6+1)/2}\ [n_5-n_6]_{q^2}\ \Phi\ u_{12}.\end{aligned} \tag{8.4}$$

We notice the appearance of terms involving the variables u_{ij}, which is natural since there is no intrinsic right action of X_i^- on the induced representations. Such actions are needed only as input in singular vectors in which all such terms involving the variables u_{ij} will vanish. Thus, it would be fine to neglect them at this stage provided they do not produce any wanted terms (i.e., terms involving l's and A's) when we act repeatedly with $\pi_R(X_i^-)$. For this we should check the action of X_i^- on u_{ij}.

Right action of X_1^- on the u's:

$$\pi_R(X_1^-)\ u_{12} = \sqrt{[2]}\ u_{13}, \tag{8.5a}$$

$$\pi_R(X_1^-)\ u_{13} = -\sqrt{[2]}\ u_{14}, \tag{8.5b}$$

$$\pi_R(X_1^-)\ u_{14} = 0, \tag{8.5c}$$

$$\pi_R(X_1^-)\ u_{23} = -\sqrt{[2]}(1-q^{-1/2}\ [2]^{-1})\ u_{23}{}^2. \tag{8.5d}$$

Right action of X_2^- on the u's:

$$\pi_R(X_2^-)\ u_{12} = -q^{1/2}\ u_{12}{}^2, \tag{8.6a}$$

$$\pi_R(X_2^-)\ u_{13} = -u_{12}\ u_{13}, \tag{8.6b}$$

$$\pi_R(X_2^-)\ u_{14} = q^{1/2}\ [2]^{-1}\ u_{13}^2, \tag{8.6c}$$

$$\pi_R(X_2^-)\ u_{23} = q(u_{12}\ u_{23}-u_{13}). \tag{8.6d}$$

We see that the u_{23} term in (8.3) would not disappear under the action of X_1^-. Similarly, the u_{12} term in (8.4) would still remain under the action of X_2^-.

IX. INTERTWINERS

There are various partial equivalences among the reducible representations. These partial equivalences are realized by intertwining operators for which a canonical derivation was given in Ref. 1. We shall follow this approach without going into details as here we would be interested in obtaining only the simplest intertwiners.

Let us denote our representation space obtained in Sec. VI by $\mathcal{V}_{\overline{n}}$ where $\overline{n}=(n_5,n_6)$ since it is characterized by the integers n_5,n_6. The corresponding representations are similarly denoted by $\pi_L=\pi_{\overline{n}}^-$. Then the intertwiner is a map from the space $\mathcal{V}_{\overline{n}}^-$ to another space $\mathcal{V}_{\overline{n}'}^-$ labeled by n_5' and n_6' such that

$$\mathcal{I}_i \ \pi_{\overline{n}}^-(X_i^-) \quad = \quad \pi_{\overline{n}'}^-(X_i^-) \ \mathcal{I}_i, \tag{9.1}$$

where $\overline{n}'$ is expected to be $-\overline{n}-1$. According to the general prescription,[1] these operators should be given by $(\pi_R(X_i^-))^s$ and the parameter s is expected to be equal to the dimension of the subspace. It is easy to check this directly. Let $s\in\mathbb{N}$ and suppose that $\Phi' = (\pi_R(X_i^-))^s \Phi$ where Φ' belongs to $\mathcal{V}_{\overline{n}'}^-$. Extending the right covariance condition (6.5a) leads to $\pi_R(X_i^+)\ \Phi' = 0$. Below we calculate this explicitly for X_1^-:

$$\begin{aligned}
\pi_R(X_1^+)\ \Phi' &= \pi_R(X_1^+)\ (\pi_R(X_1^-))^s\ \Phi \\
&= [\pi_R(X_1^+),\ (\pi_R(X_1^-))^s]\ \Phi \\
&= \pi_R([X_1^+,\ (X_1^-)^s])\ \Phi \\
&= \pi_R([s]_q (X_1^-)^{s-1}\ (q^{-(s-1)/2}\ K_1 - q^{(s-1)/2}\ K_1^{-1})/(q^{1/2}-q^{-1/2}))\ \Phi \\
&= [s]_q \pi_R(X_1^-)^{s-1}\ ((q^{-(s-1)/2+n_6} - q^{(s-1)/2-n_6})/(q^{1/2}-q^{-1/2}))\ \Phi \\
&= -[s]_q\ [s-1-2n_6]_q\ \pi_R(X_1^-)^{s-1}\ \Phi.
\end{aligned} \tag{9.2}$$

If q is a generic complex number, then, as expected, this quantity becomes zero only for $s=2n_6+1$. Next, employing the other conditions of right covariance we have $\pi_R(K_i)\ \Phi' = q^{n'}\ \Phi'$, i.e.,

$$\begin{aligned}
\pi_R(K_1)\ \Phi' &= \pi_R(K_1)(\pi_R(X_1^-))^s\ \Phi \\
&= \pi_R(q^{-s}\ (X_1^-)^s\ K_1)\ \Phi \\
&= q^{-s}\ \pi_R(X_1^-)^s\ q^{n_6}\ \Phi = q^{n_6-s}\ \Phi'.
\end{aligned} \tag{9.3}$$

So, $n_6'=n_6-s=-n_6-1$. Then the intertwining operator $\mathcal{I}_1$ (up to a multiplicative nonzero constant) is

$$\mathcal{I}_1 \quad = \quad (\pi_R(X_1^-))^{2n_6+1}. \tag{9.4}$$

Similar calculations for the other generator X_2^- yield

$$\pi_R(X_2^+)\ \Phi' = -[s]_{q^2}\ [s-1-n_5+n_6]_{q^2}\ \pi_R(X_2^-)^{s-1}\ \Phi, \tag{9.5}$$

which vanishes when $s=n_5-n_6+1$. On the other hand,

$$\pi_R(K_2)\ \Phi' \ = \ q^{n_5-n_6-2s}\ \Phi'. \tag{9.6}$$

So, $n_5'-n_6'=n_5-n_6-2s=(-n_5-1)+(n_6-1)$ and thus the second intertwining operator $\mathcal{I}_2$ is indeed given by

$$\mathcal{I}_2 \quad = \quad (\pi_R(X_2^-))^{n_5-n_6+1}. \tag{9.7}$$

The finite-dimensional invariant subspaces V_1 and V_2 discussed earlier are the kernels of these intertwining operators.

X. CONCLUDING REMARKS

In this article we have obtained induced representations of the quantum algebra $U_q so(5)$ realized on some (noncommutative) coset space of the dual quantum group $SO_q(5)$. We remark that although we have assumed integer values for the parameters n_5 and n_6 which characterize them, the formulas (of left action) define a representaion of $U_q so(5)$ also for arbitrary complex values. However, only for integer values, they comprise a deformation of representations which are integrable to a representation of the group $SO_q(5)$. We have also investigated the reducibility of these representations under restricted values of n_5, n_6 which lead to finite dimensional irreps for q generic and for root of unity.

Two basic intertwiners corresponding to the two simple roots were shown to be expressible in terms of powers of the right action. It would be interesting to find out other mixed or composite intertwiners corresponding to the nonsimple roots. For that we would need to compute the powers of the right action explicitly, i.e., by iteration of the results presented in Sec. VIII. In this way one can obtain whole new families of intertwiners. By a suitable redefinition of the generators it should be possible to realize them as q-difference operators. This yields a natural q-deformation of several equations in mathematical physics, which can be viewed as intertwiner between some representations of the underlying symmetry algebra. Also it would be interesting to explore the connection with the noncompact quantum anti-de Sitter algebra $U_q so(3,2)$ in the context of induced representations and q-difference intertwiners. We hope to address all these issues in a sequel.

ACKNOWLEDGMENTS

I thank Professor V. K. Dobrev for suggesting this problem and for useful discussions at various stages of this work. Financial support by CSIR (New Delhi) and infrastructure provided by Institute of Physics, Bhubaneswar (India), where part of the work was done, is gratefully acknowledged. I wish to express my deep gratitude to the Max-Planck Institut für Mathematik in Bonn for a visiting faculty position.

APPENDIX: COMMUTATION RELATIONS OF $SO_q(5)$

Here we give the relations which the 25 elements t_{ij} obey and which follow from (2.1) and (2.2) using (2.6) and (2.7). This explicit form is also necessary for the verification of the Gauss decomposition of Sec. III. The relations are

$$t_{ij}\ t_{i\ell}=q t_{i\ell}\ t_{ij}, \qquad i\neq 3, \quad j<\ell, j'\neq\ell, \tag{A1}$$

$$t_{ij}\ t_{kj}=q t_{kj}\ t_{ij}, \qquad j\neq 3, \quad i<k, i'\neq k, \tag{A2}$$

$$t_{ij}\ t_{ij'}=q^2\ (t_{ij'}\ t_{ij}\ +\lambda\ t_{i,j'+1}\ t_{i,j-1}\ ), \quad i\neq 3, \quad j=1,2, \tag{A3}$$

$$t_{ij}\ t_{i'j}=q^2\ (t_{i'j}\ t_{ij}\ +\lambda\ t_{i'+1,j}\ t_{i-1,j}\ ), \quad j\neq 3, \quad i=1,2, \tag{A4}$$

$$t_{3j}\ t_{3\ell}=t_{3\ell}\ t_{3j}\ +\alpha\ t_{2\ell}\ t_{4j}\ +\eta\ t_{1\ell}\ t_{5j}, \quad j<\ell, \ j'\neq\ell, \tag{A5}$$

$$t_{i3}\ t_{k3}=t_{k3}\ t_{i3}+\alpha\ t_{k2}\ t_{i4}+\eta\ t_{k1}\ t_{i5},\quad i<k,\ i'\neq k, \tag{A6}$$

$$t_{3j}^2=-q^{-1}\ [2]t_{2j}\ t_{4j}-q^{-2}\ [2]t_{1j}\ t_{5j},\quad j\neq 3, \tag{A7}$$

$$t_{i3}^2=-q^{-1}\ [2]t_{i2}\ t_{i4}-q^{-2}\ [2]t_{i1}\ t_{i5},\quad i\neq 3, \tag{A8}$$

$$t_{ij}\ t_{k\ell}=t_{k\ell}\ t_{ij}+\lambda\ t_{kj}\ t_{i\ell},\quad i<k,\ i'\neq k,\ j<\ell,\ j'\neq \ell, \tag{A9}$$

$$t_{ij}\ t_{k\ell}=t_{k\ell}\ t_{ij},\qquad i<k,\ i'\neq k,\ j>\ell, j'\neq \ell, \tag{A10}$$

$$t_{ij}\ t_{i'\ell}=q(t_{i'\ell}\ t_{ij}+\lambda\ t_{i'j}\ t_{i\ell})+\lambda\ t_{i-1,j}\ t_{i'+1,\ell},\quad i=1,2,\ j<\ell,\ j'\neq \ell, \tag{A11}$$

$$t_{ij}\ t_{i'\ell}=q(t_{i'\ell}\ t_{ij}+\lambda\ t_{i'+1,\ell}\ t_{i-1,j}),\quad i=1,2,\ j>\ell,\ j'\neq \ell, \tag{A12}$$

$$t_{ij}\ t_{kj'}=q(t_{kj'}\ t_{ij}+\lambda\ t_{ij'}\ t_{kj}),\quad i<k, i'\neq k, j=1,2, \tag{A13}$$

$$t_{ij'}\ t_{kj}=q^{-1}\ (t_{kj}\ t_{ij'}-\lambda\ t_{k,j-1}\ t_{i,j'+1}),\quad i<k,\ i'\neq k,\ j=1,2, \tag{A14}$$

$$t_{i2}\ t_{k4}=q^{-1}t_{k4}\ t_{i2}+\alpha\ t_{k3}\ t_{i3}+\beta\ t_{k2}\ t_{i4}+\gamma\ t_{k1}\ t_{i5},\quad i<k,\ i'\neq k, \tag{A15}$$

$$t_{11}\ t_{55}=t_{55}\ t_{11}+q(\xi t_{54}\ t_{12}+\eta t_{53}\ t_{13}+\gamma t_{52}\ t_{14}+\delta t_{51}\ t_{15}), \tag{A16}$$

$$t_{12}\ t_{54}=t_{54}\ t_{12}+q(\alpha t_{53}\ t_{13}+\beta t_{52}\ t_{14}+\gamma t_{51}\ t_{15}), \tag{A17}$$

$$t_{13}\ t_{53}=q(t_{53}\ t_{13}+\alpha t_{52}\ t_{14}+\eta t_{51}\ t_{15}), \tag{A18}$$

$$t_{14}\ t_{52}=t_{52}\ t_{14}-\lambda t_{51}\ t_{15}, \tag{A19}$$

$$t_{15}\ t_{51}=t_{51}\ t_{15}, \tag{A20}$$

$$t_{21}\ t_{45}=t_{45}\ t_{21}+q(\xi t_{44}\ t_{22}+\eta t_{43}\ t_{23}+\gamma t_{42}\ t_{24}+\delta t_{41}\ t_{25})+\lambda t_{11}\ t_{55}, \tag{A21}$$

$$t_{22}\ t_{44}=t_{44}\ t_{22}+q(\alpha t_{43}\ t_{23}+\beta t_{42}\ t_{24}+\gamma t_{41}\ t_{25})+\lambda t_{12}\ t_{54}, \tag{A22}$$

$$t_{23}\ t_{43}=q(t_{43}\ t_{23}+\alpha t_{42}\ t_{24}+\eta t_{41}\ t_{25})+\lambda t_{13}\ t_{53}, \tag{A23}$$

$$t_{24}\ t_{42}=t_{42}\ t_{24}+\lambda\ (t_{52}\ t_{14}-t_{51}\ t_{15}-t_{41}\ t_{25}), \tag{A24}$$

$$t_{25}\ t_{41}=t_{41}\ t_{25}+\lambda t_{51}\ t_{15}, \tag{A25}$$

$$t_{31}\ t_{35}=q(t_{35}\ t_{31}+\alpha t_{25}\ t_{41}+\eta t_{15}\ t_{51}), \tag{A26}$$

$$t_{32}\ t_{34}=q(t_{34}\ t_{32}+\alpha t_{24}\ t_{42}+\eta t_{14}\ t_{52})+\lambda t_{31}\ t_{35}. \tag{A27}$$

The additional constraints are $(i=1,2,3,4,5)$

$$\alpha t_{23}\ t_{43}+\eta t_{13}\ t_{53}=\alpha t_{32}\ t_{34}+\eta t_{31}\ t_{35}, \tag{A28}$$

$$q^3\ t_{i5}\ t_{51}+q^2\ t_{i4}\ t_{52}+q^{3/2}\ t_{i3}\ t_{53}+q\ t_{i2}\ t_{54}+t_{i1}\ t_{55}=\delta_{i1}, \tag{A29}$$

$$q^2\ t_{i5}\ t_{41}+qt_{i4}\ t_{42}+q^{1/2}\ t_{i3}\ t_{43}+t_{i2}\ t_{44}+q^{-1}\ t_{i1}\ t_{45}=\delta_{i2}, \tag{A30}$$

$$q^{3/2}\ t_{i5}\ t_{31}+q^{1/2}\ t_{i4}\ t_{32}+t_{i3}\ t_{33}+q^{-1/2}\ t_{i2}\ t_{34}+q^{-3/2}\ t_{i1}\ t_{35}=\delta_{i3}, \tag{A31}$$

$$qt_{i5}\ t_{21}+t_{i4}\ t_{22}+q^{-1/2}\ t_{i3}\ t_{23}+q^{-1}\ t_{i2}\ t_{24}+q^{-2}\ t_{i1}\ t_{25}=\delta_{i4}, \tag{A32}$$

$$t_{i5}\ t_{11}+q^{-1}\ t_{i4}\ t_{12}+q^{-3/2}\ t_{i3}\ t_{13}+q^{-2}\ t_{i2}\ t_{14}+q^{-3}\ t_{i1}\ t_{15}=\delta_{i5}, \tag{A33}$$

$$t_{55}\ t_{1i}+q^{-1}\ t_{45}\ t_{2i}+q^{-3/2}\ t_{35}\ t_{3i}+q^{-2}\ t_{25}\ t_{4i}+q^{-3}\ t_{15}\ t_{5i}=\delta_{1i}, \tag{A34}$$

$$qt_{54}\ t_{1i}+t_{44}\ t_{2i}+q^{-1/2}\ t_{34}\ t_{3i}+q^{-1}\ t_{24}\ t_{4i}+q^{-2}\ t_{14}\ t_{5i}=\delta_{2i}, \tag{A35}$$

$$q^{3/2}\ t_{53}\ t_{1i}+q^{1/2}\ t_{43}\ t_{2i}+t_{33}\ t_{3i}+q^{-1/2}\ t_{23}\ t_{4i}+q^{-3/2}\ t_{13}\ t_{5i}=\delta_{3i}, \tag{A36}$$

$$q^{2}\ t_{52}\ t_{1i}+qt_{42}\ t_{2i}+q^{1/2}\ t_{32}\ t_{3i}+t_{22}\ t_{4i}+q^{-1}\ t_{12}\ t_{5i}=\delta_{4i}, \tag{A37}$$

$$q^{3}\ t_{51}\ t_{1i}+q^{2}\ t_{41}\ t_{2i}+q^{3/2}\ t_{31}\ t_{3i}+qt_{21}\ t_{4i}+t_{11}\ t_{5i}=\delta_{5i}. \tag{A38}$$

In fact, we can obtain the set of relations (A.34)–(A.38) from (A.29)–(A.33) by $q\rightarrow q^{-1}$ and $t_{ij}\ t_{kl}\rightarrow t_{lk}\ t_{ji}$.

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Belov–Chaltikian and Blaszak–Marciniak lattice equations: Recursion operators and factorization

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(Received 14 August 2002; accepted 10 October 2002)

A systematic investigation on the construction of recursion operators for partial differential–difference equations (PDDEs) with two independent variables (one continuous and one discrete) using its generalized symmetries is presented. Also it is explained how to factorize the obtained recursion operators. The applicability of the above procedure have been illustrated for the relativistic toda (RT), Belov–Chaltikian (BC) and Blaszak–Marciniak (BM) lattice equations and shown that the former two lattice equations admit (2×2) matrix recursion operators while the latter one possesses a (3×3) matrix recursion operator. Furthermore, the constructed recursion operators can be written as a factor of 2 distinct invertible matrix operators in each of the lattice equations. It is also proved explicitly that the factorized operators are Hamiltonian and hence RT, BC and BM lattice equations are bi-Hamiltonian systems. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1530755]

I. INTRODUCTION

Integrable systems governed by nonlinear partial differential equations (PDEs) admitting solitons have a variety of rich mathematical structures such as Lax representation, certain specific singularity structure in the complex manifold of the independent variables, multi-Hamiltonian formulation, etc.[1–6] A notable characteristic of integrable nonlinear PDEs (if conservative) is the existence of a sequence of generalized symmetries (involving dependent variables and its spatial derivatives) and conserved densities. The existence of generalized symmetries quite often helps to derive other integrability properties: recursion operator, hereditary operator, bi-Hamiltonian formulation, etc., of nonlinear PDEs. This fact has been verified for a large number of nonlinear PDEs with $(1+1)$ and $(2+1)$ dimensions possessing solitons by different researchers during the past few decades[4,7–10] (see also Refs. 11–16). Recent investigation reveals that certain integrable nonlinear discrete systems characterized by nonlinear PDDEs including lattice equations have similar mathematical structures like for integrable nonlinear PDEs.[17–29]

In Ref. 21, we have considered the BC lattice equation, which is a two coupled first order lattice equation,[30] and the BM lattice equation, which is a three coupled one,[31] and shown that both the lattice equations admit a sequence of generalized symmetries (involving dependent variables and their shifts) and conserved densities. In this article, a systematic investigation on the construction of recursion operators for PDDEs with two independent variables (one continuous and one discrete) using its generalized symmetries is presented. Also, it is explained how to factorize the obtained recursion operators. We illustrate the above procedure for the RT,[32] BM and BC lattice equations, respectively, governed by

$$v_{nt}=v_n(u_{n-1}-u_n), \quad u_{nt}=u_n(u_{n-1}-u_{n+1}-v_{n+1}+v_n), \tag{1}$$

$$u_{nt}=w_{n+1}-w_{n-1}, \quad v_{nt}=u_{n-1}w_{n-1}-u_nw_n, \quad w_{nt}=w_n(v_n-v_{n+1}), \tag{2}$$

$$u_{nt}=u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n, \quad v_{nt}=v_n(u_{n+2}-u_{n-1}), \tag{3}$$

where $u_{nt}=\partial u_n/\partial t$, $v_{nt}=\partial v_n/\partial t$, $w_{nt}=\partial w_n/\partial t$, $u_n=u(n,t)$, $v_n=v(n,t)$, $w_n=w(n,t)$, t is a continuous variable and n is a discrete variable and show that the RT and BC lattice equations admit (2×2) matrix recursion operators while the BM lattice equation possesses (3×3) matrix recursion operator. Furthermore, we prove explicitly that the lattice equations (1)–(3) are bi-Hamiltonian systems.

The plan of the article is as follows. In Sec. II, we consider a first order PDDE with two independent variables (one continuous and one discrete) and show how to construct a recursion operator using its generalized symmetries. Also, we explain how to factorize the obtained recursion operator. In Sec. III, we apply the above procedure to RT, BM and BC lattice equations and construct their recursion operators which can be factorized. Section IV deals with the investigation of the nature of the operators, Hamiltonian or not, in each of the lattice equations, and we prove that all the lattice equations (1)–(3) are bi-Hamiltonian systems. Section V contains a brief summary of our results.

II. PDDES: GENERALIZED SYMMETRIES, RECURSION OPERATOR AND FACTORIZATION

A. Generalized symmetries

To be self-contained, we first explain how to derive generalized symmetries involving dependent variables and their shifts for a given PDDE. Consider, for example, a first order PDDE with two independent variables (one continuous and one discrete) of the form

$$\frac{\partial \mathbf{U}_n}{\partial t}=\mathbf{F}(\ldots,\mathbf{U}_{n-1},\mathbf{U}_n,\mathbf{U}_{n+1},\ldots), \tag{4}$$

where $\mathbf{U}_n=\mathbf{U}(n,t)$ and $\mathbf{F}(...)$ are vector quantities with same number of components, say m. The vector function $\mathbf{F}$ is assumed to be a polynomial in the dependent variable and their shifts. There are no restriction on the level of shifts or the degree of nonlinearity. We also assume that Eq. (4) is invariant under the scaling symmetry.

Let us assume that the PDDE (4) is invariant under the infinitesimal transformations:

$$n^*=n,\quad t^*=t,\quad \mathbf{U}_n^*=\mathbf{U}_n+\epsilon\mathbf{G}(n)+O(\epsilon^2), \tag{5}$$

where $\mathbf{G}(n)=\mathbf{G}(\ldots,\mathbf{U}_{n-1},\mathbf{U}_n,\mathbf{U}_{n+1},\ldots)$. Here $\mathbf{G}(n)=(\mathbf{G}_1(n),\mathbf{G}_2(n),\ldots,\mathbf{G}_m(n))$.

Then the transformed equation is

$$\begin{aligned}\frac{\partial \mathbf{U}_n^*}{\partial t^*}&=\mathbf{F}(\ldots,\mathbf{U}_{n-1}^*,\mathbf{U}_n^*,\mathbf{U}_{n+1}^*,\ldots)\\&=\mathbf{F}(\ldots,U_{n-1}+\epsilon\mathbf{G}(n-1),U_n+\epsilon\mathbf{G}(n),U_{n+1}+\epsilon\mathbf{G}(n+1),\ldots)\end{aligned} \tag{6}$$

provided $\mathbf{U}_n$ satisfy Eq. (4). Now the left hand side of Eq. (6) can be written as

$$\frac{\partial \mathbf{U}_n^*}{\partial t^*}=\frac{\partial}{\partial t}(\mathbf{U}_n+\epsilon\mathbf{G}(n)+O(\epsilon^2))\frac{\partial t}{\partial t^*}=\frac{\partial \mathbf{U}_n}{\partial t}+\epsilon[\mathbf{G}(n)]_t+O(\epsilon^2), \tag{7}$$

where $[\mathbf{G}(n)]_t$ is the first extension given by

$$[\mathbf{G}(n)]_t=\cdots+\frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_{n-1}}\frac{\partial \mathbf{U}_{n-1}}{\partial t}+\frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_n}\frac{\partial \mathbf{U}_n}{\partial t}+\frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_{n+1}}\frac{\partial \mathbf{U}_{n+1}}{\partial t}+\cdots.$$

To compute the right hand side of Eq. (6), we use the Frechet derivative of $\mathbf{F}$ defined as

$$\mathbf{F}'(\mathbf{U}_n)[\mathbf{G}(n)] = \frac{\partial}{\partial \epsilon}\mathbf{F}(\mathbf{U}_n + \epsilon \mathbf{G}(n))\big|_{\epsilon=0}$$

$$= \mathbf{F} + \epsilon\left(\cdots + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_{n-1}}E^{-1} + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_n} + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_{n+1}}E + \ldots\right)\mathbf{G}(n) + O(\epsilon^2), \tag{8}$$

Substituting Eqs. (7) and (8) in Eq. (6) and equating both sides $O(\epsilon)$ terms we obtain the following invariant equation,

$$\frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_{n-1}}\frac{\partial \mathbf{U}_{n-1}}{\partial t} + \frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_n}\frac{\partial \mathbf{U}_n}{\partial t} + \frac{\partial \mathbf{G}(\mathbf{n})}{\partial \mathbf{U}_{n+1}}\frac{\partial \mathbf{U}_{n+1}}{\partial t} + \ldots$$

$$= \left(\ldots + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_{n-1}}E^{-1} + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_n} + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_{n+1}}E + \ldots\right)\mathbf{G}(n), \tag{9}$$

where E and E^{-1} are shift operators defined by $E\mathbf{U}_n = \mathbf{U}_{n+1}$, $E^{-1}\mathbf{U}_n = \mathbf{U}_{n-1}$. Solving the invariant equation (9) we can determine the generalized symmetry $\mathbf{G}(n)$ explicitly.

B. Recursion operator

We would like to recall the following definitions required for further discussion.

Definition 1: An operator valued function $\mathcal{R}$ is said to be a recursion operator of Eq. (4) if it satisfies

$$\tilde{\mathbf{G}}(n) = \mathcal{R}\mathbf{G}(n), \tag{10}$$

where the vector functions $\mathbf{G}(n) = (\mathbf{G}_1(n), \mathbf{G}_2(n), \ldots, \mathbf{G}_m(n))$ and $\tilde{\mathbf{G}}(n) = (\tilde{\mathbf{G}}_1(n), \tilde{\mathbf{G}}_2(n), \ldots, \tilde{\mathbf{G}}_m(n))$ are generalized symmetries of (4) and $\mathcal{R}$ is a $(m \times m)$ matrix operator.

Note that there exist different methods to construct recursion operator $\mathcal{R}$ for PDDEs (see, for example, Ref. 28). In this article, we construct the recursion operator satisfying the above relation (10).

Definition 2: A local conservation law is defined by

$$\frac{\partial \rho_n}{\partial t} = J_n - J_{n+1}, \tag{11}$$

which is satisfied on all solutions of (4). The function ρ_n is the local conserved density and J_n is the associated flux.

Let us assume that the components of the generalized symmetry $\mathbf{G}(n)$ and $\tilde{\mathbf{G}}(n)$, respectively, are of ranks $(p_1, p_2, \ldots, p_m)$ and $(q_1, q_2, \ldots, q_m)$. Here $(p_1, p_2, \ldots, p_m)$ and $(q_1, q_2, \ldots, q_m)$ may be integers or rational numbers. The construction of the recursion operator essentially consists of two steps: In the first step, we determine the rank of (R_{ij}), $i, j = 1, 2, \ldots, m$, of the matrix operator $\mathcal{R}$ which must be equal to $(q_j - p_i)$ which can be determined from the following relations,

$$\text{rank } \tilde{\mathbf{G}}_1(n) = \text{rank } R_{11} + \text{rank } \mathbf{G}_1(n) = \cdots = \text{rank } R_{1m} + \text{rank } \mathbf{G}_m(n),$$

$$\text{rank } \tilde{\mathbf{G}}_m(n) = \text{rank } R_{21} + \text{rank } \mathbf{G}_1(n) = \cdots = \text{rank } R_{2m} + \text{rank } \mathbf{G}_m(n),$$

$$\vdots$$

$$\text{rank } \tilde{\mathbf{G}}_m(n) = \text{rank } R_{m1} + \text{rank } \mathbf{G}_1(n) = \cdots = \text{rank } R_{mm} + \text{rank } \mathbf{G}_m(n). \tag{12}$$

The second step involves determination of the explicit form of (R_{ij}) which may be expressed in terms of difference and inverse difference operators of the dependent variables and their inverse satisfying the relations (10) and (12).

C. Factorization of recursion operator

Having constructed the recursion operator $\mathcal{R}$ we explain how it can be factorized. For that, we first assume that the constructed $(m\times m)$ matrix recursion operator $\mathcal{R}=(R_{ij})$ of Eq. (4) can be written as a factor of 2 distinct $(m\times m)$ matrix operators $A=(A_{ij})$ and $B=(B_{ij})$. That is,

$$\begin{bmatrix} R_{11} & \dots & R_{1\mathrm{m}} \\ R_{21} & \dots & R_{2\mathrm{m}} \\ \vdots & & \vdots \\ R_{\mathrm{m}1} & \dots & R_{\mathrm{mm}} \end{bmatrix} = \begin{bmatrix} A_{11} & \dots & A_{1\mathrm{m}} \\ A_{21} & \dots & A_{2\mathrm{m}} \\ \vdots & & \vdots \\ A_{\mathrm{m}1} & \dots & A_{\mathrm{mm}} \end{bmatrix} \begin{bmatrix} B_{11} & \dots & B_{1\mathrm{m}} \\ B_{21} & \dots & B_{2\mathrm{m}} \\ \vdots & & \vdots \\ B_{\mathrm{m}1} & \dots & B_{\mathrm{mm}} \end{bmatrix}. \tag{13}$$

Equation (13) suggests that the entries of the matrix AB must be of the same rank as of $\mathcal{R}$. Accordingly, we choose the entries of (A_{ij}) and (B_{ij}) which may be expressed in terms of difference and inverse difference operators of the dependent variables and their inverse. Substituting then the expression for (A_{ij}) and (B_{ij}) in Eq. (13) and solving yields the explicit form of the matrix operators (A_{ij}) and (B_{ij}) with the required ranks.

III. RT, BM AND BC LATTICE EQUATIONS: RECURSION OPERATORS AND THEIR FACTORIZATION

A. RT lattice equation

1. Generalized symmetries

To be self-contained, in this subsection, we present computational details of the derivation of generalized symmetries for the RT lattice equation given by

$$v_{nt}=v_n(u_{n-1}-u_n), \quad u_{nt}=u_n(u_{n-1}-u_{n+1}-v_{n+1}+v_n),$$

which is invariant under the scaling symmetry

$$(t,u_n,v_n)\to(\lambda^{-1}t,\lambda u_n,\lambda v_n), \tag{14}$$

where λ is an arbitrary parameter. Assume that the RT lattice equation (1) or (14) is invariant under the infinitesimal transformations

$$n^*=n, \quad t^*=t, \quad u_n^*=u_n+\epsilon G_i^{(1)}(n)+O(\epsilon^2), \quad v_n^*=v_n+\epsilon G_i^{(2)}(n)+O(\epsilon^2), \quad i=1,2,\dots, \tag{15}$$

where

$$G_i^{(1)}(n)=G_i^{(1)}(\dots,v_{n-1},u_{n-1},u_n,v_n,u_{n+1},v_{n+1},\dots),$$

$$G_i^{(2)}(n)=G_i^{(2)}(\dots,v_{n-1},u_{n-1},u_n,v_n,u_{n+1},v_{n+1},\dots)$$

provided u_n and v_n satisfy Eq. (1). For clarity, we denote $\mathbf{G}_i(n)=(G_i^{(1)}(n),G_i^{(2)}(n))$ and the subscript i represents the ith order generalized symmetry. Consequently, we obtain the following invariant equation,

$$\frac{\partial G_i^{(1)}(n)}{\partial t}=G_i^{(1)}(n)(u_{n-1}-u_{n+1}+v_n-v_{n+1}) + u_n(G_i^{(1)}(n-1)-G_i^{(1)}(n+1)+G_i^{(2)}(n)-G_i^{(2)}(n+1)), \tag{16a}$$

$$\frac{\partial G_i^{(2)}(n)}{\partial t}=G_i^{(2)}(n)(u_{n-1}-u_n)+v_n(G_i^{(2)}(n-1)-G_i^{(2)}(n)). \tag{16b}$$

From Eq. (16) we see that

$$\mathbf{G}_2(n)=(G_2^{(1)}(n),G_2^{(2)}(n))=(v_n(u_{n-1}-u_n),u_n(u_{n-1}-u_{n+1}+v_n-v_{n+1}))$$

is a trivial generalized symmetry with rank (2,2). This suggests that the components $G_3^{(1)}(n)$ and $G_3^{(2)}(n)$ of the next generalized symmetry $\mathbf{G}_3(n)$ must have rank (3,3). With this in mind we first form monomials in u_n and v_n of rank (3,3) that lead to a set: $L=\{u_n,u_n^2,u_n^3,v_n,v_n^2,v_n^3\}$. For compactness, hereafter we use the following notation unless otherwise specified,

$$u_n=u,\quad v_n=v,\quad u_{n-1}=\underline{u},\quad v_{n-1}=\underline{v},\quad u_{n-2}=\underline{\underline{u}},\quad v_{n-2}=\underline{\underline{v}},\quad u_{n-3}=\underline{\underline{\underline{u}}},\quad v_{n-3}=\underline{\underline{\underline{v}}},$$

$$u_{n+1}=\overline{u},\quad v_{n+1}=\overline{v},\quad u_{n+2}=\bar{\bar{u}},\quad v_{n+2}=\bar{\bar{v}},\quad u_{n+3}=\overline{\overline{\overline{u}}},\quad v_{n+3}=\overline{\overline{\overline{v}}},\ \text{etc.}$$

Then the necessary partial derivatives with respect to t in each monomial of $L=\{u,v,u^2,v^2,u^3,v^3\}$ along with Eq. (14) gives the following

$$\frac{\partial^0}{\partial t^0}(u^3)=u^3,\quad \frac{\partial^0}{\partial t^0}(v^3)=v^3;\quad \frac{\partial}{\partial t}(u^2)=2u^2\ (\underline{u}-\overline{u}+v-\overline{v}),\frac{\partial}{\partial t}(v^2)=2v^2\ (\underline{u}-u),$$

$$\frac{\partial^2}{\partial t^2}(u)=u\ (\underline{u}-\overline{u}+v-\overline{v})^2+u\ \underline{u}(\underline{\underline{u}}-u+\underline{v}-v)$$
$$-u\ \overline{u}(u-\bar{\bar{u}}+\overline{v}-\bar{\bar{v}})+v\ u\ (\underline{u}-u)-u\ \overline{v}\ (u-\overline{u}),$$

$$\frac{\partial^2}{\partial t^2}(v)=v\ (\underline{u}-u)^2+v\ \underline{u}\ (\underline{\underline{u}}-u+\underline{v}-v)-u\ v(\underline{u}-\overline{u}+v-\overline{v}),$$

and a set

$$M=\{u^3,v^3,u^2\ \underline{u},u^2\overline{u},u^2\ v,u^2\ \overline{v},v^2\ \underline{u},v^2\ u,u\underline{u}^2,u\ \overline{u}^2,u\ \overline{v}^2,$$
$$u\ \underline{u}\ v,u\ \overline{u}\ v,u\ \overline{u}\ \overline{v},u\ v\ \overline{v},u\underline{u}\ \underline{\underline{u}},u\ \underline{\underline{u}}\underline{v},u\ \overline{u}\ \bar{\bar{u}},u\ \overline{u}\overline{v},v\ \underline{u}^2,\underline{u}\ \underline{\underline{u}}\ v,\underline{u}\ v\ \underline{v}\}. \tag{17}$$

Thus the most general form of the generalized symmetry $\mathbf{G}_3(n)=(G_3^{(1)}(n),G_3^{(2)}(n))$ will be

$$G_3^{(1)}(n)=a_1u^3+(a_2\ \underline{u}+a_3\ \overline{u}+a_4\ v+a_5\ \overline{v})u^2+(a_6u+a_7v)\underline{u}^2+a_8u\ \overline{u}^2$$
$$+(a_9\underline{u}\ v+a_{10}\overline{u}\overline{v}+a_{11}\overline{u}\ \overline{v}+a_{12}v\ \overline{v}+a_{13}\underline{u}\ \underline{\underline{u}}+a_{14}\underline{u}\ \underline{v}+a_{15}\overline{u}\ \bar{\bar{u}}+a_{16}\overline{u}\ \bar{\bar{v}})u$$
$$+a_{17}v^3+(a_{18}\underline{u}+a_{19}u)v^2+a_{20}u\ \overline{v}^2+(a_{21}\underline{u}\ \underline{\underline{u}}+a_{22}\underline{u}\ \underline{v})v, \tag{18a}$$

$$G_3^{(1)}(n)=b_1u^3+(b_2\ \underline{u}+b_3\ \overline{u}+b_4\ v+b_5\ \overline{v})u^2+(b_6u+b_7v)\underline{u}^2+b_8u\ \overline{u}^2$$
$$+(b_9\underline{u}\ v+b_{10}\overline{u}\overline{v}+b_{11}\overline{u}\ \overline{v}+b_{12}v\ \overline{v}+b_{13}\underline{u}\ \underline{\underline{u}}+b_{14}\underline{u}\ \underline{v}+b_{15}\overline{u}\ \bar{\bar{u}}+b_{16}\overline{u}\ \bar{\bar{v}})u$$
$$+b_{17}v^3+(b_{18}\underline{u}+b_{19}u)v^2+b_{20}u\ \overline{v}^2+(b_{21}\underline{u}\underline{\underline{u}}+b_{22}\underline{u}\ \underline{v})v, \tag{18b}$$

where a_j, b_j, $j=1,2,\ldots,22$, are arbitrary constants. We now substitute the components $G_3^{(1)}(n)$ and $G_3^{(2)}(n)$ in the invariant equation (16) with $i=3$ and making use of the RT lattice equation (1) or (14) we find, after a detailed calculation, that the consistency condition holds only for the following parametric restrictions:

$$a_4=-a_{10}=-a_{12}=a_{18}=-a_{19}=a_{21}=a_{22}=a_7=b_2=b_4=-b_5=1,$$

$$-b_3=b_{11}=-b_{20}=-b_{16}=b_{19}=-b_8=b_6=-b_{15}=b_{21}=1, b_9=2, b_{11}=-2,$$

and so the first nontrivial generalized symmetry $\mathbf{G}_3(n)=(G_3^{(1)}(n),G_3^{(2)}(n))$ with rank (3,3) becomes

$$G_3^{(1)}(n)=-vu^2+(-\overline{u}\ v-v\overline{v})u+(\underline{u}-u)v^2+(\underline{u}\ \underline{u}+\underline{u}^2+\underline{u}\ \underline{v})v, \tag{19a}$$

$$G_3^{(2)}(n)=(\underline{u}+v-\overline{v}-\overline{u})u^2+(\underline{u}\ \underline{v}-\overline{v}^2-\overline{u}\ \bar{v}+v^2-\overline{u}^2+\underline{u}^2+2\underline{u}\ v-\overline{u}\ \bar{u}-2\overline{u}\ \overline{v}+\underline{u}\ \underline{u})u. \tag{19b}$$

Next we look for the generalized symmetry $\mathbf{G}_4(n)=(G_4^{(1)}(n),G_4^{(2)}(n))$ with rank (4,4). As usual we form a monomial in u and v of rank 4 which gives $\tilde{L}=\{u,v,u^2,v^2,u^3,v^3,u^4,v^4\}$ and then, taking the necessary partial derivatives with respect to t in each monomial set $\tilde{L}$, we obtain a set like the one given in Eq. (17). Proceeding further along the lines described earlier we find that the invariant equations (16a) and (16b) with $i=4$ satisfy only if

$$\begin{aligned}G_4^{(1)}(n)=&-vu^3+(-2v\ \overline{v}-2v^2-v\underline{u}-2\overline{u}v)u^2+v\ \underline{u}^3\\&+(v\ \underline{v}+2v^2+uv+v\ \underline{u}+v^2+v\ \underline{u})\underline{u}^2-uv\ \underline{u}^2\\&+(-v\ \overline{v}^2-\overline{u}\ v\ \overline{v}+\overline{u}v^2-v^2\overline{v}+\overline{u}-\overline{u}\ v\ \overline{v}-\overline{u}\ \bar{u}\ v-v^3-\overline{u}\ \bar{u}v+\underline{u}v^2)u\\&+(-uv^2+v^2\ \underline{v}+v^2+\underline{u}v+\underline{u}\underline{v}+\underline{u}v+\underline{u}\ \underline{u})\underline{u},\end{aligned} \tag{20a}$$

$$\begin{aligned}G_4^{(2)}(n)=&(v-\underline{v}+\underline{u}+\overline{u})u^3+(2v^2+4v\ \underline{u}-2\overline{v}^2+2\underline{u}^2+\underline{u}\ \underline{v}+\underline{u}\ \underline{u}-2\overline{u}^2\\&-2\overline{u}\ \overline{v}-\overline{u}\ \bar{u}-2\overline{u}\ \overline{v}-\overline{u}\ \bar{v})u^2+(3\underline{u}\ v^2+\underline{u}\ \underline{v}^2+\underline{u}^2\underline{v}-\overline{v}^2\ \overline{u}-\overline{u}\ \bar{v}^2-\overline{u}\ \bar{u}\ \bar{v}\\&-2\overline{u}^2\bar{v}+\underline{u}^2\ \underline{v}+\underline{u}^2\ \underline{v}+\underline{u}^2v+\underline{u}\underline{u}-\overline{u}^2\ \overline{v}-\overline{u}^2\bar{u}-2\overline{v}^2\ \overline{v}-\overline{u}^2\ \bar{u}-2\overline{v}^2\ \overline{u}-2\overline{u}\bar{u}\ \overline{v}\\&-2\overline{u}\ \overline{v}\ \bar{v}-\overline{u}\ \bar{u}\ \overline{\overline{v}}+2\underline{u}^2\ v+2v\ \underline{v}\ \underline{u}+2v^2\ \underline{u}+2v\ \underline{u}\ \underline{u}-\overline{u}\bar{u}-\overline{u}\ \bar{u}\ \overline{\overline{u}}\\&+\underline{u}\ \underline{u}\ \underline{v}-\overline{v}^3-\overline{u}\ \bar{u}\ \bar{v}-\overline{u}^2\ \bar{u}+\underline{u}\ \underline{u}^2+\underline{u}\ \underline{u}\underline{v}+\underline{u}^2\underline{u}+\underline{u}\underline{u}\ \underline{v}+\underline{u}\underline{u}\ \underline{u})u.\end{aligned} \tag{20b}$$

In a similar manner we have proved that the RT lattice equation admits a sequence of generalized symmetries $\mathbf{G}_5(n)=(G_5^{(1)}(n),G_5^{(2)}(n))$, $\mathbf{G}_6(n)=(G_6^{(1)}(n),G_6^{(2)}(n))$ [with ranks (5,5),(6,6), ...] which involve a lengthy expressions.

2. Conserved densities and flux

It is easy to see that the RT lattice equation is scaling invariant,

$$(t,u,v)\to(\lambda t,\lambda^{-1}u,\lambda^{-1}v),$$

where λ is an arbitrary parameter. To derive a conserved density with rank 2, we form monomials of u and v which gives the list $L_1=\{u,u^2,v,v^2\}$. Introducing then the necessary t derivatives in each monomial of L_1 leads to $\{u^2,v^2,\overline{u}u,\underline{u}u,uv,\underline{u}v\}$. Using $u\ \overline{u}\equiv u\ \underline{u}$ we obtain $M_1=\{u^2,v^2,\overline{u}u,uv,\underline{u}v\}$. Thus the most general form of the conserved density of rank 2 will be

$$\rho_n=c_1u^2+c_2v^2+c_3\overline{u}u+c_4uv+c_5\underline{u}v, \tag{21}$$

where c_1, c_2, c_3, c_4 and c_5 are constants and so

$$\frac{\partial \rho_n}{\partial t} - J_n + J_{n+1} = (-2c_1 + c_4)u^2\ \overline{u} + (2c_1 - c_3)u^2 v + (c_5 - 2c_1)u^2\ \overline{v} + (-2c_2 + c_3)u\ v^2 + (c_4 - c_3)u\ \overline{u}\ v + (c_5 - c_3)u\ v\ \overline{u}, \tag{22a}$$

with flux

$$J_n = 2c_1 u^2\ \underline{u} + 2c_2 \underline{u}\ v^2 + 2c_3 u\ \underline{u}\ v + c_4 u \underline{u}\ \overline{u} + c_5 u\ \underline{u}\ \overline{v}. \tag{22b}$$

The definition of conservation law, Eq. (11), demands that each bracket in the right hand side of Eq. (22a) vanishes and so the conserved density ρ_n and the associated flux J_n become

$$\rho_n = \tfrac{1}{2}u^2 + (v + \overline{u} + \overline{v})u + \tfrac{1}{2}v^2, \quad J_n = u^2\ \underline{u} + (2\underline{u}\ v + \overline{u}\underline{u} + \underline{u}\ \overline{v})u + \underline{u}\ v^2.$$

To find the next conserved density ρ_n of rank 3 and the corresponding flux J_n, as usual we first form the monomials in u and v gives $L_2 = \{u, v, u^2, v^2, u^3, v^3\}$ and then the set M_2 which can be obtained by introducing the necessary t derivatives in each monomial of L_2. Proceeding as before we find the following conserved density ρ_n of rank 3 and the associated flux J_n,

$$\rho_n = \tfrac{1}{3}u^3 + (\overline{u} + v + \overline{v})u^2 + (v^2 + \overline{u^2} + \overline{v^2} + \overline{u}\ v + 2\overline{u}\ \overline{v} + v\ \overline{v} + \overline{u}\ \bar{u} + \overline{u}\ \bar{v})u + \tfrac{1}{3}v^3,$$

$$J_n = u^3\ \underline{u} + (2\overline{u}\ \underline{u} + 3\underline{u}\ v + 2\underline{u}\ \overline{v})u^2 + (\underline{u}\ \overline{u^2} + 3\underline{u}v^2 + \underline{u}\ v\ \overline{v} + 2\underline{u}\ \overline{u}\ v + 2\underline{u}\ v\ \overline{v} + 2\underline{u}\ \overline{u}\ \overline{v} + \underline{u}\ \overline{u}\ \bar{u} + \underline{u}\ \overline{u}\ \bar{v})u + \underline{u}\ v^3.$$

In a similar manner we have proved that the RT lattice equation admits a sequence of conserved densities with rank 4,5,... along with the flux which involves lengthy expressions and so the details are omitted here.

3. Recursion operator

The relation (10) for the RT lattice equation can be written as

$$\begin{bmatrix} G_{k+1}^{(1)}(n) \\ G_{k+1}^{(2)}(n) \end{bmatrix} = \mathcal{R} \begin{bmatrix} G_k^{(1)}(n) \\ G_k^{(2)}(n) \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \begin{bmatrix} G_k^{(1)}(n) \\ G_k^{(2)}(n) \end{bmatrix}, \quad k = 1,2,\ldots, \tag{23}$$

where $\mathbf{G}_k(n) = (G_k^{(1)}(n), G_k^{(2)}(n))$, $\mathbf{G}_{k+1}(n) = (G_{k+1}^{(1)}(n), G_{k+1}^{(2)}(n))$ are the generalized symmetries. The construction of the recursion operator $\mathcal{R}$ for the RT lattice equation is as follows: For $k = 3$, Eq. (23) becomes

$$\begin{bmatrix} G_4^{(1)}(n) \\ G_4^{(2)}(n) \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \begin{bmatrix} G_3^{(1)}(n) \\ G_3^{(2)}(n) \end{bmatrix}, \tag{24}$$

where $\mathbf{G}_3(n), \mathbf{G}_4(n)$ are the generalized symmetries of ranks (3,3) and (4,4) given in Eqs. (19) and (20). From Eq. (24) it is clear that the entries R_{11}, R_{12}, R_{21} and R_{22} of the matrix operator $\mathcal{R}$ must be of ranks 1 which can be determined from the following relations,

$$\text{rank}\ G_4^{(1)}(n) = \text{rank}\ R_{11} + \text{rank} G_3^{(1)}(n) = \text{rank}\ R_{12} + \text{rank}\ G_3^{(2)}(n),$$

$$\text{rank}\ G_4^{(2)}(n) = \text{rank}\ R_{21} + \text{rank} G_3^{(1)}(n) = \text{rank}\ R_{22} + \text{rank}\ G_3^{(2)}(n).$$

So we consider the entries R_{11}, R_{12}, R_{21} and R_{22} written in terms of difference and inverse difference operators of the dependent variables and their shifts having the form

$$R_{11} = e_0 v + e_1 u + e_2 u\Delta + e_3 \Delta u + e_4 \Delta v + e_5 v\Delta + e_6 v\Delta^+ u\Delta^{-1}u^{-1}, \tag{25a}$$

$$R_{12}=f_0v+f_1v\Delta^+u\Delta^{-1}u^{-1}+f_2u+f_3\Delta u+f_4u\Delta+f_5\Delta v+f_6u\Delta, \tag{25b}$$

$$R_{21}=g_0u+g_1u\Delta+g_2v\Delta+g_3\Delta u+g_4\Delta v, \tag{25c}$$

$$R_{22}=h_0u+h_1u\Delta+h_2u\Delta v\Delta^{-1}u^{-1}+h_3u\Delta u\Delta^{-1}u^{-1}+h_4u\Delta^+u\Delta^{-1}u^{-1}, \tag{25d}$$

where $e_i, f_i, i=1,2,3,4,5,6$, $h_j, g_j, j=1,2,3,4$, are arbitrary constants to be determined and Δ and Δ^+ are difference operators defined by

$$\Delta u=u_{n+1}-u_n=\overline{u}-u, \quad \Delta^+u=u_{n-1}-u_n=\underline{u}-u,$$

and Δ^{-1}, $(\Delta-\Delta^+)^{-1}$ and $(\Delta^+)^{-1}$ are inverse difference operators defined as

$$\Delta^{-1}u=\frac{1}{2}\left[\sum_{k=-\infty}^{-1}[u_{n+1+2k}+u_{n+2k}]-\sum_{k=1}^{\infty}[u_{n-1+2k}+u_{n-2+2k}]\right],$$

$$(\Delta-\Delta^+)^{-1}u=\frac{1}{2}\left[\sum_{k=-\infty}^{-1}u_{n+1+2k}-\sum_{k=1}^{\infty}u_{n-1+2k}\right],$$

$$(\Delta^+)^{-1}u=-\frac{1}{2}\left[\sum_{k=-\infty}^{-1}[u_{n+2+2k}+u_{n+1+2k}]-\sum_{k=1}^{\infty}[u_{n+2k}+u_{n-1+2k}]\right].$$

Substituting the entries R_{11}, R_{12}, R_{21} and R_{22} in Eq. (24), we have checked that it is satisfied identically only if

$$e_0=1, \quad f_0=-1, \quad -f_1=h_1=g_1=g_2=g_3=-g_4=1, \quad h_0=g_0=2,$$

and so the recursion operator for the RT lattice equation (1) becomes

$$\mathcal{R}=\begin{bmatrix} v & v+v(1-E^{-1})u(E-1)^{-1}\dfrac{1}{u} \\ u(1+E) & u(1+E)+u(E-1)v(E-1)^{-1}\dfrac{1}{u}+u(E-E^{-1})u(E-1)^{-1}\dfrac{1}{u} \end{bmatrix}, \tag{26}$$

where E and E^{-1} are the shift operators defined by $Eu_n=(1+\Delta)u_n$ and $E^{-1}u_n=(1+\Delta^+)u_n$.

4. Factorization of recursion operator

Let us assume that the constructed (2×2) matrix recursion operator $\mathcal{R}$, Eq. (26), can be written as a product of two distinct (2×2) matrix operators $A=(A_{ij})$ and $B=(B_{ij})$, $i,j=1,2$. That is,

$$\begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}=\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}. \tag{27}$$

Equation (27) suggests that the entries of the matrix AB must be of the same rank as of $\mathcal{R}$. Thus we consider the entries of the matrix operator A and B having the form

$$A_{11}=a_{11}u\Delta v+a_{12}uv\Delta+a_{13}uv\Delta^+ +a_{14}v\Delta u+a_{15}u\Delta^+u, \tag{28a}$$

$$A_{12}=b_{11}u\Delta v+b_{12}v\Delta^+u+b_{13}u\Delta u+b_{14}v\Delta u+b_{15}u\Delta^+u, \tag{28b}$$

$$A_{21}=c_{11}u\Delta v+c_{12}uv\Delta+c_{13}uv\Delta^+ +c_{14}v\Delta u+c_{15}u\Delta^+v+c_{16}v\Delta^+u+c_{17}u\Delta u+c_{18}u\Delta^+u, \tag{28c}$$

$$A_{22}=d_{11}u\Delta u+d_{12}u\Delta^{+}u+d_{13}u\Delta v+d_{14}v\Delta u+d_{15}v\Delta v+d_{16}v\Delta^{+}v, \tag{28d}$$

$$B_{11}=\tilde{a}_{11}u^{-1}\Delta^{-1}u^{-1}+\tilde{a}_{12}u^{-1}(\Delta^{+})^{-1}u^{-1}+\tilde{a}_{13}v^{-1}\Delta^{-1}u^{-1}+\tilde{a}_{14}u^{-1}(\Delta^{+})^{-1}v^{-1}, \tag{29a}$$

$$B_{12}=\tilde{b}_{11}\Delta^{-1}u^{-1}+\tilde{b}_{12}v^{-1}(\Delta^{+})^{-1}+\tilde{b}_{13}v^{-1}\Delta^{-1}+\tilde{b}_{14}(\Delta^{+})^{-1}v^{-1}+\tilde{b}_{15}u^{-1}\Delta^{-1}, \tag{29b}$$

$$B_{21}=\tilde{c}_{11}\Delta^{-1}v^{-1}+\tilde{c}_{12}u^{-1}(\Delta^{+})^{-1}+\tilde{c}_{13}v^{-1}\Delta^{-1}+\tilde{c}_{14}(\Delta^{+})^{-1}u^{-1}+\tilde{c}_{15}\Delta^{-1}u^{-1}, \tag{29c}$$

$$B_{22}=\tilde{d}_{11}v^{-1}\Delta^{-1}+\tilde{d}_{12}\Delta^{-1}u^{-1}+\tilde{d}_{13}u^{-1}(\Delta^{+})^{-1}, \tag{29d}$$

where a_{ij}, $\tilde{a}_{ij}$, b_{ij}, $\tilde{b}_{ij}$ c_{ij}, $\tilde{c}_{ij}$ d_{ij} and $\tilde{d}_{ij}$ are unknown constants to be determined. Substituting the above entries (A_{ij}) and (B_{ij}) on the right hand side of Eq. (27) and then equating with the entries on the left hand side we find that the consistency condition holds only for the following parametric restrictions:

$$b_{12}=-c_{11}=d_{11}=-d_{12}=-\tilde{b}_{11}=\tilde{c}_{12}=\tilde{d}_{13}=-\tilde{d}_{12}=1$$

and so the matrix operators A and B become

$$A=\begin{bmatrix} 0 & v\Delta^{+}u \\ -u\Delta v & u(\Delta-\Delta^{+})u \end{bmatrix}, \quad B=\begin{bmatrix} 0 & -\Delta^{-1}u^{-1} \\ u^{-1}(\Delta^{+})^{-1} & u^{-1}(\Delta^{+})^{-1}-\Delta^{-1}u^{-1} \end{bmatrix}. \tag{30}$$

We have also verified that both the matrix operators A and B are invertible. To write the recursion operator $\mathcal{R}$ in the standard form $\mathcal{R}=H_2H_1^{-1}$ we choose

$$H_2=A=\begin{bmatrix} 0 & v\Delta^{+}u \\ -u\Delta v & u(\Delta-\Delta^{+})u \end{bmatrix} \tag{31a}$$

and

$$B=H_1^{-1},$$

and so

$$H_1=\begin{bmatrix} uE-E^{-1}u & (E^{-1}-1)u \\ -u(E-1) & 0 \end{bmatrix}. \tag{31b}$$

B. BM lattice equation

1. Generalized symmetries

The invariant equation (9) takes the following form for the BM lattice equation:

$$\frac{\partial G_i^{(1)}(n)}{\partial t}=G_i^{(3)}(n+1)-G_i^{(3)}(n-1), \tag{32a}$$

$$\frac{\partial G_i^{(2)}(n)}{\partial t}=G_i^{(1)}(n-1)w_{n-1}+G_i^{(3)}(n-1)u_{n-1}-G_i^{(1)}(n)w_n-G_i^{(3)}(n)u_n, \tag{32b}$$

$$\frac{\partial G_i^{(3)}(n)}{\partial t}=G_i^{(3)}(n)(v_n-v_{n+1})+w_n(G_i^{(2)}(n)-G_i^{(2)}(n+1)). \tag{32c}$$

Solving the above invariant equations along the lines described for the RT lattice equation we have derived a sequence of generalized symmetries. The explicit forms of generalized symmetries (also

conserved densities) are given in Ref. 21. The first few generalized symmetries $\mathbf{G}_2(n)=(G_2^{(1)}(n),G_2^{(2)}(n),G_2^{(3)}(n))$, $\mathbf{G}_3(n)=(G_3^{(1)}(n),G_3^{(2)}(n),G_3^{(3)}(n))$, $\mathbf{G}_4=(G_4^{(1)}(n),G_4^{(2)}(n),G_4^{(3)}(n))$, respectively, having ranks $(\frac{3}{2},2,\frac{5}{2})$, $(\frac{5}{2},3,\frac{7}{2})$, $(\frac{7}{2},4,\frac{9}{2})$, are given by

$$G_2^{(1)}(n)=\overline{w}-\underline{w},\quad G_2^{(2)}(n)=\underline{u}\,\underline{w}-u\ \ w,\quad G_2^{(3)}(n)=w(v-\overline{v}), \tag{33}$$

$$\begin{gathered}G_3^{(1)}(n)=\underline{w}(v+\underline{v})-\overline{w}(\overline{v}+\bar{\bar{v}}),\quad G_3^{(2)}(n)=uw(v+\overline{v})-\underline{u}\,\underline{w}(v+\underline{v})+\underline{w}\,\underline{\underline{w}}-w\overline{w},\\ G_3^{(3)}(n)=w(\overline{v}^2-v^2)+w(\overline{wu}-\underline{w}\,\underline{u}),\end{gathered} \tag{34}$$

$$\begin{aligned}G_4^{(1)}(n)=&-\overline{w}\bar{\bar{v}}^2-\overline{w}\ \ \overline{v}^2-\overline{w}\bar{\bar{w}}\bar{\bar{u}}-w\ \ \overline{w}u+\underline{w}v^2+\underline{w}\underline{v}^2+w\underline{w}u+\underline{w}\,\underline{\underline{w}}\ \ \underline{\underline{u}}+v\underline{w}\,\underline{v}\\&+\underline{u}\,\underline{w}^2-\overline{u}\ \ \overline{w}^2-\overline{w}\overline{v}\bar{\bar{v}},\end{aligned}$$

$$G_4^{(2)}(n)=-uw^2v+uw^2\overline{v}-2\underline{u}\,\underline{w}wv-\underline{u}\ \ \underline{w}w\underline{v}+w\underline{w}\,\underline{\underline{w}}-wv^3+2w\overline{wuv}+w\overline{wu}\bar{\bar{v}}-w\overline{w}\bar{\bar{w}}+w\overline{v}^3, \tag{35}$$

$$\begin{aligned}G_4^{(3)}(n)=&\underline{w}\,\underline{\underline{w}}\,\underline{v}+\underline{w}\,\underline{\underline{w}}\,\underline{\underline{v}}-\underline{u}\,\underline{w}v^2-\underline{u}\,\underline{w}\underline{v}^2-\underline{w}\,\underline{\underline{w}}\,\underline{\underline{u}}\,\underline{\underline{u}}+uw\overline{v}^2+uwv^2\\&+uw\overline{uw}-w\overline{wv}-w\overline{w}\bar{\bar{v}}+u^2w^2+uv\,w\ \ \overline{v}-w\overline{w}v+\underline{w}\,\underline{\underline{w}}v-\underline{u}\,\underline{w}v\,\underline{v}-\underline{u}^2\underline{w}^2,\end{aligned}$$

where $w_n=w,w_{n+1}=\overline{w},w_{n-1}=\underline{w},\ w_{n+2}=\bar{\bar{w}},w_{n-2}=\underline{\underline{w}}$.

2. Recursion operator and factorization

Here the generalized symmetry $\mathbf{G}_k(n)=(G_k^{(1)}(n),G_k^{(2)}(n),G_k^{(3)}(n))$ and so the relation (10) takes

$$\begin{bmatrix}G_{k+1}^{(1)}(n)\\G_{k+1}^{(2)}(n)\\G_{k+1}^{(3)}(n)\end{bmatrix}=\mathcal{R}\begin{bmatrix}G_k^{(1)}(n)\\G_k^{(2)}(n)\\G_k^{(3)}(n)\end{bmatrix}=\begin{bmatrix}R_{11}&R_{12}&R_{13}\\R_{21}&R_{22}&R_{23}\\R_{31}&R_{32}&R_{33}\end{bmatrix}\begin{bmatrix}G_k^{(1)}(n)\\G_k^{(2)}(n)\\G_k^{(3)}(n)\end{bmatrix},\quad k=1,2,\ldots. \tag{36}$$

Let $k=3$. Now

$$\text{rank}\ \ G_3^{(1)}=\tfrac{5}{2},\ \text{rank}\ \ G_3^{(2)}=3,\ \text{rank}\ \ G_3^{(3)}=\tfrac{7}{2},$$

$$\text{rank}\ \ G_4^{(1)}=\tfrac{7}{2},\ \text{rank}\ \ G_4^{(2)}=4,\ \text{rank}\ \ G_4^{(3)}=\tfrac{9}{2}.$$

Then the rank of the entries of $\mathcal{R}$ can be determined from the following relations,

$$\text{rank}\ \ G_4^{(1)}(n)=\text{rank}R_{11}+\text{rank}\ \ G_3^{(1)}(n)=\text{rank}\ \ R_{12}+\text{rank}\ \ G_3^{(2)}(n)=\text{rank}\ \ R_{13}+\text{rank}\ \ G_3^{(3)}(n),$$

$$\text{rank}\ \ G_4^{(2)}(n)=\text{rank}\ \ R_{21}+\text{rank}\ \ G_3^{(1)}(n)=\text{rank}\ \ R_{22}+\text{rank}G_3^{(2)}(n)=\text{rank}\ \ R_{23}+\text{rank}\ \ G_3^{(3)}(n),$$

$$\text{rank}\ \ G_4^{(3)}(n)=\text{rank}\ \ R_{31}+\text{rank}\ \ G_3^{(1)}(n)=\text{rank}\ \ R_{32}+\text{rank}G_3^{(2)}(n)=\text{rank}\ \ R_{33}+\text{rank}\ \ G_3^{(3)}(n),$$

and so

$$\text{rank}\ \ \mathrm{R}_{11}=1,\ \text{rank}\ \ \mathrm{R}_{12}=\tfrac{1}{2},\ \text{rank}\ \ \mathrm{R}_{13}=0,$$

$$\text{rank}\ \ \mathrm{R}_{21}=\tfrac{3}{2},\ \text{rank}\ \ \mathrm{R}_{22}=1,\ \text{rank}\ \ \mathrm{R}_{23}=\tfrac{1}{2},$$

$$\text{rank}\ \ \mathrm{R}_{31}=2,\ \text{rank}\ \ \mathrm{R}_{32}=\tfrac{3}{2},\ \text{rank}\ \ \mathrm{R}_{33}=1.$$

We then choose the entries R_{11}, R_{12}, R_{13}, R_{21}, R_{22}, R_{23}, R_{31}, R_{32}, R_{33} written in terms of the difference and inverse difference operators of the dependent variables and their inverses and, proceeding further as explained for the RT lattice equation, we obtain the explicit form of the recursion operator $\mathcal{R}$,

$$\mathcal{R}=\begin{bmatrix} (Ev-vE^{-1}-u(E-1)\tilde{E}^{-1} & u(E-1)\tilde{E}^{-1} & -(EwE-E^{-1}w)\Delta^{-1}\dfrac{1}{w} \\ (E^{-1}-1)u)(\Delta-\Delta^{+})^{-1} & & \\ (wE-E^{-1}wE^{-1})(\Delta-\Delta^{+})^{-1} & v & (E^{-1}uw-uwE)\Delta^{-1}\dfrac{1}{w} \\ w(E-1)\tilde{E}^{-1}(E^{-1}-1) & w(-\tilde{E}^{-1}+(1-E))\tilde{E}^{-1} & w(E-1)v\Delta^{-1}\dfrac{1}{w} \\ u(\Delta-\Delta^{+})^{-1} & & \end{bmatrix},$$

which can be factorized into

$$\mathcal{R}=H_2H_1^{-1},$$

where

$$H_1=\begin{bmatrix} (\Delta-\Delta^{+}) & 0 & 0 \\ 0 & 0 & \Delta^{+}w \\ 0 & -w\Delta & 0 \end{bmatrix}, \tag{37}$$

$$H_2=\begin{bmatrix} Ev-vE^{-1}-u(E-1) & EwE-E^{-1}w & u(E-1) \\ (\tilde{E})^{-1}(E^{-1}-1)u & & (\tilde{E})^{-1}(E^{-1}-1)w \\ wE-E^{-1}wE^{-1} & E^{-1}uw-uwE & v(E^{-1}-1)w \\ w(E-1)(\tilde{E})^{-1} & -w(E-1)v & w(-\tilde{E}-(E-1)(\tilde{E})^{-1} \\ (E^{-1}-1)u & & (E^{-1}-1))w \end{bmatrix}, \tag{38}$$

where $\tilde{E}=\Delta-\Delta^{+}$, $(\Delta-\Delta^{+})^{-1}$ and $(\Delta^{+})^{-1}$ are inverse difference operators defined as

$$(\Delta-\Delta^{+})^{-1}u=\frac{1}{2}\left[\sum_{k=-\infty}^{-1}u_{n+1+2k}-\sum_{k=1}^{\infty}u_{n-1+2k}\right],$$

and

$$(\Delta^{+})^{-1}u=-\frac{1}{2}\left[\sum_{k=-\infty}^{-1}[u_{n+2+2k}+u_{n+1+2k}]-\sum_{k=1}^{\infty}[u_{n+2k}+u_{n-1+2k}]\right].$$

C. BC lattice equation

1. Generalized symmetries

Here the invariant equation (9) takes the following form,

$$\frac{\partial G_i^{(1)}(n)}{\partial t}=G_i^{(1)}(n)(u_{n+1}-u_{n-1})+u_n(G_i^{(1)}(n+1)-G_i^{(1)}(n-1))+G_i^{(2)}(n-1)-G_i^{(2)}(n), \tag{39a}$$

$$\frac{\partial G_i^{(2)}(n)}{\partial t} = G_i^{(2)}(n)(u_{n+2}-u_{n-1}) + v_n(G_i^{(1)}(n+2)-G_i^{(1)}(n-1)). \tag{39b}$$

In Ref. 21, we have solved the above invariant equations and shown that the BC lattice equation admits a sequence of generalized symmetries (also conserved densities). First few generalized symmetries $\mathbf{G}_2(n)=(G_2^{(1)}(n),G_2^{(2)}(n))$, $\mathbf{G}_3(n)=(G_3^{(1)}(n),G_3^{(2)}(n))$, $\mathbf{G}_4(n)=(G_4^{(1)}(n),G_4^{(2)}(n))$ having ranks (2,3), (3,4), (4,5) are

$$G_2^{(1)}(n)=u(\overline{u}-\underline{u})+\underline{v}-v, \quad G_2^{(2)}(n)=v(\bar{u}-\underline{u}), \tag{40}$$

$$G_3^{(1)}(n)=(v-u\overline{u})(u+\overline{u}+\bar{u})+(u\underline{u}-\underline{v})(u+\underline{u}+\underline{\underline{u}})-u(\underline{\underline{v}}-\overline{v}),$$

$$G_3^{(2)}(n)=\underline{u}v(u+\underline{u}+\underline{\underline{u}})-\bar{u}v(\overline{u}+\bar{u}+\overline{\overline{\overline{u}}})+v(\overline{v}+\bar{v}-\underline{v}-\underline{\underline{v}}), \tag{41}$$

$$\begin{aligned}G_4^{(1)}(n)=&-[u^3\overline{u}+2u^2\overline{u}^2+u\overline{u}^3+u^2\overline{u}\bar{u}+2u\overline{u}^2\bar{u}+u\overline{u}\bar{u}^2+u\overline{u}\bar{u}\overline{\overline{\overline{u}}}-u\underline{u}\underline{\underline{u}}\underline{\underline{\underline{u}}}-u\underline{u}\underline{\underline{u}}^2\\&-2u\underline{u}^2\underline{\underline{u}}-u\underline{u}^3-u^2\underline{u}\underline{\underline{u}}-u^3\underline{\underline{u}}-2u^2\underline{\underline{u}}^2]+3u\overline{u}\overline{v}+\overline{u}^2v+2\overline{u}\overline{\bar{u}}v+2u\overline{u}\overline{v}+u\bar{u}\overline{v}+u\overline{\overline{\overline{u}}}\,\overline{v}\\&+u^2v+u\overline{u}\overline{\bar{v}}+u\bar{u}v-u^2\underline{v}-3u\underline{u}\underline{v}-u\underline{\underline{u}}\underline{v}-u^2\underline{\underline{v}}+u^2\overline{v}-\underline{u}^2\underline{v}-2\underline{u}\underline{\underline{u}}\underline{v}-u\underline{\underline{u}}\underline{\underline{v}}\\&-u\underline{\underline{u}}\underline{\underline{v}}-u\underline{u}\underline{\underline{v}}-\underline{\underline{u}}^2\underline{v}-\underline{\underline{u}}\underline{u}\underline{\underline{v}}+\underline{v}\underline{\underline{v}}+\underline{v}\underline{\underline{v}}+\bar{u}^2v-2u\underline{u}\underline{\underline{v}}+\bar{u}\overline{\overline{\overline{u}}}v-v\overline{v}-v\bar{v}-v^2+\underline{\underline{v}}^2,\end{aligned}$$

$$\begin{aligned}G_4^{(2)}(n)=&-\overline{u}v\underline{v}+u\overline{u}\underline{u}v+\bar{u}v\bar{v}+v\bar{v}\overline{\overline{\overline{u}}}+v\bar{v}\overline{\overline{\overline{\overline{u}}}}-2\bar{u}^2\overline{\overline{u}}v-\bar{u}\overline{\overline{\overline{u}}}^2v-\bar{u}\overline{\overline{\overline{\overline{u}}}}\,\overline{\overline{\overline{\overline{u}}}}v-2\overline{u}\overline{\bar{u}}^2v-\overline{u}^2\bar{u}v\\&-u\overline{u}\bar{u}v+\bar{u}v\overline{v}+\overline{u}v\overline{v}+uv\overline{v}+v^2\bar{u}+\bar{u}v\overline{\overline{\overline{v}}}-\bar{u}^3v-\underline{u}v\underline{v}-uv\underline{v}+2u\underline{u}^2v+u^2\underline{u}v+2\underline{u}^2\underline{\underline{u}}v\\&+\underline{u}\underline{\underline{u}}^2v+\underline{u}\underline{\underline{u}}\underline{\underline{\underline{u}}}v-\underline{u}v\underline{\underline{v}}-\underline{\underline{u}}v\underline{v}-\underline{\underline{u}}v\underline{\underline{v}}-\underline{u}v\underline{\underline{v}}-v^2\underline{\underline{u}}+u\underline{u}\underline{\underline{u}}v-v\underline{\underline{v}}u-v\underline{v}\underline{\underline{u}}+v\overline{v}\overline{\overline{\overline{u}}}\,u-\overline{u}\overline{\bar{u}}\;\overline{\overline{\overline{u}}}\,v\\&+v\bar{v}\overline{u}+\underline{u}^3v.\end{aligned} \tag{42}$$

2. Recursion operator and factorization

Here the relation (10) related with the recursion operator $\mathcal{R}$ is

$$\begin{bmatrix}G_{k+1}^{(1)}(n)\\G_{k+1}^{(2)}(n)\end{bmatrix}=\mathcal{R}\begin{bmatrix}G_k^{(1)}(n)\\G_k^{(2)}(n)\end{bmatrix}=\begin{bmatrix}R_{11}&R_{12}\\R_{21}&R_{22}\end{bmatrix}\begin{bmatrix}G_k^{(1)}(n)\\G_k^{(2)}(n)\end{bmatrix}, \quad k=1,2,\ldots. \tag{43}$$

Let $k=3$. Now

$$\text{rank } G_3^{(1)}(n)=3,\ \text{rank}G_3^{(2)}(n)=4,\ \text{rank } G_4^{(1)}(n)=4, \quad \text{rank}G_4^{(2)}(n)=5.$$

The ranks of the entries of $\mathcal{R}$ can be determined from the following relations,

$$\text{rank } G_4^{(1)}(n)=\text{rank } R_{11}+\text{rank } G_3^{(1)}(n)=\text{rank } R_{12}+\text{rank } G_3^{(2)}(n),$$

$$\text{rank } G_4^{(2)}(n)=\text{rank } R_{21}+\text{rank } G_3^{(1)}(n)=\text{rank } R_{22}+\text{rank } G_3^{(2)}(n).$$

Thus

$$\text{rank } R_{11}=1,\ \text{rank } R_{12}=0,\ \text{rank}R_{21}=2,\ \text{rank } R_{22}=1.$$

Proceeding in a similar manner as for the RT and BM lattice equations (1) and (2) we construct the recursion operator $\mathcal{R}$ which can be written as a product of two invertible operators,

$$\mathcal{R}=H_2H_1^{-1},$$

where

$$H_1=\begin{bmatrix} H_{11}^{(1)} & H_{12}^{(1)} \\ H_{21}^{(1)} & H_{22}^{(1)} \end{bmatrix} \text{ and } H_2=\begin{bmatrix} H_{11}^{(2)} & H_{12}^{(2)} \\ H_{21}^{(2)} & H_{22}^{(2)} \end{bmatrix},$$

$$\begin{aligned} H_{11}^{(1)}&=uEu-uE^{-1}u+E^{-1}v-vE,\\ H_{12}^{(1)}&=-uE^{-2}v+uEv,\\ H_{21}^{(1)}&=vE^2u-vE^{-1}u,\\ H_{22}^{(1)}&=vE^2v+vEv-vE^{-2}v-vE^{-1}v. \end{aligned} \tag{44a}$$

$$\begin{aligned} H_{11}^{(2)}&=u(uE+Eu+EuE-uE^{-1}-E^{-1}u-E^{-1}uE^{-1})u+uE^{-1}v\\ &\quad -uEvE+E^{-1}vE^{-1}u-vE^2u-uvE-vEu+E^{-1}uv+uE^{-2}v),\\ H_{12}^{(2)}&=-u(-uE-Eu-EuE+uE^{-2}+E^{-1}uE^{-2}+E^{-1}uE^{-1})v\\ &\quad -v(1+E+E^2)v+E^{-1}v(1+E^{-1}+E^{-2})v-(uE^{-1}u-uEuE^{-1})v,\\ H_{21}^{(2)}&=-v(uE^{-1}+E^{-1}u+E^{-1}uE^{-1}-EuE-E^2u-E^2uE)u\\ &\quad -v[(1+E+E^2)vE-(1+E^{-1}+E^{-2})v]-v[-uE+EuE^{-1}]u,\\ H_{22}^{(2)}&=-v(E^{-1}uE^{-2}+uE^{-2}-uE-E^2uE+E^{-1}u+E^{-1}uE^{-1}\\ &\quad -E^2uE^{-1}-EuE+EuE^{-2}-E^2u)v. \end{aligned} \tag{44b}$$

IV. BI-HAMILTONIAN SYSTEM

We prove, in this section, that the factorized operators H_1 and H_2 for each of the lattice equations (1)–(3) are Hamiltonian.

A. RT lattice equation

Obviously the operators H_1 and H_2 given in Eqs. (31a) and (31b) are skew-symmetric. In order to prove that the operators H_1 and H_2 are Hamiltonian it remains to prove that they satisfy the Jacobi identity. Let us first consider the skew symmetric operator H_1. It is appropriate to mention the following theorem for a system of nonlinear PDEs $\partial\mathbf{u}/\partial t=K(\mathbf{u})$ due to Olver.[6]

Theorem: Let $\mathcal{D}$ be a skew-adjoint $q\times q$ matrix differential operator of the system of PDEs, $\partial\mathbf{u}/\partial t=K(\mathbf{u})$ and $\Theta=\frac{1}{2}\int\{\Theta\wedge\mathcal{D}\Theta\}\mathrm{d}x$, the corresponding functional bi-vector. Then $\mathcal{D}$ is Hamiltonian if and only if

$$PrV_{\mathcal{D}\theta}(\Theta)=0. \tag{45}$$

Here $\theta=\theta(\mathbf{x},\mathbf{u})$. Recent investigations by Sanders and Wang[33] suggest that the above result, Eq. (45), holds good for nonlinear PDDEs as well. Thus it remains to prove that the skew-symmetric operator H_1, Eq. (31a), of the RT lattice equation (1) satisfies Eq. (45). For nonlinear PDDEs, prolongation of the vector field is defined as[33]

$$PrV_{H\theta}=\sum_{\alpha,J}E_J\left(\sum_{\beta}H_{\alpha\beta}\theta^{\beta}\right)\frac{\partial}{\partial u_J^{\alpha}},$$

where E^J is the shift operator and H is a skew-symmetric operator. Let $\theta_1=(\theta,\varsigma)^T$. Then

$$H_1\theta_1=H_1\begin{bmatrix}\theta\\ \varsigma\end{bmatrix}=\begin{bmatrix}(uE-E^{-1}u)\theta+(E^{-1}-1)u\varsigma\\ -u\Delta\theta\end{bmatrix}=\begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix}.$$

Define a bi-vector Θ of H_1 by

$$\Theta_{H_1}=\frac{1}{2}\sum\ [\theta\wedge\Phi_1+\varsigma\wedge\Phi_2]$$

$$=\frac{1}{2}\sum\ [u\ \theta\wedge\overline{\theta}-u\ \overline{\theta}\wedge\theta+u\ \overline{\theta}\wedge\varsigma-u\ \theta\wedge\varsigma-u\ \varsigma\wedge\overline{\theta}+u\ \varsigma\wedge\theta].$$

Making use of the wedge product,

$$\theta\wedge\overline{\theta}=-\overline{\theta}\wedge\theta,\overline{\theta}\wedge\varsigma=-\varsigma\wedge\overline{\theta},\theta\wedge\theta=0,$$

we rewrite the bi-vector Θ_{H_1} as

$$\Theta_{H_1}=\sum\ [u\ \theta\wedge\overline{\theta}+u\overline{\theta}\wedge\varsigma+u\ \varsigma\wedge\theta],$$

where $\overline{\varsigma}=\varsigma_{n+1},\overline{\theta}=\theta_{n+1}$. Now

$$PrV_{H_1\theta_1}(\Theta_{H_1})=\sum\ [(-u\ \overline{\theta}+u\theta)\wedge(\theta\wedge\overline{\theta}+\overline{\theta}\wedge\varsigma+\varsigma\wedge\theta)=0.$$

Here Σ is used to denote the equivalence classes after dividing the image of $(1-E)$. These equivalence classes are called functionals. In a similar manner, we checked that for the skew-symmetric operator H_2,

$$PrV_{H_2\theta_1}(\Theta_{H_2})=0.$$

Thus the operators H_1 and H_2 are Hamiltonian. Hence the RT equation (1) can be written in the bi-Hamiltonian form. Using the compatible Hamiltonian operators H_1 and H_2, we have

$$\begin{bmatrix}v_t\\ u_t\end{bmatrix}=H_1\begin{bmatrix}\dfrac{\delta\mathcal{H}_1}{\delta u}\\ \dfrac{\delta\mathcal{H}_1}{\delta v}\end{bmatrix}=H_2\begin{bmatrix}\dfrac{\delta\mathcal{H}_0}{\delta u}\\ \dfrac{\delta\mathcal{H}_0}{\delta v}\end{bmatrix},$$

associated with the Hamiltonian functionals, $\mathcal{H}_0(u,v)=\Sigma_n\log v$ and $\mathcal{H}_1(u,v)=\Sigma_n[\frac{1}{2}(u^2+v^2)+uv+uv+uu]$. Hence the RT lattice equation (1) is a bi-Hamiltonian system. A similar observation is also pointed out by Fuchssteiner *et al.* using a different approach.[32]

B. BM lattice equation

It is straight forward to check that the operators H_1 and H_2, Eqs. (37) and (38), are skew-symmetric. In order to prove that the operators H_1 and H_2 are Hamiltonian it remains to prove that they satisfy the Jacobi identity. First consider the operator H_1. As before, let $\theta_1=(\theta,\chi,\varsigma)^T$ and

$$H_1\theta_1=H_1\begin{bmatrix}\theta\\ \chi\\ \varsigma\end{bmatrix}=\begin{bmatrix}\tilde{E}\theta\\ (E^{-1}-1)w\varsigma\\ -w(E-1)\chi\end{bmatrix}=\begin{bmatrix}\Phi_1\\ \Phi_2\\ \Phi_3\end{bmatrix}.$$

Define a bi vector Θ of H_1 by

$$\Theta_{H_1}=\frac{1}{2}\sum\ [\theta\wedge\Phi_1+\chi\wedge\Phi_2+\varsigma\wedge\Phi_3]$$

$$=\frac{1}{2}\sum\ [\theta\wedge(E-E^{-1})\theta+\chi\wedge(E^{-1}-1)w\varsigma+\varsigma\wedge(-w(E-1)\chi)]$$

$$=\frac{1}{2}\sum\ [\theta\wedge E\theta-\theta\wedge E^{-1}\theta+\chi\wedge E^{-1}w\varsigma-\chi\wedge w\varsigma-\varsigma\wedge wE\chi+\varsigma\wedge w\chi]$$

$$=\frac{1}{2}\sum\ [\theta\wedge\overline{\theta}-\overline{\theta}\wedge\theta+\overline{\chi}\wedge w\varsigma-\chi\wedge w\varsigma-\varsigma\wedge w\overline{\chi}+\varsigma\wedge w\chi]. \quad (46)$$

Making use of the property of wedge product, we simplify Eq. (46) into

$$\Theta_{H_1}=\sum\ [\theta\wedge\overline{\theta}+w\overline{\chi}\wedge\varsigma+w\varsigma\wedge\chi],$$

where $\overline{\theta}=\theta_{n+1},\overline{\chi}=\chi_{n+1}$, etc. Proceeding as before for the RT lattice equation (1), it is easy to see that

$$PrV_{H_1\theta_1}(\Theta_{H_1})=\sum\ [-w(E-1)\chi\wedge\overline{\chi}\wedge\varsigma-w(E-1)\chi\wedge\varsigma\wedge\chi]$$

$$=\sum\ [-w\ (\overline{\chi}\wedge\overline{\chi}\wedge\varsigma-\chi\wedge\overline{\chi}\wedge\varsigma)-w\ (\overline{\chi}\wedge\varsigma\wedge\chi-\chi\wedge\varsigma\wedge\chi)]=0$$

and hence H_1 is a Hamiltonian operator. Similar conclusion can also be arrived at for the operator H_2. Now the BM lattice equation (2) can be written as

$$\begin{bmatrix}u_t\\ v_t\\ w_t\end{bmatrix}=H_1\begin{bmatrix}\frac{\delta\mathcal{H}_1}{\delta u}\\ \frac{\delta\mathcal{H}_1}{\delta v}\\ \frac{\delta\mathcal{H}_1}{\delta w}\end{bmatrix}=H_2\begin{bmatrix}\frac{\delta\mathcal{H}_0}{\delta u}\\ \frac{\delta\mathcal{H}_0}{\delta v}\\ \frac{\delta\mathcal{H}_0}{\delta w}\end{bmatrix},$$

where the Hamiltonian functionals $\mathcal{H}_0(u,v,w)$ and $\mathcal{H}_1(u,v,w)$ take the forms $\mathcal{H}_0(u,v,w)=\Sigma v$ and $\mathcal{H}_1(u,v,w)=\Sigma[\frac{1}{2}v^2+uw]$ and so the BM lattice equation (2) is a bi-Hamiltonian system. The bi-Hamiltonian formulation for the BM lattice equation has also been obtained by Blaszak *et al.* using a different approach.[31]

C. BC lattice equation

It is straight forward to check that the operators H_1 and H_2 given in Eqs. (44a) and (44b) are skew-symmetric. For Hamiltonian operator, it remains to prove the Jacobi identity. First consider the operator H_1. As before, let $\theta_1=(\theta,\varsigma)^T$ and

$$H_1\theta_1=H_1\begin{bmatrix}\theta\\ \varsigma\end{bmatrix}=\begin{bmatrix}H_{11}^{(1)}\theta+H_{12}^{(1)}\varsigma\\ H_{21}^{(1)}\theta+H_{22}^{(1)}\varsigma\end{bmatrix}=\begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix},$$

where $H_{11}^{(1)},H_{12}^{(1)},H_{21}^{(1)},\ H_{22}^{(1)},H_{11}^{(2)},H_{12}^{(2)},H_{21}^{(2)}$ and $H_{22}^{(2)}$ are given in Eqs. (44a) and (44b).

Define a bi-vector Θ of H_1 by

$$\Theta_{H_1}=\frac{1}{2}\sum\,[\theta\wedge\Phi_1+\varsigma\wedge\Phi_2]$$

$$=\frac{1}{2}\sum\,[\theta\wedge(uEu-uE^{-1}u+E^{-1}v-vE)\theta+\theta\wedge(-uE^{-2}v+uEv)\varsigma$$
$$+\varsigma\wedge(vE^2u-vE^{-1}u)\theta+\varsigma\wedge(vE^2v+vEv-vE^{-2}v-vE^{-1}v)\varsigma]$$

$$=\frac{1}{2}\sum\,[\theta\wedge(uEu)\theta-\theta\wedge(uE^{-1}u)\theta+\theta\wedge(E^{-1}v)\theta-\theta\wedge(vE\theta)+\theta\wedge(-uE^{-2}v)\varsigma$$
$$+\theta\wedge(uEv)\varsigma+\varsigma\wedge(vE^2u\theta)-\varsigma\wedge(vE^{-1}u)\theta+\varsigma\wedge(vE^2v)\varsigma$$
$$+\varsigma\wedge(vEv\varsigma)-\varsigma\wedge(vE^{-2}v\varsigma)-\varsigma\wedge(vE^{-1}v)\varsigma]$$

$$=\frac{1}{2}\sum\,[\theta\wedge u\bar{u}\,\bar{\theta}-\bar{\theta}\wedge\bar{u}\,u\theta+\bar{\theta}\wedge v\,\theta-\theta\wedge v\,\bar{\theta}-\bar{\theta}\wedge\bar{u}\,v\,\varsigma+\theta\wedge u\bar{v}\,\bar{\varsigma}$$
$$+\varsigma\wedge v\,\bar{u}\,\bar{\theta}-\bar{\varsigma}\wedge\bar{v}u\,\theta+\varsigma\wedge v\bar{v}\,\bar{\varsigma}+\varsigma\wedge v\bar{v}\,\bar{\varsigma}-\bar{\varsigma}\wedge\bar{v}\,v\,\varsigma-\bar{\varsigma}\wedge\bar{v}\,v\,\varsigma], \tag{47}$$

where $\bar{\varsigma}=\varsigma_{n+1}$, $\underline{\varsigma}=\varsigma_{n-1}$, $\bar{\theta}=\theta_{n+1}$, $\underline{\theta}=\theta_{n-1}$, etc. Making use of the property of the wedge product, Eq. (47) can be written as

$$\Theta_{H_1}=\sum\,[u\,\bar{u}\,\theta\wedge\bar{\theta}+v\,\bar{\theta}\wedge\theta+\bar{u}\,v\,\varsigma\wedge\bar{\theta}+v\,\bar{v}\varsigma\wedge\bar{\varsigma}+u\,\bar{v}\,\theta\wedge\bar{\varsigma}+v\,\bar{v}\,\varsigma\wedge\bar{\varsigma}].$$

Proceeding further along the same lines as for the RT and BM lattice equations (1) and (2) we find that

$$PrV_{H_1\theta_1}(\Theta_{H_1})=0 \tag{48}$$

and so the operator H_1 is Hamiltonian. A similar conclusion can also be arrived at for the operator H_2 and therefore the BC lattice equation (3) can be written as

$$\begin{bmatrix}u_t\\ v_t\end{bmatrix}=H_1\begin{bmatrix}\dfrac{\delta\mathcal{H}_1}{\delta u}\\ \dfrac{\delta\mathcal{H}_1}{\delta v}\end{bmatrix}=H_2\begin{bmatrix}\dfrac{\delta\mathcal{H}_0}{\delta u}\\ \dfrac{\delta\mathcal{H}_0}{\delta v}\end{bmatrix},$$

where the Hamiltonian functionals are $\mathcal{H}_0(u,v)=-\Sigma\frac{1}{3}\log v$ and $\mathcal{H}_1(u,v)=\Sigma u$, indicating that it is a bi-Hamiltonian system. The bi-Hamiltonian formulation for the BC lattice equation has also been obtained by Belov *et al.* using a different approach.[30]

V. CONCLUSION

It is shown how to construct recursion operators systematically for PDDEs with two independent variables (one continuous and one discrete) using its generalized symmetries and then explained how to factorize it explicitly. This was illustrated for the relativistic toda (RT), Belov–Chaltikian (BC) and Blaszak–Marciniak (BM) lattice equations and it was shown that the RT and BC lattice equations admit (2×2) factorizable matrix recursion operators while the BM lattice equation possesses (3×3) factorizable matrix recursion operator. Furthermore, it is explicitly proved that the factorized operators are Hamiltonian in all the lattice equations. The existence of the multi-Hamiltonian structure for the above lattice equations is under investigation.

ACKNOWLEDGMENT

One of the authors (S.K.) would like to thank the University of Madras for providing a University Research Fellowship.

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Kolakoski-$(2m,2n)$ are limit-periodic model sets

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(Received 5 August 2002; accepted 29 August 2002)

We consider (generalized) Kolakoski sequences on an alphabet with two even numbers. They can be related to a primitive substitution rule of constant length ℓ. Using this connection, we prove that they have pure point dynamical and pure point diffractive spectrum, where we make use of the strong interplay between these two concepts. Since these sequences can then be described as model sets with ℓ-adic internal space, we add an approach to "visualize" such internal spaces. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1521239]

I. INTRODUCTION

A one-sided infinite sequence ω over the alphabet $\mathcal{A}=\{1,2\}$ is called a (classical) *Kolakoski sequence* (named after W. Kolakoski who introduced it in 1965, see Ref. 12), if it equals the sequence defined by its run lengths, e.g.,

$$\begin{array}{lccccccccccc} \omega= & \underbrace{22} & \underbrace{11} & \underbrace{2} & \underbrace{1} & \underbrace{22} & \underbrace{1} & \underbrace{22} & \underbrace{11} & \underbrace{2} & \underbrace{11} & \cdots \\ & 2 & 2 & 1 & 1 & 2 & 1 & 2 & 2 & 1 & 2 & \cdots=\omega. \end{array} \tag{1}$$

Here, a *run* is a maximal subword consisting of identical letters. The sequence $\omega'=1\omega$ is the only other sequence which has this property.

One way to obtain ω of (1) is by starting with 2 as a seed and iterating the two substitutions

$$\sigma_0:\ \begin{array}{l}1\mapsto 2\\ 2\mapsto 22\end{array} \quad \text{and} \quad \sigma_1:\ \begin{array}{l}1\mapsto 1\\ 2\mapsto 11,\end{array}$$

alternatingly, i.e., σ_0 substitutes letters on even positions and σ_1 letters on odd positions (we begin counting at 0):

$$2 \mapsto 22 \mapsto 2211 \mapsto 221121 \mapsto 221121221 \mapsto \cdots.$$

Clearly, the iterates converge to the Kolakoski sequence ω (in the obvious product topology), and ω is the unique (one-sided) fixed point of this iteration.

One can generalize this by choosing a different alphabet $\mathcal{A}=\{p,q\}$ [we are only looking at alphabets with $\mathrm{card}(\mathcal{A})=2$]. Such a (generalized) Kolakoski sequence, which is also equal to the sequence of its run lengths, can be obtained by iterating the two substitutions

$$\sigma_0:\ \begin{array}{l}q\mapsto p^q\\ p\mapsto p^p\end{array} \quad \text{and} \quad \sigma_1:\ \begin{array}{l}q\mapsto q^q\\ p\mapsto q^p\end{array} \tag{2}$$

alternatingly. Here, the starting letter of the sequence is p. We will call such a sequence a Kolakoski-(p,q) sequence, or Kol(p,q) for short. The classical Kolakoski sequence ω of (1) is therefore denoted by Kol(2,1) [and ω' by Kol(1,2)].

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While little is known about the classical Kolakoski sequence (see Ref. 6), and the same holds for all Kol(p,q) with p odd and q even or vice versa (see Ref. 22), the situation is more favorable if p and q are either both even or both odd. If both are odd, one can, in some cases, rewrite the substitution as a substitution of Pisot type (see Refs. 22 and 2), which can be described as (limit-) aperiodic model sets. By this method, Kol(3,1) is studied in Ref. 2 and shown to be a deformed model set. The case where both symbols are even will be studied below.

It is the aim of this article to determine structure and order of the sequences Kol$(2m,2n)$. This will require two steps: First we establish an equivalent substitution of constant length for Kol$(2m,2n)$ and analyze it with methods known from the theory of dynamical systems. Then we conclude diffractive properties from this.

Remark: Every Kol(p,q) can uniquely be extended to a bi-infinite (or two-sided) sequence. The one-sided sequence (to the right) is Kol(p,q) as explained above. The added part to the left is a reversed copy of Kol(q,p), e.g., in the case of the classical Kolakoski sequence of (1), this reads as

$$\ldots 11221221211221|22112122122112\ldots,$$

where "|" denotes the seamline between the one-sided sequences. Note that, if $q=1$ (or $p=1$), the bi-infinite sequence is mirror symmetric around the first position to the left (right) of the seamline. The bi-infinite sequence equals the sequence of its run lengths, if counting is begun at the seamline. Alternatively, one can get such a bi-infinite sequence by starting with $q|p$ and applying the two substitutions to get $\sigma_1(q)|\sigma_0(p)$ in the first step and so forth. This also implies that Kol(p,q) and Kol(q,p) will have the same spectral properties, and it suffices to study one of them.

II. Kol$(2m,2n)$ AS SUBSTITUTION OF CONSTANT LENGTH

If both letters are even numbers, i.e., $p=2m$ and $q=2n$ (with $m\neq n$, where we can concentrate on $m>n$ by the above discussion), one can build blocks of two letters and obtain an (ordinary) substitution. Setting $A=pp$ and $B=qq$, these substitutions and their *substitution matrix* $\mathbf{M}$ (sometimes called *incidence matrix* of the substitution) are given by

$$\sigma:\ \begin{matrix} A\mapsto A^mB^m \\ B\mapsto A^nB^n \end{matrix} \quad \text{and} \quad \mathbf{M}=\begin{pmatrix} m & m \\ n & n \end{pmatrix}, \tag{3}$$

where the entry M_{ij} is the number of occurrences of j in $\sigma(i)$ $(i,j\in\{A,B\}$; sometimes the transposed matrix is used). A bi-infinite fixed point can be obtained as follows:

$$B|A \mapsto A^nB^n|A^mB^m \mapsto \cdots.$$

This corresponds to the unique bi-infinite Kol$(2m,2n)$ according to our above convention.

A substitution ϱ is *primitive* if the corresponding substitution matrix $\mathbf{M}$ is primitive, i.e., $\mathbf{M}^k$ has positive entries only for some $k\in\mathbb{N}$. Equivalently, ϱ is primitive if there exists a positive integer $k\in\mathbb{N}$ such that every $i\in\mathcal{A}$ occurs in $\varrho^k(j)$ for all $j\in\mathcal{A}$. The vector $\boldsymbol{\ell}$ with components $\ell_i=|\varrho(i)|$, for $i\in\mathcal{A}$, is called the *length* of the substitution ϱ. If all ℓ_i are equal, ϱ is a substitution of *constant length*. For the substitution σ of (3), we have

$$\boldsymbol{\ell}=\begin{pmatrix} 2m \\ 2n \end{pmatrix},$$

which is therefore not of constant length (recall that $m\neq n$).

We will also need some notions from the theory of *dynamical systems*, (see Refs. 18 and 8 Chaps. 1, 5, and 7 for details). Let ϱ be a primitive substitution over $\mathcal{A}$ and $u\in\mathcal{A}^{\mathbb{Z}}$ a bi-infinite

fixed point of ϱ [i.e., $u=\varrho^k(u)$ for some $k\in\mathbb{N}$]. Denote by u_k the kth letter of $u(k\in\mathbb{Z})$ and by T the shift map [i.e., $(T(u))_k=u_{k+1}$]. Let $\mathcal{A}$ be equipped with the discrete and $\mathcal{A}^{\mathbb{Z}}$ with the corresponding product topology. If we set

$$X(\varrho)=\overline{\{T^k(u)|k\in\mathbb{Z}\}},$$

then $(X(\varrho),T)$ is a *dynamical system*. Since we require ϱ to be primitive, this dynamical system is *minimal* [i.e., $\{T^k(u)|k\in\mathbb{Z}\}$ is dense in $X(\varrho)$ for all $u\in(X(\varrho),T)$], does not depend on the chosen fixed point u (if more than one exists, which is possible in the two-sided situation) and has a unique probability measure μ associated with it. In other words, it is *strictly ergodic*. On the Hilbert space $\mathcal{L}^2(X(\varrho),\mu)$, we have the unitary operator

$$U:\ \mathcal{L}^2(X(\varrho),\mu)\to\mathcal{L}^2(X(\varrho),\mu),$$

$$f\qquad\mapsto f\circ T.$$

If $Uf=e^{i\lambda}f$ for some $0\neq f\in\mathcal{L}^2(X(\varrho),\mu)$, we call $e^{i\lambda}$ an *eigenvalue* of $(X(\varrho),T)$ and f the corresponding *eigenfunction*. The *spectrum* (of the dynamical system) is said to be a *pure point dynamical spectrum* (or *discrete spectrum*), if the eigenfunctions span $\mathcal{L}^2(X(\varrho),\mu)$. If 1 is the only eigenvalue and the only eigenfunctions are the constants, the spectrum is *continuous*. It is also possible that it has pure point and continuous components. In that case it is called *partially continuous*. Two dynamical systems (X,T) and (Y,S) are *isomorphic* (or *measure-theoretically isomorphic*), if there exists an invertible measurable map $\varphi:X\to Y$, almost everywhere defined, such that φ preserves the measure and the dynamics (i.e., $\varphi\circ T=S\circ\varphi$).

The spectral theory of primitive substitutions of constant length is well understood. By the following criterion, we know that the substitutions σ of (3) are related to substitutions of constant length.

Lemma 1 (Ref. 5, Sec. V, Theorem 1): Let ϱ *be a substitution of nonconstant length* ℓ. *If* ℓ *is a right eigenvector of the corresponding substitution matrix* $\mathbf{M}$, *then* $(X(\varrho),T)$ *is isomorphic to a substitution dynamical system generated by a substitution of constant length.* □

[Note that from (2), one can also construct a primitive substitution by distinguishing odd and even positions, e.g., for Kol(4,2) we would get (we use $\tilde{\cdot}$ as mark for even positions)

$$4\to 4\tilde{4}4\tilde{4},$$
$$\tilde{4}\to 2\tilde{2}2\tilde{2},$$
$$2\to 4\tilde{4},$$
$$\tilde{2}\to 2\tilde{2}.$$

Instead of (3), we would get a substitution with substitution matrix

$$\mathbf{M}=\begin{pmatrix} m & m & 0 & 0\\ 0 & 0 & m & m\\ n & n & 0 & 0\\ 0 & 0 & n & n\end{pmatrix}, \tag{4}$$

which is also primitive ($\mathbf{M}^2$ has positive entries only), but does not fulfill the requirements of Lemma 1. The eigenvalues of this $\mathbf{M}$ are $\{0,0,0,m+n\}$].

Since the substitutions σ of (3) fulfill the requirements of Lemma 1, the next task is now to construct the corresponding substitutions of constant length. This is achieved by numbering the A's and B's in (3), i.e., we make the substitutions $A^mB^m\to A_1\cdots A_mB_1\cdots B_m$, respectively $A^nB^n\to A_{m+1}\cdots A_{m+n}B_{m+1}\cdots B_{m+n}$. Then, the former substitutions (3) induce

$$\begin{aligned} A_1\cdots A_mB_1\cdots B_m &\mapsto (A_1\cdots A_mB_1\cdots B_m)^m(A_{m+1}\cdots A_{m+n}B_{m+1}\cdots B_{m+n})^m,\\ A_{m+1}\cdots A_{m+n}B_{m+1}\cdots B_{m+n} &\mapsto (A_1\cdots A_mB_1\cdots B_m)^n(A_{m+1}\cdots A_{m+n}B_{m+1}\cdots B_{m+n})^n. \end{aligned} \tag{5}$$

From this we get substitutions of constant length $m+n$ [the eigenvalue of the substitution matrix $\mathbf{M}$ in (3)] by parting the right sides in blocks of $m+n$ letters. For example, let $m=2$ and $n=1$. Then

$$A_1A_2B_1B_2 \mapsto A_1A_2B_1 \quad B_2A_1A_2 \quad B_1B_2A_3 \quad B_3A_3B_3,$$

$$A_3B_3 \mapsto A_1A_2B_1 \quad B_2A_3B_3,$$

and one extracts the following substitution of constant length 3:

$$\begin{aligned} A_1 &\mapsto A_1A_2B_1,\\ A_2 &\mapsto B_2A_1A_2,\\ B_1 &\mapsto B_1B_2A_3,\\ B_2 &\mapsto B_3A_3B_3,\\ A_3 &\mapsto A_1A_2B_1,\\ B_3 &\mapsto B_2A_3B_3. \end{aligned} \tag{6}$$

In the same way, we get substitutions of constant length $m+n$ from (5). Note that these substitutions are all primitive since [compare to (5)] in every block of $2m^2+2n$ successive letters (note that we use $m>n$) every letter of $\mathcal{A}=\{A_1,\ldots,A_{m+n},B_1,\ldots,B_{m+n}\}$ occurs, so if $(m+n)^{k_0} \geqslant 2m^2+2n$, then $\mathbf{M}^{k_0}$ has positive entries only (this holds for $k_0\geqslant 3$). Note also that we can reduce the alphabet by one letter by identifying $A_1=A_{m+1}$ [$A_1=A_3$ in the example (6)], because both A's always yield the same substitution.

Let us now determine the positions of A_1 in the sequence u generated by (5). They are given by $\alpha\cdot 2m+\beta\cdot 2n$ for some $\alpha,\beta\in\mathbb{Z}$ (e.g., $0, 2m, 4m,\ldots, 2m^2, 2m^2+2n, 2m^2+4n, \ldots, 2m^2+2nm,\ldots$). Therefore we get $\gcd\{i|u_i=u_0=A_1\}=\gcd(2m,2n)=2\gcd(m,n)$. The *height* $h(\varrho)$ of a primitive substitution ϱ of constant length ℓ which generates a sequence u is defined as

$$h(\varrho)=\max\{k\geqslant 1|\gcd(k,\ell)=1 \text{ and } k \text{ divides } \gcd\{i|u_i=u_0\}\}. \tag{7}$$

Then the following lemma holds.

Lemma 2: Let $(X(\varrho),T)$ be a dynamical system, where ϱ is a primitive substitution of constant length ℓ and height $h(\varrho)$. Then the pure point part of this dynamical system is isomorphic to the dynamical system $(\mathbb{Z}_\ell\times\mathbb{Z}/h(\varrho)\mathbb{Z},\tau)$, where τ is the addition of (1,1) on the Abelian group $\mathbb{Z}_\ell\times\mathbb{Z}/h(\varrho)\mathbb{Z}$, i.e., the direct product of the ℓ-adic integers $\mathbb{Z}_\ell$ and the cyclic group $\mathbb{Z}/h(\varrho)\mathbb{Z}$ of order $h(\varrho)$. Therefore the pure point dynamical spectrum is given by

$$\{e^{2\pi i\, n/\ell^m + 2\pi i k/h(\varrho)} |\, k,n\in\mathbb{Z},m\in\mathbb{N}\}.$$

Note that

$$\mathbb{Z}_\ell\simeq\mathbb{Z}_{p_1}\times\cdots\times\mathbb{Z}_{p_r}, \tag{8}$$

where $p_1,\ldots,p_r$ are the distinct primes dividing ℓ (see Ref. 16, Sec. 3.10).

Proof: The lemma is just a reformulation of Ref. 5, Theorem II.13 (compare with Ref. 18, Sec. VI and Ref. 8, Sec. 7.3). □

Proposition 1: Suppose $(X(\sigma),T)$ *has pure point dynamical spectrum, where* σ *is the substitution of (3). Then*

$$(X(\sigma),T)\simeq\begin{cases}(\mathbb{Z}_{m+n}\times\mathbb{Z}/2\mathbb{Z},\tau) & \text{if } m+n \text{ is odd,}\\ (\mathbb{Z}_{m+n},\tilde{\tau}) & \text{if } m+n \text{ is even,}\end{cases}$$

where τ *is the addition of* (1,1) and $\tilde{\tau}$ *the addition of* 1.

Proof: For the substitution (5) of constant length $\ell=m+n$, we have already seen that $\gcd\{i|u_i=u_0\}=2\gcd(m,n)$. Therefore, using (7), the height of this substitution is 2 if ℓ is odd and 1 if ℓ is even. The dynamical system of the substitution (5) is isomorphic to $(X(\sigma),T)$ by Lemma 1, therefore they have the same spectrum. The remaining statement follows from Lemma 2. □

We want to show that the spectrum of σ is indeed pure point. For this we use slightly different substitutions of constant length that we deduce from σ. We substitute $A^mB^m\to a_1\cdots a_m$ and $A^nB^n\to b_1\cdots b_n$ [so in (5) we build essentially blocks of two, e.g., $a_1=A_1A_2$]. We get

$$\begin{aligned}a_1\cdots a_m &\mapsto (a_1\cdots a_m)^m(b_1\cdots b_n)^m,\\ b_1\cdots b_n &\mapsto (a_1\cdots a_m)^n(b_1\cdots b_n)^n,\end{aligned}\tag{9}$$

which again gives substitutions of constant length $\ell=m+n$. They are all primitive substitutions by the same argument as before (in every block of m^2+n successive letters every letter occurs). In the case $n>1$, we can reduce the alphabet by one letter by identifying $a_1=b_1\mapsto a_1\cdots a_ma_1\cdots a_n$. So we have two cases, $n=1$ with substitutions

$$\tilde{\theta}:\begin{cases}a_1 \mapsto a_1\ a_2\ a_3\ \dots\ a_{m-1}\ a_m\ a_1,\\ a_2 \mapsto a_2\ a_3\ a_4\ \dots\ a_m\ a_1\ a_2,\\ \vdots\quad \dots\\ a_{m-1} \mapsto a_{m-1}\ a_m\ a_1\ \dots\ a_{m-3}\ a_{m-2}\ a_{m-1},\\ a_m \mapsto a_m\ b_1\ b_1\ \dots\ b_1\ b_1\ b_1,\\ b_1 \mapsto a_1\ a_2\ a_3\ \dots\ a_{m-1}\ a_m\ b_1,\end{cases}\tag{10}$$

and $n>1$ with substitutions θ (it is cumbersome to write down such a θ in general form, but we will investigate its structure in the next section). Now the height of θ and $\tilde{\theta}$ is always 1, because if $n>1$ we get $\gcd\{i|u_0=u_i=a_1\}=\gcd(m,n)$, and if $n=1$ we get $\gcd\{i|u_0=u_i=a_1\}=\gcd(m,m+1)=1$.

Let ϱ be a primitive substitution of constant length ℓ and height $h(\varrho)=1$. One says that ϱ admits a *coincidence*, if there exist a $k\in\mathbb{N}$ and $j<\ell^k$ such that $\varrho^k(i)_j$ is the same for all $i\in\mathcal{A}$ [the jth letter of each $\varrho^k(i)$ is the same, i.e., ϱ^k admits a column of identical values].

Lemma 3 (Ref. 5, Sec. III, Theorem 7): Let $(X(\varrho),T)$ *be a substitution dynamical system of constant length and height* $h(\varrho)=1$. *Then* $(X(\varrho),T)$ *has pure point dynamical spectrum if and only if* ϱ *admits a coincidence.* □

If a substitution has height $h>1$, one gets a substitution of height 1 by combining letters into blocks of h letters. If this new substitution has pure point dynamical spectrum, so has the original substitution of height h (see Ref. 5). Obviously, we get the following: if the substitutions θ and $\tilde{\theta}$ [which arise from (9)] admit coincidences, then the dynamical systems defined by σ of (3) have pure point dynamical spectrum.

III. COINCIDENCES AND COINCIDENCE MATRIX

Let us first check $\tilde{\theta}$ of (10) for coincidences. For this we begin by exploring the structure: $\tilde{\theta}(a_1)$ has two a_1's at position 0 and m, $\tilde{\theta}(a_2)$ has an a_1 at position $m-1$, etc. We get an a_1 in $\tilde{\theta}(a_k)$ at position $m+1-k$ for $1\leqslant k\leqslant m-1$. Similar arguments show that there is an a_m in $\tilde{\theta}(a_k)$

at position $m-k$ for $1\leqslant k\leqslant m$ and at $m-1$ in $\tilde{\theta}(b_1)$. Now, $\tilde{\theta}(a_m)$ has b_1's at all positions $1,\ldots,m$. Furthermore, $\tilde{\theta}(b_1)$ has a b_1 at position m and shares the first m letters with $\tilde{\theta}(a_1)$. Schematically, we get the following structure of $\tilde{\theta}$:

$$\begin{array}{lllllllll}
a_1 & \mapsto & * & * & * & \ldots & * & a_m & a_1, \\
a_2 & \mapsto & \cdot & \cdot & \cdot & \ldots & a_m & a_1 & \cdot, \\
\vdots & & & & & / & / & & \\
\vdots & & & & / & / & & & \\
a_{m-1} & \mapsto & \cdot & a_m & a_1 & \ldots & \cdot & \cdot & \cdot, \\
a_m & \mapsto & a_m & b_1 & b_1 & \ldots & b_1 & b_1 & b_1, \\
b_1 & \mapsto & * & * & * & \ldots & * & a_m & b_1.
\end{array} \tag{11}$$

Here we have omitted (.) all letters that are not necessary and by $*$ we denote the part that $\tilde{\theta}(a_1)$ and $\tilde{\theta}(b_1)$ share. We now check for *pairwise coincidences*, i.e., for $i_1,i_2\in\mathcal{A}$ we check whether there is a $k\in\mathbb{N}$ and a $j<\ell^k=(m+1)^k$ such that $\sigma^k(i_1)_j=\sigma^k(i_2)_j$.

So we pick $i_1,i_2\in\mathcal{A}=\{a_1,\ldots,a_m,b_1\}$, $i_1\neq i_2$. Suppose $i_1\neq a_m$ (otherwise we interchange i_1 and i_2). Then i_2 either equals a_m or at least $\tilde{\theta}(i_2)$ has an a_m [every $\tilde{\theta}(i)$, $i\in\mathcal{A}$ has one]. In the first case take $k=1$, otherwise $k=2$. Observe that there are m successive b_1's in $\tilde{\theta}(a_m)$. So, if we look at $\tilde{\theta}^k(i_1)$ and $\tilde{\theta}^k(i_2)$, we get the following: On the one hand, there are m successive b_1's somewhere in $\tilde{\theta}^k(i_2)$, say at positions $j,\ldots,j+m-1$. On the other hand, in $\tilde{\theta}^k(i_1)$, there is at one of these positions $j,\ldots,j+m-1$ either a b_1, and we have a pairwise coincidence, or an a_1. Say there is an a_1 at $\tilde{j}$ with $j\leqslant\tilde{j}\leqslant j+m-1$. Then in $\tilde{\theta}^{k+1}(i_1)$ and $\tilde{\theta}^{k+1}(i_2)$ we have pairwise coincidences at positions $\tilde{j}\cdot\ell,\ldots,\tilde{j}\cdot\ell+m$ [the $*$'s of (11)].

From this pairwise coincidences we get a coincidence inductively: We start with two letters i_1,i_2 and after $k_1\leqslant 3$ substitutions we have a pairwise coincidence, say at j_1. Now a third letter i_3 may have something else at $\tilde{\theta}^{k_1}(i_3)_{j_1}$, but whatever it is, in $\tilde{\theta}^{k_1+k_2}$ ($k_2\leqslant 3$) all three coincide somewhere at a position j_2 with $j_1\cdot\ell^{k_2}\leqslant j_2<(j_1+1)\cdot\ell^{k_2}$. Since there are $\mathrm{card}(\mathcal{A})=m+1$ letters, we get a coincidence after at most $3\cdot m$ substitutions [i.e., there is a $j<\ell^{3m}$ such that all $\tilde{\theta}^{3m}(i)_j$ are the same for all $i\in\mathcal{A}$].

The structure of θ is different. We have $\mathcal{A}=\{a_1,\ldots,a_m,b_2,\ldots b_n\}$ and therefore $\mathrm{card}(\mathcal{A})=m+n-1$. Let us first show an example, with $m=5$ and $n=3$:

$$\begin{array}{lllllllll}
a_1 & \mapsto & a_1 & a_2 & a_3 & a_4 & a_5 & a_1 & a_2 & a_3, \\
a_2 & \mapsto & a_4 & a_5 & a_1 & a_2 & a_3 & a_4 & a_5 & a_1, \\
a_3 & \mapsto & a_2 & a_3 & a_4 & a_5 & a_1 & a_2 & a_3 & a_4, \\
a_4 & \mapsto & a_5 & a_1 & b_2 & b_3 & a_1 & b_2 & b_3 & a_1, \\
a_5 & \mapsto & b_2 & b_3 & a_1 & b_2 & b_3 & a_1 & b_2 & b_3, \\
b_2 & \mapsto & a_4 & a_5 & a_1 & a_2 & a_3 & a_4 & a_5 & a_1, \\
b_3 & \mapsto & b_2 & b_3 & a_1 & b_2 & b_3 & a_1 & b_2 & b_3.
\end{array} \tag{12}$$

Since the positions of two consecutive a_1's in the sequence differ by at most m, there is an a_1 in every $\theta(i)$ with $i\in\mathcal{A}$ (note that θ is a substitution of constant length $\ell=m+n$). Again we look for pairwise coincidences, so choose $i_1,i_2\in\mathcal{A}$. Then there is (at least) one a_1 in $\theta(i_1)$, say at position j_1, and (at least) one in $\theta(i_2)$, say at position j_2. Since there can be more than one a_1 in either, we choose j_1,j_2 such that $|j_1-j_2|$ is minimal. We further choose i_1,i_2 such that $j_1<j_2$ (in the case $j_1=j_2$, e.g., $i_1=a_1$ and $i_2=a_5$ in the above example, we are already done). If we look at $\theta(i_1)$ and $\theta(i_2)$, there are two cases each (and therefore four cases, if we look at the combina-

tions): Either $\theta(i_1)_{j_1+1}=a_2,\ldots,\theta(i_1)_{j_2}=a_{j_2+1-j_1}$ or $\theta(i_1)_{j_1+1}=b_2,\ldots,\theta(i_1)_{j_2}=b_{j_2+1-j_1}$ and either $\theta(i_2)_{j_1}=a_{m+1+j_1-j_2},\ldots,\theta(i_2)_{j_2-1}=a_m$ or $\theta(i_2)_{j_1}=b_{m+1+j_1-j_2},\ldots,\theta(i_2)_{j_2-1}=b_m$. This is all that can occur by the chosen minimality of $j_2-j_1>0$.

Now we examine the case where $\theta(i_1)_{j_1+1}=a_2,\ldots,\theta(i_1)_{j_2}=a_{j_2+1-j_1}$ and $\theta(i_2)_{j_1}=a_{m+1+j_1-j_2},\ldots,\theta(i_2)_{j_2-1}=a_m$. We want to show that $\theta^2(i_1)$ and $\theta^2(i_2)$ have a pairwise coincidence. Let us look at the a_1's in $\theta(a_i)$ only (we use again the above example, but the reasons given apply for arbitrary m, n):

$$
\begin{aligned}
a_1 &\mapsto \overset{1}{\boldsymbol{a}}_1\ a_2\ a_3\ a_4\ a_5\ \overset{2}{\boldsymbol{a}}_1\ a_2\ a_3,\\
a_2 &\mapsto a_4\ a_5\ \overset{3}{\boldsymbol{a}}_1\ a_2\ a_3\ a_4\ a_5\ \overset{4}{\boldsymbol{a}}_1,\\
a_3 &\mapsto a_2\ a_3\ a_4\ a_5\ \overset{5}{\boldsymbol{a}}_1\ a_2\ a_3\ a_4,\\
a_4 &\mapsto a_5\ \overset{6}{\boldsymbol{a}}_1\ b_2\ b_3\ \overset{7}{\boldsymbol{a}}_1\ b_2\ b_3\ \overset{8}{\boldsymbol{a}}_1,\\
a_5 &\mapsto b_2\ b_3\ \overset{9}{\boldsymbol{a}}_1\ b_2\ b_3\ \overset{10}{\boldsymbol{a}}_1\ b_2\ b_3.
\end{aligned}
\tag{13}
$$

First we number the a_1's with 1,...,2m [left to right in $\theta(a_i)$ and top $(i=1)$ to bottom $(i=m)$] and we will speak of the kth a_1 (with $1\leqslant k\leqslant 2m$) according to that number. We observe the following:

(i) Let $k<m$. If the kth a_1 occurs at position $j\geqslant n$ in $\theta(a_i)$, then the $(k+1)$-st a_1 occurs at position $j-n$ in $\theta(a_{i+1})$. If the kth a_1 occurs at position $j<n$, then the $(k+1)$-st a_1 occurs at $j+m$ in the same $\theta(a_i)$.

(ii) Let $k>m+1$. If the kth a_1 occurs at position $j\geqslant n$, then the $(k-1)$-st a_1 occurs at $j-n$ in the same $\theta(a_i)$. If the kth a_1 occurs at position $j<n$ in $\theta(a_i)$, then the $(k-1)$-st a_1 occurs at position $j+m$ in $\theta(a_{i-1})$. [Notice the contrary behavior of the first two observations in going to a different or staying in the same $\theta(a_i)$ and the position of the corresponding a_1. We call this the "contrary line break property."]

(iii) The second and the $(2m)$-th a_1 occur at the same position m in $\theta(a_1)$, respectively $\theta(a_m)$. With the previous two observations we get the kth and the $(2m+2-k)$-th a_1 occur at the same position for $1<k<m$.

(iv) The first and the $(m+1)$-st a_1 occur in $\theta(a_i)$ where there is at least one more a_1. This is obvious for the first a_i; for the $(m+1)$-st observe that if it occurs at position $j<m$, then there is also one at $j+n$, and if it occurs at position $j\geqslant m$, then there is also one at $j-m$.

These observations are based on the facts that the length of the substitution is $m+n$ and that the position of the a_1's in the sequence are separated by m or n only. Now the fact that the a_i always occur in ascending order (i.e., we have $a_1a_2a_3\cdots$ and not $a_3a_1a_2\cdots$ or something else) together with the first two observations essentially gives us an algorithm, which always yields a pairwise coincidence in $\theta^2(i_1)$ and $\theta^2(i_2)$. Let us explain it in our example (13): Suppose we have $i_1=a_2$ and $i_2=a_3$. Then we have $j_1=2$ and $j_2=4$. The first step is always to reduce j_2 by one, so we have $j_2'=3$. We have $j_2'\neq j_1$, but there is a second a_1 in $\theta(a_m)$ (a_m occurs at position j_2' in i_2!), so we can increment j_1 by 1 and get $j_1'=3$. We have $j_1'=j_2'$, and $\theta(\theta(a_2)_{j_1'})=\theta(a_2)$ and $\theta(\theta(a_3)_{j_2'})=\theta(a_5)$ both have an a_1 at position 2 (the third respectively the ninth a_1). Therefore we get a pairwise coincidence in $\theta^2(a_2)$ and $\theta^2(a_3)$. This algorithm relies on the "contrary line break property."

The other three cases are mutatis mutandis the same [see the positions of the a_1's in (12)]. So, starting with any two i_1, $i_2\in\mathcal{A}$ we get a pairwise coincidence in $\theta^2(i_1)$ and $\theta^2(i_2)$. Inductively

like before, we get a coincidence after at most $2\cdot(m+n-2)$ substitutions. Therefore we have established the following.

Theorem 1: $(X(\sigma),T)$ *with* σ *of* (3) *has pure point dynamical spectrum. Also, the dynamical system of the substitutions of constant length as defined implicitly in* (5) *and* $\theta,\tilde{\theta}$ *of* (9) *and* (10) *have pure point dynamical spectrum.* □

Proposition 1′: We have

$$(X(\sigma),T)\simeq\begin{cases}(\mathbb{Z}_{m+n}\times\mathbb{Z}/2\mathbb{Z},\tau) & \text{if } m+n \text{ is odd,}\\ (\mathbb{Z}_{m+n},\tilde{\tau}) & \text{if } m+n \text{ is even,}\end{cases}\tag{14}$$

where τ *is the addition of* (1,1) *and* $\tilde{\tau}$ *the addition of* 1. □

Remark: Let ϱ be a primitive substitution of constant length ℓ and height 1 over the alphabet $\mathcal{A}=\{1,\ldots,r\}$. Then we can define the coincidence matrix $\mathbf{C}$, which is a quadratic $r\cdot(r+1)/2\times r\cdot(r+1)/2$ matrix. The entries are defined as follows (where $t\leqslant s$ and $v\leqslant u$):

$$C_{(st)(uv)}=\begin{cases}|\{j|\varrho(s)_j=u\ \wedge\ \varrho(t)_j=u\}|, & \text{if } u=v,\\ |\{j|\varrho(s)_j=u\ \wedge\ \varrho(t)_j=v\}|+|\{j|\varrho(s)_j=v\ \wedge\ \varrho(t)_j=u\}|, & \text{if } u\neq v.\end{cases}$$

Note that the substitution matrix $\mathbf{M}$ is a submatrix of $\mathbf{C}$, since $M_{su}=C_{(ss)(uu)}$. Also, $\mathbf{C}$ has row sums ℓ. With this definition, Lemma 3 reads as follows.

Proposition 2 (Ref. 18, Proposition X.1): For $(X(\varrho),T)$ *are equivalent:*

(i) $(X(\varrho),T)$ *has pure point dynamical spectrum.*
(ii) ℓ *is a simple eigenvalue of the corresponding coincidence matrix* $\mathbf{C}$. □

[Note, however, that we use a definition of $\mathbf{C}$ different from Ref. 18. The coincidence matrix there has dimension $r^2\times r^2$ and has the form (with the proper enumeration of the pairs)

$$\begin{pmatrix}M & 0 & 0\\ R & P & Q\\ R & Q & P\end{pmatrix}^t,$$

while the one defined above has the form

$$\begin{pmatrix}M & 0\\ R & P+Q\end{pmatrix}.$$

Here M, P, Q are quadratic matrices and M is the substitution matrix. Proposition 2 is true for both matrices, the proof is analogous.]

Obviously, ℓ is an eigenvalue of $\mathbf{C}$ ($\mathbf{C}/\ell$ is a stochastic matrix with row sum 1). Now the above proof of Theorem 1 translates to the following statements for $\mathbf{C}$:

(a) For $\tilde{\theta}$, the third power of the coincidence matrix, $\mathbf{C}^3$, has a column $(C^3_{(st)(a_1a_1)})$ with nonzero entries only.
(b) For θ, the square of the coincidence matrix, $\mathbf{C}^2$, has a column $(C^2_{(st)(a_1a_1)})$ with nonzero entries only.

Lemma 4 (Ref. 18, Lemma X.3): Let $\mathbf{B}$ *be a quadratic matrix with non-negative integral entries and row sums* ℓ. *If* $B_{ij}\geqslant 1$ *for all* i *and a fixed* j, *then* ℓ *is a simple eigenvalue of* $\mathbf{B}$. □

This establishes the desired result that ℓ is a simple eigenvalue for the coincidence matrix $\mathbf{C}$ of θ ($\tilde{\theta}$), since ℓ^2 (ℓ^3) is a simple eigenvalue of $\mathbf{C}^2$ ($\mathbf{C}^3$).

We end this section with an example. We take $\tilde{\theta}$ for $m=2$, $n=1$ and therefore the substitution

$$\begin{aligned} a_1 &\mapsto a_1\ a_2\ a_1,\\ a_2 &\mapsto a_2\ b_1\ b_1,\\ b_1 &\mapsto a_1\ a_2\ b_1. \end{aligned} \tag{15}$$

We get the coincidence matrix

$$\mathbf{C}=\begin{pmatrix} 2&1&0&0&0&0\\ 0&1&2&0&0&0\\ 1&1&1&0&0&0\\ 0&0&0&1&1&1\\ 1&1&0&0&1&0\\ 0&0&1&1&0&1 \end{pmatrix},\quad \mathbf{C}^2=\begin{pmatrix} 4&3&2&0&0&0\\ 2&3&4&0&0&0\\ 3&3&3&0&0&0\\ 1&1&1&2&2&2\\ 3&3&2&0&1&0\\ 1&1&2&2&1&2 \end{pmatrix}.$$

Here, already $\mathbf{C}^2$ has columns with positive entries only. The eigenvalues of $\mathbf{C}$ are $\{0,0,1,1,2,3\}$.

IV. MODEL SETS AND DIFFRACTION

A *model set* $\Lambda(\Omega)$ *(or cut-and-project set) in physical space* $\mathbb{R}^d$ is defined within the following general cut-and-project scheme (see Refs. 17 and 1)

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\ \pi\ } & \mathbb{R}^d\times H & \xrightarrow{\ \pi_{\mathrm{int}}\ } & H\\ & {\scriptstyle 1-1}\nwarrow & \cup & \nearrow{\scriptstyle \mathrm{dense}} & \\ & & \Gamma & & \end{array}$$

where the *internal space* H is a locally compact Abelian group, and $\Gamma\subset\mathbb{R}^d\times H$ is a *lattice*, i.e., a co-compact discrete subgroup of $\mathbb{R}^d\times H$. The projection $\pi_{\mathrm{int}}(\Gamma)$ is assumed to be dense in internal space, and the projection π into physical space has to be one-to-one on Γ. The model set $\Lambda(\Omega)$ is

$$\Lambda(\Omega)=\{\pi(x)\,|\,x\in\Gamma,\ \ \pi_{\mathrm{int}}(x)\in\Omega\}\subset\mathbb{R}^d,$$

where the *window* $\Omega\subset H$ is a relatively compact set with nonempty interior.

Let u be a bi-infinite sequence over $\mathcal{A}=\{1,\ldots,r\}$ and $\nu:\mathcal{A}\to\mathbb{C}$, $i\mapsto c_i$ be a (bounded) function which assigns to every letter a complex number (the *scattering strength*). Then the *autocorrelation coefficients* $\eta(z)$ are given by

$$\eta(z)=\lim_{N\to\infty}\frac{1}{2N+1}\sum_{n=-N}^{N}\overline{\nu(u_n)}\cdot\nu(u_{n+z})$$

provided the limits exist. We write δ_z for the Dirac measure at z, i.e., $\delta_z(f)=f(z)$ for f continuous. Then the *correlation measure* γ of u is given by

$$\gamma=\sum_{z\in\mathbb{Z}}\eta(z)\ \delta_z,$$

and the *diffraction spectrum* is given by the Fourier transform $\hat{\gamma}$ of this measure. [So we think of u as an atomic chain, where there is an atom of type u_n at position n with scattering strength $\nu(u_n)$. We represent this atom as $\nu(u_n)\cdot\delta_n$ and therefore get a (countable) sum of weighted Dirac measures with autocorrelation γ.] If $\hat{\gamma}$ is a sum of Dirac measures only, i.e., $\hat{\gamma}=\Sigma_{k\in S}\ d_k\cdot\delta_k$ with

a countable set S [for any choice of complex numbers $(c_i)_{i\in\mathcal{A}}$], then u is *pure point diffractive*, i.e., the diffraction spectrum consists of *Bragg peaks* only. Also, the d_k's are the square of the absolute value of the corresponding *Fourier–Bohr coefficient* at k and therefore non-negative (real) numbers. If there is no Dirac measure in $\hat{\gamma}$, except one at position 0, δ_0, which is determined by the density of the structure only, then the diffraction spectrum is *continuous*.

For substitutive systems, the diffraction spectrum and the spectrum of the corresponding dynamical system are closely related, see Refs. 7, 19, 21, 13, and 14.

Proposition 3 (Ref. 13, Corollary 1): Let ϱ be a primitive substitution of constant length ℓ with height 1 over $\mathcal{A}=\{1,\ldots,r\}$, where u is a fixed bi-infinite word of ϱ. Define $U_i=\{j\in\mathbb{Z}|u_j=i\}$ for all $i\in\mathcal{A}$. We have $\mathbb{Z}=U_1\dot{\cup}\cdots\dot{\cup}U_r$, where $\dot{\cup}$ denotes disjoint union. Then the following are equivalent:

(i) *ϱ admits a coincidence.*
(ii) *The U_i's are model sets for*

$$\begin{array}{ccccc} \mathbb{R} & \xleftarrow{\ \pi\ } & \mathbb{R}\times\mathbb{Z}_\ell & \xrightarrow{\ \pi_{\mathrm{int}}\ } & \mathbb{Z}_\ell \\ \cup & {\scriptstyle 1-1}\nwarrow & \cup & \nearrow_{\mathrm{dense}} & \cup \\ \mathbb{Z} & \longleftarrow & \Gamma=\{(z,z)|z\in\mathbb{Z}\} & \longrightarrow & \mathbb{Z} \end{array}$$

(iii) *The sequence u and the sets U_i are pure point diffractive.* (By this we mean the special choice of ν, where we set $c_i=1$ and $c_j=0$ for all $j\neq i$.) □

Note that properties ''one-to-one'' and ''dense'' are obvious; the interesting part is that there exist relatively compact windows (with respect to the ℓ-adic topology) with non-empty(!) interior. We will discuss this point in the next section.

With this Proposition, we know that θ and $\tilde{\theta}$ [as defined implicitly in (9)] generate sequences which are pure point diffractive. But we got every letter $i\in\mathcal{A}$ for the appropriate alphabet for θ, $\tilde{\theta}$ by building four-letter blocks in the substitution rule (2), e.g., in (15) we have $a_1=4444$, $a_2=2222$ and $b_1=4422$. Such a deterministic substitution rule [i.e., Kol$(2m,2n)$ is *local derivable* from the sequence generated by θ, respectively $\tilde{\theta}$] does not change the nature of the diffraction spectrum, only the Fourier-Bohr coefficients. The diffraction spectrum of Kol$(2m,2n)$ can be calculated from the one generated by θ, $\tilde{\theta}$ as follows: For Kol$(2m,2n)$ we only have scattering strengths c'_{2m} and c'_{2n}. If we therefore choose c_i ($i\in\mathcal{A}$ with respect to θ, $\tilde{\theta}$) according to its four-letter-composition in $\{2m,2n\}$, then the diffraction spectrum $\hat{\gamma}$ of θ, $\tilde{\theta}$ is also a diffraction spectrum of Kol$(2m,2n)$, where Kol$(2m,2n)$ is realized as an atom chain with atoms not on $\mathbb{Z}$ but $\mathbb{Z}/4$ [we get the diffraction spectrum of Kol$(2m,2n)$ realized on $\mathbb{Z}$ by a simple rescaling with the factor 4]. For the example (15), this means that we choose

$$c_{a_1}=c'_4\cdot(1+e^{-2\pi i/4}+e^{-2\,2\pi i/4}+e^{-3\,2\pi i/4})=0,$$

$$c_{a_2}=c'_2\cdot(1+e^{-2\pi i/4}+e^{-2\,2\pi i/4}+e^{-3\,2\pi i/4})=0,$$

$$c_{b_1}=c'_4\cdot(1+e^{-2\pi i/4})+c'_2\cdot(e^{-2\,2\pi i/4}+e^{-3\,2\pi i/4})=(1-i)(c'_4-c'_2).$$

So in this case, the diffraction spectrum of Kol(4,2) is given by the one of U_{b_1} only. All Kol$(2m,2n)$ are pure point diffractive.

Lemma 5: For a sequence $u=\phi(v)$, where v is a bi-infinite fixed point of a primitive substitution and $\phi:\mathcal{A}_v\to\mathcal{A}_u^*$ is a morphism [where u (v) is a sequence over $\mathcal{A}_u$ ($\mathcal{A}_v$)], the following statements are equivalent:

(i) *The dynamical system of u has pure point dynamical spectrum.*
(ii) *u has pure point diffraction spectrum.*

Proof: This is a (weak) conclusion of Ref. 14, Theorem 3.2. □

We therefore obtain the following.

Theorem 2: *All* Kol$(2m,2n)$ *have pure point diffraction and pure point dynamical spectrum*. □

Remarks: The dynamical system of Kol$(2m,2n)$ is isomorphic to

$$\begin{aligned}&(\mathbb{Z}_{m+n}\times\mathbb{Z}/4\mathbb{Z},\tau) \quad \text{if } m+n\equiv 1,3 \quad (4),\\ &(\mathbb{Z}_{m+n}\times\mathbb{Z}/2\mathbb{Z},\tau) \quad \text{if } m+n\equiv 2 \quad (4),\\ &(\mathbb{Z}_{m+n},\tilde{\tau}) \quad \text{if } m+n\equiv 0 \quad (4),\end{aligned} \tag{16}$$

where τ is the addition of (1,1) and $\tilde{\tau}$ the addition of 1. This can be seen by the fact that we get Kol$(2m,2n)$ from the one generated by σ of (3) by the substitution $A=pp$, $B=qq$, which corresponds just to doubling each letter in the latter one [see the substitution matrices in (3) and (4)].

If we consider how to get from (5), respectively (9), to Kol$(2m,2n)$ and compare this to Proposition 3, we get [compare with (16)] Kol$(2m,2n)$, respectively U_{2m}, U_{2n} are model sets for

$$\begin{array}{ccccc}\mathbb{R} & \xleftarrow{\pi} & \mathbb{R}\times\mathbb{Z}_{m+n}\times F & \xrightarrow{\pi_{\text{int}}} & \mathbb{Z}_{m+n}\times F\\ & {\scriptstyle 1-1}\nwarrow & \cup & \nearrow_{\text{dense}} & \\ & & \Gamma=\{(z,z,z \mod \text{ord}(F))\,|\,z\in\mathbb{Z}\} & & \end{array}$$

where

$$F\simeq\begin{cases}\mathbb{Z}/4\mathbb{Z} & \text{if } m+n\equiv 1,3 \quad (4),\\ \mathbb{Z}/2\mathbb{Z} & \text{if } m+n\equiv 2 \quad (4),\\ \{0\} & \text{if } m+n\equiv 0 \quad (4)\,.\end{cases} \tag{17}$$

(As before, $\mathbb{Z}_{m+n}\simeq\mathbb{Z}_{p_1}\times\cdots\times\mathbb{Z}_{p_r}$, where $p_1,\ldots,p_r$ are the distinct primes dividing $m+n$.) The diffraction spectrum calculated from this cut-and-project scheme is consistent with the previous one, since the Fourier–Bohr coefficients which arise in each $\mathbb{Z}_{m+n}$ separately are weighted by factors 1, $e^{-2\pi i/4}$, $e^{-2\,2\pi i/4}$ or $e^{-3\,2\pi i/4}$ which depend on the element of the cyclic group $\mathbb{Z}/4\mathbb{Z}$ (similar for the case $\mathbb{Z}/2\mathbb{Z}$) (compare with Ref. 3—but this is just how we calculated the c_i's from c'_{2m} and c'_{2n}).

Let us show how one calculates the diffraction spectrum of U_{b_1} of (15) explicitly. This substitution can be written in recursive equations for U_{a_1}, U_{a_2} and U_{b_1} by observing at which position in which substitution a certain letter occurs [e.g., b_1 occurs in $\tilde{\theta}(a_2)$ at positions 1 and 2 and in $\tilde{\theta}(b_1)$ at position 2]:

$$\begin{aligned}U_{a_1}&=(3U_{a_1})\ \cup\ (3U_{a_1}+2)\ \cup\ (3U_{b_1}),\\ U_{a_2}&=(3U_{a_1}+1)\ \cup\ (3U_{a_2})\ \cup\ (3U_{b_1}+1),\\ U_{b_1}&=(3U_{a_2}+1)\ \cup\ (3U_{a_2}+2)\ \cup\ (3U_{b_1}+2),\end{aligned}$$

where $rU_i+s=\{r\cdot z+s\,|\,z\in U_i\}$. {Note that these recursive equations form an *iterated function system* (IFS) in 3-adic space, because multiplication by a factor of 3 is a contraction in the 3-adic topology. The closure of the windows in the 3-adic internal space is therefore given by the unique

compact solution of this IFS by (a generalized version of) Hutchinson's theorem [Ref. 11 Sect. 3.1(3)]. This method is well known for unimodular substitutions of Pisot-type (see Refs. 15 and 2 and the vast literature about Rauzy fractals). Similar results apply for all primitive substitutions of constant length ℓ in ℓ-adic space.} Iterating these equations and using $U_{a_1} \cup U_{a_2} \cup U_{b_1} = \mathbb{Z}$, one gets

$$U_{b_1} = (9\mathbb{Z}+5) \cup (27\mathbb{Z}+17) \cup (27\mathbb{Z}+22) \cup (81\mathbb{Z}+53) \cup (81\mathbb{Z}+58) \cup (81\mathbb{Z}+64) \cup (81\mathbb{Z}+65) \cup \cdots .$$

The Fourier transform of each lattice coset $\omega_{r\mathbb{Z}+s} = \Sigma_{z\in\mathbb{Z}} \delta_{r\cdot z+s}$ is easy to calculate:

$$\widehat{\omega_{r\mathbb{Z}+s}} = \frac{1}{r} e^{-2\pi i k s} \omega_{\mathbb{Z}/r} .$$

Every Fourier–Bohr coefficient of $\widehat{U_{b_1}}$ is then given by the sum of the Fourier–Bohr coefficients of the corresponding $\widehat{\omega_{r\mathbb{Z}+s}}$. The structure of U_{b_1} (similar for all U_i that occur for substitutions of constant length) as a union of a countable but infinite set of (periodic) lattice cosets $r\cdot\mathbb{Z}+s$ gives rise to the name *limit-periodic* (see Ref. 9).

The *support* of the Bragg peaks of Kol$(2m,2n)$ is given by

$$\left\{ \frac{k}{4\cdot(m+n)^s} \middle| k\in\mathbb{Z},\ \ s\in\mathbb{N}_0 \right\} = \left\{ \frac{k}{2^\varepsilon \cdot p_1^{s_1} \cdot \cdots \cdot p_r^{s_r}} \middle| k\in\mathbb{Z},\ \ s_1,\ldots,s_r\in\mathbb{N}_0,\ \ \varepsilon\in\{0,\ldots,\log_2(\mathrm{ord}(F))\} \right\},$$

where $p_1,\ldots,p_r$ are the distinct primes dividing $m+n$ and F is the cyclic group of (17). However, there need not be a Bragg peak on every point of the support, e.g., Kol(8,4) is equivalent to a substitution θ of constant length $\ell = m+n = 6$, but the positions of a letter a_i, b_i are separated by multiples of 2: The support in this case is better described by $\{k/2^s \,|\, k\in\mathbb{Z},\ \ s\in\mathbb{N}_0\}$ than by $\{k/(2^s\cdot 3^r) \,|\, k\in\mathbb{Z},\ \ s,r\in\mathbb{N}_0\}$.

V. EUCLIDEAN MODELS OF ℓ-ADIC INTERNAL SPACES

So far, we have talked in an "abstract" way about the ℓ-adic internal space. Usually the discussion ends at this point, but we want to "visualize" this ℓ-adic space. We hope that by doing this, we also gain some intuition for such spaces and the meaning of p-adic internal spaces for model sets.

Recall that a p-adic integer can be written as a formal series $t = \Sigma_{i\geqslant 0} t_i \cdot p^i$ with integral coefficients t_i satisfying $0 \leqslant t_i \leqslant p-1$ (*Hensel expansion*). For the following, we identify a p-adic integer t with the sequence $(t_i)_{i\geqslant 0}$ of its coefficients. The set of all p-adic integers (a ring) is written as $\mathbb{Z}_p$, while the field of p-adic numbers is written as $\mathbb{Q}_p$ and can be seen as the set of all Laurent series $\Sigma_{i\geqslant N} t_i \cdot p^i$ with $N\in\mathbb{Z}$. There is a p-adic *valuation* $v_p : \mathbb{Q}_p \backslash \{0\} \to \mathbb{Z}$ defined by $v_p(t) = \min\{i\in\mathbb{Z} | t_i \neq 0\}$, which gives rise to the p-adic *metric* with $|t|_p = p^{-v_p(t)}$ and $|0|_p = 0$ (and $\mathbb{Q}_p$ and $\mathbb{Z}_p$ are the completions of $\mathbb{Q}$ and $\mathbb{Z}$ with respect to the p-adic metric). So with respect to the p-adic metric, two numbers in $\mathbb{Z}$ are close if their difference is divisible by a high power of p. Note that this is a *non-Archimedean* absolute value (i.e., $|x+y|_p \leqslant \max\{|x|_p, |y|_p\}$ for all $x,y \in \mathbb{Q}_p$) and we therefore get some "strange" properties: all triangles are isosceles, every point inside a ball $B_r(x) = \{y \,||y-x|_p < r\}$ is the center of this ball, all balls are open and closed, etc., (see Ref. 10).

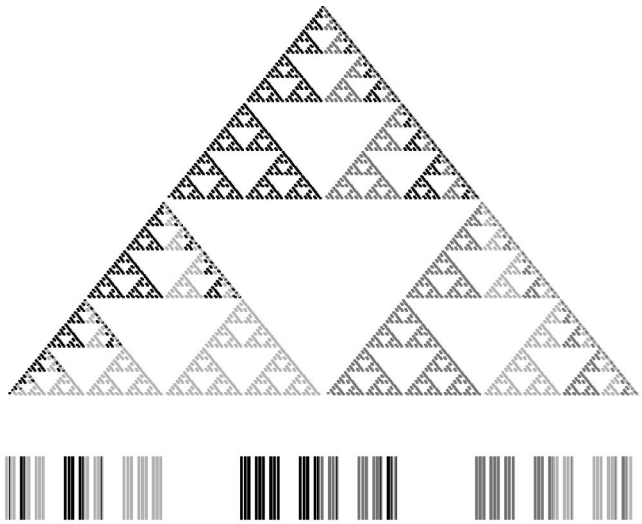
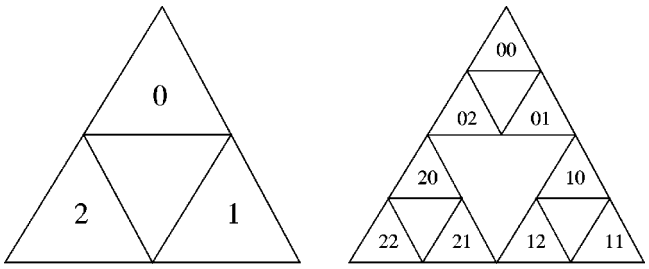


FIG. 1. 3-adic model for the internal space of (14) in $\mathbb{R}^2$ (above) and $\mathbb{R}$ (below, stretched for better representation). The colors correspond to a_1 (black), a_2 (dark gray) and b_1 (light gray).

For Euclidean models (see Ref. 20, Sec. 1.2) of $\mathbb{Z}_p$ we only need to know the formal series $t=\Sigma_{i\geqslant 0}t_i\cdot p^i$. We can even show models for $\mathbb{Z}_\ell$, where we do not make use of (8). For this, we use the addressing scheme known for fractals, for example in the Sierpinsky gasket (see Ref. 4, Chap. IV),



Now the interesting thing here is that each point in the Sierpinsky gasket has a unique address (at least if we do not take the usual connected Sierpinsky gasket but the totally disconnected version; this can be obtained by using a contraction factor less than $\frac{1}{3}$ in the IFS for the Sierpinsky gasket). So each point in the Sierpinsky gasket corresponds to a sequence $(t_i)_{i\geqslant 0}$ with elements $0\leqslant t_i \leqslant 2$—this is just the Hensel expansion of the 3-adic integers. Similarly, the Cantor set is such a geometric encoding of the 2-adic integers. ''Reasonable'' geometric representations of $\mathbb{Z}_\ell$ in $\mathbb{R}^d$ are those, where the sets $K_{\{x_0\ldots x_r\}}=\{t\in\mathbb{Z}_\ell | t_0=x_0,\ldots,t_r=x_r\}$ of points starting with the same address are represented by objects of the same size for a fixed $r\in\mathbb{N}$. Therefore we get that in d-dimension, $\mathbb{Z}_\ell$ with $d+1\leqslant\ell\leqslant$(kissing number in $\mathbb{R}^d$)$+1$ can reasonably be represented, if we do not make use of (7). Note that we can represent $\mathbb{Z}_3$ either in $\mathbb{R}^2$ or $\mathbb{R}$.

This geometric representation surely fails for some p-adic (or ℓ-adic) properties (all triangles are isosceles, every point inside a ball is its center, etc.), but some are also ''preserved:'' points which are close in the p-adic topology are also close in this geometric representation and the representation as totally disconnected fractal corresponds to the totally disconnected field $\mathbb{Q}_p$, $\mathbb{Z}_p$ and its geometric models are both compact sets. And balls in the p-adic topology correspond to scaled down copies of the whole fractal.

We like to conclude this section with our example from (15). The 3-adic geometric models are given in Fig. 1. Observe that, in the two-dimensional representation, the parts (according to our above addressing scheme for the Sierpinsky gasket) $K_{\{02\}}$, $K_{\{12\}}$ and $K_{\{21\}}$ are colored by only one

color. This corresponds to the fact that at positions $9\mathbb{Z}+6$ are a_1's, on $9\mathbb{Z}+7$ are a_2's and on $9\mathbb{Z}+5$ are b_1's only in the bi-infinite sequence. So, large patches of the same color in the geometric representations correspond to lattice cosets $\ell^r\mathbb{Z}+s$ with small r. A similar addressing scheme can be used for the one-dimensional representation (and in fact for all ℓ-adic representations).

ACKNOWLEDGMENTS

It is a pleasure to thank M. Baake, R. V. Moody and O. Redner for discussions and the German Research Council (DFG) for financial support.

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Geodesic compatibility and integrability of geodesic flows

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(Received 6 July 2001; accepted 11 October 2002)

We give a natural geometric condition called *geodesic compatibility* that implies the existence of integrals in involution of the geodesic flow of a pseudo-Riemannian metric. We prove that if two metrics satisfy the condition of geodesic compatibility then we can produce a hierarchy of metrics that also satisfy this condition. A lot of metrics studied in Riemannian and Kählerian geometry satisfy such conditions. We apply our results for obtaining an infinite family (hierarchy) of completely integrable flows on the complex projective plane $\mathbf{CP}^n$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1526939]

I. INTRODUCTION

Our main purpose in the present paper is to prove that if a pair of pseudo-Riemannian metrics g and $\bar{g}$ satisfies a natural geometric condition called *geodesic compatibility* (or PQ^{ϵ}*-projectivity*) then the geodesic flows of the metrics g and $\bar{g}$ admit integrals in involution of a special form. The integrals we find usually have singularities that can be localized out of every arbitrary taken open set D with compact closure (Theorem 1). If the manifold is compact then the integrals can be taken smooth. We prove a Kählerian analog of the results proved in Ref. 1.

In what follows we call pseudo-Riemannian metrics simply *metrics*. Positively definite metrics are called *Riemannian metrics*. All tensor object and manifolds we consider are smooth (C^{∞}). If $E \to M$ is a vector bundle over a manifold M then $\Gamma(E)$ denotes the space of the smooth sections of $E \to M$.

Let us consider some examples of metrics that satisfy the condition of the geodesic compatibility.

(a) *Geodesic equivalence*. A classical example of geodesic compatibility is the so-called *geodesic equivalence*. Recall the main definitions.
Let g and $\bar{g}$ be pseudo-Riemannian metrics given on the manifold M^n, $n = \dim M^n$.
Definition 1: The metrics g and $\bar{g}$ *are called* geodesically equivalent *iff they have the same geodesics (considered as unparametrized curves on* M^n).
We say that the metric g admits *nontrivial geodesic equivalence* iff there exists a metric $\bar{g} \neq \text{const}\, g$ such that g and $\bar{g}$ are geodesically equivalent. The first theorems concerning the existence of integrals of the geodesic flows of the metrics admitting nontrivial geodesic equivalence were proved by Dini, Painlevé, Levi-Civita and Liouville (see Ref. 2). The Liouville integrability of the corresponding geodesic flows in the case when one of the metrics g and $\bar{g}$ is Riemannian is proved in Ref. 3 (see also Refs. 4–9). The pseudo-Riemannian analogs of these theorems are proved in Ref. 11.

(b) *h-projectivity*. Another example of geodesic compatibility appears about a century later in the papers of Otsuki and Tashiro (Refs. 10 and 11).
Let M^{2n} be a $2n$-dimensional real manifold endowed with a complex structure J, $J^2 = -\mathbf{1}$, where $\mathbf{1}$ denotes the identity operator of the tangent bundle TM^{2n}. Recall that, a metric g on M^{2n} is called *Kählerian* iff the next two conditions are satisfied: (1) g is *Hermitian* metric, i.e., $g(J\xi, J\eta) = g(\xi, \eta)$, $\xi, \eta \in T_x M^{2n}$, and (2) the *Kähler form*

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$\Omega(\xi,\eta)\overset{\text{def}}{=}g(J\xi,\eta)$ is a symplectic form (i.e., Ω is nondegenerate and closed, $d\Omega=0$).
Denote by ∇ the Levi-Civita connection corresponding to the Kählerian metric g. Following Ref. 10 we give Definition 2.

Definition 2: A smooth curve $(t_1,t_2)\ni t\to\gamma(t)\in M^{2n}$, $t_1<t_2$, *is called* holomorphically planar *(with respect to the Kählerian metric g) iff*

$$\frac{\nabla\dot\gamma}{dt}(t)=a(t)\dot\gamma(t)+b(t)J\dot\gamma(t), \tag{1}$$

where a and b are smooth functions of the parameter t.

Holomorphically planar curves always exist. For example, the geodesic lines of the metric g are holomorphically planar curves. More generally, fixing any smooth functions $a,b\in C^\infty(t_1,t_2)$, a point $x_0\in M^{2n}$ and a tangent vector $\gamma_0\in T_{x_0}M^{2n}$, we can find a small $\epsilon_0>0$ and a unique solution $\gamma:(-\epsilon_0,\epsilon_0)\to M^{2n}$ of Eq. (1) with initial data $\gamma(0)=x_0$, $\dot\gamma(0)=\gamma_0$.

Let g and $\overline{g}$ be Kählerian metrics on M^{2n}.

Definition 3 (see Ref. 11): The Kählerian metrics g and $\overline{g}$ *are called* holomorphically projective *(or h-projective) iff every holomorphically planar with respect to the metric g curve* $\gamma(t)$ *is holomorphically planar with respect to the metric* $\overline{g}$ *as well, and vice versa.*

It is not hard to prove (see, for example, Refs. 11 and 12) that the condition that the Kählerian metrics g and $\overline{g}$ are h-projective is equivalent to a nonlinear partial differential equation on the ''deformation'' tensor of the Levi-Civita connections of the metrics g and $\overline{g}$. In coordinates $\{(x^1,\dots,x^{2n})\}$, the equation is

$$\overline{\Gamma}^i_{jk}-\Gamma^i_{jk}=\delta^i_j\phi_k+\delta^i_k\phi_j-\phi_\alpha J^\alpha_j J^i_k-\phi_\alpha J^\alpha_k J^i_j, \tag{2}$$

where $\phi_l(l=1,\dots,2n)$ are the components of a globally defined on an M^{2n} 1-form, Γ^i_{jk} and $\overline{\Gamma}^i_{jk}$ are the Christoffel symbols of the metrics g and $\overline{g}$, respectively, δ^i_j is the Kronecker delta and J^i_j are the components of the complex structure J. As usual, we use the standard tensor conventions and omit the summation symbols in the formulas. It can be easily seen that $\phi_k=\partial_k\phi$, where ∂_k stands for the partial derivative $\partial/\partial x^k$ and ϕ is a globally defined on an M^{2n} function (see Sec. II A). Remark that Eq. (2) cannot be obtained without using the condition that the metrics g and $\overline{g}$ are Kählerian.

(c) *PQ^ϵ-projectivity.* Here we give the definition of the geodesic compatibility that generalize the both previous notions.

Consider two metrics g and $\overline{g}$ given on the manifold M^m, $m=\dim M^m$. Let $P,Q\in\Gamma(\mathrm{End}(TM^m))$ satisfy the next properties:

(i) P and Q are antisymmetric with respect to the both metrics g and $\overline{g}$;

(ii) $PQ=\epsilon\mathbf{1}$, where ϵ is a fixed real constant such that $\epsilon\neq m+1$ and $\epsilon\neq 1$.

Denote by χ the number $\chi\overset{\text{def}}{=}m+1-\epsilon$. It follows from (ii) that $\chi\neq 0$.

Definition 4: The metrics g and $\overline{g}$ *are called* PQ^ϵ-projective *(or* geodesically compatible*) iff their Christoffel symbols satisfy the equation*

$$\overline{\Gamma}^i_{jk}-\Gamma^i_{jk}=\phi_{(j}\delta^i_{k)}-\phi_\alpha P^\alpha_{(j}Q^i_{k)}, \tag{3}$$

where ϕ_k *are the components of a globally defined on* M^m 1*-form and the operators P* and *Q satisfy relations (i)* and *(ii).*

As usual, Eq. (3) is written in a fixed coordinate chart $\{(x^1,\dots,x^m)\}$ and P^i_j and Q^i_j are the components of the operators P and Q. The brackets $(i\cdots j)$ in formula (3) denote symmetrization with respect to the pointed indices. For example, the tensor field $T_{\alpha(ij)\beta}$ stands for $T_{\alpha ij\beta}+T_{\alpha ji\beta}$. It is not hard to give an invariant definition of PQ^ϵ-projectivity.

Remark 1: If $\epsilon\neq 0$ *then the operators P and Q are nondegenerate on* M^m, $Q=\epsilon P^{-1}$ *and the dimension m of the manifold is even.*

Remark 2: Suppose that g and $\overline{g}$ *are Kählerian metrics given on the complex manifold* M^{2n}

with complex structure J. Taking $P=Q=J$ and $\epsilon=-1$ we see that h-projectivity is a particular case of PQ^{ϵ}-projectivity. Taking $P=Q=0$ and $\epsilon=0$ we obtain the notion of the geodesic equivalence.

Let us give a brief description of the results proved in the paper. Suppose that the metrics g and $\overline{g}$ given on the manifold M^m are PQ^{ϵ}-projective. Define the endomorphism $A \in \Gamma(\mathrm{End}(TM^m))$ of the tangent bundle TM^m by the formula

$$A^i_j(g,\overline{g}) \overset{\text{def}}{=} \left|\frac{\det \overline{g}}{\det g}\right|^{1/\chi} \overline{g}^{i\alpha} g_{\alpha j}. \tag{4}$$

Consider the locally defined one-parameter family of quadratic forms,

$$K_c(g,\overline{g})(\xi) \overset{\text{def}}{=} |\det(A+c\mathbf{1})|^{1/(1-\epsilon)} g((A+c\mathbf{1})^{-1}\xi,\xi), \tag{5}$$

where $\xi \in TM^m$ and c is an appropriately chosen real parameter.

Following Ref. 1 define the *rank of the pair* g and $\overline{g}$. Denote by $r(g,\overline{g})(x)$ the degree of the minimal polynomial of the operator $A(g,\overline{g})|_x$.

Definition 5: The number $r(g,\overline{g})(x)$ is called rank of the pair g and $\overline{g}$ of PQ^{ϵ}-projective metrics at the point $x \in M^m$. *The number $r(g,\overline{g}) \overset{\text{def}}{=} \max_{x\in M^m}(g,\overline{g})(x)$ is called* rank of the pair of PQ^{ϵ}-projective metrics.

Recall that the smooth functions $F_1,\ldots,F_k$ given on a smooth manifold V are called *functionally independent in V* iff the set of the points $x \in V$ where the differentials $d_xF_1,\ldots,d_xF_k$ are linearly independent is dense in V.

Theorem 1: *Suppose that the manifold M^m is connected and let the rank of the pair of PQ^{ϵ}-projective metrics g and $\overline{g}$ be r. Denote by ω_g the symplectic structure on TM^m given by the pull-back $FL_g^*\omega$ where ω is the canonical symplectic structure on T^*M^m (the form "$dp\wedge dq$") and $FL_g: TM^m \to T^*M^m$ denotes the Legendre transformation corresponding to the metric g. Then for every open set $D \subset M^m$ with compact closure in M^m there exist r quadratic in velocities functions $B^D_1(\xi),\ldots,B^D_r(\xi)$, $\xi \in TD$, such that we have the following:*

(a) $B^D_1(\xi),\ldots,B^D_r(\xi)$ are smooth functionally independent pairwise commuting integrals of the geodesic flow of the metric g on D;
(b) if the quadratic form $K_c(g,\overline{g})(\xi)$, $c=\mathrm{const}$, is correctly defined on some open set $U \subset D$ then there exist constants $\alpha_1,\ldots,\alpha_r$ such that $K_c(\xi)=\Sigma_{k=1}^r \alpha_k B^D_k(\xi)$ on D.

The integrals $B^D_1(\xi),\ldots,B^D_r(\xi)$ can be taken in the form $B^D_k(\xi) \overset{\text{def}}{=} K_{c_k}(\xi)$, where the constants $c_1,\ldots,c_r$ are appropriately chosen.

Remark 3: Actually, the constants $c_1,\ldots,c_r$ in Theorem 1 are taken "sufficiently big," i.e., $|c_k| > m_D$, $m_D \overset{\text{def}}{=} \sup_{x\in D} \max_{\lambda\in \mathrm{Spect}(A|_x)} |\lambda|$.

As a simple corollary of this theorem we obtain the next statement.

Corollary 1: The set of the points $x \in M^m$ where $r(g,\overline{g})(x)=r$ is open and dense in M^m.

We prove Theorem 1 in Sec. IV.

A Hermitian version of Theorem 1 is given in Sec. V (see Theorem 4). An important corollary is the next Kählerian analog of that proved in Ref. 1 Theorem 2. Suppose that the Kählerian metrics s and $\tilde{s}$ are h-projective. Denote by r the *Hermitian rank* of the pair s and $\tilde{s}$ (see Definition 9).

Theorem 2: *If two Kählerian metrics s and $\tilde{s}$ are h-projective then their geodesic flows admit r functionally independent integrals in involution.*

The paper is organized as follows.

In Sec. II we prove that the quadratic forms given by formula (5) are integrals of the geodesic flow of the metric g (Proposition 3, Sec. II C). In Sec. II D we prove Proposition 4. As in Ref. 1 the existence of hierarchies is a crucial point proving the commutativity of the integrals given by formula (5). We prove the commutativity of these integrals in Sec. III, Theorem 3. Section IV is devoted to the proof of Theorem 1. The Hermitian analog of this theorem is proved in Sec. V. The last section is devoted to the applications of the results. A simple geometrical construction allows us to find an infinite family (''$\mathbf{CP}^n$-hierarchy'') of completely integrable Hamiltonian systems on the complex projective plane $\mathbf{CP}^n$ (see Theorem 6). The integrals obtained by Thimm in Ref. 13 are not included in this hierarchy as a particular case.

In what follows, if a coordinate chart is fixed, we usually identify the tensor fields we consider with their coordinate (''index'') representations and denote the corresponding objects by the same letters. We use also the common tensor notations and conventions and omit the summation symbols in the formulas. An endomorphism $L \in \Gamma(\mathrm{End}(TM^n))$ is called *invertible* or *nondegenerate* on M^n iff $\det L \neq 0$ on M^n.

II. PROPERTIES OF *PQ*-PROJECTIVITY

In the present section the main properties of the PQ^{ϵ}-projective metrics are established.

A. Existence of an integral

Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective. Here we prove that the geodesic flow of the metric g admits an integral (Proposition 1).

Contracting the indices i and j in formula (3) and using that trace $Q=0$ we get $\overline{\Gamma}^i_{ik}-\Gamma^i_{ik} = \chi\phi_k$ where $\chi \overset{\text{def}}{=} m+1-\epsilon$. Using that $\Gamma^i_{ik}=\partial_k \ln\sqrt{|\det g|}$ we obtain

$$2\chi\phi_k = \frac{\partial}{\partial x^k}\left(\ln\left|\frac{\det \overline{g}}{\det g}\right|\right). \tag{6}$$

Therefore, $\phi_k=\partial_k\phi$, where ϕ is a smooth function on M^m.

The next technical lemma is needed for the sequel.

Lemma 1: The metrics g and $\overline{g}$ are PQ^{ϵ}-projective if and only if their components satisfy the next equation in covariant derivatives:

$$\nabla_k \overline{g}_{ij} = 2\phi_k \overline{g}_{ij} + \phi_{(i}\overline{g}_{j)k} - \phi_\alpha P^\alpha_{(i}\overline{g}_{j)\beta}Q^\beta_k, \tag{7}$$

where ∇ denotes the Levi-Civita connection of the metric g and the operators P and Q satisfy conditions (i) and (ii).

Proof of Lemma 1: Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective. In coordinates, we obtain

$$\begin{aligned}
\nabla_k \overline{g}_{ij} &= \partial_k \overline{g}_{ij} - \Gamma^\alpha_{ik}\overline{g}_{\alpha j} - \Gamma^\alpha_{jk}\overline{g}_{i\alpha} \\
&= \overline{\nabla}_k \overline{g}_{ij} + (\phi_{(i}\delta^\alpha_{k)} - \phi_l P^l_{(i}Q^\alpha_{k)})\overline{g}_{\alpha j} + (\phi_{(j}\delta^\alpha_{k)} - \phi_l P^l_{(j}Q^\alpha_{k)})\overline{g}_{i\alpha} \\
&= 2\phi_k\overline{g}_{ij} + \phi_{(i}\overline{g}_{j)k} - \phi_l P^l_{(i}\overline{g}_{j)\alpha}Q^\alpha_k - \phi_l P^l_k Q^\alpha_{(i}\overline{g}_{j)\alpha} \\
&= 2\phi_k\overline{g}_{ij} + \phi_{(i}\overline{g}_{j)k} - \phi_l P^l_{(i}\overline{g}_{j)\alpha}Q^\alpha_k .
\end{aligned}$$

The inverse statement immediately follows from the classical fact that the Levi-Civita connection of some metric is the unique torsion free connection that preserves the considered metric. Lemma 1 is proved.

Equations (7) are equivalent to

$$2\mu\overline{g}_{ij,k} = -2\mu_k\overline{g}_{ij} - \mu_{(i}\overline{g}_{j)k} - \mu_l P^l_{(i}\overline{\Omega}^Q_{j)k}, \tag{8}$$

where $\mu \overset{\text{def}}{=} |\det g/\det \overline{g}|^{1/\chi}$, $\mu_k \overset{\text{def}}{=} \partial\mu/\partial x^k$ $(k=1,\ldots,2n)$, and $\overline{\Omega}^Q_{kj}$ are the components of the 2-form $\overline{\Omega}^Q(\xi,\eta) \overset{\text{def}}{=} \overline{g}(Q\xi,\eta)$, $\xi,\eta \in T_xM^m$. The equivalence of Eqs. (7) and (8) easily follows from the relation $2\phi_k = -\mu_k/\mu$.

Proposition 1: Suppose that the metrics g and $\overline{g}$ are PQ^ϵ-projective. Then the quadratic form,

$$K(\xi) \overset{\text{def}}{=} \left|\frac{\det g}{\det \overline{g}}\right|^{2/\chi} \overline{g}(\xi,\xi), \tag{9}$$

is an integral of the geodesic flow of the metric g.

Proof of Proposition 1: In coordinates, we have $K_{ij} \overset{\text{def}}{=} \mu^2\overline{g}_{ij}$. Following Levi-Civita, a quadratic form $Q(\xi,\xi)=Q_{ij}\xi^i\xi^j$, $Q_{ij}=Q_{ji}$, is an integral of the geodesic flow of the metric g if and only if $Q_{(ijk)} \overset{\text{def}}{=} (Q_{ij,k}+Q_{jk,i}+Q_{ki,j})/3=0$, where $Q_{ij,k} \overset{\text{def}}{=} \nabla_k Q_{ij}$ and ∇ is the Levi-Civita connection of the metric g. Indeed, let $\gamma(s)$ $(\gamma(0)=x_0,\ \dot\gamma(0)=\xi)$ be a geodesic line of the metric g. We have $0=d/ds\,|_{s=0}(Q_{ij}\dot\gamma^i\dot\gamma^j)=Q_{ij,k}(x_0)\xi^k\xi^i\xi^j=Q_{(ijk)}(x_0)\xi^k\xi^i\xi^j$ and therefore $Q_{ij,k}+Q_{jk,i}+Q_{ki,j}=0$. Conversely, if $Q_{ij,k}+Q_{jk,i}+Q_{ki,j}=0$ then Q is an integral of the geodesic flow of the metric g.

We have

$$2K_{ij,k}=4\mu\mu_k\overline{g}_{ij}+2\mu^2\overline{g}_{ij,k},$$

$$2K_{jk,i}=4\mu\mu_i\overline{g}_{jk}+2\mu^2\overline{g}_{jk,i},$$

$$2K_{ki,j}=4\mu\mu_j\overline{g}_{ki}+2\mu^2\overline{g}_{ki,j}.$$

Summing these equations and using (8) we obtain that

$$\begin{aligned}2(K_{ij,k}+K_{jk,i}+K_{ki,j}) = -\mu(&\mu_\alpha P_i^\alpha\overline{\Omega}^Q_{jk}+\mu_\alpha P_j^\alpha\overline{\Omega}^Q_{ik}+\mu_\alpha P_j^\alpha\overline{\Omega}^Q_{ki}+\mu_\alpha P_k^\alpha\overline{\Omega}^Q_{ji}+\mu_\alpha P_k^\alpha\overline{\Omega}^Q_{ij}\\ &+\mu_\alpha P_i^\alpha\overline{\Omega}^Q_{kj})=0.\end{aligned}$$

This completes the proof of Proposition 1.

Remark 4: In the case of geodesically equivalent metrics the integral given by formula (9) coincides with the classical Painlevé integral (see Refs. 1, 2). The existence of the integral (9) in the case of h-projective Kählerian metrics is a new fact.

B. Existence of a family of *PQ*-projective metrics

Suppose that the metrics g and $\overline{g}$ are PQ^ϵ-projective. Consider the endomorphism A of the tangent bundle TM^m defined by formula (4). It is clear that A is self-adjoint with respect to the both metrics g and $\overline{g}$. Condition (i) imposed on the operators P and Q (see p. 5) yields that A commutes with P and Q. The next important technical lemma is needed for the sequel.

Lemma 2: If the metrics g and $\overline{g}$ are PQ^ϵ-projective then the metric $a_{ij} \overset{\text{def}}{=} g_{i\alpha}A_j^\alpha$ satisfies the equation

$$a_{ij,k}=\lambda_{(i}g_{j)k}-\lambda_l P^l_{(i}g_{j)q}Q^q_k, \tag{10}$$

where $\lambda_i \overset{\text{def}}{=} -\phi_l A_i^l$. The operators P and Q are antisymmetric with respect to the metric a. Inversely, consider a metric g and two antisymmetric with respect to g operators P and Q such that $PQ=\epsilon\mathbf{1}$. Suppose that P and Q are antisymmetric with respect to a nondegenerate symmet-

ric form a_{ij} and let a_{ij} satisfy Eq. (10) for some globally defined on M^{2n} 1-form λ_k. Then the metrics g and $\overline{g}\overset{\text{def}}{=}|\det \breve{g}/\det g|^{1/(1-\epsilon)}\breve{g}$, are PQ^{ϵ}-projective, where $\breve{g}_{ij}\overset{\text{def}}{=}g_{i\alpha}a^{\alpha\beta}g_{\beta j}$, $a_{i\alpha}a^{\alpha j}=\delta_i^j$.

Proof of Lemma 2: Suppose that g and $\overline{g}$ are PQ^{ϵ}-projective. Denote $\breve{g}_{ij}\overset{\text{def}}{=}\exp(-2\phi)\overline{g}_{ij}$. Using formula (7) we obtain

$$\breve{g}_{ij,k}=-2\phi_k\breve{g}_{ij}+\exp(-2\phi)\overline{g}_{ij,k}=\phi_{(i}\breve{g}_{j)k}-\phi_l P^l_{(i}\breve{g}_{j)\alpha}Q^{\alpha}_k.$$

For the inverse tensor $\breve{g}^{ij}$ ($\breve{g}_{i\alpha}\breve{g}^{\alpha j}=\delta_i^j$) we have

$$\breve{g}^{ij}_{,k}=-\breve{g}^{i\alpha}\breve{g}_{\alpha\beta,k}\breve{g}^{\beta j}=-\phi_l\breve{g}^{l(i}\delta^{j)}_k+\phi_l P^l_s\breve{g}^{s(i}Q^{j)}_k.$$

Finally, taking $a_{\alpha\beta}\overset{\text{def}}{=}g_{\alpha i}\breve{g}^{ij}g_{j\beta}$ we obtain

$$a_{\alpha\beta,k}=-\phi_l\breve{g}^{li}g_{i(\alpha}g_{\beta)k}+\phi_l P^l_r A^r_{(\alpha}g_{\beta)j}Q^j_k=\lambda_{(\alpha}g_{\beta)k}-\lambda_l P^l_{(\alpha}g_{\beta)q}Q^q_k,$$

where $\lambda_{\alpha}\overset{\text{def}}{=}-\phi_l A^l_{\alpha}$.

Let us prove the inverse part of the proposition. Suppose that the nondegenerate symmetric tensor a_{ij} satisfies Eq. (10) where P and Q are antisymmetric with respect to g and a, $PQ=\epsilon\mathbf{1}$, and λ_k are the components of a globally defined on M^m 1-form. Consider the tensor $\breve{g}^{ij}\overset{\text{def}}{=}g^{i\alpha}a_{\alpha\beta}g^{\beta j}$. For the inverse tensor $\breve{g}_{pq}$ ($\breve{g}_{p\alpha}\breve{g}^{\alpha q}=\delta^q_p$) we have

$$\breve{g}_{pq,k}=-\breve{g}_{pi}\breve{g}^{ij}_{,k}\breve{g}_{jq}=-\lambda_{\alpha}g^{\alpha i}\breve{g}_{i(p}\breve{g}_{q)k}+\lambda_l P^l_{\alpha}g^{\alpha i}\breve{g}_{i(p}\breve{g}_{q)j}Q^j_k.$$

Denoting $\phi_p\overset{\text{def}}{=}-\lambda_{\alpha}g^{\alpha i}\breve{g}_{ip}$ we obtain

$$\breve{g}_{pq,k}=\phi_{(p}\breve{g}_{q)k}-\phi_l P^l_{(p}\breve{g}_{q)j}Q^j_k. \tag{11}$$

Lemma 3: $2\phi_k=\partial_k\ln|\det\breve{g}/\det g|^{1/(1-\epsilon)}$.

Proof of Lemma 3: Denote by $\breve{\Gamma}^i_{jk}$ the Christoffel symbols of the metric $\breve{g}$. Using formula (11) we obtain

$$\begin{aligned}\breve{\Gamma}^{\alpha}_{\alpha k}&=\frac{1}{2}\breve{g}^{\alpha\beta}\frac{\partial\breve{g}_{\alpha\beta}}{\partial x^k}\\&=\frac{1}{2}\breve{g}^{\alpha\beta}(\breve{g}_{\alpha\beta,k}+\breve{g}_{l(\alpha}\Gamma^l_{\beta)k})\\&=\frac{1}{2}\breve{g}^{\alpha\beta}((\phi_{(\alpha}\breve{g}_{\beta)k}-\phi_l P^l_{(\alpha}\breve{g}_{\beta)j}Q^j_k)+\breve{g}_{l(\alpha}\Gamma^l_{\beta)k})\\&=(1-\epsilon)\phi_k+\Gamma^{\alpha}_{\alpha k}.\end{aligned}$$

Therefore, $(1-\epsilon)\phi_k=\breve{\Gamma}^{\alpha}_{\alpha k}-\Gamma^{\alpha}_{\alpha k}=\partial_k\ln|\det\breve{g}/\det g|^{1/2}$. Lemma 3 is proved.

Finally, taking $\overline{g}_{ij}\overset{\text{def}}{=}\exp(2\phi)\breve{g}_{ij}$ we obtain that $g_{ij,k}=2\phi_k\overline{g}_{ij}+\phi_{(i}\overline{g}_{j)k}-\phi_l P^l_{(i}\overline{g}_{j)\alpha}Q^{\alpha}_k$. Using Lemma 1 we complete the proof of Lemma 2.

Proposition 2: Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective and let c be a real constant such that the operator $A+c\mathbf{1}$ is invertible. Then the metrics g and

$$\overline{g}_c(g,\overline{g})\overset{\text{def}}{=}|\det(A+c\mathbf{1})|^{-1/(1-\epsilon)}g(A+c\mathbf{1})^{-1}, \tag{12}$$

where $A=A(g,\overline{g})$ is given by formula (4), are PQ^{ϵ}-projective.

Proof of Proposition 2: Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective and let c be the constant given in the statement of the corollary. It follows from Lemma 2 that the metric $a \overset{\text{def}}{=} gA$ satisfies Eq. (10). Hence, the metric $a+cg=g(A+c)$ also satisfies Eq. (10). Using the inverse part of Lemma 2 we obtain that the metrics g and $\overline{g_c} \overset{\text{def}}{=} |\det \breve{g}_c/\det g|^{1/(1-\epsilon)}\breve{g}_c$, $\breve{g}_c \overset{\text{def}}{=} g(a+cg)^{-1}g=g(A+c\mathbf{1})^{-1}$. This completes the proof of Proposition 2.

C. Existence of a family of integrals

Here we prove that the geodesic flows of a pair of PQ^{ϵ}-projective metric locally admit a family of integrals.

Proposition 3: Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective and let c be a real constant such that the operator $A+c\mathbf{1}$ is nondegenerate on M^m. Then the quadratic form,

$$K_c(g,\overline{g}) \overset{\text{def}}{=} |\det(A+c\mathbf{1})|^{1/(1-\epsilon)}g(A+c\mathbf{1})^{-1}, \tag{13}$$

is an integral of the geodesic flow of the metric g.

Remark 5: Let $D \subset M^m$ be an open set with compact closure in M^m. Taking $|c| \geqslant m_D$, $m_D \overset{\text{def}}{=} \sup_{x \in D} \max_{\lambda \in \mathrm{Spect}A|_x} |\lambda|$, we obtain a one-parameter family of integrals of the geodesic flow of the metric g.

Proof of Proposition 3: Suppose that the metrics g and $\overline{g}$ are PQ^{ϵ}-projective. It follows from Proposition 2 that g and $\overline{g_c}$ [given by formula (12)] are PQ^{ϵ}-projective. Applying Proposition 1 to these metrics we obtain that the quadratic form

$$K_c \overset{\text{def}}{=} \left|\frac{\det g}{\det \overline{g}_c}\right|^{2/\chi} \overline{g_c} = |\det(A+c\mathbf{1})|^{1/(1-\epsilon)}g(A+c\mathbf{1})^{-1}$$

is an integral of the geodesic flow of the metric g. Proposition 3 is proved.

D. Existence of hierarchies

In the present section we prove the next proposition.

Proposition 4: If the metrics g and $\overline{g}$ are PQ^{ϵ}-projective then the metrics $a \overset{\text{def}}{=} gA$ and $\overline{a} \overset{\text{def}}{=} \overline{g}A$ are $P_1Q_1^{\epsilon}$-projective, where $P_1 \overset{\text{def}}{=} PA$, $Q_1 \overset{\text{def}}{=} A^{-1}Q$, and $A=A(g,\overline{g})$ is given by formula (4).

Proof of Proposition 4: It follows from Lemma 2 that $a_{\alpha\beta,k}=\lambda_{(\alpha}g_{\beta)m}-\lambda_l P^l_{(\alpha}g_{\beta)q}Q^q_k$, where $\lambda_\alpha \overset{\text{def}}{=} -\phi_l A^l_\alpha$. We have

$$-\frac{\partial a_{\alpha\beta}}{\partial x^k}+\Gamma^l_{k(\alpha}a_{\beta)l}=-\lambda_{(\alpha}g_{\beta)k}+\lambda_l P^l_{(\alpha}g_{\beta)q}Q^q_k,$$

$$\frac{\partial a_{\alpha k}}{\partial x^\beta}-\Gamma^l_{\beta(\alpha}a_{k)l}=\lambda_{(\alpha}g_{k)\beta}-\lambda_l P^l_{(\alpha}g_{k)q}Q^q_\beta,$$

$$\frac{\partial a_{\beta k}}{\partial x^\alpha}-\Gamma^l_{\alpha(\beta}a_{k)l}=\lambda_{(\beta}g_{k)\alpha}-\lambda_l P^l_{(\beta}g_{k)q}Q^q_\alpha.$$

Summing these equations, and using the relations $\lambda_l \overset{\text{def}}{=} -\phi_\alpha A^\alpha_l$, $PA=AP$, $g(Q\xi,\eta)=-g(\xi,Q\eta)$, we obtain the next formula for the Christoffel symbols A^i_{jk} of the metric a_{ij},

$$A^k_{\alpha\beta}=\Gamma^k_{\alpha\beta}+\lambda_l a^{lk}g_{\alpha\beta}+\lambda_l P^l_{(\alpha}g_{\beta)q}Q^q_r a^{rk}=\Gamma^k_{\alpha\beta}-\phi_l g^{lk}g_{\alpha\beta}+\phi_s P^s_l A^l_{(\alpha}Q^q_{\beta)}\tilde{A}^k_q, \tag{14}$$

where $\tilde{A}^k_q$ are the components of the inverse operator A^{-1}.

By definition, $\overline{a}_{ij} \overset{\text{def}}{=} \overline{g}_{ik} A^k_j = \exp(2\phi) g_{ij}$. Using this relation we immediately obtain the next relation between the Christoffel symbols of the metrics $\overline{a}$ and g,

$$\overline{A}^k_{ij} = \Gamma^k_{ij} + \phi_{(i}\delta^k_{j)} - \phi_l g^{lk} g_{ij}. \tag{15}$$

Finally, (14) and (15) yield

$$\overline{A}^k_{ij} - A^k_{ij} = \phi_{(i}\delta^k_{j)} - \phi_s P^s_l A^l_{(i} Q^q_{j)} \tilde{A}^k_q. \tag{16}$$

This completes the proof of Proposition 4.

Suppose that a pair of PQ^ϵ-projective metrics g and $\overline{g}$ is given. It follows from Proposition 4 that *for every integer k the metrics $g^{(k)} \overset{\text{def}}{=} gA^k$ and $\overline{g}^{(k)} \overset{\text{def}}{=} gA^k$ are P_kQ_k-projective, where $P_k \overset{\text{def}}{=} PA^k$ and $Q_k \overset{\text{def}}{=} A^{-k}Q$*. Indeed, suppose that $g^{(l)}$ and $\overline{g}^{(l)}$ are P_lQ_l-projective. It follows from formula (4) that $A(g^{(l)}, \overline{g}^{(l)}) = A$ and $A(\overline{g}^{(l)}, g^{(l)}) = A^{-1}$. Applying Proposition 4 to the pair $g^{(l)}$ and $\overline{g}^{(l)}$ we obtain that $g^{(l+1)}$ and $\overline{g}^{(l+1)}$ are $P_{l+1}Q_{l+1}$-projective. Similarly, applying Proposition 4 to the pair $\overline{g}^{(l)}$ and $g^{(l)}$ we obtain that $g^{(l-1)}$ and $\overline{g}^{(l-1)}$ are $P_{l-1}Q_{l-1}$-projective.

*Definition 6: The sequence of pairs $g^{(k)}$ and $\overline{g}^{(k)}$ ($k = 0, \pm 1, \dots$) are called the PQ^ϵ-*hierarchy *corresponding to the pair g and $\overline{g}$ of PQ^ϵ-projective metrics*.

The PQ^ϵ-hierarchy is an analog of the *geodesic hierarchy* considered in Ref. 1. Proposition 4 is an analog of the Sinyukov transformation in the theory of geodesically equivalent metrics (see Refs. 14, 15). We will describe the PQ^ϵ-hierarchy by the next formal scheme,

$$\begin{array}{ccc}
\downarrow & & \downarrow \\
g^{(-1)} & \leftrightarrow & \overline{g}^{(-1)} \\
\downarrow & & \downarrow \\
g & \leftrightarrow & \overline{g} \\
\downarrow & & \downarrow \\
g^{(1)} & \leftrightarrow & \overline{g}^{(1)} \\
\downarrow & & \downarrow
\end{array}$$

where the horizontal arrows mean that the metrics $g^{(k)}$ and $\overline{g}^{(k)}$ are P_kQ_k-projective.

III. INVOLUTIVITY OF THE FAMILY OF THE INTEGRALS

In the present section we prove that the integrals given by Proposition 3 are in involution.

Theorem 3: *Suppose that the metrics g and $\overline{g}$ are PQ^ϵ-projective. Suppose in addition that the operators $A + c_1\mathbf{1}$ and $A + c_2\mathbf{1}$ are nondegenerate on M^m where c_1 and c_2 are some fixed real numbers. Then the quadratic forms $K_{c_1}(g, \overline{g})$ and $K_{c_2}(g, \overline{g})$, given by formula* (5)*, are in involution with respect to the symplectic structure $\omega_g \overset{\text{def}}{=} \mathrm{FL}_g^* \omega$, where ω denotes the canonical symplectic structure on the cotangent bundle T^*M^m and $FL_g : TM^m \to T^*M^m$ is the Legendre transformation corresponding to the metric g.*

Proof of Theorem 3: Suppose that the metrics g and $\overline{g}$ are PQ^ϵ-projective. Proposition 2 shows that the metrics g and $\overline{g}_{c_1} \overset{\text{def}}{=} |\det(A + c_1\mathbf{1})|^{-1/(1-\epsilon)} g(A + c_1\mathbf{1})^{-1}$ are PQ^ϵ-projective as well. Consider the corresponding PQ^ϵ-hierarchy,

$$\begin{array}{ccc} \downarrow & & \downarrow \\ g & \leftrightarrow & \overline{g}_{c_1} \\ \downarrow & & \downarrow \\ g^{(1)}_{c_1} & \leftrightarrow & \overline{g}^{(1)}_{c_1} \\ \downarrow & & \downarrow \\ g^{(2)}_{c_1} & \leftrightarrow & \overline{g}^{(2)}_{c_1} \\ \downarrow & & \downarrow \end{array}$$

A simple calculation shows that $A(g,\overline{g}_{c_1})=A+c_1\mathbf{1}$, and $A(\overline{g}_{c_1},g)=(A+c_1\mathbf{1})^{-1}$. Hence, $\overline{g}^{(2)}_{c_1} \overset{\text{def}}{=} \overline{g}_{c_1}A(g,\overline{g}_{c_1})^2=|\det(A+c_1\mathbf{1})|^{-1/(1-\epsilon)}g(A+c_1\mathbf{1})$. It is clear that $A(\overline{g}^{(2)}_{c_1},g^{(2)}_{c_1})=(A+c_1\mathbf{1})^{-1}$. Suppose that the nonzero real number $(-\alpha)$ is not an eigenvalue of the operator $(A+c_1\mathbf{1})^{-1}$. It follows from Proposition 3 that the quadratic form $K_\alpha(\overline{g}^{(2)}_{c_1},g^{(2)}_{c_1})$ is an integral of the geodesic flow of the metric $\overline{g}^{(2)}_{c_1}$. Applying the inverse to the Legendre transformation corresponding to the metric $\overline{g}^{(2)}_{c_1}$, we obtain that the forms

$$(\overline{g}^{(2)}_{c_1})^{-1}=|\det(A+c_1\mathbf{1})|^{1/(1-\epsilon)}(A+c_1\mathbf{1})^{-1}g^{-1} \tag{17}$$

and

$$\begin{aligned}(FL^{-1}_{\overline{g}^{(2)}_{c_1}})^*(K_\alpha) &\overset{\text{def}}{=} |\det((A+c_1)^{-1}+\alpha)|^{1/(1-\epsilon)}((A+c_1)^{-1}+\alpha)^{-1}(\overline{g}^{(2)}_{c_1})^{-1} \\ &= c(\alpha)|\det(A+(c_1+1/\alpha))|^{1/(1-\epsilon)}(A+(c_1+1/\alpha))^{-1}g^{-1},\end{aligned}$$

considered as functions on the cotangent bundle T^*M^m, are in involution with respect to the canonical symplectic structure ω on T^*M^m. Finally, applying the Legendre transformation corresponding to the metric g, we obtain that the forms $K_{c_1}(g,\overline{g})$ and $K_{c_1+\frac{1}{\alpha}}(g,\overline{g})$ are in involution with respect to ω_g. Theorem 3 is proved.

IV. FUNCTIONAL INDEPENDENCE OF THE INTEGRALS

Here we prove Theorem 1 formulated in the Introduction.

Proof of Theorem 1: We follow the idea of the proof of Theorem 2 in Ref. 1.

In what follows we use the next convention. If V is a complex vector space we assume that all linear maps and subspaces are complex linear, all tensor products are over $\mathbf{C}$, and the word ''dimension'' means the complex dimension.

Let V be a real (or complex) vector space of dimension m. Consider a nondegenerate symmetric bilinear form $s\in\mathrm{Symm}(V^*\otimes V^*)$ and a linear self-adjoint with respect to s operator $L\in\mathrm{End}(V)$. Denote by $r(L)$ *the degree of the minimal polynomial of the operator* L. Let δ be a fixed real number. Consider the curves

$$\gamma: t\to|\det(L-t\mathbf{1})|^{\delta}s(L-t\mathbf{1})^{-1}\in\mathrm{Symm}(V^*\otimes V^*)$$

and

$$\gamma_\xi: t\to|\det(L-t\mathbf{1})|^{\delta}s((L-t\mathbf{1})^{-1}\xi,\cdot)\in V^*,$$

where $\xi\in V$ is a fixed vector in V, $\mathbf{1}$ is the identity operator, and the parameter t is defined in an open set U in $\mathbf{R}$ (or $\mathbf{C}$), $U\cap\mathrm{Spect}(L)=\emptyset$. Remark that we admit three possibilities: V is real and t is real, V is complex and t is complex or real. Given a curve $l: D\to W$, where W is a vector space and D is an open domain in $\mathbf{R}$ or $\mathbf{C}$, denote by $\dim_D l$ the dimension of the linear subspace spanned

on the vectors $\{l(t)|t\in D\}$. Following our convention, if W is a complex vector space, $\dim_D l$ denotes the complex dimension of the complex linear subspace spanned on $\{l(t)|t\in D\}$.

Lemma 4:

(a) $\dim_U \gamma = r(L)$;
(b) $\dim_U \gamma_\xi \leqslant r(L)$ *and there exists an open and dense subset* $\Sigma\subset V$ *such that for every* $\xi\in\Sigma$, $\dim_U \gamma_\xi = r(L)$;
(c) *if* $t_1,\dots,t_{r(L)}\in U$, $t_i\neq t_j$ $(i\neq j)$, *then* $\gamma(t_1),\dots,\gamma(t_{r(L)})$ *are linearly independent.*

Proof of Lemma 4: Consider the case when V is a real vector space and the parameter t is real, $t\in U\subset\mathbf{R}$, $U\cap\mathrm{Spect}(L)\neq\emptyset$. The case of complex vector space is considered similarly. It follows from the nondegeneracy of the metric s that $\dim_U\gamma=\dim_U\tilde\gamma$ and $\dim_U\gamma_\xi=\dim_U\tilde\gamma_\xi$, where $\tilde\gamma(t)\overset{\text{def}}{=}\det(L-t\mathbf{1})(L-t\mathbf{1})^{-1}$ and $\tilde\gamma_\xi(t)\overset{\text{def}}{=}\det(L-t\mathbf{1})(L-t\mathbf{1})^{-1}\xi$. It is clear that $\tilde\gamma(t)=L_{m-1}t^{m-1}+\cdots+L_0$, $L_k\in\mathrm{End}(V)$, $L_{m-1}=(-1)^{m-1}\mathbf{1}$. Using the nondegeneracy of the Vandermonde determinant we obtain that $\dim_U\tilde\gamma=\mathrm{rk}\{L_{m-1},\dots,L_0\}$ and $\dim_U\tilde\gamma_\xi=\mathrm{rk}\{L_{m-1}\xi,\dots,L_0\xi\}$. Denote by $V^{\mathbf{C}}$ the complexification of V. Let $L^{\mathbf{C}},L_k^{\mathbf{C}}\in\mathrm{End}(V^{\mathbf{C}})$ be the complexifications of the real operators L and L_k $(k=0,\dots,m-1)$. Denote by r_0 the number $r_0\overset{\text{def}}{=}\max\limits_{\xi\in V}\mathrm{rk}\{L_{m-1}\xi,\dots,L_0\xi\}$.

Lemma 5:

(i) $\mathrm{rk}\{L_{m-1},\dots,L_0\}=\mathrm{rk}_{\mathbf{C}}\{L_{m-1}^{\mathbf{C}},\dots,L_0^{\mathbf{C}}\}$;
(ii) $r_0=\max_{\xi\in V^{\mathbf{C}}}\mathrm{rk}_{\mathbf{C}}\{L_{m-1}^{\mathbf{C}}\xi,\dots,L_0^{\mathbf{C}}\xi\}$;
(iii) *there exists an open dense subset* $\Sigma\subset V$ *such that for every* $\xi\in\Sigma$, $r_0=\mathrm{rk}\{L_{m-1}\xi,\dots,L_0\xi\}$.

Proof of Lemma 5: Item (i) of the lemma is obvious. Let us prove (iii). Taking a basis in V, denote by $(\xi_1,\dots,\xi_m)$ the coordinates of the vectors of V. Consider the $m\times m$ matrix T formed of the coordinates of the vectors $L_{m-1}\xi,\dots,L_0\xi$. The elements of this matrix are linear polynomials of the variables $\xi_1,\dots,\xi_m$. It is clear that there exists a nonzero minor $T_{r_0}\in\mathbf{R}^{r_0}[\xi_1,\dots,\xi_m]$ of the matrix T. The set $\Sigma\overset{\text{def}}{=}\{\xi\in V|T_{r_0}(\xi)\neq 0\}$ satisfies the statement of item (iii). The assumption that the variables $\xi_1,\dots,\xi_m$ take complex values does not change the rank of the matrix T. This proves item (ii). Lemma 5 is proved.

Consider the curves $\tilde\gamma^{\mathbf{C}}(\lambda)\overset{\text{def}}{=}(L^{\mathbf{C}}-\lambda\mathbf{1})^{-1}$ and $\tilde\gamma^{\mathbf{C}}_\xi(\lambda)\overset{\text{def}}{=}\det(L^{\mathbf{C}}-\lambda\mathbf{1})^{-1}\xi$, where $\lambda\in\mathbf{C}\backslash\mathrm{Spect}(L)$, $\xi\in V^{\mathbf{C}}$, and $\mathbf{1}$ denotes the identity operator in $V^{\mathbf{C}}$. As above, using the nondegeneracy of the Vandermonde determinant, we obtain that $\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}=\mathrm{rk}_{\mathbf{C}}\{L_{m-1}^{\mathbf{C}},\dots,L_0^{\mathbf{C}}\}$ and $\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}_\xi=\mathrm{rk}_{\mathbf{C}}\{L_{m-1}^{\mathbf{C}}\xi,\dots,L_0^{\mathbf{C}}\xi\}$. Lemma 5 shows that $\dim_U\gamma=\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}$ and $r_0=\max_{\xi\in V^{\mathbf{C}}}\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}_\xi$. Without loss of generality we can suppose that the operator $L^{\mathbf{C}}$ is given in a Jordan's basis. Using the explicit form of $L^{\mathbf{C}}$, it is not hard to see that

$$\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}=r(L)$$

and

$$\max_{\xi\in V^{\mathbf{C}}}\dim_{\mathbf{C}\backslash\mathrm{Spect}(L)}\tilde\gamma^{\mathbf{C}}_\xi=r(L).$$

The first equality proves item (a). The second one shows that $r_0=r(L)$. Applying Lemma 5(iii) we prove (b). To prove item (c) remark that instead of the curves $\gamma(t_1),\dots,\gamma(t_{r(L)})$ it is sufficient to prove the linear independence over $\mathbf{C}$ of the curves $\tilde\gamma^{\mathbf{C}}(t_1),\dots,\tilde\gamma^{\mathbf{C}}(t_{r(L)})$, where the operator $L^{\mathbf{C}}$ is given in a Jordan's basis. Using the simple form of these curves we prove item (c). Lemma 4 is proved.

Let us return to the proof of Theorem 1. Suppose that g and $\overline{g}$ are PQ^{ϵ}-projective metrics given on the connected manifold M^m. Denote by r the rank of the pair g and $\overline{g}$, and let $D\subset M^m$ be an open set with compact closure in M^m. Without loss of generality we can suppose that D is connected. Taking r different real numbers $c_1,\dots,c_r$ such that $|c_k|>m_D$, $m_D \overset{\text{def}}{=} \sup_{x\in D}\max_{\lambda\in \mathrm{Spect}(A|_x)}|\lambda|$, consider the quadratic forms $B_i^D \overset{\text{def}}{=} K_{c_i}(g,\overline{g})$ $(i=1,\dots,r)$. The forms B_i^D are well-defined on D. Considered as functions of the tangent bundle TD, B_i^D $(i=1,\dots,r)$ are pairwise commuting integrals of the geodesic flow of the metric g (Theorem 3).

Definition 7: A point $x_0\in M^m$ is called stable *iff the rank $r(g,\overline{g})(x)$ of the pair of PQ^{ϵ}-projective metrics g and $\overline{g}$ is equal to some constant q in an open neighborhood of the point x_0. We say that x_0 is a stable point of rank q.*

Definition 8: A point $x_0\in M^m$ is called singular *iff it is not stable.*

Denote the set of stable points by $\mathcal{M}(g,\overline{g})$ and the set of singular points by $\mathcal{S}(g,\overline{g})$.

Lemma 6: The set of stable points $\mathcal{M}(g,\overline{g})$ is open and dense in M^m.

Proof of Lemma 6: The set $\mathcal{M}(g,\overline{g})$ is open by its definition. It follows from Lemma 4 that *for every $x\in M^m$ there exists an open neighborhood $U(x)$ such that if $y\in U(x)$ then $r(g,\overline{g})(y)\geqslant r(g,\overline{g})(x)$.* Indeed, taking $p=r(g,\overline{g})(x)$ different real numbers $t_1,\dots,t_p$, $(-t_i)\notin \mathrm{Spect}(A|_x)$, we see [item (c), Lemma 4] that the forms $K_{t_1}|_x,\dots,K_{t_p}|_x \in \mathrm{Symm}(T_x^*M^m\otimes T_x^*M^m)$ are linearly independent. There exists an open neighborhood $U(x)$ such that if $y\in U(x)$ then $K_{t_1}|_y,\dots,K_{t_p}|_y$ are linearly independent. Finally, applying item (a) of Lemma 4 we obtain that $r(g,\overline{g})(y)\geqslant r(g,\overline{g})(x)$.

Therefore, *if x_0 is a singular point, then every open neighborhood of x_0 contains a point y such that $r(g,\overline{g})(y)>r(g,\overline{g})(x_0)$.*

Let us prove that the set of stable points $\mathcal{M}(g,\overline{g})$ is dense in M^m. Suppose that there exists an open set $Y\subset M^m$ that consists of singular points. Take a point $y_1\in Y$, $r(g,\overline{g})(y_1)=r_1$. The point y_1 is singular, and therefore there exists a point $y_2\in Y$ such that $r(g,\overline{g})(y_2)=r_2>r_1$. Applying this argument several times we find a (singular!) point $y_l\in Y$ of maximal rank m. From another side, the points of maximal rank m are stable. This contradiction proves Lemma 6.

Lemma 7: Let x_0 be a stable point of rank $q\leqslant r$, $x_0\in D$. Then there exists an open neighborhood $U(x_0)\subset D$ such that we see the following:

(a) the quadratic in velocities functions $B_1^D(\xi),\dots,B_q^D(\xi)$ are functionally independent on $TU(x_0)$. For every fixed $x\in U(x_0)$ the set of the points $\xi\in T_xM^m$ where the differentials $d_\xi B_1^D,\dots,d_\xi B_q^D$ are linearly independent is open and dense in T_xM^m;

(b) if c is a real constant such that $(A+c\mathbf{1})$ is nondegenerate on $U(x_0)$, then there exist constants $\alpha_1,\dots,\alpha_q$ such that

$$K_c(g,\overline{g})(\xi)=\sum_{k=1}^{q}\alpha_k B_k^D(\xi),\quad \xi\in TU(x_0).$$

Proof of Lemma 7: (c) of Lemma 4 shows that the forms $B_1^D|_{x_0},\dots,B_q^D|_{x_0}$, considered as elements of $\mathrm{Symm}(T_{x_0}^*M^m\otimes T_{x_0}^*M^m)$, are linearly independent. There exists an open neighborhood $U(x_0)$ of the point x_0 such that for every $y\in U(x_0)$ the forms $B_1^D|_y,\dots,B_q^D|_y$ are linearly independent and $r(g,\overline{g})(y)=q$. Hence, there exist smooth functions $\alpha_1,\dots,\alpha_q\in C^\infty(U(x_0))$ such that

$$K_c(g,\overline{g})(\xi)=\sum_{k=1}^{q}\alpha_k(y)B_k^D(\xi),$$

where $\xi\in U(x_0)$, $y=\pi(\xi)$, and $\pi:TM^m\to M^m$ is the projection on the base M^m. Denote by E_g the "energy" integral $E_g(\xi)\overset{\text{def}}{=}\frac{1}{2}g(\xi,\xi)$ and let $\{\cdot,\cdot\}_g$ be the Poisson bracket corresponding to the symplectic structure ω_g. Using that $B_1^D(\xi),\dots,B_q^D(\xi)$ and $K_c(\xi)$ are integrals of the geodesic flow of the metric g, we obtain $0=\{E_g,K_c\}_g=\Sigma_{k=1}^q\{E_g,\alpha_k\}_g B_k^D(\xi)$ for every $\xi\in TU(x_0)$. The

linear independence of the forms $B_1^D|_y,\dots,B_q^D|_y$ for every fixed $y\in U(x_0)$ shows that $\{E_g,\alpha_k\}\equiv 0$ on $TU(x_0)$, and therefore α_k are constants. Item (b) of Lemma 7 is proved.

Denote by $B_k^D|_{T_xM^m}$ the restriction of the function $B_k^D(\xi)$ on the fiber $T_xM^m\hookrightarrow TM^m$. Taking a point $\xi\in T_xM^m$, we obtain $d_\xi(B_k^D|_{T_xM^m})(\eta)=2B_k^D|_x(\xi,\eta)$, where $\eta\in T_xM^m\cong T_\xi(T_xM^m)$. It follows from Lemma 4 (b) that for every point $x\in U(x_0)$ there exists an open and dense in T_xM^m subset $\Sigma_x\subset T_xM^m$ such that if $\xi\in\Sigma_x$ then $B_1^D|_x(\xi,.),\dots,B_q^D|_x(\xi,\cdot)\in T_x^*M^m$ are linearly independent. Therefore, the functions $B_1^D(\xi),\dots,B_q^D(\xi)$ are functionally independent in $TU(x_0)$. Lemma 7 is proved.

Let us prove that the functions $B_1^D(\xi),\dots,B_r^D(\xi)$ are functionally independent in TD. According to Lemma 6 and Lemma 7, it is sufficient to prove that the stable points in D have rank r. Assume that there exists a stable point $y_0\in D$ having rank $r_0<r$. Without loss of generality we can suppose that the open set D contains a stable point $x_0\in D$ of rank r. Assume for simplicity that the points x_0 and y_0 can be connected by a geodesic line $t\to\gamma(t)\in D$, $\gamma(0)=x_0$, $\gamma(1)=y_0$. Let us take neighborhoods $U(x_0)$ and $V(y_0)$ of the points x_0 and y_0, respectively, such that the conditions of Lemma 7 are satisfied. We can suppose that the differentials $d_wB_1^D,\dots,d_wB_r^D$ are linearly independent at the point $w\overset{\text{def}}{=}\dot\gamma(0)$ (If not, we take $w'\in T_{x_0}M^m$ such that $d_{w'}B_1^D,\dots,d_{w'}B_r^D$ are linearly independent and $\exp w'\in V(y_0)$ [see Lemma 7 (a)]). Denote by $\zeta_t(\xi)$, $\xi\in TM^m$, the one-parameter family of local diffeomorphisms of TM^m corresponding to the geodesic flow of the metric g. Using the fact that the functions $B_1^D(\xi),\dots,B_r^D(\xi)$ are integrals of the geodesic flow of g, we obtain that the differentials $d_vB_1^D,\dots,d_vB_r^D$, $v\overset{\text{def}}{=}\zeta_1(w)$, are linearly independent. From another side, Lemma 7 (b) shows that $B_{r_0+1}^D(\xi)=\Sigma_{k=1}^{r_0}\alpha_kB_k^D(\xi)$ where ξ lies in $TV(y_0)$ and α_k are some constants. Hence, for every $\xi\in TV(y_0)$, $d_\xi B_{r_0+1}^D=\Sigma_{k=1}^{r_0}\alpha_kd_\xi B_k^D$. This contradiction proves that *the stable points $x\in D$, that can be connected by a geodesic line $\gamma(t)$ lying in D with another stable point $y\in D$ of rank r, are also of rank r*. By assumption, D is connected. Therefore, the stable points in D have rank r. Item (a) of Theorem 1 is proved. Item (b) easily follows from Lemma 7 (b). Theorem 1 is proved.

V. $PQ^{(-1)}$-PROJECTIVE HERMITIAN METRIC

Let M^n be a complex manifold of complex dimension n. Denote by J the complex structure of M^n, $(M^{2n},J)\cong M^n$. Consider a pair of $PQ^{(-1)}$-projective Hermitian metrics s and $\tilde s$ ($\epsilon=-1$ and $PQ=-\mathbf{1}$). Denote by $K_c(s,\tilde s)$ the local family of pairwise commuting integrals of the geodesic flow of the metric s (Theorem 3). In our case $\epsilon=-1$ and we obtain that $K_c(s,\tilde s)\overset{\text{def}}{=}|\det(A+c\mathbf{1})|^{1/2}s(A+c\mathbf{1})^{-1}$, where $A=A(s,\tilde s)$.

Fixing a complex chart $\{(z^1,\dots,z^n)\}$ consider the Hermitian matrices $S\overset{\text{def}}{=}(s_{\alpha\bar\beta})$ and $\tilde S\overset{\text{def}}{=}(\tilde s_{\alpha\bar\beta})$ related to the metrics $ds^2=2s_{\alpha\bar\beta}dz^\alpha d\bar z^\beta$ and $d\tilde s^2=2\tilde s_{\alpha\bar\beta}dz^\alpha d\bar z^\beta$, respectively. As usual, we omit the summation symbols in the formulas. Define the operator $\mathcal{A}\overset{\text{def}}{=}\mathcal{A}_\beta^\alpha(\partial/\partial z^\alpha)\otimes dz^\beta$, where

$$\mathcal{A}_\beta^\alpha\overset{\text{def}}{=}\left|\frac{\det\tilde S}{\det S}\right|^{1/(n+1)}\tilde s^{\alpha\bar\nu}s_{\bar\nu\beta},\tag{18}$$

and $\tilde s^{\alpha\bar\nu}\tilde s_{\bar\nu\beta}=\delta_\beta^\alpha$. By definition, $\mathcal{A}$ is a smooth section of the vector bundle $\mathrm{End}_{\mathbf{C}}(T^{(1,0)}M^n)$, where $T^{(1,0)}M^n$ denotes the bundle of the *holomorphic* tangent vectors to M^n. Fixing a point $x\in M^n$, denote by $\rho(s,\tilde s)(x)$ the minimal polynomial of the operator $\mathcal{A}|_x$.

Definition 9: The number $\rho(s,\tilde s)\overset{\text{def}}{=}\max_{x\in M^n}\rho(s,\tilde s)(x)$ *is called* the Hermitian rank of the pair of $PQ^{(-1)}$-projective Hermitian metrics.

Theorem 4: *Suppose that the complex manifold M^n is connected and let the Hermitian rank of the pair of $PQ^{(-1)}$-projective Hermitian metrics s and $\widetilde{s}$ be r. Then there exist r Hermitian forms $B_1,\dots,B_r$ such that we have the following:*

(a) considered as functions of the tangent bundle TM^n, the quadratic forms $B_1(\xi),\dots,B_r(\xi)$ are functionally independent pairwise commuting integrals of the geodesic flow of the metric s;

(b) for every fixed real constant c, the integral $K_c(s,\widetilde{s})(\xi)$ is well-defined and

$$K_c(s,\widetilde{s})(\xi)=\sum_{k=1}^{r}\alpha_k B_k(\xi),$$

where α_k are some constants.

The functions $B_1(\xi),\dots,B_r(\xi)$ can be taken in the form $B_k=K_{c_k}(s,\widetilde{s})$, where c_k are appropriately chosen constants.

Proof of Theorem 4: Fixing a complex chart $\{(z^1,\dots,z^n)\}$ we have $s=s_{\alpha\overline{\beta}}(dz^\alpha\otimes d\overline{z}^\beta+d\overline{z}^\beta\otimes dz^\alpha)$ and $\widetilde{s}=\widetilde{s}_{\alpha\overline{\beta}}(dz^\alpha\otimes d\overline{z}^\beta+d\overline{z}^\beta\otimes dz^\alpha)$, where $S\overset{\text{def}}{=}(s_{\alpha\overline{\beta}})$ and $\widetilde{S}\overset{\text{def}}{=}(\widetilde{s}_{\alpha\overline{\beta}})$ are Hermitian matrices. Denote by $[s]$ and $[\widetilde{s}]$ the Gramians of the metrics s and $\widetilde{s}$, respectively, i.e.,

$$[s]=\begin{bmatrix}0 & S\\ \overline{S} & 0\end{bmatrix}$$

and

$$[\widetilde{s}]=\begin{bmatrix}0 & \widetilde{S}\\ \overline{\widetilde{S}} & 0\end{bmatrix}.$$

It follows from the definition of the operator $A(s,\widetilde{s})$ [formula (4)] that in the fixed complex chart we have

$$A(s,\widetilde{s})\overset{\text{def}}{=}\left|\frac{\det[\widetilde{s}]}{\det[s]}\right|^{1/2(n+1)}[\widetilde{s}]^{-1}[s]=\left|\frac{\det\widetilde{S}}{\det S}\right|^{1/(n+1)}[\widetilde{s}]^{-1}[s].$$

Hence, $A(s,\widetilde{s})=\mathcal{A}_\beta^\alpha(\partial/\partial z^\alpha)\otimes dz^\beta+\mathcal{A}_\beta^{\overline{\alpha}}(\partial/\partial\overline{z}^\alpha)\otimes d\overline{z}^\beta$, where $\mathcal{A}_\beta^\alpha$ is given by formula (18) and $\mathcal{A}_\beta^{\overline{\alpha}}$ coincides with the complex conjugation of $\mathcal{A}_\beta^\alpha$ (i.e., $\mathcal{A}_\beta^{\overline{\alpha}}=\overline{\mathcal{A}}_\beta^\alpha$). As usual, we identify the operator $\mathcal{A}$ with the square matrix $(\mathcal{A}_\beta^\alpha)$.

Lemma 8: The degree of the minimal polynomial of the operator $\mathcal{A}(s,\widetilde{s})$ coincides with the degree of the minimal polynomial of the operator $A(s,\widetilde{s})$.

Proof of Lemma 8: A simple calculation shows that

$$\mathcal{A}-\overline{\lambda}\mathbf{1}=\widetilde{S}^{-1}(\mathcal{A}-\lambda)^*\widetilde{S},$$

where $(\cdot)^*$ denotes the Hermitian conjugation of a matrix. Hence, for every integer k we have $(\mathcal{A}-\overline{\lambda}\mathbf{1})^k=\widetilde{S}^{-1}[(\mathcal{A}-\lambda)^k]^*\widetilde{S}$. Consider the Jordan's normal form of the operator $\mathcal{A}$. The last equalities show that the Jordan's decompositions corresponding to the eigenvalues λ and $\overline{\lambda}$ coincide. Finally, we conclude the statement of the lemma from the formula $A(s,\widetilde{s})=\mathcal{A}_\beta^\alpha(\partial/\partial z^\alpha)\otimes dz^\beta+\overline{\mathcal{A}}_\beta^\alpha(\partial/\partial\overline{z}^\alpha)\otimes d\overline{z}^\beta$. Lemma 8 is proved.

It follows from Lemma 8 that the rank $r(s,\widetilde{s})$ of the pair s and $\widetilde{s}$ coincides with their Hermitian rank, i.e., $r=r(s,\widetilde{s})=\rho(s,\widetilde{s})$.

Let us fix an arbitrary real constant c. Denote by $\mathcal{K}_c(s,\widetilde{s})$ the Hermitian matrix of the form $K_c(s,\widetilde{s})$. A simple calculation shows that

$$\mathcal{K}_c(s,\tilde{s})=\det(\overline{\mathcal{A}}+c\mathbf{1})S(\overline{\mathcal{A}}+c\mathbf{1})^{-1}=\mathcal{I}_{n-1}(s,\tilde{s})c^{n-1}\cdot\cdots+\mathcal{I}_0(s,\tilde{s}).$$

The last formula is valid in every fixed complex chart. Therefore, there exist well-defined on the whole M^n Hermitian forms $I_{n-1},\ldots,I_0$ such that $K_c=I_{n-1}c^{n-1}+\cdots+I_0$. Denote by $I_{n-1}(\xi),\ldots,I_0(\xi)$ the corresponding smooth functions of the tangent bundle TM^n. We obviously have

$$K_c(\xi)=I_{n-1}(\xi)c^{n-1}+\cdots+I_0(\xi), \tag{19}$$

where $I_j\in C^\infty(TM^n)$. Denote by $\mathcal{I}(s,\tilde{s})$ the vector space spanned on the functions $I_j\in C^\infty(TM^n)$ $(j=0,\ldots,n-1)$. Take a basis $B_1(\xi),\ldots,B_{r'}(\xi)$ of the linear space $\mathcal{I}(s,\tilde{s})$. Let us fix an open set $D\subset M^n$ with compact closure in M^n and consider the quadratic forms $B_1^D(\xi),\ldots,B_r^D(\xi)$ given by Theorem 1. Item (b) of Theorem 1 and formula (19) show that $B_k|_{TD}\in\mathrm{Span}(B_1^D|_{TD},\ldots,B_r^D|_{TD})$ $(k=1,\ldots,r')$ where $\mathrm{Span}(B_1^D|_{TD},\ldots,B_r^D|_{TD})$ denotes the vector space spanned on the restrictions of the functions $B_k^D(\xi)$ on TD. From another side, $B_k^D(\xi)\overset{\text{def}}{=}K_{c_k}(s,\tilde{s})(\xi)$. Using formula (19) again we obtain that $B_k^D|_{TD}\in\mathrm{Span}(B_1|_{TD},\ldots,B_r|_{TD})$ $(k=1,\ldots,r)$. Therefore, $r=r'$. The functions $B_1^D(\xi),\ldots,B_r^D(\xi)$ are functionally independent on TD. Hence, the functions $B_1(\xi),\ldots,B_r(\xi)$ are functionally independent as well. Finally, recall that the set D was taken arbitrary. Theorem 4 is proved.

Remark 6: In the present section we do not use essentially the integrability of the complex structure J. Therefore, Theorem 4 still holds if (M^{2n},J) be an almost complex manifold of real dimension $2n$.

VI. EXAMPLES. INTEGRABLE SYSTEMS ON $\mathbf{CP}^n$

Our aim in the present section is to find a family of completely integrable systems on the complex projective space $\mathbf{CP}^n$. Denote by $\{(z_0:\cdots:z_n)\}$ the homogeneous coordinates of $\mathbf{CP}^n$ and consider the affine chart $\mathbf{C}^n\ni(z_1,\ldots,z_n)\mapsto(1:z_1:\cdots:z_n)\in\mathbf{CP}^n$. In coordinates $\{(z_1,\ldots,z_n)\}$, the Fubini metrics are given by the formula

$$dg^2\overset{\text{def}}{=}2\frac{\Sigma_{\alpha=1}^n\epsilon_\alpha|dz_\alpha|^2+\frac{K}{2}((\Sigma_{\alpha=1}^n\epsilon_\alpha|z_\alpha|^2)(\Sigma_{\alpha=1}^n\epsilon_\alpha|dz_\alpha|^2)-|\Sigma_{\alpha=1}^n\epsilon_\alpha\overline{z}_\alpha dz_\alpha|^2)}{\left(1+\frac{K}{2}\Sigma_{\alpha=1}^n\epsilon_\alpha|z_\alpha|^2\right)^2}, \tag{20}$$

where $K\neq0$ and the "signs" $\epsilon_\alpha=\pm1$ $(\alpha=1,\ldots,n)$ are fixed. Consider the hermitian form $Q(\xi,\overline{\eta})\overset{\text{def}}{=}\xi_0\overline{\eta}_0+K/2\,\Sigma_{\alpha=1}^n\epsilon_\alpha\xi_\alpha\overline{\eta}_\alpha$, $\xi,\eta\in\mathbf{C}^{n+1}$. The hypersurface $Abs\hookrightarrow\mathbf{CP}^n$ given in homogeneous coordinates by $Abs\overset{\text{def}}{=}\{Q(z)=Q(z,\overline{z})=0\}$ is called *absolute* of the corresponding Fubini metric. The Fubini metrics are smoothly defined on $\mathbf{CP}^n\backslash Abs$. If $K>0$ and $\epsilon_\alpha=1$ then $Abs=\emptyset$, and the corresponding Fubini metric is a smooth Riemannian metric on $\mathbf{CP}^n$. The Fubini metrics are usually considered only on the subset $F\overset{\text{def}}{=}\{Q(z)>0\}\subset\mathbf{CP}^n$. Nevertheless, it will be more convenient for us to think of the Fubini metrics as metrics defined on the whole $\mathbf{CP}^n$ and having "singularities" in Abs. The Fubini metrics are Hermitian and the corresponding Hermitian matrices are $g_{\alpha\overline{\beta}}=\epsilon_\alpha\delta_{\alpha\beta}/Q(z)-(K/2)[(\epsilon_\alpha\overline{z}_\alpha)(\epsilon_\beta z_\beta)/Q(z)^2]$. It is well-known that the Fubini metrics are Kählerian metrics.

Denote by ∇ the Levi-Civita connection corresponding to the Fubini metric g. The connection ∇ can be extended in a natural way to a connection on the complexification of the tangent bundle. It can be easily seen that the corresponding Christoffel symbols are given by the formula $\Gamma_{pq}^\alpha=-[K/2Q(z)](\delta_p^\alpha\epsilon_q\overline{z}_q+\delta_q^\alpha\epsilon_p\overline{z}_p)$, $\Gamma_{\overline{pq}}^{\overline{\alpha}}=\overline{\Gamma}_{pq}^\alpha$, and the other components of the Christoffel symbols vanish (see Ref. 10, Sec. 5, for the case $\epsilon_\alpha=1$).

Let $\mu_L:\mathbf{CP}^n\to\mathbf{CP}^n$ be a projective transformation induced by some (complex) linear transformation $L:\mathbf{C}^{n+1}\to\mathbf{C}^{n+1}$ given in matrix form by the nondegenerate complex matrix $L\in GL_{n+1}(\mathbf{C})$. Denote by $\tilde{g}$ the pull-back $\mu_L^* g$.

Proposition 5: The metrics g and $\tilde{g}$ are h-projective Kählerian metrics.

Proof of Proposition 5: Let L_2 be a complex 2-plane in $\mathbf{C}^{n+1}$. The set of complex lines lying in L_2 gives a natural embedding of the complex projective line $\mathbf{CP}^1$ in $\mathbf{CP}^n$. We call such embeddings *projective lines*. Proposition 5 easily follows from the next simple lemma.

Lemma 9: A smooth curve $\gamma(t)\in\mathbf{CP}^n\backslash Abs$ is holomorphically planar with respect to a fixed Fubini metric iff $\gamma(t)$ lies in a projective line.

Proof of Lemma 9: Consider the affine chart $\{(z_1,\dots,z_n)\}$ and suppose that $\gamma(t)=(\gamma^1(t),\dots,\gamma^n(t))$. The condition that $\gamma(t)$ is holomorphically planar with respect to a fixed Fubini metric g is equivalent to the equation

$$\frac{\nabla\dot{\gamma}^\alpha}{dt}(t)=\rho(t)\,\dot{\gamma}^\alpha(t),\quad \alpha=1,\dots,n,$$

where $\rho(t)$ is a smooth complex-valued function of the real parameter t and $\nabla\dot{\gamma}^\alpha/dt$ are the components of the "holomorphic" part of the real vector $\nabla\dot{\gamma}/dt$. Using the explicit form of the Christoffel symbols of the Fubini metric g we obtain

$$\frac{\nabla\dot{\gamma}^\alpha}{dt}(t)=\frac{d^2\gamma^\alpha}{dt^2}+\Gamma^\alpha_{pq}\dot{\gamma}^p\dot{\gamma}^q=\frac{d^2\gamma^\alpha}{dt^2}-\frac{K}{Q}(\epsilon_p\overline{z}_p\dot{\gamma}^p)\dot{\gamma}^\alpha.$$

Therefore, the curve $\gamma(t)$ is holomorphically planar if and only if $d^2\gamma^\alpha/dt^2=\rho_1(t)\,(d\gamma^\alpha/dt)$, where $\rho_1(t)$ is a smooth complex-valued function of t. This completes the proof of Lemma 9.

Finally, Proposition 5 follows from the fact that $\mu_L:\mathbf{CP}^n\to\mathbf{CP}^n$ maps projective lines to projective lines. Proposition 5 is proved.

An analog of Lemma 9 in the case of positive definite Fubini metrics is proved in Ref. 15, Sec. 6.

Let us take $L=\mathrm{diag}(1,\lambda_1,\dots,\lambda_n)$ where λ_α are fixed constants. In the chart $\{(z_1,\dots,z_n)\}$, the induced projective transformation $\mu_L:\mathbf{CP}^n\to\mathbf{CP}^n$ is given by the formula $(z_1,\dots,z_n)\mapsto(\lambda_1 z_1,\dots,\lambda_n z_n)$. We have

$$d\tilde{g}^2=2\,\frac{\tilde{Q}(z)(\Sigma_{\alpha=1}^n\epsilon_\alpha\rho_\alpha|dz_\alpha|^2)-\dfrac{K}{2}|\Sigma_{\alpha=1}^n\epsilon_\alpha\rho_\alpha\overline{z}_\alpha\,dz_\alpha|^2}{\tilde{Q}(z)^2},\tag{21}$$

where $\rho_\alpha\overset{\text{def}}{=}|\lambda_\alpha|^2$ and $\tilde{Q}(z)\overset{\text{def}}{=}1+K/2\,\Sigma_{\alpha=1}^n\epsilon_\alpha\rho_\alpha|z_\alpha|^2$. The components of the corresponding Hermitian matrix are $\tilde{g}_{\alpha\overline{\beta}}=\epsilon_\alpha\rho_\alpha\delta_{\alpha\beta}/\tilde{Q}(z)-(K/2)[(\epsilon_\alpha\rho_\alpha\overline{z}_\alpha)(\epsilon_\beta\rho_\beta z_\beta)/\tilde{Q}^2(z)]$. Let us remark that the metric $\tilde{g}$ is smoothly defined on $\mathbf{CP}^n\backslash\widetilde{Abs}$, where $\widetilde{Abs}\overset{\text{def}}{=}\{\tilde{Q}(z)=0\}$.

Lemma 10: Let B be a non-degenerate symmetric $n\times n$-matrix and $a,b\in\mathbf{C}^n$ are complex vectors considered as $n\times 1$-matrices. Denote by $(\cdot)'$ the transposition of a matrix and $\langle x,y\rangle\overset{\text{def}}{=}\Sigma_{\alpha=1}^n x_\alpha y_\alpha$. Then

(i) $(B+ab')^{-1}=B^{-1}-(B^{-1}a)(B^{-1}b)'/1+\langle B^{-1}a,b\rangle$;
(ii) $\det(B+ab')=(1+\langle B^{-1}a,b\rangle)\det B$.

The proof of Lemma 10 is straightforward.

Using Lemma 10 we obtain $\tilde{g}^{\alpha\overline{\beta}}=\tilde{Q}(\epsilon_\alpha\rho_\alpha^{-1}\delta_{\alpha\beta}+(K/2)\,z_\alpha\overline{z}_\beta)$. Hence, the operator $A(g,\tilde{g})$ is given by the formula $A(g,\tilde{g})=\mathcal{A}^\alpha_\beta(\partial/\partial z_\alpha)\otimes dz_\beta+\mathcal{A}^{\overline{\alpha}}_{\overline{\beta}}(\partial/\partial\overline{z}_\alpha)\otimes d\overline{z}_\beta$, where $\mathcal{A}^{\overline{\alpha}}_{\overline{\beta}}=\overline{\mathcal{A}^\alpha_\beta}$ and $\mathcal{A}^\alpha_\beta=|\det\tilde{G}/\det G|^{1/(n+1)}\tilde{g}^{\alpha\overline{\nu}}g_{\overline{\nu}\beta}$, $\tilde{G}\overset{\text{def}}{=}(\tilde{g}_{\alpha\overline{\beta}})$, $G\overset{\text{def}}{=}(g_{\alpha\overline{\beta}})$ (see Sec. 5). Applying Lemma 10 we obtain

$$\mathcal{A}_{\beta}^{\alpha}=\rho_{\beta}^{-1}\delta_{\beta}^{\alpha}-\frac{K}{2Q}((1-\rho_{\alpha})z_{\alpha}/\rho_{\alpha})(\epsilon_{\beta}\overline{z_{\beta}}). \tag{22}$$

Denote by $\mathcal{A}$ the matrix with elements $\mathcal{A}_{\beta}^{\alpha}$. Consider the sequences of Hermitian matrices $\{G^{(l)}\}_{l\in\mathbf{Z}}$ and $\{\tilde{G}^{(l)}\}_{l\in\mathbf{Z}}$ defined by the formulas $G^{(l)}\overset{\text{def}}{=}G\overline{\mathcal{A}^{l}}$ and $\tilde{G}^{(l)}\overset{\text{def}}{=}\tilde{G}\overline{\mathcal{A}^{l}}$. Denote by $g^{(l)}$ and $\tilde{g}^{(l)}$ the Hermitian metrics,

$$dg^{(l)^2}\overset{\text{def}}{=}2g_{\alpha\overline{\beta}}^{(l)}dz_{\alpha}d\overline{z}_{\beta} \tag{23}$$

and

$$d\tilde{g}^{(l)^2}\overset{\text{def}}{=}2\tilde{g}_{\alpha\overline{\beta}}^{(l)}dz_{\alpha}d\overline{z}_{\beta}, \tag{24}$$

where $g_{\alpha\overline{\beta}}^{(l)}$ and $\tilde{g}_{\alpha\overline{\beta}}^{(l)}$ are the elements of the Hermitian matrices $G^{(l)}$ and $\tilde{G}^{(l)}$, respectively.

Consider the operators $\mathcal{P}_l,\mathcal{Q}_l\in\Gamma(\mathrm{End}_{\mathbf{C}}(T^{(1,0)}(\mathbf{CP}^n\backslash Abs)))$ given in coordinates by the matrices $i\mathcal{A}^{l}$ and $i\mathcal{A}^{-l}$, respectively, and define the "real" operators $P_l\overset{\text{def}}{=}\mathcal{P}_l+\overline{\mathcal{P}_l}$ and $Q_l\overset{\text{def}}{=}\mathcal{Q}_l+\overline{\mathcal{Q}_l}$. The next theorem follows from the results proved in Sec. II D.

Theorem 5: *For every fixed integer $l\in\mathbf{Z}$ the Hermitian metrics $g^{(l)}$ and $\tilde{g}^{(l)}$ given by formulas (23) and (24) are $P_lQ_l^{(-1)}$-projective Hermitian metrics.*

The sequence of metrics $g^{(l)}$ and $\tilde{g}^{(l)}$ ($l\in\mathbf{Z}$) given by Theorem 5 is called a $\mathbf{CP}^n$*-hierarchy*.

Let us consider the one-parameter groups of transformations of $\mathbf{CP}^n$ given in coordinates by the formulas

$$T_k(\phi):(z_1,\ldots,z_k,\ldots,z_n)\mapsto(z_1,\ldots,\exp(i\phi)z_k,\ldots,z_n).$$

It follows from (20) and (21) that $T_k(\phi)$ preserve the metrics g and $\tilde{g}$, and therefore they preserve the whole $\mathbf{CP}^n$-hierarchy. Denote by T_k the corresponding Killing symmetries,

$$T_k\overset{\text{def}}{=}i\left(z_k\frac{\partial}{\partial z_k}-\overline{z_k}\frac{\partial}{\partial\overline{z_k}}\right). \tag{25}$$

Consider the "complex" impulses $p_k\overset{\text{def}}{=}\frac{1}{2}(p_{x_k}-ip_{y_k})$ and $\overline{p_k}\overset{\text{def}}{=}\frac{1}{2}(p_{x_k}+ip_{y_k})$ $(k=1,\ldots,n)$, where p_{x_k} and p_{y_k} are the impulses corresponding to the chart $\{(x_1,y_1,\ldots,x_n,y_n)\}$, $z_k\overset{\text{def}}{=}x_k+iy_k$. The chart $\{(p_1,\ldots,p_n;z_1,\ldots,z_n)\}$ is a complex chart of $T^*\mathbf{CP}^n$. The canonical symplectic structure ω on $T^*\mathbf{CP}^n$ is given by the formula $\omega=\Sigma_{k=1}^{n}dp_k\wedge dz_k+\Sigma_{k=1}^{n}d\overline{p_k}\wedge d\overline{z_k}$.

Theorem 6: *For every fixed integer $l\in\mathbf{Z}$ the functions $\mathcal{I}_{n-1}^{(l)}(p),\ldots,\mathcal{I}_0^{(l)}(p)$ given by the expansion*

$$\mathcal{K}_c^{(l)}(p)\overset{\text{def}}{=}\det(\mathcal{A}+c\mathbf{1})\langle(\mathcal{A}+c\mathbf{1})^{-1}\mathcal{A}^{l}\overline{G}^{-1}\overline{p},p\rangle=\mathcal{I}_{n-1}^{(l)}(p)c^{n-1}+\cdots+\mathcal{I}_0^{(l)}(p), \tag{26}$$

where $p\overset{\text{def}}{=}(p_1,\ldots,p_n)$, $\overline{p}\overset{\text{def}}{=}(\overline{p_1},\ldots,\overline{p_n})$ and $\langle X,Y\rangle\overset{\text{def}}{=}\Sigma_{k=1}^{n}X_kY_k$, are in involution with respect to the canonical symplectic structure ω on the cotangent bundle $T^*\mathbf{CP}^n$. If $\rho_{\alpha}\neq\rho_{\beta}$ $(\alpha\neq\beta)$ then the functions $\mathcal{I}_{n-1}^{(l)}(p),\ldots,\mathcal{I}_0^{(l)}(p)$ are functionally independent on $T^*(\mathbf{CP}^n\backslash Abs)$. Adding to the functions $\mathcal{I}_{n-1}^{(l)}(p),\ldots,\mathcal{I}_0^{(l)}(p)$ the Noether integrals $T_k(p)\overset{\text{def}}{=}i(z_kp_k-\overline{z_k}\overline{p_k})$ $(k=1,\ldots,n)$ corresponding to the Killing symmetries (25), we obtain a complete system of functionally independent functions in involutions on $T^*(\mathbf{CP}^n\backslash Abs)$.

Proof of Theorem 6: It follows from formula (22) that $\mathcal{A}_{\beta}^{\alpha}(0)=\rho_{\beta}^{-1}\delta_{\beta}^{\alpha}$. Hence, if $\rho_{\alpha}\neq\rho_{\beta}$ $(\alpha\neq\beta)$ then the Hermitian rank of the pair $g^{(l)}$ and $\tilde{g}^{(l)}$ is n. Finally, the statement of the theorem follows from Theorem 4, Sec. V, applied to the pair $g^{(-l)}$ and $\tilde{g}^{(-l)}$ from the **CP**-hierarchy. Theorem 6 is proved.

Corollary 2: Provided $\rho_\alpha \neq \rho_\beta$ $(\alpha \neq \beta)$, *the geodesic flows of the metrics* $g^{(l)}$ *and* $\tilde{g}^{(l)}$ *from the* $\mathbf{CP}^n$*-hierarchy are completely integrable.*

Remark 7: Taking $l=0$ *and* $\epsilon_\alpha = 1$, *we obtain a complete family of pairwise commuting integrals of the geodesic flow of the standard Fubini metric on* $\mathbf{CP}^n$ (see Refs. 13 and 16). *Our theorem gives an infinite family of metrics on* $\mathbf{CP}^n$ *with completely integrable geodesic flows.*

ACKNOWLEDGMENT

The author is partially supported by MESC Grant No. MM-810/98.

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Representation of semigroups in rigged Hilbert spaces: Subsemigroups of the Weyl–Heisenberg group

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(Received 12 August 2002; accepted 1 November 2002)

In this paper we study how differentiable representations of certain subsemigroups of the Weyl–Heisenberg group may be obtained in suitably constructed rigged Hilbert spaces. These semigroup representations are induced from a continuous unitary representation of the Weyl–Heisenberg group in a Hilbert space. Aspects of the rigged Hilbert space formulation of time asymmetric quantum mechanics are also investigated within the context of the results developed here. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1533835]

I. INTRODUCTION

Rigged Hilbert spaces have been used in quantum physics since the mid-1960's. Although the motivation of the first contributions[1–3] was to provide a rigorous mathematical context for Dirac's (already well-established) bra-and-ket formulation of quantum mechanics, subsequent investigations[4–7] have led to some interesting new physical results. Among these are a formulation of scattering theory which accommodates an asymmetric time evolution given by a *semigroup* of operators, and a related vector description for an (isolated) resonance state. The more recent of these works[7] extend the earlier results to relativistic resonances where it is shown that they can be characterized by irreducible representations of the causal Poincaré semigroup.

Many of the results of these theories can be subsumed under a general study of the representations of Lie groups and their subsemigroups in rigged Hilbert spaces. We call a subset S of a Lie group G a subsemigroup of the group if S contains the identity element and remains invariant under the group multiplication of G. Notice that S need not be closed under the inverse operation $x \to x^{-1}$. If S is such a subsemigroup of a Lie group G, the problem in its broadest generality can be stated as follows: If U is a continuous (often unitary) representation of G in a Hilbert space $\mathcal{H}$, does there exist a rigged Hilbert space $\Phi \subset \mathcal{H} \subset \Phi^\times$ such that Φ reduces U to a continuous representation of S?

It is clear that if $U|_\Phi$ is such a representation of S, then there also exists a dual representation $U|_\Phi^\times$ of S in $\Phi^\times$. The semigroup time evolution of Gamow vectors,[4–7] which describe the (isolated) resonance states, is given by such a representation in $\Phi^\times$ dual to a semigroup representation in Φ. In particular, in the nonrelativistic scattering theory developed in Refs. 4–6, time, i.e., the Lie group of real numbers under addition, is unitarily represented, by way of the mapping $(U(t)f)(E) = e^{iEt} f(E)$, in the Hilbert space of square integrable functions defined on the spectrum of the Hamiltonian H. The rigged Hilbert spaces $\Phi_- \subset \mathcal{H} \subset \Phi_-^\times$ and $\Phi_+ \subset \mathcal{H} \subset \Phi_+^\times$ of Hardy class functions, introduced to represent the in- and out-states, have the property that Φ_+ and Φ_- reduce the unitary group representation $U(t)$ in $\mathcal{H}$ to representations of the semigroups (under addition) of negative and positive real numbers, respectively. In the relativistic theory developed in Ref. 7, there exist two rigged Hilbert spaces which reduce a unitary representation of the Poincaré group in $\mathcal{H}$ to continuous representations of the forward and backward causal Poincaré semigroups.

These cases provide examples to the general question posed above. At present, the complete answer to this question is not known to us. It is perhaps the case that the problem is unanswerable,

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at least in the affirmative, as stated above; it may be that such rigged Hilbert spaces are possible for only certain classes of subsemigroups of G, and this then means that it is necessary to develop a classification criterion for the subsemigroups S of a Lie group G. (Recall that even in the Lie group theory, all subgroups are not considered to be of much interest. It is Lie subgroups that are generally investigated.) In this paper, we shall mainly restrict ourselves to semigroups which are the unions of the products of continuous one parameter subsemigroups.

Our purpose in this paper is to study the representations of some subsemigroups of the Weyl–Heisenberg group as illustrative of the above general question. Our treatment will also reveal the general group theoretical content underlying the rigged Hilbert space formulation of the time asymmetric quantum mechanics developed in Refs. 4–6.

It is convenient to introduce here some preliminary concepts which we shall make use of in the following sections.

Definition 1.1: A rigged Hilbert space consists of a triad of vector spaces,

$$\Phi \subset \mathcal{H} \subset \Phi^{\times}, \tag{1.1}$$

where

(1) $\mathcal{H}$ *is a Hilbert space*
(2) Φ *is a dense subspace of* $\mathcal{H}$ *and it is endowed with a complete, locally convex, nuclear topology* τ_{Φ} *that is stronger than the* $\mathcal{H}$*-topology*
(3) $\Phi^{\times}$ *is the space of continuous antilinear functionals on* Φ*. It is complete in its weak* topology* $\tau^{\times}$ *and it contains* $\mathcal{H}$ *as a dense subspace.*

Definition 1.2: A continuous representation of a Lie group G *on a topological vector space* Ψ *is a continuous mapping* $\mathcal{T}$: $G \times \Psi \to \Psi$ *such that*

(1) *for every* $g \in G$, $\mathcal{T}(g)$ *is a linear operator in* Ψ
(2) *for every* $\psi \in \Psi$ *and* $g_1, g_2 \in G$, $\mathcal{T}(g_1 g_2)\psi = \mathcal{T}(g_1)\mathcal{T}(g_2)\psi$
(3) $T(e) = I$, *the identity operator in* Ψ

Definition 1.3: A differentiable representation of a Lie group G *on a complete topological vector space* Ψ *is a mapping* $\mathcal{T}$: $G \times \Psi \to \Psi$ *which fulfills all the requirements of Definition 1.2 and has the additional property that for every one parameter subgroup* $\{g(t)\}$ *of* G, $\lim_{t \to 0} \{[\mathcal{T}(g(t))\phi - \phi]/t\}$ *exists for all* $\phi \in \Psi$ *(and, a fortiori, defines a continuous linear operator on* Ψ*).*

The semigroup analogs of these definitions are obvious. For instance, in Definition 1.3, we simply replace the one parameter subgroups $g(t)$ of G by one parameter subsemigroups $g(t)$ of S.

II. WEYL–HEISENBERG GROUP AND ITS SUBSEMIGROUPS

The three dimensional Euclidean space $\mathbb{R}^3$ is a Lie group under the associative multiplication rule, defined by

$$(a,b,c)(\alpha,\beta,\gamma) = (a+\alpha, b+\beta, c+\gamma+a\beta). \tag{2.1}$$

It is easily verified that the origin (0,0,0) of $\mathbb{R}^3$ is the identity element and that each element (a,b,c) has an inverse given by $(a,b,c)^{-1} = (-a,-b,-c+ab)$. Thus, under (2.1) $\mathbb{R}^3$ is a group, the well known Weyl–Heisenberg group. Throughout the rest of this paper we shall refer to this group by G. We shall denote an element of G by (a,b,c), or by $\boldsymbol{\xi}$, where $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)$.

The Lie algebra $\mathcal{G}$ of the group G is also isomorphic to $\mathbb{R}^3$, and the elements $\chi_1 = (1,0,0)$, $\chi_2 = (0,1,0)$ and $\chi_3 = (0,0,1)$ can be chosen as a basis for $\mathcal{G}$. In fact, $\mathcal{G}$ can be made into an associative algebra (of operators acting on $\mathbb{R}^3$ itself) by way of the multiplication rule $\mathcal{G} \otimes \mathcal{G} \to \mathcal{G}$ defined by

$$(a,b,c)(\alpha,\beta,\gamma) = (0,0,a\beta). \tag{2.2}$$

Under (2.2), the basis elements χ_i fulfill the relations $\chi_i\chi_j=\delta_{1i}\delta_{2j}\chi_3$, and thereupon we have the very well-known Heisenberg commutation relations: $[\chi_1,\chi_2]=\chi_3,[\chi_1,\chi_3]=[\chi_2,\chi_3]=0$.

Among the subsemigroups of G are the following:

$$\begin{aligned} S_1(0)&=\{\boldsymbol{\xi}:\ \xi_1\geqslant 0,\ \xi_2=0,\ \xi_3\in\mathbb{R}\},\\ S_1&=\{\boldsymbol{\xi}:\ \xi_1\geqslant 0,\ \xi_2,\xi_3\in\mathbb{R}\},\\ S_2(0)&=\{\boldsymbol{\xi}:\ \xi_1=0,\ \xi_2\geqslant 0,\ \xi_3\in\mathbb{R}\},\\ S_2&=\{\boldsymbol{\xi}:\ \xi_2\geqslant 0,\ \xi_1,\xi_3\in\mathbb{R}\},\\ S_3&=\{\boldsymbol{\xi}:\ \xi_1,\xi_2\geqslant 0,\ \xi_3\in\mathbb{R}\},\\ S_4&=\{\boldsymbol{\xi}:\ \xi_1,\xi_2\geqslant 0,\ \xi_1\xi_2\geqslant\xi_3\geqslant 0\}. \end{aligned} \tag{2.3}$$

It is readily seen that each set in (2.3) is a topological semigroup. More specifically, (2.1) reduces to a continuous, associative multiplication on every S_i, and none is closed under the inverse operation $\boldsymbol{\xi}\to\boldsymbol{\xi}^{-1}$. Thus each S_i is truly a topological subsemigroup of G. Furthermore, it is straightforward to verify that the set consisting of the inverses of the elements in each S_i of (2.3) is also a subsemigroup of G. We shall denote this complementary semigroup to S_i by S_i^{-1}.

Next, let L^2 be the Hilbert space of square integrable (with respect to Lebesgue measure) functions on the real line $\mathbb{R}$. The mapping U: $G\otimes L^2\to L^2$, defined by

$$(U(\boldsymbol{\xi})f)(x)=e^{i\xi_3}e^{ix\xi_2}f(x+\xi_1), \tag{2.4}$$

furnishes a continuous unitary representation of G in L^2. The differential of U at the identity $\mathbf{0}$, $dU|_{\mathbf{0}}$, yields a representation of the Lie algebra $\mathcal{G}$, a well known result from the classical representation theory. In particular, the basis elements χ_i acquire representation as the linear operators,

$$\begin{aligned} (dU|_{\mathbf{0}}(\chi_1)f)(x)&\equiv(Mf)(x)=ixf(x),\\ (dU|_{\mathbf{0}}(\chi_2)f)(x)&\equiv(Df)(x)=\left(\frac{df}{dx}\right)(x),\\ (dU|_{\mathbf{0}}(\chi_3)f)(x)&=if(x). \end{aligned} \tag{2.5}$$

It is clear that the first two equalities may be defined not on the whole of L^2 but on a dense subspace thereof.

In the remainder of this paper we shall discuss how a rigged Hilbert space may be constructed so that the restriction $U|_\Phi$ of U to Φ yields therein a nontrivial (i.e., one that does not extend to a representation of a subgroup of G) differentiable representation of two of the subsemigroups in (2.3). We shall also remark on how rigged Hilbert spaces may be constructed for the other subsemigroups in (2.3).

III. A DIFFERENTIABLE REPRESENTATION OF $S_1(0)$ IN A RIGGED HILBERT SPACE

In this section we shall construct a rigged Hilbert space $\Psi\subset L^2\subset\Psi^\times$ such that the restriction of U to Ψ yields a representation of the subsemigroup $S_1(0)$ of G defined in (2.3). The main technical result is the construction of the rigged Hilbert space.

A. Construction of the rigged Hilbert space

Definitions: Let L^2_+ and L^2_- be the Hilbert spaces of square integrable (with respect to Lebesgue measure) functions supported in $(0,\infty)$ and $(-\infty,0)$, respectively. Let us denote the norms

in these spaces by $\|\cdot\|_+$ and $\|\cdot\|_-$. The restriction of L^2-functions to $(0,\infty)$ and $(-\infty,0)$ define, respectively, two projection operators Q_+ and Q_- onto L^2_+ and L^2_-. Thus, $L^2_+ = Q_+L^2$, $L^2_- = Q_-L^2$, and $L^2 = L^2_- \oplus L^2_+$.

The mapping $\mathbb{H}: L^2 \to L^2$ defined by

$$(\mathbb{H}f)(t) = \frac{1}{\pi}\int_{-\infty}^{\infty} dx \frac{f(x)}{x-t},$$

where the integral is defined as the Cauchy principal value, is called the Hilbert transform. It is well known that the operators $P_+ = \frac{1}{2}(I + i\mathbb{H})$ and $P_- = \frac{1}{2}(I - i\mathbb{H})$ are projections from L^2 onto $\mathcal{H}^2_+$ and $\mathcal{H}^2_-$, the Hilbert spaces of Hardy class functions from above and below, respectively.[8] Thus, $\mathcal{H}^2_+ = P_+L^2$, $\mathcal{H}^2_- = P_-L^2$, and $L^2 = \mathcal{H}^2_- \oplus \mathcal{H}^2_+$.

For any $f \in L^1(\mathbb{R})$, the function $\hat{f}$ defined by the integral

$$\hat{f}(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ixt}\,dx, \tag{3.1}$$

is said to be the Fourier transform of f. It is well known that the mapping $\mathcal{F}: f \to \hat{f}$ defined by (3.1) extends to a unitary transformation on L^2.

Fourier transform $\mathcal{F}$ provides a unitary equivalence between the two sets of projection operators introduced above: A Paley–Wiener theorem asserts that $\mathcal{F}(Q_\pm(L^2)) = P_\mp(L^2)$, $Q_\pm(L^2) = \mathcal{F}^{-1}(P_\mp(L^2))$, $\mathcal{F}^{-1}(Q_\pm(L^2)) = P_\pm(L^2)$, and $Q_\pm(L^2) = \mathcal{F}(P_\pm(L^2))$.

A remarkable theorem of van Winter[9] states that a function in $\mathcal{H}^2_\pm$ is completely determined by its values on $(0,\infty)$ [or on $(-\infty,0)$]. Further, the restriction of $\mathcal{H}^2_\pm$-functions to $(0,\infty)$ form a dense subspace of L^2_+. Similarly, their restrictions to $(-\infty,0)$ are dense in L^2_-. Transcribed to our notation, the theorem states that the L^2-inclusions $Q_+P_\pm(L^2) \subset Q_+(L^2)$ and $Q_-P_\pm(L^2) \subset Q_-(L^2)$ are dense.

Proposition 3.1: The functions $-iP_+(L^2_-)$ form a dense subspace of $\mathcal{H}^2_+$. Similarly, the functions $iP_-(L^2_-)$ are dense in $\mathcal{H}^2_-$.

Proof: Suppose $f_0 \in \mathcal{H}^2_+$, and ϵ, any positive number. For any $h \in \mathcal{H}^2_-$, we have $P_+(f_0 + h) = P_+f_0 = f_0$. Now, by the above mentioned theorem of van Winter, we can choose $h \in \mathcal{H}^2_-$ such that

$$\|-if_0 + h\|_+ < \frac{\epsilon}{2}.$$

For such an h, let $\tilde{g} = Q_-(if_0 - h)$. Then,

$$\begin{aligned}\|-iP_+\tilde{g} - f_0\| &= \|P_+(\tilde{g} - if_0)\| = \|P_+(\tilde{g} - if_0 + h)\| \leqslant \|\tilde{g} - if_0 + h\| \\ &= (\|\tilde{g} - if_0 + h\|^2_- + \|-if_0 + h\|^2_+)^{1/2} = \|-if_0 + h\|_+ < \frac{\epsilon}{2}.\end{aligned} \tag{3.2}$$

Thus, $-iP_+(L^2_-)$ is dense in $\mathcal{H}^2_+$. The same argument shows that $iP_-(L^2_-)$ is dense in $\mathcal{H}^2_-$. □

This proposition shows that the denseness of the inclusions $Q_+P_\pm(L^2) \subset Q_+(L^2)$ and $Q_-P_\pm(L^2) \subset Q_-(L^2)$, i.e., van Winter's theorem, implies the denseness of the complementary inclusions $P_+Q_\pm(L^2) \subset P_+(L^2)$ and $P_-Q_\pm(L^2) \subset P_-(L^2)$.

Definitions: Let $\mathcal{S}$ be the space of Schwartz functions on $\mathbb{R}$. That is, if $f \in \mathcal{S}$, then we have $f \in C^\infty(\mathbb{R})$ and $\lim_{x\to\pm\infty} x^n f(x) = 0$ for $n = 0,1,2,\ldots$. It is well known that $\mathcal{S}$ is dense L^2. There exists a locally convex topology under which $\mathcal{S}$ becomes a Fréchet space, and the Fourier transform $\mathcal{F}$ defined by (3.1) is a homeomorphism on this Fréchet space. [This topology is defined by the countable family of norms $\|f\|_{mn} = \sup_{x\in\mathbb{R}}|x^m(d^n/dx^n)f(x)|$, where m and n are positive integers. Equivalently, the norms $\|f\|_n = \|(M^2 + D^2 + I)^n f\|$ can be used. See also (3.5).] Further,

$\mathcal{S}_\pm$, the space of $\mathcal{S}$-functions with the support in $(0,\pm\infty)$ is dense in $L^2_\pm$. The above mentioned Paley–Wiener theorem implies that $\mathcal{F}(\mathcal{S}_\mp)=\mathcal{S}\cap\mathcal{H}^2_\pm$ and that $\mathcal{S}\cap\mathcal{H}^2_\pm$ is dense in $\mathcal{H}^2_\pm$.

Let $\mathcal{N}$ be the subspace of Schwartz functions with vanishing moments of all orders. That is, if $f\in\mathcal{N}$, then $f\in\mathcal{S}$ and $\int_{-\infty}^{\infty}x^n f(x)dx=0$ for $n=0,1,2,\ldots$. Let $\mathcal{N}_\pm$ be the space of $\mathcal{N}$-functions supported in $(0,\pm\infty)$. It is shown in the Appendix that $\mathcal{N}_\pm$ is dense in $L^2_\pm$. Since $\mathcal{N}_-\oplus\mathcal{N}_+\subset\mathcal{N}$, it then follows that $\mathcal{N}$ is dense in L^2.

The unitarity of the Fourier transform $\mathcal{F}$ implies that the image of $\mathcal{N}$ under $\mathcal{F}$ is dense in L^2. Let this space be denoted by $\mathcal{M}$. A function f in $\mathcal{M}$, being the Fourier transform of a function in $\mathcal{N}$, is smooth, rapidly decaying and has vanishing derivatives of all orders at the origin. Further, from the Appendix, it is clear that $\mathcal{N}_-\oplus\mathcal{N}_+\subset\mathcal{N}\cap\mathcal{M}$, and so, the space $\mathcal{N}\cap\mathcal{M}$ is dense in L^2. It is also straightforward to verify that $\mathcal{N}\cap\mathcal{M}$ is a closed subspace of $\mathcal{S}$. Its invariance under the Fourier transform is an interesting property.

Proposition 3.2: $\mp iP_\pm(\mathcal{N}_-)$ *is dense in* $\mathcal{S}\cap\mathcal{H}^2_\pm$.

Proof: Let f_0, $\tilde{g}$ and ϵ be as in the proof of Proposition 3.1. The denseness of $\mathcal{N}_-$ in L^2_- (see the Appendix) allows us to choose $g\in\mathcal{N}_-$ such that

$$\|g-\tilde{g}\|<\frac{\epsilon}{2}.$$

Thus,

$$\|-iP_+g-f_0\|\leqslant\|-iP_+(g-\tilde{g})\|+\|-iP_+\tilde{g}-f_0\|<\frac{\epsilon}{2}+\frac{\epsilon}{2}=\epsilon.$$

It only remains to show that $-iP_+g\in\mathcal{S}$. To that end, recall that the Fourier transform of the Hilbert transform of a function satisfies the equality $(\mathbb{H}f)\,(y)=-i\,(y/|y|)\hat{f}(y)$. Therefore,

$$(-iP_+g)\,(y)=\left(\frac{1}{2}(\mathbb{H}-iI)g\right)(y)=-\frac{i}{2}\frac{y}{|y|}\hat{g}(y)-\frac{i}{2}\hat{g}(y). \tag{3.3}$$

Since $g\in\mathcal{N}$, $\hat{g}$ has vanishing derivatives of all orders at $y=0$. Thus, $(-iP_+g)$, and therewith also $(-iP_+g)$, belongs to $\mathcal{S}$.

The same argument proves the denseness of $iP_-(\mathcal{N}_-)$ in $\mathcal{S}\cap\mathcal{H}^2_-$. □

The proof of Proposition 3.2 also implies that $\mp iP_\pm(\mathcal{N}_+)$ is dense in $\mathcal{S}\cap\mathcal{H}^2_\pm$.

Remark: Notice that $(-iP_+g)$ is in fact an element of $\mathcal{M}$. This means that $(-iP_+g)\in\mathcal{N}\cap\mathcal{H}^2_+$ whenever $g\in\mathcal{N}$. That is, $\mathcal{N}$ has the interesting property that it is invariant under the Hilbert transform $\mathbb{H}$. Furthermore, it follows that $\mathcal{N}\cap\mathcal{H}^2_+$ is dense in $\mathcal{H}^2_+$, and therefore also in $\mathcal{S}\cap\mathcal{H}^2_+$.

Definitions: From Proposition 3.2 it follows that $-iP_+(\mathcal{N}_-)\oplus iP_-(\mathcal{N}_-)$ is a dense subspace of L^2. If f is an element of this subspace, then for unique functions $g,h\in\mathcal{N}_-$,

$$f=-iP_+g+iP_-h. \tag{3.4}$$

We may introduce a locally convex topology on $-iP_+(\mathcal{N}_-)\oplus iP_-(\mathcal{N}_-)$ by defining a family of norms $\|f\|_n$ for f:

$$\|f\|^2_n=\|-iP_+g\|^2_n+\|iP_-h\|^2_n+\|iP_-g\|^2_n+\|-iP_+h\|^2_n. \tag{3.5}$$

The norms on the right hand side of (3.5) refer to the topology that $-iP_+(\mathcal{N}_-)\oplus iP_-(\mathcal{N}_-)$ inherits as a subspace of $\mathcal{S}$. For instance, $\|-iP_+g\|_n$ can be iteratively defined by

$$\|-iP_+g\|^2_{n+1}=\|M(-iP_+g)\|^2_n+\|D(-iP_+g)\|^2_n+\|-iP_+g\|^2_n,\quad n=0,1,2,\ldots, \tag{3.6}$$

where M and D are the multiplication and differentiation operators defined in (2.5) and $\|\cdot\|_0$ is the L^2-norm. The topology induced on $\mathcal{S}$ by the norms of (3.6) is equivalent to the one given by the more customary norms $\|f\|_{mn}=\sup_{x\in\mathbb{R}}|x^m(d^n/dx^n)f(x)|$.

Let Ψ be the direct sum space $-iP_+(\mathcal{N}_-)\oplus iP_-(\mathcal{N}_-)$ endowed with the topology given by the norms (3.5).

Proposition 3.3: Ψ is a nuclear Fréchet space.

Proof: Local convexity and metrizability of Ψ are obvious from (3.5). To see that Ψ is complete, suppose that $\{f_i\}$ is a Cauchy sequence Ψ. Since each f_i has the decomposition

$$f_i=-iP_+g_i+iP_-h_i, \tag{3.7}$$

for some $g_i,h_i\in\mathcal{N}_-$, we obtain four Cauchy sequences: $\{-iP_+g_i\}$ and $\{-iP_+h_i\}$ in $\mathcal{S}\cap\mathcal{H}_+^2$; $\{iP_-g_i\}$ and $\{iP_-h_i\}$ in $\mathcal{S}\cap\mathcal{H}_-^2$. Since these two spaces are complete, we conclude that there exist functions $g,h\in\mathcal{S}\cap\mathcal{H}_+^2$ and $\tilde{g},\tilde{h}\in\mathcal{S}\cap\mathcal{H}_-^2$ such that

$$\begin{aligned} -iP_+g_i&\to g, \qquad -iP_+h_i\to h,\\ iP_-g_i&\to\tilde{g}, \qquad iP_-h_i\to\tilde{h}. \end{aligned} \tag{3.8}$$

The convergences in (3.8) are of course with respect the $\mathcal{S}$-topology (3.6). Therefore, the functions $(-iP_+g_i)$ converge to g point-wise (and similarly for the other three sequences). Next, notice that the two functions $-iP_+f$ and iP_-f obtained from any $f\in\mathcal{N}_-$ coincide on $(0,\infty)$: $(-iP_+f)(x)=(\mathbb{H}f)(x)=(iP_-f)(x)$ for $x\in(0,\infty)$. Thus, $g(x)=\tilde{g}(x)$ and $h(x)=\tilde{h}(x)$ for $x\in(0,\infty)$. Now let $g_0=i(g-\tilde{g})$, $h_0=i(h-\tilde{h})$, and

$$f_0=-iP_+g_0+iP_-h_0. \tag{3.9}$$

The function f_0 is an element of Ψ. The convergences (3.8) imply that $f_i\to f_0$. Hence, Ψ is a Fréchet space.

It is well-known that $\mathcal{S}$ is a nuclear space. Since every subspace of a nuclear space is nuclear, $-iP_+(\mathcal{N}_-)\oplus iP_-(\mathcal{N}_-)$ is nuclear. It then follows that Ψ is a nuclear space as its topology (3.5) is derived from the nuclear topology (3.6) of $\mathcal{S}$. □

Let $\Psi^\times$ be the space of continuous antilinear functionals on Ψ, endowed with the weak*-topology. Then, the triplet of spaces,

$$\Psi\subset L^2\subset\Psi^\times, \tag{3.10}$$

constitutes a rigged Hilbert space.

Remark: From the proof of Proposition 3.3, in particular from the coincidence of the functions $-iP_+f$ and iP_-f on $(0,\infty)$ for any $f\in\mathcal{N}_-$, it follows that the elements of Ψ do not vanish on any subset of $(0,\infty)$ with nonzero (finite) measure. In fact, this property could have been used to define the space Ψ. Furthermore, if f_+ is the L^2_+-function obtained from some $f\in\Psi$ by $f_+=Q_+f$, then it follows that f_+ extends to both a unique function in $\mathcal{N}\cap\mathcal{H}_+^2\subset\mathcal{S}\cap\mathcal{H}_+^2$ and a unique function in $\mathcal{N}\cap\mathcal{H}_-^2\subset\mathcal{S}\cap\mathcal{H}_-^2$. That is, $Q_+(\Psi)\subset\Phi_+\cap\Phi_-$, where $\Phi_+=Q_+(\mathcal{S}\cap\mathcal{H}_+^2)$ and $\Phi_-=Q_+(\mathcal{S}\cap\mathcal{H}_-^2)$, the spaces defined in Refs. 4 and 5 in their study of scattering and time asymmetric quantum mechanics. The denseness of Ψ in L^2 shows that [$Q_+(\Psi)$ and thus also] the intersection $\Phi_+\cap\Phi_-$ is dense in L^2_+, extending the result in Ref. 5 that it is nontrivial.

B. Representation of $S_1(0)$ in Ψ

Proposition 3.4: The restriction of U to $\mathcal{S}$, where U is the continuous unitary representation of G given in (2.4)*, yields a differentiable representation of G in $\mathcal{S}$.*

Proof: From the definition (2.4), it follows directly that $\mathcal{S}$ remains invariant under all $U(\xi)$, $\xi\in G$. Then, direct computations show,[10] for all $f\in\mathcal{S}$ and $n=0,1,2,\ldots$,

$$\|U(\boldsymbol{\xi})f\|_n \leqslant (1+\xi_1^2+\xi_2^2)^{n/2}\|f\|_n \tag{3.11}$$

and

$$\begin{aligned}
&\lim_{\xi_1\to 0}\left\|\left(\frac{U((\xi_1,0,0))-I}{\xi_1}-D\right)f\right\|_n=0,\\
&\lim_{\xi_2\to 0}\left\|\left(\frac{U((0,\xi_2,0))-I}{\xi_2}-M\right)f\right\|_n=0,\\
&\lim_{\xi_3\to 0}\left\|\left(\frac{U((0,0,\xi_3))-I}{\xi_3}-iI\right)f\right\|_n=0,
\end{aligned} \tag{3.12}$$

where the norms $\|\cdot\|_n$ are those defined in (3.6). This proves that $U|_{\mathcal{S}}$ is a differentiable representation of G. □

Remark: Equations (3.12) show that the $\mathcal{S}$-generators of the representation $U|_{\mathcal{S}}$ coincide on $\mathcal{S}$ with the L^2-generators of U. This has an interesting implication for the rigged Hilbert formulation of quantum physics in that, just as in the conventional Hilbert space theory, the concept of an observable has an interpretation as the infinitesimal form of a symmetry (or asymmetry/semigroup) transformation.

Let us next consider the action of U on the elements of Ψ.

Proposition 3.5: The restriction of U to Ψ yields a nontrivial differentiable representation of $S_1(0)$ in Ψ.

Proof: If Ψ is invariant under $U(\boldsymbol{\xi})$, $\boldsymbol{\xi}\in S_1(0)$, then it follows from the topology (3.5) and Proposition 3.4 that $U|_{\Psi}$ furnishes a differentiable representation of $S_1(0)$. Therefore, we must simply show that $U(\boldsymbol{\xi})$, $\boldsymbol{\xi}\in S_1(0)$, leaves Ψ invariant and that the resulting semigroup representation does not extend in Ψ to a representation of G or a subgroup thereof. To that end, let $f\in\Psi$. Then, there exist unique functions g and h in $\mathcal{N}_-$ such that $f=-iP_+g+iP_-h$, and

$$\begin{aligned}
U((\xi_1,0,\xi_3))f &= U((\xi_1,0,\xi_3))(-iP_+g)+U((\xi_1,0,\xi_3))iP_-h\\
&= -iP_+U((\xi_1,0,\xi_3))g+iP_-U((\xi_1,0,\xi_3))h,
\end{aligned} \tag{3.13}$$

where the second equality follows from the commutativity of translations with the Hilbert transform: $U((\xi_1,0,\xi_3))\mathbb{H}=\mathbb{H}U((\xi_1,0,\xi_3))$.

From the construction of $\mathcal{N}_-$ (the Appendix), it is clear that $U((\xi_1,0,\xi_3))g\in\mathcal{N}_-$ and $U((\xi_1,0,\xi_3))h\in\mathcal{N}_-$ if $\xi_1\geqslant 0$, or, equivalently, if $(\xi_1,0,\xi_3)\in S_1(0)$. That is, Ψ is invariant under the operator semigroup $U((\xi_1,0,\xi_3))$, $\xi_1\geqslant 0$. Furthermore, from the Appendix it is also clear that for any $\xi_1<0$, there exist functions f in $\mathcal{N}_-$ such that $U((\xi_1,0,\xi_3))f\notin\mathcal{N}_-$. Thus, the semigroup representation $U(\boldsymbol{\xi})$, $\boldsymbol{\xi}\in S_1(0)$ in Ψ does not extend to a representation of the whole of G or even the subgroup $\{(\xi_1,0,\xi_3):\ \xi_1,\xi_3\in\mathbb{R}\}$. □

IV. A DIFFERENTIABLE REPRESENTATION OF $S_2(0)$

As a corollary to the construction carried out in Sec. III, we can obtain a rigged Hilbert space $\tilde{\Psi}\subset L^2\subset\tilde{\Psi}^\times$ such that $\tilde{\Psi}$ reduces the continuous unitary representation of G given by (2.4) to a differentiable representation of subsemigroup $S_2(0)$ defined in (2.3). This can be easily achieved by letting $\tilde{\Psi}$ be the Fourier transform $\mathcal{F}(\Psi)$ of the nuclear Fréchet space Ψ constructed in the above section. Since $\mathcal{F}$ is a unitary mapping on L^2, it follows that the triad,

$$\tilde{\Psi}\subset L^2\subset\tilde{\Psi}^\times, \tag{4.1}$$

is a rigged Hilbert space. The topology on $\tilde{\Psi}$ can be induced from the topology of Ψ via the Fourier transform. That is, if $\varphi \in \tilde{\Psi}$, then $\varphi = \hat{f}$ for a unique $f \in \Psi$, and a locally convex nuclear topology can be defined on $\tilde{\Psi}$ by way of the norms

$$\|\varphi\|_n = \|f\|_n, \tag{4.2}$$

where $\|f\|_n$ are the norms in Ψ defined by (3.5).

It is well known that $\mathcal{F}$ (and $\mathcal{F}^{-1}$) establishes a unitary equivalence between the operators $U((\xi_1,0,\xi_3))$ and $U((0,\xi_1,\xi_3))$, i.e., $\mathcal{F}\circ U((\xi_1,0,\xi_3)) = U((0,\xi_1,\xi_3))$ and $U((\xi_1,0,\xi_3)) = \mathcal{F}^{-1} \circ U((0,\xi_1,\xi_3))$. It thus follows that $\tilde{\Psi}$ reduces the unitary representation U of G in L^2 given by (2.4) to a nontrivial differentiable [with respect to the topology given by (4.2)] representation of $S_2(0)$.

It is perhaps worthwhile to take a closer look at the properties of the functions in $\tilde{\Psi}$. Each such function φ is the Fourier transform of a function in Ψ, i.e.,

$$\varphi = (-iP_+ g) + (iP_- h), \tag{4.3}$$

for unique functions g and h in $\mathcal{N}_-$. From (3.3), we then have

$$\varphi(x) = -\frac{i}{2}\left(1 + \frac{x}{|x|}\right)\hat{g}(x) + \frac{i}{2}\left(1 - \frac{x}{|x|}\right)\hat{h}(x). \tag{4.4}$$

This means that the space $\tilde{\Psi}$ is the direct sum of the restrictions of $\mathcal{F}(\mathcal{N}_-)$ to $(0,\infty)$ and to $(-\infty,0)$. Since $\mathcal{F}(\mathcal{N}_-) = \mathcal{M} \cap \mathcal{H}_+^2$, we have

$$\tilde{\Psi} = Q_+(\mathcal{M} \cap \mathcal{H}_+^2) \oplus Q_-(\mathcal{M} \cap \mathcal{H}_+^2). \tag{4.5}$$

The topology of $\tilde{\Psi}$ can also be defined by way of the norms

$$\|\varphi\|_n^2 = \|\hat{g}\|_n^2 + \|\hat{h}\|_n^2, \tag{4.6}$$

where $\hat{g}$ and $\hat{h}$ are as in (4.4) and the norms on the right hand side of (4.6) are as in (3.6). This topology is clearly equivalent to one given by the norms (4.2). In this light, the differentiable representation of $S_2(0)$ in $\tilde{\Psi}$ is just that which is induced from its differentiable representation in $\mathcal{M} \cap \mathcal{H}_+^2$.

V. SUBSEMIGROUPS S_1, S_2 AND S_3

Notice that the centrally significant feature of the preceding constructions of two rigged Hilbert spaces is the existence of dense subspaces of the Hilbert space which remain invariant under the differential $dU|_{\mathbf{0}}$ but not the representation U. Once a subspace invariant under $dU|_{\mathbf{0}}$ and $U(\boldsymbol{\xi})$, $\boldsymbol{\xi} \in S_1(0)$, or $dU|_{\mathbf{0}}$ and $U(\boldsymbol{\xi})$, $\boldsymbol{\xi} \in S_2(0)$, was identified, it was possible to construct the rigged Hilbert space (3.10) or (4.1).

Such dense subspaces can be constructed also for the operator semigroups $\{U(\boldsymbol{\xi}): \boldsymbol{\xi} \in S_1\}$, $\{U(\boldsymbol{\xi}): \boldsymbol{\xi} \in S_2\}$ and $\{U(\boldsymbol{\xi}): \boldsymbol{\xi} \in S_3\}$. It is interesting to notice, however, that any subspace which remains invariant under the operator semigroup $\{U(\boldsymbol{\xi}): \boldsymbol{\xi} \in S_4\}$ will be invariant also under $\{U(\boldsymbol{\xi}): \boldsymbol{\xi} \in S_3\}$. This means that the general method implied by the preceding two constructions (by way of dense subspaces invariant under the relevant operator semigroup) does not lead to a rigged Hilbert space for a nontrivial differentiable representation of the subsemigroup S_4, i.e., such a representation naturally extends to a representation of S_3.

A dense subspace of L^2 which is invariant under the operator Lie algebra $dU|_{\mathbf{0}}$ and the semigroup $U(S_1)$ can be easily obtained from the Ψ of Sec. III. It was shown that Ψ remains

invariant under the operator semigroup $\{U(\boldsymbol{\xi}):\ \boldsymbol{\xi}\in S_1(0)\}$. However, Ψ is not invariant under any operator such as $U(\boldsymbol{\xi})$ where $\boldsymbol{\xi}=(0,\xi_2,\xi_3)$. This is easily seen when either the Hardy class property or the vanishing moment (in $\mathcal{N}$) property of the functions in Ψ is considered. For instance, for an arbitrary element $f\in\Psi$, the integrals $\int_{-\infty}^{\infty}x^n f(x)dx=0$ for $n=0,1,2,\ldots$, but the integrals of the transformed element $U(\boldsymbol{\xi})f$, $\int_{-\infty}^{\infty}x^n(U((0,\xi_2,\xi_3))f)(x)dx = e^{i\xi_3}\int_{-\infty}^{\infty}x^n e^{i\xi_2 x}f(x)dx$ do not vanish for $n=0,1,2,\ldots$, when $\xi_2\neq 0$, i.e., $U((0,\xi_2,\xi_3))f\notin\Psi$. Therefore, let $\Psi_{\boldsymbol{\xi}}=U((0,\xi_2,\xi_3))(\Psi)$. Unitarity of the operators $U((0,\xi_2,\xi_3))$ implies that $\Psi_{\boldsymbol{\xi}}$ is dense in L^2. Thus, a dense subspace of L^2 which remains invariant under the operator semigroup $U(S_1)$ can be obtained by setting

$$\Psi_1=\cup_{\boldsymbol{\xi}\in S_1}\Psi_{\boldsymbol{\xi}}, \tag{5.1}$$

and, starting from the dense subspace (5.1), a rigged Hilbert space may be built as in Sec. III for a differentiable representation of the semigroup S_1.

In complete analogy to (5.1), we can construct a dense subspace invariant under the operator semigroup $\{U(\boldsymbol{\xi}):\ \boldsymbol{\xi}\in S_2\}$, starting from the space $\tilde{\Psi}$ of Sec. IV.

As is evident from the vector space $\mathcal{N}\cap\mathcal{M}$ introduced in Sec. III, there also exist dense subspaces of L^2 which are invariant under the operator Lie algebra $dU|_{\mathbf{0}}$ but not under any nontrivial $U(\boldsymbol{\xi})$, i.e., under any $U(\boldsymbol{\xi})$ where $\boldsymbol{\xi}$ is a noncentral element of G. Now consider the vector space,

$$\Psi_3=\cup_{\boldsymbol{\xi}\in S_3}U(\boldsymbol{\xi})(\mathcal{N}\cap\mathcal{M}). \tag{5.2}$$

The unitarity of $U(\boldsymbol{\xi})$ and the denseness of $\mathcal{N}\cap\mathcal{M}$ imply that Ψ_3 is dense in L^2. By construction, Ψ_3 is invariant under both $dU|_{\mathbf{0}}$ and the operator semigroup $\{U(\boldsymbol{\xi}):\boldsymbol{\xi}\in S_3\}$, but not under any $U(\boldsymbol{\xi})$ with $\boldsymbol{\xi}\notin S_3$. Thus, a rigged Hilbert space furnishing a nontrivial differentiable representation of S_3 may be built from the dense subspace Ψ_3.

VI. CONCLUDING REMARKS—JUXTAPOSITION WITH TIME ASYMMETRIC QUANTUM THEORY

In this paper we have investigated how differentiable representations of certain subsemigroups of the Weyl–Heisenberg group may be obtained in rigged Hilbert spaces. These representations were induced from a given continuous unitary representation of the Weyl–Heisenberg group G in the Hilbert space of L^2-functions on $\mathbb{R}$. As stated earlier, the construction of the particular rigged Hilbert space, which we denote here as in Definition 1.1 generically by $\Phi\subset\mathcal{H}\subset\Phi^{\times}$, begins with the identification of a dense subspace of L^2 which stays invariant under the action of the L^2-differential $dU|_{\mathbf{0}}$ and the relevant operator subsemigroup $\{U(\boldsymbol{\xi}):\ \boldsymbol{\xi}\in S_i\}$. In order to make certain that the ensuing differentiable representation is nontrivial, i.e., that it does not extend to a representation of the group G or a subgroup thereof, it was necessary to verify that the dense subspace invariant for the subsemigroup $\{U(\boldsymbol{\xi}):\ \boldsymbol{\xi}\in S_i\}$ does not remain invariant under certain $U(\boldsymbol{\xi})$ with $\boldsymbol{\xi}\notin S_i$. Once such a dense subspace was identified, it was possible to introduce a topology on it, by means of the enveloping operator algebra of $dU|_{\mathbf{0}}$, so as to obtain a differentiable representation of S_i in the inner space Φ of the rigged Hilbert space. With respect to this topology, elements of the enveloping algebra of $dU|_{\mathbf{0}}$ become continuous as operators in Φ. Moreover, as seen from (3.12), the elements of the Φ-differential of the semigroup representation $U(S_i)$ in Φ coincide with the corresponding elements of the $\mathcal{H}$-differential $dU|_{\mathbf{0}}$ of the group representation $U(G)$ in the Hilbert space $\mathcal{H}$.

In a definite technical sense, the semigroup time evolution of the rigged Hilbert space formulation of quantum mechanics developed in Refs. 4–6 has at its heart the Weyl–Heisenberg subsemigroups S_1 and S_2 of (2.3). Recall first that the rigged Hilbert spaces of Hardy class functions constructed in Refs. 4–6 are

$$\mathcal{S}\cap\mathcal{H}^2_+|_+\subset L^2_+\subset(\mathcal{S}\cap\mathcal{H}^2_+|_+)^\times,\quad \mathcal{S}\cap\mathcal{H}^2_-|_+\subset L^2_+\subset(\mathcal{S}\cap\mathcal{H}^2_-|_+)^\times, \tag{6.1}$$

where $|_+$ indicates the restrictions of the $\mathcal{S}\cap\mathcal{H}^2_\pm$-functions to the half line $(0,\infty)$. From the above mentioned van Winter's theorem,[9] a function $f_\pm$ in $\mathcal{S}\cap\mathcal{H}^2_\pm|_+$ extends to a unique function $f^\pm$ in $\mathcal{S}\cap\mathcal{H}^2_\pm$. This property is used in Refs. 4, 5 to define a nuclear Fréchet topology on $\mathcal{S}\cap\mathcal{H}^2_\pm|_+$:

$$\|f_\pm\|_n=\|f^\pm\|_n, \tag{6.2}$$

where the norms on the right hand side refer to the Schwartz space topology (3.5) the space $\mathcal{S}\cap\mathcal{H}^2_\pm$ inherits from $\mathcal{S}^2$. [The countable family of norms used to characterize $\mathcal{S}$ in Refs. 4, 5 is not that of (3.5) but the more customary $\|f\|_n=\|(M^2+D^2+I)^n f\|_0$.] The continuous unitary representation of $\mathbb{R}$ given in L^2_+ by $(U(t)f)(E)=e^{iEt}f(E)$ reduces to a differentiable representation of $(0,\pm\infty)$ in $\mathcal{S}\cap\mathcal{H}^2_\pm|_+$. These semigroup representations can be related to the representations of S_1^{-1} and S_2 of (2.3) in the following way.

Observe that the mapping (2.4) yields a continuous representation of S_1^{-1} in L^2_+ by contractions:

$$(U(\boldsymbol{\xi})f)(x)=e^{i\xi_3}e^{ix\xi_2}f(x+\xi_1),\quad \boldsymbol{\xi}\in S_1^{-1},\ f\in L^2_+, \tag{6.3}$$

and $\|U(\boldsymbol{\xi})f\|_+\leqslant\|f\|_+$.

Further, the multiplication subgroup $\{(0,\xi_2,\xi_3):\xi_2,\xi_3\in\mathbb{R}\}$ of S_1^{-1} is unitarily represented by U in L^2_+:

$$(U((0,\xi_2,\xi_3))f)(x)=e^{i\xi_3}e^{ix\xi_2}f(x). \tag{6.4}$$

The dense subspace $\mathcal{S}_+$ remains invariant under both the operator semigroup $\{U(\boldsymbol{\xi}):\boldsymbol{\xi}\in S_1^{-1}\}$ and the basis elements M, D, I of the differential $dU|_{\mathbf{0}}$. Moreover, $\mathcal{S}_+$, a closed subspace of $\mathcal{S}$, is a nuclear Fréchet space, and therewith the triplet

$$\mathcal{S}_+\subset L^2_+\subset\mathcal{S}_+^\times \tag{6.5}$$

constitutes a rigged Hilbert space. The continuous representation (6.3) of S_1^{-1} in L^2_+ yields a differentiable representation of the semigroup in $\mathcal{S}_+$.

The Fourier transform (3.1) establishes a unitary equivalence between (6.5) and the rigged Hilbert space,

$$\mathcal{S}\cap\mathcal{H}^2_-\subset\mathcal{H}^2_-\subset(\mathcal{S}\cap\mathcal{H}^2_-)^\times, \tag{6.6}$$

while its inverse $\mathcal{F}^{-1}$ maps (6.5) unitarily onto

$$\mathcal{S}\cap\mathcal{H}^2_+\subset\mathcal{H}^2_+\subset(\mathcal{S}\cap\mathcal{H}^2_+)^\times. \tag{6.7}$$

Since $\mathcal{F}$ is a homeomorphism on $\mathcal{S}$, $\mathcal{S}\cap\mathcal{H}^2_\pm$ are closed subspaces of $\mathcal{S}$. They are thus nuclear Fréchet spaces with respect to the Schwartz space topology (3.5).

The mappings from (6.5) onto (6.6) and (6.7) given by $\mathcal{F}$ and $\mathcal{F}^{-1}$ also transform the representation of S_1^{-1} in (6.5) to a representation of S_2^{-1} and S_2 in (6.6) and (6.7), respectively. In particular,

$$\begin{aligned}\mathcal{F}U(\boldsymbol{\xi})\mathcal{F}^{-1}&=U((-\xi_2,\xi_1,\xi_3-\xi_1\xi_2)),\\ \mathcal{F}^{-1}U(\boldsymbol{\xi})\mathcal{F}&=U((\xi_2,-\xi_1,\xi_3-\xi_1\xi_2)),\end{aligned} \tag{6.8}$$

and when $\boldsymbol{\xi}\in S_1^{-1}$, the contractions $U((-\xi_2,\xi_1,\xi_3-\xi_1\xi_2))$ and $U((\xi_2,-\xi_1,\xi_3-\xi_1\xi_2))$ provide continuous representations of S_2^{-1} and S_2 in $\mathcal{H}^2_-$ and $\mathcal{H}^2_+$, respectively. Further, in the nuclear Fréchet spaces $\mathcal{S}\cap\mathcal{H}^2_-$ and $\mathcal{S}\cap\mathcal{H}^2_+$ the mappings (6.8) furnish differentiable representations of the

semigroups S_2 and S_2^{-1}, respectively. In particular, the differentiation operator D generates the one parameter group of translations in both $\mathcal{S}\cap\mathcal{H}_-^2$ and $\mathcal{S}\cap\mathcal{H}_+^2$, whereas the multiplication operator M generates only a one parameter semigroup, one in $\mathcal{S}\cap\mathcal{H}_-^2$ for negative ξ_1 and another in $\mathcal{S}\cap\mathcal{H}_+^2$ for positive ξ_1.

Consider the subsemigroup $S_2(0)$ of S_2. As just seen, it is represented differentiably by the mapping (2.4), $\boldsymbol{\xi}\to U(\boldsymbol{\xi})$, in $\mathcal{S}\cap\mathcal{H}_+^2$:

$$(U(\boldsymbol{\xi})f)(x)=e^{i\xi_3}e^{ix\xi_2}f(x),\quad \boldsymbol{\xi}\in S_2(0),\ f\in\mathcal{S}\cap\mathcal{H}_+^2. \tag{6.9}$$

The relation (6.8) and the description following it shows that this representation of $\mathcal{S}_2(0)$ in $\mathcal{S}\cap\mathcal{H}_+^2$ is nontrivial. Now, since the mapping $\mathcal{S}\cap\mathcal{H}_+^2\to\mathcal{S}\cap\mathcal{H}_+^2|_+$ is one-to-one and onto Refs. 5, 9, it follows that (6.9) induces a non-trivial differentiable representation of $S_2(0)$ in $\mathcal{S}\cap\mathcal{H}_+^2|_+$.

Observe next that the differentiable representation (6.9) of the subsemigroup $S_2(0)$ in $\mathcal{S}\cap\mathcal{H}_+^2|_+$ can be *identified* with the unitary representation (6.4) of the subgroup $\{\boldsymbol{\xi}=(0,\xi_2,\xi_3):\ \xi_2,\xi_3\in\mathbb{R}\}$ in L_+^2. Once this identification is made, we conclude that the continuous unitary representation of $\mathbb{R}$ given by (6.4),

$$(U((0,\xi_2,0))f)(x)=e^{ix\xi_2}f(x), \tag{6.10}$$

in L_+^2 is reduced by the subspace $\mathcal{S}\cap\mathcal{H}_+^2|_+$ to a representation of the half line $(0,\infty)$. This is the semigroup that is interpreted in Refs. 4–6 as governing the asymmetric time evolution of outstates and the decaying Gamow vectors. We see here that it is induced from a continuous representation of the Weyl–Heisenberg semigroup S_2 in $\mathcal{H}_+^2$. The latter representation, in turn, is equivalent to the continuous representation of the semigroup S_1^{-1} in L_+^2, given by (6.3). In this sense, it can be said that the semigroup time evolution of the quantum theory developed in Refs. 4–6, where the Hilbert space L_+^2 consists of the square integrable functions defined on the energy spectrum $(0,\infty)$ and ξ_2 is interpreted as time, t, is obtained from the semigroup of translations in L_+^2 given by (6.3), $(U(\xi)f)(E)=f(E-\xi),\ \xi\in(0,\infty)$.

ACKNOWLEDGMENT

We acknowledge the financial support from the Welch Foundation.

APPENDIX: DENSENESS OF $\mathcal{N}_+$ IN L_+^2

Proposition A.1: $\mathcal{N}_+$ is dense in L_+^2.

Proof (Ref. 11): We prove this assertion by showing that any compactly supported C^∞-function in L_+^2 can be approximated by functions in $\mathcal{N}_+$. Since the class of C^∞-functions with compact support is dense in L_+^2, the proposition follows.

Let g be a compactly supported smooth function in L_+^2 and ϵ, any positive number. Without loss of generality, let us assume that $\int_0^\infty g(x)dx\neq 0$, for otherwise we may choose a compactly supported smooth function arbitrarily close to g in the L^2-metric with this property. Now, suppose that there exists a family of compactly supported smooth functions f_k, with supports contained in, say (a_k,a_{k+1}), such that we have the following.

(1) The support of f_k is to the right of the support of f_{k-1} and disjoint from it; the support of f_0 is to the right of that of g.

(2) $\int_0^\infty x^i f_k(x)dx=0$, for $i=0,1,2,\ldots,k-1$.

(3) $\int_0^\infty x^k f_k(x)dx=-\int_0^\infty x^k(g+f_0+f_1+\cdots+f_{k-1})(x)dx$.

(4) $\|f_k\|<\epsilon/2^{k+1}a_{k+1}^k$.

If such a family $\{f_k\}$ can be found, then set

$$f=\sum_{k=0}^{\infty} f_k+g. \tag{A1}$$

The f is well defined since for each $0<x<\infty$ all but one f_k are zero.

Since the f_k have disjoint supports,

$$\int_{a_n}^{a_{n+1}} x^m \sum_{k=0}^{\infty} f_k(x)dx = \int_{a_n}^{a_{n+1}} \sum_{k=0}^{\infty} x^m f_k(x)dx = \int_{a_n}^{a_{n+1}} x^m f_n(x)dx = 0, \text{ for all } n>m, \quad \text{(A2)}$$

and so

$$\sum_{n=0}^{\infty} \left(\int_{a_n}^{a_{n+1}} \sum_{k=0}^{\infty} x^m f_k(x)dx \right) = \sum_{n=0}^{m} \left(\int_{a_n}^{a_{n+1}} \sum_{k=0}^{\infty} x^m f_k(x)dx \right) = \sum_{n=0}^{m} \int_{a_n}^{a_{n+1}} x^m f_n(x)dx. \quad \text{(A3)}$$

Therefore,

$$\int_0^{\infty} x^m f(x)dx = \int_0^{\infty} \left(\sum_{k=0}^{\infty} x^m f_k(x) + x^m g(x) \right) dx = \sum_{k=0}^{m} \int_0^{\infty} x^m f_k(x)dx + \int_0^{\infty} x^m g(x)dx = 0,$$
$$\text{for } m = 0,1,2,\ldots, \quad \text{(A4)}$$

where the above property (2) of the f_k is used in the last equality of (A2) and the property (3), in the last equality of (A4). Further, from the inequality (4), it is clear that $x^n f \in L^1((0,\infty))$. Since the functions f_k have increasing supports, it then follows that $f \in \mathcal{N}_+$.

Furthermore, from the disjointness of the supports and the property (4) above of the f_k, it follows readily that

$$\|g-f\| = \left\| \sum_{k=0}^{\infty} f_k \right\| = \left(\sum_{k=0}^{\infty} \|f_k\|^2 \right)^{1/2} \leqslant \left(\sum_{k=0}^{\infty} \frac{\epsilon^2}{2^{2k+2} a_{k+1}^{2k}} \right)^{1/2} < \epsilon, \quad \text{(A5)}$$

i.e., $\mathcal{N}_+$ is dense in L_+^2.

It remains to show that the C^∞ functions f_k can be chosen subject to the conditions (1)–(4) above. This can be done by induction. To that end, suppose the smooth functions $f_0,\ldots,f_{k-1}$ with their supports in $(a_0, a_1),\ldots,(a_{k-1}, a_k)$, respectively, have been aptly chosen. Assume further that the given smooth function is supported in $(0, a_0)$ with $a_0>1$. Define now a function f_k by setting

$$f_k(x) = \gamma_k \frac{d^k g}{dx^k} \left(\frac{a_0(x-a_k)}{a_{k+1}-a_k} \right). \quad \text{(A6)}$$

The function f_k is supported in (a_k, a_{k+1}), where a_{k+1} and the constant γ_k are to be chosen subject to the conditions (A10) and (A12) below.

From the definition (A6) it is clear that

$$\int_0^{\infty} x^i f_k(x)dx = 0, \quad \text{for } n = 0,1,2,\ldots,k-1 \quad \text{(A7)}$$

and

$$\int_0^{\infty} x^k f_k(x)dx = (-1)^k k! I \gamma_k \left(\frac{a_{k+1}-a_k}{a_0} \right)^{k+1}, \quad \text{(A8)}$$

where $I = \int_0^{\infty} g(x)dx$. Next, in accordance with condition (3) above, we require

$$\int_0^{\infty} x^k f_k(x)dx = \lambda, \quad \text{(A9)}$$

where $\lambda = -\int_0^\infty x^k(g(x)+f_0(x)+\cdots+f_{k-1}(x))dx$. Equalities (A8) and (A9) yield

$$\gamma_k = \frac{(-1)^k \lambda}{k! I}\left(\frac{a_0}{a_{k+1}-a_k}\right)^{k+1}. \tag{A10}$$

It remains only to choose a_{k+1}. By the definition (A6) of f_k and the inequality (4) on its L^2 norm, we have

$$\|f_k\| = |\gamma_k|\left(\frac{a_0}{a_{k+1}-a_k}\right)^{1/2}\left\|\frac{d^k g}{dx^k}\right\| < \frac{\epsilon}{2^{k+1}a_{k+1}^k}. \tag{A11}$$

Along with the relation (A10) above, we then observe that a_{k+1} is to be chosen subject to the inequality

$$\frac{(a_{k+1}-a_k)^{k+3/2}}{a_{k+1}^k} > \frac{|\lambda| 2^{k+1}}{\epsilon |I| k!} a_0^{k+3/2}\left\|\frac{d^k g}{dx^k}\right\|. \tag{A12}$$

By construction, $a_k > a_0 > 1$, and so it is clear that this inequality can be fulfilled by choosing a_{k+1} large enough. Once the a_{k+1} is picked out, the equation (A10) determines γ_k, and therewith the expression (A6) completely determines the function f_k. Thus, the functions f_k are simply the derivatives of the given smooth function g with their supports appropriately dilated and translated on the real axis, followed by a suitable overall scaling. □

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Erratum: Pseudo-Hermiticity for a class of nondiagonalizable Hamiltonians [J. Math. Phys. 43, 6343 (2002)]

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[DOI: 10.1063/1.1540714]

Recently, the authors of Ref. 1 used the framework provided in Ref. 2 to re-examine the consequences of pseudo-Hermiticity for the class of block-diagonalizable Hamiltonians introduced in Ref. 2. In doing so, they discovered that Theorem 2 of Ref. 2 did not hold, as they could find a counter-example. This theorem must be replaced with the following.

Theorem 2: Let H be as in Theorem 1 of Ref. 2. Then H is pseudo-Hermitian if and only if it is Hermitian with respect to an inner product $\langle\langle ,\rangle\rangle$ that supports a positive-semidefinite basis[3] including the eigenvectors of H. In particular, for every eigenvector ψ of H, $\langle\langle\psi|\psi\rangle\rangle\geqslant 0$; if the corresponding eigenvalue is real and nondefective (algebraic and geometric multiplicities are equal), $\langle\langle\psi|\psi\rangle\rangle>0$; otherwise $\langle\langle\psi|\psi\rangle\rangle=0$.

Proof: As shown in Ref. 2, pseudo-Hermiticity of H implies that H is Hermitian with respect to the inner product $\langle\langle ,\rangle\rangle_\eta$ with η given by Eq. (15) of Ref. 2 and $\sigma_{\nu_0,a}=1$. It is not difficult to check that indeed the basis vectors $|\psi_n,a,i\rangle$, constructed in Ref. 2, have the property that $\langle\langle\psi_n,a,i|\psi_n,a,i\rangle\rangle\geqslant 0$, and that $\langle\langle\psi_n,a,i|\psi_n,a,i\rangle\rangle>0$ only for the cases that $p_{n,a}=1$ and $E_n\in\mathbb{R}$, i.e., $|\psi_n,a,i=1\rangle$ is an eigenvector of H with a real eigenvalue. Furthermore, by construction, this basis includes all the eigenvectors of H. The proof of the converse is the same as the one given in Ref. 2.

It is important to note that having a positive-semidefinite basis does not imply that the inner product $\langle\langle ,\rangle\rangle_\eta$ is positive-semidefinite (unless the Hamiltonian is diagonalizable and has a real spectrum in which case both the basis and the inner product $\langle\langle ,\rangle\rangle_\eta$ are positive definite.[4]) If the Hamiltonian has defective or complex(-conjugate pair(s) of) eigenvalues, there will always be at least two null vectors with negative[3] linear combinations. Unlike positive vectors, linear combinations of nonnegative vectors need not be nonnegative.

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[3] A vector ϕ is respectively said to be positive, null (zero), negative, if $\langle\langle\phi|\phi\rangle\rangle>0$, $\langle\langle\phi|\phi\rangle\rangle=0$, $\langle\langle\phi|\phi\rangle\rangle<0$. It is said to be nonnegative if $\langle\langle\phi|\phi\rangle\rangle\geqslant 0$. A basis is called positive-semidefinite if it consists of nonnegative vectors. See, for example, J. Bognar, *Indefinite Inner Product Spaces* (Springer, Berlin, 1974).
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Critical energies in random palindrome models

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(Received 6 November 2002; accepted 15 November 2002)

We investigate the occurrence of critical energies—where the Lyapunov exponent vanishes—in random Schrödinger operators when the potentials have some local order, which we call *random palindrome models*. We give necessary and sufficient conditions for the presence of such critical energies: the commutativity of finite word elliptic transfer matrices. Finally, we perform some numerical calculations of the Lyapunov exponents showing their behavior near the critical energies and the respective time evolution of an initially localized wave packet, obtaining the exponent ruling the algebraic growth of the second momentum. We also consider special random palindrome models with one-letter bounded gap property; the transport effects of such long range order are showed numerically. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1537462]

I. INTRODUCTION

This article is concerned with the random tight-binding Hamiltonian H_v on $l^2(\mathbb{Z})$,

$$(H_v\psi)_n = v_n\psi_n + \psi_{n+1} + \psi_{n-1}, \tag{1}$$

where $v=(v_n)$ is a finitely valued sequence with some local correlation. We address the problem of occurrence of *critical energies* in the spectrum, which are those where the *Lyapunov exponent* $\gamma(E)$ vanishes. For Schrödinger operators in the one-dimensional lattice, $\gamma(E)$ is defined when the limit

$$\lim_{n\to\infty} \frac{1}{n} \log\|T_n(E)\cdots T_1(E)\| \tag{2}$$

exists, where $T_i(E)$ is a sequence of unimodular matrices of the form

$$T_i(E) = \begin{pmatrix} E-v_i & -1 \\ 1 & 0 \end{pmatrix}.$$

This question has come to surface after Dunlap, Wu and Phillips' work on the random dimer,[9] and has been addressed rigorously by some authors.[5,8,11] Although the spectrum is pure point,[8] the behavior of the Lyapunov exponent near the critical energies is responsible for dynamical delocalization, characterized by the positivity of the asymptotic growth exponent, α, of the moment

$$m_\beta(t) = \sum_{n\in\mathbb{Z}} |n|^\beta |\psi_n(t)|^2 \sim t^{\beta\alpha} \tag{3}$$

for a packet initially localized at the origin: $\psi_n(0)=\delta_{n,0}$. This is proven by Jitomirskaya, Schulz-Baldes and Stolz[11] about the time average of the above moment. In the vicinity of a critical energy, the same authors show that the Lyapunov exponent vanishes quadratically, a fact already analyzed by Bovier[5] for the dimer model with some assumptions on the density of the invariant measure

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$\lambda(E)$ of the one-dimensional dynamical system obtained from the eigenvalue equation $H_v\psi = E\psi$.

We take as our motivation this striking effect of local order on dynamical delocalization. Our contribution is on the conditions for the appearance of critical energies in random palindrome models: these are obtained as random concatenations of palindrome words (of length greater than 2). Recall that a *palindrome* is a word that reads the same from left to right or from right to left. Since the potential assumes a finite number of values, it is useful to think of a bijective nonconstant real function φ, such that $\varphi^{-1}:\varphi(B)\subset[-\Delta/2,\Delta/2]\to\mathcal{B}$, where $\mathcal{B}$ is some finite alphabet, and identify clusters with words in $\mathcal{B}$.

We are able to tackle the problem of local order fairly generally with what we call *cluster maps*. These are injective maps $\mathfrak{C}:\mathcal{A}\to\mathcal{B}^*$, taking each letter a of an alphabet $\mathcal{A}$ to a cluster $\mathfrak{C}(a)\in\mathcal{B}^*$, where $\mathcal{B}^*$ is the set of finite words in the alphabet $\mathcal{B}$ and $\mathcal{B}\supset\mathcal{A}$. Thus we think of random palindrome models as images of random sequences under a cluster map for which $\mathfrak{C}(a)$ are palindromes for all $a\in\mathcal{A}$. We make some additional assumptions on these maps in Sec. II in order to control the extent of the correlations introduced on $\mathfrak{C}(v)$ for a random v. We stress that the palindromes have appeared quite naturally, as indicated in the discussion in Sec. III D.

The critical energies in random palindrome models occur when the transfer matrices associated with each palindrome in the potential commute and are elliptic. We get a recipe for obtaining a prescribed minimum number of critical energies, in contrast with just two in the random dimer. This result is interesting in its failure to produce an interval of critical energies, which would be an absolutely continuous component of the spectrum. An absolutely continuous spectral component is (already) prohibited by Kotani's theory[12] for almost every H_v in some ergodic structure, but the reasoning which leads us to this provides further understanding of potentials assuming a finite number of values. Our second result will tell us that, apart from a set of codimension 1 in the potential intensities, $\gamma(E)>0$ for almost every E different from the above constructed critical energies, cf. Ref. 8.

The analysis of the invariant measure $\lambda(E)$,[5,13] which could yield the Taylor series of $\gamma(E)$ near these critical energies, is not possible to carry over, because the palindromes need not have the same length. To check the behavior of the Lyapunov exponent near the critical energies, we perform numerical calculations of $\gamma(E)$ using the Thouless formula, or rather its approximation in finite dimension. We also provide some numerics on the mean square displacement, for which $\beta=2$ in Eq. (3), and obtain, due to the larger number of critical energies, a superdiffusive behavior with an exponent α larger than $\frac{3}{4}$ for small disorder, as in the random dimer.[9] For sufficiently large disorder, m_2 is bounded and dynamical localization sets in.

Iterating cluster maps $\mathfrak{C}:\mathcal{A}\to\mathcal{A}^*$ such that for any $a\in\mathcal{A}$, $\mathfrak{C}^k(a)$ contains all letters of $\mathcal{A}$, i.e., *primitive* cluster maps, provides a sequence of potentials $u^{(n)}=\mathfrak{C}^{nk}(v)$, for any $v\in\mathcal{A}^{\mathbb{Z}}$ which, under some additional hypotheses, will converge to a substitution sequence. Here we do not specialize the clusters to palindromes. This is stated and proven in Sec. III F. For primitive cluster maps, for any given potential v, any letter in $\mathcal{A}$ occurs in $\mathfrak{C}(v)$ with bounded gaps. This long range order is not generally present in a random palindrome model and one applied reason for its proposal is that it yields an interesting boost in transport, measured by the second moment m_2.

The article is organized as follows: in Sec. II we give the definition of a cluster map, specialize it to give random palindrome models and state most of our analytic results. We prove them in Sec. III, where we also discuss the ergodic structure of the models and a simple particular example. In Sec. III F we discuss some random models generated by primitive cluster maps. In Sec. IV we illustrate the numerical results with plots of $\gamma(E)$ and $m_2(t)$.

II. THE MODEL AND STATEMENT OF RESULTS

We are given a random sequence in $t=(t_j)\in\mathcal{A}^{\mathbb{Z}}$ and a *cluster map*

$$\mathfrak{C}:\ \mathcal{A}\to\mathcal{B}^*,$$

$$a\mapsto\mathfrak{C}(a),$$

where $\mathcal{B}^*$ is the set of finite words in an alphabet $\mathcal{B}\supset\mathcal{A}$. We consider only cluster maps for which the whole word $\mathfrak{C}(a)$ does not occur in $\mathfrak{C}(b)$, for all $a\neq b\in\mathcal{A}$. This prevents the introduction of spurious long range correlations in $\mathfrak{C}(t)$ even if $t\in\mathcal{A}^{\mathbb{Z}}$ is random (see, however, Sec. III F).

To extend $\mathfrak{C}$ to $t\in\mathcal{A}^{\mathbb{Z}}$ by concatenation, we declare the position of the first letter of $\mathfrak{C}(t_0)$ to be -1 (this will be convenient in Sec. III F):

$$r\overset{\text{def}}{=}\mathfrak{C}(t),\quad r_{-1}r_0\cdots r_{|\mathfrak{C}(t_0)|-2}=\mathfrak{C}(t_0).$$

When $\mathcal{B}=\mathcal{A}$, $\mathfrak{C}$ is also a *substitution*.

The range of the function φ defined in the Introduction defines the *disorder* parameter Δ. Denoting the potential sequences by $v=\varphi(t)$ and $w=\varphi(\mathfrak{C}(t))$, we are interested in finding conditions for the vanishing of the Lyapunov exponent γ for some E in the spectrum of H_w, albeit γ in the spectrum of H_v is positive for almost every $v\in\mathcal{A}^{\mathbb{Z}}$.[6] With the exception of Sec. III F, we restrict our attention to cluster maps for which $\mathfrak{C}(a)$ is a palindrome, for each $a\in\mathcal{A}$. The potential $w=\mathfrak{C}(v)$ for $v\in\mathcal{A}^{\mathbb{Z}}$ is then called a *random palindrome model*. In this setting, we can get a rather complete answer to the problem of making $\gamma(E)$ vanish in the spectrum of H_w.

Consider first the case $\mathcal{A}=\{a,b\}$. Let C_a and C_b be general palindromes with sizes $|C_a|=n$ and $|C_b|=k$; and let $A=\Phi(C_a)$ and $B=\Phi(C_b)$ be their associated transfer matrices. The set of values of the potentials $\{v_i:1\leqslant i\leqslant n+k\}$ in both clusters defines an ordered s-tuple $\mathbf{v}$ taken from some open set $\mathcal{V}\subset\mathbb{R}^s$, where $s=\lceil n/2\rceil+\lceil k/2\rceil$.

Proposition 1: Let $T_i\in\{A,B\}, i\in\mathbb{Z}$, be a Bernoulli trial with A, B transfer matrices of palindromes. Then, if $[A,B]\neq 0$,

$$\Gamma=\lim_{n\to\infty}\frac{1}{n}\|T_n\cdots T_1\| \tag{4}$$

exists and is positive for almost every trial, and except for a set of codimension greater than 1 in $\mathcal{V}$.

In this excluded set of potential intensities, critical energies do occur and have appeared before in Sec. 3 of Ref. 8. There is a simple proportional relation between Γ, Eq. (4), and γ, Eq. (2), when both exist; see Corollary 2.

In proving Proposition 1, we will use the Furstenberg and Kesten theorem, thus the statement is restricted to a set of full measure μ, with μ being the product or Bernoulli measure in $\mathcal{A}^{\mathbb{Z}}$.

Define the left-shift by $(\tau(u))_n=u_{n+1}$. The left-shift translations of $\mathfrak{C}(u)$, $u\in\mathcal{A}^{\mathbb{Z}}$, generate an ergodic system $\Lambda\subset\mathcal{B}^{\mathbb{Z}}$ with a Markov measure ν. We will discuss this point in detail in Sec. III A.

Given a random sequence $u=(u_n)_{n\in\mathbb{Z}}$ in a finite alphabet $\mathcal{A}$, we assume that each letter occurring in u does so with positive probability.

Definition 1: Let $\mathfrak{C}$ be a cluster map defined on the alphabet $\mathcal{A}$, carrying each letter a_i to a palindrome $p_i=\mathfrak{C}(a_i)$. Then we say the sequence $v=\mathfrak{C}(u)$ is tessellated by palindromes.

A transversality argument together with Proposition 1 leads to the following

Theorem 1: *There is a set $Y\subset\Lambda$ of aperiodic sequences tessellated by palindromes, with $\nu(Y)=1$ such that for all $v\in Y$ the critical energies in $\sigma(H_v)$ are at most countable.*

Theorem 1 is a special case of Kotani's results[12] which rule out the absolutely continuous spectrum from potentials assuming finitely many values. However, the sets of realizations to which one and the other refer are not directly related. In order to properly make a comparison, the above mentioned ergodic structure (Λ,τ,ν) is needed. We settle this question in Sec. III A. Finally, we do not have reasons to exclude the possibility of a singular continuous spectrum in random palindrome (cluster) models, particularly with long range order.

We analyze a simple generalization of the random dimer, where $\mathcal{A}=\{a,b\}$. If we restrict C_b to a constant word of length two, $C_b=bb$, we get an open condition on the word C_a, if C_a is a palindrome of odd length, $C_a=t_0t_1\cdots t_k\cdots t_1t_0$, for small disorder. We set $v_i=\varphi(t_i)$, $v_a=\varphi(a)$, $v_b=\varphi(b)$ and

$$\Delta=\max\{|v_i-v_b|,0\leqslant i\leqslant k\}.$$

Theorem 2: *Let $C_b=bb$ and C_a be a palindrome of length $2k+1$, $k\geqslant 1$, with potentials v_i such that $|v_i-v_a|<\epsilon<\Delta$, $0\leqslant i\leqslant k$. Then*

(i) *For small enough disorder $\Delta>0$, any realization of such random palindrome model has at least $2k+1$ critical energies.*
(ii) *For $0<\Delta\leqslant 2$, the random palindrome model has at least k critical energies.*
(iii) *For $2<\Delta<4$, if k is sufficiently large, the random palindrome model has at least one critical energy.*

We build on the proof by De Bièvre and Germinet[8] on the existence of critical energies at $E=\pm v$ if $v\leqslant 1$ for the random dimer. The steps are elementary and the conclusion is based on Taylor series expansions. Bovier mentioned some plans along these lines in his paper on the random dimer.[5] Some generalizations of the random dimer were studied earlier.[13]

Applying Furstenberg and Kesten's theorem we have the following.

Corollary 1: For C_a and C_b as in Theorem 2 and sufficiently small ϵ, there exists $0<z_{\max}<2$ such that, for disorder $\Delta>2+z_{\max}$, the Lyapunov exponent $\gamma(E)$ is positive, whenever it exists.

We will say more about $z_{\max}$ for $\epsilon=0$ from the details of the proof of Theorem 2.

III. PROOFS

A. Ergodic structure

We are given two finite alphabets $\mathcal{A}$ and $\mathcal{B}$, with $\mathcal{B}\supset\mathcal{A}$, $\mathcal{A}$ having more than one element and a cluster map $\mathfrak{C}:\mathcal{A}\to\mathcal{B}^*$. We construct the Kakutani tower[15] from $\mathcal{A}^{\mathbb{Z}}$ as follows: $S_a=\{x\in\mathcal{A}^{\mathbb{Z}}:x_0=a\}\times\{1,\ldots,n_a\}$, where $n_a\overset{\text{def}}{=}|\mathfrak{C}(a)|$, for each $a\in\mathcal{A}$. Write the disjoint union $\Omega=\dot{\cup}_{a\in\mathcal{A}}S_a$ endowed with the metric

$$\rho((x,i),(y,j))=\sum_{n\in\mathbb{Z}}\frac{d(x_n,y_n)}{2^{|n|}}+d(i,j), \tag{5}$$

where d is the discrete metric. Then Ω is compact. On Ω, we have the shift transformation

$$\hat{\tau}(x,i)=\begin{cases}(x,i+1) & \text{if } i<n_a,\\ (\tau(x),1) & \text{if } i=n_a,\end{cases}$$

where τ is the shift on $\mathcal{A}^{\mathbb{Z}}$. We extend $\mathfrak{C}$ to Ω, defining $\hat{\mathfrak{C}}$ so that the diagram below commutes

$$\begin{array}{ccc}\Omega & \overset{\hat{\mathfrak{C}}}{\to} & \mathcal{B}^{\mathbb{Z}}\\ \hat{\tau}\downarrow & & \downarrow\tau\\ \Omega & \overset{\hat{\mathfrak{C}}}{\to} & \mathcal{B}^{\mathbb{Z}}\end{array}$$

and $\hat{\mathfrak{C}}(x,1)=\mathfrak{C}(x)$.

A simple averaging over the components of Ω gives an ergodic measure[11] which, however, does not account for the systematic local repetitions of letters in $\hat{\mathfrak{C}}(\Omega)$. Therefore the push-forward of this ergodic measure does not give a suitable ergodic structure. We have instead the following.

Proposition 2: Let Ω be as above and $\Lambda=\hat{\mathfrak{C}}(\Omega)\subset\mathcal{B}^{\mathbb{Z}}$ be its image under the cluster map. Then Λ is a subshift of finite type.

Let us introduce some terminology. If v is a finite word in $\mathcal{B}^*$, define

$$Y_v=\{x\in\mathcal{B}^{\mathbb{Z}}: v \text{ does not occur in } x\}.$$

We are to prove that Λ is the intersection of finitely many Y_v's. We say that a (finite) word is *acceptable* (in Λ) if it occurs in some $x\in\Lambda$; otherwise we call it *unacceptable*. We shall use *block*, cluster and word interchangeably. If the word u is contained in w, then $Y_u\subset Y_w$.

In our context, note that a word w is acceptable, i.e., $w\in\hat{\mathfrak{C}}(\Omega)$, if, and only if, w is contained in some concatenation of clusters. If an acceptable word v ends with a block and u is an acceptable word beginning with a block, then the concatenation vu is acceptable in $\hat{\mathfrak{C}}(\Omega)$.

Proof of Proposition 2: $\hat{\mathfrak{C}}$ is clearly continuous, therefore Λ is compact, and shift invariant by $\hat{\mathfrak{C}}$'s definition. Then Λ is a subshift.[14]

Note that $\mathcal{B}^*$ is partially ordered with word inclusion and the corresponding length. Fix $w=w_0\cdots w_k$ an arbitrary unacceptable word and let v be a word contained in w formed by blocks $\mathfrak{C}(a)$ which cannot be enlarged with the concatenation of another such block and still be contained in w. Finally let $\overline{v}=w_i\cdots w_j$ be an acceptable word satisfying $v\subset\overline{v}\subset w$ and which cannot be enlarged with the concatenation of any other letter of w. Put $n=\max_{a\in\mathcal{A}}|\mathfrak{C}(a)|$.

We prove that there is some unacceptable u occurring in w, with uniformly bounded length.

Case (i) v is empty. Then $|\overline{v}|\leqslant n-1$. And any word u of length n occurring in w is unacceptable.

Case (ii) v is a single cluster. Then $|\overline{v}|\leqslant n+2(n-1)$ and hence a word $u\supset\overline{v}$, whose maximum length is $3n-1$, occurring in w is unacceptable.

Case (iii) v is the concatenation of various clusters.

Suppose, without loss, that $j<k$ and let $p+1$ be such that w_{p+1} is the first letter of the rightmost cluster in v. Let $s=w_{p+1}\cdots w_{j+1}$ and $r=w_i\cdots w_p$. So, s cannot be acceptable, since otherwise we could append r to its left producing an acceptable word larger than $\overline{v}$. Note that $|s|\leqslant 2n$. □

On Λ, τ is a Markov shift[14] and we have the Markovian measure ν. Consider the projection $\pi:\Omega\to\mathcal{A}^{\mathbb{Z}}$. It is clear that to each set $Y\subset\mathcal{A}^{\mathbb{Z}}$ invariant under the shift, there corresponds an invariant set $\hat{\mathfrak{C}}(\pi^{-1}(Y))\subset\Lambda$.

Kotani's theorem[12] says there is a set $W\subset\Lambda$ with $\nu(W)=1$ such that $\sigma_{ac}(H_v)=\varnothing$ for all $v\in W$. Proposition 1 tells that there is some $Y\subset\mathcal{A}^{\mathbb{Z}}$ with $\mu(Y)=1$, μ the product measure, such that for $u\in Y$, then $\sigma_{ac}(H_{\mathfrak{C}(u)})=\varnothing$. Since $v=\hat{\mathfrak{C}}(t)$ for some t, there is a j such that $\tau^j\hat{\mathfrak{C}}(t)=\mathfrak{C}(u)$, $u\in\mathcal{A}^{\mathbb{Z}}$. The spectrum is the same for points in the same orbit, hence $W\subset\hat{\mathfrak{C}}(\pi^{-1}(Y))$. Therefore $\nu(\hat{\mathfrak{C}}(\pi^{-1}(Y)))=1$. We also have immediately the two useful corollaries:

Corollary 2: Let $Y=\{u\in\mathcal{A}^{\mathbb{Z}}:\Gamma \text{ exists}\}$ and $W=\{v\in\Lambda:\gamma(E) \text{ exists}\}$. Then $W=\hat{\mathfrak{C}}(\pi^{-1}(Y))$.

Proof: Denote by p_a the probability of the letter a appearing in a Bernoulli trial on $\mathcal{A}=\{a,b\}$ referred to in Proposition 1. p_a is the probability of $T_i=A$ in Eq. (4). Then, if γ exists, by the law of large numbers,

$$\Gamma=\lim_{n\to\infty}\frac{1}{n}\|T_n\cdots T_1\|=(p_a|\mathfrak{C}(a)|+(1-p_a)|\mathfrak{C}(b)|)\,\gamma.$$

The reciprocal is analogous. Note also that this can be extended to the case when $\mathcal{A}$ has more than two letters. □

Corollary 3: Let $Y_1 \subset \mathcal{A}^{\mathbb{Z}}$ *be an invariant set such that* $\mu(Y_1)=1$. *Then* $\nu(\hat{\mathfrak{C}}(\pi^{-1}(Y_1)))=1$.

Proof: Let Y and W be the sets of Corollary 2. Consider $Y_2=Y_1\cap Y$. Y_2 is invariant and nonempty, since $\mu(Y_1)=1$. Now $\hat{\mathfrak{C}}(\pi^{-1}(Y_2))\cap W$ is invariant and clearly nonempty, therefore $\nu(\hat{\mathfrak{C}}(\pi^{-1}(Y_2)))=1$. □

B. Some preliminaries

In this subsection, we establish conditions for the existence of critical energies on such locally correlated disordered Hamiltonians. They are preliminaries for the proofs of the main results.

Let $\rho(T)$ denote the spectral radius of the square matrix T. We begin with the following observations.

Lemma 1: Suppose that the matrices A and B commute, $[A,B]=0$, *and* $\rho(A)=\rho(B)=1$. *If* $T_i\in\{A,B\},\forall i$, *then the Lyapunov exponent* γ *vanishes.*

Proof: If n_a is the frequency of A in $T_n\cdots T_1$, then by the law of large numbers $n_a\to p_a$, and similarly $n_b\to(1-p_a)$. Hence, using the definition of the Lyapunov exponent Eq. (2), $\gamma=\log(\rho(A)^{p_a}\rho(B)^{1-p_a})=0$. □

Lemma 2: Let A,B *be* 2×2 *real matrices, and* A *not a multiple of the identity matrix* I.

(i) If $[A,B]=0$, *then there exist* $\theta,\lambda\in\mathbb{R}$ *such that* $B=\theta I+\lambda A$.

(ii) If, moreover, $\det A=\det B=1$, *then*

$$\theta^2+\lambda^2+\lambda\,\theta\,\mathrm{tr}\,A=1.$$

In this case, we denote by $B(\lambda)$ *the pencil of matrices commuting with* A. *If furthermore* $\rho(A)=1$, *then* $\rho(B(\lambda))=1$.

Proof: (*i*) and the first part of (*ii*) follow by direct calculation. To show (*ii*), note first that when $|\mathrm{tr}\,A|<2$, the pair (λ,θ) lies in an ellipse. The extrema of $\mathrm{tr}\,B=2\theta+\lambda\,\mathrm{tr}\,A$ along this ellipse occur at $\lambda=0$. □

Let A denote the transfer matrix corresponding to the cluster C_a and B the transfer matrix of the cluster C_b. For a letter t_i with corresponding potential $v_i=\varphi(t_i)$, recall that

$$T_{v_i}=\begin{pmatrix} E-v_i & -1 \\ 1 & 0 \end{pmatrix}$$

and for the word $C_a=t_0t_1\cdots t_n$, $A=T_{v_n}\cdots T_{v_1}T_{v_0}$ and correspondingly for B. Suppose we can find v_i such that, for some E, they commute. We can then write $(a_{ij})=A(E)$ and $(b_{ij}(\lambda))=B(E,\lambda)$, $\lambda\in\mathbb{R}$, with

$$\begin{aligned} b_{12}&=\lambda a_{12},\\ b_{21}&=\lambda a_{21},\\ b_{11}-b_{22}&=\lambda(a_{11}-a_{22}). \end{aligned} \tag{6}$$

Note that this system is equivalent to $[A,B]=0$, in case A is not a multiple of the identity matrix.

Let us write $\Phi(w)$ for the transfer matrix associated with the finite word w. So the notation for the basic transfer matrices of our lattice is

$$A=\Phi(C_a)\ \text{and}\ B=\Phi(C_b).$$

If t_i is the letter at position i, we have that $\Phi(t_i)$ is a function of $x_i=E-\varphi(t_i)$. The following is well known and can be checked by induction:

Lemma 3: For any word $w=t_0\cdots t_n$, *the transfer matrix* $\Phi(w)$ *has the following form,*

$$\Phi(w)=\begin{pmatrix} P_{n+1}(x_0,\ldots,x_n) & -P_n(x_1,\ldots,x_n) \\ P_n(x_0,\ldots,x_{n-1}) & -P_{n-1}(x_1,\ldots,x_{n-1}) \end{pmatrix},$$

where $P_{n+1}(x_0,\ldots,x_n)=P_n(x_0,\ldots,x_{n-1})x_n-P_{n-1}(x_0,\ldots,x_{n-2})$, $n\geqslant 0$, *with the understanding that* $P_{-1}=0$ *and* $P_0=1$ *(*P_n *is a polynomial of* E *of degree* n*).*

Note that $\Phi(bb)$ has off-diagonal elements with the property $b_{21}=-b_{12}$. An inductive argument shows that A also has this property if C_a is a palindrome:

Lemma 4: If C_a *is a palindrome, the* $A=\Phi(C_a)$ *has off-diagonal elements with the property* $a_{12}=-a_{21}$.

Proof: If C_a is a dimer, we already know A satisfies $a_{12}=-a_{21}$. If it has length $n\geqslant 3$, then $C_a=t_0Pt_0$, where P is a palindrome of length $n-2$, and we can write

$$A=\begin{pmatrix} x_0 & -1 \\ 1 & 0 \end{pmatrix} M \begin{pmatrix} x_0 & -1 \\ 1 & 0 \end{pmatrix}$$

with $M=\left(\begin{smallmatrix} a'_{11} & a'_{12} \\ -a'_{12} & a'_{22} \end{smallmatrix}\right)$, by the induction hypothesis; from this we get $a_{21}=-a_{12}$. □

Lemma 5: If C_a *and* C_b *are palindromes with* $|C_a|>|C_b|\geqslant 2$ *and* C_b *does not occur in* C_a*, then the system (6) has a finite number of solutions.*

Proof: Put $C_a=a_0\cdots a_n$ and $C_b=b_0\cdots b_k$, with $1<k<n$. We will make an induction on the size of the palindromes $|C_a|=n+1$ and $|C_b|=k+1$. Rewriting system (6) using Lemmas 3 and 4, we get

$$P_k(y_1,\ldots,y_k)=\lambda P_n(x_1,\ldots,x_n),$$

$$P_{k+1}(y_0,\ldots,y_k)+P_{k-1}(y_1,\ldots,y_{k-1})=\lambda(P_{n+1}(x_0,\ldots,x_n)+P_{n-1}(x_1,\ldots,x_{n-1})),$$

where $y_i=E-\varphi(b_i)$ and $x_i=E-\varphi(a_i)$. Eliminating λ in the system above, we get the following equation:

$$\begin{aligned} &P_k(y_1,\ldots,y_k)(P_{n+1}(x_0,\ldots,x_n)+P_{n-1}(x_1,\ldots,x_{n-1}))-P_n(x_1,\ldots,x_n)(P_{k+1}(y_0,\ldots,y_k) \\ &\quad +P_{k-1}(y_1,\ldots,y_{k-1}))=0. \end{aligned} \tag{7}$$

If there is an infinite number of energies E_i such that Eq. (7) holds, then it is a *polynomial equality*, meaning that on the left each polynomial coefficient is zero.

For $k=1$ and $k=2$, from this polynomial equation and the recursion relation given in Lemma 3, we can prove directly that C_b occurs in C_a, contrary to our hypothesis. We reduce the problem to the following.

Lemma 6: Let $|C_a|=n+1$ *and* $|C_b|=k+1$, $n>k\geqslant 3$, C_a *and* C_b *palindromes. Let* $Q(j)$ *denote the property described in items (a) and (b) below:*

(a) $$\begin{aligned} &P_{k-j}(y_1,\ldots,y_{k-j})P_{n-j-1}(x_1,\ldots,x_{n-j-1})-P_{k-j}(y_{j+1},\ldots,y_k)P_{n-j-1}(x_{j+2},\ldots,x_n) \\ &\quad \equiv P_{n-j}(x_1,\ldots,x_{n-j})P_{k-j-1}(y_1,\ldots,y_{k-j-1})-P_{n-j}(x_{j+1},\ldots,x_n)P_{k-j-1}(y_{j+2},\ldots,y_k), \end{aligned}$$

(b) $$x_0=y_0=x_n=y_k,\quad \ldots,\quad x_j=y_j=x_{n-j}=y_{k-j},$$

for some $0\leqslant j\leqslant k-2$; *then* $Q(j+2)$ *holds. In particular* $x_{j+1}=y_{j+1}=x_{n-j-1}=y_{k-j-1}$ *and* $x_{j+2}=y_{j+2}=x_{n-j-2}=y_{k-j-2}$.

Proof of Lemma 6: We use the recursion relation of Lemma 3 and

$$P_{n+1}(x_0,\ldots,x_n)=x_0P_n(x_1,\ldots,x_n)-P_{n-1}(x_2,\ldots,x_n).$$

Properties $Q(0)$ and $Q(1)$ are immediate from Eq. (7) and the recursion relations.

From point (a) of $Q(j)$, expanding the occurrences of P_{k-j} and P_{n-j},

$$\begin{aligned}
&y_{k-j}P_{k-j-1}(y_1,\ldots,y_{k-j-1})P_{n-j-1}(x_1,\ldots,x_{n-j-1})\\
&\quad -P_{k-j-2}(y_1,\ldots,y_{k-j-2})P_{n-j-1}(x_1,\ldots,x_{n-j-1})\\
&\quad -y_{j+1}P_{k-j-1}(y_{j+2},\ldots,y_k)P_{n-j-1}(x_{j+2},\ldots,x_n)\\
&\quad +P_{k-j-2}(y_{j+3},\ldots,y_k)P_{n-j-1}(x_{j+2},\ldots,x_n)\\
&\quad =x_{n-j}P_{n-j-1}(x_1,\ldots,x_{n-j-1})P_{k-j-1}(y_1,\ldots,y_{k-j-1})\\
&\qquad -P_{n-j-2}(x_1,\ldots,x_{n-j-2})P_{k-j-1}(y_1,\ldots,y_{k-j-1})\\
&\qquad -x_{j+1}P_{n-j-1}(x_{j+2},\ldots,x_n)P_{k-j-1}(y_{j+2},\ldots,y_k)\\
&\qquad +P_{n-j-2}(x_{j+3},\ldots,x_n)P_{k-j-1}(y_{j+2},\ldots,y_k).
\end{aligned}$$

Since we know that $x_{n-j}=y_{n-j}$ already, the first term and the first term after the equality sign cancel out. The terms containing the highest power in E are the third before and after the equality sign. The other terms do not affect the leading coefficient. Therefore, we have $x_{j+1}=y_{j+1}$, which are also equal to x_{n-j-1} and y_{n-j-1} by palindromicity.

We now expand $P_{k-j-1}(y_{j+2},\ldots,y_k)$ and $P_{n-j-1}(x_{j+2},\ldots,x_n)$ to conclude that $x_{j+2}=y_{j+2}$. The polynomials remaining give the equality (a) of $Q(j+2)$. □

$Q(k)$ contradicts the hypothesis that C_b does not occur in C_a. □

C. Proofs of proposition 1 and theorem 1

Proof of Proposition 1: We follow de Bièvre and Germinet[8] closely. We first note that the group generated by A and B is not compact and, resorting to Theorem II.4.4 of Ref. 3, we will prove that the orbit of any direction $x\in\mathbb{P}(\mathbb{R}^2)$ under this group contains at least three elements. It is sufficient to consider the three cases: (a) A and B elliptic, (b) A parabolic and (c) A hyperbolic, as the other cases will follow by interchanging the roles of A and B.

The noncompactness of the group is clear in cases (b) and (c). Since A and B are palindromic transfer matrices, they have the form (using Lemma 4)

$$A=\begin{pmatrix} a_1+t_A & -a_2\\ a_2 & -a_1\end{pmatrix},\quad B=\begin{pmatrix} b_1+t_B & -b_2\\ b_2 & -b_1\end{pmatrix},$$

where $t_A=\mathrm{tr}\,A$ and $t_B=\mathrm{tr}\,B$. For A and B palindromes, $[A,B]\neq 0\Leftrightarrow[A,B]$ is invertible. Hence using Theorem 7.39.2 of Ref. 2 for A and B elliptic, the noncommutativity implies $\mathrm{tr}\,(ABA^{-1}B^{-1})>2$. This shows that also in this case the group generated by A and B is not compact.

(a) If both $|t_A|<2$ and $|t_B|<2$, then from $A^2=t_AA-I$, one sees that A^2 or B^2 are elliptic, unless both $t_A=t_B=0$. In the first case, the set $\{x,Ax,A^2x,Bx,B^2x\}$ contains at least three different directions. The latter case, viewed as a geometric condition, is the intersection set of zeroes of two transverse polynomials t_A and t_B (by the same analysis of leading order coefficients given in Lemma 5). This intersection is empty unless $\gcd(t_A(E),t_B(E))\neq 1$, that is, if these polynomials have a common divisor.

Now, if for a given s-tuple $\mathbf{v}\in\mathcal{V}$, $\gcd(t_A,t_B)\neq 1$, since t_A and t_B are also polynomials in $\mathbf{v}$, it is clear that to preserve this condition $\mathbf{v}$ has to stay in an algebraic variety in parameter space $\mathcal{V}$.

(b) If $|t_A|=2$, then A has a single fixed point in $\mathbb{P}(\mathbb{R}^2)$, but it cannot be a fixed point of B since

$$[A,B]=((2a_1+t_A)a_2-(2b_1+t_B)b_2)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

is invertible. Now it is clear that the set $\{x, Bx, Ax, ABx, A^2x\}$ has at least three different directions.

(c) Again it suffices to consider the orbit of the two eigenvectors of A. If $|t_B| \geqslant 2$, we are done, again because A and B do not have eigenvectors in common. But it could be the case that B, being elliptic, exchanged the eigendirections of A. These are $e_1=(a_1+\lambda,a_2)$ and $e_2=(a_1+\overline{\lambda},a_2)$, where $\lambda=(t_A+\sqrt{t_A^2-4})/2$ and $\overline{\lambda}=1/\lambda$.

From $Be_1=ke_2$ and $Be_2=-k^{-1}e_1$, it follows that $t_B=0$. Moreover, from the system of equations

$$b_1(a_1+\lambda)-b_2a_2=k(a_1+\overline{\lambda}),$$

$$b_2(a_1+\lambda)-b_1a_2=ka_2$$

one obtains the equation $2b_2a_2=(2a_1+t_A)b_1$. Now we have again two polynomials, whose sets of zeros have, by transversality, empty intersection. □

By Corollary 2, there is a set $W\subset\Lambda$ of measure $\nu(W)=1$ which corresponds to the subset of $\mathcal{A}^{\mathbb{Z}}$ given in the proposition above. The closure of the orbit of each periodic sequence is a set of measure zero. The closure of the orbit of a sequence which is periodic except in a finite number of indices (that is, in the complement of a cylinder set[15]) is also a set of measure zero. Subtracting these sets from W we get a measurable set Y of full measure. For every $v\in Y$, $\gamma(E)>0$ except possibly when $[A,B]=0$.

Proof of Theorem 1: Fix A and B transfer matrices of palindromes C_a and C_b. As noted in the proof of Proposition 1, Eq. (6) is a system of two independent polynomials and two variables (λ,E), with a finite number of (real) roots.

A random palindrome model may have long range order; then we have to consider all possibilities of palindromes which tessellate the lattice potential. But since A, B are transfer matrices on factors in a finite alphabet, they belong to a denumerable set of unimodular matrices. Therefore the set of critical energies is at most countable. □

Lemmas 1 and 2 tell us that to find critical energies for the tight binding Hamiltonian, we have to search for commuting transfer matrices with one of them with spectral radius equals to 1. From Lemma 2, the pencil of matrices commuting with a given one is compact in $\mathrm{SL}(2,\mathbb{R})$. Hence, for each A, a choice of B from the intersection of a countable set and a compact set has generically a finite number of possibilities. This reasoning leads us to question whether the critical energies given by system (6) are real.

From Proposition 1, we also have the following.

Corollary 4: Consider Λ the set of all random palindrome models whose potentials are tessellated by palindromes $p_1,\ldots,p_n$ with p_i not contained in p_j, $i\neq j$. Let ν be the Markov measure invariant under the shift. For ν-almost every v, $\gamma(E)=0$ implies that the transfer matrices $A_i=\Phi(p_i)$ are elliptic and pairwise commuting.

D. A particular case

Now we illustrate the construction leading to critical energies in a simple situation: taking $C_a=t_0t_1t_2$ and $C_b=t_3t_4$, we shall determine transfer matrices for which the above setting applies. The potentials $v_i=\varphi(t_i)$ are allowed to take on more than two values. Note that, being the transfer matrices unimodular, the condition on the determinant is automatically fulfilled. As above, denote by A the transfer matrix of the cluster C_a and by B the transfer matrix of C_b:

$$A(E)=T_{v_2}T_{v_1}T_{v_0} \text{ and } B(E)=T_{v_4}T_{v_3}.$$

We shall use the abbreviation $x_i=E-v_i$ and drop the reference to E at our convenience in what follows. From the system of equations (6) we have the following,

$$x_3=\lambda(x_0x_1-1),$$

$$x_4=\lambda(x_1x_2-1),$$

$$x_3x_4=\lambda(x_0x_1x_2-x_0-x_2+x_1),$$

and the condition $\rho(A)=1 \Leftrightarrow |\mathrm{tr}\, A|\leqslant 2$ reads

$$|x_0x_1x_2-x_0-x_1-x_2|\leqslant 2.$$

Since the v_i are fixed values of the potential, we have three equations in two variables. We make the first two of these (algebraic) curves in the (E,λ) plane coincide by setting $v_4=v_3$, and $v_2=v_0$, but with v_0, v_1 and v_3 all different from each other. Notice that this makes C_a and C_b palindromes; that was the initial motivation for Theorem 2.

An obvious solution is $x_3=0$, that is, $E=v_3$, and $\lambda=0$. We call this the *dimer* energy, because for it $B=-I$ and the above lemmas are satisfied trivially, except for the condition $\rho(A)=1$, which remains to be verified for this energy to be critical. If $\lambda\neq 0$, we get the equation

$$x_3(x_0x_1-1)=x_0^2x_1-x_0+(v_0-v_1),$$

with the two solutions (note that $x_i-x_j=v_j-v_i$ is a constant)

$$x_{0\pm}=-\frac{v_{01}\pm\sqrt{v_{01}^2+4+4v_{01}/v_{03}}}{2},$$

where $v_{ij}=v_i-v_j$.

The three energies $E=\{v_3,v_0+x_{0+},v_0+x_{0-}\}$ will be critical energies if the following condition holds:

$$|\mathrm{tr}\, A|\leqslant 2 \;\Leftrightarrow\; |x_0^3+v_{01}x_0^2-3x_0-v_{01}|\leqslant 2.$$

One possible way to achieve this is by setting $v_{01}=2v_{03}$ and $|v_{03}|\leqslant 1$, which is enough for the purpose of showing the existence of three energies where the Lyapunov exponent vanishes.

Remark 1: (i) It may happen that $A=\pm I$ for transfer matrices, and obviously $[B,A]=0$ for any B, but the equations (6) above would have the "strange" solution $\lambda=\infty$. In this case $\rho(B)=1$ alone implies $\gamma=0$.

(ii) From the above remark, or interchanging the roles of A and B in system (6), we see that the natural domain for λ is the projective line $(-\infty,\infty]$.

(iii) We fix $C_b=bb$ from now on and will call the word C_b a dimer. *For those E^* where $A(E^*)=\pm I$, we have $\gamma(E^*)=0$ if $\rho(B)=1$, that is, if $|E^*-v_b|\leqslant 2$.*

To proceed with the generation of critical energies, we choose to enlarge the cluster C_a. For $C_b=bb$, the system of equations (6) always keeps the trivial solution coming from the dimer: $E=v_b$ and $\lambda=0$. Eliminating this solution, we get a polynomial of degree n in the variable E, which has $|C_a|-1$ roots. However, it is harder to anticipate if for these energies $|\mathrm{tr}\, A|\leqslant 2$. Providing this, Lemmas 1 and 2 will yield $\gamma(E)=0$, and since $\gamma(E)>0$ outside the spectrum, $E\in\sigma(H_v)$.

E. Proof of Theorem 2

Let us begin with the idea of the proof. The strategy is first to analyze the simple case where $C_a=a^{2k+1}$ and then make use of perturbative arguments. Without loss of generality, we suppose $v_b>v_a$, so that the disorder strength is $\Delta=v_b-v_a$. We can show that there are $2k$ energies where $A=\pm I$ (actually this is an old known fact[4]), and v_b can be chosen as in Remark 1 (iii). *This imposes the bound on the disorder $\Delta<4$, see below*. These energies are roots of a Chebyshev polynomial of degree $2k$, so they are simple. Then we consider the palindrome $C_a=a^kt'a^k$, meaning that only the central position has a different potential $\varphi(t')=v_a+\epsilon$. If $\epsilon>0$ is small, we can prove that there are $2k$ perturbed energies satisfying $|\mathrm{tr}\, A|<2$. Since this is now an open

condition on C_a, we will conclude the proof of the first part of the theorem. The second and third parts will be proven by an analysis of the sign of the second derivative of tr A in case $\Delta<4$ is arbitrary.

First, for $C_a=a^n$, we have

$$A=\begin{pmatrix} P_n(x_a) & -P_{n-1}(x_a) \\ P_{n-1}(x_a) & -P_{n-2}(x_a) \end{pmatrix},$$

where $x_a=E-v_a$. The recursion relation $P_n(x)=xP_{n-1}(x)-P_{n-2}(x)$ gives that $P_n(x)=U_n(x/2)$, where U_n are the Chebyshev polynomials of the second type, following the notation of Gradshteyn–Ryzhik.[11] The equations for commutativity of A and B read

$$x_b=\lambda P_{n-1}(x_a) \quad \text{and} \quad x_b^2=\lambda(P_n(x_a)+P_{n-2}(x_a)),$$

with $\lambda\in(-\infty,\infty]$ as noted in Remark 1 (iii). Since $x_a\neq x_b$, we have only two possibilities: $x_b=0$ or $P_{n-1}(x_a)=0$. In the latter case, tr $A=-2P_{n-2}(x_a)$. A calculation using the expression $U_n(\theta)=[\sin(n+1)\theta]/\sin\theta$, $\theta=\arccos(x/2)$ shows that at the (simple) roots of P_{n-1}, tr $A=\pm 2$.

So we have the partial conclusion that if we combine constant words of length n and dimers we get at least n critical energies for Δ small enough, namely, less than $2+\min\{z\}$, where z are the roots of $P_{n-1}(x)=0$, again using Remark 1 (iii). In general, these roots z are critical energies if, and only if, $|\Delta-z|\leqslant 2$, for $\epsilon=0$.

However, if $\Delta\geqslant 4$, since every root of $P_{n-1}(x)$ satisfies $|z|<2$, one cannot have simultaneously $\rho(B)=1$, so these critical energies cease to be so. Also, for the dimer energy $E=v_b$, a necessary condition for $|\text{tr } A|\leqslant 2$ is $\Delta\leqslant 2$. In other words, the dimer energy ceases to be critical when the disorder strength $\Delta>2$. Note that this is the same bound for the original *random dimer model*,[9] in particular, for $\Delta=2$,

$$|\text{tr } A|=|U_n(-1)-U_{n-2}(-1)|=2.$$

Now consider the case where $n=2k+1$ and $x_i=x_a$ except for $i=k$ where $x_k=x_a-\epsilon$. Let us make the abbreviation $x=x_a$ and replace $x_b=x-\Delta$. Now A reads

$$A=\begin{pmatrix} (x-\epsilon)P_k^2-2P_kP_{k-1} & -(x-\epsilon)P_kP_{k-1}+P_{k-1}^2+P_kP_{k-2} \\ (x-\epsilon)P_kP_{k-1}-P_{k-1}^2-P_kP_{k-2} & -(x-\epsilon)P_{k-1}^2+2P_{k-1}P_{k-2} \end{pmatrix}.$$

Then for $\lambda\neq 0$,

$$\begin{aligned} \text{tr } A&=(P_k^2-P_{k-1}^2)(x-\epsilon)+2P_{k-1}(xP_{k-1}-2P_k), \\ \Delta(P_k^2-P_{k-1}^2)&=\epsilon(P_k^2+P_{k-1}^2-(x-\Delta)P_kP_{k-1}). \end{aligned} \tag{8}$$

We make Taylor expansions on Eqs. (8) around the critical energies for $\epsilon=0$, namely, around the zeroes of $P_{2k}=P_k^2-P_{k-1}^2$. Let $\{z_i=2\cos[\pi i/(2k+1)];1\leqslant i\leqslant 2k\}$ be the set of roots of $P_k^2(x)=P_{k-1}^2(x)$. For $\epsilon=0$, the fact that tr $A=\pm 2$ at these $2k$ roots yields the useful relation

$$P_k(z_i)(2P_k(z_i)-z_iP_{k-1}(z_i))=1. \tag{9}$$

For small ϵ, the roots of the second equation in (8) will be $\delta(z_i,\epsilon)$ away from z_i, for each $1\leqslant i\leqslant 2k$. We fix i and write $\delta=\delta(z_i,\epsilon)$. Expanding the second equation in (8) one obtains

$$2\Delta\delta\left(\frac{2k+1}{4-z_i^2}\frac{P_{k-1}}{P_k}\right)=\epsilon(1+\Delta P_kP_{k-1})+O_2(\epsilon,\delta),$$

where $O_2(\epsilon,\delta)$ is a remainder of order 2 in ϵ and δ.

Now we compute the first terms in the power series of tr A starting from Eq. (8.949.6) in Ref. 10. To first order in δ and ϵ, $|\text{tr } A|=2$. We omit the details of the calculation of second order terms, which yields

$$\text{tr } A=\tau_0\left(1-\frac{\delta^2}{2}p(z_i,k)\right)+O(\delta^3)$$

where

$$p(x,k)=\frac{4x^2(2k+1)}{(4-x^2)^2}+f(\Delta)\frac{(2k+1)^2}{(4-x^2)^2}+\frac{(2k+1)^2}{4-x^2},$$

$$f(\Delta)=\frac{2\tau_0\Delta}{1-\tau_0\Delta P_k^2(z_i)/2},$$

$$\tau_0=-\frac{2P_{k-1}(z_i)}{P_k(z_i)}.$$

The problem is reduced to evaluating the sign of $p(z_i,k)$. We remark that δ is independent of the disorder strength Δ and therefore can be made as small as one likes by diminishing ϵ. Hence

$$p(z_i,k)>0\Leftrightarrow\ -f(\Delta)<\frac{4z_i^2}{2k+1}+4-z_i^2 \tag{10}$$

and it is clear that, for small Δ, in particular $\Delta\leqslant\sin^2[\pi/(2k+1)]$, the above holds for all $1\leqslant i\leqslant 2k$. Part (i) is proved.

We have $z_i=2\cos(\pi i/(2k+1))$, $1\leqslant i\leqslant 2k$, and for even i, $P_k(z_i)=-P_{k-1}(z_i)$ and consequently $\tau_0=2$, while for odd i, $\tau_0=-2$. If $\tau_0=2$ and $i=2j$, we note that $-f(\Delta)<0$ for small Δ. Therefore, the above inequality (10) remains true for all z_i such that

$$1-\Delta P_k^2(z_i)<0\Leftrightarrow\Delta<\frac{\sin^2[\pi i/(2k+1)]}{\sin^2[\pi ki/(2k+1)]}=4\cos^2\left(\frac{\pi i}{2(2k+1)}\right).$$

For $\tau_0=-2$ and $i=2j+1$, we have

$$\frac{4\Delta}{1+\Delta P_k^2(z_i)}\leqslant 4\sin^2\frac{\pi i}{2k+1}\Leftrightarrow\Delta\leqslant\frac{\sin^2[\pi i/(2k+1)]}{\cos^2[\pi ki/(2k+1)]}=4\cos^2\left(\frac{\pi i}{2(2k+1)}\right).$$

Note that the bound for Δ is a decreasing function of i for $1\leqslant i\leqslant 2k$. To finish, note that for $\Delta<2$, every z_i for $i\leqslant k$ satisfies the above inequality. For $\Delta<4$, the critical energy z_1 remains so for large enough k. □

Remark 2: From the condition that, for $\epsilon=0$, $|\Delta-z_i|\leqslant 2$ if, and only if, $E=v_a+z_i$ is a critical energy, we obtain $z_{\max}=2\cos[\pi/(2k+1)]$. This relates to the critical energy referred to in Theorem 2(iii). This also proves Corollary 1.

F. Primitive cluster maps

In this subsection, we comment upon cluster maps of the form $\mathfrak{C}:\mathcal{A}\to\mathcal{A}^*$, i.e., *substitutions*.[16] Fixing one such cluster map, it can be iterated on random sequences and, providing conditions so that it is a contraction, its fixed point is a substitution sequence. Thus we have a sequence of random locally correlated potentials converging to a potential with long range order (compare Ref. 1).

One extra requirement is that $\mathfrak{C}$ be *primitive:* there exists $k\geqslant 1$ such that for any $a\in\mathcal{A}$, $\mathfrak{C}^k(a)$ contains all letters of $\mathcal{A}$. Without loss of generality we assume $k=1$. We call the extension of such

$\mathfrak{C}$ to $\mathcal{A}^{\mathbb{Z}}$ a *primitive cluster map*. Note that $\mathfrak{C}(v)$, for any $v \in \mathcal{A}^{\mathbb{Z}}$, has also a long range order for primitive $\mathfrak{C}$: this is the bounded gap property for one letter. Further iterations will give rise to larger words occurring in bounded gaps in $\mathfrak{C}^n(v)$.

Theorem 3: *Let $\mathfrak{C}:\mathcal{A}^{\mathbb{Z}} \to \mathcal{A}^{\mathbb{Z}}$ be a primitive cluster map. If the second letter of $\mathfrak{C}(a)$ is the same for every $a \in \mathcal{A}$, then $\mathfrak{C}$ is a contraction.*

In this sense, given $u \in \mathcal{A}^{\mathbb{Z}}$, $\mathfrak{C}^n(u)$ provides a sequence of random cluster potentials converging to an almost periodic one.

Remarks: (i) The assumption on the second letter is due to the definition of $\mathfrak{C}(u)$, $u=(u_n)$, so that the second letter of $\mathfrak{C}(u_0)$ sits at the zeroth position of $\mathfrak{C}(u)$. This assumption in turn is necessary for

$$\lim_{n\to\infty} \mathfrak{C}^n(a)$$

to pertain to $\mathcal{A}^{\mathbb{Z}}$, for each $a \in \mathcal{A}$. In fact, here we also need $|\mathfrak{C}(a)| \geqslant 3$, but this can be accomplished by redefining the substitution $\mathfrak{C}$ on $\mathcal{A}$ as some power of itself.

(ii) It is known that, for primitive substitutions, the finite alphabet $\mathcal{A}$ splits into disjoint classes $\mathcal{A}_j$, $j=1,\ldots,r$, such that, for some $k \geqslant 1$, for each $a \in \mathcal{A}_j$, $\mathfrak{C}^k(a)$ begins with a fixed $a' \in \mathcal{A}_j$. We can relax the assumption above to

for each $a \in \mathcal{A}_j$, *the second letter in $\mathfrak{C}^k(a)$ also belongs to $\mathcal{A}_j$.*

Thus we get r fixed points. The Rudin–Shapiro substitution is an example of this more general setting.

(iii) The hull of an almost periodic sequence u, $\Omega(u)$, is the set of $v \in \mathcal{A}^{\mathbb{Z}}$ such that any finite word occurring in v occurs in u. With this definition it is clear that the limit above yields a sequence in its hull.

(iv) The above assumption can be adjusted to a given substitution: for instance, for the Thue–Morse substitution, $\mathfrak{C}(a)=abbabaab$, $\mathfrak{C}(b)=baababba$, we may use the fourth letter in place of the second.

(v) If $\mathfrak{C}$ is primitive and palindromic, critical energies appearing in $\mathfrak{C}(u)$ for a random u will be given by Theorem 1. In $\mathfrak{C}^2(u)$, these critical energies are preserved, but others may appear as other tessellations by palindromes are generated.

IV. NUMERICAL EXPERIMENTS

In these numerical experiments, we first analyze the behavior of the Lyapunov exponent $\gamma(E)$ near a critical energy E^*. Fixing $\epsilon > 0$ we perform an average of $\gamma(E)$ over a number of realizations of the Schrödinger operator for a finite size lattice. From a fitting procedure, we extract the value of the exponent ν in the expression

$$\gamma(E) \sim C|E-E^*|^{\nu} \quad \text{for small} \quad |E-E^*|.$$

We use the finite basis approximation in the Thouless formula to calculate $\gamma(E)$, $E \in [-2+v_a, 2+v_b]$ (recall that $v_b > v_a$). Fluctuations in $\gamma(E)$, when it is small, spoil the calculation of the exponent ν, and this is why we perform an average over the hull. Since we do not have actual bounds on $|E-E^*|$, a numerical calculated ν is expected to be a rough approximation. Figure 1 illustrates the procedure to estimate the exponent ν.

For the random dimer potential, Bovier[5] has found that $\nu=2$. A look at the calculations showing how the linear term vanishes in the expansion of $\gamma(E)$ and the expression of the leading (second) order term permits us to guess that ν does not increase for the random cluster model (compare Ref. 11). For comparison, we present the numerical values of ν for the dimer case as well, calculated using the same procedure. However, Bovier's hypothesis that the invariant measure (its density, in fact) has a Taylor expansion in the vicinity of the critical energy is not necessarily true in these general models.

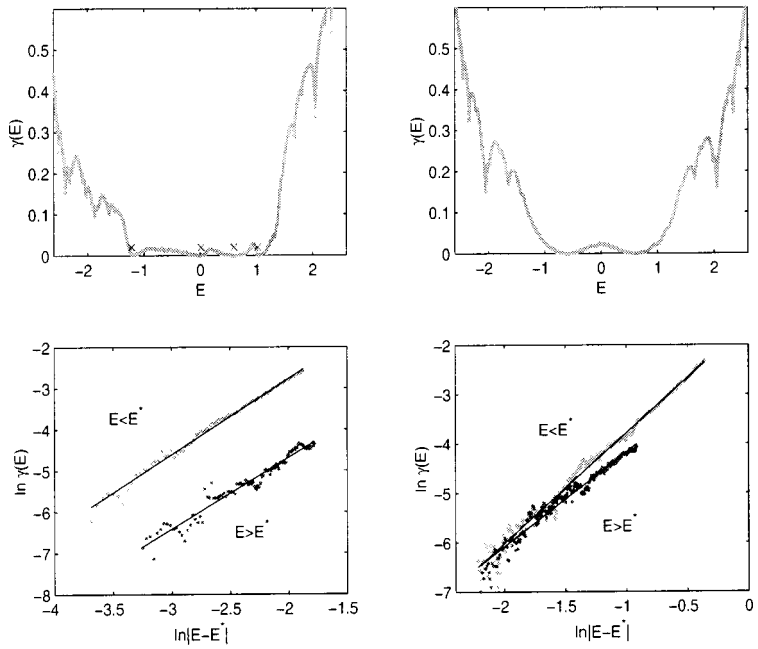

FIG. 1. On top, the graphs of the Lyapunov exponent with disorder $\Delta=1.2$, the *random palindrome model* on the left and the *random dimer* on the right. The bottom figures show examples of dilog fitting of the Lyapunov exponent: On the left, for the *random palindrome model*, near the critical energy $E^*=-1.197$, coming from the first minimum for $\epsilon=0$ (the minima for $\epsilon=0$ occur at $2\cos \pi i/5-0.6$, $i=1,2,3$, and at 0.6, positions marked with $\times$). As seen, the right branch $E<E^*$ approaches zero faster than the left branch $E>E^*$: the slopes of the fitting lines are 1.8 and 1.7, respectively. On the right, for the *random dimer* near $E^*=-0.6$, we get the slopes 2.2 for the left branch and 1.9 for the right branch.

We then perform the time evolution of a packet initially located at the central position of a finite lattice. We integrate the time-dependent Schrödinger equation using a sympletic integrator, the details of which have been explained elsewhere.[7]

We address the question whether propagation over the lattice is enhanced as an effect of the local order compared with the random dimer. We do this by computing the exponent α in the asymptotic regime of

$$[m_2(t)]^2=\sum_{n\in\mathbb{L}} n^2|\psi_n(t)|^2\sim Ct^{2\alpha},$$

where $\mathbb{L}=[-L+1,L]\cap\mathbb{Z}$ is the finite lattice [we used basis sizes up to 2 (Ref. 14)]. For the dimer, $\alpha=\frac{3}{4}$,[9] and we obtain, for the palindrome C_a of size 5, that α is higher at the beginning, but settles down to around $\frac{3}{4}$ at later times.

Table I summarizes the results on transport. For the extreme disorders considered, there is a clear transient behavior. On the one hand, for small Δ it appears that the potential is more transparent, but around $t=1000$, there is a change in slope in a curve $\log m_2$ vs $\log t$. This is why we consider the time span only for $\log t>7$ until the packet reaches the border of the lattice, with probability greater than 10^{-8}. On the other hand, for large Δ, the lattice conducts poorly at the beginning, but after $\log t>7$, m_2 also shows a power law behavior. When Δ is increased α decreases. Furthermore, the disorder can be larger than 2 maintaining superdiffusive behavior: from this we can say that conduction is enhanced in the random palindrome model as compared to the random dimer.

The reason for the higher α for short times and small disorder Δ stems from the extra critical energies, which forces $\gamma(E)$ to be small in a larger portion of the spectrum. This also explains why the ν column in Table I is not a decreasing function of the disorder. The leftmost critical energy for

TABLE I. The growth exponent α and the behavior of $\gamma(E)$ near the critical energy E^* for increasing disorder in the random palindrome model with cords $C_a=aaa'aa$ and $C_b=bb$.

Δ	ν (left branch)	E^*	α	Time span t $\ln T_1-\ln T_2$ $T_1<t<T_2$
0.2	2.2	−1.720	0.78	7–9
0.6	0.8	−0.913	0.73	7–9
1.2	1.8	−1.197	0.75	0–9
2	1.1	−0.3855	0.68	0–9.5
3	1.1	0.1826	0.67	7–10

small Δ ceases to be so around $\Delta=0.38$ for $k=5$. For $\Delta=0.6$, γ is still not growing sufficiently fast off the critical energy -0.913: it is as small as 0.036 at $E=-1.75$, just ten times its minimum value attained at 0.913. For long enough times, the exponential decay eventually sets in so only those states with localization lengths of the order of the lattice size or larger contribute to transport up until the packet reaches the border. Briefly, we have numerically found that α, the exponent measuring transport, does not increase if we have a finite number of contributing critical energies, all of them with the same exponent $\nu\leqslant 2$.

We can make the dimer critical energy and one of the critical energies due to the palindrome C_a for $\epsilon=0$ coalesce, by taking $\Delta=2\cos 2\pi/5$. It is reasonable to expect that $\gamma(E)$ will have a higher tangency at the corresponding critical energy, $E^*=\cos 2\pi/5$, or, more precisely, that $\nu(E^*)$ will be greater than 2. Even though this is apparently true (as we saw numerically), we did not observe an increase in α, which continued around 0.75.

We also investigated the following interesting example: C_a a palindrome whose potential looks like a staircase:

$$-\frac{\varphi(C_a)}{\Delta/2}=\{0.4,0.6,0.8,1,0.8,0.6,0.4\}$$

and $C_b=bb$. We obtain qualitatively the same behavior, as displayed in Figure 2, fixing $\Delta>0$, and computing $\gamma(E)$ and $m_2(t)$. We also get apparent critical energies even for $\Delta>4$, where $\gamma(E)\approx 0$ [however, this could be credited to the disorder definition, which is $\max\{\varphi(u)-v_b, u\in C_a\}$].

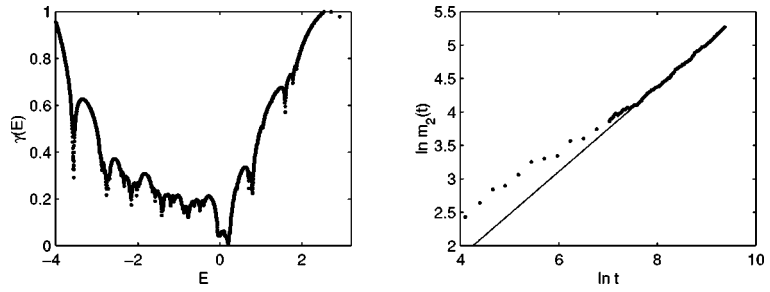

FIG. 2. The Lyapunov exponent for disorder $\Delta=4.2$ and palindrome $C_a=u_1u_2u_3u_4u_3u_2u_1$ of length 7, such that the values of the potential are $\varphi(u_i)=(\Delta/2)(1-0.2|i-4|)$. The approach to zero at $E\approx 0.2$ has $\nu=0.5$ from the left and $\nu=0.8$ from the right. On the right plot, the mean square displacement together with the linear fitting using data for $t>e^{7.5}$, from which we get the slope $\alpha=0.64$.

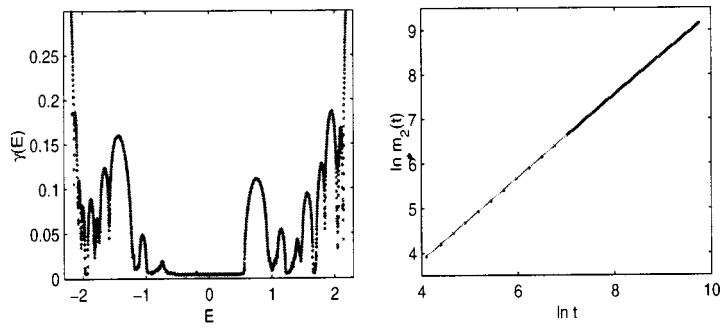

FIG. 3. The Lyapunov exponent for the sequence $\mathfrak{C}^2(u)$, u a random sequence, and disorder $\Delta=0.8$. Note the flat behavior on an interval containing the critical energies -0.4 and 0.4: there $\gamma(E)\leqslant 5\times 10^{-3}$. On the right, the mean square displacement data are shown in dots and the line obtained by a fitting has angular coefficient $\alpha=0.92$.

Finally, we consider a random palindrome model with a primitive cluster map (see Sec. III F). The map $\mathfrak{C}(a)=abbba$ and $\mathfrak{C}(b)=aba$ for $\mathcal{A}=\{a,b\}$ has the one-letter bounded gap property on the image sequence. Since the second letter of $\mathfrak{C}(a)$ and $\mathfrak{C}(b)$ is the same, then independently of the initial sequence v in $\mathcal{A}^{\mathbb{Z}}$, $\mathfrak{C}^n(v)$ tends, for $n\to\infty$, to

$$\cdots abbbaa\cdot baabbba\cdots,$$

which is the limit sequence of $\mathfrak{C}^n(b)$ (recall that the central dot marks, to its right, the zeroth position). Critical energies can be determined from the commutation of the transfer matrices $\Phi(\mathfrak{C}(a))$ and $\Phi(\mathfrak{C}(b))$.

For $\Delta\leqslant 1$ we have two critical energies, when $E=v_a$ and $E=v_b$, and only $E=v_a$ for $1<\Delta\leqslant 2$. The commutation of the transfer matrices corresponding to each cluster is the sole responsible for the critical energies upon the first iteration of $\mathfrak{C}(u)$, for a random $u\in\mathcal{A}^{\mathbb{Z}}$, cf. Proposition 1. We considered, however, the random cluster $w=\mathfrak{C}^2(u)$, with u a random sequence in $\mathcal{A}^{\mathbb{Z}}$. The sequence w has the bounded gap property for the words $\mathfrak{C}(a)$ and $\mathfrak{C}(b)$, whose corresponding transfer matrices commute at the critical energies $E=0.4$ and $E=-0.4$. There appears a new numerical behavior in both $m_2(t)$ and $\gamma(E)$, with an apparent boost in transport $\alpha\approx 0.92$, as seen in Fig. 3.

ACKNOWLEDGMENTS

T.O.C. was partially supported by FAPESP and C.R.O. was partially supported by CNPq.

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New summation technique for rapidly divergent perturbation series. Hydrogen atom in magnetic field

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(Received 7 October 2002; accepted 4 December 2002)

The perturbation series for the ground state energy of the hydrogen atom in the external magnetic field is summed via the sequence transformations. The formula for the large-order behavior of the partial sums of the series is derived. From this formula a new general sequence transformation is suggested. This transformation contains free parameters that can be further optimized. It is shown that if the renormalization approach is used, the optimal choice of these parameters leads to the previously suggested Weniger transformation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1541119]

I. INTRODUCTION

The hydrogen atom in a constant magnetic field is an elementary but tricky problem, and great deal of effort has been devoted to the solution of this problem (see, e.g., Refs. 1–20 and references therein). It is of special interest from the point of view of the summation of the divergent perturbation series. Searching for the solution of the Schrödinger equation,

$$\left[-\frac{\nabla^2}{2}-\frac{1}{r}+\frac{B^2}{8}(x^2+y^2)\right]\psi=E\psi, \tag{1}$$

in the form of the Rayleigh–Schrödinger perturbation series in the powers of the intensity of the constant magnetic field B

$$E=-\frac{1}{2}+\sum_{n=1}^{\infty}E_n\left(\frac{B^2}{8}\right)^n, \tag{2}$$

it appears that the perturbation coefficients E_n behave for large n as[1–4]

$$E_n=(-1)^{n+1}\left(\frac{4}{\pi}\right)^{5/2}\left(\frac{8}{\pi^2}\right)^n\left(2n+\frac{1}{2}\right)!\,(1+O(1/n)). \tag{3}$$

It means that the series (2) diverges for every $|B|>0$. Moreover, because of the peculiar logarithmic behavior of the energy for high magnetic fields,[5] the series is known to be one of the most difficult summable divergent series encountered in physics. Particularly, it is known[2] that the series is not efficiently summed by the Padé approximants, the most widely used summation technique (see, e.g., Refs. 21–23). Some time ago a new method for the summation of the divergent series, the so-called Weniger summation, was introduced.[24,25] This method was combined with the renormalization approach[26] and succesfully applied to the one-dimensional anharmonic oscillators.[24] Since there have been only a few attempts to sum the series for the hydrogen atom in the magnetic field,[2,6,7] we apply the Weniger summation technique to this problem to better understand its advantages and drawbacks.

The article is organized as follows. In Sec. II, the large-order behavior of the partial sums of the series (2) is derived. On the basis of this behavior a new general sequence transformation is suggested. This transformation contains free parameters that can be further optimized. In special

cases, both previously suggested Levin[23,27,28] and Weniger,[24,25] sequence transformations are obtained. In Sec. III, the renormalization of the energy and the coupling constant is made. In the final section, Sec. IV, discussion of the results and a few general remarks on the sequence transformations are made.

II. SEQUENCE TRANSFORMATIONS

On the basis of some heuristic arguments we suggest in this section a new sequence transformation. We shall proceed in an intuitive way and arguments given here should serve only as a basis for more rigorous treatment.

For the sake of simplicity, we replace the coefficients E_n of the series (2) by their large-order behavior (3) and consider the partial sums of such a series

$$s_m=\sum_{n=0}^{m} a_n, \tag{4}$$

where

$$a_n=C(-1)^{n+1}\left(\frac{B^2}{\pi^2}\right)^n\left(2n+\frac{1}{2}\right)! \tag{5}$$

and $C=(4/\pi)^{5/2}$.

Obviously, the partial sums (4) have no limit in ordinary sense and, consequently, the sum of the series Σa_n does not exist in ordinary sense. Nevertheless, we can try to give some meaning to the sum of such a series. Namely, we can try to fit the partial sums (4) to a finite number of terms. The most natural way of doing it is to write the system of l equations

$$s_m=c_0a_m+c_1a_{m-1}+\cdots+c_{l-2}a_{m-l+2}+s, \quad m=n-l+1,\ldots,n, \tag{6}$$

for l unknown coefficients $c_0,c_1,\ldots,c_{l-2}$ and s. As discussed below, the coefficient s has the meaning of the generalized sum of the series. Since the index of the coefficient a_{m-l+2} has to be greater or equal to zero, and since the smallest value of m is $n-l+1$, we take l as the integer part of $(n+3)/2$.

Now, we extend the meaning of the limit to the sequence $(-1)^{n+1}(2n+\frac{1}{2})!$. Particularly, if we say that such a sequence exhibits ''regular oscillations'' and its generalized limit is zero, then the divergent regular oscillations c_ia_i are singled out by the transformation (6) and the remaining constant term s approaches with increasing n the generalized sum of the series $\Sigma_{n=0}^{\infty}a_n$.

This transformation yields nothing but Padé approximants $[n,n]$ and $[n-1,n]$ for n even and odd, respectively. This is most easily seen by transforming the system of Equations (6) to the system of equations for computing the Padé approximants, [see, e.g., Eq. (3.10) in Ref. 24].

However, the Padé summation (6) does not work efficiently enough for the series with the coefficients growing like $(-1)^n(2n)!$ (see, e.g., Ref. 2), which is also our case. The transformation (6) for such a series is not able to single out all of the regular oscillations and a more efficient method has to be found.

Let us insert the explicit form of the coefficients a_n, Eq. (5), into the system of the equations for the partial sums (6). Then, this system can be rewritten into the form

$$s_m=C(-1)^{m+1}(2m+1/2)!(B/\pi)^{2m}\left(c_0+c_1\frac{\pi^2}{B^2(2m-\frac{1}{2})(2m-\frac{3}{2})}\right.$$
$$\left.+c_2\frac{\pi^4}{B^4(2m-\frac{1}{2})(2m-\frac{3}{2})(2m-\frac{5}{2})(2m-\frac{7}{2})}+\ldots\right)+s. \tag{7}$$

For large m, the partial sums s_m behave as

$$s_m = C(-1)^{m+1}\left(2m+\frac{1}{2}\right)!\left(\frac{B}{\pi}\right)^{2m}\left(d_0+\frac{d_1}{m+1}+\frac{d_2}{(m+1)^2}+\ldots\right)+s, \tag{8}$$

where the coefficients d_i can be obtained from the coefficients c_i by expanding Eq. (7) into the asymptotic series in the powers of $1/(m+1)$. If we fitted the partial sums s_m to the infinite number of the coefficients c_i or d_i, there would be no difference between the sequences (7) and (8). However, if we fit the partial sums s_m to a *finite* number of the coefficients c_i or d_i, the sequence transformation (8) accounts better for the large-order behavior of the partial sums s_m than the transformation (7).

On the basis of these considerations we suggest a new generalized sequence transformation

$$s_m = a_m\left(d_0+\frac{d_1}{(m+q_1)}+\frac{d_2}{(m+q_1)(m+q_2)}+\ldots+\frac{d_{l-2}}{(m+q_1)(m+q_2)\ldots(m+q_{l-2})}\right)+s, \qquad m=n,\ldots,n+l-1, \tag{9}$$

where q_i, $i=1,2,\ldots,l-2$, are arbitrary coefficients that have to be determined from some additional requirement and n denotes the index of the first partial sum taken into account. In principle, it can be arbitrary; however, for fast convergence of the method it is convenient to take it close, but not necessarily equal, to zero (see below).

Equations (9) represent a system of l equations for l unknowns $d_0, d_1, \ldots, d_{l-2}$ and s. It is remarkable that, regardless of the particular form of the coefficients q_i, the system of equations (9) can be solved in the closed form, namely

$$s = s_n + \frac{\Sigma_{j=0}^{l-1}(-1)^j[(l-1)!/(l-1-j)!j!]\,\Pi_{i=1}^{l-2}(j+n+q_i)(s_{j+n}-s_n)/a_{j+n}}{\Sigma_{j=0}^{l-1}(-1)^j[(l-1)!/(l-1-j)!j!]\,\Pi_{i=1}^{l-2}(j+n+q_i)1/a_{j+n}}. \tag{10}$$

This can be interpreted that the sum of the series is the nth partial sum plus a correction involving partial sums of higher order. This result, which is the main result of this article, was derived by generalizing the procedure for derivation of the Levin[23] and Weniger[24] transformations. In special cases $q_i=1$ and $q_i=i$, the Levin and Weniger transformations are obtained, respectively.

III. RENORMALIZATION

In this section, the renormalization of the energy and the coupling constant is discussed.

Proceeding similarly as in Ref. 26, we make the scaling transformation $x\to(1-\kappa)x$, $y\to(1-\kappa)y$ and $z\to(1-\kappa)z$. Equation (1) then becomes

$$(1-\kappa)^{-2}\left[-\frac{\nabla^2}{2}-\frac{1-\kappa}{r}+\frac{B^2}{8}(1-\kappa)^4(x^2+y^2)\right]\psi = E\psi. \tag{11}$$

Introducing the renormalized coupling constant κ related to the coupling constant B via the equation

$$\frac{B^2}{8}=\frac{\kappa}{4(1-\kappa)^4} \tag{12}$$

and the renormalized energy E_R

$$E_R(\kappa)=(1-\kappa)^2E(B) \tag{13}$$

we get from Eq. (11)

TABLE I. The energies E obtained by the summation of the ordinary series for the hydrogen atom in the magnetic field. The sequence transformation (10) for Weniger ($q_i=i$) and quadratic ($q_i=i^2$) choices of the coefficients q_i and the Padé approximants are compared. Only the numbers stabilized for l from 70 to 79 in Eq. (10) are displayed. The constant n in Eq. (10) was set to zero. "-" means that no stabilization was achieved.

B	Weniger	Quadratic	Padé [39,40]	Padé [39,39]
0.6	−0.4274622877	−0.427462287	−0.4274619	−0.4274626
1.0	−0.33116	−0.331168	−0.33105	−0.33128
2.0	-	−0.0221	−0.00648	−0.03868

$$\left[-\frac{\nabla^2}{2}-\frac{1}{r}+\kappa\left(\frac{x^2+y^2}{4}+\frac{1}{r}\right)\right]\psi=E_R\psi. \tag{14}$$

The advantages of the renormalization approach were discussed in detail in Refs. 24, 26, and 29–32 and can be summarized as follows. First, the originally unbounded interval of the magnetic fields $B\in(0,\infty)$ is shrunk to the interval $\kappa\in(0,1)$. Second, in contrast to the ordinary energy E, the renormalized energy E_R remains finite at the point $\kappa=1$ corresponding to $B\to\infty$. The constant 4 in the denominator of Eq. (12) is the result of the optimization procedure suggested in Ref. 26.

The renormalized energy $E_R(\kappa)$ can be expanded into the power series in the coupling constant κ,

$$E_R=-\frac{1}{2}+\sum_{n=1}^{\infty} b_n\kappa^n. \tag{15}$$

Proceeding analogously to Refs. 32 and 33 we find that the coefficients b_n behave for large n as

$$\lim_{n\to\infty}\frac{b_n}{E_n}=\frac{1}{4^n}. \tag{16}$$

Therefore, the rate of the divergence of the coefficients b_n, although somewhat milder, is essentially the same as that of the coefficients E_n.

IV. RESULTS AND DISCUSSION

In this section, we discuss the application of the sequence transformation (10) to the series (2) and (15).

The perturbation coefficients E_n and b_n can be calculated either by using the so(4,2) algebraic formulation of the perturbation theory[2,10] or the Bender–Wu difference equation method described in Appendix D of Ref. 2. We calculated 80 coefficients E_n and b_n in the rational form using MAPLE. The coefficients a_j in Eq. (10) were set to $a_j=E_{j+1}B^{j+1}$ or $a_j=b_{j+1}\kappa^{j+1}$ for $j=0,1,2...$ and the partial sums s_j were calculated via Eq. (4). The zeroth-order coefficient $-\frac{1}{2}$ was added to the sum s at the very end of calculations in both the ordinary and renormalized cases.

The results obtained with the sequence transformation (10) for different choices of the coefficients q_i are compared to those obtained via the Padé approximants in Tables I and II. We found, in agreement with the earlier observation made in the case of the sextic anharmonic oscillator,[24] that except for the fields smaller than $B\approx0.2$ the Levin transformation ($q_i=1$) fails to sum the series (2). The same is true also in the renormalized case. To find the reason for this failure we replaced the actual values of the E_n coefficients by the values given by the large-order formula (3). In this case the Levin choice of the coefficients q_i yields the best results. Therefore, we believe that the reason for failure of the Levin transformation to sum the series (2) is that the large-order formula (3), and consequently also the large-order formula (8), is only asymptotic, i.e., holds only for a sufficiently large m. To remain valid for small values of m, the series (8) has to be truncated after few terms. The smaller m, the sooner the series (8) has to be truncated. Therefore, it is

TABLE II. The energies E obtained by the summation of the renormalized series for the hydrogen atom in the magnetic field. The sequence transformation (10) for different choices of the coefficients q_i and n is compared with the Padé approximants and the results obtained in Ref. 12 with completely different nonperturbative method. The displayed numbers are stabilized for l from 70 to 79 and for l from 65 to 74 for $n=0$ and $n=5$ respectively.

B	Weniger ($n=0$)	Quadratic ($n=0$)	Weniger ($n=5$)	Quadratic ($n=5$)	Padé	Ref. 12
0.6	−0.4274622877571	−0.42746228	−0.4274622877571	−0.42746228775	−0.427462	−0.42746227877
1.0	−0.331168896	−0.331168	−0.3311688967	−0.33116889	−0.331	−0.33116889
2.0	−0.022213	−0.0221	−0.022213	−0.02221	−0.02	−0.0222139
3.0	0.3354	0.335	0.33546	0.33548	0.33	0.33546
10.0	3.253	3.26	3.252	3.254	3.	3.252
20.0	7.79	7.8	7.78	7.8	7.	7.784

important for efficiency of the sequence transformation (9) that the contribution of the individual terms $d_i/[(m+q_1)(m+q_2)\cdots(m+q_i)]$ in Eq. (9) decreases for small m with increasing i. This is better accomplished by the Weniger choice $q_i=i$ than by the Levin choice $q_i=1$. The decrease has to be moderate; if the growth of the coefficients q_i is too large (e.g., quadratic), the contribution of the terms $d_i/[(m+q_1)(m+q_2)\cdots(m+q_i)]$ in Eq. (9) is suppressed with increasing i not only for small m, but also for large m. Then we fit the partial sums s_m only to few constants d_i and the transformation (9) becomes inefficient again. This is well illustrated in Tables I and II. We see that if the coupling constant B or κ is sufficiently small, i.e., either the external magnetic field is small or the renormalization is made, the Weniger choice $q_i=i$ provides the best results. However, if the coupling constant is too large, the Weniger transformation becomes also unstable and the best result yields the quadratic choice $q_i=i^2$.

Further, we note that the efficiency of the Weniger sequence transformation with respect to the Padé approximants decreases with the increasing value of the coupling constant. Indeed, in the case of the ordinary series the Weniger transformation for the field $B=0.2$ gives the result $-0.490\,381\,565\,034\,762\,584\,774\,394\,74$ which is by ten orders more accurate than the result produced by the Padé approximants. However, for $B=1.0$, the Weniger transformation is only by two orders better than the Padé approximants (see Table I).

The results displayed in Table II show that the results of the summation depend slightly on the choice of n in Eq. (10). Particulary, it is seen that better results for the series (15) are achieved for $n=5$ than for $n=0$. The reason for it is the following. Due to the term $1/r$ in the interaction part of Eq. (14), the first few b_n coefficients in Eq. (15), and consequently also the first few partial sums s_n, behave irregularly (for detailed discussion see Ref. 32). Therefore, it is better to start with n around 5 when these irregularities do not play significant role.

As it is seen from Table II, the results obtained by the sequence transformation (10) agree with the results given in Ref. 12 obtained by a completely different nonperturbative method based on the rigorous Kato inequalities for the operators in the Hilbert space. The only disagreement is for the field $B=0.6$. Since otherwise our results agree with these results, the result given in Ref. 12 for $B=0.6$ contains probably a typographical error.

We also compared our method with the Borel summation and order dependent mapping (ODM) performed in Ref. 7. For this purpose we considered only the first 62 perturbation coefficients as in Ref. 7. The comparison shows that the Weniger method yields results of similar accuracy as the Borel summation up to the field strength $B=20.0$. It is of the same accuracy as ODM up to the field strength $B=1.0$. For larger fields, it yields worse results than ODM. However, it is due to the fact that we did not incorporate into our method behavior of the energy for very large magnetic fields.[5] Moreover, the method given in this paper is both conceptually and technically simpler than those given in Ref. 7.

It is worth remarking the question whether the series (2) does uniquely define the energy $E=E(B^2)$. If the series (2) is the Stieltjes series, then it does (see, e.g., Refs. 21 and 22). In such a case, $[n-1,n]$ and $[n,n]$ Padé approximants provide monotonically decreasing upper bounds and monotonically increasing lower bounds to the exact eigenvalue. Moreover, if the coefficients of

the series do not grow more rapidly than $(-1)^n(2n)!$ (which is also our case), then the sequences $[n-1,n]$ and $[n,n]$ converge to the same value. We do not know the rigorous proof that the series (2) is a Stieltjes one. However, the numerical results indicate strongly that this is really the case. Particularly, if the zeroth term of the series is excluded, then $[n,n]$ and $[n-1,n]$ Padé approximants provide lower and upper bounds to the energy $E(B^2)$ (see Table I and Ref. 2). The renormalized series (15) is not the Stieltjes series. However, it was shown in Ref. 32 on an analogous problem of the one-dimensional anharmonic oscillator that the series (15) consists of a divergent Stieltjes part and a rapidly convergent part (the rate of the convergence is geometric).

Summarizing, we found in this article the large-order behavior of the partial sums of the strongly divergent perturbation series. On the basis of this behavior a new general sequence transformation containing free parameters that can be subject of further optimalization was suggested. This sequence transformation was applied to the problem of the hydrogen atom in the constant magnetic field. Numerical analysis shows that for small values of the coupling constant, the best choice of the parameters leads to the previously suggested Weniger transformation. Such small values of the coupling constant can be achieved even for large fields, by utilizing the idea of the renormalization. Although most of our discussion was restricted to the summation of the series for the ground state energy of the hydrogen atom in magnetic field, we believe that suggestions made in this article are of much broader importance. Particulary, they show that even violently diverging series behaving as $(-1)^n(2n)!$ can be summed to accurate and realiable results.

ACKNOWLEDGMENTS

The authors would like to thank the GA UK (Grant Nos. 166/00 and 180/02), the GA CR (Grant No. 202/00/1026), the MSCR (Grant No. 100-01/206053) of the Czech Republic and NSERC of Canada (J.Z. is a NATO Science Fellow) for the support.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 3 MARCH 2003

Preserving the measure of compatibility between quantum states

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(Received 28 November 2002; accepted 12 December 2002)

In this article after defining the abstract concept of compatibility-like functions on quantum states, we prove that every bijective transformation on the set of all states which preserves such a function is implemented by an either unitary or antiunitary operator. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1545164]

In the last couple of years several communications have appeared in connection with the following problem raised by R. Peierls:[8] when different density matrices can characterize the knowledge available to different people about one and the same physical system. The first answer given by Peierls in Refs. 8 and 9 was that the density matrices under consideration must commute and their product must be nonzero. However, C. Fuchs[4] (also see Ref. 5) gave an example which made Peierls' first condition questionable. After that several attempts have been made to find the proper solution of the problem (e.g., Refs. 1 and 5). All those attempts operate with the concept of compatibility of density matrices. According to them, we say that a collection of density matrices is compatible if the supports of the matrices under consideration (i.e., the orthogonal complements of their null spaces) have nontrivial intersection. So, it is just an easy task to determine whether a pair of density matrices is compatible or not. Having this in mind, it is now a natural problem to give sense to the following question: if a pair of density matrices is compatible, then ''how much'' compatible they are. In other words, we arrive at the problem of measuring the compatibility. One possibility to define such a measure was described in Ref. 10. Namely, in some analogy with the fidelity, C. Poulin and R. Blume-Kohout defined a compatibility function (Ref. 10, Definition 1) which fulfills certain natural physical requirements and they proved some important properties.

In our recent paper[7] we have determined the structure of the bijective transformations on the set of all density operators which preserve the fidelity. This result is in close relation with Wigner's theorem on symmetry transformations. In fact, it can be considered as a Wigner-type result for the set of all mixed states (recall that Wigner's original result concerns the pure states). In Ref. 7 we proved that the transformations in question are all implemented by unitary or antiunitary operators on the underlying Hilbert space. In view of this result and the analogy between the fidelity and the measure of compatibility defined by Poulin and Blume-Kohout, it is a natural problem to determine the structure of the bijective transformations of the set of all density matrices which preserve the compatibility function. We shall see below that the solution of this problem is the same as the one concerning fidelity. This is the content of the present article.

Let us begin with the notation. Let H be a (complex, not necessarily finite dimensional) Hilbert space. If not stated otherwise, all operators on H are meant to be bounded and linear. The expression rng A denotes the range of the operator A. If A is positive, $A^{1/2}$ stands for its unique positive square root.

Denote by $S(H)$ the set of all states (or, in another terminology, density operators) on H, i.e., the positive trace-class operators on H with trace 1. The set $S(H)$ is a convex subset of the space

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of all self-adjoint operators on H and its extreme points (which are exactly the rank-one projections) are called pure states.

Now, instead of using the concept due to Poulin and Blume-Kohout, we define the abstract concept of compatibility-like functions which extends Ref. 10, Definition 1, to obtain a result of higher generality.

Definition 1: Let $C: S(H)\times S(H)\to[0,1]$ be a function such that for any pair $A,\ B\in S(H)$ of states we have

(i) $C(A,B)=0$ if and only if $\mathrm{rng}\ A^{1/2}\cap \mathrm{rng}\ B^{1/2}=\{0\}$,

(ii) $C(A,B)=C(B,A)$, and

(iii) if P is a pure state, then

$$C(A,P)^2=\sup\{\lambda\in[0,1]:\lambda P\leqslant A\}.$$

We say that C is a compatibility-like function on the set of all states on the Hilbert space H.

Several remarks should be made concerning the above definition. First, we emphasize that our definition is formulated for both finite and infinite dimensional Hilbert spaces (in Ref. 10, Definition 1, only finite dimensional spaces were considered). Concerning the correctness of the definition we note the following. The quantity on the right hand side of the equality in (iii) also appears in relation with effects. A self-adjoint operator T on H with the property $0\leqslant T\leqslant I$ (I is the identity operator) is called an effect. The effects are well-known to play important roles in the quantum theory of measurement (e.g., Ref. 3). Now, it is clear that every state on H as a linear operator can also be viewed as an effect. If T is an effect, φ is a unit vector in H, and P_φ denotes the rank-one projection onto the subspace generated by φ, then the quantity

$$\lambda(T,P_\varphi)=\sup\{\lambda\in[0,1]:\lambda P_\varphi\leqslant T\}$$

is called the strength of T along the ray represented by φ. This concept was introduced by Busch and Gudder in Ref. 2. It was proved in Ref. 2, Theorem 3, that $\lambda(T,P_\varphi)=0$ if and only if $\varphi\notin \mathrm{rng}\ T^{1/2}$, which is equivalent to $\mathrm{rng}\ T^{1/2}\cap \mathrm{rng}\ P_\varphi^{1/2}=\{0\}$. This means that there is no contradiction between the conditions (i) and (iii).

Observe that if H is finite dimensional, then the ranges of a positive operator and its square root are the same and they are automatically closed. Therefore, in the finite dimensional case we have

$$\mathrm{rng}\ A^{1/2}=\mathrm{rng}\ A=\overline{\mathrm{rng}\ A}=(\ker A)^\perp,$$

and hence (i) says that $C(A,B)>0$ if and only if $A,\ B$ are compatible in the sense mentioned in the Introduction. The meaning of (ii) is clear. Now, what about (iii)? One might think that this condition is quite restrictive and probably has no physical meaning for states. But it can be shown that the compatibility function defined by Poulin and Blume-Kohout satisfies (iii) (see either Ref. 10, Definition 1 itself or Ref. 10, Theorem 3) as well as (i) and (ii). So, to sum up, our definition is a generalization of the one given by Poulin and Blume-Kohout and hence it certainly has sense at least from the mathematical point of view.

The reason why we assume (iii) is that there is a nice formula to compute $C(A,P)$. Namely, by Ref. 2, Theorem 4, for every unit vector $\varphi\in H$ we have

$$C(A,P_\varphi)^2=\lambda(A,P_\varphi)=\begin{cases}\|A^{-1/2}\varphi\|^{-2}, & \text{if } \varphi\in\mathrm{rng}(A^{1/2});\\ 0, & \text{otherwise.}\end{cases}\tag{1}$$

(Here $A^{-1/2}$ denotes the inverse of $A^{1/2}$ on $\mathrm{rng}\ A^{1/2}$.) The proof of our result is based on this correspondence.

We further note that it would be another natural assumption to suppose that C is invariant under unitary-antiunitary transformations. But, as we do not need it in our proof, we do not assume it.

To conclude our remarks, we show a natural example for a compatibility-like function which might also justify our definition. So, for any pair $A, B \in S(H)$ define

$$C(A,B) = \sup\Bigg\{ \sum_n \sqrt{\lambda_n \mu_n} : \lambda_n, \mu_n \in [0,1], \sum_n \lambda_n = \sum_n \mu_n = 1 \text{ and}$$

$$\exists \text{ pure states } Q_n \text{ with } \sum_n \lambda_n Q_n = A, \sum_n \mu_n B_n = B \Bigg\}.$$

It is easy to verify that this function has the properties (i)–(iii). In fact, in accordance with the discussions in Refs. 1 and 5, we believe that this compatibility-like function represents the most natural way of defining a measure of compatibility between quantum states.

Now, our result reads as follows.

Theorem 2: *Let H be a Hilbert space and let C be a compatibility-like function on $S(H)$. Let $\phi: S(H) \to S(H)$ be a bijective function which preserves C, that is, assume that*

$$C(\phi(A), \phi(B)) = C(A,B) \quad (A,B \in S(H)).$$

Then there exists an either unitary or antiunitary operator U on H such that ϕ is of the form

$$\phi(A) = UAU^* \quad (A \in S(H)).$$

Proof: Clearly, we can assume that $\dim H \geqslant 2$. For temporary use, we say that the states D, A are compatible (resp. incompatible) if $C(D,A) > 0$ [resp. $C(D,A) = 0$]. It is useful to introduce the following notation. If $\mathcal{M}$ is a subset of $S(H)$, then denote

$$\mathcal{M}^{ic} = \{D \in S(H) : C(D,A) = 0 \text{ for all } A \in \mathcal{M}\}.$$

By condition (i) in Definition 1, $C(D,A) = 0$ means that the subspaces rng $D^{1/2}$, rng $A^{1/2}$ of H have trivial intersection. It can be easily verified that the operator $A \in S(H)$ has rank one (which means that A is a pure state) if and only if

$$(\{A\}^{ic})^{ic} = \{A\}.$$

Since ϕ preserves the compatibility in both directions, it follows from this characterization that ϕ preserves the pure states in both directions. This means that $A \in S(H)$ is a pure state if and only if so is $\phi(A)$.

Next we assert that ϕ maps independent pure states to independent ones. Here, a set of n pure states (rank-one projections) is called independent if their ranges generate an n-dimensional subspace of H. To prove the assertion we use induction. The statement is obvious if the set has only one element. Let $\{P_1, \ldots, P_n, P_{n+1}\}$ be a set of $n+1$ pure states such that the subset $\{P_1, \ldots, P_n\}$ is independent. It is easy to see that $\{P_1, \ldots, P_n, P_{n+1}\}$ is dependent if and only if for any $A \in S(H)$ with $C(A,P_1) > 0, \ldots, C(A,P_n) > 0$ we have that $C(A,P_{n+1}) > 0$ holds too. Indeed, this follows from the fact that for any pure state P we have $C(A,P) > 0$ if and only if the range of P is included in the range of $A^{1/2}$ (see the remarks after Definition 1). Using the above description of dependence, it is now clear that assuming ϕ maps independent sets of n pure states to sets of the same kind, we have the same property of ϕ for $n+1$ in the place of n. Since ϕ^{-1} has the same properties as ϕ, we deduce that ϕ preserves the independence of the sets of pure states in both directions.

It is easy to see that an operator $A \in S(H)$ has rank n if and only if there exists an independent set of n pure states such that $C(A,P) > 0$ for every element of that set, but there does not exist a set of $n+1$ elements having the same property. This gives us that ϕ preserves the rank.

Now we prove that ϕ preserves the transition probability between pure states. Recall that for any pair P, Q of pure states, the transition probability between them is $\mathrm{tr}PQ$, where tr is the usual trace-functional. To verify the mentioned preserver property of ϕ, first let P, Q be rank-one projections with orthogonal ranges. Define

$$A=\lambda P+\mu Q,$$

where λ, μ are fixed and satisfy $0<\lambda<\mu<1, \lambda+\mu=1$. Clearly, A acts on the two-dimensional subspace H_A of H generated by the ranges of P, Q. [Here, the phrase that A acts on H_A means that $(\ker A)^{\perp}=\mathrm{rng}\,\overline{A}=\mathrm{rng}\,A=H_A$.] We assert that $\phi(A)$ acts on the subspace generated by the ranges of the independent pure states $\phi(P)$, $\phi(Q)$. Indeed, $\phi(A)$ has rank 2 and taking into account that

$$C(\phi(A),\phi(P))=C(A,P)>0, \quad C(\phi(A),\phi(Q))=C(A,Q)>0,$$

we see that the ranges of $\phi(P)$, $\phi(Q)$ are included in $\mathrm{rng}\,\phi(A)^{1/2}=\mathrm{rng}\,\phi(A)$. This clearly implies our assertion. In what follows we restrict the considerations onto those two-dimensional subspaces, that is, to the ranges of A and $\phi(A)$, respectively. By property (iii) in the definition of compatibility-like functions, we see that

$$\lambda\leqslant C(A,R)^2\leqslant\mu$$

holds for every rank one projection R on the range of A. As ϕ preserves C, we have

$$\lambda\leqslant C(\phi(A),\phi(R))^2\leqslant\mu$$

for every rank-one projection $\phi(R)$ on the range of $\phi(A)$. Moreover, we have

$$C(\phi(A),\phi(P))^2=C(A,P)^2=\lambda, \quad C(\phi(A),\phi(Q))^2=C(A,Q)^2=\mu.$$

Now we refer to a result in Ref. 6. Namely, Lemma 3 given there states that if T is an effect and $0<\epsilon<\delta\leqslant 1$ are scalars such that $\epsilon I\leqslant T\leqslant\delta I$ and we have unit vectors φ, $\psi\in H$ such that $\lambda(T,P_{\varphi})=\epsilon$ and $\lambda(T,P_{\psi})=\delta$, then φ, ψ are eigenvectors of T and the corresponding eigenvalues are ϵ, δ, respectively. Using this result and the correspondence between compatibility-like functions and the strength, we obtain that the range of $\phi(P)$ is the eigensubspace of $\phi(A)$ corresponding to the eigenvalue λ and the range of $\phi(Q)$ is the eigensubspace of $\phi(A)$ corresponding to the eigenvalue μ. Therefore, we have

$$\phi(A)=\lambda\phi(P)+\mu\phi(Q). \tag{2}$$

Now let P, R be arbitrary rank-one projections. Pick a rank-one projection Q which is orthogonal to P such that the subspace generated by the ranges of P and Q includes the range of R. Let λ, μ and A be as above. It is easy to check that by the formula (1) we have

$$C^2(A,R)=\frac{1}{(1/\lambda)\mathrm{tr}PR+(1/\mu)\mathrm{tr}QR}=\frac{\lambda\mu}{\mu\mathrm{tr}PR+\lambda\mathrm{tr}QR}=\frac{\lambda\mu}{\mu\mathrm{tr}PR+\lambda(1-\mathrm{tr}PR)}$$
$$=\frac{\lambda\mu}{(\mu-\lambda)\mathrm{tr}PR+\lambda}. \tag{3}$$

As the spectral resolution of $\phi(A)$ is (2), we similarly have

$$C^2(\phi(A),\phi(R))=\frac{\lambda\mu}{(\mu-\lambda)\mathrm{tr}\phi(P)\phi(R)+\lambda}. \tag{4}$$

Since ϕ preserves C, it follows from (3) and (4) that

$$\mathrm{tr}\phi(P)\phi(R)=\mathrm{tr}PR,$$

which means that ϕ preserves the transition probability between pure states. It follows from Wigner's theorem that ϕ, when restricted onto the set of all pure states, is of the form

$$\phi(P)=UPU^*$$

for some unitary or antiunitary operator U on H.

It remains to show that the above formula holds for every state as well. The proof goes as follows. Let $A\in S(H)$. For every rank-one projection P we compute

$$\lambda(UAU^*,P)=\lambda(A,U^*PU)=C(A,U^*PU)^2=C(\phi(A),\phi(U^*PU))^2=C(\phi(A),P)^2$$
$$=\lambda(\phi(A),P).$$

Now we refer to Ref. 2, Corollary 1, which states that if the strengths of two effects are the same along every ray, then the effects in question are equal. This gives us that

$$\phi(A)=UAU^* \quad (A\in S(H))$$

and the proof is complete. □

ACKNOWLEDGMENTS

This article was written when the first author held a Humboldt Research Fellowship. He is very grateful to the Alexander von Humboldt Foundation for providing ideal conditions for research and to the staff of the Institute of Analysis, TU, Dresden (Germany) for the kind hospitality. The first author also acknowledges support from the Hungarian National Foundation for Scientific Research (OTKA), Grant Nos. T030082 and T031995, and from the Ministry of Education, Hungary, Grant No. FKFP 0349/2000.

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Pseudo-Hermiticity and generalized *PT*- and *CPT*-symmetries

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(Received 13 September 2002; accepted 15 November 2002)

We study certain linear and antilinear symmetry generators and involution operators associated with pseudo-Hermitian Hamiltonians and show that the theory of pseudo-Hermitian operators provides a simple explanation for the recent results of Bender, Brody and Jones (quant-ph/0208076) on the CPT-symmetry of a class of PT-symmetric non-Hermitian Hamiltonians. We present a natural extension of these results to the class of diagonalizable pseudo-Hermitian Hamiltonians H with a discrete spectrum. In particular, we introduce generalized parity ($\mathcal{P}$), time-reversal ($\mathcal{T}$), and charge-conjugation ($\mathcal{C}$) operators and establish the $\mathcal{PT}$- and $\mathcal{CPT}$-invariance of H. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1539304]

I. INTRODUCTION

Bender, Brody and Jones[1] have recently shown that for the class of PT-symmetric Hamiltonians

$$H_\nu = p^2 + x^2(ix)^\nu, \quad \nu \in [0,\infty), \tag{1}$$

one can use a complete set of eigenfunctions ψ_n to construct a linear operator C with the following properties.

(1) C is an involution generating a symmetry of the system, i.e.,

$$C^2 = 1, \quad [C,H_\nu] = 0. \tag{2}$$

In particular, H_ν is CPT-invariant.

(2) In the position representation, C has the form

$$C(x,y) = \sum_n \psi_n(x)\psi_n(y), \quad \forall x,y \in \mathbb{R}. \tag{3}$$

(3) The inner product

$$\langle \phi|\psi\rangle_{CPT} := \int_\gamma dx\,[CPT\phi(x)]\psi(x) \tag{4}$$

is positive-definite, and the eigenfunctions ψ_n are orthonormal with respect to this inner product, i.e.,

$$\langle \psi_m|\psi_n\rangle_{CPT} = \delta_{mn}. \tag{5}$$

(4) For $\nu = 0$, where the Hamiltonian H_0 is Hermitian, $C = P$.

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In Eq. (4), γ is the contour in the complex plane used to impose the vanishing boundary conditions for the eigenvalue problem of (1).[2] For $\nu\in[0,2)$, γ may be taken as the real line $\mathbb{R}$.

The purpose of this article is twofold. First, we show that the results of Ref. 1, in particular the items 1–4 of the above list, may be explained as a straightforward application of the theory of pseudo-Hermitian operators.[3–7] Second, we outline an extension of these results to the class of quasi-Hermitian Hamiltonians, i.e., diagonalizable Hamiltonians with a real spectrum, and more generally diagonalizable pseudo-Hermitian Hamiltonians. (By definition, a quasi-Hermitian operator is an operator obtained from a Hermitian operator by a similarity transformation.[8] Therefore it is diagonalizable and has a real spectrum. The converse of this statement is also true; as shown in Ref. 4, a diagonalizable operator with a real discrete spectrum is related to a Hermitian operator through a similarity transformation.) In order to achieve this purpose, we explore certain symmetry properties and involution operators associated with pseudo-Hermitian Hamiltonians.

The organization of the article is as follows. In Sec. II, we offer a discussion of pseudo-Hermitian operators and their symmetries. In Sec. III, we consider the problem of the existence and characterization of certain involution operators associated with a pseudo-Hermitian Hamiltonian. In Sec. IV, we explain the mathematical structure underlying the results of Ref. 1 for the Hamiltonians (1) with $\nu\in[0,2)$ and $\gamma=\mathbb{R}$. In Sec. V, we introduce generalized parity ($\mathcal{P}$), time-reversal ($\mathcal{T}$), and charge-conjugation ($\mathcal{C}$) operators for an arbitrary quasi-Hermitian Hamiltonian H with a discrete spectrum and establish the $\mathcal{PT}$- and $\mathcal{CPT}$-invariance of H. In Sec. VI, we extend the results of Sec. V to the more general class of diagonalizable pseudo-Hermitian operators with a discrete spectrum. Finally, in Sec. VII, we conclude the article with a summary of our main results.

II. PSEUDO-HERMITIAN OPERATORS AND THEIR SYMMETRIES

A linear operator H acting in a Hilbert space $\mathcal{H}$ is said to be pseudo-Hermitian[3] if there is a linear, invertible, Hermitian operator $\eta:\mathcal{H}\to\mathcal{H}$ such that

$$H^\dagger=\eta H\eta^{-1}. \tag{6}$$

For a given pseudo-Hermitian operator H, η is not unique.[6,9] If one fixes a particular η, one says that H is η-pseudo-Hermitian. In this case, H is Hermitian with respect to the pseudo-inner product

$$\langle\langle\phi|\psi\rangle\rangle_\eta:=\langle\phi|\eta\psi\rangle, \tag{7}$$

where $\langle\,|\,\rangle$ is the inner product of $\mathcal{H}$. [We use the term pseudo-inner product for a possibly (but not necessarily) indefinite inner product.]

For diagonalizable Hamiltonians with a discrete spectrum pseudo-Hermiticity is equivalent to the condition that the complex eigenvalues come in complex-conjugate pairs.[3] Here the discreteness of the spectrum is not essential, and as shown in Ref. 7 the diagonalizability condition may be replaced by a weaker block-diagonalizability condition. Furthermore, for the class of diagonalizable Hamiltonians with a discrete spectrum, pseudo-Hermiticity is also equivalent to the condition that the Hamiltonian admits an antilinear symmetry.[5]

Pseudo-Hermiticity also provides a characterization of the reality of the spectrum for diagonalizable Hamiltonians with a discrete spectrum. Specifically it may be used to establish the equivalence of the following statements.[4]

(1) The spectrum is real.
(2) The Hamiltonian is quasi-Hermitian.
(3) Among the operators η satisfying (6) there is a positive operator η_+, i.e., the Hamiltonian is η_+-pseudo-Hermitian for a positive operator η_+.
(4) The Hamiltonian is Hermitian with respect to a positive-definite inner product, namely $\langle\langle\,|\,\rangle\rangle_{\eta_+}$.[5,6]

One can actually construct η_+. Given a quasi-Hermitian Hamiltonian H and an associated complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, which by definition satisfies $H|\psi_n,a\rangle=E_n|\psi_n,a\rangle$, $H^\dagger|\phi_n,a\rangle=E_n^*|\phi_n,a\rangle$, and

$$\langle\phi_n,a|\psi_m,b\rangle=\delta_{nm}\delta_{ab}, \tag{8}$$

$$\sum_n\sum_{a=1}^{d_n}|\psi_n,a\rangle\langle\phi_n,a|=1, \tag{9}$$

$$H=\sum_n\sum_{a=1}^{d_n}E_n|\psi_n,a\rangle\langle\phi_n,a|, \tag{10}$$

one can express η_+ according to

$$\eta_+=\sum_n\sum_{a=1}^{d_n}|\phi_n,a\rangle\langle\phi_n,a|. \tag{11}$$

In Eqs. (8)–(11) and throughout this article n and m are spectral labels taking non-negative integer values, d_n stands for the multiplicity or degree of degeneracy of E_n, and a and b are degeneracy labels.

It turns out that η_+ is unique up to the choice of the biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$.[6] However, besides η_+, there are nonpositive invertible Hermitian operators η that are also associated with the same biorthonormal system and satisfy (6). These are determined by a sequence $\sigma:=\{\sigma_n^a\}$ of signs $\sigma_n^a=\pm$ and have the general form

$$\eta_\sigma:=\sum_n\sum_{a=1}^{d_n}\sigma_n^a|\phi_n,a\rangle\langle\phi_n,a|. \tag{12}$$

Obviously, the choice of the biorthonormal system is arbitrary. This means that given a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, we can express the most general η satisfying (6) according to (12) with $|\phi_n,a\rangle$ replaced with possibly different eigenvectors of $H^\dagger$ with the same eigenvalue as $|\phi_n,a\rangle$. Labeling these by $|\tilde\phi_n,a\rangle$ and noting that both $|\phi_n,a\rangle$ and $|\tilde\phi_n,a\rangle$ form bases of $\mathcal{H}$, we have $|\tilde\phi_n,a\rangle=A^\dagger|\phi_n,a\rangle$ for some invertible linear operator $A:\mathcal{H}\to\mathcal{H}$. Clearly, the vectors $|\tilde\phi_n,a\rangle$ and $|\tilde\psi_n,a\rangle:=A^{-1}|\psi_n,a\rangle$ form a complete biorthonormal system. Furthermore, the operator A commutes with the Hamiltonian, and

$$\eta=A^\dagger\eta_\sigma A. \tag{13}$$

This proves the following proposition. Here we include a direct proof for completeness.

Proposition 1: For a given quasi-Hermitian Hamiltonian H with a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, the most general Hermitian invertible linear operator η satisfying (6) is given by (13) where A is an invertible linear operator commuting with the Hamiltonian (a symmetry generator) and $\sigma=\{\sigma_n^a\}$ is a sequence of signs $\sigma_n^a=\pm$.

Proof: Let η be an arbitrary Hermitian invertible linear operator satisfying (6). Then one can easily check that $X:=\eta_+^{-1}\eta$ commutes with H.[3] Therefore, X is an invertible linear operator generating a symmetry of H. This implies that X and H have simultaneous eigenvectors. In particular, X has the form

$$X=\sum_n\sum_{a,b=1}^{d_n}x_{ab}^n|\psi_n,a\rangle\langle\phi_n,b|, \tag{14}$$

where x^n_{ab} are complex coefficients. Expressing η in terms of η_+ and X and using Eqs. (14), (11) and (8), we find

$$\eta=\eta_+X=\sum_n\sum_{a,b=1}^{d_n}x^n_{ab}|\phi_n,a\rangle\langle\phi_n,b|. \tag{15}$$

Taking the adjoint of both sides of this equation and making use of the Hermiticity of η, we have $x^{n*}_{ab}=x^n_{ba}$. Hence the matrices x^n with entries x^n_{ab} are Hermitian; they may be diagonalized:

$$x^n=u^n\ \ x^n_{\rm diag}\ \ u^{n\dagger}, \tag{16}$$

where u^n are $d_n\times d_n$ unitary matrices and $x^n_{\rm diag}$ are $d_n\times d_n$ diagonal real matrices. Next, we introduce

$$\begin{aligned}U&:=\sum_n\sum_{a,b=1}^{d_n}u^n_{ab}|\psi_n,a\rangle\langle\phi_n,b|,\\ D&:=\sum_n\sum_{a=1}^{d_n}\sqrt{|x^n_a|}\ \ |\psi_n,a\rangle\langle\phi_n,a|,\\ A&:=DU=\sum_n\sum_{a,b=1}^{d_n}\sqrt{|x^n_a|}\ \ u^n_{ab}|\psi_n,a\rangle\langle\phi_n,b|,\end{aligned} \tag{17}$$

where u^n_{ab} and x^n_a denote the entries of u^n and the diagonal entries of $x^n_{\rm diag}$, respectively. Note that because u^n are unitary matrices U is invertible. In fact, one can check by direct computation that

$$U^{-1}:=\sum_n\sum_{a,b=1}^{d_n}u^{*n}_{ba}|\psi_n,a\rangle\langle\phi_n,b|$$

satisfies $U^{-1}U=UU^{-1}=1$. Furthermore, because $X=\eta_+^{-1}\eta$, it is invertible, its eigenvalues x^n_a are nonzero, and D is also invertible. This in turn implies that A is invertible. Finally, using Eqs. (15)–(17), (12), (11), (8) and setting $\sigma^a_n:=x^n_a/|x^n_a|$, we can compute

$$A^\dagger\eta_\sigma A=\sum_n\sum_{abc}u^n_{ac}x^n_cu^{n*}_{bc}|\phi_n,a\rangle\langle\phi_n,b|=\eta.$$

□

Another interesting property of quasi-Hermitian Hamiltonians with a discrete spectrum is that they admit an exact antilinear symmetry. This follows from the observation that every diagonalizable pseudo-Hermitian Hamiltonian with a discrete spectrum is anti-pseudo-Hermitian with respect to the antilinear operator[5]

$$\tau_+:=\sum_n\sum_{a=1}^{d_n}|\phi_n,a\rangle\star\langle\phi_n,a|, \tag{18}$$

where $\star$ is the operation of the complex conjugation of numbers. In particular, for all $|\phi\rangle,|\psi\rangle\in\mathcal{H}$,

$$\star\,\langle\phi|\psi\rangle:=\langle\phi|\psi\rangle^*=\langle\psi|\phi\rangle.$$

Anti-pseudo-Hermiticity of H with respect to τ_+ means

$$H^\dagger=\tau_+H\tau_+^{-1}. \tag{19}$$

Again, up to the choice of a complete biorthonormal system, (18) is the unique antilinear, Hermitian, invertible operator satisfying (19). This in turn leads to the following theorem. Again here we include an explicit proof for completeness.

Proposition 2: For a given diagonalizable pseudo-Hermitian Hamiltonian H with a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, the most general antilinear, Hermitian, invertible operator satisfying (19) has the form

$$\tau=A^\dagger\tau_+A, \tag{20}$$

where A is an invertible linear operator commuting with H.

Proof: Let τ be an arbitrary antilinear, Hermitian, invertible operator satisfying (19). Then one can easily check that $X:=\tau_+^{-1}\tau$ commutes with H.[3] Therefore, X is an invertible linear operator generating a symmetry of H and having the form (14). Solving for τ in $X:=\tau_+^{-1}\tau$ and using (18), (14), and (8), we have

$$\tau=\sum_n\sum_{a,b=1}^{d_n}x^{n*}_{ab}|\phi_n,a\rangle\star\langle\phi_n,b|. \tag{21}$$

Now, we recall that τ is a Hermitian antilinear operator. Therefore $\langle\psi_n,a|\tau|\psi_n,b\rangle=\langle\psi_n,b|\tau|\psi_n,a\rangle$. Substituting (21) in this equation we find $x^n_{ab}=x^n_{ba}$, i.e., the matrices x^n formed out of x^n_{ab} are in general complex symmetric matrices. As shown in Ref. 10, the latter admit a factorization of the form

$$x^n=a^{nT}a^n, \tag{22}$$

where a^n are $n\times n$ matrices and the superscript ^{T} denotes the transpose. Next, we introduce

$$A:=\sum_n\sum_{a,b=1}^{d_n}a^n_{ab}|\psi_n,a\rangle\langle\phi_n,b|, \tag{23}$$

where a^n_{ab} are entries of a^n. Clearly, A commutes with H. Moreover, using Eqs. (18), (21)–(23), and (8), we have

$$A^\dagger\tau_+A=\sum_n\sum_{a,b=1}^{d_n}a^{n*}_{ca}a^{n*}_{cb}|\phi_n,a\rangle\star\langle\phi_n,b|=\tau.$$

For a quasi-Hermitian Hamiltonian with a discrete spectrum, we can use Eq. (20) to define antilinear analogs of the operators η_σ, namely

$$\tau_\sigma:=\sum_n\sum_{a=1}^{d_n}\sigma^a_n|\phi_n,a\rangle\star\langle\phi_n,a|, \tag{24}$$

where again $\sigma=\{\sigma^a_n\}$ is a sequence of signs $\sigma^a_n=\pm$. This is simply done by setting $a^n_{ab}=(\sqrt{\sigma^a_n})^*\delta_{ab}$ in (20).

Combining Eqs. (6) and (19), we see that H commutes with

$$\mathcal{X}:=\eta^{-1}\tau, \tag{25}$$

where η and τ are linear and antilinear Hermitian, invertible, operators such that H is η-pseudo-Hermitian and τ-anti-pseudo-Hermitian; they have the general form (13) and (20), respectively. In particular if we set $\eta=\eta_\sigma$ and $\tau=\tau_+$ in (25), we find a set of *canonical antilinear symmetry generators:*

$$\mathcal{X}_\sigma:=\eta_\sigma^{-1}\tau_+=\eta_+^{-1}\tau_\sigma. \tag{26}$$

In view of Eqs. (8) and (24) and the identity[3]

$$\eta_\sigma^{-1}=\sum_n \sum_{a=1}^{d_n} \sigma_n^a|\psi_n,a\rangle\langle\psi_n,a|, \tag{27}$$

we can easily calculate

$$\mathcal{X}_\sigma=\sum_n \sum_{a=1}^{d_n} \sigma_n^a|\psi_n,a\rangle\star\langle\phi_n,a|. \tag{28}$$

It is not difficult to show that in view of (10), (8), and (28),

$$[\mathcal{X}_\sigma,H]=0, \tag{29}$$

$$\mathcal{X}_\sigma|\psi_n,a\rangle=\sigma_n^a|\psi_n,a\rangle. \tag{30}$$

In particular,

$$\mathcal{X}_+ := \eta_+^{-1}\tau_+ = \eta_\sigma^{-1}\tau_\sigma \tag{31}$$

satisfies

$$[\mathcal{X}_+,H]=0, \tag{32}$$

$$\mathcal{X}_+|\psi_n,a\rangle=|\psi_n,a\rangle. \tag{33}$$

Hence the antilinear symmetry generated by $\mathcal{X}_\sigma$ is an exact symmetry. The converse of this statement is also valid. That is, if a diagonalizable Hamiltonian with a discrete spectrum admits an exact symmetry generated by an invertible antilinear operator, then its spectrum is real;[4] it is quasi-Hermitian. A direct consequence of this statement is that if a diagonalizable pseudo-Hermitian Hamiltonian with a discrete spectrum has nonreal eigenvalues, then it cannot support exact antilinear symmetries. Such a Hamiltonian always admits antilinear symmetries,[5] but these symmetries are necessarily broken.

We can repeat the above analysis of quasi-Hermitian Hamiltonians for the more general diagonalizable pseudo-Hermitian Hamiltonians with a discrete spectrum.[3,5] For the latter Hamiltonians nonreal eigenvalues come in complex-conjugate pairs with identical multiplicity, so we identify the spectral label n with ν_0, ν_+, or ν_- depending on whether the imaginary part of E_n is zero, positive, or negative, respectively. In this case, Eqs. (8)–(10), with $n=\nu_0,\nu_\pm$ and $m=\mu_0,\mu_\pm$, are still valid, $d_{\nu_+}=d_{\nu_-}$, and the analog of the positive operator (11) is the operator

$$\eta_+=\sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} |\phi_{\nu_0},a\rangle\langle\phi_{\nu_0},a|+\sum_\nu \sum_{a=1}^{d_\nu} (|\phi_{\nu_+},a\rangle\langle\phi_{\nu_-},a|+|\phi_{\nu_-},a\rangle\langle\phi_{\nu_+},a|). \tag{34}$$

Here we use ν to denote the common value of $\nu_\pm$.

It is not difficult to see that the proof of Proposition 1 extends to the class of diagonalizable pseudo-Hermitian Hamiltonians with a discrete spectrum; it yields the following generalization of Proposition 1, see also Ref. 5.

Proposition 3: For a given diagonalizable pseudo-Hermitian Hamiltonian H with a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, the most general Hermitian invertible linear operator η satisfying (6) is given by (13) where A is an invertible linear operator commuting with the Hamiltonian,

$$\eta_\sigma := \sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} \sigma^a_{\nu_0} |\phi_{\nu_0},a\rangle\langle\phi_{\nu_0},a| + \sum_{\nu} \sum_{a=1}^{d_\nu} (|\phi_{\nu_+},a\rangle\langle\phi_{\nu_-},a| + |\phi_{\nu_-},a\rangle\langle\phi_{\nu_+},a|), \tag{35}$$

and $\sigma=\{\sigma^a_{\nu_0}\}$ is a sequence of signs $\sigma^a_{\nu_0}=\pm$.

Similarly, one can show that every diagonalizable pseudo-Hermitian Hamiltonian H with a discrete spectrum admits antilinear symmetries generated by (25). For instance, we have the canonical antilinear symmetry generators (26) where now η_+ is given by (34) and

$$\tau_\sigma := \sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} \sigma^a_{\nu_0} |\phi_{\nu_0},a\rangle\star\langle\phi_{\nu_0},a| + \sum_{\nu} \sum_{a=1}^{d_\nu} (|\phi_{\nu_+},a\rangle\star\langle\phi_{\nu_+},a| + |\phi_{\nu_-},a\rangle\star\langle\phi_{\nu_-},a|). \tag{36}$$

We can express these symmetry generators according to

$$\mathcal{X}_\sigma = \sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} \sigma^a_{\nu_0} |\psi_{\nu_0},a\rangle\star\langle\phi_{\nu_0},a| + \sum_{\nu} \sum_{a=1}^{d_\nu} (|\psi_{\nu_+},a\rangle\star\langle\phi_{\nu_-},a| + |\psi_{\nu_-},a\rangle\star\langle\phi_{\nu_+},a|), \tag{37}$$

where we have used Eqs. (26), (34), (36), and (8) and the identity[3]

$$\eta_\sigma^{-1} = \sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} \sigma^a_{\nu_0} |\psi_{\nu_0},a\rangle\langle\psi_{\nu_0},a| + \sum_{\nu} \sum_{a=1}^{d_\nu} (|\psi_{\nu_+},a\rangle\langle\psi_{\nu_-},a| + |\psi_{\nu_-},a\rangle\langle\psi_{\nu_+},a|). \tag{38}$$

Next, we observe that in light of Eqs. (10), (8), and (37),

$$[\mathcal{X}_\sigma, H] = 0, \tag{39}$$

$$\mathcal{X}_\sigma |\psi_n,a\rangle = \begin{cases} \sigma^a_{\nu_0} |\psi_{\nu_0},\ a\rangle & \text{if } n=\nu_0, \\ |\psi_{\nu_\mp},\ a\rangle & \text{if } n=\nu_\pm. \end{cases} \tag{40}$$

In particular, the operator (31) satisfies

$$[\mathcal{X}_+, H] = 0, \tag{41}$$

$$\mathcal{X}_+ |\psi_n,a\rangle = \begin{cases} |\psi_{\nu_0},\ a\rangle, & \text{if } n=\nu_0, \\ |\psi_{\nu_\mp},\ a\rangle, & \text{if } n=\nu_\pm. \end{cases} \tag{42}$$

Therefore, $\mathcal{X}_\sigma$ generate symmetries of H which are, however, broken.

III. INVOLUTION OPERATORS ASSOCIATED WITH A PSEUDO-HERMITIAN HAMILTONIAN

Among the basic properties of the P, T, and PT operators (within the scalar/bosonic quantum mechanics) is that they are involutions of the Hilbert space, i.e., their square is the identity operator. In this section we study the problem of the existence and characterization of certain involutions of the Hilbert space which are associated with a given pseudo-Hermitian Hamiltonian.

Proposition 4: The operators $S_\sigma := \eta_+^{-1}\eta_\sigma$ and $\mathcal{X}_\sigma := \eta_+^{-1}\tau_\sigma$ are involutions.

Proof: according to Eqs. (11), (12), and (8), we have

$$S_\sigma = \sum_{\nu_0} \sum_{a=1}^{d_{\nu_0}} \sigma^a_{\nu_0} |\psi_{\nu_0},a\rangle\langle\phi_{\nu_0},a| + \sum_{\nu} \sum_{a=1}^{d_\nu} (|\psi_{\nu_+},a\rangle\langle\phi_{\nu_-},a| + |\psi_{\nu_-},a\rangle\langle\phi_{\nu_+},a|). \tag{43}$$

Squaring this expression and using (8), we find $S_\sigma^2=1$. Similarly, we have $\mathcal{X}_\sigma^2=1$. □

Corollary 1: Every diagonalizable pseudo-Hermitian Hamiltonian H with a discrete spectrum admits a symmetry generated by a linear involution S and a symmetry generated by an antilinear involution Σ, i.e., $[H,S]=[H,\Sigma]=0$ and $S^2=\Sigma^2=1$.

Proof: Again we recall that because η_+ and η_σ satisfy (6), the linear operator $S=S_\sigma := \eta_+^{-1}\eta_\sigma$ commutes with the Hamiltonian.[3] Therefore, in view of Proposition 4, S and $\Sigma=\mathcal{X}_\sigma$ are involutions generating symmetries of H. Clearly, S is linear whereas Σ is antilinear. □

Corollary 2: Let H be a diagonalizable Hamiltonian with a discrete spectrum. Then H is pseudo-Hermitian if and only if it admits an antilinear symmetry generated by an involution.

Proof: If H is pseudo-Hermitian, then according to Proposition 4 it admits such a symmetry. Conversely, suppose that H admits such a symmetry. Then because this is an antilinear symmetry, H must be pseudo-Hermitian.[5] □

Proposition 5: A diagonalizable Hamiltonian H with a discrete spectrum is anti-pseudo-Hermitian with respect to a Hermitian antilinear involution if and only if there is a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ satisfying

$$\langle\phi_n,a|\phi_m,b\rangle=\langle\psi_m,b|\psi_n,a\rangle. \tag{44}$$

Proof: Suppose H is anti-pseudo-Hermitian with respect to a Hermitian antilinear involution τ. Then there is a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ for which $\tau=\tau_+$. Now, imposing the condition that $\tau^2=1$ and using Eq. (8), one finds (44). Conversely, one can check that if a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ satisfies this equation, the Hermitian antilinear operator τ_+ given by (18) is an involution. As we mentioned above and shown in Ref. 5, H is anti-pseudo-Hermitian with respect to this operator. □

Corollary 3: A pseudo-Hermitian Hamiltonian H is anti-pseudo-Hermitian with respect to a Hermitian antilinear involution if and only if for every complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ there is an invertible linear symmetry generator A satisfying

$$\sum_n\sum_{a=1}^{d_n}\langle\psi_k,c|(AA^\dagger)^{-1}|\psi_n,a\rangle\langle\psi_m,b|(AA^\dagger)^{-1}|\psi_n,a\rangle=\delta_{km}\delta_{bc}. \tag{45}$$

Proof: According to Proposition 5, anti-pseudo-Hermiticity of H with respect to a Hermitian antilinear involution is equivalent to the existence of a complete biorthonormal system $\{|\tilde\psi_n,a\rangle,|\tilde\phi_n,a\rangle\}$ satisfying

$$\langle\tilde\phi_n,a|\tilde\phi_m,b\rangle=\langle\tilde\psi_m,b|\tilde\psi_n,a\rangle. \tag{46}$$

Now, let $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ be an arbitrary complete biorthonormal system. Then there is a linear invertible symmetry generator A satisfying $|\tilde\psi_n,a\rangle=A^{-1}|\psi_n,a\rangle$ and $|\tilde\phi_n,a\rangle=A^\dagger|\phi_n,a\rangle$. Substituting these relations in (46), we find

$$\langle\phi_n,a|AA^\dagger|\phi_m,b\rangle=\langle\psi_m,b|(AA^\dagger)^{-1}|\psi_n,a\rangle. \tag{47}$$

Next, we multiply $\langle\psi_k,c|(AA^\dagger)^{-1}|\psi_n,a\rangle$ by both sides of (47) and sum over n and a. This yields (45). Conversely, assuming the existence of an invertible symmetry generator A satisfying (45), one can easily check that the complete biorthonormal system defined by $|\tilde\psi_n,a\rangle := A^{-1}|\psi_n,a\rangle$ and $|\tilde\phi_n,a\rangle := A^\dagger|\psi_n,a\rangle$ satisfies (46). □

Equation (47) is particularly useful as it gives the necessary and sufficient conditions for a given invertible Hermitian antilinear operator τ satisfying (19) to be an involution. For example, in order to find the necessary and sufficient conditions under which τ_σ of Eq. (36) is an involution, we write $\tau_\sigma=A^\dagger\tau_+A$, where

$$A=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}(\sqrt{\sigma^a_{\nu_0}})^*\ |\psi_{\nu_0},a\rangle\langle\phi_{\nu_0},a|+\sum_\nu\sum_{a=1}^{d_\nu}(|\psi_{\nu_+},a\rangle\langle\phi_{\nu_+},a|+|\psi_{\nu_-},a\rangle\langle\phi_{\nu_-},a|),$$

and substitute this equation in (47). This yields the following conditions:

$$\langle \phi_{\nu_0},a|\phi_{\mu_0},b\rangle=\sigma^a_{\nu_0}\sigma^b_{\mu_0}\langle \psi_{\mu_0},b|\psi_{\nu_0},a\rangle, \tag{48}$$

$$\langle \phi_{\nu_0},a|\phi_{\mu_\pm},b\rangle=\sigma^a_{\nu_0}\langle \psi_{\mu_\pm},b|\psi_{\nu_0},a\rangle, \tag{49}$$

$$\langle \phi_{\nu_\pm},a|\phi_{\mu_\pm},b\rangle=\langle \psi_{\mu_\pm},b|\psi_{\nu_\pm},a\rangle. \tag{50}$$

Proposition 6: A diagonalizable Hamiltonian H with a discrete spectrum is pseudo-Hermitian with respect to a Hermitian linear involution η if and only if there is a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$, with $n=\nu_0,\nu_\pm$ as above, and a sequence of signs $\sigma=\{\sigma^a_{\nu_0}\}$ such that

$$\langle \phi_{\nu_0},a|\phi_{\mu_0},b\rangle=\sigma^a_{\nu_0}\sigma^b_{\mu_0}\langle \psi_{\nu_0},a|\psi_{\mu_0},b\rangle, \tag{51}$$

$$\langle \phi_{\nu_0},a|\phi_{\mu_\pm},b\rangle=\sigma^a_{\nu_0}\langle \psi_{\nu_0},a|\psi_{\mu_\mp},b\rangle, \tag{52}$$

$$\langle \phi_{\nu_\pm},a|\phi_{\mu_\pm},b\rangle=\langle \psi_{\nu_\mp},a|\psi_{\mu_\mp},b\rangle. \tag{53}$$

Proof: This follows from a similar argument as the one used in the proof of Proposition 5. It is based on the observation that η takes the canonical form (35) in some complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ and that in this system the condition $\eta^2=1$ is equivalent to Eqs. (51)–(53). □

Corollary 4: Let H be a diagonalizable pseudo-Hermitian Hamiltonian H with a discrete spectrum and a complete biorthonormal system $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$. Then the operators τ_σ of (36) and η_σ of (35) are involutions if and only if Eqs. (48)–(50) and (51)–(53) are satisfied. Furthermore, in this case

$$[\tau_\sigma,\eta_\sigma]=0. \tag{54}$$

Proof: The equivalence of Eqs. (48)–(50) and (51)–(53) with the condition that τ_σ and η_σ are involutions follows from Corollary 4 and Proposition 6. Finally, in view of the identities: $\tau_\sigma=\tau_\sigma^{-1}$, $\eta_\sigma=\eta_\sigma^{-1}$,

$$\tau_+^{-1}=\sum_n\sum_{a=1}^{d_n}|\psi_n,a\rangle\star\langle\psi_n,a|, \tag{55}$$

and Eqs. (36), (35), (38), and (8), we have

$$\tau_\sigma\eta_\sigma=\tau_\sigma\eta_\sigma^{-1}=\tau_+\eta_+^{-1}=\eta_+\tau_+^{-1}=\eta_\sigma\tau_\sigma.$$

□

IV. APPLICATION TO HAMILTONIANS (1) WITH $\gamma=\mathbb{R}$

Consider the class of PT-symmetric Hamiltonians H_ν of Eq. (1) with $\nu\in[0,2)$, $\gamma=\mathbb{R}$, and $\mathcal{H}=L^2(\mathbb{R})$. Then, following Ref. 1, we may choose a set of eigenvectors $|\psi_n\rangle$ of H_ν satisfying

$$PT|\psi_n\rangle=|\psi_n\rangle. \tag{56}$$

Because the eigenvalues of H_ν are nondegenerate, we have dropped the degeneracy label $a=1$. (Note that what we denote by $|\phi_n\rangle$ are eigenvectors of $H^\dagger$. This is the notation used in Refs. 3–7 which differs from that of Ref. 1.) Also as usual the PT operator is defined by $PT\psi(x):=[\psi(-x)]^*$ where $|\psi\rangle$ is an arbitrary state vector represented by the wave function $\psi(x)$. Moreover, relying on the numerical evidence[2] that is also used in Ref. 1, we assume the validity of the completeness relation

$$\sum_n (-1)^n \psi_n(x)\psi_n(y) = \delta(x-y), \tag{57}$$

and the orthogonality condition

$$(\psi_m, \psi_n) = (-1)^n \delta_{mn}, \tag{58}$$

where the indefinite inner product $(\ ,\ )$ is defined by

$$(\phi, \psi) := \int_{\mathbb{R}} dx [PT\phi(x)]\psi(x). \tag{59}$$

Introducing the functions

$$\phi_n(x) := (-1)^n \psi_n(x)^*, \tag{60}$$

which also belong to $\mathcal{H}=L^2(\mathbb{R})$, and using Eqs. (58) and (59) we can show that

$$\langle \phi_m | \psi_n \rangle := \int_{\mathbb{R}} dx \phi_m(x)^* \psi_n(x) = (-1)^m (\psi_m, \psi_n) = \delta_{mn}.$$

This coincides with the biorthonormality relation (8). Furthermore, we write Eq. (57) in the form

$$\delta(x-y) = \sum_n \phi_n(x)\psi_n(y)^* = \sum_n \langle x|\phi_n\rangle\langle \psi_n|y\rangle,$$

which is equivalent to the completeness relation (9). Therefore, $\{|\psi_n\rangle, |\phi_n\rangle\}$ forms a complete biorthonormal system, and the PT-symmetric Hamiltonians (1) are diagonalizable.[5] Moreover, because their spectrum is real and discrete, these Hamiltonians are examples of quasi-Hermitian Hamiltonians having a discrete spectrum.

Next, we calculate

$$\begin{aligned}(\phi, \psi) &= \int_{\mathbb{R}} dx \quad \phi(-x)^* \psi(x) \\ &= \int_{\mathbb{R}} dx \quad \phi(x)^* \psi(-x) \\ &= \int_{\mathbb{R}} dx \quad \phi(x)^* P\psi(x) = \langle \phi | P | \psi \rangle = \langle\langle \phi | \psi \rangle\rangle_P,\end{aligned} \tag{61}$$

where

$$\langle \phi | \psi \rangle := \int_{\mathbb{R}} dx \quad \phi(x)^* \psi(x). \tag{62}$$

According to Eq. (61), the inner product (59) is nothing but $\langle\langle\ |\ \rangle\rangle_P$. This observation together with Eqs. (58) and (60) implies

$$P = \sum_n (-1)^n |\phi_n\rangle\langle\phi_n|. \tag{63}$$

Comparing this equation with (12), we see that P is an example of the canonical operators η_σ of Eq. (12) with

$$\sigma_n=(-1)^n. \tag{64}$$

This is another verification of the fact that the Hamiltonians (1) are P-pseudo-Hermitian.[3]

Note that as a result of Eq. (56), $\psi_n(-x)^*=\psi_n(x)$. This equation together with (60) implies

$$\phi_n(x)=(-1)^n\psi_n(-x), \tag{65}$$

$$\langle\psi_m|\psi_n\rangle=\int_{\mathbb{R}}dx\,\psi_m(x)^*\psi_n(x)=\int_{\mathbb{R}}dx\,\psi_m(-x)\psi_n(-x)^*=\int_{\mathbb{R}}dx\,\psi_m(x)\psi_n(x)^*=\langle\psi_n|\psi_m\rangle, \tag{66}$$

$$\begin{aligned}\langle\phi_m|\phi_n\rangle&=\int_{\mathbb{R}}dx\,\phi_m(x)^*\phi_n\\&=(-1)^{m+n}\int_{\mathbb{R}}dx\,\psi_m(-x)^*\psi_n(-x)\\&=(-1)^{m+n}\int_{\mathbb{R}}dx\,\psi_m(x)^*\psi_n(x)=(-1)^{m+n}\langle\psi_m|\psi_n\rangle.\end{aligned} \tag{67}$$

In view of Eqs. (64) and (67), the condition (51) of Propositions 6 holds. Therefore, Eq. (63) is consistent with the fact that P is an involution.

Next, we use Eqs. (56) and (8) to calculate

$$PT=\sum_n\ |\psi_n\rangle\star\langle\phi_n|. \tag{68}$$

Then, multiplying both sides of this equation by P and using Eqs. (63) and (8), we find

$$T=\sum_n\ (-1)^n|\phi_n\rangle\star\langle\phi_n|. \tag{69}$$

This shows that the time-reversal operator T is nothing but the canonical antilinear operator (24) with σ_n given by (64). [This is consistent with the known fact[5] that the PT-symmetric standard Hamiltonians of the form $H=p^2+V(x;t)$ which have $\mathbb{R}$ as their configuration space, in general, and the Hamiltonians (1) with $\nu\in[0,2)$ and $\gamma=\mathbb{R}$, in particular, are T-anti-pseudo-Hermitian. See also Ref. 11.] Again, in view of (66) and (67), we see that the condition (48) of Corollary 4 is satisfied and the expression (69) is consistent with $T^2=1$.

Next, we consider the positive operator η_+ for the Hamiltonians (1) with $\nu\in[0,2)$ and $\gamma=\mathbb{R}$. Because these Hamiltonians are pseudo-Hermitian with respect to both η_+ and P, they admit a symmetry generated by $\eta_+^{-1}P$. This is a particular example of the symmetry generators S of Proposition 4, where $\nu_0=n$, $\sigma_{\nu_0}=(-1)^{\nu_0}=(-1)^n$, and $\nu_\pm$ are absent. We can compute $\eta_+^{-1}P$ using Eq. (43). Alternatively, we may use the identity[3]

$$\eta_+^{-1}=\sum_n\ |\psi_n\rangle\langle\psi_n| \tag{70}$$

together with Eqs. (63) and (8). This yields

$$\eta_+^{-1}P=\sum_n\ (-1)^n|\psi_n\rangle\langle\phi_n|. \tag{71}$$

The symmetry generator $\eta_+^{-1}P$ has the following form in the position representation:

$$\langle x|\,\eta_+^{-1}P|y\rangle=\sum_n\,(-1)^n\psi_n(x)^*\phi_n(y)=\sum_n\,\psi_n(x)\psi_n(y). \tag{72}$$

Comparing this equation with Eq. (3), we see that $\eta_+^{-1}P$ coincides with the charge-conjugation operator C of Ref. 1,

$$C=\eta_+^{-1}P. \tag{73}$$

Next, we use Eqs. (70), (69), (8), (67), (66), and (9) to compute

$$\begin{aligned}
T\eta_+&=\sum_{nm}\,(-1)^n|\phi_n\rangle\star\langle\phi_n|\phi_m\rangle\langle\phi_m|\\
&=\sum_{nm}\,(-1)^m|\phi_n\rangle\star\langle\psi_n|\psi_m\rangle\langle\phi_m|\\
&=\sum_{nm}\,(-1)^m|\phi_n\rangle\star\langle\psi_m|\psi_n\rangle\langle\phi_m|\\
&=\sum_{nm}\,(-1)^m|\phi_n\rangle\langle\psi_n|\psi_m\rangle\star\langle\phi_m|\\
&=\sum_{m}\,(-1)^m|\psi_m\rangle\star\langle\phi_m|\\
&=\sum_{nm}\,(-1)^m|\psi_m\rangle\langle\psi_m|\phi_n\rangle\star\langle\phi_n|=\eta_+^{-1}T=\eta_+^{-1}P^2T=CPT.
\end{aligned} \tag{74}$$

Hence,

$$\begin{aligned}
\langle\phi|\psi\rangle_{CPT}&=\int_{\mathbb{R}}dx\,[CPT\phi(x)]\psi(x)\\
&=\int_{\mathbb{R}}dx\,[T\eta_+\phi(x)]\psi(x)\\
&=\int_{\mathbb{R}}dx\,[\eta_+\phi(x)]^*\psi(x)=\int_{\mathbb{R}}dx\;\phi(x)^*[\eta_+\psi(x)]=\langle\phi|\,\eta_+\psi\rangle=\langle\!\langle\phi|\psi\rangle\!\rangle_{\eta_+},
\end{aligned} \tag{75}$$

where we have used the fact that η_+ is Hermitian. Equations (75) show that the CPT-inner product (4) advocated in Ref. 1 is nothing but the positive-definite inner product $\langle\!\langle\ |\ \rangle\!\rangle_{\eta_+}$ that was extensively used in Ref. 9. Moreover, the orthonormality relation (5) is a simple consequence of Eqs. (12) and (8).

Comparing the expressions given in (68) and (74) for the PT and CPT operators with Eq. (28), we see that the PT and CPT operators are specific examples of the canonical antilinear symmetry generators (28).

V. GENERALIZED *P*, *T*, AND *C* OPERATORS FOR QUASI-HERMITIAN OPERATORS

In the preceding section we explored the mathematical basis of the charge conjugation operator (3) for the Hamiltonians (1) with the choice $\gamma=\mathbb{R}$ which is allowed for $\nu\in[0,2)$. In this section we will demonstrate that indeed the approach based on the theory of pseudo-Hermitian operators applies to quasi-Hermitian Hamiltonians with a discrete spectrum in general and the PT-symmetric Hamiltonians (1) with $\nu\in[0,\infty)$ in particular.

As we discussed in Sec. III, every quasi-Hermitian Hamiltonian H with a discrete spectrum is η_+-pseudo-Hermitian for a positive operator η_+, and that H is Hermitian with respect to the inner product $\langle\!\langle\ |\ \rangle\!\rangle_{\eta_+}$. This in turn implies the existence of a complete set of eigenvectors $|\psi_n,a\rangle$ of H such that $|\psi_n\rangle$ are orthonormal with respect to $\langle\!\langle\ |\ \rangle\!\rangle_{\eta_+}$.

Lemma 1: Let H, η_+, and $|\psi_n,a\rangle$ be as in the preceding paragraph, and

$$|\phi_n,a\rangle := \eta_+|\psi_n,a\rangle, \tag{76}$$

$$\mathcal{P} := \sum_n \sum_{a=1}^{d_n} (-1)^n |\phi_n\rangle\langle\phi_n|, \tag{77}$$

$$\mathcal{T} := \sum_n \sum_{a=1}^{d_n} (-1)^n |\phi_n\rangle\star\langle\phi_n|, \tag{78}$$

$$\mathcal{C} := \sum_n \sum_{a=1}^{d_n} (-1)^n |\psi_n\rangle\langle\phi_n|. \tag{79}$$

Then we have the following.

(1) $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ forms a complete biorthonormal system.

(2) η_+ satisfies (11) and

$$\eta_+^{-1} = \mathcal{T}\eta_+\mathcal{T}. \tag{80}$$

(3) H is $\mathcal{P}$-pseudo-Hermitian and $\mathcal{T}$-anti-pseudo-Hermitian.

(4) $\mathcal{PT}$ and $\mathcal{CPT}$, which have the form

$$\mathcal{PT} = \sum_n \sum_{a=1}^{d_n} |\psi_n,a\rangle\star\langle\phi_n,a|, \tag{81}$$

$$\mathcal{CPT} = \sum_n \sum_{a=1}^{d_n} (-1)^n |\psi_n,a\rangle\star\langle\phi_n,a|, \tag{82}$$

are antilinear symmetry generators and $\mathcal{C}$ is a linear symmetry generator for H; the corresponding symmetries are exact, in particular $|\psi_n,a\rangle$ satisfy

$$\mathcal{PT}|\psi_n,a\rangle = |\psi_n,a\rangle, \tag{83}$$

$$\mathcal{CPT}|\psi_n,a\rangle = \mathcal{C}|\psi_n,a\rangle = (-1)^n|\psi_n,a\rangle. \tag{84}$$

(5) $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ satisfy

$$(\mathcal{PT})^2 = \mathcal{C}^2 = 1, \tag{85}$$

$$\mathcal{C} = \eta_+^{-1}P = \mathcal{T}\eta_+\mathcal{TP}. \tag{86}$$

(6) The operators $\mathcal{P}$ and $\mathcal{T}$ are involutions if and only if

$$(-1)^{m+n}\langle\phi_n,a|\phi_m,b\rangle = \langle\psi_n,a|\psi_m,b\rangle = \langle\psi_m,b|\psi_n,a\rangle. \tag{87}$$

(7) If H is a Hermitian Hamiltonian, $\mathcal{C}^{-1}\mathcal{P}$ is a Hermitian invertible linear operator commuting with H. In particular, if for all n and a, $|\phi_n,a\rangle = |\psi_n,a\rangle$, then $\mathcal{C} = \mathcal{P}$.

Proof: Statement 1 may be established by checking Eqs. (8) and (9) directly. Statements 2–4 follow from these equations and (77)–(79). $\mathcal{PT}$ and $\mathcal{CPT}$ are respectively examples of the antilinear symmetry generators $\mathcal{X}_+$ and $\mathcal{X}_\sigma$. Statement 5 is a result of Proposition 4; Eq. (86) may be checked by direct computation. Statement 6 is a consequence of Corollary 4. In order to prove statement 7, we introduce

$$\Lambda := \sum_n \sum_{a=1}^{d_n} |\psi_n,a\rangle\langle\psi_n,a|, \tag{88}$$

which is clearly a Hermitian invertible linear operator commuting with H. Now it suffices to use (8) to establish $\Lambda\mathcal{P}=\mathcal{C}$. Finally, for the case that $|\phi_n,a\rangle=|\psi_n,a\rangle$, Eq. (9) implies $\Lambda=1$. □

In view of the analogy with the systems studied in Sec. IV, we shall respectively call the operators $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ the *generalized parity, time-reversal*, and *charge conjugation* operators. The following theorem follows as a direct consequence of Lemma 1.

Theorem 1: Every diagonalizable Hamiltonian with a real discrete spectrum is invariant under the action of the generalized charge-conjugation operator $\mathcal{C}$ and the combined action of the generalized parity and time-reversal symmetry ($\mathcal{PT}$). In particular, every such Hamiltonian has exact $\mathcal{PT}$- and $\mathcal{CPT}$-symmetry.

Clearly for the Hamiltonians (1) with $\nu\in[0,2)$, the operators $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ coincide with P,T, and C. For $\nu\in[2,\infty)$, we define the vectors $|\phi_n\rangle$ according to (60) so that in the position representation

$$\eta_+(x,y)=\sum_n \phi_n(x)\phi_n(y)^*=\sum_n \psi_n(x)^*\psi_n(y), \quad \forall x,y\in\mathbb{R}. \tag{89}$$

Next, we note that Eqs. (56), (60), and consequently (65) also hold for $\nu\in[2,\infty)$. Using (65) and (57), we can show that in the position representation

$$\begin{aligned}\mathcal{P}(x,y)&=\sum_n (-1)^n\phi_n(x)\phi_n(y)^*\\ &=\sum_n (-1)^n\psi_n(-x)\psi_n(-y)^*\\ &=\sum_n (-1)^n\psi_n(-x)\psi_n(y)\\ &=\delta(x+y)=P(x,y) \quad \forall x,y\in\mathbb{R},\end{aligned} \tag{90}$$

i.e., P and $\mathcal{P}$ have the same position representations. Furthermore, we can easily see that in view of (81) and (56), $\mathcal{PT}=P\mathcal{T}$, so that T and $\mathcal{T}$ also have the same position representations. Finally, we can employ (79) and (3) to infer that C and $\mathcal{C}$ have the same position representations as well.

VI. GENERALIZED *P*, *T*, AND *C* OPERATORS FOR PSEUDO-HERMITIAN HAMILTONIANS

The construction of the operators $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ may be easily generalized to the class of all diagonalized pseudo-Hermitian operators with a discrete spectrum. Comparing the operators η_σ and $\mathcal{X}_\sigma$ for the quasi- and pseudo-Hermitian Hamiltonians discussed in Sec. III, and noting that according to Eqs. (77), (81), and (82), $\mathcal{P}$ is an example of η_σ and $\mathcal{PT}$ and $\mathcal{CPT}$ are examples of $\mathcal{X}_\sigma$, we introduce

$$\mathcal{P}:=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}} (-1)^{\nu_0}|\phi_{\nu_0},a\rangle\langle\phi_{\nu_0},a|+\sum_{\nu}\sum_{a=1}^{d_\nu}(|\phi_{\nu_+},a\rangle\langle\phi_{\nu_-},a|+|\phi_{\nu_-},a\rangle\langle\phi_{\nu_+},a|), \tag{91}$$

$$\mathcal{T}:=\sum_{\nu_0}(-1)^{\nu_0}\sum_{a=1}^{d_{\nu_0}}|\phi_{\nu_0},a\rangle\star\langle\phi_{\nu_0},a|+\sum_{\nu}\sum_{a=1}^{d_\nu}(|\phi_{\nu_+},a\rangle\star\langle\phi_{\nu_-},a|+|\phi_{\nu_-},a\rangle\star\langle\phi_{\nu_+},a|), \tag{92}$$

$$\mathcal{C}:=\sum_{\nu_0}(-1)^{\nu_0}\sum_{a=1}^{d_{\nu_0}}|\psi_{\nu_0},a\rangle\langle\phi_{\nu_0},a|+\sum_{\nu}\sum_{a=1}^{d_\nu}(|\psi_{\nu_+},a\rangle\langle\phi_{\nu_-},a|+|\psi_{\nu_-},a\rangle\langle\phi_{\nu_+},a|), \tag{93}$$

where we have used the conventions of Secs. III and IV.

Again we can check that Eqs. (85) and (86) hold. Furthermore,

$$\mathcal{PT}=\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}|\psi_{\nu_0},a\rangle\star\langle\phi_{\nu_0},a|+\sum_{\nu}\sum_{a=1}^{d_\nu}(|\psi_{\nu_+},a\rangle\star\langle\phi_{\nu_-},a|+|\psi_{\nu_-},a\rangle\star\langle\phi_{\nu_+},a|), \tag{94}$$

$$\mathcal{CPT}=\sum_{\nu_0}(-1)^{\nu_0}\sum_{a=1}^{d_{\nu_0}}|\psi_{\nu_0},a\rangle\star\langle\phi_{\nu_0},a|+\sum_{\nu}\sum_{a=1}^{d_\nu}(|\psi_{\nu_+},a\rangle\star\langle\phi_{\nu_-},a|+|\psi_{\nu_-},a\rangle\star\langle\phi_{\nu_+},a|). \tag{95}$$

In view of Eqs. (93)–(95), Proposition 4, and the construction given in the proof of Corollary 1, we can check that the operators $\mathcal{C}$, $\mathcal{PT}$, and $\mathcal{CPT}$ are involutions of the Hilbert space commuting with the Hamiltonian H. Therefore, we have the following generalization of Theorem 1.

Theorem 2: Every diagonalizable pseudo-Hermitian Hamiltonian H with a discrete spectrum is invariant under the action of $\mathcal{C}$, $\mathcal{PT}$, and $\mathcal{CPT}$. These operators which are involutions of the Hilbert space generate broken symmetries of H.

We wish to conclude this section by pointing out that the operators $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ are determined by a complete biorthonormal system associated with the Hamiltonian H. As the latter is unique only up to invertible symmetries of H, so are these operators.

VII. CONCLUSION

In this article, we discussed certain properties of pseudo-Hermitian operators and demonstrated their application in understanding the mathematical origin and exploring generalizations of the findings of Bender, Brody, and Jones.[1] In particular, for arbitrary diagonalizable pseudo-Hermitian Hamiltonians with a discrete spectrum, we introduced generalized parity, time-reversal, and charge-conjugation operators that coincide with the ordinary parity, time-reversal, and charge-conjugation for the PT-symmetric Hamiltonians (1). The generalized parity-time-reversal and charge conjugation operators are examples of generators of a set of generic symmetries of every diagonalizable pseudo-Hermitian Hamiltonians having a discrete spectrum. A common property of these symmetries is that they are generated by involutions. The generalized parity and time-reversal operators are, however, involutions only under certain conditions.

ACKNOWLEDGMENT

This work has been supported by the Turkish Academy of Sciences in framework of Young Researcher Award Program (EA-TUBA-GEBIP/2001-1-1).

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Resolvent convergence of sphere interactions to point interactions[a)]

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(Received 2 June 2000; accepted 16 October 2002)

We consider the Hamiltonian $H(a)=-\Delta+a^{-1}\lambda(a)q(\hat{x})\delta(|x|-a)$ which describes a sphere interaction ($\hat{x}=x/|x|$, $\lambda(a)=1+\alpha a+O(a^2)$). We study the convergence of $H(a)$ when $a\downarrow 0$ in the norm resolvent sense. The existence of the zero resonance of $-\Delta+q(\hat{x})\delta(|x|-1)$ affects the form of the limiting operator. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1533834]

I. INTRODUCTION

In this paper we are concerned with the Hamiltonian $H(a)$ describing a sphere interaction in $L_2(\mathbb{R}^3)$. $H(a)$ is formally given by

$$H(a)=-\Delta+a^{-1}\lambda(a)q(\hat{x})\delta(|x|-a), \tag{1.1}$$

where δ denotes the 1-dimensional delta function and $\hat{x}=x/|x|$. $q(\omega)$ is a real and smooth function on the unit sphere S_1. $\lambda(a)$ is a real valued function whose asymptotic behavior near $a=0$ is

$$\lambda(a)=1+\alpha a+O(a^2), \quad \alpha\in\mathbb{R}. \tag{1.2}$$

$H(a)$ is defined rigorously via the quadratic form h:

$$h[u,v]=(\nabla u,\nabla v)+\langle a^{-1}\lambda(a)q\gamma_a u,\gamma_a v\rangle_a,$$

$$\mathrm{Dom}[h]=H^1(\mathbb{R}^3).$$

Here $H^m(\mathbb{G})$ denotes the Sobolev space of order m over $\mathbb{G}$, $(,)$ the $L_2(\mathbb{R}^3)$ inner product, $\langle,\rangle_a$ the $L_2(S_a)$ inner product ($S_a=\{x\in\mathbb{R}^3;|x|=a\}, a>0, \langle,\rangle=\langle,\rangle_1$) and γ_a the trace operator from $H^1(\mathbb{R}^3)$ to $L_2(S_a)$. h is seen to be a lower semibounded closed form, and thus determines the unique self-adjoint operator,

$$H=H(a;a^{-1}\lambda(a)q), \tag{1.3}$$

such that

$$\mathrm{Dom}(H)\subset\mathrm{Dom}[h], \quad h[u,v]=(Hu,v),$$

for $u\in\mathrm{Dom}(H)$, $v\in\mathrm{Dom}[h]$ [(Ikebe, 1991), Theorem 1.4]. $H(a;a^{-1}\lambda(a)q)$ is seen to be $-\Delta$ with the interface condition on S_a:

$$\left(\frac{\partial u}{\partial r}\right)_+(x)-\left(\frac{\partial u}{\partial r}\right)_-(x)=a^{-1}\lambda(a)q(\hat{x})(\gamma_a u)(x), \tag{1.4}$$

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where $(\partial u/\partial r)_+(x)$ and $(\partial u/\partial r)_-(x)$ mean the limit of $\partial u/\partial r\,(x)$ obtained by approaching S_a from $\{|x|>a\}$ and $\{|x|<a\}$, respectively [(Ikebe, 1991), Theorem 1.7].

In the present paper we examine to which operator $H(a;a^{-1}\lambda(a)q)$ converges when $a\downarrow 0$. Since we have as $a\downarrow 0$,

$$a^{-2}q(\hat{x})\,\delta(|x|-a)\to\mu\,\delta(x)\quad\left(\mu=\int_{S_1}q(\omega)d\omega\right),\tag{1.5}$$

in the distribution sense, where $\delta(x)$ denotes the 3-dimensional delta function and $d\omega$ the surface measure on S_1, we may expect $-\Delta+a^{-2}q(\hat{x})\,\delta(|x|-a)$ converges to a Hamiltonian describing a point interaction $-\Delta+\mu\,\delta(x)$ in some sense. Contrary to this expectation our results (Theorems 3.3–3.6) show that we should replace a^{-2} in $-\Delta+a^{-2}q(\hat{x})\,\delta(|x|-a)$ by a^{-1} in order to obtain a meaningful limiting operator which describes a point interaction. This operator turns out to be a self-adjoint extension $H_p(\tau)$ parametrized by $\tau\in\mathbb{R}\cup\{\infty\}$ of

$$\hat{H}_{00}=-\Delta\restriction_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}.$$

That is uniquely determined by its resolvent $R_p(z;\tau)$:

$$R_p(\kappa^2;\tau)u(x)=R_0(\kappa^2)u(x)+\left(\tau-\frac{i\kappa}{4\pi}\right)^{-1}(R_0(\kappa^2)u)(0)\,\frac{e^{i\kappa|x|}}{4\pi|x|},\tag{1.6}$$

where $R_0(z)=(H_0-z)^{-1}$ and H_0 the free Hamiltonian:

$$H_0=H_p(\infty)=\overline{(-\Delta\restriction_{C_0^\infty(\mathbb{R}^3)})},$$

$\overline{T}$ being the closure of T [(Albeverio, 1988), Theorem 1.1.1, 1.1.2].

We can let $H(a;a^{-1}\lambda(a)q)$ converge to any $H_p(\tau)$ $(\tau\in\mathbb{R})$ in the norm resolvent sense if taking a suitable α in (1.2) under the condition that $H(1;q)$ has zero resonance. In this case we should note that $a^{-1}\lambda(a)q(\hat{x})$ tends to 0 in the distribution sense as $a\downarrow 0$. A similar situation occurs if we try to approximate $H_p(\tau)$ by short range Hamiltonians [(Albeverio, 1988), Theorem 1.2.10]. On the other hand, we do not have to pay any attention to the zero resonance when we approximate $H(a;q)$ by short range Hamiltonians whose potential converges to $q(\hat{x})\,\delta(|x|-a)$ for a fixed $a>0$ [(Shimada, 1992), Theorem 3].

The resolvent $R(\kappa^2;a)$ of $H(a;a^{-1}\lambda(a)q)$ is given by

$$R(\kappa^2;a)=R_0(\kappa^2)+\lambda(a)T(\kappa;a)(1-\lambda(a)\tilde{T}(\kappa;a))^{-1}\gamma_a R_0(\kappa^2)\tag{1.7}$$

[(Ikebe,1991), (7.2)]. Here, $T(\kappa;a):L_2(S_a)\to L_2(\mathbb{R}^3)$ is defined by

$$T(\kappa;a)u(x)=\frac{-1}{4\pi a}\int_{S_a}\frac{e^{i\kappa|x-y|}}{|x-y|}q(\hat{y})u(y)dS_y$$

for $u\in L_2(S_a)$,$x\in\mathbb{R}^3$ and $\tilde{T}(\kappa;a):L_2(S_a)\to L_2(S_a)$;

$$\tilde{T}(\kappa;a)u(x)=\frac{-1}{4\pi a}\int_{S_a}\frac{e^{i\kappa|x-y|}}{|x-y|}q(\hat{y})u(y)dS_y,$$

for $u\in L_2(S_a)$,$x\in S_a$. Introducing the unitary operator $U_a:L_2(S_1)\to L_2(S_a)$ defined by

$$U_a u(x)=\frac{1}{a}u(\hat{x}),$$

we can rewrite (1.7) as

$$R(\kappa^2;a)=R_0(\kappa^2)+\lambda(a)T(\kappa;a)U_a(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_0(\kappa^2), \tag{1.8}$$

where $\tilde{T}(a\kappa)=\tilde{T}(a\kappa;1)$. We shall derive the asymptotic expansions of $(1-\lambda(a)\tilde{T}(a\kappa))^{-1}$ near $a=0$ in Sec. II. In Sec. III, after examining the asymptotic behavior of $U_a^{-1}\gamma_a R_0(\kappa^2)$ and $\lambda(a)T(\kappa;a)U_a$, we prove the norm resolvent convergence of $H(a;a^{-1}\lambda(a)q)$. We shall also treat the case that q is a constant on S_1, where we can compute the zero resonance function of $H(1;q)$ explicitly.

At the end of this section, we refer to Antoine (1987), Hounkonnau (2000), and Hounkonnau (1999) (and references therein) for a recent development of this area including δ'-sphere and relativistic δ-sphere interactions. All authors mentioned above have treated Hamiltonians reduced into the direct sum of operators by a separation of variables. Among them we should mention the work of Antoine (1987). They have proved the norm resolvent convergence of their δ-sphere Hamiltonian to any Hamiltonian describing point interaction by a suitable choice of parameter. In contrast to our case, no properties of zero resonance enter into their discussion as well as into that of approximating one-dimensional point interactions by scaled short range Hamiltonians [(Albeverio, 1988), Sec. I.3.2]. They have reduced the problem to the one concerning radial Hamiltonians since their Hamiltonian is rotationally invariant. However, the author could not relate these two cases more clearly.

II. THE EXPANSION OF $(1-\lambda(a)\tilde{T}(a\kappa))^{-1}$ NEAR $a=0$

In this section, we derive the asymptotic expansion of $(1-\lambda(a)\tilde{T}(a\kappa))^{-1}$ near $a=0$. It will be done along the line of [(Shimada, 1994), Sec. 4]. The behavior depends heavily on the structure of the null space of $1-\tilde{T}(0)$.

Let us recall some results obtained in [(Shimada, 1994), Sec. 3] (up to the end of this paragraph). First, $L_2(S_1)$ is decomposed into the direct sum of subspaces:

$$L_2(S_1)=\mathcal{N}(1-\tilde{T}(0))\dot{+}\mathcal{R}(1-\tilde{T}(0)), \tag{2.1}$$

where $\mathcal{N}(T)$ means the null space of T, $\mathcal{R}(T)$ the range of T, and $\dot{+}$ the (not necessarily orthogonal) direct sum. Let Q be the projection onto $\mathcal{N}(1-\tilde{T}(0))$ along $\mathcal{R}(1-\tilde{T}(0))$. Then

$$\dim\mathcal{R}(Q)<+\infty.$$

Since $1-\tilde{T}(0)-Q$ is invertible, we define K by

$$K=(1-\tilde{T}(0)-Q)^{-1}Q_0\in\mathbf{B}(L_2(S_1)), \tag{2.2}$$

where $Q_0=1-Q$ and $\mathbf{B}(\mathcal{X},\mathcal{Y})$ denotes the set of all bounded operators from $\mathcal{X}$ to $\mathcal{Y}$ ($\mathbf{B}(\mathcal{X})=\mathbf{B}(\mathcal{X},\mathcal{X})$). We define $A_j\in\mathbf{B}(L_2(S_1))$ by

$$A_j u(\omega)=\frac{-i^j}{4\pi j!}\int_{S_1}|\omega-\omega'|^{j-1}q(\omega')u(\omega')d\omega',$$

for $u\in L_2(S_1)$. Then we have

$$\tilde{T}(\kappa)=\sum_{j=0}^{\infty}\kappa^j A_j \quad in \quad \mathbf{B}(L_2(S_1)) \quad (\kappa\in\mathbb{C}). \tag{2.3}$$

Let P_0 be the orthogonal projection onto $\mathcal{N}(H(1;q))$. Let $\hat{P}_0=\gamma_1 P_0$. Then we have

$$\tilde{P}_0 \in \mathbf{B}(L_2(\mathbb{R}^3), L_2(S_1)), \quad \mathcal{R}(\tilde{P}_0) = \mathcal{N}_2, \tag{2.4}$$

where $\mathcal{N}_2$ is the subspace of $\mathcal{N}(1-\tilde{T}(0))$ defined by

$$\mathcal{N}_2 = \{u \in L_2(S_1); u \in \mathcal{N}(1-\tilde{T}(0)), \langle u, q\rangle = 0\}. \tag{2.5}$$

We put $P = \tilde{P}_0 \tilde{P}_0^*$, where $*$ means the adjoint. We define Q_1 and Q_2 by

$$Q_1 = (1 + PqA_2)Q, \quad Q_2 = -PqA_2Q.$$

Then it is seen that Q_j $(j=0,1,2)$ are (not necessarily orthogonal) projections and satisfy the following relations:

$$Q_1 + Q_2 = Q, \quad Q_0 + Q_1 + Q_2 = 1, \quad Q_iQ_j = \delta_{ij}Q_j \ \ (i,j=0,1,2), \tag{2.6}$$

$$\mathcal{R}(Q_0) = \mathcal{R}(1-\tilde{T}(0)), \quad \mathcal{R}(Q_2) = \mathcal{N}_2. \tag{2.7}$$

If $Q_1 \neq 0$, we can find $f_0 \in \mathcal{R}(Q_1)$ such that

$$\langle f_0, q\rangle = (4\pi)^{1/2}, \quad \mathcal{R}(Q_1) = \{cf_0; c \in \mathbb{C}\}. \tag{2.8}$$

We put

$$\mathcal{N}_1 = \mathcal{R}(Q_1). \tag{2.9}$$

Then, in view of (2.1), (2.6), (2.7) and (2.9) we have the following decompositions:

$$\mathcal{N}(1-\tilde{T}(0)) = \mathcal{N}_1 \dotplus \mathcal{N}_2, \quad L_2(S_1) = \mathcal{N}_1 \dotplus \mathcal{N}_2 \dotplus \mathcal{R}(1-\tilde{T}(0)). \tag{2.10}$$

$\mathcal{N}_1$ corresponds to the zero resonance state of $H(1;q)$ in the following sense. Let $u_0 = T(0;1)f_0$. Then u_0 satisfies

$$\Delta u_0 = 0 \quad on \quad \mathbb{R}^3 \backslash S_1,$$

$$\left(\frac{\partial u_0}{\partial r}\right)_+ - \left(\frac{\partial u_0}{\partial r}\right)_- = qu_0 \quad on \quad S_1,$$

and

$$u_0(x) = -(4\pi)^{-1/2}|x|^{-1} + O(|x|^{-2}) \quad as \quad |x| \to \infty.$$

Thus, u_0 satisfies $H(1;q)u_0 = 0$ formally and does not belong to $L_2(\mathbb{R}^3)$. On the other hand, there exists a bijection between $\mathcal{N}_2$ and $\mathcal{N}(H(1;q))$ by [(Shimada, 1994), Theorem 2.4].

Now we derive the asymptotic expansion of $(1-\lambda(a)\tilde{T}(a\kappa))^{-1}$ near $a=0$ according to the possible four cases of Q_1 and Q_2.

Lemma 2.1: Assume that $Q_1 = Q_2 = 0$. Then we have as $a \downarrow 0$,

$$(1-\lambda(a)\tilde{T}(a\kappa))^{-1} = O(1),$$

where $O(a^s)$ means a bounded linear operator whose norm is $O(a^s)$ as $a \downarrow 0$.

Proof: Since $(1-\tilde{T}(0))^{-1}$ exists by (2.7), (2.9) and (2.10), we have as $a \downarrow 0$,

$$1-\lambda(a)\tilde{T}(a\kappa)=1-\tilde{T}(0)-(\tilde{T}(a\kappa)-\tilde{T}(0))+O(a)$$
$$=1-\tilde{T}(0)+o(1)$$
$$=(1-\tilde{T}(0))[1+(1-\tilde{T}(0))^{-1}o(1)],$$

where we have used (1.2) and the fact that $\tilde{T}(a\kappa)$ is a compact operator valued continuous function in a. The desired result follows immediately. □

To treat cases other than $Q_1=Q_2=0$, we use the following lemma obtained by [(Jensen, 1979), Lemma 3.12].

Lemma 2.2: Let $\mathcal{X}$, $\mathcal{Y}$, X and Y be vector spaces. Let $L:\mathcal{X}\to\mathcal{Y}, B:X\to\mathcal{X}$ and $C:\mathcal{Y}\to Y$ be linear operators. Let $A=CLB$. If A^{-1} exists, B is surjective and C is injective, then L^{-1} exists and $L^{-1}=BA^{-1}C$.

Lemma 2.3: Assume that $Q_1\neq 0$ and $\kappa\neq -i\alpha\langle qf_0,f_0\rangle$. Then $Q_1^*q(\kappa A_1+\alpha A_0)Q_1$ is invertible in $\mathbf{B}(\mathcal{R}(Q_1),\mathcal{R}(Q_1^*))$ with the inverse

$$[Q_1^*q(\kappa A_1+\alpha A_0)Q_1]^{-1}=(-i\kappa+\alpha\langle qf_0,f_0\rangle)^{-1}\langle\cdot,f_0\rangle f_0.$$

Proof: We can take $g_0\in\mathcal{R}(Q_1^*)$ such that

$$\langle f_0,g_0\rangle=1$$

by [(Shimada, 1994), Lemma 3.19]. Then $u\in\mathcal{R}(Q_1)$ is of the form

$$Q_1u=u=\langle u,g_0\rangle f_0. \tag{2.11}$$

Since $A_0=\tilde{T}(0)$ and $A_1=-i/4\pi\langle\cdot,q\rangle$, we have

$$(\kappa A_1+\alpha A_0)f_0=-i(4\pi)^{-1/2}\kappa+\alpha f_0, \tag{2.12}$$

where we used (2.8) and the fact that $f_0\in\mathcal{N}(1-\tilde{T}(0))$. Since $Q_1^*=\langle\cdot,f_0\rangle g_0$, we have by (2.8) and (2.12),

$$Q_1^*q(\kappa A_1+\alpha A_0)f_0=(-i\kappa+\alpha\langle qf_0,f_0\rangle)g_0,$$

and hence, together with (2.11),

$$Q_1^*q(\kappa A_1+\alpha A_0)Q_1u=(-i\kappa+\alpha\langle qf_0,f_0\rangle)\langle u,g_0\rangle g_0.$$

From this, the desired result follows. □

Lemma 2.4: Assume that $Q_1\neq 0$, $Q_2=0$ and $\kappa\neq -i\alpha\langle qf_0,f_0\rangle$. Then we have as $a\downarrow 0$,

$$(1-\lambda(a)\tilde{T}(a\kappa))^{-1}=-a^{-1}(-i\kappa+\alpha\langle qf_0,f_0\rangle)^{-1}\langle\cdot,qf_0\rangle f_0+O(1).$$

We should note that $\langle qf_0,f_0\rangle\neq 0$ holds if $q(\omega)\geqslant 0$ (or $q(\omega)\leqslant 0$) on S_1 under the assumption $Q_1\neq 0$ (in which case $q\not\equiv 0$). In fact, assume that $q\geqslant 0$ and $\langle qf_0,f_0\rangle=0$. Then we have

$$q^{1/2}f_0=0,$$

and hence

$$qf_0=0.$$

Thus we have

$$f_0(\omega)=\frac{-1}{4\pi}\int_{S_1}\frac{1}{|\omega-\omega'|}q(\omega')f_0(\omega')d\omega'=0,$$

which is a contradiction.

Proof: Under our assumption, we have by (2.7) and (2.10)

$$L_2(S_1)=\mathcal{R}(Q_0)\dotplus\mathcal{R}(Q_1). \tag{2.13}$$

As was shown in the proof of [(Shimada, 1994), Lemma 4.3], we have

$$L_2(S_1)=\mathcal{R}(Q_0)\dotplus\mathcal{R}(Q_1^*). \tag{2.14}$$

Now let

$$\mathcal{X}=\mathcal{Y}=L_2(S_1),\quad X=\mathcal{R}(Q_0)\dotplus\mathcal{R}(Q_1),\quad Y=\mathcal{R}(Q_0)\dotplus\mathcal{R}(Q_1^*),$$

$$L=1-\lambda(a)\tilde{T}(a\kappa),$$

$$B=[Q_0\quad a^{-1/2}Q_1],$$

$$C=\begin{bmatrix}Q_0\\ a^{-1/2}Q_1^*q\end{bmatrix}.$$

Then, from (2.13) and (2.14), B and C are well-defined bounded operators on $L_2(S_1)$. B is obviously surjective. From the proof of [(Shimada, 1994), Lemma 4.3] it follows that C is injective. Define $A=CLB$. Then A has the following form:

$$A=\begin{bmatrix}Q_0(1-\lambda(a)\tilde{T}(a\kappa))Q_0 & a^{-1/2}Q_0(1-\lambda(a)\tilde{T}(a\kappa))Q_1\\ a^{-1/2}Q_1^*q(1-\lambda(a)\tilde{T}(a\kappa))Q_0 & a^{-1}Q_1^*q(1-\lambda(a)\tilde{T}(a\kappa))Q_1\end{bmatrix}=\begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix}.$$

We have by (1.2) and (2.3),

$$1-\lambda(a)\tilde{T}(a\kappa)=1-\tilde{T}(0)-a(\kappa A_1+\alpha A_0)+O(a^2). \tag{2.15}$$

We know by [(Shimada, 1994), Lemma 3.15],

$$(1-\tilde{T}(0))Q_j=Q_j^*q(1-\tilde{T}(0))=0\quad(j=1,2). \tag{2.16}$$

Thus, using (2.15) and (2.16) we have

$$A_{11}=Q_0(1-\tilde{T}(0))Q_0+O(a),$$

$$A_{12}=O(a^{1/2})$$

$$A_{21}=O(a^{1/2})$$

$$A_{22}=-Q_1^*q(\kappa A_1+\alpha A_0)Q_1+O(a).$$

So, we can rewrite A as $A=D-E$ with

$$D=\begin{bmatrix}Q_0(1-\tilde{T}(0))Q_0 & 0\\ 0 & -Q_1^*q(\kappa A_1+\alpha A_0)Q_1\end{bmatrix},$$

$$E=\begin{bmatrix} O(a) & O(a^{1/2}) \\ O(a^{1/2}) & O(a) \end{bmatrix}.$$

We know by [(Shimada, 1994), Lemma 3.18],

$$[Q_0(1-\tilde{T}(0))Q_0]^{-1}=K|_{\mathcal{R}(Q_0)} \quad in \quad \mathbf{B}(\mathcal{R}(Q_0)) \tag{2.17}$$

[see (2.2)]. Thus, from Lemma 2.3 and (2.17), D is invertible with the inverse,

$$D^{-1}=\begin{bmatrix} K & 0 \\ 0 & -(-i\kappa+\alpha\langle qf_0,f_0\rangle)^{-1}\langle\cdot,f_0\rangle f_0 \end{bmatrix}.$$

Therefore, since A is invertible with the inverse,

$$A^{-1}=(1-D^{-1}E)^{-1}D^{-1}=D^{-1}+\sum_{j=1}^{\infty}(D^{-1}E)^jD^{-1},$$

we have by Lemma 2.2,

$$L^{-1}=BD^{-1}C+\sum_{j=1}^{\infty}B(D^{-1}E)^jD^{-1}C.$$

Direct computation shows that

$$BD^{-1}C=-a^{-1}(-i\kappa+\alpha\langle qf_0,f_0\rangle)^{-1}\langle\cdot,f_0\rangle f_0+O(1),$$

$$\sum_{j=1}^{\infty}B(D^{-1}E)^jD^{-1}C=O(1).$$

Thus we completed the proof. □

Lemma 2.5: Assuume that $Q_1=0$ *and* $Q_2\neq 0$. *Then* $Q_2^*qQ_2$ *is invertible in* $\mathbf{B}(\mathcal{R}(Q_2),\mathcal{R}(Q_2^*))$.

Proof: Since $Q_2=Q$, we have by [(Shimada, 1994), Lemma 3.3],

$$\mathcal{R}(Q_2)=\mathcal{N}(1-\tilde{T}(0)), \quad \mathcal{R}(Q_2^*)=\mathcal{N}(1-\tilde{T}(0)^*).$$

Now, since q is a bijection from $\mathcal{N}(1-\tilde{T}(0))$ to $\mathcal{N}(1-\tilde{T}(0)^*)$ ([(Shimada, 1994), Lemma 3.1]), the lemma follows. □

When $Q_1=0$ and $Q_2\neq 0$, we put $W=(Q_2^*qQ_2)^{-1}\in\mathbf{B}(\mathcal{R}(Q_2^*),\mathcal{R}(Q_2))$.

Lemma 2.6: Assume that $Q_1=0$, $Q_2\neq 0$ *and* $\alpha\neq 0$ *in* (1.2). *Then we have as* $a\downarrow 0$,

$$(1-\lambda(a)\tilde{T}(a\kappa))^{-1}=-a^{-1}\alpha^{-1}Q_2WQ_2^*q+O(1).$$

Proof: Under our assumption, we have

$$L_2(S_1)=\mathcal{R}(Q_0)\dot{+}\mathcal{R}(Q_2)=\mathcal{R}(Q_0)\dot{+}\mathcal{R}(Q_2^*).$$

Let

$$\mathcal{X}=\mathcal{Y}=L_2(S_1), \quad X=\mathcal{R}(Q_0)\dot{+}\mathcal{R}(Q_2), \quad Y=\mathcal{R}(Q_0)\dot{+}\mathcal{R}(Q_2^*),$$

$$L=1-\lambda(a)\tilde{T}(a\kappa),$$

$$B=[Q_0 \quad a^{-1/2}Q_2],$$

$$C=\begin{bmatrix} Q_0 \\ a^{-1/2}Q_2^* q \end{bmatrix}.$$

Then, from an argument similar to the proof of [(Shimada, 1994), Lemma 4.3], it follows that B is surjective and C is injective. Define $A=CLB$. Then A has the following form:

$$A=\begin{bmatrix} Q_0(1-\lambda(a)\tilde{T}(a\kappa))Q_0 & a^{-1/2}Q_0(1-\lambda(a)\tilde{T}(a\kappa))Q_2 \\ a^{-1/2}Q_2^* q(1-\lambda(a)\tilde{T}(a\kappa))Q_0 & a^{-1}Q_2^* q(1-\lambda(a)\tilde{T}(a\kappa))Q_2 \end{bmatrix}=\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}.$$

Using (2.15) and (2.16) we have

$$A_{11}=Q_0(1-\tilde{T}(0))Q_0+O(a),$$

$$A_{12}=O(a^{1/2}),$$

$$A_{21}=O(a^{1/2}),$$

$$A_{22}=-Q_2^* q(\kappa A_1+\alpha A_0)Q_2+O(a).$$

Moreover, since $A_1Q_2=0$ [(Shimada, 1994), Lemma 3.6] and $A_0=\tilde{T}(0)$, we have by (2.16),

$$A_{22}=-\alpha Q_2^* q\tilde{T}(0)Q_2+O(a)=\alpha Q_2^* q(1-\tilde{T}(0))Q_2-\alpha Q_2^* qQ_2+O(a)=-\alpha Q_2^* qQ_2+O(a).$$

So, we can rewrite A as $A=D-E$ with

$$D=\begin{bmatrix} Q_0(1-\tilde{T}(0))Q_0 & 0 \\ 0 & -\alpha Q_2^* qQ_2 \end{bmatrix},$$

$$E=\begin{bmatrix} O(a) & O(a^{1/2}) \\ O(a^{1/2}) & O(a) \end{bmatrix}.$$

From Lemma 2.5 and (2.17), D is invertible with the inverse,

$$D^{-1}=\begin{bmatrix} K & 0 \\ 0 & -\alpha^{-1}W \end{bmatrix}.$$

Thus, an application of Lemma 2.2 gives

$$L^{-1}=BD^{-1}C+O(1)=-a^{-1}\alpha^{-1}Q_2WQ_2^* q+O(1).$$

Therefore we completed the proof. □

Lemma 2.7: Assume that $Q_1\neq 0$, $Q_2\neq 0$ *and* $q(\omega)\geqslant 0$ [*or* $q(\omega)\leqslant 0$] *on* S_1. *Then* $Q_2^* qQ_2$ *is invertible in* $\mathbf{B}(\mathcal{R}(Q_2),\mathcal{R}(Q_2^*))$.

Proof: Since $\dim\mathcal{R}(Q_2)=\dim\mathcal{R}(Q_2^*)<+\infty$ [(Shimada, 1994), Theorem 2.4, Lemma 3.19]), we have only to show the injectivity of $Q_2^* qQ_2$. Assume that

$$Q_2^* qQ_2u=0, \quad u\in\mathcal{R}(Q_2).$$

Then

$$0=\langle Q_2^* q Q_2 u,u\rangle=\langle qu,u\rangle=\int_{S_1} q(\omega)|u(\omega)|^2\,d\omega,$$

and hence, by our assumption,

$$q(\omega)u(\omega)=0.$$

Thus we have

$$u(\omega)=\tilde{T}(0)u(\omega)=\frac{-1}{4\pi}\int_{S_1}\frac{1}{|\omega-\omega'|}q(\omega')u(\omega')d\omega'=0. \qquad \square$$

Lemma 2.8: Assume that $q(\omega)\geqslant 0$ [*or* $q(\omega)\leqslant 0$] *on* S_1. *Assume that* $Q_1\neq 0$, $Q_2\neq 0$, $\alpha\neq 0$ *and* $\kappa\neq -i\alpha[\det(\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}/\det(\langle f_i,qf_j\rangle)_{1\leqslant i,j\leqslant n}]$. *Define the operator* $D_1:\mathcal{R}(Q_1)\dot{+}\mathcal{R}(Q_2)\to\mathcal{R}(Q_1^*)\dot{+}\mathcal{R}(Q_2^*)$ *by*

$$D_1=\begin{bmatrix} Q_1^* q(\kappa A_1+\alpha A_0)Q_1 & \alpha Q_1^* q Q_2 \\ \alpha Q_2^* q Q_1 & \alpha Q_2^* q Q_2 \end{bmatrix}.$$

Then D_1 *is invertible. Here* $\{f_j\}_{1\leqslant j\leqslant n}$ *is a basis of* $\mathcal{R}(Q_2)$.

We put

$$D_1^{-1}=-\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22}\end{bmatrix}:\mathcal{R}(Q_1^*)\dot{+}\mathcal{R}(Q_2^*)\to\mathcal{R}(Q_1)\dot{+}\mathcal{R}(Q_2).$$

We should remark that

$$(i)\ \det(\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}\neq 0;\quad (ii)\ \det(\langle f_i,qf_j\rangle)_{1\leqslant i,j\leqslant n}\neq 0;$$

(iii) $\det(\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}/\det(\langle f_i,qf_j\rangle)_{1\leqslant i,j\leqslant n}$ does not depend on the choice of basis $\{f_j\}_{1\leqslant j\leqslant n}$. In fact, let $x=(c_0,c_1,\ldots,c_n)$. Assume that

$$(\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}x=0.$$

Then, if we assume $q\geqslant 0$, we have

$$0=((\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}x)\cdot x=\left\|q^{1/2}\left(\sum_{j=0}^{n}c_j f_j\right)\right\|^2.$$

Thus

$$q\left(\sum_{j=0}^{n}c_j f_j\right)=0.$$

Since $q:\mathcal{R}(Q)\to\mathcal{R}(Q^*)$ is bijective [(Shimada, 1994), Lemma 3.1], we have

$$\sum_{j=0}^{n}c_j f_j=0.$$

Since $f_0,f_1,\ldots,f_n$ are linearly independent, we obtain

$$c_0=c_1=\cdots=c_n=0,$$

and hence

$$x=0.$$

From this, (i) follows. We can show (ii) in a similar way. We show (iii). We use the identity

$$\det(\langle f_i, qf_j\rangle)_{1\leqslant i,j\leqslant n}=|\det(c_{ij})_{1\leqslant i,j\leqslant n}|^2\det(\langle g_i, qg_j\rangle)_{1\leqslant i,j\leqslant n}, \tag{2.18}$$

provided that

$$[f_1 f_2\cdots f_n]=[g_1 g_2\cdots g_n]\begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n}\\ c_{21} & c_{22} & \cdots & c_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ c_{n1} & c_{n2} & \cdots & c_{nn}\end{bmatrix}. \tag{2.19}$$

Let $\{g_j\}_{1\leqslant j\leqslant n}$ be another basis of $\mathcal{R}(Q_2)$. Then there exists the regular matrix $(c_{ij})_{1\leqslant i,j\leqslant n}$ such that (2.19) holds. On the other hand,

$$[f_0 f_1 f_2\cdots f_n]=[f_0 g_1 g_2\cdots g_n]\begin{bmatrix} 1 & 0 & 0 & \cdots & 0\\ 0 & c_{11} & c_{12} & \cdots & c_{1n}\\ 0 & c_{21} & c_{22} & \cdots & c_{2n}\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & c_{n1} & c_{n2} & \cdots & c_{nn}\end{bmatrix}, \tag{2.20}$$

holds. Applying (2.18) for (2.19) and (2.20), (iii) follows.

Proof of Lemma 2.8: Since

$$\dim(\mathcal{R}(Q_1)\dot{+}\mathcal{R}(Q_2))=\dim(\mathcal{R}(Q_1^*)\dot{+}\mathcal{R}(Q_2^*))<+\infty,$$

we have only to show that D_1 is injective. We can find $g_0\in\mathcal{R}(Q_1^*), g_j\in\mathcal{R}(Q_2^*)$ $(j=1,2,\ldots,n)$ such that

$$\langle f_0, g_0\rangle=1,\quad \langle f_i, g_j\rangle=\delta_{ij}\quad (i,j=1,2,\ldots,n).$$

Then we have

$$Q_1^*=\langle\cdot, f_0\rangle g_0,\quad Q_2^*=\sum_{j=1}^{n}\langle\cdot, f_j\rangle g_j. \tag{2.21}$$

Let

$$u=c_0 f_0,\quad v=\sum_{j=1}^{n} c_j f_j\ (c_k\in\mathbb{C}, k=0,1,\ldots,n). \tag{2.22}$$

Then, using (2.8), (2.12) and (2.21) we have

$$Q_1^* q(\kappa A_1+\alpha A_0)Q_1 u=c_0(-i\kappa+\alpha\langle f_0, qf_0\rangle)g_0,$$

$$\alpha Q_1^* q Q_2 v=\alpha\left(\sum_{j=1}^{n} c_j\langle f_j, qf_0\rangle\right)g_0, \tag{2.23}$$

$$\alpha Q_2^* q Q_1 u = \alpha c_0 \sum_{j=1}^{n} \langle f_0, q f_j \rangle g_j,$$

$$1\,\alpha Q_2^* q Q_2 v = \alpha \sum_{k=1}^{n} \sum_{j=1}^{n} c_j \langle f_j, q f_k \rangle g_k.$$

Thus the equation

$$D_1 \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

implies

$$\tilde{D}_1 \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix} = 0,$$

where

$$\tilde{D}_1 = \begin{bmatrix} -i\kappa + \alpha\langle f_0, q f_0 \rangle & \alpha\langle f_1, q f_0 \rangle & \cdots & \alpha\langle f_n, q f_0 \rangle \\ \alpha\langle f_0, q f_1 \rangle & \alpha\langle f_1, q f_1 \rangle & \cdots & \alpha\langle f_n, q f_1 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \alpha\langle f_0, q f_n \rangle & \alpha\langle f_1, q f_n \rangle & \cdots & \alpha\langle f_n, q f_n \rangle \end{bmatrix}. \tag{2.24}$$

Since

$$\det \tilde{D}_1 = \alpha^n (-i\kappa \det(\langle f_i, q f_j \rangle)_{1 \leqslant i,j \leqslant n} + \alpha \det(\langle f_i, q f_j \rangle)_{0 \leqslant i,j \leqslant n}) \neq 0, \tag{2.25}$$

the lemma follows. □

Lemma 2.9: Assume that $q(\omega) \geqslant 0$ [*or* $q(\omega) \leqslant 0$] *on* S_1. *Assume that* $Q_1 \neq 0$, $Q_2 \neq 0$, $\alpha \neq 0$ *and* $\kappa \neq -i\alpha \det(\langle f_i, q f_j \rangle)_{0 \leqslant i,j \leqslant n} / \det(\langle f_i, q f_j \rangle)_{1 \leqslant i,j \leqslant n}$. *Then we have as* $a \downarrow 0$,

$$(1 - \lambda(a)\tilde{T}(a\kappa))^{-1} = a^{-1}(Q_1 B_{11} Q_1^* + Q_1 B_{12} Q_2^* + Q_2 B_{21} Q_1^* + Q_2 B_{22} Q_2^*) q + O(1).$$

Proof: Under our assumption, we have

$$L_2(S_1) = \mathcal{R}(Q_0) \dotplus \mathcal{R}(Q_1) \dotplus \mathcal{R}(Q_2) = \mathcal{R}(Q_0) \dotplus \mathcal{R}(Q_1^*) \dotplus \mathcal{R}(Q_2^*).$$

Let

$$\mathcal{X} = \mathcal{Y} = L_2(S_1), \quad X = \mathcal{R}(Q_0) \dotplus \mathcal{R}(Q_1) \dotplus \mathcal{R}(Q_2),$$

$$Y = \mathcal{R}(Q_0) \dotplus \mathcal{R}(Q_1^*) \dotplus \mathcal{R}(Q_2^*),$$

$$L = 1 - \lambda(a)\tilde{T}(a\kappa),$$

$$B = [\,Q_0 \quad a^{-1/2} Q_1 \quad a^{-1/2} Q_2\,],$$

$$C = \begin{bmatrix} Q_0 \\ a^{-1/2} Q_1^* q \\ a^{-1/2} Q_2^* q \end{bmatrix}.$$

Then, it is seen that B is surjective and C is injective. Define

$$A=CLB=\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}.$$

Then, using the relations

$$(1-\tilde{T}(0))Q_j=Q_j^*q(1-\tilde{T}(0))=0 \quad (j=1,2),$$

$$A_1Q_2=Q_2^*qA_1=0$$

[(Shimada, 1994), Lemmas 3.15, 3.16], we have

$$A_{11}=Q_0(1-\tilde{T}(0))Q_0+O(a),$$

$$A_{12}=O(a^{1/2}),$$

$$A_{13}=O(a^{1/2}),$$

$$A_{21}=O(a^{1/2}),$$

$$A_{22}=-Q_1^*q(\kappa A_1+\alpha A_0)Q_1+O(a),$$

$$A_{23}=-\alpha Q_1^*qQ_2+O(a),$$

$$A_{31}=O(a^{1/2}),$$

$$A_{32}=-\alpha Q_2^*qQ_1+O(a),$$

$$A_{33}=-\alpha Q_2^*qQ_2+O(a).$$

So, we can rewrite A as $A=D-E$ with

$$D=\begin{bmatrix} Q_0(1-\tilde{T}(0))Q_0 & 0 & 0 \\ 0 & -Q_1^*q(\kappa A_1+\alpha A_0)Q_1 & -\alpha Q_1^*qQ_2 \\ 0 & -\alpha Q_2^*qQ_1 & -\alpha Q_2^*qQ_2 \end{bmatrix},$$

$$E=\begin{bmatrix} O(a) & O(a^{1/2}) & O(a^{1/2}) \\ O(a^{1/2}) & O(a) & O(a) \\ O(a^{1/2}) & O(a) & O(a) \end{bmatrix}.$$

From Lemma 2.8 and (2.17) D is invertible with the inverse,

$$D^{-1}=\begin{bmatrix} K & 0 & 0 \\ 0 & B_{11} & B_{12} \\ 0 & B_{21} & B_{22} \end{bmatrix}.$$

Thus an application of Lemma 2.2 gives the desired result. □

III. RESOLVENT CONVERGENCE OF $H(a;a^{-1}\lambda(a)q)$

In order to prove the norm resolvent convergence of $H(a;a^{-1}\lambda(a)q))$ as $a\downarrow 0$, we prepare the following two lemmas.

Lemma 3.1: Let $z\in\mathbb{C}$ be such that $\mathrm{Im}\, z\neq 0$. Then, for any $\varepsilon>0$, we have as $a\downarrow 0$,

$$U_a^{-1}\gamma_a R_0(z)=a(R_0(z)\cdot)(0)+O(a^{3/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(\mathbb{R}^3),L_2(S_1)).$$

Proof: Since $U_a^{-1}:L_2(S_a)\to L_2(S_1)$,

$$(U_a^{-1}u)(\omega)=au(a\omega) \quad (\omega\in S_1)$$

is unitary, we have only to show that

$$\gamma_a R_0(z)=(R_0(z)\cdot)(0)+O(a^{3/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(\mathbb{R}^3),L_2(S_a)), \tag{3.1}$$

as $a\downarrow 0$ for sufficiently small $\varepsilon>0$. Let $u\in\mathcal{S}$ (the Schwartz space of rapidly decreasing functions). Then, for $x\in S_a$ we have

$$(\gamma_a R_0(z)u)(x)=(R_0(z)u)(x)=(2\pi)^{-3/2}\int\frac{e^{ix\cdot\xi}}{|\xi|^2-z}\hat{u}(\xi)d\xi, \tag{3.2}$$

where $\hat{u}=\mathcal{F}u$ is the Fourier transform of u defined by

$$\mathcal{F}u(\xi)=(2\pi)^{-3/2}\int e^{-i\xi\cdot x}u(x)dx.$$

Let μ be such that $0<\mu<1/2$. Then, since

$$|e^{ix\cdot\xi}-1|\leqslant 2^{1-\mu}a^{\mu}|\xi|^{\mu} \quad (|x|=a), \tag{3.3}$$

we have by (3.2) and the Schwarz inequality,

$$|(\gamma_a R_0(z)u)(x)-(R_0(z)u)(0)|\leqslant(2\pi)^{-3/2}2^{1-\mu}a^{\mu}\left\|\frac{|\xi|^{\mu}}{|\xi|^2-z}\right\|\cdot\|u\|, \tag{3.4}$$

and hence

$$\|(\gamma_a R_0(z)u)-(R_0(z)u)(0)\|_{L_2(S_a)}\leqslant\pi^{-1}2^{1/2-\mu}a^{1+\mu}\left\|\frac{|\xi|^{\mu}}{|\xi|^2-z}\right\|\cdot\|u\|, \tag{3.5}$$

which implies (3.1). □

Lemma 3.2: Let $\kappa\in\mathbb{C}$ be such that $\mathrm{Im}\,\kappa\neq 0$. Then, for any $\varepsilon>0$, we have as $a\downarrow 0$,

$$\lambda(a)T(\kappa;a)U_a=-\frac{e^{i\kappa|x|}}{4\pi|x|}\langle\cdot,q\rangle+O(a^{1/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(S_1),L_2(\mathbb{R}^3)).$$

Proof: In view of (1.2), we have only to show that

$$T(\kappa;a)U_a=-\frac{e^{i\kappa|x|}}{4\pi|x|}\langle\cdot,q\rangle+O(a^{1/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(S_1),L_2(\mathbb{R}^3)), \tag{3.6}$$

as $a\downarrow 0$ for sufficiently small $\varepsilon>0$. Let $u\in L_2(S_1)$. Then, since

$$\mathcal{F}\left(\frac{e^{i\kappa|\cdot-y|}}{4\pi|\cdot-y|}\right)(\xi)=(2\pi)^{-3/2}\frac{e^{-i\xi\cdot y}}{|\xi|^2-\kappa^2},$$

we have by the Parseval identity,

$$\left\| T(\kappa;a)U_a u + \frac{e^{i\kappa|x|}}{4\pi|x|}\langle u,q\rangle \right\|^2 = \int d\xi \left| \frac{-(2\pi)^{-3/2}}{|\xi|^2-\kappa^2} \int_{S_1} d\omega (e^{-i\xi\cdot a\omega}-1) q(\omega)u(\omega) \right|^2 = I(a). \tag{3.7}$$

Let μ be such that $0<\mu<1/2$. Then, by (3.3) and the Schwarz inequality, we obtain

$$I(a) \leqslant (2\pi)^{-3} 2^{2(1-\mu)} a^{2\mu} \int d\xi \frac{|\xi|^{2\mu}}{||\xi|^2-\kappa^2|^2} \|q\|^2 \|u\|^2. \tag{3.8}$$

Thus (3.7) and (3.8) imply (3.6). □

Now we are in a position to prove the norm resolvent convergence of $H(a)$ as $a\downarrow 0$.

Theorem 3.3: *Assume that $Q_1=Q_2=0$. Then we have as $a\downarrow 0$,*

$$R(\kappa^2;a) = R_0(\kappa^2) + O(a) \quad in \quad \mathbf{B}(L_2(\mathbb{R}^3))$$

for $\kappa\in\mathbb{C}$ such that $Im\ \kappa^2\neq 0$.

Proof: In view of Lemmas 2.1, 3.1 and 3.2 we have

$$\lambda(a)T(\kappa;a)U_a(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_a(\kappa^2) = O(a).$$

Thus, from (1.8) we obtain the required result. □

Theorem 3.4: *Assume that $Q_1\neq 0$ and $Q_2=0$. Let $\kappa\in\mathbb{C}$ be such that $Im\ \kappa^2\neq 0$. Then, for any $\varepsilon>0$, we have as $a\downarrow 0$,*

$$R(\kappa^2;a) = R_p(\kappa^2;\tau) + O(a^{1/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(\mathbb{R}^3)),$$

where

$$\tau = \frac{\alpha\langle f_0, qf_0\rangle}{4\pi}.$$

Proof: In view of Lemmas 2.4, 3.1 and 3.2 we have by using (2.8),

$$\begin{aligned}&\lambda(a)T(\kappa;a)U_a(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_0(\kappa^2)\\ &\quad = \left(\frac{\alpha\langle f_0,qf_0\rangle}{4\pi} - \frac{i\kappa}{4\pi}\right)^{-1} (R_0(\kappa^2)\cdot)(0)\frac{e^{i\kappa|x|}}{4\pi|x|} + O(a^{1/2-\varepsilon}).\end{aligned}$$

Thus, from (1.8) we obtain the required result. □

Theorem 3.5: *Assume that $Q_1=0$, $Q_2\neq 0$ and $\alpha\neq 0$ in (1.2). Let $\kappa\in\mathbb{C}$ be such that $Im\ \kappa^2\neq 0$. Then, for any $\varepsilon>0$, we have as $a\downarrow 0$,*

$$R(\kappa^2;a) = R_0(\kappa^2) + O(a^{1/2-\varepsilon}) \quad in \quad \mathbf{B}(L_2(\mathbb{R}^3)).$$

Proof: First we show that

$$Q_2^* q\varphi = 0 \quad in \quad L_2(S_1), \tag{3.9}$$

$[\varphi(\omega)\equiv 1$ on $S_1]$. In fact, we have for $u\in L_2(S_1)$,

$$\langle u, Q_2^* q\varphi\rangle = \langle Q_2 u, q\rangle = 0,$$

since $Q_2 u\in\mathcal{N}_2$. Thus (3.9) holds. Now, in view of Lemmas 2.4, 3.1 and 3.2 we have together with (3.9),

$$\lambda(a)T(\kappa;a)U_a(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_0(\kappa^2)$$
$$=\alpha^{-1}(R_0(\kappa^2)\cdot)(0)\frac{e^{i\kappa|x|}}{4\pi|x|}\langle Q_2WQ_2^*q\varphi,q\rangle+O(a^{1/2-\varepsilon})=O(a^{1/2-\varepsilon}).$$

Thus, from (1.8) we obtain the required result. □

Theorem 3.6: *Assume that* $q(\omega)\geqslant 0$ [*or* $q(\omega)\leqslant 0$] *on* S_1. *Assume that* $Q_1\neq 0$, $Q_2\neq 0$ *and* $\alpha\neq 0$. *Let* $\kappa\in\mathbb{C}$ *be such that* $Im\ \kappa^2\neq 0$. *Then, for any* $\varepsilon>0$, *we have as* $a\downarrow 0$,

$$R(\kappa^2;a)=R_p(\kappa^2;\tau)+O(a^{1/2-\varepsilon})\quad in\quad \mathbf{B}(L_2(\mathbb{R}^3)),$$

where

$$\tau=\frac{\alpha\det(\langle f_i,qf_j\rangle)_{0\leqslant i,j\leqslant n}}{4\pi\det(\langle f_i,qf_j\rangle)_{1\leqslant i,j\leqslant n}}$$

and $\{f_1,f_2,\ldots,f_n\}$ *is a basis of* $\mathcal{R}(Q_2)$.

Proof: In view of Lemmas 2.9, 3.1 and (3.9) we have

$$(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_0(\kappa^2)=(R_0(\kappa^2)\cdot)(0)(Q_1B_{11}Q_1^*q\varphi+Q_2B_{21}Q_1^*q\varphi)+O(a^{1/2-\varepsilon}).\tag{3.10}$$

Moreover, we have

$$\lambda(a)T(\kappa;a)U_a(R_0(\kappa^2)\cdot)(0)Q_2B_{21}Q_1^*q\varphi=O(a^{1/2-\varepsilon}).\tag{3.11}$$

In fact, since $Q_2B_{21}Q_1^*q\varphi$ is of the form

$$Q_2B_{21}Q_1^*q\varphi=\sum_{j=1}^{n}c_jf_j\quad(c_j\in\mathbb{C},f_j\in\mathcal{N}_2),$$

we have

$$\langle Q_2B_{21}Q_1^*q\varphi,q\rangle=\sum_{j=1}^{n}c_j\langle f_j,q\rangle=0.$$

Thus, (3.11) holds from Lemma 3.2. Therefore we have

$$\lambda(a)T(\kappa;a)U_a(1-\lambda(a)\tilde{T}(a\kappa))^{-1}U_a^{-1}\gamma_a R_0(\kappa^2)=(R_0(\kappa^2)\cdot)(0)Q_1B_{11}Q_1^*q\varphi+O(a^{1/2-\varepsilon}).\tag{3.12}$$

Let us compute $Q_1B_{11}Q_1^*q\varphi$. We put

$$u=-Q_1B_{11}Q_1^*q\varphi,\quad v=-Q_2B_{21}Q_1^*q\varphi.$$

We note

$$\mathcal{R}(B_{11})\subset\mathcal{R}(Q_1),\quad \mathcal{R}(B_{21})\subset\mathcal{R}(Q_2).$$

Then, by (2.8) and (2.21) we have

$$-(4\pi)^{1/2}B_{11}g_0=u,\quad -(4\pi)^{1/2}B_{21}g_0=v,$$

which implies

$$D_1\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} (4\pi)^{1/2} g_0 \\ 0 \end{pmatrix}.$$

Thus, from (2.24) and (2.25) it follows that

$$u = (4\pi)^{1/2}\left(\alpha \frac{\det(\langle f_i, q f_j\rangle)_{0\leqslant i,j\leqslant n}}{\det(\langle f_i, q f_j\rangle)_{1\leqslant i,j\leqslant n}} - i\kappa \right)^{-1} f_0,$$

and hence, by (2.8), (3.12) and Lemma 3.2,

$$\begin{aligned} &\lambda(a) T(\kappa; a) U_a (1 - \lambda(a)\tilde{T}(a\kappa))^{-1} U_a^{-1} \gamma_a R_0(\kappa^2) \\ &\quad = 4\pi \left(\alpha \frac{\det(\langle f_i, q f_j\rangle)_{0\leqslant i,j\leqslant n}}{\det(\langle f_i, q f_j\rangle)_{1\leqslant i,j\leqslant n}} - i\kappa \right)^{-1} (R_0(\kappa^2)\cdot)(0) \frac{e^{i\kappa|x|}}{4\pi|x|} + O(a^{1/2-\varepsilon}), \end{aligned}$$

from which the theorem follows. □

Finally, we will give an example of the zero resonance state of $H(1;q)$. Assume that $q(\omega) = V_0$ (real constant). Then, by [S2, Theorem 7.1] we have the following.

Theorem 3.7: *If* $V_0 \neq -(2l+1)$ $(l = 0,1,2,\ldots)$, *then* $Q_1 = Q_2 = 0$. *If* $V_0 = -1$ $(V_0 = -(2l+1), l = 1,2,\ldots)$, *then* $Q_1 \neq 0$ *and* $Q_2 = 0$ $(Q_1 = 0, Q_2 \neq 0)$.

Moreover, when $V_0 = -1$, f_0 is seen to be of the form

$$f_0(\omega) = -(4\pi)^{-1/2},$$

from the proof of the theorem above. Thus the zero resonance function $u_0(x) = (T(0;1)f_0)(x)$ of $H(1;q)$ is given by

$$u_0(x) = \begin{cases} -(4\pi)^{-1/2} & (|x| \leqslant 1), \\ -(4\pi)^{-1/2}|x|^{-1} & (|x| \geqslant 1). \end{cases}$$

ACKNOWLEDGMENTS

The author wishes to express his sincere gratitude to Professor Pavel Kurasov for suggesting the present problem, and to Professor Hideo Tamura for valuable advice.

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Gauge theories of Yang–Mills vector fields coupled to antisymmetric tensor fields

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(Received 17 July 2002; accepted 10 October 2002)

A non-Abelian class of massless/massive nonlinear gauge theories of Yang–Mills vector potentials coupled to Freedman–Townsend antisymmetric tensor potentials is constructed in four space–time dimensions. These theories involve an extended Freedman–Townsend-type coupling between the vector and tensor fields, and a Chern–Simons mass term with the addition of a Higgs-type coupling of the tensor fields to the vector fields in the massive case. Geometrical, field theoretic, and algebraic aspects of the theories are discussed in detail. In particular, the geometrical structure mixes and unifies features of Yang–Mills theory and Freedman–Townsend theory formulated in terms of Lie algebra valued curvatures and connections associated to the fields and nonlinear field strengths. The theories arise from a general determination of all possible geometrical nonlinear deformations of linear Abelian gauge theory for one-form fields and two-form fields with an Abelian Chern–Simons mass term in four dimensions. For this type of deformation (with typical assumptions on the allowed form considered for terms in the gauge symmetries and field equations), an explicit classification of deformation terms at first-order is obtained, and uniqueness of deformation terms at all higher orders is proven. This leads to a uniqueness result for the non-Abelian class of theories constructed here.
[DOI: 10.1063/1.1528271]

I. INTRODUCTION

Gauge field theories continue to be fundamental in the study of many areas of mathematical physics, ranging from elementary particle interactions, and completely integrable nonlinear differential equations, to topology of three- and four-dimensional manifolds. Consequently, an effort to generalize the important types of gauge field theories is of natural interest. In recent work,[1,2] a new nonlinear gauge theory was found for massless vector fields in three space–time dimensions, describing a novel type of generalization of non-Abelian Yang–Mills theory. Its origin can be understood by considering nonlinear deformations of the Abelian linear gauge theory of one-form potentials in d dimensions.[3–5]

The deformation process considered here consists of adding linear and higher power terms to the Abelian gauge symmetry while also adding quadratic and higher power terms to the linear field equations, such that a gauge invariant action principle exists which is not equivalent to the undeformed linear theory under nonlinear field redefinitions. The property of gauge invariance is very restrictive and can be used to derive determining equations for the allowed form of the deformation terms added order by order in powers of the fields.

Non-Abelian Yang–Mills theory describes one type of allowed deformation, which works for one-form potentials in any dimension $d>1$. Interestingly, in $d=3$ dimensions, another type of deformation is allowed,[1] analogous to the Freedman–Townsend theory of antisymmetric tensor gauge fields.[6] The Freedman–Townsend theory was derived originally only for antisymmetric tensor fields in $d=4$ dimensions but it has a simple geometrical formulation in any dimension

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$d>2$ as a nonlinear gauge theory of $d-2$-form potentials, in particular, one-form potentials in $d=3$ dimensions. Moreover, this formulation of the theory has a further natural extension to a coupled tower of p-form potentials of all ranks $1\leqslant p\leqslant d-2$, in particular, coupled one-form and two-form potentials in $d=4$ dimensions.[7,8]

The novel generalization of non-Abelian Yang–Mills theory in Ref. 2 arises by combining the Yang–Mills-type and Freedman–Townsend-type deformations of the Abelian linear one-form potential gauge theory in $d=3$ dimensions. In the present paper, a similar nonlinear deformation of the Abelian linear gauge theory of one-form and two-form potentials in $d=4$ dimensions is studied, which has been announced in earlier work.[2,9] The resulting nonlinear gauge theory generalizes both non-Abelian Yang–Mills theory and Freedman–Townsend theory, describing coupled massless vector and antisymmetric tensor fields in four space–time dimensions. As a main new result, an interesting extension of this theory to include a Chern–Simons-type mass term involving both the vector and antisymmetric tensor fields is presented.

Physically speaking, the field strengths in this nonlinear gauge theory together represent coupled massive spin-one fields in the case with a Chern–Simons term, and otherwise represent massless spin-one fields coupled to massless spin-zero fields in the case with no Chern–Simons term. The construction and features of these two cases of the theory are given in Secs. II and III. The theory has a very rich and interesting geometrical structure, mixing and unifying features of Yang–Mills theory and Freedman–Townsend theory in terms of curvatures and connections associated with the fields and field strengths, which is discussed in Sec. IV. In Sec. V, the theory is derived from an analysis of allowed nonlinear geometrical deformations of the Abelian linear gauge theory of massless/massive sets of one-form and two-form potentials in four dimensions, with the mass determined by a Chern–Simons-type term. This analysis yields a novel nonlinear gauge theory for coupled massless and massive sets of vector and antisymmetric tensor fields, generalizing the two preceding cases of the new theory from Secs. II and III. Finally, some concluding remarks are made in Sec. VI.

II. DEFORMATION OF NON-ABELIAN YANG–MILLS/FREEDMAN–TOWNSEND GAUGE THEORY

First consider, as a starting point, the formulation of non-Abelian Yang–Mills theory and Freedman–Townsend theory as respective nonlinear gauge theories of massless vector and antisymmetric tensor fields on four-dimensional Minkowski space–time. For simplicity, the gauge groups will be taken to be three dimensional. Recall, in Yang–Mills theory, the Lie algebra underlying the gauge group is required to be compact semisimple, which then fixes it here to be SU(2). In Freedman–Townsend theory, however, no such condition arises on the underlying Lie algebra of the gauge group, and thus here it can be any three-dimensional non-Abelian Lie algebra, $\mathcal{G}$. From the classification of three-dimensional Lie algebras, it then follows that $\mathcal{G}$ either is semisimple and thus $\mathcal{G}=\mathrm{SU}(2)$, $\mathcal{G}=\mathrm{SU}(1,1)$, or is solvable and thus $\mathcal{G}=\mathrm{U}(1)\rtimes\mathrm{U}(1)^2$ which is a semidirect product of Abelian Lie algebras U(1) and $\mathrm{U}(1)^2$.

To formulate Yang–Mills theory with an SU(2) gauge group, introduce as the field variable a vector potential A_μ that takes values in the Lie algebra SU(2). Equivalently, with respect to a fixed SU(2) basis e_a, $a=1,2,3$, the vector potential components $A_\mu=A^a_\mu e_a$ can be regarded as a set of three ordinary vector fields A^a_μ on Minkowski space–time. Let $\varepsilon^a{}_{bc}$ denote the SU(2) structure constants, and let k_{ab} denote an SU(2) positive–definite invariant metric, related to Killing metric by $k_{ab}=-\varepsilon^c{}_{ad}\varepsilon^d{}_{bc}$, and so $\varepsilon_{abc}=\varepsilon^e{}_{bc}k_{ae}$ is totally antisymmetric.

The SU(2) Yang–Mills field strength is given by

$$F^a_{\sigma\mu}=\partial_{[\sigma}A^a_{\mu]}+\tfrac{1}{2}\varepsilon^a{}_{bc}A^b_\sigma A^c_\mu\,. \tag{2.1}$$

It is convenient in four dimensions to work with the dual field strength

$$\tilde{F}^a_{\sigma\mu}=\epsilon_{\sigma\mu}{}^{\tau\nu}F^a_{\tau\nu}, \tag{2.2}$$

which satisfies the Bianchi identity

$$D^\sigma \tilde{F}^a_{\sigma\mu} = 0, \tag{2.3}$$

where

$$D_\sigma = \partial_\sigma + \varepsilon^a{}_{bc} A^b_\sigma \tag{2.4}$$

is the SU(2) covariant derivative operator. The Yang–Mills Lagrangian is given by

$$L_{\rm YM} = \tfrac{1}{2} k_{ab} \tilde{F}^a_{\sigma\mu} \tilde{F}^b_{\tau\nu} \eta^{\sigma\tau} \eta^{\mu\nu} \tag{2.5}$$

yielding the SU(2) Yang–Mills field equation

$$E_{A^a_\tau} = \epsilon_\tau{}^{\sigma\nu\mu} D_\sigma \tilde{F}^a_{\mu\nu} = 0 \tag{2.6}$$

for A^a_τ. Under the Yang–Mills gauge symmetry on A^a_μ, given by the field variation

$$\delta_\xi A^a_\mu = D_\mu \xi^a, \tag{2.7}$$

where ξ^a are arbitrary functions that take values in the Lie algebra SU(2), the Lagrangian is gauge invariant, $\delta_\xi L_{\rm YM} = 0$. These gauge symmetries generate a SU(2) gauge group with commutator structure $[\delta_{\xi_1}, \delta_{\xi_2}] = \delta_{\xi_3}$ such that $\xi_3{}^a = \varepsilon^a{}_{bc} \xi_1{}^b \xi_2{}^c$. The Lagrangian gives rise to a gauge invariant stress-energy tensor

$$T_{\mu\nu}(\tilde{F}) = k_{ab} \eta^{\alpha\beta} (\tilde{F}^a_{\mu\alpha} \tilde{F}^b_{\nu\beta} - \tfrac{1}{4} \eta_{\mu\nu} \eta^{\sigma\tau} \tilde{F}^a_{\sigma\alpha} \tilde{F}^b_{\tau\beta}), \tag{2.8}$$

which yields a causal energy-momentum for the vector potential A^a_μ on spacelike hypersurfaces, i.e., $T_{\mu\nu}(\tilde{F}) t^\nu$ is timelike or null for all unit timelike vectors t^ν on Minkowski space–time. Gauge invariance of the Yang–Mills Lagrangian relies on the property that SU(2) is semisimple. The additional property that SU(2) is compact, corresponding to positive–definiteness of k_{ab}, is essential for causality of the Yang–Mills stress-energy tensor obtained from the Lagrangian.

Next, for formulating Freedman–Townsend theory with gauge group determined by $\mathcal{G}$, introduce as the field variable an antisymmetric tensor potential $B_{\mu\nu}$ that takes values in the Lie algebra $\mathcal{G}$. Hereafter, it is convenient to identify the vector spaces of $\mathcal{G}$ and SU(2), so the SU(2) basis provides a vector-space basis e_a, $a = 1,2,3$, for $\mathcal{G}$. Then the components of the antisymmetric tensor potential $B_{\mu\nu} = B^a_{\mu\nu} e_a$ can be regarded equivalently as a set of three ordinary antisymmetric tensor fields $B^a_{\mu\nu}$ on Minkowski space–time. Finally, introduce the Abelian field strength for $B^a_{\mu\nu}$ given by the curl

$$H^a_{\sigma\mu\nu} = \partial_{[\sigma} B^a_{\mu\nu]}, \tag{2.9}$$

along with its dual

$$\tilde{H}^a_\sigma = \epsilon_\sigma{}^{\tau\mu\nu} H^a_{\tau\mu\nu} \tag{2.10}$$

which satisfies the divergence identity

$$\partial^\sigma \tilde{H}^a_\sigma = 0. \tag{2.11}$$

Let $c^a{}_{bc}$ denote structure constants of $\mathcal{G}$, and let $c_{ab}{}^c = c^e{}_{bd} k_{ae} k^{cd}$, where the SU(2) invariant metric provides a positive–definite metric k_{ab} on $\mathcal{G}$. Note this metric is not invariant with respect to the Lie algebra product in $\mathcal{G}$ unless $\mathcal{G} \simeq$ SU(2).

Now the field strength for Freedman–Townsend theory is defined in terms of $B^a_{\mu\nu}$ and $H^a_{\tau\mu\nu}$ by the relation

$$K^a_{\sigma\mu\nu}+\tilde{K}^b_{[\sigma}B^c_{\mu\nu]}c_{cb}{}^a=H^a_{\sigma\mu\nu}, \tag{2.12}$$

where

$$\tilde{K}^a_\tau=\epsilon_\tau{}^{\sigma\mu\nu}K^a_{\sigma\mu\nu} \tag{2.13}$$

is the dual field strength. This field strength has a nonpolynomial expression in terms of $B^c_{\mu\nu}$ given by

$$\tilde{K}^a_\mu=Y^{-1}{}^{a\nu}_{\mu b}(B)\tilde{H}^b_\nu \tag{2.14}$$

with $Y^{-1}{}^{a\nu}_{\mu b}(B)$ denoting the inverse of the tensor matrix

$$Y^{a\nu}_{\mu b}(B)=\delta_\mu{}^\nu k_b{}^a+\epsilon_\mu{}^{\nu\sigma\tau}c_{cb}{}^aB^c_{\sigma\tau}, \tag{2.15}$$

where $B^c_{\sigma\tau}$ is restricted to satisfy $\det(Y^{a\nu}_{\mu b}(B))\neq 0$. Note the tensor matrix is symmetric $Y^{ab}_{\mu\nu}(B)=Y^{ba}_{\nu\mu}(B)$ due to the antisymmetry of volume tensor $\epsilon_{\mu\nu}{}^{\sigma\tau}$ and the structure constants $c^a{}_{cb}$. Then, the Freedman–Townsend Lagrangian is given by

$$L_{\rm FT}=\tfrac{1}{2}k_{ab}\tilde{K}^a_\mu\tilde{K}^b_\nu Y^{\mu\nu}_{ab}(B). \tag{2.16}$$

This yields the field equation for $B^a_{\sigma\tau}$,

$$E_{\rm B}{}^a_{\sigma\tau}=\epsilon_{\sigma\tau}{}^{\nu\mu}(\partial_\nu\tilde{K}^a_\mu+\tfrac{1}{2}c^a{}_{bc}\tilde{K}^b_\nu\tilde{K}^c_\mu)=0. \tag{2.17}$$

The gauge symmetry on $B^a_{\mu\nu}$ is given by the field variation

$$\delta_\chi B^a_{\mu\nu}=\partial_{[\mu}\chi^a_{\nu]}-c_{cb}{}^a\tilde{K}^b_{[\mu}\chi^c_{\nu]}, \tag{2.18}$$

where χ^a_ν are arbitrary covector functions that take values in the Lie algebra G. These gauge symmetries generate an Abelian gauge group $[\delta_{\chi_1},\delta_{\chi_2}]=0$ on solutions of the field equation. Off solutions, the commutator structure closes to within a trivial symmetry proportional to the field equation. Finally, the Lagrangian is gauge invariant to within a total divergence, $\delta_\chi L_{\rm FT}=\partial_\mu(\epsilon^{\mu\nu\sigma\tau}\tfrac{1}{2}c^d{}_{ab}k_{cd}\tilde{K}^a_\sigma\tilde{K}^b_\tau\chi^c_\nu)$. In particular, gauge invariance holds without the need for $\mathcal{G}$ to be semisimple. Moreover, the stress-energy tensor obtained from the Lagrangian

$$T_{\mu\nu}(\tilde{K})=k_{ab}(\tfrac{1}{2}\tilde{K}^a_\mu\tilde{K}^b_\nu-\tfrac{1}{4}\eta_{\mu\nu}\eta^{\sigma\tau}\tilde{K}^a_\sigma\tilde{K}^b_\tau) \tag{2.19}$$

yields a causal energy-momentum for the antisymmetric tensor potential $B^a_{\mu\nu}$ on spacelike hypersurfaces, i.e., $T_{\mu\nu}(\tilde{K})t^\nu$ is timelike or null for all unit timelike vectors t^ν on Minkowski space–time.

A. Nonlinear generalization

We now construct a massless gauge theory with a nonlinear interaction for the fields A^a_μ, $B^a_{\mu\nu}$, $a=1,2,3$, giving a novel generalization of the Yang–Mills/Freedman–Townsend theories above. The origin of the generalization will be explained by the deformation analysis carried out in Sec. V.

To begin, the following algebraic structure[10] is needed on the Lie algebras SU(2) and $\mathcal{G}$. Let $f_{ab}{}^c$ denote a bilinear map f from $\mathcal{G}\times\mathrm{SU}(2)$ into SU(2) defining a representation of $\mathcal{G}$ on SU(2)

$$2\,f_{[d|c}{}^af_{|e]b}{}^c=f_{cb}{}^ac^c{}_{de} \tag{2.20}$$

such that this representation acts as a derivation preserving the SU(2) commutator

$$f_{ed}{}^{c}\varepsilon^{d}{}_{ab} = 2\, f_{e[a|}{}^{d}\varepsilon^{c}{}_{d|b]}\,. \tag{2.21}$$

Since SU(2) is semisimple, any derivation is given by an adjoint representation map

$$f_{eb}{}^{c} = \varepsilon^{c}{}_{db}h_{e}{}^{d} \tag{2.22}$$

with $h_e{}^d$ denoting some linear map h from $\mathcal{G}$ into SU(2). Then, the relation (2.20) implies that h is a homomorphism (with respect to the Lie algebra product) of $\mathcal{G}$ into SU(2).

Consequently, if $\mathcal{G}$ is semisimple then clearly $h(\mathcal{G}) = \mathrm{SU}(2)$ and so $\mathcal{G} \simeq \mathrm{SU}(2)$ are isomorphic Lie algebras, with the linear map h being one-to-one. If instead $\mathcal{G}$ is solvable then the Abelian two-dimensional Lie subalgebra $\mathrm{U}(1)^2$ in $\mathcal{G}$ is the kernel of h, with $\mathcal{G}/\mathrm{U}(1)^2 \simeq h(\mathcal{G}) = \mathrm{U}(1)$ being any one-dimensional Lie subalgebra in SU(2). Hence there are two different cases allowed for the Lie algebra structures in the construction of the massless nonlinear theory. For the semisimple case when $\mathcal{G} \simeq \mathrm{SU}(2)$, since h is an isomorphism, then without loss of generality it follows that

$$h_{a}{}^{b} = \kappa\delta_{a}{}^{b}, \quad c^{a}{}_{bc} = f_{bc}{}^{a} = \kappa\varepsilon^{a}{}_{bc}\,, \tag{2.23}$$

where κ is an arbitrary nonzero constant. Alternatively, for the solvable case when $\mathcal{G} = \mathrm{U}(1) \rtimes \mathrm{U}(1)^2$, the properties of h and $\mathcal{G}$ lead to

$$h_{a}{}^{b} = v_{a}w^{b}, \quad c^{a}{}_{bc} = c^{a}{}_{[b}v_{c]}\,, \quad f_{bc}{}^{a} = \varepsilon^{a}{}_{dc}w^{d}v_{b} \tag{2.24}$$

for some fixed vectors v^a, w^a in the common vector space of $\mathcal{G}$ and SU(2), and for some fixed linear map $c^a{}_b$ such that

$$c^{a}{}_{b}v_{a} = 0, \quad c^{a}{}_{b}v^{b} = 0. \tag{2.25}$$

To proceed, the construction now follows the pattern of the novel deformation of SU(2) Yang–Mills theory in three dimensions from Ref. 2. Let $c_{ab}{}^{c} = c^{d}{}_{be}k_{ad}k^{ce}$ and $f^{a}{}_{bc} = f_{db}{}^{e}k^{ad}k_{ce}$.

Nonlinear field strengths $P^a_{\mu\nu}$, $Q^a_{\mu\nu\sigma}$ are introduced in terms of A^a_μ, $B^a_{\mu\nu}$ by

$$P^{a}_{\mu\nu} - f_{bc}{}^{a}\tilde{Q}^{b}_{[\mu}A^{c}_{\nu]} = F^{a}_{\mu\nu}\,, \tag{2.26}$$

$$Q^{a}_{\mu\nu\sigma} - f^{a}{}_{cb}\tilde{P}^{b}_{[\mu\nu}A^{c}_{\sigma]} + c_{cb}{}^{a}\tilde{Q}^{b}_{[\mu}B^{c}_{\nu\sigma]} = H^{a}_{\mu\nu\sigma}\,, \tag{2.27}$$

where

$$\tilde{P}^{a}_{\sigma\mu} = \epsilon_{\sigma\mu}{}^{\tau\nu}P^{a}_{\tau\nu}\,, \quad \tilde{Q}^{a}_{\sigma} = \epsilon_{\sigma}{}^{\tau\mu\nu}Q^{a}_{\tau\mu\nu} \tag{2.28}$$

are the duals. These field strengths depend nonpolynomially on A^a_μ, $B^a_{\mu\nu}$ in the following form. Define the tensor matrix

$$Y(A,B) = Y^{T}(A,B) = \begin{pmatrix} \delta_{b}{}^{a}\delta_{\mu}{}^{\sigma}\delta_{\nu}{}^{\alpha} & -f_{bc}{}^{a}\epsilon_{\mu\nu}{}^{\sigma\tau}A^{c}_{\tau} \\ -f^{a}{}_{cb}\epsilon_{\mu}{}^{\sigma\alpha\tau}A^{c}_{\tau} & \delta_{b}{}^{a}\delta_{\mu}{}^{\sigma} + c_{cb}{}^{a}\epsilon_{\mu}{}^{\sigma\tau\nu}B^{c}_{\tau\nu} \end{pmatrix} \tag{2.29}$$

and consider the inverse matrix $Y^{-1}(A,B)$ satisfying

$$Y^{-1}(A,B)Y(A,B) = Y(A,B)Y^{-1}(A,B) = \begin{pmatrix} \delta_{b}{}^{a}\delta_{\tau}{}^{\sigma}\delta_{\nu}{}^{\alpha} & 0 \\ 0 & \delta_{b}{}^{a}\delta_{\tau}{}^{\sigma} \end{pmatrix} \tag{2.30}$$

with A^a_τ and $B^a_{\tau\nu}$ restricted by the condition $\det(Y(A,B)) \neq 0$ necessary for invertibility of $Y(A,B)$. Assemble the field strength duals into tensor matrices

$$N=\begin{pmatrix}\tilde{P}^a_{\mu\nu}\\ \tilde{Q}^a_\mu\end{pmatrix},\quad M=\begin{pmatrix}\tilde{F}^a_{\mu\nu}\\ \tilde{H}^a_\mu\end{pmatrix}. \tag{2.31}$$

Then $N=Y^{-1}(A,B)M$, where $Y^{-1}(A,B)$ is nonpolynomial in terms of A^a_μ, $B^a_{\mu\nu}$.

The Lagrangian for the massless nonlinear theory is constructed by

$$L_{\rm N}=k_{ab}(\eta^{\sigma\tau}\eta^{\mu\nu}\tilde{P}^a_{\sigma\mu}\tilde{F}^b_{\tau\nu}+\eta^{\sigma\tau}\tilde{Q}^a_\sigma\tilde{H}^b_\tau) \tag{2.32}$$

which can be also expressed in a more symmetrical form $L=N^TY(A,B)N=M^TY^{-1}(A,B)M$. The gauge symmetries in this theory consist of the field variations given by

$$\delta_\xi A^a_\mu=D_\mu\xi^a+f_{bc}{}^a\tilde{Q}^b_\mu\xi^c, \tag{2.33}$$

$$\delta_\xi B^a_{\mu\nu}=f^a{}_{cb}\tilde{P}^b_{\mu\nu}\xi^c, \tag{2.34}$$

in terms of arbitrary functions ξ^a, and also

$$\delta_\chi A^a_\mu=0, \tag{2.35}$$

$$\delta_\chi B^a_{\mu\nu}=\partial_{[\mu}\chi^a_{\nu]}-c_{cb}{}^a\tilde{Q}^b_{[\mu}\chi^c_{\nu]}, \tag{2.36}$$

in terms of arbitrary covector functions χ^a_ν. Under both these gauge symmetries the Lagrangian is invariant to within a total divergence,

$$\delta_\xi L_{\rm N}=\partial_\mu(\epsilon^{\mu\nu\sigma\tau}2\,f_{ac}{}^dk_{bd}\tilde{Q}^a_\nu\tilde{P}^b_{\sigma\tau}\xi^c),\quad \delta_\chi L_{\rm N}=\partial_\mu(\epsilon^{\mu\nu\sigma\tau}c^c{}_{ab}k_{cd}\tilde{Q}^a_\nu\tilde{Q}^b_\sigma\chi^d_\tau) \tag{2.37}$$

as shown by results in Sec. V.

In this construction, we refer to the underlying Yang–Mills/Freedman–Townsend algebraic structure $(\mathrm{SU}(2),\mathcal{G})$ as the structure group of the massless nonlinear theory.

B. Features

The field equations for A^a_μ and $B^a_{\mu\nu}$ obtained from the Lagrangian are given by

$$E_{{\rm A}\tau}{}^a=\epsilon_\tau{}^{\nu\sigma\mu}(D_\nu\tilde{P}^a_{\sigma\mu}+f_{bc}{}^a\tilde{Q}^b_\nu\tilde{P}^c_{\sigma\mu})=0, \tag{2.38}$$

$$E_{{\rm B}\tau\sigma}{}^a=\epsilon_{\tau\sigma}{}^{\nu\mu}(\partial_\nu\tilde{Q}^a_\mu+\tfrac{1}{2}c^a{}_{bc}\tilde{Q}^b_\nu\tilde{Q}^c_\mu)=0. \tag{2.39}$$

Both these field equations are of second order in derivatives of A^a_μ, $B^a_{\mu\nu}$, with the second derivatives appearing linearly and first derivatives appearing quadratically, while A^a_μ, $B^a_{\mu\nu}$ appear nonpolynomially. As a consequence of gauge invariance, the field equations satisfy nonlinear divergence identities

$$D^\tau E_{{\rm A}\tau}{}^a=-\eta^{\tau\mu}f_{bc}{}^a\tilde{Q}^b_\mu E_{{\rm A}\tau}{}^c-\eta^{\tau\mu}\eta^{\sigma\nu}f_{cb}{}^a\tilde{P}^b_{\mu\nu}E_{{\rm B}\tau\sigma}{}^c, \tag{2.40}$$

$$\partial^\tau E_{{\rm B}\tau\sigma}{}^a=-\eta^{\tau\mu}c^a{}_{bc}\tilde{Q}^b_\mu E_{{\rm B}\tau\sigma}{}^c. \tag{2.41}$$

There are also nonlinear divergence identities that arise on the dual field strengths

$$\eta^{\sigma\mu}(D_\sigma\tilde{P}^a_{\mu\nu}+f_{bc}{}^a\tilde{Q}^b_\sigma\tilde{P}^c_{\mu\nu})=\eta^{\sigma\mu}f_{bc}{}^aE_{{\rm B}\mu\nu}{}^bA^c_\sigma, \tag{2.42}$$

$$\eta^{\sigma\mu}(\partial_\sigma\tilde{Q}^a_\mu-c_{bc}{}^a\tilde{Q}^b_\sigma\tilde{Q}^c_\mu-f^a{}_{bc}\eta^{\tau\nu}\tilde{P}^b_{\sigma\tau}\tilde{P}^c_{\mu\nu})=-\eta^{\sigma\mu}f^a{}_{bc}E_{{\rm A}\mu}{}^cA^b_\sigma-\eta^{\sigma\mu}\eta^{\tau\nu}c_{bc}{}^aE_{{\rm B}\mu\nu}{}^cB^b_{\sigma\tau}, \tag{2.43}$$

due to the SU(2) Bianchi identity (2.3) on $\tilde{F}^a_{\mu\nu}$ and the linear divergence identity (2.11) on $\tilde{H}^a_{\sigma\mu\nu}$. Consequently, for solutions of the field equations, the field strengths satisfy a system of divergence and curl equations

$$D_{[\nu}\tilde{P}^a_{\sigma\mu]} = -f_{bc}{}^a \tilde{Q}^b_{[\nu}\tilde{P}^c_{\sigma\mu]}, \quad D^\nu \tilde{P}^a_{\mu\nu} = -\eta^{\sigma\nu} f_{bc}{}^a \tilde{Q}^b_\sigma \tilde{P}^c_{\mu\nu}, \tag{2.44}$$

$$\partial_{[\nu}\tilde{Q}^a_{\mu]} = -\tfrac{1}{2} c^a{}_{bc} \tilde{Q}^b_{[\nu}\tilde{Q}^c_{\mu]}, \quad \partial^\mu \tilde{Q}^a_\mu = \eta^{\sigma\mu} c_{bc}{}^a \tilde{Q}^b_\sigma \tilde{Q}^c_\mu + \eta^{\sigma\mu}\eta^{\tau\nu} f^a{}_{bc} \tilde{P}^b_{\sigma\tau}\tilde{P}^c_{\mu\nu}, \tag{2.45}$$

with quadratic source terms. In the divergence equation on $\tilde{Q}^a_\mu$, the source terms identically vanish when $c_{(ab)c} = k_{d(a}c^d{}_{b)c} = 0$, which occurs in the case $\mathcal{G} \simeq \mathrm{SU}(2)$.

In both cases $\mathcal{G} \simeq \mathrm{SU}(2)$ or $\mathrm{U}(1) \rtimes \mathrm{U}(1)^2$, the divergence and curl equations (2.44) and (2.45) together with equations (2.26) and (2.27) constitute a first-order nonlinear field theory for A^a_μ, $B^a_{\mu\nu}$, $\tilde{P}^a_{\mu\nu}$, $\tilde{Q}^a_\nu$. Moreover, its linearization reduces to the Abelian linear gauge theory of vector potentials and antisymmetric tensor potentials (see Sec. V A), whose field strengths represent free massless spin-one and spin-zero fields. Hence, in physical terms, solutions of the nonlinear field strength equations (2.44) and (2.45) describe a set of nonlinearly interacting massless fields of spin-one and spin-zero, respectively, in Minkowski space–time.

Under the gauge symmetries the field strengths have the transformation

$$\delta_\xi \tilde{P}^a_{\mu\nu} = \varepsilon^a{}_{bc}\tilde{P}^b_{\mu\nu}\xi^c + (Y^{-1}\xi\cdot E)^a_{\mu\nu}, \quad \delta_\xi \tilde{Q}^a_\mu = (Y^{-1}\xi\cdot E)^a_\mu, \tag{2.46}$$

$$\delta_\chi \tilde{P}^a_{\mu\nu} = (Y^{-1}\chi\cdot E)^a_{\mu\nu}, \quad \delta_\chi \tilde{Q}^a_\mu = (Y^{-1}\chi\cdot E)^a_\mu, \tag{2.47}$$

where $Y^{-1}\xi\cdot E$ and $Y^{-1}\chi\cdot E$ are the respective products of the inverse of the tensor matrix (2.29) with the field equation tensor matrices

$$\xi\cdot E = \begin{pmatrix} f_{bc}{}^a E_{\mathrm{B}\mu\nu}{}^b \xi^c \\ -f^a{}_{cb} E_{\mathrm{A}\mu}{}^b \xi^c \end{pmatrix}, \quad \chi\cdot E = \begin{pmatrix} 0 \\ \eta^{\sigma\nu} c_{cb}{}^a E_{\mathrm{B}\sigma\mu}{}^b \chi^c_\nu \end{pmatrix}. \tag{2.48}$$

Hence, for solutions of the field equations, $\tilde{P}^a_{\mu\nu}$ and $\tilde{Q}^a_\mu$ are gauge invariant with respect to δ_χ, while with respect to δ_ξ, $\tilde{Q}^a_\mu$ is gauge invariant and $\tilde{P}^a_{\mu\nu}$ transforms homogeneously by the adjoint representation of the Lie algebra SU(2).

The gauge symmetries on solutions of the field equations have the commutator structure

$$[\delta_{\xi_1}, \delta_{\xi_2}] = \delta_{\xi_3}, \quad [\delta_{\chi_1}, \delta_{\chi_2}] = 0, \quad [\delta_{\xi_1}, \delta_{\chi_1}] = 0, \tag{2.49}$$

where $\xi_3{}^a = \varepsilon^a{}_{bc}\xi_1{}^b \xi_2{}^c$. Exponentiating these gauge symmetries leads to a group of finite gauge transformations closed on solutions for A^a_μ, $B^a_{\mu\nu}$. In particular, δ_χ generates a $\mathrm{U}(1)^3$ Abelian group of nonlinear gauge transformations, while δ_ξ generates an SU(2) non-Abelian group of nonlinear gauge transformations, with δ_χ and δ_ξ commuting. Thus the complete gauge group for the nonlinear theory has the direct product structure $\mathrm{SU}(2) \times \mathrm{U}(1)^3$.

The spin-one field strength equations (2.44) lead to conserved electric and magnetic type currents $J_{\mathrm{e}\mu}{}^a = \partial^\nu P^a_{\mu\nu}$, $J_{\mathrm{m}\mu}{}^a = \partial^\nu \tilde{P}^a_{\mu\nu}$ in the nonlinear theory. Corresponding sets of electric and magnetic charges are given by

$$Q_{\mathrm{e}}{}^a = \frac{1}{4\pi}\int_S P^a_{\nu\mu} t^\nu \, dS^\mu, \quad a = 1,2,3, \tag{2.50}$$

$$Q_{\mathrm{m}}{}^a = \frac{1}{4\pi}\int_S \tilde{P}^a_{\nu\mu} t^\nu \, dS^\mu, \quad a = 1,2,3 \tag{2.51}$$

for any closed surface S in a constant time hypersurface in Minkowski space–time, with surface element dS^μ and hypersurface unit normal t^ν. If the closed surface is taken to be a sphere S_∞ at spatial infinity, the resulting enclosed total charges are time-independent constants, $t^\nu \partial_\nu Q_{\mathrm{e}}{}^a = t^\nu \partial_\nu Q_{\mathrm{m}}{}^a = 0$, provided there is no current flow normal to S_∞. These total charges are gauge invariant with respect to δ_χ and transform by the adjoint representation of the Lie algebra SU(2) with respect to δ_ξ if the functions ξ^a are constant on S_∞,

$$\delta_\xi Q_{\mathrm{e}}{}^a = \varepsilon^a{}_{bc} Q_{\mathrm{e}}{}^b \xi^c, \quad \delta_\xi Q_{\mathrm{m}}{}^a = \varepsilon^a{}_{bc} Q_{\mathrm{m}}{}^b \xi^c, \tag{2.52}$$

$$\delta_\chi Q_{\mathrm{e}}{}^a = \delta_\chi Q_{\mathrm{m}}{}^a = 0. \tag{2.53}$$

Similarly, the spin-zero field strength equations (2.45) yield a conserved tensor $J_{\mathrm{s}\sigma\mu}^a = \partial^\nu Q^a_{\sigma\mu\nu}$, which leads to a set of scalar type charges

$$Q_{\mathrm{s}}{}^a = \frac{1}{2\pi} \int_C Q^a_{\sigma\nu\mu} n^\sigma t^\nu \, ds^\mu, \quad a = 1,2,3 \tag{2.54}$$

for any closed curve C on a surface S in a constant time hypersurface in Minkowski space–time, with line element ds^μ, surface unit normal n^σ, and hypersurface unit normal t^ν. If the closed curve is taken to be a circle C_∞ at spatial infinity, the resulting enclosed total charges are time-independent constants, $t^\nu \partial_\nu Q_{\mathrm{s}}{}^a = 0$, provided there is no current flow normal to C_∞. These total charges are gauge invariant with respect to both δ_ξ and δ_χ,

$$\delta_\xi Q_{\mathrm{s}}{}^a = \delta_\chi Q_{\mathrm{s}}{}^a = 0. \tag{2.55}$$

Note that, due to the source terms in the spin-one and spin-zero field strength equations, the total charges (2.50), (2.51), (2.54) are, in general, nonzero for solutions.

The Lagrangian gives rise in the standard manner (under diffeomorphisms on Minkowski space–time) to a stress-energy tensor

$$T_{\mu\nu}(\tilde{P},\tilde{Q}) = k_{ab}(\tilde{P}^a_{\mu\sigma}\tilde{P}^b_{\nu\tau}\eta^{\sigma\tau} + \tfrac{1}{2}\tilde{Q}^a_\mu \tilde{Q}^b_\nu - \tfrac{1}{4}\eta_{\mu\nu}(\tilde{P}^a_{\sigma\alpha}\tilde{P}^b_{\tau\beta}\eta^{\sigma\tau}\eta^{\alpha\beta} + \tilde{Q}^a_\sigma \tilde{Q}^b_\tau \eta^{\sigma\tau})). \tag{2.56}$$

This tensor is conserved and gauge invariant on solutions. The conservation equation $\partial^\mu T_{\mu\nu}(\tilde{P},\tilde{Q}) = 0$ can be derived in a standard manner from the space–time covariance of the theory, while gauge invariance $\delta_\xi T_{\mu\nu}(\tilde{P},\tilde{Q}) = \delta_\chi T_{\mu\nu}(\tilde{P},\tilde{Q}) = 0$ manifestly holds due to the gauge transformation properties of the field strengths.

Conserved currents $J_\mu(\zeta) = \zeta^\nu T_{\mu\nu}(\tilde{P},\tilde{Q})$ are obtained from the stress-energy tensor by contraction with a Killing vector field ζ^ν on Minkowski space–time. These conserved currents define gauge invariant fluxes of energy momentum and stress carried by the fields on a constant time hypersurface Σ, when ζ^ν is taken to be a time translation and space translation, respectively. Fluxes of angular momentum and boost momentum are defined similarly with ζ^ν taken to be a rotation or boost. In particular, for $\zeta^\nu = t^\nu$ given by the timelike unit normal t^μ to Σ, a positive energy $t^\mu t^\nu T_{\mu\nu}(\tilde{P},\tilde{Q})$ and a causal energy-momentum $t^\mu T_{\mu\nu}(\tilde{P},\tilde{Q})$ is obtained for solutions. The corresponding total fluxes are given by

$$Q(\zeta) = \int_\Sigma t^\mu \zeta^\nu T_{\mu\nu}(\tilde{P},\tilde{Q}) dV, \tag{2.57}$$

where dV is the volume element on Σ.

An extension of this theory from an (SU(2),$\mathcal{G}$) structure group to a general non-Abelian structure group is presented in Sec. IV.

III. EXTENDED DEFORMATION WITH CHERN–SIMONS MASS TERM

The nonlinear generalization of Yang–Mills/Freedman–Townsend gauge theories in Sec. II has an interesting extension to include a Chern–Simons mass term. This construction yields a novel gauge theory for massive vector potentials A^a_μ coupled to massive antisymmetric tensor potentials $B^a_{\mu\nu}$, $a=1,2,3$, presented here. For simplicity, the Lie algebra of the underlying Yang–Mills and Freedman–Townsend gauge groups will again be given by the most general three-dimensional possibilities, respectively, SU(2) and $\mathcal{G}\simeq \mathrm{SU}(2)$ or $\mathrm{U}(1)\rtimes \mathrm{U}(1)^2$.

The natural starting point is a non-Abelian Chern–Simons-type term[11]

$$L_{\mathrm{CS}}=m\epsilon^{\nu\mu\sigma\tau}k_{ab}(B^a_{\sigma\tau}\partial_\nu A^b_\mu+\lambda A^d_\nu A^e_\mu B^a_{\sigma\tau}\varepsilon^b{}_{de}), \tag{3.1}$$

where $m\neq 0$ is the Chern–Simons mass, λ is a coupling constant, and, recall, $k_{ab}=-\varepsilon^c{}_{ad}\varepsilon^d{}_{bc}$ is a positive definite metric on the common three-dimensional vector space of the Lie algebras SU(2),$\mathcal{G}$. In the case $\mathcal{G}=\mathrm{SU}(2)$, the addition of this Lagrangian to the pure Yang–Mills and Freedman–Townsend Lagrangians (2.5) and (2.16) gives a gauge invariant Lagrangian $L=L_{\mathrm{YM}}+L_{\mathrm{FT}}+L_{\mathrm{CS}}$ if a SU(2) Yang–Mills–Higgs-type coupling is added between the antisymmetric tensor potentials $B^a_{\mu\nu}$ and the Yang–Mills vector potentials A^a_μ. Gauge invariance also determines the Chern–Simons coupling to be $\lambda=\frac{1}{2}$. This yields a massive SU(2) Yang–Mills/Freedman–Townsend gauge theory[6] with the mass arising from the nonlinear interaction of the fields A^a_μ and $B^a_{\mu\nu}$ through the Chern–Simons Lagrangian. The origin of the Yang–Mills–Higgs coupling of $B^a_{\mu\nu}$ with A^a_μ will be explained by the deformation analysis in Sec. V. Remarkably, this coupling also allows the Chern–Simons Lagrangian (3.1) to be compatible with the nonlinear generalization of massless Yang–Mills/Freedman–Townsend theory constructed in Sec. II A, as we now carry out.

To begin, we replace the ordinary curl (2.9) of $B^a_{\mu\nu}$ in the nonlinear field strengths (2.26) and (2.27) by the Yang–Mills covariant curl

$$H^a_{\sigma\mu\nu}=D_{[\sigma}B^a_{\mu\nu]} \tag{3.2}$$

using the SU(2) covariant derivative operator (2.4). Note the dual (2.10) of $H^a_{\sigma\mu\nu}$ now satisfies an SU(2) divergence identity

$$D^\sigma \tilde{H}^a_\sigma=\tilde{F}^b_{\mu\nu}B^c_{\sigma\tau}\varepsilon^a{}_{bc}\eta^{\mu\sigma}\eta^{\nu\tau}. \tag{3.3}$$

We also covariantly modify the nonlinear gauge symmetries (2.34) and (2.36) on $B^a_{\mu\nu}$ to involve an SU(2) covariant curl $D_{[\mu}\chi^a_{\nu]}$ in $\delta_\chi B^a_{\mu\nu}$ and an SU(2) commutator $\varepsilon^a{}_{bc}B^b_{\mu\nu}\xi^c$ in $\delta_\xi B^a_{\mu\nu}$. The nonlinear gauge symmetries (2.33) and (2.35) on A^a_μ remain unchanged. Furthermore, in the algebraic structure used to construct the massless nonlinear theory, the bilinear map defined by $f_{ab}{}^c$ from $\mathcal{G}\times\mathrm{SU}(2)$ into SU(2) remains a representation of $\mathcal{G}$ and a derivation of SU(2). However, consistency of the Yang–Mills–Higgs coupling between $B^a_{\mu\nu}$ and A^a_μ requires that the SU(2) commutator needs to act as a derivation of $\mathcal{G}$,

$$\varepsilon^c{}_{de}c^d{}_{ab}=2\varepsilon^d{}_{[a|e}c^c{}_{d|b]}. \tag{3.4}$$

This holds only if $\mathcal{G}\simeq\mathrm{SU}(2)$, and therefore excludes the possibility $\mathcal{G}\simeq\mathrm{U}(1)\rtimes\mathrm{U}(1)^2$. Hence, we thereby have

$$c^c{}_{ab}=\kappa\varepsilon^c{}_{ab}, \tag{3.5}$$

where κ is a nonzero constant. Since $f_{ab}{}^c$ is then both a derivation of and representation of $\mathcal{G}$, these properties fix $f_{ab}{}^c$ to be the adjoint representation

$$f_{ab}{}^c=c^c{}_{ab}. \tag{3.6}$$

As a result, with the underlying Yang–Mills/Freedman–Townsend algebraic structure $\mathcal{G} \simeq \mathrm{SU}(2)$, the nonlinear field strengths are given by

$$P^a_{\mu\nu} - \kappa\varepsilon^a{}_{bc}\tilde{Q}^b_{[\mu}A^c_{\nu]} = F^a_{\mu\nu}, \tag{3.7}$$

$$Q^a_{\mu\nu\sigma} - \kappa\varepsilon^a{}_{bc}(\tilde{Q}^b_{[\mu}B^c_{\nu\sigma]} - \tilde{P}^b_{[\mu\nu}A^c_{\sigma]}) = H^a_{\mu\nu\sigma}, \tag{3.8}$$

while the nonlinear gauge symmetries take the form

$$\delta_\xi A^a_\mu = D_\mu\xi^a + \kappa\varepsilon^a{}_{bc}\tilde{Q}^b_\mu\xi^c, \tag{3.9}$$

$$\delta_\chi A^a_\mu = 0, \tag{3.10}$$

and

$$\delta_\xi B^a_{\mu\nu} = \varepsilon^a{}_{bc}(B^b_{\mu\nu} + \kappa\tilde{P}^b_{\mu\nu})\xi^c, \tag{3.11}$$

$$\delta_\chi B^a_{\mu\nu} = D_{[\mu}\chi^a_{\nu]} + \kappa\varepsilon^a{}_{bc}\tilde{Q}^b_{[\mu}\chi^c_{\nu]}, \tag{3.12}$$

in terms of arbitrary scalar functions ξ^a and covector functions χ^a_ν. The complete Lagrangian is then constructed by adding the Chern–Simons Lagrangian (3.1) to the nonlinear field strength Lagrangian (2.32), $L = L_{\mathrm{N}} + L_{\mathrm{CS}}$. This Lagrangian depends on A^a_μ and $B^a_{\mu\nu}$ in the nonpolynomial form

$$L = M^T Y^{-1}(A,B)M + mM^T((2-2\lambda)B + (2\lambda-1)A), \tag{3.13}$$

where $Y(A,B)$ is the symmetric tensor matrix (2.29) constructed linearly from A^a_μ, $B^a_{\mu\nu}$, and M is the tensor matrix (2.31) of the SU(2) field strengths of A^a_μ, $B^a_{\mu\nu}$, and where, in the Chern–Simons term,

$$A = \begin{pmatrix} 0 \\ A^a_\mu \end{pmatrix}, \quad B = \begin{pmatrix} B^a_{\mu\nu} \\ 0 \end{pmatrix}, \tag{3.14}$$

are tensor matrices defined by the fields. Note $N = Y^{-1}(A,B)M$ yields the tensor matrix (2.31) of the nonlinear field strengths.

Under both gauge symmetries (3.9) to (3.12), the Lagrangian (3.13) is invariant to within a total divergence,

$$\delta_\xi L = \partial_\mu(\epsilon^{\mu\nu\sigma\tau}\kappa k_{cd}\varepsilon^c{}_{ba}\tilde{Q}^a_\nu(2\tilde{P}^b_{\sigma\tau} + mB^b_{\sigma\tau})\xi^d), \tag{3.15}$$

$$\delta_\chi L = \partial_\mu(\epsilon^{\mu\nu\sigma\tau}k_{cd}(\kappa\varepsilon^c{}_{ab}\tilde{Q}^a_\nu\tilde{Q}^b_\sigma + m\tilde{F}^c_{\nu\sigma})\chi^d_\tau), \tag{3.16}$$

provided the coupling constants κ and λ are fixed such that

$$\kappa = 1/m, \quad \lambda = 1/2 \tag{3.17}$$

as shown by results in Sec. V. This gauge theory gives a nonlinear deformation of the massive SU(2) Yang–Mills/Freedman–Townsend theory from Ref. 6. We refer to the underlying algebraic structure SU(2) as the structure group of the massive nonlinear theory.

A. Features

The Lagrangian (3.13) yields the following field equations for A^a_μ and $B^a_{\mu\nu}$:

$$E_{\mathrm{A}\tau}{}^a = \epsilon_\tau{}^{\nu\sigma\mu}(D_\nu \tilde{P}^a_{\sigma\mu} + \varepsilon^a{}_{bc}((1/m)\tilde{Q}^b_\nu - A^b_\nu)\tilde{P}^c_{\sigma\mu}) + m\tilde{Q}^a_\tau = 0, \tag{3.18}$$

$$E_{\mathrm{B}\tau\sigma}{}^a = \epsilon_{\tau\sigma}{}^{\nu\mu}(D_\nu \tilde{Q}^a_\mu + \varepsilon^a{}_{bc}((1/(2m))\,\tilde{Q}^b_\nu - A^b_\nu)\tilde{Q}^c_\mu) + m\tilde{P}^a_{\tau\sigma} = 0. \tag{3.19}$$

These field equations are of second order in derivatives of A^a_μ, $B^a_{\mu\nu}$, with the second derivatives appearing linearly and first derivatives appearing quadratically, while A^a_μ, $B^a_{\mu\nu}$ appear nonpolynomially through the nonlinear field strengths. Due to the SU(2) Bianchi identity (2.3) and SU(2) divergence identity (3.3), these field strengths satisfy nonlinear divergence identities

$$\eta^{\nu\sigma}(D_\nu \tilde{P}^a_{\sigma\mu} + \varepsilon^a{}_{bc}((1/m)\,\tilde{Q}^b_\nu - A^b_\nu)\tilde{P}^c_{\sigma\mu}) = (1/m)\,\eta^{\nu\sigma}\varepsilon^a{}_{bc}E_{\mathrm{B}\nu\mu}{}^b A^c_\sigma, \tag{3.20}$$

$$\eta^{\nu\sigma}(D_\nu \tilde{Q}^a_\mu - \varepsilon^a{}_{bc}A^b_\nu \tilde{Q}^c_\sigma) = (1/m)\,\eta^{\nu\sigma}\varepsilon^a{}_{bc}(E_{\mathrm{A}\nu}{}^b A^c_\sigma + \eta^{\mu\tau}E_{\mathrm{B}\nu\mu}{}^b B^c_{\sigma\tau}). \tag{3.21}$$

Consequently, for solutions of the field equations, the field strengths satisfy a system of divergence and curl equations. Here, in contrast to the massless nonlinear theory in Sec. II A, this system can be written in terms of the field strengths alone

$$\partial_{[\sigma}\tilde{P}^a_{\nu\mu]} + mQ^a_{\sigma\nu\mu} = -(1/m)\,\varepsilon^a{}_{bc}\tilde{Q}^b_{[\sigma}\tilde{P}^c_{\nu\mu]}, \quad \partial^\nu \tilde{P}^a_{\nu\mu} = -(1/m)\,\eta^{\sigma\nu}\varepsilon^a{}_{bc}\tilde{Q}^b_\sigma P^c_{\nu\mu}, \tag{3.22}$$

$$\partial_{[\sigma}\tilde{Q}^a_{\nu]} + mP^a_{\sigma\nu} = -(1/(2m))\,\varepsilon^a{}_{bc}\tilde{Q}^b_{[\sigma}\tilde{Q}^c_{\nu]}, \quad \partial^\nu \tilde{Q}^a_\nu = 0, \tag{3.23}$$

constituting a first-order nonlinear field theory for $\tilde{P}^a_{\nu\mu}$, $\tilde{Q}^a_\nu$.

Linearization of the equations (3.22) and (3.23) produces a system of linear massive spin-one field strength equations, with the mass given by m. The corresponding linearization in terms of A^a_μ and $B^a_{\mu\nu}$ thus reduces to the Abelian linear gauge theory of massive vector potentials and antisymmetric tensor potentials (see Sec. V A). Hence, solutions of the nonlinear field theory for A^a_μ and $B^a_{\mu\nu}$ together describe a set of nonlinearly interacting massive spin-one fields in Minkowski space–time, where the coupling constant of the interaction is proportional to the inverse mass. A connection between this massive nonlinear theory and pure massive SU(2) Yang–Mills theory is discussed in Sec. IV.

Some additional features of the massive nonlinear theory will now be highlighted and compared to the massless nonlinear theory from Sec. II A.

The gauge symmetries on solutions of the field equations have the commutator structure

$$[\delta_{\xi_1}, \delta_{\xi_2}] = \delta_{\xi_3}, \quad [\delta_{\chi_1}, \delta_{\chi_2}] = 0, \quad [\delta_{\xi_1}, \delta_{\chi_1}] = \delta_{\chi_3}, \tag{3.24}$$

where $\xi_3{}^a = \varepsilon^a{}_{bc}\xi_1{}^b\xi_2{}^c$ and $\chi_{3\mu}{}^a = \varepsilon^a{}_{bc}\xi_1{}^b\chi_{1\mu}{}^c$. Thus the gauge group generated by exponentiation of these gauge symmetries is the semidirect product $\mathrm{SU}(2) \rtimes \mathrm{U}(1)^3$ which differs from the direct product structure in the massless nonlinear theory. Surprisingly, under this gauge group the nonlinear field strengths for solutions of the field equations are gauge invariant

$$\delta_\xi \tilde{P}^a_{\mu\nu} = \delta_\chi \tilde{P}^a_{\mu\nu} = 0, \quad \delta_\xi \tilde{Q}^a_\nu = \delta_\chi \tilde{Q}^a_\nu = 0. \tag{3.25}$$

Off solutions, the gauge symmetries are closed to within trivial gauge symmetries proportional to the field equations.

Conserved electric, magnetic, and scalar type charges are given by the same currents (2.50), (2.51), and (2.54) as derived for the massless nonlinear theory. These currents are gauge invariant on solutions of the field equations, due to the gauge transformation properties of the field strengths.

More remarkably, the conserved stress-energy tensor obtained from the Lagrangian (3.13) is of the same form (2.56) as in the massless nonlinear theory. In particular, the Chern–Simons term (3.1) makes no contribution to the stress-energy, as it has no dependence on the space–time metric $\eta_{\mu\nu}$ other than through the associated (metric compatible) volume tensor $\epsilon^{\mu\nu\sigma\tau}$. This stress-energy tensor (2.56) is again conserved and gauge invariant on solutions of the field equations in the massive nonlinear theory. Likewise it again yields a positive energy $t^\mu t^\nu T_{\mu\nu}(\tilde{P},\tilde{Q})$ and a causal energy momentum $t^\mu T_{\mu\nu}(\tilde{P},\tilde{Q})$ carried by the fields on any constant time hyperplane, with a unit timelike normal t^μ.

An extension of this theory from an SU(2) structure group to a general non-Abelian structure group is presented in the next section.

IV. GEOMETRICAL ASPECTS

The massless and massive nonlinear deformations of SU(2) Yang–Mills/Freedman–Townsend gauge theory constructed in Secs. II and III have a straightforward extension from a SU(2) structure group to a general non-Abelian structure group. The resulting non-Abelian massless and massive theories of coupled vector and antisymmetric tensor potentials possess a geometrically rich structure involving connections on Lie group bundles and associated covariant derivative operators and curvatures, which blend geometrical features of pure Yang–Mills theory and pure Freedman–Townsend theory, as will be discussed here. In particular, this structure exposes a striking equivalence between the massless/massive Yang–Mills equations for a Lie group connection and the field strength equations in the massless/massive nonlinear deformation. An interesting duality between the massive Yang–Mills equations and massive Freedman–Townsend equations will also be noted.

To begin, recall, the field variables consist of a set of three vector fields A^a_μ and three antisymmetric tensor fields $B^a_{\mu\nu}$, $a=1,2,3$, with which is associated an internal three-dimensional real vector space. We fix a basis e_a, $a=1,2,3$, for the Lie algebra SU(2) on this vector space and formulate the field variables geometrically as an SU(2)-valued one-form $A=A^a_\mu e_a\,dx^\mu$ and an SU(2)-valued two-form $B=B^a_{\mu\nu}e_a\,dx^\mu\,dx^\nu$. Similarly, the nonlinear field strengths are represented geometrically as an SU(2)-valued two-form $P=P^a_{\mu\nu}e_a\,dx^\mu\,dx^\nu$ and an SU(2)-valued three-form $Q=Q^a_{\mu\nu\sigma}e_a\,dx^\mu\,dx^\nu\,dx^\sigma$, whose duals are the two-form $*P=\tilde{P}^a_{\mu\nu}e_a\,dx^\mu\,dx^\nu$ and the one-form $*Q=\tilde{Q}^a_\mu e_a\,dx^\mu$.

We now introduce the following SU(2) covariant derivative operators, using A and $*Q$ as connection one-forms:

$$D_A=d+[A,\cdot\,], \tag{4.1}$$

$$D_{*Q}=d+[\lambda *Q,\cdot\,], \tag{4.2}$$

$$D_{A+*Q}=d+[A+\lambda *Q,\cdot\,], \tag{4.3}$$

where λ is a coupling constant, and $[\,\cdot\,,\cdot\,]$ denotes the SU(2) Lie bracket. The corresponding SU(2) curvatures are given by the two-forms

$$R_A=dA+\tfrac{1}{2}[A,A], \tag{4.4}$$

$$R_{*Q}=\lambda(d*Q+\tfrac{1}{2}\lambda[*Q,*Q]), \tag{4.5}$$

$$R_{A+*Q}=R_A+R_{*Q}+\lambda[A,*Q], \tag{4.6}$$

which satisfy

$$(D_A)^2=[R_A,\cdot], \quad (D_{*Q})^2=[R_{*Q},\cdot], \quad (D_{A+*Q})^2=[R_{A+*Q},\cdot]. \tag{4.7}$$

A. Massless SU(2) theory

The nonlinear massless field equations (2.38) and (2.39) for A,B together with the massless field strength equations (2.26) and (2.27) which define P,Q are given in geometrical form by

$$P=R_{A+*Q}-R_{*Q}, \tag{4.8}$$

$$Q=D_{*Q}B+\lambda[A,*P], \tag{4.9}$$

and

$$D_{A+*Q}*P=0, \tag{4.10}$$

$$R_{*Q}=0. \tag{4.11}$$

Thus, $*Q$ is a zero-curvature connection, while $*P$ is covariantly curl-free.

Hence, on solutions, it follows that

$$P=R_{A+*Q} \tag{4.12}$$

is a curvature, while

$$Q=D_{*Q}(B-\lambda*P) \tag{4.13}$$

is a covariant curl. In addition, the field strength identities (2.42) and (2.43) become

$$D_{A+*Q}P=0 \tag{4.14}$$

due to the SU(2) Bianchi identity, and

$$D_{*Q}Q=dQ=0 \tag{4.15}$$

since $[*Q,Q]=0$ is an identity.

Now, consider the SU(2)-valued one-form,

$$A_{\mathrm{SU}(2)}=A+\lambda*Q. \tag{4.16}$$

Under the gauge symmetry δ_ξ, $A_{\mathrm{SU}(2)}$ transforms as a SU(2) connection

$$\delta_\xi A_{\mathrm{SU}(2)}=D_{A_{\mathrm{SU}(2)}}\xi, \tag{4.17}$$

where

$$D_{A_{\mathrm{SU}(2)}}=d+[A_{\mathrm{SU}(2)},\cdot]. \tag{4.18}$$

This connection is invariant under the gauge symmetry δ_χ,

$$\delta_\chi A_{\mathrm{SU}(2)}=0. \tag{4.19}$$

Moreover, in terms of $A_{\mathrm{SU}(2)}$, the nonlinear field strength equations (4.10) and (4.12) involving P are simply the SU(2) Yang–Mills equations. In particular,

$$F_{\mathrm{SU}(2)} = P \tag{4.20}$$

is the SU(2) curvature of $A_{\mathrm{SU}(2)}$, satisfying the Yang–Mills connection equation

$$D_{A_{\mathrm{SU}(2)}} * F_{\mathrm{SU}(2)} = 0 \tag{4.21}$$

and the Bianchi identity

$$D_{A_{\mathrm{SU}(2)}} F_{\mathrm{SU}(2)} = 0. \tag{4.22}$$

Similarly, consider the SU(2)-valued two-form

$$B_{\mathrm{SU}(2)} = B - \lambda * P. \tag{4.23}$$

From the field strength equation (4.13), note $Q = D_{*Q} B_{\mathrm{SU}(2)}$ is equivalent to

$$*Q = Y^{-1}_{B_{\mathrm{SU}(2)}}(*dB_{\mathrm{SU}(2)}), \tag{4.24}$$

where $Y^{-1}_{B_{\mathrm{SU}(2)}}$ is the inverse of the linear map

$$Y_{B_{\mathrm{SU}(2)}} = \mathbb{I} + \lambda * [B_{\mathrm{SU}(2)}, \cdot\,] \tag{4.25}$$

acting on SU(2)-valued one-forms. Thus,

$$K_{\mathrm{SU}(2)} = *Q \tag{4.26}$$

is the SU(2) Freedman–Townsend three-form field strength of $B_{\mathrm{SU}(2)}$. In particular, under the gauge symmetry δ_χ, $B_{\mathrm{SU}(2)}$ transforms as a Freedman–Townsend antisymmetric tensor potential

$$\delta_\chi B_{\mathrm{SU}(2)} = D_{K_{\mathrm{SU}(2)}} \chi \tag{4.27}$$

and is invariant under the gauge symmetry δ_ξ,

$$\delta_\xi B_{\mathrm{SU}(2)} = 0. \tag{4.28}$$

Here

$$D_{K_{\mathrm{SU}(2)}} = d + [*K_{\mathrm{SU}(2)}, \cdot\,] \tag{4.29}$$

is an SU(2) covariant derivative using the dual field strength as the connection one-form. Moreover, $K_{\mathrm{SU}(2)}$ satisfies both the Freedman–Townsend field equation

$$R_{K_{\mathrm{SU}(2)}} = 0 \tag{4.30}$$

and field strength identity

$$dK_{\mathrm{SU}(2)} = 0, \tag{4.31}$$

which follow from the field strength equations (4.11) and (4.15) involving Q.

Interestingly, we therefore see that pure SU(2) Yang–Mills theory for a vector potential $A_{\mathrm{SU}(2)}$ and pure SU(2) Freedman–Townsend theory for an antisymmetry tensor potential $B_{\mathrm{SU}(2)}$ possess a combined formulation as a massless nonlinear gauge theory given by a nonlinear deformation of SU(2) Yang–Mills gauge theory for $A = A_{\mathrm{SU}(2)} - \lambda K_{\mathrm{SU}(2)}$ and SU(2) Freedman–Townsend gauge theory for $B = \lambda * F_{\mathrm{SU}(2)} + B_{\mathrm{SU}(2)}$.

B. Massive SU(2) theory

Compared to the massless case, the massive nonlinear theory has some significant geometrical differences. The nonlinear massive field equations (3.18) and (3.19) for A, B together with the field strength equations (3.7) and (3.8) which define P, Q take the geometrical form

$$P = R_{A+*Q} - R_{*Q}, \tag{4.32}$$

$$Q = D_{A+*Q}B + \frac{1}{m}[A, *P], \tag{4.33}$$

with $\lambda = 1/m$ in the covariant derivatives (4.2) and (4.3), and

$$\frac{1}{m} D_{*Q} *P = -Q, \tag{4.34}$$

$$R_{*Q} = -P. \tag{4.35}$$

By substitution of equations (4.35) and (4.34), respectively, into expressions (4.32) and (4.33), it follows that

$$R_{A+*Q} = 0 \tag{4.36}$$

and

$$D_{A+*Q}(*P + mB) = 0. \tag{4.37}$$

Hence, on solutions, $A + (1/m)*Q$ is a zero-curvature connection, while $*P + mB$ is covariantly curl-free. In addition, the field strength identities (3.20) and (3.21) become

$$D_{*Q}P = 0 \tag{4.38}$$

due to the SU(2) Bianchi identity, and

$$D_{*Q}Q = dQ = 0 \tag{4.39}$$

since $[*Q, Q] = [*P, P] = 0$ is an identity.

Now, in analogy with the massless case, consider the SU(2)-valued one-form

$$A_{\mathrm{SU}(2)} = \frac{1}{m} *Q. \tag{4.40}$$

In terms of $A_{\mathrm{SU}(2)}$, the nonlinear field strength equations (4.34), (4.35), and (4.38) involving P are simply the massive SU(2) Yang–Mills equations, in particular,

$$*D_{A_{\mathrm{SU}(2)}} *F_{\mathrm{SU}(2)} + m^2 A_{\mathrm{SU}(2)} = 0 \tag{4.41}$$

and the Bianchi identity

$$D_{A_{\mathrm{SU}(2)}} F_{\mathrm{SU}(2)} = 0, \tag{4.42}$$

where

$$F_{\mathrm{SU}(2)} = -P \tag{4.43}$$

is the SU(2) curvature of $A_{\mathrm{SU}(2)}$. Moreover, $A_{\mathrm{SU}(2)}$ satisfies Lorentz gauge

$$d*A_{\mathrm{SU}(2)}=0 \tag{4.44}$$

due to the field strength identity (4.39). Correspondingly, under the SU(2) gauge symmetry δ_ξ, $A_{\mathrm{SU}(2)}$ is gauge invariant

$$\delta_\xi A_{\mathrm{SU}(2)}=0. \tag{4.45}$$

Finally, from the remaining field strength equations (4.36) and (4.37), it follows that the SU(2)-valued one-form

$$A_{\mathrm{flat}}=A+\frac{1}{m}*Q \tag{4.46}$$

is a flat connection, with respect to which the SU(2)-valued two-form

$$B_{\text{curl-free}}=B+\frac{1}{m}*P \tag{4.47}$$

is covariantly curl-free. Thus, up to gauge transformations, $B_{\text{curl-free}}$ is an exact two-form and A_{flat} vanishes. This two-form has no apparent geometrical relation to Freedman–Townsend theory, in contrast to the situation in the massless case.

Interestingly, however, the nonlinear field strength equations (4.34), (4.35), (4.38), (4.39) exhibit a direct relation to massive SU(2) Freedman–Townsend theory as follows. Consider the SU(2)-valued two-form

$$B_{\mathrm{SU}(2)}=-\frac{1}{m}*P. \tag{4.48}$$

From the field strength equation (4.34), we see that

$$K_{\mathrm{SU}(2)}=\frac{1}{m}Q \tag{4.49}$$

is the SU(2) Freedman–Townsend field strength three-form determined by

$$D_{K_{\mathrm{SU}(2)}}B_{\mathrm{SU}(2)}=K_{\mathrm{SU}(2)}, \tag{4.50}$$

and hence

$$Y^{-1}_{B_{\mathrm{SU}(2)}}(*dB_{\mathrm{SU}(2)})=*K_{\mathrm{SU}(2)}. \tag{4.51}$$

We then see that the field strength equation (4.35) is simply the massive Freedman–Townsend field equation

$$R_{K_{\mathrm{SU}(2)}}=m^2*B_{\mathrm{SU}(2)}, \tag{4.52}$$

while the field strength equation (4.38) yields the SU(2) Freedman–Townsend field strength identity

$$dK_{\mathrm{SU}(2)}=0. \tag{4.53}$$

Finally, from the field strength equation (4.39), we obtain

$$D_{K_{\mathrm{SU}(2)}}*B_{\mathrm{SU}(2)}=0, \tag{4.54}$$

which is a nonlinear SU(2) Lorentz gauge on $B_{\mathrm{SU}(2)}$.

It now follows through the duality

$$A_{\mathrm{SU}(2)} = *K_{\mathrm{SU}(2)}, \quad mB_{\mathrm{SU}(2)} = *F_{\mathrm{SU}(2)}, \quad m \neq 0 \tag{4.55}$$

given by Eqs. (4.40), (4.43), (4.48), and (4.49) that this massive Freedman–Townsend theory for $B_{\mathrm{SU}(2)}$ is equivalent to the massive Yang–Mills theory for $A_{\mathrm{SU}(2)}$.

Consequently, we see that pure massive SU(2) Yang–Mills theory for a vector potential $A_{\mathrm{SU}(2)}$ [or equivalently pure massive SU(2) Freedman–Townsend theory for an antisymmetric tensor potential $B_{\mathrm{SU}(2)}$], along with a SU(2) theory of a covariantly exact antisymmetric tensor potential $B_{\text{curl-free}}$ with respect to a flat connection A_{flat}, together possess a reformulation as a massive nonlinear gauge theory given by a nonlinear deformation of SU(2) Yang–Mills/Freedman–Townsend theory with a Chern–Simons mass term for $A = A_{\mathrm{flat}} - A_{\mathrm{SU}(2)}$ and $B = B_{\text{curl-free}} - (1/m)*F_{\mathrm{SU}(2)}$.

C. General non-Abelian theory

The SU(2) massless and massive nonlinear theories are easily generalized so that in place of the SU(2) structure group we have a non-Abelian structure group based on any semisimple Lie algebra, $\mathcal{A}$. Geometrically, A, $*Q$, B, $*P$ thereby are generalized to be $\mathcal{A}$-valued one-forms and two-forms. The field strength equations in Secs. IV A and IV B retain the same geometrical form with $[\cdot,\cdot]$ given by the Lie bracket of $\mathcal{A}$. As shown by the deformation analysis in Sec. V, this provides the most general non-Abelian massless and massive nonlinear theories representing a geometrical deformation of semisimple Yang–Mills/Freedman–Townsend gauge theory for Lie-algebra valued field variables A, B.

A further type of extension arises from considering non-semisimple structure groups. Recall from Sec. II, for the massless nonlinear theory an allowed structure group is $(\mathrm{SU}(2), \mathcal{G} = \mathrm{U}(1) \rtimes \mathrm{U}(1)^2)$, based on using the Lie algebras SU(2) for the Yang–Mills algebraic structure and $\mathcal{G}$ for the Freedman–Townsend algebraic structure underlying the construction of the theory. A more general non-semisimple structure group is allowed for both the massless as well as the massive nonlinear theories, which will now be presented. This extension involves some unexpected, novel algebraic features compared to the SU(2) case.

To proceed, we first introduce two Lie algebras $\mathcal{A}$ and $\mathcal{A}'$ along with a homomorphism h from $\mathcal{A}'$ into $\mathcal{A}$. Thus, $h(\mathcal{A}') \subseteq \mathcal{A}$ is a subalgebra of $\mathcal{A}$ while $\ker(h) \subseteq \mathcal{A}'$ is an invariant subalgebra of $\mathcal{A}'$. (In particular, note $\mathcal{A}' \simeq \mathcal{A}$ are isomorphic Lie algebras iff the kernel of h is empty and h is surjective.) Then the algebraic structure common to both the massless and massive nonlinear theories consists of the Lie brackets $[\cdot,\cdot]_{\mathcal{A}}$, $[\cdot,\cdot]_{\mathcal{A}'}$, and inner products $(\cdot,\cdot)_{\mathcal{A}}$, $(\cdot,\cdot)_{\mathcal{A}'}$ fixed on $\mathcal{A}$ and $\mathcal{A}'$, and a bilinear map $f(\cdot,\cdot) = [\cdot, h(\cdot)]_{\mathcal{A}}$ from $\mathcal{A} \times \mathcal{A}'$ into $\mathcal{A}$. There are additional properties required to hold on this algebraic structure in the separate massless and massive cases. An explanation for the origin of these properties will be provided by the deformation analysis in Sec. V.

We begin with some algebraic preliminaries of a techincal nature. Associated with the Lie brackets and bilinear map, introduce the linear maps $ad_{\mathcal{A}}(\cdot)$ and $ad_{\mathcal{A}'}(\cdot)$ denoting the adjoint representation of the Lie algebras $\mathcal{A}$ and $\mathcal{A}'$,

$$ad_{\mathcal{A}}(v)u = [v,u]_{\mathcal{A}}, \quad ad_{\mathcal{A}'}(v')u' = [v',u']_{\mathcal{A}'}, \tag{4.56}$$

and the additional linear maps $ad_{\mathcal{A}} \circ h(\cdot)$ and $ad_{h,\mathcal{A}}(\cdot)$ defined via $f(\cdot,\cdot)$ by

$$ad_{\mathcal{A}} \circ h(v')u = ad_{\mathcal{A}}(u)h(v') = [u, h(v')]_{\mathcal{A}} = f(u,v'), \tag{4.57}$$

$$ad_{h,\mathcal{A}}(v)u' = ad_{\mathcal{A}} \circ h(u')v = f(v,u'), \tag{4.58}$$

for all u, v in $\mathcal{A}$, and all u', v' in $\mathcal{A}'$. Let $h^T(\cdot)$ denote the adjoint map of $h(\cdot)$ from $\mathcal{A}$ into $\mathcal{A}'$ defined in the natural manner with respect to the inner products on $\mathcal{A}$ and $\mathcal{A}'$. This gives a bilinear map $f^T(\cdot,\cdot)=[\cdot,h^T(\cdot)]_{\mathcal{A}'}$ from $\mathcal{A}'\times\mathcal{A}$ into $\mathcal{A}'$. Now, introduce the associated linear maps $ad_{\mathcal{A}'}\circ h^T(\cdot)$ and $ad_{h,\mathcal{A}'}(\cdot)$, defined via $f^T(\cdot,\cdot)$ by

$$ad_{\mathcal{A}'}\circ h^T(v)u'=ad_{\mathcal{A}'}(u')h^T(v)=[u',h^T(v)]_{\mathcal{A}'}=f^T(u',v), \tag{4.59}$$

$$ad_{h,\mathcal{A}'}(v')u=ad_{\mathcal{A}'}\circ h^T(u)v'=f^T(v',u), \tag{4.60}$$

for all u, v in $\mathcal{A}$, and all u', v' in $\mathcal{A}'$.

Similarly, let $ad^T_{\mathcal{A}}(\cdot)$ and $ad^T_{\mathcal{A}'}(\cdot)$ denote the adjoint maps of $ad_{\mathcal{A}}(\cdot)$,$ad_{\mathcal{A}'}(\cdot)$ and define the related adjoints $ad^*_{\mathcal{A}}(\cdot)$ and $ad^*_{\mathcal{A}'}(\cdot)$ by

$$ad^*_{\mathcal{A}}(v)u=ad^T_{\mathcal{A}}(u)v, \quad ad^*_{\mathcal{A}'}(v')u'=ad^T_{\mathcal{A}'}(u')v', \tag{4.61}$$

as well as the analogous adjoint maps $ad^T_{h,\mathcal{A}}(\cdot)$, $ad^T_{h,\mathcal{A}'}(\cdot)$, $ad^*_{h,\mathcal{A}}(\cdot)$, $ad^*_{h,\mathcal{A}'}(\cdot)$ given via

$$ad^*_{h,\mathcal{A}}(u)v=-h^T(ad^*_{\mathcal{A}}(u)v)=-h^T(ad^T_{\mathcal{A}}(v)u)=ad^T_{h,\mathcal{A}}(v)u, \tag{4.62}$$

$$ad^*_{h,\mathcal{A}'}(u')v'=-h(ad^*_{\mathcal{A}'}(u')v')=-h(ad^T_{\mathcal{A}'}(v')u')=ad^T_{h,\mathcal{A}'}(v')u', \tag{4.63}$$

again for all u, v in $\mathcal{A}$, and all u', v' in $\mathcal{A}'$. Since h is a homomorphism of $\mathcal{A}'$ into $\mathcal{A}$, it follows that

$$ad^*_{h,\mathcal{A}}(\cdot)h=-ad^*_{\mathcal{A}'}(h^T(\cdot)). \tag{4.64}$$

The appearance of these adjoint maps is an essential feature in the general non-Abelian algebraic structure of the massless and massive nonlinear theories. Note, we have $ad^*_{\mathcal{A}}(\cdot)=ad_{\mathcal{A}}(\cdot)$ and $ad^*_{\mathcal{A}'}(\cdot)=ad_{\mathcal{A}'}(\cdot)$ if and only if the inner products are invariant with respect to the Lie brackets, which holds whenever $\mathcal{A}$ and $\mathcal{A}'$ are semisimple and the inner products are given by the Cartan–Killing metrics of $\mathcal{A}$ and $\mathcal{A}'$.

Next, we take A, $*Q$ to be $\mathcal{A}$-,$\mathcal{A}'$-valued one-forms and B, $*P$ to be $\mathcal{A}'$-,$\mathcal{A}$-valued two-forms, respectively. For later use in formulating $*Q$, $*P$ geometrically in terms of A, B, we first introduce the following inner product norm on pairs (α,β) consisting of a $\mathcal{A}$-valued two-form α and a $\mathcal{A}'$-valued one-form β:

$$Y_{A,B}((\alpha,\beta),(\alpha,\beta))=(\alpha,\alpha)_{\mathcal{A}}+(\beta,\beta)_{\mathcal{A}'}-2([h(\beta),A]_{\mathcal{A}},*\alpha)_{\mathcal{A}}-([\beta,\beta]_{\mathcal{A}'},*B)_{\mathcal{A}'}, \tag{4.65}$$

where $(\cdot,\cdot)_{\mathcal{A}}$ and $(\cdot,\cdot)_{\mathcal{A}'}$ are extended to act on $\mathcal{A}$-,$\mathcal{A}'$-valued forms via the Hodge inner product. Then let $Y_{A,B}(\cdot)=Y^{\mathrm{T}}_{A,B}(\cdot)$ be the associated symmetric linear map on pairs (α,β).

Finally, we also introduce the following covariant derivative operators:

$$D_A=d+ad_{\mathcal{A}}(A), \tag{4.66}$$

$$D_{*Q}=d+ad_{\mathcal{A}}\circ h(*Q), \tag{4.67}$$

$$D_{A+*Q}=d+ad_{\mathcal{A}}(A+h(*Q)), \tag{4.68}$$

which act on $\mathcal{A}$-valued functions and forms, and

$$D'_{*Q}=d-ad^T_{\mathcal{A}'}(*Q), \tag{4.69}$$

$$D'_A=d-ad^T_{\mathcal{A}'}\circ h^{-1}(A), \tag{4.70}$$

$$D'_{A+*Q}=d-ad^T_{\mathcal{A}'}(h^{-1}(A)+*Q), \tag{4.71}$$

which act on $\mathcal{A}'$-valued functions and forms, where the last two derivative operators are defined only when h is invertible. The Lie-algebra valued curvature two-forms associated with these connections are determined by

$$R_A=dA+\tfrac{1}{2}[A,A]_{\mathcal{A}}, \tag{4.72}$$

$$R'_{*Q}=d*Q+\tfrac{1}{2}[*Q,*Q]_{\mathcal{A}'}, \tag{4.73}$$

which satisfy

$$(D_A)^2=ad_{\mathcal{A}}(R_A), \tag{4.74}$$

$$(D'_{*Q})^2=-ad^T_{\mathcal{A}'}(R'_{*Q}). \tag{4.75}$$

Moreover, note that since h is a homomorphism of $\mathcal{A}'$ into $\mathcal{A}$, we have

$$R_{*Q}=h(R'_{*Q}), \tag{4.76}$$

while from the property that $-ad^T_{\mathcal{A}'}(\cdot)$ is the coadjoint representation of $\mathcal{A}'$, we also have

$$R'_A=-ad^T_{\mathcal{A}'}\circ h^{-1}(R_A) \tag{4.77}$$

since when h^{-1} exists it gives a homomorphism of $\mathcal{A}$ onto $\mathcal{A}'$.

1. Massless theory

In the massless nonlinear theory, the Lie algebra $\mathcal{A}$ is required to be semisimple, and hence

$$ad^*_{\mathcal{A}}(\cdot)=-ad^T_{\mathcal{A}}(\cdot)=ad_{\mathcal{A}}(\cdot), \tag{4.78}$$

with the inner product $(\cdot,\cdot)_{\mathcal{A}}$ given by the Cartan–Killing metric of $\mathcal{A}$. Note that, consequently,

$$ad^T_{\mathcal{A}'}\circ h^T(\cdot)=h^T\circ ad_{\mathcal{A}}\circ h(\cdot) \tag{4.79}$$

and so

$$h^T(D_{*Q}(\cdot))=D'_{*Q}(h^T(\cdot)). \tag{4.80}$$

No further properties are needed on the Lie algebra structure of $\mathcal{A}$, $\mathcal{A}'$. Now the entire theory can be constructed geometrically in terms of the covariant derivatives (4.66), (4.68), (4.69) and curvatures (4.72) and (4.73) along with the linear map (4.65). First, the massless nonlinear field strengths are defined by

$$(*P,*Q)=Y^{-1}_{A,B}(*R_A,*dB), \tag{4.81}$$

where $Y^{-1}_{A,B}(\cdot)$ is the inverse of the linear map $Y_{A,B}(\cdot)$. In terms of these field strengths, the gauge symmetries on A, B are given by

$$\delta_\xi A=D_{A+*Q}\xi, \quad \delta_\xi B=\Gamma'_{*P}\xi, \tag{4.82}$$

for arbitrary $\mathcal{A}$-valued functions ξ on M, and

$$\delta_\chi A=0, \quad \delta_\chi B=D'_{*Q}\chi, \tag{4.83}$$

for arbitrary $\mathcal{A}'$-valued one-forms χ on M. Here $\Gamma'_{*P}(\cdot)$ is a linear map associated with $*P$ by

$$\Gamma'_{*P}=ad^T_{h,\mathcal{A}'}(*P). \tag{4.84}$$

Finally, the Lagrangian is given by

$$L=\tfrac{1}{2}(*P,R_A)_{\mathcal{A}}+\tfrac{1}{2}(*Q,*dB)_{\mathcal{A}'}=\tfrac{1}{2}(*P,*Q)\cdot Y_{A,B}(*P,*Q), \tag{4.85}$$

where $(\alpha,\beta)\cdot(\alpha,\beta)=(\alpha,\alpha)_{\mathcal{A}}+(\beta,\beta)_{\mathcal{A}'}$ for any $\mathcal{A}$-valued forms α, $\mathcal{A}'$-valued forms β. This yields the field equations for A, B:

$$*E_{\mathrm{A}}=D_{A+*Q}*P=0, \quad *E_{\mathrm{B}}=R'_{*Q}=0. \tag{4.86}$$

Thus, on solutions, $*Q$ is a zero-curvature connection, while $*P$ is covariantly curl-free.

From the field strength equation (4.81), $*P$ and $*Q$ have the form

$$P=R_{A+*Q}-R_{*Q}, \quad Q=D'_{*Q}B-\Gamma'_{*P}A. \tag{4.87}$$

Hence, since $R_{*Q}=h(R'_{*Q})=0$ and $ad_{\mathcal{A}}(*P)A=D_{*Q}*P$ on solutions, it respectively follows that

$$P=R_{A+*Q} \tag{4.88}$$

is a curvature, while

$$Q=D'_{*Q}(B-h^T(*P)) \tag{4.89}$$

is a covariant curl, using in addition the algebraic relation

$$ad^T_{h,\mathcal{A}}(\cdot)=h^T\circ ad_{\mathcal{A}}(\cdot). \tag{4.90}$$

Then, the covariant exterior derivatives D'_{*Q} of Q and D_{A+*Q} of P yield

$$D_{A+*Q}P=0 \tag{4.91}$$

and

$$D'_{*Q}Q=0. \tag{4.92}$$

These are the same geometrical expressions as those in the SU(2) case.

Therefore, geometrically, $ad_{\mathcal{A}}(A+h^T(*Q))=A_{\mathrm{YM}}$ is a Yang–Mills connection one-form, whose curvature $ad_{\mathcal{A}}(P)=F_{\mathrm{YM}}$ satisfies the massless Yang–Mills equations $D_{A_{\mathrm{YM}}}*F_{\mathrm{YM}}=0$ and the Bianchi identity $D_{A_{\mathrm{YM}}}F_{\mathrm{YM}}=0$, with $D_{A_{\mathrm{YM}}}=d+ad_{\mathcal{A}}(A_{\mathrm{YM}})$, based on the gauge group associated to the semisimple Lie algebra $\mathcal{A}$.

2. Massive theory

In the massive nonlinear theory, the homomorphism h is required to be a Lie-algebra isomorphism

$$h(\cdot)=\frac{1}{m}\,\mathrm{id}(\cdot) \tag{4.93}$$

so $\mathcal{A}=h(\mathcal{A}')\simeq\mathcal{A}'$, where $m\neq 0$ is the mass, and id is a linear map identifying the vector spaces of $\mathcal{A}$ and $\mathcal{A}'$. But, $\mathcal{A}$ and $\mathcal{A}'$ need not be semisimple here, and there are no further properties

required on the Lie algebra structure of $\mathcal{A}$, $\mathcal{A}'$. Thus, surprisingly, compared to massive Yang–Mills/Freedman–Townsend theory[6] as well as to pure massless Yang–Mills theory, a more general structure group is allowed for the massive nonlinear theory.

First, the massive nonlinear field strengths are defined by

$$(*P,*Q)=Y^{-1}_{A,B}(*R_A,*D'_AB), \tag{4.94}$$

where $Y^{-1}_{A,B}(\cdot)$ is the inverse of the linear map $Y_{A,B}(\cdot)$. In terms of these field strengths, the gauge symmetries on A, B are given by

$$\delta_\xi A=D_{A+*Q}\xi, \quad \delta_\xi B=\Gamma'_{B+*P}\xi, \tag{4.95}$$

for arbitrary $\mathcal{A}$-valued functions ξ on M, and

$$\delta_\chi A=0, \quad \delta_\chi B=D'_{A+*Q}\chi, \tag{4.96}$$

for arbitrary $\mathcal{A}'$-valued one-forms χ on M, where now

$$\Gamma'_{B+*P}=-ad^*_{h,\mathcal{A}'}(*P)+ad_{h,\mathcal{A}'}(B). \tag{4.97}$$

The Lagrangian is given by

$$L=\tfrac{1}{2}(*P+m^2h(B),R_A)_{\mathcal{A}}+\tfrac{1}{2}(*Q,*D'_AB)_{\mathcal{A}'}, \tag{4.98}$$

which yields the field equations for A, B:

$$*E_{\mathrm{A}}=h(D'_{*Q}h^{-1}(*P))+m^2h(Q)=0, \quad *E_{\mathrm{B}}=R'_{*Q}+h^{-1}(P)=0, \tag{4.99}$$

where h^{-1} is the inverse of the isomorphism h,

$$h^{-1}(\cdot)=m\,\mathrm{id}(\cdot)=m^2h^T(\cdot). \tag{4.100}$$

From the field strength equation (4.94), $*P$ and $*Q$ have the form

$$P=R_{A+*Q}-R_{*Q}, \quad Q=D'_{A+*Q}B-\Gamma'_{*P}A. \tag{4.101}$$

Hence, since

$$R_{*Q}=-P \tag{4.102}$$

holds on solutions, it follows that

$$R_{A+*Q}=0 \tag{4.103}$$

and so $A+*Q$ is a zero-curvature connection. Furthermore, from

$$D'_{*Q}h^T(*P)=-Q \tag{4.104}$$

on solutions, and from $\Gamma'_{*P}A=ad^T_{\mathcal{A}'}\circ h^{-1}(A)h^T(*P)$ through the algebraic relation

$$ad^T_{h,\mathcal{A}}(\cdot)=-ad^T_{\mathcal{A}'}\circ h^{-1}(\cdot)h^T \tag{4.105}$$

obtained from the homomorphism equation (4.64), it follows that

$$D'_{A+*Q}(B+h^T(*P))=0 \tag{4.106}$$

and so $B+h^T(*P)$ is covariantly curl-free. Then, the covariant exterior derivatives D'_{*Q} of Q and D_{*Q} of P yield

$$D_{*Q}P=0 \tag{4.107}$$

and

$$D'_{*Q}Q=h^T(ad^T_{\mathcal{A}}(*P)P). \tag{4.108}$$

Therefore, geometrically, $ad_{\mathcal{A}}\circ h(*Q)=A_{\rm YM}$ is a Yang–Mills connection one-form, whose curvature $-ad_{\mathcal{A}}(P)=F_{\rm YM}$ satisfies an adjoint version of the massive Yang–Mills equations

$$*D^T_{A_{\rm YM}}*F_{\rm YM}+m^2A_{\rm YM}=0 \tag{4.109}$$

and the Bianchi identity

$$D^T_{A_{\rm YM}}F_{\rm YM}=0, \tag{4.110}$$

where

$$D^T_{A_{\rm YM}}=d-ad^T_{\mathcal{A}}(A_{\rm YM}). \tag{4.111}$$

In addition, $A_{\rm YM}$ satisfies a nonlinear covariant gauge condition

$$D^T_{A_{\rm YM}}*A_{\rm YM}=-ad^T_{\mathcal{A}}(*F_{\rm YM})F_{\rm YM}. \tag{4.112}$$

Interestingly, this adjoint modification is based on having a non-semisimple Lie algebra $\mathcal{A}$, so that $ad^*_{\mathcal{A}}(\cdot)\neq ad_{\mathcal{A}}(\cdot)$. Its consistency relies on the property that, for any Lie algebra $\mathcal{A}$, $-ad^T_{\mathcal{A}}(\cdot)$ is the coadjoint representation of $\mathcal{A}$. If $\mathcal{A}$ is chosen to be semisimple, then note the standard massive Yang–Mills theory is obtained.

Similarly to the SU(2) case, the non-semisimple massive Yang–Mills theory (4.109) to (4.112) here is equivalent to a non-semisimple massive Freedman–Townsend theory given by the duality

$$A_{\rm YM}=*K_{\rm YM}, \quad mB_{\rm YM}=*F_{\rm YM} \tag{4.113}$$

as follows from the field strength equations (4.102), (4.104), (4.107), and (4.108).

V. DEFORMATION ANALYSIS

Here a systematic determination of the most general nonlinear geometrical deformation will be given for the linear gauge theory of $n\geqslant 1$ vector potentials A^a_μ, $a=1,\ldots,n$, and $n'\geqslant 1$ antisymmetric tensor potentials $B^{a'}_{\mu\nu}$, $a'=1,\ldots,n'$, with a Chern–Simons-type mass term, on a four-dimensional space–time manifold M. The method used is a geometrical version of the field theoretic approach to deformations developed in Refs. 3, 1, and 12.

A. Linear theory

We formulate the linear theory geometrically, using a set of one-forms $A^a=A^a_\mu\,dx^\mu$ and two-forms $B^{a'}=B^{a'}_{\mu\nu}\,dx^\mu\,dx^\nu$. These field variables are regarded as taking values in respective internal vector spaces $\mathcal{A}$, $\mathcal{A}'$ of dimensions n, n'.

To proceed, the only structure we require on the space–time manifold M is the exterior derivative operator d and the Hodge dual $*$ such that $*^2=\pm 1$ where 1 is the identity operator. Hereafter, products of fields will be understood to be wedge products of forms on M (and tensor products with respect to $\mathcal{A}$, $\mathcal{A}'$). Recall, in terms of $*$, there is a standard Hodge inner product on pairs (α,β) of one-forms and two-forms, $(\alpha,\beta)\cdot(\alpha,\beta)=*(\alpha*\alpha)-*(\beta*\beta)$.

The linear field strengths associated with the field variables are given by the $\mathcal{A}$-valued two-form $F^a = dA^a$ and $\mathcal{A}'$-valued three-form $H^{a'} = dB^{a'}$. Then the Lagrangian is given by the following real-valued four-form:

$$\overset{(2)}{L} = \tfrac{1}{2}\delta_{ab}F^a * F^b - \tfrac{1}{2}\delta_{a'b'}H^{a'} * H^{b'} + m_{aa'}F^a B^{b'}, \tag{5.1}$$

where δ_{ab}, $\delta_{a'b'}$ represent components of respective inner products on $\mathcal{A}$, $\mathcal{A}'$, and $m_{aa'}$ represents components of a bilinear form on $\mathcal{A}\times\mathcal{A}'$. We refer to $m_{aa'}$ as the mass tensor. This Lagrangian is invariant to within an exact four-form under the separate Abelian gauge symmetries given by

$$\overset{(0)}{\delta}_\xi A^a = d\xi^a, \quad \overset{(0)}{\delta}_\xi B^{a'} = 0, \tag{5.2}$$

for arbitrary $\mathcal{A}$-valued functions ξ^a, and

$$\overset{(0)}{\delta}_\chi A^a = 0, \quad \overset{(0)}{\delta}_\xi B^{a'} = d\chi^{a'}, \tag{5.3}$$

for arbitrary $\mathcal{A}'$-valued one-forms $\chi^{a'}$. Under variations of the fields A^a and $B^{a'}$, the Lagrangian yields the Euler–Lagrange field equations

$$*\overset{(1)}{E}_{\mathrm{A}}{}^a = d*F^a + m_{a'}{}^a H^{a'} = 0, \tag{5.4}$$

$$*\overset{(1)}{E}_{\mathrm{B}}{}^{a'} = d*H^{a'} + m_a{}^{a'} F^a = 0, \tag{5.5}$$

where $m_{a'}{}^a = \delta^{ab}m_{ba'}$ and $m_a{}^{a'} = \delta^{a'b'}m_{ab'}$ are components of linear maps $m_{\mathcal{A}}(\cdot)$ from $\mathcal{A}$ into $\mathcal{A}'$, and $m_{\mathcal{A}'}(\cdot)$ from $\mathcal{A}'$ into $\mathcal{A}$.

Note, in the case when the mass tensor vanishes, $m_{aa'} = 0$, the fields A^a and $B^{a'}$ are decoupled and the linear theory reduces to massless Abelian Yang–Mills gauge theory for A^a and massless Abelian Freedman–Townsend gauge theory for $B^{a'}$. The field strengths F^a and $H^{a'}$ obviously then describe free massless spin-one and spin-zero fields.

In contrast, in the opposite case when the mass tensor is fully nondegenerate, $m_{aa'} = m\,\delta_{aa'}$ where $\delta_a{}^{a'}$ is a vector-space isomorphism of $\mathcal{A}$ and $\mathcal{A}'$ (and hence $n = n'$), the fields A^a and $B^{a'}$ are coupled through a Chern–Simons mass term. The linear theory then reduces to massive Abelian Yang–Mills/Freedman–Townsend gauge theory, which is the linearization of the nonlinear theory given in Ref. 6. Consequently, the field strengths F^a and $H^{a'}$ together describe free massive spin-one fields, with the mass given by m. (In particular, A^a supplies two of the three spin-one helicity components while $B^{a'}$ supplies the third.)

To continue, we consider the general case with no conditions assumed on the mass tensor. Let $\mathcal{A}_0$ and $\mathcal{A}'_0$ denote the kernels of the maps $m_{\mathcal{A}}(\cdot)$ and $m_{\mathcal{A}'}(\cdot)$, and let $\mathcal{A}_m$ and $\mathcal{A}'_m$ denote the orthogonal complements of these kernels. Note there is a direct sum decomposition, $\mathcal{A} = \mathcal{A}_0 \oplus \mathcal{A}_m$, $\mathcal{A}' = \mathcal{A}'_0 \oplus \mathcal{A}'_m$, with respect to the inner products on the internal vector spaces. Moreover, $\mathcal{A}_m$ and $\mathcal{A}'_m$ are isomorphic vector subspaces, with a common dimension denoted by $0 \leqslant k \leqslant n, n'$.

Fix a basis for these vector subspaces so that the fields A^a and $B^{a'}$ belong to $\mathcal{A}_0$ and $\mathcal{A}'_0$ for $a = a' = 1,\ldots,k$ and belong to $\mathcal{A}_m$ and $\mathcal{A}'_m$ for $a = k+1,\ldots,n$, $a' = k+1,\ldots,n'$. Then, physically speaking, it follows from the linear field equations that the field strengths F^a and $H^{a'}$ given by $a = a' = 1,\ldots,k$, together describe a set of k free massive spin-one fields with mass equal to the nonzero eigenvalues of $m_{aa'}$, while the remaining field strengths F^a and $H^{a'}$ given by $a = k+1,\ldots,n$ and $a' = k+1,\ldots,n'$ describe separate sets of $n-k$ free massless spin-one fields and $n'-k$ free massless spin-zero fields, respectively.

B. Determining equations for nonlinear deformations

We now consider nonlinear deformations of the linear Abelian gauge theory for A^a and $B^{a'}$, with the deformation terms being locally constructed in a geometrical manner from the fields by using only the exterior derivative d and Hodge dual $*$ on M. Here, a deformation consists of adding linear and higher power terms to the Abelian gauge symmetries (5.2) and (5.3),

$$\delta_\xi A^a = \overset{(0)}{\delta}_\xi A^a + \overset{(1)}{\delta}_\xi A^a + \cdots, \quad \delta_\xi B^{a'} = \overset{(0)}{\delta}_\xi B^{a'} + \overset{(1)}{\delta}_\xi B^{a'} + \cdots, \tag{5.6}$$

and

$$\delta_\chi A^a = \overset{(0)}{\delta}_\chi A^a + \overset{(1)}{\delta}_\chi A^a + \cdots, \quad \delta_\chi B^{a'} = \overset{(0)}{\delta}_\chi B^{a'} + \overset{(1)}{\delta}_\chi B^{a'} + \cdots, \tag{5.7}$$

while simultaneously adding quadratic and higher power terms to the linear field equations (5.4) and (5.5),

$$E_{\mathrm{A}}{}^a = \overset{(1)}{E}_{\mathrm{A}}{}^a + \overset{(2)}{E}_{\mathrm{A}}{}^a + \cdots, \quad E_{\mathrm{B}}{}^{a'} = \overset{(1)}{E}_{\mathrm{B}}{}^{a'} + \overset{(2)}{E}_{\mathrm{B}}{}^{a'} + \cdots, \tag{5.8}$$

such that there exists a locally constructed Lagrangian four-form that is gauge invariant to within an exact four-form. The condition of gauge invariance is expressed by

$$\delta_\xi L = \overset{(0)\ (2)}{\delta}_\xi L + \overset{(1)\ (2)}{\delta}_\xi L + \overset{(0)\ (3)}{\delta}_\xi L + \cdots = d\Theta_\xi, \tag{5.9}$$

$$\delta_\chi L = \overset{(0)\ (2)}{\delta}_\chi L + \overset{(1)\ (2)}{\delta}_\chi L + \overset{(0)\ (3)}{\delta}_\chi L + \cdots = d\Theta_\chi, \tag{5.10}$$

holding for some locally constructed three-forms Θ_ξ and Θ_χ, where the Lagrangian is related to the field equations through

$$\delta L = \delta A^a * E_{\mathrm{A}}{}^b \delta_{ab} + \delta B^{a'} * E_{\mathrm{B}}{}^{b'} \delta_{a'b'} + d\Gamma, \tag{5.11}$$

holding for some locally constructed three-form Γ, under arbitrary variations δA^a, $\delta B^{a'}$.

For writing down deformation terms and analyzing the deformation equations, a precise formal setting is provided by the field space $\mathcal{S}=\{(A^a(x), B^{a'}(x))\}$ defined as the set of all sections of the vector bundle of $\mathcal{A}$-valued one-forms and $\mathcal{A}'$-valued two-forms on M. Hereafter, geometrically, a field variation $(\delta A^a,\ \delta B^{a'})$ is regarded as a vector field on $\mathcal{S}$ while field equations $(E^A{}_a,\ E^B{}_{a'})$ are regarded as a covector field on $\mathcal{S}$, where $E^{\mathrm{A}}{}_a$, $E^{\mathrm{B}}{}_{a'}$ are related to $E_{\mathrm{A}}{}^a$, $E_{\mathrm{B}}{}^{a'}$ by

$$\delta_{ab} * E_{\mathrm{A}}{}^a \cdot \delta A^b = \delta A^a \rfloor E^{\mathrm{A}}{}_a, \quad \delta_{a'b'} * E_{\mathrm{A}}{}^{a'} \cdot \delta B^{b'} = \delta B^{a'} \rfloor E^{\mathrm{B}}{}_{a'}. \tag{5.12}$$

Here the hook $\rfloor$ denotes interior product of a vector field with a covector field on $\mathcal{S}$. Associated to $\mathcal{S}$ is the jet space defined using local coordinates

$$J^{(\infty)}(\mathcal{S}) = (x, A^a, B^{a'}, dA^a, dB^{a'}, d*dA^a, d*dB^{a'}, \ldots), \tag{5.13}$$

where x represents a point in M; A^a, dA^a, $d*dA^a, \ldots$, represent the values of the $\mathcal{A}$-valued one-form field $A^a(x)$ and its exterior derivatives at x; and $B^{a'}$, $dB^{a'}$, $d*dB^{a'}, \ldots$, represent the values of the $\mathcal{A}'$-valued two-form field $B^{a'}(x)$ and its exterior derivatives at x. In this setting, a locally constructed function or p-form on M is a function purely of the jet variables $(A^a, B^{a'}, dA^a, dB^{a'}, d*dA^a, d*dB^{a'}, \ldots)$ and their Hodge duals $(*A^a, *B^{a'}, *dA^a, *dB^{a'}, *d*dA^a, *d*dB^{a'}, \ldots)$, up to some finite order. Let ∂_{A^a}, $\partial_{B^{a'}}$, and $\partial_{(d*)^k dA^a}$, $\partial_{(d*)^k dB^{a'}}$, $k=0,1,2,\ldots$, denote derivatives with respect to the jet variables. Note the derivatives ∂_{A^a}, $\partial_{B^{a'}}$

produce covector fields on $\mathcal{S}$. We define contravariant derivatives $\partial^{\flat}_{A^a}$, $\partial^{\flat}_{B^{a'}}$ that produce vector fields on $\mathcal{S}$ via the natural pairing $\partial^{\flat}_{A^a} g \rfloor \partial_{A^a} f = \delta^{ab} \partial_{A^a} g \cdot \partial_{A^b} f$ and $\partial^{\flat}_{B^{a'}} g \rfloor \partial_{B^{a'}} f = \delta^{a'b'} \partial^{\flat}_{B^{a'}} g \cdot \partial_{B^{b'}} f$, for any locally constructed functions f, g. Likewise we define $\partial^{\flat}_{(d*)^k\, dA^a}$, $\partial^{\flat}_{(d*)^k\, dB^{a'}}$. Then, we introduce Euler–Lagrange operators given by

$$E^{\flat}_{A^a} = \partial^{\flat}_{A^a} - \sum_{k\geqslant 0} (*d*)^{k+1} \partial^{\flat}_{(d*)^k\, dA^a}, \quad E^{\flat}_{B^{a'}} = \partial^{\flat}_{B^{a'}} - \sum_{k\geqslant 0} (*d*)^{k+1} \partial^{\flat}_{(d*)^k\, dB^{a'}}. \tag{5.14}$$

These operators take locally constructed functions f into vector fields $(E^{\flat}_{A^a}(f), E^{\flat}_{B^{a'}}(f))$ on $\mathcal{S}$ and have the property that $E^{\flat}_{A^a}(f) = E^{\flat}_{B^{a'}}(f) = 0$ annihilates a locally constructed function f if and only if $*f = d\Gamma$ for some locally constructed three-form Γ. The related operators

$$E^{\sharp}_{A^a} = \partial_{A^a} - \sum_{k\geqslant 0} (*d*)^{\sharp k+1} \partial_{(d*)^k\, dA^a}, \quad E^{\sharp}_{B^{a'}} = \partial_{B^{a'}} - \sum_{k\geqslant 0} (*d*)^{\sharp k+1} \partial_{(d*)^k\, dB^{a'}} \tag{5.15}$$

yield covector fields on $\mathcal{S}$, where $*^{\sharp}$ and $d^{\sharp}$ denote the contravariant Hodge dual operator and contravariant exterior derivative operator on vectors and antisymmetric tensors on M.

The relation between the deformation terms in the field equations and Lagrangian is most naturally expressed through the Euler–Lagrange operators by

$$\overset{(k)}{E}{}^{\mathrm{A}}{}_a = E^{\sharp}_{A^a}(*\overset{(k+1)}{L}), \quad \overset{(k)}{E}{}^{\mathrm{B}}{}_{a'} = E^{\sharp}_{B^{a'}}(*\overset{(k+1)}{L}), \tag{5.16}$$

which determines

$$\overset{(k+1)}{L} = -\frac{1}{k+1}(\overset{(k)}{E}{}_{\mathrm{A}}{}^a A^b \delta_{ab} - \overset{(k)}{E}{}_{\mathrm{B}}{}^{a'} B^{b'} \delta_{a'b'}) \tag{5.17}$$

to within an exact four-form.

In terms of the Euler–Lagrange operators, the condition for existence of a gauge-invariant Lagrangian is equivalent to the equations

$$E^{\flat}_{A^a}(\delta_\xi A^a \cdot *E_{\mathrm{A}}{}^b \delta_{ab} + \delta_\xi B^{a'} \cdot *E_{\mathrm{B}}{}^{b'} \delta_{a'b'}) = 0, \tag{5.18}$$

$$E^{\flat}_{A^a}(\delta_\chi A^a \cdot *E_{\mathrm{A}}{}^b \delta_{ab} + \delta_\chi B^{a'} \cdot *E_{\mathrm{B}}{}^{b'} \delta_{a'b'}) = 0, \tag{5.19}$$

$$E^{\flat}_{B^{a'}}(\delta_\xi A^a \cdot *E_{\mathrm{A}}{}^b \delta_{ab} + \delta_\xi B^{a'} \cdot *E_{\mathrm{B}}{}^{b'} \delta_{a'b'}) = 0, \tag{5.20}$$

$$E^{\flat}_{B^{a'}}(\delta_\chi A^a \cdot *E_{\mathrm{A}}{}^b \delta_{ab} + \delta_\chi B^{a'} \cdot *E_{\mathrm{B}}{}^{b'} \delta_{a'b'}) = 0. \tag{5.21}$$

These four equations are the determining system for all allowed deformations.

Remark: To proceed, we restrict attention to deformations that involve at most one derivative of A^a, $B^{a'}$, ξ^a, $\chi^{a'}$ in the gauge symmetries and at most two derivatives of A^a, $B^{a'}$ in the field equations. Such deformations automatically preserve the number of gauge degrees of freedom and initial-data degrees of freedom in the nonlinear theory to be the same as those in the linear theory. Also, we consider only nontrivial deformations such that the field equations and gauge symmetries in the nonlinear theory are not equivalent to those in the linear theory by a change either of field variables or of gauge symmetry variables (see Ref. 3).

The determining system can be reformulated more usefully and geometrically as Lie derivative equations. We introduce the Lie derivative $\mathcal{L}_\delta$ with respect to a vector field $(\delta A^a, \delta B^{a'})$ on $\mathcal{S}$ acting on a locally constructed covector field $(f^{\mathrm{A}}_a, f^{\mathrm{B}}_{a'})$ by

$$(\mathcal{L}_\delta f)^{\mathrm{A}}_a = \left(\delta A^b \rfloor \partial_{A^b} f^{\mathrm{A}}_a + \delta B^{b'} \rfloor \partial_{B^{b'}} f^{\mathrm{A}}_a + \sum_{k\geqslant 0} (d*)^k\, d\,\delta A^b \rfloor \partial_{(d*)^k\, dA^b} f^{\mathrm{A}}_a + (d*)^k\, d\,\delta B^{b'} \rfloor \partial_{(d*)^k\, dB^{b'}} f^{\mathrm{A}}_a \right)$$
$$- \left(\partial_{A^a} \delta A^b \rfloor f^{\mathrm{A}}_b + \partial_{A^a} \delta B^{b'} \rfloor f^{\mathrm{B}}_{b'} - \sum_{k\geqslant 0} (*d*)^{\sharp k+1} (\partial_{(d*)^k\, dA^a} \delta A^b \rfloor f^{\mathrm{A}}_b + \partial_{(d*)^k\, dA^a} \delta B^{b'} \rfloor f^{\mathrm{B}}_{b'}) \right), \tag{5.22}$$

$$(\mathcal{L}_\delta f)^{\mathrm{B}}_{a'} = \left(\delta A^b \rfloor \partial_{A^b} f^{\mathrm{B}}_{a'} + \delta B^{b'} \rfloor \partial_{B^{b'}} f^{\mathrm{B}}_{a'} + \sum_{k\geqslant 0} (d*)^k\, d\,\delta A^b \rfloor \partial_{(d*)^k\, dA^b} f^{\mathrm{B}}_{a'} + (d*)^k\, d\,\delta B^{b'} \rfloor \partial_{(d*)^k\, dB^{b'}} f^{\mathrm{B}}_{a'} \right)$$
$$- \left(\partial_{B^{a'}} \delta A^b \rfloor f^{\mathrm{A}}_b + \partial_{B^{a'}} \delta B^{b'} \rfloor f^{\mathrm{B}}_{b'} - \sum_{k\geqslant 0} (*d*)^{\sharp k+1} (\partial_{dB^{a'}} \delta A^b \rfloor f^{\mathrm{A}}_b + \partial_{dB^{a'}} \delta B^{b'} \rfloor f^{\mathrm{B}}_{b'}) \right). \tag{5.23}$$

Theorem 1: *Local gauge invariance holds if and only if the Lie derivative of the field equations with respect to the gauge symmetries vanishes*

$$\mathcal{L}_{\delta_\xi}(E^{\mathrm{A}}{}_a, E^{\mathrm{B}}{}_{a'}) = 0, \quad \mathcal{L}_{\delta_\chi}(E^{\mathrm{A}}{}_a, E^{\mathrm{B}}{}_{a'}) = 0. \tag{5.24}$$

Geometrically, these equations assert that the gauge symmetries are vector fields tangential to the surface in $\mathcal{S}$ corresponding to the field equations. Due to gauge invariance, the commutators of these vector fields have the same property.

Theorem 2: *Local gauge invariance holds only if the Lie derivative of the field equations with respect to the gauge symmetry commutators vanishes*

$$\mathcal{L}_{[\delta_{\xi_1}, \delta_{\xi_2}]}(E^{\mathrm{A}}{}_a, E^{\mathrm{B}}{}_{a'}) = 0, \quad \mathcal{L}_{[\delta_{\chi_1}, \delta_{\chi_2}]}(E^{\mathrm{A}}{}_a, E^{\mathrm{B}}{}_{a'}) = 0, \quad \mathcal{L}_{[\delta_{\xi_1}, \delta_{\chi_1}]}(E^{\mathrm{A}}{}_a, E^{\mathrm{B}}{}_{a'}) = 0. \tag{5.25}$$

An expansion of these equations in powers of A^a and $B^{a'}$ (and their derivatives) gives a hierarchy of determining equations whose solutions yield all allowed deformation terms in the field equations and gauge symmetries. We now find the solution of these determining equations explicitly at the lowest orders to give all first-order deformations and then outline an induction analysis to obtain a uniqueness result for the higher-order deformations.

C. First-order deformations and uniqueness of higher-order deformations

Up to a change of field variables and gauge symmetry variables, the most general possible first-order deformation terms for the gauge symmetries are given by

$$\overset{(1)}{\delta}_\xi A^a = a^a{}_{bc} A^b \xi^c + b^a{}_{b'c} * H^{b'} \xi^c + c^a{}_{b'c} * (B^{b'}\, d\xi^c) + \tilde{c}^a{}_{b'c} * (*B^{b'}\, d\xi^c), \tag{5.26}$$

$$\overset{(1)}{\delta}_\xi B^{a'} = d^{a'}{}_{b'c} B^{b'}\, \xi^c + \tilde{d}^{a'}{}_{b'c} * B^{b'}\, \xi^c + e^{a'}{}_{bc} F^b \xi^c + \tilde{e}^{a'}{}_{bc} * F^b \xi^c + f^{a'}{}_{bc} * (A^b\, d\xi^c), \tag{5.27}$$

with

$$e^{a'}{}_{[bc]} = f^{a'}{}_{[bc]} = 0, \tag{5.28}$$

and by

$$\overset{(1)}{\delta}_\chi A^a = g^a{}_{b'c'} * (B^{b'}\chi^{c'}) + \tilde{g}^a{}_{b'c'} * (*B^{b'}\chi^{c'}) + h^a{}_{bc'} * (F^b\chi^{c'}) + \tilde{h}^a{}_{bc'} * (*F^b\chi^{c'}) + i^a{}_{bc'} A^b * d * \chi^{c'} + \tilde{i}^a{}_{bc'} (*d*A^b)\chi^{c'}, \tag{5.29}$$

$$\overset{(1)}{\delta}_\chi B^{a'} = j^{a'}{}_{bc'} A^b \chi^{c'} + \tilde{j}^{a'}{}_{bc'} * (A^b\chi^{c'}) + k^{a'}{}_{b'c'} * H^{b'}\chi^{c'} + \tilde{k}^{a'}{}_{b'c'} * (*H^{b'}\chi^{c'}) + l^{a'}{}_{b'c'} * d * (B^{b'}\chi^{c'}) + \tilde{l}^{a'}{}_{b'c'} * d * (*B^{b'}\chi^{c'}) + m^{a'}{}_{bc'} B^{b'} * d * \chi^{c'} + \tilde{m}^{a'}{}_{bc'} * B^{b'} * d * \chi^{c'}, \tag{5.30}$$

where the coefficients are constants, which represent the components of bilinear maps from $\mathcal{A}\times\mathcal{A}$, $\mathcal{A}\times\mathcal{A}'$, $\mathcal{A}'\times\mathcal{A}$, $\mathcal{A}'\times\mathcal{A}'$ into $\mathcal{A}$ and $\mathcal{A}'$. These coefficients are determined by solving the zeroth-order part of the Lie derivative commutator equation from Theorem 2 (using the methods of Refs. 3 and 12). This yields the linear algebraic relations

$$a_{a(bc)} = 0, \quad f_{a'(bc)} = 0, \tag{5.31}$$

$$l_{a'b'c'} = \tilde{l}_{a'b'c'} = m_{a'b'c'} = \tilde{m}_{a'b'c'} = 0, \quad g_{ab'c'} = \tilde{g}_{ab'c'} = 0, \tag{5.32}$$

$$c_{ab'c} = \tilde{c}_{ab'c} = 0, \quad \tilde{j}_{a'bc'} = \tilde{d}_{a'cb'} = 0, \quad d_{a'b'c} + j_{a'cb'} = 0. \tag{5.33}$$

Additional linear algebraic relations arise from the first-order part of the Lie derivative equation from Theorem 1 applied to the rigid symmetries

$$(\delta_\xi)_{\text{rigid}} = \delta_\xi|_{d\xi=0}, \quad (\delta_\chi)_{\text{rigid}} = \delta_\chi|_{d\chi=0} \tag{5.34}$$

given by restricting the gauge symmetry variables so that $d\xi^a = d\chi^{a'} = 0$. This leads to (by the methods of Refs. 3 and 12)

$$\tilde{e}_{a'bc} + b_{ba'c} = 0, \tag{5.35}$$

$$m_a{}^{a'} j_{a'cb'} - m_{b'}{}^b a_{bac} = 0, \quad a_{(ab)c} - m_{(b}{}^{b'} b_{a)b'c} = 0, \quad j_{(a'|c|b')} - m_{(a'}{}^a b_{|a|b')c} = 0, \tag{5.36}$$

$$k_{(a'b')e'} = 0, \quad m_a{}^{a'} k_{a'b'c'} + j_{b'ac'} = 0, \tag{5.37}$$

$$h_{abc'} = \tilde{h}_{abc'} = 0, \quad \tilde{k}_{a'b'c'} = 0. \tag{5.38}$$

Then, we return to the first-order part of the Lie derivative equation with ξ^a and $\chi^{a'}$ now taken to be arbitrary, which determines the first-order deformation terms in the field equations (by the methods of Ref. 1). This yields

$$\overset{(2)}{*E}{}_A{}^a = d * (\tfrac{1}{2} a^a{}_{bc} A^b A^c + b^a{}_{b'c} * H^{b'} A^c) - a_{cb}{}^a A^b * F^c - b_{cb'}{}^a * H^{b'} F^c + (2F^b * H^{c'} - A^b d * H^{c'}) e^{a'}{}_{bc} + j_{b'}{}^a{}_{c'} * H^{b'} B^{c'} - m_{c'}{}^c a_{cb}{}^a A^b B^{c'}, \tag{5.39}$$

$$\overset{(2)}{E}{}_B{}^{a'} = d * (j^{a'}{}_{bc'} A^b B^{c'} - k^{a'}{}_{b'c'} * H^{b'} B^{c'} + b_b{}^{a'}{}_c * F^b A^c) + \tfrac{1}{2} k_{b'c'}{}^{a'} * H^{b'} * H^{c'} - d(A^b * F^c) e^{a'}{}_{bc} - j_{c'b}{}^{a'} A^b * H^{c'} + m_a{}^{a'} a^a{}_{bc} A^b A^c, \tag{5.40}$$

together with the linear algebraic relation

$$m_{(a|}{}^{a'} e_{a'b|c)} + m_b{}^{b'} e_{b'ac} = 0. \tag{5.41}$$

The corresponding Lagrangian is given by

$$\overset{(3)}{L} = \tfrac{1}{2} a_{abc} * F^a A^b A^c + j_{a'bc'} * H^{a'} A^b B^{c'} + b_{ab'c} * F^a * H^{b'} A^c - \tfrac{1}{2} k_{a'b'c'} * H^{a'} * H^{b'} B^{c'}$$
$$- e_{a'bc} * H^{a'} F^b A^c + \tfrac{1}{2} m_{aa'} a^a{}_{bc} B^{a'} A^b A^c. \tag{5.42}$$

These deformation terms are related to the deformation terms in the gauge symmetries (as follows from general results in Ref. 3) by being the Noether currents of the rigid symmetries associated to the first-order deformed gauge symmetries

$$\overset{(1)}{\delta}_\xi A^a = a^a{}_{bc} A^b \xi^c + b^a{}_{b'c} * H^{b'} \xi^c, \tag{5.43}$$

$$\overset{(1)}{\delta}_\xi B^{a'} = - j^{a'}{}_{cb'} B^{b'} \xi^c - b_b{}^{a'}{}_c * F^b \xi^c + e^{a'}{}_{bc} F^b \xi^c, \tag{5.44}$$

$$\overset{(1)}{\delta}_\chi A^a = 0, \tag{5.45}$$

$$\overset{(1)}{\delta}_\chi B^{a'} = j^{a'}{}_{bc'} A^b \chi^{c'} + k^{a'}{}_{b'c'} * H^{b'} \chi^{c'}. \tag{5.46}$$

In particular, we have $*d(\overset{(2)}{E}{}_{\rm A}{}^a \xi^b \delta_{ab}) = (\overset{(1)}{\delta}_\xi A^a)_{\rm rigid} \rfloor \overset{(1)}{E}{}^{\rm A}{}_a$ and $*d(\overset{(2)}{E}{}_{\rm B}{}^{a'} \chi^{b'} \delta_{a'b'}) = (\overset{(1)}{\delta}_\xi B^{a'})_{\rm rigid} \rfloor \overset{(1)}{E}{}^{\rm B}{}_{a'}$, where $d\xi^b = d\chi^{b'} = 0$.

We next note that, from (5.43) to (5.46),

$$[\overset{(0)}{\delta}_{\xi_1}, \delta_{\xi_2}] = \overset{(0)}{\delta}_{\xi_3}, \quad \xi_3{}^a = a^a{}_{bc} \xi_1{}^b \xi_2{}^c, \tag{5.47}$$

$$[\overset{(0)}{\delta}_{\chi_1}, \delta_{\chi_2}] = 0, \tag{5.48}$$

$$[\overset{(0)}{\delta}_{\xi_1}, \delta_{\chi_2}] = \overset{(0)}{\delta}_{\chi_3}, \quad \chi_3{}^{a'} = j^{a'}{}_{bc'} \xi_1{}^b \chi_2{}^{c'}. \tag{5.49}$$

Now we consider the first-order part of the Lie derivative commutator equation from Theorem 2 and subtract the first-order part of the Lie derivative equation from Theorem 1 with the gauge symmetry variables given by the commutators (5.47)–(5.49). This combined equation leads to the result (by the methods of Refs. 3 and 12) that the gauge symmetry commutators are closed to first-order when $A^a, B^{a'}$ satisfy the linear field equations $\overset{(1)}{E}{}_{\rm A}{}^a = 0$ and $\overset{(1)}{E}{}_{\rm B}{}^{a'} = 0$. Then if the gauge symmetry variables are taken to be rigid, $d\xi_1{}^a = d\xi_2{}^a = 0$ and $d\chi_1{}^{a'} = d\chi_2{}^{a'} = 0$, we obtain an integrability condition involving just the first-order deformation terms,

$$([\overset{(1)}{\delta}_{\xi_1}, \overset{(1)}{\delta}_{\xi_2}])_{\rm rigid} A^a - (\overset{(1)}{\delta}_{\xi_3})_{\rm rigid} A^a = d\, \overset{(1)}{\xi}{}^a_{(\xi_1,\xi_2)}, \quad ([\overset{(1)}{\delta}_{\xi_1}, \overset{(1)}{\delta}_{\xi_2}])_{\rm rigid} B^{a'} - (\overset{(1)}{\delta}_{\xi_3})_{\rm rigid} B^{a'} = d\, \overset{(1)}{\chi}{}^{a'}_{(\xi_1,\xi_2)}, \tag{5.50}$$

$$([\overset{(1)}{\delta}_{\chi_1}, \overset{(1)}{\delta}_{\chi_2}])_{\rm rigid} A^a = d\, \overset{(1)}{\xi}{}^a_{(\chi_1,\chi_2)}, \quad ([\overset{(1)}{\delta}_{\chi_1}, \overset{(1)}{\delta}_{\chi_2}])_{\rm rigid} B^{a'} = d\, \overset{(1)}{\chi}{}^{a'}_{(\chi_1,\chi_2)}, \tag{5.51}$$

$$([\overset{(1)}{\delta}_{\xi_1}, \overset{(1)}{\delta}_{\chi_2}])_{\rm rigid} A^a - (\overset{(1)}{\delta}_{\chi_3})_{\rm rigid} A^a = d\, \overset{(1)}{\xi}{}^a_{(\xi_1,\chi_2)}, \quad ([\overset{(1)}{\delta}_{\xi_1}, \overset{(1)}{\delta}_{\chi_2}])_{\rm rigid} B^{a'} - (\overset{(1)}{\delta}_{\chi_3})_{\rm rigid} B^{a'} = d\, \overset{(1)}{\chi}{}^{a'}_{(\xi_1,\chi_2)}, \tag{5.52}$$

which hold for some locally constructed $\mathcal{A}$-valued functions $\overset{(1)}{\xi}{}^{a}_{(\cdot,\cdot)}$ and $\mathcal{A}'$-valued one-forms $\overset{(1)}{\chi}{}^{a'}_{(\cdot,\cdot)}$ depending linearly on $\xi_1{}^a, \xi_2{}^a, \chi_1{}^{a'}, \chi_2{}^{a'}$. The solution of these six equations (using the methods of Ref. 12) yields the quadratic algebraic relations

$$a_{adb}a^{b}{}_{ec} - 2a_{ab[c|}a^{b}{}_{d|e]} = 0, \tag{5.53}$$

$$2a_{ab[c}b^{b}{}_{|d'|e]} - b_{ad'b}a^{b}{}_{ec} + 2b_{ab'[c|}b^{db'}{}_{|e]}m_{d'd} - 2b_{ab'[c|}j^{b'}{}_{|e]d'} = 0, \tag{5.54}$$

$$j_{a'be'}a^{b}{}_{dc} - 2j_{a'[d|b'}j^{b'}{}_{|c]e'} = 0, \tag{5.55}$$

plus three others that are redundant as a consequence of (5.36) and (5.37).

Another integrability condition arises for the first-order deformation terms if we consider the second-order part of the Lie derivative equation from Theorem 1 under the previous conditions imposed on $A^a, B^{a'}, \xi^a, \chi^{a'}$. Contracting this equation with $(A^a, B^{a'})$, we obtain

$$(\overset{(1)}{\delta}{}_{\xi})_{\text{rigid}}A^{a}\rfloor\overset{(2)}{E}{}^{\mathrm{A}}{}_{a} + (\overset{(1)}{\delta}{}_{\xi})_{\text{rigid}}B^{a'}\rfloor\overset{(2)}{E}{}^{\mathrm{B}}{}_{a'} = d\overset{(3)}{\Theta}{}_{\xi}, \tag{5.56}$$

$$(\overset{(1)}{\delta}{}_{\chi})_{\text{rigid}}A^{a}\rfloor\overset{(2)}{E}{}^{\mathrm{A}}{}_{a} + (\overset{(1)}{\delta}{}_{\chi})_{\text{rigid}}B^{a'}\rfloor\overset{(2)}{E}{}^{\mathrm{B}}{}_{a'} = d\overset{(3)}{\Theta}{}_{\chi}, \tag{5.57}$$

holding for some locally constructed three-forms $\Theta_{(3)\xi}, \Theta_{(3)\chi}$ which depend linearly on $\xi^a, \chi^{a'}$. The solution of these two equations (again using the methods of Ref. 12) yields the additional quadratic algebraic relations

$$k_{[a'b'|c'}k^{c'}{}_{|d']e'} = 0, \tag{5.58}$$

$$b_{ab'c}k_{d'e'}{}^{b'} - 2b_{a[d'|b}b^{b}{}_{|e']c} = 0, \tag{5.59}$$

$$2e_{a'(b|c}a^{c}{}_{|d)e} - e_{c'bd}j^{c'}{}_{ea'} - 2e_{a'c(d}m_{b)b'}b^{cb'}{}_{e} = 0, \tag{5.60}$$

plus others that reduce to combinations of (5.53) to (5.55) through (5.36) and (5.37). Moreover, the quadratic relation (5.55) itself is a consequence of (5.58) and (5.37).

It can be shown that the integrability relations (5.53)–(5.55) are necessary and sufficient to allow solving for the second order deformation terms in the gauge symmetries from the first-order part of the Lie derivative commutator equation in Theorem 2. The additional integrability relations (5.58)–(5.60) are necessary in then solving the second-order part of the Lie derivative equation from Theorem 1 for the second order deformation terms in the field equations. However, it is found that a solution exists if and only if the following additional algebraic relation holds on the coefficients of the field equation deformation terms,

$$k_{d'e'}{}^{c'}e_{c'ab} - 2e_{[d'|ca}b^{c}{}_{|e']b} - 2e_{[d'|cb}b^{c}{}_{|e']a} = 0. \tag{5.61}$$

This relation imposes in effect a further integrability relation on allowed first-order deformations.

Theorem 3: *Up to a change of field variables and gauge symmetry variables, all first-order geometrical deformations are given by Eqs. (5.43)–(5.46), Eqs. (5.39) and (5.40), with the coefficients satisfying the linear relations (5.36) and (5.37) and the quadratic relations (5.53)–(5.55) and (5.58)–(5.61). There are no further algebraic obstructions to the existence of second-order geometrical deformations.*

These first-order deformations have the following classification: the a_{abc} terms represent a massless Yang–Mills self-coupling of A^a, the $k_{a'b'c'}$ terms represent a massless Freedman–Townsend self-coupling of $B^{a'}$, and the $b_{ab'c}$ terms represent an extended Freedman–Townsend coupling between A^a and $B^{a'}$, while the $j_{a'bc'}$ terms represent a Higgs-type coupling of $B^{a'}$ to A^a

which is nontrivial only when the mass tensor $m_{aa'}$ is nonzero. The $e_{a'bc}$ terms, in contrast, represent a different type of coupling between A^a and $B^{a'}$ unrelated to Yang–Mills and Freedman–Townsend type couplings. It is similar in form to the coupling known for one-form and two-form fields in extended supergravity theory.[13,14] Moreover, the deformation corresponding to the $e_{a'bc}$ terms is characterized by possessing opposite parity compared to the parity of the other deformation terms. In particular, consider the parity operator $\mathcal{P}$ defined by $d\mathcal{P}=\mathcal{P}d$, $*\mathcal{P}=-\mathcal{P}*$. If we assign even parity to A^a and odd parity to $B^{a'}$,

$$\mathcal{P}A^a=A^a, \quad \mathcal{P}B^{a'}=-B^{a'}, \tag{5.62}$$

which thus determines

$$\mathcal{P}*F^a=-F^a, \quad \mathcal{P}*H^{a'}=H^{a'}, \tag{5.63}$$

and

$$\mathcal{P}\xi^a=\xi^a, \quad \mathcal{P}\chi^{a'}=-\chi^{a'}, \tag{5.64}$$

then it follows that all the deformation terms except for the $e_{a'bc}$ terms have even parity.

To proceed, we now consider the uniqueness of the higher-order deformation terms determined by the first-order terms in Theorem 3. Let $\Delta\overset{(k+1)}{E}_{\mathrm{A}}{}^a$, $\Delta\overset{(k+1)}{E}_{\mathrm{B}}{}^{a'}$, $\Delta\overset{(k)}{\delta}_\xi A^a$, $\Delta\overset{(k)}{\delta}_\chi A^a$, $\Delta\overset{(k)}{\delta}_\xi B^{a'}$, $\Delta\overset{(k)}{\delta}_\chi B^{a'}$ denote the difference of any two deformations that agree up to some given order $k\geqslant 1$. Then the $k+1$st-order part of the Lie derivative equation from Theorem 1 yields

$$\overset{(0)}{\delta}_\xi\Delta\overset{(k+2)}{E}_{\mathrm{A}}{}^a=\overset{(0)}{\delta}_\chi\Delta\overset{(k+2)}{E}_{\mathrm{A}}{}^a=0, \quad \overset{(0)}{\delta}_\xi\Delta\overset{(k+2)}{E}_{\mathrm{B}}{}^{a'}=\overset{(0)}{\delta}_\chi\Delta\overset{(k+2)}{E}_{\mathrm{B}}{}^{a'}=0. \tag{5.65}$$

Similarly, the kth order part of the Lie derivative commutator equation from Theorem 2 yields the result that, after a change of field variables and gauge symmetry variables,

$$\overset{(0)}{\delta}_{\xi_2}\Delta\overset{(k+1)}{\delta}_{\xi_1}A^a=\overset{(0)}{\delta}_{\chi_2}\Delta\overset{(k+1)}{\delta}_{\xi_1}A^a=0, \quad \overset{(0)}{\delta}_{\xi_2}\Delta\overset{(k+1)}{\delta}_{\chi_1}A^a=\overset{(0)}{\delta}_{\chi_2}\Delta\overset{(k+1)}{\delta}_{\chi_1}A^a=0, \tag{5.66}$$

$$\overset{(0)}{\delta}_{\xi_2}\Delta\overset{(k+1)}{\delta}_{\xi_1}B^{a'}=\overset{(0)}{\delta}_{\chi_2}\Delta\overset{(k+1)}{\delta}_{\xi_1}B^{a'}=0, \quad \overset{(0)}{\delta}_{\xi_2}\Delta\overset{(k+1)}{\delta}_{\chi_1}B^{a'}=\overset{(0)}{\delta}_{\chi_2}\Delta\overset{(k+1)}{\delta}_{\chi_1}B^{a'}=0. \tag{5.67}$$

Under the assumptions on the number of derivatives considered for possible deformation terms (see Remark in Sec. V B), the solution of Eqs. (5.65)–(5.67) is immediately given by

$$\Delta\overset{(k+2)}{E}_{\mathrm{A}}{}^a=0, \quad \Delta\overset{(k+2)}{E}_{\mathrm{B}}{}^{a'}=0, \quad k\geqslant 1, \tag{5.68}$$

$$\Delta\overset{(k+1)}{\delta}_\xi A^a=\Delta\overset{(k+1)}{\delta}_\chi A^a=0, \quad \Delta\overset{(k+1)}{\delta}_\xi B^{a'}=\Delta\overset{(k+1)}{\delta}_\chi B^{a'}=0, \quad k\geqslant 1. \tag{5.69}$$

Hence, we have established the following uniqueness result.

Theorem 4: *If two deformations agree at all orders* $1\leqslant l\leqslant k$, $\Delta\overset{(l+1)}{E}_{\mathrm{A}}{}^a=\Delta\overset{(l+1)}{E}_{\mathrm{B}}{}^{a'}=0$, $\Delta\overset{(l)}{\delta}_\xi A^a=\Delta\overset{(l)}{\delta}_\chi A^a=0$, $\Delta\overset{(l)}{\delta}_\xi B^{a'}=\Delta\overset{(l)}{\delta}_\chi B^{a'}=0$, *then up to a change of field variables and gauge symmetry variables, the deformations also agree at order* $l=k+1$.

D. Deformations to all orders

Hereafter we restrict attention to parity-invariant and opposite-parity deformations separately and proceed to write down a complete deformation to all orders in each case. A full discussion of the combined parity non-invariant deformations from Theorem 3 is given in Ref. 15.

For a deformation determined at first-order purely by the $e_{a'bc}$ terms, note that the linear algebraic relations (5.28) and (5.41) imply

$$m_{a'}{}^{a}e^{a'}{}_{bc}=0 \tag{5.70}$$

and hence the $e_{a'bc}$ terms are incompatible with a nonzero mass tensor. However, in the massless case, the $e_{a'bc}$ terms produce a nontrivial deformation, which we now write down to all orders.

The algebraic structure on $\mathcal{A},\mathcal{A}'$ associated to $e^{a'}{}_{bc}$ consists of a symmetric product from $\mathcal{A}\times\mathcal{A}$ into $\mathcal{A}'$. Then the gauge symmetries are given by

$$\delta_\xi A^a=d\xi^a,\quad \delta_\xi B^{a'}=e^{a'}{}_{bc}F^b\xi^c, \tag{5.71}$$

$$\delta_\chi A^a=0,\quad \delta_\chi B^{a'}=d\chi^{a'}, \tag{5.72}$$

while the Lagrangian is constructed by

$$L=\tfrac{1}{2}F^a{*}F^b\delta_{ab}-\tfrac{1}{2}H^{a'}{*}H^{b'}\delta_{a'b'}-{*}H^{a'}F^bA^ce_{a'bc}+\tfrac{1}{2}F^bA^c{*}(F^dA^e)e^{a'}{}_{bc}e_{a'de}. \tag{5.73}$$

It is straightforward to see that this Lagrangian is gauge invariant, $\delta_\xi L=\delta_\chi L=0$, and that the gauge symmetries commute, $[\delta_{\xi_1},\delta_{\xi_2}]=[\delta_{\chi_1},\delta_{\chi_2}]=[\delta_{\xi_1},\delta_{\chi_2}]=0$. From the Lagrangian, the field equations are given by

$$E_{\mathrm{A}}{}^{a}=d{*}F^a+(2F^b{*}H^{c'}-A^bd{*}H^{c'})e_{c'b}{}^{a}-(2F^b{*}(F^cA^d)+A^bd{*}(F^cA^d))e^{a'}{}_{cd}e_{a'b}{}^{a}=0, \tag{5.74}$$

$$E_{\mathrm{B}}{}^{a'}=d(*H^{a'}-{*}(F^bA^c))e^{a'}{}_{bc}=0. \tag{5.75}$$

Theorem 5: *The massless nonlinear theory (5.71)–(5.75) is the unique nonlinear geometrical deformation of the Abelian linear theory (5.1)–(5.5) determined by the first-order deformation terms* $e_{a'bc}$.

Next we consider a general deformation determined at first-order by all terms except $e_{a'bc}$. This deformation is more general than the massless/massive nonlinear theories constructed in Secs. II and III, since it includes a mixing of massless and massive fields $A^a,B^{a'}$, controlled by the eigenvalues of the mass tensor $m_{aa'}$.

Let $a^a{}_{bc},b^a{}_{b'c},j^{a'}{}_{bc'},k_{a'b'}{}^{c'}$ be the components of respective bilinear maps from $\mathcal{A}\times\mathcal{A}$ into $\mathcal{A}$, $\mathcal{A}'\times\mathcal{A}$ into $\mathcal{A}$, $\mathcal{A}\times\mathcal{A}'$ into $\mathcal{A}'$, $\mathcal{A}'\times\mathcal{A}'$ into $\mathcal{A}'$, fixed to satisfy the linear and quadratic relations (5.36) and (5.37), (5.53)–(5.55), (5.58), and (5.59). Thus, it follows that $a^a{}_{bc}$ and $k_{a'b'}{}^{c'}$ define the commutator structure constants (5.53) and (5.58) of respective Lie algebras on $\mathcal{A},\mathcal{A}'$, while $j^{a'}{}_{bc'}$ and $b^a{}_{b'c}$ define linear maps that are representations (5.55) and (5.59) of these Lie algebras on the vector spaces of $\mathcal{A}',\mathcal{A}$, respectively. Further discussion of the additional algebraic structure imposed by the relations (5.36), (5.37), (5.54) is given in the next section.

To write down the deformation to all orders, we first define a Yang–Mills field strength two-form and a related antisymmetric tensor field strength three-form by

$$F^a_A=dA^a+\tfrac{1}{2}a^a{}_{bc}A^bA^c,\quad H^{a'}_A=dB^{a'}+j^{a'}{}_{bc'}A^bB^{c'}. \tag{5.76}$$

Geometrically, F^a_A is the curvature of the connection one-form $a^a{}_{bc}A^b$, and $H^{a'}_A$ is the covariant curl of $B^{a'}$ in terms of the associated connection $j^{a'}{}_{bc'}A^b$. Consequently, using the covariant exterior derivative operators given by

$$D_A=d+a^a{}_{bc}A^b,\quad D'_A=d+j^{a'}{}_{bc'}A^b, \tag{5.77}$$

we have

$$D'_A B^{a'} = H_A^{a'}, \tag{5.78}$$

$$[D_A, D_A] = a^a{}_{bc} F_A^b, \quad [D'_A, D'_A] = j^{a'}{}_{bc'} F_A^b, \tag{5.79}$$

due to the algebraic structure (5.53) and (5.55). Next we define a nonlinear field strength two-form P^a and three-form Q^a by the equations

$$P^a - *Q^{b'} A^c b^a{}_{b'c} = F_A^a, \tag{5.80}$$

$$Q^{a'} - *P^b A^c b_b{}^{a'}{}_c - *Q^{b'} B^{c'} k^{a'}{}_{b'c'} = H_A^{a'}. \tag{5.81}$$

These field strengths are nonpolynomial expressions in terms of $A^a, B^{a'}$, as given by

$$(P^a, Q^{a'}) = Y^{-1}{}_{A,B}(F_A^a, H_B^{a'}), \tag{5.82}$$

where $Y^{-1}{}_{A,B}$ is the inverse of the linear map

$$Y_{A,B} = \begin{pmatrix} \mathrm{id} & A^b b^a{}_{c'b} * \\ -A^b b_c{}^{a'}{}_b * & \mathrm{id} - B^{b'} k^{a'}{}_{c'b'} * \end{pmatrix} \tag{5.83}$$

defined to act on the vector space of pairs of $\mathcal{A}$-valued two-forms, $\mathcal{A}'$-valued three-forms.

Now we write down the deformation, using the previous structure. The gauge symmetries on $A^a, B^{a'}$ are given by the field variations

$$\delta_\xi A^a = D_A \xi^a + b^a{}_{b'c} * Q^{b'} \xi^c, \tag{5.84}$$

$$\delta_\xi B^{a'} = -j^{a'}{}_{cb'} B^{b'} \xi^c - b_b{}^{a'}{}_{c} * P^b \xi^c, \tag{5.85}$$

$$\delta_\chi A^a = 0, \tag{5.86}$$

$$\delta_\chi B^{a'} = D'_A \chi^{a'} + k^{a'}{}_{b'c'} * Q^{b'} \chi^{c'}, \tag{5.87}$$

where ξ^a is an arbitrary $\mathcal{A}$-valued function, and $\chi^{a'}$ is an arbitrary $\mathcal{A}'$-valued one-form. The Lagrangian four-form for $A^a, B^{a'}$ is constructed by

$$L = \tfrac{1}{2} * P^a F_A^b \delta_{ab} + \tfrac{1}{2} * Q^{a'} H^{b'}{}_A \delta_{a'b'} + F_A^a B^{b'} m_{ab'}. \tag{5.88}$$

Gauge invariance of this Lagrangian is established as follows.

The variation of L under the gauge symmetry δ_ξ yields

$$\begin{aligned} \delta_\xi L = {} & m_{ab'} (D_A \delta_\xi A^a B^{b'} + F_A^a \delta_\xi B^{b'}) + *P^e (D_A \delta_\xi A^a + b^a{}_{b'c} * Q^{b'} \delta_\xi A^c) \delta_{ae} \\ & + *Q^{e'} (D'_A \delta_\xi B^{a'} + j^{a'}{}_{bc'} \delta_\xi A^b B^{c'} + \tfrac{1}{2} k^{a'}{}_{b'c'} * Q^{b'} \delta_\xi B^{c'}) \delta_{a'e'}. \end{aligned} \tag{5.89}$$

To proceed, collecting all terms $d\xi^c$ we obtain $-(*P^b b_{ba'c} + B^{b'} m_{bb'} b^b{}_{a'c}) * Q^{a'} d\xi^c$. Next we integrate by parts and use the field strength equations (5.76), (5.80), (5.81) to eliminate $dA^a, dB^{a'}$ algebraically in terms of $P^a, Q^{a'}, A^a, B^{a'}$. This yields terms of the type $P^a * P^b \xi^c$, $Q^{a'} * Q^{b'} \xi^c$, $*Q^{a'} * Q^{b'} * P^c \xi^d$, $*P^a * Q^{b'} A^c \xi^d$, $*Q^{a'} * Q^{b'} B^{c'} \xi^d$. Then we find that the coefficients of these terms vanish, respectively, due to the algebraic relations (5.36), (5.59), (5.54), (5.55). Hence, it follows that

$$\delta_\xi L = d((b_{ba'c} P^b + m_{bb'} b^b{}_{a'c} B^{b'}) * Q^{a'} \xi^c). \tag{5.90}$$

Similarly, under the gauge symmetry δ_χ, the variation of L is given by

$$\delta_\chi L = m_{ab'} F^a_A \delta_\chi B^{b'} + *Q^{e'}(D'_A \delta_\chi B^{a'} + \tfrac{1}{2} k^{a'}{}_{b'c'} * Q^{b'} \delta_\chi B^{c'})\delta_{a'e'}. \tag{5.91}$$

Proceeding as before, we find that all $d\chi^{c'}$ terms yield $(-\frac{1}{2} * Q^{a'} * Q^{b'} k_{a'b'c'} + F^a_A m_{ac'}) d\chi^{c'}$. An integration by parts and use of the field strength equations (5.76), (5.80), and (5.81) leaves terms of the type $*Q^{a'} P^b \chi^{c'}$, $*Q^{a'} * Q^{b'} * Q^{c'} \chi^{d'}$, $*Q^{a'} * Q^{b'} A^c \chi^{d'}$, $P^a A^b \chi^{c'}$, $A^a A^b * Q^{c'} \chi^{d'}$. Then we find that the coefficients of these terms vanish, respectively, due to the algebraic relations (5.37), (5.58), (5.55), (5.36). Hence, it follows that

$$\delta_\chi L = d((\tfrac{1}{2} k_{a'b'c'} * Q^{a'} * Q^{b'} + m_{ac'} F^a_A)\chi^{c'}. \tag{5.92}$$

Proposition: The Lagrangian (5.88) *is invariant to within an exact four-form (5.90) and (5.92) under the gauge symmetries (5.84)–(5.87).*

The field equations for $A^a, B^{a'}$ are given by

$$E_{\mathrm{A}}{}^a = D_A * P^a + (b^a{}_{c'b} m_c{}^{c'} A^b - b_{cb'}{}^a * Q^{b'}) * P^c + Q^{b'} m_{b'}{}^a = 0, \tag{5.93}$$

$$E_{\mathrm{B}}{}^{a'} = D'_A * Q^{a'} + \tfrac{1}{2} k_{b'c'}{}^{a'} * Q^{b'} * Q^{c'} - b_c{}^{a'}{}_b m_{c'}{}^c A^b * Q^{c'} + P^b m_b{}^{a'} = 0. \tag{5.94}$$

On solutions of these field equations, the gauge symmetries on $A^a, B^{a'}$ have the commutator structure

$$[\delta_{\xi_1}, \delta_{\xi_2}] = \delta_{\xi_3}, \quad [\delta_{\chi_1}, \delta_{\chi_2}] = 0, \quad [\delta_{\xi_1}, \delta_{\chi_2}] = \delta_{\chi_3}, \tag{5.95}$$

where

$$\xi_3{}^a = a^a{}_{bc} \xi_1{}^b \xi_2{}^c, \quad \chi_3{}^{a'} = j^{a'}{}_{bc'} \xi_1{}^b \chi_2{}^{c'}. \tag{5.96}$$

Off solutions, the commutator structure remains closed to within trivial symmetries proportional to the field equations

$$\delta_E A^a = 2 b^{ab'}{}_{[c|} b_{db'|e]} \xi_1{}^c \xi_2{}^e * E_{\mathrm{A}}{}^d - b^{ab'}{}_c k_{b'd'e'} \xi_1{}^c * (\chi_2{}^{e'} E_{\mathrm{B}}{}^{d'}), \tag{5.97}$$

$$\begin{aligned}\delta_E B^{a'} = {} & 2 b^{a'b}{}_{[c|} b_{bd'|e]} \xi_1{}^c \xi_2{}^e * E_{\mathrm{B}}{}^{d'} + k^{a'b'}{}_{e'} b_{db'c} \xi_1{}^c \chi_2{}^{e'} * E_{\mathrm{A}}{}^d - k^{a'b'}{}_{c'} k_{b'd'e'} \chi_1{}^{c'} * (\chi_2{}^{e'} E_{\mathrm{B}}{}^{d'}) \\ & + k^{a'b'}{}_{e'} k_{b'd'c'} \chi_2{}^{e'} * (\chi_1{}^{c'} E_{\mathrm{B}}{}^{d'}).\end{aligned} \tag{5.98}$$

Theorem 6: *The nonlinear theory (5.84)–(5.94) is the unique nonlinear geometrical deformation of the Abelian linear theory (5.1)–(5.5) determined by the first-order deformation terms* $a^a{}_{bc}, b^a{}_{b'c}, j^{a'}{}_{bc'}, k^{a'}{}_{b'c'}$.

We remark that the pure massless/massive SU(2) case of this theory, given by

$$a^a{}_{bc} = \epsilon_{bc}{}^a, \quad b^a{}_{b'c} = \lambda \epsilon_{b'c}{}^a, \quad j^{a'}{}_{bc'} = \epsilon_{bc'}{}^{a'}, \quad k^{a'}{}_{b'c'} = \lambda \epsilon_{b'c'}{}^{a'} \tag{5.99}$$

(where $a, a', \ldots = 1,2,3$) with $\lambda = 1/m$ and $m = \mathrm{const} \neq 0$ in the massive case, and $\lambda = \mathrm{const} \neq 0$ in the massless case, yields the SU(2) theories from Secs. II and III.

E. Algebraic structure in the nonlinear theory

Finally, we discuss the full algebraic structure on $\mathcal{A}, \mathcal{A}'$ underlying the nonlinear theory (5.84)–(5.94) given by the general parity-invariant deformation.

We start from the vector space decompositions $\mathcal{A} = \mathcal{A}_0 \oplus \mathcal{A}_m$ and $\mathcal{A}' = \mathcal{A}'_0 \oplus \mathcal{A}'_m$ into massless and massive subspaces defined by the mass tensor $m_{aa'}$. Let $\mathcal{P}_0, \mathcal{P}_m, \mathcal{P}'_0, \mathcal{P}'_m$ be the respective

projection operators onto these subspaces in $\mathcal{A},\mathcal{A}'$. Thus we have $m_{\mathcal{A}}(u_0)=m_{\mathcal{A}'}(v'_0)=0$ and $u'_{\rm m}=m_{\mathcal{A}}(u_m)\neq 0$, $v_m=m_{\mathcal{A}'}(v'_{\rm m})\neq 0$, with subscripts denoting subspace projections for all u,v in $\mathcal{A}$ and u',v' in $\mathcal{A}'$. Let $(u,v)_{\mathcal{A}}=u^a v^b \delta_{ab}$ and $(u',v')_{\mathcal{A}'}=u'^a v'^b \delta_{a'b'}$ denote the vector space inner products on $\mathcal{A},\mathcal{A}'$. We denote the Lie algebra multiplication $a^a{}_{bc}u^b v^c$ and $k_{b'c'}{}^{a'}u'^b v'^c$ on $\mathcal{A}$ and $\mathcal{A}'$ by the brackets $[u,v]_{\mathcal{A}}$ and $[u',v']_{\mathcal{A}'}$. In addition we denote the Lie algebra representations $j^{a'}{}_{bc'}u^b$ and $b^a{}_{b'c}u'^b$ by the linear maps $\rho'(u)$ and $\rho(u')$. Similarly, $ad_{\mathcal{A}}(u)$ and $ad_{\mathcal{A}'}(u')$ denote the adjoint representations given by $a^a{}_{bc}u^b$ and $k_{b'c'}{}^{a'}u'^b$ on $\mathcal{A}$ and $\mathcal{A}'$.

We begin by noting Eqs. (5.58) and (5.59) show that ρ' is a derivation of the Lie algebra $\mathcal{A}'$,

$$\rho'(w)[u',v']_{\mathcal{A}'}=[\rho'(w)u',v']_{\mathcal{A}'}+[u',\rho'(w)v']_{\mathcal{A}'}, \tag{5.100}$$

for all w in $\mathcal{A}$, $u'v'$ in $\mathcal{A}'$.

We now consider the additional algebraic structure imposed by the algebraic relations (5.36) and (5.37). To proceed, first note that, by Eq. (5.37),

$$\rho'(u_0)=0, \quad \rho'(u_m)=ad_{\mathcal{A}'}(m_{\mathcal{A}}(u_m)), \tag{5.101}$$

which completely determines ρ' in terms of the adjoint representation of $\mathcal{A}'$. Next, by Eq. (5.36), it follows that

$$m_{\mathcal{A}}([u,v]_{\mathcal{A}})=[m_{\mathcal{A}}(u),m_{\mathcal{A}}(v)]_{\mathcal{A}'}. \tag{5.102}$$

Hence, $\mathcal{A}'_m$ is a Lie subalgebra of $\mathcal{A}'$, and $\mathcal{A}_0$ is an invariant Lie subalgebra of $\mathcal{A}$, namely $[\mathcal{A}'_m,\mathcal{A}'_m]\subseteq\mathcal{A}'_m$, $[\mathcal{A},\mathcal{A}_0]\subseteq\mathcal{A}_0$. Furthermore, it also follows from Eq. (5.36) that

$$(u_0,[v_0,w]_{\mathcal{A}})_{\mathcal{A}}=-(v_0,[u_0,w]_{\mathcal{A}})_{\mathcal{A}} \tag{5.103}$$

and thus the inner product on $\mathcal{A}$ is an invariant metric with respect to the massless subspace $\mathcal{A}_0$. Consequently, since $\mathcal{A}_0$ is a Lie subalgebra, it must be a direct sum of an Abelian Lie algebra $\mathcal{A}_0^c$ and a semisimple Lie algebra $\mathcal{A}_0^s$. However, the inner product is not required to be invariant with respect to the whole Lie algebra $\mathcal{A}$, since

$$(u,[v,w]_{\mathcal{A}})_{\mathcal{A}}+(v,[u,w]_{\mathcal{A}})_{\mathcal{A}}=(u,\rho(m_{\mathcal{A}}(v))w)_{\mathcal{A}}+(v,\rho(m_{\mathcal{A}}(u))w)_{\mathcal{A}}, \tag{5.104}$$

which need not vanish for u,v in $\mathcal{A}_m$. Thus, surprisingly, $\mathcal{A}$ need not be semisimple unless its massive subspace $\mathcal{A}_m$ is empty. Moreover, the inner product on the Lie algebra $\mathcal{A}'$ likewise is not required to be invariant except on the massless subspace $\mathcal{A}'_0$,

$$(u'_0,[v'_0,w']_{\mathcal{A}'})_{\mathcal{A}'}=-(v'_0,[u'_0,w']_{\mathcal{A}'})_{\mathcal{A}'}, \tag{5.105}$$

since, by Eq. (5.37),

$$(u',[v',m_{\mathcal{A}}(w)]_{\mathcal{A}'})_{\mathcal{A}'}+(v',[u',m_{\mathcal{A}}(w)]_{\mathcal{A}'})_{\mathcal{A}'}=(u',m_{\mathcal{A}}(\rho(v')w))_{\mathcal{A}'}+(v',m_{\mathcal{A}}(\rho(u')w))_{\mathcal{A}'}, \tag{5.106}$$

which need not vanish for u',v' in $\mathcal{A}'_m$. Hence, as $\mathcal{A}'_m$ is a Lie subalgebra, it need not be semisimple and therefore, again, the whole Lie algebra $\mathcal{A}'$ is not required to be semisimple unless its massive subspace $\mathcal{A}'_m$ is empty.

Finally, we consider the remaining algebraic relation (5.54). This imposes further structure on the Lie algebras $\mathcal{A},\mathcal{A}'$, and on the representation ρ as follows. We first examine, separately, the pure massless case $m_{aa'}=0$ and pure massive case $m_{aa'}=m\delta_{aa'}$, $m\neq 0$.

In the massless case,

$$\mathcal{A}=\mathcal{A}_0, \quad \mathcal{A}'=\mathcal{A}'_0, \tag{5.107}$$

and so $\mathcal{A}$ and $\mathcal{A}'$ are each a direct sum of Abelian Lie algebras $\mathcal{A}^c,\mathcal{A}'^c$ and semisimple Lie algebras $\mathcal{A}^s,\mathcal{A}'^s$, respectively. Now, Eq. (5.54) reduces to

$$\rho(w')[u,v]_{\mathcal{A}}=[\rho(w')u,v]+[u,\rho(w')v], \tag{5.108}$$

which states that the linear map ρ is a derivation of the Lie algebra $\mathcal{A}'$. Since the quotient of $\mathcal{A}'$ by its center $\mathcal{A}'^c$ is semisimple, ρ must take the form

$$\rho(w')=ad_{\mathcal{A}}(h(w')) \tag{5.109}$$

for some linear map h from $\mathcal{A}'$ into $\mathcal{A}$. It then follows that

$$[h(u'),h(v')]_{\mathcal{A}}=h([u',v']_{\mathcal{A}'}). \tag{5.110}$$

Hence, the kernel of h is an invariant Lie subalgebra of $\mathcal{A}'$. As a consequence of the decomposition $\mathcal{A}'=\mathcal{A}'^c\oplus\mathcal{A}'^s$, any such subalgebra must belong to $\mathcal{A}'^c$. Furthermore, the image of h is a Lie subalgebra of $\mathcal{A}$ isomorphic to $\mathcal{A}'^s$. Hence, $h(\mathcal{A}'^s)\subseteq\mathcal{A}^s$ yields a Lie algebra homomorphism. This now fully describes the structure imposed on $\mathcal{A}$ and $\mathcal{A}'$ by the algebraic relations (5.36) and (5.37), (5.53)–(5.55), (5.58), and (5.59) in the massless case.

In the massive case, note

$$\mathcal{A}=\mathcal{A}_m, \quad \mathcal{A}'=\mathcal{A}'_m \tag{5.111}$$

are isomorphic as vector spaces under the map $m_{\mathcal{A}'}(\mathcal{A}'_m)=m\,\mathrm{id}(\mathcal{A}'_m)=m\mathcal{A}_m$. Since this map is a Lie algebra homomorphism by Eq. (5.102), then $\mathcal{A}$ and $\mathcal{A}'$ are isomorphic Lie algebras. Consequently, Eq. (5.54) becomes

$$\begin{aligned}&[\rho_m(w)u,v]_{\mathcal{A}}+[u,\rho_m(w)v]_{\mathcal{A}}-\rho_m(w)[u,v]_{\mathcal{A}}\\&\quad=\rho_m(\rho_m(w)u)v-\rho_m(\rho_m(w)v)u-\rho_m([w,u]_{\mathcal{A}})v+\rho_m([w,v]_{\mathcal{A}})u,\end{aligned} \tag{5.112}$$

where $\rho_m(w)=\rho(m_{\mathcal{A}}(w))$. Taking into account Eq. (5.36), the relation (5.112) states that the linear map on $\mathcal{A}$ defined by

$$\tilde{\rho}_m(u)v=\rho_m(v)u-ad_{\mathcal{A}}(v)u \tag{5.113}$$

must be a skew-adjoint representation of the Lie algebra $\mathcal{A}$,

$$(u,\tilde{\rho}_m(w)v)_{\mathcal{A}}=-(v,\tilde{\rho}_m(w)u)_{\mathcal{A}}, \quad [\tilde{\rho}_m(u),\tilde{\rho}_m(v)]=\tilde{\rho}_m([u,v]_{\mathcal{A}}). \tag{5.114}$$

This is satisfied if $\rho_m=ad_{\mathcal{A}}$, in which case $\tilde{\rho}_m=0$ is a trivial representation, or if $\rho_m=0$, in which case $\tilde{\rho}_m=-ad^T_{\mathcal{A}}$ is the coadjoint representation. In either case, there is no further algebraic structure imposed by Eq. (5.112). Note then, surprisingly, $\mathcal{A}$ is thus not required to be semisimple in massive case with $\rho_m=ad_{\mathcal{A}}$.

To conclude the discussion, we return to the general situation when $\mathcal{A}$ and $\mathcal{A}'$ contain both massless and massive nonempty subspaces. In this case, from Eq. (5.54), it follows that

$$\begin{aligned}&[\rho(w')u,v]_{\mathcal{A}}+[u,\rho(w')v]_{\mathcal{A}}-\rho(w)[u,v]_{\mathcal{A}}\\&\quad=\rho(m_{\mathcal{A}}(\rho(w')u))v-\rho(m_{\mathcal{A}}(\rho(w')v))u-\rho([w',m_{\mathcal{A}}(u)]_{\mathcal{A}'})v+\rho([w',m_{\mathcal{A}}(v)]_{\mathcal{A}'})u.\end{aligned} \tag{5.115}$$

We now show that this equation is satisfied by

$$\rho(w')=ad_{\mathcal{A}}(h(w')) \tag{5.116}$$

for some linear map h from $\mathcal{A}'$ into $\mathcal{A}$ if

$$h(m_{\mathcal{A}}(\mathcal{A}_m))=\mathcal{A}_m, \quad m_{\mathcal{A}}(h(\mathcal{A}'_m))=\mathcal{A}'_m, \quad h(\mathcal{A}'_0)\subseteq\mathcal{A}_0 \tag{5.117}$$

and if

$$[\mathcal{A}_m,\mathcal{A}_m]\subseteq\mathcal{A}_m, \quad [\mathcal{A}_m,\mathcal{A}_0]\subseteq\mathcal{A}_0^c, \quad [ad_{\mathcal{A}_0}(\mathcal{A}_m),ad_{\mathcal{A}_0}(\mathcal{A}_m)]=0, \tag{5.118}$$

where $\mathcal{A}_0^c$ is the center of the Lie algebra $\mathcal{A}$. To begin the proof, first note that if Eq. (5.116) holds then the left-hand side of Eq. (5.115) directly vanishes for any h since $ad_{\mathcal{A}}$ is a derivation of $\mathcal{A}$. Next, from Eq. (5.59), the last two terms on the right-hand side of Eq. (5.115) become

$$\begin{aligned}&-[ad_{\mathcal{A}}(w_m),ad_{\mathcal{A}}(u_m)]v+[ad_{\mathcal{A}}(w_m),ad_{\mathcal{A}}(v_m)]u\\&\quad=-ad_{\mathcal{A}}([w_m,u_m]_{\mathcal{A}})v+ad_{\mathcal{A}}([w_m,v_m]_{\mathcal{A}})u\\&\quad=-[[w_m,u_m]_{\mathcal{A}},v]_{\mathcal{A}}+[[w_m,v_m]_{\mathcal{A}},v]_{\mathcal{A}},\end{aligned} \tag{5.119}$$

where $w_m=m_{\mathcal{A}'}(w')$. Then, by Eq. (5.118), the first two terms on the right-hand side of Eq. (5.115) reduce to

$$ad_{\mathcal{A}}(ad_{\mathcal{A}}(w_m)u_m)v-ad_{\mathcal{A}}(ad_{\mathcal{A}}(w_m)v_m)u=[[w_m,u_m]_{\mathcal{A}},v]_{\mathcal{A}}-[[w_m,v_m]_{\mathcal{A}},u]_{\mathcal{A}}. \tag{5.120}$$

Hence, the right-hand side of Eq. (5.115) vanishes, which completes the proof.

Consequently, note that Eqs. (5.116)–(5.118) determine

$$\rho(w'_m)=ad_{\mathcal{A}_m}(m_{\mathcal{A}'}^{-1}(w'_m)), \quad \rho(w'_0)=ad_{\mathcal{A}_0}(h_0(w'_0)) \tag{5.121}$$

in terms of some linear map $h_0=h\circ\mathcal{P}'_0$ from $\mathcal{A}'_0$ into $\mathcal{A}_0$, and using the inverse $m_{\mathcal{A}'}^{-1}$ from $\mathcal{A}_m$ into $\mathcal{A}'_m$ of the linear map $m_{\mathcal{A}'}\circ\mathcal{P}'_m$. It then follows that

$$m_{\mathcal{A}'}([u',v']_{\mathcal{A}'})=[m_{\mathcal{A}'}(u'),m_{\mathcal{A}'}(v')]_{\mathcal{A}}. \tag{5.122}$$

Hence, $\mathcal{A}'_0$ is an invariant Lie subalgebra of $\mathcal{A}'$, and $\mathcal{A}_m$ is a Lie subalgebra of $\mathcal{A}$. Consequently, since by Eq. (5.105) the inner product on $\mathcal{A}'_0$ is an invariant metric with respect to $\mathcal{A}'$, the Lie subalgebra $\mathcal{A}'_0$ is a direct sum of an Abelian Lie algebra $\mathcal{A}'^c_0$ and a semisimple Lie algebra $\mathcal{A}'^s_0$. Furthermore, from Eq. (5.122), it follows that $\mathcal{A}_m$ and $\mathcal{A}'_m$ are isomorphic Lie algebras, but note that they are not required to be semisimple. This now gives a complete description of the algebraic structure imposed by the relations (5.36) and (5.37), (5.53)–(5.55), (5.58), and (5.59) in the case given by Eqs. (5.116)–(5.118).

Thus, the previous algebraic analysis leads to an interesting generalization of the massless/massive nonlinear theories in Secs. II and III given by the nonlinear theory (5.84)–(5.94) with the following algebraic structure:

(i) The massless and massive subspaces $\mathcal{A}_0,\mathcal{A}'_0,\mathcal{A}_m,\mathcal{A}'_m$ are Lie subalgebras of $\mathcal{A},\mathcal{A}'$ with $\mathcal{A}'_m$ and $\mathcal{A}_m$ being isomorphic under the linear maps $m_{\mathcal{A}},m_{\mathcal{A}'}$ given by the mass tensor.

(ii) $\mathcal{A}_0$ and $\mathcal{A}'_0$ are semisimple Lie algebras and ideals in $\mathcal{A},\mathcal{A}'$, such that $\mathcal{A}_0$ and $\mathcal{A}_m$ commute; however, the Lie algebras $\mathcal{A}_m\simeq\mathcal{A}'_m$ are not restricted to be semisimple (they may be nilpotent or solvable) and $\mathcal{A}'_m$ is not restricted to commute with $\mathcal{A}'_0$.

(iii) The representation ρ' is the adjoint representation of $\mathcal{A}'_m=m_{\mathcal{A}}(\mathcal{A}_m)$ on $\mathcal{A}'$, while the representation ρ is the sum of the adjoint representations of $\mathcal{A}_m=m_{\mathcal{A}'}^{-1}(\mathcal{A}'_m)$ and of $\mathcal{A}_0=h_0(\mathcal{A}'_0)$ on $\mathcal{A}$, for any linear map h_0.

In physical terms, the resulting nonlinear theory (5.84)–(5.94) is a novel generalization of Yang–Mills gauge theory for vector potentials A^a coupled to Freedman–Townsend gauge theory for antisymmetric tensor potentials $B^{a'}$, involving a Chern–Simons-type mass term. It describes a set of nonlinearly interacting massive spin-one fields and massless spin-one and spin-zero fields, with a mutual interaction between the massive and massless fields.

VI. CONCLUDING REMARKS

This paper has developed in detail the geometrical, field theoretic, and algebraic aspects of an interesting nonlinear generalization of massless/massive Yang–Mills/Freedman–Townsend gauge theory in four dimensions. The generalization involves an extended Freedman–Townsend coupling between the Yang–Mills one-form gauge fields and Freedman–Townsend two-form gauge fields, in addition to a Higgs-type coupling tied to a Chern–Simons mass term, and accompanied by a novel form of generalized Yang–Mills and Freedman–Townsend gauge symmetries and field equations in both the massless and massive cases. In particular, the geometrical structure of the resulting nonlinear gauge theory mixes and unifies well-known features of Yang–Mills theory and Freedman–Townsend theory in terms of Lie algebra valued curvatures and connections associated to the gauge fields and nonlinear field strengths.

This generalization was found by a general determination of the geometrical nonlinear deformations of linear Abelian gauge theory for one-form fields and two-form fields with an Abelian Chern–Simons mass term. The deformation framework used here is a geometrical version of the field theoretic approach developed in Refs. 3, 1, and 12. It exposes clearly the existence of two integrability conditions on the first-order parts of possible deformations and leads to a simple uniqueness argument for the higher-order parts of allowed deformations.

Another approach to deformations (see Ref. 4 for an overview), which is based on BRST cohomology,[5,16,17] has recently yielded important results on the classification of allowed first-order deformations of the free gauge theory for a set of p-form fields, $p=1,\ldots,n-1$, in $n\geqslant 2$ dimensions.[7,18] While this classification analysis is complete for massless p-form fields with $p\geqslant 2$ and lists the extended Freedman–Townsend and Yang–Mills types of first-order deformations, it did not explicitly treat deformations of massive p-form fields with the mass given by an Abelian Chern–Simons term in the free gauge theory. Moreover, integrability conditions (i.e., obstructions to the existence of higher-order deformation terms) associated with combining the distinct types of allowed first-order deformations were not obtained for any $p\geqslant 1$. In the case $p\leqslant 2$, these gaps are closed by the deformation results obtained in Sec. V. In particular, a complete classification of first-order geometrical deformations of the free gauge theory for a massive/massless set of one-form and two-form fields has been obtained in $n=4$ dimensions, including all integrability conditions that arise on such deformations (with typical assumptions on the allowed number of derivatives considered for terms in the gauge symmetries and field equations). Also, uniqueness results on deformations to all orders in this setting have been proved. (Interestingly, if the restriction to geometrical deformations is relaxed, then an additional type of deformation is known to exist in the case $p=1$.[19])

There are several directions in which the main results in this paper could be generalized. First, an extension of the general massless/massive nonlinear theory constructed here for Yang–Mills one-form gauge fields coupled to Freedman–Townsend two-form gauge fields with a Chern–Simons mass term in four dimensions is expected to exist in n dimensions, involving a tower of Lie-algebra valued p-form fields $A_{(p)}$, $p=1,\ldots,n-2$, with a Yang–Mills self-coupling on $A_{(1)}$, a Freedman–Townsend self-coupling on $A_{(n-2)}$, and an extended Freedman–Townsend coupling between $A_{(1)},\ldots,A_{(n-2)}$, in addition to a Higgs coupling of $A_{(2)},\ldots,A_{(n-2)}$ with $A_{(1)}$ in the massive case.

Second, it is straightforward to couple such a geometrical nonlinear gauge theory to gravity. In particular, on a space–time with metric tensor g, the only structure needed is the Hodge dual operator $*$ determined by g, and the exterior derivative d operator (which is independent of g). For the case $n=4$ dimensions, if the Lagrangian of the nonlinear gauge theory given in this paper for $A_{(1)}$ and $A_{(2)}$ is combined with the Einstein gravitational Lagrangian for g, then this achieves an interesting generalization of the Einstein–Yang–Mills theory (and there is obvious extension to n dimensions for $A_{(1)},\ldots,A_{(n-2)}$). Of particular interest would be to consider its field theoretic features, such as black hole solutions, non-Abelian monopole solutions, and critical behavior in the initial value problem.

ACKNOWLEDGMENTS

The author would like to thank the organizers of the First and Second Workshops on Formal Geometry and Mathematical Physics where some of the results in this paper were first presented.

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Thermodynamic properties of the $2N$-piece relativistic string

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(Received 17 April 2002; accepted 19 November 2002)

The thermodynamic free energy $F(\beta)$ is calculated for a gas consisting of the transverse oscillations of a piecewise uniform bosonic string. The string consists of $2N$ parts of equal length, of alternating type I and type II material, and is relativistic in the sense that the velocity of sound everywhere equals the velocity of light. The present paper is a continuation of two earlier papers, one dealing with the Casimir energy of a $2N$-piece string [I. Brevik and R. Sollie, J. Math. Phys. **38**, 2774 (1997)], and another dealing with the thermodynamic properties of a string divided into two (unequal) parts [I. Brevik, A. A. Bytsenko, and H. B. Nielsen, Class. Quantum Grav. **15**, 3383 (1998)]. Making use of the Meinardus theorem, we calculate the asymptotics of the level state density, and show that the critical temperatures in the individual parts are equal, for arbitrary space–time dimension D. If $D=26$, we find $\beta=(2/N)\sqrt{2\pi/T_{II}}$, T_{II} being the tension in part II. Thermodynamic interactions of parts related to high genus g is also considered. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1540235]

I. INTRODUCTION

Whereas the bosonic string of length L in D-dimensional space–time is assumed to be uniform, the *composite* string is imagined to consist of two or more uniform pieces. In a Casimir context, such a model was introduced in 1990.[1] The string was assumed to be divided into two pieces, of lengths L_I and L_{II}, and the model was relativistic in the sense that the velocity of sound was everywhere required to be equal to the velocity of light. With this contraint imposed on the model, the Casimir energy of the string, i.e., the zero-point energy associated with its discontinuity properties, was easily calculable as a function of the length ratio $s=L_{II}/L_I$. Later, various aspects of the relativistic piecewise uniform string model were studied.[2–12] One may note, for instance, the paper of Lu and Huang[12] in which the model finds application in relation to the Green–Schwarz superstring.

The present article focuses attention on the thermodynamic free energy $F(\beta)$ at inverse temperature $\beta=1/T$ of a $2N$-piece string, made up of $2N$ parts of equal length, of alternating type I and type II material. The model is relativistic, in the sense explained above. In an earlier paper[7] we developed the Casimir theory for a string of this type, whereas in another paper[8] we considered the free energy for the case where the string consists of *two* pieces only, i.e., the model of Ref. 4. The calculation of $F(\beta)$ for a $2N$-piece string has to our knowledge not been undertaken before.

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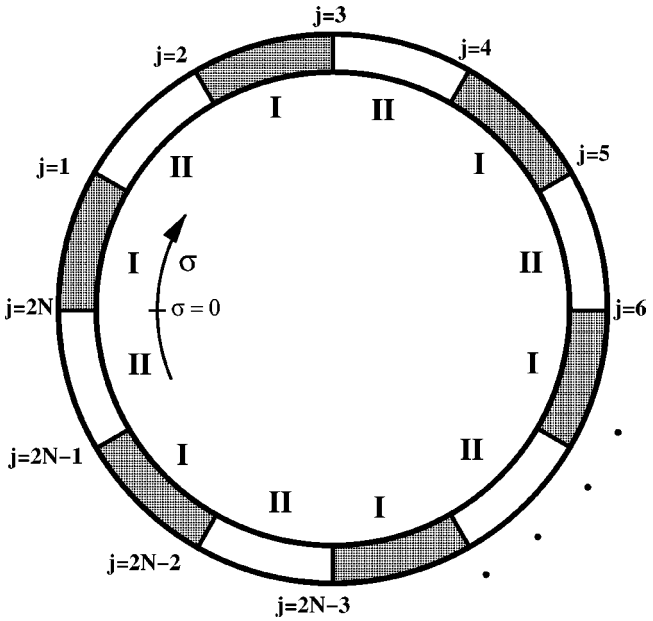

FIG. 1. Sketch of the composite $2N$ string, when $N=6$.

It turns out, similarly as in Ref. 10, that the Meinardus theorem[13–15] is powerful, allowing us to find the asymptotics of the level state density. Using this we find, for a general space–time dimension D, that the critical (Hagedorn) temperatures for the two kinds of pieces are the same. When $D=26$, the common space–time dimension for a bosonic string, we find $\beta_c = (2/N)\sqrt{2\pi/T_{II}}$, T_{II} being the tension in region II. This result is derived in Sec. VI. In Sec. VII, we comment upon the thermodynamic properties of the composite string for arbitrary genus g.

II. RESUMÉ OF THE 2*N*-PIECE STRING THEORY

Assume, as mentioned, that the string of total length L is divided into $2N$ equally large pieces, of alternating type I and type II material; see Fig. 1. The string is relativistic, in the sense that the velocity of sound is everywhere equal to the velocity of light, $v_s=\sqrt{T_I/\rho_I}=\sqrt{T_{II}/\rho_{II}}=c$, where T_I, T_{II} are the tensions and ρ_I, ρ_{II} the mass densities in the two pieces. We will study the transverse oscillations $\psi=\psi(\sigma,\tau)$ of the string, σ denoting as usual the position coordinate and τ the time coordinate of the string. We can thus write in the two regions

$$\begin{aligned}\psi_I &= \xi_I e^{i\omega(\sigma-\tau)} + \eta_I e^{-i\omega(\sigma+\tau)},\\ \psi_{II} &= \xi_{II} e^{i\omega(\sigma-\tau)} + \eta_{II} e^{-i\omega(\sigma+\tau)},\end{aligned} \tag{1}$$

where ξ and η are constants. The junction conditions are that ψ itself as well as the transverse elastic force $T\partial\psi/\partial\sigma$ are continuous, i.e.,

$$\psi_I=\psi_{II}, \quad T_I\partial\psi_I/\partial\sigma = T_{II}\partial\psi_{II}/\partial\sigma, \tag{2}$$

at each of the $2N$ junctions. We define x as the tension ratio, $x=T_I/T_{II}$, and define also the symbols p_N and α by $p_N=\omega L/N$, $\alpha=(1-x)/(1+x)$. Now introduce the matrix Λ,

$$\Lambda(\alpha,p_N)=\begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \tag{3}$$

with

$$a=e^{-ip_N}-\alpha^2, \quad b=\alpha(e^{-ip_N}-1). \tag{4}$$

Then, as shown in Ref. 7, the eigenfrequencies ω are determined from the equation

$$\mathrm{Det}[(1-\alpha^2)^{-N}\Lambda^N(\alpha,p_N)-1]=0. \tag{5}$$

For practical purposes it is convenient to reformulate the condition (5). Let us define two new quantities $\lambda_\pm$:

$$\lambda_\pm(p_N)=\cos p_N-\alpha^2\pm[(\cos p_N-\alpha^2)^2-(1-\alpha^2)^2]^{1/2}. \tag{6}$$

Then, we can reexpress the condition (5) as[7]

$$\lambda_+^N+\lambda_-^N=2(1-\alpha^2)^N. \tag{7}$$

We can now make use of the following recursion formula for the quantity $S_N\equiv\lambda_+^N+\lambda_-^N$:

$$S_N=2(\cos p-\alpha^2)S_{N-1}-(1-\alpha^2)^2S_{N-2}, \quad N\geqslant 2, \tag{8}$$

in which it is assumed that $\omega L/N$ is constant, at all recursive steps. The initial values of S_N are $S_0=2$, $S_1=\lambda_++\lambda_-=2(\cos p-\alpha^2)$.

Assume now that $L=\pi$, in conformity with usual practice. Thus $p_N=\pi\omega/N$. We let $X^\mu(\sigma,\tau)$, with $\mu=0,1,2,...,(D-1)$, specify the coordinates on the world sheet. For each of the eigenvalue branches determined by the dispersion equation (5) we can write X^μ on the form

$$X^\mu=x^\mu+\frac{p^\mu\tau}{\pi T_0}+X_I^\mu, \quad \text{region I}, \tag{9}$$

$$X^\mu=x^\mu+\frac{p^\mu\tau}{\pi T_0}+X_{II}^\mu, \quad \text{region II}, \tag{10}$$

where x^μ is the center-of-mass position, p^μ is the total momentum of the string, and $T_0=\frac{1}{2}(T_I+T_{II})$ is the mean tension. Further, X_I^μ and X_{II}^μ are decomposed into oscillator coordinates,

$$X_I^\mu=\frac{i}{2}\ell_s\sum_{n\neq 0}\frac{1}{n}[\alpha_{nI}e^{i\omega(\sigma-\tau)}+\tilde{\alpha}_{nI}e^{-i\omega(\sigma+\tau)}], \tag{11}$$

$$X_{II}^\mu=\frac{i}{2}\ell_s\sum_{n\neq 0}\frac{1}{n}[\alpha_{nII}e^{i\omega(\sigma-\tau)}+\tilde{\alpha}_{nII}e^{-i\omega(\sigma+\tau)}]. \tag{12}$$

Here, ℓ_s is the fundamental string length, unspecified so far, and $\alpha_n,\tilde{\alpha}_n$ are oscillator coordinates of the right- and left-moving waves, respectively. A characteristic property of the composite string is that the oscillator coordinates have to be specified for each of the various branches determined by Eq. (5). This makes the handling of the formalism complicated, in general. A significant simplification can be obtained if, following Ref. 8, we limit ourselves to the case of extreme string ratios only. Since α occurs quadratically in Eqs. (6) and (7), the eigenvalue spectrum has to be invariant under the transformation $x\to 1/x$. It is sufficient, therefore, to consider the tension ratio interval $0<x\leqslant 1$ only. The case of extreme tensions corresponds to $x\to 0$. We will consider only this case in the following.

III. THE CASE OF EXTREME TENSIONS

We assume that T_{II} has a finite value, so that the limiting case $x\to 0$ corresponds to $T_I\to 0$. Thus $T_0\to\frac{1}{2}T_{II}$. Since now $\alpha\to 1$ we get from Eq. (6) $\lambda_-=0$, $\lambda_+=\cos p_N-1$, so we obtain from

Eq. (7) the remarkable simplification that all the eigenfrequency branches degenerate into one single branch determined by $\cos p_N=1$. That is, the eigenvalue spectrum becomes

$$\omega_n=2Nn, \quad n=\pm 1,\pm 2,\pm 3,\ldots . \tag{13}$$

Then, choosing the fundamental length equal to $\ell_s=(\pi T_I)^{-1/2}$, we can write the expansion (11) in region I as (with subscript I on the α_n's omitted)

$$X_I^\mu=\frac{i}{2\sqrt{\pi T_I}}\sum_{n\neq 0}\frac{1}{n}[\alpha_n^\mu e^{2iNn(\sigma-\tau)}+\tilde{\alpha}_n^\mu e^{-2iNn(\sigma+\tau)}]. \tag{14}$$

The junction conditions (2) permit all waves to propagate from region I to region II. When $x\rightarrow 0$, they reduce to the equations

$$\xi_I+\eta_I=2\xi_{II}=2\eta_{II}, \tag{15}$$

which show that the right- and left-moving amplitudes ξ_I and η_I in region I can be chosen freely and that the amplitudes ξ_{II}, η_{II} in region II are thereafter fixed. This means, in oscillator language, that α_n^μ and $\tilde{\alpha}_n^\mu$ can be chosen freely. The expansion in region II can in view of Eq. (15) be written as

$$X_{II}^\mu=\frac{i}{2\sqrt{\pi T_I}}\sum_{n\neq 0}\frac{1}{n}\gamma_n^\mu e^{-2iNn\tau}\cos(2Nn\sigma), \tag{16}$$

where we have defined γ_n^μ as

$$\gamma_n^\mu=\alpha_n^\mu+\tilde{\alpha}_n^\mu, \quad n\neq 0. \tag{17}$$

The oscillations in region II are thus standing waves. This is the same kind of behavior as that found for the two-piece string.[8]

The action of the string is

$$S=-\frac{1}{2}\int \mathrm{d}\tau\mathrm{d}\sigma T(\sigma)\eta^{\alpha\beta}\partial_\alpha X^\mu\partial_\beta X_\mu, \tag{18}$$

where $\alpha,\beta=0,1$ and $T(\sigma)=T_I$ in region I, $T(\sigma)=T_{II}$ in region II. The momentum conjugate to X^μ is $P^\mu(\sigma)=T(\sigma)\dot{X}^\mu$, and the Hamiltonian is accordingly

$$H=\int_0^\pi [P_\mu(\sigma)\dot{X}^\mu-\mathcal{L}]\mathrm{d}\sigma=\frac{1}{2}\int_0^\pi T(\sigma)(\dot{X}^2+X'^2)\mathrm{d}\sigma, \tag{19}$$

where $\mathcal{L}$ is the Lagrangian.

As for the constraint equation for the string, some care has to be taken. Conventionally, in the classical theory for the uniform string the constraint equation reads $T_{\alpha\beta}=0$, $T_{\alpha\beta}$ being the energy–momentum tensor. As discussed in Ref. 8, the situation is here more complicated, since the junctions restrict the freedom one has to take the variations δX^μ. We thus have to replace the strong condition $T_{\alpha\beta}=0$ by a weaker condition, and the most natural choice, which we will adopt, is to impose that $H=0$ when applied to the physical states.

Let us introduce lightcone coordinates, $\sigma^-=\tau-\sigma$ and $\sigma^+=\tau+\sigma$. The derivatives conjugate to $\sigma^\mp$ are $\partial_\mp=\frac{1}{2}(\partial_\tau\mp\partial_\sigma)$. In region I,

$$\partial_- X^\mu = \frac{N}{\sqrt{\pi T_I}} \sum_{-\infty}^{\infty} \alpha_n^\mu e^{2iNn(\sigma-\tau)},$$
$$\partial_+ X^\mu = \frac{N}{\sqrt{\pi T_I}} \sum_{-\infty}^{\infty} \tilde{\alpha}_n e^{-2iNn(\sigma+\tau)}, \tag{20}$$

and in region II

$$\partial_\mp X^\mu = \frac{N}{2\sqrt{\pi T_I}} \sum_{-\infty}^{\infty} \gamma_n^\mu e^{\pm 2in(\sigma\mp\tau)}, \tag{21}$$

where we have defined

$$\alpha_0^\mu = \tilde{\alpha}_0^\mu = \frac{p^\mu}{NT_{II}} \sqrt{\frac{T_I}{\pi}}, \qquad \gamma_0^\mu = 2\alpha_0^\mu. \tag{22}$$

Inserting these expressions into the Hamiltonian

$$H = \int_0^\pi T(\sigma)(\partial_- X \cdot \partial_- X + \partial_+ X \cdot \partial_+ X)\mathrm{d}\sigma$$
$$= NT_I \int_0^{\pi/(2N)} (\partial_- X \cdot \partial_- X + \partial_+ X \cdot \partial_+ X)\mathrm{d}\sigma$$
$$+ NT_{II} \int_{\pi/(2N)}^{\pi/N} (\partial_- X \cdot \partial_- X + \partial_+ X \cdot \partial_+ X)\mathrm{d}\sigma \tag{23}$$

we get

$$H = \frac{1}{2} N^2 \sum_{-\infty}^{\infty} (\alpha_{-n} \cdot \alpha_n + \tilde{\alpha}_{-n} \cdot \tilde{\alpha}_n) + \frac{N^2}{4x} \sum_{-\infty}^{\infty} \gamma_{-n} \cdot \gamma_n. \tag{24}$$

Now consider the expression for the square M^2 of the mass of the string. One must have $M^2 = -p^\mu p_\mu$, as in the case of a uniform string.[16] We start from the constraint $H=0$ when applied to physical states, making use of Eq. (24) in which we separate out the $n=0$ terms. Using that $\alpha_0 \cdot \alpha_0 = -M^2 x/(\pi N^2 T_{II})$ according to Eq. (22) we obtain in this way, when again observing that $x \ll 1$,

$$M^2 = \pi N^2 T_{II} \sum_{n=1}^{\infty} \left[\alpha_{-n} \cdot \alpha_n + \tilde{\alpha}_{-n} \cdot \tilde{\alpha}_n + \frac{1}{2x} \gamma_{-n} \cdot \gamma_n \right]. \tag{25}$$

The following point ought to be stressed in order to prevent misunderstanding. The reason why we have dealt with the limit of extreme tensions, $x = T_I/T_{II} \to 0$, is merely practical; therewith the eigenvalue branches degenerate into one single branch, Eq. (13). This simplification is however not of fundamental importance; in particular, it has no bearing on the general problem of how to distinguish between the actions for massive and massless particles. We never put T_I exactly equal to zero.

IV. QUANTIZATION

The momentum conjugate to X^μ is at any position on the string equal to $T(\sigma)\dot{X}^\mu$. We accordingly require the commutation rules in region I to be

$$T_I[\dot{X}^\mu(\sigma,\tau), X^\nu(\sigma',\tau)] = -i\,\delta(\sigma-\sigma')\,\eta^{\mu\nu}, \tag{26}$$

and in region II

$$T_{II}[\dot{X}^{\mu}(\sigma,\tau),X^{\nu}(\sigma',\tau)]=-i\,\delta(\sigma-\sigma')\,\eta^{\mu\nu}, \tag{27}$$

$\eta^{\mu\nu}$ being the D-dimensional flat metric. The other commutators vanish. The quantities to be promoted to Fock state operators are $\alpha_{\mp n}$ and $\gamma_{\mp n}$. We insert the expansions for X^{μ} and $\dot{X}^{\mu}$ in regions I and II into Eqs. (26) and (27) and make use of the effective relationship

$$\sum_{n=-\infty}^{\infty} e^{2iNn(\sigma-\sigma')}=2\sum_{n=-\infty}^{\infty}\cos 2Nn\sigma\cos 2Nn\sigma'\rightarrow\frac{\pi}{N}\delta(\sigma-\sigma'). \tag{28}$$

We then get in region I

$$[\alpha_n^{\mu},\alpha_m^{\nu}]=n\,\delta_{n+m,0}\eta^{\mu\nu}, \tag{29}$$

with a similar relation for $\tilde{\alpha}_n$. In region II,

$$[\gamma_n^{\mu},\gamma_m^{\nu}]=4nx\;\delta_{n+m,0}\;\eta^{\mu\nu}. \tag{30}$$

We introduce annihilation and creation operators by

$$\begin{aligned}\alpha_n^{\mu}&=\sqrt{n}\,a_n^{\mu}, \quad \alpha_{-n}^{\mu}=\sqrt{n}\,a_n^{\mu\dagger},\\ \gamma_n^{\mu}&=\sqrt{4nx}\,c_n^{\mu}, \quad \gamma_{-n}^{\mu}=\sqrt{4nx}\,c_n^{\mu\dagger},\end{aligned} \tag{31}$$

and find for $n\geqslant 1$ the standard form

$$\begin{aligned}[a_n^{\mu},a_m^{\nu\dagger}]&=\delta_{nm}\eta^{\mu\nu},\\ [c_n^{\mu},c_m^{\nu\dagger}]&=\delta_{nm}\eta^{\mu\nu}.\end{aligned} \tag{32}$$

These expressions are formally the same as those found for a two-piece string.[8] From Eq. (24) we get, when separating out the $n=0$ term,

$$H=-\frac{M^2}{\pi T_{II}}+\frac{1}{2}N\sum_{n=1}^{\infty}\omega_n(a_n^{\dagger}\cdot a_n+\tilde{a}_n^{\dagger}\cdot\tilde{a}_n+2\,c_n^{\dagger}\cdot c_n). \tag{33}$$

Here $a_n^{\dagger}\cdot a_n\equiv a_n^{\mu\dagger}a_{n\mu}$, and $\omega_n=2Nn$ as before. From the condition $H=0$ we now get

$$M^2=\frac{1}{2}\pi NT_{II}\sum_{i=1}^{24}\sum_{n=1}^{\infty}\omega_n(a_{ni}^{\dagger}a_{ni}+\tilde{a}_{ni}^{\dagger}\tilde{a}_{ni}+2\,c_{ni}^{\dagger}c_{ni}-\mathcal{C}), \tag{34}$$

where we have put $D=26$ and summed over the transverse 24 oscillator operators. Further, we have introduced a constant $\mathcal{C}$ in order to account for ordering ambiguities. Note that in Eq. (20) the denominator goes to zero when T_I does, but the same T_I is restored again in Eqs. (22) and (26). The result is that the commutation rules for the creation and annihilation operators, Eq. (29), take the same form as usual in quantum field theory.

V. QUANTUM THERMODYNAMICS

The constraint for the closed string (fat circles at Fig. 2), expressing the invariance of the theory in the region I under shifts of the origin of the coordinate, has the form

$$\sum_{i=1}^{24}\sum_{n=1}^{\infty}\omega_n[a_{ni}^{\dagger}a_{ni}-\tilde{a}_{ni}^{\dagger}\tilde{a}_{ni}]=0. \tag{35}$$

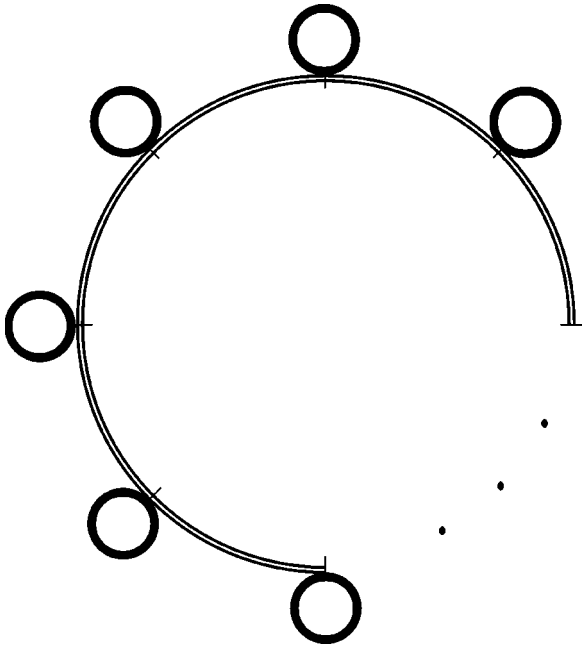

FIG. 2. Fat circles correspond to closed strings, double lines correspond to open strings.

The commutation relations for the above operators are given by Eq. (32). The mass of state (obtained by acting on the Fock vacuum $|0\rangle$ with creation operators) can be written as follows: $(\text{mass})^2 \sim a_{n1}^{\dagger} \cdots a_{ni}^{\dagger} c_{n1}^{\dagger} \cdots c_{ni}^{\dagger} |0\rangle$.

Let us start with the discussion of the free energy in field theory at nonzero temperature $T = \beta^{-1}$ (we put $k_B = 1$). As usual the physical Hilbert space consists of all Fock space states obeying the condition (35), which can be implemented by means of the integral representation for Kronecker deltas. Thus the free energy of the field content in the ''proper time'' representation becomes

$$F(\beta) = \mathcal{F}(\beta = \infty) - \pi (2\pi)^{-14} \int_0^{\infty} \frac{\mathrm{d}\tau_2}{\tau_2^{14}} \left[\theta_3 \left(0 \,\middle|\, \frac{i\beta^2}{2\pi\tau_2} \right) - 1 \right] \mathrm{Tr} \exp\left\{ -\frac{\tau_2 M^2}{2} \right\}$$
$$\times \int_{-\pi}^{\pi} \frac{\mathrm{d}\tau_1}{2\pi} \mathrm{Tr} \exp\left\{ iN\tau_1 \sum_{i=1}^{24} \sum_{n=1}^{\infty} \omega_n [a_{ni}^{\dagger} a_{ni} - \tilde{a}_{ni}^{\dagger} \tilde{a}_{ni}] \right\}, \tag{36}$$

where $\mathcal{F}(\beta = \infty)$ is the temperature independent part of $F(\beta)$ (the Casimir energy), while the second term in (36) presents the temperature dependent part (the statistical sum). Once the free energy has been found, the other thermodynamic quantities can readily be calculated. For instance, the energy U and the entropy S of the system are $U = (\partial/\partial\beta)(\beta F(\beta))$, $S = \beta^2 (\partial/\partial\beta)(F(\beta))$.

VI. THE CRITICAL TEMPERATURE

First we consider some mathematical results on the asymptotics of the level degeneracy which leads to the asymptotics of the level state density. Let

$$\mathcal{G}(z) = \prod_{n=1}^{\infty} [1 - e^{-zn}]^{-a_n} = 1 + \sum_{n=1}^{\infty} \Xi(n) e^{-zn} \tag{37}$$

be the generating function, where $\Re z > 0$ and a_n are non-negative real numbers. Let us consider the associated Dirichlet series

$$\mathcal{D}(s)=\sum_{n=1}^{\infty} a_n n^{-s}, \qquad s=\sigma+it, \tag{38}$$

which converges for $0<\sigma<p$. We assume that $\mathcal{D}(s)$ can be analytically continued in the region $\sigma\geqslant -C_0$ $(0<C_0<1)$ and here $\mathcal{D}(s)$ is analytic except for a pole of order one at $s=p$ with residue A. Besides we assume that $\mathcal{D}(s)=\mathcal{O}(|t|^{C_1})$ uniformly in $\sigma\geqslant -C_0$ as $|t|\to\infty$, where C_1 is a fixed positive real number. The following lemma[13–15] is useful with regard to the asymptotic properties of $\mathcal{G}(z)$ at $z=0$:

Lemma 1: If $\mathcal{G}(z)$ and $\mathcal{D}(s)$ satisfy the above assumptions and $z=y+2\pi ix$, then

$$\mathcal{G}(z)=\exp\left\{A\Gamma(p)\zeta_R(1+p)z^{-p}-\mathcal{D}(0)\log z+\frac{d}{ds}\mathcal{D}(s)\bigg|_{s=0}+\mathcal{O}(y^{C_0})\right\} \tag{39}$$

uniformly in x as $y\to 0$, provided $|\arg z|\leqslant\pi/2$ and $|x|\leqslant\frac{1}{2}$. Moreover, there exists a positive number ε such that

$$\mathcal{G}(z)=\mathcal{O}(\exp\{A\Gamma(p)\zeta_R(1+p)y^{-p}-Cy^{-\varepsilon}\}), \tag{40}$$

uniformly in x with $y^{\alpha}\leqslant|x|\leqslant\frac{1}{2}$ as $y\to 0$, C being a fixed real number and $\alpha=1+p/2-p\nu/4$, $0<\nu<\frac{2}{3}$.

The main result below follows from the lemma and permits one to calculate the complete asymptotics of $\Xi(n)$.

Theorem 1: (Meinardus[13,14]) *For $n\to\infty$ one has*

$$\Xi(n)=C_p n^k \exp\left\{\frac{1+p}{p}[A\Gamma(1+p)\zeta_R(1+p)]^{1/(1+p)}n^{p/(1+p)}\right\}(1+\mathcal{O}(n^{-k_1}))\,, \tag{41}$$

$$C_p=[A\Gamma(1+p)\zeta_R(1+p)]^{(1-2\mathcal{D}(0))/2(1+p)}\frac{\exp((d/\mathrm{d}s)\mathcal{D}(s)|_{s=0})}{[2\pi(1+p)]^{1/2}}, \tag{42}$$

$$k=\frac{2\mathcal{D}(0)-p-2}{2(1+p)}\,, \qquad k_1=\frac{p}{1+p}\min\left(\frac{C_0}{p}-\frac{\nu}{4},\frac{1}{2}-\nu\right). \tag{43}$$

Coming back to the composite string problem, note that the generation function has the form

$$W(\beta)=\mathrm{Tr}[e^{-\beta M^2}]_{(\mathcal{C}=0)}=W^{(I)}(\beta)W^{(II)}(\beta)\equiv\prod_{n=1}^{\infty}[1-e^{-n\beta Q(N)}]^{-48}\prod_{n=1}^{\infty}[1-e^{-2n\beta Q(N)}]^{-24}, \tag{44}$$

where $Q(N)=\pi T_{II}N^2$. Some remarks are in order. Taking into account $a_n=D-2$ [or $a_n=2(D-2)$ in the case of region II], we have $p=1$. In fact, Eq. (38) gives the Riemann zeta function. Therefore, from the Meinardus theorem, Eqs. (41)–(43), it follows that

$$\Xi^{(I)}(n)=C_1^{(I)}n^{k^{(I)}}\exp\left\{\pi\sqrt{\frac{4n\pi(D-2)}{3Q(N)}}\right\}(1+\mathcal{O}(n^{-k_1}))\,, \tag{45}$$

$$\Xi^{(II)}(n)=C_1^{(II)}n^{k^{(II)}}\exp\left\{\pi\sqrt{\frac{2n(D-2)}{3Q(N)}}\right\}(1+\mathcal{O}(n^{-k_1}))\,. \tag{46}$$

Using the mass formula $M^2=n$ (for the sake of simplicity we assume a tension parameter, with dimensions of $(\text{mass})^{p+1}$, equal to 1) we find for the number of bosonic string states of mass M to $M+dM$

$$\nu(M)dM \simeq 2C_1 M^{(1-D)/2}\exp(bM)dM\,, \qquad b=\pi\sqrt{\frac{D-2}{3Q(N)}}\,. \tag{47}$$

One can show that the constant b is the inverse of the Hagedorn temperature.

For the closed bosonic string in the region I the constraint $N_0=\tilde{N}_0$ should be taken into account, where N_0 is a number operator related to M^2. As a result, in Eq. (45) the total degeneracy of the level n is simply the square of $\Xi^{(I)}(n)$. Therefore the critical temperatures of composite string are given by

$$\beta_c^{(I)}=\pi\sqrt{\frac{D-2}{3Q(N)}}=\frac{2}{N}\sqrt{\frac{2\pi}{T_{II}}}\,, \tag{48}$$

$$\beta_c^{(II)}=\pi\sqrt{\frac{D-2}{3Q(N)}}=\frac{2}{N}\sqrt{\frac{2\pi}{T_{II}}}\,, \tag{49}$$

and so $\beta_c^{(I)}=\beta_c^{(II)}=\beta_c$.

VII. HIGH GENERA

The aim of this section is to consider thermodynamic properties of the composite string to arbitrary genus g associated with Riemann surface world-sheet $\Sigma_{\rm g}$. Such considerations allow us to identify the critical temperature at arbitrary loop order. It is well-known that the genus-g temperature contribution to the free energy for the bosonic string can be written as[17]

$$F_{\rm g}(\beta)=\sum_{\mathbf{m},\mathbf{n}\in\mathbf{Z}^{2g}/\{\mathbf{0}\}}\int (d\tau)_{WP}\,(\det P^{+}P)^{1/2}(\det\Delta_{\rm g})^{-13}e^{-\Delta S(\beta;\mathbf{m},\mathbf{n})}\,, \tag{50}$$

where $(\mathrm{d}\tau)_{WP}$ is the Weil–Petersson measure on the Teichmüller space. This measure as well as the factors $\det(P^{+}P)$ and $\det\Delta_{\rm g}$ are each individually modular invariant.[17] In addition,

$$I_{\rm g}(\tau)=(\det P^{+}P)^{1/2}(\det\Delta_{\rm g})^{-13}=e^{c(2{\rm g}-2)}\left(\frac{d}{ds}Z(s)\bigg|_{s=1}\right)^{-13}Z(2)\,, \tag{51}$$

where $Z(s)$ is the Selberg zeta function and c an absolute constant.[18] Furthermore, the winding-number factor has the form of a metric over the space of windings, namely

$$\Delta S(\beta;\mathbf{m},\mathbf{n})=\frac{\pi}{2}NT_{II}\beta^2[m_\ell\Omega_{\ell i}-n_i]((\Im\Omega)^{-1})_{ij}[\overline{\Omega}_{jk}m_k-n_j]={\rm g}^{\mu\nu}(\Omega)\mathcal{N}_\mu\mathcal{N}_\nu\,, \tag{52}$$

where $\mu,\nu=1,2,\ldots,2g$, $\{\mathcal{N}_1,\ldots,\mathcal{N}_{2{\rm g}}\}\equiv\{m_1,n_1,\ldots,m_{\rm g},n_{\rm g}\}$. The periodic matrix Ω, corresponding to the string world-sheet of genus g, is a holomorphic function of the moduli, $\Omega_{ij}=\Omega_{ji}$ and $\Im\Omega>0$. The matrix Ω admits a decomposition into real symmetric g$\otimes$g matrices: $\Omega=\Omega_1+i\Omega_2$. As a result

$${\rm g}(\Omega_1+i\Omega_2)=\begin{pmatrix}\Omega_1\Omega_2^{-1}\Omega_1+\Omega_2 & -\Omega_1\Omega_2^{-1}\\ -\Omega_2^{-1}\Omega_1 & \Omega_2^{-1}\end{pmatrix}. \tag{53}$$

Besides, ${\rm g}(\Omega)=\hat{\Lambda}^t{\rm g}(\Lambda(\Omega))\hat{\Lambda}$,[18] where Λ is an element of the symplectic modular group $Sp(2{\rm g},\mathbf{Z})$ and the associated tranformation of the periodic matrix reads $\Omega\mapsto\Omega'=\Lambda(\Omega)=(A\Omega+B)(C\Omega+D)^{-1}$. As a consequence, the winding factor $\Sigma_{\mathbf{m},\mathbf{n}}\exp[-\Delta S(\beta;\mathbf{m},\mathbf{n})]$ is also modular invariant. It can be shown that the 2g summations present in the expression for $F_{\rm g}(\beta)$ can be

replaced by a single summation together with a change in the region of integration from the fundamental domain to the analog of the strip S_{a_1} related to the cycle a_1, whose choice is entirely arbitrary.[17,19] Then, one has

$$F_{\mathrm{g}}(\beta)=\sum_{r=1}^{\infty}\int (\mathrm{d}\tau)_{WP}\, I_{\mathrm{g}}(\tau)\exp\left\{-\frac{\pi}{2}NT_{II}\beta^2 r^2(\Omega_{1i}((\Im\Omega)^{-1})_{ij}\overline{\Omega}_{j1})\right\}. \tag{54}$$

To make use of the Mellin transform the genus-g free energy can be present in the form[20–22]

$$F_g(\beta)=\frac{1}{2\pi i}\int_{\Re\, s=s_0}\mathrm{d}s\Gamma(s)\zeta(2s)\left(\frac{\pi}{2}NT_{II}\beta^2\right)^{-s} \times\left\{\int (\mathrm{d}\tau)_{WP}\, I_{\mathrm{g}}(\tau)[\Omega_{1i}((\Im\Omega)^{-1})_{ij}\overline{\Omega}_{j1}]^{-s}\right\}_{(\mathrm{Reg})}. \tag{55}$$

In order to deal with Eq. (55) the integrals on a suitable variable in $(\mathrm{d}\tau)_{WP}$ should be understood as the regularized ones. In this way the order of integration may be interchanged.

The critical behaviors of closed and open strings of the composite model coincide (at least at level $\mathrm{g}=1$). Let us consider, for example, the open string genus-g contribution to the free energy. The matrix Ω may be chosen as $\Omega=\mathrm{diag}(\Omega_2,\Omega_2^{-1})$. In the limit $\Omega_2\to 0$, one has

$$\exp\left\{-\frac{\pi}{2}NT_{II}\beta^2(\mathcal{N}^t\Omega\mathcal{N})^{-s}\right\}\to\exp\left\{-\frac{\pi}{2}NT_{II}\beta^2\Omega_2^{-1}\mathcal{N}^t\mathcal{N}\right\}, \tag{56}$$

and

$$\left(\sum_{\mathcal{N}\in\mathbf{Z}^{2g}/\{\mathbf{0}\}}(\mathcal{N}^t\Omega\mathcal{N})^{-s}\right)_{(\Omega_2\to 0)}\to\Omega_2^s\sum_{\mathcal{N}\in\mathbf{Z}^g/\{\mathbf{0}\}}(\mathcal{N}^t\mathcal{N})^{-s}=\Omega_2^s Z_{\mathrm{g}}|^{\mathbf{0}}_{\mathbf{0}}|(2s), \tag{57}$$

where the Epstein zeta function of order g is defined by

$$Z_{\mathrm{g}}|^{\mathbf{b}}_{\mathbf{h}}|(s)=\sum_{\mathcal{N}\in\mathbf{Z}^g/\{\mathbf{0}\}}[(n_1+b_1)^2+\cdots+(n_{\mathrm{g}}+b_{\mathrm{g}})^2]^{-s/2}\exp[2\pi i(\mathcal{N}^t,\mathbf{h})]. \tag{58}$$

The corresponding contribution is given by

$$\frac{1}{2\pi i}\int_{\Re\, s=s_0}\mathrm{d}s\,\Gamma(s)\left(\frac{\pi}{2}NT_{II}\beta^2\right)^{-s}Z_{\mathrm{g}}|^{\mathbf{0}}_{\mathbf{0}}|(2s)\left\{\int \mathrm{d}\tau_{WP}\Omega_2^s I_{\mathrm{g}}(\tau)\right\}_{(\mathrm{Reg})}. \tag{59}$$

Since a tachyon is present in the spectrum, the total free energy will be divergent, for any g. The infrared divergence may be regularized by means of a suitable cutoff parameter. This divergence could be associated with pinching a cycle nonhomologous at zero. The behavior of the factor $(\mathrm{d}\tau)_{WP}\, I_{\mathrm{g}}(\tau)$ is given by the Belavin–Knizhnik double-pole result and has a universal character for any g. It should also be noticed that this divergence is β independent and the meromormphic structure is similar to the genus-one case. As a consequence, the whole genus dependence of the critical temperature is encoded in the Epstein zeta function $Z_{\mathrm{g}}|^{\mathbf{0}}_{\mathbf{0}}|(2s)$ (see for details Ref. 20).

For this reason, we mention the asymptotic properties of function $Z_{\mathrm{g}}|^{\mathbf{0}}_{\mathbf{0}}|(2s)$. The following result holds:

Corollary 1 (Ref. 20):

$$B_g \equiv \lim_{\Re s \to +\infty} \frac{Z_g|^{\mathbf{b}}_{\mathbf{0}}|(2s+2)}{Z_g|^{\mathbf{b}}_{\mathbf{0}}|(2s)} = [(\hat{b}_1 - \eta_1)^2 + \cdots + (\hat{b}_g - \eta_g)^2]^{-1}, \tag{60}$$

where at least one of the b_i *is noninteger,* $\hat{b}_i = b_i - [b_i]$ *with* $[b_i]$ *the noninteger (decimal) part of* b_i *and*

$$\eta_i = \begin{cases} 0\,, & 0 \leqslant \hat{b}_i \leqslant \frac{1}{2}, \\ 1\,, & \frac{1}{2} \leqslant \hat{b}_i < 1. \end{cases} \tag{61}$$

Furthermore, if $\mathbf{b} = (0,0,\ldots,0)$, *then* $B_g = 1$.

As a consequence, the interactions of bosonic strings do not modify the critical temperature. However, one can consider different linear real bundles over compact Riemann surfaces and spinorial structures on them. The procedure of evaluation of the free energy in terms of the path integral over the metrics does not depend on whatever type of real scalars are considered. This fact leads to new contributions to the genus-g integral (50).

One could investigate the role of these contributions for the torus compactification.[2,18,23] In this case, the sum in Eq. (50) should be taken over the vectors on the lattice on which some space dimensions are compactified. The half-lattice vectors can be labelled by the multiplets $(b_1, \ldots, b_p)$, with $b_i = \frac{1}{2}$. The critical temperature related to the multiplet $\mathbf{b} = (b_1, \ldots, b_p, 0, \ldots, 0)$ can be easily evaluated by means of Eq. (60), which gives $B_p = 4p^{-1}$. As a result $\beta_{c,p} = (2/\sqrt{p})\,\beta_c$. As an example, we note the particular multiplets $(0, \ldots, \frac{1}{2}, \ldots, 0)$ and $(0,..\frac{1}{2},\frac{1}{2},...,0)$, where only one b_i and two b_i are different from zero. In this case we have ''minimal'' critical temperatures given by $\beta_{c,1}^{-1} = \beta_c^{-1}/2$ and $\beta_{c,2}^{-1} = \beta_c^{-1}/\sqrt{2}$, respectively.

VIII. CONCLUDING REMARKS

Making use of the Meinardus theorem in Sec. VI, we found the critical temperatures of the two kinds of pieces in the string (I and II) to be equal and to be given by Eqs. (48) and (49) for arbitrary space–time dimension D. The calculation generalizes earlier calculations of the Casimir energy of the $2N$-piece string in Ref. 7, and of thermodynamics of the two-piece string in Ref. 8. Interactions of bosonic parts of a piecewice uniform string do not modify the critical temperatures. However, for the sectors of parts having a spinor structure, the critical temperatures, associated with genus g, depend on the windings.

It ought to be emphasized again that a fundamental property of this kind of string theory is its *relativistic invariance*. It means the velocity of sound is everywhere required to be equal to the velocity of light. If this requirement were to be abandoned, the regularization procedure would be more difficult. The requirement about relativistic invariance makes the string theory quite analogous to the Casimir theory in a continuous medium satisfying the condition $\varepsilon\mu = 1$, ε being the premittivity and μ the permeability (cf., for instance, Refs. 24 and 25, and also the recent discussion in Ref. 26).

The theory above was worked out in explicit form, making the simplifying assumption $x = T_I/T_{II} \to 0$. It should be noted, however, that no important physical property of the string model is lost by going to the case of extreme string tensions. In particular, as already mentioned, this simplification does not prevent one from distinguishing between the actions for massive and massless particles.

As for physical implications of the string model, we note that it can be looked upon as the vacuum state of a quantum field theory in a two-dimensional space–time endowed with special properties. One of the most fundamental properties of the string is the *negativity* of the Casimir energy. Moreover, as we would expect, the Casimir energy can always be made more negative if the string chooses to divide itself into a larger number of pieces. It becomes natural to suggest that the model could be of some importance for cosmology. Perhaps a ''phase transition'' of this sort played a physical role in the early universe.

Let us also mention another argument, taken from the theory of superstrings, which similarly points towards the physical importance of two-dimensional field theory. In Ref. 27 it is argued that at high temperatures, the free energy for a superstring is $F_{\text{string}} \sim -VT^2$, where V is the volume and T is the temperature. One can compare this with the quantum field theory behavior of the free energy in d spatial dimensions, $F_{QFT} \sim -VT^{d+1}$. It becomes natural to interpret this to mean that the fundamental degrees of freedom in string theory are much less than in quantum field theory in the same dimensions, and that the underlying string theory should be like a two-dimensional quantum field theory. See also the recent discussion in Ref. 28.

ACKNOWLEDGMENT

The research of A. A. Bytsenko has been supported in part by the Russian Foundation for Basic Research (Grant No. 01-02-17157).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 3 MARCH 2003

Adjoint operators, gauge invariant perturbations, and covariant symplectic form for black holes in string theory

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(Received 1 February 2002; accepted 5 December 2002)

Using a scheme of adjoint operators, we give a covariant and gauge invariant treatment for the perturbation theory of static charged black holes in string theory, valid for curvature below the Planck scale; conserved quantities and a covariant symplectic form on the phase space are explicitly constructed. Future extensions of the present results are discussed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1542661]

I. INTRODUCTION

At present, the theories of extended objects such as membranes and strings represent the more viable candidates for a quantum theory of gravity. Particularly, there have been many efforts studying black holes in string theory from different points of view, with the main task of elucidating on the problem of quantum gravity embedded in them, since such objects appear to play a crucial role in the subject. However, because of the many technical and conceptual difficulties in treating the full theory, the low-energy limit of string theory has been developed as a more pragmatic approach. This low-energy physics emerges as an effective action obtained from the lowest order in the world-sheet and string loop expansion, where the usual Einstein–Hilbert gravity is supplemented by gauge fields, scalar fields such as the axion and the dilaton, which couple in a nontrivial way to the other matter fields.[1] As it is well known, the presence of the dilaton changes drastically the dynamical properties of the systems, and new features arise in this theory due to the nontrivial coupling of this field. In particular, dilaton black holes have shown to have novel thermodynamics properties,[2,3] and to behave like elementary particles in the sense that the excitation spectrum has an energy gap.[4–6] Besides, it has been explored the viewpoint that quantum black holes are massive excitations of extended objects and also correspond, in this sense, to elementary particles (Ref. 7, and references cited therein).

In all issues discussed above, the first-order perturbation analysis plays a fundamental role. Perturbation theory revels important physical information of the system under study. As we shall see, the adjoint operators approach will cover, in a unified way, various aspects of the same problem (in this case, the perturbation analysis of string black holes), which traditionally have been treated separately. In the remainder of this Introduction, we discuss such aspects, pointing out our aims and successes in the present work, and we make a review of previous works in which the present approach has been employed.

In the scheme of the perturbation theory, the black holes (and other space–times) have been studied from different approaches. The traditional approaches consist of trying to solve the original set of equations for the field perturbations directly. This approach has several disadvantages and difficulties that can be overcome by means of an alternative and more convenient approach based on the concept of the adjoint of a differential operator (Wald's method). The reach and differences of this approach with respect to the usual ones have been already discussed widely in previous works; in fact, in the cases where string fields are involved, the approach has been

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applied successfully in the setting of the Einstein–Maxwell-dilaton-axion (EMDA) theory, which contains the low-energy limit of string theory as a particular case.[8,9] Additionally, as we shall see, with the connection recently established between adjoint operators and conserved currents,[10–12] Wald's method becomes the more convenient and powerful approach for facing the study of perturbations.

At a more general context, the study of conservation laws in field theories involving gravity becomes particularly interesting because of the lack of conserved currents representing the conservation of energy and momentum. Additionally, in the construction of a *covariant symplectic structure* on the phase space of classical systems, a bilinear product on first-order deformations of classical solutions on such phase space is required.[13–15] In both cases, the problem is to find a local expression physically meaningful and coming from some continuity equation. As we shall see, the present adjoint operators scheme allows us to establish a local continuity law with the features described above, from which conserved quantities and a covariant symplectic structure (in terms of Debye potentials) are derived.

In this manner, the purpose of the present work is to perform an analysis of the first-order perturbations of the dilatonic charged black holes employing Wald's method. Previously, the self-adjointness of the operator governing the field perturbations in the EMDA theory has been demonstrated,[10] leaving only the finding of the corresponding decoupled set of equations in the case where the background space–time corresponds to the solution considered, in order to establish our results.

For this purpose, the outline of this article is as follows. The relevant information on the background solution is given in Sec. II. In Sec. III, a decoupled set of equations for metric, vector potential, and dilaton perturbations is obtained from the original equations for the field perturbations using the Newman–Penrose formulation. Employing the results of Sec. III, the equations for the Debye potentials, and the expressions for the metric, vector potential, and dilaton perturbations in terms of those, are found in Sec. IV A. In Sec. IV B, our fundamental continuity equation is established and a symplectic structure is derived in Sec. IV C. The separation of variables for the equations for the Debye potentials and for the continuity equation is performed in Sec. V, such that two conserved quantities are obtained. Finally, we finish with some concluding remarks and future extensions of the present results.

It is worth pointing out some issues on the notation. The first-order field variations appearing in Refs. 8 and 9 are denoted by a superscript B. On the other hand, the field variations coincide, according to Witten's interpretation,[13,14] with an infinite-dimensional generalization of the usual exterior derivative, which is traditionally represented by the symbol δ. However, in Refs. 8 and 9 and the present work, the Newman–Penrose formalism is used, in which the symbol δ is employed for denoting one of the directional derivatives defined by the null tetrad. In this manner, for avoiding confusion, we will maintain the symbol δ as usual in the Newman–Penrose notation, and the superscript B for the first-order field variations (the exterior derivative of background fields). In the present article, the exterior derivative will not be performed explicitly, and it will be sufficient for our purposes to understand any quantity with the superscript B as a one-form on the phase space. Quantities without such a superscript will correspond to background fields, which mean zero-forms on the phase space. With these previous considerations, formulas and notation of Refs. 8 and 9 will be used throughout this article; the concepts and definitions on differential forms, exterior derivatives, etc., come from Ref. 14.

II. BACKGROUND SPACE–TIME

Static, spherically symmetric solutions of the Einstein–Maxwell-dilaton equations have been found, representing charged black holes for curvature below the Planck scale.[2,3] The solutions for magnetically charged dilaton black holes have, using the metric convention $(+---)$, the line element

$$ds^2=\chi^2 dt^2-\chi^{-2}dr^2-R^2 d\Omega, \tag{1}$$

where χ and R depend only on r:

$$\chi^2=\left(1-\frac{r_+}{r}\right)\left(1-\frac{r_-}{r}\right)^{(1-a^2)/(1+a^2)},\quad R=r\left(1-\frac{r_-}{r}\right)^{a^2/(1+a^2)}, \tag{2}$$

where r_+ and r_- are the values of the parameter r at the outer and the inner horizons, respectively, and are related to the physical mass (M) and charge (Q); a is the dilaton coupling parameter. The Maxwell and dilaton fields are given by

$$F=Q\sin\theta d\theta\wedge d\varphi,\quad e^{-2a\phi}=\left(1-\frac{r_-}{r}\right)^{2a^2/(a^2+1)}\qquad(\xi\equiv -e^{-2a\phi}). \tag{3}$$

There are also electrically charged solutions which may be obtained by a duality rotation. For more details see Refs. 2 and 3.

For our present purpose, it is more convenient to specify the line element (2) by the null tetrad

$$\begin{gathered}D\equiv l^\mu\partial_\mu=\frac{1}{\chi^2}\partial_t+\partial_r,\qquad \Delta\equiv n^\mu\partial_\mu=\frac{1}{2}(\partial_t-\chi^2\partial_r),\\ \delta\equiv m^\mu\partial_\mu=\frac{1}{\sqrt{2}R}(\partial_\theta+i\csc\theta\partial_\varphi),\quad \bar{\delta}\equiv\bar{m}^\mu\partial_\mu=\frac{1}{\sqrt{2}R}(\partial_\theta-i\csc\theta\partial_\varphi).\end{gathered} \tag{4}$$

Using the commutation relations of the tetrad (4), the nonvanishing spin coefficients can be conveniently expressed as

$$\begin{gathered}\rho=D\ln R^{-1},\quad \mu=\Delta\ln R,\quad \gamma=\Delta\ln\chi^{-1},\\ \beta=\delta\ln\sin^{1/2}\theta,\quad \alpha=-\bar{\delta}\ln\sin^{1/2}\theta,\end{gathered} \tag{5}$$

where ρ, μ, and γ depend only on r, and β and α on both r and θ.

On the other hand, considering the first of Eqs. (3) and the definitions $\varphi_0\equiv l^\mu m^\nu F_{\mu\nu}$, $\varphi_1\equiv\frac{1}{2}(l^\mu n^\nu+\bar{m}^\mu m^\nu)F_{\mu\nu}$, and $\varphi_2\equiv\bar{m}^\mu n^\nu F_{\mu\nu}$, the Newman–Penrose components of the electromagnetic field are given by

$$\varphi_0=0=\varphi_2,\quad \varphi_1(r)=\frac{iQ}{2R^2}. \tag{6}$$

Note that $\varphi_1+\bar{\varphi_1}=0=\delta\phi_1$, which will be used implicitly below. On the other hand, from Eqs. (3) and (4), the only nonvanishing derivatives of the dilaton field are $D\phi$ and $\Delta\phi$, which depend only on r, and

$$\delta\phi=0=\bar{\delta}\phi. \tag{7}$$

Thus, the only nonvanishing Ricci scalars are (see Appendix of Ref. 8)

$$\begin{gathered}\Phi_{00}=-(D\phi)^2,\quad \Phi_{22}=-(\Delta\phi)^2,\\ \Phi_{11}=-\tfrac{1}{2}(D\phi)(\Delta\phi)-2\xi\varphi_1^2,\quad \Lambda=-\tfrac{1}{6}(D\phi)(\Delta\phi),\end{gathered} \tag{8}$$

and the only nonvanishing component of the Weyl spinor can be expressed as

$$\Psi_2(r)=2\gamma\rho-\tfrac{2}{3}D\phi\Delta\phi. \tag{9}$$

Furthermore, the background Maxwell equations take the form[8]

$$(D-2\rho)\varphi_1=0, \quad (\Delta+2\mu)\varphi_1=0, \tag{10}$$

and, similarly, the background dilaton equation is

$$D\Delta\phi+2\mu D\phi-2a\xi\varphi_1^2=0. \tag{11}$$

Additionally, using Eqs. (4)–(9) and the commutation relations, we can find the following relations:

$$\begin{aligned}(D+p\rho)(\delta+q\beta)&=(\delta+q\beta)[D+(p+1)\rho],\\ (\Delta+p\gamma+p'\mu)(\delta+q\beta)&=(\delta+q\beta)[\Delta+p\gamma+(p'-1)\mu],\end{aligned} \tag{12}$$

where p, q, and p' are arbitrary constants.

In the Newman–Penrose formalism, the adjoints of the tetrad components (4) are given, in general, by Eqs. (16) of Ref. 8, which reduce to

$$D^\dagger=-(D-2\rho), \quad \Delta^\dagger=-(\Delta-2\gamma+2\mu), \quad \delta^\dagger=-(\delta+2\beta), \quad \overline{\delta}^\dagger=-(\overline{\delta}+2\overline{\beta}), \tag{13}$$

for the present background solution. These equations will be used below.

III. DECOUPLED SET OF EQUATIONS FOR GAUGE INVARIANT PERTURBATIONS

The notation, conventions, and Appendix of Ref. 8 will be used extensively throughout this article. In particular, the metric, vector potential, and dilaton variations are represented by $h_{\mu\nu}$, b_μ, and ϕ^{B}, respectively. The metric and vector potential perturbations are defined modulo gauge transformations. Since the dilaton is a fundamental physical field, no gauge invariance associated with this field exists.

On the other hand, it is well known that when the perturbation analysis is performed using the Newman–Penrose formalism, one is faced with the perturbed tetrad gauge freedom. The traditional approaches make use of this gauge freedom in order to simplify the equations for the perturbations (Ref. 8 and references therein). However, we shall see that in the present case, although including string fields, there is no need to invoke perturbed tetrad rotations, but that appropriate combinations of the perturbed quantities, which are independent on the perturbed tetrad gauge freedom, lead in a natural way to a decoupled set of equations from the original set. Such combinations prove to be also independent on the ordinary gauge transformations of the electromagnetic potential perturbations. This system of equations consists of five second-order linear partial differential equations for five unknowns, Ψ_0^{B}, $\overline{\Psi_4^{\mathrm{B}}}$, $\tilde{\sigma}$, $\tilde{\lambda}$, and $(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}$, and can be expressed in the following matrix form (a detailed derivation of this system is given in Ref. 12):

$$\mathcal{O}(\Psi^{\mathrm{B}})=\mathcal{S}\begin{pmatrix}(T_{\mu\nu})\\(j_\mu)\\ \phi_s\end{pmatrix}, \tag{14}$$

where $\mathcal{O}$ is the 5×5 matrix

$$\mathcal{O}\equiv\begin{pmatrix}\mathcal{O}_{11} & 0 & \mathcal{O}_{13} & -F_1D\phi & F_1\\ 0 & \mathcal{O}_{22} & \frac{\chi^4}{4}\Delta\phi F_1 & \mathcal{O}_{24} & \frac{\chi^4}{4}F_1\\ \mathcal{O}_{31} & 0 & \mathcal{O}_{33} & \mathcal{O}_{34} & \mathcal{O}_{35}\\ 0 & \mathcal{O}_{42} & \mathcal{O}_{43} & \mathcal{O}_{44} & \mathcal{O}_{45}\\ \frac{\chi^4}{8}F_1 & \frac{1}{2}F_1 & \mathcal{O}_{53} & \mathcal{O}_{54} & \mathcal{O}_{55}\end{pmatrix}, \tag{15}$$

$$(\Psi^{\mathrm{B}})\equiv\begin{pmatrix}\dfrac{\Psi_0^{\mathrm{B}}}{\Psi_4^{\mathrm{B}}}\\ \tilde{\sigma}^{\mathrm{B}}\\ \tilde{\lambda}^{\mathrm{B}}\\ (\delta-2\beta)\tilde{\phi}^{\mathrm{B}}\end{pmatrix}, \tag{16}$$

and $\mathcal{S}$ is the 5×3 matrix

$$\mathcal{S}\equiv\begin{pmatrix}\mathcal{S}_{11} & 0 & 0\\ \mathcal{S}_{21} & 0 & 0\\ \mathcal{S}_{31} & \mathcal{S}_{32} & 0\\ \mathcal{S}_{41} & \mathcal{S}_{42} & 0\\ \mathcal{S}_{51} & \mathcal{S}_{52} & \mathcal{S}_{53}\end{pmatrix}, \tag{17}$$

where the entries are given explicitly by

$$\mathcal{O}_{11}=(D-5\rho)(\Delta-4\gamma+\mu)-(\delta-2\beta)(\bar{\delta}+4\bar{\beta})-(3\Psi_2-2\Phi_{11}+2D\phi\Delta\phi),$$

$$\mathcal{O}_{13}=-8\xi\varphi_1^2D-4D\phi(\gamma D\phi-3a\xi\varphi_1^2),$$

$$F_1(r)=8\chi^{-2}D\phi\left(\gamma+\frac{a\xi\varphi_1^2}{D\phi}\right),$$

$$\mathcal{O}_{22}=(\Delta+2\gamma+5\mu)(D-\rho)-(\delta-2\beta)(\bar{\delta}+4\bar{\beta})-(3\Psi_2+2D\phi\Delta\phi-2\Phi_{11}),$$

$$\mathcal{O}_{24}=8\xi\varphi_1^2(\Delta+2\gamma)+4\Delta\phi(\gamma D\phi-3a\xi\varphi_1^2),$$

$$\mathcal{O}_{31}=\Delta-4\gamma+2\mu,$$

$$\mathcal{O}_{33}=(\Delta-4\gamma)(D-2\rho)-aD\phi(\Delta-2\gamma)-(\delta-2\beta)(\bar{\delta}+4\bar{\beta})-2(3\Psi_2+2\Phi_{11}),$$

$$\mathcal{O}_{34}=-aD\phi D+2\Phi_{00},$$

$$\mathcal{O}_{35}=a(D-2\rho)-2D\phi, \tag{18}$$

$$\mathcal{O}_{42}=D-2\rho,$$

$$\mathcal{O}_{43}=a\Delta\phi(\Delta-2\gamma)-2\Phi_{22},$$

$$\mathcal{O}_{44}=-D(\Delta+2\gamma+2\mu)+a\Delta\phi D+(\delta-2\beta)(\bar{\delta}+4\bar{\beta})+2(3\Psi_2+2\Phi_{11}),$$

$$\mathcal{O}_{45}=a(\Delta+2\mu)-2\Delta\phi,$$

$$\mathcal{O}_{53}=-\frac{\chi^4}{8}F_1(D-2\rho)+[\Delta\phi(D-\rho)-2a\xi\varphi_1^2](\Delta-2\gamma+\mu)$$
$$-\Delta\phi(\delta-2\beta)(\bar{\delta}+4\bar{\beta})-\mu F_2-\Phi_{22}D\phi,$$

$$\mathcal{O}_{54}=(F_2-\mu D\phi)(D-\rho)-(D-3\rho)D\phi(\Delta+2\gamma+2\mu)+D\phi(\delta-2\beta)(\bar{\delta}+4\bar{\beta})$$
$$+[(\Delta\phi D-2a\xi\varphi_1^2)\rho]+D\phi(3\Psi_2+2\Phi_{11}),$$

$$\mathcal{O}_{55}=(D-3\rho)(\Delta+3\mu)-(\delta-2\beta)(\overline{\delta}+4\overline{\beta})-3\Psi_2+2\mu\rho-3D\phi\Delta\phi-4(a^2-1)\xi\varphi_1^2,$$

$$F_2\equiv 2D\phi\left(\mu+\frac{a\xi\varphi_1^2}{D\phi}\right),$$

and

$$\mathcal{S}_{11}=2(\delta-2\beta)(D-3\rho)l^{(\mu}m^{\nu)}-[(D-5\rho)(D-\rho)+\Phi_{00}]m^\mu m^\nu-(\delta-2\beta)\delta l^\mu l^\nu,$$

$$\mathcal{S}_{21}=2(\delta-2\beta)(\Delta+2\gamma+3\mu)n^{(\mu}m^{\nu)}-[(\Delta+2\gamma+5\mu)(\Delta+\mu)+\Phi_{22}]m^\mu m^\nu-(\delta-2\beta)\delta n^\mu n^\nu,$$

$$\mathcal{S}_{31}=2(\delta-2\beta)l^{(\mu}m^{\nu)}-2(D-\rho)m^\mu m^\nu,$$

$$\mathcal{S}_{32}=\frac{1}{2\varphi_1}(\delta-2\beta)[(D-3\rho)\xi^{-1}m^\mu-\delta\xi^{-1}l^\mu],$$

$$\mathcal{S}_{41}=2(\delta-2\beta)n^{(\mu}m^{\nu)}-2(\Delta+\mu)m^\mu m^\nu, \tag{19}$$

$$\mathcal{S}_{42}=\frac{1}{2\varphi_1}(\delta-2\beta)[(\Delta+3\mu)\xi^{-1}m^\mu-\delta\xi^{-1}n^\mu],$$

$$\mathcal{S}_{51}=2D\phi(\delta-2\beta)n^{(\nu}m^{\nu)}+2\Delta\phi(\delta-2\beta)l^{(\nu}m^{\nu)}+(4a\xi\varphi_1^2-\Delta\phi D-D\phi\Delta)m^\mu m^\nu,$$

$$\mathcal{S}_{52}=-4a\varphi_1(\delta-2\beta)m^\mu,$$

$$\mathcal{S}_{53}=\tfrac{1}{2}(\delta-2\beta)\delta.$$

Note that both $\mathcal{O}$ and $\mathcal{S}$ depend only on the background fields. As mentioned previously, a gauge-fixing condition on the perturbed tetrad is unnecessary for obtaining the complete system (14). Furthermore, the entries of the matrix (Ψ^{B}) are automatically independent on the gauge transformations of the vector potential variations b_μ: $(\Psi^{\mathrm{B}})(h_{\mu\nu},b_\mu)=(\Psi^{\mathrm{B}})(h_{\mu\nu},b_\mu+\nabla_\mu\varepsilon)$. In this manner, the invariance under the gauge freedoms of the matter fields and the perturbed tetrad is guaranteed. This issue will be particularly important below, when we discuss the bilinear forms on the reduced phase space.

In the traditional approach, the field perturbations are separated in polar and axial perturbations (and some gauge-fixing conditions are imposed) with the purpose of reducing the equations governing the perturbations to Schrödinger-type equations, and then to apply semiclassical methods based on the Hermiticity of such a system of equations. However, as shown in Ref. 11, such treatment is unnecessary, and for many aims one can obtain essentially the same physical results working directly with the original non-Hermitian system of equations. In fact, when string fields are involved, such as the present case, those reductions seem to be very difficult to carry out, or, when possible, the interaction matrix is too complex to be displayed in explicit form.[5] Therefore, Eqs. (14) in their original form, without separations nor reductions, are sufficient for our present purposes.

IV. LOCAL CONTINUITY LAWS ON THE PHASE SPACE AND DEBYE POTENTIALS

A. Equations for the Debye potentials

Following that made in Ref. 12, if the matrix potential (ψ) satisfies $\mathcal{O}^{\dagger}(\psi)=0$, with

$$(\psi)=\begin{pmatrix}\psi_G\\ \psi_H\\ \psi_E\\ \psi_F\\ \psi_D\end{pmatrix}, \tag{20}$$

then the metric, vector potential, and dilaton *real* variations are given by

$$\begin{pmatrix}-\frac{1}{2}h_{\mu\nu}\\ 2b_{\mu}\\ \phi^{\mathrm{B}}\end{pmatrix}=\mathcal{S}^{\dagger}(\psi)=\begin{pmatrix}\mathcal{S}^{\dagger}_{11}\psi_G+\mathcal{S}^{\dagger}_{21}\psi_H+\mathcal{S}^{\dagger}_{31}\psi_E+\mathcal{S}^{\dagger}_{41}\psi_F+\mathcal{S}^{\dagger}_{51}\psi_D+\text{c.c.}\\ \mathcal{S}^{\dagger}_{32}\psi_E+\mathcal{S}^{\dagger}_{42}\psi_F+\mathcal{S}^{\dagger}_{52}\psi_D+\text{c.c.}\\ \mathcal{S}^{\dagger}_{53}\psi_D+\text{c.c.}\end{pmatrix}; \tag{21}$$

from Eqs. (13), and (19), we have explicitly that

$$\mathcal{S}^{\dagger}_{11}=2l_{(\mu}m_{\nu)}(D+\rho)(\delta+4\beta)-m_{\mu}m_{\nu}[(D-\rho)(D+3\rho)+\Phi_{00}]-l_{\mu}l_{\nu}(\delta+2\beta)(\delta+4\beta),$$

$$\mathcal{S}^{\dagger}_{21}=2n_{(\mu}m_{\nu)}(\Delta-4\gamma-\mu)(\delta+4\beta)-m_{\mu}m_{\nu}[(\Delta-2\gamma+\mu)(\Delta-4\gamma-3\mu)+\Phi_{22}]$$
$$-n_{\mu}n_{\nu}(\delta+2\beta)(\delta+4\beta),$$

$$\mathcal{S}^{\dagger}_{31}=2m_{\mu}m_{\nu}(D-\rho)-2l_{(\mu}m_{\nu)}(\delta+4\beta),$$

$$\mathcal{S}^{\dagger}_{41}=2m_{\mu}m_{\nu}(\Delta-2\gamma+\mu)-2n_{(\mu}m_{\nu)}(\delta+4\beta),$$

$$\mathcal{S}^{\dagger}_{51}=-2D\phi n_{(\mu}m_{\nu)}(\delta+4\beta)-2\Delta\phi l_{(\mu}m_{\nu)}(\delta+4\beta)+m_{\mu}m_{\nu}(8a\xi\varphi_1^2+\Delta\phi D+D\phi\Delta), \tag{22}$$

$$\mathcal{S}^{\dagger}_{32}=\frac{1}{2\xi}[m_{\mu}(D+\rho)-l_{\mu}(\delta+2\beta)](\delta+4\beta)\frac{1}{\varphi_1},$$

$$\mathcal{S}^{\dagger}_{42}=\frac{1}{2\xi}[m_{\mu}(\Delta-2\gamma-\mu)-n_{\mu}(\delta+2\beta)](\delta+4\beta)\frac{1}{\varphi_1},$$

$$\mathcal{S}^{\dagger}_{52}=4a\varphi_1 m_{\mu}(\delta+4\beta),$$

$$\mathcal{S}^{\dagger}_{53}=\frac{1}{2}(\delta+2\beta)(\delta+4\beta).$$

In this manner, the complete field variations are given by Eqs. (21) in terms of the Debye potentials, which satisfy a system of five second-order linear partial differential equations:

$$\mathcal{O}^{\dagger}(\psi)=\begin{pmatrix} \mathcal{O}^{\dagger}_{11} & 0 & \mathcal{O}^{\dagger}_{31} & 0 & \frac{\chi^4}{8}F_1 \\ 0 & \mathcal{O}^{\dagger}_{22} & 0 & \mathcal{O}^{\dagger}_{42} & \frac{1}{2}F_1 \\ \mathcal{O}^{\dagger}_{13} & \frac{\chi^4}{4}\Delta\phi F_1 & \mathcal{O}^{\dagger}_{33} & \mathcal{O}^{\dagger}_{43} & \mathcal{O}^{\dagger}_{53} \\ -F_1 D\phi & \mathcal{O}^{\dagger}_{24} & \mathcal{O}^{\dagger}_{34} & \mathcal{O}^{\dagger}_{44} & \mathcal{O}^{\dagger}_{54} \\ F_1 & \frac{\chi^4}{4}F_1 & \mathcal{O}^{\dagger}_{35} & \mathcal{O}^{\dagger}_{45} & \mathcal{O}^{\dagger}_{55} \end{pmatrix}\begin{pmatrix} \psi_G \\ \psi_H \\ \psi_E \\ \psi_F \\ \psi_D \end{pmatrix}=0, \tag{23}$$

where

$$\mathcal{O}^{\dagger}_{11}=(\Delta+2\gamma+\mu)(D+3\rho)-(\bar{\delta}-2\bar{\beta})(\delta+4\beta)-(3\Psi_2-2\Phi_{11}+2D\phi\Delta\phi),$$

$$\mathcal{O}^{\dagger}_{13}=8\xi\varphi_1^2(D+2\rho)+F_1\Delta\phi,$$

$$\mathcal{O}^{\dagger}_{22}=(D-\rho)(\Delta-4\gamma-3\mu)-(\bar{\delta}-2\bar{\beta})(\delta+4\beta)-(3\Psi_2-2\Phi_{11}+2D\phi\Delta\phi),$$

$$\mathcal{O}^{\dagger}_{24}=-8\xi\varphi_1^2(\Delta-4\gamma-2\mu)+\frac{\chi^2}{2}F_1\Delta\phi,$$

$$\mathcal{O}^{\dagger}_{31}=-(\Delta+2\gamma),$$

$$\mathcal{O}^{\dagger}_{33}=D(\Delta+2\gamma+2\mu)+aD\phi(\Delta+2\mu)-(\bar{\delta}-2\bar{\beta})(\delta+4\beta)-2(3\Psi_2+2\Phi_{11})+a\Delta D\phi,$$

$$\mathcal{O}^{\dagger}_{34}=aD\phi(D-2\rho)+aD^2\phi+2\Phi_{00}, \tag{24}$$

$$\mathcal{O}^{\dagger}_{35}=-aD-2D\phi, \quad \mathcal{O}^{\dagger}_{42}=-D, \quad \mathcal{O}^{\dagger}_{43}=-a\Delta\phi(\Delta+2\mu)-a\Delta^2\phi-2\Phi_{22},$$

$$\mathcal{O}^{\dagger}_{44}=-(\Delta-4\gamma+a\Delta\phi)(D-2\rho)+(\bar{\delta}-2\bar{\beta})(\delta+4\beta)+2(3\Psi_2+2\Phi_{11})-aD\Delta\phi,$$

$$\mathcal{O}^{\dagger}_{45}=-a(\Delta-2\gamma)-2\Delta\phi,$$

$$\mathcal{O}^{\dagger}_{53}=\tfrac{1}{8}D\chi^4F_1+(\Delta+\mu)(4a\xi\varphi_1^2-\mu D\phi+\Delta\phi D)-\Delta\phi(\bar{\delta}-2\bar{\beta})(\delta+4\beta)-\Phi_{22}D\phi-\mu F_2,$$

$$\mathcal{O}^{\dagger}_{54}=-(D-\rho)(F_2-\mu D\phi)-(\Delta-4\gamma)D\phi(D+\rho)+D\phi(\bar{\delta}-2\bar{\beta})(\delta+4\beta)$$
$$+[(\Delta\phi D-2a\xi\varphi_1^2)\rho]+D\phi(3\Psi_2+2\Phi_{11}),$$

$$\mathcal{O}^{\dagger}_{55}=(\Delta-2\gamma-\mu)(D+\rho)-(\bar{\delta}-2\bar{\beta})(\delta+4\beta)-3\Psi_2+2\mu\rho-3D\phi\Delta\phi+4(a^2-1)\xi\varphi_1^2,$$

and Eqs. (13), and (18) have been used. Equations (23) are our fundamental equations since, as we shall see, all conserved quantities and bilinear forms on the phase space are defined in terms of the Debye potentials. Although these equations admit separable solutions in a simple way, we will use them first in the form (23) in order to establish a *covariant* conservation law, and subsequently to carry out such separation.

B. Covariant continuity equation and bilinear forms on the phase space

Since the decoupled system (14) and the system of equations for the Debye potentials (23) are adjoints to each other, we have that[12]

$$(\psi)\mathcal{O}(\Psi^{\mathrm{B}})-\mathcal{O}^{\dagger}(\psi)(\Psi^{\mathrm{B}})=\nabla_{\mu}J^{\mu}(\psi,\Psi^{\mathrm{B}}). \tag{25}$$

The left-hand side contains terms of the form $\psi_G\mathcal{O}_{11}\Psi_0^{\mathrm{B}}-\mathcal{O}_{11}^{\dagger}\psi_G\Psi_0^{\mathrm{B}}$ [see Eqs. (15), and (23)], which can be expressed in the following form, considering the explicit forms of the operators $\mathcal{O}_{11}$, and $\mathcal{O}_{11}^{\dagger}$ given in Eqs. (18) and (24), respectively, that $D\equiv l^{\mu}\partial_{\mu}$, $\Delta\equiv n^{\mu}\partial_{\mu}$, $\delta\equiv m^{\mu}\partial_{\mu}$, $\overline{\delta}\equiv\overline{m}^{\mu}\partial_{\mu}$, and that they are acting on scalar fields:

$$\begin{aligned}\psi_G\mathcal{O}_{11}\Psi_0^{\mathrm{B}}-\mathcal{O}_{11}^{\dagger}\psi_G\Psi_0^{\mathrm{B}}=\nabla_{\mu}[&l^{\mu}\psi_G(\Delta-4\gamma+\mu)\Psi_0^{\mathrm{B}}-n^{\mu}(D+3\rho)\psi_G\Psi_0^{\mathrm{B}}-m^{\mu}\psi_G(\overline{\delta}+4\overline{\beta})\Psi_0^{\mathrm{B}}\\&+\overline{m}^{\mu}(\delta+4\beta)\psi_G\Psi_0^{\mathrm{B}}],\end{aligned} \tag{26}$$

and similarly for the remaining terms:

$$\begin{aligned}
&\psi_G\mathcal{O}_{13}\tilde{\sigma}^{\mathrm{B}}-\mathcal{O}_{13}^{\dagger}\psi_G\tilde{\sigma}^{\mathrm{B}}=\nabla_{\mu}(-8\xi\varphi_1^2l^{\mu}\psi_G\tilde{\sigma}^{\mathrm{B}}),\\
&\psi_H\mathcal{O}_{22}\overline{\Psi_4^{\mathrm{B}}}-\mathcal{O}_{22}^{\dagger}\psi_H\overline{\Psi_4^{\mathrm{B}}}=\nabla_{\mu}[n^{\mu}\psi_H(D-\rho)\overline{\Psi_4^{\mathrm{B}}}-l^{\mu}(\Delta-4\gamma-3\mu)\psi_H\overline{\Psi_4^{\mathrm{B}}}-m^{\mu}\psi_H(\overline{\delta}+4\overline{\beta})\overline{\Psi_4^{\mathrm{B}}}\\
&\qquad+\overline{m}^{\mu}(\delta+4\beta)\psi_H\overline{\Psi_4^{\mathrm{B}}}],\\
&\psi_H\mathcal{O}_{24}\tilde{\lambda}^{\mathrm{B}}-\mathcal{O}_{24}^{\dagger}\psi_H\tilde{\lambda}^{\mathrm{B}}=\nabla_{\mu}[8\xi\varphi_1^2n^{\mu}\psi_H\tilde{\lambda}^{\mathrm{B}}),\\
&\psi_E\mathcal{O}_{31}\Psi_0^{\mathrm{B}}-\mathcal{O}_{31}^{\dagger}\psi_E\Psi_0^{\mathrm{B}}=\nabla_{\mu}[n^{\mu}\psi_E\Psi_0^{\mathrm{B}}],\\
&\psi_E\mathcal{O}_{33}\tilde{\sigma}^{\mathrm{B}}-\mathcal{O}_{33}^{\dagger}\psi_E\tilde{\sigma}^{\mathrm{B}}=\nabla_{\mu}[n^{\mu}\psi_E(D-2\rho-aD\phi)\tilde{\sigma}^{\mathrm{B}}-l^{\mu}(\Delta+2\gamma+2\mu)\psi_E\tilde{\sigma}^{\mathrm{B}}\\
&\qquad-m^{\mu}\psi_E(\overline{\delta}+4\overline{\beta})\tilde{\sigma}^{\mathrm{B}}+\overline{m}^{\mu}(\delta+4\beta)\psi_E\tilde{\sigma}^{\mathrm{B}}],\\
&\psi_E\mathcal{O}_{34}\tilde{\lambda}^{\mathrm{B}}-\mathcal{O}_{34}^{\dagger}\psi_E\tilde{\lambda}^{\mathrm{B}}=\nabla_{\mu}(-aD\phi l^{\mu}\psi_E\tilde{\lambda}^{\mathrm{B}}),\\
&\psi_E\mathcal{O}_{35}(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}-\mathcal{O}_{35}^{\dagger}\psi_E(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}=\nabla_{\mu}[al^{\mu}\psi_E(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}],\\
&\psi_F\mathcal{O}_{42}\overline{\Psi_4^{\mathrm{B}}}-\mathcal{O}_{42}^{\dagger}\psi_F\overline{\Psi_4^{\mathrm{B}}}=\nabla_{\mu}(l^{\mu}\psi_F\overline{\Psi_4^{\mathrm{B}}}),\\
&\psi_F\mathcal{O}_{43}\tilde{\sigma}^{\mathrm{B}}-\mathcal{O}_{43}^{\dagger}\psi_E\tilde{\sigma}^{\mathrm{B}}=\nabla_{\mu}[a\Delta\phi n^{\mu}\psi_F\tilde{\sigma}^{\mathrm{B}}],\\
&\psi_F\mathcal{O}_{44}\tilde{\lambda}^{\mathrm{B}}-\mathcal{O}_{44}^{\dagger}\psi_F\tilde{\lambda}^{\mathrm{B}}=\nabla_{\mu}[n^{\mu}(D-2\rho)\psi_F\tilde{\lambda}^{\mathrm{B}}-l^{\mu}\psi_F(\Delta+2\gamma+2\mu-a\Delta\phi)\tilde{\lambda}^{\mathrm{B}}+m^{\mu}\psi_F(\overline{\delta}+4\overline{\beta})\tilde{\lambda}^{\mathrm{B}}\\
&\qquad-\overline{m}^{\mu}(\delta+4\beta)\psi_F\tilde{\lambda}^{\mathrm{B}}],\\
&\psi_F\mathcal{O}_{45}(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}-\mathcal{O}_{45}^{\dagger}\psi_F(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}=\nabla_{\mu}[an^{\mu}\psi_F(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}],\\
&\psi_D\mathcal{O}_{53}\tilde{\sigma}^{\mathrm{B}}-\mathcal{O}_{53}^{\dagger}\psi_D\tilde{\sigma}^{\mathrm{B}}=\nabla_{\mu}\Bigg[-n^{\mu}(\Delta\phi D-\mu D\phi+4a\xi\varphi_1^2)\psi_D\tilde{\sigma}^{\mathrm{B}}+l^{\mu}\Delta\phi\psi_D\left(\Delta+\mu+\frac{2a\xi\varphi_1^2}{D\phi}\right)\tilde{\sigma}^{\mathrm{B}}\\
&\qquad-\Delta\phi m^{\mu}\psi_D(\overline{\delta}+4\overline{\beta})\tilde{\sigma}^{\mathrm{B}}+\Delta\phi\overline{m}^{\mu}(\delta+4\beta)\psi_D\tilde{\sigma}^{\mathrm{B}}\Bigg],\\
&\psi_D\mathcal{O}_{54}\tilde{\lambda}^{\mathrm{B}}-\mathcal{O}_{54}^{\dagger}\psi_D\tilde{\lambda}^{\mathrm{B}}=\nabla_{\mu}\Bigg[D\phi n^{\mu}(D+\rho)\psi_D\tilde{\lambda}^{\mathrm{B}}-D\phi l^{\mu}\psi_D\left(\Delta+2\gamma+\mu-\frac{2a\xi\varphi_1^2}{D\phi}\right)\tilde{\lambda}^{\mathrm{B}}\\
&\qquad+D\phi m^{\mu}\psi_D(\overline{\delta}+4\overline{\beta})\tilde{\lambda}^{\mathrm{B}}-D\phi\overline{m}^{\mu}(\delta+4\beta)\psi_D\tilde{\lambda}^{\mathrm{B}}\Bigg],
\end{aligned} \tag{27}$$

$$\psi_D \mathcal{O}_{55}(\delta-2\beta)\tilde{\phi}^{\mathrm{B}} - \mathcal{O}^{\dagger}_{55}\psi_D(\delta-2\beta)\tilde{\phi}^{\mathrm{B}} = \nabla_\mu[-n^\mu(D+\rho)\psi_D(\delta-2\beta)\tilde{\phi}^{\mathrm{B}} + l^\mu\psi_D(\Delta+3\mu) \times(\delta-2\beta)\tilde{\phi}^{\mathrm{B}} - m^\mu\psi_D(\bar{\delta}+4\bar{\beta})(\delta-2\beta)\tilde{\phi}^{\mathrm{B}} + \bar{m}^\mu(\delta+4\beta)\psi_D(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}].$$

Moreover, from Eqs. (14) and (23) $\mathcal{O}(\Psi^{\mathrm{B}})=0$ and $\mathcal{O}^{\dagger}(\psi)=0$. [The presence of an inhomogeneous term corresponding to the additional sources of the field variations in Eqs. (14) is only a *knack* for finding the operator $\mathcal{S}$. Finally we set $T_{\mu\nu}=0$, $j_\mu=0$, $\phi_s=0$.] Hence, from Eq. (25) we have the local continuity law:

$$\nabla_\mu J^\mu(\Psi^{\mathrm{B}},\psi)=0,$$
$$J^\mu = J^\mu_{11}+J^\mu_{13}+J^\mu_{22}+J^\mu_{24}+J^\mu_{31}+J^\mu_{33}+J^\mu_{34}+J^\mu_{35}+J^\mu_{42}+J^\mu_{43}+J^\mu_{44}+J^\mu_{45}+J^\mu_{53}+J^\mu_{54}+J^\mu_{55}, \tag{28}$$

and, of course, the J^μ_{ij}'s $(i,j=1,2,3,4,5)$ are the components coming from Eqs. (26), and (27); for example, $J^\mu_{34}=-aD\phi l^\mu\psi_E\tilde{\lambda}^{\mathrm{B}}$. Thus, J^μ is a *covariantly* conserved current. We will discuss now the properties and physical meaning of J^μ.

It is easy to verify that, such as (Ψ^{B}) in Eq. (16), the matrix potential (ψ) in Eq. (20) is made out of one-forms. Equations (21) give the field variations $h_{\mu\nu}$, b_μ, and ϕ^{B} (one-forms), in terms of (ψ). Since the operator $\mathcal{S}^\dagger$ is dependent only on background fields (zero-forms), thus (ψ) corresponds to one-forms. This implies automatically that $J^\mu=J^\mu(\Psi^{\mathrm{B}},\psi)$ in Eq. (28) is a (non-degenerate) two-form on the corresponding phase space of the solution considered (the matrix operators $\mathcal{O}$ and $\mathcal{O}^\dagger$ involved in the construction of J^μ are also dependent only on the background fields). In next section, we will demonstrate that J^μ is a *closed* two-form on the phase space, from which a symplectic structure will be constructed.

C. Covariant symplectic structure on the phase space

For demonstrating that J^μ is a closed two-form, we need to rewrite the J^μ_{ij}'s in Eq. (28). For example, J^μ_{11} [see Eq. (26)] can be rewritten as

$$\begin{aligned} &l^\mu\psi_G(\Delta-4\gamma+\mu)\Psi_0^{\mathrm{B}} - n^\mu(D+3\rho)\psi_G\Psi_0{}^{\mathrm{B}} - m^\mu\psi_G(\bar{\delta}+4\bar{\beta})\Psi_0^{\mathrm{B}} + \bar{m}^\mu(\delta+4\beta)\psi_G\Psi_0^{\mathrm{B}} \\ &\quad = -[l^\mu\psi_G(\Delta-4\gamma+\mu)\Psi_0]^{\mathrm{B}} + [n^\mu(D+3\rho)\psi_G\Psi_0]^{\mathrm{B}} + [m^\mu\psi_G(\bar{\delta}+4\bar{\beta})\Psi_0]^{\mathrm{B}} \\ &\qquad -[\bar{m}^\mu(\delta+4\beta)\psi_G\Psi_0]^{\mathrm{B}}, \end{aligned} \tag{29}$$

where we have considered that Ψ_0 vanishes at the background, and the Leibniz rule for the exterior derivative. Eq. (29), implies that J^μ_{11} is an *exact* two-form, and automatically a closed two-form. Similarly, using the fact that $\overline{\Psi_4^{\mathrm{B}}}$, $\tilde{\sigma}^{\mathrm{B}}$, $\tilde{\lambda}^{\mathrm{B}}$, and $(\delta-2\beta)\tilde{\phi}^{\mathrm{B}}$ can be expressed as variations of vanishing background fields, and the property of exterior derivative used above, we can find that

$$(J^\mu_{ij})^{\mathrm{B}}=0, \tag{30}$$

which makes that J^μ itself to be closed. In this manner, the geometrical structure defined as $\omega \equiv \int_\Sigma J^\mu d\Sigma_\mu$, where Σ is an initial value hypersurface, corresponds to a symplectic structure on the phase space. As J^μ is conserved, ω is independent of the choice of Σ and, in particular, is Poincaré invariant. Since (Ψ^{B}) is invariant under gauge transformation of b_μ, J^μ and ω have the same invariance properties. Hence, we have constructed a gauge-invariant closed two-form ω on the reduced phase space, which means the phase space modulo gauge transformations. Similarly, J^μ and ω are independent of the perturbed tetrad gauge freedom.

V. SEPARATION OF VARIABLES AND CONSERVED QUANTITIES

Our fundamental equations for the Debye potentials (23) and the continuity equation (28) admit separation of variables in terms of harmonic time and the spin-weighted spherical harmonics. The first ones are reduced to a system of *ordinary* differential equations for the radial parts of the potentials, the second one yields two conserved quantities expressed in terms of such radial parts.

A. Separable solutions for the potentials

An advantage of using the Newman–Penrose formalism is that each quantity has a type, and its corresponding boost weight and spin weight. This property suggests the separable solutions more convenient for the equations under study.

More specifically, the effect of the (relevant) Geroch–Held–Penrose operators on the spin-weighted spherical harmonics is given by[16]

$$\begin{aligned} \text{Þ}_s Y_{lm} &= (\delta - 2s\beta)\,{}_sY_{lm} = \frac{1}{\sqrt{2}R}[(l-s)(l+s+1)]^{1/2}\,{}_{s+1}Y_{lm}, \\ \text{Þ}'_s Y_{lm} &= (\bar{\delta} + 2s\bar{\beta})\,{}_sY_{lm} = -\frac{1}{\sqrt{2}R}[(l+s)(l-s+1)]^{1/2}\,{}_{s-1}Y_{lm}, \end{aligned} \tag{31}$$

where Eqs. (4) and (5) have been used. On the other hand, from Eqs. (23), it is easy to determine that the potentials ψ_G, ψ_H, ψ_E, ψ_F, and ψ_D have types $\{-4,0\}$, $\{0,4\}$, $\{-3,1\}$, $\{-1,3\}$, and $\{-2,2\}$, respectively. Therefore, all potentials have spin weight -2. Thus, making use of the fact that the background solution is static and spherically symmetric, we seek for solutions for the potentials of the form:

$$\psi_I = \psi_i(r)\,{}_{-2}Y_{lm}(\theta,\varphi)e^{-i\omega t}, \tag{32}$$

where the subscripts $I=G,H,E,F,D$ and $i=g,h,e,f,d$, respectively. Since $(\bar{\delta}-2\bar{\beta})(\delta+4\beta)$ is the only operator appearing in Eqs. (23) that involves angular variables, we only need to know that

$$(\bar{\delta}-2\bar{\beta})(\delta+4\beta)\psi_I = -\frac{L^2}{2R^2}\psi_I, \quad L=[(l-1)(l+2)]^{1/2}, \tag{33}$$

where Eqs. (31) and (32) have been employed. The remaining terms correspond to functions and differential operators involving only radial and time variables. In fact, from Eqs. (4) and (32) we have that

$$D\psi_I = \mathcal{D}\psi_I, \quad \Delta\psi_I = -\frac{\chi^2}{2}\bar{\mathcal{D}}\psi_I \quad \left(D\bar{\psi}_I = \overline{\mathcal{D}\psi_I}, \quad \Delta\bar{\psi}_I = -\frac{\chi^2}{2}\mathcal{D}\bar{\psi}_I\right), \tag{34}$$

where

$$\mathcal{D} = \partial_r - \frac{i\omega}{\chi^2}, \quad \bar{\mathcal{D}} = \partial_r + \frac{i\omega}{\chi^2}. \tag{35}$$

In this manner, it suffices to substitute the operators D and Δ, according to Eqs. (34), by $\mathcal{D}$ and $-(\chi^2/2)\bar{\mathcal{D}}$, respectively, $(\bar{\delta}-2\bar{\beta})(\delta+4\beta)$ by $-(L^2/2R^2)$ [according to Eq. (33)], and ψ_I by ψ_i (the corresponding radial part) into Eqs. (23), for reducing them to a system of ordinary equations for the radial parts ψ_i's of the potentials. Hence, the separation of variables proposed in Eq. (32) applies in a natural and straightforward way.

B. Separation of variables for the continuity equation

In this section we will see that the covariant continuity equation (28), together with the separable solutions admitted for the potentials [Eq. (32)], and the corresponding separation of variables for the field variations[12] (where a more detailed version of the present work is presented), lead to the existence of two conserved quantities.

As we have seen, at each space–time point, J^μ in Eq. (28) is a two-form on the phase space. Regardless of the last interpretation, we can maintain J^μ as a bilinear product on field perturbations on the space–time manifold. In this manner, the covariantly conserved current (28) can be rewritten, grouping conveniently its components on the null tetrad, in the form

$$J^\mu = V_l l^\mu + V_n n^\mu + V_m m^\mu + V_{\bar{m}} \bar{m}^\mu, \tag{36}$$

where

$$\begin{aligned}
V_l \equiv{}& \psi_{\mathrm{G}}(\Delta - 4\gamma + \mu)\Psi_0^{\mathrm{B}} - 8\xi\varphi_1^2\psi_{\mathrm{G}}\tilde{\sigma}^{\mathrm{B}} - \overline{\Psi_4^{\mathrm{B}}}(\Delta - 4\gamma - 3\mu)\psi_H - \tilde{\sigma}^{\mathrm{B}}(\Delta + 2\gamma + 2\mu)\psi_{\mathrm{E}} - aD\phi\psi_E\tilde{\lambda}^{\mathrm{B}} \\
&+ a\psi_E(\delta - 2\beta)\tilde{\phi}^{\mathrm{B}} + \psi_{\mathrm{F}}\overline{\Psi_4^{\mathrm{B}}} - \psi_{\mathrm{F}}(\Delta + 2\gamma + 2\mu - a\Delta\phi)\tilde{\lambda}^{\mathrm{B}} + \Delta\phi\psi_d\left(\Delta + \mu + \frac{2a\xi\varphi_1^2}{D\phi}\right)\tilde{\sigma}^{\mathrm{B}} \\
&- D\phi\psi_d\left(\Delta + 2\gamma + \mu - \frac{2a\xi\varphi_1^2}{D\phi}\right)\tilde{\lambda}^{\mathrm{B}} + \psi_{\mathrm{D}}(\Delta + 3\mu)(\delta - 2\beta)\tilde{\phi}^{\mathrm{B}}, \\
V_n \equiv{}& -\Psi_0^{\mathrm{B}}(D + 3\rho)\psi_{\mathrm{G}} + \psi_{\mathrm{H}}(D - \rho)\overline{\Psi_4^{\mathrm{B}}} + 8\xi\varphi_1^2\psi_{\mathrm{H}}\tilde{\lambda}^{\mathrm{B}} + \psi_{\mathrm{E}}\Psi_0^{\mathrm{B}} + \psi_{\mathrm{E}}(D - 2\rho - aD\phi)\tilde{\sigma}^{\mathrm{B}} \\
&+ a\Delta\phi\psi_{\mathrm{F}}\tilde{\sigma}^{\mathrm{B}} + \tilde{\lambda}^{\mathrm{B}}(D - 2\rho)\psi_{\mathrm{F}} + a\psi_{\mathrm{F}}(\delta - 2\beta)\tilde{\phi}^{\mathrm{B}} - \tilde{\sigma}^{\mathrm{B}}[4a\xi\varphi_1^2 - \mu D\phi + \Delta\phi D]\psi_{\mathrm{D}} \\
&+ D\phi\tilde{\lambda}^{\mathrm{B}}(D + \rho)\psi_{\mathrm{D}} - [(D + \rho)\psi_{\mathrm{D}}](\delta - 2\beta)\tilde{\phi}^{\mathrm{B}}, \\
V_m \equiv{}& -\psi_{\mathrm{G}}(\bar{\delta} + 4\bar{\beta})\Psi_0^{\mathrm{B}} - \psi_{\mathrm{H}}(\bar{\delta} + 4\bar{\beta})\overline{\Psi_4^{\mathrm{B}}} - \psi_{\mathrm{E}}(\bar{\delta} + 4\bar{\beta})\tilde{\sigma}^{\mathrm{B}} + \psi_{\mathrm{F}}(\bar{\delta} + 4\bar{\beta})\tilde{\lambda}^{\mathrm{B}} - \Delta\phi\psi_{\mathrm{D}}(\bar{\delta} + 4\bar{\beta})\tilde{\sigma}^{\mathrm{B}} \\
&+ D\phi\psi_{\mathrm{D}}(\bar{\delta} + 4\bar{\beta})\tilde{\lambda}^{\mathrm{B}} - \psi_{\mathrm{D}}(\bar{\delta} + 4\bar{\beta})(\delta - 2\beta)\tilde{\phi}^{\mathrm{B}}, \\
V_{\bar{m}} \equiv{}& \Psi_0^{\mathrm{B}}(\delta + 4\beta)\psi_{\mathrm{G}} + \overline{\Psi_4^{\mathrm{B}}}(\delta + 4\beta)\psi_{\mathrm{H}} + \tilde{\sigma}(\delta + 4\beta)\psi_{\mathrm{E}} - \tilde{\lambda}^{\mathrm{B}}(\delta + 4\beta)\psi_{\mathrm{F}} + \Delta\phi\tilde{\sigma}^{\mathrm{B}}(\delta + 4\beta)\psi_{\mathrm{D}} \\
&- D\phi\tilde{\lambda}^{\mathrm{B}}(\delta + 4\beta)\psi_{\mathrm{D}} + (\delta + 4\beta)\psi_{\mathrm{D}}(\delta - 2\beta)\tilde{\phi}^{\mathrm{B}}.
\end{aligned} \tag{37}$$

Therefore, considering that in the Newman–Penrose formalism $\partial_\mu l^\mu = -2\rho$, $\partial_\mu n^\mu = 2\mu - 2\gamma$, $\partial_\mu m^\mu = 2\beta$, the continuity equation (28) can be rewritten in the following form:

$$\partial_\mu(V_l l^\mu + V_n n^\mu + V_m m^\nu + V_{\bar{m}}\bar{m}^\mu) = (D - 2\rho)V_l + (\Delta + 2\mu - 2\gamma)V_n = 0, \tag{38}$$

where we have considered that $(\delta + 2\beta)V_m + (\bar{\delta} + 2\bar{\beta})V_{\bar{m}} = 0$, which can be shown using the explicit forms of V_m and $V_{\bar{m}}$ in Eqs. (37), and considering that all components of (Ψ^{B}) have spin weight 2.[12]

Thus, the whole physical information about our conserved quantities is contained in V_l and V_n. Furthermore, direct substitutions of the separable solutions for the potentials [Eq. (32)], and field variations[12] into the expressions for the bilinear products V_l and V_n given in Eqs. (37), lead to a splitting of such products in terms of the form e^0 and $e^{-2i\omega t}$:

$$\begin{aligned}
V_n &= \left[V_n^+ + \frac{i\omega}{\chi^2}G^+\right]{}_{-2}Y_{lm}\,\overline{{}_{-2}Y_{lm}} + e^{-2i\omega t}\left[V_n^- + \frac{i\omega}{\chi^2}G^-\right]{}_{-2}Y_{lm}\,{}_2Y_{lm}, \\
V_l &= \left[V_l^+ + \frac{i\omega}{2}G^+\right]{}_{-2}Y_{lm}\,\overline{{}_{-2}Y_{lm}} + e^{-2i\omega t}\left[V_l^- - \frac{i\omega}{2}G^-\right]{}_{-2}Y_{lm}\,{}_2Y_{lm},
\end{aligned} \tag{39}$$

where

$$
\begin{aligned}
V_n^{\pm} \equiv & \Psi_0^{\mathrm{B}\pm}[\psi_e - R^3\partial_r(R^{-3}\psi_g)] + \psi_h[R^{-1}\partial_r(R\,\overline{\Psi_4^{\mathrm{B}\pm}}) + 8\xi\varphi_1^2\tilde{\lambda}^{\mathrm{B}\pm}] + \psi_e R^{-2}\xi^{-1/2}\partial_r(R^2\xi^{1/2}\tilde{\sigma}^{\mathrm{B}\pm}) \\
& + a\psi_f[\Delta\phi\tilde{\sigma}^{\mathrm{B}\pm} + \tilde{\phi}^{\mathrm{B}\pm}] + \tilde{\lambda}^{\mathrm{B}\pm}R^2\partial_r(R^2\psi_f) - \tilde{\sigma}^{\mathrm{B}\pm}[\Delta\phi R\partial_r(R^{-1}\psi_d) + 4a\xi\varphi_1^2\psi_d] \\
& + R[D\phi\tilde{\lambda}^{\mathrm{B}\pm} - \tilde{\phi}^{\mathrm{B}\pm}]\partial_r(R^{-1}\psi_d), \\
V_l^{\pm} \equiv & \overline{\Psi_4^{\mathrm{B}\pm}}[\psi_f + \tfrac{1}{2}\chi^{-2}R^3\partial_r(R^{-3}\chi^2\psi_h)] - \psi_g[\tfrac{1}{2}\chi^{-2}R^{-1}\partial_r(R\chi^4\Psi_0^{\mathrm{B}\pm}) + 8\xi\varphi_1^2\tilde{\sigma}^{\mathrm{B}\pm}] \\
& + \tfrac{1}{2}\psi_f\chi^4R^{-2}\xi^{-1/2}\partial_r(\xi^{1/2}R^2\chi^{-2}\tilde{\lambda}^{\mathrm{B}\pm}) + a\psi_e[\tilde{\phi}^{\mathrm{B}\pm} - \Delta\phi\tilde{\lambda}^{\mathrm{B}\pm}] + \tfrac{1}{2}\tilde{\sigma}^{\mathrm{B}\pm}\chi^4R^{-2}\partial_r(R^2\chi^{-2}\psi_e) \\
& + \Delta\phi\psi_d\left[-\frac{1}{2}\chi^2R^{-1}\partial_r(R\tilde{\sigma}^{\mathrm{B}\pm}) + \frac{2a\xi\varphi_1^2}{D\phi}\tilde{\sigma}^{\mathrm{B}\pm}\right] \\
& + D\phi\psi_d\left[\frac{1}{2}\chi^4R^{-1}\partial_r(R\chi^{-2}\tilde{\lambda}^{\mathrm{B}\pm}) + \frac{2a\xi\varphi_1^2}{D\phi}\tilde{\lambda}^{\mathrm{B}\pm}\right] - \frac{1}{2}\chi^2R^{-3}\psi_d\partial_r(R^3\tilde{\phi}^{\mathrm{B}\pm}),
\end{aligned}
\tag{40}
$$

and

$$
\begin{aligned}
G^+ &\equiv \psi_g\Psi_0^{\mathrm{B}+} + \psi_h\overline{\Psi_4^{\mathrm{B}+}} + \psi_e\tilde{\sigma}^{\mathrm{B}+} - \psi_f\tilde{\lambda}^{\mathrm{B}+} + \psi_d[\Delta\phi\tilde{\sigma}^{\mathrm{B}+} - D\phi\tilde{\lambda}^{\mathrm{B}+} + \tilde{\phi}^{\mathrm{B}+}], \\
G^- &\equiv \psi_g\Psi_0^{\mathrm{B}-} - \psi_h\overline{\Psi_4^{\mathrm{B}-}} - \psi_e\tilde{\sigma}^{\mathrm{B}-} - \psi_f\tilde{\lambda}^{\mathrm{B}-} + \psi_d[\Delta\phi\tilde{\sigma}^{\mathrm{B}-} - D\phi\tilde{\lambda}^{\mathrm{B}-} + \tilde{\phi}^{\mathrm{B}-}] = \frac{L^2l(l+1)}{8R^4}\psi_d^2
\end{aligned}
\tag{41}
$$

are only functions of r. Since the components $(\Psi^{\mathrm{B}})^-$ are directly proportional to the potentials,[12] V_n^- and V_l^- in Eqs. (40) have remarkable reductions (unlike V_n^+ and V_l^+):

$$
\begin{aligned}
V_n^- &= -\frac{L^2l(l+1)}{8R^4}\left[-2\psi_g\psi_h\partial_r\ln R^3 + R\psi_d\partial_r\left(\frac{\psi_d}{R}\right)\right], \\
V_l^- &= -\frac{L^2l(l+1)\chi^2}{16R^4}\left[2\psi_g\psi_h\partial_r\ln R^3 + R\psi_d\partial_r\left(\frac{\psi_d}{R}\right)\right],
\end{aligned}
\tag{42}
$$

therefore, from Eqs. (41), and (42), is very easy to show that

$$
\begin{aligned}
& V_n^- + 2\chi^{-2}V_l^- + R^{-2}\partial_r(R^2G^-) = 0, \\
& V_l^- - \frac{\chi^2}{2}V_n^- = -\frac{L^2l(l+1)\chi^2}{4R^4}(\partial_r\ln R^3)\psi_g\psi_h,
\end{aligned}
\tag{43}
$$

which will be useful below.

C. Conserved quantities

Substituting expressions (39) into Eq. (38), using the explicit form for D, Δ, ρ, μ, and γ we obtain, after some simplification and suitably grouping, that

$$
\begin{aligned}
& \frac{1}{R^2}\partial_rR^2\left[V_l^+ - \frac{\chi^2}{2}V_n^+\right]\,{}_{-2}Y_{lm}\,\overline{{}_{-2}Y_{lm}} + \frac{e^{-2i\omega t}}{R^2}\partial_rR^2\left[V_l^- - \frac{\chi^2}{2}V_n^-\right]\,{}_{-2}Y_{lm}\,{}_2Y_{lm} \\
& \quad - i\omega e^{-2i\omega t}\left[2\frac{V_l^-}{\chi^2} + V_n^- + R^{-2}\partial_r(R^2G^-)\right]\,{}_{-2}Y_{lm}\,{}_2Y_{lm} = 0,
\end{aligned}
\tag{44}
$$

the last term vanishes according to the first of Eqs. (43), thus Eq. (44) reduces to

$$\partial_r R^2\left[V_l^+ - \frac{\chi^2}{2}V_n^+\right]{}_{-2}Y_{lm}\,\overline{{}_{-2}Y_{lm}} + e^{-2i\omega t}\partial_r R^2\left[V_l^- - \frac{\chi^2}{2}V_n^-\right]{}_{-2}Y_{lm}\,{}_{2}Y_{lm} = 0, \tag{45}$$

which implies (using the linear independence of terms of the form $e^{i\omega t}$ and $e^{-i\omega t}$) that there exist two conserved quantities, which we denote by $K^{(\pm)}$:

$$R^2\left[V_l^{(\pm)} - \frac{\chi^2}{2}V_n^{(\pm)}\right] \equiv K^{(\pm)}. \tag{46}$$

Although K^+ has a complicated form in terms of the potentials, K^- has a remarkably simple form, in accordance with the last expression in Eq. (43):

$$K^- \equiv R^2\left[V_l^- - \frac{\chi^2}{2}V_n^-\right] = -\frac{L^2 l(l+1)}{4}\,\frac{\chi^2(\partial_r \ln R^3)}{R^2}\,\psi_g\psi_h\,. \tag{47}$$

Note that, since $(\Psi^{\mathrm{B}})^+$ depends on $(\overline{\psi_i})$, K^+ depends on (ψ_i) and $(\overline{\psi_i})$, whereas K^- directly on the potentials without involving its complex conjugates.

The existence of these two conserved quantities deserves some important comments. First: although the equations used for obtaining such quantities are not Hermitian ones (for which the constancy of the Wronskian yields traditionally conserved quantities), one can obtain, without any restrictions and full generality, conserved quantities, provided that the original system of equations and its adjoint system are used. Second: as we have seen, if the potentials have a time dependence of the form $e^{-i\omega t}$, the field perturbations appearing in the decoupled system contain terms proportional to $e^{-i\omega t}$ and $e^{i\omega t}$ (in the classical cases, unlike the present case involving string fields, only terms proportional to $e^{i\omega t}$ are present[11]), which lead finally to two conserved quantities. In the classical cases, only a conserved quantity analogous to the present K^+ is obtained. In fact, the bilinear terms depending on $\Psi_0^{\mathrm{B}+}$ and ψ_g in the expression for K^+ [see the explicit forms for V_n^+ and V_l^+ in Eqs. (40)] yield a conservation relation for the energy of gravitational perturbations in the classical Schwarzschild black hole (and something similar for electromagnetic perturbations).[11] In this manner, it is possible that K^+ has the same physical meaning for the present string black hole: the conservation of the energy for the coupled field perturbations. However, this question will require a long asymptotic analysis and will be studied in a subsequent work. On the other hand, K^- is a novel conserved quantity apparently without classical analogy; it is also an open question to investigate its physical meaning.

VI. CONCLUDING REMARKS

We summarize some questions that remain open and will be the subject of forthcoming works.

First, although string black holes are considered as classical black holes plus Planck-scale corrections, they are not actually *quantum black holes*. Hence, for example, the thermodynamics properties argued in Refs. 2 and 3 are limited in this sense; a proper quantization will give a more complete and satisfactory description of such objects (see the paragraph before final comments of Ref. 5). The idea is, of course, that the symplectic structure constructed in the present work is to be the starting point for such a (canonical) quantization, which will give us a consistent quantum extension of string black holes.

Second, as mentioned, the physical meaning of the conserved quantities obtained in the present work remains to be worked out. This subject will include the calculation of physical quantities such as scattering amplitudes, reflection and transmission coefficients, etc.

Finally, the scheme of adjoint operators employed in the present work can be understood as an important extension of the original Wald's method: wherever there exists an appropriate decoupled equation, it is not only possible to express the complete solution in terms of scalar potentials, but also to find automatically a corresponding (covariantly) conserved current.

ACKNOWLEDGMENTS

This work was supported by CONACYT and the Sistema Nacional de Investigadores (México).

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Spherically symmetric solutions of a boundary value problem for monopoles

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(Received 28 October 2002; accepted 9 December 2002)

In this article we study spherically symmetric monopoles, which are critical points for the Yang–Mills–Higgs functional over a disk in three dimensions, with prescribed degree and covariant constant at the boundary. This is a three-dimensional gauge-theory generalization of the Ginzburg-Landau model in two dimensions. [DOI: 10.1063/1.1543226]

I. INTRODUCTION

In this article we treat a three-dimensional analog of the vortex equations in two dimensions and look for solutions with spherical symmetry as described in Sec. II. The domain considered is a three-dimensional disk and we prescribe the degree of the monopole at the boundary. Unlike in two dimensions, where Ginzburg–Landau-type functionals appear either with or without gauge potentials, the problem in three dimensions is well-posed only in gauge theory. Without a curvature term in the action, a minimizing sequence for the action would yield a trivial limit.[2] In the presence of a gauge potential, this problem is well-posed, natural and has physical meaning.

The most general Yang–Mills–Higgs functional takes the form

$$\mathcal{YMH}(A,\phi)=\frac{\epsilon}{2}\|F\|_{L^2}^2+\frac{\rho}{2}\|D_A\phi\|_{L^2}^2+\frac{\lambda}{8}\|\,|\phi|^2-a^2\|_{L^2}^2\ , \tag{1.1}$$

for appropriate constants ϵ, ρ, λ and a. Working on $\mathbb{R}^3$, one usually applies a rescaling of ϕ, a rescaling of space, and a rescaling of the action to set $\epsilon=\rho=a=1$, so the action functional depends on a single parameter, λ. On the unit ball, however, we cannot rescale space, so we can only eliminate two of the four parameters. We set $\rho=a=1$, and obtain a two-parameter family of functionals

$$\mathcal{YMH}_{\epsilon,\lambda}(A,\phi)=\frac{\epsilon}{2}\|F\|_{L^2(B^3)}^2+\frac{1}{2}\|D_A\phi\|_{L^2(B^3)}^2+\frac{\lambda}{8}\|\,|\phi|^2-1\|_{L^2(B^3)}^2. \tag{1.2}$$

(Alternatively, we could work on a sphere of radius R. One can then rescale to set $\epsilon=1$, at the cost of varying R. We then obtain a two-parameter family of functionals indexed by λ and R.) We know from the general theory for monopoles (cf. Ref. 2 for $\epsilon=1$, $\lambda\geqslant 0$) that there exists a minimum for this functional which satisfies the Euler Lagrange equations

$$\begin{aligned}\epsilon *D_A *F&=[D_A\phi,\phi],\\ *D_A *D_A\phi&=\frac{\lambda}{2}(|\phi|^2-1)\phi,\end{aligned} \tag{1.3}$$

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and suitable boundary conditions on $\partial B^3 \equiv S^2$ (cf. Sec. IV and Refs. 2 and 3), and is smooth. In this article we prove the existence, and describe the form, of spherically symmetric solutions to these equations.

We note that, even for $\lambda = 0$, these are not solutions to the Bogomolnyi equations found in Ref. 1. The Bogomolnyi solutions are obtained only in the limit $\lambda \to 0$, $R \to \infty$, or equivalently $\lambda \to 0$, $\epsilon \to 0$.

II. SPHERICALLY SYMMETRIC CONNECTIONS, MONOPOLES, AND GAUGE TRANSFORMATIONS

We work on the trivial principal SU(2)-bundle $P = B^3 \times \mathrm{SU}(2)$ and its associated vector bundles. A is a connection on P, which can be viewed as a one-form on B^3 with values in su(2). The Higgs field ϕ is a section of the adjoint bundle, i.e., a map $\phi : B^3 \to \mathrm{su}(2)$. Here $\mathrm{su}(2) \equiv \{X \in \mathcal{M}_{2\times 2} : tr\, X = 0\, ;\, X + \overline{X^T} = 0\}$ is the Lie algebra of SU(2). We identify su(2) with the imaginary quaternions $\mathrm{Im}\,\mathbb{H} \equiv \{x_1 i + x_2 j + x_3 k : (x_1, x_2, x_3) \in \mathbb{R}^3\}$ by identifying the matrices

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix},$$

with i, j, k, respectively, and extending this mapping to a Lie-algebra isomorphism. It is also convenient to define the three-vector of Lie-algebra elements $\vec{\sigma} = (i, j, k)$.

The symmetry group SO(3) acts on pairs (A, ϕ), simultaneously rotating the three-dimensional base space and the three-dimensional Lie algebra. That is, the triple (i, j, k) transforms in the same way as the triple (x_1, x_2, x_3), so quantities such as $\vec{\sigma} \cdot \vec{x}$ are invariant.

We are interested in finding Yang–Mills–Higgs fields (A, ϕ) which are invariant under this group action. To this purpose, one needs to specify the value of the connection one-form $A : B^3 \to \Lambda^1(B^3) \otimes \mathrm{Im}\,\mathbb{H}$ and of the Higgs field $\phi : B^3 \to \mathrm{Im}\,\mathbb{H}$ at one point of each group orbit (on the base) and impose invariance under the isotropy group of that point. We find it convenient to fix the values of (A, ϕ) on the slice $L \equiv \{\vec{x} \in B^3 : x_2 = x_3 = 0, x_1 \in (0,1]\}$. The isotropy group at $(x,0,0) \in L$ is SO(2), i.e., rotations about the x_1-axis (and about the i axis in the Lie algebra). For the Higgs field ϕ one has in general

$$\phi(x,0,0) = \varphi_1(x) i + \varphi_2(x) j + \varphi_3(x) k \in \mathrm{Im}\,\mathbb{H} \simeq \mathrm{su}(2)\,,$$

where $\varphi_l(x)$, $l = 1,2,3$ are real-valued functions. Imposing invariance under SO(2) forces $\varphi_2(x) = \varphi_3(x) = 0$ for all $x \in (0,1]$. Applying the action of SO(3), one obtains the symmetric form of the Higgs field ϕ

$$\phi = \frac{\varphi(r)}{r} \vec{\sigma} \cdot \vec{x} \equiv \frac{\varphi(r)}{r} (x_1 i + x_2 j + x_3 k)\,, \tag{2.1}$$

with $r \equiv |\vec{x}|$, $\vec{x} \equiv (x_1, x_2, x_3) \in \mathbb{R}^3$, $\vec{\sigma} \equiv (i, j, k) \in \mathrm{Im}\,\mathbb{H}$.

An su(2)-valued connection on the slice L is given in general by

$$\begin{aligned} A(x,0,0) = {} & a_{11}(x) i\, dx_1 + a_{12}(x) i\, dx_2 + a_{13}(x) i\, dx_3 + a_{21}(x) j\, dx_1 + a_{22}(x) k\, dx_2 + a_{23}(x) j\, dx_3 \\ & + a_{31}(x) k\, dx_1 + a_{32}(x) k\, dx_2 + a_{33}(x) k\, dx_3\,. \end{aligned} \tag{2.2}$$

Imposing SO(2)-invariance yields $a_{12} = a_{13} = a_{21} = a_{31} = 0$, $a_{22} = a_{33}$, and $a_{23} = -a_{32}$. Thus the final form of the SO(2)-invariant connection evaluated at the points $(x,0,0) \in L$ is

$$A(x,0,0) = a(x) i\, dx_1 + b(x)(j\, dx_2 + k\, dx_3) + c(x)(k\, dx_2 - j\, dx_3)\,.$$

Transporting this slice via the SO(3) group action on B^3 one obtains the invariant version

$$A(x_1,x_2,x_3)=\frac{\alpha(r)}{r}\vec{\sigma}\cdot\vec{dx}+\frac{\beta(r)}{r^3}(\vec{x}\times\vec{dx})\cdot(\vec{x}\times\vec{\sigma})+\frac{\gamma(r)}{r^2}\vec{\sigma}\cdot(\vec{x}\times\vec{dx}), \tag{2.3}$$

where "×" denotes the cross product of vectors and $\vec{dx}\equiv(dx_1,dx_2,dx_3)$.

At this point there is still some gauge freedom available to further specify the connection A, namely that provided by "symmetric" gauge transformations. Such a transformation g is determined by its values on the slice L, which must be SO(2)-invariant. This yields $i\,g(x,0,0)=g(x,0,0)\,i$, thus $g(x,0,0)=\exp(i\,h(x))$. Therefore, symmetric gauge transformations are of the type

$$g(x_1,x_2,x_3)=\exp\left(h(r)\frac{\vec{\sigma}\cdot\vec{x}}{|\vec{x}|}\right), \tag{2.4}$$

where $h(r)$ is an arbitrary function of the radius r. Performing such a gauge transformation does not change the form (2.1) of the Higgs field ϕ. However, A transforms nontrivially. In particular, setting $h(r)\equiv\int\alpha(r)/r\,dr$ exactly cancels the α-piece in $g^{-1}dg+g^{-1}A\,g$. Thus, one can impose $\alpha(r)=0$. The final version of A is then

$$A(x_1,x_2,x_3)=\frac{\beta(r)}{r^3}(\vec{x}\times\vec{dx})\cdot(\vec{x}\times\vec{\sigma})+\frac{\gamma(r)}{r^2}\vec{\sigma}\cdot(\vec{x}\times\vec{dx}). \tag{2.5}$$

The only gauge freedom remaining is from the constant of integration in the indefinite integral $\int[\alpha(r)/r]\,dr$ (cf. Sec. IV).

Note that the β and γ terms have opposite parities. The isometry $\vec{x}\to-\vec{x}$ sends β to $-\beta$ but sends γ to $+\gamma$.

III. THE YANG–MILLS–HIGGS FUNCTIONAL ON SPHERICALLY SYMMETRIC CONFIGURATIONS

In this section we explicity compute the Yang–Mills–Higgs functional, and the resulting equations of motion, for symmetric pairs (A,ϕ). Our connection is a sum of two terms,

$$A=B+C,$$

where

$$\begin{aligned}B&=\frac{\beta(r)}{r^3}(\vec{x}\times\vec{dx})\cdot(\vec{x}\times\vec{\sigma})\\&=\frac{\beta(r)}{r^3}[(r^2-x_1^2)i-x_1x_3k-x_1x_2j]\,dx_1+\frac{\beta(r)}{r^3}[(r^2-x_2^2)j-x_2x_3k-x_1x_2i]\,dx_2\\&\quad+\frac{\beta(r)}{r^3}[(r^2-x_3^2)k-x_1x_3i-x_2x_3j]\,dx_3,\end{aligned} \tag{3.1}$$

and

$$\begin{aligned}C&=\frac{\gamma(r)}{r^2}\vec{\sigma}\cdot(\vec{x}\times\vec{dx})\\&=\frac{\gamma(r)}{r^2}(x_3j-x_2k)\,dx_1+\frac{\gamma(r)}{r^2}(x_1k-x_3i)\,dx_2+\frac{\gamma(r)}{r^2}(x_2i-x_1j)\,dx_3.\end{aligned} \tag{3.2}$$

A. Preliminary computations

The curvature of A is given by

$$F = dA + A \wedge A = dB + dC + B \wedge B + C \wedge C ,$$

since the cross term $B \wedge C + C \wedge B$ is identically zero.

Computing F_{12}, the various nonzero terms are

$$(d\,B)_{12} = \frac{\beta'}{r^2}(-x_2 i + x_1 j), \tag{3.3}$$

$$(d\,C)_{12} = \left(\frac{-\gamma}{r^2}\right)' \left(\frac{x_1 x_3}{r} i + \frac{x_2 x_3}{r} j\right) + \left(\frac{2\gamma}{r^2} + \left(\frac{\gamma}{r^2}\right)' \left(\frac{x_2^2}{r} + \frac{x_1^2}{r}\right)\right) k, \tag{3.4}$$

$$(B \wedge B)_{12} = \frac{2\beta^2}{r^4}[x_1 x_3 i + x_2 x_3 j + x_3^2 k], \tag{3.5}$$

$$(C \wedge C)_{12} = \frac{2\gamma^2}{r^4}[x_1 x_3 i + x_2 x_3 j + x_3^2 k]. \tag{3.6}$$

By rotational symmetry, the contributions to F_{13} and F_{23} are similar.

The covariant derivative of the monopole $\phi = [\varphi(r)/r]\vec{\sigma} \cdot \vec{x}$ is given by

$$D_A \phi \equiv d\phi + [B, \phi] + [C, \phi] , \tag{3.7}$$

where

$$d\phi = \frac{\vec{\sigma} \cdot \vec{x}}{r} d\varphi + \varphi\, d\left(\frac{\vec{\sigma} \cdot \vec{x}}{r}\right) \quad , \tag{3.8}$$

$$[B, \phi] \equiv B\phi - \phi B = \frac{2\beta\varphi}{r^2}(-x_3 j + x_2 k)\, d\,x_1 + \text{cyclic permutations}, \tag{3.9}$$

$$[C, \phi] \equiv C\phi - \phi C = \frac{2\gamma\varphi}{r^3}[(r^2 - x_1^2) i - x_1 x_3 k - x_1 x_2 j] d\,x_1 + \text{cyclic permutations}. \tag{3.10}$$

At this point we are ready to compute the three terms involved in the Yang–Mills–Higgs functional (1.2). They are

(1) $|F|^2 \equiv F \wedge *F$,
(2) $|D\phi|^2 \equiv D\phi \wedge *D\phi$,
(3) $(|\phi|^2 - 1)^2$.

Computation of (1): One shows easily that

$$dB \wedge *dC = dC \wedge *dB = 0 ,$$

$$dB \wedge *(B \wedge B) = (B \wedge B) \wedge *dB = 0 ,$$

$$dB \wedge *(C \wedge C) = (C \wedge C) \wedge *dB = 0 ,$$

thus

$$
\begin{aligned}
|F|^2 &= |dB|^2 + |dC|^2 + dC\wedge *(B\wedge B) + dC\wedge *(C\wedge C) + (B\wedge B)\wedge *(B\wedge B) \\
&\quad + (B\wedge B)\wedge *(C\wedge C) + (C\wedge C)\wedge *(C\wedge C) \\
&= 2\frac{\beta'^2}{r^2} + 2\frac{\gamma'^2}{r^2} + 4\frac{\gamma^2}{r^4} + 4\frac{\beta^2\gamma}{r^4} + 4\frac{\gamma^3}{r^4} + 4\frac{\beta^4}{r^4} + 8\frac{\beta^2\gamma^2}{r^4} + 4\frac{\gamma^4}{r^4} \\
&= \frac{2\beta'^2}{r^2} + \frac{2\gamma'^2}{r^2} + \frac{4(\beta^2+\gamma^2+\gamma)^2}{r^4}. \qquad (3.11)
\end{aligned}
$$

Computation of (2): One shows that

$$d\phi\wedge *[B,\phi] = [B,\phi]\wedge *d\phi = 0\,,$$

$$[B,\phi]\wedge *[C,\phi] = [C,\phi]\wedge *[B,\phi] = 0\,,$$

thus

$$|D\phi|^2 = |d\phi|^2 + |[B,\phi]|^2 + |[C,\phi]|^2 + 2\,d\phi\wedge *[C,\phi] \qquad (3.12)$$

$$= \left(\varphi'^2 + 2\frac{\varphi^2}{r^2}\right) + 8\frac{\beta^2\varphi^2}{r^2} + 8\frac{\gamma^2\varphi^2}{r^2} + 8\frac{\gamma\varphi^2}{r^2}. \qquad (3.13)$$

Computation of (3): One easily obtains

$$(|\phi|^2 - 1)^2 = \left(\frac{\varphi^2}{r^2} - 1\right)^2.$$

Collecting terms, the Yang–Mills–Higgs functional calculated on spherically symmetric configurations is given by

$$
\begin{aligned}
\mathcal{SYMH}(\gamma,\varphi) = 4\pi\int_0^1 \Bigg[& 2\epsilon\left(\beta'^2 + \gamma'^2 + \frac{2}{r^2}(\beta^2+\gamma^2+\gamma)^2\right) + r^2\varphi'^2 \\
& + 2\varphi^2[1 + 4(\beta^2+\gamma^2+\gamma)] + \lambda r^2(\varphi^2-1)^2 \Bigg] \mathrm{d}r\ . \qquad (3.14)
\end{aligned}
$$

IV. FURTHER GAUGE TRANSFORMATIONS AND THE EULER–LAGRANGE EQUATIONS

We want to search for absolute minima of the functional (3.14) among all finite-action spherically symmetric configurations (β, γ, φ). The following theorem restricts the possibilities:

Theorem 4.1: *If the functional (3.14) has a minimum, then this minimum is achieved by functions* (β, γ, φ) *with* β *identically zero and* $\gamma(0) = 0$.

Proof: First we find a gauge transformation that yields $\beta(0) = \gamma(0) = 0$. In that gauge, we then show that minimization requires $\beta/(\gamma + \frac{1}{2})$ to be constant, hence for β to be identically zero.

If $\mathcal{SYMH}(\beta,\gamma,\varphi) < \infty$, then β and γ much approach well-defined limits as $r \to 0$, and $\beta^2(0) + \gamma^2(0) + \gamma(0) = 0$. If $\beta(0)$ and $\gamma(0)$ are not already zero, we let θ be the argument of the complex number $\beta(0) + i\,\gamma(0)$, and define

$$g = \exp\left(\theta\frac{\vec{\sigma}\cdot\vec{x}}{|\vec{x}|}\right) \equiv \exp\left(\theta\frac{x_1 i + x_2 j + x_3 k}{|\vec{x}|}\right) \equiv \cos(\theta) + \sin(\theta)\frac{\vec{\sigma}\cdot\vec{x}}{|\vec{x}|}\,. \qquad (4.1)$$

Then

$$d\,g(x_1,x_2,x_3)=\sin(\theta)\left[\frac{\vec{\sigma}\cdot\vec{dx}}{|\vec{x}|}+d\left(\frac{1}{|\vec{x}|}\right)\vec{\sigma}\cdot\vec{x}\right]\ , \tag{4.2}$$

and evaluating on our slice gives

$$d\,g(r,0,0)=\frac{\sin(\theta)}{r}(j\,d\,x_2+k\,d\,x_3). \tag{4.3}$$

Our transformed connection on the slice is then

$$\begin{aligned}[g^{-1}d\,g+g^{-1}A\,g](r,0,0)&=\left[\frac{\cos(2\theta)\,\beta(r)}{r}+\frac{\sin(2\theta)\,\gamma(r)}{r}+\frac{\cos(\theta)\sin(\theta)}{r}\right](j\,d\,x_2+k\,d\,x_3)\\&\quad+\left[-\frac{\sin(2\theta)\,\beta(r)}{r}+\frac{\cos(2\theta)\,\gamma(r)}{r}-\frac{\sin^2(\theta)}{r}\right](k\,d\,x_2-j\,d\,x_3)\\&\equiv\frac{\hat{\beta}(r)}{r}(j\,d\,x_2+k\,d\,x_3)+\frac{\hat{\gamma}(r)}{r}(k\,d\,x_2-j\,d\,x_3).\end{aligned} \tag{4.4}$$

Plugging in the values of $\sin(\theta)$, $\cos(\theta)$, etc., gives

$$\hat{\beta}(r)=\frac{(\beta^2(0)-\gamma^2(0))\beta(r)+2\beta(0)\gamma(0)\gamma(r)+\beta(0)\gamma(0)}{\beta^2(0)+\gamma^2(0)}, \tag{4.5}$$

$$\hat{\gamma}(r)=\frac{(-2\beta(0)\gamma(0))\beta(r)+(\beta^2(0)-\gamma^2(0))\gamma(r)-\gamma^2(0)}{\beta^2(0)+\gamma^2(0)}. \tag{4.6}$$

As $r\to 0$, both these terms go to zero, since $\beta^2(0)+\gamma^2(0)+\gamma(0)=0$.

Having set $\beta(0)=\gamma(0)=0$, we now show that β must be identically zero. We choose polar coordinates in the $(\beta,\gamma+\frac{1}{2})$-plane:

$$\begin{aligned}\beta&=\nu\cos t,\\ \gamma+\tfrac{1}{2}&=\nu\sin t.\end{aligned} \tag{4.7}$$

In these coordinates, the functional (3.14) becomes

$$\mathcal{SYMH}(\nu,t)=4\pi\int_0^1\left[\ 2\epsilon\left(\nu'^2+t'^2\nu^2+\frac{2}{r^2}\left(\nu^2-\frac{1}{4}\right)^2\right)+r^2\varphi'^2+8\varphi^2\nu^2+\lambda r^2(\varphi^2-1)^2\ \right]dr, \tag{4.8}$$

with $\nu^2(0)=\frac{1}{4}$. The only dependence on t is in the $t'^2\nu^2$ term, which is minimized by setting $t=$const. But then $\cot(t)=\beta/(\gamma+\frac{1}{2})$ must be constant, and equal to $\beta(0)/(\gamma(0)+\frac{1}{2})=0$, so β is identically zero. □

We may therefore restrict our attention to the functional

$$\mathcal{S}(\gamma,\varphi)=4\pi\int_0^1\left[\ 2\epsilon\left(\gamma'^2+\frac{2}{r^2}(\gamma^2+\gamma)^2\right)+r^2\varphi'^2+2\varphi^2(1+2\gamma)^2+\lambda r^2(\varphi^2-1)^2\ \right]dr. \tag{4.9}$$

The Euler–Lagrange equations for this functional together with the appropriate boundary conditions are then

$$\gamma'' - \frac{2}{\epsilon}\varphi^2(1+2\gamma) - \frac{2}{r^2}(\gamma^2+\gamma)(1+2\gamma) = 0 \quad \text{on } (0,1),$$

$$\varphi'' + \frac{2\varphi'}{r} - \frac{2\varphi}{r^2}(1+2\gamma)^2 - 2\lambda\varphi(\varphi^2-1) = 0 \quad \text{on } (0,1),$$

$$\gamma(1) = -\tfrac{1}{2}, \tag{4.10}$$

$$\gamma(0) = 0,$$

$$\varphi(1) = +1 \quad (\text{or } \varphi(1) = -1).$$

The boundary conditions above come directly from the variational principle. In fact, to cancel the boundary terms one needs to either restrict the space of connections to those with prescribed boundary data, or to impose Neumann-type boundary conditions. The boundary condition $\varphi(1) = \pm 1$ comes from $|\phi| = 1$ on ∂B^3 and $\gamma(1) = -\frac{1}{2}$ comes from

$$(D\phi)_\tau = (d\phi)_\tau + [A_\tau, \phi] = (1+2\gamma)\phi \quad d\left(\frac{\vec{\sigma}\cdot\vec{x}}{r}\right) = 0 \tag{4.11}$$

on ∂B^3, where the subscript τ denotes tangential components (cf. Refs. 2 and 3).

Observation: After some computation, the system (4.10) could also be obtained by imposing spherical symmetry in (1.3), thus critical symmetric points for the action (4.9) are symmetric critical points (not necessarily minima) for (1.2). This is also known *a priori* from the ''principle of symmetric criticality.'' [4]

V. EXISTENCE OF SPHERICALLY SYMMETRIC MONOPOLES

Our basic existence result is the following.

Theorem 5.1: *For all values of* $\lambda \geqslant 0$, $\epsilon > 0$, *there exists a symmetric solution of*

$$\begin{gathered} \epsilon * D_A * F = [D_A\phi, \phi] \quad \text{on } B^3, \\ * D_A^* D_A \phi = \frac{\lambda}{2}(|\phi|^2 - 1)\phi \quad \text{on } B^3, \\ (D\phi)_\tau = 0 \quad \text{on } \partial B^3, \\ |\varphi| = 1 \quad \text{on } \partial B^3. \end{gathered} \tag{5.1}$$

Observation: These equations do not reduce to the Bogomolnyi equations, even if $\lambda = 0$. The Bogolmolnyi argument involves an integration by parts; on a finite domain, this results in a boundary contribution.[1]

Proof: Because of the derivative terms in the action, the natural space for γ (denoted $\mathcal{H}_\gamma$) is $H^1(0,1)$, while the natural space $\mathcal{H}_\varphi$ for φ is the weighted Sobolev space $H^1((0,1), r^2 dr)$. By the Sobolev embedding theorem, functions in $\mathcal{H}_\gamma$ are continuous on $[0,1]$. Functions in $\mathcal{H}_\varphi$ are continuous on $(0,1]$, but may not have a limit at $r = 0$. We may therefore apply boundary conditions to γ at $r = 0$ and at $r = 1$, and to φ at $r = 1$.

Let

$$\mathcal{F} = \{(\gamma, \varphi) \in \mathcal{H}_\gamma \times \mathcal{H}_\varphi \ : \ \gamma(1) = -\tfrac{1}{2},\ \gamma(0) = 0, \varphi(1) = 1\}. \tag{5.2}$$

The action functional (4.9) is well-defined on $\mathcal{F}$, and is finite whenever φ is bounded. In particular, $\mu \equiv Inf_{\mathcal{F}} \mathcal{S}$ is finite. We follow the direct method in the calculus of variations. That is, take a minimizing sequence for $\mathcal{S}$, show that it converges weakly in $\mathcal{F}$, and then show that the weak limit minimizes the action and so solves the Euler–Lagrange equations.

Let (γ_n, φ_n) be a minimizing sequence for $\mathcal{S}$. Since $\lambda \geqslant 0$, the action is not increased if we make the replacement

$$\varphi(r) \to \begin{cases} -1, & \text{if } \varphi(r) < -1; \\ \varphi(r), & \text{if } -1 \leqslant \varphi(r) \leqslant 1; \\ 1, & \text{if } \varphi(r) > 1. \end{cases} \tag{5.3}$$

As a result, we can assume that each $\varphi_n(r)$ is bounded in magnitude by 1. Under these circumstances, the sequence (γ_n, φ_n) is bounded in $\mathcal{F} \subset \mathcal{H}_\gamma \times \mathcal{H}_\varphi$. However, balls in $\mathcal{H}_\gamma$ are weakly compact, as are balls in $\mathcal{H}_\varphi$, so the pair (γ_n, φ_n) converges weakly in $\mathcal{H}_\gamma \times \mathcal{H}_\varphi$ to a limit $(\gamma_\infty, \varphi_\infty)$.

By Sobolev, $\gamma_n(r)$ and $\varphi_n(r)$ converge pointwise to $\gamma_\infty(r)$ and $\varphi_\infty(r)$, so the limiting values $\gamma(0)$, $\gamma(1)$, and $\varphi(1)$ are preserved, and $(\gamma_\infty, \varphi_\infty) \in \mathcal{F}$. Moreover, terms in $\mathcal{S}(\gamma_n, \varphi_n)$ that do not involve derivatives converge to the corresponding terms in $\mathcal{S}(\gamma_\infty, \varphi_\infty)$. The derivative terms are quadratic, hence weakly semicontinuous. As a result, $\mathcal{S}(\gamma_\infty, \varphi_\infty)$ is bounded above by μ, and therefore must equal μ.

Showing that γ_∞ and φ_∞ satisfy the Euler–Lagrange equations (4.10) is then a standard exercise in the calculus of variations. Smoothness of $(\gamma_\infty, \varphi_\infty)$ away from $r=0$ follows by elliptic regularity of the equations (4.10). Smoothness at $r=0$ follows from regular singular-point analysis, combined with the fact that both functions are bounded (see Sec. VI for details). This in turn implies that the connection and Higgs field (A, ϕ) constructed from $(\gamma_\infty, \varphi_\infty)$ comprise a smooth, symmetric classical solution to the PDE system (5.1). [Alternatively, one can establish regularity of (A, ϕ) from the ellipticity of the PDE system (5.1), since we are working in a gauge with $d^*A = 0$.]

VI. REGULAR SINGULAR POINT ANALYSIS

In Sec. V we demonstrated the existence of symmetric monopoles for arbitrary $\lambda \geqslant 0$ and $\epsilon > 0$. In this section we explore their form near the regular singular point of the equations (4.10), namely $r=0$.

Theorem 6.1: *Let (γ, φ) be a bounded finite-action solution to the ODE system (4.10) for some fixed $\epsilon > 0$ and $\lambda \geqslant 0$. Then there exist constants a_1 and b_2 such that*

$$\begin{aligned} \varphi(r) &= a_1 r + O(r^3), \\ \gamma(r) &= b_2 r^2 + O(r^4), \\ \gamma'(r) &= 2 b_2 r + O(r^3), \end{aligned} \tag{6.1}$$

near $r=0$. In particular, $\varphi(0) = \gamma'(0) = 0$.

Proof: We begin with the equation for φ, which we write as

$$\varphi'' + \frac{2\varphi'}{r} - \frac{2\varphi}{r^2} = \frac{8\varphi}{r^2}(\gamma + \gamma^2) + 2\lambda\varphi(\varphi^2 - 1). \tag{6.2}$$

Since φ is bounded and $\gamma(0) = 0$, the terms on the right hand side are less singular than those on the left hand side, and to leading order φ resembles the solution to the homogeneous equation

$$\varphi'' + \frac{2\varphi'}{r} - \frac{2\varphi}{r^2} = 0. \tag{6.3}$$

The general solution to this equation is $\varphi = a_1 r + a_{-2} r^{-2}$. However, φ is bounded by assumption, so $a_{-2} = 0$. Thus the solution to (6.2) is, to leading order, $a_1 r$.

Next we turn to the equation for γ, namely

$$\gamma'' - \frac{2\gamma}{r^2} = \frac{2}{\epsilon}\varphi^2(1+2\gamma) + \frac{2\gamma}{r^2}(2\gamma^2+3\gamma). \tag{6.4}$$

Again, since φ is bounded and $\gamma(0)=0$, this may be viewed as a perturbation of the homogeneous linear equation

$$\gamma'' - \frac{2\gamma}{r^2} = 0, \tag{6.5}$$

whose solution is $\gamma = b_{-1} r^{-1} + b_2 r^2$. Since γ is bounded, $b_{-1} = 0$. Thus our solution to (6.4) is, to leading order, $b_2 r^2$.

With these basic results, we can estimate the right hand sides of (6.2) and (6.4). The right hand side of (6.2) is $O(r)$, which gives an $O(r)$ correction to φ'', hence an $O(r^3)$ correction to φ. The right hand side of (6.4) is $O(r^2)$, thus giving an $O(r^3)$ correction to γ' and an $O(r^4)$ correction to γ. □

One can do an expansion for φ and γ in powers of r. Indeed, only odd powers contribute to φ and only even powers contribute to γ. This is seen by induction. By Theorem 6.1, φ is odd and γ is even through order r^2. However, if φ is odd and γ is even through order r^k, then the right hand sides of (6.2) and (6.4) are odd and even, respectively, to order r^k, and so φ and γ are odd and even, respectively, to order r^{k+2}. Thus φ and γ are odd and even to all orders in r.

We can therefore write an asymptotic expansion

$$\begin{aligned} \varphi(r) &\sim \sum_{n \text{ odd}} a_n r^n, \\ \gamma(r) &\sim \sum_{n \text{ even}} b_n r^n. \end{aligned} \tag{6.6}$$

Plugging this expansion into Eqs. (6.2) and (6.4) and equating coefficients of r^{n-2} gives recursion relations of the form

$$\begin{aligned} (2k)(2k+3)a_{2k+1} &= \text{algebraic expression involving } a_1, b_2, \ldots, b_{2k}, \\ (2k+1)(2k-2)b_{2k} &= \text{algebraic expression involving } a_1, b_2, \ldots, b_{2k-2}. \end{aligned} \tag{6.7}$$

These relations do not constrain a_1 or b_2. However, once we have a_1 and b_2, the remaining coefficients are determined. The first few are

$$\begin{aligned} a_3 &= (4a_1 b_2 - \lambda a_1)/5, \\ b_4 &= (3b_2^2 + \epsilon^{-1} a_1^2)/5, \\ a_5 &= (4a_1 b_4 + 4a_3 b_2 + 4a_1 b_2^2 + \lambda(a_1^3 - a_3))/14, \\ b_6 &= (b_2^3 + 3b_2 b_4 + \epsilon^{-1}(a_1 a_3 + a_1^2 b_2))/7, \\ a_7 &= [4(a_1 b_6 + a_3 b_4 + a_5 b_2 + a_3 b_2^2 + 2a_1 b_2 b_4) + \lambda(3a_1^2 a_3 - a_5)]/27, \\ b_8 &= [3(2b_2^2 b_4 + b_4^2 + 2b_2 b_6) + \epsilon^{-1}(a_3^2 + 2a_1 a_5 + 2a_1^2 b_4 + 4a_1 a_3 b_2)]/27, \end{aligned} \tag{6.8}$$

TABLE I. Taylor coefficients (a_1, b_2) for various values of (ϵ, λ).

ϵ	λ	a_1	b_2
0.1	0	2.829 090 77	−4.474 602 32
0.1	1	3.147 735 51	−4.920 725 56
0.1	3	3.626 927 66	−5.571 109 38
0.1	10	4.628 924 07	−6.819 479 99
0.1	30	6.192 746 93	−8.464 748 94
0.3	0	2.019 049 55	−1.885 499 02
0.3	1	2.261 181 76	−2.049 949 84
0.3	3	2.665 179 94	−2.316 736 22
0.3	10	3.595 504 62	−2.868 170 01
0.3	30	5.125 103 42	−3.583 740 45
1	0	1.670 981 22	−1.028 947 46
1	1	1.859 737 04	−1.075 046 39
1	3	2.195 729 81	−1.155 777 83
1	10	3.048 984 41	−1.340 418 24
1	30	4.553 843 41	−1.589 104 70
3	0	1.570 810 44	−0.806 159 86
3	1	1.741 842 36	−0.820 788 59
3	3	2.051 561 43	−0.846 952 10
3	10	2.867 501 86	−0.909 244 87
3	30	4.357 761 01	−0.995 512 35
10	0	1.536 222 87	−0.731 466 86
10	1	1.700 996 54	−0.735 764 32
10	3	2.001 022 88	−0.743 501 47
10	10	2.801 981 39	−0.762 191 07
10	30	4.285 717 13	−0.788 386 76

$$a_9=[4(a_1b_8+a_3b_6+a_5b_4+a_7b_2+a_5b_2^2+2a_3b_2b_4+a_1b_4^2+2a_1b_2b_6)+\lambda(3a_1^2a_5+3a_1a_3^2-a_7)]/44,$$

$$b_{10}=[3(b_2^2b_6+b_2b_4^2+b_2b_8+b_4b_6)+\epsilon^{-1}(a_1a_7+a_3a_5+a_1^2b_6+a_3^2b_2+2a_1a_3b_4+2a_1a_5b_2)]/22.$$

VII. SYMMETRIES AND STABILITY

The action functional and the resulting Euler–Lagrange equations are invariant under two natural symmetries,

$$\varphi(r)\to-\varphi(r),\quad \gamma(r)\to+\gamma(r); \tag{7.1}$$

$$\varphi(r)\to\varphi(r),\quad \gamma(r)\to-1-\gamma(r). \tag{7.2}$$

The first symmetry (7.1) comes from the isometry $\vec{x}\to-\vec{x}$ of B^3, which of course respects rotational symmetry. Since $\vec{\sigma}\cdot\vec{x}$ is odd and $\vec{\sigma}\cdot(\vec{x}\times\overrightarrow{dx})$ is even, pulling the pair (A,ϕ) back by this isometry flips the sign of φ while preserving γ. Using this symmetry, we can fix the sign of $\varphi(1)$, which we henceforth take to be positive.

The second symmetry (7.2) is a gauge transformation by $(\vec{\sigma}\cdot\vec{x})/r$. This is of the form of (4.2), with $\theta=\pi/2$. From (4.4) it is clear that this transformation sends γ to $-1-\gamma$ without generating a β term or changing φ. Applying this to a connection with $\gamma(0)=0$ yields a new connection with $\gamma(0)=-1$. This connection has finite action but is singular at the origin, reflecting the singular gauge transformation that generated it.

We now consider stability properties of the ODE system (4.10). These ODEs have several fixed points, namely

$$(\gamma,\varphi)=(-\tfrac{1}{2},1),\ (-\tfrac{1}{2},-1),\ (-\tfrac{1}{2},0),\ (0,0)\ \text{ or }\ (-1,0). \tag{7.3}$$

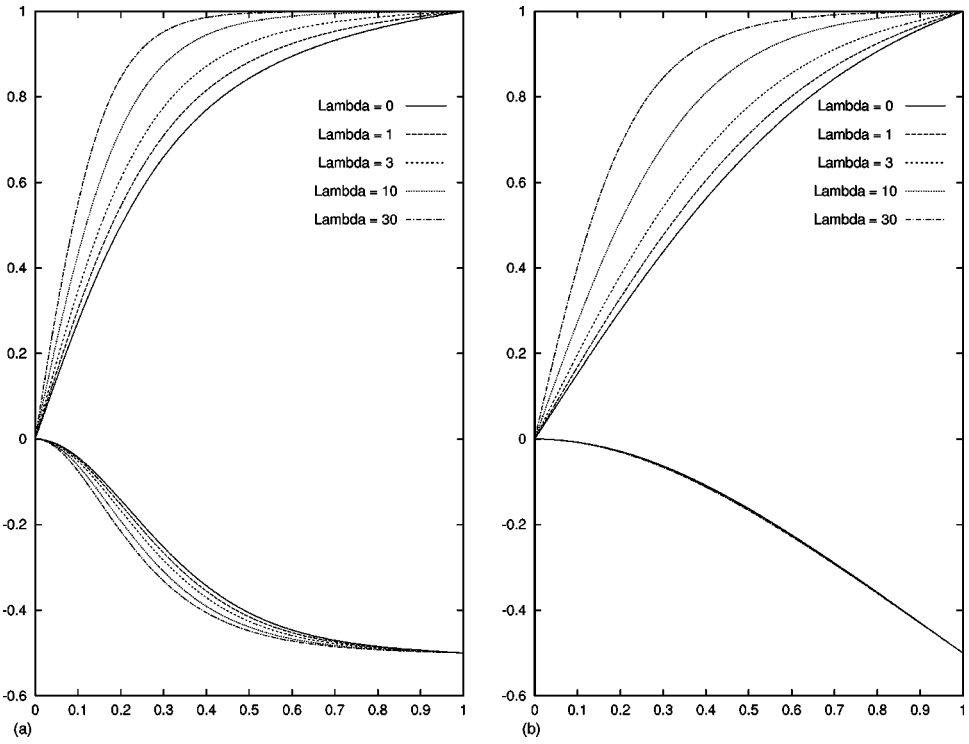

FIG. 1. Trajectories with fixed ϵ.

The point $(-\frac{1}{2},-1)$ is related to $(-\frac{1}{2},1)$ by the symmetry (7.1), while $(-1,0)$ is related to $(0,0)$ by (7.2), so we do not need to study these. What remains is $(-\frac{1}{2},1)$, $(-\frac{1}{2},0)$, and $(0,0)$.

For the $\gamma=-1/2$ fixed points, we define $\delta=\gamma+1/2$, and the equation for γ becomes

$$\delta''=4\delta\left(\frac{\varphi^2}{\epsilon}-\frac{1}{4r^2}+\frac{\delta^2}{r^2}\right). \tag{7.4}$$

The fixed point $\gamma=-\frac{1}{2}$ is stable for $\varphi=1$ when $r^2<\epsilon/4$, but is unstable if $r^2>\epsilon/4$. This defines a natural length scale to the problem, namely $\sqrt{\epsilon}/2$. We should expect our solutions to behave qualitatively differently for r less than or greater than this length scale. Of course, if $\epsilon>4$, then all radii r are less than this length scale. In the case of $\varphi=0$, the value $\gamma=\frac{1}{2}$ is always stable, regardless of ϵ or r.

Near $\gamma=-\frac{1}{2}$, the equation for φ becomes

$$\varphi''+2\frac{\varphi'}{r}=2\varphi\left(\frac{4\delta^2}{r^2}+\lambda(\varphi^2-1)\right). \tag{7.5}$$

The behavior of this fixed point depends on the value of φ. Near $\varphi=0$ we have

$$(r\varphi)''=-2\lambda r\varphi+O(\delta^2)+O(\varphi^2),$$

which is stable for all positive values of r. Near $\varphi=1$, however, we write $\varphi=1+\zeta$ and have

$$(r\zeta)''=4\lambda(r\zeta)+O(\zeta^2)+O(\delta^2).$$

This is unstable as long as $\lambda>0$, and has natural length scale $1/\sqrt{4\lambda}$.

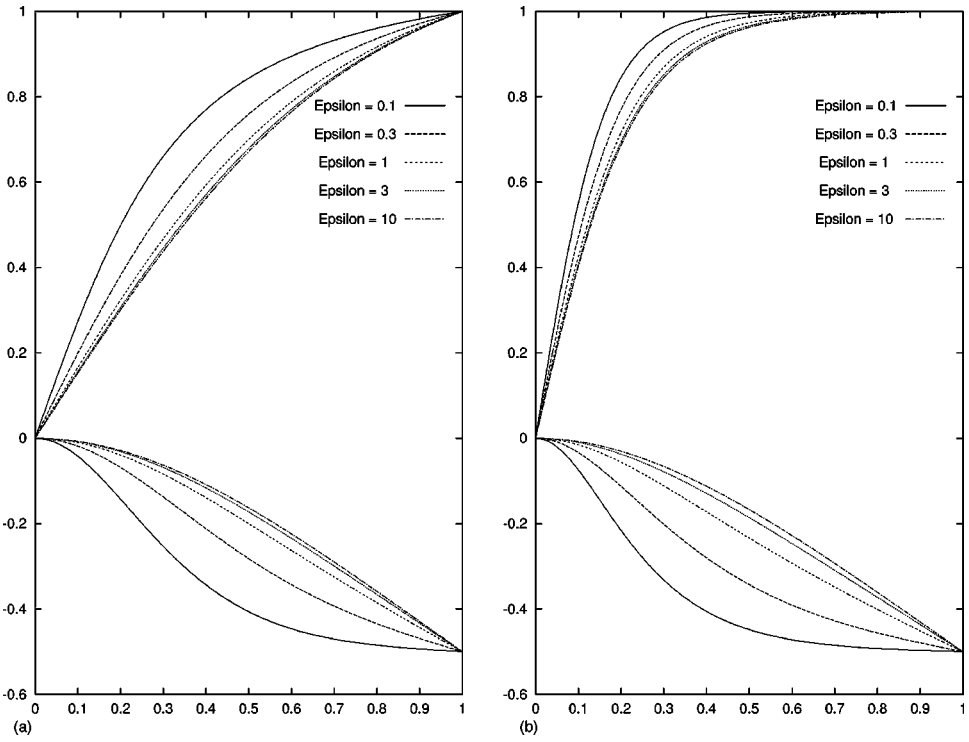

FIG. 2. Trajectories with λ fixed.

To summarize, the fixed point $(-\frac{1}{2},0)$ is stable, while the fixed point $(-\frac{1}{2},1)$ is unstable. If $r^2<\epsilon/4$, then there is one unstable mode, corresponding to growth of $\varphi-1$. If $r^2>\epsilon/4$, then there are two unstable modes, one for φ and one for γ.

Finally, there is the fixed point (0,0). Near (0,0) we have

$$\begin{aligned}\gamma'' &= 2\gamma/r^2 + \text{higher order},\\ \varphi'' + 2\varphi'/r &= 2\varphi(r^{-2}-\lambda) + \text{higher order}.\end{aligned} \tag{7.6}$$

This fixed point is always unstable, with γ growing rapidly. φ will grow exponentially if $r<1/\sqrt{\lambda}$, and will oscillate if $r>1/\sqrt{\lambda}$.

VIII. NUMERICAL RESULTS AND QUALITATIVE ANALYSIS

For any fixed ϵ and λ, and given a_1 and b_2, one can in principle integrate the differential equations out to $r=1$. In practice, numerical errors due to the discretization of the interval [0,1] can be very bad near the origin, due to the singular nature of the ODE system there. A better method is to use the power series (6.6) in a neighborhood of the origin and to numerically integrate from there. In a discretization of 10 000 points, we use the power series out to $r=0.01$, or 100 lattice spacings from the origin.

In this way we get a pair $(\gamma(1),\varphi(1))$ for each (a_1,b_2). Using Newton's method, we then find values of (a_1,b_2) such that $(\gamma(1),\varphi(1))=(-\frac{1}{2},1)$. Table I lists the correct values of a_1 and b_2 for several values of ϵ and λ.

The resulting functions $\varphi(r)$ and $\gamma(r)$ are sketched in Figs. 1 and 2. Figure 1 shows the functions for different values of λ and ϵ fixed at 0.1 or at 10. Figure 2 is similar, only with λ fixed and ϵ variable. In each case the positive function is φ and the negative function is γ.

From these figures several qualitative features are clear. Although φ depends significantly on both ϵ and λ, γ is practically independent of λ, especially when ϵ is large. The length scale on

which γ changes from 0 to $-\frac{1}{2}$ is the smaller of $\sqrt{\epsilon}$ and 1. The length scale on which φ changes from 0 to 1 is the smallest of $\sqrt{\epsilon}$, $1/\sqrt{\lambda}$, and 1. Thus changing λ has the greatest effect when λ is greater than 1, while changing ϵ has the greatest effect when $\epsilon<1$.

The source code for these numerical results can be obtained from the authors.

ACKNOWLEDGMENT

The authors thank Professor Karen K. Uhlenbeck for useful conversations on this subject.

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Massive complex scalar field in the Kerr–Sen geometry: Exact solution of wave equation and Hawking radiation

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(Received 4 September 2001; accepted 2 December 2002)

The separated radial part of a massive complex scalar wave equation in the Kerr–Sen geometry is shown to satisfy the generalized spheroidal wave equation which is, in fact, a confluent Heun equation up to a multiplier. The Hawking evaporation of scalar particles in the Kerr–Sen black hole background is investigated by the Damour–Ruffini–Sannan method. It is shown that quantum thermal effect of the Kerr–Sen black hole has the same character as that of the Kerr–Newman black hole. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1539899]

I. INTRODUCTION

In a recent paper,[1] we have investigated exact solution of a massive complex scalar field equation in the Kerr–Newman black hole background, and demonstrated that both its radial part and its angular part can be transformed into the form of a generalized spheroidal wave equation.[2] Previous work on solution of a massive scalar wave equation in the Kerr(–Newman) space–time had been completed in Refs. 3 and 4. It is interesting to extend our analysis to solution of a scalar wave equation in a Kerr–Sen black hole background.[5] The Kerr–Sen solution arising in the low energy effective string field theory is a rotating charged black hole generated from the Kerr solution. The thermodynamic property of this twisted Kerr black hole was discussed in Ref. 6 by using separation of the Hamilton–Jacobi equation of a test particle. The aim of this paper is to study some exact solutions to a massive charged scalar wave equation and to find its connection to the confluent Heun equation[7] as well as to investigate quantum thermal effect of scalar particles on the Kerr–Sen space–time.

The paper is organized as follows: In Sec. II, we separate a massive charged scalar field equation on the Kerr–Sen black hole background into the radial and angular parts. Section III is devoted to transforming the radial part into a generalized spheroidal wave equation and to relating it to the confluent Heun equation. Then, we investigate quantum thermal effect of scalar particles in the Kerr–Sen space–time in Sec. IV. Finally, we summarize our discussions in the conclusion section.

II. SEPARATING VARIABLES OF KLEIN–GORDON EQUATION ON THE KERR–SEN BLACK HOLE BACKGROUND

Constructed from the charge neutral rotating (Kerr) black hole solution, the Kerr–Sen solution[5] is an exact classical four dimensional black hole solution in the low energy effective heterotic string field theory. In the Boyer–Lindquist coordinates, the Kerr–Sen metric and the electromagnetic field vector potential can be rewritten as[6]

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$$ds^2=-\frac{\Delta}{\Sigma}(dt-a\sin^2\theta\, d\varphi)^2+\frac{\sin^2\theta}{\Sigma}[a\,dt-(\Sigma+a^2\sin^2\theta)d\varphi]^2+\Sigma\left(\frac{dr^2}{\Delta}+d\theta^2\right),$$
$$\mathcal{A}=\frac{-Qr}{\Sigma}(dt-a\sin^2\theta\, d\varphi), \tag{1}$$

where $\Delta=r^2+2(b-M)r+a^2=(r-r_+)(r-r_-)$, $\Sigma=r^2+2br+a^2\cos^2\theta$ and $r_\pm=M-b\pm\epsilon$ with $\epsilon=\sqrt{(M-b)^2-a^2}$.

This metric describes a black hole carrying mass M, charge Q, angular momentum $J=Ma$, and magnetic dipole moment Qa. The twist parameter b is related to the Sen's parameter α via $b=Q^2/2M=M\tanh^2(\alpha/2)$. Because $M\geqslant b\geqslant 0$, $r=r_-$ is a new singularity in the region $r\leqslant 0$, the event horizon of the Kerr–Sen black hole is located at $r=r_+$. The area of the outer event horizon of the twisted Kerr solution[5] is given by $A_+=4\pi(r_+^2+2br_++a^2)=8\pi Mr_+$.

We consider the solution of a massive charged test scalar field on the Kerr–Sen black hole background (we use Planck unit system $G=\hbar=c=k_B=1$ throughout the paper). Because the Kerr–Sen metric (1) only differs from the Kerr(–Newman) solution by the form of two functions Δ and Σ, the minimal electromagnetic coupling Klein–Gordon field equation satisfied by the complex scalar wave function Φ with mass μ and charge q in such a space–time can be separated as $\Phi(t,r,\theta,\varphi)=R(r)S^{\not<}_{m,0}(ka,\theta)e^{i(m\varphi-\omega t)}$, in which the angular part $S^{\not<}_{m,0}(ka,\theta)$ is an ordinary spheroidal angular wave function with spin weight $s=0$, while the radial part can be given as follows:

$$\partial_r[\Delta\,\partial_r R(r)]+\left[\frac{(Ar-ma)^2}{\Delta}+k^2\Delta+2Dr-\lambda\right]R(r)=0, \tag{2}$$

here λ is a separation constant, $A=2M\omega-qQ$, $D=A\omega-M\mu^2$, $k=\sqrt{\omega^2-\mu^2}$ (we assume that $\omega>\mu$). For later convenience, we also denote $\epsilon B=A(M-b)-ma$ and introduce $W_\pm=(A\pm B)/2$.

With further substitution $R(r)=(r-r_+)^{i(A+B)/2}(r-r_-)^{i(A-B)/2}F(r)$, we can transform Eq. (2) for $R(r)$ into a modified generalized spheroidal wave equation with imaginary spin weight iA and boost weight iB for $F(r)$,[1]

$$\Delta\partial_r^2F(r)+2[i\epsilon B+(1+iA)(r-M+b)]\partial_rF(r)+[k^2\Delta+2Dr+iA-\lambda]F(r)=0. \tag{3}$$

Equation (2) has two regular singular points $r=r_\pm$ with indices $\pm iW_+$ and $\pm iW_-$, respectively, whereas Eq. (3) has indices $\rho_+=0$, $-2iW_+$ and $\rho_-=0$, $-2iW_-$ at two singularities $r=r_\pm$, respectively. The infinity is an irregular singularity of Eqs. (2) and (3). Equation (3) has the same form as the radial part of the massive complex scalar wave equation in the Kerr–Newman geometry[1] with its solution (when $\mu=0$) named as the generalized spheroidal wave function.[2] It is interesting to note that a special solution of function $F(r)$ satisfies the Jacobi equation of imaginary index when $\omega=\pm\mu=qQ/M$ (namely, $k=D=0$).

III. GENERALIZED SPHEROIDAL WAVE FUNCTION AND HEUN EQUATION

In this section, we shall show that the generalized spheroidal wave equation (3) of imaginary number order is, in fact, a confluent form of Heun equation.[7] To this end, let us make a coordinate transformation $r=M-b+\epsilon z$ and substitute $R(r)=(z-1)^{i(A+B)/2}(z+1)^{i(A-B)/2}F(z)$ into Eq. (2), then we can reduce it to the following standard forms of a generalized spheroidal wave equation:[1,7]

$$(z^2-1)R''(z)+2zR'(z)+\left[(\epsilon k)^2(z^2-1)+2D\epsilon z+\frac{(Az+B)^2}{z^2-1}+2D(M-b)-\lambda\right]R(z)=0 \tag{4}$$

and

$$(z^2-1)F''(z)+2[iB+(1+iA)z]F'(z)+[(\epsilon k)^2(z^2-1)+2D\epsilon z+2D(M-b)+iA-\lambda]F(z)=0\,, \tag{5}$$

where a prime denotes the derivative with respect to its argument.

The spin-weighted spheroidal wave function $F(z)$ is symmetric under the reflect $k\to -k$. Letting $F(z)=e^{i\epsilon kz}G(z)$ without loss of generality, we can transform Eq. (5) to

$$(z^2-1)G''(z)+2[iB+(1+iA)z+i\epsilon k(z^2-1)]G'(z)+[2i\epsilon k(1+iA-iD/k)z-2\epsilon kB+iA+2D(M-b)-\lambda]G(z)=0\,. \tag{6}$$

By means of changing variable $z=1-2x$, we arrange the singularities $r=r_+$ $(z=1)$ to $x=0$ and $r=r_-$ $(z=-1)$ to $x=1$, respectively, and reduce Eq. (6) to a confluent form of Heun's equation[7,8]

$$G''(x)+\left(\beta+\frac{\gamma}{x}+\frac{\delta}{x-1}\right)G'(x)+\frac{\alpha\beta x-h}{x(x-1)}G(x)=0\,, \tag{7}$$

with $\gamma=1+2iW_+$, $\delta=1+2iW_-$, $\beta=4i\epsilon k$, $\alpha=-(1+iA)+iD/k$, $h=\lambda-2i\epsilon k-iA+4\epsilon kW_+-2Dr_+$.

This confluent Heun equation (7), with h its accessory parameter, has two regular singular points at $x=0,\ 1$ with exponents $(0,\ 1-\gamma)$ and $(0,\ 1-\delta)$, respectively, as well as an irregular singularity at the infinity point. The power series solution in the vicinity of the point $x=0$ for Eq. (7) can be written as

$$G(\alpha,\beta,\gamma,\delta,h;x)=\sum_{n=0}^{\infty} g_n x^n\,, \tag{8}$$

and the coefficient g_n satisfies a three-term recurrence relation[7,8]

$$\begin{gathered} g_0=1\,,\quad g_1=-h/\gamma\,,\\ (n+1)(n+\gamma)g_{n+1}-\beta(n-1+\alpha)g_{n-1}=[n(n-1-\beta+\gamma+\delta)-h]g_n\,. \end{gathered} \tag{9}$$

It is not difficult to deduce the exponent $1-\gamma$ solution[8] for $x=0$ and obtain the power series solution in the vicinity of the point $x=1$ by a linear transformation interchanging the regular singular points $x=0$ and $x=1$: $x\to 1-x$. Expansion of solutions to the confluent Heun's equation in terms of hypergeometric and confluent hypergeometric functions has been presented in Refs. 2 and 7. The confluent Heun's functions can be normalized to constitute a group of orthogonal complete functions.[7] It should be noted that Heun's confluent equation also admits quasipolynomial solutions for particular values of the parameters.[7,8] It follows from the three-term recurrence relation that $G(\alpha,\beta,\gamma,\delta,h;x)$ is a polynomial solution if

$$\begin{gathered} \alpha=-N\,,\quad \text{with integer } N\geqslant 0\,,\\ g_{N+1}(h)=0\,, \end{gathered} \tag{10}$$

where g_{N+1} being a polynomial of degree $N+1$ in h, that is, there are $N+1$ eigenvalues h_i for h such that $g_{N+1}(h_i)\equiv 0$.

IV. HAWKING RADIATION OF SCALAR PARTICLES

Now we investigate the Hawking evaporation[9] of scalar particles in the Kerr–Sen black hole by using the Damour–Ruffini–Sannan's (DRS) method.[10] This approach only requires the exis-

tence of a future horizon and is completely independent of any dynamical details of the process leading to the formation of this horizon. The DRS method assumes analyticity properties of the wave function in the complexified manifold.

In the following, we shall consider a wave outgoing from the event horizon r_+ over interval $r_+<r<\infty$. According to the DRS method, a correct outgoing wave $\Phi^{\text{out}}=\Phi^{\text{out}}(t,r,\theta,\varphi)$ is an adequate superposition of functions $\Phi^{\text{out}}_{r>r_+}$ and $\Phi^{\text{out}}_{r<r_+}$,

$$\Phi^{\text{out}}=C[\,\eta(r-r_+)\Phi^{\text{out}}_{r>r_+}+\eta(r_+-r)\Phi^{\text{out}}_{r<r_+}e^{2\pi W_+}], \tag{11}$$

where η is the conventional unit step function, C is a normalization factor.

In fact, components $\Phi^{\text{out}}_{r>r_+}$ and $\Phi^{\text{out}}_{r<r_+}$ have asymptotic behaviors,

$$\Phi^{\text{out}}_{r>r_+}=\Phi^{\text{out}}_{r>r_+}(t,r,\theta,\varphi)\to c_1(r-r_+)^{iW_+}S^{\swarrow}_{m,0}(ka,\theta)e^{i(m\varphi-\omega t)}\quad(r\to r_+), \tag{12}$$

$$\Phi^{\text{out}}_{r<r_+}=\Phi^{\text{out}}_{r<r_+}(t,r,\theta,\varphi)\to c_2(r-r_+)^{-iW_+}S^{\swarrow}_{m,0}(ka,\theta)e^{i(m\varphi-\omega t)}\quad(r\to r_+) \tag{13}$$

when $r\to r_+$. Clearly, the outgoing wave $\Phi^{\text{out}}_{r>r_+}$ cannot be directly extended from $r_+<r<\infty$ to $r_-<r<r_+$, but it can be analytically continued to an outgoing wave $\Phi^{\text{out}}_{r<r_+}$ that inside event horizon r_+ by the lower half complex r-plane around unit circle $r=r_+-i0$:

$$r-r_+\to(r_+-r)e^{-i\pi}.$$

By this analytical treatment, we have

$$\Phi^{\text{out}}_{r<r_+}\sim c_2(r-r_+)^{-iW_+}S^{\ell}_{m,0}(ka,\theta)e^{i(m\varphi-\omega t)}. \tag{14}$$

Equation (13) just takes one solution to the radial equation inside the event horizon r_+, it has the same form of Eq. (14) generated by the analytical method. As $\Phi^{\text{out}}_{r>r_+}$ differs $\Phi^{\text{out}}_{r<r_+}$ by a factor $(r-r_+)^{-2iW_+}$, then a difference factor $e^{2\pi W_+}$ emerges due to the above analytical treatment. Thus we can derive the relative scattering probability of the scalar wave at the event horizon

$$\left|\frac{\Phi^{\text{out}}_{r>r_+}}{\Phi^{\text{out}}_{r<r_+}}\right|^2=e^{-4\pi W_+}, \tag{15}$$

and obtain the thermal radiation spectrum with the Hawking temperature $T=\kappa/2\pi$.

$$\begin{aligned}\langle\mathcal{N}\rangle&=|C|^2=\frac{1}{e^{4\pi W_+}-1},\\ W_+&=\frac{Ar_+-ma}{2\epsilon}=\frac{\omega-m\Omega-q\Phi}{2\kappa},\end{aligned} \tag{16}$$

where the angular velocity at the horizon is $\Omega=a/2Mr_+$, the electric potential is $\Phi=Q/2M=b/Q$, the surface gravity at the pole is $\kappa=(r_+-M+b)/2Mr_+=\epsilon/2Mr_+$.

The black body radiation spectrum (16) demonstrates that the thermal property of Kerr–Sen black hole is similar to that of Kerr–Newman black hole though its geometry character is like that of the Kerr solution.[6] Correspondingly, there exist four thermodynamical laws of the Kerr–Sen black hole, similar to those of Kerr–Newman black hole thermodynamics.

V. CONCLUSION

In this paper, we have shown that the separation of variables of the scalar wave equation in the Kerr–Newman black hole background can apply completely to the case of the twisted Kerr solution. The separated radial part can be recast into the generalized spheroidal wave equation, which is, in fact, a confluent form of Heun equation.

In addition, we find that the thermal property of the twisted Kerr black hole resembles that of Kerr–Newman black hole though its geometry character likes that of the Kerr solution. The Kerr–Sen solution shares similar four black hole thermodynamical laws and quantum thermal effect as the Kerr–Newman space–time does.

ACKNOWLEDGMENTS

One of us (S.Q.W.) is very indebted to Dr. Jeff Zhao and Dr. C. B. Yang for their help in finding some useful references.

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Quasi-homogeneous thermodynamics and black holes

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(Received 14 October 2002; accepted 29 November 2002)

We propose a generalized thermodynamics in which quasi-homogeneity of the thermodynamic potentials plays a fundamental role. This thermodynamic formalism arises from a generalization of the approach presented in Ref. 1, and it is based on the requirement that quasi-homogeneity is a nontrivial symmetry for the Pfaffian form $\delta Q_{\text{rev.}}$ It is shown that quasi-homogeneous thermodynamics fits the thermodynamic features of at least some self-gravitating systems. We analyze how quasi-homogeneous thermodynamics is suggested by black hole thermodynamics. Then, some existing results involving self-gravitating systems are also shortly discussed in the light of this thermodynamic framework. The consequences of the lack of extensivity are also recalled. We show that generalized Gibbs–Duhem equations arise as a consequence of quasi-homogeneity of the thermodynamic potentials. An heuristic link between this generalized thermodynamic formalism and the thermodynamic limit is also discussed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1542922]

I. INTRODUCTION

In Ref. 1 we have shown that, by choosing the extensive variables $(U,V,X^1,\ldots,X^n)$ as independent variables, and by postulating that the integrable Pfaffian form δQ_{rev} representing the infinitesimal heat exchanged reversibly is homogeneous of degree one and that the homogeneity symmetry is nontrivial (for the definition of nontrivial symmetry see the next section), it is possible to find immediately an integrating factor for δQ_{rev}. In fact, if $Y=U\partial_U+V\partial_V+\Sigma_i X^i\partial_{X^i}$ is the Liouville vector field associated with the homogeneity symmetry, one has that an integrating factor is given by $f=\delta Q_{\text{rev}}(Y)=i_Y\delta Q_{\text{rev}}\not\equiv 0$ (see Ref. 1 and references therein). The entropy $S(U,V,X^1,\ldots,X^n)$, which represents the fundamental equation in the entropy representation, is then straightforwardly recovered. The framework presented in Ref. 1 can be generalized in the following sense. A generalized thermodynamics where δQ_{rev} is a quasi-homogeneous integrable Pfaffian form is proposed. Quasi-homogeneity is realized to be a property which characterizes the behavior of thermodynamic functions like, e.g., the entropy in the black hole case, in some statistical mechanical models involving nonrelativistic matter interacting via the Newtonian potential and also in the case of self-gravitating radiation. When gravity plays an important role the standard extensivity property of thermodynamics does not hold; nevertheless, one can still find a form of thermodynamics in which each thermodynamic variable follows a power scaling law where the power can be different from one or zero, i.e., the variables are allowed to be neither extensive nor intensive. Black hole thermodynamics is the most evident and special thermodynamics belonging to this framework.

The plan of the paper is the following. In Sec. II we give some definitions and then in Sec. III, we propose a theoretical framework for quasi-homogeneous thermodynamics, by generalizing the standard thermodynamics case.[1] In Secs. IV, V, and VI examples displaying a quasi-homogeneous thermodynamics are discussed. In Sec. IV, the role of quasi-homogeneity in black hole thermodynamics is shown; in Sec. V, we discuss a model of fermionic nonrelativistic matter with Newtonian interaction which displays a quasi-homogeneous behavior. In Sec. VI, the general relativistic case of thermal geons and self-gravitating radiation are discussed. Sec. VII concerns the

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discussion of the physical consequences for thermodynamics when the requirement of homogeneity is relaxed. In Sec. VIII a summary of constructive assumptions is made. In Sec. IX the generalized Gibbs–Duhem identities are discussed. In Sec. X the energy representation and the Legendre transform are analyzed. In Sec. XI some further suggestions from black hole thermodynamics are discussed. Section XII has an heuristic nature, a link between the thermodynamic limit and the formalism of quasi-homogeneous thermodynamics is proposed. In the Appendix further mathematical and physical aspects are explored.

II. QUASI-HOMOGENEOUS PFAFFIAN FORMS

Given a set of real coordinates $x \equiv (x^1,\ldots,x^n)$ and a set of weights $\boldsymbol{\alpha} \equiv (\alpha_1,\ldots,\alpha_n) \in \mathbb{R}^n$, a real-valued function $G(x^1,\ldots,x^n)$ is quasi-homogeneous of degree r and type $\boldsymbol{\alpha}$ if, under the action of the one-parameter group of quasi-homogeneous dilatations

$$g^\tau : (x^1,\ldots,x^n) \to (e^{\alpha_1 \tau} x^1,\ldots,e^{\alpha_n \tau} x^n), \tag{1}$$

where $\tau \in \mathbb{R}$, one finds

$$G(g^\tau x) = e^{r\tau} G(x). \tag{2}$$

A differentiable function G on a open connected domain

$$\mathcal{D} = \{x \in \mathcal{D} \,|\, g^\tau x \in \mathcal{D} \;\; \forall \;\; x \in \mathcal{D}, \tau \in \mathbb{R}\} \subseteq \mathbb{R}^n \tag{3}$$

is quasi-homogeneous of degree r, if and only if,[2,3]

$$DG = rG, \tag{4}$$

where the Euler vector field

$$D \equiv \alpha_1 x^1 \frac{\partial}{\partial x^1} + \cdots + \alpha_n x^n \frac{\partial}{\partial x^n} \tag{5}$$

is the infinitesimal generator of the transformation. Notice that a quasi-homogeneous transformation is also called ''similarity transformation'' and ''stretching transformation.'' [4] The identity (4) is a generalization of the Euler identity for homogeneous functions. Quasi-homogeneity for functions and vector fields is defined in Ref. 2. Notice that, according to the definition given above, one cannot avoid specifying, together with the degree of quasi-homogeneity, the type of the quasi-homogeneous object one is considering.

Homogeneous functions are a subset of quasi-homogeneous functions, in fact they have all the weights equal to 1. We define *strictly quasi-homogeneous functions* the functions which satisfy the above definition with weights which cannot be all equal. A quasihomogeneous function of n variables is characterized by n weights and its degree. If all the weights are undetermined and arbitrary, or if they are in part undetermined and in part equal to 1, then all the weights can be set equal to 1, and then the function is actually homogeneous. The vice versa is not true, because there are homogeneous functions which do not admit different weights (i.e., they are not strictly quasi-homogeneous). A trivial example is given by $g(x,y) = x^2 + y^2$, which is homogeneous of degree 2 but it is not also strictly quasihomogeneous. Instead, the function $h(x,y) = xy$ is homogeneous of degree 2 and it is also quasi-homogeneous with undetermined weights. In the following, ''quasi-homogeneous'' is used as synonymous of strictly quasi-homogeneous, unless a more general discussion is required.

A Pfaffian form

$$\omega = \sum_{i=1}^{n} \omega_i(x) dx^i \tag{6}$$

is defined to be quasi-homogeneous of degree $r \in \mathbb{R}$ if, under the scaling

$$x^1,\ldots,x^n \mapsto \lambda^{\alpha_1} x^1,\ldots,\lambda^{\alpha_n} x^n \tag{7}$$

one finds

$$\omega \mapsto \lambda^r \omega. \tag{8}$$

This happens if and only if the degree of quasi-homogeneity $\deg(\omega_i(x))$ of $\omega_i(x)$ is such that $\deg(\omega_i(x)) = r - \alpha_i \ \forall i = 1,\ldots,n$. Let us assume that a quasi-homogeneous ω is integrable, i.e., $\omega \wedge d\omega = 0$. A quasi-homogeneous transformation is a symmetry for ω (see, e.g., Refs. 5 and 6), in the sense that

$$(L_D \omega) \wedge \omega = 0 \tag{9}$$

where L_D is the Lie derivative associated with D defined in (5). An integrating factor f such that the form ω/f is closed can then be constructed by contracting the vector field D with ω:

$$f \equiv \omega(D) = i_D(\omega), \tag{10}$$

and $\omega(D) \not\equiv 0$ is to be assumed. This means that the symmetry generated by D is nontrivial, in the sense that it does not belong to the distribution of codimension one which is associated with the kernel of ω. Then, the symmetry is not tangent to each leaf of the foliation associated with the integrable one-form ω, but it carries leaves onto other leaves. In this sense, a nontrivial symmetry is transversal with respect to the foliation.
One gets

$$d\left(\frac{\omega}{f}\right) = 0. \tag{11}$$

The integrating factor f is a quasi-homogeneous function of degree r, because $D i_D(\omega) = i_D L_D \omega = r i_D(\omega)$ (due to the Cartan formula $L_X i_Y - i_Y L_X = i_{[X,Y]}$ and to $i_0 = 0$). Then ω/f is of degree zero and its integral can be found only by quadratures (cf. Sec. III); one gets

$$\hat{S} - \hat{S}_0 \equiv \int_\Gamma \frac{\omega}{f}. \tag{12}$$

It can be shown that there exists a quasi-homogeneous function F of degree one with respect to D such that

$$\hat{S} = \log(F), \tag{13}$$

$$DF = F, \tag{14}$$

thus it holds $D\hat{S} = 1$ and $\hat{S}$ is not quasi-homogeneous. On this topic see Appendix A, where the case of a generic transversal symmetry is treated. The above construction is completely analogous to the construction developed for homogeneous integrable Pfaffian forms in Ref. 1.

III. A GENERAL FRAMEWORK

Quasi-homogeneous thermodynamics (recall that we mean strictly quasi-homogeneous) overcomes the standard distinction between extensive and intensive variables. We propose the following generalization for the integrable Pfaffian form δQ_{rev} which represents the infinitesimal heat exchanged by the system:

$$\delta Q_{\mathrm{rev}} = dU^* - \sum_{i=1}^{n} \xi_i^* \, dX^{i*} \tag{15}$$

where the asterisk indicates that both the independent variables $U^*, X^{1*}, \ldots, X^{n*}$ and the dependent ones $\xi_1^*, \ldots, \xi_n^*$ in (15) are generalizations of the usual ones in the sense that they are not simply intensive and/or extensive but quasi-homogeneous, in such a way that the Pfaffian form δQ_{rev} is quasi-homogeneous of degree r. Moreover, for the sake of definiteness and in order to fit some requirements for the validity of Frobenius' theorem, δQ_{rev} is assumed to be of class at least C^1 in the thermodynamic domain (except, maybe, on the boundary as, e.g., the surface $T=0$).

The thermodynamic domain $\mathcal{D}$ is assumed to be a simply connected set which satisfies (3). A further requirement for $\mathcal{D}$ has to be introduced if the entropy S^* is required to be superadditive: $\mathcal{D}$ has to be closed with respect to the sum (see Sec. VII for further details). Compare also Sec. III B. [In standard homogeneous thermodynamics, the thermodynamic domain can be assumed to be a convex cone,[1] which is a cone with the property to be closed under addition (Ref. 7, pp. 13–14). One can also assume that the domain $\mathcal{D}$ is still a convex cone with the further requirement that it has to be invariant under quasi-homogeneous transformations. This can be obtained by considering a set $\mathcal{C} \subset \mathbb{R}^{n+1}$ which is invariant under quasi-homogeneous transformations and then the set $\mathcal{K}$ of all the positive linear combinations of elements of $\mathcal{C}$. The set $\mathcal{K}$ is the smallest convex cone containing $\mathcal{C}$ (Ref. 7, p. 14). This cone $\mathcal{K}$ is trivially still invariant under quasi-homogeneous transformations.]

In the following, it is useful to refer to the variables $U^*, X^{1*}, \ldots, X^{n*}$ as would-be extensive variables, and to the variables $\xi_1^*, \ldots, \xi_n^*$ (and also T^*) as would-be intensive variables. The variables $U^*, X^{1*}, \ldots, X^{n*}$ could also be chosen to be such that they are additive, i.e., if one considers a system which is composed by two noninteracting subsystems, then $X^* = X_1^* + X_2^*$. See also Ref. 8.

We assume that the X^{i*} are of degree α_i; notice that the degree of U^* is $\alpha = r$, i.e., the degree r of δQ_{rev} and the weight α of U^* have to coincide in every case. The Euler vector field is

$$D = \alpha U^* \frac{\partial}{\partial U^*} + \sum_i \alpha_i X^{i*} \frac{\partial}{\partial X^{i*}}. \tag{16}$$

An integrating factor for δQ_{rev} is given by

$$f^* = \alpha U^* - \sum_i \alpha_i \xi_i^* X^{i*}, \tag{17}$$

and it is assumed that $f^* \not\equiv 0$ as in standard thermodynamics and, moreover, it is assumed that $f^* \geqslant 0$, which is related to the positivity of the absolute temperature. Then, it is possible to show that, as in standard thermodynamics, the potential $\hat{S}^*$, which is not quasi-homogeneous, is associated with a positive definite potential S^* which is a quasi-homogeneous function of degree 1 with respect to the Euler vector field D:

$$\hat{S}^* - \hat{S}_0^* = \int_\Gamma \frac{\omega}{f^*} = \log\left(\frac{S^*}{S_0^*}\right). \tag{18}$$

The proof is found in Appendix A.

Before continuing our analysis, we recall that a detailed and important study on quasi-homogeneous functions and their application to scaling and universality is the subject of Refs. 9 and 10 (therein, quasi-homogeneous functions are called ''generalized homogeneous functions,'' which is a better denomination, but we adopt a common mathematical denomination). See also Ref. 11. Further mathematical properties are found in Ref. 12 [note that, therein, quasi-homogeneous functions are called ''almost-homogeneous functions'' (Ref. 12, p. 231), whereas

the definition ''generalized homogeneous functions'' is assigned to a further generalization of the equation defining homogeneous and almost-homogeneous functions (Ref. 12, p. 304)].

A. Metrical entropy

By analogy with the construction for standard thermodynamics, a possibility is that S^* is the metrical entropy for the system. This is what happens in standard homogeneous thermodynamics and also in black hole thermodynamics, and we conjecture that this occurrence is not special. See however the discussion at the end of this section.

We define $T^* \geqslant 0$ by means of

$$\frac{\partial S^*}{\partial U^*} \equiv \frac{1}{T^*} > 0, \tag{19}$$

which means that S^* is assumed to be monotonically increasing in U^*. T^* is another integrating factor for (15), it is such that

$$\delta Q_{\text{rev}} = T^* \, dS^*. \tag{20}$$

T^* is a quasi-homogeneous function of degree $r-1$ (see theorem 1 of Ref. 9, where it is shown that the partial derivative $\partial g/\partial X$ of a quasi-homogeneous function g of degree a with respect to a variable X of weight b is a quasi-homogeneous function of degree $a-b$ and the same type as g). When $r \neq 1$, the function T is not intensive, but changes under quasi-homogeneous rescalings of the system. In the case of a Kerr–Newman black hole, one finds, e.g., that, by doubling the mass and the charge, and by quadruplicating the angular momentum, the temperature becomes one-half the temperature of the original black hole state. This behavior is well justified in the light of the Hawking effect.

As a consequence of (19) and of (18), one finds

$$\frac{\partial \hat{S}^*}{\partial U^*} = \frac{1}{f^*} = \frac{1}{S^*} \, \frac{\partial S^*}{\partial U^*} = \frac{1}{T^* S^*}, \tag{21}$$

thus

$$f^* = T^* S^*, \tag{22}$$

as in standard thermodynamics. From (20) it is easy to show that the quasi-homogeneous entropy can be written as

$$S^* = \alpha \frac{U^*}{T^*} - \sum_i \alpha_i \frac{\xi_i^*}{T^*} X^{i*}. \tag{23}$$

In fact, T^* is an integrating factor of degree $r-1$ for δQ_{rev}, and $dS^* \equiv \delta Q_{\text{rev}}/T^*$ is an exact quasi-homogeneous Pfaffian form of degree 1. Then, as a consequence of lemma 1 in Appendix A (cf. also result 1 therein), one finds $S^* = i_D(\delta Q_{\text{rev}}/T^*)$, i.e., Eq. (23) holds. When all the weights in (23) are equal to 1, the well-known expression for the homogeneous thermodynamic entropy is recovered.

B. Thermodynamic foliation

As in the case of standard thermodynamics, one can require that the thermodynamic foliation is defined by the leaves $\hat{S}^* = \text{const}$ everywhere in the thermodynamic manifold, except maybe on the boundary. Singularities for $\hat{S}^*$ can occur where $f^* = 0$, i.e., in the set $Z(f^*) = Z(T^*) \cup Z(S^*)$.

The surface $T^*=0$ is expected to represent an adiabatic boundary of the thermodynamic manifold. Notice that, as in the case of standard thermodynamics, the set $Z(S^*)$ of zeroes of the function S^*, if nonempty, is assumed to be contained in the set $Z(T^*)$. In standard thermodynamics the occurrence of a zero for S at a temperature $T>0$ can be considered pathological, a system in such a state should necessarily absorb heat in a neighborhood of this state, whichever reversible process could be considered. Compare Ref. 1. The same would happen in the quasi-homogeneous case.

Because of (18), the singular values for the thermodynamic foliation are represented by the points where $S^*=0$ (if any).

A stronger assumption on the domain: One could also assume that

$$f^*\geqslant 0 \Leftrightarrow U^*\geqslant b(X^{1*},\ldots,X^{n*}), \tag{24}$$

where $b(X^{1*},\ldots,X^{n*})$ is a quasi-homogeneous function of degree α and weights $(\alpha_1,\ldots,\alpha_n)$. This function $b(X^{1*},\ldots,X^{n*})$ plays the role of lowest energy for the system, because by definition $U^*\geqslant b$. The domain $\mathcal{D}$ has to include the following set:

$$epi(b)\equiv\{(U^*,X^{1*},\ldots,X^{n*})|(X^{1*},\ldots,X^{n*})\in\mathcal{K}_{(n)},\ \ U^*\geqslant b(X^{1*},\ldots,X^{n*})\}, \tag{25}$$

where $\mathcal{K}_{(n)}\subseteq\mathbb{R}^n$ is an open connected set. $epi(b)$ is by definition the epigraph of the function b. If $\mathcal{K}_{(n)}$ is closed under quasi-homogeneous dilatations $(X^{1*},\ldots,X^{n*})\mapsto(\lambda^{\alpha_1}X^{1*},\ldots,\lambda^{\alpha_n}X^{n*})$, then $epi(b)$ is closed under quasi-homogeneous dilatations involving also U^*, because $b(\lambda^{\alpha_1}X^{1*},\ldots,\lambda^{\alpha_n}X^{n*})=\lambda^{\alpha}b(X^{1*},\ldots,X^{n*})\leqslant\lambda^{\alpha}U^*$. Moreover, if $\mathcal{K}_{(n)}$ is also closed under the sum and if b is subadditive, then $epi(b)$ is closed under the sum too, thus the closure of $\mathcal{K}_{(n)}$ under quasi-homogeneous dilatations and under the sum allows us to choose $\mathcal{D}=epi(b)$, in analogy with the standard homogeneous case. (Notice that if, e.g., $\mathcal{K}_{(n)}=\mathbb{R}^n_+$, then it is a convex cone which is invariant under quasi-homogeneous dilatations.) An example where the domain $\mathcal{D}$ coincides with the epigraph of a quasi-homogeneous function is furnished by black hole thermodynamics.

Under this assumption on the structure of the domain, one finds that it is not possible to find a state having $S^*=0$ at $T^*>0$, because by introducing

$$B^*\equiv U^*-b(X^{1*},\ldots,X^{n*})\geqslant 0 \tag{26}$$

one finds

$$S^*(B^*,X^{1*},\ldots,X^{n*})=S^*(0,X^{1*},\ldots,X^{n*})+\int_0^{B^*}dY\,\frac{1}{T^*(Y,X^{1*},\ldots,X^{n*})}, \tag{27}$$

which cannot be zero for any $B^*>0$ (in the last formula mathematical conditions ensuring a continuous entropy at $T^*=0$ have been implicitly assumed, cf. Ref. 1).

As far as the reference state is concerned, we assume that states like the one where all the variables $U^*,X^{1*},\ldots,X^{n*}$ are zero, and any states which imply the absence of the system, are unphysical. The thermodynamic description starts being meaningful if a statistically relevant number of degrees of freedom is available. Compare Sec. II of Ref. 1.

C. Possible ambiguities

One may wonder what should happen if one finds that ω is quasi-homogeneous but the exact weights are not *a priori* known. In particular, one can assume that their ratio is known, i.e., α/α_i and α_j/α_i are known for all $i\neq j$; then, there is an overall undetermined multiplicative constant $q\neq 0$, in the sense that these ratios do not change if one multiplies all the weights by the same constant. One could, e.g., know $r^{(1)}\equiv\alpha/\alpha_1$ and $r_j^{(1)}\equiv\alpha_j/\alpha_1$ for $\alpha_1\neq 0$ and for all $j\neq 1$, but the absolute weight α_1 is not known, thus the weights are $(\alpha_1 r^{(1)},\alpha_1,\alpha_1 r_2^{(1)},\ldots,\alpha_1 r_n^{(1)})$. An example where this ambiguity appears is represented by black hole thermodynamics (see Sec. IV). One can

also assign the weights with respect to a scale λ whose absolute weight could be unknown. The absolute weights are then of the form $(q\alpha, q\alpha_1, \ldots, q\alpha_n)$ with q undetermined. We treat the latter case without loss of generality, being the former equivalent to it under the map $\alpha_1 \mapsto q\alpha_1$, $q\alpha_1 r^{(1)} \mapsto q\alpha, q\alpha_1 r_i^{(1)} \mapsto q\alpha_i$ for all $i \neq 1$. As a consequence of the undetermined overall factor q, one has a one-parameter family of Euler vector fields $\{D_{(q)}\}$, with

$$D_{(q)} = q\alpha U^* \frac{\partial}{\partial U^*} + \sum_i q\alpha_i X^{i*} \frac{\partial}{\partial X^{i*}}. \tag{28}$$

Thus, there exist a one-parameter family $\{f^*_{(q)}\}$ of integrating factors, with $f^*_{(q)} = \delta Q_{\text{rev}}(D_{(q)})$, and a one-parameter family $\{\hat{S}_{(q)}\}$ of potentials such that

$$\frac{\delta Q_{\text{rev}}}{f^*_{(q)}} = d\hat{S}_{(q)} \tag{29}$$

and a one-parameter family of entropies $\{S^*_{(q)}\}$ satisfying

$$d\hat{S}_{(q)} = \frac{dS^*_{(q)}}{S^*_{(q)}}, \tag{30}$$

$$D_{(q)} S^*_{(q)} = S^*_{(q)}. \tag{31}$$

The true metrical entropy S^*, according to our conjecture, belongs to the family $\{S^*_{(q)}\}$ but is undetermined because the overall factor q is undetermined. In order to see which relation occurs between the various entropies in this family, let us consider a fixed value $\overline{q}$ of the parameter q. Then we obtain the entropy $S^*_{(\overline{q})}$. If one considers a generic $\hat{q} \neq \overline{q}$, one has

$$D_{(\hat{q})} = \frac{\hat{q}}{\overline{q}} D_{(\overline{q})} \tag{32}$$

and

$$f^*_{(\hat{q})} = \frac{\hat{q}}{\overline{q}} f^*_{(\overline{q})}. \tag{33}$$

Then,

$$\frac{\delta Q_{\text{rev}}}{f^*_{(\hat{q})}} = \frac{\overline{q}}{\hat{q}} \frac{\delta Q_{\text{rev}}}{f^*_{(\overline{q})}} \tag{34}$$

$$\Leftrightarrow$$

$$d \log(S^*_{(\hat{q})}) = \frac{\overline{q}}{\hat{q}} d \log(S^*_{(\overline{q})}). \tag{35}$$

As a consequence, by assuming in the integral of $\delta Q_{\text{rev}}/f$ the same reference state $(U_0^*, X_0^{1*}, \ldots, X_0^{n*})$, one finds

$$S^*_{(\hat{q})}(U^*, X^{1*}, \ldots, X^{n*}) = \frac{S^*_{(\hat{q})}(U_0^*, X_0^{1*}, \ldots, X_0^{n*})}{(S^*_{(\overline{q})}(U_0^*, X_0^{1*}, \ldots, X_0^{n*}))^{\overline{q}/\hat{q}}} \; (S^*_{(\overline{q})}(U^*, X^{1*}, \ldots, X^{n*}))^{\overline{q}/\hat{q}}, \tag{36}$$

i.e.,

$$S^*_{(\hat{q})} = \zeta_{\hat{q},\overline{q}} (S^*_{(\overline{q})})^{\overline{q}/\hat{q}}, \tag{37}$$

where $\zeta_{\hat{q},\overline{q}} \equiv S^*_{(\hat{q})}(U^*_0, X^1_0{}^*, \ldots, X^n_0{}^*)/(S^*_{(\overline{q})}(U^*_0, X^1_0{}^*, \ldots, X^n_0{}^*))^{\overline{q}/\hat{q}}$ is a constant, once one has fixed the reference state. The metrical entropy S^* is related with the entropy $S^*_{(\overline{q})}$ by a simple power law. Compare also Appendix A.

The one-parameter family of temperatures $\{T^*_{(q)}\}$, with

$$\frac{1}{T^*_{(q)}} \equiv \frac{\partial S^*_{(q)}}{\partial U^*}, \tag{38}$$

is such that

$$\frac{1}{T^*_{(\hat{q})}} = \zeta_{\hat{q},\overline{q}} \frac{\overline{q}}{\hat{q}} (S^*_{(\overline{q})})^{\overline{q}/\hat{q}-1} \frac{1}{T^*_{(\overline{q})}}. \tag{39}$$

Analogous relations exist for the other partial derivatives of $S^*_{(\overline{q})}$ and $S^*_{(\hat{q})}$. Notice that it holds $f^*_{(q)} = T^*_{(q)} \; S^*_{(q)}$, because

$$\frac{\partial \hat{S}^*_{(q)}}{\partial U^*} = \frac{1}{f^*_{(q)}} = \frac{1}{S^*_{(q)}} \frac{\partial S^*_{(q)}}{\partial U^*} = \frac{1}{T^*_{(q)} S^*_{(q)}}. \tag{40}$$

1. Phenomenological resolution of the ambiguity

The metrical entropy S^* could be phenomenologically identified by means of an absolute temperature thermometer, made of standard matter, allowing to find, as the parameters $U^*, X^1{}^*, \ldots, X^n{}^*$ are varied, the function T^* describing the absolute temperature of the system. As a consequence, also S^* can be recovered. We remark that the resolution of the above ambiguity by means of a phenomenological input is completely in the spirit of thermodynamics, which has a phenomenological nature as far as statistical mechanics is not taken into account.

2. How to fix the absolute weights by means of statistical mechanics

A priori, even in statistical mechanics, there is a scaling ambiguity, unless the absolute weights are somehow fixed. On this topic, see also Sec. XII. In fact, let us assume that the statistical mechanical entropy (calculated by means of some sort of thermodynamic limit or by means of some mean field approximation; cf. Sec. XII) under rescaling by means of a scale λ is a quasi-homogeneous function of degree α_S and weights $\alpha_1, \ldots, \alpha_n$. This means that $S_{sm}(\lambda^{\alpha} U, \lambda^{\alpha_1} X^1, \ldots, \lambda^{\alpha_n} X^n) = \lambda^{\alpha_S} S_{sm}(U, X^1, \ldots, X^n)$. By changing the scale $\lambda = \overline{\lambda}^{q}$, the scaling of the variables becomes $\overline{\lambda}^{q\alpha_i}$. Thus, there is an overall factor q of ambiguity. Such a redefinition of the scale, unless the absolute weights are somehow fixed, allows to remap any quasi-homogeneous function of degree $\alpha \neq 0$ into a quasi-homogeneous function of degree one, as noticed in Ref. 10. The statistical mechanical entropy is then assumed to satisfy

$$S_{sm}(\lambda^{q\alpha} U, \lambda^{q\alpha_1} X^1, \ldots, \lambda^{q\alpha_n} X^n) = \lambda^{q\alpha_S} S_{sm}(U, X^1, \ldots, X^n), \tag{41}$$

where the overall factor ambiguity is enhanced. With respect to the Euler vector field $D_{(q)}$ which corresponds to the above weights it holds $D_{(q)} S_{sm} = q \alpha_S S_{sm}$.

We know that from a thermodynamic point of view there is a one-parameter family of possible metrical entropies, each of which is of degree one. The statistical mechanical entropy S_{sm} has to coincide with the metrical thermodynamic entropy S^* and it has to hold $T \, dS_{sm} = T^* \, dS^* = \delta Q_{\text{rev}}$. As a consequence, the statistical mechanical entropy has to be a degree one quasi-homogeneous function. This requirement fixes $q \alpha_S = 1$, and fixes unambiguously the weights (then, it eliminates also the ambiguity in the one-parameter family of thermodynamic entropies).

We could also relax our conjecture about the identification of S^* in formula (18) as the metrical entropy. The Clausius-type formula (18) gives in general an empirical entropy which is to be uniquely related with the metrical entropy by identifying the absolute temperature scale as in the standard procedure. One could still assume that the metrical entropy is quasi-homogeneous, but it would be possible in line of principle to require that its degree is q, with q non-necessarily equal to 1. Then, even in the case where all the weights are known, one would find $S^*_{\text{metric}} \propto (S^*)^q$, where S^* is obtained from formula (18). Compare also Appendix A. The above phenomenological procedure could be still allowed. Compare also Sec. XII and the conclusions herein.

A further consideration is in order, and it concerns the possible presence of variables of weight zero. All the mathematical approach developed in this section remains unaltered. It is to be noted that, if a variable I^* having weight zero is present, the term $I^* \partial / I^*$ does not appear in the Euler operator and in the integrating factor f the term proportional to I^* is missing.

Notice that it is possible that the thermodynamic description allows a reducing/enlarging of the thermodynamic space as the one discussed in Ref. 1. This means that part of the variables X^i* appearing in δQ_{rev} and in S^* could be set equal to zero consistently, which means that a meaningful thermodynamic description is still allowed when $X^i* = 0$ (in standard thermodynamics such variables play, e.g., the role of external fields[1]); consistency requires that, if $X^i* = 0$ is allowed, then $\xi_i^* = 0$ as $X^i* = 0$.[1] Black hole thermodynamics represents a good example, and this topic is discussed in Sec. XI.

We underline that this kind of generalization of thermodynamics can be considered as a subcase of a generalization proposed by Landsberg in Ref. 13. Therein, a discussion of generalized ideal gases appears, where the properties of the following generalized entropy are analyzed:

$$S = bN \log\left(a \frac{UV^g}{N^h} \right). \tag{42}$$

Given the Euler field

$$D_{\alpha\beta\gamma} = \alpha U \frac{\partial}{\partial U} + \beta V \frac{\partial}{\partial V} + \gamma N \frac{\partial}{\partial N}, \tag{43}$$

it is easy to show that S in (42) is quasi-homogeneous (of degree γ) if and only if $\alpha + g\beta - h\gamma = 0$. If the latter constraint is not implemented, then S is not quasi-homogeneous. Homogeneity requires $h = g + 1$.

IV. THE BLACK HOLE CASE

We summarize herein the results obtained in Ref. 14 in the black hole case (we set $\hbar = c = G = k_b = 1$, where k_b is the Boltzmann constant; moreover, we work with unrationalized electrical units). For a general discussion about black hole thermodynamics see, e.g., Refs. 15 and 16. Herein, as well as in Sec. V and in Sec. VI, we do not use the asterisk, which is in general used only in theoretical sections. The Pfaffian form of black hole thermodynamics for black holes of the Kerr–Newman family is

$$\delta Q_{\text{rev}} \equiv dM - \Phi\, dQ - \Omega\, dJ, \tag{44}$$

where the parameters M, Q, J are the mass M, the angular momentum J and the charge Q of the black hole; the angular velocity

$$\Omega = \frac{J}{M} \frac{1}{2M^2 - Q^2 + 2M\sqrt{M^2 - Q^2 - J^2/M^2}} \tag{45}$$

and the electric potential

$$\Phi = \frac{Q(M + \sqrt{M^2 - Q^2 - J^2/M^2})}{2M^2 - Q^2 + 2M\sqrt{M^2 - Q^2 - J^2/M^2}} \tag{46}$$

are associated with the black hole horizon. M in (44) plays the role of internal energy, the remaining terms in (44) being ''standard'' work terms. Each black hole of the Kerr–Newman family is a stationary solution of the Einstein equations, and it can be considered, from the thermodynamic point of view we develop here, rather loosely speaking, as an ''equilibrium state of the geometry.'' The variation occurring in (44) is taken along such stationary solutions. The thermodynamic domain for the nonextremal black holes is the (open) nonextremal manifold implicitly defined by the inequality $M^4 - M^2Q^2 - J^2 > 0$; the extremal submanifold $M^4 - M^2Q^2 - J^2 = 0$ is a boundary of the former, and its status is analyzed in Ref. 17 (therein a discussion of the third law of thermodynamics also in the light of this approach is found). (We limit ourselves to recall that in black hole thermodynamics the entropic form of the third law is violated[18] but still the unattainability of $T = 0$ holds under suitable hypotheses.)

The Pfaffian form (44) is integrable, it satisfies the condition $\delta Q_{\text{rev}} \wedge d(\delta Q_{\text{rev}}) = 0$, i.e.,

$$-\partial_J \Phi + \partial_Q \Omega + \Phi \partial_M \Omega - \Omega \partial_M \Phi = 0. \tag{47}$$

Moreover, the Pfaffian form (44) is quasi-homogeneous. In fact, under $M \to \lambda^{\alpha} M$; $Q \to \lambda^{\alpha} Q$; $J \to \lambda^{2\alpha} J$, one obtains $\delta Q_{\text{rev}} \to \lambda^{\alpha} \delta Q_{\text{rev}}$, where $\lambda > 0$. The weights α, α, 2α are not known, only their ratio is determined. Then, the degree of δQ_{rev} is not fixed.[14] Nevertheless, a thermodynamic construction is allowed. One finds that the integrating factor for δQ_{rev} is given by $f = \alpha(M - \Phi Q - 2\Omega J)$, that is

$$f = \alpha \sqrt{M^2 - Q^2 - J^2/M^2} \tag{48}$$

(it is interesting to notice that this integrating factor is proportional to the horizon coordinate c introduced by Carter in Ref. 19, thus, it is constant on the horizon). Then, one gets[14]

$$\int \frac{\delta Q_{\text{rev}}}{f} \equiv \hat{S} - \hat{S}_0 = \frac{1}{2\alpha} \log\left(\frac{A}{A_0}\right), \tag{49}$$

where $A = 4\pi(M^2(1 + \sqrt{1 - Q^2/M^2 - J^2/M^4})^2 + J^2/M^2)$ is the black hole area and is positive definite. The main difficulty is in finding the metrical entropy, because of the undetermined overall multiplicative constant α. Both $\alpha = 1/2$ and a undetermined proportionality constant c_0 appearing in the Bekenstein–Hawking law $S = c_0 A$ are recovered, e.g., by comparing the temperature of the black hole with the Hawking temperature, and one finds $c_0 = 1/4$; also the Euclidean path integral method can be used with this aim[20] (see also the papers collected in Ref. 21), as well as a phenomenological plot of the temperature as a function of M, Q, J. [Moreover, we notice that the same result $S \propto A$ could be obtained by requiring that the metrical entropy is quasi-homogeneous of degree one with respect to the Euler field D which is obtained by normalizing to one the biggest weight 2α:

$$D = \frac{1}{2} M \frac{\partial}{\partial M} + \frac{1}{2} Q \frac{\partial}{\partial Q} + J \frac{\partial}{\partial J}. \tag{50}$$

But this normalization rule should be justified on a general thermodynamic footing, and the case $J = 0$ (Reissner–Nordström solution), being homogeneous in M, Q, shows that the physically correct value $\alpha = 1/2$ cannot be found on the ground of such a rule.]

S is quasi-homogeneous of degree one and of type (1/2,1/2,1) and it is well defined everywhere in the thermodynamic manifold. It is such that $S = 0$ only for $M = Q = J = 0$, which should not be considered as a state belonging to the thermodynamic manifold (see the discussion in Sec. III; moreover, near $M = 0$ quantum gravity effects are non-negligible and general relativity is

expected to be nonviable). Thus, $Z(S)=\varnothing$ and one finds $Z(f)=Z(T)$, and $\hat{S}$ is regular everywhere; as a consequence, $\hat{S}$ and S could be continued even on the extremal submanifold (but see Ref. 17 for arguments against this continuation). All nonextremal states have $T>0$, whereas the extremal boundary corresponds to $T=0$. As it is well-known, one obtains an entropy which is not concave, but simply strictly superadditive when the merging of two black holes is considered. This ensures the second law of thermodynamics.[13,22,23] See also Sec. VII.

By introducing

$$b(Q,J)\equiv\frac{1}{\sqrt{2}}\sqrt{Q^2+\sqrt{Q^4+4J^2}}, \tag{51}$$

which is a quasi-homogeneous function of degree 1/2 and weights (1/2,1), as it can be easily verified (see also Ref. 17), the domain can be also written as follows:

$$\mathcal{D}=\{(M,Q,J)|(Q,J)\in\mathbb{R}^2,M\geqslant b(Q,J)\}\equiv \mathrm{epi}(b). \tag{52}$$

In fact, $M=b(Q,J)$ is the physical (i.e., having positive mass) solution of $M^4-M^2Q^2-J^2=0$ and the black hole manifold is $M^4-M^2Q^2-J^2\geqslant 0$, which means $M\geqslant b$. The function $b(Q,J)$ indicates, for given values of Q,J, which is the lowest mass such that a black hole solution can exist. The lowest mass coincides with the mass of the extremal black hole having Q,J as charge and angular momentum, respectively.

We point out that the quasi-homogeneous behavior of black hole thermodynamics is not a special feature of the Kerr–Newman family. In fact, it can be realized easily, e.g., in the case of the Kerr–Newman–anti–de-Sitter (KN–AdS) case.[24] A peculiar feature arises, one has to define a thermodynamic angular velocity Ω as the difference between the angular velocity of the horizon and the angular velocity at infinity, and the same is true in the case of the electric potential.[24] Nevertheless, these definitions are necessary, e.g., the ''electric'' work term has to involve the difference between the potential at the horizon and the potential at infinity when the latter is not zero, and, on the same footing, the redefinition of Ω is due to the fact that the angular velocity is not zero at infinity. The change in the energy associated with these work terms has to involve such a difference, which does not appear in the KN case because of the vanishing of Φ and of Ω at infinity.

General relativity is surprising from a thermodynamic point of view. Black hole solutions of the Einstein equations are involved with an integrability condition (47), and they allow a fine explicit thermodynamic construction via Carathéodory. One finds a link with thermodynamics which is *a priori* unexpected and it is not simply the formal analogy between laws of thermodynamics and laws of black hole mechanics, because the above construction belongs to the thermodynamic framework, apart from the geometric inputs Ω, Φ, which come from general relativity. See also the discussion in Ref. 14.

V. NEWTONIAN GRAVITY. A MODEL OF HERTEL, NARNHOFER, AND THIRRING

There exists an interesting statistical mechanical calculation for gravitating fermions which corroborates the idea that, in presence of gravity, a quasi-homogeneous thermodynamics is allowed.[25–27] The model (HNT model in the following) involves nonrelativistic fermions interacting by means of a Coulomb potential and a Newtonian potential, with vanishing (or small) total charge. Thus, the calculation does not involve general relativity but only Newtonian gravity. Nevertheless, the result is still interesting and, to some extent, puzzling. The quantum mechanical Hamiltonian which is considered is

$$H=\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2M_i}+\sum_{i<j}\frac{e_ie_j-Gm_im_j}{|\vec{x}_i-\vec{x}_j|}. \tag{53}$$

The authors state that a thermodynamic limit exists if the following asymptotic behavior is allowed for U,V: $V\sim 1/N$, $U\sim N^{7/3}$, and the microcanonical entropy is of degree 1 in the number N of fermions. The scaling properties of U, V with N are peculiar, they are homogeneous of degree 1 if the potential term in (53) is suppressed by means of a multiplicative factor $1/N^{2/3}$, which means that, as the system gets larger, the interaction becomes weaker.[27] If this suppression is not in agreement with the physics, and if the fermions do not become relativistic, then the microcanonical entropy $S(U,V,N)$ is a quasi-homogeneous function of degree 1, and the weights of U,V,N are $7/3,-1,1$, respectively. Compare also Sec. XII, where the notion of quasi-homogeneous thermodynamic limit is introduced. The Euler field is

$$D_{UVN}=\frac{7}{3}\,U\,\frac{\partial}{\partial U}-V\,\frac{\partial}{\partial V}+N\,\frac{\partial}{\partial N}. \tag{54}$$

For details of the highly nontrivial calculations, see Refs. 25,26 and 28. We are interested here in pointing out that, as stressed in Ref. 25, there is a one-parameter family of equivalent limits $N\to\infty$, whose parameter γ remains fixed by the requirement that the ground state energy goes like $N^{7/3}$, according to a result of Ref. 29. A scaling ambiguity, which would reflect itself in the undetermined weights $(-2\gamma+5/3,3\gamma,1)$ of (U,V,N), respectively, is thus solved by comparing with the scaling behavior of the ground state. See also Ref. 28. Another important point is that the temperature-dependent Thomas–Fermi equation, which allows these scaling properties, becomes exact in the thermodynamic limit for the system under discussion.[25] We limit ourselves to underline that Newtonian gravity furnishes a statistical mechanical example where unusual scaling laws for the ''extensive'' variables are allowed. The purely attractive nature of gravity plays a major role, because it does not saturate, i.e., it does not allow to obtain a ground state proportional to the number of particles.[29] Notice also that a lack of concavity is allowed.[27]

It is interesting to notice that another model involving different scaling relations has been developed in Ref. 30. Therein, a classical gas of nonrelativistic particles which interact by means of Newtonian gravity is considered in a diluted regime where particles of mass m are enclosed in a box; the following behavior is recovered in a nonconventional thermodynamic limit where $V/N^3\to$const. as $N\to\infty$. A dilution parameter

$$\xi\equiv\frac{1}{Gm^2}\,\frac{UV^{1/3}}{N^2} \tag{55}$$

is kept constant in the thermodynamic limit. One finds that $S(U,V,N)$ is quasi-homogeneous of degree 1 and weights (1,3,1), as can be inferred from Ref. 30. Compare also Sec. XII. This model differs from the previous one because it involves classical matter, the gas is kept diluted in the thermodynamic limit, no collapse is considered. Note that even the HNT model can be related with the parameter ξ introduced in (55), in fact even in HNT model this parameter is constant in the appropriate thermodynamic limit. ξ can be qualitatively interpreted as the ratio between the internal energy and the Newtonian gravitational energy, in fact the gravitational energy of a homogeneous sphere of mass $M\equiv N^2m$ is proportional to $GM^2/V^{1/3}$. Thus, in both cases, the requirement of a non-negligible contribution of the gravitational energy to the internal energy is realized in the thermodynamic limit. In the HNT model, a self-bounded system is considered, like a (cold) star, where V contracts as the mass is increased; in the model of Ref. 30, the physical conditions are different, a gaseous system is considered, the energy per particle remains constant and small, and the systems remains gaseous in the thermodynamic limit.

In the regime where gravitational forces cannot be neglected, one can expect that a different kind of quasi-homogeneous thermodynamics can arise, with different weights, depending on the actual physical conditions, e.g., the amount and the type of matter. Semirelativistic matter is expected to behave in a different manner (cf. Ref. 29). The point is that a different scaling behavior of the ground state of the matter can be expected if relativistic effects in the kinetic energy are non-negligible. A self-consistent calculation taking into account general relativity is

expected to give another kind of contribution. An approach, combining in a self-consistent way general-relativistic equations and finite-temperature Thomas–Fermi approximation for the thermodynamic functionals would be required. In this direction, see Ref. 31. It is also interesting to point out that such an approach probably would not be useful for understanding black hole thermodynamics, in fact no stable ground state for the matter could exist by hypothesis (a collapse of the matter beyond the possible stable states represented by white dwarf and neutron stars should take place, with no possibility to prevent the formation of an event horizon).

VI. A LOOK AT THE THERMAL GEON AND AT SELF-GRAVITATING RADIATION

We discuss naively the scaling properties of the so-called thermal geons.[32] A geon is a ''gravitational electromagnetic entity'' which consists in a self-gravitating ensemble of electromagnetic modes.[33] The most stable configuration is such that the photons are distributed within a toroidal region of the space–time, but also a spherical distribution can be allowed. Geons do not represent strictly stationary solutions of the Einstein equations, because a leakage of photons to infinity is allowed. Nevertheless, they can be considered as metastable quasistationary solutions. Moreover, sizes are considered where no contribution of electron physics, due to pair creation by the electromagnetic field, is considered, and no zero-point energy is taken into account. In Ref. 32 the idea of a geon has been generalized to the case of thermally distributed electromagnetic modes. The main assumptions are the following ones: (a) the metric is a spherosymmetric static diagonal metric in the Schwarzschild gauge; (b) there exist two separate classes of electromagnetic modes; the first class is constituted by bounded null geodesics which represent modes whose energy cannot escape to infinity (the actual rate of flux to infinity goes to zero exponentially with the ratio between the dimensions of the geon and the wavelength λ). The second class is constituted by free electromagnetic modes, i.e., by null geodesics which reach infinity. (c) The energy of the free modes is zero, the energy of the bounded modes of frequency Ω is (in natural units)

$$E_\Omega = \Omega \frac{1}{\exp\left(\frac{\Omega}{T}\right) - 1}, \tag{56}$$

which is the usual distribution for black-body radiation and T is the temperature. See also Ref. 32 on this topic. The active region of the geon is defined as the region where the metric coefficient g_{00} satisfies $|g_{00}| < 1$. By defining R as the radius of the active region and M as its mass, the following scaling laws can be deduced:[32]

$$R \sim R_T \equiv \left(\frac{15\hbar^3 c^7}{8\pi^3 G}\right)^{1/2} \frac{1}{(k_b T)^2} \propto \frac{1}{T^2}, \tag{57}$$

$$M \sim M_T \equiv \left(\frac{15\hbar^3 c^{11}}{8\pi^3 G^3}\right)^{1/2} \frac{1}{(k_b T)^2} \propto \frac{1}{T^2}. \tag{58}$$

As an order of magnitude estimation on the same footing of the previous evaluations, one can see that the entropy behaves as $S \propto VT^3$, where V is the volume of the active region, thus $S \propto T^{-3}$. From the above naive considerations, one finds that S is a quasi-homogeneous function

$$S(\lambda^{-2}M, \lambda^{-6}V) = \lambda^{-3} S(M, V). \tag{59}$$

In the case of a massless gas, there is an ambiguity in the identification of the absolute weights of the variables. There is an overall multiplicative factor to be determined in the Euler vector field. Let us assume that S is of degree 1, as suggested by the formal picture of thermodynamics (cf. Sec. III and Sec. XII); then T has degree $-1/3$ and the scaling law for the fundamental equation is

$$S(\lambda^{2/3}M,\lambda^2 V)=\lambda S(M,V), \tag{60}$$

i.e., M has weight 2/3 and V has weight 2. We note that the ratio $M/V^{1/3}$ is scale-invariant and it is the same ratio which is kept constant in the thermodynamic limit discussed in Ref. 30. The above result about thermal radiation can be confirmed by comparing it with the study of Ref. 34. Black-body self-gravitating radiation enclosed in a spherical box of radius R is considered in Ref. 34. It is shown that the maximization of the entropy in a spherosymmetric geometry leads to the following results: (i) the metric is static; (ii) the perfect fluid of photons satisfies the Tolman–Oppenheimer–Volkov (TOV) equation. In particular, the TOV equation one obtains is scale invariant. By introducing the density $\rho(r)$, the mass $m(r)=\int_0^r dy\, 4\pi y^2\rho(y)$ (r is the radial coordinate) one can define, by following Ref. 34, the dimensionless variables

$$\mu=m(r)/r, \tag{61}$$

$$q=dm/dr=4\pi r^2\rho(r), \tag{62}$$

and the TOV becomes equivalent to the following couple of equations:

$$r\frac{dq}{dr}=\frac{2q}{1-2\mu}\left(1-4\mu-\frac{2}{3}\,q\right), \tag{63}$$

$$r\frac{d\mu}{dr}=q-\mu. \tag{64}$$

No equilibrium is attained if $\mu>0.25$.[34] We are interested here in the scaling properties of the Pfaffian form

$$\delta Q_{\mathrm{rev}}=dM+p\,dV, \tag{65}$$

where $M\equiv m(R)$ is the mass, V is the volume (as seen from infinity) and $p=\rho(R)/3$ is the pressure as a function of the box radius. These variations are to be intended, as in the black hole case, as ''on shell,'' i.e., along static spherosymmetric equilibrium solutions of the TOV. Each solution represents a thermodynamic equilibrium state. Under the scaling $M\to\lambda M$; $V\to\lambda^3 V$; $p\to\lambda^{-2}p$, which corresponds to (30) of Ref. 34 and is allowed by the scale invariance of the TOV, one finds $\delta Q_{\mathrm{rev}}\to\lambda\,\delta Q_{\mathrm{rev}}$. Particularly, one has

$$D=\alpha\left(M\,\frac{\partial}{\partial M}+3V\,\frac{\partial}{\partial V}\right), \tag{66}$$

where α has to be determined. From $dV=4\pi R^2\,dR$ and from (64) one finds

$$\delta Q_{\mathrm{rev}}=\tfrac{4}{3}\,q\,dR \tag{67}$$

and the integrating factor

$$\delta Q_{\mathrm{rev}}(D)=\alpha(M+3pV)=\alpha\tfrac{1}{3}(3\mu+q)R. \tag{68}$$

Thus,

$$\frac{\omega}{f}=\frac{4}{\alpha}\,\frac{q}{3\mu+q}\,\frac{dR}{R}. \tag{69}$$

By comparing this result with the ratio dS/S which can be obtained by the exact result (34) of Ref. 34, one finds that $\alpha=2/3$. As the consequence, the weights of D are the same as in the case of

thermal geons [notice that the requirement for S to be quasi-homogeneous of degree one in the scale factor λ would lead to the scaling $r\to\lambda^{2/3}r$; $m\to\lambda^{2/3}m$; $\rho\to\lambda^{-4/3}\rho$ in (30) of Ref. 34].

VII. CONSEQUENCES OF THE NONEXTENSIVITY OF *S*

We have to underline that the lack of extensivity has important consequences on the properties of the entropy. In fact, if one considers for a continuous entropy S superadditivity (S), concavity (C) and homogeneity (H), one finds:
(a) (H) and (S) imply (C);[35]
(b) (H) and (C) imply (S);[36]
(c) (S), with the condition $S(0)=0$, and (C) imply (H).[8,22]

We recall that a function $h(x)$ of n variables, collectively indicated with x in this section, is superadditive if $h(x+y)\geqslant h(x)+h(y)$ for all x,y in its domain. Superadditivity, in the case of entropy, means that the principle of entropy increase in a irreversible adiabatic process is respected. Moreover, (C) requires a convex domain, (S) a domain which has to be closed under addition, and (H) a domain which has to be closed under multiplication of x by a real scalar $\lambda>0$ (a cone).

Notice that the condition $S(0)=0$ appearing in (c) is a mathematical condition which could be required even if the state $x=0$ does not belong to the thermodynamic space, in the light of our discussion in Sec. III; see however also Ref. 22, where $x=0$ is included in the thermodynamic space. One could consider an extended domain including $x=0$, on a purely mathematical ground, even if the thermodynamic formalism at such a point is meaningless. Moreover, S is required to be a continuous function. Then, if homogeneity does not hold and $S(0)=0$, either superadditivity or concavity has to be violated. It can be easily shown that the condition $S(0)=0$ in (c) can be replaced by the (natural) requirement that $S(x)\geqslant 0$ for any state x in the thermodynamic domain. In fact, (C) implies

$$S(\tfrac{1}{2}y+\tfrac{1}{2}z)\geqslant\tfrac{1}{2}S(y)+\tfrac{1}{2}S(z) \tag{70}$$

for any y,z; moreover, (S) implies

$$S(2x)\geqslant 2S(x). \tag{71}$$

If $z=0$ and $y=2x$, from (70) one obtains

$$S(x)\geqslant\tfrac{1}{2}S(2x)+\tfrac{1}{2}S(0). \tag{72}$$

Then, $1/2\ S(2x)+1/2\ S(0)\leqslant S(x)\leqslant 1/2\ S(2x)$, which implies $S(0)\leqslant 0$. As a consequence, the requirement of a non-negative entropy S, together with (S) and (C), implies $S(0)=0$, thus also (H) has to hold. This shows that the condition $S(0)=0$, in the framework of thermodynamics, where $S\geqslant 0$, cannot be actually considered as a true restriction leaving room for a thermodynamics in which a concave and superadditive but nonhomogeneous entropy is allowed if S is defined in $x=0$ (of course, this holds as far as negative values of S are forbidden). Notice that $S^*(0)=0$ for a continuous quasi-homogeneous entropy defined in 0.

Superadditivity of the entropy means that for the thermodynamic system the entropy does not increase by fragmenting the system.[8] From the point of view of the energy representation, to be discussed in Sec. X, superadditivity of the entropy is equivalent to the subadditivity of the energy under the condition (19) (for a proof, see Refs. 35 and 36). [This equivalence holds even if conditions (C), (H) are violated.] Subadditivity of the energy means that exploding is not energetically advantageous for the system.[37,38] The relevance of (S) for the second law of thermodynamics is discussed and underlined in Ref. 13. Accordingly, one should privilege the superadditivity property against the concavity, and superadditivity should be required as a fundamental property for the quasi-homogeneous picture of thermodynamics. Notice that a lack of concavity for thermodynamics in presence of gravity is verified in Refs. 39 and 40, where negative heat

capacities in presence of gravity are calculated. Therein, a discussion on how to deal with the lack of the standard stability properties of thermodynamics is sketched. See also Refs. 41 and 42. It is to be noted that this lack of concavity in presence of gravity forces to abandon the usual Gibbsian scheme for thermodynamics, and the homogeneity property has to be withdrawn because of (a), if one adopts the superadditivity as a fundamental property for the metrical entropy of a system. Due to the above equivalence between superadditivity of the entropy and subadditivity of the internal energy, one can naively justify this choice by underlining that, because of the purely attractive nature of gravity, internal energy of a self-gravitating system should be strictly subadditive, in fact energy decreases as the accretion of matter increases. Thus, there is an implosive instability of gravity, which eventually leads to the formation of black holes, to be identified as very long-lived metastable states. By passing, we note that there is another instability which is opposite in character with respect to the one implied by gravity. It involves system fragmentation/explosion because of a superadditive energy.[37,38] It should be characterized only by unstable states (systems with a suitable charge excess would be explosive[28]). (See also the works of Lieb collected in Ref. 43, in particular the review in Ref. 44; see also Ref. 45.)

VIII. SUMMARY OF CONSTRUCTIVE ASSUMPTIONS

We summarize the set of constructive assumptions upon which our approach is based. They correspond to the assumptions leading to standard homogeneous thermodynamics,[1] the difference consists in the substitution of the homogeneity symmetry with the quasihomogeneity symmetry and also in the explicit request that the entropy is superadditive. We comment only some assumptions which require further remarks with respect to the discussion developed in the text.

(**a1**) The quasi-homogeneity symmetry which characterizes the thermodynamic system is translated into the quasi-homogeneity of the Pfaffian form $\delta Q_{\mathrm{rev}}=dU^*-\Sigma_{i=1}^{n}\xi_i^*\,dX^{i*}$.

(**a2**) The quasi-homogeneity symmetry of δQ_{rev} is nontrivial.

(**a3**) The thermodynamic foliation is defined by the leaves $\hat{S}^{*-1}(c)$, where $c\in\mathbb{R}$ is a constant, everywhere in $\mathcal{D}$.

This assumption does not leave room for foliations which are based on a quasi-homogeneous S^* which is allowed to be negative. Compare the discussion in Ref. 1 for the homogeneous case.

(**a4**) The integrating factor f^* is non-negative.

(**a5**) The metrical entropy S^* is quasi-homogeneous of degree 1.

This assumption could also be weakened, as discussed in the text.

(**a6**) The metrical entropy S^* is superadditive.

This assumption substitutes the requirement for a concave entropy occurring in standard homogeneous thermodynamics. Notice that in standard thermodynamics it would lead again to a concave metrical entropy, because of the implication (a) of Sec. VII (cf. Ref. 35).

(**a7**) We require that $Z(S^*)\subseteq Z(T^*)$.

This assumption is, e.g., implemented as in Sec. III B. One can also add the following assumptions which appear to be physically appealing.

(**a8**) We require that to each level set $S^*=\mathrm{const}$ corresponds a unique leaf.

This assumption means that two states of the same quasi-homogeneous system lying on the same isoentropic surface are path-connected, i.e., it is possible to find a reversible adiabatic path connecting each other.

(**a9**) We require that $\partial S^*/\partial V^*$ is positive if V^* is the volume of the system.

This simply means that the pressure p^* is positive whenever it is definite.

(**a10**) We require that $f^*=0$ corresponds to an integral manifold of δQ_{rev}.

This assumption is natural and is related to the problem of the third law. Compare Ref. 1 for standard thermodynamics; see also Ref. 17 for the black hole case and also Appendix B.

IX. GENERALIZED GIBBS–DUHEM EQUATION

Quasi-homogeneity of S^* allows to find a generalization of the standard Gibbs–Duhem equation.[46]

A. Case where none independent variable of weight zero appears

We first discuss the case where none independent variable of weight zero appears. By differentiating (23) one finds

$$dS^*=\alpha\,\frac{1}{T^*}\,dU^*+\alpha U^* d\left(\frac{1}{T^*}\right)-\sum_i \alpha_i\,\frac{\xi_i^*}{T^*}dX^{i*}-\sum_i \alpha_i X^{i*} d\left(\frac{\xi_i^*}{T^*}\right) \tag{73}$$

and by comparing with

$$dS^*=\frac{1}{T^*}\,dU^*-\sum_i\,\frac{\xi_i^*}{T^*}\,dX^{i\ *} \tag{74}$$

one finds that the following generalized Gibbs–Duhem equation has to hold:

$$\alpha U^{*-[(\alpha-1)/\alpha]+1} d\left(\frac{U^{*[(\alpha-1)/\alpha]}}{T^*}\right)-\sum_i \alpha_i X^{i*-[(\alpha_i-1)/\alpha_i]+1} d\left(\frac{X^{i*[(\alpha_i-1)/\alpha_i]}\xi_i^*}{T^*}\right)=0. \tag{75}$$

This equation, as in the usual thermodynamic case, allows to express the differential of a would-be intensive variable as a function of all the other ones, and then to find such a would-be intensive variable apart from a integration constant (cf. Ref. 46 for the case of standard thermodynamics). In fact, one could, e.g., find for $1/T^*$:

$$d\log\left(\frac{1}{T^*}\right)=-\frac{\alpha-1}{f^*}\;\;dU^*+\frac{1}{f^*}\sum_i \alpha_i X^{i*-[(\alpha_i-1)/\alpha_i]+1} d(X^{i*[(\alpha_i-1)/\alpha_i]}\xi_i^*). \tag{76}$$

Notice that

$$d\log\left(\frac{1}{T^*}\right)=-d\log(f^*)+\frac{\delta Q_{\rm rev}}{f^*}. \tag{77}$$

Equation (76) is implemented if (18) and (74) hold. Let us consider the inverse problem where one assigns n would-be intensive functions $\xi_1^*,\ldots,\xi_n^*$ which are quasi-homogeneous in $U^*,X^{1*},\ldots,X^{n*}$ and such that $\delta Q_{\rm rev}$ is quasi-homogeneous as well. Equation (76), or, equivalently, Eq. (77) can be used for recovering T^*, and then for reconstructing S^* by means of (18), if and only if one has ensured that $\delta Q_{\rm rev}/f^*$ is an exact differential, i.e., that $\delta Q_{\rm rev}$ is integrable and f^* is an integrating factor for $\delta Q_{\rm rev}$. Otherwise, (76) is not even meaningful [a closed form on the left-hand side of (77) should be equal to a nonclosed form on the right-hand side of the same equation]. Compare also Ref. 1.

Notice that, if S^* has degree q, then (75) becomes

$$\frac{\alpha}{q}\,U^{*-[(\alpha-q)/\alpha]+1} d\left(\frac{U^{*[(\alpha-q)/\alpha]}}{T^*}\right)-\sum_i\,\frac{\alpha_i}{q}\,X^{i*-[(\alpha_i-q)/\alpha_i]+1} d\left(\frac{X^{i*[(\alpha_i-q)/\alpha_i]}\xi_i^*}{T^*}\right)=0. \tag{78}$$

See also Appendix C.

B. Case where independent variables of weight zero appear

Let us assume that, the independent variables X^{i*} have weight zero for $i=p+1,\ldots,n$, with $p<n$. This means that ξ_i^* have degree α for $i=p+1,\ldots,n$. The Euler vector field is

$$D=\alpha U^*\frac{\partial}{\partial U^*}+\sum_{i\leqslant p}\alpha_i X^{i*}\frac{\partial}{\partial X^{i*}}, \tag{79}$$

and the integrating factor is

$$f^* = \alpha U^* - \sum_{i \leqslant p} \alpha_i \xi_i^* X^{i*}. \tag{80}$$

Then, one has

$$S^* = \frac{1}{T^*} \left(\alpha U^* - \sum_{i \leqslant p} \alpha_i \xi_i^* X^{i*} \right). \tag{81}$$

It is easy to show that the Gibbs–Duhem equation in this case is

$$\alpha U^{*-[(\alpha-1)/\alpha]+1} d\left(\frac{U^{*[(\alpha-1)/\alpha]}}{T^*} \right) - \sum_{i \leqslant p} \alpha_i X^{i*-[(\alpha_i-1)/\alpha_i]+1} d\left(\frac{X^{i*[(\alpha_i-1)/\alpha_i]} \xi_i^*}{T^*} \right)$$
$$+ \sum_{p<i \leqslant n} \frac{\xi_i^*}{T^*} dX^{i*} = 0. \tag{82}$$

One can also obtain the analogous of Eq. (76),

$$d \log\left(\frac{1}{T^*} \right) = -\frac{\alpha-1}{f^*} dU^* + \frac{1}{f^*} \sum_{i \leqslant p} \alpha_i X^{i*-[(\alpha_i-1)/\alpha_i]+1} d(X^{i*[(\alpha_i-1)/\alpha_i]} \xi_i^*) - \frac{1}{f^*} \sum_{p<i \leqslant n} \xi_i^* dX^{i*}. \tag{83}$$

Equation (77) still holds.

Concerning the Gibbs–Duhem equation in standard thermodynamics, see Ref. 47.

C. Examples

In the black hole case, as well known, one has (we do not write the asterisk in what follows)

$$S = \frac{M}{2T} - \frac{\Phi Q}{2T} - \frac{\Omega J}{T} \tag{84}$$

and

$$dS = \frac{1}{T} dM - \frac{\Phi}{T} dQ - \frac{\Omega}{T} dJ; \tag{85}$$

the generalized Gibbs–Duhem equation, associated with the quasi-homogeneity of S, is

$$-\frac{1}{2T} dM + \frac{M}{2} d\left(\frac{1}{T} \right) + \frac{\Phi}{2T} dQ - \frac{Q}{2} d\left(\frac{\Phi}{T} \right) - J d\left(\frac{\Omega}{T} \right) = 0, \tag{86}$$

which can be rewritten as[14]

$$\frac{1}{2} M^2 d\left(\frac{1}{MT} \right) - \frac{1}{2} Q^2 d\left(\frac{\Phi}{QT} \right) - J d\left(\frac{\Omega}{T} \right) = 0. \tag{87}$$

Then, one can find $1/T$ from

$$d \log\left(\frac{1}{T} \right) = \frac{1}{f} \left(\frac{1}{2} dM + \frac{1}{2} Q^2 d\left(\frac{\Phi}{Q} \right) + J \, d\Omega \right). \tag{88}$$

It can be easily shown that $1/T$ can be determined apart from an undetermined multiplicative constant.

X. ENERGY REPRESENTATION AND LEGENDRE TRANSFORM

In the energy representation, the fundamental equation is $U^*=U^*(S^*,X^{1*},\ldots,X^{n*})$. One has

$$dU^*=T^*\,dS^*+\sum_i \xi_i^* dX^{i*}. \tag{89}$$

U^* is a quasi-homogeneous function of degree r and type $(1,\alpha_1,\ldots,\alpha_n)$; T^* is quasi-homogeneous of degree $r-1$, ξ_i^* are quasi-homogeneous of degree α_i-r. Equation (89) represents an exact quasi-homogeneous Pfaffian form of degree r. The Euler operator is

$$D=S^*\,\frac{\partial}{\partial S^*}+\sum_i \alpha_i X^{i*}\,\frac{\partial}{\partial X^{i*}}. \tag{90}$$

One has then

$$U^*=\frac{1}{r}\left(T^*S^*+\sum_i \alpha_i \xi_i^* X^{i*}\right). \tag{91}$$

(Notice that the generalization to the case where S^* is quasi-homogeneous of degree q is trivial.)

As far as the Gibbs–Duhem equation is concerned, one easily finds (we shift to the case where S^* has degree q)

$$\frac{q}{r}\;S^{*-[(q-r)/q]+1}d(S^{*[(q-r)/q]}T^*)+\sum_i \frac{\alpha_i}{r}\,X^{i*-[(\alpha_i-r)/\alpha_i]+1}d(X^{i*[(\alpha_i-r)/\alpha_i]}\xi_i^*)=0. \tag{92}$$

For a proof see Appendix C. One can, e.g., determine T^* from

$$d(S^{*[(q-r)/q]}T^*)=-S^{*[(q-r)/q]-1}\,\frac{1}{q}\sum_i \alpha_i X^{i*-[(\alpha_i-r)/\alpha_i]+1}d(X^{i*[(\alpha_i-r)/\alpha_i]}\xi_i^*). \tag{93}$$

A formula analogous to (82) can be obtained if some independent zero-weight variables appear; one obtains (cf. Appendix C)

$$\frac{q}{r}\,S^{*-[(q-r)/q]+1}d(S^{*[(q-r)/q]}T^*)+\sum_{i\leqslant p}\frac{\alpha_i}{r}\,X^{i*-[(\alpha_i-r)/\alpha_i]+1}d(X^{i*[(\alpha_i-r)/\alpha_i]}\xi_i^*)$$

$$-\sum_{p<i\leqslant n}\xi_i^* dX^{i*}=0. \tag{94}$$

A. Legendre transforms

Legendre transforming of the potentials involves the usual procedure. A noticeable difference, with respect to standard thermodynamics, is that, if, between the $n+1$ independent variables, no variable of weight zero appears and no intensive dependent variable occurs, then one can iterate the Legendre transformations of the potential $n+1$ times and find a potential which is not identically vanishing. Moreover, the would-be intensive variables appear in the Euler operator involving the new independent variables. Let us, e.g., consider the quasi-homogeneous free energy

$$F^*(T^*,X^{1*},\ldots,X^{n*})=U^*-T^*\quad S^*. \tag{95}$$

It is a quasi-homogeneous function of degree r with respect to the Euler operator

$$D_1=(r-1)T^*\,\frac{\partial}{\partial T^*}+\sum_i \alpha_i X^{i*}\,\frac{\partial}{\partial X^{i*}}. \tag{96}$$

One can Legendre transform also with respect to the remaining n variables $X^{1*},\ldots,X^{n*}$:

$$G^*_{n+1}(T^*,\xi^*_1,\ldots,\xi^*_n)=U^*-T^*S^*-\sum_{i=1}^{n} X^{i*}\xi^*_i\not\equiv 0. \tag{97}$$

The corresponding Euler operator is

$$D_{n+1}=(r-1)T^*\,\frac{\partial}{\partial T^*}+\sum_i\,(r-\alpha_i)\xi^*_i\,\frac{\partial}{\partial \xi^*_i}. \tag{98}$$

Notice that, all the potentials which are obtained by Legendre transforming the internal energy U^* are quasi-homogeneous of degree r with respect to the corresponding Euler operator; all the Massieu–Planck potentials, which are obtained by Legendre transforming the entropy S^*, are quasi-homogeneous of degree 1. In other terms, the Legendre transform preserves the degree of quasi-homogeneity [but it changes variables and weights: the function

$$h^*(\xi^*,Y^*)=g^*-\xi^*X^* \tag{99}$$

which is obtained by a Legendre transform with respect to a variable ξ of weight α of a function $g(X^*,Y^*)$ which is quasi-homogeneous of degree r and weights $(r-\alpha,r-\beta)$, has weight $(\alpha,r-\beta)$]. For a proof, see Ref. 9 (theorem 2, Appendix A therein).

1. Case where weight-zero independent variables appear

Let us consider the case where a variable η^* of degree r and a variable I^* of weight zero appears:

$$dU^*=T^*\,dS^*+\xi^*\,dX^*+\eta^*\,dI^*. \tag{100}$$

The Euler operator is

$$D=S^*\,\frac{\partial}{\partial S^*}+\beta X^*\,\frac{\partial}{\partial X^*}. \tag{101}$$

One can Legendre transform three times, obtaining

$$G_3(T^*,\xi^*,\eta^*)=\frac{1}{r}\,[(1-r)T^*S^*-(r-\beta)\xi^*X^*-r\,\eta^*I^*] \tag{102}$$

and

$$D_3=(r-1)T^*\,\frac{\partial}{\partial T^*}+(r-\beta)\xi^*\,\frac{\partial}{\partial \xi^*}+r\,\eta^*\,\frac{\partial}{\partial \eta^*}. \tag{103}$$

2. Case with would-be intensive variable of degree zero

Let us consider the case where a variable ζ^* of degree zero and a variable Z^* of weight r appears,

$$dU^*=T^*\,dS^*+\xi^*\,dX^*+\zeta^*\,dZ^*. \tag{104}$$

The Euler operator is

$$D = S^* \frac{\partial}{\partial S^*} + \beta X^* \frac{\partial}{\partial X^*} + rZ^* \frac{\partial}{\partial Z^*}. \tag{105}$$

One can Legendre transform three times, obtaining

$$G_3(T^*, \xi^*, \zeta^*) = \frac{1}{r}[(1-r)T^*S^* - (r-\beta)\xi^* X^*] \tag{106}$$

and

$$D_3 = (r-1)T^* \frac{\partial}{\partial T^*} + (r-\beta)\xi^* \frac{\partial}{\partial \xi^*}. \tag{107}$$

This case is analogous to what happens in standard thermodynamics, e.g., when one passes from $U(S,V,N)$ to $F(T,V,N)$ and then to $G(T,p,N)$.

B. From the entropy to the energy representation and further considerations

In order to pass from the entropy representation $S^*(U^*, X^{1\,*}, \ldots, X^{n\,*})$ to the energy representation $U^*(S^*, X^{1*}, \ldots, X^{n*})$, one inverts the first relation with respect to U^*, which is possible because $\partial S^*/\partial U^* > 0$. If S^* has degree 1 and weights $(r, \alpha_1, \ldots, \alpha_n)$, then U^* has degree r and weights $(1, \alpha_1, \ldots, \alpha_n)$. Analogous considerations hold when passing from the energy to the entropy representation. We show that, when it is possible to invert, at least locally, a quasi-homogeneous function with respect to one variable, a quasi-homogeneous function is obtained again, having obvious degree and weights.

In the general case, let us consider a quasi-homogeneous function $w = g(x^1, \ldots, x^n)$ of degree r and weights $(a_1, \ldots, a_n)$; the partial derivatives

$$p_i \equiv \frac{\partial w}{\partial x^i} \tag{108}$$

are quasi-homogeneous functions of degree $r - a_i$ for $i = 1, \ldots, n$. Let us assume, e.g., that $p_1 \neq 0$. Then, at least locally, one can invert w with respect to x^1 and find $x^1 = h(w, x^2, \ldots, x^n)$ such that $g(h(w, x^2, \ldots, x^n), x^2, \ldots, x^n) = w$. The inverse function h (where it exists and it is sufficiently smooth) is easily shown to be a quasi-homogeneous function of degree a_1 and weights $(r, a_2, \ldots, a_n)$. In fact, one has

$$g(\lambda^{a_1} x^1, \lambda^{a_2} x^2, \ldots, \lambda^{a_n} x^n) = g(\lambda^{a_1} h(w, x^2, \ldots, x^n), \lambda^{a_2} x^2, \ldots, \lambda^{a_n} x^n) = \lambda^r g(x^1, \ldots, x^n). \tag{109}$$

Moreover, one has

$$g(h(\lambda^r w, \lambda^{a_2} x^2, \ldots, \lambda^{a_n} x^n), \lambda^{a_2} x^2, \ldots, \lambda^{a_n} x^n) = \lambda^r w = \lambda^r g(x^1, \ldots, x^n), \tag{110}$$

thus it has to hold

$$h(\lambda^r w, \lambda^{a_2} x^2, \ldots, \lambda^{a_n} x^n) = \lambda^{a_1} h(w, x^2, \ldots, x^n). \tag{111}$$

Compare Ref. 35, where an analogous property is shown in passing from the entropy representation to the energy representation in standard (homogeneous) thermodynamics. See also Ref. 48.

As a further example, let us consider Kerr–Newman black holes. By inverting (where possible) the relation $T = T(M,Q,J)$ with respect to M, one obtains (at least formally) $M = M(T,Q,J)$. We know that M and Q have degree 1/2, J has degree one and T has degree $-1/2$. In the new variables, $M = M(T,Q,J)$ is a quasi-homogeneous function of degree 1/2 and weights $(-1/2, 1/2, 1)$. The Euler operator corresponding to the independent variables (T,Q,J) is

$$\overline{D} = -\frac{1}{2} T \frac{\partial}{\partial T} + \frac{1}{2} Q \frac{\partial}{\partial Q} + J \frac{\partial}{\partial J} \tag{112}$$

and it holds

$$\overline{D} M = \tfrac{1}{2} M. \tag{113}$$

XI. FURTHER INSIGHTS FROM BLACK HOLES

A feature of quasi-homogeneous thermodynamics, shared also with homogeneous thermodynamics, is that in the expression of the metrical entropy and of the absolute temperature a undetermined multiplicative constant appears (cf. also Ref. 1). Such a constant is phenomenologically fixed once the absolute scale of temperature is chosen. From the point of view of the actual analytic expression of this constant, it should be furnished by a statistical mechanical calculation. The black hole case can be again useful. By dimensional analysis, if we make the hypothesis that the entropy of a black hole can depend only on $\hbar, c, G, k_b$, we find that

$$S \propto \frac{k_b c^3}{\hbar G} A; \tag{114}$$

this is the same procedure as in the original proposal of Bekenstein.[49] For the temperature one obtains

$$T \propto \frac{\hbar c}{k_b} \left(\frac{\partial A}{\partial (GM/c^2)} \right)^{-1}. \tag{115}$$

A dimensionless constant has still to be determined.

If one considers standard thermodynamics cases, this hypothesis which allows to recover the dimensions of the entropy by involving only the above constants works for the photon gas but it does not work in other cases; e.g., in the case of a Fermi gas of electrons, the electron mass represents a further scale, related to a microscopic analysis of the system, to be taken into account. In our case, the confirmation of the above hypothesis comes from the Hawking effect, which gives us the behavior of the black hole temperature, to be compared with (115). Then, because of the absence of a particle mass scale and, e.g., in the Schwarzchild and in the Kerr cases being involved only vacuum solutions of the Einstein equations, one could be tempted to think about some sort of ''graviton gas,'' but, actually, this is far from being evident. See also Ref. 14.

Black holes represent an example of the the procedure of reducing/enlarging consistently the thermodynamics space discussed in Sec. III. In fact, the construction of the fundamental equation sketched in Sec. IV is allowed also in the case of a black hole with $J=0$ and of a black hole with $Q=0$. Two parameters appear, M,Q and M,J, respectively. The integrability condition is then trivially satisfied, but a well-defined potential S is obtained everywhere. Moreover, black holes of the Kerr–Newman family are a consistent extension of the black holes of the Reissner–Nordström family (by adding J) or of the Kerr family (by adding Q). To this family belong also a thermodynamically degenerate case: the Schwarzschild case $J=0=Q$, which is described only by one variable M. Notice also that the Kerr–Newman family can be obtained by setting $\Lambda=0$ in the KN–AdS family.

In the case of black hole thermodynamics, it is tempting to conjecture that the quasi-homogeneous behavior of the thermodynamic potentials could be related to an explanation, to some extent, analogous to the one for the quasi-homogeneous behavior of the thermodynamic potentials in standard thermodynamics near the critical point:[50,51] As in standard thermodynamics the (leading order) quasi-homogeneous behavior can be related to the conformal invariance of the underlying quantum field theory near criticality,[51] one could conjecture that the quasi-homogeneous behavior of black hole thermodynamics could be related to some sort of conformal invariance of the quantum theory underlying general relativity (superstring theory). This field

deserves further investigation. We however point out that it does not seem to be necessary that quasi-homogeneous thermodynamics should be related to some sort of conformal invariance in every case. For black holes, as well as for the general case, one should determine the reason of a quasi-homogeneous behavior by means of statistical mechanical calculations. In the following section, a further discussion is found.

XII. HEURISTICS: QUASI-HOMOGENEOUS THERMODYNAMICS AND THERMODYNAMIC LIMIT

In this section we suggest that the thermodynamic limit, under suitable hypotheses, can lead only to quasi-homogeneous thermodynamics. The thermodynamic limit should not be intended in a literal sense, of course, but as a tool which allows to determine the leading terms in the statistical mechanical functionals as large systems occur. Compare e.g., Ref. 52, Chap. 4, and also Ref. 53. Thermodynamics of macrosystems emerges as an asymptotic law which is extrapolated from the asymptotic behavior of statistical mechanics. To some extent, the thermodynamic limit is also a tool by means of which the vague notion of ''macroscopic system'' is meant to be implemented, and a proper thermodynamic behavior recovered. Such a behavior depends on the interactions and on the nature of the system involved (e.g., fermionic or bosonic matter), together with a dependence on the initial conditions (from a quantum-mechanical point of view, a sort of ''preparation'' of the system, even if it is of ''astrophysical size''). As far as the gravitational interaction can be neglected, the standard thermodynamic behavior emerges, with the usual asymptotic laws which justify the extensivity of standard thermodynamics. At the same time, extensivity cannot be considered as an absolute and unmodifiable property of thermodynamics, because of the purely attractive nature of gravity. One can also expect a different asymptotic behavior for different systems at different scales. See also the discussion in the following sections.

The basic set (B) of assumptions is the following.

Assumptions (B): Let $\{Z_i\}$ *be the set of the thermodynamic variables, both independent* $(Z_i^{(I)})$ *and dependent* $(Z_i^{(D)})$ *ones. Let the independent variables describe the Gibbs thermodynamic space. Let* λ *be the parameter such that, by taking* $\lambda \to \infty$*, one recovers the thermodynamic limit. Assume that the thermodynamic limit properly describes the bulk properties of the system under consideration.*

Assume that the thermodynamic limit of the statistical mechanical quantities, like, e.g., the entropy or the free energy, exists under the hypothesis that, in the limit $\lambda \to \infty$*, the independent thermodynamic variables* $Z_i^{(I)}(\lambda)$ *are rescaled as*

$$Z_i^{(I)} = g_i^{(I)}(\lambda) Z_i^{(I)\ 0}, \tag{116}$$

where $g_i^{(I)}(\lambda)$ *is a positive function which is either an invertible function of* λ *or it is one (or a constant), and* $Z_i^{(I)\ 0}$ *is the value of the i-esime variable* $Z_i^{(I)}$ *at an arbitrary reference state (cf. Ref. 53 for the extensive case).*

We now state the following result (R-group).

Result (R-group): Let us assume the set of assumptions (B) and that for the rescalings of the independent variables the group property holds,

$$g_i^{(I)}(\lambda\mu) = g_i^{(I)}(\lambda) g_i^{(I)}(\mu). \tag{117}$$

This implies that for each independent variable there exists a real number $\alpha_i^{(I)}$ *such that* $g_i^{(I)}(\lambda) = \lambda^{\alpha_i^{(I)}}$.

Let us assume that the dependent thermodynamic variables

$$Z_i^{(D)} = Z_i^{(D)}(Z_1^{(I)}, \ldots, Z_n^{(I)}), \tag{118}$$

are obtained as leading terms in the asymptotic expansion of the corresponding statistical mechanical functionals $\mathcal{Z}_i^{(D)}$ *in the following sense: for each* i *there exists a positive continuous function* $\rho_i(\lambda)$ *such that*

$$\lim_{\lambda\to\infty}\frac{1}{\rho_i(\lambda)}\,\mathcal{Z}_i^{(D)}(g_1^{(I)}(\lambda)Z_1^{(I)},\ldots,g_n^{(I)}(\lambda)Z_n^{(I)})=Z_i^{(D)}(Z_1^{(I)},\ldots,Z_n^{(I)}),\tag{119}$$

and let us assume that the domain of the functionals $\mathcal{Z}_i^{(D)}$ *is invariant under the above rescalings. Then, the dependent thermodynamic variables are quasi-homogeneous, i.e., they satisfy*

$$Z_i^{(D)}(g_1^{(I)}(\lambda)Z_1^{(I)},\ldots,g_n^{(I)}(\lambda)Z_n^{(I)})=g_i^{(D)}(\lambda)Z_i^{(D)}(Z_1^{(I)},\ldots,Z_n^{(I)}),\tag{120}$$

where $g_i^{(D)}(\lambda)=\lambda^{\alpha_i^{(D)}}$ *and* $\alpha_i^{(D)}\in\mathbb{R}$.

Moreover, for all i, *the functions* $\rho_i(\lambda)$ *are regularly varying functions*:[54] *for all* $\mu\in\mathbb{R}_+$,

$$\lim_{\lambda\to\infty}\frac{\rho_i(\lambda\mu)}{\rho_i(\lambda)}=\mu^{\alpha_i^{(D)}}\tag{121}$$

($\alpha_i^{(D)}$ *is also called degree of* ρ_i).

In order to be more explicit, let us consider (R-group) for a specific case. Let us, e.g., assume that the thermodynamic limit for the statistical mechanical functional $\mathcal{S}$ representing the entropy exists in the sense that

$$\lim_{\lambda\to\infty}\frac{1}{\rho_S(\lambda)}\,\mathcal{S}(\lambda^{\alpha_U}U,\lambda^{\alpha_V}V,\lambda^{\alpha_N}N)=S(U,V,N),\tag{122}$$

where the function ρ_S is positive and $\alpha_U,\alpha_V,\alpha_N$ are real numbers. Then for each real $\mu>0$ the function ρ_S satisfies

$$\lim_{\lambda\to\infty}\frac{\rho_S(\lambda\mu)}{\rho_S(\lambda)}=\mu^{\gamma}\tag{123}$$

for some $\gamma\in\mathbb{R}$. Moreover, S is quasi-homogeneous of degree γ. In fact, from (122) it follows

$$\lim_{\lambda\to\infty}\frac{1}{\rho_S(\lambda\mu)}\,\mathcal{S}((\lambda\mu)^{\alpha_U}U,(\lambda\mu)^{\alpha_V}V,(\lambda\mu)^{\alpha_N}N)=S(U,V,N).\tag{124}$$

Moreover, it holds

$$\lim_{\lambda\to\infty}\frac{1}{\rho_S(\lambda)}\,\mathcal{S}(\lambda^{\alpha_U}(\mu^{\alpha_U}U),\lambda^{\alpha_V}(\mu^{\alpha_V}V),\lambda^{\alpha_N}(\mu^{\alpha_N}N))=S(\mu^{\alpha_U}U,\mu^{\alpha_V}V,\mu^{\alpha_N}N).\tag{125}$$

Then

$$\lim_{\lambda\to\infty}\frac{\rho_S(\lambda)}{\rho_S(\lambda\mu)}\,\frac{\mathcal{S}((\lambda\mu)^{\alpha_U}U,(\lambda\mu)^{\alpha_V}V,(\lambda\mu)^{\alpha_N}N)}{\mathcal{S}(\lambda^{\alpha_U}(\mu^{\alpha_U}U),\lambda^{\alpha_V}(\mu^{\alpha_V}V),\lambda^{\alpha_N}(\mu^{\alpha_N}N))}$$

$$=\frac{S(U,V,N)}{S(\mu^{\alpha_U}U,\mu^{\alpha_V}V,\mu^{\alpha_N}N)}=\lim_{\lambda\to\infty}\frac{\rho_S(\lambda)}{\rho_S(\lambda\mu)},\tag{126}$$

which is possible only if the above conditions are implemented. A general proof is found in Appendix E. Compare Ref. 55, where a rigorous approach for asymptotics of tempered distributions is developed.

The case where one or more variables are ''intensive,'' i.e., are not rescaled, presents no difficulty. The above reasoning about the leading order in the asymptotic law identified in the thermodynamic limit is corroborated b y the standard thermodynamic limit, which allows to find a leading-order homogeneous thermodynamics. We define *quasi-homogeneous thermodynamic limit* the thermodynamic limit satisfying the group property.

Moreover, we notice that, if, e.g., for the thermodynamic entropy $S(U,V,N)$ it holds

$$S(g_U(\lambda)U_0,g_V(\lambda)V_0,g_N(\lambda)N_0)=g_S(\lambda)S_0=g_S(\lambda)S(U_0,V_0,N_0), \tag{127}$$

where the functions g_U,g_V,g_N,g_S are positive and the group property holds, then S has to be quasi-homogeneous and the g_i are power-like functions. The key point is that a behavior like the one in (127) under the group property is necessarily quasi-homogeneous; as it is shown in Ref. 9, ''powers need no generalization'' (see Appendix A in Ref. 9 and Appendix C in Ref. 10). A different proof is sketched in Appendix D for the sake of completeness. The aforementioned theorem implies that actually one has

$$S(g(\lambda)^{\alpha_U}U,g(\lambda)^{\alpha_V}V,g(\lambda)^{\alpha_N}N)=g(\lambda)^{\alpha_S}S(U,V,N) \tag{128}$$

with the same scaling function $g(\lambda)$. By defining

$$\overline{\lambda}\equiv g(\lambda) \tag{129}$$

one finds $S(\overline{\lambda}^{\alpha_U}U,\overline{\lambda}^{\alpha_V}V,\overline{\lambda}^{\alpha_N}N)=\overline{\lambda}^{\alpha_S}S(U,V,N)$, i.e., the standard definition of quasi-homogeneous behavior for a function. A generalization of the quasi-homogeneous behavior of a function under rescaling with the group property is not allowed.

We now relax the requirement for the group property, one can still make a conjecture (C-reg) which would allows a quasi-homogeneous behavior under rather general conditions.

Conjecture (C-reg): Let us assume the set (B) and that g,g_i (for $i=1,\ldots,n$) are positive and continuous functions which are regularly varying functions of real degree $\gamma,\alpha_1,\ldots,\alpha_n$ respectively.

Assume that the statistical mechanical functional $\mathcal{Z}$ satisfies

$$\lim_{\lambda\to\infty}\frac{1}{g(\lambda)}\,\mathcal{Z}(g_1(\lambda)Z^1,\ldots,g_n(\lambda)Z^n)=Z(Z^1,\ldots,Z^n), \tag{130}$$

where Z^i are the independent thermodynamic variables [we omit the suffix (I)].

We conjecture that, under suitable hypotheses, the asymptotic $Z(Z^1,\ldots,Z^n)$ is quasi-homogeneous of degree γ and weights $(\alpha_1,\ldots,\alpha_n)$.

For each positive real μ one should find

$$\lim_{\lambda\to\infty}\frac{1}{g(\lambda\mu)}\,\mathcal{Z}(g_1(\lambda\mu)Z^1,\ldots,g_n(\lambda\mu)Z^n)=Z(Z^1,\ldots,Z^n) \tag{131}$$

$$\text{``}=\text{''}\lim_{\lambda\to\infty}\frac{1}{g(\lambda)\mu^{\gamma}}\,\mathcal{Z}(g_1(\lambda)\mu^{\alpha_1}Z^1,\ldots,g_n(\lambda)\mu^{\alpha_n}Z^n) \tag{132}$$

$$=\frac{1}{\mu^{\gamma}}\,Z(\mu^{\alpha_1}Z^1,\ldots,\mu^{\alpha_n}Z^n), \tag{133}$$

where "=" indicates that further hypotheses on the statistical mechanical functional should be satisfied. Notice that the case $g_i(\lambda)=\lambda^{\alpha_i}$ is a subcase of the preceding one and requires only that the limit (130) exists and that the state $(\mu^{\alpha_1}Z^1,\ldots,\mu^{\alpha_n}Z^n)$ belongs to the domain of the statistical mechanical functional $\mathcal{Z}$.

From a physical point of view, it can be noticed that, when passing from the statistical mechanical functional $\mathcal{S}$ representing the entropy to its asymptotic S_{sm} under dilatations, as in the standard thermodynamic limit, it would be not strictly necessary, *a priori*, to impose that $g(\lambda)=\lambda$ in order to obtain an homogeneous S_{sm} [herein we indicate by S_{sm} the asymptotic which is indicated by S in (122)]. (S_{sm} corresponds to the statistical mechanical entropy one takes into account in Sec. III C 2.) A generic regularly varying function of degree one could also be allowed [e.g., $g(\lambda)=\lambda\log(\lambda)$ could be allowed]. The requirement

$$\lim_{\lambda\to\infty}\frac{1}{\lambda}\,\mathcal{S}(\lambda x)=S_{\mathrm{sm}}(x) \tag{134}$$

amounts to the requirement that in some sense also $\mathcal{S}$ is extensive.

We have found that, under rather general hypotheses, the only possible outcome of the thermodynamic limit is a form of quasi-homogeneous thermodynamics. The thermodynamic limit, at the same time, is not expected to describe all possible systems; e.g., it cannot be applied to a thin (molecular thickness) metallic film.[56] Nevertheless, it can be safely applied to a huge class of macroscopic systems, and, in the nonrelativistic case, it allows to conclude that the Thomas–Fermi approximation becomes exact in the limit.

In partially concluding these heuristic considerations, we point out that a relation between a so-called pseudoextensive thermodynamics and the thermodynamic limit has been postulated in Ref. 57 and an analysis of Newtonian self-gravitating systems is made in Ref. 58. We limit ourselves to refer the reader to the aforementioned papers.

A. Nonconventional thermodynamic limit

A nonconventional thermodynamic limit has already been proposed. A very interesting discussion of the thermodynamic limit in physical systems is found in Ref. 59. Therein, physical systems are divided into two classes each of which can be associated with its own thermodynamic limit; one can distinguish between the standard thermodynamic limit (STL) and the inhomogeneous mean field thermodynamic limit (IMFTL) which occurs, e.g., in self-gravitating systems as the one of HNT model. The latter kind of thermodynamic limit can be related with the presence of long-range forces.[59] In order to identify the correct limit, the key notion of characteristic bulk length scale is introduced, which corresponds to a typical length scale λ_{typ} resulting from the interaction of many particles in the system. Such length scale λ_{typ} plays the role of characteristic invariant in the thermodynamic limit. In the case of a classical self-gravitating isothermal gas, the Jeans length λ_{Jeans} is such a typical length. Moreover, the requirement that mean thermodynamic quantities exist almost everywhere in the thermodynamic limit is a tool for selecting the appropriate thermodynamic limit at constant λ_{typ}.[59] A complementarity between STL and IMFTL can also be allowed for the same system, in the sense that STL and IMFTL can describe complementary asymptotic properties for the same large but finite system (the case of classical Coulomb systems is discussed). We do not discuss further on this approach herein, we limit ourselves to point out that one obtains the same limit, in the case of classical self-gravitating matter, if one keeps λ_{Jeans} fixed or ξ fixed (cf. Sec. V). Notice that ξ is an intensive function with respect to the Euler operator relative to the HNT model. At an heuristic level one expects that in general there exists a physically meaningful function which is left invariant under a quasi-homogeneous thermodynamic limit and which is intensive under the corresponding Euler operator.

A nonconventional discussion of the thermodynamic limit is found also in Secs. 1.2 and 4.2 of Ref. 27. Both for stable and for unstable interactions are discussed, and the criterion for selecting the limit is a comparison between the kinetic and the potential energies involved in the system. According to Ref. 28 (pp. 1–3), a nonconventional thermodynamic limit has to be associated with

the peculiar scaling behavior for ''nonstable interactions;'' the notion of ''Thomas–Fermi thermodynamic limit'' is also introduced for nonextensive systems. Note that a more general thermodynamic limit can also be allowed, where also the coupling constants are allowed to vary in the limit. Compare Refs. 25, 28, and 59.

B. Absolute weights again

It is evident that one has a reference quantity with respect to which all the others are ''weighted'' in the thermodynamic limit. Then an overall undetermined scale factor q is expected to appear, unless an absolute weight is known.

In the standard homogeneous case, the problem of assigning absolute weights does not arise, they are all equal to 1 for extensive variables and 0 for intensive ones, the thermodynamic limit is performed with the aim of studying bulk properties of the system, and the ratios U/N and V/N are kept constant. Roughly, one fixes the energy per particle and the volume per particle (or, equivalently, the density N/V and the energy density U/V) and then performs the limit with the aim of neglecting any finite-size effect. The same is true also for a massless particle gas, like the photon gas, where the limit $U,V\to\infty, U/V=\text{const}$ is performed.

If a strict quasi-homogeneous picture is required, then the above problem is instead present. When N is available, as it is when nonzero rest-mass particles are considered, it is to some extent natural to assume that its weight is 1. Such a special role of N can be justified. In the model of Hertel, Narnhofer, and Thirring, the existence of the Boltzmann's entropy per particle in the thermodynamic limit $\lim_{N\to\infty}\log(\Omega)/N$ is ensured, in agreement with Boltzmann's postulate, which states that the entropy per particle $\log(\Omega)/N$ exists for an equilibrium system. As a consequence of the coincidence of $\lim_{N\to\infty}\log(\Omega)/N$ with the thermodynamic entropy density (per particle), one can justify *a posteriori* the assumption that N has weight 1, in fact $\log(\Omega)$ in the thermodynamic limit coincides with the thermodynamic entropy which has degree 1. The other weights α_i appropriate to the physical condition one is considering for the system are recovered in the asymptotic limit. Then, no ambiguity for an overall multiplicative constant in the definition of the weight like the one discussed in Sec. III C appears. Note also that the Boltzmann's entropy, being the logarithm of the number of microstates compatible with a given macrostate, by involving the (vague) concept of macrostate and thus of macroscopic system can legitimately related to the thermodynamic limit (again in the sense of asymptotic law). [About Boltzmann's entropy and its coincidence with the Gibbs entropy (which, in the quantum case, corresponds to the von Neumann entropy) see, e.g., Ref. 60.] A more puzzling case is represented by a self-gravitating massless gas, but weights can be still fixed. See Sec. VI.

In general, if $\lambda\to\infty$ corresponds to the thermodynamic limit, one could also require the existence of the Boltzmann entropy density functional as $\lambda\to\infty$, to be defined as

$$s_{\text{boltz}}\equiv\lim_{\lambda\to\infty}\frac{1}{\lambda^{\alpha_S}}\log(\Omega), \tag{135}$$

where α_S is a constant which is fixed by the requirement of finiteness of the above limit. α_S has to be introduced because the scale λ can also be such that λ/N is not asymptotically a positive constant, i.e., $\lambda\not\sim N$ in the sense of the asymptotic behavior. This more general choice for the scale is also necessary if N is not a good thermodynamic variable (as in the massless gas case). We know that it is consistent to fix the weights by choosing the Boltzmann entropy to be of degree 1.

If another variable, e.g., the internal energy, would be used as reference variable, the relative weights could be still recovered in line of principle, but the aforementioned ambiguity would emerge in absence of a criterion for finding the absolute weight of at least one (independent or dependent) variable.

One could also choose to work in the energy representation, and decide to fix the weight of the internal energy to be 1. Then the entropy in general would not be a degree 1 quasi-homogeneous function; in the HNT model, one would obtain $\deg(V)=-3/7$; $\deg(N)=3/7$; $\deg(S)=3/7$,

against the weight 7/3 of U resulting by assuming that N has weight 1. This procedure, although legitimate because of the overall ambiguity, is less satisfactory, because the thermodynamic construction, in the case the entropy is a quasi-homogeneous function and the weights present the overall factor ambiguity, allows naturally the thermodynamic entropy to be of degree 1. The only exception which, in line of principle could be admitted, is given by the case where the weights in the Gibbs space are all fixed and the statistical-mechanical entropy is not of degree 1, but it is apparently not allowed (unless some reason for fixing the absolute weight of a variable appears).

C. Thermodynamics, weights and gravity

As far as gravity is negligible, one finds the standard extensivity property for the fundamental equation in the entropy (energy) representation; when the scale of the system is such that is no more possible to neglect self-gravity effects, then the weights of the thermodynamic variables change according to the nature of the system and to the scale itself. The quasi-homogeneous character of thermodynamics with fixed weights $(\alpha_1,\ldots,\alpha_n)$ has to be intended as relative to the validity range of the asymptotic expansion which leads to those particular $(\alpha_1,\ldots,\alpha_n)$, whose nature is thus nonabsolute. [One could also be tempted to write $\alpha_i=\alpha_i(\lambda)$, in order to recall that the weights can change with the scale. Nevertheless, in light of the above theorem about quasi-homogeneity, such a dependence is not allowed. The quasi-homogeneity is extrapolated at each fixed scale, and it is made ''absolute'' by the thermodynamic formalism.] Also an estimate of the error for finite λ should be allowed.[52] One could think also to a sort of ''evolving picture'' for the formalism, in which one starts from standard homogeneous systems, characterized by stable interactions, and then, as far as gravity becomes non-negligible, a quasi-homogeneous behavior is allowed. Weights can change, even in a discontinuous way, depending on the physical conditions leading to the new stationary equilibrium state. Because of the Hawking effect, the ''end of the story'' does not occur even when the scale and the physical conditions are such that a black hole forms, whose ''classical'' weights are the ones presented in Sec. IV.

It is interesting to underline again that ordinary thermodynamics implements the picture described above, as discussed in several fundamental papers on the stability of matter.[29,61–63] See also Refs. 43 and 64. Strict quasi-homogeneity is expected to be effective when gravitation begins playing an essential role in the physics of the system. Moreover, the so-called fourth law of thermodynamics[13] should be generalized in such a way to include the general quasi-homogeneous behavior of the thermodynamic variables (dependent as well as independent ones).

XIII. CONCLUSIONS

Quasi-homogeneous thermodynamics is proposed as the unifying picture for thermodynamics where both stationary black holes, fermionic nonrelativistic matter, and self-gravitating electromagnetic radiation are found.

We have chosen to introduce quasi-homogeneity in thermodynamics by generalizing the formalism developed for standard homogeneous thermodynamics.[1] The basic requirement is that the Euler vector field which generates quasi-homogeneous dilatations in the Gibbs' thermodynamic space is a nontrivial symmetry for the integrable Pfaffian form δQ_{rev}. This means that the symmetry maps leaves of the thermodynamic foliation onto other leaves. The leaves of the foliation are naturally associated with a quasi-homogeneous function S^* of degree 1, which is suggested to be the (unique apart from a multiplicative constant) metrical entropy corresponding to the fundamental equation in the entropy representation. This is true also in the case one knows the weights of the thermodynamics variables apart from an overall unknown factor. Notice that quasi-homogeneity could be introduced also at the level of the fundamental equation in the entropy representation or in the energy one, but, in the case where only the relative weights of the independent thermodynamic variables are known, it should be considered equivalent the choice of a degree one internal energy with respect to the choice of a degree 1 entropy (cf. also Ref. 9), whereas the aforementioned approach privileges a degree 1 entropy.

The consequences of the lack of homogeneity are recalled, and superadditivity of the metrical entropy is a privileged property ensuring the second law even in absence of concavity for S^*.

The generalized Gibbs–Duhem identities are also derived, and the energy representation and the behavior under Legendre transforms is analyzed.

An heuristic argument which can relate quasi-homogeneous thermodynamics to the thermodynamic limit in statistical mechanics (even if in a nonconventional framework) has been introduced. According to this argument, under the group property only a form of quasi-homogeneous thermodynamics can be recovered in the thermodynamic limit. Moreover, a mean field thermodynamic limit appears to be appropriate; the suggestion from the existing models is that one has to search for asymptotic scaling properties of the equations allowing to find out the mean field thermodynamics for the system, in fact the scaling properties of a finite temperature Thomas–Fermi equation appears to be involved in the quasi-homogeneity of the HNT model, whereas the scaling properties of the TOV equations are related with the quasi-homogeneity of self-gravitating radiation.

Gravity appears to play a fundamental role in allowing a generalization of the standard scheme for thermodynamics. The purely attractive nature of gravity, as well-known, is the reason for the failure of the extensivity property in thermodynamics of self-gravitating systems, because of the absence of saturation which leads to an implosive instability, and matter systems eventually can implode into a black hole if the mass is sufficiently large. Moreover, the thermodynamic ensembles become inequivalent,[28] and the lack of concavity leads to phase transitions in matter systems in the canonical ensemble.[27,28] Negative heat capacities arise in the microcanonical ensemble. Also black holes present this feature.

Black hole thermodynamics requires some special comments. From the point of view of thermodynamic formalism, black hole thermodynamics can be realized to be a rather straightforward generalization of the formalism developed for standard thermodynamics in Ref. 1; moreover, its quasi-homogeneous behavior can no more be considered as exceptional, because self-gravitating systems exist where quasi-homogeneous scaling laws are satisfied. Nevertheless, from other points of view black hole thermodynamics is still to be considered special, also because it is still unclear which statistical mechanics should lie beyond it.

We limit ourselves herein to this proposal for a generalization of the thermodynamic formalism, without pursuing it further on (apart from a note on the third law in Appendix B). For future investigations, it would be interesting to develop a statistical mechanical formalism where general relativity is self-consistently included.

It would be also interesting to explore, if other long range forces are allowed to be included in the framework of quasi-homogeneous thermodynamics. Classical two-component Coulomb matter seems to belong to this framework,[59] further investigations are required in order to see if this is true also for quantum Coulomb matter.

APPENDIX A: INTEGRAL OF ω/μ AND POTENTIALS ASSOCIATED WITH QUASI-HOMOGENEOUS EXACT PFAFFIAN FORMS

We first present some results in the general case of a generic symmetry X for a Pfaffian form ω. Then we translate the results for the case of the quasi-homogeneity symmetry. We recall that a vector field X is defined to be a symmetry for a Pfaffian form ω if

$$(L_X\omega)\wedge\omega=0. \tag{A1}$$

This means that there exists a function h such that

$$L_X\omega=h\omega. \tag{A2}$$

See Refs. 5 and 6.

We need the following two lemmas.

Lemma 1: Let $\overline{\omega}$ be an exact Pfaffian form; let X be a symmetry such that

$$L_X\overline{\omega}=q\,\overline{\omega}, \tag{A3}$$

where $q\neq 0$ *is a constant. Then, one finds that* $\overline{\omega}=d\phi$ *is implemented by*

$$\phi\equiv\frac{1}{q}\,i_X\overline{\omega}. \tag{A4}$$

Proof: The proof is elementary. One has trivially

$$d\phi=\frac{1}{q}\,d(i_X\overline{\omega})=-\frac{1}{q}\,i_X(d\overline{\omega})+\frac{1}{q}\,L_X\overline{\omega}. \tag{A5}$$

From $d\overline{\omega}=0$ because $\overline{\omega}$ is closed and from the symmetry of $\overline{\omega}$, which implies $L_X\overline{\omega}=q\,\overline{\omega}$ the thesis follows. Notice that ϕ satisfies $X\phi=q\phi$. □

Lemma 2: Let $\omega_{(0)}$ *be an exact Pfaffian form; let* $\hat{W}$ *be the associated potential:* $d\hat{W}\equiv\omega_{(0)}$*; let* X *be a symmetry such that* $L_X\omega_{(0)}=0$*. Then*

$$d\hat{W}=\frac{dF}{F}, \tag{A6}$$

where F *satisfies*

$$XF=qF, \tag{A7}$$

with $q\in\mathbb{R}$ *constant. Moreover,*

$$i_X\omega_{(0)}=q. \tag{A8}$$

As a consequence, $q=0$ *is allowed if and only if the symmetry is tangent (i.e., trivial).*

Proof: We have

$$0=L_X\omega_{(0)}=L_X\,d\hat{W}=dL_X\hat{W}. \tag{A9}$$

As a consequence,

$$L_X\hat{W}=X\hat{W}=q, \tag{A10}$$

where q is a constant. We can define a positive definite function F such that

$$\hat{W}\equiv\log(F). \tag{A11}$$

Then we get that (A10) is equivalent to the following equation for F:

$$XF=qF; \tag{A12}$$

moreover

$$d\hat{W}=\frac{dF}{F}, \tag{A13}$$

and

$$i_X\omega_{(0)}=i_X\,d\hat{W}=L_X\hat{W}=\frac{1}{F}\,XF=q. \tag{A14}$$

If the symmetry is tangent, then $i_X\omega_{(0)}\equiv 0$. Then $q=0$ necessarily. If $q=0$, then F and $\hat{W}$ satisfy $XF=0$ and $X\hat{W}=0$, respectively. As a consequence, $i_X\omega_{(0)}=i_X\,d\hat{W}=L_X\hat{W}=0$, which completes the proof. □

Notice that $\hat{W}$ has to be found by quadratures, the contraction of the Pfaffian form with the vector field X is not useful in order to find a potential without explicit integration.

One can in general show that the following theorem holds.

Theorem 1: *Let ω be a integrable Pfaffian form which is defined in a simply connected domain; let X be a nontrivial symmetry for ω; let $\mu=i_X\omega$. Then μ is an integrating factor for ω and the foliation corresponding to the Pfaffian equation $\omega=0$ is associated with a potential F which satisfies the following equation*:

$$XF=F. \tag{A15}$$

Proof: The proof that ω/μ is closed is trivial. See also Refs. 6 and 1. Moreover

$$L_X\,\frac{\omega}{\mu}=0, \tag{A16}$$

being X a symmetry for ω. In fact,

$$L_X\,\frac{\omega}{\mu}=\frac{1}{\mu^2}((L_X\omega)\mu-(L_X\mu)\omega)=\frac{1}{(i_X\omega)^2}((L_X\omega)(i_X\omega)-(L_Xi_X\omega)\omega) \tag{A17}$$

$$=\frac{1}{(i_X\omega)^2}\,i_X(\omega\wedge(L_X\omega)), \tag{A18}$$

where the rules $i_XL_X=L_Xi_X$ and $i_X(\alpha\wedge\beta)=(i_X\alpha)\wedge\beta+(-)^n\alpha\wedge(i_X\beta)$ for a n-form α and a m-form β are used. Compare Ref. 65.

As a consequence, ω/μ is an exact one-form such that the previous lemma applies. One has

$$\frac{\omega}{\mu}=d\hat{W}=\frac{dF}{F}, \tag{A19}$$

where F satisfied Eq. (A7) with $q\neq 0$, because of the hypothesis of nontrivial symmetry. Then one finds

$$dF=\frac{F}{\mu}\,\omega, \tag{A20}$$

which satisfies $L_X\,dF=q\,dF$ and is closed. Then, from (A4), we obtain

$$F=\frac{1}{q}\,\frac{F}{\mu}\,i_X\omega, \tag{A21}$$

which, because of the definition of μ, implies $q=1$. □

Notice that the integrating factor satisfies

$$L_X\mu=L_Xi_X\omega=i_XL_X\omega=h\mu. \tag{A22}$$

It is interesting to underline that this theorem allows to construct a general theory of thermodynamics if δQ_{rev} has a nontrivial symmetry. It is easy to see that the constructions of Secs. III A and III B remain unaltered, and also the constructive assumptions of Sec. VIII can be trivially generalized [it is sufficient to delete "quasi-homogeneous" in (a1) and (a2) and to change (a5) into "the metrical entropy S satisfies $X\ \ S=S$"]. The case of quasi-homogeneous symmetry is immediately

obtained by requiring that each independent variable in the thermodynamic space has the same kind of symmetry as the potential S. More general symmetries can also be introduced. Further details will be given elsewhere.[66]

1. The quasi-homogeneous case

The following results are immediate consequences of the previous lemmas and theorem in the case of quasi-homogeneous symmetry.

Result 1: Let

$$\omega=\sum_{i=1}^{n}\omega_i\,dx^i \tag{A23}$$

be an exact quasi-homogeneous Pfaffian form of degree $r\neq 0$ *and weights* $(\alpha_1,\ldots,\alpha_n)$; *let*

$$D\equiv\sum_{i=1}^{n}\alpha_i x^i\,\frac{\partial}{\partial x^i} \tag{A24}$$

be the Euler operator; let the symmetry be nontrivial (or transversal), i.e.,

$$\omega(D)=i_D\omega=\sum_{i=1}^{n}\alpha_i\omega_i x^i\not\equiv 0. \tag{A25}$$

Then, one finds that $\omega=d\phi$ *is implemented by*

$$\phi\equiv\frac{1}{r}\,\omega(D). \tag{A26}$$

The above result can be used even when some zero weights occur. It cannot be used if $r=0$, in which case the potential can be found only by quadratures. When one considers, e.g., $\delta Q_{\mathrm{rev}}/f$, the potential has to be found by integrating the exact form.

Result 2: Let $\omega_{(0)}$ *be an exact quasi-homogeneous Pfaffian form of degree* $r=0$; *let* W *be the associated potential:* $d\hat{W}\equiv\omega_{(0)}$. *Then*

$$d\hat{W}=\frac{dF}{F}, \tag{A27}$$

where F *is a quasi-homogeneous function of degree* q *with respect to the Euler vector field* D. *Moreover,*

$$i_D\omega_{(0)}=q. \tag{A28}$$

As a consequence, $q=0$ *is allowed if and only if the symmetry is tangent.*

Notice that $\hat{W}$ has to be found by quadratures, the contraction of the Pfaffian form with the Euler vector field is not useful in order to find a potential without explicit integration.

Result 3: If $\omega_{(r)}$ *is a quasi-homogeneous integrable Pfaffian form of degree* r *defined in a connected, simply connected domain, if the symmetry is nontrivial and if* μ *is the corresponding integrating factor* $\omega(D)$, *then*

$$d\hat{W}\equiv\frac{\omega_{(r)}}{\mu}=\frac{dF}{F}, \tag{A29}$$

where F *is a quasi-homogeneous function of degree 1 with respect to the Euler vector field* D.

The degree r of $\omega_{(r)}$ can also be zero in the case where at least one weight, say α_1, is different from zero (the would-be intensive variable ω_1 has then weight $-\alpha_1$). Herein examples are given where $0<r<\infty$. It would be interesting to see if $r\leqslant 0$ is physically meaningful.

Notice that the fact that the case $q=0$ is not allowed by the requirement of nontriviality for the symmetry can be verified by direct inspection, in fact from Eq. (A20) it follows

$$\partial_i F=\frac{F}{\mu}\,\omega^i \quad \forall i=1,\ldots,n, \tag{A30}$$

thus $DF=0$ becomes

$$\sum_{i=1}^{n}\alpha_i x^i\,\frac{F}{\mu}\,\omega^i=0, \tag{A31}$$

which is not allowed, in fact, because of $\mu=\Sigma_{i=1}^{n}\alpha_i x^i\omega^i$, it would imply $F\equiv 0$. It is interesting to note that, from a mathematical point of view, $\hat{W}$ is an almost quasi-homogeneous function of degree zero with first order deficiency index identically equal to 1 (cf. Ref. 3), i.e., its behavior under quasi-homogeneous scaling is

$$\hat{W}(\lambda^{\alpha_1}x^1,\ldots,\lambda^{\alpha_n}x^n)=\hat{W}(x^1,\ldots,x^n)+\log(\lambda). \tag{A32}$$

This property of $\hat{W}$ is to be related with the nontriviality of the symmetry, which allows to find an integrating factor $\mu\not\equiv 0$.

2. Some more results on quasi-homogeneous integrable Pfaffian forms

We have found that, for nontrivial symmetry,

$$\omega_{(r)}=g_{(r-1)}dF, \tag{A33}$$

where $g_{(r-1)}$ is quasi-homogeneous of degree $r-1$. If G is a quasi-homogeneous function of degree q such that

$$\omega_{(r)}=g_{(r-q)}\,dG \tag{A34}$$

then necessarily

$$G=\zeta F^q, \tag{A35}$$

where $\zeta=\text{const}$. In fact, one has

$$\omega_{(r)}=g_{(r-q)}\,dG=g_{(r-1)}\,dF \tag{A36}$$

and

$$g_{(r-q)}=\frac{g_{(r-1)}}{dG/dF}. \tag{A37}$$

Moreover, the quasi-homogeneity of $G(F)$ implies

$$DG=qG=\frac{dG}{dF}\,F, \tag{A38}$$

that is,

$$\frac{dG}{dF} = q\,\frac{G}{F}, \tag{A39}$$

whose solution is (A35). For $q=1$, one obtains that the quasi-homogeneous function F of degree one implementing (A33) is unique apart from a multiplicative constant. [Notice that this result can be generalized easily to the case of a generic symmetry X. By referring to theorem 1, if G satisfies $XG=qG$ and $\omega = b\,dG$, then $G=G(F)$, where F is the potential (A15), and $G=\kappa F^q$, where κ is a constant.]

It is evident that, if D is a symmetry generator, $D_q = qD$ is another symmetry generator for $q \in \mathbb{R}-\{0\}$. It is also interesting that, by changing q, the integrating factor f_q changes in such a way that $\omega/f_q = d\log(F_q)$, where $F_q = F^{1/q}$ is quasi-homogeneous of degree 1 with respect to D_q (i.e., $D_q F_q = F_q$). In fact, one has $f_q = qf$ and

$$\frac{\omega}{f_q} = \frac{1}{q}\,\frac{\omega}{f} = \frac{1}{q}\,d\log(F) = d\log(F^{1/q}); \tag{A40}$$

then, $D_q F^{1/q} = qDF^{1/q} = q1/qF^{1/q-1}DF = F^{1/q}$.

APPENDIX B: *S* AS A FUNCTION OF *T* IN QUASI-HOMOGENEOUS THERMODYNAMICS AND THE THIRD LAW IN ENTROPIC FORM

We assume that the metrical entropy S^* is quasi-homogeneous of degree 1, and that $\alpha, \alpha_1, \ldots, \alpha_n$ are the weights of the independent variables $U^*, X^{1*}, \ldots, X^{n*}$. The temperature is then a quasi-homogeneous function of degree $\alpha - 1$. Let us consider $S^* = S^*(T^*, X^{1*}, \ldots, X^{n*})$. The entropic form of the third law, for standard thermodynamics, states that $S \to S_0$ as $T \to 0$, where S_0 is a constant which has to be zero.[1] Planck's restatement of the third law $S \to 0$ as $T \to 0$ is mandatory, if the third law holds, also in the case of quasi-homogeneous thermodynamics. In fact, if, for any fixed value of $X^{1*}, \ldots, X^{n*}$,

$$\lim_{T^* \to 0} S^*(T^*, X^{1*}, \ldots, X^{n*}) = S^*(0, X^{1*}, \ldots, X^{n*}) \equiv S_0^* \tag{B1}$$

holds, then, from

$$\lim_{T^* \to 0} S^*(\lambda^{\alpha-1}T^*, \lambda^{\alpha_1}X^{1*}, \ldots, \lambda^{\alpha_n}X^{n*}) = \lambda \lim_{T^* \to 0} S^*(T^*, X^{1*}, \ldots, X^{n*}) = \lambda \quad S_0^* \tag{B2}$$

and

$$\lim_{T^* \to 0} S^*(\lambda^{\alpha-1}T^*, \lambda^{\alpha_1}X^{1*}, \ldots, \lambda^{\alpha_n}X^{n*}) = S^*(0, \lambda^{\alpha_1}X^{1*}, \ldots, \lambda^{\alpha_n}X^{n*}) = S_0^* \tag{B3}$$

one finds $S_0^* = 0$. In the above formulas, continuity of S^* at $T^* = 0$ is assumed (otherwise the third law is violated[67]).

We know that black hole thermodynamics violates the entropic form of the third law. This behavior is not a general feature of quasi-homogeneous thermodynamics. We construct a toy-entropy which is both quasi-homogeneous and superadditive and implements the third law. Herein, as in Sec. VII, with x we indicate collectively the n variables appearing in S. Our starting point consists in realizing that, given two non-negative superadditive functions $g(x), h(x)$, the function

$$F(x) \equiv g(x)h(x) \tag{B4}$$

is superadditive too. In fact,

$$F(x_1+x_2) = g(x_1+x_2)h(x_1+x_2) \geqslant (g(x_1)+g(x_2))(h(x_1)+h(x_2)) \tag{B5}$$

$$= g(x_1)h(x_1) + g(x_2)h(x_2) + g(x_1)h(x_2) + g(x_2)h(x_1) \tag{B6}$$

$$\geqslant g(x_1)h(x_1) + g(x_2)h(x_2) = F(x_1) + F(x_2). \tag{B7}$$

Then, let us consider $g = 2\sqrt{U^* X^*}$ and $h = X^{*2}$. Both are superadditive functions (g is superadditive because of its homogeneity and concavity). Then $S^* \equiv 2\sqrt{U^* X^* X^{*2}}$ is superadditive and quasi-homogeneous. For S^* as a function of T^*, one finds

$$S^* = 2T^* X^{*5} \tag{B8}$$

which satisfies $S^* \to 0$ as $T^* \to 0$.

It is also interesting to notice that, in general, if S is a strictly superadditive function everywhere (i.e., also on the boundary $T=0$) then the entropic version of the third law in Planck's form has to be violated; in fact, if $(U_0, X_0^1, \ldots, X_0^n)$ is such that $T(U_0, X_0^1, \ldots, X_0^n) = 0$, then

$$S(U + U_0, X^1 + X_0^1, \ldots, X^n + X_0^n) > S(U_0, X_0^1, \ldots, X_0^n) + S(U, X_1, \ldots, X^n) \tag{B9}$$

is possible with the strict inequality only if $S(U_0, X_0^1, \ldots, X_0^n) > 0$. In the case of a self-gravitating system belonging to quasi-homogeneous thermodynamics framework, if the energy is strictly subadditive everywhere, then the third law cannot hold.

As far as mathematical properties of the Pfaffian form δQ_{rev} ensuring the validity of the entropic form of the third law are concerned, it can be shown that a quasi-homogeneous δQ_{rev} which is C^1 everywhere is a sufficient condition, in analogy with standard thermodynamics.[1,67] In fact, a superadditive non-negative function $S: \mathcal{D} \to \mathbb{R}_+ \cup \{\infty\}$ cannot be divergent at a limit point x_0 of its domain (we mean that all the points x in the domain satisfy $\|x\| < \infty$, where $\|\cdot\|$ stays for the Euclidean norm and that x_0 can be included in the domain by setting $S(x_0) = \infty$). This is evident if one translates rigidly the domain in such a way that $x_0 \equiv 0$. Then, if z_0 is another point in the domain of S one has $S(z_0) = S(z_0 + 0) \geqslant S(0) + S(z_0) = \infty$. Thus, if $S \not\equiv \infty$, then S has to be finite. Then S has to be finite in the limit as $T \to 0$. As a consequence, if f^* is the integrating factor, one has

$$\frac{\partial f}{\partial U^*} = 1 + S^* \frac{\partial T^*}{\partial U^*} \tag{B10}$$

and $\partial T^*/\partial U^* = 1/C$, where C is the heat capacity at fixed parameters X^{i*}, which has to tend to zero if S^* is finite and non-negative as $T^* \to 0$. Then, if f^* is everywhere C^1 (and it is such if δQ_{rev} is C^1 everywhere), it holds $S^* \to 0$ as $T^* \to 0$. Moreover, it is evident from (18) that $\lim_{T^* \to 0} S^* = 0$ holds if and only if $\int_\gamma \delta Q_{\text{rev}}/f^* \to -\infty$ as $T^* \to 0$ whichever path is chosen in approaching $T^* = 0$. Even the latter is an extension to the quasi-homogeneous case of the standard case.[1,67] See also Ref. 68 for further conditions.

APPENDIX C: GIBBS–DUHEM EQUATION REVISITED

Let us consider a quasi-homogeneous function $g(x^1, \ldots, x^n)$ of degree $q \neq 0$ and of weights $(\alpha_1, \ldots, \alpha_p, 0, \ldots, 0)$ where $1 \leqslant p \leqslant n$ is an integer and the last $n-p$ weights are all zero. It satisfies

$$Dg = qg, \tag{C1}$$

where

$$D = \sum_{i \leqslant p} \alpha_i x^i \frac{\partial}{\partial x^i}. \tag{C2}$$

If one defines

$$g_i \equiv \frac{\partial g}{\partial x^i} \quad \forall i = 1,\ldots,n, \tag{C3}$$

and

$$\omega_g \equiv \sum_i g_i \, dx^i = dg, \tag{C4}$$

one finds

$$g = \frac{1}{q} \, i_D \omega_g \, . \tag{C5}$$

This formal manipulation is useful in order to derive the Gibbs–Duhem equation. In fact, one has

$$dg = d\left(\frac{1}{q} \, i_D \omega_g\right) = \frac{1}{q} \, (-i_D \, d\omega_g + L_D \omega_g), \tag{C6}$$

where $L_D \omega_g = q \omega_g$ holds. Moreover, $d\omega_g = 0$ because $dg = \omega_g$ by construction. The Gibbs–Duhem equation is shown to be equivalent to

$$-\frac{1}{q} \, i_D \, d\omega_g = 0. \tag{C7}$$

One can easily see that

$$d\omega_g = \sum_i dg_i \wedge dx^i \tag{C8}$$

and that

$$\begin{aligned} i_D \, d\omega_g &= \sum_i (i_D \, dg_i) dx^i - \sum_i dg_i (i_D \, dx^i) \\ &= \sum_i (Dg_i) dx^i - \sum_{i \leqslant p} dg_i (\alpha_i x^i) \\ &= \sum_{i \leqslant p} (q - \alpha_i) g_i \, dx^i - \sum_{i \leqslant p} dg_i (\alpha_i x^i) + \sum_{p < i \leqslant n} q g_i \, dx^i. \end{aligned} \tag{C9}$$

As a consequence, (C7) becomes

$$\sum_{i \leqslant p} \frac{\alpha_i}{q} \, (x^i)^{q/\alpha_i} d((x^i)^{1 - q/\alpha_i} g_i) - \sum_{p < i \leqslant n} g_i \, dx^i = 0. \tag{C10}$$

If none independent variable of weight zero appears, then one finds

$$\sum_i \frac{\alpha_i}{q} \, (x^i)^{q/\alpha_i} d((x^i)^{1 - q/\alpha_i} g_i) = 0. \tag{C11}$$

Let us consider the inverse problem, where one assigns n would-be intensive variables g_i and the quasi-homogeneous one-form of degree $\omega_g = \Sigma_i g_i \, dx^i$ such that $L_D \omega_g = q \omega_g$ [one has to require

that $\deg(g_i)=q-\alpha_i$, where the weights of the independent variables x^i are the same as above]. Then one can also define a function $g\equiv i_D\omega_g/q$. From $dg=(-i_D\,d\omega_g)/q+\omega_g$ follows that ω_g is closed if $i_D\,d\omega_g=0$, i.e., if the Gibbs–Duhem equation is satisfied.

We limit ourselves to point out that more general Gibbs–Duhem equations are obtained in the generic symmetric case.[66] The generalization of (83) is

$$(i_X\delta Q_{\rm rev})d\log\left(\frac{1}{T}\right)-i_X\,d\,\delta Q_{\rm rev}+(L_X-1)\,\delta Q_{\rm rev}=0. \tag{C12}$$

APPENDIX D: QUASI-HOMOGENEITY (SCALING) CANNOT BE GENERALIZED

We show that, if $f(x^1,\ldots,x^n)$ is a C^1 function on a open connected set which satisfies the following identity:

$$f(g_1(\lambda)x^1,\ldots,g_n(\lambda)x^n)=g(\lambda)f(x^1,\ldots,x^n) \tag{D1}$$

and the functions $g(\lambda),g_i(\lambda)$ for $i=1,\ldots,n$ are positive definite and invertible, then $f(x^1,\ldots,x^n)$ is necessarily quasi-homogeneous. The above transformation is meant to be obtained by a "generalized similarity transformation" which carries $x^1,\ldots,x^n$ into $g_1(\lambda)x^1,\ldots,g_n(\lambda)x^n$. Let us consider $u\equiv g(\lambda)$ and the inverse $\lambda=g^{-1}(u)$. Define

$$h_i(u)\equiv g_i(g^{-1}(u))\quad\forall i=1,\ldots,n. \tag{D2}$$

It is also useful to define

$$u\equiv e^s. \tag{D3}$$

Then we obtain

$$f(h_1(e^s)x^1,\ldots,h_n(e^s)x^n)=e^sf(x^1,\ldots,x^n). \tag{D4}$$

Note that, for $s=0$, one finds

$$f(h_1(1)x^1,\ldots,h_n(1)x^n)=f(x^1,\ldots,x^n). \tag{D5}$$

This *a priori* does not imply that $h_i(1)=1\ \forall i=1,\ldots,n$, but the one-parameter $s\in\mathbb{R}_+$ "generalized similarity transformation" $\mathcal{T}_s$: $(x^1,\ldots,x^n)\to(h_1(e^s)x^1,\ldots,h_n(e^s)x^n)$ is consistently defined if $\mathcal{T}_{s=0}$ is the identity, i.e., if $h_i(1)=1\ \forall i=1,\ldots,n$.

We introduce the auxiliary function

$$F(s;x^1,\ldots,x^n)\equiv e^{-s}f(h_1(e^s)x^1,\ldots,h_n(e^s)x^n). \tag{D6}$$

It is such that $\partial_sF=0$, i.e.,

$$F=\sum_{i=1}^n e^sh_i'(e^s)x^i\left(\frac{\partial F}{\partial x^i}\right)(h_1(e^s)x^1,\ldots,h_n(e^s)x^n), \tag{D7}$$

where $h_i'(u)\equiv dh_i/du$. For $s=0$ one obtains

$$f(x^1,\ldots,x^n)=\sum_{i=1}^n h_i'(1)x^i\left(\frac{\partial f}{\partial x^i}\right)(x^1,\ldots,x^n). \tag{D8}$$

Thus, $f(x^1,\ldots,x^n)$ is a quasi-homogeneous function of degree 1 and weights $(h_1'(1),\ldots,h_n'(1))\equiv(\alpha_1,\ldots,\alpha_n)$. As a consequence, one has

$$f(e^{\alpha_1s}x^1,\ldots,e^{\alpha_ns}x^n)=e^sf(x^1,\ldots,x^n), \tag{D9}$$

i.e.,

$$h_i(e^s)=e^{\alpha_i s} \quad \forall i=1,\ldots,n. \tag{D10}$$

By resorting the original dependence on λ, one finds

$$f((g(\lambda))^{\alpha_1}x^1,\ldots,(g(\lambda))^{\alpha_n}x^n)=g(\lambda)f(x^1,\ldots,x^n), \tag{D11}$$

i.e.,

$$g_i(\lambda)=(g(\lambda))^{\alpha_i} \quad \forall i=1,\ldots,n. \tag{D12}$$

If some $g_i=1$ above, then one simply finds that the variable x^i is quasi-homogeneous of degree zero, i.e., it has weight zero. If instead $g(\lambda)=1$, then f is quasi-homogeneous of degree zero. The proof is straightforward. Let λ_0 be such that $g_i(\lambda_0)=1 \ \forall i=1,\ldots,n$. We have that

$$\frac{\partial f}{\partial \lambda}=0=\sum_{i=1}^{n} g_i'(\lambda)x^i\left(\frac{\partial f}{\partial x^i}\right)(g_1(\lambda)x^1,\ldots,g_n(\lambda)x^n). \tag{D13}$$

By setting $\lambda=\lambda_0$, one finds

$$0=\sum_{i=1}^{n} g_i'(\lambda_0)x^i\left(\frac{\partial f}{\partial x^i}\right)(x^1,\ldots,x^n), \tag{D14}$$

i.e., f is quasi-homogeneous of degree zero and weights $(g_1'(\lambda_0),\ldots,g_n'(\lambda_0))$.

APPENDIX E: SCALING AND ASYMPTOTICS

Let us assume that $f(x)$ is a function of n variables collectively indicated with x. Let the domain of f be invariant under quasi-homogeneous transformations. Let $\{\mathcal{T}_\lambda\}$ be a one-parameter quasi-homogeneous transformation. If we require that there exist a positive continuous function $\rho(\lambda)$ and a continuous function $g(x)\not\equiv 0$ such that g is an asymptotic of f in the following sense:

$$\lim_{\lambda\to\infty}\frac{1}{\rho(\lambda)}f(\mathcal{T}_\lambda x)=g(x), \tag{E1}$$

where the limit is assumed to exist. Then, (a) the function $\rho(\lambda)$ is a regularly varying function, i.e., it satisfies for all $a>0$,

$$\lim_{\lambda\to\infty}\frac{\rho(\lambda a)}{\rho(\lambda)}\equiv C(a), \tag{E2}$$

where $C(a)C(b)=C(ab)$, i.e., $C(a)=a^\gamma$ for some $\gamma\in\mathbb{R}$; γ is also defined the order of the regularly varying function $\rho(\lambda)$; (b) the function satisfies the ''homogeneity'' relation

$$g(\mathcal{T}_\mu x)=\mu^\gamma g(x), \tag{E3}$$

i.e., $g(x)$ is quasi-homogeneous of degree γ.

Proof: for each real $s>0$ it holds

$$\lim_{\lambda\to\infty}\frac{1}{\rho(\lambda s)}f(\mathcal{T}_{\lambda s}x)=g(x), \tag{E4}$$

and, because of $\mathcal{T}_{\lambda s}=\mathcal{T}_\lambda\mathcal{T}_s$,

$$\lim_{\lambda\to\infty}\frac{1}{\rho(\lambda)}\,f(\mathcal{T}_\lambda(\mathcal{T}_s x))=g(\mathcal{T}_s x). \tag{E5}$$

As a consequence,

$$\lim_{\lambda\to\infty}\frac{\rho(\lambda)}{\rho(\lambda s)}\,\frac{f(\mathcal{T}_{\lambda s}x)}{f(\mathcal{T}_\lambda(\mathcal{T}_s x))}=\frac{g(x)}{g(\mathcal{T}_s x)}=\lim_{\lambda\to\infty}\frac{\rho(\lambda)}{\rho(\lambda s)}. \tag{E6}$$

This is possible only if the following conditions:

$$\lim_{\lambda\to\infty}\frac{\rho(\lambda s)}{\rho(\lambda)}=C(s) \tag{E7}$$

and

$$g(\mathcal{T}_s x)=C(s)g(x) \tag{E8}$$

are both satisfied. Moreover, it is easy to see that it holds

$$C(st)=C(s)C(t), \tag{E9}$$

which implies that there exists a real number γ such that $C(s)=s^\gamma$. Thus, one obtains

$$g(\mathcal{T}_s x)=s^\gamma g(x), \tag{E10}$$

which concludes the proof. □

Compare also Ref. 55.

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Leibnizian, Galilean and Newtonian structures of space–time[a)]

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(Received 28 October 2002; accepted 2 December 2002)

The following three geometrical structures on a manifold are studied in detail: *Leibnizian*: a nonvanishing one-form Ω plus a Riemannian metric $\langle\cdot,\cdot\rangle$ on its annhilator vector bundle. In particular, the possible dimensions of the automorphism group of a Leibnizian G-structure are characterized. *Galilean*: Leibnizian structure endowed with an affine connection ∇ (gauge field) which parallelizes Ω and $\langle\cdot,\cdot\rangle$. For any fixed vector field of observers $Z(\Omega(Z)\equiv 1)$, an explicit Koszul-type formula which reconstructs bijectively all the possible ∇'s from the gravitational $\mathcal{G}:=\nabla_Z Z$ and vorticity $\omega:=\frac{1}{2}$ rot Z fields (plus eventually the torsion) is provided. *Newtonian*: Galilean structure with $\langle\cdot,\cdot\rangle$ flat and a field of observers Z which is inertial (its flow preserves the Leibnizian structure and $\omega\equiv 0$). Classical concepts in Newtonian theory are revisited and discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1541120]

I. INTRODUCTION

It is well-known since Cartan's era[2] that Newtonian theory can be stated in the language of differential geometry, and many authors have studied this geometrization on its own and in comparison with (or as a limit of) Einstein's general relativity [see for example, Refs. 3–8, 11, 12, 13 (Box 12.4), 14–16, 18, and 21]. The aim of this article is to carry out a geometrization from a more general viewpoint, which arises from the fundamental considerations on measurements of space and time in Ref. 1.

A *Leibnizian* structure on an m-manifold M is a pair $(\Omega,\langle\cdot,\cdot\rangle)$ consisting of a nonvanishing one-form Ω and a (positive definite) Riemannian metric $\langle\cdot,\cdot\rangle$ on its kernel. When $m=4$, this structure appears naturally as a consequence of our methods of measurement of space–time; in fact, it is natural to assume the existence of a Leibnizian (or dual *anti-Leibnizian*) structure in the degenerate part of a signature-changing metric from Lorentzian to Riemannian.[1] When Ω is exact, i.e., $\Omega=dT$ for an *absolute time* function T, the intuitive idea ''at each instant of time there exist a Riemannian metric on space'' is geometrized. Given the Leibnizian space–time a *Galilean* connection is an affine connection which parallelizes Ω and $\langle\cdot,\cdot\rangle$. As a difference with the Levi-Civita connection for a semi-Riemannian (Riemannian, Lorentzian or with any index) manifold, symmetric Galilean connections are not univocally determined by the Leibnizian structure. Moreover, there exists a symmetric Galilean connection if and only if Ω is closed (i.e., locally, $\Omega=dT$). Galilean connections can be seen as gauge fields, which are necessary to preserve the covariance of physical laws under the change of ''Galilean reference frames.'' A Newtonian space–time will be a Galilean one $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ where ∇ satisfies certain symmetries. In the present article we study the mathematical properties of each level (Leibnizian/Galilean/Newtonian) and the corresponding physical interpretations.

From the purely mathematical viewpoint, some questions arise naturally: which are the pos-

[a)]Part of the results of this article has been announced at the RSME meeting ''Encuentros de Otoño de Geometría y Física'' Miraflores de la Sierra (Madrid), September 2001.

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sible dimensions of the group of automorphisms of a Leibnizian space–time? How many Galilean connections admit a Leibnizian structure? Is there an explicit way to construct them? The answers to such questions are interesting also from the physical viewpoint. The cornerstone of our approach can be stated as follows (see Lemma 25, Theorem 27, and Corollary 28): *given a Leibnizian space–time, a field of observers Z and an (unknown) Galilean connection ∇, the gravitational field $\mathcal{G}$ and the vorticity/Coriolis field ω measured by Z* (plus, eventually, any skew-symmetric tensor Tor representing the torsion, subject to the restriction $\Omega\circ \mathrm{Tor}=d\Omega$) *permit us to reconstruct univocally the connection ∇*. Even though partial versions of this result are well-known (*ad nauseam* if $\langle\cdot,\cdot\rangle$ is flat and Z determines an ''inertial reference frame''), the full result is new, as far as we know. In fact, it relies on formula (13), which plays a similar role to Koszul's formula in semi-Riemannian geometry, and introduces a type of ''sub-Riemannian'' geometry with interest of its own. Then, classical Newtonian concepts are revisited under this viewpoint.

In the comparison with classical geometrizations of Newtonian theory (see, e.g., Refs. 21, 13, Box 12.4, and 5), where one assumes first that the space is flat and then some sort of assumptions to make inertial references frames appear, the advantages of our approach become apparent not only for its bigger generality but also for the sake of clarity: the detailed study of the structures at each level Leibnizian/Galilean/Newtonian clarifies both the mathematical results and the physical interpretations. It is also worth pointing out that Kunzle and some co-workers[11,12,4] have also studied some Leibnizian structures; in fact, they call $(M,\Omega,\langle\cdot,\cdot\rangle)$ with Ω closed ''Galilei structure'' and the corresponding compatible connections ''Galilei connections.'' Nevertheless, our constructive procedure of all Galilean connections and associated physical interpretations go further [see Remark 29(2)]. (In fact, our study led us to put different names to the structures depending on if ∇ was fixed or not, as in Ref. 5. The names Leibnizian, Galilean and Newtonian are suggested by some famous historical facts–Galilean studies on freely moving bodies, controversy between Leibniz and Newton, and Newton's discussion of the spinning water-bucket.)

The present article is divided into three parts. In the first one (Sec. II), the properties of pure Leibnizian structures are studied. Leibnizian vector fields and fields of Leibnizian observers (FLOs) are introduced, as infinitesimal generators of automorphisms. In Theorem 8, the possible dimensions of these vector fields are characterized, in agreement with some known properties of classical *kinematical group*.

The second part (Sec. III) is devoted to Galilean structures. Apart from the commented results on our Koszul-type formula (13), we introduce both Galilean vector fields and fields of Galilean observers (i.e., the corresponding Leibnizian fields which preserve infinitesimally the connection ∇), see Table I. In Sec. III C, coordinate expressions for the connection, geodesics and curvature (for coordinates adapted to general fields of observers as well as more restricted ones: Leibnizian, Galilean or *inertial*) are also provided.

Finally, in the third part (Sec. IV) the Newtonian case is specifically revised, discussing the classical concepts. In fact, our definition of Newtonian space–time is a Galilean one which admits an inertial field of observers and with $(\mathrm{an}\Omega,\langle\cdot,\cdot\rangle)$ flat. This definition avoids conditions at infinity, which are discussed in relation to the properties of gravitational fields and the uniqueness of Poisson's equation. Even though from the mathematical viewpoint the results are clearer when nonsymmetric connections are also taken into account [see Remark 29(1)], we restrict to symmetric connections for physical concepts or coordinate expressions, in particular along all the third part.

II. LEIBNIZIAN STRUCTURES

A. Leibnizian space–times

1. Setup

A *Leibnizian* space–time is a triad, $(M,\Omega,\langle\cdot,\cdot\rangle)$, consisting of a smooth connected manifold M, of any dimension $m=n+1\geqslant 2$, a differential one-form $\Omega\in\Lambda^1(M)$, nowhere null ($\Omega_p\neq 0, \forall p\in M$), and a smoth, bilinear, symmetric and positive definite map

TABLE I. Semi-Riemannian versus Leibnizian/Galilean.

● Structure	Semi-Riemannian, (M,g) $\dim M=m$, index $g=s$	Leibnizian, $(M,\Omega,<,>)$ $\dim M=m\ (=n+1)$
● Structural group	Orthonormal, $O_s(m)$ $\dim O_s(m)=m(m-1)/2$	Galilean, $G_m(\mathbb{R})$ $\dim G_m(\mathbb{R})=m(m-1)/2$
● Infinitesimal automorphisms	Killing vector fields Possible dimensions: $0,1,\ldots,m(m+1)/2$	Leibnizian vector fields Possible dimensions $(d\Omega=0)$: 0, 1 or ∞
● Possible connections ∇ which parallelize the structure	Determined by all torsion tensors, bijective correspondence: Connections$\leftrightarrow$two-covar. one-contrav. skew-symmetric tensors Unique connection without torsion (Levi-Civita)	Determined by: (a) Possible torsions: $\Omega\circ$ Tor$=d\,\Omega$ (b) Fixed Z $(\Omega(Z)=1)$: $\nabla_Z Z$ and $\omega=rot\,Z/2$ Existence of ∇ without Tor $\Leftrightarrow d\,\Omega=0$
● Fixed a connection ∇ which parallelizes the structure	Canonically, Tor$=0$ Killing$\Rightarrow$Affine No new definition of vector fields required	Even if Tor$=0$, Leibnizian$\not\Rightarrow$Affine Galilean vector fields: Leibnizian+affine Dimension Galilean: $0,1,\ldots,m(m+1)/2$

$$\langle\cdot,\cdot\rangle:\Gamma(\mathrm{an}\Omega)\times\Gamma(\mathrm{an}\Omega)\to C^\infty(M),\quad (V,W)\mapsto\langle V,W\rangle,$$

where $\mathrm{an}\Omega=\{v\in TM\,|\,\Omega(v)=0\}$, is the n-distribution induced by Ω, and the symbol Γ denotes the corresponding vector fields, so $\Gamma(\mathrm{an}\Omega)=\{V\in\Gamma(TM)\,|\,V_p\in\mathrm{an}\Omega,\ \forall p\in M\}$. [As usual, M will be assumed Hausdorff and paracompact; "smooth" will mean C^∞ (even though C^2 is enough).] Summing up, the Leibnizian structure on M is the nonvanishing one-form Ω plus the Riemannian vector bundle $(\mathrm{an}(\Omega),\langle\cdot,\cdot\rangle)$.

Note: Let the superscript * denote dual space. For any $p\in M$ there exists a canonical isomorphism between $(\mathrm{an}\Omega_p)^*$ and the quotient vector space $(T_pM)^*/\mathrm{Span}\Omega_p$. Therefore, the metric $\langle\cdot,\cdot\rangle_p$ induces a canonical Euclidean product on $(T_pM)^*/\mathrm{Span}\Omega_p$, as well as a positive semidefinite metric on $(T_pM)^*$, with radical generated by Ω_p. Thus, a Leibnizian structure is equivalent to a degenerate semidefinite positive metric of constant rank n in the cotangent bundle TM^*, plus a one-form generating its radical. In Ref. 1, an *anti-Leibnizian* structure on M is defined as a degenerate semidefinite positive metric of constant rank n in the tangent bundle TM, plus a vector field Z generating its radical. Thus, the study of anti-Leibnizian structures is analogous (dual) to the study of the Leibnizian ones.

According to Ref. 1, Euclidean space $(\mathrm{an}(\Omega_p),\langle\cdot,\cdot\rangle_p)$ is called the *absolute space* at $p\in M$, and the linear form Ω_p is the *absolute clock* at p. A tangent vector $Z_p\in T_pM$ is *timelike*, if $\Omega_p(Z_p)\neq 0$ (*spacelike*, otherwise). If, additionally, $\Omega_p(Z_p)>0$ [resp. $\Omega_p(Z_p)<0$], Z_p *points out the future* (resp. *the past*). Any normalized timelike vector Z_p [that is, with $\Omega_p(Z_p)=1$] is a *standard timelike unit* (or *instantaneous observer*) at p; any (ordered) orthonormal base of the absolute space at p is a *set of standard spacelike units* at p.

Let us introduce definitions for the concepts of observer and field of observers (or reference frame) analogous to the Lorentzian ones; compare with Ref. 17, Chap. 2. An *observer* is a smooth curve, $\gamma:I\to M$ ($I\subseteq\mathbb{R}$, interval), such that its velocity is always a standard timelike unit, $\Omega_{\gamma(s)}(\gamma'(s))=1$, $\forall s\in I$. The parameter of this curve is the *proper time* of the observer γ. A *field of (instantaneous) observers* (FO) is a vector field $Z\in\Gamma(TM)$ with $\Omega(Z)\equiv 1$, that is, integral curves of Z are observers. The existence of a FO on any Leibnizian space–time is straightforward from the paracompactness of M. [Conversely, if we assume the existence of a FO, then Lemma 25 and Remark 26 permit us to construct an affine connection on M; thus, we could deduce the

paracompactness of M by using Ref. 19, Vol. II, Addendum 1, p. 8-52.] Let $\mathcal{Z}(M)\equiv\mathcal{Z}(M,\Omega)$ be the set of all the FOs. Clearly, $\mathcal{Z}(M)$ has a structure of affine space with associated vector field $\Gamma(\mathrm{an}\Omega)$. For each FO, $Z\in\mathcal{Z}(M)$, define the field of endomorphisms:

$$P^Z(v)=v-\Omega(v)Z, \qquad \forall v\in TM, \tag{1}$$

or *spacelike projection along* Z. Obviously, the image of P^Z is $\mathrm{an}(\Omega)$.

When the absolute clock Ω satisfies $\Omega\wedge d\Omega=0$ (i.e., the distribution $\mathrm{an}\Omega$ is involutive: $[V,W]\in\Gamma(\mathrm{an}\Omega),\forall V,W\in\Gamma(\mathrm{an}\Omega)$), we say that $(M,\Omega,\langle\cdot,\cdot\rangle)$ is *locally sincronizable*; if $d\Omega=0$ (Ω is closed), then $(M,\Omega,\langle\cdot,\cdot\rangle)$ is *proper time locally syncronizable*. In fact, it is well-known that the equality $\Omega\wedge d\Omega=0$ is equivalent, locally, to $\Omega=f\,dt$, for some smooth functions $f>0$, t. That is, in the domain of f and t, hipersuperfaces $t\equiv$const are tangent to the absolute space at each point. Thus, in principle, any observer could be "syncronized," that is, it can regard t as a compromise time, obtained by rescaling its proper time. In the more restrictive case $d\Omega=0$, one has locally $\Omega=dt$. Thus, any observer γ is direcly "syncronized," up to a constant c_γ [i.e., $t\circ\gamma(s)=s+c_\gamma,\forall s\in I$]. Notice that these concepts about local syncronizability are intrinsic to the Leibnizian structure and, then, applicable to each particular observer γ. This is a clear difference with the Lorenzian case, where the analogous concepts have meaning only for fields of observers. [If (M,g) is a time-oriented Lorentzian manifold, a FO is a unit future-pointing timelike vector field Z. If $Z^\flat$ is the metrically associated one-form, Z is said locally syncronizable (resp. proper time locally sincronizable) if $Z^\flat\wedge dZ^\flat=0$ (resp. $dZ^\flat=0$). It is not difficult to prove that, in the neighborhood of any point, *a proper time locally syncronizable vector field can be always constructed* (compare with Ref. 17, Sec. 2.3).]

When Ω is exact, that is, $\Omega=dT$ for some (unique up to a constant) $T\in C^\infty(M)$, T will be called the function *absolute time*. In this case, any observer γ will be assumed to be parametrized with T ($T\circ\gamma(s)=s,\forall s\in I$). When M is simply connected, local proper time synchronizability is equivalent to the existence of such an absolute time function.

2. Coordinates

Given a Leibnizian space–time $(M,\Omega,\langle\cdot,\cdot\rangle)$ and a FO, $Z\in\mathcal{Z}(M)$, for each $p\in M$ there exist charts $(U,y^0,\ldots,y^n)$ such that $\partial_{y^0}=Z|_U$. We can wonder if, additionally, these charts may be adapted to the absolute spaces. More precisely, we have the following.

Definition 1: Let $(M,\Omega,\langle\cdot,\cdot\rangle)$ *a Leibnizian space–time and* $(U',t,x^1,\ldots,x^n)$ *a coordinate system in* M. $(U',t,x^1,\ldots,x^n)$ *is* adapted to the absolute space *if*

$$\Omega(\partial_{x_i})=0, \qquad \forall i\in\{1,\ldots,n\}$$

(in particular, hipersuperfaces $t\equiv$const *are integral manifolds of the distribution* $\mathrm{an}\Omega$*).*

Given a FO, $Z\in\mathcal{Z}(M)$, $(U',t,x^1,\ldots,x^n)$ *is* adapted to Z *if, on* U',

$$\partial_t=Z \quad and \quad \Omega=dt.$$

If the chart is adapted to the absolute space, then $\Omega=\Omega(\partial_t)dt$; if it is adapted to Z, then it is adapted to the absolute space too. Clearly, if $(U',t,x^1,\ldots,x^n)$ is adapted to the absolute space (resp. a Z), then $\Omega\wedge d\Omega=0$ (resp. $d\Omega=0$) on U'. The converse also holds; in fact, the following result yields adapted charts constructively.

Proposition 2: Let Z *be a FO on a Leibnizian space–time* $(M,\Omega,\langle\cdot,\cdot\rangle)$. *Fix a chart* $(U,y^0,\ldots,y^n)$ *such that* $\partial_{y^0}=Z|_U$, *and put*

$$V_k=P^Z(\partial_{y^k})\in\mathrm{an}\Omega, \quad \forall k\in\{1,\ldots,n\}, \tag{2}$$

with P^Z *in (1). Then*

(i) $(Z,V_1,\ldots,V_n)$ *is a local base of vector fields* (moving frame) *with* $\Omega(V_k)=0$ *and*

$$d\Omega(Z,V_j)=-\Omega([Z,V_j]),\qquad d\Omega(V_i,V_j)=-\Omega([V_i,V_j]),\qquad \forall i,j\in\{1,\dots n\}. \tag{3}$$

(ii) If $\Omega\wedge d\Omega=0$, *then, at some neighborhood* U' *of each* $p\in U$, *there exist coordinates* $(t,x^1,\dots,x^n)$ *satisfying on* U':

$$\Omega=\Omega(\partial_t)dt,\quad \partial_{x^k}=V_k,\quad \forall k\in\{1,\dots,n\}.$$

Thus, such coordinates are adapted to the absolute space.

(iii) If $d\Omega=0$, *then, in addition to (ii), one has*

$$\partial_t=Z,$$

on U' (*i.e., the coordinates are adapted to* Z).

Proof: (i) Obvious.

(ii) As the distribution anΩ is involutive, $\Omega([V_i,V_j])=0$ and, from (2), $[V_i,V_j]=0$. Thus, it is enough to apply classical Frobenius' theorem (see, for example, Ref. 23 Chap. 1).

(iii) By using (3), one checks $[Z,V_j]=0$ and, again, the result follows from Frobenius' theorem. □

From now on, Latin indexes i, j, k will vary in $1,\dots,n$. We will simplify the notation, too: $\partial_{x^k}\equiv\partial_k$.

3. Galilean group at a point

Fix $p\in M$. An (ordered) base $B=(Z_p,e_1,\dots,e_n)$ of T_pM is a *Galilean base at* p if $\Omega(Z_p)=1$ and $\{e_1,\dots,e_n\}$ is an orthonormal base of an(Ω_p), that is, if Z_p is a standard timelike unit at p and $e_1,\dots,e_n$ are standard spacelike units.

A *Galilean transformation at* p is a linear map, $A:T_pM\to T_pM$, which maps some (and thus, any) Galilean base onto a Galilean base. Or, equally, $\Omega_p(A(X_p))=\Omega_p(X_p)$ *and* $\langle A(V_p),A(W_p)\rangle_p=\langle V_p,W_p\rangle_p$, $\forall X_p\in T_pM$, $\forall V_p,W_p\in$ an(Ω_p). The group of all such transformations will be called the *Galilean group* at p.

Matricial Galilean group $G_m(\mathbb{R})$, $m=n+1$, is the group of the matrixes

$$\begin{pmatrix}1 & 0\\ a & A\end{pmatrix},\qquad \text{where}\quad a=\begin{pmatrix}a^1\\ \vdots\\ a^n\end{pmatrix}\in\mathbb{R}^n\quad\text{and}\quad A\cdot A^t=I_n \tag{4}$$

(A is an orthogonal matrix $n\times n$).

It is straightforward to check that, given a Galilean base B and any other base $B'=(Z'_p,e'_1,\dots,e'_n)$ in T_pM, the base B' is Galilean if and only if the transition matrix belongs to $G_m(\mathbb{R})$, that is,

$$Z'_p=Z_p+\sum_{i=1}^{n}a^ie_i,\qquad e'_j=\sum_{i=1}^{n}a^i_je_i,\quad \forall j\in\{1,\dots,n\},$$

where $A=(a^i_j)$ is a orthogonal matrix. In this case, $v=\Sigma_j a^je_j$ is the *velocity of* Z'_p *measured by* Z_p.

B. Leibnizian vector fields

1. Automorphisms of Leibnizian G-structures

Let LM be the linear frame bundle of M, that is, each element of LM can be seen as a (ordered) base of the tangent space at some point of M. The Leibnizian structure $(\Omega,\langle\cdot,\cdot\rangle)$ on M determines the fiber bundle of all the Galilean bases $GM\subset LM$. As $G_m(\mathbb{R})$ acts freely and transively on each fiber, GM is a G-structure with $G=G_m(\mathbb{R})$ [i.e., a principal fiber bundle with structural group $G_m(\mathbb{R})$, obtained as a reduction of LM]. Recall that the set of the orthonormal

bases for any semi-Riemannian metric (in particular, Riemannian or Lorentzian) is a well-known example of G-structure; the dimension of its structural group is equal to the dimension of $G_m(\mathbb{R})$, i.e., $m(m-1)/2$ $(m=n+1)$. G-structures have mathematical interest in their own right (see, for example, Ref. 9), and we will be interested in two properties of Leibnizian G-structures with striking differences with respect to the semi-Riemannian case: their infinitesimal automorphisms (studied below) and the set of all the compatible affine connections (Sec. III B).

An infinitesimal automorphism of a G-structure is a vector field K generating a group of automorphisms of the principal fiber bundle. In the semi-Riemannian case, such a K is called a Killing vector field. In the Leibnizian one, the following definition is equivalent.

Definition 3: Given $(M,\Omega,\langle\cdot,\cdot\rangle)$, *a vector field* $K\in\Gamma(TM)$ *is* Leibnizian (Killing) *if its local flows* ψ_s *preserve the absolute clock and space, that is,*

$$\psi_s^*\Omega=\Omega \qquad \text{and} \qquad \psi_s^*\langle\cdot,\cdot\rangle=\langle\cdot,\cdot\rangle.$$

$\mathrm{Leib}(M)\equiv\mathrm{Leib}(M,\Omega,\langle\cdot,\cdot\rangle)$ *will denote the set of all the Leibnizian vector fields.*

As $\mathcal{L}_K$, the Lie derivative along K, can be recovered from the local flows of K, the following characterizations of Leibnizian vector fields are straightforward.

Proposition 4: Let $(M,\Omega,\langle\cdot,\cdot\rangle)$ *be a Leibnizian space–time, and* $K\in\Gamma(TM)$ *be a vector field. The following assertions are equivalent:*

(1) K *is a Leibnizian vector field.*
(2) $\mathcal{L}_K\Omega=0$ *and* $\mathcal{L}_K\langle\cdot,\cdot\rangle=0$,
(3) The following two properties hold:
(a) $\Omega([K,Y])=K(\Omega(Y))$, $\forall Y\in\Gamma(TM)$ *[equally:* $-d\Omega(K,Y)=Y(\Omega(K))$*].*
(b) $K\langle V,W\rangle=\langle[K,V],W\rangle+\langle V,[K,W]\rangle$, $\forall V,W\in\Gamma(\mathrm{an}\Omega)$.

In particular, $\mathrm{Leib}(M)$ *is a Lie algebra.*

Remark 5: (1) The right hand side of *3(b)* makes sense [i.e., $[K,V]$, $[K,W]\in\Gamma(\mathrm{an}\Omega)$] when *3(a)* holds.

(2) When $d\Omega=0$, property $3(a)$ holds if and only if $\Omega(K)=cte$. We will put then, for each $c\in\mathbb{R}$,

$$\mathrm{Leib}_c(M)=\{K\in\mathrm{Leib}(M)\,|\,\Omega(K)=c\} \tag{5}$$

(clearly, the relevant cases will be $c=0,1$).

(3) As we will see, the dimension of $\mathrm{Leib}(M)$ may be infinite. This was expected from a purely algebraic viewpoint: a straightforward computation from (4) shows that the Lie algebra $G_m(\mathbb{R})$ contains elements of rank 1 and, thus, this algebra is of finite type (see Ref. 9, Proposition 1.4). As a consequence, the automorphisms of a Leibnizian manifold are not necessarily a (finite dimensional) Lie group.

2. Fields of Leibnizian observers

Consider now the case that Z is a *field of Leibnizian observers (FLO)*, that is, $Z\in\mathcal{Z}(M)$, and Z is Leibnizian. (The name of *rigid vector fields* is also natural for FLO's, see Ref. 17, Sec. 2.3). We will be interested in the classical interpretations of these vector fields; thus, we assume now $d\Omega=0$. According to formula (5) the set of all the FLOs will be denoted as $\mathrm{Leib}_1(M)$.

From Proposition 2, given $Z\in\mathcal{Z}(M)$ a chart $(t,x^1,\ldots,x^n)$ adapted to Z exists. Put

$$h_{ij}=\langle\partial_i,\partial_j\rangle, \qquad h\equiv\langle\cdot,\cdot\rangle.$$

The following characterization of the FLOs is immediate from its definition and Proposition 4.

Proposition 6: Let $(M,\Omega,\langle\cdot,\cdot\rangle)$ *be a Leibnizian space–time with* $d\Omega=0$ *and* $Z\in\mathcal{Z}(M)$. *The field of observers* Z *is a FLO if and only if for each* $p\in M$ *there exists a chart* $(t,x^1,\ldots,x^n)$ *adapted to* Z *such that*

$$\partial_t h_{ij}=0, \quad \forall i,j\in\{1,\dots n\}. \tag{6}$$

Remark 7: Of course, in this case equality (6) holds for any chart adapted to Z. Thus, the FLOs are those fields of observers satisfying the following: their observers see that, locally, the metric $\langle\cdot,\cdot\rangle$ does not change with the local absolute time t (they are always at the same distance of the neighboring observers).

3. Main result

Now, let us characterize the dimension of the Lie algebra Leib(M). For simplicity, we will assume the existence of a globally defined time function T (of course, the results hold locally if only $d\Omega=0$).

Notice first that $\mathrm{Leib}_1(M)$ may be empty [and then $\mathrm{Leib}(M)=\mathrm{Leib}_0(M)$], no matter the dimension of $\mathrm{Leib}_0(M)$ be. Recall also that a vector field $Z\in\Gamma(TM)$ is called *complete* if it admits a globally defined flow ϕ, i.e., $\phi_t: M\to M$, for all $t\in\mathbb{R}$ [for $Z\in\mathcal{Z}(M)$, one can say, equally, that the—inextendable—observers in Z are defined on all $\mathbb{R}$].

Theorem 8: *Consider the Leibnizian space–time* $(M,dT,\langle\cdot,\cdot\rangle)$.

(1) (a) Let $K\in\mathrm{Leib}_0(M)$ *be. The restriction of* K *to each hypersurface* $T\equiv T_0$ *(constant) is a Killing vector field of the Riemannian manifold* $(T^{-1}(T_0),\langle\cdot,\cdot\rangle)$.
(b) If $\mathrm{Leib}_0(M)\neq 0$, *then* $\dim(\mathrm{Leib}_0(M)=\infty)$.
(2) If $\mathrm{Leib}_1(M)$ *is not empty, then it is an affine space of associated vector space* $\mathrm{Leib}_0(M)$. *Thus,* $\dim(\mathrm{Leib}(M))\in\{0,1,\infty\}$.
(3) If there exists a complete FLO, $Z\in\mathrm{Leib}_1(M)$, *then we have the following.*
(a) All the hypersurfaces $T\equiv$ const *are isommetric*.
(b) If one of the $T^{-1}(T_0)$ *admits a Killing vector field* $K_0(\not\equiv 0)$, *then* $dim\,\mathrm{Leib}_0(M)=\infty$.

Proof: (1) Assertion (a) is obvious. For (b) take any $K\in\mathrm{Leib}_0(M)$. Notice that, for any function $a:\mathbb{R}\to\mathbb{R}$, the vector field

$$K^a(p)=a(T(p))K(p), \quad \forall p\in M,$$

satisfies $K^a\in\mathrm{Leib}_0(M)$ too. If $K\not\equiv 0$, one can choose a neighborhood U where K does not vanish, and some interval $]T_1,T_2[$, $T_1<T_2$ included in $T(U)$. Now, just take infinite independient functions $a(T)$ vanishing outside of $]T_1,T_2[$.

(2) Obvious.

(3) For (a) recall that the flow ϕ_t of Z generates an isommetry between $T^{-1}(T_0)$ and $T^{-1}(T_0+t),\forall t\in\mathbb{R}$. For (b), we have just to find some $K\in\mathrm{Leib}_0(M)$, $K\not\equiv 0$ and apply *1(b)*. Such a vector field can be constructed from K_0 and the flow of Z as follows:

$$K_p=d\phi_{(T(p)-T_0)}(K_0[\phi_{-(T(p)-T_0)}(p)]) \tag{7}$$

{with the notation: $K_0[q]\equiv(K_0)_q$, for $q=\phi_{-(T(p)-T_0)}(p)$}, □

Remark 9: Choosing $M=\mathbb{R}\times S$ (S any manifold) with $T:\mathbb{R}\times S\to\mathbb{R}$ the natural projection, it is not difficult to prove that all the dimensions of $\mathrm{Leib}_c(M)$ permited by Theorem 8 can occur. Substracting a small neighborhood of some point, the importance of the hypothesis of completeness in *(3)* can be easily verified (even though this result is always true locally, for any FLO).

Moreover, locally, when there exists a FLO and there are r independent Killing vector fields $K_{01},\dots,K_{0r}$ in the neighborhood of some point at a hypersurface $T\equiv T_0$, then infinitely many new FLOs can be constructed, type $Z^*=Z+\Sigma_i a^i(T)K_i$, for any functions $a^1,\dots,a^r$ and K_i's as in (7). That is, as the time T varies, all the observers in Z^* can move in the direction of a spacelike Killing vector field with a speed which depends arbitrarily on T; this generalizes well-known properties of the *kinematical group*, see Ref. 5.

III. GALILEAN STRUCTURES

A. Galilean space–times

1. Galilean connections

As already commented, a Leibnizian structure has no canonical affine connection associated. Now, affine connections preserving the Leibnizian structure will be studied. The existence of such a fixed connection can be seen as a physical requirement from gauge covariance. In fact, if no connection is fixed, then all the the sections of the principal fiber bundle GM, or *Galilean reference frames*, are physically equivalent. But, in this case, physical laws as Newton's second one should be covariant under changes of Galilean reference frames. This forces the existence of a gauge field (i.e., a compatible connection) which restates covariance. Recall that general relativity can also be seen as a gauge theory, where the gauge invariance under different choices of sections in the principle fiber bundle of the orthonormal basis must be preserved. Nevertheless, in this theory the gauge field (the gravitational field) is canonically fixed as the unique torsionless connection of the bundle.

Definition 10: A Galilean connection *in a Leibnizian space–time* $(M,\Omega,\langle\cdot,\cdot\rangle)$, *is a connection* ∇ *such that its parallel transport maps Galilean bases onto Galilean bases.*

A Galilean space–time $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *is a Leibnizian space–time* $(M,\Omega,\langle\cdot,\cdot\rangle)$ *endowed with a Galilean connection* ∇.

As the connection can be reconstructed from the parallel transport, it is not difficult to check the following characterization.

Proposition 11: An affine connection ∇ *on a Leibnizian space–time* $(M,\Omega,\langle\cdot,\cdot\rangle)$ *is Galilean if and only if the following two conditions hold:*

(1) $\nabla\Omega=0$ [i.e., $\nabla_X\Omega=0, \quad \forall X\in\Gamma(TM)$].
(2) $\nabla\langle\cdot,\cdot\rangle=0$, *that is,* $X\langle V,W\rangle=\langle\nabla_X V,W\rangle+\langle V,\nabla_X W\rangle, \quad \forall X\in\Gamma(TM), \quad \forall V,W\in\Gamma(\mathrm{an}\Omega)$.

Remark 12: Item (*1*) holds if and only if $\Omega(\nabla_X Y)=X(\Omega(Y)), \ \forall Y\in\Gamma(TM)$. Thus, if $\Omega(Y)$ is constant, then $\nabla_X Y\in\Gamma(\mathrm{an}\Omega), \forall X\in\Gamma(TM)$. In particular, this happens if $Y=Z\in\mathcal{Z}(M)$ or if $Y=V,W\in\Gamma(\mathrm{an}\Omega)$; therefore, the right-hand side of item (*2*) is well defined.

Equally, a Galilean connection can be seen as a connection in the fiber bundle of the Galilean bases GM. As any principal fiber bundle, GM admits connections, but it does not admit necessarily a symmetric connection. Thus, in principle, Galilean connections are not assumed symmetric. Even more, our results on existence of Galilean connections will be mathematically clearer without this restriction. Thus, the *torsion*

$$\mathrm{Tor}(X,Y)=\nabla_X Y-\nabla_Y X-[X,Y],$$

which measures the lack of symmetry of the connection, will be relevant. The existence of a symmetric Galilean connection implies restrictions on the one-form Ω, as the following result shows.

Lemma 13: For any Galilean space–time $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$,

$$\Omega\circ\mathrm{Tor}=d\Omega. \tag{8}$$

Therefore, if there exists a symmetric Galilean connection, then $d\Omega=0$.

Proof: By using Remark 12,

$$\begin{aligned} d\Omega(X,Y)&=X(\Omega(Y))-Y(\Omega(X))-\Omega([X,Y])\\ &=\Omega(\nabla_X Y)-\Omega(\nabla_Y X)-\Omega([X,Y])\\ &=\Omega(\mathrm{Tor}(X,Y)), \quad \forall X,Y\in\Gamma(TM), \end{aligned}$$

which proves (8). □

Remark 14: If a G-structure is parallelizable, then it admits a symmetric connection (Ref. 9, Proposition 1.2), but the converse is clearly false. Nevertheless, as we will see in Sec. III B, if $d\Omega=0$, then there are symmetric connections. Thus, for Leibnizian G-structures one can say: *there exists a symmetric connection if and only if* "Ω *is parallelizable*" (i.e., locally $\Omega=dt$).

When $d\Omega\neq 0$, only "connections symmetric for a field of observers" can be defined:

Definition 15: Let $Z\in\mathcal{Z}(M)$ *be a FO, and* P^Z *its associated projection [formula (1)]. A Galilean connection is* Z-symmetric, *if*

$$P^Z\circ \mathrm{Tor}\equiv 0.$$

If $d\Omega=0$, then $\Omega\circ\mathrm{Tor}\equiv 0$ and, therefore, $P^Z\circ\mathrm{Tor}\equiv\mathrm{Tor}$; that is symmetric and Z-symmetric connections are equal. More precisely, we have the following.

Proposition 16: Let $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *be a Galilean space–time. The following assertions are equivalent:*

(1) ∇ *is symmetric.*
(2) $d\Omega=0$ *and, given any point* $p\in M$*, there exist a neighborhood* U *and a FO on* U*,* $Z\in\mathcal{Z}(U)$*, such that* ∇ *is* Z*-symmetric on* U*.*
(3) Fix any point $p\in M$*; there exists a neighborhood* U *and two FOs* Z,Z' *on* U*, which are independent at* p *and such that* ∇ *is* Z *and* Z'*-symmetric on* U*.*
(4) ∇ *is* Z*-symmetric for any FO,* $Z\in\mathcal{Z}(M)$*.*

Proof: By using Lemma 13 and the above comments, the implications $1\Rightarrow 2\Rightarrow 1\Rightarrow 4\Rightarrow 3$ are obvious. For $3\Rightarrow 2$, notice that

$$0=(P^Z-P^{Z'})\circ\mathrm{Tor}(v,w)=(Z-Z')_p\,d\Omega(v,w),\quad \forall v,w\in T_pM. \qquad \square$$

Finally, let us define the following fundamental concepts (see Sec. III A 3 for interpretations).

Definition 17: Let $Z\in\mathcal{Z}(M)$*, a FO in a Galilean space–time,* $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$*. The gravitational field induced by* ∇ *in* Z *is the vector field:*

$$\mathcal{G}=\nabla_Z Z.$$

The vorticity *or* Coriolis field *induced by* ∇ *in* Z *is the skew-symmetric two covariant tensor field* $\omega\equiv\frac{1}{2}\mathrm{rot}Z$ *defined by*

$$\omega(V,W)=\tfrac{1}{2}(\langle\nabla_V Z,W\rangle-\langle V,\nabla_W Z\rangle),\quad \forall V,W\in\Gamma(\mathrm{an}\Omega).$$

An observer $\gamma:I\to M$*,* $\Omega(\gamma')\equiv 1$*, is freely falling if it is a geodesic for* ∇*.*

Remark 18: Recall that $\Omega(\mathcal{G})=\Omega(\nabla_Z Z)=Z(\Omega(Z))=0$, that is, as the Galilean connection parallelizes Ω, the gravitational field is always spacelike.

Analogously, the definition of ω makes sense because ω is applied only on spacelike vector fields (Remark 12). In general, the *rotational* of a vector field $\mathrm{rot}X$, as in Definition 17, makes sense when $\Omega(X)$ is constant (in particular, if X is spacelike or a FO) and it is applied on pairs of spacelike tangent vectors.

2. Galilean vector fields

As for the Leibnizian case, vector fields (and, in particular, FOs) with flows preserving the Galilean structure become natural now. Recall first that, given an affine conection ∇, a vector field K with local flows preserving ∇ (i.e., $\mathcal{L}_K\nabla=0$) is called affine (Killing) and is characterized by the equality

$$[K,\nabla_Y X]=\nabla_{[K,Y]}X+\nabla_Y[K,X],\quad \forall X,Y\in\Gamma(TM) \tag{9}$$

(when K, X and Y are coordinate vector fields, this means that the Christoffel symbols are independent of the coordinate associated to K).

Definition 19: Given a Galilean structure $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$, *a vector field* $K\in\Gamma(TM)$ *is* Galilean *(Killing) if* K *is Leibnizian for* $(M,\Omega,\langle\cdot,\cdot\rangle)$ *and affine for* ∇. *If, additionally,* K *is a FO, then* K *is a* field of Galilean observers *(FGO).*

Denote by $\mathrm{Gal}(M)\equiv\mathrm{Gal}(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ the Lie algebra of all the Galilean vector fields. If $d\Omega=0$, $\mathrm{Gal}_1(M)$ will denote the affine space of all the FGOs, in agreement with the notation in Remark 5(2). Although Leibnizian vector fields might have infinite dimension, this cannot hold for the Galilean ones, which are always affine; recall that the maximum dimension for affine vector fields is $m(m+1)$. Therefore, from the classical results by Palais, the diffeomorphisms of M preserving the Galilean structure are a (finite dimensional) Lie group, and its associated algebra is the subalgebra of $\mathrm{Gal}(M)$ generated by its complete vector fields (see, for example, Ref. 10, Vol. I, Note 9). It is not difficult to find the best bound for the dimension of $\mathrm{Gal}(M)$:

Proposition 20: If $m=\dim M$, *then* $\dim(\mathrm{Gal}(M))\leqslant m(m+1)/2$.

Proof: Choose $p\in M$ and take coordinates $(t,x^1,\ldots,x^n)$ such that the corresponding set of coordinate vector fields (∂_μ) is a Galilean base at p. Each Galilean vector field $K\in\mathrm{Gal}(M)$ is determined by the values of $K^\mu(p)$ and $\partial_\nu K^\mu(p)$. (This holds for any affine vector field. The proof is analogous to the one for the Killing case in Ref. 22 p. 442-3.) Condition *3(b)* of Proposition 4 imposes $m(m-1)/2$ independent linear equations for the values of $\partial_i K^j(p)$; Condition *3(a)* fixes the values of $\partial_\nu K^0,\forall\,\nu\in\{0,1,\ldots,n\}$, that is, it imposes m independent conditions more. □

Remark 21: This bound for $\dim(\mathrm{Gal}(M))$ is the best one, as one can check in the standard example: $(\mathbb{R}^{n+1},dt^2,\langle\cdot,\cdot\rangle_0,\nabla^0)$, t being the usual projection on the first variable and $\langle\cdot,\cdot\rangle_0$ (resp. ∇^0) the usual metric on each hypersuperface (resp. usual connection).

Remarkably, the maximum dimension of $\mathrm{Gal}(M)$ is equal to the maximum dimension for the Killing vector fields of a semi-Riemannian metric on M. This was expected because, on one hand, the groups $G_m(\mathbb{R})$ and orthogonal $O_s(n+1,\mathbb{R})$ have the same dimensión and, on the other, Killing vector fields are automatically affine for the Levi-Civita connection of the semi-Riemannian metric.

Finally, we give the following consequence on gravitational and Coriolis fields (Definition 17), interesting for its classical physical interpretation.

Proposition 22: Let $Z\in\mathcal{Z}(M)$ *be a FGO of* $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$. *Then*

$$\mathcal{L}_Z\mathcal{G}(=[Z,\mathcal{G}])=0,\quad \mathcal{L}_Z\omega=0,\quad \mathcal{L}_Z\mathrm{Tor}=0.$$

If $d\Omega=0$, *then the first (resp. second, third) equality is equivalent to the following fact: for any chart* $(t,x^1,\ldots,x^n)$ *adapted to* Z, *the field* $\mathcal{G}$ *(resp.* ω, *Tor) is independent of the coordinate* t.

Proof: The first equality is a consequence of (9) with $K=X=Y=Z$. From this formula one also has

$$[Z,\nabla_X Z]=\nabla_{[Z,X]}Z. \tag{10}$$

Then, for any spacelike vector fields V,W,

$$2\mathcal{L}_Z\omega(V,W)=2(Z(\omega(V,W))-\omega([Z,V],W)-\omega(V,[Z,W]))=Z(\langle\nabla_V Z,W\rangle-\langle V,\nabla_W Z\rangle)$$
$$-\langle\nabla_{[Z,V]}Z,W\rangle+\langle[Z,V],\nabla_W Z\rangle-\langle\nabla_V Z,[Z,W]\rangle+\langle V,\nabla_{[Z,W]}Z\rangle.$$

But this expression vanishes, by using Proposition 4 [formula *3(b)*] and (10). For the torsion, we can assume that X, Y, Z, at any fixed point, commute and then

$$\mathcal{L}_Z\mathrm{Tor}(X,Y)=[Z,\nabla_X Y]-[Z,\nabla_Y X].$$

By (9), the last two terms vanish.

Finally, the last assertion is straightforward from the expressions in coordinates. □

3. Classical physical interpretations

Next, some definitions will suggest the classical interpretations for observers in $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$. For simplicity, we will consider the case $d\Omega=0$ and ∇ symmetric, but the definitions can be extended formally to the general case.

Fix a FO, $Z\in\mathcal{Z}(M)$. Denote, as usual,

$$A_Z:\mathrm{an}\Omega\to\mathrm{an}\Omega,\quad A_Z(V)=-\nabla_V Z,\quad \forall V\in\Gamma(\mathrm{an}\Omega),$$

and decompose $-A_Z$ in its symmetric $\hat{S}$ and skew-symmetric $\hat{\omega}$ parts. [The sign $-$ in the definition of A_Z is a usual convention differential geometry: A_Z is then the Weingarten endomorphism for the hypersuperficies $t\equiv\mathrm{const}$ (see, for example, Ref. 10). Nevertheless, this sign is ruled out in the decomposition.] That is,

$$-A_Z=\hat{S}+\hat{\omega}$$

where $\hat{S}$ is self-adjoint for $\langle\cdot,\cdot\rangle$, and $\hat{\omega}$ skew-adjoint. Denote by S,ω the corresponding fields of two-covariant associated tensors:

$$S(V,W)=\langle\hat{S}(V),W\rangle=\tfrac{1}{2}(\langle\nabla_V Z,W\rangle+\langle V,\nabla_W Z\rangle),$$

$$\omega(V,W)=\langle\hat{\omega}(V),W\rangle=\tfrac{1}{2}(\langle\nabla_V Z,W\rangle-\langle V,\nabla_W Z\rangle).$$

Tensor ω is, then, the vorticity or Coriolis field in Definition 17. The name ''vorticity'' means that, if Z represents the trajectories of the particles of a fluid, then ω measures how, given a fixed trajectory, the others turn around. The name ''Coriolis field'' appears because ω measures the ''lack of inerciality'' of Z due to the spinning of the observers (even though this lack of inerciality maybe intrinsic, see Remark 36). In fact, when $n=3$ and M (or, equally, anΩ) is orientable, ω can be represented by a *Coriolis vector field* C_ω in a standard way. Indeed, fix an orientation continuously at each fiber of anΩ; the metric $\langle\cdot,\cdot\rangle$ yields a standard *oriented volume element*, dv, which is a skew-symmetric three-covariant tensor. Now, define C_ω by the equality $\omega(V,W)=dv(C_\omega,V,W),\forall V,W\in\Gamma(\mathrm{an}\Omega)$. $\hat{S}$ (or, S) will be called the *intrinsic Leibnizian part of* A_Z, because of the following result.

Proposition 23: Fix $Z\in\mathcal{Z}(M)$. The endomorphism field $\hat{S}$ (and, thus, S) depends only on the Leibnizian structure $(M,\Omega,\langle\cdot,\cdot\rangle)$; thus, it is independent of the Galilean connection ∇.

Moreover, Z is Leibnizian if and only if $\hat{S}=0$.

Proof: From the definition of S (recall that we assume now Tor$=0$)

$$S(V,V)=\langle\nabla_V Z,V\rangle=(\langle[V,Z],V\rangle+\langle\nabla_Z V,V\rangle)=-\langle[Z,V],V\rangle+\tfrac{1}{2}Z\langle V,V\rangle,\tag{11}$$

and the first assertion holds. The last assertion is straightforward from (11), the third characterization in Proposition 4, and Remark 5(2). □

Now, $\hat{S}$ can be decomposed as

$$\hat{S}=\frac{\theta}{n}I+\sigma,$$

where I is the identity endomorphism, σ is the *shear*, characterized because it must be traceless, and θ is the *expansion*. So, θ measures how, with an observer fixed, neighboring observers go away on average, and σ is the deviations of this average. From Proposition 23, each observer γ in a FLO, Z, stands at a constant distance from any other observer $\overline{\gamma}$ in Z; nevertheless, depending on the Galilean connection, they may rotate when $\omega\neq 0$. Then, the gravitational field of a FLO Z

measures the forces which must be used, in order to compensate gravity and maintain a constant distance between its observers. Alternatively, Z may represent a *rigid solid*, and $\mathcal{G}$ measures gravitational tensions.

Finally, fields of inertial observers will be defined. Notice that, from a classical physical viewpoint, it is natural to assume that they are FLOs without ''rotations.'' But, under our mathematical approach, it is also natural to assume that they are FGO. Thus, we give two definitions.

Definition 24: Let $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *be a Leibnizian space–time with symmetric* ∇, *and* $Z \in \mathcal{Z}(M)$. *We will say that* Z *is a* field of inertial observers (FIO) *if* Z *is a FLO and* $\omega=0$.

In this case, the FIO Z *is* proper *if it is a FGO.*

B. Existence of Galilean connections: Fundamental theorem

Next, we determine all the Galilean connections compatible with a fixed Leibnizian structure.

Recall that, for a semi-Riemannian metric g, all the connections which parallelize g can be computed from their torsion, Tor and Koszul's formula (which determines the Levi-Civita connection, i.e., the unique one with $\mathrm{Tor}=0$). The only condition for Tor is to be a two-skew-symmetric covariant, one-contravariant tensor field, $\mathrm{Tor}\in\Lambda^2(TM,TM)$. Thus, there exists a natural bijection between the connections which parallelize g and the tensors field in $\Lambda^2(TM,TM)$.

On the contrary, formula (8) does represent an obstruction for the possible torsions associated to a Galilean connection. As a consequence, we will have to consider tensors fields in $\Lambda^2(TM,TM)$ under a restriction type (8). In addition, we will need so many new parameters as restrictions in (8). As we will see, gravitational and Coriolis fields will be these new parameters.

Our study will be carried out in two steps. In the first one (Sec. III B 1) we will see how, given a Galilean structure and fixed Z, the values of $\mathcal{G}$, ω and Tor fix the Galilean connection. In the second step (Sec. III B 2) we will see how, given a Leibnizian structure and fixed Z, the permitted values of $\mathcal{G}$, ω and Tor are in bijective correspondence with the space of all the Galilean connections.

1. Formula "à la Koszul"

Our aim is to prove formula (13), which plays a role similar to the Koszul formula in semi-Riemannian geometry. Our next result is, then, the ''fundamental lemma of the Galilean geometry'' (compare, for example, with Ref. 19, Vol. IV, Chap. 6). As in previous notation, put, for any Galilean connection ∇,

$$A(X,Y)=\mathrm{Tor}(X,Y)+[X,Y]=\nabla_X Y-\nabla_Y X, \qquad \forall X,Y\in\Gamma(TM). \tag{12}$$

That is, A is two times the skew-symmetric part of ∇, and it depends just on its torsion. Notice that $A(Z,W)\in\Gamma(\mathrm{an}\Omega)$, $\forall Z\in\mathcal{Z}(M),\forall W\in\Gamma(\mathrm{an}\Omega)$ and $A(W_1,W_2)\in\Gamma(\mathrm{an}\Omega)$, $\forall W_1,W_2\in\Gamma(\mathrm{an}\Omega)$.

Lemma 25: Let $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *be a Galilean space–time, and* $Z\in\mathcal{Z}(M)$ *a FO with gravitational field* $\mathcal{G}$ *and Coriolis* ω. *Then,* ∇ *satisfies the following formula:*

$$\begin{aligned}2\langle P^Z(\nabla_X Y),V\rangle=&X\langle P^Z(Y),V\rangle+Y\langle P^Z(X),V\rangle-V\langle P^Z(X),P^Z(Y)\rangle+2(\Omega(X)\,\Omega(Y)\langle\mathcal{G},V\rangle\\&+\Omega(X)\,\omega(P^Z(Y),V)+\Omega(Y)\,\omega(P^Z(X),V))+\Omega(X)(\langle A(Z,P^Z(Y)),V\rangle\\&-\langle A(Z,V),P^Z(Y)\rangle)-\Omega(Y)(\langle A(Z,P^Z(X)),V\rangle+\langle A(Z,V),P^Z(X)\rangle)\\&+\langle A(P^Z(X),P^Z(Y)),V\rangle-\langle A(P^Z(Y),V),P^Z(X)\rangle-\langle A(P^Z(X),V),P^Z(Y)\rangle,\end{aligned} \tag{13}$$

where $X,Y\in\Gamma(TM)$ *and* $V\in\Gamma(\mathrm{an}\Omega)$ *is any spacelike vector field.*

Proof: From the cyclic identities,

$$V\langle P^Z(X),P^Z(Y)\rangle=\langle\nabla_V P^Z(X),P^Z(Y)\rangle+\langle P^Z(X),\nabla_V P^Z(Y)\rangle, \tag{14}$$

$$P^Z(X)\langle P^Z(Y),V\rangle=\langle\nabla_{P^Z(X)}P^Z(Y),V\rangle+\langle P^Z(Y),\nabla_{P^Z(X)}V\rangle, \tag{15}$$

$$P^Z(Y)\langle V, P^Z(X)\rangle = \langle \nabla_{P^Z(Y)} V, P^Z(X)\rangle + \langle V, \nabla_{P^Z(Y)} P^Z(X)\rangle, \tag{16}$$

compute (15)+(16)−(14) to obtain

$$\begin{aligned}\langle \nabla_{P^Z(X)} P^Z(Y) + \nabla_{P^Z(Y)} P^Z(X), V\rangle = {} & P^Z(X)\langle P^Z(Y), V\rangle + P^Z(Y)\langle V, P^Z(X)\rangle - V\langle P^Z(X), P^Z(Y)\rangle \\ & - \langle A(P^Z(Y), V), P^Z(X)\rangle - \langle A(P^Z(X), V), P^Z(Y)\rangle. \end{aligned}\tag{17}$$

On the other hand, using (1) and (12),

$$\begin{aligned} 2\langle \nabla_X P^Z(Y), V\rangle &= 2\langle \nabla_{P^Z(X)} P^Z(Y), V\rangle + 2\,\Omega(X)\langle \nabla_Z P^Z(Y), V\rangle \\ &= \langle \nabla_{P^Z(X)} P^Z(Y), V\rangle + \langle \nabla_{P^Z(Y)} P^Z(X), V\rangle + \langle A(P^Z(X), P^Z(Y)), V\rangle \\ &\quad + 2\,\Omega(X)\langle \nabla_Z P^Z(Y), V\rangle. \end{aligned}\tag{18}$$

Substituing (17) in (18),

$$\begin{aligned} 2\langle \nabla_X P^Z(Y), V\rangle = {} & P^Z(X)\langle P^Z(Y), V\rangle + P^Z(Y)\langle V, P^Z(X)\rangle - V\langle P^Z(X), P^Z(Y)\rangle \\ & - \langle A(P^Z(Y), V), P^Z(X)\rangle - \langle A(P^Z(X), V), P^Z(Y)\rangle + \langle A(P^Z(X), P^Z(Y)), V\rangle \\ & + 2\,\Omega(X)\langle \nabla_Z P^Z(Y), V\rangle. \end{aligned}\tag{19}$$

Substituting also, in the two first terms on the right-hand side of (19), the values of $P^Z(X), P^Z(Y)$ by its expresion (1),

$$\begin{aligned} 2\langle \nabla_X P^Z(Y), V\rangle = {} & \Omega(X)\langle \nabla_Z P^Z(Y), V\rangle - \Omega(X)\langle P^Z(Y), \nabla_Z V\rangle - \Omega(Y)\langle \nabla_Z V, P^Z(X)\rangle \\ & - \Omega(Y)\langle V, \nabla_{P^Z(X)} Z\rangle - \Omega(Y)\langle V, A(Z, P^Z(X))\rangle + \{\text{Koszul}\}, \end{aligned}\tag{20}$$

where

$$\begin{aligned} \{\text{Koszul}\} = {} & X\langle P^Z(Y), V\rangle + Y\langle V, P^Z(X)\rangle - V\langle P^Z(X), P^Z(Y)\rangle + \langle A(P^Z(X), P^Z(Y)), V\rangle \\ & - \langle A(P^Z(Y), V), P^Z(X)\rangle - \langle A(P^Z(X), V), P^Z(Y)\rangle. \end{aligned}$$

But, using $\nabla_X(\Omega(Y)Z) = \Omega(\nabla_X Y)Z + \Omega(Y)(\Omega(X)\nabla_Z Z + \nabla_{P^Z(X)} Z)$, one has

$$\begin{aligned} P^Z(\nabla_X Y) = \nabla_X Y - \Omega(\nabla_X Y)Z &= \nabla_X(\Omega(Y)Z) + \nabla_X P^Z(Y) - \Omega(\nabla_X Y)Z \\ &= \Omega(X)\Omega(Y)\mathcal{G} + \Omega(Y)\nabla_{P^Z(X)} Z + \nabla_X P^Z(Y). \end{aligned}\tag{21}$$

Thus, substitute (20) in (21):

$$\begin{aligned} 2\langle P^Z(\nabla_X Y), V\rangle = {} & 2\,\Omega(X)\,\Omega(Y)\langle \mathcal{G}, V\rangle + \Omega(Y)\langle \nabla_{P^Z(X)} Z, V\rangle + \Omega(X)\langle \nabla_{P^Z(Y)} Z, V\rangle \\ & + \Omega(X)\langle A(Z, P^Z(Y)), V\rangle - \Omega(X)\langle P^Z(Y), \nabla_V Z\rangle - \Omega(X)\langle P^Z(Y), A(Z, V)\rangle \\ & - \Omega(Y)\langle \nabla_V Z, P^Z(X)\rangle - \Omega(Y)\langle A(Z, V), P^Z(X)\rangle - \Omega(Y)\langle V, A(Z, P^Z(X))\rangle \\ & + \{\text{Koszul}\} \\ = {} & 2\,\Omega(X)\,\Omega(Y)\langle \mathcal{G}, V\rangle + 2\,\Omega(X)\,\omega(P^Z(Y), V) + 2\,\Omega(Y)\,\omega(P^Z(X), V) \\ & + \Omega(X)(\langle A(Z, P^Z(Y)), V\rangle - \langle A(Z, V), P^Z(Y)\rangle) - \Omega(Y)(\langle A(Z, P^Z(X)), V\rangle \\ & + \langle A(Z, V), P^Z(X)\rangle) + \{\text{Koszul}\}, \end{aligned}$$

as required. □

Remark 26: As $\nabla_X Y = P^Z(\nabla_X Y) + X(\Omega(Y))Z$, *formula (13) permits us to reconstruct* ∇ *from* $\Omega, \langle\cdot,\cdot\rangle$, Tor, *and the values of* $\mathcal{G}, \omega$ *associated to* Z.

2. Natural bijection

Let us see how, for fixed FO, formula (13) determines all the Galilean connections of a Leibnizian space–time. As in previous notation, let (i) $\Lambda^2(\mathrm{an}\Omega)$ be the vector space of all the two-covariant skew-symmetric tensors defined on spacelike vectors [that is, $\vartheta\in\Lambda^2(\mathrm{an}\Omega)$, if and only if, $\vartheta:\mathrm{an}\Omega\times\mathrm{an}\Omega\to C^\infty(M)$, ϑ is $C^\infty(M)$–bilinear and skew-symmetric] and (ii) $\Lambda^2(TM,\mathrm{an}\Omega)$ be the vector space of all the two-covariant skew-symmetric tensors, one-contravariant spacelike valued [that is, $\Theta\in\Lambda^2(TM,\mathrm{an}\Omega)$, if and only if, $\Theta:\Gamma(TM)\times\Gamma(TM)\to\Gamma(\mathrm{an}\Omega)$, Θ is $C^\infty(M)$–bilinear and skew-symmetric].

Theorem 27: *Given a Leibnizian space–time* $(M,\Omega,\langle\cdot,\cdot\rangle)$, *let* $\mathcal{D}(\Omega,\langle\cdot,\cdot\rangle)$ *be the set of all its Galilean connections. For fixed FO, Z, the map,* $D^Z:\mathcal{D}(\Omega,\langle\cdot,\cdot\rangle)\to\Gamma(\mathrm{an}\Omega)\times\Lambda^2(\mathrm{an}\Omega)\times\Lambda^2(TM,\mathrm{an}\Omega)$, *given by*

$$D^Z(\nabla)=(\mathcal{G}(\equiv\nabla_Z Z),\ \omega(\equiv\tfrac{1}{2}\mathrm{rot}Z),\ P^Z\circ\mathrm{Tor}),\qquad\forall\nabla\in\mathcal{D}(\Omega,\langle\cdot,\cdot\rangle),$$

is one-to-one and onto.

Proof: Obviously, this map is well-defined. Let us prove that it is one-to-one. By using (8) and (12)

$$P^Z\circ\mathrm{Tor}=A(\cdot,\cdot)-d\,\Omega(\cdot,\cdot)Z-[\cdot,\cdot]\tag{22}$$

and

$$D^Z(\tilde{\nabla})=D^Z(\nabla)\Rightarrow\tilde{\mathcal{G}}=\mathcal{G},\quad\tilde{\omega}=\omega,\quad\tilde{A}=A.$$

Thus, from formula (13),

$$\langle P^Z(\tilde{\nabla}_X Y)-P^Z(\nabla_X Y),V\rangle=0,\qquad\forall X,Y\in\Gamma(TM),\forall V\in\Gamma(\mathrm{an}\Omega)\Rightarrow\tilde{\nabla}_X Y-\nabla_X Y=P^Z(\tilde{\nabla}_X Y)-P^Z(\nabla_X Y)=0,\qquad\forall X,Y\in\Gamma(TM),$$

as required.

In order to check that D^Z is onto, fix $\mathcal{G}\in\mathrm{an}\Omega$, $\omega\in\Lambda^2(\mathrm{an}\Omega)$ and $\Theta\in\Lambda^2(TM,\mathrm{an}\Omega)$. Taking into account (22), define

$$A(X,Y)=\Theta(X,Y)+d\,\Omega(X,Y)Z+[X,Y],\qquad\forall X,Y\in\Gamma(TM).$$

Then

$$\Omega(A(X,Y))=d\,\Omega(X,Y)+\Omega([X,Y])=X(\Omega(Y))-Y(\Omega(X)),$$

and $A(Z,W)\in\Gamma(\mathrm{an}\Omega)$, $\forall W\in\Gamma(\mathrm{an}\Omega)$, $A(W_1,W_2)\in\Gamma(\mathrm{an}\Omega)$, $\forall W_1,W_2\in\Gamma(\mathrm{an}\Omega)$. As a consequence, there exists an unique map $\Pi:\Gamma(TM)\times\Gamma(TM)\to\Gamma(\mathrm{an}\Omega)$, such that

$$2\,\langle\Pi(X,Y),V\rangle,\qquad\forall X,Y\in\Gamma(TM),\forall V\in\Gamma(\mathrm{an}\Omega),$$

satisfies formula (13) for previously fixed $\mathcal{G}$, ω and A. Define then

$$\nabla_X Y=X(\Omega(Y))Z+\Pi(X,Y),\qquad\forall X,Y\in\Gamma(TM).$$

A straightforward computation shows that the so-defined ∇ is a Galilean connection, with $D^Z(\nabla)$ equal to the initial $(\mathcal{G},\omega,\Theta)$. □

According to this theorem, there exists a canonical way to construct a Galilean connection from $Z\in\mathcal{Z}(M)$, and a gravitational and Coriolis field: the unique ∇ such that $D^Z(\nabla)=(\mathcal{G},\omega,0)$. If, additionally, the space–time satisfies $d\Omega=0$, we can consider only symmetric connections, that is, as in the following.

Corollary 28: Let $(M,\Omega,\langle\cdot,\cdot\rangle)$ *be a Leibnizian space–time, and fix* $Z\in\mathcal{Z}(M)$. *The set of all the Z-symmetric Galilean connections is mapped bijectively onto the set of all the possible gravitational* $\mathcal{G}\in\Gamma(\mathrm{an}\Omega)$ *and Coriolis* $\omega\in\Lambda^2(\mathrm{an}\Omega)$ *fields.*

In particular, if $d\Omega=0$, *then the set of all the symmetric Galilean connections is also mapped bijectively onto* $\Gamma(\mathrm{an}\Omega)\times\Lambda^2(\mathrm{an}\Omega)$.

Notice also that, when $d\Omega=0$, if nonsymmetric connections are considered, then Theorem 27 can be rewritten putting Tor instead of $P^Z\circ\mathrm{Tor}$.

Remark 29: (1) It is well-known that the set of all the affine connections on a manifold M has a natural structure of affine space, the associated vector space being the one of all the two-covariant, one-contravariant tensors fields. As commented at the beginning of this section, if a semi-Riemannian metric g is fixed, the set of all the connections parallelizing g has a natural structure of vector space (the Levi-Civita connection would play the role of vector 0), isomorphic to the vector space of all the possible torsions, i.e., the space $\Lambda^2(TM,TM)$. Recall that $\Lambda^2(TM,TM)$ is a vector fiber bundle, with fiber of dimension $m^2(m-1)/2$. Theorem 27 shows that, for fixed Z, the space $\mathcal{D}(\Omega,\langle\cdot,\cdot\rangle)$ admits a natural structure of vector space (the Z-symmetric connection with null gravitational and Coriolis fields would play the role of vector 0), isomorphic to the vector space $\Gamma(\mathrm{an}\Omega)\times\Lambda^2(\mathrm{an}\Omega)\times\Lambda^2(TM,\mathrm{an}\Omega)$. Recall that this vector space is also a vector fiber bundle, with fiber of equal dimension $n+n(n-1)/2+n^2(n+1)/2=m^2(m-1)/2$.

(2) Corollary 28 can be seen as an improved version of Ref. 11, Theorem 7. In fact, this result asserts that the degrees of freedom for the symmetric Galilean connections can be put in one-to-one correspondence with the set $\Lambda^2(TM)$ of all two-forms on M. Thus, we obtain not only the further splitting of such two forms in $\mathcal{G}$ and ω but also the more precise associated physical interpretations, which are developed in the remainder of the article.

C. Formulas for the connection, geodesics and curvature

Next, we will give explicit formulas in coordinates for the different geometric elements (Christoffel symbols, geodesics, curvature) associated to a Galilean connection. By using Lemma 25, these formulas can be given in terms of the Leibnizian estructure, and the fields $\mathcal{G}$, ω, Tor. For simplicity, we will assume that the connection is symmetric and, thus, $d\Omega=0$, but it is not difficult to give general expressions (see the computations following Remark 33).

Thus, fix $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ with a symmetric ∇, and a FO, $Z\in\mathcal{Z}(M)$. Let $(t,x^1,\ldots,x^n)$ be a chart adapted to Z as in Proposition 2, and let $\mathcal{G}^k$ (resp. ω_{ij}) be the components of the gravitational field $\mathcal{G}$ (resp. Coriolis field ω) for Z. Let $(h^{kl})_{n\times n}$, be the smooth local functions obtained from the inverse of the matrix $(h_{ij}=\langle\partial_i,\partial_j\rangle)_{n\times n}$ at each point. Indices will be raised as usual, thus $\omega_i^k(=\omega_i{}^k)=\Sigma_l\omega_{il}h^{kl}$.

Theorem 30: *The Christoffel symbols of* ∇ *in any chart adapted to* $Z\in\mathcal{Z}(M)$ *are*

$$\Gamma^0_{\mu\nu}=0,\quad \Gamma^k_{00}=\mathcal{G}^k,\quad \Gamma^k_{i0}=\omega_i^k+\frac{1}{2}\sum_{l=1}^{n}h^{kl}\frac{\partial h_{il}}{\partial t},$$

$\forall\,\mu,\nu\in\{0,1,\ldots,n\}$, $\forall\,i,k\in\{1,\ldots,n\}$, *the remainder being equal to the symbols for the hypersurfaces* $t\equiv\mathrm{const}$ *with the induced metric, i.e.,*

$$\Gamma^k_{ij}=\frac{1}{2}\sum_{l=1}^{n}h^{kl}\left(\frac{\partial h_{il}}{\partial x^j}+\frac{\partial h_{jl}}{\partial x^i}-\frac{\partial h_{ij}}{\partial x^l}\right),\qquad \forall\,i,j,k\in\{1,\ldots,n\}.$$

As a consequence, for any freely falling observer $\gamma:I\to M$ *(Definition 17), the following equations of the motion hold, putting* $\gamma^i=x^i\circ\gamma$:

$$\frac{d^2\gamma^k}{dt^2}+\frac{1}{2}\sum_{i,j,l=1}^{n}(h^{kl}\circ\gamma)\left(\frac{\partial h_{il}}{\partial x^j}+\frac{\partial h_{jl}}{\partial x^i}-\frac{\partial h_{ij}}{\partial x^l}\right)\circ\gamma\cdot\frac{d\gamma^i}{dt}\frac{d\gamma^j}{dt}$$

$$=-\mathcal{G}^k\circ\gamma-\sum_{i,l=1}^{n}(h^{kl}\circ\gamma)\left(\frac{\partial h_{il}}{\partial t}\circ\gamma\right)\frac{d\gamma^i}{dt}-2\sum_{i=1}^{n}(\omega_i^k\circ\gamma)\frac{d\gamma^i}{dt}, \tag{23}$$

for all $k\in\{1,\ldots,n\}$.

Proof: From Remark 26, one has $\Gamma^0_{\mu\nu}=0$. For the remainder, just apply formula (13) with $P^Z(\partial_i)=\partial_i$ and $A(\partial_\mu,\partial_\nu)=0$, [recall that $A(X,Y)=[X,Y]$, $\forall X,Y\in\Gamma(TM)$, because of the symmetry of ∇]. □

Notice that, if h_{ij} is independent of t (i.e., Z is a FLO, Proposition 6), the left-hand side of (23) yields the acceleration of the curve obtained as the projection of γ in a hypersurface $t\equiv$const (acceleration computed with the metric $\langle\cdot,\cdot\rangle$ on this hypersurface). Denote this left-hand side as $D^h(\gamma^k)'/dt$. On the other hand, recall that Z is an affine vector field if and only if

$$\partial_t\Gamma^\rho_{\mu\nu}=0,$$

for all μ, ν, ρ. Thus, the following characterization of a previously defined field of observers is straightforward (see also Propositions 6 and 22).

Corollary 31: Let $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *be a Galilean space–time with symmetric* ∇, *and* $Z\in\mathcal{Z}(M)$. *Then, in the domain of any chart adapted to* Z,

(1) Z *is a FLO if and only if* $\partial_t h_{ij}=0$.

In this case, $\Gamma^k_{i0}=\omega_i^k$ *and, for freely falling observers,*

$$\frac{D^h(\gamma^k)'}{dt}=-\mathcal{G}^k\circ\gamma-2\sum_{i}^{n}(\omega_i^k\circ\gamma)\frac{d\gamma^i}{dt}. \tag{24}$$

(2) Z *is a FGO if and only if* $\partial_t h_{ij}=\partial_t\omega_{ij}=\partial_t\mathcal{G}^k=0$.

In this case, (24) holds with $\mathcal{G}^k=\mathcal{G}^k(x^1,\ldots,x^n),\omega_i^k=\omega_i^k(x^1,\ldots,x^n)$.

(3) Z *is a FIO if and only if* $\partial_t h_{ij}=0,\omega_{ij}=0$.

In this case, $\Gamma^k_{i0}=0$ *and, for freely falling observers,*

$$\frac{D^h(\gamma^k)'}{dt}=-\mathcal{G}^k\circ\gamma. \tag{25}$$

(4) Z *is a proper FIO if and only if* $\partial_t h_{ij}=\partial_t\mathcal{G}^k=0,\omega_{ij}=0$.

In this case, (25) holds with $\mathcal{G}^k=\mathcal{G}^k(x^1,\ldots,x^n)$.

From the Christoffel symbols one can readily compute the curvature tensor R (we will follow the convention of sign $R(X,Y)=[\nabla_X,\nabla_Y]-\nabla_{[X,Y]}$). As

$$\Omega(R(X,Y)Q)=0,\ \forall X,Y,Q\in\Gamma(M), \tag{26}$$

the operator R is spacelike-valued; moreover,

$$\langle V,R(X,Y)W\rangle=-\langle R(X,Y)V,W\rangle,\quad \forall X,Y\in\Gamma(TM),\forall V,W\in\mathrm{an}\Omega \tag{27}$$

[notice that (26) and (27) are also valid if ∇ is not symmetric]. Recall that, in a Galilean space–time, neither the four-covariant curvature tensor nor the scalar curvature make sense, but the Ricci tensor, Ric, does make sense. For each Riemanian hypersurface $t\equiv$const, the symbol ∇^h will denote the Levi-Civita connection (as well as the gradient), and the corresponding curvature and Ricci tensors (defined on spacelike vectors) will be R^h, Ric^h, resp. If $R^h\equiv 0$, we will say that the space $(\mathrm{an}\Omega,\langle\cdot,\cdot\rangle)$ is flat. In this case, if Z is a FLO, we can assume that the spacelike coordinates are parallel, i.e., $\Gamma^k_{ij}\equiv 0$ (see Proposition 35 for a general result).

Corollary 32: Given a Galilean space–time $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *with symmetric* ∇*, for any chart adapted to* $Z\in\mathcal{Z}(M)$ *we have the following.*

(1) $R(\partial_i,\partial_j)\partial_k=R^h(\partial_i,\partial_j)\partial_k$ *and* $\mathrm{Ric}(\partial_i,\partial_j)=\mathrm{Ric}^h(\partial_i,\partial_j)$.

(2) If Z is a FLO, $R(\partial_i,\partial_t)\partial_t=\nabla^h_{\partial_i}\mathcal{G}-\Sigma_k(\partial_t\omega^k_i+\Sigma_l\omega^l_i\omega^k_l)\partial_k$. *[In particular, if Z is a FIO,* $R(\partial_i,\partial_t)\partial_t=\nabla^h_{\partial_i}\mathcal{G}$.*]*

Moreover, $\mathrm{Ric}(\partial_t,\partial_t)=\mathrm{div}^h\mathcal{G}+\|\omega\|^2$, *where* div^h *denotes the divergence with respect to* $\langle\cdot,\cdot\rangle$ *in the corresponding hypersurface* $t\equiv\mathrm{const}$, *and* $\|\omega\|^2=-\Sigma_{i,j}\omega^i_j\omega^j_i$. *[In particular, if Z is a FIO,* $\mathrm{Ric}(\partial_t,\partial_t)=\mathrm{div}^h\mathcal{G}$.*]*

(3) If Z is a FLO, $R(\partial_t,\partial_i)\partial_j=\Sigma_k(-\partial_i\omega^k_j+\Sigma_l(\Gamma^l_{ij}\omega^k_l-\Gamma^k_{il}\omega^l_j))\partial_k$.

In particular, (a) if Z is a FIO, then $R(\partial_t,\partial_i)\partial_j=0$, *and (b) if the space is flat, and parallel spacelike coordinates are taken,* $R(\partial_t,\partial_i)\partial_j=-\Sigma_k\partial_i\omega^k_j\partial_k$.

(4) If Z is a FLO, $R(\partial_i,\partial_j)\partial_t=\Sigma_k(\partial_i\omega^k_j-\partial_j\omega^k_i+\Sigma_l(\Gamma^k_{il}\omega^l_j-\Gamma^k_{jl}\omega^l_i))\partial_k$.

In particular, (a) if Z is a FIO, then $R(\partial_i,\partial_j)\partial_t=0$, *and (b) if the space is flat, and parallel spacelike coordinates are taken,* $R(\partial_i,\partial_j)\partial_t=\Sigma_k(\partial_i\omega^k_j-\partial_j\omega^k_i)\partial_k$.

Remark 33: Item (*1*) makes it natural to define the *sectional curvature* of a tangent plane included in an absolute space $\pi_p\subset\mathrm{an}\Omega_p$ as the curvature of π_p for the hypersurface $T\equiv T(p)$ endowed with the Riemannian metric $\langle\cdot,\cdot\rangle$, i.e., $K(\pi_p)=\langle R^h(v,w)w,v\rangle$, where v,w is any orthonormal base of π_p. If $\pi_p\subset T_pM$ does not lie in the absolute space $\mathrm{an}\Omega_p$, we can define:

$$K(\pi_p)=\langle R(v,Z_p)Z_p,v\rangle,$$

where v is any unit vector of $\pi_p\cap\mathrm{an}\Omega_p$ and $Z_p\in\pi_p$ satisfies $\Omega(Z_p)=1$. Thus, from a purely geometrical viewpoint, a rich ''sub-Riemannian'' geometry is introduced in this way, with interest on its own (compare with Ref. 20).

Alternatively, it is not difficult to study the curvature tensor by means of moving frames *à la Cartan*. For the sake of completeness, we sketch the structural equations. Locally, fix a field of observers Z and an orthonormal base of vector fields $E_1,\ldots,E_n$ of $\mathrm{an}\Omega$, and consider the dual base $(\Omega,\varphi^1,\ldots,\varphi^n)$ of $(E_0=Z,E_1,\ldots,E_n)$, plus the one-forms $\varphi^i{}_\rho$:

$$\varphi^i{}_\rho(X)=\varphi^i(\nabla_X E_\rho),\qquad \forall i\in\{1,\ldots,n\},\ \forall\rho\in\{0,1,\ldots,n\},\ \forall X\in\Gamma(TM).$$

Then, a straightforward computation shows the following three properties, valid even if ∇ is not symmetric:

(1) The curvature tensor

$$R(X,Y)E_\rho=\sum_{k=1}^{n}\Upsilon^k{}_\rho(X,Y)E_k$$

is univocally determined by the *second structural equation:*

$$\Upsilon^k{}_\rho=d\,\varphi^k{}_\rho+\sum_{l=1}^{k}\varphi^k{}_l\wedge\varphi^l{}_\rho,\qquad \forall k\in\{1,\ldots,n\},\ \forall\rho\in\{0,1,\ldots,n\}.$$

(2) For the gravitational and Coriolis fields $\mathcal{G}$, ω of the FO, Z, the one-forms $\varphi^i{}_0$ satisfy

$$2P^{Z^*}\omega=P^{Z^*}\mathcal{G}^\flat\wedge\Omega+\sum_{k=1}^{n}\varphi^k{}_0\wedge\varphi^k,$$

where $\mathcal{G}^\flat(V)=\langle\mathcal{G},V\rangle$, for all $V\in\mathrm{an}\Omega$.

(3) $\Upsilon^j{}_i=-\Upsilon^i{}_j$ and $\varphi^j{}_i=-\varphi^i{}_j$, for all $i,j\in\{1,\ldots,n\}$.

Therefore, if ∇ is Z-symmetric, the *connection one-forms* $\varphi^i{}_\rho$, are the unique one-forms satisfying the *first structural equation:*

$$2P^{Z^*}\omega = P^{Z^*}\mathcal{G}^\flat \wedge \Omega + \sum_{k=1}^{n} \varphi^k{}_0 \wedge \varphi^k,$$

$$d\,\varphi^i = -\varphi^i{}_0 \wedge \Omega - \sum_{k=1}^{n} \varphi^i{}_k \wedge \varphi^k,$$

plus the skew-symmetry relations $\varphi^j{}_i = -\varphi^i{}_j$.

IV. NEWTONIAN STRUCTURES

A. Newtonian space–times

As a difference with most previous references, our definition of Newtonian space–time is independent of hypotheses at infinity, i.e., it would be locally testable.

Definition 34: A Galilean space–time $(M,\Omega,\langle\cdot,\cdot\rangle,\nabla)$ *with symmetric* ∇ *is* Newtonian *if its space is flat and it admits a FIO.*

In this case, the Newtonian space–time will be proper *if some of its FIOs are proper.*

Now, it is natural to wonder: (a) which hypotheses imply the existence of a FIO? and (b) under these hypotheses, how many FIO's exist? In order to answer (a), we will assume for simplicity some global hypotheses, as the existence of a function absolute time T.

Proposition 35: Let $(M,dT,\langle\cdot,\cdot\rangle,\nabla)$ *be a Galilean space–time with* ∇ *symmetric and geodesically complete. Assume that each hypersurface* $T\equiv$const *is flat and simply connected. Then we have the following.*

(1) There exist a FLO, Z*, and the Leibnizian structure* $(M,dT,\langle\cdot,\cdot\rangle)$ *isomorphic to the standard one* $(\mathbb{R}^{n+1},dt,\langle\cdot,\cdot\rangle_0)$ [*with* $\langle\cdot,\cdot\rangle_0=\Sigma_{i=1}^n(dx^i)^2$ *and* $(t,x^1,\ldots,x^n)$ *the usual coordinates of* $\mathbb{R}^{n+1}$], *being identifiable under the isomorphism* $T\equiv t, Z\equiv\partial_t$.

(2) For fixed FLO Z *with vorticity* ω*, there exists a FIO (and, then, the space–time is Newtonian) if and only if there exists a spacelike vector field* $A\in\Gamma(\mathrm{an}\Omega)$ *such that* $2\omega=\mathrm{rot}A$.

Equally, under the identification with $(\mathbb{R}^{n+1},dt,\langle\cdot,\cdot\rangle_0)$*, there exists a FIO if and only if there exist* n *functions* $a^i:\mathbb{R}^{n+1}\to\mathbb{R}$ *such that* $2\omega_{ji}(\equiv 2\omega^i_j)=\partial_j a^i-\partial_i a^j$.

(3) If there exists a FLO, Z*, with vorticity* ω *depending only on* T $(\partial_i\omega_{jk}\equiv 0)$*, then there exists a FIO.*

Proof: Recall first that $\Omega(\beta')$ is a constant c_β for any geodesic β. Taking β with $c_\beta\neq 0$, the range of T must be all $\mathbb{R}$. By using geodesics with $c_\beta=0$, each hypersurface $T\equiv$const must be isommetric to $\mathbb{R}^n$.

(1) The flow ϕ_s of Z can be defined directly as follows. Fix any geodesic $\gamma(s)$ parametrized by T, i.e., $T\circ\gamma(s)=s,\forall s\in\mathbb{R}$. For each $p\in M$, take the unique spacelike geodesic $\alpha:[0,1]\to T^{-1}(T(p))$ connecting $\gamma(T(p))$ with p. Let $v_s, s\in\mathbb{R}$, be the vector field along γ obtained by parallel transport of $\alpha'(0)$ along γ, from $\gamma(T(p))$ to $\gamma(T(p)+s)$. If α_s^* is the geodesic with initial velocity v_s, define $\phi_s(p)=\alpha_s^*(1)$. It is straightforward to check that the infinitesimal generator Z of ϕ_s is a FLO and, fixing an orthonormal base of the absolute space at $\gamma(0)$, the isomorphism with the standard Leibnizian structure is straightforward.

(2) Fix the FLO Z. Put $\overline{Z}=Z-A$, where, using the isomorphism of item *(1)*, $A=\Sigma_k a^k\partial_k$ for some functions a^k on $\mathbb{R}^{n+1}$. Easily, $\mathrm{rot}\overline{Z}(\partial_i,\partial_j)=2\omega_{ij}-\partial_i a^j+\partial_j a^i$, and the result follows.

(3) Use item *(2)* with $a^j=-\Sigma_k\omega_{jk}x^k$. □

Remark 36: (1) For all Newtonian space–times the Leibnizian structure must be locally isomorphic to the standard one on $\mathbb{R}^m$. For the sake of simplicity, we will assume from now on that this standard Leibnizian structure underlies globally on any Newtonian space–time.

(2) From item *(2)* it is clear that if, for some indexes i,j,k, one has $\partial_i\omega_{jk}+\partial_k\omega_{ij}+\partial_j\omega_{ki}\neq 0$, ($\omega$ is not "spatially closed"), then there are no FIOs. Notice that, when Z is a FLO but not a FIO, (i) if the space–time is Newtonian (i.e., there exists a FIO), then ω represents "inertial (Coriolis) forces," (ii) otherwise, ω represents "true" gravitational forces (which cannot be "gauged away").

(3) An alternative formulation of Definition 34 is to impose the "gyroscope principle:" $R(X,Y)V=0$ whenever V is spacelike [see, for example, Ref. 13, Box 12.4, Axiom (3); and Ref. 14, Def. 1.1, Axiom 5]. In this case, Corollary 32(*1*) implies that the space is flat and Corollary 32(*4*) plus Proposition 35(*3*) implies the existence of a FIO.

Next, we will focus on the question (b) at the beginning of this section. Recall first the following straighforward result.

Lemma 37: Let $(\mathbb{R}^{n+1},dt,\langle\cdot,\cdot\rangle_0,\nabla)$ *be a Newtonian space–time and fix a FIO,* $Z\in\mathcal{Z}(M)$. *Consider a generic FO,* $\overline{Z}=Z+\Sigma_i a^i\partial_i$ *for some functions* a^i *on* $\mathbb{R}^{n+1}$.

(1) The relation between the gravitational fields $\mathcal{G},\overline{\mathcal{G}}$ *of* Z, $\overline{Z}$ is

$$\overline{\mathcal{G}}=\mathcal{G}+\sum_{i=1}^{n}\partial_t a^i\partial_i+\sum_{i,j=1}^{n}(a^i\partial_i a^j)\partial_j. \tag{28}$$

(2) $\overline{Z}$ *is a FIO if and only if the* a^i*'s are independent of* x, $a^i\equiv a^i(t)$, *and, thus,*

$$\overline{\mathcal{G}}=\mathcal{G}+(a^i)'(t)\partial_i. \tag{29}$$

(3) If Z *and* $\overline{Z}$ *are proper FIOs then (28) and (29) hold with constant derivatives* $(a^i)'$, *for all* i.

Therefore, if Z is a FIO, then $\overline{Z}=Z+\Sigma_i a^i(t)\partial_i$ is a FIO for any $a^i(t)$, and the FIOs have infinite dimension. If Z is proper, $\overline{Z}$ will be proper if and only if $a^i(t)=\alpha_1^i\cdot t+\alpha_0^i$ for some constants α_1^i,α_0^i. And if Z and $\overline{Z}$ are FIOs (proper or not) with the same gravitational field, then $a^i(t)\equiv\alpha_0^i$ for all i. Summing up, we have the following.

Theorem 38: *Let* $(\mathbb{R}^{n+1},dt,\langle\cdot,\cdot\rangle_0,\nabla)$ *be a Newtonian space–time.*

(1) The set of all the FIOs is an affine space of infinite dimension.
(2) If the Newtonian space–time is proper, proper FIOs are a $2n$*-dimensional subspace.*
(3) For fixed FIO, Z, *with gravitational field* $\mathcal{G}$, *the set* $FIO(\mathcal{G})=\{\overline{Z}\in\mathcal{Z}(M)|\overline{Z}$ *is a FIO and* $\overline{\mathcal{G}}=\mathcal{G}\}$ *is an* n*-dimensional subspace.*

Remark 39: (1) When Z is a proper FIO, one can also put $\mathrm{FIO}(\mathcal{G})=\{\overline{Z}\in\mathcal{Z}(M)|\overline{Z}$ is a FIO and $[Z,\overline{Z}]=0\}$. In this case, $\mathrm{FIO}(\mathcal{G})$ is the set of all the FOs *whose observers move with constant velocity respect to* Z. Of course, there are only n independent directions for such velocities. Any other proper FIO $\overline{Z}$ measures a gravitational field $\overline{\mathcal{G}}=\mathcal{G}+\mathcal{G}_0$, where $\mathcal{G}_0$ is parallel ("a uniform gravitational field cannot be distinguished from a uniform acceleration").

(2) Any possible gravitational field $\mathcal{G}$ for ∇ fixes the n-dimensional set of fields of observers $\mathrm{FIO}(\mathcal{G})$. One of such gravitational fields $\mathcal{G}_0$ maybe privileged by some physical or mathematical reason. For example, $\mathcal{G}_0$ may be the unique gravitational field vanishing at infinity (this is a natural condition for Poisson's equation) or the unique one vanishing along a concrete observer γ_0. (This observer can be called "the center of the Universe" following ideas of Newton himself—"the center of the Universe is not accelerated by gravitation.") In this case, $\mathrm{FIO}(\mathcal{G}_0)$ is a distinguished n-dimensional set of fields of inertial observers.

(3) It is commonly accepted that "inertial reference frames" [see (4) below] can be defined only if there exist a privileged $\mathcal{G}_0$ which vanishes at infinity (see, for example, Ref. 21). Under our viewpoint, it is preferable to maintain our definition of FIOs and, when necessary, to speak about proper FIOs or $\mathrm{FIO}(\mathcal{G}_0)$ (as in the next section). Recall that, under our definition, the question whether a field of observers is inertial or not is *purely local* and can be determined, in principle, from Corollaries 31 and 32. In any case, those who prefer more classical names can call our inertial observers "Newtonian observers" and reserve the name "inertial" for our $\mathrm{FIO}(\mathcal{G}_0)$ when $\mathcal{G}_0$ vanishes at infinity.

(4) From our definition of FIO, we can give a natural definition of *inertial reference frame* (IRF), as a particular case of Galilean reference frame (see Sec. III A 1), i.e., as the choice of a

privileged gauge. Consider a Newtonian space–time, and fix any $p \in M$. Each orthonormal base $(e_1,\ldots,e_n)$ of the absolute space $(\mathrm{an}\Omega_p, \langle\cdot,\cdot\rangle_p)$ can be parallelly propagated to obtain a orthonormal base of vector fields $(E_1,\ldots,E_n)$. A *IRF* is a base of vector fields (moving frame) $(Z,E_1,\ldots,E_n)$ where Z is a FIO and $E_1,\ldots,E_n \in \Gamma(\mathrm{an}\Omega)$ is a parallel orthonormal base of vector fields. The gravitational field of the IRF is, by definition, the one of Z (the IRF will be *proper* if Z is a proper FIO). [Notice that this gravitational field is a gauge field; thus, FIO($\mathcal{G}$) characterizes all the IRFs with the same gauge field $\mathcal{G}$.] For fixed $\mathcal{G}_0$, all the IRF's with gravitational field equal to $\mathcal{G}_0$ are determined by the value of $(Z,E_1,\ldots,E_n)$ at p. Thus, the Galilean group $G_m(\mathbb{R})$ acts freely and transitively on the set of all the IRF's with gravitational field $\mathcal{G}_0$ (*classical homogeneous Galilean transformations*).

B. Poisson's equation

Up to now, Newtonian space–times have been described in a purely geometric way. Notice that the knowledge of a FIO Z and its corresponding $\mathcal{G}$ allows one to reconstruct ∇ [as a very particular case of formula (13)]. Poisson's equation relates geometry to the ''source'' of the gravitational field, by connecting $\mathcal{G}$ to the density of mass. Units with gravitational Newton's constant $G=1$ will be assumed. Recall first the following result [straightforward from (29) and Corollary 32]:

Lemmma 40: For any Newtonian space–time, we have the following.

(1) The spatial divergence of the gravitational field $\mathrm{div}^h\mathcal{G}$ *is equal for all the FIOs.*

Moreover, $Ric(Z_p,Z_p)=\mathrm{div}^h\mathcal{G}(p)$ *for all* Z_p with $dt(Z_p)=1$ *and, thus,* $Ric=4\pi\rho dt\otimes dt$ *where* ρ *is the* density of mass *defined as*

$$\rho(t,x)=\mathrm{div}^h\mathcal{G}(t,x)/4\pi.$$

(2) If, for some FIO Z, the gravitational field $\mathcal{G}$ *is a spatial gradient, i.e.,* $\mathcal{G}=\nabla^h\Phi$ *for some function* Φ*, then the gravitational field* $\overline{\mathcal{G}}$ *of any other FIO* $\overline{Z}=Z+\Sigma_i a^i(t)\partial_i$ *is the spatial gradient* $\overline{\mathcal{G}}=\nabla^h\overline{\Phi}$ *with*

$$\overline{\Phi}(t,x)=\Phi(t,x)+\sum_{i=1}^{n}(a^i)'(t)x^i+b^0(t)$$

and $b^0(t)$ *arbitrary.*

Thus, classical Newton's gravitational law and Poisson's equation suggest the following.

Definition 41: A Newtonian (resp. proper Newtonian) space–time $(\mathbb{R}^{n+1},dt,\langle\cdot,\cdot\rangle_0,\nabla)$ *is* Poissonian *(resp.* proper Poissonian*) if the following two conditions hold:*

(i) The density of mass is non-negative, $\rho\geqslant 0$.

(ii) The gravitational field $\mathcal{G}$ *of a FIO is a spatial gradient* $\mathcal{G}=\nabla^h\Phi$*, for some* $\Phi \in C^2(\mathbb{R}^{n+1})$.

Remark 42: An alternative assumption to *(ii)* is to impose the conservative character of gravitational forces by means of an assumption on the curvature, say, for some $Z\in\mathcal{Z}(M)$, $\langle R(V,Z)Z,W\rangle=\langle R(W,Z)Z,V\rangle$ whenever V,W are spacelike [use Corollary 32; compare with Ref. 14 [Def. 1, Axiom 4], and Ref. 13, Box 12.4, Axiom (7)]. From Lemma 40, assumption (i) can also be formulated as $\mathrm{Ric}(v,v)\geqslant 0$ for all v. Recall that, in any case, our axioms avoid any type of redundancy (as, for example, those in Ref. 13, Box 12.4).

In any Poissonian space–time, denoting by Δ^h the spacelike Laplacian, intrinsic *Poisson's equation*

$$\Delta^h\Phi=4\pi\rho \tag{30}$$

holds. Taking coordinates adapted to some FIO Z (and spacelike parallel), it is well-known that if $\Phi(t,x)$ is a solution of (30), then $\Phi^*(t,x)=\Phi(t,x)+\Sigma_i b^i(t)x^i+b^0(t)$ is a new solution. Thus, Poisson's equation does not determine univocally the value of $\mathcal{G}$ for $Z=\partial_t$, but the value of all the

possible $\mathcal{G}$'s for all the FIOs [this happens even in the proper case, where ρ is necessarily independent of t, and the solutions of (30) can be chosen independent of t]. But this is not surprising, because, in principle, (30) should not privilege any particular inertial gauge.

In order to avoid this difficulty, one assumes usually that (30) can be written in coordinates such that $Z=\partial_t$ is not an arbitrary FIO but one in a priviledged set FIO($\mathcal{G}_0$). The classical assumption for $\mathcal{G}_0$ is to assume that it vanishes at spatial infinity [thus, if such a $\mathcal{G}_0$ exists, then (29) implies that it is unique], and this can be always assumed if ρ has spatial compact support.

Nevertheless, when $\rho(t,\cdot)$ does not have compact support for some t, perhaps no $\mathcal{G}_0$ vanishes at spatial infinity. The simplest case happens for a nonempty spatially homogeneous Universe, i.e., when $\rho(t,x)\equiv\rho_0(t)$ with $\rho_0(t)\not\equiv 0$ [even though perhaps $\rho_0(t)\equiv$const]. Then, a typical solution of (30) when $n=3$ is, in spatial spherical coordinates, $\Phi(t,x)=2\pi\rho_0(t)r^2/3$. The corresponding gravitational field $\mathcal{G}_0$ is null at $r=0$, i.e., along the observer $\gamma_0(t)=(t,0)$ (the ''center of the Universe''). Thus, if one chooses such a γ_0, then a tridimensional set of fields of inertial observers FIO($\mathcal{G}_0$) is privileged, and $\mathcal{G}_0$ can be reconstructed from ρ.

ACKNOWLEDGMENTS

The authors acknowledge Professor Mariano Santander from the Universidad de Valladolid for some comments. The second-named author has been partially supported by MCyT-FEDER Grant No. BFM2001-2871-C04-01.

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Reciprocal transformations of Hamiltonian operators of hydrodynamic type: Nonlocal Hamiltonian formalism for linearly degenerate systems

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(Received 7 February 2002; accepted 9 December 2002)

Reciprocal transformations of Hamiltonian operators of hydrodynamic type are investigated. The transformed operators are generally nonlocal, possessing a number of remarkable algebraic and differential-geometric properties. We apply our results to linearly degenerate semi-Hamiltonian systems in Riemann invariants, a typical example being $R^i_t=(\Sigma^n_{m=1}R^m-R^i)R^i_x$, $\quad i=1,2,\ldots,n$. Since all such systems are linearizable by appropriate (generalized) reciprocal transformations, our formulas provide an infinity of mutually compatible nonlocal Hamiltonian structures, explicitly parametrized by n arbitrary functions of one variable. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1542921]

I. INTRODUCTION

Equations of hydrodynamic type,

$$u^i_t=v^i_j(u)u^j_x, \qquad i,j=1,\ldots,n,$$

naturally arise in applications such as gas dynamics, hydrodynamics, chemical kinetics, the Whitham averaging procedure, differential geometry and topological field theory (see, e.g., Refs. 9, 10, 27, 28, 8, 21, and 22). In this article we study Hamiltonian systems,

$$u^i_t=v^i_j(u)u^j_x=J^{ij}\frac{\partial h}{\partial u^j}, \quad i=1,2,\ldots,n, \tag{1}$$

where

$$J^{ij}=g^{ij}(u)\frac{d}{dx}-g^{is}(u)\Gamma^j_{sk}(u)u^k_x \tag{2}$$

is the Hamiltonian operator and $h(u)$ is the density. As pointed out by Dubrovin and Novikov,[9] expression (2) defines a Hamiltonian operator if and only if the metric g^{ij} ($g^{ij}=g^{ji}$, $\det g^{ij}\neq 0$) is flat and Γ^j_{sk} are the Christoffel symbols of the corresponding Levi-Civita connection. Notice that Eqs. (1) and (2) imply that v^i_j is the matrix of second covariant derivatives of the density h,

$$v^i_j=\nabla^i\nabla_j h,$$

where $\nabla^i\equiv g^{ij}\nabla_j$. The theory of integrability of Hamiltonian systems of hydrodynamic type was proposed by Tsarev.[27,28] He demonstrated that if a Hamiltonian system (1) is diagonalizable, that is, can be written in the diagonal form

$$R^i_t=v^i(R)R^i_x$$

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(the corresponding coordinates R^i are called the Riemann invariants), then it necessarily possesses an infinity of conservation laws and commuting flows and, moreover, is integrable by the so-called "generalized hodograph transform." In Riemann invariants R^i, the flat metric g^{ij} also becomes diagonal, $g^{ij}=g^{ii}\delta^{ij}$, thus establishing a correspondence between Hamiltonian diagonalizable systems (1) and n-orthogonal curvilinear coordinates in flat spaces. This shows that the theory of Hamiltonian systems of hydrodynamic type is deeply rooted in classical differential geometry.

There exists an important class of nonlocal transformations which act on hydrodynamic-type systems. Unlike the classical Bäcklund transformations (Miura-type transformations) familiar from the soliton theory, these transformations change the *independent* variables of a system. They are defined as follows. Let $B(u)dx+A(u)dt$ and $N(u)dx+M(u)dt$ be two conservation laws of system (1), understood as one-forms which are closed by virtue of (1). In the new independent variables $\tilde{x}$ and $\tilde{t}$ defined by

$$d\tilde{x}=B(u)dx+A(u)dt, \quad d\tilde{t}=N(u)dx+M(u)dt, \tag{3}$$

Eqs. (1) take the form

$$u^i_{\tilde{t}}=\tilde{v}^i_j(u)u^j_{\tilde{x}}, \tag{4}$$

where the transformed matrix $\tilde{v}$ is $\tilde{v}=(Bv-AE)(ME-Nv)^{-1}$, $E=id$. Transformations of the type (3) originate from gas dynamics and are known as *reciprocal*.[26] The simplest example is, probably, the passage from Eulerian to Lagrangian coordinates in one-dimensional gas dynamics. Reciprocal transformations are known to preserve the class of diagonalizable systems, which is an immediate corollary of the form of the transformed matrix $\tilde{v}$. Moreover, all conservation laws and commuting flows of the initial system can easily be recalculated in the new independent variables. Therefore, reciprocal transformations preserve the whole class of integrable systems of hydrodynamic type.

The only object which, under reciprocal transformations, behaves in a nontrivial way is the Hamiltonian structure. Generic reciprocal transformations destroy the local Hamiltonian formalism of the form (2). To the best of our knowledge, the behavior of Hamiltonian structures under reciprocal transformations (and their appropriate generalizations) has not been discussed in the literature. Investigation of this problem is, thus, the main objective of our article.

In Secs. III and IV we study the behavior of Hamiltonian structures (2) under reciprocal transformations (3). The main conclusion is that local Hamiltonian structures generally become nonlocal, so that the transformed system (4) is still Hamiltonian, $u^i_{\tilde{t}}=\tilde{J}^{ij}\partial\tilde{h}/\partial u^j$, however, with the nonlocal Hamiltonian operator

$$\tilde{J}^{ij}=\tilde{g}^{ij}\frac{d}{d\tilde{x}}-\tilde{g}^{is}\tilde{\Gamma}^j_{sk}u^k_{\tilde{x}}+\sum \varepsilon^\alpha w^i_{(\alpha)k}u^k_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}w^j_{(\alpha)s}u^s_{\tilde{x}}. \tag{5}$$

Here $\varepsilon^\alpha=\pm 1$; the explicit form of the transformed metric $\tilde{g}^{ij}$ and the nonlocal terms is stated in Secs. III and IV.

Remark: In the particular case of constant A, B, M, N, transformations (3) reduce to linear changes of the independent variables, $\tilde{x}=bx+at$, $\tilde{t}=nx+mt$, (a, b, m, n are constants). As pointed out by Tsarev,[28] transformations of this type preserve the locality of Hamiltonian structures of hydrodynamic type (see also Ref. 24).

Nonlocal operators of the form (5) have been extensively investigated in Refs. 20, 11, 13, 25, 1, 18, 5, and 2, and have a remarkable differential-geometric interpretation. The general theory is briefly recalled in Sec. II. As an illustration of our approach, we discuss Hamiltonian formalism of linearly degenerate semi-Hamiltonian systems in Riemann invariants,

$$R^i_t=v^i(R)R^i_x,$$

where the characteristic speeds $v^i(R)$ satisfy the identities

(1) $\partial_i v^i = 0$ for any $i = 1,2,\ldots n$, $\partial_i = \partial/\partial R^i$ (linear degeneracy);
(2) $\partial_k[\partial_j v^i/(v^j - v^i)] = \partial_j[\partial_k v^i/(v^k - v^i)]$ for any $i \neq j \neq k$ (semi-Hamiltonian property).

Linearly degenerate semi-Hamiltonian systems have interesting interrelations with separable (Stäckel) systems in classical mechanics[15,16,4,12,14] and finite-gap solutions of integrable soliton equations. For instance, the linearly degenerate semi-Hamiltonian system $R^i_t = (\Sigma R^m - R^i)R^i_x$ governs the evolution of zeros of the n-gap ψ-function in the KdV theory.[6,7,12] For $n=2$ we have essentially one nontrivial linearly degenerate system,

$$u_t = v u_x, \quad v_t = u v_x, \tag{6}$$

arising in gas dynamics (Chaplygin gas), field theory (Born–Infeld equation) and classical differential geometry (minimal surfaces in Minkowski three-space, improper affine spheres). Theorem 1 of Sec. III provides infinitely many Hamiltonian representations of system (6),

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = J \begin{pmatrix} \partial h/\partial u \\ \partial h/\partial v \end{pmatrix}, \tag{7}$$

with nonlocal operators

$$\begin{aligned} J = {} & (u-v)^2 \begin{pmatrix} f(u) & 0 \\ 0 & \varphi(v) \end{pmatrix} \frac{d}{dx} + (u-v) \\ & \times \begin{pmatrix} \frac{1}{2}(u-v)f'(u)u_x + f(u)(u_x - v_x) & \varphi(v)u_x + f(u)v_x \\ -\varphi(v)u_x - f(u)v_x & \frac{1}{2}(u-v)\varphi'(v)v_x + \varphi(v)(u_x - v_x) \end{pmatrix} \\ & + \begin{pmatrix} w^1 u_x & u_x \\ w^2 v_x & v_x \end{pmatrix} \begin{pmatrix} d \\ \overline{dx} \end{pmatrix}^{-1} \begin{pmatrix} u_x & v_x \\ w^1 u_x & w^2 v_x \end{pmatrix}, \end{aligned}$$

where $w^1 = \frac{1}{2}[(u-v)f'(u) - f(u) - \varphi(v)]$ and $w^2 = \frac{1}{2}[(v-u)\varphi'(v) - f(u) - \varphi(v)]$ are the characteristic speeds of commuting flows of system (6), and the corresponding Hamiltonian densities

$$h = \frac{1}{4(v-u)} \left(\left[\int^u \frac{\mathrm{d}\nu}{\sqrt{f(\nu)}} \right]^2 - \left[\int^v \frac{\mathrm{d}\nu}{\sqrt{\varphi(\nu)}} \right]^2 \right),$$

parametrized by two arbitrary functions $f(u)$ and $\varphi(v)$. In view of the linearity of J in $f(u)$ and $\varphi(v)$, all these Hamiltonian structures are mutually compatible. Notice that the local part of the operator J is of the form (2), corresponding to the metric

$$(u-v)^{-2} \left(\frac{du^2}{f(u)} + \frac{dv^2}{\varphi(v)} \right),$$

which is not flat for generic $f(u)$ and $\varphi(v)$. Particular choices of $f(u)$ and $\varphi(v)$ lead to local Hamiltonian structures which were first discovered in Refs. 23 and 3 (see Example 1 in Sec. III).

Another example of this type is the three-component linearly degenerate semi-Hamiltonian system

$$u_t = (v+w)u_x, \quad v_t = (u-w)v_x, \quad w_t = \tfrac{1}{2}(u+v)w_x, \tag{8}$$

which is the Riemann invariant form of non-isentropic gas dynamics with the special equation of state $P(\rho,s)=s-1/\rho$ (see Refs. 29 and 19). Our approach provides infinitely many nonlocal Hamiltonian structures of the form

$$J=\frac{4}{\rho^2}\begin{pmatrix} f(u) & 0 & 0\\ 0 & \varphi(v) & 0\\ 0 & 0 & \psi(w)\end{pmatrix}\frac{d}{dx}$$
$$+\frac{2}{\rho}\begin{pmatrix} \frac{1}{\rho}f'(u)u_x+2f(u)\left(\frac{1}{\rho}\right)_x & -\varphi(v)u_x-f(u)v_x & -2\psi(w)u_x-f(u)w_x\\ \varphi(v)u_x+f(u)v_x & \frac{1}{\rho}\varphi'(v)v_x+2\varphi(v)\left(\frac{1}{\rho}\right)_x & -2\psi(w)v_x+\varphi(v)w_x\\ 2\psi(w)u_x+f(u)w_x & 2\psi(w)v_x-\varphi(v)w_x & \frac{1}{\rho}\psi'(w)v_x+2\psi(w)\left(\frac{1}{\rho}\right)_x\end{pmatrix}$$
$$+\begin{pmatrix} w^1u_x & u_x\\ w^2v_x & v_x\\ w^3w_x & w_x\end{pmatrix}\left(\frac{d}{dx}\right)^{-1}\begin{pmatrix} u_x & v_x & w_x\\ w^1u_x & w^2v_x & w^3w_x\end{pmatrix},\quad \rho=\left(w+\frac{v-u}{2}\right)^{-1}.$$

Here the local part is of the form (2), generated by the diagonal metric

$$(2w+v-u)^{-2}\left(\frac{du^2}{f(u)}+\frac{dv^2}{\varphi(v)}+\frac{dw^2}{\psi(w)}\right),\tag{9}$$

which is not flat in general, and w^1, w^2, w^3 are the characteristic speeds of commuting flows of system (8):

$$w^1=-\tfrac{1}{2}(2w+v-u)f'(u)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)],$$
$$w^2=\tfrac{1}{2}(2w+v-u)\varphi'(v)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)],$$
$$w^3=(2w+v-u)\psi'(w)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)].$$

These Hamiltonian operators depend linearly on three arbitrary functions $f(u)$, $\varphi(v)$ and $\psi(w)$, and are mutually compatible (Example 2 in Sec. III).

Similar arguments applied to the three-component linearly degenerate semi-Hamiltonian system

$$u_t=(v+w)u_x,\quad v_t=(u+w)v_x,\quad w_t=(u+v)w_x\tag{10}$$

provide infinitely many nonlocal Hamiltonian structures

$$J=\begin{pmatrix} g^{11} & 0 & 0\\ 0 & g^{22} & 0\\ 0 & 0 & g^{33}\end{pmatrix}\frac{d}{dx}$$
$$+\begin{pmatrix} g^{11}\left[\frac{f'(u)}{2f(u)}u_x+\frac{u_x-v_x}{u-v}+\frac{u_x-w_x}{u-w}\right] & \frac{g^{22}u_x+g^{11}v_x}{u-v} & \frac{g^{33}u_x+g^{11}w_x}{u-w}\\ -\frac{g^{22}u_x+g^{11}v_x}{u-v} & g^{22}\left[\frac{\varphi'(v)}{2\varphi(v)}v_x+\frac{u_x-v_x}{u-v}+\frac{v_x-w_x}{v-w}\right] & \frac{g^{33}v_x+g^{22}w_x}{v-w}\\ -\frac{g^{33}u_x+g^{11}w_x}{u-w} & -\frac{g^{33}v_x+g^{22}w_x}{v-w} & g^{33}\left[\frac{\psi'(w)}{2\psi(w)}w_x+\frac{w_x-v_x}{w-v}+\frac{u_x-w_x}{u-w}\right]\end{pmatrix}$$

$$+\begin{pmatrix} \lambda^1 u_x & \mu^1 u_x & \eta^1 u_x & u_x \\ \lambda^2 v_x & \mu^2 v_x & \eta^2 v_x & v_x \\ \lambda^3 w_x & \mu^3 w_x & \eta^3 w_x & w_x \end{pmatrix} \left(\frac{d}{dx}\right)^{-1} \begin{pmatrix} u_x & v_x & w_x \\ \eta^1 u_x & \eta^2 v_x & \eta^3 w_x \\ \mu^1 u_x & \mu^2 v_x & \mu^3 w_x \\ \lambda^1 u_x & \lambda^2 v_x & \lambda^3 w_x \end{pmatrix}.$$

Here the metric components are

$$g^{11}=(u-v)^2(u-w)^2 f(u), \quad g^{22}=(v-u)^2(v-w)^2\varphi(v), \quad g^{33}=(w-u)^2(w-v)^2\psi(w),$$

the coefficients $\eta^1=v+w$, $\eta^2=u+w$ and $\eta^3=v+w$ are the characteristic speeds of system (10), and μ^k, λ^k are the characteristic speeds of its commuting flows:

$$\mu^1=-\frac{1}{2}(u-v)(u-w)f'(u)+uf(u)+v\varphi(v)+w\psi(w)-\int^u f(\nu)\mathrm{d}\nu-\int^v \varphi(\nu)\mathrm{d}\nu$$
$$-\int^w \psi(\nu)\mathrm{d}\nu-\frac{1}{2}(v+w)(f(u)+\varphi(v)+\psi(w)),$$

$$\lambda^1=(u-v)(u-w)[2f(u)+uf'(u)]-2[u^2f(u)+v^2\varphi(v)+w^2\psi(w)]$$
$$+(v+w)\left[uf(u)+v\varphi(v)+w\psi(w)+\int^u f(\nu)\mathrm{d}\nu+\int^v \varphi(\nu)\mathrm{d}\nu+\int^w \psi(\nu)\mathrm{d}\nu\right].$$

(μ^2, μ^3 and λ^2, λ^3 can be obtained by a cyclic permutation of u, v, w and f, φ, ψ.) These operators depend linearly on three arbitrary functions $f(u)$, $\varphi(v)$ and $\psi(w)$ and are mutually compatible. The details can be found in Example 3 in Sec. IV.

Generalized reciprocal transformations and their action on the local Poisson brackets of Dubrovin–Novikov type are discussed in Sec. V.

II. NONLOCAL HAMILTONIAN OPERATORS OF HYDRODYNAMIC TYPE. NONLOCAL HAMILTONIAN FORMALISM FOR SEMI-HAMILTONIAN SYSTEMS

In this section we recall the necessary information about nonlocal Hamiltonian operators of hydrodynamic type

$$J^{ij}=g^{ij}\frac{d}{dx}-g^{is}\Gamma^j_{sk}u^k_x+\sum_\alpha \varepsilon^\alpha w^i_{(\alpha)k}u^k_x\left(\frac{d}{dx}\right)^{-1} w^i_{(\alpha)n}u^n_x, \quad \varepsilon^\alpha=\pm 1, \tag{11}$$

which are defined by a metric g^{ij} ($g^{ij}=g^{ji}$, $\det g^{ij}\neq 0$), the corresponding Levi-Civita connection Γ^j_{sk} and a set of affinors $w_{(\alpha)}$ forming the nonlocal "tail."

Theorem 1:[11] *The operator J^{ij} is Hamiltonian if and only if the affinors $w_{(\alpha)}$ satisfy the equations*

$$g_{ik}w^k_{(\alpha)j}=g_{jk}w^k_{(\alpha)i}, \tag{12}$$

$$\nabla_k w^i_{(\alpha)j}=\nabla_j w^i_{(\alpha)k}, \tag{13}$$

and the curvature tensor of the metric g^{ij} has the expansion

$$R^{ij}_{kl}=\sum_\alpha \varepsilon^\alpha(w^i_{(\alpha)k}w^j_{(\alpha)l}-w^i_{(\alpha)l}w^j_{(\alpha)k}). \tag{14}$$

Moreover, the set of affinors $w_{(\alpha)}$ must be commutative,

$$[w_{(\alpha)}, \quad w_{(\beta)}]=0. \tag{15}$$

As pointed out in Ref. 11, Eqs. (12)–(15) constitute the Gauss–Codazzi–Ricci equations of submanifolds of pseudo-Euclidean spaces with flat normal bundle. There are three particularly interesting special cases of the general formula (11).

Hamiltonian operators associated with *constant curvature* metrics, first introduced in Ref. 20 (see also Ref. 25), are of the form

$$J^{ij}=g^{ij}\frac{d}{dx}-g^{is}\Gamma^j_{sk}u^k_x+cu^i_x\left(\frac{d}{dx}\right)^{-1}u^j_x. \tag{16}$$

Here g^{ij} is a metric of constant curvature c, so that the Gauss equation (14) takes the form

$$R^{ij}_{kl}=c(\delta^i_k\delta^j_l-\delta^i_l\delta^j_k).$$

Hamiltonian operators associated with *conformally flat* metrics are of the form[13]

$$J^{ij}=g^{ij}\frac{d}{dx}-g^{is}\Gamma^j_{sk}u^k_x+w^i_ku^k_x\left(\frac{d}{dx}\right)^{-1}u^j_x+u^i_x\left(\frac{d}{dx}\right)^{-1}w^j_ku^k_x. \tag{17}$$

The corresponding equations (12)–(14) reduce to

$$g_{ik}w^k_j=g_{jk}w^k_i,$$

$$\nabla_kw^i_j=\nabla_jw^i_k,$$

while the curvature tensor of the metric g^{ij} has the expansion

$$R^{ij}_{kl}=w^i_k\delta^j_l+w^j_l\delta^i_k-w^j_k\delta^i_l-w^i_l\delta^j_k,$$

implying that the metric g^{ij} is conformally flat.

Hamiltonian operators associated with *hypersurfaces of the Euclidean space* are[11]

$$J^{ij}=g^{ij}\frac{d}{dx}-g^{is}\Gamma^j_{sk}u^k_x+w^i_ku^k_x\left(\frac{d}{dx}\right)^{-1}w^j_nu^n_x. \tag{18}$$

The corresponding equations (12)–(14),

$$g_{ik}w^k_j=g_{jk}w^k_i,$$

$$\nabla_kw^i_j=\nabla_jw^i_k,$$

$$R^{ij}_{kl}=w^i_kw^j_l-w^i_lw^j_k,$$

are the Gauss–Codazzi equations governing the first fundamental form g^{ij} and the shape operator w^i_j of a hypersurface in the Euclidean space.

Nonlocal Hamiltonian operators of the form (11) and their particular instances (16)–(18) appear in a variety of applications including the Whitham theory [where operators of the form (11) arise as a result of the Whitham averaging of nonlocal higher order Poisson brackets of integrable PDEs[1,2]], recursion scheme, Dirac reduction, etc.[11] Canonical coordinates for these operators were introduced in a recent paper by Maltsev and Novikov.[18] The corresponding nonlocal symplectic structures were investigated in Ref. 17.

Notice that Eqs. (11)–(14) simplify if the metric g and affinors $w_{(\alpha)}$ are diagonal, $g^{ij}=g^{ii}\delta^{ij}$, $w^i_{(\alpha)j}=w^i_{(\alpha)}\delta^i_j$. In this case the operator (11) takes the form

$$J^{ij}=g^{ii}\delta^{ij}\frac{d}{dx}-g^{ii}\Gamma^j_{ik}u^k_x+\sum_\alpha\varepsilon^{(\alpha)}w^i_{(\alpha)}u^i_x\left(\frac{d}{dx}\right)^{-1}w^j_{(\alpha)}u^j_x, \tag{19}$$

while Eqs. (12)–(14) reduce to

$$\partial_j \ln \sqrt{g_{ii}} = \frac{\partial_j w^i_{(\alpha)}}{w^j_{(\alpha)} - w^i_{(\alpha)}}, \tag{20}$$

$$R^{ij}_{ij} = \sum_\alpha \varepsilon^{(\alpha)} w^i_{(\alpha)} w^j_{(\alpha)} \tag{21}$$

for any $i \neq j$. Nonlocal Hamiltonian operators of the form (19) naturally arise as Hamiltonian structures of semi-Hamiltonian systems in Riemann invariants.[11,5] Let us recall the main construction. Following Tsarev,[28] a system in Riemann invariants

$$R^i_t = v^i(R) R^i_x, \quad i = 1,2,\ldots,n, \tag{22}$$

is called semi-Hamiltonian if the characteristic speeds $v^i(R)$ satisfy the identities

$$\partial_k \frac{\partial_j v^i}{v^j - v^i} = \partial_j \frac{\partial_k v^i}{v^k - v^i}$$

for any triple $i \neq j \neq k$. Let us introduce the diagonal metric $g_{ii} dR^{i^2}$ by the formulas

$$\partial_j \ln \sqrt{g_{ii}} = \frac{\partial_j v^i}{v^j - v^i} \tag{23}$$

for any $i \neq j$. Notice that g_{ii} is defined up to a multiple $g_{ii} \to g_{ii}/f^i(R^i)$, where $f^i(R^i)$ is an arbitrary function of R^i.

Although the metric g_{ii} may happen to be flat for particular choices of $f^i(R^i)$ (in this case our system is Hamiltonian with the local Hamiltonian operator of Dubrovin–Novikov type corresponding to the metric g_{ii}), it is not flat in general. Suppose one can find the expansion of the curvature tensor of this metric in the form (21), where $w^i_{(\alpha)}$ are characteristic speeds of commuting flows of system (22):

$$R^i_{t^\alpha} = w^i_{(\alpha)}(R) R^i_x. \tag{24}$$

Notice that the flows (22) and (24) commute if and only if

$$\frac{\partial_j v^i}{v^j - v^i} = \frac{\partial_j w^i_{(\alpha)}}{w^j_{(\alpha)} - w^i_{(\alpha)}} \tag{25}$$

for any $i \neq j$. In this case the system (22) will be Hamiltonian with the nonlocal Hamiltonian operator (19) [indeed, both conditions (20) and (21) are satisfied]. The main problem is thus to find the expansion (21) for a metric satisfying (23). We point out that the sum in (21) is infinite in general.

Remarkably, there exist semi-Hamiltonian systems for which one can explicitly construct the expansion (21) for an arbitrary metric g_{ii} satisfying (23). Moreover, for any choice of $f^i(R^i)$ the summation in (21) is *finite*, so that the corresponding systems possess infinitely many Hamiltonian structures explicitly parametrized by n arbitrary functions of one variable. Among the most interesting examples of this type are systems of Temple's class and linearly degenerate semi-Hamiltonian systems. The construction of nonlocal Hamiltonian formalism for linearly degenerate semi-Hamiltonian systems is based on the formulas for reciprocal transformations of local Hamiltonian operators which we derive in Secs. III–V.

III. RECIPROCAL TRANSFORMATIONS WHICH CHANGE ONLY THE SPACE VARIABLE *x*

Consider a Hamiltonian system (1),

$$u_t^i = v_j^i(u)u_x^j = (\nabla^i\nabla_j h)u_x^j = J^{ij}\frac{\partial h}{\partial u^j},$$

with the local Hamiltonian operator (2),

$$J^{ij} = g^{ij}\frac{d}{dx} - g^{is}\Gamma_{sk}^j u_x^k.$$

In this section we discuss special reciprocal transformations of the form (3) which change the space variable x only,

$$d\tilde{x} = B(u)dx + A(u)dt, \quad \tilde{t} = t. \tag{26}$$

Notice that an arbitrary reciprocal transformation (3) can be represented as a composition

$$R_1 \circ T \circ R_2$$

where R_1 and R_2 are reciprocal transformations of the form (26) and T is the transformation interchanging the independent variables: $\tilde{x} = t$, $\tilde{t} = x$. After the transformation (26), system (1) takes the form

$$u_t^i = \tilde{v}_j^i(u)u_{\tilde{x}}^j = (\nabla^i\nabla_j h \cdot B - \delta_j^i A)u_{\tilde{x}}^j, \tag{27}$$

while the Hamiltonian operator J^{ij} undergoes a nontrivial transformation and becomes nonlocal. To write down the transformed operator $\tilde{J}^{ij}$, we introduce the Hamiltonian system

$$u_\tau^i = w_j^i(u)u_x^j = J^{ij}\frac{\partial B}{\partial u^j} = (\nabla^i\nabla_j B)u_x^j \tag{28}$$

generated by the Hamiltonian operator J^{ij} and the density B. Clearly, systems (1) and (28) commute. Since the flux of the conserved density B corresponding to the flow (28) is given by the formula $\frac{1}{2}(\nabla B)^2$ [here $\nabla B = B_i du^i$ is the gradient of B and $(\nabla B)^2 = g^{ij}B_iB_j$], we can incorporate the time τ into the reciprocal transformation (26) as follows:

$$d\tilde{x} = Bdx + Adt + \tfrac{1}{2}(\nabla B)^2 d\tau.$$

Therefore, the transformed system (28) takes the form

$$u_\tau^i = \tilde{w}_j^i(u)u_{\tilde{x}}^j = (\nabla^i\nabla_j B \cdot B - \tfrac{1}{2}\delta_j^i(\nabla B)^2)u_{\tilde{x}}^j. \tag{29}$$

The transformed systems (27) and (29) commute. Now we can formulate the main result of this section.

Theorem 2: *The transformed system (27) is Hamiltonian,*

$$u_t^i = \tilde{J}^{ij}\frac{\partial \tilde{h}}{\partial u^j},$$

with the nonlocal operator

$$\tilde{J}^{ij}=\tilde{g}^{ij}\frac{d}{d\tilde{x}}-\tilde{g}^{is}\tilde{\Gamma}^{j}_{sk}u^{k}_{\tilde{x}}+\tilde{w}^{i}_{k}u^{k}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}u^{j}_{\tilde{x}}+u^{i}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\tilde{w}^{j}_{k}u^{k}_{\tilde{x}} \tag{30}$$

and the Hamiltonian density $\tilde{h}(u)=h(u)/B(u)$. *Here the transformed metric is* $\tilde{g}^{ij}=B^2g^{ij}$, $\tilde{\Gamma}$ *is the Levi-Civita connection of* $\tilde{g}$, *and* $\tilde{w}^{i}_{j}$ *is given by (29). Notice that the transformed metric is conformally flat with the curvature tensor*

$$\tilde{R}^{ij}_{kl}=\tilde{w}^{i}_{k}\delta^{j}_{l}+\tilde{w}^{j}_{l}\delta^{i}_{k}-\tilde{w}^{j}_{k}\delta^{i}_{l}-\tilde{w}^{i}_{l}\delta^{j}_{k}.$$

The proof follows directly from results of Ref. 13 where nonlocal Hamiltonian operators of the form (30) associated with conformally flat metrics were investigated. As an illustration of the procedure outlined in Theorem 1, we explicitly construct nonlocal Hamiltonian formalism for the two-component linearly degenerate system (6).

Example 1: The linear system

$$u_t=u_x,\quad v_t=-v_x \tag{31}$$

possesses infinitely many Hamiltonian representations

$$\begin{pmatrix}u\\v\end{pmatrix}_t=J\begin{pmatrix}\partial h/\partial u\\ \partial h/\partial v\end{pmatrix} \tag{32}$$

with local Hamiltonian operators J of the type (2),

$$J=4\begin{pmatrix}f(u)&0\\0&\varphi(v)\end{pmatrix}\frac{d}{dx}+2\begin{pmatrix}f'(u)u_x&0\\0&\varphi'(v)v_x\end{pmatrix}, \tag{33}$$

corresponding to flat metrics

$$ds^2=\frac{du^2}{4f(u)}+\frac{dv^2}{4\varphi(v)} \tag{34}$$

[here $f(u)$ and $\varphi(v)$ are arbitrary functions]. The corresponding Hamiltonian densities are

$$h(u,v)=\frac{1}{8}\left[\int^{u}\frac{\mathrm{d}\nu}{\sqrt{f(\nu)}}\right]^2-\frac{1}{8}\left[\int^{v}\frac{\mathrm{d}\nu}{\sqrt{\varphi(\nu)}}\right]^2. \tag{35}$$

Consider the reciprocal transformation

$$d\tilde{x}=Bdx+Adt=\tfrac{1}{2}(v-u)dx-\tfrac{1}{2}(v+u)dt,\quad \tilde{t}=t, \tag{36}$$

mapping the linear system (31) to the linearly degenerate system

$$u_t=vu_{\tilde{x}},\quad v_t=uv_{\tilde{x}}. \tag{37}$$

To write down the transformed Hamiltonian operators (33), we first introduce the transformed metric

$$d\tilde{s}^2=\frac{ds^2}{B^2}=(u-v)^{-2}\left(\frac{du^2}{f(u)}+\frac{dv^2}{\varphi(v)}\right), \tag{38}$$

which is no longer flat for generic $f(u)$ and $\varphi(v)$. Following the procedure outlined in Theorem 1, we calculate the Hamiltonian flow generated by the Hamiltonian operator (33) and the Hamiltonian density $B=\frac{1}{2}(v-u)$. A simple computation gives the system

$$u_\tau = -f'(u)u_x, \quad v_\tau = \varphi'(v)v_x, \tag{39}$$

which clearly commutes with (31). To incorporate the time τ into the reciprocal transformation (36), we calculate the flux of the density B corresponding to the flow (39),

$$\tfrac{1}{2}(\nabla B)^2 = \tfrac{1}{2}[f(u)+\varphi(v)].$$

Thus, reciprocal transformation (36) takes the form

$$d\tilde{x} = Bdx + Adt + \tfrac{1}{2}(\nabla B)^2 d\tau = \tfrac{1}{2}(v-u)dx - \tfrac{1}{2}(v+u)dt + \tfrac{1}{2}[f(u)+\varphi(v)]d\tau, \quad \tilde{t} = t,$$

so that the transformed system (39) is

$$u_\tau = w^1 u_{\tilde{x}}, \quad v_\tau = w^2 v_{\tilde{x}}, \tag{40}$$

where

$$w^1 = \tfrac{1}{2}[(u-v)f'(u) - f(u) - \varphi(v)], \quad w^2 = \tfrac{1}{2}[(v-u)\varphi'(v) - f(u) - \varphi(v)] \tag{41}$$

[notice that Eqs. (40) and (41) constitute a general commuting flow of the linearly degenerate system (37)]. According to Theorem 1, system (37) is Hamiltonian,

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \tilde{J}\begin{pmatrix} \partial\tilde{h}/\partial u \\ \partial\tilde{h}/\partial v \end{pmatrix},$$

with nonlocal operators $\tilde{J}$ of the form

$$\begin{aligned} &(u-v)^2\begin{pmatrix} f(u) & 0 \\ 0 & \varphi(v) \end{pmatrix}\frac{d}{d\tilde{x}} + (u-v) \\ &\quad\times\begin{pmatrix} \tfrac{1}{2}(u-v)f'(u)u_{\tilde{x}} + f(u)(u_{\tilde{x}} - v_{\tilde{x}}) & \varphi(v)u_{\tilde{x}} + f(u)v_{\tilde{x}} \\ -\varphi(v)u_{\tilde{x}} - f(u)v_{\tilde{x}} & \tfrac{1}{2}(u-v)\varphi'(v)v_{\tilde{x}} + \varphi(v)(u_{\tilde{x}} - v_{\tilde{x}}) \end{pmatrix} \\ &\quad+\begin{pmatrix} w^1 u_{\tilde{x}} & u_{\tilde{x}} \\ w^2 v_{\tilde{x}} & v_{\tilde{x}} \end{pmatrix}\left(\frac{d}{d\tilde{x}}\right)^{-1}\begin{pmatrix} u_{\tilde{x}} & v_{\tilde{x}} \\ w^1 u_{\tilde{x}} & w^2 v_{\tilde{x}} \end{pmatrix} \end{aligned} \tag{42}$$

and the Hamiltonian densities

$$\tilde{h} = h/B = \frac{1}{4(v-u)}\left(\left[\int^u \frac{d\nu}{\sqrt{f(\nu)}}\right]^2 - \left[\int^v \frac{d\nu}{\sqrt{\varphi(\nu)}}\right]^2\right).$$

All these operators are mutually compatible. Let us discuss some particular cases. For $f(u)=1$, $\varphi(v)=-1$ and $f(u)=u$, $\varphi(v)=-v$ we have $w^1=w^2=0$, so that the transformed operators take local forms

$$(u-v)^2\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{d}{d\tilde{x}} + (u-v)\begin{pmatrix} u_{\tilde{x}} - v_{\tilde{x}} & v_{\tilde{x}} - u_{\tilde{x}} \\ u_{\tilde{x}} - v_{\tilde{x}} & v_{\tilde{x}} - u_{\tilde{x}} \end{pmatrix} \tag{43}$$

and

$$(u-v)^2\begin{pmatrix} u & 0 \\ 0 & -v \end{pmatrix}\frac{d}{d\tilde{x}}+(u-v)\begin{pmatrix} (\frac{3}{2}u-\frac{1}{2}v)u_{\tilde{x}}-uv_{\tilde{x}} & uv_{\tilde{x}}-vu_{\tilde{x}} \\ vu_{\tilde{x}}-uv_{\tilde{x}} & (\frac{3}{2}v-\frac{1}{2}u)v_{\tilde{x}}-vu_{\tilde{x}} \end{pmatrix}, \tag{44}$$

the corresponding Hamiltonian densities being

$$h(u,v)=\frac{u^2+v^2}{4(v-u)} \quad \text{and} \quad h(u,v)=\frac{u+v}{v-u},$$

respectively. In the case $f(u)=u^2$, $\varphi(v)=-v^2$ we have $w^1=-w^2=\frac{1}{2}(u-v)^2$ so that the operator $\tilde{J}$ takes the form

$$\begin{aligned}(u-v)^2\begin{pmatrix} u^2 & 0 \\ 0 & -v^2 \end{pmatrix}\frac{d}{d\tilde{x}}+(u-v)\begin{pmatrix} u(2u-v)u_{\tilde{x}}-u^2v_{\tilde{x}} & u^2v_{\tilde{x}}-v^2u_{\tilde{x}} \\ v^2u_{\tilde{x}}-u^2v_{\tilde{x}} & v(2v-u)v_{\tilde{x}}-v^2u_{\tilde{x}} \end{pmatrix} \\ +\begin{pmatrix} \frac{1}{2}(u-v)^2u_{\tilde{x}} & u_{\tilde{x}} \\ -\frac{1}{2}(u-v)^2v_{\tilde{x}} & v_{\tilde{x}} \end{pmatrix}\left(\frac{d}{d\tilde{x}}\right)^{-1}\begin{pmatrix} u_{\tilde{x}} & v_{\tilde{x}} \\ \frac{1}{2}(u-v)^2u_{\tilde{x}} & -\frac{1}{2}(u-v)^2v_{\tilde{x}} \end{pmatrix}\end{aligned} \tag{45}$$

with the corresponding density

$$h(u,v)=\frac{(\ln u)^2+(\ln v)^2}{4(v-u)}.$$

Notice that the local part of the Hamiltonian operator (45),

$$(u-v)^2\begin{pmatrix} u^2 & 0 \\ 0 & -v^2 \end{pmatrix}\frac{d}{d\tilde{x}}+(u-v)\begin{pmatrix} u(2u-v)u_{\tilde{x}}-u^2v_{\tilde{x}} & u^2v_{\tilde{x}}-v^2u_{\tilde{x}} \\ v^2u_{\tilde{x}}-u^2v_{\tilde{x}} & v(2v-u)v_{\tilde{x}}-v^2u_{\tilde{x}} \end{pmatrix}, \tag{46}$$

is itself Hamiltonian, indeed, the metric

$$(u-v)^{-2}\left(\frac{du^2}{u^2}-\frac{dv^2}{v^2}\right)$$

is flat.

One can show that the operators (43), (44) and (46) (are arbitrary linear combinations thereof) are the only local Hamiltonian structures of Dubrovin–Novikov type of the system (37). This follows from the fact that the metric

$$(u-v)^{-2}\left(\frac{du^2}{f(u)}-\frac{dv^2}{\varphi(v)}\right)$$

is flat if and only if

$$f(u)=\alpha u^2+\beta u+\gamma, \quad \varphi(v)=-\alpha v^2-\beta v-\gamma,$$

where α, β and γ are arbitrary constants. These local structures were first discovered in Refs. 23 and 3, and subsequently generalized to polytropic gas dynamics in Refs. 21 and 22. The general nonlocal operator (42) first appeared in Ref. 5.

Example 2: The linear system

$$u_t = u_x, \quad v_t = -v_x, \quad w_t = 0 \tag{47}$$

possesses infinitely many Hamiltonian representations

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_t = J \begin{pmatrix} \partial h/\partial u \\ \partial h/\partial v \\ \partial h/\partial w \end{pmatrix}$$

with local operators

$$J = 4\begin{pmatrix} f(u) & 0 & 0 \\ 0 & \varphi(v) & 0 \\ 0 & 0 & \psi(w) \end{pmatrix} \frac{d}{dx} + 2\begin{pmatrix} f'(u)u_x & 0 & 0 \\ 0 & \varphi'(v)v_x & 0 \\ 0 & 0 & \psi'(w)w_x \end{pmatrix}.$$

corresponding to flat metrics

$$ds^2 = \frac{du^2}{4f(u)} + \frac{dv^2}{4\varphi(v)} + \frac{dw^2}{4\psi(w)}$$

[here $f(u)$, $\varphi(v)$ and $\psi(w)$ are arbitrary functions]. The corresponding Hamiltonian densities are

$$h(u,v) = \frac{1}{8}\left[\int^u \frac{\mathrm{d}\nu}{\sqrt{f(\nu)}}\right]^2 - \frac{1}{8}\left[\int^v \frac{\mathrm{d}\nu}{\sqrt{\varphi(\nu)}}\right]^2.$$

Consider the reciprocal transformation

$$d\tilde{x} = B\,dx + A\,dt = [w + \tfrac{1}{2}(v-u)]\,dx - \tfrac{1}{2}(u+v)\,dt, \quad \tilde{t} = t, \tag{48}$$

mapping the system (47) to the linearly degenerate semi-Hamiltonian system

$$u_t = (v+w)u_{\tilde{x}}, \quad v_t = (u-w)v_{\tilde{x}}, \quad w_t = \tfrac{1}{2}(u+v)w_{\tilde{x}}. \tag{49}$$

Notice that under the change of variables

$$u = -c + s - \frac{1}{\rho}, \quad v = -c - s + \frac{1}{\rho}, \quad w = s, \tag{50}$$

system (49) takes the form of equations of gas dynamics

$$\rho_t + \partial_{\tilde{x}}(\rho c) = 0, \quad c_t + c c_{\tilde{x}} + \frac{1}{\rho}\partial_{\tilde{x}} P(\rho, s) = 0, \quad s_t + c s_{\tilde{x}} = 0 \tag{51}$$

with the special equation of state $P = s - 1/\rho$ generalizing isentropic Chaplygin gas [see Refs. 29 and 19].

To calculate the transformed Hamiltonian operators (3), we introduce the conformal metric (9),

$$d\tilde{s}^2 = \frac{ds^2}{B^2} = (2w + v - u)^{-2}\left(\frac{du^2}{f(u)} + \frac{dv^2}{\varphi(v)} + \frac{dw^2}{\psi(w)}\right),$$

which is no longer flat in general. Following the recipe of Theorem 1, we introduce the Hamiltonian flow generated by the Hamiltonian operator (3) and the Hamiltonian density $B = w + \frac{1}{2}(v - u)$. A simple computation gives the system

$$u_\tau=-f'(u)u_x,\quad v_\tau=\varphi'(v)v_x,\quad w_\tau=2\psi'(w)w_x, \tag{52}$$

which commutes with (47). To incorporate the time τ into the reciprocal transformation (48), we calculate the flux of the density B corresponding to the flow (52),

$$\tfrac{1}{2}(\nabla B)^2=\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)].$$

Thus, transformation (48) takes the form

$$d\tilde{x}=Bdx+Adt+\tfrac{1}{2}(\nabla B)^2d\tau=[w+\tfrac{1}{2}(v-u)]dx-\tfrac{1}{2}(v+u)dt+\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)]d\tau,$$

$$\tilde{t}=t,$$

so that the transformed flow (52) is

$$u_\tau=w^1u_{\tilde{x}},\quad v_\tau=w^2v_{\tilde{x}},\quad w_\tau=w^3w_{\tilde{x}}, \tag{53}$$

where

$$\begin{aligned}
w^1&=-\tfrac{1}{2}(2w+v-u)f'(u)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)],\\
w^2&=\tfrac{1}{2}(2w+v-u)\varphi'(v)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)],\\
w^3&=(2w+v-u)\psi'(w)-\tfrac{1}{2}[f(u)+\varphi(v)+4\psi(w)].
\end{aligned} \tag{54}$$

Notice that Eqs. (53) and (54) constitute a general commuting flow of the linearly degenerate system (49). According to Theorem 1, the system (49) is Hamiltonian,

$$\begin{pmatrix} u\\ v\\ w\end{pmatrix}_t=\tilde{J}\begin{pmatrix}\partial\tilde{h}/\partial u\\ \partial\tilde{h}/\partial v\\ \partial\tilde{h}/\partial w\end{pmatrix},$$

with nonlocal operators $\tilde{J}$ of the form

$$\begin{aligned}
&\frac{4}{\rho^2}\begin{pmatrix} f(u) & 0 & 0\\ 0 & \varphi(v) & 0\\ 0 & 0 & \psi(w)\end{pmatrix}\frac{d}{d\tilde{x}}\\
&\quad+\frac{2}{\rho}\begin{pmatrix} \frac{1}{\rho}f'(u)u_{\tilde{x}}+2f(u)\left(\frac{1}{\rho}\right)_{\tilde{x}} & -\varphi(v)u_{\tilde{x}}-f(u)v_{\tilde{x}} & -2\psi(w)u_{\tilde{x}}-f(u)w_{\tilde{x}}\\ \varphi(v)u_{\tilde{x}}+f(u)v_{\tilde{x}} & \frac{1}{\rho}\varphi'(v)v_{\tilde{x}}+2\varphi(v)\left(\frac{1}{\rho}\right)_{\tilde{x}} & -2\psi(w)v_{\tilde{x}}+\varphi(v)w_{\tilde{x}}\\ 2\psi(w)u_{\tilde{x}}+f(u)w_{\tilde{x}} & 2\psi(w)v_{\tilde{x}}-\varphi(v)w_{\tilde{x}} & \frac{1}{\rho}\psi'(w)v_{\tilde{x}}+2\psi(w)\left(\frac{1}{\rho}\right)_{\tilde{x}}\end{pmatrix}\\
&\quad+\begin{pmatrix} w^1u_{\tilde{x}} & u_{\tilde{x}}\\ w^2v_{\tilde{x}} & v_{\tilde{x}}\\ w^3w_{\tilde{x}} & w_{\tilde{x}}\end{pmatrix}\left(\frac{d}{d\tilde{x}}\right)^{-1}\begin{pmatrix} u_{\tilde{x}} & v_{\tilde{x}} & w_{\tilde{x}}\\ w^1u_{\tilde{x}} & w^2v_{\tilde{x}} & w^3w_{\tilde{x}}\end{pmatrix}
\end{aligned} \tag{55}$$

and the Hamiltonian densities

$$\tilde{h}=h/B=\frac{\rho}{8}\left(\left[\int^{u}\frac{d\nu}{\sqrt{f(\nu)}}\right]^2-\left[\int^{v}\frac{d\nu}{\sqrt{\varphi(\nu)}}\right]^2\right),$$

where $2w+v-u=2/\rho$ [see (50)]. We point out that the corresponding metric (9) is flat if and only if

$$f(u)=\varepsilon u+\alpha,\quad \varphi(v)=\varepsilon v+\beta,\quad \psi(w)=-\frac{\varepsilon}{2}w+\gamma,$$

where the constants α, β, γ and ε are constrained by $\alpha+\beta+4\gamma=0$. In this case $w^1=w^2=w^3=0$, so that the corresponding operators (55) are local, thus providing three nonequivalent Hamiltonian structures of Dubrovin–Novikov type.

IV. RECIPROCAL TRANSFORMATIONS WHICH CHANGE BOTH *x* AND *t*

Consider again the Hamiltonian system (1),

$$u^i_t=v^i_j(u)u^j_x=(\nabla^i\nabla_j h)u^j_x=J^{ij}\frac{\partial h}{\partial u^j},$$

with the local Hamiltonian operator

$$J^{ij}=g^{ij}\frac{d}{dx}-g^{is}\Gamma^j_{sk}u^k_x$$

corresponding to the flat metric g^{ij}. In this section we discuss the behavior of Hamiltonian operators (2) under general reciprocal transformations

$$d\tilde{x}=B(u)dx+A(u)dt,\quad d\tilde{t}=N(u)dx+M(u)dt$$

of the form (3) which map system (1) to the system (4),

$$u^i_{\tilde{t}}=\tilde{v}^i_j(u)u^j_{\tilde{x}},\quad \tilde{v}=(Bv-AE)(ME-Nv)^{-1},\quad E=id.$$

First of all, we introduce the transformed metric

$$\tilde{g}_{ij}=\frac{(M\delta^s_i-Nv^s_i)(M\delta^r_j-Nv^j_r)}{(BM-AN)^2}g_{sr},\tag{56}$$

which is no longer flat in general. This metric will generate the local part of the transformed Hamiltonian operator $\tilde{J}$.

Remark: In the particular case of reciprocal transformations changing only the variable x, we have $N=0$, $M=1$ so that formula (56) reduces to the conformal transformation

$$\tilde{g}_{ij}=g_{ij}/B^2.$$

Similarly, if we interchange the independent variables (that is, if $A=N=1$, $B=M=0$), we have

$$\tilde{g}_{ij}=v^s_i g_{sr}v^r_j,$$

which coincides with the formula proposed in Ref. 28. Notice that in the second case the metric $\tilde{g}_{ij}$ is automatically flat, which means that the local Hamiltonian formalism is invariant under the interchange of independent variables.

To calculate the nonlocal "tail" of the transformed operator $\widetilde{J}$, we introduce the Hamiltonian flows

$$u^i_\tau=(\nabla^i\nabla_j N)u^j_x=J^{ij}\frac{\partial N}{\partial u^j} \tag{57}$$

and

$$u^i_\zeta=(\nabla^i\nabla_j B)u^j_x=J^{ij}\frac{\partial B}{\partial u^j}, \tag{58}$$

generated by the Hamiltonian operator J^{ij} and the Hamiltonian densities N and B which enter the reciprocal transformation (3). Clearly, systems (57) and (58) commute with (1). To incorporate the times τ and ζ into the reciprocal transformation (3), we calculate the fluxes P, Q and R, S of the Hamiltonian densities B and N,

$$d\tilde{x}=Bdx+Adt+Pd\tau+Qd\zeta,$$

$$d\tilde{t}=Ndx+Mdt+Rd\tau+Sd\zeta,$$

that is, the coefficients which make these one-forms closed by virtue of (1), (57) and (58). Here

$$Q=\tfrac{1}{2}(\nabla B)^2=\tfrac{1}{2}g^{ij}B_iB_j,$$

$$R=\tfrac{1}{2}(\nabla N)^2=\tfrac{1}{2}g^{ij}N_iN_j,$$

(see Ref. 28) and P, S are normalized as

$$P+S=(\nabla B,\nabla N)=g^{ij}B_iN_j.$$

Therefore, the transformed flows (57) and (58) take the forms

$$u^i_\tau=\mu^i_j(u)u^j_{\tilde{x}} \tag{59}$$

and

$$u^i_\zeta=\lambda^i_j(u)u^j_{\tilde{x}}, \tag{60}$$

where the matrices μ^i_j and λ^i_j are

$$\mu^i_j=B\nabla^i\nabla_jN-P\delta^i_j+N\tilde{v}^k_j\nabla^i\nabla_kN-R\tilde{v}^i_j \tag{61}$$

and

$$\lambda^i_j=B\nabla^i\nabla_jB-Q\delta^i_j+N\tilde{v}^k_j\nabla^i\nabla_kB-S\tilde{v}^i_j, \tag{62}$$

respectively [these formulas readily follow from (57) and (58) after one changes from x, t, τ, ζ to $\tilde{x}$, $\tilde{t}$, τ, ζ]. The transformed flows (59) and (60) commute with (4). Now we can formulate the main result of this section.

Theorem 3: *After the reciprocal transformation* (3), *the local Hamiltonian operator* (2) *corresponding to the flat metric* g^{ij} *becomes nonlocal of the form*

$$\tilde{J}^{ij}=\tilde{g}^{ij}\frac{d}{d\tilde{x}}-\tilde{g}^{is}\tilde{\Gamma}^{j}_{sk}u^{k}_{\tilde{x}}+\lambda^{i}_{k}u^{k}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}u^{j}_{\tilde{x}}+u^{i}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\lambda^{j}_{k}u^{k}_{\tilde{x}}$$
$$+\mu^{i}_{k}u^{k}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\tilde{v}^{j}_{n}u^{n}_{\tilde{x}}+\tilde{v}^{i}_{n}u^{n}_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\mu^{j}_{k}u^{k}_{\tilde{x}}.$$

Here the local part is defined by the metric $\tilde{g}^{ij}$ given by (56), $\tilde{\Gamma}$ is the Levi-Civita connection of $\tilde{g}$, and the nonlocal terms λ^{i}_{j}, μ^{i}_{j} and $\tilde{v}^{i}_{j}$ are defined in (61), (62) and (4). In particular, the curvature tensor of $\tilde{g}^{ij}$ is

$$\tilde{R}^{ij}_{kl}=\lambda^{i}_{k}\delta^{j}_{l}+\lambda^{j}_{l}\delta^{i}_{k}-\lambda^{j}_{k}\delta^{i}_{l}-\lambda^{i}_{l}\delta^{j}_{k}+\mu^{i}_{k}\tilde{v}^{j}_{l}+\mu^{j}_{l}\tilde{v}^{i}_{k}-\mu^{j}_{k}\tilde{v}^{i}_{l}-\mu^{i}_{l}\tilde{v}^{j}_{k}.$$

The proof of Theorem 3 will follow from general results of Sec. V.

As an illustration of this procedure, we explicitly calculate nonlocal Hamiltonian operators associated with the three-component linearly degenerate system (10).

Example 3: We start with the same linear system (47) as in Example 2,

$$u_t=u_x,\qquad v_t=-v_x,\qquad w_t=0,$$

which possesses infinitely many Hamiltonian structures with operators

$$J=\begin{pmatrix} f(u) & 0 & 0\\ 0 & \varphi(v) & 0\\ 0 & 0 & \frac{1}{4}\psi(w)\end{pmatrix}\frac{d}{dx}+\frac{1}{2}\begin{pmatrix} f'u_x & 0 & 0\\ 0 & \varphi'v_x & 0\\ 0 & 0 & \frac{1}{4}\psi'w_x\end{pmatrix} \tag{63}$$

corresponding to flat metrics

$$ds^2=\frac{du^2}{f(u)}+\frac{dv^2}{\varphi(v)}+4\frac{dw^2}{\psi(w)} \tag{64}$$

[here $f(u)$, $\varphi(v)$ and $\psi(w)$ are arbitrary functions; the multiple 4 is chosen for convenience].

Consider the reciprocal transformation

$$\begin{aligned} d\tilde{x}&=Bdx+Adt=(2w^2-u^2-v^2)dx+(v^2-u^2)dt,\\ d\tilde{t}&=Ndx+Mdt=(u+v-2w)dx+(u-v)dt,\end{aligned} \tag{65}$$

which maps system (47) to the three-component linearly degenerate semi-Hamiltonian system

$$u^{\sim}_{\tilde{t}}=(v+w)u_{\tilde{x}},\quad v^{\sim}_{\tilde{t}}=(u+w)v_{\tilde{x}},\quad w^{\sim}_{\tilde{t}}=(u+v)w_{\tilde{x}}. \tag{66}$$

The transformed metric (64) [apply formula (56)],

$$d\tilde{s}^2=\frac{du^2}{(u-v)^2(u-w)^2f(u)}+\frac{dv^2}{(v-u)^2(v-w)^2\varphi(v)}+\frac{dw^2}{(w-u)^2(w-v)^2\psi(w)}, \tag{67}$$

is no longer flat for generic $f(u)$, $\varphi(v)$ and $\psi(w)$. The commuting flows of system (47) generated by the Hamiltonian densities $N=u+v-2w$ and $B=2w^2-u^2-v^2$ are

$$u_\tau=\tfrac{1}{2}f'u_x,\quad v_\tau=\tfrac{1}{2}\varphi'v_x,\quad w_\tau=-\tfrac{1}{4}\psi'w_x \tag{68}$$

and

$$u_\zeta=-(2f+uf')u_x,\quad v_\zeta=-(2\varphi+v\varphi')v_x,\quad w_\zeta=(\psi+\tfrac{1}{2}w\psi')w_x, \tag{69}$$

respectively. To incorporate the times τ and ζ into the reciprocal transformation (65), we have to calculate the fluxes P, Q and R, S of the Hamiltonian densities B and N,

$$\begin{aligned} d\tilde{x}&=Bdx+Adt+Pd\tau+Qd\zeta,\\ d\tilde{t}&=Ndx+Mdt+Rd\tau+Sd\zeta, \end{aligned} \tag{70}$$

that is, the coefficients which make these one-forms closed by virtue of (47), (68) and (69). Here

$$Q=\tfrac{1}{2}(\nabla B)^2=2[u^2f(u)+v^2\varphi(v)+w^2\psi(w)],$$

$$R=\tfrac{1}{2}(\nabla N)^2=\tfrac{1}{2}[f(u)+\varphi(v)+\psi(w)],$$

while P and S are of the form

$$P=-uf-v\varphi-w\psi+\int^u f(\nu)\mathrm{d}\nu+\int^v \varphi(\nu)\mathrm{d}\nu+\int^w \psi(\nu)\mathrm{d}\nu,$$

$$S=-uf-v\varphi-w\psi-\int^u f(\nu)\mathrm{d}\nu-\int^v \varphi(\nu)\mathrm{d}\nu-\int^w \psi(\nu)\mathrm{d}\nu,$$

respectively. Notice that $P+S=(\nabla B,\,\nabla N)=g^{ij}B_iN_j$. Under the extended reciprocal transformation (70), the commuting flows (68) and (69) take the form

$$u_\tau=\mu^1u_{\tilde{x}},\quad v_\tau=\mu^2v_{\tilde{x}},\quad w_\tau=\mu^3w_{\tilde{x}} \tag{71}$$

and

$$u_\zeta=\lambda^1u_{\tilde{x}},\quad v_\zeta=\lambda^2v_{\tilde{x}},\quad w_\zeta=\lambda^3w_{\tilde{x}}, \tag{72}$$

where the characteristic speeds are

$$\mu^1=-\tfrac{1}{2}(u-v)(u-w)f'-(v+w)R-P,$$

$$\mu^2=-\tfrac{1}{2}(v-u)(v-w)\varphi'-(u+w)R-P,$$

$$\mu^3=-\tfrac{1}{2}(w-u)(w-v)\psi'-(u+v)R-P,$$

and

$$\lambda^1=(u-v)(u-w)(2f+uf')-(v+w)S-Q,$$

$$\lambda^2=(v-u)(v-w)(2\varphi+v\varphi')-(u+w)S-Q,$$

$$\lambda^3=(w-u)(w-v)(2\psi+w\psi')-(u+v)S-Q,$$

respectively. The transformed flows (71) and (72) commute with (66). According to Theorem 2, the transformed metric (67) and the transformed flows (71) and (72) generate the nonlocal Hamiltonian operator which, in matrix form, is

$$\tilde{J}=\begin{pmatrix}\tilde{g}^{11}&0&0\\0&\tilde{g}^{22}&0\\0&0&\tilde{g}^{33}\end{pmatrix}\frac{d}{d\tilde{x}}$$
$$+\begin{pmatrix}\tilde{g}^{11}\left[\frac{f'(u)}{2f(u)}u_{\tilde{x}}+\frac{u_{\tilde{x}}-v_{\tilde{x}}}{u-v}+\frac{u_{\tilde{x}}-w_{\tilde{x}}}{u-w}\right] & \frac{\tilde{g}^{22}u_{\tilde{x}}+\tilde{g}^{11}v_{\tilde{x}}}{u-v} & \frac{\tilde{g}^{33}u_{\tilde{x}}+\tilde{g}^{11}w_{\tilde{x}}}{u-w}\\ -\frac{\tilde{g}^{22}u_{\tilde{x}}+\tilde{g}^{11}v_{\tilde{x}}}{u-v} & \tilde{g}^{22}\left[\frac{\varphi'(v)}{2\varphi(v)}v_{\tilde{x}}+\frac{u_{\tilde{x}}-v_{\tilde{x}}}{u-v}+\frac{v_{\tilde{x}}-w_{\tilde{x}}}{v-w}\right] & \frac{\tilde{g}^{33}v_{\tilde{x}}+\tilde{g}^{22}w_{\tilde{x}}}{v-w}\\ -\frac{\tilde{g}^{33}u_{\tilde{x}}+\tilde{g}^{11}w_{\tilde{x}}}{u-w} & -\frac{\tilde{g}^{33}v_{\tilde{x}}+\tilde{g}^{22}w_{\tilde{x}}}{v-w} & \tilde{g}^{33}\left[\frac{\psi'(w)}{2\psi(w)}w_{\tilde{x}}+\frac{w_{\tilde{x}}-v_{\tilde{x}}}{w-v}+\frac{u_{\tilde{x}}-w_{\tilde{x}}}{u-w}\right]\end{pmatrix}$$
$$+\begin{pmatrix}\lambda^1u_{\tilde{x}}&\mu^1u_{\tilde{x}}&\eta^1v_{\tilde{x}}&u_{\tilde{x}}\\ \lambda^2v_{\tilde{x}}&\mu^2v_{\tilde{x}}&\eta^2v_{\tilde{x}}&v_{\tilde{x}}\\ \lambda^3w_{\tilde{x}}&\mu^3w_{\tilde{x}}&\eta^3w_{\tilde{x}}&w_{\tilde{x}}\end{pmatrix}\left(\frac{d}{d\tilde{x}}\right)^{-1}\begin{pmatrix}u_{\tilde{x}}&v_{\tilde{x}}&w_{\tilde{x}}\\ \eta^1u_{\tilde{x}}&\eta^2v_{\tilde{x}}&\eta^3w_{\tilde{x}}\\ \mu^1u_{\tilde{x}}&\mu^2v_{\tilde{x}}&\mu^3w_{\tilde{x}}\\ \lambda^1u_{\tilde{x}}&\lambda^2v_{\tilde{x}}&\lambda^3w_{\tilde{x}}\end{pmatrix},$$

where $\tilde{g}^{ii}$ are components of the transformed metric (67), $\eta^1=v+w$, $\eta^2=u+w$ and $\eta^3=u+v$ are the characteristic speeds of system (66), and λ^k, μ^k are the characteristic speeds of its commuting flows (71) and (72). In the particular case $f(u)=\alpha$, $\varphi(v)=\beta$ and $\psi(w)=\gamma$, where α, β, γ are constants subject to a single constraint $\alpha+\beta+\gamma=0$, we have $\lambda^k=\mu^k=0$, so that the transformed operator takes the local Dubrovin–Novikov form, the corresponding flat metric being

$$d\tilde{s}^2=\frac{du^2}{\alpha(u-v)^2(u-w)^2}+\frac{dv^2}{\beta(v-u)^2(v-w)^2}+\frac{dw^2}{\gamma(w-u)^2(w-v)^2}.$$

As shown in Ref. 23, these are the only local Hamiltonian structures of hydrodynamic type of the three-component system (66).

Remark: Modifying the reciprocal transformation (65) from Example 3 as

$$d\tilde{x}=[2R(w)-P(u)-Q(v)]dx+[Q(v)-P(u)]dt,$$

$$d\tilde{t}=[A(u)+B(v)-2C(w)]dx+[A(u)-B(v)]dt,$$

we obtain the transformed system

$$u_{\tilde{t}}=\frac{R(w)-Q(v)}{C(w)-B(v)}u_{\tilde{x}},\quad v_{\tilde{t}}=\frac{P(u)-R(w)}{A(u)-C(w)}v_{\tilde{x}},\quad w_{\tilde{t}}=\frac{Q(v)-P(u)}{B(v)-A(u)}w_{\tilde{x}},\tag{73}$$

where $A(u)$, $B(v)$, $C(w)$ and $P(u)$, $Q(v)$, $R(w)$ are arbitrary functions. As shown in Ref. 12, formulas (73) define a general three-component linearly degenerate semi-Hamiltonian system. Repeating the construction of Example 3, one can obtain the associated family of nonlocal Hamiltonian structures.

V. GENERALIZED RECIPROCAL TRANSFORMATIONS

Consider N commuting flows of hydrodynamic type

$$R^i_{t^\beta}=v^i_\beta(R)R^i_{t^1},\quad i=1,2,\ldots n,\quad \beta=1,2,\ldots,N,\tag{74}$$

where we have set $t^1\equiv x$ and $t^2\equiv t$ (so that $v^i_1\equiv 1$). We assume that the flows (74) are Hamiltonian with the local Hamiltonian operator (2) generated by the flat metric $ds^2=g_{ii}(R)dR^{i^2}$, so that $v^i_\beta=\nabla^i\nabla_i h_\beta$, where h_β are the corresponding Hamiltonian densities. Let us change from t^1, $t^2,\ldots,t^N$ to the new independent variables $\tilde{t}^1$, $\tilde{t}^2,\ldots,\tilde{t}^N$ defined as

$$d\tilde{t}^\gamma=a^\gamma_\beta(R)dt^\beta,\quad \gamma,\beta=1,2,\ldots N,\tag{75}$$

where $a_1^\gamma(R)$ are the conserved densities of systems (74), and $a_\beta^\gamma(R)$ are the corresponding fluxes:

$$\partial_{t^\beta} a_1^\gamma = \partial_{t^1} a_\beta^\gamma. \tag{76}$$

Transformations of the type (75) naturally generalize reciprocal transformations (the case $N=2$). Under the *generalized* reciprocal transformation (75), the commuting flows (74) transforms to

$$R^i_{\tilde{t}^\beta} = \tilde{v}^i_\beta(R) R^i_{\tilde{t}^1}, \tag{77}$$

where

$$\tilde{v}^i_\beta = \frac{A^\gamma_\beta v^i_\gamma}{A^\nu_1 v^i_\nu}, \tag{78}$$

while the metric ds^2 transforms to

$$d\tilde{s}^2 = \tilde{g}_{ii} dR^{i^2}, \quad \tilde{g}_{ii} = g_{ii}(A^\nu_1 v^i_\nu)^2. \tag{79}$$

Here A^β_γ is the inverse of a^ν_β,

$$dt^\beta = A^\beta_\gamma d\tilde{t}^\gamma. \tag{80}$$

We emphasize that the transformed metric $d\tilde{s}^2$ is no longer flat in general. In the particular case $N=2$ formula (79) reduces to (56). To calculate the curvature tensor of the metric $d\tilde{s}^2$ we introduce N extra flows

$$R^i_{\tau^\gamma} = w^i_\gamma(R) R^i_{t^1}, \quad i=1,2,\ldots,n, \quad \gamma=1,2,\ldots,N, \tag{81}$$

generated by the Hamiltonian operator (2) and the Hamiltonian densities $a_1^\beta(R)$:

$$w^i_\beta = \nabla^i \nabla_i a_1^\beta.$$

Clearly, the flows (81) commute with (74). To calculate the transformed flows (81), we have to incorporate the times τ^β into the generalized reciprocal transformation (75), namely,

$$d\tilde{t}^\gamma = a^\gamma_\beta dt^\beta + c^\gamma_\beta d\tau^\beta, \quad \gamma,\beta = 1,2,\ldots,N.$$

Here the fluxes c^γ_β are restricted by

$$c^\beta_\gamma + c^\gamma_\beta = (\nabla a_1^\beta, \quad \nabla a_1^\gamma) = \sum g^{kk} (\partial_k a_1^\beta)(\partial_k a_1^\gamma), \tag{82}$$

where $(\nabla f, \nabla g)$ denotes a scalar product of the gradients of f and g in the metric ds^2. Finally, the transformed flows (81) take the form

$$R^i_{\tau^\gamma} = \tilde{w}^i_\gamma(R) R^i_{\tilde{t}^1}, \tag{83}$$

with

$$\tilde{w}^i_\gamma = \frac{w^i_\gamma - c^\beta_\gamma A^\varepsilon_\beta v^i_\varepsilon}{A^\nu_1 v^i_\nu}. \tag{84}$$

Theorem 4: *The curvature tensor of the transformed metric $d\tilde{s}^2$ is*

$$\tilde{R}^{ij}_{ij}=\sum_{\beta=1}^{N}(\tilde{v}^i_\beta\tilde{w}^j_\beta+\tilde{v}^j_\beta\tilde{w}^i_\beta).$$

The metric $d\tilde{s}^2$ generates the nonlocal Hamiltonian operator

$$\tilde{J}^{ij}=\tilde{g}^{ii}\delta^{ij}\frac{d}{d\tilde{x}}-\tilde{g}^{ii}\tilde{\Gamma}^j_{ik}R^k_{\tilde{x}}+\sum_{\beta=1}^{N}\tilde{v}^i_\beta R^i_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\tilde{w}^j_\beta R^j_{\tilde{x}}+\sum_{\beta=1}^{N}\tilde{w}^i_\beta R^i_{\tilde{x}}\left(\frac{d}{d\tilde{x}}\right)^{-1}\tilde{v}^j_\beta R^j_{\tilde{x}}.$$

Proof: Let us introduce the Lame coefficients $H_{1i}=\sqrt{g_{ii}}$ and the rotation coefficients $\beta_{ik}=\partial_i H_{1k}/H_{1i}$ (for any $i\neq k$). According to Ref. 28, the linear problem

$$\partial_i H_k=\beta_{ik}H_i,\quad i\neq k,$$

has N particlular solutions $H_{\beta i}$, where $H_{\beta i}=v^i_\beta H_{1i}$, and N other solutions H^β_i, where $H^\beta_i=w^i_\beta H_{1i}$. Since commuting flows (74) and (81) are locally Hamiltonian ($v^i_\beta=\nabla^i\nabla_i h_\beta$ and $w^i_\beta=\nabla^i\nabla_i a^\beta_1$), the relationship between conserved densities (h_β and a^β_1) and the corresponding commuting flows (v^i_β and w^i_β) can be written as

$$H_{\beta i}=\psi_{\beta i,i}+\sum_{m\neq i}\beta_{mi}\psi_{\beta m},\quad H^\beta_i=\psi^\beta_{i,i}+\sum_{m\neq i}\beta_{mi}\psi^\beta_m, \tag{85}$$

where $\psi_{\beta i}$ and ψ^β_i are defined by the equations $\partial_i h_\beta=\psi_{\beta i}H_{1i}$ and $\partial_i a^\beta_1=\psi^\beta_i H_{1i}$. In this notation the formulas (78), (84) and (79) become

$$\tilde{H}_{\beta i}=A^\gamma_\beta H_{\gamma i},\quad \tilde{H}^\beta_i=H^\beta_i-\tilde{H}_{\gamma i}c^\gamma_\beta$$

(where $\tilde{v}^i_\beta=\tilde{H}_{\beta i}/\tilde{H}_{1i}$ and $\tilde{w}^i_\beta=\tilde{H}^\beta_i/\tilde{H}_{1i}$) and the transformed rotation coefficients are

$$\tilde{\beta}_{ik}=\beta_{ik}-\psi^\beta_i\tilde{H}_{\beta k}.$$

Since the metric ds^2 is flat, the curvature components R^i_{jik} ($i\neq j\neq k$) vanish identically, that is, $\partial_i\beta_{jk}=\beta_{ji}\beta_{ik}$ ($i\neq j\neq k$). This identity is preserved under generalized reciprocal transformations: $\partial_i\tilde{\beta}_{jk}=\tilde{\beta}_{ji}\tilde{\beta}_{ik}$. However, the components $\tilde{R}^{ij}_{ij}$ defined as

$$\tilde{R}^{ij}_{ij}=-\frac{\tilde{\Delta}_{ij}}{\tilde{H}_{1i}\tilde{H}_{1j}},$$

where

$$\tilde{\Delta}_{ij}\equiv\partial_i\tilde{\beta}_{ij}+\partial_j\tilde{\beta}_{ji}+\sum_{m\neq i}\tilde{\beta}_{mi}\tilde{\beta}_{mj},$$

will no longer be zero. Indeed,

$$\begin{aligned}\tilde{\Delta}_{ij}&=\partial_i\tilde{\beta}_{ij}+\partial_j\tilde{\beta}_{ji}+\sum_{m\neq i\neq k}\tilde{\beta}_{mi}\tilde{\beta}_{mj}\\&=\partial_i[\beta_{ij}-\psi^\gamma_i\tilde{H}_{\gamma j}]+\partial_j[\beta_{ji}-\psi^\gamma_j\tilde{H}_{\gamma i}]+\sum_{m\neq i\neq j}(\beta_{mi}-\psi^\gamma_m\tilde{H}_{\gamma i})(\beta_{mj}-\psi^\beta_m\tilde{H}_{\beta j})\\&=\Delta_{ij}-\tilde{H}_{\gamma j}\left[\psi^\gamma_{i,i}+\sum_{m\neq i}\beta_{mi}\psi^\gamma_m\right]\end{aligned}$$

$$-\tilde{H}_{\gamma i}\left[\psi^{\gamma}_{j,j}+\sum_{m\neq j}\beta_{mj}\psi^{\gamma}_{m}\right]+\tilde{H}_{\beta i}\tilde{H}_{\gamma j}\sum\ \psi^{\beta}_{m}\psi^{\gamma}_{m}.$$

Since $\Delta_{ij}\equiv 0$, Eqs. (85) and (82) imply

$$\begin{aligned}\tilde{\Delta}_{ij}&=-\tilde{H}_{\gamma j}H^{\gamma}_{i}-\tilde{H}_{\gamma i}H^{\gamma}_{j}+\tilde{H}_{\gamma i}\tilde{H}_{\beta j}(c^{\beta}_{\gamma}+c^{\gamma}_{\beta})\\&=-\tilde{H}_{\beta j}[H^{\beta}_{i}-\tilde{H}_{\gamma i}c^{\gamma}_{\beta}]-\tilde{H}_{\beta j}[H^{\beta}_{i}-\tilde{H}_{\gamma i}c^{\gamma}_{\beta}]\\&=-\tilde{H}_{\beta j}\tilde{H}^{\beta}_{i}-\tilde{H}_{\beta i}\tilde{H}^{\beta}_{j}.\end{aligned}$$

Thus, the transformed curvature tensor is

$$\tilde{R}^{ij}_{ij}=-\frac{1}{\tilde{H}_{1i}\tilde{H}_{1j}}\tilde{\Delta}_{ij}=\frac{\tilde{H}_{\beta j}\tilde{H}^{\beta}_{i}+\tilde{H}_{\beta i}\tilde{H}^{\beta}_{j}}{\tilde{H}_{1i}\tilde{H}_{1j}}=\tilde{v}^{i}_{\beta}\tilde{w}^{j}_{\beta}+\tilde{v}^{j}_{\beta}\tilde{w}^{i}_{\beta}.$$

For $N=2$ this proves Theorem 2 formulated in Sec. IV.

As shown in Ref. 12, any linearly degenerate semi-Hamiltonian system in Riemann invariants can be linearized by a generalized reciprocal transformation. Applying the results of Sec. V to local Hamiltonian structures of a linear system, one can explicitly construct an infinity of mutually compatible nonlocal Hamiltonian structures for an arbitrary linearly degenerate semi-Hamiltonian system in the same way as it was done in Examples 1–3. In the example below we explicitly construct nonlocal Hamiltonian formalism for the n-component linearly degenerate system mentioned in the abstract.

Example 4: As shown in Ref. 12, the linearly degenerate semi-Hamiltonian system

$$R^{i}_{\tilde{t}^2}=\left(R^{i}-\sum_{m=1}^{n}R^{m}\right)R^{i}_{\tilde{t}^1},\quad i=1,2,\ldots,n, \tag{86}$$

and its linearly degenerate commuting flows

$$R^{i}_{\tilde{t}^{\beta}}=(-1)^{\beta+1}(\partial_i\tilde{h}_{\beta})R^{i}_{\tilde{t}^1},\quad i=1,2,\ldots,n,\quad \beta=3,4,\ldots,n,$$

where

$$\tilde{h}=\prod_{k=1}^{n}(1+\lambda R^{k})=1+\lambda\tilde{h}_1+\lambda^2\tilde{h}_2+\lambda^3\tilde{h}_3+\cdots+\lambda^n\tilde{h}_n,$$

can be obtained from a set of commuting linear flows

$$R^{i}_{t^{\beta}}=(\varepsilon^{i})^{\beta-1}R^{i}_{t^1},\quad \beta=1,2,\ldots,n$$

(ε^{i} are arbitrary constants) by a generalized reciprocal transformation,

$$d\tilde{t}^{\beta}=a^{\beta}_{\gamma}dt^{\gamma},$$

where

$$a^{\beta}_{\gamma}=\sum_{k=1}^{n}(\varepsilon^{k})^{\gamma-1}(R^{k})^{n-\beta}.$$

In the two- and three-component cases the explicit form of this transformation is stated in Examples 1 and 3. The inverse reciprocal transformation is

$$dt^{\beta}=A^{\beta}_{\gamma}d\tilde{t}^{\gamma},$$

where

$$A^{\beta}_{\gamma}=\sum_{k=1}^{n}(-1)^{n+\gamma+\beta+1}\frac{\partial_k\tilde{\varepsilon}_{n+1-\gamma}}{\Pi^{n}_{m\neq k}(\varepsilon^k-\varepsilon^m)}\frac{\partial_k\tilde{h}_{\beta}}{\Pi^{n}_{s\neq k}(R^k-R^s)}$$

and

$$\tilde{\varepsilon}=\prod_{k=1}^{n}(1+\lambda\varepsilon^k)=1+\lambda\tilde{\varepsilon}_1+\lambda^2\tilde{\varepsilon}_2+\lambda^3\tilde{\varepsilon}_3+\cdots+\lambda^n\tilde{\varepsilon}_n.$$

Applying Theorem 4 to local Hamiltonian structures of the corresponding linear systems, we obtain infinitely many nonlocal Hamiltonian operators associated with the system (86):

$$A^{ij}=g^{ii}\delta^{ij}\frac{d}{dx}-g^{ii}\Gamma^{j}_{ik}R^k_x+\sum_{\beta=1}^{n-1}\left[\tilde{v}^i_{\beta}R^i_x\left(\frac{d}{dx}\right)^{-1}\tilde{w}^j_{\beta}R^j_x+\tilde{w}^i_{\beta}R^i_x\left(\frac{d}{dx}\right)^{-1}\tilde{v}^j_{\beta}R^j_x\right]. \tag{87}$$

Here $g_{ii}(dR^i)^2$ is the diagonal metric of the form

$$\frac{dR^{1^2}}{\Pi_{k\neq 1}(R^1-R^k)f^1(R^1)}+\cdots+\frac{dR^{n^2}}{\Pi_{k\neq n}(R^n-R^k)f^n(R^n)}, \tag{88}$$

with the curvature tensor

$$\tilde{R}^{ik}_{ik}=\sum_{\beta=1}^{n-1}(\tilde{v}^i_{\beta}\tilde{w}^k_{\beta}+\tilde{v}^k_{\beta}\tilde{w}^i_{\beta}),$$

where

$$\tilde{v}^i_{\beta}=\partial_i\tilde{h}_{\beta},$$

$$\tilde{w}^i_{\beta}=(n-\beta)\prod_{k\neq i}(R^i-R^k)\left[\frac{1}{2}f_i'(R^i)(R^i)^{n-\beta-1}+(n-\beta-1)f_i(R^i)(R^i)^{n-\beta-2}\right]-\sum_{\gamma=1}^{n-1}\tilde{v}^i_{\gamma}c^{\gamma}_{\beta},$$

$$\partial_i c^{\gamma}_{\beta}=(n-\beta)(n-\gamma)\left[\tfrac{1}{2}f_i'(R^i)(R^i)^{2n-\beta-\gamma-2}+(n-\beta-1)f_i(R^i)(R^i)^{2n-\beta-\gamma-3}\right].$$

Operators (87) depend on n arbitrary functions $f^1(R^1),\ \ldots,\ f^n(R^n)$, and are mutually compatible. It was demonstrated in Ref. 23 that the metric (88) is not flat for $n\geqslant 4$, whatever $f^i(R^i)$ are.

ACKNOWLEDGMENTS

We thank the Royal Society for their financial support of M.V.P. to Loughborough, making this collaboration possible. M.V.P. is also partially supported by the Russian Foundation for Fundamental Research (Grant Nos. 00-01-00210 and 00-01-00366).

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Involution analysis of the partial differential equations characterizing Hamiltonian vector fields

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(Received 4 February 2002; accepted 8 November 2002)

In a recent article, certain underdetermined linear systems of partial differential equations connected with Lie–Poisson structures have been studied. They were constructed via power series solutions of the evolution equation for a given Hamiltonian. We extend the results to arbitrary Poisson manifolds, correct an error in the case of degenerate Poisson structures, and show that these linear systems simply characterize Hamiltonian vector fields. Our basic tool is the formal theory of differential equations with its central concept of an involutive system. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1536021]

I. INTRODUCTION

In a recent article, Bender *et al.*[1] studied certain underdetermined linear systems of partial differential equations connected with Lie–Poisson structures. These systems arose from considering power series solutions of the corresponding evolution equations. In the present work their results are extended to arbitrary Poisson manifolds and the relation to Poisson geometry is clarified. In particular, it turns out that these systems are simply the equations characterizing the Hamiltonian vector fields on the manifold.

Furthermore, we correct an error in the cited work. For degenerate Poisson structures, i.e., if the Poisson matrix J is singular, the claimed expression is *not* the general solution of the underdetermined system; further solutions exist. Let us take for example the system related to the Lie–Poisson structure induced by the Lie algebra E_2:

$$\begin{aligned} y\frac{\partial G}{\partial z}+x\frac{\partial F}{\partial z}&=0\,,\\ y\frac{\partial H}{\partial z}+y\frac{\partial F}{\partial x}-x\frac{\partial F}{\partial y}-G&=0\,,\\ x\frac{\partial H}{\partial z}-y\frac{\partial G}{\partial x}+x\frac{\partial G}{\partial y}-F&=0\,. \end{aligned} \tag{1}$$

Bender *et al.*[1] claimed that its general solution was

$$F=-y\frac{\partial K}{\partial z},\quad G=x\frac{\partial K}{\partial z},\quad H=y\frac{\partial K}{\partial x}-x\frac{\partial K}{\partial y}, \tag{2}$$

with an arbitrary function $K(x,y,z)$. However, one easily checks that $F=c_1/x$, $G=c_2/y$ and $H=(c_1/x^2+c_2/y^2)z$ solves (1) for arbitrary values of the constants c_1, c_2 and only for $c_1=-c_2=c$ these expressions are contained in the solution family (2), namely for the choice $K=-cz/xy$. We will show that (2) represents the general solution only, if we augment (1) by the algebraic constraint $xF+yG=0$.

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Our basic tool will be the formal theory of differential equations.[2–4] Some elements of this theory are about a century old, but it still seems to be fairly unknown. In fact, Bender *et al.*[1] mentioned a number of questions concerning the arbitrariness of the general solution of a system of partial differential equations many of which can be answered with the help of the formal theory (see, e.g., Ref. 5).

A key concept within the formal theory is *involution*. For lack of space, we cannot give a detailed introduction but must refer to the above cited works. Any serious analysis of a system of differential equations not in Cauchy–Kovalevskaya form requires usually that the system is involutive. Involution comprises in particular the absence of integrability conditions. Any system can be completed to an involutive one (under some mild regularity assumptions). Fortunately, we do not have to bother with a completion, as it turns out that due to the properties of Poisson manifolds our system is already involutive.

In the next section those basic properties of Poisson manifolds that are needed later are reviewed. In Sec. III an underdetermined system of partial differential equations characterizing Hamiltonian vector fields is derived and the conditions under which it is involutive are analyzed. The relation to the work of Bender *et al.*[1] is found in Sec. IV, studying the fundamental power series solutions of the Hamiltonian evolution equation. Finally, after considering explicitly the case of the Lie–Poisson structure of E_2, some conclusions are given in Sec. VI.

II. POISSON MANIFOLDS

For easier comparison with the results presented by Bender *et al.*,[1] we use throughout local coordinates; the intrinsic theory of Poisson manifolds can be found in the book of Vaisman[6] (with an emphasis on the geometry; see also Ref. 7) or in the books of Marsden and Ratiu,[8] resp., Libermann and Marle[9] (with an emphasis on applications in mechanics).

A *Poisson manifold* is a (smooth) manifold M equipped with a bracket structure on the ring $\mathcal{F}(M)$ of smooth functions on M. This bracket $\{\cdot,\cdot\}:\mathcal{F}(M)\times\mathcal{F}(M)\to\mathcal{F}(M)$ must satisfy four axioms for arbitrary functions $F,G,H\in\mathcal{F}(M)$ and real constants λ,μ:

(i) $\{F,G\}=-\{G,F\}$ (skew-symmetry),
(ii) $\{\lambda F+\mu G,H\}=\lambda\{F,H\}+\mu\{G,H\}$ (linearity),
(iii) $\{FG,H\}=F\{G,H\}+\{F,H\}G$ (Leibniz rule),
(iv) $\{F,\{G,H\}\}+\{G,\{H,F\}\}+\{H,\{F,G\}\}=0$ (Jacobi identity).

Thus the ring $\mathcal{F}(M)$ acquires the structure of an infinite-dimensional Lie algebra.

In terms of local coordinates $(z^1,\ldots,z^n)$ on the manifold M, the bracket is uniquely determined by the *Poisson matrix* $J^{kl}=\{z^k,z^l\}$. For two arbitrary functions $F,G\in\mathcal{F}(M)$ we find $\{F,G\}=(\nabla F)^t J\nabla G$. The matrix J is obviously skew-symmetric and the Jacobi identity induces the following differential equations for its components:

$$J^{kl}\frac{\partial J^{ij}}{\partial z^l}+J^{il}\frac{\partial J^{jk}}{\partial z^l}+J^{jl}\frac{\partial J^{ki}}{\partial z^l}=0\,,\quad 1\leqslant i,j,k\leqslant n\,. \tag{3}$$

In an intrinsic language, the Poisson bracket is defined in terms of the Poisson bivector $w\in\Lambda^2(TM)$ by $\{F,G\}=w(dF,dG)$. The matrix J is a coordinate representation of this bivector, $w=J^{kl}\partial_{z^k}\wedge\partial_{z^l}$, and the Jacobi identity (3) expresses the vanishing of the Schouten–Nijenhuis bracket of w with itself.

If the matrix J is regular (which obviously can only happen on even-dimensional manifolds), then M is in fact a symplectic manifold with the symplectic structure locally defined by the inverse of J. If $\mathcal{A}$ is an n-dimensional Lie algebra, then its dual space $\mathcal{A}^*$ carries a canonical *Lie–Poisson structure*. Since $T\mathcal{A}^*\cong\mathcal{A}^*\times\mathcal{A}^*$, we may identify for any smooth function $\phi\in\mathcal{F}(\mathcal{A}^*)$ at the point $\lambda\in\mathcal{A}^*$ the tangent map $T_\lambda\phi:\mathcal{A}^*\to\mathbb{R}$ with an element of $\mathcal{A}^{**}=\mathcal{A}$ and define for $\phi,\psi\in\mathcal{F}(\mathcal{A}^*)$,

$$\{\phi,\psi\}(\lambda)=\lambda([T_\lambda\phi,T_\lambda\psi])\,.$$

If C_{kl}^i denotes the structure constants of $\mathcal{A}$ for some basis $\{A_1,\ldots,A_n\}$, i.e. $[A_k,A_l]=C_{kl}^i A_i$, then in coordinates $(z_1,\ldots,z_n)$ with respect to the dual basis $\{A^1,\ldots,A^n\}$ of $\mathcal{A}^*$ the Poisson matrix is given by $J_{kl}=C_{kl}^i z_i$. It is trivial to check that it satisfies (3). Bender *et al.*[1] considered exclusively Poisson structures of this form.

A Poisson structure defines a homomorphism $\sharp: T^*M\to TM$ by $\omega_1(\omega_2^\sharp)=w(\omega_1,\omega_2)$ for arbitrary one-forms $\omega_1,\omega_2\in T^*M$. The structure w is *nondegenerate*, if $\sharp$ is an isomorphism or, equivalently, the Poisson matrix J is regular. More generally, the rank of a Poisson structure is defined as the dimension of $\operatorname{im}\sharp$ (we restrict here and in the sequel to the case that $\operatorname{im}\sharp$ defines a regular distribution on M). If $\operatorname{rank} w=n-r$, then r linearly independent one-forms $\chi^{(a)}=\chi_k^{(a)}\,dz^k$ exist on M such that $\ker\sharp=\langle\chi^{(1)},\ldots,\chi^{(r)}\rangle$. If a function $C\in\mathcal{F}(M)$ is such that $dC\in\ker\sharp$, then $\{C,F\}=0$ for all $F\in\mathcal{F}(M)$ and C is called a *Casimir function.*

We associate with any function $H\in\mathcal{F}(M)$ its *Hamiltonian vector field*,

$$X_H=(dH)^\sharp=\{\cdot,H\}=J^{kl}\frac{\partial H}{\partial z^l}\frac{\partial}{\partial z^k}.$$

For a Casimir function C, X_C is obviously the zero vector field. For later use, we introduce as a special case the short hand

$$X^{(k)}=X_{-z^k}=\{z^k,\cdot\}=J^{kl}\frac{\partial}{\partial z^l}.$$

The Poisson bracket may now conveniently be expressed with these fields:

$$\{F,G\}=\frac{\partial F}{\partial z^k}X^{(k)}G=-\frac{\partial G}{\partial z^k}X^{(k)}F.$$

The Hamiltonian vector fields form a Lie algebra under the Lie bracket. Indeed, one easily obtains for arbitrary functions $F,G,H\in\mathcal{F}(M)$ with the help of the Jacobi identity,

$$X_{\{F,G\}}(H)=\{H,\{F,G\}\}=\{\{H,F\},G\}-\{\{H,G\},F\}=[X_G,X_F](H). \tag{4}$$

Thus the mapping $F\mapsto X_F$ defines a Lie algebra *anti*homomorphism between $\mathcal{F}(M)$ and the Hamiltonian vector fields (if we had defined $X_F=\{F,\cdot\}$, we would have obtained a homomorphism[6]). It follows from (4) that the distribution $\operatorname{im}\sharp$ is involutive and thus defines a foliation of the manifold M. By a classical result in Poisson geometry, the leaves are $(n-r)$-dimensional symplectic manifolds, i.e., they carry a nondegenerate Poisson structure. Obviously, the codistribution $\ker\sharp$ is just the annihilator of $\operatorname{im}\sharp$.

A Hamiltonian vector field X_H may be written either in the form $X_H=(X^{(k)}H)\partial_{z^k}$ or as $X_H=-H_{z^k}X^{(k)}$. Thus the fields $X^{(k)}$ span the distribution $\operatorname{im}\sharp$ and (4) takes the form

$$[X^{(k)},X^{(l)}]=\frac{\partial J^{kl}}{\partial z^j}X^{(j)}. \tag{5}$$

Note that in the special case of a Lie–Poisson structure the vector fields $X^{(k)}$ provide us with a representation of the underlying Lie algebra, as then $\partial J_{kl}/\partial z_j=C_{kl}^j$.

The vector field X_H defines a dynamical system on the Poisson manifold M. We denote its flow by ϕ, i.e., ϕ is a map $\mathbb{R}\times M\to M$ (as we are only interested in local properties, we do not bother about the precise domain of definition of ϕ) and $\phi_z(t)=\phi(t,z)$ yields the integral curve of X_H passing through the point $z\in M$. A central property of Hamiltonian flows is that they preserve the Poisson structure. Indeed, it follows again from the Jacobi identity that for arbitrary functions $F,G,H\in\mathcal{F}(M)$,

$$(L_{X_H}w)(dF,dG)=X_H(w(dF,dG))-w(L_{X_H}dF,dG)-w(dF,L_{X_H}dG)$$
$$=X_H(\{F,G\})-\{X_HF,G\}-\{F,X_HG\}=0,$$

where L_X denotes the Lie derivative with respect to the vector field X. Thus $L_{X_H}w=0$ for every Hamiltonian vector field X_H.

If we consider how functions $F\in\mathcal{F}(M)$ vary along the integral curves of the Hamiltonian vector field X_H, then we find for arbitrary points $z\in M$,

$$\frac{d}{dt}(\phi_z^*F)(t)=\phi_z^*(dF(X_H))(t)=\phi_z^*(\{F,H\})(t)\,. \tag{6}$$

Often this equation is briefly written as $\dot{F}=\{F,H\}$.

Let us expand the function ϕ^*F in a formal power series in t,

$$(\phi^*F)(t,z)=\sum_{\alpha=0}^{\infty}F_\alpha(z)t^\alpha, \tag{7}$$

with coefficients $F_\alpha\in\mathcal{F}(M)$. A trivial computation shows then that

$$(\{F,G\})_\alpha=\sum_{\beta=0}^{\alpha}\{F_{\alpha-\beta},G_\beta\}\,. \tag{8}$$

Since, by definition of a flow, $(\phi^*F)(0,z)=F(z)$, we may express the coefficients F_α in a closed form: entering the expansion (7) into the differential equation (6) yields the relation $\alpha F_\alpha=\{F_{\alpha-1},H\}$ and thus

$$F_0=F\,,\quad F_1=\{F,H\}\,,\quad F_2=\tfrac{1}{2}\{\{F,H\},H\}\,,$$
$$F_\alpha=\frac{1}{\alpha!}\{\cdots\{\{F,\underbrace{H\},H\}\cdots,H\}}_{\alpha\ \text{brackets}}\,. \tag{9}$$

III. A PARTIAL DIFFERENTIAL SYSTEM AND ITS INVOLUTION ANALYSIS

Assume we are given an arbitrary vector field X on the Poisson manifold M. A natural question is whether or not a function $H\in\mathcal{F}(M)$ exists such that $X=X_H=(dH)^\sharp$. By the results of Sec. II, this corresponds in local coordinates where $X=\xi^k\partial_{z^k}$ to studying the solvability of the following overdetermined inhomogeneous linear first-order system for H:

$$X^{(k)}H=J^{kl}\frac{\partial H}{\partial z^l}=\xi^k\,. \tag{10}$$

It should be noted that we consider in the sequel only the *formal* solvability, i.e., the existence of formal power series solutions H.

In the language of the formal theory, conditions on the right hand side $\vec{\xi}$ for the existence of solutions are called *compatibility conditions*. They are determined by rendering (10) involutive. For linear first-order systems with one unknown function this is a classical problem much studied in the 19th century (see, e.g., the references in the textbooks[10,11]); in modern geometric language it leads to the Frobenius theorem. The system (10) is involutive, if and only if the vector fields $X^{(k)}$ span an involutive distribution, i.e., if the distribution is closed under the Lie bracket.

But we have already determined in (5) that this is indeed the case. Applying these commutator relations to the function H and using (10) immediately yields the following compatibility conditions for the right hand side $\vec{\xi}$:

$$X^{(k)}\xi^l - X^{(l)}\xi^k = \frac{\partial J^{kl}}{\partial z^j}\xi^j, \quad 1 \leqslant k < l \leqslant n. \tag{11}$$

Restricted to the special case of a Lie–Poisson manifold, this is the underdetermined system studied by Bender *et al.*[1] In general, (11) does *not* contain all compatibility conditions of (10). If the Poisson structure is degenerate, the vector fields $X^{(k)}$ are not linearly independent, as trivially $\chi_k^{(a)} X^{(k)} = 0$ for the one-forms $\chi^{(a)}$ spanning $\ker \sharp$. Thus we find in addition,

$$\chi_k^{(a)}\xi^k = 0, \quad 1 \leqslant a \leqslant r. \tag{12}$$

Bender *et al.*[1] ignored these equations and they are the reason for the problem mentioned in the Introduction.

In an intrinsic language, (11) is (up to a constant factor) the local coordinate form of $L_X w = 0$ and (12) of $\chi^{(a)}(X) = 0$. This observation is not too surprising: by definition of the one-forms $\chi^{(a)}$, the second equation simply says that the vector field X must lie in $\operatorname{im} \sharp$ and we showed above that for every Hamiltonian vector field the Lie derivative of the Poisson bivector w vanishes. Thus both conditions are obviously *necessary* for X being Hamiltonian. Because of the involution of the linear system (10), they are also *sufficient* for the vector field X being (formally) Hamiltonian.

It follows from these considerations that the general formal solution of (11), (12) is

$$\xi^k = X^{(k)}H = J^{kl}\frac{\partial H}{\partial z^l},$$

where the function $H \in \mathcal{F}(M)$ is arbitrary. Hence (11), (12) indeed always represents an underdetermined system, although it comprises more equations than unknown functions.

We proceed with an involution analysis of the combined system (11), (12). We first analyze whether it is possible to generate integrability conditions via cross-differentiations within the differential equations (11). We introduce the short hand $A^{kl} = X^{(k)}\xi^l - X^{(l)}\xi^k - (\partial J^{kl}/\partial z^j)\xi^j$ (the antisymmetric tensor corresponding to the bivector $L_X w$) and thus (11) may be written as $A^{kl} = 0$. If we take the cyclic combination

$$X^{(m)}A^{kl} + X^{(k)}A^{lm} + X^{(l)}A^{mk} = 0, \tag{13}$$

all second-order derivatives vanish and thus an integrability condition might be hidden here.

Here (13) contains the difference $(X^{(m)}X^{(k)} - X^{(k)}X^{(m)})\xi^l$ (and cyclic permutations of it). Here we enter the commutation relation (5). The arising equation contains expressions of the form $(\partial J^{mk}/\partial z^j)(X^{(j)}\xi^l - X^{(l)}\xi^j)$ which are simplified using (11). These operations finally yield the algebraic integrability conditions

$$\left(\frac{\partial J^{mk}}{\partial z^i}\frac{\partial J^{il}}{\partial z^n} + \frac{\partial J^{lm}}{\partial z^i}\frac{\partial J^{ik}}{\partial z^n} + \frac{\partial J^{kl}}{\partial z^i}\frac{\partial J^{im}}{\partial z^n} + J^{il}\frac{\partial^2 J^{mk}}{\partial z^n \partial z^i} + J^{ik}\frac{\partial^2 J^{lm}}{\partial z^n \partial z^i} + J^{im}\frac{\partial^2 J^{kl}}{\partial z^n \partial z^i} \right)\xi^n = 0.$$

As the coefficient of ξ^n is just the z^n-derivative of the Jacobi identity (3), this condition is always satisfied. If our Poisson structure is nondegenerate [so that the equations (12) do not arise], this result suffices to conclude that (11) is involutive, as (13) is the only linear combination of differentiated equations where all second-order derivatives vanish.

In the case of a degenerate Poisson structure we must also analyze prolongations of the algebraic equations (12). We first consider the application of one of the vector fields $X^{(l)}$. Upon entering the differential equations (11), a trivial computation yields

$$X^{(l)}(\chi_k^{(a)}\xi^k) = \left(J^{lm}\frac{\partial \chi_k^{(a)}}{\partial z^m} + \frac{\partial J^{lm}}{\partial z^k}\chi_m^{(a)} \right)\xi^k.$$

Exploiting the relation $J^{lm}\chi_m^{(a)}=0$ we have thus found the integrability conditions

$$J^{lm}\left(\frac{\partial\chi_k^{(a)}}{\partial z^m}-\frac{\partial\chi_m^{(a)}}{\partial z^k}\right)\xi^k=0\,,\quad 1\leqslant l\leqslant n\,. \tag{14}$$

A necessary condition for involution is that these conditions are linearly dependent of the algebraic equations (12) or, equivalently, that contracting the coefficients with J^{nk} yields zero. Relabeling the indices m and k in the second term, we arrive at the condition

$$(J^{nk}J^{lm}-J^{lk}J^{nm})\frac{\partial\chi_k^{(a)}}{\partial z^m}=0\,.$$

Exploiting again the relation $J^{lm}\chi_m^{(a)}=0$ and using the Jacobi identity (3) we find

$$(J^{nk}J^{lm}-J^{lk}J^{nm})\frac{\partial\chi_k^{(a)}}{\partial z^m}=\left(J^{lm}\frac{\partial J^{kn}}{\partial z^m}+J^{nm}\frac{\partial J^{lk}}{\partial z^m}\right)\chi_k^{(a)}=J^{km}\frac{\partial J^{ln}}{\partial z^m}\chi_k^{(a)}=0,$$

and hence this condition is always satisfied by the definition of the one-forms $\chi^{(a)}$.

As the vector fields $X^{(l)}$ are not linearly independent, the analysis above does not cover all possible prolongations of the constraints (12). Let $Y^{(b)}$ be r further vector fields such that together with the fields $X^{(l)}$ they span the full tangent space TM. This implies the existence of functions A_k^{lb} and B_c^{lb} such that

$$[X^{(l)},Y^{(b)}]=A_k^{lb}X^{(k)}+B_c^{lb}Y^{(c)}\,. \tag{15}$$

Applying the vector fields $Y^{(b)}$ to (12) yields differential equations

$$Y^{(b)}(\chi_k^{(a)}\xi^k)=0, \tag{16}$$

which are obviously algebraically independent of the system (11). In a strict geometric sense, they represent integrability conditions, albeit of a rather trivial nature. The more interesting question is whether it is possible to derive further integrability conditions via cross-differentiations between equations in (16) and (11), respectively. But one fairly easily sees that this cannot be the case.

A further integrability condition could only be generated by applying one of the vector fields $X^{(l)}$ to (16) and eliminating all arising second-order derivatives using equations obtained by applying some of the fields $Y^{(b)}$ to (11). But according to (15) we may write

$$X^{(l)}Y^{(b)}(\chi_k^{(a)}\xi^k)=(Y^{(b)}X^{(l)}+A_k^{lb}X^{(k)}+B_c^{lb}Y^{(c)})(\chi_k^{(a)}\xi^k)\,.$$

The second and the third terms on the right hand side consist of linear combinations of equations already present in the augmented system (11), (12), (16). In the first term we find the expression $X^{(l)}(\chi_k^{(a)}\xi^k)$ of which we have shown above that it may also be written as a linear combination of equations in (11), (12). Thus the right hand side is algebraically dependent of (11), (12), (16) plus the equations obtained by applying $Y^{(b)}$ to (11) and there are no further integrability conditions hidden.

Hence we have proven that for nondegenerate Poisson structures the system (11) is directly involutive, whereas in the degenerate case we must only add the trivial integrability conditions (16) to the system (11), (12) in order to achieve involution.

The Schouten–Nijenhuis bracket allows us to reformulate these lengthy coordinate calculations in an intrinsic language. As already mentioned, the system (11) is equivalent to $L_Xw=-[X,w]=0$. Let Y be an arbitrary vector field; then the prolongation of (11) in the direction Y is simply given by $L_YL_Xw=[Y,[X,w]]=0$. The graded Jacobi identity of the Schouten–Nijenhuis bracket yields $L_YL_Xw=L_XL_Yw-L_{[X,Y]}w$. On the right hand side, all second-order derivatives of

X are located in the second term. It vanishes if Y is a Hamiltonian vector field (i.e., a linear combination of the fields $X^{(k)}$), as $[X,Y]$ is then Hamiltonian, too. However, in this case we also have $L_Y w=0$, so that no integrability conditions appear.

In a similar manner, we can analyze the prolongation of the equations $\chi^{(a)}(X)=0$. If Y is a Hamiltonian vector field, then $L_Y(\chi^{(a)}(X))=(L_Y\chi^{(a)})(X)-\chi^{(a)}([X,Y])=(L_Y\chi^{(a)})(X)$. By Cartan's formula, $L_Y\chi^{(a)}=\iota_Y d\chi^{(a)}+d(\iota_Y\chi^{(a)})$ where ι_Y denotes the interior derivative with respect to Y. The second term vanishes, as Y is Hamiltonian and thus $\iota_Y\chi^{(a)}=0$. For the first term, we exploit that the codistribution $\ker\sharp$ spanned by the forms $\chi^{(a)}$ is involutive, as it annihilates the involutive distribution $\operatorname{im}\sharp$. This implies by the Frobenius theorem that $d\chi^{(a)}=\omega_b^{(a)}\wedge\chi^{(b)}$ for some one-forms $\omega_b^{(a)}$ and hence $\iota_X\iota_Y d\chi^{(a)}=0$. Thus no integrability conditions appear in the prolongation with respect to a Hamiltonian vector fields and the trivial ones (16) in any other prolongation.

IV. THE FUNDAMENTAL POWER SERIES SOLUTIONS

Bender *et al.*[1] derived the underdetermined system (11) differently. They considered in some local coordinate chart the n special functions $F^{(k)}\in\mathcal{F}(M)$ given by $F^{(k)}(z)=z^k$. We may call the functions $\phi^*F^{(k)}$ the *fundamental solutions* of the differential equation (6), as it obeys a kind of nonlinear superposition principle: for any function $F\in\mathcal{F}(M)$ we have

$$(\phi^*F)(t,z)=F((\phi^*F^{(1)})(t,z),\ldots,(\phi^*F^{(n)})(t,z)).$$

Indeed, the functions $\phi^*F^{(k)}$ are obviously nothing but the components of the flow in the local coordinates $(z^1,\ldots,z^n)$.

Bender *et al.*[1] expanded the fundamental solutions into power series of the form (7) and determined partial differential equations for the coefficients $F_\alpha^{(k)}$. Using our results above it is straightforward to find these equations. We first apply the relation (8) for $\alpha=1$:

$$(\{F^{(k)},F^{(l)}\})_1=\{F_1^{(k)},F_0^{(l)}\}+\{F_0^{(k)},F_1^{(l)}\}.$$

By the definition of the functions $F^{(k)}$, the right hand side may obviously be written in the form $X^{(k)}F_1^{(l)}-X^{(l)}F_1^{(k)}$. Because of $(\{F^{(k)},F^{(l)}\})_0=\{F_0^{(k)},F_0^{(l)}\}=J^{kl}$, the left hand side evaluates to

$$(\{F^{(k)},F^{(l)}\})_1=\{J^{kl},H\}=\frac{\partial J^{kl}}{\partial z^j}\{z^j,H\}=\frac{\partial J^{kl}}{\partial z^j}\{F_0^{(j)},H\}=\frac{\partial J^{kl}}{\partial z^j}F_1^{(j)}.$$

Putting the pieces together, we find that the first-order coefficients $F_1^{(k)}$ satisfy the compatibility conditions (11). This is of course not surprising: by definition of the flow ϕ and the functions $F^{(k)}$, the coefficients $F_1^{(k)}$ are nothing but the components ξ^k of the Hamiltonian vector field X_H in the given local coordinates.

We may derive similarly systems of partial differential equations for the higher-order coefficients $F_k^{(i)}$. In second order, the starting point is the relation

$$(\{F^{(k)},F^{(l)}\})_2=\{F_2^{(k)},F_0^{(l)}\}+\{F_1^{(k)},F_1^{(l)}\}+\{F_0^{(k)},F_2^{(l)}\}.$$

The right hand side equals $X^{(k)}F_2^{(l)}-X^{(l)}F_2^{(k)}+\{F_1^{(k)},F_1^{(l)}\}$. Using the results above we evaluate the left hand side to

$$(\{F^{(k)},F^{(l)}\})_2=\{(\{F^{(k)},F^{(l)}\})_1,H\}=\left\{\frac{\partial J^{kl}}{\partial z^j}F_1^{(j)},H\right\}=\frac{\partial J^{kl}}{\partial z^j}F_2^{(j)}+\left\{\frac{\partial J^{kl}}{\partial z^j},H\right\}F_1^{(j)}.$$

Thus we obtain the following system for the second-order coefficients:

$$X^{(k)}F_2^{(l)}-X^{(l)}F_2^{(k)}-\frac{\partial J^{kl}}{\partial z^j}F_2^{(j)}=\left\{\frac{\partial J^{kl}}{\partial z^j},H\right\}F_1^{(j)}-\{F_1^{(k)},F_1^{(l)}\}. \tag{17}$$

Note that the homogeneous part of this linear system is identical with our compatibility conditions (11). It is easy to see that if we continue in this manner, the homogeneous part always remains unchanged. Only the right hand side becomes a more and more complicated expression in the coefficients of lower order. More precisely, we find

$$X^{(k)}F_\alpha^{(l)}-X^{(l)}F_\alpha^{(k)}-\frac{\partial J^{kl}}{\partial z^j}F_\alpha^{(j)}=R_\alpha^{kl}-\sum_{\beta=1}^{\alpha-1}\{F_{\alpha-\beta}^{(k)},F_\beta^{(l)}\}, \tag{18}$$

where the term R_α^{kl} is determined by the recurrence relation

$$R_{\alpha+1}^{kl}=\left\{\frac{\partial J^{kl}}{\partial z^j},H\right\}F_\alpha^{(j)}+\{R_\alpha^{kl},H\}, \quad R_1^{kl}=0\,.$$

It should be noted that so far we have only shown that the functions $F_\alpha^{(k)}$ satisfy certain differential equations. We have *not* shown that they form their respective general solution. Indeed, we already know from the last section that this is the case only for nondegenerate Poisson structures. It is trivial to see that

$$\chi_k^{(a)}F_1^{(k)}=\chi_k^{(a)}\{F_0^{(k)},H\}=\chi_k^{(a)}X^{(k)}H=0\,, \quad 1\leqslant a\leqslant r\,.$$

Thus we recover (12). However, using the power series approach we still have no rigorous proof that we have found all equations satisfied by the first-order coefficients $F_1^{(\alpha)}$ whereas this followed trivially from our compatibility analysis in the last section.

The higher-order coefficients $F_\alpha^{(k)}$ also satisfy some algebraic constraints which may be determined recursively. If we set $G_\alpha^{(a)}=\chi_k^{(a)}F_\alpha^{(k)}$, then a trivial computation yields

$$G_{\alpha+1}^{(a)}=\{G_\alpha^{(a)},H\}-\{\chi_k^{(a)},H\}F_\alpha^{(k)}\,. \tag{19}$$

Of course, such a relation holds for arbitrary one-forms χ. The special property of the one-forms $\chi^{(a)}\in\ker\sharp$ is that for them $G_1^{(a)}=0$.

Bender *et al.*,[1] explicitly determined and solved for several concrete instances of a Lie-Poisson manifold the inhomogeneous system (17) for the second-order coefficients. They used the traditional approach of finding a particular solution of the inhomogeneous system and adding the general solution of the homogenous system. But obviously, (9) provides us with simpler closed form expressions for the general solution of the combined system (18), (19) for any order α.

V. AN EXPLICIT EXAMPLE

We detail the calculations presented so far for the Lie–Poisson structure associated with the three-dimensional Lie algebra E_2 generating the Euclidean motions in $\mathbb{R}^2$. This structure is characterized by the Poisson matrix

$$J=\begin{pmatrix}0 & 0 & -y\\ 0 & 0 & x\\ y & -x & 0\end{pmatrix}.$$

If we exclude the origin and confine ourselves to $M=\mathbb{R}^2\backslash\{0\}$, its constant rank is 2 and $\ker\sharp$ is spanned by the single one-form $\chi=x\,dx+y\,dy$. The vector fields $X^{(k)}$ have the form

$$X^{(1)}=-y\partial_z\,, \quad X^{(2)}=x\partial_z\,, \quad X^{(3)}=y\partial_x-x\partial_y\,.$$

They yield a representation of E_2 on $\mathbb{R}^3$, as the only nonvanishing Lie brackets are

$$[X^{(1)},X^{(3)}]=-X^{(2)}\,, \quad [X^{(2)},X^{(3)}]=X^{(1)}\,.$$

If we write $\xi^1=F$, $\xi^2=G$, $\xi^3=H$, then the evaluation of (11) yields the system (1).

Obviously, $X^{(1)}$ and $X^{(2)}$ are linearly dependent: $\chi_k X^{(k)}=xX^{(1)}+yX^{(2)}=0$. Hence (12) takes the form $xF+yG=0$ and all solutions given by (2) satisfy this equation. However, the system (1) implies only the relations $\partial/\partial z(xF+yG)=0$ and $(y\partial/\partial x-x\partial/\partial y)(xF+yG)=0$. Thus it possesses further solutions for which $xF+yG\neq 0$; one example has been given in the Introduction.

The Hamiltonian vector field X_K associated to an arbitrary function K is of the form $X_K=-yK_z\partial_x+xK_z\partial_y+(yK_x-xK_y)\partial_z$. As expected, the components are just the components of the general solution (2). A direct compatibility analysis yields that a general vector field $X=F\partial_x+G\partial_y+H\partial_z$ is Hamiltonian, if and only if its components satisfy

$$xF+yG=0\,,\quad F_x+G_y+H_z=0\,.$$

This system is equivalent to (1) *plus* the algebraic constraint $xF+yG=0$.

Let us perform an involution analysis of the system consisting of (1) and the constraint $xF+yG=0$. Cross-differentiations of the equations within (1) do not lead to any new equations. There is not short-cut for showing this; one must perform some lengthy computations which are equivalent to our analysis of (13).

The z-prolongation of the constraint is already contained in (1); thus applying neither $X^{(1)}$ nor $X^{(2)}$ to the constraint yields an integrability condition. If we apply $X^{(3)}$ to it, we obtain an equation which is a linear combination of the second and the third equation in the system (1). Indeed, it is easy to see that in our special case the one-form χ is such that in (14) the expression in the parentheses vanishes.

However, the vector fields $X^{(k)}$ do not form a basis of TM. Thus we must also study either the x- or the y-prolongation of the constraint. Either one leads to a trivial integrability condition, say, $xF_x+yG_x+F=0$, if we choose $Y=\partial_x$. Now, as a last step, we must check whether a cross-differentiation of this equation with some equation contained in (1) yields something nontrivial. But it is easy to see that this is not the case and we have arrived at an involutive system.

VI. CONCLUSIONS

We rederived the results of Bender *et al.*[1] on Lie–Poisson structures in a more geometric fashion using the formal theory of differential equations and generalized them to arbitrary Poisson manifolds. It turned out that their system simply describes necessary and sufficient conditions on the components of a vector field for the field to be Hamiltonian with respect to the given Poisson structure. We also corrected an error of Bender *et al.*,[1] in the case of degenerate Poisson structures where the Poisson matrix admits nontrivial null vectors.

We studied only the formal solvability of our differential systems. In the analytic category we could use the Cartan–Kähler theorem for proving the existence of analytic solutions (because of the linearity of the systems, the Holmgren theorem ensures that these solutions are unique even in much larger function spaces). The assumption that the Poisson matrix is analytic is not so restrictive, as it is for example trivially true for any Lie–Poisson structure. In contrast, the restriction to analytic vector fields is surely too severe for applications.

An existence theory in more general function spaces would require a deeper analysis of the systems. In the case of a nondegenerate Poisson structure it is not difficult to prove that both (10) and (11), (12) form elliptic systems in the sense that their symbol maps are injective. Thus one could apply the results outlined in the encyclopaedia article by Dudnikov and Samborski.[12] But as for our purposes the formal analysis was sufficient, we refrain from going further in this direction.

It is very instructive to see how deeply the involution analysis of our partial differential system (11), (12) is related to Poisson geometry. The two characteristic properties of the Poisson matrix J, skew-symmetry and the Jacobi identity (3), must be applied repeatedly for showing the vanishing of all integrability conditions. It is tempting to conjecture that conversely the system has the wanted properties, if and only if the matrix J defines a Poisson structure, but we have not been able to prove this. Such a proof would require to solve the *inverse* problem of compatibility for the

system (11), (12). Fairly recently, an algorithmic solution of this inverse problem has been developed.[13,14] However, the involved computations are rather tedious and it seems hopeless to perform them for our system.

We studied in this article only classical Poisson systems. Bender *et al.*[1] also considered quantum systems where the coordinates z^j become noncommutative. We developed recently a theory of involutive bases in a fairly large class of algebras, the polynomial algebras of solvable type.[4] This class contains in particular the universal enveloping algebras of finite-dimensional Lie algebras. The latter should provide the right setting for an analogous analysis of the quantum version of the evolution equation (6).

ACKNOWLEDGMENTS

The constructive remarks of an anonymous referee lead to a considerable improvement of the article. This work has been financially supported by Deutsche Forschungsgemeinschaft and by INTAS (Project No. 99-1222).

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Discrete symmetry's chains and links between integrable equations

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(Received 13 August 2002; accepted 5 September 2002)

We consider the discrete symmetry's dressing chains of the nonlinear Schrödinger equation (NLS) and Davey–Stewartson equations (DS). The modified NLS (mNLS) equation and the modified DS (mDS) equations are obtained. The explicitly reversible Bäcklund auto-transformations for the mNLS and mDS equations are constructed. We demonstrate discrete symmetry's conjugate chains of the KP and DS models. The two-dimensional generalization of the P_4 equation is obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1523641]

I. INTRODUCTION

Darboux transformations (DT) are very useful method to construct exact solutions of integrable PDE.[1] Some time ago a new approach to the DT (called dressing chains of discrete symmetries) emerged at the horizon of soliton's mathematics. This approach to proliferate integrable equations was proposed in the example of the Korteweg–de Vries (KdV) and sine-Gordon equations.[2] The scheme to proliferate the integrable equation (we choose the KdV for definiteness) starts out from Lax pair and DT of this equation. After very simple transformations (see Sec. II) we obtain new integrable equations with their Lax pairs. The modified KdV (mKdV$=$m^{1}KdV), m^{2}KdV, and m^{3}KdV equations were thus constructed, the second of which can be reduced to the exponential Calogero–Degasperis (CD) equation by an exponential point change of variables and the third contains the elliptic CD equation. The only price we have to pay for this simplicity is a rapidly growing amount of calculation.

Despite its apparent simplicity, the method of dressing chains is an extremely powerful method, as can be illustrated in following example (see details in Refs. 2–4): as noted in Refs. 2 and 3, the m^{n}KdV equations ($n=0,\ldots,3$), together with the Krichever–Novikov equation, exhaust all the integrable equations of the form $u_t+u_{xxx}+f(u_{xx},u_x,u)=0$. In Ref. 4 we generalized the dressing-chain method to considerably $(1+2)$-dimensional nonlinear equations: the Kadomtsev–Petviashvili (KP) and the Boiti–Leon–Pempinelli (BLP) equations. A new result, which is characteristic precisely of multidimensional equations, is the discovery of two types of dressing chains for the KP equation (we call these the conjugate chains). The new chain can be constructed with the help of binary DT.

The aim of this work is the generalization of the dressing-chains method for the nonlinear Schrödinger (NLS) and Davey–Stewartson (DS) equations. The plan of this paper is as follows. In Secs. II and III we review the dressing-chains method for the higher and lower KdV equations and for the higher KP equations. The dressing chains for the NLS and for the DS equations are discussed in Secs. IV and V. In Sec. VI we develop a technique for constructing exact localized solution of DS equations with a reduction constraint imposed and give some of these solutions. We conclude with a discussion on possible role of discrete symmetry's dressing chains in the theory of integrable PDE.

Last but not least, the dressing-chains method allows us to construct new integrable equations and, on the other hand, to find a link between known ones. For example, the sine-Gordon, KdV,

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and CD equations can be constructed starting out from the KdV equation via dressing chains. *Maybe it is really only one integrable equation*?

II. 2D-P_4 EQUATION

Let us begin our discussion of the Borisov–Zykov method by analyzing the simplest of all possible integrable systems, the KdV equation. The starting point is the Lax pair for the KdV equation

$$\psi_{xx}=(u-\lambda)\psi, \quad \psi_t=2(u+2\lambda)\psi_x-u_x\psi, \tag{1}$$

where the KdV equation

$$u_t-6uu_x+u_{xxx}=0. \tag{2}$$

Setting $\tau=\phi_x/\phi$, where ϕ is a partial solution of (2) with the $\lambda=\mu$, we can write the Lax pair as

$$\tau_x=-\tau^2+u-\mu, \quad \tau_t=[2(u+2\mu)\tau-u_x]_x. \tag{3}$$

Exempting u from (4), we get

$$\tau_t=6\tau^2\tau_x-\tau_{xxx}+6\mu\tau_x. \tag{4}$$

If $\mu=0$ then we have the well-known mKdV equation. To construct Lax pair for (4) we use the DT

$$u_1=u-2\tau_x, \quad \psi_1=\psi_x-\tau\psi.$$

Setting $\sigma=\psi_{1,x}/\psi_1$, we get the x chain

$$(\sigma+\tau)_x=-\sigma^2+\tau^2-\lambda+\mu \tag{5}$$

and t chain

$$(\sigma+\tau)_t=[2(-\tau_x+\tau^2+\mu+2\lambda)\sigma-2\tau\tau_x+6\mu\tau+2\tau^3]_x.$$

At last, after introduction of the auxiliary function (denoted by Ψ)

$$\sigma+\tau=\Psi,$$

we obtain the Lax pair for (4)

$$\Psi_x=-\Psi^2+2\tau\Psi-\lambda+\mu, \quad \Psi_t=2[(\tau^2-\tau_x+\mu+2\lambda)\Psi+2(\mu-\lambda)\tau]_x. \tag{6}$$

Starting out from (6), we can find the m^{2}KdV (which can be reduced to the exponential CD equation by an exponential point change of variables) with its Lax pair. Continuing this procedure, we obtain the elliptic CD equation (m^{3}KdV) and *it is the end of this way*. The m^{3}KdV equation is the last equation which can be obtained by this method.

At first, one may wonder why the limitation appears by the $n=3$. However, we can write the Lax pairs for the m^{n}KdV with $n<4$ as two Riccati equations. It is incorrect for the m^{4}KdV.[2] This equation, therefore, is different from the ones found earlier and cannot be used by the old scheme. On the other hand, as we have mentioned in the Introduction, the m^{n}KdV equations ($n=0,\ldots,3$), together with the Krichever–Novikov equation, exhaust all the integrable equations of the form $u_t+u_{xxx}+f(u_{xx},u_x,u)=0$. So, this limitation is something beyond that. We can understand the triviality of this limitation with the help of the Painleve property. Let consider the m^{1}KdV equation (4). The function τ is the solution of both this equation and two Riccati equations

(3) [inserting τ_x from the first equation (3) in the second one we obtain the second Riccati equation], so it is obvious that the function τ has the Painleve property and that it is incorrect for the solutions of the m^{3}KdV with $n>3$.

In Ref. 5 the continuation of the KdV equation hierarchy in the direction corresponding to the negative power of the spectral parameter is constructed in the following way: let the L operator have the form (1)

$$L=-\partial_x^2+u(x,t),$$

and the nonlinear equations are

$$L_t=[L,A_N].$$

The operators A_N have the form

$$A_N=\sum_{m=-1}^{N} K_m(L)^m,$$

where $N=-1,-2,\ldots,$ and K_m are some operators.

The first lower KdV ($N=-1$) equation has the form (see Ref. 5),

$$\mathrm{KdV}_{-1}(\sigma)\equiv(\sigma_x^2+\sigma_{xx})_t-(e^{2\sigma})_x=0,$$

where σ is connected with u in the following way:

$$u=-\sigma_{xx}-\sigma_x^2.$$

Let $\sigma=iq/2$, where $q=q(x,t)$. It easy to see that

$$\mathrm{KdV}_{-1}(\sigma)=\tfrac{1}{2}(i\partial_x-q_x)(q_{xt}-2\sin q)=0, \tag{7}$$

so we have the Miura transformation between the KdV_{-1} equation and the sine-Gordon equation.

Lax pair for the (7) has the form

$$\psi_{xx}=\left(\frac{iq_{xx}}{2}-\frac{q_x^2}{4}+\lambda^2\right)\psi,\quad \psi_t=\frac{1}{2\lambda^2}e^{iq}\left(\psi_x-\frac{iq_x}{2}\psi\right). \tag{8}$$

Starting out from (8), we can find the Lax pair for the sine-Gordon equation. To do this we introduce a new function $\tilde{\psi}$

$$\tilde{\psi}=\frac{1}{\lambda}\left(\psi_x-\frac{i}{2}q_x\psi\right). \tag{9}$$

Therefore

$$\tilde{\psi}_x=\lambda\psi-\frac{i}{2}q_x\tilde{\psi},\quad \psi_t=\frac{1}{2\lambda}e^{iq}\tilde{\psi},\quad \tilde{\psi}_t=-\frac{1}{2\lambda}(iq_{xt}-e^{iq})\psi. \tag{10}$$

Substituting $2\sin q$ in place of q_{xt} (in the equation for the $\tilde{\psi}_t$) we can see that (9) and (10) are the well-known Lax pair for the sine-Gordon equation.

Thus, we can use the method of dressing chains for both higher and lower KdV equations. The sine-Gordon, KdV, and CD equations can be constructed starting out from the KdV equation via dressing chains of discrete symmetries. These are simply different representations of the same equation. From this standpoint, *the difference between sine-Gordon, KdV, mKdV, and CD equations is similar to the difference between the Maxwell equations in different gauges*!

Surprisingly, much of the analysis of the simple system carries over directly to the multidimensional case. The KP equations are given by

$$u_t+6uu_x+u_{xxx}=-3\alpha^2v_y, \quad v_x=u_y,$$

where $u=u(x,y,t)$, $v=v(x,y,t)$, $\alpha^2=\pm1$. The Lax pair for the KP equations is

$$\alpha\psi_y+\psi_{xx}+u\psi=0, \quad \psi_t+4\psi_{xxx}+6u\psi_x+3(u_x-\alpha v)\psi=0. \tag{11}$$

Setting $f\equiv\log\phi$, $\tau\equiv f_x$, where ϕ is a partial solution of (11), we can write Lax pair (11) as

$$\begin{gathered}\alpha\tau_y+(\tau_x+\tau^2+u)_x=0,\\ \tau_t+(4\tau_{xx}+12\tau\tau_x+4\tau^3+6u\tau+3u_x-3\alpha v)_x=0.\end{gathered} \tag{12}$$

It follows from the first equation in (12) that

$$u=-\tau_x-\tau^2-\alpha F, \quad F_x=\tau_y. \tag{13}$$

Substituting (12) into the second equation in (13) and making some simple transformations, we obtain the well-known mKP equation[6]

$$\tau_t-6\tau^2\tau_x+\tau_{xxx}=3\alpha(2\tau_xF-\alpha F_y), \quad F_x-\tau_y=0. \tag{14}$$

We now construct dressing chains of discrete symmetries. The KP equation admits the Darboux transformation[1]

$$\psi_1=\psi-\tau\psi, \quad u_1=u+2\tau_x, \quad v_1=v+2\tau_y. \tag{15}$$

Setting $s\equiv\log\psi_1$, $\sigma=s_x$, we see that σ satisfies the system of equations obtained from (12) by replacing $u\to u_1$ and $v\to v_1$. Comparing these equations with (12) and eliminating the potentials u and v, we obtain

$$\begin{gathered}\alpha(s-f)_y+(s+f)_{xx}+s_x^2-f_x^2=0,\\ (s-f)_t+[2(2s+f)_{xx}+6s_x^2-3f_x^2]_x+4s_x^3+6(f_{xx}-f_x^2-\alpha f_y)s_x-6\alpha(f_{xy}-f_xf_y)+2f_x^3=0.\end{gathered} \tag{16}$$

The first equation in (16) determines the y chain and the second determines the t chain, denoted by $C_y^{(+)}$ and $C_t^{(+)}$, respectively. Later (in Sec. III) we will generalize the Borisov–Zykov approach for the case of the KP equation, and we will find that the results of Borisov–Zykov carry over with only one important change.

As we have seen, the Painleve property is connected with the dressing chains. The approach of using dressing chain (5) to construct the P_4 equation was proposed in Ref. 7. It is interesting to apply this method to the chain (16).

To do this, it is helpful to insert the periodic condition. It is well known that the periodic condion for (5) led to the P_4 equations. Let us consider the dressing chain $C_y^{(+)}$ (16). Setting $f=f_n$, $s=f_{n+1}$, we use the condition of periodic

$$f_{n+N}=f_n+c(y). \tag{17}$$

It easy to see that

$$u_{n+N}=u_n+\alpha c',$$

so the condition (17) gets us some generalization of the harmonic oscillator. We choose $N=3$ and $c=-2y/\alpha$. Introducing new fields g_n, $n=1,2,3$

$$f_1=\tfrac{1}{2}(g_1-g_2+g_3+c),\quad f_2=\tfrac{1}{2}(g_1+g_2-g_3-c),\quad f_3=\tfrac{1}{2}(-g_1+g_2+g_3+c),$$

we can now rewrite the equations for the f_n in the following way:

$$\alpha(g_{2_y}-g_{3_y}-c_y)+(g_{2_x}-g_{3_x})g_{1_x}+g_{1_{xx}}=0,$$

$$\alpha(-g_{1_y}+g_{3_y}+c_y)+(g_{3_x}-g_{1_x})g_{2_x}+g_{2_{xx}}=0,$$

$$\alpha(g_{1_y}-g_{2_y}-c_y)+(g_{1_x}-g_{2_x})g_{3_x}+g_{3_{xx}}=0.$$

Excluding g_3, and using thecompatibility condition $\partial_y(g_{2,xx})=\partial_x^2(g_{2,y})$, we get the nonlinear equation which can be written via some transformation as

$$z_{xx}=\frac{1}{2}\frac{z_x^2}{z}+\frac{3}{2}z^3+4xz^2+2(x^2-2)z+\frac{\beta}{z}+\frac{3\alpha^2q^2}{2z}-3\alpha qz+\frac{\alpha}{z}\partial_x^{-1}\partial_y(z^3+2xz^2-3\alpha qz),$$

$$z_y=q_x, \tag{18}$$

where $z=g_{1_x}$ and $q=g_{1_y}$. The one-dimensional limit (where $\partial_y=q=0$) of Eq. (18) is the P_4 equation, so (18) is the two-dimensional generalization of the P_4 equation and should be called the 2D-P_4 equation.

The price we pay for the D=2 is that locality in x is lost, that is, in the usual run of things for the multidimensional integrable systems.

III. CONJUGATE CHAINS FOR THE KP EQUATIONS

The correspondence between the KdV dressing-chains formalism that we developed in the previous section and the KP dressing-chains formalism is quite remarkable. We find that almost the entire KdV formalism can be imported into the KP chains.

Chains (16) involve two Lax pairs for Eqs. (14), which arise after introducting the auxiliary function (denoted by Ψ) according to one of two rules

$$\Psi=s-f,\quad \Psi=s+f. \tag{19}$$

Using the first rule, we obtain

$$\alpha\Psi_y+(2f+\Psi)_{xx}+2f_x\Psi_x+\Psi_x^2=0,$$

$$\Psi_t+2(2\Psi_{xx}+6f_x\Psi_x+3\Psi_x^2+3\theta)_x+6\theta\Psi_x+4(3f+\Psi)_x\Psi_x^2=0, \tag{20}$$

$$\theta\equiv f_{xx}+f_x^2-\alpha f_y,$$

from (16). The compatibility condition for these equations is

$$(f_t-2f_x^3+f_{xxx})_x=3\alpha(2f_{xx}f_y-\alpha f_{yy}), \tag{21}$$

which is merely another form of the mKP equation (for $\tau=f_x$ and $F=f_y$).

This process can be repeated. In particular, the system (20) contains a new nonlinear equation obtained by eliminating the potential f. For this purpose, we linearize the first equation in (20) by substituting

$$f=-\tfrac{1}{2}(\Psi+\alpha\xi), \tag{22}$$

where $\xi=\xi(x,y,t)$. Inserting (22) in the second equation in (20), differentiating it with respect to x, and introducing $S\equiv\Psi_x$, we obtain the system

$$S_t+S_{xxx}-\tfrac{3}{2}S^2S_x=-3\alpha^2[(\tfrac{1}{2}\xi_x^2+\xi_y)S+(\tfrac{1}{2}\xi_x^2+\xi_y)_x]_x,$$
$$S_y=(\xi_{xx}+\xi_xS)_x. \tag{23}$$

Although Eq. (23) looks like a two-dimensional generalization of the mKdV equation, the one-dimensional limit (where $\partial_y=0$) of (20) is

$$g_t+\left(g_{xx}-\frac{\alpha^2}{2}g^3-\frac{3}{2}\frac{g_x^2}{g}\right)_x=0$$

[where $g(x,t)\equiv\xi_x=\exp(-\Psi)$] rather than the mKdV equation. After an exponential point change of variable, this equation reduced to the exponential CD equation. Therefore, Eq. (23) should be called the two-dimensional CD equation rather than the two-dimensional mKdV equation.

In Ref. 2, another representation for Ψ was used in the derivation of the CD equation, namely, the representation determined by the second formula in (19). We have used this representation in Ref. 4.

In addition to the usual DT, the KP equations admit the so-called binary Darboux transformations,[1] which, as we now show, allow us to construct new KP dressing chains.

It is obvious that the KP equation admits the Lax pair

$$-\alpha\chi_y+\chi_{xx}+u\chi=0,\quad \chi_t+4\chi_{xxx}+6u\chi_x+3(u_x+\alpha v)\chi=0, \tag{24}$$

which can be obtained from (11) by simply replacing $\alpha\to-\alpha$. Let

$$dQ(\chi,\psi)=\chi\psi dx+\frac{1}{\alpha}(\chi_x\psi-\chi\psi_x)dy+4\left(\psi_x\chi_x-\chi_{xx}\psi-\chi\psi_{xx}-\frac{3}{2}u\chi\psi\right)dt,$$

$$Q(\chi,\psi)\equiv\int dQ(\chi,\psi).$$

It is easy to see that the one-form $dQ(\chi,\psi)$ is closed if ψ and χ are solutions of Eqs. (11) and (24). Pair (24) also admits the Darboux transformation

$$\chi_{-1}=\chi-\rho\chi,\quad u_{-1}=u+2\rho_x,\quad v_{-1}=v+2\rho_y, \tag{25}$$

where $\rho=(\log\tilde{\chi})_x$, and $\tilde{\chi}$ is a partial solution of (24). Applying DT (15), we have

$$\chi_1=\frac{A+BQ(\chi,\psi)}{\psi},$$

where A and B are arbitrary constants. Now, using (25) we obtain

$$u_{1,-1}=u+2[\log(A+BQ(\chi,\psi))]_{xx},\quad v_{1,-1}=v+2[\log(A+BQ(\chi,\psi))]_{xy}.$$

We set $\sigma\equiv\chi_{1,x}/\chi_1$. This function satisfies the equations obtained from (12) by replacing $u\to u_1$, $v\to v_1$, and $\alpha\to-\alpha$. In other words, this yields new integrable y- and t-chains ($C_y^{(-)}$ and $C_t^{(-)}$), which can be called *conjugate* to the $C^{(+)}$ chains discussed above

$$-\alpha(s+f)_y+(s+f)_{xx}+s_x^2-f_x^2=0,$$

$$(s+f)_t+[4(s+f)_{xx}+6s_x^2-3f_x^2]_x+4s_x^3+6(f_{xx}-f_x^2-\alpha f_y)s_x-6\alpha f_xf_y-2f_x^3=0,$$

where we still have $\tau=f_x$ and $\sigma=s_x$. Comparing the expressions for $C^{(-)}$ and $C^{(+)}$ from (16), we see that these chains do not reduce to each other, thereby justifying the term "conjugate." This implies that the chains $C^{(-)}$ lead to new integrable equations and also to the corresponding Lax

pairs. To construct these, we should again use two possibilities to define Ψ; see Eq. (19). In the present case, it is convenient to choose the second formula. As a result, we obtain yet another Lax pair for the mKP equation (21)

$$-\alpha\Psi_y+\Psi_{xx}-2f_x\Psi_x+\Psi_x^2=0,$$

$$\Psi_t+2(2\Psi_{xx}-3f_x\Psi_x+3\Psi_x^2)_x+6(f_x^2-\alpha f_y)\Psi_x-6f_x\Psi_{xx}+4(\Psi-3f)_x\Psi_x^2=0.$$

Linearizing the first equation by the substitution that differs from (22) only by the sign of the right-hand side and defined as $S\equiv\Psi_x$, we get

$$\begin{gathered}S_t+4S_{xxx}-\tfrac{3}{2}S^2S_x=3\alpha[\xi_{xx}S+2\xi_xS_x+\alpha(\xi_y-\tfrac{1}{2}\xi_x^2)S]_x,\\ \alpha S_y=(S_x-\alpha\xi_xS)_x.\end{gathered}\tag{26}$$

Equations (26) are similar to (23) and also reduce to the CD equation in the one-dimensional limit (for $\alpha^2=1$). At the same time, as follows from the method of their construction, Eqs. (26) do not reduce to system (23) via a 1:1 change of dependent variables (by a gauge transformation); therefore, Eqs. (26) can be called conjugate to the Eqs. (23).

IV. DRESSING CHAINS FOR THE NLS EQUATION

The results in the last section indicate that generalizing the dressing-chain method to considerably more complicated NLS and DS equations can be very fruitful. In this section we use the dressing chains of discrete symmetries to proliferate the NLS equation. Recently, Shabat has studied such chains for the Zakharov–Shabat spectral problem in some unusual gauge.[8] We have another aim: to construct higher mNLS equations. We can do it in two gauges, each with its own advantages and disadvantages.

(1) *Standard symmetric Zakharov–Shabat gauge*. In this gauge we have very clear connections between NLS and m^{n}NLS equations. The disadvantage of this gauge is a very rapidly growing amount of calculations. For the $n>2$ we obtain very cumbersome equations.
(2) *New Shabat gauge*.[8] The advantage of this gauge is that the equations have more compact form. However, the connection between real NLS and real mNLS equations is not obvious in this gauge. The reconstruction of the m^{n}NLS for a $n>2$ must be checked tediously.

Here, we choose the standard gauge for the spectral problem; therefore, the Lax pair for the NLS equation is

$$\Psi_t=-2i\sigma_3\Psi\Lambda^2+2iU\Psi\Lambda+V\Psi,\quad \Psi_x=-i\sigma_3\Psi\Lambda+iU\Psi,\tag{27}$$

where

$$U=\begin{pmatrix}0 & u\\ v & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad V=\sigma_3(iU^2-U_x),$$

and Λ is an arbitrary constant matrix. The compatibility condition gets us the NLS equations

$$iu_t+u_{xx}+2u^2v=0,\quad -iv_t+v_{xx}+2v^2u=0.$$

Let Φ is a partial solution of (27) with the $\Lambda=\mathrm{diag}((\lambda+\mu)/2,(\lambda-\mu)/2)$, Ψ is the same for the $\Lambda_1=\mathrm{diag}((\lambda_1+\mu_1)/2,(\lambda_1-\mu_1)/2)$ and $\tau\equiv\Phi\Lambda\Phi^{-1}$. This matrix function is the solution of the system

$$\tau_x=i[\tau,\sigma_3]\tau+i[U,\tau],\quad \tau_t=2\tau_x\tau+[V,\tau].\tag{28}$$

The Darboux transformation has the form

$$\Psi\to\Psi_1=\Psi\Lambda_1-\tau\Psi,\quad U\to U_1=U+[\tau,\sigma_3]. \tag{29}$$

There are two discrete symmetries of the Zakharov–Shabat spectral problem: S- and T symmetries. The transformation (29) is S^2 symmetry. We must use squared S symmetry because an elementary S symmetries are insufficient to construct exact solutions of the NLS.

Using (29), we obtain

$$u\to u_1=u-2b,\quad v\to v_1=v+2c, \tag{30}$$

where

$$\tau=\begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{31}$$

Substituting (31) into (28), we get

$$a_x=-d_x=-i(2bc-uc+vb),\quad b_x=-i(2bd+(a-d)u), \tag{32}$$

$$c_x=i(2ac+(a-d)v),$$

and

$$\begin{gathered} a_t=(a^2)_x+2b_xc-bv_x-cu_x,\quad d_t=(d^2)_x+2bc_x+bv_x+cu_x, \\ b_t=2(ibuv+a_xb+b_xd)+(a-d)u_x,\quad c_t=2(-icuv+ac_x+cd_x)+(a-d)v_x. \end{gathered} \tag{33}$$

Calculating the determinant and trace of matrix τ we get

$$ad-bc=\frac{\lambda^2-\mu^2}{4},\quad a+d=\lambda. \tag{34}$$

Using (34), we get

$$a=\tfrac{1}{2}(\lambda\pm\sqrt{\mu^2-4bc}). \tag{35}$$

Eliminating u and v from the last two Eqs. (32) and putting everything together, we find mNLS (m^1NLS) equation

$$\begin{gathered} (\mu^2-4bc)(ib_t+b_{xx}-2b^2c)+2\lambda(\lambda c+2ic_x)b^2+2(b_xc+2bc_x)b_x\equiv(\mu^2-4bc)\beta(b,c)=0, \\ (\mu^2-4bc)(-ic_t+c_{xx}-2c^2b)+2\lambda(\lambda b-2ib_x)c^2+2(bc_x+2b_xc)c_x\equiv(\mu^2-4bc)\gamma(b,c)=0. \end{gathered} \tag{36}$$

The designations $\beta(b,c)$ and $\gamma(b,c)$ will be useful [see (41), (42)].

As we have mentioned above, the NLS equation has a broader set of symmetries. In addition to the Darboux transformations, the discrete symmetries include the Schlesinger transformations or T symmetries. The T symmetries produce an explicity invertible Bäcklund auto-transformations for the NLS equation

$$u\to u_1=u_{xx}+u^2v-\frac{u_x^2}{u},\quad v\to v_1=\frac{1}{u},$$

and

$$u\to u_{-1}=\frac{1}{v},\quad v\to v_{-1}=v_{xx}+v^2u-\frac{v_x^2}{v},$$

where

$$(u_1)_{-1}=(u_{-1})_1=u,\quad (v_1)_{-1}=(v_{-1})_1=v.$$

These symmetries are related to the Toda chain and some of its generalizations.[9]

The mNLS equation (36) has the similar property. We have very cumbersome Schlesinger transformations for (36) so we show ones when $\lambda=\mu=0$. In this case, (36) has an elegant form

$$\begin{aligned} &ib_t+b_{xx}-2b^2c-\frac{b_xc_x}{c}-\frac{1}{2}\frac{b_x^2}{b}=0,\\ &-ic_t+c_{xx}-2bc^2-\frac{b_xc_x}{b}-\frac{1}{2}\frac{c_x^2}{c}=0. \end{aligned} \tag{37}$$

The explicity invertible Bäcklund auto-transformations for (37) are

$$b\to b_1=\frac{1}{4}\frac{(2cb_x^2-2cbb_{xx}+c_xb_xb+4c^2b^3)^2}{c^2b(b_x^2-4cb^3)},\quad c\to c_1=\frac{4cb^2}{b_x^2-4cb^3},$$

$$b\to b_{-1}=\frac{4bc^2}{c_x^2-4bc^3},\quad c\to c_{-1}=\frac{1}{4}\frac{(2bc_x^2-2bcc_{xx}+b_xc_xc+4b^2c^3)^2}{b^2c(c_x^2-4bc^3)}.$$

It is easy to verify that

$$(b_1)_{-1}=(b_{-1})_1=b,\quad (c_1)_{-1}=(c_{-1})_1=c.$$

To obtain dressing chains of discrete symmetries S^2, we construct new matrix function $\tau_1=\Psi_1\Lambda_1\Psi_1^{-1}$ with Ψ_1 from (29). Its elements a_1, b_1, c_1, and d_1 are solutions of (32)–(35) by replacing $\lambda\to\lambda_1$, $\mu\to\mu_1$, $u\to u_1$, and $v\to v_1$ [see (30)]. Eliminating potentials u and v, we obtain our chains

$$\begin{aligned} &(\lambda-2a)b_{1,x}-(\lambda_1-2a_1)b_x+2i(\lambda_1-a_1)(\lambda-2a)b_1-2i(\lambda_1-2a_1)ab=0,\\ &(\lambda-2a)c_{1,x}-(\lambda_1-2a_1)c_x-2i(\lambda-2a)a_1c_1+2i(\lambda_1-2a_1)(\lambda-a)c=0,\\ &b_{1,t}b-b_1b_t+2[(\lambda-a)b_1b_x-(\lambda_1-a_1)b_{1,x}b]+(\lambda_1-2a_1)(b^2)_x+K_1b_1+M_1b=0,\\ &c_{1,t}c-c_1c_t+2(ac_1c_x-a_1c_{1,x}c)+(\lambda_1-2a_1)(c^2)_x+K_2c_1+M_2c=0, \end{aligned} \tag{38}$$

where

$$\begin{aligned} &K_1=4iC(2,2)b^2+2[(a-a_1)_x+2iB(-2,-2)c]b-(\lambda-2a)B_x(-2,-2),\\ &K_2=-4iB(0,2)c^2-2[(a-a_1)_x+2iC(0,-2)b]c-(\lambda-2a)C_x(0,-2),\\ &M_1=(\lambda_1-2a_1)B_x(-2,-2),\quad M_2=(\lambda_1-2a_1)C_x(0,-2),\\ &B(n,k)=\frac{ib_x+(n\lambda-ka)b}{\lambda-2a},\quad C(n,k)=\frac{ic_x+(n\lambda-ka)c}{\lambda-2a}, \end{aligned}$$

and fields a, d (a_1, d_1) are expressed in term of b, c (b_1, c_1) via (34)–(35).

Chains (38) involve Lax pair for the mNLS (36), which arise after introducing the auxiliary fields

$$\psi \equiv \frac{b_1}{b}, \quad \phi \equiv \frac{c_1}{c}, \quad A \equiv a_1 .$$

After some calculations, we obtain

$$\psi_x = \left(2i(A-\lambda_1) - \frac{b_x}{b} \right) \psi + \frac{i(2A-\lambda_1)}{b} B(0,2),$$

$$\phi_x = \left(2iA - \frac{c_x}{c} \right) \phi + \frac{i(2A-\lambda_1)}{c} C(2,2),$$

$$\begin{aligned}
\psi_t &= 2(\lambda_1 - A)\psi_x - 4ibc\phi\psi^2 - 2i(bC(2,2)\psi + cB(0,2)\phi)\psi + P\psi + \frac{\lambda_1 - 2A}{b} B_x(0,2), \\
\phi_t &= 2A\phi_x + 4ibc\psi\phi^2 + 2i(bC(2,2)\psi + cB(0,2)\phi)\phi + Q\phi - \frac{\lambda_1 - 2A}{c} C_x(2,2),
\end{aligned} \tag{39}$$

$$A_x = -i[2bc\phi\psi + bC(2,2)\psi + cB(0,2)\phi],$$

$$A_t = -4i\lambda_1 bc\phi\psi - b[2iAC(2,2) + C_x(2,2)]\psi + c[2i(A-\lambda_1)B(0,2) + B_x(0,2)]\phi,$$

where

$$P = \frac{[2b_x(\lambda_1 - A) - ib_{xx}](\mu^2 - 4bc) + 2(bc)_x[2b(\lambda - a) - ib_x]}{b(\mu^2 - 4bc)},$$

$$Q = \frac{(2c_x A + ic_{xx})(\mu^2 - 4bc) + 2(bc)_x(2ca + ic_x)}{c(\mu^2 - 4bc)}.$$

The mNLS equation (36) arises from the compatibility condition of (39)

$$(\psi_x)_t = (\psi_t)_x, \quad (\phi_x)_t = (\phi_t)_x, \quad (A_x)_t = (A_t)_x . \tag{40}$$

From the first two equations (40), we get two nonlinear equations

$$\beta_1(b,c) = 0, \quad \gamma_1(b,c) = 0.$$

The connection between these equations and the mNLS (36) is given by

$$\beta_1(b,c) = b\left(\frac{\beta(b,c)}{b} \right)_x, \quad \gamma_1(b,c) = c\left(\frac{\gamma(b,c)}{c} \right)_x , \tag{41}$$

so we have not (36) but

$$\beta(b,c) = mb, \quad \gamma(b,c) = m'c, \tag{42}$$

where m and m' are arbitrary constants. Substituting b_t and c_t [which are expressed from (42)] into the third equation of the system (40), we obtain $m' = m$. Thus, using the gauge transformation

$$b \to e^{-imt} b, \quad c \to e^{imt} c,$$

we can reduce (42) to mNLS (36)

$$\beta(b,c)-mb\to e^{-imt}\beta(b,c)=0,\quad \gamma(b,c)-mc\to e^{-imt}\gamma(b,c)=0.$$

This completes the proof that the system (39) is the Lax pair of mNLS. We are giving two formulas (for convenience of reader) which are useful to check for this Lax pair

$$a_x=\frac{(bc)_x}{\lambda-2a},\quad a_t=\lambda a_x+b_xc-bc_x-bC_x(0,-2)+cB_x(-2,-2).$$

We will shortly see the advantage of carefully working out the details of the NLS dressing chains. We will find that almost all of this formalism carried over directly into the more complicated DS dressing chains. Formulas for the DS dressing chains are very bulky but have the same structure.

V. CONJUGATE CHAINS OF THE DS EQUATIONS

The DS equations has the form

$$iu_t+u_{xx}+\frac{1}{\alpha^2}u_{yy}-\frac{2}{\alpha^2}u^2v+qu=0,\quad -iv_t+v_{xx}+\frac{1}{\alpha^2}v_{yy}-\frac{2}{\alpha^2}v^2u+qv=0, \tag{43}$$

$$q_{yy}-\alpha^2q_{xx}=-4(uv)_{xx},$$

where $u=u(x,y,t)$, $v=v(x,y,t)$, $q=q(x,y,t)$. We have the DS-I system if $\alpha=1$, and DS-II if $\alpha=i$. Under the reduction $v=\pm\bar{u}$, one obtains a known model that describes the propagation of a small amplitude wave packet that is quasi-one-dimensional and quasi-monochromatic over the surface of a nonviscous curl-free liquid.[10] The quantity u is the envelope of the velocity potential, while q describes the nonlocal flow generated by the wave packet. A different application of (43) is related to the dynamics of plasma waves.[11] We will not use this reduction restriction in this section.

Lax pair for the (43) has the form

$$\begin{gathered}\psi_y=\alpha\psi_x+u\phi,\quad \phi_y=-\alpha\phi_x+v\psi,\\ \psi_t=2i\psi_{xx}+\frac{2i}{\alpha}u\phi_x+\left(\frac{1}{2}\left[\frac{1}{\alpha}F_y+F_x\right]-\frac{i}{\alpha^2}uv\right)\psi+\frac{i}{\alpha^2}(\alpha u_x+u_y)\phi,\\ \phi_t=-2i\phi_{xx}+\frac{2i}{\alpha}v\psi_x+\left(\frac{1}{2}\left[\frac{1}{\alpha}F_y-F_x\right]+\frac{i}{\alpha^2}uv\right)\phi+\frac{i}{\alpha^2}(\alpha v_x-v_y)\psi,\end{gathered} \tag{44}$$

where $q=-iF_x$.

Let $\{\psi_1,\phi_1;\psi_2,\phi_2;\psi,\phi\}$ be solutions of (44) for the same u, v, and F. DT is given by

$$\begin{gathered}\psi\to\psi_1=\psi_x-a\psi-b\phi,\quad \phi\to\phi_1=\phi_x-c\psi-d\phi,\\ u\to u_1=u+2\alpha b,\quad v\to v_1=v-2\alpha c,\quad F\to F_1=F+4i(a+d),\end{gathered} \tag{45}$$

where

$$a=\frac{\psi_{1,x}\phi_2-\psi_{2,x}\phi_1}{\Delta},\quad b=\frac{\psi_{2,x}\psi_1-\psi_{1,x}\psi_2}{\Delta},\quad c=\frac{\phi_{1,x}\phi_2-\phi_{2,x}\phi_1}{\Delta}, \tag{46}$$

$$d=\frac{\phi_{2,x}\psi_1-\phi_{1,x}\psi_2}{\Delta},\quad \Delta=\psi_1\phi_2-\psi_2\phi_1.$$

The quantities a, b, c, d are solutions of the system

$$
\begin{aligned}
&a_y=\alpha(a_x+2bc)+uc-vb,\quad b_y=\alpha(b_x+2bd)+(d-a)u+u_x,\\
&c_y=-\alpha(c_x+2ac)+(a-d)v+v_x,\quad d_y=-\alpha(d_x+2bc)-uc+vb,\\
&a_t=2i\left[\left(a_x+2bc+a^2+\frac{q}{4}\right)_x+2(a+d)bc\right]+\frac{i}{\alpha^2}[bv_y+cu_y-(uv)_x]\\
&\quad+\frac{i}{\alpha}\left[cu_x-bv_x+2(cdu-abv+(uc)_x)+\frac{q_y}{2}\right],\\
&b_t=2i\left[(b_x+2bd)_x+2\left(a_x+bc+d^2+\frac{q}{4}\right)b\right]+\frac{i}{\alpha^2}[u_{xy}+(d-a)u_y-2buv]\\
&\quad+\frac{i}{\alpha}[u_{xx}+(3d-a)u_x+2(d_x+d^2-ad+bc)u-2b^2v],\\
&c_t=-2i\left[(c_x+2ac)_x+2\left(d_x+bc+a^2+\frac{q}{4}\right)c\right]-\frac{i}{\alpha^2}[v_{xy}+(a-d)v_y-2cuv]\\
&\quad+\frac{i}{\alpha}[v_{xx}+(3a-d)v_x+2(a_x+a^2-ad+bc)v-2c^2u],\\
&d_t=-2i\left[\left(d_x+2bc+d^2+\frac{q}{4}\right)_x+2(a+d)bc\right]-\frac{i}{\alpha^2}[bv_y+cu_y-(uv)_x]\\
&\quad-\frac{i}{\alpha}\left[cu_x-bv_x+2(cdu-abv-(bv)_x)-\frac{q_y}{2}\right].
\end{aligned}
\tag{47}
$$

These equations can be obtained from (44). Equations (47) are similar to (32) and (33). The Lax pair (44) and Eqs. (47) are simply two different representations of the same equation. To construct mDS equations we must first express fields a and d via one function $\theta=\theta(x,y,t)$, defined by the relations

$$
a=\frac{\alpha\theta_x+\theta_y}{2\alpha},\quad d=\frac{\alpha\theta_x-\theta_y}{2\alpha}. \tag{48}
$$

It is easy to check the accuracy of this representation by the substitution (48) into the first and fourth equations (47). Second, we must exclude potentials u and v from the first four equations (47). Introducing new fields $\xi=\xi(x,y,t)$, $X=\theta_x$, $Y=\theta_y$

$$
q=-2X_x-X^2-4bc+\frac{1}{\alpha^2}(\xi-Y^2),
$$

and putting everything together, we find mDS (mDS-I if $\alpha=1$ and mDS-II if $\alpha=i$) equations as the system of five equations for the five functions b, c, ξ, X, and Y:

$$
\begin{aligned}
&ib_t+2(bX+b_x)_x+\frac{1}{\alpha}[(UX+U_x)_x+2b(Uc-Vb)-2Y(bX+b_x)]\\
&\quad+\frac{1}{\alpha^2}[U_{xy}-U(X_y+XY)-2(U_xY+bUV)+\xi b]+\frac{1}{\alpha^3}Y(UY-U_y)=0,
\end{aligned}
$$

$$
\begin{aligned}
&-ic_t+2(cX+c_x)_x-\frac{1}{\alpha}[(VX+V_x)_x-2c(Uc-Vb)-2Y(cX+c_x)]\\
&\quad+\frac{1}{\alpha^2}[V_{xy}-V(X_y+XY)-2(V_xY+cUV)+\xi c]-\frac{1}{\alpha^3}Y(VY-V_y)=0,\\
&iX_t+4[(bc)_x+2Xbc]-\frac{2}{\alpha}[X(Vb-Uc)+4cb_y-2(cU)_x+bV_x-cU_x-YX_x]\\
&\quad-\frac{2}{\alpha^2}[(UV)_x-Vb_y-Uc_y+Y(bV+cU)]-\frac{1}{\alpha^3}(Y^2-\xi)_y=0,\\
&iY_t+4(b_yc-bc_y)+\frac{1}{\alpha}[2(U_yc-Uc_y+V_yb-Vb_y)+\xi_x]=0,\\
&X_y-Y_x=0,
\end{aligned}
\tag{49}
$$

where

$$
U=\frac{G_1}{2\alpha(2bcY+\alpha(bc_x-b_xc))},\quad V=\frac{G_2}{2\alpha(2bcY+\alpha(bc_x-b_xc))},
$$

$$
\begin{aligned}
G_1&=\alpha^3[b_xX_x-bX_{xx}+2b(2bcX+b_xc-bc_x)]\\
&\quad+\alpha^2[2(bc_y-b_yc)-(X_x+4bc)Y]b+\alpha(bX_{yy}-b_xY_y)+bYY_y,\\
G_2&=\alpha^3[c_xX_x-cX_{xx}+2c(2bcX-b_xc+bc_x)]\\
&\quad+\alpha^2[2(bc_y-b_yc)+(X_x+4bc)Y]c+\alpha(cX_{yy}-c_xY_y)-cYY_y.
\end{aligned}
$$

As we have mentioned above, the NLS equation has two types of discrete symmetries: Darboux and Schlesinger transformations. In just the same way, the discrete symmetries of the DS equations include T symmetry. These transformations are given by[12,13]

$$
u\to u_1=u(uv+\alpha^2(\log u)_{xx}-(\log u)_{yy}),\quad v\to v_1=\frac{1}{u},\quad q\to q_1=q+4(\log u)_{xx},
$$

$$
u\to u_{-1}=\frac{1}{v},\quad v\to v_{-1}=v(uv+\alpha^2(\log v)_{xx}-(\log v)_{yy}),\quad q\to q_{-1}=q+4(\log v)_{xx}.
$$

Similar transformations for (49) are given by

$$
b\to b_1=\frac{M_1}{\alpha U(U+2\alpha b)},\quad c\to c_1=\frac{b}{U(U+2\alpha b)},
$$

$$
X\to X_1=X+2\alpha\frac{Ub_x-U_xb}{U(U+2\alpha b)},\quad Y\to Y_1=\frac{-U^2Y+2\alpha[UU_x-bU_y+\alpha U(b_x+bX)]}{U(U+2\alpha b)},
$$

$$
\xi\to\xi_1=\xi+4\alpha\frac{\alpha^2U(b_{xx}+(bX)_x)+\alpha[b(UY_x-U_{xy})+U(U_{xx}-b_xY)]-UU_xY}{U(U+2\alpha b)},
$$

and

$$c\to c_{-1}=\frac{M_{-1}}{\alpha V(V-2\alpha c)},\quad b\to b_{-1}=\frac{c}{V(V-2\alpha c)},$$

$$X\to X_{-1}=X-2\alpha\frac{Vc_x-V_xc}{V(V-2\alpha c)},\quad Y\to Y_{-1}=\frac{V^2Y+2\alpha[VV_x-cV_y-\alpha V(c_x+cX)]}{V(V-2\alpha c)},$$

$$\xi\to\xi_{-1}=\xi-4\alpha\frac{\alpha^2V(c_{xx}+(cX)_x)-\alpha[c(VY_x-V_{xy})+V(V_{xx}-c_xY)]-VV_xY}{V(V-2\alpha c)},$$

where

$$\begin{aligned}M_1=&\alpha^3[U^2b(2X_x-X^2)+2U((U_xb-Ub_x)X+(U^2)_xb_x+4(Ub)^2c+(U_x^2-2UU_{xx})b]\\&+\alpha^2U[U(UX_x+2bY_x)+(2U_yb-UU_x)X-2Ub_xY+4U^2cb-2U_{xy}b-UU_{xx}+2b_xU_y\\&+2U_x^2]+\alpha[U^3(Y_x+XY+Uc)+U^2(bY^2-2U_xY-U_{xy})+U_y((U^2)_x-bU_y)]\\&+U^2Y(UY-U_y),\end{aligned}$$

$$\begin{aligned}M_{-1}=&\alpha^3[V^2c(X^2-2X_x)-2V(V_xc-Vc_x)X-(V^2)_xc_x-4(Vc)^2b-(V_x^2-2VV_{xx})c]\\&+\alpha^2V[V(VX_x+2cY_x)+(2V_yc-VV_x)X-2Vc_xY+4V^2bc-2V_{xy}c-VV_{xx}+2c_xV_y\\&+2V_x^2]-\alpha[V^3(Y_x+XY+Vb)+V^2(cY^2-2V_xY-V_{xy})+V_y((V^2)_x-cV_y)]\\&+V^2Y(VY-V_y).\end{aligned}$$

It is possible to verify that $X_{\pm1,y}=Y_{\pm1,x}$, $(b_1)_{-1}=(b_{-1})_1=b$, and so on.

To obtain dressing chains of discrete symmetries, we must exclude potentials u, v, q from the two systems: (47) and the system of equations obtained from (47) by replacing $a\to a_1$, $b\to b_1$, $c\to c_1$, $d\to d_1$, $q\to q_1=q+4(a+d)_x$, $u\to u_1$, $v\to v_1$ [it is necessary to use (45)]. As a result, we have y chains

$$\begin{aligned}&[2bc(d-a)+b_xc-bc_x](a_{1,y}-\alpha a_{1,x})+(bc_1-b_1c)(a_y-\alpha a_x)_x+(bc_1-b_1c)(bc_y-b_yc)\\&+\alpha[(b_1c+2b_1c_1+bc_1)(bc_x-b_xc)+4bc(ac_1(b+b_1)-b_1d(c+c_1))]\\&+[(bc_1+b_1c)(a-d)+b_1c_x-b_xc_1](a_y-\alpha a_x)=0,\\&(bc_1-b_1c)[(b_1-b)_y-\alpha(b+b_1)_x]+(a-a_1-d+d_1)[\alpha(a_{1,x}b-a_xb_1)+a_yb_1-a_{1,y}b]\\&+2\alpha[(b+b_1)(abc_1+cb_1d_1)-bb_1(c+c_1)(a_1+d)]=0,\\&(b_1c-bc_1)[(c_1-c)_y+\alpha(c+c_1)_x]+(a-a_1-d+d_1)[\alpha(a_{1,x}c-a_xc_1)+a_yc_1-a_{1,y}c]\\&-2\alpha[(c+c_1)(a_1c_1b+cdb_1)-cc_1(b+b_1)(a+d_1)]=0,\\&(a_1+d_1)_y-\alpha(a_1-d_1)_x=0,\end{aligned}\tag{50}$$

and t chains

$$\begin{aligned}&\alpha^2(a_1-a)_t+i[2\alpha^2((a^2-a_1^2-2b_1c_1-a_{1,x}-d_x)_x+2((a+d)bc-(b+b_1)c_1d_1-(c+c_1)a_1b_1\\&-(bc_1)_x)-b_xc_1-b_1c_x)+\alpha((c-3c_1)U_x+(b+b_1)V_x+2(b_1c_y-b_yc_1-(a+d)_{xy}\\&+(b_x+a_1b_1-ab)V-(c_{1,x}+c_1d_1-cd)U))+(b-b_1)V_y+(c-c_1)U_y]=0,\end{aligned}$$

$$
\begin{aligned}
&\alpha^2(bb_{1,t}-b_tb_1)+i[2\alpha^2(2b^2(a_1d_1-b_1c_1)-2bb_1^2(c_1+c)+b_{xx}b_1-b_{1,xx}b-2bd_{1,x}(b+b_1)\\
&\quad+2(b_xdb_1-b_{1,x}d_1b)+b[a_1b_x-2a_{1,x}b_1-b_{xx}-3b_xd_1+2(b_1(d^2-bc)-d_1^2(b+b_1))])\\
&\quad+\alpha((b_1-b)U_{xx}+(3(b_1d-bd_1)+a_1b-ab_1)U_x+2[b_1bV(b+b_1)+bb_y(a_1-d_1)-bb_{xy}\\
&\quad+U(b_1d_x-bd_{1,x}+b_1d^2-bd_1^2-bb_1(c+c_1)+ba_1d_1-b_1ad)])+U_{xy}(b_1-b)+U_y(b(a_1\\
&\quad-d_1)-b_1(a-d))]=0,\\
&\alpha^2(cc_{1,t}-c_tc_1)+i[2\alpha^2(2c^2(b_1c_1-a_1d_1)+2cc_1^2(b_1+b)+c_{1,xx}c-c_1c_{xx}+2ca_{1,x}(c+c_1)\\
&\quad+2(ca_1c_{1,x}-c_1ac_x)+c[2c_1d_{1,x}-d_1c_x+c_{xx}+3c_xa_1+2(c_1(bc-a^2)+a_1^2(c+c_1))])\\
&\quad+\alpha((c_1-c)V_{xx}+(3(ac_1-a_1c)+cd_1-c_1d)V_x+2[c_1cU(c+c_1)+cc_y(d_1-a_1)-cc_{xy}\\
&\quad+V(c_1a_x-ca_{1,x}+c_1a^2-ca_1^2-cc_1(b+b_1)+ca_1d_1-c_1ad)])+V_{xy}(c-c_1)+V_y(c(a_1-d_1)\\
&\quad-c_1(a-d))]=0,\\
&\alpha^2(d_1-d)_t+i[2\alpha^2((d_1^2-d^2+2b_1c_1+a_x+d_{1,x})_x-2((a+d)bc-(b+b_1)c_1d_1-(c+c_1)a_1b_1\\
&\quad-(b_1c)_x)+b_xc_1+b_1c_x)+\alpha((b-3b_1)V_x+(c+c_1)U_x+2(c_1b_y-b_1c_y-(a+d)_{xy}\\
&\quad+(c_x+c_1d_1-cd)U-(b_{1,x}+a_1b_1-ab)V))+(c_1-c)U_y+(b_1-b)V_y]=0.
\end{aligned}
\tag{51}
$$

These formulas are an awful sight! Unfortunately, I don't know how to write them in more compact form in our gauge. Equation (51) has the best form I could imagine.

Although these equations are long and difficult, the end result is quite simple. We can see that all of the $(1+1)$ NLS formalism carried over directly into the $(2+1)$ DS dressing chains. In particular, the chains (51) involve Lax pair for the mDS (49). We do not give it here.

As noted in Sec. III, the KP equations admit two types of chains, which we call conjugate. It is a new result, which is characteristic precisely of multidimensional systems. Of course, it is true for the DS equations.

To construct the chains which are conjugate to (50)–(51), we must introduce the new Lax pair for the DS equations $[p=p(x,y,t),\ f=f(x,y,t)]$

$$
\begin{aligned}
&p_y=\alpha p_x-vf,\quad f_y=-\alpha f_x-up,\\
&p_t=-2ip_{xx}+\frac{2i}{\alpha}vf_x-\left(\frac{1}{2}\left[\frac{1}{\alpha}F_y+F_x\right]-\frac{i}{\alpha^2}uv\right)p+\frac{i}{\alpha^2}(\alpha v_x+v_y)f,\\
&f_t=2if_{xx}+\frac{2i}{\alpha}up_x-\left(\frac{1}{2}\left[\frac{1}{\alpha}F_y-F_x\right]+\frac{i}{\alpha^2}uv\right)f+\frac{i}{\alpha^2}(\alpha u_x-u_y)p,
\end{aligned}
\tag{52}
$$

two matrix functions

$$
\Psi=\begin{pmatrix}\psi_1 & \psi_2\\ \phi_1 & \phi_2\end{pmatrix},\quad \Phi=\begin{pmatrix}p_1 & f_1\\ p_2 & f_2\end{pmatrix},
$$

and one form

$$
d\Omega=\Phi\Psi\,dx+\alpha\Phi\sigma_3\Psi\,dy+2i\left(\Phi\sigma_3\Psi_x-\Phi_x\sigma_3\Psi+\frac{1}{\alpha}\Phi\sigma_3\Psi\right),\quad \Omega=\int d\Omega.
$$

This one form is closed if $\psi_{1,2}$, $\phi_{1,2}$, $p_{1,2}$, and $f_{1,2}$ are solutions of Eqs. (44) and (52) for the same u, v, F. It is easy to see that the quantities

$$A=\frac{p_{1,x}f_2-p_{2,x}f_1}{\Delta},\quad B=\frac{f_{1,x}f_2-f_{2,x}f_1}{\Delta},\quad C=\frac{p_{2,x}p_1-p_{1,x}p_2}{\Delta},$$

$$D=\frac{f_{2,x}p_1-f_{1,x}p_2}{\Delta},\quad \Delta=p_1f_2-p_2f_1.$$

are solutions of the y system

$$\begin{gathered}A_y=\alpha(A_x+2BC)+uC-vB,\quad B_y=-\alpha(B_x+2AB)+(D-A)u-u_x,\\ C_y=\alpha(C_x+2CD)+(A-D)v-v_x,\quad D_y=-A_y+\alpha(A-D)_x.\end{gathered}\tag{53}$$

Here, we don't need t system (four equations for the A_t, B_t, C_t, and D_t).

The Darboux transformation (45) [for the system (44)] give us the transformation rule for the functions A, B, C, D

$$A\to a_1=\Lambda_{11}-a,\quad B\to b_1=\Lambda_{12}-b,\quad C\to c_1=\Lambda_{21}-c,\quad D\to d_1=\Lambda_{22}-d,$$

where a, b, c, and d are defined in (46), and Λ_{ik} are elements of the matrix $\Lambda=\Psi\Omega^{-1}\Phi$, $i,k=1,2$. Transforming the system (53) and exluding potentials u and v from this system and from the first four equations (47), we get y chains which are conjugate to (50). There are four equations; two of them are equaivalent to the first and fourth equations (50). The remaining two equations are given by

$$\begin{aligned}&(bc_1-b_1c)[(b+b_1)_y+\alpha(b+b_1)_x]+(a+a_1-d-d_1)[\alpha(a_xb_1-a_{1,x}b)+a_{1,y}b-a_yb_1]\\&\quad-2\alpha[(b+b_1)(abc_1+a_1b_1c)-bb_1(c+c_1)(d+d_1)]=0,\end{aligned}$$

$$\begin{aligned}&(b_1c-bc_1)[(c+c_1)_y-\alpha(c+c_1)_x]+(a+a_1-d-d_1)[\alpha(a_xc_1-a_{1,x}c)+a_{1,y}c-a_yc_1]\\&\quad+2\alpha[(c+c_1)(bc_1d_1+b_1cd)-cc_1(b+b_1)(a+a_1)]=0.\end{aligned}$$

The conjugate t chains can be obtained by the same way. We do not give them here.

VI. ON THE LOCALIZED SOLUTIONS OF THE DS EQUATIONS

Discrete symmetries are a good way to obtain exact solutions of the nonlinear integrable equations. In Ref. 14 we applied the DT (S symmetry) to construct exact solutions to the DS-I and DS-II equations (the same to the BLP equations; see Ref. 15). In particular, we have obtained the dromion solutions of the DS-I equations. In this section we use the T symmetry to construct nonsingular solutions to the DS-I that fall off according to the exponential and/or rational low along *all* directions in the plan (see also Ref. 16). In the rest of this section we present (via S symmetry) novel exact solution of the DS-II equations describing the soliton on the plane-wave background.

A. DS-I equations

To study the DS-I equations it is convenient to use the following change of variables:

$$\partial_x\to\frac{1}{\sqrt{2}}(\partial_x+\partial_y),\quad \partial_y\to\frac{1}{\sqrt{2}}(\partial_x-\partial_y),\quad v\to-\frac{\overline{u}}{2}.$$

We are interested in localized solutions to the DS-I equations which move without shape distortions, and we look for these solutions in the form

$$u(t,x,y)=\overline{v(t,x,y)}=U(\xi,\eta)\exp(i\theta),\quad q(t,x,y)=Q(\xi,\eta),$$

where

$$\xi = x - 2at, \quad \eta = x - 4bt, \quad \theta = ax + by - (a^2 + b^2)t,$$

and $U(\xi, \eta)$ is the real function. It was shown in Ref. 16 that a solution to the DS-I equations can be found in this setting from the nonlinear Liouville equation

$$\partial_x \partial_y \Phi = \tfrac{1}{2} \exp(\Phi), \tag{54}$$

for the function $\Phi \equiv \log(U^2)$. This result was obtained via the T symmetries (see the previous section).

It is convenient to introduce the boundary conditions for the $U(x,y)$ as

$$U(x,0) = A(x), \quad U(0,y) = B(y), \quad A(0) = B(0) = C, \tag{55}$$

where $A(x)$ and $B(y)$ are the given functions. Now, we can use the solution to the Gousat problem for (54) given in Ref. 17, from which we find

$$U(x,y) = \frac{4CA(x)B(y)}{4C^2 - \int_0^x dp A^2(p) \int_0^y dq B^2(q)}. \tag{56}$$

Using T symmetries, one can also find the explicit expression for the $Q(x,y)$ field

$$Q(x,y) = \frac{1}{2}\left(P'\left(\frac{1}{P'}\right)'' + G'\left(\frac{1}{G'}\right)''\right) - \frac{3}{4}([(\log P')']^2 + [(\log G')']^2) + \frac{2}{PG-4}\left(PG'' + P''G - \frac{(PG')^2 + (P'G)^2 + 8P'G'}{PG-4}\right),$$

where

$$P(x) = \frac{1}{C}\int_0^x dp A^2(p), \quad G(y) = \frac{1}{C}\int_0^y dq\, B^2(q).$$

Expression (56) also allows us to construct localized solutions. For example, choosing the boundary functions in the form of two solutions of the NLS equation, we obtain the well-known ''one-dromion'' solution.[18] Other localized objects are found by choosing the boundary conditions appropriately. Thus, assuming $A(x)$ and $B(y)$ to be solutions of the KdV equation, we obtain a new solution that decays exponentially in **all directions**.[16] It is possible to show that these equations are different from the (L,M) dromions[19] and N^2-soliton solutions built in Refs. 20 and 21.

The rational localized solutions (''lamps'') are obtained in the same way. We get the two-lamp solution and the four-lamp solution in Ref. 16. One can always choose the parameters such that the solutions falling off in all directions according to rational law are nonsingular. Finally, we can obtain the localized solution falling off according to the exponential law as a function of x and according to the ratianol law as a function of x.

B. DS-II equations

We couldn't find a localized nonstationary solution of the DS-II equation. We present only soliton on the plane-wave background. We choose the initial solution of the DS-II equations as

$$u = A\exp(iS), \quad S = -(2A^2 + a^2 - b^2)t + ax + by, \quad q = 0,$$

where A, a and b are real constants. The solutions of the Lax pair (44)

$$\psi_1 = f \exp\left(i\frac{S}{2} + M \right), \quad \psi_2 = \frac{\overline{i(2m-b)-p}}{2A}\left(f - 2i\frac{\alpha_1}{p} \right)\exp\left(i\frac{S}{2} + \overline{M} \right),$$

where

$$f = \alpha_1\left[x + \frac{1}{p}((b-2m)y + 2(2(bm - A^2 - 2m^2) - ap)t) \right] + \alpha_2,$$

$$M = mx + \tfrac{1}{2}((p-a)y + [p(b+2m) - 4am]t), \quad p^2 + [4A^2 + (b-2m)^2]^2 = 0.$$

Using (45) (with $\overline{m} = m$, $\overline{\alpha_1} = \alpha_1$, and $\alpha_2 = 0$) we get nonsingular solution u_1 which is the soliton on the plane-wave background

$$|u_1|^2 \to A^2 \quad \text{at} \quad x^2 + y^2 \to \infty.$$

This solution is a two-dimensional generalization of the ''exulton'' solution of the NLS built in Ref. 1.

VII. CONCLUSION

The past years of intense theoretical research have made it increasingly clear that the secret to integrability most likely lies in the power of discrete symmetries. Let us summarize some of the promising features of the discrete symmetries.

(1) It is an extremely powerful method to construct exact solutions of integrable equations.
(2) This approach includes all ''soliton miracles:'' finite-gap solutions, the Painleve property, etc.
(3) Discrete symmetries allow us to proliferate integrable equations. For example, the whole MKdV theory can be considered as the DT theory and the Toda–Volterra theory can be considered as the theory of S- and T symmetries of the NLS equations (Ref. 9).
(4) Discrete symmetries led to a connection between integrable system and supersymmetry.
(5) Discrete symmetries allow us to construct discrete integrable systems.

Ideally, we would want a unified theory to unite and understand all soliton miracles. There are two ways to find this unified theory. The first path is connected with the Hirota bilinear difference equation.[22] This famous equation is known to provide a canonical integrable discretization for most important types of soliton equation.

The second path is the theory of dressing chains. This approach allows us to proliferate integrable equations and, at the same time, to establish a link between known integrable equations (it is clear that the Miura map can be obtained from the dressing chains). Ideally, we want to show that all integrable equations are nothing but different forms of a single equation!

Even if this direction is right, it is still a long way off. Now, the theory itself often seems like a confused jumble of random (but useful) rules and random (but remarkable) observations. It remains to be seen how useful the dressing chains will become in the future.

ACKNOWLEDGMENT

This work was supported by the Grant of Education Department of the Russian Federation, No. E00-3.1-383.

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Scattering of solitons of the Klein–Gordon equation coupled to a classical particle

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(Received 21 January 2002; accepted 28 November 2002)

Long-time asymptotics are established for finite energy solutions of the scalar Klein–Gordon equation coupled to a relativistic classical particle: any ''scattering'' solution is asymptotically a sum of a soliton and of a dispersive free wave packet as $t \to \pm\infty$. These asymptotics mean the nonlinear scattering of free wave packets by the soliton. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1539900]

I. INTRODUCTION: KLEIN–GORDON FIELD COUPLED TO A CLASSICAL PARTICLE

In this paper we consider the classical scalar Klein–Gordon equation coupled (noncovariantly) to a relativistic classical particle subjected to an external potential V of compact support. The system is a finite-range perturbation of the corresponding translation-invariant system without V that admits soliton-type solutions describing a particle traveling with constant velocity that is dressed by a comoving wave field. The set of all such solutions forms a finite-dimensional manifold, called the *soliton manifold*, in the phase space (a Hilbert space) of the unperturbed system. We are interested in *scattering* solutions of the perturbed system in which the particle travels to infinity as $t \to \pm\infty$.

The reason for the name *soliton manifold* resides the fact, proven in this paper, that it is an attracting set for the scattering solutions of the perturbed dynamical system. The attraction holds in the Fréchet topology defined by the local energy seminorms.

Our main result is the long-time asymptotics in the global energy norm: each scattering solution is asymptotically the sum of a soliton and a dispersive free wave as $t \to \pm\infty$. This means that the solution is scattering of the free wave by a soliton. This representation of the solutions gives a mathematical description of the wave-particle duality: for $t = -\infty$ such solution is a union of a ''particle'' = soliton and ''photon'' = free wave, for finite t the solution in general does not admit such a representation, and for $t = \infty$ the representation again appears.

Previously similar results have been proved for relativistic charged particles coupled, respectively, to the wave equation corresponding to $m = 0$ (Refs. 11 and 13) and to Maxwell's equations.[2,10,16] The proof of these results is based on the nonautonomous integral inequality method[19] that uses essentially the strong Huygen's principle. In the case of the Klein–Gordon equation with $m > 0$ the strong Huygen's principle fails. That is why we develop a new more general version of the integral inequality method that does not use the strong Huygen's principle. An important role play the known time decay of the Green function for the Klein–Gordon equation and a sufficiently fast spatial decay of the solitons in the case $m > 0$.

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We consider a scalar wave field $\psi(x)\in\mathbb{R}$, $x\in\mathbb{R}^3$, coupled to a relativistic particle with position q and momentum p, governed by

$$\dot{\psi}(x,t)=\pi(x,t),\quad \dot{\pi}(x,t)=\Delta\psi(x,t)-m^2\psi(x,t)-\rho(x-q(t)),$$
$$\dot{q}(t)=p(t)/(1+p^2(t))^{1/2},\quad \dot{p}(t)=-\nabla V(q(t))+\int d^3x\ \psi(x,t)\,\nabla\rho(x-q(t)) \tag{1}$$

subject to appropriate initial conditions determining the dynamics. This is a Hamiltonian system with the Hamiltonian functional

$$\mathcal{H}(\psi,\pi,q,p)=(1+p^2)^{1/2}+V(q)+\frac{1}{2}\int d^3x(|\nabla\psi(x)|^2+m^2|\psi(x)|^2+|\pi(x)|^2)$$
$$+\int d^3x\ \psi(x)\rho(x-q). \tag{2}$$

We have set the mechanical mass of the particle and the speed of wave propagation equal to one. The case of the point particle corresponds to $\rho(x)=\delta(x)$ and then the interaction term in the Hamiltonian is simply $\psi(q)$. This would result however in an energy which is not bounded from below implying for the scattering theory the well-known ultraviolet divergence. Therefore we smooth the coupling by the function $\rho(x)$ following the strategy proposed by Abraham[1] for the Maxwell field. Respectively, the system (1) is not relativistic covariant. In analogy to the Maxwell–Lorentz equations we call ρ the ''charge distribution.'' We assume the real-valued function ρ to be in the Sobolev space H^1 and of compact support, i.e.,

$$\rho,\nabla\rho\in L^2(\mathbb{R}^3),\quad \rho(x)=0\ \text{ for }\ |x|\geqslant R_\rho. \tag{C}$$

An important assumption is that the norm of ρ in L^2 is sufficiently small,

$$\gamma_\rho:=\|\rho\|_{L^2}\ll 1 \tag{3}$$

meaning *weak* field-particle interaction.

For the potential V we introduce two sets of assumptions: smooth and bounded from below,

$$V\in C^2(\mathbb{R}^3),\quad V_0:=\inf_{q\in\mathbb{R}^3}V(q)>-\infty; \tag{$P_{\min}$}$$

and of a compact support,

$$V(x)\equiv 0\quad \text{for }\ |x|>R_V>0. \tag{K}$$

Consider the corresponding nonperturbed system with $V\equiv 0$:

$$\dot{\psi}(x,t)=\pi(x,t),\quad \dot{\pi}(x,t)=\Delta\psi(x,t)-m^2\psi(x,t)-\rho(x-q(t)),$$
$$\dot{q}(t)=p(t)/(1+p^2(t))^{1/2},\quad \dot{p}(t)=\int d^3x\ \psi(x,t)\,\nabla\rho(x-q(t)). \tag{4}$$

The system (4) has solutions traveling with constant velocity $v,|v|<1$. Up to spatial translations they are given by

$$S_v(t)=(\psi_v(x-vt),\pi_v(x-vt),vt,p_v) \tag{5}$$

with

$$\psi_v(x) = -\frac{1}{4\pi}\int \frac{e^{-m|(y-x)_\parallel + \lambda(y-x)_\perp|}\rho(y)d^3y}{|(y-x)_\parallel + \lambda(y-x)_\perp|},$$
$$\pi_v(x) = -v\cdot\nabla\psi_v(x), \quad p_v = v/\lambda. \tag{6}$$

Here we set $\lambda = \sqrt{1-v^2}$ and $x = x_\parallel + x_\perp$, where $v \| x_\parallel \in \mathbb{R}^3$ and $v \perp x_\perp \in \mathbb{R}^3$ for $x \in \mathbb{R}^3$. We call $S_v(t)$ the *soliton* with velocity v centered at $q(t) = vt$.

Let us discuss and summarize now our main results, the precise theorems to be stated in the following sections. Consider the set of scattering solutions to (1) for which $|q(t)| \to \infty$ as $t \to \infty$. Below we discuss the properties of these solutions. Since only a finite amount of energy can be dissipated to infinity, we shall show the relaxation of acceleration,

$$\ddot{q}(t) \to 0, \quad t \to \pm\infty. \tag{7}$$

More precisely, we shall establish the rate of convergence $|\ddot{q}(t)| \sim t^{-1-\sigma}$ with a $\sigma > 0$. This is a crucial point of our asymptotic analysis. It implies that

$$\dot{q}(t) \to v_\pm, \quad t \to \pm\infty. \tag{8}$$

Also we show that the fields are asymptotically traveling waves in the sense

$$(\psi(x,t), \pi(x,t)) \sim (\psi_{v_\pm}(x - q(t)), \pi_{v_\pm}(x - q(t))), \quad t \to \pm\infty. \tag{9}$$

Since the energy is conserved, the convergence here is in the sense of local energy seminorms, cf. Sec. II. Further, we shall establish the corresponding asymptotics in the *global* energy norm,

$$(\psi(x,t), \pi(x,t)) \sim (\psi_{v_\pm}(x - q(t)), \pi_{v_\pm}(x - q(t))) + U(t)\Psi_\pm, \quad t \to \pm\infty, \tag{10}$$

where $U(t)$ is the unitary group generated by the free Klein–Gordon equation, and $\Psi_\pm$ are the scattering states. At last we suggest simple sufficient conditions for solutions to be scattering. Note that all finite energy solutions are scattering if $V(x) \equiv 0$. We prove (8), (9), and (10) with the assumption (3), however we suggest the same asymptotics hold in more general framework.

We mention now some previous results which reflect the gradual progress in investigating the long-time asymptotics for coupled field-particle equations.

The results of Ref. 14 for the wave equation, $m = 0$, imply the long-time convergence to the set of solitons of type (5) in the sense of local energy seminorms, as in (9).

Soliton-type asymptotics were proved for certain translation invariant completely integrable 1D equations.[18] Soliton-type asymptotics in *local* energy seminorms was proved for a translation invariant 3D system of a scalar field coupled to a particle[15] and for translation invariant 1D kinetic-reaction systems.[8]

Soliton-type asymptotics of type (10) in *global* energy norm were proved initially for *small perturbations* of soliton-type solutions of 1D nonlinear Schrödinger equations.[3,4]

Soliton-type asymptotics of type (10) in the energy norm for all finite energy scattering solutions is proved here for the first time for coupled particle-field equations (1). The asymptotics is provided by radiation of the energy to infinity which leads to the relaxation (7). The relaxation in classical electrodynamics is known as ''radiative damping'' studied by Lorentz,[17] Dirac,[5] Feynman[7] and others.[9]

Note that a lot of numerical experiments[12] confirm the long-time convergence of an arbitrary finite energy solution of a general relativistic equation to a finite sum of solitons with velocities less than the light speed and of ''photons'' propagating at the light speed. Nevertheless the proof remains an absolutely open problem.

II. EXISTENCE OF DYNAMICS, *A PRIORI* ESTIMATES

To formulate our results precisely, we need some definitions. We introduce the phase space suitable for the Cauchy problem corresponding to (1) and (2). Let L^2 be the real Hilbert space $L^2(\mathbb{R}^3)$ with scalar product $\langle\cdot,\cdot\rangle$ and norm $|\cdot|$, and let H^1 be the Sobolev space $H^1=\{\psi \in L^2: |\nabla\psi| \in L^2\}$ with the norm $\|\psi\|=|\psi|+|\nabla\psi|$. Let $|\psi|_R$ denote the norm in $L^2(B_R)$ for $R>0$, where $B_R=\{x\in\mathbb{R}^3:|x|\leqslant R\}$. Then the seminorms $\|\psi\|_R=|\psi|_R+|\nabla\psi|_R$ are continuous on H^1.

Definition 1: (i) The phase space $\mathcal{E}$ is the Hilbert space $H^1\times L^2\times\mathbb{R}^3\times\mathbb{R}^3$ of states $Y=(\psi,\pi,q,p)$ with finite norm

$$\|Y\|_{\mathcal{E}}=\|\psi\|+|\pi|+|q|+|p|\,.$$

(ii) $\mathcal{E}_F$ is the space $\mathcal{E}$ endowed with the Fréchet topology defined by the local energy seminorms

$$\|Y\|_R=\|\psi\|_R+|\pi|_R+|q|+|p|,\quad \forall R>0\,.$$

(iii) $\mathcal{F}$ is the Hilbert space $H^1\times L^2$ of fields $\Psi=(\psi,\pi)$ with finite norm

$$\|\Psi\|_{\mathcal{F}}=\|\psi\|+|\pi|\,.$$

(iv) $\mathcal{F}_F$ is the space $\mathcal{F}$ endowed with the Fréchet topology defined by the local energy seminorms

$$\|\Psi\|_R=\|\psi\|_R+|\pi|_R\,,\quad \forall R>0\,.$$

Note that both spaces $\mathcal{E}$ and $\mathcal{E}_F$ are metrisable. For $\psi\in L^2$ we have

$$-\frac{1}{2m^2}|\rho|^2\leqslant\frac{m^2}{2}|\psi|^2+\langle\psi,\rho(\cdot-q)\rangle\leqslant\frac{m^2+1}{2}|\psi|^2+\frac{1}{2}|\rho|^2. \tag{11}$$

Therefore $\mathcal{E}$ is the space of finite energy states. The Hamiltonian functional $\mathcal{H}$ is continuous on the space $\mathcal{E}$ and the lower bound in (11) implies that the energy functional (2) is bounded from below, namely,

$$\inf_{Y\in\mathcal{E}}\mathcal{H}(Y)\geqslant 1+V_0-\frac{1}{2m^2}|\rho|^2. \tag{12}$$

We consider the Cauchy problem for the Hamiltonian system (1), which we write as

$$\dot{Y}(t)=\mathcal{V}_0(Y(t))+\mathcal{V}_1(Y(t)),\quad t\in\mathbb{R},\quad Y(0)=Y^0. \tag{13}$$

All derivatives are understood in the sense of distributions. Here $Y(t)=(\psi(t),\pi(t),q(t),p(t))$, $Y^0=(\psi^0,\pi^0,q^0,p^0)\in\mathcal{E}$, and $\mathcal{V}_0: Y\mapsto(\pi,\Delta\psi-m^2\psi,0,0)$. Recall that we are interested in situations where the particle is allowed to travel to infinity, e.g., when the external potential $V(q)$ vanishes identically. The existence of dynamics is true under such conditions ($P_{\min}$).

Theorem 2: *Let (C) and $(P_{\min})$ hold. Then (i) for every $Y^0\in\mathcal{E}$ the Cauchy problem (13) has a unique solution $Y(t)\in C(\mathbb{R},\mathcal{E})$. (ii) For every $t\in\mathbb{R}$ the map $W_t: Y^0\mapsto Y(t)$ is continuous both on $\mathcal{E}$ and on $\mathcal{E}_F$. (iii) The energy is conserved, i.e.,*

$$\mathcal{H}(Y(t))=\mathcal{H}(Y^0)\quad \text{for } t\in\mathbb{R}. \tag{14}$$

(iv) The speed is bounded,

$$|\dot{q}(t)|\leqslant\overline{v}<1\quad \text{for } t\in\mathbb{R}. \tag{15}$$

Proof: We follow Ref. 14, where the case $m=0$ is considered. Let us fix an arbitrary $b>0$ and prove (i)–(iii) for $\|Y^0\|_{\mathcal{E}}\leqslant b$ and $|t|\leqslant\varepsilon=\varepsilon(b)$ for some sufficiently small $\varepsilon(b)>0$.

ad (i) Fourier transform provides the existence and uniqueness of solution $Y_0(t) \in C(\mathbb{R},\mathcal{E})$ to the linear problem (13) with $\mathcal{V}_1 = 0$. Let $W_t^0 : Y^0 \mapsto Y_0(t)$ be the corresponding strongly continuous group of bounded linear operators on $\mathcal{E}$. Then uniqueness of solution to the (inhomogeneous) linear problem implies that (13) for $Y(t) \in C(\mathbb{R},\mathcal{E})$ is equivalent to

$$Y(t) = W_t^0 Y^0 + \int_0^t ds\, W_{t-s}^0 \mathcal{V}_1(Y(s)), \tag{16}$$

because $\mathcal{V}_1(Y(\cdot)) \in C(\mathbb{R},\mathcal{E})$ in this case. The latter follows from a local Lipschitz continuity of the map $\mathcal{V}_1$ in $\mathcal{E}$: for each $b>0$ there exist a $\kappa = \kappa(b) > 0$ such that for all $Y, Z \in \mathcal{E}$ with $\|Y\|_{\mathcal{E}}, \|Z\|_{\mathcal{E}} \leqslant b$,

$$\|\mathcal{V}_1(Y) - \mathcal{V}_1(Z)\|_{\mathcal{E}} \leqslant \kappa \|Y - Z\|_{\mathcal{E}}. \tag{17}$$

For example, we have

$$\left| \int d^3x\, (\psi_1(x) - \psi_2(x)) \nabla \rho(x-q) \right| \leqslant |\nabla(\psi_1 - \psi_2)||\rho|.$$

Moreover, by the contraction mapping principle, Eq. (16) has a unique local solution $Y(\cdot) \in C([-\varepsilon,\varepsilon],\mathcal{E})$ with $\varepsilon > 0$ depending only on b. Then the existence of the global dynamics will follow from the *a priori* estimate, see in *ad (iii)* below.

ad (ii) The map $W_t : Y^0 \mapsto Y(t)$ is continuous in the norm $\|\cdot\|_{\mathcal{E}}$ for $|t| \leqslant \varepsilon$ and $\|Y^0\| \leqslant b$. To prove continuity of W_t in $\mathcal{E}_F$, let us consider Picard's successive approximation scheme

$$Y^N(t) = W_t^0 Y^0 + \int_0^t ds\, W_{t-s}^0 \mathcal{V}_1(Y^{N-1}(s)), \quad N = 1,2,\ldots .$$

The equation for q^N in this system implies $|\dot{q}^N(t)| < 1$ and therefore $|q(t)| < |q^0| + |t|$. Now we fix $t \in \mathbb{R}$ and choose $R > |q^0| + |t| + R_\rho$ with R_ρ from (C). From the explicit solution of the free Klein–Gordon equation $W_t^0 Y^0$ (see Sec. III) we conclude that every Picard's approximation $Y^N(t)$ and hence the solution $Y(t) = (\psi(x,t), \pi(x,t), q(t), p(t))$ for $|x| < R$ depends only on the initial data $(\psi^0(x), \pi^0(x), q^0, p^0)$ with $|x| < R + |t|$. Thus the continuity of W_t in $\mathcal{E}_F$ follows from the continuity in $\mathcal{E}$.

ad (iii) For $k = 0,1,\ldots$ denote by $C_0^k(\mathbb{R}^3)$ the space of functions $\psi(x) \in C^k(\mathbb{R}^3)$ with compact support. For initial data $(\psi^0, \pi^0) \in C^3(\mathbb{R}^3) \times C^2(\mathbb{R}^3)$ the solution $\psi = \psi(x,t)$ satisfies $\psi \in C^2(\mathbb{R}^3 \times \mathbb{R})$. Indeed, this is well known for the solution $W_t^0 Y^0$ of the linear Klein–Gordon equation. The integral representation (16) then implies the same property for ψ. In addition, let Y^0 have compact support, i.e.,

$$\psi^0(x) = \pi^0(x) = 0 \quad \text{for} \quad |x| > R^0 \tag{18}$$

with some $R^0 > 0$. Since $|q(t)| < |q^0| + |t|$, (16) implies

$$\psi(x,t) = 0 \quad \text{for } |x| \geqslant |t| + \max\{R^0, R_\rho + |q^0| + |t|\}.$$

Thus, for such initial data energy conservation can be shown by integration by parts. Hence (iii) follows from the continuity of W_t and the fact that $C_0^3(\mathbb{R}^3) \oplus C_0^2(\mathbb{R}^3) \oplus \mathbb{R}^3 \oplus \mathbb{R}^3$ is dense in $\mathcal{E}$.

We use now energy conservation to ensure the existence of a global solution and its continuity. Similar to (11) we have

$$\mathcal{H}(Y) \geqslant \frac{1}{2}|\pi|^2 + \frac{1}{2}|\nabla\psi|^2 + \frac{m^2}{4}|\psi|^2 + \sqrt{1+p^2} + V(q) - \frac{1}{m^2}|\rho|^2,$$

and by energy conservation, for $|t| \leqslant \varepsilon$,

$$\frac{1}{2}|\pi(t)|^2+\frac{1}{2}|\nabla\psi(t)|^2+\frac{m^2}{4}|\psi|^2+\sqrt{1+p^2(t)}+V(q(t))-\frac{1}{m^2}|\rho|^2\leqslant\mathcal{H}(Y(t))=\mathcal{H}(Y^0). \quad (19)$$

Therefore $(P_{\min})$ implies the *a priori* estimate

$$\|\psi(t)\|+|\pi(t)|+|p(t)|\leqslant B \text{ for } t\in\mathbb{R} \quad (20)$$

with B depending only on the norm $\|Y^0\|_{\mathcal{E}}$ of the initial data and on $|\rho|$. Properties (i)–(iii) for arbitrary $t\in\mathbb{R}$ now follow from the same properties for small $|t|$ and from the *a priori* bound (20).

ad (iv) Note first that (20) implies $|p(t)|\leqslant p_0<\infty$. Hence

$$|\dot{q}(t)|/(1-\dot{q}^2(t))^{1/2}=|p(t)|\leqslant p_0<\infty,$$

which yields $|\dot{q}(t)|\leqslant q_1=:\overline{v}<1$. □

III. INTEGRAL INEQUALITY ARGUMENT

Definition 3: Let $0<\sigma<1/2$ *and let* $\alpha=(1-2\sigma)/3$. *The set* $\mathcal{E}^\sigma$ *is the set of the states* $(\psi,\pi,q,p)\in\mathcal{E}$ *such that*

$$\int_{R\leqslant|x|}d^3x(R^2|\psi(x)|^2+|\nabla\psi(x)|^2)=\mathcal{O}(R^{-(4+2\sigma)}) \quad (21)$$

and

$$\int_{R^\alpha\leqslant|x|}d^3x\ (|\psi(x)|^2+|\pi(x)|^2)=\mathcal{O}(R^{-(4+2\sigma)}) \quad (22)$$

as $R\to+\infty$.

If the soliton-type asymptotics is approximately valid, then the field should be close to the soliton centered at $q(t)$ with velocity $v(t)=\dot{q}(t)$. We therefore consider the difference

$$Z(x,t)=\Psi(x,t)-\Psi_{v(t)}(x-q(t)), \quad (23)$$

where

$$\Psi(x,t)=(\psi(x,t),\pi(x,t))$$

and $\Psi_v(x)=(\psi_v(x),\pi_v(x))$ is the field part of the soliton. Defining $\overline{\rho}(x)=(0,\rho(x))$ and $A(\psi,\pi)=(\pi,\Delta\psi-m^2\psi)$, it follows that Ψ obeys the equations of motion:

$$\dot{\Psi}(x,t)=A\Psi(x,t)-\overline{\rho}(x-q(t)). \quad (24)$$

On the other hand, for the soliton field Ψ_v with a fixed v, the equation

$$-\frac{\partial\Psi_v}{\partial x}(x-q(t))v=A\Psi_v(x-q(t))-\overline{\rho}(x-q(t)) \quad (25)$$

holds. Then (24) and (25) imply the following equation for Z:

$$\dot{Z}(x,t)=AZ(x,t)-\frac{\partial\Psi_{v(t)}}{\partial p}(x-q(t))\dot{p}(t). \quad (26)$$

Here, according to the chain rule,

$$\frac{\partial \Psi_v}{\partial p} = \frac{\partial \Psi_v}{\partial v}\frac{\partial v}{\partial p}, \tag{27}$$

where $\partial v/\partial p$ is the Jacobi matrix of the map $p \mapsto v(p) = p/\sqrt{1+p^2}$.

Proposition 4: Let (C), $(P_{\min})$, (K) *hold, let the solution* $Y(t)$ *to the system (1) be scattering and* $Y(0) \in \mathcal{E}^\sigma$ *for a certain* $\sigma \in (0;1/2)$. *Then for any* $R>0$ *and sufficiently small* $\gamma_\rho := |\rho|$,

$$\|Z(\cdot + q(t),t)\|_R \leqslant C_R(Z(0),q^0,\overline{v},R_\rho)(1+|t|)^{-1-\sigma}. \tag{28}$$

Proof: First, we prove the estimate with $R = R_\rho$. Definition (23) implies $Z(\cdot,t) \in \mathcal{F}$. Solving the equations (26) we get the mild solution representation,

$$Z(t) = U(t)Z(0) - \int_0^t U(t-s)\left[\frac{\partial \Psi_{v(s)}}{\partial p}(\cdot - q(s))\dot{p}(s)\right] ds, \tag{29}$$

with $U(t)$ the group generated by the free Klein–Gordon equation in $H^1 \oplus L^2$, see the explicit formulas in Sec. III A below.

Thus, the proof consists of two essential parts: (1) estimating, in local seminorms, the action of the free Klein–Gordon group $U(t)Z(0)$ and (2) estimating, in local seminorms, the free Klein–Gordon group applied to the Jacobian of the soliton field, $U(t-s)[\partial \Psi_{v(s)}/\partial p(\cdot - q(s))]$.

A. Local decay for the free Klein–Gordon group

Let us denote $S_t(x) = \{y\colon |y-x| = t\}$, $B_t(x) = \{y\colon |y-x| \leqslant t\}$. For sufficiently smooth initial data, say $u_0, v_0 \in C_0^\infty(\mathbb{R}^3)$, the action of the free Klein–Gordon group in $\mathbb{R}^3$ reads [Ref. 6, Chap. 5, formulas (6.4), (6.11), (6.12)],

$$U(t)(u_0(x),v_0(x)) = (u(x,t),v(x,t)) = (u_w(x,t) - u_m(x,t), v_w(x,t) - v_m(x,t))$$

with

$$u_w(x,t) = \frac{1}{4\pi t^2}\int_{S_t(x)} d^2y\, u_0(y) + \frac{1}{4\pi t}\int_{S_t(x)} d^2y \frac{\partial u_0(y)}{\partial n} + \frac{1}{4\pi t}\int_{S_t(x)} d^2y\, v_0(y), \tag{30}$$

$$u_m(x,t) = \frac{m^2}{8\pi}\int_{S_t(x)} d^2y\, u_0(y) + \frac{m}{4\pi}\int_{B_t(x)} d^3y\, \dot{F}(t,x-y)u_0(y) + \frac{m}{4\pi}\int_{B_t(x)} d^3y\, F(t,x-y)v_0(y), \tag{31}$$

and

$$\begin{aligned} v_w(x,t) = \dot{u}_w(x,t) = {} & \frac{1}{2\pi t^2}\int_{S_t(x)} d^2y \frac{\partial u_0(y)}{\partial n} + \frac{1}{4\pi t}\int_{S_t(x)} d^2y \frac{\partial^2 u_0(y)}{\partial n^2} \\ & + \frac{1}{4\pi t^2}\int_{S_t(x)} d^2y\, v_0(y) + \frac{1}{4\pi t}\int_{S_t(x)} d^2y \frac{\partial v_0(y)}{\partial n}, \end{aligned} \tag{32}$$

$$\begin{aligned} v_m(x,t) = \dot{u}_m(x,t) = {} & \frac{m^2}{4\pi t}\int_{S_t(x)} d^2y\, u_0(y) - \frac{m^4 t}{32\pi}\int_{S_t(x)} d^2y\, u_0(y) + \frac{m^2}{8\pi}\int_{S_t(x)} d^2y \frac{\partial u_0(y)}{\partial n} \\ & + \frac{m}{4\pi}\int_{B_t(x)} d^3y\, \ddot{F}(t,x-y)u_0(y) + \frac{m^2}{8\pi}\int_{S_t(x)} d^2y\, v_0(y) \\ & + \frac{m}{4\pi}\int_{B_t(x)} d^3y\, \dot{F}(t,x-y)v_0(y). \end{aligned} \tag{33}$$

Here $n = (y-x)/|y-x|$ is the exterior unit normal vector of the sphere $S_t(x)$ at a point y,

$$F(t,z)=\frac{J_1(m\sqrt{t^2-z^2})}{\sqrt{t^2-z^2}},$$

J_1 being the Bessel function of order 1. Note that $(u_w(x,t),v_w(x,t))$ is the solution to the free wave equation corresponding to $m=0$, with the same initial conditions (u_0,v_0). From the well-known asymptotics

$$|J_1(s)|+|J_1'(s)|+|J_1''(s)|=\mathcal{O}(|s|^{-1/2}) \quad \text{as } s\to\infty$$

of the Bessel function, see Ref. 20, Chap. XVII, it follows that

$$|F(t,z)|+|\dot{F}(t,z)|+|\ddot{F}(t,z)|+|\nabla_z F(t,z)|=\mathcal{O}(|t|^{-3/2}) \quad \text{as } t\to\infty, \tag{34}$$

if $|z|\leqslant\nu|t|$ with $0<\nu<1$. However, near the boundary of the cone $|z|=|t|$ only some weaker decay is valid, namely for $|z|\leqslant|t|-1$,

$$|F(t,z)|+|\dot{F}(t,z)|+|\ddot{F}(t,z)|+|\nabla_z F(t,z)|=\mathcal{O}(|t|^{-3/4}) \quad \text{as } t\to\infty, \tag{35}$$

Definition 5: The set $\mathcal{F}^\sigma$ for $0<\sigma<1/2$ is the set of the fields $(\psi,\pi)\in\mathcal{F}$ satisfying the conditions (21),(22).

Lemma 6: Let $(u_0,v_0)\in\mathcal{F}^\sigma$ with some $\sigma\in(0;1/2)$. Then $\forall R>0$,

$$\|U(t)(u_0,v_0)\|_R\leqslant C(u_0,v_0,R)(1+|t|)^{-1-\sigma}. \tag{36}$$

Proof: Note that for any fixed t the map $U(t):(u_0,v_0)\to(u(t),v(t))$ is continuous in $\mathcal{F}$. For initial data $(u_0,v_0)\in\mathcal{F}^\sigma$ we can approximate them with u_0^n, $v_0^n\in C_0^\infty$ such that the bounds (21), (22) hold for u_0, v_0 uniformly in n. Hence, it is sufficient to obtain the estimate (36) for $u_0,v_0\in C_0^\infty$, with $C(u_0,v_0,R)$ depending only on the constant of (21), (22) and on the norm of u_0,v_0 in $\mathcal{F}$. Thus, we may use the integral representation (30) to (33).

At first consider (u_w,v_w). For the free wave equation the following energy inequality is well known:

$$\int_{B_R}d^3x(|\nabla u_w(x,t)|^2+|v_w(x,t)|^2)\leqslant\int_{B_{t+R}}d^3x(|\nabla u_0(x)|^2+|v_0(x)|^2).$$

Further, from the strong Huygen's principle it follows that for $t>R$ the solution $(u_w(x,t),v_w(x,t))$ does not change if one replaces $u_0(x)$, $v_0(x)$ by zero inside the ball B_{t-R}. Hence,

$$\int_{B_R}d^3x(|\nabla u_w(x,t)|^2+|v_w(x,t)|^2)\leqslant\int_{B_{t-R,t+R}}d^3x(|\nabla u_0(x)|^2+|v_0(x)|^2),$$

where $B_{t-R,t+R}=\{x\in\mathbb{R}^3: t-R\leqslant|x|\leqslant t+R\}$. Then the conditions (21), (22) imply, for sufficiently large t,

$$|\nabla u_w(\cdot,t)|_R+|v_w(\cdot,t)|_R\leqslant C(R,u_0,v_0)(1+|t|)^{-1-\sigma}. \tag{37}$$

It remains to estimate $|u_w(\cdot,t)|_R$, $\|u_m(\cdot,t)\|_R$, and $|v_m(\cdot,t)|_R$. We claim that if $(u_0,v_0)\in\mathcal{F}^\sigma$, then for sufficiently large t any of the norms $|I(\cdot,t)|_R$, $\|J(\cdot,t)\|_R$, $|K(\cdot,t)|_R$ is bounded by $C(u_0,v_0,R)(1+|t|)^{-1-\sigma}$ for any integral $I(x,t)$ of (30), $J(x,t)$ of (31), $K(x,t)$ of (33). At first consider the spherical integrals. For example, let us prove these estimates for the integrals

$$I(x,t)=\frac{1}{4\pi t}\int_{S_t(x)}d^2y\,\frac{\partial u_0(y)}{\partial n},\quad J(x,t)=\frac{m^2}{8\pi}\int_{S_t(x)}d^2y\,u_0(y),\quad K(x,t)=\frac{m^4t}{32\pi}\int_{S_t(x)}d^2y\,u_0(y).$$

For $I(x,t)$ we should estimate $|I(\cdot,t)|_R$. We have

$$|I(\cdot,t)|_R^2=\int_{B_R} d^3x(I(x,t))^2$$
$$=\frac{C}{t^2}\int_{B_R} d^3x\left(\int_{S_t(x)} d^2y\,\frac{\partial u_0(y)}{\partial n}\right)^2$$
$$\leqslant\frac{C}{t^2}\int_{B_R} d^3x\ 4\pi t^2\int_{S_t(x)} d^2y\left(\frac{\partial u_0(y)}{\partial n}\right)^2=C_1\int_{B_R} d^3x\int_{S_t(x)} d^2y\left(\frac{\partial u_0(y)}{\partial n}\right)^2.$$

For a non-negative continuous function u and $t\geqslant R$ the following bound follows by integration in polar coordinates and geometric argument:

$$\int_{B_R} d^3x\int_{S_t(x)} d^2y\,u(y)\leqslant 8\pi R^2\int_{B_{t-R,t+R}} d^3x\,u(x). \tag{38}$$

Hence

$$|I(\cdot,t)|_R^2\leqslant C_2R^2\int_{B_{t-R,t+R}} d^3x\left(\frac{\partial u_0(x)}{\partial n}\right)^2 \tag{39}$$

for $t>R$. Thus, from the condition (21) the stated bound follows.

For $J(x,t)$ we should estimate $\|J(\cdot,t)\|_R=|J(\cdot,t)|_R+|\nabla J(\cdot,t)|_R$. Consider $|J(\cdot,t)|_R$. Similar to (39) we obtain

$$|J(\cdot,t)|_R^2\leqslant CR^2t^2\int_{B_{t-R,t+R}} d^3x(u_0(x))^2.$$

Then from the condition (21) the required estimate follows. For $\nabla J(x,t)=(m^2/8\pi)\int_{S_t(x)}d^2y\,\nabla u_0(y)$ the estimate is analogous. Consider $|K(\cdot,t)|_R$. Similarly to (39) we obtain

$$|K(\cdot,t)|_R^2\leqslant CR^2t^4\int_{B_{t-R,t+R}} d^3x(u_0(x))^2.$$

Then the estimate we need follows from the condition (21).

Now estimate the integrals over the balls. For example, consider the integral

$$J(x,t)=\frac{m}{4\pi}\int_{B_t(x)} d^3y\,F(t,x-y)v_0(y).$$

We should estimate $|J(\cdot,t)|_R$ and $|\nabla J(\cdot,t)|_R$. We have

$$|J(x,t)|=C\left|\int_{B_t(x)} d^3y\,F(t,x-y)v_0(y)\right|$$
$$\leqslant C\left|\int_{B_{t^\alpha}(x)} d^3y\,F(t,x-y)v_0(y)\right|+C\left|\int_{B'_{t^\alpha}(x)} d^3y\,F(t,x-y)v_0(y)\right|,$$

where $B_{t^\alpha}(x)=\{y:|y-x|\leqslant t^\alpha\}$, $B'_{t^\alpha}(x)=\{y:t^\alpha\leqslant|y-x|\leqslant t\}$. The first integral is bounded by

$$\left(\int_{B_{t^\alpha}(x)} d^3y\,F^2(t,x-y)\right)^{1/2}\left(\int_{B_{t^\alpha}(x)} d^3y\,v_0^2(y)\right)^{1/2}\leqslant C_1t^{(3\alpha-3)/2}|v_0|\leqslant C_1t^{-1-\sigma}|v_0|$$

for $\alpha=(1-2\sigma)/3$. The second integral is bounded by

$$\left|\int_{B_{t^\alpha,t-1}(x)} d^3y\, F(t,x-y)v_0(y)\right| + \left|\int_{B_{t-1,t}(x)} d^3y\, F(t,x-y)v^0(y)\right|, \tag{40}$$

where $B_{t^\alpha,t-1}(x)=\{y:t^\alpha\leqslant|y-x|\leqslant t-1\}$, $B_{t-1,t}(x)=\{y:t-1\leqslant|y-x|\leqslant t\}$. Further, for sufficiently large t the first integral of (40) is bounded by

$$\left(\int_{B_{t^\alpha,t-1}(x)} d^3y\, F^2(t,x-y)\right)^{1/2}\left(\int_{B_{t^\alpha,t-1}(x)} d^3y\, v_0^2(y)\right)^{1/2}\leqslant C(t^{3-3/2})^{1/2}(t^{-7/2-2\sigma})^{1/2}=Ct^{-1-\sigma},$$

due to (35) and (22). The second integral of (40) is bounded by

$$C\,t\left(\int_{B_{t-1,t}(x)} d^3y\, v_0^2(y)\right)^{1/2}\leqslant Ct^{-1-\sigma}$$

by (22). Thus we have the pointwise bound $|J(x,t)|\leqslant Ct^{-1-\sigma}$ that implies the stated integral bound.

Now let us estimate $|\nabla J(\cdot,t)|_R$. Note that

$$\nabla J(x,t)=\frac{m}{4\pi}\int_{B_t(x)} d^3y\, F(t,x-y)\nabla v_0(y).$$

Since $F(t,x-y)=m/2$ for $|x-y|=t$, the partial integration gives

$$\left|\int_{B_t(x)} d^3y\, F(t,x-y)\frac{\partial}{\partial y_i}v_0(y)\right|\leqslant\frac{m}{2}\int_{S_t(x)} d^2y\,|v_0(y)|+\int_{B_t(x)} d^3y\left|\frac{\partial}{\partial x_i}F(t,x-y)v_0(y)\right|.$$

Then the estimates for both the spherical integral and the integral over the ball are made as above. Hence, the bound $|\nabla J(\cdot,t)|_R\leqslant C(v_0,R)(1+|t|)^{-1-\sigma}$ follows from the condition (22).

Altogether, we obtain that for sufficiently large t the estimate (36) is true. For bounded t this estimate follows from the energy conservation for the free Klein–Gordon equation.

□

Remark: The statement of the lemma is true under some weaker conditions on initial data, than (21), (22). Namely, it suffices to assume that

$$\int_{R\leqslant|x|\leqslant R+1} d^3x(R^2|u_0(x)|^2+|\nabla v_0(x)|^2)=\mathcal{O}(R^{-(4+2\sigma)}),$$

$$\int_{R^\alpha\leqslant|x|\leqslant R} d^3x\ (|u_0(x)|^2+|v_0(x)|^2)=\mathcal{O}(R^{-(4+2\sigma)})$$

as $R\to+\infty$; $\alpha=(1-2\sigma)/3$.

Thus, for the first term on the right-hand side of (29) we have

$$\|U(t)Z(0)\|_{R_\rho}\leqslant\frac{C(Z(0),\overline{v},R_\rho)}{(1+|t|)^{1+\sigma}}.$$

Then from (15) the estimate

$$\|U(t)Z(0)(\cdot+q(t))\|_{R_\rho}\leqslant\frac{C(Z(0),q^0,\overline{v},R_\rho)}{(1+|t|)^{1+\sigma}} \tag{41}$$

follows.

B. Decay of the soliton field subject to free Klein–Gordon group

Denote by $Z_1(x,t)=\psi(x,t)-\psi_{v(t)}(x-q(t))$ the first component of $Z(x,t)$ and observe that $\langle \psi_v, \nabla\rho\rangle=0$ for $|v|<1$ because the soliton (5) is a solution to (4). Note that for scattering solutions, for sufficiently large $|t|$, the fourth equation of the system (1) transforms to the fourth nonperturbed equation of the system (4) Then for these $|t|$,

$$\dot p(t)=\langle Z_1(x+q(t),t),\nabla\rho(x)\rangle\,. \tag{42}$$

Thus we obtain,

$$|\dot p(t)|\leqslant C\|Z(\cdot+q(t),t)\|_{R_\rho}\gamma_\rho\,. \tag{43}$$

Denote $S_{t-s}(x)=\{y\colon |y-x|=t-s\}$, $B_{t-s}(x)=\{y\colon |y-x|\leqslant t-s\}$, $\psi_v^p=\partial\psi_v/\partial p$, $\pi_v^p=\partial\pi_v/\partial p$, and

$$(\psi^U(\cdot,t,s),\pi^U(\cdot,t,s))=U(t-s)\left[\frac{\partial\Psi_{v(s)}}{\partial p}(\cdot-q(s))\right]. \tag{44}$$

Then the formulas (30), (31) for $U(t-s)$ imply

$$\begin{aligned}\psi^U(x,t,s)=&\frac{1}{4\pi(t-s)}\int_{S_{t-s}(x)}d^2y\;\pi^p_{v(s)}(y-q(s))-\frac{m}{4\pi}\int_{B_{t-s}(x)}d^3y\,F(t-s,x-y)\,\pi^p_{v(s)}(y-q(s))\\&+\frac{1}{4\pi(t-s)^2}\int_{S_{t-s}(x)}d^2y\;\psi^p_{v(s)}(y-q(s))+\frac{1}{4\pi(t-s)}\int_{S_{t-s}(x)}d^2y\,\frac{\partial}{\partial n}\psi^p_{v(s)}(y-q(s))\\&-\frac{m^2}{8\pi}\int_{S_{t-s}(x)}d^2y\;\psi^p_{v(s)}(y-q(s))-\frac{m}{4\pi}\int_{B_{t-s}(x)}d^3y\,\dot F(t-s,x-y)\,\psi^p_{v(s)}(y-q(s)).\end{aligned} \tag{45}$$

From this one derives the explicit formula for $\nabla\psi^U(x,t,s)$; (32) and (33) give the formula for $\pi^U(x,t,s)$.

Now $\psi^U(x+q(t),t,s)$ can be represented as the sum of type (45) of integrals over the shifted sphere $S_{t-s}(x+q(t))$ and ball $B_{t-s}(x+q(t))$ and with $x+q(t)$ replacing x in F and $\dot F$. Denote $\psi^U_S(x+q(t),t,s)$ the sum of the integrals over the sphere $S_{t-s}(x+q(t))$ and $\psi^U_B(x+q(t),t,s)$ the sum of the integrals over the ball $B_{t-s}(x+q(t))$. Let us estimate $\psi^U_S(x+q(t),t,s)$. If $|x|\leqslant R_\rho$, we have on the sphere $S_{t-s}(x+q(t))$,

$$|y-q(s)|=|(y-x-q(t))+(x+q(t)-q(s))|\geqslant(t-s)-|x|-\overline{v}(t-s)\geqslant(1-\overline{v})(t-s)-R_\rho \tag{46}$$

by the bound (15) on $\dot q(t)$. On the other hand, the integral representation (6) yields by Cauchy–Schwartz inequality,

$$\sup_{|v|\leqslant\overline{v}}\sup_{|x|\geqslant 2R_\rho} e^{m|x|}(|\partial^\alpha\psi^p_v(x)|+|\partial^\beta\pi^p_v(x)|)\leqslant C(\overline{v},R_\rho)\,\gamma_\rho<\infty \tag{47}$$

for all multi-indices α,β with $|\alpha|\leqslant 2$, $|\beta|\leqslant 1$, recall that $\gamma_\rho:=|\rho|$. Then (47) and (46) imply the following pointwise bound for $\psi^U_S(x+q(t),t,s)$:

$$|\psi^U_S(x+q(t),t,s)|\leqslant C_1(\overline{v},R_\rho)\,\gamma_\rho e^{-m(t-s)} \tag{48}$$

for $|x|\leqslant R_\rho$ and provided $t-s\geqslant 3R_\rho/(1-\overline{v})$.

Now let us estimate $\psi^U_B(x+q(t),t,s)$. Set $\mu=(1-2\sigma)/6$ and consider two regions $B_\mu=\{y\colon |y-q(s)|\leqslant(t-s)^\mu\}$ and

$$B'_\mu = B_{t-s}(x+q(t)) - B_\mu = \{y : |y-(x+q(t))| \leqslant (t-s) \ \& \ |y-q(s)| > (t-s)^\mu\}.$$

Represent every integral over the ball $B_{t-s}(x+q(t))$ as the sum of the integrals over B_μ and B'_μ. Note that the volume of B_μ is of order $(t-s)^{3\mu}$, the volume of B'_μ is of order $(t-s)^3-(t-s)^{3\mu}$. Furthermore, for sufficiently large $t-s$ and $y \in B_\mu$ we have $|y-x| \leqslant \nu|t|$ with some positive $\nu<1$. Hence, by (34) the following estimate is true:

$$|F(t-s,x-y)| + |\dot{F}(t-s,x-y)| + |\ddot{F}(t-s,x-y)| \leqslant C|t-s|^{-3/2}.$$

Then for the integrals over B_μ we have

$$\left| \int_{B_\mu} \cdots \right| \leqslant C_1(t-s)^{3\mu}(t-s)^{-3/2} C_2 \gamma_\rho = C_3 \gamma_\rho (t-s)^{3\mu-3/2} = C_3 \gamma_\rho (t-s)^{-1-\sigma}$$

for $\mu = (1-2\sigma)/6$.

For the integrals over B'_μ we obtain, due to (47), provided $t-s \geqslant (2R_\rho)^{1/\mu}$,

$$\left| \int_{B'_\mu} \cdots \right| \leqslant C_4((t-s)^3-(t-s)^{3\mu}) C_5 \exp(-m(t-s)^\mu)\, \gamma_\rho \leqslant \frac{C_6 \gamma_\rho}{(t-s)^{1+\sigma}}$$

for sufficiently large $t-s$. Thus, the sum of the integrals over B'_μ is bounded by $(C_7(\overline{v},R_\rho)\gamma_\rho)/(1+(t-s)^{1+\sigma})$. So we come to

$$|\psi_B^U(x+q(t),t,s)| \leqslant \frac{C_8(\overline{v},R_\rho)\gamma_\rho}{1+(t-s)^{1+\sigma}} \tag{49}$$

for $|x| \leqslant R_\rho$ and sufficiently large $t-s$. Therefore (48) and (49) imply for large $t-s$, together with similar bounds for $\nabla\psi^U(x+q(t),t,s)$ and $\pi^U(x+q(t),t,s)$, the integral estimate

$$\|(\psi^U(\cdot+q(t),t,s), \pi^U(\cdot+q(t),t,s))\|_{R_\rho} \leqslant \frac{C_9(\overline{v},R_\rho)\gamma_\rho}{1+(t-s)^{1+\sigma}}. \tag{50}$$

On the other hand, for bounded $t-s$ this integral estimate follows from (44) by energy conservation for the group $U(t-s)$ since $\|\partial\Psi_v/\partial p\|_{\mathcal{F}} \leqslant C(\overline{v},R_\rho)\gamma_\rho$ by (C). Finally, (43) and (50) imply

$$\|\dot{p}(s)\cdot(\psi^U(\cdot+q(t),t,s), \pi^U(\cdot+q(t),t,s))\|_{R_\rho} \leqslant C_{10}(\overline{v},R_\rho)\gamma_\rho \frac{\|Z(\cdot+q(s),s)\|_{R_\rho}\gamma_\rho}{1+(t-s)^{1+\sigma}}. \tag{51}$$

C. Completing the proof of Proposition 4

The method was initially developed in Ref. 13 for $m=0$, see also Ref. 11. Combining (29) to (51) and (41) we arrive at

$$\|Z(\cdot+q(t),t)\|_{R_\rho} \leqslant \frac{C(Z(0),q^0,\overline{v},R_\rho)}{(1+|t|)^{1+\sigma}} + \gamma_\rho^2 C_{10}(\overline{v},R_\rho) \int_0^t \frac{\|Z(\cdot+q(s),s)\|_{R_\rho}}{1+(t-s)^{1+\sigma}} ds, \quad t \geqslant 0. \tag{52}$$

Therefore, setting $M(t) = \max_{0\leqslant s\leqslant t}(1+|s|)^{1+\sigma}\|Z(\cdot+q(s),s)\|_{R_\rho}$, we have

$$M(t) \leqslant C_0(Z(0),q^0,\overline{v},R_\rho) + \gamma_\rho^2 C(\overline{v},R_\rho) I_\sigma M(t),$$

where

$$I_\sigma = \sup_{t\geqslant 0}(1+|t|)^{1+\sigma} \int_0^t \frac{(1+|s|)^{-1-\sigma}}{(1+|t-s|^{1+\sigma})}\, ds < \infty.$$

It remains to choose $\gamma_\rho^2 C(\overline{v},R_\rho)I_\sigma<1$, then (28) with $R=R_\rho$ follows.

Remark: It is important that $\overline{v}$ is bounded for bounded γ_ρ and fixed initial data.

At last, we claim that the bound (28) with $R=R_\rho$ implies (28) for any $R>0$. Indeed, (50)–(52) hold with the norm $\|\cdot\|_R$ instead of $\|\cdot\|_{R_\rho}$ on the *left*-hand sides and with $C_i(\overline{v},\rho,R)$ instead of $C_i(\overline{v},R_\rho)$ on the *right*-hand sides. Then (52) with this generalization and (28) with $R=R_\rho$ imply (28) for any $R>0$. □

IV. SCATTERING

Theorem 7: *Under the conditions of Proposition 4, for sufficiently small γ_ρ, the convergence (7) holds, and the solution $Y(t)$ displays the following long-time asymptotics:*

(i) There exist $v_\pm=\lim_{t\to\pm\infty}\dot q(t)\in\mathcal{V}$ such that

$$|\dot q(t)-v_\pm| \leqslant C\ (1+|t|)^{-\sigma}, \tag{53}$$

$$\|\Psi(\cdot+q(t),t)-\Psi_{v_\pm}\|_R\leqslant C_R(1+|t|)^{-\sigma},\quad \forall R>0. \tag{54}$$

(ii) There exist $\Psi_\pm\in\mathcal{F}$ such that

$$\|\Psi(\cdot,t)-\Psi_{v(t)}(\cdot-q(t))-U(t)\Psi_\pm\|_{\mathcal{F}}\leqslant C(1+|t|)^{-\sigma}. \tag{55}$$

Proof: (i) Equation (28) with $R=R_\rho$ and (43) imply

$$|\dot p(t)|\leqslant C(1+|t|)^{-1-\sigma}\Leftrightarrow|\ddot q(t)|\leqslant C_1(1+|t|)^{-1-\sigma}. \tag{56}$$

Then the limits (8) exist, and (53) follows. Therefore, (28) implies (54).

(ii) We have to prove that $\|Z(x,t)-U(t)F_\pm\|_{\mathcal{F}}\leqslant C(1+|t|)^{-\sigma}$. This is equivalent to $\|U(-t)Z(x,t)-F_\pm\|_{\mathcal{F}}\leqslant C(1+|t|)^{-\sigma}$ since the group $U(t)$ is isometric in $\mathcal{F}$. Apply $U(-t)$ to the integral equation (29). We obtain

$$U(-t)Z(t)=Z(0)-\int_0^t U(-s)\left[\frac{\partial\Psi_{v(s)}}{\partial p}(\cdot-q(s))\dot p(s)\right]ds.$$

The condition (15) implies that the norm of $\Psi_{v(s)}(\cdot-q(s))$ in $\mathcal{F}$ is bounded uniformly with respect to s. Then (56) implies the convergence of the integral in $\mathcal{F}$ at the stated rate and Theorem 7 is proved. □

A. Constructing scattering solutions

Let us formulate a criterion for a solution $Y(t)$ to be scattering. Introduce the energy of the field part of a solution

$$h(t)=\frac{1}{2}\int d^3x(|\nabla\psi(x,t)|^2+m^2|\psi(x,t)|^2+|\pi(x,t)|^2).$$

Set $G=\sup_{x\in\mathbb{R}^3}|\nabla V(x)|$ and $v(t)=\dot q(t)$.

Theorem 8: *Let (C), $(P_{\min})$, (K) hold. Consider solutions $Y(t)$ to the system (1) with initial data $Y(0)\in\mathcal{E}^\sigma$, $0<\sigma<1/2$. Let $R_V,G,h(0),|q(0)|$ be finite. Then for $|\dot q(0)|$ close enough to 1 and sufficiently small γ_ρ, we have*

$$\lim_{t\to\pm\infty}|q(t)|=\infty. \tag{57}$$

Proof: Since the system (1) is time invertible, we consider only the case $t\to+\infty$. Consider the particle with initial data $q(0),v(0):=\dot q(0)$. Introduce $e=v(0)/|v(0)|$. The orthogonal projection of the vectors $v(t),p(t),q(t)$ onto e read $v_e(t)e$, $p_e(t)e$, $q_e(t)e$, respectively, with $v_e(t):=v(t)\cdot e$, $p_e(t):=p(t)\cdot e$, $q_e(t):=q(t)\cdot e$, here the dot means the scalar product in $\mathbb{R}^3$. Note that

the vectors $v(t)$ and $p(t)$, $v_e(t)$ and $p_e(t)$ are of the same directions and $v_e(0)=|v(0)|$, $p_e(0)=|p(0)|$. Introduce the layer in $\mathbb{R}^3$, $L(e,R_V)=\{x:|x\cdot e|\leqslant R_V\}$, then $\operatorname{supp} V\subset L(e,R_V)$.

The statement of the theorem follows from the three propositions below. Since the system (1) is invariant with respect to time translations, we start from $t=0$ in either proposition.

Proposition 9: Let $|q(0)|>R_V$, $|v(0)|$ be close enough to 1, let e be directed toward $L(e,R_V)$. Then the particle enters $L(e,R_V)$ at a certain moment τ with $|v_e(\tau)|$ close to 1.

Proposition 10: Let $|q(0)|\leqslant R_V$, let $|v(0)|$ be close to 1. Then the particle leaves $L(e,R_V)$ at a certain moment τ such that $|v_e(\tau)|>0$ and $v_e(\tau)e$ is directed outside $L(e,R_V)$.

Proposition 11: Let $|q(0)|\geqslant R_V$, $|v(0)|>0$ and e is directed outside $L(e,R_V)$. Then the particle never enters $L(e,R_V)$ and $|q_e(t)|\to\infty$ as $t\to+\infty$.

Proof of Proposition 9: For $v_e(t)$ we have the estimate

$$v_e(t)\geqslant v_e(0)-\int_0^t|\dot v(s)|ds=|v(0)|-\int_0^t|\dot v(s)|ds.$$

Since outside $L(e,R_v)$ the free equations (4) are satisfied, the following estimate (see [28) and (43)] is valid:

$$|\dot v(t)|\leqslant\frac{C(Z(0),q(0),\overline{v},R_\rho)\,\gamma_\rho}{(1+|t|)^{\sigma+1}}. \tag{58}$$

Here $C(Z(0),q(0),\overline{v},R_\rho)$ is bounded uniformly with respect to the values $q(0),\psi(0),\pi(0)$ under consideration. Thus,

$$v_e(t)\geqslant|v(0)|-\int_0^\infty\frac{C\gamma_\rho\,dt}{(1+|t|)^{\sigma+1}}=|v(0)|-\frac{C\gamma_\rho}{\sigma},$$

and we obtain the required result for sufficiently small γ_ρ. □

Proof of Proposition 10: First we check that the growth of the field energy is not very fast.

Lemma 12: The following bound holds:

$$h(t)\leqslant(\sqrt{h(0)}+\sqrt{2}\,\gamma_\rho t)^2. \tag{59}$$

Proof: Multiply the equation $\ddot\psi=\Delta\psi-m^2\psi-\rho$ by $\dot\psi$ and integrate over $\mathbb{R}^3$. We obtain $\dot h(t)=-\int d^3x\,\rho\dot\psi$ and hence $\dot h(t)\leqslant\sqrt{2}\,\gamma_\rho\sqrt{h}$. Integrating this differential inequality in t we come to $\sqrt{h(t)}\leqslant\sqrt{h(0)}+\sqrt{2}\,\gamma_\rho t$ which proves (59). □

Let us now prove the proposition. Recall that $v=p/\sqrt{1+p^2}$ and hence, $p=v/\sqrt{1-v^2}$. Thus, $|v|$ is close to 1 if and only if $|p|$ is large. From the equation

$$\dot p(t)=-\nabla V(q(t))+\int d^3x\,\psi(x,t)\,\nabla\rho(x-q(t))$$

we obtain, due to (59), $|\dot p|\leqslant G+\|\psi\|\gamma_\rho\leqslant G+(2h(t))^{1/2}\gamma_\rho\leqslant G+((2h(0))^{1/2}+2\gamma_\rho t)\gamma_\rho=G_1+2\gamma_\rho^2 t$ with $G_1=G+(2h(0))^{1/2}\gamma_\rho$. The conditions of the theorem imply that G_1 is bounded. We obtain the following lower and upper bounds:

$$p_e(t)\geqslant p_e(0)-\int_0^t|\dot p(s)|ds\geqslant|p(0)|-G_1t-\gamma_\rho^2t^2=P-f(t),$$

$$|p(t)|\leqslant|p(0)|+\int_0^t|\dot p(s)|ds\leqslant|p(0)|+G_1t+\gamma_\rho^2t^2=P+f(t),$$

where $P:=|p(0)|$, $f(t):=G_1t+\gamma_\rho^2t^2$. These estimates imply for $v_e(t)$,

$$v_e(t)=\frac{p_e(t)}{|p(t)|}\left(1+\frac{1}{|p(t)|^2}\right)^{-1/2}\geqslant\frac{P-f(t)}{P+f(t)}\left(1-\frac{1}{(P-f(t))^2}\right)$$
$$=\frac{1-a^2-2af(t)+a^2f^2(t)}{1-a^2f^2(t)}$$
$$\geqslant(1-a^2-2af(t)+a^2f^2(t))(1+a^2f^2(t))=1-a^2+g(t), \tag{60}$$

where $a:=P^{-1}$, $g(t):=-2af(t)+(2a^2-a^4)f^2(t)-2a^3f^3(t)+a^4f^4(t)$. The corresponding estimate for $q_e(t)$ is

$$q_e(t)\geqslant q_e(0)+(1-a^2)t+\int_0^t g(s)ds. \tag{61}$$

Take sufficiently large P, that is small a, then from the estimates (61), (60) the statement of the proposition follows. □

Proof of Proposition 11: We claim that there exist such small $\gamma_\rho>0,\underline{v}>0$ that $\forall\, t>0 v_e(t)\geqslant\underline{v}$. Indeed, set $T=\sup\{t>0\colon v_e(t)>\underline{v}\}$. If $\underline{v}<v_e(0)/2$, then, by continuity, $T>0$. We claim that it is possible to choose such small $\gamma_\rho>0$, $\underline{v}>0$ that $T=+\infty$. Indeed, for $t\in[0,T]$ the free equations (4) are satisfied, hence the estimate (58) is valid. Take

$$0<\underline{v}<v_e(0)-\int_0^\infty\frac{C\gamma_\rho}{(1+|t|)^{\sigma+1}}=v_e(0)-\frac{C\gamma_\rho}{\sigma};$$

this choice is possible for sufficiently small γ_ρ. If $T<+\infty$, then $v_e(T)>\underline{v}$, hence, by continuity, $v_e(T+\varepsilon)>\underline{v}$ for some $\varepsilon>0$. This contradicts to the definition of T. Thus, $T=+\infty$. Hence, for $t>0$ one obtains $q_e(t)\geqslant q_e(0)+\underline{v}t$. □

Note that from the proof of the theorem the following statement follows.

Corollary 13: Let (C), ($P_{\min}$), (K) hold, let $Y(0)\in\mathcal{E}^\sigma,0<\sigma<1/2$. Let $R_V,h(0),|q(0)|$ be finite. Then for $\dot{q}(0)\neq0$ and sufficiently small γ_ρ, G the solution $Y(t)$ is scattering.

ACKNOWLEDGMENTS

The work is supported by the Wittgenstein 2000 Award of Peter Markowich, funded by the Austria Research Fund and by the Erwin–Schrödinger–Institute, Vienna, Austria.

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Transport of energy in dissipative advection phenomena

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(Received 4 November 2002; accepted 26 November 2002)

A study of the distribution of energy among the different scales is performed for several systems in fluid mechanics, including the Navier–Stokes, magnetohydrodynamics and active scalars equations. It is found that all these systems possess a common structure which enables us to deduce how the energy introduced by the forcing is transferred to the scales present in the flow. It is also shown that in special cases an energy cascade will occur. The limits of this method are also considered. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1540237]

I. INTRODUCTION

It is well known that the energy injected into a fluid by some forcing will be distributed among all the scales of the flow. In a general sense this is true for all phenomena governed by nonlinear equations: for every decomposition of the solution in different modes representing the scales, the nonlinearity will make interact different modes so that they do not evolve independently. The details of how this interaction occurs depend essentially on the particular equation modeling the phenomenon. However, for certain equations, prevalent in several processes in fluid mechanics, the transfer of energy may be studied with some generality. These equations could be called dissipative advection phenomena by the two terms of their expression:

$$\frac{\partial w}{\partial t} = Aw + Tw + f, \tag{1}$$

where w is the magnitude under study. It is assumed that the solution of our initial value problem exists for all time, and that $w(t)$ belongs to a certain Hilbert space H. A is a linear self-adjoint dissipative operator; it is defined in a dense domain

$$A: D(A) \to H,$$

and it satisfies, for some constant $\alpha > 0$ and all $w \in D(A)$,

$$-(Aw, w) \geqslant \alpha \|w\|^2. \tag{2}$$

Thus the whole spectrum of A is contained in $(-\infty, -\alpha]$. For simplicity purposes we will assume that H is separable and the spectrum of A discrete, although it is not really necessary. T is a generally nonlinear and time-dependent operator densely defined in H, satisfying the orthogonality property:

$$(Tw, w) = 0, \tag{3}$$

for every w in the domain of T. A represents the dissipation and T the advective effect in the evolution of w. As we will see, condition (3) means that the energy injected by the forcing f will be distributed without loss by this advective term among all scales, while dissipation acts in a different way on each of them.

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The present article represents a simplification of the arguments advanced in Ref. 1 for the study of hydrodynamics turbulence. The Navier–Stokes case is analyzed there in more generality and depth, without making use of some of our hypotheses concerning uniqueness of the solution, which in fact are not proved in general. While it is probably overoptimistic to think that Ref. 1 answers all the questions on the origin and behavior of cascades in turbulence, it represents a valuable attempt to rigorize a classical and difficult problem. The method developed there is not difficult and we have been able to extend its range beyond the original hydrodynamic problem: in addition to the Navier–Stokes equations, the magnetohydrodynamics (MHD) system possesses also the required form, along with several equations describing passive and active scalars. Among the latter we may mention the vorticity in plane flows, the magnetic potential in two-dimensional plasmas, the temperature in Bénard convection, the salinity in oceanic waters and other magnitudes relevant in geophysical phenomena.

In a limit case we can prove something similar to energy cascades in the sense of Kolmogorov: energy is transferred without loss to smaller (direct cascade) or larger scales (inverse cascade) in a form independent of A, i.e., of viscosity.[2] However, the assumptions needed to prove this are probably excessive and the fact that there is no discernible influence of the space dimension, unlike what is experimentally known, seems to indicate that physical cascades have their own phenomenology not covered by this case.

II. THE MAIN RESULTS

Let (e_n) be a basis of H formed by eigenfunctions of A, $-Ae_n=\lambda_n e_n$, with $\lambda_1=\alpha$, $\lambda_1 \leqslant \lambda_2 \leqslant \cdots$. We will consider that the scales of the problem are given by the orthogonal decomposition $w=\Sigma(w,e_n)e_n$, so that a large-scale function is one limited to the lower eigenfunctions. When, as usual, A is essentially the Laplacian, certainly the higher eigenfunctions are more irregular than the lower ones. In particular, if H is formed by periodic functions, the basis is formed by the trigonometric functions $\mathbf{x}\rightarrow\exp(i\mathbf{k}\cdot\mathbf{x})$ and the spectral decomposition is the Fourier one, so that the concept coincides with the classical one.

The energy estimates are classical: by making the scalar product of (1) with w,

$$\frac{1}{2}\frac{\partial}{\partial t}(w,w)-(Aw,w)=(Tw,w)+(f,w)=(f,w). \tag{4}$$

Thus

$$\frac{1}{2}\frac{d}{dt}\|w\|^2-(Aw,w)=(f,w)\leqslant\|f\|\,\|w\|\leqslant\frac{1}{2\alpha}\|f\|^2+\frac{\alpha}{2}\|w\|^2. \tag{5}$$

Since $-(Aw,w)\geqslant\alpha\|w\|^2$,

$$\frac{d}{dt}\|w\|^2+\alpha\|w\|^2\leqslant\frac{1}{\alpha}\|f\|^2, \tag{6}$$

so that

$$\|w(t)\|^2\leqslant\|w(0)\|^2e^{-\alpha t}+\frac{1}{\alpha}\int_0^t e^{-\alpha(t-s)}\|f(s)\|^2\,ds, \tag{7}$$

which is bounded in particular if $\|f\|$ is bounded for all time: e.g., if it does not depend on time. In the absence of forcing the solution tends exponentially to zero. We will only need to assume

$$\lim_{t\rightarrow\infty}\frac{1}{T}\|w(T)\|^2=0, \tag{8}$$

which certainly happens if w remains bounded. Our remaining hypotheses are as follows: let us denote by $\langle\ \rangle$ the time mean of a magnitude:

$$\langle g\rangle = \lim_{T\to\infty}\frac{1}{T}\int_0^T g(s)\,\mathrm{d}s, \tag{9}$$

provided it exists. We will assume that the time mean of all the magnitudes occurring in Eqs. (11)–(16) exists. This is not an unreasonable hypothesis, since turbulent phenomena are usually considered decaying or statistically stationary.

Let H_1 be the finite-dimensional subspace of H whose basis is $\{e_k, e_{k+1}, \ldots, e_l\}$. We will consider that H_1 is the space of some intermediate range of scales, called the injection range because we will assume that f lies within this range for all time; if f is large-scale, then $k=1$. Let H_2 be the subspace orthogonal to H_1, a Hilbert basis of whom is formed by the remaining e_j. Let $w = w_1 + w_2$ be the orthogonal decomposition of an element of H in the subspaces H_1 and H_2. The condition $(Tw,w)=0$ means therefore

$$(Tw,w_2) = -(Tw,w_1). \tag{10}$$

By taking the scalar product of (1) with w_1 and w_2 we obtain, analogously to (4),

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|w_1\|^2 - (Aw_1,w_1) &= (Tw,w_1) + (f,w_1), \\ \frac{1}{2}\frac{d}{dt}\|w_2\|^2 - (Aw_2,w_2) &= (Tw,w_2) = -(Tw,w_1), \end{aligned} \tag{11}$$

since $(f,w_2)=0$. We also have

$$\left\langle \frac{d}{dt}\|w_i\|^2 \right\rangle = \lim_{T\to\infty}\frac{1}{T}(\|w_i(T)\|^2 - \|w_i(0)\|^2) = 0, \tag{12}$$

and therefore

$$\begin{aligned} \langle(-Aw_1,w_1)\rangle &= \langle(Tw,w_1)\rangle + \langle(f,w_1)\rangle, \\ \langle(-Aw_2,w_2)\rangle &= \langle(Tw,w_2)\rangle = -\langle(Tw,w_1)\rangle. \end{aligned} \tag{13}$$

Now $(-Aw_i,w_i)\geqslant 0$ may be regarded as the dissipation of the component w_i, whereas (Tw,w_i) is the energy transferred by the advection to that component. Therefore the mean energy transferred to the noninjective scales is positive and identical to the mean dissipation of them, and also equal to the energy lost by the injective scales. Notice that this does not yield any information about if the energy goes to larger or smaller scales than the injective range, or more likely to both. If we decompose again w_2 in $w_2^+ + w_2^-$, formed respectively by smaller scales (projection in the $e_j : j>l$) and larger (projection in $e_i : i<k$), what we can deduce is

$$\langle(Tw,w_2^+)\rangle + \langle(Tw,w_2^-)\rangle = \langle(-Aw_2,w_2)\rangle = \langle(-Aw_2^+,w_2^+)\rangle + \langle(-Aw_2^-,w_2^-)\rangle. \tag{14}$$

Cascades are not merely energy transfer. In the Kolmogorov[2] theory of homogeneous turbulence, it is admitted that there exists a range of scales (called inertial) where energy is transferred without viscous loss. To prove something similar we need to make an additional hypothesis, also made in Ref. 3: we assume that there is a range outside the injection one such that the projection of w there is zero, or very small. Take the injection range generated by $e_k, \ldots, e_l$, and assume that from e_l to e_n there is no projection of w. Let E_h^+ be the energy transferred to modes larger than e_h, i.e., the product of Tw with the projection $w_h^+ = \Sigma_{j>h}(w,e_j)e_j$. Then

$$\langle(-Aw_2^+,w_2^+)\rangle=E_{l+1}^+=E_{l+2}^+=\cdots=E_n^+=\langle(Tw,w_2^+)\rangle. \tag{15}$$

Thus the energy passes without loss through this inertial range. Since it goes to smaller scales, it is called a direct cascade. The same could be done for larger scales if we assume that the projection of w in some range e_i, $e_{i+1},\ldots,e_{k-1}$ is zero: then, with an obvious notation,

$$\langle(-Aw_2^-,w_2^-)\rangle=E_{k-1}^-=E_{k-2}^-=\cdots=E_i^-=\langle(Tw,w_2^-)\rangle. \tag{16}$$

This should be an inverse cascade. For the direct one, however, there is a more manageable criterion to ascertain that the projection of w in small ranges is itself small: if the energy satisfies the inequality

$$\|w\|^2=\sum\ |(w,e_n)|^2\ll\sum\ \lambda_n|(w,e_n)|^2=(-Aw,w), \tag{17}$$

it is because large λ_n must play the main role, i.e., w is localized at the higher frequencies. Thus a much larger ''enstrophy'' $(-Aw,w)$ than energy means that a direct cascade is more likely, as stated in Ref. 3. This, however, does not seem to be a prerequisite for the actual cascades observed in turbulent phenomena.

III. EXAMPLES

A. The Navier–Stokes equations

The original example, developed as stated in much more depth and detail in Ref. 1, is the Navier–Stokes system for incompressible Newtonian fluids. It is worth to study how the abstract framework applies to this classical case. The Navier–Stokes equations are

$$\begin{gathered}\frac{\partial\mathbf{u}}{\partial t}=\nu\Delta\mathbf{u}-\mathbf{u}\cdot\nabla\mathbf{u}-\nabla p+\mathbf{f},\\ \nabla\cdot\mathbf{u}=0,\end{gathered} \tag{18}$$

where $\mathbf{u}$ represents the fluid velocity, ν the viscosity, p the kinetic pressure and $\mathbf{f}$ the forcing. Boundary conditions determine the space H. By taking the divergence of the first equation, one finds that p is in fact a (nonlocal) function of the velocity gradient, the solution of an elliptic problem (see, e.g., Ref. 1). We may either define

$$\begin{gathered}T\mathbf{u}=-\mathbf{u}\cdot\nabla\mathbf{u}+\nabla p(\mathbf{u}),\\ A=\nu\Delta,\end{gathered} \tag{19}$$

or, as usual, project (18) into the space of functions with null divergence. Denoting by P this projection, one gets the Stokes system:

$$\frac{\partial\mathbf{u}}{\partial t}=\nu P\Delta\mathbf{u}-P\mathbf{u}\cdot\nabla\mathbf{u}+P\mathbf{f}. \tag{20}$$

Then we may define $T\mathbf{u}=-P\mathbf{u}\cdot\nabla\mathbf{u}$, $A=\nu P\Delta$. The space H is defined by the boundary conditions. For periodic ones in a box Ω, one sets

$$H=\left\{\mathbf{u}\in L^2(\Omega)^N:\nabla\cdot\mathbf{u}=0,\ \int_\Omega\mathbf{u}\,dV=\mathbf{0},\mathbf{u}\cdot\mathbf{n}\Big|_{\partial\Omega}\ \text{antiperiodic}\right\}. \tag{21}$$

N is the space dimension. The condition $\nabla \cdot \mathbf{u}=0$ is to be understood in the sense of distributions. For these functions the trace of $\mathbf{u}\cdot\mathbf{n}$ at the boundary makes sense. The domain of A is defined as $D(A)=H^2(\Omega)^N \cap H$.

For no-slip boundary conditions, the velocity at the boundary of the smooth bounded domain Ω is taken as zero: we therefore set

$$\begin{aligned} H&=\{\mathbf{u}\in L^2(\Omega)^N:\nabla\cdot\mathbf{u}=0,\mathbf{u}\cdot\mathbf{n}|_{\partial\Omega}=0\},\\ D(A)&=H^2(\Omega)^N\cap H_0^1(\Omega)^N\cap H. \end{aligned} \tag{22}$$

That T and A satisfy the previous conditions is classical (see, e.g., Ref. 1 or 4).

B. Magnetohydrodynamics

The MHD system for an incompressible plasma with velocity $\mathbf{u}$ and magnetic field $\mathbf{B}$ are

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t}&=\nu\Delta\mathbf{u}-\mathbf{u}\cdot\nabla\mathbf{u}+\mathbf{B}\cdot\nabla\mathbf{B}-\nabla\left(p+\frac{B^2}{2}\right)+\mathbf{f}_1,\\ \frac{\partial \mathbf{B}}{\partial t}&=\eta\Delta\mathbf{B}-\mathbf{u}\cdot\nabla\mathbf{B}+\mathbf{B}\cdot\nabla\mathbf{u}+\mathbf{f}_2,\\ \nabla\cdot\mathbf{u}&=0,\\ \nabla\cdot\mathbf{B}&=0. \end{aligned} \tag{23}$$

$\eta>0$ is the plasma resistivity. Again a projection P to the space of fields with null divergence is applied to the equations, obtaining

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t}&=\nu P\Delta\mathbf{u}-P\mathbf{u}\cdot\nabla\mathbf{u}+P\mathbf{B}\cdot\nabla\mathbf{B}+P\mathbf{f}_1,\\ \frac{\partial \mathbf{B}}{\partial t}&=\eta P\Delta\mathbf{B}-P\mathbf{u}\cdot\nabla\mathbf{B}+P\mathbf{B}\cdot\nabla\mathbf{u}+P\mathbf{f}_2. \end{aligned} \tag{24}$$

Now we define $\mathbf{w}=(\mathbf{u};\mathbf{B})$,

$$\begin{aligned} T\mathbf{w}&=(-P\mathbf{u}\cdot\nabla\mathbf{u}+P\mathbf{B}\cdot\nabla\mathbf{B};\ -P\mathbf{u}\cdot\nabla\mathbf{B}+P\mathbf{B}\cdot\nabla\mathbf{u}),\\ A\mathbf{w}&=(\nu P\Delta\mathbf{u};\ \eta P\Delta\mathbf{B}). \end{aligned} \tag{25}$$

The space H again depends on the boundary conditions. It is defined essentially as (21) for periodic problems, with the exception that now both components $\mathbf{u}$ and $\mathbf{B}$ of $\mathbf{w}$ must be periodic. $D(A)$ is defined as $H^2(\Omega)^{2N}\cap H$. For Dirichlet homogeneous problems, the analog of (22) is used; in this case $D(A)=H^2(\Omega)^{2N}\cap H_0^1(\Omega)^{2N}\cap H$. For the case where the boundary of Ω is supposed to be a perfect conductor, i.e., $\mathbf{u}|_{\partial\Omega}=\mathbf{0}$, $\mathbf{B}\cdot\mathbf{n}|_{\partial\Omega}=0$, $(\nabla\times\mathbf{B})\times\mathbf{n}|_{\partial\Omega}=\mathbf{0}$, one sets

$$\begin{aligned} H&=\{(\mathbf{u};\mathbf{B})\in L^2(\Omega)^{2N}:\nabla\cdot\mathbf{u}=\nabla\cdot\mathbf{B}=0,\mathbf{u}\cdot\mathbf{n}|_{\partial\Omega}=\mathbf{B}\cdot\mathbf{n}|_{\partial\Omega}=0\},\\ D(A)&=\{(\mathbf{u};\mathbf{B})\in H^2(\Omega)^{2N}\cap H:\mathbf{u}\in H_0^1(\Omega)^N,\ (\nabla\times\mathbf{B})\times\mathbf{n}|_{\partial\Omega}=\mathbf{0}\}. \end{aligned} \tag{26}$$

(See, e.g., Refs. 4, 5.) Again A and T satisfy the main conditions and therefore one should expect an analogous transfer of energy for MHD problems. However, it is known that cascades in MHD are very different from the hydrodynamic ones (see, e.g., Ref. 6), which is a warning not to expect fine details from our calculations on energy transfer.

C. Passive scalars

These are magnitudes ϕ that are transported and diffused by an incompressible flow with a given velocity $\mathbf{u}$. They evolve according to

$$\frac{\partial \phi}{\partial t} = \kappa \Delta \phi - \mathbf{u} \cdot \nabla \phi + f. \tag{27}$$

The velocity is a datum of the problem. It satisfies $\nabla \cdot \mathbf{u} = 0$, $\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0$. $\kappa > 0$ is a diffusion coefficient; as we see ϕ has no influence on $\mathbf{u}$. Boundary conditions depend on the meaning of ϕ, and these define the domain of $A = \kappa\Delta$. Set $H = L^2(\Omega)$; for Dirichlet problems, $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$; for periodic ones, $D(A) = \{\phi \in H^2(\Omega) : \phi|_{\partial\Omega} \text{ periodic}\}$; for Neumann ones, $D(A) = \{\phi \in H^2(\Omega) : \partial\phi/\partial n \in H_0^1(\Omega)\}$. The condition of symmetry for A,

$$\int_{\partial\Omega} \phi \frac{\partial \phi}{\partial n} \mathrm{d}\sigma = 0,$$

is satisfied for all $\phi \in D(A)$. Tracers in a fluid are assumed to behave as passive scalars, provided they are not dense enough to modify the density or other properties of the fluid. For instance, salt in ocean water is not taken as a passive, but as an active scalar.

D. Active scalars

The equation is formally similar to (27), but now $\mathbf{u}$ depends on ϕ through some other equation, making $\mathbf{u}$ a (usually nonlocal) function of ϕ. These equations are rather common in fluid mechanics (see, e.g., Ref. 7). We will consider two examples: the magnetic potential in two-dimensional MHD and the temperature in Bénard convection.

E. Magnetic potential

Two-dimensional magnetic fields $\mathbf{B} = (B_1, B_2)$ in a simply connected domain Ω are of the form $B_1 = \partial A/\partial x_2$, $B_2 = -\partial A/\partial x_1$ for some scalar field A, called the magnetic potential. With this variable the MHD equations (without forcing on the magnetic field) become

$$\frac{\partial A}{\partial t} = \eta \Delta A - \mathbf{u} \cdot \nabla A + C(t),$$

$$\frac{\partial \mathbf{u}}{\partial t} = \nu \Delta \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u} + \Delta A \nabla A + f, \tag{28}$$

$$\nabla \cdot \mathbf{u} = 0.$$

$C(t)$ is some time-dependent constant depending on the choosing of A, which is indifferent to the addition of any gradient. Boundary conditions and the gauge constant C are linked. We may choose $C = 0$, but at the expense of not being able to precise the values of A at any point. If $\mathbf{B} \cdot \mathbf{n}|_{\partial\Omega} = 0$, A is constant along every connected component of $\partial\Omega$. By allowing $C \neq 0$ and choosing $A = 0$ at a given point of $\partial\Omega$, we have $A|_{\partial\Omega} = 0$. Thus we may take $H = L^2(\Omega)$, $A = \eta\Delta$, $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$. The second equation of (28) is ignored; we may study the transfer of energy without knowing the full evolution of the system. The magnetic potential is reputed to possess an inverse cascade,[6] such as the velocity in two-dimensional turbulence.

F. Temperature in Bénard convection

In a simple model, this satisfies

$$\frac{\partial T}{\partial t}=\kappa\Delta T-\mathbf{u}\cdot\nabla T+f,$$

$$\frac{\partial \mathbf{u}}{\partial t}=\nu\Delta\mathbf{u}-\mathbf{u}\cdot\nabla\mathbf{u}-\nabla p+\mathbf{e}_2(T-T_1), \tag{29}$$

$$\nabla\cdot\mathbf{u}=0.$$

T is the temperature in a box $[0,1]\times[0,1]$, κ is a thermal diffusion constant, $\mathbf{e}_2=(1,0)$, T_1 is the temperature at the upper lid $x_2=1$, and T_1+1 is the temperature at the lower one $x_2=0$. p, $\mathbf{u}$, T, $\partial\mathbf{u}/\partial x_1$ and $\partial T/\partial x_1$ are assumed one-periodic in the x_1-direction, $\mathbf{u}=\mathbf{0}$ at $x_2=0$ and $x_2=1$.[4,8] f is a possible injection of temperature.

These conditions make it possible to find $\mathbf{u}$ as a nonlocal function of T (since $\mathbf{u}$ satisfies a parabolic equation on a cylinder) so that we may define for the temperature the spaces

$$H=L^2[0,1]\times L^2[0,1], \tag{30}$$

$$D(A)=D(\kappa\Delta)$$
$$=\left\{T\in H^2(\Omega):\, T(x,1)=T_1,\, T(x,0)=T_1+1, T(0,y)=T(1,y),\, \frac{\partial T}{\partial x_1}(0,y)=\frac{\partial T}{\partial x_1}(1,y)\right\}.$$

Neumann conditions on the lateral walls are also admissible. Conditions are easily seen to be satisfied (the integral at the boundary of $T\partial T/\partial n$ always vanishes) so that we may ignore $\mathbf{u}$ to see that the temperature is transferred to the different scales according to our model.

IV. CONCLUSIONS

It is found that the transfer of energy among the different scales acts in a similar way in several processes of fluid mechanics, including the Navier–Stokes equations, the magnetohydrodynamics system, and passive and active scalar equations. The essence of this fact is that these magnitudes follow an evolution equation formed by the addition of a linear dissipative term which determines the scales of the flow and an advective one which distributes the energy injected by the forcing among the different scales. In some extreme cases the presence of a direct or inverse cascade, where energy is transferred without dissipative loss through some inertial range, may also be proved. However, it is pointed that these results do not yield precise information on the transfer of energy in some specific direction, which is known to differ according to the magnitude and the space dimension.

ACKNOWLEDGMENT

This work was partially supported by the Ministry of Science of Spain under Grant No. BMF2000-0814.

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The partial averaging method

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(Received 28 October 2002; accepted 5 December 2002)

The partial averaging technique is defined and used in conjunction with the random series implementation of the Feynman–Kaç formula. It enjoys certain properties such as good rates of convergence and convergence for potentials with coulombic singularities. In this work, I introduce the reader to the technique and I analyze the basic mathematical properties of the method. I show that the method is convergent for all Kato class potentials that have finite Gaussian transform. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1541933]

I. INTRODUCTION

The thermodynamic properties of a monodimensional spinless quantum system characterized by the inverse temperature $\beta=1/(k_BT)$ are completely determined by the canonical partition function

$$Z(\beta)=\int_{\mathbb{R}}\rho(x,x;\beta)\mathrm{d}x, \tag{1}$$

where the (unnormalized) density matrix

$$\rho(x,x';\beta)=\langle x|e^{-\beta H}|x'\rangle$$

can be computed with the help of the Feynman–Kaç representation formula[1,2]

$$\frac{\rho(x,x';\beta)}{\rho_{fp}(x,x';\beta)}=\mathbb{E}\exp\left\{-\beta\int_0^1 V[x_0(u)+\sigma B_u^0]\mathrm{d}u\right\} \tag{2}$$

for a large class of potentials. In Eq. (2), m_0 is the mass of the particle, $x_0(u)$ is a shorthand for $x+(x'-x)u$, $\sigma=(\hbar^2\beta/m_0)^{1/2}$, and

$$\rho_{fp}(x,x';\beta)=\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(x-x')^2}{2\sigma^2}\right]$$

is the density matrix of a similar free particle. The stochastic element that appears in Eq. (2), $\{B_u^0, 0\leqslant u\leqslant 1\}$, is a so-called standard Brownian bridge defined as follows: if $\{B_u, u\geqslant 0\}$ is a standard Brownian motion starting at zero, then the Brownian bridge is the stochastic process $\{B_u-uB_1, 0\leqslant u\leqslant 1\}$. Unless otherwise stated, in this article, we shall reserve the symbol $\mathbb{E}$ to denote the expected value (average value) of a certain random variable against the underlying probability measure of the Brownian bridge B_u^0.

The generalization of Eq. (2) to a d-dimensional system is straightforward. The symbol B_u^0 now denotes a d-dimensional standard Brownian bridge, which is a vector $(B_{u,1}^0, B_{u,2}^0, \ldots, B_{u,d}^0)$ with the components being independent standard Brownian bridges. The symbol σ stands for the

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vector $(\sigma_1,\sigma_2,\ldots,\sigma_d)$ with components defined by $\sigma_i^2=\hbar^2\beta/m_{0,i}$. The product σB_u^0 is interpreted as the d-dimensional vector of components $\sigma_i B_{u,i}^0$. Finally, x and x' are points in the configuration space $\mathbb{R}^d$ connected by the line $x_0(u)=x+(x'-x)u$.

As emphasized in Ref. 3, the success of the Feynman–Kaç formula in the computation of the thermodynamic properties of quantum systems is fortuitously due to another remarkable result: the Metropolis *et al.*[4] sampling algorithm of arbitrary finite-dimensional probability distributions, which lies at the heart of the Monte Carlo integration schemes.[5] This leads to the related but separate problem of finding a rapidly convergent sequence of finite-dimensional approximations of the stochastic integral (2). The main techniques found in literature can be classified in two categories: the discrete path integral methods and the random series techniques (for reviews, see Refs. 6 and 7, respectively). The latter methods lend themselves to various modifications which result in convergence for a wider class of potentials $V(x)$ or/and improved asymptotic convergence. One such method is the partial averaging (PA) technique, which was initially introduced by Doll, Coalson, and Freeman[8] as a way to accelerate the convergence of the ''primitive'' Fourier path integral method (FPI).[9]

As we shall see, the partial averaging method requires the Gaussian transform of the potential V for its implementation. For real life potentials this is a difficult but not impossible task. However, it was generally considered that the improvement the technique brings in does not warrant the effort of computing the Gaussian transform of the potential and therefore, the so-called gradient corrected partial averaging method was used instead. It has been shown that this latter method has general $\mathcal{O}(1/n^2)$ asymptotic behavior for sufficiently smooth potentials and it has been argued that there is not much reason to suspect a better convergence rate for the full partial averaging method.[10] However, more accurate numerical evidence recently presented in Ref. 7 suggests that the full partial averaging method does have in fact a better behavior: if the technique is used in conjunction with the FPI approach and if the potential is smooth enough, the asymptotic convergence is $\mathcal{O}(1/n^3)$. The importance of the partial averaging method resides also in the fact that it acts as a prototypical strategy for improving the asymptotic rate of convergence of the random series path integral methods. As such, the reweighted random series technique[7] achieves superior asymptotic convergence by simulating the partial averaging approach.

In this work, I shall argue for one more property of the partial averaging method which is not shared by the gradient corrected version and in general by the nonaveraged methods. More specifically, I shall show that the method can be employed for potentials having negative coulombic singularities, for which standard discrete path integral techniques (and also the primitive random series ones) fail to converge.[11,12] In this respect, it is quite surprising that the technique has been scarcely used for this purpose, despite the fact that in several instances its application for the polaron problem[13,14] and for the computation of statistical properties of quantum systems[15] was numerically successful. Though several other methods for dealing with the coulombic singularities have been proposed (see, for instance, Ref. 16), I appreciate that the advantage of the partial averaging strategy can be best emphasized by its ability of handling such systems.

In this article, I establish a sufficiently large class of potentials for which the partial averaging sequence of approximations converges to the correct Feynman–Kaç result, though I only study the convergence of the density matrix and of the partition function. This class includes most of the smooth and bounded from below potentials as well as most of the potentials having coulombic singularities. The proofs I perform are of a rather trivial nature, as they are direct consequences of well established convergence theorems from general probability theory. In fact, they exploit the martingale property of the partial averaging method. Besides their intrinsic value, these convergence theorems are important because they set the proper mathematical context in which the partial averaging method should be further discussed or utilized.

II. FORMULATION OF THE PROBLEM

A. A chemically relevant class of (scalar) potentials

A sufficiently large class of potentials for which the Feynman–Kaç formula (2) and its multidimensional analog hold is the so-called Kato class, which we define below. If

$$g(y)=\begin{cases}|y|, & d=1,\\ \ln(\|y\|^{-1}), & d=2,\\ \|y\|^{2-d}, & d\geqslant 3,\end{cases}$$

then the Kato class K_d is made up of all measurable functions $f:\mathbb{R}^d\to\mathbb{R}$ such that

$$\limsup_{\alpha\downarrow 0}\sup_{x\in\mathbb{R}^d}\int_{\|x-y\|\leqslant\alpha}|f(y)g(x-y)|\mathrm{d}y=0. \tag{3}$$

We also say that f is in K_d^{loc} if $1_D f\in K_d$ for all bounded domains $D\subset\mathbb{R}^d$. We say that the potential $V(x)$ is of Kato class if its negative part $V_-=\max\{0,-V\}$ is in K_d, while its positive part $V_+=\max\{0,V\}$ is in K_d^{loc}. In these conditions, as shown in Refs. 17 and 18, the Feynman–Kaç formula (2) holds. Moreover, Theorem B.7.5 of Ref. 18 shows that the density matrix $\rho(x,x';\beta)$ is continuous on $\mathbb{R}^d\times\mathbb{R}^d\times(0,\infty)$, while Theorem B.6.7 of the same reference shows that for a given $\beta>0$, the density matrix is uniformly bounded in the variables (x,x').

A remarkable theorem due to Aizenman and Simon[19] gives an alternative definition for the Kato class K_d. More precisely, Theorem 4.5 of Ref. 19 says that $V\in K_d$ if and only if

$$\limsup_{\epsilon\downarrow 0}\sup_{x\in\mathbb{R}^d}\mathbb{E}\left[\int_0^{\epsilon}|V(x+\sigma B_u)|\mathrm{d}u\right]=0, \tag{4}$$

where $\mathbb{E}$ denotes the expectation value against the d-dimensional Brownian motion B_u. Inverting the order of integration in Eq. (4) and remembering that B_u is a Gaussian distributed variable of variance u, we obtain the equivalent condition

$$\limsup_{\epsilon\downarrow 0}\sup_{x\in\mathbb{R}^d}\int_0^{\epsilon}\mathrm{d}u\int_{\mathbb{R}^d}(2\pi u)^{-d/2}e^{-\|z\|^2/(2u)}|V(x+\sigma z)|\mathrm{d}z=0. \tag{5}$$

We leave it for the reader to perform the substitutions $u'=u/\epsilon$ and then $z'=z/\sqrt{\epsilon}$ in successive order and prove the following reformulation of the condition given by Eq. (5):

$$\limsup_{\epsilon\downarrow 0}\sup_{x\in\mathbb{R}^d}\epsilon\int_0^{1}\mathrm{d}u\int_{\mathbb{R}^d}(2\pi u)^{-d/2}e^{-\|z\|^2/(2u)}|V(x+\sigma\sqrt{\epsilon}z)|\mathrm{d}z=0. \tag{6}$$

In the Appendix, we shall use Eq. (4) in the proof of Theorem 5 and Eq. (6) in the proof of Theorem 4, respectively.

As far as the chemical physicist is concerned, the Kato class of potentials is sufficiently general. It contains, for instance, the coulombic potential as it appears in electronic structure calculations. For another example, the *ab initio* intermolecular potential computed at the level of the Born-Oppenheimer approximation cannot have singularities worse than the coulombic ones and therefore it is of Kato class. However, we do not consider certain empirical potentials which are not of Kato class, as for example the Leonard-Jones potential. Nevertheless, this can be brought into the Kato class if the unphysical r^{-12} singularity is removed by truncation or by other approximations.

Let us anticipate a little and also demand that the potential V have finite Gaussian transform. The reader may read ahead in the next subsection and see that this condition is natural for the proper definition of the partial averaging method. More precisely, we require that

$$\overline{|V|}_{\alpha}(x)=\left(\prod_{i=1}^{d}\frac{1}{2\pi\alpha_i^2}\right)^{1/2}\int_{\mathbb{R}}\mathrm{d}z_1\cdots\int_{\mathbb{R}}\mathrm{d}z_d\exp\left(-\sum_{i=1}^{d}\frac{z_i^2}{2\alpha_i^2}\right)|V(x+z)|<\infty, \tag{7}$$

for all $x \in \mathbb{R}^d$ and $\alpha \in \mathbb{R}_+^d$. [In this article, $\mathbb{R}_+ = (0,\infty)$.] Certain properties of the potentials having finite Gaussian transform are given by Theorem 3 of the Appendix.

From the thermodynamic point of view, only the diagonal density matrix $\rho(x,x;\beta)$ is of interest. Moreover, in order to have a physically relevant statistics, the condition

$$0 < Z(\beta) < \infty, \quad \forall \beta > 0 \tag{8}$$

must hold, but the inequality (8) is not a requirement for the results obtained in this article to be valid. In practice, the condition is achieved by the addition of a *constraining* potential, which is usually a continuous and bounded from below function (thus still in the Kato class). The constraining potential is intended to simulate, for example, the effect of the container in which a reaction takes place. A sufficient condition for the quantum partition function to be finite is that the analog classical partition function be finite. This follows from the following inequality:

Proposition 1: Set

$$Z_{cl}(\beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} e^{-\beta V(x)} \mathrm{d}x.$$

Then, $Z(\beta) \leqslant Z_{cl}(\beta)$.

Proof: By Jensen's inequality and Tonelli theorem,

$$\begin{aligned} Z(\beta) &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} \mathrm{d}x\, \mathbb{E}\, e^{-\beta \int_0^1 V(x+\sigma B_u^0)\mathrm{d}u} \\ &\leqslant \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} \mathrm{d}x\, \mathbb{E} \int_0^1 \mathrm{d}u\, e^{-\beta V(x+\sigma B_u^0)} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \mathbb{E} \int_0^1 \mathrm{d}u \int_{\mathbb{R}} \mathrm{d}x\, e^{-\beta V(x+\sigma B_u^0)} = Z_{cl}(\beta). \end{aligned}$$

□

As stated, Proposition 1 remains true for multidimensional systems. In this article, we shall perform the proofs only for monodimensional systems. The reader should notice that our arguments are purely measure theoretic, in fact irrespective of the dimensionality of the physical systems. On the other hand, in the chemical physics literature it is customary to perform the analysis in ''monodimensional'' notation. I consider that the mathematician will have little trouble generalizing the proofs, yet the chemist may find it hard to accommodate a more complicated notation.

B. The partial averaging strategy

In this section, we shall give a short review of the partial averaging method for monodimensional systems (the multidimensional generalization is straightforward). For a more complete discussion, the reader should consult Ref. 7. The most general series representation of the Brownian bridge is given by the Ito-Nisio theorem,[20] the statement of which is reproduced below. Assume given $\{\lambda_k(\tau)\}_{k \geqslant 1}$ a system of functions on the interval $[0,1]$ which, together with the constant function $\lambda_0(\tau) = 1$, makes up an orthonormal basis in $L^2[0,1]$. Let $\Lambda_k(u)$ denote the primitives

$$\Lambda_k(u) = \int_0^u \lambda_k(\tau)\mathrm{d}\tau$$

of the functions $\lambda_k(u)$. If Ω is the space of infinite sequences $\overline{a} \equiv (a_1, a_2, \ldots)$ and

$$P[\overline{a}] = \prod_{k=1}^{\infty} \mu(a_k) \tag{9}$$

is the (unique by the Kolmogorov extension theorem) probability measure on Ω such that the coordinate maps $\overline{a}\to a_k$ are independent identically distributed (i.i.d.) variables with distribution probability

$$\mu(a_k\in A)=\frac{1}{\sqrt{2\pi}}\int_A e^{-z^2/2}\,\mathrm{d}z, \tag{10}$$

then

$$B_u^0(\overline{a})=\sum_{k=1}^{\infty} a_k\Lambda_k(u),\quad 0\leqslant u\leqslant 1 \tag{11}$$

is equal in distribution to a standard Brownian bridge. Moreover, the convergence of the above series is almost surely uniform on the interval [0,1].

Using the Ito–Nisio representation of the Brownian bridge, the Feynman–Kaç formula (2) takes the form

$$\frac{\rho(x,x';\beta)}{\rho_{fp}(x,x';\beta)}=\int_\Omega \mathrm{d}P[\overline{a}]\exp\left\{-\beta\int_0^1 V\left[x_0(u)+\sigma\sum_{k=1}^{\infty} a_k\Lambda_k(u)\right]\mathrm{d}u\right\}.$$

The independence of the coordinates a_k, which physically amounts to choosing those representations in which the kinetic energy operator is diagonal, is the key to the use of the partial averaging method. Denoting by $\mathbb{E}_n$ the average over the coefficients beyond the rank n, the partial averaging formula reads

$$\frac{\rho_n^{PA}(x,x';\beta)}{\rho_{fp}(x,x';\beta)}=\int_{\mathbb{R}}\mathrm{d}\mu(a_1)\ldots\int_{\mathbb{R}}\mathrm{d}\mu(a_n)\exp\left\{-\beta\ \ \mathbb{E}_n\int_0^1 V\left[x_0(u)+\sigma\sum_{k=1}^{\infty} a_k\Lambda_k(u)\right]\mathrm{d}u\right\}. \tag{12}$$

Assuming that the Fubini theorem holds (this is proved in the next section), one may invert the order of integration in the exponent and compute

$$\mathbb{E}_n\int_0^1 V[x_0(u)+\sigma B_u^0(\overline{a})]\mathrm{d}u=\int_0^1 \mathbb{E}_n V[x_0(u)+\sigma B_u^0(\overline{a})]\mathrm{d}u=\int_0^1 \overline{V}_{u,n}\left[x_0(u)+\sigma\sum_{k=1}^{n} a_k\Lambda_k(u)\right]\mathrm{d}u, \tag{13}$$

where

$$\overline{V}_{u,n}(y)=\int_{\mathbb{R}}\frac{1}{\sqrt{2\pi\Gamma_n^2(u)}}\exp\left[-\frac{z^2}{2\Gamma_n^2(u)}\right]V(y+z)\mathrm{d}z. \tag{14}$$

The function $\Gamma_n^2(u)$ is defined by

$$\Gamma_n^2(u)=\sigma^2\sum_{k=n+1}^{\infty}\Lambda_k(u)^2=\sigma^2\left[u(1-u)-\sum_{k=1}^{n}\Lambda_k(u)^2\right]. \tag{15}$$

[Again, the reader is referred to Ref. 7 for additional explanations. It is customary to use the notation $\Gamma_n^2(u)$ to mean the square of $\Gamma_n(u)$.] To summarize, we *define* the nth order partial averaging approximation to the diagonal density matrix by the formula

$$\frac{\rho_n^{PA}(x,x';\beta)}{\rho_{fp}(x,x';\beta)} = \int_{\mathbb{R}} \mathrm{d}\mu(a_1)\ldots \int_{\mathbb{R}} \mathrm{d}\mu(a_n) \exp\left\{ -\beta \int_0^1 \overline{V}_{u,n}\left[x_0(u) + \sigma \sum_{k=1}^{n} a_k \Lambda_k(u) \right] \mathrm{d}u \right\}. \tag{16}$$

III. MARTINGALE PROPERTY AND CONVERGENCE RESULTS

This section establishes the martingale property of the partial averaging method. One may notice that we obtain some important convergence results without actually doing much work other than citing some well-established theorems. The chemical physicist will probably be more interested in Corollary 1, which is for that matter presented separately.

On the set Ω of sequences $\overline{a} \equiv (a_1, a_2, \ldots)$, consider the σ-algebra generated by the finite-dimensional Borel sets $\mathcal{F}_\infty = \sigma(\cup_{n \geqslant 0} \mathcal{F}_n)$, where $\mathcal{F}_n = \sigma(a_1, a_2, \ldots, a_n)$ and $\mathcal{F}_0 = \{\varnothing, \Omega\}$. By construction, $\{\mathcal{F}_n\}_{n \geqslant 0}$ is a filtration. Also, the probability measure $\mathrm{d}P[\overline{a}]$ introduced in the previous section is, of course, defined over $\mathcal{F}_\infty$ so that the default probability space we refer to in this work is $(\Omega, \mathcal{F}_\infty, P)$. If f is an integrable random variable on Ω, we shall sometimes denote the conditional expectation $\mathbb{E}[f \,|\, \mathcal{F}_n]$ simply by $\mathbb{E}_n f$.

To continue with the introduction of the notations, we define

$$U_n(x,x',\beta;\overline{a}) = \int_0^1 \overline{V}_{u,n}\left[x_0(u) + \sigma \sum_{k=1}^{n} a_k \Lambda_k(u) \right] \mathrm{d}u$$

and

$$U_\infty(x,x',\beta;\overline{a}) = \int_0^1 V\left[x_0(u) + \sigma \sum_{k=1}^{\infty} a_k \Lambda_k(u) \right] \mathrm{d}u.$$

The variables x, x', and β are interpreted here as parameters and, just as a reminder, we separate them by a semicolon from the "true" variable $\overline{a}$. By construction, $U_n(x,x',\beta;\overline{a})$ is $\mathcal{F}_n$ measurable, while $U_\infty(x,x',\beta;\overline{a})$ is $\mathcal{F}_\infty$ measurable. Let us prove that $U_n(x,x',\beta;\overline{a}) = \mathbb{E}_n[U_\infty(x,x',\beta;\overline{a})]$ for P-almost every $\overline{a}$. As shown in the previous section, this boils down to proving

$$\mathbb{E}_n \int_0^1 V[x_0(u) + \sigma B_u^0(\overline{a})]\mathrm{d}u = \int_0^1 \mathbb{E}_n V[x_0(u) + \sigma B_u^0(\overline{a})]\mathrm{d}u$$

P-almost surely. The relation follows from the Fubini–Tonelli theorem provided that

$$\int_0^1 \mathbb{E}_n |V[x_0(u) + \sigma B_u^0(\overline{a})]| \mathrm{d}u \tag{17}$$

is finite P-a.s. Since the above integrand is non-negative, it is enough to show that its P-expectation is finite. Let

$$\mathrm{d}\mu_\epsilon(z) = \frac{1}{\sqrt{2\pi\epsilon^2}} e^{-z^2/(2\epsilon^2)} \mathrm{d}z$$

denote the respective Gaussian measure on $\mathbb{R}$. Using the Tonelli theorem to invert the order of integration, one computes

$$\mathbb{E}\left\{\int_0^1 \mathbb{E}_n\left|V[x_0(u)+\sigma B_u^0(\overline{a})]\right|\mathrm{d}u\right\}=\int_0^1 \mathbb{E}|V[x_0(u)+\sigma B_u^0(\overline{a})]|\mathrm{d}u$$

$$=\int_0^1 \mathrm{d}u\int_{\mathbb{R}}|V[x_0(u)+z]|\mathrm{d}\mu_{\Gamma_0(u)}(z)<\infty. \tag{18}$$

The last expression is finite for all $(x,x';\beta)\in\mathbb{R}^2\times\mathbb{R}_+$ by Theorem 4 of the Appendix. Equation (18) also shows that $U_\infty(x,x',\beta;\overline{a})$ is P-integrable for all $(x,x';\beta)$. Then, standard theorems from martingale theory show [see Theorem 5.7 of Ref. 21] the following:

Theorem 1: *For all $(x,x',\beta)\in\mathbb{R}^2\times\mathbb{R}_+$, the sequence $U_n(x,x',\beta;\overline{a})$ is a martingale adapted to the filtration $\mathcal{F}_n$ and is a.s. and L^1 convergent to $\mathbb{E}[U_\infty(x,x',\beta;\overline{a})|\mathcal{F}_\infty]=U_\infty(x,x',\beta;\overline{a})$.*

Let us define

$$X_n(x,x',\beta;\overline{a})=\rho_{fp}(x,x';\beta)\exp[-\beta\,U_n(x,x',\beta;\overline{a})]$$

and

$$X_\infty(x,x',\beta;\overline{a})=\rho_{fp}(x,x';\beta)\exp[-\beta\,U_\infty(x,x',\beta;\overline{a})].$$

Then, we have

$$\rho(x,x';\beta)=\mathbb{E}[X_\infty(x,x',\beta;\overline{a})] \tag{19}$$

and

$$\rho_n^{PA}(x,x';\beta)=\mathbb{E}[X_n(x,x',\beta;\overline{a})], \tag{20}$$

respectively.

Theorem 2: *(PA Convergence Theorem) For all $(x,x',\beta)\in\mathbb{R}^2\times\mathbb{R}_+$, the sequence $X_n(x,x',\beta;\overline{a})$ is a submartingale adapted to the filtration $\mathcal{F}_n$ and is a.s. and L^1 convergent to $X_\infty(x,x',\beta;\overline{a})$.*

Proof: We notice that $X_n(x,x',\beta;\overline{a})$ is the exponential of a martingale. Thus, by the conditional Jensen's inequality (see p. 225 of Ref. 21), we have

$$X_n\leqslant\mathbb{E}[X_{n+1}|\mathcal{F}_n]\leqslant\mathbb{E}[X_\infty|\mathcal{F}_n]. \tag{21}$$

The above inequality establishes the submartingale property because, as mentioned in Sec. II A,

$$\rho(x,x';\beta)=\mathbb{E}[\mathbb{E}[X_\infty|\mathcal{F}_n]]=\mathbb{E}X_\infty$$

is uniformly bounded in the variables (x,x') for all $\beta>0$. An elementary proof of this assertion is given in the Appendix (see Theorem 5). Finally, the a.s. convergence follows directly from Theorem 1, while the L^1 convergence follows from the Dominated convergence theorem and the inequality (21). □

We define the nth order partial averaging partition function by the formula

$$Z_n^{PA}(\beta)=\int_{\mathbb{R}}\rho_n^{PA}(x,x;\beta)\mathrm{d}x.$$

Using the symbol ↑ to mean "monotonically increasing to," a direct consequence of Theorem 2 is the following.

Corollary 1: As $n\to\infty$,

$$\rho_n^{PA}(x,x';\beta)\uparrow\rho(x,x';\beta)\text{ and }Z_n^{PA}(\beta)\uparrow Z(\beta). \tag{22}$$

Proof: The pointwise monotonic convergence of the density matrix is a direct consequence of the submartingale property and of the $L^1(\Omega,P)$ convergence of the partial averaging method. Then, the convergence of the partition functions follows from the monotone convergence theorem. □

IV. SUMMARY

In this article, I presented the basic properties of the partial averaging method. I demonstrated that the method can be employed for a quite general class of potentials by proving several convergence results of interest for the chemical physicist. In particular, I proved that the PA method is convergent for most of the potentials having negative coulombic singularities. The value of the convergence theorems deduced in the present article consists of the fact that they establish the mathematical context in which the partial averaging method should be utilized or discussed. I also anticipate that the martingale property will play an important role in establishing the asymptotic rates of convergence for different partial averaging schemes and, in fact, it may explain the superior asymptotic behavior of these methods.

ACKNOWLEDGMENTS

The author acknowledges support from the National Science Foundation through awards CHE-0095053 and CHE-0131114. He also would like to thank Professor J. D. Doll for continuing discussions concerning the present developments.

APPENDIX: SOME USEFUL THEOREMS

The following theorem consists of well known facts about the Gaussian transform and I present it here for ease of reference.

Theorem 3: *Let* $f:\mathbb{R}^d\to\mathbb{R}$ *be a Borel measurable function, let* $\alpha=(\alpha_0,\ldots,\alpha_d)\in\mathbb{R}_+^d$, *and let* $\|\alpha\|=\max_{1\leqslant i\leqslant d}\alpha_i$. *Consider the d-dimensional Gaussian measure*

$$\mathrm{d}\mu_\alpha(z)=\prod_{i=1}^{d}\left[\frac{1}{\sqrt{2\pi\alpha_i^2}}e^{-z_i^2/(2\alpha_i^2)}\mathrm{d}z_i\right] \tag{A1}$$

and let

$$F(x,\alpha)=\int_{\mathbb{R}^d}|f(x+z)|\mathrm{d}\mu_\alpha(z)$$

be defined on $\mathbb{R}^d\times\mathbb{R}_+^d$. *Assume there is* $(y,\eta)\in\mathbb{R}^d\times\mathbb{R}_+^d$ *such that* $F(y,\eta)<\infty$ *and let* $D=\mathbb{R}^d\times\Pi_{i=1}^d(0,\eta_i)$. *Then the following are true:*

(a) f *is locally integrable.*

(b) $F(x,\alpha)<\infty$ *for all* $(x,\alpha)\in D$.

(c)

$$G(x,\alpha)=\int_{\mathbb{R}^d}f(x+z)\mathrm{d}\mu_\alpha(z)$$

is well defined, continuous and infinitely differentiable in both arguments on D.

(d) $\lim_{\|\alpha\|\to 0}G(x,\alpha)=f(x)$ *a.e. More strongly,*

$$\lim_{\|\alpha\|\to 0}\int_{\mathbb{R}^d}|f(x+z)-f(x)|\mathrm{d}\mu_\alpha(z)=0 \quad \text{a.e.}$$

Theorem 4: *Let x and x' be arbitrary points in $\mathbb{R}^d$, let $\beta>0$, and let B_u^0 be a standard d-dimensional Brownian bridge on $[0,1]$. Pick some arbitrary $\sigma=(\sigma_1,\ldots,\sigma_d)\in\mathbb{R}_+^d$ and set $y=x'-x$. If $V\in K_d^{loc}$ and V has finite Gaussian transform, then*

$$\int_0^1 \mathbb{E}|V(x+yu+\sigma B_u^0)|\mathrm{d}u=\int_0^1 \mathrm{d}u\int_{\mathbb{R}^d}|V(x+yu+z)|\mathrm{d}\mu_{\Gamma_0(u)}(z)<\infty, \tag{A2}$$

where $\Gamma_0^2(u)=u(1-u)(\sigma_1^2,\ldots,\sigma_d^2)$ and the Gaussian measure $\mathrm{d}\mu_\alpha(z)$ is defined by the relation (A1).

Observation: We stated this theorem separately because its proof depends upon the dimensionality of the problem. More precisely, if the system is monodimensional, one may use $\Gamma_0^2(u)\leqslant\sigma^2$ to show that the integral (A2) is smaller than

$$\int_0^1 \mathrm{d}u\,\frac{1}{\sqrt{u(1-u)}}\int_{\mathbb{R}}|V(x+yu+z)|\mathrm{d}\mu_\sigma(z). \tag{A3}$$

By Theorem 3(c), the integral

$$\int_{\mathbb{R}}|V(x+yu+z)|\mathrm{d}\mu_\sigma(z)$$

as a function of u is continuous on $[0,1]$, thus bounded. Then, by the integrability of $[u(1-u)]^{-1/2}$, it follows that the integral (A3) is finite. However, this reasoning is not valid for higher dimensions because $[u(1-u)]^{-d/2}$ is not integrable for $d\geqslant 2$ and the additional condition $V\in K_d^{loc}$ is needed.

Proof of the theorem: The equality (A2) was discussed in the text. From Theorem 3(c), it follows that

$$\int_{\mathbb{R}^d}|V(x+yu+z)|\mathrm{d}\mu_{\Gamma_0(u)}(z)$$

as a function of u is continuous on all compact intervals $[\epsilon,1-\epsilon]$ with $0<\epsilon<\frac{1}{2}$, thus bounded and integrable. It is then enough to show that

$$I_\epsilon(x,y)=\int_0^\epsilon \mathrm{d}u\int_{\mathbb{R}^d}|V(x+yu+z)|\mathrm{d}\mu_{\Gamma_0(u)}(z)=\int_0^\epsilon \mathrm{d}u\int_{\mathbb{R}^d}|V(x+z)|\mathrm{d}\mu_{\Gamma_0(u)}(z-yu)<\infty$$

for all x and y and small enough ϵ. This is so because the integral over the end $[1-\epsilon,1]$ can be shown to equal $I_\epsilon(x+y,-y)$ by the change of variable $u'=1-u$. We shall prove the above inequality in two steps.

Step 1: In the first step, we prove the inequality

$$I_\epsilon(x,y)\leqslant 2^d\exp\left(\sum_{i=1}^d\frac{y_i^2}{4\sigma_i^2}\right)\int_0^\epsilon \mathrm{d}u\int_{\mathbb{R}^d}|V(x+z)|\mathrm{d}\mu_{\sigma\sqrt{2u}}(z). \tag{A4}$$

The inequality $0<u<\frac{1}{2}$ implies

$$\prod_{i=1}^d\left\{\frac{1}{\sqrt{2\pi\sigma_i^2u(1-u)}}\exp\left[-\frac{(z_i-y_iu)^2}{2\sigma_i^2u(1-u)}\right]\right\}\leqslant 2^{d/2}\prod_{i=1}^d\left\{\frac{1}{\sqrt{2\pi\sigma_i^2u}}\exp\left[-\frac{(z_i-y_iu)^2}{2\sigma_i^2u}\right]\right\}. \tag{A5}$$

On the other hand, the minimum of the expression

$$z_i^2/2-2z_iy_iu+y_i^2u^2$$

as a quadratic function of z_i is attained at $z_i=2y_iu$ and has the value $-y_i^2u^2$. Therefore,

$$\frac{(z_i-y_iu)^2}{2\sigma_i^2u}=\frac{z_i^2/2+z_i^2/2-2z_iy_iu+y_i^2u^2}{2\sigma_i^2u}\geqslant\frac{z_i^2}{4\sigma_i^2u}-\frac{y_i^2u}{2\sigma_i^2}\geqslant\frac{z_i^2}{4\sigma_i^2u}-\frac{y_i^2}{4\sigma_i^2},$$

where we used again the condition $u<\frac{1}{2}$. Replacing the last inequality in Eq. (A5), we obtain

$$\prod_{i=1}^{d}\left\{\frac{1}{\sqrt{2\pi\sigma_i^2u(1-u)}}\exp\left[-\frac{(z_i-y_iu)^2}{2\sigma_i^2u(1-u)}\right]\right\}\leqslant 2^d\exp\left(\sum_{i=1}^{d}\frac{y_i^2}{4\sigma_i^2}\right)\prod_{i=1}^{d}\left[\frac{1}{\sqrt{4\pi\sigma_i^2u}}\exp\left(-\frac{z_i^2}{4\sigma_i^2u}\right)\right]$$

and, consequently, the inequality given by Eq. (A4) is proven.

Step 2: By the results from the first step, it suffices to show that the last integral in Eq. (A4) is finite. By appropriate transformation of coordinates, we may rewrite this last integral as

$$\begin{aligned}\int_0^{\epsilon}du\int_{\mathbb{R}^d}|V(x+z)|\,d\mu_{\sigma\sqrt{2u}}(z)&=\epsilon\int_0^1du\int_{\mathbb{R}^d}|V(x+z)|\,d\mu_{\sigma\sqrt{2\epsilon u}}(z)\\&=\epsilon\int_0^1du\int_{\mathbb{R}^d}|V(x+z\sigma\sqrt{2\epsilon})|\,d\mu_{\sqrt{u}}(z).\end{aligned}$$

Even more, the integral over $\mathbb{R}^d$ in the last relation can be restricted to the ball $\|z\|<1$. Indeed if $\|z\|\geqslant 1$, we have

$$\begin{aligned}(2\pi u)^{-d/2}\exp\left\{-\frac{\|z\|^2}{2u}\right\}&=u^{-d/2}\exp\left\{-\frac{\|z\|^2}{2}\left(\frac{1}{u}-1\right)\right\}(2\pi)^{-d/2}\exp(-\|z\|^2/2)\\&\leqslant u^{-d/2}e^{1/2}e^{-1/(2u)}(2\pi)^{-d/2}\exp(-\|z\|^2/2).\end{aligned}$$

Notice that

$$M_0=\sup_{u>0}\ e^{1/2}u^{-d/2}\exp[-1/(2u)]<\infty.$$

Then, a little calculus and Theorem 3(c) show that

$$\epsilon\int_0^1du\int_{\|z\|\geqslant 1}|V(x+z\sigma\sqrt{2\epsilon})|\,d\mu_{\sqrt{u}}(z)\leqslant\epsilon M_0\int_{\mathbb{R}^d}|V(x+z\sigma\sqrt{2\epsilon})|\,d\mu_1(z)<\infty.$$

To conclude the theorem, we only need to prove that

$$\epsilon\int_0^1du\int_{\|z\|<1}|V(x+z\sigma\sqrt{2\epsilon})|\,d\mu_{\sqrt{u}}(z)<\infty$$

for ϵ small enough. Pick an arbitrary $\eta>0$. Remembering that $\epsilon<\frac{1}{2}$ and taking x such that $\|x\|<\eta$, we notice that in order to compute the integral over z in the above formula, we only need to know the potential over the ball D of radius $\eta+\max_{1\leqslant i\leqslant d}\sigma_i$ centered at origin. Therefore, if we set $V_D=1_DV$, then

$$\epsilon\int_0^1du\int_{\|z\|<1}|V(x+z\sigma\sqrt{2\epsilon})|\,d\mu_{\sqrt{u}}(z)\leqslant\epsilon\int_0^1du\int_{\mathbb{R}^d}|V_D(x+z\sigma\sqrt{2\epsilon})|\,d\mu_{\sqrt{u}}(z)\qquad\text{(A6)}$$

for all x such that $\|x\|<\eta$. Since D is bounded and $V\in K_d^{\mathrm{loc}}$, it follows that $V_D\in K_d$ and then Eq. (6) guarantees that there is $\epsilon_0>0$ such that the last integral in Eq. (A6) is uniformly bounded for all x. Consequently,

$$\epsilon_0 \int_0^1 \mathrm{d}u \int_{\|z\|<1} |V(x+z\sigma\sqrt{2\epsilon_0})| \mathrm{d}\mu_{\sqrt{u}}(z)$$

is bounded for all x such that $\|x\|<\eta$. Since η is arbitrary, we are done. □

Theorem 5: *Assume V is a Kato-class potential. Then there is $M_\beta>0$ a constant depending upon the inverse temperature β such that $\rho(x,x';\beta)\leqslant M_\beta$ for all $(x,x')\in\mathbb{R}^d\times\mathbb{R}^d$.*

Observation: The proof of this theorem will show why the Kato class is the natural class for the treatment of Feynman–Kaç semigroups. Most of the arguments used in the proof are borrowed from Aizenman and Simon.[19]

Proof of the theorem: If V_- denotes the negative part of V, we notice that

$$\mathbb{E}\exp\left\{-\beta\int_0^1 V[x_0(u)+\sigma B_u^0]\right\}\leqslant \mathbb{E}\exp\left\{\beta\int_0^1 V_-[x_0(u)+\sigma B_u^0]\right\},$$

so, without loss of generality, we may assume that V is of class K_d. The proof of this theorem is organized in three steps, each step reducing the problem to a simpler statement.

Step 1: In the first step, we prove that it suffices to show that

$$\sup_x \int_{\mathbb{R}^d} \rho(x,x';\beta)\mathrm{d}x'<\infty \tag{A7}$$

for all $\beta>0$ and $V\in K_d$.

In this part of the proof, it is convenient to denote the density matrix by $\rho_V(x,x';\beta)$, the index V indicating the potential from which the density matrix is derived. For the proof, we need two well-known properties of the density matrix $\rho_V(x,x';\beta)$: it is symmetrical

$$\rho_V(x,x';\beta)=\rho_V(x',x;\beta)$$

and it satisfies the Trotter product rule

$$\rho_V(x,x';\beta)=\int_{\mathbb{R}^d}\rho_V(x,y;\beta/2)\rho_V(y,x';\beta/2)\mathrm{d}y.$$

These two properties can be established by direct computation starting with the definition of the Brownian bridge. The first one is a consequence of the symmetry of the standard Brownian bridge, that is $\{B_{1-u}^0:0\leqslant u\leqslant 1\}$ is also a Brownian bridge and is equal in distribution to $\{B_u^0:0\leqslant u\leqslant 1\}$. The Trotter product rule is a consequence of the Markov property of the Brownian motion B_u entering the definition of the Brownian bridge. The simple proofs are left to the reader.

Now, the Cauchy–Schwartz inequality gives the estimate

$$\rho_V(x,x';\beta)\leqslant\left[\int_{\mathbb{R}^d}\rho_V(x,y;\beta/2)^2\mathrm{d}y\right]^{1/2}\left[\int_{\mathbb{R}^d}\rho_V(y,x';\beta/2)^2\mathrm{d}y\right]^{1/2}.$$

Taking the supremum over x and x' and using the symmetry of the density matrix, one concludes that

$$\sup_{x,x'}\ \rho_V(x,x';\beta)\leqslant\sup_x\int_{\mathbb{R}^d}\rho_V(x,y;\beta/2)^2\mathrm{d}y. \tag{A8}$$

Again by the Cauchy–Schwartz inequality,

$$\frac{\rho_V(x,x';\beta/2)^2}{\rho_{fp}(x,x';\beta/2)^2}=\left(\mathbb{E}\exp\left\{-\frac{\beta}{2}\int_0^1 V\left[x_0(u)+\frac{\sigma}{\sqrt{2}}B_u^0\right]\mathrm{d}u\right\}\right)^2$$
$$\leqslant\mathbb{E}\exp\left\{-\frac{\beta}{2}\int_0^1 2V\left[x_0(u)+\frac{\sigma}{\sqrt{2}}B_u^0\right]\mathrm{d}u\right\}.$$

Next, we combine the last equation with the bound

$$\rho_{fp}(x,x';\beta/2)^2\leqslant\left(\prod_{i=1}^d\frac{1}{\sqrt{\pi\sigma_i^2}}\right)\rho_{fp}(x,x';\beta/2)$$

to obtain the inequality

$$\rho_V(x,x';\beta/2)^2\leqslant\left(\prod_{i=1}^d\frac{1}{\sqrt{\pi\sigma_i^2}}\right)\rho_{2V}(x,x';\beta/2). \tag{A9}$$

Substituting Eq. (A9) in Eq. (A8), one obtains

$$\sup_{x,x'}\ \rho_V(x,x';\beta)\leqslant\left(\prod_{i=1}^d\frac{1}{\sqrt{\pi\sigma_i^2}}\right)\sup_x\int_{\mathbb{R}^d}\rho_{2V}(x,y;\beta/2)\mathrm{d}y$$

and the claim of Step 1 is concluded because $\beta/2>0$ and $2V\in K_d$.

Step 2: Simple transformations of coordinates show that

$$\int_{\mathbb{R}^d}\rho(x,x';\beta)\mathrm{d}x'=\int_{\mathbb{R}^d}\mathrm{d}\mu_1(z)\,\mathbb{E}\,e^{-\beta\int_0^1 V[x+zu\sigma+\sigma B_u^0]\mathrm{d}u}$$

and from the very definition of the Brownian bridge, we learn that $zu+B_u^0$ is in fact a Brownian motion B_u starting at zero. Thus,

$$\int_{\mathbb{R}^d}\rho(x,x';\beta)\mathrm{d}x'=\mathbb{E}\,e^{-\beta\int_0^1 V(x+\sigma B_u)\mathrm{d}u}.$$

For the remainder of the proof, $\mathbb{E}$ stands for the expectation value with respect to the underlying measure of the standard Brownian motion B_u.

In this second step, we use the Markov property of the Brownian motion to show that if there is $\epsilon_0>0$ such that the inequality

$$\sup_x\ \mathbb{E}\ \ e^{-\beta\int_0^\epsilon V(x+\sigma B_u)\mathrm{d}u}<\infty$$

holds for all $\epsilon<\epsilon_0$, then Eq. (A7) also holds.

Let θ and τ be some positive real numbers such that $\theta+\tau=1$. We break the integrand in the above equation in two parts:

$$e^{-\beta\int_0^1 V(x+\sigma B_u)\mathrm{d}u}=e^{-\beta\int_0^\theta V(x+\sigma B_u)\mathrm{d}u}e^{-\beta\int_\theta^1 V(x+\sigma B_u)\mathrm{d}u}=e^{-\beta\int_0^\theta V(x+\sigma B_u)\mathrm{d}u}e^{-\beta\int_0^\tau V(x+\sigma B_{\theta+u})\mathrm{d}u}.$$

Using the Markov property, we learn that the expected value of the above integrand conditioned on the random variables B_u with $u\in[0,\theta]$ is

$$e^{-\beta\int_0^\theta V(x+\sigma B_u)\mathrm{d}u}\mathbb{E}'\,e^{-\beta\int_0^\tau V(x+\sigma B_\theta+\sigma B'_u)\mathrm{d}u}.$$

Here, the symbol $\mathbb{E}'$ denotes the expected value against the standard Brownian motion starting at zero B'_u, Brownian motion that is independent from B_u. The above conditional expectation is smaller than or equal to

$$e^{-\beta\int_0^\theta V(x+\sigma B_u)\mathrm{d}u}\sup_x \mathbb{E}\, e^{-\beta\int_0^\tau V(x+\sigma B_u)\mathrm{d}u},$$

where the prime sign becomes superfluous and is therefore dropped. Taking the total expectation and then the supremum over x, we obtain the inequality

$$\sup_x \mathbb{E}\, e^{-\beta\int_0^1 V(x+\sigma B_u)\mathrm{d}u}\leqslant \sup_x \mathbb{E}\, e^{-\beta\int_0^\theta V(x+\sigma B_u)\mathrm{d}u}\times\sup_x \mathbb{E}\, e^{-\beta\int_0^\tau V(x+\sigma B_u)\mathrm{d}u}.$$

A simple inductive argument then shows that

$$\sup_x \mathbb{E}\, e^{-\beta\int_0^1 V(x+\sigma B_u)\mathrm{d}u}\leqslant\left\{\sup_x \mathbb{E}\, e^{-\beta\int_0^{1/n} V(x+\sigma B_u)\mathrm{d}u}\right\}^n \tag{A10}$$

for all $n\geqslant 1$. Clearly, the claim of Step 2 is concluded because the right-hand side of Eq. (A10) is finite for all n such that $1/n<\epsilon_0$.

Step 3: In this final step, we prove that there is ϵ_0 small enough such that

$$\sup_x \mathbb{E}\, e^{-\beta\int_0^\epsilon V(x+\sigma B_u)\mathrm{d}u}<\infty$$

for all $\epsilon<\epsilon_0$. Equation (4) allows us to pick some $\epsilon_0>0$ such that

$$\sup_x \mathbb{E}\left[\beta\int_0^\epsilon |V|(x+\sigma B_u)\mathrm{d}u\right]<\frac{1}{2} \tag{A11}$$

for all $\epsilon<\epsilon_0$. Next, we consider the inequality

$$\sup_x \mathbb{E}\, e^{-\beta\int_0^\epsilon V(x+\sigma B_u)\mathrm{d}u}\leqslant\sup_x \mathbb{E}\, e^{\beta\int_0^\epsilon |V|(x+\sigma B_u)\mathrm{d}u}=\sup_x\sum_{k=1}^\infty \frac{\beta^k}{k!}\mathbb{E}\left[\int_0^\epsilon |V|(x+\sigma B_u)\mathrm{d}u\right]^k\leqslant\sum_{k=0}^\infty A_k, \tag{A12}$$

where

$$A_k=\sup_x\frac{\beta^k}{k!}\mathbb{E}\left[\int_0^\epsilon |V|(x+\sigma B_u)\mathrm{d}u\right]^k=\beta^k\mathbb{E}\int_{0\leqslant s_1\leqslant\ldots\leqslant s_k\leqslant\epsilon}|V|(x+\sigma B_{s_1})\cdots|V|(x+\sigma B_{s_k})\mathrm{d}s_1\cdots\mathrm{d}s_k. \tag{A13}$$

Notice that the term by term integration of the first series appearing in Eq. (A12) is guaranteed by the monotone convergence theorem. The last equality in Eq. (A13) follows by symmetry arguments.

To construct a bound for the terms A_k, we first condition on the random variables B_u with $u\in[0,s_{k-1}]$ and use the Markov property of B_u to show that this conditional expectation has the value

$$\beta^{k-1}\int_{0\leqslant s_1\leqslant\ldots\leqslant s_{k-1}\leqslant\epsilon}|V|(x+\sigma B_{s_1})\cdots|V|(x+\sigma B_{s_{k-1}})\times\left[\mathbb{E}'\beta\int_0^{\epsilon-s_{k-1}}|V|(x+\sigma B_{s_{k-1}}+\sigma B'_u)\mathrm{d}u\right]\mathrm{d}s_1\cdots\mathrm{d}s_{k-1}. \tag{A14}$$

Equation (A11) shows that the quantity in the square brackets is bounded by $\frac{1}{2}$. Therefore, the conditional expectation given by Eq. (A14) is bounded by

$$\frac{1}{2}\beta^{k-1}\int_{0\leqslant s_1\leqslant\ldots\leqslant s_{k-1}\leqslant\epsilon}|V|(x+\sigma B_{s_1})\cdots|V|(x+\sigma B_{s_{k-1}})\mathrm{d}s_1\cdots\mathrm{d}s_{k-1}. \tag{A15}$$

Taking the total expectation in Eqs. (A14) and (A15) and then the supremum over x, we learn that

$$A_k\leqslant A_{k-1}/2,$$

from which the inequality $A_k\leqslant 1/2^k$ follows by induction. Substituting this last inequality in Eq. (A12), we obtain

$$\sup_x \mathbb{E}\, e^{-\beta\int_0^\epsilon V(x+\sigma B_u)\mathrm{d}u}\leqslant\sum_{k=0}^{\infty}\frac{1}{2^k}=2<\infty$$

for all $\epsilon<\epsilon_0$ and the proof of Step 3 and of the theorem is concluded. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 3 MARCH 2003

Limits of a Ginzburg–Landau model with codimension-one defects

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(Received 11 December 2002; accepted 20 December 2002)

We derive a nondimensional Ginzburg–Landau energy functional that does not use temperature-dependent scaling quantities. Using the machinery of gamma-convergence, the asymptotic limits of the functional are computed in the presence of thin defects centered around co-dimension 1 manifolds. We classify the defects into three groups depending on the L^1-norm of the defect potential. We show that each group has its own distinguished asymptotic limit as the thickness of the defect converges to zero. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1545165]

I. INTRODUCTION

The Ginzburg–Landau model has successfully captured a wide range of phenomena associated with the behavior of a superconducting material subjected to external magnetic fields. This includes the analysis of the relation between the transition temperature below which one first observes superconductivity and the strength of the applied field. In this article we present a modification of the standard Ginzburg–Landau model that incorporates the presence of normal—that is, non-superconducting—material appearing as thin inclusions within the superconducting bulk. We study the effect of this modification in the asymptotic regime where the thickness of the normal inclusions is small. Particular attention is paid to the effect on the transition temperature of the material.

As we shall see, in our model the normal inclusions are broken into three distinct regimes involving a weak, critical and strong influence on the behavior of the superconductor. Previous attempts by physicists to model the presence of normal defects in a superconducting material via Ginzburg–Landau theory include Refs. 1 and 9. In Refs. 2, 5 and 6, a modification of the Ginzburg–Landau model is studied which corresponds in our language to the case of weak inclusions only. The identification of the three regimes was set forth in Ref. 7 for the case of a one-dimensional superconductor and a primary purpose of the present study is to extend this model and analysis to the more physically interesting cases of two- and three-dimensional samples.

Because a central application we have in mind concerns the temperature versus external field transition curve, we shall begin our analysis with a careful nondimensionalization of the unmodified Ginzburg–Landau model. Commonly used nondimensionalizations typically involve scaling space as well as the order parameter and field by temperature-dependent quantities. This can lead to inappropriate formulations for our purposes. Consequently, in Sec. II we present in some detail a nondimensionalization that involves scaling only by temperature-independent quantities. We believe this formulation may prove useful in other investigations stressing temperature dependence in superconducting materials.

We follow this in Sec. III with a presentation of the modified Ginzburg–Landau model to incorporate the normal inclusions. A central component of the standard Ginzburg–Landau energy[11] is a bulk term depending on the complex-valued order parameter $\tilde{u}$ of the form

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$$\int_{\tilde{\Omega}} -\alpha|\tilde{u}|^2+\frac{\beta}{2}|\tilde{u}|^4\,\mathrm{d}\tilde{x},$$

where $\tilde{\Omega}$ is the region occupied by the superconductor. The factor β is a positive, temperature-independent constant but α is a factor depending on temperature. For temperatures below the critical temperature T_c, where onset first occurs in the absence of magnetic fields, α is positive, while it is negative above this value where superconductivity is precluded. Since the physically relevant quantity here is $|\tilde{u}|^2$, which measures the density of superconducting electron pairs, this sign change in α allows for the emergence of the stable state $|\tilde{u}|^2=\alpha/\beta$ signaling the presence of superconductivity in the model. In the modification we pursue, we model the presence of normal regions within $\tilde{\Omega}$ by taking α to be negative, regardless of temperature, in certain small portions of the sample. It is the size of the positive factor $-\alpha$, taken to be of the form $-\alpha=a/\delta^p$, that distinguishes the three different asymptotic regimes alluded to earlier. Here a is a positive constant, p is non-negative and $0<\delta\ll 1$ corresponds to the thickness of the normal region. What turns out to be relevant is the L^1-norm of this factor a/δ^p taken over the normal region, thus leading to the regimes $p<1$, $p=1$ and $p>1$.

In Sec. IV we invoke the theory of gamma-convergence (cf. Ref. 4) to study the limit of the modified Ginzburg–Landau energy for small δ. We review the definition of this convergence at the outset of the section. The identification of the gamma-limits allows one to characterize minimizers, both global and local, of the original energies as being minimizers of the identified limiting energies.

Finally, in Sec. V we focus on the issue of transition temperatures in the presence of normal inclusions by calculating the second variation of the limiting energies taken about the purely normal state. This leads to concrete eigenvalue problems whose first eigenvalue corresponds to the shift down in transition temperature due to the presence of applied magnetic fields for this superconducting/normal sample in the $\delta\to 0$ first approximation.

II. FORMULATION OF THE NONDIMENSIONAL PROBLEM FOR A CLEAN SUPERCONDUCTOR

The dimensional Ginzburg–Landau functional is given by

$$G(\tilde{u},\tilde{\mathbf{A}})=\int_{\tilde{D}}\frac{1}{2m}\left|\left(i\hbar\tilde{\nabla}-\frac{e}{c}\tilde{\mathbf{A}}\right)\tilde{u}\right|^2-\alpha|\tilde{u}|^2+\frac{\beta}{2}|\tilde{u}|^4\mathrm{d}\tilde{x}+\int_{\mathbb{R}^n}\frac{1}{8\pi}|\tilde{\nabla}\times\tilde{\mathbf{A}}-\tilde{\mathbf{H}}_{\mathbf{e}}|^2\mathrm{d}\tilde{x}. \tag{2.1}$$

Here $\tilde{D}\subset\mathbb{R}^n$ ($n=1$, 2 or 3) is the bounded domain occupied by the superconducting sample, c is the speed of light, $\hbar$ is Planck's constant, e and m are the electron's charge and half-mass, $\tilde{\mathbf{H}}_{\mathbf{e}}:\mathbb{R}^n\to\mathbb{R}^n$ and $\tilde{\mathbf{A}}:\mathbb{R}^n\to\mathbb{R}^n$ are the applied magnetic field and the total magnetic potential, respectively, $u:\tilde{D}\to\mathbb{C}$ is the order parameter, and α and β are material parameters. The dependence of β on the temperature T is weak. Since in most applications one works at temperatures that are not too far from the critical temperature, we can assume that β is temperature-independent. The parameter α, on the other hand, is sensitive to the temperature. The standard model is to take

$$\alpha\sim\alpha_0(T_c-T)\quad\text{for}\quad T_c-T\ll 1, \tag{2.2}$$

where α_0 is a positive constant and T_c is the critical temperature for the material, below which superconductivity is observable in the absence of any applied field (cf. Ref. 3).

We wish to nondimensionalize the various terms in the energy functional (2.1) without scaling by any temperature-dependent quantities. We start with generic scalings: $\overline{H}$ for the magnetic field, l for lengthscale, and $\sqrt{M}$ for u, and later we shall make judicious choices for these three factors. It is useful to recall the definitions of four fundamental parameters that appear frequently in superconductivity: the coherence length

$$\xi = \sqrt{\frac{\hbar^2}{2m\alpha}}, \tag{2.3}$$

the penetration depth

$$\lambda = \sqrt{\frac{m\beta c^2}{4\pi\alpha e^2}}, \tag{2.4}$$

the (dimensionless) Ginzburg–Landau parameter

$$\kappa = \frac{\lambda}{\xi}, \tag{2.5}$$

and the basic flux quantum

$$\Phi_0 = 2\pi\frac{\hbar c}{e}. \tag{2.6}$$

We now scale:

$$u = \frac{\tilde{u}}{\sqrt{M}}, \quad x = \frac{\tilde{x}}{l}, \quad \mathbf{H_e} = \frac{\tilde{\mathbf{H}}_\mathbf{e}}{2(2\pi)^{1/2}\overline{H}}, \quad \mathbf{A} = \frac{\tilde{\mathbf{A}}}{2(2\pi)^{1/2}l\overline{H}}. \tag{2.7}$$

Under this scaling, the Ginzburg–Landau functional becomes

$$G(u,\mathbf{A}) = \int_D \left(\frac{M\hbar^2}{2m}\frac{1}{l^2}\left| \left(i\nabla - \frac{2(2\pi)^{1/2}\overline{H}el^2}{c\hbar}\mathbf{A} \right) u \right|^2 - \alpha M|u|^2 + \frac{\beta M^2}{2}|u|^4 \right) l^n \, \mathrm{d}x$$

$$+ \int_{\mathbb{R}^n} \overline{H}^2 |\nabla\times\mathbf{A} - \mathbf{H_e}|^2 \, l^n \, \mathrm{d}x$$

$\Rightarrow$

$$\frac{1}{l^n\overline{H}^2}G(u,\mathbf{A}) = \int_D \left(\frac{M\hbar^2}{2m\overline{H}^2}\frac{1}{l^2}\left| \left(i\nabla - \frac{2(2\pi)^{1/2}\overline{H}el^2}{c\hbar}\mathbf{A} \right) u \right|^2 - \frac{\alpha M}{\overline{H}^2}|u|^2 + \frac{\beta M^2}{2\overline{H}^2}|u|^4 \right) \mathrm{d}x$$

$$+ \int_{\mathbb{R}^n} |\nabla\times\mathbf{A} - \mathbf{H_e}|^2 \, \mathrm{d}x. \tag{2.8}$$

Here D denotes the original domain $\tilde{D}$ scaled by l.

Again, our goal is to find a nondimensionalization such that M, $\overline{H}$ and l are not temperature-dependent. Before proceeding, we should perhaps mention that in addition to the coherence length and the penetration depth, there is another length-scale in the problem given by

$$\zeta = \frac{2m\beta}{\hbar^2}.$$

An elementary calculation shows that ζ and κ are related through

$$\zeta = 4\pi\kappa r_0, \tag{2.9}$$

where $r_0 = e^2/mc^2$ is the classical radius of the electron. Since λ and ξ depend on temperature through α, we are left with only two choices for scaling length in a temperature-independent manner. One is ζ and the other one is some typical length l associated with the domain $\tilde{D}$ such as

its diameter. The former choice is not desirable since $r_0 \sim 10^{-15}$ m, which is much smaller than any other length in the problem. We therefore opt for the latter choice that *uses the problem's specific geometry to fix its length-scale*. Thus we are guaranteed to end up working with a domain D whose size is $\mathcal{O}(1)$.

Choosing a value for M is trickier. It is not desirable to use the geometrical quantity l. If we choose ζ, we end up with a representation for G that has terms such as r_0/l that are extremely small as explained above. We cannot use ξ and λ since this will lead to a formulation where the temperature appears implicitly in u, and this causes difficulties in any phase transition analysis. To remedy the situation we use the formula (2.2) to define

$$\xi_0 = \sqrt{\frac{\hbar^2}{2m\alpha_0}} \quad \text{and} \quad \lambda_0 = \sqrt{\frac{m\beta c^2}{4\pi\alpha_0 e^2}}. \tag{2.10}$$

These definitions imply that $\lambda = \lambda_0 \rho(T)$ and $\xi = \xi_0 \rho(T)$, with $\rho(T) \sim (T_c - T)^{-1/2}$. We can therefore use ξ_0, or, even better, α_0, as a natural scaling length for M:

$$M = \frac{\overline{H}^2}{\alpha_0}. \tag{2.11}$$

Scaling H is to a large extent dependent on the specific problem at hand. For example, if we are interested in mesoscopic domains, we can use the number of fluxoids in $\tilde{D}$ as a scaling parameter and set

$$\overline{H} = \frac{\Phi_0}{2(2\pi)^{3/2} l^2} = \frac{\hbar c}{2(2\pi)^{1/2} e l^2}. \tag{2.12}$$

Up to a factor and an additive constant, we obtain that the energy is given by

$$G(u, \mathbf{A}) = \int_D \left(\left(\frac{\xi_0}{l} \right)^2 |(i\nabla - \mathbf{A})u|^2 + \frac{\nu^2}{2} (|u|^2 - \mu^2)^2 \right) dx + \int_{\mathbb{R}^n} |\nabla \times \mathbf{A} - \mathbf{H_e}|^2 \, dx. \tag{2.13}$$

Here

$$\nu^2 = \frac{\beta \overline{H}^2}{\alpha_0^2} \tag{2.14}$$

and is independent of temperature, while the temperature dependence is captured in the parameter μ^2 given by

$$\mu^2 \sim \frac{\alpha_0^2 (T_c - T)}{\beta \overline{H}^2} \quad \text{for} \quad T_c - T \ll 1. \tag{2.15}$$

It is also useful to write the energy in another form that exposes the parameter κ. It follows from (2.10) and (2.12) that

$$\frac{l^2 \nu^2}{\xi_0^2} = \frac{\lambda_0^2}{l^2}.$$

Substituting this into (2.13) and noting that $\kappa = \lambda_0 / \xi_0$ we obtain (after multiplying G by a constant)

$$G(u,\mathbf{A})=\int_D\left(|(i\nabla-\mathbf{A})u|^2+\frac{\sigma}{2}(|u|^2-\mu^2)^2\right)\,dx+\sigma^{-1}\kappa^2\int_{\mathbb{R}^n}|\nabla\times\mathbf{A}-\mathbf{H_e}|^2\,dx, \tag{2.16}$$

where $\sigma=(\lambda_0/l)^2$.

III. FORMULATION OF THE VARIATIONAL PROBLEM WITH NORMAL INCLUSIONS

In this section we discuss the incorporation of normal inclusions into the Ginzburg–Landau model. This will be carried out through an appropriate modification of the nondimensional energy (2.13). We wish to consider three possible geometries for the region occupied by the superconductor: that of a thin film, an infinite cylinder and an arbitrary smooth, bounded three-dimensional domain. For the first two, we denote by $D\subset\mathbb{R}^2$ a smooth, bounded, connected open set. In the case of the film, D will represent the planar region covered by the film. In the case of an infinite cylinder, D represents the $2d$ cross-section. In all cases, we study the behavior of the superconductor when exposed to an applied magnetic field $\mathbf{H_e}$. In the first two cases, we take $\mathbf{H_e}$ to be directed orthogonally to D, that is, $\mathbf{H_e}$ takes the form $(0,0,h_e)$ for some $h_e:\mathbb{R}^2\to\mathbb{R}^1$, while $\mathbf{H_e}:\mathbb{R}^3\to\mathbb{R}^3$ is at this point taken to be arbitrary in the fully $3d$ case.

To model the normal inclusions in the sample, we first introduce $\Gamma=(\cup_{i=1}^N\Gamma_i)\subset D$ to be a finite union of nonintersecting C^2 curves (surfaces) for $D\subset\mathbb{R}^2$ ($\subset\mathbb{R}^3$). We assume that for each i, either Γ_i has no boundary or else that its boundary lies in ∂D. We shall denote by $d_\Gamma:D\to\mathbb{R}^1$ the Euclidean distance from a point in D to Γ and we note that under the assumption that $\Gamma\in C^2$ we can conclude that $d_\Gamma\in C^2$ in a sufficiently small neighborhood of Γ. We also note that the (mean) curvature of Γ, denoted by κ_Γ, is bounded in L^∞. Then, for $\delta>0$ and small, define a δ-neighborhood D_δ around Γ by

$$D_\delta=\{x\in D:\, d_\Gamma(x)<\delta\}. \tag{3.1}$$

In what follows, D_δ will represent the region taken up by the normal inclusions.

The impurity is modeled by the potential V_δ defined through

$$V_\delta=\frac{a}{\delta^p}\chi_{D_\delta}, \tag{3.2}$$

where a is a fixed positive constant, p is a positive parameter that characterizes the ''strength'' of the impurity, and χ_{D_δ} denotes the characteristic function of the set D_δ.

We begin with the case of a thin film. In this case, to leading order in the film thickness, one may ignore the field induced by any supercurrents[10] and thereby obtain the following modified Ginzburg–Landau model with inclusions:

$$E_\delta(u)=\int_D|(i\nabla-\mathbf{A}_e)u|^2dx+\int_D V_\delta(x)|u|^2dx+\int_{D\setminus D_\delta}\frac{\nu^2}{2}(|u|^2-\mu^2)^2dx. \tag{3.3}$$

Here $\mathbf{A}_e:\mathbb{R}^2\to\mathbb{R}^2$ is the magnetic potential associated with $\mathbf{H_e}$; that is,

$$\nabla\times\mathbf{A}_e=\mathbf{H_e}. \tag{3.4}$$

To simplify the presentation of the asymptotic analysis we take $\xi_0/l=1$ in (2.13).

For the case of an infinite cylinder with cross-section $D\subset\mathbb{R}^2$ and the case where $D\subset\mathbb{R}^3$, we may not ignore the induced magnetic field and so the energy includes the total magnetic potential $\mathbf{A}$ and takes the form

$$G_\delta(u,\mathbf{A})=\int_D|(i\nabla-\mathbf{A})u|^2dx+\int_D V_\delta(x)|u|^2dx+\int_{D\setminus D_\delta}\frac{\nu^2}{2}(|u|^2-\mu^2)^2dx+\int_{R^n}|\nabla\times\mathbf{A}-\mathbf{H_e}|^2\,dx, \tag{3.5}$$

for $n=2,3$.

We note that the functional E_δ is well-defined for Sobolev functions $u \in H^1(D;\mathbb{C})$ consisting of all square-integrable, complex-valued functions having (weak) square-integrable gradients. The functional G_δ makes sense for $u \in H^1(D;\mathbb{C})$ and $\mathbf{A}$ such that $\mathbf{A} \in H^1_{\mathrm{loc}}(\mathbb{R}^n;\mathbb{R}^n)$ ($n=2$ or 3) and such that $\nabla \times \mathbf{A} - \mathbf{H_e} \in L^2(\mathbb{R}^n;\mathbb{R}^n)$. We will denote this space of admissible magnetic potentials by $H^1_e(\mathbb{R}^n;\mathbb{R}^n)$.

IV. ASYMPTOTIC LIMITS OF E_δ AND G_δ

The characterization of the minimizers of the functionals E_δ and G_δ depends on the value taken by the parameter p. We investigate the asymptotic limits using the method of gamma-convergence.

To describe these asymptotic limits, we need to recall the notion of the trace of a Sobolev function (cf. Ref. 12). The trace of a Sobolev function is a measure-theoretic means to describe the restriction of a Sobolev function defined on $\mathbb{R}^n$ to an $(n-1)$-dimensional set. It is not obvious that such a restriction is sensible since Sobolev functions are only defined up to sets of n-measure zero. However, for $u \in H^1(D;\mathbb{C})$, one can define the trace of u on the smooth curves (surfaces) Γ previously introduced, which we denote by $\mathrm{tr}_\Gamma u$. In particular, one has $\mathrm{tr}_\Gamma u \in L^2(\Gamma;\mathbb{C})$ and there exists a positive constant $C=C(\Gamma,D)$ such that

$$\int_\Gamma |\mathrm{tr}_\Gamma u|^2 \, dH^{n-1}(x) \leqslant C \int_D |u|^2 + |\nabla u|^2 \, dx. \tag{4.1}$$

Here dH^{n-1} corresponds to $(n-1)$-dimensional Hausdorf measure, that is, essentially d(arc length) in two dimensions and d(surface area) in three dimensions. Of course, (4.1) in particular implies that if a sequence of functions defined on D converges in $H^1(D;\mathbb{C})$, then necessarily their traces converge in $L^2(\Gamma;\mathbb{C})$. We also record here the fact that the $L^2(\Gamma;\mathbb{C})$-norm of the trace can be approached through integral averages in the sense that for any $u \in H^1(D;\mathbb{C})$ one has

$$\int_\Gamma |\mathrm{tr}_\Gamma u|^2 \, dH^{n-1}(x) = \lim_{\delta \to 0} \frac{1}{2\delta} \int_{D_\delta} |u|^2 \, dx. \tag{4.2}$$

Throughout the article, we shall generally suppress the notation $\mathrm{tr}_\Gamma u$ and write simply u when considering the restriction of a Sobolev function u to the set Γ. However, it should be interpreted in terms of trace.

We now recall the characterization of gamma-convergence of a sequence of functionals (cf., e.g., Ref. 4). A family of functionals $\{F_\delta\}$, all defined on Banach space X and mapping into $\mathbb{R}^1$, are said to gamma-converge to a functional $F: X \to \mathbb{R}^1$ with respect to the topology of X if

$$\forall u \in X, \exists \text{a sequence } \{u_\delta\} \subset X \quad \text{such that } u_\delta \overset{X}{\to} u \quad \text{and } \lim_{\delta \to 0} F_\delta(u_\delta) = F(u), \tag{4.3}$$

and

$$\forall u \in X, \quad \forall \{v_\delta\} \subset X \quad \text{such that } v_\delta \overset{X}{\to} u, \text{ we have } \liminf F_\delta(v_\delta) \geqslant F(u). \tag{4.4}$$

A useful consequence of this definition is that if a class of functionals $\{F_\delta\}$ has a gamma-limit F, then any limit u of minimizers $\{u_\delta\}$ of F_δ must minimize the limiting functional F.

We shall apply this machinery to the sequence $\{E_\delta\}$ in the topology $X=H^1(D;\mathbb{C})$, to obtain the following result:

Theorem 4.1: *(i) For $0 \leqslant p < 1$, the $H^1(D;\mathbb{C})$ gamma-limit of the sequence $\{E_\delta\}$ as $\delta \to 0$ is the functional $E^{(0)}$ given by*

$$E^{(0)}(u)=\int_D|(i\nabla-\mathbf{A}_e)u|^2\mathrm{d}x+\int_D\frac{\nu^2}{2}(|u|^2-\mu^2)^2\mathrm{d}x. \tag{4.5}$$

(ii) For $p=1$, the gamma-limit of the $\{E_\delta\}$ as $\delta\to0$ is $E^{(1)}$ given by

$$E^{(1)}(u)=E^{(0)}(u)+2a\int_\Gamma|u|^2\mathrm{d}H^1(x). \tag{4.6}$$

(iii) For $p>1$, the gamma-limit of the $\{E_\delta\}$ as $\delta\to0$ is $E^{(2)}$ given by

$$E^{(2)}(u)=\begin{cases}E^{(0)}(u), & \text{if } \mathrm{tr}_\Gamma u(x)=0 \quad \text{for} \quad H^{n-1}\,a.e.\,x\in\Gamma,\\ +\infty, & \text{otherwise.}\end{cases} \tag{4.7}$$

In a similar fashion, we shall obtain the gamma-limit of $\{G_\delta\}$. In this case, we take the $H^1(D;\mathbb{C})$ topology for u, and the $H^1_{\mathbf{e}}$ topology for $\mathbf{A}$.

Theorem 4.2: *(i) For $0\leqslant p<1$, the $H^1(D;\mathbb{C})\times H^1_{\mathbf{e}}(\mathbb{R}^n;\mathbb{R}^n)$ gamma-limit of the sequence $\{G_\delta\}$ as $\delta\to0$ is the functional $G^{(0)}$ given by*

$$G^{(0)}(u,\mathbf{A})=\int_D|(i\nabla-\mathbf{A})u|^2\mathrm{d}x+\int_D\frac{\nu^2}{2}(|u|^2-\mu^2)^2\mathrm{d}x+\int_{\mathbb{R}^n}|\nabla\times\mathbf{A}-\mathbf{H}_e|^2\,\mathrm{d}x. \tag{4.8}$$

(ii) For $p=1$, the gamma-limit of the $\{G_\delta\}$ as $d\to0$ is $G^{(1)}$ given by

$$G^{(1)}(u,\mathbf{A})=G^{(0)}(u,\mathbf{A})+2a\int_\Gamma|u|^2\mathrm{d}H^{n-1}(x). \tag{4.9}$$

(iii) For $p>1$, the gamma-limit of the $\{G_\delta\}$ as $\delta\to0$ is $G^{(2)}$ given by

$$G^{(2)}(u,\mathbf{A})=\begin{cases}G^{(0)}(u,\mathbf{A}), & \text{if } \mathrm{tr}_\Gamma u(x)=0 \quad \text{for} \quad H^{n-1}\,a.e.\,x\in\Gamma,\\ +\infty, & \text{otherwise.}\end{cases} \tag{4.10}$$

Proof of Theorems 4.1 and 4.2: Since the two theorems are proved in a similar manner, we shall present both proofs simultaneously.

Case 1: $0\leqslant p<1$.

We begin with the construction required by (4.3). For both E_δ and G_δ we choose the trivial sequence. That is, given any $u\in H^1(D;\mathbb{C})$ and $\mathbf{A}$ such that $\mathbf{A}-\mathbf{A}_e\in H^1(\mathbb{R}^n;\mathbb{R}^n)$ we take for the required construction $\{u_\delta\}$ simply $u_\delta=u$ and for $\{\mathbf{A}_\delta\}$ simply $\mathbf{A}_\delta=\mathbf{A}$ for all δ. Then the properties

$$\lim_{\delta\to0}E_\delta(u_\delta)=E^{(0)}(u) \quad \text{and} \quad \lim_{\delta\to0}G_\delta(u_\delta,\mathbf{A}_\delta)=G^{(0)}(u,\mathbf{A})$$

follow immediately from (4.1) and (4.2) since

$$\int_D V_\delta(x)|u_\delta|^2\mathrm{d}x=\frac{a}{\delta^p}\int_{D_\delta}|u|^2\,\mathrm{d}x=a\,\delta^{1-p}\left(\frac{1}{\delta}\int_{D_\delta}|u|^2\,\mathrm{d}x\right)\approx2a\,\delta^{1-p}\int_\Gamma|u|^2\,\mathrm{d}H^{n-1}(x)\to0$$
$$\text{as} \quad \delta\to0.$$

The convergence of the other terms in E_δ and G_δ to the appropriate terms in $E^{(0)}$ and $G^{(0)}$ are trivial. The lower semi-continuity property (4.4) follows at once since the non-negative term in the energies E_δ and G_δ involving V_δ can be ignored and all other terms are in fact continuous in the H^1 topology.

Case 2: $p=1$.

In light of (4.2), one may again take the trivial sequences $u_\delta = u$ and $\mathbf{A}_\delta = \mathbf{A}$ in order to establish the construction (4.3) for E_δ and G_δ.

The lower semi-continuity condition (4.4)—in fact, continuity under in the H^1 topology—will follow from (4.1) and (4.2) and the fact that if $u_\delta \to u$ in $H^1(D;\mathbb{C})$, then

$$\lim_{\delta\to 0}\left|\frac{1}{\delta}\int_{D_\delta}|u_\delta|^2\,\mathrm{d}x - 2\int_\Gamma |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\right| = 0. \tag{4.11}$$

To verify (4.11), we use the co-area formula to compute

$$\begin{aligned}
&\left|\frac{1}{\delta}\int_{\{0<d_\Gamma(x)<\delta\}}|u_\delta|^2\,\mathrm{d}x - \int_\Gamma |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\right| \\
&\quad = \left|\frac{1}{\delta}\int_0^\delta \int_{\{d_\Gamma(x)=\eta\}} |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\,\mathrm{d}\eta - \int_\Gamma |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\right| \\
&\quad = \frac{1}{\delta}\left|\int_0^\delta \left\{\int_{\{d_\Gamma(x)=\eta\}} |u_\delta|^2\,\mathrm{d}H^{n-1}(x) - \int_{\{d_\Gamma(x)=0\}}\right\}\right| |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\,\mathrm{d}\eta.
\end{aligned}$$

This last difference is controlled using the divergence theorem, yielding

$$\begin{aligned}
&\left|\frac{1}{\delta}\int_{\{0<d_\Gamma(x)<\delta\}}|u_\delta|^2\,\mathrm{d}x - \int_\Gamma |u_\delta|^2\,\mathrm{d}H^{n-1}(x)\right| \\
&\quad \leqslant \frac{1}{\delta}\left|\int_0^\delta \int_{\{0<d_\Gamma(x)<\eta\}} \mathrm{div}(|u_\delta|^2\nabla d_\Gamma)\,\mathrm{d}x\right| \\
&\qquad + \frac{1}{\delta}\left|\int_0^\delta \int_{\partial D\cap\{0<d_\Gamma(x)<\eta\}} |u_\delta|^2\,(\nabla d_\Gamma\cdot \nu_{\partial D})\,\mathrm{d}H^{n-1}(x)\,\mathrm{d}\eta\right| \\
&\quad \leqslant \frac{1}{\delta}\int_0^\delta \int_{\{0<d_\Gamma(x)<\eta\}} (|u_\delta|^2\|\kappa_\Gamma\|_{L^\infty(\Gamma)} + 2|u_\delta||\nabla u_\delta|)\,\mathrm{d}x + \int_{\partial D\cap\{0<d_\Gamma(x)<\delta\}} |u_\delta|^2\,\mathrm{d}H^{n-1}(x) \\
&\quad \leqslant (\|\kappa_\Gamma\|_{L^\infty(\Gamma)}+1)\|u_\delta\|^2_{H^1(\{0<d_\Gamma(x)<\delta\})} \\
&\qquad + \|u_\delta\|^2_{L^2(\partial D\cap\{0<d_\Gamma(x)<\delta\})} \to 0 \quad \text{as} \quad \delta\to 0.
\end{aligned}$$

Case 3: $p>1$.

To establish property (4.3), fix any $u\in H^1(D;\mathbb{C})$. If $u(x)\neq 0$ for H^{n-1} a.e. $x\in\Gamma$, then take the trivial sequence $u_\delta = u$ for the constructive part (4.3). Using (4.2), one finds

$$\int_D V_\delta |u_\delta|^2\,\mathrm{d}x = \frac{\alpha}{\delta^{p-1}}\left(\frac{1}{\delta}\int_{D_\delta}|u|^2\right) \approx \frac{2\alpha}{\delta^{p-1}}\int_\Gamma |u|^2\,\mathrm{d}H^{n-1}(x) \to \infty. \tag{4.12}$$

Hence, $\lim_{\delta\to 0} E_\delta(u_\delta) = E^{(2)}(u) = \infty$ and the same reasoning applies to G_δ.

If, on the other hand, $u(x)=0$, then we introduce a smooth sequence $\rho_\delta:[0,\infty)\to[0,\infty)$ such that (i) $\rho_\delta(s)=0$ for $0\leqslant s\leqslant\delta$, (ii) $\rho_\delta(s)=1$ for $s\geqslant\delta^{1/2}$ and (iii) $|\rho_\delta'(s)|\leqslant 2/\delta^{1/2}$ for all s. Then define the sequence $\{u_\delta\}$ through the formula

$$u_\delta(x) = u(x)\rho_\delta(d_\Gamma(x)).$$

Clearly $u_\delta\to u$ in $L^2(D;\mathbb{C})$ and since

$$|\nabla u_\delta|^2 \leq 2\left(|\nabla u|^2 + \frac{1}{\delta}|u|^2\right)$$

one finds that

$$\int_{\{\delta<d_\Gamma(x)<\delta^{1/2}\}} |\nabla u_\delta|^2 \, dx \leq 2\left(\int_{\{\delta<d_\Gamma(x)<\delta^{1/2}\}} |\nabla u|^2 \, dx + \frac{1}{\delta}\int_{\{d_\Gamma(x)<\delta^{1/2}\}} |u|^2 \, dx\right). \quad (4.13)$$

Since $u \in H^1(D;\mathbb{C})$, the first term on the right in (4.13) clearly approaches zero with δ. Now since smooth functions are dense in H^1, we may assume that $u \in H^1(D;\mathbb{C}) \cap C^1(D;\mathbb{C})$. Then the assumption $u=0$ implies that for any $\eta>0$ and any $x \in D$ such that $d_\Gamma(x)=\eta$ one has

$$u(x) = \int_0^\eta \frac{d}{dt} u(y + t\nu(y)) \, dt,$$

where $y=y(x)$ is the closest point of Γ to x and $\nu(y)$ is the unit normal of Γ at y pointing towards x. Consequently, we have

$$|u(x)|^2 \leq \eta \int_0^\eta |\nabla u(y + t\nu(y))|^2 \, dt \quad \text{for any } x \text{ such that } d_\Gamma(x)=\eta. \quad (4.14)$$

We then handle the second term in (4.13) again through an appeal to the co-area formula, Fubini's theorem and (4.14) as follows:

$$\begin{aligned}
\frac{1}{\delta}\int_{\{\delta<d_\Gamma(x)<\delta^{1/2}\}} |u(x)|^2 \, dx &\leq \frac{1}{\delta}\int_\delta^{\delta^{1/2}} \int_{\{d_\Gamma(x)=\eta\}} \eta \int_0^\eta |\nabla u(y+t\nu(y))|^2 \, dt \, dH^{n-1}(x) \, d\eta \\
&\leq \frac{1}{\delta}\int_0^{\delta^{1/2}} \eta \int_{\{d_\Gamma(x)=\eta\}} \int_0^{\delta^{1/2}} |\nabla u(y+t\nu(y))|^2 \, dt \, dH^{n-1}(x) \, d\eta \\
&= \frac{1}{\delta}\int_0^{\delta^{1/2}} \eta \int_0^{\delta^{1/2}} \int_{\{d_\Gamma(x)=\eta\}} |\nabla u(y+t\nu(y))|^2 \, dH^{n-1}(x) \, dt \, d\eta \\
&\leq \frac{1}{\delta}\int_0^{\delta^{1/2}} \eta \int_0^{\delta^{1/2}} \int_{\{d_\Gamma(x)=t\}} |\nabla u(x)|^2 (1 + C_0\delta^{(n-1)/2}) \, dH^{n-1}(x) \, dt \, d\eta,
\end{aligned}$$

where the factor of $C_0\delta^{(n-1)/2}$ appearing in the last integral arises from the difference in dH^{n-1} along $\{d_\Gamma(x)=\eta\}$ versus $\{d_\Gamma(x)=t\}$ where $|t-\eta| \leq \delta^{1/2}$. We conclude that

$$\frac{1}{\delta}\int_{\{\delta<d_\Gamma(x)<\delta^{1/2}\}} |u(x)|^2 \, dx \leq C \int_{\{d_\Gamma(x)<\delta^{1/2}\}} |\nabla u|^2 \, dx \to 0 \text{ as } \delta \to 0.$$

It easily follows that $u_\delta \to u$ in $H^1(D;\mathbb{C})$ as well. Then, since

$$\int_D V_\delta(x)|u_\delta|^2 \, dx = \int_{\{d_\Gamma(x)<\delta\}} \frac{a}{\delta^p} \cdot 0 \, dx = 0,$$

one concludes that $E_\delta(u_\delta) \to E^{(2)}(u)$ and $G_\delta(u_\delta, \mathbf{A}) \to G^{(2)}(u, \mathbf{A})$ as $\delta \to 0$, thus establishing (4.3) in this case.

The lower semi-continuity property (4.4) is clear in the case where $u=0$ since again one may simply ignore the non-negative term involving the potential V_δ. To establish the lower semi-continuity for the case $u \not\equiv 0$, we let $\{u_\delta\}$ be any sequence converging in $H^1(D;\mathbb{C})$ to u, and use (4.1) and (4.2) to see that

$$\frac{1}{\delta^p}\int_{D_\delta}|u_\delta|^2\,dx=\frac{1}{\delta^{p-1}}\left\{\left(\frac{1}{\delta}\int_{D_\delta}|u_\delta|^2\,dx-2\int_\Gamma|u_\delta|^2\,dH^{n-1}(x)\right)\right\}$$
$$+\frac{2}{\delta^{p-1}}\left\{\left(\int_\Gamma|u_\delta|^2-|u|^2\,dH^{n-1}(x)\right)+\int_\Gamma|u|^2\,dH^{n-1}(x)\right\}$$
$$=\frac{1}{\delta^{p-1}}\left(2\int_\Gamma|u|^2\,dH^{n-1}(x)+o(1)\right)\to\infty=E^{(2)}(u)=G^{(2)}(u,\mathbf{A}).$$

□

V. VARIATIONAL CHARACTERIZATION OF TRANSITION TEMPERATURE WITH NORMAL INCLUSIONS

One application of the analysis of the previous section concerns the transition temperature $T=T(\mathbf{H_e})$ below which the normal state in a superconductor with normal inclusions loses stability. Recall that within Ginzburg–Landau theory, the normal state prevails when the order parameter vanishes identically while the applied magnetic field completely penetrates the sample so that $\mathbf{A}=\mathbf{A_e}$ where $\mathbf{A_e}$ is given by (3.4). Then the loss of stability of the state $u=0$ in (3.3) or of the pair $(u,\mathbf{A})=(0,\mathbf{A_e})$ in (3.5) for $\delta\ll 1$ should be related to the corresponding loss of stability of their gamma-limits given by Theorems 4.1 and 4.2. This claim is supported by the fact that limits of minimizers of a gamma-converging sequence will minimize the gamma-limit and even an isolated local minimizer of a gamma-limit will be a limit point of a sequence of local minimizers of the gamma-converging sequence (see Ref. 8 in this regard).

Stability or instability of a critical point is most easily classified in terms of the sign of the second variation taken about the point in question. Starting from (4.5) and (4.7), a straightforward calculation yields the second variation formula for the gamma-limits of E_δ when $p<1$ or $p>1$:

$$\delta^2E^{(j)}(0;u)\equiv\left.\frac{d^2E^{(j)}(0+\varepsilon u)}{d\varepsilon^2}\right|_{\varepsilon=0}=2\int_D\{|(i\nabla-\mathbf{A}_e)u|^2-\nu^2\mu^2|u|^2\}\,dx \tag{5.1}$$

for $j=0$ or 2 where for $j=0$ $(p<1)$, the variation is taken over arbitrary functions in $u\in H^1(D;\mathbb{C})$ while for $j=2$ $(p>1)$, we additionally require $u=0$ on Γ in the sense of traces.

For E_δ in the critical case $p=1$, we obtain from (4.6) that

$$\delta^2E^{(1)}(0;u)=2\int_D\{|(i\nabla-\mathbf{A}_e)u|^2-\nu^2\mu^2|u|^2\}\,dx+4a\int_\Gamma|u|^2\,dH^{n-1}(x) \tag{5.2}$$

for any $u\in H^1(D;\mathbb{C})$.

Now if our goal is to understand the phase transition curve $T=T(\mathbf{H_e})$, we can capture this through the parameter μ [cf. (2.15)]. Loss of stability of the normal state corresponds to the value of μ where the second variations calculated above vanish. Hence we can characterize $\mu^2(\mathbf{H_e})$ and through (2.15) obtain $T(\mathbf{H_e})$ via the formulas

$$\mu^2(\mathbf{H_e})=\inf_{\{u\in H^1(D;\mathbb{C})\}}\frac{\int_D|(i\nabla-\mathbf{A}_e)u|^2\,dx}{\nu^2\int_D|u|^2\,dx}\quad\text{for}\quad p<1,$$

$$\mu^2(\mathbf{H_e})=\inf_{\{u\in H^1(D;\mathbb{C})\}}\frac{\int_D|(i\nabla-\mathbf{A}_e)u|^2\,dx+2a\int_\Gamma|u|^2\,dH^{n-1}(x)}{\nu^2\int_D|u|^2\,dx}\quad\text{for}\quad p=1, \tag{5.3}$$

$$\mu^2(\mathbf{H_e})=\inf_{\{u\in H^1(D;\mathbb{C}),\ u=0\ \text{on}\ \Gamma\}}\frac{\int_D|(i\nabla-\mathbf{A}_e)u|^2\,dx}{\nu^2\int_D|u|^2\,dx}\quad\text{for}\quad p>1.$$

A similar set of calculations on the three gamma-limits of G_δ given by (4.8)–(4.10) yield corresponding formulas

$$\delta^2 G^{(j)}(0,\mathbf{A_e};u,\mathbf{A}) \equiv \left.\frac{d^2 G^{(j)}(0+\varepsilon u,\mathbf{A_e}+\varepsilon \mathbf{A})}{d\varepsilon^2}\right|_{\varepsilon=0}$$

$$= 2\int_D \{|(i\nabla - \mathbf{A}_e)u|^2 - \nu^2\mu^2|u|^2\}\,dx + 2\int_{\mathbb{R}^n} |\nabla\times\mathbf{A}|^2\,dx \tag{5.4}$$

for $j=0$ or 2 where for $j=0$ $(p<1)$, the variation is taken over arbitrary functions $u \in H^1(D;\mathbb{C})$ and $\mathbf{A}\in H^1_e(\mathbb{R}^n;\mathbb{R}^n)$ while for $j=2$ $(p>1)$, we additionally require $u=0$ on Γ in the sense of traces.

For the second variation of $G^{(1)}$ in the critical case $p=1$ we obtain from (4.9) that

$$\delta^2 G^{(1)}(0,\mathbf{A_e};u,\mathbf{A}) = 2\int_D \{|(i\nabla - \mathbf{A}_e)u|^2 - \nu^2\mu^2|u|^2\}\,dx + 4a\int_\Gamma |u|^2\,dH^{n-1}(x) + 2\int_{\mathbb{R}^n} |\nabla\times\mathbf{A}|^2\,dx$$

for any $u\in H^1(D;\mathbb{C})$ and $\mathbf{A}\in H^1_{\mathbf{e}}(\mathbb{R}^n;\mathbb{R}^n)$.

Since the convex term $\int_{\mathbb{R}^n}|\nabla\times\mathbf{A}|^2\,dx$ will never lead to instability, the value of $\mu^2(\mathbf{H_e})$ yielding zero second variation will again be achieved by (5.3) for the cases $p<1$, $p=1$ and $p>1$ by taking $\mathbf{A}=0$.

We point out that in the absence of any applied field where one can take $\mathbf{A_e}=0$, the presence of the normal junction will still cause a shift down in the critical temperature when $p\geqslant 1$, that is, when the junction is sufficiently strong. In other words, $\mu^2(0)>0$ in (5.3) for E_δ or G_δ for the cases $p=1$ and $p>1$. On the other hand, for a weak junction $(p<1)$, one finds that $\mu^2(0)=0$ so that to leading order in δ, there is no shift in the critical temperature in the absence of applied fields.

VI. SUMMARY

We have calculated several canonical limits of the Ginzburg–Landau energy functional for superconducting samples with defects. The defect is centered around a co-dimension-one manifold in the domain. The defect is defined through a penalizing potential in a small neighborhood of that manifold. The different limits are distinguished by the strength of the defect, which, in turn, is controlled by the L_1-norm of the penalizing potential.

One of the interesting conclusions we obtain is that when the defect is sufficiently strong, the minimizer must vanish along the defect. This result has a number of consequences; in particular, it affects the phase transition temperature. It is well known that this temperature is determined by the first eigenvalue of the magnetic Schrödinger operator. Typically one considers this spectral problem under Neumann boundary conditions. Our results indicate that in the presence of strong defects, one should compute the leading eigenvalue of the magnetic Schrödinger operator for functions that satisfy Dirichlet boundary conditions along the defect and Neumann boundary conditions along the rest of the sample boundary.

ACKNOWLEDGMENTS

J.R. was partially supported by NSF Grant No. DMS-0203312. P.S. was partially supported by NSF Grant No. DMS-0100540.

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Twisted super-Yangians and their representations

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(Received 18 November 2002; accepted 22 November 2002)

Starting with the super-Yangian $Y(M|N)$ based on $\mathrm{gl}(M|N)$, we define twisted super-Yangians $Y(M|N)^{\pm}$. Only $Y^{+}(M|2n)$ and $Y^{-}(2m|N)$ can be defined, and appear to be isomorphic one with each other. We study their finite-dimensional irreducible highest weight representations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1542662]

I. INTRODUCTION

Quite recently, a revival of interest has been put on coideal algebras of Hopf algebras, both from mathematical and physical points of view. Among these algebras, let us note the twisted Yangians $Y^{\pm}(N)$, introduced by Olshanski[1] and widely studied (see, for instance Ref. 2 and references therein), or the reflection algebras, introduced by Sklyanin[3] and studied in Refs. 4 and 5.

From the mathematical point of view, it seems that such coideal condition is quite restrictive, leading to a very small class of subalgebras, for a given Hopf algebra.[6,7] Indeed, for quantum algebras $\mathcal{U}_q(\mathrm{gl}_N)$, it has been proven that they are natural deformations of symmetric spaces.[6]

From a physical point of view, such ideals appear to play an important role in integrable systems with boundaries.[4,8,9] They appear to be the integrals of motion of such systems,[4,9] and also naturally deduced from the boundary condition.[8]

It thus appears natural to look for such coideals when the underlying algebra is not gl_N anymore. Such types of algebras have been introduced in Ref. 10 for the case of Yangians based on orthogonal and symplectic algebras, and orthosymplectic superalgebras. They are defined as the ''twist'' of the (super)Yangian based on the corresponding Lie (super)algebra.

The aim of the present work is to complete the picture with the case of super-Yangians based on $\mathrm{gl}(M|N)$. After recalling the basic definitions and properties of the super-Yangians $Y(\mathrm{gl}(M|N)) \equiv Y(M|N)$ in Sec. II, we will define the twisted super-Yangians $Y(M|N)^{+}$ in Sec. III. Their finite-dimensional irreducible representations are studied in Sec. IV. We conclude in Sec. V.

II. SUPER-YANGIANS $Y(M|N)$

The super-Yangian $Y(M|N)$ based on the $\mathrm{gl}(M|N)$ superalgebra has been introduced in Ref. 11, and its irreducible finite-dimensional representations studied in Ref. 12. Since it is a $\mathbb{Z}_2$-graded (Hopf) algebra, different conventions can be chosen: the ones we choose are given below. We will rephrase the properties given in Ref. 12 in this context.

A. Graded spaces

We start with $K\times K$ matrices acting on the vector space $\mathbb{C}^K$, and introduce a $\mathbb{Z}_2$-grading $[.]$ on these spaces. We will denote by E_{ij} the usual $K\times K$ matrices which have 1 in position (i,j), and by e_i the basic vectors of $\mathbb{C}^K$ which have 1 in position i:

$$E_{ij}e_k = \delta_{jk}e_i\,. \tag{2.1}$$

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The $\mathbb{Z}_2$-grade is defined by

$$[E_{ij}]=[i]+[j];\ \ [e_i]=[i]\ \text{ and }\ [i]\in\{0,1\}\ \ \forall i,\ \ j=1,\ldots,K. \tag{2.2}$$

We will call even the matrices and vectors such that

$$A=A_{ij}E_{ij}\quad\text{ with }\quad [A_{ij}]=[i]+[j];\quad u=u_ie_i\quad\text{ with }\quad [u_i]=[i]. \tag{2.3}$$

The tensor product of graded matrices is chosen to be graded:

$$(E_{ij}\otimes E_{kl})(E_{ab}\otimes E_{cd})=(-1)^{([k]+[l])([a]+[b])}(E_{ij}E_{ab})\otimes(E_{kl}E_{cd}). \tag{2.4}$$

On the tensor product of $\mathbb{C}^K$ vector spaces, one has

$$(E_{ij}\otimes E_{kl})(e_a\otimes e_b)=(-1)^{([k]+[l])[a]}(E_{ij}e_a)\otimes(E_{kl}e_b). \tag{2.5}$$

We introduce the graded permutation operator:

$$P_{12}=\sum_{i,j}(-1)^{[j]}E_{ij}\otimes E_{ji}, \tag{2.6}$$

which obeys $P^2=\mathbb{I}$ and

$$P(e_i\otimes e_j)=(-1)^{[i][j]}e_j\otimes e_i,\ P(E_{ij}\otimes E_{kl})P=(-1)^{([i]+[j])([k]+[l])}E_{kl}\otimes E_{ij}. \tag{2.7}$$

B. Definition and first properties of $Y(M|N)$

We set $K=M+N$ and define the $\mathbb{Z}_2$-grade by

$$\begin{gathered}[i]=0\ \ \text{for}\ \ 1\leqslant i\leqslant M,\\ [i]=1\ \ \text{for}\ \ M+1\leqslant i\leqslant M+N.\end{gathered} \tag{2.8}$$

The super-Yangian $Y(M|N)$ has generators $T^{ab}_{(n)}$ (of $\mathbb{Z}_2$-grade $[a]+[b]$), gathered in

$$T(u)=\sum_{a,b=1}^{K}\sum_{n\geqslant 0}u^{-n}T^{ab}_{(n)}E_{ab}=\sum_{a,b=1}^{K}T^{ab}(u)E_{ab}=\sum_{n\geqslant 0}u^{-n}T_{(n)}\ \ \text{with}\ \ T_{(0)}=\mathbb{I}_K. \tag{2.9}$$

The even matrix $T(u)\in M_K[Y(M|N)]$ obeys

$$R_{12}(u-v)\,T_1(u)\,T_2(v)=T_2(v)\,T_1(u)\,R_{12}(u-v), \tag{2.10}$$

$$\text{with } R_{12}(u-v)=\mathbb{I}\otimes\mathbb{I}-\frac{1}{u-v}P_{12}, \tag{2.11}$$

or equivalently

$$[T^{ab}(u)\,,T^{cd}(v)\}=\frac{(-1)^{[a][b]+([a]+[b])[c]}}{u-v}(T^{cb}(u)T^{ad}(v)-T^{cb}(v)T^{ad}(u)), \tag{2.12}$$

where the graded commutator is defined by

$$[A,B\}=AB-(-1)^{[A][B]}BA. \tag{2.13}$$

It is a Hopf algebra:

$$\Delta(T^{ab}(u))=\sum_{c=1}^{M+N} T^{ac}(u)\otimes T^{cb}(u);\quad \epsilon(T^{ab}(u))=\delta^{ab};\quad S(T^{ab}(u))=(T^{-1}(u))^{ab}. \tag{2.14}$$

Note that $Y(M|N)$ contains several subalgebras:[12]

Property 2.1 (Subalgebras of $Y(M|N)$):

(i) *The generators $T^{ab}(u)$ with $a,b=1,\ldots,M$ (resp. $T^{ab}(u)$, $a,b=M+1,\ldots,M+N$) define the algebra inclusion $Y(M)\subset Y(M|N)$ [resp. $Y(N)\subset Y(M|N)$].*

(ii) *The generators $T^{ab}_{(1)}$ with $a,b=1,\ldots,M+N$ form a $\mathrm{gl}(M|N)$ Lie sub-superalgebra of $Y(M|N)$.*

(iii) *The generators $T^{ab}(u)$ with $a,b\in\{M,M+1\}$ define the algebra inclusion $Y(1|1)\subset Y(M|N)$.*

Remark: The above subalgebras are *not* Hopf subalgebras of $Y(M|N)$. Indeed, the coproduct (2.14) is based on all the generators of $Y(M|N)$, so that it does not induce the coproduct of $Y(M)$ and $Y(N)$.

We have also the following property.

Property 2.2 (Isomorphism between $Y(M|N)$ and $Y(N|M)$): Let

$$\widetilde{T}^{ab}(u)=(-1)^{[\overline{a}]([\overline{b}]+1)}T^{\overline{b}\,\overline{a}}(u)\quad with\quad \overline{a}=K+1-a,$$
$$[a]'=[\overline{a}]+1. \tag{2.15}$$

$\widetilde{T}(u)$ obey the Hopf algebra relations of $Y(N|M)$, with $\Delta'(x)=P\Delta(x)P$. We have thus a Hopf algebra isomorphism between $Y(M|N)$ and $Y(N|M)$.

Proof: One first proves that $\widetilde{T}(u)$ satisfies the commutation relations of $Y(N|M)$.

To prove that, we need

$$T^{cb}(u)T^{ad}(v)-T^{cb}(v)T^{ad}(u)=-(-1)^{([a]+[d])([b]+[c])}(T^{ad}(u)T^{cb}(v)-T^{ad}(v)T^{cb}(u)),$$

which can be proven either by a direct calculation, or by using the graded antisymmetry of the commutator,

$$[T^{ab}(u),T^{cd}(v)\}=-(-1)^{([a]+[d])([b]+[c])}[T^{cd}(v),T^{ab}(u)\}, \tag{2.16}$$

and computing $[T^{cd}(v),T^{ab}(u)\}$ using (2.12) with the replacements $(a,b,u)\leftrightarrow(c,d,v)$.

With the help of the above calculation one gets

$$\begin{aligned}
[\widetilde{T}^{ab}(u),\widetilde{T}^{cd}(v)\} &= (-1)^{[\overline{a}][\overline{b}]+[\overline{c}][\overline{d}]}[T^{\overline{b}\,\overline{a}}(u),T^{\overline{d}\,\overline{c}}(v)\}\\
&= \frac{(-1)^{[\overline{a}][\overline{b}]+[\overline{c}][\overline{d}]+[\overline{b}][\overline{a}]+([\overline{b}]+[\overline{a}])[\overline{d}]}}{u-v}(T^{\overline{d}\,\overline{a}}(u)T^{\overline{b}\,\overline{c}}(v)-T^{\overline{d}\,\overline{a}}(v)T^{\overline{b}\,\overline{c}}(u))\\
&= \frac{(-1)^{([\overline{a}]+[\overline{b}]+[\overline{c}])[\overline{d}]+([\overline{b}]+[\overline{c}])([\overline{a}]+[\overline{d}])}}{u-v}(T^{\overline{b}\,\overline{c}}(u)T^{\overline{d}\,\overline{a}}(v)-T^{\overline{b}\,\overline{c}}(v)T^{\overline{d}\,\overline{a}}(u))\\
&= \frac{(-1)^{[a]'[b]'+([a]'+[b]')[c]'}}{u-v}(\widetilde{T}^{cb}(u)\widetilde{T}^{ad}(v)-\widetilde{T}^{cb}(v)\widetilde{T}^{ad}(u)),
\end{aligned}$$

which is the correct expression for the commutator in $Y(N|M)$, since $[\ ]'$ is the correct gradation of $Y(N|M)$.

For the Hopf structure, one has

$$\begin{aligned}\Delta_{M|N}\tilde{T}^{ab}(u)&=\sum_{c=1}^{K}(-1)^{[\bar{a}]([\bar{b}]+1)}T^{\bar{b}\bar{c}}(u)\otimes T^{c\bar{a}}(u)\\&=\sum_{c=1}^{K}(-1)^{[\bar{a}]([\bar{b}]+1)+[\bar{c}]([\bar{b}]+1)+[\bar{a}]([\bar{c}]+1)}\tilde{T}^{cb}(u)\otimes\tilde{T}^{ac}(u)\\&=P\,\tilde{T}^{ac}(u)\otimes\tilde{T}^{cb}(u)\,P\\&=\Delta'_{N|M}\,\tilde{T}^{ab}(u),\end{aligned}$$

where we have denoted by $\Delta_{M|N}$ (resp. $\Delta_{N|M}$) the coproduct on $Y(M|N)$ [resp. on $Y(N|M)$].

A simple calculation shows

$$\epsilon_{M|N}(\tilde{T}^{ab}(u))=\epsilon'_{N|M}(\tilde{T}^{ab}(u)),\tag{2.17}$$

where $\epsilon'=\epsilon$ is the counit associated to Δ', while for the antipode

$$S'_{M|N}(\tilde{T}^{ab}(u))=(-1)^{[\bar{a}]([\bar{b}]+1)}\theta_a\theta_b(T^{-1}(u))^{\bar{a}\bar{b}}=S'_{N|M}(\tilde{T}^{ab}(u))=(\tilde{T}^{-1\prime}(u))^{ab},\tag{2.18}$$

where, in the last equality, the inverse $\tilde{T}^{-1\prime}(u)$ is computed using m' instead of m:

$$m'(\tilde{T}^{ab}(u)\otimes\tilde{T}^{-1\prime}(u)^{bc})=(-1)^{([a']+[b'])([b']+[c'])}\tilde{T}^{-1\prime}(u)^{bc}\cdot\tilde{T}^{ab}(u)=\delta^{ac}.\tag{2.19}$$

$S'_{M|N}$ obeys the relations

$$m'(S'\otimes id)\Delta'=\epsilon'=m'(id\otimes S')\Delta'.\tag{2.20}$$

■

C. Finite-dimensional irreducible representations of $Y(M|2n)$

The finite-dimensional irreducible representations of the super-Yangian $Y(M|N)$ have been studied in Ref. 12. We recall here its main results, referring to Ref. 12 for the proofs.

We will specify to the case $N=2n$, for it is the only case that is needed for twisted super-Yangians. Moreover, in order to be able to deal with the twisted super-Yangians, we need to choose a positive root system different from the one chosen in Ref. 12. Indeed, the situation is analogous to the one encountered in the case of simple Lie superalgebras, which admit different *inequivalent* systems of simple roots (see, for instance, Ref. 13). For our purpose, we define the following.

Definition 2.3 (Positive roots): Let $\Phi^{\pm,0}\subset\mathbb{N}_K^2$, *where* $\mathbb{N}_K=\mathbb{N}_{M+2n}=[1,M+2n]\cap\mathbb{N}$, *be defined by*

$$\Phi^+=\left\{(a,b)\in\mathbb{N}_K^2,\ \text{with either}\ \left|\begin{array}{c}1\leqslant a<b\leqslant M\\ M+1\leqslant a<b\leqslant M+2n\\ 1\leqslant a\leqslant M,\ M+n+1\leqslant b\leqslant M+2n\\ M+1\leqslant a\leqslant M+n,\ 1\leqslant b\leqslant M\end{array}\right.\right.\tag{2.21}$$

$$\Phi^-=\{(a,b)\in\mathbb{N}_{M+2n}^2,\ \text{such that}\ (b,a)\in\Phi^+\},\tag{2.22}$$

$$\Phi^0=\{(a,a),\ with\ a\in\mathbb{N}_{M+2n}\}.\tag{2.23}$$

We have $\mathbb{N}_{M+2n}^2=\Phi^-+\Phi^0+\Phi^+$, *and the positive roots will be associated to* $T^{ab}(u)$ *with* $(a,b)\in\Phi^+$.

Once a positive root system is chosen, one can introduce the notion of highest weight vectors:

Definition 2.4 (Highest weight vectors): Let $\mathcal{M}$ be a module of $Y(M|2n)$. A highest weight vector $\xi \in \mathcal{M}$ is defined by

$$T^{aa}(u)\xi = \lambda^a(u)\xi, \quad \forall a = 1,\ldots,M+2n,$$
$$T^{ab}(u)\xi = 0, \quad \forall (a,b) \in \Phi^+. \tag{2.24}$$

$\lambda(u) = (\lambda^1(u),\ldots,\lambda^{M+2n}(u)) \in \mathbb{C}[[u^{-1}]]$ *is the highest weight associated to* ξ.

The notion of highest weight vectors grounds in the following properties:

Property 2.5: Any irreducible finite-dimensional representation of $Y(M|N)$ admits a unique (up to multiplication by scalars) highest weight vector.

Property 2.6: The irreducible representation of $Y(M|N)$ with highest weight $\lambda(u)$ is finite dimensional if and only if we have

$$\frac{\lambda^a(u)}{\lambda^{a+1}(u)} = \frac{P_a(u+1)}{P_a(u)}, \quad 1 \leqslant a \leqslant M+N-1, \quad a \neq M, \tag{2.25}$$

$$\frac{\lambda^M(u)}{\lambda^{M+1}(u)} = \frac{P_M(u)}{P_{M+N}(u)}, \tag{2.26}$$

where $P_a(u)$ are monic polynomials.

Let us remark that some signs differ between our presentation and the presentation given in Ref. 12 because of the definition for $T(u)$: the relation between these two notations is given by $T^{ab}_{(n)} = (-1)^{[b]} t^a_b[n]$.

Definition 2.7 (Evaluation representations): Let J^{ab} be the generators of the gl$(M|N)$ *superalgebra and $\pi^{ab} = \pi(J^{ab})$ a finite-dimensional representation of* gl$(M|N)$. *Then, the morphism*

$$ev(T(u)) = 1 + \frac{\mathbb{E}}{u} \quad \textit{with} \quad \mathbb{E} = \pi^{ab} E_{ab} \tag{2.27}$$

provides a finite-dimensional representation of $Y(M|N)$, called an evaluation representation.

The usefulness of evaluation representations reveals in the following theorem:

Theorem 2.8: *Any irreducible finite-dimensional representation of $Y(M|N)$ is isomorphic to the irreducible part of tensor products of evaluation representations.*

III. TWISTED SUPER-YANGIANS

A. Introduction to $Y(M|N)^\tau$

We now introduce the notion of twisted super-Yangian, in the same way twisted Yangians have been defined from the Yangians $Y(N)$.

We first introduce the transposition t on matrices:

$$E^t_{ab} = (-1)^{[a]([b]+1)} \theta_a \theta_b E_{\bar{b}\bar{a}} \text{ with } \quad \theta_a = \pm 1,$$
$$\bar{a} = M+1-a \quad \text{for } 1 \leqslant a \leqslant M, \tag{3.1}$$
$$\bar{a} = 2M+N+1-a \quad \text{for } M+1 \leqslant a \leqslant M+N,$$

which satisfies

$$(AB)^t = B^t A^t. \tag{3.2}$$

Demanding the transposition to be of order 2 leads to the constraint

$$(-1)^{[a]}\, \theta_a \theta_{\bar{a}} = \theta_0 = \pm 1 \quad \forall \quad a. \tag{3.3}$$

Note that for superalgebras, one could ask the transposition to be of order 4 only. We will not consider this case in the following.

Let us stress that $\overline{a}$ has *not* the same meaning as in Sec. II: from now on, we will use this notation to denote (3.1). These new $\overline{a}$ satisfy $[a]=[\overline{a}]$.

Let us also note that there is a freedom on the definition of the transposition, $\theta_a \to (-1)^{[a]}\theta_a$: this freedom is fixed when imposing $\mathbb{I}^t=\mathbb{I}$. Remark also the useful identity

$$(-1)^{[a]([b]+1)}\theta_a\theta_b=(-1)^{[\overline{a}]([\overline{b}]+1)}\theta_{\overline{a}}\theta_{\overline{b}}. \tag{3.4}$$

Then, we define on $Y(M|N)$

$$\tau[T(u)]=\sum_{a,b}\tau[T^{ab}(u)]\,E_{ab}=\sum_{a,b}T^{ab}(-u)\,E^t_{ab}, \tag{3.5}$$

which reads for the super-Yangian generators

$$\tau(T^{ab}(u))=(-1)^{[a]([b]+1)}\theta_a\theta_b\;T^{\overline{b}\overline{a}}(-u). \tag{3.6}$$

Property 3.1: τ is an algebra automorphism for $Y(M|2n)$ and $Y(2m|N)$ only.
In that case, one must choose $\theta_0=+1$ for $Y(M|2n)$ and $\theta_0=-1$ for $Y(2m|N)$.

Proof: Considering subalgebras mentioned in Property 2.1, one can see that τ acts as an automorphism of $Y(M)$ of the type defined in Ref. 14, with $\theta_a\theta_{\overline{a}}=\theta_0$, and an automorphism of $Y(N)$ with $\theta_a\theta_{\overline{a}}=-\theta_0$. Using the results of Ref. 14, where it is proved that when M is odd, one must have $\theta_0=+1$ in $Y(M)$, one immediately concludes that we cannot have MN odd, and that the values for θ_0 are the ones given in the property.

Then, it is a simple matter of calculation to show that τ is an automorphism of the superalgebra $Y(M|N)$:

$$\tau([T^{ab}(u),T^{cd}(v)\})=[\tau(T^{ab}(u)),\tau(T^{cd}(v))\}. \tag{3.7}$$

■

One then defines in $Y(M|N)$ (we take MN even):

$$S(u)=T(u)\,\tau[T(u)]=\sum_{a,b=1}^{M+N}S^{ab}(u)E_{ab}=\mathbb{I}+\sum_{a,b=1}^{M+N}\sum_{n>0}u^{-n}S^{ab}_{(n)}E_{ab}, \tag{3.8}$$

$$S^{ab}_{(n)}=\sum_{c=1}^{M+N}\sum_{p=0}^{n}(-1)^p(-1)^{[c]([b]+1)}\theta_c\theta_b T^{ac}_{(n-p)}T^{\overline{b}\overline{c}}_{(p)}, \tag{3.9}$$

$$S^{ab}(u)=\sum_{c=1}^{M+N}(-1)^{[c]([b]+1)}\theta_c\theta_b T^{ac}(u)T^{\overline{b}\overline{c}}(-u). \tag{3.10}$$

$S(u)$ defines a subalgebra of the super-Yangian:

Theorem 3.2: *$S(u)$ obey the following relations:*

$$R_{12}(u-v)\,S_1(u)\,R'_{12}(u+v)\,S_2(v)=S_2(v)\,R'_{12}(u+v)\,S_1(u)\,R_{12}(u-v), \tag{3.11}$$

$$\tau(S(u))=S(u)+\frac{\theta_0}{2u}(S(u)-S(-u)), \tag{3.12}$$

where $R(x)$ is the super-Yangian R-matrix,

$$R'(x)=\mathbb{I}+\frac{1}{x}Q=R^{t_1}(-x) \quad with \quad Q=P^{t_1}, \tag{3.13}$$

and t_1 is the transposition (3.1) in the first space. These two relations uniquely define a subalgebra $Y(M|N)^\tau$ in the super-Yangian.

Proof: One starts with the relation (2.10) and applies the transposition t_1 and the sign operation $(u,v)\to(-u,-v)$ to get

$$\tau[T_1(u)]R'_{12}(u+v)T_2(v)=T_2(v)R'_{12}(u+v)\tau[T_1(u)]. \tag{3.14}$$

A direct calculation shows that

$$P\,Q=Q\,P=\theta_0 Q;\quad P^2=\mathbb{I} \text{ and } \quad Q^2=(M-N)Q. \tag{3.15}$$

Thus, applying $P(.)P$ on (3.14) leads to (after the exchange $u\leftrightarrow v$)

$$T_1(u)R'_{12}(u+v)\tau[T_2(v)]=\tau[T_2(v)]R'_{12}(u+v)T_1(u). \tag{3.16}$$

Finally, applying once again the transposition t_1 and $(u,v)\leftrightarrow(-u,-v)$, we obtain

$$R_{12}(u-v)\tau[T_1(u)]\tau[T_2(v)]=\tau[T_2(v)]\tau[T_1(u)]R_{12}(u-v), \tag{3.17}$$

which is another way to prove that τ is an automorphism. A simple calculation using (2.10), (3.14), (3.16) and (3.17) shows then that (3.11) is satisfied.

The second relation is also proved directly:

$$(\tau[S(u)])^{ab}=\sum_{c=1}^{M+N}(-1)^{[a]([b]+1)+[c]([a]+1)}\theta_a\theta_b\theta_{\bar{a}}\theta_{\bar{c}}T^{\bar{b}\bar{c}}(-u)T^{a\bar{c}}(u) \tag{3.18}$$

$$=S(u)+\sum_{c=1}^{M+N}(-1)^{[a]([b]+[c])}\theta_b\theta_c[T^{\bar{b}\bar{c}}(-u),T^{a\bar{c}}(u)\} \tag{3.19}$$

$$=\left(S(u)+\frac{\theta_0}{2u}(S(u)-S(-u))\right)^{ab}, \tag{3.20}$$

where, in the last step, we have used the graded commutator (2.12).

Conversely, let us start with an abstract algebra $\mathcal{A}$ whose generators $\sigma^{ab}_{(n)}$ obey (3.11) and (3.12). There is an obvious surjective morphism j from $\mathcal{A}$ to $Y(M|N)^\tau$. Thus, it remains to show that this morphism is injective. We follow the argumentation done in Ref. 15 for the case of (non-super) twisted Yangians.

We first introduce a filtration on $Y(M|N)$ induced by

$$\deg(T^{ab}_{(p)})=p \quad \text{and} \quad \deg(XY)=\deg(X)\deg(Y),\ \ \forall X,Y\in Y(M|N). \tag{3.21}$$

The graded algebra $grY(M|N)$ is defined as usual by

$$Y_p(M|N)=\{X\in Y(M|N),\quad \text{with}\quad \deg(X)\leqslant p\};\ \ p>0, \tag{3.22}$$

$$Y_0(M|N)=\mathbb{C};\ \ gr_0Y(M|N)=\mathbb{C}, \tag{3.23}$$

$$gr_pY(M|N)=Y_p(M|N)\,/\,Y_{p-1}(M|N);\ \ p>0, \tag{3.24}$$

$$grY(M|N)=\oplus_{p\geqslant 0}gr_pY(M|N). \tag{3.25}$$

Since for $X \in gr_p Y(M|N)$ and $Y \in gr_q Y(M|N)$, we have $[X,Y\} \in gr_{p+q-1} Y(M|N)$, we deduce that $grY(M|N)$ is commutative. (During this proof, and to avoid confusion with the gradation deg, we will write commutative and commutator where one should has written $\mathbb{Z}_2$-graded commutative and $\mathbb{Z}_2$-graded commutator.) The same is true for $grY(M|N)^\tau$; here the filtration is induced by the $Y(M|N)$ one.

Similarly, on $\mathcal{A}$, we introduce a filtration given by

$$\deg(\sigma_{(n)}^{ab}) = n. \tag{3.26}$$

This makes $gr\mathcal{A}$ a commutative algebra, for the same reasons as above. Moreover, since the morphism j preserves the filtration, it is enough to show that the induced morphism $\overline{j}$ between graded algebras is injective.

Let $\overline{T}_{(p)}^{ab}$ and $\overline{S}_{(p)}^{ab}$ be the image of $T_{(p)}^{ab}$ and $S_{(p)}^{ab}$ in $grY(M|N)^\tau$. The expression (3.9) is still valid for the elements of $grY(M|N)^\tau$, so that we deduce

$$\overline{S}_{(p)}^{ab} = \overline{T}_{(p)}^{ab} + (-1)^p (-1)^{[a]([b]+1)} \theta_a \theta_b \overline{T}_{(p)}^{\overline{b}\overline{a}} = (-1)^p (-1)^{[a]([b]+1)} \theta_a \theta_b \overline{S}_{(p)}^{\overline{b}\overline{a}}. \tag{3.27}$$

In Ref. 12, it has been proven that the generators $\overline{T}_{(p)}^{ab}$ are independent. [Strictly speaking, the proof is lacking in Ref. 12, but it can be done following the steps given in Ref. 15 for Yangians $Y(N)$.] Thus, we conclude that $grY(M|N)^\tau$ is isomorphic to the algebra of polynomials in the ($\mathbb{Z}_2$-graded) letters $x_{(p)}^{ab}$ submitted to the constraints (3.27).

Finally, the symmetry relation (3.12) in the algebra $gr\mathcal{A}$ just takes the form (3.27), so that $gr\mathcal{A}$ is also isomorphic to the algebra of polynomials in the ($\mathbb{Z}_2$-graded) letters $x_{(p)}^{ab}$ submitted to the constraints (3.27). Hence, $\overline{j}$ is injective. ■

Corollary 3.3 (PBW basis for $Y(M|N)^\tau$): Given an arbitrary linear order on the following set of generators (for $p=1,2,\ldots$),

$$\begin{gathered}
S_{(2p)}^{ij} \ \text{for } 1 \leqslant i,j \leqslant M \quad \text{and} \quad i+j \leqslant M+1, \\
S_{(2p+1)}^{ij} \ \text{for } 1 \leqslant i,j \leqslant M \quad \text{and} \quad i+j < M+1, \\
S_{(2p)}^{ij} \ \text{for } M+1 \leqslant i,j \leqslant M+2n \ \text{ and } \ i+j < 2M+2+2n, \\
S_{(2p+1)}^{ij} \ \text{for } M+1 \leqslant i,j \leqslant M+2n \ \text{ and } \ i+j \leqslant 2M+2+2n, \\
S_{(2p)}^{ij} \ \text{for } M+1 \leqslant i \leqslant M+2n \ \text{ and } \ 1 \leqslant j \leqslant M,
\end{gathered} \tag{3.28}$$

any element of $Y(M|2n)^\tau$ is uniquely written as a linear combination of the ordered monomials in these generators.

The same type of basis exists for $Y(2m|N)^\tau$ with an obvious exchange of M and N (and m and n).

Proof: It is a direct consequence of the proof of Theorem 3.2. Indeed, considering $grY(M|2n)^\tau$, it is sufficient to find a basis for it, i.e., for the algebra of polynomials in the ($\mathbb{Z}_2$-graded) letters $x_{(p)}^{ab}$ submitted to the constraints (3.27). From the property $a+b \leqslant M+1 \Leftrightarrow \overline{a}+\overline{b} \geqslant M+1$, $\overline{a}=b \Leftrightarrow a+b=M+1$ when $a,b \leqslant M$, and $a+b \leqslant M+n+2 \Leftrightarrow \overline{a}+\overline{b} \geqslant M+n+2$, $\overline{a}=b \Leftrightarrow a+b=M+n+2$ when $a,b \geqslant M+1$, an analysis of these constraints lead to the above basis. ■

Although several automorphisms τ can be defined (depending upon the choices for the θ's), they all lead to the same subalgebra $Y(M|N)^\tau$:

Property 3.4: All the θ_a dependence, but the value of θ_0, can be removed in the commutation relations of $Y(M|N)^\tau$.

Proof: We prove the property by exhibiting a basis in which the θ dependence has disappeared. We give this basis for the case $Y(M|2n)^{\tau}$ and $\theta_0=+1$, the other case being similar. When restricted to the bosonic part, it is the same basis as the one given in Ref. 14 for (bosonic) twisted Yangians.

For $Y^-(2n)$,

$$J^{ij}(u)=\theta^i\theta^j S^{ij}(u);\quad K^{ij}(u)=\theta^i S^{i,\bar{j}}(u);\quad \overline{K}^{ij}(u)=\theta^j S^{\bar{i},j}(u);\quad i,j=1,\ldots,n. \tag{3.29}$$

For $Y^+(M)$, the redefinition is the same as before, plus for the remaining generators which appear when $M=2m+1$ (we set $\tilde{m}=m+1$):

$$J_0(u)=\theta^{\tilde{m}} S^{\tilde{m}\tilde{m}}(u);\quad L^i(u)=\theta^i S^{\tilde{m},i}(u);\quad \overline{L}^i(u)=\theta^{\tilde{m}}\theta^i S^{i,\tilde{m}}(u);\quad i=1,\ldots,m. \tag{3.30}$$

This proves that the commutation relations among generators of $Y^-(2n)$ and those among $Y^+(M)$ are free from θ's in this basis. Commuting an element of $Y^-(2n)$ with one of $Y^+(M)$ provides the change of basis for the fermionic generators:

$$\begin{aligned} &F^{ai}(u)=\theta_a\theta_i S^{ai}(u),\quad \overline{F}^{ia}(u)=\theta_a\theta_i S^{ai}(u),\quad i=M+1,\ldots,M+n,\\ &G^{ai}(u)=\theta_a S^{\bar{ai}}(u),\quad \overline{G}^{ia}(u)=\theta_i S^{\bar{ai}}(u)\quad a=1,\ldots,M,\\ &H^i(u)=\theta_i S^{m+1,i}(u),\quad \overline{H}^i(u)=\theta_{m+1}\theta_i S^{i,m+1}(u),\quad \text{if } M=2m+1. \end{aligned} \tag{3.31}$$

All the $Y(M|2n)^+$-generators are expressible in terms of the generators (3.29)–(3.31) using the symmetry relation (3.12). Then, one can check that all the graded commutators in this basis are free from θ. ■

Using the isomorphism 2.2, one can focus on either one of the two cases given in Proposition 3.1. From now on, we will consider the case $Y(M|2n)$ and $\theta_0=+1$. Since it is only the value of θ_0 which is relevant for our study, we will use it to label the automorphism τ.

Definition 3.5: The twisted super-Yangian $Y(M|2n)^+\equiv Y(2n|M)^-$ is the subalgebra generated by $S(u)=T(u)\tau[T(u)]$, with τ given in (3.6) and

$$\begin{aligned} &\theta_a=1\quad for\ 1\leqslant a\leqslant M,\\ &\theta_a=sg\left(\frac{2M+2n+1}{2}-a\right)\quad for\ M+1\leqslant a\leqslant M+2n. \end{aligned} \tag{3.32}$$

B. Few properties of $Y(M|2n)^+$

Proposition 3.6: The relation (3.11) is equivalent to the following commutator:

$$\begin{aligned} [S_1(u),S_2(v)]=&\frac{1}{u-v}(P_{12}S_1(u)S_2(v)-S_2(v)S_1(u)P_{12})-\frac{1}{u+v}(S_1(u)Q_{12}S_2(v)\\ &-S_2(v)Q_{12}S_1(u))+\frac{1}{u^2-v^2}(P_{12}S_1(u)Q_{12}S_2(v)-S_2(v)Q_{12}S_1(u)P_{12}) \end{aligned} \tag{3.33}$$

and also to

$$
\begin{aligned}
[S^{ab}(u),S^{cd}(v)\}=&\frac{(-1)^{([a]+[b])[c]}}{u-v}(-1)^{[a][b]}(S^{cb}(u)S^{ad}(v)-S^{cb}(v)S^{ad}(u))\\
&-\frac{(-1)^{([a]+[b])[c]}}{u+v}((-1)^{[a][c]}\theta_b\theta_{\bar{c}}S^{a\bar{c}}(u)S^{\bar{b}d}(v)\\
&-(-1)^{[b][d]}\theta_{\bar{a}}\theta_d S^{c\bar{a}}(v)S^{\bar{d}b}(u))\\
&+\frac{(-1)^{([a]+[b])[c]}}{u^2-v^2}(-1)^{[a]}\theta_a\theta_b(S^{c\bar{a}}(u)S^{\bar{b}d}(v)\\
&-S^{c\bar{a}}(v)S^{\bar{b}d}(u)).
\end{aligned}
\tag{3.34}
$$

Proof: Equation (3.33) follows from a direct calculation using (3.11), (2.11) and (3.13). ■

As an obvious consequence, we get the following.

Corollary 3.7: The twisted super-Yangian $Y(M|2n)^+$ *contains* osp$(M|2n)$ *as Lie subsuperalgebra. It is generated by*

$$
S^{ab}_{(1)}=T^{ab}_{(1)}-(-1)^{[a]([b]+1)}\theta_a\theta_b T^{\bar{b}\bar{a}}_{(1)} \quad a,b=1,\ldots,M+2n, \tag{3.35}
$$

which obey

$$
S^{ab}_{(1)}=-(-1)^{[a]([b]+1)}\theta_a\theta_b S^{\bar{b}\bar{a}}_{(1)}, \tag{3.36}
$$

and defines a morphism of algebra $\mathcal{U}[\text{osp}(M|2n)]\to Y(M|2n)^+$.

The action of the osp$(M|2n)$ *generators on the twisted Yangian is given by*

$$
\begin{aligned}
[S^{ab}_{(1)},S^{cd}(v)\}=&(-1)^{([a]+[b])[c]}\{(-1)^{[a][b]}(\delta_{cb}S^{ad}(v)-\delta_{ad}S^{cb}(v))\\
&-\theta_{\bar{a}}\theta_b(\delta_{a\bar{c}}S^{\bar{b}d}(v)-\delta_{\bar{d}b}S^{c\bar{a}}(v))\}.
\end{aligned}
\tag{3.37}
$$

Proof: Expanding $(u\pm v)^{-1}=u^{-1}(1\mp vu^{-1}+\cdots)$ and taking the coefficient of $u^{-1}v^{-1}$ in (3.33) leads to

$$
[S_{1(1)},S_{2(1)}\}=P_{12}S_{2(1)}-S_{2(1)}P_{12}-Q_{12}S_{2(1)}+S_{2(1)}Q_{12}, \tag{3.38}
$$

where the subscript (1) refers to the coefficient of u^{-1} and v^{-1}, while the indices 1,2 label the auxiliary spaces. The symmetry relation projected on the u^{-1} term reads

$$
S^t_{(1)}=-S_{(1)}. \tag{3.39}
$$

Equations (3.38) and (3.39) are just the defining relations of osp$(M|2n)$.

Starting now from (3.34) and taking the coefficient of u^{-1} gives the relation (3.37). Note that taking the coefficient of v^{-1} in this last relation gives again the commutation relations of osp$(M|2n)$. ■

Let us denote the osp$(M|2n)$ generators by J^{ab} and gather them in the matrix

$$
F=\sum_{a,b=1}^{M+N}J^{ab}F_{ab} \quad \text{with} \quad F_{ab}=E_{ab}-(-1)^{[a]([b]+1)}\theta_a\theta_b E^{\bar{b}\bar{a}}. \tag{3.40}
$$

It satisfies

$$
\begin{aligned}
F^t&=-F,\\
[F_1,F_2\}&=P_{12}F_2-F_2P_{12}+F_2Q_{12}-Q_{12}F_2,
\end{aligned}
\tag{3.41}
$$

where t is the transposition (3.1).

Property 3.8: The following map defines an algebra homomorphism:

$$\begin{aligned} &Y(M|2n)^+ \to \mathcal{U}[\mathrm{osp}(M|2n)], \\ &S(u) \to \mathbb{F}(u) = \mathbb{I} + \frac{1}{u+\frac{1}{2}} F. \end{aligned} \tag{3.42}$$

Proof: We have to prove that $\mathbb{F}$ obeys to the relations (3.11) and (3.12). A direct calculation shows

$$\mathbb{F}^t(-u) = \mathbb{I} + \frac{1}{u-\frac{1}{2}} F = \mathbb{F}(u) + \frac{1}{2u}(\mathbb{F}(u) - \mathbb{F}(-u)).$$

Moreover, using (3.15), the commutator (3.41) and the relations

$$\begin{aligned} &P_{12}F_2 = F_1 P_{12} \Rightarrow Q_{12}F_2 = -Q_{12}F_1, \\ &P_{12}F_1 = F_2 P_{12} \Rightarrow F_1 Q_{12} = -F_2 Q_{12}, \end{aligned} \tag{3.43}$$

one proves that we have

$$\begin{aligned} [\mathbb{F}_1(u), \mathbb{F}_2(v)\} = &\frac{1}{u-v}(P_{12}\mathbb{F}_1(u)\mathbb{F}_2(v) - \mathbb{F}_2(v)\mathbb{F}_1(u)P_{12}) - \frac{1}{u+v}(\mathbb{F}_1(u)Q_{12}\mathbb{F}_2(v) \\ &- \mathbb{F}_2(v)Q_{12}\mathbb{F}_1(u)) + \frac{1}{u^2-v^2}(P_{12}\mathbb{F}_1(u)Q_{12}\mathbb{F}_2(v) - \mathbb{F}_2(v)Q_{12}\mathbb{F}_1(u)P_{12}). \end{aligned}$$

■

The relation between $\mathrm{osp}(M|2n)$ and $Y(M|2n)^+$ also reveals in the following.

Property 3.9: $Y(M|2n)^+$ is a deformation of $\mathcal{U}(\mathrm{osp}(M|2n)[x])$, the (positive modes) loop algebra based on $\mathrm{osp}(M|2n)$.

Proof: We start with $S(u) = \mathbb{I} + s(u)$, and make a change of basis $\tilde{s}(u) = \hbar^{-1} s(u/\hbar)$. In this basis, the commutation relations read

$$\begin{aligned} [\tilde{s}_1(u), \tilde{s}_2(v)\} = &\frac{1}{u-v}(P_{12}\tilde{s}_1(u) + P_{12}\tilde{s}_2(v) - \tilde{s}_1(u)P_{12} - \tilde{s}_2(v)P_{12}) - \frac{1}{u+v}(\tilde{s}_1(u)Q_{12} + Q_{12}\tilde{s}_2(v) \\ &- Q_{12}\tilde{s}_1(u) - \tilde{s}_2(v)Q_{12}) + \frac{\hbar}{u-v}(P_{12}\tilde{s}_1(u)\tilde{s}_2(v) - \tilde{s}_2(v)\tilde{s}_1(u)P_{12}) \\ &- \frac{\hbar}{u+v}(\tilde{s}_1(u)Q_{12}\tilde{s}_2(v) - \tilde{s}_2(v)Q_{12}\tilde{s}_1(u)) + \frac{\hbar}{u^2-v^2}(P_{12}\tilde{s}_1(u)Q_{12} + P_{12}\tilde{s}_2(v) \\ &- Q_{12}\tilde{s}_1(u)P_{12} - \tilde{s}_2(v)P_{12}) + \frac{\hbar^2}{u^2-v^2}(P_{12}\tilde{s}_1(u)Q_{12}\tilde{s}_2(v) - \tilde{s}_2(v)Q_{12}\tilde{s}_1(u)P_{12}). \end{aligned}$$

For $\hbar \neq 0$ all the algebras $Y_\hbar(M|2n)^+$ are isomorphic, while in the limit $\hbar \to 0$, $Y_{\hbar=0}(M|2n)^+$ reduces to $\mathcal{U}(\mathrm{osp}(M|2n)[x])$. ■

Note also the following isomorphism.

Property 3.10 (Automorphism of $Y(M|2n)^+$): The transformations

$$S(u) \to g(u)\, S(u) \quad \textit{with } g(u) \textit{ even } \mathbb{C}\textit{-function} \tag{3.44}$$

are automorphisms of $Y(M|2n)^+$.

Proof: Multiplying (3.11) by $g(u)g(v)$ shows that it is invariant under the transformation (3.44), for any function g. The symmetry relation (3.12) is preserved for $g(u)$ even only. ■

There is another of type of automorphism that we will need when looking at the representations of twisted super-Yangians:

Definition 3.11 (# involution): For any index $i=1,\ldots,M+N$, *we define* i' *by*

$$i'=\begin{cases}\tilde{m}+1 & \text{if} \quad i=m,\\ m & \text{if} \quad i=\tilde{m}+1 \qquad \text{where} \quad m=\left[\frac{M}{2}\right] \quad \text{and} \quad \tilde{m}=\left[\frac{M+1}{2}\right]\\ i & \text{otherwise}.\end{cases} \tag{3.45}$$

The # involution acts on $S(u)$ *by*

$$S^{ij}_{\#}(u)=S^{i'j'}(u) \tag{3.46}$$

and is an order 2 automorphism of $Y(M|2n)^+$.

Proof: Obvious direct calculation from the relations (3.34) and (3.12). ■

For the Hopf structure, and mimicking again the case of twisted Yangians, one can show the following.

Property 3.12: $Y(M|2n)^+$ *is a left coideal of* $Y(M|2n)$*:*

$$\Delta(Y(M|2n)^+)\subset Y(M|2n)\otimes Y(M|2n)^+. \tag{3.47}$$

More precisely,

$$\Delta(S^{ab}_{(p)})=\sum_{y=0}^{p}\sum_{q=0}^{y}\sum_{d,e=1}^{M+2n}(-1)^q(-1)^{[d]([e]+[b])}\theta_b\theta_e T^{ad}_{(y-q)}\overline{T^{be}_{(q)}}\otimes S^{de}_{(y)},$$

$$\Delta[S^{ab}(u)]=\sum_{d,e=1}^{M+2n}(-1)^{[d]([e]+[b])}\theta_b\theta_e T^{ad}(u)\overline{T^{be}}(-u)\otimes S^{de}(u).$$

Proof: Direct calculation using (2.14) and (3.9). ■

C. Subalgebras of $Y(M|2n)^+$

Property 3.13: The twisted super-Yangian $Y(M|N)^+$ *contains as subalgebras* $Y(M)^+$, $Y(N)^-$ *and* $\mathrm{osp}(M|N)$.

Proof: A direct examination on the commutator (2.12) and the symmetry relation (3.12) shows that $S^{ab}(u)$ with $a,b=1,\ldots,M$ (resp. $a,b=M+1,\ldots,M+N$) generates the twisted Yangian $Y(M)^+$ [resp. $Y(N)^-$]. The last inclusion has been proved in Corollary 3.7. ■

Property 3.14: As algebra embeddings, we have

$$Y(1|2)^+\subset Y(2m+1|2n)^+ \quad \text{and} \quad Y(2|2)^+\subset Y(2m|2n)^+. \tag{3.48}$$

Proof: We consider the generators $S^{ij}(u)$, with $i,j=m+1,2m+n+1,2m+n+2$ in $Y(2m+1|2n)^+$ and $S^{ij}(u)$, with $i,j=m,m+1,2m+n,2m+n+1$ in $Y(2m|2n)^-$: they obey the commutation and symmetry relations of $Y(1|2)^+$ and $Y(2|2)^+$, respectively. ■

Note that there is no regular embedding of $Y(1|2)^+$ into $Y(2m|2n)^+$. The circumstances are here different from both simple superalgebras and non-super twisted Yangians cases: in the first case, it always exists a regular $\mathrm{osp}(1|2)$ embedding, and in the second case, one can always construct a regular $Y(2)^{\pm}$ embedding in the twisted Yangian $Y(M)^{\pm}$. It is the symmetry relation which causes this unusual situation.

Property 3.15: As algebra embedding, we have

$$Y(2m|2n)^+ \subset Y(2m+1|2n)^+. \tag{3.49}$$

Let us stress, however, that $Y(2m|2n)^+$ is not a Hopf coideal of $Y(2m+1|2n)^+$.

The same results apply for $Y(2m)^+$ and $Y(2m+1)^+$.

Proof: Let $s^{ij}(u)$ be the generators of $Y(2m+1|2n)^+$. We set $M=2m+1$ and introduce

$$\sigma^{ij}(u)=s^{ij}(u) \quad \text{for } 1\leqslant i,j\leqslant m \text{ and } M+1\leqslant i,j\leqslant M+n+1,$$

$$\sigma_{i,j}(u)=s^{i-1,j-1}(u) \quad \text{for } m+2\leqslant i,j\leqslant M \text{ and } M+n+2\leqslant i,j\leqslant M+2n,$$

$$\sigma^{ij}(u)=s^{i-1,j}(u) \quad \text{for } \begin{cases} 1\leqslant j\leqslant m \text{ or } M+1\leqslant j\leqslant M+n+1, \\ m+2\leqslant i\leqslant M \text{ or } M+n+2\leqslant i\leqslant M+2n, \end{cases}$$

$$\sigma^{ij}(u)=s^{i,j-1}(u) \quad \text{for } \begin{cases} 1\leqslant i\leqslant m \text{ or } M+1\leqslant i\leqslant M+n+1, \\ m+2\leqslant j\leqslant M \text{ or } M+n+2\leqslant j\leqslant M+2n. \end{cases}$$

We prove that the generators $\sigma^{ij}(u)$ generate $Y(2m|2n)^+$. We denote by $x\to\overline{x}$ the "bar" operator introduced in (3.6) for $Y(2m+1|2n)^+$, and by $x\to\tilde{x}$ this "bar" operator for $Y(2m|2n)^+$. In the same way, we call τ and θ (resp. $\tilde{\tau}$ and $\tilde{\theta}$) the corresponding operations in $Y(2m+1|2n)^+$ [resp. $Y(2m|2n)^+$]. It is easy to see that

$$\overline{\imath}=\tilde{\imath}, \quad \theta_i=\tilde{\theta}_i, \quad \text{for } i\leqslant m \text{ and } M+1\leqslant i\leqslant M+n+1,$$

$$\overline{\imath-1}=\tilde{\imath}, \qquad \theta_{i-1}=\tilde{\theta}_i, \quad \text{for } m+2\leqslant i\leqslant M \text{ and } M+n+2\leqslant i,j\leqslant M+2n,$$

so that the action of τ on $s(u)$ is equivalent to the action of $\tilde{\tau}$ on $\sigma(u)$. It also proves that the symmetry relation of $s(u)$ [coming from $Y(2m+1|2n)^+$] implies the symmetry relation for $\sigma(u)$ [as $Y(2m|2n)^+$ generator].

In the same way, one shows, starting with the commutation relations of $s(u)$, that the commutation relations of $\sigma(u)$ are those of $Y(2m|2n)^+$.

Finally, computing $\Delta\sigma^{ij}(u)$ as it is induced from the $Y(2m+1|2n)^+$ coproduct does not lead to the coproduct formula for $Y(2m|2n)^+$. ■

IV. FINITE-DIMENSIONAL IRREDUCIBLE REPRESENTATIONS OF $Y(M|2n)^+$

We study here the finite-dimensional irreducible representations of $Y(M|2n)^+$ starting from $Y(M|2n)$ in the same way those of $Y(M)^\pm$ have been studied starting from $Y(M)$.[16]

As a shorthand notation, we note irreps for irreducible representations.

A. Generalities

Definition 4.1 (Highest weight vector): Let $\mathcal{M}$ be a module of $Y(M|2n)^+$. A nonzero vector $\xi\in\mathcal{M}$ is called highest weight if it satisfies

$$S^{ij}(u)\xi=0 \quad \textit{for } (i,j)\in\Phi^+, \tag{4.1}$$

$$S^{ii}(u)\xi=\mu_i(u)\xi \quad \textit{for } i=1,\ldots,M+2n, \tag{4.2}$$

for some formal series $\mu_i(u)\in 1+u^{-1}\mathbb{C}[[u^{-1}]]$. The set $\mu(u)\equiv(\mu_1(u),\ldots,\mu_{M+2n}(u))$ is the highest weight of $\mathcal{M}$.

Remark 1: Due to the symmetry relation (3.12), some of the relations (4.1) are redundant, and one could reduce Φ^+: we keep it as it is to make the comparison with the $Y(M|N)$ case.

Note also that, in the basis of Ref. 12, the symmetry relation would have led to $S^{ij}(u)\xi=0$, $\forall i\neq j$, hence the present choice for the positive root system.

Remark 2: The symmetry relation also implies for the highest weight

$$\mu_{\bar{a}}(u)=\frac{1}{2u}\mu_a(u)+\frac{2u-1}{2u}\mu_a(-u), \tag{4.3}$$

so that, in the $Y(2m+1|2n)^+$ case, $\mu_{m+1}(u)$ is an even function of u.

Definition 4.2 (Highest weight representations): A representation V of the twisted super-Yangian $Y(M|2n)^+$ is called highest weight if it is generated by a highest weight vector ξ. If $\mu(u)$ is the highest weight of ξ, we will use the notation $V[\mu(u)]$ for V.

Theorem 4.3: *Every finite-dimensional irrep V of $Y(M|2n)^+$ is highest weight. Moreover, V contains a unique (up to scalar multiples) highest weight vector.*

Proof: We define

$$V_+=\{v\in V|S^{ab}_{(p)}v=0,\ \forall(a,b)\in\Phi^+ \ \text{ and } \ p>0\}. \tag{4.4}$$

We first prove that V_+ is not empty.

Let $m\equiv[M/2]$. The generators $S^{11}_{(1)},\ldots,S^{mm}_{(1)},S^{M+1,M+1}_{(1)},\ldots,S^{M+n,M+n}_{(1)}$ form a Cartan subalgebra of $\mathrm{Osp}(M|2n)$, so there exists at least one eigenvector v common to all $S^{aa}_{(1)}$ and with eigenvalue $\mu=(\mu^{(1)}_1,\ldots,\mu^{(1)}_{M+2n})$.

If $v\in V_+$, then we have $V_+\neq\varnothing$. If $v\notin V_+$, by applying $S^{ab}_{(p)},(a,b)\in\Phi^+$, to v we obtain an other common eigenvector of the $S^{aa}_{(1)}$ with eigenvalue $\mu+\omega$, where ω is a $\mathbb{Z}_{>0}$-linear combination of the positive roots. As V is finite dimensional, repeated applications of generators $S^{ab}_{(n)}$, $(a,b)\in\Phi^+$, $n>0$, will lead to a nonvanishing vector $v_+\in V$ such that

$$S^{ab}_{(p)}v_+=0\ \forall(a,b)\in\Phi^+,\ \ p>0, \tag{4.5}$$

$$S^{aa}_{(1)}v_+=\lambda^{(1)}v_+\ \forall a. \tag{4.6}$$

So $v_+\in V_+$ and V_+ contains at least one nonzero element.

One defines

$$\mathcal{T}_\pm=\{S^{ab}(u),\forall(a,b)\in\Phi^\pm\} \tag{4.7}$$

and L (resp. R) the left (resp. right) ideal generated by $\mathcal{T}_+$ (resp. $\mathcal{T}_-$). We also introduce the subalgebra

$$\mathcal{Y}_0=\{y\in Y(M|2n)^+,\ \text{such that}\ \ [S^{aa}_{(1)},y]=0\ \forall a=1,\ldots,M+2n\} \tag{4.8}$$

and correspondingly

$$L_0=\mathcal{Y}_0\cap L\quad\text{and}\quad R_0=\mathcal{Y}_0\cap R. \tag{4.9}$$

Using the PBW Theorem 3.3, one shows that $L_0=R_0\equiv I_0$ is a two-sided ideal so that $\mathcal{G}=\mathcal{Y}_0/I_0$ is an algebra. From the commutation relations (3.34), one gets that $[S^{aa}(u),S^{bb}(v)]\in I_0$, i.e., $\mathcal{G}$ is a commutative algebra.

By construction, $\forall v\in V_+$ and $i\in I_0$, one has $iv=0$, so that V_+ is a $\mathcal{G}$-module. Since $\mathcal{G}$ is commutative, there exists a nonzero common eigenvector $\xi\in V_+$. Now, let $V'=\mathcal{U}(\mathcal{T}_-)\xi$: it is a nonzero submodule of V, and since V is supposed irreducible, it must equal V. Thus, ξ is a highest weight vector of V.

Finally, if there is another highest weight vector ξ', the above construction ensures that $V=\mathcal{U}(\mathcal{T}_-)\xi=\mathcal{U}(\mathcal{T}_-)\xi'$ which is possible only for ξ and ξ' proportional. ■

Theorem 4.4: *(Necessary conditions for finite-dimensional irreps) If the irreducible highest weight representation $V[\mu(u)]$ of $Y(M|2n)^+$ is finite dimensional, then the following relations hold*:

$$\frac{\mu_i(u)}{\mu_{i+1}(u)}=\frac{P_{i+1}(u+1)}{P_{i+1}(u)}\quad \textit{for}\quad \begin{cases} m+2\leqslant i\leqslant M-1,\\ M+n+1\leqslant i\leqslant M+2n-1, \end{cases} \tag{4.10}$$

$$\frac{\mu_{M+n+1}(-u)}{\mu_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)P_{M+n+1}(-u)}{P_{M+n+1}(u)P_{M+n+1}(1-u)}. \tag{4.11}$$

If $M=2m+1$, we have also the relation

$$\gamma(u)\frac{\mu_{m+1}(u)}{\mu_{m+2}(u)}=\frac{P_{m+1}(u+1)}{P_{m+1}(u)}, \quad \textit{where} \quad \gamma(u) \quad \textit{is either} \quad 1 \quad \textit{or} \quad \frac{2u}{2u+1}. \tag{4.12}$$

If $M=2$, we have the additional condition

$$\frac{\mu_2(-u)}{\mu_2(u)}=\frac{P(u+1)P(-u)}{P(u)P(1-u)}\frac{(u+\gamma)(2u-1)}{(u-\gamma)(2u+1)}, \quad \textit{with} \quad P(-\gamma)P(\gamma+1)\neq 0. \tag{4.13}$$

Finally, for $M=2m>2$, we have the relations

$$\frac{\mu^o_{m+1}(u)}{\mu_{m+2}(u)}=\frac{P_{m+2}(u+1)}{P_{m+2}(u)},$$

$$\gamma(u)\frac{\mu^o_{m+1}(-u)}{\mu^o_{m+1}(u)}=\frac{P_{m+1}(u+1)P_{m+1}(-u)}{P_{m+1}(u)P_{m+1}(1-u)}, \tag{4.14}$$

where $\gamma(u)$ is either 1 or $(2u-1)/(2u+1)$, and $\mu^o_{m+1}(u)$ is either $\mu_{m+1}(u)$ or $\mu^{\#}_{m+1}(u)$. We have introduced $\mu^{\#}_{m+1}(u)$, which is deduced from $\mu_{m+1}(u)$ by the action of the # automorphism (see Definition 3.11 and Ref. 16 for more details).

Proof: It is a direct consequence of the classification of finite-dimensional irreps for the algebras $Y(M)^{\pm}$ done in Ref. 16. Since $Y(M)^{+}$ and $Y(2n)^{-}$ are subalgebras of $Y(M|2n)^{+}$, starting with an $Y(M|2n)^{+}$-irrep with highest weight ξ and considering the cyclic span of ξ with each of these subalgebras leads to the result. ■

B. Finite-dimensional irreps of $Y(1|2)^{+}$

Let $V[\mu(u)]$ be an irrep of $Y(1|2)^{+}$ with highest weight $\mu(u)\equiv(\mu_1(u),\mu_2(u),\mu_3(u))$. From the symmetry relation (4.3) we obtain that $\mu_1(u)$ is an even series in u^{-1} and $\mu_2(u)$ can be deduced from $\mu_3(u)$.

Property 4.5: If $V[\mu_1(u),\mu_3(u)]$ is finite dimensional, then there exists a formal even series $\psi(u)$ in u^{-1} such that

$$\psi(u)\mu_1(u)=(1-\alpha_1^2u^{-2})\cdots(1-\alpha_k^2u^{-2}), \tag{4.15}$$

$$\psi(u)\mu_3(u)=(1-\alpha_1u^{-1})\cdots(1-\alpha_ku^{-1})(1+\beta_1u^{-1})\ldots(1+\beta_ku^{-1}). \tag{4.16}$$

Proof: Let ξ be the highest weight vector of $V[\mu(u)]$.

Under $(S^{22}_{(1)},S^{33}_{(1)})$, $S^{32}_{(l_1)}\cdots S^{32}_{(l_s)}S^{31}_{(p_1)}\cdots S^{31}_{(p_r)}\xi$ has weight $(\mu_2^{(1)}+2s+r,\mu_3^{(1)}-2s-r)$ whereas $S^{31}_{(i)}\xi$ has weight $(\mu_2^{(1)}+1,\mu_3^{(1)}-1)$. So $S^{31}_{(i)}\xi$ can only be written as a linear combination of vectors $S^{31}_{(j)}\xi$. Let k be the minimum non-negative integer such that $S^{31}_{(k+1)}\xi$ is a linear combination of the vectors $\xi_1\equiv S^{31}_{(1)}\xi,\ldots,\xi_k\equiv S^{31}_{(k)}\xi$ (such k exists because $V[\mu(u)]$ is finite dimensional).

We will prove that for any vector $S^{31}_{(r)}\xi$ with $r\geqslant k+1$ we have

$$S^{31}_{(r)}\xi=a_1^{(r)}\xi_1+\cdots+a_k^{(r)}\xi_k, \tag{4.17}$$

where the $a_i^{(r)}$ are complex numbers.

Equation (4.17) is true for $r=k+1$ by definition of k. Taking $i=k=l=3$, $j=1$ in the commutation relation and exchanging u and v, we get

$$[S^{33}(u),S^{31}(v)]=-\frac{1}{u-v}(S^{31}(v)S^{33}(u)-S^{31}(u)S^{33}(v))-\frac{1}{u+v}S^{32}(u)S^{21}(v)$$
$$+\frac{1}{u^2-v^2}S^{32}(u)S^{13}(v)+\frac{-1+u-v}{u^2-v^2}S^{32}(v)S^{13}(u). \tag{4.18}$$

We multiply by (u^2-v^2) and take the coefficient at u^0v^{-p} $(p\geqslant 1)$. Using the fact that $S^{21}(u)\xi=S^{13}(u)\xi=0$ we obtain

$$S^{33}_{(2)}S^{31}_{(p)}\xi=-S^{31}_{(p+1)}\xi+S^{31}_{(1)}S^{33}_{(p)}\xi+S^{31}_{(p)}(S^{33}_{(2)}-S^{33}_{(1)})\xi. \tag{4.19}$$

For $i=1,\ldots,k-1$ (4.19) gives

$$S^{33}_{(2)}\xi_i=-\xi_{i+1}+\mu_3^{(i)}\xi_1+(\mu_3^{(2)}-\mu_3^{(1)})\xi_i\,. \tag{4.20}$$

For $i=k$, using $S^{31}_{(k+1)}\xi=a_1^{(k+1)}\xi_1+\cdots+a_k^{(k+1)}\xi_k$ in (4.19) gives

$$S^{33}_{(2)}\xi_k=-(a_1^{(k+1)}\xi_1+\cdots+a_k^{(k+1)}\xi_k)+\mu_3^{(k)}\xi_1+(\mu_3^{(2)}-\mu_3^{(1)})\xi_k\,. \tag{4.21}$$

So $\forall i\in\{1,\ldots,k\}$, $S^{33}_{(2)}\xi_i$ is a linear combination of the $\{\xi_j\}_{j=1,\ldots,k}$.

Now suppose that $\forall r\in\{k+1,\ldots,p\}$ (where $p\geqslant k+1$), Eq. (4.17) holds. We then have

$$S^{31}_{(p+1)}\xi=-S^{33}_{(2)}S^{31}_{(p)}+\mu_3^{(p)}\xi_1+(\mu_3^{(2)}-\mu_3^{(1)})S^{31}_{(p)}\xi$$
$$=-\sum_{i=1}^{k}(a_i^{(p)}S^{33}_{(2)}\xi_i)+\mu_3^{(p)}\xi_1+(\mu_3^{(2)}-\mu_3^{(1)})\sum_{i=1}^{k}(a_i^{(p)}\xi_i), \tag{4.22}$$

so $S^{31}_{(p+1)}\xi$ is a linear combination of the $\{\xi_j\}_{j=1,\ldots,k}$ and Eq. (4.17) is proved by induction on p. We can therefore write

$$S^{31}(u)\xi=a_1(u)\xi_1+\cdots+a_k(u)\xi_k\,, \tag{4.23}$$

where $a_i(u)=u^{-i}+\Sigma_{s=k+1}^{\infty}a_i^{(s)}u^{-s}$.

We can rewrite (4.19) as

$$S^{33}_{(2)}S^{31}(v)\xi=-vS^{31}(v)\xi+\mu_3(v)\xi_1+(\mu_3^{(2)}-\mu_3^{(1)})S^{31}(v)\xi. \tag{4.24}$$

On the other hand, applying $S^{33}_{(2)}$ on (4.23) and using (4.20) and (4.21) we have

$$S^{33}_{(2)}S^{31}(v)\xi=\sum_{i=1}^{k}a_i(v)S^{33}_{(2)}\xi_i$$
$$=\left(\sum_{i=1}^{k}(a_i(v)\mu_3^{(i)})+(\mu_3^{(2)}-\mu_3^{(1)})-a_k(v)a_1^{(k+1)}\right)\xi_1$$
$$+\sum_{i=2}^{k}(-a_{i-1}(v)+(\mu_3^{(2)}-\mu_3^{(1)})a_i(v)-a_k(v)a_i^{(k+1)})\xi_i\,. \tag{4.25}$$

Taking the coefficient at ξ_i for $i=2,\ldots,k$ in (4.24) and (4.25) leads to

$$-a_{i-1}(v)+va_i(v)-a_i^{k+1}a_k(v)=0, \tag{4.26}$$

so that

$$a_i(v)=a_k(v)\underbrace{(v^{k-i}-v^{k-1-i}a_k^{k+1}-v^{k-i-2}a_{k-1}^{(k+1)}-\cdots-va_{i+2}^{(k+1)}-a_{i+1}^{(k+1)}}_{A_i(v)} \tag{A27}$$

for $i=1,\ldots,k-1$. The coefficient at ξ_1 in (4.24) and (4.25) leads to

$$\mu_3(v)=\underbrace{\sum_{i=1}^{k}\mu_3^{(i)}a_k(v)A_i(v)}_{\text{pol. of degree } k-1}-a_1^{(k+1)}a_k(v)+\underbrace{va_k(v)A_1(v)}_{\text{monic pol. of degree } k} \tag{4.28}$$

So $\mu_3(v)=a_k(v)B(v)$ where $B(v)$ is a monic polynomial in v of degree k.

For $\mu_1(v)$ we use

$$[S^{11}(u),S^{31}(v)]=\frac{u+v+1}{u^2-v^2}S^{31}(u)S^{11}(v)-\frac{1}{u+v}S^{12}(u)S^{11}(v)-\frac{2v+1}{u^2-v^2}S^{31}(v)S^{11}(u).$$

Notice that $S^{11}(u)$ is an even series in u^{-1}. Using the same procedure we find that $\mu_1(v)=a_k(v)C(v)$ where $C(v)$ is a monic polynomial in v of degree k.

Defining $\varphi(u)=(a_k(u)u^k)^{-1}$, we have

$$\varphi(u)\mu_1(u)=(1+\alpha_1u^{-1})\cdots(1+\alpha_ku^{-1}), \tag{4.29}$$

$$\varphi(u)\mu_3(u)=(1+\beta_1u^{-1})\cdots(1+\beta_ku^{-1}), \tag{4.30}$$

where the α_i's and the β_i's are complex numbers.

The formal series

$$\psi(u)\equiv\varphi(u)(1-\alpha_1u^{-1})\cdots(1-\alpha_ku^{-1})=\frac{(1-\alpha_1^2u^{-2})\cdots(1-\alpha_k^2u^{-2})}{\mu_1(u)}. \tag{4.31}$$

is an even series in u^{-1}. The composition of the automorphism $S(u)\to\psi(u)S(u)$ with $V[\mu(u)]$ is an irrep with the following highest weight which we shall again denote by $\mu(u)$:

$$\mu_1(u)=(1-\alpha_1^2u^{-2})\cdots(1-\alpha_k^2u^{-2}), \tag{4.32}$$

$$\mu_3(u)=(1-\alpha_1u^{-1})\cdots(1-\alpha_ku^{-1})(1+\beta_1u^{-1})\cdots(1+\beta_ku^{-1}). \tag{4.33}$$

■

Thus, up to an automorphism of $Y(1|2)^+$, we can assume that $\mu_1(u)$ and $\mu_3(u)$ are polynomials in u^{-1}.

Theorem 4.6: *Let $V[\mu_1(u),\mu_3(u)]$ be an irrep of $Y(1|2)^+$. Suppose $\mu_1(u)$ and $\mu_3(u)$ satisfy*

$$\frac{\mu_1(u)}{\mu_3(u)}=\frac{P(u+1)}{P(u)}\frac{R(u)}{Q(u)}, \tag{4.34}$$

$$\frac{\mu_3(-u)}{\mu_3(u)}=\frac{P(u+1)P(-u)}{P(u)P(1-u)}, \tag{4.35}$$

where $P(u)$, $Q(u)$ and $R(u)$ are a monic polynomial, $Q(u)$ and $R(u)$ are even in u and of same degree.

Then V is finite-dimensional.

Proof: We call p (resp. $2r$) the degree of $P(u)$ [resp. $Q(u)$ and $R(u)$]. Since $R(u)$ and $Q(u)$ are even, they write

$$R(u)=R_0(u)R_0(-u); \quad Q(u)=Q_0(u)Q_0(-u) \quad \text{with} \quad dg(R_0)=dg(Q_0)=r. \tag{4.36}$$

We introduce

$$\lambda_1(u)=u^{-s-r}P(u+1)R_0(u), \tag{4.37}$$

$$\lambda_2(u)=u^{-s-r}P(u+1)Q_0(u), \tag{4.38}$$

$$\lambda_3(u)=u^{-s-r}P(u)Q_0(u). \tag{4.39}$$

Let $L[\lambda(u)]$ be the corresponding irreducible highest weight module of $Y(1|2)$. Since $\lambda_1(u)/\lambda_2(u)=R_0(u)/Q_0(u)$ and $\lambda_2(u)/\lambda_3(u)=P(u+1)/P(u)$, according to Ref. 12 $L[\lambda(u)]$ is finite dimensional. The cyclic $Y(1|2)^+$-span of its highest weight vector is a finite-dimensional representation $V[\mu'(u)]$ of $Y(1|2)^+$ with $\mu_1'(u)=\lambda_1(u)\lambda_1(-u)$ and $\mu_3'(u)=\lambda_3(u)\lambda_2(-u)$. By construction, the polynomials $\mu_i'(u)$ satisfy (4.34) and (4.35). This implies that

$$\psi(u)\equiv\frac{\mu_3(u)}{\mu_3'(u)}=\frac{\mu_3(-u)}{\mu_3'(-u)} \tag{4.40}$$

is an even series in u^{-1} and

$$\mu_1(u)=\frac{\mu_3(u)}{\mu_3'(u)}\mu_1'(u)=\psi(u)\mu_1'(u). \tag{4.41}$$

Thus, there exists an automorphism $S(u)\to\psi(u)S(u)$ of $Y(1|2)^+$ such that its composition with the representation $V[\mu'(u)]$ is isomorphic to $V[\mu(u)]$:$V[\mu(u)]$ is therefore finite dimensional. ■

Conjecture 1: The sufficient condition (4.34) of Theorem 4.6 for the existence of finite-dimensional irreps of $Y(1|2)^+$ is also a necessary condition.

We remind that the condition (4.35) has been proved to be necessary (see Theorem 4.6), so that Conjecture 1 just says that Theorem 4.6 states necessary and sufficient conditions for finite-dimensional irreps of $Y(1|2)^+$.

C. The general case $Y(2m+1|2n)^+$

Theorem 4.7: *Let $V=V[\mu_{m+1}(u),\ldots,\mu_{2m+1}(u),\mu_{M+n+1}(u),\ldots,\mu_{M+2n}(u)]$ be an irrep of $Y(2m+1|2n)^+$. We take $m\geqslant 1$ and note $M=2m+1$.*

Suppose the weights $\mu_i(u)$ obey

$$\frac{\mu_i(u)}{\mu_{i+1}(u)}=\frac{P_{i+1}(u+1)}{P_{i+1}(u)} \quad \textit{for} \quad \begin{cases} m+2\leqslant i\leqslant 2m, \\ M+n+1\leqslant i\leqslant M+2n-1, \end{cases} \tag{4.42}$$

$$\frac{\mu_{M+n+1}(-u)}{\mu_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)P_{M+n+1}(-u)}{P_{M+n+1}(u)P_{M+n+1}(1-u)}, \tag{4.43}$$

$$\gamma(u)\frac{\mu_{m+1}(u)}{\mu_{m+2}(u)}=\frac{P_{m+2}(u+1)}{P_{m+2}(u)}, \tag{4.44}$$

$$\frac{\mu_{m+1}(u)}{\mu_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)}{P_{M+n+1}(u)}\frac{R(u)}{Q(u)}, \tag{4.45}$$

with $R(u)$ and $Q(u)$ even and of same degree. In the above formulas, $\gamma(u)$ is either 1 *or* $2u/(2u+1)$.

Then V is finite dimensional.

Under the assumption of Conjecture 1, the above sufficient conditions are also necessary ones.

Proof: First, let $\gamma(u)$ be 1. We note s_i the degree of the polynomials $P_i(u)$, decompose $R(u)$ and $Q(u)$ as in (4.36), and note

$$P_+(u)=\prod_{a=m+2}^{M} P_a(u); \quad P_-(u)=\prod_{a=M+n+1}^{M+2n} P_a(u); \quad s_0=r+\sum_{i=m+1}^{M} s_i+\sum_{i=M+n+1}^{M+2n} s_i. \tag{4.46}$$

We also define

$$\lambda_i(u)=u^{-s_0}P_+(u+1)P_-(u+1)R_0(u), \qquad i=1,\ldots,m+1, \tag{4.47}$$

$$\lambda_i(u)=u^{-s_0}P_-(u+1)R_0(u)\prod_{a=m+2}^{i} P_a(u)\prod_{a=i+1}^{2m+1} P_a(u+1), \qquad i=m+2,\ldots,M, \tag{4.48}$$

$$\lambda_i(u)=u^{-s_0}P_+(u+1)P_-(u+1)Q_0(u), \qquad i=M+1,\ldots,M+n, \tag{4.49}$$

$$\lambda_i(u)=u^{-s_0}P_+(u+1)Q_0(u)\prod_{a=M+n+1}^{i} P_a(u)\prod_{a=i+1}^{M+2n} P_a(u+1),$$

$$i=M+n+1,\ldots,M+2n. \tag{4.50}$$

We therefore have

$$\frac{\lambda_i(u)}{\lambda_{i+1}(u)}=\frac{P_{i+1}(u+1)}{P_{i+1}(u)} \quad \text{for} \quad \begin{cases} i=m+1,\ldots,M-1, \\ i=M+n,\ldots,M+2n-1, \end{cases} \tag{4.51}$$

$$\frac{\lambda_i(u)}{\lambda_{i+1}(u)}=1 \quad \text{for} \quad \begin{cases} i=1,\ldots,m, \\ i=M+1,\ldots,M+n-1, \end{cases} \tag{4.52}$$

$$\frac{\lambda_M(u)}{\lambda_{M+1}(u)}=\frac{R_0(u)}{Q_0(u)}\frac{P_+(u)}{P_+(u+1)}. \tag{4.53}$$

We consider the highest weight irrep $L[\lambda(u)]$ of $Y(2m+1|2n)$. According to Property 2.6, the relations (4.51)–(4.53) ensure that $L[\lambda(u)]$ is finite dimensional. The cyclic $Y(2m+1|2n)^+$-span of its highest weight vector is a finite-dimensional representation with highest weights $\mu_i'(u)=\lambda_i(u)\overline{\lambda_i}(-u)$ for $i=m+1,\ldots,2m+1$ and $i=M+n+1,\ldots,M+2n$. Its irreducible quotient is a finite-dimensional irrep $V[\overline{\mu}(u)]$ of $Y(2m|2n)^+$.

Moreover, the $\mu_i'(u)$ verify

$$\frac{\mu_i'(u)}{\mu_{i+1}'(u)}=\frac{P_{i+1}(u+1)}{P_{i+1}(u)}=\frac{\mu_i(u)}{\mu_{i+1}(u)}, \quad \begin{cases} i=m+1,\ldots,M-1, \\ i=M+n+1,\ldots,M+2n-1, \end{cases} \tag{4.54}$$

$$\frac{\mu'_{M+n+1}(-u)}{\mu'_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)P_{M+n+1}(-u)}{P_{M+n+1}(u)P_{M+n+1}(1-u)}=\frac{\mu_{M+n+1}(-u)}{\mu_{M+n+1}(u)}, \tag{4.55}$$

$$\frac{\mu'_{m+1}(u)}{\mu'_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)}{P_{M+n+1}(u)}\frac{R(u)}{Q(u)}=\frac{\mu_{m+1}(u)}{\mu_{M+n+1}(u)}. \tag{4.56}$$

The formal series

$$\psi(u)=\frac{\mu_{M+n+1}(-u)}{\mu'_{M+n+1}(u)} \tag{4.57}$$

is an even series in u^{-1} and we have

$$\frac{\mu_i(u)}{\mu'_i(u)}=\psi(u), \quad \forall i. \tag{4.58}$$

Hence there exists an automorphism $S(u)\to\psi(u)S(u)$ of $Y(2m+1|2n)^+$ such that its composition with $V[\mu'(u)]$ is isomorphic to $V[\mu(u)]$. The latter is thus finite dimensional.

Now, let $\gamma(u)=2u/(2u+1)$ holds. We introduce the osp$(2m+1|2n)$ representation V_0, of highest weight $l_i=-\frac{1}{2}$ for $i=m+2,\ldots,2m+1$ and $l_i=0$ for $i=m+1,M+n+1,\ldots,M+2n$ and promote it to a $Y(2m+1|2n)^+$ representation using the evaluation map. The corresponding highest weight has components $l_i(u)=2u/(2u+1)$ for $i=m+2,\ldots,2m+1$, and $l_i(u)=1$ for $i=m+1,M+n+1,\ldots,M+2n$.

Moreover, making the same construction as for the case $\gamma(u)=1$, and considering the tensor product $L[\lambda(u)]\otimes V_0$, we get a finite-dimensional representation $V[\mu''(u)]$ obeying the relations (4.42)–(4.45) with $\gamma(u)=2u/(2u+1)$. Its irreducible subquotient is isomorphic to $V[\mu(u)]$, which is therefore finite dimensional.

Conversely, let us suppose that the irrep $V[\mu(u)]$ is finite dimensional. From Theorem 4.4, one already knows that the conditions (4.42)–(4.44) must be satisfied.

Suppose also that Conjecture 1 holds. The subalgebra generated by the coefficients of $S^{ij}(u)$, $i,j=m+1,M+n,M+n+1$, is isomorphic to $Y(1|2)^+$. The cyclic span of the highest weight vector of $V[\mu(u)]$ with respect to this subalgebra is a representation with highest weight $(\mu_{m+1}(u),\mu_{M+n+1}(u))$. Its irreducible quotient is finite dimensional and, so, we have relation (4.45). ■

D. Finite-dimensional irreps of $Y(2|2)^+$

Let $V=V[\mu(u)]$ be an irrep of $Y(2|2)^+$ with highest weight $\mu(u)$.

Proposition 4.8: If $V[\mu(u)]$ is finite dimensional, then there exists a formal even series $\psi(u)$ in u^{-1} such that

$$\psi(u)\mu_2(u)=(1-\alpha_1u^{-1})\cdots(1-\alpha_ku^{-1}), \tag{4.59}$$

$$\psi(u)\mu_4(u)=(1-\beta_1u^{-1})\cdots(1-\beta_ku^{-1}). \tag{4.60}$$

Proof: The proof is very similar to the case of $Y(1|2)^+$, and we leave it to the reader. Note that for the calculation being achieved using the fermionic generator $S_{13}(u)$ [instead of the even bosonic one $S_{12}(u)$], there is no difference in the proof for $Y(1|2)^+$ and $Y(2|2)^+$, in opposition with the $Y(2)^+$ and $Y(2)^-$ cases.[16] ■

Theorem 4.9: *Let $V[\mu_2(u),\mu_4(u)]$ be an irrep of $Y(2|2)^+$. If $\mu_2(u)$ and $\mu_4(u)$ satisfy*

$$\frac{\mu_2(u)}{\mu_4(u)}=\frac{u-\gamma}{u+\frac{1}{2}}\frac{P_4(u+1)\,P_2(u)}{P_4(u)\,P_2(u+1)}\frac{R(u)}{Q(u)}, \tag{4.61}$$

$$\frac{\mu_4(-u)}{\mu_4(u)}=\left(\frac{u+\frac{1}{2}}{u-\frac{1}{2}}\right)^2\frac{P_4(u+1)\,P_4(-u)}{P_4(u)\,P_4(1-u)}, \tag{4.62}$$

then V is finite dimensional.

In the above formulas, $P_2(u)$, $P_4(u)$, $Q(u)$ and $R(u)$ are monic polynomials, $Q(u)$ and $R(u)$ are even in u and of same degree, and $\gamma \in \mathbb{C}$.

Proof: We call p_2 (resp. p_4, resp. $2r$) the degree of $P_2(u)$ [resp. $P_4(u)$, resp. $Q(u)$ and $R(u)$] and decompose $Q(u)$ and $R(u)$ as in (4.36). Let $L[\lambda(u)]$ be the irrep of $Y(2|2)$ with weights

$$\lambda_1(u) = u^{-p_2-p_4-r} P_4(u+1) P_2(u+1) R_0(u), \tag{4.63}$$

$$\lambda_2(u) = u^{-p_2-p_4-r} P_4(u+1) P_2(u) R_0(u), \tag{4.64}$$

$$\lambda_3(u) = u^{-p_2-p_4-r} P_4(u+1) P_2(u+1) Q_0(u), \tag{4.65}$$

$$\lambda_4(u) = u^{-p_2-p_4-r} P_4(u) P_2(u+1) Q_0(u). \tag{4.66}$$

Since we have

$$\frac{\lambda_1(u)}{\lambda_2(u)} = \frac{P_2(u+1)}{P_2(u)}, \quad \frac{\lambda_2(u)}{\lambda_3(u)} = \frac{P_2(u+1) R_0(u)}{P_2(u)\, Q_0(u)}, \quad \frac{\lambda_3(u)}{\lambda_4(u)} = \frac{P_4(u+1)}{P_4(u)}, \tag{4.67}$$

$L[\lambda(u)]$ is finite dimensional. The $Y(2|2)^+$-cyclic span of its highest weight vector is a finite-dimensional $Y(2|2)^+$-representation $V[\mu'(u)]$ of weights $\mu_2'(u) = \lambda_2(u)\lambda_1(-u)$ and $\mu_4'(u) = \lambda_4(u)\lambda_3(-u)$. These weights obey the relations

$$\frac{\mu_2'(u)}{\mu_4'(u)} = \frac{P_4(u+1)\, P_2(u)}{P_4(u)\, P_2(u+1)} \frac{R(u)}{Q(u)}, \tag{4.68}$$

$$\frac{\mu_4'(-u)}{\mu_4'(u)} = \frac{P_4(u+1)\, P_4(-u)}{P_4(u)\, P_4(1-u)}. \tag{4.69}$$

We now consider the osp(2|2) finite-dimensional irrep V_0 with weights $l_2 = -\gamma - \frac{1}{2}$ and $l_4 = -1$. Through the evaluation map, its provides a finite-dimensional representation of $Y(2|2)^+$ with weights

$$l_2(u) = \frac{u-\gamma}{u+\frac{1}{2}} \quad \text{and} \quad l_4(u) = \frac{u-\frac{1}{2}}{u+\frac{1}{2}}. \tag{4.70}$$

The tensor product $L[\lambda(u)] \otimes V_0$ is thus a finite-dimensional representation of $Y(2|2)^+$, with weights $\mu_i''(u) = \mu_i'(u) l_i(u)$, $i = 2,4$. They obey relations (4.61) and (4.62), so that the irreducible quotient provide a finite-dimensional irrep isomorphic to V. Thus, V finite dimensional. ■

Note that the polynomial $P(u) = (u - \frac{1}{2})^2$ obeys the relation $P(1-u) = P(u)$, so that the condition on $\mu_4(u)$ does not differ from the one obtained for $Y(2)^-$.

Conjecture 2: The sufficient condition (4.61) *of Theorem 4.9 for the existence of finite-dimensional irreps of $Y(2|2)^+$ is also a necessary condition.*

E. The general case $Y(2m|2n)^+$

Theorem 4.10: *(Case of $Y(2|2m)^+$) Let $V = V[\mu_2(u), \mu_{n+3}(u), \ldots, \mu_{2+2n}(u)]$ be an irrep of $Y(2|2n)^+$.*

Suppose the weights $\mu_i(u)$ obey

$$\frac{\mu_i(u)}{\mu_{i+1}(u)} = \frac{P_{i+1}(u+1)}{P_{i+1}(u)} \quad \text{for} \quad n+3 \leqslant i \leqslant 2n+1, \tag{4.71}$$

$$\frac{\mu_{n+3}(-u)}{\mu_{n+3}(u)}=\left(\frac{u-\frac{1}{2}}{u+\frac{1}{2}}\right)^2\frac{P_{n+3}(u+1)P_{n+3}(-u)}{P_{n+3}(u)P_{n+3}(1-u)}, \tag{4.72}$$

$$\frac{\mu_2(u)}{\mu_{n+3}(u)}=\frac{u-\gamma}{u+\frac{1}{2}}\frac{P_{n+3}(u+1)\,P_2(u)}{P_{n+3}(u)\,P_2(u+1)}\frac{R(u)}{Q(u)}, \tag{4.73}$$

with $R(u)$ and $Q(u)$ even and of same degree, and $\gamma\in\mathbb{C}$.

Then V is finite dimensional.

Under the assumption of Conjecture 2, the conditions (4.71)–(4.73) are necessary and sufficient conditions for V to be a finite-dimensional irrep.

Proof: The proof is similar to the previous ones. One constructs a finite-dimensional irrep for $Y(2|2n)^+$ which fulfills the conditions (4.71)–(4.73). It takes the form $V'=L[\lambda(u)]\otimes V_\gamma$. $L[\lambda(u)]$ is constructed as in Theorem 4.7. The finite-dimensional osp$(2|2n)$-irrep V_γ has weight

$$l_2=-\gamma-\tfrac{1}{2}\quad\text{and}\quad l_i=-1,\quad\text{for}\quad n+3\leqslant i\leqslant 2n. \tag{4.74}$$

Looking at the osp$(2|2n)$-span of the highest weight vector and taking the irreducible subquotient, we get a finite-dimensional irrep V' with highest weight obeying (4.71)–(4.73). V being isomorphic to V', it is therefore finite dimensional.

Conversely, assuming Conjecture 2, and looking at the subalgebras $Y(2|2)^+$ and $Y(2n)^-$, one easily proves that the conditions (4.71)–(4.73) are necessary conditions. ■

Theorem 4.11: *(Case of $m>1$) Let $V=V[\mu_{m+1}(u),\ldots,\mu_M(u),\mu_{M+n+1}(u),\ldots,\mu_{M+2n}(u)]$ be an irrep of $Y(2m|2n)^+$. We note $M=2m$ and take $m>1$.*

Suppose the weights $\mu_i(u)$ obey

$$\frac{\mu_i(u)}{\mu_{i+1}(u)}=\frac{P_{i+1}(u+1)}{P_{i+1}(u)}\quad\text{for}\quad\begin{cases}m+1\leqslant i\leqslant 2m-1,\\ M+n+1\leqslant i\leqslant M+2n-1,\end{cases} \tag{4.75}$$

$$\frac{\mu_{M+n+1}(-u)}{\mu_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)P_{M+n+1}(-u)}{P_{M+n+1}(u)P_{M+n+1}(1-u)}, \tag{4.76}$$

$$\gamma(u)\frac{\mu_{m+1}(u)}{\mu_{M+n+1}(u)}=\frac{P_{M+n+1}(u+1)\,P_{m+1}(u)}{P_{M+n+1}(u)\,P_{m+1}(u+1)}\frac{R(u)}{Q(u)}, \tag{4.77}$$

with $R(u)$ and $Q(u)$ even and of same degree, and $\gamma(u)$ is either 1 or $(2u-1)/(2u+1)$.

Then V is finite dimensional.

Proof: We start with the case $\gamma(u)=1$, and do the same construction as in Theorem 4.7, to get weights $\lambda_i(u)$ defined as in Eqs. (4.47)–(4.50), with now $M=2m$. We introduce

$$\lambda_i'(u)=P_{m+1}(u+1)\lambda_i(u)\quad\text{for}\quad\begin{cases}i=1,\ldots,m,\\ i=M+1,\ldots,M+2n,\end{cases} \tag{4.78}$$

$$\lambda_i'(u)=P_{m+1}(u)\lambda_i(u)\quad\text{for}\quad i=m+1,\ldots,M. \tag{4.79}$$

For these new weights, the relations (4.51)–(4.53) are still valid when $i\neq m,M$. In these latter cases, we get

$$\frac{\lambda_m'(u)}{\lambda_{m+1}'(u)}=\frac{P_{m+1}(u+1)}{P_{m+1}(u)}, \tag{4.80}$$

$$\frac{\lambda_M'(u)}{\lambda_{M+1}'(u)}=\frac{P_{m+1}(u)}{P_{m+1}(u+1)}\frac{P_+(u)}{P_+(u+1)}\frac{R_0(u)}{Q_0(u)}. \tag{4.81}$$

Thus, the $Y(2m|2n)$-irrep $L[\lambda'(u)]$ is still finite dimensional. The cyclic $Y(2m|2n)^+$-span of its highest weight vector is a representation with highest weight $\overline{\mu}_i(u)=\lambda'_i(u)\lambda'_i(-u)$ for $i=m+1,\ldots,2m$ and $i=M+n+1,\ldots,M+2n$. Its irreducible quotient is a finite-dimensional irrep $V[\overline{\mu}(u)]$ of $Y(2m|2n)^+$.

Moreover, the weights $\overline{\mu}_i(u)$ for $i=m+1,\ldots,M-1$ on the one hand, and $i=M+n+1,..,M+2n-1$ on the other hand, verify the same relations as the $\mu'_i(u)$, i.e., the conditions (4.75) and (4.76). For the remaining relation, one computes

$$\frac{\overline{\mu}_{m+1}(u)}{\overline{\mu}_{M+n+1}(u)}=\frac{P_{m+1}(u)}{P_{m+1}(u+1)}\,\frac{\mu'_{m+1}(u)}{\mu'_{M+n+1}(u)}, \tag{4.82}$$

which gives the relation (4.77).

The weights $\mu_i(u)$ and $\overline{\mu}_i(u)$ both obeying the relations (4.75)–(4.77), there exists an automorphism $S(u)\to\psi(u)S(u)$ of $Y(2m|2n)^+$ such that its composition with $V[\overline{\mu}(u)]$ is isomorphic to $V[\mu(u)]$. The latter is thus finite dimensional.

If now $\gamma(u)=2u/(2u-1)$, we construct the tensor product of the above representation by the osp$(2m|2n)$ finite-dimensional irrep V_0 with weights $l_i=-\frac{1}{2}$ for $m+1\leqslant i\leqslant 2m$ and $l_i=-1$ for $2m+n+1\leqslant i\leqslant 2m+2n$. V_0 provides a finite-dimensional representation for $Y(2m|2n)^+$ with weights $l_i(u)=2u/(2u+1)$ for $m+1\leqslant i\leqslant 2m$ and $l_i(u)=2u/(2u-1)$ for $2m+n+1\leqslant i\leqslant 2m+2n$. The weights of the tensor product obey the relations (4.75)–(4.77), and we conclude as in Theorem 4.7. ■

Remark: Conversely, let us suppose that the irrep $V[\mu(u)]$ is finite dimensional and that Conjecture 2 holds. From Theorem 4.4, one already knows that the conditions (4.75) and (4.76) must be satisfied (for $i\neq m+1$). Moreover, we get also

$$\gamma(u)\,\frac{\mu^o_{m+1}(-u)}{\mu^o_{m+1}(u)}=\frac{P_m(u+1)P_m(-u)}{P_m(u)P_m(1-u)} \tag{4.83}$$

with $\gamma(u)$ and $\mu^o_{m+1}(u)$ defined as in Theorem 4.4.

We suppose also that $\mu^o_{m+1}(u)=\mu_{m+1}(u)$, which turns out to suppose that (4.75) is valid for $i=m+1$.

The subalgebra generated by the coefficients of $S^{ij}(u)$, $i,j=m,m+1,M+n,M+n+1$, is isomorphic to $Y(2|2)^+$. The cyclic span of the highest weight vector of $V[\mu(u)]$ with respect to this subalgebra is a representation with highest weight $(\mu_{m+1}(u),\mu_{M+n+1}(u))$. Its irreducible quotient is finite dimensional and, so, we have

$$\frac{\mu_{m+1}(u)}{\mu_{M+n+1}(u)}=\frac{u-\gamma}{u+\frac{1}{2}}\,\frac{P_{M+n+1}(u+1)\,P_{m+1}(u)}{P_{M+n+1}(u)\,P_{m+1}(u+1)}\,\frac{R(u)}{Q(u)}. \tag{4.84}$$

We look at the osp$(2m|2n)$ irrep induced by the generators $S^{ab}_{(1)}$ acting on the highest weight vector. It is finite dimensional, so we must have

$$l_{i+1}-l_i\in\mathbb{Z}_+ \quad \text{for} \begin{cases} m+2\leqslant i\leqslant 2m, \\ M+n+1\leqslant i\leqslant M+2n-1, \end{cases} \tag{4.85}$$

$$-(l_{m+2}+l_{m+1})\in\tfrac{1}{2}\mathbb{Z}_+ \quad \text{and} \quad -l_{M+n+1}\in\mathbb{Z}_+, \tag{4.86}$$

$$l_{m+1}-l_{M+n+1}\in\tfrac{1}{2}\mathbb{Z}_+, \tag{4.87}$$

where $\mu_i(u)=1+u^{-1}l_i+\cdots$. The above relations [on the weights $\mu_i(u)$] imply the following constraints:

$$l_{i+1}-l_i\in\mathbb{Z}_+ \quad \text{for} \quad \begin{cases} m+2\leqslant i\leqslant 2m, \\ M+n+1\leqslant i\leqslant M+2n-1, \end{cases} \tag{4.88}$$

$$-(l_{m+1}+l_{m+2})\in\mathbb{Z}_+ \quad \text{and} \quad -l_{M+n+1}\in\mathbb{Z}_+, \tag{4.89}$$

$$l_{m+1}-l_{M+n+1}\in\mathbb{Z}_+ +(-\gamma-\tfrac{1}{2}). \tag{4.90}$$

This implies in particular that $\gamma\in-\frac{1}{2}\mathbb{Z}_+$, so that we are back to the conditions (4.77). Thus, we are led to the following:

Conjecture 3: The sufficient conditions of Theorem 4.11 for the existence of finite-dimensional irreps of $Y(2m|2n)^+$ are also necessary conditions.

V. CONCLUSION

We have defined the notion of twisted Yangians in the context of superalgebra gl$(M|N)$. It appears that most of the properties of the twisted Yangians $Y^{\pm}(N)$ can be exhibited in the superalgebra case. However, only $Y^+(M|2n)$ and $Y^-(2m|N)$ can be defined, and appear to be isomorphic. We thus concentrate on $Y^+(M|2n)$. Its finite-dimensional irreducible representations have been studied. $Y^+(M|2n)$ is also a coideal subalgebra of $Y(M|2n)$, and is a deformation of the polynomial superalgebra $\mathcal{U}(\mathrm{osp}(M|2n)[x])$.

From a mathematical point of view, the center of this algebra remains to be studied, and in particular the notion of Sklyanin determinant (which appears in the context of twisted Yangians) has to be generalized to this case. Note that the notion of quantum Berezinian, which generates central elements of $Y(M|N)$, has been introduced in Ref. 11.

From the physical of view, the integrable systems with boundary that could be relevant for such an algebra has to be determined. Nonlinear sigma models based on a supergroup seem to be a good candidate.

ACKNOWLEDGMENTS

We warmly thank D. Arnaudon, L. Frappat and A. Molev for fruitful comments. A part of the redaction was done at the School of Mathematics, Sydney University, and E.R. thanks them for hospitality.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 3 MARCH 2003

The dynamical Yang–Baxter relation and the minimal representation of the elliptic quantum group

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(Received 25 March 2002; accepted 10 December 2002)

In this article, we give the general forms of the minimal L matrix (the elements of the L-matrix are c numbers) associated with the Boltzmann weights of the A_{n-1}^{1} interaction-round-a-face (IRF) model and the minimal representation of the A_{n-1} series elliptic quantum group given by Felder and Varchenko. The explicit dependence of elements of L-matrices on spectral parameter z are given. They are of five different forms [A(1-4) and B]. The algebra for the coefficients (which do not depend on z) are given. The algebra of form A is proved to be trivial, while that of form B obeys Yang–Baxter equation (YBE). We also give the PBW base and the centers for the algebra of form B. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1543635]

I. INTRODUCTION

Recently, many papers have focused on the many-body long-distance integrable dynamical system, such as the Ruijsenaar Schneider model and the Calogero Moser (CM) model.[1–3] They are closely connected with the quantum Hall effect in the condense matter physics and the Seiberg Witten (SW) theory in the field theory, especially for the equations of the spectral curve in the SW theory, namely, the modified eigenvalue equations of the Lax matrices in the above integrable models.[4–6] These Lax matrices are the classical limit of the L matrices which is associated with the interaction-round-a-face (IRF) model of Lie group[7–9] and the modified Yang–Baxter relation (NSF equation).[10–13] All these L-matrices are corresponding to the representation of the elliptic quantum group which was proposed by Felder and Varchenko.[11,12] So it is very interesting to study the general solution of the L-matrices.

In this article, we study the simplest case of L-matrices which satisfy the dynamical Yang–Baxter relation (DYBR) for the A_{n-1} group. The deep study of the A_{n-1} group case can help us to understand the other Lie group cases because a subset of the other Lie groups can be constructed by the A_{n-1} group. We only study the simplest case of L matrices, that is to say, the Hilbert space of the L-operator is a scale function space. We find that the L matrices can only have five possible forms, form A(1), A(2), A(3), A(4) and form B. The form A(1) and B can be constructed by the factorized L matrices.[14–17] And the coefficient part of form B obeys a set of quadratic equations which can be related to the Shibukawa–Ueno operator.[18] The algebra of these quadratic relations have explicit PBW base and satisfy the YBE without spectral parameter z. We find that all known L-matrices[9,12,16] of related problem are equivalent to one representation of this algebra. But it is still an open question as to whether it is the unique one.

The present article is organized as follows. In Sec. II, we study the dependence of the elements of L-matrix with spectral parameter z. In Sec. III, we study the dependence of the essential

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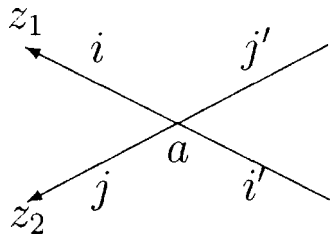

FIG. 1. The element of R-matrix $R(a|z_1-z_2)_{ij}^{i'j'}$.

part of these elements, which are functions of both z and (a,b), with respect to the indices of the elements. We prove that there are five possible classes of the minimal L-matrices. We then relate the elements of adjacent lattice points (a,b) and $(a+\hat{i}',b+\hat{i})$ in the end of this section. Section IV is written for the equations of the coefficient part of the elements of L-matrices, as a necessary and sufficient condition of L-matrices to satisfy the DYBR. This leads to two kinds of algebras. The A algebra, which is corresponding to the form A(i) ($i=1,2,3,4$), is trivially commutative and thus the coefficients of form A(i) can be determined completely. The algebra for form B coefficients is studied further in Sec. V, which satisfies YBE, and we establish the PBW base for it. We also give center elements for this algebra. In the last section, we give a known solution to the equations of form B. Throughout this article, we always assume all elements of L-matrix are c number functions which are not identically zero and $n\geqslant 4$.

II. DYBR AND THE RELATION BETWEEN FACTORIZED *L*-MATRIX AND MINIMAL *L*-MATRIX

It is well known that the Boltzmann weight of the $A_{n-1}^{(1)}$ IRF[7–9] model can be written as

$$R(a|z)_{ii}^{ii}=\frac{\sigma(z+w)}{\sigma(w)},\quad R(a|z)_{ij}^{ij}=\frac{\sigma(z)\sigma(a_{ij}-w)}{\sigma(w)\sigma(a_{ij})}\qquad \text{for}\qquad i\neq j,$$
$$R(a|z)_{ij}^{ji}=\frac{\sigma(z+a_{ij})}{\sigma(a_{ij})}\qquad \text{for}\qquad i\neq j,\quad R(a|z)_{i'j'}^{ij}=0\quad \text{for other cases,} \tag{1}$$

where $a\equiv(m_0,m_1,\ldots,m_{n-1})$ is an n-vector, and $a_{ij}=a_i-a_j$, $a_i=w(m_i-(1/n)\Sigma_l m_l+w_i)$, m_i ($i=0,1,\ldots,n-1$) are integers which describe the state of model, while $\{w,w_i\}$ are generic c-numbers which are the parameters of the model, and $\sigma(z)\equiv\theta[{}^{1/2}_{1/2}](z,\tau)$, with

$$\theta[{}^{a}_{b}](z,\tau)\equiv\sum_{m\in Z}e^{i\pi(m+a)^2\tau+2i\pi(m+a)(z+b)}.$$

We define an n-dimension vector $\hat{j}=(0,0,\ldots,0,1,0,\ldots)$, in which the jth component is 1.

We consider a matrix whose elements are linear operators. We denote the elements of the matrix as $L({}^{a}_{b}|z)_{i}^{j}$. The R-matrix and the L-matrix can also be depicted by Figs. 1 and 2.

The dynamical Yang–Baxter relation (DYBR) is written as (also see Fig. 3)

$$\sum_{i',j'}R(b|z_1-z_2)_{ij}^{i'j'}L({}^{a}_{b}|z_1)_{i'}^{i''}L({}^{a+\hat{i}''}_{b+\hat{i}'}|z_2)_{j'}^{j''}=\sum_{i',j'}L({}^{a}_{b}|z_2)_{j}^{j'}L({}^{a+\hat{j}'}_{b+\hat{j}}|z_1)_{i}^{i'}R(a|z_1-z_2)_{i'j'}^{i''j''},\tag{2}$$

where $b\equiv(m_0^b,m_1^b,\ldots,m_{n-1}^b)$, $a\equiv(m_0^a,m_1^a,\ldots,m_{n-1}^a)$. We note that Eq. (2) gives the quadratic relation of the elements of L. If we let $b=a+h$, the form of the equation will be the same as that given in Refs. 11 and 12, and the relation which L satisfies is the definition relation of the elliptic quantum group proposed by Felder and Varchenko. Here, the elements of the L-matrix are operators, and Eq. (2) is the algebra of these operators. In this article, we only discuss the minimal form

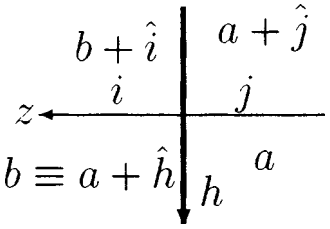

FIG. 2. The element of L-matrix, $L(a,h|z)^j_i \equiv L(^a_b|z)^j_i$.

of the operators, namely, we only consider the simplest case that all elements are c numbers. In this situation, the $L(^a_b|z)^j_i$ is scalar functions of (a,b,z,i,j). We will try to find the general form of such L-matrix. From Eq. (2), we have

$$\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z_1)^{i'}_i}{L(^a_b|z_1)^{i'}_i}=\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{i'}_i}{L(^a_b|z_2)^{i'}_i}, \tag{3}$$

$$R(b|z_1-z_2)^{ii}_{ii}=R(a|z_1-z_2)^{i'j'}_{i'j'}\frac{L(^a_b|z_2)^{j'}_i}{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{j'}_i}\frac{L(^{a+\hat{j}'}_{b+\hat{i}}|z_1)^{i'}_i}{L(^a_b|z_1)^{i'}_i}$$

$$+R(a|z_1-z_2)^{i'j'}_{j'i'}\frac{L(^a_b|z_2)^{i'}_i}{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{j'}_i}\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z_1)^{j'}_i}{L(^a_b|z_1)^{i'}_i}\quad (i'\neq j'), \tag{4}$$

$$R(a|z_1-z_2)^{i'i'}_{i'i'}=R(b|z_1-z_2)^{ij}_{ij}\frac{L(^a_b|z_1)^{i'}_i}{L(^{a+\hat{i}'}_{b+\hat{j}}|z_1)^{i'}_i}\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{i'}_j}{L(^a_b|z_2)^{i'}_j}$$

$$+R(b|z_1-z_2)^{ji}_{ij}\frac{L(^a_b|z_1)^{i'}_j}{L(^{a+\hat{i}'}_{b+\hat{j}}|z_1)^{i'}_i}\frac{L(^{a+\hat{i}'}_{b+\hat{j}}|z_2)^{i'}_i}{L(^a_b|z_2)^{i'}_j}\quad (i\neq j). \tag{5}$$

By solving Eqs. (4) and (5), we can determine $L(^a_b|z)^j_i$ as the function of z. Let

$$\frac{L(^a_b|z_2)^{j'}_i}{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{j'}_i}\equiv g(z_2),\quad \frac{L(^{a+\hat{j}'}_{b+\hat{i}}|z_1)^{i'}_i}{L(^a_b|z_1)^{i'}_i}\equiv h(z_1),\qquad \frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z)^{j'}_i}{L(^a_b|z)^{i'}_i}\equiv f(z), \tag{6}$$

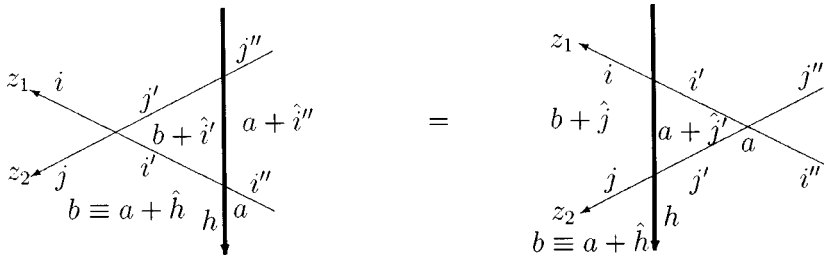

FIG. 3. The dynamical Yang–Baxter relation.

$$\frac{R(b|z_1-z_2)^{ii}_{ii}}{R(a|z_1-z_2)^{i'j'}_{i'j'}}\equiv A(z_1-z_2), \qquad -\frac{R(a|z_1-z_2)^{i'j'}_{j'i'}}{R(a|z_1-z_2)^{i'j'}_{i'j'}}\equiv B(z_1-z_2). \tag{7}$$

We then rewrite Eq. (4) as

$$g(z_2)h(z_1)=A(z_1-z_2)+B(z_1-z_2)f(z_1)/f(z_2)\equiv F(z_1,z_2). \tag{8}$$

We find that the left hand side of the above equation is factorized by the functions of z_1 and z_2. So taking logarithm to the both sides of the above equation and taking the derivative with respect to z_1 and z_2, we have

$$\frac{\partial^2}{\partial z_1\partial z_2}\ln F(z_1,z_2)=0. \tag{9}$$

Hence the above equation gives

$$F(z_1,z_2)\frac{\partial^2}{\partial z_1\partial z_2}F(z_1,z_2)-\frac{\partial}{\partial z_1}F(z_1,z_2)\frac{\partial}{\partial z_2}F(z_1,z_2)=0. \tag{10}$$

By using Eqs. (8) and (10), we can get an algebraic equation of second order about $f(z_1)$,

$$\begin{aligned} &f(z_1)^2[d_1f'(z_2)+d_2f(z_2)]+f(z_1)[d_3f'(z_2)^2+d_4f'(z_2)f(z_2)+d_5f(z_2)^2]\\ &\quad+d_6f'(z_2)f(z_2)^2+d_7f(z_2)^3=0, \end{aligned} \tag{11}$$

where d_i $(i=1, 2, \ldots, 7)$ are known functions of z_1-z_2. Define

$$y=\frac{f(z_1)}{f(z_2)},$$

$$\theta\equiv\frac{f'(z_2)}{f(z_2)}=\frac{\partial}{\partial z_2}\ln\left\{\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z_2)^{j'}_{i}}{L(^{a}_{b}|z_2)^{i'}_{i}}\right\}.$$

Then, Eq. (11) can be rewritten as

$$y^2(d_1\theta+d_2)+y(d_3\theta^2+d_4\theta+d_5)+(d_6\theta+d_7)=0. \tag{12}$$

When z_2 is fixed, the coefficients of Eq. (12) are the functions of z_1. So y is also a function of z_1. Since Eq. (12) is of second order, the y can only have two solutions $y_1(z_1,z_2)$ and $y_2(z_1,z_2)$ at most. If we can find two different L-matrices $L_1(^a_b|z)$ and $L_2(^a_b|z)$ which satisfy the DYBR with same θ, we must have $f(z_1)/f(z_2)=f_1(z_1)/f_1(z_2)$ or $f(z_1)/f(z_2)=f_2(z_1)/f_2(z_2)$, where f_1 and f_2 are obtained by the two different L's. Then, we can obtain $f(z_1)\sim f_1(z_1)$ or $f(z_1)\sim f_2(z_1)$, where ''$\sim$'' implies that, as the function of z_1, two sides of it can only be different with a constant respect to z_1. Thus, we can conclude that if there are two $L_i(^a_b|z)$ $(i=1,2)$ which satisfy the DYBR and are not proportional to each other, and when $z=z_2$, they have the same $\theta=\theta_1(z_2)=\theta_2(z_2)$, then every $f(z)$ related with $L(^a_b|z)$ satisfying $f'(z)/f(z)=\theta$ when $z=z_2$ must satisfy

$$f(z)=f_1(z)\text{const} \quad \text{or} \quad f(z)=f_2(z)\text{const}, \tag{13}$$

where the constants do not depend on z.

Now we consider the factorized L-matrix[14–17] which has an adjustable parameter δ. We will show that for the given z_2 and θ, there are generally two different δ's which can give $f'_{\delta_1}(z_2)/f_{\delta_1}(z_2)=f'_{\delta_2}(z_2)/f_{\delta_2}(z_2)=\theta$.

Considering the intertwiner of the Z_n Belavin model and the $A_{n-1}^{(1)}$ IRF model,[19,20] we have

$$\varphi^{(j)}_{a+\hat{i},a}(z)=\theta\begin{bmatrix}\frac{1}{2}-\frac{j}{n}\\ \frac{1}{2}\end{bmatrix}(z+n(a+\hat{i})_i,n\tau)\equiv\theta^{(j)}(nz_i),$$

$$(a+\hat{i})_i=w\left(m_i+1-\frac{1}{n}\sum_l(m_l+\delta_{il})+w_i\right)=a_i+w\left(1-\frac{1}{n}\right).$$

Define $\tilde{\varphi}^{(j)}_{a+\hat{\nu},a}(z)$ which satisfies

$$\sum_{j=0}^{n-1}\tilde{\varphi}^{(j)}_{a+\hat{\nu},a}(z)\varphi^{(j)}_{a+\hat{\mu},a}(z)=\delta_{\mu\nu}.$$

Let

$$\overline{L}_s\left(\begin{matrix}a\\ b\end{matrix}|z\right)^{\nu}_{\mu}=\sum_{j=0}^{n-1}\tilde{\varphi}^{(j)}_{a+\hat{\nu},a}(z)\varphi^{(j)}_{b+\hat{\mu},b}(z+s),\tag{14}$$

where s is an arbitrary parameter. Then by using the correspondence relation between face and vertex,[20] we can prove that the L-matrix above satisfies the DYBR Eq. (2). After some derivation, we have[17]

$$\overline{L}_s\left(\begin{matrix}a\\ b\end{matrix}|z\right)^{\nu}_{\mu}=\frac{\sigma(z+\Delta+(n-1)w-(n-1)/2+s/n+b_\mu-a_\nu)}{\sigma(z+\Delta+(n-1)w-(n-1)/2)}\prod_{j(\neq\nu)}\frac{\sigma(s/n+b_\mu-a_j)}{\sigma(a_\nu-a_j)}$$

with $\Delta=w\Sigma_j w_j$. Let $\delta=\Delta+(n-1)w-(n-1)/2+s/n=\delta(s)$, $\delta'=s/n$. Since $\sigma(z+\Delta+(n-1)w-(n-1)/2)$ is irrelevant with a,b,μ,ν, from the above formula, we can prove that

$$L_\delta\left(\begin{matrix}a\\ b\end{matrix}|z\right)^{\nu}_{\mu}=\overline{L}_s\left(\begin{matrix}a\\ b\end{matrix}|z\right)^{\nu}_{\mu}\sigma\left(z+\Delta+(n-1)w-\frac{n-1}{2}\right)=\sigma(z+\delta+b_\mu-a_\nu)\prod_{j\neq\nu}\frac{\sigma(\delta'+b_\mu-a_j)}{\sigma(a_\nu-a_j)}\tag{15}$$

also satisfy the DYBR [Eq. (2)].

Considering the definition of θ, we have

$$\theta(z)=\frac{f'_\delta(z)}{f_\delta(z)}=\frac{\sigma'(z+\delta+b_i-a_{j'}+w)}{\sigma(z+\delta+b_i-a_{j'}+w)}-\frac{\sigma'(z+\delta+b_i-a_{i'})}{\sigma(z+\delta+b_i-a_{i'})}.\tag{16}$$

By using the properties of the θ-function, one can show that for a given θ, there generally exist two different δ's satisfying Eq. (16).

From Eq. (13), we know that for the L-matrix which satisfies the DYBR,

$$f(z)\sim f_\delta(z)\tag{17}$$

must be held for certain δ. And from Eq. (8), we know that $g(z)$ and $h(z)$ can be determined completely by $f(z)$ up to a scale. So we have

$$g(z)\sim g_\delta(z),\quad h(z)\sim h_\delta(z).\tag{18}$$

Here the parameter δ is the same as that in Eq. (17). Then, from Eqs. (17) and (18), we have

$$\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z)^{j'}_{i}}{L(^{a}_{b}|z)^{i'}_{i}}\sim\frac{\sigma(z+\delta+b_i-a_{j'}+w)}{\sigma(z+\delta+b_i-a_{i'})}, \tag{19}$$

$$\frac{L(^{a+\hat{j}'}_{b+\hat{i}}|z)^{i'}_{i}}{L(^{a}_{b}|z)^{i'}_{i}}\sim\frac{\sigma(z+\delta+b_i-a_{i'}+w)}{\sigma(z+\delta+b_i-a_{i'})}, \tag{20}$$

$$\frac{L(^{a}_{b}|z)^{j'}_{i}}{L(^{a+\hat{i}'}_{b+\hat{i}}|z)^{j'}_{i}}\sim\frac{\sigma(z+\delta+b_i-a_{j'})}{\sigma(z+\delta+b_i-a_{j'}+w)}. \tag{21}$$

So from Eqs. (19) and (21), we can obtain

$$\frac{L(^{a}_{b}|z)^{j'}_{i}}{L(^{a}_{b}|z)^{i'}_{i}}\sim\frac{\sigma(z+\delta+b_i-a_{j'})}{\sigma(z+\delta+b_i-a_{i'})}. \tag{22}$$

In Eqs. (19)–(22), all δ's are the same. We note here that the δ may depend on i,i',j',a,b, but it does not depend on z, i.e., $\delta=\delta_i(abi'j')$. One sees from Eqs. (19), (20) and (22) $\delta_i(i'j')\cong\delta_i(j'i')\ (\mathrm{mod}\ \Lambda_\tau)$.

Similarly, from Eq. (5), we have

$$\frac{L(^{a+\hat{i}'}_{b+\hat{j}}|z)^{i'}_{i}}{L(^{a}_{b}|z)^{i'}_{j}}\sim\frac{\sigma(z+\delta+b_i-a_{i'}-w)}{\sigma(z+\delta+b_j-a_{i'})}, \tag{23}$$

$$\frac{L(^{a+\hat{i}'}_{b+\hat{i}}|z)^{i'}_{j}}{L(^{a}_{b}|z)^{i'}_{j}}\sim\frac{\sigma(z+\delta+b_j-a_{i'}-w)}{\sigma(z+\delta+b_j-a_{i'})}, \tag{24}$$

$$\frac{L(^{a+\hat{i}'}_{b+\hat{j}}|z)^{i'}_{i}}{L(^{a}_{b}|z)^{i'}_{i}}\sim\frac{\sigma(z+\delta+b_i-a_{i'}-w)}{\sigma(z+\delta+b_i-a_{i'})}, \tag{25}$$

$$\frac{L(^{a}_{b}|z)^{i'}_{j}}{L(^{a}_{b}|z)^{i'}_{i}}\sim\frac{\sigma(z+\delta+b_j-a_{i'})}{\sigma(z+\delta+b_i-a_{i'})}. \tag{26}$$

Here the dependence of the δ's are similar with the former. We also have $\delta=\delta^{i'}(abij)$ and $\delta^{i'}(ij)\cong\delta^{i'}(ji)\ (\mathrm{mod}\ \Lambda_\tau)$.

III. DEPENDENCE OF ELEMENTS OF *L*-MATRIX WITH SPECTRAL PARAMETER *z*

In this section, we study the dependence of $L(^{a}_{b}|z)^{j}_{i}$ with respect to z. It is found that there are only five possible forms of L-matrices in the whole lattice. We prove this in the following steps.

Step 1: Assume $i\neq i'$, $j\neq j'$. From Eqs. (22) and (26), we have

$$\frac{L(^{a}_{b}|z)^{j}_{i}}{L(^{a}_{b}|z)^{j'}_{i'}}=\frac{L(^{a}_{b}|z)^{j}_{i}L(^{a}_{b}|z)^{j'}_{i'}}{L(^{a}_{b}|z)^{j'}_{i}L(^{a}_{b}|z)^{j'}_{i'}}\sim\frac{\sigma(z+\delta_i+b_i-a_j)}{\sigma(z+\delta_i+b_i-a_{j'})}\frac{\sigma(z+\delta^{j'}+b_i-a_{j'})}{\sigma(z+\delta^{j'}+b_{i'}-a_{j'})}, \tag{27}$$

$$\frac{L(^{a}_{b}|z)^{j}_{i}}{L(^{a}_{b}|z)^{j'}_{i'}}=\frac{L(^{a}_{b}|z)^{j}_{i}L(^{a}_{b}|z)^{j}_{i'}}{L(^{a}_{b}|z)^{j}_{i'}L(^{a}_{b}|z)^{j'}_{i'}}\sim\frac{\sigma(z+\delta^{j}+b_i-a_j)}{\sigma(z+\delta^{j}+b_{i'}-a_j)}\frac{\sigma(z+\delta_{i'}+b_{i'}-a_j)}{\sigma(z+\delta_{i'}+b_{i'}-a_{j'})}, \tag{28}$$

giving

$$\frac{\sigma(z+\delta_i+b_i-a_j)}{\sigma(z+\delta_i+b_i-a_{j'})}\frac{\sigma(z+\delta_{i'}+b_{i'}-a_{j'})}{\sigma(z+\delta_{i'}+b_{i'}-a_j)}\frac{\sigma(z+\delta^{j'}+b_i-a_{j'})}{\sigma(z+\delta^{j'}+b_{i'}-a_{j'})}\frac{\sigma(z+\delta^{j}+b_{i'}-a_j)}{\sigma(z+\delta^{j}+b_i-a_j)}$$

$$\equiv\frac{(1)\ (2)\ (3)\ (4)}{(1')(2')(3')(4')}\sim 1, \tag{29}$$

where

$$\delta_i=\delta_i(a,b,j,j'),\quad \delta^j=\delta^j(a,b,i,i'),$$

$$\delta_{i'}=\delta_{i'}(a,b,j,j'),\quad \delta^{j'}=\delta^{j'}(a,b,i,i').$$

Obviously in Eq. (29), the zeroes of the numerator must coincide with those of the denominator. From this fact and noticing that a_j and $a_{j'}$, b_i and b_i' are generic complex numbers, we analyze all cases and obtain

$$\delta_i-\delta_{i'}\cong K(b_{i'}-b_i)\quad\text{and}\quad \delta^j-\delta^{j'}\cong K(a_j-a_{j'}),\quad K=0,1,2, \tag{30}$$

where $\delta_i=\delta_i(j\ j')$, $\delta_{i'}=\delta_{i'}(j\ j')$, $\delta^j=\delta^j(i\ i')$, $\delta^{j'}=\delta^{j'}(i\ i')$ and $K=K(i\ i'\ j\ j')$. From Eq. (29), we also have

$$\delta_i\cong\delta^{j'}\cong\delta_{i'}\cong\delta^j,\quad\text{when}\ \ K=0, \tag{31}$$

$$\delta_i(j\ \ j')-\delta^{j'}(i\ \ i')\cong b_{i'}-b_i+a_j-a_{j'},\quad\text{when}\ \ K=2. \tag{32}$$

Step 2: Since the dimension $n\geqslant 4$, we may choose three different i_1,i_2,i_3 and substitute $\{i_1,i_2\}$, $\{i_2,i_3\}$, $\{i_1,i_3\}$ as $\{i,i'\}$ into Eq. (30). This leads to the conclusion that K is independent of the indices i,i',j and j'.

These are the rules for the differences between $\delta_i(jj')$ and $\delta_{i'}(jj')$ and for the differences between $\delta^j(ii')$ and $\delta^{j'}(ii')$.

Step 3: Now let us study the differences between $\delta_i(j_1j_2)$ and $\delta_i(j_3j_4)$. Consider different indices j_1, j_2, j_3. We have from Eq. (22)

$$\frac{L(^a_b|z)^{j_1}_i}{L(^a_b|z)^{j_2}_i}\frac{L(^a_b|z)^{j_2}_i}{L(^a_b|z)^{j_3}_i}\sim\frac{\sigma(z+\delta_i(j_1j_2)+b_i-a_{j_1})}{\sigma(z+\delta_i(j_1j_2)+b_i-a_{j_2})}\frac{\sigma(z+\delta_i(j_2j_3)+b_i-a_{j_2})}{\sigma(z+\delta_i(j_2j_3)+b_i-a_{j_3})},$$

$$LHS=\frac{L(^a_b|z)^{j_1}_i}{L(^a_b|z)^{j_3}_i}\sim\frac{\sigma(z+\delta_i(j_1j_3)+b_i-a_{j_1})}{\sigma(z+\delta_i(j_1j_3)+b_i-a_{j_3})}.$$

This implies

$$\frac{\sigma(z+\delta_i(j_1j_2)+b_i-a_{j_1})}{\sigma(z+\delta_i(j_1j_2)+b_i-a_{j_2})}\frac{\sigma(z+\delta_i(j_2j_3)+b_i-a_{j_2})}{\sigma(z+\delta_i(j_2j_3)+b_i-a_{j_3})}\frac{\sigma(z+\delta_i(j_1j_3)+b_i-a_{j_3})}{\sigma(z+\delta_i(j_1j_3)+b_i-a_{j_1})}$$

$$\equiv\frac{(1)\ (2)\ (3)}{(1')\ (2')\ (3')}\sim 1.$$

From this equation, we obtain

$$\delta_i(j_1j_2)-k(a_{j_1}+a_{j_2})\cong\delta_i(j_2j_3)-k(a_{j_2}+a_{j_3})\cong\delta_i(j_1j_3)-k(a_{j_1}+a_{j_3}),\quad k=0,1, \tag{33}$$

where $k=k(ij_1j_2j_3)$.

Step 4: Consider unequal j_a, j_b, j_c, j_d, and substitute $\{j_a, j_b, j_c\}, \{j_b, j_c, j_d\}, \{j_a, j_c, j_d\}$ as $\{j_1, j_2, j_3\}$ into Eq. (33), we may show that k is also independent of the indices.

Therefore, from Eqs. (30) and (33), we conclude that one can always find a number C independent of indices $i\ j\ j'$ such that

$$C \cong \delta_i(jj') - k_0(a_j + a_{j'}) + Kb_i. \tag{34}$$

Similarly, we also find a number D satisfying

$$D \cong \delta^j(ii') + k^0(b_i + b_{i'}) - Ka_j, \tag{35}$$

where D, K, k_0, k^0 are independent of indices, and are fixed for a given lattice point (a,b).

Step 5: In the following, we discuss the cases $K=0$ and 2. For $K=0$, one has from Eqs. (30), (31), (34) and (35),

$$\delta_i(jj') \cong C + k_0(a_j + a_{j'}) \cong \delta^j(ii') \cong D - k^0(b_i + b_{i'}) \Rightarrow D - C = k_0(a_j + a_{j'}) + k^0(b_i + b_{i'}).$$

Thus, the k_0 and k^0 must be zero since C and D are independent of the indices. We have

$$\delta \cong C \cong D \cong \delta_i \cong \delta^j. \tag{36}$$

When $K=2$, from Eq. (32), we can find a number E satisfying

$$E \cong C \cong D \quad \text{and} \quad k_0 = k^0 = 1. \tag{37}$$

Step 6: We next study the relations for C, D, K, k_0, K^0 between adjacent lattice point (a,b) and $(a+\hat{i}', b+\hat{i})$. Equations (19) and (23) intertwine two lattice points. Notice that in Eqs. (19)–(22) [or in Eqs. (23)–(26)] the δ's are the same. By using these equations, we can prove that k, k_0, k^0 are unchanged for adjacent lattice points while

$$C(a+\hat{i}', b+\hat{i}) - C(a,b) = C' - C \cong -k_0 w\left(1 - \frac{2}{n}\right) + Kw\left(1 - \frac{1}{n}\right), \tag{38}$$

$$D(a+\hat{i}', b+\hat{i}) - D(a,b) = D' - D \cong k^0 w\left(1 - \frac{2}{n}\right) - Kw\left(1 - \frac{1}{n}\right). \tag{39}$$

These equations imply that Eq. (37) cannot be realized in two adjacent lattice points. Thus $K=2$ must be discarded.

According to K, k_0, k^0, when (a,b) is given, the elements of the L-matrix can take five forms.

(1) Form A(1). $K=1$, $k_0 = k^0 = 0$, from Eqs. (22), (34) and (35), we have

$$\frac{L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_i^j}{L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_i^0} \sim \frac{\sigma(z + \delta_i(0j) + b_i - a_j)}{\sigma(z + \delta_i(0j) + b_i - a_0)} \sim \frac{\sigma(z + C - b_i + b_i - a_j)}{\sigma(z + C - b_i + b_i - a_0)} = \frac{\sigma(z + C - a_j)}{\sigma(z + C - a_0)},$$

and from Eq. (26), we have

$$\frac{L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_i^0}{L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_0^0} \sim \frac{\sigma(z + \delta^0(i0) + b_i - a_0)}{\sigma(z + \delta^0(i0) + b_0 - a_0)} \sim \frac{\sigma(z + D + a_0 + b_i - a_0)}{\sigma(z + D + a_0 + b_0 - a_0)} = \frac{\sigma(z + D + b_i)}{\sigma(z + D + b_0)}.$$

Therefore, we obtain

$$L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_i^j \sim \frac{\sigma(z + C - a_j)}{\sigma(z + C - a_0)} \frac{\sigma(z + D + b_i)}{\sigma(z + D + b_0)} L\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right)_0^0 \sim \sigma(z + C - a_j)\sigma(z + D + b_i) F\left(\begin{smallmatrix} a \\ b \end{smallmatrix}|z\right). \tag{40}$$

By using Eqs. (27), (34) and (35), we can similarly derive other forms as follows.
(2) Form A(2). $K=1$, $k_0=0$, $k^0=1$, we have

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_i^j \sim \frac{\sigma(z+C-a_j)}{\sigma(z+D-b_i)} F\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right). \tag{41}$$

(3) Form A(3). $K=1$, $k_0=1$, $k^0=1$, we have

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_i^j \sim \frac{1}{\sigma(z+C+a_j)\sigma(z+D-b_i)} F\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right). \tag{42}$$

(4) Form A(4). $K=1$, $k_0=1$, $k^0=0$, we have

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_i^j \sim \frac{\sigma(z+D+b_i)}{\sigma(z+C+a_j)} F\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right). \tag{43}$$

(5) Form B. $K=0$, $k_0=0$, $k^0=0$; from Eqs. (27) and (36), one obtains

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_i^j \sim \sigma(z+\delta+b_i-a_j) F\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right). \tag{44}$$

The relation of $F(z)$ between adjacent lattice points (a,b) and (a',b') is discussed in Appendix A.

In conclusion, there can be at most five classes of L-matrices in the whole lattice. Each of them is of the same form at all lattice points.

We must check if these inductive relations are integrable in the whole lattice. That is, if one goes from (a,b) to $(a''=a+\hat{i}'+\hat{j}', b''=b+\hat{i}+\hat{j})$ via different paths, the resulting C'' D'' $F''(z)$ should be the same. The conclusion is affirmative.

For $a\equiv(m_0,m_1,\ldots,m_{n-1})$, define $m\equiv\Sigma_i m_i$. Thus $m(a'=a+\hat{i}', b'=b+\hat{i})=m(a,b)+1$. We can express five forms as follows, which satisfy all relations of adjacent lattice points,
(1) Form A(1). Let $C=C_0+mw(1-1/n)$, $D=D_0-mw(1-1/n)$. Then

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_k^l \sim \sigma\left(z+C_0+mw\left(1-\frac{1}{n}\right)-a_l\right)\sigma\left(z+D_0-mw\left(1-\frac{1}{n}\right)+b_k\right)F_0(z) \tag{45}$$

and C_0, D_0, $F_0(z)$ are unchanged in the whole lattice.
(2) Form A(2). Let

$$C=C_0+mw\left(1-\frac{1}{n}\right), \qquad D=D_0-m\frac{w}{n},$$

$$F(z)=F_0(z)\prod_{j=0}^{n-1}\sigma\left(z+D_0-m\frac{w}{n}-b_j\right).$$

We then have

$$\frac{F'(z)}{F(z)}=\frac{\sigma(z+D_0-(m+1)\,w/n-b_i-w(1-1/n))}{\sigma(z+D_0-m\,w/n-b_i)}=\frac{\sigma(z+D-b_i-w)}{\sigma(z+D-b_i)}.$$

Thus,

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_k^l \sim \sigma\left(z+C_0+mw\left(1-\frac{1}{n}\right)-a_l\right)\prod_{j(\neq k)}\sigma\left(z+D_0-m\frac{w}{n}-b_j\right)F_0(z) \tag{46}$$

and C_0, D_0, $F_0(z)$ are unchanged in the whole lattice.

(3) Form A(3). Let

$$C=C_0+m\frac{w}{n},\qquad D=D_0-m\frac{w}{n},$$

$$F(z)=F_0(z)\prod_{j=0}^{n-1}\sigma\left(z+C_0+m\frac{w}{n}+a_j\right)\sigma\left(z+D_0-m\frac{w}{n}-b_j\right).$$

We then have

$$\frac{F'(z)}{F(z)}=\frac{\sigma(z+C+a_{i'}+w)}{\sigma(z+C+a_{i'})}\frac{\sigma(z+D-b_i-w)}{\sigma(z+D-b_i)}.$$

Thus,

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_k^l\sim\prod_{j(\neq l)}\sigma\left(z+C_0+m\frac{w}{n}+a_j\right)\prod_{j(\neq k)}\sigma\left(z+D_0-m\frac{w}{n}-b_j\right)F_0(z) \tag{47}$$

and C_0, D_0, $F_0(z)$ are unchanged in the whole lattice.

(4) Form A(4). Let

$$C=C_0+m\frac{w}{n},\qquad D=D_0-mw\left(1-\frac{1}{n}\right),$$

$$F(z)=F_0(z)\prod_{j=0}^{n-1}\sigma\left(z+C_0+m\frac{w}{n}+a_j\right).$$

We then have

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_k^l\sim\sigma\left(z+D_0-mw\left(1-\frac{1}{n}\right)+b_k\right)\prod_{j(\neq l)}\sigma\left(z+C_0+m\frac{w}{n}+a_j\right)F_0(z) \tag{48}$$

and C_0, D_0, $F_0(z)$ are unchanged in the whole lattice.

(5) Form B.

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_k^l\sim\sigma(z+\delta_0+b_k-a_l)F_0(z) \tag{49}$$

and δ_0, $F_0(z)$ are unchanged in the whole lattice.

Thus we can establish the L-matrix in the whole lattice, if we can properly choose the coefficients of the elements of L-matrix. We will discuss this problem in the next section.

IV. THE COEFFICIENTS IRRELEVANT WITH *z* OF THE ELEMENTS OF *L*-MATRIX

In this section, we study the sufficient condition of L-matrices for DYBR and derive the equations satisfied by the coefficients irrelevant with z of the elements of L-matrix.

As an example, we study the form B which is useful in the later. From Eq. (44) for the form B, the L-matrix takes the form

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)_i^j=\left(\begin{smallmatrix}a\\b\end{smallmatrix}\right)_i^j\sigma(z+\delta+b_i-a_j)F(z), \tag{50}$$

$$L\left(\begin{smallmatrix}a+\hat{i}'\\b+\hat{i}\end{smallmatrix}|z\right)_j^{j'}=\left(\begin{smallmatrix}a+\hat{i}'\\b+\hat{i}\end{smallmatrix}\right)_j^{j'}\sigma(z+\delta+b'_j-a'_{j'})F(z). \tag{51}$$

Then, substituting the above equation and Eq. (1) for the R-matrix into the DYBR Eq. (2) and noticing the fact

$$a'_{j'}=a_{j'}+w\left(\delta_{i'j'}-\frac{1}{n}\right),\quad b'_j=b_j+w\left(\delta_{ij}-\frac{1}{n}\right)\quad(\text{for } a'=a+\hat{i}',\ b'=b+\hat{i}),$$

we obtain the equations for the coefficients:

$$\binom{a}{b}_i^{i'}\binom{a+\hat{i}'}{b+\hat{i}}_i^{i'}=\binom{a}{b}_i^{i'}\binom{a+\hat{i}'}{b+\hat{i}}_i^{i'},\tag{52}$$

which is trivially satisfied, and

$$\binom{a}{b}_i^{i'}\binom{a+\hat{i}'}{b+\hat{i}}_{i'}^{j'}-\frac{\sigma(a_{i'j'}-w)}{\sigma(a_{i'j'}+w)}\binom{a}{b}_i^{j'}\binom{a+\hat{j}'}{b+\hat{i}}_i^{i'}=0\quad(i'\neq j'),\tag{53}$$

$$\binom{a}{b}_i^{i'}\binom{a+\hat{i}'}{b+\hat{i}}_j^{i'}-\binom{a}{b}_j^{i'}\binom{a+\hat{i}'}{b+\hat{j}}_i^{i'}=0\quad(i\neq j),\tag{54}$$

$$\begin{aligned}&\binom{a}{b}_j^{i'}\binom{a+\hat{i}'}{b+\hat{j}}_i^{j'}\sigma(a_{i'j'}+b_{ij})\sigma(w)+\binom{a}{b}_i^{i'}\binom{a+\hat{i}'}{b+\hat{i}}_j^{j'}\sigma(b_{ij}-w)\sigma(a_{i'j'})\\&-\binom{a}{b}_j^{j'}\binom{a+\hat{j}'}{b+\hat{j}}_i^{i'}\sigma(a_{i'j'}-w)\sigma(b_{ij})=0\quad(i\neq j,\ i'\neq j'),\end{aligned}\tag{55}$$

respectively. In the derivation, we have used the addition formula

$$\begin{aligned}&\sigma(u+x)\sigma(u-x)\sigma(v+y)\sigma(v-y)-\sigma(u+y)\sigma(u-y)\sigma(v+x)\sigma(v-x)\\&=\sigma(u+v)\sigma(u-v)\sigma(x+y)\sigma(x-y).\end{aligned}\tag{56}$$

Define

$$\begin{aligned}&\binom{a}{b}_i^{i'}\times\prod_{l(\neq i')}\sigma(a_l-a_{i'})=\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]_i^{i'},\\&\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]_i^{i'}\left[\begin{smallmatrix}a+\hat{i}'\\b+\hat{i}\end{smallmatrix}\right]_{j'}^{j'}=Y_i^{i'j'}{}_{j'}.\end{aligned}\tag{57}$$

Then for form B, we rewrite Eqs. (53)–(55) as

$$Y_i^{i'j'}{}_{i'}-Y_i^{j'i'}{}_{i'}=0\quad(i'\neq j'),\tag{58}$$

$$Y_i^{i'i'}{}_{j'}-Y_j^{i'i'}{}_{i'}=0\quad(i\neq j),\tag{59}$$

$$\sigma(w)\sigma(a_{i'j'}+b_{ij})Y_j^{i'j'}{}_{i'}+\sigma(a_{i'j'})\sigma(b_{ij}-w)Y_i^{i'j'}{}_{j'}-\sigma(a_{i'j'}+w)\sigma(b_{ij})Y_j^{j'i'}{}_{i'}=0\quad(i\neq j,\ i'\neq j').\tag{60}$$

With the same procedure, one can also show that all A forms [forms A(1)–A(4)] share common coefficient relations

$$Y_i^{i'j'}{}_{i'}-\frac{\sigma(a_{i'j'}-w)}{\sigma(a_{i'j'}+w)}Y_i^{j'i'}{}_{i'}=0\quad(i'\neq j'),\tag{61}$$

$$Y_i^{i'i'}{}_{j'}-Y_j^{i'i'}{}_{i'}=0\quad(i\neq j),\tag{62}$$

$$Y_j^{i'j'}{}_{i'}=Y_i^{i'j'}{}_{j'}=\frac{\sigma(a_{i'j'}-w)}{\sigma(a_{i'j'}+w)}Y_j^{j'i'}{}_{i'}\quad(i\neq j,\ i'\neq j').\tag{63}$$

For the coefficients of form A(i) ($i=1,2,3,4$), we can easily find the rule. Consider a function $G(a,b)$ on a lattice points ($a=\Sigma_j m_j^a \hat{j}, b=\Sigma_i m_i^b \hat{i}$). From the lattice (a,b), by using the relation $G(a+\hat{i}',b+\hat{i})=G(a,b)[{}_b^a]_i^{i'}$, we can construct the function on the other lattice point. Because of Eqs. (61)–(63), we can obtain the same $G(a+\hat{i}'+\hat{j}',b+\hat{i}+\hat{j})$ through different paths from (a,b) to $(a+\hat{i}'+\hat{j}',b+\hat{i}+\hat{j})$. So this procedure is integrable. This implies that there must exist a function $G(a,b)$ which can determine $[{}_b^a]_i^{i'}$ with

$$[{}_b^a]_i^{i'}=G(a+\hat{i}',b+\hat{i})/G(a,b). \tag{64}$$

Hence, we can solve the problem of form A completely. However, to the coefficients of the form B, its rule is more complicated and we will discuss it in the next section.

Obviously, if we take a gauge transformation

$$[{}_b^a]_i^j \to \overline{[{}_b^a]}_i^j = [{}_b^a]_i^j \frac{g(a+\hat{j},b+\hat{i})}{g(a,b)},$$

and if $[{}_b^a]_i^j$ satisfies Eqs. (61)–(63), $\overline{[{}_b^a]}_i^j$ also satisfies these equations. In this sense, all form A coefficients are gauge equivalent to a constant.

V. THE ALGEBRA FOR FORM B COEFFICIENTS

A. The PBW base of the algebra

In this section, we give the PBW base of the algebra for form B coefficients. The main result is Theorem 1. We also give the center of this algebra. Equations (58)–(60) can be regarded as the algebraic relations which are satisfied by the operators in the lattice ($a=\Sigma_{j=0}^{n-1} m_j^a \hat{j}, b=\Sigma_{i=0}^{n-1} m_i^b \hat{i}$). We define a new operator

$$A_i^{i'} \equiv [{}_b^a]_i^{i'} \Gamma_i^{i'}, \tag{65}$$

where

$$\Gamma_i^{i'} f(a,b) = f(a+\hat{i}',b+\hat{i}) \Gamma_i^{i'}. \tag{66}$$

Namely, we regard the a,b as operators; $\Gamma_i^{i'}$ is not commutative with the function of a,b. In this way, we have the following exchange relations of the operators $\{A_i^{i'}\}$

$$A_i^{i'} A_i^{j'} = A_i^{j'} A_i^{i'} \qquad (i' \neq j'), \tag{67a}$$

$$\sigma(a_{i'j'}+w)\sigma(b_{ij}) A_j^{j'} A_i^{i'} = \sigma(a_{i'j'})\sigma(b_{ij}-w) A_i^{i'} A_j^{j'} + \sigma(w)\sigma(a_{i'j'}+b_{ij}) A_j^{i'} A_i^{j'} \qquad (i \neq i',\ j \neq j'), \tag{67b}$$

$$A_i^{i'} A_j^{i'} = A_j^{i'} A_i^{i'} \qquad (i \neq j). \tag{67c}$$

These equations are equivalent relations to the Felder and Varchenko elliptic quantum algebra under special condition. It is worth noting that in Eq. (67b), the coefficients should be regarded as the functions of operators and they do not commute with A_i^j. These equations are irrelevant with the parameter z. This situation is similar to the relation between the Sklyanin algebra[21–25] and the YBR of the Belavin model.[26–28] In formulation, Eq. (67b) is also similar to the function R-matrices given by Shibukawa and Ueno.[18]

Using the (a) and (b) of Eq. (67), we can exchange the order of the up-indices of a pair of operators $A_i^{j'} A_j^{i'}$. So $A_i^{j'} A_j^{i'}$ can be written as linear combination of $A_i^{i'} A_j^{j'}$ and $A_j^{i'} A_i^{j'}$. Therefore,

we can write the product of three operators $A_i^{i'}A_j^{j'}A_k^{k'}$ as the linear combination of $A_\cdot^{k'}A_\cdot^{j'}A_\cdot^{i'}$. This procedure can be done in two different ways. For the two ways, by using Eqs. (58)–(60), we can show that according to the rules (67a) and (67b) [we will simplify it as (ab)], if the product of three operators $A_i^{i'}A_j^{j'}A_k^{k'}$ is changed to the linear combination of $A_\cdot^{k'}A_\cdot^{j'}A_\cdot^{i'}$ by two different paths, their results are equal. The paths are as follows:

$$(A)\quad i'j'k'\to i'k'j'\to k'i'j'\to k'j'i',$$

$$(B)\quad i'j'k'\to j'i'k'\to j'k'i'\to k'j'i'.$$

In the above transformation, we think that the result of the (ab) transformation on two adjacent operators with the same up-indices does not change the order of them, namely, $A_i^{i'}A_j^{i'}\Rightarrow A_i^{i'}A_j^{i'}$. And we think the associative and the distributive law are satisfied in the transformation.

Furthermore, if we consider the rule (67c), the linear expansions of operator products $A_i^{i'}A_j^{j'}A_k^{j'}$ and $A_i^{i'}A_k^{j'}A_j^{j'}$ by $A_\cdot^{j'}A_\cdot^{j'}A_\cdot^{i'}$ via the (ab) transformation are equal. Therefore, we also call this fact the Yang–Baxter equation (YBE).

Similarly, after $A_i^{j'}A_j^{j'}A_k^{i'}$ and $A_j^{j'}A_i^{j'}A_k^{i'}$ change to the linear combination of the $A_\cdot^{i'}A_\cdot^{j'}A_\cdot^{j'}$ by (ab), these two expansion are equal via the rule (67c).

For the coefficient algebra (or Yang–Baxter algebra) which we discussed above, we will give it a PBW base in the following. We first give some definitions for establishing the base.

Definition 1: Bunch: A bunch is a polynomial (or monomial) of operator A's, in which all terms have the same number of A's and the upper indices of A's in all terms are arranged in the same way.

Example:

$$B=\sum_{i_1i_2i_3i_4} C_{i_1i_2i_3i_4}A_{i_1}^{j_1}A_{i_2}^{j_2}A_{i_3}^{j_3}A_{i_4}^{j_4}$$

is a bunch. A polynomial is always a bunch.

Definition 2: Inverse order number: To any two integers i',j' with a given order, we say the inverse order number is 1 if $i'>j'$ and it is 0 if $i'\leqslant j'$. And the inverse order number of a successive product $A_\cdot^{i'}A_\cdot^{j'}A_\cdot^{k'}\cdots$ is the sum of the inverse order numbers of all up-index pairs.

Definition 3: Normal order product: The (ab) normal order product is a successive product of operators in which the up-indices are arranged from smaller to bigger when inspecting from the left to the right, while the arrangement of the down-indices can be arbitrary. The (abc) normal order product is that the up-indices are arranged from the smaller to the bigger and the down-indices of the operators with the same up-indices are also arranged from smaller to bigger. Their inverse order numbers are zero.

Example: $A_2^1A_1^1A_1^2A_3^2A_5^3A_1^4A_3^5A_1^5$ is an (ab) normal order product but is not an (abc) normal order product. By using the rule (67c), we can change it to the (abc) normal order product $A_1^1A_2^1A_1^2A_3^2A_5^3A_1^4A_1^5A_3^5$.

Definition 4: Normal order expansion: The (ab) normal order expansion of a polynomial of A's is a procedure in which we change each term of the polynomial into a bunch of (ab) normal order products by only using rules (67a) and (67b). We also call the final resulting polynomial as the (ab) normal expansion of the original polynomial.

The (abc) normal order expansion is a procedure, in which we first perform the (ab) normal order expansion and then we rearrange each term of the resulting polynomial into (abc) normal order product by using rule (67c). We also call the final result as an (abc) normal expansion of the original polynomial.

Then, we have a theorem.

Theorem 1: *Transforming on a polynomial of operators A_i^j by using the rules (abc) of Eq. (67) does not change its (abc) normal order expansion.*

It is worth noting that the coefficients of the expansions are functions of the parameters $\{a,b\}$, and they do not commute with operator A_i^j.

The detailed proof of the theorem will be given in Appendix B.

Corollary: The (abc) normal order products are linearly independent.

Proof: If there were a linear relation $\Sigma C_i g_i=0$, where g_i are (abc) normal order products, the LHS must be able to be changed to zero via Eq. (67). However, each operation does not change the (abc) expansion. Thus it is impossible since C_i are not all zero. □

Thus the set of all (abc) normal order products is the PBW base of the algebra defined by Eq. (67).

B. The center of the algebra

By standard procedure, we may obtain the center of elliptic quantum group (the detail will be given elsewhere),

$$I=\frac{\Delta(a)}{\Delta(b)}\mathrm{Det}\ L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right),$$

where $\Delta(a)=\Pi_{i<j}\sigma(a_{ij}),\Delta(b)=\Pi_{i<j}\sigma(b_{ij})$,

$$\mathrm{Det}\ L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)=\sum_P (-1)^{[\mathrm{Sign}P\left(\begin{smallmatrix}0&1&\cdots&n-1\\ \mu_0&\mu_1&\cdots&\mu_{n-1}\end{smallmatrix}\right)]}\ L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)^0_{\mu_0}L\left(\begin{smallmatrix}a+\hat{0}\\b+\hat{\mu}_0\end{smallmatrix}|z+w\right)^1_{\mu_1}\cdots L\left(\begin{smallmatrix}a+\hat{0}+\hat{1}+\cdots+\widehat{n-2}\\b+\hat{\mu}_0+\hat{\mu}_1+\cdots+\hat{\mu}_{n-2}\end{smallmatrix}|z+(n-1)w\right)^{n-1}_{\mu_{n-1}},$$

and P's are permutations of integers 0, 1, …, $n-1$. This agrees with that of Ref. 12 for $n=2$.

In the case of

$$L\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)^{i'}_i=\sigma(z+\delta+b_i-a_{i'})A_i^{i'},$$

the quantum determinant can be written as

$$I\left(\begin{smallmatrix}a\\b\end{smallmatrix}|z\right)=\sum_P (-1)^{[\mathrm{Sign}P\left(\begin{smallmatrix}0&1&\cdots&n-1\\ \mu_0&\mu_1&\cdots&\mu_{n-1}\end{smallmatrix}\right)]}\sigma(z+\delta+b_{\mu_0}-a_0)\sigma(z+w+\delta+b_{\mu_1}-a_1)\cdots$$
$$\times\sigma(z+(n-1)w+\delta+b_{\mu_{n-1}}-a_{n-1})A^0_{\mu_0}A^1_{\mu_1}\cdots A^{n-1}_{\mu_{n-1}}.$$

It is easy to check

$$\Phi(z)_{\mu_0\cdots\mu_{n-1}}\equiv\sigma(z+\delta+b_{\mu_0}-a_0)\cdots\sigma(z+(n-1)w+\delta+b_{\mu_{n-1}}-a_{n-1})$$

is quasi-doubly periodic in τ and 1:

$$\Phi(z+1)=(-1)^n\Phi(z),$$

$$\Phi(z+\tau)=\exp\left[-2\pi i\left(\frac{n\tau}{2}+n\delta+nz+\frac{n(n-1)}{2}w+\frac{n}{2}+\sum_i b_{\mu_i}-\sum_i a_i\right)\right]\Phi(z)$$
$$=\exp\left[-2\pi i\left(\frac{n\tau}{2}+n\delta+nz+\frac{n(n-1)}{2}w+\frac{n}{2}\right)\right]\Phi(z)$$

for all $\mu_0,\ldots,\mu_{n-1}$ being a permutation of $(0,1,\ldots,n-1)$. Therefore, from a theorem of such function (see Ref. 29), we have

$$\Phi(z)_{\mu_0,\ldots,\mu_{n-1}}=\sum_{i=0}^{n-1} C^i_{\mu_0,\ldots,\mu_{n-1}} f_i(z), \tag{68}$$

where $\{f_i(z)\}$ are base functions of the space of such quasi-double periodic function. For example, we may choose

$$f_i(z)=\theta\begin{bmatrix}\frac{1}{2}-\frac{i}{n}\\ \frac{1}{2}\end{bmatrix}\left(nz+n\delta+\frac{n(n-1)w}{2}+\frac{n-1}{2},\ n\tau\right).$$

One can obtain $C^i_{\mu_0,\ldots,\mu_{n-1}}$ by choosing n points $z_1,\ldots,z_n$ in the above equation and solve a set of n linear equations. We then derive the n center elements for the algebra. From

$$I(^a_b|z)=\sum_i f_i(z)\left\{\sum_P (-1)^{[\mathrm{Sign}P(^{0\ 1\ \cdots n-1}_{\mu_0\mu_1\cdots\mu_{n-1}})]} C^i_{\mu_0,\ldots,\mu_{n-1}} A^0_{\mu_0}A^1_{\mu_1}\cdots A^{n-1}_{\mu_{n-1}}\right\}\equiv\sum_i f_i(z)J_i,$$

we see that $[\Delta(a)/\Delta(b)]J_i$ are the center elements of the algebra.

VI. A KNOWN SOLUTION FOR THE FORM B COEFFICIENTS

The equations [Eqs. (58)–(60)] of form B coefficients seem simple but they interrelate the values of the coefficients $[^a_b]^{i'}_i$ between different lattice points. To our best knowledge, we only know the analytic solution

$$[^a_b]^{i'}_i=\prod_{j(\neq i')}\sigma(\delta'+b_i-a_{j'}), \tag{69}$$

which can be derived by the factorized operator of Eq. (15),

$$L_\delta(^a_b|z)^{i'}_i=\sigma(z+\delta+b_i-a_{i'})\prod_{j(\neq i')}\frac{\sigma(\delta'+b_i-a_j)}{\sigma(a_{i'}-a_j)}\equiv(-1)^{n-1}\sigma(z+\delta+b_i-a_{i'})(^a_b)^{i'}_i$$

and

$$[^a_b]^{i'}_i=(^a_b)^{i'}_i\prod_{j(\neq i')}\sigma(a_j-a_{i'}).$$

The corresponding $Y^{i'j'}_i$ is

$$Y^{i'j'}_i=[^a_b]^{i'}_i[^{a+\hat{i}'}_{b+\hat{i}}]^{j'}_j=\prod_{l(\neq i')}\sigma(\delta'+b_i-a_l)\prod_{m(\neq j')}\sigma(\delta'+b'_j-a'_m). \tag{70}$$

By using the addition formula (56), we can check that the solution satisfies Eqs. (58)–(60) directly.

This solution can be proved to be equivalent with the results obtained by using the symmetry fusion method for the $A^{(1)}_{n-1}$ model in Ref. 9. And it is also equivalent with the evaluation modules $(n=2)$ obtained by Felder and Varchenko in Ref. 12.

Equation (69) is the only known solution for the form B coefficients. We do not know if there are other analytic solutions. This is still an open question worthy of study.

APPENDIX A: THE RELATION $F(z)$ BETWEEN ADJACENT LATTICE POINTS

Suppose we go from (a,b) to $(a+\hat{i}',b+\hat{i})$. Then we have $a_j'=a_j+w(\delta_{i'j}-1/n)$, $b_j'=b_j+w(\delta_{ij}-1/n)$. From Eqs. (38) and (39), we may choose

$$C'-C=-k_0w\left(1-\frac{2}{n}\right)+Kw\left(1-\frac{1}{n}\right), \tag{A1}$$

$$D'-D=k^0w\left(1-\frac{2}{n}\right)-Kw\left(1-\frac{1}{n}\right) \tag{A2}$$

without loss of generality. This is the explicit relation of CD (δ E) between adjacent lattice points for each form of L-matrices. From Eq. (19)

$$\frac{L\binom{a+\hat{i}'}{b+\hat{i}}|z)_i^{j'}}{L\binom{a}{b}|z)_i^{i'}}\sim\frac{\sigma(z+\delta_i(i'j')+b_i-a_{j'}+w)}{\sigma(z+\delta_i(i'j')+b_i-a_{i'})}$$

and from Eq. (34)

$$\delta_i(i'j')\cong C-Kb_i+k_0(a_{i'}+a_{j'}),$$

we have

$$\frac{L\binom{a+\hat{i}'}{b+\hat{i}}|z)_i^{j'}}{L\binom{a}{b}|z)_i^{i'}}\sim\frac{\sigma(z+C+(1-K)b_i+k_0a_{i'}+(k_0-1)a_{j'}+w)}{\sigma(z+C+(1-K)b_i+(k_0-1)a_{i'}+k_0a_{j'})}. \tag{A3}$$

The relations of $F(z)$ and $F'(z)$ [the new function at lattice point (a',b')] can be obtained by putting the explicit forms of five forms of L-matrices [Eqs. (40)–(44)] into Eq. (A3). For example, we study the A(1) form.

(1) $A(1)\overset{i\,i'}{\rightarrow}A(1)$ $K=1$, $k_0=k^0=0$.

From Eqs. (A1) and (A2), one has

$$C'=C+w\left(1-\frac{1}{n}\right),\quad D'=D-w\left(1-\frac{1}{n}\right). \tag{A4}$$

Then Eqs. (40) and (A3) yield

$$\begin{aligned}\frac{L\binom{a'}{b'}|z)_i^{j'}}{L\binom{a}{b}|z)_i^{i'}}&\sim\frac{\sigma(z+C'-a_{j'}')\sigma(z+D'+b_i')F'(z)}{\sigma(z+C-a_{i'})\sigma(z+D+b_i)F(z)}\\&\sim\frac{\sigma(z+C-a_{j'}+w)\sigma(z+D+b_i)F'(z)}{\sigma(z+C-a_{i'})\sigma(z+D+b_i)F(z)}\\&\sim\frac{\sigma(z+C-a_{j'}+w)}{\sigma(z+C-a_{i'})}\Rightarrow\frac{F'(z)}{F(z)}\sim1.\end{aligned} \tag{A5}$$

Other A(i)'s are similar. We list them in the following.

(2) $A(2)\overset{i\,i'}{\rightarrow}A(2)$ $K=1$, $k_0=0$, $k^0=1$.

Equations (A1) and (A2) give

$$C'=C+w\left(1-\frac{1}{n}\right),\quad D'=D-\frac{w}{n}. \tag{A6}$$

From Eqs. (41) and (A3), we have

$$\frac{F'(z)}{F(z)} \sim \frac{\sigma(z+D-b_i-w)}{\sigma(z+D-b_i)}.$$

(3) $A(3) \overset{i\,i'}{\to} A(3)$ $K=1,\ k_0=k^0=1.$

$$\frac{F'(z)}{F(z)} \sim \frac{\sigma(z+C+a_{i'}+w)\sigma(z+D-b_i-w)}{\sigma(z+C+a_{i'})\sigma(z+D-b_i)}. \tag{A7}$$

(4) $A(4) \overset{i\,i'}{\to} A(4)$ $K=1,\ k_0=1,\ k^0=0.$

$$\frac{F'(z)}{F(z)} \sim \frac{\sigma(z+C+a_{i'}+w)}{\sigma(z+C+a_{i'})}. \tag{A8}$$

(5) $B \overset{i\,i'}{\to} B$ $K=0,\ k_0=k^0=0.$

From Eq. (A1) and noting $\delta \cong C \cong D$ for this class, we have $C' \cong D' \cong \delta' \cong C \cong D \cong \delta$. We may choose $\delta' = \delta$ without loss of generality. Equations (44) and (A3) imply

$$\begin{aligned}\frac{L(^{a'}_{b'}|z)^{j'}_{i}}{L(^{a}_{b}|z)^{i'}_{i}} &\sim \frac{\sigma(z+\delta'+b'_i-a'_{j'})F'(z)}{\sigma(z+\delta+b_i-a_{i'})F(z)} \\ &= \frac{\sigma(z+\delta+b_i-a_{j'}+w)F'(z)}{\sigma(z+\delta+b_i-a_{i'})F(z)} \\ &\sim \frac{\sigma(z+\delta+b_i-a_{j'}+w)}{\sigma(z+\delta+b_i-a_{i'})} \\ \Rightarrow \frac{F'(z)}{F(z)} &\sim 1. \end{aligned} \tag{A9}$$

APPENDIX B: THE PROOF OF THEOREM 1

To prove the theorem, first, we prove the following lemma.

Lemma 1: To any successive product of operators, if we transform it by using Eqs. (67a) and (67b) such that at each step its inverse order number is reduced (the adjacent up-indices are exchanged when the left one is bigger than that of the right one), the final result of the (ab) normal order expansion is unique.

Here we assume that in this transformation, two adjacent operators with the same up-indices do not change the order. And we think that in every step of the transformation, the location of two exchanged operators in all terms of the linear combination after the previous step are same.

Proof: We can do the procedure by different paths. For example, if we want to obtain (ab) normal order expansion of $A^4_{\cdot}A^4_{\cdot}A^6_{\cdot}A^5_{\cdot}A^2_{\cdot}A^2_{\cdot}$, we may do this in following different paths:

(1) $$A^4_{\cdot}A^4_{\cdot}A^6_{\cdot}A^5_{\cdot}A^2_{\cdot}A^2_{\cdot} \equiv (446522) \underset{Q_{2,3}}{\to} (446252) \underset{Q_{1,2}}{\to} (442652) \underset{Q_{2,3}}{\to} (442625) \underset{Q_{5,6}}{\to} (442265) \underset{Q_{4,5}}{\to} (424265) \underset{Q_{3,4}}{\to} (422465) \underset{Q_{4,5}}{\to} (242465) \underset{Q_{3,4}}{\to} (224465) \underset{Q_{2,3}}{\to} (224456),$$

(2) $$A^4_{\cdot}A^4_{\cdot}A^6_{\cdot}A^5_{\cdot}A^2_{\cdot}A^2_{\cdot} \equiv (446522) \underset{Q_{1,2}}{\to} (445622) \underset{Q_{5,6}}{\to} (445262) \underset{Q_{4,5}}{\to} (442562) \underset{Q_{3,4}}{\to} (424562) \underset{Q_{2,3}}{\to} (244562) \underset{Q_{3,4}}{\to} (244526) \underset{Q_{4,5}}{\to} (244256) \underset{Q_{3,4}}{\to} (242456) \underset{Q_{2,3}}{\to} (224456),$$

where $Q_{i,i+1}$ denotes the exchange of the ith operator A and $i+1$th operator A by using rules (67a) and (67b). We may denote such a procedure by the product of a set of exchange operators $\{Q_{i,i+1}\}$ acting on the bunch. For the path (1) in the example, we have

$$Q_{5,6}Q_{2,3}Q_{1,2}Q_{3,4}Q_{2,3}Q_{4,5}Q_{5,6}Q_{3,4}Q_{4,5}A^4_{\cdot}A^4_{\cdot}A^6_{\cdot}A^5_{\cdot}A^2_{\cdot}A^2_{\cdot} = \sum \cdots A^2_{\cdot}A^2_{\cdot}A^4_{\cdot}A^4_{\cdot}A^5_{\cdot}A^6_{\cdot}.$$

For the path (2), we have

$$Q_{2,3}Q_{3,4}Q_{4,5}Q_{5,6}Q_{1,2}Q_{2,3}Q_{3,4}Q_{4,5}Q_{3,4}A^4_{\cdot}A^4_{\cdot}A^6_{\cdot}A^5_{\cdot}A^2_{\cdot}A^2_{\cdot}=\sum \cdots A^2_{\cdot}A^2_{\cdot}A^4_{\cdot}A^4_{\cdot}A^5_{\cdot}A^6_{\cdot}.$$

In general cases, a path of such procedure is denoted by

$$Q_{i_1,i_1+1}Q_{i_2,i_1+1}\cdots Q_{i_s,i_s+1}(A^{j_1}_{k_1}A^{j_2}_{k_2}\cdots A^{j_l}_{k_l})=\sum_{j'k'} c^{t_1\cdots k'_1\cdots}_{j_1\cdots k_1\cdots}A^{j_{t_1}}_{k'_1}A^{j_{t_2}}_{k'_2}\cdots A^{j_{t_l}}_{k'_l} \tag{B1}$$

with $j_{t_1}\leqslant j_{t_2}\leqslant\cdots\leqslant j_{t_l}$. Note that the original arrangement $\{j_1j_2\cdots j_l\}$ and the final arrangement $\{j_{t_1}j_{t_2}\cdots j_{t_l}\}$ are same for whatever path of the (ab) normal product expansion we choose.

Assume there is another path for (ab) normal product expansion

$$Q_{i'_1,i'_1+1}Q_{i'_2,i'_1+1}\cdots Q_{i'_s,i'_s+1}(A^{j_1}_{k_1}A^{j_2}_{k_2}\cdots A^{j_l}_{k_l})=\sum_{j'k'} d^{t_1\cdots k'_1\cdots}_{j_1\cdots k_1\cdots}A^{j_{t_1}}_{k'_1}A^{j_{t_2}}_{k'_2}\cdots A^{j_{t_l}}_{k'_l}. \tag{B2}$$

Consider the corresponding two products of exchange operators in the permutation group

$$P^{(1)}=P_{i_1,i_1+1}P_{i_2,i_2+1}\cdots P_{i_s,i_s+1}$$

and

$$P^{(2)}=P_{i'_1,i'_1+1}P_{i'_2,i'_2+1}\cdots P_{i'_s,i'_s+1}.$$

They must all be able to permute the arrangement $\{j_1\cdots j_l\}$ into $\{j_{t_1}j_{t_2}\cdots j_{t_l}\}$. Although some of the j's may be the same, the permutation $\{^{1\,2\cdots l}_{t_1t_2\cdots t_l}\}$ is unique, however. This is due to the rule we do not exchange adjacent operators with same upper indices. In permutation group, we can express an arbitrary element by product of exchange operators in different ways. However, we can always make them equal step by step using the following equations:

$$P_{i,i+1}P_{i,i+1}=id, \tag{B3}$$

$$P_{i,i+1}P_{j,j+1}=P_{j,j+1}P_{i,i+1}\quad (i+1<j), \tag{B4}$$

$$P_{i,i+1}P_{i+1,i+2}P_{i,i+1}=P_{i+1,i+2}P_{i,i+1}P_{i+1,i+2}. \tag{B5}$$

Thus $P^{(1)}$ can be changed to $P^{(2)}$ by using these equations step by step.

On the other hand, the $\{Q_{i,i+1}\}$ operators have the same properties. We have checked

$$Q_{i,i+1}Q_{i,i+1}=id \tag{B6}$$

for two adjacent operators $A^{j_1}_{k_1}A^{j_2}_{k'_2}$ $(j_1\neq j_2)$, and thus it is also valid for all bunches due to distribution law. We also have

$$Q_{i,i+1}Q_{j,j+1}=Q_{j,j+1}Q_{i,i+1}\quad (i+1<j) \tag{B7}$$

because of the distribution law. Finally we have

$$Q_{i,i+1}Q_{i+1,i+2}Q_{i,i+1}=Q_{i+1,i+2}Q_{i,i+1}Q_{i+1,i+2} \tag{B8}$$

due to YBE for any polynomial $A^{j_1}_{k_1}A^{j_2}_{k_2}A^{j_3}_{k_3}$ with different indices. Due to distribution law, this equation is also true for any bunch. Therefore, we can also change $Q^{(1)}=Q_{i_1,i_1+1}Q_{i_2,i_2+1}\cdots Q_{i_s,i_s+1}$ into $Q^{(2)}=Q_{i'_1,i'_1+1}Q_{i'_2,i'_2+1}\cdots Q_{i'_s,i'_s+1}$ in Eqs. (B1) and (B2), re-

spectively, by using Eqs. (B6)–(B8) step by step since $P^{(1)}$ and $P^{(2)}$ can be equaled in such a way by using Eqs. (B3)–(B5), respectively. Thus we have $c^{j_{t_1}\cdots k_1'\cdots}_{j_1\cdots k_1\cdots}=d^{j_{t_1}\cdots k_1'\cdots}_{j_1\cdots k_1\cdots}$.

We then conclude that the resulting (ab) normal order expansion of the two paths gives the same result. Therefore, all paths give the same result. □

Corollaries then follow:

Corollary 1: If in a product of successive product of operators $CA_i^{i'}A_j^{j'}D$ where C,D are all products of operators, we obtain the combination of $CA_\cdot^{j'}A_\cdot^{i'}D$ [it is $C(\alpha A_i^{j'}A_j^{i'}+\beta A_j^{j'}A_i^{i'})D$]. By changing [with rule (ab) in Eq. (67)] two adjacent operators whose up-indices are unequal, the results of their (ab) normal order expansions are same, if the procedure is done according to the rules described in Lemma 1.

Proof: If $i'>j'$, we can regard this changing procedure as the first step of the (ab) normal order expansion. Thus, we can prove it. If $i'<j'$, we can do the (ab) normal order expansion of $C(\alpha A_i^{j'}A_j^{i'}+\beta A_j^{j'}A_i^{i'})D$, and let the first step as the changing of $A_\cdot^{j'}A_\cdot^{i'}$ into $A_\cdot^{i'}A_\cdot^{j'}$. Then, by using the rule (ab), we can prove that $i'j'\to j'i'\to i'j'$ is the identical transformation. So with the distributive law, the (ab) normal order expansion of bunch $C(\alpha A_i^{j'}A_j^{i'}+\beta A_j^{j'}A_i^{i'})D=$the (ab) normal order expansion of $CA_i^{i'}A_j^{j'}D$. Therefore, this corollary is proved. □

Corollary 2: With the rules of Eqs. (67a) and (67b), if a polynomial (a linear combination of products) of operators C can be changed to D ($C\overset{(ab)}{\to}D$), the (ab) normal order expansions of C and D are same, if the expansion is done according to the rules described in Lemma 1.

Proof: Because each step of the transformation does not affect the result of the expansion.□

Thus Eqs. (67a) and (67b) are compatible with the (ab) normal order expansion and the (abc) normal order expansion.

Here we note that same results of the (ab) normal order expansion give the same results of the (abc) normal order expansion, so the above two corollaries are also true for the (abc) normal order expansion.

Next, we prove the following lemma.

Lemma 2: The (abc) normal order expansion of the bunch $CA_j^{i'}A_k^{i'}D$ and the bunch $CA_k^{i'}A_j^{i'}D$ are same.

Proof: We need only to prove this when they are monomials. We prove the following propositions by using the mathematical inductive method:

Proposition (i): This lemma is true when the inverse order number is zero.

Proposition (ii): If the lemma is true when the inverse order number is smaller than m, it is also true when the inverse order number is equal to m.

The first proposition is obvious, because in this case, $CA_j^{i'}A_k^{i'}D$ and $CA_k^{i'}A_j^{i'}D$ are all (ab) normal order products. To obtain the (abc) normalization, we only need to rearrange the down-indices of the part of the product where the up-indices are the same from the smaller to the bigger by rule (67c). Both of the bunches have the same sets of the down-indices for up-indices i'. Therefore, the (abc) normal order products of them are same.

To the second proposition, we have the following cases:

(α). If in C or D, we can rearrange the up-indices $\{i'\}$ of them to reduce the inverse order number, for example, $D\overset{(ab)}{\to}D'$, we can obtain $CA_j^{i'}A_k^{i'}D'$ and $CA_k^{i'}A_j^{i'}D'$. According to Corollary 2 of Lemma 1, the (ab) normal order expansions of both of them will keep unchanged. However, because the inverse order number must be smaller that m now, according to assumption of proposition (ii), their (abc) normal order expansions are same. Therefore, the (abc) normal order expansions of the $CA_j^{i'}A_k^{i'}D$ and the $CA_k^{i'}A_j^{i'}D$ are same.

(β). If C and D have already been normalized but the inverse order number of the bunch as a whole can be reduced, namely, the bunch is not an (ab) normal order product. We can let $C=C_1A_{i_c}^{i_c'}$, $D=A_{i_d}^{i_d'}D_1$. Then we must have $i_c'>i'$ or (and) $i'>i_d'$. Let us assume $i_c'>i'$. These two

bunches can be rewritten as $T_1=C_1A_{i_c}^{i_c'}A_j^{i'}A_k^{i'}D$ and $T_2=C_1A_{i_c}^{i_c'}A_k^{i'}A_j^{i'}D$, respectively. According to the rule (ab) in Eq. (67), we can change them as $T_1\Rightarrow T_1'=C_1\Sigma_{rst}a_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}D$ and $T_2\Rightarrow T_2'=C_1\Sigma_{rst}b_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}D$, where a_{rst} and b_{rst} are some coefficients. With the help of the YBE which we studied in Sec. V, one can see that these two combinations $\Sigma_{rst}a_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}$ and $\Sigma_{rst}b_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}$ are the same if we take the rule (67c) into account. Thus we must have

$$\sum_{rst}a_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}-\sum_{rst}b_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}=\sum_t\left(\sum_{rs}(a_{rst}-b_{rst})A_r^{i'}A_s^{i'}\right)A_t^{i_c'}$$

with $\Sigma_{rs}(a_{rst}-b_{rst})A_r^{i'}A_s^{i'}=0$ if we take the rule (67c) into account. This is to say

$$a_{rst}+a_{srt}=b_{rst}+b_{srt}=2c_{rst}\quad\text{for each } t. \tag{B9}$$

Thus we have

$$T_1'=\sum_{rst}C_1a_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}D\equiv\sum_t\sum_{rs}(C_1a_{rst}A_r^{i'}A_s^{i'}D_t)$$

and

$$T_2'=\sum_{rst}C_1b_{rst}A_r^{i'}A_s^{i'}A_t^{i_c'}D\equiv\sum_t\sum_{rs}(C_1b_{rst}A_r^{i'}A_s^{i'}D_t).$$

From Eq. (B9) and due to the assumption of proposition (ii), the (abc) normal order expansions of T_1' and T_2' are the same. According to the procedure of the (abc) normal order expansion, we see that the (abc) normal order expansions of T_1 and T_2 are same.

If $i'>i_d'$, the proof is similar. So we see that proposition (ii) is true.

Thus, with the mathematical inductive method, we prove Lemma 2. □

From Corollary 2 of Lemmas 1 and 2, we obtain Theorem 1.

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Unbraiding the braided tensor product

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(Received 20 August 2002; accepted 16 September 2002)

We show that the braided tensor product algebra $\mathcal{A}_1 \underline{\otimes} \mathcal{A}_2$ of two module algebras $\mathcal{A}_1, \mathcal{A}_2$ of a quasitriangular Hopf algebra H is isomorphic to the ordinary tensor product $\mathcal{A}_1 \otimes \mathcal{A}_2$, provided there exists a realization of H within $\mathcal{A}_1$. In other words, under this assumption we construct a transformation of generators which decouples $\mathcal{A}_1, \mathcal{A}_2$ (i.e., makes them commuting). We apply the theorem to the braided tensor product algebras of two or more quantum group covariant quantum spaces, deformed Heisenberg algebras and q-deformed fuzzy spheres. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1522818]

I. INTRODUCTION AND MAIN THEOREM

As is well known, given two associative unital algebras $\mathcal{A}_1, \mathcal{A}_2$ (over the field $\mathbb{C}$, say), one can build a new module algebra $\mathcal{A}$ which is as a vector space the tensor product $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$ of the two vector spaces (over the same field) by postulating the product law

$$(a_1 \otimes a_2)(b_1 \otimes b_2) = a_1 b_1 \otimes a_2 b_2 . \tag{1.1}$$

The resulting algebra is the ordinary tensor product algebra. Equation (1.1) is equivalent to the set of relations

$$(a_1 \otimes \mathbf{1}_2)(b_1 \otimes \mathbf{1}_2) = a_1 b_1 \otimes \mathbf{1}_2 , \tag{1.2}$$

$$(a_1 \otimes \mathbf{1}_2)(\mathbf{1}_1 \otimes a_2) = a_1 \otimes a_2 , \tag{1.3}$$

$$(\mathbf{1}_1 \otimes a_2)(\mathbf{1}_1 \otimes b_2) = \mathbf{1}_1 \otimes a_2 b_2 , \tag{1.4}$$

$$(\mathbf{1}_1 \otimes a_2)(a_1 \otimes \mathbf{1}_2) = (a_1 \otimes \mathbf{1}_2)(\mathbf{1}_1 \otimes a_2). \tag{1.5}$$

However, in many cases the same goal can be reached also by replacing (1.5) by some suitable nontrivial commutation relations. With a standard abuse of notation we shall denote in the sequel $a_1 \otimes a_2$ by $a_1 a_2$ for any $a_1 \in \mathcal{A}_1$, $a_2 \in \mathcal{A}_2$ and omit all units $\mathbf{1}_i$ when multiplied by non-unit elements; consequently (1.2)–(1.4) take trivial forms, whereas (1.5) becomes the commutation relation

$$a_2 a_1 = a_1 a_2 . \tag{1.6}$$

If $\mathcal{A}_1,\mathcal{A}_2$ are module algebras of a Lie algebra $\mathbf{g}$, and we require $\mathcal{A}$ to be too, then (1.6) has essentially no alternative (apart from the case of superalgebras, where a minus sign may appear at the right-hand side, according to the Grassman parity of a_1,a_2), because any $g\in\mathbf{g}$ acts as a derivation on the (algebra as well as tensor) product of any two elements or, in Hopf algebra language, because the coproduct $\Delta(g)=g_{(1)}\otimes g_{(2)}$ [at the right-hand side (rhs) we have used Sweedler notation] of the Hopf algebra $H\equiv U\mathbf{g}$ is cocommutative. In the main part of this paper we shall work with right-module algebras (instead of left ones), and denote by $\triangleleft:(a_i,g)\in\mathcal{A}_i\times H\to a_i\triangleleft g\in\mathcal{A}_i$ the right action; the reason is that they are equivalent to left comodule algebras, which are used in much of the literature. In Sec. V we shall give the formulas for left module algebras. We recall that a right action $\triangleleft:(a,g)\in\mathcal{A}\times H\to a\triangleleft g\in\mathcal{A}$ by definition fulfills

$$a\triangleleft(gg')=(a\triangleleft g)\triangleleft g', \tag{1.7}$$

$$(aa')\triangleleft g=(a\triangleleft g_{(1)})(a'\triangleleft g_{(2)}). \tag{1.8}$$

If we "q-deform" this setting by taking as Hopf algebra H the quantum group $U_q\mathbf{g}$, and as $\mathcal{A}_i$ the corresponding q-deformed module algebras, then it is also known[21,24,25] that although $\Delta(g)$ is no longer cocommutative, it is still possible to build the deformed counterpart of $\mathcal{A}$ if one replaces (1.6) with nontrivial commutation relations of the form

$$a_2a_1=(a_1\triangleleft\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)}). \tag{1.9}$$

Here $\mathcal{R}\equiv\mathcal{R}^{(1)}\otimes\mathcal{R}^{(2)}\in H^+\otimes H^-$ denotes the so-called universal R-matrix of $H\equiv U_q\mathbf{g}$,[10] and $H^\pm$ denote the Hopf positive and negative Borel subalgebras of H. This yields instead of $\mathcal{A}$ a *braided* tensor product algebra $\mathcal{A}^+=\mathcal{A}_1\underline{\otimes}^+\mathcal{A}_2$.[25] An alternative one $\mathcal{A}^-=\mathcal{A}_1\underline{\otimes}^-\mathcal{A}_2$ is obtained by replacing in the previous formula $\mathcal{R}$ by $\mathcal{R}_{21}^{-1}$:

$$a_2a_1=(a_1\triangleleft\mathcal{R}^{-1(2)})(a_2\triangleleft\mathcal{R}^{-1(1)}). \tag{1.10}$$

Both $\mathcal{A}^+$ and $\mathcal{A}^-$ go to the ordinary tensor product algebra $\mathcal{A}$ in the limit $q\to1$.

This is a particular example of a more general notion, that of a *crossed (or twisted) tensor product*[3] of two unital associative algebras.

In view of (1.9) or (1.10) studying representations of $\mathcal{A}^\pm$ is a more difficult task than just studying the representations of $\mathcal{A}_1,\mathcal{A}_2$, taking their tensor products and studying the irreducible ones there contained. The degrees of freedom of $\mathcal{A}_1,\mathcal{A}_2$ are so to say "coupled." One might ask whether one can "decouple" them by a transformation of generators.

In this work we present a sufficient condition for the construction of a transformation making $\mathcal{A}^+$ isomorphic to the ordinary tensor product algebra $\mathcal{A}_1\otimes\mathcal{A}_2$, more precisely equal to the product $\mathcal{A}_1\tilde{\mathcal{A}}_2^+$, with $\tilde{\mathcal{A}}_2^+$ a subalgebra of $\mathcal{A}^+$ isomorphic to $\mathcal{A}_2$ and *commuting* [in the sense (1.6)] with $\mathcal{A}_1$, although—of course—no longer a H-submodule; and similarly for $\mathcal{A}^-$. In a quantum theory framework one could thus interpret the generators of $\mathcal{A}_1,\tilde{\mathcal{A}}_2^\pm$ as pertaining to decoupled degrees of freedom, describing, e.g., some composite or "quasiparticle" excitations. Reducing $\mathcal{A}^\pm$ to a form $\mathcal{A}_1\tilde{\mathcal{A}}_2^\pm$ will be called an *unbraiding* of the braided tensor product algebra $\mathcal{A}^\pm=\mathcal{A}_1\underline{\otimes}^\pm\mathcal{A}_2$. The sufficient condition is that there, respectively, exists an algebra homomorphism φ_1^+ or an algebra homomorphism φ_1^-

$$\varphi_1^\pm:\mathcal{A}_1\rtimes H^\pm\to\mathcal{A}_1, \tag{1.11}$$

acting as the identity on $\mathcal{A}_1$, namely for any $a_1\in\mathcal{A}_1$,

$$\varphi_1^\pm(a_1)=a_1. \tag{1.12}$$

[Note that, as a consequence of (1.12), $\varphi_1^{\pm}$ is idempotent, $(\varphi_1^{\pm})^2=\varphi_1^{\pm}$.] Here $\mathcal{A}_1 \rtimes H^{\pm}$ denotes the cross product between $\mathcal{A}_1$ and $H^{\pm}$. In other words, this amounts to assuming that $\varphi_1^{+}(H^{+})$ [respectively, $\varphi_1^{-}(H^{-})$] provides a *realization* of H^{+} (respectively, H^{-}) within $\mathcal{A}_1$. In fact, $\tilde{\mathcal{A}}_2$ is found using the main result of this work.

Theorem 1: *Let $\{H,\mathcal{R}\}$ be a quasitriangular Hopf algebra and H^{+},H^{-} be Hopf subalgebras of H such that $\mathcal{R}\in H^{+}\otimes H^{-}$. Let $\mathcal{A}_1,\mathcal{A}_2$ be, respectively, a H^{+}- and a H^{-}-module algebra, so that we can define $\mathcal{A}^{+}$ as in (1.9), and φ_1^{+} be a homomorphism of the type (1.11), (1.12), so that we can define the "unbraiding" map $\chi^{+}:\mathcal{A}_2\to\mathcal{A}^{+}$ by*

$$\chi^{+}(a_2):=\varphi_1^{+}(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)}). \tag{1.13}$$

Alternatively, let $\mathcal{A}_1,\mathcal{A}_2$ be, respectively, a H^{-}- and a H^{+}-module algebra, so that we can define $\mathcal{A}^{-}$ as in (1.10), and φ_1^{-} be a homomorphism of the type (1.11), (1.12), so that we can define the "unbraiding" map $\chi^{-}:\mathcal{A}_2\to\mathcal{A}^{-}$ by

$$\chi^{-}(a_2):=\varphi_1^{-}(\mathcal{R}^{-1(2)})(a_2\triangleleft\mathcal{R}^{-1(1)}). \tag{1.14}$$

In either case $\chi^{\pm}$ are then injective algebra homomorphisms and

$$[\chi^{\pm}(a_2),\mathcal{A}_1]=0, \tag{1.15}$$

namely the subalgebras $\tilde{\mathcal{A}}_2^{\pm}:=\chi^{\pm}(\mathcal{A}_2)\approx\mathcal{A}_2$ commute with $\mathcal{A}_1$. Moreover $\mathcal{A}^{\pm}=\mathcal{A}_1\tilde{\mathcal{A}}_2^{\pm}$.

Proof: We start by recalling the content of the hypotheses stated in the theorem. The algebra $\mathcal{A}_1\rtimes H^{\pm}$ as a vector space is the tensor product of $\mathcal{A}_1$ and $H^{\pm}$, whereas its product law is obtained combining the product laws of these two tensor factors with the cross-product law,

$$a_1 g=g_{(1)}(a_1\triangleleft g_{(2)}), \tag{1.16}$$

for any $a_1\in\mathcal{A}_1$ and $g\in H^{\pm}$. $\varphi_1^{\pm}$ being an algebra homomorphism means that for any $\xi,\xi'\in\mathcal{A}_1\rtimes H^{\pm}$,

$$\varphi_1^{\pm}(\xi\xi')=\varphi_1^{\pm}(\xi)\varphi_1^{\pm}(\xi'). \tag{1.17}$$

For $\xi\equiv a\in\mathcal{A}_1\subset\mathcal{A}_1\rtimes H^{\pm}$, $\xi'\equiv g\in H^{\pm}\subset\mathcal{A}_1\rtimes H^{\pm}$ this implies

$$a\varphi^{\pm}(g)=\varphi^{\pm}(g_{(1)})(a\triangleleft g_{(2)}). \tag{1.18}$$

Hereby we have also used (1.12) and (1.16). After these preliminaries, note that under the assumption (1.9), for any $a_1\in\mathcal{A}_1$ and $a_2\in\mathcal{A}_2$

$$\begin{aligned}
a_1\chi^{+}(a_2) &\overset{(1.13)}{=} a_1\varphi_1^{+}(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)})\\
&\overset{(1.18)}{=} \varphi^{+}(\mathcal{R}^{(1)}_{(1)})(a_1\triangleleft\mathcal{R}^{(1)}_{(2)})(a_2\triangleleft\mathcal{R}^{(2)})\\
&\overset{(A3)}{=} \varphi^{+}(\mathcal{R}^{(1)})(a_1\triangleleft\mathcal{R}^{(1')})(a_2\triangleleft\mathcal{R}^{(2)}\mathcal{R}^{(2')})\\
&\overset{(1.9)}{=} \varphi^{+}(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)})a_1\\
&\overset{(1.13)}{=} \chi^{+}(a_2)a_1,
\end{aligned}$$

which proves (1.15) in this case. Moreover

$$\begin{aligned}
\chi^+(a_2a_2') &\overset{(1.13)}{=} \varphi_1^+(\mathcal{R}^{(1)})(a_2a_2'\triangleleft\mathcal{R}^{(2)})\\
&\overset{(1.8)}{=} \varphi^+(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)}_{(1)})(a_2'\triangleleft\mathcal{R}^{(2)}_{(2)})\\
&\overset{(A4)}{=} \varphi^+(\mathcal{R}^{(1')}\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)})(a_2'\triangleleft\mathcal{R}^{(2')})\\
&\overset{(1.17)}{=} \varphi^+(\mathcal{R}^{(1')})\varphi(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)})(a_2'\triangleleft\mathcal{R}^{(2')})\\
&\overset{(1.13)}{=} \varphi^+(\mathcal{R}^{(1')})\chi^+(a_2)(a_2'\triangleleft\mathcal{R}^{(2')})\\
&\overset{(1.15)}{=} \chi^+(a_2)\varphi(\mathcal{R}^{(1')})(a_2'\triangleleft\mathcal{R}^{(2')})\\
&\overset{(1.13)}{=} \chi^+(a_2)\chi^+(a_2'),
\end{aligned}$$

proving that χ^+ is a homomorphism. To prove injectivity we show that χ^+ can be inverted on $\chi^+(\mathcal{A}_2)$, and the inverse is given by

$$(\chi^+)^{-1}(\tilde{a}_2)=V^{-1}([\varphi^+(S^{-1}\mathcal{R}^{(1)})\tilde{a}_2]\triangleleft\mathcal{R}^{(2)}), \tag{1.19}$$

where $V\in\mathcal{A}_1$ is the invertible element defined by $V:=\varphi_1^+(S^{-1}\mathcal{R}^{(1)})\triangleleft\mathcal{R}^{(2)}$ (V is invertible because $\mathcal{R}$ is). In fact,

$$\begin{aligned}
&V^{-1}[\varphi_1^+(S^{-1}\mathcal{R}^{(1)})\chi^+(a_2)]\triangleleft\mathcal{R}^{(2)}\\
&\overset{(1.13)}{=} V^{-1}[\varphi_1^+(S^{-1}\mathcal{R}^{(1)})\varphi_1^+(\mathcal{R}^{(1')})(a_2\triangleleft\mathcal{R}^{(2')})]\triangleleft\mathcal{R}^{(2)}\\
&\overset{(A.1.5),(1.17)}{=} V^{-1}\{\varphi_1^+[S^{-1}(\mathcal{R}^{-1(1')}\mathcal{R}^{(1)})](a_2\triangleleft\mathcal{R}^{-1(2')})\}\triangleleft\mathcal{R}^{(2)}\\
&\overset{(1.8)}{=} V^{-1}\varphi_1^+[S^{-1}(\mathcal{R}^{-1(1')}\mathcal{R}^{(1)})]\triangleleft\mathcal{R}^{(2)}_{(1)}(a_2\triangleleft\mathcal{R}^{-1(2')})\triangleleft\mathcal{R}^{(2)}_{(2)}\\
&\overset{(A.1.4)}{=} V^{-1}\varphi_1^+[S^{-1}(\mathcal{R}^{-1(1')}\mathcal{R}^{(1)}\mathcal{R}^{(1'')})]\triangleleft\mathcal{R}^{(2'')}(a_2\triangleleft\mathcal{R}^{-1(2')})\triangleleft\mathcal{R}^{(2)})\\
&\overset{(1.7)}{=} V^{-1}\varphi_1^+[S^{-1}(\mathcal{R}^{(1'')})]\triangleleft\mathcal{R}^{(2'')}a_2=V^{-1}Va_2=a_2.
\end{aligned}$$

In fact, if φ_1^+ can be extended to an algebra homomorphism $\varphi_1:\mathcal{A}_1\rtimes H\to\mathcal{A}_1$ a little calculation with the help of Eqs. (A32) and (A7) shows that $V=\varphi_1(v)$, where $v\in H$ is the invertible central element defined by (A8). We know that $\mathcal{A}_1\tilde{\mathcal{A}}_2^+\subset\mathcal{A}^+$. To prove that $\mathcal{A}^+=\mathcal{A}_1\tilde{\mathcal{A}}_2^+$ note first that by (1.9) any element in $\mathcal{A}^+$ can be written as a sum of products a_1a_2, with $a_1\in\mathcal{A}_1$ and $a_2\in\mathcal{A}_2$. So we need to show that

$$a_1a_2=b^{(1)}\chi^+(b^{(2)}) \tag{1.20}$$

for some $b^{(1)}\in\mathcal{A}_1$, $b^{(2)}\in\mathcal{A}_2$ (at the rhs a sum of many terms is implicitly understood). Now this can be proved as follows:

$$\begin{aligned}
a_1a_2&=a_1\varphi_1^+(\mathbf{1}_H)(a_2\triangleleft\mathbf{1}_H)=a_1\varphi_1^+(\mathcal{R}^{-1(1)}\mathcal{R}^{(1')})[a_2\triangleleft(\mathcal{R}^{-1(2)}\mathcal{R}^{(2')})]\\
&\overset{(1.7)}{=} a_1\varphi_1^+(\mathcal{R}^{-1(1)})\varphi_1^+(\mathcal{R}^{(1')})(a_2\triangleleft\mathcal{R}^{-1(2)})\triangleleft\mathcal{R}^{(2')}\overset{(1.13)}{=}a_1\varphi_1^+(\mathcal{R}^{-1(1)})\chi^+(a_2\triangleleft\mathcal{R}^{-1(2)}),
\end{aligned}$$

which is of the form (1.20).

The proof for χ^- under the corresponding assumptions is completely analogous. □

In the next section we shall need an alternative expression for $\chi^\pm$, which we prove in the appendix:

Proposition 1:

$$\chi^+(a_2)=(a_2\triangleleft\mathcal{R}^{-1(2)})\varphi_1^+(S\mathcal{R}^{-1(1)}), \tag{1.21}$$

$$\chi^-(a_2)=(a_2\triangleleft\mathcal{R}^{(1)})\varphi_1^-(S\mathcal{R}^{(2)}). \tag{1.22}$$

The rest of the paper is essentially devoted to illustrate the application of Theorem 1 to some algebras $\mathcal{A}_i$ for which homomorphisms $\varphi_1^\pm$ are known. In Ref. 5 algebra homomorphisms $\varphi_1^\pm$ have been found for (a slightly enlarged version $\mathcal{A}_1$ of) the algebra of functions on the N-dimensional quantum Euclidean space[13] $\mathbb{R}_q^N$, corresponding to $H=U_q\,\mathrm{so}(N)$. The explicit forms of $\varphi_1^\pm$ on the Faddeev–Reshetikhin–Takhtadjan (FRT) generators $\mathcal{L}_j^{\pm i}$ of $U_q\,\mathrm{so}(N)$ are recalled in the third part of the Appendix. The maps $\varphi_1^\pm$ for $N=3$ are given also in Refs. 6 and 7. The same maps do the job also on the quotient spaces obtained by setting $x^i x_i=1$ [quantum $(N-1)$-dimensional spheres S_q^{N-1}], and the appropriate maps for the q-deformed fuzzy sphere $S_{q,M}^2$ have been found in Ref. 20. Therefore $U_q\,\mathrm{so}(N)$ and the quantum Euclidean spaces/spheres provide nontrivial H and $\mathcal{A}_1$ for the application of the above theorem. In fact, the constructions of the frame given in Refs. 18 and 5 can be interpreted as an application of the theorem with $\mathcal{A}_1\equiv\mathbb{R}_q^N$ and $\mathcal{A}_2$ the $N!$-dim exterior algebra generated by the differentials dx^i of the $U_q\,\mathrm{so}(N)$-covariant differential calculus (although with a universal R-matrix $\mathcal{R}$ slightly modified by multiplication by the coproduct $\Delta(\Lambda)=\Lambda\otimes\Lambda$ of a new element Λ generating dilatations); consequently, in agreement with the philosophy of Ref. 26, the algebra of differential forms on $\mathbb{R}_q^N$ can be written as $\mathbb{R}_q^N\otimes\tilde{\mathcal{A}}_2$, where $\tilde{\mathcal{A}}_2$ is the $N!$-dim exterior algebra generated by the frame elements. On the other hand, the existence of algebra homomorphisms $\varphi:\mathcal{A}_1\rtimes H\to\mathcal{A}_1$, for $H=U_q\,\mathrm{so}(N), U_q\mathrm{sl}(N)$ and $\mathcal{A}_1$, respectively, equal to (a suitable completion of) the $U_q\,\mathrm{so}(N)$-covariant Heisenberg algebra or the $U_q\,\mathrm{sl}(N)$-covariant Heisenberg or Clifford algebras, has been known for even a longer time,[14,9,22] so the theorem also applies if we choose as $(H,\mathcal{A}_1)$ one of these pairs of algebras.

Of course the above theorem can be used iteratively to completely unbraid an algebra $\mathcal{A}$ obtained by repeated braided tensor product [through prescription (1.9), or prescription (1.10)] of an arbitrary number of H-module algebras $\mathcal{A}_1,\mathcal{A}_2,\ldots,\mathcal{A}_M$. We shall explicitly consider the particular case that the latter be M identical copies of the $U_q\,\mathrm{so}(N)$-covariant quantum space/sphere (Sec. III), of the $U_q\,\mathrm{so}(3)$-covariant q-fuzzy sphere (Sec. VI), or of the $U_q\,\mathrm{so}(N)$- or $U_q\,\mathrm{sl}(N)$-covariant Heisenberg algebra (Sec. IV). There we shall explicitly write down the generators of $\tilde{\mathcal{A}}_2^\pm$ for the lowest N examples. Also the results appeared in Section 3.3 of Ref. 2 can be reinterpreted as an application (at the representation level) of the above iterated unbraiding procedure to a particular iterated braided tensor product algebra, namely a lattice current algebra. In the latter both H and all the $\mathcal{A}_i$ are copies of one and the same quasitriangular semisimple Hopf algebra $\mathcal{G}$.

In the third part of the Appendix we analyze the properties of $\varphi^\pm$ under the main real sections of $U_q\,\mathrm{so}(N)$, what was left aside in Ref. 5. In Sec. II we investigate in the context of general position the properties of $\chi^\pm$ under the $*$-structures.

II. THE UNBRAIDING UNDER THE $*$-STRUCTURES

Assume H is a Hopf $*$-algebra, namely the coproduct Δ and counit ε are $*$-homomorphisms,

$$\Delta(g^*)\equiv(g^*)_{(1)}\otimes(g^*)_{(2)}=(g_{(1)})^*\otimes(g_{(2)})^*, \tag{2.1}$$

and $\mathcal{A}_1$, $\mathcal{A}_2$ are H-module $*$-algebras, namely for any $a_i\in\mathcal{A}_i$,

$$(a_i \triangleleft g)^* = a_i^* \triangleleft S^{-1} g^* \tag{2.2}$$

(here S denotes the antipode of H); we have used and shall use the same symbol $*$ for the $*$-structure on all algebras $H, \mathcal{A}_1$, etc. Then $*$ is a $*$-structure also for $\mathcal{A}_1 \rtimes H$. The same statement is not automatically true for the braided tensor product algebra $\mathcal{A}^{\pm} = \mathcal{A}_1 \underline{\otimes}^{\pm} \mathcal{A}_2$, because the basic requirement that the latter be antimultiplicative

$$(a_2 a_1)^* = a_1^* a_2^* \tag{2.3}$$

(note that this would make $\mathcal{A}^{\pm}$ also a H-module $*$-algebra) is not automatically guaranteed. In fact, applying this would-be $*$ to rhs of (1.9) one finds

$$\begin{aligned}
(a_2 a_1)^* &\overset{(1.9)}{=} [(a_1 \triangleleft \mathcal{R}^{(1)})(a_2 \triangleleft \mathcal{R}^{(2)})]^* \\
&\overset{(2.3)}{=} (a_2 \triangleleft \mathcal{R}^{(2)})^* (a_1 \triangleleft \mathcal{R}^{(1)})^* \\
&\overset{(2.2)}{=} (a_2^* \triangleleft S^{-1}\mathcal{R}^{(2)*})(a_1^* \triangleleft S^{-1}\mathcal{R}^{(1)*}) \\
&\overset{(1.9)}{=} (a_1^* \triangleleft S^{-1}\mathcal{R}^{(1)*}\mathcal{R}^{(1')})(a_2^* \triangleleft S^{-1}\mathcal{R}^{(2)*}\mathcal{R}^{(2')});
\end{aligned} \tag{2.4}$$

in order that this be equal to the rhs of (2.3) it is necessary that $(S^{-1} \otimes S^{-1})\mathcal{R}^* = \mathcal{R}^{-1}$, which upon use of (A5) is equivalent to

$$\mathcal{R}^* = \mathcal{R}^{-1} \tag{2.5}$$

(here $\mathcal{R}^*$ means $\mathcal{R}^{(1)*} \otimes \mathcal{R}^{(2)*}$). This condition is fulfilled only for the standard noncompact sections (A28) of $U_q\mathbf{g}$, for $|q| = 1$; as a consequence, $\mathcal{A}^+ = \mathcal{A}_1 \underline{\otimes}^+ \mathcal{A}_2$ becomes a H-module $*$-algebra if one extends the $*$-structures of the tensor factors to $\mathcal{A}$ using (2.3). The same holds for $\mathcal{A}^-$.

On the contrary, the compact section, which requires $q \in \mathbb{R}$, is characterized by

$$\mathcal{R}^* = \mathcal{R}_{21}. \tag{2.6}$$

In the latter case the map $*$ introduced through (2.3) makes sense only as an involutive antimultiplicative antilinear map $\mathcal{A}^+ \to \mathcal{A}^-$, if both $\mathcal{A}^+$ and $\mathcal{A}^-$ exist. In fact, in this case the last line in (2.4) will be replaced by

$$\overset{(1.10),(2.6)}{=} (a_1^* \triangleleft S^{-1}\mathcal{R}^{(2)}\mathcal{R}^{-1(2')})(a_2^* \triangleleft S^{-1}\mathcal{R}^{(1)}\mathcal{R}^{-1(1')}) \overset{(A5)}{=} a_1^* a_2^*,$$

as required. Alternatively, if $\mathcal{A}_1, \mathcal{A}_2$ are two copies of the same algebra and we denote by $\psi: \mathcal{A}_1 \to \mathcal{A}_2$ the map associating to each $a_1 \in \mathcal{A}_1$ the equivalent element in $\mathcal{A}_2$, one can define an alternative $*$-structure $\star$ in $\mathcal{A}^{\pm}$ by setting

$$a_1^\star = \psi(a_1^*), \quad a_2^\star = \psi^{-1}(a_2^*), \tag{2.7}$$

since this is instead compatible with (1.9). In fact, (2.4) will become

$$
\begin{aligned}
(a_2 a_1)^{\star} &\overset{(1.9)}{=} [(a_1 \triangleleft \mathcal{R}^{(1)})(a_2 \triangleleft \mathcal{R}^{(2)})]^{\star} \\
&\overset{(2.3)}{=} (a_2 \triangleleft \mathcal{R}^{(2)})^{\star}(a_1 \triangleleft \mathcal{R}^{(1)})^{\star} \\
&\overset{(2.2)}{=} \psi^{-1}(a_2^{*} \triangleleft S^{-1}\mathcal{R}^{(2)*})\psi(a_1^{*} \triangleleft S^{-1}\mathcal{R}^{(1)*}) \\
&\overset{(1.9)}{=} \psi(a_1^{*} \triangleleft S^{-1}\mathcal{R}^{(2)}\mathcal{R}^{-1(2')})\psi^{-1}(a_2^{*} \triangleleft S^{-1}\mathcal{R}^{(1)}\mathcal{R}^{-1(1')}) \\
&\overset{(A5)}{=} \psi(a_1^{*})\psi^{-1}(a_2^{*})a_1 \\
&\overset{(2.7)}{=} a_1^{\star}a_2^{\star}. \qquad (2.8)
\end{aligned}
$$

A similar trick can be used also if one considers an iterated braided tensor product of $M>2$ copies of the same algebra, see next section. However, such $\star$'s have not the standard commutative limit, because of the presence of the map ψ.

Inspired by the applications of the next two sections, we now assume that $\varphi_1^{\pm}$ fulfill some specific conditions relating its action before and after the application of the involution $*$, and analyze the identities relating the action of $\chi^{\pm}$ before and after the application of $*$ which follow herefrom.

Proposition 2: Assume that the conditions of Theorem 1 for defining χ^{+} or χ^{-} are fulfilled. If $\mathcal{R}^{*}=\mathcal{R}^{-1}$ and for any $g^{\pm}\in H^{\pm}$,

$$[\varphi_1^{\pm}(g^{\pm})]^{*}=\varphi_1^{\pm}(g^{\pm *}), \qquad (2.9)$$

in other words $\varphi_1^{\pm}$ are $*$-homomorphisms, then

$$[\chi^{\pm}(a_2)]^{*}=\chi^{\pm}(a_2^{*}). \qquad (2.10)$$

If $\mathcal{R}^{*}=\mathcal{R}_{21}$ and $*:H^{\pm}\to H^{\mp}$ fulfills

$$[\varphi_1^{\pm}(g)]^{*}=\varphi_1^{\mp}(g^{*}), \qquad (2.11)$$

then

$$[\chi^{\pm}(a_2)]^{*}=\chi^{\mp}(a_2^{*}). \qquad (2.12)$$

Proof: Under the first assumptions, for any $a_2\in\mathcal{A}_2$,

$$
\begin{aligned}
[\chi^{+}(a_2)]^{*} &\overset{(1.21)}{=} [(a_2 \triangleleft \mathcal{R}^{-1(2)})\varphi_1^{+}(S\mathcal{R}^{-1(1)})]^{*} \\
&= [\varphi_1^{+}(S\mathcal{R}^{-1(1)})]^{*}(a_2 \triangleleft \mathcal{R}^{-1(2)})^{*} \\
&\overset{(2.9),(2.2)}{=} \varphi_1^{+}(S^{-1}\mathcal{R}^{-1(1)*})(a_2^{*} \triangleleft S^{-1}\mathcal{R}^{-1(2)*}) \\
&\overset{(2.5)}{=} \varphi_1^{+}(S^{-1}\mathcal{R}^{(1)})(a_2^{*} \triangleleft S^{-1}\mathcal{R}^{(2)})
\end{aligned}
$$

$$\overset{(A5)}{=} \varphi_1^+(\mathcal{R}^{(1)})(a_2^* \triangleleft \mathcal{R}^{(2)})$$

$$\overset{(1.13)}{=} \chi^+(a_2^*).$$

Similarly one proves (2.10) for χ^-. Under the second assumptions, for any $a_2 \in \mathcal{A}_2$,

$$[\chi^+(a_2)]^* \overset{(1.21)}{=} [(a_2 \triangleleft \mathcal{R}^{-1(2)})\varphi_1^+(S\mathcal{R}^{-1(1)})]^*$$
$$= [\varphi_1^+(S\mathcal{R}^{-1(1)})]^*(a_2 \triangleleft \mathcal{R}^{-1(2)})^*$$

$$\overset{(2.11),(2.2)}{=} \varphi_1^-(S^{-1}\mathcal{R}^{-1(1)*})(a_2^* \triangleleft S^{-1}\mathcal{R}^{-1(2)*})$$

$$\overset{(2.6)}{=} \varphi_1^-(S^{-1}\mathcal{R}^{-1(2)})(a_2^* \triangleleft S^{-1}\mathcal{R}^{-1(1)})$$
$$\overset{(A5)}{=} \varphi_1^-(\mathcal{R}^{-1(2)})(a_2^* \triangleleft \mathcal{R}^{-1(1)})$$

$$\overset{(1.14)}{=} \chi^-(a_2^*).$$

By similar arguments one proves the claim for χ^-. □

It should be noted that there also exist nonstandard star structures on $U_q\mathbf{g}$ for $|q|=1$, in particular the compact form $X_i^{\pm *} = X_i^{\mp}$, $K_i^* = K_i^{-1}$ in terms of the Cartan–Weyl generators. Then

$$\mathcal{R}^* = \mathcal{R}_{21}^{-1}, \tag{2.13}$$

while the coproduct does not fulfill (2.1) as in a standard Hopf $*$-algebra but becomes flipped under the star. This nevertheless has the correct classical limit, because the coproduct is cocommutative for $q=1$. In certain cases (in particular on the fuzzy quantum sphere[20] discussed in Sec. VI, but see also Ref. 31), it is then possible to define a star structure on each $\mathcal{A}_i$, which takes the form $a_{i;k}^* = \pm \Omega_i a_{i;k} \Omega_i^{-1}$ on the generators $a_{i;k}$ of $\mathcal{A}_i$. Here $\Omega_i = \sqrt[4]{v_i}^{-1}\omega_i$, where v_i and ω_i are the realizations in $\mathcal{A}_i$ (using an algebra map from $U_q\mathbf{g}$ to $\mathcal{A}_i$ as above) of the central element $v \in U_q\mathbf{g}$ (A8) and the "universal Weyl element" ω in an extension of $U_q\mathbf{g}$.[23] All this must be defined in some representation of $\mathcal{A}_i$; for more details see Refs. 20 and 31. (The v in Refs. 20 and 31 is the square root of our v here.) If moreover there exists an element Ω which realizes $\sqrt[4]{v}^{-1}\omega$ in $\mathcal{A}^+ = \mathcal{A}_1 \otimes^+ \mathcal{A}_2$ or a "physical" subspace thereof, then it follows easily from (2.13) that the star structure $a_{i;k}^* = \pm \Omega a_{i;k} \Omega^{-1}$ on $\mathcal{A}^+$ is consistent with the commutation relations of the braided tensor product algebra $\mathcal{A}^+$. This star then has the correct classical limit, and the same construction also works for $\mathcal{A}^-$.

III. UNBRAIDING CHAINS OF BRAIDED QUANTUM EUCLIDEAN SPACES OR SPHERES

In this section we consider the braided tensor product of $M \geqslant 2$ copies $\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_M$ of the quantum Euclidean space $\mathbb{R}_q^N$ (Ref. 13) [the U_q so(N)-covariant quantum space], i.e., of the unital associative algebra generated by x^i fulfilling the relations

$$\mathcal{P}^{ij}_{a_{hk}} x^h x^k = 0, \tag{3.1}$$

where $\mathcal{P}_a$ denotes the q-deformed antisymmetric projector appearing in the decomposition of the braid matrix $\hat{R}$ of $U_q\,\mathrm{so}(N)$ [given in formula (A23)], or of the quotient space of the latter obtained by setting $r^2 := x^i x_i = 1$ [the quantum $(N-1)$-dimensional sphere S_q^{N-1}]. The multiplet (x^i) carries the fundamental vector representation ρ of $U_q\,\mathrm{so}(N)$: for any $g \in U_q\,\mathrm{so}(N)$

$$x^i \triangleleft g = \rho^i_j(g) x^j. \tag{3.2}$$

We shall enumerate the different copies of the quantum Euclidean space or sphere by attaching an additional greek index to them, e.g., $\alpha = 1,2,\ldots,M$. The prescription (1.10) to glue $\mathcal{A}_1,\ldots,\mathcal{A}_M$ into a $U_q\,\mathrm{so}(N)$-module associative algebra $\mathcal{A}^-$ gives the following cross commutation relations between their respective generators:

$$x^{\alpha,i} x^{\beta,j} = \hat{R}^{ij}_{hk} x^{\alpha,h} x^{\beta,k} \tag{3.3}$$

whenever $\alpha < \beta$. Note that prescriptions (1.10) and (1.9) go into each other under the inverse reordering $1,2,\ldots,M \to M,\ldots,2,1$. Applying iteratively Theorem 1 we shall be able to completely unbraid this iterated tensor product.

To define $\varphi_1^{\pm}$ one actually needs a slightly enlarged version[5] of $\mathbb{R}_q^N$ (or S_q^{N-1}). One has to introduce some new generators $\sqrt{r_a}$, with $1 \leqslant a \leqslant N/2$, together with their inverses $(\sqrt{r_a})^{-1}$, requiring that

$$r_a^2 = \sum_{h=-a}^{a} x^h x_h = \sum_{h=-a}^{a} g_{hk} x^h x^k \tag{3.4}$$

(note that, having set $n := [N/2]$, r_n^2 coincides with r^2). Moreover for odd N we add also $\sqrt{x^0}$ and its inverse as new generators. In fact, the commutation relations involving these new generators can be fixed consistently, and turn out to be simply q-commutation relations. r plays the role of deformed Euclidean distance of the generic point of coordinates (x^i) of $\mathbb{R}_q^N$ from the origin; r_a is the projection of r on the subspace $x^i = 0$, $|i| > a$. In the previous equation g_{hk} denotes the metric matrix of $\mathrm{SO}_q(N)$:

$$g_{ij} = g^{ij} = q^{-\rho_i} \delta_{i,-j}\,. \tag{3.5}$$

It is a $\mathrm{SO}_q(N)$-isotropic tensor and is a deformation of the ordinary Euclidean metric. Here and in the sequel $n := [N/2]$ is the rank of $\mathrm{so}(N)$, the indices take the values $i = -n,\ldots,-1,0,1,\ldots n$ for N odd, and $i = -n,\ldots,-1,1,\ldots n$ for N even. Moreover, we have introduced the notation $(\rho_i) = (n - \frac{1}{2},\ldots,\frac{1}{2},0,-\frac{1}{2},\ldots,\frac{1}{2}-n)$ for N odd, $(n-1,\ldots,0,0,\ldots,1-n)$ for N even. In the case of even N one needs to include also the FRT generator $\mathcal{L}_1^{-1}$ and its inverse $\mathcal{L}_1^{+1}$ [which are generators of $U_q\,\mathrm{so}(N)$ belonging to the Cartan subalgebra] among the generators of $\mathcal{A}_1$. They satisfy the commutation relations

$$\mathcal{L}_1^{-1} x^{\pm 1} = q^{\pm 1} x^{\pm 1} \mathcal{L}_1^{-1}, \quad \mathcal{L}_1^{-1} x^{\pm i} = x^{\pm i} \mathcal{L}_1^{-1} \quad \text{for} \quad i > 1 \tag{3.6}$$

with $\mathcal{A}_1$, and the standard FRT relations with the rest of $U_q\,\mathrm{so}(N)$. One can easily show that the extension of the action of $U_q\,\mathrm{so}(N)$ to $\sqrt{r_a}$ $(\sqrt{r_a})^{-1}$ is uniquely determined by the constraints the latter fulfill; it is a bit complicated and therefore will be omitted, since we will not need its explicit expression. The action of H on $\mathcal{L}_1^{-1}$ is the standard (right) adjoint action. Note that the maps $\varphi_1^{\pm}$ have no analog in the "undeformed" case $(q=1)$, because $\mathcal{A}_1 \equiv \mathbb{R}^N$ is abelian, whereas $H \equiv U_q\,\mathrm{so}(N)$ is not.

The unbraiding procedure is recursive. We use the homomorphism φ_1 found in Ref. 5 and start by unbraiding the first copy from the others. Following Theorem 1, we perform the following change of generators in $\mathcal{A}^-$,

$$y^{1,i} := x^{1,i},$$

$$y^{\alpha,i}:=\chi^{-}(x^{\alpha,i}) \overset{(1.14)}{=} \varphi_1(\mathcal{R}^{-1(2)})\rho^i_j(\mathcal{R}^{-1(1)})x^{\alpha,j}=\varphi_1(\mathcal{L}^{-i}_{\ j})x^{\alpha,j},\quad \alpha>1.$$

In the last equality we have used the definition (A15) of the FRT generators[13] of $U_q\,\mathrm{so}(N)$. In the third part of the Appendix we recall the $\varphi^{\pm}$ images of the latter. In view of formula (A36) we thus find

$$y^{1,i}:=x^{1,i},$$

$$y^{\alpha,i}:=g^{ih}[\mu^1_h,x^{1,k}]_q g_{kj}x^{\alpha,j},\quad \alpha>1. \tag{3.7}$$

The suffix 1 in μ^1_a means that the special elements μ_a defined in (A37) must be taken as elements of the first copy of $\mathbb{R}^N_q$. In view of (A37) we see that $g^{ih}[\mu^1_h,x^{1,k}]_q g_{kj}$ are rather simple polynomials in x^i and r_a^{-1}, homogeneous of total degree 1 in the coordinates x^i and r_a. Hence (3.7) is a transformation of polynomial type and therefore likely to be implemented as a well-defined operator transformation also when representing $\mathcal{A}^-$ as an algebra of operators on some linear space. Using the results (A42) given in the appendix we give now the explicit expression of (3.7) for $N=3$:

$$y^{\alpha,-}=-qh\gamma_1\frac{r}{x^0}x^{\alpha,-},$$

$$y^{\alpha,0}=\sqrt{q}(q+1)\frac{1}{x^0}x^+x^{\alpha,-}+x^{\alpha,0}, \tag{3.8}$$

$$y^{\alpha,+}=\frac{\sqrt{q}(q+1)}{h\gamma_1 r x^0}(x^+)^2x^{\alpha,-}+\frac{q^{-1}+1}{h\gamma_1 r}x^+x^{\alpha,0}-\frac{1}{qh\gamma_1 r}x^0x^{\alpha,+}$$

for any $\alpha=2,\ldots,M$. Here we have set $x^i\equiv x^{1,i}$, $h\equiv\sqrt{q}-1/\sqrt{q}$, replaced for simplicity the values $-1,0,1$ of the indices by the ones $-,0,+$ and denoted by $\gamma_1\in\mathbb{C}$ a free parameter.

As a consequence of the theorem we find the following.

Corollary 1:

$$[y^{1,i},y^{\alpha,j}]=0,\quad \alpha>1, \tag{3.9}$$

$$y^{\alpha,i}y^{\beta,j}=\hat{R}^{ij}_{hk}y^{\alpha,h}y^{\beta,k},\quad 1<\alpha<\beta, \tag{3.10}$$

$$\mathcal{P}^{ij}_{a_{hk}}y^{\alpha,h}y^{\alpha,k}=0. \tag{3.11}$$

By (3.9) the subalgebra $\tilde{\mathcal{A}}_1^-\equiv\mathcal{A}_1$ of $\mathcal{A}^-$ generated by $y^{1,i}\equiv x^{1,i}$ commutes with the subalgebra generated by $y^{2,i},\ldots,y^{M,i}$, which we shall call $\tilde{\mathcal{A}}^-$. This was the first step of the unbraiding procedure. Now we can reiterate the latter for $\tilde{\mathcal{A}}^-$, with $y^{2,i}$ playing the role of $x^{1,i}$. After $M-1$ steps, we shall have determined M independent commuting subalgebras of $\mathcal{A}^-$ which we shall call $\tilde{\mathcal{A}}^-_\alpha$, $\alpha=1,\ldots,M$.

The unbraiding procedure for the alternative braided tensor product stemming from prescription (1.9) arises by iterating the change of generators

$$y'^{M,i}:=x^{M,i},$$

$$y'^{\alpha,i}:=\varphi_M(\mathcal{L}^{+i}_{\ j})x^{\alpha,j}=g^{ih}[\overline{\mu}^M_h,x^{M,k}]_{q^{-1}}g_{kj}x^{\alpha,j},\quad \alpha<M. \tag{3.12}$$

$\overline{\mu}_a^M$ are the special elements defined in (A40) belonging to the Mth copy of $\mathbb{R}_q^N$. Using the results (A43) given in the appendix we give the explicit expression of (3.12) for $N=3$: for any $\alpha=1,\ldots,M-1$,

$$y'^{\alpha,-}=-h\overline{\gamma}_1\frac{z^0}{r_z}x^{\alpha,-}+\frac{k\overline{\gamma}_1}{\sqrt{q}r_z}z^-x^{\alpha,0}+\frac{q^{-2}k\overline{\gamma}_1}{r_z z^0}(z^-)^2x^{\alpha,+},$$

$$y'^{\alpha,0}=x^{\alpha,0}+q^{-1/2}(q^{-1}+1)\frac{1}{z^0}z^-x^{\alpha,+}, \tag{3.13}$$

$$y'^{\alpha,+}=-\frac{r_z}{h\overline{\gamma}_1 z^0}x^{\alpha,+}.$$

Here we have set $z^i\equiv x^{M,i}$, $r_z^2\equiv x^{M,i}x_i^M$, $k\equiv q-q^{-1}$, and $\overline{\gamma}_1\in\mathbb{C}$ is a free parameter.

Again, the subalgebra $\tilde{\mathcal{A}}_M^+\approx\mathbb{R}_q^N$ of $\mathcal{A}^+$ generated by $y^{M,i}\equiv x^{M,i}$ commutes with the subalgebra generated by $y^{1,i},\ldots,y^{M-1,i}$, which we shall call $\tilde{\mathcal{A}}^+$. This was the first step of the unbraiding procedure. Now we can reiterate the latter for $\tilde{\mathcal{A}}^+$, with $y^{M-1,i}$ playing the role of $x^{M,i}$. After $M-1$ steps, we shall have determined M independent commuting subalgebras of $\mathcal{A}^+$ which we shall call $\tilde{\mathcal{A}}_\alpha^+$.

We summarize the results of this section.

Proposition 3: Let $\mathcal{A}_1,\mathcal{A}_2,\ldots,\mathcal{A}_M$ be M copies of the U_q so(N)-covariant quantum Euclidean space (or sphere). Then $\mathcal{A}_1\underline{\otimes}^{\pm}\mathcal{A}_2\underline{\otimes}^{\pm}\cdots\underline{\otimes}^{\pm}\mathcal{A}_M=\mathcal{A}_1\tilde{\mathcal{A}}_2^{\pm}\cdots\tilde{\mathcal{A}}_M^{\pm}$, where $\tilde{\mathcal{A}}_2^{\pm},\ldots,\tilde{\mathcal{A}}_M^{\pm}$ are subalgebras of the left-hand side (lhs) isomorphic to $\mathcal{A}_1$ and commuting with each other.

By a suitable choice of $\gamma_1,\overline{\gamma}_1$, as well as of the other free parameters appearing in the definitions of $\varphi^{\pm}$ for $N>3$ (see Part 3 of the Appendix), one can make $\varphi^{\pm}$ into $*$-homomorphisms when $|q|=1$, and make them satisfy the relation

$$[\varphi^{\pm}(g)]^*=\varphi^{\mp}(g^*) \tag{3.14}$$

when $q\in\mathbb{R}^+$. Since these relations are of the type considered in proposition 2, the claims of the latter for $\chi^{\pm}$ and their consequences hold. In particular, when $|q|=1$ one has a well-defined $*$ on the braided tensor product of $\mathcal{A}_1,\ldots,\mathcal{A}_M$ mapping each of the independent, commuting subalgebras $\tilde{\mathcal{A}}_i^{\pm}$ into itself. On the contrary for real q one can consider the map $*:\mathcal{A}^+\to\mathcal{A}^-$ defined by (2.3) or a $*$-structure on $\mathcal{A}^{\pm}$ defined in a way similar to what we have done in (2.7),

$$(x^{\alpha,i})^\star=x^{M-\alpha+1,j}g_{ji}. \tag{3.15}$$

The latter has not the standard classical limit. A short calculation shows that the latter implies

$$(y^{\alpha,i})^\star=y'^{M-\alpha+1,j}g_{ji}. \tag{3.16}$$

IV. UNBRAIDING CHAINS OF BRAIDED HEISENBERG ALGEBRAS

In this section we consider the braided tensor product of $M\geqslant 2$ copies $\mathcal{A}_1,\mathcal{A}_2,\ldots,\mathcal{A}_M$ of the $U_q\mathbf{g}$-covariant deformed Heisenberg algebra $\mathcal{D}_{\epsilon,\mathbf{g}}$, $\mathbf{g}=\mathrm{sl}(N)$, so$(N)$,[29,32,4] i.e., the unital associative algebra generated by x^i,∂_j fulfilling the relations

$$\mathcal{P}^{ij}_{a_{hk}}x^hx^k=0,$$

$$\mathcal{P}^{ij}_{a_{hk}}\partial_j\partial_i=0, \tag{4.1}$$

$$\partial_ix^j=\delta_j^i+(q\gamma\hat{R})^{\epsilon jk}_{ih}x^h\partial_k,$$

where $\gamma=q^{1/N}$,1 respectively, for $\mathbf{g}=\mathrm{sl}(N)$, $\mathrm{so}(N)$, and the exponent ϵ can take either value $\epsilon=1,-1$. $\hat{R}$ denotes the braid matrix of $U_q\mathbf{g}$ [given in formulas (A22) and (A23)], and again $\mathcal{P}_a$ the antisymmetric projector appearing in the decomposition of the latter. The coordinates x^i transform according to the fundamental vector representation of $U_q\mathbf{g}$, as in (3.2), whereas the partial derivatives trasform according to the contragredient representation,

$$\partial_i \triangleleft g = \partial_h \rho_i^h(S^{-1}g). \tag{4.2}$$

The indices will take the values $i=1,\ldots,N$ if $\mathbf{g}=\mathrm{sl}(N)$, the same values considered in the preceding section if $\mathbf{g}=\mathrm{so}(N)$. Clearly in the latter case $\mathcal{D}_\epsilon,\mathbf{g}$ has the quantum Euclidean space generated by x^i as a module subalgebra.

Again, we shall enumerate the different copies by attaching to them an additional greek index, e.g., $\alpha=1,2,\ldots,M$. The prescription (1.9) to glue $\mathcal{A}_1,\ldots,\mathcal{A}_M$ into a $U_q\mathbf{g}$-module associative algebra $\mathcal{A}^+$ (see also Ref. 15) gives the following cross commutation relations between their respective generators:

$$\begin{aligned} &x^{\alpha,i}x^{\beta,j}=\hat{R}^{ij}_{hk}x^{\beta,h}x^{\alpha,k}, \quad \partial_{\alpha,i}\partial_{\beta,j}=\hat{R}^{kh}_{ji}\partial_{\beta,h}\partial_{\alpha,k}, \\ &\partial_{\alpha,i}x^{\beta,j}=\hat{R}^{-1\,jh}_{ik}x^{\beta,k}\partial_{\alpha,h}, \quad \partial_{\beta,i}x^{\alpha,j}=\hat{R}^{jh}_{ik}x^{\alpha,k}\partial_{\beta,h} \end{aligned} \tag{4.3}$$

when $\alpha>\beta$. With respect to Ref. 15 we have called the generators x^i,∂_j instead of A^i,A^+_j, inverted the order of the product due to covariance with respect to the *right* (instead of the *left*) $U_q\mathbf{g}$-action, and for the sake of simplicity we have put equal to one possible factors at the rhs of (4.3).

In Refs. 14 and 9 algebra homomorphisms $\varphi:\mathcal{D}_\epsilon,\mathbf{g}\rtimes H\to\mathcal{D}_\epsilon,\mathbf{g}$ have been determined for $\mathbf{g}=\mathrm{so}(n)$ and $\mathbf{g}=\mathrm{sl}(N),\mathrm{so}(N)$, respectively. This is the q-analog of vector field realization of $\mathbf{g}$ on the corresponding $\mathbf{g}$-covariant (undeformed) space, e.g., $\varphi_1(E^i_j)=x^i\partial_j-(1/N)\,\delta^i_j$ in the $\mathbf{g}=\mathrm{sl}(N)$ case. The searched maps $\varphi^\pm$ will be simply the restrictions of φ to $\mathcal{D}_\epsilon,\mathbf{g}\rtimes H^\pm$. In Ref. 14 there are among others the φ-images of the Chevalley generators of $U_q\,\mathrm{so}(N)$ [one should take care of the fact that in Ref. 14 we considered $U_q\,\mathrm{so}(N)$ acting by a *left* action, instead of a right one, what manifests itself in a replacement $q\to q^{-1}$, or equivalently in an opposite coproduct; the rules for passing from right to left are described in Sec. V], in Ref. 9 there are the φ-images of the generators of $U_q\mathbf{g}$ playing the role of "vector fields" on G_q. By the change of generators described in Ref. 13 one can easily pass from the Chevalley to the FRT generators $\mathcal{L}^{\pm i}_j$ (A15), whereas the relation between the latter and the vector fields is recalled in (A52). The FRT generators are the ones explicitly needed in writing down $\chi^\pm(x^i)$ and $\chi^\pm(\partial_i)$. For example, for $\mathbf{g}=\mathrm{sl}(2)$ and $\epsilon=1$ one finds

$$\begin{aligned} &\varphi(\mathcal{L}_1^{+1})=\varphi(\mathcal{L}_2^{-2})=[\varphi(\mathcal{L}_1^{-1})]^{-1}=[\varphi(\mathcal{L}_2^{+2})]^{-1}=\alpha\Lambda^{1/2}[1+(q^2-1)x^2\partial_2]^{1/2}, \\ &\varphi(\mathcal{L}_2^{+1})=-\alpha k q^{-1}\Lambda^{1/2}[1+(q^2-1)x^2\partial_2]^{-1/2}x^1\partial_2, \\ &\varphi(\mathcal{L}_1^{-2})=\alpha k q^3\Lambda^{1/2}[1+(q^2-1)x^2\partial_2]^{-1/2}x^2\partial_1, \end{aligned} \tag{4.4}$$

where α is fixed by (A14) to be $\alpha=\pm1,\pm i$ and we have set

$$\Lambda^{-2}:=1+(q^2-1)x^i\partial_i. \tag{4.5}$$

Whereas for $\mathbf{g}=\mathrm{so}(3)$ and $\epsilon=1$ one finds on the positive Borel subalgebra

$$\begin{aligned} &\varphi(\mathcal{L}_-^{+-})=-\alpha\Lambda[1+(q-1)x^0\partial_0+(q^2-1)x^+\partial_+], \\ &\varphi(\mathcal{L}_0^{+-})=\alpha k\Lambda(x^-\partial_0-\sqrt{q}x^0\partial_+), \end{aligned}$$

$$\begin{gathered}\varphi(\mathcal{L}_{+}^{+-})=\frac{1}{1+q^{-1}}\varphi(\mathcal{L}_{0}^{+-})\varphi(\mathcal{L}_{+}^{+0}),\\ \varphi(\mathcal{L}_{0}^{+0})=1,\\ \varphi(\mathcal{L}_{+}^{+0})=-q^{-1/2}[\varphi(\mathcal{L}_{-}^{+-})]^{-1}\varphi(\mathcal{L}_{0}^{+-}),\\ \varphi(\mathcal{L}_{+}^{++})=[\varphi(\mathcal{L}_{-}^{+-})]^{-1},\end{gathered}\tag{4.6}$$

and on the negative Borel subalgebra

$$\begin{gathered}\varphi(\mathcal{L}_{-}^{--})=-(\alpha\Lambda[1+(q-1)x^0\partial_0+(q^2-1)x^+\partial_+])^{-1},\\ \varphi(\mathcal{L}_{-}^{-0})=-\alpha q^2 k\varphi(\mathcal{L}_{-}^{--})\Lambda(x^0\partial_- -\sqrt{q}x^+\partial_0),\\ \varphi(\mathcal{L}_{-}^{-+})=\frac{1}{1+q}\varphi(\mathcal{L}_{0}^{-+})\varphi(\mathcal{L}_{-}^{-0}),\\ \varphi(\mathcal{L}_{0}^{-0})=1,\\ \varphi(\mathcal{L}_{0}^{-+})=-\alpha q^{3/2}k\Lambda(x^0\partial_- -\sqrt{q}x^+\partial_0),\\ \varphi(\mathcal{L}_{+}^{-+})=[\varphi(\mathcal{L}_{-}^{--})]^{-1}.\end{gathered}\tag{4.7}$$

Here we have set

$$\Lambda^{-2}:=\left[1+(q^2-1)x^i\partial_i+\frac{(q^2-1)^2}{\omega_1^2}(g_{ij}x^ix^j)(g^{hk}\partial_k\partial_h)\right],\tag{4.8}$$

where

$$\omega_a:=(q^{\rho_a}+q^{-\rho_a}),$$

and replaced for simplicity the values $-1,0,1$ of the indices by the ones $-,0,+$. In either case the φ-images of $\mathcal{L}_{j}^{+i}$ and $\mathcal{L}_{i}^{-j}$ for $i>j$ vanish, because the latter do.

We see that strictly speaking φ takes values in some appropriate completion of $\mathcal{D}_{\epsilon,\mathbf{g}}$, containing at least the square root and inverse square root of the polynomial Λ^{-2}, respectively, defined in (4.5), (4.8), as well as the square root of $[1+(q^2-1)x^2\partial_2]$ and its inverse, when $\mathbf{g}=\mathrm{sl}(2)$, and the inverses $(4.6)_6$, $(4.7)_6$, when $\mathbf{g}=\mathrm{so}(3)$. Apart from this minimal completion, another possible one is the so-called h-adic, namely the ring of formal power series in $h=\log q$ with coefficients in $\mathcal{D}_{\epsilon,\mathbf{g}}$. Other completions, e.g., in operator norms, can be considered according to the needs. One can easily show that the extension of the action of H to any such completion is uniquely determined (we omit to write down its explicit expression, since we do not need it).

According to the main theorem, we set

$$\begin{gathered}y^{1,i}\equiv x^{1,i},\\ \partial_{y,1,a}\equiv\partial_{1,a},\\ y^{\alpha,i}\equiv\chi^-(x^{\alpha,i})=\varphi_1(\mathcal{L}_{j}^{-1})x^{\alpha,j},\quad \alpha>1,\\ \partial_{y,\alpha,a}\equiv\chi^-(\partial_{\alpha,a})=\varphi_1(S\mathcal{L}_{a}^{-d})\partial_{\alpha,d},\quad \alpha>1,\end{gathered}\tag{4.9}$$

and we find the following.

Corollary 2:

$$\mathcal{P}^{ij}_{a_{hk}} y^{\alpha,h} y^{\alpha,k} = 0,$$

$$\mathcal{P}^{hk}_{a_{ij}} \partial_{y\alpha,k} \partial_{y,\alpha,h} = 0, \tag{4.10}$$

$$\partial_{y,\alpha,i} y^{\alpha,j} = \delta^j_i + (q\hat{R})^{\epsilon_\alpha jl}_{im} y^{\alpha,m} \partial_{y,\alpha,l}$$

for all $\alpha = 1, \ldots, M$, *together with*

$$[y^{1,i}, y^{\alpha,j}] = 0, \quad [\partial_{y,1,i}, y^{\alpha,j}] = 0,$$
$$[\partial_{y,\alpha,i}, y^{1,j}] = 0, \quad [\partial_{y,1,i}, \partial_{y,\alpha,j}] = 0 \tag{4.11}$$

when $\alpha > 1$, *and*

$$y^{\alpha,i} y^{\beta,j} = \hat{R}^{ij}_{hk} y^{\beta,h} y^{\alpha,k},$$

$$\partial_{y,\alpha,i} \partial_{y,\beta,j} = \hat{R}^{kh}_{ji} \partial_{y,\beta,h} \partial_{y,\alpha,k},$$

$$\partial_{y,\alpha,i} y^{\beta,j} = \hat{R}^{-1\,jh}_{ik} y^{\beta k} \partial_{y,\alpha,h}, \tag{4.12}$$

$$\partial_{y,\beta,i} y^{\alpha,j} = \hat{R}^{jh}_{ik} y^{\alpha,k} \partial_{y,\beta,h}$$

when $1 < \beta < \alpha$.

By (4.11) $y^{1,i} \equiv x^{1,i}$ and $\partial_{y,1,i} \equiv \partial_{1,i}$ commute with the subalgebra generated by $y^{2,i}, \ldots, y^{M,i}$ and $\partial_{y,2,i}, \ldots, \partial_{y,M,i}$ which we shall call $\tilde{\mathcal{A}}^+$. This was the first step of the unbraiding procedure. Now we can reiterate the latter for $\tilde{\mathcal{A}}^+$, with $y^{2,i}, \partial_{y,2,i}$ playing the role of $x^{1,i}, \partial_{1,i}$. After $M-1$ steps, we shall have determined M independent commuting subalgebras of $\mathcal{A}^+$ which we shall call $\tilde{\mathcal{A}}^+_\alpha$.

For the sake of brevity we omit the unbraiding procedure for the alternative braided tensor product algebra stemming from prescription (1.10), which can be found following arguments completely analogous to the ones presented at the end of Sec. III. We summarize the results of this section by the following.

Proposition 4: Let $\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_M$ *be M copies of the* $U_q\mathbf{g}$*-covariant Heisenberg algebra* $\mathcal{D}_{\epsilon,\mathbf{g}}$, $\mathbf{g} = \mathrm{sl}(N)$, $\mathrm{so}(N)$. *Then* $\mathcal{A}_1 \underline{\otimes}^{\pm} \mathcal{A}_2 \underline{\otimes}^{\pm} \ldots \underline{\otimes}^{\pm} \mathcal{A}_M = \mathcal{A}_1 \tilde{\mathcal{A}}^{\pm}_2 \cdots \tilde{\mathcal{A}}^{\pm}_M$, *where* $\tilde{\mathcal{A}}^{\pm}_2, \ldots, \tilde{\mathcal{A}}^{\pm}_M$ *are subalgebras of the lhs isomorphic to* $\mathcal{D}_{\epsilon,\mathbf{g}}$ *and commuting with each other*.

Relations (A28), (2.2), (3.2), (4.2) and (4.1) fix the $*$-structure of $\mathcal{A}_1$ to be

$$(x^i)^* = x^i, \quad (\partial_i)^* = -\partial_i \begin{cases} q^{\pm 2(N-i+1)} & \text{if } H = U_q\,\mathrm{sl}(N), \\ q^{\pm N + \rho_i} & \text{if } H = U_q \mathrm{so}(N), \end{cases} \tag{4.13}$$

if $|q| = 1$, and

$$(x^h)^* = x^k g_{kh}, \quad (\partial_i)^* = -\frac{\Lambda^{\pm 2}}{q^{\pm N} + q^{\pm 2}} [(g^{jh}\partial_h \partial_j), x^i], \tag{4.14}$$

if $H = U_q\,\mathrm{so}(N)$ and $q \in \mathbb{R}^+$. The upper or lower sign, respectively, refer to the choices $\epsilon = 1$, -1 in $(4.1)_3$, and $\Lambda^{\pm 2}$ are, respectively, defined by

$$\Lambda^{\pm 2} := \left[1 + (q^{\pm 2} - 1) x^i \partial_i + \frac{(q^{\pm 2} - 1)^2}{\omega_n^2} r^2 (g^{ji} \partial_i \partial_j) \right]^{-1}. \tag{4.15}$$

The map φ is a $*$-homomorphism both for q real and $|q|=1$. If we denote by $\varphi^{\pm}$ its restrictions to $\mathcal{A}\rtimes H^{\pm}$, then they are $*$-homomorphisms when $|q|=1$ (see the fourth part of the Appendix), and fulfill the relation

$$[\varphi^{\pm}(g)]^*=\varphi^{\mp}(g^*) \tag{4.16}$$

when $q\in\mathbb{R}^+$.[14] Since these relations are of the type considered in proposition 2, the claims of the latter for $\chi^{\pm}$ and their consequences hold. In particular, when $|q|=1$ one has a well-defined $*$ on the braided tensor product of $\mathcal{A}_1,\ldots,\mathcal{A}_M$ mapping each of the independent, commuting subalgebras $\tilde{\mathcal{A}}_\alpha^{\pm}$ into itself.

Finally, the above results have an important corollary. According to Hochschild cohomology arguments developed by Gerstenhaber[19] and applicable to Heisenberg algebras because of the results found by Du Cloux in Ref. 12, any deformed Heisenberg algebra, in particular the braided tensor products of $\mathcal{A}_1,\ldots,\mathcal{A}_M$ considered in this section, can be realized simply by a change of generators in the h-adic completion, $h=\log q$, of its undeformed counterpart (but in general *not* in other, e.g., *operator-norm*, completions). However explicit realizations are not provided by these results. The results presented here, combined to some older ones, allow to determine one such realization. In Ref. 27 Ogievetsky found an explicit realization ϕ or deforming map of the elements of $\mathcal{D}_\epsilon,\mathbf{g}$ in terms of formal power series in $h=\log q$ with coefficients in the corresponding undeformed Heisenberg algebra. Another, less explicit, one was found in Ref. 16. The composition of the unbraiding map found in this section, which allows to decouple M different copies of $\mathcal{D}_\epsilon,\mathbf{g}$ from each other, with the map ϕ provides an explicit realization or deforming map of the larger Heisenberg algebra $\mathcal{A}$ (what we have called the braided chain of Heisenberg algebras), in the h-adic completion of the undeformed $(N\cdot M)$-dimensional Heisenberg algebra.

V. FORMULAS FOR THE LEFT ACTION

For psychological reasons we often prefer to work with a left action rather than with a right one. In this section we give the analogs for left H-module algebras of the main results found so far for right H-module algebras. The left action of $g\in H$ on a product fulfills

$$(gg')\triangleright a=g\triangleright(g'\triangleright a), \tag{5.1}$$

$$g\triangleright(aa')=(g_{(1)}\triangleright a)(g_{(2)}\triangleright a'). \tag{5.2}$$

The product laws in the braided tensor product algebras $\hat{\mathcal{A}}^+,\hat{\mathcal{A}}^-$ are, respectively, given by

$$a_2a_1=(\mathcal{R}^{-1(1)}\triangleright a_1)(\mathcal{R}^{-1(2)}\triangleright a_2), \tag{5.3}$$

$$a_2a_1=(\mathcal{R}^{(2)}\triangleright a_1)(\mathcal{R}^{(1)}\triangleright a_2). \tag{5.4}$$

The analog of Theorem 1 reads as follows.

Theorem 2: *Let $\{H,\mathcal{R}\}$ be a quasitriangular Hopf algebra and H^+,H^- be Hopf subalgebras of H such that $\mathcal{R}\in H^+\otimes H^-$. Let $\hat{\mathcal{A}}_1,\hat{\mathcal{A}}_2$ be, respectively, a (left) H^+- and a H^--module algebra, so that we can define $\hat{\mathcal{A}}^+$ as in (5.3), and $\hat{\varphi}_1^+:H^+\ltimes\hat{\mathcal{A}}_1\to\hat{\mathcal{A}}_1$ be an algebra homomorphism fulfilling (1.12), so that we can define a map $\hat{\chi}^+:\hat{\mathcal{A}}_2\to\hat{\mathcal{A}}^+$ by*

$$\hat{\chi}^+(a_2):=(\mathcal{R}^{(2)}\triangleright a_2)\,\hat{\varphi}_1^+(\mathcal{R}^{(1)}). \tag{5.5}$$

Alternatively, let $\hat{\mathcal{A}}_1,\hat{\mathcal{A}}_2$ be, respectively, a (left) H^--and a H^+-module algebra, so that we can define $\hat{\mathcal{A}}^-$ as in (5.4), and $\hat{\varphi}_1^+:H^+\ltimes\hat{\mathcal{A}}_1\to\hat{\mathcal{A}}_1$ be an algebra homomorphism fulfilling (1.12), so that we can define a map $\hat{\chi}^-:\hat{\mathcal{A}}_2\to\hat{\mathcal{A}}^-$ by

$$\hat{\chi}^-(a_2):=(\mathcal{R}^{-1(1)}\triangleright a_2)\,\hat{\varphi}_1^-(\mathcal{R}^{-1(2)}). \tag{5.6}$$

In either case $\hat{\chi}^{\pm}$ *are then injective algebra homomorphisms and*

$$[\hat{\chi}^{\pm}(a_2),\hat{\mathcal{A}}_1]=0, \tag{5.7}$$

namely the subalgebras $\tilde{\hat{\mathcal{A}}}_2^{\pm}:=\hat{\chi}^{\pm}(\hat{\mathcal{A}}_2)\approx\hat{\mathcal{A}}_2$ *commute with* $\hat{\mathcal{A}}_1$. *Moreover* $\hat{\mathcal{A}}^{\pm}=\hat{\mathcal{A}}_1\tilde{\hat{\mathcal{A}}}_2^{\pm}$.

The results of Sec. II apply without modifications (one just has to place a $\hat{}$ in the appropriate places).

To enumerate the generators of the algebras considered in Secs. III and IV we shall exchange lower with upper indices, so the generators will read $x_{\alpha,i}, \partial^{\alpha,i}$. This is necessary if we wish the x's to carry what we shall consider the fundamental (vector) representation ρ of $U_q\mathbf{g}$,

$$g\triangleright x_i=x_j\rho_i^j(g), \tag{5.8}$$

rather than its contragredient $\rho^T\circ S$, because this follows from the row×column multiplication law $\rho_h^i(gg')=\rho_j^i(g)\rho_h^j(g')$. Apart from this replacement, all the commutation relations remain the same, but can be rephrased in an equivalent way exchanging lower with upper indices also in the braid matrices and in the projectors $\mathcal{P}_a$, because $\hat{R}^T=\hat{R}$, ${\mathcal{P}_a}^T=\mathcal{P}_a$. For instance, the analog of (3.1) will read

$$\mathcal{P}_{aij}^{hk}x_hx_k=0. \tag{5.9}$$

The analogs of (3.2) and (4.2) read

$$g\triangleright x_i=\rho_i^j(g)x_j, \tag{5.10}$$

$$g\triangleright \partial^i=\partial^h\rho_h^i(Sg). \tag{5.11}$$

Algebra homomorphisms $\hat{\varphi}_1^{\pm}$ for the algebras considered in Secs. III and IV are immediately obtained in terms of the $\varphi_1^{\pm}$ described there, according to the rule

$$\hat{\varphi}_1^{\pm}(\mathcal{L}_j^{\pm h})=U_a^{-1j}\varphi_1^{\mp}(\mathcal{L}_b^{\mp a})U_h^b. \tag{5.12}$$

Here

$$U_c^b:=\rho_c^b(u), \tag{5.13}$$

$u\in H$ is a special element as in (A6), and at the rhs the correct expression in the new notation has lower and upper indices exchanged. If $\hat{\mathcal{A}}_1$ is the quantum Euclidean space $\mathbb{R}_q^N$ one finds, for instance,

$$\hat{\varphi}_1^-(\mathcal{L}_j^{-h})=U_a^{-1j}g_{ac}[\overline{\mu}^c,x_k]_{q^{-1}}g^{kb}U_b^h \overset{(A30)}{=} g_{cj}[\overline{\mu}^c,x_k]_qg^{hk}, \tag{5.14}$$

where μ^c is the same as μ_c [see (A3)], but in the new notation. For instance, when $|c|>1$ it reads

$$\overline{\mu}^c=\overline{\gamma}_cr_{|c|}^{-1}r_{|c|-1}^{-1}x_{-c}, \tag{5.15}$$

with γ_c defined as in (A41) and r_a $(a\geqslant 0)$ defined by the condition

$$r_a^2=\sum_{h=-a}^{a}x_hx^h=\sum_{h=-a}^{a}g^{hk}x_hx_k.$$

The analog of (3.7) is therefore (with $\alpha>1$)

$$y_{1,i}:=x_{1,i}, \tag{5.16}$$

$$y^{\alpha,i} := \hat{\chi}^-(x_{\alpha,i}) = x_{\alpha,j}\hat{\varphi}_1(\mathcal{L}_i^{-j}) = x_{\alpha,j} g_{hi}[\overline{\mu}^{1,h}, x_{1,k}]_{q^{-1}} g^{jk}. \tag{5.17}$$

VI. UNBRAIDING CHAINS OF FUZZY QUANTUM SPHERES

As a last example, we consider the braided tensor product of M copies $\mathcal{A}_1, \ldots, \mathcal{A}_M$ of the q-deformed fuzzy sphere $\hat{S}^2_{q,N}$ (Ref. 20) (to relate this to our conventions, the q in Ref. 20 should be replaced by $q^{-1/2}$), which we consider as a left $U_q\,\mathrm{so}(3)$ module algebra. It is generated by x_i fulfilling the relations

$$\begin{aligned} \varepsilon_k^{ij} x_i x_j &= \Lambda_N \;\; x_k, \\ g^{ij} x_i x_j &= R^2. \end{aligned} \tag{6.1}$$

Here $R>0$,

$$C_N = \frac{[N]_q[N+2]_q}{[2]_q^2}, \quad \Lambda_N = R\,\frac{[2]_{q^{N+1}}}{\sqrt{[N]_q[N+2]_q}}, \tag{6.2}$$

where $[n]_q := (q^{n/2} - q^{-n/2})/(q^{1/2} - q^{-1/2})$, and

$$\begin{gathered} \varepsilon_1^{10} = q^{1/2}, \quad \varepsilon_1^{01} = -q^{-1/2}, \\ \varepsilon_0^{00} = q^{1/2} - q^{-1/2}, \quad \varepsilon_0^{1-1} = 1 = -\varepsilon_0^{-11}, \\ \varepsilon_{-1}^{0-1} = q^{1/2}, \quad \varepsilon_{-1}^{-10} = -q^{-1/2} \end{gathered} \tag{6.3}$$

are the spin-1 Clebsch–Gordan coefficients. The multiplet (x_i) carries the fundamental vector representation ρ of $H = U_q\,\mathrm{so}(3)$:

$$g \triangleright x_i = x_j \rho_i^j(g). \tag{6.4}$$

There is no obvious generalization to higher dimensions, but this algebra appears to be relevant, e.g., to D-branes on the SU(2) WZW model.[1] It has a unique irreducible representation, which is equivalent to $\mathrm{Mat}(N+1)$. Here we only consider the case $q \in \mathbb{R}^+$, where the star structure is given by $x_i^* = g^{ij} x_j$. Then $\hat{S}^2_{q,N}$ is simply the "discrete series" of Podles's spheres.[28] It was shown in Ref. 20 that there is a star-algebra homomorphism $\hat{\varphi}: H \ltimes \hat{S}^2_{q,N} \to \hat{S}^2_{q,N}$, which takes a particularly simple form

$$\hat{\varphi}(E^+) = \frac{1}{R}\sqrt{q^{-1}[2]_q C_N}\, x_1, \quad \hat{\varphi}(E^-) = -\frac{1}{R}\sqrt{q[2]_q C_N}\, x_{-1},$$

$$\hat{\varphi}(q^{H/2}) = \frac{[2]_{q^{N+1}}}{[2]_q}\left(1 - \frac{q^{1/2} - q^{-1/2}}{\Lambda_N} x_0\right)$$

where $E^\pm = X^\pm q^{H/4} \in U_q\,\mathrm{so}(3)$. Note that $(1 - [(q^{1/2} - q^{-1/2})/\Lambda_N] x_0)$ is invertible since the eigenvalues of $q^{H/2}$ are positive (assuming $q>0$), therefore $\hat{\varphi}(q^{-H/2}) \in \hat{S}^2_{q,N}$ is well-defined also. Hence the algebra homomorphisms $\hat{\varphi}$ is defined on the entire algebra $U_q\,\mathrm{so}(3)$. Using the definition (A15) and the explicit form for the universal $\mathcal{R}$ (see, e.g., Ref. 8), one finds

$$[\mathcal{L}_j^{-i}] = \begin{bmatrix} q^{H/2}, & 0, & 0 \\ -(1-q^{-1})\sqrt{[2]_q}E^-, & 1, & 0 \\ q^{-1/2}(1-q^{-1})^2 q^{-H/2}(E^-)^2, & -(1-q^{-1})\sqrt{[2]_q} q^{-H/2} E^-, & q^{-H/2} \end{bmatrix} \tag{6.6}$$

and

$$[\mathcal{L}_j^{+i}]=\begin{bmatrix} q^{-H/2}, & (q-1)\sqrt{[2]_q}q^{-H/2}E^+, & (q-1)^2q^{-H/2}(E^+)^2, \\ 0, & 1, & q^{-1/2}(q-1)\sqrt{[2]_q}E^+ \\ 0, & 0, & q^{H/2} \end{bmatrix}. \tag{6.7}$$

The unbraiding procedure then works as in Theorem 2. To be specific, assume that the braided tensor product algebra is as in (5.3). Then we set

$$y_{1,i}:=x_{1,i}\,, \tag{6.8}$$

$$y_{\alpha,i}:=\hat{\chi}(x_{\alpha,i})=x_{\alpha,j}\hat{\varphi}_1(\mathcal{L}_i^{+j}), \quad \alpha>1, \tag{6.9}$$

without spelling out these expressions further. According to Theorem 2, they satisfy

Corollary 3:

$$\varepsilon_k^{ij}y_{\alpha,i}y_{\alpha,j}=\Lambda_N y_{\alpha,k}\,,$$

$$g^{ij}y_{\alpha,i}y_{\alpha,j}=R^2$$

for all $\alpha=1,\ldots,M$, *together with*

$$[y_{1,i}\,,y_{\alpha,j}]=0, \tag{6.10}$$

$$y_{\alpha,i}y_{\beta,j}=\hat{R}_{ij}^{hk}y_{\beta,h}y_{\alpha,k} \tag{6.11}$$

when $1<\alpha$ *and* $\alpha\beta$.

Iterating this procedure as before, we find the following.

Proposition 5: Let $\mathcal{A}_1,\mathcal{A}_2,\ldots,\mathcal{A}_M$ *be M copies of the* $U_q\mathrm{so}(3)$*-covariant fuzzy quantum sphere. Then* $\mathcal{A}_1\underline{\otimes}^{\pm}\mathcal{A}_2\underline{\otimes}^{\pm}\cdots\ \underline{\otimes}^{\pm}\mathcal{A}_M=\mathcal{A}_1\tilde{\mathcal{A}}_2^{\pm}\cdots\ \tilde{\mathcal{A}}_M^{\pm}$, *where* $\tilde{\mathcal{A}}_2^{\pm},\ldots,\tilde{\mathcal{A}}_M^{\pm}$ *are subalgebras of the lhs isomorphic to* $\mathcal{A}_1$ *and commuting with each other.*

APPENDIX

1. The universal *R*-matrix

In this appendix we recall the basics about the universal R-matrix[10] of the quantum groups $U_q\mathbf{g}$, while fixing our conventions. Recall that the universal R-matrix $\mathcal{R}$ is a special element

$$\mathcal{R}\equiv\mathcal{R}^{(1)}\otimes\mathcal{R}^{(2)}\in U_q\mathbf{g}\otimes U_q\mathbf{g} \tag{A1}$$

intertwining between Δ and opposite coproduct Δ^{op}, and so does also $\mathcal{R}_{21}^{-1}$:

$$\begin{aligned}\mathcal{R}(g_{(1)}\otimes g_{(2)})&=(g_{(2)}\otimes g_{(1)})\mathcal{R},\\ \mathcal{R}_{21}^{-1}(g_{(1)}\otimes g_{(2)})&=(g_{(2)}\otimes g_{(1)})\mathcal{R}_{21}^{-1}\,.\end{aligned} \tag{A2}$$

In (A1) we have used a Sweedler notation with upper indices: the right-hand side is a short-hand notation for a sum $\Sigma_I\mathcal{R}_I^{(1)}\otimes\mathcal{R}_I^{(2)}$ of infinitely many terms. We recall some useful formulas

$$(\Delta\otimes\mathrm{id})\mathcal{R}=\mathcal{R}_{13}\mathcal{R}_{23}\,, \tag{A3}$$

$$(\mathrm{id}\otimes\Delta)\mathcal{R}=\mathcal{R}_{13}\mathcal{R}_{12}\,, \tag{A4}$$

$$(S\otimes\mathrm{id})\mathcal{R}=\mathcal{R}^{-1}=(\mathrm{id}\otimes S^{-1})\mathcal{R}, \tag{A5}$$

$$S^{-1}(g)=u^{-1}S(g)u. \tag{A6}$$

Here u is any of the elements $u_1,u_2,\ldots,u_8$ defined below

$$\begin{aligned} u_1&:=(S\mathcal{R}^{(2)})\mathcal{R}^{(1)}, \quad u_2:=(S\mathcal{R}^{-1(1)})\mathcal{R}^{-1(2)},\\ u_3&:=\mathcal{R}^{(2)}S^{-1}\mathcal{R}^{(1)}, \quad u_4:=\mathcal{R}^{-1(1)}S^{-1}\mathcal{R}^{-1(2)},\\ (u_5)^{-1}&:=\mathcal{R}^{(1)}S\mathcal{R}^{(2)}, \quad (u_6)^{-1}:=(S^{-1}\mathcal{R}^{(1)})\mathcal{R}^{(2)},\\ (u_7)^{-1}&:=\mathcal{R}^{-1(2)}S\mathcal{R}^{-1(1)}, \quad (u_8)^{-1}:=(S^{-1}\mathcal{R}^{-1(2)})\mathcal{R}^{-1(1)}. \end{aligned} \tag{A7}$$

In fact, using the results of Drinfel'd[10,11] one can show that

$$u_1=u_3=u_7=u_8=vu_2=vu_4=vu_5=vu_6, \tag{A8}$$

where v is a suitable element belonging to the center of $U_q\,\mathrm{so}(N)$.

From (A2) and (A3), (A4) it follows the universal Yang–Baxter relation

$$\mathcal{R}_{12}\mathcal{R}_{13}\mathcal{R}_{23}=\mathcal{R}_{23}\mathcal{R}_{13}\mathcal{R}_{12}, \tag{A9}$$

whence the other two relations follow

$$\mathcal{R}^{-1}{}_{12}\mathcal{R}^{-1}{}_{13}\mathcal{R}^{-1}{}_{23}=\mathcal{R}^{-1}{}_{23}\mathcal{R}^{-1}{}_{13}\mathcal{R}^{-1}{}_{12}, \tag{A10}$$

$$\mathcal{R}_{13}\mathcal{R}_{23}\mathcal{R}^{-1}{}_{12}=\mathcal{R}^{-1}{}_{12}\mathcal{R}_{23}\mathcal{R}_{13}. \tag{A11}$$

As before, let ρ be the fundamental N-dimensional representation of $\mathbf{g}=\mathrm{sl}(N),\mathrm{so}(N),\mathrm{sp}(N)$. By applying $\mathrm{id}\otimes\rho^a_c\otimes\rho^b_d$ to (A9), $\rho^a_c\otimes\rho^b_d\otimes\mathrm{id}$ to (A10) and $\rho^a_c\otimes\mathrm{id}\otimes\rho^b_d$ to (A11) we, respectively, find the commutation relations

$$\hat{R}^{ab}_{cd}\mathcal{L}^{+d}_f\mathcal{L}^{+c}_e=\mathcal{L}^{+b}_c\mathcal{L}^{+a}_d\hat{R}^{dc}_{ef}, \tag{A12}$$

$$\hat{R}^{ab}_{cd}\mathcal{L}^{-d}_f\mathcal{L}^{-c}_e=\mathcal{L}^{-b}_c\mathcal{L}^{-a}_d\hat{R}^{dc}_{ef}, \tag{A13}$$

$$\hat{R}^{ab}_{cd}\mathcal{L}^{+d}_f\mathcal{L}^{-c}_e=\mathcal{L}^{-b}_c\mathcal{L}^{+a}_d\hat{R}^{dc}_{ef}, \tag{A14}$$

where $\mathcal{L}^{\pm a}_l$ are the Faddeev–Reshetikin–Takhtadjan generators[13] of $U_q\mathbf{g}$, defined by

$$\mathcal{L}^{+a}_l:=\mathcal{R}^{(1)}\rho^a_l(\mathcal{R}^{(2)}), \quad \mathcal{L}^{-a}_l:=\rho^a_l(\mathcal{R}^{-1(1)})\mathcal{R}^{-1(2)}. \tag{A15}$$

It is known[13] that $\{\mathcal{L}^{+i}_j,\mathcal{L}^{-i}_j\}$ and the square roots of the elements $\mathcal{L}^{\pm i}_i$ provide a (overcomplete) set of generators of $U_q\mathbf{g}$. Since in our conventions

$$\mathcal{R}\in H^+\otimes H^-, \tag{A16}$$

then $\mathcal{L}^{+a}_l\in H^+$ and $\mathcal{L}^{-a}_l\in H^-$. Beside (A12)–(A14) these generators fulfill

$$\mathcal{L}^{+i}_j=0, \quad \text{if } i>j, \tag{A17}$$

$$\mathcal{L}^{-i}_j=0, \quad \text{if } i<j, \tag{A18}$$

$$\mathcal{L}^{-i}_i\mathcal{L}^{+i}_i=\mathcal{L}^{+i}_i\mathcal{L}^{-i}_i=1, \quad \forall i \tag{A19}$$

$$\mathcal{L}^{\pm-n}_{-n}\cdots\ \mathcal{L}^{\pm n}_n=1, \tag{A20}$$

and, when $\mathbf{g}=\mathrm{so}(N),\mathrm{sp}(N)$, some additional relations. When $\mathbf{g}=\mathrm{so}(N)$ the latter read

$$\mathcal{L}_j^{\pm i}\mathcal{L}_k^{\pm h}g^{kj}=g^{hi},\quad \mathcal{L}_i^{\pm j}\mathcal{L}_h^{\pm k}g_{kj}=g_{hi}, \tag{A21}$$

where g_{ij} has been defined in (3.5). The braid matrix $\hat{R}$ is related to $\mathcal{R}$ by $\hat{R}^{ij}_{hk}\equiv R^{ji}_{hk}:=(\rho^j_h\otimes\rho^i_k)\mathcal{R}$. With the indices' convention described in Secs. III and IV $\hat{R}$ is given by

$$\hat{R}=q^{-1/N}\left[q\sum_i e^i_i\otimes e^i_i+\sum_{i\neq j}e^j_i\otimes e^i_j+k\sum_{i<j}e^i_i\otimes e^j_j\right] \tag{A22}$$

when $\mathbf{g}=\mathrm{sl}(N)$, and by

$$\hat{R}=q\sum_{i\neq 0}e^i_i\otimes e^i_i+\sum_{\substack{i\neq j,-j\\ \text{or } i=j=0}}e^j_i\otimes e^i_j+q^{-1}\sum_{i\neq 0}e^{-i}_i\otimes e^i_{-i}+k\left(\sum_{i<j}e^i_i\otimes e^j_j-\sum_{i<j}q^{-\rho_i+\rho_j}e^{-j}_i\otimes e^j_{-i}\right) \tag{A23}$$

when $\mathbf{g}=\mathrm{so}(N)$. Here e^i_j is the $N\times N$ matrix with all elements equal to zero except for a 1 in the ith column and jth row. The braid matrix of $\mathrm{sl}(N)$ admits the orthogonal projector decomposition

$$\hat{R}=q\mathcal{P}_S-q^{-1}\mathcal{P}_a,\quad \mathbf{g}=\mathrm{sl}(N); \tag{A24}$$

$\mathcal{P}_a$, $\mathcal{P}_S$ are the $U_q\,\mathrm{sl}(N)$-covariant deformed antisymmetric and symmetric projectors. The braid matrix of $\mathrm{so}(N)$ admits the orthogonal projector decomposition

$$\hat{R}=q\mathcal{P}_s-q^{-1}\mathcal{P}_a+q^{1-N}\mathcal{P}_t,\quad \mathbf{g}=\mathrm{so}(N); \tag{A25}$$

$\mathcal{P}_a$, $\mathcal{P}_t$, $\mathcal{P}_s$ are the q-deformed antisymmetric, trace, trace-free symmetric projectors.

The compact section of $U_q\mathbf{g}$ requires $q\in\mathbb{R}^+$ if $\mathbf{g}=\mathrm{so}(N)$, $q\in\mathbb{R}$ if $\mathbf{g}=\mathrm{sl}(N)$ and is characterized by the $*$-structure,

$$(\mathcal{L}_j^{\pm i})^*=S\mathcal{L}_i^{\mp j}. \tag{A26}$$

For $\mathbf{g}=\mathrm{so}(N)$ this amounts to

$$(\mathcal{L}_j^{\pm i})^*=g_{ih}\mathcal{L}_k^{\mp h}g^{kj}. \tag{A27}$$

The noncompact sections of $U_q\mathbf{g}$ require $|q|=1$ and are characterized by the $*$-structure,

$$(\mathcal{L}_j^{\pm i})^*=U_r^{-1i}\mathcal{L}_s^{\pm r}U_j^s=u\mathcal{L}_j^{\pm i}u^{-1}. \tag{A28}$$

This can be checked using the property $(\hat{R}^{ij}_{hk})^*=\hat{R}^{-1ji}_{kh}$. Here we have defined

$$U^i_j=\rho^i_j(u) \tag{A29}$$

with u any of the elements defined in (A7). For $\mathbf{g}=\mathrm{so}(N)$ one can take

$$U^i_j:=g^{ih}g_{jh}. \tag{A30}$$

From formulas (A3) and (A4) in the Appendix one finds that the coproducts are given by

$$\Delta(\mathcal{L}_j^{+i})=\mathcal{L}_h^{+i}\otimes\mathcal{L}_j^{+h},\quad \Delta(\mathcal{L}_j^{-i})=\mathcal{L}_h^{-i}\otimes\mathcal{L}_j^{-h}. \tag{A31}$$

2. Proof of proposition 1

We make use of the identity

$$\varphi^{\pm}(g^{\pm})\triangleleft h^{\pm}=\varphi^{\pm}(g^{\pm}\triangleleft h^{\pm}), \tag{A32}$$

for any $g^{\pm}$, $h^{\pm}\in H^{\pm}$, which we prove in Ref. 17. The right action appearing at the rhs is the (right) adjoint action on itself

$$h\triangleleft g=Sg_{(1)}hg_{(2)}, \quad g,h\in H; \tag{A33}$$

where S denotes the antipode of the Hopf algebra H. We shall also need the inverse of (1.9),

$$a_1a_2=(a_2\triangleleft\mathcal{R}^{-1(2)})(a_1\triangleleft\mathcal{R}^{-1(1)}). \tag{A34}$$

Now,

$$\begin{aligned}
\chi^{+}(a_2) &\overset{(1.13)}{=} \varphi_1^{+}(\mathcal{R}^{(1)})(a_2\triangleleft\mathcal{R}^{(2)})\\
&\overset{(A34)}{=} (a_2\triangleleft\mathcal{R}^{(2)}\mathcal{R}^{-1(2')})[\varphi_1^{+}(\mathcal{R}^{(1)})\triangleleft\mathcal{R}^{-1(1')}]\\
&\overset{(A32)}{=} (a_2\triangleleft\mathcal{R}^{(2)}\mathcal{R}^{-1(2')})\varphi_1^{+}(\mathcal{R}^{(1)}\triangleleft\mathcal{R}^{-1(1')})\\
&\overset{(A33)}{=} (a_2\triangleleft\mathcal{R}^{(2)}\mathcal{R}^{-1(2')})\varphi_1^{+}(S\mathcal{R}_{(1)}^{-1(1')}\mathcal{R}^{(1)}\mathcal{R}_{(2)}^{-1(1')})\\
&\overset{(A3)}{=} (a_2\triangleleft\mathcal{R}^{(2)}\mathcal{R}^{-1(2')}\mathcal{R}^{-1(2'')})\varphi_1^{+}(S\mathcal{R}^{-1(1'')}\mathcal{R}^{(1)}\mathcal{R}^{-1(1')})\\
&=(a_2\triangleleft\mathcal{R}^{-1(2'')})\varphi_1^{+}(S\mathcal{R}^{-1(1'')}),
\end{aligned}$$

which proves (1.21). Similarly one proves (1.22).

3. The maps $\varphi^{\pm}$ for the quantum Euclidean spaces or spheres

We introduce the short-hand notation

$$[A,B]_x=AB-xBA. \tag{A35}$$

In Ref. 5 we have found algebra homomorphisms $\varphi^{\pm}:\mathbb{R}_q^N\rtimes U_q^{\pm}\,\mathrm{so}(N)\to\mathbb{R}_q^N$. The images of φ^{-} on the negative FRT generators read

$$\varphi^{-}(\mathcal{L}_j^{-i})=g^{ih}[\mu_h,x^k]_q g_{kj}, \tag{A36}$$

where

$$\begin{aligned}
\mu_0&=\gamma_0(x^0)^{-1} \quad \text{for } N \text{ odd},\\
\mu_{\pm1}&=\gamma_{\pm1}(x^{\pm1})^{-1}\mathcal{L}_1^{\pm1} \quad \text{for } N \text{ even},\\
\mu_a&=\gamma_a r_{|a|}^{-1}r_{|a|-1}^{-1}x^{-a} \quad \text{otherwise},
\end{aligned} \tag{A37}$$

and $\gamma_a\in\mathbb{C}$ are normalization constants fulfilling the conditions

$$\gamma_0=-q^{-1/2}h^{-1} \quad \text{for } N \text{ odd},$$
$$\gamma_1\gamma_{-1}=\begin{cases}-q^{-1}h^{-2} & \text{for } N \text{ odd},\\ k^{-2} & \text{for } N \text{ even},\end{cases} \tag{A38}$$
$$\gamma_a\gamma_{-a}=-q^{-1}k^{-2}\omega_a\omega_{a-1} \quad \text{for } a>1.$$

h, k, ω_a are defined as in Secs. III and IV. On the other hand, the images of φ^+ on the positive FRT generators read

$$\varphi^+(\mathcal{L}_j^{+i})=g^{ih}[\overline{\mu}_h,x^k]_{q^{-1}}g_{kj}, \tag{A39}$$

where

$$\overline{\mu}_0=\overline{\gamma}_0(x^0)^{-1} \quad \text{for } N \text{ odd},$$
$$\overline{\mu}_{\pm1}=\overline{\gamma}_{\pm1}(x^{\pm1})^{-1}\mathcal{L}_1^{\pm1} \quad \text{for } N \text{ even}, \tag{A40}$$
$$\overline{\mu}_a=\overline{\gamma}_a r_{|a|}^{-1}r_{|a|-1}^{-1}x^{-a} \quad \text{otherwise},$$

and $\overline{\gamma}_a\in\mathbb{C}$ normalization constants fulfilling the conditions

$$\overline{\gamma}_0=q^{1/2}h^{-1} \quad \text{for } N \text{ odd},$$
$$\overline{\gamma}_1\overline{\gamma}_{-1}=\begin{cases}-qh^{-2} & \text{for } N \text{ odd},\\ k^{-2} & \text{for } N \text{ even},\end{cases} \tag{A41}$$
$$\overline{\gamma}_a\overline{\gamma}_{-a}=-qk^{-2}\omega_a\omega_{a-1} \quad \text{for } a>1.$$

If we require $\varphi^+=\varphi^-$ on the Cartan subalgebra $H_c=H^+\cap H^+$ then it must be

$$\overline{\gamma}_i=-\gamma_{-i}\begin{cases}1 & \text{if } i>1, \text{ or } i=1 \text{ and } N \text{ odd}\\ q^2 & \text{if } i<-1, \text{ or } i=-1 \text{ and } N \text{ odd}.\end{cases}$$

Incidentally, for odd N one can choose the free parameters $\gamma_a,\overline{\gamma}_a$ in such a way that in addition φ^+,φ^- can be glued into an algebra homomorphism $\varphi:\mathbb{R}_q^N\rtimes U_q\,\mathrm{so}(N)\to\mathbb{R}_q^N$:[5] It must be $\gamma_1{}^2=-q^{-2}h^{-2}$, $\gamma_{-1}{}^2=-h^{-2}$, $\gamma_a{}^2=-q^{-2}k^{-2}\omega_a\omega_{a-1}$, $\gamma_{-a}{}^2=-k^{-2}\omega_a\omega_{a-1}$ $(a>1)$, and $\overline{\gamma_i}=-q\gamma_i$, $i=-n,1-n,\ldots,n$.

We give the following explicit expression for $\varphi^{\pm}(\mathcal{L}_j^{\pm i})$ in the case $N=3$:

$$[\varphi^-(\mathcal{L}_j^{-i})]=\begin{bmatrix}-qh\gamma_1(x^0)^{-1}r & & \\ q^{1/2}(q+1)(x^0)^{-1}x^+ & 1 & \\ q^{1/2}(q+1)(h\gamma_1 rx^0)^{-1}(x^+)^2 & (1+q^{-1})(h\gamma_1 r)^{-1} & -(qh\gamma_1 r)^{-1}x^0\end{bmatrix} \tag{A42}$$

and

$$[\varphi^+(\mathcal{L}_j^{+i})]=\begin{bmatrix}-h\overline{\gamma}_1 r^{-1}x^0 & q^{-1/2}\overline{\gamma}_1 kr^{-1}x^- & q^{-2}k\overline{\gamma}_1(rx^0)^{-1}(x^-)^2\\ & 1 & q^{-1/2}(q^{-1}+1)(x^0)^{-1}x^-\\ & & -(h\overline{\gamma}_1x^0)^{-1}r\end{bmatrix}. \tag{A43}$$

When $q\in\mathbb{R}^+$ the real structure of $\mathbb{R}_q^N$ is given by

$$(x^i)^*=x^jg_{ji}. \tag{A44}$$

Note that when N is odd $\mu_0,\overline{\mu}_0$, which are completely determined by their definitions, are such that $\mu_0^*=-q^{-1}\overline{\mu}_0$. We fix the other $\gamma_a,\overline{\gamma}_a$ so that for any a

$$\mu_a^*=-q^{-1}g_{ab}\overline{\mu}_b. \tag{A45}$$

This was already considered in Ref. 5 and requires

$$\gamma_{\pm 1}^* = -\overline{\gamma}_{\mp 1} \quad \text{if } N \text{ even},$$

$$\gamma_a^* = -\overline{\gamma}_{-a} \begin{cases} 1 & \text{if } a<0, \\ q^{-2} & \text{if } a>0, \end{cases} \quad \text{otherwise.} \tag{A46}$$

As a consequence,

$$[\varphi^-(\mathcal{L}_j^{-i})]^* \overset{(A36)}{=} (g^{ih}[\mu_h, x^k]_q g_{kj})^*$$

$$\overset{(A44)}{=} g^{ih}[x^j, \mu_h^*]_q$$

$$\overset{(A45)}{=} [\overline{\mu}_i, x^j]_{q^{-1}}$$

$$\overset{(A39)}{=} g_{ih}\varphi^+(\mathcal{L}_k^{+h})g^{kj}$$

$$\overset{(A27)}{=} \varphi^+[(\mathcal{L}_j^i)^*].$$

In other words

$$[\varphi^{\pm}(g)]^* = \varphi^{\mp}(g^*). \tag{A47}$$

When $|q|=1$

$$(x^i)^* = x^i. \tag{A48}$$

Note that when N is odd $\mu_0, \overline{\mu}_0$, which are completely determined by their definitions, are such that $\mu_0^* = -q\mu_0 = \overline{\mu}_0$. We fix the other $\gamma_a, \overline{\gamma}_a$ so that for any a

$$\mu_a^* = -q\mu_a, \quad \overline{\mu}_a^* = -q^{-1}\overline{\mu}_a. \tag{A49}$$

This requires

$$\gamma_{\pm 1}^* = -\gamma_{\pm 1} \quad \text{if } N \text{ even},$$

$$\gamma_a^* = -\gamma_a \begin{cases} 1 & \text{if } a<0 \\ q^{+2} & \text{if } a>0 \quad \text{otherwise.} \end{cases} \tag{A50}$$

As a consequence,

$$[\varphi^-(\mathcal{L}_j^{-i})]^* \overset{(A36)}{=} (g^{ih}[\mu_h, x^k]_q g_{kj})^*$$

$$\overset{(A48)}{=} -q^{-1}g^{hi}[\mu_h^*, x^k]_q g_{jk}$$

$$\overset{(A49)}{=} g^{hi}[\mu_h, x^k]_q g_{jk}$$

$$\overset{(A30),(A36)}{=} U_r^{-1i}\varphi^-(\mathcal{L}_s^{-r})U_r^i$$

$$\overset{(A28)}{=} \varphi^-[(\mathcal{L}_j^{-i})^*].$$

Similarly one proves that $[\varphi^-(\mathcal{L}_j^{-i})]^*=\varphi^-[(\mathcal{L}_j^{-i})^*]$. In other words, $\varphi^\pm$ are $*$-homomorphisms.

4. The maps φ for the deformed Heisenberg algebras

In Ref. 14 we constructed an algebra homomorphism $\varphi: U_q\,\mathrm{so}(N)\ltimes\mathcal{A}_1\to\mathcal{A}_1$, where $\mathcal{A}_1$ denotes the $U_q\,\mathrm{so}(N)$-covariant (deformed) Heisenberg algebra, such that φ is a $*$-homomorphism

$$\varphi(g^*)=\varphi(g)^* \tag{A51}$$

on the compact section of $U_q\,\mathrm{so}(N)$ (what requires $q\in\mathbb{R}^+$). One can easily prove the same result also for the noncompact section (A28) of $\mathbf{g}=\mathrm{so}(N)$ as well as the compact and noncompact sections of $\mathbf{g}=\mathrm{sl}(N)$. This can be done maybe most rapidly using as a set of generators the so-called vector fields Z_j^i,[30] which are related to the FRT generators by

$$Z_j^i=\mathcal{L}_h^{+i}S\mathcal{L}_j^{-h}. \tag{A52}$$

From (A26) and (A28) one immediately finds

$$(Z_j^i)^*=Z_i^j \quad \text{if } q\in\mathbb{R}^+, \tag{A53}$$

$$(Z_j^i)^*=U_a^{-1i}(S^{-1}\mathcal{L}_b^{-h})\mathcal{L}_h^{+a}U_j^b \quad \text{if } |q|=1; \tag{A54}$$

if $\mathbf{g}=\mathrm{so}(N)$ the second relation reduces to

$$(Z_j^i)^*=U_b^{-1a}Z_c^b\hat{R}_{aj}^{-1ci}. \tag{A55}$$

In Ref. 9 the explicit expression of $\varphi(Z_j^i)$ in terms of the x's and ∂'s is given both for $g=\mathrm{sl}(N)$ and $\mathbf{g}=\mathrm{so}(N)$, and it is not difficult to show that on these generators (and therefore on all of $U_q\mathbf{g}$) (A51) is satisfied. In performing the calculations one has to keep in mind that the authors of Ref. 9 work with the left action, rather than with the right, so one has to switch to the conventions described in Sec. V, but, as explained there, this wil not modify the result (A51). As an intermediate step, we give the action of the $*$-structure on the coordinates and derivatives for the case $\mathbf{g}=\mathrm{so}(N)$, in the notation used there:

$$(x_h)^*=g^{hk}x_k, \quad (\partial^i)^*=-q^{-N}\hat{\partial}_i \quad \text{if } q\in\mathbb{R}^+, \tag{A56}$$

$$(x_h)^*=x_h, \quad (\partial^i)^*=-q^N U_j^{-1i}\partial^j, \quad (\hat{\partial}_i)^*=-q^{-N}\partial_i \quad \text{if } |q|=1. \tag{A57}$$

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Spin networks for noncompact groups

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(Received 25 June 2002; accepted 12 September 2002)

Spin networks are a natural generalization of Wilson loop functionals. They have been extensively studied in the case where the gauge group is compact and it has been shown that they naturally form a basis of gauge invariant observables. Physically the restriction to compact gauge groups is enough for the study of Yang–Mills theories, however it is well known that noncompact groups naturally arise as internal gauge groups for Lorentzian gravity models. In this context, a proper construction of gauge invariant observables is needed. The purpose of the present work is to define the notion of spin network states for noncompact groups. We first build, by a careful gauge fixing procedure, a natural measure and a Hilbert space structure on the space of gauge invariant graph connections. Spin networks are then defined as generalized eigenvectors of a complete set of hermitic commuting operators. We show how the delicate issue of taking the quotient of a space by noncompact groups can be address in term of algebraic geometry. We finally construct the full Hilbert space containing all spin network states. Having in mind applications to gravity, we illustrate our results for the groups SL(2,**R**) and SL(2,**C**). © *2003 American Institute of Physics.* [DOI: 10.1063/1.1521522]

I. INTRODUCTION

The purpose of this paper is to generalize the construction of an Hilbert space of spin network states to the case in which the gauge group is noncompact. Spin network states arise naturally in many fields of physics since they form a basis of gauge invariant functionals in Yang–Mills-type theories.[1] In the context of gravity they were introduced by Rovelli and Smolin[2,3] and they were promoted as a basis of an Hilbert space of gauge and diffeomorphism invariant functionals in works by Ashtekar and Lewandowski[4–6] and by Baez.[7] This series of works have been focused on the case where the gauge group is compact. Compact gauge groups are natural as symmetry groups of gauge theory and Euclidean gravity, however noncompact gauge groups arise as symmetry groups of Lorentzian gravity.

For instance, SL(2,**C**) arises in the original Ashtekar formulation of $3+1$ gravity in terms of self-dual variables. However, in this context, the lack of properly well-defined spin network states has forced the community to work with the real SU(2) Barbero[8] connection at the price of introducing a new constant (Immirzi parameter), a more complicated dynamics[9] and the loss of a natural four-dimensional geometrical interpretation of the phase space variables.[10] In the case of $2+1$ Lorentzian gravity, the partition function and the transition amplitudes have been computed in terms of spin networks (recoupling coefficients) of SL(2,**R**).[11] In this context, geometrical

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interpretation of the representation labels has led to the conclusion that space is continuous whereas time is discrete,[11,12] in agreement with former results from 't Hooft.[13]

In order to put these results on a firmer basis and construct geometrical operators in the Lorentzian context, one needs to understand better the nature of noncompact spin networks and how they form a natural Hilbert space related to the Hilbert space of gauge and diffeomorphism invariant connections. This is the purpose of this work.

Several issues concerning noncompact spin network have already been raised in the literature. First, Ashtekar and Lewandowski have already addressed the issue of completeness of the spin network functionals[14] versus the separability of the space of gauge invariant connections. We shall come back to these issues in Sec. III B. There also has been some attempts to define noncompact spin networks. Marolf[15] was the first one to show, in the context of $2+1$ gravity on the torus, that the loop transform using finite dimensional representation is ill defined when the group is noncompact. He and, Ashtekar and Loll,[16] have studied the possibility to overcome this difficulty at the price of introducing additional and non-natural structures.

Our approach shed new lights on this problem, it leads to a different point of view since we do not insist on having spin networks labeled by finite dimensional representations. We show that one should work instead with the infinite dimensional unitary representations of the group. The emergence of spin networks labeled by infinite dimensional representation is not new. They already appeared in the context of spin foams models for Lorentzian 3D gravity[11,17] and 4D gravity.[18,19]

Moreover our formalism is more general since it sets a framework for all noncompact groups. Indeed, our purpose is to give a general account of the construction of noncompact spin networks and the structure of the stratified space of gauge invariant connections. Our presentation is valid for any semisimple reductive group. The general exposition is therefore quite mathematical. Having in mind further application to gravity we will illustrate the main problems and results in the context of SL(2,**C**) and SL(2,**R**).

Connection space and cylindrical functions: We choose once for all a manifold Σ and P a locally trivial smooth principal G-bundle over Σ, with G a semisimple reductive group. We denote by $\mathcal{A}$ the space of gauge G-connections and by $\mathcal{G}$ the gauge group acting on connection by $A^k = k^{-1}Ak + k^{-1}\,dk$. The theories we are interested in are Yang–Mills type in the sense that the phase space conjugate variables are given by a G-connection A (a magnetic potential) and a $a\,dP$ valued densitized vector field E, both are anti-Hermitian. This phase space is the cotangent bundle to the space of connection $T^*(\mathcal{A})$. On such a phase space we want to impose the Gauss laws (gauge invariance) and eventually the diffeomorphism constraint. The representation of the operator algebra is done in the polarization where the wave functionals depend on the connection and therefore the Hilbert space structure is formally $L^2(\mathcal{A}/\mathcal{G}, d\mu)$. The purpose of this work is to study the structure of this space. In fact we will first restrict our intention to special gauge invariant functionals of the connections called cylindrical functionals and we will study the possibility to give the space of cylindrical functions an Hilbert space structure. In the gauge invariant context, cylindrical functions are associated with graphs. Given a smooth *oriented* graph Γ composed of E oriented edges and V vertices we have the holonomy map:

$$\Gamma:\ \mathcal{A} \to G^{\otimes E}$$

$$A \to (g_{e_1}, \ldots, g_{e_E}), \tag{1.1}$$

where $g_e(A) \in G$ denotes the holonomy of the connection along the edge e of the graph Γ, which associates to any connection the holonomy of this connection along the E edges of the graph Γ. The space of cylindrical functionals associated with Γ is the pullback by Γ of $C^\infty(G^{\otimes E})$ defined by

$$\Gamma^* \phi(A) = \phi(g_e(A)). \tag{1.2}$$

The action of the gauge group on $\mathcal{A}$ translates into an action at the vertices of the graph Γ, if we denote by $s(e)$ and $t(e)$ the source and target of the edge e the gauge group action is given by

$$g_e(A^k)=k_{s(e)}^{-1}g_e(A)k_{t(e)} \tag{1.3}$$

The space of gauge invariant graph connection is denoted $A_\Gamma=G^{\otimes E}/G^{\otimes V}$ and cylindrical gauge invariant functionals are functionals on A_Γ. We want to construct a measure $d\mu_\Gamma$ on A_Γ which provides an Hilbert space structure to the space of gauge invariant cylindrical functional $\mathcal{H}_\Gamma=L^2(\Gamma,d\mu_\Gamma)$. This Hilbert space structure should give a representation of the Yang–Mills operator algebra restricted to Γ. This operator algebra denoted O_Γ is the quantization of the cotangent structure $T^*(G^{\otimes E}/G^{\otimes V})$ generated by the multiplication by gauge invariant function on $G^{\otimes E}$ and by the gauge invariant derivation operators. We will see that this algebra is the operator algebra of a system of gauged particles (see Sec. VIII D). The main constraint which determines (almost but not totally) the measure $d\mu_\Gamma$ is the fact that real classical quantities should be quantized as Hermitian operators. In the case of a compact group, there is a unique solution up to an overall factor: the product of normalized Haar measures over each edge group element.

$$d\mu_\Gamma=\prod_{e\in E_\Gamma} dg_e. \tag{1.4}$$

This measure is then consistently extended to the space of all cylindrical functions and defines a measure on the space of generalized connection modulo gauge invariance.[4,20] In the noncompact case, it is no longer possible to integrate gauge invariant functional with (1.4) since the volume of the group is infinite. In order to construct the correct measure, we need to divide by the infinite volume of the gauge group, hence to gauge fix the gauge group action. We will do so in the following by showing that A_Γ is isomorphic to $G^{h_\Gamma-1}$ where h_Γ is the genus-handle number of the surface obtained by blowing up the graph Γ. To be precise the isomorphism is only between dense subspaces. The measure we are looking for is obtained as the pushforward of the Haar measure on $G^{h_\Gamma-1}$.

The isomorphism is constructed by a gauge fixing procedure. This gauge fixing procedure is done in two steps. First in Sec. II. we choose a maximal tree in Γ and we show that $A_\Gamma\sim G^{h_\Gamma}/\mathrm{Ad}(G)$ where $\mathrm{Ad}(G)$ denotes the adjoint diagonal action. In Sec. III. we introduce general useful facts about noncompact groups and present some important results of algebraic geometry allowing us to understand the geometry of noncompact quotient spaces. Then in Sec. IV, we continue the gauge fixing by showing that there exists an isomorphism between (dense subsets of) $G^{h_\Gamma}/\mathrm{Ad}(G)$ and $G^{h_\Gamma-1}$. The isomorphism constructed being far from obvious. We finally show that the pull back measure is independent from all gauge choices leading to a well-defined canonical measure $d\mu_\Gamma$ on A_Γ. In Sec. V. we show that $\mathrm{Ad}\,G$-invariant and naively hermitic differential operators are indeed hermitic operator for the measure $d\mu_\Gamma$, we can define spin networks states as eigenvectors of a complete basis of such operators. In Sec. VI and VII, we present explicit results for the rank one groups SU(2),SL(2,**C**),SL(2,**R**). Section VI is devoted to the case where h_Γ, the genus of the graph, is one. This case is very different from the generic case treated in Sec. VII. Finally in Sec. VIII we discuss the construction of the full Hilbert space of all spin networks and show that it exhibits some interesting Fock substructure.

II. GAUGE FIXING CYLINDRICAL FUNCTIONS

A. Constructing flowers

$A_\Gamma=G^{\otimes E}/G^{\otimes V}$ is the space of graph invariant gauge connections. If $\Gamma=\cup_i\Gamma_i$ is a non connected graph then A_Γ decomposes as the cross product $\otimes_i A_{\Gamma_i}$. It is therefore enough to understand the construction for the case of connected graphs and we will restrict in the following, unless specified otherwise, to connected graphs only.

Γ is composed of E oriented edges and V vertices. Each oriented edge e starts at the source vertex $s(e)$ and ends at the target vertex $t(e)$. A function on A_Γ is a function on $G^{\otimes E}$ which satisfies gauge invariance at each vertex. More precisely, given group elements k_v at each vertex v, ϕ satisfies:

$$\phi(g_{e_i}) = \phi(k_{s(e_i)}^{-1} g_{e_i} k_{t(e_i)}), \quad i = 1, \ldots, E. \tag{2.1}$$

Our first goal is to define a measure to integrate such a function. For this purpose, we would like to identify the ''true'' degrees of freedom of ϕ: we are going to gauge fix the gauge invariance (2.1).

There is a very simple and natural gauge fixing for graph connections which consists in eliminating as many variables g_e as possible by fixing them to, say, the identity 1. More precisely, we choose a maximal tree T on our graph Γ. T is a subset of edges which touches every vertex without ever forming a loop. The characteristic property of a maximal tree is that there exists a unique path along the tree T which connects any two given vertices of Γ. In particular, T is made up of $V-1$ edges. Given two vertices A and B, we can define the oriented product of group elements h_{AB}^T along the path in T connecting A and B. Now, using the gauge invariance (2.1), we can fix all the group elements on the edges of T to 1. To achieve this, we first need to choose a vertex A from which we are going to write our gauge fixing procedure. And we use (2.1) with

$$k_v = h_{vA}^T. \tag{2.2}$$

For an arbitrary edge e, the transformation reads

$$G_e^{(T)} = h_{As(e)}^T g_e h_{t(e)A}^T. \tag{2.3}$$

Let us consider an edge $e \in T$. There exists an unique path in T linking it to A, else there would be a loop in the tree T. There are two situations: either the path connects A to $s(e)$ or it connects A and $t(e)$. Reversing the orientation of e, we can choose, for example, that the path connects A to $t(e)$. Then, $h_{s(e)A}^T = g_e h_{t(e)A}^T$ and $h_{As(e)}^T = (h_{s(e)A}^T)^{-1}$ so that (2.3) reads $G_e^{(T)} = 1$. So (2.2) fixes all the group elements living on the edges of the tree T to 1. This defines a function ϕ_T depending on the $g_\Gamma = E - V + 1$ group elements living on the edges not in T:

$$\phi_T(\{G_e^{(T)}, e \notin T\}) = \phi(g_e = G_e^{(T)} \quad \text{if } e \notin T \text{ or } = 1 \text{ else}). \tag{2.4}$$

This new function has a simple residual gauge invariance

$$\forall k \in G, \phi_T(G_{f_i}^{(T)}) = \phi_T(k^{-1} G_{f_i}^{(T)} k), \quad i = 1, \ldots, g_\Gamma. \tag{2.5}$$

In other word, this gauge fixing procedure is an isomorphism

$$T: \; G^{h_\Gamma}/\mathrm{Ad}(G) \to A_\Gamma \tag{2.6}$$

and ϕ_T is the pull back of ϕ by this isomorphism.

The residual gauge invariance corresponds to a graph with a single vertex which we call a *flower*. What happens is that we have contracted the whole tree T to the single A, which is the remaining vertex. *A priori*, this construction and therefore the function ϕ_T depends on the choice of the point A. In fact, the whole construction is independent of this choice. Shifting from the vertex A to another vertex B, we can define the product of the group elements along the path in T going from A to B; let us note it as $h = h_{AB}^T$. The gauge fixing procedure carried from B will create variables:

$$\tilde{G}_e^{(T)} = h_{Bs(e)}^T g_e h_{t(e)B}^T = h^{-1} h_{As(e)}^T g_e h_{t(e)A}^T h = h^{-1} G_e^{(T)} h. \tag{2.7}$$

We will define a new function $\tilde{\phi}_T$ based on these new variables, but it will be *equal* to ϕ_T due to the gauge invariance (2.5) for $k = h$.

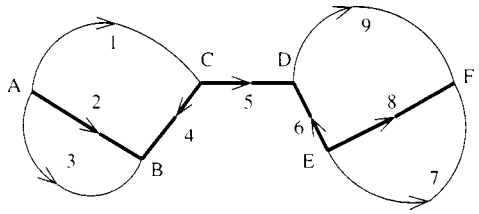
One important issue for later is the way the function ϕ_T changes when we modify the maximal tree T on which it is based. Let us therefore choose another maximal tree U. We can follow the same gauge fixing procedure based on the vertex A to define variables $G_e^{(U)}$ for each

edge e not belonging to U and define a function on the flower ϕ_U. To relate ϕ_T and ϕ_U, we would like to decompose the variables $G_e^{(U)}$ onto the variables $G_e^{(T)}$. Let us more generally consider any oriented loop $\mathcal{L}$ starting at the point A and coming back to the point A and try to express the oriented product of the group elements along it—say H—in terms of the $G_e^{(T)}$. Such a loop must contain at least an edge not belonging to T; else the tree T would contain a loop, which is impossible. Then, it is easy to realize that H is the oriented product—following the orientation of the loop $\mathcal{L}$—of the variables $G_e^{(T)}$ for e on $\mathcal{L}$ and not belonging to T. For an edge $e \notin U$, the group element $G_e^{(U)}$ can be expressed as the holonomy around the loop $\mathcal{L}^{(U)}[e]$ following U from A to $s(e)$ and back from $t(e)$ to A. We can therefore decomposes $G_e^{(U)}$ into an oriented product of $G_f^{(T)}$. Coming back to the function ϕ_T and ϕ_U, this implies that

$$\phi_T(G_e^{(T)}) = \phi_U\left(G_e^{(U)} = \overrightarrow{\prod_{f \in \mathcal{L}[e]\setminus T}} G_f^{(T)} \right). \tag{2.8}$$

B. Examples

In the following we give some illustration of all these procedures for the following simple graph:

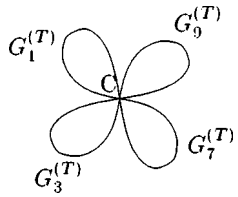


The function ϕ satisfies the following relation for every variables $k \in G$:

$$\begin{aligned}&\phi(g_1,\ldots,g_9)\\ &\quad = \phi(k_A^{-1}g_1k_C, k_A^{-1}g_2k_B, k_A^{-1}g_3k_B, k_C^{-1}g_4k_B, k_C^{-1}g_5k_D, k_E^{-1}g_7k_F, k_E^{-1}g_8k_F, k_D^{-1}g_9k_F).\end{aligned} \tag{2.9}$$

We choose the tree T as indicated on the above graph and we write down the gauge fixed variables $G^{(T)}$ based on the vertex C,

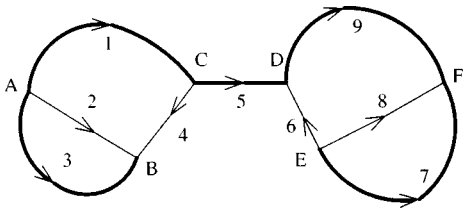
$$\begin{aligned}&G_1^{(T)} = g_4g_2^{-1}g_1, \quad G_3^{(T)} = g_4g_2^{-1}g_3g_4^{-1},\\ &G_7^{(T)} = g_5g_6^{-1}g_7g_8^{-1}g_6g_5^{-1}, \quad G_9^{(T)} = g_5g_9g_8^{-1}g_6g_5^{-1},\end{aligned} \tag{2.10}$$



Then one defines the function on the four petal flower by the following relation:

$$\phi_T(G_1^{(T)}, G_3^{(T)}, G_7^{(T)}, G_9^{(T)}) = \phi(G_1^{(T)}, 1, G_3^{(T)}, 1, 1, 1, G_7^{(T)}, 1, G_9^{(T)}). \tag{2.11}$$

One can do the same for another tree U:



(2.12)

Still based on the vertex C, we define the $G^{(U)}$ variables,

$$G_2^{(U)}=g_1^{-1}g_2g_3^{-1}g_1,\quad G_4^{(U)}=g_4g_3^{-1}g_1,$$
$$G_6^{(U)}=g_5g_9g_7^{-1}g_6g_5^{-1},\quad G_8^{(U)}=g_5g_9g_7^{-1}g_8g_9^{-1}g_5^{-1}. \tag{2.13}$$

Then, we can also define the function ϕ_U as done above for the tree T. Now, following the procedure (2.8) of change of tree, we find the decomposition of the $G^{(U)}$ variables in terms of the $G^{(T)}$ variables

$$G_2^{(U)}=(G_1^{(T)})^{-1}(G_3^{(T)})^{-1}G_1^{(T)},\quad G_4^{(U)}=(G_3^{(T)})^{-1}G_1^{(T)},$$
$$G_8^{(U)}=G_9^{(T)}(G_7^{(T)})^{-1}(G_9^{(T)})^{-1},\quad G_6^{(U)}=G_9^{(T)}(G_7^{(T)})^{-1}. \tag{2.14}$$

If one is skeptical, one can check these relations directly using the initial g variables. Finally, we get the relation between the two functions on the flower

$$\phi_T(G_1^{(T)},G_3^{(T)},G_7^{(T)},G_9^{(T)})$$
$$=\phi_U((G_1^{(T)})^{-1}(G_3^{(T)})^{-1}G_1^{(T)},(G_3^{(T)})^{-1}G_1^{(T)},G_9^{(T)}(G_7^{(T)})^{-1},G_9^{(T)}(G_7^{(T)})^{-1}(G_9^{(T)})^{-1}). \tag{2.15}$$

III. REDUCTIVE GROUPS, QUOTIENT SPACE, AND ALGEBRAIC GEOMETRY

We have reduced so far the problem of constructing a measure on A_Γ to the problem of constructing invariant measures on the spaces $A_h=G\times\cdots\times G/\mathrm{Ad}(G)$, where $\mathrm{Ad}(G)$ denotes the diagonal adjoint action of G.

$$g\cdot(g_1,\ldots,g_h)\to(gg_1g^{-1},\ldots,gg_hg^{-1}). \tag{3.1}$$

The measure we are seeking for should be symmetric and invariant under right and left multiplication,

$$d\mu(g_{\sigma_1},\ldots,g_{\sigma_h})=d\mu(g_1,\ldots,g_h), \tag{3.2}$$

$$d\mu(kg_1h,\ldots,g_h)=d\mu(g_1,\ldots,g_h), \tag{3.3}$$

where σ is a permutation. It should also satisfy reality conditions.

More precisely, suppose $P(X_1,\ldots,X_h)$ is a real ($P^\dagger=P$) $\mathrm{Ad}(G)$-invariant element of $U(\mathcal{G}^h)-U(\mathcal{G})$ being the universal enveloping algebra of G. P can be realized as a differential operator on A_h using the correspondence between a Lie algebra element X and left invariant derivative operator

$$\partial_X^i\phi(g_1,\cdot,g_i,\ldots,g_h)\equiv\phi(g_1,\cdot,g_iX,\ldots,g_h). \tag{3.4}$$

This differential operator P should be Hermitian with respect to the measure $d\mu$ we are seeking for. In the case of a compact group, there is only one measure satisfying this conditions; $d\mu$ is just the product of normalized Haar measures for each group factor. The symmetry property is obvious and the implementation of the reality conditions are equivalent to the right and left invariance of the Haar measure. The integral of a gauge invariant function ϕ over $G^{\otimes 2}$ factorizes

$$\int_{G^{\otimes 2}} dg_1\, dg_2\, \phi(g_1,g_2) = \mathrm{vol}(G) \int_{A_2} d\mu(g_1,g_2)\phi(g_1,g_2), \tag{3.5}$$

since the volume of a compact group is finite, and we can normalize the Haar measure such that it is one. In the case of a noncompact group, this is no longer possible since one would have to divide by the volume of the gauge group which is obviously infinite. We therefore have to be more cautious in the construction.

Before constructing explicitly the measure on A_h, we need to introduce some results concerning Lie algebras and Lie groups (all these facts can be studied more thoroughly in, e.g., Ref. 21).

A. Reductive Lie group and Cartan subalgebra

The theory we are developing is valid for all, so-called, linear connected reductive semisimple groups, i.e., algebraic matrix subgroups which are connected, invariant under conjugate transpose and of finite center. This contains all compact Lie groups but also noncompact ones which will be our main interest. Among these, we distinguish complex groups [$\mathrm{SL}(N,\mathbf{C})$, $\mathrm{SO}(N,\mathbf{C})$, and $\mathrm{Sp}(N,\mathbf{C})$] from real noncompact groups [e.g., $\mathrm{SL}(2,\mathbf{R})$, $\mathrm{SO}(N,1)$, or $\mathrm{SL}(N,\mathbf{R})$,…].

Given a Lie group G and its Lie algebra $\mathcal{G}$, a Cartan Lie subalgebra $\mathcal{H}$ is a maximal abelian subalgebra of $\mathcal{G}$ stable under the conjugate transpose. A Cartan subgroup H is the centralizer of a Cartan subalgebra $\mathcal{H}$ (i.e., the subgroup of element of G commuting with all the elements of $\mathcal{H}$). For each Cartan subgroup, we define the Weyl group as $W(H)=N(H)/H$, where $N(H)$ denotes the normalizer of H. In the case of compact groups, there is only one Cartan subalgebra, moreover any group element can be conjugated to the Cartan subgroup. In the noncompact case, this is no longer true. First, in general, there is a finite number of nonconjugate Cartan subalgebras, which all have the same rank [e.g., 2 for $\mathrm{SL}(2,\mathbf{R})$, 1 for $\mathrm{SO}(2N+1,1)$, N for $\mathrm{SL}(N,\mathbf{R})$]. Note that for complex groups [e.g., $\mathrm{SL}(N,\mathbf{C})$] there is only one Cartan subgroup. Second, not all elements of G can be conjugated to a Cartan subgroup. The elements which can and which commute only with carbon elements are called regular and the corresponding set is denoted G_1. G_1 consists of elements x such that $\mathrm{Ad}\,x$ is diagonalizable and such that 1 is an eigenvalue with multiplicity equal to the rank of the group. It is an open set in G and its complement is of Haar measure 0. Moreover the action of $\mathrm{Ad}(G)$ on G_1 is regular, $G_1/\mathrm{Ad}(G)$ is equal to the disjoint union $\sqcup_i H_i/W(H_i)$ of the Cartan subgroups modulo their Weyl group.

Given a Cartan subgroup H of G, we define a measure on G/H as follows:

$$\int_G f(g)dg = \int_{G/H}\left[\int_H f(xh)dh\right]dx, \tag{3.6}$$

where dg,dh are the invariant Haar measures on G,H, and f is a compactly supported function on G. If we interchange the x and h integration and note that dx is still invariant under left multiplication, therefore, we have the identity

$$\int_G f(g)dg = \int_H\left[\int_{G/H} f(h^{-1}xh)dx\right]dh. \tag{3.7}$$

Note that we cannot in the RHS of (3.7) innocently interchange the x and h integration as in (3.6). G_1 can be decomposed in a union of conjugacy classes $G_1=\sqcup_i G_i^H$, where G_i^H

$=\{ghg^{-1}, h\in H_i, g\in G\}$, each conjugacy class covers $w(H_i)=\#W(H_i)$ times a connected component of G_1. The integral over G can therefore be re-expressed as an integral over conjugacy classes, this is the Weyl integration formula

$$\int_G f(g)dg=\sum_i \frac{1}{w(H_i)}\int_{H_i}\left[\int_{G/H_i} f(xhx^{-1})dx\right]|\Delta_i(h)|^2\,dh, \tag{3.8}$$

where

$$\Delta(e^H)=\prod_{\alpha\in\Delta^+(H_i)}\sinh\frac{\alpha(H)}{2}, \tag{3.9}$$

for $H\in\mathcal{H}_i^{\mathbf{C}}$, $e^H\in H_i$. Contrary to the case of compact groups, not all group elements can be obtained as an exponential e^X with $X\in\mathcal{G}$. However we can realize any group element as e^X with X in the complexified Lie algebra $\mathcal{G}^{\mathbf{C}}$.

B. Orbit space invariant theory and algebraic geometry

A_h is defined as a quotient space by the action of a group G. We know that in general we do not get as a result a nice Haussdorf manifold. Several types of singularity can arise when we consider orbit spaces. Let us look for instance at the case of $A_2=G\times G/\mathrm{Ad}(G)$. If (g_1,g_2) are generic (noncommuting) elements of G, the isotropy group of these points is the center of G hence a finite subgroup. But, if g_1 and g_2 are commuting elements of G, the isotropy group is nontrivial. It is the intersection of the centralizer of g_1 and g_2. If say g_1 is regular, it is a Cartan subgroup and in general the dimension of the isotropy subgroup is, at least, the rank of the group when g_1 and g_2 commute. These nongeneric points can act like attractors for the action of $\mathrm{Ad}(G)$. Suppose, for instance, that $G=\mathrm{SL}(2,\mathbf{R})$ and $(g_1,g_2)=(1,e^{\sigma_3})$ where $\sigma_3=\mathrm{diag}(+1,-1)$. The isotropy group of this point is the group $e^{t\sigma_3}$. This point is non-Haussdorf and is an attractor for some neighboring orbits. To see that, lets consider $g_u=(e^{u\sigma_+},e^{\sigma_3})$ where $\sigma_+=\left(\begin{smallmatrix}0&1\\0&0\end{smallmatrix}\right)$. Then $\lim_{t\to\infty} e^{-t\sigma_3}g_u e^{t\sigma_3}=(1,e^{\sigma_3})$. The orbit $\mathrm{Ad}(G).(e^{u\sigma_+},e^{\sigma_3})$ is not closed since it contains the point $(1,e^{\sigma_3})$. Therefore any neighborhood of the orbit $\mathrm{Ad}(G)\cdot(e^{u\sigma_+},e^{\sigma_3})$ contains $(1,e^{\sigma_3})$. So two different orbits associated with $u>0$ and $u'<0$ have nondisjoint neighborhoods which means that the quotient space is not Haussdorf. One way to cure this problem is to exclude from the beginning the set of commuting elements, so that all orbits are closed. However this is not enough. Suppose, for instance, that $G=\mathrm{SL}(2,\mathbf{R})$ and denote by $(x,y)\in\mathbf{R}^2$ the group element $(e^{\sigma_3}e^{x\sigma_+},e^{\sigma_3}e^{y\sigma_-})$. The action of $e^{t\sigma_3}$ translates into the action $(x,y)\to(e^t x,e^{-t}y)$. The exclusion of the commuting elements translates into the condition $(x,y)\neq(0,0)$. In this space, all orbits are closed. But one can see that any neighborhood of the orbit of $(x,0)$ will intersect a neighborhood of the orbit of $(0,y)$ and the quotient is once again not Haussdorf. The solution is to exclude the points $(x,0)$ or $(0,y)$, then we obtain a nice quotient.

This example illustrates the general problematic in defining quotient spaces. In fact, since G is an algebraic group (being a subgroup of matrices) and since the $\mathrm{Ad}(G)$ action is also algebraic, this problem has received a lot of attention in the mathematical literature when the group is complex[22,23] under the name of invariant theory.

First, one needs to recall general facts from algebraic geometry and then give the definition of a regular or *geometric quotient space*. An affine algebraic variety X over $\mathbf{C}$ is defined as being the set of zeros of a collection of polynomials of $\mathbf{C}^N$, $X=\cap_i V(P_i)$, where $V(P)=\{x\in\mathbf{C}^N | P(x)=0\}$. The topology which is useful in this context is the Zariski topology where the closed sets are the algebraic subvariety of X, generated by $X(P)=X\cap V(P)$. The open sets are finite union of standard open sets $X_P=\{x\in X, P(x)\neq 0\}$. It is important to note that the open sets in Zariski topology are much bigger than in the usual topology. For instance any nonempty open set of X is a dense subset of X and any finite intersection of nonempty open sets is also dense. Given an affine

algebraic variety X, one defines the algebra of *regular* functions, denoted $\mathbf{C}[X]$, as the algebra of polynomials on $\mathbf{C}^N$ restricted to X, it is clear that $\mathbf{C}[X]=\mathbf{C}[\mathbf{C}^N]/I(X)$, where $I(X)$ is the ideal of polynomials which are zero on X.

One of the basic theorems in this context is that any subalgebra A of $\mathbf{C}[\mathbf{C}^N]$ (or any commutative algebra) which is finitely generated and does not contain nilpotent elements is the algebra of regular functions on an affine variety X. Such an algebra is called affine. X is called the spectrum of A and defined as the set of homomorphism $A\to\mathbf{C}$. This theorem translates geometry into algebra.

Given an affine variety X, we say that it is irreducible if it cannot be decomposed as the union of two subvarieties. In the algebraic language, this translates into the condition that $\mathbf{C}[X]$ is integral. Given $\mathbf{C}[X]$, we can define the field of rational functions and we denote it $\mathbf{C}(X)$. We say that an application between two affine varieties $\phi:X\to Y$ is a morphism iff ϕ^* maps regular functions of Y onto regular functions of X.

We are now ready to precise the good notion of a quotient. Roughly a good quotient space is one for which orbits are separated by rational invariant functions. Let G be an algebraic group acting on an affine irreducible variety X. A geometrical quotient of X by the action of G is an affine variety Y together with a surjective morphism $\pi:X\to Y$ such that

(i) π induces an isomorphism between $\mathbf{C}(Y)$ and $\mathbf{C}(X)^G$.
(ii) The fibers of π are the orbits of G in X.

The condition (ii) tells us that Y is a quotient space since it is an orbit space. The condition (i) tells us that this quotient space is an algebraic variety where points are separated by rational functions. We saw in the previous examples that such a good quotient space does not exist in general. Hopefully there is a fundamental theorem of Rosenlicht[22] which states that given a variety X and an algebraic action of G on X, it is always possible to choose an open dense set X_0 stable under G such that X_0/G is a good quotient. The proof of this theorem goes as follows. We first restrict Y such that hypothesis (i) is satisfied. Then, hypothesis (i) implies that the orbit of x is dense in $\pi^{-1}(x)$. However, in general, hypothesis (ii) is not true. What we do next is to restrict ourself to a subset X_0 of X which contains only orbits of maximal dimension. This implies (ii). Then the geometric quotient X_0/G exists as an algebraic variety.

In the case the group G is reductive, there exists a fundamental theorem due to Hilbert and Nagata which states that if X is irreducible and G reductive then $\mathbf{C}[X]^G$ is finitely generated. Since $\mathbf{C}[X]^G$ does not contain nilpotent elements, this means that it is an affine algebra and therefore that it is the algebra of regular functions over its spectrum, which is denoted $X//G \equiv \mathrm{spec}(\mathbf{C}[X]^G)$. It is equipped with a surjective morphism $\pi:X\to X//G$ and called the *quotient* of X by G. The quotient of X by G is universal in the sense that any G-invariant morphism $p:X\to Y$ can be factorized over $X//G$, i.e., there exists a morphism $q:X//G\to Y$ such that $p=q\circ\pi$. It is then possible to show that any fiber of π contains a *unique* closed orbit. Geometrically this means that $X//G$ is the space of closed orbits of G in X. This is a little bit disappointing since this means that $X//G$ could be a very rough description of the space of orbits. For instance $X//G$ is generally not a geometric quotient. For instance Let $X=\mathbf{C}^2$ and $G=\mathbf{C}^*$ acts by multiplication $(x,y)\to(tx,ty)$. The only invariant polynomials $P(x,y)$ are the constant polynomials, so that $X//G$ is reduced to a point. In other words, there is one unique closed orbit, the one of $(0,0)$. Fortunately, the following property is true if G is linear reductive connected and *semisimple*. In this case, the algebra of fractions of $\mathbf{C}[X]^G$ [i.e., $\mathbf{C}(X//G)$] is equal to $\mathbf{C}(X)^G$. Equivalently this means that $X//G$ is the space of closed and dense orbits, i.e., any fiber $\pi:X\to X//G$ contains a dense closed orbit. Therefore this theorem imply that in the case we consider, e.g., linear reductive group we can define the geometrical quotient space X/G as the algebraic dual of the space of invariant polynomial.

Coming back to our specific problem we have G a linear reductive connected semisimple Lie group acting on $X=G^n$ by the adjoint action. By the general theory just exposed, we know that, in the case G is complex, the universal orbit space $G^n//\mathrm{Ad}\,G$ consisting of dense orbits separated

by invariant polynomials on G^n is well defined. Moreover by the Rosenlicht theorem, we know that it is always possible to exclude from G^n a closed set such that the universal orbit space is well defined as a geometric quotient. However the drawbacks of these general methods, despite their beauty and generality, are that they say nothing about the real case in which we are interested and that they are not constructive.

It is therefore still interesting to understand better and explicitly which closed set we have to exclude from G^n in order to get a geometric quotient space (which is then a well-defined affine variety). Moreover we are interested in the measure theoretical property of the quotient and we would like to show that the difference between the geometrical quotient and the quotient space $G^n//G$ is of measure zero.

First we know from Rosenlich theorem that it is possible to obtain a geometrical quotient by excluding a closed (in the Zariski topology) set from G^n.

In the case of $G/\mathrm{Ad}(G)$, this problem is well known. The solution is to exclude from G the points at which the $\mathrm{Ad}(G)$ action is not regular. The set of regular elements of G is denoted by G_1 and this is the set of $g \in G$ for which $\mathrm{Ad}(G)$ is diagonalizable and such that 1 is an eigenvalue with multiplicity equal to the rank of the group. The quotient space $G_1/\mathrm{Ad}(G)$ is equal to the union of the regular elements of Cartan subgroups modulo their Weyl group $\sqcup_i H_i/W(H_i)$.

In the case of $G\times G$, the same strategy is working and we need to exclude from it nonregular points. We therefore consider the action of $\mathrm{Ad}(G)$ not on $G\times G$ but on a subspace. For a general group even if we know the existence of such a maximal subspace we do not have an explicit description and this deserves a full mathematical study. We can however give an explicit description in the case of rank 1 groups, in that case we define

$$G_2 \equiv \{(g_1,g_2) \in G\times G; g_1 \in G_1 \text{ or } g_2 \in G_1, \text{ and } \det[g_1,g_2] \neq 0\}, \tag{3.10}$$

where $[g_1,g_2]=g_1g_2-g_2g_1$ is the commutation in the algebra.

We then have the following proposition.

Proposition 1: G_2 is a dense subset of $G\times G$, its complement is of Haar measure zero and $G_2/Ad(G)$ is a geometric quotient when G is of rank one. Therefore, $A_2=G_2/Ad(G)$ is an Haussdorff manifold of dimension $dimG$ which separates rational functions and it is the base manifold of a homogeneous fiber bundle whose fiber is G and total space $G_2 \approx A_2\times G$.

This proposal is proved in the Sec. VII where we construct the dual spectrum space to the space of invariant polynomials and show that it is isomorphic to $G_2/\mathrm{Ad}(G)$. The main point is that the condition of being in G_2 can be implemented as algebraic inequalities.

Note that, in the definition (3.10), G_2 is such that the centralizer of any element of G_2 is trivial. Suppose g commutes with $(g_1,g_2) \in G_2$, since we can take, e.g., g_1 to be regular hence g can be diagonalized in the same basis as g_1 (the regularity assumption is essential here). g cannot be regular since it commutes with g_2 and therefore it would mean that g_2 is also diagonal in the same basis, hence commutes with g_1, which is impossible. So the definition of G_2 implies that g is diagonal and nonregular. If the rank of the group is 1, this means that g is the identity. In the case of $\mathrm{SL}(N,\mathbf{C})$ it is easy to check that the additional determinant condition is enough to conclude that g should lie in the center. It is important to understand that the definition of G_2 is not the naive definition where one just excludes from $G\times G$ the group elements which have a nontrivial centralizer: in order to get a nice quotient, we need to take away more points and this is dictated by the fact that we want the quotient space to be the spectrum of the algebra of invariant functionals.

In the general case of higher rank group we define G_2 to be the following space:

$$G_2 \equiv \{(g_1,g_2) \in G\times G; g_1 \in G_1 \text{ or } g_2 \in G_1, \text{ and } C(g_1,g_2)=Z_G\}, \tag{3.11}$$

where, $C(g_1,g_2)$ denotes the centralizer of g_1 and g_2 and Z_G denotes the center of the group. We have seen that for $\mathrm{SL}(N,\mathbf{C})$ this can be achieved by implementing an algebraic inequality. We expect this to be true for all groups. We will see in the next section that G_2 admits a quotient by

$\mathrm{Ad}(G)$ and we denote by A_2 the quotient. However, contrary to the definition (3.10) valid for rank 1 group, the definition (3.11) is not equivalent to a definition of G_2 as an algebraic dual.

IV. CONSTRUCTION OF THE MEASURE ON A_H

This section is central to our paper. In this section we go back to our problem which is the construction of a measure on A_h. We show, by a nontrivial gauge fixing procedure, that a dense subset of $G^h/\mathrm{Ad}(G)$ can be identified with a dense subset of G^{h-1} when $h>1$. We first consider A_2, the case of one Cartan subgroup, then the case of several Cartan subgroups, we then consider the case of A_h. Finally, setting everything together we show that the measure on A_Γ does not depend on all the gauge fixing choices, leading to the definition of a canonical measure.

A. Construction of the measure on A_2

1. Case of a unique Cartan subgroup H

Let us consider the following embedding of G_1 into A_2. Given $g\in G_1$, we can conjugate it to the Cartan subgroup H of G, i.e., there exists $h\in H$, $x\in G/H$ such that $g=xhx^{-1}$. We choose a section $s:G/H\to G$ and we define the map

$$j_s:\ G_1\to A_2$$

$$g=xhx^{-1}\to \mathrm{Ad}(G)\cdot(h,s(x)), \tag{4.1}$$

where $\mathrm{Ad}(G)\cdot(h,s(x))$ is the orbit of $(h,s(x))$ under the conjugation by G. This is a gauge fixing since given $(g_1,g_2)\in A_2$ we can conjugate g_1 to the Cartan subgroup H of G, i.e., there exists $h\in H$, $y\in G/H$ such that $g_1=yhy^{-1}$. Then $\mathrm{Ad}(G)\cdot(g_1,g_2)=\mathrm{Ad}(G)\cdot(h,y^{-1}g_2y)$. This fixes only partially the gauge since H can act on y by $y\to yk$ which means that we can still conjugate $\tilde{g}_2=y^{-1}g_2y$ by a Cartan group element. Nevertheless, since we are in A_2, the centralizer of g_1 and g_2 is trivial, this means that the centralizer of $h\in H$ and $\tilde{g}_2$ is trivial. Since the centralizer of $h\in H\cap G_1$ is H, this implies that the conjugate action of H on $\tilde{g}_2$ has no other fixed point than the center elements. Let us suppose for the following that the center of G is trivial. Then, if we exclude a set of measure zero to G, there exists a section $s:G/H\to G$, such that we can use the residual symmetry coming from the conjugation by H to impose that $\tilde{g}_2$ belongs to the image of s. For instance in the case of SL(N,C), we exclude the points such that $a_{ij}+1=0$, where a_{ij} are the matrix elements, and we choose the section to be such that $\prod_{i=1}^{N-1} a_{ij}+1=1$, for all $i=1,\ldots,N-1$. Finally, the gauge fixing we impose is $(g_1,g_2)\to(h,s(x))\in H\times G/H$. We just have argued that every element of G_2 can be brought to this form. Moreover the condition that the centralizer of (g_1,g_2) is trivial is implemented if we ask $g=s(x)h(s)x^{-1}\notin H$. Indeed, $s(x)h(s)x^{-1}\in H$ would mean that either $s(x)\in H$ or that $s(x)$ is a Weyl transformation. The first possibility, $s(x)\in H$ is impossible since $s(x)$ and h do not commute. So that j_s gives a map from $G_1\backslash H$ to A_2. The second possibility is related to the Gribov ambiguity, which makes the definition of j_s still ambiguous.

This can be traced back to the fact that a given group element g can be conjugated to different Cartan elements related by the action of the Weyl group $W(H)$, which is the residual conjugation action on the Cartan subgroup. There is two ways to solve this problem. First, we can require good transformations of the section s under the action of the Weyl group

$$\forall x\in G/H,\ \ \forall w\in W(H),\ \ s(xw)=w^{-1}s(x)w. \tag{4.2}$$

This renders j_s well defined and this is the hypothesis we will suppose in the following. Or we can impose h to be in a fixed Weyl chamber. In this case, one must remove all the $1/w(H)$ factors from the following proofs.

With this map, we can pullback functions on A_2, or equivalently invariant functions on G_2, to functions on G_1 by $j_s^*F(xhx^{-1})=F(h,s(x))$.

Definition 1: Let μ be a measure on A_2 defined by

$$\int_{A_2} F(g_1,g_2)d\mu(g_1,g_2)\equiv\int_G j_s^* F(g)dg. \tag{4.3}$$

Proposition 2: Let F be a L^1 function on G_2 with respect to the Haar measure. We also require that its gauge invariant version ${}^GF$ is well defined:

$${}^GF(g_1,g_2)=\int_G F(gg_1g^{-1},gg_2g^{-1})dg. \tag{4.4}$$

Then we have

$$\int_{G\times G} F(g_1,g_2)dg_1dg_2=\int_{A_2} {}^GF(g_1,g_2)d\mu(g_1,g_2). \tag{4.5}$$

In order to prove this, let $F(g_1,g_2)$ be a L^1 function on $G\times G$.

$$\int_{G\times G} F(g_1,g_2)dg_1\,dg_2 \tag{4.6}$$

$$=\frac{1}{w(H)}\int_{G/H\times H\times G} F(xhx^{-1},g_2)\Delta(h)dx\,dh\,dg_2 \tag{4.7}$$

$$=\frac{1}{w(H)}\int_{G/H\times H\times G} F(xhx^{-1},xg_2x^{-1})\Delta(h)dx\,dh\,dg_2, \tag{4.8}$$

where we have used the Weyl integration formula (3.8) in the first equality and the invariance under right and left translation of the Haar measure dg_2 in the second. Using the identity (3.7) for the integration on G_2 the integral can be expanded as

$$\begin{aligned}&\frac{1}{w(H)}\int_{G/H\times H\times H\times H\backslash G} F(xhx^{-1},xkyk^{-1}x^{-1})\Delta(h)dx\,dh\,dk\,dy\\&=\frac{1}{w(H)}\int_{H\times H\backslash G}\left[\int_{G/H\times H} F(xhx^{-1},xky(xk)^{-1})dx\,dk\right]\Delta(h)dh\,dy\\&=\frac{1}{w(H)}\int_{H\times H\backslash G}\left[\int_{G/H\times H} F(xkh(xk)^{-1},xky(xk)^{-1})dx\,dk\right]\Delta(h)dh\,dy,\end{aligned} \tag{4.9}$$

where we have used the fact that H is abelian to derive the last equality. Then using the definition of the G/H measure (3.6), we finally get

$$\int_{G\times G} F(g_1,g_2)dg_1\,dg_2=\frac{1}{w(H)}\int_{H\times H\backslash G} {}^GF(h,y)\Delta(h)dh\,dy, \tag{4.10}$$

where ${}^GF$ is the gauge invariant version of F:

$${}^GF(g_1,g_2)=\int_G F(gg_1g^{-1},gg_2g^{-1})dg. \tag{4.11}$$

Theorem 1: *μ is independent of s, symmetric, invariant under right and left multiplication and invariant under taking the inverse:*

$$d\mu(g_1,g_2)=d\mu(g_2,g_1), \tag{4.12}$$

$$d\mu(kg_1h,g_2)=d\mu(g_1,g_2), \tag{4.13}$$

$$d\mu(g_1,g_2)=d\mu(g_1^{-1},g_2). \tag{4.14}$$

Let us prove the above theorem for $d\mu(kg_1,g_2)$ (left multiplication). One will be able to prove the other properties following the same line of thoughts. The easiest way to prove the theorem is to use a Faddev–Popov gauge fixing procedure using the proposition 2. Let us choose an invariant function F on G_2. We can choose any function φ on G_2 such that ${}^G\varphi=1$ and create the (gauge fixed) function $\tilde{F}=F\varphi$. In the usual Faddeev–Popov procedure one would choose φ to be proportional to a δ function of a gauge fixing condition, but this is not necessary. Applying proposition 2,

$$\int_{A_2} F(g_1,g_2)d\mu(g_1,g_2)=\int_{G\times G}\tilde{F}(g_1,g_2)dg_1\,dg_2. \tag{4.15}$$

Using the freedom in the choice of the function φ in proposition 2 and the fact that if $\varphi(g_1,g_2)$ is a gauge fixing so is $\varphi_k(g_1,g_2)=\varphi(k^{-1}g_1,g_2)$, we get

$$\begin{aligned}\int_{A_2} F(g_1,g_2)d\mu(kg_1,g_2)&=\int_{G\times G}F(k^{-1}g_1,g_2)\varphi(k^{-1}g_1,g_2)dg_1\,dg_2\\&=\int_{G\times G}F(g_1,g_2)\varphi(g_1,g_2)dg_1\,dg_2\\&=\int_{A_2}F(g_1,g_2)d\mu(g_1,g_2).\end{aligned} \tag{4.16}$$

So we conclude to the left invariance of the measure $d\mu$ defined on A_2.

2. The case of many Cartan subgroups

In general, we have many Cartan subgroups and let's note them $H_1,H_2,\ldots,H_n$. G_1 can be decomposed in disconnected components $G^{(i)}=\mathrm{Ad}(G)\cdot H_i$, each conjugated to the Cartan subgroup H_i. For each of these components, one can choose a section $s_i:G/H_i\to G$ and define a map

$$\begin{aligned}&j_i:\ G^{(i)}\subset G_1\to A_2\\&g=yhy^{-1}\to\mathrm{Ad}(G)\cdot(h,s_i(y)).\end{aligned} \tag{4.17}$$

From this map, one can define a measure $d\mu_i$ on A_2 as in the definition (1) by

$$\int_{A_2}F(g_1,g_2)d\mu_i(g_1,g_2)\equiv\int_{G_i}j_i^*F(g)dg. \tag{4.18}$$

Proposition 3: Given any L^1 function F on G_2 we have

$$\int_{G\times G}F(g_1,g_2)dg_1\,dg_2=\int_{A_2}{}^GF(g_1,g_2)d\mu(g_1,g_2), \tag{4.19}$$

where

$$d\mu(g_1,g_2)=\sum_i\frac{1}{w(H_i)}d\mu_i(g_1,g_2) \tag{4.20}$$

and where ${}^GF$ is the gauge invariant version of F:

$$ {}^{G}F(g_1,g_2)=\int_G F(gg_1g^{-1},gg_2g^{-1})dg. \tag{4.21}$$

Let $F(g_1,g_2)$ be a L^1 function on $G\times G$.

$$\int_{G\times G} F(g_1,g_2)dg_1\,dg_2 \tag{4.22}$$

$$=\sum_i \frac{1}{w(H_i)}\int_{G/H_i\times H_i\times G} F(xhx^{-1},g_2)\Delta(h)dx\,dh\,dg_2 \tag{4.23}$$

$$=\sum_i \frac{1}{w(H_i)}\int_{G/H_i\times H_i\times G} F(xhx^{-1},xg_2x^{-1})\Delta(h)dx\,dh\,dg_2, \tag{4.24}$$

where we have used the Weyl integration formula (3.8) in the first equality and the invariance under right and left translation of the Haar measure in the second. Using the identity (3.7) for the integration on G_2 the integral can be expanded as

$$\sum_i \frac{1}{w(H_i)}\int_{G/H_i\times H_i\times H_i\backslash G} F(xhx^{-1},xkyk^{-1}x^{-1})\Delta(h)dx\,dh\,dk\,dy \tag{4.25}$$

$$=\sum_i \frac{1}{w(H_i)}\int_{H_i\times H_i\backslash G}\left[\int_{G/H_i\times H_i} F(xhx^{-1},xky(xk)^{-1})dx\,dk\right]\Delta(h)dh\,dy. \tag{4.26}$$

Using the fact that H_i is abelian and the definition of the G/H_i measure (3.6) we finally get

$$\begin{aligned}\int_{G\times G} F(g_1,g_2)dg_1\,dg_2&=\sum_i \frac{1}{w(H_i)}\int_{H_i\times H_i\backslash G} {}^{G}F(h,y)\Delta(h)dh\,dy\\ &=\sum_i \frac{1}{w(H_i)}\int_{G^{(i)}} dg\, j_i^*({}^{G}F)(g)\\ &=\sum_i \frac{1}{w(H_i)}\int_{A_2} d\mu_i(g_1,g_2)\,{}^{G}F(g_1,g_2).\end{aligned} \tag{4.27}$$

Using the above proposition, we can generalize theorem 1 to the multi-Cartan case using the same proof as done before.

B. The measure on A_h

We are now interested in generalizing the case of A_2 to A_h. Applying the Rosenlich theorem stated in (Sec. III B), it is always possible to choose an open dense set $G_h\subset G^h$ such that the geometric quotient $A_h=G_h/\mathrm{Ad}(G)$ is well-defined as in proposition 1. Following the choice made for the 2-petals case we get the following definition when G is rank one:

$$G_h\equiv\{(g_1,\ldots,g_h)\in G^{\otimes h}\,|\,\exists(i,j)\in[1,\ldots,h],(g_i,g_j)\in G_2\}. \tag{4.28}$$

Definition 2: Note that G_h is such that the centralizer of any element in G_h is the identity.

Definition 3: We choose two edges i,j on the n-petal flower. Then, we can define a measure on A_h

$$\mu^{(ij)}[f(g_1,g_2,\ldots,g_n)]=\int_{G_2^{(ij)}} d\mu(g_i,g_j)\int\prod_{k\neq i,j} dg_k\, f(g_1,g_2,\ldots,g_n), \tag{4.29}$$

where we have taken the measure gauge fixed measure $d\mu(g_i,g_j)$ on the two chosen edges and the Haar measure on the other edges.
This measure is well defined since $\int \Pi_{k\neq i,j} dg_k f(g_1,g_2,\ldots,g_n)$ is an invariant function on $G_2^{(ij)}$ [and therefore a function on A_2, which we can integrate using $d\mu(g_i,g_j)$].

Proposition 4: Given any L^1 function F on G^n we have

$$\int_{G^n} F(g_1,\ldots,g_n)dg_1\cdots dg_n = \int_{A_n} {}^G F(g_1,\ldots,g_n)d\mu(g_1,\ldots,g_n), \tag{4.30}$$

where ${}^G F$ is the gauge invariant version of F:

$${}^G F(g_1,\ldots,g_n) = \int_G F(gg_1g^{-1},\ldots,gg_ng^{-1})dg. \tag{4.31}$$

This proposition is easily proved using the proposition 2 and the invariance of the Haar measure under right and left multiplication. And its leads to the following theorem:

Theorem 2: *The measures $d\mu^{(ij)}$ do not depend on the choice of edges i,j. And one defines a unique measure $d\mu(g_1,g_2,\ldots,g_n)$ on A_h. Moreover, this measure is symmetric under permutation of $g_1,\ldots,g_n$, under right and left multiplication and under taking the inverse of one of its argument:*

$$\begin{aligned} d\mu(g_{\sigma_1},\ldots,g_{\sigma_n}) &= d\mu(g_1,\ldots,g_n),\\ d\mu(kg_1h,\ldots,g_n) &= d\mu(g_1,\ldots,g_n),\\ d\mu(g_1^{-1},\ldots,g_n) &= d\mu(g_1,\ldots,g_n). \end{aligned} \tag{4.32}$$

C. Measure on an arbitrary graph

To construct the measure on an arbitrary graph Γ, we are going to choose a maximal tree T and carry on the gauge fixing procedure described in the first section in order to reduce the graph Γ to a flower. We then define the measure $d\mu_T$ such that for all gauge invariant functions ϕ on Γ, we have

$$\int d\mu_T(g_1,\ldots,g_E)\phi(g_1,\ldots,g_E) = \int \widetilde{d\mu}(g_1,\ldots,g_F)\phi_T(g_1,\ldots,g_F), \tag{4.33}$$

where $\widetilde{d\mu}$ is the measure on the F petal flower.

This definition *a priori* depends on the choice of the tree T. We are going to prove that this is not the case. So we choose two maximal trees T and U. The gauge fixed function are related by (2.8):

$$\phi_T(G_e^{(T)}) = \phi_U\left(G_e^{(U)} = \overrightarrow{\prod_{f\in \mathcal{L}[e]\setminus T}} G_f^{(T)} \right)$$

and we want to prove that

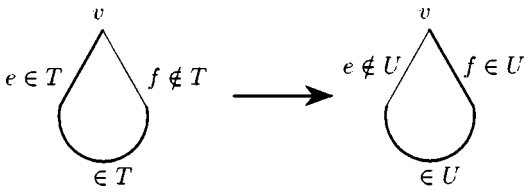
$$\int \widetilde{d\mu}(G_1^{(T)},\ldots,G_F^{(T)})\phi_T(G_1^{(T)},\ldots,G_F^{(T)}) = \int \widetilde{d\mu}(G_1^{(U)},\ldots,G_F^{(U)})\phi_U(G_1^{(U)},\ldots,G_F^{(U)}) \tag{4.34}$$

or equivalently

$$\int \widetilde{d\mu}(G_1^{(U)},\ldots,G_F^{(U)})\phi_U(G_1^{(U)},\ldots,G_F^{(U)}) = \int \widetilde{d\mu}(G_1^{(T)},\ldots,G_F^{(T)})\phi_U\left(G_e^{(U)}=\overrightarrow{\prod_{f\in\mathcal{L}[e]\setminus T}} G_f^{(T)}\right). \tag{4.35}$$

We are going to show this equality by doing some elementary changes of variables which would correspond to elementary moves between the two maximal trees and we will show that the measure is invariant under each such move. Let us first define what we mean by an elementary move.

Definition 4: Given a graph Γ *and a maximal tree* T *on it, let us choose a vertex* v *such that there is at least one edge linked to it which is not in the tree* T. *Let us pick one and call it* f. *There exists an unique path in* T *linking the other vertex of* f *to* v. *This path goes along an unique edge* $e\in T$ *linked to* v. *Then an elementary change of tree, or elementary move, is exchanging the role of* e *and* f *and considering the maximal tree* $U=T\cup f\setminus e$.



The interest in such a definition lies into the following proposition.

Proposition 5: Having chosen two maximal trees T *and* U *on a graph* Γ, *there exists a sequence of elementary moves going from* T *to* U.

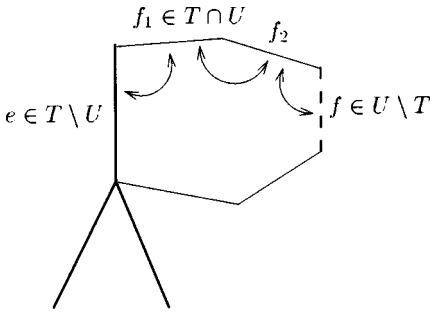
Then, as we will see, the change of variable from $G^{(U)}$ to $G^{(T)}$ is very simple for such a move since it is implemented either by an inversion or by left multiplication, so that it will simplify the study of change of trees.

Let us first prove the proposition. Given Γ and two maximal trees T,U in it we can distinguish four types of edges: edges belonging to both trees T and U, edges in $V=T\setminus U$, edges in $W=U\setminus T$ and edges in neither trees. By elementary moves on either the tree T or the tree U, we would like to reduce the sets V and W down to nothing. Let us take a closer look at the set V. First, V might not be connected. In this case, we would carry on the following procedure on each of its connected parts. Let's denote one of the connected part V_1 and work on it. V_1 is a tree as part of the tree T. In particular, it is not closed and has some open ends, i.e., edges connected to V_1 only by one vertex. By doing elementary moves, we are going to remove them from V_1, and then, by repeating the same operations, one could erase completely the set V_1. And finally, by repeating the procedure on the other connected parts of V, one could absorb completely the set $T\setminus U$.

So let us choose an edge e at an open end of V_1. It has two vertices: v in the exterior of V_1 and w in the interior of V_1. There exists an unique path $\mathcal{P}$ along U which links these two vertices and $e\notin U$ is not in it. In $\mathcal{P}$, there exists at least one edge in U but not in T else there would be a loop in the tree T.

Let us suppose that such an edge $f\in U\setminus T$ touches directly the edge e (at the vertex v). Then, we can do an elementary move exchanging $e\leftrightarrow f$ and create a tree $\widetilde{U}=U\cup e\setminus f$ closer to the tree

T than the tree U.



Let us now come back to the general case in which we have to follow a sequence of edges $f_1,\ldots,f_n \in T \cap U$ starting from the vertex v along the path $\mathcal{P}$ to an edge f in $U \backslash T$. Then, we do the allowed elementary moves on the tree U exchanging $e \leftrightarrow f_1,\ldots,f_{n-1} \leftrightarrow f_n$, thus creating the trees $U_1,\ldots,U_n$. Starting from v, all the edges $e,f_1,\ldots,f_{n-1}$ are both in T and U_n, f_n is in $T \backslash U_n$, f is in $U_n \backslash T$, and all the other edges on the way back to w are in U_n. So that we are in the same simple case as above and we finally do the move $f_n \leftrightarrow f$ on the tree U_n creating a tree $\tilde{U}$ such that the whole loop $\mathcal{P}$ from v to v is in both T and $\tilde{U}$ except the edge f which is in neither. Practically, we had a loop with all the edges in U but one which is in T (it is e), and by elementary moves, we move it around until it meets an edge which is not in T and they ''cancel'' each other.

This ends the absorbtion of the edge e: the set $T \backslash \tilde{U}$ contains one edge less than $T \backslash U$. And we now repeat the same procedure using the new tree $\tilde{U}$.

We now are able to prove the following.

Theorem 3: *The Jacobian of the change of variables (4.35) is 1, so that the measure $d\mu_T$ is invariant under changes of tree.*

This theorem will assure the existence of a measure $d\mu^{(\Gamma)} = d\mu_T$ independent from the choice of the tree T and therefore from the whole gauge fixing procedure, which is the measure we will use to integrate our gauge invariant functions and define a space of L^2 gauge invariant functions. This space will in fact be the Hilbert space of spin networks defined on the graph Γ.

Proposition 5 means that we only have to prove the theorem 3 for elementary moves. So, let us realize an elementary move on the tree T around the vertex v and define the new maximal tree $U = T \cup f \backslash e$. For every edge $a \notin U$ on the U flower, we define the variables $G_a^{(U)}$. And we want to express them in terms of the variables $G_b^{(U)}$. For $a \notin U$ and $\notin T$, we want to relate $G_a^{(U)}$ to $G_a^{(T)}$. It can be easily seen that these two variables are equal up to a multiplication on the left or right or on both sides by $G_f^{(T)}$ or its inverse. And for the only other case $a = e$, we will have $G_e^{(U)} = (G_f^{(T)})^{\pm 1}$. Then using the invariance of the measure of the flower by multiplication or by taking the inverse of one of its argument (theorem 2), we can conclude that the above change of variables has a trivial Jacobian.

V. SPIN NETWORKS STATES

In this section, we are going to define the spin networks as eigenvectors of a set of commuting Laplacian operators, which will be shown to be hermitian.

A. Laplacian operators

Let us consider a graph Γ and a gauge invariant function defined on it. These functions depend on E group elements $g_1,\ldots,g_E$. Let's denote by X an element of the Lie algebra and by $\partial_X^{R_e}$ (respectively, $\partial_X^{L_e}$) the right (respectively, left) invariant derivative acting on the jth group element associated with the edge e:

$$\partial_X^{R_1} f(g_1,\ldots,g_N) = f(Xg_1,\ldots,g_N), \tag{5.1}$$

$$\partial_X^{L_1} f(g_1,\ldots,g_N) = f(g_1(-X),\ldots,g_N), \tag{5.2}$$

The gauge group action acts on derivative operators by conjugation at each vertex :

$$\partial_X^{R_e} \to \partial^{R_e}_{k_{s(e)} X k_{s(e)}^{-1}}.$$

We are interested in gauge invariant differential operators. The algebra of such operators is generated by Laplacian operators $\Delta_e^{(i)}$ where e labels the edges of Γ and i runs from 1 to the rank r of the group. For each edge e, the space of Laplacians is in one to one correspondence with the Casimir operators of the Lie algebra. Therefore this set of Laplacians gives a complete basis of commuting operators. Indeed, they are commuting since for a given e two Casimirs commute and for different edges e's the differential operators $\partial_X^{R_e}$ commute with each other.

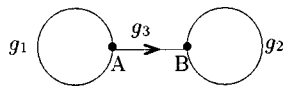
We want to define the spin networks as the basis of eigenstates vectors for this complete set of gauge invariant differential operators. In order to do that, we need to show that these operators are Hermitian with respect to the measure $d\mu^{(\Gamma)}$ that we have just constructed. We are going to give the proof for the quadratic Laplacian operator $\Delta_e = \Sigma_i \partial^{R_e}_{X_i} \partial^{R_e}_{X_i}$ ($\Delta_e = \partial^{R_e}\partial^{R_e}$ for short), where X_i denotes an orthonormal basis of the Lie algebra. The general case is similar, it simply needs more cumbersome notations.

Because of the measure $d\mu^{(\Gamma)}$ has being defined on the gauge fixed flower corresponding to Γ, we have to follow the gauge fixing procedure leading to group variables $G_i,\ldots,G_F$ on the flower and express the operators Δ_e in term of the derivatives $\tilde{\partial}_i^{L,R}$ with respect to these new variables.

To start with, let us look at an example, the case of the two petal flower coming from either the Θ graph or the eyeglass graph. Let's first gauge fix the Θ graph:

We gauge fix from the point A. We have $G_1 = g_1 g_3^{-1}$ and $G_2 = g_2 g_3^{-1}$. It is then easy to check that $\partial_1^R = \tilde{\partial}_1^R$, $\partial_2^R = \tilde{\partial}_2^R$, and $\partial_3^R = \tilde{\partial}^{L_1} + \tilde{\partial}^{L_2}$ so that $\Delta_1 = \tilde{L}_1$, $\Delta_2 = \tilde{L}_2$, and $\Delta_3 = \tilde{\Delta}_1 + \tilde{\Delta}_2 + 2\tilde{\Delta}_{12}$, where $\tilde{\Delta}_{12} = \tilde{\partial}_1^L . \tilde{\partial}_2^L$.

In the case of the eyeglass graph



We have $G_1 = g_1$ and $G_2 = g_3 g_2 g_3^{-1}$. Thus $\Delta_1 = \tilde{\Delta}_1$, $\Delta_2 = \tilde{\Delta}_2$ as the Laplacian is invariant under $\mathrm{Ad}(G)$ and $\Delta_3 = (\tilde{\partial}_2^R - \tilde{\partial}_2^L)^2$.

In the generic case, for a given edge e, if there exists a maximal tree T which does not go through e, then e will be on the gauge fixed flower and Δ_e will simply be the Laplacian $\tilde{\Delta}_e$ with derivatives with respect to the flower variable G_e.

What happens to edges which are in every possible trees, such as the middle edge in the eyeglass graph, is slightly more tricky. For such an edge e, we choose to gauge fix from its departure vertex v. Then ∂_e^R will be equal to the sum of $\tilde{\partial}_f^R$ for all edges f whose loop starts with e and $\tilde{\partial}_f^L$ for all edges whose loop finishes with e.

In any case, the initial differential operators Δ_e can be written as a sum of $\tilde{\Delta}_{ij}^{RR}=\tilde{\partial}_i^R.\tilde{\partial}_j^R$ and $\tilde{\Delta}_{ij}^{LR}=\tilde{\partial}_i^L.\tilde{\partial}_j^R$ where $i,j=1,\ldots,g$. These operators are Ad(G) invariant operators on G^h. This is easily seen since the gauge invariance of a function ϕ_Γ is equivalent to

$$\left(\sum_{e|s(e)=v}\partial^{R_e}+\sum_{e|t(e)=v}\partial^{L_e}\right)\phi=0, \tag{5.3}$$

for all vertices v. Choosing a tree amounts to use these equations to express all derivatives along edges belonging to the tree in terms of the other ones that we named $\tilde{\partial}_i^{L,R}$. We are then left with only one relation $\Sigma_{i=1}^h(\tilde{\partial}_i^R+\tilde{\partial}_i^L)\phi=0$.

B. Spin networks as Laplacian eigenvectors

Theorem 4: *The Laplacian operators* $\tilde{\Delta}_{ij}^{RR},\tilde{\Delta}_{ij}^{LR}$ *are Hermitian with respect to the measure* $d\mu_h, h>1$.

We will give the proof for $\tilde{\Delta}_i\equiv\tilde{\Delta}_{ii}^{RR}$. The proof for a general operator is similar.

Let us consider

$$\int_{A_h}(\varphi\tilde{\Delta}_i\psi-\psi\tilde{\Delta}_i\varphi)d\mu_h, \tag{5.4}$$

where φ,ψ are gauge invariant functions. And let us introduce a gauge fixing function ϕ, which is such that

$$\int_G {}^g\phi\, dg=1, \tag{5.5}$$

where ${}^g\phi(g_1,\ldots,g_N)=\phi(gg_1g^{-1},\ldots,gg_Ng^{-1})$. The integral (5.4) can be written as

$$\int_{G^h}(\varphi\tilde{\Delta}_i\psi-\psi\tilde{\Delta}_i\varphi)\,\phi\, dg_1\cdots dg_h. \tag{5.6}$$

Using the invariance of the Haar measure under left multiplication we can integrate by part the right invariant derivatives, this leads to (we take off the tilde for simplicity of the notations)

$$\int_{A_h}(\varphi\Delta\psi-\psi\Delta\varphi)d\mu=\int_{G^h}\psi\partial_{X_j}^{R_i}\varphi\partial_{X_j}^{R_i}\phi-\varphi\partial_{X_j}^{R_i}\psi\partial_{X_j}^{R_i}\phi\, dg_1\cdots dg_h. \tag{5.7}$$

Let us look at the first term, we can write it as

$$\int_{G^h}dg_1\cdots dg_h\,\psi\partial_{X_j}^{R_i}\varphi\partial_{X_j}^{R_i}\phi=\int_{A_h}\psi\left[\int_G dg^g\,\partial_{X_i}^{R_k}\varphi^g\partial_{X_i}^{R_l}\phi\right]d\mu_h, \tag{5.8}$$

where we have used the definition of the invariant measure (4) and ${}^g\psi=\psi$. Using the following identity

$${}^g\partial_{X_i}\phi=\partial_{Ad(g)^{-1}X_i}{}^g\phi, \tag{5.9}$$

and the invariance of the quadratic differential operator

$$\sum_i\partial_{Ad(g)\cdot X_i}^R\otimes\partial_{Ad(g)\cdot X_i}^R=\sum_i\partial_{X_i}^R\otimes\partial_{X_i}^R \tag{5.10}$$

one gets

$$\int_{A_h} \psi \left[\int_G dg\, \partial_{X_i}{}^g\varphi \partial_{X_i}{}^g\phi\, dg \right] d\mu_h . \tag{5.11}$$

Using that ${}^g\varphi = \varphi$ since φ is gauge invariant and that the condition (5.5) implies $\partial_{X_i} \int {}^g\phi\, dg = 0$, we conclude that the integral (5.4) is zero.

Definition 5: Since the operators Δ_e form a set of commuting Hermitian operators on the Hilbert space $L^2(d\mu^{(\Gamma)})$, we can diagonalize them and their eigenvectors form an orthonormal basis of $L^2(d\mu^{(\Gamma)})$. We call these eigenvectors spin networks.

It should be clear that these vectors should be considered as generalized δ normalizable vectors if one of the eigenvalues they carry is part of a continuous spectrum: one should consider them as invariant distributions and not invariant functions.

We obtain a basis of functions which are labeled by the eigenvalues of the Laplacians—the Casimirs of the group—on each edge of the graph Γ. In other words, if we call $d\rho(\lambda)$ the spectral measure of the Laplacian operator one gets

$$H_\Gamma \equiv L^2(d\mu^{(\Gamma)}) = \oplus_e \int d\rho(\lambda_e) \otimes_v I_v(\lambda), \tag{5.12}$$

where $I_v(\lambda)$ is the space of intertwiners between the representations carried by the edges meeting at the vertex v.

In the case of $G = \mathrm{SU}(2)$, there is a one-to-one correspondence between the eigenvalues of the Casimir and the irreducible unitary representations. And by the previous reasoning, we have totally reconstructed the usual structure of spin networks with representations labeling the edges of the spin networks if the graph is trivalent. In a more general context, one should be careful that the eigenvalues of the Laplacians do not always completely characterize the representations, there can be a degeneracy where several representations carry the same Laplacians. This is the case, for instance, of the series of discrete representations of SL(2,**R**), where the degeneracy is 2. This is not the case however for the unitary representations of SL(2,**C**) which are totally determined by the values of their two Casimirs. We have presented the spin networks in the particular case of rank 1 but as we said in the beginning, all the propositions work the same for a more general group.

C. Unfolding vertices and SU(2) spin networks

Using the gauge fixing procedure, we can unfold all the vertices of a given graph Γ. By this, we mean replace each vertex by a (minimal) tree which has only 3-valent vertices. More explicitly, let us consider a vertex v. We can match the edges meeting at v two by two (if their number is odd, we leave one edge on its own) and create a 3-valent vertex for each of these pairs. Then we repeat this process until over.

Let us call the unfolded graph Γ_0. As the flowers corresponding to Γ and to Γ_0 are the same, we have $L^2(d\mu^{(\Gamma)}) = L^2(d\mu^{(\Gamma_0)})$. We can then construct spin networks on the graph Γ_0, by labeling all its edges—both the ones already in Γ and the new ones which are *inside* the vertices of Γ—with representations of the group G. These spin networks span $L^2(d\mu^{(\Gamma_0)})$ and therefore also $L^2(d\mu^{(\Gamma)})$. That way, we have unfolded the structure of the vertices of the spin networks based on the graph Γ. We have reduced the problem of characterizing nodes to the case of 3-valent ones. One thing which one should be aware of is that for high rank groups, it happens that the space of trivalent interwiners is infinite dimensional, e.g., sl(3,**R**).

In the case of $G = \mathrm{SU}(2)$, the 3-valent nodes are 3-valent intertwiners intertwining between the representations labeling the three edges. These intertwiners are unique to a normalization. So we have fully characterized SU(2) spin networks—both their edges and nodes—by the above unfolding procedure. In the general case, we can have many possible 3-valent intertwiners and their space has to be studied in order to fully characterize the nodes of the spin networks.

VI. THE ONE LOOP CASE

In this section, we restrict ourselves to rank one groups and we deal with the graph made of a single loop with a single bivalent vertex, which describes the quotient space $G/\mathrm{Ad}(G)$. This case is essentially different from the cases of flowers with higher $h \geqslant 2$ number of petals for which the quotient space $G^h/\mathrm{Ad}(G)$ can be mapped onto G^{h-1} as described in the preceding section. And both the techniques used and the problems encountered differ from the other cases. Nevertheless, this study is important since the characters of the unitary representations are supposed to be orthonormal vectors of $L^2(G/\mathrm{Ad}(G))$, therefore it is interesting as the simplest part of the gauge invariant connection space and it illustrates the problem of the possible nonconnectivity of the quotient space and the (super)selection rule issue which comes with it.[25]

A. SL(2,C)

In this section, we consider the case where the group is $\mathrm{SL}(2,\mathbf{C})$ and we are interested in describing the quotient $(\mathrm{SL}(2,\mathbf{C}))//\mathrm{Ad}(\mathrm{SL}(2,\mathbf{C}))$ as defined in Sec. III B. Let $g=\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbf{C})$, the algebra $\mathbf{C}[\mathrm{SL}(2,\mathbf{C})]^{\mathrm{SL}(2,\mathbf{C})}$ of polynomials invariant under the adjoint action is generated by $X(g)=(1/2)tr(g)$, since such polynomials are linear combination of $tr(g^n)$. $tr(g^n)$ can be expressed as a polynomial in X due to the relation $g^2-tr(g)g+1=0$, more precisely $tr(g^n)=T_n(X)$ with T_n the Chebichev's polynomials of the first kind. Therefore the spectrum of the invariant polynomial affine algebra is just $\mathbf{C}$ and the quotient morphism is the trace. Moreover $tr^{-1}(2x), x \neq \pm 1$ is exactly an orbit of a strictly regular element. $\mathrm{tr}^{-1}(\pm 2)$ contain several orbits but only the orbit of the identity matrix is closed. One can therefore think of $\mathrm{SL}(2,\mathbf{C})//\mathrm{Ad}(\mathrm{SL}(2,\mathbf{C}))$ as the geometric quotient of $G_1 \cup \pm Id$. The G-invariant measure (Weyl measure) induced by the $\mathrm{SL}(2,\mathbf{C})$ Haar measure is given by

$$\mu(f)=\int_{\mathbf{C}} |X^2-1| f(X) dX, \tag{6.1}$$

where the integration region is over the complex plane minus the interval $[-1,+1]$ with the usual Lebesgue measure on $\mathbf{C}$.

More explicitly, $\mathrm{SL}(2,\mathbf{C})$ has only one Cartan subgroup H which is the set of diagonal matrices $\mathrm{diag}(\lambda,\lambda^{-1})$, $\lambda \in \mathbf{C}$. The Weyl group is Z_2 and $\mathrm{diag}(\lambda,\lambda^{-1})$ is conjugate to $\mathrm{diag}(\lambda^{-1},\lambda)$. The Weyl integration formula reads:

$$\int_{\mathrm{SL}(2,\mathbf{C})} f(g) dg = \int_H dh \left[\int_{\mathrm{SL}(2,\mathbf{C})/H} f(xhx^{-1}) dx \right] |\Delta(h)|^2. \tag{6.2}$$

The invariant measure is obtained by removing the redundant integration over $\mathrm{SL}(2,\mathbf{C})/H$ and integration solely on H and one finds back the measure (6.1).

The unitary principal series of $\mathrm{SL}(2,\mathbf{C})$ is a family of unitary irreducible representations of $\mathrm{SL}(2,\mathbf{C})$ indexed by pairs (j,ρ) with $j \in \mathbf{Z}/2$ and $\rho \in \mathbf{R}$. There are realized in $L^2(\mathbf{C})$ and the action $R_{j,\rho}$ of $\mathrm{SL}(2,\mathbf{C})$ is given by

$$R_{j,\rho}\begin{pmatrix} a & b \\ c & d \end{pmatrix} f(z) = |bz+d|^{-2-2i\rho} \left(\frac{bz+d}{|bz+d|} \right)^{2j} f\left(\frac{az+c}{bz+d} \right) \tag{6.3}$$

for $z \in \mathbf{C}$ and $f \in L^2(\mathbf{C})$. The characters are

$$\chi_{j,\rho}\begin{pmatrix} e^{x+i\theta} & 0 \\ 0 & e^{-x-i\theta} \end{pmatrix} = \frac{e^{i\rho x}e^{ij\theta}+e^{-i\rho x}e^{-ij\theta}}{|e^{x+i\theta}-e^{-x-i\theta}|^2}. \tag{6.4}$$

Using the measure (6.1) on $X=(e^{x+i\theta}+e^{-x-i\theta})/2$ and making a change of variables to x,θ, it is straightforward to check that

$$\mu(\chi_{j_1,\rho_1}\chi_{j_2,\rho_2})=\delta_{j_1 j_2}\delta(\rho_1-\rho_2) \tag{6.5}$$

so that the above characters form an orthonormal basis of the Hilbert space $L^2(A_1)=L^2(\mathrm{SL}(2,\mathbf{C})//Ad(\mathrm{SL}(2,\mathbf{C})))$.

B. SU(2)

In the case of SU(2), there is again a unique Cartan subgroup H, composed of the diagonal matrices $h_\theta=\mathrm{diag}(e^{i\theta},e^{-i\theta}),\theta\in[-\pi,\pi]$. The Weyl group is Z_2: h_θ and $h_{-\theta}$ are conjugate. The SU(2)-invariant measure is

$$\mu_{\mathrm{SU}(2)}(f)=\frac{2}{\pi}\int_{-1}^{+1}dX\sqrt{1-X^2}f(X)=\frac{2}{\pi}\int_0^{\pi}d\theta\sin^2\theta f(\theta), \tag{6.6}$$

where $X=1/2\,\mathrm{tr}(g)=\cos\theta$.

An orthonormal basis of $L^2(\mathrm{SU}(2)/\mathrm{Ad}(\mathrm{SU}(2)))$ is given by the characters of the irreducible (finite dimensional) representation of SU(2):

$$\chi_j(h_\theta)=\frac{\sin(j+1)\theta}{\sin(\theta)}, \tag{6.7}$$

where j runs over the non-negative integers (twice the spin). For making a change of variable from X to θ, it is easy to check that

$$\mu_{\mathrm{SU}(2)}(\chi_j\chi_k)=\delta_{jk}. \tag{6.8}$$

C. SL(2,R)

In the case of $\mathrm{SL}(2,\mathbf{R})$, we have two Cartans subgroups; a compact one, which corresponds to space rotations

$$H_0=\left\{k_\theta=\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix},\quad 0\leqslant\theta\leqslant 2\pi\right\} \tag{6.9}$$

and a noncompact one, which corresponds to boosts

$$H_1=\pm\left\{a_t=\begin{pmatrix}e^t & 0\\ 0 & e^{-t}\end{pmatrix},t\in R\right\}. \tag{6.10}$$

$W(H_0)$ is trivial but $W(H_1)=Z_2$ and a_t is conjugate to a_{-t}. A regular element of $\mathrm{SL}(2,\mathbf{R})$ can be conjugated to H_0 or to H_1 and an $\mathrm{Ad}(\mathrm{SL}(2,\mathbf{R}))$ invariant function f will be described by its action on both Cartan subgroups, i.e., by two functions $f_0(\theta)$ and $f_1^{\pm}(t),t\geqslant 0$.

We would like to divide by the volume of G/H_0 and of G/H_1. These two volumes are infinite and the ratio of these two volumes is also infinite. So this leads to an ambiguity and we are left with a one-parameter family (up to normalization) of possible $\mathrm{Ad}(\mathrm{SL}(2,\mathbf{R}))$ invariant measures

$$\mu_{\mathrm{SL}(2,\mathbf{R})}(f)=\alpha_0\int_0^{2\pi}d\theta\sin^2\theta f_0(\theta)+\alpha_1\int_0^{+\infty}dt\sinh^2 t f_1^{\pm}(t). \tag{6.11}$$

The formal property that we want our measure to satisfy is

$$\mu({}^G f)=\int_G dg\, f(g), \tag{6.12}$$

where ${}^{G}f$ denotes the averaging over the gauge group G of a compact supported noninvariant function f. The subtle point is that the centralizer of a generic group element under the adjoint action is (conjugated to) either H_0 or H_1 depending on the group element. So the averaging should take this into account. Therefore if f_0 (respectively, f_1) is supported on the space $G_{(0)}$ (respectively, $G_{(1)}$) of group elements which can be conjugated to H_0 (respectively, H_1), we define

$$ {}^{G}f_i(g=xh_ix^{-1})=\int_{G/H_i} dx_i\, f(x_ih_ix_i^{-1}). \tag{6.13}$$

In this case, we easily prove using (3.8) that (6.12) is satisfied for the unique choice $\alpha_i=1$.

However, this is not the whole story. The natural way to get an invariant measure is to choose a cutoff λ and G_λ a compact subset of G, with $G_\lambda\to G$ when λ grows to infinity. Then we take the invariant measure to be the limit

$$ \mu(f)=\lim_{\lambda\to\infty}\frac{\int_{G_\lambda} f(g)dg}{\int_{G_\lambda} dg}, \tag{6.14}$$

for a G invariant function f. The resulting measure that it leads to is $(\alpha_0=1,\alpha_1=0)$. And this measure gives a zero weight to function with support on $G_{(1)}$.

The way to reconcile these points of view is the following. One needs to define two Hilbert spaces, one (denoted $\mathcal{H}_0$) for the functions with support on $G_{(0)}$ which is given by the measure $(\alpha_0=1,\alpha_1=0)$ and one (denoted $\mathcal{H}_1$) for the functions with support on $G_{(1)}$ which is given by the measure $(\alpha_0=0,\alpha_1=1)$. This would take into account the fact that the space of $\mathrm{Ad}(G)$ invariants is disconnected with incommensurable volume of centralizer. Physically, this means that the two sectors cannot communicate, i.e., we can not find physical operators mapping physical states between the two sectors. This was rigorously shown by Gomberoff and Marolf[25] in a similar context but in the language of group averaging and rigging maps.

$\mathrm{SL}(2,\mathbf{R})$ has three series of principal unitary representations: the continuous series $\mathcal{C}_s$ labeled by a positive real number s and two discrete series $\mathcal{D}_n^{\pm}$ both labeled by a integer $n\geqslant 1$ and a sign. The characters of the continuous series are

$$ \chi_s(k_\theta)=0, \tag{6.15}$$

$$ \chi_s(\pm a_t)=\frac{\cos st}{|\sinh t|} \tag{6.16}$$

and the characters of the discrete series $\mathcal{D}_n^{\pm}$ are

$$ \chi_n^{\pm}(k_\theta)=\mp\frac{e^{\pm i(n-1)\theta}}{2i\sin\theta}, \tag{6.17}$$

$$ \chi_n^{\pm}(a_t)=\frac{e^{-(n-1)|t|}}{2|\sinh t|}\ \text{with a factor}\ (-1)^n\ \text{for}\ -a_t. \tag{6.18}$$

It is clear that the characters of the discrete series (respectively, continuous series) are orthonormal with respect to the Hilbert space structure $\mathcal{H}_0$ (respectively, $\mathcal{H}_1$). Moreover both characters are eigenvalues of the Laplacian. More explicitly, the Laplacian reads

$$ \Delta=\frac{1}{\sin\theta}\frac{\partial^2}{\partial\theta^2}\sin\theta+\frac{1}{4}\ \text{on}\ H_0,\quad \Delta=-\frac{1}{\sinh t}\frac{\partial^2}{\partial t^2}\sinh t+\frac{1}{4}\ \text{on}\ H_1\ \text{for}\ t\geqslant 0 \tag{6.19}$$

so that the eigenvalue of χ_s is $s^2+1/4$ and the one corresponding to $\chi_n^{\pm}$ is $m(1-m)$ with $m=n-1/2$. Moreover, one could notice that, for a generic measure (6.11) with arbitrary (α_0,α_1),

the discrete characters $\chi_n^{\pm}$ are not orthonormal, which would be in contradiction with the fact that the Laplacian is Hermitian, unless we restrict ourself to the choice $\mathcal{H}_0$, i.e., $(\alpha_0=1,\alpha_1=0)$ which appear to be the only self-consistent choice of measure when taking into account the discrete series.

The characters of the continuous series are fully characterized as distributions which are eigenvectors of the Laplacian, invariant under the Weyl group (residual gauge symmetry) and with full support only on $G_{(1)}$. However, this is not the case for the discrete series. There are several distributions which are both eigenvector of the Laplacian and invariant with support in $G_{(0)}$. The solution of this puzzle lies in the definition of the Laplacian and more particularly in the space of functions on which it is defined. Indeed, among all the invariant distributions, one should choose the ones which are not only a distribution on $G_{(0)}\amalg G_{(1)}$ but on the full group G: one asks $\chi_n^{\pm}$ to be an eigenvalue of the Laplacian as a distribution on G. More precisely, in order to satisfy the eigenvalue equation $\int_G \chi(g)\Delta f(g)dg=\lambda\int_G \chi(g)f(g)dg$, one needs to integrate by parts. If f is a compact supported function on $G_{(0)}\amalg G_{(1)}$, all the boundary terms vanishes trivially. However, if f is a compact supported function on G, the vanishing of the boundary terms leads to some boundary conditions on χ. The eigen-distributions that can be extended to distributions on G are called regular. Now it is easy to check that such distributions (normalizable with respect to the scalar product on $\mathcal{H}_0$) are in one-to-one correspondence with unitary representations. This was first shown by Harish–Chandra and was the foundation of his works on harmonic analysis on the noncompact group.[26]

To sum up, the issue is about the domain of definition of the Laplacian Δ. We make it act on the Hilbert spaces $\mathcal{H}_0$ and $\mathcal{H}_1$ for consistency of the group averaging, but the eigenvalue problems is well defined for distributions on the whole group G (taking into account the null elements, which are not regular). Nevertheless, we can conclude that the discrete characters χ_n restricted to $G_{(0)}$ form a basis of $\mathcal{H}_0$ and the continuous characters χ_s form a basis of $\mathcal{H}_1$. And the tail of χ_n on $G_{(1)}$ is due to nontrivial boundary conditions in the eigenvalue problem.

The case of one petal graph is quite complicated, this is essentially due to the fact that the space A_1 is not connected, since we have excluded all null rotations and that taking them into account is not straightforward. Fortunately, as we shall now see, the situation for higher loop graphs is simpler since the generic centralizer of a point of G^h is G for all elements.

VII. THE TWO PETAL FLOWER: EXAMPLES

A. SL(2,C)

In this section, we consider the case where the group is $\mathrm{SL}(2,\mathbf{C})$ and we are interested in describing the quotient $(\mathrm{SL}(2,\mathbf{C}))^2//\mathrm{Ad}(\mathrm{SL}(2,\mathbf{C}))$ as defined in Sec. III B. Let $(g_1,g_2)\in\mathrm{SL}(2,\mathbf{C})^2$ and denote $X_1(g_1,g_2)=(1/2)tr(g_1)$, $X_2(g_1,g_2)=(1/2)tr(g_2)$, and $X_3(g_1,g_2^{-1})=(1/2)\mathrm{tr}(g_1g_2)$. This defines an $\mathrm{Ad}(\mathrm{SL}(2,\mathbf{C}))$-invariant morphism $\pi:\mathrm{SL}(2,\mathbf{C})^2\to\mathbf{C}^3$. We have the following property.

Proposition 6: π gives an isomorphism between the algebra of invariant polynomials $\mathbf{C}[\mathrm{SL}(2,\mathbf{C})^2]^{\mathrm{SL}(2,\mathbf{C})}$ and $\mathbf{C}[X_1,X_2,X_3]$.

Proof: Let

$$G_2(\mathrm{SL}(2,\mathbf{C}))=\{(g_1,g_2)\in\mathrm{SL}(2,\mathbf{C})\,|\,tr(g_1)^2\neq 4 \text{ or } tr(g_2)^2\neq 4, \text{ and } tr([g_1,g_2]_G)\neq 2\}.$$

The image of this set by π is the complement in $\mathbf{C}^3$ of Δ, where Δ is the closed subset of $\mathbf{C}^3$ such that the polynomials X_1^2-1 or X_2^2-1, and $\Theta(X_1,X_2,X_3)\equiv(X_3-X_1X_2)^2-(X_1^2-1)(X_2^2-1)$ are equal to zero ($[,]_G$ denotes the group commutator). This is clear since $tr([g_1,g_2]_G)-2=-\det(g_1g_2-g_2g_1)=4\Theta(X_1,X_2,X_3)$. The key point is that this gives an isomorphism between $G_2(\mathrm{SL}(2,\mathbf{C}))/\mathrm{SL}(2,\mathbf{C})$ and $\mathbf{C}^3\backslash\Delta$. We can construct explicitly the inverse map, Let $s(\vec{X})=(s_1,s_2)$ be defined by

$$s_1(\vec{X})=\begin{pmatrix} X_1+\sqrt{X_1^2-1} & 0 \\ 0 & X_1-\sqrt{X_1^2-1}\end{pmatrix}, \tag{7.1}$$

$$s_2(\vec{X})=\begin{pmatrix} X_2-\dfrac{X_1X_2-X_3}{\sqrt{X_1^2-1}} & 1 \\ -\dfrac{\Theta(\vec{X})}{X_1^2-1} & X_2+\dfrac{X_1X_2-X_3}{\sqrt{X_1^2-1}}\end{pmatrix}. \tag{7.2}$$

One should be careful since s needs the definition of a square root, this means that this is a multivalued function on $\mathbf{C}^3\backslash\Delta$, however any change in the choice of the square root determination is implemented by a gauge transformation, therefore s is well defined as a function valued into $G_2(\mathrm{SL}(2,\mathbf{C}))/\mathrm{SL}(2,\mathbf{C})$. Suppose we define $\tilde{s}(\vec{X})$ the map corresponding to another determination of the square root, i.e., the one obtained from s by replacing $\sqrt{X_1^2-1}\to-\sqrt{X_1^2-1}$ we have that

$$\tilde{s}(\vec{X})=\mathrm{Ad}\begin{pmatrix} 0 & i \\ i & 0\end{pmatrix}\cdot s(\vec{X}). \tag{7.3}$$

It is easy to see that $\pi\circ s$ is the identity mapping on $\mathbf{C}^3\backslash\Delta$. It is also true that $s\circ\pi$ is the identity mapping on $G_2(\mathrm{SL}(2,\mathbf{C}))/\mathrm{SL}(2,\mathbf{C})$. First, given $(g_1,g_2)\in G_2(\mathrm{SL}(2,\mathbf{C}))$ we can diagonalize g_1 since it is regular. This does not fix completely the action of the gauge group since one can still act by a diagonal gauge transformation and a Weyl transformation (i.e., $g_1\to g_1^{-1}$). Any diagonal transformation $\mathrm{diag}(\lambda,\lambda^{-1})$ is acting on $g_2=\left(\begin{smallmatrix} a & b \\ c & d\end{smallmatrix}\right)\to\left(\begin{smallmatrix} a & \lambda^2 b \\ \lambda^{-2}c & d\end{smallmatrix}\right)$. Now, $tr(g_1g_2g_1^{-1}g_2^{-1})-2=-(\lambda-\lambda^{-1})^2bc$. The condition $\Theta\neq0$ translates into $bc\neq0$, so that one can fix the residual action by asking $b=1$.

Proposition 7: The invariant measure μ defined in definition (1) is simply the Lebesgue measure in $\mathbf{C}^3$ when translated in terms of X_1, X_2, X_3. More precisely, let F be a function on $\mathbf{C}^3$, π^*F is an invariant function and

$$\int_{(\mathrm{SL}(2,\mathbf{C}))^2//\mathrm{SL}(2,\mathbf{C})}\pi^*F(g_1,g_2)d\mu(g_1,g_2)=\int_{\mathbf{C}^3}F(\vec{X})d^2X_1\,d^2X_2\,d^2X_3. \tag{7.4}$$

Proof: Let us recall that the Haar measure for $\mathrm{SL}(2,\mathbf{C})$ is defined as $dg=d^2a\,d^2b\,d^2c\,d^2d\,\delta^2(ad-bc-1)$ if $g=\left(\begin{smallmatrix} a & b \\ c & d\end{smallmatrix}\right)$. Let

$$y=\begin{pmatrix} a & 1 \\ c & d\end{pmatrix},\quad h=\begin{pmatrix} \lambda & 0 \\ 0 & \lambda^{-1}\end{pmatrix},\quad g=yhy^{-1}. \tag{7.5}$$

The measure on A_2 is defined by $d\mu=dg$ it is easy to see that

$$dg=|\lambda-\lambda^{-1}|^2d^2(\lambda+\lambda^{-1})d^2a\,d^2d. \tag{7.6}$$

Moreover $X_1=\lambda+\lambda^{-1}$, $X_2=a+d$, and $X_3=\lambda a+\lambda^{-1}d$ thus $dg=d^2X_1\,d^2X_2\,d^2X_3$.

Let us define the invariant functionals

$$\Phi^{\vec{\jmath},\vec{\rho}}(g_1,g_2)=\chi_{j_1,\rho_1}(g_1)\chi_{j_2,\rho_2}(g_2)\chi_{j_3,\rho_3}(g_1g_2). \tag{7.7}$$

An explicit computation gives

$$\int\Phi^{\vec{\jmath},\vec{\rho}}\,d\mu(g_1,g_2)=\prod_{i=1}^{3}\delta(\rho_i)\,\delta_{j_i}. \tag{7.8}$$

B. SU(2)

We can deduce the SU(2) case from the previous formalism. We have the constraint $\vec{X}(g_1,g_2)\in I_3$ where

$$I_3\equiv\{X_i\in]-1,1[,\Theta(\vec{X})=(X_3-X_1X_2)^2-(X_1^2-1)(X_2^2-1)<0\} \tag{7.9}$$

and the invariant measure is

$$\int_{I_3} d\vec{X}. \tag{7.10}$$

Writing $X=\cos\theta$, we can re-express the above constraint in term of $\theta_{1,2,3}\in[0,\pi]$:

$$\cos(\theta_1+\theta_2)\leqslant\cos\theta_3\leqslant\cos(\theta_1-\theta_2) \tag{7.11}$$

which is simply the constraint arising when multiplying two elements of SU(2) or equivalently summing two vectors in a spherical space. Indeed two group elements g_1,g_2 in $\mathrm{SU}(2)\sim S^3$ determine a triangle in S^3 with vertices $1,g_1,g_2$. The invariant geometry of this triangle is determined by the three edges length which are θ_1, θ_2, θ_3. In these variables, the measure is $\sin\theta_1\sin\theta_2\sin\theta_3\,d\theta_1\,d\theta_2\,d\theta_3$ and the domain of integration is

$$\theta_1+\theta_2\leqslant\theta_3 \quad \text{and cyclic perm}, \tag{7.12}$$

$$\theta_1+\theta_2+\theta_3\leqslant 2\pi. \tag{7.13}$$

One can also express the invariant geometry of the triangle in terms of two edges: their lengths θ_1, θ_2 and the angle $\tilde{\theta}_3$ they form. This angle is determined by the edges lengths by $\cos\theta_3=\cos\theta_1\cos\theta_2-\sin\theta_1\sin\theta_2\cos\tilde{\theta}_3$. In these geometric variables, the condition on the variables reads $\Theta=-\sin^2\theta_1\sin^2\theta_2\sin^2\tilde{\theta}_3\neq 0$ which means that we exclude degenerate triangles. In these new variables, the measure is $\sin^2\theta_1\sin^2\theta_2\,d\theta_1\,d\theta_2\sin\tilde{\theta}_3\,d\tilde{\theta}_3$. Now one can easily check that

$$\int_{I_3}\chi_{j_1}(X_1)\chi_{j_2}(X_2)\chi_{j_3}(X_3)d\vec{X}=\delta_{j_1,j_2}\delta_{j_2,j_3}\frac{1}{d_{j_3}} \tag{7.14}$$

as expected.

Let us note that one gets the measure (7.10) directly by a gauge fixing procedure without having to appeal to the general theorem 1. Let $g_i=\left(\begin{smallmatrix}a_i & b_i\\ -\bar{b}_i & \bar{a}_i\end{smallmatrix}\right)$, $i=1,2$. The gauge conditions we want to impose are $b_1(g_1)=0$ and $\mathrm{Im}(b_2)(g_2)=0$, Im denotes the imaginary part. The Faddeev–Popov determinant is the determinant of the 3×3 matrix $(\mathrm{Re}(b_1)([X_i,g_1]);\mathrm{Im}(b_1)([X_i,g_1]);\mathrm{Im}(b_2)([X_i,g_2]))$, where X_i, $i=1,\ldots,3$ is a basis of su(2). This determinant is proportional to $(a_1-(a_1)^{-1})^2 b_2$, it should multiply the gauge fixed measure $dg_1\,dg_2\,\delta^2(b_1)\delta(\mathrm{Im}(b_2))$, a direct computation leads to the results (7.10).

C. SL(2,R)

In the case of $\mathrm{SL}(2,\mathbf{R})$, the constraint reads $\vec{X}(g_1,g_2)\in J_3$ where

$$J_3\equiv\{X_i\in\mathbf{R},\,\Theta(\vec{X})\neq 0,(X_1^2\neq 1 \ \text{ or } \ X_2^2\neq 1)\} \ \text{ and } \ \{\vec{X}\neq I_3\}. \tag{7.15}$$

The invariant measure is given by

$$\int_{J_3} d\vec{X}. \tag{7.16}$$

This result can be obtain using both previous methods, gauge fixing or application of the general formulas in the context of SL(2,**R**). It is interesting to note that J_3 correspond to a real section of $\mathbf{C}^3$ which is complementary to I_3 describing SU(2). As in the case of SU(2), one can give a geometrical interpretation of the configuration space J_3 and the nondegeneracy condition. This will lead to a nice understanding of the singularity properties.

It is well known that SL(2,**R**) is isomorphic to $\mathrm{Ad}\,S_3$, the anti-de-Sitter space in three dimensions, which can be described as an hyperboloid in flat four dimension space, $\mathrm{Ad}\,S_3=\{-(X_0)^2+(X_1)^2+(X_2)^2-(X_3)^2=-1\}$, the isomorphism being

$$g(X)=\begin{pmatrix} X_0+X_1 & X_2+X_3 \\ X_2-X_3 & X_0-X_1 \end{pmatrix}. \tag{7.17}$$

$\mathrm{Ad}\,S_3$ is a Lorentzian space and SO(2,2) is its isometry group. Then the space of couples of group elements (g_1,g_2) corresponds to the space of geodesic triangles in $\mathrm{Ad}\,S_3$ with one vertex fixed to be the identity. The adjoint action of SL(2,**R**) on (g_1,g_2) translates into the action of the subgroup of SO(2,2) which fixes the identity, hence into the action of the Lorentz group SO(2,1) which rotates the triangles. So the space of orbits is the space which describes the intrinsic geometry of anti-de-Sitter triangles. Such triangles can be of four types: they can be spacelike, timelike, null or degenerate (meaning that the three vertices of the triangle belong to the same geodesic), depending on whether they lay in a spacelike, timelike or null plane. The edges of the triangles can also be of four types: they can be timelike, spacelike, null or degenerate (meaning that the two vertices of the edge coincide). Unlike the SU(2) case, the invariant geometry cannot be fully characterized by the edge lengths since the length (more precisely the square length) is zero for both a null edge and a degenerate edge. However, the following proposition 8 shows that if we restrict the space of triangles to triangles which satisfy the condition $\Theta\neq 0$ then the geometry of the triangle is uniquely determined by the lengths of its edges. The geometrical meaning of this condition is the following:

Proposition 8: The condition $\Theta(g_1,g_2)=0$ *is equivalent to the condition that the AdS triangle* $(1,g_1,g_2)$ *is either null or degenerate. Moreover* $\Theta(g_1,g_2)<0$ *[respectively* $\Theta(g_1,g_2)>0$*] iff the Ad S triangle* $(1,g_1,g_2)$ *is spacelike (respectively timelike).*

In order to prove this proposition, we need to do some $\mathrm{Ad}\,S$ geometry. It is convenient to consider $\mathrm{Ad}\,S$ space as embedded in the projective space $\mathbf{R}^+P^3$, which is the space of half lines in $\mathbf{R}^4$: $\mathrm{Ad}\,S_3=\{(X_0:X_1:X_2:X_3)\in\mathbf{R}^+P^3|-(X_0)^2+(X_1)^2+(X_2)^2-(X_3)^2<0\}$. The advantages of such a representation of the $\mathrm{Ad}\,S$ space is to simplify the geodesic geometry of $\mathrm{Ad}\,S$. First the geodesics of $\mathrm{Ad}\,S$ are the straight lines of $\mathbf{R}^+P^3$. Moreover the geodesic planes of $\mathrm{Ad}\,S_3$ are the intersection of $\mathbf{R}^+P^3$ planes with $\mathrm{Ad}\,S$, they are therefore given by linear equations $P_{(Y_0:Y_1:Y_2:Y_3)}=\{(X_0:X_1:X_2:X_3)\in\mathbf{R}^+P^3|X_iY^j=0\}$ [the indices are raised using a Lorentzian $(-,+,+,-)$ metric]. Thus the geodesic hyperplanes of $\mathrm{Ad}\,S$ are in one to one correspondence with points of R^+P^3. Geometrically this means that all the geodesics orthogonal to a given plane meet in one point. If the plane P_Y is spacelike then $Y\cdot Y<0$ and the refocusing point is in $\mathrm{Ad}\,S$. This corresponds to the attractive nature of negative cosmological constant where all timelike geodesics refocus in a finite proper time. If the plane P_Y is timelike then $Y\cdot Y>0$. And if the plane P_Y is null then $Y\cdot Y=0$. Moreover, in this latter case, P_Y is tangent to the quadric $Y\cdot Y=0$.

Next, we identify $\mathbf{R}^+P^3$ with the space of 2×2 matrices modulo multiplication by a positive scalar using $Y\in\mathbf{R}^+P^3\rightarrow g(Y)$ as in (7.17). Now let us consider the triangle $(1,g_1,g_2)$ and suppose that it is nondegenerate, i.e., $[g_1,g_2]=g_1g_2-g_2g_1\neq 0$. Let us denote by $Y(g_1,g_2)$ the $\mathbf{R}^+P^3$ element satisfying $g(Y(g_1,g_2))=[g_1,g_2]$. It is clear that $P_{Y(g_1,g_2)}$ is the plane of the triangle $(1,g_1,g_2)$ since $tr([g_1,g_2]g)=0$ if $g=1,g_1$ or g_2. Then a straightforward computation shows that

$$Y(g_1,g_2)\cdot Y(g_1,g_2)\equiv\det([g_1,g_2])=8\Theta(g_1,g_2), \tag{7.18}$$

and leads to the conclusion of the proposition 8.

This proposition tells us that the space J_3 is the space of nondegenerate and non-null triangles. This space is disconnected, and has two disconnected regions depending on whether the normal to the triangle is timelike or spacelike. There is no natural distinction between past and future in $\mathrm{Ad}\,S_3$ since it is periodic in time and a timelike geodesic will come back to the initial normal surface. Therefore we can define two Hilbert space structures, one for the functions with support on spacelike triangles and one for the functions with support on timelike triangles, with the scalar product defined by the measure (7.16). The situation is however drastically different from the one loop case where the invariant space was also disconnected but in that case the centralizer group was drastically different in both regions. In the present two petals case, we see that the centralizer, i.e., the group which fixes a given triangle, is trivial in both sectors. This means that there is no superselection rule avoiding to construct invariant operators mapping one sector to another. Indeed one realizes that, even when we extend the space J_3 to the space $\tilde{J}_3$ of all nondegenerate triangles (allowing null cases), the centralizer of any triangle of $\tilde{J}_3$ is still trivial. Therefore we can extend the definition of the measure to $\tilde{J}_3$ which is connected and there exists one unique invariant measure on this space. In other words, we see that if $\phi(g_1,g_2)$ is a function with compact support on $\tilde{J}_3$ then ${}^G\phi(g_1,g_2)=\int \phi(gg_1g^{-1},gg_2g^{-1})dg$ is well defined for all $(g_1,g_2)\in\tilde{J}_3$. This means that the invariant distributions on J_3 obtained by group averaging can be extended to invariant distributions on $\tilde{J}_3$. We expect the spin network functionals to be of this type and therefore the Hilbert space structure to be uniquely fixed in that case.

VIII. THE HILBERT SPACE OF SPIN NETWORKS

A. The compact group case: The Ashtekar–Lewandowski construction

The Ashtekar–Lewandowski approach consists in the use projective techniques in the *compact* group case to define the space of generalized connections, a space of continuous functions upon it (cylindrical functions) and a measure called the Ashtekar–Lewandowski (AL) measure[20] which endow this space with a Natural and difeomorphism invariant Hilbert space structure. For a recent and complete review of this approach, one can look at Ref. 9.

First, we define a space of gauge invariant ''connections'' for each graph Γ, embedded in a spacelike manifold.

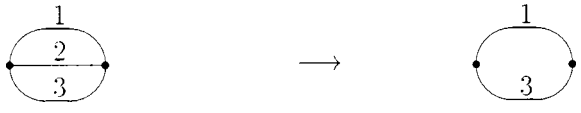
$$A_\Gamma=G^{\otimes E}/G^{\otimes V}=\{[(g_{e_1},\ldots,g_{e_E})]_{G^{\otimes V}}\}=\{\{(k^{-1}_{s(e_i)}g_{e_i}k_{t(e_i)},\ i=1,\ldots,E),k_v\in G\}\}. \tag{8.1}$$

We define a partial order $\prec$ over the set of graphs: $\Gamma_1\prec\Gamma_2$ iff Γ_1 can be obtained from Γ_2 by removing edges and bivalent vertices. We then define projections $p_{\Gamma_2\Gamma_1}:A_{\Gamma_2}\to A_{\Gamma_1}$ for $\Gamma_1\prec\Gamma_2$, by removing the extra edges and contracting the extra bivalents vertices:

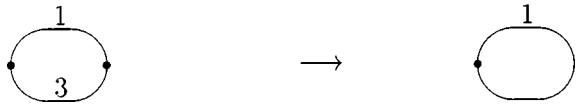
$$\begin{gathered}\text{removing the edge } i \quad (g_1,\ldots,g_i,\ldots,g_E)\to(g_1,\ldots,g_{i-1},g_{i+1},\ldots,g_E)\\ \text{bivalent vertex between 1 and 2} \quad (g_1,g_2,\ldots,g_E)\to(g_1g_2^{\epsilon},\ldots,g_E)\end{gathered} \tag{8.2}$$

with $\epsilon=\pm1$ depending on the relative orientation on g_1 and g_2.

Let us illustrate these rules with the example of the reduction of the Θ graph to a single loop:



$$(g_1,g_2,g_3)\sim(h^{-1}g_1k,h^{-1}g_2k,h^{-1}g_3k)\to(g_1,g_3)\sim(h^{-1}g_1k,h^{-1}g_3k), \tag{8.3}$$



$$(g_1,g_3)\sim(h^{-1}g_1k,h^{-1}g_3k)\rightarrow G_1=g_1g_3^{-1}\sim h^{-1}G_1h.$$

Then, we can define the projective limit $\overline{A}$ as the set of families of elements of A_Γ consistent with the projections:

$$\overline{A}=\{(a_\Gamma)_{\Gamma\,\text{graph}}\in\times_\Gamma A_\Gamma/\forall\Gamma_{1,2},\Gamma_1\prec\Gamma_2\Rightarrow p_{\Gamma_2\Gamma_1}a_{\Gamma_2}=a_{\Gamma_1}\}. \tag{8.4}$$

In the case of a compact group G, the spaces A_Γ are topological, compact and Haussdorf and the projections are continuous, therefore $\overline{A}$ with the Tychonov topology (product topology) is compact and Haussdorf. We can now construct continuous function on $\overline{A}$. We start by defining the spaces:

$$C^0(A_\Gamma)=\{f\in\mathcal{F}(A_\Gamma,\mathbf{C}),f\ \ \text{continuous}\}. \tag{8.5}$$

The projections p induce some injections between the spaces of functions $C^0(A_{\Gamma_1})$ and $C^0(A_{\Gamma_2})$ for $\Gamma_1\prec\Gamma_2$:

$$i_{\Gamma_1\Gamma_2}:C^0(A_{\Gamma_1})\rightarrow C^0(A_{\Gamma_2}) \tag{8.6}$$

$$\phi(\{g_e\}_{e\in\Gamma_1})\rightarrow\tilde{\phi}(\{g_e\}_{e\in\Gamma_2})=\phi(p_{\Gamma_2\Gamma_1}\{g_e\}_{e\in\Gamma_2}). \tag{8.7}$$

We define the following equivalence relation:

$$f_{\Gamma_1}\in C^0(A_{\Gamma_1})\sim f_{\Gamma_2}\in C^0(A_{\Gamma_2})\Leftrightarrow\exists\Gamma_3\succ\Gamma_1,\Gamma_2,i_{\Gamma_1\Gamma_3}f_{\Gamma_1}=i_{\Gamma_2\Gamma_3}f_{\Gamma_2}\Leftrightarrow\forall\Gamma_3\succ\Gamma_1,\Gamma_2,i_{\Gamma_1\Gamma_3}f_{\Gamma_1}=i_{\Gamma_2\Gamma_3}f_{\Gamma_2}. \tag{8.8}$$

This allows us to define the space of cylindrical functions:

$$\text{Cyl}(\overline{A})=\bigcup_\Gamma C^0(A_\Gamma)/\sim \tag{8.9}$$

We divide by the previous equivalence relation in order to remove the redundancies due to the existence of the injections. On $\text{Cyl}(\overline{A})$, we can define a norm

$$\|[f_\Gamma]_\sim\|=\sup_{x_\Gamma\in A_\Gamma}|f_\Gamma(x_\Gamma)|. \tag{8.10}$$

Then the completed space is an abelian C^* algebra, to which we can apply the Gelfand–Naimark theorem. It states that it is the algebra of continuous functions on a certain compact Haussdorf space called the Gelfand spectrum of the C^* algebra. In Ref. 20, Ashtekar and Lewandowski prove that its Gelfand spectrum is simply $\overline{A}$ i.e., that we have the following isomorphism:

$$\text{Cyl}(\overline{A})\approx C^0(\overline{A}). \tag{8.11}$$

Choosing measures $d\mu^{(\Gamma)}$—the Haar measure—on the spaces of discrete connections A_Γ and checking that they are consistent with the injections

$$\forall\Gamma_1\prec\Gamma_2,i_{\Gamma_1\Gamma_2}\,d\mu^{(\Gamma_2)}=d\mu^{(\Gamma_1)} \tag{8.12}$$

we can define a measure $\overline{d\mu}$—the *Ashtekar–Lewandowski* measure—on $\overline{A}$ by considering their projective limit. And our final Hilbert space will be $\mathcal{H}_{\text{cyl}}=L^2(\overline{A},\overline{d\mu})$.

B. An alternative: the GNS construction

An elegant way of constructing the Hilbert space $\mathcal{H}_{\text{cyl}}$ is using the GNS (Gelfand–Naimark–Segal) construction.[24,27] One considers the algebra $\mathcal{A}$ of all cylindrical functions f_Γ (on all graphs Γ) with the normal multiplication law between functions. One defines the norm sup on this space as in the previous paragraph:

$$\|f_\Gamma\| = \sup_{A_\Gamma} |f_\Gamma|. \tag{8.13}$$

One can then complete $\mathcal{A}$ to a C^* algebra $\overline{\mathcal{A}}$. On $\overline{\mathcal{A}}$, we define a *state* ω—a positive linear form—which is simply the integration:

$$\omega(f_\Gamma) = \int_{A_\Gamma} d\mu^{(\Gamma)} f_\Gamma = \int_{SU(2)^E} dg_1 \ldots dg_E \, f_\Gamma(g_1, \ldots, g_E), \tag{8.14}$$

ω induced an inner product $\langle f_{\Gamma_1} | f_{\Gamma_2} \rangle = \omega(f^*_{\Gamma_1} f_{\Gamma_2})$ remembering that the product of the two cylindrical functions is a cylindrical function based on any graph bigger than both Γ_1 and Γ_2. We then define the Gelfand ideal

$$\mathcal{I} = \{a \in \overline{\mathcal{A}} | \, \omega(a^* a) = 0\}. \tag{8.15}$$

We get a positive definite scalar product on the space $\mathcal{H}_{\text{gns}} = \overline{\mathcal{A}}/\mathcal{I}$. And we get the physical Hilbert space by completing this space to $\overline{\mathcal{H}_{\text{gns}}}$. It is straightforward to check that the equivalence relation $\sim$ is the same as defined by $\mathcal{I}$ so that $\overline{\mathcal{H}_{\text{gns}}} = \mathcal{H}_{\text{cyl}}$.

Let us make this construction explicit using the spaces $\mathcal{H}_\Gamma = L^2(A_\Gamma, d\mu^{(\Gamma)}) = L^2(A_\Gamma, d\mu^E)$ = with $d\mu$ being the Haar measure on SU(2). $\mathcal{H}_\Gamma$ is the Hilbert space of spin networks based on the graph Γ. The usual basis is indeed the spin networks basis. These spin networks are labeled by irreducible representations j of SU(2) on each edge and intertwiners i for each vertex. Then, the function is defined by taking the group elements in the edge representations and contracting them using the intertwiners.

Let us give a decomposition of $\mathcal{H}_\Gamma$ on which it will be easy to implement the equivalence relation$\sim$. If an edge e of Γ is labeled by the representation $j=0$, then the corresponding spin network function will not depend on the group element g_e: it will be equal to the spin network defined on $\Gamma' = \Gamma \backslash \{e\}$ with the same labels. So we can decompose $\mathcal{H}_\Gamma$ into the direct sum of Hilbert spaces $\tilde{\mathcal{H}}_{\Gamma'}$, $\Gamma' \subset \Gamma$, of spin networks based on Γ' with no trivial representations $j=0$. Furthermore, if we consider an arbitrary graph Γ_1 (which is not the single loop with a single vertex) and a graph Γ_2 obtained by removing a bivalent vertex from Γ_1, the space $\tilde{\mathcal{H}}_{\Gamma_1}$ and $\tilde{\mathcal{H}}_{\Gamma_2}$ are isomorphic using the restriction of the injection $i_{\Gamma_2 \Gamma_1}$ to $\tilde{\mathcal{H}}_{\Gamma_2}$. This means that we can decompose $\mathcal{H}_\Gamma$ as the direct sum of spaces $\mathcal{H}'_\Gamma$ with $\Gamma' \subset \Gamma$ containing no bivalent vertex (including loops with no vertex at all). To sum up this, we define $\mathcal{G}$ the set of all graphs and $\tilde{\mathcal{G}}$ *the set of all graphs which don't contain bivalent vertices*. We have

$$\mathcal{H}_\Gamma = \bigoplus_{\Gamma' \in \tilde{\mathcal{G}}, \Gamma' \subset \Gamma} (i_{\Gamma' \Gamma}) \tilde{\mathcal{H}}_{\Gamma'}. \tag{8.16}$$

Using these new notations, we have $\mathcal{H}_{\text{gns}} = \oplus_{\Gamma \in \tilde{\mathcal{G}}} \tilde{\mathcal{H}}_\Gamma$ which implements in a practical way the nondirect sum $+_{\Gamma \in \tilde{\mathcal{G}}} \mathcal{H}_\Gamma \equiv \oplus_{\Gamma \in \mathcal{G}} \mathcal{H}_\Gamma / \sim$.

C. The noncompact group case

Let us now assume the group G is noncompact. The obstacle to applying the AL construction is the noncompactness of the A_Γ spaces. There is no problem defining the projections and injec-

tions. However, the space $\overline{A}$ is noncompact and therefore we cannot obtain it as Gelfand spectrum. Moreover, we cannot define a norm $\|f_\Gamma\|$ on the spaces of continuous functions $C^0(A_\Gamma)$ so that $Cyl(\overline{A})$ does not have any norm and cannot be completed into a C^* algebra. And finally, the family of measures $d\mu^{(\Gamma)}$ is not consistent with the partial order on the set of graphs. To save some results of the AL approach, one could try to compactify the spaces A_Γ or to impose some cutoff on the group. Nevertheless, this makes it hard to deal with the gauge invariance. One could also change the definition of $C^0(A_\Gamma)$ by taking the bounded continuous functions in order to define a norm on these spaces. Nevertheless, it is not clear what would be its Gelfand spectrum.

One promising approach would be to use the fact that A_Γ is an algebraic space. It can therefore be recovered not as a Gelfand spectrum but as an algebraic spectrum of the affine algebra $P(A_\Gamma)$ of polynomial function. The problem is that the union of all such affine algebras modulo $\sim$ in no longer finitely generated so the usual theorems of algebraic geometry cannot be applied and it is not clear if one can define an algebraic dual of that space. But we still think that this road is worth pursuing.

Here, we choose to concentrate on defining a Hilbert space—the Hilbert space of spin networks—and we do not tackle the problem of constructing it as a L^2 space. Our construction will be based on the results obtained from the GNS approach; in particular, we will not need the projections/injections structure. The drawback of this approach is that we do not construct the space of generalized connections $\overline{A}$. So we cannot interpret our Hilbert space as a L^2 space: we lose some aspects of the ''wave function'' interpretation. But for all practical purposes the Hilbert space structure is all of what we need.

So, what is the structure we are left with? In the noncompact group case the trivial representation $j=0$ is not a L^2 representation. Any function not depending on a group element is clearly not normalizable. In other words the trivial representation does not appear in the decomposition of $L^2(A_\Gamma)$. This mean that we have built directly the spaces $\tilde{\mathcal{H}}$ defined in the previous paragraph. And we build the configuration space as a direct sum of these spaces:

$$\mathcal{H}_{\text{config}}=\bigoplus_{\Gamma\in\tilde{\mathcal{G}}}\tilde{\mathcal{H}}_\Gamma\,. \tag{8.17}$$

There is a possible normalization ambiguity in the above summation. *A priori*, we are free to normalize the different $\tilde{\mathcal{H}}_\Gamma$ spaces as we wish. This relative normalization of the Hilbert spaces can be traced down to an ambiguity in the definition of the Haar measure used to define the measure $d\mu^{(\Gamma)}$ of each Hilbert space. In the compact case, we fix these measures to be probability measures[7] and we normalize the Haar measure such that the group gets a unit volume. This makes the measures consistent with the projection structure of the Ashtekar–Lewandowski construction. In the noncompact group case, it is impossible to define such a normalization. However, looking at the way the Haar measure comes into the definition of (3) the measures over different graphs, it is natural to require that the Haar measure be normalized the same way for all measures. More precisely, if we take an integrable function over $G^{(n+1)}/\mathrm{Ad}(G)$, we can integrate out one of its variable using the Haar measure, and we would get an integrable function over $G^n/\mathrm{Ad}(G)$. Then, it is natural to require that the integrals of the two functions be equal.

This argument fixes the Haar measure up to a constant. And if we rescale the Haar measure by a factor α, then the measures $d\mu_n$ are to be scaled by $\alpha^{(n-1)}$. And we can think of the normalization of the Haar measure as the choice of a scale in our physical theory.

Now the space $\mathcal{H}_{\text{config}}$ defined in (8.17) does not seem to be a L^2 space. Nevertheless, it carries some Fock space structure. In that frame, the projection/injection structure of the AL approach would be replaced by creation and annihilation operators. These would act like isometries between the different Hilbert spaces $\tilde{\mathcal{H}}_\Gamma=L^2(G^E/G^V)=L^2(G^{h_\Gamma}/\mathrm{Ad}(G))$ and could fix the normalization ambiguity. More precisely, let's consider an infinite graph Γ_∞, i.e., a sequence of graphs $(\Gamma_i)_{i\in N}, \Gamma_i\in\tilde{\mathcal{G}}$ such that $\Gamma_i<\Gamma_{i+1}$ and the inclusion is strict. Then the space

$$\mathcal{F}_{\Gamma_\infty} = \bigoplus_i \tilde{\mathcal{H}}_{\Gamma_i}, \tag{8.18}$$

looks like a Fock space where the addition of a loop would be a creation operator.

The difficulty of endowing $\mathcal{F}_{\Gamma_\infty}$ of a Fock space structure comes from the residual Ad(G) noncompact gauge symmetry. There exists a natural gauge fixing through the possibility of erasing this remaining symmetry by considering cylindrical functions which are gauge invariant but at a single vertex of the graph. Indeed, following the gauge fixing procedure described in Sec. II based at the point A, the space of such graph connections is simply $G^{\otimes h_\Gamma}$ and the corresponding Hilbert space of states is $L^2(G^{\otimes h_\Gamma}, dg^{\otimes h_\Gamma})$. It is then possible to pile these spaces into a Fock space of states $\mathcal{F}$ by carefully summing over graphs. The connection states can be seen as a set of loops whose base point is A (flower around the vertex A). The creation and annihilation operators acting as usually to go from $L^2(G^N)$ to $L^2(G^{N\pm 1})$ then create or destroy a loop from A. Thus, from this point of view, $\mathcal{F}$ represents the fluctuations of the connection around the point A. Then, what about the gauge invariance at the point A? Imposing it directly on $\mathcal{F}$ leads to divergence problems. Nevertheless, instead of imposing gauge invariance, we could place ourself at the point A and ignore the gauge invariance but instead impose that the considered states transform nicely under G and belong to a given representation of the group G. However this means introducing by hand in the theory an observer at the point A, represented by the chosen representation. And in the present work, we prefer to tackle the issue of considering fully gauge invariant functionals and study the sum of the spaces $L^2(G^{\otimes h_\Gamma}/\mathrm{Ad}(G))$.

D. Towards a Fock space for the space of connections

We are interested by gluing together $L^2(G^n/\mathrm{Ad}(G))$ spaces. An useful analogy is interpreting these spaces as state spaces of particles living on the group G.[28] Indeed, $L^2(G^n,(dg)^n)$—dg is the Haar measure on G—is the space corresponding to a free particle living on the group G^n or equivalently n free particles living on the group G. Its action evaluated on a function $g(t)$:$\mathbf{R} \to G^n$ is

$$S_{\text{free}} = \frac{1}{2}\int dt\, \mathrm{Tr}((g^{-1}\partial_t g)^2). \tag{8.19}$$

One can check this action is invariant under (constant) left and right multiplication in G^n. We can do the Hamiltonian analysis of this system and the phase space is the tangent bundle of the group G. The equation of motion is

$$\partial_t(g^{-1}\partial_t g) = 0. \tag{8.20}$$

We choose $\pi^{(l)} = g^{-1}\partial_t g$ as momentum (instead of the canonical momentum), it is the Noether charge associated to the left invariance. The solutions are then parametrized as

$$g(t,g_0) = g_0 \exp(\pi^{(l)} t). \tag{8.21}$$

We could also choose the right momentum defined by $\pi^{(r)} = -\partial_t g g^{-1}$ and then the solutions would be

$$g(t,g_0) = \exp(-\pi^{(r)} t) g_0 \tag{8.22}$$

which are the geodesics.

The Poisson bracket reads

$$\{g,\hat{g}\}=0,$$
$$\{g,\pi_X^{(l)}\}=Xg, \tag{8.23}$$
$$\{\pi_X^{(l)},\pi_Y^{(l)}\}=\pi_{[X,Y]}^{(l)},$$

where g, $\hat{g}$ are group elements, X, Y are in the Lie algebra, and $\pi_X^{(l)}=\mathrm{Tr}(X\pi^{(l)})$ is the component of $\pi^{(l)}$ in the X direction.

One can create a Fock space for the free particles states

$$\mathcal{F}=\bigoplus_{n\geqslant 0} L^2(G^n). \tag{8.24}$$

We can construct creation operators $a_\varphi^\dagger$ and annihilation operators a_φ which are adding or removing a one particle state to a (symmetrized) n particle state—let us call it ψ:

$$(a_\varphi\psi)(g_1,g_2,\ldots,g_{n-1})=\int dg_n\psi(g_1,g_2,\ldots,g_n)\overline{\varphi}(g_n), \tag{8.25}$$

$$(a_\varphi^\dagger\psi)(g_1,g_2,\ldots,g_{n+1})=\sum_i \psi(g_1,\ldots,g_{i-1},g_{i+1},\ldots,g_n)\varphi(g_i). \tag{8.26}$$

We can also write a (free) field theory corresponding to this Fock space. Indeed, let us define a field operator $\Phi(g)=a_{\delta_g}$, $\Phi^\dagger(g)=a_{\delta_g}^\dagger$, where δ_g denote the Dirac delta function supported at g. Then, the action of the total impulsion operator on the Hilbert space of N particles can be written in terms of the field operators $\Sigma_{i=1}^N\pi_X^{i(l/r)}=\int_G dg\,\Phi^\dagger(g)(-i\nabla_X^{(l/r)})\Phi(g)$, where $\nabla_X^{(l/r)}$ denote the left or right invariant derivative operator in the direction of X. In the same way the Hamiltonian operator can be written as

$$H=-\int_G dg\,\Phi^\dagger(g)\Delta\Phi(g), \tag{8.27}$$

and the action governing the quantization and the dynamic of the field is expressed in terms of a space–time field $\Phi(t,g)$:

$$S[\Phi(t,g)]=\int_{\mathbf{R}\times G} dt\,dg\Phi^\dagger(g)\left(i\frac{\partial}{\partial t}+\Delta\right)\Phi(g). \tag{8.28}$$

We now wish to follow the same steps for gauged particles, i.e., in the case that we gauge the global $\mathrm{Ad}(G)$ symmetry. This can be achieved by introducing a gauge fields A living in the Lie algebra $\mathcal{G}$, and the action reads (we have slightly modified the action given in Ref. 28):

$$S_{\text{gauged}}[g(t)\in G^n,A]=-\frac{1}{2}\int dt\,\mathrm{Tr}((g^{-1}\partial_t g)^2)$$
$$+\int dt\,\mathrm{Tr}((g\partial_t g^{-1})A+A(g^{-1}\partial_t g)+gAg^{-1}A-A^2). \tag{8.29}$$

This action is invariant under the following $\mathrm{Ad}(G)$ gauge invariance for arbitrary G-valued $h(t)$:

$$g\to hgh^{-1}$$
$$A\to hAh^{-1}+h\partial_t h^{-1} \tag{8.30}$$

The space of states of our system will be $L^2(G^n/\mathrm{Ad}(G))$. For these gauged particles, we would like to do the same thing as for the free particles, i.e., write down creation and annihilation operators and a corresponding field theory. The problem is the change of symmetry: the symmetry in $L^2(G^n/\mathrm{Ad}(G))$ is a global symmetry $\mathrm{Ad}(G)$ on the system of n particles and it is hard to have a Fock space interpretation. An analogy would be to study a system of N particles in space–time which would be invariant under global Poincaré transformations.

The easiest way to write creation and annihilation operators would be through gauge fixing. Starting from a graph Γ and going through the gauge fixing procedure, we have seen that the space $L^2(A_\Gamma)$ is naturally isomorphic to $L^2(G^n)$. Therefore the space associated with an infinite graph is similar Fock space. And in this context creation and annihilation operators are adding or removing a loop to the graph. We feel that it will be interesting to have a deeper understanding of this ideas and of the field theory behind this. Note that the action of the field theory behind the gauged particle is obtain by introducing a gauge field $A(t)$ and a term to the action (8.28):

$$\int dt\, dg\, A(t)(\nabla^{(l)}-\nabla^{(r)})\Phi(g,t). \tag{8.31}$$

IX. CONCLUSION

In this paper, we have defined the notion of Spin network states for noncompact reductive groups. We have shown how to construct the quotient space of graph connections as the algebraic dual of a polynomial algebra. We have also constructed, by a careful gauge fixing procedure, a canonical measure on this space which turned out to be independent of any gauge fixing choices. This measure defines a Hilbert space structure for each graph, and spin networks states are defined as generalized eigenvectors of invariant, hermitic differential operators. We have explicitly realized all these ideas in the context of $\mathrm{SL}(2,\mathbf{R})$ and $\mathrm{SL}(2,\mathbf{C})$ by a direct analysis of the quotient space and measure in the simplest cases. Finally we have discussed the nature of the full Hilbert space based on all graphs and we have shown that a natural Fock structure appears in this context.

The work we have done is the first step toward a full comprehension of noncompact spin networks, i.e., identical to the one we have for the compact ones. As we have stressed in our paper, an understanding of the full Hilbert space as an L^2 space is still missing. We expect that this should come together with an interpretation of the full space of gauged connections as an algebraic dual. Also, a more detailed and explicit study of the space of spin networks would be interesting to pursue in order to reach a deeper understanding of their analytic properties, in the spirit of the work of Harish–Chandra on characters of noncompact groups. Finally, we feel that the Fock space structure which is emerging in our construction is something important that should be put on firmer basis. Nevertheless, this work opens the possibility to study the Hilbert spaces of noncompact spin networks that arises in Lorentzian formulations of gravity and allows us to discuss the spectra of geometrical operators in this context.[12]

ACKNOWLEDGMENTS

L.F. would like to thank F. Delduc for a discussion. This work has been supported by an ACI-blanche grant.

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An operator method for finding exact solutions to vector Korteweg–de Vries equations

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(Received 24 January 2002; accepted 13 December 2002)

We develop an operator method which helps finding exact solutions to nonlinear evolution equations (NLEs). Our working schema goes as follows: First we translate the given (NLE) into an appropriate operator version (ONLE). Second, we look for solutions to (ONLE) of the form $U=(I+L)^{-1}M$, where both L and M are operator-valued functions of the space–time variables and the range of M locates in some appropriate Banach algebras which admits a functional ϕ that preserves the squares [i.e., $\phi(A^2)=\phi(A)^2$]. Finally, a solution u of the given (NLE) can be obtained by setting $u:=\phi(U)$. This method is named by the LM method. Using the LM method, we have rederived the famous Cole–Hopf transformation which reduces the nonlinear Burgers equation into the linear heat equation. The main part of this article is to use the LM method to study the vector Korteweg–de Vries (KdV) equations $\mathbf{u}_t=\mathbf{u}_{xxx}+3(\mathbf{u}^2)_x$ settled in finite-dimensional unital Banach algebras $\mathcal{J}$. It is shown that these vector KdV equations admit soliton solutions. Specially, we have carried out a thorough study of the quaternionic KdV equation (i.e., the vector KdV equation settled in the Hamilton quaternion algebra $\mathbb{H}$) and shown many interesting and surprising aspects of the quaternionic KdV solitons. Two of them read as follows. (a) The paradoxical energy symmetry breaking phenomenon: Two quaternionic KdV solitons with different energies can annihilate each other. (b) The surprising low-dimensional phenomenon: The interaction of any finitely many quaternionic KdV solitons which live in a unital three-dimensional subspace Π of $\mathbb{H}$ does not yield any effect to the part outside that subspace Π and thus their interaction behaves as if it were linear although the interaction between quaternionic KdV solitons is really nonlinear. The LM method can be thought as a complement to the famous bilinear operator method of Hirota. Hirota's method works very powerful for solving scalar equation but has difficulty with vector equations. The LM method helps overcoming this difficulty. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1544414]

I. THE METHODOLOGY AND OVERVIEW OF THE RESULTS

We are given the following nonlinear evolution equation:

$$\text{(NLE)}\quad u_t=L(u,u_x,u_{xx},\dots)+N(u,u_x,u_{xx},\dots),x\in\mathbb{R},t\in\mathbb{R},$$

where $L(u,u_x,u_{xx},\dots)$ is the linear part and $N(u,u_x,u_{xx},\dots)$ the nonlinear part of the equation. Our working scheme for finding exact solutions of NLE consists of four steps.

(1) First we interpret the NLE in an appropriate operator version, i.e., for an appropriate Banach algebra $\mathcal{A}$ we will solve the corresponding operator-valued equation

$$\text{(ONLE)}\quad U_t=L(U,U_x,\dots)+N(U,U_x,\dots),x\in\mathbb{R},t\in\mathbb{R},\quad U(x,t)\in\mathcal{A}.$$

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Because of the noncommutativity of operators the product of scalar functions such as uu_x could be interpreted as UU_x or U_xU or the combination $(UU_x+U_xU)/2$ as operator product. Hence, the NLE can be interpreted in general in different ways and thus one should choose carefully one of them that is suitable to solve. Moreover, if the absolute value $|u|^2$ appears in the NLE, then the Banach algebra $\mathcal{A}$ should be also a C^* algebra so that the absolute value $|u|^2$ can be interpreted as either the product UU^* or U^*U or combinations of them.

The Banach algebras, that we will use frequently, are those $\mathcal{L}(\mathcal{E})$ generated by all linear bounded operators on Banach spaces $\mathcal{E}$.

(2) Let M be an operator-valued function solving the linearized equation of ONLE, i.e., M solves

$$M_t=L(M),x\in\mathbb{R},t\in\mathbb{R},\quad M(x,t)\in\mathcal{A}.$$

(3) We search an operator-valued function L such that $U:=(1+L)^{-1}M$ solves the ONLE. The function L will be coupled with the function M and solves sometimes also the linearized equation of ONLE.

(4) To recover scalar solutions from solutions U of ONLE, the following trace method (TM) will be used.

(TM) Assume that there exists a $\xi\in\mathcal{E}'$ and an $\mathcal{E}$-valued function η such that all of the operators $U(x,t)$ can be written as $U(x,t)=\xi\otimes\eta(x,t)$. Using the trace functional tr and setting $u:=\mathrm{tr}(U)$ we will obtain a solution of the NLE, since the trace functional obeys the following elementary but important property.

Lemma 1.1: Let $\mathcal{E}$ be a Banach space and $\xi\in\mathcal{E}'$. Denote by $\xi\otimes\mathcal{E}$ the set consisting of all operators $\xi\otimes a$ $(a\in\mathcal{E})$. Then, $\xi\otimes\mathcal{E}$ is a closed subalgebra of $\mathcal{L}(\mathcal{E})$ and the trace functional tr *is an algebraic homomorphism from $\xi\otimes E$ into $\mathbb{C}$, i.e.,*

$$\mathrm{tr}(\xi\otimes a\cdot\xi\otimes b)=\mathrm{tr}(\xi\otimes a)\cdot\mathrm{tr}(\xi\otimes b),\quad a,b\in\mathcal{E}.$$

Proof: We have $\xi\otimes a\cdot\xi\otimes b=\langle\xi,b\rangle\xi\otimes a=\mathrm{tr}(\xi\otimes b)\cdot(\xi\otimes a)$. This implies that $\xi\otimes\mathcal{E}$ is a subalgebra of $\mathcal{L}(\mathcal{E})$ as well as the multiplicative property of the trace tr in $\xi\otimes\mathcal{E}$. □

The above lemma implies in particular that for an operator-valued function U given by $U=\xi\otimes\eta(x)$ for some fixed ξ there holds

$$\mathrm{tr}((\partial_x^jU)\cdot(\partial_x^kU))=(\mathrm{tr}(\partial_x^jU))\cdot(\mathrm{tr}(\partial_x^kU))\quad(j,k=0,1,2,\ldots).$$

This observation enables one to freely interpret the product uu_x of functions as UU_x or U_xU or the combination $(UU_x+U_xU)/2$ in the sense of operator product. Sometimes an appropriate choice of the interpretations will make the equation solvable.

It follows from the general theory of linear PDE's that the generic solutions of the linearized equation $P_t=L(P)$ of ONLE are performed by appropriate linear operators, i.e., $P_x=AP$ and $P_t=BP$. Therefore, the following observation will be very useful.

Lemma 1.2: Let J be an open interval in $\mathbb{R}$ and $\mathcal{E}$ be a Banach space. Assume $L,M:J\to\mathcal{L}(\mathcal{E})$ to be two C^∞ operator valued functions such that for some fixed closed, densely defined operator A in $\mathcal{E}$ there holds

$$L_x=AL,\quad M_x=AM,\quad x\in J.$$

Let

$$\Omega:=\{x\in J:I+L(x)\quad \textit{is invertible}\}$$

and define on Ω the function $U:=(I+L)^{-1}M$. Then,

$$(I+L)U_x=AU,\quad (I+L)U_{xx}=A(I-L)U_x,$$

$$(I+L)U_{xxx}=3AU_{xx}-A^2(2I-L)U_x.$$

In general, each of the x-derivatives $U^{(n)}\equiv\partial_x^n U$ *can be written as a product of some appropriate linear operator* T_n *with* U. *More precisely,* $U^{(n)}=T_nU$ *and the class of linear operators* $(T_n)_{n\geqslant 1}$ *obeys the following recursion formula:*

$$T_1=(I+L)^{-1}A,\quad T_{n+1}=(T_n)_x+T_nT_1\quad (n\geqslant 1).$$

Proof: Taking x-derivatives in both sides of the equality $(I+L)U=M$ and using the Leibniz rule. □

It is suggested by this observation that if higher order derivatives in the NLE are involved then the similarity

$$L_x=AL,\quad M_x=AM\quad \text{as well as}\quad L_t=BL,\quad M_x=BM$$

should be verified in order to simplify the computation of higher order derivatives of the product $U=(I+L)^{-1}M$. Moreover, the common factor U in the representations of derivatives can be extracted and finally eliminated.

Since the searched solutions U for ONLE has the representation $U=(I+L)^{-1}M$, we will name the above method the LM method. Correspondingly, an NLE which can be solved by this method will be called an LM-solvable equation. As illustrated above, the solutions of an LM-solvable NLE admit the following very important superposition property: If u_1,u_2 are solutions of the NLE generated by the pair (L_1,M_1) and (L_2,M_2), respectively, then the pair (L_1+L_2,M_1+M_2) will generate a solution u for NLE that describes the interaction of the two solutions u_1 and u_2. Thus, if u is a solution generated by the pair (L,M), then the interaction of u and the solution $\hat{u}$ generated by the counterpart $(-L,-M)$ of (L,M) is described by the solution generated by the pair $(L-L,M-M)=(0,0)$ which is just the vacuum solution 0. In other words, $\hat{u}$ and u annihilate each other. In particular, if u is a soliton then the counterpart $\hat{u}$ should be understood as an antisoliton.

Certainly, the chance of success in applying the LM method heavily depends on the special structure of the ONLE. Therefore, in translating a scalar nonlinear evolution equation into an operator nonlinear equation one should measure, as the first thing of all, the degree of nonlinearity (DNL) of each term involved. Roughly speaking, if $U=(I+L)^{-1}M$, then the DNL of U is -1, since the only nonlinear term in the product is $(I+L)^{-1}$. In general, the DNL of the nth order derivative of U is $-(n+1)$. We note that the DNL of U_t is -2. Therefore, the following compatibility for the degree of the nonlinearity (C4DNL) should be followed in principle, in order to find an appropriate operator version of NLE that is solvable by the LM method.

(C4DNL) The total DNL of the terms in the right-hand side of the OLNE should be -2.

Further contents of the paper are organized as follows. In Sec. II we begin to illustrate the LM method with the Burgers equation, there the well-known Cole–Hopf transformation will be re-derived in a natural way by appealing to the LM method. In Sec. III we show how the LM method can be used to solve the usual scalar KdV equation. As a by-product, solution formula for operator KdV equation (OKDV) has been found. It reveals what one should do in finding solutions of the KdV equation is to solve the operator equation $GL+LG=M$. The starting point of Sec. IV is to translate the vector KdV equation

$$\mathbf{u}_t-\mathbf{u}_{xxx}-3(\mathbf{uu})_x=0,\quad \mathbf{u}\in\mathcal{J} \tag{1.1}$$

settled in a unital Banach algebra $\mathcal{J}$ into an appropriate operator form. The price paid by the LM method is the solvability of equations (1.1), i.e., it can be solved by a linearization process. In Sec. V we concentrate on the concrete case $\mathcal{J}=\mathbb{H}$, i.e., on the vector KdV equation settled in the Hamilton quaternionic algebra $\mathbb{H}$. Such a consideration is stimulated by the work of *quaternionic quantum mechanics*.[3] Our study of the quaternionic KdV equation provides a prototype for the further study of other quaternionic soliton equations.

Using the LM method we show that the quaternionic KdV equation is a soliton equation; interaction of two solitary wave solutions has been described in an explicit way. Our result reveals that the structure of solitary wave solutions of the quaternionic KdV equation is much richer than the ones for the real and complex KdV equations. In particular, we discover the following low-dimensional linear phenomenon of the interaction of the quaternionic KdV solitons: the interaction of any finitely many quaternionic KdV solitons which live in a unital three-dimensional subspace does not yield any effect outside that three-dimensional subspace and thus their interaction behaves as if it were linear although the interaction between quaternionic KdV solitons is really nonlinear. We find also, as a by-product, a noncommutative soliton system of three components which is the reduction from the quaternionic KdV equation by switching one of the vector part into zero. The remarkable aspect of this new noncommutative soliton system is that it can not be derived from a vector KdV equation of the form (1.1) by choosing some appropriate three-dimensional unital Banach algebra $\mathcal{J}$, since any three-dimensional unital Banach algebra is commutative.

The LM method should be considered as a solution method for general nonlinear equations, although here we have only described its working scheme for nonlinear evolution equations of Burgers/KdV type. Moreover, the LM method can be thought also as a complement to the famous bilinear operator method of Hirota.[11] Hirota's method works very powerful for solving scalar equation (cf. Refs. 1, 5, 8, and 17) but has difficulty with vector equations. As seen above, the LM method may help to overcome this difficulty.

Related results to the LM method can be found in the works of Aden and Carl,[2] Carl and Huang[6] for the scalar KdV equation, and of Schiebold[18] for the scalar Toda lattice equation.

We remark that the vector KdV equation (1.1) can be reduced from a symmetry reduction of ordinary self-dual Yang–Mills equations with supergauge groups, see, e.g., Ref. 12. We refer the reader to Refs. 21, 16, 14, 15, and 1 for more information on the physical origin and the mathematical studies of the scalar KdV equations and to Ref. 7 (cf. also Ref. 8) for a detailed study of the vector KdV equations in the context of Lie symmetries.

II. THE STARTING POINT: BURGERS EQUATION AND COLE–HOPF TRANSFORMATION

As a first test of the LM method we consider Burgers equation,

$$(\mathrm{BE}) \quad u_t - u_{xx} - 2uu_x = 0.$$

By letting $u = v_x$ we obtain the corresponding potential Burgers equation,

$$(\mathrm{PBE}) \quad v_t - v_{xx} - v_x^2 = 0.$$

However, the DNL of the term $v_{xx} + v_x^2$ is dominated by the DNL of the term v_x^2, which is -4. According to C4DNL, the PBE cannot be solved by the LM method. On the other hand, the DNL of the term $u_{xx} + 2uu_x$ is the same as that of the term u_t. Therefore, a successful use of the LM method could be expected.

The operator version of the product uu_x can be taken as either UU_x or U_xU, i.e., we can interpret BE in two ways

$$(\mathrm{OBE}) \quad U_t - U_{xx} - 2UU_x = 0$$

and

$$(\mathrm{OBE}') \quad U_t - U_{xx} - 2U_xU = 0.$$

The solutions of (OBE') can be obtained by taking adjoints of solutions of OBE, i.e., if U solves OBE, then U' solves OBE', and *vice versa*.

According to this observation, for a given Banach space $\mathcal{E}$ we need only to solve OBE. Starting with two smooth operator-valued functions L and M we consider $U := (I+L)^{-1}M$. Then

$$(I+L)U_x=M_x-L_xU, \quad (I+L)U_{xx}=M_{xx}-L_{xx}U-2L_xU_x.$$

Similarly,

$$(I+L)U_t=M_t-L_tU.$$

Assume U solves OBE, i.e.,

$$(I+L)(U_t-U_{xx}-2UU_x)=0. \tag{2.1}$$

Substituting the above relations into (2.1) and rearranging the terms yields

$$(M_t-M_{xx})-(L_t-L_{xx})U+2(L_x-M)U_x=0.$$

Therefore, the functions L and M are expected to satisfy the following equations:

$$L_t-L_{xx}=0, \quad M_t-M_{xx}=0, \quad L_x-M=0.$$

Solving them yields $M=L_x$ and that L satisfies the operator heat equation

$$L_t-L_{xx}=0. \tag{2.2}$$

In conclusion, $U=(I+L)^{-1}L_x$ solves OBE whenever L solves (2.2).

To extract scalar solutions for BE we use the trace method. For this purpose we assume that the solution L of (2.2) is given by

$$L(x,t)=\xi\otimes l(x,t),$$

where $\xi\in\mathcal{E}'$ is fixed and the function l solves the $\mathcal{E}$ valued heat equation

$$l_t-l_{xx}=0. \tag{2.3}$$

In this case, the scalar function $u:=\mathrm{tr}(U)=\langle\xi,(I+\xi\otimes l)^{-1}l_x\rangle$ which can be rewritten as

$$u=\phi_x/\phi \quad \text{with} \quad \phi:=1+\langle\xi,l\rangle, \tag{2.4}$$

solves the Burgers equation (BE). Note that the scalar function ϕ solves the heat equation

$$\phi_t-\phi_{xx}=0. \tag{2.4$'$}$$

Summing up, we have just recovered the well-known Cole–Hopf transformation (2.4) which reduces the viscid Burgers equation to the linear heat equation (2.4′). We refer the reader to the work of Gesztesy and Holden[9] for a new review and extensions of the Cole–Hopf transformation.

By settling the operator equation (OBE) in appropriate Banach algebras the above procedure will produce solutions to vector equations $\mathbf{u}_t-\mathbf{u}_{xx}-2\mathbf{u}\mathbf{u}_x=0$ of Burgers type. However, in this paper we shall concentrate on the vector KdV equations.

III. KdV EQUATION AND OPERATOR EQUATION $GL+LG=M$

The Korteweg–de Vries (KdV) equation which we shall consider has the form

$$(\mathrm{KdV}) \quad u_t-u_{xxx}-6uu_x=0.$$

By letting $u=v_x$ we obtain the corresponding potential KdV equation,

$$(\mathrm{PKdV}) \quad v_t-v_{xxx}-3(v_x)^2=0.$$

On the one hand, the DNL of the term $u_{xxx}+6uu_x$ is dominated by the DNL of the term u_{xxx}, which is -4. According to C4DNL, the KdV cannot be solved directly by the LM method.

On the other hand, the DNL of the term $v_{xxx}+3v_x^2$ could be reduced to -2 by the interaction of the linear term v_{xxx} with the nonlinear term v_x^2. Therefore, it is valuable to try to solve PKdV with the LM method.

The operator version of PKdV is the same one, i.e.,

$$(\text{OPKdV}) \quad V_t-V_{xxx}-3(V_x)^2=0.$$

Let L and M be two $\mathcal{L}(\mathcal{E})$-valued solutions of the linearized equation of OPKdV, i.e.,

$$M_t-M_{xxx}=0, \quad L_t-L_{xxx}=0. \tag{3.1}$$

For $V:=(I+L)^{-1}M$ we have

$$M_t=(I+L)V_t+L_tV,$$

$$M_{xxx}=(I+L)V_{xxx}+3L_xV_{xx}+3L_{xx}V_x+L_{xxx}V.$$

It follows that

$$(I+L)(V_t-V_{xxx})=3(L_xV_{xx}+L_{xx}V_x).$$

Therefore, if V solves OPKdV, then $3(L_xV_{xx}+L_{xx}V_x)=3(I+L)V_x^2$, i.e.,

$$(L_xV_{xx}+L_{xx}V_x)=(M_x-L_xV)V_x, \tag{3.2}$$

since $(I+L)V_x=M_x-L_xV$.

A known fact is that the $\mathcal{L}(\mathcal{E})$-valued solutions of the linear evolution equation $N_t-N_{xxx}=0$ are performed by operators in the Banach space $\mathcal{E}$, i.e., they are given by the relation $N_x=GN$ with some appropriate densely defined, closed operators G in the Banach space $\mathcal{E}$. For this reason, we assume

$$L_x=GL, \quad M_x=GM \tag{3.3}$$

with some appropriate densely defined, closed operator G in the Banach space $\mathcal{E}$. Then, (3.2) becomes

$$(GLV_{xx}+G^2LV_x)=(GM-GLV)V_x.$$

Killing G yields

$$(LV_{xx}+GLV_x)=(M-LV)V_x.$$

Multiplying both sides by $I+L$ and using

$$(I+L)(M-LV)=(I+L)V=M,$$

$$(I+L)V_{xx}=M_{xx}-2L_xV_x-L_{xx}V=G(I-L)V_x,$$

we obtain

$$[LG(I-L)+(I+L)GL]V_x=MV_x.$$

Killing V_x yields

$$M=GL+LG. \tag{3.4}$$

In conclusion, the following result has been established: The $\mathcal{L}(\mathcal{E})$-valued function $V=(I+L)^{-1}M$ solves OPKdV whenever L and M satisfy (3.1) and (3.3) and are coupled by the relation (3.4).

It follows that if M can be written as $M(x,t)=\xi\otimes m(x,t)$ for some fixed $\xi\in\mathcal{E}'$, then a scalar solution u of the KdV equation will be extracted through $u=\mathrm{tr}(V)_x$. Furthermore, if the operator X which solves the operator equation $GX+XG=\xi\otimes a$ belongs to a quasi-Banach ideal $\mathcal{Y}$ that admits a continuous determinant $\det_\lambda$, then the solution u can be represented by (see Refs. 2 or 6)

$$u(x,t)=2(\ln w(x,t))_{xx} \quad \text{with} \quad w(x,t)=\det_\lambda(I+L).$$

As an illustration of this method, we take G to be an $N\times N$ matrix such that G and $-G$ have no eigenvalues in common. Then, it is well known (see e.g., Ref. 13, p. 414 or Ref. 6) that for each $N\times N$ matrix C the matrix equation $GX+XG=C$ has a unique solution. In particular, we take C to be an $N\times N$ matrix of rank 1 and let X be the unique solution of the matrix equation $GX+XG=C$. Define

$$L(x,t):=e^{xG+tG^3}X, \quad M:=e^{xG+tG^3}C.$$

Then, L and M are solutions of Eqs. (3.1), (3.3), and (3.4). By letting

$$w(x,t):=\det(I+L(x,t)), \quad (x,t)\in\mathbb{R}^2$$

we find from the above result that $u(x,t):=2(\ln w(x,t))_{xx}$ solves the KdV equation in the domain where $w(x,t)$ does not vanish. The usual N-soliton solution can be obtained in this way by taking a diagonal matrix G. More results can be found in recent work.[6]

IV. SOLVING VECTOR KdV EQUATIONS BY LM METHOD

In the sequel $\mathcal{J}$ denotes a unital real Banach algebra of finite dimension $d:=\dim(\mathcal{J})<\infty$, with unit $I_{\mathcal{J}}$. The vector KdV equation in $\mathcal{J}$ has the form

$$\mathbf{u}_t-\mathbf{u}_{xxx}-3(\mathbf{uu})_x=0, \quad \mathbf{u}\in\mathcal{J}. \tag{4.1a}$$

The solutions

$$\mathbf{u}:\mathbb{R}^2\ni(x,t)\to\mathbf{u}(x,t)\in\mathcal{J} \tag{4.1b}$$

are $\mathcal{J}$-valued smooth functions. We call (4.1a) the $\mathcal{J}$-KdV equation.

A. Nonlinear systems equivalent to $\mathcal{J}$-KdV equations

If we choose a basis $\{e_1,\ldots,e_d\}$ of the finite-dimensional algebra $\mathcal{J}$, then there exist coefficients $(c_{ijk})\subset\mathbb{R}$ such that the products of the base elements are given by

$$e_ie_j=\sum_{m=1}^{d}c_{ijm}e_m \quad (i,j=1,2,\ldots,d). \tag{4.2a}$$

Moreover, the associativity $(e_ie_j)e_k=e_i(e_je_k)$ yields the following relation of these coefficients:

$$\sum_{m=1}^{d}c_{ijm}c_{mkl}=\sum_{m=1}^{d}c_{jkm}c_{iml} \quad (i,j,k,l=1,2,\ldots,d). \tag{4.2b}$$

We write a solution $\mathbf{u}$ of (4.1a) in its components form

$$\mathbf{u}=\sum_{j=1}^{d}u_je_j \tag{4.2c}$$

and substitute it into (4.1a), using (4.2a) to develop the product **uu**, we obtain the following nonlinear system:

$$(u_k)_t=(u_k)_{xxx}+3\sum_{1\leqslant i,j\leqslant d} c_{ijk}(u_iu_j)_x, \quad k=1,2,\ldots,d. \tag{4.2d}$$

We remark that the relation (4.2b) for the coefficients is also sufficient for a nonlinear system of the form (4.2d) being equivalent to a vector KdV equation (4.1a) settled in some appropriate Banach algebra $\mathcal{J}$. To see this, we assume (4.2b) and define by (4.2a) the products of the classic base elements $\{e_1,\ldots,e_d\}$ of the Euclid space $\mathbb{R}^d$. Then $\mathbb{R}^d$ under this product rule becomes to be an associative algebra and thus a Banach algebra. In this way, the given system (4.2d) is equivalent to the vector KdV equation (4.1a) settled in $\mathcal{J}=\mathbb{R}^d$ with the above defined product rule.

Clearly, only those nonlinear systems (4.2d) generated by noncommutative algebras $\mathcal{J}$ are of great interest. All noncommutative unital Banach algebras have dimension at least four. The first two noncommutative four-dimensional unital Banach algebras are the matrix algebra $M_2(\mathbb{R})$ and the Hamilton quaternion algebra $\mathbb{H}$; both of them belong to the class of the so-called *Clifford algebras*.[19] The four-dimensional vector KdV equation settled on $\mathbb{H}$, called the *quaternionic KdV equation*, has many very interesting properties, see Sec. V.

B. $\mathcal{J}$-Banach spaces

A $\mathcal{J}$-banach space $\mathcal{E}$ is a Banach space over the unital Banach algebra $\mathcal{J}$, i.e., it is a real Banach space with the additional property that the product operation

$$\mathcal{J}\times\mathcal{E}\ni(\alpha,u)\mapsto\alpha u\in\mathcal{E}$$

has been defined and satisfies the associativity

$$\beta(\alpha u)=(\beta\alpha)u \quad \forall\,\alpha,\beta\in\mathcal{J},u\in\mathcal{E}.$$

We say that a mapping $S:\mathcal{E}\to\mathcal{E}_1$ between two $\mathcal{J}$-Banach spaces is *$\mathcal{J}$-linear* if it is a real-linear mapping such that

$$S(\alpha u)=\alpha(Su) \quad \forall\,\alpha\in\mathcal{J},u\in\mathcal{E}.$$

$\mathcal{J}$-Banach spaces can be constructed from the usual real Banach spaces as follows. We take a real Banach space $\mathcal{E}_0$ and consider the algebraic tensor product $\mathcal{J}\otimes\mathcal{E}_0$. Since $\mathcal{J}$ is of finite dimension d, $\mathcal{J}\otimes\mathcal{E}_0$ is a Banach space isomorphic to the product space $\mathcal{E}_0^d$. We define a product rule by

$$\alpha(\beta\otimes u):=(\alpha\beta)\otimes u \quad (\alpha,\beta\in\mathcal{J},u\in\mathcal{E}_0).$$

Then we have a $\mathcal{J}$-linear space $\mathcal{J}\otimes\mathcal{E}_0$. As examples, we have $\mathcal{J}\otimes\mathbb{R}^n=\mathcal{J}^n$ and $\mathcal{J}\otimes\mathbb{C}^n=(\mathcal{J}^n)_{\mathbb{C}}$ the complexification of the product space $\mathcal{J}^n$.

A linear bounded operator $T:\mathcal{E}_1\to\mathcal{E}_2$ between two real Banach spaces can be extended to a $\mathcal{J}$-linear bounded operator $\tilde{T}:\mathcal{J}\otimes\mathcal{E}_1\to\mathcal{J}\otimes\mathcal{E}_2$ by setting

$$\tilde{T}(\beta\otimes u):=\beta\otimes(Tu) \quad (\beta\in\mathcal{J},u\in\mathcal{E}_1).$$

We call $\tilde{T}$ the *$\mathcal{J}$-extension* of T.

The generally used notations for the usual Banach spaces adopt their extensions to the $\mathcal{J}$-Banach spaces. For example, the dual space $\mathcal{E}'$ of a $\mathcal{J}$-Banach space $\mathcal{E}$ is the $\mathcal{J}$-Banach space consisting of all $\mathcal{J}$-linear continuous functionals on $\mathcal{E}$. Similarly, $\mathcal{L}(\mathcal{E})$ is used to denote the space of all $\mathcal{J}$-linear bounded operators on a $\mathcal{J}$-Banach space $\mathcal{E}$. $\mathcal{L}(\mathcal{E})$ is also a $\mathcal{J}$-algebra. As usual, the tensor product $\xi\otimes\eta$ with $\xi\in\mathcal{E}'$ and $\eta\in\mathcal{E}$ denotes the operator defined by

$$\xi\otimes\eta(u):=\langle\xi,u\rangle\,\eta \quad (u\in\mathcal{E}). \tag{4.3a}$$

Correspondingly, an operator $S\in\mathcal{L}(\mathcal{E})$ is called a *rank one operator* if $S=\xi\otimes\eta$ for some $\xi\in\mathcal{E}'$ and $\eta\in\mathcal{E}$.

As seen in Sec. III, the notion ''trace'' defined for real-linear rank one operators plays an important role in finding exact solutions of the scalar KdV equation. Encouraged by this success, in finding exact solutions to the $\mathcal{J}$-KdV equation (4.1a) we are hoping certainly that analogies of the notion ''trace'' will work in a similar way. Because we are working in general with a noncommutative Banach algebra $\mathcal{J}$, it remains a question as to whether the ''trace'' of a $\mathcal{J}$-linear operator could be defined and how. Naively, one might define the trace of a rank one operator $S=\xi\otimes\eta$ by $\mathrm{trace}(S)=\langle\xi,\eta\rangle$. However, the following observation reveals that this is not well defined if we are working in a noncommutative Banach algebra $\mathcal{J}$. We consider the easiest case $\mathcal{E}=\mathcal{J}$ and let $\xi_0\in\mathcal{J}'$ be the functional given by

$$\xi_0(u):=u \quad (u\in\mathcal{J}).$$

For two elements $\eta_1,\eta_2\in\mathcal{J}$ we consider the operator $S:\mathcal{J}\to\mathcal{J}$ given by

$$Su:=u(\eta_2\eta_1) \quad \forall u\in\mathcal{J}.$$

On the one hand, since $Su=\xi_0(u)(\eta_2\eta_1)$, we see that S is a rank one operator and can be represented as $S=\xi_0\otimes(\eta_2\eta_1)$. On the other hand, by considering the functional $\xi_1\in\mathcal{J}'$ given by $\xi_1(u):=u\eta_2$ $(u\in\mathcal{J})$ we find that $Su=\xi_1(u)\eta_1$ and thus $S=\xi_1\otimes\eta_1$. Therefore, the rank one operator S admits the following representations:

$$S=\xi_0\otimes(\eta_2\eta_1)=\xi_1\otimes\eta_1.$$

We have

$$\langle\xi_0,(\eta_2\eta_1)\rangle=\eta_2\eta_1 \quad \text{and} \quad \langle\xi_1,\eta_1\rangle=\eta_1\eta_2.$$

Thus, if η_1,η_2 are not commutative, then

$$\langle\xi_0,(\eta_2\eta_1)\rangle=\eta_2\eta_1\neq\eta_1\eta_2=\langle\xi_1,\eta_1\rangle.$$

Consequently, if the Banach algebra $\mathcal{J}$ is noncommutative, then there does not exist a nontrivial extension of the notion trace which is defined for all rank one operators over the easiest $\mathcal{J}$-Banach space $\mathcal{E}=\mathcal{J}$!

This nonexistence forces us to correct our goal. For this purpose, We take a fixed $\xi\in\mathcal{E}'$ and use $\xi\otimes\mathcal{E}$ to denote the set of all rank one operators of the form $\xi\otimes\eta$ with some $\eta\in\mathcal{E}$. It follows from the property $S(\xi\otimes\eta)=\xi\otimes(S\eta)$ that $\xi\otimes\mathcal{E}$ is a left ideal of the $\mathcal{J}$-Banach algebra $\mathcal{L}(\mathcal{E})$. We consider the $\mathcal{J}$-linear operator $\mathrm{tr}_\xi:\xi\otimes\mathcal{E}\to\mathcal{J}$ given by

$$\mathrm{tr}_\xi(A):=\langle\xi,\eta\rangle \quad \text{for } A=\xi\otimes\eta\in\xi\otimes\mathcal{E}. \tag{4.3a}$$

Note that here we have marked tr_ξ with the suffix ξ in order to stress its restriction that it is only defined on the left ideal $\xi\otimes\mathcal{E}$.

Now, since $(\xi\otimes\eta_1)(\eta\otimes\eta_2)=\xi\otimes(\langle\xi,\eta_2\rangle\eta_1)$ for all $\eta_1,\eta_2\in\mathcal{E}$, we find that tr_ξ is an antihomomorphism, i.e.,

$$\mathrm{tr}_\xi(AB)=\mathrm{tr}_\xi(B)\cdot\mathrm{tr}_\xi(A) \quad \forall A,B\in\xi\otimes\mathcal{E}. \tag{4.3b}$$

In particular,

$$\mathrm{tr}_\xi(A^2)=\mathrm{tr}_\xi(A)^2 \quad \forall A\in\xi\otimes\mathcal{E}. \tag{4.3c}$$

As seen later, all what we need for finding exact solutions of the $\mathcal{J}$-KdV equation is just only the property that tr_ξ is an antihomomorphism.

C. Solutions of $\mathcal{J}$-KdV equations

Let $\mathcal{E}$ be a $\mathcal{J}$-Banach space and fix an element $\xi \in \mathcal{E}'$. As seen above, the functional

$$\mathrm{tr}_\xi : \xi \otimes \mathcal{E} \to \mathcal{J}$$

defined by (4.3a) is an antihomomorphism on the left ideal $\xi \otimes \mathcal{E}$ of $\mathcal{L}(\mathcal{E})$.

In the $\mathcal{J}$-Banach algebra $\xi \otimes \mathcal{E}$, the operator version of (4.1a) in its potential form reads as

$$V_t - V_{xxx} - 3(V_x)^2 = 0. \tag{4.4}$$

Following the result in Sec. III we assume that L, M are solutions of the corresponding linearized equation which are realized by an operator $G \in \mathcal{L}(\mathcal{E})$, i.e.,

$$L_x = GL, \quad L_t = G^3 L, \quad L \in \mathcal{L}(\mathcal{E}), \tag{4.5a}$$

$$M_x = GM, \quad M_t = G^3 M, \quad M \in \xi \otimes \mathcal{E}, \tag{4.5b}$$

and the couple relation

$$GL + LG = M. \tag{4.5c}$$

Note that the solutions for M are searched in the left ideal $\xi \otimes \mathcal{E}$ while the solutions for L should be found in general in the bigger space $\mathcal{L}(\mathcal{E})$.

The solution of (4.4) is given by

$$V = (I + L)^{-1} M \tag{4.6a}$$

and thus $U := V_x$ solves the following operator KdV equation:

$$U_t - U_{xxx} - 3(UU)_x = 0. \tag{4.6b}$$

Let

$$\mathbf{u} := \mathrm{tr}_\xi(U) = \mathrm{tr}_\xi(V)_x. \tag{4.6c}$$

Then an application of the antihomomorphism tr_ξ to both sides of (4.6b) yields that $\mathbf{u}$ is a solution of the $\mathcal{J}$-KdV equation (4.1a).

Again, this approach has also reduced a nonlinear problem (4.1a) of KdV type into a process of solving linear equations (4.5a)–(4.5c).

To find a more transparent representation for the solutions given in (4.6c), we impose the following spectral condition on the generator G:

$$0 \notin \mathrm{Sp}(G) + \mathrm{Sp}(G), \tag{4.7a}$$

where $\mathrm{Sp}(G)$ denotes the spectrum of G. It is known (cf. Refs. 4 and 6) that (4.7a) guarantees that the operator equation $GA + AG = B$ has a unique solution $A \in \mathcal{L}(\mathcal{E})$ for each given operator $B \in \mathcal{L}(\mathcal{E})$.

We take the following solutions of M:

$$M(x,t) = e^{xG + tG^3} Y \quad \text{with some} \quad Y \in \xi \otimes \mathcal{E}. \tag{4.7b}$$

Then the solution of the operator equation $GL + LG = M$ has the form

$$L(x,t)=e^{xG+tG^3}X, \tag{4.7c}$$

where $X\in\mathcal{L}(\mathcal{E})$ is uniquely determined by the operator equation

$$GX+XG=Y. \tag{4.7d}$$

As seen before, the solvability of the operator equation (4.7d) is guaranteed by the spectral condition (4.7a). Thus, each element $Y\in\xi\otimes\mathcal{E}$ has generated a solution of the $\mathcal{J}$-KdV equation (4.1a). We denote this solution as $\mathbf{u}[G,Y]$, i.e.,

$$\mathbf{u}[G,Y]:=\mathrm{tr}_{\xi}((I_{\mathcal{E}}+e^{xG+tG^3}X)^{-1}e^{xG+tG^3}Y)_x, \tag{4.8a}$$

in order to indicate its dependence on the generator G and the given element $Y\in\xi\otimes\mathcal{E}$. In the practical computation we use the following equivalent form of (4.8a):

$$\mathbf{u}[G,Y]=\mathrm{tr}_{\xi}((e^{-xG-tG^3}+X)^{-1}Y)_x. \tag{4.8a$'$}$$

According to the above construction, in the following context we shall call the triple

$$\{\mathcal{E},G,\xi\}$$

a solving process. That is, here $\mathcal{E}$ is a $\mathcal{J}$-Banach space, G a bounded $\mathcal{J}$-linear operator on $\mathcal{E}$ satisfying the spectral condition (4.7a), and ξ an element in the dual space $\mathcal{E}'$.

The vacuum solution is obtained by switching the rank one operator Y into zero, i.e.,

$$\mathbf{u}[G,0]\equiv 0. \tag{4.8b}$$

Since $\xi\otimes\mathcal{E}$ is a Banach space, the sum $Y+Z$ of $Y,Z\in\xi\otimes\mathcal{E}$ belongs again to $\xi\otimes\mathcal{E}$ and thus defines a solution $\mathbf{u}[G,Y+Z]$. Since the two old solutions $\mathbf{u}[G,Y]$ and $\mathbf{u}[G,Z]$ are the result of switching Z and Y into zero, respectively, the new solution $\mathbf{u}[G,Y+Z]$ describes the interaction between the two old ones and hence it is the result of joining the two old solutions. In notation, we have

$$\mathbf{u}[G,Y]\bowtie\mathbf{u}[G,Z]=\mathbf{u}[G,Y+Z],\quad Y,Z\in\xi\otimes\mathcal{E} \tag{4.9}$$

or say that the "$\bowtie$" defines an operation between solutions.

The "$\bowtie$" operation has richer properties. We give some of them.

1. Existence of annihilator

It follows from the definition combining with the property (4.8b) that

$$\mathbf{u}[G,Y]\bowtie\mathbf{u}[G,-Y]=\mathbf{u}[G,Y+(-Y)]=\mathbf{u}[G,0]\equiv 0.$$

Equivalently,

$$\mathbf{u}[G,Y]\bowtie\mathbf{u}[G,-Y]\equiv 0.$$

This means, the solutions $\mathbf{u}[G,Y]$ and $\mathbf{u}[G,-Y]$ annihilate each other.

2. Generating new solutions by prolongation

Given are two solving processes $\{\mathcal{E}_1,H_1,\xi_1\}$ and $\{\mathcal{E}_2,H_2,\xi_2\}$. Under appropriate additional spectral conditions we shall construct a new solving process, namely, the so-called direct sum

$$\{\mathcal{E}_1,H_1,\xi_1\}\oplus\{\mathcal{E}_2,H_2,\xi_2\}\equiv\{\mathcal{E}_1\oplus\mathcal{E}_2,H_1\oplus H_2,\xi_1\oplus\xi_2\}.$$

We set

$$\mathcal{E}:=\mathcal{E}_1\oplus\mathcal{E}_2,\quad H:=H_1\oplus H_2\in\mathcal{L}(\mathcal{E}),\quad \xi:=\xi_1\oplus\xi_2\in\mathcal{E}'.$$

The following identifications

$$\mathcal{E}_1 \cong \mathcal{E}_1 \oplus \mathbf{0}_2, \quad \mathcal{E}_2 \cong \mathbf{0}_1 \oplus \mathcal{E}_2$$

prolongate vectors in $\mathcal{E}_1$ and $\mathcal{E}_2$ as vectors in the direct sum $\mathcal{E}$. Here, $\mathbf{0}_i$ is the zero vector of $\mathcal{E}_i$. More precisely, a vector $\eta_1 \in \mathcal{E}_1$ is identified with the vector $\eta_1 \oplus \mathbf{0}_2$. Similarly, a vector $\eta_2 \in \mathcal{E}_2$ is identified with the vector $\mathbf{0}_1 \oplus \eta_2$ in $\mathcal{E}$. In this way, both $\mathcal{E}_1$ and $\mathcal{E}_2$ are identified as subspaces of $\mathcal{E}$. Moreover, the antihomomorphism $\mathrm{tr}_\xi : \xi \otimes \mathcal{E} \to \mathcal{J}$ extends both antihomomorphisms $\mathrm{tr}_{\xi_j} : \xi_j \otimes \mathcal{E}_j \to \mathcal{J}$ $(j=1,2)$ in the sense that

$$\mathrm{tr}_\xi(\xi \otimes \eta_j) = \langle \xi_j, \eta_j \rangle = \mathrm{tr}_{\xi_j}(\xi_j \otimes \eta_j) \quad \text{for all} \quad \eta_j \in \mathcal{E}_j.$$

We have $\mathrm{Sp}(H_1 \oplus H_2) = \mathrm{Sp}(H_1) \cup \mathrm{Sp}(H_2)$. Therefore, the spectral condition (4.7a) for $H = H_1 \oplus H_2$ is equivalent to the following:

$$0 \notin \{\lambda + \mu : \lambda, \mu \in \mathrm{Sp}(H_1) \cup \mathrm{Sp}(H_2)\}. \tag{4.10}$$

Consequently,

$$\{\mathcal{E}, H, \xi\} \equiv \{\mathcal{E}_1 \oplus \mathcal{E}_2, H_1 \oplus H_2, \xi_1 \oplus \xi_2\}$$

gives a solving process whenever the additional spectral condition (4.10) is satisfied.

Now we assume (4.10). For each pair $(\eta_1, \eta_2) \in \mathcal{E}_1 \otimes \mathcal{E}_2$ we have two solutions $s_j := \mathbf{u}[H_j, \xi_j \otimes \eta_j]$ $(j=1,2)$ of the $\mathcal{J}$-KdV equation (4.1a). Moreover, for $\eta := \eta_1 \oplus \eta_2 \in \mathcal{E}$ we have also a solution $s := \mathbf{u}[H_1 \oplus H_2, \xi \otimes \eta]$ which can be rewritten as

$$\mathbf{u}[H_1 \oplus H_2, \xi \otimes \eta] = \mathbf{u}[H_1 \oplus H_2, Y_1 + Y_2]$$

with

$$Y_j := \xi \otimes \eta_j \in \xi \otimes \mathcal{E}_j \quad (j=1,2).$$

Note that each rank one operator Y_j generates a solution

$$S_j := \mathbf{u}[H_1 \oplus H_2, Y_j] \quad (j=1,2).$$

As interpreted before, the new solution s is just the result of joining the two solutions S_1 and S_2 together, i.e.,

$$S_1 \bowtie S_2 = s. \tag{4.11a}$$

We want to show that the solutions S_1, S_2 are nothing but the old ones s_1, s_2 and thus s describes the interaction of the two old solutions. Hence, we can extend the "$\bowtie$" operation given in (4.9) to any solutions and denote it by

$$\mathbf{u}[H_1, \xi_1 \otimes \eta_1] \bowtie \mathbf{u}[H_2, \xi_2 \otimes \eta_2] = \mathbf{u}[H_1 \oplus H_2, (\xi_1 \oplus \xi_2) \otimes (\eta_1 \oplus \eta_2)]. \tag{4.11b}$$

Below we establish the expected equalities $S_j = s_j$ $(j=1,2)$. For this purpose, we represent each operator A on the direct sum $\mathcal{E}$ as a 2×2 operator matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{with operators } A_{ij} : \mathcal{E}_j \to \mathcal{E}_i. \tag{4.12a}$$

In the computation of the inverses we will use the following important rule: Assume A_{11} to be invertible. Then A is invertible if and only if its *Schur complement*

$$\Delta(A) := A_{22} - A_{21}A_{11}^{-1}A_{12} \tag{4.12b}$$

is invertible as an operator on $\mathcal{E}_2$. In case A is invertible, its inverse is given by

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} + A_{11}^{-1}A_{12}\Delta^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}\Delta^{-1} \\ -\Delta^{-1}A_{21}A_{11}^{-1} & \Delta^{-1} \end{pmatrix}, \tag{4.12c}$$

where $\Delta^{-1} := \Delta(A)^{-1}$. The matrix representation of the direct sum H is the diagonal ones $H = \mathrm{diag}(H_1, H_2)$ and thus its exponentials $T = T(x,t) := \exp(-xH - tH^3)$ have the matrix form

$$T = e^{-xH - tH^3} = \mathrm{diag}(T_1, T_2), \quad T_j := e^{-xH_j - tH_j^3}. \tag{4.13}$$

The sum $Y = Y_1 + Y_2 = (Y_{ij})_{2\times 2}$ has entries

$$Y_{ij} := \xi_j \otimes \eta_i \in \xi_j \otimes \mathcal{E}_i \quad (i,j = 1,2) \tag{4.14a}$$

and the entries of the unique solution $X = (X_{ij})_{2\times 2}$ of the operator equation $HX + XH = Y$ are uniquely determined by the operator equations

$$\begin{aligned} &H_1X_{11} + X_{11}H_1 = \xi_1 \otimes \eta_1, \quad H_1X_{12} + X_{12}H_2 = \xi_2 \otimes \eta_1, \\ &H_2X_{21} + X_{21}H_1 = \xi_1 \otimes \eta_2, \quad H_2X_{22} + X_{22}H_2 = \xi_2 \otimes \eta_2. \end{aligned} \tag{4.14b}$$

By definition, we have

$$s = \mathbf{u}[H_1 \oplus H_2, Y_1 + Y_2] = \mathrm{tr}_\xi (K^{-1}Y)_x, \tag{4.15a}$$

where $K = (K_{ij})_{2\times 2} := T + X$ has entries

$$\begin{aligned} &K_{11} := T_1 + X_{11}, \quad K_{12} := X_{12}, \\ &K_{21} := X_{21}, \quad K_{22} := T_2 + X_{22}. \end{aligned} \tag{4.15b}$$

Recall that the old solutions s_1, s_2 are given by

$$s_j = \mathrm{tr}_{\xi_j}(K_{jj}^{-1}Y_{jj})_x, \quad j = 1,2.$$

Since the restriction of tr_ξ in each of the subspaces $\xi_j \otimes \mathcal{E}_j \subset \xi \otimes \mathcal{E}$ is tr_{ξ_j}, we can rewrite the solutions s_j as

$$s_j = \mathrm{tr}_\xi (K_{jj}^{-1}Y_{jj})_x, \quad j = 1,2.$$

In case K_{11} is invertible we can apply the rule in (4.12c) to find that $K = T + X$ is invertible if and only if its Schur complement

$$\Delta \equiv \Delta(K) = K_{22} - K_{21}K_{11}^{-1}K_{12} \tag{4.16a}$$

is invertible and therefore we can compute the inverse of K by (4.12c). It follows that the sum of the diagonal entries of $K^{-1}Y$ is

$$K_{11}^{-1}Y_{11} + K_{11}^{-1}K_{12}\Delta^{-1}(K_{21}K_{11}^{-1}Y_{11} - Y_{21}) - \Delta^{-1}K_{21}K_{11}^{-1}Y_{12} + \Delta^{-1}Y_{22} = K_{11}^{-1}Y_{11} + K_{22}^{-1}Y_{22} + C_{12},$$

where

$$C_{12} := K_{11}^{-1}K_{12}\Delta^{-1}(K_{21}K_{11}^{-1}Y_{11} - Y_{21}) + \Delta^{-1}K_{21}K_{11}^{-1}(K_{22}^{-1}Y_{22} - Y_{12}). \tag{4.16b}$$

Consequently, the newly generated solution $s=\mathbf{u}[H_1\oplus H_2, Y_1+Y_2]$, as the spatial derivative of the trace of the sum of the diagonal entries of $K^{-1}Y$, is equal to

$$s=s_1+s_2+c_{12}, \quad c_{12}:=\mathrm{tr}_{\xi}(C_{12})_x. \tag{4.16c}$$

The cross term c_{12} reflects the interaction of the two old solutions s_1 and s_2.

Now we switch η_2 into zero, i.e., we set $\eta_2=0$. Then $Y_{21}=0, Y_{22}=0$ and thus $X_{21}=0, X_{22}=0$, $K_{21}=X_{21}=0$. It yields that $c_{12}=0$ and $s_2=0$, hence $s=s_1+s_2+c_{12}=s_1$. In other words, we have established the desired equality $s_1=\mathbf{u}[H,Y_1]=S_1$. The other equality $s_2=S_2$ can be proved in the same spirit.

The above approach yields simultaneously the following criterion for the smoothness of the newly generated solution $\mathbf{u}[H_1,\xi_1\otimes\eta_1]\bowtie\mathbf{u}[H_2,\xi_2\otimes\eta_2]$: Assume both of the old solutions $\mathbf{u}[H_1,\xi_1\otimes\eta_1], \mathbf{u}[H_2,\xi_2\otimes\eta_2]$ are smooth, i.e., both $K_{11}(x,t)$ and $K_{22}(x,t)$ are invertible for each point $(x,t)\in\mathbb{R}^2$. Then $\mathbf{u}[H_1,\xi_1\otimes\eta_1]\bowtie\mathbf{u}[H_2,\xi_2\otimes\eta_2]$ is a smooth solution whenever the Schur complement $\Delta(K)$ is invertible everywhere, i.e., for each $(x,t)\in\mathbb{R}^2$ the operator $\Delta(K)(x,t)$ is invertible.

In case the newly generated solution $\mathbf{u}[H_1,\xi_1\otimes\eta_1]\bowtie\mathbf{u}[H_2,\xi_2\otimes\eta_2]$, which describes the interaction of the old solutions $\mathbf{u}[H_1,\xi_1\otimes\eta_1]$ and $\mathbf{u}[H_2,\xi_2\otimes\eta_2]$, is smooth, we say that $\mathbf{u}[H_1,\xi_1\otimes\eta_1]$ and $\mathbf{u}[H_2,\xi_2\otimes\eta_2]$ interact *smoothly*; otherwise *singularly*.

As it will be seen later, the interaction of two smooth solutions might be singular, i.e., they might undergo a blow-up by interaction.

D. Solitary wave solutions and their interaction

We shall use the solution program written in Sec. IV C to find solitary wave solutions of the $\mathcal{J}$-KdV equation and to study their interaction.

Fix $n\in\mathbb{N}$. The product $\mathcal{J}^n$ is a $\mathcal{J}$-Banach space as well as a $\mathcal{J}$-Banach algebra. We take $\mathcal{E}\equiv\mathcal{J}^n$ as the underlying Banach space. Elements in $\mathcal{J}^n$ are written as vector columns $(b_1,\ldots,b_n)^T$ with $b_1,\ldots,b_n\in\mathcal{J}$.

For each $\mathbf{a}\in\mathcal{J}$ we defined an element $\hat{\mathbf{a}}\in\mathcal{L}(\mathcal{J})$ by

$$\hat{\mathbf{a}}(\mathbf{b}):=\mathbf{ba} \quad (\mathbf{b}\in\mathcal{J}). \tag{4.17a}$$

The mapping $\mathcal{J}\ni\mathbf{a}\mapsto\hat{\mathbf{a}}\in\mathcal{L}(\mathcal{J})$ is an antihomomorphism:

$$\widehat{\mathbf{ab}}=\hat{\mathbf{b}}\hat{\mathbf{a}} \quad (\mathbf{a},\mathbf{b}\in\mathcal{J}). \tag{4.17b}$$

Below we will identify a real constant $r\in\mathbb{R}$ with $\hat{r}\in\mathcal{L}(\mathcal{J})$.

Let $\xi:=(1,1,\ldots,1)$ be the functional on $(\mathcal{J}^n)'$ defined by

$$\xi(\mathbf{a}):=\sum_{j=1}^{n}\mathbf{a}_j \quad \text{for } \mathbf{a}=(\mathbf{a}_1,\ldots,\mathbf{a}_n)^T\in\mathcal{J}^n.$$

Let $\lambda_1,\ldots,\lambda_n$ be real numbers such that

$$\lambda_i+\lambda_j\neq 0, \quad \forall i,j. \tag{4.18a}$$

We call readers' attention to the fact that all of our calculations below will be carried out with the special functional ξ defined by (4.18a). In particular, the reader should remember that the antihomomorphism tr_{ξ} is only well defined on the left ideal $\xi\otimes\mathcal{J}^n$.

We consider the generator $G:=\mathrm{diag}(\lambda_1,\ldots,\lambda_n)\in\mathcal{L}(\mathcal{J}^n)$. Then

$$T:=\exp(-xG-tG^3)=\mathrm{diag}(w_1,w_2,\ldots,w_n) \tag{4.18b}$$

has entries

$$w_j \equiv w_j(\lambda_j, x, t) := e^{-x\lambda_j - t\lambda_j^3}. \tag{4.18c}$$

For given $\mathbf{a} := (\mathbf{a}_1, \ldots, \mathbf{a}_n)^T \in \mathcal{J}^n$ we set $\eta \equiv \eta[\lambda, \mathbf{a}] := ((2\lambda_1)\mathbf{a}_1, \ldots, (2\lambda_n)\mathbf{a}_n)^{T\cdot} \in \mathcal{J}^n$. Then the rank one operator $Y[\lambda, \mathbf{a}] := \xi \otimes \eta$ has the matrix representation

$$Y[\lambda, \mathbf{a}] = \begin{pmatrix} (2\lambda_1)\hat{\mathbf{a}}_1 & \cdots & (2\lambda_1)\hat{\mathbf{a}}_1 \\ \cdots & \cdots & \cdots \\ (2\lambda_n)\hat{\mathbf{a}}_n & \cdots & (2\lambda_n)\hat{\mathbf{a}}_n \end{pmatrix}. \tag{4.19a}$$

The unique solution of the operator equation $GX + XG = Y[\lambda, \mathbf{a}]$, denoted by $X[\lambda, \mathbf{a}]$, is given by

$$X[\lambda, \mathbf{a}] = \begin{pmatrix} k_{11}\hat{\mathbf{a}}_1 & \cdots & k_{1n}\hat{\mathbf{a}}_1 \\ \cdots & \cdots & \cdots \\ k_{n1}\hat{\mathbf{a}}_n & \cdots & k_{nn}\hat{\mathbf{a}}_n \end{pmatrix}, \quad k_{ij} := \frac{2\lambda_i}{\lambda_i + \lambda_j}. \tag{4.19b}$$

We denote the generated solutions $\mathbf{u}[G, \xi \otimes \eta[\lambda, \mathbf{a}]]$ by $\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n]$ in order to indicate their dependence on the spectral parameters $\lambda_j' s$ and the vector rows $\mathbf{a}$. We have

$$\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n] = \mathrm{tr}_\xi((T + X[\lambda, \mathbf{a}])^{-1} Y[\lambda, \mathbf{a}])_x \tag{4.20}$$

[cf. (4.8a')]. Since $\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n]$ depends on the vector $\mathbf{w} = (w_1, w_2, \ldots, w_n)$ as well as on the vectors $\lambda = (\lambda_1, \ldots, \lambda_n)$ and $\mathbf{a} = (\mathbf{a}_1, \ldots, \mathbf{a}_n)$, we represent this solution as

$$\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n] \equiv \mathbf{u}(\mathbf{w}, \lambda, \mathbf{a}). \tag{4.21a}$$

The annihilator (cf. Sec. IV C 1) of $\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n]$ is the solution

$$\mathbf{u}[\lambda_1, -\mathbf{a}_1, \ldots, \lambda_n, -\mathbf{a}_n] = \mathrm{tr}_\xi((T + X[\lambda, -\mathbf{a}])^{-1} Y[\lambda, -\mathbf{a}])_x.$$

Note that $Y[\lambda, -\mathbf{a}] = -Y[\lambda, \mathbf{a}]$ and $X[\lambda, -\mathbf{a}] = -X[\lambda, \mathbf{a}]$. We have

$$\mathrm{tr}_\xi((T + X[\lambda, -\mathbf{a}])^{-1} Y[\lambda, -\mathbf{a}])_x = \mathrm{tr}_\xi((-T + X[\lambda, \mathbf{a}])^{-1} Y[\lambda, \mathbf{a}])_x.$$

Therefore, if we have calculated the solution $\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n]$ and written it in the form (4.21a), then its annihilator $\mathbf{u}[\lambda_1, -\mathbf{a}_1, \ldots, \lambda_n, -\mathbf{a}_n]$ is just the result of the replacement of $\mathbf{w}$ by $-\mathbf{w}$, i.e.,

$$\mathbf{u}[\lambda_1, -\mathbf{a}_1, \ldots, \lambda_n, -\mathbf{a}_n] \equiv \mathbf{u}(-\mathbf{w}, \lambda, \mathbf{a}). \tag{4.21b}$$

Another useful property is that if ϕ is an automorphism on $\mathcal{J}$, then

$$\mathbf{u}[\lambda_1, \phi\mathbf{a}_1, \ldots, \lambda_n, \phi\mathbf{a}_n] = \phi\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n]. \tag{4.21c}$$

We remark (cf. Refs. 2 or 6 and 10) that the class of scalar solutions $\mathbf{u}[\lambda_1, \mathbf{a}_1, \ldots, \lambda_n, \mathbf{a}_n] \in \mathbb{R} \cdot I_{\mathcal{J}}$ generated by positive parameters $\lambda_j > 0$ and $\mathbf{a}_j = a_j I_{\mathcal{J}}$ with $a_j > 0$ coincides with the class of multisoliton solutions of the scalar KdV equation constructed by the Hirota method[11] or the inverse scattering method.[1]

1. Solitary waves

These solutions will be obtained by switching all $\mathbf{a}_2, \mathbf{a}_3, \ldots, \mathbf{a}_n$ into zeros. Therefore, by setting $\mathbf{a}_2 = \cdots = \mathbf{a}_n = 0$ in (4.20) and then dropping the suffices we obtain the solitary wave solution with velocity λ and a parameter $\mathbf{a} \in \mathcal{J}$

$$\mathbf{u}[\lambda, \mathbf{a}] := (2\lambda) \cdot ((e^{-x\lambda - t\lambda^3} + \mathbf{a})^{-1} \mathbf{a})_x. \tag{4.22a}$$

Here and later, we use the abbreviation $c+\mathbf{a}\equiv cI_{\mathcal{J}}+\mathbf{a}$ for real numbers c. By writing the product $(e^{-x\lambda-t\lambda^3}+\mathbf{a})^{-1}\mathbf{a}$ as the difference $1-(1+e^{x\lambda+t\lambda^3}\mathbf{a})^{-1}$ we simplify the representation of $\mathbf{u}$ into

$$\mathbf{u}[\lambda,\mathbf{a}](x,t)=(-2\lambda)\cdot((1+e^{x\lambda+t\lambda^3}\mathbf{a})^{-1})_x, \tag{4.22b}$$

or equivalently, with $w=w(\lambda,x,t):=e^{-x\lambda-t\lambda^3}$,

$$\mathbf{u}[\lambda,\mathbf{a}](x,t)=(2\lambda^2)\cdot(w\mathbf{a})(w+\mathbf{a})^{-2}. \tag{4.22c}$$

This gives the parametrized representation of all nonperiodic solitary wave solutions of (4.1a), where the parameter $(\lambda, \mathbf{a})$ runs through the set $\mathbb{R}\times\mathcal{J}$.

It is easily seen that a solitary wave solution $\mathbf{u}[\lambda,\mathbf{a}]$ with $\lambda\neq 0$ is a smooth solution if and only if the parameter $\mathbf{a}$ locates in the subset $\mathcal{J}_s$ of $\mathcal{J}$:

$$\mathcal{J}_s:=\{\mathbf{b}\in\mathcal{J}:\mathbf{b}+\mu I_{\mathcal{J}} \text{ is invertible for all } \mu\geqslant 0\}. \tag{4.23}$$

Note that a smooth solitary wave solution $\mathbf{u}[\lambda,\mathbf{a}]$ is also bounded and localized in the sense that

$$\mathbf{u}[\lambda,\mathbf{a}]\to 0 \quad \text{as } x\lambda+t\lambda^3\to\pm\infty.$$

Now the meaning of the solution $\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]$ in (4.20) becomes clear. It just describes the interaction of the given n solitary waves $\mathbf{u}[\lambda_i,\mathbf{a}_i]$ $(i=1,2,\ldots,n)$. Therefore, using our "$\bowtie$" operation, it can be represented as

$$\bowtie_{i=1}^{k}\mathbf{u}[\lambda_i,\mathbf{a}_i]=\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n].$$

2. Interaction of two solitary waves

To study the interaction of two solitary waves, we apply the formula (4.19) with a replacement of $\mathbf{a}_1,\mathbf{a}_2$ by the letters $\mathbf{a}$, $\mathbf{b}$. We have

$$\mathbf{u}[\lambda_1,\mathbf{a}]\bowtie\mathbf{u}[\lambda_2,\mathbf{b}]=\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=\mathrm{tr}_{\xi}(K^{-1}\xi\otimes\eta)_x,$$

where $K=T+X=(K_{ij})_{2\times 2}$ has entries

$$K_{11}=w_1+\hat{\mathbf{a}},K_{12}=k_1\hat{\mathbf{a}},\quad K_{21}=k_2\hat{\mathbf{b}},\quad K_{22}=w_2+\hat{\mathbf{b}},$$

$$w_j\equiv w_j(\lambda_j,x,t)=\exp(-x\lambda_j-t\lambda_j^3),\quad j=1,2,$$

$$k_j:=(2\lambda_j)/(\lambda_1+\lambda_2),\quad j=1,2,$$

and

$$\xi=(1,1)\in(\mathcal{J}^2)',\quad \eta=(2\lambda_1\mathbf{a},2\lambda_2\mathbf{b})^T\in\mathcal{J}^2.$$

We assume further that both $\mathbf{a},\mathbf{b}\in\mathcal{J}$ have no real spectra, i.e., for each real number r both sums $\mathbf{a}+r$ and $\mathbf{b}+r$ are invertible. In particular, the sum $w_1+\hat{\mathbf{a}}$ is invertible and thus the Schur complement of K is

$$\Delta(K)=K_{22}-K_{21}K_{11}^{-1}K_{12}=(w_2+\hat{\mathbf{b}})-(k_2\hat{\mathbf{b}})(w_1+\hat{\mathbf{a}})^{-1}(k_1\hat{\mathbf{a}}),$$

which can be rewritten as $\Delta(K)=\hat{\delta}\cdot(w_1+\hat{\mathbf{a}})^{-1}$ with

$$\delta\equiv\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]:=(w_1+\mathbf{a})(w_2+\mathbf{b})-(k_1k_2)\mathbf{ab}. \tag{4.24}$$

Hence, $\Delta(K)$ at the point $(x,t)\in\mathbb{R}^2$ is invertible if and only if so is δ at that point. δ is called the *determinant* of the matrix K.

Since $\mathrm{tr}_\xi(K^{-1}\xi\otimes\eta)=\mathrm{tr}_\xi(\xi\otimes(K^{-1}\eta))$, we have

$$\mathrm{tr}_\xi(K^{-1}\xi\otimes\eta)=2(\eta_1+\eta_2),$$

where $\eta_{1,2}\in\mathcal{J}$ are determined by the equation $\eta=K(\eta_1,\eta_2)^T$, or equivalently,

$$\begin{aligned}\eta_1(w_1+\mathbf{a})+k_1\eta_2\mathbf{a}&=\lambda_1\mathbf{a},\\ k_2\eta_1\mathbf{b}+\eta_2(w_2+\mathbf{b})&=\lambda_2\mathbf{b}.\end{aligned}\tag{4.25a}$$

We need to find the sum $\eta_1+\eta_2$. For this purpose, we set $\eta_3:=(\eta_1+\eta_2)/2$, $\eta_4:=(\eta_1-\eta_2)/2$ and substitute them into (4.25a). Then the equations for η_3,η_4 are

$$\eta_3(w_1+\mathbf{a}+k_1\mathbf{a})(w_1+\mathbf{a}-k_1\mathbf{a})^{-1}+\eta_4=\lambda_1\mathbf{a}(w_1+\mathbf{a}-k_1\mathbf{a})^{-1},$$

$$\eta_3(w_2+\mathbf{b}+k_2\mathbf{b})(w_2+\mathbf{b}-k_2\mathbf{b})^{-1}-\eta_4=\lambda_2\mathbf{b}(w_2+\mathbf{b}-k_2\mathbf{b})^{-1}.$$

Summing up the two equations, we obtain that

$$2\eta_3=(w_1+(1-k_1)\mathbf{a})^{-1}\cdot\alpha\cdot\delta^{-1}\cdot(w_1+(1-k_1)\mathbf{a}),$$

where δ is the determinant given by (4.24a) and

$$\alpha:=(\lambda_1\mathbf{a})(w_2+(1-k_2)\mathbf{b})+(w_1+(1-k_1)\mathbf{a})(\lambda_2\mathbf{b}).$$

Using the definition $k_j=\lambda_j/(\lambda_1+\lambda_2)$ $(j=1,2)$ we rewrite the term α as

$$2(\lambda_1+\lambda_2)\cdot\alpha=2\delta-(2w_1w_2+k_2w_2\mathbf{a}+k_1w_1\mathbf{b}).$$

It follows that $4(\lambda_1+\lambda_2)\eta_3=2-\eta_3'$ with

$$\eta_3':=[w_1+(1-k_1)\mathbf{a}]^{-1}\cdot(2w_1w_2+k_2w_2\mathbf{a}+k_1w_1\mathbf{b})\cdot\delta^{-1}\cdot[w_1+(1-k_1)\mathbf{a}]\tag{4.25b}$$

and thus

$$\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=\mathrm{tr}_\xi(K^{-1}\xi\otimes\eta)_x=-(\lambda_1+\lambda_2)^{-1}\cdot(\eta_3')_x.\tag{4.25c}$$

The above approach yields also the following smoothness criterion: Assume both solutions $\mathbf{u}[\lambda_1,\mathbf{a}]$ and $\mathbf{u}[\lambda_2,\mathbf{b}]$ are smooth, i.e., both $w_1(x,t)+\mathbf{a}$ and $w_2(x,t)+\mathbf{b}$ are invertible for each $(x,t)\in\mathbb{R}^2$. Then the newly generated solution $\mathbf{u}[\lambda_1,\mathbf{a}]\bowtie u[\lambda_2,\mathbf{b}]$ is a smooth solution if and only $\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}](x,t)$ is invertible for every $(x,t)\in\mathbb{R}^2$. We note that the first condition in the above criterion is equivalent to that both **a** and **b** generate localized solitary wave solutions. However, the second ones implies that two localized solitary waves might interact singularly. Such examples for the case $\mathcal{J}=\mathbb{H}$ the Hamilton quaternions will be seen in the next section.

The asymptotic behavior of the interaction $\mathbf{u}[\lambda_1,\mathbf{a}]\bowtie\mathbf{u}[\lambda_2,\mathbf{b}]$ is easily to describe if both **a** and **b** are invertible. The result is that if the interaction is asymptotically smooth then the only effect of the interaction of these two solitary waves is asymptotically a phase shift and thus these two solitary waves interact asymptotically elastic.

To see this, we assume both $\mathbf{a},\mathbf{b}\in\mathcal{J}_s$ are invertible and that for $|x|,|t|$ sufficiently large the term $\delta(x,t)\equiv(w_1(x,t)+\mathbf{a})(w_2(x,t)+\mathbf{b})-(k_1k_2)\mathbf{ab}$ is always invertible. We consider the trajectory $w_1=\text{constant}$, and assume $\lambda_1>0,\lambda_2>0$. Then

$$\delta\sim(w_1+\gamma\mathbf{a})\mathbf{b}\quad\text{as}\quad t\to+\infty,$$

$$\delta \sim (w_1 + \mathbf{a})(w_2 + \mathbf{b}) \quad \text{as} \quad t \to -\infty,$$

where

$$\gamma := 1 - (k_1 k_2) = (\lambda_1 - \lambda_2)^2/(\lambda_1 + \lambda_2)^2 > 0.$$

This implies by (4.25b) and (4.25c) that

$$\mathbf{u}[\lambda_1, \mathbf{a}] \bowtie \mathbf{u}[\lambda_2, \mathbf{b}] \sim \mathbf{u}[\lambda_1, \gamma \mathbf{a}] \quad \text{as} \quad t \to +\infty,$$

$$\mathbf{u}[\lambda_1, \mathbf{a}] \bowtie \mathbf{u}[\lambda_2, \mathbf{b}] \sim \mathbf{u}[\lambda_1, \mathbf{a}] \quad \text{as} \quad t \to -\infty.$$

Similarly, for fixed w_2

$$\mathbf{u}[\lambda_1, \mathbf{a}] \bowtie \mathbf{u}[\lambda_2, \mathbf{b}] \sim \mathbf{u}[\lambda_2, \gamma \mathbf{b}] \quad \text{as} \quad t \to +\infty,$$

$$\mathbf{u}[\lambda_1, \mathbf{a}] \bowtie \mathbf{u}[\lambda_2, \mathbf{b}] \sim \mathbf{u}[\lambda_2, \mathbf{b}] \quad \text{as} \quad t \to -\infty.$$

Note that the difference between the two solitary waves $\mathbf{u}[\lambda_1, \gamma \mathbf{a}]$ (respectively, $\mathbf{u}[\lambda_2, \gamma \mathbf{b}]$) and $\mathbf{u}[\lambda_1, \mathbf{a}]$ (respectively, $\mathbf{u}[\lambda_1, \mathbf{b}]$) is only a phase shift. In other words, we have proved that the interaction of such two solitary waves is asymptotically elastic.

3. Condition for smoothness of interaction

Let $\{\mathcal{E}, G, \xi\}$ be a real solution process, i.e., $\mathcal{E}$ is a real Banach space and $G \in \mathcal{L}(\mathcal{E})$ a generator satisfying the spectral condition (4.7a): $0 \notin \mathrm{Sp}(G) + \mathrm{Sp}(G)$. We consider a real valued solution

$$\mathbf{u}[G, \xi \otimes \eta] = \mathrm{tr}((T + X)^{-1}(\xi \otimes \eta))_x$$

and assume it is smooth in the sense that

$$(T + X)(x, t) = \exp(-xG - tG^3) + X$$

is invertible for every $(x, t) \in \mathbb{R}^2$. As seen in Sec. IV B, the algebraic tensor product $\tilde{\mathcal{E}} := \mathcal{J} \otimes \mathcal{E}$ is a $\mathcal{J}$-Banach space and the operators G, X, T, the vector $\eta \in \mathcal{E}$ as well as the functional $\xi \in \mathcal{E}'$ admit their $\mathcal{J}$-extensions; denoted by $\tilde{G}$, $\tilde{T}$, $\tilde{X}$, $\tilde{\eta}$, and $\tilde{\xi}$.

Let $\lambda \in \mathbb{R}$ be such that

$$-\lambda \notin \{0\} \cup \mathrm{Sp}(G). \tag{4.26}$$

The generator $H := \tilde{G} \oplus \lambda$ on the direct product $\tilde{\mathcal{E}} \oplus \mathcal{J}$ has spectrum $\mathrm{Sp}(H) = \{\lambda\} \cup \mathrm{Sp}(G)$ and thus, by (4.26), satisfies the required spectral condition (4.7a), i.e., $0 \notin \mathrm{Sp}(H) + \mathrm{Sp}(H)$. Hence, we have a new solution process $\{\tilde{\mathcal{E}} \oplus \mathcal{J}, H, \tilde{\xi} \oplus 1\}$ (cf. Sec. IV C 2). Moreover, since

$$\mathbf{u}[\tilde{G}, \tilde{\xi} \otimes \tilde{\eta}] = \mathbf{u}[G, \xi \otimes \eta] \cdot I_{\mathcal{J}},$$

for each $\mathbf{a} \in \mathcal{J}$ the solution

$$s := \mathbf{u}[H, (\tilde{\xi} \oplus 1) \otimes (\tilde{\eta} \oplus \mathbf{a})] = (\mathbf{u}[G, \xi \otimes \eta] \cdot I_{\mathcal{J}}) \bowtie \mathbf{u}[\lambda, \mathbf{a}]$$

describes the interaction of the solution $\mathbf{u}[G, \xi \otimes \eta]$ of the scalar KdV equation with the solitary wave solution $\mathbf{u}[\lambda, \mathbf{a}]$ of the $\mathcal{J}$-KdV equation. We want to find the condition on the parameter $\mathbf{a}$ which ensures the smoothness of this interaction.

For this purpose, we note that

$$s = \mathrm{tr}_{\xi}(K^{-1}(\xi \oplus 1))_x,$$

and the entries of the 2×2 operator matrix $K=(K_{ij})_{2\times 2}$ are given by

$$K_{11}=\widetilde{T+X},\quad K_{21}:=((\lambda+\tilde{G}')^{-1}\tilde{\xi})\otimes\mathbf{a},\quad K_{22}:=w+\hat{\mathbf{a}}$$

($w:=e^{-x\lambda-t\lambda^3}$) and K_{12} is determined by the relation

$$K_{12}\mathbf{b}:=\mathbf{b}(\lambda+\tilde{G})^{-1}\tilde{\eta}\quad(\mathbf{b}\in\mathcal{J}).$$

Since $(\widetilde{T+X})(x,t)$ is everywhere invertible, we can use the results in Sec. IV C 2 to find that $K(x,t)$ is everywhere invertible if and only if so is its Schur complement $\Delta(K)=K_{22}-K_{21}K_{11}^{-1}K_{12}$ [see (4.16a)].

To find a more transparent representation of $\Delta(K)$, we apply the operator $K_{21}K_{11}^{-1}K_{12}$ to an element $\mathbf{b}\in\mathcal{J}$ and obtain

$$\begin{aligned}K_{21}K_{11}^{-1}K_{12}\mathbf{b}&=((\lambda+\tilde{G}')^{-1}\tilde{\xi}\otimes\mathbf{a})(\tilde{T}+\tilde{X})^{-1}\mathbf{b}(\lambda+\tilde{G})^{-1}\tilde{\eta}\\&=\mathbf{b}\langle(\lambda+\tilde{G}')^{-1}\tilde{\xi},(\tilde{T}+\tilde{X})^{-1}(\lambda+\tilde{G})^{-1}\tilde{\eta}\rangle\mathbf{a}\\&=\mathbf{b}\langle\xi,(\lambda+G)^{-1}(T+X)^{-1}(\lambda+G)^{-1}\eta\rangle\mathbf{a}.\end{aligned}$$

Here for the second equality we have used the $\mathcal{J}$-linearity of all the involved operators. It yields that

$$\Delta(K)=w+\hat{\mathbf{a}}-\langle\xi,(\lambda+G)^{-1}(T+X)^{-1}(\lambda+G)^{-1}\eta\rangle\hat{\mathbf{a}}.$$

We observe that for each $(x,t)\in\mathbb{R}$ the term $\langle\xi,(\lambda+G)^{-1}(T(x,t)+X)^{-1}(\lambda+G)^{-1}\eta\rangle$ is a real number. Hence, we have proved the following.

Assertion: If

$$\mathbf{a}\in\mathcal{J}_0:=\{\mathbf{b}\in\mathcal{J}:\mathbf{b}+r\ \text{ is invertible for each }\ r\in\mathbb{R}\},$$

then the interaction $\mathbf{u}[\lambda,\mathbf{a}]\bowtie\mathbf{u}[G,\xi\otimes\eta]$ is smooth.

V. SOLITON SOLUTIONS OF QUATERNIONIC KdV EQUATION

In this section we will apply our general theory to the special case $\mathcal{J}=\mathbb{H}$, the Hamilton quaternion algebra. The vector KdV equation settled in $\mathcal{J}=\mathbb{H}$ is called the *quaternionic KdV equation*.

Why is the quaternionic KdV equation especially interesting? To this question two answers can be given, one mathematical and one physical. The mathematical answer is based on the Frobenius theorem which asserts that there exist exactly three division algebras over $\mathbb{R}$: the real field $\mathbb{R}$, the complex field $\mathbb{C}$ and the Hamilton quaternion algebra $\mathbb{H}$. Sometimes, quaternions are named also by hypercomplex numbers. The vector KdV equation over $\mathbb{C}$ is just the complexification of the real KdV equation. However, the complex field $\mathbb{C}$, like the base field $\mathbb{R}$, is commutative. Among all noncommutative associative algebras, $\mathbb{H}$ is the simplest one and is the unique noncommutative associative division algebra. Moreover, $\mathbb{H}$ together with the matrix algebra $M_2(\mathbb{R})$ are the two simplest Clifford algebras over the real field. The standard fact of Clifford algebras[19] is that every Clifford algebra over $\mathbb{R}$ can be decomposed into disjoint sums of $\mathbb{H}$ and $M_2(\mathbb{R})$. These observations force one to answer the question as to which special features can be expected from the quaternionic KdV equation. The physical consideration is stimulated by the need of the study of the so-called *quaternionic quantum mechanics*.[3] As pointed out by Adler, one of the physical reasons which motivates this study is that "a successful unification of the fundamental forces will require a generalization beyond complex quantum mechanics." The quaternionic KdV equation, like the usual real and complex KdV equations for the scalar soliton theory, should serve as a model equation in the quaternionic soliton theory.

The noncommutativity of $\mathbb{H}$ makes the study of quaternionic equations being challenging. For example, the classical Hirota formalism in solving scalar soliton equations cannot be used directly

to equations settled in $\mathbb{H}$. Our approach below will show a way to study quaternionic equations and will reveal that the structure of soliton solutions of the quaternionic KdV equation is much richer than the ones for the real and complex KdV equations.

A. Basic properties of $\mathbb{H}$

Recall that $\mathbb{H}$ is a four-dimensional *Clifford algebra* with a basis

$$\{e_1=1, e_2=\mathbf{i}, e_3=\mathbf{j}, e_4=\mathbf{k}\}$$

which obeys the following product rule:

$$\mathbf{i}^2=\mathbf{j}^2=\mathbf{k}^2=\mathbf{ijk}=-1.$$

The usual matrix realization of the basis elements by 2×2 complex matrices are given by $e_1 \cong I_2$ the identity matrix and

$$e_2\cong\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad e_3\cong\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad \text{and } e_4\cong\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

In this way, we have the identification

$$a_1e_1+a_2\mathbf{i}+a_3\mathbf{j}+a_4\mathbf{k}\cong\begin{pmatrix} a_1+a_2i & a_3+a_4i \\ -a_3+a_4i & a_1-a_2i \end{pmatrix}\in M_2(\mathbb{C}).$$

This matrix realization of $\mathbb{H}$ helps a lot in the practical calculations using a computer algebra program such as *Mathematica*.

Elements of the linear subspace spanned by **i**, **j**, and **k** are called vectors. The following convention will be used: We write an element $\mathbf{a}=\Sigma_{l=1}^4 a_l e_l\in\mathbb{H}$ as

$$\mathbf{a}=a_1+\tilde{\mathbf{a}}, \quad \tilde{\mathbf{a}}:=\sum_{l=2}^{4} a_l e_l .$$

a_1 is called the *scalar part* of **a** and $\tilde{\mathbf{a}}$ the *vector part* of **a**.

Each nonzero element $\mathbf{a}=a_1+\tilde{\mathbf{a}}$ possesses an inverse given by $\mathbf{a}^{-1}=|\mathbf{a}|^{-2}\overline{\mathbf{a}}$. Here, $|\mathbf{a}| := \sqrt{a_1^2+a_2^2+a_3^2+a_4^2}$ is the *norm* of **a** and $\overline{\mathbf{a}}:=a_1-\tilde{\mathbf{a}}$ is the *conjugation* of **a**. It follows that

$$\mathbb{H}_0:=\{\mathbf{a}\in\mathbb{H}:(\mathbf{a}+r)^{-1}\in\mathbb{H} \quad \forall r\in\mathbb{R}\}=\{\mathbf{a}\in\mathbb{H}:\tilde{\mathbf{a}}\neq 0\}. \tag{5.1}$$

For our purpose, we need also the following basic property of $\mathbb{H}$.

Lemma 5.1: Let **a**, **b** *be two vectors in* $\mathbb{H}$ *such that the four elements* 1, **a**, **b** and **ab** *are linearly dependent, i.e., there exists a nonzero vector* $(c_1,c_2,c_3,c_3)\in\mathbb{R}^4$ *such that*

$$c_1+c_2\mathbf{a}+c_3\mathbf{b}+c_4\mathbf{ab}=0.$$

Then **a** *and* **b** *are parallel, i.e., the cross product* $\mathbf{a}\times\mathbf{b}=0$.

This result means that each unital proper subalgebra of $\mathbb{H}$ has dimension smaller than or equal to 2.

B. The quaternionic KdV equation

We call the following vector KdV equation

$$\mathbf{u}_t=\mathbf{u}_{xxx}+3(\mathbf{u}^2)_x, \quad \mathbf{u}\in\mathbb{H}, \tag{5.2a}$$

the *quaternionic KdV equation*.

1. The equivalent nonlinear system

Writing

$$\mathbf{u}=u_1+u_2\mathbf{i}+u_3\mathbf{j}+u_4\mathbf{k}$$

and using the product rule in Sec. V A we see that the nonlinear system equivalent to (5.2a) has the form

$$\begin{aligned} &u_{1t}-u_{1xxx}-3(u_1^2-u_2^2-u_3^2-u_4^2)_x=0,\\ &u_{\sigma t}-u_{\sigma xxx}-6(u_1u_\sigma)_x=0, \quad \sigma=2,3,4. \end{aligned} \tag{5.2b}$$

2. The first two conserved quantities

Obviously, the momentum

$$m(\mathbf{u}):=\int_{-\infty}^{\infty}\mathbf{u}(x,\cdot)\,dx \tag{5.2c}$$

is a conserved quantity. Below we want to show that the second order momentum

$$m_2(\mathbf{u}):=\int_{-\infty}^{\infty}\mathbf{u}(x,\cdot)^2\,dx \tag{5.2d}$$

is also a conserved quantity, i.e.,

$$m_2(\mathbf{u})=\int_{-\infty}^{\infty}\mathbf{u}(x,\cdot)^2\,dx\equiv\text{const.} \tag{5.2e}$$

The noncommutativity of $\mathbb{H}$ makes the proof of (5.2e) being a little difficult.

To prove (5.2e), we let $\mathbf{u}$ be a solution of (5.2a) which vanishes as $x\to\pm\infty$ and has finite energy

$$E(\mathbf{u}):=\int_{-\infty}^{\infty}|\mathbf{u}(x,\cdot)|^2\,dx<\infty. \tag{5.2f}$$

We have

$$\frac{d}{dt}m_2(\mathbf{u})=\int[\mathbf{u}\mathbf{u}_{xxx}+\mathbf{u}_{xxx}\mathbf{u}]\,dx+3\int[\mathbf{u}(\mathbf{u}^2)_x+(\mathbf{u}^2)_x\mathbf{u}]\,dx.$$

The first integral is equal to zero, as can be seen by taking part integration. Hence

$$\frac{1}{3}\cdot\frac{d}{dt}m_2(\mathbf{u})=\int[\mathbf{u}(\mathbf{u}^2)_x+(\mathbf{u}^2)_x\mathbf{u}]\,dx:=I.$$

On the one hand, we use the identity

$$\mathbf{u}(\mathbf{u}^2)_x+(\mathbf{u}^2)_x\mathbf{u}=[\mathbf{u}(\mathbf{u}\mathbf{u}_x)+(\mathbf{u}\mathbf{u}_x)\mathbf{u}]+[(\mathbf{u}\mathbf{u}_x)\mathbf{u}+(\mathbf{u}\mathbf{u}_x)\mathbf{u}]$$

combining with the fact that the sum $\mathbf{ab}+\mathbf{ba}$ for any $\mathbf{a},\mathbf{b}\in\mathbb{H}$ is real to find that I is real. On the other hand, we use the identity

$$[\mathbf{u}(\mathbf{u}^2)_x+(\mathbf{u}^2)_x\mathbf{u}]=\tfrac{4}{3}(\mathbf{u}^3)_x+\tfrac{1}{3}\cdot[\mathbf{u}(\mathbf{u}\mathbf{u}_x-\mathbf{u}_x\mathbf{u})-(\mathbf{u}\mathbf{u}_x-\mathbf{u}_x\mathbf{u})\mathbf{u}]$$

combining with the fact that the difference $\mathbf{ab}-\mathbf{ba}$ for any $\mathbf{a},\mathbf{b}\in\mathbb{H}$ is either zero or a pure vector to see that I is either zero or a pure vector. But I is real, we conclude that $I=0$ and thus $(d/dt)\,m_2(\mathbf{u})\equiv 0$. This is just the desired result (5.2e).

The scalar KdV equation possesses infinite number of conservation laws which have been established under the help of the Miura transformation. Since we are in a noncommutative algebra $\mathbb{H}$, the Miura transformation works no longer and thus it left an interesting problem which quantities will be conserved by the quaternionic KdV equation.

As it will be shown later, the energy is not a conserved quantity of the quaternionic KdV equation.

C. Quaternionic KdV solitons and their interaction

Using (4.22c), a general solitary wave solution of the quaternionic KdV equation (5.2a) has the form

$$\mathbf{u}[\lambda,\mathbf{a}]=(2\lambda^2)(w\mathbf{a})(w+\mathbf{a})^{-2},\quad w\equiv w(\lambda,x,t):=e^{-x\lambda-t\lambda^3}, \tag{5.3a}$$

which, represented in its coordinates form, reads as

$$\begin{aligned} u_1[\lambda,\mathbf{a}]&=(2\lambda^2 w)(a_1 w^2+2|\mathbf{a}|^2 w+a_1|\mathbf{a}|^2)/Q[\lambda,\mathbf{a}],\\ u_\sigma[\lambda,\mathbf{a}]&=(2\lambda^2 w)(w^2-|\mathbf{a}|^2)a_\sigma/Q[\lambda,\mathbf{a}],\quad \sigma=2,3,4,\\ Q[\lambda,\mathbf{a}]&:=(w^2+2a_1 w+|\mathbf{a}|^2)^2. \end{aligned} \tag{5.3b}$$

Since the wave velocity of the solitary wave $\mathbf{u}[\lambda,\mathbf{a}]$ is equal to λ^2, we call the nonzero real number λ the *velocity parameter*. Correspondingly, we call the nonzero quaternion $\mathbf{a}$ the *position parameter*.

The solitary wave solution $\mathbf{u}[\lambda,\mathbf{a}]$ is smooth and thus localized if and only if the position parameter $\mathbf{a}$ locates at the subset $\mathbb{H}_s:=\mathbb{H}\backslash\mathbb{R}_-$. Solitary wave solutions $\mathbf{u}[\lambda,\mathbf{a}]$ corresponding to positive parameters $\mathbf{a}\in\mathbb{R}_+$ are nothing but the scalar KdV solitons. Hence, we call a solitary wave solution in the class

$$\mathcal{S}_{\mathbb{H}}:=\{\mathbf{u}[\lambda,\mathbf{a}]:0\neq\lambda\in\mathbb{R},\tilde{\mathbf{a}}\neq 0\}$$

a *quaternionic soliton*. Note that here we have used the name ''soliton'' instead of ''solitary wave.'' The reason is, as it will be seen soon in Sec. V C 2, that any two elements in the class $\mathcal{S}_{\mathbb{H}}$ interact asymptotically smoothly and elastically.

Let $\mathbf{u}[\lambda,\mathbf{a}]$ be a quaternionic soliton. Then, its time-independent momentum

$$m(\mathbf{u}[\lambda,\mathbf{a}])=\int_{-\infty}^{\infty}(-2\lambda)((w+\mathbf{a})^{-1}\mathbf{a})_x\,dx=2|\lambda| \tag{5.3c}$$

is independent from the position parameter $\mathbf{a}$. To compute its time-independent energy, we use the solution formula (5.3a) and obtain

$$\begin{aligned} E(\mathbf{u}[\lambda,\mathbf{a}])&=(4\lambda^4|\mathbf{a}|^2)\cdot\int_{-\infty}^{\infty}\frac{w^2}{[(w+a_1)^2+|\tilde{\mathbf{a}}|^2]^2}\,dx\\ &=(4|\lambda|^3|\mathbf{a}|^2)\cdot\int_0^{\infty}\frac{w}{[(w+a_1)^2+|\tilde{\mathbf{a}}|^2]^2}\,dw\\ &=4|\lambda|^3|\cdot(1+s^2)\cdot\int_0^{\infty}\frac{v}{[(v+s)^2+1]^2}\,dv\ \ (\text{with}\ \ v:=w/|\tilde{\mathbf{a}}|,\quad s:=a_1/|\tilde{\mathbf{a}}|). \end{aligned}$$

Therefore, with $s:=a_1/|\tilde{\mathbf{a}}|$,

$$E(\mathbf{u}[\lambda,\mathbf{a}])=|\lambda|^3\cdot(1+s^2)\cdot[2+s(2\arctan s-\pi)]. \tag{5.3d}$$

Similarly, we compute the energy distribution in the real part and find

$$E(u_1[\lambda,\mathbf{a}])=\frac{|\lambda|^3}{3}+\frac{1}{2}E(\mathbf{u}[\lambda,\mathbf{a}]). \tag{5.3e}$$

Equations (5.3d) and (5.3e) imply that the energy and its distribution in the real part are strictly decreasing functions of the parameter $s:=a_1/|\tilde{\mathbf{a}}|$ and the energy becomes unbounded as $s\to-\infty$ and converges to the value $2|\lambda|^3/3$ as $s\to+\infty$. Note that the value $2|\lambda|^2/3$ is just equal to the energy of a scalar KdV soliton with velocity λ^2. Thus, the energy of a scalar KdV soliton is always smaller than the energy of a quaternionic KdV soliton moving with the same velocity.

1. Energy symmetry breaking and energy conservation breaking

On the one hand, the quaternionic KdV solitons $\mathbf{u}[\lambda,\mathbf{a}]$ and $\mathbf{u}[\lambda,-\mathbf{a}]$ annihilate each other, i.e.,

$$\mathbf{u}[\lambda,\mathbf{a}]\bowtie\mathbf{u}[\lambda,-\mathbf{a}]=\mathbf{u}[\lambda,\mathbf{a}+(-\mathbf{a})]=\mathbf{u}[\lambda,0]\equiv 0.$$

On the other hand, using (5.3d) and (5.3e) we find that

$$E(\mathbf{u}[\lambda,\mathbf{a}])-E(\mathbf{u}[\lambda,-\mathbf{a}])=-2\pi s(1+s^2)\cdot|\lambda|^3$$

with $s:=a_1/|\tilde{\mathbf{a}}|$. Hence, the *energy symmetry is broken*: The energy of a quaternionic KdV soliton $\mathbf{u}[\lambda,\mathbf{a}]$ with positive charge (i.e., $a_1>0$) is smaller than the energy of its counterpart $\mathbf{u}[\lambda,-\mathbf{a}]$, although they annihilate each other.

Using the algorithm which will be given in Sec. V C 4 we compute the two-soliton solution $\mathbf{u}[1,\mathbf{i},2,\mathbf{j}]$ and obtain that $\mathbf{u}[1,\mathbf{i},2,\mathbf{j}]=f_1/f+(f_2/f)\mathbf{i}+(f_3/f)\mathbf{j}$ with

```
f_1:=2*(4*v^2+324*u^4*v^2+u^2*(1+90*v^2+81*v^4)),

f_2:=u*(-1/729+(22*v^2)/81-v^4+u^2*(1/9-(22*v^2)/9+v^4)),

f_3:=4*v*(-1+81*v^2+729*u^4*(-1+v^2)+18*u^2*(-1+9*v^2))/729,

f:=(1/81+u^2+v^2+u^2*v^2)^2,  u==Exp[-x-t], v==Exp[-2x-8t].
```

Set $s:=\mathrm{Exp}[-6t]$. Then we have

$$\text{energy}(t):=\int_{\mathbb{R}}|\mathbf{u}(x,t)|^2\,dx=\int_0^{\infty}\frac{(f_1^2+f_2^2+f_3^2)}{uf^2}[u=u,v=s*u^2]\,du.$$

For each fixed $s>0$ the integrand is a rational function of u. We use *Mathematica* to compute this integral. After that, we draw the energy evolution in time [see Fig. 1(a) the Appendix]. It shows that the energy is time-dependent and thus the energy is not a conserved quantity of the quaternionic KdV equation.

2. Two-points blow-up

Consider two quaternionic soliton solutions $\mathbf{u}[\lambda_1,\mathbf{a}]$ and $\mathbf{u}[\lambda_2,\mathbf{b}]$ for which

$$\lambda_1\neq\pm\lambda_2 \quad\text{and}\quad \mathbf{a},\mathbf{b}\in\mathbb{H}_0.$$

It follows from Sec. IV D 2 [see (4.24)] that the singularity set of the solution

$$\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=\mathbf{u}[\lambda_1,\mathbf{a}]\bowtie\mathbf{u}[\lambda_2,\mathbf{b}]$$

just consists of the points $(x,t)\in\mathbb{R}^2$ such that

$$\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=(w_1+\mathbf{a})(w_2+\mathbf{b})-(k_1k_2)\mathbf{ab}$$

are not invertible at these points. Since each nonzero element in $\mathbb{H}$ possesses an inverse, the above is equivalent to say that the singularity set of the solution $\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]$ is nothing but the zero set of $\delta[\lambda_2,\mathbf{b},\lambda_1,\mathbf{a}]$. In notation, we write this fact as

$$\mathrm{Sing}(\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}])=\{(x,t)\in\mathbb{R}^2:\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}](x,t)=0\}. \tag{5.4}$$

It is left to determine when and at which point $\delta[\lambda_2,\mathbf{b},\lambda_1,\mathbf{a}]$ becomes zero.

To this end, we rewrite $\delta\equiv\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]$ as

$$\delta=(w_1w_2+a_1w_2+b_1w_1+\gamma a_1b_1)+\gamma\tilde{\mathbf{a}}\tilde{\mathbf{b}}+(w_1+\gamma a_1)\tilde{\mathbf{b}}+(w_2+\gamma b_1)\tilde{\mathbf{a}}, \tag{5.5a}$$

where

$$\gamma:=1-(k_1k_2)=(\lambda_1-\lambda_2)^2/(\lambda_1+\lambda_2)^2 \tag{5.5b}$$

and

$$w_l=w_l(\lambda_l,x,t)=e^{-x\lambda_l-t\lambda_l^3},\quad l=1,2. \tag{5.5c}$$

Since we have assumed $\lambda_1\neq\lambda_2$, the parameter γ is positive. Therefore, Lemma 5.1 applies and yields that $\delta[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=0$ at (x,t) if and only if

$$\tilde{\mathbf{a}}\|\tilde{\mathbf{b}} \tag{5.6a}$$

and

$$\begin{array}{c}(w_1w_2+a_1w_2+b_1w_1+\gamma a_1b_1)+\gamma\tilde{\mathbf{a}}\tilde{\mathbf{b}}=0\\ (w_1+\gamma a_1)\tilde{\mathbf{b}}+(w_2+\gamma b_1)\tilde{\mathbf{a}}=0\end{array}\quad\text{at } (x,t). \tag{5.6b}$$

Equation (5.6a) gives the first condition for the nonemptyness of the singularity set $\mathrm{Sing}(\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}])$. Further conditions will be determined by (5.6b).

Since both $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$ are nonzero, condition (5.6a) is equivalent to the following more transparent ones:

$$\tilde{\mathbf{b}}=-\alpha\tilde{\mathbf{a}}\quad\text{for some } 0\neq\alpha\in\mathbb{R}. \tag{5.7}$$

Substituting (5.7) into (5.6b) we have

$$\begin{array}{c}(w_1w_2+a_1w_2+b_1w_1+\gamma a_1b_1)+(\alpha\gamma)\cdot|\tilde{\mathbf{a}}|^2=0\\ (w_2+\gamma b_1)=\alpha(w_1+\gamma a_1)\end{array}\quad\text{at } (x,t). \tag{5.8}$$

We solve w_2 from the second equation in (5.8), substitute it into the first equation in (5.8), and obtain the following equivalent equations of (5.8):

$$\begin{array}{c}w_1^2+[(1+\gamma)a_1+(1-\gamma)b_1\alpha^{-1}]w_1+\gamma\cdot|\mathbf{a}|^2=0,\\ w_2=\alpha w_1+\gamma(\alpha a_1-b_1).\end{array} \tag{5.9}$$

An elementary manipulation shows that the condition that (5.9) has two pair (w_1,w_2) of positive solutions $w_1>0,w_2>0$ is equivalent to the following ones:

$$(1+\gamma)a_1+(1-\gamma)b_1\alpha^{-1} \leqslant -2\sqrt{\gamma}\cdot|\mathbf{a}|,$$
$$(1+\gamma)b_1+(1-\gamma)a_1\alpha<0, \tag{5.10a}$$

which can be simplified into

$$\alpha(\lambda_1\lambda_2)>0, \quad b_1\leqslant -\left(\frac{\alpha}{2\lambda_1\lambda_2}\right)\cdot[(\lambda_1^2+\lambda_2^2)a_1+|\lambda_1^2-\lambda_2^2|\cdot|\mathbf{a}|]. \tag{5.10b}$$

Note that if $a_1\geqslant 0$ and $b_1\geqslant 0$, then the conditions in (5.10b) cannot be satisfied.

We collect these results as follows.

(c1) The singularity set $\mathrm{Sing}(\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}])$ is nonempty if and only if both conditions in (5.10b) are satisfied. In case the singularity set is nonempty, then it contains at most two points in the space–time plane whose coordinates are determined by the equations

$$x\lambda_1+t\lambda_1^3=-\ln w_1,$$
$$x\lambda_2+t\lambda_2^3=-\ln[\alpha(w_1+\gamma a_1)-\gamma b_1],$$

w_1 are positive solutions of the first equation of (5.9).

This implies the following smoothing effect of the interaction: If the interaction $\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]$ possess a singularity at a space–time point (x_1,t_1), then the singularity will soon vanish as time going forward and backward. The singularity will be recovered once again at a certain space–time point (x_2,t_2). After or before that time point t_2, the interaction keeps always smooth. As result, the interaction of any two quaternionic KdV solitons is asymptotically smooth and elastic.

(c2) The singularity set $\mathrm{Sing}(\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}])$ becomes empty whenever one of the following conditions hold true:

$$\text{Either} \quad a_1\geqslant 0, b_1\geqslant 0 \quad \text{or} \quad \tilde{\mathbf{a}}\not\parallel\tilde{\mathbf{b}}.$$

(c3) For any given quaternionic KdV soliton there always exists another quaternionic soliton which interacts the former in a singular way. This implies particularly that there exists a solution of the form

$$\mathbf{u}[\lambda_1,\mathbf{a},\lambda_2,\mathbf{b}]=\mathbf{u}[\lambda_1,\mathbf{a}]\bowtie\mathbf{u}[\lambda_2,\mathbf{b}]$$

whose initial profile is smooth but which undergoes a blow-up at a finite time.

3. Smooth interaction with scalar solitons

Since the subset $\mathbb{H}_0$, which consists of all elements $\mathbf{a}\in\mathbb{H}$ such that $\mathbf{a}+r$ is invertible for each $r\in\mathbb{R}$, is just the set $\{\mathbf{a}\in\mathbb{H}:\tilde{\mathbf{a}}\neq 0\}$ [see (5.1)], we derive the following result immediately from Sec. IV D 3:

(c4) Assume $\mathbf{u}[G,\xi\otimes\eta]$ to be a smooth solution of the scalar KdV equation. Then the interaction $\mathbf{u}[G,\xi\otimes\eta]\bowtie\mathbf{u}[\lambda,\mathbf{a}]$ between the scalar solution $\mathbf{u}[G,\xi\otimes\eta]$ and the quaternionic soliton solutions $\mathbf{u}[\lambda,\mathbf{a}]$ with parameters $\lambda\notin-\mathrm{Sp}(G)$ is smooth. In particular, a quaternionic KdV soliton $\mathbf{u}[\lambda,\mathbf{a}]$ with positive parameter $\lambda>0$ interacts smoothly with any scalar multisoliton solution $\mathbf{u}[\lambda_1,a_1,\ldots,\lambda_n,a_n]$ (where $\lambda_j>0,a_j>0$).

4. A practical guide to computing multisoliton solutions

This guide is for the purpose of working with the computer algebra program like *Mathematica*.[20]

We recall the formulas (4.19) and (4.20) for computing a general quaternionic n-soliton solution $s=\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]$. We have

$$s=2\,\mathrm{tr}_{\xi}(\xi\otimes(K^{-1}\eta))_x$$

with $\xi=(1,1,\ldots,1)\in(\mathcal{J}^n)'$, $\eta=(\lambda_1\mathbf{a}_1,\lambda_2\mathbf{a}_2,\ldots,\lambda_n\mathbf{a}_n)^T\in\mathcal{J}^n$, and the $n\times n$ quaternionic matrix $K=T+X[\lambda,\mathbf{a}]$ with T and $X[\lambda,\mathbf{a}]$ given by (4.18b) and (4.19b), respectively. Writing $K^{-1}\eta=(\gamma_1,\ldots,\gamma_n)^T$, we have

$$s=2\,\mathrm{tr}_{\xi}(\xi\otimes(K^{-1}\eta))_x=2(\gamma_1+\gamma_2+\cdots+\gamma_n)_x$$

and the components γ_j are determined by the equation

$$(\gamma_1,\ldots,\gamma_n)\hat{K}=(\lambda_1\mathbf{a}_1,\ldots,\lambda_n\mathbf{a}_n)=\eta^T,$$

where $\hat{K}\equiv\hat{K}[\lambda,\mathbf{a}]$ is the $n\times n$ quaternionic matrix

$$\hat{K}=\begin{pmatrix} w_1+\mathbf{a}_1 & k_{21}\mathbf{a}_2 & \cdots & k_{n1}\mathbf{a}_n \\ k_{12}\mathbf{a}_1 & w_2+\mathbf{a}_2 & \cdots & k_{n2}\mathbf{a}_n \\ & \cdots & \cdots & \\ k_{1n}\mathbf{a}_1 & k_{2n}\mathbf{a}_2 & \cdots & w_n+\mathbf{a}_n \end{pmatrix}\equiv\begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ \cdots \\ \mathbf{R}_n \end{pmatrix} \tag{5.11}$$

with constants $k_{ij}:=2\lambda_i/\lambda_i+\lambda_j$ and functions $w_j\equiv w_j(x,t)=\exp(-x\lambda_j-t\lambda_j^3)$. We note that the given row η^T and the row $(\gamma_1,\ldots,\gamma_n)$ of the unknowns are understood as $1\times n$ quaternionic matrices and the product $(\gamma_1,\ldots,\gamma_n)\hat{K}$ is just the product of the quaternionic matrices.

What we should compute is the sum $\gamma_1+\gamma_2+\cdots+\gamma_n$. In the practical performance of the calculation, we use the following transformation:

$$\gamma_1:=\zeta_1-\zeta_2,\gamma_2:=\zeta_2-\zeta_3,\ldots,\gamma_n:=\zeta_n,$$

so that $\gamma_1+\gamma_2+\cdots+\gamma_n=\zeta_1$. This reduces our need to calculate the single component ζ_1. The equation $(\gamma_1,\ldots,\gamma_n)\hat{K}=\eta^T$ can be rewritten in the new variables $(\zeta_1,\ldots,\zeta_n)$ as follows:

$$(\zeta_1,\ldots,\zeta_n)A=(\lambda_1\mathbf{a}_1,\ldots,\lambda_n\mathbf{a}_n)=\eta^T, \tag{5.12a}$$

where $A\equiv A[\lambda,\mathbf{a}]$ is the $n\times n$ quaternionic matrix

$$A=\begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2-\mathbf{R}_1 \\ \cdots \\ \mathbf{R}_n-\mathbf{R}_{n-1} \end{pmatrix}. \tag{5.12b}$$

That is, the first row of A is the first row of $\hat{K}$, and up to the second row the m-row of A is equal to the m-row of $\hat{K}$ minus the $(m-1)$-row of $\hat{K}$.

To make the calculation with *Mathematica* being possible, we use the following matrix realization of the quaternion algebra $\mathbb{H}$:

$$a_1e_1+a_2\mathbf{i}+a_3\mathbf{j}+a_4\mathbf{k}\cong\begin{pmatrix} z_1 & z_2 \\ -\overline{z}_2 & \overline{z}_1 \end{pmatrix}\in M_2(\mathbb{C})$$

with $z_1:=a_1+a_2i$ and $z_2:=a_3+a_4i$. In this way, each $m\times n$ quaternionic matrix is identified with a $(2m)\times(2n)$ complex matrix. In particular, both $(\zeta_1,\ldots,\zeta_n)$ and η^T are identified as $2\times(2n)$ complex matrices and A is identified as a $(2n)\times(2n)$ matrix.

We set

$$(\zeta_1,\ldots,\zeta_n)=\left(\begin{array}{cc|c|cc} y_1 & z_1 & \cdots & y_n & z_n \\ -\overline{z_1} & \overline{y_1} & \cdots & -\overline{z_n} & \overline{y_n} \end{array}\right)_{2\times(2n)}.$$

Then Eq. (5.12a) is equivalent to the following linear system of $2n$ unknowns:

$$(y_1,z_1,\ldots,y_n,z_n)A=\text{the first row of } \eta^T. \tag{5.12c}$$

All information of the solution $s=\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]$ is stored in the components y_1,z_1 of ζ_1. More precisely, we have

$$\begin{aligned} 2(\mathrm{Re}\,y_1)_x&=\text{the real part of } s,\\ 2(\mathrm{Im}\,y_1)_x&=\text{the } \mathbf{i} \text{ part of } s,\\ 2(\mathrm{Re}\,z_1)_x&=\text{the } \mathbf{j} \text{ part of } s,\\ 2(\mathrm{Im}\,z_1)_x&=\text{the } \mathbf{k} \text{ part of } s. \end{aligned} \tag{5.12d}$$

We use Cramer's formula[13] to solve the linear system (5.12c). It yields that

$$y_1=\frac{\det(A_1)}{\det(A)},\quad z_1=\frac{\det(A_2)}{\det(A)}, \tag{5.12e}$$

where $A_1\equiv A_1[\lambda,\mathbf{a}]$ (respectively, $A_2\equiv A_2[\lambda,\mathbf{a}]$) is the $(2n)\times(2n)$ complex matrix obtained from the $(2n)\times(2n)$ complex matrix A by replacing the first (respectively, second) row of A by the first row of the $2\times(2n)$ complex matrix η^T.

Replacing each element $\mathbf{a}_s\in\mathbb{H}$ by its conjugation $\overline{\mathbf{a}_s}$, we have the following relation for the involved three matrices:

$$A[\lambda,\overline{\mathbf{a}}]=\overline{A}[\lambda,\mathbf{a}],\quad A_l[\lambda,\overline{\mathbf{a}}]=\overline{A_l}[\lambda,\mathbf{a}]\quad (l=1,2).$$

Here $\overline{B}$ for a $(2n)\times(2n)$ complex matrix B is defined as the matrix obtained from B by replacing all of its entries by their complex conjugates. In particular, we have

$$\det(A[\lambda,\overline{\mathbf{a}}])=\overline{\det(A[\lambda,\mathbf{a}])},\quad \det(A_l[\lambda,\overline{\mathbf{a}}])=\overline{\det(A_l[\lambda,\mathbf{a}])}\quad (l=1,2).$$

Therefore, by the solution formula (5.12e) we obtain the following relation:

$$\mathbf{u}[\lambda_1,\overline{\mathbf{a}_1},\ldots,\lambda_n,\overline{\mathbf{a}_n}]=\overline{\mathbf{u}}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]\equiv\overline{\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]}. \tag{5.12f}$$

Consider the special case where all $\mathbf{a}_s$ are pure vectors, i.e., $\mathbf{a}_s=\tilde{\mathbf{a}}_s$ for $s=1,2,\ldots,n$. Then $\overline{\tilde{\mathbf{a}}_s}=-\tilde{\mathbf{a}}_s$ and thus, by (5.12f),

$$\mathbf{u}[\lambda_1,-\tilde{\mathbf{a}}_1,\ldots,\lambda_n,-\tilde{\mathbf{a}}_n]=\overline{\mathbf{u}}[\lambda_1,\tilde{\mathbf{a}}_1,\ldots,\lambda_n,\tilde{\mathbf{a}}_n]. \tag{5.12g}$$

In other words, the annihilator of a multisoliton solution generated by pure vectors is just given by its conjugation.

The above working scheme reduces the calculation of an n-soliton solution into calculating the determinants of three $(2n)\times(2n)$ complex matrices A and $A_{1,2}$. The number of variables involved in these matrices are $5n$: among them are n spectral parameters $\lambda_1,\ldots,\lambda_n$ and $4n$ further real parameters for the position parameters $\mathbf{a}_1,\ldots,\mathbf{a}_n$; each element $\mathbf{a}_j$ in $\mathbb{H}$ shares four real parameters. In order to reduce the number of the involved variables, we need simplifying our situation as follows. First, since the quaternionic KdV equation is invariant under the scaling $(x,t,\mathbf{u})\to(x\lambda,t\lambda^3,\lambda^{-2}\mathbf{u})$, we can set $\lambda_1=1$. Second, for any given two elements $\mathbf{a}_1,\mathbf{a}_2\in\mathbb{H}$ whose vector parts $\tilde{\mathbf{a}}_1$ and $\tilde{\mathbf{a}}_2$ expand a two-dimensional subspace we can always find an automorphism

γ of $\mathbb{H}$ such that either $\gamma\tilde{\mathbf{a}}_1=|\tilde{\mathbf{a}}_1|\cdot\mathbf{i}$ and $\gamma\tilde{\mathbf{a}}_2=c_1\mathbf{i}+c_2\mathbf{j}$ for some $c_2>0$ or $\gamma\tilde{\mathbf{a}}_2=|\tilde{\mathbf{a}}_2|\cdot\mathbf{i}$ and $\gamma\mathbf{a}_1=c_3\mathbf{i}+c_4\mathbf{j}$ for some $c_4>0$. Without loss of generality we assume the first case occurs, i.e., there exists an automorphism ϕ of $\mathbb{H}$ such that $\phi\tilde{\mathbf{a}}_1=|\tilde{\mathbf{a}}_1|\cdot\mathbf{i}$ and $\phi\tilde{\mathbf{a}}_2=c_1\mathbf{i}+c_2\mathbf{j}$ for some $c_2>0$. In this case, we set $\lambda_1=1$. Then for any given $\mathbf{a}_3,\ldots,\mathbf{a}_n\in\mathbb{H}$ we have

$$\phi\mathbf{u}[1,\mathbf{a}_1,\lambda_2,\mathbf{a}_2,\ldots,\lambda_n,\mathbf{a}_n]=\mathbf{u}[1,r+|\tilde{\mathbf{a}}|\mathbf{i},\lambda_2,s+c_1\mathbf{i}+c_2\mathbf{j},\ldots,\lambda_n,\phi\mathbf{a}_n]$$

with some $r,s\in\mathbb{R}$. Choosing a shift transformation $x\to x+x_0$ and $t\to t+t_0$ in the space–time plane, the latter reduces into the following standard ones $\mathbf{u}[1,r_1+\mathbf{i},\lambda_2,s_1+c_3\mathbf{i}+\mathbf{j},\ldots,\lambda_n,\phi\mathbf{a}_n]$. In conclusion, what we need computing is the following standard form of the n-soliton solutions $\mathbf{u}[1,r+\mathbf{i},\lambda_2,s+p\mathbf{i}+\mathbf{j},\ldots,\lambda_n,\mathbf{a}_n]$ with $r,s,p\in\mathbb{R}$. The number of variables involved in the standard form is $5n-6$. This reduction of the variables helps the practical performance of the calculation a little.

D. Noncommutative soliton system of three components as reduction of quaternionic KdV equation

Switching the $\mathbf{k}$ component u_4 of a solution $\mathbf{u}=u_1+u_2\mathbf{i}+u_3\mathbf{j}+u_4\mathbf{k}$ of the quaternionic KdV equation (5.2a), (5.2b) into zero, we have a nonlinear system of three components:

$$\begin{aligned} &u_{1t}-u_{1xxx}-3(u_1^2-u_2^2-u_3^2)_x=0,\\ &u_{\sigma t}-u_{\sigma xxx}-6(u_1u_\sigma)_x=0,\quad \sigma=2,3. \end{aligned} \tag{5.13}$$

Let $\Pi(\mathbf{i},\mathbf{j})$ be the unital three-dimensional subspace of $\mathbb{H}$ spanned by the base elements $\mathbf{1}$, $\mathbf{i}$, and $\mathbf{j}$. Then a solution $\mathbf{u}$ of the quaternionic KdV equation is a solution of the system (5.13) if and only if $\mathbf{u}$ lives in $\Pi(\mathbf{i},\mathbf{j})$, or equivalently, the $\mathbf{k}$ part of $\mathbf{u}$ vanishes.

All quaternionic KdV solitons $\mathbf{u}[\lambda,\mathbf{a}]$ with position parameters $\mathbf{a}$ locating at $\Pi(\mathbf{i},\mathbf{j})$ are solitary wave solutions to the system (5.13). However, since the interaction between quaternionic KdV solitons is nonlinear, it is certainly not allowed to expect that the result of their interaction

$$\mathbf{u}[\lambda_1,\mathbf{a}_1,\lambda_2,\mathbf{a}_2,\ldots,\lambda_n,\mathbf{a}_n]=\mathbf{u}[\lambda_1,\mathbf{a}_1]\bowtie\mathbf{u}[\lambda_2,\mathbf{a}_2]\bowtie\cdots\bowtie\mathbf{u}[\lambda_n,\mathbf{a}_n]$$

[with $\mathbf{a}_j\in\Pi(\mathbf{i},\mathbf{j})$] lives also in $\Pi(\mathbf{i},\mathbf{j})$; recalling that $\mathbf{ij}=\mathbf{k}$ which says that $\Pi(\mathbf{i},\mathbf{j})$ is not closed under multiplication. In other words, it should be wrong if one expects that the system (5.13) is a soliton system.

Another reason why this should be wrong is that a system of the form (5.13) cannot be derived from a $\mathcal{J}$-KdV equation with some appropriate three-dimensional unital Banach algebra $\mathcal{J}$. This is because any three-dimensional unital Banach algebra $\mathcal{J}$ is commutative and thus any two solitary wave solutions of the corresponding $\mathcal{J}$-KdV equation have commutative position parameters while the two solitary wave solutions $\mathbf{u}[1,\mathbf{i}]$ and $\mathbf{u}[1,\mathbf{j}]$ to the system (5.13) do not.

Against all of the above ''wrong'' thinking, we have the following assertion, which is certainly very surprising.

Assertion: The nonlinear system (5.13) is a soliton system. More precisely, the $\mathbf{k}$ parts of the interactions $\mathbf{u}[\lambda_1,\mathbf{a}_1,\lambda_2,\mathbf{a}_2,\ldots,\lambda_n,\mathbf{a}_n]$ with position parameters $\mathbf{a}_j\in\Pi(\mathbf{i},\mathbf{j})$ do vanish and thus all such quaternionic multisoliton solutions are simultaneously multisoliton solutions to (5.13).

Since any unital three-dimensional subspace $\Pi(\mathbf{v}_1,\mathbf{v}_2)$ of $\mathbb{H}$ spanned by the unit $\mathbf{1}$ and further two vectors $\mathbf{v}_1,\mathbf{v}_2\in\mathbb{H}$ can be transformed into the standard ones $\Pi(\mathbf{i},\mathbf{j})$ by an appropriate automorphism of $\mathbb{H}$, the above assertion implies also the following very interesting low-dimensional phenomenon of the interaction of quaternionic KdV solitons:

(c5) Let $\mathbf{u}[\lambda_j,\mathbf{a}_j]$ $(1\leqslant j\leqslant n)$ be any finitely many quaternionic KdV solitons which live in a unital three-dimensional linear subspace $\Pi(\mathbf{v}_1,\mathbf{v}_2)$ [i.e., all $\mathbf{a}_j\in\Pi(\mathbf{v}_1,\mathbf{v}_2)$]. Then their interaction $\mathbf{u}[\lambda_1,\mathbf{a}_1,\lambda_2,\mathbf{a}_2,\ldots\lambda_n,\mathbf{a}_n]$ lives again in $\Pi(\mathbf{v}_1,\mathbf{v}_2)$. More precisely, for each $(x,t)\in\mathbb{R}^2$ the value $\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots\lambda_n,\mathbf{a}_n](x,t)$ does belong again to $\Pi(\mathbf{v}_1,\mathbf{v}_2)$.

This result, roughly speaking, implies that the interaction of any finitely many quaternionic KdV solitons with position parameters locating in a unital three-dimensional subspace behaves as if the interaction were linear although it is really nonlinear.

The proof of the above Assertion is unbelievable easy and goes as follows. We consider the automorphism $\psi:\mathbb{H}\to\mathbb{H}$ induced by the element $\mathbf{k}$, i.e.,

$$\psi(u):=\mathbf{k}u\mathbf{k}^{-1} \quad (u\in\mathbb{H}). \tag{5.14a}$$

We have

$$\psi(\mathbf{k})=\mathbf{k}, \quad \psi(u)=\overline{u} \quad \forall u\in\Pi(\mathbf{i},\mathbf{j}). \tag{5.14b}$$

To prove our Assertion, we fix n elements $\mathbf{a}_l\in\Pi(\mathbf{i},\mathbf{j})$ $(l=1,2,\ldots,n)$ and set

$$s=\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]=u_1+u_2\mathbf{i}+u_3\mathbf{j}+u_4\mathbf{k}.$$

Applying (4.21c) with the above automorphism ψ, we obtain

$$\psi\mathbf{u}[\lambda_1,\mathbf{a}_1,\ldots,\lambda_n,\mathbf{a}_n]=\mathbf{u}[\lambda_1,\psi\mathbf{a}_1,\ldots,\lambda_n,\psi\mathbf{a}_n].$$

The latter is equal to $\mathbf{u}[\lambda_1,\overline{\mathbf{a}_1},\ldots,\lambda_n,\overline{\mathbf{a}_n}]$ by (5.14b) and furthermore, equal to the conjugation $\overline{s}$ by (5.12f). Hence, we have $\psi(s)=\overline{s}$, i.e.,

$$(u_1+u_4\mathbf{k})-(u_2\mathbf{i}+u_3\mathbf{j})=\psi(s)=\overline{s}=(u_1-u_4\mathbf{k})-(u_2\mathbf{i}+u_3\mathbf{j}),$$

yielding the desired result $u_4\equiv 0$.

The discovery of the above low-dimensional phenomenon is as follows. Initialized by the wish of finding the concrete representations of two-soliton solutions in their standard forms $s=\mathbf{u}[1,r+\mathbf{i},\lambda_2,s+p\mathbf{i}+\mathbf{j}]$, the author calculated them with *Mathematica*.[20] After several seconds the computer gives an unbelievable result: The $\mathbf{k}$ part of s does vanish, i.e., the nonlinear interaction between the $\mathbf{i}$ part of the soliton $\mathbf{u}[1,r+\mathbf{i}]$ and the $\mathbf{j}$ part of the soliton $\mathbf{u}[\lambda_2,s+p\mathbf{i}+\mathbf{j}]$ does not generate any contribution to the $\mathbf{k}$ part although $\mathbf{ij}=\mathbf{k}$! Carefully checking the inputs and computing it in another computer again, the result keeps unchanged. With very uncertain feeling the author tried with three-soliton and then with four-soliton solutions, what the computer told is the above described surprising low-dimensional phenomenon of the interaction. However, the trying with five solitons was likely an adventure. The number of variables involved in the computing is $5\times 5-6=19$, which yielded a very high capacity need and caused a crash of the computer. Giving up computing with computer, the author found by luck, 2 days later, the easy proof for the above most wanted result.

E. Properties of quaternionic KdV solitons: a summary

The first component a_1 of the position parameter $\mathbf{a}$ of a quaternionic soliton $\mathbf{u}[\lambda,\mathbf{a}]$ should be considered as the *charge* of that soliton. Accordingly, we can decompose the quaternionic KdV solitons into three classes,

$$\mathcal{S}_+:=\{\mathbf{u}[\lambda,\mathbf{a}]:a_1>0,\tilde{\mathbf{a}}\neq 0\},$$

$$\mathcal{S}_0:=\{\mathbf{u}[\lambda,\mathbf{a}]:a_1=0,\tilde{\mathbf{a}}\neq 0\},$$

$$\mathcal{S}_-:=\{\mathbf{u}[\lambda,\mathbf{a}]:a_1<0,\tilde{\mathbf{a}}\neq 0\}.$$

A soliton of class $\mathcal{S}_\pm$ is said to be *positively* and *negatively* charged, respectively, while a soliton of class $\mathcal{S}_0$ is said to be *neutral*. Since the result of the interaction between $\mathbf{u}[\lambda,\mathbf{a}]$ and $\mathbf{u}[\lambda,$

$-\mathbf{a}]$ is the vacuum solution, i.e., $\mathbf{u}[\lambda,\mathbf{a}]\bowtie\mathbf{u}[\lambda,-\mathbf{a}]\equiv 0$, each element in the class $\mathcal{S}_+$ finds its annihilator in the class $\mathcal{S}_-$ and *vice versa*. However, the class $\mathcal{S}_0$ is closed in the sense that the annihilator of each element in $\mathcal{S}_0$ locates again in $\mathcal{S}_0$.

The main properties of quaternionic KdV solitons are collected as follows.

A positively charged soliton annihilates a negatively charged soliton, although the energy of the former is less than the energy of the latter.

Any two non-negatively charged solitons interact smoothly.

Only under the very restrictive conditions (5.10b) the interaction between two quaternionic KdV solitons undergoes a blow-up, and the blow-up occurs at most at two points of the space–time plane. Hence, the interaction is asymptotically smooth and elastic.

The interaction between a quaternionic KdV soliton and a smooth solution of the scalar KdV equation is smooth. In particular, a quaternionic soliton interacts smoothly with any smooth scalar multisoliton solution.

The annihilator of a multisoliton solution generated by pure vectors is just given by its conjugation.

The nonlinear interaction between any finitely many quaternionic solitons which live in a unital three-dimensional subspace Π of $\mathbb{H}$ does not yield any effect to the part outside that subspace Π.

APPENDIX

(A) Representation formula for two-solitons. We use the scheme described in Sec. V C 4 to compute the typical two-solitons solutions

$$s\equiv\mathbf{u}[1,\mathbf{i},b/(1-b),s+p*\mathbf{i}+\mathbf{j}]$$

under the help of the computer algebra program *Mathematica*.[20] It yields [cf. (5.12d) and (5.12e)] that

$$s=2\left(\frac{\mathrm{Re}[\det(\mathrm{A1})]}{\det(\mathrm{A})}+\frac{\mathrm{Im}[\det(\mathrm{A1})]}{\det(\mathrm{A})}\cdot\mathbf{i}+\frac{\det(\mathrm{A2})}{\det(\mathrm{A})}\cdot\mathbf{j}\right)_x,$$

where

```
det(A)==-32*b^3*(1+r^2)*(1+p^2+s^2)+16*b^4*(1+r^2)*(1+p^2+s^2) +
    (1+u^2)*(1+p^2+v^2)-8*b*(p^2*(1+r*u)-p*(r-u)*(s-u) +
    (1+r*u)*(1+s*v))+8*b^2*(3+2*s^2+2*r^2*(1+s^2) +
    p^2*(3+2*r^2+r*u)-p*(r-u)*(s-v)+s*v+r*(u+s*u*v)),

det(A1)==(-I+u)*(((-1+2*b)*(I+r+4*b^2*(I+r)+b*(-4*I-5*r+u)))/(-1+b) +
    (I*(-1+2*b)*p-2*b*s+v)*((b*(p-I*s)*(-1+b*(2-(2*I)*r) +
    (2*I)*r-I*u))/(-1+b)+(I+r)*(I*p-2*b*(I*p+s)+v))) -
    (2*b*(I-2*r+2*b*(-I+r)+u)*(4*b^2*(I+r)*(1+p^2+s^2) +
    (I+r)*(1+p^2+I*p*(s-v)+s*v)-b*(4*I+(3*I)*s^2+p^2*(4*I+5*r-u)
    -u-s^2*u+I*p*(I+r)*(s-v)+I*s*v+r*(5+4*s^2+s*v))))/(-1+b),

det(A2)==(b*(I-2*r+2*b*(-I+r)+u)*(-I-2*r+2*b*(I+r)+u)*(s-v))/(-1+b),
    u==r+Exp[-x-t],  v==s+Exp[-x*b/(1-b)-t*(b/(1-b))^3].
```

(B) Some plots for quaternionic KdV solitons. (Figures 1 and 2.)

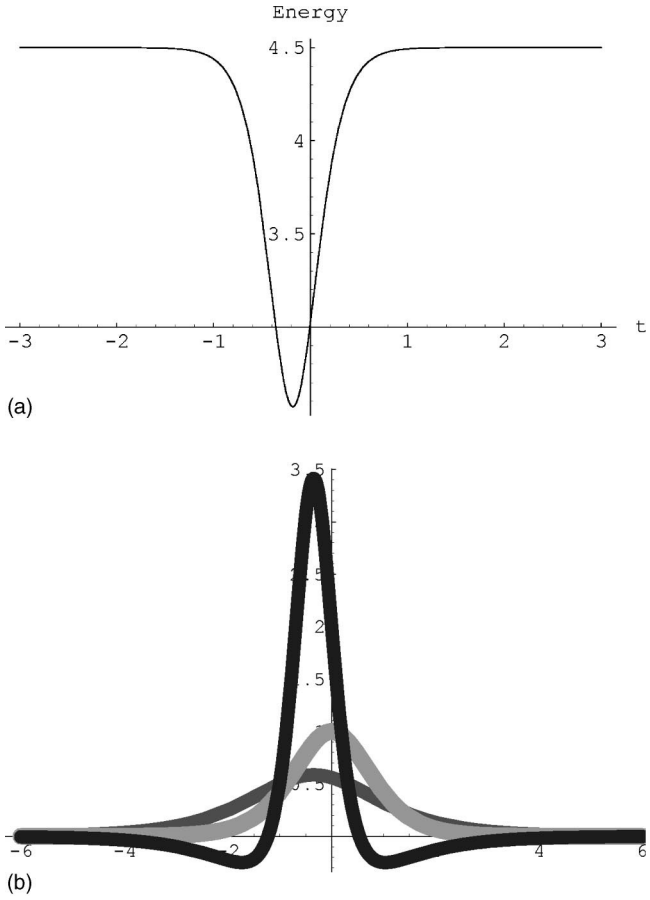

FIG. 1. (a) The time-dependent energy of the solution $\mathbf{u}[1,\mathbf{i},2,\mathbf{j}]$. (b) The initial profiles of the real parts of the three different one-solitons $\mathbf{u}[1,1+\mathbf{i}]\in\mathcal{S}_+$ of positive charge (with the lowest peak), $\mathbf{u}[1,\mathbf{i}]\in\mathcal{S}_0$ of zero charge (with the moderate peak), and $\mathbf{u}[1,-1+\mathbf{i}]\in\mathcal{S}_-$ of negative charge (with the highest peak).

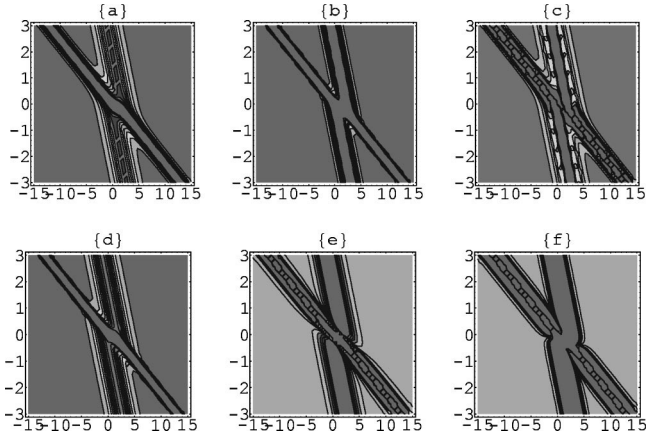

FIG. 2. The contour plots of the real parts of the interactions of the three different classes $\mathcal{S}_\pm$ and $\mathcal{S}_0$ of one-solitons. The typical **X** form of the patterns reveals the elasticity of the interaction. (a) For $\mathbf{u}[1,1+\mathbf{i}]\bowtie\mathbf{u}[2,1+\mathbf{j}]\cdots\mathcal{S}_+-\mathcal{S}_+$ interaction. (b) For $\mathbf{u}[1,1+\mathbf{i}]\bowtie\mathbf{u}[2,\mathbf{j}]\cdots\mathcal{S}_+-\mathcal{S}_0$ interaction. (c) For $\mathbf{u}[1,-1+\mathbf{i}]\bowtie\mathbf{u}[2,-1+\mathbf{j}]\cdots\mathcal{S}_--\mathcal{S}_-$ interaction. (d) For $\mathbf{u}[1,1+\mathbf{i}]\bowtie\mathbf{u}[2,\mathbf{j}]\cdots\mathcal{S}_+-\mathcal{S}_0$ interaction. (e) For $\mathbf{u}[1,1+\mathbf{i}]\bowtie\mathbf{u}[2,-1+\mathbf{j}]\cdots\mathcal{S}_+-\mathcal{S}_-$ interaction. (f) For $\mathbf{u}[1,\mathbf{i}]\bowtie\mathbf{u}[2,-1+\mathbf{j}]\cdots\mathcal{S}_0-\mathcal{S}_-$ interaction.

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N-point deformation of algebraic K3 surfaces

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(Received 2 April 2002; accepted 13 December 2002)

We construct a set of noncommutative geometries by performing N-point deformation of algebraic K3 surfaces. First, we consider two-point deformation of algebraic K3 surfaces by performing algebraic deformation of a pair of commutative algebraic K3 surfaces. In this case, the moduli space of the noncommutative deformations is of dimension 19, the same as the moduli dimension of the complex deformations of commutative algebraic K3 surfaces. Then, we extend this method to the N-point case. In the N-point case, the dimension of deformation moduli space becomes $19N(N-1)/2$. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1545163]

I. INTRODUCTION

Ever since the work of Connes, Douglas, and Schwarz[1] connecting the noncommutative torus and the T-duality in the M theory context appeared in the string/M theory arena, the field related with noncommutaive geometry[2] becomes an industry in the string/M theory circle. Notably, noncommutative torus[3,4] and its varieties have been studied intensively.[5–8] However, noncommutative versions of the K3 surfaces and the Calabi–Yau (CY) threefolds have been rarely studied[9–11] (see also Refs. 12–14). Only recently, noncommutative tori with complex structures have been studied.[15,16]

In Ref. 17, Berenstein, Jejjala, and Leigh initiated an algebraic geometry approach to noncommutative moduli space. Then in Ref. 9, Berenstein and Leigh discussed noncommutative CY threefold from the viewpoint of algebraic geometry. They considered two examples: a toroidal orbifold $T^6/\mathbb{Z}_2\times\mathbb{Z}_2$ and an orbifold of the quintic in $\mathbb{CP}^4$, each with discrete torsion.[18–22] There, they explained the fractionation of branes at singularities from a noncommutative geometric viewpoint under the presence of discrete torsion.

In Ref. 9, Berenstein and Leigh considered the $T^6/\mathbb{Z}_2\times\mathbb{Z}_2$ case and recovered a large slice of the moduli space of complex structures of the CY threefold from the deformation of the noncommutative resolution of the orbifolds via central extension of the local algebra of holomorphic functions. In the commutative K3 case, the moduli space for the K3 space itself has been known already (see, for instance, Ref. 23), and even the moduli space for the bundles on K3 surfaces has been studied.[24] In the noncommutative deformation of CY threefolds in Ref. 9, the three holomorphic coordinates y_i anticommute with each other to be compatible with $\mathbb{Z}_2$ discrete torsion.

In our previous work,[10] we applied this algebraic approach to K3 surfaces in the cases of the orbifolds $T^4/\mathbb{Z}_2$. We constructed a family of noncommutative K3 surfaces by algebraically deforming $T^4/\mathbb{Z}_2$ in both complex and noncommutative directions altogether. In that construction the dimensions of moduli spaces for the complex structures and the noncommutative deformations were the same 18, which is the dimension of the moduli space of the complex structures of K3 surfaces constructed with two elliptic curves.

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However, in the commutative case the complete family of complex deformations of K3 surfaces is of 20 dimension inside which that of the algebraic K3 surfaces is of 19 dimension.[23] In this article, we first construct a 19 dimensional family of the noncommutative moduli of general algebraic K3 surfaces by considering algebraic deformation of a pair of K3 surfaces. This construction apparently looks similar to the Connes–Lott's ''two-point space'' construction of the standard model.[25] Thus, we will call it ''two-point deformation.'' Next, we extend this method directly to the N-point case by deforming N-tuple of commutative algebraic K3 surfaces embedded in $\mathbb{P}^2(x_1,x_2)\times\mathbb{P}^1(t_1)\times\cdots\times\mathbb{P}^1(t_N)$.

In Sec. II, we construct a two-point deformation for general algebraic K3 surfaces. In Sec. III, we extend the method to the N-point case. In Sec. IV, we conclude with discussion.

II. TWO-POINT DEFORMATION

In this section, we first consider the ''two-point space'' version of noncommutative deformation for general algebraic K3 surfaces in the direct extension of our previous work on noncommutative $T^4/\mathbb{Z}_2$.[10] General algebraic K3 surfaces are given by the following form and with a point added at infinity:

$$y^2=f(x_1,x_2). \tag{1}$$

Here f is a function with total degree 6 in x_1,x_2.

Now, we compare this with the Kummer surface, the orbifold of $T^4/\mathbb{Z}_2$ case.[10] There we considered T^4 as the product of two elliptic curves, each given in Weierstrass form

$$y_i^2=x_i(x_i-1)(x_i-a_i), \tag{2}$$

with a point added at infinity for $i=1,2$. By the following change of variables, the point at infinity is brought to a finite point:

$$\begin{aligned} y_i\to y_i'&=\frac{y_i}{x_i^2},\\ x_i\to x_i'&=\frac{1}{x_i}. \end{aligned} \tag{3}$$

For algebraic K3 surfaces, we first consider a function with total degree 6 in complex variables u,v,w, for instance,

$$F(u,v,w)=u^2v^3w+u^4v^2.$$

In a patch where the point at infinity of w can be brought to a finite point, this can be written as

$$\frac{F}{w^6}=\left(\frac{u}{w}\right)^2\left(\frac{v}{w}\right)^3+\left(\frac{u}{w}\right)^4\left(\frac{v}{w}\right)^2$$

and may be denoted as

$$f(x_1,x_2)=x_1^2x_2^3+x_1^4x_2^2,$$

where $x_1=u/w, x_2=v/w$. Then, an algebraic K3 surface is given by

$$y^2=f(x_1,x_2)=x_1^2x_2^3+x_1^4x_2^2. \tag{4}$$

Similarly, in a patch where the point at infinity of u can be brought to a finite point, we consider a function

$$\frac{F}{u^6}=\left(\frac{v}{u}\right)^3\frac{w}{u}+\left(\frac{v}{u}\right)^2,$$

and this can be written as

$$y'^2=f'(x_1',x_2')=x_1'^3x_2'+x_1'^2, \tag{5}$$

where $x_1'=v/u=x_2/x_1, x_2'=w/u=1/x_1$. This can be also obtained directly from (4) by dividing it with x_1^6:

$$\frac{y^2}{x_1^6}=\frac{x_1^2x_2^3}{x_1^6}+\frac{x_1^4x_2^2}{x_1^6}=\left(\frac{x_2}{x_1}\right)^3\frac{1}{x_1}+\left(\frac{x_2}{x_1}\right)^2.$$

Thus, in the case of the general algebraic K3, a point at infinity in one patch can be brought to a finite point in another patch by the following change of variables:

$$y\to y'=\frac{y}{x_1^3}, \tag{6}$$

$$\begin{aligned} x_1&\to x_1'=\frac{x_2}{x_1},\\ x_2&\to x_2'=\frac{1}{x_1}. \end{aligned} \tag{7}$$

We now consider a deformation of algebraic K3 surfaces in a noncommutative direction. Following the same reasoning in our previous work,[10] we consider two commuting complex variables x_1,x_2 and two noncommuting variables t_1,t_2 such that

$$\begin{aligned} t_1^2&=h_1(x_1,x_2),\\ t_2^2&=h_2(x_1,x_2), \end{aligned} \tag{8}$$

where h_1,h_2 are commuting functions of total degree 6 in x_1,x_2. To be consistent with the condition that t_1^2,t_2^2 belong to the center, one can allow the following deformation for t_1,t_2:

$$t_1t_2+t_2t_1=P(x_1,x_2). \tag{9}$$

Here the right hand side should be a polynomial and free of poles in each patch. Thus, under the change of variables (7),

$$x_1\to x_1'=\frac{x_2}{x_1},$$

$$x_2\to x_2'=\frac{1}{x_1},$$

t_i should be changed into

$$t_i\to t_i'=\frac{t_i}{x_1^3},\quad \text{for } i=1,2. \tag{10}$$

This is due to the fact that t's transform just like y in (6). Therefore, P transforms as

$$P(x_1,x_2)\to x_1^6 P'\left(\frac{x_2}{x_1},\frac{1}{x_1}\right). \tag{11}$$

This implies that P' should be of total degree 6 in x_1',x_2', at most. Interchanging the role of P and P' one can see that P should also be of total degree 6 in x_1,x_2.

The above structure can be understood in the following manner. If we do not impose the condition (9), and if we have only one of the t_i's satisfying the condition (8), then we have only one copy of an algebraic K3 surface. If we have both t_i's without the condition (9), then we have two copies of K3 surfaces. If we have both t_i's and impose the condition (9), then we have noncommutatively deformed K3 surfaces in which the above mentioned two K3 surfaces intertwined each other everywhere on their surfaces, becoming fuzzy. This seems to be similar to the ''two-point space'' version of the Connes–Lott model.[25] In the Connes–Lott model, every point of the space becomes fuzzy due to the 1-to-2 correspondence at each point in the space, where the two corresponding points at each classical location are prefixed. On the other hand, ours are more or less like position x and momentum p in quantum mechanics at every point in the space. However, since we started with two copies of the classical space just like the Connes–Lott model, and combined them to become a noncommutative space, we will call our construction ''two-point deformation,'' though our construction is not exactly the same as Connes–Lott's in its nature.

Now, we count the dimension of the moduli space of our deformation. In our previous work for noncommutative $T^4/\mathbb{Z}_2$,[10] t_1 for y_1y_2 and t_2 for y_2y_1 were all invariants of the K3 surface. The dimensions of the moduli spaces of these deformations were 18 for both the noncommutative and complex deformation cases, matching the moduli space dimension of the complex deformation for $T^4/\mathbb{Z}_2$. In the present case, from Eq. (11) we can see that the dimension of the moduli spaces of these deformations are 19 for both the noncommutative and complex deformation cases. In fact, to show this we need to count the dimension of the polynomials of degree 6 in three variables up to constant modulo projective linear transformations of three variables. We get $19=28-1-8$, where 28 is the dimension of polynomials of degree 6 in three variables and 1 and 8 correspond to a constant and $PGL(3,\mathbb{C})$, respectively.

III. *N*-POINT DEFORMATION

In this section, we follow the method in the previous section and consider the ''N-point space'' of the noncommutative deformation of the general algebraic K3 surfaces.

First, we consider N-tuple of commutative algebraic K3 surfaces,

$$\begin{aligned} t_1^2&=h_1(x_1,x_2),\\ &\vdots\\ t_N^2&=h_N(x_1,x_2), \end{aligned} \tag{12}$$

where $h_1,\ldots,h_N$ are commuting functions of total degree 6 in x_1,x_2. This can be regarded as embedding the ith copy of algebraic K3 surface X_i in $\mathbb{P}^2(x_1,x_2)\times\mathbb{P}^1(t_i)$ as $t_i^2=h_i(x_1,x_2)$ of a degree 6 polynomial. Locally the algebra representing the functions on X_i can be expressed as $\mathbb{C}[x_1,x_2,t_i]/I_i$, where I_i is a principal ideal generated by $t_i^2-h_i(x_1,x_2)$ and $\mathbb{C}[x_1,x_2,t_1,\ldots,t_N]$ is a local polynomial algebra of $\mathbb{P}^2(x_1,x_2)\times\mathbb{P}^1(t_1)\times\cdots\times\mathbb{P}^1(t_N)$. Thus embedding X_i in $\mathbb{P}^2(x_1,x_2)\times\mathbb{P}^1(t_1)\times\cdots\times\mathbb{P}^1(t_N)$ induces a natural quotient map from $\mathbb{C}[x_1,x_2,t_1,\ldots,t_N]$ to $\mathbb{C}[x_1,x_2,t_i]/I_i$ by putting t_j as 0 for $j\neq i$.

Now, we consider the deformation of this embedded space in the noncommutative direction as in the two-point case. In order to be consistent with the condition that $t_1^2,\ldots,t_N^2$ belong to the center along with x_1,x_2, we can allow the following deformation for $t_1,\ldots,t_N$:

$$t_it_j+t_jt_i=P_{ij}(x_1,x_2),\quad \text{for } i,j=1,\ldots,N,\ i\neq j. \tag{13}$$

Here the right hand side should be a polynomial and free of poles in each patch. Thus, under the change of variables (7),

$$x_1 \to x_1' = \frac{x_2}{x_1},$$

$$x_2 \to x_2' = \frac{1}{x_1},$$

t_i's should be changed into

$$t_i \to t_i' = \frac{t_i}{x_1^3}, \quad \text{for } i = 1,\ldots,N. \tag{14}$$

This is due to the fact that t_i's transform just like y in (6). Therefore, P_{ij} transforms as

$$P_{ij}(x_1,x_2) \to x_1^6 P_{ij}'\left(\frac{x_2}{x_1}, \frac{1}{x_1}\right). \tag{15}$$

This implies that P_{ij}' should be of total degree 6 in x_1', x_2', at most. Interchanging the role of P_{ij} and P_{ij}' one can see that P_{ij} should be also of total degree 6 in x_1, x_2.

If we forget the embedded N K3 surfaces given by the constraints (12) for the time being, the above defined $\{P_{ij}(x_1,x_2)\}$ given by (13) define a deformation of the ambient space $\mathbb{P}^2(x_1,x_2) \times \mathbb{P}^1(t_1) \times \cdots \times \mathbb{P}^1(t_N)$. So, we can understand that imposing the condition of the change of chart (14) and (15) compatible to the complex structures coming from (12) induces a restriction on P_{ij} being of total degree 6 in x_1, x_2. We might call this deformation a deformation of N K3 surfaces. The choice of P_{ij} is independent of the choice of h_i, which means that the deformations of the classical complex structure and of the noncommutative structure are independent of each other as expected. Now, we count the dimension of the moduli space of our deformation. In the two-point case of the previous section, the dimension of the moduli space of the deformation was 19. In that case, we counted the dimension of the polynomials of degree 6 in three variables up to constant modulo projective linear transformations of three variables. Thus, we got $19 = 28 - 1 - 8$, where 28 is the dimension of polynomials of degree 6 in three variables and 1 and 8 correspond to a constant and $PGL(3,\mathbb{C})$, respectively. Thus, in the N-point case the dimension of the moduli space of the deformation is the number of independent P_{ij} times the deformation dimension of the two-point case. Namely, we have $19N(N-1)/2$ as the dimension of the deformation moduli for the N-point deformation case.

IV. DISCUSSION

In this article, we deformed N K3 surfaces in the noncommutative sense and computed the dimension for the moduli space.

In the first part of the article, we constructed the two-point deformation of algebraic K3 surfaces by considering algebraic deformation of a pair of commutative algebraic K3 surfaces. Doing this, we used the same method as in the case of the Kummer K3 surface[10] which is the $\mathbb{Z}_2$ quotient of two elliptic curves E_1, E_2 where E_i satisfies $y_i^2 = f_i(x_i)$. In Ref. 10, we defined $t_1 = y_1 y_2$, $t_2 = y_2 y_1$ and introduced the deformation $t_1 t_2 + t_2 t_1 = P_{12}(x_1,x_2)$. In that case t_1, t_2 were functions on the Kummer K3 surface, so that the deformation was a noncommutative deformation of one Kummer K3 surface. However, the moduli dimension of that deformation was of 18,[10] not the same as the moduli dimension of algebraic K3 surfaces. Here, we recovered the same moduli dimension of deformation, 19 by algebraically deforming a pair of algebraic K3 surfaces in a manner similar to the Connes–Lott construction.[25]

Then we considered the extension of this method to the N-point case. Notice that in the N-point deformation case, t_j in the $t_i t_j + t_j t_i = P_{ij}(x_1,x_2)$ is not a function on the ith copy of

commutative K3 surface X_i for $i \neq j$. Rather, this can be thought of as noncommutative deformation of N K3 surfaces or a noncommutative deformation of the ambient space $\mathbb{P}^2(x_1,x_2) \times \mathbb{P}^1(t_1) \times \cdots \times \mathbb{P}^1(t_N)$ compatible to the complex structure of each K3 surface. In the N-point case, we obtained $19N(N-1)/2$ as the dimension of deformation moduli.

When $N=3$, it is interesting whether we can find an analog of the classical hyperkähler structure of K3 surface. First, we recall the property of the moduli space of Ricci flat metrics on a K3 surface S. If a given metric g satisfies $g(Jv,Jw)=g(v,w)$ for any tangent vector v,w, then we say that the metric g is compatible with the complex structure J. If the two form $\Omega(\cdot,\cdot) = g(J\cdot,\cdot)$ is closed, then it is called a Kähler metric and Ω is called a Kähler form. Any given Ricci-flat metric g induces a Hodge $*$ operator on $H^2(S,\mathbb{R}) \cong \mathbb{R}^{3,19}$ by which $H^2(S,\mathbb{R})$ can be decomposed as a direct sum of two eigenspaces, self-dual part (eigenvalue 1) of dimension 3 and anti-self-dual part (eigenvalue -1) of dimension 19.

In this setting, for the given Ricci-flat metric g, the self-dual part Λ^+ is a three-dimensional real vector space consisting of vectors whose self intersection is positive. Different compatible structures J to g correspond to different unit vectors in Λ^+, and they form S^2 isomorphic to $\mathbb{P}^1$. Here we choose three orthogonal unit vectors $\Omega_1,\Omega_2,\Omega_3$ in Λ^+ such that corresponding complex structures J_1,J_2,J_3 satisfy the relation $J_iJ_j=\epsilon_{ijk}J_k$ for $i,j,k=1,2,3$. This is called a hyperkähler structure on S. We wonder whether we can see the three-point deformation case as the deformation of this hyperkähler structure on S by relating t_i's with J_i's.

Fröhlich *et al.*[26,27] defined a spectral triple for this hyperkähler case introducing the operators $\partial, \overline{\partial}, T^i, \overline{T^i}$, $i=1,2,3$, acting on the differential forms. Here, $\partial = \frac{1}{2}(D - i\overline{D})$, where D is the Dirac operator and T^i, $i=1,2,3$, are operators coming from the hyperkähler structure. Then they extended this definition to the noncommutative case. We also wonder whether we can relate our t_i with their T_i.

Finally, we wonder whether we can find a sort of Clifford structures on $\mathbb{P}^2(x_1,x_2)$ with the fiber $\mathbb{P}^1(t_1) \times \cdots \times \mathbb{P}^1(t_N)$. This may be considered by regarding $t_it_j+t_jt_i=P_{ij}(x_1,x_2)$, $i,j=1,\ldots,N$, $i \neq j$ and $t_i^2=h_i(x_1,x_2)$, $i=1,\ldots,N$, not as constraints giving noncommutative deformation and complex structures for K3 surfaces but as the components of a symmetric matrix giving the metric on the fiber.

ACKNOWLEDGMENT

This work was supported by KOSEF Interdisciplinary Research Grant No. R01-2000-00022.

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Riccati solutions of discrete Painlevé equations with Weyl group symmetry of type $E_8^{(1)}$

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(Received 26 September 2002; accepted 8 October 2002)

We present special solutions of the discrete Painlevé equations associated with $A_0^{(1)}$, $A_0^{(1)}*$ and $A_0^{(1)}**$-surfaces. These solutions can be expressed by solutions of linear difference equations. Here the $A_0^{(1)}$-surface discrete Painlevé equation is the most generic difference equation, as all discrete Painlevé equations can be obtained by its degeneration limit. These special solutions exist when the parameters of the discrete Painlevé equation satisfy a particular constraint. We consider that these special functions belong to the hypergeometric family although they seem to go beyond the known discrete and q-discrete hypergeometric functions. We also discuss the degeneration scheme of these solutions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1531216]

I. INTRODUCTION

Discrete Painlevé equations are studied with various views of integrable systems.[1,2,6] One of the authors presented the list of all difference Painlevé equations from the view point of algebraic geometry. For a rational surface, we can obtain a birational representation of certain affine Weyl groups as its symmetry. We regard a translation part of the symmetry as a difference system. Discrete Painlevé equations were classified on the basis of the types of rational surfaces, and some new equations were discovered by this classification.[8]

Let X be a smooth projective surface. We denote by $\mathcal{K}_X$ the canonical divisor class on X, and by $|-\mathcal{K}_X|$ the set of all positive divisors on X such that is linearly equivalent to $-\mathcal{K}_X$. We call an element of $|-\mathcal{K}_X|$ an anticanonical divisor. Generalized Halphen surfaces are smooth projective rational surfaces with an anticanonical divisor of canonical type. If $|-\mathcal{K}_X|$ has a unique divisor D, then X is classified according to the type R of D, where R is in Table II. The list of R can be obtained from the list of sublattices of $Q(E_8^{(1)})$ which are indecomposable and of affine type (see Table I). We call a surface X an R-surface.

In this article, we consider the case that the root lattice $Q(R)=\mathbb{Z}\delta$ (δ: null root) especially. It is the case that D itself is irreducible. Usually this lattice is not a root lattice, but we assign the symbol $A_0^{(1)}$ to the type of lattice. The divisor D has the three types; a smooth curve, a curve with a double point, and a curve with a cusp. We assign the symbols $A_0^{(1)}$, $A_0^{(1)}*$ and $A_0^{(1)}**$ to each type, respectively. This $A_0^{(1)}$ is the most generic case in this list. These three types of surfaces have Weyl group symmetry of type $E_8^{(1)}$.

The types of surfaces are divided into three classes naturally. We call them the elliptic type, the multiplicative type and the additive type, respectively. This classification corresponds to the types of discrete equation, what we call elliptic-difference equation, q-difference equation and usual difference equation. See Ref. 8 in detail.

In this list, $D_l^{(1)}$, $E_l^{(1)}$-surface can be constructed as a space of initial conditions for Painlevé differential equations (see Table III).

Each discrete Painlevé equation is usually named by the form of discrete equation and the differential equation obtained at the limit, for example $q\text{-}P_{IV}$, $d\text{-}P_I$. But, in view of the list, we cannot name all equations in this way. Ramani *et al.* named these equations from the symmetry

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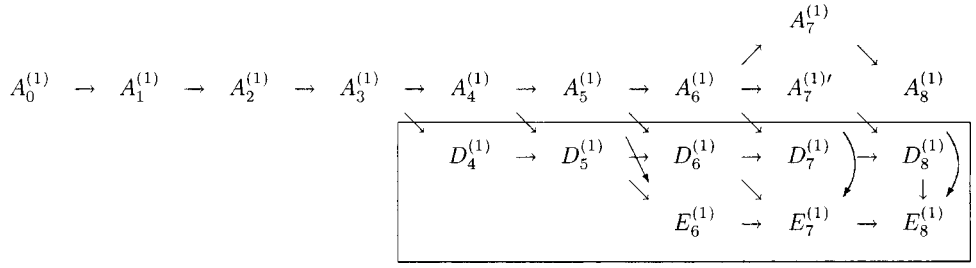
TABLE I. The list of indecomposable affine root subsystem of $E_8^{(1)}$.



The arrows mean inclusions ($R \to R' \Leftrightarrow Q(R) \subset Q(R')$).

that the equation has.[7] But there is a case that different equations have the same symmetry, and it is not trivial whether a discrete system with a given symmetry exists or not. For example, $A_3^{(1)}$-surface has Weyl group symmetry of type $D_5^{(1)}$ but there is no surface with Weyl group symmetry of type $D_6^{(1)}$. So, in this article, we distinguish each discrete Painlevé equation by the rational surface on which the equation is defined, and call, for example, the $A_0^{(1)}$-surface discrete Painlevé equation ($dP(A_0^{(1)})$).

We know many results about special solutions with respect to Painlevé differential equations whose parameters satisfy particular conditions (Ref. 5, etc.). These solutions are divided into algebraic solutions and what we call Riccati solutions. Riccati solutions are expressed by solutions of linear equations of the second order. For example, the sixth Painlevé equation P_{VI} has special solutions expressed in terms of the Gauss hypergeometric functions. The discrete Painlevé equations also possess Riccati solutions for particular values of the parameter. For example, the $A_3^{(1)}$-surface discrete Painlevé equation (q-P_{VI}) has solutions expressed by the q-hypergeometric functions.[3]

In Ref. 7, Ramani *et al.* presented special solutions of the $A_1^{(1)}$-surface discrete Painlevé equation and its degenerations. But they did not mention about the discrete Painlevé equations corresponding to the surfaces of types $A_0^{(1)}$, $A_0^{(1)*}$ and $A_0^{(1)**}$.

In this article, we obtain special solutions for these discrete Painlevé equations. We also discuss the degeneration scheme of these equations.

The article is organized as follows:

In Sec. II, we show a geometrical construction of the $A_0^{(1)}$-surface discrete Painlevé equation and a Riccati solution of this equation in Theorem 2.

In Sec. III, we obtain the $A_0^{(1)*}$-surface discrete Painlevé equation in the geometric approach, and a special solution of this equation. And we show a degeneration scheme of these equations in Theorem 3, 5.

In Sec. IV, we obtain the $A_0^{(1)**}$-surface discrete Painlevé equation in the geometric approach, and a special solution of this equation in a similar way. And we show a degeneration scheme of these equations in Theorem 8.

TABLE II. Classification of generalized Halphen surfaces with $\dim|-K_X| = 0$.

Type	R
Elliptic type	$A_0^{(1)}$
Multiplicative type	$A_0^{(1)*}$ $A_1^{(1)}$ $A_2^{(1)}$ $A_3^{(1)}$ $A_4^{(1)}$ $A_5^{(1)}$ $A_6^{(1)}$ $A_7^{(1)}$ $A_7^{(1)\prime}$ $A_8^{(1)}$
Additive type	$A_0^{(1)**}$ $A_1^{(1)*}$ $A_2^{(1)*}$
	$D_4^{(1)}$ $D_5^{(1)}$ $D_6^{(1)}$ $D_7^{(1)}$ $D_8^{(1)}$
	$E_6^{(1)}$ $E_7^{(1)}$ $E_8^{(1)}$

TABLE III. The Painlevé differential equations.

Type of surface	$D_4^{(1)}$	$D_5^{(1)}$	$D_6^{(1)}$	$D_7^{(1)}$	$D_8^{(1)}$	$E_6^{(1)}$	$E_7^{(1)}$	$E_8^{(1)}$
Painlevé equation	P_{VI}	P_V	$P_{III}^{D_6^{(1)}}$	$P_{III}^{D_7^{(1)}}$	$P_{III}^{D_8^{(1)}}$	P_{IV}	P_{II}	P_I

In Sec. V, we show as Theorem 9 a degeneration scheme between a special solution of the $A_0^{(1)*}$-surface discrete Painlevé equation in Sec. III and a special solution of the $A_1^{(1)}$-surface discrete Painlevé equation.

II. ELLIPTIC TYPE

A. Discrete Painlevé equation

We present the $A_0^{(1)}$-surface discrete Painlevé equation ($dP(A_0^{(1)})$). This system is equivalent to ell.P derived in Ref. 4. In this article, all 2×2 matrices represent PGL(2)-action on $\mathbb{P}^1$, i.e., $w=\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)z$ means $w=(az+b)/(cz+d)$.

The $A_0^{(1)}$-surface discrete Painlevé equation is the following difference system for unknown functions f(t), g(t):

$$\overline{g}=M\left(f,c_7,c_8,t-\frac{1}{4}\sum_{i=1}^{6}c_i\right)M\left(f,c_5,c_6,t-\frac{1}{4}\sum_{i=1}^{4}c_i\right)M\left(f,c_3,c_4,t-\frac{1}{4}(c_1+c_2)\right)\times M(f,c_1,c_2,t)g, \tag{2.1}$$

$$\underline{f}=M\left(g,d_7,d_8,t-\frac{1}{4}\sum_{i=1}^{6}d_i\right)M\left(g,d_5,d_6,t-\frac{1}{4}\sum_{i=1}^{4}d_i\right)M\left(g,d_3,d_4,t-\frac{1}{4}(d_1+d_2)\right)\times M(g,d_1,d_2,t)f, \tag{2.2}$$

where $\overline{g}=g(t+\lambda)$, $\underline{f}=f(t-\lambda)$ *and*

$$\begin{aligned}M(h,\kappa_1,\kappa_2,s)&=\begin{pmatrix}-\wp\left(2s-\frac{-\kappa_1+\kappa_2}{2}\right) & \wp\left(2s-\frac{\kappa_1-\kappa_2}{2}\right)\\ -1 & 1\end{pmatrix}\\&\times\begin{pmatrix}(h-\wp(\kappa_2))(\wp(2s)-\wp(2s-\kappa_2))\left(\wp\left(2s-\frac{\kappa_1+\kappa_2}{2}\right)-\wp\left(2s-\frac{\kappa_1-\kappa_2}{2}\right)\right) & 0\\ 0 & (h-\wp(\kappa_1))(\wp(2s)-\wp(2s-\kappa_1))\left(\wp\left(2s-\frac{\kappa_1+\kappa_2}{2}\right)-\wp\left(2s-\frac{-\kappa_1+\kappa_2}{2}\right)\right)\end{pmatrix}\\&\times\begin{pmatrix}1 & -\wp(2s-\kappa_1)\\ 1 & -\wp(2s-\kappa_2)\end{pmatrix}.\end{aligned} \tag{2.3}$$

Here b_i $(i=1,\ldots,8)$ *are constant parameters and set* $\lambda=\frac{1}{2}\Sigma_{i=1}^{8}b_i$, $c_i=b_i+t$, $d_i=t-b_i$. *Note that we will regard* $(f(t),g(t))$ *as inhomogeneous coordinates of* $\mathbb{P}^1\times\mathbb{P}^1$.

We derive this discrete equation as a translation of $W(E_8^{(1)})$ again.

We construct the $A_0^{(1)}$-surface by blowing up $\mathbb{P}^1\times\mathbb{P}^1$ at eight points $p_i(i=1,\ldots,8)$. For generic eight points there is an elliptic curve which passes through these eight points. We parametrize these eight points and the curve as follows:

$$(f+g+\wp(2t))(4\wp(2t)fg-g_3)=\left(fg+\wp(2t)(f+g)+\frac{g_2}{4}\right)^2, \tag{2.4}$$

$$p_i: \quad (\wp(b_i+t),\wp(t-b_i)) \quad (i=1,\ldots,8). \tag{2.5}$$

Remark 2.1: We can parametrize an isomorphism class of surfaces by using the period mapping. The period mapping maps the elements of the second homology to $\mathbb{C}$.

Let ω be a meromorphic two-form on X with $\mathrm{div}(\omega)=-D$. Then ω determines the period mapping $\hat{\chi}:H_2(X-D,\mathbb{Z})\to\mathbb{C}$ which sends $\Gamma\in H_2(X-D,\mathbb{Z})$ to $\int_\Gamma\omega$.

Now, there exists the short exact sequence:

$$0\to H_1(D,\mathbb{Z})\to H_2(X-D,\mathbb{Z})\to Q(E_8^{(1)})\to 0,$$

where $Q(E_8^{(1)})=\Sigma_{i=0}^{8}\mathbb{Z}\alpha_i$ is the root lattice of type $E_8^{(1)}$. So we obtain the mapping

$$\chi: \quad Q(E_8^{(1)})\to\mathbb{C} \quad \mathrm{mod}\ \hat{\chi}(H_1(D,\mathbb{Z}))$$

through the period mapping $\hat{\chi}$. In the case, the parametrization is the following:

$$\begin{gathered}\chi(\alpha_1)=-4t, \quad \chi(\alpha_2)=b_1+b_2+2t, \quad \chi(\alpha_i)=b_i-b_{i-1} \ (i=3,\ldots,7),\\ \chi(\alpha_8)=b_2-b_1, \quad \chi(\alpha_0)=b_8-b_7.\end{gathered} \tag{2.6}$$

Here $Q(E_8^{(1)})$ is realized in $\mathrm{Pic}(X)=H_2(X,\mathbb{Z})$. And α_i's are represented by the elements of the Picard group as follows:

$$\begin{gathered}\alpha_1=H_1-H_0, \quad \alpha_2=H_0-E_1-E_2, \quad \alpha_i=E_{i-1}-E_i \ (i=3,\ldots,7),\\ \alpha_8=E_1-E_2, \quad \alpha_0=E_7-E_8.\end{gathered} \tag{2.7}$$

We denote the total transform of $f=\mathrm{const}$ (or $g=\mathrm{const}$) on X by H_0 (or H_1, respectively) and the total transform of the point p_i by E_i. The Picard group $\mathrm{Pic}(X)$ and the canonical divisor $\mathcal{K}_X$ are

$$\mathrm{Pic}(X)=\mathbb{Z}H_0+\mathbb{Z}H_1+\sum_{i=1}^{8}\mathbb{Z}E_i, \quad \mathcal{K}_X=-2H_0-2H_1+\sum_{i=1}^{8}E_i,$$

where the intersection numbers of pairs of base elements are

$$H_i\cdot H_j=1-\delta_{i,j}, \quad E_i\cdot E_j=-\delta_{i,j}, \quad H_i\cdot E_j=0, \quad \text{where } \delta_{i,j}=\begin{cases}1 & i=j,\\ 0 & i\neq j.\end{cases}$$

□

Generators of affine Weyl group $W(E_8^{(1)})=\langle w_i \ (i=0,1,\ldots,8)\rangle$ act on these coordinates and parameters. We give a representation of these actions in order to construct $dP(A_0^{(1)})$:

$$w_2: \quad \left(\begin{matrix}b_1 & b_2 & b_3 & b_4\\ b_5 & b_6 & b_7 & b_8\end{matrix}, t, g\right)$$

$$\mapsto\left(\begin{matrix}b_1-3\dfrac{2t+b_1+b_2}{4} & b_2-3\dfrac{2t+b_1+b_2}{4} & b_3+\dfrac{2t+b_1+b_2}{4} & b_4+\dfrac{2t+b_1+b_2}{4}\\ b_5+\dfrac{2t+b_1+b_2}{4} & b_6+\dfrac{2t+b_1+b_2}{4} & b_7+\dfrac{2t+b_1+b_2}{4} & b_8+\dfrac{2t+b_1+b_2}{4}\end{matrix}, t-\frac{2t+b_1+b_2}{4}, \tilde{g}\right),$$

$$w_1:\quad (t,f,g)\mapsto(-t,g,f),\quad w_i:\quad (b_{i-1},b_i)\mapsto(b_i,b_{i-1})\quad (i=3,\ldots,7),$$

$$w_8:\quad (b_1,b_2)\mapsto(b_2,b_1),\quad w_0:\quad (b_7,b_8)\mapsto(b_8,b_7),$$

where $\tilde{g}$ is given by

$$\frac{\tilde{g}-\wp(2t-(b_1-b_2)/2)}{\tilde{g}-\wp(2t-(-b_1+b_2)/2)}$$
$$=\frac{f-\wp(b_2+t)}{f-\wp(b_1+t)}\,\frac{\wp(t-(b_1+b_2)/2)-\wp(2t-(b_1-b_2)/2)}{\wp(t-(b_1+b_2)/2)-\wp(2t-(-b_1+b_2)/2)}\,\frac{\wp(2t)-\wp(t-b_2)}{\wp(2t)-\wp(t-b_1)}\,\frac{g-\wp(t-b_1)}{g-\wp(t-b_2)}.$$

Notice that we can rewrite the action of w_2 into the following form:

$$w_2:\quad (c_1,c_2,t,g)\mapsto\left(-c_2,-c_1,t-\frac{c_1+c_2}{4},M(f,c_1,c_2,t)g\right),$$

where we use the notation $c_i=b_i+t$ and $M(f,c_1,c_2,t)$ is defined by (2.3).

By taking a translation of $W(E_8^{(1)})$, we obtain a nonlinear difference equation. The translation can be described by a product of simple reflections w_i's:

$$\begin{aligned}dP(A_0^{(1)})=&w_1\circ w_2\circ w_3\circ w_8\circ w_4\circ w_3\circ w_2\circ w_5\circ w_4\circ w_3\circ w_8\circ w_6\circ w_5\circ w_4\\&\circ w_3\circ w_2\circ w_7\circ w_6\circ w_5\circ w_4\circ w_3\circ w_8\circ w_0\circ w_7\circ w_6\circ w_5\circ w_4\circ w_3\circ w_2\\&\circ w_1\circ w_2\circ w_3\circ w_4\circ w_5\circ w_6\circ w_7\circ w_0\circ w_8\circ w_3\circ w_4\circ w_5\circ w_6\circ w_7\circ w_2\\&\circ w_3\circ w_4\circ w_5\circ w_6\circ w_8\circ w_3\circ w_4\circ w_5\circ w_2\circ w_3\circ w_4\circ w_8\circ w_3\circ w_2:\end{aligned}\tag{2.8}$$

$$(b_i,t,f,g)\mapsto(b_i,t+\lambda,\overline{f},\overline{g})\quad (i=1,\ldots,8),\quad \lambda=\frac{1}{2}\sum_{i=1}^{8}b_i,\tag{2.9}$$

where mappings of f,g are defined by (2.1) and (2.2).

Remark 2.2: In Ref. 8, we obtain $A_0^{(1)}$-surface by blowing up $\mathbb{P}^2$ with the centers at nine points:

$$\begin{gathered}y^2z=4x^3-g_2x^2z-g_3z^3,\\ p_i:\quad (\wp(\theta_i):\wp'(\theta_i):1)\quad (i=1,\ldots,9),\end{gathered}\tag{2.10}$$

$$\chi(\alpha_i)=\theta_{i+1}-\theta_i\ \ (i=1,\ldots,7),\quad \chi(\alpha_8)=\theta_1+\theta_2+\theta_3,\quad \chi(\alpha_0)=\theta_9-\theta_8.\tag{2.11}$$

Both parameters and coordinates correspond as follows:

$$b_1=-\tfrac{3}{4}(\theta_1+\theta_2),\quad b_i=\theta_{i+1}+\tfrac{1}{4}(\theta_1+\theta_2)\ \ (i=2,\ldots,8),\quad t=\tfrac{1}{4}(\theta_1-\theta_2),\tag{2.12}$$

$$f=\frac{(4\wp(\theta_1/2)^3-3g_2\wp(\theta_1/2)-4g_3)x-2\wp(\theta_1/2)\wp'(\theta_1/2)y-(g_2\wp(\theta_1/2)^2+6g_3\wp(\theta_1/2)+g_2^2/4)z}{-(12\wp(\theta_1/2)^2-g_2)x-2\wp'(\theta_1/2)y+(4\wp(\theta_1/2)^3+g_2\wp(\theta_1/2)+2g_3)z},\tag{2.13}$$

$$g=\frac{(4\wp(\theta_2/2)^3-3g_2\wp(\theta_2/2)-4g_3)x-2\wp(\theta_2/2)\wp'(\theta_2/2)y-(g_2\wp(\theta_2/2)^2+6g_3\wp(\theta_2/2)+g_2^2/4)z}{-(12\wp(\theta_2/2)^2-g_2)x-2\wp'(\theta_2/2)y+(4\wp(\theta_2/2)^3+g_2\wp(\theta_2/2)+2g_3)z}. \tag{2.14}$$

We note that the next formula holds for any θ, φ.

$$\wp(\theta+\varphi)$$
$$=\frac{(4\wp(\varphi)^3-3g_2\wp(\varphi)-4g_3)\wp(\theta)-2\wp(\varphi)\wp'(\varphi)\wp'(\theta)-(g_2\wp(\varphi)^2+6g_3\wp(\varphi)+g_2^2/4)}{-(12\wp(\varphi)^2-g_2)\wp(\theta)-2\wp'(\varphi)\wp'(\theta)+(4\wp(\varphi)^3+g_2\wp(\varphi)+2g_3)}. \tag{2.15}$$

This formula is a kind of additive formula of $\wp$-function. □

Note that points on the elliptic curve (2.4) move to points on this elliptic curve.

Proposition 1: $dP(A_0^{(1)})$ has the following trivial solution:

$$f=\wp(q+2t^2/\lambda+t),\quad g=\wp(-q-2t^2/\lambda+t), \tag{2.16}$$

where q is a constant determined by initial condition.

Proof: We suppose that the solution's form is $f=\wp(p+t)$, $g=\wp(t-p)$, where $p=p(t)$. We input them into (2.1) and (2.2). We note that the following identity holds for arbitrary c,

$$\frac{\wp(2t-(c_1+c_2)/2-c)-\wp(2t-(c_1+c_2)/2+c_2)}{\wp(2t-(c_1+c_2)/2-c)-\wp(2t-(c_1+c_2)/2+c_1)}\frac{\wp(c)-\wp(c_1)}{\wp(c)-\wp(c_2)}\frac{\wp(2t-c)-\wp(2t-c_2)}{\wp(2t-c)-\wp(2t-c_1)}$$
$$=\frac{\wp(2t-(c_1+c_2)/2)-\wp(2t-(c_1+c_2)/2+c_2)}{\wp(2t-(c_1+c_2)/2)-\wp(2t-(c_1+c_2)2+c_1)}\frac{\wp(2t)-\wp(2t-c_2)}{\wp(2t)-\wp(2t-c_1)}, \tag{2.17}$$

because both sides equal to

$$\frac{\sigma(2t-(c_1+c_2)/2+c_1)^2\sigma(c_2)^2\sigma(2t-c_1)^2}{\sigma(2t-(c_1+c_2)/2+c_2)^2\sigma(c_1)^2\sigma(2t-c_2)^2}.$$

Since (2.17) is equivalent to

$$\wp\left(2t-\frac{c_1+c_2}{2}-c\right)=M(\wp(c),c_1,c_2,t)\wp(2t-c), \tag{2.18}$$

we obtain

$$\wp(t+\lambda-\overline{p})=\wp(-3t-\lambda-p), \tag{2.19}$$

$$\wp(t-\lambda+\underline{p})=\wp(-3t+\lambda+p). \tag{2.20}$$

The compatibility condition of them leads one difference equation,

$$\overline{p}=p+4t+2\lambda, \tag{2.21}$$

so that

$$p=q+2t^2/\lambda, \tag{2.22}$$

where q is a constant determined by initial condition.

B. Linear equation

We derive the following theorem in this section.

Theorem 2: *A solution of the following system of equations is written by a solution of linear equation:*

$$\begin{vmatrix} fg & g & f & 1 \\ \wp(b_1+t)\wp(t-b_1) & \wp(t-b_1) & \wp(b_1+t) & 1 \\ \wp(b_3+t)\wp(t-b_3) & \wp(t-b_3) & \wp(b_3+t) & 1 \\ \wp(b_5+t)\wp(t-b_5) & \wp(t-b_5) & \wp(b_5+t) & 1 \end{vmatrix} = 0, \tag{2.23}$$

$$\begin{vmatrix} f\overline{g} & \overline{g} & f & 1 \\ \wp(b_8+t)\wp(\overline{t}-b_8) & \wp(\overline{t}-b_8) & \wp(b_8+t) & 1 \\ \wp(b_6+t)\wp(\overline{t}-b_6) & \wp(\overline{t}-b_6) & \wp(b_6+t) & 1 \\ \wp(b_4+t)\wp(\overline{t}-b_4) & \wp(\overline{t}-b_4) & \wp(b_4+t) & 1 \end{vmatrix} = 0, \tag{2.24}$$

where $\overline{t}=t+\lambda$. *When* $b_1+b_3+b_5+b_7=0$, *a solution of this system is a special solution of* $dP(A_0^{(1)})$ *(2.1) and (2.2).* □

Transforming these equations,

$$\overline{g}=\frac{\begin{vmatrix} \wp(b_8+\overline{t})\wp(\overline{t}-b_8) & \wp(\overline{t}-b_8) & 1 \\ \wp(b_6+\overline{t})\wp(\overline{t}-b_6) & \wp(\overline{t}-b_6) & 1 \\ \wp(b_4+\overline{t})\wp(\overline{t}-b_4) & \wp(\overline{t}-b_4) & 1 \end{vmatrix} f+ \begin{vmatrix} \wp(b_8+\overline{t})\wp(\overline{t}-b_8) & \wp(b_8+\overline{t}) & \wp(\overline{t}-b_8) \\ \wp(b_6+\overline{t})\wp(\overline{t}-b_6) & \wp(b_6+\overline{t}) & \wp(\overline{t}-b_6) \\ \wp(b_4+\overline{t})\wp(\overline{t}-b_4) & \wp(b_4+\overline{t}) & \wp(\overline{t}-b_4) \end{vmatrix}}{\begin{vmatrix} \wp(b_8+\overline{t}) & \wp(\overline{t}-b_8) & 1 \\ \wp(b_6+\overline{t}) & \wp(\overline{t}-b_6) & 1 \\ \wp(b_4+\overline{t}) & \wp(\overline{t}-b_4) & 1 \end{vmatrix} f+ \begin{vmatrix} \wp(b_8+\overline{t})\wp(\overline{t}-b_8) & \wp(b_8+\overline{t}) & 1 \\ \wp(b_6+\overline{t})\wp(\overline{t}-b_6) & \wp(b_6+\overline{t}) & 1 \\ \wp(b_4+\overline{t})\wp(\overline{t}-b_4) & \wp(b_4+\overline{t}) & 1 \end{vmatrix}}, \tag{2.25}$$

$$f=\frac{\begin{vmatrix} \wp(b_1+t)\wp(t-b_1) & \wp(b_1+t) & 1 \\ \wp(b_3+t)\wp(t-b_3) & \wp(b_3+t) & 1 \\ \wp(b_5+t)\wp(t-b_5) & \wp(b_5+t) & 1 \end{vmatrix} g+ \begin{vmatrix} \wp(b_1+t)\wp(t-b_1) & \wp(t-b_1) & \wp(b_1+t) \\ \wp(b_3+t)\wp(t-b_3) & \wp(t-b_3) & \wp(b_3+t) \\ \wp(b_5+t)\wp(t-b_5) & \wp(t-b_5) & \wp(b_5+t) \end{vmatrix}}{\begin{vmatrix} \wp(t-b_1) & \wp(b_1+t) & 1 \\ \wp(t-b_3) & \wp(b_3+t) & 1 \\ \wp(t-b_5) & \wp(b_5+t) & 1 \end{vmatrix} g+ \begin{vmatrix} \wp(b_1+t)\wp(t-b_1) & \wp(t-b_1) & 1 \\ \wp(b_3+t)\wp(t-b_3) & \wp(t-b_3) & 1 \\ \wp(b_5+t)\wp(t-b_5) & \wp(t-b_5) & 1 \end{vmatrix}}. \tag{2.26}$$

Eliminating f, we can obtain a difference equation of the first order with respect to the variable g. When g is expressed by homogeneous coordinate ($g=g_1/g_2$), $\overline{g}=(Ag+B)/(Cg+D)$ leads to $\overline{g_1}/\overline{g_2}=(Ag_1+Bg_2)/(Cg_1+Dg_2)$. The solution g is represented by solution of linear equation:

$$\begin{pmatrix} \overline{g_1} \\ \overline{g_2} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}.$$

Now we demonstrate Theorem 2. On the condition $b_1+b_3+b_5+b_7=0$, we consider the curve $I=0$, where

$$I=\begin{vmatrix} fg & g & f & 1 \\ \wp(b_1+t)\wp(t-b_1) & \wp(t-b_1) & \wp(b_1+t) & 1 \\ \wp(b_3+t)\wp(t-b_3) & \wp(t-b_3) & \wp(b_3+t) & 1 \\ \wp(b_5+t)\wp(t-b_5) & \wp(t-b_5) & \wp(b_5+t) & 1 \end{vmatrix}$$

$$=\begin{vmatrix} fg & g & f & 1 \\ \wp(c_1)\wp(2t-c_1) & \wp(2t-c_1) & \wp(c_1) & 1 \\ \wp(c_3)\wp(2t-c_3) & \wp(2t-c_3) & \wp(c_3) & 1 \\ \wp(c_5)\wp(2t-c_5) & \wp(2t-c_5) & \wp(c_5) & 1 \end{vmatrix}. \tag{2.27}$$

Remark 2.3: On this condition, p_i $(i=1,3,5,7)$ lie on $I=0$, because the following formula holds:

$$\begin{vmatrix} \wp(b_1+t)\wp(t-b_1) & \wp(t-b_1) & \wp(b_1+t) & 1 \\ \wp(b_3+t)\wp(t-b_3) & \wp(t-b_3) & \wp(b_3+t) & 1 \\ \wp(b_5+t)\wp(t-b_5) & \wp(t-b_5) & \wp(b_5+t) & 1 \\ \wp(b_7+t)\wp(t-b_7) & \wp(t-b_7) & \wp(b_7+t) & 1 \end{vmatrix}=0. \tag{2.28}$$

The curve $I=0$ has the divisor class $C=H_0+H_1-E_1-E_3-E_5-E_7$, and the self-intersection number of C is -2. In this case, we can restrict affine Weyl group action on the curve $I=0$, which is isomorphic to $\mathbb{P}^1$, and the translation is automorphism on $\mathbb{P}^1$, namely homographic transformation. □

Calculating w_2 acting I, we set $\tilde{I}$ as follows:

$$\tilde{I}=\begin{vmatrix} f\tilde{g} & \tilde{g} & f & 1 \\ \wp(c_2)\wp(2\tilde{t}+c_2) & \wp(2\tilde{t}+c_2) & \wp(c_2) & 1 \\ \wp(c_3)\wp(2\tilde{t}-c_3) & \wp(2\tilde{t}-c_3) & \wp(c_3) & 1 \\ \wp(c_5)\wp(2\tilde{t}-c_5) & \wp(2\tilde{t}-c_5) & \wp(c_5) & 1 \end{vmatrix}, \tag{2.29}$$

where $\tilde{t}=t-(c_1+c_2)/4$. Then

$$\tilde{I}=I\left(\frac{\wp(2\tilde{t})-\wp(2\tilde{t}+c_2)}{\wp(2\tilde{t})-\wp(2\tilde{t}+c_1)}\frac{\wp(2t)-\wp(2t-c_2)}{\wp(2t)-\wp(2t-c_1)}\right)^2(f-\wp(c_2))(\wp(c_2)-\wp(c_3))(\wp(c_2)-\wp(c_5))$$

$$\times(\wp(2t-c_1)-\wp(2t-c_2))(\wp(2\tilde{t}+c_2)-\wp(2\tilde{t}+c_1))^2\times\left(\begin{vmatrix} f & g & 1 \\ \wp(c_1) & \wp(2t-c_1) & 1 \\ \wp(c_2) & \wp(2t-c_2) & 1 \end{vmatrix}\right.$$

$$\left.\times\begin{vmatrix} \wp(c_1) & \wp(2t-c_1) & 1 \\ \wp(c_2) & \wp(2t-c_2) & 1 \\ \wp(c_3) & \wp(2t-c_3) & 1 \end{vmatrix}\begin{vmatrix} \wp(c_1) & \wp(2t-c_1) & 1 \\ \wp(c_2) & \wp(2t-c_2) & 1 \\ \wp(c_5) & \wp(2t-c_5) & 1 \end{vmatrix}\right)^{-1}. \tag{2.30}$$

Therefore $I=0\Rightarrow\tilde{I}=0$. Similarly we consider the curve $\mathcal{I}=0$,

$$\mathcal{I}=\begin{vmatrix} f\overline{g} & \overline{g} & f & 1 \\ \wp(b_8+t)\wp(\overline{t}-b_8) & \wp(\overline{t}-b_8) & \wp(b_8+t) & 1 \\ \wp(b_6+t)\wp(\overline{t}-b_6) & \wp(\overline{t}-b_6) & \wp(b_6+t) & 1 \\ \wp(b_4+t)\wp(\overline{t}-b_4) & \wp(\overline{t}-b_4) & \wp(b_4+t) & 1 \end{vmatrix}. \tag{2.31}$$

Then $I=0\Rightarrow\mathcal{I}=0$ holds, and we consider the curve $\overline{I}=0$,

$$\overline{I}=\begin{vmatrix} \overline{f\overline{g}} & \overline{g} & \overline{f} & 1 \\ \wp(b_1+\overline{t})\wp(\overline{t}-b_1) & \wp(\overline{t}-b_1) & \wp(b_1+\overline{t}) & 1 \\ \wp(b_3+\overline{t})\wp(\overline{t}-b_3) & \wp(\overline{t}-b_3) & \wp(b_3+\overline{t}) & 1 \\ \wp(b_5+\overline{t})\wp(\overline{t}-b_5) & \wp(\overline{t}-b_5) & \wp(b_5+\overline{t}) & 1 \end{vmatrix}. \tag{2.32}$$

Then $I=0\Rightarrow\overline{I}=0$. This means that f,g which satisfy $I=0$ are a special solution on the condition $b_1+b_3+b_5+b_7=0$.

III. MULTIPLICATIVE TYPE

We can obtain the $A_0^{(1)}*$-surface from the $A_0^{(1)}$-surface by degeneration. By the same process the $A_0^{(1)}*$-surface discrete Painlevé equation and the linear equation also can be obtained.

A. Discrete Painlevé equation

We discuss the following theorem in this section. The equations obtained by the degeneration in the theorem coincide with the equations in Ref. 4.

Put $g_2=\frac{4}{3}(1+3\varepsilon^2)$, $g_3=-\frac{8}{27}(1-9\varepsilon^2)$ in the $A_0^{(1)}$-surface discrete Painlevé equations (2.1) and (2.2) and let ε tend to 0. Then we obtain the $A_0^{(1)}*$-surface discrete Painlevé equation. Moreover, the change of the variables and parameters $e^{2t}=t_1, e^{2\lambda}=\lambda_1, f=\frac{1}{3}(f_1+10)/(f_1-2), g=\frac{1}{3}(g_1+10)/(g_1-2), e^{2b_i}=\beta_i$ yields the expression in the following theorem. In the expression we replace again t_1 by t and λ_1, f_1, g_1, β_i by λ, f, g, b_i, respectively. For the sake of simplification of notation, the replacement process will be written as follows:

$$e^{2t}\to t,\quad e^{2\lambda}\to\lambda,\quad f\to\frac{1}{3}\frac{f+10}{f-2},\quad g\to\frac{1}{3}\frac{g+10}{g-2},\quad e^{2b_i}\to b_i.$$

These are summarized as follows:

Theorem 3: *Make the substitution:* $g_2=\frac{4}{3}(1+3\varepsilon^2)$, $g_3=-\frac{8}{27}(1-9\varepsilon^2)$ *in* $dP(A_0^{(1)})$ *(2.1) and (2.2). Take the limit* $\varepsilon\to 0$. *Moreover, by the change of variables and parameters,* $e^{2t}\to t, e^{2\lambda}\to\lambda, f\to\frac{1}{3}(f+10)/(f-2), g\to\frac{1}{3}(g+10)/(g-2), e^{2b_i}\to b_i$, *we obtain* $dP(A_0^{(1)}*)$*:*

$$\begin{aligned}&\frac{(\overline{g}t^2\lambda-f)(gt^2-f)-(t^4\lambda^2-1)(t^4-1)}{(\overline{g}/(t^2\lambda)-f)(g/t^2-f)-(1-1/(t^4\lambda^2))(1-1/t^4)}\\ &\quad=\lambda^2(f^4-m_1tf^3+(m_2t^2-3-m_8t^8)f^2+(m_7t^7-m_3t^3+2m_1t)f+m_8t^8-m_6t^6+m_4t^4\\ &\qquad-m_2t^2+1)\times(m_8f^4-m_7f^3/t+(m_6/t^2-3m_8-1/t^8)f^2+(m_1/t^7-m_5/t^3+2m_7/t)f\\ &\qquad+1/t^8-m_2/t^6+m_4/t^4-m_6/t^2+m_8)^{-1},\end{aligned} \tag{3.1}$$

$$\frac{(\underline{f}t^2/\lambda-g)(ft^2-g)-(t^4/\lambda^2-1)(t^4-1)}{(\underline{f}\lambda/t^2-g)(f/t^2-g)-(1-\lambda^2/t^4)(1-1/t^4)}$$

$$=\frac{1}{\lambda^2}(m_8g^4-m_7tg^3+(m_6t^2-3m_8-t^8)g^2+(m_1t^7-m_5t^3+2m_7t)g+t^8-m_2t^6+m_4t^4$$
$$-m_6t^2+m_8)\times(g^4-m_1g^3/t+(m_2/t^2-3-m_8/t^8)g^2+(m_7/t^7-m_3/t^3+2m_1/t)g$$
$$+m_8/t^8-m_6/t^6+m_4/t^4-m_2/t^2+1)^{-1}, \tag{3.2}$$

where $\overline{g}=g(t\lambda),\underline{f}=f(t/\lambda),\lambda=\sqrt{\Pi_{i=1}^8 b_i}$, m_i *is the ith elementary symmetric function of* b_j $(j=1,\ldots,8)$. □

The above theorem shows that we can obtain $dP(A_0^{(1)*})$ from $dP(A_0^{(1)})$. But, for readers' convenience, we describe geometrical construction of this discrete equation similar to the previous section.

We construct $A_0^{(1)*}$-surface by blowing up $\mathbb{P}^1\times\mathbb{P}^1$ at eight points. These eight points and a curve which these points lie on are as follows:

$$f^2+g^2-\left(t^2+\frac{1}{t^2}\right)fg+\left(t^2-\frac{1}{t^2}\right)^2=0, \tag{3.3}$$

$$p_i:\quad \left(b_it+\frac{1}{b_it},\frac{t}{b_i}+\frac{b_i}{t}\right)\quad (i=1,\ldots,8), \tag{3.4}$$

$$e^{2\chi(\alpha_1)}=t^{-4},\quad e^{2\chi(\alpha_2)}=b_1b_2t^2,\quad e^{2\chi(\alpha_i)}=b_i/b_{i-1}\ \ (i=3,\ldots,7),$$
$$e^{2\chi(\alpha_8)}=b_2/b_1,\quad e^{2\chi(\alpha_0)}=b_8/b_7. \tag{3.5}$$

Generators of affine Weyl group $W(E_8^{(1)})=\langle w_i\ (i=0,1,\ldots,8)\rangle$ act on these coordinates and parameters. We give a representation of these actions in order to construct $dP(A_0^{(1)*})$:

$$w_2:\quad \left(\begin{matrix}b_1 & b_2 & b_3 & b_4\\ b_5 & b_6 & b_7 & b_8\end{matrix},t,g\right)$$
$$\mapsto\left(\begin{matrix}b_1/(\sqrt[4]{b_1b_2t^2})^3 & b_2/(\sqrt[4]{b_1b_2t^2})^3 & b_3\sqrt[4]{b_1b_2t^2} & b_4\sqrt[4]{b_1b_2t^2}\\ b_5\sqrt[4]{b_1b_2t^2} & b_6\sqrt[4]{b_1b_2t^2} & b_7\sqrt[4]{b_1b_2t^2} & b_8\sqrt[4]{b_1b_2t^2}\end{matrix},t/\sqrt[4]{b_1b_2t^2},\tilde{g}\right),$$

$$w_1:\quad (t,f,g)\mapsto(1/t,g,f),\quad w_i:\quad (b_{i-1},b_i)\mapsto(b_i,b_{i-1})\quad (i=3,\ldots,7),$$

$$w_8:\quad (b_1,b_2)\mapsto(b_2,b_1),\quad w_0:\quad (b_7,b_8)\mapsto(b_8,b_7),$$

where $\tilde{g}$ is given by

$$\frac{\tilde{g}-(\sqrt{b_2/b_1}t^2+\sqrt{b_1/b_2}/t^2)}{\tilde{g}-(\sqrt{b_1/b_2}t^2+\sqrt{b_2/b_1}/t^2)}=\frac{f-(b_2t+1/(b_2t))}{f-(b_1t+1/(b_1t))}\,\frac{g-(t/b_1+b_1/t)}{g-(t/b_2+b_2/t)}.$$

Notice that we can rewrite the action of w_2 for $c_i=b_it$ into the following form:

$$w_2:\quad (c_1,c_2,t,g)\mapsto(1/c_2,1/c_1,t/\sqrt[4]{c_1c_2},\tilde{g}.$$

Here we put Γ and $\tilde{\Gamma}$ as

$$\Gamma=\frac{gt^2-f}{t^4-1},\quad \tilde{\Gamma}=\frac{\tilde{g}t^2/\sqrt{c_1c_2}-f}{t^4/c_1c_2-1},$$

then the relation between Γ and $\tilde{\Gamma}$ can be simply represented as

$$\tilde{\Gamma}=\frac{(c_1c_2f-c_1-c_2)\Gamma-(c_1c_2-1)}{(c_1c_2-1)\Gamma+(f-c_1-c_2)}. \tag{3.6}$$

So this transformation can be represented by PGL(2)-action:

$$\tilde{\Gamma}=\begin{pmatrix} c_1c_2f-c_1-c_2 & -(c_1c_2-1) \\ c_1c_2-1 & f-c_1-c_2 \end{pmatrix}\Gamma. \tag{3.7}$$

By taking a translation of $W(E_8^{(1)})$, we obtain a nonlinear difference equation. The translation can be described by a product of simple reflections w_i's. This representation is the same as the case of $dP(A_0^{(1)})$, that is, (2.8).

Now we calculate $\overline{g}$ from g and f. Putting Γ, $\acute{\Gamma}$,

$$\Gamma=\frac{gt^2-f}{t^4-1}, \quad \acute{\Gamma}=\frac{\overline{g}t^2/\sqrt{\Pi_{i=1}^8 c_i}-f}{t^4/\Pi_{i=1}^8 c_i-1}=\frac{\overline{g}/(t^2\lambda)-f}{1/(t^4\lambda^2)-1},$$

$\overline{g}$ can be described as follows:

$$\begin{aligned}\acute{\Gamma}=&\begin{pmatrix} c_7c_8f-c_7-c_8 & -(c_7c_8-1) \\ c_7c_8-1 & f-c_7-c_8 \end{pmatrix}\begin{pmatrix} c_5c_6f-c_5-c_6 & -(c_5c_6-1) \\ c_5c_6-1 & f-c_5-c_6 \end{pmatrix} \\ &\times\begin{pmatrix} c_3c_4f-c_3-c_4 & -(c_3c_4-1) \\ c_3c_4-1 & f-c_3-c_4 \end{pmatrix}\begin{pmatrix} c_1c_2f-c_1-c_2 & -(c_1c_2-1) \\ c_1c_2-1 & f-c_1-c_2 \end{pmatrix}\Gamma \\ =&\begin{pmatrix} t^8D & -(t^8D-N)/f \\ (t^8D-N)/f & N \end{pmatrix}\Gamma.\end{aligned} \tag{3.8}$$

Here N and D are as follows:

$$N=f^4-m_1tf^3+(m_2t^2-3-m_8t^8)f^2+(m_7t^7-m_3t^3+2m_1t)f+m_8t^8-m_6t^6+m_4t^4-m_2t^2+1, \tag{3.9}$$

$$\begin{aligned}D=&m_8f^4-m_7f^3/t+(m_6/t^2-3m_8-1/t^8)f^2+(m_1/t^7-m_5/t^3+2m_7/t)f \\ &+1/t^8-m_2/t^6+m_4/t^4-m_6/t^2+m_8,\end{aligned} \tag{3.10}$$

where m_i is the ith elementary symmetric function of b_j's. This equation can be modified

$$t^8\frac{\Gamma(\acute{\Gamma}-f)+1}{\acute{\Gamma}(\Gamma-f)+1}=\frac{N}{D}.$$

This equation is (3.1).

Similarly putting Φ, $\acute{\Phi}$,

$$\Phi=\frac{f/t^2-g}{1/t^4-1}, \quad \acute{\Phi}=\frac{\underline{f}/(t^2\sqrt{\Pi_{i=1}^8 d_i})-g}{1/(t^4\Pi_{i=1}^8 d_i)-1}=\frac{\underline{f}t^2/\lambda-g}{t^4/\lambda^2-1},$$

$\underline{f}$ can be described as follows:

$$\begin{aligned}\acute{\Phi}=&\begin{pmatrix} d_7d_8g-d_7-d_8 & -(d_7d_8-1)\\ d_7d_8-1 & g-d_7-d_8\end{pmatrix}\begin{pmatrix} d_5d_6g-d_5-d_6 & -(d_5d_6-1)\\ d_5d_6-1 & g-d_5-d_6\end{pmatrix}\\ &\times\begin{pmatrix} d_3d_4g-d_3-d_4 & -(d_3d_4-1)\\ d_3d_4-1 & g-d_3-d_4\end{pmatrix}\begin{pmatrix} d_1d_2g-d_1-d_2 & -(d_1d_2-1)\\ d_1d_2-1 & g-d_1-d_2\end{pmatrix}\Phi\\ =&\begin{pmatrix} \nabla/t^8 & -(\nabla/t^8-\Delta)/g\\ (\nabla/t^8-\Delta)/g & \Delta\end{pmatrix}\Phi. \end{aligned}\tag{3.11}$$

Here ∇ and Δ are as follows:

$$\nabla=m_8g^4-m_7tg^3+(m_6t^2-3m_8-t^8)g^2+(m_1t^7-m_5t^3+2m_7t)g+t^8-m_2t^6+m_4t^4-m_6t^2+m_8,\tag{3.12}$$

$$\begin{aligned}\Delta=&g^4-m_1g^3/t+(m_2/t^2-3-m_8/t^8)g^2+(m_7/t^7-m_3/t^3+2m_1/t)g\\ &+m_8/t^8-m_6/t^6+m_4/t^4-m_2/t^2+1.\end{aligned}\tag{3.13}$$

This equation can be modified:

$$t^8\frac{\acute{\Phi}(\Phi-g)+1}{\Phi(\acute{\Phi}-g)+1}=\frac{\nabla}{\Delta}.$$

This is (3.2).

Remark 3.1: In Ref. 8, we obtain the $A_0^{(1)}*$-surface by blowing up $\mathbb{P}^2$ with the centers at nine points:

$$\begin{gathered}y^2z=4x^2(x+z),\\ p_i:\quad\left(\frac{1}{\sinh^2\theta_i}:\frac{-2\cosh\theta_i}{\sinh^3\theta_i}:1\right)\quad(i=1,\ldots,9),\end{gathered}\tag{3.14}$$

$$\chi(\alpha_i)=\theta_{i+1}-\theta_i\ \ (i=1,\ldots,7),\quad \chi(\alpha_8)=\theta_1+\theta_2+\theta_3,\quad \chi(\alpha_0)=\theta_9-\theta_8.\tag{3.15}$$

Both parameters and coordinates correspond as follows:

$$\begin{gathered}b_1=\exp(-\tfrac{3}{2}(\theta_1+\theta_2)),\quad b_i=\exp(2\theta_{i+1}+\tfrac{1}{2}(\theta_1+\theta_2))\ \ (i=2,\ldots,8),\\ t=\exp(\tfrac{1}{2}(\theta_1-\theta_2)),\end{gathered}\tag{3.16}$$

$$f=\frac{-2(1-6e^{2\theta_1}+e^{4\theta_1})x-(1-e^{4\theta_1})y+16e^{2\theta_1}z}{e^{\theta_1}(2(1+e^{2\theta_1})x-(1-e^{2\theta_1})y)},\tag{3.17}$$

$$g=\frac{-2(1-6e^{2\theta_2}+e^{4\theta_2})x-(1-e^{4\theta_2})y+16e^{2\theta_2}z}{e^{\theta_2}(2(1+e^{2\theta_2})x-(1-e^{2\theta_2})y)}.\tag{3.18}$$

□

Similar to the case of $A_0^{(1)}$, $dP(A_0^{(1)}*)$ has a trivial solution.

Proposition 4: $dP(A_0^{(1)}*)$ has the following trivial solution:

$$f=tq\exp\left(\frac{2(\log t)^2}{\log\lambda}\right)+\frac{1}{tq\exp\left(\frac{2(\log t)^2}{\log\lambda}\right)},\quad g=\frac{t}{q\exp\left(\frac{2(\log t)^2}{\log\lambda}\right)}+\frac{q\exp\left(\frac{2(\log t)^2}{\log\lambda}\right)}{t},\tag{3.19}$$

where q is determined by initial condition.

B. Linear equation

We present a special solution of $dP(A_0^{(1)*})$ in this section.

Theorem 5: *By the limiting process*: $g_2=\frac{4}{3}(1+3\varepsilon^2)$, $g_3=-\frac{8}{27}(1-9\varepsilon^2)$ $(\varepsilon\to 0)$ *in (2.23), (2.24), and the change of variables and parameters:* $e^{2t}\to t$, $e^{2\lambda}\to\lambda$, $f\to\frac{1}{3}(f+10)/(f-2)$, $g\to\frac{1}{3}(g+10)/(g-2)$, $e^{2b_i}\to b_i$, *we obtain the system of equations:*

$$\begin{vmatrix} fg & g & f & 1\\ \left(b_1t+\frac{1}{b_1t}\right) & \left(\frac{t}{b_1}+\frac{b_1}{t}\right) & \frac{t}{b_1}+\frac{b_1}{t} & b_1t+\frac{1}{b_1t} & 1\\ \left(b_3t+\frac{1}{b_3t}\right) & \left(\frac{t}{b_3}+\frac{b_3}{t}\right) & \frac{t}{b_3}+\frac{b_3}{t} & b_3t+\frac{1}{b_3t} & 1\\ \left(b_5t+\frac{1}{b_5t}\right) & \left(\frac{t}{b_5}+\frac{b_5}{t}\right) & \frac{t}{b_5}+\frac{b_5}{t} & b_5t+\frac{1}{b_5t} & 1 \end{vmatrix}=0,\tag{3.20}$$

$$\begin{vmatrix} f\overline{g} & \overline{g} & f & 1\\ \left(b_8t+\frac{1}{b_8t}\right) & \left(\frac{\overline{t}}{b_8}+\frac{b_8}{\overline{t}}\right) & \frac{\overline{t}}{b_8}+\frac{b_8}{\overline{t}} & b_8t+\frac{1}{b_8t} & 1\\ \left(b_6t+\frac{1}{b_6t}\right) & \left(\frac{\overline{t}}{b_6}+\frac{b_6}{\overline{t}}\right) & \frac{\overline{t}}{b_6}+\frac{b_6}{\overline{t}} & b_6t+\frac{1}{b_6t} & 1\\ \left(b_4t+\frac{1}{b_4t}\right) & \left(\frac{\overline{t}}{b_4}+\frac{b_4}{\overline{t}}\right) & \frac{\overline{t}}{b_4}+\frac{b_4}{\overline{t}} & b_4t+\frac{1}{b_4t} & 1 \end{vmatrix}=0,\tag{3.21}$$

where $\overline{t}=t\lambda$.

A solution of this system is a special solution of $dP(A_0^{(1)*})$ *with* $b_1b_3b_5b_7=1$. □

We can easily check that the equations (3.20) and (3.21) define a special solution of $dP(A_0^{(1)*})$ similar to the case of $A_0^{(1)}$.

Transforming these equations,

$$\begin{aligned}\overline{g}=&\left(f\left((b_2+b_4+b_6+b_8)t-\left(\frac{1}{b_2}+\frac{1}{b_4}+\frac{1}{b_6}+\frac{1}{b_8}\right)\frac{1}{t}\right)-(b_2b_4+b_2b_6+b_2b_8+b_4b_6+b_4b_8\right.\\ &\left.+b_6b_8)\left(t^2-\frac{1}{\overline{t}^2}\right)+\left(t^2\overline{t}^2-\frac{1}{t^2\overline{t}^2}\right)\right)\Big/\\ &\left(f\left(t\overline{t}-\frac{1}{\overline{t}t}\right)-\left(\left(\frac{1}{b_2}+\frac{1}{b_4}+\frac{1}{b_6}+\frac{1}{b_8}\right)\overline{t}-(b_2+b_4+b_6+b_8)\frac{1}{\overline{t}}\right)\right),\end{aligned}\tag{3.22}$$

$$f=\left(g\left(\left(\frac{1}{b_1}+\frac{1}{b_3}+\frac{1}{b_5}+\frac{1}{b_7}\right)t-(b_1+b_3+b_5+b_7)\frac{1}{t}\right)-(b_1b_3+b_1b_5+b_1b_7+b_3b_5+b_3b_7+b_5b_7)\left(t^2-\frac{1}{t^2}\right)+\left(t^4-\frac{1}{t^4}\right)\right)\Bigg/$$

$$\left(g\left(t^2-\frac{1}{t^2}\right)-\left((b_1+b_3+b_5+b_7)t-\left(\frac{1}{b_1}+\frac{1}{b_3}+\frac{1}{b_5}+\frac{1}{b_7}\right)\frac{1}{t}\right)\right). \tag{3.23}$$

Eliminating f, we obtain a difference equation of the first order with respect to the variable g.

IV. ADDITIVE TYPE

We can obtain the $A_0^{(1)}{}^{**}$-surface from the $A_0^{(1)}{}^{*}$-surface by a degeneration process. By the same process the $A_0^{(1)}{}^{**}$-surface discrete Painlevé equation and linear equation also can be obtained.

A. Discrete Painlevé equation

We discuss about the following theorem in this section.

Theorem 6 (ORG[4]): *By the limiting process, $t\to e^{\varepsilon t}$, $\lambda\to 1+\varepsilon\lambda$, $f\to 2+\varepsilon^2 f$, $g\to 2+\varepsilon^2 g$, $b_i\to e^{\varepsilon b_i}$, $(\varepsilon\to 0)$, we obtain the $dP(A_0^{(1)}{}^{**})$ from $dP(A_0^{(1)}{}^{*})$ (3.1) and (3.2):*

$$\frac{(f-\overline{g}+(2t+\lambda)^2)(f-g+4t^2)+4f(2t+\lambda)2t}{2t(f-\overline{g}+(2t+\lambda)^2)+(2t+\lambda)(f-g+4t^2)}=2\,\frac{f^4+S_2f^3+S_4f^2+S_6f+S_8}{S_1f^3+S_3f^2+S_5f+S_7}, \tag{4.1}$$

$$\frac{(g-\underline{f}+(2t-\lambda)^2)(g-f+4t^2)+4g(2t-\lambda)2t}{2t(g-\underline{f}+(2t-\lambda)^2)+(2t-\lambda)(g-f+4t^2)}=2\,\frac{g^4+\Sigma_2g^3+\Sigma_4g^2+\Sigma_6g+\Sigma_8}{\Sigma_1g^3+\Sigma_3g^2+\Sigma_5g+\Sigma_7}, \tag{4.2}$$

where $\overline{g}=g(t+\lambda)$, $\underline{f}=f(t-\lambda)$, $\lambda=\frac{1}{2}\Sigma_{i=1}^{8}b_i$, S_i is the ith elementary symmetric function of the quantities $c_j=b_j+t$ $(j=1,\ldots,8)$, and Σ_i is the ith elementary symmetric function of the quantities $d_j=t-b_j$. □

The above theorem shows that we can obtain $dP(A_0^{(1)}{}^{**})$ from $dP(A_0^{(1)}{}^{*})$. But we describe geometrical construction of this discrete equation similar to the previous section.

We construct the $A_0^{(1)}{}^{**}$-surface by blowing up $\mathbb{P}^1\times\mathbb{P}^1$ at eight points. These eight points and a curve which these points lie on are as follows:

$$(f-g)^2-8t^2(f+g)+16t^4=0, \tag{4.3}$$

$$p_i:\quad ((b_i+t)^2,(t-b_i)^2)\quad (i=1,\ldots,8), \tag{4.4}$$

$$\chi(\alpha_1)=-2t,\quad \chi(\alpha_2)=\tfrac{1}{2}(b_1+b_2)+t,\quad \chi(\alpha_i)=\tfrac{1}{2}(b_i-b_{i-1})\ \ (i=3,\ldots,7)$$
$$\chi(\alpha_8)=\tfrac{1}{2}(b_2-b_1),\quad \chi(\alpha_0)=\tfrac{1}{2}(b_8-b_7). \tag{4.5}$$

Generators of affine Weyl group $W(E_8^{(1)})=\langle w_i\ (i=0,1,\ldots,8)\rangle$ act on these coordinates and parameters. We give a representation of these actions in order to construct $dP(A_0^{(1)}{}^{**})$.

$$w_2:\ \begin{pmatrix} b_1 & b_2 & b_3 & b_4 \\ b_5 & b_6 & b_7 & b_8 \end{pmatrix}, t, g \Bigg) \mapsto \left(\begin{matrix} b_1 - 3\frac{2t+b_1+b_2}{4} & b_2 - 3\frac{2t+b_1+b_2}{4} & b_3 + \frac{2t+b_1+b_2}{4} & b_4 + \frac{2t+b_1+b_2}{4} \\ b_5 + \frac{2t+b_1+b_2}{4} & b_6 + \frac{2t+b_1+b_2}{4} & b_7 + \frac{2t+b_1+b_2}{4} & b_8 + \frac{2t+b_1+b_2}{4} \end{matrix}, t - \frac{2t+b_1+b_2}{4}, \tilde{g} \right),$$

$$w_1:\quad (t,f,g) \mapsto (-t,g,f), \quad w_i:\quad (b_{i-1},b_i) \mapsto (b_i,b_{i-1}) \quad (i=3,\ldots,7),$$

$$w_8:\quad (b_1,b_2) \mapsto (b_2,b_1), \quad w_0:\quad (b_7,b_8) \mapsto (b_8,b_7),$$

where $\tilde{g}$ is given by

$$\frac{\tilde{g}-(2t-(b_1-b_2)/2)^2}{\tilde{g}-(2t-(-b_1+b_2)/2)^2} = \frac{f-(b_2+t)^2}{f-(b_1+t)^2}\,\frac{g-(t-b_1)^2}{g-(t-b_2)^2}.$$

Notice that we can rewrite the action of w_2 for $c_i = b_i + t$ into the following form:

$$w_2:\quad (c_1,c_2,t,g) \mapsto (-c_2,-c_1,t-(c_1+c_2)/4,\tilde{g}).$$

Here we put Γ, $\tilde{\Gamma}$,

$$\Gamma = \frac{f-g+4t^2}{4t}, \quad \tilde{\Gamma} = \frac{f-\tilde{g}+(2t-(c_1+c_2)/2)^2}{4t-c_1-c_2},$$

then the relation between Γ and $\tilde{\Gamma}$ can be simply represented by PGL(2)-action:

$$\tilde{\Gamma} = \begin{pmatrix} f+c_1c_2 & -(c_1+c_2)f \\ -(c_1+c_2) & f+c_1c_2 \end{pmatrix} \Gamma. \tag{4.6}$$

By taking a translation of $W(E_8^{(1)})$, we obtain a nonlinear difference equation. The translation can be described by a product of simple reflections w_i's. This representation is same as the case of $dP(A_0^{(1)})$, that is (2.8).

Now we calculate $\overline{g}$ from g and f. Putting Γ, $\acute{\Gamma}$,

$$\Gamma = \frac{f-g+4t^2}{4t}, \quad \acute{\Gamma} = \frac{f-\overline{g}+\left(2t-\frac{1}{2}\Sigma_{i=1}^8 c_i\right)^2}{4t-\Sigma_{i=1}^8 c_i} = \frac{f-\overline{g}+(2t+\lambda)^2}{-4t-2\lambda},$$

$\overline{g}$ can be described as follows:

$$\begin{aligned}\acute{\Gamma}=&\begin{pmatrix} f+c_7c_8 & -(c_7+c_8)f \\ -(c_7+c_8) & f+c_7c_8 \end{pmatrix}\begin{pmatrix} f+c_5c_6 & -(c_5+c_6)f \\ -(c_5+c_6) & f+c_5c_6 \end{pmatrix}\begin{pmatrix} f+c_3c_4 & -(c_3+c_4)f \\ -(c_3+c_4) & f+c_3c_4 \end{pmatrix}\\ &\times\begin{pmatrix} f+c_1c_2 & -(c_1+c_2)f \\ -(c_1+c_2) & f+c_1c_2 \end{pmatrix}\Gamma\\ =&\begin{pmatrix} f^4+S_2f^3+S_4f^2+S_6f+S_8 & -(S_1f^3+S_3f^2+S_5f+S_7)f \\ -(S_1f^3+S_3f^2+S_5f+S_7) & f^4+S_2f^3+S_4f^2+S_6f+S_8 \end{pmatrix}\Gamma,\end{aligned} \tag{4.7}$$

where S_i is the ith elementary symmetric function of c_j's. This equation can be modified.

$$\frac{\acute{\Gamma}\Gamma-f}{\acute{\Gamma}-\Gamma}=\frac{f^4+S_2f^3+S_4f^2+S_6f+S_8}{S_1f^3+S_3f^2+S_5f+S_7}.$$

This equation is (4.1).

Similarly putting Φ, $\acute{\Phi}$,

$$\Phi=\frac{g-f+4t^2}{-4t},\quad \acute{\Phi}=\frac{g-\underline{f}+(-2t+\frac{1}{2}\Sigma_{i=1}^{8}d_i)^2}{-4t+\Sigma_{i=1}^{8}d_i}=\frac{g-\underline{f}+(2t-\lambda)^2}{4t-2\lambda},$$

$\underline{f}$ can be described as follows:

$$\begin{aligned}\acute{\Phi}=&\begin{pmatrix} g+d_7d_8 & (d_7+d_8)g \\ d_7+d_8 & g+d_7d_8 \end{pmatrix}\begin{pmatrix} g+d_5d_6 & (d_5+d_6)g \\ d_5+d_6 & g+d_5d_6 \end{pmatrix}\begin{pmatrix} g+d_3d_4 & (d_3+d_4)g \\ d_3+d_4 & g+d_3d_4 \end{pmatrix}\\ &\times\begin{pmatrix} g+d_1d_2 & (d_1+d_2)g \\ d_1+d_2 & g+d_1d_2 \end{pmatrix}\Phi\\ =&\begin{pmatrix} g^4+S_2g^3+\Sigma_4g^2+\Sigma_6g+\Sigma_8 & (\Sigma_1g^3+\Sigma_3g^2+\Sigma_5g+\Sigma_7)g \\ \Sigma_1g^3+\Sigma_3g^2+\Sigma_5g+\Sigma_7 & g^4+\Sigma_2g^3+\Sigma_4g^2+\Sigma_6g+\Sigma_8 \end{pmatrix}\Phi,\end{aligned} \tag{4.8}$$

where $d_i=t-b_i$ $(i=1,\ldots,8)$, and Σ_i is the ith elementary symmetric function of d_j's. This equation can be modified:

$$\frac{\acute{\Phi}\Phi-g}{\Phi-\acute{\Phi}}=\frac{g^4+\Sigma_2g^3+\Sigma_4g^2+\Sigma_6g+\Sigma_8}{\Sigma_1g^3+\Sigma_3g^2+\Sigma_5g+\Sigma_7}.$$

This is (4.2).

Remark 4.1: In Ref. 8, we obtain the $A_0^{(1)}{}^{**}$-surface by blowing up $\mathbb{P}^2$ with the centers at nine points:

$$\begin{gathered}y^2z=4x^3,\\ p_i:\quad (a_i:-2:a_i^3)\quad (i=1,\ldots,9),\end{gathered} \tag{4.9}$$

$$\begin{gathered}\chi(\alpha_i)=(a_{i+1}-a_i)/\lambda\quad (i=1,\ldots,7),\quad \chi(\alpha_8)=(a_1+a_2+a_3)/\lambda,\\ \chi(\alpha_0)=(a_9-a_8)/\lambda,\quad \lambda=\sum_{i=1}^{9}a_i.\end{gathered} \tag{4.10}$$

Both parameters and coordinates correspond as follows:

$$b_1=-\tfrac{3}{2}(a_1+a_2),\quad b_i=2a_{i+1}+\tfrac{1}{2}(a_1+a_2)\ \ (i=2,\ldots,8),\quad t=\tfrac{1}{2}(a_1-a_2), \tag{4.11}$$

$$f=\frac{-6a_1^2x+a_1^3y+8z}{2x+a_1y},\quad g=\frac{-6a_2^2x+a_2^3y+8z}{2x+a_2y}. \tag{4.12}$$

□

Proposition 7: $dP(A_0^{(1)}{}^{**})$ has the following trivial solution:

$$f=(q+2t^2/\lambda+t)^2,\ \ g=(-q-2t^2/\lambda+t)^2, \tag{4.13}$$

where q is determined by initial condition.

B. Linear equation

We present a special solution of $dP(A_0^{(1)}{}^{**})$ in this section.

Theorem 8: *By the limiting process, $t\to e^{\varepsilon t}$, $\lambda\to 1+\varepsilon\lambda$, $f\to 2+\varepsilon^2 f$, $g\to 2+\varepsilon^2 g$, $b_i\to e^{\varepsilon b_i}$ $(\varepsilon\to 0)$ in (3.20), and (3.21), we obtain the system of equations:*

$$\begin{vmatrix} fg & g & f & 1\\ (b_1+t)^2(t-b_1)^2 & (t-b_1)^2 & (b_1+t)^2 & 1\\ (b_3+t)^2(t-b_3)^2 & (t-b_3)^2 & (b_3+t)^2 & 1\\ (b_5+t)^2(t-b_5)^2 & (t-b_5)^2 & (b_5+t)^2 & 1 \end{vmatrix}=0, \tag{4.14}$$

$$\begin{vmatrix} f\overline{g} & \overline{g} & f & 1\\ (b_8+t)^2(\overline{t}-b_8)^2 & (\overline{t}-b_8)^2 & (b_8+t)^2 & 1\\ (b_6+t)^2(\overline{t}-b_6)^2 & (\overline{t}-b_6)^2 & (b_6+t)^2 & 1\\ (b_4+t)^2(\overline{t}-b_4)^2 & (\overline{t}-b_4)^2 & (b_4+t)^2 & 1 \end{vmatrix}=0, \tag{4.15}$$

where $\overline{t}=t+\lambda$.

A solution of this system is a special solution of $dP(A_0^{(1)}{}^{**})$ with $b_1+b_3+b_5+b_7=0$. □

We can easily check that the equations (4.14) and (4.15) define a special solution of $dP(A_0^{(1)}{}^{**})$.

Transforming these equations,

$$\overline{g}=\frac{-A_{2468}(-(t+\overline{t})/2)f+B_{2468}((t+\overline{t})/2)}{128(t+\overline{t})f-A_{2468}((t+\overline{t})/2)},\quad f=\frac{A_{1357}(t)g+B_{1357}(t)}{256tg+A_{1357}(-t)}, \tag{4.16}$$

where

$$\begin{aligned}A_{ijkl}(t)=&-8(b_i+b_j-b_k-b_l)(b_i-b_j+b_k-b_l)(b_i-b_j-b_k+b_l)+16((b_i+b_j-b_k-b_l)^2\\&+(b_i-b_j+b_k-b_l)^2+(b_i-b_j-b_k+b_l)^2)t-256t^3,\end{aligned}$$

$$\begin{aligned}B_{ijkl}(t)=&-(3b_i-b_j-b_k-b_l)(3b_j-b_i-b_k-b_l)(3b_k-b_i-b_j-b_l)(3b_l-b_i-b_j-b_k)t\\&-32((b_i+b_j-b_k-b_l)^2+(b_i-b_j+b_k-b_l)^2+(b_i-b_j-b_k+b_l)^2)t^3+768t^5.\end{aligned}$$

Eliminating f, we obtain a difference equation of the first order with respect to the variable g.

V. RICCATI SOLUTION OF $dP(A_1^{(1)})$

We can obtain the $A_1^{(1)}$-surface from the $A_0^{(1)}*$-surface by a degeneration process. By the same process the $A_1^{(1)}$-surface discrete Painlevé equation and linear equation also can be obtained.

Theorem 9: *By the limiting process,* $t\to\sqrt{t}$, $\lambda\to\sqrt{\lambda}$, $f\to fp^{1/4}/(\varepsilon\sqrt{t})$, $g\to\sqrt{t}p^{1/4}/(\varepsilon g)$, $b_i\to b_i p^{1/4}/\varepsilon(i=1,\ldots,4)$, $b_i\to\varepsilon p^{1/4}/b_i(i=5,\ldots,8)$ $(\varepsilon\to 0)$ *in (3.20) and (3.21), where* $p=\sqrt{b_1b_2b_3b_4/(b_5b_6b_7b_8)}$, *we obtain the system of equations:*

$$\begin{vmatrix} fg & g & f & 1\\ t^2 & t/b_1 & b_1t & 1\\ t^2 & t/b_3 & b_3t & 1\\ 1 & 1/b_5 & b_5 & 1 \end{vmatrix}=0,\qquad \begin{vmatrix} f\overline{g} & \overline{g} & f & 1\\ 1 & 1/b_8 & b_8 & 1\\ 1 & 1/b_6 & b_6 & 1\\ t\overline{t} & \overline{t}/b_4 & b_4t & 1 \end{vmatrix}=0, \tag{5.1}$$

where $\overline{t}=t\lambda$.

A solution of this system is a special solution of $dP(A_1^{(1)})$ *with* $b_5b_7=b_1b_3p$. □

We introduce this theorem in this section.

By the limiting procedure on the $A_0^{(1)}*$-surface discrete Painlevé equations (3.1) and (3.2), we obtain the $A_1^{(1)}$-surface discrete Painlevé equation:[4]

$$\frac{(f\overline{g}-t\overline{t})(fg-t^2)}{(f\overline{g}-1)(fg-1)}=\frac{(f-b_1t)(f-b_2t)(f-b_3t)(f-b_4t)}{(f-b_5)(f-b_6)(f-b_7)(f-b_8)}, \tag{5.2}$$

$$\frac{(fg-t^2)(\underline{f}g-\underline{t}t)}{(fg-1)(\underline{f}g-1)}=\frac{(g-t/b_1)(g-t/b_2)(g-t/b_3)(g-t/b_4)}{(g-1/b_5)(g-1/b_6)(g-1/b_7)(g-1/b_8)}. \tag{5.3}$$

We can construct $dP(A_1^{(1)})$ by geometrical approach similar to the above discussions, but we only show the construction of surface. Here $A_1^{(1)}$-surface is obtained by blowing up $\mathbb{P}^1\times\mathbb{P}^1$ at eight points. These eight points and a curve which these points lie on are as follows:

$$\begin{gathered}(fg-t^2)(fg-1)=0,\\ p_i:\quad \left(b_it,\frac{t}{b_i}\right)\quad (i=1,\ldots,4),\quad p_i:\quad \left(b_i,\frac{1}{b_i}\right)\quad (i=5,\ldots,8).\end{gathered} \tag{5.4}$$

By the same limiting procedure on the system of equations (3.20) and (3.21), we obtain the system of equations (5.1), or

$$\overline{g}=\frac{f(1-t\overline{t})+t(\overline{t}(b_6+b_8)-b_2-b_4)}{g(b_6+b_8-t(b_2+b_4))+b_6b_8(t\overline{t}-1)}, \tag{5.5}$$

$$f=\frac{gb_5b_7(t^2-1)+t(b_1+b_3-t(b_5+b_7))}{g(t(b_1+b_3)-b_5-b_7)+1-t^2}. \tag{5.6}$$

These equations coincide with the equations in Ref. 7.

VI. DISCUSSION

In the article, we derive the linear equations as the special solutions of discrete Painlevé equations. So that we show that these equations belong to the hypergeometric family, we will seek the series solutions of them like the q-hypergeometric series. If there exists the series solutions of $dP(A_0^{(1)})$, it should be called elliptic-hypergeometric series.

ACKNOWLEDGMENTS

The authors would like to thank K. Okamoto and M. Jimbo for discussions and advice. The authors are also grateful to Y. Ohta, T. Takebe, T. Takenawa, and T. Tsuda for useful comments.

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W. Gordon's integral (1929) and its representations by means of Appell's functions F_2, F_1, and F_3

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(Received 29 October 2002; accepted 29 October 2002)

Exact analytical representations for W. Gordon's integral by means of Appell's functions are given. It is shown, that they correlate between each other. But representation of this integral by means of Appell's function F_2 is more attractive.
 [DOI: 10.1063/1.1539305]

I. INTRODUCTION

In W. Gordon's original work,[1] the first attempt was given to evaluate the integral of the form

$$J_c^{jp}(a,a')=\int_0^\infty e^{-\lambda z} z^{c+j-1}\,{}_1F_1(-a;c;kz)\,{}_1F_1(-a';c';k'z)\,dz, \tag{1.1}$$

where $\lambda=(k+k')/2$, $c'=c\pm p$, $j\in\mathbb{Z}$, $\mathrm{Re}(c+j)>0$, $\mathrm{Re}\,\lambda>0$, p, a, $a'\geqslant 0$ are integers, c, $c'\neq 0,-1,-2,\ldots$. As the authors of Ref. 2 noted, the general formula for this integral can be derived, but it is so complex that it cannot be used conveniently; recursion relations which facilitate the reduction integrals of type (1) to the integral with $j=p=0$, are more convenient.

In the present paper for this integral, three different representations by means of Appell's functions F_1, F_2, and F_3 (1880)[3] are obtained. The latter are

$$F_1\left(\alpha\left|\begin{matrix}\beta,\beta\\ -\ -\end{matrix}\right|x,y\right)=\sum_{m=0}^\infty A_m x^m\,{}_2F_1\left(\begin{matrix}\alpha+m,\beta'\\ \gamma+m\end{matrix}\right|y\Big),$$

$$F_2\left(\alpha\left|\begin{matrix}\beta,\beta'\\ \gamma,\gamma'\end{matrix}\right|x,y\right)=\sum_{m=0}^\infty A_m x^m\,{}_2F_1\left(\begin{matrix}\alpha+m,\beta'\\ \gamma'\end{matrix}\right|y\Big),$$

$$F_3\left(\begin{matrix}-\\ \gamma\end{matrix}\left|\begin{matrix}\alpha,\alpha';\beta,\beta'\\ -\ -\quad -\ -\end{matrix}\right|x,y\right)=\sum_{m=0}^\infty A_m x^m\,{}_2F_1\left(\begin{matrix}\alpha',\beta'\\ \gamma+m\end{matrix}\right|y\Big),$$

where $A_m=(\alpha)_m(\beta)_m/((\gamma)_m(l)_m)$.

These double hypergeometric series absolutely converge interior to the domains:

$$D_1=D_3:|x|<1,|y|<1 \quad \text{and} \quad D_2:|x|+|y|<1.$$

All the main symbols are standard,[4] e.g., we have Pochhammer's symbol $(a)_k=\Gamma(a+k)/\Gamma(a)$, $(a)_0=1$, etc.

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II. SOME ADDITIONAL INFORMATION

It is well-known[3–5] that the following formulas are true:

$$\int_0^1 e^{xt}t^{\alpha-1}(1-\mathrm{t})^{\gamma-\alpha-1}\mathrm{d}t=\frac{\Gamma(\alpha)\Gamma(\gamma-\alpha)}{\Gamma(\gamma)}\,{}_1F_1(\alpha;\gamma;x), \tag{2.1}$$

$$\int_0^\infty e^{-\lambda z}z^{\alpha-1}\,{}_1F_1(\beta;\gamma;kz)dz=\frac{\Gamma(\alpha)}{\lambda^\alpha}\,{}_2F_1\left(\begin{matrix}\alpha,\beta\\ \gamma\end{matrix}\middle| x\right), \tag{2.2}$$

$${}_2F_1\left(\begin{matrix}\alpha,\beta\\ \gamma\end{matrix}\middle| x\right)=(1-x)^{-\alpha}\,{}_2F_1\left(\begin{matrix}\alpha,\gamma-\beta\\ \gamma\end{matrix}\middle|\frac{x}{x-1}\right), \tag{2.3}$$

$$\int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1}(1-xt)^{-\beta}(1-yt)^{-\beta'}\mathrm{d}t=\frac{\Gamma(\alpha)\Gamma(\gamma-\alpha)}{\Gamma(\gamma)}F_1\left(\begin{matrix}\alpha\\ \gamma\end{matrix}\middle|\begin{matrix}\beta,\beta'\\ -\ -\end{matrix}\middle| x,y\right), \tag{2.4}$$

$$F_1\left(\begin{matrix}\alpha\\ \gamma\end{matrix}\middle|\begin{matrix}\beta,\beta'\\ -\ -\end{matrix}\middle| x,y\right)=(1-x)^{-\alpha}F_1\left(\begin{matrix}\alpha\\ \gamma\end{matrix}\middle|\begin{matrix}\gamma-\beta-\beta',\beta'\\ -\qquad -\end{matrix}\middle|\frac{x}{x-1},\frac{x-y}{x-1}\right) \tag{2.5}$$

$$=(1-x)^{-\beta}F_3\left(\begin{matrix}-\\ \gamma\end{matrix}\middle|\begin{matrix}\alpha,\gamma-\alpha;\beta,\beta'\\ -\quad -\quad -\ -\end{matrix}\middle|\frac{x}{x-1},y\right), \tag{2.6}$$

$$=\left(\frac{x}{y}\right)^{\beta'}F_2\left(\beta+\beta'\middle|\begin{matrix}\alpha,\beta'\\ \gamma,\beta+\beta'\end{matrix}\middle| x,1-\frac{x}{y}\right), \tag{2.7}$$

All parameters take values such that the integrals and the series have meaning.

III. REPRESENTATION BY MEANS OF APPELL'S FUNCTION F_2

As is seen in Ref. 6, integral (1.1) is a special case of off-diagonal matrix elements $\langle q|z^k|q'\rangle$, where q is a set of parameters of Schrödinger's radial function; therefore we have the following representation:[6]

$$J_c^{jp}(a,a')=\frac{\Gamma(c+j)}{\lambda^{c+j}}F_2\left(c+j\middle|\begin{matrix}-a,-a'\\ c,c'\end{matrix}\middle| x,y\right), \tag{R2}$$

where $x=k/\lambda$ and $y=k'/\lambda$.

Many recursion relations, reduction formulas, and special cases for Appell's functions F_1, F_2, and F_3 may be found in Refs. 6 and 7 (and references therein). In particular, for Appell's function F_2 we have

$$F_2\left(c\middle|\begin{matrix}-a,-a'\\ c,c\end{matrix}\middle| x,y\right)=(1-x)^a(1-y)^{a'}\,{}_2F_1\left(\begin{matrix}-a,-a'\\ c\end{matrix}\middle|\frac{xy}{(1-x)(1-y)}\right),\quad x\neq y\neq 1,$$

$$F_2\left(c+j\middle|\begin{matrix}-a,-a\\ c,c\end{matrix}\middle|1,1\right)=F_2\left(c-j-1\middle|\begin{matrix}-a,-a\\ c,c\end{matrix}\middle|1,1\right)=\frac{(1)_a}{(c)_a}\,{}_3F_2\left(\begin{matrix}-a,-j,j+1\\ c,1\end{matrix}\middle|1\right),\quad j\leftrightarrow -j-1;$$

$$F_2\left(c+j\middle|\begin{matrix}\alpha,\alpha'\\ c,c+p\end{matrix}\middle| x,y\right)=\frac{(c)_p}{y^p(c+j-p)_p}\sum_{m=0}^{p}(-1)^mC_p^mF_2\left(c+j-p\middle|\begin{matrix}\alpha,\alpha'-m\\ c,c\end{matrix}\middle| x,y\right),$$

where $C_p^m=p!/(m!(p-m)!)$, $\mathrm{Re}(c+j-p)>0$, and

$$y(c+\sigma-1)F_2\left(c+\sigma\left|\begin{matrix}\alpha,\beta\\ c,c\end{matrix}\right|x,y\right)$$
$$=\beta F_2\left(c+\sigma-1\left|\begin{matrix}\alpha,\beta+1\\ c,c\end{matrix}\right|x,y\right)+(c-2\beta)F_2\left(c+\sigma-1\left|\begin{matrix}\alpha,\beta\\ c,c\end{matrix}\right|x,y\right)$$
$$+(\beta-c)F_2\left(c+\sigma-1\left|\begin{matrix}\alpha,\beta-1\\ c,c\end{matrix}\right|x,y\right),$$

where $\sigma\geqslant 1$, $\mathrm{Re}(c+\sigma-1)>0$.

IV. REPRESENTATIONS BY MEANS OF APPELL'S FUNCTIONS F_1 AND F_3

Considering formulas (2.1)–(2.3), we get

$$J_c^{jp}(a,a')=\frac{1}{\lambda^{c+j}}\Gamma\left[\begin{matrix}c,c+j\\ -a,c+a\end{matrix}\right]\int_0^1\frac{t^{-a-1}(1-t)^{c+a-1}}{(1-xt)^{c+j+a'}}(1-y-xt)^{a'}$$
$$\times{}_2F_1\left(\begin{matrix}-a',c'-c-j\\ c'\end{matrix}\middle|\frac{y}{xt-y-1}\right)\mathrm{d}t.$$

Here, the parameter $c'-c-j=(-j\pm p)\in\mathbb{Z}$, that is why we "open" Gauss's function *only* with respect to $a'\geqslant 0$ and integrate over t; then taking into consideration the E. Picard integral (2.4), we have:

$$J_c^{jp}(a,a')=\frac{\Gamma(c+j)}{\lambda^{c+j}}(1-y)^{a'}\sum_{m=0}^{a'}B_m\left(\frac{y}{y-1}\right)^m F_1\left(\begin{matrix}-a\\ c\end{matrix}\middle|\begin{matrix}c+j+a',m-a'\\ -\qquad -\end{matrix}\middle|x,\frac{x}{1-y}\right),$$

where $B_m=(-a')_m(c'-c-j)_m/((c')_m(1)_m)$.

From here, using Appell's transform (2.5), we have the following representation:

$$J_c^{jp}(a,a')=\frac{\Gamma(c+j)}{\lambda^{c+j}}(1-x)^a(1-y)^{a'}\sum_{m=0}^{a'}B_m\left(\frac{y}{y-1}\right)^m$$
$$\times F_1\left(\begin{matrix}-a\\ c\end{matrix}\middle|\begin{matrix}-j-m,m-a'\\ -\qquad -\end{matrix}\middle|\frac{x}{x-1},\frac{xy}{(1-x)(1-y)}\right),\tag{R1}$$

where $x\neq y\neq 1$. We rewrite F_1 in the form

$$F_1\equiv\sum_{\mu=0}^{a'-m}\frac{(-a)_\mu(-j-m)_\mu}{(c)_\mu(1)_\mu}\left(\frac{x}{x-1}\right)^\mu{}_2F_1\left(\begin{matrix}-a,\mu-a'\\ c+\mu\end{matrix}\middle|\frac{xy}{(1-x)(1-y)}\right).$$

From here, using Appell's transform (2.6), we have the following representation:

$$J_c^{jp}(a,a')=\frac{\Gamma(c+j)}{\lambda^{c+j}}(1-\mathrm{x})^{a-j-m}(1-y)^{a'}\sum_{m=0}^{a'}B_m\left(\frac{y}{y-1}\right)^m$$
$$\times F_3\left(\begin{matrix}-\\ c\end{matrix}\middle|\begin{matrix}-a,c+a;-j-m,m-a'\\ -\quad -\quad -\quad -\end{matrix}\middle|x,\frac{xy}{(1-x)(1-y)}\right),\tag{R3}$$

where $x\neq y\neq 1$. We rewrite F_3 in the form

$$F_3 \equiv \sum_{\mu=0}^{a'-m} \frac{(-a)_\mu (-j-m)_\mu}{(c)_\mu (1)_\mu} x^\mu \, {}_2F_1\left(\begin{matrix} c+a, m-a' \\ c+\mu \end{matrix} \middle| \frac{xy}{(1-x)(1-y)} \right).$$

From expressions (2.7) and (R1), we have:

$$F_1\left(\begin{matrix} -a \\ c \end{matrix} \middle| \begin{matrix} -j-m, m-a' \\ - \quad - \end{matrix} \middle| \frac{x}{x-1}, \frac{xy}{(1-x)(1-y)} \right) = \left(\frac{y}{y-1} \right)^{a'-m} F_2\left(\begin{matrix} -j-a' \\ c, -j-a' \end{matrix} \middle| \begin{matrix} -a, m-a' \\ \end{matrix} \middle| \frac{x}{x-1}, \frac{1}{y} \right), \tag{R1$'$}$$

where $x \neq y \neq 1$. Finally, we rewrite F_2 in the form

$$F_2 \equiv \sum_{\mu=0}^{a'-m} \frac{(-a)_\mu (-j-a')_\mu}{(c)_\mu (1)_\mu} \left(\frac{x}{x-1} \right)^\mu {}_2F_1\left(\begin{matrix} \mu-j-a', m-a' \\ -j-a' \end{matrix} \middle| \frac{1}{y} \right).$$

Note that in Ref. 8 only one special case of (R1) was considered, when $c' = c-p, j, p \geqslant 0$.

ACKNOWLEDGMENTS

I thank Professor N. N. Bogolubov, Jr. and Professor N. M. Matveev for enlightening discussion and encouragement.

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Addendum: "The two-dimensional hydrogen atom revisited" [J. Math. Phys. 43, 4681 (2002)]

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[DOI: 10.1063/1.1541121]

After publication of this paper we became aware that some of the results contained therein had previously been published in Ref. 1. We wish to thank G. F. Torres del Castillo for bringing this to our attention.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

An investigation of entanglement and quasiprobability distribution in a generalized Jaynes-Cummings model

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(Received 29 October 2002; accepted 13 January 2003)

In this paper, we consider a unified approach to study the degree of entanglement of two-level systems interacting with a quantized electromagnetic field. We investigate a range of parameters in a generalized Jaynes–Cummings model (JC-model) with intensity-dependent, field nonlinearity and nonresonant coupling. In terms of the density matrix and without the diagonal approximation we derive an explicit expression for the entanglement degree using a function analogous to mutual entropy. This notion is inspired by the fact that the quantum state may be interpreted as a measure of information. With the aid of the quasiprobability distribution function, the statistical properties of the field are analyzed. It is shown that when the atom is initially in its upper-level and the one-photon at resonance, the Q-function splits into two peaks and counter rotate in phase space. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1559643]

I. OVERVIEW

Entanglement is arguably the key property distinguishing quantum and classical systems, and lies at the heart of recent proposals for quantum communication and computation. Recently, entanglement as a physical resource has been used in quantum information such as quantum teleportation, superdense coding and quantum cryptography.[1] Consequently, to understand and develop the quantum theory of information it is necessary to quantify the entanglement. The research on quantifying entangled states has been considered by several authors (see, e.g., Ref. 2). To quantify entangled states, we have to know whether the states are pure or mixed states. Thus, if the entangled state is pure, then it is sufficient to use the von Neumann entropy, which is unique in several ways.[3] These situations have been considered and the reduced von Neumann entropy used to analyze the quantum fluctuations.[4–6] In general, the final state is not necessarily pure, and therefore we need to adopt a new method to measure the degree of entanglement in mixed state. Here we may refer to the method which has been adopted in Ref. 7 for using quantum mutual entropy to measure the degree of entanglement in the time development of the JC-model. The entanglement for the time development of the JC-model has been investigated,[8,9] and we established that the entanglement can be controlled by means of squeezing.[8]

It is well known that the simplest and most fundamental system to study the coupling between radiation and matter is a single two-level atom interacting with a single mode of an electromagnetic field in a cavity. This problem has received a great deal of interest, especially since the maser was invented. However, at that time, the problem was of purely academic interest as the matrix elements describing the radiation–atom interaction are usually so small that the field of a single photon is not sufficient to lead to an atom field evolution time shorter than the other characteristic times of the system, such as the excited state lifetime (the time of flight of the atom through the cavity and the cavity mode damping time). It was therefore not possible to test experimentally the fundamental theories of radiation–matter interaction, which predicted other effects.[10] The well-known solvable model describing this interaction is the JC-model[11] which is the basis for a vast

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array of the current experiments on foundations of quantum mechanics. This involves entangled states,[12] new ideas of quantum optics,[13] and novel device structures such as a micromaser, single-atom laser.[14] Thus this model contains all the subtle features of quantum entanglement albeit dependent on the interaction strength.

In this paper, we study the problem of a two-level atom interacting with a single-mode field, allowing the nonlinearities of both field and intensity-dependent coupling to be arbitrary in the presence of the Stark shift. However, we shall put no restriction on the derivation of the entanglement degree ignoring any approximation such as diagonal approximation which has been used in earlier studies.[7–9] We shall show that as should be expected, the entanglement still exhibits a quasi-period which is strongly affected by different parameters of the present system. In classical information theory, the mutual entropy is a very important quantity to analyze the communication processes and physical transformations. In handling the present paper we emphasis on applying the quasi-mutual entropy not the quantum mutual entropy. We also aim to analyze the effect of different forms of the nonlinearities on the Q-function as well as the atomic level occupation probabilities.

We organize the paper as follows. In Sec. II, we rewrite the dynamics of the Jaynes–Cummings model from a point of view based on the entangled dressed-state eigenbasis. Section III begins with a derivation of an expression for the entanglement due to quasi-mutual entropy in a general two-level system interacting with a coherent state, without the diagonal approximation. In Sec. III A, we analyze the role of the different parameters and verify that the strong entanglement will occur for particular choices. We devote Sec. IV to consider the statistical properties of the field with the help of the quasiprobability distribution function (Q-function). Our conclusions are summarized in Sec. V.

II. THE MODEL

We devote this section to a brief discussion of the most general class of JC-model which describes the interaction between a single few-level atom and the quantized cavity field. In fact, the JC-model has been extensively studied by many authors and numerous nonclassical effects have been predicted and in some cases verified in the laboratory.[10] The Hamiltonian of the JC-model concerns a two-level atom interacting with a single mode of quantized radiation (boson) field of a given frequency ω, is described in terms of the usual creation $\hat{a}^{\dagger}$, and annihilation $\hat{a}$ operators of the boson field satisfying $[\hat{a},\hat{a}^{\dagger}]=1$, the two-level system is represented by the z-component of the Pauli matrix operator with the energy separation of the two atomic levels $\omega_0=(E_e-E_g)$, where E_i is the energy for level $|i\rangle$, and their mutual interaction is expressed in the rotating wave approximation which can be represented by the generic formula as

$$\frac{\hat{H}}{\hbar}=\Re(\hat{A})+S(\hat{A})(\hat{G}_{ee}-\hat{G}_{gg})+\hat{A}(\beta_2\hat{G}_{ee}+\beta_1\hat{G}_{gg})+\lambda(\hat{A}_k\hat{G}_{eg}+\hat{G}_{eg}\hat{A}_k^{\dagger}), \tag{1}$$

where $\hat{A}$ is some generalized number operator for the photon field, while $\hat{A}_k$ and $\hat{A}_k^{\dagger}$ represent generalized raising (lowering) operators. We denote by λ the dipole-interaction strength between the radiation and the atom or in the generic model represents the coupling between the boson field and the pseudo-spin matrices $\hat{G}_{ij}$. The third term of $\hat{H}$ describes the dynamic Stark shifts of the ground and excited levels of the atom which depends on the one-photon coupling constant. This coupling depends on the mismatch $|\Delta|$ (the detuning parameter $\Delta=\omega_0-k\omega$) and the intensity and statistics of the cavity field. β_1 and β_2 are parameters describing the intensity-dependent Stark shifts ($k>1$) of the two-level atom which is due to the virtual transitions to the intermediate relay level. Also, λ is related to λ_1 the coupling constant for the ($|e\rangle\leftrightarrow|j\rangle$ transition) and λ_2 for the ($|g\rangle\leftrightarrow|j\rangle$ transition) by the relation

$$\lambda=\frac{\lambda_1\lambda_2}{\Delta},\quad \beta_1=\frac{\lambda_1^2}{\Delta},\quad \beta_2=\frac{\lambda_2^2}{\Delta}. \tag{2}$$

It is worth noting here that the form of the Hamiltonian (1), in the absence of Stark shifts ($\beta_i = 0$) and the nonlinearities reduces to (up to constant factors) that of Ref. 15. We assume that the injected atom is prepared before entering the cavity in the following form:

$$\rho = \cos^2\left(\frac{\varrho}{2}\right)\hat{G}_{ee} + \sin^2\left(\frac{\varrho}{2}\right)\hat{G}_{gg} \in \mathsf{S}_A . \tag{3}$$

Also, we suppose that the initial state of the radiation field is a coherent state. Then we may write the initial state of the field as

$$\varpi = |\eta\rangle\langle\eta| \in \mathsf{S}_F , \quad |\eta\rangle = \sum_{n=0}^{\infty} b_n |n\rangle, \tag{4}$$

where, $b_n = \exp(-\frac{1}{2}\overline{n})(\overline{n}^{n/2}/\sqrt{n!})$, and $\overline{n} = |\eta|^2$ is the intensity of the initial coherent field. The continuous map $\mathcal{E}_t^*$ describing the time evolution between the atom and the field is defined by the unitary operator generated by $\hat{H}$ such that

$$\begin{gathered} \mathcal{E}_t^* : \mathsf{S}_A \to \mathsf{S}_A \otimes \mathsf{S}_F , \\ \mathcal{E}_t^* \rho = \hat{U}_t(\rho \otimes \varpi)\hat{U}_t^* , \\ \hat{U}_t \equiv \exp\left(-it\frac{\hat{H}}{\hbar}\right). \end{gathered} \tag{5}$$

The quantity expressed in Eq. (5) is to be calculated using quantum states evolving in time under the action of Hamiltonian $\hat{H}$.

Entanglement is a feature of the fully-quantized matter–radiation interaction, for example, the steady states of Eq. (1) are entangled states known as ''dressed states.'' Before proceeding further, we give a specific example for the sake of concreteness. We consider the case of the k-photon JC-model with arbitrary forms of the nonlinearities of both the field and the intensity-dependent coupling in the presence of the Stark shifts. Here, we assume that $\hat{A}_k = f(\hat{a}^\dagger\hat{a}) \otimes \hat{a}^k$, $\hat{A} = \hat{a}^\dagger\hat{a}$, $S(\hat{A}) = \omega_0/2$, and $\Re(\hat{A}) = \omega\hat{a}^\dagger\hat{a} + \Re_1(\hat{a}^\dagger\hat{a})$. The first term in the $\Re(\hat{A})$ obviously stands for the energy of a free photon field, whereas $\omega_0/2$ stands for the two-level atom, the level splitting depending on the strength of the photon field. We denote by $\Re_1(\hat{a}^\dagger\hat{a})$ the one-mode field nonlinearity and $\lambda f(\hat{a}^\dagger\hat{a})$ represents an arbitrary intensity-dependent coupling. Switching to an interaction-picture representation for convenience, it can be shown that exact solutions of this interacting system are

$$\begin{gathered} \hat{H}|s,g\rangle = E_0|s,g\rangle, \quad 0 \leqslant s < k, \\ \hat{H}|\Psi_{\pm}^{(n)}\rangle = E_{\pm}^{(n)}|\Psi_{\pm}^{(n)}\rangle, \end{gathered} \tag{6}$$

where the eigenvalues E_0 and $E_{\pm}^{(n)}$ are given by

$$\begin{gathered} E_{\pm}^{(n)} = \omega\left(n + \frac{k}{2}\right) + \frac{\omega_0}{2} + \frac{1}{2}(\Re_1(n) - \Re_1(n+k)) + \frac{1}{2}[n\beta_2 + \beta_1(n+k)] \pm \mu_n , \\ E_0 = \left(s\beta_1 - \frac{\Delta}{2}\right), \end{gathered} \tag{7}$$

and the eigenstates $|\Psi_{\pm}^{(n)}\rangle$ are

$$|\Psi_{+}^{(n)}\rangle = \sin\theta_n|n,e\rangle + \cos\theta_n|n+k,g\rangle,$$
$$|\Psi_{-}^{(n)}\rangle = \cos\theta_n|n,e\rangle - \sin\theta_n|n+k,g\rangle, \tag{8}$$

with

$$\mu_n = \sqrt{\nu_n^2+\tau_n^2},$$
$$\nu_n = \frac{\Delta}{2} + \frac{1}{2}(\beta_2 n - \beta_1(n+k)) + \frac{1}{2}(\Re_1(n) - \Re_1(n+k)), \tag{9}$$
$$\tau_n = \lambda f(n+k)\sqrt{\frac{(n+k)!}{n!}},$$

where μ_n is a modified Rabi frequency. The angle θ_n is given by

$$\theta_n = \sin^{-1}\left(\frac{\tau_n}{\sqrt{(\nu_n-\mu_n)^2+\tau_n^2}}\right). \tag{10}$$

The entangled states $|s,g\rangle$ and $|\Psi_{\pm}^{(n)}\rangle$ are orthonormal and complete. Here $\pm$ labels the entangled states which in their bare condition are the ground $|g\rangle$ and the excited $|e\rangle$ states, and n, the states of the boson field. The condition for $\theta_n=\pi/4$ is $\nu_n=0$ for which it is sufficient that $\Delta=\beta_1=\beta_2=\Re_1(n)$.

The unitary evolution operator $\hat{U}_t$ can be written as

$$\hat{U}_t = \sum_{n=0}^{\infty}\{\exp(-itE_{+}^{(n)})|\Psi_{+}^{(n)}\rangle\langle\Psi_{+}^{(n)}| + \exp(-itE_{-}^{(n)})|\Psi_{-}^{(n)}\rangle\langle\Psi_{-}^{(n)}|\}$$
$$+\sum_{s=0}^{k-1}\exp(-itE_0)|s,g\rangle\langle g,s|. \tag{11}$$

Despite being straightforwardly solvable in this way, the JC-model is well-known for the fact that the time-evolution of most expectation values is usually expressible only in series form. Having obtained the explicit forms of the unitary operator $\hat{U}_t$, for the system under consideration then the eigenvalues and the eigenfunctions can be used to discuss many features concerning the field or the atom. Given the impressive technological advances in several experimental areas of quantum optics, condensed matter, atomic physics, etc..., it is nowadays possible to realize a system of two interacting degrees of freedom and watch the time evolution of the corresponding entanglement process.[16] It is therefore also of importance to understand the entanglement process in simple Hamiltonian systems. Hamiltonian systems with two degrees of freedom often present a very rich dynamics, which in many cases is not yet completely understood from a general point of view. In particular, if the interaction is nonlinear the system may present chaotic behavior in the classical limit. The consequences of this fact for the quantum dynamics are as yet unsettled. A step in this direction was taken a few years ago, as it was conjectured that "the rate of entropy production can be used as an intrinsically quantum test of the chaotic versus regular nature of the evolution."[17] The idea has been tested in some models.[18] In the next section we are going to discuss the degree of entanglement due to quantum quasi-mutual entropy which is a special case of the quantum relative entropy.

III. DERIVATION OF ENTANGLEMENT DEGREE

Quantum entanglement is one of the paradigmatic ingredients of quantum theory. In the following we are interested in studying the entanglement for an initial mixed state of the cavity

field, as mixed states are the true representation of the state of the field at a finite temperature. However, it is difficult to define the entanglement for mixed states. This is because we cannot easily define an analogu of the Schmidt decomposition for a general mixed state of a composite system. Such a mixed state can be expanded in terms of pure states in infinitely many different ways and it is not clear which, if any, decomposition should be favored. Mixing two entangled pure states could result in a mixed state with entanglement much less than the average entanglement of the states mixed. Mixed state entanglement is thus a very different entity to either correlations or pure state entanglement. At least three different measures have been used to quantify entanglement for a mixed state. One of these measures, the relative entropy of entanglement,[2] is defined for mixed state of a composite system (such as the atom-field system) as[7,8]

$$E_{re}(\mathcal{E}_t^*\rho,\mathcal{E}_t^*\sigma)=\mathrm{Tr}\,\mathcal{E}_t^*\rho(\log\mathcal{E}_t^*\rho-\log\mathcal{E}_t^*\sigma), \tag{12}$$

where $E_{re}(\mathcal{E}_t^*\rho,\mathcal{E}_t^*\sigma)$ measures the difficulty of distinguishing between the states $\mathcal{E}_t^*\rho$ and $\mathcal{E}_t^*\sigma$. A state $\mathcal{E}_t^*\sigma$ of a bipartite system $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$ is called separable if $\mathcal{E}_t^*\sigma$ is a mixture of product states, i.e., if $\mathcal{E}_t^*\sigma$ can be written as[19]

$$\mathcal{E}_t^*\sigma=\sum_k\ p_k\sigma_k^A\otimes\sigma_k^F, \tag{13}$$

where $\sigma_k^A\in\mathsf{S}(\mathcal{H}_1)$, $\sigma_k^F\in\mathsf{S}(\mathcal{H}_2)$, $p_k>0$, and $\Sigma_k p_k=1$. A separable state can be prepared by local means, that is, by performing local quantum operations on a product state. The relative entropy of entanglement measure tells us how difficult it is to distinguish the given entangled state from its closest approximation in the set of separable states. The other measures of entanglement are associated with formation and distillation of entangled states.

In Refs. 7–9, a method using quasi-mutual entropy to measure the degree of entanglement in the time development of a two-level system has been adopted. This measure quantifies how much the correlated systems know about the state of each other. However, in the present paper, we will derive the entanglement degree without the diagonal approximation which has been used in Refs. 7–9. The final state is given by

$$\mathcal{E}_t^*\rho=U_t(\rho\otimes\varpi)U_t^*=\cos^2\left(\frac{\varrho}{2}\right)U_t|\,\eta;e\rangle\langle\,\eta;e|U_t^*+\sin^2\left(\frac{\varrho}{2}\right)U_t|\,\eta;g\rangle\langle\,\eta;g|U_t^*\,. \tag{14}$$

Then the von Neumann entropy for the reduced state $\mathcal{E}_t^*\rho$ is given by

$$S(\mathcal{E}_t^*\rho)=\lambda_1^{AF}(t)\log\lambda_1^{AF}(t)+\lambda_2^{AF}(t)\log\lambda_2^{AF}(t), \tag{15}$$

where $\lambda_1^{AF}(t)=\cos^2(\varrho/2)$, $\lambda_2^{AF}(t)=\sin^2(\varrho/2)$.

Taking the partial trace over the atomic system, we obtain

$$\begin{aligned}\rho_t^F=\mathrm{tr}_A\,\mathcal{E}_t^*\rho=&\cos^2\left(\frac{\varrho}{2}\right)(|\psi_1(t)\rangle\langle\psi_1(t)|+|\psi_2(t)\rangle\langle\psi_2(t)|)\\&+\sin^2\left(\frac{\varrho}{2}\right)(|\psi_3(t)\rangle\langle\psi_3(t)|+|\psi_4(t)\rangle\langle\psi_4(t)|),\end{aligned} \tag{16}$$

where

$$
\begin{aligned}
|\psi_1(t)\rangle &= \sum_{n=0}^{\infty} b_n e^{-i\gamma_n t}(\cos\mu_n t + i\cos 2\theta_n \sin\mu_n t)|n\rangle,\\
|\psi_2(t)\rangle &= -i\sum_{n=0}^{\infty} b_{n-k} e^{-i\gamma_{n-k} t}\sin 2\theta_{n-k}\sin\mu_{n-k} t|n\rangle,\\
|\psi_3(t)\rangle &= -i\sum_{n=0}^{\infty} b_{n+k} e^{-i\gamma_n t}\sin 2\theta_n \sin\mu_n t|n\rangle,\\
|\psi_4(t)\rangle &= \sum_{n=0}^{\infty} b_n e^{-i\gamma_{n-k} t}(\cos\mu_{n-k} t + i\cos 2\theta_{n-k}\sin\mu_{n-k} t)|n\rangle,
\end{aligned}
\tag{17}
$$

with

$$
\gamma_n = \tfrac{1}{2}(\Re(n)+\Re(n+k)) + \tfrac{1}{2}[n\beta_2 + \beta_1(n+k)]. \tag{18}
$$

The von Neumann entropy for the reduced state $S(\rho_t^F)$ is computed by

$$
S(\rho_t^F) = -\lambda_1^F(t)\log\lambda_1^F(t) - \lambda_2^F(t)\log\lambda_2^F(t) - \lambda_3^F(t)\log\lambda_3^F(t) - \lambda_4^F(t)\log\lambda_4^F(t), \tag{19}
$$

where $\lambda_i^F(t)$ are the solutions of the following equation:

$$
\det[\hat{\rho}(t) - \lambda(t)\hat{N}(t)] = 0, \tag{20}
$$

$\hat{\rho}(t)$ and $\hat{N}(t)$ are 4×4 matrices having the following elements:

$$
\begin{aligned}
[\hat{\rho}(t)]_{ij} &\equiv \langle\psi_i(t)|\rho_t^F|\psi_j(t)\rangle \quad (i,j=1,2,3,4),\\
[\hat{N}(t)]_{ij} &\equiv \langle\psi_i(t)|\psi_j(t)\rangle \quad (i,j=1,2,3,4).
\end{aligned}
\tag{21}
$$

For the reduced state $S(\rho_t^A)$ we find that the von Neumann entropy takes the form

$$
S(\rho_t^A) = -\lambda_+^A(t)\log\lambda_+^A(t) - \lambda_-^A(t)\log\lambda_-^A(t), \tag{22}
$$

where $\lambda_i^A(t)$ is given by

$$
\lambda_\pm^A(t) = \tfrac{1}{2}\{1 \pm \sqrt{(2\mathsf{C}_{ee}(t)-1)^2 + 4|\mathsf{C}_{eg}(t)|^2}\}. \tag{23}
$$

In this case, the probability of finding the atom in its excited or ground states are expressed as the diagonal element of the reduced atomic density matrix; thus

$$
\begin{aligned}
\mathsf{C}_{ee}(t) = \sum_{n,l=0} b_{n,l}\Bigg\{ & \tilde{E}_{++}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2 |\sin\theta_n|^2|\sin\theta_l|^2 + \frac{1}{4}\left|\sin\left(\frac{\varrho}{2}\right)\right|^2 \sin 2\theta_n \sin 2\theta_l\right]\\
& + \tilde{E}_{+-}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2 |\sin\theta_n|^2|\cos\theta_l|^2 - \frac{1}{4}\left|\sin\left(\frac{\varrho}{2}\right)\right|^2 \sin 2\theta_n \sin 2\theta_l\right]\\
& + \tilde{E}_{-+}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2 |\cos\theta_n|^2|\sin\theta_l|^2 - \frac{1}{4}\left|\sin\left(\frac{\varrho}{2}\right)\right|^2 \sin 2\theta_n \sin 2\theta_l\right]\\
& + \tilde{E}_{--}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2 |\cos\theta_n|^2|\cos\theta_l|^2 + \frac{1}{4}\left|\sin\left(\frac{\varrho}{2}\right)\right|^2 \sin 2\theta_n \sin 2\theta_l\right]\Bigg\},
\end{aligned}
\tag{24}
$$

$$
\mathsf{C}_{ee}(t) = 1 - \mathsf{C}_{gg}(t),
$$

and the off-diagonal element $\mathsf{C}_{eg}(t)$ is given by

$$
\begin{aligned}
\mathsf{C}_{eg}(t)=\frac{1}{2}\sum_{n,l=0}^{\infty} b_{n,l}\Bigg\{ & \widetilde{E}_{++}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2|\sin\theta_n|^2\sin 2\theta_l+\left|\sin\left(\frac{\varrho}{2}\right)\right|^2\sin 2\theta_n|\cos\theta_l|^2\right] \\
& -\widetilde{E}_{+-}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2|\sin\theta_n|^2\sin 2\theta_l-\left|\sin\left(\frac{\varrho}{2}\right)\right|^2\sin 2\theta_n|\sin\theta_l|^2\right] \\
& +\widetilde{E}_{-+}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2|\cos\theta_n|^2\sin 2\theta_l-\left|\sin\left(\frac{\varrho}{2}\right)\right|^2\sin 2\theta_n|\cos\theta_l|^2\right] \\
& -\widetilde{E}_{--}^{(nl)}\left[\left|\cos\left(\frac{\varrho}{2}\right)\right|^2|\cos\theta_n|^2\sin 2\theta_l+\left|\sin\left(\frac{\varrho}{2}\right)\right|^2\sin 2\theta_n|\sin\theta_l|^2\right]\Bigg\}, \qquad (25)
\end{aligned}
$$

where $\widetilde{E}_{ij}^{(nl)}=\exp[-it(E_i^{(n)}-E_j^{(l)})]$. Thus we rigorously obtain the entanglement degree in the system under consideration in the following form:[7,8]

$$
\begin{aligned}
\mathrm{DEM}(\mathcal{E}_t^*\rho) &\equiv \mathrm{tr}\,\mathcal{E}_t^*\rho(\log\mathcal{E}_t^*\rho-\log(\rho_t^A\otimes\rho_t^F)) \\
&= S(\rho_t^A)+S(\rho_t^F)-S(\mathcal{E}_t^*\rho) \\
&= -\lambda_1^F(t)\log\lambda_1^F(t)-\lambda_2^F(t)\log\lambda_2^F(t)-\lambda_3^F(t)\log\lambda_3^F(t)-\lambda_4^F(t)\log\lambda_4^F(t) \\
&\quad -\lambda_+^A(t)\log\lambda_+^A(t)-\lambda_-^A(t)\log\lambda_-^A(t)+\lambda_1^{AF}(t)\log\lambda_1^{AF}(t) \\
&\quad +\lambda_2^{AF}(t)\log\lambda_2^{AF}(t). \qquad (26)
\end{aligned}
$$

Note that the tensor product state $\rho_t^A\otimes\rho_t^F$ is one of the disentangled states. From the above equations and the matrix elements which represent the state of the field, we are able to determine under which conditions we may attain a reasonable entanglement degree. In what follows, we shall analyze numerically whether and how it would be possible to increase the amount of entanglement of the output state. Therefore, we consider the situation where the initial field state is a coherent state.

A. Discussion

In the previous section we have assumed perfect unitary evolution and initial state preparation for the system. This assumption is partially justified for the following reasons: (1) a very good control of the quantum dynamics has been achieved for a single atom (or trapped ion); (2) they are well isolated from their environment. In this section we present several results related to a general definition of entanglement degree, denoted $\mathrm{DEM}(\mathcal{E}_t^*\rho)$. Although it has already been used in the past in the framework of the diagonal approximation formalism, such an entanglement degree becomes particularly interesting when we consider a general mixed state. It is then possible to show that $\mathrm{DEM}(\mathcal{E}_t^*\rho)$ possesses a number of interesting properties. Comparing to the quantum von Neumann entropy the advantage of this entanglement degree measure, is that for the mixed state which is a general case one just needs to compute $\mathrm{DEM}(\mathcal{E}_t^*\rho)$. No more knowledge of the final state is required, neither does it need to be diagonalized, as in the von Neumann entropy case.

We inspect the time-evolution of the entanglement degree for a two-level system, choosing the initial state of the radiation field to be a coherent state. The importance of studying in detail the entanglement degree in different initial states is twofold. It may be viewed as a key to the understanding of some of the striking differences between the quantum and classical description of the world such as the nonexistence at the classical level of the majority of states allowed by quantum mechanics. In particular, if the interaction is nonlinear the system may present chaotic behavior in the classical limit. We should note that if we set the angle $\varrho=0(\pi)$ (i.e., the atom

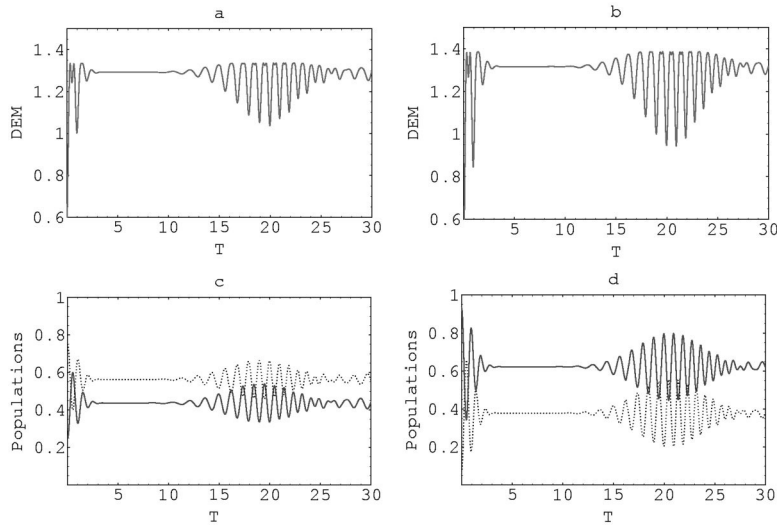

FIG. 1. The entanglement degree DEM($\mathcal{E}_t^*\rho$) in (a), (b) and the atomic populations of the excited and ground states in (c), (d) as functions of the scaled time $T=\lambda t$. Calculations assume that $\beta_1=0$, $\beta_2=0$, $f(n)=1$, ($\phi=0$) and the field in the coherent state, the detuning parameter Δ has zero value, $k=1$ (one-photon resonance), the mean-photon number $\bar{n}=10$ and for different values of ϱ, where (a), (c) $\varrho=\pi/3$ and (b), (d) $\varrho=\pi/12$.

initially in the excited (ground) state) the final state of the system is a pure entangled state. Therefore it is sufficient to use von Neumann entropy in order to measure the degree of entanglement for the above cases and the entanglement degree is just twice the reduced von Neumann entropy i.e., DEM($\mathcal{E}_t^*\rho$)$=2S(\rho_t^A)$. These situations have been considered and the reduced von Neumann entropy has been applied to analyze the quantum fluctuations.[4–6] In a general case (i.e., $\varrho\neq 0$ or π), the final state is not necessarily pure, so that we need to adopt the DEM($\mathcal{E}_t^*\rho$) in order to measure the degree of entanglement in the present model. In fact, the initial state of the atomic system was considered as an exited state or a ground state in Ref. 6, however, we start from a mixed state, namely Eq. (3) as an initial state of the atomic system. Thus our initial setting enables us to discuss the variation of the entanglement degree for different values of the angle ϱ of the initial atomic system.

In order to explore the effects of parameters of the system on the entanglement degree, we plot the entanglement degree for (i) different values of the angle ϱ, in Fig. 1; (ii) different values of the detuning parameter Δ/λ in Fig. 2; (iii) different values of the intensity-dependent coupling in Fig. 3; (iv) different values of Stark shift parameters β_1 and β_2, in Fig. 4 and finally, different values of the field nonlinearity in Fig. 5. One of the interesting phenomenon described by a two-level system is the dynamical behavior of the system. When we consider that the atom is initially in the upper state (i.e., $\varrho=0$) in the absence of both the detuning and Stark shift, the upper state population $\mathsf{C}_{ee}(t)$ is reduced to $\mathsf{C}_{ee}(t)=\Sigma_n b_n^2\cos^2\mu_n t$, where the field is initially described by photon statistics b_n^2. This shows that the upper state population oscillates periodically at the Rabi-flopping frequency, similar to the case of classical fields. In the vacuum field at $n=0$ and on resonance $\Delta=0$, the dressed states are separated by the frequency $\mu_0=2\lambda$, generally called vacuum Rabi splitting. Intuitive pictures of the interaction between a two-level atom and an electric field commonly involve the expectation that the atomic level populations must change as both systems exchange excitations over the course of time. This is due to the absence of further atomic levels, which precludes the existence of destructive interference between different atomic transitions. However, in a fully-quantized interaction model such as the Jaynes-Cummings model, it is indeed possible to have states in which the atomic populations are completely or nearly completely trapped. This can be ultimately traced to the fact that the eigenstates of this model are entangled.

In order to get a deeper insight into modulation effect of the parameter ϱ on the entanglement

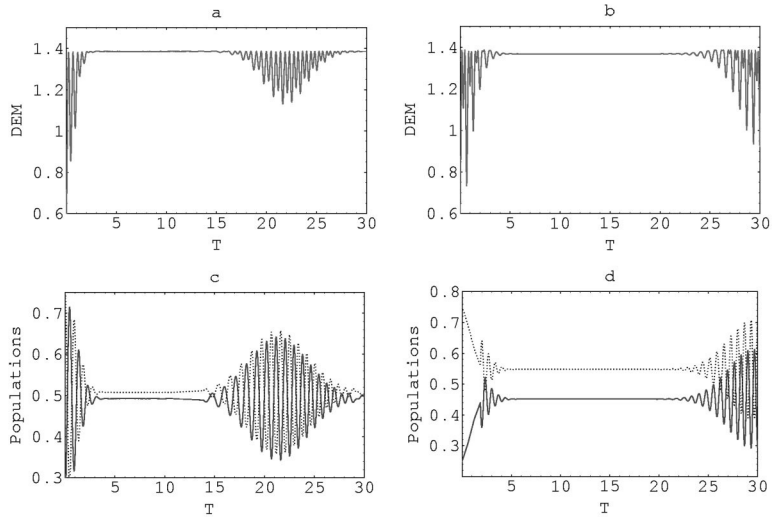

FIG. 2. The entanglement degree DEM($\mathcal{E}_t^*\rho$) in (a), (b) and the atomic populations of the excited and ground states in (c), (d) as functions of the scaled time $T=\lambda t$. Calculations assume that $\beta_1=0$, $\beta_2=0$, $f(n)=1$, ($\varrho=\pi/3,\phi=0$) and the field in the coherent state, $k=1$ (one-photon resonance), the mean-photon number $\overline{n}=10$ and for different values of the detuning parameter Δ, where (a), (c) $\Delta/\lambda=3$ and (b), (d) $\Delta/\lambda=6$.

degree, in Fig. 1, we plot the entanglement degree for different values of the parameter ϱ. It is remarkable that, the first maximum of the entanglement degree at $t>0$ is achieved at the collapse time, that is when the average photon number in the cavity mode reaches its steady value, and at one-half the revival time, the entanglement degree reaches its local minimum. Meanwhile, the general feature of the entanglement degree in the case ϱ takes very small values is also almost identical to that in the previous cases [see Fig. 1(a)]. As $\varrho=\pi/12\approx 0.08\pi$, we find that the maximum value of the entanglement degree increases, such as DEM($\mathcal{E}_t^*\rho$)$\approx$1.4, [see Fig. 1(b)]. When we further decrease the angle $\varrho\approx 0$ we find that our degree of entanglement takes just twice

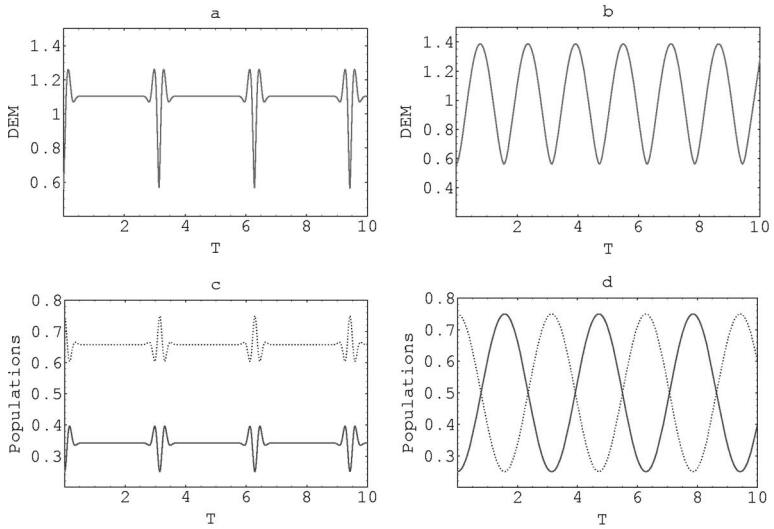

FIG. 3. The entanglement degree DEM($\mathcal{E}_t^*\rho$) in (a), (b) and the atomic populations of the excited and ground states in (c), (d) as functions of the scaled time $T=\lambda t$. Calculations assume that $\beta_1=0$, $\beta_2=0$, ($\varrho=\pi/3,\phi=0$) and the field in the coherent state, the detuning parameter Δ has zero value, $k=1$ (one-photon resonance), the mean-photon number $\overline{n}=10$ and for different values of the intensity-dependent coupling $f(n)$, where (a), (c) $f(n)=\sqrt{n}$, and (b), (d) $f(n)=1/\sqrt{n}$.

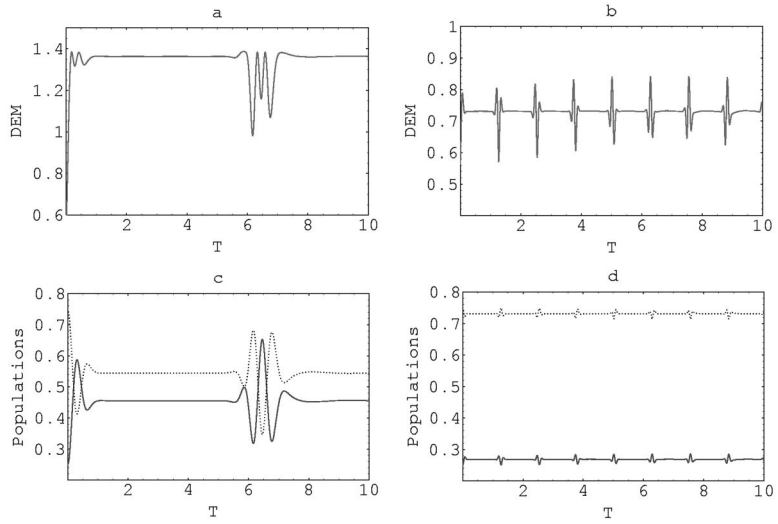

FIG. 4. The entanglement degree DEM($\mathcal{E}_t^*\rho$) in (a), (b) and the atomic populations of the excited and ground states in (c), (d) as functions of the scaled time $T=\lambda t$. Calculations assume that $(\varrho=\pi/3,\phi=0)$ and the field in the coherent state, the detuning parameter Δ has zero value, $k=2$ (two-photon process), the mean-photon number $\bar{n}=10$ and for different values of the Stark shift parameter where (a), (c) $\beta_1=1$, $\beta_2=2$, and (b), (d) $\beta_1=1$, $\beta_2=7$.

the value of the von Neumann entropy, i.e., DEM($\mathcal{E}_t^*\rho$)$\approx$ 2 log 2. It has been shown that the atomic occupation probability undergoes a collapse followed by a series of revivals.[1] The collapse is due to the destructive interference of quantum Rabi flopping at different frequencies; a similar phenomenon may also occur with a classical field, however, the revivals are a purely quantum mechanical effect that originates in the discreteness of the quantum field. Collapse and revivals have been observed in a micromaser experiment.[20]

As soon as we take the detuning effects into consideration, it is easy to realize the general behavior is affected by increasing the value of the detuning parameter, where the revival time is elongated to have the value $\tau_R\simeq 2\pi\sqrt{\delta^2+n+1}$, $(\delta=\Delta/2\lambda)$; see Fig. 2. However, any change of

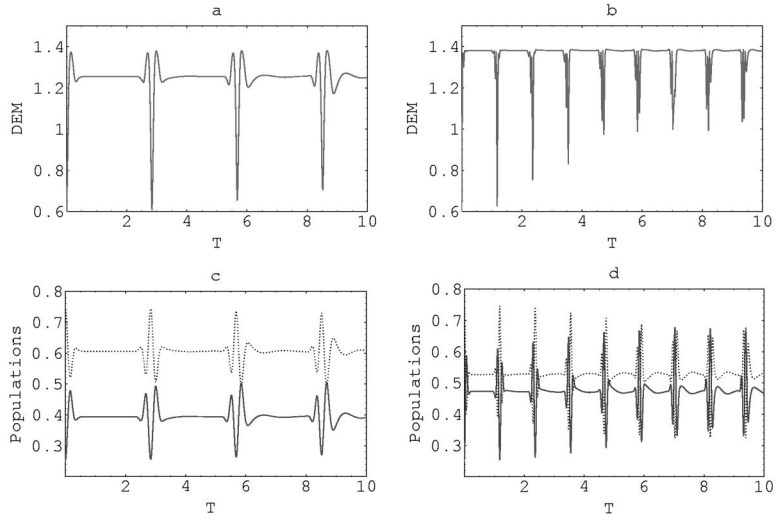

FIG. 5. The entanglement degree DEM($\mathcal{E}_t^*\rho$) in (a), (b) and the atomic populations of the excited and ground states in (c), (d) as functions of the scaled time $T=\lambda t$. Calculations assume that $(\varrho=\pi/3,\phi=0)$ and the field in the coherent state, the detuning parameter Δ has zero value, $k=1$ (one-photon resonance), the mean-photon number $\bar{n}=10$, $\beta_1=0$, $\beta_2=0$ and for different values of the Kerr-like medium, where (a), (c) $\chi/\lambda=0.1$, and (b), (d) $\chi/\lambda=0.5$.

the detuning parameter leads to changes in the entanglement degree and increasing the detuning parameter Δ leads the entanglement degree to survive for a long period. It is worthwhile pointing out the availability of the longer period entanglement, meaning that the entanglement is high for a longer interval of time. The entanglement as a physical resource is available on the condition that the entanglement could keep long enough so that we can accomplish some task. For example, in Ref. 21 to generate the entangled atomic state, the entanglement between the atom and the cavity field must survive long enough so that it can be transferred to a next atom via a coherent interaction. At this point, the increasingly long period of entanglement has some advantages. Although some authors use another method to prepare multiparticle entanglement,[22] this method of lengthening the period of entanglement is available.

Figure 3, is plotted in the setting of the detuning parameter $\Delta=0$, and $\varrho=\pi/3$ and different values of the intensity-dependent coupling $f(n)=\sqrt{n}$ for Fig. 3(a) and $f(n)=1/\sqrt{n}$ for Fig. 3(b). We note that the maximum value of the entanglement degree is approximately ≈ 1.25. In this case, we can say that the entanglement degree is a periodical function of time with period $t=\pi/\lambda$. This is essentially because of the nonlinear nature of the coupling in this case which results in the Rabi frequency being proportional to the photon number as opposed to its square root, as is the case in one-photon JC-model. The situation is completely changed when we consider $f(n)=1/\sqrt{n}$ [see Fig. 3(b)] where the maximum value of the entanglement degree increases and reaches ≈ 1.4, and the entanglement degree is a periodical function of time with period $t=\pi/2\lambda$.

Figure 4, shows the basic features of the behavior of the entanglement degree in the two-photon case ($k=2$) with different values of the Stark shift parameters β_1 and β_2. Except for β_1 and β_2, we choose the same values as in Fig. 1(a). We remark that the entanglement degree has some kind of periodicity [see Fig. 4(a)]. This behavior is affected if the deviation between β_1 and β_2 is increased [see Fig. 4(b)]. Note that the behavior of the entanglement degree is complicated, reflecting local maxima and minima in wave packet trajectory. The local maxima and minima is due to the field interaction with an atom, corresponding to entanglement and disentanglement. Because of the influence of Stark shift on entanglement, the amplitude of local maxima and minima decrease with increasing the deviation of $r=\sqrt{\beta_1/\beta_2}$ from the unity ($r\gg 1$ or $r\ll 1$). However, as r takes values close to unity, we return to the same behavior as in the absenceof Stark shift parameters. Due to the repeated period of entanglement and disentanglement the state of the atom and field lose and gain coherence but the coherence recovered by the atom is never that which was lost. Obviously, the arbitrariness of n leads to the fact that the factor $\frac{1}{4}[\beta_2 n-\beta_1(n+2)]^2$, which appears in μ_n, fails to vanish for general single-mode field state, i.e., in most situations the Stark shifts cannot be ignored, even the two levels $|e\rangle$ and $|g\rangle$ are equally coupled to the virtual level $|i\rangle$. If the final states is free of the Stark effects and is in the case of exact resonance, the system will evolve periodically in the presence of the coherent states. However, for the phase sensitive averages of the cavity field, the Stark shifts still cannot be ignored in any case. Once the Stark shift is taken into account, this interesting feature disappears. Further, it seen that Rabi frequency depends on the square root of the product of $(n+1)$ and $(n+2)$, rather than a linear dependence on them required for large detuning. It is therefore vital that Stark shifts are included in any analysis of a multiphoton effective two-level system.

We see that the evolution of the entanglement degree is almost similar for both $\beta_2=\beta_1$ and the absence of Stark shift cases. This may be interpreted as follows, physically, this result corresponds to the fact that the Stark shift creates an effective intensity-dependent detuning $\Delta_N=\beta_2-\beta_1$.[23] When $\beta_2=\beta_1=1$, $\Delta_N=0$, in this case, the Stark shift does not affect the time evolution of the entanglement degree. As is visible from the figures, the effects of the dynamic Stark shift are more pronounced when r deviates from unity. Interestingly, when r is decreased, the values of the maximum entanglement are increased, indicating that the Stark shift leads to an increasing of the degree of entanglement of the field and atom. A slight change in r, therefore, dramatically alters the entanglement. Periodic models therefore may be more robust in this sense. Such models may physically consist of, for example, Raman scattering and equal or unequal two-photon absorption. An appropriate choice of detuning leads to periodicity which in fact is a manifestation of the commensurate Rabi frequencies proportional to n.

Now we turn our attention to see the effect of the nonlinearity of the field with a Kerr-type medium on the entanglement degree, i.e., we take $\Re(n)=\chi n(n-1)$, where χ is related to the third-order nonlinear succeptibility. In fact, the optical Kerr effect is one of the most extensively studied phenomenon in the field of nonlinear optics because of its applications that range from frequency conversions to quantum nondemolition measurements.[24] The optical Kerr effect can be used to construct a quantum phase gate.[25] From Figs. 5(a), 5(b), where the effect of the Kerr is shown for values of $\chi/\lambda=0.1$ and $\chi/\lambda=0.5$, it is observed that the Kerr-like medium with the field mode is very weak when we take $\chi/\lambda=0.01$. In fact, this weakness of the nonlinear interaction leads to increasing the values of the minimum entanglement degree and consequently the sustainment time of the maximum entanglement. In this case, the field and the atom almost retain in strong entanglement in the time evolution process. However, as we increase the value of χ/λ, we find the value of the maximum entanglement degree begins to decrease [see Fig. 5(b)]. Further we noticed that the degree of entanglement between the field and the atom is also reduced. Collapse and revivals in the JC-model have been known for some time. With the addition of a Kerr-like medium the revival time decreases along with the peak-to-peak amplitude of the oscillations. In the usual model the revivals tend to be irregular and indistinguishable after several sequences, but with a Kerr-type nonlinear medium included many more distinct revival-collapse sequences occur. In the meantime we realize that the amplitude of the oscillations decreases as χ/λ increases. Here we may mention that if the coupling parameter of a Kerr-like medium is stronger than the atom-field coupling one can see the system starts to dominate the dynamics (there is nearly decoupling of the atom and field) and there is a repetition for some kind of regularity in the evolution of the system. This is apparent from the regular spikes present in Fig. 5(b). This result is in agreement with the fact that in the limit for strong nonlinear interaction of the Kerr-like medium with the field mode, the field and the atom are almost decoupled. Also, we can see that the amplitude of the oscillation becomes smaller but with more revivals in the same time. These numerical illustrations provide evidence that in cases of physical interest entanglement can be significant and can be reliably estimated for a broad range of field parameters using the present formalism.

As we see from the above figures the field is initially in a mixed state. As time goes on we note a growth in DEM$(\mathcal{E}_t^*\rho)$, followed by a sudden decrease, almost at half of the revival time. Of course, the total atom-field state cannot have its entanglement degree diminished, which means that as the field becomes more pure the atomic state must be closer to a mixed state. Although this behavior is not obvious, exists a neat explanation from the phase space point of view, as we are going to show in the rest of the paper.

IV. PHASE SPACE APPROACH

In the previous section we discussed a particular aspect of the entanglement degree and collapses-revivals phenomenon in the multi-photon model with the initial field prepared in the coherent state. Now we are going to try to understand better the behavior of the system by focusing our attention on the field dynamics. The representation of fields in phase space has been providing new insights of the JC field dynamics.[26] Perhaps the most convenient quasiprobability to be used in this kind of problem is the Q-function. The first step to be taken is the calculation of the final state of the system $\mathcal{E}_t^*\rho$ [see Eq. (14)], and then we get the Q-function as

$$Q(x,y,t)=\frac{1}{\pi}\langle\zeta|\rho_F(t)|\zeta\rangle, \tag{27}$$

where $|\zeta\rangle$ is a coherent state with amplitude $\zeta=x+iy$, and $\rho_F(t)$ is the reduced density operator for the field. More than just a theoretical curiosity, $Q(x,y,t)$ can be detected in homodyne experiments.[27] The Q-function is not only a convenient tool to calculate expectation values of anti-normally ordered products of operators, but also gives us a new insight into the mechanism of interaction in the model under consideration.

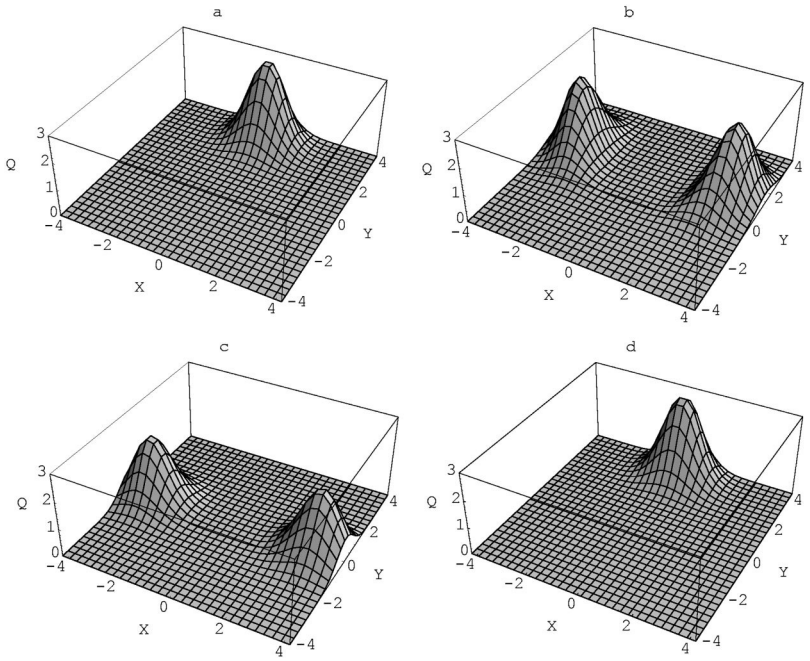

FIG. 6. A plot of Q-function of the cavity field with the initial mean photon number $\bar{n}=5$, (a) $f(n)=1$, $\lambda t=0$, (b) $f(n)=1$, $\lambda t=5\pi/2$, (c) $f(n)=\sqrt{n}$, $\lambda t=5\pi/2$ and (d) $f(n)=1/\sqrt{n}$, $\lambda t=5\pi/2$.

We present the results of this section mainly in graphical form with the initial mean photon number $\bar{n}=5$. The splitting and recombination of branches of the Q-function in phase space is clearly associated with the collapses and revivals phenomenon, when a splitting of the Q-function occurs, we have a complicated evolution of the field. In this case the field is no longer in a pure state at the time when branches in the Q-function occur. In Fig. 6, the Q-function shows a very clear picture of the field dynamics; in Fig. 6(a) the Q-function shows that the initial coherent state at $\lambda t=0$, centered at the point $(-\pi,0)$, splits into two symmetric peaks in phase space located at $(\pi,1)$ and $(-\pi,1)$, respectively, at one-half of the characteristic time T_R, i.e., $\lambda t=5\pi/2$ [see Fig. 6(b)]. It is already well-known that for an initial coherent state the collapse is associated to a split of the Q-function in two branches, and that at half the revival time, when the field becomes very close to a pure state, the two branches are most far apart.[28]

Once the intensity-dependent coupling $f(n)$ is taken into account, the two symmetric peaks in phase space located at $(\pi,0)$ and $(-\pi,0)$, where we have chosen $f(n)=\sqrt{n}$, [see Fig. 6(c)]. However, we see the one-peak structure of the Q-function is recovered at this moment for $f(n)=1/\sqrt{n}$, i.e., we have returned to the case in Fig. 6(a). In Fig. 7, we plot the Q-function of the cavity field with the initial mean photon number $\bar{n}=5$, at $\lambda t=5\pi/2$, and for different values of the field nonlinearity. In Fig. 7(a), we see that for small values of the Kerr-type nonlinear medium the Q-function of the field mode shows asymmetric splitting [see Fig. 7(a)]. One peak is stationary in the given rotating frame, while the other moves clockwise around the origin of the phase space. Further increasing of the Kerr-type nonlinear medium leads to the Q-function splits into four rather than two components, as in the case of the absence of the field nonlinearity [compare Figs. 6(b) and 7(b)]. In Fig. 7(c) we consider the intensity-dependent coupling effect in the presence of the field nonlinearity, we see that the Q-function of the cavity field splits into two peaks which move clockwise and anticlockwise around the origin of the phase space.

We can say that the time scale T_R represents the main characteristic of the dynamics in those particular phase spaces that are not affected by quantum entanglement. For $t>0$ the two peaks split into two sets of counter-rotating peaks during the collapse. At longer times the Q-function is spread out over an angular region in the xy-plane, as shown in Figs. 6–7. If we combine this

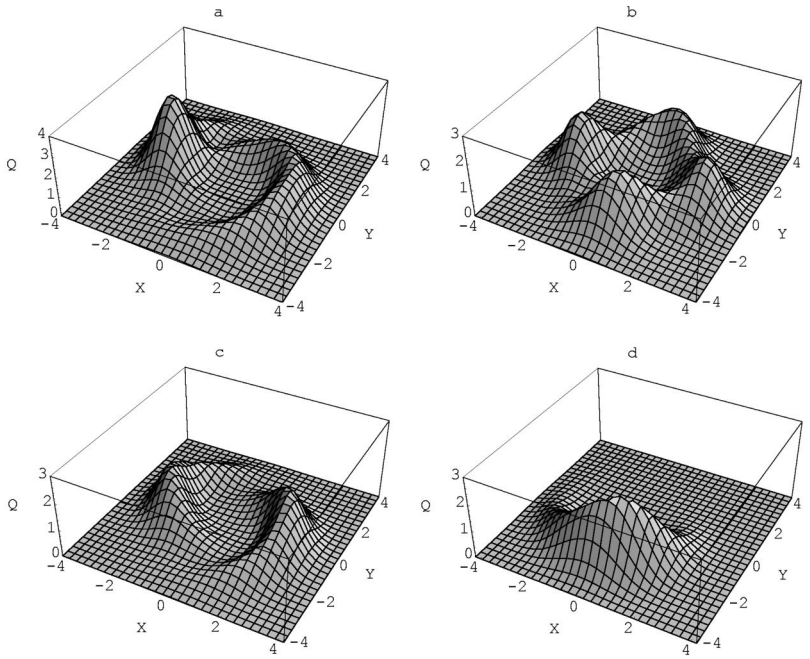

FIG. 7. A plot of Q-function of the cavity field with the initial mean photon number $\bar{n}=5$, at $\lambda t=5\pi/2$, where (a) $\chi/\lambda=0.02$, $f(n)=1$, (b) $\chi/\lambda=0.1$, $f(n)=1$, (c) $\chi/\lambda=0.02$, $f(n)=\sqrt{n}$ and (d) $\chi/\lambda=0.02$, $f(n)=1/\sqrt{n}$.

observation with the fact that the entanglement degree at this moment is almost maximum we can conclude that the cavity field is in a pure state.

V. CONCLUDING REMARKS

Despite the relative simplicity of the generalized JC-model, the full theoretical treatment of its dynamics is a nontrivial problem. In the present work we have attempted to delve into a detailed analysis of the dynamics of the process of entanglement in a two-level system interacting with a coherent state. We have derived a general entanglement degree expression without the diagonal approximation which has been adopted previously in Refs. 7–9. This represents an attempt of establishing a connection between a mixed state of physical systems and the measure of the degree of entanglement due to a quasi-mutual entropy between different subsystems. The entanglement process of the model is very rich and much more can be learned from specific features of the entanglement degree due to the quasi-mutual entropy such as its oscillations (recoherences in time, periodic or not). We have found an intimate connection between these features and the different forms of the nonlinearities of both the field and intensity-dependent coupling. We have shown here by exploring numerically in different parameters of the exactly soluble model that important changes occur in the generalized quasi-mutual entropy, which measures the degree of entanglement. The significant effect of the Stark shift parameter appears when r deviates from unity. An interesting characteristic feature is that the entanglement degree tends to its minimum value for a strong Kerr-type ($\chi \gg \lambda$). In view of the recent advances in single-atom quantum optics, we hope these fully quantum correlated states will be explored experimentally in the near future. Further analysis using the evolution of the field Q-function showed us that for a given field coherent intensity $\bar{n}$, there is an optimum value of the nonlinear parameters for which the entanglement is a minimum.

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Wigner functions for curved spaces. II. On spheres

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(Received 12 November 2002; accepted 10 December 2002)

The form of the Wigner distribution function for Hamiltonian systems in spaces of constant negative curvature (i.e., hyperboloids) proposed in M. A. Alonso, G. S. Pogosyan, and K. B. Wolf, ''Wigner functions for curved spaces. I. On hyperboloids'' [J. Math. Phys. **43**, 5857 (2002)], is extended here to spaces whose curvature is constant and positive, i.e., spheres. An essential part of this construction is the use of the functions of Sherman and Volobuyev, which are an overcomplete set of plane-wave-like solutions of the Laplace–Beltrami equation for this space. Rotations that displace the poles transform these functions with a multiplier factor, and their momentum direction becomes formally complex; the covariance properties of the proposed Wigner function are understood in these terms. As an example for the one-dimensional case, we consider the energy eigenstates of the oscillator on the circle in a Pöschl–Teller potential. The standard theory of quantum oscillators is regained in the contraction limit to the space of zero curvature. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1559644]

I. INTRODUCTION

In the first part of this series[1] we proposed a generic form for the Wigner quasiprobability distribution function defined in terms of the generalized basis of plane waves; this form may be extended in a natural way to curved configuration spaces, provided that an analogous basis of plane-wave-like solutions can be found on those manifolds; the new functions will correspondingly endow their argument and index with the physical meaning of position and momentum. Although one may think to generalize the Wigner function to any manifold, the hyperboloid and the sphere are the two simplest cases to start such a study. In Ref. 1 we considered spaces of constant negative curvature, i.e., the upper sheet of a two-sheeted hyperboloid, where the basic plane waves were the set of Shapiro functions.[2] That Wigner function has the desired marginal projections, and its properties of covariance under rotations and hyperbolic translations were shown to stem from those of the Shapiro functions. The goal of this second part is the study of the Wigner function on spaces of positive constant curvature, i.e., on spheres.

As was the case in Ref. 1, the generalization offered in our approach results from recognizing that the Wigner function on flat phase space $(\mathbf{p},\mathbf{x}) \in \mathfrak{R}^{2D}$,[3] in addition to its usual expression as a single integral, can be written also in the following twofold integral form with a Dirac δ,

$$W_{\mathfrak{R}^D}(f,g|\mathbf{x},\mathbf{p}) := \frac{1}{(2\pi)^D}\int_{\mathfrak{R}^D} d^D\mathbf{z} f(\mathbf{x}-\tfrac{1}{2}\mathbf{z})^* e^{-i\mathbf{p}\cdot\mathbf{z}} g(\mathbf{x}+\tfrac{1}{2}\mathbf{z})$$
$$= \frac{1}{(2\pi)^D}\int_{\mathfrak{R}^D} d^D\mathbf{x}' \int_{\mathfrak{R}^D} d^D\mathbf{x}'' f(\mathbf{x}')^* g(\mathbf{x}'')\,\phi_{\mathbf{p}}(\mathbf{x}')\,\delta^D(\mathbf{x}-\tfrac{1}{2}(\mathbf{x}'+\mathbf{x}''))\,\phi_{\mathbf{p}}(\mathbf{x}'')^*, \tag{1}$$

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where the function $\phi_{\mathbf{p}}(x)$ and its complex conjugate $\phi_{\mathbf{p}}(x)^*$, whose argument and index variables bind the position and momentum variables, are the plane waves

$$\phi_{\mathbf{p}}(\mathbf{x}) := \exp(i\mathbf{p}\cdot\mathbf{x}), \quad -\Delta\phi(\mathbf{x}) = p^2\phi(\mathbf{x}), \tag{2}$$

where $p := |\mathbf{p}|$, and which are solutions of the Helmholtz (Laplace–Beltrami) equation on flat space. Momentum $\mathbf{p}$ has units of inverse length when $\hbar = 1$; in optics, p is the wave number of light.

The form (1) of the Wigner function again suggests its generalization to the sphere $\mathcal{S}^D$ through replacing the integration over flat space ($\int_{\Re^D} d^D\mathbf{x}$) by an integration over the new D-dimensional manifold ($\int_{\mathcal{S}^D} dx$), replacing the plane waves $\phi_{\mathbf{p}}(\mathbf{x})$ of flat space by *plane-wave-like* solutions of the Laplace–Beltrami equation on that manifold, and replacing the Dirac delta $\delta^D(\mathbf{x} - \frac{1}{2}(\mathbf{x}' + \mathbf{x}''))$ in (1) by an appropriate distribution on the sphere. The new reproducing kernel should guarantee that, if $\mathbf{x}'$ and $\mathbf{x}''$ are on the manifold, then $\mathbf{x}$ should lie halfway along a geodesic.

In flat space, the transformation between the position and momentum representations arises from the basis of plane wave functions (2) that defines the Fourier transform; on the hyperboloid, it is a Mellin transform. Here, this transform will relate wave functions on the sphere with functions over a momentum space, through a summation over the discrete values that the wave number can have on the sphere, and an integral over the directions of the plane waves. Both the hyperboloid and the sphere are characterized by the radius R (curvature $\pm 1/R$), which will serve as the contraction parameter whose limit $R \to \infty$ represents flat space, and where the traditional phase space and Wigner function are recovered.

Let us stress that, unlike previous studies where the sphere is the symplectic manifold on which the Wigner function is drawn, as in the cases for spin[4] and finite systems,[5,6] or of the Wigner function defined on the coadjoint orbits of a Lie algebra[7] which may have a similar or more complicated topology, this Wigner function describes wave fields whose configuration space is the sphere. Also, we distinguish the present case from other previous definitions describing Helmholtz wave fields in flat free space, where momentum is constrained to the so-called Descartes sphere of ray directions.[8]

In Sec. II we concentrate the necessary definitions and relevant properties of these plane-wave-like solutions, and our understanding of the momentum space conjugate to the sphere. In Sec. III we develop the new Wigner function on the direct product phase space, making explicit its covariance properties and its contraction limit. As in Ref. 1, we illustrate some of these results in Sec. IV with an example: the harmonic oscillator analog on the circle ($D = 1$) that corresponds to the bounded-interval Pöschl–Teller potential. In Sec. V we recapitulate our results in the context of other approaches in the literature.

II. SPHERICAL SPACES AND MOMENTUM

We follow the plan of Ref. 1 to present the Laplace–Beltrami operator on the curved space—here a D-dimensional spherical manifold—and its corresponding basis of plane-wave functions.[9,10] This is the basis we choose to define the momentum manifold that will appear in the definition of the Wigner function in the next section.

A. Laplace–Beltrami operator on the sphere

Consider the D-dimensional manifold of a sphere $\mathcal{S}^D$ of radius $R > 0$, embedded in the ambient space $x \in \Re^{D+1}$,

$$|x|^2 := x_0^2 + \mathbf{x}^2 = R^2, \quad \mathbf{x}^2 := x_1^2 + x_2^2 + \cdots + x_D^2. \tag{3}$$

The isometry group of the manifold of $\mathbf{x}$'s is the real orthogonal group in $D+1$ dimensions; for simplicity we disregard reflections and use the proper rotation group $\mathrm{SO}(D+1)$. This will replace the Euclidean isometry $\mathrm{ISO}(D)_+$ of flat configuration space. The standard realization of the Lie algebra $\mathrm{so}(D+1)$ by generators of rotations of the ambient $(D+1)$-dimensional space (3), is

$$M_{j,k} := x_j \partial_{x_k} - x_k \partial_{x_j}, \quad j,k = 0,1,2,\ldots,D. \tag{4}$$

The Laplace–Beltrami operator on $\mathcal{S}^D_+$ is (R^{-2} times) the second-order invariant Casimir operator, namely,

$$\Delta_{\mathrm{LB}} := \frac{1}{R^2}\mathcal{C} = \frac{1}{R^2} \sum_{0 \leqslant j < k \leqslant D} M^2_{j,k}. \tag{5}$$

The spectrum of the Casimir operator of so($D+1$) is well known to be the lower bound, discrete but infinite set of values

$$\Sigma(\mathcal{C}) = \{\ell(\ell+D-1) \,|\, \ell \in \mathcal{Z}^+_0\}, \quad \mathcal{Z}^+_0 := \{0,1,2,\ldots\}. \tag{6}$$

Corresponding to each value of ℓ there is a unitary irreducible representation belonging to the most degenerate (also called most symmetric) series, which is of finite dimension [$2\ell+1$ in so(3) for $D=2$]. The free wave functions on the sphere are the solutions to the Laplace–Beltrami equation characterized by those eigenvalues (6), that we choose to write as

$$\Delta_{\mathrm{LB}} f(\mathbf{x}) = -\frac{\ell(\ell+D-1)}{R^2} f(\mathbf{x}) = -\left[p^2 - \left(\frac{D-1}{2R}\right)^2\right] f(\mathbf{x}), \tag{7}$$

$$p := [\ell + \tfrac{1}{2}(D-1)]/R, \quad \ell = -\tfrac{1}{2}(D-1) + pR \in \mathcal{Z}^+_0. \tag{8}$$

B. Sherman–Volobuyev functions on the sphere

In Ref. 1 we used the Shapiro functions, introduced by Gel'fand, Graev, and Shapiro in Ref. 2 as Fourier-type plane waves on a D-dimensional space of negative curvature (the upper sheet of the hyperboloid $\mathcal{H}^D_+$). Close analogs to these functions on the (compact) space of positive curvature—the sphere $\mathcal{S}^D \subset \Re^{D+1}$, were given by Sherman in Ref. 9 and were independently used by Volobuyev in Ref. 10, who wrote his work in the context of a phase space model where momentum space is the hyperboloid of Kadyshevsky and Mir–Kasimov,[11] and translated this to a spherical case with the Laplace–Beltrami equation on this manifold. In contrast to the denumerable basis of spherical harmonics, which are orthonormal and complete on $\mathcal{S}^D$, the generalized basis of Sherman–Volobuyev functions (as is the case with coherent states on flat space) are neither. Thus, this basis must be complemented by a distinct *dual* basis. In the following, we keep the notation in direct correspondence with that used in Ref. 1.

By vertical projection, the upper and lower hemispheres of a sphere $\mathcal{S}^D \subset \Re^{D+1}$ map on the same open equatorial disk $\mathcal{D}^D \subset \Re^D$ (and the equator on its common closure—a lower-dimensional $\mathcal{S}^{D-1}$ manifold). For convenience, functions $f(x)$ on the sphere $x \in \mathcal{S}^D$, $|x|^2 = R^2$, will be sometimes written as functions on $[\{-1,1\} \otimes \mathcal{D}^D] \oplus \mathcal{S}^{D-1}$ with colatitude angle χ as

$$f(x) \equiv f(x_0, \mathbf{x}) \equiv f_\sigma(\mathbf{x}),$$

$$x_0 = \sigma\sqrt{R^2 - \mathbf{x}^2} = R\cos\chi, \quad \sigma \in \{-1,1\}, \quad 0 \leqslant \chi < \pi, \quad \text{or} \quad \sigma = 0, \ \chi = \frac{1}{2}\pi, \tag{9}$$

$$\mathbf{x} = R\boldsymbol{\xi}\sin\chi \in \mathcal{D}^D \subset \Re^D, \quad \boldsymbol{\xi} \in \mathcal{S}^{D-1}.$$

The $\sigma = 0$ submanifold is the equator of the sphere, but its explicit inclusion is not crucial to our work. Integration over the sphere will be written as

$$\int_{\mathcal{S}^D} dx\, f(x) := R \sum_{\sigma=-1,+1} \int_{\mathcal{D}^D} \frac{d\mathbf{x}}{\sqrt{R^2 - \mathbf{x}^2}} f_\sigma(\mathbf{x}), \tag{10}$$

and the $\sigma=0$ submanifold will be normally ignored.

The Sherman–Volobuyev functions and their duals are complex functions on the sphere that are solutions to the Laplace–Beltrami equation (7); they are classified according to (6) by the index $\ell \in \mathcal{Z}_0^+$ of completely symmetric representations in SO(D), or equivalently, by the discrete *wave number* p in (7), whose values are spaced by $1/R$. The functions in the Sherman–Volobuyev generalized basis of plane waves are characterized by a real *momentum* vector

$$\mathbf{p} := p\mathbf{n}, \quad p = \frac{1}{R}[\tfrac{1}{2}(D-1)+\ell], \quad \ell \in \mathcal{Z}_0^+, \quad \mathbf{n} \in \mathcal{S}^{D-1}. \tag{11}$$

which has the direction indicated by the unit vector on the sphere in the equatorial subspace. Using the relations (8) between the representation index ℓ and the absolute value of the momentum vector, $p=|\mathbf{p}|>0$ (for $D>1$), these functions and their duals are

$$\Phi_{\mathbf{p}}^{(D)}(x) := \left(\frac{x_0 + i\mathbf{n}\cdot\mathbf{x}}{R}\right)^{\ell} = (\cos\chi + i\mathbf{n}\cdot\boldsymbol{\xi}\sin\chi)^{\ell} = \Phi_{p(-\mathbf{n})}^{(D)}(x)^*, \tag{12}$$

$$\begin{aligned}\overline{\Phi}_{\mathbf{p}}^{(D)}(x) &:= (\operatorname{sign}\mathbf{n}\cdot\mathbf{x})^{D-1}\left(\frac{x_0 + i\mathbf{n}\cdot\mathbf{x}}{R}\right)^{1-D-\ell} \\ &= (\operatorname{sign}\mathbf{n}\cdot\mathbf{x})^{D-1}(\cos\chi + i\mathbf{n}\cdot\mathbf{x}\sin\chi)^{1-D-\ell} \\ &= (\operatorname{sign}\mathbf{n}\cdot\mathbf{x})^{D-1}/\Phi_{((D-1)/R+p)\mathbf{n}}^{(D)}(x) = \overline{\Phi}_{p(-\mathbf{n})}^{(D)}(x)^*. \end{aligned} \tag{13}$$

In Fig. 1 we show Sherman–Volobuyev functions for the case $D=2$, which can be readily plotted on the sphere $\mathcal{S}^2$. The functions (12) can be equivalently characterized as the highest-weight solid $\mathcal{S}^D$-hyperspherical harmonics $\mathcal{Y}_{\ell,\ldots,\ell}(x) \sim (x_1+ix_2)^{\ell}$ (which are solutions of the Laplace equation in the ambient space), rotated so as to bring the x_1-x_2 plane to the plane x_0-$\mathbf{n}$, for each equatorial direction $\mathbf{n} \in \mathcal{S}^{D-1}$. Their dual functions (13) are the second solutions of the Laplace equation, which are obtained by replacing $\ell \to 1-D-\ell$, and formally correspond to the same eigenvalues (6) of the Casimir operator on the sphere; they are singular on the $\mathcal{S}^{D-2}$ submanifold orthogonal to the x_0-$\mathbf{n}$ plane. In the $D=2$ case, these are the two points at right angles to the wavetrain.

C. Properties and limits

The Sherman–Volobuyev functions satisfy the following completeness and orthogonality relations:

$$\frac{1}{(2\pi)^D}\sum_{\ell=0}^{\infty} N^{(D)}(p)\int_{\mathcal{S}^{D-1}} d\mathbf{n}\,\Phi_{p\mathbf{n}}^{(D)}(x)\overline{\Phi}_{p\mathbf{n}}^{(D)}(x') = \delta_{\mathcal{S}^D}(x,x'), \tag{14}$$

$$\frac{1}{(2\pi)^D}\int_{\mathcal{S}^D} dx\,\overline{\Phi}_{p\mathbf{n}}^{(D)}(x)\Phi_{p'\mathbf{n}'}^{(D)}(x) = \frac{1}{N^{(D)}(p)}\,\delta_{p,p'}d_p(\mathbf{n},\mathbf{n}'), \tag{15}$$

where the Plancherel weight of the irreducible representations is

$$\begin{aligned} N^{(D)}(p) &:= pR\,\Gamma(\tfrac{1}{2}(D-1)+pR)/\Gamma(-\tfrac{1}{2}(D-3)+pR) = \tfrac{1}{2}(D-1)!\,\Delta_{\ell}^{(D)}, \\ \Delta_{\ell}^{(D)} &:= \text{dim irrep } \ell \text{ of SO}(D+1). \end{aligned} \tag{16}$$

Writing $|\mathcal{S}^{D-1}| = 2\pi^{\frac{1}{2}D}/\Gamma(\frac{1}{2}D)$ for the surface of the sphere, the $\delta_{\mathcal{S}^D}(x,x')$ on the ambient sphere $\mathcal{S}^D$, and the $d_p(\mathbf{n},\mathbf{n}')$ on the momentum direction spheres $\mathbf{n},\mathbf{n}' \in \mathcal{S}^{D-1}$, are

$$\delta_{\mathcal{S}^D}(x,x') = \delta_{\sigma,\sigma'}\sqrt{R^2-\mathbf{x}^2}\,\delta^D(\mathbf{x}-\mathbf{x}'), \quad \mathbf{x},\mathbf{x}' \in \mathcal{D}^D, \tag{17}$$

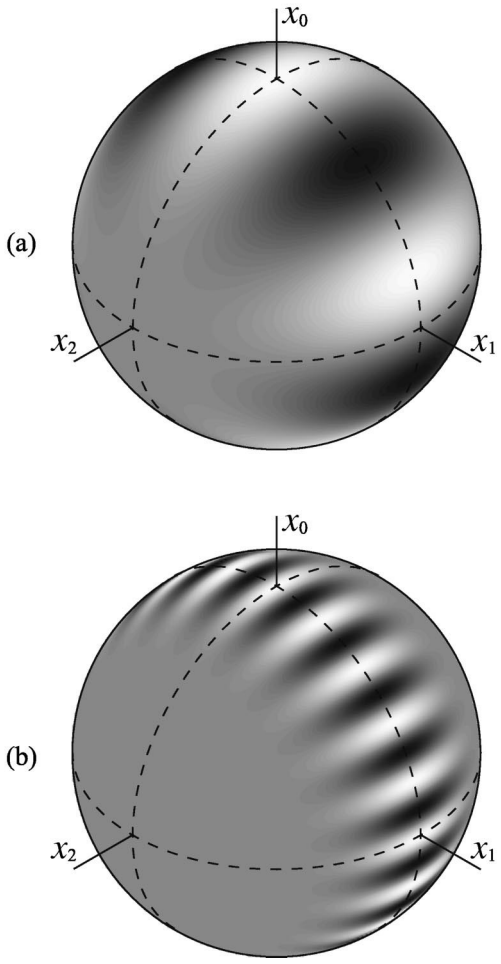

FIG. 1. Sherman–Volobuyev functions for the case $D=2$, $\Phi^{(2)}_{\mathbf{p}}(x)$ on the sphere $x\in\mathcal{S}^2$. The real part is shown for $\ell=5$ and 20, for momenta $\mathbf{p}=p\,\mathbf{n}$ with $p=11/2R$ and $41/2R$, in the same direction $\mathbf{n}(\theta)\in\mathcal{S}^1$ along 1-axis ($\theta=0$). White and black correspond to values $+1$ and -1 of the function; the 2ℓ extrema occur along the meridian at the x_0-x_1 plane; at the two points on the x_2 axis of the sphere the complex functions are zero. The imaginary part is identical to the real part except for a rotation of $\pi/2\ell$ around the x_2 axis, i.e., by a displacement of $\frac{1}{4}$ wavelength.

$$d_p(\mathbf{n},\mathbf{n}')=\frac{1}{|\mathcal{S}^{D-1}|}\left(C_\ell^{D/2}(\mathbf{n}\cdot\mathbf{n}')+C_{\ell-1}^{D/2}(\mathbf{n}\cdot\mathbf{n}')\right),\quad \mathbf{n},\mathbf{n}'\in\mathcal{S}^{D-1},\tag{18}$$

where $\delta^D(\mathbf{x}-\mathbf{x}')$ is the D-dimensional Dirac delta on the disk $\mathcal{D}^D$, and there is the Kronecker delta $\delta_{p,p'}:=\delta_{\ell,\ell'}$ between spheres of discrete radii p and p'. The $C_\ell^{1/2\,D}(\kappa)$ are the Gegenbauer polynomials of degree ℓ in $\kappa=\mathbf{n}\cdot\mathbf{n}'$, i.e., the cosine of the angle between the two momentum vectors, $\mathbf{p}$ and $\mathbf{p}'$. In particular, note that for $\ell=0$, $N^{(D)}=\frac{1}{2}\Gamma(D)$.

As pointed out by Sherman and by Volobuyev,[9,10] the last $d_p(\mathbf{n},\mathbf{n}')$ in (18) is not a true Dirac δ, but a reproducing kernel in the $\Delta_\ell^{(D)}$-dimensional vector space spanned by the functions $\{\Phi^{(D)}_{p\mathbf{n}}(x)\}_{\mathbf{n}\in\mathcal{S}^{D-1}}$ of fixed wave number $p\leftrightarrow\ell$,

$$\int_{\mathcal{S}^{D-1}}d\mathbf{n}'\;d_p(\mathbf{n},\mathbf{n}')\Phi^{(D)}_{p\mathbf{n}'}(x)=\Phi^{(D)}_{p\mathbf{n}}(x),\tag{19}$$

and the same property holds for the duals $\{\overline{\Phi}^{(D)}_{p\mathbf{n}}(x)\}_{\mathbf{n}\in\mathcal{S}^{D-1}}$. In the limit of large wave numbers, $\lim_{pR\to\infty}d_p(\mathbf{n},\mathbf{n}')=\delta_{\mathcal{S}^{D-1}}(\mathbf{n},\mathbf{n}')$.

The Inönu–Wigner contraction limit of the rotation to the Euclidean group $\mathrm{SO}(D+1) \to \mathrm{ISO}(D)$ is the limit $R\to\infty$ in our expressions for vectors with $x_0 \approx R$, $\mathbf{x}^2 \ll R^2$, and $\mathbf{p}=p\,\mathbf{n}$ as before with discrete values of p separated by a decreasing R^{-1}, i.e.,

$$\lim_{R\to\infty} \Phi^{(D)}_{\mathbf{p}}(x) = \lim_{R\to\infty} \left(\frac{x_0 + i\mathbf{n}\cdot\mathbf{x}}{R} \right)^{-1/2(D-1)+pR} \approx \lim_{R\to\infty} \left(1 + i\frac{\mathbf{n}\cdot\mathbf{x}}{R} \right)^{pR} = \exp(i\mathbf{x}\cdot\mathbf{p}), \tag{20}$$

$$\lim_{R\to\infty} \overline{\Phi}^{(D)}_{\mathbf{p}}(x) = \exp(-i\,\mathbf{x}\cdot\mathbf{p}). \tag{21}$$

Correspondingly, $\lim_{R\to\infty} N^{(D)}(p)=1$ and $\delta^D(x,x') \to \delta^D(\mathbf{x}-\mathbf{x}')$. Ordinary Fourier analysis and synthesis are thus recovered in the contraction limit; this justifies the name of plane waves for the Sherman–Volobuyev functions, as well as our expectation that they will provide the bridge between the position on the sphere and a physically appropriate momentum space.

D. Momentum space for the sphere

The basis of Sherman–Volobuyev functions is nonorthonormal and overcomplete, as can be seen from (15), (18), and (19), but allows the synthesis of functions $f(x)$ on the sphere $x\in\mathcal{S}^D$, with coefficients in a space that we recognize as the *momentum* manifold, $\mathbf{p}=p\mathbf{n}\in\mathcal{Z}_0^+\otimes\mathcal{S}^{D-1}$ of the D-dimensional system on configuration space $x\in\mathcal{S}^D$.

The Sherman–Volobuyev synthesis of a complex function $f(x)$ over the sphere $x\in\mathcal{S}^D$, involves a sum of integrals over spheres; the sum ranges over the radii $p=\frac{1}{2}(D-1)/R, \frac{1}{2}(D+1)/R, \frac{1}{2}(D+3)/R,\ldots$ (corresponding to $\ell=0,1,2,\ldots$), and the integrals over $\mathbf{n}\in\mathcal{S}^{D-1}$, with both the functions and their duals, as follows:[9,10]

$$f(x) = \frac{1}{(2\pi)^{D/2}} \sum_{\ell=0}^{\infty} N^{(D)}(p) \int_{\mathcal{S}^{D-1}} d\mathbf{n}\, \Phi^{(D)}_{p\mathbf{n}}(x) \tilde{f}(p\mathbf{n}), \tag{22}$$

$$f(x)^* = \frac{1}{(2\pi)^{D/2}} \sum_{\ell=0}^{\infty} N^{(D)}(p) \int_{\mathcal{S}^{D-1}} d\mathbf{n}\, \overline{\Phi}^{(D)}_{p\mathbf{n}}(x) \tilde{\bar{f}}(p\mathbf{n}). \tag{23}$$

The coefficients are found by

$$\tilde{f}(p\mathbf{n}) = \frac{1}{(2\pi)^{D/2}} \int_{\mathcal{S}^D} dx\, \overline{\Phi}^{(D)}_{p\mathbf{n}}(x)\, f(x), \tag{24}$$

$$\tilde{\bar{f}}(p\mathbf{n}) = \frac{1}{(2\pi)^{D/2}} \int_{\mathcal{S}^D} dx\, \Phi^{(D)}_{p\mathbf{n}}(x)\, f(x)^*. \tag{25}$$

This means that there are *two* (rather than a single) mutually dual momentum representations for any one wave function on the sphere. That both should be considered on equal footing is indicated by the Parseval relation,

$$(f,g)_{\mathcal{S}^D} := \int_{\mathcal{S}^D} dx\, f(x)^* g(x) \tag{26}$$

$$= \sum_{\ell=0}^{\infty} N^{(D)}(p) \int_{\mathcal{S}^{D-1}} d\mathbf{n}\, \tilde{\bar{f}}(p\mathbf{n})\, \tilde{g}(p\mathbf{n}) \tag{27}$$

$$= \sum_{\ell=0}^{\infty} N^{(D)}(p) \int_{\mathcal{S}^{D-1}} d\mathbf{n}\, \tilde{f}(p\mathbf{n})^* \tilde{g}(p\mathbf{n})^*. \tag{28}$$

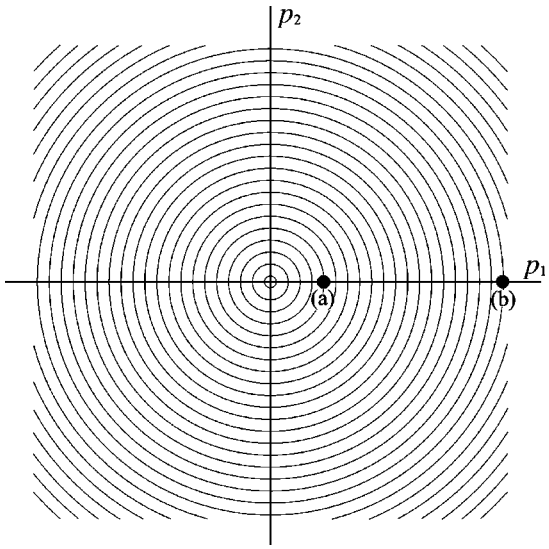

FIG. 2. Momentum space and the Sherman–Volobuyev functions $\Phi^{(2)}_{\mathbf{p}}(x)$. The momentum space $\mathbf{p}=p\,\mathbf{n}$ is composed by concentric circles $\mathbf{n}(\theta)\in\mathcal{S}^1$, of radii $p\in\{\frac{1}{2},\frac{3}{2},\ldots\}/R$ (for $\ell\in\{0,1,\ldots\}$). The two functions of Fig. 1 are shown for $\ell=5$ and 20, with direction $\mathbf{n}$ along the 1-axis.

It will help intuition to consider again the case $D=2$ for wave fields on the ordinary two-sphere $\mathcal{S}^2$, where $x_0^2+x_1^2+x_2^2=R^2$. While in Fig. 1 we show the complex Sherman–Volobuyev functions, Figure 2 schematizes their representation in the momentum space $\mathbf{p}=p\mathbf{n}$ of concentric circles with discrete radii $p\leftrightarrow\ell$ and direction $\mathbf{n}\in\mathcal{S}^1$. The length of the momentum vector $p=|\mathbf{p}|$ is associated to the number ℓ of wavelengths around the meridian indicated by $\mathbf{n}$, which is normal to all wave fronts. There is an evident covariance between the SO(2) rotations of the circles of momentum and rotations of the configuration-space sphere around its x_0 axis.

E. Covariance properties

Because the basis of Sherman–Volobuyev functions (12) and their duals (13) depends on the scalar product $\mathbf{n}\cdot\mathbf{x}$, they will be covariant in $\mathbf{x}$ and $\mathbf{n}$ under rotations $\mathbf{R}\in\mathrm{SO}(D)$ of the sphere $\mathcal{S}^D$ within its equatorial disk $\mathbf{x}\in\mathcal{D}^D$, *viz.*,

$$T(\mathbf{R}):\Phi^{(D)}_{p\mathbf{n}}(x_0,\mathbf{x}):=\Phi^{(D)}_{p\mathbf{n}}(x_0,\mathbf{R}^{-1}\mathbf{x})=\Phi^{(D)}_{p\mathbf{Rn}}(x_0,\mathbf{x}), \tag{29}$$

and similarly for the dual $\overline{\Phi}^{(D)}_{p\mathbf{n}}(x_0,\mathbf{x})$'s.

We now analyze further the transformation properties of the Sherman–Volobuyev plane-wave-like basis under $\mathrm{SO}(D+1)$ rotations *out of* the equatorial disk $\mathbf{x}\in\mathcal{D}^D$ (i.e., mixing x_0 and components of $\mathbf{x}$), and the covariant transformations of the sphere of momentum directions $\mathbf{n}\in\mathcal{S}^{D-1}$. Under these transformations, the direction vector $\mathbf{n}$ of momentum may become complex, as we now show. Indeed, the functions (12) can be written as the power ℓ of a scalar product between one complex and one real $(D+1)$-vectors (Refs. 9 and 10) also indicated by $\cdot$:

$$x_0+i\,\mathbf{n}\cdot\mathbf{x}=\begin{pmatrix}1\\ i\mathbf{n}\end{pmatrix}\cdot\begin{pmatrix}x_0\\ \mathbf{x}\end{pmatrix}=:\nu\cdot x,\quad \mathbf{n}\cdot\mathbf{n}=1,\quad \nu\cdot\nu=0, \tag{30}$$

To find the transformation of the Sherman–Volobuyev function set under rotations of the ambient-space vectors $x\in\mathcal{S}^D$ in the plane of x_0 and a unit vector $\mathbf{m}\in\mathcal{S}^{D-1}$ in the equatorial subspace of the sphere, we decompose the position vectors as $\mathbf{x}=\mathbf{x}_{\|\mathbf{m}}+\mathbf{x}_{\perp\mathbf{m}}$, into their components parallel and perpendicular to the direction of $\mathbf{m}$. The latter are invariant under all rotations

of the x_0-$\mathbf{m}$ plane, that we indicate by $\mathbf{R}_\mathbf{m} \in \mathrm{SO}(D+1)$. Then we can write $x=(x_0,\mathbf{x}_{\parallel\mathbf{m}},\mathbf{x}_{\perp\mathbf{m}})^{\mathsf{T}}$ and $\mathbf{n}=(\mathbf{n}_{\parallel\mathbf{m}},\mathbf{n}_{\perp\mathbf{m}})^{\mathsf{T}}$, so the action of a rotation by $\alpha \in \mathcal{S}^1$ on ambient space will be

$$T(\mathbf{R}_\mathbf{m}(\alpha)):\begin{pmatrix} x_0 \\ \mathbf{x}_{\parallel\mathbf{m}} \\ \mathbf{x}_{\perp\mathbf{m}} \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ \mathbf{x}_{\parallel\mathbf{m}} \\ \mathbf{x}_{\perp\mathbf{m}} \end{pmatrix}. \tag{31}$$

The corresponding transformation of the momentum vector $\mathbf{p}=p\mathbf{n}$ will leave the irreducible representation index p invariant, and the action on the unit direction vectors $\mathbf{n}$ which characterize the Sherman–Volobuyev functions can be found from (30), through the $(D+1)$-dimensional inner product form $\nu\cdot x' = \nu'\cdot x$. This yields the transformation of the complex vector $\nu=(1,i\mathbf{n})^{\mathsf{T}}$ to

$$\nu'(\alpha) = \begin{pmatrix} 1 \\ i\mathbf{n}_{\parallel\mathbf{m}} \\ i\mathbf{n}_{\perp\mathbf{m}} \end{pmatrix} \cdot \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mu(\mathbf{m},\alpha;\mathbf{n}) \begin{pmatrix} 1 \\ i\mathbf{n}'_{\parallel\mathbf{m}} \\ i\mathbf{n}'_{\perp\mathbf{m}} \end{pmatrix}, \tag{32}$$

with a *multiplier* function (which is independent of x),

$$\mu(\mathbf{m},\alpha;\mathbf{n}) := \cos\alpha + i\mathbf{m}\cdot\mathbf{n}\sin\alpha \tag{33}$$

and a new direction vector

$$\mathbf{n}' = \begin{pmatrix} \mathbf{n}'_{\parallel\mathbf{m}} \\ \mathbf{n}'_{\perp\mathbf{m}} \end{pmatrix} = \frac{1}{\mu(\mathbf{m},\alpha;\mathbf{n})} \begin{pmatrix} (\mathbf{m}\cdot\mathbf{n}\cos\alpha + i\sin\alpha)\mathbf{m} \\ \mathbf{n}_{\perp\mathbf{m}} \end{pmatrix}, \tag{34}$$

of real norm $\mathbf{n}'\cdot\mathbf{n}'=1$.

The action of $\mathbf{R}_\mathbf{m} \in \mathrm{SO}(D+1)$ on the Sherman–Volobuyev functions of fixed wave number $p \leftrightarrow \ell$ [recall (11)], and their duals is therefore

$$T(\mathbf{R}_\mathbf{m}(\alpha)):\Phi^{(D)}_{p\mathbf{n}}(x) = \mu(\mathbf{m},\alpha;\mathbf{n})^{\ell}\Phi^{(D)}_{p\mathbf{n}'}(x), \tag{35}$$

$$T(\mathbf{R}_\mathbf{m}(\alpha)):\overline{\Phi}^{(D)}_{p\mathbf{n}}(x) = \mu(\mathbf{m},\alpha;\mathbf{n})^{1-D-\ell}\overline{\Phi}^{(D)}_{p\mathbf{n}'}(x). \tag{36}$$

The transformations that rotate out of the equatorial subspace thus produce ''complex momentum direction vectors.'' We use quotes around this phrase because the Sherman–Volobuyev functions are already an overcomplete set, and those whose $\mathbf{n}$'s are complex are in any case expressible in terms of the real-$\mathbf{n}$ set, as we shall note below. But formally, the complexification of the direction sphere $\mathbf{n}$ can be a useful tool for intuition. When we separate the real and imaginary parts of $\mathbf{n}'(\alpha)=\mathbf{r}'(\alpha)+i\mathbf{s}'(\alpha)$, we see that

$$\begin{pmatrix} \mathbf{r}'_{\parallel\mathbf{m}} \\ \mathbf{r}'_{\perp\mathbf{m}} \end{pmatrix} = \frac{1}{|\mu(\mathbf{m},\alpha;\mathbf{n})|^2} \begin{pmatrix} \mathbf{n}\cdot\mathbf{m}\mathbf{m} \\ \mathbf{n}_{\perp\mathbf{m}}\sin\alpha\cos\alpha \end{pmatrix}, \tag{37}$$

$$\begin{pmatrix} \mathbf{s}'_{\parallel\mathbf{m}} \\ \mathbf{s}'_{\perp\mathbf{m}} \end{pmatrix} = \frac{-1}{|\mu(\mathbf{m},\alpha;\mathbf{n})|^2} \begin{pmatrix} ((\mathbf{m}\cdot\mathbf{n})^2-1)\mathbf{m}\sin\alpha\cos\alpha \\ -\mathbf{n}\cdot\mathbf{m}\mathbf{n}_{\perp\mathbf{m}}\sin\alpha \end{pmatrix}. \tag{38}$$

Here we note that $\mathbf{r}'\cdot\mathbf{s}'=0$ for all α, and this implies $|\mathbf{r}'|^2-|\mathbf{s}'|^2=1$; this is the surface of a hyperboloid, of signature $(+,-)$ in the D real and D imaginary components. This confines $\mathbf{s}$ to an independent $\mathcal{S}^{D-2}$-sphere.

In dimension D, the complex sphere $\mathcal{C}^{D-1}$ is a homogeneous space for the action of $\mathrm{SO}(D)$, which is determined by its natural action on $\mathcal{S}^D$ through (31)–(34). When we shall discuss in Sec. III C the behavior of the Wigner function under translations (i.e., rotations) of space, the transformations of position and of momentum that are correlated by the map (31)–(34) will define the

Sherman–Volobuyev covariance of the proposed Wigner function. The two lowest-dimensional cases will now be examined to show how the above formalism reduces to the analysis of the well-known Fourier series.

F. The cases $D=1$ (circle) and $D=2$ (sphere)

The $D=1$ case of Sherman–Volobuyev functions (39) on the circle $\chi\in\mathcal{S}^1$ may appear trivial, but it is important to note that we recover the Fourier series that we use in the example of Sec. IV. Momentum space is now the set of points $p=\ell n/R$, $\ell\in\mathcal{Z}_0^+$, and $n\in\mathcal{S}^0=\{-1,+1\}$ is a sign. Moreover, the duals are now the complex conjugate functions,

$$\Phi^{(1)}_{\pm\ell/R}(x)=e^{\pm i\ell\chi}=\overline{\Phi}^{(1)}_{\pm\ell/R}(x)^*. \tag{39}$$

The discrete measure over momentum space $N^{(1)}(p)$ in (16) is, in the $D=1$ case,

$$N^{(1)}(\ell\geqslant 1)=1,\quad N^{(1)}(\ell=0)=\tfrac{1}{2}. \tag{40}$$

In particular the two $\ell=0$ functions $\Phi^{(1)}_{\pm 0}(x)=1$ will sum with the factor $\frac{1}{2}$ from (40) to provide a single $e^{i0\chi}=1$ basis element. This is the full Fourier basis $e^{im\chi}$, with $m=n\ell\in\mathcal{Z}$, reproduced with the correct unit normalization coefficients. The multiplier function in (33) is $\mu(\cdot,\alpha;n)=e^{in\alpha}$ [$n=\operatorname{sign} m\in\{-1,+1\}$, cf. (39)]. Under rotations of the χ-circle therefore, the functions $e^{im\chi}$ are multiplied by the correct phase $e^{in\ell\alpha}$, as follows from (35)–(36). The Sherman–Volobuyev synthesis and analysis (22)–(25) in the $D=1$ case on the circle are given by the well-known Fourier series

$$f(\chi)=\frac{1}{\sqrt{2\pi}}\sum_{m\in\mathcal{Z}}e^{im\chi}\tilde{f}(m),\quad \tilde{f}(m)=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}d\chi\, e^{-im\chi}f(\chi). \tag{41}$$

For $D\geqslant 2$, the Sherman–Volobuyev basis functions are an overcomplete set. This overcompleteness is transparent in the case $D=2$ of the sphere $\mathcal{S}^2$, where the momentum direction $\mathbf{n}(\theta)$ is parametrized around the circle $\theta\in\mathcal{S}^1$, and $\mathbf{n}(\theta)\cdot\mathbf{n}(\theta')=\cos(\theta-\theta')$—see Fig. 2. For fixed $p\leftrightarrow\ell$, the dimension of the space of functions $f_{(p)}(\theta)$ is $\Delta^{(2)}_\ell=2\ell+1$, where a better known, orthonormal and complete basis is that of solid spherical harmonics $\{\mathcal{Y}_{\ell,m}(x)\}_{m=-\ell}^{\ell}$. In other words, although the momentum circles in Fig. 2 appear continuous, only $2\ell+1$ points on each circle correspond to independent functions. On these circles, the Gegenbauer polynomials in (18) reduce to Chebyshev polynomials of the second kind, $C^1_\ell(\kappa)=U_\ell(\kappa)=\sin[(\ell+1)\theta]/\sin\theta$, and reproduce the well-known Dirichlet kernel,

$$d_p(\mathbf{n},\mathbf{n}')=\frac{1}{2\pi}\sum_{m=-\ell}^{\ell}e^{im(\theta-\theta')}=\frac{\sin[(\ell+\frac{1}{2})(\theta-\theta')]}{2\pi\sin\frac{1}{2}(\theta-\theta')}\xrightarrow[\ell\to\infty]{}\delta(\theta). \tag{42}$$

Since the functions $\Phi^{(2)}_{\mathbf{p}}(x)$ are polynomials of integer degree $\ell=pR-\frac{1}{2}$ in $\mathbf{n}\cdot\mathbf{x}\sim\cos\theta=\frac{1}{2}(e^{i\theta}+e^{-i\theta})$, then any function $f_{(p)}(\theta)$ in this space is fully reproduced by (42), i.e.,

$$\int_{\mathcal{S}^1}d\theta\, d_p(\mathbf{n}(\theta),\mathbf{n}'(\theta'))f_{(p)}(\theta)=f_{(p)}(\theta'). \tag{43}$$

Also visible in the $D=2$ case of Fig. 1 is the covariance of the Sherman–Volobuyev functions under rotations out of the equatorial plane, Eqs. (31)–(38), leading to complex direction vectors $\mathbf{n}=\mathbf{r}+i\mathbf{s}$. The real part $\mathbf{r}\in\mathfrak{R}^2$ of $\mathbf{n}$ here determines the imaginary part $\mathbf{s}$ up to a sign (the two points of $\mathcal{S}^0\subset\mathfrak{R}$). When $\mathbf{n}=\mathbf{r}$ is real, $|\mathbf{r}|^2=1\Rightarrow\mathbf{s}=\mathbf{0}$. The vector $\mathbf{n}$ is complex when and only when $|\mathbf{r}|^2>1$, and then its imaginary part $\mathbf{s}$ has magnitude $|\mathbf{s}|^2=|\mathbf{r}|^2-1$, and lies at right angles to $\mathbf{r}$.

To examine the multiplier function (33), we consider the Sherman–Volobuyev functions $\Phi^{(2)}_{\mathbf{p}}(x)$ on the sphere $x\in\mathcal{S}^2$ [shown in Fig. 1 and Eq. (12)] whose real momentum direction vector is along the 1-axis, $\mathbf{n}=\binom{1}{0}$. When we rotate by α the x-sphere in the 0-1 plane [Eq. (35) with $\mathbf{m}\|\mathbf{n}$, so $\mathbf{m}\cdot\mathbf{n}=1$], then for p and ℓ related by (8), the multiplier factor is

$$\mu(\mathbf{m},\alpha,\mathbf{m})=e^{i\alpha}, \tag{44}$$

and the transformed Sherman–Volobuyev function will be

$$\mathbf{R}_{\mathbf{m}}(\alpha):\Phi^{(2)}_{p\mathbf{m}}(x)=[(x'_0+ix'_1)/R]^{\ell}=e^{i\ell\alpha}\Phi^{(2)}_{p\mathbf{m}}(x), \tag{45}$$

i.e., they eigenfunctions of rotations in the direction of the momentum $\mathbf{n}=\mathbf{m}$ [cf. the extreme spherical harmonics $\mathcal{Y}_{\ell,\ell}(x)$ under rotations about x_0]. On the other hand, when the rotation is performed in the 0-2 plane, then instead of (45) we use (35), now with $\binom{0}{1}=\mathbf{m}\perp\mathbf{n}=\binom{1}{0}$, so $\mathbf{m}\cdot\mathbf{n}=0$, and the multiplier is

$$\mu(\mathbf{m},\alpha,\perp\mathbf{m})=\cos\alpha. \tag{46}$$

Thus rotated, the Sherman–Volobuyev functions remain plane-wave-like solutions of the Laplace–Beltrami equation,

$$\mathbf{R}_{\mathbf{m}}(\alpha):\Phi^{(2)}_{p(\perp\mathbf{m})}(x)=(x_0\cos\alpha-x_2\sin\alpha+ix_1)^{\ell}=(\cos\alpha)^{\ell}\Phi^{(2)}_{p\mathbf{n}''(\alpha)}(x),\quad \mathbf{n}''(\alpha)=\begin{pmatrix}\sec\alpha\\ i\tan\alpha\end{pmatrix}, \tag{47}$$

whose wave fronts are normal to a maximal circle, which is no longer a sphere meridian, as those in Fig. 1. The real part of $\mathbf{n}''$ points in the same direction as $\mathbf{n}$, but the imaginary part is responsible for displacing the wave train laterally, along the 2-axis. We underline again that when $\mathbf{n}''$ is not real, $\Phi^{(2)}_{p\mathbf{n}''}(x)$ does not belong to the Sherman–Volobuyev function basis [which by itself satisfies (14)–(15)], but to an analytic continuation of their continuous direction label $\mathbf{n}$ to the complex unit circle $\mathcal{C}^1$.

G. Oscillators on the sphere

Free fields on the sphere, whose energy is purely kinetic, are ruled by the Laplace–Beltrami equation (5)–(7). A second energy term is introduced by adding a function $V(\mathbf{x})$ of position,

$$\left(\frac{-1}{2\mu}\Delta_{\mathrm{LB}}+R^2V(\mathbf{x})\right)f(\mathbf{x})=R^2Ef(\mathbf{x}). \tag{48}$$

In Schrödinger quantum mechanics this describes a particle of mass $m=\hbar^2\mu$ in a potential $V(\mathbf{x})$.[12–14] In wave optics, the interpretation of the extra term comes from the refractive index anomaly of the medium $n(\mathbf{x})=\mu-V(\mathbf{x})$, with $\mu\gg V$ and $V^2\approx 0$.

An SO($D-1$)-isotropic harmonic oscillator potential on the sphere $\mathcal{S}^D$, depending only on the colatitude angle $\chi\in[0,\pi]$ of (9), can be generalized in many ways. An especially useful model is, as in the hyperbolic case,[1] the Pöschl–Teller potential in D-dimensional configuration space[13] given by

$$V(\mathbf{x})=\frac{1}{2}\mu\omega^2R^2\frac{|\mathbf{x}|^2}{x_0^2}=\frac{1}{2}\mu\omega^2R^2\tan^2\chi=\frac{1}{2}\mu\omega^2R^2(\sec^2\chi-1). \tag{49}$$

The wave functions of this model are also the Wigner (Clebsch–Gordan) coupling coefficients for the three-dimensional Lorentz algebra so(2,1) between representations belonging to the discrete, lower-bound Bargmann D_k^+ series.[15]

III. WIGNER FUNCTION ON THE SPHERE

Here we construct the Wigner function for the sphere in the same way as for the hyperboloid in Ref. 1, namely generalizing the double-integral form in Eq. (1), replacing the plane waves over $\mathfrak{R}^D$ with the Sherman–Volobuyev functions and their duals over $\mathcal{S}^D$.

A. Definition

With the measure (10) and the functions in (12)–(13), we define the Wigner function on the sphere as

$$W_{\mathcal{S}}(f,g|x,\mathbf{p}) := \frac{1}{(2\pi)^D}\int_{\mathcal{S}^D} d^D x' \int_{\mathcal{S}^D} d^D x''\, f(x')^* \Delta^D(x;x',x'') g(x'') \times \frac{1}{2}[\Phi^{(D)}_{\mathbf{p}}(x')\overline{\Phi}^{(D)}_{\mathbf{p}}(x'') + \overline{\Phi}^{(D)}_{\mathbf{p}}(x')^* \Phi^{(D)}_{\mathbf{p}}(x'')^*]. \tag{50}$$

We now describe each of the elements of this definition.

We denote the position argument $x=(x_0,\mathbf{x})$ of the Wigner function by the ambient vector, with the understanding that it is the position on the sphere; contrary to the hyperbolic case, where the surface can be mapped 1:1 on $\mathbf{x}$, the sign of x_0 distinguishes between the two hemispheres [and we prefer not to write $(\sigma,\mathbf{x})$ as in (9)]. As in Ref. 1, the $\Delta^D(x;x',x'')$ which takes the place of the flat Dirac delta $\delta^D(\mathbf{x}-\frac{1}{2}(\mathbf{x}'+\mathbf{x}''))$ in Eq. (1), should guarantee that x be the midpoint of the shortest *geodesic* between x' and x'', and lie on the sphere $\mathcal{S}^D$ of radius R. To this end, we choose any $(D+1)$-vector $y=(y_0,\mathbf{y})\in\mathcal{S}^D$ which is orthogonal to $x=(x_0,\mathbf{x})\in\mathcal{S}^D$, $x\cdot y=0$. Then, we write

$$\begin{aligned} x' &:= x\cos\tfrac{1}{2}\alpha - y\sin\tfrac{1}{2}\alpha \\ x'' &:= x\cos\tfrac{1}{2}\alpha + y\sin\tfrac{1}{2}\alpha \end{aligned} \quad \Rightarrow x = \frac{x'+x''}{2\cos\frac{1}{2}\alpha}, \tag{51}$$

so $|x|=R=|y|\Leftrightarrow|x'|=R=|x''|$ for all $\alpha\in[0,\pi]$ and any y on the $\mathcal{S}^{D-1}$ sphere orthogonal to x. From (51) it also follows that $x\cdot x'=R^2\cos\frac{1}{2}\alpha=x\cdot x''$ and $x'\cdot x''=R^2\cos\alpha$, so x indeed lies at angles $\frac{1}{2}\alpha$ between x' and x'' on the sphere. When the signs of the 0-components match, the binding Δ in (50) that enforces (51) on the equatorial projection disks $\mathcal{D}^D_{+}$, can be written as

$$\Delta^D(x;x',x'') = \frac{x_0}{R}\,\delta^D\left(\mathbf{x}-\frac{\mathbf{x}'+\mathbf{x}''}{2\cos\frac{1}{2}\alpha}\right). \tag{52}$$

More generally, when we denote by $v_{\perp x}$ the component of $v\in\mathfrak{R}^{D+1}$ which is orthogonal to x, the binding Δ is

$$\Delta^D(x;x',x'') = \delta^D\left(\frac{(x'+x'')_{\perp x}}{2\cos\frac{1}{2}\alpha}\right). \tag{53}$$

This distribution has the properties

$$\Delta^D(x;x',x') = \frac{x_0}{R}\,\delta^D(\mathbf{x}-\mathbf{x}'), \quad \int_{\mathcal{S}^D} d^D x \Delta^D(x;x',x'') = 1. \tag{54}$$

Through complex conjugation, we verify that the Wigner function (50) satisfies the necessary property

$$W_{\mathcal{S}}(f,g|x,\mathbf{p})^* = W_{\mathcal{S}}(g,f|x,\mathbf{p}). \tag{55}$$

This is the reason for the factor $\frac{1}{2}[\Phi_{\mathbf{p}}^{(D)}(x')\,\overline{\Phi}_{\mathbf{p}}^{(D)}(x'')+\overline{\Phi}_{\mathbf{p}}^{(D)}(x')^*\,\Phi_{\mathbf{p}}^{(D)}(x'')^*]$; only this combination turns into itself with x' and x'' exchanged, and has the correct contraction limit detailed in Sec. III D. Equation (55) guarantees that, for $f=g$, the Wigner function is real.

By means of this binding Δ and the change of variables in (51), the $2D$-fold integration in the Wigner function (50) reduces to the D-fold integral form

$$\begin{aligned}W_{\mathcal{S}}(f,g|x,\mathbf{p})=&[1/(2\pi)^D]\int_0^{\pi}(\sin\alpha)^{D-1}\,d\alpha\int_{\mathcal{S}^{D-1}_{\perp x}}d^{D-1}y\\&\times f(x\cos\tfrac{1}{2}\alpha-y\sin\tfrac{1}{2}\alpha)^*g(x\cos\tfrac{1}{2}\alpha+y\sin\tfrac{1}{2}\alpha)\\&\times\tfrac{1}{2}[\Phi_{\mathbf{p}}^{(D)}(x\cos\tfrac{1}{2}\alpha-y\sin\tfrac{1}{2}\alpha)\overline{\Phi}_{\mathbf{p}}^{(D)}(x\cos\tfrac{1}{2}\alpha+y\sin\tfrac{1}{2}\alpha)\\&+\overline{\Phi}_{\mathbf{p}}^{(D)}(x\cos\tfrac{1}{2}\alpha-y\sin\tfrac{1}{2}\alpha)^*\Phi_{\mathbf{p}}^{(D)}(x\cos\tfrac{1}{2}\alpha+y\sin\tfrac{1}{2}\alpha)^*].\end{aligned}\tag{56}$$

B. Marginal projections

The integral of the Wigner function $W_{\mathcal{S}}(f,g|x,\mathbf{p})$ in (50) over momentum space yields the cross-probability distribution over configuration space, and conversely, integration over the sphere yields a function of momentum shown below. The two marginal distributions derive from the orthogonality and completeness relations of the Sherman–Volobuyev basis and its dual, Eqs. (15)–(14) and (54). They are

$$\begin{aligned}M_{\mathcal{S}}(f,g|x)=&\int_{\mathbf{p}\in\Re^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\,W_{\mathcal{S}}(f,g|x,\mathbf{p})\\=&\int_{\mathcal{S}^D}d^Dx'\int_{\mathcal{S}^D}d^Dx''\,f(x')^*g(x'')\Delta^D(x;x',x'')\,\delta^D(x',x'')\\=&\int_{\mathcal{S}^D}d^Dx'\,f(x')^*g(x')\Delta^D(x;x',x')=f(x)^*g(x),\end{aligned}\tag{57}$$

$$\begin{aligned}M_{\mathcal{S}}(f,g|\mathbf{p})=&\int_{\mathcal{S}^D}d^Dx\,W_{\mathcal{S}}(f,g|x,\mathbf{p})\\=&\frac{1}{2(2\pi)^D}\Bigg[\int_{\mathcal{S}^D}d^Dx'\,f(x')^*\Phi_{\mathbf{p}}^{(D)}(x')\int_{\mathcal{S}^D}d^Dx''\,g(x'')\,\overline{\Phi}_{\mathbf{p}}^{(D)}(x'')\\&+\int_{\mathcal{S}^D}d^Dx'\,f(x')^*\overline{\Phi}_{\mathbf{p}}^{(D)}(x')^*\int_{\mathcal{S}^D}d^Dx''g(x'')\Phi_{\mathbf{p}}^{(D)}(x'')^*\Bigg]\\=&\frac{1}{2}[\tilde{\bar{f}}(\mathbf{p})\tilde{g}(\mathbf{p})+\tilde{f}(\mathbf{p})^*\tilde{\bar{g}}(\mathbf{p})^*].\end{aligned}\tag{58}$$

We note that both the momentum representation and its dual appear on equal footing. The Parseval relation (27)–(28) provides the overlap

$$\int_{\mathcal{S}^D}d^Dx\,M_{\mathcal{S}}(f,g|x)=(f,g)_{\mathcal{S}^D}=\int_{\mathbf{p}\in\mathcal{S}^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\,M_{\mathcal{S}}(f,g|\mathbf{p}).\tag{59}$$

C. Covariance under SO($D+1$) rotations

Under rotations $\mathbf{R}\in\mathrm{SO}(D+1)$ of the ambient space around the x_0 axis, the basis of Sherman–Volobuyev functions (12)–(13) on the $\mathcal{S}^D$-sphere transform as given by (29). Since the

integrations and binding Δ in (53) that appear in the definition (50) are invariant [$\Delta^D(\overline{x};\overline{x'},\overline{x''}) = \Delta^D(x;x',x'')$ for $\overline{\mathbf{x}}=\mathbf{R}^{-1}\mathbf{x}$, etc.], it follows that the proposed Wigner function is covariant under SO(D) rotations, fulfilling

$$W_{\mathcal{S}}(T(\mathbf{R}):f,T(\mathbf{R}):g|x,\mathbf{p}) = W_{\mathcal{S}}(f,g|x_0,\mathbf{R}^{-1}\mathbf{x},\mathbf{R}^{-1}\mathbf{p}). \tag{60}$$

But now consider the rotations of the sphere $\mathcal{S}^D$ out of the equatorial $\mathbf{x}\in\Re^D$ subspace, $\mathbf{R}_{\mathbf{m}}(\alpha)\in \mathrm{SO}(D+1)$, as was done in (35)–(47) for the Sherman–Volobuyev functions and their duals of direction $\mathbf{n}$, and $\ell\leftrightarrow p$ characterizing the invariant wave number [SO(D,1) irreducible representation] as given by (8), and $\mathbf{n}'$ by (34). The Wigner function (50) is bilinear in $\Phi^{(D)}_{p\,\mathbf{n}}(x)$ and $\overline{\Phi}^{(D)}_{p\,\mathbf{n}}(x)$, and so it will transform with a multiplier factor that is extracted from the integral, as

$$\begin{aligned} &W_{\mathcal{S}}(T[\mathbf{R}_{\mathbf{m}}(\alpha)]:f,T[\mathbf{R}_{\mathbf{m}}(\alpha)]:g|x,p\mathbf{n}) \\ &\quad = \mathrm{Re}[(\mu(\mathbf{m},\alpha,\mathbf{n}))^{-D+1}]W_{\mathcal{S}}(f,g|\mathbf{R}_{\mathbf{m}}(\alpha)^{-1}:x,p\mathbf{R}_{\mathbf{m}}(\alpha)^{-1}:\mathbf{n}). \end{aligned} \tag{61}$$

We call (61) the Sherman–Volobuyev covariance of Wigner functions on the sphere. This concept is the analog of that introduced for the hyperbolic case in Ref. 1. Since volume elements of the momentum direction sphere $\mathbf{n}\in\mathcal{S}^D$ are not conserved under rotations $\mathbf{R}_{\mathbf{m}}\in\mathrm{SO}(D+1)$, the multiplier for the Wigner function, $\mu(\mathbf{m},\alpha,\mathbf{n})$ in (33), is necessary to offset this change of measure and ensure the total conservation of probability contained in (59). A new feature that appears in the sphere, however, is that an analytic continuation of the momentum direction is implied by this covariance.

D. Contraction limit

When the radius of the sphere grows and the functions $f(x)$ and $g(x)$ in the Wigner function remain significantly different from zero only within a given area around $x=(R,\mathbf{0})$ that becomes increasingly a flat patch, the Wigner function (56) reduces to the standard Wigner function for flat space, Eq. (1). In (56), the integrand will be significant only when $\mathcal{S}^D$-norms of the vectors fulfill

$$|\mathbf{x}\cos\tfrac{1}{2}\alpha \pm \mathbf{y}\sin\tfrac{1}{2}\alpha| \ll R \Rightarrow \begin{cases} |\mathbf{x}|\cos\frac{1}{2}\alpha \ll R & \Rightarrow \sin\chi \ll 1, \\ |\mathbf{y}|\sin\frac{1}{2}\alpha \ll R & \Rightarrow \sin\alpha \ll 1, \end{cases} \tag{62}$$

$$\Rightarrow x\approx R(1,\chi\boldsymbol{\xi})^{\mathrm{T}}, \quad y\approx R(\chi\boldsymbol{\xi}\cdot\boldsymbol{\eta},\boldsymbol{\eta})^{\mathrm{T}}, \tag{63}$$

where $\boldsymbol{\eta}\in\mathcal{S}^{D-1}$ is a unit vector in the direction of $\mathbf{y}$. The limit (20) and the approximations $\sin\alpha\approx\alpha$ and $\cos\frac{1}{2}\alpha\approx\cos\chi\approx 1$, bring the Wigner function (56) to

$$\begin{aligned} W_{\mathcal{S}}(f,g|x,\mathbf{p}) = \frac{R^D}{(2\pi)^D}\int_0^\infty \alpha^{D-1}\,d\alpha \int_{\mathcal{S}^{D-1}} d^{D-1}\boldsymbol{\eta} \\ \times f(x_0,\mathbf{x}-\tfrac{1}{2}R\alpha\boldsymbol{\eta})^*\exp(-iR\alpha\boldsymbol{\eta}\cdot\mathbf{p})g(x_0,\mathbf{x}+\tfrac{1}{2}R\alpha\boldsymbol{\eta}). \end{aligned} \tag{64}$$

Changing variables to $\mathbf{z}=R\alpha\,\boldsymbol{\eta}$ and integrations by $\int_{\Re^D} d^D\mathbf{z} = R^D\int_0^\infty \alpha^{D-1}\,d\alpha\times\int_{\mathcal{S}^{D-1}} d^{D-1}\boldsymbol{\eta}$, completes the proof that (64) reduces to (1) in the limit $R\to\infty$.

IV. PÖSCHL–TELLER OSCILLATOR ON THE CIRCLE

We saw in Eqs. (39)–(41) that in the case $D=1$, the Sherman–Volobuyev basis coincides with the Fourier series basis of complex exponential functions on the circle, and that momentum space is a set of equally spaced points on a line,

$$\Phi^{(1)}_p(x_1) = \exp(i\chi pR), \quad x_1 = R\sin\chi, \quad \chi\in\mathcal{S}^1, \quad p=m/R, \quad m\in\mathcal{Z}. \tag{65}$$

A. Wigner function on the circle

The Wigner function of wave functions on the circle, Eq. (56), has the same structure as the standard flat-space Wigner function (1) except for the integration ranges. The displaced arguments of the two functions f and g in (56), in the form (65) where $x_1 = R\sin\chi$ and $y_1 = R\sin\eta$, are

$$x\cos\tfrac{1}{2}\alpha \pm y\sin\tfrac{1}{2}\alpha = R\begin{pmatrix}\cos(\chi \pm \frac{1}{2}\eta\alpha)\\ \sin(\chi \pm \frac{1}{2}\eta\alpha)\end{pmatrix}, \tag{66}$$

with $\eta\alpha \in (-\pi,\pi)$. The Wigner function (56), indicating $f(R\cos\chi, R\sin\chi) = f(\chi)$ and $p = m/R$, thus becomes

$$W_{\mathcal{S}}(f,g|x,p) = \frac{R}{2\pi}\int_{-\pi}^{\pi} d\alpha\, f\left(\chi - \frac{1}{2}\alpha\right)^* e^{-im\alpha} g\left(\chi + \frac{1}{2}\alpha\right) \tag{67}$$

$$= \frac{1}{2\pi}\sum_{m',m''=-\infty}^{\infty} \tilde{f}(m')^*\,\mathrm{sinc}\left[\frac{1}{2}(m'+m'') - m\right] e^{i(m''-m')\chi}\tilde{g}(m''), \tag{68}$$

where $\mathrm{sinc}\,\nu := \sin(\pi\nu)/\pi\nu$ is $\delta_{\nu,0}$ when ν is integer, and $(-1)^{\nu-1/2}/\pi\nu$ when ν is half-integer; therefore the double sum in (68) cannot be reduced to a single one except when the coefficients $\tilde{f}(m)$ vanish for a given parity of m. Finally, we recall that for $D=1$ the multiplier function (61) for rotations of the circle is unity.

B. Oscillator on the circle

We now consider the oscillator on the circle which obeys the $D=1$ case of the Schrödinger equation (48) with the Pöschl–Teller potential given in Eq. (49), and written

$$V(\chi) = \sqrt{r(r-1)}(\sec^2\chi - 1), \quad r := \tfrac{1}{2} + \tfrac{1}{2}\sqrt{(2\mu\omega R^2)^2 + 1}. \tag{69}$$

This potential exhibits two inpenetrable barriers at $\chi = \pm\frac{1}{2}\pi$ on $\mathcal{S}_1$. We thus expect two independent solutions in the two disconnected open intervals $\chi \in (-\frac{1}{2}\pi, \frac{1}{2}\pi)$ and $\chi \in (\frac{1}{2}\pi, \frac{3}{2}\pi)$.

Changing variables and placing the potential (69) into the Schrödinger equation on the circle (48), one obtains the Pöschl–Teller equation,[16]

$$\frac{d^2\psi}{d\theta^2} + [4\varepsilon - r(r-1)(\sec^2\theta + \csc^2\theta)]\psi = 0, \quad \theta := \tfrac{1}{2}\chi \pm \tfrac{1}{4}\pi \in (0, \tfrac{1}{2}\pi); \quad \varepsilon := 2\mu R^2(E + \tfrac{1}{2}\mu\omega^2 R^2). \tag{70}$$

Writing $\chi^{\pm} = 2\theta \mp \frac{1}{2}\pi \in (-\frac{1}{2}\pi, \frac{1}{2}\pi)$ and $\psi^{\pm}(\chi) = \psi(\chi^{\pm}) = \psi(\theta)$, the solutions to this equation are

$$\psi_n^{r,\pm}(\chi) = 2^{2r}\sqrt{\frac{n!(n+r)}{\pi\Gamma(n+2r)}}\,\Gamma(r)\left(\frac{1}{2}\sin 2\theta\right)^r C_n^r(\cos 2\theta)$$

$$= \Theta(\pm\cos\chi)\sqrt{\frac{n!(n+r)}{2\pi\Gamma(n+2r)}}\,\Gamma(r)|2\cos\chi|^r C_n^r(\sin\chi), \tag{71}$$

where $\Theta(x)$ is the Heaviside function that determines the well in which the particle is confined, so that $\psi_n^{r,-}(\chi) = \psi_n^{r,+}(\chi+\pi)$. In what follows we assume the particle is in $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$ and disregard the index $\pm$. The spectrum of values of ε is quantized in the quadratic series $(n+r)^2$, so the energy values are

$$E_n^r=\frac{(r+n)^2}{2\mu R^2}-\frac{1}{2}\mu\omega^2R^2=\frac{1}{2\mu R^2}\left(n^2+2r\left(n+\frac{1}{2}\right)\right). \tag{72}$$

C. Contractions to the square box and oscillator in flat space

It is interesting to consider two limiting cases of the Pöschl–Teller potential on the two half-circles in Eqs. (71) and (72). The first is the limit of weak potentials $\omega\to 0$ (so $r\to 1$), and the second is the analog of the previous contraction, now from the circle to the line.

In the limit of weak potential barrier, one could *prima facie* expect that the Pöschl–Teller eigenstates (71) may reduce to the free eigenstates (39) on the circle. This is not the case however, as can be seen by setting $r=1$ in Eqs. (71) and using the property[17] that $\cos\chi\, C_n^1(\sin\chi)$ is $\cos[(n+1)\chi]$ for n even, and $\sin[(n+1)\chi]$ for n odd,

$$\psi_n^1(\chi)=\Theta(\cos\chi)\sqrt{\frac{2}{\pi}}\begin{cases}\cos[(n+1)\chi], & n \text{ even},\\ \sin[(n+1)\chi], & n \text{ odd},\end{cases}\qquad E_n^1=\frac{(n+1)^2}{2\mu R^2}. \tag{73}$$

The energies (72) for the limit states form a quadratic sequence characteristic of a square well with impenetrable barriers at $\chi=\pm\pi/2$. This, rather than the free circle, is the limit $r\to 1$ of the Pöschl–Teller potential.

The second limit of interest is the contraction $r\to\infty$ of the Pöschl–Teller potential on the circle to the harmonic oscillator on flat space,

$$r\gg 1\Leftarrow r\sim\mu\omega R^2,$$

$$(1-z^2)^{r/2}\sim\exp(-rz^2/2)\quad \text{for } z^2<1.$$

Then, Eq. (71) becomes

$$\begin{aligned}\psi_n^r(\chi)&=\Theta(\cos\chi)\sqrt{\frac{n!(n+r)\Gamma^2(r)}{2^n\sqrt{\pi}\Gamma(r+\frac{1}{2}n)\Gamma(r+\frac{1}{2}[n+1])}}\,|\cos\chi|^r C_n^r(\sin\chi)\\ &\sim\sqrt{\frac{n!}{\sqrt{2\pi}}}(2r)^{1/4-n/2}e^{-\frac{1}{2}r\sin^2\chi}C_n^r(\sin\chi)\\ &\sim\frac{1}{\sqrt{n!2^n\sqrt{\pi/r}}}e^{-\frac{1}{2}r\sin^2\chi}H_n(\sqrt{r}\sin\chi)\\ &=\frac{\sqrt{R}}{\sqrt{n!\,2^n\sqrt{\pi/\mu\omega}}}e^{-\mu\omega x_1^2/2}H_n(\sqrt{\mu\omega}x_1).\end{aligned} \tag{74}$$

In the last expression we replaced $z=\sin\chi=x_1/R$, and again, these are the energy eigenstates of the harmonic oscillator in flat space. The energies of these limit states, from (72), now exhibit the linear harmonic oscillator spectrum $E_n=\omega(n+\frac{1}{2})$. The $\sqrt{R}$ factor compensates the normalization on x_1.

D. Wave functions in momentum representation

The momentum representation of the wave functions $\psi_n^r(\chi)$ can be found from the Fourier series coefficients $\tilde{\psi}_n^{r,\pm}(m)$ in (41) of the functions $\psi_n^{r,\pm}(\chi)$ in (71). It is convenient to expand the Gegenbauer polynomials as

$$C_n^r(\sin\chi)=\frac{e^{in\pi/2}}{[\Gamma(r)]^2}\sum_{j=0}^{n}(-1)^j\frac{\Gamma(j+r)\Gamma(n-j+r)}{j!(n-j)!}e^{i(2j-n)\chi}. \tag{75}$$

The integral can be then performed[17] and yields the momentum representation of the wave functions of $p=m/R$ in terms of the hypergeometric ${}_3F_2$ function of unit argument, as

$$\begin{aligned}\tilde{\psi}_n^r(m) &:= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\chi\,\psi_n^r(\chi)e^{im\chi}\\ &= \frac{e^{in\pi/2}}{\sqrt{8\pi}}\sqrt{\frac{n+r}{n!\Gamma(n+2r)}}\,\frac{\Gamma(n+r)\Gamma(r+1)}{\Gamma(\frac{1}{2}(r+m+n)+1)\Gamma(\frac{1}{2}(r-m-n)+1)}\\ &\quad\times{}_3F_2\left(\begin{matrix}-n,\ -\frac{1}{2}(r+m+n),\ r\\ -r-n+1,\ \frac{1}{2}(r-m-n)+1\end{matrix}\,\middle|\,1\right).\end{aligned} \tag{76}$$

Because the wave functions $\psi_n^r(\chi)$ vanish on one half-circle, it turns out that it is sufficient to determine the coefficients for m even; in fact, any periodic function $f(\chi)$ vanishing in the interval $(\frac{1}{2}\pi,\frac{3}{2}\pi)$ will have its odd-m coefficients determined by the even-m ones through the relation

$$\tilde{f}(2m+1)=(-1)^m\sum_{k\in\mathcal{Z}}\frac{(-1)^k}{\pi(m-k+\frac{1}{2})}\tilde{f}(2k). \tag{77}$$

E. Wigner function for the Pöschl–Teller states

The Wigner function (50) in the case $D=1$ for two functions f,g on the circle $\chi\in\mathcal{S}_1$ was written in Eqs. (67)–(68). For the energy eigenstates $\psi_n^r(\chi)$ of the Pöschl–Teller potential given in (71), the Wigner functions can be computed numerically; we have not been able to find a closed expression for them. They are plotted in Fig. 3 along with their marginal projections, for $n=0,1,5,10$.

V. CONCLUDING REMARKS

We have defined the analog of the Wigner function of Ref. 1 for the case of a spherical configuration space. We have observed remarkably different properties between the hyperbolic and spherical cases. First, unlike the Shapiro functions of the former, the Sherman–Volobuyev functions of real momentum are an overcomplete set; a dual basis is thus required and this implies the existence of two dual momentum representations. Further, a coordinate translation which displaces the poles causes the momentum of a Sherman–Volobuyev function to become complex. As a consequence, the covariance of the momentum representation(s) as well as the that of Wigner function under this type of translation are meaningful only as an analytic continuation of the momentum direction vector. The appearance of a multiplier is analogous to the hyperbolic case in Ref. 1.

These features derive from the definition of momentum afforded by the Shapiro and the Sherman–Volobuyev plane-wave-like solutions of the Laplace–Beltrami equation on the hyperbolic and spherical manifolds, and are reflected by the Wigner function introduced here. In trying to fit the definition (50) and the corresponding one for the hyperbolic case in Ref. 1, into the existing plethora of Wigner functions defined in Refs. 3–7, 18 and others found in the literature, it seems increasingly clear that the concept of a Wigner function is not unique. Perhaps a working definition of such a class of functions $W(f,g|x,p)$ should include only (cf. Ref. 19) sesquilinearity in the wave fields ($\sim f(x')^*\,g(x'')$), a symmetric correlation between their arguments x',x'' to a point x in the manifold [determined by a Dirac-type $\Delta(x;x',x'')$], and a complete (or overcomplete) basis (or generalized basis) $\{\Phi_p(x)\}$ which will provide p as conjugate coordinate for a momentum manifold to complete phase space. The minimal properties to be expected of such

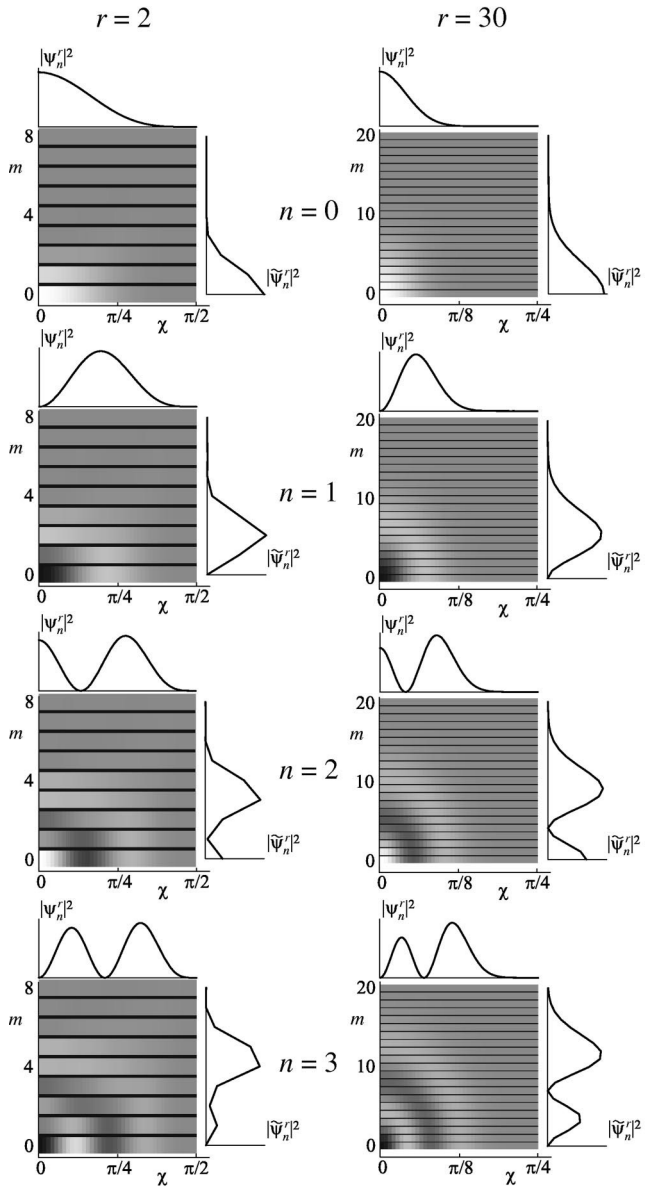

FIG. 3. Wigner functions of the Pöschl–Teller eigenstates $\psi_n^r(\chi)$, on rows of mode $n=0,1,2,3$, for values of the parameter r of the sphere [Eq. (69)], $r=2$ (left) and $r=30$ (right); we show a quadrant of position $x_1=R\sin\chi$, $\chi\in[0,\frac{1}{2}\pi]$ and momentum/angular momentum $p=m/R$ [Eqs. (65)]. The quadrants have reflection symmetry across the axes. White is the maximum, black is the minimum; the shade at the upper right corner corresponds to zero. The marginal projection $|\psi_n^r(\chi)|^2$ is plotted at top, and $|\tilde{\psi}_n^r(m)|^2$ is plotted to the right.

Wigner functions should include the correct marginals, a useful form of covariance between the wave fields and the phase space coordinates, and a natural contraction limit to flat space returning the traditional Wigner function.

To test Wigner function models, it is also important to have a number of basic systems, such as the harmonic or Pöschl–Teller potentials, or Coulomb systems, that should substantiate intuition and the usefulness of the representation. A practical example could be the description of surface waves on sperical bubbles. Let us not forget that the Wigner function does not provide

more information than the wave fields do (in fact, overall phases are lost), but displays this information in a manner that should be more amenable to our understanding.

ACKNOWLEDGMENTS

We thank the support of the Dirección General de Asuntos del Personal Académico, Universidad Nacional Autónoma de México (DGAPA–UNAM) grant IN112300 *Optica Matemática*. M.A.A. and K.B.W. thank Professor Harrison Barrett for the hospitality at the Optical Sciences Center (Tucson, Arizona), and Dana Clarke for introducing to us the objective of an interesting research project. G.S.P. acknowledges the Consejo Nacional de Ciencia y Tecnología (México) for a Cátedra Patrimonial Nivel II, and the Armenian National Science and Engineering Foundation for Grant No. PS124–01.

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On the boson spectrum of the *N* particle Schrödinger operator with periodic binary potential (dense matter)

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(Received 29 July 2002; accepted 21 September 2002)

A new asymptotic method is proposed for calculation of spectral series and corresponding asymptotic eigenfunctions for the spinless N particle Schrödinger equation when N tends to infinitum but the physical parameters and the volume are fixed (dense matter case). © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1523640]

I. INTRODUCTION

Let us consider the N particle Schrödinger spinless equation with binary potential $\alpha V_0(|x-y|r_0^{-1})$ where $x,\ y\in\mathbb{R}^3,\ \alpha$ is its characteristic value, and r_0 is its characteristic radius. As an approximation to the real problems, in the statistical physics is considered[1] the N particle Schrödinger operator with periodic conditions at a period L and with regularized periodic binary potential.

Following that approximation, we obtain in the dimensionless coordinates $x=x'/L$ the spectral problem for the N particle Schrödinger operator on the torus $M=(\mathbb{R}^3/\mathbb{Z}^3)^N$:

$$\sum_{i=1}^{N} -\varepsilon^2\Delta_{x_i}\psi+\sum_{1\leqslant i<j\leqslant N} V(x_i-x_j,\delta)\psi=\lambda\psi, \tag{1}$$

considered at the subspace $L_2^B(M)$ of symmetric functions from $L_2(M)$. Here $x_i=(x_{i1},x_{i2},x_{i3})$;

$$\delta=r_0/L,\quad \varepsilon^2=h^2(2m\alpha)^{-1}/L^2.$$

The regularized binary potential $V(x-y)$ is defined in Ref. 1 as

$$V(x_i-x_j,\delta)=\delta^3\sum_{|k|=0}^{\infty}\nu_k\exp\{i2\pi(k,(x-y))\};$$
$$\nu_k=\int_{\mathbb{R}^3}\exp\{i2\pi\delta(z,k)\}V_0(|z|)dz;\quad \nu_k=\nu_{-k}. \tag{2}$$

It is considered the case when ν_k are not negative, and as a function of index k decrease quickly:

$$0\leqslant\nu_k\leqslant C_m/(1+|k|)^m;\quad m=0,1,\ldots;C_m<\infty. \tag{3}$$

The eigenvalue E of the dimension problem is equal to $\lambda\alpha$ where λ is the eigenvalue of operator (1). It is well known[2] that symmetric operator (1), denoted by H, with $D(H)=C^\infty(M)$, is essentially self-adjoint. In the following by H we also define its closure (which is a self-adjoint operator), and consider the spectral problem

$$H\psi=\lambda\psi. \tag{4}$$

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In that paper the asymptotic method is proposed for the spectral problem (4) in the case when $N\to\infty$ but the physical parameters δ, ε, L are fixed (dense matter).

In the following the abbreviation NSO will be used for the "*N* particle Schrödinger operator."

The presented asymptotical method is based on the approach proposed in Refs. 3–5.

II. ASYMPTOTIC REPRESENTATION FOR THE NSO

It is well known that every periodical symmetrical function in N variables x_i can be expanded into the Fourier series with respect to the symmetrized harmonics $S\exp\{i2\pi((k_1,x_1)+\cdots+(k_N,x_N))\}$, where S is the operator of symmetrization.

Now let us introduce the simplest symmetrized harmonics:

$$u_k=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}\exp\{i2\pi(k,x_j)\};\quad k\in\mathbb{Z}^3. \tag{5}$$

In Sec. IV the next lemma is proved.

Lemma 1: Let us consider infinite algebra A generated by the set of functions (5) for all integer vector-index $k\in\mathbb{Z}^3$. *Then, for all sets of integer vector-index* $k_1,\ldots,k_N$ *the functions* $S\exp\{i2\pi\Sigma_{j=1}^{N}(k_i,x_j)\}$ *belong to the algebra A*.

Consequently, every symmetric and periodic function can be considered as a composite function of infinite number functions u_k, $|k|\geqslant 1$. This situation resembles the functional method in the second quantization problems.

We shall construct below asymptotic solutions to the problem (1) which expand into a converging series with respect to the functions u_k, $\overline{u_k}$, $|k|\geqslant 1$. On such solutions $f(\ldots,u_k,\overline{u_k},\ldots)$ we reduce the equation $H\psi=\lambda\psi$ to such a one that has derivatives only in u_k, $\overline{u_k}$, $|k|\geqslant 1$, and its coefficients also depend only on u_k, $\overline{u_k}$, $|k|\geqslant 1$. Therefore, u_k, $\overline{u_k}$ can be considered as the new variables. As $u_{-k}=\overline{u_k}$, we have to exclude dependent variables. Hence, in the following, we divide the infinite set of indexes $\{1\leqslant|k|\}$ into a sum of two infinite, nonintersecting subsets P, $\overline{P}$ such that every subset does not have two indexes which sum is equal to zero. Evidently, in that case $P=-\overline{P}$ and $P\cup(-P)=\mathbb{Z}^3\setminus 0$.

The eigenfunctions of the operator (1) are approximated by the WKB type functions

$$P(u_{k_1},\ldots,u_{k_l};\overline{u_{k_1}},\ldots,\overline{u_{k_l}})\exp\left\{-\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi(u)\right\},$$
$$\Phi(u)=\sum_{k\in P}|\beta_k|u_k\overline{u_k},\quad \sum_{k\in P}|\beta_k|<\infty, \tag{6}$$

where $P(u_{k_1},\ldots,u_{k_l};\overline{u_{k_1}},\ldots,\overline{u_{k_l}})$ are polynomial functions.

The functions u_k with $N\to\infty$ converge to the normally distributed random variables.[6] That will be used in justification of spectral asymptotics.

In what follows we transform the equations (1) and (4) at the composite functions to the new variables u_k, $\overline{u_k}$, $k\in P$. To that end let us introduce derivatives in variables $u_k=u_k^1+iu_k^2$:

$$\frac{\partial}{\partial u_k}=2^{-1}\left(\frac{\partial}{\partial u_k^1}-\frac{i\partial}{\partial u_k^2}\right);\quad \frac{\partial}{\partial\overline{u_k}}=2^{-1}\left(\frac{\partial}{\partial u_k^1}+\frac{i\partial}{\partial u_k^2}\right).$$

Direct calculations give

$$\sum_{j=1}^{N}\Delta_{x_j}\ f(\ldots,u_k,\overline{u_k}\ldots)=\sum_{m,k\in P}\frac{\partial^2 f}{\partial u_k\partial u_m}\sum_{j=1}^{N}\frac{\partial u_k}{\partial x_j}\frac{\partial u_m}{\partial x_j}+2\sum_{m,k\in P}\frac{\partial^2 f}{\partial u_k\partial\overline{u_m}}\sum_{j=1}^{N}\frac{\partial u_k}{\partial x_j}\frac{\partial\overline{u_m}}{\partial x_j}$$
$$+\sum_{m,k\in P}\frac{\partial^2 f}{\partial\overline{u_k}\partial\overline{u_m}}\sum_{j=1}^{N}\frac{\partial\overline{u_k}}{\partial x_j}\frac{\partial\overline{u_m}}{\partial x_j}+\sum_{k\in P}\frac{\partial f}{\partial u_k}\sum_{j=1}^{N}\Delta_{x_j}u_k$$
$$+\sum_{k\in P}\frac{\partial f}{\partial\overline{u_k}}\sum_{j=1}^{N}\Delta_{x_j}\overline{u_k}. \tag{7}$$

Now it will be shown that all coefficients in (7) depend only on u_k, $\overline{u_k}$. To that end one can easily check that

$$\sum_{j=1}^{N}\frac{\partial u_k}{\partial x_j}\frac{\partial u_m}{\partial x_j}=-(k,m)4\pi^2N^{-1/2}u_{k+m},\quad \sum_{j=1}^{N}\Delta_{x_j}u_k=-k^2 4\pi^2u_k,$$
$$\sum_{j=1}^{N}\frac{\partial u_k}{\partial x_j}\frac{\partial\overline{u_m}}{\partial x_j}=(k,m)4\pi^2N^{-1/2}u_{k-m},\quad u_0=N^{1/2}. \tag{8}$$

Further, let us express the sum of binary potentials through u_k, $k\in P$.

Proposition 2: The sum of binary potentials satisfies the relation

$$\sum_{1\leqslant i<j\leqslant N}V(x_i-x_j,\delta)=\left(\frac{1}{2}\right)\sum_{1\leqslant i,j\leqslant N}V(x_i-x_j,\delta)-\frac{N}{2}\delta^3\sum_{k\in\mathbb{Z}^3}\nu_k=\frac{\delta^3N(N-1)}{2}\nu_0-\delta^3N\sum_{k\in P}\nu_k$$
$$+\delta^3N\sum_{k\in P}\nu_ku_k\overline{u_k}. \tag{9}$$

That formula follows from (3) and (5) as a consequence of relations $Im\,\nu_k=0$, $\nu_k=\nu_{-k}$.

Let us introduce notations:

$$L_1\left(\ldots,\frac{\partial}{\partial u_k},\frac{\partial}{\partial\overline{u}_k},\ldots,u_k,\overline{u_k},\ldots\right)=:-2\varepsilon^2 4\pi^2\sum_{m\in P}m^2\frac{\partial^2}{\partial u_m\partial\overline{u}_m}+N\delta^3\left(\sum_{k\in P}\nu_ku_k\overline{u_k}\right)$$
$$+\varepsilon^2 4\pi^2\sum_{m\in P}m^2\left(u_m\frac{\partial}{\partial u_m}+\overline{u_m}\frac{\partial}{\partial\overline{u}_m}\right); \tag{10}$$

$$L_2\left(\ldots,\frac{\partial}{\partial u_k},\frac{\partial}{\partial\overline{u}_k},\ldots,u_k,\overline{u_k},\ldots\right)=:-2\varepsilon^2 4\pi^2\sum_{k\neq m,k,m\in P}(k,m)u_{k-m}\frac{\partial^2}{\partial u_k\partial\overline{u}_m}$$
$$+\varepsilon^2 4\pi^2\sum_{k,m\in P}(k,m)u_{k+m}\frac{\partial^2}{\partial u_k\partial u_m}$$
$$+\varepsilon^2 4\pi^2\sum_{k,m\in P}(k,m)\overline{u_{k+m}}\frac{\partial^2}{\partial\overline{u}_k\partial\overline{u}_m}. \tag{11}$$

In the following will be used the constant

$$\mu=:\frac{\delta^3N(N-1)}{2}\nu_0-\delta^3N\sum_{k\in P}\nu_k, \tag{12}$$

and notation

$$f(\ldots,u_k,\overline{u_k}\ldots)\circ J=:f\left(\ldots,\frac{1}{\sqrt{N}}\sum_{j=1}^{N}\exp\{i2\pi(k,x_j)\},\frac{1}{\sqrt{N}}\sum_{j=1}^{N}\exp\{-i2\pi(k,x_j)\},\ldots\right). \quad (13)$$

Summing up the above consideration we obtain from formulas (7)–(13) the following lemma.

Lemma 3: The operator (1) at the functions (6) has the form

$$H(f\circ J)=\left\{\left(L_1+\frac{1}{\sqrt{N}}L_2+\mu\right)f\right\}\circ J. \quad (14)$$

We would like to mention that the binary interaction is completely included in the right-hand side of formula (14). The impulse is decomposed into two parts, and the second part, L_2, contains small parameter $1/\sqrt{N}$.

Near the operator L_2 on the right-hand side of (14), there is the small parameter $1/\sqrt{N}$; therefore, it is natural to consider the operator L_1 as the main term in approximation of operator H. Consider the eigenfunction of the operator L_1 and prove that the second term $(1/\sqrt{N})L_2$ is small at that eigenfunction. It means[7] that an asymptotics of some spectral series for the operator (1) is defined by the operator L_1.

We will follow that scheme, and now the operator L_1 will be studied. The operator L_1 is the infinite sum of noninteracting (modified) harmonic oscillators and its spectrum and eigenfunctions can be calculated exactly.

Let

$$L_{1,k}=:\varepsilon^2 4\pi^2k^2\left\{-2\frac{\partial^2}{\partial u_k\partial\overline{u_k}}+u_k\frac{\partial}{\partial u_k}+\overline{u_k}\frac{\partial}{\partial\overline{u_k}}\right\}+N\delta^3\nu_k u_k\overline{u_k}. \quad (15)$$

Evidently, at the functions (6) the equality

$$L_1=\sum_{k\in P}L_{1,k} \quad (16)$$

is true. Now let us make more precise the coefficients β_k in the functions (6), such that the $\exp\{-(\sqrt{N\delta^3}/\varepsilon)\Phi\}$ is eigenfunction of the operator L_1.

Proposition 4: Let

$$\beta_k=\frac{\varepsilon}{2\sqrt{N\delta^3}}\left(1-\sqrt{1+\frac{2\nu_k\delta^3N}{4\pi^2\varepsilon^2k^2}}\right). \quad (17)$$

Then

$$0\leqslant-\beta_k\leqslant\frac{\sqrt{\nu_k}}{\pi|k|}, \quad (18)$$

the series $\Phi=:\Sigma_{k\in P}|\beta_k|u_k\overline{u_k}$ *is convergent and the function* $\exp\{-(\sqrt{N\delta^3}/\varepsilon)\Phi\}$ *is an eigenfunction of the operator* L_1.

In the following the values β_k from that proposition will be used. Further, commutation of the operator L_1 with exponential function is considered. Evidently operator L_1 satisfies the commutation relation

$$L_1\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in P}\beta_k u_k\overline{u_k}\right\}\varphi=\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in P}\beta_k u_k\overline{u_k}\right\}\left\{\sum_{k\in P}\widetilde{L_{1,k}}\varphi\right\}, \quad (19)$$

where

$$\widetilde{L_{1,k}}=:4\pi^2k^2\left\{-2\varepsilon^2\frac{\partial^2}{\partial u_k\partial u_k}+\alpha_k u_k\frac{\partial}{\partial u_k}+\alpha_k\overline{u_k}\frac{\partial}{\partial u_k}\right\}-4\pi^2 2\varepsilon\sqrt{N\delta^3}\beta_k k^2,$$
$$\alpha_k=\varepsilon^2\sqrt{1+\frac{2\nu_k\delta^3N}{4\pi^2\varepsilon^2k^2}}. \tag{20}$$

The eigenfuntions of operators $\widetilde{L_{1,k}}$, and hence the eigenfuntions of operator L_1, can be more easily calculated. Let us introduce a pair of integer non-negative indexes n_k^+, n_k^- such that if $n_k^+>0$, then $n_k^-=0$, and, conversely, if $n_k^->0$, then $n_k^+=0$. Define functions $\varphi(n_k^+,n_k^-,d_k)=:u_k^{n_k^+}\overline{u}_k^{n_k^-}(u_k\overline{u}_k)^{d_k}$, $d_k\geqslant 0$, $d_k\in\mathbb{Z}$.

Lemma 5: 1° Let Q be a finite subset of indexes from P and let

$$\psi(\ldots;n_k^+,n_k^-,d_k;\ldots)=:\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in P}\beta_k u_k\overline{u_k}\right\}\prod_{k\in Q}\varphi(n_k^+,n_k^-,d_k), \tag{21}$$

where β_k are defined by the formulas (17). (a) If $d_k=0$ for $k\in Q$, then, for any pair (n_k^+,n_k^-), $k\in Q$, the functions (21) are eigenfuntions of the operator L_1 with eigenvalues

$$\lambda(\ldots,n_k^+,n_k^-,0,\ldots)=-2\varepsilon\sqrt{N\delta^3}\sum_{k\in P}4\pi^2\beta_k k^2+\sum_{m\in Q}(n_m^++n_m^-)4\pi^2\varepsilon^2m^2\sqrt{1+\frac{2\nu_m\delta^3N}{4\pi^2\varepsilon^2m^2}}. \tag{22}$$

(b) If $d_k>0$, the eigenfunctions of the operator L_1 are

$$\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in P}\beta_k u_k\overline{u_k}\right\}\prod_{k\in Q}\left\{\varphi(n_k^+,n_k^-,d_k)+\sum_{l=1}^{d_k}c_{k,l}\varphi(n_k^+,n_k^-,d_k-l)\right\} \tag{23}$$

with some coefficients $c_{k,l}$. The correspondent eigenvalues are

$$\lambda(\ldots,n_k^+,n_k^-,d_k,\ldots)=-2\varepsilon\sqrt{N\delta^3}\sum_{k\in P}\beta_k k^2 4\pi^2+\sum_{m\in Q}(n_m^++n_m^-+2d_m)4\pi^2\varepsilon^2m^2\sqrt{1+\frac{2\nu_m\delta^3N}{4\pi^2\varepsilon^2m^2}}. \tag{24}$$

2° (a) The operator $\widetilde{L_{1,k}}$ is symmetric in the space $L_2(R,\rho d\xi_k d\eta_k)$; $u_k=:\xi_k+i\eta_k$; $\rho=:\exp\{-(\alpha_k/\varepsilon^2)u_k\overline{u_k}\}$. (b) The operators of creation and annihilation,

$$a_\xi^+=\frac{\varepsilon}{\sqrt{2\alpha_k}}\left(-\frac{\partial}{\partial\xi_k}+2\frac{\alpha_k}{\varepsilon^2}\xi_k\right),$$
$$a_\xi^-=\frac{\varepsilon}{\sqrt{2\alpha_k}}\frac{\partial}{\partial\xi_k},\quad [a_\xi^-,a_\xi^+]=1, \tag{25}$$

$$a_\eta^+=\frac{\varepsilon}{\sqrt{2\alpha_k}}\left(-\frac{\partial}{\partial\eta_k}+2\frac{\alpha_k}{\varepsilon^2}\eta_k\right),$$
$$a_\eta^-=\frac{\varepsilon}{\sqrt{2\alpha_k}}\frac{\partial}{\partial\eta_k},\quad [a_\eta^-,a_\eta^+]=1, \tag{26}$$

are formally conjugated in the space $L_2(R,\rho d\xi_k d\eta_k)$. *(c) The operator* $\widetilde{L_{1,k}}$ *can be represented in the form*

$$\widetilde{L_{1,k}}=4\pi^2k^2\alpha_k a_\xi^+ a_\xi^- +4\pi^2k^2\alpha_k a_\eta^+ a_\eta^- -4\pi^2 2\varepsilon\sqrt{N\delta^3}\beta_k k^2. \tag{27}$$

(1) Let us prove at first the statements 2° (b) and 2° (c). Evidently,

$$2\frac{\partial^2}{\partial u_k\partial\overline{u_k}}=\frac{1}{2}\left(\frac{\partial^2}{\partial\xi_k^2}+\frac{\partial^2}{\partial\eta_k^2}\right),$$

$$u_k\frac{\partial}{\partial u_k}+\overline{u_k}\frac{\partial}{\partial\overline{u_k}}=\xi_k\frac{\partial}{\partial\xi_k}+\eta_k\frac{\partial}{\partial\eta_k}.$$

Therefore, the formula (20) can be rewritten as

$$\widetilde{L_{1,k}}=\frac{1}{2}\varepsilon^2 4\pi^2k^2\left(-\frac{\partial}{\partial\xi_k}+2\frac{\alpha_k}{\varepsilon^2}\xi_k\right)\frac{\partial}{\partial\xi_k}+\frac{1}{2}\varepsilon^2 4\pi^2k^2\left(-\frac{\partial}{\partial\eta_k}+2\frac{\alpha_k}{\varepsilon^2}\eta_k\right)\frac{\partial}{\partial\eta_k}$$
$$-4\pi^2 2\varepsilon\sqrt{N\delta^3}\beta_k k^2.$$

Now, the formula (27) follows directly from the definitions (25) and (26) of operators $a_\xi^\pm$, $a_\eta^\pm$. (2) The formula (22) for the operator L_1 spectrum follows directly from the representation (27). The statement 1(a) about the eigenfunctions (21) and (23) of operator L_1 can be checked by direct calculations. (3) The statement 2(a) can be proved integrating by parts. The lemma is proved.

It is useful to find the space where the operator L_1 is symmetric. To that end let us define at topological space with the elements $u=\{u_{k_1},u_{k_2},\ldots;k_i\in P\}$ the finite dimension projection P_n:

$$P_n u=:\{P_n'u_{k_1},P_n'u_{k_2},\ldots,P_n'u_{k_l},\ldots\}, \tag{28}$$

where $P_n'u_k=:0$ if $|k|>n$, and $P_n'u_k=:u_k$ if $|k|\leqslant n$.

At the functions $f(\ldots,u_k,\overline{u_k},\ldots)$ and $g(\ldots,u_k,\overline{u_k},\ldots)$ the scalar product is introduced in Refs. 8 and 9 as

$$\langle f,g\rangle=:\lim_{n\to\infty}(\pi)^{-\sigma(n)}\int_{R^{2\sigma(n)}}\exp\left\{-\sum_{k\in P}P_n'u_k\overline{P_n'u_k}\right\}f(P_nu)\overline{g}(P_nu)$$
$$\times\prod_{k\in P,|k|<n}d\,\mathrm{Re}\,P_n'u_k\,d\,\mathrm{Im}\,P_n'u_k; \tag{29}$$

here the value $\sigma(n)$ is the number of indexes from P which comply with restriction $|k|\leqslant n$.

Evidently, the scalar product (29) is defined on the functions (6).

Lemma 6: 1°. The operator L_1 *is symmetric at the functions (6) with respect to the scalar product (29). 2°. Linear combinations of the functions* $\psi(\ldots;n_k^+,n_k^-,d_k;\ldots)\circ J$ *are dense in the space* $L_2^B(M)$.

1°. Let us fix that $-1+2(\sqrt{N\delta^3}/\varepsilon)\beta_k=-(\alpha_k/\varepsilon^2)$. Hence, at the functions type (6) $f=\exp\{\Sigma_{k\in P}\beta_k u_k\overline{u_k}\}P_f(u)$, $g=\exp\{\Sigma_{k\in P}\beta_k u_k\overline{u_k}\}P_g(u)$, where $P_f(u)$, $P_g(u)$ are polynomials, the next integral formula is accomplished due to the symmetry of the operator $\widetilde{L_{1,k}}$ at the space $L_2(R,\rho d\xi_k d\eta_k)$ with the weight $\rho=:\exp\{-(\alpha_k/\varepsilon^2)u_k\overline{u_k}\}$ (the item 2° of Lemma 5), and, due to the commutation formula (19),

$$\lim_{n\to\infty}\pi^{-\sigma(n)}\int_{\mathbb{R}^{2\sigma(n)}}\exp\left\{-\sum_{k\in P}P'_nu_k\overline{P'_nu_k}\right\}(L_1f)(P_nu)\overline{g}(P_nu)\prod_{k\in P,|k|<n}d\,\mathrm{Re}\,P'_nu_k d\,\mathrm{Im}\,P'_nu_k$$

$$=\lim_{n\to\infty}\pi^{-\sigma(n)}\int_{\mathbb{R}^{2\sigma(n)}}\exp\left\{-\sum_{k\in P}\frac{\alpha_k}{\varepsilon^2}P'_nu_k\overline{P'_nu_k}\right\}$$

$$\times\left(\sum_{k\in P}\widetilde{L_{1,k}}P_f\right)\overline{P_g}(P_nu)\prod_{k\in P,|k|<n}d\,\mathrm{Re}\,P'_nu_k d\,\mathrm{Im}\,P'_nu_k$$

$$=\lim_{n\to\infty}\pi^{-\sigma(n)}\int_{\mathbb{R}^{2\sigma(n)}}\exp\left\{-\sum_{k\in P}P'_nu_k\overline{P'_nu_k}\right\}$$

$$\times f(P_nu)\overline{L_1g}(P_nu)\prod_{k\in P,|k|<n}d\,\mathrm{Re}\,P'_nu_k d\,\mathrm{Im}\,P'_nu_k\,. \tag{30}$$

Therefore the item 1° is proved. Item 2° follows directly from Lemma 1. The lemma is proved.

The eigenfunctions of the operator $\widetilde{L_{1,k}}$, and, hence, of the operator L_1 [see (19)] can also be found from the representation (27). But the eigenfunctions in the form (21) are useful because they are also eigenfunctions of complete impulse operator:

$$\sum_{j=1}^{N}-i\nabla_{x_j}. \tag{31}$$

By direct calculations we get

$$\left(\sum_{j=1}^{N}-i\nabla_{x_j}\right)u_k^n=2\pi knu_k^n,$$

$$\sum_{j=1}^{N}-i\nabla_{x_j}|u_k|^2=0, \tag{32}$$

and hence prove the proposition.

Proposition 7: Functions (21) are the eigenfunctions of the complete impulse operator with eigenvalues $2\pi(\Sigma_{k\in Q}(n_k^+ + n_k^-)k)$.

So, it follows from the formula (14) that if the operator $N^{-(1/2)}L_2$ does not contribute in the main terms of low energy eigenvalues, then the main terms of low energy asymptotics is defined completely by the spectrum of the operator L_1 [formulas (22) and (24)]. Therefore, we can expect for the low energy spectral series of NSO (1) and (4) asymptotic behavior:

$$\lambda(\ldots,n_k,\ldots)=\frac{\nu_0N(N-1)\delta^3}{2}-\frac{N\delta^3}{2}\sum_{|k|=1}^{\infty}\nu_k+\sum_{k\in P}4\pi^2\varepsilon^2k^2\left(\sqrt{1+\frac{2\nu_k\delta^3N}{4\pi^2\varepsilon^2k^2}}-1\right)$$

$$+\sum_{k\in G}n_k\sqrt{\varepsilon^4 16\pi^4k^4+2(4\pi^2\varepsilon^2k^2)\nu_kN\delta^3},\quad n_k\geqslant 0; \tag{33}$$

here G is some finite subset of P. All variation of the L_1 spectrum can be taken into consideration by means of non-negative integers n_k.

At first the spectrum (33) was deduced in the physical works[10] by N. N. Bogolubov for the rarefied medium in the statistical limit. In a series of publication[11–18] it was proved by the method of second quantization that the formulas (33) provide the spectral asymptotics when δ, ε, L are

fixed and the Fourier coefficients ν_k are of order $1/N$: $0 \leqslant \nu_k \leqslant c(k\delta)/N$ and $c(k\delta)$ quickly tends to zero as $|k| \to \infty$. The complete theory of quadratic bosons operators and their normal forms are in Refs. 1, 16, 17, and 35.

Many scientists thought that the asymptotics (33) are valid only for the weak interaction and rarefied medium. In some physical papers were stated doubts that formulas (33) are valid in the statistical limit. In Ref. 19 it was shown by numerical experiments at one dimension ($x = x_1$) for the case $V(x-y) = \alpha\delta(x-y)$ that the minimal eigenvalue from the series (33) is valid for the NSO if $0 < \alpha$ and less some constant. That result can be considered like a hint that the spectrum (33) could not work in the statistical limit for all values of binary potential.

Proposed in that paper was a new asymptotic approach that allows us to construct and unexpectedly justify the asymptotics (33) for the strong binary interaction (that is, $\nu_k \sim 1$) in the case when the physical parameters δ, ε, L are fixed and $N \to \infty$ (strong interaction and dense matter). The success was achieved because the new operator L_1 and new WKB type functions (6) are involved.

In the next paragraph the theorem will be proved.

Theorem 8 (Main): *Let the physical parameters δ, ε, L be fixed but $N \to \infty$. 1°. Let us suppose that $\nu_k \to 0$ as $|k| \to \infty$ more quickly than any power $|k|$:*

$$0 \leqslant \nu_k \leqslant \frac{c_m}{(1+|k|)^m}; \quad m \in \mathbb{Z}_+; \quad |c_m| < \infty. \tag{34}$$

Then the value $\lambda(\ldots,0,\ldots)$ in the formula (33) is the asymptotics of the minimal eigenvalue λ_0 of the NSO (1) with the precision $O(N^{1/2-\gamma})$ for some $\gamma > 0$:

$$\lambda_0 = \frac{\nu_0 N(N-1)\delta^3}{2} - \frac{N\delta^3}{2} \sum_{|k| \geqslant 1, k \in P} \nu_k + \sum_{k \in P} 4\pi^2\varepsilon^2 k^2 \left(\sqrt{1 + \frac{2\nu_k \delta^3 N}{4\pi^2\varepsilon^2 k^2}} - 1 \right) + O(N^{1/2-\gamma}). \tag{35}$$

2°. Let us suppose that the Fourier coefficients $\nu_k \geqslant 0$ and $\nu_k = 0$ for $k \notin Q$ where Q is some finite subset of the set P. Then for every finite subset $\{n_k\} = \{n_{k_1}, \ldots, n_{k_m}\}, k_i \in Q \subset P$, $n_{k_j} > 0$ there is eigenvalue $\lambda\{n_k\}$ of the NSO (1) such that

$$|\lambda\{n_k\} - \lambda(\ldots,n_k,\ldots)| \leqslant \varepsilon\delta^{3/2} C\left(\sum_{k \in Q} n_k \right); \tag{36}$$

$$if \sum_{k \in Q} n_k \to \infty, \ then \ C\left(\sum_{k \in Q} n_k \right) \to \infty, \tag{37}$$

where $\lambda(\ldots,n_k,\ldots)$ is the eigenvalue of the series (33).

The main theorem tells that the asymptotic series (33) is started near the minimal eigenvalue of the NSO at the dense matter case.

It also follows from the item 2° [see (36) and (37)] that there are $g(N,\gamma_0)$ points of the NSO spectrum which have asymptotics (33) with the precision $O(N^{1/2-\gamma_0})$, $0 < \gamma_0 < \frac{1}{2}$, where $g(N,\gamma_0)$ is some increasing function of N which tends to infinitum when N tends to infinitum.

The NSO have many other spectral series which can be described by that approach. For example, if the movement of mass center is considered, then eigenfunction approximation is reasonable to look for in a form

$$f(\ldots u_k, \overline{u_k} \ldots) \exp\left\{ \sum_{j=1}^{N} i2\pi(l,x_j) \right\}, l \in \mathbb{Z}^3, \tag{38}$$

where f is the function of type (6).

Evidently,

$$\sum_{j=1}^{N} \Delta_{x_j} f \exp\left\{ i2\pi \sum_{j=1}^{N} (l,x_j) \right\} = \exp\left\{ i2\pi \sum_{j=1}^{N} (l,x_j) \right\} \left\{ \sum_{j=1}^{N} \Delta_{x_j} f - 4\pi^2 N l^2 f + i4\pi \sum_{j=1}^{N} \left(l, \frac{\partial f}{\partial x_j} \right) \right\}. \tag{39}$$

Next, let us introduce the operator L_3:

$$L_3 =: -8\pi^2 \sum_{k \in P} (k,l) \left\{ u_k \frac{\partial}{\partial u_k} - \overline{u_k} \frac{\partial}{\partial \overline{u_k}} \right\}. \tag{40}$$

It is clear that $L_3 f = i4\pi \Sigma_{j=1}^{N} (l, \partial f / \partial x_j)$.

Proposition 9: The NSO operator (1) at the functions (38) has the form

$$H\left(f \circ J \exp\left\{ i2\pi \sum_{j=1}^{N} (l,x_j) \right\} \right) = \exp\left\{ i2\pi \sum_{j=1}^{N} (l,x_j) \right\} \left\{ \left(L_1 - \varepsilon^2 L_3 + \frac{1}{\sqrt{N}} L_2 + \mu + 4\pi^2 \varepsilon^2 N l^2 \right) f \right\} \circ J. \tag{41}$$

Formula (41) is a direct consequence of the formulas (39), (40), and (14).

It is not difficult to show that new spectral series $\lambda(l, \ldots, n_m, \ldots)$, corresponding to the functions (38), can be calculated through the series (34):

$$\lambda(l, \ldots, n_m, \ldots) = \lambda(\ldots, n_m, \ldots) + 4\pi^2 \varepsilon^2 N l^2 \pm 8\pi^2 \varepsilon^2 \sum_{m \in G} (l,m) n_m. \tag{42}$$

Under the condition 2° (b) of the main theorem the series (42) gives the asymptotics of the NSO (1) with the same precision $O(\varepsilon \delta^{3/2})$.

III. PROOF OF THE MAIN THEOREM

At first we prove the item 2° of the theorem, employing the averaging.[6] Then, we divide the proof of estimate (35) for the minimal eigenvalue into two parts, as estimated from below and from above.

A. Proof of the item 2°

At the eigenfunctions $\psi(\ldots; n_k^+, n_k^-, d_k; \ldots)$ of the operator L_1 the NSO operator (1), due to the formula (14), satisfies the relation

$$H\psi(\ldots; n_k^+, n_k^-, d_k; \ldots) = (\mu + \lambda(\ldots, n_k^+, n_k^-, d_k, \ldots))\psi(\ldots; n_k^+, n_k^-, d_k; \ldots) + \frac{1}{\sqrt{N}} L_2 \psi(\ldots; n_k^+, n_k^-, d_k; \ldots). \tag{43}$$

It follows from formula (43) and Ref. 7 that there is an eigenvalue λ of the operator H such that

$$|\lambda - \{\mu + \lambda(\ldots, n_k^+, n_k^-, d_k, \ldots)\}| \leq N^{-1/2} \| L_2 \psi(\ldots; n_k^+, n_k^-, d_k; \ldots) \|_{L_2(M)} \times \| \psi(\ldots; n_k^+, n_k^-, d_k; \ldots) \|_{L_2(M)}^{-1}. \tag{44}$$

The norms on the right-hand side of inequality (44) can be calculated accordance with the averaging theory.[6,20] To that end we consider the vectors $X_j = \{\cos 2\pi(k_1, x_j),$

$\ldots,\cos 2\pi(k_q,x_j);\sin 2\pi(k_1,x_j),\ldots,\sin 2\pi(k_q,x_j)\}^T$; here $\{k_1,\ldots,k_q\}=Q\subset P$ and all $k_i\neq k_j$ for $i\neq j$. The set P does not contain indexes k, $-k$ simultaneously. Hence, in the subset Q the indexes comply with conditions at Q:

$$\pm k_i\neq k_j, \quad if \quad i\neq j, \tag{45}$$

which will be used afterwards.

Now, by the Wiener construction a space will be produced at which X_j are identically distributed independent (idi) random vectors. For simplicity let us describe that Wiener construction for the one-dimensional case $x_j\in R^1$, $j=1,\ldots,N$. Consider space Ω with points $\{x\}=:\{x_1,\ldots,x_n,\ldots\}$; $0\leqslant x_k\leqslant 1$. For the open sets in the space Ω are selected cylindrical sets:[8,9]

$$\Omega(a_{i_1},b_{i_1};\ldots;a_{i_n},b_{i_n})=:\{x:a_{i_\alpha}<x_{i_\alpha}<b_{i_\alpha},\alpha=1,\ldots,n;0\leqslant a_{i_\alpha}\leqslant b_{i_\alpha};$$
$$\text{if } i\notin\{i_1,\ldots,i_n\} \text{ then } x_i \text{ is any point at } [0,1]\}.$$

The measure of open sets is defined as

$$\mu\{\Omega(a_{i_1},b_{i_1};\ldots;a_{i_n},b_{i_n})\}=:\prod_{\alpha=1}^{n}(b_{i_\alpha}-a_{i_\alpha}), \tag{46}$$

and evidently exists its Lebesgue extension[8] μ_L. It is clear that

$$\mu_L\{x:a_i\leqslant x_i\leqslant b_i;a_j\leqslant x_j\leqslant b_j;i\neq j\}=\mu_L\{x:a_i\leqslant x_i\leqslant b_i\}\mu_L\{x:a_j\leqslant x_j\leqslant b_j\}$$
$$=(b_i-a_i)(b_j-a_j), \tag{47}$$

and $\mu_L(\Omega)=1$. Therefore, functions x_i and x_j, $0<i,\ j<\infty$, are independent identically distributed functions at $\{\Omega,\mu_L\}$. Consequently, X_j, $j=1,\ldots,$ are idi random vectors at $\{\Omega,\mu_L\}$. It is clear that the vector average of X_j is $(1/\sqrt{N})\Sigma_{j=1}^{N}X_j=\{\xi_{k_1},\ldots,\xi_{k_q};\eta_{k_1},\ldots,\eta_{k_q}\}^T$, where $\xi_k=\mathrm{Re}\,u_k;\eta_k=\mathrm{Im}\,u_k$. In the same manner we can construct $\{\Omega,\mu_L\}$ for the three-dimensional case $x_j\in R^3$, $j=1,\ldots,N$.

The averaging theory[6,20] provides

$$\int_M f(\xi_{k_1},\ldots,\xi_{k_q};\eta_{k_1},\ldots,\eta_{k_q})\circ J\,dx_1\cdots dx_N$$
$$=\pi^{-q}\int f(\xi_{k_1},\ldots,\xi_{k_q};\eta_{k_1},\ldots,\eta_{k_q})\left\{1+\sum_{r=1}^{s}\frac{1}{N^{r/2}}P_r(\xi,\eta)\right\}$$
$$\times\exp\left\{-\sum_{\alpha=1}^{q}(\xi_{k_\alpha}^2+\eta_{k_\alpha}^2)\right\}\prod_{\alpha=1}^{q}d\xi_{k_\alpha}d\eta_{k_\alpha}+o\left(\frac{1}{N^{s/2}}\right) \tag{48}$$

under some conditions on the function f and random vectors X_j, that is, on ξ_k,η_k. Here $P_r(\xi,\eta)$ are some polynomial functions independent on f.

We will use the estimations of the theorem[6] 20.1. The theorem 20.1 conditions demand that the random vectors X_j obey the Cramér's condition.

Let

$$f(t_1,\ldots,t_{2q})=:\int_T\exp\left\{i\sum_{j=1}^{q}(t_j\cos 2\pi(k_j,x)+t_{j+q}\sin 2\pi(k_j,x))\right\}dx,$$
$$\pm k_i\neq k_j;1\leqslant i,\ j\leqslant q;\quad T=:\mathbb{R}^3/\mathbb{Z}^3. \tag{49}$$

The Cramér's condition on the idi X_j is

$$\overline{\lim}_{|t|\to\infty}|f(t_1,\ldots,t_{2q})|<1. \tag{50}$$

To estimate the norms on the right-hand side of inequality (44), consider the integral

$$I(\{P_k\})=:\int_M \exp\left\{\frac{2\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in Q}\beta_k(\xi_k^2+\eta_k^2)\right\}\prod_{k\in Q}(\xi_k^2+\eta_k^2)^{P_k}\prod_{l\in G}(\xi_l^2+\eta_l^2)^{P_l}dx_1\cdots dx_N, \tag{51}$$

where $Q\cap G=\varnothing$ and the number of elements in the sets Q,G are finite: $|Q|$, $|G|<\infty$.

Lemma 10: Let $|Q|$, $|G|$ be finite; δ, ε and ν_k are fixed. Then, for $N\to\infty$, the integral (51) has asymptotics

$$I(\{P_k\})=\prod_{k\in Q}\left(1+2|\beta_k|\frac{\sqrt{N\delta^3}}{\varepsilon}\right)^{-(P_k+1)}\prod_{k\in Q\cup G}\Gamma(P_k+1)\left\{1+O\left(\frac{1}{\sqrt{N}}\right)\right\}. \tag{52}$$

Lemma 10 is a direct consequence of the theorem[6] 20.1 and Lemma 11:

Lemma 11: The function (49) with fixed q obeys the Cramér's condition (50).

Consider the function

$$g(\omega,x)=:\sum_{j=1}^{q}(\omega_j\cos 2\pi(k_j,x)+\omega_{j+q}\sin 2\pi(k_j,x)),\quad\text{where}\quad \omega=t/|t|\quad\text{and}\quad|\omega|=1. \tag{53}$$

Evidently,

$$f(t_1,\ldots,t_{2q})=\int_{T^3}\exp\{i\ \ |t|g(\omega,x)\}dx. \tag{54}$$

The behavior of the function f as $|t|\to\infty$ can be studied by integration by parts. Let e_1, e_2 be the partition of unity in $\mathbb{R}$ such that $supp e_1\in[-2,2]$ and $e_1(t)=1$ if $|t|\leqslant 1$. Evidently,

$$|f(t_1,\ldots,t_{2q})|\leqslant\int e_1(|\nabla g|^2|t|^{2\varepsilon})+\left|\int e_2(|\nabla g|^2|t|^{2\varepsilon})\exp\{i\ \ |t|g(\omega,x)\}dx\right|. \tag{55}$$

There is obtained integrating by parts[21] for $\varepsilon<1/4$ that the second integral on the right-hand side of (55) is about $|t|^{4\varepsilon-1}$ and tends to zero as $|t|\to\infty$. Now consider the first integral on the right-hand side of (55). Let us suppose opposite, that

$$\overline{\lim}_{|t|\to\infty}\int_T e_1(|\nabla g(\omega,x)|^2|t|^{2\varepsilon})dx\geqslant 1. \tag{56}$$

The measure $\mu\{x:x\in T\}=1$, and $e(|\nabla g|^2|t|^{2\varepsilon})\leqslant 1$. Therefore integral on the left-hand side of (56) is bounded by 1. Therefore, it follows from (56) that the upper limit is equal to 1. Hence, exist ω_k; $|t_k|\to\infty$ such that

$$a_k=:\int e_1(|\nabla g(\omega_k,x)|^2|t_k|^{2\varepsilon})dx\to 1. \tag{57}$$

The points ω_k are at unit sphere in R^{2q}; hence, some subsequence $\omega_{k'}$ converge: $\lim_{k'\to\infty}\omega_{k'}=\overline{\omega}$. Now, let us show that for $k'>N(\beta)$ the next inclusion is true:

$$M_{k'}=:\left\{x:|\nabla g(\omega_{k'},x)|^2<\frac{2}{|t_{k'}|^{2\varepsilon}}\right\}\subset M_\beta, \tag{58}$$

here $M_\beta =: \{x: |\nabla g(\bar{\omega},x)|^2 \leqslant \beta\}$. Indeed,

$$|\nabla g(\omega_{k'},x)|^2 = |\nabla g(\bar{\omega},x)|^2 + (\bar{\omega}-\omega_{k'})\frac{\partial}{\partial\omega}|\nabla g(\theta,x)|^2 < \frac{2}{|t_{k'}|^{2\varepsilon}} \tag{59}$$

at the points of the set $M_{k'}$. Hence at the points of $M_{k'}$: $|\nabla g(\bar{\omega},x)|^2 < 2/|t_{k'}|^{2\varepsilon} + \text{const}$, $|\omega_k - \bar{\omega}| < \beta$ if $k' > N(\beta)$. It proves the inclusion (58). According to the definition of functions e_1, e_2, and due to the inclusion (58), an inequality

$$\int_{\{x:|\nabla g(\bar{\omega},x)|^2<\beta\}} dx \geqslant \int_{\{x:|\nabla g(\omega_{k'},x)|^2<2/|t_{k'}|^{2\varepsilon}\}} dx \geqslant a_{k'}, k' > N(\beta), \tag{60}$$

is satisfied. Then, when $k' \to \infty$, we obtain that

$$\mu ess M_\beta \geqslant 1 \quad \text{for all} \quad \beta > 0. \tag{61}$$

Due to the Lebesgue theorem

$$\mu ess M_0 = \lim_{\beta \to +0} \mu ess M_\beta \geqslant 1. \tag{62}$$

It means that if $\overline{\lim}_{|t|\to\infty} f(t_1,\ldots,t_{2q}) \geqslant 1$, then there exists the point $\bar{\omega}$ such that

$$\mu ess\{x: |\nabla g(\bar{\omega},x)|^2 = 0\} \geqslant 1. \tag{63}$$

Let us show that for every ω the function $|\nabla g(\omega_{k'},x)|^2$ is not equal to zero almost every where on T. Its integral

$$\begin{aligned}\int_T |\nabla g(\omega,x)|^2 dx &= 4\pi^2 \sum_{i,j=1}^{q} \omega_i \omega_j (k_i,k_j) \int_T \cos 2\pi(k_i,x)\cos 2\pi(k_j,x)dx \\ &\quad - 8\pi^2 \sum_{j=1}^{q}\sum_{l=q}^{2q} \omega_j \omega_l (k_j,k_l) \int_T \cos 2\pi(k_l,x)\sin 2\pi(k_j,x)dx \\ &\quad + 4\pi^2 \sum_{i=q+1}^{2q}\sum_{j=q+1}^{2q} \omega_i \omega_j (k_i,k_j) \int_T \sin 2\pi(k_i,x)\sin 2\pi(k_j,x)dx \\ &= 2\pi^2 \sum_{j=1}^{2q} \omega_j^2 k_j^2 \neq 0,\end{aligned}$$

because $\pm k_i \neq k_j$ and $k_j \neq 0$ at Q [see (45)]. Hence, the function $|\nabla g(\bar{\omega},x)|^2$ is not equal to zero almost everywhere. It contradicts (63), which indicates that $|\nabla g(\bar{\omega},x)| = 0$ almost everywhere. The contradiction proves (50).

Observation: The result of the lemma can be improved on the basis of analytic sets in such form: $\lim_{|t|\to\infty} f(t_1,\ldots,t_{2q}) = 0$.

There are many publications on the problem of averaging by probability approach.[22–26] But they do not allow us to consider the case $q = \infty$, though it looks like, in our case, the asymptotic formula of Lemma 10 will be true with some modification and for $q = \infty$.

The study of integrals $\int u_k u_m \exp\{(\sqrt{N\delta^3}/\varepsilon)\Sigma_{k\in Q}\beta_k |u_k|^2\}$ is important for the statistical physics and in the case $|Q| = \infty$ some estimate were obtained in Refs. 27–29. All those estimates are less exact than asymptotic expansion (52) which yet has been known only for the case $|Q| < \infty$.

Now let us apply the asymptotic (52) to estimate the right-hand side of the inequality (44). Without loss of generality the case $k_1 \in Q$, $n_{k_1}^{+} > 0$, $n_{k_1}^{-} = 0$, $d_{k_1} = 0$ and $n_k^{\pm} = 0$, $d_k = 0$ for $k \in (Q \backslash k_1)$ will be considered.

It follows from the formula (11) for the operator L_2 that

$$L_2 \exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in Q}\beta_k u_k\overline{u_k}\right\} u_{k_1}^{n_{k_1}^+} = \frac{1}{\sqrt{N}}\{R_1(n_{k_1}^+)+R_2(n_{k_1}^+)+R_3(n_{k_1}^+)\}; \tag{64}$$

$$R_1(n_{k_1}^+) = N\delta^3 \exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in Q}\beta_k u_k\overline{u_k}\right\} u_{k_1}^{n_{k_1}^+}\left\{-8\pi^2\sum_{k\neq m;k,m\in Q}(k,m)\beta_k\beta_m\overline{u_k}u_m u_{k-m}\right.$$
$$\left.+8\pi^2\,\mathrm{Re}\left\{\sum_{k,m\in Q}(k,m)\beta_k\beta_m\overline{u_k u_m}u_{k+m}\right\}\right\}; \tag{65}$$

$$R_2(n_{k_1}^+) = \varepsilon\sqrt{N\delta^3}\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in Q}\beta_k u_k\overline{u_k}\right\} u_{k_1}^{n_{k_1}^+-1} n_{k_1}^+$$
$$\times\left\{-8\pi^2\sum_{k_1\neq m;m\in Q}(k_1,m)\beta_m u_m u_{k_1-m}+8\pi^2\sum_{m\in Q}(k_1,m)\beta_m\overline{u_m}u_{k_1+m}\right\}; \tag{66}$$

$$R_3(n_{k_1}^+) = (-4\pi^2k_1^2)\varepsilon^2 n_{k_1}^+(n_{k_1}^+-1)\exp\left\{\frac{\sqrt{N\delta^3}}{\varepsilon}\sum_{k\in Q}\beta_k u_k\overline{u_k}\right\} u_{k_1}^{n_{k_1}^+-2}u_{2k_1}. \tag{67}$$

Direct application of the Cauchy inequality and asymptotic formula (52) to the functions (64)–(67) produces the estimate

$$\frac{1}{\sqrt{N}}\|L_2\psi(\ldots,n_k^+,n_k^-,d_k;\ldots)\|_{L_2(M)}\|\psi(\ldots,n_k^+,n_k^-,d_k;\ldots)\|_{L_2(M)}^{-1}\leqslant \mathrm{const}\times\varepsilon\,\delta^{3/2}. \tag{68}$$

Therefore, estimate (36) of the item 2° is a consequence of estimates (44) and (68).

B. Proof of estimation from below for the minimal eigenvalue of NSO

This section is devoted to the proof of the minimal eigenvalue estimate from below, that is

$$\lambda_0 \geqslant (\mu+\overline{\lambda_0})+O(N^{1/2-\gamma}),$$

where γ is some positive constant, the constant μ defined in (12), and

$$\overline{\lambda_0} =: \sum_{k\in P} 4\pi^2\varepsilon^2k^2\left\{\sqrt{1+\frac{2\nu_k\delta^3N}{k^2 4\pi^2\varepsilon^2}}-1\right\}.$$

To that end let us introduce some approximation of the operator H which has as minimal eigenfunction the exponent from the formula (21).

It follows from the formulas (43), (64), and (65) that the positive function $\psi_0 =: \exp\{(\sqrt{N\delta^3}/\varepsilon)\Sigma_{k\in P}\beta_k u_k\overline{u_k}\}$, where β_k are defined by (17), satisfies the equation

$$\{H-r\}\psi_0 = (\mu+\overline{\lambda_0})\psi_0,$$
$$r =: \sqrt{N}\delta^3 8\pi^2\left\{-\sum_{k\neq m;k.,m\in P}(k,m)\beta_k\beta_m\overline{u_k}u_m u_{k-m}+\mathrm{Re}\left\{\sum_{k,m\in P}(k,m)\beta_k\beta_m\overline{u_k u_m}u_{k+m}\right\}\right\}. \tag{69}$$

Evidently ψ_0 is the minimal eigenfuction, and minimal eigenvalue $\lambda(\ldots,0,\ldots)$ of the series (33), which is equal to $(\mu+\overline{\lambda_0})$, is the minimal eigenvalue of the operator $H-r$. Otherwise the positive function ψ_0 has to be orthogonal and a minimal eigenfunction of the operator $H-r$,

which is, due to Ref. 30, non-negative. But the two non-negative functions cannot be orthogonal. The operator $H-r$ will be used for estimation from below the minimal eigenvalue λ_0 of the operator H.

Let us introduce some partition of unity at the $3N$ dimensional torus M such that $e_1^2+e_2^2=1$; $e_j\in C^\infty(M)$.

Then[31]

$$H=\sum_{j=1}^{2} e_j H e_j-\sum_{j=1}^{2}(\nabla e_j)^2,$$

where $\nabla=:\Sigma_{j=1}^{N}\nabla_{x_j}$ is a complete gradient. Evidently

$$H=e_1(H-r)e_1+e_1re_1+e_2He_2-(\nabla e_1)^2-(\nabla e_2)^2. \tag{70}$$

The functions e_j will be chosen so that at the minimal eigenfunction φ_0 of the operator H are satisfied inequalities:

$$(e_1|r|e_1\varphi_0,\varphi_0)\leqslant c_1\frac{\overline{\lambda_0}}{N^{\gamma_1}}(\varphi_0,\varphi_0), \tag{71}$$

$$(e_2He_2\varphi_0,\varphi_0)\geqslant(\mu+c_2N^{1/2+\gamma_2})(e_2\varphi_0,e_2\varphi_0), \tag{72}$$

$$\sum_{j=1}^{2}((\nabla e_j)^2\varphi_0,\varphi_0)\leqslant c_3N^{-\gamma_3}(\varphi_0,\varphi_0), \tag{73}$$

for some positive values $\gamma_1,\ \gamma_2,\ \gamma_3;\ c_1,\ c_2,\ c_3$.

As the operator $(H-r)$ has minimal eigenvalue $(\mu+\overline{\lambda_0})$, then it follows from the formula (70), inequalities (71)–(73), and property $e_1^2+e_2^2=1$ that

$$\lambda_0(\varphi_0,\varphi_0)=(H\varphi_0,\varphi_0)\geqslant\left\{\mu+\overline{\lambda_0}\left(1+\frac{c}{N^{\gamma_1}}\right)\right\}(\varphi_0,\varphi_0)-cN^{-\gamma_3}(\varphi_0,\varphi_0). \tag{74}$$

That is,

$$\lambda_0\geqslant(\mu+\overline{\lambda_0})+O(N^{1/2-\gamma_1}), \tag{75}$$

which is the desired estimate from below. The construction of the functions e_j is based on the lemma.

Lemma 12: 1° *Let* $d_p(\sigma)=:\Sigma_{k+m=p}|\beta_k|^\sigma|\beta_m|^\sigma$, $0<\sigma<1$, *where* β_k *is an even function of* k. *Then*

$$|r(x)|\leqslant 48\pi^2\delta^3\sqrt{N}\left(\sum_{k\in P}k^2|\beta_k|^{2-\sigma}|u_k|^2\right)\left(\sum_{q\in P}d_q(\sigma)|u_q|^2\right)^{1/2}, \tag{76}$$

and $d_q(\sigma)$ *complies with conditions (34).*

2°: For $0\leqslant\sigma\leqslant 1$ *is satisfied inequality*

$$4^{1-\sigma/2}\left(\frac{N\delta^3}{\varepsilon^2}\right)^{-\sigma/2}|\beta_k|^{2-\sigma}\leqslant\frac{\nu_k}{4\pi^2k^2}. \tag{77}$$

1° The conditions (34) for the coefficients $d_q(\sigma)$ are a direct consequence of (34) on ν_k. The inequality (76) is a consequence of the Cauchy inequality. 2° Evidently, $|\beta_k|=(\varepsilon/\sqrt{N\delta^3})\times(\nu_kN\delta^3/4\pi^2\varepsilon^2k^2)/\{1+\sqrt{1+2\nu_kN\delta^3/4\pi^2\varepsilon^2k^2}\}$, and, therefore,

$$|\beta_k|^{2-\sigma} \leqslant \left(\frac{4\nu_k^2/(4\pi^2k^2)^2}{\varepsilon^2/N\delta^3 + 2\nu_k/4\pi^2k^2} \right)^{1-\sigma/2} \frac{1}{4^{1-\sigma/2}}. \tag{78}$$

To transform the right-hand side (78) the evident inequality will be used:

$$\frac{a^2}{b+a} = \frac{a^2}{(b+a)^x} \frac{1}{(b+a)^{1-x}} \leqslant \frac{a^{2-x}}{b^{1-x}} \tag{79}$$

at $a,b>0$; $0 \leqslant x \leqslant 1$. Let us choose x such that $(2-x)(1-\sigma/2)=1$, which gives $x=2(1-\sigma)/(2-\sigma)$. The condition $0 \leqslant x \leqslant 1$ implies that $0 \leqslant \sigma \leqslant 1$. Let $b =: \varepsilon^2/N\delta^3$; $a =: 2\nu_k/4\pi^2k^2$. Then (77) follows from (78) and (79). The lemma is proved.

The estimate

$$|r(x)| \leqslant \left(\frac{4\delta^3}{\varepsilon^2} \right)^{\sigma/2} N^{1/2+\sigma/2} \left\{ \sum_{k \in P} \delta^3 \nu_k |u_k|^2 \right\} \left\{ \sum_{q \in P} d_q(\sigma) |u_q|^2 \right\}^{1/2} \tag{80}$$

is obtained by application of the inequality (77) to inequality (76). Consequently, at the set $D(\sigma_1)$,

$$D(\sigma_1) =: \left\{ x : \sum_{q \in P} d_q(\sigma) |u_q|^2 < 5c_o N^{2\sigma_1} \right\}, \tag{81}$$

inequality

$$|r(x)| \leqslant 36 \left(\frac{4\delta^3}{\varepsilon^2} \right)^{\sigma/2} \sqrt{5c_0} N^{1/2+\sigma/2+\sigma_1} \left\{ \sum_{k \in P} \delta^3 \nu_k |u_k|^2 \right\} \tag{82}$$

is satisfied. The parameters σ, σ_1 will be chosen in the intervals

$$\sigma_1 > \frac{1}{4}; \quad \frac{\sigma}{2} + \sigma_1 < \frac{1}{2}; \quad \sigma > 0 \tag{83}$$

such that

$$\gamma_1 =: \frac{1}{2} - \frac{\sigma}{2} - \sigma_1 > 0. \tag{84}$$

Now let us calculate functions e_1, e_2. Let functions $e_1'(t)$, $e_2'(t) \in C^\infty(\mathbb{R}^1)$; and $(e_1'(t))^2 + (e_2'(t))^2 = 1$, $supp e_2'(t) \in [\frac{1}{2}, +\infty)$, $supp e_1'(t) \in [-1,1]$. Definition:

$$e_1(x) =: e_1' \left\{ \left(\sum_{q \in P} d_q(\sigma) |u_q|^2 \right) \Big/ 5c_0 N^{2\sigma_1} \right\}, \tag{85}$$

$$e_2(x) =: e_2' \left\{ \left(\sum_{q \in P} d_q(\sigma) |u_q|^2 \right) \Big/ 5c_0 N^{2\sigma_1} \right\}, \tag{86}$$

where c_0 is some positive constant which will be chosen later in the proof of Lemma 15.

Proposition 13: The functions e_1, r, φ_0 satisfy inequality (71).

Evidently $supp e_1(x) \subseteq D(\sigma_1)$ and $0 \leqslant e_1 \leqslant 1$. Therefore, due to inequality (82), we obtain

$$(|r|e_1\varphi_0, e_1\varphi_0) \leqslant 36 \left(\frac{4\delta^3}{\varepsilon^2} \right)^{\sigma/2} \sqrt{5c_0} N^{1-\gamma_1} \int_M \left(\sum_{k \in P} \delta^3 \nu_k |u_k|^2 \right) e_1^2 \varphi_0^2 dx. \tag{87}$$

But the minimal eigenfunction φ_0 satisfies the energy equality

$$\int_M \varepsilon^2|\nabla\varphi_0|^2+N\int_M\left(\sum_{k\in P}\delta^3\nu_k|u_k|^2\right)\varphi_0^2dx=(\lambda_0-\mu)\int_M|\varphi_0|^2dx. \tag{88}$$

It follows from relations (87) and (88) and estimate from above (111) that

$$(|r|e_1\varphi_0,e_1\varphi_0)\leqslant 36\left(\frac{4\delta^3}{\varepsilon^2}\right)^{\sigma/2}\sqrt{5c_0}\frac{\overline{\lambda_0}}{N^{\gamma_1}}(\varphi_0,\varphi_0). \tag{89}$$

[The estimate from above (111) is proved independent of estimate from below.] The inequality (89) is exactly equivalent to the inequality (71).

Proposition 14: The functions e_1, e_2 satisfy the inequality (73).

We prove that

$$|\nabla e_j|^2\leqslant CN^{-2\sigma_1};\quad j=1,2; \tag{90}$$

where (90) is a stronger inequality than (73). Let us prove (90) for $j=1$; for $j=2$ the proof is the same. Direct calculations provide

$$\nabla e_1=\frac{\partial e_1'}{\partial t}\sum_{q\in P}d_q(\sigma)(u_q\nabla\overline{u_q}+\overline{u_q}\nabla u_q)/5c_0N^{2\sigma_1},$$

$$\frac{\partial u_k}{\partial x_j}=\frac{i2\pi k}{\sqrt{N}}\exp\{i2\pi(k,x_j)\}.$$

Hence,

$$\begin{aligned}|\nabla e_1|&\leqslant 4\pi\left|\frac{\partial e_1'}{\partial t}\right|(5c_0N^{2\sigma_1})^{-1}\sum_{q\in P}|q|d_q(\sigma)|u_q|\\&\leqslant 4\pi\left|\frac{\partial e_1'}{\partial t}\right|(5c_0N^{2\sigma_1})^{-1}\sqrt{\sum_{q\in P}|q|^2d_q(\sigma)}\sqrt{\sum_{q\in P}d_q(\sigma)|u_q|^2}\\&\leqslant 4\pi c_eN^{-\sigma_1}(5c_0)^{-1/2}\sqrt{\sum_{q\in P}|q|^2d_q(\sigma)},\end{aligned} \tag{91}$$

where $c_e=\max_{\mathbb{R}}|\partial e_1'/\partial t|$.

In the last reduction we use that at the set support $\partial e_1'/\partial t$ $(\Sigma_{q\in P}d_q(\sigma)|u_q|^2/c_0N^{2\sigma_1})$ there is inequality $\sqrt{\Sigma_{q\in P}d_q(\sigma)|u_q|^2}\leqslant\sqrt{5c_0}N^{\sigma_1}$. So the functions e_j satisfy inequality (90) with the constant

$$c=(5c_0)^{-1}\left\{\sum_{j=1}^{2}\max_{\mathbb{R}}\left|\frac{\partial e_j'}{\partial t}\right|\right\}16\pi^2\left\{\sum_{q\in P}q^2d_q(\sigma)\right\}. \tag{92}$$

The proof is over.

Now let us consider the inequality (72). To that end the next lemma will be proved.

Lemma 15: Any function $\varphi\in W_2^1(M)$ with $\mathrm{supp}\varphi\subseteq\mathrm{supp}e_2$ satisfies inequality

$$\int_M|\nabla\varphi|^2dx\geqslant\frac{1}{4}\frac{N^{2\sigma_1}}{\ln 6N}\{1+o(1)\}\int_M|\varphi|^2dx, \tag{93}$$

where $o(1)\to\infty$ as $N\to\infty$.

Let $c_{k_1 \dots k_N}$ be the Fourier coefficients of the function φ with respect to the simple harmonics $\exp\{i2\pi(k_1x_1+\cdots+k_Nx_N)\}$. Evidently for any positive value d^2 there is inequality

$$\int_M |\varphi|^2 dx \leqslant \sum_{k_1^2+\cdots+k_N^2 \leqslant d^2} |c_{k_1 \cdots k_N}|^2 + d^{-2} \sum_{k_1^2+\cdots+k_N^2 \geqslant d^2} (k_1^2+\cdots+k_N^2)|c_{k_1 \cdots k_N}|^2. \tag{94}$$

Further,

$$d^{-2} \sum_{k_1^2+\cdots+k_N^2 \geqslant d^2} (k_1^2+\cdots+k_N^2)|c_{k_1 \cdots k_N}|^2 \leqslant d^{-2} \int_M |\nabla \varphi|^2 dx; \tag{95}$$

$$|c_{k_1 \cdots k_N}|^2 \leqslant \mu ess\{suppe_2\} \int_M |\varphi|^2 dx. \tag{96}$$

To make an advance we have to estimate (a) the number of combinations such that $\Sigma_{i=1}^N k_i^2 \leqslant d^2$, $k_i \in \mathbb{Z}^3$, which will be designate as N_a and (b) estimate $\mu ess\{suppe_2\}$.

(a) *The number of combinations*. Evidently $N_a \leqslant 2^{d^2} \times N_a'$, where N_a' is the number of combinations for which $\Sigma_{j=1}^{3N} k_j^2 \leqslant d^2$; $k_j \geqslant 0$, $k_j \in \mathbb{Z}$.

The factor 2^{d^2} is introduced to take into consideration all combinations $\pm k_1, \dots, \pm k_{3N}$; $k_j \in \mathbb{Z}_+$. As in the succession $\pm k_1, \dots, \pm k_{3N}$ there are not more then d^2 terms which are not equal to zero; therefore the factor 2^{d^2} considers all additional combinations which happened because of sign $\pm$ variation near k_j.

The number N_a' is less than or equal to the number of combinations at which

$$\sum_{j=1}^{3N} k_j \leqslant d^2, \quad k_j \geqslant 0, \quad k_j \in \mathbb{Z}, \tag{97}$$

because $k_j^2 \geqslant k_j$ for $k_j \geqslant 0$, $k_j \in \mathbb{Z}$. The number of combinations (97) is calculated in Ref. 32. Therefore,

$$N_a \leqslant 2^{d^2} \sum_{n=0}^{d^2} \sum_{r_1+\cdots+r_{3N}=n} \frac{n!}{r_1! \cdots r_{3N}!} = 2^{d^2} \sum_{n=0}^{d^2} (3N)^n \leqslant 2^{d^2+1} (3N)^{d^2}. \tag{98}$$

(b) *Estimate for* $\mu ess\{suppe_2\}$. The coefficients $d_q(\sigma) \leqslant c_l(\delta,\sigma)/(1+|q|)^l$, $0 \leqslant l < \infty$; and $|u_q| \leqslant \sqrt{N}$. Hence, for a fixed positive constant c_0, there exist values $f > 0$ such that

$$\sum_{q \geqslant N^f} d_q(\sigma)|u_q|^2 \leqslant \frac{c_0}{8}. \tag{99}$$

It means that the set

$$\Gamma(\sigma_1) = \left\{ x: \sum_{q \in P, q \leqslant N^f} d_q(\sigma)|u_q|^2 \geqslant \frac{5}{4} c_0 N^{2\sigma_1} \right\} \tag{100}$$

includes the set $\mathsf{C}D(\sigma_1)$ [complement to $D(\sigma_1)$, which is defined in (81)].

Further, let us consider the set

$$\omega(\sigma_1) = \cap_{|k|=0}^{N^f} \{x: |u_k| \leqslant N^{\sigma_1}\}. \tag{101}$$

Evidently, at the set $\omega(\sigma_1)$ the inequality

$$\left\{\sum_{q\in P,q\leqslant N^f} d_q(\sigma)|u_q|^2\right\}\Big|_{\omega(\sigma_1)} \leqslant \left\{\sum_{q\in P,q\leqslant N^f} d_q(\sigma)\right\} N^{2\sigma_1} \tag{102}$$

is satisfied. *Let us define the positive constant* c_0, *which is used in definitons of functions* e_1, e_2, *as*

$$c_0=\sum_{q\in P} d_q(\sigma). \tag{103}$$

Hence, due to inequality (102) the set $\Gamma(\sigma_1)$, and therefore the set $\mathsf{C}D(\sigma_1)$, are included into the complement $\mathsf{C}\omega(\sigma_1)$. These inclusions imply inequality

$$\mu ess\mathsf{C}D(\sigma_1)\leqslant \mu ess\Gamma(\sigma_1)\leqslant \mu ess\mathsf{C}\omega(\sigma_1). \tag{104}$$

It is well known that $\mathsf{C}\omega(\sigma_1)=\cup_{|k|=0}^{N^f}\mathsf{C}\{x:|u_k|\leqslant N^{\sigma_1}\}=\cup_{|k|=0}^{N^f}\{x:|u_k|>N^{\sigma_1}\}$ [due to the formula (101)] and

$$\mu ess\mathsf{C}\omega(\sigma_1)\leqslant \sum_{|k|=0}^{N^f} \mu ess\{x:|u_k|\geqslant N^{\sigma_1}\}. \tag{105}$$

Employing the large deviations theorem[33] for values $\sigma_1<\frac{1}{2}$ we obtain from (105) the estimate

$$\mu ess\mathsf{C}\omega(\sigma_1)\leqslant \frac{4\pi^2}{3}(N^f+1)^3\exp\left\{-\frac{N^{2\sigma_1}}{2}\right\}. \tag{106}$$

The estimates (104) and (106) prove that

$$\mu ess\{suppe_2\}\leqslant \frac{4\pi^2}{3}(N^f+1)^3\exp\left\{-\frac{N^{2\sigma_1}}{2}\right\}. \tag{107}$$

Now the parameter d^2 is chosen so that

$$\mu ess\{suppe_2\}N_a\leqslant \tfrac{1}{2}. \tag{108}$$

Due to the inequalities (98) and (107), for that aim it is sufficient that $(4\pi^2/3)(N^f+1)^3\times\exp\{-(N^{2\sigma_1}/2)\}2(6N)^{d^2}=\frac{1}{2}$; namely,

$$d^2=\frac{N^{2\sigma_1}}{2\ln 6N}\{1+o(1)\}. \tag{109}$$

With the estimates (108) and (109) we can prove the main inequality (93). It follows from (94)–(96) that

$$\int_M|\nabla\varphi|^2dx\geqslant d^2\{1-N_a\mu ess\{suppe_2\}\}\int_M|\varphi|^2dx. \tag{110}$$

Now the estimate (93) follows from inequalities (108) and (109) and formula (110). The lemma is proved.

So, if the parameters σ_1, σ are chosen in the interval (83), the inequality (75) follows from the inequalities (71)–(73). Hence, the estimate from below (75) is proved.

C. Proof of the estimate from above for the minimal eigenvalue of NSO

Here the estimate from above

$$\lambda_0 \leqslant (\mu + \overline{\lambda_0}) + O(N^{1/2-\gamma}), \tag{111}$$

will be proved.

We use the designation of item 2. It follows from (69) that

$$\begin{aligned} N\delta^3 \int_M \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}\left\{|\nabla\Phi|^2 + \sum_{k\in P} \nu_k |u_k|^2\right\} dx \\ \leqslant \int_M |r| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx + \overline{\lambda_0} \\ \times \int_M \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}, \end{aligned} \tag{112}$$

where the remainder term r is defined in (69) and $\Phi =: \Sigma_{k\in P}|\beta_k||u_k|^2$.

The integral from $|r|$ on the right-hand side of (112) can be estimated through a sum of integrals

$$\delta^3 |k||m||\beta_k\beta_m| \int_M |u_k u_m u_{k\pm m}| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx. \tag{113}$$

The next lemma is proved following that idea.

Lemma 16: The integral from the residual term satisfies the inequality

$$\begin{aligned} \int_M |r| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx \leqslant c\left(\frac{\delta^3}{\varepsilon^2}\right)^{\gamma/2} N^{1/2+\sigma_0+\gamma/2}\left\{\sum_{k\in P} |\beta_k|^\gamma\right\} \int_M \left(\sum_{k\in P} \delta^3 \nu_k |u_k|^2\right) \\ \times \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}, \end{aligned} \tag{114}$$

where parameters σ_0, γ *satisfy conditions* $\frac{1}{4} < \sigma_0 < \frac{1}{2}$, $0 < \gamma < 1$; $\frac{1}{2} + \sigma_0 + \gamma/2 < 1$.

1°. As was said above, the left-hand side of (114) is estimated by the sum of integrals (113). Every integral (113) can be presented as the sum of the integral over the set $\Omega_{k\pm m} = \{x : |u_{k\pm m}| < N^{\sigma_0}\}$ and the integral over its complement $\mathrm{C}\Omega_{k\pm m} = \{x : |u_{k\pm m}| \geqslant N^{\sigma_0}\}$. By the theorem of large deviation[33] $\mu ess \mathrm{C}\Omega_{k\pm m} \leqslant c(\sigma_0)\exp\{-(N^{2\sigma_0}/2)\}$ uniform in $k, m \in \mathbb{Z}^3$. Hence

$$\begin{aligned} \sum_{k,m\in P} \sqrt{N}\delta^3 8\pi^2 \int_M |k||m||\beta_k\beta_m||u_k u_m u_{k\pm m}| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx \\ \leqslant \sum_{k,m\in P} N^{1/2+\sigma_0} \delta^3 8\pi^2 |k||m||\beta_k\beta_m| \int_M |u_k u_m| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx \\ + N^2 8\pi^2 c(\sigma_0)\left\{\sum_{k,m\in P} \delta^3 |k||m||\beta_k\beta_m|\right\} \exp\left\{-\frac{N^{2\sigma_0}}{2}\right\}. \end{aligned} \tag{115}$$

2°. We would like to neglect the second term on the right-hand side of the formula (115). To that end let us estimate from below the integral

$$I(k,m) = \int_M |u_k u_m| \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\} dx. \tag{116}$$

The Jensen inequality for the convex functions produces $\int_{\mathbb{R}} f(t)\,d\mu \geqslant f(\int_{\mathbb{R}} t\,d\mu)$, where $\int_{\mathbb{R}} d\mu = 1$.

To apply the Jensen inequality to the integral (116) let us define[34,36] measure

$$d\mu=(-1)d_t\int_{\Phi\geqslant t}|u_ku_m|dx/(-1)\int_{\mathbb{R}}d_t\left\{\int_{\Phi\geqslant t}|u_ku_m|dx\right\}. \tag{117}$$

Then, by Jensen inequality, it is obtained that

$$I(k,m)\geqslant\left\{\int_M|u_ku_m|dx\right\}\exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\int_M\Phi d\mu\right\}, \tag{118}$$

because it is clear that by the Fubini theorem[34] and by the averaging theory[6] one can obtain

$$\int_{\mathbb{R}}(-1)d_t\left\{\int_{\Phi\geqslant t}|u_ku_m|dx\right\}=\int_M|u_ku_m|dx=(\pi)^{-1}\left\{\int|\eta|e^{-\eta^2}d\eta\right\}^2+O\left(\frac{1}{\sqrt{N}}\right); \tag{119}$$

$$\begin{aligned}\int_{\mathbb{R}}(-1)td_t\left\{\int_{\Phi\geqslant t}|u_ku_m|dx\right\}&=\int_M\Phi|u_ku_m|dx=\sum_{l\in P}|\beta_l|\int_M|u_l|^2|u_ku_m|dx\\&=\left\{\sum_{l\in P}|\beta_l|\right\}\left\{\pi^{-3/2}\left(\int\eta_1^2e^{-\eta_1^2}d\eta_1\right)\left(\int|\eta|e^{-\eta^2}d\eta\right)^2\right\}+O\left(\frac{1}{\sqrt{N}}\right).\end{aligned} \tag{120}$$

Inequalities (118)–(120) provide

$$I(k,m)\geqslant c_2\exp\left\{-c_1\frac{\sqrt{N\delta^3}}{\varepsilon}\right\}dx,$$

$$c_1=:\frac{2}{\pi^{3/2}}\left\{\sum_{l\in P}|\beta_l|\right\}\left\{1+O\left(\frac{1}{\sqrt{N}}\right)\right\}\left(\int\eta^2e^{-\eta^2}d\eta\right), \tag{121}$$

$$c_2=:\frac{1}{\pi^{3/2}}\left\{\int|\eta|e^{-\eta^2}d\eta\right\}^2\left\{1+O\left(\frac{1}{\sqrt{N}}\right)\right\}.$$

3°. Inequality (121) tells that the second term on the right-hand side of inequality (115) is much less than the first term on the right-hand side of (115) if $\sigma_0>\frac{1}{4}$ and physical parameters δ, ε are fixed. Therefore, it follows from the (121), (115), and (77) that

$$\begin{aligned}&\sqrt{N}\delta^3 8\pi^2\sum_{k,m\in P}|k||m||\beta_k\beta_m|\int_M|u_ku_mu_{k\pm m}|\exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}dx\\&\leqslant\text{const}\frac{1}{4\pi^2}\left(\frac{\delta^3}{\varepsilon^2}\right)^{\gamma/2}N^{1/2+\sigma_0+\gamma/2}\left\{\sum_{k\in P}|\beta_k|^\gamma\right\}\int_M\left(\sum_{k\in P}\delta^3\nu_k|u_k|^2\right)\exp\left\{-\frac{2\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}dx\end{aligned} \tag{122}$$

for any $1>\gamma>0$.

We showed above that the left-hand side of inequality (122) estimates the left-hand side of (114). Therefore, (114) is a direct consequence of (122). The lemma is proved.

Now, substituting the estimate (114) into the right-hand side of the inequality (112), an estimate is obtained:

$$\int N\delta^3 \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}\left\{|\nabla\Phi|^2 dx+\sum_{k\in P}\delta^3\nu_k|u_k|^2\right\}\leqslant\frac{\overline{\lambda_0}}{1+c/N^\alpha}\int_M \exp\left\{-2\frac{\sqrt{N\delta^3}}{\varepsilon}\Phi\right\}dx \tag{123}$$

$\alpha=:\frac{1}{2}-\sigma_0-\gamma/2$.

Due to the variational principle the inequality (123) produces the inequality (111). So, from estimation from below (75) and estimation from above (111), estimate (35) of the main theorem follows. The theorem is proved.

IV. PROOF OF THE LEMMA 1

Let us consider function $S\exp\{i2\pi\Sigma_{j=1}^N(k_j,x_j)\}$ and suppose that in the set of the vector indexes $k_1,\ldots,k_N$ there are only l vector indexes $k_{j_1},\ldots,k_{j_l}$ different from zero. Without any restriction we can consider that $k_{j_1}=k_1,\ldots,k_{j_l}=k_l$. The number l is called the lengths of the vector index set. Evidently $1\leqslant l\leqslant N$. We prove the lemma by induction on the lengths l at any fixed N. So, for the $l=1$, evidently, $S\exp\{i2\pi\Sigma_{j=1}^N(k_j,x_j)\}=\sqrt{N}u_{k_1}$. Now let us suppose that for the length $1\leqslant l\leqslant n$ the symmetrized harmonic, which is defined as $S\exp\{i2\pi\Sigma_{j=1}^l(k_j,x_j)\}=(1/N!)\,\Sigma_\beta\exp\{i2\pi\Sigma_{m=1}^l(k_m,x_{\beta^{-1}(m)})\}$, can be presented as polynomials in the functions u_k, and prove that it is true for the $l=n+1\leqslant N$. To that end we consider the product

$$N^{(n+1)/2}u_{k_1}\cdots u_{k_{n+1}}=\sum_{m=1}^{n+1}\sum_{\{i_1,\ldots,i_m\}}\sum_{\{\alpha^1\},\ldots,\{\alpha^m\}}A\{i_1,\ldots,i_m;\{\alpha^1,\ldots\alpha^m\}\}\exp(i2\pi)$$
$$\times\left\{\left(\left(\sum_{\nu=1}^{r_1}k_{\alpha_\nu^1}\right),x_{i_1}\right)+\cdots+\left(\left(\sum_{\nu=1}^{r_m}k_{\alpha_\nu^m}\right),x_{i_m}\right)\right\}, \tag{124}$$

where $r_k=|\{\alpha^k\}|$, $A\{\ldots\}$ some integer coefficients.

In that sum at fixed m all subsets $\{i_1,\ldots,i_m\}$ are ordered: $i_1<\cdots<i_m$ and belong to the set $\{1,\ldots,N\}$. Further, at fixed subset $\{i_1,\ldots,i_m\}$ we consider all nonintersecting ordered subsets $\{\alpha^1\},\ldots,\{\alpha^m\}$ of the set $\{1,\ldots,n+1\}$ such that $\Sigma_{i=1}^m r_i=n+1$. It is clear that the terms of the sum (124), corresponding to the values m, are functions depending on m arguments, and the length of vector index sets corresponding to those functions is equal to $n+1$ only at $m=n+1$. In the case $m=n+1$ all subsets $\{\alpha^1\},\ldots,\{\alpha^m\}$ in the summa (124) have only one element $\{\alpha^j\}=\alpha_j$, $j=1,\ldots,n+1$, and $\{\alpha_1,\ldots,\alpha_{n+1}\}$ is some permutation of $\{1,\ldots,n+1\}$. Moreover, in that case, all coefficients $A\{i_1,\ldots,i_m;\{\alpha^1,\ldots\alpha^m\}\}$ are the same, and will be denoted by A. Therefore, subsume from (124), corresponding to the value $m=n+1$ can be presented as follows:

$$\sum_{\{i_{1,\ldots,i_{n+1}}\}}\sum_\alpha A\exp\left\{i2\pi\sum_{j=1}^{n+1}(k_{\alpha_{(j)}^{-1}},x_{i_j})\right\}, \tag{125}$$

where the sum is taken over all permutation α of the set $\{1,\ldots,n+1\}$ and over all ordered subsets $\{i_1,\ldots,i_{n+1}\}$ of the set $\{1,\ldots,N\}$. Evidently, $\Sigma_{j=1}^{n+1}(k_{\alpha_{(j)}^{-1}},x_{i_j})=\Sigma_{m=1}^{n+1}(k_m,x_{i_{\alpha(m)}})$; hence, the sum (125) can be presented as the sum $\Sigma_{\{i_1,\ldots,i_{n+1}\}}\Sigma_\alpha A\exp\{i2\pi\Sigma_{m=1}^{n+1}(k_m,x_{i_{\alpha(m)}})\}$, where the second sum with respect to α is taken over all permutations α of the set $\{1,\ldots,n+1\}$. It is clear that

$$A\sum_{\{i_1,\ldots,i_{n+1}\}}\sum_\alpha\exp\left\{i2\pi\sum_{m=1}^{n+1}(k_m,x_{i_{\alpha(m)}})\right\}=\frac{A}{(N-n-1)!}\sum_\beta\exp\left\{i2\pi\sum_{m=1}^{n+1}(k_m,x_{\beta^{-1}(m)})\right\}, \tag{126}$$

where summa with respect to β is taking over all permutations β of the set $\{1,\ldots,N\}$. Evidently the sum on the right-hand side of (126) is equal to $[AN!/(N-n-1)!]\,S\exp\{i2\pi\Sigma_{j=1}^{n+1}(k_j,x_j)\}$. Hence, a function

$$N^{(n+1)/2}u_{k_1}\cdots u_{k_{n+1}} - \frac{AN!}{(N-n-1)!}S\exp\left\{i2\pi\sum_{j=1}^{n+1}(k_j,x_j)\right\} \tag{127}$$

is the symmetrical function which is equal to the sum of symmetrized harmonics, having the length of the vector index sets not more than n. Therefore, by inductive supposition the function (127) and, hence, the function $S\exp\{i2\pi\Sigma_{j=1}^{n+1}(k_j,x_j)\}$, can be presented as a polynomial in u_k. The lemma is proved.

ACKNOWLEDGMENT

This work was possible through the partial financial support EDI-IPN, CGEPI-IPN 20021170, and CONACYT Project No. 35009-E.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Duality versus dual flatness in quantum information geometry

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(Received 16 August 2002; accepted 20 December 2002)

We investigate questions in quantum information geometry which concern the existence and nonexistence of dual and dually flat structures on stratified sets of density operators on finite-dimensional Hilbert spaces. We show that the set of density operators of a given rank admits dually flat connections for which one connection is complete if and only if this rank is maximal. We prove, moreover, that there is never a dually flat structure on the set of pure states. Thus any general theory of quantum information geometry that involves duality concepts must inevitably be based on dual structures which are nonflat. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556192]

I. INTRODUCTION

The power and strength of classical information geometry and its applications rely in many respects on the fact that in basic situations of interest the spaces under investigation are naturally endowed with the structure of a dually flat manifold (cf. Refs. 1 and 3, see also Sec. II). Of utmost importance is then that naturally associated with the dually flat structure is a distancelike *canonical divergence function*. This divergence yields a variational characterization of geodesic projections on submanifolds by a minimizing property which is crucial for applications (cf. Refs. 2 and 3).

In the last years there has also been great progress in generalizing and extending fundamental concepts and results from classical information geometry to the quantum setting. One now disposes in particular of quantum analogs and versions of the Fisher metric (cf. Refs. 20, 23, 11, 5, and 17) and of α-connections (cf. Refs. 21, 12, 13, and 10). These advances allow, for example, to extend Cramér–Rao type inequalities to the information geometry of positive density operators as well as to pure state estimation theory (cf. Refs. 15, 16, 8, 9, and 18).

On the other hand, for the fundamental spaces of study in quantum information geometry, i.e., the sets of density operators of a given rank on a finite-dimensional Hilbert space, projections and divergence functions which have properties as nice and special as in the classical setting are till now only known to exist in the special case where the operators have maximal rank. Their existence in the full rank case is a simple consequence of dual flatness, using the well-known fact that when equipped with the Boguliobov–Kobu–Mori (BKM) inner product, the complete exponential connection and the (incomplete) mixture connection define a dually flat structure on the set of positive density operators of (cf. Refs. 21 and 3). On the sets of density operators of a given general rank, distinguished dual structures have been constructed by Fujiwara using symmetric logarithmic derivatives (cf. Ref. 7). However, none of the Fujiwara structures is dually flat.

In view of these facts and the importance of the existence of canonical divergence functions one is therefore naturally led to ask to which extent the concept of dual flatness can be carried over and put to use on the sets of density operators of a given nonmaximal rank.

By employing general structure theorems for dually flat manifolds which were obtained in our

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previous work,[4] the present note sets out to answer this question in a systematic way. Motivated by the fact that for the above-mentioned canonical dually flat structure on the set of positive density operators, the exponential connection is complete, we also investigate the existence of dually flat structures with a complete connection. Our main results can be stated as follows:

Theorem A: *There is never a dually flat structure on the set of pure states.*

Theorem B: *The set $\mathcal{S}_r$ of density operators of a given rank r on a Hilbert space of complex dimension $n \in \mathbb{N}$ admits dually flat connections for which one connection is complete if and only if r is maximal, i.e., if and only if $r=n$.*

The remaining parts of the present article are organized as follows: In Sec. II we briefly recall some basic definitions and results from Ref. 4. Section III is the heart of the article. It contains a detailed description of our approach, which emphasizes the differences and similarities between the classical and the quantum setting, and here the proofs of Theorems A and B are given. Section IV is the final one, containing further conclusions and a discussion of other points of interest.

II. PRELIMINARIES

As described in Refs. 1 and 3, a *dual structure* on a Riemannian manifold (M,g) is given by a pair of affine connections ∇ and ∇^* which are dual to each other in the sense that for all vector fields X,Y,Z on M,

$$Xg(Y,Z)=g(\nabla_X Y,Z)+g(Y,\nabla^*_X Z).$$

If in addition both connections ∇ and ∇^* have vanishing torsion and curvature, the pair (∇,∇^*) is said to define a *dually flat structure* on (M,g).

In our previous work[4] we obtained general obstruction and structure results for dually flat manifolds. The ones we will employ in the present note may be stated as follows:

Proposition 2.1:[4] *Compact manifolds with finite fundamental group never admit dually flat structures.*

Proposition 2.2:[4] *Let (M,g,∇,∇^*) be a dually flat manifold. If one of the two connections is complete in the sense that all of its geodesics are defined on the whole real line, then the homotopy groups $\pi_k(M)$ vanish for $2 \leqslant k \in \mathbb{N}$.*

The completeness assumption in Proposition 2.2 guarantees that any two points of the manifold can be joined by a geodesic of the complete connection (cf. Ref. 4). This latter property is, e.g., of special interest in dealing with the problem to define geodesic projections onto general submanifolds.

III. STRATIFICATIONS AND DUALLY FLAT STRUCTURES

To illustrate our results and approach we shall first discuss the following

A. Basic example

Consider the set $X=\{1,2\}$ of elementary events. The set $\overline{\mathcal{P}}$ of classical probability distributions on X consists of the disjoint union of the line segment $\mathcal{P}_2=\{(p_1,p_2)\in\overline{\mathcal{P}} \;:\; p_1,p_2>0\}$ and the two Dirac measures $\mathcal{P}_1=\{\delta_1,\delta_2\}$: $\overline{\mathcal{P}}=\mathcal{P}_1 \uplus \mathcal{P}_2$. Extending this situation to the quantum setting leads to the set $\overline{\mathcal{S}}$ of density operators on $\mathbb{C}^X \cong \mathbb{C}^2$. A concrete realization of $\overline{\mathcal{S}}$ by matrices, the Stokes parametrization (compare, for example, Ref. 22), is given as follows:

$$\overline{\mathcal{S}} \;\cong\; \left\{ \frac{1}{2}\begin{pmatrix} 1+x & y+iz \\ y-iz & 1-x \end{pmatrix} \;:\; x,y,z\in\mathbb{R},\;\; x^2+y^2+z^2 \leqslant 1 \right\}.$$

The set $\overline{\mathcal{S}}$ is diffeomorphic to the closed unit ball in $\mathbb{R}^3$. It can be stratified as $\overline{\mathcal{S}}=\mathcal{S}_1 \uplus \mathcal{S}_2$, where $\mathcal{S}_2$ denotes the set of positive density operators of (maximal) rank two, and $\mathcal{S}_1$ denotes the density operators of rank one. The sets $\mathcal{S}_2$ and $\mathcal{S}_1$ are diffeomorphic to the open three-ball and the two-sphere, respectively.

For $r=2$, both $\mathcal{P}_r$ and $\mathcal{S}_r$ admit a dually flat structure with one complete connection (compare Ref. 4). For $r=1$, $\mathcal{P}_r$ admits a trivial dually flat structure. But according to our first result, Theorem A, there is no dually flat structure on the stratum $\mathcal{S}_1$.

In what follows, we shall show that the main features of the above example generalize to states of any rank and all higher dimensions.

As we shall briefly discuss in the following section, the sets $\mathcal{P}_r$ always admit a dually flat structure with one complete connection. In contrast to this fact, in Sec. III C we will prove that the quantum analog of $\mathcal{P}_r$, the set $\mathcal{S}_r$ of density operators of a given rank r, enjoys this property iff the rank r is maximal, and that the set of pure states $\mathcal{S}_1$ never admits a dually flat structure.

B. The classical setting

Consider a nonempty finite set X and the closed simplex

$$\overline{\mathcal{P}} = \overline{\mathcal{P}}(X) = \left\{ p=(p_x)_{x\in X}\in \mathbb{R}^X \ : \ p_x \geqslant 0 \quad \text{for all } x\in X, \ \sum_{x\in X} p_x = 1 \right\}.$$

The support set of a probability distribution $p\in\overline{\mathcal{P}}(X)$ is defined as $\operatorname{supp} p := \{x\in X \ : \ p_x>0\}$. To each nonempty subset A of X one may associate the corresponding (open) "face"

$$\mathcal{P}(A) := \{p\in\overline{\mathcal{P}} \ : \ \operatorname{supp} p = A\}. \tag{1}$$

Each open face $\mathcal{P}(A)$ is a differentiable submanifold of $\mathbb{R}^X$ of dimension $|A|-1$. It is well known that $\mathcal{P}(A)$ carries a natural dually flat structure which is given by

$$(\mathcal{P}(A), g_A, \nabla_A^{(e)}, \nabla_A^{(m)}), \tag{2}$$

where g_A denotes the Fisher metric, $\nabla_A^{(e)}$ denotes the exponential connection, and $\nabla_A^{(m)}$ denotes the mixture connection. The mixture connection is not complete, whereas the exponential connection is.

We have the stratification

$$\overline{\mathcal{P}} = \biguplus_{\emptyset\neq A\subset X} \mathcal{P}(A). \tag{3}$$

Collecting all faces $\mathcal{P}(A)$ with $|A|=r$ for a fixed r, one obtains

$$\mathcal{P}_r := \{p\in\overline{\mathcal{P}} \ : \ |\operatorname{supp} p| = r\} = \biguplus_{\substack{\emptyset\neq A\subset X \\ |A|=r}} \mathcal{P}(A). \tag{4}$$

Given a subset A of X with r elements, the set $\mathcal{P}_r$ may be considered as the orbit of $\mathcal{P}(A)$ under the permutation group of X. This gives rise to a new stratification

$$\overline{\mathcal{P}} = \biguplus_{r=1}^{|X|} \mathcal{P}_r, \tag{5}$$

which is coarser than the stratification (3). Obviously, each stratum $\mathcal{P}_r$ admits the dually flat structure given by (2).

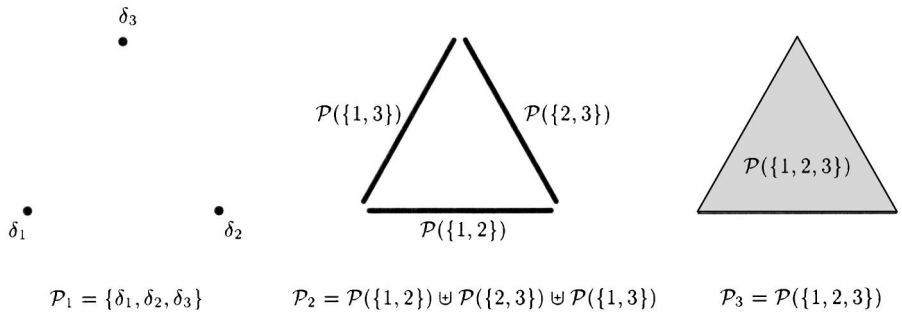

FIG. 1. The two stratifications of $\overline{\mathcal{P}} = \overline{\mathcal{P}}(X)$ for $X = \{1,2,3\}$.

Figure 1 depicts the situation in the case where $X = \{1,2,3\}$.

C. The quantum setting

Let $(H, \langle \cdot, \cdot \rangle)$ be a complex Hilbert space of finite (complex) dimension n, and let $\mathcal{A}$ denote the algebra of linear operators on H. A *density operator* $\rho \in \mathcal{A}$ is characterized by the properties

$$\rho = \rho^*, \quad \rho \geqslant 0, \quad \operatorname{tr} \rho = 1.$$

The set of density operators is denoted by $\overline{\mathcal{S}}$ or $\overline{\mathcal{S}}(H)$. This is a compact and convex set of real dimension

$$\dim_{\mathbb{R}} \overline{\mathcal{S}} \;=\; n^2 - 1.$$

In order to extend the definitions of $\mathcal{P}(A)$ and $\mathcal{P}_r$ to the Hilbert space setting, we have to find a generalized version of the maps $p \mapsto \operatorname{supp} p$ and $A \mapsto |A|$.

A natural candidate for the "support" of a density operator is given by its image:

$$\text{im:} \quad \overline{\mathcal{S}} \quad \to \quad \mathcal{G}(H) := \biguplus_{r=1}^{n} \mathcal{G}_r(H), \quad \rho \mapsto \operatorname{im} \rho.$$

Here, $\mathcal{G}_r(H)$ denotes the Grassmann manifold of (complex) r-dimensional complex subspaces of H, which has real dimension $2r(n-r)$.

Considering the "cardinality" of a subspace A of H to be given by the complex dimension of A, by making use of an orthonormal basis $X = \{x_1, \ldots, x_n\}$ of H we obtain the following commutative diagram:

$$\begin{array}{ccc}
\bar{\mathcal{P}}(X) & \xrightarrow{\iota} & \bar{\mathcal{S}}(H) \\
\Big\downarrow \text{supp} & & \Big\downarrow \text{im} \\
2^X & \xrightarrow{\text{span}} & \mathcal{G}(H) \\
\Big\downarrow |\cdot| & & \Big\downarrow \dim \\
\{1, \ldots, n\} & \xrightarrow{\text{id}} & \{1, \ldots, n\}
\end{array}$$

Here ι is the inclusion map

$$(p_x)_{x \in X} \;\mapsto\; \sum_{x \in X} p_x \, \pi_x \,,$$

where for $x \in X$ the symbol π_x denotes the orthogonal projection onto the subspace $\mathbb{C} \cdot x$, and where "span" assigns to each subset A of X the linear hull of A.

As in (1), to each subspace $A \subset H$ we now associate the (open) A-face of $\overline{\mathcal{S}}$, defined by

$$\mathcal{S}(A) \;:=\; \{\rho \in \overline{\mathcal{S}} \;:\; \operatorname{im} \rho = A\}.$$

This is a convex subset of $\overline{\mathcal{S}}$ of real dimension

$$\dim_{\mathbb{R}} \mathcal{S}(A) = (\dim_{\mathbb{C}} A)^2 - 1,$$

which can be identified with the set of all positive density operators on the Hilbert space A.

It is well known that $\mathcal{S}(A)$ carries a dually flat structure with one complete connection. Moreover, this structure can be chosen in such a way that for each orthonormal basis $X = \{x_1, \ldots, x_r\}$ of A, the ι-pullback of this structure coincides with the structure on $\mathcal{P}(X)$ discussed in Sec. III B (cf. Ref. 3).

We obtain the following analog to the stratification (3):

$$\overline{\mathcal{S}} = \biguplus_{A \in \mathcal{G}(H)} \mathcal{S}(A). \tag{6}$$

Collecting all faces $\mathcal{S}(A)$ with $\dim A = r$ for a fixed r yields now the set of density operators of rank r:

$$\mathcal{S}_r := \{\rho \in \overline{\mathcal{S}} : \operatorname{rank} \rho = r\} = \biguplus_{A \in \mathcal{G}_r(H)} \mathcal{S}(A).$$

The sets $\mathcal{S}_r$ are differentiable manifolds of real dimension $2nr - r^2 - 1$. Notice also that the manifold $\mathcal{S}_1$ is diffeomorphic to $\mathbb{CP}^{n-1}$, the complex projective space of real dimension $2(n-1)$. Its elements are also known as the *pure states*.

Given a subspace $A \in \mathcal{G}_r$, the set $\mathcal{S}_r$ may be considered as the orbit of $\mathcal{S}(A)$ under the unitary group on H. This leads to the following stratification:

$$\overline{\mathcal{S}} = \biguplus_{r=1}^{n} \mathcal{S}_r. \tag{7}$$

The stratification (7) is obviously coarser than the stratification (6). The natural question is therefore if there is also in this case a dually flat structure on the individual strata $\mathcal{S}_r$. Notice also that from $\mathcal{S}_n = \mathcal{S}(H)$ we know that the largest stratum admits a natural dually flat structure.

We first treat the case of pure states (i.e., $r = 1$) which is of special importance in the statistical estimation theory of pure state models (cf. Refs. 8, 9, and 18). The quantum analog of the Fisher metric is here given by the Fubini-Study metric on $\mathcal{S}_1 \cong \mathcal{G}_1$, and it is clear that $\mathcal{S}_1$ admits a multitude of dual structures. However, in contrast to this fact one has the following.

Theorem 3.1: *There exists no dually flat structure on the set $\mathcal{S}_1$ of pure states.*

Proof: The stratum $\mathcal{S}_1$ is diffeomorphic to a complex projective space so that, in particular, its fundamental group is trivial. Proposition 2.1 implies therefore that $\mathcal{S}_1$ does not admit any dually flat structure. □

To deal with the existence problem for dually flat structures on sets of mixed states, we shall employ the following proposition.

Proposition 3.2: The stratum $\mathcal{S}_r$ and the Grassmann manifold $\mathcal{G}_r$ are homotopy equivalent and therefore have isomorphic homotopy groups.

Proof: Given a complex subspace $A \subset H$ of complex dimension r, define the center of the face $\mathcal{S}(A)$ as

$$\rho_A := \frac{1}{\dim A} \text{orthogonal projection onto } A.$$

We will now construct a homotopy equivalence between $\mathcal{G}_r$ and $\mathcal{S}_r$ as follows (compare Fig. 2 for an illustration).

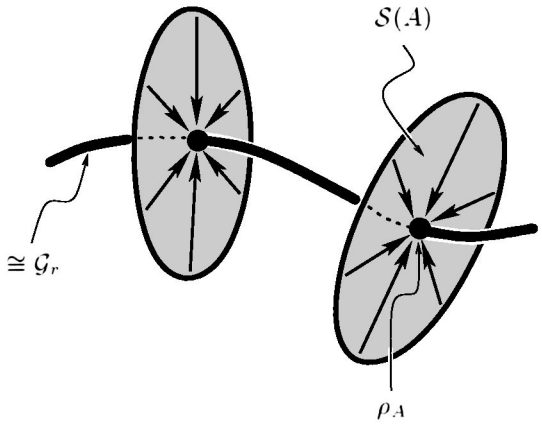

FIG. 2. Homotoping $\mathcal{S}_r$ to $\mathcal{G}_r$.

Consider the following maps:

$$f:\mathcal{G}_r \to \mathcal{S}_r, \quad A \mapsto \rho_A,$$

$$g:\mathcal{S}_r \to \mathcal{G}_r, \quad \rho \mapsto \mathrm{im}\,\rho.$$

Obviously, the composition $g \circ f$ is equal to the identity on $\mathcal{G}_r$. Furthermore, the homotopy

$$F:[0,1]\times\mathcal{S}_r \to \mathcal{S}_r, \quad (t,\rho) \mapsto (1-t)\,\rho + t\,\rho_{\mathrm{im}\,\rho},$$

which satisfies

$$F(0,\cdot) = \mathrm{id}_{\mathcal{S}_r}, \quad F(1,\cdot) = f \circ g,$$

provides a homotopic deformation of the composition $f \circ g$ to the identity on $\mathcal{S}_r$. □

Theorem 3.3: *The set $\mathcal{S}_r$ of density operators of a given rank r on a Hilbert space of complex dimension $n \in \mathbb{N}$ admits dually flat connections for which one connection is complete if and only if r is maximal, i.e., if and only if $r = n$.*

Proof: Notice first that when equipped with the Boguliobov–Kobu-Mori inner product, the exponential and mixture connection define a dually flat structure on the set of density operators of full rank, and that the exponential connection is complete.

Assume now that for $r < n$ there is a dually flat structure with one complete connection on $\mathcal{S}_r$.

According to Proposition 3.2, the manifold $\mathcal{S}_r$ and the Grassmann manifold $\mathcal{G}_r$ have isomorphic homotopy groups.

Using the coset representation $\mathcal{G}_r = \mathrm{SU}(n)/(\,\mathrm{SU}(n) \cap (\mathrm{U}(r) \times \mathrm{U}(n-r))\,)$ of the Grassmannian as a symmetric space (cf., e.g., Ref. 14), one easily sees that $\mathcal{G}_r$ is simply connected. The Hurewicz isomorphism theorem in algebraic topology (cf. Ref. 24) implies therefore that $\mathcal{G}_r$ and $\mathcal{S}_r$ possess at least one higher-dimensional homotopy group which is nontrivial. This, however, contradicts Proposition 2.2.

□

IV. CONCLUSIONS AND FURTHER REMARKS

Any general theory of quantum information geometry must include as a special case a theory of density operators on finite-dimensional Hilbert spaces and, in particular, the estimation theory of quantum pure state models. An important consequence of our results is therefore that any such general theory that involves duality concepts must inevitably be based on dual structures which are nonflat.

As we mentioned in the Introduction, for dually flat manifolds there is a natural as well as important variational characterization of geodesic projections by distancelike divergence func-

tions. We feel that a general theory of dual but not necessarily dually flat structures must extend this divergence concept appropiately. In this regard, special emphasis should be placed on the investigation of dual structures for which the associated connections have vanishing torsion. In fact, for torsion-free dual structures one knows from work of Matumoto (cf. Ref. 19) that any such structure can—though, however, not in a canonical way—be obtained from divergence functions in the sense of Eguchi (cf. Ref. 6).

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Multiresolution analysis generated by a seed function

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(Received 14 October 2002; accepted 17 December 2002)

In this paper we use the equivalence result originally proved by the author, which relates a multiresolution analysis (MRA) of $\mathcal{L}^2(\mathbf{R})$ and an orthonormal set of single electron wave functions in the lowest Landau level, to build up a procedure which produces, starting with a certain square-integrable function, a MRA of $\mathcal{L}^2(\mathbf{R})$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556193]

I. INTRODUCTION

In a series of recent papers,[1–3] we have shown the existence of a relation between any multiresolution analysis (MRA) of $\mathcal{L}^2(\mathbf{R})$ and an orthonormal (o.n.) set of functions of $\mathcal{L}^2(\mathbf{R}^2)$ which (1) belong to the lowest Landau level (LLL), (2) are closed under the action of two commuting unitary translation operators, and (3) can be used to produce a normalized trial ground state for the gas of N electrons. This method has been used up to now to produce different trial ground states for the well-known fractional quantum Hall effect (FQHE). In our previous papers we were mainly interested in using known facts from MRA in order to get information about FQHE. However, already in Refs. 1 and 2, we have also discussed the possibility of reversing the construction, in order to get the coefficients of a MRA, in the sense of Refs. 6 and 7, simply starting from a given single electron o.n. basis closed under the action of two (magnetic) translation operators. To implement this proposal we only need such a set of wave functions: then we immediately have the coefficients of the related MRA.[1,2] However, this approach is not really easy to use, the reason being that there are not many examples of this kind of wave function in the LLL in the literature.[4,5]

In this paper we consider a different possibility. We will show how a given function of $\mathcal{L}^2(\mathbf{R})$ satisfying some extra condition can be used to generate a set of coefficients related to a MRA of $\mathcal{L}^2(\mathbf{R})$.[6,7]

The paper is organized as follows. In Sec. II we quickly review the method proposed in Refs. 1 and 2, without insisting too much on its physical aspects. In Secs. III and IV we show how to use a seed function in order to construct a set of coefficients giving rise to a MRA. In Sec. V we discuss some examples, and we discuss our conclusions in Sec. VI. In the Appendix we prove some easy results on the convolution of sequences which are used in the main body of the paper, results which we were not able to find in the existing literature.

II. THE METHOD

We begin this section with the following remark: in Refs. 2 and 3 the method originally introduced in Ref. 1 has been generalized. This generalization, which is crucial for concrete applications in the analysis of the FQHE, is only an unnecessary complication here and, for this reason, will not be used.

The many-body model of the FQHE consists simply in a two-dimensional electron gas (2DEG)—that is a gas of electrons constrained in a two-dimensional layer—in a positive uniform background and subjected to a uniform magnetic field along z, whose Hamiltonian (for N electrons) is[1]

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$$H^{(N)}=H_0^{(N)}+\lambda(H_C^{(N)}+H_B^{(N)}), \tag{2.1}$$

where $H_0^{(N)}$ is the sum of N contributions:

$$H_0^{(N)}=\sum_{i=1}^{N} H_0(i). \tag{2.2}$$

Here $H_0(i)$ describes the minimal coupling of the ith electron with the magnetic field:

$$H_0=\frac{1}{2}(\underline{p}+\underline{A}(r))^2=\frac{1}{2}\left(p_x-\frac{y}{2}\right)^2+\frac{1}{2}\left(p_y+\frac{x}{2}\right)^2. \tag{2.3}$$

$H_C^{(N)}$ is the canonical Coulomb interaction between charged particles,

$$H_C^{(N)}=\frac{1}{2}\sum_{i\neq j}^{N}\frac{1}{|\underline{r}_i-\underline{r}_j|},$$

and $H_B^{(N)}$ is the interaction of the charges with the background, Ref. 4.

We now consider $\lambda(H_C^{(N)}+H_B^{(N)})$ as a perturbation of the free Hamiltonian $H_0^{(N)}$, and we look for eigenstates of $H_0^{(N)}$ in the form of Slater determinants built up with single electron wave functions. The easiest way to approach this problem consists in introducing the new variables

$$P'=p_x-y/2, \quad Q'=p_y+x/2. \tag{2.4}$$

In terms of P' and Q' the single electron Hamiltonian, H_0, can be written as

$$H_0=\tfrac{1}{2}(Q'^2+P'^2). \tag{2.5}$$

The transformation (2.4) can be seen as a part of a canonical map from (x,y,p_x,p_y) into (Q,P,Q',P') where

$$P=p_y-x/2, \quad Q=p_x+y/2. \tag{2.6}$$

These operators satisfy the following commutation relations:

$$[Q,P]=[Q',P']=i, \quad [Q,P']=[Q',P]=[Q,Q']=[P,P']=0. \tag{2.7}$$

It is shown in Refs. 8 and 9 that a wave function in the (x,y) space is related to its PP' expression by

$$\Psi(x,y)=\frac{e^{ixy/2}}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{i(xP'+yP+PP')}\Psi(P,P')\,\mathrm{d}P\,\mathrm{d}P', \tag{2.8}$$

which can be easily inverted:

$$\Psi(P,P')=\frac{e^{-iPP'}}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(xP'+yP+xy/2)}\Psi(x,y)\,\mathrm{d}x\,\mathrm{d}y. \tag{2.9}$$

The usefulness of the PP' representation stems from the expression (2.5) of H_0. Indeed, in this representation, the single electron Schrödinger equation admits eigenvectors $\Psi(P,P')$ of H_0 of the form $\Psi(P,P')=f(P')h(P)$. Thus the ground state of (2.5) must have the form $f_0(P')h(P)$, where

$$f_0(P')=\pi^{-1/4}e^{-P'^2/2}, \tag{2.10}$$

while the function $h(P)$ is arbitrary, which manifests the degeneracy of the LLL, and should be fixed by the interaction. With f_0 as in Eq. (2.10), formula (2.8) becomes

$$\psi(x,y)=\frac{e^{ixy/2}}{\sqrt{2}\,\pi^{3/4}}\int_{-\infty}^{\infty}e^{iyP}e^{-(x+P)^2/2}h(P)\,\mathrm{d}P, \tag{2.11}$$

while, using (2.9), $h(P)$ can be written in terms of $\psi(x,y)$ as

$$h(P)=\frac{e^{-iPP'+P'^2/2}}{2\,\pi^{3/4}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(xP'+yP+xy/2)}\Psi(x,y)\,\mathrm{d}x\,\mathrm{d}y\,. \tag{2.12}$$

Let us now define the so-called magnetic translation operators $T(\vec{a}_i)$ for a square lattice with basis $\vec{a}_1=a(1,0)$, $\vec{a}_2=a(0,1)$, $a^2=2\pi$,[1] by

$$T_1:=T(\vec{a}_1)=e^{iaQ},\quad T_2:=T(\vec{a}_2)=e^{iaP}. \tag{2.13}$$

We see that, due to (2.7) and to the condition on the cell of the lattice, $a^2=2\pi$,

$$[T(\vec{a}_1),T(\vec{a}_2)]=[T(\vec{a}_1),H_0]=[T(\vec{a}_2),H_0]=0. \tag{2.14}$$

The action of the T's on a generic function $f(x,y)\in\mathcal{L}^2(\mathbf{R}^2)$ is the following:

$$f_{m,n}(x,y):=T_1^mT_2^nf(x,y)=(-1)^{mn}e^{i(a/2)(my-nx)}f(x+ma,y+na). \tag{2.15}$$

This formula shows that, if for instance $f(x,y)$ is localized around the origin, then $f_{m,n}(x,y)$ is localized around the site $a(-m,-n)$ of the square lattice.

Now we have all the ingredients to construct the ground state of $H_0^{(N)}$ mimicking the classical procedure. We simply start from the single electron ground state of H_0 given in (2.11), $\psi(x,y)$. Then we construct a set of copies $\psi_{m,n}(x,y)$ of ψ as in (2.15), with $m,n\in\mathbf{Z}$. All these functions still belong to the lowest Landau level for any choice of the function $h(P)$ due to (2.14). N of these wave functions $\psi_{m,n}(x,y)$ are finally used to construct a Slater determinant for the finite system:

$$\psi^{(N)}(\underline{r}_1,\underline{r}_2,\ldots,\underline{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_{m_1,n_1}(\underline{r}_1) & \psi_{m_1,n_1}(\underline{r}_2) & \cdots & \psi_{m_1,n_1}(\underline{r}_N)\\ \psi_{m_2,n_2}(\underline{r}_1) & \psi_{m_2,n_2}(\underline{r}_2) & \cdots & \psi_{m_2,n_2}(\underline{r}_N)\\ . & . & \cdots & .\\ . & . & \cdots & .\\ . & . & \cdots & .\\ \psi_{m_N,n_N}(\underline{r}_1) & \psi_{m_N,n_N}(\underline{r}_2) & \cdots & \psi_{m_N,n_N}(\underline{r}_N)\end{vmatrix}. \tag{2.16}$$

It is known, Ref. 4, that in order to have $\langle\psi^{(N)},\psi^{(N)}\rangle=1$ for all N we need to have

$$\langle\psi_{m_i,n_i}\psi_{m_j,n_j}\rangle=\delta_{m_i,m_j}\delta_{n_i,n_j}. \tag{2.17}$$

Let $\psi(x,y)$ be as in (2.11) and $\psi_{m,n}(x,y)=T_1^mT_2^n\psi(x,y)=(-1)^{mn}e^{i(a/2)(my-nx)}\psi(x+ma,y+na)$. After few computations and again using condition $a^2=2\pi$, we get

$$\psi_{m,n}(x,y)=\frac{e^{i(xy/2)+iamy}}{\sqrt{2}\,\pi^{3/4}}\int_{-\infty}^{\infty}\mathrm{d}P\,e^{i(y+na)P-(x+ma+P)^2/2}h(P). \tag{2.18}$$

We have discussed in Ref. 1 conditions on $h(P)$ such that equality (2.17), or its equivalent form

$$\tilde{S}_{m,n} := \langle \psi_{0,0}, \psi_{m,n} \rangle = \delta_{m,0}\delta_{n,0}, \quad \forall m,n \in \mathbf{Z}, \tag{2.19}$$

are satisfied. With the above-given definitions we find

$$\tilde{S}_{l_1,l_2} = \int_{-\infty}^{\infty} \mathrm{d}p\, e^{-il_2 ap}\overline{h(p-l_1 a)}h(p), \tag{2.20}$$

which restates the problem of the orthonormality of the wave functions in terms of $h(P)$. In particular we see that, for $m=n=0$, this equation implies that ψ_{00} is normalized in $\mathcal{L}^2(\mathbf{R}^2)$ if and only if $h(P)$ is normalized in $\mathcal{L}^2(\mathbf{R})$. This reflects the unitarity of the transformation (2.8), which, more in general, implies that any o.n. set in $\mathcal{L}^2(\mathbf{R})$ is mapped into an o.n. set in $\mathcal{L}^2(\mathbf{R}^2)$.

In the above-given construction we are considering a square lattice in which all the lattice sites are occupied by an electron. We say that the *filling factor* ν is equal to 1. We have seen in Ref. 1 that, in order to construct an o.n. set of functions in the LLL corresponding to a filling $\nu=\frac{1}{2}$ (only half of the lattice sites are occupied), we have to replace (2.19) and (2.20) with the following slightly weaker condition:

$$S_{l_1,l_2} = \tilde{S}_{l_1,2l_2} = \int_{-\infty}^{\infty} \mathrm{d}p\, e^{-2il_2 ap}\overline{h(p-l_1 a)}h(p) = \int_{-\infty}^{\infty} \mathrm{d}p\, e^{il_1 ap}\overline{\hat{h}(p-2l_2 a)}\hat{h}(p) = \delta_{l_1,0}\delta_{l_2,0}, \tag{2.21}$$

for all $l_1, l_2 \in \mathbf{Z}$, where $\hat{h}(p) = (1/\sqrt{2\pi}) \int_{\mathbf{R}} e^{-ipx}h(x)\mathrm{d}x$ is the Fourier transform of $h(x)$. If $h(x)$ satisfies (2.21), then, defining

$$h_n = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} \mathrm{d}p\, e^{-inxa}h(x), \tag{2.22}$$

it is easily checked that

$$\sum_{n\in\mathbf{Z}} h_n\overline{h_{n+2l}} = \delta_{l,0}. \tag{2.23}$$

The proof of this claim, contained in Ref. 1, is based on condition (2.21) and on the use of the Poisson summation formula (PSF), which we write here as

$$\sum_{n\in\mathbf{Z}} e^{inxc} = \frac{2\pi}{|c|}\sum_{n\in\mathbf{Z}} \delta\left(x - n\frac{2\pi}{c}\right). \tag{2.24}$$

It is well known that the PSF does not always hold, and conditions for its validity are given in several papers and books, see Ref. 10, p. 298, and references therein, for instance. In this paper we will always assume its validity, and from time to time we will check it explicitly.

Equation (2.23) shows how a function $h(x)$, satisfying the orthonormality condition (ONC) (2.21), can be used to generate, via (2.22), a set of coefficients which are related to a MRA.[6,7,11] This procedure can be extended in many ways which are not relevant here,[1–3] and therefore will not be considered in this paper. In Ref. 2 is also discussed in some detail the role of the Zak transform in our procedure, while a detailed summary of our results can be found in Ref. 12.

Several problems arise at this point.

(1) Is there any simple way to construct functions $h(x)$ which solve the ONC (2.21)? Of course, any o.n. basis $\Psi_{n,m}(x,y)$ arising in the analysis of the FQHE could be used to construct such a $h(x)$, but the literature is rather poor of these examples.[4,5]
(2) Equation (2.23) is not the only condition which should be satisfied by a set of complex numbers in order to get a MRA of $\mathcal{L}^2(\mathbf{R})$, see Refs. 6, 7, and 11 and the following definition. What can be said about the other conditions?

We will consider the first point above in Sec. III. Point (2) will be analyzed in Sec. IV.

We end this section by the following.

Definition: We call *relevant* any sequence $h=\{h_n, n\in\mathbf{Z}\}$ which satisfies the following properties:

$$\text{(r1)} \qquad \sum_{n\in\mathbf{Z}} h_n\overline{h_{n+2l}}=\delta_{l,0};$$

$$\text{(r2)} \qquad h_n=O\left(\frac{1}{1+|n|^2}\right), \quad n\gg 1;$$

$$\text{(r3)} \qquad \sum_{n\in\mathbf{Z}} h_n=\sqrt{2};$$

$$\text{(r4)} \qquad H(\omega)=\frac{1}{\sqrt{2}}\sum_{n\in\mathbf{Z}} h_n e^{-i\omega n}\neq 0, \ \forall\,\omega\in\left[-\frac{\pi}{2},\frac{\pi}{2}\right].$$

The role of relevant sequences in connection with MRA is explained in Refs. 6, 7, and 11, for instance, and will not be discussed here.

III. THE SEED FUNCTION, PART ONE

In this section we will show how to find, under very general assumptions, sequences satisfying condition (r1) by making use of the approach outlined in Sec. II. In particular we will show how, starting with a given *seed function* $h\in\mathcal{L}^2(\mathbf{R})$, we can obtain another function H satisfying the ONC (2.21) and, as a consequence, a set of coefficients defined as in (2.22) which satisfies condition (r1). As will appear evident, a crucial role is played by formulas (2.8) and (2.12).

Let $h(P)$ be a generic square integrable function. Using formula (2.8) we get a function

$$\Psi_h(x,y)=\frac{e^{ixy/2}}{\sqrt{2}\,\pi^{3/4}}\int_{-\infty}^{\infty} e^{iyP}e^{-(x+P)^2/2}h(P)\,\mathrm{d}P,$$

which belongs to the LLL independently of the choice of $h(P)$. Using T_1 and T_2 we define other functions, still belonging to the LLL, as in (2.15):

$$\Phi_{h,\underline{l}}(\underline{r})=T_1^{l_1}T_2^{2l_2}\Psi_h(x,y)=e^{-i/2(\tilde{X}_{\underline{l}}y-\tilde{Y}_{\underline{l}}x)}\Psi_h(\underline{r}-\tilde{\underline{R}}_{\underline{l}}), \tag{3.1}$$

where we use the notation $\underline{l}=(l_1,l_2)$, and we have defined $\tilde{\underline{R}}_{\underline{l}}=(\tilde{X}_{\underline{l}},\tilde{Y}_{\underline{l}})=-a(l_1,2l_2)$. Notice that, since we are considering even powers of T_2, we obtain a set of normalized wave functions of the LLL corresponding to a filling $\nu=\frac{1}{2}$ which are mutually orthogonal whenever the seed function $h(P)$ satisfies the ONC (2.21),[1] and, via (2.22) also a set of coefficients h_n satisfying (r1). However, in general, $h(P)$ does not satisfy (2.21). We want to show here the way in which a function $H(P)$ satisfying the ONC can be obtained starting from this original h. The function $H(P)$ will be used to define some coefficients as shown in (2.22).

First of all we use the set $\mathcal{I}_\Phi=\{\Phi_{h,\underline{l}}, \underline{l}\in\mathbf{Z}^2\}$ to construct another set of functions, still belonging to the LLL, by considering the following superposition:

$$\chi_{\underline{n}}(\underline{r})=\sum_{\underline{l}\in\mathbf{Z}^2} f_{\underline{l}}\Phi_{h,\underline{l}+\underline{n}}(\underline{r}), \tag{3.2}$$

where $\underline{n}=(n_1,n_2)$. The set $\mathcal{I}_\chi=\{\chi_{\underline{n}}, \underline{n}\in\mathbf{Z}^2\}$ shares with $\mathcal{I}_\Phi$ the property of being closed under the action of the magnetic translations:

$$\chi_{\underline{n}}(\underline{r}) = T_1^{n_1} T_2^{n_2} \chi_{\underline{0}}(\underline{r}). \tag{3.3}$$

For this reason we can consider $\chi_{\underline{0}}(\underline{r})$ as a function in the LLL obtained from a $H(P)$, different from the seed function h, via the same transformation (2.8), $\chi_{\underline{0}}(\underline{r}) = \phi_H(\underline{r})$, so that $H(P)$ can be obtained from $\chi_{\underline{0}}(\underline{r})$ by considering the inverse transformation (2.12). The coefficients $f_{\underline{l}}$ will now be fixed by requiring that the set $\mathcal{I}_\chi$ is made of o.n. functions:

$$\langle \chi_{\underline{n}}, \chi_{\underline{0}} \rangle = \delta_{\underline{n},\underline{0}} = \delta_{n_1,0}\delta_{n_2,0}, \tag{3.4}$$

for all integers n_1 and n_2. Using (3.2) and the following equality,

$$S^{(h)}_{\underline{l}+\underline{n}} = \langle \Phi_{h,\underline{l}+\underline{n}}, \Phi_{h,\underline{0}} \rangle = \langle \Phi_{h,\underline{l}}, \Phi_{h,-\underline{n}} \rangle, \tag{3.5}$$

which follows from the unitarity of T_i and from (3.3), the orthonormality constraint (3.4) becomes

$$\sum_{\underline{l},\underline{s} \in \mathbf{Z}^2} \overline{f_{\underline{l}}} f_{\underline{s}} S^{(h)}_{\underline{l}+\underline{n}-\underline{s}} = \delta_{\underline{n},\underline{0}}. \tag{3.6}$$

Incidentally we recall that $S^{(h)}_{\underline{l}}$ can be rewritten in terms of the seed function as in (2.21). We use here $S^{(h)}_{\underline{l}}$ instead of the simplest $S_{\underline{l}}$ to emphasize the role of the seed function h. Introducing the following functions:

$$F(\underline{p}) = \sum_{n \in \mathbf{Z}^2} f_{\underline{n}} e^{i\underline{p}\cdot\underline{n}}, \quad S^{(h)}(\underline{p}) = \sum_{n \in \mathbf{Z}^2} S^{(h)}_{\underline{n}} e^{i\underline{p}\cdot\underline{n}}, \tag{3.7}$$

Eq. (3.6) can be rewritten as $|F(\underline{p})|^2 S^{(h)}(\underline{p}) = 1$, whose solution is

$$F(\underline{p}) = \frac{e^{i\varphi(\underline{p})}}{\sqrt{S^{(h)}(\underline{p})}}, \tag{3.8}$$

$\varphi(\underline{p})$ being a generic real function. To simplify the treatment, we will put $\varphi(\underline{p}) = 0$ from now on. We will comment on this choice at the end of Sec. V. Notice that since the coefficients $S^{(h)}_{\underline{n}}$ satisfy the relation $S^{(h)}_{\underline{n}} = \overline{S^{(h)}_{-\underline{n}}}$, then $S^{(h)}(\underline{p})$ is a real function, which is surely non-negative. In order to avoid problems with possible divergences arising when $S^{(h)}(\underline{p}) = 0$, we will try to consider in the following only those seed functions for which $S^{(h)}(\underline{p})$ is strictly positive.

Once the function $F(\underline{p})$ is known, obtaining the coefficients $f_{\underline{s}}$ is quite straightforward:

$$f_{\underline{s}} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} d^2\underline{p} \frac{e^{-i\underline{p}\cdot\underline{s}}}{\sqrt{S^{(h)}(\underline{p})}}. \tag{3.9}$$

It is not difficult to explicitly check this result: if we use (3.9) in the expansion (3.2), we recover $\langle \chi_{\underline{n}}, \chi_{\underline{0}} \rangle = \delta_{\underline{n},\underline{0}}$, as expected. In the proof of this statement the PSF has to be used.

The coefficients $f_{\underline{s}}$ and Eq. (3.2) produce a function $\chi_{\underline{0}}(\underline{r})$ which, together with its magnetic translated $\chi_{\underline{n}} = T_1^{n_1} T_2^{2n_2} \chi_{\underline{0}}$, gives rise to an o.n. set in the LLL, for $\nu = \frac{1}{2}$. By making use of Eq. (2.12) we obtain a square integrable function $H(P)$ which, as a consequence of this fact, satisfies the ONC (2.21):

$$H(P) = \frac{e^{-iPP' + P'^2/2}}{2\pi^{3/4}} \sum_{\underline{l} \in \mathbf{Z}^2} f_{\underline{l}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(xP' + yP + xy/2)} \Phi_{h,\underline{l}}(x,y)\, dx\, dy.$$

After some minor computation and using the integral expression for $\Phi_{h,\underline{l}}$, we get

$$H(P)=\sum_{\underline{l}\in\mathbf{Z}^2} f_{\underline{l}}h(P-al_1)e^{-2iaPl_2}. \tag{3.10}$$

In other words, we conclude that, given a seed function $h(P)$, the function $H(P)$ as defined earlier, with the coefficients $f_{\underline{l}}$ given in (3.9), satisfies the following ONC:

$$\int_{-\infty}^{\infty} H(P)\overline{H(P-al_1)}e^{-2iaPl_2}\,\mathrm{d}P=\int_{-\infty}^{\infty} H(P)\overline{H(P+\tilde{X}_{\underline{l}})}e^{iP\tilde{Y}_{\underline{l}}}\,\mathrm{d}P=\delta_{l_1,0}\delta_{l_2,0}. \tag{3.11}$$

We can now use $H(P)$ to find the coefficients of the MRA as in (2.22):

$$H_n=\frac{1}{\sqrt{a}}\int_{-\infty}^{\infty}\mathrm{d}p\, e^{-inxa}H(x)=\sqrt{a}\hat{H}(na), \tag{3.12}$$

where $\hat{H}(p)$ is the Fourier transform of the function $H(x)$. These coefficients, for what has been discussed in Sec. II, automatically satisfy condition (r1):

$$\sum_{n\in\mathbf{Z}} H_n\overline{H_{n+2l}}=\delta_{l,0}, \tag{3.13}$$

simply as a consequence of (3.11). Introducing the Fourier transform of the function $h(x)$, $\hat{h}(p)$, the integral in (3.12) can be written as

$$H_n=\sqrt{a}\sum_{\underline{l}\in\mathbf{Z}^2} f_{\underline{l}}\hat{h}((n+2l_2)a), \tag{3.14}$$

which is the expression of the coefficients in terms of the seed function. Making use of the PSF this expression can be further simplified. In fact, summing over l_1, we get

$$H_n=\sqrt{a}\sum_{s\in\mathbf{Z}} c_s\hat{h}((n+2s)a), \tag{3.15}$$

where we have defined the new coefficients c_s as follows:

$$c_s=\frac{1}{2\pi}\int_0^{2\pi}\frac{e^{-ips}\,\mathrm{d}p}{\sqrt{S^{(h)}(0,p)}}. \tag{3.16}$$

Remark: In the above-mentioned procedure we have made essentially no requirement on $h(x)$. In particular, we have not assumed that h satisfies the ONC (2.21) from the very beginning, but we have asked $S^{(h)}(0,p)$ to be nonzero in $[0,2\pi[$. This is the reason why we had to construct, starting from h, a new function H which *does satisfy* the ONC. It is interesting to remark that, whenever h is already a solution of condition (2.21), $H(x)$ coincides with $h(x)$. In fact, under this assumption, $S^{(h)}_{\underline{l}}=\delta_{\underline{l},\underline{0}}$, so that $S^{(h)}(\underline{p})=1$. Therefore $f_{\underline{l}}=\delta_{\underline{l},\underline{0}}$ and, see (3.10), $H(P)=h(P)$. This will happen, for instance, in Examples 1 and 2 in the following.

Before going on to consider the other requirements of the relevant sequences, we give the following summation rules, which can be deduced from the above-given definitions and from the PSF. We have

$$\sum_{r_1\in\mathbf{Z}} S^{(h)}_{r_1,r_2}=a\sum_{r_1\in\mathbf{Z}}\hat{h}(ar_1)\overline{\hat{h}((r_1-2r_2)a)},\quad \text{for all fixed } r_2\in\mathbf{Z}, \tag{3.17}$$

$$\sum_{r_2\in\mathbf{Z}} S^{(h)}_{r_1,r_2}=\frac{a}{2}\sum_{r_2\in\mathbf{Z}} h\left(\frac{ar_2}{2}\right)\overline{h\left(\frac{a}{2}(r_2-2r_1)\right)},\quad \text{for all fixed } r_1\in\mathbf{Z}, \tag{3.18}$$

$$\sum_{\underline{r}\in\mathbf{Z}^2} S^{(h)}_{\underline{r}}=a\sum_{\underline{r}\in\mathbf{Z}^2}\hat{h}(ar_1)\overline{\hat{h}((r_1-2r_2)a)}=\frac{a}{2}\sum_{\underline{r}\in\mathbf{Z}^2} h\left(\frac{ar_2}{2}\right)\overline{h\left(\frac{a}{2}(r_2-2r_1)\right)}=S^{(h)}(\underline{0}), \tag{3.19}$$

$$\sum_{s\in\mathbf{Z}}|c_s|^2=\frac{1}{2\pi}\int_0^{2\pi}\frac{\mathrm{d}p}{|S^{(h)}(0,p)|}, \tag{3.20}$$

$$\sum_{s\in\mathbf{Z}} c_s=\frac{1}{\sqrt{S^{(h)}(\underline{0})}}. \tag{3.21}$$

The proofs of all these equalities are trivial and will not be given here.

IV. THE SEED FUNCTION, PART TWO

In the following we move our attention to the conditions that a seed function $h(x)$ must satisfy in order to produce, via formula (3.15), a set of coefficients $\{H_n\}$ which satisfies conditions (r2)–(r4) of Sec. II. This will conclude the construction of our relevant sequences.

A. On the asymptotic behavior of H_n

We are interested here in finding conditions on $h(x)$ which implies condition (r2). Before considering this problem, it may be interesting to observe that, due to definition (3.12), there exists an easy way to characterize the situation which produces a finite sequence of coefficients H_n: using the same notations as in Ref. 13 we say that $H=\{H_n, n\in\mathbf{Z}\}$ belongs to f, the set of all the complex sequences with only a finite number of nonzero entries, if and only if $\hat{H}(p)$ is compactly supported. Unfortunately, the analysis of the support of $\hat{H}(p)$ could be a hard problem, so that this result is of little practical use. More useful is to approach this problem within the framework of convolutions of sequences. We refer to the Appendix for some results on this topic which will be used here. In fact, it is not hard to check that formula (3.15) can be rewritten in terms of convolutions. Defining two sequences related to $\hat{h}(na)$ as

$$\hat{h}^{(\mathrm{even})}_k=\hat{h}(2ka),\quad \hat{h}^{(\mathrm{odd})}_k=\hat{h}((2k+1)a), \tag{4.1}$$

which share with $\hat{h}$ the same asymptotic behavior, we can write $H_n=\sqrt{a}\Sigma_{s\in\mathbf{Z}} c_s\hat{h}((n+2s)a)$ as follows:

$$\begin{aligned} H_{2n}&=\sqrt{a}(\overline{c}*\hat{h}^{(\mathrm{even})})_n,\\ H_{2n+1}&=\sqrt{a}(\overline{c}*\hat{h}^{(\mathrm{odd})})_n, \end{aligned} \tag{4.2}$$

where we have used that $\overline{c_s}=c_{-s}$ and we have defined $(a*b)_n=\Sigma_{s\in\mathbf{Z}} a_s b_{n-s}$.

We see from (4.2) that H_n has the same behavior for large n as $(\overline{c}*\hat{h})_n$, where $\hat{h}_n=\hat{h}(na)$. In order to get information about the asymptotic behavior of H_n, we therefore have to consider the behavior of the sequences $\{c_n\}$ and $\{\hat{h}_n\}$. In particular, the decay features of $\hat{h}_n$ are given by the explicit expression of the seed function $h(x)$ and of its Fourier transform $\hat{h}(p)$. The situation is not so simple for the coefficients c_n, whose definition (3.16) refers to the function

$$\sigma(p)=\frac{1}{\sqrt{S^{(h)}(0,p)}},$$

and, via ((2.21),(3.7)), to the seed function itself. The asymptotic behavior of the c_n can be deduced using standard techniques in the Fourier series theory: whenever $\sigma(p)$ has $n-1$ continuous derivatives and the nth derivative has a finite number of discontinuities in $[0,2\pi[$, then the c_s goes like $1/|s|^{n+1}$. Of course, this hypothesis is satisfied whenever $S^{(h)}(0,p)$ is n-times differentiable and is strictly positive for $p\in[0,2\pi[$. Instead of finding conditions on the seed function for this hypothesis to be satisfied we mention here a class of *good* examples which will be discussed in more detail in the next section, together with many other examples.

Let k be a natural number and let $\hat{h}_k(p)$ be defined as follows;

$$\hat{h}_k(p)=\begin{cases}\dfrac{1}{\sqrt{(2k+1)a}}, & p\in[0,(2k+1)a[\\ 0 \quad \text{otherwise,}\end{cases} \tag{4.3}$$

then the related coefficients $H_n^{(k)}$ satisfy condition (r1) for all values of k and decrease faster than any inverse power of $|n|$, so that they also satisfy condition (r2). This follows from the compact support of $\hat{h}_k(p)$ and from the C^∞ nature of the function $\sigma(p)$ generated by $\hat{h}_k(p)$.

B. About the condition $\Sigma_{n\in\mathbf{Z}} H_n=\sqrt{2}$

Here we want to find conditions on the seed function $h(x)$ which ensures the validity of condition (r3). Again, we will make use several times of the PSF, which will be assumed to hold.

Under this assumption it is not difficult to prove that

Proposition: The set of coefficients (3.15) satisfies condition (r3) if and only if

$$\sum_{n\in\mathbf{Z}}\hat{h}(na)=\sqrt{\frac{2}{a}S^{(h)}(0)}. \tag{4.4}$$

Proof: From the definition (3.15) we see that (r3) is satisfied whenever $\Sigma_{s,n\in\mathbf{Z}}c_s\hat{h}((n+2s)a)=\sqrt{2/a}$. Introducing the integer $m=n+2s$ and using Eq. (3.21), we get equality (4.4). The converse is straightforward.

Another result related to this is the following.

Corollary: Whenever the PSF can be applied, a necessary condition for (r3) to hold is that

$$\sum_{n,m\in\mathbf{Z}}\hat{h}(na)\overline{[\hat{h}(ma)-2\hat{h}((n-2m)a)]}=0 \tag{4.5}$$

is satisfied. Furthermore, if $\hat{h}(p)$ has a finite support in $\mathbf{R}$, then the above-given condition reads

$$\sum_{n\in\mathbf{N}}(-1)^n\hat{h}(na)=0. \tag{4.6}$$

Proof: The first statement directly follows from the previous proposition and from Eq. (3.19). Formula (4.6) follows from (4.5) and from a direct computation, assuming that $\hat{h}(p)$ is equal to zero outside a given interval $[-N_1a,N_2a[$, for any $N_1,N_2=0,1,2,3,\ldots$. Under these conditions it is easy to check that

$$\sum_{n,m\in\mathbf{Z}}\hat{h}(na)\overline{[\hat{h}(ma)-2\hat{h}((n-2m)a)]}=-\left|\sum_{n\in\mathbf{Z}}(-1)^n\hat{h}(na)\right|^2,$$

so that (4.6) follows.

C. About the condition $H(\omega)\neq 0,\ \forall \omega\in[-\pi/2,\pi/2]$

Let $H(\omega)$ be defined as in (r4),

$$H(\omega)=\frac{1}{\sqrt{2}}\sum_{n\in\mathbf{Z}} H_n e^{-i\omega n}, \tag{4.7}$$

with H_n as in (3.15). Then we can rewrite $H(\omega)$ as follows:

$$H(\omega)=\sqrt{\frac{a}{2}}\mathcal{K}(2\omega)\mathcal{H}(-\omega),$$

where

$$\mathcal{K}(\omega)=\sum_{s\in\mathbf{Z}} c_s e^{i\omega s},\quad \mathcal{H}(\omega)=\sum_{s\in\mathbf{Z}} \hat{h}(sa)^{i\omega s}. \tag{4.8}$$

Due to the equality $c_{-s}=\overline{c_s}$ we can check that $\mathcal{K}$ is a real function. Moreover, we can also check that $\mathcal{K}(2\omega)\neq 0$ for all $\omega\in[-\pi/2,\pi/2]$ or, equivalently, that $\mathcal{K}(\nu-\pi)\neq 0$ for all $\nu\in[0,2\pi]$. The proof of this statement follows again from the PSF. In particular we can check that

$$\mathcal{K}(\nu-\pi)=\begin{cases}\dfrac{1}{\sqrt{S^{(h)}(0,\nu+\pi)}} & \text{if } 0\leqslant\nu<\pi\\[2ex] \dfrac{1}{\sqrt{S^{(h)}(0,\nu-\pi)}} & \text{if } \pi\leqslant\nu\leqslant 2\pi,\end{cases} \tag{4.9}$$

and for this reason $H(\omega)$ is different from 0 in $[-\pi/2,\pi/2]$ if and only if $\mathcal{H}(\omega)\neq 0$ in $[-\pi/2,\pi/2]$, condition which is easier to verify since it is directly linked to the seed function $\hat{h}(p)$. In the next section we will discuss examples of seed functions satisfying this condition.

Remarks: (1) One can think that analogous results could be obtained in a completely different (and, maybe, more natural) way, that is by starting from a given *seed sequence* $\{h_n, n\in\mathbf{Z}\}$, normalized in $l^2(\mathbf{Z})$, and by defining a new sequence $H_n=\Sigma_{s\in\mathbf{Z}} c_s h_{n+s}$. The problem should be now finding conditions on c_s such that properties (r1)–(r4) are satisfied. It is not very hard to check that, even if this approach does not seem to be very different from what we have done, it is quite difficult to obtain reasonable conditions on c_s: what is missing, from our point of view, is the possibility of mapping the problem into complete different settings, in which the requirement $\Sigma_{n\in\mathbf{Z}} H_n\overline{H}_{n+2l}=\delta_{l,0}$ can be considered simply as an orthonormality requirement between wave functions in a certain subspace of $\mathcal{L}^2(\mathbf{R}^2)$.

(2) It may be useful to remark also that the generic use of the sentence *whenever the PSF holds* is related to the fact that several inequivalent hypotheses could be checked in order to ensure the validity of the PSF. For instance, multiplying formula (2.24) for a function $\varphi(x)$ and integrating over $\mathbf{R}$, we know that the equality holds for instance (1) if φ belongs to $\mathcal{S}$ or (2) if φ belongs to $\mathcal{L}^1(\mathbf{R})$ and is continuous and with bounded variation or (3) if φ is continuous and if $\sup_{x\in\mathbf{R}}(|\varphi(x)|+|\hat{\varphi}(x)|)(1+|x|)^{1+\epsilon}<\infty$. Moreover, we will find in the next section other situations in which none of these conditions are satisfied but, nevertheless, the validity of the PSF can be explicitly proved. In conclusion, we find that the most economical way to handle with the PSF is simply to check its validity whenever it is needed.

V. EXAMPLES

This section is devoted to an analysis of several applications of the construction outlined in Secs. III and IV.

Example 1: Let us consider the following function, defined in the momentum space:

$$\hat{h}(p)=\begin{cases}\dfrac{1}{\sqrt{a}}, & p\in[0,a[\\ 0 \quad \text{otherwise.}\end{cases} \tag{5.1}$$

This is a normalized function in $\mathcal{L}^2(\mathbf{R})$, and the coefficients $S_{\underline{l}}^{(h)}$, defined as in (2.21), are all zero but when $l_1=l_2=0$: $S_{\underline{l}}^{(h)}=\delta_{\underline{l},\underline{0}}$. Therefore $S^{(h)}(\underline{p})=1$ and, as a consequence of (3.16), $c_s=\delta_{s,0}$. Therefore $H_n=\sqrt{a}\hat{h}(na)=\delta_{n,0}$, which clearly satisfies (r1), (r2), and (r4) but does not satisfy condition (r3). Furthermore, it is easy to check that all the sum rules given in Sec. III are satisfied. For instance, it is straightforward to check explicitly Eq. (3.21). This shows that the PSF can be applied also for a function $\sigma(p)=1$, which does not fit any of the hypotheses given before.

Example 2: Let us consider the following function, defined again in the momentum space:

$$\hat{h}(p)=\begin{cases}\dfrac{1}{\sqrt{2a}}, & p\in[0,2a[\\ 0 \quad \text{otherwise.}\end{cases} \tag{5.2}$$

As before we find $S_{\underline{l}}^{(h)}=\delta_{\underline{l},\underline{0}}$, $S^{(h)}(\underline{p})=1$ and $c_s=\delta_{s,0}$. Therefore, $H_n=\sqrt{a}\hat{h}(na)=(1/\sqrt{2})(\delta_{n,0}+\delta_{n,1})$. We have therefore obtained the coefficients of the Haar MRA: all the properties (r1)–(r4) are obviously satisfied, as well as all the sum rules given before.

We want to remark that in both these examples the ONC (2.21) was already satisfied by the seed function itself, and for this reason it is not a surprise that the new function H in (3.10) coincides with h.

Example 3: Let us consider

$$h(x)=\begin{cases}\dfrac{1}{\sqrt{da}}, & p\in[0,da[\\ 0 \quad \text{otherwise,}\end{cases} \tag{5.3}$$

where $d=1,2,3,\ldots$. This time the seed function has compact support in the position space, so that $\hat{h}(p)$ decayes rather slowly. $S^{(h)}(0,p)$ is, in general, different from 1 but is independent of p, so that c_s is again proportional to $\delta_{s,0}$. Moreover an explicit computation shows that $\hat{h}(na)$ is different from zero only if $n=0$, so that H_n turns out to be nonzero only if $n=0$. Therefore, even if the seed function is quite different from that of Example 1, the resulting coefficients essentially coincide with those obtained there. The sum rules again are verified.

Example 4: Let us define now

$$\hat{h}(p)=\begin{cases}\dfrac{1}{\sqrt{3a}}, & p\in[0,3a[\\ 0 \quad \text{otherwise.}\end{cases} \tag{5.4}$$

We get easily $S_{\underline{r}}^{(h)}=\delta_{r_1,0}[\delta_{r_2,0}+\frac{1}{3}(\delta_{r_2,1}+\delta_{r_2,-1})]$, which implies that $S^{(h)}(\underline{p})=1+\frac{2}{3}\cos(p_2)$. We see that $S^{(h)}(0,p)$ is always positive in $[0,2\pi]$ and infinitely differentiable. We can deduce, therefore, that the c_s's decay faster than any inverse power of $|s|$. Since $\hat{h}(p)$ is different from zero only in the finite set $[0,3a[$ we can use the result of the Proposition given in the Appendix, statement (1), to conclude that the sequence H_n in (3.15) satisfies conditions (r1) and (r2). However, since (4.4) is not verified, we do not expect condition (r3) to hold. All the sum rules can be explicitly checked.

Example 5: Let $h(x)=(1/\pi^{1/4})e^{-x^2/2}$. Its Fourier transform is $\hat{h}(p)=(1/\pi^{1/4})e^{-p^2/2}$. Using formula (2.21) we find $S_{\underline{r}}^{(h)}=e^{-(\pi/2)(r_1^2+4r_2^2)}$, which implies that $S^{(h)}(0,p)$

$=\Sigma_{r_1\in\mathbf{Z}}e^{-(\pi/2)r_1^2}\Sigma_{r_2\in\mathbf{Z}}e^{-2\pi r_2^2}e^{ipr_2}$. The sum in r_1 can be performed numerically and it gives $\Sigma_{r_1\in\mathbf{Z}}e^{-(\pi/2)r_1^2}=1.4195$. Using now the usual techniques outlined earlier and in the Appendix we can easily deduce that, not only condition (r1) but also conditions (r2) and (r4) are automatically satisfied, the reason being the very fast decay properties of both c_s and $\hat{h}$. However, condition (r3) is not verified since equality (4.4) does not hold. On the contrary, all the sum rules deduced in Sec. III are verified.

Let us work out this example in more detail. Since the explicit computation of $S^{(h)}(0,p)$ is difficult, we consider here a perturbative computation. We will show that already a very crude approximation gives interesting results, and that a slightly better approximation makes the result almost exact. The main difficulty consists in the computation of c_s in (3.16). Using the expansion

$$\frac{1}{\sqrt{1+x}}=1-\frac{1}{2}x+\frac{3}{8}x^2+\cdots,$$

and observing that $\Sigma_{r_2=1}^{\infty}e^{-2\pi r_2^2}\simeq 0.001\,86$, we can proced as follows:

$$\frac{1}{\sqrt{S^{(h)}(0,p)}}=\frac{1}{\sqrt{1.4195}}\frac{1}{\sqrt{1+2\Sigma_{r_2=1}^{\infty}e^{-2\pi r_2^2}\cos(pr_2)}}$$

$$\simeq\frac{1}{\sqrt{1.4195}}\left(1-\sum_{r_2=1}^{\infty}e^{-2\pi r_2^2}\cos(pr_2)\right)\simeq\frac{1}{\sqrt{1.4195}}$$

considering the crudest approximation (the rest is only 2/1000 of the main contribution!). In this way we get $c_s\simeq\delta_{s,0}/\sqrt{1.4195}$, and therefore $H_n\simeq(2^{1/4}/\sqrt{1.4195})\,e^{-\pi n^2}$. It is clear that both (r2) and (r4) are satisfied. As for the (r1), a numerical computation shows that $\Sigma_{n\in\mathbf{Z}}H_n^2\simeq 0.999\,992$, $\Sigma_{n\in\mathbf{Z}}H_nH_{n\pm 2}\simeq 0.001\,86$, and $\Sigma_{n\in\mathbf{Z}}H_nH_{n\pm 2l}$ is even smaller for $|l|$ larger than 1. We see that this is already a good approximation of (2.23). Better results can be obtained simply considering the next contribution in the previous expansion, which means considering also the term with $r_2=1$ in the above-given sum. In this case we get $c_s\simeq(1/\sqrt{1.4195})\,(\delta_{s,0}-\frac{1}{2}(\delta_{s,1}+\delta_{s,-1}))$, and

$$H_n\simeq\frac{2^{1/4}}{\sqrt{1.4195}}\left[e^{-\pi n^2}-\frac{1}{2}e^{-2\pi}(e^{-\pi(n+2)^2}+e^{-\pi(n-2)^2})\right].$$

We find now that $\Sigma_{n\in\mathbf{Z}}H_n^2\simeq 0.999\,992$, while $\Sigma_{n\in\mathbf{Z}}H_nH_{n\pm 2}\simeq 10^{-8}$, which is much smaller than before. As for (r3), a numerical computation gives $\Sigma_{n\in\mathbf{Z}}H_n\simeq 1.0844\neq\sqrt{2}$, as expected. Again, all the sum rules are satisfied.

Example 6: This example generalizes Example 2, in the sense that we still require $\hat{h}(p)$ to be zero outside $[0,2a[$ but we do not fix the analytic expression of $\hat{h}$ inside $[0,2a[$. Without going into all the details we just want to remark that also now c_s is proportional to $\delta_{s,0}$, so that H_n is proportional to $\hat{h}(na)$. More in detail we find

$$H_n=\frac{1}{\sqrt{|\hat{h}(0)|^2+|\hat{h}(a)|^2}}(\hat{h}(0)\,\delta_{n,0}+\hat{h}(a)\,\delta_{n,1}).$$

It is clear that conditions (r1), (r2), and (r4) are automatically satisfied, while (r3) holds whenever $\hat{h}(p)$ is such that

$$\frac{\hat{h}(0)+\hat{h}(a)}{\sqrt{|\hat{h}(0)|^2+|\hat{h}(a)|^2}}=\sqrt{2}.$$

Example 7: This example can be considered as a generalization of Examples 1 and 4 and was already mentioned in Sec. IV. Let k be a fixed natural: $k=0,1,2,...,$ and let

$$\hat{h}_k(p)=\begin{cases}\dfrac{1}{\sqrt{(2k+1)a}}, & p\in[0,(2k+1)a[\\ 0 \quad \text{otherwise.}\end{cases} \tag{5.5}$$

Obviously, $k=0$ returns Example 1, while $k=1$ gives Example 4. Computing the integral in (2.21) we find

$$S^{(h_k)}(0,p)=1+(1-\delta_{k,0})\frac{2}{2k+1}\sum_{j=0}^{k-1}(2j+1)\cos(p(k-j)),$$

which turns out to be strictly positive for all values of k. This claim was analytically and numerically checked for many values of k. For k increasing it is possible to see that the function $S^{(h_k)}(0,p)$ approaches more and more zero, but, at least for $k\leqslant 100$, it is always strictly positive. We guess that this same positivity also holds for k bigger than 100, but an analytical control is quite difficult in this case and it is not very relevant here. Incidentally, this is the reason why the seed function $\hat{h}_k(p)$ is defined on, say, odd intervals. For even ones, in fact, $(p\in[0,2ka[)$, it is easy to check that $S^{(h_k)}(0,p)$ has a zero inside $[0,2\pi[$, and the integral defining c_s may diverge.

It is now clear that, for any fixed k, the function $1/S^{(h_k)}(0,p)$ is in C^∞, so that c_s decays faster than any inverse power of $|s|$. Now, since $\hat{h}(p)$ is different from zero only in a finite interval, it is also clear that for the asymptotic behavior of the coefficients $H_n=\sqrt{a}\Sigma_{s\in\mathbf{Z}}c_s\hat{h}((n+2s)a)$ we can apply the Proposition given in the Appendix, statement (1), so that we conclude that $H_n\in s$, where s is defined in the Appendix. Condition (r3) does not hold since Eq. (4.4) is not verified.

Example 8: Let us fix $l\in\mathbf{N}$ and define

$$h_l(x)=0\begin{cases}\sqrt{\dfrac{2}{la}}, & x\in\left[0,\dfrac{la}{2}\right[\\ 0 \quad \text{otherwise.}\end{cases} \tag{5.6}$$

This class of seed functions is interesting because it produces, after the usual procedure, a set of coefficients c_s which are always zero but if $s=0$. Therefore we obtain

$$H_n=\sqrt{\frac{a}{S^{(h_l)}(0)}}\hat{h}_l(na).$$

Whenever l is even the situation is not very interesting, since we get $H_n\propto\delta_{n,0}$. On the contrary, if l is odd, $l=2k+1$, we find that

$$\hat{h}_{2k+1}(na)=\begin{cases}\sqrt{\dfrac{2k+1}{2a}}, & n=0\\ 0, \quad n=\pm 2,\pm 4,\pm 6,\ldots\\ \sqrt{\dfrac{2}{ina\sqrt{\pi a(2k+1)}}}, & n=\pm 1,\pm 3,\pm 5,\ldots.\end{cases}$$

We therefore see that, even if (r1) is satisfied, (r2) is not. Also (r3) does not hold since Eq. (4.4) is not verified.

Example 9: As a final example here we consider the following seed function

$$\hat{h}(p)=\frac{2}{a(1+p^2)},$$

which produces the following coefficients

$$S_{\underline{r}}^{(h)}=\frac{e^{-|r_1|a}}{1+2\pi r_2^2}$$

and the following function $S^{(h)}(\underline{p})$:

$$S^{(h)}(\underline{p})=\frac{1+e^{-a}}{1-e^{-a}}\varphi(p_2) \quad \text{with} \quad \varphi(p_2)=\sum_{r_2\in\mathbf{Z}}\frac{e^{ip_2r_2}}{1+2\pi r_2^2}.$$

It is an easy estimate to check that $\varphi(p_2)\neq 0$ in $[0,2\pi[$. However, we cannot use the same arguments as for Example 5 to conclude that $\varphi(p_2)$ belongs to C^∞, the reason being that the Fourier coefficients $(1/1+2\pi r_2^2)$ of φ do not decay very fast. For this reason it is not difficult to understand that condition (r2) is not satisfied whereas conditions (r1) and (r3) hold. In particular this last condition can be controlled by checking directly Eq. (4.4).

Let us now go back to Eq. (3.8), where the phase $\varphi(\underline{p})$ was chosen to be equal to zero. We want to show here that this is really a very special choice. In fact, the following two simple examples point out that a different choice of $\varphi(\underline{p})$ produces coefficients H_n which can be significantly different from the ones we get if $\varphi(\underline{p})=0$.

First we remark that the expression for c_s must be a little bit modified. Instead of (3.16) we have

$$c_s=\frac{1}{2\pi}\int_0^{2\pi}\frac{e^{-ips+i\varphi(0,p)}\,\mathrm{d}p}{\sqrt{S^{(h)}(0,p)}}. \tag{5.7}$$

A first application of this formula consists in choosing $\varphi(0,p)=pK_0$, K_0 being a fixed integer. If we consider, for instance, Example 2, we see that the only difference, in this case is that, instead of having $c_s=\delta_{s,0}$, we find $c_s=\delta_{s,K_0}$, so that $H_n=(1/\sqrt{2})\,(\delta_{n,K_0}+\delta_{n,K_0+1})$. More interesting is the situation if φ is not linear. Let us consider here $\varphi(0,p)=\gamma p^2$, $\gamma\in\mathbf{R}$. Restricting ourselves again to Example 2, for which $S^{(h)}(\underline{0})=1$, we can still compute analytically the coefficients c_s, which turn out to be

$$c_s=\frac{-1}{4\pi}\sqrt{\frac{\pi}{-i\gamma}}e^{-(is^2/4\gamma}\left(\Phi\left(\frac{i(4\pi\gamma-s)}{2\sqrt{-i\gamma}}\right)+\Phi\left(\frac{is}{2\sqrt{-i\gamma}}\right)\right),$$

where Φ is the erf function.[14] Using its well-known asymptotic behavior, we find that c_s decays as $|s|^{-1}$, which is a very slow behavior when compared with that obtained for $\varphi=0$.

VI. CONCLUSIONS

We have shown how to use the relation between the FQHE and the MRA recently established by the author in order to construct a set of coefficients which produce a MRA of $\mathcal{L}^2(\mathbf{R})$. The examples given show that while it is essentially automatic to obtain a sequence satisying condition (r1), more care must be used to find a seed function which produces a relevant sequence. Conditions on the seed function for the set $\{H_n, n\in\mathbf{Z}\}$ to be relevant are discussed.

ACKNOWLEDGMENT

This work has been financially supported in part by M.U.R.S.T., within the project *Problemi Matematici Non Lineari di Propagazione e Stabilità nei Modelli del Continuo*, coordinated by Professor T. Ruggeri.

APPENDIX: CONVOLUTIONS OF SEQUENCES

In this appendix we prove some results concerning the asymptotic behavior of convolutions in view of applications. We wish to stress that these results are given here since, though being quite reasonable, they were not found by the author in the existing literature.

We use here the same notation as in Ref. 13: f, s, and l_p are well-known spaces of sequences, the first containing all the *finite* sequences, that is, those sequences which are zero outside of a finite set of indexes. The other sets are defined as follows:

$$s=\{a:\lim_{|n|,\infty}|n|^p a_n=0,\quad \forall p\in\mathbb{N}\},\quad l_p=\left\{a:\|a\|_p=\left(\sum_{p\in\mathbf{Z}}|a_n|^p\right)^{1/p}<\infty\right\}. \tag{A1}$$

Given two sequences a,b we define a third sequence $c=a*b$ as $c_n=\Sigma_{s\in\mathbf{Z}}a_s b_{n-s}=\Sigma_{s\in\mathbf{Z}}a_{n-s}b_s$. We have the following.

Proposition: Let a,b, and c be as above. Then the following statements hold:

(1) if $a\in f$ then the asymptotic behavior of c is the same of that of b;
(2) if $a\in l_1$ and $b\in l_p$ then $c\in l_p$, for all $1\leqslant p<\infty$;
(3) if $a,b\in s$ then $c\in s$.

Proof:

(1) This is clear because $a_n=0$ but for a finite number of indexes n. Of course the same result can be obtained simply by exchanging the roles of a and b.

(2) The proof of this statement follows from well-known properties of the convolutions of functions. We start defining two functions, defined in $\mathbf{R}$, as follows:

$$a(x)=|a_s|,\quad x\in[s,s+1[,\quad b(x)=|b_s|,\quad x\in[s,s+1[,\quad s\in\mathbf{Z}.$$

It is clear that $a(x)\in\mathcal{L}^1(\mathbf{R})$, while $b(x)\in\mathcal{L}^p(\mathbf{R})$. Then it is well known that $a*b\in\mathcal{L}^p(\mathbf{R})$, where $(a*b)(x)=\int_{\mathbf{R}}a(y)b(x-y)\mathrm{d}y$. In order to conclude that $c\in l_p$ we consider that

$$c(x)=\int_{\mathbf{R}}a(y)b(x-y)\mathrm{d}y=\sum_{s\in\mathbf{Z}}\int_s^{s+1}a(y)b(x-y)\mathrm{d}y=\sum_{s\in\mathbf{Z}}|a_s|\int_s^{s+1}b(x-y)dy.$$

Using now the definition of $b(x)$ it is easy to check that, for all integers l and for $0\leqslant\alpha<1$, we have

$$c(l+\alpha)=\sum_{s\in\mathbf{Z}}|a_s|((1-\alpha)|b_{l-s-1}|+\alpha|b_{l-s}|)=(1-\alpha)d_{l-1}+\alpha d_l, \tag{A2}$$

where we have defined $d_l=\Sigma_{s\in\mathbf{Z}}|a_s b_{l-s}|\geqslant 0$, for all $l\in\mathbf{Z}$. The conclusion now follows from the fact that $c(x)$ belongs to $\mathcal{L}^p(\mathbf{R})$ and from the inequality $(\gamma_1+\gamma_2+\cdots+\gamma_n)^p\geqslant\gamma_1^p+\gamma_2^p+\cdots+\gamma_n^p$, which holds whenever $\gamma_j\geqslant 0$ and for all $p\geqslant 1$. In fact we have

$$\infty>\int_{\mathbf{R}}|c(x)|^p\mathrm{d}x=\sum_{l\in\mathbf{Z}}\int_l^{l+1}|c(x)|^p\mathrm{d}x=\sum_{l\in\mathbf{Z}}\int_0^1|c(l+x)|^p\mathrm{d}x=\sum_{l\in\mathbf{Z}}\int_0^1((1-\alpha)d_{l-1}+\alpha d_l)^p\mathrm{d}\alpha$$

$$\geqslant\frac{2}{p+1}\sum_{l\in\mathbf{Z}}d_l^p\geqslant\frac{2}{p+1}\sum_{l\in\mathbf{Z}}c_l^p,$$

which proves that $c \in l_p$.

(3) From the definition $c_n = \Sigma_{s \in \mathbf{Z}} a_s b_{n-s}$ we easily get the following equality between functions: $C(p) = A(p)B(p)$, where $A(p) = \Sigma_{s \in \mathbf{Z}} a_s e^{isp}$, $B(p) = \Sigma_{s \in \mathbf{Z}} b_s e^{isp}$, and $C(p) = \Sigma_{s \in \mathbf{Z}} c_s e^{isp}$. The coefficients c_l can now be found simply by

$$c_l = \frac{1}{2\pi} \int_0^{2\pi} C(p) e^{-ipl} \, dp = \frac{1}{2\pi} \int_0^{2\pi} A(p)B(p) e^{-ipl} \, dp, \tag{A3}$$

which is the starting point of our asymptotic analysis. In fact, due to the fact that a, $b \in s$, the functions $A(p)$ and $B(p)$ belong to C^∞, and so their product does. This implies, using well-known fact about the Fourier series, that the coefficients c_l in (A3) decay faster than every inverse power of $|l|$, so that $c \in s$.

Remark: It is clear that statement (2) is not enough to ensure validity of (r2), which is satisfied, on the contrary, if a and b are both in s or if, e.g., a is in f and b decays like $1/n^2$.

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Continuum quantum systems as limits of discrete quantum systems. IV. Affine canonical transforms

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(Received 4 June 2002; accepted 30 December 2002)

Affine canonical transforms, complex-order Fourier transforms, and their associated coherent states appear in two scenarios: finite-discrete and continuum. We examine the relationship between the two scenarios, making systematic use of inductive limits, which were developed in the preceding articles in this series. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1557331]

I. INTRODUCTION

Inductive limits provide a clear and precise means whereby objects associated with a continuum system can be realized as limits of objects associated with a sequence of discrete systems. Three preceding papers[1–3] discuss inductive limits of vectors and operators. Another work[4] concerns inductive limits of representations. In the present article, we illustrate the approach by applying it to a continuum scenario and a discrete scenario that lie in the core of quantum physics.

Our main results are as follows. Theorem 6.1 realizes Glauber coherent states as inductive limits of spin coherent states. A practical version of the result goes back to Radcliffe[5] and Arecchi *et al.*[6] Theorem 5.3 realizes the group of continuum motion canonical transforms as an inductive limit of the group of discrete motion canonical transforms. A practical version was initiated in Ref. 6 and considerably developed by Atakishiyev *et al.*[7,8] Theorem 5.1 and Corollary 5.2 realize single-parameter groups of continuum affine canonical transforms as inductive limits of single-parameter groups of discrete affine canonical transforms. Practical versions can be found in Dobrev *et al.*[9] Theorem 6.2 realizes continuum complex-order Fourier transforms as inductive limits of discrete complex-order Fourier transforms. From a practical point of view, that can be seen as a mild generalization of the fractional Fourier transforms in Ref. 10. In Ref. 4, Corollary 5.2 and Theorem 5.3 are expressed explicitly as inductive limits of representations but, in the present article, they are expressed simply as inductive limits of operators.

In using the adjective ''practical,'' rather than ''heuristic,'' we have erred towards understatement rather than overstatement. There is a vast body of literature on discrete to continuum correspondences that seem to be potential applications of inductive limits; see Sec. VII for a sample of further citations. Sometimes, in those works, the practical versions of the results have involved expressions of the form $\mathcal{O}=\lim_n \mathcal{O}_n$ or $\mathcal{O}_n \to \mathcal{O}$ that do not conform to any evident definition of limit. Sometimes, comparatively weak results have been stated and proved, yet with an apparently suggested meaning that goes beyond the literal interpretation; for instance, parallel discussion of continuum and discrete scenarios, the latter implicitly understood to be an approximation to the former. Actually, our use of inductive limits does have a practical intention, as we shall explain in Sec. VII.

Let us indicate the nature of the general kind of problem that concerns us. The limit equations in question are of the form $\mathcal{O}=\lim_n \mathcal{O}_n$, where $\mathcal{O}$ is an object (say, a vector, an operator or a representation) associated with Hilbert space $\mathcal{L}$, and each $\mathcal{O}_n$ is an object associated with a Hilbert space $\mathcal{L}_n$. In this article, $\mathcal{L}=L^2(\mathbb{R})$ and $\mathcal{L}_n$ is of finite dimension n. The problem is to select appropriate definitions so as to make such limit equations potentially provable or refutable; or, at least, true or false. One approach is to embed the spaces $\mathcal{L}_n$ in the space $\mathcal{L}$, and to replace

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differential equations with corresponding difference equations. In general form, this is, of course, a numerical approximation technique that has been in widespread use ever since the emergence of statistical analysis in the 18th century. We must be very selective with our citations, since otherwise there would be no end to them. The convergence of eigenvectors examined in Ref. 11 may be applicable to the operators we consider below; this is significant, because convergence of spectral measures may be an interesting avenue for research into discrete to continuum limits of representations (see Ref. 3, Sec. V). In Ref. 12, groups acting on $\mathcal{L}_n$ are embedded in groups acting on $\mathcal{L}$, and the discrete to continuum correspondence is characterized in terms of module induction. Another approach, proposed by Parthasarathy[13,14] and Lindsay–Parthasarathy,[15] is to collect all the spaces $\mathcal{L}_n$ together in a Fock space where limits can be examined without mentioning the space $\mathcal{L}$. Arguably, our approach is the most flexible of the three, since the definitions of inductive limits of vectors and operators do not require any constraints on the Hilbert spaces $\mathcal{L}$ and $\mathcal{L}_n$ (except for separability). However, it seems very probable that the particular limit equations in the present article can also be realized through the other two approaches.

Although some of the material below is in the nature of a review, this is a side-effect of a need to reformulate known results before presenting our own. We must also point out that although some of our limit formulas are unitary versions of accepted heuristic limits of Hermitian operators, the assertions that the formulas now express are new, since the kinds of limit involved had not previously been supplied with definitions.

II. CONTINUUM AFFINE CANONICAL TRANSFORMS

We shall introduce a six-dimensional connected real Lie group $\mathrm{HSA}=\mathrm{HSA}(2,\mathbb{R})$ and an action of HSA as unitary operators on the continuum state space $L^2(\mathbb{R})$. As we shall see in the next section, HSA is a central extension of the special affine group SA on the plane; SA is also the Schorödinger group with one space dimension and one time dimension. The group HSA, and its representation on $L^2(\mathbb{R})$, are discussed by Dobrev *et al.*,[9] and Neiderer;[16] for some other sources—oriented more towards the phase space picture—see Sec. III. Our main target, in this section, is to obtain explicit matrix representations for some generators of the Lie algebra of HSA. We shall also examine a subgroup HM of HSA. The group HM is a central extension of the Euclidian motion group.

The real Lie algebra $\mathrm{hsa}=\mathrm{hsa}(2,\mathbb{R})$ has a basis $\{iB,iC,iD,iP,iQ,iI\}$. The notation indicates that B, C, D, P, Q, I are elements of the complexification. The commutation relations are defined to be such that I is central, $[Q,P]=iI$ and, in the universal enveloping algebra,

$$B=\tfrac{1}{2}P^2, \qquad C=\tfrac{1}{2}Q^2, \qquad D=\tfrac{1}{2}(PQ+QP).$$

It is not hard to show that the commutation relations involving B, C, D are

$$\begin{gathered}[B,P]=0=[C,Q], \qquad [C,P]=iQ=-[D,Q], \qquad [D,P]=iP=-[B,Q],\\ [B,C]=-iD, \qquad [B,D]=-2iB, \qquad [C,D]=2iC.\end{gathered} \tag{1}$$

For instance,

$$\begin{aligned}[B,C]&=\tfrac{1}{4}(P^2Q^2-PQPQ+PQPQ-PQ^2P+PQ^2P-QPQP+QPQP-Q^2P^2)\\ &=\tfrac{1}{4}(P[P,Q]Q+PQ[P,Q]+[P,Q]QP+Q[P,Q]P)=-iD.\end{aligned}$$

Let $\hat{B}$, $\hat{C}$, $\hat{D}$, $\hat{P}$, $\hat{Q}$, $\hat{I}$ be the Hermitian operators on $L^2(\mathbb{R})$ such that $\hat{I}$ is the identity operator and

$$(\hat{P}\phi)(q)=-i\frac{d}{dq}\phi(q), \qquad (\hat{Q}\phi)(q)=q\phi(q), \tag{2}$$

$$\hat{B}=\tfrac{1}{2}\hat{P}^2, \qquad \hat{C}=\tfrac{1}{2}\hat{Q}^2, \qquad \hat{D}=\tfrac{1}{2}(\hat{P}\hat{Q}+\hat{Q}\hat{P}), \tag{3}$$

where ϕ belongs to the Schwartz space $\mathcal{S}(\mathbb{R})$. The operators $\hat{P}$ and $\hat{Q}$ are sometimes understood to correspond to momentum and position, respectively (or frequency and time, in signal processing, or frequency and position, in optics).

Let σ be the anti-Hermitian representation of hsa on $L^2(\mathbb{R})$ such that the elements B, C, D, P, Q, I act as $\hat{B}$, $\hat{C}$, $\hat{D}$, $\hat{P}$, $\hat{Q}$, $\hat{I}$, respectively. We introduce a real Lie group HSA=HSA(2,$\mathbb{R}$) and a faithful unitary representation ρ of HSA such that HSA has associated Lie algebra hsa and such that ρ has differential representation σ. The elements of the group ρ(HSA) are called **continuum affine canonical transforms**. Of course, there is no essential difference between the abstract Lie group HSA and the group of unitary operators ρ(HSA). Each is isomorphic to the other via the isomorphism ρ. Nevertheless, we do sometimes find it useful to distinguish between the two groups. Given real β, γ, δ, μ, ν, κ, we write

$$\hat{H}(\beta,\gamma,\delta,\mu,\nu,\kappa)=\beta\hat{B}+\gamma\hat{C}+\delta\hat{D}+\mu\hat{P}+\nu\hat{Q}+\kappa\hat{I}, \tag{4}$$

$$\hat{U}(\beta,\gamma,\delta,\mu,\nu,\kappa)=\exp(-i\hat{H}(\beta,\gamma,\delta,\mu,\nu,\kappa)). \tag{5}$$

The continuum affine canonical transforms are the composites of operators that have the form $\hat{U}(\beta,\ldots,\kappa)$.

Warning: some affine canonical transforms do not have the exponential form $\hat{U}(\beta,\ldots,\kappa)$. We shall not be making use of this negative result, but we mention that it can be proved by considering the subquotient SL(2,$\mathbb{R}$) of HSA, and using Eq. (19).

As an element of the Lie algebra hsa, we define

$$N=B+C-I/2\,.$$

The corresponding Hermitian operator on $L^2(\mathbb{R})$ is

$$\hat{N}=\sigma(N)=\hat{B}+\hat{C}+\hat{I}/2.$$

Let hm=hm(2,$\mathbb{R}$) be the subalgebra of hsa with basis $\{iI,iN,iP,iQ\}$ and let HM=HM(2,$\mathbb{R}$) be the subgroup of HSA with associated Lie algebra hm. We call HM the group of **Heisenberg motions**, and we call the elements of the group ρ(HM) the **continuum motion canonical transforms**. Again, there is no essential difference between the two isomorphic groups HM and ρ(HM). The commutation relations for HM are given by Eq. (1) together with

$$[N,I]=0, \qquad [N,P]=iQ, \qquad [N,Q]=-iP. \tag{6}$$

The continuum (and discrete) motion canonical transforms will be of particular importance to us, and it is worth introducing some special notation for them. Given $\kappa,\lambda,\mu,\nu\in\mathbb{R}$, we define

$$\hat{E}(\kappa,\lambda,\mu,\nu)=\exp(-i(\kappa\hat{I}+\lambda\hat{N}+\mu\hat{P}+\nu\hat{Q})). \tag{7}$$

By passing to the quotient group HM/Z(HM)$\cong$EM (see Sec. III), it can easily be shown that the operators having the form $\hat{E}(\kappa,\lambda,\mu,\nu)$ are closed under composition. In other words, the continuum motion canonical transforms are precisely the operators having the form $\hat{E}(\kappa,\lambda,\mu,\nu)$.

We shall give some explicit matrix equations for the infinitesmal generators $\hat{B}$, $\hat{C}$, $\hat{D}$, $\hat{P}$, $\hat{Q}$, $\hat{I}$ of the continuum affine canonical transforms. For that, we need to specify a complete orthonormal set. Recall that, for $s\in\mathbb{N}$, the s-**th Hermite polynomial** H_s and the s-**th Hermite function** h_s are the functions $\mathbb{R}\to\mathbb{C}$ given by

$$(-1)^s \exp(q^2/2)\frac{d^s}{dq^s}\exp(-q^2) = H_s(q) = \sqrt{s!\,2^s\sqrt{\pi}}\exp(q^2/2)h_s(q). \tag{8}$$

Switching to Dirac notation, we write $|s\rangle = h_s$. Note that the zeroth Hermite function $|0\rangle = h_0$ is the Gaussian function

$$h_0(q) = \pi^{-1/4}\exp(-q^2/2). \tag{9}$$

Recall that $\{|s\rangle : s \in \mathbb{N}\}$ is a complete orthonormal set in $L^2(\mathbb{R})$. Also recall that the annihilation operator $\hat{A} = (\hat{Q} + i\hat{P})/\sqrt{2}$ and its Hermitian conjugate, the creation operator $\hat{A}^\dagger = (\hat{Q} - i\hat{P})/\sqrt{2}$, act by

$$\hat{A}|s\rangle = \sqrt{s}|s-1\rangle, \qquad \hat{A}^\dagger|s\rangle = \sqrt{s+1}|s+1\rangle. \tag{10}$$

By direct calculation using Eq. (10), we obtain

$$\hat{B}\,|s\rangle = \frac{-1}{4}\sqrt{s(s-1)}|s-2\rangle + \frac{2s+1}{4}|s\rangle + \frac{-1}{4}\sqrt{(s+1)(s+2)}\,|s+2\rangle, \tag{11}$$

$$\hat{C}\,|s\rangle = \frac{1}{4}\sqrt{s(s-1)}\,|s-2\rangle + \frac{2s+1}{4}|s\rangle + \frac{1}{4}\sqrt{(s+1)(s+2)}\,|s+2\rangle, \tag{12}$$

$$\hat{D}\,|s\rangle = \frac{-i}{2}\sqrt{s(s-1)}\,|s-2\rangle + \frac{i}{2}\sqrt{(s+1)(s+2)}\,|s+2\rangle, \tag{13}$$

$$\hat{P}\,|s\rangle = -i\sqrt{\frac{s}{2}}|s-1\rangle + i\sqrt{\frac{s+1}{2}}|s+1\rangle, \tag{14}$$

$$\hat{Q}\,|s\rangle = \sqrt{\frac{s}{2}}|s-1\rangle + \sqrt{\frac{s+1}{2}}|s+1\rangle, \tag{15}$$

$$\hat{I}\,|s\rangle = |s\rangle, \tag{16}$$

$$\hat{N}\,|s\rangle = s\,|s\rangle. \tag{17}$$

In Sec. IV, we shall find discrete analogues of these seven matrix equations.

Let us end this section with an example. Recall that the continuum Fourier transform is the unitary operator $\hat{F}$ on $L^2(\mathbb{R})$ such that $\hat{F}\,|s\rangle = i^s\,|s\rangle$. More generally, after Namias,[17] the continuum fractional Fourier transform of order $t \in \mathbb{R}$ is the unitary operator $\hat{F}^t$ on $L^2(\mathbb{R})$ such that $\hat{F}^t\,|s\rangle = \exp(2\pi i s t)\,|s\rangle$. In other words,

$$\hat{F}^t = \exp(2\pi i t\hat{N}) = e^{-\pi i t}\exp(2\pi i(\hat{B}+\hat{C})). \tag{18}$$

III. THE CONTINUUM PHASE SPACE PICTURE

This section has two purposes. One of them is to fulfill the promise, made above, to explain how the groups HSA and HM are central extensions of the groups SA and EM, which act on the real plane. The other purpose is to clarify the relationship between the Hermitian operators and their corresponding unitary operators. In Refs. 6–9 and 12, and many other works, limits are described mainly in terms of Hermitian operators. But inductive limits are defined for unitary operators; they are not defined for unbounded Hermitian operators. So we do need to be able to move freely from Hermitian operators to unitary operators, and in reverse.

The phase space picture provides much insight into these matters. There is a vast literature on phase space, and much attention has been paid to affine canonical transforms, especially special linear canonical transforms. See, for instance work by Folland,[18] Hillery *et al.*,[19] Littlejohn,[20] Ozorio de Almeida;[21] we also mention two collections of papers edited by Forbes *et al.*[22] (on applications to optics) and Mecklenbräuker–Hlawatsch[23] (on applications to signal processing). The relevant material, though, is not easy to extract from the literature. Let us give a brief self-contained account of it.

The **phase space plane**, denoted $\mathcal{P}$, is defined to be a copy of $\mathbb{R}^2$. We regard $\mathcal{P}$ as a Euclidean plane equipped with a fixed coordinate system; the vectors are written as coordinate vectors (p,q) where p and q are formal variables.

Recall that the group of special linear transforms of the real plane, denoted $\mathrm{SL}=\mathrm{SL}(2,\mathbb{R})$, has Lie algebra $\mathrm{sl}=\mathrm{sl}(2,\mathbb{R})$ with basis $\{i\overline{B},i\overline{C},i\overline{D}\}$ where

$$\overline{B}=\begin{pmatrix}0 & -i\\ 0 & 0\end{pmatrix},\qquad \overline{C}=\begin{pmatrix}0 & 0\\ i & 0\end{pmatrix},\qquad \overline{D}=\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}.$$

Thus, SL is generated by the elements having the form

$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\exp(-i(\beta\overline{B}+\gamma\overline{C}+\delta\overline{D}))=\exp\begin{pmatrix}\delta & -\beta\\ \gamma & -\delta\end{pmatrix},$$

where $\beta,\gamma,\delta\in\mathbb{R}$. Diagonalizing, a straightforward calculation shows that

$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}\cos\alpha+\delta\alpha^{-1}\sin\alpha & -\beta\alpha^{-1}\sin\alpha\\ \gamma\alpha^{-1}\sin\alpha & \cos\alpha-\delta\alpha^{-1}\sin\alpha\end{pmatrix},\tag{19}$$

where α is the real or imaginary number such that $\alpha^2=\beta\gamma-\delta^2$ and, for imaginary α, we understand that $\cos\alpha=\cosh i\alpha$ and $\sin\alpha=i\sinh i\alpha$. Note that, for given real a, b, c, d satisfying $ad-bc=1$, Eq. (19) has a solution in reals β, γ, δ if and only if $a+d\geqslant -2$. The natural action of SL on the real plane is given by

$$\exp(-i(\beta\overline{B}+\gamma\overline{C}+\delta\overline{D}))\begin{pmatrix}x\\ y\end{pmatrix}=\begin{pmatrix}a & b\\ c & d\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}=\begin{pmatrix}ax+by\\ cx+dy\end{pmatrix}.\tag{20}$$

The Euclidean special affine group $\mathrm{SA}=\mathrm{SA}(2,\mathbb{R})$ (which coincides with the Schrödinger group with one space and one time dimension) is generated by SL and the plane translates. The associated Lie algebra $\mathrm{sa}=\mathrm{sa}(2,\mathbb{R})$ has basis $\{i\overline{B},i\overline{C},i\overline{D},i\overline{P},i\overline{Q}\}$, where

$$\exp(-i(\mu\overline{P}+\nu\overline{Q}))\begin{pmatrix}x\\ y\end{pmatrix}=\begin{pmatrix}x+\mu\\ y+\nu\end{pmatrix}.\tag{21}$$

Evidently, $[\overline{P},\overline{Q}]=0$. It is easy to check that the 14 other commutation relations are as in Eq. (1). We allow SA to act on $\mathcal{P}$ via the identification $(p,q)=(-y,x)$. Thus

$$\exp(-i(\beta\overline{B}+\gamma\overline{C}+\delta\overline{D}))\begin{pmatrix}p\\ q\end{pmatrix}=\begin{pmatrix}d & -c\\ b & a\end{pmatrix}\begin{pmatrix}p\\ q\end{pmatrix},$$

$$\exp(-i(\mu\overline{P}+\nu\overline{Q}))\begin{pmatrix}p\\ q\end{pmatrix}=\begin{pmatrix}p-\nu\\ q+\mu\end{pmatrix}.$$

By comparing commutation relations, we see that there is a Lie algebra epimorphism $\mathrm{hsa}\to\mathrm{sa}$ mapping B, C, D, P, Q, I to $\overline{B}$, $\overline{C}$, $\overline{D}$, $\overline{P}$, $\overline{Q}$, 0, respectively. The group epimorphism $\mathrm{HSA}\to\mathrm{SA}$ has kernel

$$\mathrm{Ker}(\mathrm{HSA}\to\mathrm{SA})=Z(\mathrm{HSA})=\{\exp(-it\pi I):t\in\mathbb{R}\}.$$

We allow HSA to act on $\mathcal{P}$ by inflation from SA. Thus

$$\exp(-i(\beta B+\gamma C+\delta D))\begin{pmatrix}p\\q\end{pmatrix}=\begin{pmatrix}d&-c\\b&a\end{pmatrix}\begin{pmatrix}p\\q\end{pmatrix}, \tag{22}$$

$$\exp(-i(\mu P+\nu Q+\kappa I))\begin{pmatrix}p\\q\end{pmatrix}=\begin{pmatrix}p-\nu\\q+\mu\end{pmatrix}. \tag{23}$$

The state space $L^2(\mathbb{R})$ and the phase space plane $\mathcal{P}$ are related to each other via the continuous function

$$\omega:L^2(\mathbb{R})\ni\psi\mapsto\omega[\psi]\in L^2_{\mathbb{R}}(\mathcal{P}),$$

$$\omega[\phi](p,q)=\frac{1}{\pi}\int_{-\infty}^{\infty}dt\,\overline{\phi(q+t)}\,\phi(q-t)\exp(2ipt).$$

The function ω is essentially a specialization of the famous Weyl–Wigner correspondence; see the references at the beginning of this section, especially Refs. 19 and 18. Given $g\in\mathrm{HSA}$ and $\psi\in L^2(\mathbb{R})$, then

$$\omega[\rho(g)\psi](g(p,q))=\omega[\psi](p,q).$$

In other words, ω is covariant with the actions of HSA on the signal space $L^2(\mathbb{R})$ and on the phase space $\mathcal{P}$. The result is proved in, for instance, Ref. 20 (Equations 6.18, 6.23, 6.27), and Ref. 18 (Proposition 2.13, Theorem 2.15). The rationale for our terminology should now be apparent: the ''Heisenberg'' groups HSA and HM are central extensions (or quantized versions) of the groups SA and EM.

The special linear canonical transforms are usually understood to be unitary actions of SL on the state space $L^2(\mathbb{R})$. For an element of SL as in Eq. (19), the action on state space is taken to be the unitary operator

$$\lambda(a,b,c,d)\hat{U}(\beta,\gamma,\delta,0,0,0)=\lambda(a,b,c,d)\exp(-i(\beta\hat{B}+\gamma\hat{C}+\delta\hat{D})),$$

where $\lambda(a,b,c,d)$ is a phase. The phases $\lambda(a,b,c,d)$ cannot be chosen so as to yield a unitary representation of SL. True enough, they can be chosen so as to preserve composition up to $\pm$ signs, thus determining a unitary representation of the metaplectic group $\mathrm{Mp}(2,\mathbb{R})$, which is the double cover of SL. But that observation has limited practical use, since the description of the metaplectic group is very complicated; see Ref. 18, Chap. 4. For practical purposes, the special linear canonical transforms comprise a four-dimensional group, one of the degrees of freedom being the multiplications by phases. In fact, to establish a clear correspondence with the discrete scenario, we have no choice but to include the momentum and position translates, as well as the multiplications by phases. Thus, even if one is primarily concerned with the three-parameter group SL, the connection with the discrete scenario demands that we consider all six degrees of freedom in the group HSA.

IV. DISCRETE AFFINE CANONICAL TRANSFORMS

We shall introduce some discrete affine canonical transforms whose infinitesmal generators satisfy matrix equations analogous to Eqs. (11)–(17). First, we need to look at the Kravchuk functions, which are discrete analogs of the Hermite functions. We closely follow the representation-theoretic discussion of the Kravchuk functions in Ref. 24 (Chap. 6) and, to a lesser extent, Ref. 25 (Chap. 8). For parallel discussions of the Kravchuk and Hermite functions in

connection with discrete and continuum oscillator algebras, see Refs. 10 and 26. An alternative approach to the comparison of Kravchuk and Hermite functions, making systematic use of creation and annihilation operators, can be found in Ref. 27.

All lemmas that we state without proof can be obtained from the earlier lemmas together with routine calculations as in Ref. 24. There is only one argument that is not straightforward, namely, the proof of Lemma 4.5. For this, Ref. 24 invokes the theory of hypergeometric functions, and that requires some delicate analysis, the Kravchuk functions being specializations of hypergeometric functions at singular points. Our more direct argument is purely algebraic. The results proved below concerning Kravchuk functions and Kravchuk polynomials are summarized in Appendix B.

Let n be a positive integer. Write $n=2\ell+1$. Let $[n]$ denote the set of k such that $\ell+k$ and $\ell-k$ are natural numbers. Thus, $[n]$ consists of n integers or n halves of odd integers. Let $\mathcal{L}_n$ be the n-dimensional Hilbert space of functions $[n]\to\mathbb{C}$, the inner product being

$$\langle\psi|\chi\rangle=\sum_{k=-\ell}^{\ell}\overline{\psi(k)}\chi(k),$$

where $\psi,\chi\in\mathcal{L}_n$, and the bar denotes complex conjugation. Let $|k\rangle_n^Z$ denote the vector in $\mathcal{L}_n$ such that, given $\psi\in\mathcal{L}_n$, then $\psi(k)=\langle\psi|k\rangle_n^Z$. The set $\{|k\rangle_n^Z:k\in[n]\}$ is an orthonormal basis for $\mathcal{L}_n$. Via the equation

$$|k\rangle_n^Z=\frac{u^{\ell+k}v^{\ell-k}}{\sqrt{(\ell+k)!(\ell-k)!}} \tag{24}$$

we identify $\mathcal{L}_n$ with the space of homogenous polynomials of degree 2ℓ in variables u and v.

Later, we shall be realizing $\mathcal{L}_n$ as a representation space of the Lie group U(2). For the following three preliminary results, though, we may as well consider, more generally, the Lie group GL(2,$\mathbb{C}$). We define a group representation ρ_n of GL(2,$\mathbb{C}$) on $\mathcal{L}_n$ such that

$$(\rho_n(g)F)(u,v)=F(au+cv,bu+dv),\qquad g=\begin{pmatrix}a&b\\c&d\end{pmatrix}. \tag{25}$$

Lemma 4.1: Let $j,k\in[n]$. Put $\max=\max(0,j+k)$ *and* $\min=\min(\ell+j,\ell+k)$. *Then, with respect to the orthonormal basis $\{|k\rangle_n^Z:k\in[n]\}$, the (j,k) entry of the matrix representing $\rho_n(g)$ is*

$${}_n^Z\langle j|\rho_n(g)|k\rangle_n^Z=\sqrt{\frac{(\ell+j)!(\ell-j)!}{(\ell+k)!(\ell-k)!}}\sum_{r=\max}^{\min}\binom{\ell+k}{r}\binom{\ell-k}{\ell+j-r}a^r b^{\ell+j-r}c^{\ell+k-r}d^{r-j-k}.$$

Henceforth, we work directly from Lemma 4.1, and we can forget about the characterization of $\mathcal{L}_n$ as a space of polynomials.

Lemma 4.2: Now suppose that $g\in\mathrm{SL}(2,\mathbb{C})$, and that the matrix entries b, c, d are nonzero. Given $j,k\in[n]$, then

$${}_n^Z\langle j|\rho_n(g)|k\rangle_n^Z=\frac{b^{\ell+j}c^{\ell+k}}{d^{j+k}}\sqrt{\frac{(\ell+j)!(\ell+k)!}{(\ell-j)!(\ell-k)!}}\sum_{r=0}^{\min(\ell+j,\ell+k)}\frac{(2\ell-r)!(bc)^{-r}}{\nu!(\ell+j-r)!(\ell+k-r)!}.$$

Let $c_r=\ell(\ell+1)-\kappa^2+\frac{1}{4}$ for $2\kappa\in\mathbb{Z}$. Thus

$$c_{k+1/2}=(\ell-k)(\ell+k+1),\qquad c_{k-1/2}=(\ell+k)(\ell-k+1).$$

Let σ_n be the differential representation of ρ_n.

Lemma 4.3: Given an element $H=\left(\begin{smallmatrix}A&B\\C&D\end{smallmatrix}\right)$ of $\mathrm{gl}(2,\mathbb{C})$ *and an element $k\in[n]$, then*

$$\sigma_n(H)\,|k\rangle_n^Z=\sqrt{c_{k-1/2}}\,C\,|k-1\rangle_n^Z+((\ell+k)A+(\ell-k)D)\,|k\rangle_n^Z+\sqrt{c_{k+1/2}}\,B\,|k+1\rangle_n^Z.$$

The real Lie algebra u(2) and its subalgebra su(2) have bases $\{-iW,-iX,-iY,-iZ\}$ and $\{-iX,-iY,-iZ\}$, respectively, where

$$W=\frac{1}{2}\begin{pmatrix}1&0\\0&1\end{pmatrix},\qquad X=\frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix},\qquad Y=\frac{1}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix},\qquad Z=\frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Note that W commutes with X, Y, Z, and the other commutation relations are $[X,Y]=iZ$ and $[Y,Z]=iX$ and $[Z,X]=iY$. Let

$$\hat{W}_n=\sigma_n(W),\qquad \hat{X}_n=\sigma_n(X),\qquad \hat{Y}_n=\sigma_n(Y),\qquad \hat{Z}_n=\sigma_n(Z_n).$$

Given $k\in[n]$, then, by Lemma 4.3,

$$\hat{W}_n\,|k\rangle_n^Z=\ell\,|k\rangle_n^Z\,, \tag{26}$$

$$\hat{X}_n\,|k\rangle_n^Z=\tfrac{1}{2}(\sqrt{c_{k-1/2}}\,|k-1\rangle_n^Z+\sqrt{c_{k+1/2}}\,|k+1\rangle_n^Z), \tag{27}$$

$$\hat{Y}_n\,|k\rangle_n^Z=\frac{i}{2}(\sqrt{c_{k-1/2}}\,|k-1\rangle_n^Z-\sqrt{c_{k+1/2}}\,|k+1\rangle_n^Z), \tag{28}$$

$$\hat{Z}_n\,|k\rangle_n^Z=k|k\rangle_n^Z\,. \tag{29}$$

Thus, the algebra representation σ_n of $\mathrm{gl}(2,\mathbb{C})$ restricts to anti-Hermitian representations of u(2) and isu(2). In other words, the group representation ρ_n of $\mathrm{GL}(2,\mathbb{C})$ restricts to unitary representations of U(2) and SU(2). It is well-known (by an easy ladder argument) that the two restricted representations are irreducible.

For each $k\in[n]$, we define a vector

$$|k\rangle_n^X=\exp(-i\pi\hat{Y}_n/2)\,|k\rangle_n^Z. \tag{30}$$

To rewrite Eqs. (26)–(29) with respect to the orthonormal basis $\{|k\rangle_n^X:k\in[n]\}$, let us first determine the exponentials of iW, iX, iY, iZ. By evaluating derivatives at $t=0$, or by appealing to Eq. (19) (with complex values of β, γ, δ), we have

$$\begin{gathered}\exp(-itW)=\begin{pmatrix}e^{-it/2}&0\\0&e^{-it/2}\end{pmatrix},\quad \exp(-itX)=\begin{pmatrix}\cos t/2&-i\sin t/2\\-i\sin t/2&\cos t/2\end{pmatrix},\\ \exp(-itY)=\begin{pmatrix}\cos t/2&-\sin t/2\\\sin t/2&\cos t/2\end{pmatrix},\quad \exp(-itZ)=\begin{pmatrix}e^{-it/2}&0\\0&e^{it/2}\end{pmatrix}.\end{gathered} \tag{31}$$

By direct calculation, $e^{-itY}Ze^{itY}=Z\cos t+X\sin t$ for all $t\in\mathbb{R}$. So

$$\exp(-i\pi\hat{Y}_n/2)\hat{Z}_n\exp(i\pi\hat{Y}_n/2)=\hat{X}_n,\quad \exp(-i\pi\hat{Y}_n/2)\hat{X}_n\exp(i\pi\hat{Y}_n/2)=-\hat{Z}_n.$$

We can now rewrite Eqs. (26)–(29) as

$$\hat{W}_n\,|k\rangle_n^X=\ell\,|k\rangle_n^X\,, \tag{32}$$

$$\hat{X}_n\,|k\rangle_n^X=k|k\rangle_n^X\,, \tag{33}$$

$$\hat{Y}_n\,|k\rangle_n^X=\frac{i}{2}(\sqrt{c_{k-1/2}}\,|k-1\rangle_n^X-\sqrt{c_{k+1/2}}\,|k+1\rangle_n^X), \tag{34}$$

$$\hat{Z}_n |k\rangle_n^X = \frac{-1}{2}\left(\sqrt{c_{k-1/2}}\,|k-1\rangle_n^X + \sqrt{c_{k+1/2}}\,|k+1\rangle_n^X\right). \tag{35}$$

Lemmas 4.1 and 4.2 now yield the following result.

Lemma 4.4: Given $j,k\in[n]$, then

$$(1)\quad {}_n^Z\langle j|k\rangle_n^X = \frac{(-1)^{\ell+j}}{2^\ell}\sqrt{\frac{(\ell+j)!(\ell-j)!}{(\ell+k)!(\ell-k)!}}\sum_r \binom{\ell+k}{r}\binom{\ell-k}{\ell+j-r}(-1)^r,$$

$$(2)\quad {}_n^Z\langle j|k\rangle_n^X = \frac{(-1)^{\ell+j}}{2^\ell}\sqrt{\frac{(\ell+j)!(\ell+k)!}{(\ell-j)!(\ell-k)!}}\sum_s \frac{(2\ell-s)!(-2)^s}{s!(\ell+j-\nu)!(\ell+k-s)!},$$

where the indices of the sums run over the values for which the terms are defined, namely, $\max(0,j+k)\leqslant r\leqslant\min(\ell+j,\ell+k)$ *and* $0\leqslant s\leqslant\min(\ell+j,\ell+k)$.

Lemma 4.5: Given $j,k\in[n]$, then

$${}_n^Z\langle k|j\rangle_n^X=(-1)^{j-k}\quad {}_n^Z\langle j|k\rangle_n^X=(-1)^{\ell+k}\quad {}_n^Z\langle k|-j\rangle_n^X=(-1)^{\ell-j}\quad {}_n^Z\langle k|j\rangle_n^X.$$

Proof: Throughout the argument, when multiplying powers of -1, we must bear in mind that j,k,ℓ are all integers or all halves of odd integers. By Lemma 4.4(2),

$$(-1)^{\ell+j}\quad {}_n^Z\langle j|k\rangle_n^X=(-1)^{\ell+k}\quad {}_n^Z\langle k|j\rangle_n^X\ .$$

The first asserted equality follows.

Since the eigenvalues of $\hat{X}_n$ are distinct, the eigenvector equations $\hat{X}_n|j\rangle_n^X=|j\rangle_n^X$ and $\hat{X}_n|-j\rangle_n^X=-j\,|j\rangle_n^X$ determine the unit vectors $|j\rangle_n^X$ and $|-j\rangle_n^X$ up to phase factors. By Eqs. (27) and (33), the matrix entry ${}_n^Z\langle j|\hat{X}_n|k\rangle_n^X$ is zero unless $|j-k|=1$. Therefore, fixing j, there is a phase ω such that, for all k, we have

$${}_n^Z\langle k|-j\rangle_n^X=\omega(-1)^{\ell+k}\,{}_n^Z\langle k|j\rangle_n^X\ .$$

(In other words, if we multiply the Z-coordinates of $|j\rangle_n^X$ by an alternating ±1, then we get a multiple of $|-j\rangle_n^X$.) Putting $k=-\ell$, and noting that, by Lemma 4.4(1),

$${}_n^Z\langle-\ell|-j\rangle_n^X=\frac{1}{2}\sqrt{\binom{2\ell}{\ell+j}}\quad {}_n^Z\langle-\ell|j\rangle_n^X,$$

we deduce that $\omega=1$. The second asserted equality follows and, hence, the third. □

Lemma 4.6: Given $j,k\in[n]$, then

$$(1)\quad \sqrt{c_{k-1/2}}\quad {}_n^Z\langle k-1|j\rangle_n^X-2j\,{}_n^Z\langle k|j\rangle_n^X+\sqrt{c_{k+1/2}}\quad {}_n^Z\langle k+1|j\rangle_n^X=0,$$

$$(2)\quad \sqrt{c_{j-1/2}}\quad {}_n^Z\langle k|j-1\rangle_n^X-2k\,{}_n^Z\langle k|j\rangle_n^X+\sqrt{c_{j+1/2}}\quad {}_n^Z\langle k|j+1\rangle_n^X=0.$$

Let $\mathbb{N}_n$ denote the set of natural numbers less than n. For each $s\in\mathbb{N}_n$, we define the **Kravchuk polynomial** $K_{s,n}:\mathbb{N}_n\to\mathbb{C}$ and the **Kravchuk function** $h_{s,n}:[n]\to\mathbb{C}$ such that

$$\frac{(-1)^{\ell+j}}{2^\ell}\sqrt{\binom{2\ell}{\ell+j}\binom{2\ell}{\ell+k}}K_{\ell+j,n}(\ell+k)=h_{\ell+j,n}(k)={}_n^Z\langle j|k\rangle_n^X$$

for $j,k\in[n]$. The formulas in Appendix B are precisely Lemmas 4.4–4.6.

Proposition 4.7: The set of Kravchuk functions $\{h_{s,n}:s\in\mathbb{N}_n\}$ is an orthonormal basis for $\mathcal{L}_n$.

Proof: The values of the Kravchuk functions are the overlaps of two orthonormal bases. □

We now rewrite the Kravchuk functions as $|s\rangle_n=h_{s,n}$.

Proposition 4.8: Given $s\in[n]$, *then* $|s\rangle_n=(-1)^s\,|\ell-s\rangle_n^X$.
Proof: Apply Lemma 4.5. □
Via Proposition 4.8, we can rewrite Eqs. (32)–(35) as

$$\hat{W}_n\,|s\rangle_n=\ell\,|s\rangle_n\ , \tag{36}$$

$$\hat{X}_n\,|s\rangle_n=(\ell-s)\,|s\rangle_n\ , \tag{37}$$

$$\hat{Y}_n\,|s\rangle_n=\frac{i}{2}(-\sqrt{s(2\ell+1-s)}\,|s-1\rangle_n+\sqrt{(s+1)(2\ell-s)}\,|s+1\rangle_n), \tag{38}$$

$$\hat{Z}_n\,|s\rangle_n=\tfrac{1}{2}(\sqrt{s(2\ell+1-s)}\,|s-1\rangle_n+\sqrt{(s+1)(2\ell-s)}\,|s+1\rangle_n). \tag{39}$$

We define Hermitian operators

$$\hat{I}_n=\hat{X}_n/\ell,\quad \hat{P}_n=-\hat{Y}_n/\sqrt{\ell},\qquad \hat{Q}_n=\hat{Z}_n/\sqrt{\ell},$$

$$2\hat{B}_n=\hat{P}_n^2,\qquad 2\hat{C}_n=\hat{Q}_n^2,\quad 2\hat{D}_n=\hat{P}_n\hat{Q}_n+\hat{Q}_n\hat{P}_n\,.$$

We can understand $\hat{P}_n$ as discrete momentum (or frequency) and $\hat{Q}_n$ as discrete position (or time). For real $\beta,\ \gamma,\ \delta,\ \mu,\ \nu,\ \kappa$, we introduce a Hermitian operator

$$\hat{H}_n(\beta,\gamma,\delta,\mu,\nu,\kappa)=\beta\hat{B}_n+\gamma\hat{C}_n+\delta\hat{D}_n+\mu\hat{P}_n+\nu\hat{Q}_n+\kappa\hat{I}_n\,. \tag{40}$$

We define a **discrete affine canonical transform** to be a unitary operator having the form

$$\hat{U}_n(\beta,\gamma,\delta,\mu,\nu,\kappa)=\exp(-i\hat{H}_n(\beta,\gamma,\delta,\mu,\nu,\kappa)). \tag{41}$$

Recall that, in the continuum scenario, we defined the continuum affine canonical transforms to be the composites of the unitary operators having the form $\hat{U}(\beta,\ldots,\kappa)$. Our reason for not defining the discrete affine canonical transforms in the same way is that the infinitesmal generators $\hat{H}_n(\beta,\ldots,\kappa)$ do not span a Lie algebra. We can work with single-parameter groups of discrete affine canonical transforms—including fractional Fourier transforms, chirps and dilations—and these single-parameter groups, of course, have the index-additivity property $\hat{U}^s\hat{U}^t=\hat{U}^{s+t}$. In general, though, we do not retain any tractible closure property if we compose elements of distinct single-parameter groups.

However, in the continuum scenario, we defined the motion canonical transforms to be precisely the unitary operators having the form $\hat{E}(\kappa,\lambda,\mu,\nu)$, these operators being closed under composition. That feature can be retained in the discrete scenario. Let

$$\hat{N}_n=\hat{W}_n-\hat{X}_n=\ell(\hat{1}-\hat{I}_n).$$

The operators $\hat{I}_n,\ \hat{N}_n,\ \hat{P}_n,\ \hat{Q}_n$ are closed under commutators. We define a **discrete motion canonical transform** to be a unitary operator having the form

$$\hat{E}_n(\kappa,\lambda,\mu,\nu)=\exp(-i(\kappa\hat{I}_n+\lambda\hat{N}_n+\mu\hat{P}_n+\nu\hat{Q}_n))=\rho(E_n(\kappa,\lambda,\mu,\nu)), \tag{42}$$

where $\kappa,\lambda,\mu,\nu\in\mathbb{R}$. Let us put it in the language of representations. The Lie group u(2) has a basis $\{I_n,N_n,P_n,Q_n\}$ where

$$I_n=X/\ell\,,\quad N_n=W-X,\quad P_n=-Y/\sqrt{\ell}\,,\quad Q_n=Z/\sqrt{\ell}\,.$$

The commutation relations are

$$[I_n,N_n]=0,\quad [I_n,P_n]=-iQ_n/\ell\,,\quad [I_n,Q_n]=iP_n/\ell\,,$$
$$[N_n,P_n]=iQ_n\,,\quad [N_n,Q_n]=-iP_n\,,\quad [P_n,Q_n]=iI_n\,. \tag{43}$$

The algebra representation σ_n maps I_n, N_n, P_n, Q_n to $\hat{I}_n$, $\hat{N}_n$, $\hat{P}_n$, $\hat{Q}_n$, respectively. Observe that, as $\ell\to\infty$, the structural constants for I_n, N_n, P_n, Q_n converge to those given in Sec. 2 for the basis elements I, N, P, Q of hm. The algebra iu(2) and the group U(2) are to serve as the discrete analogs of the algebra hm and the group HM.

Now let us write down the matrices for $\hat{B}_n$, $\hat{C}_n$, $\hat{D}_n$, $\hat{P}_n$, $\hat{Q}_n$, $\hat{N}_n$, $\hat{I}_n$ with respect to the basis of Kravchuk functions. For $2r+1\in\mathbb{N}$, let

$$t_n(r)=\sqrt{(2r+1)(4\ell-2r+1)/16\ell}.$$

Given $s\in\mathbb{N}_n$, then

$$t_n\left(s+\frac{1}{2}\right)=\sqrt{\frac{s+1}{2}\left(1-\frac{s}{2\ell}\right)},\quad t_n\left(s-\frac{1}{2}\right)=\sqrt{\frac{s}{2}\left(1-\frac{s-1}{2\ell}\right)}.$$

By Eqs. (36)–(39),

$$\hat{B}_n|s\rangle_n=-\frac{1}{2}t_n\left(s-\frac{1}{2}\right)t_n\left(s-\frac{3}{2}\right)|s-2\rangle_n+\left(\frac{s}{2}\left(1-\frac{s}{2\ell}\right)+\frac{1}{4}\right)|s\rangle_n$$
$$-\frac{1}{2}t_n\left(s+\frac{1}{2}\right)t_n\left(s+\frac{3}{2}\right)|s+2\rangle_n\,, \tag{44}$$

$$\hat{C}_n|s\rangle_n=\frac{1}{2}t_n\left(s-\frac{1}{2}\right)t_n\left(s-\frac{3}{2}\right)|s-2\rangle_n+\left(\frac{s}{2}\left(1-\frac{s}{2\ell}\right)+\frac{1}{4}\right)|s\rangle_n+\frac{1}{2}t_n\left(s+\frac{1}{2}\right)t_n\left(s+\frac{3}{2}\right)|s+2\rangle_n\,, \tag{45}$$

$$\hat{D}_n|s\rangle_n=-it_n(s-\tfrac{1}{2})t_n(s-\tfrac{3}{2})|s-2\rangle_n+it_n(s+\tfrac{1}{2})t_n(s+\tfrac{3}{2})|s+2\rangle_n\,, \tag{46}$$

$$\hat{P}_n|s\rangle_n=-it_n(s-\tfrac{1}{2})|s-1\rangle_n+it_n(s+\tfrac{1}{2})|s+1\rangle_n\,, \tag{47}$$

$$\hat{Q}_n|s\rangle_n=t_n(s-\tfrac{1}{2})|s-1\rangle_n+t_n(s+\tfrac{1}{2})|s+1\rangle_n\,, \tag{48}$$

$$\hat{I}_n|s\rangle_n=(1-s/\ell)|s\rangle_n\,, \tag{49}$$

$$\hat{N}_n|s\rangle_n=s|s\rangle_n\,. \tag{50}$$

Again, we observe a suggestive connection with the continuum scenario. As $\ell\to\infty$, the matrix entries in Eqs. (44)–(50) converge to the matrix entries in Eqs. (11)–(17).

In Sec. II, we ended with an example. Let us end the present section with the analogous example. The discrete Fourier transform of Atakishiyev–Wolf[10] is the unitary operator $\hat{F}_n$ on $\mathcal{L}_n$ such that $\hat{F}_n|s\rangle_n=i^s|s\rangle_n$. More generally, their discrete fractional Fourier transform of order $t\in\mathbb{R}$ is the unitary operator $\hat{F}_n^t$ on $\mathcal{L}_n$ such that $\hat{F}_n^t|s\rangle_n=\exp(2\pi ist)|s\rangle_n$. In other words,

$$\hat{F}_n^t=\exp(2\pi it\hat{N}_n). \tag{51}$$

V. CONVERGENCE OF UNITARY TRANSFORMS

We wish to say that the continuum affine canonical transforms are limits of discrete affine canonical transforms. The whole problem lies in making the assertion absolutely unambiguous; then the proof will follow purely by deductive reasoning. Parts of the proof are deferred to Ref. 4.

Usually, when one writes an equation of the form $x=\lim_{n\to\infty}x_n$, the object x and the objects x_n all belong to the same space (or category). Such is not the case in our situation. We need to specify an interface between the continuum scenario and the discrete scenario. Let us describe the interface in two different ways, the first one clear and precise, the second one more illuminating from a practical perspective.

The clear description of the interface makes use of inductive limits, which are introduced in Refs. 1–3. A summary is given in Ref. 4, Sec. 2. Let $\mathcal{S}(\mathbb{R})$ be the Schwartz subspace of $L^2(\mathbb{R})$. For each positive integer n, let res_n be the linear map $\mathcal{S}(\mathbb{R})\to\mathcal{L}_n$ such that, given $\phi\in\mathcal{S}(\mathbb{R})$, and writing $\phi_n=\mathrm{res}_n(\phi)$, then

$$\phi_n(k)=\ell^{-1/4}\phi(\ell^{-1/2}k), \tag{52}$$

where $k\in[n]$. The linear maps res_n comprise an inductive resolution of $L^2(\mathbb{R})$. We are now in a position to realize vectors ψ in $L^2(\mathbb{R})$ as limits $\psi=\lim_n\psi_n$, where each ψ_n is a vector in the n-dimensional space $\mathcal{L}_n$. We can do the same for bounded operators and, in particular, for unitary operators.

The following alternative description is rather more intuitive. Let ϕ be a continuous and well-behaved complex-valued function with one real variable. For each n, let ϕ_n be a vector in $\mathcal{L}_n$. We regard ϕ_n as a good approximation to ϕ provided

$$\phi_n(k)\approx\ell^{-1/4}\phi(\ell^{-1/2}k)$$

for almost all $k\in[n]$. As the number of sample points $n=2\ell+1$ increases, the mesh $\ell^{-1/2}$ decreases and the width of the sample window $2\ell^{1/2}$ increases. If ϕ_n becomes an arbitrarily good approximation to ϕ in a certain manner that preserves everything involving inner products, then we say that ϕ_n converges to ϕ, and we write $\phi=\lim_n\phi_n$. Limits of unitary operators are required to preserve limits of vectors.

For example, Ref. 2, Theorem 5.1, says that

$$|s\rangle=\lim_n|s\rangle_n, \tag{53}$$

for all natural numbers s. In other words, the Hermite functions are the inductive limits of the Kravchuk functions.

Theorem 5.1: *Let* $\beta=\lim_n\beta_n$, $\gamma=\lim_n\gamma_n$, $\delta=\lim_n\delta_n$, $\mu=\lim_n\mu_n$, $\nu=\lim_n\nu_n$, $\kappa=\lim_n\kappa_n$ *as limits of real sequences. Then*

$$\hat{U}(\beta,\gamma,\delta,\mu,\nu,\kappa)=\lim_n\hat{U}_n(\beta_n,\gamma_n,\delta_n,\mu_n,\nu_n,\kappa_n).$$

Proof: This is part of Ref. 4, Theorem 7.2. □

A comparison of Eqs. (11)–(16) with Eqs. (44)–(49) provides a heuristic justification for Theorem 5.1, but not a proof. Convergence of matrix entries of infinitesmal generators does not, in general, imply convergence of the corresponding unitary operators.

Although arbitrary pairs of discrete affine canonical transforms do not compose in a tractible way, let us draw attention to the index-additivity property of single-parameter groups of discrete affine canonical transforms. Fix reals β, γ, δ, μ, ν, κ. Theorem 5.1 tells us that

$$\hat{U}(t\beta,t\gamma,t\delta,t\mu,t\nu,t\kappa)=\lim_n\hat{U}_n(t\beta_n,t\gamma_n,t\delta_n,t\mu_n,t\nu_n,t\kappa_n) \tag{54}$$

for all $t\in\mathbb{R}$. Since $\hat{B}_n,\hat{C}_n,\hat{D}_n,\hat{P}_n,\hat{Q}_n,\hat{I}_n$ are linearly independent for $n\geqslant 3$, we have the following.

Corollary 5.2: For fixed $n\geqslant 3$, *Eq. (54) describes a bijective correspondence between the single-parameter groups of continuum affine canonical transforms and the single-parameter*

groups of discrete affine canonical transforms on $\mathcal{L}_n$. Now let n vary. The elements of a single-parameter group of continuum affine canonical transforms are inductive limits of sequences of elements of the corresponding single-parameter groups of discrete affine canonical transforms.

We now turn to motion canonical transforms.

Theorem 5.3: *Let* $\kappa=\lim_n \kappa_n$, $\lambda=\lim_n \lambda_n$, $\mu=\lim_n \mu_n$, $\nu=\lim_n \nu_n$ *as limits of real sequences. Then*

$$\hat{E}(\kappa,\lambda,\beta,\gamma)=\lim_n \hat{E}_n(\kappa_n,\lambda_n,\beta_n,\delta_n).$$

Proof: The limit of representations in Ref. 4, Theorem 10.2, is a stronger result. □

Warning: Theorem 5.3 is not a special case of Theorem 5.1. Not all of the discrete motion canonical transforms are discrete affine canonical transforms.

Comparing Eqs. (18) and (51), we see that Theorem 5.3 recovers the convergence of fractional Fourier transforms

$$\hat{F}^t=\lim_n \hat{F}_n^t. \tag{55}$$

A more direct proof of Eq. (55) is given in Ref. 3, Example 4.F. The equation (not expressed in the form of an inductive limit) is due to Atakishiyev–Wolf.[10]

VI. COMPLEX-ORDER FOURIER TRANSFORMS AND COHERENT STATES

We introduce two more objects to the continuum scenario: the system of Glauber coherent states (Gabor functions) and the continuum Hermite semigroup (the semigroup of complex-order Fourier transforms). Then we introduce the analogous objects to the discrete scenario: the system of spin coherent states and the discrete Hermite semigroup (discrete complex-order Fourier transforms). As in the previous section, the analogy between the discrete and continuum objects is plain enough; our purpose is to express the analogy precisely using inductive limits.

For an introduction to the Glauber and spin coherent states, see Ref. 28, Chap. 1 or Ref. 29. To fix notation, we shall recall the relevant definitions, but we shall not discuss the measures on the label spaces. The **Glauber coherent state** $|z\rangle^C$ with **label** $z\in\mathbb{C}$ can be defined as

$$|z\rangle^C=\exp(-|z|^2/2)\exp(z\hat{A}^\dagger)|0\rangle=\exp(-|z|^2/2)\sum_{s=0}^{\infty}\frac{z^s}{\sqrt{s!}}|s\rangle. \tag{56}$$

Writing g_z to denote $|z\rangle^C$ regarded as a (rapidly decreasing) function $\mathbb{R}\to\mathbb{C}$, we have

$$\pi^{1/4}g_z(q)=\exp\left(-\frac{q^2}{2}+\sqrt{2}zq-\frac{z^2}{2}-\frac{|z|^2}{2}\right)=\exp\left(-\frac{q^2}{2}-(u+iv)q-\frac{u^2}{2}-\frac{iuv}{2}\right), \tag{57}$$

where $\sqrt{2}z=u+iv$ with $u,v\in\mathbb{R}$. We note one other useful characterization:

$$|z\rangle^C=\exp(-iu\hat{P}+iv\hat{Q}))|0\rangle. \tag{58}$$

In electrical enginnering and signal processing, Glauber coherent states are usually called **Gabor functions**, and are usually expressed in the form of Eq. (57). The other two equations are more normally used in quantum physics. As a gesture of mediation between the two disciplines, let us give a quick proof that the three equations are mutually equivalent. From Eq. (58), rewritten as

$$g_z=\exp(-iu\hat{P}+iv\hat{Q})h_0,$$

it is easy to obtain Eq. (57) using the identities

$$\exp(-i(u\hat{P}+v\hat{Q}))=\exp(iuv/2)\exp(iv\hat{Q})\exp(-iu\hat{P}),$$

$$\exp(-iu\hat{P})\phi(q)=\phi(q-u),\quad \exp(-iv\hat{Q})\phi(q)=\exp(ivq)\phi(q),$$

where $\phi\in\mathcal{S}(\mathbb{R})$. Using the generating function

$$\exp(2qt-t^2)=\sum_{s=0}^{\infty}\frac{t^s}{s!}H_s(q)$$

together with Eq. (57), straightforward manipulation yields

$$\sum_{s=0}^{\infty}\frac{t^s}{s!}\int_{-\infty}^{\infty}dqH_s(q)\exp(-q^2/2)g_z(q)=\pi^{1/4}\exp(-|z|^2/2)\exp(\sqrt{2}zt).$$

Comparing coefficients of powers of t, we obtain $\langle s|z\rangle^C=\exp(-|z|^2/2)/\sqrt{s!}$. The equivalence of Eqs. (56)–(58) is now established.

For $\zeta\in\mathbb{C}$ with $|\zeta|\leqslant 1$, the **continuum complex-order Fourier transform** $\hat{F}(\zeta)$ is defined to be the bounded operator on $L^2(\mathbb{R})$ such that

$$\hat{F}(\zeta)\,|s\rangle=\zeta^s\,|s\rangle\,. \tag{59}$$

The integral kernel for $\hat{F}(\zeta)$ may be found in Ref. 30. An optical realization of $\hat{F}(\zeta)$ is discussed in Ref. 31. We have an obvious composition law

$$\hat{F}(\zeta)\hat{F}(\zeta')=\hat{F}(\zeta\zeta'). \tag{60}$$

The commutative semigroup $\{\hat{F}(\zeta):|\zeta|\leqslant 1\}$, called the **continuum Hermite semigroup**, is evidently isomorphic to the semigroup $\{\zeta\in\mathbb{C}:|\zeta|\leqslant 1\}$. Writing

$$\zeta=\exp(2\pi it), \tag{61}$$

we say that $\hat{F}(\zeta)$ has **order** t. Given $\hat{F}(\zeta)$, the real part of t is well-defined up to congruence modulo 1. The condition $|\zeta|\leqslant 1$ is precisely the condition that t lies in the closed upper half of the complex plane. By Eq. (17),

$$\hat{F}(\zeta)=\exp(2\pi it\hat{N}).$$

The continuum fractional Fourier transforms are precisely the unitary continuum complex-order Fourier transforms. By Eqs. (56) and (59), the continuum Hermite semigroup permutes the Glauber coherent states (up to scalar factors) according to the equation

$$\hat{F}(\zeta)\,|z\rangle^C=\exp(|z\zeta|^2/2-|z|^2/2)\,|\zeta z\rangle^C\,. \tag{62}$$

Now let us look at the discrete scenario. The **discrete annihilation operator** $\hat{A}_n$ and its Hermitian conjugate, the **discrete creation operator** $\hat{A}_n^\dagger$, are defined to be

$$\hat{A}_n=(\hat{Q}_n+i\hat{P}_n)/\sqrt{2}\,,\quad \hat{A}_n^\dagger=(\hat{Q}_n-i\hat{P}_n)/\sqrt{2}\,.$$

From Eqs. (47) and (48) we have

$$\hat{A}_n\,|s\rangle_n=\sqrt{s\left(1-\frac{s-1}{2\ell}\right)}\,|s-1\rangle_n\,,\quad \hat{A}_n^\dagger|s\rangle_n=\sqrt{(s+1)\left(1-\frac{s}{2\ell}\right)}\,|s+1\rangle_n\,.$$

The **spin coherent state** $|z\rangle_n^C$ with **label** $z \in \mathbb{C}$ is defined by

$$\left(1+\frac{|z|^2}{2\ell}\right)^{\ell} |z\rangle_n^C = \exp(z\hat{A}_n^\dagger)|0\rangle_n = \sum_{s=0}^{2\ell} \sqrt{\binom{2\ell}{s}} \left(\frac{z}{\sqrt{2\ell}}\right)^s |s\rangle_n \ . \tag{63}$$

We also allow a spin coherent state

$$|\infty\rangle_n^C = \lim_{z\to\infty} |z\rangle_n^C = |2\ell\rangle_n^C \ .$$

For arbitrary $\zeta \in \mathbb{C}$, the **discrete complex-order Fourier transform** $\hat{F}_n(\zeta)$ is defined to be the operator on $L^2(\mathbb{R})$ such that

$$\hat{F}_n(\zeta)\,|s\rangle_n = \zeta^s\,|s\rangle_n \ . \tag{64}$$

Using Eqs. (30) and (31), followed by Lemma 4.1 and Proposition 4.8, it can be shown that

$$\hat{F}_n(\zeta) = \rho_n(K(\zeta)), \qquad K(\zeta) = \frac{1}{2}\begin{pmatrix} 1+\zeta & 1-\zeta \\ 1-\zeta & 1+\zeta \end{pmatrix}. \tag{65}$$

Evidently, we have a composition law

$$\hat{F}_n(\zeta)\hat{F}_n(\zeta') = \hat{F}_n(\zeta\zeta'). \tag{66}$$

The semigroup $\{\hat{F}(\zeta):\zeta\in\mathbb{C}\}$ is called the **discrete Hermite semigroup**. Letting t be as in Eq. (61), we say that $\hat{F}_n(\zeta)$ has **order** t. The real part of t is still well-defined only up to congruence modulo 1, but there are now no constraints on the range of t. By Eq. (50),

$$\hat{F}_n(\zeta) = \exp(2\pi i t \hat{N}_n).$$

The discrete fractional Fourier transforms are precisely the unitary discrete complex-order Fourier transforms. By Eqs. (63) and (59), the discrete Hermite semigroup permutes the spin coherent states (up to scalar factors) according to the equation

$$\hat{F}_n(\zeta)\,|z\rangle_n^C = \left(\frac{2\ell+|\zeta z|^2}{2\ell+|z|^2}\right)^{\ell} |\zeta z\rangle_n^C . \tag{67}$$

Theorem 6.1: *Given* $z\in\mathbb{C}$, *then* $|z\rangle^C = \lim_n |z\rangle_n^C$.

Proof: Consider a vector $\psi\in L^2(\mathbb{R})$ and vectors $\psi_n \in L_n$ such that the set $\{\|\psi_n\|:n\in\mathbb{N}\}$ is bounded. By Eq. (53) and Ref. 1, Theorem 3.4, $\psi = \lim_n \psi_n$ if and only if

$$\langle s|\psi\rangle = \lim_n {}_n\langle s|\psi_n\rangle$$

for all $s\in\mathbb{N}$. These two equivalent conditions hold when $\psi = |z\rangle^C$ and $\psi_n = |z\rangle_n^C$ because

$$\frac{\exp(-|z|^2/2)}{\sqrt{s!}} = \lim_{\ell\to\infty}\left(1+\frac{|z|^1}{2\ell}\right)^{-\ell} \sqrt{\binom{2\ell}{s}}\left(\frac{1}{\sqrt{2\ell}}\right)^s .$$

□

Theorem 6.2: *Given* $\zeta\in\mathbb{C}$ *with* $|\zeta|\leqslant 1$, *then* $\hat{F}(\zeta) = \lim_n \hat{F}_n(\zeta)$.

Proof: Let $\psi\in L^2(\mathbb{R})$ and $\psi_n\in\mathcal{L}_n$ such that $\psi = \lim_n \psi_n$. Using the criterion for limits noted in the previous argument,

$$\langle s|\hat{F}(\zeta)\psi\rangle=\zeta^s\langle s|\psi\rangle=\lim_n \zeta^s\ {}_n\langle s|\psi_n\rangle=\lim_n\ {}_n\langle s|\hat{F}_n(\zeta)\psi_n\rangle,$$

and $\hat{F}(\zeta)\psi=\lim_n \hat{F}_n(\zeta)\psi_n$. □

VII. CONCLUSIONS

We have used inductive limits to express the way in which the discrete scenario and the continuum scenario are related to each other. From a procedural point of view (oriented, say, towards implementation of numerical calculations), the relationships between the two scenarios has two significant aspects: *approximation* and *analogy*. Not only do the discrete objects serve as approximations to their corresponding continuum objects, but they are also analogs in the sense that the algebraic structures in the discrete scenario mirror the algebraic structures in the continuum scenario. For the purpose of numerical calculation, that feature is important, because it ensures that errors due to inaccuracy of the approximating formulas are not compounded under repeated composition. Our approach provides some rationale for both of those aspects: inductive limits serve as approximations; they also preserve algebraic structures, specifically, they preserve inner products, operator-vector compositions, and operator-operator compositions.

We propose inductive limits as a way of providing theoretical justification for discrete approximations in cases where precise error analysis would be too difficult. As concrete examples become more complicated, intuition may become unreliable, and a precise criterion for the limits may become increasingly useful. Inductive limits of representations, as in Sec. V and Ref. 4, appears to be applicable to various other limits of representations. See, for instance, Refs. 8 and 32–35. It is to be expected that, through moderately complicated but routine exercises in epsilonics, the limits of operators in those works can be shown to be inductive limits.

However, to plough through such calculations would be to overlook a more interesting line of study. Limits of representations are more subtle than limits of individual operators. The result (Ref. 4, Theorem 9.4) on convergence of structural constants requires, in addition to convergence of individual operators, an analytic convergence hypothesis. The hypothesis is potentially verifiable, in practice, for concrete examples, but some simplifications may be possible; perhaps it suffices to check the uniformity condition in Ref. 4, Sec. 8 only for a spanning set of infinitesmal generators. Thus, at the time of writing, the criterion for inductive limits of representations should be regarded as subject to simplification or modification.

Besides, in order to be of significant practical use, the theory of inductive limits of representations is in need of general theorems. For a limit of representations $\rho=\lim_n \rho_n$ (Ref. 4. Proposition 9) asserts that, if ρ is faithful, then ρ_n is faithful for large n. That result is unlikely to be useful in application to concrete examples, since faithfulness is usually obvious to start with. However, the result may point the way forwards: if ρ is irreducible, must ρ_n be irreducible for large n? To prove theorems, of course, it is sometimes necessary to tinker with definitions. So, again, we conclude that the present criterion for inductive limits of representations should be regarded as subject to change.

It appears that inductive limits can also be used to describe a correspondence between a finite-discrete periodic scenario based on the integers modulo p^m and a continuous periodic scenario based on the p-adic integers. Here, p is a rational prime. For the discrete context, see Refs. 36 and 37; for the continuous context, see Refs. 38, and 39. In this p-adic scenario, purely intuitive arguments are to be distrusted, so the use of some or another precise notion of limit is essential.

Discrete versus continuum correspondences of operators and representations arise frequently. Without attempting to classify the various directions of study, let us list some papers on the topic where the term *limit* is used explicitly and is probably interpretable as *inductive limit:* Refs. 40, 6, 7, 8, 32, 10, 41, 42, 5, 43, 44, 35, and 45–47. We have given a broad spread of citations so as to provide evidence that an intuitive equivalent of the notion of an inductive limit is in widespread use. The list could be extended considerably. The author has come across only one paper (citation

omitted) in which the limits of operators are nonsensical (arbitrary $\mathrm{SL}(2,\mathbb{R})$ canonical transforms written as ''limits'' of $\mathrm{SL}(2,p)$ canonical transforms, where p runs over the rational primes).

There are also a great many works where the term *limit* is not used for our purpose, but inductive limits seem to be involved implicitly. This point pertains, in particular, to many single-parameter discrete systems used as approximations to continuum systems in signal processing. For some examples, see Refs. 48 and 49 and references therein.

APPENDIX A: A COUNTER-EXAMPLE

By the definition of inductive limits of operators, Theorem 6.2 can be expressed as follows.

Theorem A.1: *Given a vector* $\psi\in L^2(\mathbb{R})$ *and vectors* $\psi_n\in\mathcal{L}_n$ *such that* $\psi=\lim_n \psi_n$, *then, for all* $\zeta\in\mathbb{C}$ *with* $|\zeta|\leqslant 1$, *we have* $\hat{F}(\zeta)\psi=\lim_n \hat{F}_n(\zeta)\psi_n$.

For arbitrary $\zeta\in\mathbb{C}^\times$, we can still define $\hat{F}(\zeta)$ to be the operator on $L^2(\mathbb{R})$ satisfying Eq. (59). If $|\zeta|>1$, then $\hat{F}(\zeta)$ is unbounded. The domain of $\hat{F}(\zeta)$, in this case, has been studied by Byun.[50] Plainly, for arbitrary ζ, the conclusion of Theorem A.1 still holds when ψ is a Glauber cat state (linear combination of coherent states) in $L^2(\mathbb{R})$ and ψ is the corresponding spin cat state in $\mathcal{L}_n$. However, for arbitrary ζ and arbitrary ψ in the domain of $\hat{F}(\zeta)$, the conclusion of Theorem A.1 can fail. A counter-example is $\psi=0$ and $\psi_n=2^{-2\ell}|2\ell\rangle$ with $\zeta=3$.

It is difficult to imagine how the mainstream techniques (formal manipulation) could be used to ''derive'' Theorem A.1 without also ''deriving'' the fallacy refuted in the previous paragraph.

APPENDIX B: IDENTITIES FOR THE KRAVCHUK FUNCTIONS

Let n be a positive integer. As in Sec. IV, we write $n=2\ell+1$ and $[n]=\{-\ell,1-\ell,\ldots,\ell-1,\ell\}$ and we define $c_{k+1/2}=(\ell-k)(\ell+k+1)$, equivalently, $c_{k-1/2}=(\ell+k)(\ell-k+1)$, where $2k\in\mathbb{Z}$. The **Kravchuk polynomials** $K_{0,n},K_{1,n},\ldots,K_{2\ell,n}$ are the functions $\{0,1,\ldots,2\ell\}\to\mathbb{C}$ given by

$$K_{\ell+j,n}(\ell+k)=\binom{2\ell}{l+j}^{-1}\sum_{\mu=\max(0,j+k)}^{\min(\ell+j,\ell+k)}\binom{\ell+k}{\mu}\binom{\ell-k}{\ell+j-\mu}(-1)^\mu$$
$$=\sum_{\nu=0}^{\min(\ell+j,\ell+k)}\binom{2\ell}{\nu}^{-1}\binom{\ell+j}{\nu}\binom{\ell+k}{\nu}(-2)^\nu,$$

where $j,k\in[n]$. Note that, in each of the two formulas, the index μ or ν runs over all values for which the terms are defined. In Sec. IV, it is shown that the two formulas are equivalent to each other. It is also shown that the Kravchuk polynomials satisfy

$$K_{\ell+k,n}(\ell+j)=K_{\ell+j,n}(\ell+k), \tag{B1}$$

$$K_{\ell+j,n}(\ell-k)=(-1)^{\ell+j}K_{\ell+j,n}(\ell+k), \tag{B2}$$

$$K_{\ell-j,n}(\ell+k)=(-1)^{\ell+k}K_{\ell+j,n}(\ell+k), \tag{B3}$$

$$(\ell-k)K_{\ell+j,n}(\ell+k+1)+2jK_{\ell+j,n}(\ell+k)+(\ell+k)K_{\ell+j,n}(\ell+k-1)=0, \tag{B4}$$

$$(\ell-j)K_{\ell+j+1,n}(\ell+k)+2kK_{\ell+j,n}(\ell+k)+(\ell+j)K_{\ell+j-1,n}(\ell+k)=0. \tag{B5}$$

The **Kravchuk functions** $h_{0,n},h_{1,n},\ldots,h_{2\ell,n}$ are the functions $[n]\to\mathbb{C}$ given by

$$h_{s,n}(k)=\frac{(-1)^s}{2^\ell}\sqrt{\binom{2\ell}{s}\binom{2\ell}{\ell+k}}K_{s,n}(\ell+k). \tag{B6}$$

In other words,

$$h_{\ell+j,n}(k)=\frac{(-1)^{\ell+j}}{2^{\ell}}\sqrt{\frac{(\ell+j)!(\ell-j)!}{(\ell+k)!(\ell-k)!}}\sum_{\mu}\binom{\ell+k}{\mu}\binom{\ell-k}{\ell+j-\mu}(-1)^{\mu}$$

$$=\frac{(-1)^{\ell+j}}{2^{\ell}}\sqrt{\frac{(\ell+j)!(\ell+k)!}{(\ell-j)!(\ell+k)!}}\sum_{\nu}\frac{(2\ell-\nu)!(-2)^{\nu}}{\nu!(\ell+j-\nu)!(\ell+k-\nu)!}. \tag{B7}$$

Equations (B1–B5) can be rewritten as

$$h_{\ell+k,n}(j)=(-1)^{k-j}h_{\ell+j,n}(k), \tag{B8}$$

$$h_{\ell+j,n}(-k)=(-1)^{\ell+j}h_{\ell+j,n}(k), \tag{B9}$$

$$h_{\ell-j,n}(k)=(-1)^{\ell-k}h_{\ell+j,n}(k), \tag{B10}$$

$$\sqrt{c_{k+1/2}}h_{\ell+j,n}(k+1)+2jh_{\ell+j,n}(k)+\sqrt{c_{k-1/2}}h_{\ell+j,n}(k-1)=0, \tag{B11}$$

$$\sqrt{c_{j+1/2}}h_{\ell+j+1,n}(k)-2kh_{\ell+j,n}(k)+\sqrt{c_{j-1/2}}h_{\ell+j-1,n}(k)=0. \tag{B12}$$

Proposition 4.7 says that Kravchuk functions comprise an orthonormal basis for the space of functions $[n]\to\mathbb{C}$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Upper and lower limits for the number of S-wave bound states in an attractive potential

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(Received 11 September 2002; accepted 22 October 2002)

New upper and lower limits are given for the number of S-wave bound states yielded by an attractive (monotonic) potential in the context of the Schrödinger or Klein–Gordon equation. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1532107]

I. INTRODUCTION AND MAIN RESULTS

The determination in the framework of nonrelativistic quantum mechanics of necessary and sufficient conditions for the existence of bound states in a given potential and, more generally, of upper and lower limits for the number of bound states yielded by such a potential, has engaged the attention of theoretical and mathematical physicists since the early 1950s, and, notwithstanding the fact that, with modern computers, the numerical evaluation of the number of bound states for a given potential is an easy task, it continues to be actively pursued: see, for instance, Refs. 1,2,5–7,10–17,19–26, 28–30, as well as the surveys of (some of) these results in Refs. 8 and 32. In this article we provide new upper and lower limits for the number of S-wave bound states possessed by a central potential vanishing at infinity and yielding a nowhere repulsive force and we compare them, for some test potentials, with the exact results and with previously known upper and lower limits. These comparisons indicate that these new limits are generally more stringent than hitherto known results and indeed remarkably cogent, especially for potentials possessing many bound states.

Let us briefly review (some of) the previous findings, focusing on those relevant to our treatment, hence restricting attention to the S-wave case (even when results are also known for higher partial waves). Hereafter—except in Sec. IV—we use the standard nonrelativistic quantum mechanical units such that $\hbar^2/(2m)=1$, which entail that the potential $V(r)$ has the dimension of an inverse square length, and we indicate with N the number of S-wave bound states. We also assume throughout that the potential $V(r)$ is less singular than the inverse square radius at the origin and that it vanishes asymptotically faster than the inverse square radius, say (for some *positive* ε)

$$\lim_{r\to 0}\lfloor r^{2-\varepsilon}V(r)\rfloor=0, \tag{1.1a}$$

$$\lim_{r\to \infty}\lfloor r^{2+\varepsilon}V(r)\rfloor=0. \tag{1.1b}$$

Note that these assumptions entail that the square root of the (modulus of the) potential is integrable both at the origin and at infinity.

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Bargmann[2] and Schwinger[30] obtained the following upper limit for N:

$$\text{BS:}\quad N \leqslant \int_0^\infty \mathrm{d}r\, r|V(r)|. \tag{1.2}$$

This result is generally referred to as the Bargmann–Schwinger bound; we hereafter refer to it as the BS (upper) limit. This result was obtained after Jost and Pais[22] had shown that the fact that the right-hand side of (1.2) exceeds unity is a *necessary* condition for the existence of bound states (namely, the special case of the BS limit with $N=1$).

Cohn[15,16] and Calogero[6,7] later obtained another upper limit for N, which is valid provided the force associated with the potential $V(r)$ is nowhere repulsive, namely the potential $V(r)$ is a monotonically nondecreasing function of the radius r,

$$dV(r)/dr \geqslant 0, \tag{1.3}$$

entailing of course that the potential is everywhere negative, $V(r)=-|V(r)|$. This upper limit reads

$$\text{CC:}\quad N \leqslant \frac{2}{\pi}\int_0^\infty \mathrm{d}r|V(r)|^{1/2}. \tag{1.4}$$

This result has been referred to as the Calogero–Cohn bound;[11] hereafter we shall refer to it as the CC (upper) limit. This CC limit, (1.4), in contrast to the BS limit (1.2), features the correct dependence on the strength of the potential; indeed it has been shown[8] that, for any potential $V(r)$, if a measure of the strength of the potential is introduced via the introduction of a ''coupling constant'' g^2 by setting

$$V(r)=g^2 v(r), \tag{1.5}$$

then as g diverges to positive infinity, N grows proportionally to g. But it is also known[10] (see also Refs. 7, 14, and 19) that asymptotically, as g diverges, $g\to\infty$,

$$N \approx \frac{1}{\pi}\int_0^\infty \mathrm{d}r|V(r)|^{1/2}=\frac{g}{\pi}\int_0^\infty \mathrm{d}r|v(r)|^{1/2}. \tag{1.6}$$

Hence for strongly attractive potentials featuring many bound states the CC limit (1.4) tends to overestimate N by a factor 2. The main merit of the new limits provided in this article is to remedy this defect (see below).

Some modifications of the inequality (1.4) and of the condition (1.3) on the shape of the potential have been introduced by Chadan *et al.*[11] These modifications lead to less restrictive inequalities but more flexible conditions on the shape of the potential, allowing for some oscillations.

Another upper bound, which also gives the correct power behavior of the number of bound states when the strength of the potential diverges, has been obtained by Martin:[25]

$$\text{M:}\quad N \leqslant \left[\int_0^\infty \mathrm{d}r\, r^2 V^-(r)\int_0^\infty \mathrm{d}r\, V^-(r)\right]^{1/4}, \tag{1.7}$$

where $V^-(r)$ is the *negative* part of $V(r)$. This limit is applicable even if the potential does not satisfy the property to yield a nowhere repulsive force, see (1.3), but it is nontrivial only for potentials the nonpositive part of which is integrable at the origin. Hereafter we refer to it as the M (upper) limit.

The known lower limits on N are scarcer and less neat. A result[7] states that

$$N \geqslant \frac{1}{\pi} \int_0^\infty dr \, \min[1/a, -a\, V(r)] - \frac{1}{2}, \tag{1.8a}$$

where a is an arbitrary *positive* constant, $a>0$, and

$$\min[x,y]=x \quad \text{if} \quad x \leqslant y, \qquad \min[x,y]=y \quad \text{if} \quad y \leqslant x. \tag{1.8b}$$

By choosing a proportional to g^{-1} [see (1.5)] it is clear that this limit has the correct power growth when g diverges. The most stringent version of this limit obtains by performing first the integration on the right-hand side of (1.8a), and by then maximizing the result over all *positive* values of the parameter a. For everywhere nondecreasing potentials, see (1.3), the minimum definition (1.8b) is easily implemented by splitting the integration range in (1.8a) in two parts, and, thereby, via standard computations, one arrives at the somewhat neater lower limit

$$\text{C:} \quad N \geqslant \frac{2}{\pi} \rho |V(\rho)|^{1/2} - \frac{1}{2}, \tag{1.9a}$$

where ρ is a root of the equation

$$\rho\, V(\rho) = \int_\rho^\infty dr\, V(r). \tag{1.9b}$$

This limit will be hereafter referred to as the C (lower) limit.

If the potential, besides satisfying the monotonicity condition (1.3), is finite at the origin, a more explicit if less cogent result obtains by setting $a=|V(0)|^{-1/2}$ in (1.8):

$$\text{C}_0\text{:} \quad N \geqslant \frac{1}{\pi} \int_0^\infty dr \, \frac{|V(r)|}{|V(0)|^{1/2}} - \frac{1}{2}. \tag{1.10}$$

Hereafter we shall refer to this result as the C_0 (lower) limit.

By setting $N=1$ in (1.8) and (1.9), respectively (1.10), one obtains the following three conditions, each of which is *sufficient* to guarantee the existence of (at least) one bound state:

$$\int_0^\infty dr \, \min[1/a, -a\, V(r)] > \frac{3\pi}{2}, \tag{1.11a}$$

$$\rho |V(\rho)|^{1/2} > \frac{3\pi}{4} \tag{1.11b}$$

with ρ again a root of (1.9b),

$$\int_0^\infty dr |V(r)| > \frac{3\pi}{2} |V(0)|^{1/2}. \tag{1.11c}$$

In the first of these inequalities, (1.11a), a is an arbitrary *positive* constant; the most stringent condition obtains of course by performing first the integration on the left-hand side and by then minimizing the result over all *positive* values of a; the other two inequalities, (1.11b) and (1.11c), are neater but for their validity it is required that the potential satisfies the monotonicity condition (1.3) [and of course (1.11c) is only applicable if the potential is finite at the origin].

In view of future applications (see below) let us also report two other conditions which are *sufficient* to guarantee that the potential $V(r)$ possesses (at least) one bound state:[5,8]

$$a^{-1}\int_0^a \mathrm{d}r\, r^2|V(r)|+a\int_a^\infty \mathrm{d}r\,|V(r)|>1, \tag{1.12}$$

$$a\int_0^\infty \mathrm{d}r|V(r)|/[1+a^2|V(r)|]>1. \tag{1.13}$$

Both these conditions apply provided the potential is nowhere positive, $V(r)=-|V(r)|$; in both of them a is an arbitrary *positive* constant, and of course the most stringent conditions obtain by minimizing the left-hand sides over all *positive* values of a. It is easily seen that, in the case of (1.12), the minimizing value of a is the root of the equation

$$\int_0^a \mathrm{d}r\, r^2|V(r)|=a^2\int_a^\infty \mathrm{d}r|V(r)| \tag{1.14}$$

[entailing that the two terms on the left-hand side of (1.12) yield equal contributions] and in the case of (1.13) it is the root of the equation

$$\int_0^\infty \mathrm{d}r|V(r)|(1-a^2|V(r)|)(1+a^2|V(r)|)^{-2}=0. \tag{1.15}$$

After this terse survey of previous results let us now report the new upper and lower limits on the number N of S-wave bound states obtained in this article, in which we restrict for simplicity attention to potentials that satisfy the monotonicity condition (1.3) (we plan to report results applicable to more general potentials, as well as to higher partial waves, in a subsequent paper). These limits are of two different types.

The (new) upper limit of the first type reads as follows:

$$N\leqslant \frac{1}{\pi}\int_0^\infty \mathrm{d}r|V(r)|^{1/2}+\frac{1}{4\pi}\log\left|\frac{V(p)}{V(q)}\right|+\frac{1}{2}, \tag{1.16a}$$

with the two distances p and q defined by the relations

$$\int_0^p \mathrm{d}r|V(r)|^{1/2}=\pi/2, \tag{1.16b}$$

$$\int_q^\infty \mathrm{d}r|V(r)|^{1/2}=\pi/2. \tag{1.16c}$$

Clearly these two formulas, (1.16b), respectively (1.16c), provide an unambiguous definition of the two quantities p, respectively q, provided the potential $V(r)$ possesses at least one bound state, since it must then satisfy the following *necessary* condition for the existence of bound states[6] [corresponding to (1.4) with $N=1$]:

$$\int_0^\infty \mathrm{d}r|V(r)|^{1/2}\geqslant \pi/2. \tag{1.17}$$

And also note that, due to the assumed monotonicity of the potential, see (1.3), (1.16) entails that a neater albeit less stringent upper limit to N is provided by the formula

$$N\leqslant \frac{1}{\pi}\int_0^\infty \mathrm{d}r|V(r)|^{1/2}+\frac{1}{4\pi}\log\left|\frac{V(0)}{V(q)}\right|+\frac{1}{2}, \tag{1.18}$$

with q always defined by (1.16c). This upper limit is, however, nontrivial only for potentials that are finite at the origin.

The (new) lower limit of the first type reads (for potentials that are finite at the origin)

$$N > \frac{1}{\pi}\int_0^s dr\,|V(r)|^{1/2} - \frac{1}{4\pi}\log\left|\frac{V(0)}{V(s)}\right| - \frac{1}{2}, \tag{1.19}$$

with s an arbitrary (of course *positive*) radius. The choice of s that produces the most stringent bound is the root of the following nondifferential equation in s (here, and always below, appended primes denote differentiations):

$$V'(s) = 4|V(s)|^{3/2}. \tag{1.20}$$

Indeed, the values of s which satisfy this last equation maximize the right-hand side of (1.19). If this equation possesses more than one positive root, generally the most stringent bound obtains by choosing the largest.

A neater, if generally less stringent, lower bound obtains by choosing $s=q$, since via (1.16c) one then gets

$$N > \frac{1}{\pi}\int_0^\infty dr\,|V(r)|^{1/2} - \frac{1}{4\pi}\log\left|\frac{V(0)}{V(q)}\right| - 1. \tag{1.21}$$

The analogy of this formula, (1.21), to (1.18) is remarkable, and of course this lower limit to N is also nontrivial only if the potential $V(r)$ is finite at the origin.

If the potential is singular at the origin, a neat lower bound, analogous to (1.16a), reads

$$N \geqslant \frac{1}{\pi}\int_0^\infty dr\,|V(r)|^{1/2} - \frac{1}{4\pi}\log\left|\frac{V(p)}{V(q)}\right| - \frac{3}{2}, \tag{1.22}$$

with p and q defined by (1.16b) and (1.18c).

A less neat but generally more stringent (albeit only marginally so) lower bound that looks somewhat analogous to (1.19) and is also applicable to potentials that are singular at the origin reads

$$N > \frac{1}{\pi}\int_t^s dr\,|V(r)|^{1/2} - \frac{1}{4\pi}\log\left|\frac{V(p)}{V(s)}\right|, \tag{1.23a}$$

with p defined by (1.16b) and $s \geqslant t$ but otherwise *arbitrary*. As for the *positive* quantity t, a characterization of it adequate to guarantee validity of this lower limit, (1.23a), is the requirement that it be the smallest positive root of the (nondifferential) equation

$$t = \int_0^t dr\, r^2 |V(r)|. \tag{1.23b}$$

Another characterization of t, which leads to a (generally only marginally) more stringent lower limit, is provided in Sec. III. Note that, as above, the choice of s in (1.23a) that yields the most stringent bound is the root of the nondifferential equation (1.20) (provided, of course, such a choice of s is compatible with the condition $s \geqslant t$, as it is certainly the case for strong potentials possessing many bound states). And again, as above, a neater, if generally less stringent, lower bound obtains by choosing $s=q$, since via (1.16c) one then gets, in place of (1.23a),

$$N > \frac{1}{\pi}\int_t^\infty dr\,|V(r)|^{1/2} - \frac{1}{4\pi}\log\left|\frac{V(p)}{V(q)}\right| - \frac{1}{2}, \tag{1.23c}$$

again of course with q, respectively t, defined by (1.16b) and (1.23b) (of course provided $q \geqslant t$, as it is certainly the case for strong potentials).

Let us now report a second type of (new) limits on the number N of S-wave bound states, which are particularly suitable for numerical computations, although there exist also cases amenable to analytic treatment (see Sec. II).

First we report an upper limit, valid for potentials finite at the origin, to which consideration is, for simplicity, here restricted. Let us define the radius q via (1.16c), and the sequence of *increasing* radii $r_j^{(+)}$ via the explicit recursion relation

$$r_{j+1}^{(+)} = r_j^{(+)} + (\pi/2)\left|V(r_j^{(+)})\right|^{-1/2}, \quad r_0^{(+)} = 0, \tag{1.24}$$

and let the positive integer $J^{(+)}$ be defined by the condition that the radius $r_{J^{(+)}+1}^{(+)}$ yielded by this recursion (be the first one to) exceed or equal q,

$$r_{J^{(+)}}^{(+)} < q \leqslant r_{J^{(+)}+1}^{(+)}. \tag{1.25}$$

The upper limit is then provided by the inequality

$$N \leqslant \{\{(J^{(+)}+1)/2\}\} + 1. \tag{1.26}$$

Here and always below the double braces denote the integer part: $\{\{J/2\}\} = J/2$ if J is *even* and $\{\{J/2\}\} = (J-1)/2$ if J is *odd*.

Finally we report an analogous lower limit to N, which does not require that $V(r)$ be finite at the origin to yield a nontrivial result. Again, one first defines the radius q via (1.16c), and then introduces a series of *decreasing* radii $r_j^{(-)}$ via the explicit recursion relation

$$r_{j+1}^{(-)} = r_j^{(-)} - (\pi/2)\left|V(r_j^{(-)})\right|^{-1/2}, \quad r_0^{(-)} = q. \tag{1.27}$$

Now let the positive integer $J^{(-)}$ be defined by the condition that the quantity $r_{J^{(-)}}^{(-)}$ yielded by this recursion be the last one to be *positive*,

$$r_{J^{(-)}+1}^{(-)} \leqslant 0 < r_{J^{(-)}}^{(-)}. \tag{1.28}$$

The lower limit is then provided by the inequality

$$N \geqslant \{\{J^{(-)}/2\}\}. \tag{1.29}$$

In Sec. II we provide several tests of the efficacy of our upper and lower limits; in Sec. III, we prove them; in Sec. IV we point out that all the results reported herein in the (nonrelativistic) context of the Schrödinger equation can be easily extended to the (kinematically relativistic, if only first-quantized) Klein–Gordon case.

II. TESTS

Most of the limits on the number of S-wave bound states reported in Sec. I are ''best possible,'' namely, it is generally possible to find potentials that saturate them. The shape of these saturating potentials can generally be easily inferred from the very procedure whereby the limits were derived; in particular for our new limits the saturating potentials are generally of ladder type (including the simplest such potential, the square-well), since for such potentials the second term on the right-hand side of (3.7) tends to vanish (as discussed in some detail in the last part of Sec. III). But while the fact that the formula providing a limit has the property to be ''best possible'' entails that there can be no hope to make it more stringent by just modifying some constant appearing in it [it is, for instance, impossible to obtain a more stringent upper limit than (1.4) by just replacing the constant $2/\pi$ on the right-hand side by a smaller number], it does by no means imply that such a bound provides a stringent limitation for all potentials; far from it (as we will

presently see). Indeed, a more interesting question is how different limits behave for a variety of (test) potentials. This section is devoted to such an assessment, for which we use six different potentials: the square-well potential (hereafter referred to as SW)

$$\text{SW:}\quad V(r)=-g^2R^{-2}\quad \text{for}\quad r\leqslant R, \tag{2.1a}$$

$$\text{SW:}\quad V(r)=0\quad \text{for}\quad r>R; \tag{2.1b}$$

the Pöschl–Teller[27] (or "single-soliton," see for instance Ref. 9) potential (hereafter referred to as PT),

$$\text{PT:}\quad V(r)=-g^2R^{-2}[\cosh(r/R)]^{-2}; \tag{2.2}$$

the exponential potential (hereafter referred to as E),

$$\text{E:}\quad V(r)=-g^2R^{-2}\exp(-r/R); \tag{2.3}$$

the Hulthén potential (hereafter referred to as H),

$$\text{H:}\quad V(r)=-g^2R^{-2}[\exp(r/R)-1]^{-1}; \tag{2.4}$$

the Yukawa potential (hereafter referred to as Y),

$$\text{Y:}\quad V(r)=-g^2(rR)^{-1}\exp(-r/R); \tag{2.5}$$

and the following shifted and truncated inverse square potential (hereafter referred to as STIS), which has the merit to allow analytic computation of all limits as well as of the exact number of bound states (see below):

$$\text{STIS:}\quad V(r)=-g^2(R+r)^{-2}\quad \text{for}\quad 0\leqslant r\leqslant \alpha R, \tag{2.6a}$$

$$\text{STIS:}\quad V(r)=0\quad \text{for}\quad r>\alpha R. \tag{2.6b}$$

In all these equations, and below, R is an arbitrary (of course *positive*) given radius, and g, as well as α in the last equation, (2.6), are arbitrary dimensionless *positive* constants.

We only report, for the new limits of the first type, tests of the *neatest* limits given in Sec. I, namely we consider the upper, respectively lower, limits (1.18), respectively (1.21), for regular potentials, and the upper, respectively lower, limits (1.16), respectively (1.22), (only) for singular potentials; indeed, for regular potentials, the difference between the neater upper limit (1.18) and the more stringent upper limit (1.16) is generally negligibly small (namely, less than one unit), and likewise for the difference between the neater lower limit (1.21) and the more stringent lower limits (1.19) or (1.23). (Let us however emphasize that when one considers potentials with few bound states or searches for constraints on potential parameters necessary or sufficient for the existence of one bound state, it is advisable to use the most stringent available limits.) As for the new limits of the second type, we test the upper, respectively lower, limits (1.26), respectively (1.29), for regular potentials, and the lower limit (1.29) for singular potentials. The tests are performed by comparing the new limits with the exact results, and with the previously known limits reported (and named) in Sec. I.

The simplest test is provided by the (nonsingular) SW potential (2.1), for which the exact number of bound states is given by the formula

$$N=\{\{\nu\}\}, \tag{2.7}$$

with

$$\nu = \frac{g}{\pi} + \frac{1}{2}. \tag{2.8}$$

In this case the new limits obtained in this article tend to give the exact result (as explained above), except for the approximations introduced in order to obtain neater formulas. Indeed the upper, respectively lower, limits of the first type (1.18), respectively (1.21) [with $q<R$ as implied by (1.16c), so that the logarithmic terms in both these formulas vanish], yield $N \leqslant \nu$ respectively, $N > \nu - \frac{3}{2}$, while the more stringent lower bound (1.19) with $s=R$ yields $N \geqslant \nu - 1$. The upper, respectively lower, limits of the second type, (1.26), respectively (1.29), can as well be computed analytically for this potential, yielding $N \leqslant \nu + \frac{1}{2}$, respectively $N \geqslant \nu - 1$. The BS, CC and M upper limits do not produce such good results. The BS upper limit yields $N \leqslant g^2/2$, which gives a very poor limitation when g (hence the number of bound states) grows (indeed we know that the BS upper limit is always very poor for strong potentials, see also below). The CC, respectively M, upper limits do give the correct linear behavior in g, but with too big a slope, respectively $N \leqslant 2g/\pi = 2\ (\nu - \frac{1}{2})$ and $N \leqslant 3^{-1/4} g = 3^{-1/4}\pi(\nu - \frac{1}{2}) = 2.387\,(\nu - \frac{1}{2})$. Finally, in this particular case the C and C_0 lower limits coincide and yield $N \geqslant \nu - 1$, namely a slightly more stringent limit than (1.21) [indeed, just the same result as (1.19), see above].

The second test is performed with the (nonsingular) PT potential (2.2). For this potential the exact number of bound states is again given by (2.7) but now with

$$\nu = (\sqrt{1+4g^2}+1)/4, \tag{2.9a}$$

which, in the limit of large g, yields

$$\nu = \frac{1}{2}g + \frac{1}{4} + \frac{1}{16g} + O(g^{-3}). \tag{2.9b}$$

In this case the new upper and lower limits of the first type, (1.18), respectively (1.21), can as well be computed analytically, and they read

$$N \leqslant \frac{g}{2} - \frac{1}{2\pi}\log\left[\sin\left(\frac{\pi}{2g}\right)\right] + \frac{1}{2}, \tag{2.10a}$$

respectively

$$N > \frac{g}{2} + \frac{1}{2\pi}\log\left[\sin\left(\frac{\pi}{2g}\right)\right] - 1, \tag{2.11a}$$

entailing, in the limit of large g,

$$N \leqslant \frac{g}{2} + \frac{1}{2\pi}\log\left(\frac{2g}{\pi}\right) + \frac{1}{2} + \frac{1}{12\pi}\left(\frac{\pi}{2g}\right)^2 + O(g^{-4}), \tag{2.10b}$$

respectively

$$N > \frac{g}{2} - \frac{1}{2\pi}\log\left(\frac{2g}{\pi}\right) - 1 - \frac{1}{12\pi}\left(\frac{\pi}{2g}\right)^2 + O(g^{-4}). \tag{2.11b}$$

As for the new limits of the second type, (1.26) and (1.29), in this case they can only be evaluated numerically. In Fig. 1 we present, for this potential, a comparison between the exact number of bound states, the new limits of the first and of the second type, and the previously known C, C_0 lower limits, and BS, CC, M upper limits, all of which can be computed analytically: BS: $N \leqslant \log(2)g^2$ (very bad at large g); CC: $N \leqslant g$; M: $N \leqslant (\pi^2/12)^{1/4} g \approx 0.95g$ (both of which give roughly twice the correct result at large g); C: $N \geqslant (2/\pi)\exp(-x)g - \frac{1}{2} \approx 0{,}336g - \frac{1}{2}$ [where x is the

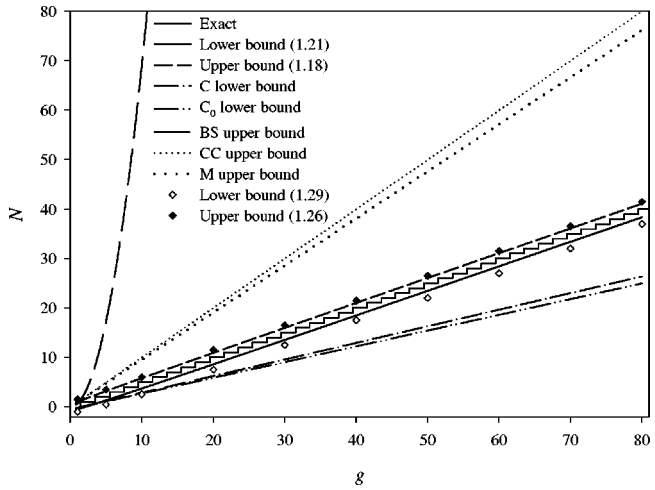

FIG. 1. Comparison between the exact number of bound states for the PT potential (2.2) (ladder curve), the limits of the first type (1.18) (short-dash curve) and (1.21) (solid curve), the C (dash-dot curve) and C_0 (dash-double-dot curve) lower limits, the BS (long-dash curve), the CC (small-dot curve) and M(sparse-dot curve) upper limits, and the limits of the second type (1.26) (black diamond) and (1.29) (white diamond).

root of $2x=1+\exp(-2x)$]; C_0: $N\geqslant g/\pi-\frac{1}{2}\approx 0{,}318g-\frac{1}{2}$ [the C and the C_0 lower bounds are less stringent than the lower bound (2.11) as soon as g exceeds 3.98 and 3.48, respectively]. As it is clear from Fig. 1, the new bounds are quite cogent. From (2.10b) and (2.11b) one sees that those of the first type remain quite stringent as well for rather large values of g: for instance, when the exact number N of bound states is equal to 5000, these upper and lower limits restrict it to the rather small interval [4998,5001]. Likewise, at this value of g, the new limits of the second type, (1.26), respectively (1.29), entail the restrictions $4996\leqslant N\leqslant 5002$; while the corresponding value of the BS upper limit exceeds 6.9×10^7, the CC upper limit only informs us that $N\leqslant 10^4$, and the lower limit C that $N\geqslant 3360$.

The third test is performed with the (regular) E potential (2.3). In this case the exact number of bound states coincides with the number of zeros of the zeroth-order Bessel function $J_0(x)$ in the interval $0<x\leqslant 2g$ (see, for example, Ref. 18, p. 196). Also in this case the new upper and lower limits of the first type (1.18) and (1.21) can be computed analytically:

$$N\leqslant \frac{2}{\pi}g+\frac{1}{2\pi}\log\left(\frac{4}{\pi}g\right)+\frac{1}{2}, \tag{2.12}$$

$$N>\frac{2}{\pi}g-\frac{1}{2\pi}\log\left(\frac{4}{\pi}g\right)-1, \tag{2.13}$$

while those of the second type must be evaluated numerically. In this case all the previously known limits can as well be computed analytically: BS: $N\leqslant g^2$; CC: $N\leqslant 4/\pi g$; M: $N\leqslant 2^{1/4}g$; C: $N\geqslant 2/(\pi\sqrt{e})g-\frac{1}{2}$; C_0: $N\geqslant g/\pi-\frac{1}{2}$. A comparison between these results is presented in Fig. 2. It is again clear that the new limits are remarkably effective.

The fourth test is performed with the (singular) H potential (2.4). In this case the exact number of bound states is given simply by the integer part of g:

$$N=\{\{g\}\}. \tag{2.14}$$

The new upper, respectively lower, limits of the first type applicable to singular potentials, (1.16), respectively (1.22), can in this case be computed analytically as well:

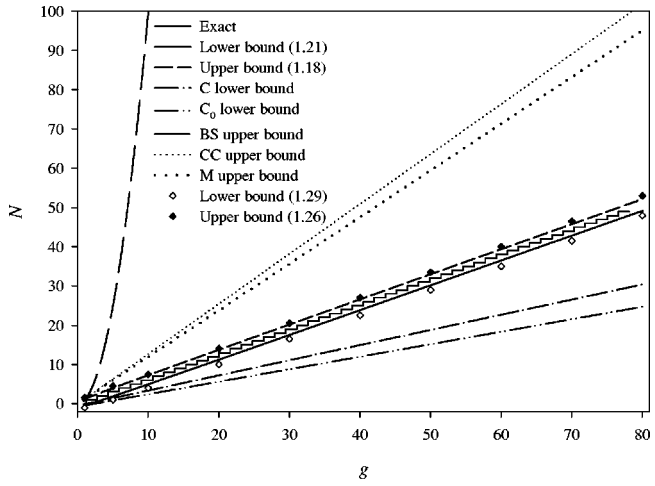

FIG. 2. Comparison between the exact number of bound states for the E potential (2.3) (ladder curve), the limits of the first type (1.18) (short-dash curve) and (1.21) (solid curve), the C (dash-dot curve) and C_0 (dash-double-dot curve) lower limits, the BS (long-dash curve), the CC (small-dot curve) and M (sparse-dot curve) upper limits, and the limits of the second type (1.26) (black diamond) and (1.29) (white diamond).

$$N \leqslant g - \frac{1}{\pi}\log\left(\tan\frac{\pi}{4g}\right) + \frac{1}{2}, \tag{2.15a}$$

$$N > g + \frac{1}{\pi}\log\left(\tan\frac{\pi}{4g}\right) - \frac{3}{2}, \tag{2.16a}$$

yielding asymptotically, for large g,

$$N \leqslant g - \frac{1}{\pi}\log\left(\frac{\pi}{4g}\right) + \frac{1}{2} - \frac{\pi}{48g^2} + O(g^{-4}), \tag{2.15b}$$

$$N > g + \frac{1}{\pi}\log\left(\frac{\pi}{4g}\right) - \frac{3}{2} + \frac{\pi}{48g^2} + O(g^{-4}). \tag{2.16b}$$

The new lower limit of the second type (1.29) must in this case be evaluated numerically, while all the previously known limits (relevant to the case of singular potentials) can be computed analytically: BS: $N \leqslant (\pi^2/6)g^2$; CC: $N \leqslant 2g$; C: $N \geqslant (2/\pi)\log(2)g - \frac{1}{2}$. A comparison between these results is presented in Fig. 3. It is again clear that the new limits are remarkably effective. And it is again clear from a comparison of the asymptotic formulas (2.15b) and (2.16b) that the new upper and lower limits of the first type remain remarkably cogent even at large values of g: for instance, when the exact number of bound states is equal to $N = 5000$, these limits, (2.15a) and (2.16a), restrict N to the relatively small interval $[4996,\ 5003]$. For comparison, the corresponding value of the BS upper limit exceeds 4×10^7, the CC upper limit is 10^4, and the lower limit C only informs us that $N \geqslant 2207$, while the new lower limit of the second type, (1.29), informs us that $N \geqslant 4994$.

The fifth test is performed with the (singular) Y potential (2.5). In this case the exact number of bound states must be evaluated numerically: we employed two different methods of calculation, in order to check the numerical results[3,4] (note that these two methods possess a natural link[31]). The new upper and lower limits, (1.16) and (1.22), respectively, can instead be computed analytically:

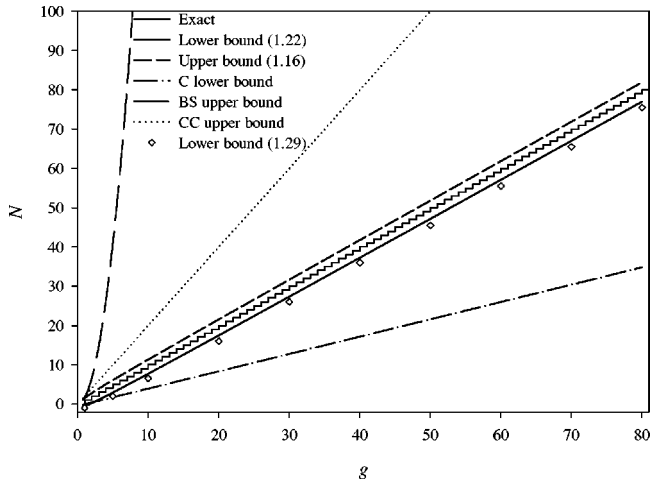

FIG. 3. Comparison between the exact number of bound states for the H potential (2.4) (ladder curve), the limits of the first type (1.16) (short-dash curve) and (1.22) (solid curve), the C lower limit (dash-dot-curve), the BS (long-dash curve) and CC (dot curve) upper limits, and the lower limit of the second type (1.29) (white diamond).

$$N \leqslant \sqrt{\frac{2}{\pi}}g + \frac{x^2-y^2}{2\pi} + \frac{1}{2\pi}\log\left(\frac{x}{y}\right) + \frac{1}{2}, \tag{2.17a}$$

$$N > \sqrt{\frac{2}{\pi}}g - \frac{x^2-y^2}{2\pi} - \frac{1}{2\pi}\log\left(\frac{x}{y}\right) - \frac{3}{2}, \tag{2.18a}$$

with

$$\mathrm{erf}(y)=\alpha, \quad \mathrm{erf}(x)=1-\alpha, \quad \alpha=(\pi/8)^{1/2}g^{-1}, \tag{2.19}$$

so that asymptotically (as $g\to\infty$, and keeping only the first correction term)

$$N \leqslant \sqrt{\frac{2}{\pi}}g + \frac{1}{\pi}\log(g), \tag{2.17b}$$

$$N > \sqrt{\frac{2}{\pi}}g - \frac{1}{\pi}\log(g). \tag{2.18b}$$

The new lower bound of the second type must also be evaluated numerically, while the previously known limits relevant to the singular case can all be evaluated (almost completely) analytically: BS: $N\leqslant g^2$; CC: $N\leqslant 2(2/\pi)^{1/2}g$; C: $N\geqslant(2/\pi)x^{1/2}\exp(-x/2)g-\frac{1}{2}=0.531(2/\pi)g-\frac{1}{2}$ [where x is the root of $\exp(-x)=\int_x^\infty dy\, y^{-1}\exp(-y)$]. A comparison between these results is presented in Fig. 4. It is again clear that the new limits are remarkably effective. And it is again clear from a comparison of the asymptotic formulas (2.17b) and (2.18b) that the new upper and lower limits of the first type remain remarkably cogent even at large values of g: for instance, when the exact number of bound states is equal to $N=50$, these limits, (2.17a) and (2.18a), restrict N to the relatively small interval [49,53]. For comparison, the corresponding value of the BS upper limit exceeds 4000, while the CC upper limit and the C lower limit only informs us that $22\leqslant N \leqslant 103$; as for the new lower limit, (1.29), it entails that $N\geqslant 48$.

Finally, the sixth test is performed with the (regular) STIS potential (2.6). As already mentioned, this test potential is particularly appealing because in this case *all* the relevant calculations can be performed analytically; moreover, in contrast to the five previous cases, this potential features two dimensionless parameters rather than only one.

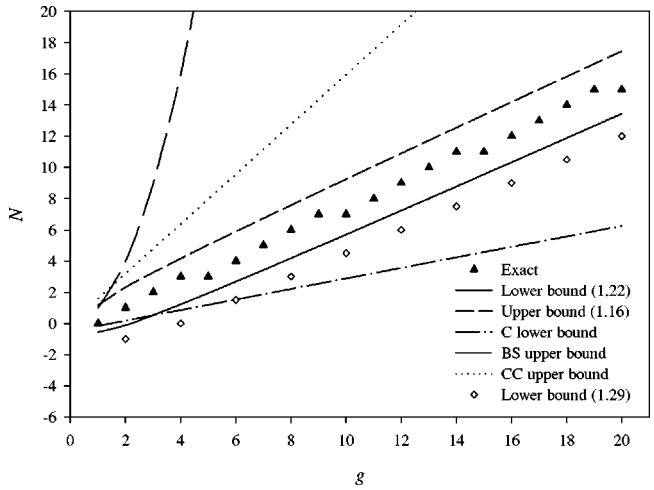

FIG. 4. Comparison between the exact number of bound states for the Y potential (2.5) (black triangle), the limits of the first type (1.16) (short-dash curve) and (1.22) (solid curve), the C lower limit (dash-dot curve), the BS (long-dash curve) and CC (dot curve) upper limits, and the lower limit of the second type (1.29) (white dimaond).

This potential possesses bound states only if the ''coupling constant'' g exceeds $\frac{1}{2}$, $g>\frac{1}{2}$ (irrespective of the value of the other, *positive*, parameter it features, $\alpha>0$), and the exact number N of its bound states is then given again by (2.7), but now with

$$\nu=\frac{1}{2\pi}(\lambda\,\log(1+\alpha)+2\,\arctan(\lambda)) \tag{2.20a}$$

with $\lambda=\sqrt{4g^2-1}$, entailing at large g

$$\nu=\frac{1}{\pi}\left(g-\frac{1}{8g}\right)\log(1+\alpha)-\frac{1}{2\pi g}+\frac{1}{2}+O(g^{-3}), \tag{2.20b}$$

and at large α

$$\nu=\frac{\lambda}{2\pi}\left[\log(\alpha)+\frac{1}{\alpha}\right]+\frac{1}{\pi}\arctan(\lambda)+O(\alpha^{-2}). \tag{2.20c}$$

The new upper and lower limits of the first type, (1.18) and (1.21), respectively, yield

$$\{\{\nu_{\rm lo}\}\}\leqslant N\leqslant\{\{\nu_{\rm up}\}\} \tag{2.21a}$$

with

$$\nu_{\rm up}=\frac{1}{\pi}\left(g+\frac{1}{2}\right)\log(1+\alpha)-\frac{1}{4g}+\frac{1}{2}, \tag{2.21b}$$

respectively

$$\nu_{\rm lo}=\frac{1}{\pi}\left(g-\frac{1}{2}\right)\log(1+\alpha)+\frac{1}{4g}, \tag{2.21c}$$

entailing at large g

$$\frac{\nu_{\rm up}-\nu_{\rm lo}}{\nu}=\frac{1}{g}\left[1+\frac{\pi}{2\log(1+\alpha)}\right]-\frac{1}{g^2}\left[\frac{\pi}{\log(1+\alpha)}+\frac{\pi^2}{4\log^2(1+\alpha)}\right]+O(g^{-3}), \quad (2.21d)$$

and at large α

$$\frac{\nu_{\rm up}-\nu_{\rm lo}}{\nu}=\frac{2}{\lambda}\left\{1+\frac{\pi}{2\log(\alpha)}\left[1-\frac{1}{g}-\frac{4}{\pi\lambda}\arctan(\lambda)\right]\right\}+O([\log(\alpha)]^{-2}). \quad (2.21e)$$

The new upper and lower limits of the second type, (1.26) and (1.29), respectively, yield

$$\{\{\nu_-\}\}\leqslant N\leqslant\{\{\nu_+\}\} \quad (2.22a)$$

with

$$\nu_\pm=\frac{1}{2}\left\{\left\{\frac{2}{\pi}g_\pm\log(1+\alpha)-\frac{g_\pm}{g}\right\}\right\}+\frac{3\pm 3}{4} \quad (2.22b)$$

where

$$g_\pm=\frac{\pm(\pi/2)}{\log[1\pm\pi/(2g)]}, \quad (2.22c)$$

so that, at large g,

$$g_\pm=g\pm\frac{\pi}{4}+O(g^{-1}) \quad (2.22d)$$

entailing

$$\nu_\pm=\frac{1}{2}\left\{\left\{\left(\frac{2}{\pi}g\pm\frac{1}{2}\right)\log(1+\alpha)\right\}\right\}+\frac{1\pm 3}{4}+O(g^{-1}), \quad (2.22e)$$

hence

$$\frac{\nu_+-\nu_-}{\nu}=O(g^{-1}). \quad (2.22f)$$

Note that the formulas for the lower limit are only applicable if $g>\pi/2$ [see (2.22c)].

The previously known upper and lower limits can also be evaluated in closed form for this potential:

$$\text{BS:}\quad N\leqslant g^2\left[\log(1+\alpha)-\frac{\alpha}{1+\alpha}\right], \quad (2.23)$$

$$\text{CC:}\quad N\leqslant\frac{2}{\pi}g\log(1+\alpha), \quad (2.24)$$

$$\text{M:}\quad N\leqslant g\left[\left(\alpha-2\log(1+\alpha)+\frac{\alpha}{1+\alpha}\right)\frac{\alpha}{1+\alpha}\right]^{1/4}, \quad (2.25)$$

$$\text{C:}\quad N\geqslant\frac{2}{\pi}g\left(1-\frac{1}{\sqrt{1+\alpha}}\right)-\frac{1}{2}, \quad (2.26)$$

TABLE I. Comparison between the exact number of bound states N, the bounds of the first type (1.18) and (1.21), see (2.21), the limits of the second type (1.26) and (1.29), see (2.22), the BS, CC and M upper limits, and the C and C_0 lower limits, for the STIS potential (2.6) with a representative set of values of α and g.

(α,g)	N	$\{\{\nu_{lo}\}\}$	$\{\{\nu_{up}\}\}$	$\{\{\nu_-\}\}$	$\{\{\nu_+\}\}$	BS	CC	M	C	C_0
(1,10)	2	2	2	2	4	19	4	4	2	2
$(1,10^2)$	22	21	22	22	24	1931	44	48	19	16
$(1,10^3)$	221	220	221	220	222	$>10^5$	441	488	186	159
$(10^2,10)$	15	13	15	13	17	362	29	30	6	3
$(10^2,10^2)$	147	146	148	146	150	36250	293	308	57	32
$(10^4,10)$	29	27	31	27	33	821	58	99	6	3
$(10^4,10^2)$	293	291	295	291	297	82105	586	999	63	32
$(10^6,10)$	44	41	46	40	49	1281	87	316	6	3
$(10^6,10^2)$	440	437	442	436	445	$>10^5$	879	3162	64	32

$$C_0: \quad N \geqslant \frac{1}{\pi} g \frac{\alpha}{1+\alpha} - \frac{1}{2}. \tag{2.27}$$

The merits of the new limits are already apparent from these formulas. Representative examples are given in Table I.

In conclusion it seems justified to conclude from these tests that the new limits presented in this article are rather cogent and generally superior to those hitherto known. They are particularly effective for strong potentials possessing many bound states, thanks to their capability to generally reproduce the correct asymptotic (semiclassical) result (1.6) when the coupling constant diverges. Let us also emphasize that, from a computational point of view, the limits of the second type presented herein are particularly convenient, especially in the case of regular potentials.

III. PROOFS

In this section we prove the new results reported in Sec. I. We assume throughout that the potential satisfies the conditions (1.1) as well as (1.3).

Let $u(r)$ be the zero-energy S-wave Schrödinger wave function, characterized by the second-order ordinary differential equation

$$u''(r) - V(r)u(r) = 0, \tag{3.1a}$$

with boundary condition

$$u(0) = 0. \tag{3.1b}$$

It is well known (see, for instance, Ref. 8) that the number of zeros of the solution of (3.1a) with (3.1b) in the interval $0 < r < \infty$ coincides with the number N of S-wave bound states supported by the potential $V(r)$ (we always exclude, for simplicity, the marginal case of a potential that features a "zero-energy bound state or resonance"). Let us indicate with z_n the successive zeros of $u(r)$, and with b_n the successive zeros of $u'(r)$ [namely, the locations of the successive extrema of the wave function $u(r)$],

$$u(z_n) = 0, \; u'(b_n) = 0. \tag{3.2}$$

It is then clear that, since the potential $V(r)$ is nowhere *positive* [as implied by (1.1) with (1.3)],

$$V(r) = -|V(r)|, \tag{3.3}$$

the zero-energy wave function $u(r)$ is an everywhere convex function of r, entailing the "interlacing" relations

$$0=z_0<b_1<z_1<b_2<\cdots<z_{N-1}<b_N<z_N<\infty. \tag{3.4}$$

Note that these formulas imply that $u'(r)$ does *not* vanish in the interval $z_N\leqslant r<\infty$, namely a $b_{N+1}<\infty$ does not exist [otherwise it would be inevitably followed by $z_{N+1}<\infty$, and this is excluded since N is the number of zeros of $u(r)$].

Following Refs. 7 and 8 we now introduce a function $\eta(r)$ defined via the relation

$$\tan[\eta(r)]=|V(r)|^{1/2}u(r)/u'(r), \tag{3.5a}$$

with

$$\eta(0)=0, \tag{3.5b}$$

and the requirement that $\eta(r)$ be a continuous function of r [to lift the mod(π) ambiguity entailed by the definition (3.5a)]. It is then clear that the properties (3.4) together with the definition (3.5a) imply the relations

$$\eta(z_n)=n\pi, \quad \eta(b_{n+1})=(2n+1)\pi/2, \ n=0,1,\ldots,N-1, \tag{3.6a}$$

$$\eta(z_N)=\eta(\infty)=N\pi, \tag{3.6b}$$

and that the value of $\eta(r)$ inside the intervals (3.4) lies between the values taken at the extremal points of these intervals, namely, for $z_n\leqslant r\leqslant b_{n+1}$ with $n=0,\ldots,N-1$, $n\pi\leqslant\eta(r)\leqslant(2n+1)\pi/2$, and for $b_n\leqslant r\leqslant z_n$ with $n=1,\ldots,N$, $(2n-1)\pi/2\leqslant\eta(r)\leqslant n\pi$, except of course for the last interval, $z_N\leqslant r<\infty$, where $N\pi\leqslant\eta(r)<(2N+1)\pi/2$. Note that these results also imply that, for *all* values of r,

$$0\leqslant\eta(r)<(N+\tfrac{1}{2})\pi \tag{3.6c}$$

(indeed the value at which the second inequality was violated would qualify as b_{N+1}, which, as already noted, would then inevitably be followed by z_{N+1}, violating the hypothesis that the number of zeros be N).

Moreover, from (3.1a) we obtain via (3.5a) and (3.3) the nonlinear first-order differential equation

$$\eta'(r)=|V(r)|^{1/2}-\frac{V'(r)}{4|V(r)|}\sin[2\eta(r)], \tag{3.7}$$

which, together with the ''initial condition'' (3.5b), determines the function $\eta(r)$ and, therefore, via (3.6b), the number N of S-wave bound states. This equation will be our main tool to derive (upper and lower) limits on N.

It is indeed clear from (3.7) and (1.3) that

$$\eta'(r)\leqslant|V(r)|^{1/2}+\frac{V'(r)}{4|V(r)|}, \tag{3.8}$$

$$\eta'(r)\geqslant|V(r)|^{1/2}-\frac{V'(r)}{4|V(r)|}. \tag{3.9}$$

These inequalities (3.8), respectively (3.9), together with (3.5b) and (3.6), will be our main tool to derive upper, respectively lower, limits on N. (Note that more stringent conditions might be written by considering separately all the intervals of type $z_n\leqslant r\leqslant b_{n+1}$ where $\sin[2\eta(r)]$ is clearly *non-negative*, see (3.4) and (3.6a), respectively, and all the intervals of type $b_n\leqslant r\leqslant z_n$ where $\sin[2\eta(r)]$ is clearly *nonpositive*, see (3.4) and (3.6a); but it does not appear that such a distinction

might be maintained to the end without having to renounce the goal to obtain reasonably neat final formulas for the limits; we will, however, take advantage of this improvement for certain intervals, see below.)

Let us now focus first on the derivation of the upper limit (1.16). To this end we integrate (3.8) from b_1 to z_{N-1}, and via (3.6a) and (3.3) we get

$$\left(N-\frac{3}{2}\right)\pi \leqslant \int_{b_1}^{z_{N-1}} \mathrm{d}r\,|V(r)|^{1/2}+\frac{1}{4}\log\left|\frac{V(b_1)}{V(z_{N-1})}\right|. \tag{3.10}$$

On the other hand we know, as already noted above, that in the intervals $0\leqslant r\leqslant b_1$ and $z_{N-1}\leqslant r\leqslant b_N$ (where $\sin[2\eta(r)]$ is *non-negative*, see (3.4) and (3.6a)] (3.8) can be replaced by the more stringent inequality [see (3.7)]

$$\eta'(r)\leqslant |V(r)|^{1/2}, \tag{3.11a}$$

and the integration of this inequality over these intervals yields [via (3.6a)]

$$\frac{\pi}{2}\leqslant \int_0^{b_1} \mathrm{d}r\,|V(r)|^{1/2}, \tag{3.11b}$$

$$\frac{\pi}{2}\leqslant \int_{z_{N-1}}^{b_N} \mathrm{d}r\,|V(r)|^{1/2}. \tag{3.11c}$$

Hence by summing (3.10), (311b) and (3.11c) (and dividing by π) we get

$$N-\frac{1}{2}\leqslant \frac{1}{\pi}\int_0^{b_N} \mathrm{d}r\,|V(r)|^{1/2}+\frac{1}{4\pi}\log\left|\frac{V(b_1)}{V(z_{N-1})}\right|, \tag{3.12}$$

and therefore *a fortiori* [thanks to the monotonicity of $V(r)$, see (1.3)]

$$N\leqslant \frac{1}{\pi}\int_0^{\infty} \mathrm{d}r\,|V(r)|^{1/2}+\frac{1}{4\pi}\log\left|\frac{V(p)}{V(q)}\right|+\frac{1}{2}, \tag{3.13a}$$

provided

$$p\leqslant b_1, \tag{3.13b}$$

$$q\geqslant z_{N-1}. \tag{3.13c}$$

To complete the proof of the first upper limit reported in Sec. I, see (1.16), we must show that the radii p, respectively q, defined by (1.16b), respectively (1.16c), satisfy (3.13b), respectively (3.13c). For p this is immediately implied by a comparison of (1.16b) and (3.11b); and, likewise, indeed *a fortiori*, this is as well implied for q by a comparison of (1.16c) and (3.11c).

Let us now proceed and prove the first lower limit of Sec. I. We treat firstly the case in which the potential is finite at the origin, see (1.19). To this end we integrate (3.9) from 0 to an arbitrary (of course *positive*) radius s getting thereby the inequality

$$\eta(s)\geqslant \int_0^{s} \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(0)}{V(s)}\right|, \tag{3.14}$$

namely *a fortiori*, via (3.6c),

$$\left(N+\frac{1}{2}\right)\pi > \int_0^{s} \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(0)}{V(s)}\right|, \tag{3.15}$$

which clearly immediately implies (1.19).

If the potential diverges at the origin, to get the lower bound (1.22) we integrate (3.9) from p to q and we then get via (1.16b) and (1.16c)

$$\eta(q)-\eta(p)\geqslant\int_p^q \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(p)}{V(q)}\right|=\int_0^\infty \mathrm{d}r\,|V(r)|^{1/2}-\pi-\frac{1}{4}\log\left|\frac{V(p)}{V(q)}\right|, \tag{3.16}$$

and via (3.6c) this clearly yields (1.22).

A generally more stringent but less explicit bound obtains by integrating (3.9) from b_1 to s getting thereby [see (3.6a)]

$$\eta(s)-\frac{\pi}{2}\geqslant\int_{b_1}^s \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(b_1)}{V(s)}\right|, \tag{3.17a}$$

hence *a fortiori*, via (3.6c),

$$N\pi>\int_{b_1}^s \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(b_1)}{V(s)}\right|, \tag{3.17b}$$

hence *a fortiori* [see (3.13b) and (1.3)]

$$N\pi>\int_{b_1}^s \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(p)}{V(s)}\right|, \tag{3.18}$$

hence finally

$$N\pi>\int_t^s \mathrm{d}r\,|V(r)|^{1/2}-\frac{1}{4}\log\left|\frac{V(p)}{V(s)}\right|, \tag{3.19a}$$

provided there holds the inequality

$$t\geqslant b_1. \tag{3.19b}$$

This condition is clearly equivalent to the requirement that the potential $V(r)$ amputated of its part extending beyond t possess at least one bound state. [Since when $V(r)$ vanishes, $u(r)$ is linear, $u(r)=\alpha r+\beta$, see (3.1a), hence the condition (3.19b) with $V(r)$ vanishing beyond t guarantees the existence of $z_1<\infty$.] It is therefore sufficient, to make sure that (3.19b) holds, that this amputated potential, $V(r)\,\theta(t-r)$ [where $\theta(x)$ is the step function, $\theta(x)=1$ if $x\geqslant 0$, $\theta(x)=0$ if $x<0$] satisfy one of the *sufficient* conditions for the existence of at least one bound state reported in Sec. I, see (1.11)–(1.13). Here for simplicity we restrict attention to the *sufficient* condition (1.12), and we thereby conclude that a formula adequate to guarantee that the inequality (3.19b) be satisfied is validity, for some *positive* value of a of either one of the following two inequalities, see (1.12) [below we write $\geqslant$ in place of $>$, since t might coincide with b_1, see (3.19b), which would correspond to an amputated potential possessing only a zero-energy bound state or resonance]:

$$a^{-1}\int_0^a \mathrm{d}r\,r^2|V(r)|+a\int_a^t \mathrm{d}r|V(r)|\geqslant 1 \quad \text{with} \quad a\leqslant t, \tag{3.20a}$$

$$a^{-1}\int_0^a \mathrm{d}r\,r^2|V(r)|\geqslant 1 \quad \text{with} \quad a\geqslant t. \tag{3.20b}$$

And clearly the choice $a=t$ leads to (1.23b), thereby completing the proof of the first lower limit to N for potentials singular at the origin as reported in Sec. I, see (1.23).

Let us now proceed and prove the second type of limits to N. For simplicity, in the case of the upper bound we restrict attention to the case of potentials which are finite at the origin, and of course we always assume the potential to satisfy the monotonicity condition (1.3).

First of all we introduce the potential amputated of its part beyond q

$$\overline{V}(r)=V(r) \quad \text{for} \quad 0\leqslant r<q, \tag{3.21a}$$

$$\overline{V}(r)=0 \quad \text{for} \quad r\geqslant q. \tag{3.21b}$$

Here q is defined by (1.16c), hence it satisfies the condition (3.13c); therefore, if we indicate with $\overline{N}$ the number of bound states possessed by the potential $\overline{V}(r)$, either $\overline{N}=N-1$ [if $z_{N-1}\leqslant q<b_N$; indeed the zero-energy wave function $\overline{u}(r)$ corresponding to the potential $\overline{V}(r)$ is linear for $r>q$, see (3.21b), hence it has one less zero than the zero-energy wave function $u(r)$ corresponding to the potential $V(r)$ if the cutoff point q comes before the point, b_N, at which $u(r)$ bends over for the last time, namely where it has its last extremum] or $\overline{N}=N$ [if $q\geqslant b_N$; we include in the count of the number $\overline{N}$ of bound states of $\overline{V}(r)$ also a zero-energy one, should it happen that there be one, namely that $q=b_N$]. So, in any case,

$$\overline{N}\leqslant N\leqslant\overline{N}+1. \tag{3.22}$$

Our strategy is now to introduce two monotonically increasing ladder-type potentials, $V^{(+)}(r)$, respectively $V^{(-)}(r)$, both vanishing beyond q just as $\overline{V}(r)$ does [see (3.21b)], which minorize, respectively majorize, $\overline{V}(r)$,

$$V^{(+)}(r)\leqslant\overline{V}(r)\leqslant V^{(-)}(r), \tag{3.23}$$

so that the number of bound states, $N^{(+)}$, respectively $N^{(-)}$, possessed by them majorize, respectively minorize, $\overline{N}$, yielding, via (3.22),

$$N^{(-)}\leqslant N\leqslant N^{(+)}+1. \tag{3.24}$$

And these potentials, $V^{(+)}(r)$, respectively $V^{(-)}(r)$, shall now be manufactured so that one can easily compute the numbers of bound states they possess.

Indeed the potential $V^{(+)}(r)$ is now defined by the rule

$$V^{(+)}(r)=V(r_j^{(+)}) \quad \text{for} \quad r_j^{(+)}\leqslant r<r_{j+1}^{(+)}, \quad j=0,1,\ldots,J^{(+)}-1, \tag{3.25a}$$

$$V^{(+)}(r)=V(r_{J^{(+)}}^{(+)}) \quad \text{for} \quad r_{J^{(+)}}^{(+)}\leqslant r<q, \tag{3.25b}$$

$$V^{(+)}(r)=0 \quad \text{for} \quad r\geqslant q, \tag{3.25c}$$

with the increasing radii $r_j^{(+)}$ defined by the recurrence relation (1.24), and the *positive* integer $J^{(+)}$ defined by the condition that the radius $r_{J^{(+)}+1}^{(+)}$ yielded by this recursion (be the first one to) exceed or equal q, see (1.25). It is plain that this potential minorizes, see (3.23), the truncated potential $\overline{V}(r)$ for all values of r (if in doubt, draw a graph), and it is moreover easy to compute the number $N^{(+)}$ of bound states it possesses, since for this potential

$$\eta^{(+)}(r_j^{(+)})=j\ \pi/2, \quad j=0,1,\ldots,J^{(+)}+1. \tag{3.26}$$

This result is implied by the differential equation satisfied by $\eta^{(+)}(r)$, which reads simply

$$\eta'^{(+)}(r)=|V^{(+)}(r)|^{1/2}, \tag{3.27a}$$

namely [see (3.25a)]

$$\eta'^{(+)}(r)=|V^{(+)}(r_j^{(+)})|^{1/2} \quad \text{for} \quad r_j^{(+)}\leqslant r<r_{j+1}^{(+)}, \quad j=0,1,\ldots,J^{(+)}, \tag{3.27b}$$

since the second term on the right-hand side of (3.7) vanishes for $r_j^{(+)}<r<r_{j+1}^{(+)}$ because $V^{(+)}(r)=V^{(+)}(r_j^{(+)})$ is constant there hence its derivative vanishes, and at $r=r_j^{(+)}$ because $\sin[2\eta^{(+)}(r_j^{(+)})]$ vanishes due to (3.26) and therefore kills the contribution that would otherwise come from the delta function produced by the derivative of the discontinuity of the potential occurring there. And the consistency of (3.26) with (3.27) is of course guaranteed by (3.25b) and (1.24).

We now note that, for this potential $V^{(+)}(r)$, (3.26) implies

$$r_j^{(+)}=z_{j/2}^{(+)} \quad \text{if} \quad j \quad \text{is} \quad even, \quad j=0,2,\ldots,J^{(+)}-1 \quad \text{or} \quad J^{(+)}, \tag{3.28a}$$

$$r_j^{(+)}=b_{(j+1)/2}^{(+)} \quad \text{if} \quad j \quad \text{is} \quad odd, \quad j=1,3,\ldots,J^{(+)}-1 \quad \text{or} \quad J^{(+)}, \tag{3.28b}$$

where the radii $z_j^{(+)}$, respectively $b_j^{(+)}$, are of course the successive zeros, respectively the extrema, of the zero-energy wave function $u^{(+)}(r)$ corresponding to the potential $V^{(+)}(r)$ [see (3.4)]. Moreover, for a potential amputated of its part beyond q [as is the case of $V^{(+)}(r)$], the number $N^{(+)}$ of bound states is characterized by the condition $b_{N^{(+)}}^{(+)}\leqslant q$ [since the zero-energy wave function is a straight line for $r>q$, see (3.1a) and (3.25c)]. Hence after considering the two possible parities, even or odd, of $J^{(+)}$, we conclude that, in both cases,

$$N^{(+)}=\{\{(J^{(+)}+1)/2\}\}, \tag{3.29}$$

and via (3.24) this completes our proof of the upper limit (1.26).

To prove the lower limit (1.29) we introduce the following ladder-type potential:

$$V^{(-)}(r)=V(r_{J^{(-)}}^{(-)}) \quad \text{for} \quad 0\leqslant r\leqslant r_{J^{(-)}}^{(-)}, \tag{3.30a}$$

$$V^{(-)}(r)=V(r_{j-1}^{(-)}) \quad \text{for} \quad r_j^{(-)}<r\leqslant r_{j-1}^{(-)}, \quad j=J^{(-)},J^{(-)}-1,\ldots,2,1, \tag{3.30b}$$

$$V^{(-)}(r)=0 \quad \text{for} \quad q=r_0^{(-)}<r<\infty, \tag{3.30c}$$

with the sequence of *decreasing* radii $r_j^{(-)}$ defined by the recursion relation (1.27). It is plain that this potential majorizes, see (3.23), the truncated potential $\overline{V}(r)$ for all values of r (if in doubt, draw a graph); hence if $N^{(-)}$ is the number of S-wave bound states possessed by this potential, the (first part of the) inequality (3.24) holds. As we know, since the potential $V^{(-)}(r)$ vanishes identically beyond q (and $b_{N^{(-)}}^{(-)}\leqslant q$), see (3.30c), this number $N^{(-)}$ is given by

$$N^{(-)}=\{\{\eta^{(-)}(q)/\pi\}\}. \tag{3.31}$$

Here $\eta^{(-)}(r)$ is of course the solution of the differential equation (3.7) for the potential $V^{(-)}(r)$, namely

$$\eta'^{(-)}(r)=|V^{(-)}(r)|^{1/2}-\frac{V'^{(-)}(r)}{4|V^{(-)}(r)|}\sin[2\eta^{(-)}(r)], \tag{3.32}$$

with the initial condition

$$\eta^{(-)}(0)=0. \tag{3.33}$$

Since the ladder-type potential $V^{(-)}(r)$ presents some discontinuities, see (3.30), the integration of (3.32) from the initial condition (3.33) onward shall encounter some delta functions, but these integrable singularities of the right-hand side of (3.32) do not destroy the properties of existence, uniqueness and continuity of the solution $\eta^{(-)}(r)$ of (3.32) with (3.33).

Let now $\tilde{\eta}(r)$ be another solution of the same differential equation (3.32), characterized by the initial condition

$$\tilde{\eta}(0) = -r_{J(-)}^{(-)} |V(r_{J(-)}^{(-)})|^{1/2}. \tag{3.34}$$

Since clearly [see (3.33) and (1.28)]

$$\eta^{(-)}(0) > \tilde{\eta}(0) \tag{3.35a}$$

and the two functions $\eta^{(-)}(r)$ and $\tilde{\eta}(r)$ satisfy the same differential equation, there follows that, for every finite value of r an analogous inequality holds [indeed, the graph of the continuous function $\tilde{\eta}(r)$ as function of r can never overtake the graph of the continuous function $\eta^{(-)}(r)$ as function of r, since at the point of crossing their slopes must coincide because $\tilde{\eta}(r)$ satisfies the same differential equation as $\eta^{(-)}(r)$, see (3.32), hence no crossing can occur]:

$$\eta^{(-)}(r) > \tilde{\eta}(r). \tag{3.35b}$$

Hence as well

$$\eta^{(-)}(q) > \tilde{\eta}(q), \tag{3.35c}$$

entailing *a fortiori*, via (3.31),

$$N^{(-)} \geqslant \{\{\tilde{\eta}(q)/\pi\}\}. \tag{3.36}$$

[Note that, though a strict inequality sign appears in (3.35c), one must allow for the possibility of equality in this formula, (3.36), because two *different* numbers may have the *same* integer part].

But the initial condition (3.34) and the recursion relation (1.27) defining the radii $r_j^{(-)}$ have been adjusted, as it can be easily verified in analogy to the argument used above, so that $\tilde{\eta}(r_{J(-)}^{(-)}) = 0$, $\tilde{\eta}(r_{J(-)-1}^{(-)}) = \pi/2$, $\tilde{\eta}(r_{J(-)-2}^{(-)}) = \pi$, and so on, entailing [see (1.27)]

$$\tilde{\eta}(r_0^{(-)}) = \tilde{\eta}(q) = J^{(-)}\,\pi/2. \tag{3.37}$$

Via (3.31) and (3.24) this implies the lower limit (1.29), which is thereby proven.

IV. THE KLEIN–GORDON CASE

In the context of first-quantized mechanics with relativistic kinematics, a zero-spin particle of (*positive*) mass m moving in an external potential $W(\mathbf{r})$, which is the fourth-component of a relativistic four-vector, is described (in self-evident notation, and with an appropriate choice of units) by the following Klein–Gordon equation:

$$(\mathbf{P}^2 + m^2)\,\psi(\mathbf{r}) = [E - W(\mathbf{r})]^2 \psi(\mathbf{r}). \tag{4.1}$$

In the spherically symmetrical case, $W(\mathbf{r}) = W(r)$, the zero-kinetic-energy (namely, $E = m$) S-wave radial equation coincides with the corresponding equation for the Schrödinger case, (3.1), with the following definition of $V(r)$ in terms of $W(r)$:

$$V(r) = 2mW(r) - W^2(r). \tag{4.2}$$

Note that, if the potential $W(r)$ is monotonically nondecreasing and vanishes at infinity [and is therefore *nonpositive*, $W(r) = -|W(r)|$], the same property, see (1.3), holds as well for the potential $V(r)$. And the following conditions on the behavior of $W(r)$ at the origin and at infinity are clearly sufficient to guarantee the validity of (1.1):

$$\lim_{r \to 0} \lfloor r^{1-\varepsilon} W(r) \rfloor = 0, \tag{4.3a}$$

$$\lim_{r\to\infty}[r^{2+\varepsilon}W(r)]=0. \tag{4.3b}$$

All the results reported above in the Schrödinger context can therefore be immediately taken over to the Klein–Gordon case. Note, however, that, as a consequence of the relation (4.2), if one introduces a ''coupling constant'' g as a measure of the strength of the potential by setting $W(r)=g^2w(r)$, then one sees that in the Klein–Gordon case as g diverges the number of S-wave bound states grows proportionally to g^2 [rather than proportionally to g as is the case in the Schrödinger context, see (1.6)].

ACKNOWLEDGMENTS

One of us (F.B.) would like to thank Professor F. Michel for its interest, Dr. C. Semay for checking some numerical results, and FNRS for financial support (FNRS Postdoctoral Researcher position).

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Multiple algebraisations of an elliptic Calogero–Sutherland model

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(Received 22 July 2002; accepted 18 December 2002)

Recently, Gómez-Ullate *et al.* [Phys. Lett. B **511**, 112 (2001)] have studied an N-particle quantum problem with elliptic-function potentials. They have shown that the Hamiltonian operator preserves a finite dimensional space of functions and as such is quasi-exactly solvable (QES). In this article we show that other types of invariant function spaces exist, which are in close relation to the algebraic properties of the elliptic functions. Accordingly, series of new algebraic eigenfunctions can be constructed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1557788]

I. INTRODUCTION

The first example of a nontrivial, integrable quantum many-body Hamiltonian was found by Calogero.[1] It describes a system of N particles in one dimension interacting pairwise by means of an inverse square potential. The similar model endowed with an inverse sine-square potential is also integrable as shown by Sutherland.[2] In fact these two potentials are particular cases of a two-parameter family of potentials defined by the Weierstrass function.[3,4] A detailed analysis of these models generalizing the Calogero–Sutherland (CS) quantum models was reported in Ref. 5. Their classical counterparts are discussed, e.g., in Ref. 6.

While integrable models (classical or quantum) can be studied because of their mathematical interest, it became apparent in recent years that the CS models can be applied to a large number of fields of physics. These range from condensed matter (quantum Hall liquids, quantum spin chains,...)[7] to gauge theories,[8] soliton theory[9] as well as recently to questions related to black holes and (anti)-deSitter space.[10,11] In particular, it was shown in Ref. 11 that the asymptotic dynamics of two-dimensional gravity in anti-deSitter and deSitter space respectively can be described by a generalized two-body CS model.

The property of a model to be integrable (i.e., to have a complete set of commuting constants of motion) does not necessarily imply that the spectrum and the eigenfunctions of the corresponding Hamiltonian can be constructed explicitly. The models which have this property are called *solvable*. From the beginning the CS models were known to be solvable, while further properties of their spectrum were obtained only recently, see, e.g., Ref. 12 and 13. However, the explicit form of the spectrum is still missing as far as the full Weierstrass-function potential is considered for generic values of N.

A step forward in the construction of solvable N-body problems interacting via a Weierstrass function was achieved in Ref. 14. The authors indeed showed that, when the Weierstrass potential is supplemented by a suitable external potential, a finite number of eigenvectors can be computed explicitly in terms of special functions. Stated differently, the model is quasi-exactly solvable (QES) according to the definition of Ref. 15. In fact, the kind of interaction considered in Ref. 14

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and in the present article generalizes a potential first introduced in Ref. 16.

Following the ideas of Ref. 15, the QES property holds when the Hamiltonian operator possesses a finite-dimensional invariant vector space of functions. Such a vector space was indeed constructed in Ref. 14 for the Hamiltonian considered. The purpose of this article is to demonstrate that this Hamiltonian possesses alternative invariant finite-dimensional vector spaces of functions. The way these new vector spaces are constructed is very reminiscent to the multiple algebraizations of the Lamé equations (see, e.g., Ref. 17), which occur due to the properties of the Jacobi elliptic functions.

The Hamiltonian is presented in Sec. II. In this section we also give the transformation putting the Hamiltonian in a Lie-algebraic form which reveals its QES property. The new invariant vector spaces are constructed in Sec. III and the Hamiltonian is studied for particular values of the parameters. The results are summarized in Sec. IV.

II. AN ELLIPTIC CALOGERO–SUTHERLAND MODEL

The quantum Hamiltonian proposed recently by Gómez-Ullate *et al.*[14] is given by

$$H_N(\mathbf{x}) = -\sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} + V_N(\mathbf{x}) \quad , \quad \mathbf{x} = (x_1, x_2, \ldots, x_N). \tag{1}$$

It describes N particles on a line interacting through the potential

$$V_N(\mathbf{x}) = c_m \sum_{k=1}^{N} \mathcal{P}(x_k + i\beta) + 4b(b-1) \sum_{k=1}^{N} \mathcal{P}(2x_k) + a(a-1) \sum_{\substack{j,k=1 \\ j \neq k}}^{N} [\mathcal{P}(x_j + x_k) + \mathcal{P}(x_j - x_k)]. \tag{2}$$

Here $\mathcal{P}(z) \equiv \mathcal{P}(z; g_2, g_3)$ denotes the Weierstrass function with invariants g_2, g_3. The constants a, b are real and positive, c_m is real. The term proportional to c_m can be interpreted as the potential of an external field.

The Hamiltonian (1) was shown to admit an invariant, finite-dimensional vector space of functions.[14] Restricting the operator to this vector space, the eigenvalue equation $H_N \psi = E \psi$ is reduced to a matrix equation and, accordingly, a finite number of eigenvectors can be determined algebraically. Following the definition of Ref. 15 the operator H_N is called quasi-exactly solvable (QES).

To reveal this property H_N has to be transformed appropriately. The authors of Ref. 14 introduced the function (called ''gauge factor'')

$$\mu(\mathbf{x}) = \prod_{j<k} [\mathcal{P}(x_j + i\beta) - \mathcal{P}(x_k + i\beta)]^a \prod_k [\mathcal{P}'(x_k + i\beta)]^b \tag{3}$$

and the new variables

$$z_k = \mathcal{P}(x_k + i\beta), \quad k = 1, \ldots, N. \tag{4}$$

Then a Hamiltonian $\bar{H}_N$—spectrally equivalent to H_N—is constructed according to $\bar{H}_N(\mathbf{z}) = \mu^{-1}(\mathbf{z}) H_N(\mathbf{x}) \mu(\mathbf{z})$. If the coupling constant c_m is chosen according to

$$c_m = [2m + 2a(N-1) + 4b][2m + 1 + 2a(N-1) + 2b], \quad m \in \mathbb{N}, \tag{5}$$

$\bar{H}_N(\mathbf{z})$ preserves the finite dimensional polynomial space[18]

$$\mathcal{M}_m = \mathrm{span}\left\{ \tau_1^{l_1} \tau_2^{l_2} \cdots \tau_N^{l_N} \ ; \ \sum_{i=1}^{N} l_i \leqslant m \right\} \tag{6}$$

with the kth elementary symmetric function

$$\tau_k \equiv \sum_{i_1<i_2<\cdots<i_k} z_{i_1} z_{i_2} \cdots z_{i_k}, \quad 1 \leqslant k \leqslant N. \tag{7}$$

A lengthy calculation leads to

$$\overline{H}_N(\mathbf{z}) = -\sum_{k=1}^{N} p_k \frac{\partial^2}{\partial z_k^2} - 2a \sum_{\substack{k,l=1 \\ k\neq l}}^{N} \frac{p_k}{z_k - z_l} \frac{\partial}{\partial z_k} - \left(b + \frac{1}{2}\right) \sum_{k=1}^{N} p_k' \frac{\partial}{\partial z_k} + \overline{V}_N(\mathbf{z}), \tag{8}$$

where $p_k \equiv p(z_k)$ and $p_k' \equiv p'(z_k)$ with

$$p(z) = 4z^3 - g_2 z - g_3, \quad p'(z) \equiv \frac{dp}{dz} = 12z^2 - g_2. \tag{9}$$

In the following we will use the roots, e_i, $i=1,2,3$, of $p(z)$:

$$p(z) = 4(z-e_1)(z-e_2)(z-e_3) = 4z^3 - g_2 z - g_3. \tag{10}$$

These numbers are equal to the values of the Weierstrass function at its half-periods.

The potential $\overline{V}_N$ in (8) is given by

$$\overline{V}_N(\mathbf{z}) = m(12b + 8a(N-1) + 4m + 2)\tau_1, \quad \tau_1 = \sum_{k=1}^{N} z_k. \tag{11}$$

The crucial observation is that the Hamiltonian $\overline{H}_N(\mathbf{z})$ can be written as a quadratic polynomial of the differential operators

$$\mathcal{D}_k = \frac{\partial}{\partial \tau_k}, \quad \mathcal{N}_{jk} = \tau_j \frac{\partial}{\partial \tau_k}, \quad \mathcal{U}_k = \tau_k \left(r - \sum_{i=1}^{N} \tau_i \frac{\partial}{\partial \tau_i} \right), \quad j,k = 1,2,\ldots,N, \tag{12}$$

with $r=m$. These operators form a representation of the Lie algebra $\mathrm{sl}(N+1)$ for generic value of the real parameter r; for $r=m$ they preserve the vector space $\mathcal{M}_m$ and the representation is finite dimensional.

Denoting by $\overline{H}_N^{(+)}$ the part of $\overline{H}_N$ which increases the degree of elements of $\mathcal{M}_m$, we find

$$\overline{H}_N^{(+)} = -4\tau_1(\mathcal{N} - m)\left(\mathcal{N} + m + \frac{1}{2} + 2a(N-1) + 3b \right), \quad \mathcal{N} \equiv \sum_{k=1}^{N} \mathcal{N}_{kk}. \tag{13}$$

Obviously, the factor $(\mathcal{N}-m)$ leads to the annihilation of all the monomials in $\mathcal{M}_m$ which have overall degree m. Therefore, we find $\overline{H}_N \mathcal{M}_m \subseteq \mathcal{M}_m$. As a consequence, eigenvectors of $\overline{H}_N$ (and therefore also of H_N) can be constructed in $\mathcal{M}_m$. In the following we will refer to this property as an ''algebraization'' of H_N.

III. ADDITIONAL GAUGE FACTORS

Inspired by the construction of the Lamé polynomials (see, e.g., Ref. 17), we introduce one further transformation of the Hamiltonian H_N:

$$\overline{H}_N \to \tilde{H}_N = \tilde{\mu}^{-1} \overline{H}_N \tilde{\mu} \tag{14}$$

with the gauge factor $\tilde{\mu}$ of the form

$$\tilde{\mu}(\mathbf{z})=\prod_{k=1}^{N}(z_k-e_1)^{\nu_1}(z_k-e_2)^{\nu_2}(z_k-e_3)^{\nu_3}. \tag{15}$$

The choice $\nu_1=\nu_2=\nu_3=0$ obviously corresponds to Ref. 14. After a calculation, we find that for each value of the form

$$\nu_i=0 \quad \text{or} \quad \nu_i=\tfrac{1}{2}-b, \quad i=1,2,3, \tag{16}$$

the Hamiltonian $\tilde{H}_N$ can be expressed as a quadratic combination of the operators (12) with suitable values (depending on the values of ν_i's) of the parameter r. We then found eight gauge factors (15) leading to algebraizations of the initial operator H_N. Let us now investigate the relations between r and the different parameters involved in the equations.

We find that the degree-increasing part, say $\tilde{H}_N^{(+)}$, of $\tilde{H}_N$ is given by

$$\tilde{H}_N^{(+)}=-4\tau_1(\mathcal{N}-(m+bn_f-\tfrac{1}{2}n_f))(\mathcal{N}+m+2a(N-1)+(3-n_f)b+\tfrac{1}{2}(1+n_f)). \tag{17}$$

Here, n_f denotes the number of nonzero exponents ν_i, $i=1,2,3$, in (15), i.e., is either 0,1,2 or 3. Note that for $n_f=1$ and $n_f=2$ three different algebraizations are available.

If we allow m to be a noninteger and require instead that $\tilde{m}$ with

$$\tilde{m}\equiv m+bn_f-\tfrac{1}{2}n_f \tag{18}$$

is an integer, we conclude that now

$$\tilde{H}_N\mathcal{M}_{\tilde{m}}\subseteq\mathcal{M}_{\tilde{m}}. \tag{19}$$

In the special case $b=0$, we can distinguish two different cases: (1) both m and $\tilde{m}$ are integers and (2) only $\tilde{m}$ is an integer. For item (1) we find a quadruple algebraization of the Hamiltonian $\tilde{H}_N$ (one algebraization for $n_f=0$ and three for $n_f=2$):

$$\tilde{H}_N\mathcal{M}_m\subseteq\mathcal{M}_m \quad \text{for} \quad n_f=0, \tag{20a}$$

$$\tilde{H}_N\mathcal{M}_{m-1}\subseteq\mathcal{M}_{m-1} \quad \text{for} \quad n_f=2. \tag{20b}$$

Similarly, for item (2) we find

$$\tilde{H}_N\mathcal{M}_{m-1/2}\subseteq\mathcal{M}_{m-1/2} \quad \text{for} \quad n_f=1, \tag{21a}$$

$$\tilde{H}_N\mathcal{M}_{m-3/2}\subseteq\mathcal{M}_{m-3/2} \quad \text{for} \quad n_f=3. \tag{21b}$$

Now, $\tilde{m}=m-1/2$ should be an integer. Again, this is a quadruple algebraization of the Hamiltonian $\tilde{H}_N$ (one algebraization for $n_f=3$ and three for $n_f=1$).

A. $a=b=0$: Relation between the Hamiltonian H_N and the Lamé operators

In order to understand the pattern of the algebraic solutions obtained for the model (1) and (2), it is useful to study the limit $a=b=0$. Using the relation

$$\mathcal{P}(x+i\beta)=e_3+(e_2-e_3)\mathrm{sn}^2(\sqrt{e_1-e_3}x,k), \quad k^2\equiv\frac{e_2-e_3}{e_1-e_3}, \tag{22}$$

it is easy to see that for $a=b=0$ the operator (1) takes the form

$$H_N(\mathbf{u})=(e_1-e_3)\sum_{j=1}^{N}\left\{-\frac{\partial^2}{\partial u_j^2}+2m(2m+1)k^2\mathrm{sn}^2(u_j,k)\right\}+2m(2m+1)e_3N \tag{23}$$

with $u_j\equiv\sqrt{e_1-e_3}x_j$. The operator inside the brackets $\{\}$ of (23) constitutes N decoupled copies of the Lamé operator $L(u)$:

$$L(u)=-\frac{d^2}{du^2}+2m(2m+1)k^2\mathrm{sn}^2(u,k),\quad 0\leqslant k\leqslant 1, \tag{24}$$

which admits $(4m+1)$ algebraic eigenvalues if m is an integer or a half integer.

If m is an integer, $(m+1)$ eigenvectors of $L(u)$ are of the form $p_m(\mathrm{sn}^2)$ and $(3m)$ eigenvectors are of the form $\mathrm{cn}\cdot p_{m-1}(\mathrm{sn}^2)$, $\mathrm{sn}\cdot p_{m-1}(\mathrm{sn}^2)$, $\mathrm{dn}\cdot p_{m-1}(\mathrm{sn}^2)$. sn, cn, dn are abbreviations for the Jacobi elliptic functions $\mathrm{sn}(u,k),\mathrm{cn}(u,k),\mathrm{dn}(u,k)$ and p_n denotes a polynomial of degree n in its argument. If m is a half integer $3(m+\frac{1}{2})$, eigenvectors of $L(u)$ are of the form $\mathrm{sn}\cdot\mathrm{cn}\cdot p_{m+1/2}(\mathrm{sn}^2)$, $\mathrm{sn}\cdot\mathrm{dn}\cdot p_{m+1/2}(\mathrm{sn}^2)$, $\mathrm{cn}\cdot\mathrm{dn}\cdot p_{m+1/2}(\mathrm{sn}^2)$ and $(m-\frac{1}{2})$ eigenvectors are of the form $\mathrm{sn}\cdot\mathrm{cn}\cdot\mathrm{dn}\cdot p_{m-1/2}(\mathrm{sn}^2)$.

Therefore, a total number of $(4m+1)^N$ algebraic eigenvectors of the Hamiltonian (23) can be constructed. However, not all of them are completely symmetric under the permutations of the coordinates. Since the procedure of algebraization is crucially related to the symmetrized variables τ_k [see (7)], only the completely symmetric solutions can be hoped to be recovered in the generic case for which $a\neq 0$ and/or $b\neq 0$.

Studying the solutions of the operator (23) and the structure of the eigenfunctions of the Lamé operator, it is not difficult to see that the number of completely symmetric solutions is given by

$$C_{m+N}^N+3C_{m+N-1}^N \tag{25a}$$

if m is an integer and

$$3C_{m'+N}^N+C_{m'+N-1}^N,\quad m'\equiv m+\tfrac{1}{2}, \tag{25b}$$

if m is a half integer, respectively. C_q^p denotes the usual combinatoric symbol.

We find that for $b=0$ the number of algebraic solutions available by applying the method described here agrees nicely with these above numbers. Moreover, we checked for several particular cases that, indeed, the relevant Lamé solutions are reproduced in the limit $a\to 0$. Note that in Ref. 14 only C_{m+N}^N solutions were found for integer values of m. Our supplementary factorizations therefore complete the pattern.

B. The case $N=m=2$, $b=0$

For the choice $N=m=2$, (20a) leads to a 6×6 matrix with respect to the basis $\{1,\tau_1,\tau_2,\tau_1^2,\tau_1\tau_2,\tau_2^2\}$:[14]

$$\begin{pmatrix} 0 & g_2(2a+2b+1) & -2ag_3 & 4g_3 & 0 & 0\\ 16a+24b+20 & 0 & g_2(b+\frac{1}{2}) & 4g_2(a+b+1) & 2g_3(1-a) & 0\\ 0 & 8a+24b+12 & 0 & 0 & g_2(2a+2b+5) & -4g_3(a+1)\\ 0 & 8a+12b+14 & 0 & 0 & g_2(b+\frac{1}{2}) & 2g_3\\ 0 & 0 & 8a+12b+14 & 16(a+3b+3) & 0 & g_2(2b+3)\\ 0 & 0 & 0 & 0 & 8a+24b+28 & 0 \end{pmatrix}. \tag{26}$$

For (20b) we obtain three different 3×3 matrices with respect to the basis $\{1,\tau_1,\tau_2\}$:

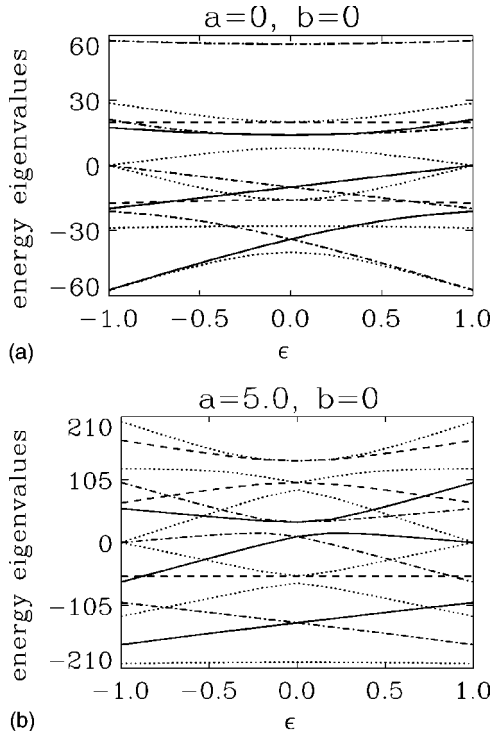

FIG. 1. (a) The energy eigenvalues of the 6×6 matrix (dotted) and of the 3×3 matrices h_i ($i=1$ dashed, $i=2$ solid, $i=3$ dotted-dashed), which correspond to the choice $N=m=2$, are shown for $a=b=0$ as a function of ϵ, where $e_1=2$, $e_2=-1+\epsilon$ and $e_3=-1-\epsilon$. (b) Same as (a), but for $a=5.0$.

$$h_i=\begin{pmatrix} (6+4a)e_i & g_2(2a+1)+8e_i^2 & -2ag_3 \\ 14+8a & (10+4a)e_i & g_2/2+4e_i^2 \\ 0 & 28+8a & (14+4a)e_i \end{pmatrix}, \quad i=1,2,3. \tag{27}$$

We thus obtain 15 algebraic solutions, i.e., an additional nine to the ones obtained in Ref. 14.

In Figs. 1(a) and 1(b) we show the energy eigenvalues as functions of ϵ for

$$e_1=2, \quad e_2=-1+\epsilon, \quad e_3=-1-\epsilon \tag{28}$$

and $a=0$ and $a=5.0$, respectively. Figure 1(a) corresponds to two decoupled Lamé operators. The limit $\epsilon=0$ further corresponds to the completely integrable case of two decoupled oscillators [$e_2=e_3$, so $k=0$ and the potential vanishes in (22) and (23)]. The eigenvalues of this system are of the form $3(j_1^2+j_2^2)-40$ where j_1,j_2 are integers. The set of algebraic eigenvalues obtained with our factorization (15) represents just the completely symmetric case, i.e., $j_1+j_2=2n$, $n=0,1,2,\ldots$, in this limit. This can be checked in Fig. 1(a). In Fig. 1(b) the effect of an interaction potential on the energy eigenvalues is demonstrated for $a=5.0$.

The case for which two of the numbers e_1,e_2,e_3 are equal is in itself special, since the 15 eigenvalues can be expressed as linear functions of a and the system is highly degenerated, irrespectively of a. E.g., for $e_1=2$, $e_2=e_3=-1$, three eigenvalues of the 6×6 matrix are not degenerate:

$$-8(5+4a), \quad -4(7+2a), \quad 8(1+2a), \tag{29a}$$

the other three eigenvalues of the 6×6 matrix coincide with those of the 3×3 matrix h_1:

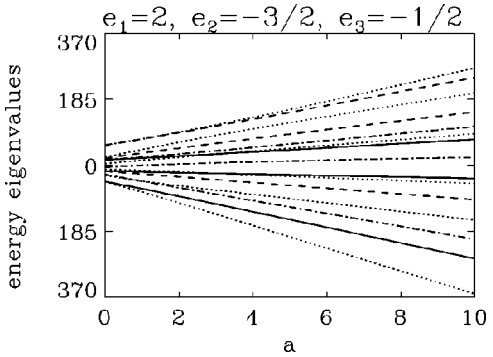

FIG. 2. The energy eigenvalues of the 6×6 matrix (dotted) and of the 3×3 matrices h_i ($i=1$ dashed, $i=2$ solid, $i=3$ dotted-dashed), which correspond to the choice $N=m=2$, are shown for $b=0$ and $e_1=2$, $e_2=-\frac{3}{2}$, $e_3=-\frac{1}{3}$ as a function of a.

$$-8(2+a), \quad 4(5+4a), \quad 8(7+2a), \tag{29b}$$

and finally the eigenvalues of the 3×3 matrices h_2 and h_3 coincide and read

$$-2(17+10a), \quad -2(5-2a), \quad 2(7+2a). \tag{29c}$$

This is clearly shown in Figs. 1(a) and 1(b), where at $\epsilon=0$ three of the dotted curves, which correspond to three of the eigenvalues of the 6×6 matrix, and the three dashed curves, which correspond to the three eigenvalues of h_1, cross both for $a=0$ and $a=5.0$, respectively. Similarly, the three solid lines and the three dotted-dashed lines, which correspond to the three eigenvalues of the matrices h_2 and h_3, respectively, cross at $\epsilon=0$. How these degeneracies disappear for a generic choice of e_i, $i=1,2,3$, is also shown in these figures

Finally, in Fig. 2 we demonstrate the dependence of the eigenvalues on the parameter a for the special choice $e_1=2$, $e_2=-\frac{3}{2}$, $e_3=-\frac{1}{2}$.

IV. SUMMARY

The construction of integrable models of Calogero–Sutherland (CS) type has recently received a lot of attention in relation to new applications related to different domains of theoretical physics. The class of N-body integrable models remains, however, very tiny, and several generalizations are worth considering. The construction of quasi-exactly solvable Hamiltonians describing N degrees of freedom appears to be a possible extension of the notion of integrable systems. As seen in Refs. 14 and 16, the potential can be more general than those related to the root system of a Lie algebra (typically of the type A_N for potentials depending on the differences of the particles' coordinates).

In this article, we reconsidered such a QES model proposed recently in Ref. 14. It depends on four parameters: two coupling constants a,b and the two periods of the Weierstrass function $\mathcal{P}$, parametrized by g_2,g_3. More popular models are recovered for special limits of these constants: an Inozemtsev model for $b=0$, a system of N decoupled Lamé equations if $a=b=0$ and a system of N decoupled oscillators if, in addition, $e_2=e_3$ (or equivalently $g_2^3=27g_3^2$). We have seen that the case $b=0$ possesses a particularly rich algebraic spectrum.

By investigation of the spectrum available in these limits, it appears that the solutions constructed in Ref. 14 do not constitute the full set of completely symmetric algebraic eigenfunctions of the initial Hamiltonian (1). Following closely the construction of the Lamé polynomials we have found additional algebraizations of the operator H_N. The set of algebraic eigenfunctions obtained in this way coincides exactly with the number of possible algebraic functions. We assume that an extension of the type of Hamiltonian considered here to 2×2 matrix valued operators[19] might be possible, but leave this construction as a future project.[20]

Note added: After this article was finished several papers appeared dealing with the same topic. These are, e.g., K. Takemura, math.QA/0205274 and O. Chalykh *et al.*, math.QA/0212029.

ACKNOWLEDGMENTS

Y.B. acknowledges discussions with N. Nachez. B.H. was supported by an EPSRC grant.

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Positive measure spectrum for Schrödinger operators with periodic magnetic fields

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(Received 7 October 2002; accepted 20 December 2002)

We study Schrödinger operators with periodic magnetic field in $\mathbb{R}^2$, in the case of irrational magnetic flux. Positive measure Cantor spectrum is generically expected in the presence of an electric potential. We show that, even without electric potential, the spectrum has positive measure if the magnetic field is a perturbation of a constant one. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556551]

I. INTRODUCTION

Magnetic Schrödinger operators have been studied in solid state physics, especially in connection with the quantum Hall effect, as well as in their own right. In a regular crystal ''physics'' is periodic, i.e., the electric potential—caused by the background field of the ions—is a periodic function. Magnetic fields—internal as well as external ones—are periodic as well, the latter ones typically being constant. Alas, as is well known, magnetic fields enter the Schrödinger operator through a vector potential, so that the resulting operator is not necessarily periodic. Indeed, it is so only in the simple and well-understood case of ''zero flux,'' where one has absolutely continuous spectrum and band-structure (Birman and Suslina, 1998; Sobolev, 1999). Here, the magnetic flux (in units of flux quanta) is defined by

$$\Phi = \frac{1}{2\pi} \int_{\mathcal{F}} B(x,y)\, \mathrm{d}x\, \mathrm{d}y, \tag{1}$$

where B is the magnetic field and $\mathcal{F}$ is a lattice cell (fundamental domain for the action of the group). Note that in our units with $\hbar = e = 1$, the magnetic flux quantum is just 2π.

For integer or rational flux the spectrum will still consist of bands (possibly degenerating into points), but pure point spectrum is possible.

For irrational flux one expects Cantor spectrum (i.e., a nowhere dense set, no isolated points). The question is now: If B is constant, what ''defines the lattice,'' thus defining $\mathcal{F}$ and the flux? A potential $V(x,y) = \cos(2\pi x) + \cos(2\pi y)$ has periods (1,1); one might consider any pair (m,n) of integers as periods of V, i.e., one can consider any coarser superlattice of $\mathbb{Z}\times\mathbb{Z}$ as the lattice of symmetry, but no finer lattice. Indeed, in this case one finds Cantor structure for a certain set of irrational values of Φ (Helffer and Sjöstrand, 1989).

On the other hand, $V(x,y) = \cos(2\pi x)$ has periods $(1,c)$ for any real c; it does not define a fixed ''minimally coarse'' lattice. Indeed, the Schrödinger operator with constant magnetic field and this potential V has band spectrum. This is still true for every potential $V(x,y) = V_0(x)$ with reasonably non-degenerate V_0. Now, if we perturb such a V by a periodic V_1 we expect Cantor spectrum, although this is not known. We only know that the Schödinger operator can be approximated in norm resolvent sense by operators from a natural algebra which have Cantor spectra (Gruber, 2001).

Setting the Cantor issue aside, Dinaburg *et al.* (1997) showed that what survives under this kind of perturbation is the positive measure of the bands, although the bands might dissolve into a Cantor set.

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We ask the same question for Schrödinger operators with periodic magnetic field B, without electric potential V. For constant B the spectrum is pure-point and infinitely degenerate (Landau levels). Is a periodic (zero-flux) perturbation of B enough to cause the same effects as the potential V?

In the course of giving an affirmative answer, we construct the generalized eigenfunctions and give estimates on the measure of the ''bands.''

II. OUTLINE

In Sec. III we describe the setup and perform a first perturbation by one-dimensional magnetic potentials. For the general case, we give the direct integral decomposition and express the operator in an appropriate basis ''moving along the fiber.'' In Sec. IV we give concise formulations of the main results. The resulting double-infinite matrix problem is reduced in Sec. V to a problem which is almost diagonal in a sense made precise there. In Sec. VI we prove the main reduction lemma, using estimates on Weber–Hermite functions. Section VII finishes the proof of the main results.

III. SETUP AND FIRST PERTURBATION

For simplicity of notation we assume that the lattice is $\mathbb{Z}\times\mathbb{Z}$. Let B be an arbitrary smooth periodic magnetic field and Φ its flux through a fundamental cell of the lattice in units of flux quanta. Then we can decompose B as

$$B=B_c+B_z$$

with

$$B_c=2\pi\Phi$$

and

$$B_z=B-B_c\,.$$

Note that B_z has zero flux! Therefore, B_z has a periodic vector potential A_z, and we can choose it to be of the form

$$A_z(x,y)=\begin{pmatrix}\varepsilon_0 A^0(y)\\ \varepsilon_1 A^1(x,y)\end{pmatrix} \tag{2}$$

with periodic smooth A^0 and A^1, where we introduced parameters $\varepsilon_0,\varepsilon_1$ for later convenience.

B_c is obviously constant, and we choose a vector potential

$$A_z(y)=B_c\begin{pmatrix}y\\ 0\end{pmatrix} \tag{3}$$

for it. In this gauge, the magnetic Schrödinger operator takes on the form

$$H=\frac{1}{2}\left[\left(\frac{1}{\imath}\frac{\partial}{\partial x}-B_c y-\varepsilon_0 A^0(y)\right)^2+\left(\frac{1}{\imath}\frac{\partial}{\partial y}-\varepsilon_1 A^1(x,y)\right)^2\right]. \tag{4}$$

Note that, in order to emphasize the dependencies, we write out the arguments of A^0 and A^1 even though they are multiplication operators; in the following we will keep sacrificing strictness of notation for better clarity in cases such as this one.

First we will set $\varepsilon_1=0$ and study the effect of switching on ε_0. The operator (4) does not depend on x if $\varepsilon_1=0$. Using Fourier transform on $L^2(\mathbb{R}_x)$, we can decompose $L^2(\mathbb{R}^2)$ into a direct integral $\int_{\mathbb{R}}^{\oplus}L^2(\mathbb{R}_y)\,\mathrm{d}\xi$ such that

$$L^2(\mathbb{R}^2) \ni f \mapsto \hat{f}, \quad \hat{f}_\xi(y) = \int_{\mathbb{R}} f(x,y) e^{-2\pi\imath\xi x}\, \mathrm{d}x, \tag{5a}$$

$$f(x,y) = \int_{\mathbb{R}} f_\xi(y) e^{2\pi\imath\xi x}\, \mathrm{d}\xi, \tag{5b}$$

$$H = \int_{\mathbb{R}}^{\oplus} \hat{H}_\xi\, \mathrm{d}\xi, \quad \hat{H}_\xi = V_\xi(y) - \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} \tag{5c}$$

with

$$V_\xi(y) = \tfrac{1}{2}(2\pi\xi - B_c y - \varepsilon_0 A^0(y))^2. \tag{5d}$$

In the case $\varepsilon_0 = \varepsilon_1 = 0$ we are dealing with the Landau Hamiltonian. We will go through its analysis since we will use its eigenfunctions later on as a basis.

A. $\varepsilon_0 = 0 = \varepsilon_1$

$$V_\xi(y) = \frac{1}{2}(2\pi\xi - B_c y)^2 = \frac{B_c^2}{2}(y - \beta\xi)^2 \tag{6}$$

is a harmonic oscillator potential with frequency B_c, shifted by $\beta\xi$ with $\beta = 2\pi/B_c = 1/\Phi$ (we assume $B_c \neq 0$, or else there is not much to do). If we denote by

$$\Omega_m(y) = \frac{(-1)^m}{\sqrt{\sqrt{\pi} 2^m m!}} \exp\left(\frac{y^2}{2}\right) \frac{\mathrm{d}^m}{\mathrm{d}y^m} \exp(-y^2), \quad m \in \mathbb{Z}_+, \tag{7}$$

the Weber–Hermite functions, i.e., the standard normalized eigenfunctions of the harmonic oscillator with frequency 1, then

$$\Psi_{\xi,m} = \sqrt[4]{B_c}\, \Omega_m(\sqrt{B_c}(y - \beta\xi)), \quad m \in \mathbb{Z}_+, \tag{8}$$

are the eigenfunctions of $\hat{H}_\xi$, and the corresponding eigenvalues are $B_c(\frac{1}{2} + m)$. Since the spectrum of $\hat{H}_\xi$ is independent of ξ it coincides with the spectrum of H as a set, and both are pure-point. On the other hand, since H is invariant in x, it has infinitely degenerate spectrum.

B. $\varepsilon_0 \neq 0 = \varepsilon_1$

Introducing the shifted variable $\tilde{y} = y - \beta\xi$, we can write the potential (5d) as

$$V_\xi(\tilde{y}) = \frac{B_c^2}{2}(\tilde{y} + \varepsilon_0 A^0(\tilde{y} + \beta\xi))^2. \tag{9}$$

Since A^0 is periodic and smooth (and therefore bounded), this is just a perturbation of the harmonic oscillator potential. $V_\xi(\tilde{y})$ will still tend to infinity as $|\tilde{y}|$ does, so that $\hat{H}_\xi$ has discrete spectrum. Some simple estimates using test functions show that for small ε_0 the eigenvalues will be within $C_m \varepsilon_0 \max|A^0|$ of the Landau levels, for some constants C_m (involving the maximum of $|y\Omega_m(y)|$) depending on m and B_c only; in particular, they are independent of ξ. A closer investigation shows that C_m is indeed bounded with respect to m.

Note that V_ξ is periodic in ξ with period $B_c/2\pi = \Phi$. Therefore, the spectrum of $H = \int_{\mathbb{R}}^{\oplus} \hat{H}_\xi\, \mathrm{d}\xi$ consists of bands whose size is bounded by $2C_m\varepsilon_0 \max|A^0|$. These bands might degenerate into points.

C. $\varepsilon_0 \neq 0 \neq \varepsilon_1$

Now H is not independent of x anymore. But at least it will be periodic in x with period 1, since A^1 is periodic. Using Fourier series on $L^2([0,1]_x)$, we can decompose $L^2(\mathbb{R}^2)$ into a direct integral $\int_{[0,1]}^{\oplus} L^2([0,1]_x \times \mathbb{R}_y)\, \mathrm{d}\xi$ such that

$$L^2(\mathbb{R}^2) \ni f \mapsto \hat{f}, \quad \hat{f}_\xi(x,y) = \sum_{l \in \mathbb{Z}} f(x+l,y) e^{-2\pi \imath \xi (x+l)}, \tag{10a}$$

$$f(x,y) = \int_{[0,1]} \hat{f}_\xi(x,y) e^{2\pi \imath \xi x}\, \mathrm{d}\xi, \tag{10b}$$

$$H = \int_{[0,1]}^{\oplus} \hat{H}_\xi\, \mathrm{d}\xi, \quad \hat{H}_\xi = \frac{1}{2}\left[\left(\frac{1}{\imath}\frac{\partial}{\partial x} + 2\pi\xi - B_c y - \varepsilon_0 A^0(y)\right)^2 + \left(\frac{1}{\imath}\frac{\partial}{\partial y} - \varepsilon_1 A^1(x,y)\right)^2\right] \tag{10c}$$

acting on functions periodic in x. Note that we keep denoting the fiber operator $\hat{H}_\xi$ for the new direct integral, in order to avoid an inflation of notation.

If we now choose the basis $(e^{2\pi \imath n x})_{n \in \mathbb{Z}}$ in $L^2([0,1]_x)$, defining an isomorphism with $\ell^2(\mathbb{Z})$, and combine this with the isomorphism defining the direct integral above, we arrive at the direct integral $L^2(\mathbb{R}^2) = \int_{[0,1]}^{\oplus} \ell^2(\mathbb{Z}) \otimes L^2(\mathbb{R})\, \mathrm{d}\xi$ with

$$L^2(\mathbb{R}^2) \ni f \mapsto \hat{f}, \quad \hat{f}_{\xi,n}(y) = \int_{[0,1]} \sum_{l \in \mathbb{Z}} f(x+l,y) e^{-2\pi \imath [\xi l + (\xi+n)x]}\, \mathrm{d}x, \tag{11a}$$

$$f(x,y) = \int_{[0,1]} \sum_{n \in \mathbb{Z}} \hat{f}_{\xi,n}(y) e^{2\pi \imath (\xi+n)x}\, \mathrm{d}\xi, \tag{11b}$$

$$H = \int_{[0,1]}^{\oplus} \hat{H}_\xi\, \mathrm{d}\xi, \quad \hat{H}_\xi = \frac{1}{2}\left[(2\pi(\nu+\xi) - B_c y - \varepsilon_0 A^0(y))^2 + \left(\frac{1}{\imath}\frac{\mathrm{d}}{\mathrm{d}y} - \varepsilon_1 \widehat{A^1}(y)\star\right)^2\right]. \tag{11c}$$

Here, ν is the operator of multiplication on $\ell^2(\mathbb{Z})$, i.e., $(\nu g)(n) = n g(n)$, and $\widehat{A^1}(y)\star$ is convolution with the Fourier series of $A^1(x,y)$ in x:

$$(\widehat{A^1}(y) \star g)(n) = \sum_{l \in \mathbb{Z}} g(l) \widehat{A^1}_{n-l}(y), \tag{12a}$$

$$\widehat{A^1}_n(y) = \int_{[0,1]} A^1(x,y) e^{-2\pi \imath n x}\, \mathrm{d}x. \tag{12b}$$

Note that, of course, our basis functions belong to the domain of the operator.

As a final step, we choose a special basis in $L^2(\mathbb{R})$, namely the eigenfunctions $(\Psi_{\xi,m})_{m \in \mathbb{Z}_+}$ described in Sec. III A, Eq. (8). Thus we arrive at

Lemma 1: There is a decomposition of $L^2(\mathbb{R}^2)$ *into* $\int_{[0,1]}^{\oplus} \ell^2(\mathbb{Z} \times \mathbb{Z}_+)\, \mathrm{d}\xi$ *with*

$$L^2(\mathbb{R}^2) \ni f \mapsto \hat{f}, \tag{13a}$$

$$\hat{f}_{\xi,n,m} = \int_{[0,1] \times \mathbb{R}} \sum_{l \in \mathbb{Z}} f(x+l,y) e^{-2\pi \imath [\xi l + (\xi+n)x]} \Psi_{\xi+n,m}(y)\, \mathrm{d}x\, \mathrm{d}y, \tag{13b}$$

$$f(x,y) = \int_{[0,1]} \sum_{n \in \mathbb{Z}} \sum_{m \in \mathbb{Z}_+} \hat{f}_{\xi,n,m} e^{2\pi \imath (\xi+n)x} \Psi_{\xi+n,m}(y)\, \mathrm{d}\xi \tag{13c}$$

such that H decomposes as

$$H=\int_{[0,1]}^{\oplus}\hat{H}_\xi\,\mathrm{d}\xi, \tag{14a}$$

$$(\hat{H}_\xi\hat{f}_\xi)_{m,n}=B_c(\tfrac{1}{2}+m)\hat{f}_{\xi,m,n} \tag{14b}$$

$$+\frac{1}{2}\varepsilon_0^2\sum_{l\in\mathbb{Z}_+}\widetilde{A^0}_{l,m}(\beta(\xi+n))\hat{f}_{\xi,l,n} \tag{14c}$$

$$-\varepsilon_0\sum_{l\in\mathbb{Z}_+}A^0_{l,m}(\beta(\xi+n))\hat{f}_{\xi,l,n} \tag{14d}$$

$$+\frac{1}{2}\varepsilon_1^2\sum_{l\in\mathbb{Z}_+}\sum_{k\in\mathbb{Z}}\widetilde{A^{1(n-k)}_{l,m}}(\beta(\xi+n))\hat{f}_{\xi,l,k} \tag{14e}$$

$$-\varepsilon_1\sum_{l\in\mathbb{Z}_+}\sum_{k\in\mathbb{Z}}\widehat{A^{1(n-k)}_{l,m}}(\beta(\xi+n))\hat{f}_{\xi,l,k}, \tag{14f}$$

where

$$\widetilde{A^0}_{l,m}(p)=\sqrt{B_c}\int_{\mathbb{R}}(A^0)^2(y+p)\Omega_l(\sqrt{B_c}y)\Omega_m(\sqrt{B_c}y)\,\mathrm{d}y, \tag{15a}$$

$$A^0_{l,m}(p)=B_c^{3/2}\int_{\mathbb{R}}A^0(y+p)y\Omega_l(\sqrt{B_c}y)\Omega_m(\sqrt{B_c}y)\,\mathrm{d}y, \tag{15b}$$

$$\widetilde{A^{1(k)}_{l,m}}(p)=\sqrt{B_c}\int_{\mathbb{R}}\widehat{(A^1)^2}_k(y+p)\Omega_l(\sqrt{B_c}(y+\beta k))\Omega_m(\sqrt{B_c}y)\,\mathrm{d}y, \tag{15c}$$

$$\widehat{A^{1(k)}_{l,m}}(p)=\frac{1}{\imath}B_c\int_{\mathbb{R}}\widehat{A^1}_k(y+p)[\Omega_l'(\sqrt{B_c}(y+\beta k))\Omega_m(\sqrt{B_c}y)-\Omega_l(\sqrt{B_c}(y+\beta k))\Omega_m'(\sqrt{B_c}y)]\,\mathrm{d}y. \tag{15d}$$

As above, $\widehat{A^1}_k$ denotes the kth Fourier coefficient of A^1 with respect to x, and analogously for $(A^1)^2$.

Proof: We have

$$(\hat{H}_\xi\hat{f}_\xi)_{m,n}=\sum_{l\in\mathbb{Z}_+}\sum_{k\in\mathbb{Z}}\hat{H}_{\xi,m,n;l,k}\hat{f}_{\xi,l,k},$$

so that we just have to compute the matrix elements in the given basis, for all the terms in (11c).

(14b) These are just the Landau eigenvalues in the case $\varepsilon_0=0=\varepsilon_1$.

(14c) and (15a) For the terms with coefficient ε_0^2 we have to compute the matrix element of the square term $(A^0)^2$, which is

$$\sqrt{B_c}\int_{\mathbb{R}}(A^0)^2(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l(\sqrt{B_c}(y-\beta(\xi+n)))\,\mathrm{d}y.$$

(14d) and (15b) The terms with coefficient ε_0 in (11c) give the matrix element of the mixed term $(B_cy-2\pi(\nu+\xi))A^0$, the calculation is the same as above.

(14e) and (15c) The coefficient ε_1^2 singles out the square term $\widehat{A^1}\star\widehat{A^1}\star=\widehat{(A^1)^2}\star$, i.e., convolution with the Fourier series of $(A^1)^2$. Its matrix element is

$$\sqrt{B_c}\int_{\mathbb{R}}\widehat{(A^1)^2}_{n-k}(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l(\sqrt{B_c}(y-\beta(\xi+k)))\,dy$$

so that shifting y as above gives the desired result.

(14f) and (15d) The term with coefficient ε_1 is

$$\imath\left(\frac{d}{dy}\circ\widehat{A^1}\star+\widehat{A^1}\star\frac{d}{dy}\right).$$

The first part can be written $d/dy\circ\widehat{A^1}\star=\widehat{A^1}'\star+\widehat{A^1}\star d/dy$ which has matrix element

$$\sqrt{B_c}\int_{\mathbb{R}}[\widehat{A^1}'_{n-k}(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l(\sqrt{B_c}(y-\beta(\xi+k)))$$
$$+\sqrt{B_c}\widehat{A^1}_{n-k}(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l'(\sqrt{B_c}(y-\beta(\xi+k)))]\,dy.$$

On the other hand, we can use partial integration for the matrix element of the second part, which is $\widehat{A^1}\star d/dy$:

$$B_c\int_{\mathbb{R}}\widehat{A^1}_{n-k}(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l'(\sqrt{B_c}(y-\beta(\xi+k)))\,dy$$
$$=\sqrt{B_c}\int_{\mathbb{R}}[-\widehat{A^1}'_{n-k}(y)\Omega_m(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l(\sqrt{B_c}(y-\beta(\xi+k)))$$
$$-\sqrt{B_c}\,\widehat{A^1}_{n-k}(y)\Omega_m'(\sqrt{B_c}(y-\beta(\xi+n)))\Omega_l(\sqrt{B_c}(y-\beta(\xi+k)))]\,dy.$$

These two parts add up to the desired result. □

Remark 1: Note that the functions $\widetilde{A^0}_{l,m}(p)$, $A^0_{l,m}(p)$, $\widetilde{A^{1(k)}_{l,m}}(p)$, $\widehat{A^{1(k)}_{l,m}}(p)$ have period 1 in p. Also, due to the decay of the Weber–Hermite functions $\Omega_m(y)$ in y, the functions $\widetilde{A^{1(k)}_{l,m}}(p)$, $\widehat{A^{1(k)}_{l,m}}(p)$ exhibit exponential decay in k.

Remark 2: If A^1 depends on x only then $\widetilde{A^{1(k)}_{l,m}}(p)=\delta_{k,0}\delta_{l,m}\overline{(A^1)^2}$ with the average $\overline{(A^1)^2}$ of $(A^1)^2$ with respect to x. If we assume that $\overline{A^1}=0$ (we can always add a constant to A^1 to achieve this, without changing the magnetic field) then $\widehat{A^{1(k)}_{l,m}}(p)=0$.

Remark 3: In the simplest nontrivial case $A^0(y)=\cos(2\pi y)$, using parity of the Weber–Hermite functions we get

$$A^0{}_{l,m}(p)=a_{l,m}\cos(2\pi p)+b_{l,m}\sin(2\pi p),$$

where $a_{l,m}=0$ if $m+l$ is even, and $b_{l,m}=0$ if $m+l$ is odd. Similarly,

$$\widetilde{A^0}_{l,m}(p)=\tfrac{1}{2}\delta_{l,m}+c_{l,m}\cos(4\pi p)+d_{l,m}\sin(4\pi p),$$

where $c_{l,m}=0$ if $m+l$ is odd, and $d_{l,m}=0$ if $m+l$ is even.

Remark 4: Creation and annihilation operators on harmonic oscillator functions yield

$$\Omega_m'(y)=\sqrt{\frac{m}{2}}\,\Omega_{m-1}-\sqrt{\frac{m+1}{2}}\,\Omega_{m+1},\tag{16a}$$

$$y\Omega_m(y) = \sqrt{\frac{m}{2}}\,\Omega_{m-1} + \sqrt{\frac{m+1}{2}}\,\Omega_{m+1}. \tag{16b}$$

Using these we can express ${A^0}_{l,m}$ and $\widehat{A^1}^{(k)}_{l,m}$ solely in terms of A^0, A^1 and Weber–Hermite functions, without referring to their derivatives or multiplication by y.

IV. MAIN RESULTS

Let $P^0_{\xi,m}$ denote the projection on the eigenspace of the mth Landau level. Lemma 1 tells us that the action of $\hat{H}_\xi$ in this eigenspace, i.e., the part of $\hat{H}_\xi$ which is "diagonal in m," amounts to

$$\begin{aligned}(P^0_{\xi,m}\hat{H}_\xi P^0_{\xi,m})\hat{f}_{\xi,m,n} = {} & (B_c(\tfrac{1}{2}+m) + \tfrac{1}{2}\varepsilon_0^2\widetilde{A^0}_{m,m}(\beta(\xi+n)) - \varepsilon_0 A^0_{m,m}(\beta(\xi+n)))\hat{f}_{\xi,m,n} \\ & + \sum_{k\in\mathbb{Z}} [\tfrac{1}{2}\varepsilon_1^2\widetilde{A^1}^{(n-k)}_{m,m}(\beta(\xi+n)) - \varepsilon_1\widehat{A^1}^{(n-k)}_{m,m}(\beta(\xi+n))]\hat{f}_{\xi,m,k}.\end{aligned} \tag{17}$$

For fixed ξ and m this is a one-dimensional difference operator with quasiperiodic coefficients and exponentially decaying off-diagonal (i.e., $k\neq 0$) terms. If we choose A^1 to be independent of y as in Remark 2 there are no off-diagonal terms at all. If we furthermore choose $A^0(y)=\cos(2\pi y)$ as in Remark 3 then (17) will be similar to the almost Matthieu operator, with a slightly more complicated potential. Indeed, if we look at terms of order up to ε_0 only it will be exactly the almost Matthieu operator. In the case of constant magnetic field this observation goes back to Hofstadter (1976).

If ε_0 and ε_1 are small enough then H will have invariant subspaces E_m which are close to the eigenspaces of the Landau levels. We will construct a unitary transformation which shows that H is close to an almost Matthieu operator, and that the difference can be controlled.

In the course of this section we will need the following assumptions.

Diophantine: There are $C>0$, $\kappa>0$ such that $|\{\beta n\}|>C/|n|^\kappa$ for all $n\in\mathbb{Z}\backslash 0$. Here, $\beta = 2\pi/B_c = 1/\Phi$ as before, and $\{\cdot\}$ denotes the fractional part.

Smoothness: A^0 and $A^1(x,y)$ are smooth; furthermore, all derivatives $(\partial^j A^1/\partial y^j)(x,y)$ are analytic in $|\Im x|<\delta$ for some common $\delta>0$.

Morse: $A^0_{m,m}$ is a Morse function on S^1 with exactly two critical points.

Theorem 1: *Assume that A^0 and $A^1(x,y)$ are smooth as defined above. Then, for every small enough ε_0 and ε_1 there is an $M(\varepsilon_0,\varepsilon_1)$ such that $M(\varepsilon_0,\varepsilon_1)\to\infty$ as both $\varepsilon_0,\varepsilon_1\to\infty$, and such that for $m\leqslant M(\varepsilon_0,\varepsilon_1)$ the invariant subspace E_m of H and the restriction of H to E_m have a direct integral decomposition*

$$E_m = \int_{[0,1]}^{\oplus} \ell^2(\mathbb{Z})\,\mathrm{d}\xi, \tag{18a}$$

$$H_m := H|_{E_m} = \int_{[0,1]}^{\oplus} H_{m,\xi}\,\mathrm{d}\xi. \tag{18b}$$

Furthermore, $H_{m,\xi}$ acts on $g\in\ell^2(\mathbb{Z})$ as a one-dimensional difference operator with exponentially decaying coefficients close to those of (17):

$$(H_{m,\xi}g)(n) = d_m(\beta(\xi+n))g(n) + \sum_{k\in\mathbb{Z}} a_m(n-k,\beta(\xi+n))g(k), \tag{19a}$$

$$\|d_m(\cdot) - [B_c(\tfrac{1}{2}+m) - \varepsilon_0 A^0_{m,m}(\cdot)]\|_{C^2(S^1)} < C_0\varepsilon_0^2, \tag{19b}$$

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} \|a_m(k,\cdot)e^{\delta|k|}\|_{C^2(S^1)} < C_1\varepsilon_0 \tag{19c}$$

for some $\delta>0$.

We denote by $\|\cdot\|_{C^2(S^1)}$ the sum of the supremum norms of the derivatives of order 0,1,2.

As in Dinaburg *et al.* (1997) we can now make use of the results of Dinaburg (1997) on ergodic families of operators:

Theorem 2: *Let* $\beta=2\pi/B_c$ *be diophantine and* A^0, A^1 *smooth as defined above, and* $M>0$ *such that* $A^0_{m,m}$ *is a Morse function with exactly two critical points for all* $m\leqslant M$. *Then there are* $\tilde{\varepsilon}_0,\tilde{\varepsilon}_1>0$ *depending on* M *such that for all* $\varepsilon_0<\tilde{\varepsilon}_0,\varepsilon_1<\tilde{\varepsilon}_1$ *the following are true for all* $m\leqslant M$.

1. There are 1-periodic measurable functions λ_m *such that for every* $n\in\mathbb{Z}$ *and almost every* $\xi\in[0,1]$, $\lambda_m(\beta(\xi+n))$ *is an eigenvalue of* $H_{m,\xi}$ *and therefore in the spectrum of* H_m. *Furthermore,*

$$\|\lambda_m(\cdot)-[B_c(\tfrac{1}{2}+m)-\varepsilon_0 A^0_{m,m}(\cdot)]\|_{L^\infty(S^1)} < \text{const}\,\varepsilon_0^2. \tag{20}$$

2. There are 1-periodic measurable functions $f_{m,l,k}, l\in\mathbb{Z}_+, n\in\mathbb{Z}$, *decaying exponentially in n such that for almost every* $\xi\in[0,1]$,

$$\sum_{\substack{l\in\mathbb{Z}_+\\ k\in\mathbb{Z}}} |f_{m,l,n}(\beta\xi)|(l^2+1)e^{2\delta|n|}<\infty, \tag{21}$$

and for every $k\in\mathbb{Z}$, *the series*

$$\Phi_{m,\xi,k}(x,y)=\sum_{\substack{l\in\mathbb{Z}_+\\ n\in\mathbb{Z}}} f_{m,l,n-k}(\beta(\xi+k))e^{2\pi i(\xi+n)x}\Psi_{\xi+n,l}(y) \tag{22}$$

and all its derivatives converge uniformly in x,y. $\Phi_{m,\xi,k}$ *is an eigenfunction of* $H_{m,\xi}$ *and therefore a generalized eigenfunction of* H, *with eigenvalue* $\lambda_m(\beta(\xi+k))$. *Moreover, for every* $N>0$ *and for* $\varepsilon_0,\varepsilon_1$ *small enough* (*depending on* N),

$$|\Phi_{m,\xi,k}(x,y)|\leqslant \frac{\text{const}}{y^{2N}+1} \tag{23}$$

with the constant depending on ξ,k,m,N.

3. H_m *is uniformly* ε_0*-close to band structure:* H_m *is unitarily equivalent to multiplication by the function* $\lambda_m(\beta\cdot)$. *The Lebesgue measure of the spectrum of* H_m *is* $\varepsilon_0|\operatorname{ran}A^0_{m,m}|+O(\varepsilon_0^2)$.

Remark 5: One can reduce the smoothness requirements somewhat (to analyticity in x of a finite number of derivatives in y), thereby weakening the result on decay of the generalized eigenfunctions in y.

Remark 6: Of course one can also include an electric potential into the picture; Dinaburg *et al.* (1997) did so in the case of constant magnetic field, i.e., $A^0\equiv A^1\equiv 0$. The point in our work is that the magnetic field perturbation alone is strong enough to deform the Landau levels into a spectral set with positive measure.

V. REDUCTION

$\hat{H}_\xi$ is a double matrix operator on $\ell^2(\mathbb{Z}_+\times\mathbb{Z})$ with indices $(m,n)\in\mathbb{Z}_+\times\mathbb{Z}$. We decompose it as $\hat{H}_\xi=\mathcal{D}_1+\mathcal{M}_1+\mathcal{O}_1$, where $\mathcal{D}_1$ is diagonal in m and n, $\mathcal{O}_1$ is off-diagonal in m and contains only the first row and the first column, and $\mathcal{M}_1$ is the remainder. Note that both $\mathcal{O}_1$ and $\mathcal{M}_1$ are of order ε_0 (we always assume $\varepsilon_1<\varepsilon_0$).

Our goal is to find a unitary transformation U which kills the terms in $\mathcal{O}$ (they represent the interaction between different Landau levels). U should leave the rest of the structure basically untouched. We will show how to accomplish this for the interaction between the 0-th and all other bands; extending this to M off-diagonal terms is a trivial generalization.

The strategy is as follows: We define U as $U=\Pi_{j\in\mathbb{N}}U_j$, where U_j eliminates off-diagonal terms up to (and including) order ε_0^j. Each transformation is of the form $U_j=e^{\imath W_j}$ for a Hermitian bounded W_j whose coefficients are of order ε_0^j. We use the Baker–Hausdorff formula

$$e^{-\imath A}Be^{\imath A}=\sum_{r\in\mathbb{Z}_+}\frac{\imath^r}{r!}[B,A]_r, \tag{24a}$$

$$[B,A]_0=B, \tag{24b}$$

$$[B,A]_{r+1}=[[B,A]_r,A] \tag{24c}$$

in order to find W_j. In fact, in the jth step we will only have to consider the terms up to order ε_0^j in this formula, which are the terms $r=0$ and $r=1$. This gives us

$$\mathcal{O}_1+\imath[\mathcal{D}_1,W_1]=0,$$

which reads as follows for the coefficients:

$$W_1(m,n;l,k)=0 \quad \text{for } m>0, \tag{25a}$$

$$W_1(0,n;l,k)=\mathcal{O}_1(0,n;l,k)+\imath[\mathcal{D}_1(0,n;0,n)-\mathcal{D}_1(l,k;l,k)]W_1(0,n;l,k) \quad \text{for } m=0. \tag{25b}$$

Because of

$$|\mathcal{D}_1(0,n;0,n)-\mathcal{D}_1(l,k;l,k)|>B_cl-\tfrac{1}{2}\varepsilon_0^2(\|\widetilde{A^0}_{0,0}\|_\infty+\|\widetilde{A^0}_{l,l}\|_\infty)-\varepsilon_0(\|A^0{}_{0,0}\|_\infty+\|A^0{}_{l,l}\|_\infty)$$
$$-\tfrac{1}{2}\varepsilon_1^2(\|\widetilde{A^{1(0)}}_{0,0}\|_\infty+\|\widetilde{A^{1(0)}}_{l,l}\|_\infty)-\varepsilon_1(\|\widehat{A^{1(0)}}_{0,0}\|_\infty+\|\widehat{A^{1(0)}}_{l,l}\|_\infty)>\tfrac{1}{2}B_cl$$

we can choose ε_0 small enough so that for all $l>0$ there is no small denominator problem when solving Eq. (25b) for W_1.

Defining $H_2=U_1^*HU_1$ and repeating the above-mentioned steps we arrive at the following:

Lemma 2: We define W_j inductively by $[\mathcal{D}_j,W_j]=\imath\mathcal{O}_j$ as in (25a), (25b), and furthermore $U_j=e^{\imath W_j}$, $H_{j+1}=U_j^*H_jU_j$. Then we have the following.

Closeness to diagonal operator:

$$\|\mathcal{D}_j(m,n;m,n)-[B_c(\tfrac{1}{2}+m)-\varepsilon_0A^0_{m,m}]\|_{C^2(S^1)}<\varepsilon_0\delta_j. \tag{26}$$

Off-diagonal smallness:

$$\sum_{l\in\mathbb{Z}_+}\|\mathcal{O}_j(0,n;l,n)\|_{C^2(S^1)}(l^s+1)<\gamma_j, \tag{27a}$$

$$\sum_{k\in\mathbb{Z}\setminus\{n\}}\sum_{l\in\mathbb{Z}_+}\|\mathcal{O}_j(0,n;l,k)\|_{C^2(S^1)}e^{2\delta|n-k|}(l^s+1)<\varepsilon_1\gamma_j. \tag{27b}$$

Smallness of mixed terms:

$$\sum_{l\in\mathbb{Z}_+}\|\mathcal{M}_j(m,n;l,n)\|_{C^2(S^1)}(l^s+1)<(m^{s+1}+1)\delta_j, \tag{28a}$$

$$\sum_{k\in\mathbb{Z}\setminus\{n\}}\sum_{l\in\mathbb{Z}_+}\|\mathcal{M}_j(m,n;l,k)\|_{C^2(S^1)}e^{2\delta|n-k|}(l^s+1)<(m^{s+1}+1)\varepsilon_1\delta_j. \tag{28b}$$

Furthermore, we have

$$\gamma_{j+1}=\text{const}\,\gamma_j\delta_j, \tag{29a}$$

$$\delta_{j+1}=\delta_j(1+\text{const}\,\gamma_j), \tag{29b}$$

$$W_j(0,n;l,k)\sim\frac{1}{\imath B_c}\frac{\mathcal{O}_j(0,n;l,k)}{l}\quad\text{as } l\to\infty, \tag{29c}$$

where the constants depend on s, and $\gamma_1=\delta_1=\text{const}\,\varepsilon_0$.

We will prove the induction hypothesis for $j=1$ in Sec. VI, the inductive step is a standard exercise.

Remark 7: Note that we keep using the same hypotheses as in Theorem 1.

Remark 8: As a consequence of the recursive relations (29a), (29b) one gets inductively

$$\delta_j<\text{const}_s\,\varepsilon_0,$$

$$\gamma_j<(\text{const}_s\,\varepsilon_0)^j$$

because

$$\delta_{j+1}=\delta_j(1+\text{const}\,\gamma_j)=\delta_j+\text{const}\,\gamma_{j+1}=\cdots=\text{const}\sum_{i=1}^{j+1}\gamma_i$$

$$<\text{const}\sum_{i=1}^{j+1}(\text{const}\,\varepsilon_0)^i<\text{const}\frac{\text{const}\,\varepsilon_0}{1-\text{const}\,\varepsilon_0}<\text{const}\,\varepsilon_0,$$

where the "const" denote possibly different constants.

VI. ESTIMATES

In order to prove Lemma 2 we only need to check the assertion for $j=1$ where we have the following nonvanishing matrix elements:

$$\mathcal{D}_1(m,n;m,n)=B_c(\tfrac{1}{2}+m)+\tfrac{1}{2}\varepsilon_0^2\widetilde{A^0}_{m,m}(\beta(\xi+n))-\varepsilon_0A^0_{m,m}(\beta(\xi+n))$$
$$+\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(0)}}_{m,m}(\beta(\xi+n))-\varepsilon_1\widehat{A^{1(0)}}_{m,m}(\beta(\xi+n)), \tag{30a}$$

$$\mathcal{M}_1(m,n;l,k)\overset{n\neq k}{=}\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(n-k)}}_{m,l}(\beta(\xi+n))-\varepsilon_1\widehat{A^{1(n-k)}}_{m,l}(\beta(\xi+n)), \tag{30b}$$

$$\mathcal{M}_1(m,n;l,n)=\tfrac{1}{2}\varepsilon_0^2\widetilde{A^0}_{m,l}(\beta(\xi+n))-\varepsilon_0A^0_{m,l}(\beta(\xi+n))+\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(0)}}_{m,l}(\beta(\xi+n))$$
$$-\varepsilon_1\widehat{A^{1(0)}}_{m,l}(\beta(\xi+n)), \tag{30c}$$

$$\mathcal{O}_1(m,n;0,n)=\tfrac{1}{2}\varepsilon_0^2\widetilde{A^0}_{m,0}(\beta(\xi+n))-\varepsilon_0A^0_{m,0}(\beta(\xi+n))+\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(0)}}_{m,0}(\beta(\xi+n))$$
$$-\varepsilon_1\widehat{A^{1(0)}}_{m,0}(\beta(\xi+n)), \tag{30d}$$

$$\mathcal{O}_1(m,n;0,k)\overset{n\neq k}{=}\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(n-k)}}_{m,0}(\beta(\xi+n))-\varepsilon_1\widehat{A^{1(n-k)}}_{m,0}(\beta(\xi+n)). \tag{30e}$$

Note that we may assume $\widehat{A^{1(0)}}_{m,l}=0$; we can always achieve this by changing A^1 by a function of y only, this does not change B. $\widetilde{A^{1(0)}}_{m,l}=0$ cannot be made to disappear in the same way because it involves the average of $(A^1)^2$ instead of A^1.

If we rewrite the induction hypotheses (26)–(29c) in terms of the coefficients of the vector potential we get

$$\sum_{l\in\mathbb{Z}_+} \left\| \tfrac{1}{2}\varepsilon_0^2\widetilde{A^0}_{m,l}(\beta(\xi+n))-\varepsilon_0 A^0_{m,l}(\beta(\xi+n))+\tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(0)}}_{m,l}(\beta(\xi+n))-\varepsilon_1\widehat{A^{1(0)}}_{m,l}(\beta(\xi+n))\right\| < \text{const}\,\varepsilon_0(m^{s+1}+1), \tag{31a}$$

$$\sum_{k\in\mathbb{Z}}\sum_{l\in\mathbb{Z}_+} \left\| \tfrac{1}{2}\varepsilon_1^2\widetilde{A^{1(n-k)}}_{m,l}(\beta(\xi+n))-\varepsilon_1\widehat{A^{1(n-k)}}_{m,l}(\beta(\xi+n))\right\| e^{2\delta|n-k|} < \text{const}\,\varepsilon_1(m^{s+1}+1). \tag{31b}$$

Since the vector potentials A^0, A^1 are periodic in y, inequalities of the type (31a) and (31b) can be derived independently for the individual terms appearing there from the smoothness (analyticity) assumption and estimates for

$$\int_{\mathbb{R}} e^{\imath\eta y}\Omega_m(y)\Omega_l(y)\,dy$$

in η. For this we can use the estimates from the case of constant magnetic field (Dinaburg *et al.*, 1997, lemmata 6–8). Because of our Remark 4 there are no new estimates to prove.

Finally, we note that the asymptotic equation (29c) follows from

$$|\mathcal{D}_1(0,n;0,n)-\mathcal{D}_1(l,k;l,k)+lB_c| < \varepsilon_0\,\text{const},$$

which implies

$$\frac{1}{\mathcal{D}_1(0,n;0,n)-\mathcal{D}_1(l,k;l,k)} \sim -\frac{1}{B_c l}$$

for $l\to\infty$.

VII. FINISHING THE PROOF

The columns of the tranformation U define new basis vectors $b_{\xi,n,m}, n\in\mathbb{Z}, m\in\mathbb{Z}_+$. From the induction hypothesis (27b) we get

$$|b_{\xi,n,m}|(m^{N+1}+1)e^{2\delta|n-j|} < \text{const}. \tag{32}$$

This implies that for each m, we can apply the main results of Dinaburg (1997) to the operator H_m, which is an ergodic family (in ξ) of difference operators with exponentially decaying almost periodic coefficients. As a consequence we get Sec. III and the eigenfunction expansion in Sec. IV, Eqs. (21) and (22), of Theorem 2.

Uniform convergence of (22) and its derivatives follows from (32) and the relation (16a) for the derivatives. As in (Dinaburg *et al.*, 1997), (32) also gives the estimate on the rate of decay in y, (23).

Finally, from Sec. III we know that, for almost every ξ, the spectrum of $H_{m,\xi}$ is given by $(\lambda_m(\beta(\xi+n)))_{n\in\mathbb{Z}}$. If $E_{\xi,m,n}$ are the corresponding eigenspaces, then $E_{m,n}:=\int^{\oplus} E_{\xi,m,n}\,d\xi$ are invariant subspaces such that the restriction of H to $E_{m,n}$ is unitarily equivalent to multiplication with the function $\xi\mapsto\lambda_m(\beta(\xi+n))$. On the other hand, $H_m=\oplus_{n\in\mathbb{Z}}E_{m,n}$. Therefore, since $H_m=\int^{\oplus}H_{m,\xi}\,d\xi$, the operator H_m is unitarily equivalent to multiplication with the function λ_m.

This together with the quantitive estimate (20) finally gives the assertion in Sec. V about the measure of the spectrum.

ACKNOWLEDGMENT

We thank Leonid Friedlander for fruitful discussions and exchange of ideas.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Wave function confinement via transfer matrix methods

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(Received 21 August 2002; accepted 11 December 2002)

The exact transfer matrix approach used in studying sectionally constant potentials in one dimension is generalized to cylindrical and spherical geometries, where the potential depends only on radius. In each geometry two transfer matrices suffice to completely describe the wave function: one for handling a discontinuity in potential and one for handling a delta-function potential barrier. This method is then applied to the problem of confining a wave function in a cylindrical configuration using only a series of carefully placed delta function potential barriers. It is found that confinement can be made to increase nearly exponentially with the number of barriers if placed correctly, but that this arrangement has an exponentially sharp dependence on both barrier position and energy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1554763]

I. INTRODUCTION

It is a well known result in one-dimensional quantum mechanics that a lattice of evenly spaced potential barriers, such as delta functions, can give rise to bands of perfect transmission by particles with energies in allowable ranges, even when that energy is significantly less than the potentials involved in the lattice. This is due to how the boundary conditions imposed on the particle's wave function by the laws of quantum mechanics give rise to resonances. It seems like it should be possible to exploit this feature of wave mechanics in geometries other than that of planar lattices. For example, can an arrangement of cylindrically symmetric concentric barriers be found that amplifies the probability for a particle of a particular energy to be found in the interior region of the barriers? The same question could be asked of an arrangement of spherically symmetric barriers. In seeking to answer this question we found that it was necessary to extend a particularly useful method used in studying one-dimensional planar quantum system to cylindrical and spherical geometries: namely, the method of transfer matrices.

Transfer matrices have long been used in studying one-dimensional scattering problems not only in quantum mechanics,[1–5] but in electrodynamics and optics as well. The primary advantage of using transfer matrices is the systematic manner in which wave functions are matched at potential boundaries. This allows for systematic calculation of scattering parameters such as transmittance and reflectance. The ease with which the approach can be implemented on a computer allows calculations with large numbers of barriers that would be otherwise intractable. Walker and Gathright's article[5] provides a thorough survey of the principals and methods involved. It turns out that the basic idea can be extended to cylindrical and spherical systems. This has recently been done for the electromagnetic problem[6,7] while the corresponding problem in quantum mechanics has only been briefly covered. One study[8] develops the transfer matrices for the spherical case, while another[9] makes some use of cylindrical transfer matrices in investigating a double barrier problem. Neither study presents the general transfer matrix for the planar/cylindrical/spherical problem, nor do either of them derive the transfer matrix for a delta function potential. Both

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problems are addressed here. It is found that, independent of geometry, two matrices suffice to completely describe the propagation of the wave function: one for transferring over a discontinuity in the potential and one for transferring over a delta function barrier. In the general formulation it is no longer possible to separate out the propagation matrix from the other two matrices as is done for the planar case in Ref. 5. Each matrix is dependent on where the discontinuity or delta function is located. Hence we lose some of the power of planar transfer matrices. Nevertheless, the matrices developed are fully rigorous and applicable to any quantum system possessing the necessary symmetries.

In the first section of this article we present the derivation of the generalized transfer matrices and highlight some of their important properties. We then consider the question of confinement in a cylindrically symmetric system composed of an array of delta function potentials. We make use of the transfer matrices developed to find a configuration of barriers that gives near optimal confinement. We also develop the analogous problem in a planar system for purposes of comparison. We then provide some numerical results for the confinement problem obtained from our solution. Finally, in the appendixes we highlight some properties of the algebraic group that arises when studying generalized transfer matrices.

II. MATRIX DEVELOPMENT

Consider the dimensionless version of the time independent Schrödinger equation

$$\nabla^2\psi(\mathbf{r})+\rho^2(e-v)\psi(\mathbf{r})=0. \tag{1}$$

Here the constant ρ is given by

$$\rho=\frac{\sqrt{2mV_0}}{\hbar}a_0,$$

where V_0 and a_0 are the units of energy and length, respectively. The quantities $\mathbf{r}$, e, and v in (1) are given by taking their dimensional counterparts and dividing by a_0 or V_0 as appropriate. We phrase the problem in dimensionless terms in order to ease computer implementation (for which the transfer matrix method is particularly well suited). In a region where v is constant, Eq. (1) is simply Helmholtz's equation with $k=\rho\sqrt{e-v}$:

$$(\nabla^2+k^2)\psi(\mathbf{r})=0. \tag{2}$$

Using separation of variables[10] gives the radial equations

$$\left[\frac{d^2}{dr^2}+k^2\right]\psi(r)=0, \quad n=1, \tag{3a}$$

$$\left[\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+k^2-\frac{\nu^2}{r^2}\right]\psi(r)=0, \quad n=2, \tag{3b}$$

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{\ell(\ell+1)}{r^2}\right]\psi(r)=0, \quad n=3, \tag{3c}$$

where ν and ℓ are the azimuthal quantum numbers and n indicates whether we are working in planar $(n=1)$, cylindrical $(n=2)$, or spherical $(n=3)$ coordinates. The general solution to (3) can be written as

$$\psi(r)=A\phi(r)+B\chi(r), \tag{4}$$

where $\phi(r)$ and $\chi(r)$ are linearly independent solutions. Of the possible choices for $\phi(r)$ and $\chi(r)$ we will use forms that represent outgoing and incoming waves, respectively:

$$\phi(r)=e^{ikr}, \quad \chi(r)=e^{-ikr}, \quad n=1, \tag{5a}$$

$$\phi(r)=H_\nu^{(1)}(kr), \quad \chi(r)=H_\nu^{(2)}(kr), \quad n=2, \tag{5b}$$

$$\phi(r)=h_\ell^{(1)}(kr), \quad \chi(r)=h_\ell^{(2)}(kr), \quad n=3, \tag{5c}$$

where H_ν and h_ℓ are the cylindrical and spherical Hankel functions. We make this choice simply because scattering problems are best phrased in terms of incoming and outgoing waves. However, the transfer matrices we will derive are independent of the choice made for $\phi(r)$ and $\chi(r)$.

A. Discontinuity

Suppose we have a discontinuity in the potential at $r=a$. Say that it rises from v_1 to v_2. We demand that the radial wave function and its first derivative be continuous at $r=a$:

$$\psi_1(a)=\psi_2(a),$$

$$\psi_1'(a)=\psi_2'(a).$$

These conditions can be written nicely in a matrix form:

$$\begin{pmatrix} \phi_1 & \chi_1 \\ \phi_1' & \chi_1' \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}=\begin{pmatrix} \phi_2 & \chi_2 \\ \phi_2' & \chi_2' \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{6}$$

where everything is evaluated at $r=a$. Note that the subscripts on the functions refer to the constant k. Thus $\phi_i(a)$ has $k=k_i=\rho\sqrt{e-v_i}$. To simplify we introduce the following notation:

$$\mathbf{M}_i(a)\equiv\begin{pmatrix} \phi_i(a) & \chi_i(a) \\ \phi_i'(a) & \chi_i'(a) \end{pmatrix}, \quad \mathbf{\Psi}_i\equiv\begin{pmatrix} A_i \\ B_i \end{pmatrix}.$$

Thus (6) can be rewritten as

$$\mathbf{M}_1(a)\mathbf{\Psi}_1=\mathbf{M}_2(a)\mathbf{\Psi}_2. \tag{6'}$$

Solving for $\mathbf{\Psi}_2$, we get

$$\mathbf{\Psi}_2=\mathbf{M}_2^{-1}(a)\mathbf{M}_1(a)\mathbf{\Psi}_1. \tag{7}$$

This gives us the desired transfer matrix for going from region 1 to region 2:

$$\begin{aligned}\mathbf{\Gamma}_n\equiv\mathbf{M}_2^{-1}(a)\mathbf{M}_1(a)&=\frac{1}{\phi_2\chi_2'-\phi_2'\chi_2}\begin{pmatrix} \chi_2' & -\chi_2 \\ -\phi_2' & \phi_2 \end{pmatrix}\begin{pmatrix} \phi_1 & \chi_1 \\ \phi_1' & \chi_1' \end{pmatrix} \\ &=\frac{1}{\phi_2\chi_2'-\phi_2'\chi_2}\begin{pmatrix} \phi_1\chi_2'-\phi_1'\chi_2 & \chi_1\chi_2'-\chi_1'\chi_2 \\ \phi_2\phi_1'-\phi_2'\phi_1 & \phi_2\chi_1'-\phi_2'\chi_1 \end{pmatrix}.\end{aligned} \tag{8}$$

Again, everything is evaluated at $r=a$. We can simplify the notation somewhat if we introduce a generalized Wronskian:

$$\mathfrak{m}(\phi_i,\chi_j)\equiv\phi_i\chi_j'-\phi_i'\chi_j. \tag{9}$$

When $i=j$, this generalized Wronskian is just the normal Wronskian. For the particular forms of $\phi(r)$ and $\chi(r)$ we have chosen, the normal Wronskian is given by

$$\mathfrak{m}(\phi_i,\chi_i)=\begin{cases} -2ik_i, & n=1,\\ -\dfrac{4i}{a\pi}, & n=2,\\ -\dfrac{2i}{a^2k_i}, & n=3. \end{cases} \tag{10}$$

Note that none of these are ever zero since we deliberately choose $\phi(r)$ and $\chi(r)$ to be linearly independent solutions. With this notation we can rewrite (8) as

$$\mathbf{\Gamma}_n=\frac{1}{\mathfrak{m}(\phi_2,\chi_2)}\begin{pmatrix} \mathfrak{m}(\phi_1,\chi_2) & \mathfrak{m}(\chi_1,\chi_2)\\ \mathfrak{m}(\phi_2,\phi_1) & \mathfrak{m}(\phi_2,\chi_1)\end{pmatrix}. \tag{11}$$

Any solution to (4) can be used in the above expression for the discontinuity transfer matrix. For reference, the explicit components of $\mathbf{\Gamma}_n$ for each n and for the $\phi(r)$ and $\chi(r)$ that we have chosen are listed in Appendix B.

B. Delta function barrier

Now suppose we have two shells separated by a delta function barrier at $r=a$:

$$v(r)=\frac{\alpha}{c_n r^{n-1}}\,\delta(r-a),$$

where the constant c_n is given by

$$c_n=\begin{cases} 1, & n=1,\\ 2\pi, & n=2,\\ 4\pi, & n=3, \end{cases}$$

and α is the strength of the barrier. We still demand that the radial wave function be continuous at the boundary, but the first derivative will suffer a discontinuity due to the delta function. We can calculate the discontinuity by integrating (1) from $r=a-\epsilon$ to $r=a+\epsilon$:

$$0=c_n\int_{a-\epsilon}^{a+\epsilon}\mathrm{d}r\;\; r^{n-1}\times\left[\frac{d^2}{dr^2}+\frac{n-1}{r}\frac{d}{dr}+\frac{\gamma_n}{r^2}+\rho^2(e-v(r))\right]\psi(r),$$

where γ_n is given by

$$\gamma_n=\begin{cases} 0, & n=1,\\ \nu^2, & n=2,\\ \ell(\ell-1), & n=3. \end{cases}$$

First, note that the integral over the terms involving e and γ_n will vanish due to the continuity of ψ. If we rewrite the remaining terms slightly, we get

$$\int_{a-\epsilon}^{a+\epsilon}\frac{d}{dr}\left(r^{n-1}\frac{d}{dr}\psi(r)\right)\mathrm{d}r=\int_{n-\epsilon}^{a+\epsilon}\rho^2 v(r)\psi(r)r^{n-1}\mathrm{d}r=\frac{\alpha\rho^2}{c_n}\int_{a-\epsilon}^{a+\epsilon}\psi(r)\,\delta(r-a)\,\mathrm{d}r.$$

Integrating both sides gives us

$$r^{n-1}\frac{d}{dr}\psi(r)\Big|_{a-\epsilon}^{a+\epsilon}=\frac{\alpha\rho^2}{c_n}\psi(a),$$

$$\psi_2'(a)-\psi_1'(a)=\frac{\alpha\rho^2}{c_n a^{n-1}}\psi(a),$$

$$\psi_2'(a)-\psi_1'(a)=\frac{\alpha\rho^2}{2c_n a^{n-1}}(\psi_1(a)+\psi_2(a)),$$

the last line holding since ψ is continuous at $r=a$. We rewrite this as

$$\psi_1'(a)+\zeta_n\psi_1(a)=\psi_2'(a)-\zeta_n\psi_2(a), \tag{12}$$

where

$$\zeta_n=\frac{\alpha\rho^2}{2c_n a^{n-1}}. \tag{13}$$

Again we can write the boundary conditions on ψ at $r=a$ in a convenient matrix form,

$$\begin{pmatrix} \phi & \chi \\ \phi'+\zeta_n\phi & \chi'+\zeta_n\chi \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}=\begin{pmatrix} \phi & \chi \\ \phi'-\zeta_n\phi & \chi'-\zeta_n\chi \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{14}$$

where everything is evaluated at $r=a$. We introduce the following notation:

$$\mathbf{N}_{\pm}(a)\equiv\begin{pmatrix} \phi(a) & \chi(a) \\ \phi'(a)\pm\zeta_n\phi(a) & \chi'(a)\pm\zeta_n\chi(a) \end{pmatrix}.$$

We can then rewrite (14) as

$$\mathbf{N}_+(a)\mathbf{\Psi}_1=\mathbf{N}_-(a)\mathbf{\Psi}_2. \tag{14'}$$

Solving for $\mathbf{\Psi}_2$ we have

$$\mathbf{\Psi}_2=\mathbf{N}_-^{-1}(a)\mathbf{N}_+(a)\mathbf{\Psi}_1. \tag{15}$$

We now have the desired transfer matrix for going from region 1 to region 2 over a delta function barrier:

$$\begin{aligned}\mathbf{\Delta}_n\equiv\mathbf{N}_-^{-1}(a)\mathbf{N}_+(a)&=\frac{1}{\mathfrak{m}(\phi,\chi)}\begin{pmatrix} \chi'-\zeta_n\chi & -\chi \\ -\phi'+\zeta_n\phi & \phi \end{pmatrix}\begin{pmatrix} \phi & \chi \\ \phi'+\zeta_n\phi & \chi'+\zeta_n\chi \end{pmatrix}\\ &=\mathbb{1}-\frac{2\zeta_n}{\mathfrak{m}(\phi,\chi)}\begin{pmatrix} \phi\chi & \chi\chi \\ -\phi\phi & -\phi\chi \end{pmatrix},\end{aligned} \tag{16}$$

where again everything is evaluated at $r=a$. As we explained above the Wronskian is never zero, so this matrix always exists. For convenience we define the constant

$$\xi_n=-i\frac{2\zeta_n}{\mathfrak{m}(\phi,\chi)}, \tag{17}$$

and write the delta function transfer matrix as

$$\mathbf{\Delta}_n=\mathbb{1}-i\xi_n\begin{pmatrix} \phi\chi & \chi^2 \\ -\phi^2 & -\phi\chi \end{pmatrix}. \tag{18}$$

For the $\phi(r)$ and $\chi(r)$ listed in (5) the constant ξ_n is given by

$$\xi_n = \begin{cases} \dfrac{\rho^2\alpha}{2k}, & n=1, \\ \dfrac{\rho^2\alpha}{8}, & n=2, \\ \dfrac{\rho^2\alpha k}{8\pi}, & n=3. \end{cases} \tag{19}$$

Note that when k is real, ξ_n is also real. Recall that k will be real (and positive) when the potential v is less than the particle energy e. When this is true $\phi(r)$ and $\chi(r)$ will be complex conjugates, and (18) can be put into a more convenient form:

$$\mathbf{\Delta}_n = \begin{pmatrix} 1-i\xi_n|\phi|^2 & -i\xi_n(\phi^*)^2 \\ i\xi_n\phi^2 & 1+i\xi_n|\phi|^2 \end{pmatrix}. \tag{20}$$

C. Properties

By exploiting a few simple symmetry and conservation properties, we can make some general statements about the transfer matrices linking various regions without resorting to explicit calculations.[1,11–13] Recall that the probability current density in the radial direction is given by

$$j_r = -\frac{i\hbar}{2m}\left(\psi^*\frac{d\psi}{dr} - \psi\frac{d\psi^*}{dr}\right). \tag{21}$$

When ψ is of the form (4) with $\phi(r)=\chi(r)^*$ $(e>v)$ we can express this current as a sum of incident and reflected current densities (without any interference terms):

$$j_r = -\frac{i\hbar}{2m}(|A|^2-|B|^2)\left(\phi^*\frac{d\phi}{dr} - \phi\frac{d\phi^*}{dr}\right). \tag{22}$$

Probability flux conservation requires that the quantity $|A|^2-|B|^2$ be invariant in regions of the same potential [so that $\phi(r)$ is the same]. This, in turn, imposes the restriction

$$M^\dagger\sigma_z M = \sigma_z \tag{23}$$

on the transfer matrices linking two such regions. In addition, the principle of symmetry under time reversal requires that the transfer matrix M satisfy

$$M^* = \sigma_x M \sigma_x . \tag{24}$$

The matrices σ_z and σ_x in these equations are the usual Pauli spin matrices (though, of course, no spin is involved here). Together these two conditions require that the transfer matrix linking any two regions of the same potential (less than e) must belong to the pseudo-unitary group SU(1,1). Every matrix in this group can be written in the form

$$\begin{pmatrix} a & b^* \\ b & a^* \end{pmatrix} \quad \text{with} \quad |a|^2-|b|^2=1. \tag{25}$$

Pseudo-unitary matrices are less common, and hence less familiar to physicists, than unitary or Hermitian matrices. Some of the relevant properties of this group are reviewed in Appendix A as well as in Ref. 11.

It happens to be the case that the determinant of a matrix connecting two regions of the same potential is equal to unity regardless of the value of the potential v. An explicit calculation will show that the determinants of the transfer matrices given in (11) and (18) are

$$\det(\mathbf{\Gamma}_n) = \frac{\mathfrak{m}(\phi_1, \chi_1)}{\mathfrak{m}(\phi_2, \chi_2)}, \tag{26a}$$

$$\det(\mathbf{\Delta}_n) = 1. \tag{26b}$$

According to Eq. (10) the determinant of $\mathbf{\Gamma}_n$ depends only on the ratio k_1/k_2. By taking a product of discontinuity and delta function transfer matrices one can see that the determinant of an arbitrary transfer matrix linking a region at potential v_1 to a region at potential v_2 depends only on the ratio k_1/k_n.

As a check on the logical consistency of the arguments leading to the expressed forms for the transfer matrices one should verify that they give reasonable answers in certain limits. First off, if one transfers over a discontinuity of zero height or over a delta function barrier of zero strength one would expect to get the identity for a transfer matrix. Inspection of (11) and (18) shows that this is the case:

$$\mathbf{\Gamma}_n(v, v, a) = \mathbb{1}, \tag{27a}$$

$$\mathbf{\Delta}_n(v, 0, a) = \mathbb{1}. \tag{27b}$$

Physical intuition also suggests expected inverses for the various transfer matrices. Namely jumping from v_2 to v_1 should cancel a transfer from v_1 to v_2 at the same location, and a transfer over a $-\alpha$ strength delta function should cancel a transfer over an α strength delta function at the same location. A slightly longer inspection will reveal this to be the case:

$$\mathbf{\Gamma}_n^{-1}(v_1, v_2, a) = \mathbf{\Gamma}_n(v_2, v_1, a), \tag{28a}$$

$$\mathbf{\Delta}_n^{-1}(v, \alpha, a) = \mathbf{\Delta}_n(v, -\alpha, a). \tag{28b}$$

III. WAVE FUNCTION CONFINEMENT

Consider a cylindrically symmetric potential in two dimensions that is zero everywhere except in some annular region centered at the origin. One can pose the question of how to configure the potential in that region to maximally amplify an incoming matter wave so as to effectively trap it in the center region. Given the infinite number of ways in which one might configure a potential, this could be a very difficult problem. We will consider only a very restricted subcase. Namely we will allow our potential to consist of only delta function potential barriers of all the same strength, so that the only free parameters are the number of barriers and their locations. Furthermore, we will assume that the incoming matter wave is cylindrically symmetric: $\nu = 0$. In order to attack this problem we must first make precise what we mean by maximally confining a wave function in the internal region.

Let us suppose that our potential has m delta function barriers. There are then $m+1$ regions: the internal region containing the origin, the external region containing infinity and $m-1$ interbarrier regions (see Fig. 1). In each region we will assume that $\psi(r)$ is written in the form (4) with ϕ and χ as given in (5b). We label the coefficients in the internal region A_0 and B_0, and successively label the coefficients in each region by A_j and B_j. The coefficients in the external region are then A_m and B_m. Since the imaginary parts of the Hankel functions go to infinity at the origin we must have

$$A_0 = B_0 \tag{29}$$

to insure that the wave function be physical.

According to (22) the total probability current in the internal region must then be zero. That is, any probability that enters that region must eventually be reflected back out. By conservation of probability the total current in each successive region must also be zero. This in turn implies that

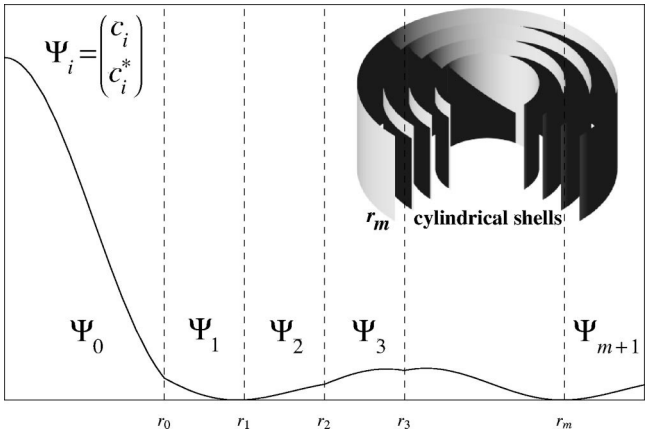

FIG. 1. A cylindrical setup with m barriers at radii r_i and corresponding wave functions $\mathbf{\Psi}_i$.

$|A_j| = |B_j|$ for each j in the range $[0,m]$. Specifically, we must have $|A_m| = |B_m|$. Any incoming matter wave will eventually be reflected back out. We can then define the confinement coefficient as the ratio of internal to external probability amplitudes:

$$\mathcal{C} \equiv \frac{|A_0|^2}{|A_m|^2} = \frac{|B_0|^2}{|B_m|^2}. \tag{30}$$

It is this quantity that we wish to maximize by choosing m positions at which to place the barriers. We will label these optimal positions r_0 through r_{m-1}. At each of these positions there will be a corresponding delta function transfer matrix connecting the coefficients in the adjoining regions:

$$\mathbf{\Psi}_{j+1} = \mathbf{\Delta}_j \mathbf{\Psi}_j .$$

Connecting the internal and external regions will be the total transfer matrix

$$\mathbf{T}_m = \mathbf{\Delta}_{m-1} \cdots \mathbf{\Delta}_1 \mathbf{\Delta}_0$$

with

$$\mathbf{\Psi}_m = \mathbf{T}_m \mathbf{\Psi}_0 . \tag{31}$$

Of course, we are free to choose the phase of the wave function at will. Equation (31) together with (29) provides a relation between the phase of A_m and that of B_m. Using this relation we can always choose the phase so that $A_m = B_m^*$ (we already know that their magnitudes are the same). As each of the delta function transfer matrices $\mathbf{\Delta}_j$ are of the form given in (25), Eq. (A12) in Appendix A guarantees that the coefficients in each region will satisfy

$$A_j = B_j^* .$$

Thus, from here onward we will denote $\mathbf{\Psi}_j$ in each region by

$$\mathbf{\Psi}_j = \begin{pmatrix} c_j \\ c_j^* \end{pmatrix}. \tag{32}$$

The confinement coefficient then becomes

$$\mathcal{C} = \frac{|c_0|^2}{|c_m|^2}. \tag{33}$$

Although we have only been talking about a cylindrical configuration, we can pose a similar problem in planar or spherical configurations. In the planar case we need only put an infinitely high barrier at the origin, so that any wave coming in from infinity is reflected back no matter what the energy. The constraint on the internal coefficients in this situation is that the wave function be exactly zero at the origin. This requires that

$$A_0 = -B_0 .$$

Thus all of our comments on zero total probability current hold in the planar case as well, and we can again choose the phase so that $A_j = B_j^*$. The spherical case is identical to the cylindrical case in form, the only real difference being that the transfer matrices have a different dependence on r. We can then summarize the necessary constraints on the internal coefficients in planar, cylindrical and spherical configurations:

$$c_0^* = -c_0 \quad \text{pure imaginary} \quad n=1,$$

$$c_0^* = c_0 \quad \text{pure real} \quad n=2,$$

$$c_0^* = c_0 \quad \text{pure real} \quad n=3.$$

Before looking specifically at any one particular geometry we will first outline the general solution, and only then examine the special cases of the planar and cylindrical configurations.

A. General solution

For m barriers we have the relation

$$\mathbf{\Psi}_m = \mathbf{T}_m(r_0, r_1, \ldots, r_{m-1})\mathbf{\Psi}_0 ,$$

where

$$\mathbf{\Psi}_0 = \begin{pmatrix} c_0 \\ c_0^* \end{pmatrix}, \quad \Psi_m = \begin{pmatrix} c_m \\ c_m^* \end{pmatrix}.$$

What we want to do is choose the r_j's so that the quantity

$$\mathcal{C} = \frac{|c_0|^2}{|c_m|^2}$$

is maximized. One can either think of this as fixing the magnitude of c_m and maximizing the internal amplitude c_0 or, equivalently, as fixing the magnitude of c_0 and minimizing that of c_m. Our point of view will typically be the latter.

Strictly speaking, this is an optimization problem in m variables. One obvious approach would be to write down the confinement coefficient as a function of the r_j's, take m partial derivatives and set them all equal to zero simultaneously. Not only does this approach become quickly intractable for more than a small number of barriers but, in general, it does not give the global minimum, only a local one.

A much simpler approach is to independently attack each successive barrier starting with the first one. That is, choose r_0 to minimize the ratio $|c_1|/|c_0|$. Having fixed r_0, choose r_1 to minimize the ratio $|c_2|/|c_1|$ and so on out to r_{m-1}, the rationale being that the product of these ratios will give a near minimal total ratio:

$$\frac{|c_m|}{|c_0|} = \frac{|c_1|}{|c_0|}\frac{|c_2|}{|c_1|}\cdots\frac{|c_m|}{|c_{m-1}|}.$$

This approach fails when choosing a suboptimal ratio $|c_j|/|c_{j-1}|$ that affects the phase of c_j in such a way as to make another ratio small enough to more than compensate for the increase in $|c_j|/|c_{j-1}|$. In the planar problem, this turns out not to be possible, so that the above approach does indeed give the optimal solution. The cylindrical and spherical cases are not so well behaved. However, trial and error suggests that while this approach is not optimal it gives fairly good results.

So now the question becomes how to find $r_j > r_{j-1}$ that minimizes the ratio $|c_{j+1}|/|c_j|$ assuming that c_j and r_{j-1} are known. We will call this ratio the *amplification ratio* at the jth barrier. It turns out that we can place some immediate bounds on the extent to which we can minimize (or maximize) such a ratio. Since $\mathbf{\Psi}_j$ is of the form

$$\mathbf{\Psi}_j = \begin{pmatrix} c_j \\ c_j^* \end{pmatrix},$$

Eq. (A25) of Appendix A tells us that $|c_j|$ is proportional to the vector norm $\|\mathbf{\Psi}_j\|$, so that the amplification ratio can be written

$$\frac{|c_{j+1}|}{|c_j|} = \frac{\|\mathbf{\Psi}_{j+1}\|}{\|\mathbf{\Psi}_j\|} = \frac{\|\mathbf{\Delta}(r)\mathbf{\Psi}_j\|}{\|\mathbf{\Psi}_j\|}. \tag{34}$$

Furthermore, from Eq. (A26) we know that this quantity will always lie between the singular values of $\mathbf{\Delta}(r)$:

$$\sigma_2(r) \leqslant \frac{\|\mathbf{\Delta}(r)\mathbf{\Psi}_0\|}{\|\mathbf{\Psi}_0\|} \leqslant \sigma_1(r). \tag{35}$$

Thus, no matter what r_j we pick we will always have

$$\frac{|c_{j+1}|}{|c_j|} \geqslant \sigma_2(r_j).$$

So before attempting to minimize the amplification ratio, we will take a look at the singular values of the delta function transfer matrix.

In the long run, the solution of this problem is facilitated by first casting the delta function transfer matrix in a slightly different form (which may appear more complicated at first). Since we are assuming here that $e > v = 0$ (so that the wave function may propagate freely) we start with Eq. (20) ($\alpha > 0$ is assumed to be given):

$$\mathbf{\Delta}(r) = \begin{pmatrix} 1 - i\xi|\phi(r)|^2 & -i\xi\phi^2(r)^* \\ i\xi\phi^2(r) & 1 + i\xi|\phi(r)|^2 \end{pmatrix},$$

and make the following definition,

$$\eta(r) = \tan^{-1}(\xi|\phi(r)|^2). \tag{36}$$

Since $\xi|\phi(r)|^2$ is always real and in the range $(0,\infty)$, $\eta(r)$ will be real and in the range $(0,\pi/2)$. Furthermore, $\eta(r)$ is either constant or a monotonically decreasing function of r for the ϕ's given in (5). From here on out we will assume that the r dependence of ϕ and η is understood, and we will not indicate it expressly.

Using (36) we proceed to write the elements of $\mathbf{\Delta}(r)$ in polar form:

$$1 + i\xi|\phi|^2 = \sqrt{1 + \xi^2|\phi|^4}\, e^{i \tan^{-1}(\xi|\phi|^2)} = \sqrt{1 + \tan^2 \eta}\, e^{i\eta} = \sec \eta\, e^{i\eta} \tag{37}$$

and

$$\phi^2 = |\phi|^2 \frac{\phi^2}{\phi^* \phi} = |\phi|^2 \frac{\phi}{\phi^*}$$

so that

$$i\xi\phi^2 = i\xi|\phi|^2 \frac{\phi}{\phi^*} = i\tan(\eta)\frac{\phi}{\phi^*}. \tag{38}$$

Equations (37) and (38) together with their complex conjugates give us the following form for $\mathbf{\Delta}(r)$:

$$\mathbf{\Delta}(r) = \begin{pmatrix} \sec(\eta)e^{-i\eta} & -i\tan(\eta)\dfrac{\phi^*}{\phi} \\ i\tan(\eta)\dfrac{\phi}{\phi^*} & \sec(\eta)e^{i\eta} \end{pmatrix}. \tag{39}$$

In this form it is easy to see that the determinant of $\mathbf{\Delta}(r)$ is unity:

$$\det(\mathbf{\Delta}(r)) = \sec^2\eta - \tan^2\eta = 1$$

Utilizing Eq. (A21) we can easily write down the singular values for $\mathbf{\Delta}(r)$:

$$\sigma_1(r) = \sec\eta + \tan\eta, \tag{40a}$$

$$\sigma_2(r) = \sec\eta - \tan\eta. \tag{40b}$$

Moreover, since the determinant of $\mathbf{\Delta}(r)$ is 1, these singular values are inverses of each other:

$$\sigma_1(r)\sigma_2(r) = 1.$$

As we remarked earlier our amplification ratio will always lie between these singular values. We can show this explicitly by finding an expression for the amplification ratio. This is facilitated by first calculating the polar decomposition of $\mathbf{\Delta}(r)$,

$$\mathbf{\Delta}(r) = \begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix} \begin{pmatrix} \sec(\eta) & -i\tan(\eta)\dfrac{\phi^*}{\phi}e^{i\eta} \\ i\tan(\eta)\dfrac{\phi}{\phi^*}e^{-i\eta} & \sec(\eta) \end{pmatrix}. \tag{41}$$

Note that the first matrix in this decomposition is unitary and that the second is Hermitian and has the same singular values as $\mathbf{\Delta}(r)$. This is the nature of the polar decomposition. Unitary matrices only rotate vectors, leaving the Hermitian matrix to do the stretching. Hence, we will focus on it. If we multiply this matrix on the right by $(c_j, c_j^*)^T$, we get

$$\begin{pmatrix} d_{j+1} \\ d_{j+1}^* \end{pmatrix} = \begin{pmatrix} \sec(\eta) & -i\tan(\eta)\dfrac{\phi^*}{\phi}e^{i\eta} \\ i\tan(\eta)\dfrac{\phi}{\phi^*}e^{-i\eta} & \sec(\eta) \end{pmatrix} \begin{pmatrix} c_j \\ c_j^* \end{pmatrix}$$

$$= \begin{pmatrix} c_j\sec(\eta) - ic_j^*\tan(\eta)\dfrac{\phi^*}{\phi}e^{i\eta} \\ c_j^*\sec(\eta) + ic_j\tan(\eta)\dfrac{\phi}{\phi^*}e^{-i\eta} \end{pmatrix}.$$

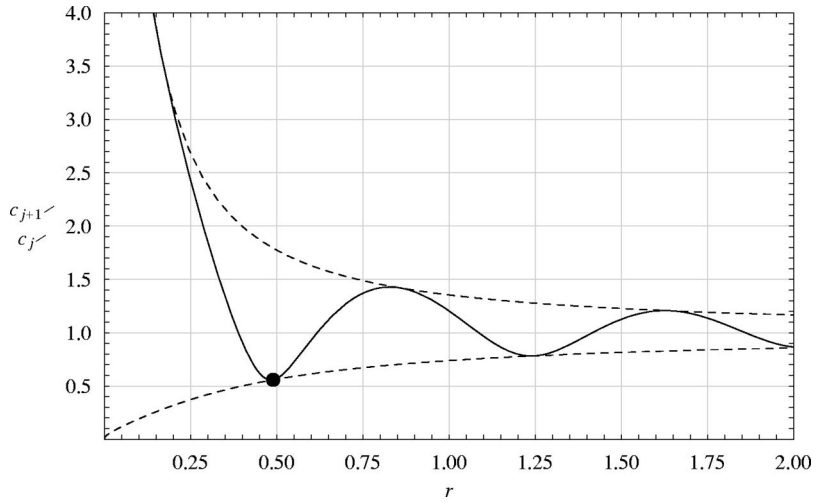

FIG. 2. Bounded amplification ratio.

We have used d_{j+1} here instead of c_{j+1} because we have not yet multiplied by the unitary matrix in (41). However, we still have $|d_{j+1}|=|c_{j+1}|$. Taking the ratio of d_{j+1} and c_j we get

$$\frac{d_{j+1}}{c_j}=\sec(\eta)-i\tan(\eta)\frac{\phi^* c_j^*}{\phi c_j}e^{i\eta}. \tag{42}$$

Now define

$$\beta(r)=-i\frac{\phi^* c_j^*}{\phi c_j}e^{i\eta}. \tag{43}$$

Note that β is of the form

$$\beta(r)=e^{i\theta(r)}, \quad |\beta|=1.$$

We can then write (42) as

$$\frac{d_{j+1}}{c_j}=\sec\eta+\beta\tan\eta. \tag{44}$$

The absolute value of this ratio is equal to our amplification ratio,

$$\frac{|d_{j+1}|}{|c_j|}=\frac{|c_{j+1}|}{|c_j|}=|\sec\eta+\beta\tan\eta|.$$

As $|\beta|=1$ this quantity clearly lies between the singular values σ_2 and σ_1:

$$\sigma_2\leqslant|\sec\eta+\beta\tan\eta|\leqslant\sigma_1. \tag{45}$$

When $\beta=-1$ the amplification ratio equals σ_2 and when $\beta=1$ the ratio equals σ_1. Figure 2 shows a typical plot of Eq. (45). The solid line is the amplification ratio, while the dashed lines are the bounding singular values σ_2 and σ_1. The point indicated in the figure is the first point at which the amplification ratio is equal to σ_2.

A more explicit form for the amplification ratio is

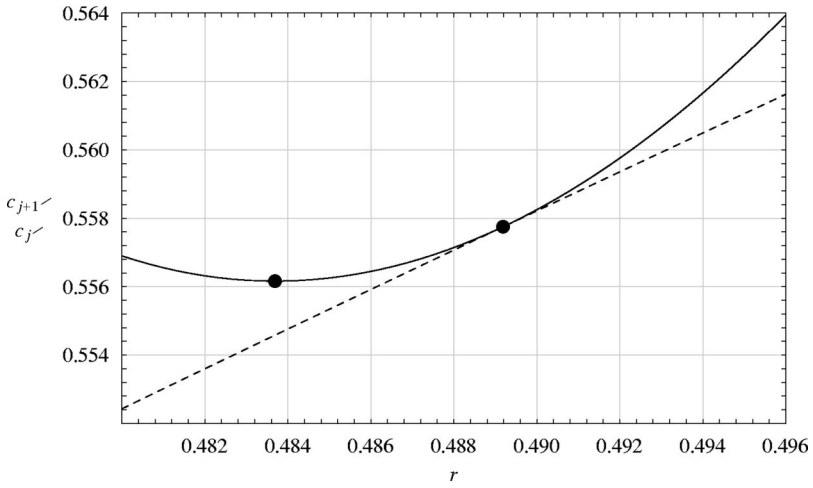

FIG. 3. The tangent point versus the true minimum.

$$\frac{|c_{j+1}|}{|c_j|}=[\sec^2\eta+\tan^2\eta+2\sec\eta\tan\eta\cos\theta]^{1/2}. \tag{46}$$

Note that choosing $\beta=-1$ ($\theta=\pi$) does not necessarily give the minimum value for the amplification ratio as η is, in general, a function of r. However, it should be clear from Fig. 2 that the true minimum will always occur very near $\beta=-1$. Figure 3 shows a blowup of the region around this point showing the true minimum versus the tangent point.

Instead of choosing the true minimum of the amplification ratio for r_j we will use the point at which the amplification ratio is equal to σ_2, the reason being that the equation determining the singular values is simpler in form than the equation determining the amplification ratio. This allows us to write down both the transfer matrix at r_j and the overall confinement coefficient in a particularly simple form.

Going back to (43) and setting $\beta=-1$ gives us the following condition on ϕ and η at r_j:

$$\frac{\phi}{\phi^*}=i\frac{c_j^*}{c_j}e^{i\eta}. \tag{47}$$

This is the critical equation that must be solved for r_j. Note that it is recursive in nature. One must first solve it for r_0 in order to find c_1, and then solve it for r_1 in order to find c_2, and so on. As the equation usually permits multiple solutions, it is the first solution larger than r_{j-1} that is chosen, as this will give the smallest ratio.

Applying this to Eq. (41) gives us the form of the transfer matrix at r_j:

$$\mathbf{\Delta}_j=\begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix}\begin{pmatrix} \sec(\eta) & -\tan(\eta)\dfrac{c_j}{c_j^*} \\ -\tan(\eta)\dfrac{c_j^*}{c_j} & \sec(\eta) \end{pmatrix}. \tag{48}$$

Knowing $\mathbf{\Delta}_j$, r_j and c_j we can find c_{j+1} and repeat the process:

$$\mathbf{\Delta}_j\begin{pmatrix} c_j \\ c_j^* \end{pmatrix}=\begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix}\begin{pmatrix} c_j\sec\eta-c_j\tan\eta \\ c_j^*\sec\eta-c_j^*\tan\eta \end{pmatrix}=\begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix}\begin{pmatrix} \sigma_2 c_j \\ \sigma_2 c_j^* \end{pmatrix}=\begin{pmatrix} \sigma_2 e^{-i\eta}c_j \\ \sigma_2 e^{+i\eta}c_j^* \end{pmatrix}=\begin{pmatrix} c_{j+1} \\ c_{j+1}^* \end{pmatrix}. \tag{49}$$

We now have a recursive function for determining the c_j's in each region (assuming all of the r_j's are known):

$$c_1 = \sigma_2(r_0) e^{-i\eta(r_0)} c_0,$$

$$c_2 = \sigma_2(r_1) e^{-i\eta(r_1)} c_1 = \sigma_2(r_0)\sigma_2(r_1) e^{-i(\eta(r_0)+\eta(r_1))} c_0,$$

$$\vdots$$

$$c_m = \left(\prod_{j=0}^{m-1} \sigma_2(r_j) e^{-i\eta(r_j)} \right) c_0, \tag{50}$$

giving us the ratio

$$\frac{|c_m|}{|c_0|} = \prod_{j=0}^{m-1} \sigma_2(r_j) \tag{51}$$

and the confinement coefficient

$$C = \frac{|c_0|^2}{|c_m|^2} = \left(\prod_{j=0}^{m-1} \sigma_1(r_j) \right)^2, \tag{52}$$

recalling that $\sigma_1(r) = \sigma_2(r)^{-1}$. By (40) we know that $\sigma_1(r)$ is always greater than 1. If η happens to be constant (as in the planar problem), then σ_1 will be constant as well and (52) reduces to

$$\mathcal{C} = \sigma_1^{2m}.$$

Here the confinement coefficient rises exponentially with the number of barriers. If η is a decreasing function of r (as is the case in cylindrical and spherical geometries), $\sigma_1(r)$ will fall and eventually approach unity as $r \to \infty$. Therefore the dependence on the number of barriers is high at first but tapers as more barriers are added.

Note that Eq. (50) also gives us an expression for the c_j / c_j^* ratio that occurs in the jth transfer matrix. This will be useful for finding an explicit form for the total transfer matrix:

$$\frac{c_j}{c_j^*} = \left(e^{-2i\Sigma_{k=0}^{j-1}\eta(r_k)}\right) \frac{c_0}{c_0^*}. \tag{53}$$

B. Planar case

As we mentioned earlier, the planar case turns out to be exactly solvable by the method of the previous section. This is largely a result of the simple fact that here η is a constant:

$$\eta(r) = \tan^{-1} \xi = \text{const.}$$

This in turn implies that singular values of the transfer matrix are also both constant:

$$\sigma_1(r) = \sec \eta + \tan \eta = \text{const},$$

$$\sigma_2(r) = \sec \eta - \tan \eta = \text{const}.$$

At each stage, therefore, we are free to choose an r_j that achieves the minimum possible amplification ratio no matter what the positions of the other barriers. The only problem remaining is whether or not we can find an exact expression for each of these r_j's. Due to the simplicity of $\phi(r)$ this, too, is possible.

Starting with (47),

$$\frac{\phi}{\phi^*} = i\frac{c_j^*}{c_j}e^{i\eta}$$

and, using the form for ϕ from (5a), we get

$$e^{2ikr_j} = i\frac{c_j^*}{c_j}e^{i\eta}.$$

We can then use Eq. (53), recalling that η is constant, to write the ratio of c_j^* and c_j as

$$\frac{c_j^*}{c_j} = e^{2ij\eta}\frac{c_0^*}{c_0} = -e^{2ij\eta}, \tag{54}$$

leaving us with

$$e^{2ikr_j} = -ie^{i(1+2j)\eta}.$$

Taking the logarithm of both sides and solving we find that

$$r_j = \frac{1}{2k}\left(\frac{3\pi}{2} + (1+2j)\tan^{-1}\xi\right). \tag{55}$$

As one might expect this gives us a constant spacing between barriers:

$$r_j - r_{j-1} = \frac{1}{k}\tan^{-1}\xi.$$

Note, however, that the distance between the origin and the first barrier (at r_0) is different than the interbarrier spacing:

$$r_0 = \frac{3\pi}{4k} + \frac{1}{2k}\tan^{-1}\xi.$$

We can write out an explicit form for the transfer matrix at the jth barrier by applying (54) to the general form (48):

$$\mathbf{\Delta}_j = \begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix}\begin{pmatrix} \sec(\eta) & \tan(\eta)e^{-2ij\eta} \\ \tan(\eta)e^{2ij\eta} & \sec(\eta) \end{pmatrix} = \mathbf{U}\mathbf{H}_j.$$

Note here that the unitary matrix $\mathbf{U}$ is independent of j by virtue of the constant nature of η. Having an expression for the individual transfer matrices we would also like to write out an explicit form for the total transfer matrix over m barriers:

$$\mathbf{T}_m = \mathbf{\Delta}_{m-1}\mathbf{\Delta}_{m-2}\cdots\mathbf{\Delta}_1\mathbf{\Delta}_0.$$

Though this may appear complicated at first, a few simple matrix manipulations will make it possible. The first step is to notice that

$$\mathbf{H}_j\mathbf{U} = \mathbf{U}\mathbf{H}_{j-1}.$$

Multiplying both sides by $\mathbf{U}^{-1}$ on the right gives

$$\mathbf{H}_j = \mathbf{U}\mathbf{H}_{j-1}\mathbf{U}^{-1} = \mathbf{U}^j\mathbf{H}_0\mathbf{U}^{-j}.$$

Applying this result to $\mathbf{\Delta}_j$ gives

$$\mathbf{\Delta}_j = \mathbf{U}^{j+1}\mathbf{H}_0\mathbf{U}^{-j}. \tag{56}$$

In this form the product of successive transfer matrices is made easier since the internal $\mathbf{U}$'s all cancel:

$$\mathbf{T}_m = \mathbf{\Delta}_{m-1}\mathbf{\Delta}_{m-2}\cdots\mathbf{\Delta}_1\mathbf{\Delta}_0 = (\mathbf{U}^m\mathbf{H}_0\mathbf{U}^{-m+1})(\mathbf{U}^{m-1}\mathbf{H}_0\mathbf{U}^{-m+2})\cdots(\mathbf{U}^2\mathbf{H}_0\mathbf{U}^{-1})(\mathbf{U}\mathbf{H}_0) = \mathbf{U}^m\mathbf{H}_0^m. \tag{57}$$

Due to their simple forms the mth powers of $\mathbf{U}$ and $\mathbf{H}_0$ are not hard to calculate:

$$\mathbf{T}_m = \begin{pmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{pmatrix}^m \begin{pmatrix} \sec\eta & \tan\eta \\ \tan\eta & \sec\eta \end{pmatrix}^m = \frac{1}{2}\begin{pmatrix} e^{-im\eta} & 0 \\ 0 & e^{im\eta} \end{pmatrix}\begin{pmatrix} \sigma_1^m+\sigma_2^m & \sigma_1^m-\sigma_2^m \\ \sigma_1^m-\sigma_2^m & \sigma_1^m+\sigma_2^m \end{pmatrix}. \tag{58}$$

We have inadvertently given the polar decomposition of the total transfer matrix as $\mathbf{U}^m$ is unitary and $\mathbf{H}_0^m$ is Hermitian (actually symmetric) and positive-definite. Taking this matrix and operating on $\mathbf{\Psi}_0$ we expect to recover the confinement coefficient:

$$\mathbf{T}_m\begin{pmatrix} i \\ -i \end{pmatrix} = \begin{pmatrix} i\sigma_2^m e^{-im\eta} \\ -i\sigma_2^m e^{im\eta} \end{pmatrix}$$

and as expected

$$\mathcal{C} = \left(\frac{1}{\sigma_2^m}\right)^2 = \sigma_1^{2m}.$$

In terms of ξ this is

$$\mathcal{C} = (\sqrt{1+\xi^2}+\xi)^{2m}.$$

C. Cylindrical case

The cylindrical case is necessarily more complicated than the planar one as η is no longer constant, but depends on r. More specifically it is a monotonically decreasing function of r:

$$\eta(r) = \tan^{-1}(\xi(J_\nu(kr)^2 + Y_\nu(kr)^2)).$$

In order to simplify notation we will denote η and ϕ at the jth barrier by

$$\eta_j \equiv \eta(r_j) = \tan^{-1}(\xi|\phi(r_j)|^2),$$

$$\phi_j \equiv \phi(r_j).$$

As the ratio c_0/c_0^* is 1 for the cylindrical case we can write (53) as

$$\frac{c_j^*}{c_j} = e^{2i\Sigma_{k=0}^{j-1}\eta_k}\frac{c_0^*}{c_0} = e^{2i\Sigma_{k=0}^{j-1}\eta_k}. \tag{59}$$

Our equation for determining r_j is then

$$\frac{\phi_j}{\phi_j^*} = i\frac{c_j^*}{c_j}e^{i\eta_j} = ie^{i(\eta_j+2\Sigma_{k=0}^{j-1}\eta_k)}. \tag{60}$$

Unfortunately this equation is transcendental in form and must be solved numerically for each of the r_j.

Calculating the explicit forms for the transfer matrices in the cylindrical case is more complicated as well, but here the approach used in the planar case is at least generalizable. The specific polar decomposed form for the jth transfer matrix is readily found from (59) and (48):

$$\mathbf{\Delta}_j=\begin{pmatrix} e^{-i\eta_j} & 0 \\ 0 & e^{i\eta_j} \end{pmatrix}\begin{pmatrix} \sec(\eta_j) & -\tan(\eta_j)e^{-2i\Sigma_{k=0}^{j-1}\eta_k} \\ -\tan(\eta_j)e^{2i\Sigma_{k=0}^{j-1}\eta_k} & \sec(\eta_j) \end{pmatrix}=\mathbf{U}_j\mathbf{H}_j\,.$$

Now the unitary part depends on j as expected. We would like to perform some analogous matrix manipulations to those used in the planar case in order to arrive at the total transfer matrix. More care must be taken here, though, as $\mathbf{U}$ now depends on j. We first define the matrix

$$\mathbf{S}_j=\begin{pmatrix} \sec\eta_j & -\tan\eta_j \\ -\tan\eta_j & \sec\eta_j \end{pmatrix}. \tag{61}$$

Some algebra will show that $\mathbf{H}_j$ can be written as

$$\mathbf{H}_j=(\mathbf{U}_{j-1}\mathbf{U}_{j-2}\cdots\mathbf{U}_0)\mathbf{S}_j(\mathbf{U}_{j-1}\mathbf{U}_{j-2}\cdots\mathbf{U}_0)^{-1}$$

with

$$\mathbf{H}_0=\mathbf{S}_0\,.$$

To further simplify notation we define the product matrix

$$(\Pi\mathbf{U})_j\equiv\mathbf{U}_{j-1}\mathbf{U}_{j-2}\cdots\mathbf{U}_1\mathbf{U}_0\,,$$

$$(\Pi\mathbf{U})_0\equiv\mathbb{1},$$

so that

$$\mathbf{H}_j=(\Pi\mathbf{U})_j\mathbf{S}_j(\Pi\mathbf{U})_j^{-1}. \tag{62}$$

As in the planar case, if we multiply two consecutive transfer matrices together the internal unitary matrices cancel:

$$\mathbf{\Delta}_j\mathbf{\Delta}_{j-1}=\mathbf{U}_j\mathbf{H}_j\mathbf{U}_{j-1}\mathbf{H}_{j-1}=(\Pi\mathbf{U})_{j+1}\mathbf{S}_j(\Pi\mathbf{U})_j^{-1}(\Pi\mathbf{U})_j\mathbf{S}_{j-1}(\Pi\mathbf{U})_{j-1}^{-1}=(\Pi\mathbf{U})_{j+1}\mathbf{S}_j\mathbf{S}_{j-1}(\Pi\mathbf{U})_{j-1}^{-1}.$$

Doing this for the whole sequence of transfer matrices gives us the total transfer matrix:

$$\mathbf{T}_m=(\Pi\mathbf{\Delta})_m=(\Pi\mathbf{U})_m(\Pi\mathbf{S})_m\,, \tag{63}$$

It turns out that it does not matter in which order the $\mathbf{U}_j$ matrices or $\mathbf{S}_j$ matrices are multiplied since they are self-commuting:

$$[\mathbf{U}_i,\mathbf{U}_j]=0, \tag{64a}$$

$$[\mathbf{S}_i,\mathbf{S}_j]=0. \tag{64b}$$

Again we have inadvertently arrived at a polar decomposition for the total transfer matrix. This time, however, instead of two matrices both raised to the mth power we have two products of m different matrices. Fortunately the products are not hard to compute, even if they look a bit complicated:

$$(\Pi\mathbf{U})_m=\begin{pmatrix} e^{-i(\eta_0+\cdots+\eta_{m-1})} & 0 \\ 0 & e^{i(\eta_0+\cdots+\eta_{m-1})} \end{pmatrix}, \tag{65}$$

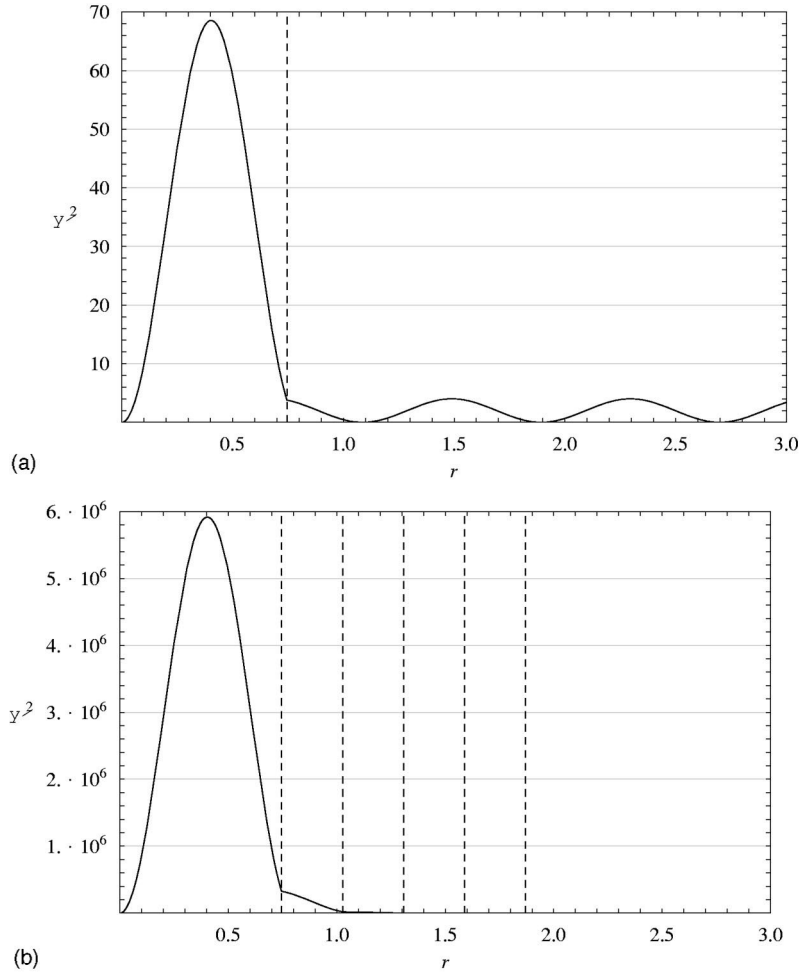

FIG. 4. A wave function in a planar configuration. Note the even spacing of the barriers. $e=1$, $\rho=3.898$.

$$(\Pi \mathbf{S})_m = \frac{1}{2}\begin{pmatrix} \prod' \sigma_{1j} + \prod' \sigma_{2j} & \prod' \sigma_{2j} - \prod' \sigma_{1j} \\ \prod' \sigma_{2j} - \prod' \sigma_{1j} & \prod' \sigma_{1j} + \prod' \sigma_{2j} \end{pmatrix}, \tag{66}$$

where Π' is shorthand for $\Pi_{j=0}^{m-1}$. Applying $\mathbf{T}_m$ to $\boldsymbol{\Psi}_0$ one obtains the confinement coefficient given in (52) as we would hope.

D. Results

Now that we have calculated explicit forms for the barrier positions and the transfer matrices for both the planar and cylindrical configurations, we can run some numerical trials and verify that we indeed have the predicted confinement.

Figures 4(a) and 4(b) show probability densities in a planar configuration. Figures 5(a), 5(b), and 6 show corresponding probability densities in a cylindrical configuration. Note here the strong dependence on ρ. Figure 7 shows how the confinement coefficient varies with the number of barriers in both planar and cylindrical configurations.

One, perhaps unexpected, result found in these numerical trials was how sensitive the confinement coefficient was to both the energy of the particle and the positions of the barriers. Figures

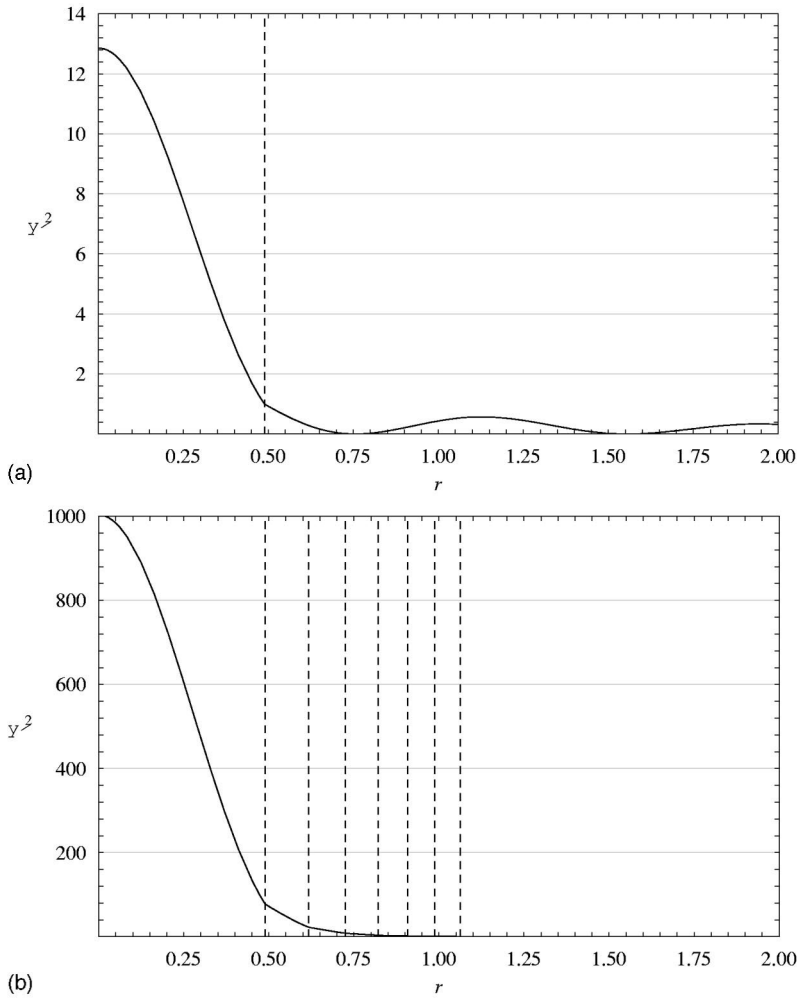

FIG. 5. A wave function in a cylindrical configuration. Note how the barrier spacing decreases with increasing r. $e=1$, $\rho=3.898$.

8(a) and 8(b) show the extremely sharp energy dependence. In general it is found for both the planar and cylindrical configurations that the higher the spike the sharper it is, much as for a sequence of functions approaching a delta function. Figures 9(a) and 9(b) show the dependence on the barrier positions for a three barrier system. As one might expect, the confinement coefficient is much more sensitive to the position of the first barrier than it is to the last. This is because each of the r_j's depend only the positions preceding it. If the first barrier position is perturbed, everything is destroyed, but if the last barrier position is perturbed, we are still guaranteed confinement at least as good as in the case of $m-1$ barriers.

IV. CONCLUSIONS

We have found that we can write down generalized transfer matrices for wave functions propagating in sectionally constant potentials in planar, cylindrical, and spherical geometries. Two matrices suffice to describe how the wave function propagates across potential boundaries: one for moving over a discontinuity in potential and one for moving past a delta function potential barrier. The form of these matrices is independent of the geometry. One simply needs to choose the appropriate linear independent solutions to the radial equation and insert these into the transfer

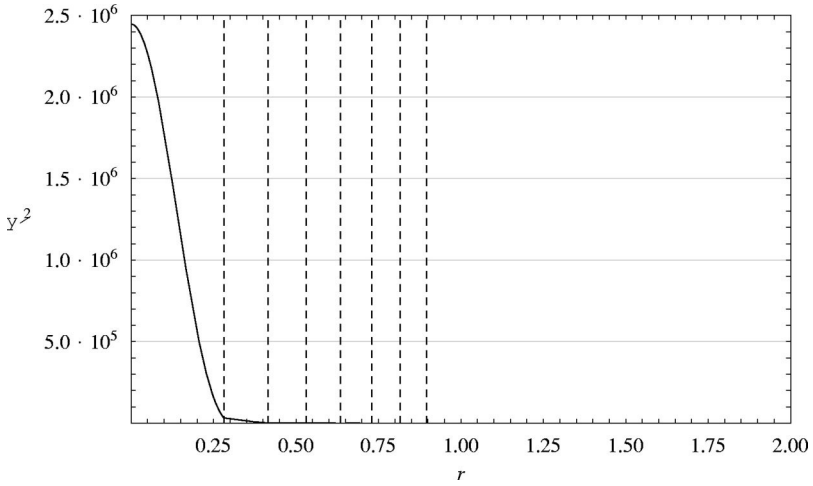

FIG. 6. A cylindrical configuration with seven barriers. By doubling ρ we have increased the confinement coefficient by three orders of magnitude. $e=1$, $\rho=7.797$ and $C=6.12\times10^5$.

matrix expressions. By approximating a real potential with sectionally constant pieces the transfer matrices can be used to find the wave function in any quantum system possessing the necessary symmetries.

In considering the confinement problem we find that it is indeed possible to achieve an extremely large confinement ratio with an arrangement of only a few carefully placed delta function barriers. In the planar problem an analytic, closed form expression was found for not only the transfer matrix and confinement coefficient, but the optimal barrier positions as well. The exact solution gives a truly exponential dependence for the confinement coefficient on the number of barriers. In the cylindrical arrangement an analytic form was found for the transfer matrix and confinement coefficient when specific near-optimal barrier positions were chosen. However, these barrier positions need to be solved for numerically. It was found that this approximate solution gives a decreasing exponential dependence on the number of barriers, while still allowing a confinement ratio several orders of magnitude larger than unity. The analysis and arguments for

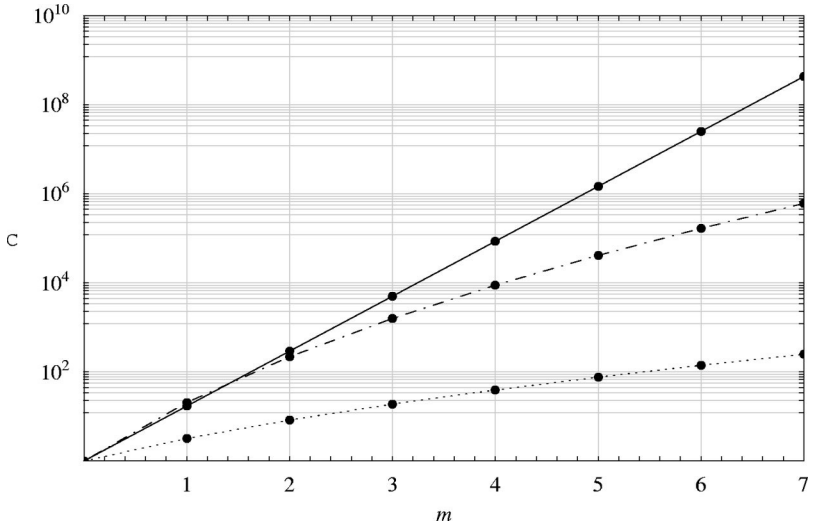

FIG. 7. Confinement coefficient as a function of the number of barriers in a cylindrical and planar configurations. The solid line is for a planar configuration with $\rho=3.898$. The dotted and dashed lines are for a cylindrical configuration with $\rho=3.898$ and $\rho=7.797$ respectively. $e=1$ for all.

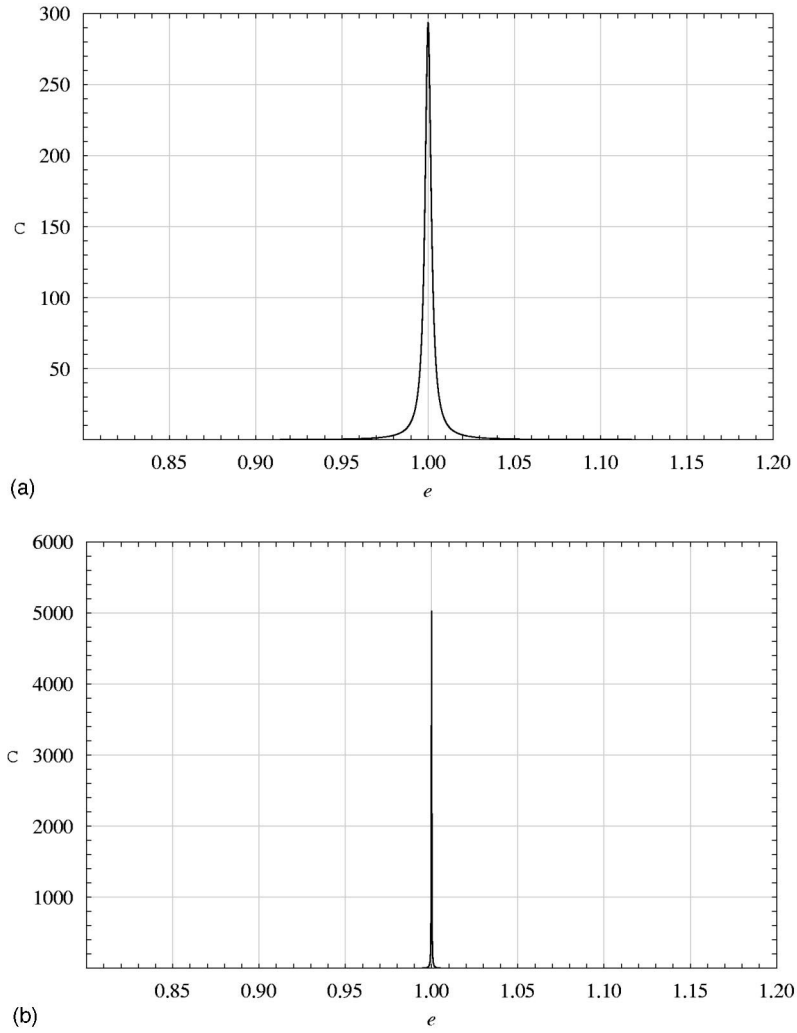

FIG. 8. Dependence of the confinement coefficient on energy in a planar configuration with $\rho = 3.898$.

the cylindrical problem apply equally well to the spherical problem. One simply needs to replace the cylindrical Hankel or Bessel functions with the corresponding spherical ones. Independent of geometry, however, it is found that the confinement coefficient is extremely sensitive to both the barrier positions and the energy of the particle. Without an extreme fine tuning of both of these parameters the confinement disappears.

APPENDIX A: THE TRANSFER MATRIX GROUP SU(1,1)

Flux conservation (FC) together with symmetry under time reversal (T) requires that the transfer matrix linking any two regions of the same potential in planar, cylindrical, or spherical geometries belong to the special pseudo-unitary group SU(1,1). We review some of the properties of this group here.

The pseudo-unitary group U(1,1) is defined as group of linear transformations on $\mathbb{C}^2$ that preserves the *indefinite* sesquilinear form

$$\langle u,v\rangle = u_1^* v_1 - v_2^* v_2 \tag{A1}$$

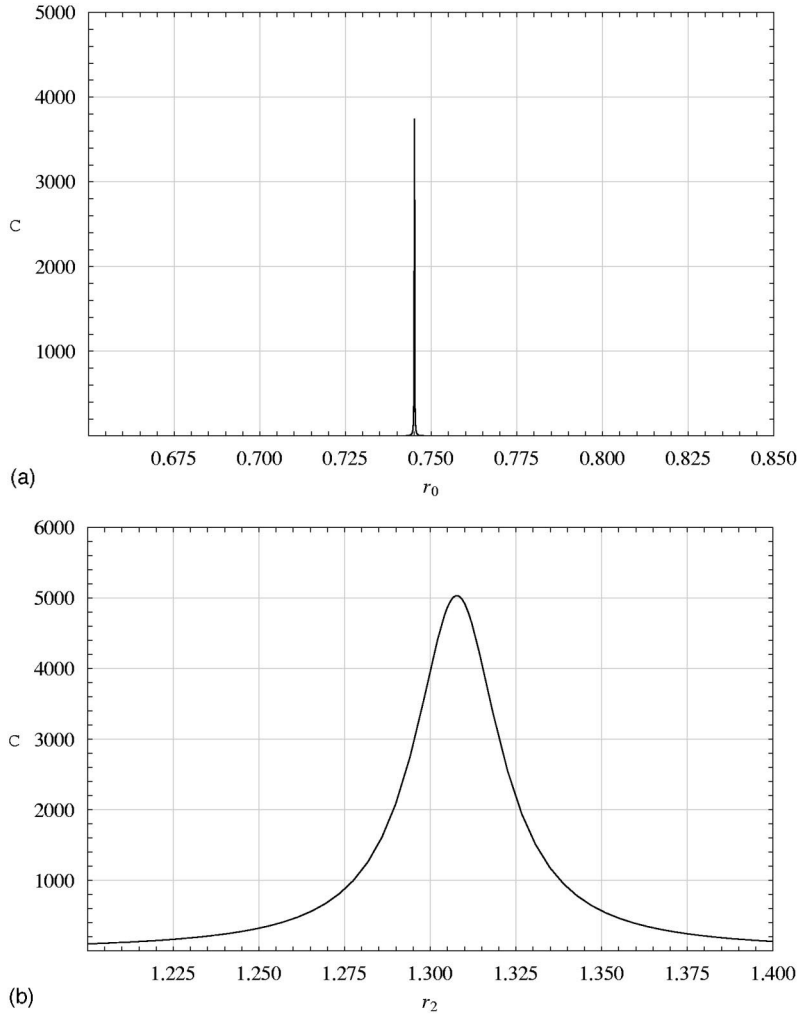

FIG. 9. Dependence of the confinement coefficient on barrier positions in a planar configuration with three barriers. $m=3$, $e=1$ and $\rho=3.898$

or equivalently as the set of nonsingular matrices that preserves the indefinite metric σ_z (the usual Pauli spin matrix)

$$M^{\dagger}\sigma_z M=\sigma_z\,. \tag{A2}$$

Transformations of this form leave the pseudo-norm

$$\langle u,u\rangle=|u_1|^2-|u_2|^2 \tag{A3}$$

invariant and so are flux conserving. The addition of T symmetry requires that the matrices belong to the subgroup of U(1,1) possessing unit determinant, denoted SU(1,1). This group can be written as the following set of 2×2 complex matrices:

$$\mathrm{SU}(1,1)=\left\{\begin{pmatrix} a & b^* \\ b & a^* \end{pmatrix}\middle|\,|a|^2-|b|^2=1\right\}. \tag{A4}$$

Unlike unitary and Hermitian matrices, pseudo-unitary matrices are not normal (they do not commute with their adjoint) but rather pseudo-normal (i.e., normal with respect to the given indefinite metric). In particular, if $A \in \mathrm{U}(1,1)$, then

$$A^{-1} = \sigma_z A^\dagger \sigma_z . \tag{A5}$$

For an arbitrary element of SU(1,1) this is

$$\begin{pmatrix} a & b^* \\ b & a^* \end{pmatrix}^{-1} = \begin{pmatrix} a^* & -b^* \\ -b & a \end{pmatrix}. \tag{A6}$$

1. Isomorphisms

As noted in Ref. 11 there are other realizations of the group SU(1,1) that are sometimes convenient. In particular, SU(1,1) is isomorphic to both $\mathrm{SL}(2,\mathbb{R})$, the group of 2×2 real matrices with unit determinant, and $\mathrm{Sp}(2,\mathbb{R})$, the real symplectic group.

The isomorphism between SU(1,1) and $\mathrm{SL}(2,\mathbb{R})$ is suggested by the fact that both the trace and determinant of elements in SU(1,1) are real. If $A \in \mathrm{SU}(1,1)$ is given by

$$A = \begin{pmatrix} a & b^* \\ b & a^* \end{pmatrix},$$

then

$$\mathrm{tr}(A) = 2\,\mathrm{Re}(a), \tag{A7a}$$

$$\det(A) = 1, \tag{A7b}$$

from which it immediately follows that the eigenvalues of A are either purely real and inverses or each other or complex conjugates of modulus one. That the same is true of matrices in $\mathrm{SL}(2,\mathbb{R})$ suggests that elements in SU(1,1) are related to real matrices by a similarity transformation. In fact, for any $A \in \mathrm{SU}(1,1)$,

$$SAS^{-1} \in \mathrm{SL}(2,\mathbb{R}), \tag{A8a}$$

where S is the unitary matrix

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}, \quad S^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}. \tag{A8b}$$

Likewise, for any $B \in \mathrm{SL}(2,\mathbb{R})$,

$$S^{-1} B S \in \mathrm{SU}(1,1). \tag{A9}$$

Thus, SU(1,1) and $\mathrm{SL}(2,\mathbb{R})$ are conjugate subgroups of $\mathrm{GL}(2,\mathbb{C})$ and so isomorphic.

The real symplectic group $\mathrm{Sp}(2,\mathbb{R})$ is defined as the group of linear transformations that preserve an antisymmetric bilinear form on $\mathbb{R}^2$, or, equivalently, as the group of real matrices that satisfy

$$M^{\mathrm{T}} J M = J, \tag{A10a}$$

where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{A10b}$$

One can show that a matrix M satisfies this equation if and only if $M \in \mathrm{SL}(2,\mathbb{R})$ so that $\mathrm{Sp}(2,\mathbb{R}) = \mathrm{SL}(2,\mathbb{R})$. Hence, we have the isomorphisms

$$\mathrm{SU}(1,1) \cong \mathrm{SL}(2,\mathbb{R}) = \mathrm{Sp}(2,\mathbb{R}). \tag{A11}$$

2. Action

As a subgroup of $\mathrm{GL}(2,\mathbb{C})$, the group SU(1,1) acts on $\mathbb{C}^2$. Due to its relationship with $\mathrm{SL}(2,\mathbb{R})$, however, it leaves some important subsets of $\mathbb{C}^2$ invariant. In addition, via conjugation by S, SU(1,1) acts directly on $\mathbb{R}^2$.

Define $\Omega = \{v \in \mathbb{C}^2 | v_1 = v_2^*\}$. That is, Ω consists of all vectors of the form

$$\begin{pmatrix} c \\ c^* \end{pmatrix}, \quad c \in \mathbb{C}.$$

It is important to note that Ω is *not* a subspace of $\mathbb{C}^2$, as it is not closed under scalar multiplication. In fact, the subspace spanned by Ω is all of $\mathbb{C}^2$. However, one may note that Ω *is* a subspace of $\mathbb{C}^2$ when considered as a (four-dimensional) vector space over $\mathbb{R}$. In either case, it is easy to see that SU(1,1) leaves Ω invariant: $\mathrm{SU}(1,1)\Omega = \Omega$,

$$\begin{pmatrix} a & b^* \\ b & a^* \end{pmatrix} \begin{pmatrix} c \\ c^* \end{pmatrix} = \begin{pmatrix} ac + b^* c^* \\ a^* c^* + bc \end{pmatrix} = \begin{pmatrix} d \\ d^* \end{pmatrix}. \tag{A12}$$

Another way to see this is to first observe that

$$S\Omega = \mathbb{R}^2, \quad S^{-1}\mathbb{R}^2 = \Omega. \tag{A13}$$

Indeed, for $x, y \in \mathbb{R}$ we have

$$S \begin{pmatrix} x+iy \\ x-iy \end{pmatrix} = \sqrt{2} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{A14}$$

It is then easy to see that the action of SU(1,1) on Ω is entirely equivalent to the action of $\mathrm{SL}(2,\mathbb{R})$ on $\mathbb{R}^2$:

$$\mathrm{SU}(1,1)\Omega = (S^{-1}\mathrm{SL}(2,\mathbb{R})S)\Omega = S^{-1}\mathrm{SL}(2,\mathbb{R})(S\Omega) = S^{-1}\mathrm{SL}(2,\mathbb{R})\mathbb{R}^2 = S^{-1}\mathbb{R}^2 = \Omega.$$

Going back to (A12) we note that

$$d = ac + b^* c^* = c\left(a + b^* \frac{c^*}{c}\right) = c(a + b^* \,\mathrm{sgn}(c^*)^2), \tag{A15}$$

so that the ratio d/c is a complex number depending only on a, b, and $\angle c$ ($\mathrm{sgn}(c^*) = \mathrm{sgn}(c)^{-1} = e^{-i\angle c}$). In particular,

$$\frac{|d|}{|c|} = [|a|^2 + |b|^2 + 2|a||b|\cos(\angle a + \angle b + 2\angle c)]^{1/2},$$

$$\angle d - \angle c = \angle(a + b^* \,\mathrm{sgn}(c^*)^2).$$

We noted that Ω is not closed under multiplication by $\mathbb{C}$. However, it should be noted that the set so obtained is also invariant under SU(1,1):

$$\Omega' = \{zv | z \in \mathbb{C} \text{ and } v \in \Omega\}. \tag{A16}$$

If we write

$$z = re^{i\theta}, \quad v = s\begin{pmatrix} e^{+i\varphi} \\ e^{-i\varphi} \end{pmatrix},$$

then we can write an arbitrary member of Ω' as

$$u = rs\begin{pmatrix} e^{i(\theta+\phi)} \\ e^{i(\theta-\phi)} \end{pmatrix}. \tag{A17}$$

In this form it should be clear that Ω' consists of all those vectors in $\mathbb{C}^2$ whose components have equal magnitude:

$$\Omega' = \{u \in \mathbb{C}^2 | |u_1| = |u_2|\}. \tag{A18}$$

It is easy to see that SU(1,1) leaves Ω' invariant: Let $A \in \mathrm{SU}(1,1)$, $z \in \mathbb{C}$, $v \in \Omega$ and $u = zv \in \Omega'$. Then

$$Au = A(zv) = z(Av) = zv' = u' \in \Omega',$$

so that

$$\mathrm{SU}(1,1)\Omega' = \Omega'. \tag{A19}$$

3. Singular value decomposition

The singular value decomposition (SVD) of a matrix A is given by

$$A = U\Sigma V^\dagger,$$

where U and V are unitary matrices and Σ is a diagonal matrix with decreasing but non-negative values on the main diagonal. If A is square and nonsingular, then Σ will be positive definite. The diagonal elements of Σ are called the singular values of A. They are given by the positive square roots of the eigenvalues of $A^\dagger A$. The SVD of a matrix is important because it reveals clearly how much the matrix can stretch or shrink an arbitrary vector. The singular values of A are precisely the (2-norm) lengths of the semi-major axes of the hyperellipsoid defined by $\{Av | \|v\| = 1\}$. (See Ref. 14 for more information.)

For $A \in \mathrm{SU}(1,1)$ the SVD is straightforward to calculate. The eigenvalues of

$$A^\dagger A = \begin{pmatrix} |a|^2 + |b|^2 & 2a^* b^* \\ 2ab & |a|^2 + |b|^2 \end{pmatrix} \tag{A20}$$

are given by

$$\lambda_\pm(A^\dagger A) = \lambda_\pm(AA^\dagger) = (|a| \pm |b|)^2,$$

so that the singular values of A are

$$\sigma_{1,2} = |a| \pm |b|. \tag{A21}$$

We have taken the positive square root in both cases as $\det(A) = 1$ and so $|a| > |b|$. It is then straightforward to calculate the SVD of A:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{sgn}(a) & \mathrm{sgn}(a) \\ \mathrm{sgn}(b) & -\mathrm{sgn}(b) \end{pmatrix}, \tag{A22a}$$

$$V=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ \operatorname{sgn}(ab) & -\operatorname{sgn}(ab)\end{pmatrix}, \tag{A22b}$$

and

$$\Sigma=\begin{pmatrix}|a|+|b| & 0\\ 0 & |a|-|b|\end{pmatrix}. \tag{A22c}$$

Note that this decomposition takes us out of the group SU(1,1) as U and V are unitary not pseudo-unitary.

4. Polar decomposition

The polar decomposition of a matrix A is the equivalent of the complex number decomposition $z=re^{i\theta}$. It gives a unitary matrix Θ times a positive-definite Hermitian matrix R (or vice versa):

$$A=\Theta R=R'\Theta.$$

This decomposition is useful for separating the actions of rotation and stretching. The matrix R (or R') will be seen to contain the singular values of A and is thus responsible for stretching, while U, being unitary, only rotates.

The polar decomposition of a matrix A is easily calculated from the SVD. For $A\in \mathrm{SU}(1,1)$ we have

$$A=\Theta R=(UV^{\dagger})(V\Sigma V^{\dagger})=\begin{pmatrix}\operatorname{sgn}(a) & 0\\ 0 & \operatorname{sgn}(a^*)\end{pmatrix}\begin{pmatrix}|a| & b^*\operatorname{sgn}(a^*)\\ b\operatorname{sgn}(a) & |a|\end{pmatrix} \tag{A23a}$$

or

$$A=R'\Theta=(U\Sigma U^{\dagger})(UV^{\dagger})=\begin{pmatrix}|a| & b^*\operatorname{sgn}(a)\\ b\operatorname{sgn}(a^*) & |a|\end{pmatrix}\begin{pmatrix}\operatorname{sgn}(a) & 0\\ 0 & \operatorname{sgn}(a^*)\end{pmatrix}. \tag{A23b}$$

Unlike the SVD, the polar decomposition of A leaves us in SU(1,1) as the matrix Θ is both unitary and pseudo-unitary.

5. Norm

An interesting property of SU(1,1) is that p-norm of any matrix in SU(1,1) appears to be independent of p. In particular, let $A\in \mathrm{SU}(1,1)$. Then

$$\|A\|_1=\|A\|_2=\|A\|_\infty=|a|+|b|. \tag{A24}$$

Recall that the p-norm of a matrix A is defined as

$$\|A\|_p=\sup_{v\neq 0}\frac{\|Av\|_p}{\|v\|_p},$$

where the vector p-norm is given by

$$\|v\|_p=(|v_1|^p+|v_2|^p+\cdots+|v_n|^p)^{1/p}.$$

Thus the p-norm of A is the maximal amount that A will stretch a vector. Note that if $v\in\Omega'$ (defined in Appendix A, Sec. 2), then

$$\|v\|_p = 2^{1/p}|v_i|. \tag{A25}$$

Since A leaves Ω' invariant, $\|Av\|_p = 2^{1/p}|v_i'|$ and the quantity

$$\frac{\|Av\|_p}{\|v\|_p} = \frac{|v_i'|}{|v_i|}$$

is independent of p. However, such a statement is not generally true for $v \notin \Omega'$.

The 2-norm, or spectral norm, of a matrix is the most important. One can show that it is given by its largest singular value,

$$\|A\| \equiv \|A\|_2 = \sigma_1.$$

Moreover, one can show that for any $A \in \mathrm{GL}(2,\mathbb{C})$ and any $v \in \mathbb{C}^2$ that

$$\sigma_2 \leqslant \frac{\|Av\|}{\|v\|} \leqslant \sigma_1. \tag{A26}$$

For $A \in \mathrm{SU}(1,1)$ and $v = (c, c^*)^{\mathrm{T}} \in \Omega$ we can write

$$\frac{\|Av\|_p}{\|v\|_p} = [|a|^2 + |b|^2 + 2|a||b|\cos(\angle a + \angle b + 2\angle c)]^{1/2},$$

which, by varying the cosine, obviously lies between

$$|a| - |b| \leqslant \frac{\|Av\|_p}{\|v\|_p} \leqslant |a| + |b| \tag{27}$$

for $|a| > |b|$.

APPENDIX B: TRANSFER MATRIX EXPRESSIONS

For reference, we list here the components of the discontinuity and delta function transfer matrices for the choices for $\phi(r)$ and $\chi(r)$ made in (5).

1. Discontinuity

Equation (11) for the discontinuity transfer matrix is

$$\mathbf{\Gamma}_n(v_1, v_2, a) = \frac{1}{\mathfrak{m}(\phi_2, \chi_2)} \begin{pmatrix} \mathfrak{m}(\phi_1, \chi_2) & \mathfrak{m}(\chi_1, \chi_2) \\ \mathfrak{m}(\phi_2, \phi_1) & \mathfrak{m}(\phi_2, \chi_1) \end{pmatrix}.$$

Using (9) and (10) for the generalized Wronskian gives us

$$\mathbf{\Gamma}_1 = \frac{1}{2k} \begin{pmatrix} (k_1 + k_2)e^{ia(k_1 - k_2)} & (k_2 - k_1)e^{-ia(k_1 + k_2)} \\ (k_2 - k_1)e^{ia(k_1 + k_2)} & (k_1 + k_2)e^{-ia(k_1 - k_2)} \end{pmatrix},$$

$$\mathbf{\Gamma}_2 = \frac{ia\pi}{8} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix},$$

$$\mathbf{\Gamma}_3 = \frac{ia^2 k_2}{2(2\ell + 1)} \begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix},$$

where

$$m_{11}=k_2H_\nu^{(1)}(ak_1)[H_{\nu-1}^{(2)}(ak_2)-H_{\nu+1}^{(2)}(ak_2)]-k_1H_\nu^{(2)}(ak_2)[H_{\nu-1}^{(1)}(ak_1)-H_{\nu+1}^{(1)}(ak_1)],$$

$$m_{12}=k_2H_\nu^{(2)}(ak_1)[H_{\nu-1}^{(2)}(ak_2)-H_{\nu+1}^{(2)}(ak_2)]-k_1H_\nu^{(2)}(ak_2)[H_{\nu-1}^{(2)}(ak_1)-H_{\nu+1}^{(2)}(ak_1)],$$

$$m_{21}=-k_2H_\nu^{(1)}(ak_1)[H_{\nu-1}^{(1)}(ak_2)-H_{\nu+1}^{(1)}(ak_2)]+k_1H_\nu^{(1)}(ak_2)[H_{\nu-1}^{(1)}(ak_1)-H_{\nu+1}^{(1)}(ak_1)],$$

$$m_{22}=-k_2H_\nu^{(2)}(ak_1)[H_{\nu-1}^{(1)}(ak_2)-H_{\nu+1}^{(1)}(ak_2)]+k_1H_\nu^{(1)}(ak_2)[H_{\nu-1}^{(2)}(ak_1)-H_{\nu+1}^{(2)}(ak_1)],$$

and

$$n_{11}=k_2h_\ell^{(1)}(ak_1)[\ell h_{\ell-1}^{(2)}(\dot{a}k_2)-(\ell+1)h_{\ell+1}^{(2)}(ak_2)]-k_1h_\ell^{(2)}(ak_2)[\ell h_{\ell-1}^{(1)}(ak_1)-(\ell+1)h_{\ell+1}^{(1)}(ak_1)],$$

$$n_{12}=k_2h_\ell^{(2)}(ak_1)[\ell h_{\ell-1}^{(2)}(ak_2)-(\ell+1)h_{\ell+1}^{(2)}(ak_2)]-k_1h_\ell^{(2)}(ak_2)[\ell h_{\ell-1}^{(2)}(ak_1)-(\ell+1)h_{\ell+1}^{(2)}(ak_1)],$$

$$n_{21}=-k_2h_\ell^{(1)}(ak_1)[\ell h_{\ell-1}^{(1)}(ak_2)-(\ell+1)h_{\ell+1}^{(1)}(ak_2)]+k_1h_\ell^{(1)}(ak_2)[\ell h_{\ell-1}^{(1)}(ak_1)-(\ell+1)h_{\ell+1}^{(1)}(ak_1)],$$

$$n_{22}=-k_2h_\ell^{(2)}(ak_1)[\ell h_{\ell-1}^{(1)}(ak_2)-(\ell+1)h_{\ell+1}^{(1)}(ak_2)]+k_1h_\ell^{(1)}(ak_2)[\ell h_{\ell-1}^{(2)}(ak_1)-(\ell+1)h_{\ell+1}^{(2)}(ak_1)].$$

2. Delta function

Equation (18) for the delta function transfer matrix is

$$\mathbf{\Delta}_n=\mathbb{1}-i\xi_n\begin{pmatrix}\phi\chi & \chi^2\\ -\phi^2 & -\phi\chi\end{pmatrix}.$$

Using (19) for ξ_n we get

$$\mathbf{\Delta}_1=\mathbb{1}-i\frac{\rho^2\alpha}{2k}\begin{pmatrix}1 & e^{-2iak}\\ -e^{2iak} & -1\end{pmatrix},$$

$$\mathbf{\Delta}_2=\mathbb{1}-i\frac{\rho^2\alpha}{8}\begin{pmatrix}H_\nu^{(1)}(ak)H_\nu^{(2)}(ak) & [H_\nu^{(2)}(ak)]^2\\ -[H_\nu^{(1)}(ak)]^2 & -H_\nu^{(1)}(ak)H_\nu^{(2)}(ak)\end{pmatrix},$$

$$\mathbf{\Delta}_3=\mathbb{1}-i\frac{\rho^2\alpha k}{8\pi}\begin{pmatrix}h_\ell^{(1)}(ak)h_\ell^{(2)}(ak) & [h_\ell^{(2)}(ak)]^2\\ -[h_\ell^{(1)}(ak)]^2 & -h_\ell^{(1)}(ak)h_\ell^{(2)}(ak)\end{pmatrix}.$$

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Boundary behavior of quantum Green's functions

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(Received 28 May 2002; accepted 16 December 2002)

We consider the time-independent Green's function for the Schrödinger operator with a one-particle potential, defined in a d-dimensional domain. Recently, in one dimension (1D), the Green's function problem was solved explicitly in inverse form, with diagonal elements of the Green's function as prescribed variables. In this article, the 1D inverse solution is used to derive leading behavior of the Green's function close to the domain boundary. The emphasis is put onto ''universal'' expansion terms which are dominated by the boundary and do not depend on the particular shape of the applied potential. The inverse formalism is extended to higher dimensions, especially to 3D, and subsequently the boundary form of the Green's function is predicted for an arbitrarily shaped domain boundary. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1557330]

I. INTRODUCTION

For a connected finite domain, the eigenvalue spectrum of an operator with a boundary condition depends strongly on the shape of the smooth boundary. A rigorous analysis of the eigenvalue density was first done by Weyl[1] for the 3D Laplacian in the asymptotic limit of an infinite volume (at short wavelengths of eigenstates). The next surface and curvature contributions to the eigenvalue density were derived for the Dirichlet and Neumann boundary conditions first in 3D,[2] and then, by using the path integral method, in 2D.[3] In this connection, Kac posed a question whether there is a one-to-one correspondence between the boundary shape and the corresponding eigenvalue spectrum of the Laplacian. The answer is negative:[4] there exist nonisometric pairs of 2D flat shapes which are isospectral.[5,6] An important progress in calculations was made within a time-independent Green's function method in Ref. 7. Here, a multiple reflection expansion was used to get Green's function for an arbitrary domain, in the limit of small wavelengths. This technique, applied to physical problems like electromagnetic field in a cavity,[8] evoked numerous research activities.[9] Its extension to the Schrödinger operator[10] resulted in semiclassical expansions for quantum mechanical system valid for finite domains.[11,12] The influence of spatial confinement on the energy spectra of simple quantum systems, like harmonic oscillator or hydrogen atom, was investigated in many other works (see, e.g., Refs. 13–17).

This article deals with local effects of a domain boundary on the Green's function of a Schrödinger operator. The topic is studied within an ''inverse'' formulation for Green's functions. The motivation for this formulation comes from the seemingly unrelated density-functional theory.

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The latter is based on the famous Hohenberg–Kohn uniqueness theorem,[18] having a practical realization in the Kohn–Sham separation ansatz.[19] In the density-functional theory, the usual ''direct'' formulation, i.e., the ground-state expectation value of an observable in terms of some prescribed external fields, is replaced by the ''inverse'' one, with the particle density as the controlling variable. In a series of works,[20–22] we have developed an infinite gradient series expansion of the kinetic-energy density functional for 1D noninteracting Fermion systems in the ground state by applying the Green's function method. By definition, the expansion in potential gradients and correspondingly in density gradients does not allow us to consider discontinuities, say at hard particles or extended regions. The ''inverse'' formulation of Green's functions arised as a natural means for their explicit representation in any situation.

To introduce the inverse format for Green's functions, let us first specify notation. We consider a d-dimensional domain Ω of points $\mathbf{r}=(x_1,x_2,\ldots,x_d)$, infinite ($\mathbf{r}\in R^d$) or finite, bounded by hard walls at the domain boundary $\partial\Omega$. Selecting units so that $\hbar^2/(2m)=1$ with m being the particle mass, the general one-particle Hamiltonian formulated within the domain Ω is given by

$$\hat{\mathbf{H}}=-\Delta_{\mathbf{r}}+u(\mathbf{r}). \tag{1.1}$$

Here, $u(\mathbf{r})$ is an arbitrary external potential, continuous inside Ω, which does not include the infinite potential due to the presence of domain walls at $\partial\Omega$. The time-independent Schrödinger equation reads

$$\hat{\mathbf{H}}\psi_k(\mathbf{r})=\lambda_k\psi_k(\mathbf{r}) \tag{1.2}$$

with the Dirichlet boundary condition (b.c.) $\psi_k(\mathbf{r})=0$ at the domain boundary $\mathbf{r}\in\partial\Omega$. $\psi_k(\mathbf{r})$ and λ_k are respectively the eigenstates and the eigenvalues of Hamiltonian $\hat{\mathbf{H}}$, and index k can be either discrete (localized eigenstates) or continuous (extended eigenstates). The time-independent Green's function is defined by[23] $\mathbf{G}_z=(z-\hat{\mathbf{H}})^{-1}$, where z is a complex variable with components $\lambda=\mathrm{Re}(z)$ and $s=\mathrm{Im}(z)$. $\mathbf{G}_z$ is an analytic function of z except of those points on the real z-axis which correspond to the eigenvalues of $\hat{\mathbf{H}}$: it exhibits simple poles at discrete eigenvalues of $\hat{\mathbf{H}}$ and a branch cut along fragments of the real z-axis which correspond to the continuous spectrum of $\hat{\mathbf{H}}$. In the latter case, the discontinuity of the transverse limits $\mathbf{G}_\lambda^{\pm}=\lim_{s\to 0^+}\mathbf{G}_{\lambda\pm is}$ yields the density of states at λ. In the vector-space representation,

$$G_z(\mathbf{r},\mathbf{r}')=\sum_k \frac{\psi_k^*(\mathbf{r})\psi_k(\mathbf{r}')}{z-\lambda_k}, \tag{1.3}$$

the Green's function satisfies the two-point differential equation

$$[\Delta_{\mathbf{r}}+z-u(\mathbf{r})]G_z(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}') \tag{1.4}$$

with the b.c. at the domain boundary, $G_z(\mathbf{r},\mathbf{r}')=0$ at $\mathbf{r}\in\partial\Omega$. We notice that in one dimension (1D), diagonal elements of the Green's function, denoted by

$$n_z(x)=\sum_k \frac{\psi_k(x)\psi_k^*(x)}{z-\lambda_k}, \tag{1.5}$$

are well defined finite quantities. This is no longer true in dimensions $\geqslant 2$ where the equal-argument Green's function diverges. One can avoid this divergence by redefining new one-point quantities, whose choice is crucial from the point of view of this work. In 3D, which is of practical interest, the finite quantity

$$\nu_z(\mathbf{r})=\lim_{\mathbf{r}'\to\mathbf{r}} 4\pi\frac{\partial}{\partial z}G_z(\mathbf{r},\mathbf{r}'), \quad d=3, \tag{1.6}$$

will be especially useful. The function ν_z remains informative since the differentiation of the Green's function with respect to z keeps the poles of the latter. One can reconstruct the original Green's function by using the relation

$$\int_0^z \mathrm{d}s \quad \nu_s(\mathbf{r}) = 4\pi \langle \mathbf{r}| \frac{1}{z-\hat{\mathbf{H}}} + \frac{1}{\hat{\mathbf{H}}} |\mathbf{r}\rangle, \quad d=3. \tag{1.7}$$

The z-independent term in (1.7), which subtracts the diverging part of the diagonal Green's function element, has no effect on the density-functional formalism developed in Refs. 20–22.

The above format is the direct one: for a given constraining domain Ω and a given external field $u(\mathbf{r})$, find the corresponding Green's function. For continuum 1D space[20,21] and for simply connected lattice structures,[22] the direct problem was replaced by the inverse one with diagonal elements of Green's function as controlling variables: (i) the external field in terms of the diagonal elements of Green's function (the inverse profile relation) and (ii) off-diagonal Green's function elements in terms of the diagonal ones. The 1D inverse profile relation was found explicitly in the form

$$z-u(x) = -\frac{1}{4}\frac{1}{n_z^2(x)} + \frac{1}{4}\left[\frac{n_z'(x)}{n_z(x)}\right]^2 - \frac{1}{2}\frac{n_z''(x)}{n_z(x)}, \tag{1.8}$$

with the standard b.c. $n_z(x)=0$ at $x \in \partial\Omega$. A prime means the derivative with respect to the argument. Equation (1.8) with b.c. determines $n_z(x)$ uniquely up to the sign. When compared to the basic equation (1.4) of the direct format, it has the virtue of being a one-point differential equation without the appearance of a δ-function. As concerns the off-diagonal elements of the Green's function, they can be expressed in terms of the diagonal ones as follows:

$$G_z(x,x') = [n_z(x)]^{1/2}[n_z(x')]^{1/2} \exp\left[\mathrm{sign}(x-x') \int_{x'}^{x} \frac{\mathrm{d}s}{2n_z(s)}\right]. \tag{1.9}$$

As was already mentioned, in this article we use the inverse formalism to study behavior of the Green's function close to the confining domain boundary. In the leading and some higher orders of the distance from the boundary, the Green's function is shown to exhibit "universal" terms which are dominated by the boundary and do not depend on the applied potential. These boundary terms are derived first in 1D, and subsequently predicted in 3D for an arbitrarily shaped domain boundary. The results are exact at all wavelengths.

The article is organized as follows. In Sec. II, we derive in the inverse format the boundary form of the 1D Green's function. Before extending the inverse formalism to higher dimensions, in particular to 3D, we first treat, in the direct format with the zero potential, two special cases which can be treated exactly as one-dimensional. Systems that are stratified to only one Cartesian coordinate (Sec. III) justify the choice of the one-point quantity ν_z (1.6). Spherically symmetric systems (Sec. IV) reveal unexpected logarithmic terms in the boundary expansion of the Green's function. In the latter case, as a by-product of the formalism, we derive general behavior of the Green's functions close to the center of radial symmetry. A technique for systematic construction of the inverse profile relation in an arbitrary dimension and for any potential is developed in Sec. V. As a consequence, the (universal) boundary terms in the 3D Green's function are suggested for an arbitrarily shaped domain boundary.

II. 1D GREEN'S FUNCTION

We start with 1D Green's function $G_z(x,x')$ defined in a domain $\Omega=(0,X)$, and look for its behavior close to a wall, say as $x,x' \to 0$. The potential $u(x)$ is assumed to be regular at $x=0$, and its Taylor expansion for $x>0$ is written as

$$u(x)=\sum_{n=0}^{\infty} u_n x^n, \qquad u_n=\frac{1}{n!}\left.\frac{\mathrm{d}^n u(x)}{\mathrm{d}x^n}\right|_{x=0}. \tag{2.1}$$

The first coefficient u_0 only shifts $z\to z-u_0$, so without any loss of generality it is set equal to 0.

Let us suppose that the diagonal element of the Green's function $n_z(x)$, satisfying the b.c. $n_z(0)=0$, also has the Taylor series expansion around $x=0$,

$$n_z(x)=\sum_{n=1}^{\infty} c_n x^n, \qquad c_n=\frac{1}{n!}\left.\frac{\mathrm{d}^n n_z(x)}{\mathrm{d}x^n}\right|_{x=0}, \tag{2.2}$$

and insert this expansion into the exact inverse profile relation (1.8). The requirement of the vanishing of the prefactors attached to x^{-2},x^{-1},x^0, etc., implies the following sequence of equations for the coefficients $\{c_n\}$:

$$(c_1)^2-1=0, \tag{2.3a}$$

$$c_2[(c_1)^2-1]=0, \tag{2.3b}$$

$$2zc_1+3c_3=0, \tag{2.3c}$$

etc. Equation (2.3a) tells us that $[n_z'(0)]^2=1$. Actually, we observe in 1D examples with boundaries, like free particle or harmonic oscillator in bounded well, that

$$n_z'(0)=-1. \tag{2.4}$$

This means that n_z goes to zero at the boundary from below. The universal slope -1 depends neither on details of the applied potential nor on the b.c. at the opposite boundary X. Relation (2.4) also tells us that the functional series, which determines $n_z(x)$ via formula (1.5), is not uniformly convergent. In the opposite case, we could differentiate this functional series term by term with respect to x, which leads to the contradiction $n_z'(0)=0$. Equation (2.3b) is fulfilled identically, leaving the coefficient c_2 unspecified: the value of $c_2(z)$, which depends on z and $\{u_n\}$, is fixed by the requirement of the vanishing of $n_z(x)$ at the opposite X-boundary. Equation (2.3c) determines the coefficient c_3, which, being the function of only z (trivially shifted by u_0), is universal in the same sense as c_1. The next coefficients $c_4,c_5,\ldots$ are analytic functions of both $\{u_n\}$ and c_2, which confirms the adequacy of the analyticity assumption (2.2). We conclude that

$$n_z(x)\sim -x+c_2(z)x^2+\frac{2z}{3}x^3 \qquad \text{as } x\to 0^+. \tag{2.5}$$

When the two points x and x' are close to the boundary at 0, the leading terms of $G_z(x,x')$ can be evaluated by inserting (2.5) into (1.9), with the result

$$G_z(x,x')\sim -x_<+c_2(z)xx'+\frac{z}{6}x_<(x_<^2+3x_>^2) \qquad \text{as both } x,x'\to 0^+. \tag{2.6}$$

Here, we have introduced the standard notation $x_<\equiv\min\{x,x'\}$ and $x_>\equiv\max\{x,x'\}$.

III. *d*-DIMENSIONAL GREEN'S FUNCTION WITH A 1D CONFINEMENT TO POTENTIAL

There exists a large family of d-dimensional models whose Green's function can be explicitly expressed in terms of a related 1D Green's function. The family is defined by potentials that are stratified in one dimension, i.e., depend on only one Cartesian coordinate of $\mathbf{r}=(x_1,\ldots,x_d)$, say $x_1=x\in\Omega_x$, $u(\mathbf{r})=u(x)$. For simplicity, the subspace of vectors $\mathbf{r}_\perp=(x_2,\ldots,x_d)$ perpendicular to

the x-axis will be infinite, $\Omega=\Omega_x\otimes R^{d-1}$. Using the separation-of-variables treatment with plane waves $\mathbf{k}_\perp=(k_2,\ldots,k_d)$ in the perpendicular subspace, the d-dimensional Green's function is expressible as

$$G_z(\mathbf{r},\mathbf{r}')=\int_{-\infty}^{\infty}\frac{\mathrm{d}k_2}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{\mathrm{d}k_d}{2\pi}G^{1\mathrm{D}}_{z-k_2^2-\cdots-k_d^2}(x,x')\mathrm{e}^{\mathrm{i}\mathbf{k}_\perp\cdot(\mathbf{r}_\perp-\mathbf{r}'_\perp)}, \tag{3.1}$$

where $\mathbf{G}^{1\mathrm{D}}$ is a 1D Green's function associated with the potential $u(x)$ and the domain Ω_x. In $d=3$ dimensions, passing to polar coordinates, formula (3.1) takes form

$$G_z^{3\mathrm{D}}(\mathbf{r},\mathbf{r}')=\frac{1}{2\pi}\int_0^\infty \mathrm{d}k\ \ kG^{1\mathrm{D}}_{z-k^2}(x,x')J_0(k\rho_\perp). \tag{3.2}$$

Here, $\rho_\perp=|\mathbf{r}_\perp-\mathbf{r}'_\perp|$ is the perpendicular distance of points $\mathbf{r},\mathbf{r}'$ and J_0 denotes the Bessel function of the first kind.[24]

Let the 3D domain Ω be the half-space $\langle 0,\infty)\otimes R^2$. The corresponding 1D Green's function $G^{1\mathrm{D}}_{z-k^2}(x,x')$ in (3.2), formulated within $\Omega_x=\langle 0,\infty)$, can be expanded in x and x' near the rectilinear hard wall at 0 using the previously derived formula (2.6). It might be tempting to insert this expansion directly into (3.2), but already the leading term $\sim -x_<$ implies a diverging integral over k. This indicates that a renormalization procedure is needed for a 1D Green's function.

We first assume that $\rho_\perp\neq 0$, i.e., the two points $\mathbf{r}$ and $\mathbf{r}'$ do not lie on the same line perpendicular to the surface of the wall. $G^{1\mathrm{D}}$ can be split into two parts

$$G_z^{1\mathrm{D}}(x,x')=\frac{1}{2\mathrm{i}\sqrt{z}}[\mathrm{e}^{\mathrm{i}\sqrt{z}|x-x'|}-\mathrm{e}^{\mathrm{i}\sqrt{z}(x+x')}]+\delta G_z^{1\mathrm{D}}(x,x'),\qquad x,x'\geqslant 0, \tag{3.3}$$

where one assumes that $\mathrm{Im}(\sqrt{z})>0$ in order to ensure the regularity at $|x-x'|\to\infty$. The first part, which is nothing but a 1D Green's function of free particle in the half-space $x\geqslant 0$, contains all universal terms of the small-x,x' expansion (2.6). The remainder does not contain the universal terms and behaves like

$$\delta G_z^{1\mathrm{D}}(x,x')=[c_2^{1\mathrm{D}}(z)+\mathrm{i}\sqrt{z}]xx'+O[xx'(x^2+x'^2)], \tag{3.4}$$

where the model-dependent $c_2^{1\mathrm{D}}(z)$ is defined by (2.5) or (2.6). Substituting (3.3) and (3.4) in the basic formula (3.2), one gets

$$G_z^{3\mathrm{D}}(\mathbf{r},\mathbf{r}')=-\frac{1}{4\pi}\left[\frac{\exp(\mathrm{i}\sqrt{z}|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}-\frac{\exp(\mathrm{i}\sqrt{z}\sqrt{(x+x')^2+\rho_\perp^2})}{\sqrt{(x+x')^2+\rho_\perp^2}}\right]+\delta G_z^{3\mathrm{D}}(\mathbf{r},\mathbf{r}'), \tag{3.5a}$$

where

$$\delta G_z^{3\mathrm{D}}(\mathbf{r},\mathbf{r}')=-\frac{z}{2\pi}\int_1^\infty \mathrm{d}s\ \ s[c_2^{1\mathrm{D}}(zs^2)+\mathrm{i}\sqrt{z}s]I_0(\sqrt{z}\rho_\perp\sqrt{s^2-1})\ \ xx'+O[xx'(x^2+x'^2)]. \tag{3.5b}$$

It can be easily shown that $c_2^{1\mathrm{D}}(z)+\mathrm{i}\sqrt{z}\sim O(1/z)$ as $|z|\to\infty$, so the integral in (3.5b) has the necessary convergence property. Consequently, the total $G_z^{3\mathrm{D}}(x,x';\rho_\perp\neq 0)\propto xx'$ does not exhibit universal expansion terms near the boundary, as is intuitively anticipated.

When $\rho_\perp=0$, i.e., the two points $\mathbf{r}$ and $\mathbf{r}'$ lie on the same line perpendicular to the surface of the wall, relation (3.2) can be transformed to

$$G_z^{3\mathrm{D}}(x,x';\rho_\perp=0)=G_0^{3\mathrm{D}}(x,x';\rho_\perp=0)+\frac{1}{4\pi}\int_0^z \mathrm{d}s\ \ G_s^{1\mathrm{D}}(x,x'). \tag{3.6}$$

It is straightforward to show that the small-x,x' expansion of G_0^{3D} is determined by the free-particle limit plus a model-dependent term $\sim O(xx')$. From (2.6), $G_s^{1D}(x,x')=-x_<+O(xx')$. Substituting this in (3.6), one observes that

$$G_z^{3D}(x,x';\rho_\perp=0)=-\frac{x_<}{2\pi|x-x'|(x+x')}-\frac{z}{4\pi}x_<+O(xx'). \tag{3.7}$$

The first two leading terms on the rhs of (3.7) are universal, the applied potential contributes starting from the term of order $O(xx')$.

We add that the 3D one-point quantity ν_z, introduced in (1.6), equals the diagonal element of the 1D Green's function associated with the potential $u(x)$, and therefore satisfies the inverse relation of type (1.8),

$$z-u(x)=-\frac{1}{4}\frac{1}{\nu_z^2(x)}+\frac{1}{4}\left[\frac{\nu_z'(x)}{\nu_z(x)}\right]^2-\frac{1}{2}\frac{\nu_z''(x)}{\nu_z(x)}, \tag{3.8}$$

and exhibits the small-x expansion (2.5).

IV. RADIAL GREEN'S FUNCTION

We now consider a 3D quantum system with radial symmetry, confined to the domain $\Omega=\{|\mathbf{r}|\leqslant R\}$ (radius R may be either finite or infinite). The external potential $u(r)$ depends only on the magnitude r of $\mathbf{r}$. The radial problem can be reduced to 1D by factoring out the angular dependence of the Hamiltonian eigenfunctions in terms of the spherical harmonics. Let us introduce for each angular momentum quantum number $l=0,1,2,\ldots$ the 1D Green's function associated with the Hamiltonian

$$\hat{\mathbf{H}}^{(l)}=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)}{r^2}+u(r), \tag{4.1}$$

$\mathbf{G}_z^{(l)}=(z-\hat{\mathbf{H}}^{(l)})^{-1}$, with zero b.c. at the origin $r=0$ and at the boundary $r=R$. The total 3D radial Green's function is then expressible as

$$G_z^{3D}(\mathbf{r},\mathbf{r}')=\sum_{l=0}^{\infty}\frac{(2l+1)}{4\pi rr'}P_l(\cos\omega)G_z^{(l)}(r,r'), \tag{4.2}$$

where ω is the angle between $\mathbf{r}$, $\mathbf{r}'$ and P_l denotes the Legendre polynomial of degree l.[24] The radial analog of the 1D inverse profile Eq. (1.8) for the diagonal elements of $\mathbf{G}_z^{(l)}$, $n_z^{(l)}(r)=G_z^{(l)}(r,r)$, reads

$$z-u(r)-\frac{l(l+1)}{r^2}=-\frac{1}{4}\frac{1}{n_z^{(l)}(r)^2}+\frac{1}{4}\left[\frac{n_z^{(l)\prime}(r)}{n_z^{(l)}(r)}\right]^2-\frac{1}{2}\frac{n_z^{(l)\prime\prime}(r)}{n_z^{(l)}(r)}, \tag{4.3}$$

with the obvious b.c. $n_z^{(l)}(0)=n_z^{(l)}(R)=0$. According to (1.9), the off-diagonal elements of $\mathbf{G}_z^{(l)}$ are expressible in terms of the diagonal ones as follows:

$$G_z^{(l)}(r,r')=[n_z^{(l)}(r)]^{1/2}[n_z^{(l)}(r')]^{1/2}\exp\left[\mathrm{sign}(r-r')\int_{r'}^{r}\frac{\mathrm{d}s}{2n_z^{(l)}(s)}\right]. \tag{4.4}$$

A. Behavior close to the center

Although the additional potential term $l(l+1)/r^2$ $(l\neq 0)$ is singular at $r=0$, the $r\to 0$ analysis of Eq. (4.3) is similar to that of the 1D inverse profile relation (1.8) close to a boundary (see Sec. II). Let us assume that the potential $u(r)$ is regular at the origin. Inserting into (4.3) the Taylor expansion of $n_z^{(l)}$ around $r=0$,

$$n_z^{(l)}(r)=\sum_{n=1}^{\infty} c_n^{(l)} r^n, \qquad c_n^{(l)}=\frac{1}{n!}\left.\frac{\mathrm{d}^n n_z^{(l)}(r)}{\mathrm{d}r^n}\right|_{r=0}, \tag{4.5}$$

one gets a sequence of equations for the coefficients $\{c_n^{(l)}\}$ which implies

$$n_z^{(l)}(r)\sim -\frac{r}{2l+1}+\delta_{l,0}c_2^{(0)}(z)r^2-\frac{2z}{(2l-1)(2l+1)(2l+3)}r^3 \qquad \text{as } r\to 0. \tag{4.6}$$

The leading terms of the expansion of the Green's function $G_z^{(l)}(r,r')$ in r and r' can be evaluated by inserting (4.6) into (4.4). The total 3D Green's function (4.2) can be obtained by applying the generating formula for Legendre polynomials, with the result

$$G_z^{3\mathrm{D}}(\mathbf{r},\mathbf{r}')\sim -\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}+\frac{c_2^{(0)}(z)}{4\pi}+\frac{z}{8\pi}|\mathbf{r}-\mathbf{r}'| \qquad \text{as both } r,r'\to 0. \tag{4.7}$$

Here, the potential $u(r)$ and the presence of the boundary at $r=R$ are reflected only in the model-dependent coefficient $c_2^{(0)}(z)$.

B. Behavior close to the boundary

We introduce a new variable, the distance from the wall $x=R-r$, and redefine $u(r)\to u(x)$, $n_z^{(l)}(r)\to n_z^{(l)}(x)$, $G_z^{(l)}(r,r')\to G_z^{(l)}(x,x')$. The total 3D Green's function (4.2) is expressible simply as

$$G_z^{3\mathrm{D}}(x,x';\omega)=\frac{1}{4\pi(1-x/R)(1-x'/R)}\frac{1}{R}\sum_{l=0}^{\infty}\frac{(2l+1)}{R}P_l(\cos\omega)G_z^{(l)}(x,x'). \tag{4.8}$$

The "angular momentum" potential $l(l+1)/(R-x)^2$ is an analytic function of x close to the boundary. Provided that $u(x)$ is also regular at $x=0$, it holds $G_z^{(l)}(x,x')\sim -x_<$ as $x,x'\to 0$. Inserting this into (4.8), the 3D Green's function becomes proportional to the nonconverging series $\Sigma_{l=0}^{\infty}(2l+1)P_l(\cos\omega)$ and we face the same problem as in the previous case of the 3D rectilinear boundary (Sec. III).

Since we know how to solve the divergence problem for the rectilinear hard wall, our strategy is first to reproduce the result (3.2), valid for the 3D rectilinear wall, as the $R\to\infty$ limit of the relation (4.8), and then to get the leading $1/R$ correction due to the curvature of the wall surface. We have treated the angular momentum potential $l(l+1)/(R-x)^2$ as a perturbative series in $1/R$, then used the standard Green's function perturbation theory for $\mathbf{G}^{(l)}$ and finally performed a convenient continualization of the sum on the rhs of (4.8) setting $l=kR-1/2$ (k fixed) and

$$P_l(\cos\omega)=J_0(k\rho_\perp)-\frac{k\rho_\perp(x+x')}{2R}J_1(k\rho_\perp)+O\left(\frac{1}{R^2}\right).$$

Here, $\rho_\perp$, defined by $\rho_\perp^2=|\mathbf{r}-\mathbf{r}'|^2-(x-x')^2$, is the analog of the perpendicular distance $|\mathbf{r}_\perp-\mathbf{r}'_\perp|$ in the case of the rectilinear wall. The final result is

$$G_z^{3\mathrm{D}}(x,x';\rho_\perp)=\frac{1}{2\pi}\int_0^\infty \mathrm{d}k\ \ kG_{z-k^2}^{1\mathrm{D}}(x,x')J_0(k\rho_\perp)+\frac{1}{R}\mathcal{G}_z(x,x';\rho_\perp)+O\left(\frac{1}{R^2}\right), \tag{4.9}$$

where

$$\mathcal{G}_z(x,x';\rho_\perp)=\frac{(x+x')}{2\pi}\int_0^\infty \mathrm{d}k\ \ kG^{1\mathrm{D}}_{z-k^2}(x,x')J_0(k\rho_\perp)$$
$$-\frac{\rho_\perp(x+x')}{4\pi}\int_0^\infty \mathrm{d}k\ \ k^2G^{1\mathrm{D}}_{z-k^2}(x,x')J_1(k\rho_\perp)$$
$$+\frac{1}{\pi}\int_0^\infty \mathrm{d}k\ \ k^3J_0(k\rho_\perp)\int_0^\infty \mathrm{d}y\ \ G^{1\mathrm{D}}_{z-k^2}(x,y)yG^{1\mathrm{D}}_{z-k^2}(y,x'). \tag{4.10}$$

$\mathbf{G}^{1\mathrm{D}}$ is the 1D Green's function corresponding to the given potential $u(x)$, with the zero b.c. at $x=0$ and the regularity condition at $x\to\infty$.

The first term in (4.9) is nothing but the exact result (3.2) valid for the $R\to\infty$ rectilinear hard wall. Its expansion for small x,x' coordinates was discussed in Sec. III. The next term $\mathcal{G}_z(x,x';\rho_\perp)/R$ represents the leading correction due to the curvature of the wall surface. In the particular case of the zero potential, when $\mathbf{G}^{1\mathrm{D}}$ is given by (3.3) with $\delta\mathbf{G}^{1\mathrm{D}}=0$, the small-$x,x'$ expansion of $\mathcal{G}_z$ reads:

$$\mathcal{G}_z(x,x';\rho_\perp\neq 0)=\frac{xx'z}{4\pi}K_0(-\mathrm{i}\sqrt{z}\rho_\perp)+O[xx'(x+x')], \tag{4.11}$$

where K_0 is a modified Bessel function;[24]

$$\mathcal{G}_z(x,x';\rho_\perp=0)=\frac{xx'}{4\pi(x+x')^2}-\frac{xx'z}{4\pi}\ln[-\mathrm{i}\sqrt{z}(x+x')]+O(xx'). \tag{4.12}$$

Worked-out examples with nonzero potentials tell us that for $\rho_\perp\neq 0$ the leading term $\propto xx'$ on the rhs of (4.11) depends on the applied potential, while there is evidence that for $\rho_\perp=0$ the first two leading terms on the rhs of (4.12) are universal (i.e., independent of the applied potential) and the potential enters into the next term of order $O(xx')$. From (4.12), the one-point quantity of interest ν_z has the following short-distance expansion from the wall,

$$\nu_z(x)=-x-\frac{1}{R}x^2\ln\left(\frac{x}{x_0}\right)+O(x^2), \tag{4.13}$$

where $x_0=\mathrm{i}/\sqrt{z}$ is the length parameter. We see that the nonzero curvature of the sphere surface induces a nonanalyticity, namely, divergence of the second and higher-order derivatives of ν_z with respect to x at the sphere surface $x=0$. In the following section, we will prove the universality of the logarithmic term in the expansion (4.13) and derive its general form for an arbitrarily shaped domain boundary.

V. *d*-DIMENSIONAL GREEN'S FUNCTION

Let us now consider a d-dimensional quantum system with the general Hamiltonian (1.1) and Green's function satisfying Eq. (1.5). Representing the δ-function by $\delta(\mathbf{r}-\mathbf{r}')=\int \exp[\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]\mathrm{d}\mathbf{k}/(2\pi)^d$, $\mathbf{k}=(k_1,\ldots,k_d)$, we rewrite (1.5) as follows:

$$G_z(\mathbf{r},\mathbf{r}')=[z-u(\mathbf{r})+\Delta_{\mathbf{r}}]^{-1}\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}\exp[\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]. \tag{5.1}$$

It is easy to derive the commutation rule

$$[z-u(\mathbf{r})+\nabla^2_{\mathbf{r}}]^{-1}\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r})=\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r})[z-u(\mathbf{r})+(\nabla_{\mathbf{r}}+\mathrm{i}\mathbf{k})^2]^{-1}. \tag{5.2}$$

Consequently,

$$G_z(\mathbf{r},\mathbf{r}')=\int \frac{d\mathbf{k}}{(2\pi)^d}\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')][z-u(\mathbf{r})+(\nabla_{\mathbf{r}}+i\mathbf{k})^2]^{-1}$$
$$=\int \frac{d\mathbf{k}}{(2\pi)^d}\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]\left[1+\frac{\nabla_{\mathbf{r}}^2+2i\mathbf{k}\cdot\nabla_{\mathbf{r}}}{z-u(\mathbf{r})-k^2}\right]^{-1}\frac{1}{z-u(\mathbf{r})-k^2}. \tag{5.3}$$

The standard expansion of the inverse operator in (5.3) then results in an infinite series

$$\frac{1}{z-u(\mathbf{r})-k^2}-\frac{1}{z-u(\mathbf{r})-k^2}(\nabla^2+2i\mathbf{k}\cdot\nabla)\frac{1}{z-u(\mathbf{r})-k^2}$$
$$+\frac{1}{z-u(\mathbf{r})-k^2}(\nabla^2+2i\mathbf{k}\cdot\nabla)\frac{1}{z-u(\mathbf{r})-k^2}(\nabla^2+2i\mathbf{k}\cdot\nabla)\frac{1}{z-u(\mathbf{r})-k^2}-\cdots, \tag{5.4}$$

where we have dropped the subscript $\mathbf{r}$ from ∇. Writing the series (5.4) formally as the sum $\Sigma_n\alpha_n(\mathbf{r},\mathbf{k})/[z-u(\mathbf{r})-k^2]^n$, we have at once

$$\sum_{n=1}^{\infty}\frac{\alpha_n(\mathbf{r},\mathbf{k})}{[z-u(\mathbf{r})-k^2]^n}=\frac{1}{z-u(\mathbf{r})-k^2}-\frac{1}{z-u(\mathbf{r})-k^2}(\nabla^2+2i\mathbf{k}\cdot\nabla)\sum_{n=1}^{\infty}\frac{\alpha_n(\mathbf{r},\mathbf{k})}{[z-u(\mathbf{r})-k^2]^n}. \tag{5.5}$$

This differential equation implies the following recursion for the coefficients $\{\alpha(\mathbf{r},\mathbf{k})\}$:

$$\alpha_n=\delta_{n,1}-[\nabla^2\alpha_{n-1}+2i\mathbf{k}\cdot\nabla\alpha_{n-1}]-(n-2)[2i\alpha_{n-2}\mathbf{k}\cdot\nabla u+2\nabla\alpha_{n-2}\cdot\nabla u+\alpha_{n-2}\nabla^2 u]$$
$$-(n-2)(n-3)\alpha_{n-3}|\nabla u|^2. \tag{5.6}$$

Green's function (5.3) is expressible in terms of the coefficients $\{\alpha_n\}$ as follows:

$$G_z(\mathbf{r},\mathbf{r}')=\int \frac{d\mathbf{k}}{(2\pi)^d}\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]\sum_{n=1}^{\infty}\frac{\alpha_n(\mathbf{r},\mathbf{k})}{[z-u(\mathbf{r})-k^2]^n}. \tag{5.7}$$

Introducing spherical coordinates in $\mathbf{k}$-space, the integrals on the rhs of (5.7) can be evaluated by using the residue theorem in the complex k-plane.

It is straightforward to retrieve the 1D profile relation (1.8) by using the above scheme. The calculations are more tedious in 3D. Generating the coefficients $\{\alpha_n\}$ from the recursion (5.6), formula (5.7) gives, in the direct format,

$$i\nu_z(\mathbf{r})=\frac{1}{2}\frac{1}{\sqrt{z-u(\mathbf{r})}}-\frac{1}{16}\frac{\Delta u(\mathbf{r})}{[z-u(\mathbf{r})]^{5/2}}-\frac{5}{64}\frac{|\nabla u(\mathbf{r})|^2}{[z-u(\mathbf{r})]^{7/2}}+\frac{1}{64}\frac{\Delta^2 u(\mathbf{r})}{[z-u(\mathbf{r})]^{7/2}}+O([z-u(\mathbf{r})]^{-9/2}). \tag{5.8}$$

The inversion of (5.8) starting from the local-homogeneity reference $z-u(\mathbf{r})=-1/[4\nu_z^2(\mathbf{r})]$ results in the inverse profile equation

$$z-u(\mathbf{r})=-\frac{1}{4\nu_z^2(\mathbf{r})}[1-|\nabla\nu_z|^2+2\nu_z\Delta\nu_z]-\sum_{n=1}^{\infty}\varphi_n(\mathbf{r}). \tag{5.9}$$

Here, the terms which involves just $2n$ ν_z-functions are grouped into φ_n. In particular,

$$\varphi_1=\frac{1}{6}\left[(\Delta\nu_z)^2-\sum_{i,j=1}^{3}(\partial_i\partial_j\nu_z)^2\right], \tag{5.10a}$$

$$\varphi_2=\frac{1}{6}\sum_{i,j,k}[3(\partial_i\partial_j\nu_z)^2(\partial_k\nu_z)^2+2(\partial_i\partial_k\nu_z)(\partial_j\partial_k\nu_z)(\partial_i\nu_z)(\partial_j\nu_z)-4(\partial_k^2\nu_z)(\partial_i\partial_j\nu_z)(\partial_i\nu_z)(\partial_j\nu_z)$$
$$-(\partial_i^2\nu_z)(\partial_j^2\nu_z)(\partial_k\nu_z)^2]+\frac{1}{3}\nu_z\sum_{i,j,k}[4(\partial_k^2\nu_z)(\partial_i^2\partial_j\nu_z)(\partial_j\nu_z)-2(\partial_i^2\partial_j\nu_z)(\partial_j\partial_k\nu_z)(\partial_k\nu_z)$$
$$-2(\partial_i\partial_j\partial_k\nu_z)(\partial_i\partial_j\nu_z)(\partial_k\nu_z)-2(\partial_i\partial_j\nu_z)(\partial_j\partial_k\nu_z)(\partial_i\partial_k\nu_z)+(\partial_i\partial_j\nu_z)^2(\partial_k^2\nu_z)$$
$$+(\partial_i^2\nu_z)(\partial_j^2\nu_z)(\partial_k^2\nu_z)]+\frac{1}{6}\nu_z^2\sum_{i,j,k}[2(\partial_i^2\partial_j^2\nu_z)(\partial_k^2\nu_z)-2(\partial_i\partial_j\nu_z)(\partial_i\partial_j\partial_k^2\nu_z)$$
$$+(\partial_i^2\partial_k\nu_z)(\partial_j^2\partial_k\nu_z)-(\partial_i\partial_j\partial_k\nu_z)^2], \tag{5.10b}$$

etc. Note that the convergence of the direct series (5.8) is restricted to the high-energy part of the spectrum, $z-u(\mathbf{r})\gg 1$, and to slowly varying potentials $u(\mathbf{r})$. These are the attributes of extended states, and, indeed, ν_z given by (5.8) exhibits a branch cut along real z-axis. On the other hand, the inverse profile relation (5.9), being supplemented by the appropriate b.c. for ν_z, holds in the whole complex z-plane, including simple poles induced by discrete localized states of the Hamiltonian spectrum. This is an important feature of the inverse format.

As a check, we know from Sec. III that (5.9) must reduce to the 1D profile relation (3.8) when both $u(\mathbf{r})$ and $\nu_z(\mathbf{r})$ are stratified in one dimension. Under these circumstances $\varphi_1=\varphi_2=\cdots=0$, and indeed (5.9) becomes identical to (3.8).

Like in the 1D case, the 3D inverse relation (5.9) is very appropriate to describe the behavior of $\nu_z(\mathbf{r})$ close to the boundary $\partial\Omega$, where $\nu_z\to 0$. Provided that $u(\mathbf{r})$ is regular at $\mathbf{r}\in\partial\Omega$, the lhs of (5.9) is regular at $\mathbf{r}\in\partial\Omega$ and so must be also the corresponding rhs. The cancellation of the leading diverging terms on the rhs of Eq. (5.9) is determined exclusively by the terms $\propto 1/\nu_z^2$, i.e., by

$$z-u(\mathbf{r})\sim -\frac{1}{4\nu_z^2(\mathbf{r})}[1-|\nabla\nu_z|^2+2\nu_z\Delta\nu_z]. \tag{5.11}$$

This relation implies all universal terms of the ν_z-expansion around the boundary.

Let us analyze relation (5.11) for the general potential $u(\mathbf{r})$ and the general 3D domain Ω with a smooth 2D boundary $\partial\Omega$ of points $\mathbf{r}_0$ defined implicitly as follows:

$$\partial\Omega: \qquad \phi(\mathbf{r}_0)=C_0. \tag{5.12}$$

The function ϕ is such that C_0 has the dimension of length [for example, $\phi(\mathbf{r}_0)=\sqrt{x_0^2+y_0^2+z_0^2}$ $(=R)$ for the sphere]. The set of points $\{\mathbf{r}_0\}\in\partial\Omega$ can be parametrized by two curvilinear coordinates θ and φ, $\mathbf{r}_0=\mathbf{r}_0(\theta,\varphi)$, which are chosen to form an orthogonal coordinate system. To every point $\mathbf{r}\in\Omega$, we attach the number $C=\phi(\mathbf{r})$ (with the dimension of length) and introduce the coordinate $\xi=C_0-C$. The point $\mathbf{r}_0\in\partial\Omega$ adjoint to a given $\mathbf{r}$ results as the intersection of the surface $\partial\Omega$ with a curve which passes through $\mathbf{r}$ and simultaneously is perpendicular at every point $\mathbf{r}'$ to the surface $\phi(\mathbf{r}')=C'$. The relationship between $\mathbf{r}$ and $\mathbf{r}_0$ reads

$$\mathbf{r}=\mathbf{r}_0+\sum_{n=1}^{\infty}\mathbf{u}_n(\mathbf{r}_0)\xi^n, \tag{5.13}$$

where

$$\mathbf{u}_1=-\frac{\nabla\phi(\mathbf{r}_0)}{|\nabla\phi(\mathbf{r}_0)|^2}, \tag{5.14a}$$

$$(\mathbf{u}_2)_i=\frac{1}{2|\nabla\phi(\mathbf{r}_0)|^4}\sum_j\ \partial_i\partial_j\phi(\mathbf{r}_0)\partial_j\phi(\mathbf{r}_0)-\frac{\partial_i\phi(\mathbf{r}_0)}{|\nabla\phi(\mathbf{r}_0)|^6}\sum_{j,k}\ \partial_j\partial_k\phi(\mathbf{r}_0)\partial_j\phi(\mathbf{r}_0)\partial_k\phi(\mathbf{r}_0), \tag{5.14b}$$

etc. The relationship (5.13) determines $\mathbf{r}$ as a function of the curvilinear coordinates ξ, θ and φ, which are orthogonal by construction. Thus[24]

$$|\nabla\nu_z|^2=\frac{1}{h_\xi^2}\left(\frac{\partial\nu_z}{\partial\xi}\right)^2+\frac{1}{h_\theta^2}\left(\frac{\partial\nu_z}{\partial\theta}\right)^2+\frac{1}{h_\varphi^2}\left(\frac{\partial\nu_z}{\partial\varphi}\right)^2, \tag{5.15a}$$

$$\Delta\nu_z=\frac{1}{h_\xi^2}\left(\frac{\partial^2\nu_z}{\partial\xi^2}\right)+\frac{1}{h_\xi h_\theta h_\varphi}\left(\frac{\partial}{\partial\xi}\frac{h_\theta h_\varphi}{h_\xi}\right)\frac{\partial\nu_z}{\partial\xi}+\hat{\mathbf{\Phi}}_{\theta,\varphi}\nu_z, \tag{5.15b}$$

where h_ξ, h_θ and h_φ are metrical coefficients, and $\hat{\mathbf{\Phi}}_{\theta,\varphi}$ is the operator containing derivatives only with respect to θ and φ. It is useful to express the coefficients in (5.15) in terms of Cartesian coordinates:

$$\frac{1}{h_\xi^2}=|\nabla\phi(\mathbf{r})|^2=|\nabla\phi(\mathbf{r}_0)|^2-\frac{2\xi}{|\nabla\phi(\mathbf{r}_0)|^2}\sum_{i,j}\ \partial_i\partial_j\phi(\mathbf{r}_0)\partial_i\phi(\mathbf{r}_0)\partial_j\phi(\mathbf{r}_0)+O(\xi^2), \tag{5.16}$$

and

$$\frac{1}{h_\xi h_\theta h_\varphi}\left(\frac{\partial}{\partial\xi}\frac{h_\theta h_\varphi}{h_\xi}\right)=-\Delta\phi(\mathbf{r})=-\Delta\phi(\mathbf{r}_0)+O(\xi). \tag{5.17}$$

Inspired by our previous result (4.13) valid for the sphere, the function ν_z is sought in the limit $\xi\to 0$ in the form

$$\nu_z(\mathbf{r})=c_1(\theta,\varphi)\xi+c_2(\theta,\varphi)\xi^2+\cdots+d_1(\theta,\varphi)\xi\ln(\xi/\xi_0)+d_2(\theta,\varphi)\xi^2\ln(\xi/\xi_0)+\cdots, \tag{5.18}$$

where the formal parameter $\xi_0=\mathrm{i}/\sqrt{z}$ makes the argument of the logarithm dimensionless. The removal of diverging singularities on the rhs of Eq. (5.11), namely, the vanishing of the coefficients attached to terms $\ln^2\xi$, $\ln\xi$, ξ^0, $\xi\ln\xi$, $\xi\ln^2\xi$ and ξ^1 in the square bracket, fixes

$$c_1=-\frac{1}{|\nabla\phi(\mathbf{r}_0)|},\quad d_1=0,\quad d_2=-\frac{\Delta\phi(\mathbf{r}_0)}{2|\nabla\phi(\mathbf{r}_0)|^3}. \tag{5.19}$$

Consequently, one arrives at

$$\nu_z(\mathbf{r})=-\frac{1}{|\nabla\phi(\mathbf{r}_0)|}\xi-\frac{\Delta\phi(\mathbf{r}_0)}{2|\nabla\phi(\mathbf{r}_0)|^3}\xi^2\ln(\xi/\xi_0)+O(\xi^2). \tag{5.20}$$

We present two examples. For the sphere, $\phi(\mathbf{r}_0)=\sqrt{x_0^2+y_0^2+z_0^2}(=R)$, one has

$$\nabla\phi(\mathbf{r}_0)=\frac{\mathbf{r}_0}{|\mathbf{r}_0|},\qquad \Delta\phi(\mathbf{r})=\frac{2}{|\mathbf{r}_0|}. \tag{5.21}$$

Since $|\mathbf{r}_0|=R$ and $\xi=R-r$, one recovers (4.13) with $x\equiv\xi$. For the cylinder infinite in the z-direction, $\phi(\mathbf{r}_0)=\sqrt{x_0^2+y_0^2}(=R)$, one has

$$\nabla\phi(\mathbf{r}_0)=\frac{\mathbf{r}_\perp}{|\mathbf{r}_\perp|},\qquad \Delta\phi(\mathbf{r})=\frac{1}{|\mathbf{r}_\perp|}, \tag{5.22}$$

where $\mathbf{r}_\perp=(x_0,y_0,0)$. Thus,

$$\nu_z(\mathbf{r})=-\xi-\frac{1}{2R}\xi^2\ln(\xi/\xi_0)+O(\xi^2), \tag{5.23}$$

with $\xi=R-\sqrt{x^2+y^2}$.

We would like to add that although ξ has the dimension of length, it does not represent in general the metric distance $\tau=|\mathbf{r}-\mathbf{r}_0|$. Since one has

$$\tau=\frac{1}{|\nabla\phi(\mathbf{r}_0)|}\xi+O(\xi^2), \tag{5.24}$$

Eq. (5.20) can be expressed in terms of τ as follows:

$$\nu_z(\mathbf{r})=-\tau-\frac{\Delta\phi(\mathbf{r}_0)}{2|\nabla\phi(\mathbf{r}_0)|}\tau^2\ln(\tau/\tau_0)+O(\tau^2) \tag{5.25}$$

with the obvious definition of τ_0.

As was mentionned in the Introduction, ν_z, used through relation (1.7), is the crucial one-point quantity in the density-functional formalism developed in Refs. 20–22. From a general point of view it is desirable to have at one's disposal also off-diagonal elements of the Green's function. The knowledge of ν_z is not sufficient to get the complete Green's function within the present method (except of the case of the rectilinear hard wall). However, the short-distance expansion of ν_z (5.25), derived with the aid of curvilinear coordinates which mimic the global shape of the domain, depends only on the local surface characteristic. Since this one-point quantity is generated from the Green's function itself, it is reasonable to expect the local shape dependence of the latter as well. This assumption, together with the explicitly worked-out examples of the sphere (Sec. IV) and of the infinite cylinder, indicates the following boundary behavior of the Green's function. For the considered pair of points $\mathbf{r},\mathbf{r}'\in\Omega$ with the respective adjoint points $\mathbf{r}_0,\mathbf{r}_0'\in\partial\Omega$, the perpendicular distance is defined by $\rho_\perp=|\mathbf{r}_0-\mathbf{r}_0'|$ and $\tau=|\mathbf{r}-\mathbf{r}_0|$, $\tau'=|\mathbf{r}'-\mathbf{r}_0'|$. If $\rho_\perp\neq 0$, the 3D Green's function is supposed to exhibit the leading term $\propto\tau\tau'$ with a potential-dependent prefactor. If $\rho_\perp=0$, the analog of the sphere result (4.9) reads

$$G_z^{3\mathrm{D}}(\tau,\tau';\rho_\perp=0)=G_z^{3\mathrm{D}}(\tau,\tau';\rho_\perp=0)\big|_{\text{half-space}} + \frac{\Delta\phi(\mathbf{r}_0)}{2|\nabla\phi(\mathbf{r}_0)|}\left\{\frac{\tau\tau'}{4\pi(\tau+\tau')}-\frac{\tau\tau' z}{4\pi}\ln[-\mathrm{i}\sqrt{z}(\tau+\tau')]+O(\tau\tau')\right\}+\cdots. \tag{5.26}$$

The first term on the rhs of (5.26) corresponds to the Green's function evaluated in presence of the rectilinear hard wall tangent to the domain surface at point $\mathbf{r}_0$. The equation of the tangent plane is $\nabla\phi(\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0)=0$. The next term is the first correction due to the curvature of the wall surface; the applied potential is supposed to contribute to the term of order $O(\tau\tau')$. A rigorous proof of the conjecture (5.26) is a challenge for the future.

In conclusion, we have shown that, close to a hard wall, time-independent Green's functions exhibit a short-distance expansion which is to a relatively high order universal, i.e., it does not depend on the applied potential, only the local shape of the wall is relevant. The universal terms are analytic in 1D, and some of them are singular in 3D provided that the boundary curvature is nonzero. This information was obtained due to the inverse formalism developed in this article, and cannot be deduced directly from the definition of the Green's function.

ACKNOWLEDGMENTS

This work was supported by a grant from the National Science Foundation and by Grant VEGA 2/7174/2.

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Renormalization of Coulomb interactions for the 1D Dirac equation

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(Received 1 February 2002; accepted 18 December 2002)

The Coulomb interaction $1/|x|$ for the Dirac equation in one space dimension is singular in the sense that there exists a four-parameter family of self-adjoint extensions of the associated Hamiltonian operator. The purpose of this paper is to represent the dynamical group generated by some of the self-adjoint extensions as a path integral. The Feynman–Kac functional we use is constructed by a renormalization process that subtracts divergences as paths cross the isolated singularity $x=0$ of the interaction. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1555683]

I. INTRODUCTION

In its traditional form, the Feynman–Kac formula gives an expression for the solution u of the heat equation

$$\frac{\partial u}{\partial t}(x,t)=\frac{1}{2}\Delta u(x,t)-V(x)u(x,t),\quad u(x,0)=\psi(x),\quad x\in\mathbb{R}^d,\quad t>0, \tag{1.1}$$

with a source or sink term Vu, in terms of an integral

$$u(x,t)=\int_\Omega e^{-\int_0^t V(\omega(s))\,ds}\psi(\omega(t))\,dW^x(\omega) \tag{1.2}$$

over the space Ω of continuous paths $\omega:[0,\infty)\to\mathbb{R}^d$. For each $x\in\mathbb{R}^d$, Wiener measure W^x is concentrated on those paths $\omega\in\Omega$ with $\omega(0)=x$.

Suppose that the inital value ψ belongs to a function space X. If $\frac{1}{2}\Delta-V$ is the generator of C_0-semigroup $e^{t(\frac{1}{2}\Delta-V)}$, $t\geqslant 0$ acting on X, then the problem of solving the heat equation (1.1) may be viewed in terms of the theory of C_0-semigroups as finding

$$u(\cdot,t)=e^{t(\frac{1}{2}\Delta-V)}\psi,\quad t\geqslant 0.$$

Suppose now that $X=L^2(\mathbb{R}^d)$. The C_0-semigroup $t\mapsto e^{t(\frac{1}{2}\Delta-V)}$ itself may also be expressed directly in terms of an integral over a space of paths by setting

$$\langle M_t(E)\phi,\psi\rangle=\int_{\mathbb{R}^d}\left(\int_E\overline{\psi}(\omega(t))\,dW^x(\omega)\right)\phi(x)\,dx,\quad \phi,\psi\in L^2(\mathbb{R}^d), \tag{1.3}$$

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with respect to the inner product $\langle \cdot\,,\,\cdot \rangle$ of $L^2(\mathbb{R}^d)$. Then for each Borel subset E of Ω (in the compact-open topology), the estimate $|\langle M_t(E)\phi,\psi\rangle| \leqslant \|\phi\|_2\|\psi\|_2$ ensures that $M_t(E)$ is a bounded linear operator on $L^2(\mathbb{R}^d)$ and $E \mapsto M_t(E)$ is an operator valued measure in the strong operator topology, so that

$$e^{t(\frac{1}{2}\Delta - V)} = \int_\Omega e^{-\int_0^t V(\omega(s))ds}\, dM_t(\omega) \tag{1.4}$$

for suitable functions $V:\mathbb{R}^d \to \mathbb{R}$. Equation (1.2) may be written as

$$u(x,t) = (e^{t(\frac{1}{2}\Delta - V)}\psi)(x) = \left(\int_\Omega e^{-\int_0^t V(\omega(s))\, ds} d(M_t^*\psi)(\omega) \right)(x), \quad x \in \mathbb{R}^d,$$

with respect to the $L^2(\mathbb{R}^d)$-valued measure $M_t^*\psi: E \mapsto M_t(E)^*\psi$.

The advantage of working with the operator valued measures M_t instead of the dual measures M_t^* is apparent when we look at the value M_t gives to a cylinder set

$$E = \{\omega \in \Omega : \omega(t_1) \in B_1, \omega(t_2) \in B_2, \ldots, \omega(t_n) \in B_n\} \tag{1.5}$$

with $0 \leqslant t_1 < \cdots < t_n \leqslant t$ and $B_1, \ldots, B_n$ Borel subsets of $\mathbb{R}^d$. From Eq. (1.3) and the definition of Wiener measure W^x, we have

$$M_t(E) = e^{(t-t_n)\Delta/2} Q(B_n) e^{(t_n - t_{n-1})\Delta/2} \cdots Q(B_2) e^{(t_2 - t_1)\Delta/2} Q(B_1) e^{t_1 \Delta/2}. \tag{1.6}$$

Here $Q(B)$ is the operator of multiplication by the characteristic function χ_B of the Borel set $B \subset \mathbb{R}^d$ acting on $L^2(\mathbb{R}^d)$. If μ is the initial distribution of a diffusing substance, then $M_t(E)\mu$ may be interpreted as the distribution of the substance at time t after it has been subjected to a perturbation represented by the event E.

Equation (1.6) suggests replacing the heat semigroup $e^{t\Delta/2}$, $t \geqslant 0$, by a general C_0-semigroup $S(t) = e^{-At}$, $t \geqslant 0$, acting on a function space X on which the spectral measure Q of multiplication by characteristic functions acts as well. The formula

$$M_t(E) = S(t - t_n) Q(B_n) S(t_n - t_{n-1}) \cdots Q(B_2) S(t_2 - t_1) Q(B_1) S(t_1) \tag{1.7}$$

does define an additive operator valued function M_t on the algebra $\mathcal{S}_t$ generated by all cylinder sets E of the form (1.5). If M_t is the restriction to $\mathcal{S}_t$ of an operator valued measure (necessarily unique) defined on the σ-algebra $\sigma(\mathcal{S}_t)$ generated by $\mathcal{S}_t$, then the analogue

$$e^{-t(A+V)} = \int_\Omega e^{-\int_0^t V(\omega(s))ds}\, dM_t(\omega) \tag{1.8}$$

of Eq. (1.4) is still valid for a large class of function $V:\mathbb{R}^d \to \mathbb{R}$ (Ref. 13, Chap. 3). We shall also call (1.8) a Feynman–Kac formula, although there may be no probability measure associated with the semigroup S of operators.

The present work is concerned with the Dirac equation in one space dimension. We take the free Dirac equation for a particle of mass $m \geqslant 0$ to be given by

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left(-i\hbar c\, \boldsymbol{\alpha} \frac{\partial}{\partial x} + mc^2 \boldsymbol{\beta} \right) \psi(x,t) = (H_0\psi)(x,t)$$

with $\psi(x,t) \in \mathbb{C}^2$ for $x \in \mathbb{R}$ and $t \geqslant 0$. The (2×2) matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ satisfy $\boldsymbol{\alpha}^2 = \boldsymbol{\beta}^2 = Id$ and $\boldsymbol{\alpha}\boldsymbol{\beta} + \boldsymbol{\beta}\boldsymbol{\alpha} = 0$. With an interaction represented by a potential $V:\mathbb{R} \to \mathbb{R}$, the Dirac equation becomes

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = (H_0 + V)\psi(x,t), \tag{1.9}$$

so in a coordinate system in which $\hbar = c = 1$, solutions of the initial value problem associated with Eq. (1.9) define a group $e^{-it(H_0+V)}$, $t \in \mathbb{R}$, of operators for suitable potentials V. By the usual abuse of notation, in the expression $H_0 + V$ the symbol V is interpreted as a multiplication operator acting in $L^2(\mathbb{R},\mathbb{C}^2)$.

Now suppose that $S(t) = e^{-itH_0}$ for $t \in \mathbb{R}$. Then formula (1.7) defines an additive operator valued set function M_t on the algebra $\mathcal{S}_t$. The set function M_t is actually the restriction to $\mathcal{S}_t$ of an operator valued measure $\widetilde{M}_t : \sigma(\mathcal{S}_t) \to \mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$ that is σ additive for the strong operator topology of $\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$. One way to see this is to take $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ to be the Pauli matrices

$$\boldsymbol{\alpha} = \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\beta} = -\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}. \tag{1.10}$$

Other possible representations are unitarily equivalent to this choice of matrices (known as the *Chiral representation*). Then $im\boldsymbol{\sigma}_1$ is a bounded perturbation of the operator $\boldsymbol{\sigma}_3(\partial/\partial x)$, which is the generator of a direct sum of translations acting on $L^2(\mathbb{R},\mathbb{C}^2)$ and $L^p(\mathbb{R},\mathbb{C}^2)$, for all $1 \leqslant p < \infty$.

It follows that for each $1 \leqslant p \leqslant \infty$, the inequality $\|S(t)\psi\|_p \leqslant e^{m|t|}\|\psi\|_p$ holds for all $t \in \mathbb{R}$ and $\psi \in L^p(\mathbb{R},\mathbb{C}^2_p) \cap L^2(\mathbb{R},\mathbb{C}^2)$. Here $\mathbb{C}^2_p$ denotes $\mathbb{C}^2$ with the ℓ^p-norm. The set functions defined by Eq. (1.7) are therefore bounded on the algebra $\mathcal{S}_t$ in operator norm by e^{mt} for $p = 1$ and $p = \infty$, and so for all $1 \leqslant p \leqslant \infty$ by the Riesz–Thorin interpolation theorem (Ref. 13, Chap. 2).

Further analysis shows that the operator valued measures M_t so defined are actually supported on the space Ω of all continuous paths $\omega : [0,\infty) \to \mathbb{R}$ with velocity equal to ± 1 and only finitely many changes of direction in each bounded time interval, see Ref. 11 or Sec. VII below.

A similar argument shows that the operator valued measures M_t, $t \geqslant 0$, also act on the space $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ of $\mathbb{C}^2$-valued Borel measures equipped with the total variation norm and on the space $\mathcal{L}^\infty(\mathbb{R},\mathbb{C}^2)$ of bounded Borel measurable functions with the weak topology $\sigma(\mathcal{L}^\infty(\mathbb{R},\mathbb{C}^2),\mathcal{M}(\mathbb{R},\mathbb{C}^2))$ defined by the duality between $\mathcal{L}^\infty(\mathbb{R},\mathbb{C}^2)$ and $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$.

Denote the constant function equal to one on $\mathbb{R}$ by $\mathbf{1}$. The space of all $n \times n$ matrices over $\mathbb{C}$ is denoted by $\mathbf{M}_n(\mathbb{C})$. The matrix valued measures $\nu_{t,x} : \sigma(\mathcal{S}_t) \to \mathbf{M}_2(\mathbb{C})$ defined by

$$\nu_{t,x}(E)v = (M_t(E)(\mathbf{1}v))(x), \quad E \in \sigma(\mathcal{S}_t), \quad v \in \mathbb{C}^2, \quad x \in \mathbb{R}, \quad t > 0, \tag{1.11}$$

were constructed by Ichinose[10] using the method of Nelson.[16] Representations of $\nu_{t,x}$ using a Poisson process have been obtained by Blanchard *et al.*[4] and Zastawniak,[19] see also Ref. 11 for a survey. The sample space properties mentioned above follow immediately from the Poisson process representations, see Proposition 6.1 below.

For suitable functions $V : \mathbb{R} \to \mathbb{R}$, we obtain the Feynman–Kac formula

$$e^{-it(H_0+V)} = \int_\Omega e^{-i\int_0^t V(\omega(s))ds}\, dM_t(\omega). \tag{1.12}$$

In order that $\int_0^t |V(\omega(s))|\, ds < \infty$ for all $\omega \in \Omega$ and $t > 0$, the function V must be *locally integrable* on $\mathbb{R}$. The set of paths with no changes in direction and crossing zero has nonzero M_t measure, so the same conclusion holds if $\int_0^t |V(\omega(s))|\, ds < \infty$ for M_t almost all $\omega \in \Omega$ and all $t > 0$.

Now suppose that V is locally integrable on $\mathbb{R}$. Because $H_0 + V$ is in the limit point case at $\pm\infty$ (Ref. 18, Theorem 6.8), the minimal operator (Ref. 18, p. 41) associated with the differential expression $H_0 + V$ is essentially self-adjoint (Ref. 18, Theorem 5.7). The functional calculus for self-adjoint operators makes sense of the left-hand side of Eq. (1.12). Note that the symbol $H_0 + V$ must be interpreted in this special sense, because we are not assuming that $H_0 + V$ is densely defined as the sum of two self-adjoint operators or as a quadratic form sum. Finally, the equality (1.12) follows after approximating V by cutoff functions $V_k = \chi_{\{|V| \leqslant k\}} V$, $k = 1,2,\ldots$.

We are concerned in this work with the potential $V(x) = (\gamma/|x|)$, $x \in \mathbb{R}\backslash\{0\}$, which is not a locally integrable function on $\mathbb{R}$. The operator $H_0 + V$ with domain $C_0^\infty(\mathbb{R}\backslash\{0\},\mathbb{C}^2)$ of all smooth

functions $\mathbb{C}^2$-valued with compact support in $\mathbb{R}\backslash\{0\}$ has a four parameter family of self-adjoint extensions studied by Benvegnù.[3] For every path $\omega\in\Omega$ passing through zero, $\int_0^t|V(\omega(s))|\,ds=\infty$ and Eq. (1.12) now makes no sense. In particular, there is no uniquely determined self-adjoint operator H_0+V associated with the left-hand side of (1.12).

By analogy with the three dimensional case, V is called a *Coulomb potential* and H_0+V is sometimes called the Hamiltonian of a one dimensional hydrogen atom. Models of this type arise in the investigation of quantum wires and in the description of electrons near the surface of liquid helium, see Ref. 3 for the references.

Another motivation for investigating self-adjoint extensions of H_0+V is that it is a particularly simple example of a singular perturbation of the free Hamiltonian H_0, in the sense that the differential expression H_0+V does not have an essentially self-adjoint minimal operator (Ref. 18, p. 41). Other examples include point interactions $H_0+c\,\delta$ and $H_0+c\,\delta'$ which have been the subject of recent investigations in both the nonrelativistic[2] and relativistic settings.[8]

Singular perturbations also arise in the perturbative approach to quantum field theory where renormalization of the interaction terms involving the subtraction of divergences is necessary. In order to make sense of the Feynman–Kac formula (1.12) for the Coulomb potential V, we find an analogous subtraction of divergences from the expression $\int_0^t V(\omega(s))\,ds$. The exponential functional $e^{-i\int_0^t V(\omega(s))\,ds}$ is thereby modified in the limit by terms whose modulus is one. By adjusting the subtraction of the divergence, we obtain a two-parameter family of self-adjoint extensions of $(H_0+V)|C_0^\infty(\mathbb{R}\backslash\{0\},\mathbb{C}^2)$. This is the origin of the word renormalization in the title. Our renormalization of the interaction is achieved by specifying the behavior of the interaction term for specific paths that cross the singularity at zero.

The appropriate modification of the Feynman–Kac formula (1.12) is given by

$$e^{-it(H_0+{}_\Gamma V)}=\int_\Omega F_t^\Gamma(\omega)\,dM_t(\omega). \tag{1.13}$$

Here $H_0+{}_\Gamma V$ is an element of the two-parameter family of self-adjoint extensions of $H_0+V|C_0^\infty(\mathbb{R}\backslash\{0\},\mathbb{C}^2)$ corresponding to certain boundary conditions denoted by Γ, and F_t^Γ is a *multiplicative functional* of the modulus one associated with Γ.

The term multiplicative functional is borrowed from the theory of Markov processes. To say that F_t, $t\geqslant 0$ is a multiplicative functional means that for each $t\geqslant 0$, the function $F_t:\Omega\to\mathbb{C}$ is measurable with respect to the σ-algebra $\sigma(\mathcal{S}_t)$ (or perhaps, an appropriate completion) and $F_{s+t}=F_t\circ\theta_s F_s$, M_{t+s}, a.e., where $\theta_s:\Omega\to\Omega$ is the shift map defined by $\theta_s\omega=\omega(s+\,\cdot\,)$, for all $s\geqslant 0$ and $\omega\in\Omega$.

It follows from the properties of the operator valued measures M_t that $t\mapsto\int_\Omega F_t\,dM_t$, $t>0$, is necessarily a *semigroup of operators* if F_t is M_t integrable for each $t>0$. The point of the Feynman–Kac formula is to represent the dynamical group of an interacting quantum system in terms of the integral of such a multiplicative functional with respect to the measures associated with a free system. More accurately, it is usually the analytic continuation of the dynamical group to imaginary time for which such a representation is obtained, otherwise, there may be no *measure* associate with the free system.

The usual example of a multiplicative functional is the Feynman–Kac functional $F_t(\omega)=e^{-i\int_0^t V(\omega(s))\,ds}$. The multiplicative functional F_t^Γ mentioned above is obtained by subtracting divergences from the expression $\int_0^t V(\omega(s))\,ds$ in a way prescribed by the boundary conditions Γ. In the case of the nonrelativistic hydrogen atom in one dimension, Fischer, Leschke, and Müller[7] show that the multiplicative functional

$$F_t(\omega)=\chi_{\{\int_0^t|V(\omega(s))|\,ds<\infty\}}e^{-\int_0^t V(\omega(s))ds}$$

is associated with the Dirichlet boundary condition at zero, but they do not investigate the possibility of obtaining semigroups associated with other self-adjoint extensions by multiplicative functionals.

The paper is organized as follows. Section II sets some terminology and notation concerning vector integration. An explicit formula for the operator valued measures associated with zero-mass case of the Dirac equation is given in Sec. III. Here the path space consists of all paths with constant velocity 1 or -1. In Sec. IV the Feynman–Kac formula for a nonsingular perturbation is calculated explicitly in the zero-mass case of the Dirac equation. Although this is an easy calculation, it sets the stage for the later arguments. The operator valued measures associated with point interactions in the zero-mass case of the Dirac equation can also be calculated explicitly. In Sec. V, we present the formula in Theorem 5.1 and we find that paths reflected at zero are introduced into the path space. The relative weight assigned to these paths is determined by the boundary conditions at zero that give the associated self-adjoint extension of the one dimensional Dirac operator. Next, in Sec. VI, we look at Coulomb potentials in the zero-mass case. An explicit calculation of the Feynman–Kac formula is possible here too, but we must subtract a logarithmic divergence from the exponent of the Feynman–Kac functional in a manner prescribed by the boundary conditions at zero for those paths which hit the origin. The case of nonzero mass treated in Sec. VII is more complicated. The path space consists of continuous paths with velocity ± 1 and finitely many changes of direction in any bounded time interval, but we still obtain the Feynman–Kac formula for Coulomb potentials by subtracting a logarithmic divergence from the exponent of the Feynman–Kac functional in a manner prescribed by the boundary conditions at zero.

II. OPERATOR VALUED MEASURES

Because we shall be dealing with operator valued measures, we make a few remarks about vector integration. Details may be found in Ref. 15. Let X be a Banach space, $(\Sigma,\mathcal{E})$ a measurable space and $m:\mathcal{E}\to X$ a vector measure, that is, an X-valued set function σ-additive for the norm topology of X. Here σ-additive has the same meaning as it does for scalar valued measures: $m(\cup_{j=1}^{\infty}E_j)=\Sigma_{j=1}^{\infty}m(E_j)$ for all pairwise disjoint elements E_j, $j=1,2,\ldots$, of $\mathcal{E}$. The vector space of all continuous linear functionals on X is denoted by X'

A function $f:\Sigma\to\mathbb{C}$ is said to be *m-integrable* if for each $\xi\in X'$, the function f is integrable with respect to the scalar measure $\langle m,\xi\rangle:E\mapsto\langle m(E),\xi\rangle$, $E\in\mathcal{E}$, and for each $E\in\mathcal{E}$, there exists a vector $(f.m)(E)$ belonging to X such that the equality

$$\langle (f.m)(E),\xi\rangle=\int_E f d\langle m,\xi\rangle$$

holds for every $\xi\in X'$. It turns out that the mapping $E\mapsto(f.m)(E)$, $E\in\mathcal{E}$, is necessarily σ-additive for the norm topology of X, that is, the indefinite integral $f.m=fm$ of an m-integrable function f is again a vector measure. We shall also write $\int_E f\,dm$ for the vector $(f.m)(E)$, $E\in\mathcal{E}$.

Let $\mathcal{L}(X)$ denote the space of bounded linear operators acting on X, equipped with the strong operator topology. A similar notion of integrability applies to a function $f:\Sigma\to\mathbb{C}$ with respect to an operator valued measure $M:\mathcal{E}\to\mathcal{L}(X)$, that is, an $\mathcal{L}(X)$-valued set function σ-additive for the *strong operator topology*. For each $x\in X$ and $\xi\in X'$, the function f is integrable with respect to the scalar measure $\langle Mx,\xi\rangle:E\mapsto\langle M(E)x,\xi\rangle$, $E\in\mathcal{E}$, and for each $E\in\mathcal{E}$, there exists an operator $(f.M)(E)$ belonging to $\mathcal{L}(X)$ such that the equality

$$\langle (f.M)(E)x,\xi\rangle=\int_E f\,d\langle Mx,\xi\rangle$$

holds for every $x \in X$ and $\xi \in X'$. The indefinite integral $fM: E \mapsto (f.M)(E)$, $E \in \mathcal{E}$, is σ-additive for the strong operator topology of $\mathcal{L}(X)$. We shall also write $\int_E f\, dM$ for the bounded linear operator $(f.M)(E)$, $E \in \mathcal{E}$.

With integration understood in the above sense, the usual monotone and dominated convergence theorems are valid. In particular, bounded measurable functions are integrable. If $\phi: \Sigma \to \Xi$ is a measurable map into the measurable space $(\Xi, \mathcal{S})$, then $M \circ \phi^{-1}$ denotes the operator valued measure $S \mapsto M(\phi^{-1}(S))$, $S \in \mathcal{S}$. Notation applied to bounded linear operators will also be adopted for operator valued measures. If $S: X \to X$ and $T: X \to X$ are bounded linear operators, then the operator valued measure $E \mapsto SM(E)T$, $E \in \mathcal{E}$, is denoted by SMT. The direct sum $M_1 \oplus M_2$ of two operator valued measures $M_1: \mathcal{E} \to \mathcal{L}(H_1)$, $M_2: \mathcal{E} \to \mathcal{L}(H_2)$ acting on Hilbert spaces H_1, H_2 is defined by $M_1 \oplus M_2: E \mapsto M_1(E) \oplus M_2(E)$, $E \in \mathcal{E}$.

An operator valued measure $M: \mathcal{E} \to \mathcal{L}(X)$ is said to be *concentrated* on a set A if $M(E) = 0$ for all $E \in \mathcal{E}$ disjoint from A.

III. THE TRANSLATION MEASURES

The path space measures associated with translation on $\mathbb{R}$ are particularly simple. We shall construct the operator valued measures associated with the one dimensional Dirac equation out of these, so we give the explicit calculation of this special case here.

Let $Q: \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mathbb{R}))$ be the spectral measure of multiplication by characteristic functions of Borel subsets of $\mathbb{R}$. Let p be the self-adjoint operator $(1/i)(\partial/\partial x)$ acting in $L^2(\mathbb{R})$. We can explicitly calculate the operator valued measures defined by formula (1.7) in the case that $S(t) = e^{ipt}$, $t \in \mathbb{R}$.

Then for n times $0 < t_1 < \cdots < t_n < t$ and n Borel subsets $B_1, \ldots, B_n$ of $\mathbb{R}$,

$$\begin{aligned}
&(e^{ip(t-t_n)} Q(B_n) e^{ip(t_n - t_{n-1})} \cdots Q(B_1) e^{ipt_1} f)(x) \\
&\quad = \chi_{B_n}(x + t - t_n)(e^{ip(t_n - t_{n-1})} Q(B_{n-1}) \cdots Q(B_1) e^{ipt_1} f)(x + t - t_n) \\
&\quad = \chi_{B_n}(x + t - t_n) \chi_{B_{n-1}}(x + t - t_{n-1}) \cdots \chi_{B_1}(x + t - t_1) f(x + t) \\
&\quad = (e^{ipt} Q \circ \gamma_+^{-1}(E) f)(x). \qquad (3.1)
\end{aligned}$$

Here $E \subset \Omega$ is the cylinder set (1.5) and Ω is the collection of all paths $\omega: [0, \infty) \to \mathbb{R}$ for which there exists $x \in \mathbb{R}$ such that either

(a) $\omega(s) = x + s$, for all $s \geqslant 0$, or,

(b) $\omega(s) = x - s$, for all $s \geqslant 0$.

The mapping $\gamma_+: \mathbb{R} \to \Omega$ is defined by $\gamma_+(x)(s) = x - s$ for $s \geqslant 0$ and analogously, $\gamma_-: \mathbb{R} \to \Omega$ is defined by $\gamma_-(x)(s) = x + s$ for $x \geqslant 0$ and $s \geqslant 0$. The set Ω has the finest topology for which the maps $\gamma_\pm$ are continuous. Then

$$M_t^+ := e^{ipt} Q \circ \gamma_+^{-1}$$

is an $\mathcal{L}(L^2(\mathbb{R}))$-valued Borel measure on Ω. Similarly, set

$$M_t^- := e^{-ipt} Q \circ \gamma_-^{-1}.$$

The range of $\gamma_\pm$ is the set of characteristic lines of the equation

$$\frac{\partial u}{\partial t} = \pm ipu = \pm \frac{\partial u}{\partial x}$$

defining translations on $\mathbb{R}$.

Remark 3.1: The same argument as above applies to a classical dynamical system with the maps $\gamma_\pm$ replaced by the flow of the system.

Now suppose that A is the self-adjoint differential operator

$$A=\boldsymbol{\sigma}_3\frac{1}{i}\frac{\partial}{\partial x}=\frac{1}{i}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{\partial}{\partial x} \tag{3.2}$$

acting in $L^2(\mathbb{R},\mathbb{C}^2)$. Set $S(t)=e^{-iAt}$ for all $t\in\mathbb{R}$ and $Q:\mathcal{B}(\mathbb{R})\to\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$ is multiplication by characteristic functions. For every set E of the form (1.5), $M_t(E)\in\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$ is the operator given by formula (1.7). Then $A=p\oplus(-p)$ in $L^2(\mathbb{R},\mathbb{C}^2)$ and M_t defines an $\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$-valued Borel measure on Ω given by

$$M_t=(e^{-ipt}Q\circ\gamma_-^{-1})\oplus(e^{ipt}Q\circ\gamma_+^{-1})=M_t^-\oplus M_t^+. \tag{3.3}$$

IV. THE FEYNMAN–KAC FORMULA FOR NONSINGULAR POTENTIALS

Let $V:\mathbb{R}\to\mathbb{R}$ be a locally integrable function. In the present context, this is what is meant by a nonsingular interaction. The spectral measure $Q:\mathcal{B}(\mathbb{R})\to\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$ of multiplication by characteristic functions is the spectral resolution of the position operator for a Dirac particle on the line. Then

$$Q(V):=\int_{\mathbb{R}}V\,dQ$$

is the self-adjoint operator of multiplication by V acting in $L^2(\mathbb{R},\mathbb{C}^2)$. The symbol $\int_{\mathbb{R}}V\,dQ$ is interpreted literally because

$$\mathcal{D}(Q(V))=\{f\in L^2(\mathbb{R},\mathbb{C}^2):V\ \text{is}\ (Qf)\ \text{integrable}\}$$

and $Q(V)f:=\int_{\mathbb{R}}V\,d(Qf)$ for all $f\in\mathcal{D}(Q(V))$.

As mentioned in the Introduction, the operator $A+Q(V)$ whose domain is the set of all functions $u\in L^2(\mathbb{R},\mathbb{C}^2)$, absolutely continuous on bounded intervals such that $Au+Vu\in L^2(\mathbb{R},\mathbb{C}^2)$ is self-adjoint. Therefore, $e^{-it(A+Q(V))}$, $t\in\mathbb{R}$, is a continuous unitary group of operators. The following Feynman–Kac formula represents the semigroup of operators as a functional integral. In this special case, both sides of the formula can be calculated explicitly. The proof below sets the stage for the more involved calculations later. For each $\omega\in\Omega$, set $X_s(\omega)=\omega(s)$, $s\geqslant 0$.

According to the notation mentioned above, the value of the operator valued measure

$$e^{-ipt}Q\circ\gamma_-^{-1}:\mathcal{B}(\Omega)\to\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$$

on the Borel subset E of Ω is the bounded linear operator $e^{-ipt}Q(\gamma_-^{-1}(E))$.

Proposition 4.1: The function $\omega\mapsto e^{-i\int_0^t V\circ X_s(\omega)\,ds}$, $\omega\in\Omega$, exists and is M_t-integrable for each $t\geqslant 0$. Furthermore,

$$e^{-it(A+Q(V))}=\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,dM_t. \tag{4.1}$$

Proof: Because V is locally integrable, $\int_0^t|V(x-s)|\,ds<\infty$ and $\int_0^t|V(x+s)|\,ds<\infty$ for every $x\in\mathbb{R}$. Hence, $\int_0^t|V(\omega(s))|\,ds<\infty$ for every $\omega\in\Omega$. The measurable function $\omega\mapsto e^{-i\int_0^t V\circ X_s(\omega)\,ds}$, $\omega\in\Omega$, has absolute value one, so it is integrable with respect to the operator valued measure M_t. We calculate its integral from Eq. (3.3) by observing that

$$\begin{aligned}\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,dM_t &= \int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,d(M_t^-\oplus M_t^+)\\ &= \left(\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,dM_t^-\right)\oplus\left(\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,dM_t^+\right)\\ &= \left(\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,d(e^{-ipt}Q\circ\gamma_-^{-1})\right)\oplus\left(\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,d(e^{ipt}Q\circ\gamma_+^{-1})\right)\\ &= \left(e^{-ipt}\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,d(Q\circ\gamma_-^{-1})\right)\oplus\left(e^{-ipt}\int_\Omega e^{-i\int_0^t V\circ X_s\,ds}\,d(Q\circ\gamma_+^{-1})\right)\\ &= (e^{-ipt}Q(e^{-i\int_0^t V\circ X_s\circ\gamma_-\,ds}))\oplus(e^{ipt}Q(e^{-i\int_0^t V\circ X_s\circ\gamma_+\,ds})).\end{aligned}\tag{4.2}$$

Now let $v\in L^2(\mathbb{R})$. Then for almost all $x\in\mathbb{R}$, we have

$$(Q(e^{-i\int_0^t V\circ X_s\circ\gamma_+\,ds})v)(x)=e^{-i\int_0^t V\circ X_s\circ\gamma_+(x)\,ds}v(x)=e^{-i\int_0^t V(x-s)\,ds}v(x)$$

so we have

$$\begin{aligned}(e^{ipt}Q(e^{-i\int_0^t V\circ X_s\circ\gamma_+\,ds})v)(x) &= e^{-i\int_0^t V\circ X_s\circ\gamma_+(x+t)\,ds}v(x+t)\\ &= e^{-i\int_0^t V(x+t-s)\,ds}v(x+t)\\ &= e^{-i\int_0^t V(x+s)\,ds}v(x+t)\\ &= e^{-i\int_x^{x+t} V(s)\,ds}v(x+t).\end{aligned}$$

Similarly,

$$(e^{-ipt}Q(e^{-i\int_0^t V\circ X_s\circ\gamma_-\,ds})u)(x)=e^{-i\int_{x-t}^{x} V(s)\,ds}u(x-t).$$

Integration by parts verifies that for $\phi=\binom{\phi_1}{\phi_2}\in L^2(\mathbb{R},\mathbb{C}^2)$, the equality

$$(e^{-it(A+Q(V))}\phi)(x)=\begin{pmatrix} e^{-i\int_{x-t}^{x} V(s)\,ds}\phi_1(x-t)\\ e^{-i\int_x^{x+t} V(s)\,ds}\phi_2(x+t)\end{pmatrix}$$

holds for almost all $x\in\mathbb{R}$, so now equality (4.1) follows from (4.2). □

V. POINT INTERACTIONS: ZERO MASS

Let A_Γ be the operator (3.2) with the boundary condition

$$\begin{pmatrix}\phi_1(0+)\\ \phi_2(0-)\end{pmatrix}=\Gamma\begin{pmatrix}\phi_1(0-)\\ \phi_2(0+)\end{pmatrix}\tag{5.1}$$

at zero with respect to the unitary matrix

$$\Gamma=\eta\begin{pmatrix}\alpha & -\overline{\beta}\\ \beta & \overline{\alpha}\end{pmatrix}\tag{5.2}$$

with $\alpha,\beta,\eta\in\mathbb{C}$ satisfying $|\alpha|^2+|\beta|^2=1$ and $|\eta|=1$.

In this simple case, a calculation shows that the matrix Γ corresponds to a unitary map from one deficiency subspace of $A|C_0^\infty(\mathbb{R}\setminus\{0\},\mathbb{C}^2)$ onto another, so A_Γ is self-adjoint and every self-adjoint extension of $A|C_0^\infty(\mathbb{R}\setminus\{0\},\mathbb{C}^2)$ may be obtained in this way (Ref. 18, Theorem 4.4); see also Ref. 5 for further discussion of this point.

A careful analysis of the self-adjoint operator $A_\Gamma - m\boldsymbol{\sigma}_1$ (or rather, a self-adjoint operator unitarily equivalent to this one) is given in Ref. 9. Certain choices of the boundary condition Γ are associated with point interactions.

The present chiral representation is better adapted to the calculation of functional integrals, but the Dirac representation of Refs. 3 and 9 leads to a simpler determination of the boundary conditions that arise from taking the nonrelativistic limit.

For suitable $\phi\in L^2(\mathbb{R},\mathbb{C}^2)$ the function

$$\begin{pmatrix} u(x,t)\\ v(x,t)\end{pmatrix}=(e^{-itA_\Gamma}\phi)(x),\quad x\in\mathbb{R}, \tag{5.3}$$

is a solution $\psi(x,t)=\binom{u(x,t)}{v(x,t)}$ of the equation

$$\frac{\partial\psi}{\partial t}+\boldsymbol{\sigma}_3\frac{\partial\psi}{\partial x}=0,\quad \psi(\,\cdot\,,t)\in L^2(\mathbb{R},\mathbb{C}^2)$$

satisfying the initial condition $\psi(x,0)=\phi(x)$, $x\in\mathbb{R}$, and satisfying the boundary condition (5.1).

Let $t>0$. If $x>0$ or $x<-t$, then $v(x,t)=\phi_2(x+t)$ and if $x<0$ or $x>t$, then $u(x,t)=\phi_1(x-t)$. In the region $-t<x<0$, there exists another function Φ such that $v(x,t)=\Phi(x+t)$. To ensure that the boundary condition (5.1) is satisfied, we must have

$$\Phi(t-)=\eta[\beta\phi_1((-t)-)+\overline{\alpha}\phi_2(t+)]$$

for all $t>0$. Therefore, if ϕ_1,ϕ_2 are absolutely continuous on subintervals of $\mathbb{R}\setminus\{0\}$ and satisfy the boundary condition (5.1), it follows that

$$v(x,t)=\eta[\beta\phi_1((-(x+t))+\overline{\alpha}\phi_2(x+t)],\quad -t<x<0.$$

Similarly, we have

$$u(x,t)=\eta[\alpha\phi_1(x-t)-\overline{\beta}\phi_2(-(x-t))],\quad 0<x<t.$$

It follows that for any $\phi\in L^2(\mathbb{R},\mathbb{C}^2)$, Eq. (5.3) holds with

$$u(x,t)=\begin{cases}\phi_1(x-t) & \text{for all } x>t,\ x<0\\ \eta[\alpha\phi_1(x-t)-\overline{\beta}\phi_2(-(x-t))] & \text{for all } 0<x<t,\end{cases} \tag{5.4}$$

$$v(x,t)=\begin{cases}\phi_2(x+t) & \text{for all } x<-t,\ x>0\\ \eta[\beta\phi_1(-(x+t))+\overline{\alpha}\phi_2(x+t)] & \text{for all } -t<x<0.\end{cases} \tag{5.5}$$

Let $S(t)=e^{-itA_\Gamma}$ for all $t\geqslant 0$ and let M_t^Γ be the additive set function defined by Eq. (1.7) for cylinder sets E given by formula (1.5). Define the paths $\zeta_\pm:\mathbb{R}\to\Omega$ which reflect at $x=0$ by the formulas

$$\zeta_+(x)(s)=\operatorname{sgn}(x)|x-s|,\quad s\geqslant 0,\ x\in\mathbb{R}, \tag{5.6}$$

$$\zeta_-(x)(s)=\operatorname{sgn}(x)|x+s|,\quad s\geqslant 0,\quad x\in\mathbb{R}. \tag{5.7}$$

Here we enlarge Ω so as to include not only the ranges of the characteristic mappings $\gamma_\pm$, but also of the reflected paths $\zeta_\pm(x)$, $x\in\mathbb{R}$, that is, set $\Omega_0=\gamma_+(\mathbb{R})\cup\gamma_-(\mathbb{R})$, Ω_1

$=\zeta_+((0,\infty))\cup\zeta_-((-\infty,0))$ and $\Omega=\Omega_0\cup\Omega_1$. Then Ω_0 is the set of paths with no reflection at zero and Ω_1 is the set of paths with a reflection at zero for some positive time.

Theorem 5.1: *Let $S(t)=e^{-iA_\Gamma t}$ for all $t\in\mathbb{R}$ and for each $t\geqslant 0$ let M_t be the operator valued measure acting on $L^2(\mathbb{R},\mathbb{C}^2)$ defined by formula (1.5).*

Then there exist operator valued measures M_t^0 and $M_t^{\Gamma,1}$ such that $M_t^\Gamma=M_t^0+M_t^{\Gamma,1}$, where M_t^0 is concentrated on paths $\omega\in\Omega$ which do not hit zero in the interval $(0,t)$ and $M_t^{\Gamma,1}$ is concentrated on those paths $\omega\in\Omega$ that do.

More precisely, set $(Rf)(x)=f(-x)$ for $f\in L^2(\mathbb{R},\mathbb{C})$, $x\in\mathbb{R}$. Then

$$M_t^0=\chi_{\{X_0X_t>0\}}.[(e^{-ipt}Q\circ\gamma_-^{-1})\oplus(e^{ipt}Q\circ\gamma_+^{-1})], \tag{5.8}$$

$$M_t^{\Gamma,1}=\eta\begin{pmatrix}\alpha\chi_{\{X_0X_t<0\}}.(e^{-ipt}Q\circ\gamma_-^{-1}) & -\overline{\beta}(\chi_{(0,t)}.[e^{-ipt}QR])\circ\zeta_-^{-1}\\ \beta(\chi_{(-t,0)}.[e^{ipt}QR])\circ\zeta_+^{-1} & \overline{\alpha}\chi_{\{X_0X_t<0\}}.(e^{ipt}Q\circ\gamma_+^{-1})\end{pmatrix}. \tag{5.9}$$

The operator valued measure M_t^0 is concentrated on the Borel set $\Omega_0\cap\{X_0X_t>0\}$ and $M_t^{\Gamma,1}$ is concentrated on $(\Omega_0\cap\{X_0X_t<0\})\cup\zeta_+((0,t))\cup\zeta_-((-t,0))$.

Proof: Let $E\subset\Omega$ be a nonempty cylinder set (1.5) and $f\in L^2(\mathbb{R},\mathbb{C}^2)$. Then for almost all x outside the interval $[-t,t]$, a calculation similar to (3.1) holds because the formula for e^{-iAt} applies, so that

$$(M_t^\Gamma(E)f)(x)=([(e^{-ipt}Q\circ\gamma_-^{-1}(E))\oplus(e^{ipt}Q\circ\gamma_+^{-1}(E))]f)(x).$$

Then neither path $\gamma_\pm(x\pm t)$ hits zero in the time interval $[0,t]$. Hence, $(M_t^\Gamma(E)f)(x)$ is equal to

$$\begin{aligned}&((\chi_{\{X_0X_t>0\}}.[(e^{-ipt}Q\circ\gamma_-^{-1})\oplus(e^{ipt}Q\circ\gamma_+^{-1})])(E)f)(x)\\&\quad+\left(\eta\begin{pmatrix}\alpha\chi_{\{X_0X_t<0\}}.(e^{-ipt}Q\circ\gamma_-^{-1})(E) & -\overline{\beta}(\chi_{(0,t)}.[e^{-ipt}QR])\circ\zeta_-^{-1}(E)\\ \beta(\chi_{(-t,0)}.[e^{ipt}QR])\circ\zeta_+^{-1}(E) & \overline{\alpha}\chi_{\{X_0X_t<0}.(e^{ipt}Q\circ\gamma_+^{-1})(E)\end{pmatrix}f\right)(x)\end{aligned} \tag{5.10}$$

for almost all of these x because the second term is zero.

Now suppose that $-t<x<0$ and E is a nonempty cylinder set (1.5). Then there exists $k=0,\ldots,n$ such that $x+t-t_k>0$ and $x+t-t_{k+1}<0$, where we have set $t_0=0$ and $t_{n+1}=t$. Then we have

$$\begin{aligned}(M_t^\Gamma(E)f)_2(x)&=(e^{-i(t-t_n)A_\Gamma}Q(B_n)e^{-i(t_n-t_{n-1})A_\Gamma}\cdots Q(B_1)e^{-it_1A_\Gamma}f)_2(x)\\&=\chi_{B_n}(x+t-t_n)(e^{-i(t_n-t_{n-1})A_\Gamma}Q(B_{n-1})\cdots Q(B_1)e^{-it_1A_\Gamma}f)_2(x+t-t_n)\\&\vdots\\&=\chi_{B_n}(x+t-t_n)\cdots\chi_{B_{k+1}}(x+t-t_{k+1})\\&\quad\times(e^{-i(t_{k+1}-t_k)A_\Gamma}Q(B_k)\cdots Q(B_1)e^{-it_1A_\Gamma}f)_2(x+t-t_{k+1})\\&=\eta\chi_{B_n}(x+t-t_n)\cdots\chi_{B_{k+1}}(x+t-t_{k+1})\\&\quad\times[\beta\chi_{B_k}(-(x+t-t_k))(e^{-i(t_k-t_{k-1})A_\Gamma}Q(B_{k-1})\cdots Q(B_1)e^{-it_1A_\Gamma}f)_1(-(x\\&\quad+t-t_k))+\overline{\alpha}\chi_{B_k}(x+t-t_k)(e^{-i(t_k-t_{k-1})A_\Gamma}Q(B_{k-1})\cdots Q(B_1)e^{-it_1A_\Gamma}f)_2(x\\&\quad+t-t_k)]\end{aligned}$$

[by Eq. (5.5)]

$$\vdots$$

$$\begin{aligned}
&= \eta\chi_{B_n}(x+t-t_n)\cdots\chi_{B_{k+1}}(x+t-t_{k+1})\\
&\quad\times[\beta\chi_{B_k}(-(x+t-t_k))\cdots\chi_{B_1}(-(x+t-t_1))f_1(-(x+t))\\
&\quad+\overline{\alpha}\chi_{B_k}(x+t-t_k)\cdots\chi_{B_1}(x+t-t_1)f_2(x+t)]\\
&= \eta(\beta e^{itp}Q\circ\zeta_+^{-1}(E)Rf_1+\overline{\alpha}e^{itp}Q\circ\gamma_+^{-1}(E)f_2)(x).
\end{aligned}$$

These equalities hold true for almost all $-(t-t_k)<x<-(t-t_{k+1})$.

Because $x<0$, we have $x-(t-t_j)<0$ for all $j=0,\ldots,n+1$. It follows that

$$\begin{aligned}
(M_t^\Gamma(E)f)_1(x) &= (e^{-i(t-t_n)A_\Gamma}Q(B_n)e^{-i(t_n-t_{n-1})A_\Gamma}\cdots Q(B_1)e^{-it_1A_\Gamma}f)_1(x)\\
&= \chi_{B_n}(x-(t-t_n))(e^{-ip(t_n-t_{n-1})}Q(B_{n-1})\cdots Q(B_1)e^{-ipt_1}f)_1(x-(t-t_n))\\
&= \chi_{B_n}(x-(t-t_n))\chi_{B_{n-1}}(x-(t-t_{n-1}))\cdots\chi_{B_1}(x-(t-t_1))f_1(x-t)\\
&= (e^{-ipt}Q\circ\gamma_-^{-1}(E)f_1)(x).
\end{aligned}$$

Hence, the equality

$$(M_t^\Gamma(E)f)(x)=\begin{pmatrix} e^{-ipt}Q\circ\gamma_-^{-1}(E)f_1\\ \eta(\beta e^{itp}Q\circ\zeta_+^{-1}(E)Rf_1+\overline{\alpha}e^{itp}Q\circ\gamma_+^{-1}(E)f_2)\end{pmatrix}(x) \tag{5.11}$$

holds for almost all $-(t-t_k)<x<-(t-t_{k+1})$. As k varies from 0 to n, we obtain the representation (5.11) almost everwhere on the interval $(-t,0)$ for the given cylinder set E. Because E is any cylinder set, the representation (5.11) holds on every cylinder set for almost all $x\in(-t,0)$. We need to check that the right-hand side of Eq. (5.11) is given by the expression (5.10) for almost all $x\in(-t,0)$.

Now the element $((\chi_{\{X_0X_t>0\}}.[(e^{-ipt}Q\circ\gamma_-^{-1})\oplus(e^{ipt}Q\circ\gamma_+^{-1})])(E)f)_1$ of $L^2(\mathbb{R})$ is equal to $e^{-ipt}\chi_{\gamma_-^{-1}(\{X_0X_t>0\}\cap E)}f_1$, which, at $x\in(-t,0)$ is $\chi_{\gamma_-^{-1}(\{X_0X_t>0\}\cap E)}(x-t)f_1(x-t)$. But $X_0(\gamma_-(x-t))X_t(\gamma_-(x-t))>0$ for $x<0$, so this is just

$$\chi_{\gamma_-^{-1}(E)}(x-t)f_1(x-t)=(e^{-ipt}Q\circ\gamma_-^{-1}(E)f_1)(x),$$

corresponding to the first element of (5.11). Because $X_0(\gamma_-(x-t))X_t(\gamma_-(x-t))>0$ for $x<0$, no other contribution is made by the first elements of (5.10).

On the other hand, $((\chi_{\{X_0X_t>0\}}.[(e^{-ipt}Q\circ\gamma_-^{-1})\oplus(e^{ipt}Q\circ\gamma_+^{-1})])(E)f)_2(x)=0$ for $-t<x<0$, because then $X_0(\gamma_+(x+t))X_t(\gamma_+(x+t))<0$. It follows that $(M_t^\Gamma(E)f)(x)$ is equal to the expression (5.10).

A similar argument applies to the interval $(0,t)$, for then $X_0(\gamma_+(x+t))X_t(\gamma_+(x+t))>0$.

Let ϕ be an integrable $\mathbb{C}^2$-valued simple function. Replacing f by ϕ, the formulas above make sense for *each* $x\in\mathbb{R}$. But, for each $x\in\mathbb{R}$ and $t>0$, there is at most one path $\omega\in\Omega$ such that $\omega=\gamma_\pm(x\pm t)$ or $\omega=\zeta_\pm(x\pm t)$ and $X_0(\omega)X_t(\omega)=0$.

Then $(M_t^\Gamma(E\cap\{X_0X_t=0\})\phi)(x)=0$ for all $E\in\mathcal{S}_t$ and almost all $x\in\mathbb{R}$. The image $[\phi]$ of ϕ in $L^2(\mathbb{R},\mathbb{C}^2)$ has the property that $M_t^\Gamma(E\cap\{X_0X_t=0\})[\phi]=0$ as an element of $L^2(\mathbb{R},\mathbb{C}^2)$ for every $E\in\mathcal{S}_t$. Integrable simple functions are dense in $L^2(\mathbb{R},\mathbb{C}^2)$, so the cylinder set $\{X_0X_t=0\}$ is an M_t^Γ-null set. This establishes the representation $M_t^\Gamma(E)=M_t^0(E)+M_t^{\Gamma,1}(E)$ on all cylinder sets E. Both sides of the equation are σ additive, so we have equality on all Borel subsets E of Ω.□

Remark 5.2: (a) According to Theorem 5.1, relativistic point interactions in one dimension are also associated with $\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$-valued measures on the path space Ω. Nevertheless, the smallest number $C>0$ for which $\|e^{-itA_\Gamma}f\|_\infty\leqslant C\|f\|_\infty$ for all $t\in\mathbb{R}$ and $f\in L^2(\mathbb{R},\mathbb{C}^2)\cap L^\infty(\mathbb{R},\mathbb{C}^2)$ is

$|\alpha|+|\beta|$. Because

$$\sup\{|a|+|b|: a,b\in\mathbb{C},\ |a|^2+|b|^2=1\}=\sqrt{2},$$

the group e^{-itA_Γ} need not be similar to a group of contractions on $L^\infty(\mathbb{R},\mathbb{C}^2)$—this is the usual condition for constructing path space measures. In the case of point interactions δ associated with the Laplacian Δ in $\mathbb{R}^d$, the positive operators $e^{t(\Delta-\delta)}$, $t>0$, are not even *bounded* on $L^\infty(\mathbb{R}^d)$ for $d=1,2,3$.[6,1]

(b) The effect of off-diagonal terms in the unitary matrix Γ is to introduce paths $\zeta_\pm(x)$, $x\in\mathbb{R}$, that scatter off the singular interaction at the origin. The off-diagonal terms of Γ are the reflection coefficients and the diagonal terms are the transmission coefficients of the transmitted path. An operator valued measure $M_t^{\Gamma,1}$ concentrated on the associated reflected or transmitted paths is associated with each of these coefficients via formula (5.9).

VI. THE FEYNMAN–KAC FORMULA FOR SINGULAR POTENTIALS: ZERO MASS

Let $\gamma\in\mathbb{R}$ and $V(x)=\gamma/|x|$ for all $x\in\mathbb{R}$ with $x\neq 0$. Let Γ be a (2×2) unitary matrix—any such matrix can be expressed in the form (5.2). Then the operator

$$\frac{1}{i}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{\partial}{\partial x}+\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\frac{\gamma}{|x|} \tag{6.1}$$

satisfying the boundary conditions

$$\begin{pmatrix}\lim_{x\to 0+}|x|^{i\gamma}u(x)\\ \lim_{x\to 0-}|x|^{i\gamma}v(x)\end{pmatrix}=\Gamma\begin{pmatrix}\lim_{x\to 0-}|x|^{-i\gamma}u(x)\\ \lim_{x\to 0+}|x|^{-i\gamma}v(x)\end{pmatrix} \tag{6.2}$$

is self-adjoint and written as $A+_\Gamma Q(V)$. As mentioned above in the case $\gamma=0$, the collection of all unitary matrices Γ is in one-to-one correspondence with isometries from one deficiency subspace of $(A+Q(V))|C_0^\infty(\mathbb{R}\backslash\{0\},\mathbb{C}^2)$ onto another.

Then $e^{-it(A+_\Gamma Q(V))}$, $t\in\mathbb{R}$, is a continuous unitary group of operators. Calculations similar to those of Sec. V show that for $\phi\in L^2(\mathbb{R},\mathbb{C}^2)$, the function

$$\begin{pmatrix}u(x,t)\\ v(x,t)\end{pmatrix}=(e^{-it(A+_\Gamma Q(V))}\phi)(x),\quad x\in\mathbb{R}, \tag{6.3}$$

is given by

$$u(x,t)=\begin{cases}e^{-i\int_{x-t}^{x}V(s)\,ds}\phi_1(x-t) & \text{for all } x>t,\ x<0\\ \eta e^{-i\gamma(\ln|x|+\ln|x-t|)}[\alpha\phi_1(x-t)-\overline{\beta}\phi_2(-(x-t))] & \text{for all } 0<x<t,\end{cases}$$

$$v(x,t)=\begin{cases}e^{-i\int_{x}^{x+t}V(s)\,ds}\phi_2(x+t) & \text{for all } x<-t,\ x>0\\ \eta e^{-i\gamma(\ln|x|+\ln(x+t))}[\beta\phi_1(-(x+t))+\overline{\alpha}\phi_2(x+t)] & \text{for all } -t<x<0.\end{cases}$$

Suppose that $\beta=0$ and $\eta\alpha=e^{-i\kappa_1}$, $\eta\overline{\alpha}=e^{-i\kappa_2}$ for numbers $0\leqslant\kappa_j<2\pi$.

For the moment, we take Ω to be the collection of all paths that lie in the range of the maps $\gamma_\pm$, that is, there exists $x\in\mathbb{R}$ such that either $\omega(s)=x+s$ for all $s\geqslant 0$, or $\omega(s)=x-s$. Suppose that $\omega\in\Omega$ is a path for which $X_0(\omega)X_t(\omega)<0$, which is to say that the path ω hits the origin at some time in the open interval $(0,t)$. Set

$$\left\langle\int_0^t V\circ X_s(\omega)\,ds\right\rangle_\Gamma=\begin{cases}\gamma(\ln|\omega(0)|+\ln|\omega(t)|)+\kappa_1 & \text{if } \omega'(s)=1,\ s>0\\ \gamma(\ln|\omega(0)|+\ln|\omega(t)|)+\kappa_2 & \text{if } \omega'(s)=-1,\ s>0.\end{cases} \tag{6.4}$$

Then the measurable function $F_t^\Gamma:\Omega\to\mathbb{C}$ is defined by

$$F_t^\Gamma = \chi_{\{X_0 X_t > 0\}} . e^{-i\int_0^t V\circ X_s\, ds} + \chi_{\{X_0 X_t < 0\}} . e^{-i\langle \int_0^t V\circ X_s\, ds\rangle_\Gamma}. \tag{6.5}$$

Here F_t^Γ is a *multiplicative functional*. The multiplicative property is borrowed from the theory of Markov processes:

$$F_{s+t}^\Gamma(\omega) = F_t^\Gamma(\omega_s) F_s^\Gamma(\omega) \quad \text{a.e.}, \tag{6.6}$$

with $\omega_s(r) = \omega(s+r)$. It is natural to view

$$\left\langle \int_0^t V\circ X_s\, ds \right\rangle_\Gamma$$

as a renormalization of the expression $\int_0^t V\circ X_s\, ds$ on the set of all paths $\omega \in \Omega$ such that $X_0(\omega) X_t(\omega) < 0$. For example, suppose that $0 < x < t$ and $\omega(s) = x - s$. Then

$$\begin{aligned}\int_{[0,t]\cap\{|\omega(s)|>\epsilon\}} V(\omega(s))\, ds &= \int_{x+\epsilon}^t \frac{\gamma}{|x-s|}\, ds + \int_0^{x-\epsilon} \frac{\gamma}{|x-s|}\, ds \\ &= \gamma(\ln|\omega(0)| + \ln|\omega(t)|) - 2\gamma \ln \epsilon,\end{aligned}$$

as $\epsilon \to 0+$, so we are subtracting a logarithmic divergence. Nevertheless, for each $\epsilon > 0$ sufficiently small, $e^{-i\int_{[0,t]\cap\{|\omega(s)|>\epsilon\}} V(\omega(s))\, ds}$ and $e^{-i\langle \int_0^t V\circ X_s\, ds\rangle_\Gamma}$ differ by a complex factor with modulus one.

Lemma 6.1: F_t^Γ is a continuous multiplicative functional, that is, $s \mapsto F_s^\Gamma(\omega), s \in [0,t]$ is continuous for M_t almost all $\omega \in \Omega$.

Proof: We look at the case $\omega'(s) = -1$ for all $s > 0$. The argument is similar for the other type of path. We have

$$F_s^\Gamma(\omega) = e^{-i\int_0^s V(\omega(r))\, dr} \chi_{\{X_s > 0\}\cup\{X_s < -s\}}(\omega) + e^{-i\langle \int_0^s V(\omega(r))\, dr\rangle_\Gamma} \chi_{\{-s < X_s < 0\}}(\omega),$$

$$\begin{aligned}F_t^\Gamma(\omega_s) &= e^{-i\int_0^t V(\omega_s(r))\, dr} \chi_{\{X_t > 0\}\cup\{X_t < -t\}}(\omega_s) + e^{-i\langle \int_0^t V(\omega_s(r))\, dr\rangle_\Gamma} \chi_{\{-t < X_t < 0\}}(\omega_s) \\ &= e^{-i\int_s^{s+t} V(\omega(r))\, dr} \chi_{\{X_{s+t} > 0\}\cup\{X_{s+t} < -t\}}(\omega) + e^{-i\langle \int_0^t V(\omega_s(r))\, dr\rangle_\Gamma} \chi_{\{-t < X_{s+t} < 0\}}(\omega) \\ &= e^{-i\int_s^{s+t} V(\omega(r))\, dr} \chi_{\{X_s > t\}\cup\{X_s < 0\}}(\omega) + e^{-i\langle \int_0^t V(\omega_s(r))\, dr\rangle_\Gamma} \chi_{\{0 < X_s < t\}}(\omega).\end{aligned}$$

The last line follows from the observation $X_r(\omega) = X_0(\omega) - r$ for all $r \geqslant 0$. Then

$$\begin{aligned}F_t^\Gamma(\omega_s) F_s^\Gamma(\omega) &= e^{-i\int_0^{s+t} V(\omega(r))\, dr} \chi_{\{X_s > t\}\cup\{X_s < -s\}}(\omega) \\ &\quad + e^{-i\int_s^{s+t} V(\omega(r))\, dr} e^{-i\langle \int_0^s V(\omega(r))\, dr\rangle_\Gamma} \chi_{\{-s < X_s < 0\}}(\omega) \\ &\quad + e^{-i\int_0^s V(\omega(r))\, dr} e^{-i\langle \int_0^t V(\omega_s(r))\, dr\rangle_\Gamma} \chi_{\{0 < X_s < t\}}(\omega) \\ &= e^{-i\int_0^{s+t} V(\omega(r))\, dr} \chi_{\{X_{s+t} > 0\}\cup\{X_{s+t} < -s-t\}}(\omega) \\ &\quad + e^{-i\int_s^{s+t} V(\omega(r))\, dr} e^{-i\langle \int_0^s V(\omega(r))\, dr\rangle_\Gamma} \chi_{\{-s-t < X_{s+t} < -t\}}(\omega) \\ &\quad + e^{-i\int_0^s V(\omega(r))\, dr} e^{-i\langle \int_0^t V(\omega_s(r))\, dr\rangle_\Gamma} \chi_{\{-t < X_{s+t} < 0\}}(\omega).\end{aligned}$$

But from Eq. (1.9),

$$\left\langle \int_0^t V(\omega_s(r))\,dr \right\rangle_\Gamma = \gamma(\ln(\omega_s(0))+\ln|\omega_s(t)|)+\kappa_2 = \gamma(\ln(\omega(s))+\ln|\omega(s+t)|)+\kappa_2$$

and for $s<\omega(0)<s+t$, we have $\int_0^s V(\omega(r))\,dr=\gamma(\ln(\omega(0))-\ln(\omega(s))$. Hence,

$$e^{-i\int_0^s V(\omega(r))\,dr}e^{-i\langle\int_0^t V(\omega_s(r))\,dr\rangle_\Gamma}=e^{-i\gamma(\ln(\omega(0))+\ln(\omega(s+t)))+i\kappa_2}=e^{-i\langle\int_0^{s+t}V(\omega(r))\,dr\rangle_\Gamma}.$$

For $0<\omega(0)<s$, we have $\int_s^{s+t}V(\omega(r))\,dr=\gamma(\ln(|\omega(s+t)|-\ln(|\omega(s)|))$. Hence,

$$e^{-i\int_s^{s+t}V(\omega(r))\,dr}e^{-i\langle\int_0^s V(\omega(r))\,dr\rangle_\Gamma}=e^{-i\gamma(\ln(|\omega(0)|)+\ln(|\omega(s+t)|)+i\kappa_2}=e^{-i\langle\int_0^{s+t}V(\omega(r))\,dr\rangle_\Gamma}.$$

The equality $F^\Gamma_{s+t}(\omega)=F^\Gamma_t(\omega_s)F^\Gamma_s(\omega)$ therefore holds unless $\omega(0)$ belongs to the finite set $\{0,s,s+t\}$. However, the set of all such ω has M_{t+s} measure zero.

Continuity of $s\mapsto F^\Gamma_s(\omega)$ at $s_0\in[0,t]$ follows from formulas (6.4) and (6.5) and the fact that the set of all ω with $\omega(0)=0$ or $\omega(s_0)=0$ has M_t measure zero. □

The following result represents the operator $e^{-it(A+_\Gamma Q(V))}$ as an integral with respect to the free Dirac measure M_t for each $t>0$.

Theorem 6.2: *The function F^Γ_t is M_t integrable for each $t\geqslant 0$. Furthermore,*

$$e^{-it(A+_\Gamma Q(V))}=\int_\Omega F^\Gamma_t\,dM_t. \tag{6.7}$$

Proof: As in the proof of Theorem 2.1,

$$\int_\Omega F^\Gamma_t\,dM_t=(e^{-ipt}Q(F^\Gamma_t\circ\gamma_-))\oplus(e^{ipt}Q(F^\Gamma_t\circ\gamma_+)).$$

Now let $\phi_2\in L^2(\mathbb{R})$. Then for almost all $x\in\mathbb{R}$, we have

$$\begin{aligned}(Q(F^\Gamma_t\circ\gamma_+)\phi_2)(x)&=F^\Gamma_t\circ\gamma_+(x)\,\phi_2(x)\\&=\chi_{\{X_0X_t>0\}}(\gamma_+(x)).e^{-i\int_0^t V(x-s)\,ds}\phi_2(x)\\&\quad+\chi_{\{X_0X_t<0\}}(\gamma_+(x)).e^{-i\langle\int_0^t V\circ X_s\circ\gamma_+(x)\,ds\rangle_\Gamma}\phi_2(x)\\&=\chi_{\{x'>t\}\cup\{x'<0\}}(x).e^{-i\int_0^t V(x-s)\,ds}\phi_2(x)\\&\quad+\chi_{\{0<x'<t\}}(x).e^{-i\langle\int_0^t V\circ X_s\circ\gamma_+(x)\,ds\rangle_\Gamma}\phi_2(x),\end{aligned}$$

so we have

$$\begin{aligned}(e^{ipt}Q(F^\Gamma_t\circ\gamma_+)\phi_2)(x)&=F^\Gamma_t\circ\gamma_+(x+t)\,\phi_2(x+t)\\&=\chi_{\{x'>t\}\cup\{x'<0\}}(x+t).e^{-i\int_0^t V(x+t-s)\,ds}\phi_2(x+t)+\chi_{\{0<x'<t\}}(x\\&\quad+t).e^{-i\langle\int_0^t V\circ X_s\circ\gamma_+(x+t)\,ds\rangle_\Gamma}\phi_2(x+t)\\&=\chi_{\{x'>0\}\cup\{x'<-t\}}(x).e^{-i\int_x^{x+t}V(s)\,ds}\phi_2(x+t)\\&\quad+\chi_{\{-t<x'<0\}}(x).e^{-i\langle\int_0^t V\circ X_s\circ\gamma_+(x+t)\,ds\rangle_\Gamma}\phi_2(x+t)\\&=\chi_{\{x'>0\}\cup\{x'<-t\}}(x).e^{-i\int_0^t V(x+s)\,ds}\phi_2(x+t)\\&\quad+\chi_{\{-t<x'<0\}}(x).e^{-i\gamma(\ln|x|+\ln|x+t|)-i\kappa_2}\phi_2(x+t).\end{aligned}$$

Similarly,

$$(e^{-ipt}Q(F_t^\Gamma\circ\gamma_-)\phi_1)(x)=\chi_{\{x'<0\}\cup\{x'>t\}}(x).e^{-i\int_{x-t}^{x}V(s)\,ds}\phi_1(x-t)$$
$$+\chi_{\{0<x'<t\}}(x).e^{-i\gamma(\ln|x|+\ln|x-t|)-i\kappa_1}\phi_1(x-t).$$

Comparison with formula (6.3) for $e^{-it(A+\Gamma Q(V))}\phi$ for $\phi\in L^2(\mathbb{R},\mathbb{C}^2)$ establishes the result. □

Suppose that Γ is *any* (2×2) unitary matrix. Another representation of $e^{-it(A+\Gamma Q(V))}$ is possible by using the measures M_t^Γ associated with point interactions (5.8). Take the path space Ω to be the union of the ranges of the functions $\gamma_\pm$ and $\zeta_\pm$. For each $\omega\in\Omega$, set $\tau(\omega)=\inf\{s\geqslant0:\omega(s)=0\}$, where we allow the possibility that $\tau(\omega)=\infty$ if ω never hits the origin.

The integral $\int_0^t V\circ X_s\,ds$ does not converge on the set $\{0<\tau<t\}$ of paths, so we use the following renormalization or principal value. Let

$$\left\langle\int_0^t V\circ X_s(\omega)\,ds\right\rangle=\gamma(\ln|\omega(0)|+\ln|\omega(t)|) \tag{6.8}$$

for all $\omega\in\Omega$ for which $0<\tau(\omega)<t$ and set

$$F_t=\chi_{\{\tau>t\}}.e^{-i\int_0^t V\circ X_s\,ds}+\chi_{\{0<\tau<t\}}.e^{-i\langle\int_0^t V\circ X_s\,ds\rangle}. \tag{6.9}$$

Note that according to formula (5.8), the sets $\{\tau=0\}$ and $\{\tau=t\}$ are M_t^Γ null. The proof of the following statement is similar to that above.

Theorem 6.3: *Let Γ be any (2×2) unitary matrix. The function F_t, $t>0$, is a multiplicative functional and F_t is M_t^Γ integrable for each $t\geqslant0$. Furthermore,*

$$e^{-it(A+\Gamma Q(V))}=\int_\Omega F_t\,dM_t^\Gamma. \tag{6.10}$$

VII. THE FEYNMAN–KAC FORMULA FOR SINGULAR POTENTIALS: NONZERO MASS

Let A be the self-adjoint operator (3.2) and let β be the Hermitian matrix $\left(\begin{smallmatrix}0&-1\\-1&0\end{smallmatrix}\right)$ and $m>0$. Then $A+m\beta$ is a self-adjoint operator acting in $L^2(\mathbb{R},\mathbb{C}^2)$. Let $S(t)=e^{-it(A+m\beta)}$ and suppose that $M_{t,m}$ is the measure defined by formula (1.7).

The matrix $m\boldsymbol{\beta}$ is a bounded perturbation of A, so the Dyson series expansion (Ref. 14, Theorem IX.2.1)

$$S(t)=e^{-it(A+m\boldsymbol{\beta})}=e^{-itA}+\sum_{n=1}^{\infty}(-im)^nR_n(t),$$
$$R_n(t)=\int_0^t\cdots\int_0^{s_2}e^{-i(t-s_n)A}\boldsymbol{\beta}e^{-i(s_n-s_{n-1})A}\cdots\boldsymbol{\beta}e^{-i(s_2-s_1)A}\boldsymbol{\beta}e^{-is_1A}\,ds_1\cdots ds_n \tag{7.1}$$

converges absolutely in the operator norm of $\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$. Set $R_0(t)=e^{-itA}$ for $t\geqslant0$.

Denote the algebra generated by cylinder sets (1.5) by $\mathcal{Z}_t(\Omega)$. For each set E of the form (1.5), set

$$M_t^{(n)}(E)=\sum_{\substack{n_0+\cdots+n_k=n\\ n_0,\ldots,n_k\geqslant0}}R_{n_k}(t-t_k)Q(B_k)R_{n_{k-1}}(t_k-t_{k-1})\cdots Q(B_1)R_{n_0}(t_1). \tag{7.2}$$

The identities

$$\sum_{\substack{l+m=n\\ l,m\geqslant 0}} R_l(s)R_m(t)=R_n(s+t), \quad n=0,1,2,\ldots, \quad s,t\geqslant 0,$$

ensure that (7.2) defines an additive operator valued set function $E\mapsto M_t^{(n)}(E)$, $E\in\mathcal{Z}_t(\Omega)$. Furthermore, the sum $M_{t,m}(E)=\Sigma_{n=0}^{\infty}(-im)^n M_t^{(n)}(E)$ converges uniformly in the operator norm of $\mathcal{L}(L^2(\mathbb{R},\mathbb{C}^2))$ for each $E\in\mathcal{Z}_t(\Omega)$. For each $n=0,1,2\ldots$, the operator valued measure $M_t^{(n)}$ is supported on the set of those paths belonging to Ω with exactly n changes in direction in the interval $[0,t]$. This follows immediately from the Poisson process representation of Zastawniak[19] to which we now turn.

As mentioned in the Introduction, the operator valued measures $M_{t,m}$ and $M_t^{(n)}$ may be viewed as acting on the space $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ of $\mathbb{C}^2$-valued measures defined on the Borel σ-algebra $\mathcal{B}(\mathbb{R})$ of $\mathbb{R}$ with the total variation norm. We shall identify this action more carefully now.

In the case that $\mu\in\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ has a density $f:\mathbb{R}\to\mathbb{C}^2$ with respect to Lebesgue measure on $\mathbb{R}$, then according to formula (3.2), we have $(e^{-iAs}f)(x)=(f_1(x-s),f_2(x+s))$ for almost all $x\in\mathbb{R}$, because the expression is valid on the dense subspace $L^1\cap L^2(\mathbb{R},\mathbb{C}^2)$ of $L^1(\mathbb{R},\mathbb{C}^2)$. For any continuous function $\phi:\mathbb{R}\to\mathbb{C}^2$ with compact support,

$$\begin{aligned}\langle\phi,e^{-iAs}f\rangle&=\int_{\mathbb{R}}\phi_1(x)(e^{-iAs}f)_1(x)\,dx+\int_{\mathbb{R}}\phi_2(x)(e^{-iAs}f)_2(x)\,dx\\&=\int_{\mathbb{R}}\phi_1(x+s)f_1(x)\,dx+\int_{\mathbb{R}}\phi_2(x-s)f_2(x)\,dx=\langle e^{iAs}\phi,f\rangle,\end{aligned}$$

with respect to the duality between $L^\infty(\mathbb{R},\mathbb{C}^2)$ and $L^1(\mathbb{R},\mathbb{C}^2)$.

For cylinder sets (1.5), it is therefore consistent to interpret formulas (1.7) and (7.1) with $S(s)=e^{-iAs}$ acting on a measure $\mu\in\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ for each $s\in\mathbb{R}$ by the formula

$$\begin{aligned}\langle\phi,S(s)\mu\rangle&=\int_{\mathbb{R}}\phi_1(x)\,d[(S(s)\mu)_1](x)+\int_{\mathbb{R}}\phi_2(x)\,d[(S(s)\mu)_2](x)\\&=\int_{\mathbb{R}}\phi_1(x+s)\,d\mu_1(x)+\int_{\mathbb{R}}\phi_2(x-s)\,d\mu_2(x)=\langle S(-s)\phi,\mu\rangle\end{aligned}\tag{7.3}$$

for all continuous functions $\phi:\mathbb{R}\to\mathbb{C}^2$ with compact support. The embedding of $L^1(\mathbb{R},\mathbb{C}^2)$ in $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ induces the direct sum of translations on $L^1(\mathbb{R},\mathbb{C}^2)$ given above. Note that the group S of operators is not actually a C_0 group acting on $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$.

Let δ_x denote the unit point mass at $x\in\mathbb{R}$. In the same spirit as above, the operator $e^{ipy}:L^1(\mathbb{R})\to L^1(\mathbb{R})$ defined for all $f\in L^1(\mathbb{R})$ by $(e^{ipy}f)(x)=f(x+y)$, $x\in\mathbb{R}$, is translation by $y\in\mathbb{R}$. Then denoting the induced operator on $\mathcal{M}(\mathbb{R})$ by the same symbol, we have $e^{ipy}\delta_x=\delta_{x-y}$ for all $x\in\mathbb{R}$. The standard basis vectors of $\mathbb{C}^2$ are written as e_1,e_2.

Proposition 7.1 (Zastawniak[19]): Let $(\Xi,\mathcal{E},P,\langle N_t\rangle_{t\geqslant 0})$ be the standard Poisson process with intensity one. Let $\tau_k(\xi)=\inf\{t\geqslant 0:N_t(\xi)=k\}$ be the kth jump time of $\xi\in\Xi$. For each $t\geqslant 0$, $j=1,2$ and $x\in\mathbb{R}$, let $Y_t^{(x,j)}:\Xi\to\mathbb{R}$ be the random variable defined by

$$Y_t^{(x,j)}=x-(-1)^j\int_0^t(-1)^{N_s}\,ds.$$

Then for each $x\in\mathbb{R}$ and $j=1,2$ and cylinder set (1.5), the $\mathbb{C}^2$ valued Borel measure $M_t^{(n)}(X_{t_1}\in B_1,\ldots,X_{t_k}\in B_k)(\delta_x e_j)$ equals

$$B\mapsto e^t \sum_{\substack{n_0+\cdots+n_k=n\\ n_0,\ldots,n_k\geqslant 0}} \int_{E_{n_0,\ldots,n_k}(t_1,\ldots,t_k)} \chi_{B_k}\circ Y_{t_k}^{(x,j)}\cdots\chi_{B_1}\circ Y_{t_1}^{(x,j)} \times[e^{i(t-\tau_n)A}\boldsymbol{\beta}e^{-i(\tau_n-\tau_{n-1})A}\cdots\boldsymbol{\beta}e^{-i\tau_1 A}(\delta_x e_j)](B)\,dP,\quad B\in\mathcal{B}(\mathbb{R}).$$

Here $E_{n_0,\ldots,n_k}(t_1,\ldots,t_k)$ is the set of $\xi\in\Xi$ with n_{j-1} jumps at times greater than t_{j-1} but less than or equal to t_j for each $j=1,\ldots,k+1$.

Let $\Phi_{x,j}:\Xi\to\Omega$ denote the map sending $\xi\in\Xi$ onto the path $\omega:[0,\infty)\to\mathbb{R}$ defined by $\omega(s)=Y_s^{(x,j)}(\xi)$ for all $s\geqslant 0$. Let $P_t^{(n)}=\chi_{\{N_t=n\}}P$. Now let $\tau_k(\omega)$, $k=1,\ldots,K(\omega)$ be the consecutive times where $\omega\in\Omega$ changes direction in the time interval $[0,t]$. It follows from Proposition 7.1 that

$$M_t^{(n)}(E)(\delta_x e_j)=e^t\int_E e^{i(t-\tau_n)A}\boldsymbol{\beta}e^{-i(\tau_n-\tau_{n-1})A}\cdots\boldsymbol{\beta}e^{-i\tau_1 A}(\delta_x e_j)\,d(P_t^{(n)}\circ\Phi_{x,j}^{-1})$$

for all elements E of the σ-algebra $\sigma(\mathcal{Z}_t(\Omega))$ generated by the algebra $\mathcal{Z}_t(\Omega)$ of cylinder sets. In other words, the $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$-valued measure $E\mapsto M_t^{(n)}(E)(\delta_x e_j)$ has an $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$-valued density

$$e^t e^{-i(t-\tau_n)A}\boldsymbol{\beta}e^{-i(\tau_n-\tau_{n-1})A}\cdots\boldsymbol{\beta}e^{-i\tau_1 A}(\delta_x e_j) \tag{7.4}$$

with respect to the finite measure $P_t^{(n)}\circ\Phi_{x,j}^{-1}$.

We may take $\Omega=\cup_{x\in\mathbb{R},j=1,2}\Phi_{x,j}(\Xi)$. For each $v\in\mathbb{C}^2$, the $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$-valued measure $M_t^{(n)}(\,\cdot\,)[\delta_x v]$ is therefore concentrated on all paths ω with $\omega(0)=x$, velocity ± 1 and exactly n changes of direction in the interval $[0,t]$. Each operator $M_t^{(n)}(E)$ is also continuous for the weak topology of the duality between $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$ and the space $\mathcal{L}^\infty(\mathbb{R},\mathbb{C}^2)$ of bounded Borel measurable functions. Because the set of all measures $\delta_x v$ for $x\in\mathbb{R}$ and $v\in\mathbb{C}^2$ separates the vector space $\mathcal{L}^\infty(\mathbb{R},\mathbb{C}^2)$, it follows that $M_t^{(n)}$ is concentrated on all paths ω with velocity ± 1 and exactly n changes of direction in the interval $[0,t]$, as mentioned above.

Lemma 7.2: Suppose that $G_{u,v}^{(j)}$, $j=0,\ldots,n$ are bounded random variables such that $G_{u,v}^{(j)}$ is measurable with respect to $\sigma\{X_s:u\leqslant s\leqslant v\}$ for every $0\leqslant u<v\leqslant t$. Let $\omega_{-r}(s)=\omega(s-r)$ for all $s\geqslant r$.

Then $G_{0,\tau_1}^{(0)}\cdots G_{\tau_{n-1},\tau_n}^{(n-1)}G_{\tau_n,t}^{(n)}$ is $M_t^{(n)}$ integrable and

$$\int_\Omega G_{0,\tau_1}^{(0)}\cdots G_{\tau_{n-1},\tau_n}^{(n-1)}G_{\tau_n,t}^{(n)}\,dM_t^{(n)} = \int_0^t\cdots\int_0^{s_2}\left(\int_\Omega G_{s_n,t}^{(n)}(\omega_{-s_n})\,dM_{t-s_n}(\omega)\right)\boldsymbol{\beta}\left(\int_\Omega G_{s_{n-1},s_n}^{(n-1)}(\omega_{-s_{n-1}})\,dM_{s_n-s_{n-1}}(\omega)\right)\cdots \times\boldsymbol{\beta}\left(\int_\Omega G_{s_1,s_2}^{(1)}(\omega_{-s_1})\,dM_{s_2-s_1}(\omega)\right)\boldsymbol{\beta}\left(\int_\Omega G_{0,s_1}^{(0)}(\omega)\,dM_{s_1}(\omega)\right)ds_1\cdots ds_n.$$

Proof: The density of the $\mathcal{M}(\mathbb{R},\mathbb{C}^2)$-valued measure $M_t^{(n)}(\,\cdot\,)(\delta_x e_j)$ with respect to the probability measure $P_t^{(n)}\circ\Phi_{x,j}^{-1}$ is given by (7.4). For each $0<s_1<\cdots<s_n<t$, let $\xi_{s_1,\ldots,s_n}\in\Xi$ be a sample point with $N_{s_k}(\xi_{s_1,\ldots,s_n})=k$ and $N_{s_k-}(\xi_{s_1,\ldots,s_n})=k-1$, $k=1,\ldots,n$. The jump time corresponding to the kth time $\tau_k(\omega)$ of changing direction of the sample path ω is written as $\tau_k'(\xi)$.

Then we have

$$\int_\Omega G^{(0)}_{0,\tau_1}\cdots G^{(n-1)}_{\tau_{n-1},\tau_n} G^{(n)}_{\tau_n,t}\, d(M^{(n)}_t(\delta_x e_j))$$

$$= e^t \int_\Omega G^{(0)}_{0,\tau_1}\cdots G^{(n-1)}_{\tau_{n-1},\tau_n} G^{(n)}_{\tau_n,t} e^{-i(t-\tau_n)A}\boldsymbol{\beta} e^{-i(\tau_n-\tau_{n-1})A}\cdots\boldsymbol{\beta} e^{-i\tau_1 A}(\delta_x e_j)\, dP^{(n)}_t\circ\Phi^{-1}_{x,j}$$

$$= e^t \int_{\{N_t=n\}} (G^{(0)}_{0,\tau_1}\circ\Phi_{x,j})\cdots(G^{(n-1)}_{\tau_{n-1},\tau_n}\circ\Phi_{x,j})(G^{(n)}_{\tau_n,t}\circ\Phi_{x,j})$$
$$\times e^{-i(t-\tau'_n)A}\boldsymbol{\beta} e^{-i(\tau'_n-\tau'_{n-1})A}\cdots\boldsymbol{\beta} e^{-i\tau'_1 A}(\delta_x e_j)\, dP$$
$$= \int_0^t\cdots\int_0^{s_2} (G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\ldots,s_n}))\cdots(G^{(n)}_{s_n,t}\circ\Phi_{x,j}(\xi_{s_1,\ldots,s_n}))$$
$$\times e^{-i(t-s_n)A}\boldsymbol{\beta} e^{-i(s_n-s_{n-1})A}\cdots\boldsymbol{\beta} e^{-is_1 A}(\delta_x e_j)\, ds_1\cdots ds_n, \tag{7.5}$$

because the joint distribution of $(\tau'_1,\ldots,\tau'_n)$ on $\{N(t)=n\}$ is the measure $e^{-t}ds_1\cdots ds_n$ on $\{s\in\mathbb{R}^n: 0<s_1<\cdots<s_n<t\}$ [Ref. 19, Eq. (17)].

Now $\Phi_{x,j}(\xi_{s_1,\ldots,s_n})(s)=Y^{(x,j)}_s(\xi_{s_1,\ldots,s_n})=x-(-1)^j\int_0^s(-1)^{N_r(\xi_{s_1,\ldots,s_n})}\,dr$. We can write this expression as

$$x-(-1)^j\int_0^{s_k}(-1)^{N_r(\xi_{s_1,\ldots,s_n})}\,dr-(-1)^j\int_{s_k}^{s}(-1)^{N_r(\xi_{s_1,\ldots,s_n})}\,dr$$
$$= x_{k,j}-(-1)^j\int_{s_k}^{s}(-1)^{N_r(\xi_{s_1,\ldots,s_n})}\,dr$$
$$= x_{k,j}-(-1)^{j+k}(s-s_k)=\gamma_{(-1)^{j+k}}(x_{k,j})(s-s_k),\quad s_k\leqslant s<s_{k+1}$$
$$= \theta_{-s_k}(\gamma_{(-1)^{j+k}}(x_{k,j}))(s),\quad s_k\leqslant s<s_{k+1}. \tag{7.6}$$

Here we have set $\theta_u(\xi):s\to\xi(u+s)$ for $s+u\geqslant 0$, $u\in\mathbb{R}$ and $\xi\in\Xi$ and

$$x_{k,j}=x-(-1)^j\int_0^{s_k}(-1)^{N_r(\xi_{s_1,\ldots,s_n})}\,dr$$
$$=\Phi_{x,j}(\xi_{s_1,\ldots,s_n})(s_k)\quad\text{for } k=0,\ldots,n, \text{ and } j=1,2,$$

with the convention $x_{0,j}=x$, $s_0=0$ and $s_{n+1}=t$.

Now from (3.3),

$$\int_\Omega G^{(0)}_{0,s_1}(\omega)\, dM_{s_1}(\omega)=\left(\int_\Omega G^{(0)}_{0,s_1}(\omega)\, dM^-_{s_1}(\omega)\right)\oplus\left(\int_\Omega G^{(0)}_{0,s_1}(\omega)\, dM^+_{s_1}(\omega)\right)$$
$$=\left(e^{-ipt}\int_\Omega G^{(0)}_{0,s_1}(\omega)\, d(Q\circ\gamma^{-1}_-)(\omega)\right)\oplus\left(e^{ipt}\int_\Omega G^{(0)}_{0,s_1}(\omega)\, d(Q\circ\gamma^{-1}_+)(\omega)\right)$$
$$=(e^{-ipt}Q(G^{(0)}_{0,s_1}\circ\gamma_-))\oplus(e^{ipt}Q(G^{(0)}_{0,s_1}\circ\gamma_+)).$$

Hence,

$$\int_\Omega G^{(0)}_{0,s_1}(\omega)\, M_{s_1}(d\omega)(\delta_x e_j) = e^{(-1)^j ips_1}([G^{(0)}_{0,s_1}\circ\gamma_{(-1)^j}].\delta_x)e_j$$
$$= [G^{(0)}_{0,s_1}(\gamma_{(-1)^j}(x))].(e^{(-1)^j ips_1}\delta_x)e_j$$
$$= [G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n})]e^{-is_1A}(\delta_x e_j).$$

Similarly,

$$\left(\int_\Omega G^{(1)}_{s_1,s_2}(\omega_{-s_1})\, dM_{s_2-s_1}(\omega)\right)\beta\left(\int_\Omega G^{(0)}_{0,s_1}(\omega)\, dM_{s_1}(\omega)\right)(\delta_x e_j)$$
$$= [G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n})][(e^{-ip(s_2-s_1)}Q(G^{(1)}_{s_1,s_2}\circ\theta_{-s_1}\circ\gamma_-))$$
$$\oplus(e^{ip(s_2-s_1)}Q(G^{(1)}_{s_1,s_2}\circ\theta_{-s_1}\circ\gamma_+))]\beta e^{-is_1A}(\delta_x e_j). \tag{7.7}$$

To see what this expression is, let $j=1$. Then $\beta e^{-is_1A}(\delta_x e_1)=\delta_{x+s_1}\beta e_1$. Now $\beta e_1=-e_2$, so

$$(e^{-ip(s_2-s_1)}Q(G^{(1)}_{s_1,s_2}\circ(\gamma_-)_{-s_1}))\oplus(e^{ip(s_2-s_1)}Q(G^{(1)}_{s_1,s_2}\circ(\gamma_+)_{-s_1}))\beta e^{-is_1A}(\delta_x e_1)$$
$$= -e^{ip(s_2-s_1)}[(G^{(1)}_{s_1,s_2}\circ\theta_{-s_1}\circ\gamma_+).\delta_{x+s_1}]e_2$$
$$= -G^{(1)}_{s_1,s_2}(\theta_{-s_1}(\gamma_+(x+s_1)))[e^{ip(s_2-s_1)}\delta_{x+s_1}]e_2$$
$$= G^{(1)}_{s_1,s_2}(\theta_{-s_1}(\gamma_+(x+s_1)))e^{-i(s_2-s_1)A}\beta e^{-is_1A}(\delta_x e_1).$$

The sample path $\theta_{-s_1}(\gamma_+(x+s_1))$ is $s\mapsto\gamma_+(x+s_1)(s-s_1)$ for $s\geqslant s_1$. But

$$\gamma_+(x+s_1)(s-s_1)=x+s_1-(s-s_1)=\Phi_{x,1}(\xi_{s_1,\dots,s_n})(s)$$

for all $s_1\leqslant s\leqslant s_2$, as in formula (7.6). A similar argument works for $j=2$. The general formula for the left-hand side of Eq. (7.7) is therefore

$$[G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n})][G^{(1)}_{s_1,s_2}(\gamma_{(-1)^{j+1}}(x_{1,j})_{-s_1})]e^{-i(s_2-s_1)A}\beta e^{-is_1A}(\delta_x e_j)$$
$$= [G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n})].[G^{(1)}_{s_1,s_2}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n})]e^{-i(s_2-s_1)A}\beta e^{-is_1A}(\delta_x e_j).$$

Continuing in this way, we obtain

$$\left(\int_\Omega G^{(n)}_{s_n,t}(\omega_{-s_n})\, dM_{t-s_n}(\omega)\right)\beta\left(\int_\Omega G^{(n-1)}_{s_{n-1},s_n}(\omega_{-s_{n-1}})\, dM_{s_n-s_{n-1}}(\omega)\right)\cdots$$
$$\times\beta\left(\int_\Omega G^{(1)}_{s_1,s_2}(\omega_{-s_1})\, dM_{s_2-s_1}(\omega)\right)\beta\left(\int_\Omega G^{(0)}_{0,s_1}(\omega)\, dM_{s_1}(\omega)\right)(\delta_x e_j)$$
$$= (G^{(0)}_{0,s_1}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n}))\cdots(G^{(n)}_{s_n,t}\circ\Phi_{x,j}(\xi_{s_1,\dots,s_n}))$$
$$\times e^{-i(t-s_n)A}\beta e^{-i(s_n-s_{n-1})A}\cdots\beta e^{-is_1A}(\delta_x e_j). \tag{7.8}$$

Combining Eqs. (7.5) and (7.8) completes the proof. □

Let Γ be the (2×2) unitary matrix (5.2). Suppose that $\beta=0$ and $\eta\alpha=e^{i\kappa_1}$, $\eta\overline{\alpha}=e^{i\kappa_2}$ for numbers $0\leqslant\kappa_j<2\pi$. As above, denote the consecutive times where $\omega\in\Omega$ changes direction by $\tau_k(\omega)$, $k=1,\dots,K(\omega)$ with $\tau_{K+1}(\omega)=t$. The shift operator θ_u maps $\omega\in\Omega$ into the path $\theta_u(\omega)(s)=\omega(s+u)$ defined for all $s\geqslant -u$.

Lemma 7.3: There is essentially only one right continuous multiplicative functional F_t^Γ on Ω satisfying (6.4) and (6.5) on $\{\tau_1>t\}$. It is given M_t almost everywhere by

$$F_t^\Gamma=\exp\left[-i\sum_{k=0}^{n}\chi_{\{X_{\tau_k}X_{\tau_{k+1}}>0\}}\left(\int_{\tau_k}^{\tau_{k+1}}V\circ X_s\,ds\right)+\chi_{\{X_{\tau_k}X_{\tau_{k+1}}<0\}}\left\langle\int_{\tau_k}^{\tau_{k+1}}V\circ X_s\,ds\right\rangle_\Gamma\right], \quad (7.9)$$

on $\{N_t=n\}$ where $\tau_0=0$ and $\tau_{n+1}=t$. The expression $\langle\int_{\tau_k}^{\tau_{k+1}}V\circ X_s\,ds\rangle_\Gamma$ is given by

$$\begin{aligned}&\gamma(\ln|\omega(\tau_k)|+\ln|\omega(\tau_{k+1})|)+\kappa_1, \quad \text{if } \omega'(s)=1,\ \tau_k(\omega)<s<\tau_{k+1}(\omega),\\ &\gamma(\ln|\omega(\tau_k)|+\ln|\omega(\tau_{k+1})|)+\kappa_2, \quad \text{if } \omega'(s)=-1,\ \tau_k(\omega)<s<\tau_{k+1}(\omega).\end{aligned} \quad (7.10)$$

Furthermore, the multiplicative functional F_t^Γ satisfies

$$F_t^\Gamma=F_{\tau_1}^\Gamma.(F_{\tau_2-\tau_1}^\Gamma\circ\theta_{\tau_1})\cdots(F_{t-\tau_n}^\Gamma\circ\theta_{\tau_n}), \quad (7.11)$$

M_t almost everywhere on $\{N_t=n\}$.

Proof: Suppose first that F_t^Γ is a multiplicative functional satisfying Eqs. (6.4) and (6.5) on the set $\{\tau_1>t\}$ of all paths with no change in direction before time t.

Then for every $0<t_1<\cdots<t_n<t$,

$$F_t^\Gamma=F_{t_1}^\Gamma.(F_{t_2-t_1}^\Gamma\circ\theta_{t_1})\cdots(F_{t-t_n}^\Gamma\circ\theta_{t_n}),$$

a.e., on $\{N_t=n\}$, because F_t^Γ is a multiplicative functional. Right continuity ensures that we can replace $t_1,\ldots,t_n$ by the jump times $\tau_1,\ldots,\tau_n$ so that Eq. (7.11) holds.

Now suppose that $\omega\in\Omega$ and $\tau_k(\omega)=t_k$, $\tau_{k+1}(\omega)=t_{k+1}$ with $0<t_k<t_{k+1}<t$, $k=0,\ldots,n-1$, $\tau_{n+1}=t$. Then on the interval $[0,t_{k+1}-t_k]$, the sample path $\theta_{t_k}(\omega)$ is equal to the restriction of an element of $\{\tau_1>t_{k+1}-t_k\}$ to $[0,t_{k+1}-t_k]$, so that by Eqs. (6.4) and (6.5) we have

$$\begin{aligned}(F_{\tau_{k+1}-\tau_k}^\Gamma\circ\theta_{\tau_1})(\omega)&=(F_{t_{k+1}-t_k}^\Gamma\circ\theta_{t_k})(\omega)\\ &=\chi_{\{X_0X_{t_{k+1}-t_k}>0\}}(\theta_{t_k}(\omega))e^{-i\int_0^{t_{k+1}-t_k}V\circ X_s(\theta_{t_k}(\omega))\,ds}\\ &\quad+\chi_{\{X_0X_{t_{k+1}-t_k}<0\}}(\theta_{t_k}(\omega))e^{-i\langle\int_0^{t_{k+1}-t_k}V\circ X_s(\theta_{t_k}(\omega))\,ds\rangle_\Gamma}\\ &=\chi_{\{X_{t_k}X_{t_{k+1}}>0\}}(\omega)e^{-i\int_{t_k}^{t_{k+1}}V\circ X_s(\omega)\,ds}+\chi_{\{X_{t_k}X_{t_{k+1}}<0\}}(\omega)e^{-i\langle\int_{t_k}^{t_{k+1}}V\circ X_s(\omega)\,ds\rangle_\Gamma}\\ &=\chi_{\{X_{\tau_k}X_{\tau_{k+1}}>0\}}(\omega)e^{-i\int_{\tau_k}^{\tau_{k+1}}V\circ X_s(\omega)\,ds}+\chi_{\{X_{\tau_k}X_{\tau_{k+1}}<0\}}(\omega)e^{-i\langle\int_{\tau_k}^{\tau_{k+1}}V\circ X_s(\omega)\,ds\rangle_\Gamma}.\end{aligned}$$

Hence Eq. (7.9) follows by applying Eq. (7.11).

On the other hand, Eq. (7.11) follows from the definition (7.9). To check that (7.9) defines a multiplicative functional, it is enough to check that Eq. (6.6) holds for almost all $\omega\in\{N_{t+s}=n\}$, for each $n=1,2,\ldots$ and on each set $\{\tau_{k-1}\leqslant s<\tau_k\}$, $k=1,\ldots,n$.

According to formula (7.9) and Lemma 5.1, we have

$$F_{\tau_k-\tau_{k-1}}\circ\theta_{\tau_k}=(F_{s-\tau_{k-1}}\circ\theta_{\tau_{k-1}})(F_{\tau_k-s}\circ\theta_s),$$

$$F_t\circ\theta_s=(F_{\tau_k-s}\circ\theta_s)(F_{s+t-\tau_k}\circ\theta_{\tau_k})$$

on the set $\{N_{t+s}=n,\tau_{k-1}\leqslant s<\tau_k\}$. Then

$$
\begin{aligned}
F^{\Gamma}_{s+t} &= F^{\Gamma}_{\tau_1}(F^{\Gamma}_{\tau_2-\tau_1}\circ\theta_{\tau_1})\cdots(F^{\Gamma}_{s+t-\tau_n}\circ\theta_{\tau_n}) \\
&= F^{\Gamma}_{\tau_1}(F^{\Gamma}_{\tau_2-\tau_1}\circ\theta_{\tau_1})\cdots(F_{s-\tau_{k-1}}\circ\theta_{\tau_{k-1}})(F_{\tau_k-s}\circ\theta_s)\cdots(F^{\Gamma}_{s+t-\tau_n}\circ\theta_{\tau_n}) \\
&= F_s(F_{\tau_k-s}\circ\theta_s)(F^{\Gamma}_{s+t-\tau_k}\circ\theta_{\tau_k}) = F_sF_t\circ\theta_s .
\end{aligned}
$$

Hence, formula (7.9) does indeed define a multiplicative functional. □

The operator $H_0+_{\Gamma}Q(V) \coloneqq A+_{\Gamma}Q(V)+m\beta$ is interpreted as a bounded perturbation of the self-adjoint operator $A+_{\Gamma}Q(V)$, so it is itself self-adjoint. A careful study of the operator $H_0+_{\Gamma}Q(V)$ in the Dirac representation is given in Ref. 3.

Theorem 7.4: *For every $t\geqslant 0$, the equality*

$$
e^{-it(H_0+_{\Gamma}Q(V))} = \int_{\Omega} F^{\Gamma}_t \, dM_{t,m} \tag{7.12}
$$

holds.

Proof: It suffices to establish that for each $n=1,2,\ldots,$ the equality

$$
\begin{aligned}
\int_{\Omega} F^{\Gamma}_t \, dM^{(n)}_t = \int_0^t\cdots\int_0^{s_2} & e^{-i(t-s_n)(A+_{\Gamma}Q(V))}\beta e^{-i(s_n-s_{n-1})(A+_{\Gamma}Q(V))}\cdots \\
& \times\beta e^{-i(s_2-s_1)(A+_{\Gamma}Q(V))}\beta e^{-is_1(A+_{\Gamma}Q(V))}\, ds_1\cdots ds_n
\end{aligned} \tag{7.13}
$$

is valid, for then the operator coefficients of the Taylor expansion in powers of m on the right- and left-hand sides of Eq. (7.12) agree. The equality

$$
\int_{\Omega} F^{\Gamma}_t \, dM^{(0)}_t = \int_{\Omega} F^{\Gamma}_t \, dM_t = e^{-it(A+_{\Gamma}Q(V))}
$$

corresponding to $n=0$ is proved in Theorem 6.2.

Appealing to Theorem 6.2 again, we can write the right-hand side of Eq. (7.13) as

$$
\begin{aligned}
\int_0^t\cdots\int_0^{s_2}\left(\int_{\Omega} F^{\Gamma}_{t-s_n}\, dM_{t-s_n}\right)\beta\left(\int_{\Omega} F^{\Gamma}_{s_n-s_{n-1}}\, dM_{s_n-s_{n-1}}\right)\cdots \\
\times\beta\left(\int_{\Omega} F^{\Gamma}_{s_2-s_1}\, dM_{s_2-s_1}\right)\beta F^{\Gamma}_{s_1}\, dM_{s_1}\, ds_1\cdots ds_n .
\end{aligned}
$$

By Eq. (7.11), we have

$$
F^{\Gamma}_t = F^{\Gamma}_{\tau_1}(F^{\Gamma}_{\tau_2-\tau_1}\circ\theta_{\tau_1})\cdots(F^{\Gamma}_{t-\tau_n}\circ\theta_{\tau_n}),
$$

so Lemma 7.2 shows that Eq. (7.13) holds. □

We also state the following Feynman–Kac formula with respect to the measure $M^{\Gamma}_{t,m}$ associated with point interactions. The proof is similar to that above, except we replace the appeal to Theorem 6.2 by Theorem 6.3.

Let Γ be an arbitrary (2×2) unitary matrix (5.2), A_{Γ} the operator (3.2) with the boundary condition (5.1), $S(s)=e^{-is(A_{\Gamma}+m\beta)}$ for every $s\in\mathbb{R}$ and suppose that $M^{\Gamma}_{t,m}$ is the measure defined by formula (1.7). The multiplicative functional F_t is defined by formulas (7.9) and (7.10), but with $\kappa_1=\kappa_2=0$.

Theorem 7.5: *For every $t\geqslant 0$, the equality*

$$
e^{-it(H_0+_{\Gamma}Q(V))} = \int_{\Omega} F_t \, dM^{\Gamma}_{t,m} \tag{7.14}
$$

holds.

Remark 7.6: (a) In the case that Γ is a unitary diagonal matrix, the equality

$$F_t^{\Gamma}.M_{t,m}=F_t.M_{t,m}^{\Gamma}$$

holds for all $t\geqslant 0$.

(b) The argument of Sec. VII should admit considerable generalization. The operator valued measures $M_{t,m}$ are obtained from the zero-mass measures M_t by the concatenation of finitely many paths in any bounded time interval and this result should extend to generators other than $-iA$ and other bounded perturbations. The appropriate renormalization for other types of singular potentials should be determined by the boundary conditions at the singularities.

(c) One point of view of Feynmanism is that the evolution of the states of an interacting quantum system can be written as integrals $t\mapsto\int_{\Omega}F_t\,dM_t$, $t\geqslant 0$, over path space Ω. The process of renormalization in perturbative quantum field theory is required to construct the multiplicative functional $\langle F_t\rangle_{t\geqslant 0}$, just as it is required to obtain the representations (7.12) and (7.14) for the Dirac equation with a Coulomb interaction in one space dimension. Because interactions in quantum field theory are never defined at a point, the process of renormalization is necessarily more involved.[12,17]

ACKNOWLEDGMENT

The first author would like to thank the School of Mathematics, UNSW for warm hospitality during his visit to Sydney, during which most of the research was done.

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General relations between radial integrals in nonrelativistic and relativistic calculation schemes

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(Received 27 September 2002; accepted 9 December 2002)

Using the equivalent relativistic operator and the correspondence of its terms to the operators in the Breit–Pauli approximation the relativistic analogs for the integrals of Coulomb, spin–contact, spin–orbit, spin–spin and other interactions are obtained. They give the possibility to take into account not only direct but also indirect relativistic effects by performing the calculations of atomic structure with existing general programs in a nonrelativistic scheme with relativistic Breit–Pauli corrections. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1557769]

I. INTRODUCTION

The effective relativistic operator can be introduced,[1–3] which matrix elements with respect to nonrelativistic wave functions give the same result as the relativistic Hamiltonian in the basis of relativistic wave functions. The effective operator is expressed in terms of standard operators, acting in the space of spin–angular nonrelativistic wave functions; the relativistic integrals only play the role of coefficients at various parts of such an operator. The separate terms of the effective operator asymptotically turn into the operators of relativistic corrections in the Breit–Pauli approximation.[2,4] The ranks and consequently the spin-angular parts of matrix elements of corresponding operators are equal; it enables us to establish the general relations between the radial integrals in both approximations. The future development of the method of equivalent relativistic operator and interpretation of its separate terms in a case of nonequivalent electrons[4] gives the possibility of deriving such general relations. This is our aim in this work.

The relativistic analogs of some nonrelativistic integrals were obtained earlier in works.[5,6] For this purpose the two-electron average energy in nonrelativistic and relativistic approximations was compared.[5] In such a way the analogs of single-configuration Slater integrals F^k and G^k were derived. However, several averaged coefficients at the radial integrals vanish, the same also happens for the spin–orbit constant. In Ref. 6 the method of effective operator was applied for the expression of Coulomb integrals R^k in terms of relativistic integrals, but the general formula did not given. For the spin–orbit constant only the approximate formula in terms of the differences of average energies for the highest and lowest relativistic configurations was proposed. We investigate the relativistic analogs of radial integrals for various relativistic corrections in the configuration interaction approximation.

II. RELATIVISTIC ANALOGS OF INTEGRALS

Let us consider the relativistic Dirac–Breit Hamiltonian:

$$H^{\mathrm{rel}} = H_{\alpha_1} + H_{\alpha_2} + H_\beta + H_\gamma + H_\delta, \tag{1}$$

where

$$H_{\alpha_1} = \sum_i \left[(\alpha_i \mathbf{p}_i) + (\beta_i - 1)\, mc^2 \right], \tag{2}$$

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$$H_{\alpha_2}=-\sum_i \frac{Ze^2}{r_i}, \qquad H_\beta=\sum_{i<j}\frac{e^2}{r_{ij}},$$
$$H_\gamma=-\frac{e^2}{2}\sum_{i<j}\frac{(\alpha_i\cdot\alpha_j)}{r_{ij}}, \qquad H_\delta=-\frac{e^2}{2}\sum_{i<j}\frac{(\alpha_i\cdot\mathbf{r}_{ij})(\alpha_j\cdot\mathbf{r}_{ij})}{r_{ij}^3}. \tag{3}$$

Here the usual notations are employed. The rest mass of electrons is excluded from H_{α_1} in order to have the Hamiltonian corresponding to its nonrelativistic analog.

The equivalent operators for one-electron and two-electron terms of the relativistic Hamiltonian,

$$H_1=\sum_i h_i, \quad H_2=\sum_{i<j}\sum_k (g_i^{(k)}\cdot g_j^{(k)}), \tag{4}$$

obtain the following expressions in the second quantization form:[1,3,4]

$$O_1=\sum_{\substack{jk\\ n_1l_1n_2l_2}}(-1)^{l_2+1/2+j+k}[j,k]^{1/2}\begin{Bmatrix} l_1 & 1/2 & j\\ 1/2 & l_2 & k\end{Bmatrix}(n_1l_1j\|h_1\|n_2l_2j)W^{(kk0)}(n_1l_1,n_2l_2), \tag{5}$$

$$\begin{aligned}O_2=&\frac{1}{2}\sum_{\substack{k\\ \{n_il_ij_i\}}}(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_3l_3j_3n_4l_4j_4)\\ &\times\Bigg\{\sum_{\varkappa k_1K_1k_2K_2}(-1)^{\varkappa+k_2+K_1}[\varkappa,k_1,K_1,k_2,K_2,j_1,j_2,j_3,j_4]^{1/2}\\ &\times\begin{Bmatrix} k_1 & K_1 & k\\ K_2 & k_2 & \varkappa\end{Bmatrix}\begin{Bmatrix} l_1 & l_3 & k_1\\ 1/2 & 1/2 & K_1\\ j_1 & j_3 & k\end{Bmatrix}\begin{Bmatrix} l_2 & l_4 & k_2\\ 1/2 & 1/2 & K_2\\ j_2 & j_4 & k\end{Bmatrix}\\ &\times[W^{(k_1K_1)}(n_1l_1,n_3l_3)\times W^{(k_2K_2)}(n_2l_2,n_4l_4)]^{(\varkappa\varkappa0)}-\delta(n_2,n_3)\delta(l_2,l_3)\delta(j_2,j_3)\\ &\times\delta(j_1,j_4)\sum_{k_1}(-1)^{k_1+l_1+j_3+1/2}[k_1]^{1/2}\begin{Bmatrix} 1/2 & 1/2 & k_1\\ l_1 & l_4 & j_1\end{Bmatrix}W^{(k_1k_10)}(n_1l_1,n_4l_4)\Bigg\}.\end{aligned} \tag{6}$$

The quantities in braces are $6j$ and $9j$ coefficients; $[k_1,k_2,\dots]$ means $(2k_1+1)(2k_2+1)\cdots$ and $\{n_il_ij_i\}$ means all sets of these quantum numbers with $i=1-4$. $W^{(k_1k_2)}$ is the standard operator with the orbital rank k_1 and spin rank k_2, in $W^{(kk0)}$ the two equal ranks are joined into the zero rank with respect to the total momentum. The single electron reduced matrix element of $w^{(k_1k_2)}$ is defined as follows:

$$\langle n_\alpha l_\alpha s\|w^{(k_1k_2)}(n_1l_1,n_2l_2)\|n_\beta l_\beta s\rangle=[k_1,k_2]^{1/2}\delta(n_1,n_\alpha)\delta(n_\beta,n_2)\delta(l_1,l_\alpha)\delta(l_\beta,l_2). \tag{7}$$

The separate terms of equivalent operators in the α^2 limit turn into various Breit–Pauli operators. This correspondence for equivalent electrons was considered in Ref. 2 and for nonequivalent electrons in Ref. 4. Since the spin–angular parts of corresponding operators with the same tensorial ranks are equal, the relations between the relativistic and nonrelativistic radial integrals can be obtained. In order to derive them, it is sufficient to compare the one-electron or two-electron nondiagonal matrix or reduced matrix elements with respect to nonantisymmetrized wave functions.

Expanding the small component of orbital in powers of the fine structure constant α the scalar part of the relativistic one-electron operators O_{α_1} and O_{α_2} turns into various operators: nonrelativistic operators of kinetic energy and Coulomb interaction with the nucleus as well as to the operators of electron mass and Darwin relativistic corrections (see Table 1 of Ref. 4). In order to obtain the separate relations for the integrals of all these operators it would be necessary to separate the matrix elements of single electron operators O_{α_1} and O_{α_2}, since they are calculated jointly as a rule by relativistic programs. It is more useful to include the contributions of Darwin and mass corrections into the relations for the nonrelativistic integrals of kinetic energy and Coulomb interaction with nucleus.[7] Then the nonrelativistic radial integral,

$$I(nl,n'l)=-\frac{1}{2}\int_0^\infty P_{nl}(r)\left[\frac{d^2}{dr^2}+\frac{2Z}{r}-\frac{l(l+1)}{r^2}\right]P_{n'l}(r)\,dr, \tag{8}$$

must be replaced by the average of relativistic integrals,

$$I(nl,n'l)=\frac{1}{4l+2}\sum_j\ [j]\,I(nlj,n'lj), \tag{9}$$

where

$$I(nlj,n'lj)=\int_0^\infty\left\{-2c^2Q_{n\bar{l}j}(r)Q_{n'\bar{l}j}(r)+cQ_{n\bar{l}j}(r)\left[\frac{dP_{n'lj}(r)}{dr}+\frac{\varkappa}{r}P_{n'lj}(r)\right]-cP_{nlj}(r)\right.$$
$$\left.\times\left[\frac{dQ_{n'\bar{l}j}(r)}{dr}-\frac{\varkappa}{r}Q_{n'\bar{l}j}(r)\right]-\frac{Z}{r}(P_{nlj}(r)P_{n'lj}(r)+Q_{n\bar{l}j}(r)Q_{n'\bar{l}j}(r))\right\}dr. \tag{10}$$

$P_{nlj}(r)$ and $Q_{n\bar{l}j}(r)$ are correspondingly the large and small components of a relativistic single electron wave function.

The terms of operator O_β with spin ranks $K_1=K_2=0$ turn into the nonrelativistic operator of Coulomb interaction as well as to the Darwin two-electron (contact) interaction. Evaluating the matrix element of equivalent operator (6) the second term cancels out some contribution of the first term.[3] The comparison of the matrix elements for the Coulomb interaction operator and the corresponding terms of operator (6) gives the necessary substitution for a general nonrelativistic integral of Coulomb interaction:

$$R^k(n_1l_1n_2l_2,n_3l_3n_4l_4)=\frac{1}{4}\sum_{j_1j_2j_3j_4}[j_1,j_2,j_3,j_4]\begin{Bmatrix}j_1 & j_3 & k\\ l_3 & l_1 & 1/2\end{Bmatrix}^2\begin{Bmatrix}j_2 & j_4 & k\\ l_4 & l_2 & 1/2\end{Bmatrix}^2$$
$$\times[R^k(n_1l_1j_1n_2l_2j_2,n_3l_3j_3n_4l_4j_4)+R^k(n_1l_1j_1n_2\bar{l}_2j_2,n_3l_3j_3n_4\bar{l}_4j_4)$$
$$+R^k(n\bar{l}_1j_1n_2l_2j_2,n_3\bar{l}_3j_3n_4l_4j_4)+R^k(n_1\bar{l}_1j_1n_2\bar{l}_2j_2,n_3\bar{l}_3j_3n_4\bar{l}_4j_4)]. \tag{11}$$

In the integrals the sets of quantum numbers of electron are indicated in the same order as in a matrix element; set nlj corresponds to the large component and $n\bar{l}j$ to the small component of the wave function. The first integral in the brackets of (11) presents the relativistic analog of the Coulomb interaction integral, the two following take into account the two-electron Darwin correction. The last one integral is of order α^4. It can be omitted and is only retained for the reason that the relativistic programs usually present the sum of all four integrals.

The other relativistic correction in the Breit–Pauli approximation having the term-dependent matrix element is the spin–contact term. It is coming from the parts of O_γ and O_δ operators with the ranks $k_1=k_2=k$, $K_1=K_2=1$. In the Breit–Pauli approximation their common matrix element is expressed by the single integral:

$$R_2'(n_1l_1n_2l_2,n_3l_3n_4l_4)=\frac{\alpha^2}{4}\int_0^\infty r^{-2}P_{n_1l_1}(r)P_{n_2l_2}(r)P_{n_3l_3}(r)P_{n_4l_4}(r)dr. \tag{12}$$

It can be replaced by the following relativistic form:

$$R_2'(n_1l_1n_2l_2,n_3l_3n_4l_4)=\frac{3}{4}\sum_k(-1)^{k+k_1}\sum_{j_1j_2j_3j_4}[j_1,j_2,j_3,j_4]^{1/2}\begin{Bmatrix} l_1 & l_3 & k_1\\ 1/2 & 1/2 & 1\\ j_1 & j_3 & k\end{Bmatrix}$$
$$\times\begin{Bmatrix} l_2 & l_4 & k_1\\ 1/2 & 1/2 & 1\\ j_2 & j_4 & k\end{Bmatrix}\frac{(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_3l_3j_3n_4l_4j_4)_{\gamma+\delta}}{\langle l_1\|C^{(k_1)}\|l_3\rangle\langle l_2\|C^{(k_1)}\|l_4\rangle}, \tag{13}$$

where $\langle l_1\|C^{(k)}\|l_3\rangle$ is the reduced matrix element of spherical function (relativistic states are indicated by a rounded ket whereas the nonrelativistic ones by an angular ket). In this and the following relations the summary contribution of γ and δ operators is taken into account by using the expressions for their reduced matrix elements given in Refs. 3 and 4.

Because in the nonrelativistic approximation the spin–contact correction has the same spin-angular part as the matrix element of Coulomb interaction between electrons,[7] this correction is usually taken into account by adding the term $(2k+1)R_2'$ to the Slater integral R^k. In Eq. (13), k_1 obtains any value permitted by the triangular condition, thus the relativistic analog of such a correction to various integrals R^{k_1} is obtained different.

Approximately this relatively small relativistic interaction can be taken into account in a more simple way. In nonrelativistic approximation the matrix elements of Darwin two-electron (H_{D}) and spin–contact (H_{sc}) interactions differ only by a constant:[7]

$$\langle n_1l_1n_2l_2LSJ|h^D|n_3l_3n_4l_4L'S'J\rangle=-2\langle n_1l_1n_2l_2LSJ|h^{sc}|n_3l_3n_4l_4L'S'J\rangle. \tag{14}$$

Thus the contribution of spin–contact interaction asymptotically correct in order of α^2 can be introduced in the relation (11) simply changing the sign at the second and third integrals R^k.

The spin–spin interaction corresponds to the terms of O_γ and O_δ operators with the ranks $k_1=k\pm1$, $k_2=k\mp1$, $K_1=K_2=1$. Two-electron spin–spin matrix element is presented in Ref. 8. Its comparison with the matrix element for the corresponding terms of $O_\gamma+O_\delta$ gives the relation

$$I^k(n_1l_1n_2l_2,n_3l_3n_4l_4)=\frac{\alpha^2}{4}\int_0^\infty dr_1\int_0^{r_1}P_{n_1l_1}(r_1)P_{n_2l_2}(r_2)\frac{r_2^k}{r_1^{k+3}}P_{n_3l_3}(r_1)P_{n_4l_4}(r_2)dr_2$$
$$=\frac{3}{2\,(2k+3)}\left[\frac{(2k+1)\,(2k+5)}{(k+1)\,(k+2)}\right]^{1/2}$$
$$\times\sum_{j_1j_2j_3j_4}[j_1,j_2,j_3,j_4]^{1/2}\begin{Bmatrix} l_1 & l_3 & k+2\\ 1/2 & 1/2 & 1\\ j_1 & j_3 & k+1\end{Bmatrix}\begin{Bmatrix} l_2 & l_4 & k\\ 1/2 & 1/2 & 1\\ j_2 & j_4 & k+1\end{Bmatrix}$$
$$\times\frac{(n_1l_1j_1n_2l_2j_2\|g_1^{(k+1)}g_2^{(k+1)}\|n_3l_3j_3n_4l_4j_4)_{\gamma+\delta}}{\langle l_1\|C^{(k+2)}\|l_3\rangle\langle l_2\|C^{(k+2)}\|l_4\rangle}. \tag{15}$$

In the nonrelativistic approximation the one-electron spin–orbit and the main part of spin–other–orbit interactions are taken into account using the spin–orbit constant. In a general case of the configuration mixing this constant can be presented as follows:

$$\zeta_{nl,n'l}=\zeta^{Z}_{nl,n'l}+\sum_{n''l''}\zeta_{nl\,n''l'',n'l\,n''l''}+\zeta'_{nl,n'l}, \tag{16}$$

where the first part $\zeta^{Z}_{nl,n'l}$ corresponds to the spin–orbit interaction in the field of nucleus, the second part to the spin–other orbit interaction with the various closed shells $n''l''^{4l''+2}$ and the last one to this interaction between configurations $nl^{N}n'l^{N'}$ and $nl^{N-1}n'l^{N'+1}$. Equation (16) turns into a single-configuration case at $n'=n$.

According to Table 1 of Ref. 4, $\zeta^{Z}_{nl,n'l}$ corresponds to the contribution of operator O_{α_2} with the rank $k=1$. It obtains the following relativistic expression:[6]

$$\zeta^{Z}_{nl,n'l}=-Z\alpha^2[l(l+1)(2l+1)]^{-1}\sum_{j}(2j+1)[j(j+1)-l(l+1)-3/4](nlj|r^{-1}|n'lj). \tag{17}$$

In nonrelativistic approximation the other two parts of $\zeta_{nl,n'l}$ contain the same integrals I^k (15) as the matrix element of the spin–spin interaction and additional integrals depending on the derivative of the radial orbital. The simpler way to obtain the relativistic formulas for the second and third parts of (16) is not to derive and substitute expressions for the separate radial integrals, but to evaluate the matrix element of corresponding equivalent relativistic operator having a form of the one-electron type. Using the standard formulas of tensorial operators we obtain

$$\begin{aligned}\zeta_{nl\,n''l'',n'l\,n''l''}=&[l(l+1)(2l+1)]^{-1}\sum_{j_1j_2}[j_2(j_2+1)-l(l+1)-3/4]\\&\times\Bigg\{[j_1,j_2]^{1/2}(n''l''j_1nlj_2\|g_1^{(0)}g_2^{(0)}\|n''l''j_1n'lj_2)_{\beta+\gamma+\delta}\\&+(-1)^{j_1+j_2}\sum_{k}(n''l''j_1nlj_2\|g_1^{(k)}g_2^{(k)}\|n'lj_2n''l''j_1)_{\beta+\gamma+\delta}\Bigg\},\end{aligned} \tag{18}$$

$$\begin{aligned}\zeta'_{nl,n'l}=&[l(l+1)(2l+1)]^{-1}\sum_{j_1j_2}[j_2(j_2+1)-l(l+1)-3/4]\\&\times\Bigg\{\frac{N}{4(2l+1)}(1+\delta_{n,n'})[j_1,j_2]^{1/2}(nlj_1nlj_2\|g_1^{(0)}g_2^{(0)}\|nlj_1n'lj_2)_{\beta+\gamma+\delta}\\&+(-1)^{j_1+j_2}\sum_{k}(nlj_1nlj_2\|g_1^{(k)}g_2^{(k)}\|n'lj_2nlj_1)_{\beta+\gamma+\delta}\Bigg\}.\end{aligned} \tag{19}$$

The spin–other–orbit and orbit–orbit operators consist from several terms[9,10] and for each term with different ranks the relativistic analog of the same integral obtains a different expression. They turn to the same integral only asymptotically when the small component of the orbital is expanded by the large component in powers of α^2. These expressions are not presented in this paper since it is a simpler way to calculate exactly the contributions of these operators by the equivalent operator method.

III. CONCLUSIONS

The nonrelativistic approximation with relativistic corrections in the Breit–Pauli form is widely used due to its simplicity as compared with a relativistic approximation as well as due to the possibility to classify the terms in more realistic manner, even for the rather heavy atoms in a LS coupling scheme. However, the use of relativistic wave functions becomes necessary not only at high values of effective nuclear charge, but also for the outer shells of heavy atoms due to a shrinking of inner shells.

In this work the general relations between radial integrals in nonrelativistic and relativistic calculation schemes are obtained. They enable us to perform the relativistic CI calculations in the nonrelativistic scheme using the existing general programmes for the Breit–Pauli approximation.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Moment problems and the causal set approach to quantum gravity

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(Received 24 May 2002; accepted 6 September 2002)

We study a collection of discrete Markov chains related to the causal set approach to modeling discrete theories of quantum gravity. The transition probabilities of these chains satisfy a general covariance principle, a causality principle, and a renormalizability condition. The corresponding dynamics are completely determined by a sequence of non-negative real coupling constants. Using techniques related to the classical moment problem, we give a complete description of any such sequence of coupling constants. We prove a representation theorem: every discrete theory of quantum gravity arising from causal set dynamics satisfying covariance, causality, and renormalizability corresponds to a unique probability distribution function on the non-negative real numbers, with the coupling constants defining the theory given by the moments of the distribution. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1519668]

I. INTRODUCTION

There are currently a number of approaches aimed at formulating a successful theory of quantum gravity undergoing development, the most familiar being string theory. This article concerns an alternative to string theory: the *causal set* approach to quantum gravity. In its current state of development, the causal set approach provides a classical analog to a true quantum theory; work focusing on the development of a full quantum analog is currently underway (cf. Sec. II here and Ref. 1 for basic axioms of the causal set theory, and Refs. 2 and 3 for physical discussions concerning the causal set approach). We study the causal set approach as a classical precursor to a theory of quantum gravity.

At first glance, the most natural way to combine quantum theory and general relativity would be to quantize the space–time metric. As is well known, such a direct approach must contend with a number a significant obstructions, including the existence of unrenormalizable divergences. There is currently no clear consensus as to how these divergences are to be addressed. Many believe that the source of the problem (if not the solution) might lie in the basic assumptions involving the underlying structure of space–time. More precisely, it has been suggested that treating space–time as a discrete combinatorial object as opposed to a manifold could lead to insight towards removing the divergences in the quantum field theoretic approach, if not to a substitute for such an approach (cf. Refs. 4 and 5 and references therein).

Discrete approaches to gravity initially arose as an attempt to circumvent many of the difficulties arising in classical general relativity (e.g., existence of singularities, the difficulty of solving Einstein's field equations for general systems). Roughly speaking, the idea behind early discretization procedures involved replacing the space–time continuum with a triangulation, the construction being either a triangulation of four-dimensional space–time, or later $3+1$ in nature (triangulate a three-dimensional hypersurface at a fixed time, triangulate a second hypersurface

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considered as a time evolution of the first hypersurface, and connect vertices between triangulated hypersurfaces). In such an approach the vertices are taken to be (discrete) events, the edges between vertices in different hypersurfaces spacelike or timelike curves, and the salient relation between two such events whether one can cause the other or not.

Over the last two decades, discretization procedures have been further developed and refined, and their applications in gravity greatly expanded (cf. Ref. 6 for a recent survey of discrete approaches to gravity, both classical and quantum). One particular line of development, pioneered by Sorkin and his co-workers,[4] deemphasized the role of the metric in favor of focusing on the causal structure of space–time. This approach, the so-called causal set approach, is motivated in part by two observations. First, the causal structure of the space–time continuum determines the topological, differentiable, and conformal Lorentzian metric structure of the space–time continuum (cf. Refs. 4, 2, and 5). Second, the causal structure of the space–time continuum and the corresponding discrete causal structure are very simple mathematical objects: *posets* (partially ordered sets). Taking the primary relationship between two events to be causation, the causal set approach to gravity posits that the deep structure of space–time should be modeled by the discrete causal structures which arise as natural abstractions of the posets occuring when the causal structure of the space–time continuum is discretized (in the context of gravity, these posets are called *causets*). The causal set approach to gravity then seeks ''natural'' dynamics under which causets evolve. In Ref. 1, Rideout and Sorkin propose such dynamics (formulated probabilistically) for the (classical) evolution of causets.

Thus, the search for an appropriate dynamical framework for a quantum theory of gravity has recently led to interest in stochastic dynamical systems taking their values in certain locally finite partially ordered sets (*causets*). As discussed in Ref. 1, these systems can be realized as Markov chains whose transition probabilities are required to satisfy a discrete covariance principle and a discrete causality principle. We call such Markov chains ''generic'' if all of the transition probabilities which could be nonzero are positive (cf. Definition 2.1). Given the appropriate mathematical formalism (cf. Ref. 1, and Sec. II of this work), it is possible to classify all such generic chains: there is a 1–1 correspondence between generic chains satisfying covariance and causality and nonnegative sequences of real numbers, $T=\{t_n\}_{n=0}^{\infty}$, satisfying $t_0=1$ (the coupling constants t_n are given explicitly in terms of the Markov chain—cf. Ref. 1 and Sec. II of this work).

It is easy to see that an arbitrary sequence T is unlikely to have physical significance, and therefore we want to find additional natural conditions which restrict the collection of sequences under consideration to those sequences which are ''physical.'' Thus, in addition to covariance and causality one might expect, as first suggested in Ref. 7, that a discrete theory of quantum gravity should satisfy a cosmological renormalizability condition under cycles of expansion and contraction. Given the framework of Ref. 1 such a condition can be formulated as an additional constraint on the coupling constants defining the theory. To make this precise, we introduce the required notation.

We will denote by $\mathcal{S}$ the collection of sequences of non-negative real numbers. We will denote elements of $\mathcal{S}$ by upper case roman letters, and, as above, we will use the corresponding lower case letter to denote specific elements of a given sequence. We will denote by $\mathcal{S}_1$ the subset of $\mathcal{S}$ consisting of those sequences which begin with 1. We define a *cosmological renormalization operator* $\mathcal{R}:\mathcal{S}\to\mathcal{S}$ by

$$(\mathcal{R}(T))_n=t_n+t_{n+1}. \tag{1}$$

The operator $\mathcal{R}$ admits a stable manifold, $\mathrm{Stab}(\mathcal{R})\subset\mathcal{S}$, defined by

$$\mathrm{Stab}(\mathcal{R})=\left\{T\in\mathcal{S}:T\in\bigcap_{k=0}^{\infty}\mathcal{R}^k(\mathcal{S})\right\}. \tag{2}$$

We call elements of $\mathrm{Stab}(\mathcal{R})$ *stable sequences* and we note that (cf. Ref. 7 and Sec. II in this work) there is a 1–1 correspondence between generic chains satisfying causality, covariance and cosmo-

logical renormalizability under cycles of expansion and contraction and elements of $\mathbb{S} = \mathcal{S}_1 \cap \mathrm{Stab}(\mathcal{R})$. Our main result, a representation theorem, gives a complete description of $\mathrm{Stab}(\mathcal{R})$ in terms of measures on $\mathbb{R}^+ = [0,\infty)$:

Theorem 1.1: *Let T be a sequence of non-negative real numbers. Then $T \in \mathrm{Stab}(\mathcal{R})$ if and only if there is a nondecreasing function $\alpha: \mathbb{R}^+ \to \mathbb{R}$ such that*

$$t_n = \int_0^\infty s^n d\alpha(s). \tag{3}$$

For T and α as in Theorem 1.1, we will say that T is represented by α.

Our theorem is motivated by an observation of Ref. 7: *transitive percolation*, the theory which is determined by choosing $t \in \mathbb{R}^+$ and defining associated coupling constants by

$$t_n = t^n, \tag{4}$$

defines a stable sequence (by convention $0^0 = 1$). Transitive percolation as given by (4) is represented by a probability measure on $\mathbb{R}^+$; a delta-mass of weight one concentrated at $t \in \mathbb{R}^+$ has moments which coincide with the sequence. This measure can in turn be represented by its probability distribution function, a translate of the Heaviside function. Our theorem can be seen as quantifying to what extent transitive percolation is representative of the general behavior of stable sequences. Namely, any stable sequence is a ''linear combination'' of percolation sequences.

As is clear from the statement of Theorem 1.1, our result is closely related to the classical moment problem of Stieltjes type (cf. Sec. III to follow). As a consequence, Theorem 1.1 and its proof provide a means of applying the extensive collection of sophisticated mathematical tools developed in the context of the moment problem to questions related to quantum gravity. We provide a number of straightforward corollaries of our technique. These corollaries include an explicit representation of the transition probabilities associated to any generic Markov chain which defines a discrete theory satisfying covariance, causality and cosmological renormalizability, as well as a second representation theorem which associates to any such theory a natural self-adjoint non-negative operator acting on a model Hilbert space (cf. Sec. V to follow).

II. BACKGROUND AND DEFINITIONS FROM DISCRETE QUANTUM GRAVITY

In this section we present the mathematical formulation for a classical precursor of a discrete theory of quantum gravity. We follow the development of Refs. 1 and 7.

The fundamental object of study, a *causet*, is a locally finite partially ordered set. Throughout this article we will denote causets with upper case roman letters and, when needed, indicate the partial order relation using the symbol $\lll$. We assume throughout that $\lll$ is irreflexive.

An isomorphism of causets is a bijection which preserves the partial orders. Isomorphism defines an equivalence relation on causets. We will denote by $\mathcal{C}_n$ the collection of equivalence classes of causets with n elements indexed by $\{0,1,\ldots,n-1\}$, with partial order consistent with indexing. Thus, up to equivalence,

$$\mathcal{C}_n = \{C : C \text{ a causet}, \ C = \{a_0,\ldots,a_{n-1}\}, \ a_k \lll a_l \Rightarrow k < l\}. \tag{5}$$

We write

$$\mathcal{C} = \bigcup_{n \in \mathbb{N}} \mathcal{C}_n \tag{6}$$

and we note that $\mathcal{C}$ carries a natural partial order given as follows: $C \prec D$ if and only if $C \in \mathcal{C}_n$, $D \in \mathcal{C}_m$ with $n < m$, and there exists an order preserving function $f: C \to D$ such that $f(C)$ is an initial segment of D.

Informally, we can describe the dynamic evolution of causets as follows: Initially, the state of the system is given by the trivial causet consisting of a single point. At each increment of time, an

element comes into existence as the ''offspring'' of elements already in existence. That is, at the beginning of the nth increment of time we have a causet $C \in \mathcal{C}_n$ which we evolve to a causet $D \in \mathcal{C}_{n+1}$ by adding an element to C together with relations between the new element and a subset of elements of C (those elements in the past of the new element, i.e., those which bear some causal relationship to the new element). The new relations are determined randomly; the probability that any given collection of relations is added is given by a collection of transition probabilities which define the theory. We can now proceed to formalize this description.

Given a causet C and an element $x \in C$, we define the past of x by

$$\text{past}_C(x) = \{y \in C : y \lll x\}. \tag{7}$$

We will regard $\text{past}_C(x)$ as a poset with partial order given by the partial order of C. A *link* in a partially ordered set is an irreducible relation (i.e., a relation that contains no other relation). A *path* in a partially ordered set is a sequence of elements of the set, each related to the next by a link.

Given $C \in \mathcal{C}_n$, we will define the family of C, denoted $F(C)$, as those elements $D \in \mathcal{C}_{n+1}$ such that $C \prec D$, where $\prec$ denotes the partial order of elements of $\mathcal{C}$:

$$F(C) = \{D \in \mathcal{C}_{n+1} : C \prec D\}. \tag{8}$$

Given $C \in \mathcal{C}_n$ and $D \in F(C)$, the precursor set of the transition $C \to D$, denoted $\text{Prec}(C,D)$, is the past of the element $x \in D \backslash C$:

$$\text{Prec}(C,D) = \text{past}_D(x) \subset D. \tag{9}$$

Note that $\text{Prec}(C,D)$ is a poset with partial order given by its description as the past of an element $x \in D$. The collection of *maximal elements associated to the transition* $C \to D$ is the collection of elements of D with links to the element x:

$$\max(C,D) = \{y \in D : y \text{ linked to } x,\ x \in D \backslash C\}. \tag{10}$$

A special role in the theory will be played by those causets with no relations. We will denote the element of $\mathcal{C}_n$ with no relations by A_n:

$$A_n = ((a_0, a_1, \ldots, a_{n-1}), \varnothing). \tag{11}$$

We note that there is a natural path in $\mathcal{C}$ of length n from A_0 to A_n.

We define a collection of Markov chains with state space $\mathcal{C}$ as follows:

Definition 2.1: *We say that a Markov chain M with state space $\mathcal{C}$ belongs to the collection $\mathcal{M}$ if the transition probabilities of M satisfy the following.*

(1) Given $C \in \mathcal{C}_n$, let $\text{Prob}(C \to D)$ denote the transition probability corresponding to an evolution from causet C to causet D. Then $\text{Prob}(C \to D) = 0$ if $D \notin F(C)$ and $\Sigma_{D \in F(C)} \text{Prob}(C \to D) = 1$.

(2) (General Covariance) Let $C \in \mathcal{C}_n$. Suppose $\mathcal{P}_1$ and $\mathcal{P}_2$ are two paths from A_0 to C and write $\mathcal{P}_I = \{l_{i1}, \ldots, l_{in}\}$ where the l_{ij} are the links defining the path $\mathcal{P}_i$. Then

$$\prod_{k=1}^{n} \text{Prob}(l_{1k}) = \prod_{k=1}^{n} \text{Prob}(l_{2k}).$$

(3) (Causality) Suppose that $C \in \mathcal{C}_n$ and for $i = 1, 2$, suppose that $C_i \in F(C)$. Let $B \in \mathcal{C}_m$, $m \leqslant n$, be defined by

$$B = \text{Prec}(C, C_1) \cup \text{Prec}(C, C_2)$$

with poset structure induced by that of C. Let $B_i \in \mathcal{C}_{m+1}$ be B with an element added in the same manner as in the transitions $C \to C_i$. Then we require

$$\frac{\text{Prob}(C \to C_1)}{\text{Prob}(C \to C_2)} = \frac{\text{Prob}(B \to B_1)}{\text{Prob}(B \to B_2)}. \tag{12}$$

It is a theorem of Rideout and Sorkin that any generic element of $\mathcal{M}$ is completely determined by a discrete collection of coupling constants given by transitions between causets with no relations. More precisely, let $M \in \mathcal{M}$, and suppose that A_n is given as in (11). Associate to M a sequence of positive coupling constants $\{q_n\}_{n=0}^{\infty}$ defined by

$$q_0 = 1, \tag{13}$$

$$q_n = \text{Prob}(A_{n-1} \to A_n), \tag{14}$$

where, as above, the expression appearing on the right hand side of (14) denotes the probability of transition from A_{n-1} to A_n. In Ref. 1, Rideout and Sorkin prove that the sequence $\{q_n\}_{n=0}^{\infty}$ completely determines the theory associated to M. More precisely, given an element $C \in \mathcal{C}_n$, and $D \in F(C)$ [cf. (8)], let max(C,D) be the collection of maximal elements associated to the transition $C \to D$ [cf. (10)] and let Prec(C,D) be the precursor set of the transition $C \to D$ [cf. (9)]. Suppose the cardinality of Prec(C,D) is ρ and that the cardinality of max(C,D) is m. Then the transition probability for the evolution $C \to D$ is given by (cf. Ref. 1)

$$\text{Prob}(C \to D) = q_n \sum_{k=0}^{m} (-1)^k \binom{m}{k} \frac{1}{q_{\rho-k}}, \tag{15}$$

which indicates that the Markov chain M is completely determined by the sequence of q_n defined as in (14).

Following Ref. 1, we define a sequence t_n by

$$t_n = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} \frac{1}{q_k}. \tag{16}$$

Then we can recover the coupling constants q_n from the sequence of t_n:

$$\frac{1}{q_n} = \sum_{k=0}^{n} \binom{n}{k} t_k. \tag{17}$$

As in the Introduction, let $\mathcal{S}_1$ be defined by $\mathcal{S}_1 = \{T \in \mathcal{S} : t_0 = 1\}$. There is a bijection between generic elements of $\mathcal{M}$ and elements of $\mathcal{S}_1$ given by associating to each element of $\mathcal{S}_1$ the associated collection of coupling constants $\{q_n\}_{n=0}^{\infty}$ given by (17).

Amongst additional constraints that one might impose to restrict further the collection of chains that could serve as classical precursor for a discrete model of quantum gravity, there is a natural choice involving cosmological renormalizability under cycles of expansion and contraction. More precisely, given a causet C, we call an element $\gamma \in C$ a *post*, if every element of C is either in the past of γ or in the future of γ in C [denoted future$_C(\gamma)$]:

$$C = \text{past}_C(\gamma) \cup \{\gamma\} \cup \text{future}_C(\gamma). \tag{18}$$

Physically, the occurence of a post corresponds to a collapse of the universe to zero diameter, followed by reexpansion.

Given a causet C and a post γ, there is a simple relationship between the coupling constants t_n governing the evolution of C and the coupling constants governing the evolution of the causet $\{\gamma\}\cup \text{future}_C(\gamma)$ (cf. Ref. 7): If $p=|\text{past}_C(\gamma)|$, then the coupling constants for $\{\gamma\}\cup \text{future}_C(\gamma)$ are given by

$$\tilde{t}_n=\sum_{k=0}^{p}\binom{p}{k}t_{n+k}, \tag{19}$$

where $n>0$. This relationship is concisely described in terms of the cosmological renormalization operator $\mathcal{R}:\mathcal{S}\to\mathcal{S}$ defined by

$$(\mathcal{R}(T))_n=t_n+t_{n+1}. \tag{20}$$

Using the renormalization operator we can write the right hand side of (19) as $(\mathcal{R}^p(T))_n$. We use this concise notation to define the collection of Markov chains which we intend to study.

Definition 2.2: *We say that a Markov chain M with state space $\mathcal{C}$ belongs to the collection $\mathbb{M}$ if*

(1) $M\in\mathcal{M}$ is generic, and
(2) If M is represented by the sequence $T\in\mathcal{S}$, then

$$T\in\bigcap_{n=0}^{\infty}\mathcal{R}^n(\mathcal{S}). \tag{21}$$

As in the Introduction, we call the right hand side of (21) the stable set of the renormalization operator and we write

$$\text{Stab}(\mathcal{R})=\bigcap_{n=0}^{\infty}\mathcal{R}^n(\mathcal{S}). \tag{22}$$

If we set $\mathbb{S}=\mathcal{S}_1\cap\text{Stab}(\mathcal{R})$, then it is clear from the definition that there is a bijection between elements of $\mathbb{M}$ and elements of $\mathbb{S}$. It is also clear that $\text{Stab}(\mathcal{R})$ is a convex set.

As discussed in Refs. 1 and 7 and our introduction, there are a number of interesting special cases of processes which satisfy the conditions defining $\mathbb{M}$. Of particular interest from our point of view are theories of *transitive percolation* defined by fixing $t\in\mathbb{R}^+$ and setting

$$t_n=t^n. \tag{23}$$

As mentioned in the Introduction, the sequence defined by (23) can be represented by a probability measure on $\mathbb{R}$: a delta-mass of weight 1 concentrated at $t\in\mathbb{R}^+$. This fact, together with the observed convexity of $\text{Stab}(\mathcal{R})$, suggests that we develop a representation of $\text{Stab}(\mathcal{R})$ in terms of the moments of probability measures on $\mathbb{R}^+$.

III. MOMENT PROBLEMS

In this section we develop material related to the classical moment problem which we will need in the sequel. References to this material include Refs. 8 and 9.

Let $[a,b]$ be an interval in the real line, $\alpha:[a,b]\to\mathbb{R}$ a function of bounded variation. Given $t\in(a,b)$, we write

$$\alpha(t\pm)=\lim_{s\to t^{\pm}}\alpha(s).$$

We say that α is *normalized* if $\alpha(a)=0$ and for all $t\in(a,b)$,

$$\alpha(t)=\frac{\alpha(t-)+\alpha(t+)}{2}. \tag{24}$$

If f is continuous on $[a,b]$ and α is of bounded variation, we will denote the Stieltjes integral of f with respect to α by $\int_a^b f(s)d\alpha(s)$. Functions of bounded variation behave well with respect to Stieltjes integration: if α is of bounded variation on $[a,b]$, if f is continuous, and if $c\in[a,b]$, then

$$\beta(x)=\int_c^x f(s)d\alpha(s) \tag{25}$$

defines a function of bounded variation. Moreover, if g is continuous, then

$$\int_a^b g(s)d\beta(s)=\int_a^b g(s)f(s)d\alpha(s). \tag{26}$$

Stieltjes integration behaves as expected under change of coordinates: if α is of bounded variation on $[a,b]$, if f is continuous on $[a,b]$ and if γ is continuous and strictly increasing on $[a,b]$, then

$$\int_a^b f(s)d\alpha(s)=\int_c^d f(\gamma(s))d\alpha(\gamma(s)), \tag{27}$$

where $a=\gamma(c)$ and $b=\gamma(d)$.

Stieltjes integration can be extended to improper integrals. For example, if $\alpha:\mathbb{R}^+\to\mathbb{R}$ is of bounded variation, and f is continuous on $(0,\infty)$, we write

$$\int_0^\infty f(s)d\alpha(s)=\lim_{R\to\infty,\epsilon\to 0}\int_\epsilon^R f(s)d\alpha(s)$$

when the limit exists and is finite. The formulas (26) and (27) are easily extended to improper integrals.

Definition 3.1: *Let $T\in\mathcal{S}$. We say that a nondecreasing function $\alpha:[0,1]\to\mathbb{R}$ is a solution of the* Hausdorff moment problem for *T if, for all n,*

$$t_n=\int_0^1 s^n d\alpha(s). \tag{28}$$

We say that a nondecreasing function $\alpha:\mathbb{R}^+\to\mathbb{R}$ is a solution of the Stieltjes moment problem for *T if, for all n,*

$$t_n=\int_0^\infty s^n d\alpha(s). \tag{29}$$

The solution of the Stieltjes moment problem played a fundamental role in the development of modern analysis. We recall the material relevant to our purpose.

Definition 3.2: *Let T be a sequence of real numbers. The* difference operator, Δ, *mapping sequences of real numbers to sequences of real numbers is defined by*

$$(\Delta(T))_n=t_{n+1}-t_n. \tag{30}$$

A sequence $T\in\mathcal{S}$ is said to be completely monotonic *if for all n and for all k,*

$$(\Delta^k(T))_n\geqslant 0. \tag{31}$$

We can now state Hausdorff's solution to the moment problem bearing his name:

Theorem 3.1: *(Hausdorff) Suppose $T \in \mathcal{S}$. Then the Hausdorff moment problem for T has a solution if and only if the sequence T is completely monotonic. When T is completely monotonic, the solution of the moment problem is unique.*

The solution of the moment problem associated to Stieltjes is given in the following.

Theorem 3.2: *(Stieltjes) Suppose $T \in \mathcal{S}$. Then the Stieltjes moment problem for T has a solution if and only if the Hankel determinants*

$$H_{0,n} = \begin{vmatrix} t_0 & t_1 & \dots & t_n \\ t_1 & t_2 & \dots & t_{n+1} \\ \dots & \dots & \dots & \dots \\ t_n & t_{n+1} & \dots & t_{2n} \end{vmatrix}, \tag{32}$$

$$H_{1,n} = \begin{vmatrix} t_1 & t_2 & \dots & t_{n+1} \\ t_2 & t_3 & \dots & t_{n+2} \\ \dots & \dots & \dots & \dots \\ t_{n+1} & t_{n+2} & \dots & t_{2n+1} \end{vmatrix} \tag{33}$$

are nonnegative for all values of n.

IV. PROOF OF THE MAIN RESULT

We begin with a definition:

Definition 4.1. Let $X=(X_{i,j})$, $0 \leqslant i, j < \infty$, be a doubly infinite matrix with real entries. We say that X is a tableau *if we have the following.*

(1) $X_{i,j} \geqslant 0$ *for all i, j.*
(2) *If $X_k = \{X_{k,j}\}_{j=0}^{\infty}$ is the sequence whose terms are given by the kth row of X and $\mathcal{R}$ is the renormalization operator defined by (20), then $\mathcal{R}(X_k) = X_{k-1}$ for all k.*

Given $n \in \mathbb{N}$, a partial n-tableau *is a matrix of n rows and an infinite number of columns which satisfies the two defining conditions of a tableau. If $\mathcal{P}_n$ is the collection of partial n-tableau, if $P \in \mathcal{P}_n$ and $m \leqslant n$, the m-corner operator $\mathcal{O}_m : \mathcal{P}_n \to \mathbb{R}^m \times \mathbb{R}^m$ is the map defined by truncation*:

$$\mathcal{O}_m(P) = (P_{i,j}), \quad 0 \leqslant i, j \leqslant m-1. \tag{34}$$

Tableaux are closely related to stable sequences: It is clear from Definitions 2.2 and 4.1 that if X is a tableau and $X_0 = \{X_{0,n}\}_{n=0}^{\infty}$ is the first row of X, then $X_0 \in \mathrm{Stab}(\mathcal{R})$. Conversely, we have the following.

Lemma 4.1: Suppose that $T \in \mathrm{Stab}(\mathcal{R})$. Then there is a tableau whose first row is T.

Proof: Let $T \in \mathrm{Stab}(\mathcal{R})$. For each $n \in \mathbb{N}$ we can find a partial n-tableau with first row T. We will create an infinite sequence, $\{Y^{\alpha}\}_{\alpha=1}^{\infty}$. Each Y^{α} is itself an infinite sequence of partial tableaux where the number of rows will tend to infinity as $\alpha \to \infty$. Then we will use a diagonal trick to finish the proof.

Define a sequence of partial tableau, $Y^1 = \{Y_n^1\}_{n=1}^{\infty}$, where for each n, Y_n^1 is a partial n-tableau with T as first row. Having chosen subsequences $Y^{m-1} \subset Y^{m-2} \subset \cdots \subset Y^1$, choose a subsequence Y^m of Y^{m-1} which satisfies the following.

(1) Y_n^m is a partial k_n-tableau with $k_n \geqslant m$.
(2) If $\mathcal{O}_m$ is the m-corner operator defined in (34), then $\mathcal{O}_m(Y_n^m)$ converges as $n \to \infty$.

Consider the sequence of matrices $Z_k = Y_k^k$. Then Z_k converges to a doubly infinite matrix with non-negative entries and first row given by T. That Z is a tableau follows from the continuity of the m-corner operator acting on Z_k. □

Lemma 4.2: Suppose that X is a tableau and let $\{X_{k,n}\}=\{X_{k,n}\}_{k=0}^{\infty}$ be the sequence whose terms are given by the nth column of X. Then $\{X_{k,n}\}$ is a completely monotonic sequence.

Proof: An explicit computation shows that the diagonal entries of X are given by

$$X_{k,k}=\sum_{l=0}^{k}(-1)^l\binom{k}{l}X_{l,0}. \tag{35}$$

By assumption the terms of X are all non-negative. This proves that the first column of X is completely monotonic. To finish the proof, note that tableaux are stable under truncation of their first n columns. Carrying out such a truncation, the argument above establishes that the $(n+1)$th column of X (the first column of the truncated matrix) is completely monotonic. □

Lemma 4.3: Suppose $\{y_i\}_{i=1}^{\infty}$ is a completely monotonic sequence. Let $\alpha:[0,1]\to\mathbb{R}$ be the normalized nondecreasing function such that, for $1\leqslant i$,

$$y_i=\int_0^1 s^{i-1}d\alpha(s). \tag{36}$$

Then there exists y_0 such that $\{y_i\}_{i=0}^{\infty}$ is completely monotonic if and only if

$$\int_0^1 s^{-1}d\alpha(s) \quad converges. \tag{37}$$

Moreover, if $\int_0^1 s^{-1}d\alpha(s)=L$, then

$$L=\inf\{y_0:\{y_i\}_{i=0}^{\infty}\ is\ completely\ monotonic\}. \tag{38}$$

Proof: Suppose that (37) holds. Define $\beta:[0,1]\to\mathbb{R}$ by

$$\beta(t)=\int_0^t s^{-1}d\alpha(s).$$

Then β is nondecreasing and for $i\geqslant 1$,

$$\int_0^1 s^i d\beta(s)=\int_0^1 s^{i-1}d\alpha(s).$$

Setting $y_0=\int_0^1 s^{-1}d\alpha(s)$, we see that there is a solution to the Hausdorff moment problem for the augmented sequence $\{y_i\}_{i=0}^{\infty}$. By Hausdorff's theorem (cf. Theorem 3.1), the augmented sequence is completely monotonic.

Conversely, suppose there is a $y_0\in\mathbb{R}$ such that the augmented sequence $\{y_i\}_{i=0}^{\infty}$ is completely monotonic. Let $\beta:[0,1]\to\mathbb{R}$ be the normalized nondecreasing solution of the Hausdorff moment problem for the augmented sequence. Then, for all $i\geqslant 1$,

$$\int_0^1 s^{i-1}d\alpha(s)=\int_0^1 s^{i-1}sd\beta(s). \tag{39}$$

Define continuous linear functionals, L_α, L_β, on the space of continuous functions on [0,1]:

$$L_\alpha(f)=\int_0^1 f(s)d\alpha(s),$$

$$L_\beta(f)=\int_0^1 f(s)sd\beta(s).$$

From (39) we conclude that L_α and L_β agree on polynomials. By the Weierstrass theorem and continuity of the integral, we conclude that $L_\alpha = L_\beta$. Choose $f_n(s)$ the increasing sequence of non-negative continuous functions equal to $1/s$ on $[1/n,1]$ and equal to n on $[0,1/n]$ so that

$$\lim_{n\to\infty} \int_0^1 f_n(s) s d\beta(s) = y_0.$$

Then,

$$\int_{1/n}^1 f_n(s) d\alpha(s) \leqslant \int_0^1 f_n(s) s d\beta(s). \tag{40}$$

Since the right hand side of (40) converges as $n\to\infty$, we conclude that (37) holds. Since the right hand side converges to y_0, we conclude that $L = \int_0^1 s^{-1} d\alpha(s)$ is a lower bound for any y_0 augmenting the original sequence. Since we have already established that when the integral converges, $y_0 = L$ gives a completely monotonic augmented sequence, we are done. □

Remark: With $\{y_i\}_{i=1}^\infty$ and L as in Lemma 4.3, any $y_0 \geqslant L$ gives a completely monotonic augmented sequence.

Lemma 4.4: Let X be a tableau. Then X is determined by its first column. In fact, if $\{X_{n,0}\} = \{X_{n,0}\}_{n=0}^\infty$ *is the first column of X and* $\alpha:[0,1]\to\mathbb{R}$ *is the normalized nondecreasing function representing* $\{X_{n,0}\}$,

$$X_{n,0} = \int_0^1 s^n d\alpha(s), \tag{41}$$

then

$$X_{0,p} = \int_0^1 s^{-p}(1-s)^p d\alpha(s). \tag{42}$$

Proof: By Lemma 4.2 $\{X_{n,0}\} = \{X_{n,0}\}_{n=0}^\infty$ is a completely monotonic sequence and thus admits a representation by α as in (41). By definition of a tableau, $X_{n,0} + X_{n,1} = X_{n-1,0}$ for all $n \geqslant 1$, and thus for $n \geqslant 1$,

$$X_{n,1} = \int_0^1 s^{n-1}(1-s) d\alpha(s).$$

Since $\{X_{n,1}\}_{n=1}^\infty$ is represented as a moment sequence, by Hausdorff's theorem $\{X_{n,1}\}_{n=1}^\infty$ is completely monotonic. Since $\{X_{n,1}\}_{n=1}^\infty$ is part of a column of a tableau, $\{X_{n,1}\}_{n=1}^\infty$ extends to a completely monotonic sequence $\{X_{n,1}\}_{n=0}^\infty$. By Lemma 4.3, we conclude that

$$\int_0^1 s^{-1}(1-s) d\alpha(s)$$

converges and we set

$$L = \int_0^1 s^{-1}(1-s) d\alpha(s).$$

Let $\beta:[0,1]\to\mathbb{R}$ be a normalized nondecreasing function representing the completely monotone sequence $L, X_{1,1}, X_{2,1}, \ldots$. Let $\epsilon = X_{0,1} - L$ and let $h(t)$ be the Heaviside function:

$$h(t)=\begin{cases}1 & \text{if } t>0\\ 0 & \text{if } t\leqslant 0.\end{cases}$$

Define $\gamma:[0,1]\to\mathbb{R}$ by

$$\gamma(t)=\beta(t)+\epsilon h(t). \tag{43}$$

Then γ is nondecreasing and for all $n\geqslant 0$,

$$X_{n,1}=\int_0^1 s^n d\gamma(s).$$

Let $f_n(s)$ be as defined in the proof of Lemma 4.3. Consider the pair of columns $\{X_{n,1}\}$ and $\{X_{n,2}\}$. By the analysis given for the pair $\{X_{n,0}\}$ and $\{X_{n,1}\}$, we know that

$$\int_0^1 s^{-1}(1-s)d\gamma(s)$$

converges and therefore $\int_0^1 f_n(s)(1-s)d\gamma(s)$ converges as $n\to\infty$. But $\int_0^1 f_n(s)(1-s)d\beta(s)$ is non-negative and $\int_0^1 f_n(s)(1-s)dh(s)$ diverges as $n\to\infty$, from which we conclude that $\epsilon=0$. Thus, $X_{0,1}=L$ and the column $\{X_{n,0}\}$ determines the column $\{X_{n,1}\}$. The lemma follows by induction. □

Proof of Theorem 1.1: Suppose that $T\in\mathcal{S}$ and suppose that $\alpha:\mathbb{R}^+\to\mathbb{R}$ is a normalized nondecreasing function representing T:

$$t_n=\int_0^\infty s^n d\alpha(s).$$

Fix $p\in\mathbb{N}$ and define $\beta:\mathbb{R}^+\to\mathbb{R}^+$ by

$$\beta(s)=\int_0^s \frac{1}{(1+u)^p} d\alpha(u).$$

Then β is nondecreasing on $\mathbb{R}^+$ and of bounded variation. Let S be the sequence corresponding to the moments of β:

$$s_n=\int_0^\infty u^n d\beta(u).$$

A direct computation using (26) gives $\mathcal{R}^p(S)=T$. This proves that every moment sequence is stable.

To establish the converse, suppose that T is a stable sequence. By Lemma 4.1, there is a tableau, X, which has T as its first row. By Lemma 4.4, X is determined by its first column. By Lemma 4.3, the first column of X is completely monotonic and thus, by Hausdorff's theorem, there is a unique normalized nondecreasing $\alpha:[0,1]\to\mathbb{R}$ which represents $\{X_{n,0}\}$:

$$X_{n,0}=\int_0^1 s^n d\alpha(s).$$

Thus, T is determined by α. To complete the proof, we use α to construct a measure on $\mathbb{R}^+$ with moments given by T.

Write $u=(1-s)/s$ and $s=1/(1+u)$. The function $\gamma:\mathbb{R}^+\to\mathbb{R}$ defined as the composition $\gamma(u)=-\alpha(s)$ is nondecreasing with total variation bounded by the variation of α. By Lemma 4.4,

$$X_{0,n}=\int_0^\infty u^n d\gamma(u), \tag{44}$$

which exhibits the first row of X as a moment sequence and completes our proof. □

V. APPLICATIONS

Theorem 1.1 provides for a representation of the transition probabilities for a Markov chain which provides a classical precursor for a discrete theory of quantum gravity satisfying causality, covariance and cosmological renormalizability:

Corollary 5.1: Suppose that $M \in \mathbb{M}$ is a Markov chain satisfying Definition 2.2. Suppose that $T \in \mathbb{S}$ is the sequence of coupling constants defining M and that $\alpha: \mathbb{R}^+ \to \mathbb{R}$ is a nondecreasing function representing T. Suppose that $\{q_n\}_{n=0}^{\infty}$ are the transition probabilities defined in (14). Then

$$\frac{1}{q_n} = \int_0^{\infty} (1+s)^n d\alpha(s). \tag{45}$$

Proof: This follows immediately from (17) and the binomial theorem. □

Using Corollary 5.1 we obtain an attractive representation for general transition probabilities:

Corollary 5.2: Suppose that $C \in \mathcal{C}_n$ and that $D \in F(C)$. Suppose that the cardinality of $\mathrm{Prec}(C,D)$ *is ρ and that the cardinality of* $\max(C,D)$ *is m. Suppose that $M \in \mathbb{M}$ is a Markov chain satisfying Definition 2.2. Suppose that $T \in \mathbb{S}$ is the sequence of coupling constants defining M and that $\alpha: \mathbb{R}^+ \to \mathbb{R}$ is a nondecreasing function representing T. Then*

$$\mathrm{Prob}(C \to D) = \frac{\int_0^{\infty} s^m (1+s)^{\rho - m} d\alpha(s)}{\int_0^{\infty} (1+s)^n d\alpha(s)}. \tag{46}$$

Proof: This follows immediately from Corollary 5.1, (15), and the binomial theorem applied to $s^m = ((1+s)-1)^m$. □

Our next result establishes that *all* positive sequences which grow fast enough are stable:

Corollary 5.3: Any monotonic sequence which grows sufficiently quickly defines an element of $\mathrm{Stab}(\mathcal{R})$.

Proof: For a quickly growing sequence, the positivity conditions on the Hankel determinants (32) and (33) are trivially satisfied as the value of the determinant is controlled by the entry in the lower right hand corner. Thus, any monotonic sequence which grows sufficiently quickly is a moment sequence and Corollary 5.3 follows from Theorem 1.1. □

Corollaries 5.2 and 5.3 provide a means of quantifying the evolution of causets under dynamics which provide for rapidly increasing coupling constants. We hope to return to this in a future paper.

Our final result uses Hankel determinants to associate to any stable sequence which is not a finite linear combination of percolation sequences, a model Hilbert space and a non-negative self-adjoint operator. Our development follows that of Simon.[10]

The Hankel determinants appearing in (32) and (33) are associated to quadratic forms which arise naturally in the analysis of the Stieltjes moment problem. More precisely, given a sequence $T \in \mathrm{Stab}(\mathcal{R})$, consider the sesquilinear forms $H_N^i: \mathbb{C}^N \to \mathbb{C}$ defined by

$$H_N^0(\rho,\sigma) = \sum_{0 \leqslant n,m \leqslant N-1} \overline{\rho}_n \sigma_m t_{n+m}, \tag{47}$$

$$H_N^1(\rho,\sigma) = \sum_{0 \leqslant n,m \leqslant N-1} \overline{\rho}_n \sigma_m t_{n+m+1}. \tag{48}$$

Let $\mathcal{H}_N^i$ be the matrices associated to the forms H_N^i via the relation

$$H_N^i(\rho,\sigma) = \langle \rho, \mathcal{H}_N^i \sigma \rangle, \tag{49}$$

where the pairing is Euclidean. Then the Hankel determinants appearing in Theorem 3.2 are given by $\det(\mathcal{H}_N^i) = H_{i,N}$ and the forms H_N^i are strictly positive definite if and only if the corresponding Hankel determinants are positive (cf. Ref. 10). Following Ref. 10, we use this material to reformulate the Stieltjes result in the language of self-adjoint operators.

For the remainder of the article we assume that the sequence T is not a finite linear combination of percolation sequences, so that the Hankel determinants are all strictly positive definite.

Suppose that $\mathbb{C}[x]$ is the algebra of polynomials with complex coefficients. Define a positive definite inner product on $\mathbb{C}[x]$ by

$$\langle p,q\rangle = H_N^0(\rho,\sigma), \tag{50}$$

where $p(x) = \Sigma_{n=0}^{N-1}\rho_n x^n$ and $q(x) = \Sigma_{n=0}^{N-1}\sigma_n x^n$. Using this inner product, we complete $\mathbb{C}[x]$ to a Hilbert space $\mathbb{H}_T$, where the subscript T denotes the dependence on the moment sequence T.

Let A be the operator with domain $D(A) = \mathbb{C}[x] \subset \mathbb{H}_T$ defined by

$$A(p)(x) = xp(x). \tag{51}$$

Then A is densely defined, symmetric and non-negative. Thus, by the theory of von Neumann, A admits self-adjoint extensions. Amongst the (possibly many) self-adjoint extensions of A there is a distinguished extension, the *minimal* non-negative self-adjoint extension (the Friedrichs extension) of A to an operator A_F with domain contained in $\mathbb{H}_T$.

It is a theorem of Simon that the collection of such extensions of A parametrizes solutions to the (nondegenerate) Stieltjes moment problem.[10] We summarize these results in the following.

Theorem 5.1: *(Simon) Suppose that $T \in \mathcal{S}$ is a sequence which is not a finite linear combination of percolation sequences and whose corresponding Stieltjes problem admits a solution. Let $\mathbb{H}_T$ be the corresponding Hilbert space completion of the algebra of polynomials with inner product defined by* (50)*, and let $A: D(A) \to \mathbb{C}[x]$ be the operator defined by (51). Then every solution to the Stieltjes problem for the sequence T corresponds to a unique non-negative self-adjoint extension of A to an operator $\tilde{A}: \mathbb{H}_T \to \mathbb{H}_T$ with spectral measure $\mu_{\tilde{A}}$ satisfying*

$$t_n = \int_0^\infty s^n d\mu_{\tilde{A}}(s).$$

With the conventions established above, we have the following corollary:

Corollary 5.4: To every sequence $T \in \mathcal{S}_1 \cap \mathrm{Stab}(\mathcal{R})$, which is not a finite linear combination of percolation sequences, there corresponds a pair $(\mathbb{H}_T, A_F)$ where $\mathbb{H}_T$ is the Hilbert space completion of $\mathbb{C}[x]$ defined by inner products (50) and A_F is the minimal non-negative self-adjoint extension of the densely defined operator $A: \mathbb{C}[x] \to \mathbb{C}[x]$ defined in (51). Thus, there is a distinguished spectral measure whose moments are given by the sequence T.

ACKNOWLEDGMENTS

We thank Rafael Sorkin for suggesting the problem and for a number of helpful conversations.

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A new approach of the stationary axisymmetric vacuum S(A) solutions

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(Received 19 March 2002; accepted 15 November 2002)

We revisit axisymmetric stationary vacuum solutions of the Einstein equations, like we did for the cylindrical case [J. Math. Phys. **41**, 7535 (2000)]. We explicitly formulate the simplest hypothesis under which the S(A) solutions, or axisymmetric Lewis solutions can be found and demonstrate that this hypothesis leads to a linear relation between the potentials. We show that the field equations still can be associated to the motion of a classical particle in a central field, where an arbitrary harmonic χ function plays the role of time. Three classes of solutions are obtained without the need of invoking the Papapetrou class. They depend on two real parameters, and the potentials are functions of χ only. The new approach exempts the need of complex parameters. We interpret one of the parameters as related to the vorticity of the source. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1556191]

I. INTRODUCTION

Axially symmetric stationary vacuum space–times in Einstein's theory are important because they can describe the exterior fields of massive rotating astrophysical objects.[1,2] Here we reexamine the S(A) class of solutions of these space–times (see Ref. 3, p. 204).

In a preceding paper[4] we have already reexamined the vacuum solutions obtained by Lewis,[5] and van Stockum,[6] for a stationary cylindrically symmetric space–time. Lewis established the existence of three classes of solutions in terms of four parameters. One of these classes appeared by the introduction of complex parameters. Through our approach the three classes arose without the need of complexification. We cannot use the Ernst formalism[7,8] in the cylindrical case since the partial differential equations which link the dragging ω to the twist potential Φ become ill defined. Furthermore, we showed that the structure of the field equations can be associated with the motion of a classical particle in a central field. This association allowed a kinematical interpretation of the parameters, describing the Lewis space–time without the need of specifying a particular matter source of the field.

Here we extend our analysis to the axisymmetric case. In order to proceed, we formulate the fundamental hypothesis (Sec. III) which allows the employment of our method. By doing this we obtain directly the S(A) solutions without making use of the Papapetrou class[3] as is usually done. Thus the S(A) solutions arise as a natural extension to the axisymmetric case of the Lewis solutions. Hence these solutions could be appropriately called the axisymmetric Lewis solutions. Then we follow some similar steps of Ref. 4 and show that the classification and mechanical interpretation used in the cylindrical case can be extended, also, to the axisymmetric case.

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The paper is organized as follows. In Sec. II we recall the system of equations to be solved for the axially symmetric stationary vacuum metrics. We introduce in Sec. III the fundamental hypothesis from which the linear dependence between the potentials is deduced. In Sec. IV, we examine the main consequence of the kinematical role of the arbitrary harmonic functions of these solutions. The solutions and classification are presented in Sec. V and its vorticity is calculated. We end with a brief conclusion.

II. FIELD EQUATIONS

The general line element for a stationary axisymmetric space–time, with signature $+2$, can be written like

$$ds^2 = -f\,dt^2 + 2k\,dt\,d\phi + e^{\mu}(dr^2+dz^2) + l\,d\phi^2, \tag{1}$$

where f, l, k, and μ are all functions of the Weyl coordinates r and z. Defining for convenience,

$$f = rF(r,z), \quad l = rL(r,z), \quad k = rK(r,z), \tag{2}$$

we obtain from Einstein's vacuum field equations,[5,6]

$$\Delta F = -F\Omega, \tag{3}$$

$$\Delta L = -L\Omega, \tag{4}$$

$$\Delta K = -K\Omega, \tag{5}$$

$$\mu_r = -\frac{1}{2r}[1 + r^2(F_rL_r - F_zL_z + K_r^2 - K_z^2)], \tag{6}$$

$$\mu_z = -\frac{r}{2}(F_rL_z + F_zL_r + 2K_rK_z), \tag{7}$$

with

$$FL + K^2 = 1, \tag{8}$$

where the Laplacian Δ and Ω are defined by

$$\Delta F = F_{rr} + \frac{1}{r}F_r + F_{zz}, \tag{9}$$

$$\Omega = F_rL_r + K_r^2 + F_zL_z + K_z^2, \tag{10}$$

with the indexes standing for differentiation. The function μ is obtained by quadratures and, thus, we have only to determine F, L, and K. Let us note that the field equations (3)–(5) can also be written in the more symmetric form,

$$F\Delta L = L\Delta F, \tag{11}$$

$$L\Delta K = K\Delta L, \tag{12}$$

$$K\Delta F = F\Delta K. \tag{13}$$

III. THE FUNDAMENTAL HYPOTHESIS ON THE *F*, *L*, AND *K* FUNCTIONS

In the cylindrically symmetric case, where in (2) F, L, and K, depend only on r, we have demonstrated the existence of a linear dependence between the potentials.[4] However, in the axially symmetric case, when F, L, and K are functions of r and z, such a general demonstration is no longer possible. Thus, we have to introduce some further hypothesis to solve the field equations.

Keeping in mind the method used in the cylindrical case[4] we make the hypothesis that there exists a functional relation, different from (8), between F, L, and K,

$$\Phi(F,L,K)=0. \tag{14}$$

Then, from (8) and (14) we can obtain two general relations that can be expressed, for example, as

$$F=F(K), \quad L=L(K). \tag{15}$$

From (15) we have the identities,

$$\nabla F\cdot\nabla L+(\nabla K)^2\equiv(1+F_K L_K)(\nabla K)^2, \tag{16}$$

$$\Delta F\equiv F_K\Delta K+F_{KK}(\nabla K)^2, \tag{17}$$

$$\Delta L\equiv L_K\Delta K+L_{KK}(\nabla K)^2, \tag{18}$$

where ∇ is the gradient operator. With (15)–(18), we can rewrite the two first field equations (3) and (4) like

$$(1+F_K L_K)(KF_K-F)=F_{KK}, \tag{19}$$

$$(1+F_K L_K)(KL_K-L)=L_{KK}, \tag{20}$$

which is a system of two differential equations permitting one to determine the functions (15), as we shall see (Eq. (41)). Hence, the only partial derivative equation to solve is the third field equation, (5), for the function $K(r,z)$,

$$\Delta K=-K(1+F_K L_K)(K_r^2+K_z^2). \tag{21}$$

A kinematical interpretation can be given from (19) to (21). Indeed, considering (19) multiplied by L and (20) by F and subtracting both equations, we obtain

$$(1+F_K L_K)K=\frac{(LF_K-FL_K)_K}{LF_K-FL_K}. \tag{22}$$

Without any loss of generality, we can make an arbitrary change of unknown function by putting $K=K(\chi)$, where $\chi(r,z)$ is a new unknown function. Then (21) becomes

$$K_\chi\Delta\chi=[f(K)-K_{\chi\chi}](\nabla\chi)^2, \tag{23}$$

where

$$f(K)=-K(1+F_K L_K). \tag{24}$$

Always without loss of generality, we can fix this change of function such that $K(\chi)$ satisfies the differential equation

$$\frac{K_{\chi\chi}}{K_\chi^2}=f(K), \tag{25}$$

implying that χ is an harmonic function.

Let us examine what (25) implies on the two first field equations (19) and (20). Substituting (25) into (22) and integrating we obtain

$$LF_\chi - FL_\chi = C_1, \tag{26}$$

where C_1 is an integration constant. In a similar way, but starting from (4) and (5) with $L=L(F)$ and $K=K(F)$, and considering (3) with $F(\chi)$; and repeating again from (3) and (5) with $F(L)$ and $K(L)$ and considering (4) with $L(\chi)$, we obtain

$$KL_\chi - LK_\chi = C_2, \tag{27}$$

$$FK_\chi - KF_\chi = C_3, \tag{28}$$

respectively, where C_2 and C_3 are also integration constants.

Equations (26)–(28) express the conservation of an *angular momentum* $\vec{C}=(C_1,C_2,C_3)$ in the *space* (F,L,K), like in the cylindrical case,[4] but here it is χ which plays the role of *time*, instead of $\tau=\ln r$ in Ref. 4. In Sec. IV we study consequences of this fact. Besides, from (26) to (28), we can immediately deduce a linear relation between the potentials,

$$K=\alpha L+\beta F, \tag{29}$$

where α and β are constants. The relation (29) is the one that we were looking for when we stated (14), and it describes a family of two parameter planes in the space (F,L,K). Hence, most of the interpretation in terms of a classical particle in a central field made in Ref. 4 holds here again. In particular, the discussion about the nature of the conic, which is the intersection of the surfaces (8) and (29) in the (F,L,K) space, followed in Ref. 4 for the cylindrical case, remains the same in the axisymmetric case.

Let us stress that all the results of this section can be obtained in the axisymmetric case only under the hypothesis (14), which we call the *fundamental hypothesis* for the S(A) class, while in the cylindrical case they were general, i.e., valid without any hypothesis. A well-known counterexample of an axisymmetric solution that does not satisfy this hypothesis is Kerr solution.

The linear dependence between the potentials (29) allows us to write this relation using the well-known Papapetrou functions f_P and ω giving

$$f_P=r\left(\omega^2+\frac{\omega}{\alpha}-\frac{\beta}{\alpha}\right)^{-1/2}. \tag{30}$$

We recognize from (30) the class S(A) (see Ref. 3, p. 204) of stationary vacuum solutions, which thus presents itself as the most natural generalization of the cylindrical class of Lewis solutions. These solutions can also be named the axisymmetric Lewis solutions.

IV. CONSEQUENCES OF THE KINEMATICAL ROLE OF THE HARMONIC FUNCTION χ

In order to analyze these consequences we return to the cylindrically symmetric case. We now give an integration method of the $K(r)$ equation slightly different from the one presented in Ref. 4. By doing this, we want to enlighten the common feature of the two types of Lewis solutions, cylindric and axisymmetric, namely the fact that they only depend on a harmonic function. However, this function is imposed in the cylindric case, whereas it is arbitrary in the axial case.

In the cylindrical case, (21) with (29) reduces to

$$K_{rr}+\frac{1}{r}K_r-\frac{\delta K K_r^2}{\Delta}=0, \tag{31}$$

with

$$\Delta\equiv\delta K^2-4\alpha\beta, \quad \delta\equiv 1+4\alpha\beta. \tag{32}$$

Changing the unknown function $K=K(\chi)$ in (31) in such a way that

$$\frac{K_{\chi\chi}}{K_\chi}=\frac{\delta K K_\chi}{\Delta} \tag{33}$$

leads to

$$\frac{\chi_{rr}}{\chi_r}=-\frac{1}{r}. \tag{34}$$

Consequently, after integration of (34), we obtain

$$\chi=k_1\ln\left(\frac{r}{r_0}\right), \tag{35}$$

where k_1 and r_0 are integration constants, and, by integration of (33),

$$\int\frac{\mathrm{d}K}{\sqrt{\Delta}}=k_1\ln\frac{r}{r_0}+k_2, \tag{36}$$

where k_2 is an integration constant. The study of the integral (36) leads to the cylindrical solutions of Lewis.[4] Let us note that all these solutions depend only on the solution of the differential equation (34), i.e.,

$$\Delta\chi=\chi_{rr}+\frac{1}{r}\chi_r=0, \tag{37}$$

which means that χ is a harmonic function. In this special case of cylindrical symmetry, the differential equation (37) can be explicitly integrated, giving the only solution (35).

It is no longer the case in the more general axisymmetric situation, for which the corresponding equation (hereafter (40)) is a partial differential equation, even though the line reasoning remains the same. Indeed, coming back to (21), it can be written as

$$\Delta K=f(K)(\nabla K)^2. \tag{38}$$

The standard procedure of changing the unknown function $K=K(\chi)$ used in (23), gives now with (29),

$$\frac{K_{\chi\chi}}{K_\chi}-\frac{\delta K K_\chi}{\Delta}=0. \tag{39}$$

With (39), (38) reduces to

$$\Delta\chi=0. \tag{40}$$

We have that (39) is (33) with $\chi(r,z)$ arbitrary harmonic functions in place of the particular harmonic function, $\ln r$, convenient for the cylindrical case.

So, we can obtain from the functional hypothesis (14) the different classes of the Lewis solution by an analysis similar to the one used in the cylindric case (Ref. 4).

V. THREE CLASSES OF AXISYMMETRIC SOLUTIONS OBTAINED FROM (29)

The solutions $K(\chi)$ of (39), expressed in terms of an arbitrary harmonic function $\chi(r,z)$ can be classified following the sign of δ, defined in (32), like in the procedure used in the cylindrical case (Ref. 4).

The corresponding functions $F(\chi)$ and $L(\chi)$ are deduced from the relations

$$F=\frac{K\mp\sqrt{\Delta}}{2\alpha},\quad L=\frac{K\pm\sqrt{\Delta}}{2\beta}, \tag{41}$$

obtained from (8) and (29). From (6) to (8) and (41) the potential μ obeys

$$\mu_r=-\frac{1}{2r}+\epsilon\frac{r}{2}(\chi_r^2-\chi_z^2), \tag{42}$$

$$\mu_z=\epsilon r\chi_r\chi_z, \tag{43}$$

with the following values for ϵ,

$$\epsilon=\begin{cases}+1, & \delta>0\\ 0, & \delta=0\\ -1, & \delta<0\end{cases}.$$

For this axisymmetric space–time we can calculate its vorticity vector Ω^α given by

$$\Omega^\alpha=\frac{\epsilon^{\alpha\beta\gamma\delta}}{2\sqrt{g}}u_\beta(u_{[\gamma;\delta]}+u_{[\alpha;\mu}u_{\delta]}u^\mu), \tag{44}$$

where u^α is a time like vector

$$u^\alpha=\frac{1}{\sqrt{-g_{tt}}}\delta_t^\alpha.$$

Calculating the scalar of (44) for (1) we obtain

$$\Omega^2=g_{\alpha\beta}\Omega^\alpha\Omega^\beta=\frac{(KF_\chi-FK_\chi)^2}{4e^\mu F^2}(\chi_r^2+\chi_z^2). \tag{45}$$

Some remarks about the vorticity of the S(A) solutions is presented in the conclusion. Finally, we present the three classes of solutions obtained, which are the following.

A. Class I: $\delta>0$

1. $\alpha\beta>0$

$$K=2\left(\frac{\alpha\beta}{\delta}\right)^{1/2}\cosh\chi, \tag{46}$$

$$F=\left(\frac{\alpha}{\beta}\right)^{1/2}\left(\frac{1}{\sqrt{\delta}}\cosh\chi\mp\sinh\chi\right), \tag{47}$$

$$L=\left(\frac{\beta}{\alpha}\right)^{1/2}\left(\frac{1}{\sqrt{\delta}}\cosh\chi\pm\sinh\chi\right). \tag{48}$$

2. $\alpha\beta<0$ with $-\alpha\beta<1/4$

$$K=2\left(-\frac{\alpha\beta}{\delta}\right)^{1/2}\sinh\chi, \tag{49}$$

$$F=\left(-\frac{\alpha}{\beta}\right)^{1/2}\left(\frac{1}{\sqrt{\delta}}\sinh\chi\mp\cosh\chi\right), \tag{50}$$

$$L=\left(-\frac{\beta}{\alpha}\right)^{1/2}\left(\frac{1}{\sqrt{\delta}}\sinh\chi\pm\cosh\chi\right). \tag{51}$$

3. $\alpha\beta=0$

Here we use (8) and (29), instead of (41).

Case $\alpha=0$ and $\beta\neq0$:

$$K=e^{\chi}, \tag{52}$$

$$F=\frac{1}{\beta}e^{\chi}, \tag{53}$$

$$L=\beta(e^{-\chi}-e^{\chi}). \tag{54}$$

From (45) with (52) and (53) we have $\Omega^2=0$.

Case $\alpha\neq0$ and $\beta=0$:

$$K=e^{\chi}, \tag{55}$$

$$F=\alpha(e^{-\chi}-e^{\chi}), \tag{56}$$

$$L=\frac{1}{\alpha}e^{\chi}. \tag{57}$$

From (45) with (55) and (56) we have $\Omega^2\neq0$.

Case $\alpha=\beta=0$: We use (3), (8), and (29) obtaining the Weyl static metric,

$$K=0, \tag{58}$$

$$F=e^{\chi}, \tag{59}$$

$$L=e^{-\chi}. \tag{60}$$

This solution, without dragging, is an axisymmetric extension of the cylindrical Levi-Civita solution.

B. Class II: $\delta<0$

We remark here, as we did in Ref. 4, that there is no need to introduce complex parameters in our approach, as is usually done in the corresponding cylindrical case,[3,9,10]

$$K=2\left(\frac{\alpha\beta}{\delta}\right)^{1/2}\sin\chi, \tag{61}$$

$$F=\left(-\frac{\alpha}{\beta}\right)^{1/2}\left(\frac{1}{\sqrt{-\delta}}\sin\chi\mp\cos\chi\right), \tag{62}$$

$$L=\left(-\frac{\beta}{\alpha}\right)^{1/2}\left(\frac{1}{\sqrt{-\delta}}\sin\chi\pm\cos\chi\right). \tag{63}$$

C. Class III: $\delta=0$ or $\alpha\beta=-1/4$

$$K=\chi, \tag{64}$$

$$F=\frac{1}{2\beta}(\chi\mp 1), \tag{65}$$

$$L=\frac{1}{2\alpha}(\chi\pm 1). \tag{66}$$

Here we can integrate (42) and (43) obtaining $e^{\mu}=c/\sqrt{r}$ where c is an integration constant. This class corresponds to the van Stockum's class[6] (see Ref. 3, p. 205).

VI. CONCLUSION

The general solution of the cylindrically symmetric stationary vacuum Einstein's field equations is the Lewis solution. It is no longer the case for the more general equations with axial symmetry. We precised here the most general hypothesis under which we can find the axisymmetric solutions obtained by Lewis.[5,6] This hypothesis (14) is a functional dependence between the potentials F, L, and K different from (8), and allowed us to demonstrate a linear relation between the potentials. This fact implied that the field equations can be interpreted as describing the motion of a classical particle in a central force field, like in the cylindrical symmetric case.[4] We can recognize the solutions as belonging to the S(A) class (see Ref. 3, p. 204). We obtained these solutions without recalling the Papapetrou class, as is usually done. These solutions depend upon an arbitrary harmonic function, and its classification in three classes is similar to the cylindrically symmetric case. Here again, as in Ref. 4, we do not need to appeal to complex constants, like in Refs. 9 and 10. This harmonic function plays the role of time in the motion of the precedent classical particle interpretation.

It is interesting to observe in Sec. V A 3, that for $\alpha=0$ and $\beta\neq 0$ the vorticity scalar Ω vanishes, while for $\alpha\neq 0$ and $\beta=0$ it does not. This shows a similarity with the corresponding solutions for the cylindrical case[4] where α is associated with the parameter that produces the vorticity of the source, as shown by Refs. 11 and 9. On the other hand, β in spite of also being associated with the stationarity of the source does not produce vorticity, but topological defect as shown in Ref. 11 and topological frame dragging demonstrated in Ref. 12.

For $\delta=0$, in Sec. V C, we have $e^{\mu}=c/\sqrt{r}$, which has the same r dependence as in the cylindrical system[11,9] with energy density per unit length $\sigma=1/4$. This class of solutions, like in the cylindrical case, is in the frontier between the two other corresponding classes.

ACKNOWLEDGMENT

N.O.S. gratefully acknowledges financial assistance from CNPq, Brazil.

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Total variation in Hamiltonian formalism and symplectic-energy integrators

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(Received 4 December 2001; accepted 9 January 2003)

We present a discrete total variation calculus in Hamiltonian formalism in this paper. Using this discrete variation calculus and generating functions for the flows of Hamiltonian systems, we derive symplectic-energy integrators of any finite order for Hamiltonian systems from a variational perspective. The relationship between the symplectic integrators derived directly from the Hamiltonian systems and the variationally derived symplectic-energy integrators is explored. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1559642]

I. INTRODUCTION

We begin by recalling the ordinary variational principle in Hamiltonian formalism. Suppose Q denotes the configuration space with coordinates q^i, and T^*Q the phase space with coordinates (q^i,p^i), $i=1,2,\ldots,n$. Consider a Hamiltonian H: $T^*Q\to\mathbb{R}$. The corresponding action functional is defined by

$$S((q^i(t),p^i(t)))=\int_a^b (p^i\dot{q}^i-H(q^i,p^i))\,\mathrm{d}t, \tag{I.1}$$

where $(q^i(t),p^i(t))$ is a C^2 curve in phase space T^*Q.

The variational principle in Hamiltonian formalism seeks the curves $(q^i(t),p^i(t))$ for which the action functional S is stationary under variations of $(q^i(t),p^i(t))$ with fixed end points. We first define the variation of $(q^i(t),p^i(t))$.

Let

$$V=\sum_{i=1}^{n}\phi^i(\mathbf{q},\mathbf{p})\frac{\partial}{\partial q^i}+\sum_{i=1}^{n}\psi^i(\mathbf{q},\mathbf{p})\frac{\partial}{\partial p^i} \tag{I.2}$$

be a vector field on T^*Q. Here $\mathbf{q}=(q^1,\ldots,q^n)$, $\mathbf{p}=(p^1,\ldots,p^n)$. For simplicity, we will use Einstein convention and omit the summation notation Σ in the following.

Denote the flow of V by F^ϵ: $F^\epsilon(\mathbf{q},\mathbf{p})=(\tilde{\mathbf{q}},\tilde{\mathbf{p}})$, which is written in components as

$$\tilde{q}^i=f^i(\epsilon,\mathbf{q},\mathbf{p}), \tag{I.3}$$

$$\tilde{p}^i=g^i(\epsilon,\mathbf{q},\mathbf{p}), \tag{I.4}$$

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where $(\mathbf{q},\mathbf{p}) \in T^*Q$ and

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} f^i(\epsilon,\mathbf{q},\mathbf{p}) = \phi^i(\mathbf{q},\mathbf{p}),$$

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} g^i(\epsilon,\mathbf{q},\mathbf{p}) = \psi^i(\mathbf{q},\mathbf{p}).$$

Let $(q^i(t),p^i(t))$ be a curve in T^*Q. The transformation (I.3) and (I.4) transforms $(q^i(t),p^i(t))$ into a family of curves

$$(\tilde{q}^i(t),\tilde{p}^i(t)) = (f^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)),g^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t))).$$

Now we are ready to define the variation of $(q^i(t),p^i(t))$:

$$\delta(q^i(t),p^i(t)) =: \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} (\tilde{q}^i(t),\tilde{p}^i(t)) = (\phi^i(\mathbf{q},\mathbf{p}),\psi^i(\mathbf{q},\mathbf{p})). \tag{I.5}$$

Next, we calculate the variation of S at $(q^i(t),p^i(t))$ as follows:

$$\begin{aligned}
\delta S &= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} S((\tilde{q}^i(t),\tilde{p}^i(t))) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} S((f^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)),g^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)))) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \int_a^b \left(g^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)) \frac{\mathrm{d}}{\mathrm{d}t} f^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)) - H(f^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t)),g^i(\epsilon,\mathbf{q}(t),\mathbf{p}(t))) \right) \mathrm{d}t \\
&= \int_a^b \left[\left(\dot{q}^i - \frac{\partial H}{\partial p^i} \right) \psi^i + \left(-\dot{p}^i - \frac{\partial H}{\partial q^i} \right) \phi^i \right] \mathrm{d}t + p^i \phi^i |_a^b .
\end{aligned} \tag{I.6}$$

If $\phi^i(\mathbf{q}(a),\mathbf{p}(a)) = \phi^i(\mathbf{q}(b),\mathbf{p}(b)) = 0$, the requirement of $\delta S = 0$ yields the Hamilton equation for $(q^i(t),p^i(t))$:

$$\begin{aligned}
\dot{q}^i &= \frac{\partial H}{\partial p^i}, \\
\dot{p}^i &= -\frac{\partial H}{\partial q^i}.
\end{aligned} \tag{1.7}$$

If we drop the requirement of $\phi^i(\mathbf{q}(a),\mathbf{p}(a)) = \phi^i(\mathbf{q}(b),\mathbf{p}(b)) = 0$, we can naturally obtain the canonical one form on T^*Q from the second term in (I.6): $\theta = p^i \mathrm{d}q^i$. Furthermore, restricting $(\tilde{q}^i(t),\tilde{p}^i(t))$ to the solution space of (I.7), we can prove that the solution of (I.7) preserves the canonical two-form $\omega = \mathrm{d}\theta_L = \mathrm{d}p^i \wedge \mathrm{d}q^i$.

On the other hand, it is not necessary to restrict $(\tilde{q}^i(t),\tilde{p}^i(t))$ to the solution space of (I.7). Introducing the Euler–Lagrange one-form

$$E(q^i,p^i) = \left(\dot{q}^i - \frac{\partial H}{\partial p^i} \right) \mathrm{d}p^i + \left(-\dot{p}^i - \frac{\partial H}{\partial q^i} \right) \mathrm{d}q^i, \tag{I.8}$$

the nilpotency of d leads to

$$dE(q^i,p^i)+\frac{d}{dt}\omega=0. \tag{I.9}$$

Namely, the necessary and sufficient condition for symplectic structure preserving is that the Euler–Lagrange one form is closed.[1–3]

Based on the above-given variational principle in Hamiltonian formalism and using the ideas of discrete Lagrange mechanics,[4–8] we can develop a natural version of discrete Hamilton mechanics with fixed time steps and derive symplectic integrators for Hamilton canonical equations from a variational perspective.[3]

However the symplectic integrators obtained in this way are not energy-preserving in general because of its fixed time steps.[9,10] An energy-preserving symplectic integrator is a more preferable and natural candidate of approximations for conservative Hamilton equations since the solution of conservative Hamilton equations is not only symplectic but also energy-preserving. To attain this goal, we use variable time steps and a discrete total variation calculus developed in Refs. 11–15. The basic idea is to construct a discrete action functional with variable time steps and then apply a discrete total variation calculus. In this way, we can derive symplectic integrators and their associated energy conservation laws. These variationally derived symplectic integrators are two-step integrators. If we take fixed time steps, the resulting integrators are equivalent to the symplectic integrators derived directly from the Hamiltonian systems in some special cases.

An outline of this paper is as follows. In Sec. II, we present total variation for continuous variational principle in Hamiltonian formalism. Section III is devoted to deriving symplectic-energy integrators. In Sec. IV, using generating function methods, we obtain high order symplectic-energy integrators. In Sec. V, we present an example. We finish this paper by making some conclusions and comments in Sec. VI.

II. TOTAL VARIATION IN HAMILTONIAN FORMALISM

In order to discuss total variation in Hamiltonian formalism, we will work with extended phase space $\mathbb{R}\times T^*Q$ with coordinates (t,q^i,p^i). Here t denotes time. For details, see Ref. 16. by total variation, we refer to variations of both (q^i,p^i) and t. Consider a vector field on $\mathbb{R}\times T^*Q$,

$$V=\xi(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial t}+\phi^i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial q^i}+\psi^i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial p^i}. \tag{II.1}$$

Let F^ϵ be the flow of V. For $(t,q^i,p^i)\in\mathbb{R}\times T^*Q$, we have $F^\epsilon(t,q^i,p^i)=(\tilde{t},\tilde{q}^i,\tilde{p}^i)$:

$$\tilde{t}=h(\epsilon,t,\mathbf{q},\mathbf{p}), \tag{II.2}$$

$$\tilde{q}^i=f^i(\epsilon,t,\mathbf{q},\mathbf{p}), \tag{II.3}$$

$$\tilde{p}^i=g^i(\epsilon,t,\mathbf{q},\mathbf{p}), \tag{II.4}$$

where

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h(\epsilon,t,\mathbf{q},\mathbf{p})=\xi(t,\mathbf{q},\mathbf{p}), \tag{II.5}$$

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} f^i(\epsilon,t,\mathbf{q},\mathbf{p})=\phi^i(t,\mathbf{q},\mathbf{p}), \tag{II.6}$$

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} g^i(\epsilon,t,\mathbf{q},\mathbf{p})=\psi^i(t,\mathbf{q},\mathbf{p}). \tag{II.7}$$

The transformation (II.2)–(II.4) transforms a curve $(q^i(t),p^i(t))$ into a family of curves $(\tilde{q}^i(\epsilon,\tilde{t}),\tilde{p}^i(\epsilon,\tilde{t}))$ determined by

$$\tilde{t}=h(\epsilon,t,\mathbf{q}(t),\mathbf{p}(t)), \tag{II.8}$$

$$\tilde{q}^i=f^i(\epsilon,t,\mathbf{q}(t),\mathbf{p}(t)), \tag{II.9}$$

$$\tilde{p}^i=g^i(\epsilon,t,\mathbf{q}(t),\mathbf{p}(t)). \tag{II.10}$$

Suppose we can solve (II.8) for t: $t=h^{-1}(\epsilon,\tilde{t})$. Then we have

$$\tilde{q}^i(\epsilon,\tilde{t})=f^i(\epsilon,h^{-1}(\epsilon,\tilde{t}),\mathbf{q}(h^{-1}(\epsilon,\tilde{t})),\mathbf{p}(h^{-1}(\epsilon,\tilde{t}))), \tag{II.11}$$

$$\tilde{p}^i(\epsilon,\tilde{t})=g^i(\epsilon,h^{-1}(\epsilon,\tilde{t}),\mathbf{q}(h^{-1}(\epsilon,\tilde{t})),\mathbf{p}(h^{-1}(\epsilon,\tilde{t}))). \tag{II.12}$$

Before calculating the variation of S directly, we first consider the first-order prolongation of V,

$$\mathrm{pr}^1V=\xi(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial t}+\phi^i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial q^i}+\psi^i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial p^i}+\alpha^i(t,\mathbf{q},\mathbf{p},\dot{\mathbf{q}},\dot{\mathbf{p}})\frac{\partial}{\partial \dot{q}^i}+\beta^i(t,\mathbf{q},\mathbf{p},\dot{\mathbf{q}},\dot{\mathbf{p}})\frac{\partial}{\partial \dot{p}^i}, \tag{II.13}$$

where pr^1V denote the first-order prolongation of V and

$$\alpha^i(t,\mathbf{q},\mathbf{p},\dot{\mathbf{q}},\dot{\mathbf{p}})=D_t\phi^i(t,\mathbf{q},\mathbf{p})-\dot{q}^iD_t\xi(t,\mathbf{q},\mathbf{p}), \tag{II.14}$$

$$\beta^i(t,\mathbf{q},\mathbf{p},\dot{\mathbf{q}},\dot{\mathbf{p}})=D_t\psi^i(t,\mathbf{q},\mathbf{p})-\dot{p}^iD_t\xi(t,\mathbf{q},\mathbf{p}), \tag{II.15}$$

where D_t denotes the total derivative. For example

$$D_t\phi^i(t,\mathbf{q},\mathbf{p})=\phi^i_t+\phi_{\mathbf{q}}\dot{\mathbf{q}}+\phi_{\mathbf{p}}\dot{\mathbf{p}}.$$

For prolongation of vector field and formulas (II.14) and (II.15), we refer the reader to Ref. 17.

Now we calculate the variation of S directly as follows:

$$\begin{aligned}
\delta S&=\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}S\Big((\tilde{q}^i(\epsilon,\tilde{t}),\tilde{p}^i(\epsilon,\tilde{t}))\\
&=\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}\int_{\tilde{a}}^{\tilde{b}}(\tilde{p}^i(\epsilon,\tilde{t}))\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t})-H(\tilde{q}^i(\epsilon,\tilde{t}),\tilde{p}^i(\epsilon,\tilde{t}))\Big)\,\mathrm{d}\tilde{t}\\
&=\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}\int_{a}^{b}(\tilde{p}^i(\epsilon,\tilde{t}))\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t})-H(\tilde{q}^i(\epsilon,\tilde{t}),\tilde{p}^i(\epsilon,\tilde{t}))\big)\frac{\mathrm{d}\tilde{t}}{\mathrm{d}t}\mathrm{d}t\quad(\tilde{t}=h(\epsilon,t,\mathbf{q}(t),\mathbf{p}(t)))\\
&=\int_a^b\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}(\tilde{p}^i(\epsilon,\tilde{t}))\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t})-H(\tilde{q}^i(\epsilon,\tilde{t}),\tilde{p}^i(\epsilon,\tilde{t}))\,\mathrm{d}t\\
&\quad+\int_a^b(p^i(t)\dot{q}^i(t)-H(q^i(t),p^i(t)))D_t\xi\,\mathrm{d}t
\end{aligned} \tag{II.16}$$

$$=\int_a^b\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}H(q^i(t),p^i(t))\right)\xi+\left(-\dot{p}^i-\frac{\partial H}{\partial q^i}\right)\phi^i+\left(\dot{q}^i-\frac{\partial H}{\partial p^i}\right)\psi^i\right]\mathrm{d}t+[p^i\phi^i-H(q^i,p^i)\xi]\big|_a^b. \tag{II.17}$$

Here in (II.16), we used (II.5) and the fact

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}\frac{\mathrm{d}\tilde{t}}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}\tilde{t}=D_t\xi.$$

In (II.17), we used the prolongation formula (II.14).

If $\xi(a,\mathbf{q}(a),\mathbf{p}(a))=\xi(b,\mathbf{q}(b),\mathbf{p}(b))=0$ and $\phi^i(a,\mathbf{q}(a),\mathbf{p}(a))=\phi^i(b,\mathbf{q}(b),\mathbf{p}(b))=0$, the requirement of $\delta S=0$ yields the Hamilton canonical equation

$$\begin{aligned}\dot{q}^i&=\frac{\partial H}{\partial p^i},\\ \dot{p}^i&=-\frac{\partial H}{\partial q^i},\end{aligned}\tag{II.18}$$

from the variation ϕ^i,ψ^i and the energy conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t}H(q^i,p^i)=0\tag{II.19}$$

from the variation ξ.
Since

$$\frac{\mathrm{d}}{\mathrm{d}t}H(q^i,p^i)=\frac{\partial H}{\partial q^i}\dot{q}^i+\frac{\partial H}{\partial p^i}\dot{p}^i,$$

we can easily see that the energy conservation law (II.19) is a natural consequence of the Hamilton canonical equation (II.18).

If we drop the requirement

$$\xi(a,\mathbf{q}(a),\mathbf{p}(a))=\xi(b,\mathbf{q}(b),\mathbf{p}(b))=0,$$

$$\phi^i(a,\mathbf{q}(a),\mathbf{p}(a))=\phi^i(b,\mathbf{q}(b),\mathbf{p}(b))=0,$$

we can define the extended canonical one form on $\mathbb{R}\times T^*Q$ from the second term in (II.17)

$$\theta=p^i\mathrm{d}q^i-H(q^i,p^i)\mathrm{d}t.\tag{II.20}$$

Furthermore, restricting $(\tilde{q}^i(t),\tilde{p}^i(t))$ to the solution space of (II.18), we can prove the solution of (II.18) preserves the extended canonical two form

$$\omega=\mathrm{d}\theta=\mathrm{d}p^i\wedge\mathrm{d}q^i-\mathrm{d}H(q^i,p^i)\wedge\mathrm{d}t,\tag{II.21}$$

by using the same method in Ref. 8.

III. A DISCRETE TOTAL VARIATION CALCULUS IN HAMILTONIAN FORMALISM AND SYMPLECTIC-ENERGY INTEGRATORS

In this section, we develop a discrete version of total variation in Hamiltonian formalism. Using this discrete total variation calculus, we will derive symplectic-energy integrators.

Let

$$L(q^i,p^i,\dot{q}^i,\dot{p}^i)=p^i\dot{q}^i-H(q^i,p^i)$$

be a function from $\mathbb{R}\times T(T^*Q)$ to $\mathbb{R}$. Here L does not depend on t explicitly.

We use $P\times P$ for the discrete version of $\mathbb{R}\times T(T^*Q)$. Here P is the discrete version of $\mathbb{R}\times T^*Q$. A point $(t_0,\mathbf{q}_0,\mathbf{p}_0;t_1,\mathbf{q}_1,\mathbf{p}_1)\in P\times P$ corresponds to a tangent vector

$$\left(\frac{q_1-q_0}{t_1-t_0}\,\frac{p_1-p_0}{t_1-t_0}\right).$$

For simplicity, the vector symbols $\mathbf{q}=(q^1,\ldots,q^n)$ and $\mathbf{p}=(p^1,\ldots,p^n)$ are used throughout this section. A discrete L is defined to be $\mathbb{L}$: $P\times P\to\mathbb{R}$ and the corresponding discrete action to be

$$\mathbb{S}=\sum_{k=0}^{N-1}\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})(t_{k+1}-t_k), \tag{III.1}$$

where $t_0=a,t_N=b$.

The discrete variational principle in total variation is to extremize $\mathbb{S}$ for variations of both $\mathbf{q}_k,\mathbf{p}_k$ and t_k holding the end points $(t_0,\mathbf{q}_0,\mathbf{p}_0)$ and $(t_N,\mathbf{q}_N,\mathbf{p}_N)$ fixed. This discrete variational principle determines a discrete flow Φ: $P\times P\to P\times P$ by

$$\Phi(t_{k-1},\mathbf{q}_{k-1},\mathbf{p}_{k-1},t_k,\mathbf{q}_k,\mathbf{p}_k)=(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1}). \tag{III.2}$$

Here $(t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})$ is found from the following discrete Hamilton canonical equation:

$$\begin{aligned}&(t_{k+1}-t_k)D_2\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})\\&\quad+(t_k-t_{k-1})D_5\mathbb{L}(t_{k-1},\mathbf{q}_{k-1},\mathbf{p}_{k-1},t_k,\mathbf{q}_k,\mathbf{p}_k)=0,\\&(t_{k+1}-t_k)D_3\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})\\&\quad+(t_k-t_{k-1})D_6\mathbb{L}(t_{k-1},\mathbf{q}_{k-1},\mathbf{p}_{k-1},t_k,\mathbf{q}_k,\mathbf{p}_k)=0,\end{aligned} \tag{III.3}$$

and the discrete energy conservation law

$$\begin{aligned}&(t_{k+1}-t_k)D_1\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})+(t_k-t_{k-1})D_4\mathbb{L}(t_{k-1},\mathbf{q}_{k-1},\mathbf{p}_{k-1},t_k,\mathbf{q}_k,\mathbf{p}_k)\\&\quad-\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})+\mathbb{L}(t_{k-1},\mathbf{q}_{k-1},\mathbf{p}_{k-1},t_k,\mathbf{q}_k,\mathbf{p}_k)=0.\end{aligned} \tag{III.4}$$

Here D_i denotes the partial derivative of $\mathbb{L}$ with respect to the ith argument. Equation (III.3) is the discrete Hamilton canonical equation (variational integrator). Equation (III.4) is the discrete energy conservation law associated with (III.3). Unlike the continuous case, the variational integrator (III.3) does not satisfy (III.4) for arbitrarily given t_{k+1} in general. Therefore, we need to solve (III.3) and (III.4) simultaneously with q_{k+1}, p_{k+1} and t_{k+1} being unknowns.

Now we prove that the discrete flow determined by (III.3) and (III.4) preserves a discrete version of the extended Lagrange two form ω defined in (II.21). Therefore, we call (III.3) and (III.4) a symplectic-energy integrator. We do this directly from the variational point of view, consistent with the continuous case.[8]

As in the continuous case, we calculate $\mathrm{d}\mathbb{S}$ for variations with varied end points.

$$
\begin{aligned}
&\mathrm{d}\mathbb{S}(t_0,\mathbf{q}_0,\mathbf{p}_0,\ldots,t_N,\mathbf{q}_N,\mathbf{p}_N)\cdot(\delta t_0,\delta\mathbf{q}_0,\delta\mathbf{p}_0,\ldots,\delta t_N,\delta\mathbf{q}_N,\delta\mathbf{p}_N)\\
&\quad=\sum_{k=0}^{N-1}(D_2\mathbb{L}(\mathbf{v}_k)\,\delta\mathbf{q}_k+D_5\mathbb{L}(\mathbf{v}_k)\,\delta\mathbf{q}_{k+1}+D_3\mathbb{L}(\mathbf{v}_k)\,\delta\mathbf{p}_k+D_6\mathbb{L}(\mathbf{v}_k)\,\delta\mathbf{p}_{k+1})(t_{k+1}-t_k)\\
&\qquad+\sum_{k=0}^{N-1}(D_1\mathbb{L}(\mathbf{v}_k)\,\delta t_k+D_4\mathbb{L}(\mathbf{v}_k)\,\delta t_{k+1})(t_{k+1}-t_k)+\mathbb{L}(\mathbf{v}_k)(\delta t_{k+1}-\delta t_k)\\
&\quad=\sum_{k=1}^{N-1}(D_2\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)+D_5\mathbb{L}(\mathbf{v}_{k-1})(t_k-t_{k-1}))\,\delta\mathbf{q}_k\\
&\qquad+\sum_{k=1}^{N-1}(D_3\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)+D_6\mathbb{L}(\mathbf{v}_{k-1})(t_k-t_{k-1}))\,\delta\mathbf{p}_k\\
&\qquad+\sum_{k=1}^{N-1}(D_1\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)+D_4\mathbb{L}(\mathbf{v}_{k-1})(t_k-t_{k-1})+\mathbb{L}(\mathbf{v}_{k-1})-\mathbb{L}(\mathbf{v}_k))\,\delta t_k\\
&\qquad+D_2\mathbb{L}(\mathbf{v}_0)(t_1-t_0)\,\delta\mathbf{q}_0+D_3\mathbb{L}(\mathbf{v}_0)(t_1-t_0)\,\delta p_0+(D_1\mathbb{L}(\mathbf{v}_0)(t_1-t_0)-\mathbb{L}(\mathbf{v}_0))\,\delta t_0\\
&\qquad+D_5\mathbb{L}(\mathbf{v}_{N-1})(t_N-t_{N-1})\,\delta\mathbf{q}_N+D_6\mathbb{L}(\mathbf{v}_{N-1})(t_N-t_{N-1})\,\delta\mathbf{p}_N\\
&\qquad+(D_4\mathbb{L}(\mathbf{v}_{N-1})(t_N-t_{N-1})-\mathbb{L}(\mathbf{v}_{N-1}))\,\delta t_N,
\end{aligned}
\tag{III.5}
$$

where $\mathbf{v}_k=(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})$, $k=0,1,\ldots,N-1$.

We can see that the last six terms in (III.5) come from the boundary variations. Based on the boundary variations, we can define two one forms on $P\times P$,

$$
\begin{aligned}
\theta_{\mathrm{L}}^{-}(\mathbf{v}_k)&=D_2\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)\mathrm{d}\mathbf{q}_k+D_3\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)\mathrm{d}\mathbf{p}_k\\
&\quad+(D_1\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)-\mathbb{L}(\mathbf{v}_k))\mathrm{d}t_k
\end{aligned}
\tag{III.6}
$$

and

$$
\begin{aligned}
\theta_{\mathrm{L}}^{+}(\mathbf{v}_k)&=D_5\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)\mathrm{d}\mathbf{q}_{k+1}+D_6\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)\mathrm{d}\mathbf{p}_{k+1}\\
&\quad+(D_4\mathbb{L}(\mathbf{v}_k)(t_{k+1}-t_k)+\mathbb{L}(\mathbf{v}_k))\mathrm{d}t_{k+1}.
\end{aligned}
\tag{III.7}
$$

Here we have used the notation in Ref. 8. We regard the pair $(\theta_{\mathrm{L}}^{-},\theta_{\mathrm{L}}^{+})$ as being the discrete version of the extended canonical one form θ defined in (II.20).

Now we parametrize the solutions of the discrete variational principle by (t_0,q_0,t_1,q_1), and restrict $\mathbb{S}$ to that solution space. Then Eq. (III.5) becomes

$$
\begin{aligned}
&\mathrm{d}\mathbb{S}(t_0,\mathbf{q}_0,\mathbf{p}_0,\ldots,t_N,\mathbf{q}_N,\mathbf{p}_N)\cdot(\delta t_0,\delta\mathbf{q}_0,\delta\mathbf{p}_0,\ldots,\delta t_N,\delta\mathbf{q}_N,\delta\mathbf{p}_N)\\
&\quad=\theta_{\mathrm{L}}^{-}(t_0,\mathbf{q}_0,\mathbf{p}_0,t_1,\mathbf{q}_1,\mathbf{p}_1)\cdot(\delta t_0,\delta\mathbf{q}_0,\delta\mathbf{p}_0,\delta t_1,\delta\mathbf{q}_1,\delta\mathbf{p}_1)\\
&\qquad+\theta_{\mathrm{L}}^{+}(t_{N-1},\mathbf{q}_{N-1},\mathbf{p}_{N-1},t_N,\mathbf{q}_N,\mathbf{p}_N)\cdot(\delta t_{N-1},\delta\mathbf{q}_{N-1},\delta\mathbf{p}_{N-1},\delta t_N,\delta\mathbf{q}_N,\delta\mathbf{p}_N)\\
&\quad=\theta_{\mathrm{L}}^{-}(t_0,\mathbf{q}_0,\mathbf{p}_0,t_1,\mathbf{q}_1,\mathbf{p}_1)\cdot(\delta t_0,\delta\mathbf{q}_0,\delta\mathbf{p}_0,\delta t_1,\delta\mathbf{q}_1,\delta\mathbf{p}_1)\\
&\qquad+(\Phi^{N-1})^{*}\theta_{\mathrm{L}}^{+}(t_0,\mathbf{q}_0,\mathbf{p}_0,t_1,\mathbf{q}_1,\mathbf{p}_1)\cdot(\delta t_0,\delta\mathbf{q}_0,\delta\mathbf{p}_0,\delta t_1,\delta\mathbf{q}_1,\delta\mathbf{p}_1).
\end{aligned}
\tag{III.8}
$$

From (III.8), we can obtain

$$
\mathrm{d}\mathbb{S}=\theta_{\mathrm{L}}^{-}+(\Phi^{N-1})^{*}\theta_{\mathrm{L}}^{+}.
\tag{III.9}
$$

The Eq. (III.9) holds for arbitrary $N>1$. Taking $N=2$ leads to

$$\mathrm{d}\mathbb{S}=\theta_{\mathbb{L}}^{-}+\Phi^{*}\theta_{\mathbb{L}}^{+}. \tag{III.10}$$

Taking exterior differentiation of (III.10) reveals that

$$\Phi^{*}(d\theta_{\mathbb{L}}^{+})=-\mathrm{d}\theta_{\mathbb{L}}^{-}. \tag{III.11}$$

From the definition of $\theta_{\mathbb{L}}^{-}$ and $\theta_{\mathbb{L}}^{+}$, we know that

$$\theta_{\mathbb{L}}^{-}+\theta_{\mathbb{L}}^{+}=\mathrm{d}\mathbb{L}. \tag{III.12}$$

Taking exterior differentiation of (III.12), we obtain $\mathrm{d}\theta_{\mathbb{L}}^{+}=-\mathrm{d}\theta_{\mathbb{L}}^{-}$. Define

$$\omega_{\mathbb{L}}\equiv\mathrm{d}\theta_{\mathbb{L}}^{+}=-\mathrm{d}\theta_{\mathbb{L}}^{-}. \tag{III.13}$$

Finally, we have shown that the discrete flow Φ preserves the discrete extended canonical two form $\omega_{\mathbb{L}}$:

$$\Phi^{*}(\omega_{\mathbb{L}})=\omega_{\mathbb{L}}. \tag{III.14}$$

We call the coupled difference system (III.3) and (III.4) a symplectic-energy integrator in the sense that it satisfies the discrete energy conservation law (III.4) and preserves the discrete extended canonical two form $\omega_{\mathbb{L}}$.

To illustrate the above-mentioned discrete total variation calculus, we now present an example. We choose $\mathbb{L}$ in (III.1) as

$$\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})=\mathbf{p}_{k+1/2}\frac{\mathbf{q}_{k+1}-\mathbf{q}_k}{t_{k+1}-t_k}-H(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}), \tag{III.15}$$

where

$$\mathbf{p}_{k+1/2}=\frac{\mathbf{p}_k+\mathbf{p}_{k+1}}{2},\quad \mathbf{q}_{k+1/2}=\frac{\mathbf{q}_k+\mathbf{q}_{k+1}}{2}.$$

Using (III.3), we can obtain the corresponding discrete Hamilton equation

$$\begin{aligned}
&\frac{\mathbf{q}_{k+1}-\mathbf{q}_{k-1}}{2}-\frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+(t_k-t_{k-1})\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right)=0,\\
&\frac{\mathbf{p}_{k+1}-\mathbf{p}_{k-1}}{2}+\frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+(t_k-t_{k-1})\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right)=0,
\end{aligned} \tag{III.16}$$

where

$$p_{k-1/2}=\frac{\mathbf{p}_k+\mathbf{p}_{k-1}}{2},\quad \mathbf{q}_{k-1/2}=\frac{\mathbf{q}_k+\mathbf{q}_{k-1}}{2}.$$

Using (III.4), we can obtain the corresponding discrete energy conservation law

$$H(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})=H(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2}). \tag{III.17}$$

The symplectic-energy integrator (III.16) and (III.17) preserves the discrete two form:

$$\frac{1}{2}(\mathrm{d}\mathbf{p}_k\wedge\mathrm{d}\mathbf{q}_{k+1}+\mathrm{d}\mathbf{p}_{k+1}\wedge\mathrm{d}\mathbf{q}_k)-H(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})\wedge\left(\frac{\mathrm{d}t_k+\mathrm{d}t_{k+1}}{2}\right). \tag{III.18}$$

If we take fixed time steps $t_{k+1}-t_k=h$ (h is a constant), then (III.16) becomes

$$\frac{\mathbf{q}_{k+1}-\mathbf{q}_{k-1}}{2h}=\frac{1}{2}\left(\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right),$$
$$\frac{\mathbf{p}_{k+1}-\mathbf{p}_{k-1}}{2h}=-\frac{1}{2}\left(\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right). \tag{III.19}$$

Now we explore the relationship between (III.19) and the midpoint integrator for the Hamiltonian system

$$\dot{\mathbf{q}}=\frac{\partial H}{\partial \mathbf{p}},$$
$$\dot{\mathbf{p}}=-\frac{\partial H}{\partial \mathbf{q}}. \tag{III.20}$$

The midpoint symplectic integrator for (III.20) is

$$\frac{\mathbf{q}_{k+1}-\mathbf{q}_{k}}{h}=\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}),$$
$$\frac{\mathbf{p}_{k+1}-\mathbf{p}_{k}}{h}=-\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}). \tag{III.21}$$

In (III.21), we replace k by $k-1$ and obtain

$$\frac{\mathbf{q}_{k}-\mathbf{q}_{k-1}}{h}=\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2}),$$
$$\frac{\mathbf{p}_{k}-\mathbf{p}_{k-1}}{h}=-\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2}). \tag{III.22}$$

Adding (III.22) to (III.21) results in (III.19). Therefore, if we use (III.21) to obtain $\mathbf{p}_k,\mathbf{q}_k$, the two-step integrator (III.19) is equivalent to the midpoint integrator (III.21). However, the equivalence does not hold in general. For example, choose $\mathbb{L}$ in (III.1) as

$$\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})=\mathbf{p}_k\frac{\mathbf{q}_{k+1}-\mathbf{q}_k}{t_{k+1}-t_k}-H(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}), \tag{III.23}$$

and take fixed time steps $t_{k+1}-t_k=h$. Then (III.3) becomes

$$\frac{\mathbf{q}_{k+1}-\mathbf{q}_{k}}{h}=\frac{1}{2}\left(\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+\frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right),$$
$$\frac{\mathbf{p}_{k}-\mathbf{p}_{k-1}}{h}=-\frac{1}{2}\left(\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right). \tag{III.24}$$

The integrator (III.24) is a two-step integrator which preserves $\mathrm{d}p_k\wedge\mathrm{d}q_{k+1}$. In this case, we cannot find one-step integrator which is equivalent to (III.24). In conclusion, using discrete total variation calculus, we derive two-step symplectic-energy integrators. When taking fixed time steps, some of them are equivalent to one-step integrators derived directly from the Hamiltonian system while the others do not have this equivalence.

IV. HIGH ORDER SYMPLECTIC-ENERGY INTEGRATORS BY GENERATING FUNCTIONS

In this section, we develop high order symplectic-energy integrators by using the generating function of the flow of the Hamiltonian system

$$\dot{\mathbf{z}}=J\nabla H(\mathbf{z}), \tag{IV.1}$$

where

$$\mathbf{z}=(\mathbf{p},\mathbf{q})^T, \quad J=\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}.$$

We first recall the generating function with normal Darboux matrix of a symplectic transformation. For details, see Refs. 18 and 19.

Suppose α is a $4n\times 4n$ nonsingular matrix with the form

$$\alpha=\begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where A, B, C, and D are both $2n\times 2n$ matrices.

We denote the inverse of α by

$$\alpha^{-1}=\begin{pmatrix} A_1 & B_1 \\ C_1 & D_1 \end{pmatrix},$$

where A_1, B_1, C_1, and D_1 are both $2n\times 2n$ matrices.

We call a $4n\times 4n$ matrix α *a Darboux matrix* if

$$\alpha^T J_{4n}\alpha=\tilde{J}_{4n}, \tag{IV.2}$$

where

$$J_{4n}=\begin{pmatrix} 0 & -I_{2n} \\ I_{2n} & 0 \end{pmatrix}, \quad \tilde{J}_{4n}=\begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix}, \quad J_{2n}=\begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix},$$

where I_n is an $n\times n$ identity matrix and I_{2n} is a $2n\times 2n$ identity matrix.

Every Darboux matrix induces a *fractional transform* between symplectic and symmetric matrices

$$\sigma_\alpha: \quad \mathrm{Sp}(2n)\to \mathrm{Sm}(2n),$$

$$\sigma_\alpha=(AS+B)(CS+D)^{-1}=M, \quad \text{for } S\in \mathrm{Sp}(2n),\ \det(CS+D)\neq 0$$

with the inverse transform $\sigma_\alpha^{-1}=\sigma_{\alpha_{-1}}$

$$\sigma_\alpha^{-1}: \quad \mathrm{Sm}(2n)\to \mathrm{Sp}(2n),$$

$$\sigma_\alpha^{-1}=(A_1M+B_1)(C_1M+D_1)^{-1}=S,$$

where $\mathrm{Sp}(2n)$ is the group of symplectic matrices and $\mathrm{Sm}(2n)$ the set of symmetric matrices.

We can generalize the above discussions to generally nonlinear transformations on $\mathbb{R}^{2n}$. Denote by $\mathrm{Spnl}(2n)$ the set of symplectic transformations on $\mathbb{R}^{2n}$ and $\mathrm{Smnl}(2n)$ the set of symmetric transformations (i.e., transformations with symmetric Jacobian) on $\mathbb{R}^{2n}$. Every $f\in \mathrm{Smnl}(2n)$ corresponds, at least locally, to a real function ϕ (unique to a constant) such that f is the gradient of ϕ:

$$f(\mathbf{w})=\nabla\phi(\mathbf{w}), \tag{IV.3}$$

where $\nabla\phi(\mathbf{w})=(\phi_{w_1}(\mathbf{w}),\ldots,\phi_{w_{2n}}(\mathbf{w}))$ and $\mathbf{w}=(w_1,w_2,\ldots,w_{2n})$.

Then we have

σ_α: $\mathrm{Spnl}(2n)\to\mathrm{Smnl}(2n)$,

$$\sigma_\alpha=(A\circ g+B)\circ(C\circ g+D)^{-1}=\nabla\phi,\ \text{for } g\in\mathrm{Spnl}(2n),\ \det(Cg_{\mathbf{z}}+D)\neq 0$$

or alternatively

$$Ag(\mathbf{z})+B\mathbf{z}=(\nabla\phi)(Cg(\mathbf{z})+D\mathbf{z}),$$

where $\circ$ denotes the composition of transformation and the $2n\times 2n$ constant matrices A, B, C, and D are regarded as linear transformations. $g_{\mathbf{z}}$ denotes the Jacobian of the symplectic transformation g.

We call ϕ the *generating function* of Darboux type α for the symplectic transformation g.

Conversely, we have

σ_α: $\mathrm{Smnl}(2n)\to\mathrm{Spnl}(2n)$,

$$\sigma_\alpha^{-1}(\nabla\phi)=(A_1\circ\nabla\phi+B_1)\circ(C_1\circ\nabla\phi+D_1)^{-1}=g \quad \text{for} \quad \det(C_1\phi_{\mathbf{ww}}+D_1)\neq 0,$$

or alternatively

$$A_1\nabla\phi(\mathbf{w})+B_1\mathbf{w}=g(C_1\nabla\phi(\mathbf{w})+D_1\mathbf{w}),$$

where g is called the symplectic transformation of Darboux type α for the generating function ϕ.

For the study of integrators, we may restrict ourselves to the *normal Darboux matrices*, i.e., those satisfying $A+B=0$, $C+D=I_{2n}$. The normal Darboux matrices can be characterized as

$$\alpha=\begin{pmatrix} J_{2n} & -J_{2n} \\ E & I_{2n}-E \end{pmatrix}, \quad E=\frac{1}{2}(I_{2n}+J_{2n}F), \quad F^T=F, \tag{IV.4}$$

and

$$\alpha^{-1}=\begin{pmatrix} (E-I_{2n})J_{2n} & I_{2n} \\ EJ_{2n} & I_{2n} \end{pmatrix}. \tag{IV.5}$$

The fractional transform induced by a normal Darboux matrix establishes a one–one correspondence between symplectic transformations near *identity* and symmetric transformations near *nullity*.

For simplicity, we take $F=0$, then $E=\frac{1}{2}I_{2n}$ and

$$\alpha=\begin{pmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2}I_{2n} & \frac{1}{2}I_{2n} \end{pmatrix}. \tag{IV.6}$$

Now we consider the generating function of the flow of (IV.1). Denote the flow of (IV.1) by e_H^t. The generating function $\phi(\mathbf{w},t)$ for the flow e_H^t of Darboux type (IV.6) is given by

$$\nabla\phi=(J_{2n}\circ e_H^t-J_{2n})\circ(\tfrac{1}{2}e_H^t+\tfrac{1}{2}I_{2n})^{-1} \quad \text{for small} \quad |t|, \tag{IV.7}$$

where $\phi(\mathbf{w},t)$ satisfies the Hamilton–Jacobi equation

$$\frac{\partial}{\partial t}\phi(\mathbf{w},t)=-H\left(\mathbf{w}+\frac{1}{2}J_{2n}\nabla\phi(\mathbf{w},t)\right) \tag{IV.8}$$

and can be expressed by Taylor series in t,

$$\phi(\mathbf{w},t)=\sum_{k=1}^{\infty}\phi^k(w)t^k,\quad \text{for small}\quad |t|. \tag{IV.9}$$

The coefficients $\phi^k(w)$ can be determined recursively

$$\begin{aligned}&\phi^1(\mathbf{w})=-H(w),\\ &\phi^{k+1}(\mathbf{w})=\frac{-1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{j_1+\cdots+j_m=k\\ j_l\geqslant 1}}D^mH\left(\frac{1}{2}J_{2n}\nabla\phi^{j_1},\ldots,\frac{1}{2}J_{2n}\nabla\phi^{j_m}\right),\end{aligned} \tag{IV.10}$$

where $k\geqslant 1$, and we use the notation of the m-linear form

$$\begin{aligned}&D^mH\left(\frac{1}{2}J_{2n}\nabla\phi^{j_1},\ldots,\frac{1}{2}J_{2n}\nabla\phi^{j_m}\right)\\ &\quad:=\sum_{i_1,\ldots,i_m=1}^{2n}H_{\mathbf{z}_{i_1}\cdots\mathbf{z}_{i_m}}(\mathbf{w})\left(\frac{1}{2}J_{2n}\nabla\phi^{j_1}(\mathbf{w})\right)_{i_1}\cdots\left(\frac{1}{2}J_{2n}\nabla\phi^{j_m}(\mathbf{w})\right)_{i_m}.\end{aligned}$$

From (IV.7), we can see that the phase flow $\hat{\mathbf{z}}:=e_H^t\mathbf{z}$ satisfies

$$J_{2n}(\hat{\mathbf{z}}-\mathbf{z})=\nabla\phi\left(\frac{\hat{\mathbf{z}}-\mathbf{z}}{2}\right)=\sum_{j=1}^{\infty}t^j\nabla\phi^j\left(\frac{\hat{\mathbf{z}}+\mathbf{z}}{2}\right). \tag{IV.11}$$

Now we choose $\mathbb{L}$ in (III.1) as

$$\mathbb{L}(t_k,\mathbf{q}_k,\mathbf{p}_k,t_{k+1},\mathbf{q}_{k+1},\mathbf{p}_{k+1})=\mathbf{p}_{k+1/2}\frac{\mathbf{q}_{k+1}-\mathbf{q}_k}{t_{k+1}-t_k}-\psi^m(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}), \tag{IV.12}$$

where

$$\psi^m(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})=\sum_{j=1}^{m}t^j\phi^j(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2}). \tag{IV.13}$$

The corresponding symplectic-energy integrator (III.3) and (III.4) is

$$\begin{aligned}&\frac{\mathbf{q}_{k+1}-\mathbf{q}_{k-1}}{2}-\frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial\psi^m}{\partial\mathbf{p}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+(t_k-t_{k-1})\frac{\partial\psi^m}{\partial\mathbf{p}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right)=0,\\ &\frac{\mathbf{p}_{k+1}-\mathbf{p}_{k-1}}{2}+\frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial\psi^m}{\partial\mathbf{q}}(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})+(t_k-t_{k-1})\frac{\partial\psi^m}{\partial\mathbf{q}}(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2})\right)=0,\\ &\psi^m(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})=\psi^m(\mathbf{q}_{k-1/2},\mathbf{p}_{k-1/2}),\end{aligned} \tag{IV.14}$$

which satisfies the discrete extended canonical two form

$$\frac{1}{2}(\mathrm{d}\mathbf{p}_k\wedge\mathrm{d}\mathbf{q}_{k+1}+\mathrm{d}\mathbf{p}_{k+1}\wedge\mathrm{d}\mathbf{q}_k)-\psi^m(\mathbf{q}_{k+1/2},\mathbf{p}_{k+1/2})\wedge\left(\frac{\mathrm{d}t_k+\mathrm{d}t_{k+1}}{2}\right). \tag{IV.15}$$

The integrator (IV.14) is a two-step symplectic-energy integrator with $2m$th order of accuracy.

V. AN EXAMPLE AND AN OPTIMIZATION METHOD

In this section, we will present an example. We take the Hamiltonian as

$$H(q,p)=\tfrac{1}{2}p^2+\tfrac{1}{2}(q^4-q^2), \tag{V.1}$$

where for clarity q and p are scalars.

Corresponding to (V.1), the discrete Lagrangian (III.1) is chosen as

$$\mathbb{L}(t_k,q_k,p_k,t_{k+1},q_{k+1},p_{k+1})=p_{k+1/2}\frac{q_{k+1}-q_k}{t_{k+1}-t_k}-\frac{1}{2}p_{k+1/2}^2-\frac{1}{2}(q_{k+1/2}^4-q_{k+1/2}^2). \tag{V.2}$$

The corresponding symplectic-energy integrator (III.3) and (III.4) becomes

$$\begin{gathered}\frac{q_{k+1}-q_{k-1}}{2}-\frac{1}{2}((t_{k+1}-t_k)p_{k+1/2}+(t_k-t_{k-1})p_{k-1/2})=0,\\ \frac{p_{k+1}-p_{k-1}}{2}+\frac{1}{2}((t_{k+1}-t_k)(2q_{k+1/2}^3-q_{k+1/2})+(t_k-t_{k-1})(2q_{k-1/2}^3-q_{k-1/2}))=0,\\ \frac{1}{2}p_{k+1/2}^2+\frac{1}{2}(q_{k+1/2}^4-q_{k+1/2}^2)=\frac{1}{2}p_{k-1/2}^2+\frac{1}{2}(q_{k-1/2}^4-q_{k-1/2}^2),\end{gathered} \tag{V.3}$$

where t_{k-1}, q_{k-1}, p_{k-1} and t_k,q_k,p_k are given and t_{k+1}, q_{k+1}, p_{k+1} are unknowns.

In the following numerical experiment, we will use a robust optimization method suggested in Ref. 14 to solve (V.3). Concretely, let

$$A=\frac{q_{k+1}-q_{k-1}}{2}-\frac{1}{2}((t_{k+1}-t_k)p_{k+1/2}+(t_k-t_{k-1})p_{k-1/2}),$$

$$B=\frac{p_{k+1}-p_{k-1}}{2}+\frac{1}{2}((t_{k+1}-t_k)(2q_{k+1/2}^3-q_{k+1/2})+(t_k-t_{k-1})(2q_{k-1/2}^3-q_{k-1/2})),$$

$$C=\frac{1}{2}p_{k+1/2}^2+\frac{1}{2}(q_{k+1/2}^4-q_{k+1/2}^2)-\frac{1}{2}p_{k-1/2}^2-\frac{1}{2}(q_{k-1/2}^4-q_{k-1/2}^2).$$

Then we minimize the quantity

$$F=A^2+B^2+C^2 \tag{V.4}$$

over q_{k+1}, p_{k+1}, and t_{k+1} under the constraint $t_{k+1}>t_k$. This constraint guarantees that no singularities occur in choosing time steps.

We will compare (V.3) with the following integrator with fixed time steps:

$$\begin{gathered}\frac{q_{k+1}-q_{k-1}}{2h}-\frac{1}{2}(p_{k+1/2}+p_{k-1/2})=0,\\ \frac{p_{k+1}-p_{k-1}}{2h}+\frac{1}{2}((2q_{k+1/2}^3-q_{k+1/2})+(2q_{k-1/2}^3-q_{k-1/2}))=0.\end{gathered} \tag{V.5}$$

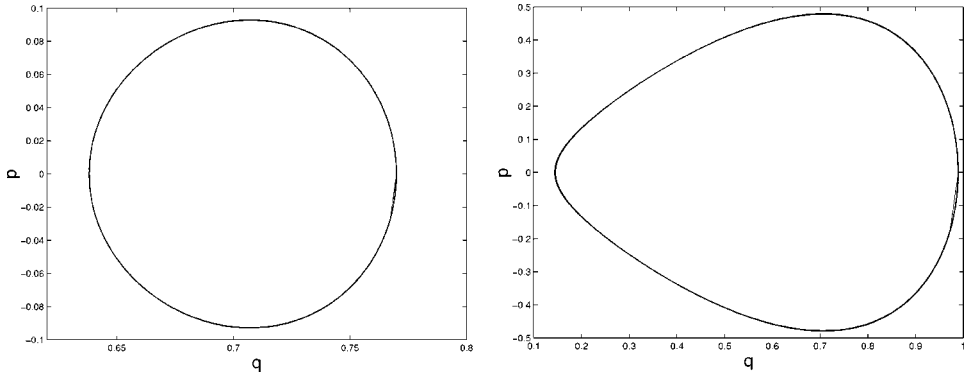

FIG. 1. The orbits calculated by (V.3) and (V.5). Left-hand plot: $q_0=0.77$, $p_0=0$; right-hand plot: $q_0=0.99$, $p_0=0$.

In our numerical experiment, we use two initial conditions $q_0=0.77$, $p_0=0$, $t=0$ and $q_0=0.99$, $p_0=0$, $t=0$. To obtain q_1 and p_1, we apply the midpoint integrator with $t_1=0.1$.

In Fig. 1, the orbits calculated by (V.3) and (V.5) are shown for the two initial conditions. The two orbits in each initial condition are almost indistinguishable. In Fig. 2, we plot the evolution of the energy $H(q_{k+1/2},p_{k+1/2})$ for both (V.3) and (V.5). The oscillating curve is for (V.5) and the lower line for (V.3).

For more numerical examples, see Ref. 14 in the Lagrangian setting. In principle, the results in Ref. 14 apply to the Hamiltonian setting in the present paper as well, noticing that $(q_{k+1}-q_k)/h=p_{k+1/2}$. The purpose of this paper is to develop a discrete total variation calculus in the Hamiltonian setting and obtain the symplectic-energy integrators. The comprehensive implementation of the obtained integrators is not the subject of this paper and will be the topic for future research.

VI. CONCLUDING REMARKS

We develop a discrete total variation calculus in Hamiltonian formalism in this paper. This calculus provides a new method for constructing structure-preserving integrators for Hamiltonian system from a variational point of view. Using this calculus, we derive energy conservation laws associated with the integrators. The coupled integrators are two-step integrators and preserve a discrete version of the extended canonical two form. If we take fixed time steps, the resulting integrators are equivalent to the symplectic integrators derived directly from the Hamiltonian systems only in special cases. Thus, new two-step symplectic integrators are variationally obtained. Using generating function method, we also obtain higher order symplectic-energy integrators.

In principle, our discussions can be generalized to multisymplectic Hamiltonian system

$$M\mathbf{z}_t+K\mathbf{z}_x=\nabla_{\mathbf{z}}H(\mathbf{z}),\quad \mathbf{z}\in\mathbf{R}^n, \tag{VI.1}$$

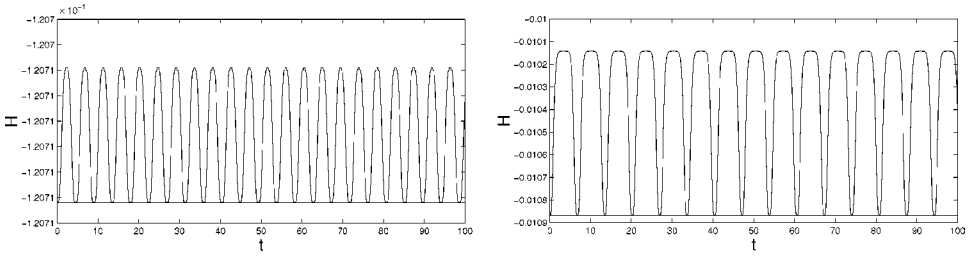

FIG. 2. The energy evolution for (V.3) and (V.5). Left-hand plot: $q_0=0.77$, $p_0=0$; right-hand plot: $q_0=0.99$, $p_0=0$.

where M and K are skew-symmetric matrices on $\mathbf{R}^n, n \geqslant 3$ and $S: \mathbf{R}^n \to \mathbf{R}$ is a smooth function.[20,21] We call the above-mentioned system a multisymplectic Hamiltonian system, since it possesses a multisymplectic conservation law

$$\frac{\partial}{\partial t}\omega + \frac{\partial}{\partial x}\kappa = 0, \tag{VI.2}$$

where ω and κ are the presymplectic forms

$$\omega = \tfrac{1}{2}\mathrm{d}\mathbf{z} \wedge M\,\mathrm{d}\mathbf{z}, \qquad \kappa = \tfrac{1}{2}\mathrm{d}\mathbf{z} \wedge K\mathrm{d}\mathbf{z}.$$

Construct the action functional

$$S = \int \left(\frac{1}{2}\mathbf{z}^T(M\mathbf{z}_t + K\mathbf{z}_x) - H(\mathbf{z}) \right) \mathrm{d}x \wedge \mathrm{d}t. \tag{VI.3}$$

Performing total variation on (VI.3), we can obtain the multisymplectic Hamiltonian system (VI.1) and the corresponding local energy conservation law

$$\frac{\partial}{\partial t}\left(S(z) - \frac{1}{2}z^T K z_x \right) + \frac{\partial}{\partial x}\left(\frac{1}{2}z^T K z_t \right) = 0, \tag{VI.4}$$

and the local momentum conservation law

$$\frac{\partial}{\partial t}\left(\frac{1}{2}z^T M z_x \right) + \frac{\partial}{\partial x}\left(S(z) - \frac{1}{2}z^T M z_t \right) = 0. \tag{VI.5}$$

In the same way, we can develop a discrete total variation calculus in the multisymplectic form and obtain multisymplectic-energy-momentum integrators.

ACKNOWLEDGMENTS

This work is supported by the National Natural Science Foundation of China (Grant Nos. 90103004, 10171096) and the National Key Project for Basic Research of China (G1998030601).

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Integrability of Kersten–Krasil'shchik coupled KdV–mKdV equations: singularity analysis and Lax pair

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(Received 26 September 2002; accepted 10 December 2002)

The integrability of a coupled KdV–mKdV system is tested by means of singularity analysis. The true Lax pair associated with this system is obtained by the use of prolongation technique. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1558903]

I. INTRODUCTION

Very recently, Kersten and Krasil'shchik[1] constructed the recursion operator for symmetries of a coupled KdV–mKdV system

$$\begin{aligned} u_t &= -u_{xxx}+6uu_x-3ww_{xxx}-3w_xw_{xx}+3u_xw^2+6uww_x, \\ w_t &= -w_{xxx}+3w^2w_x+3uw_x+3u_xw, \end{aligned} \tag{1}$$

which arises as the classical part of one of the superextensions of the KdV equation. In this work, we study the integrability of this system using the Painlevé test. Then, we use Dodd–Fordy[2] algorithm of the Wahlquist–Estabrook[3] prolongation technique in order to obtain the Lax pair. We find a 3×3 matrix spectral problem for the Kersten–Krasil'shchik system.

II. SINGULARITY ANALYSIS

Let us study the integrability of (1) following the Weiss–Kruskal algorithm of singularity analysis.[4,5] The algorithm is well known and widely used, therefore we omit unessential computational details.

First, we find that a hypersurface $\phi(x,t)=0$ is noncharacteristic for the system (1) if $\phi_x\neq0$ and set $\phi_x=1$ without loss of generality. Then we substitute the expansions

$$\begin{aligned} u &= u_0(t)\phi^{\alpha}+\cdots+u_r(t)\phi^{r+\alpha}+\cdots, \\ w &= w_0(t)\phi^{\beta}+\cdots+w_r(t)\phi^{r+\beta}+\cdots, \end{aligned} \tag{2}$$

into (1), and find the following branches (i.e., admissible choices of α, β, u_0, and w_0), together with the positions r of resonances (where arbitrary functions can enter the expansions):

$$\begin{aligned} &\alpha=-2, \quad \beta=-1, \quad u_0=1, \quad w_0=\pm i, \\ &r=-1,1,2,3,4,6, \end{aligned} \tag{3}$$

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$$\alpha=-2,\quad \beta=-1,\quad u_0=2,\quad w_0=\pm 2i,$$
$$r=-2,-1,3,3,4,8, \tag{4}$$

$$\alpha=-2,\quad \beta=2,\quad u_0=2,\quad \forall w_0(t),$$
$$r=-4,-1,0,1,4,6, \tag{5}$$

$$\alpha=-2,\quad \beta=3,\quad u_0=2,\quad \forall w_0(t),$$
$$r=-5,-1,-1,0,4,6, \tag{6}$$

besides those which correspond to the Taylor expansions governed by the Cauchy–Kovalevskaya theorem.

The branch (3) is generic: the expansions (2) with (3) describe the behavior of a generic solution near its singularity. The nongeneric branches (4), (5), and (6) correspond to singularities of special solutions. The branches (4) and (5) admit the following interpretation, in the spirit of Ref. 6: (4) describes the collision of two generic poles (3) with same sign of w_0, whereas (5) describes the collision of two generic poles (3) with opposite signs of w_0. The branch (6) corresponds to (5) with $w_0\to 0$.

Next, we find from (1) the recursion relations for the coefficients $u_n(t)$ and $w_n(t)$ $(n=0,1,2,\ldots)$ of the expansions (2), separately for each of the branches, and check the consistency of those recursion relations at the resonances. The recursion relations turn out to be consistent, therefore the expansions (2) of solutions of (1) are free from logarithmic terms. We conclude that the system (1) passes the Painlevé test for integrability successfully and must be expected to possess a Lax pair.

III. PROLONGATION STRUCTURE

By introducing the variables $p=u_x$, $q=w_x$, $r=p_x$, $s=q_x$, we assume that there exist $N\times N$ matrix functions F and G, depending upon u,w,p,q,r,s, such that

$$y_x=-yF,$$
$$y_t=-yG, \tag{7}$$

where y is a row matrix with elements y^A, $A=1,\ldots,N$. The system of equations in (1) can be represented as the compatibility conditions of (7) if

$$F_t-G_x+[F,G]=0, \tag{8}$$

where $[F,G]$ is the matrix commutator. This requirement gives the set of partial differential equations for F and G:

$$F_p=F_q=F_r=F_s=0,\quad F_u=-G_r,\quad 3wF_u+F_w=-G_s,$$
$$pG_u+qG_w+rG_p+sG_q-3(2up-qs+pw^2+2uwq)F_u-3(w^2q+uq+pw)F_w-[F,G]=0. \tag{9}$$

Next, we integrate equations (9) and find

$$F=\left(uw-\frac{w^3}{2}\right)X_1+\frac{w^2}{2}X_2+uX_3+wX_4+X_5, \tag{10}$$

where X_1,X_2,X_3,X_4,X_5 are constant matrices of integration. It is immediately seen that X_1 is in the center of prolongation algebra.[3] Hence, we can take it to be zero and find G as

$$G=(-r-ws-q^2+2u^2-w^4-w^2u)X_3-(s-w^3-3uw)X_4-(p+wq)X_6-uwX_7-\left(\frac{w^2}{2}+u\right)X_8$$
$$-qX_9-\frac{w^2}{2}X_{10}-wX_{11}+X_0, \tag{11}$$

where X_0 is a constant matrix of integration. The remaining elements are

$$X_6=[X_5,X_3],\quad X_7=[X_4,X_6],\quad X_8=[X_5,X_6],$$
$$X_9=[X_5,X_4],\quad X_{10}=[X_4,X_9],\quad X_{11}=[X_5,X_9]. \tag{12}$$

The integrability conditions impose the following restrictions on X_i $(i=0,\ldots,11)$:

$$[X_2,X_3]=0,\quad [X_5,X_0]=0,\quad [X_3,[X_3,X_6]]=0,\quad [X_2,[X_4,X_3]]=0,$$
$$[X_3,[X_4,X_3]]=0,\quad [X_3,[X_4,[X_4,X_3]]]=0,\quad [[X_4,[X_4,X_3]],[X_3,X_6]]=0,$$
$$2X_6+[X_5,X_2]=0,\quad [X_3,X_0]-[X_5,X_8]=0,\quad [X_4,X_2]+4[X_4,X_3]=0,$$
$$[X_4,X_0]-[X_5,X_{11}]=0,\quad 3X_6-\tfrac{1}{2}[X_5,[X_3,X_6]]-[X_3,X_8]=0,$$
$$3X_2-3[X_4,[X_4,X_3]]-[X_2,X_6]+[X_3,X_6]=0,$$
$$X_7+2[X_5,[X_4,X_3]]-[X_3,X_9]=0,$$
$$[X_2,X_0]-2[X_4,X_{11}]-[X_5,X_8]-[X_5,X_{10}]=0,$$
$$[X_2,[X_5,[X_4,X_3]]]+[X_2,X_7]+\tfrac{1}{2}[X_2,[X_2,X_9]]=0,$$
$$3X_9-[X_3,X_{11}]-[X_4,X_8]-[X_5,X_7]-2[X_5,[X_5,[X_4,X_3]]]=0,$$
$$[X_3,X_7]+\tfrac{1}{2}[X_4,[X_3,X_6]]+[X_3,[X_5,[X_4,X_3]]]=0,$$
$$X_9-\tfrac{1}{2}([X_2,X_{11}]+[X_4,X_8]+[X_4,X_{10}])-\tfrac{1}{3}([X_5,[X_5,[X_4,X_3]]]+[X_5,X_7])-\tfrac{1}{6}[X_5,[X_2,X_9]]$$
$$=0,$$
$$\tfrac{1}{2}[X_2,X_5]+\tfrac{1}{4}([X_2,X_8]+[X_2,X_{10}])+\tfrac{1}{3}([X_4,X_7]+[X_4,[X_5,[X_4,X_3]]])+\tfrac{1}{6}[X_4,[X_2,X_9]]=0,$$
$$3X_6-\tfrac{1}{2}([X_2,X_8]+[X_3,X_8]+[X_3,X_{10}])-[X_4,X_7]-2[X_5,[X_3,X_6]]-[X_4,[X_5,[X_4,X_3]]]$$
$$-2[X_5,[X_4,[,X_4,X_3]]]=0,$$
$$8[X_4,X_3]+\tfrac{1}{4}[X_2,[X_2,X_9]]-2[X_4,[X_4,[X_4,X_3]]]-\tfrac{1}{6}([X_3,[X_2,X_9]]+11[X_4,[X_3,X_6]])=0..$$

Together with the Jacobi identities we obtain further relations

$$[X_2,X_6]+2[X_3,X_6]=0,\quad [X_4,X_{11}]-[X_5,X_{10}]=0,$$
$$[X_5,[X_3,X_6]]-[X_3,X_8]=0,\quad [X_2,X_8]-[X_5,[X_2,X_6]]=0,$$
$$[X_5,[X_4,X_3]]+[X_3,X_9]-X_7=0,$$

$$
\begin{gathered}
-4[X_5,[X_4,X_3]]+[X_2,X_9]+2X_7=0,\\
[X_2,[X_5,[X_4,X_3]]]+2[[X_4,X_3],X_6]=0,\\
[X_3,[X_5,[X_4,X_3]]]-[[X_4,X_3],X_6]=0,\\
[X_3,[X_2,X_9]]-[X_2,[X_3,X_9]]=0,\\
[X_4,X_3]=0,\quad [X_2,X_7]=0,\quad [X_3,X_7]=0,\\
[X_3,X_{10}]=0,\quad [X_4,X_7]=0,\quad [X_5,X_7]=X_9,\\
[X_2,[X_2,X_9]]=0,\quad [X_4,[X_3,X_6]]=0,\\
[X_5,X_8]+[X_5,X_{10}]=0.
\end{gathered}
\tag{14}
$$

In order to find the Lie algebra generated by F and matrix representations of the generators $\{X_i\}_0^{11}$, we follow the strategy of Dodd–Fordy.[3] First we reduce the number of elements. By using Eqs. (12)–(14), we get $X_2=-2X_3$. Next, we locate nilpotent and neutral elements. The Eqs. (12) and (13) together with $X_2=-2X_3$ give that $[X_5,X_3]=X_6$ and $[X_3,X_6]=2X_3$, hence X_3 is nilpotent and X_6 is the neutral element. Let us note that the system of equations in (1) has the following scale symmetry:

$$
x\to\lambda^{-1}x,\quad t\to\lambda^{-3}t,\quad u\to\lambda^2u,\quad w\to\lambda w,
\tag{15}
$$

which implies that the elements X_i must satisfy

$$
\begin{gathered}
X_0\to\lambda^3X_0,\quad X_3\to\lambda^{-1}X_3,\quad X_4\to X_4,\quad X_5\to\lambda X_5,\\
X_6\to X_6,\quad X_7\to X_7,\quad X_8\to\lambda X_8,\quad X_9\to\lambda X_9,\\
X_{10}\to\lambda X_{10},\quad X_{11}\to\lambda^2X_{11},
\end{gathered}
\tag{16}
$$

where λ is a constant. By using the basis elements, we try to embed the prolongation algebra into $\mathrm{sl}(n+1,c)$. Starting from the case $n=1$, we found that $\mathrm{sl}(2,c)$ cannot be the whole algebra. The simplest nontrivial closure is in terms of $\mathrm{sl}(3,c)$. We take

$$
X_3=e_{-\alpha_1},\quad X_6=h_1,
\tag{17}
$$

where we use the standart Cartan–Weyl basis[7] of A_2. Together with the scale symmetries we find that

$$
\begin{gathered}
X_0=-4c_2^2\lambda^4e_{-\alpha_1}-36c_1^3\lambda^3(h_1+2h_2)-4c_2\lambda^2e_{\alpha_1},\\
X_4=d_1(h_1+2h_2)+d_2\lambda^{-1}e_{\alpha_2}+d_3\lambda^2e_{-\alpha_1-\alpha_2},\\
X_5=e_{\alpha_1}+c_1\lambda(h_1+2h_2)+c_2\lambda^2e_{-\alpha_1},\\
X_7=d_2\lambda^{-1}e_{\alpha_2}+d_3\lambda^2e_{-\alpha_1-\alpha_2},\\
X_8=-2e_{\alpha_1}+2c_2\lambda^2e_{-\alpha_1},\\
X_9=d_2\lambda^{-1}e_{\alpha_1+\alpha_2}-d_3\lambda^2e_{-\alpha_2}+3c_1d_2e_{\alpha_2}-3c_1d_3\lambda^3e_{-\alpha_1-\alpha_2},
\end{gathered}
\tag{18}
$$

$$X_{10}=-d_2d_3\lambda(h_1+2h_2)-6c_1d_2d_3\lambda^2e_{-\alpha_1},$$

$$X_{11}=(9c_1^2+c_2)d_2\lambda e_{\alpha_2}+6c_1d_3\lambda^3e_{-\alpha_2}+6c_1d_2e_{\alpha_1+\alpha_2}+(9c_1^2+c_2)d_3\lambda^4e_{-\alpha_1-\alpha_2},$$

where $\{c_i\}_1^2$ and $\{d_i\}_1^3$ are constants with conditions

$$d_1d_2=0,\quad d_1d_3=0,\quad d_2d_3=6c_1,\quad c_2=9c_1^2. \tag{19}$$

We choose $d_1=0$, $c_1=d_2=1$. So that, $X_7=X_4$ and $X_0=-36\lambda^2X_5$. Then, we obtain the matrix representations of the generators X_i as

$$X_3=\begin{pmatrix}0&0&0\\0&0&0\\1&0&0\end{pmatrix},\quad X_4=\begin{pmatrix}0&0&0\\-\lambda^{-1}&0&0\\0&6\lambda^2&0\end{pmatrix},$$

$$X_5=\begin{pmatrix}-\lambda&0&1\\0&2\lambda&0\\9\lambda^2&0&-\lambda\end{pmatrix},\quad X_6=\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix},$$

$$X_8=\begin{pmatrix}0&0&-2\\0&0&0\\18\lambda^2&0&0\end{pmatrix},\quad X_9=\begin{pmatrix}0&6\lambda^2&0\\-3&0&\lambda^{-1}\\0&-18\lambda^3&0\end{pmatrix}, \tag{20}$$

$$X_{10}=\begin{pmatrix}6\lambda&0&0\\0&-12\lambda&0\\-36\lambda^2&0&6\lambda\end{pmatrix},\quad X_{11}=\begin{pmatrix}0&-36\lambda^3&0\\-18\lambda&0&6\\0&108\lambda^4&0\end{pmatrix}.$$

By substituting the matrix representations of the generators into Eqs. (10) and (11) we can construct the Lax pair, $\Psi_x=X\Psi$, $\Psi_t=T\Psi$, for the system (1), with the following matrices X and T:

$$X=\begin{pmatrix}\lambda&w\lambda^{-1}&w^2-u-9\lambda^2\\0&-2\lambda&-6w\lambda^2\\-1&0&\lambda\end{pmatrix}, \tag{21}$$

$T=\{\{p+wq+3\lambda w^2-36\lambda^3,(w^3+2uw-s)\lambda^{-1}-3q-18\lambda w,r+ws+q^2-2u^2+w^4+w^2u-9\lambda^2$ $w^2+18\lambda^2u+324\lambda^4\}$, $\{6q\lambda^2-36\lambda^3w,-6\lambda w^2+72\lambda^3$, $6(s-w^3-2uw)\lambda^2-18q\lambda^3+108\lambda^4w\}$, $\{-w^2-2u+36\lambda^2,q\lambda^{-1}+6w,-p-wq+3\lambda w^2-36\lambda^3\}\}$, where the matrix T is written by rows and $X=-F^\dagger$, $T=-G^\dagger$, $\Psi=y^\dagger$.

The forms of X and T are unusual in the sense of the dependence on λ. It is possible to obtain equivalent matrices by the gauge transformation,

$$X'=SXS^{-1},\quad T'=STS^{-1}, \tag{22}$$

where

$$S=\begin{pmatrix}1&0&0\\0&0&-1\\0&\lambda^{-1}&0\end{pmatrix}. \tag{23}$$

The result is

$$X' = \begin{pmatrix} \lambda & u - w^2 + 9\lambda^2 & w \\ 1 & \lambda & 0 \\ 0 & 6\lambda w & -2\lambda \end{pmatrix}, \tag{24}$$

$T' = \{\{p + wq + 3\lambda w^2 - 36\lambda^3, \quad -r - ws - q^2 + 2u^2 - w^4 - w^2 u + 9\lambda^2 w^2 - 18\lambda^2 u - 324\lambda^4, \quad w^3 + 2uw - s - 3q\lambda - 18\lambda^2 w\}, \quad \{w^2 + 2u - 36\lambda^2, \quad -p - wq + 3\lambda w^2 - 36\lambda^3, -q - 6w\lambda\}, \quad \{6q\lambda - 36\lambda^2 w, -6(s - w^3 - 2uw)\lambda + 18q\lambda^2 - 108\lambda^3 w, -6\lambda w^2 + 72\lambda^3\}\}$.

IV. CONCLUDING REMARKS

The matrix X' gives us exactly the spectral problem for the KdV equation when $w = 0$. But X' does not reduce to the one for mKdV equation when $u = 0$. This result should be expected because the Kersten–Krasil'shchik system, when $u = 0$, gives not only mKdV equation, as stated in Ref. 1, but also an ordinary differential equation in w. Finally, we note that the Lax pair obtained from (7) with (24) is a true Lax pair since the parameter λ cannot be removed from X' by a gauge transformation, as can be proven by a gauge-invariant technique.[8]

ACKNOWLEDGMENT

This work is supported in part by the Scientific and Technical Research Council of Turkey (TUBITAK).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Legendre transformation and analytical mechanics: A geometric approach

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(Received 14 October 2002; accepted 26 November 2002)

A revisitation of the Legendre transformation in the context of affine principal bundles is presented. The argument, merged with the gauge-theoretical considerations developed by Massa *et al.*, provides a unified representation of Lagrangian and Hamiltonian mechanics, extending to arbitrary nonautonomous systems the symplectic approach of Tulczyjew. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1555684]

I. INTRODUCTION

In recent papers[1–4] a new geometrical framework for analytical mechanics has been developed. The formulation automatically embodies the invariance of Lagrange's equations under gauge transformations of the form $L \to L + \dot{f}$, $\dot{f}$ denoting the total time derivative of an arbitrary smooth function over the configuration manifold. Within this context we shall introduce an enhanced version of the Legendre transformation, and discuss its significance in the representation of the equations of motion. The argument extends to arbitrary dynamical systems the symplectic framework originally developed by Tulczyjew in time-independent mechanics.[5–9]

The mathematical foundations of the method are dealt with in Sec. II. The central point is the introduction of an involutory notion of duality between affine principal bundles. On this basis, the stated ''enhanced version'' of the Legendre transformation is established.

The subsequent analysis, in Sec. III, shows that the Lagrangian and Hamiltonian bundles, i.e., the cornerstones of the gauge-theoretical formulation of dynamics developed in Ref. 1, satisfy the duality criterion. A straightforward comparison with the results of Sec. II completes the construction, giving rise to a canonical diffeomorphism between higher jet bundles, essentially equivalent to the so-called *Tulczyjew triple* $T^*(T^*(M)) \leftrightarrow T(T^*(M)) \leftrightarrow T^*(T(M))$. The dynamical implications of the scheme are discussed.

II. AFFINE SPACES AND AFFINE BUNDLES

A. Algebraic preliminaries

Let Q and X, respectively, denote an $(n+1)$-dimensional affine space and a free vector on Q, or, what is the same, a constant vector field on Q.

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The quotient of Q by the one-parameter group of translations $\varphi_\xi : x \to x + \xi X$ generated by X is then an n-dimensional affine space M, while the quotient map $\pi : Q \to M$ is an affine surjection, making Q into a principal fiber bundle over M, with structural group $(\Re, +)$ and fundamental vector field X.

In what follows, we shall refer M to (global) affine coordinates $x^1, \ldots, x^n$, and Q to fibered affine coordinates $x^1, \ldots, x^n, u$, with $\langle X, du \rangle = 1 \Leftrightarrow X = \partial / \partial u$.

Let Q^* denote the family of *affine sections* $\sigma : M \to Q$. In coordinates, every $\sigma \in Q^*$ admits a representation of the form

$$u = v + y_i x^i. \tag{2.1}$$

The coefficients $y_1, \ldots, y_n$, v form a global coordinate system on Q^*. The following assertions are entirely straightforward.

Q^* is an $(n+1)$-dimensional affine space, modeled on the vector space W^* formed by the totality of *affine functions* over M (known in the literature as the *extended dual* of M).

The one-parameter group of translations $\varphi_\xi : Q \to Q$ acts in an obvious way on Q^*, sending each section $\sigma : u = v + y_i x^i$ into the section $\varphi_\xi \cdot \sigma : u = v + \xi + y_i x^i$. The generator of this action is a constant vector field Y on Q^*, expressed in coordinates as $Y = \partial / \partial v$. Viewed as an element of the modeling space W^*, the vector Y coincides with the constant function $f(x) \equiv 1 \quad \forall \; x \in M$.

Let M^* denote the quotient of Q^* by the action $\sigma \to \varphi_\xi \cdot \sigma$ described above. A straightforward argument shows that the variables $y_1, \ldots, y_n$ form an affine coordinate system on M^*, and that the quotient map $Q^* \to M^*$ is an affine surjection, making Q^* into a principal fiber bundle over M^*, with structural group $(\Re, +)$ and fundamental vector field Y.

For each $\sigma \in Q^*$, let $F_\sigma : Q \to \Re$ denote the associated *trivialization* of the bundle $Q \to M$. The correspondence $z, \sigma \to F_\sigma(z)$ is then a function on $Q \times Q^*$, henceforth denoted by $F(z, \sigma)$. In coordinates, Eq. (2.1) provides the expression

$$F_\sigma = u - v(\sigma) - y_i(\sigma)\, x^i$$

mathematically equivalent to the representation

$$F(x^i, u, y_i, v) = u - v - x^i y_i. \tag{2.2}$$

Equation (2.2) establishes a *bi-affine pairing* between the spaces Q and Q^*, *invariant* under the one-parameter group of translations

$$(z, \sigma) \mapsto (\varphi_\xi(z),\, \varphi_\xi \cdot \sigma). \tag{2.3}$$

In terms of this pairing, the condition for a point $z \in Q$ to belong to an affine section $\sigma \in Q^*$, or, equivalently, for a section $\sigma \in Q^*$ to contain a point $z \in Q$, is expressed by the relation $F(z, \sigma) = 0$. In this respect, precisely in the same way as an element $\sigma \in Q^*$ is an affine section $\sigma : M \to Q$, a point $z \in Q$ may be viewed as an affine section $z : M^* \to Q^*$, described in coordinates as

$$v = u(z) - x^i(z)\, y_i \tag{2.4}$$

and with image space $z(M^*)$ identical to the affine subspace of Q^* formed by the totality of hyperplanes containing z.

The previous arguments allow a simple characterization of the first jet spaces $j_1(Q, M)$ and $j_1(Q^*, M^*)$ associated with the fibrations $Q \to M$ and $Q^* \to M^*$. Recalling the interpretation of the bi-affine pairing (2.2) we have in fact the following.

Theorem 2.1: *Both manifolds $j_1(Q, M)$ and $j_1(Q^*, M^*)$ are diffeomorphic to the submanifold $\mathcal{S} \subset Q \times Q^*$ described by the equation $F(z, \sigma) = 0$.*

Proof: By definition, every pair $(z, \sigma) \in \mathcal{S}$, meant as a point $z \in Q$ and a hyperplane $\sigma : M \to Q$ through z is an element of $j_1(Q, M)$, while, meant as a point $\sigma \in Q^*$ and a hyperplane

$z:M^*\to Q^*$ containing σ, it belongs to $j_1(Q^*,M^*)$. A straightforward argument (left to the reader) shows that both correspondences $\mathcal{S}\to j_1(Q,M)$ and $\mathcal{S}\to j_1(Q^*,M^*)$ obtained in this way are in fact diffeomorphisms. □

In view of Theorem 2.1, the bundles $j_1(Q,M)$ and $j_1(Q^*,M^*)$ may be identified. Depending on the context, we shall refer them to global coordinates x^i,u,y_i or x^i,v,y_i, related to each other by the correspondence

$$u-v-x^iy_i=0. \tag{2.5}$$

The content of Theorem 2.1 is completed by the following observations.

(a) Both manifolds $j_1(Q,M)$ and $j_1(Q^*,M^*)$ are *principal fiber bundles*, with structural group $(\Re,+)$, and group actions obtained as jet extensions of the maps $\varphi_\xi:Q\to Q$ and $\varphi_\xi:Q^*\to Q^*$ described above. With the identifications stated in Theorem 2.1, the resulting bundle structures are unified into the principal fibration $\mathcal{S}\to M\times M^*$ associated with the one-parameter group of translations (2.3).

Both coordinate systems x^i,u,y_i and x^i,v,y_i are fibered over $M\times M^*$, with u,v playing the role of *trivializations* of the bundle $\mathcal{S}\to M\times M^*$, and with the fundamental vector field expressed indifferently as $\hat{X}=\partial/\partial u=\partial/\partial v$.

(b) By construction, each manifold $j_1(Q,M)$, $j_1(Q^*,M^*)$ carries a distinguished contact one-form, known as the *Liouville* 1-*form*. Once again, with the identification stated in Theorem 2.1, both Liouville one-forms are unified into a single geometrical object, expressed in coordinates as

$$\vartheta \;=\; du-y_i\,dx^i \;=\; dv+x^i\,dy_i \tag{2.6}$$

and playing the role of a *connection one-form* over the bundle $\mathcal{S}\to M\times M^*$.

The exterior two-form,

$$\Omega:=-d\vartheta=dy_i\wedge dx^i, \tag{2.7}$$

identical, up to a sign, to the *curvature* of ϑ, endows the manifold $M\times M^*$ with a canonical *symplectic structure*.

The previous discussion, summarized into the diagram

$$\begin{array}{ccccc} j_1(Q,M) & = & \mathcal{S} & = & j_1(Q^*,M^*) \\ \downarrow & & \downarrow & & \downarrow \\ Q & & M\times M^* & & Q^* \\ \downarrow & & & & \downarrow \\ M & & & & M^* \end{array} \tag{2.8}$$

is the core of the Legendre transformation between affine bundles.

Every section $\varphi:M\to Q$ may in fact be lifted to a map $j_1(\varphi):M\to j_1(Q,M)$, thereby giving rise, through the diagram (2.8), to correspondences $\Lambda_\varphi:M\to Q^*$, $\lambda_\varphi:M\to M^*$, and $\kappa_\varphi:M\to M\times M^*$.

The last one is nothing but the *graph* $\kappa_\varphi(x)=(x,\lambda_\varphi(x))$ of the map λ_φ. As far as the other two are concerned, expressing φ as $u=\varphi(x^1,\ldots,x^n)$, and recalling Eq. (2.5), as well as the definition of $j_1(\varphi)$, we get the coordinate representations

$$\Lambda_\varphi:\quad y_i=\frac{\partial\varphi}{\partial x^i},\quad v=\varphi-x^i\frac{\partial\varphi}{\partial x^i}; \tag{2.9a}$$

$$\lambda_\varphi:\quad y_i=\frac{\partial\varphi}{\partial x^i}. \tag{2.9b}$$

In view of Eqs. (2.7) and (2.9b), the map κ_φ satisfies the identity

$$\kappa_\varphi^*(\Omega)=\lambda_\varphi^*(dy_i)\wedge dx^i=d\left(\frac{\partial\varphi}{\partial x^i}dx^i\right)=0 \tag{2.10}$$

indicating that the graph of λ_φ is a *Lagrangian submanifold* of $M\times M^*$.

In a perfectly symmetric way, every section $\psi: M^*\to Q^*$, lifted to a map $j_1(\psi): M^*\to j_1(Q^*,M^*)$, gives rise, through the diagram (2.8), to correspondences $\Lambda_\psi: M^*\to Q$, $\lambda_\psi: M^*\to M$, and $\kappa_\psi: M^*\to M\times M^*$, with κ_ψ representing the graph of λ_ψ. In coordinates, expressing ψ as $v=-\psi(y_1,\ldots,y_n)$, we have the representations

$$\Lambda_\psi: \quad x^i=\frac{\partial\psi}{\partial y_i}, \quad u=-\psi+y_i\frac{\partial\psi}{\partial y_i}; \tag{2.11a}$$

$$\lambda_\psi: \quad x^i=\frac{\partial\psi}{\partial y_i}. \tag{2.11b}$$

Once again, in view of Eq. (2.11b), the graph of λ_ψ is easily recognized to be a Lagrangian submanifold of $M\times M^*$.

A special instance of the previous construction occurs when the map λ_φ associated with the section $\varphi: M\to Q$ is a *diffeomorphism*, i.e., when the graph $\kappa_\varphi(M)\subset M\times M^*$ projects injectively onto M^*. Under the stated assumption, the correspondence $\psi:=\Lambda_\varphi\cdot\lambda_\varphi^{-1}: M^*\to Q^*$ is a *section* of the bundle $Q^*\to M^*$, described in coordinates as

$$v=-y_i x^i+\varphi(x^1,\ldots,x^n):=-\psi(y_1,\ldots,y_n) \tag{2.12}$$

with the variables x^i defined implicitly in terms of the y_i's through Eq. (2.9b).

From Eqs. (2.9b) and (2.12), by elementary computations, we get the identities

$$\frac{\partial\psi}{\partial y_i}=x^i-y_j\frac{\partial x^j}{\partial y_i}-\frac{\partial\varphi}{\partial x^j}\frac{\partial x^j}{\partial y_i}=x^i, \quad \varphi=-\psi+y_i\frac{\partial\psi}{\partial y_i}. \tag{2.13}$$

Comparison with Eqs. (2.11a) and (2.11b) provides the identifications

$$\lambda_\psi=\lambda_\varphi^{-1}, \quad \varphi=\Lambda_\psi\cdot\lambda_\varphi$$

pointing out the perfectly symmetric role played by the sections φ and ψ. Consistently with the current terminology, every diffeomorphism $M\leftrightarrow M^*$ arising from a section $\varphi: M\to Q$ through the algorithm indicated above will be called a *Legendre transformation*.

B. Affine principal fibrations

The construction of Sec. II A is easily extended to the context of affine bundles over an arbitrary base manifold N. The basic structure is summarized into the diagram

$$\begin{array}{ccc} Q & \longrightarrow & M \\ {\scriptstyle\pi}\downarrow & & \downarrow{\scriptstyle\pi} \\ N & = & N \end{array} \tag{2.14}$$

in which $Q\to N$ and $M\to N$ are affine fibrations, while $Q\to M$ is both an affine bundle homomorphism, fibered over N, and a principal fiber bundle, with structural group $(\Re,+)$. [Basically, this means that M is the quotient of Q by the action of the one-parameter group of affine translations generated by an everywhere nonzero vector field X tangent to the fibers of $Q\to N$, and constant along each fiber.]

We shall refer the manifold N to local coordinates $\xi^1,\ldots,\xi^r$. The bundles M and Q will be, respectively, referred to affine fibered coordinates $\xi^1,\ldots,\xi^r,x^1,\ldots,x^n$ and $\xi^1,\ldots,\xi^r,x^1,\ldots,x^n,u$. The fibers of $M\to N$ and $Q\to N$ will be denoted by M_ξ, Q_ξ, $\xi\in N$.

For each $\xi\in N$ let us now consider the family of affine sections $\sigma_\xi:M_\xi\to Q_\xi$. As pointed out in Sec. II A, these form an affine space $Q_\xi{}^*$ carrying an affine principal fibration $Q_\xi{}^*\to M_\xi{}^*$ "dual" of the fibration $Q_\xi\to M_\xi$ in the sense described by Eq. (2.2).

Introducing the spaces $Q^*:=\cup_{\xi\in N} Q_\xi{}^*$, $M^*:=\cup_{\xi\in N} M_\xi{}^*$, the situation is summarized into the commutative diagram

$$\begin{array}{ccc} Q^* & \longrightarrow & M^* \\ {\scriptstyle\pi}\downarrow & & \downarrow{\scriptstyle\pi} \\ N & = & N \end{array} \tag{2.15}$$

in which all vertical arrows represent affine fibrations, while $Q^*\to M^*$ is an affine bundle homomorphism and a principal fibration.

Exactly as in Sec. II A, every coordinate system ξ^α,x^i,u on Q determines coordinates ξ^α,y_i,v on Q^* and ξ^α,y_i on M^* on the basis of the requirement

$$\xi^\alpha(\sigma):=\xi^\alpha(\pi(\sigma)),\quad v(\sigma)+y_i(\sigma)\,x^i(x)=u(\sigma(x))\quad\forall\ x\in M_{\pi(\sigma)}. \tag{2.16}$$

Once again, the fibrations $Q\to M$ and $Q^*\to M^*$ are *dual* of each other under the bi-affine pairing $(z,\sigma)\to F(z,\sigma)$ defined on the fibered product $Q\times_N Q^*$ by

$$F(z,\sigma)=u(z)-v(\sigma)-y_i(\sigma)\,x^i(z). \tag{2.17}$$

In particular, denoting by $\mathcal{S}$ the submanifold of $Q\times_N Q^*$ described by the equation $F(z,\sigma)=0$ and recalling the proof of Theorem 2.1, we get the identifications

$$\mathcal{S}=\bigcup_{\xi\in N} j_1(Q_\xi,M_\xi)=\bigcup_{\xi\in N} j_1(Q_\xi{}^*,M_\xi{}^*). \tag{2.18}$$

Depending on the context, we shall refer $\mathcal{S}$ to coordinates ξ^α,x^i,u,y_i or ξ^α,x^i,y_i,v, with transformation law

$$u-v-x^i\,y_i=0. \tag{2.19}$$

The previous arguments help analyzing the relationship between the first jet spaces $j_1(Q,M)$ and $j_1(Q^*,M^*)$. To this end, prior to any further consideration, we recall that both spaces carry natural actions of the group $(\Re,+)$, respectively, obtained by lifting the group actions on $Q\to M$ and on $Q^*\to M^*$. Introducing the notation $B:=j_1(Q,M)/(\Re,+)$, $B^*:=j_1(Q^*,M^*)/(\Re,+)$, the situation is expressed diagrammatically as

$$\begin{array}{ccc} j_1(Q,M) & \longrightarrow & Q \\ \downarrow & & \downarrow \\ B & \longrightarrow & M \end{array} \qquad\qquad \begin{array}{ccc} j_1(Q^*,M^*) & \longrightarrow & Q^* \\ \downarrow & & \downarrow \\ B^* & \longrightarrow & M^* \end{array} \tag{2.20}$$

the vertical arrows denoting affine principal fibrations.

Using jet coordinates $\xi^\alpha,x^i,u,u_\alpha,u_i$ on $j_1(Q,M)$ and $\xi^\alpha,y_i,v,v_\alpha,v^i$ on $j_1(Q^*,M^*)$, the fundamental vector fields over $j_1(Q,M)\to B$ and $j_1(Q^*,M^*)\to B^*$ coincide, respectively, with the fields $\partial/\partial u$ and $\partial/\partial v$.

In addition to this, the manifolds $j_1(Q,M)$, $j_1(Q^*,M^*)$ are endowed with corresponding *Liouville one-forms*, expressed in coordinates as

$$\Theta_1=du-u_\alpha\,d\xi^\alpha-u_i\,dx^i, \tag{2.21a}$$

$$\Theta_2 = dv - v_\alpha\, d\xi^\alpha - v^i\, dy_i\,, \tag{2.21b}$$

and playing the role of connection one-forms with respect to the principal fibrations $j_1(Q,M) \to B$ and $j_1(Q^*,M^*) \to B^*$ discussed above.

Finally, by definition, for each $z \in Q$, the elements of the fiber $j_1(Q,M)_{|z}$ are equivalence classes of sections $\varphi: M \to Q$ having a first order contact at z. Setting $\xi := \pi(z) \in N$, the restriction of each such φ to the fiber M_ξ is a section $\varphi_\xi: M_\xi \to Q_\xi$. Moreover, if two sections φ, φ' have a first order contact at z, the restrictions φ_ξ, φ'_ξ also do.

In this way, by varying z, we obtain a surjection $j_1(Q,M) \to \cup_{\xi \in N} j_1(Q_\xi, M_\xi)$. A similar argument establishes the surjection $j_1(Q^*,M^*) \to \cup_{\xi \in N} j_1(Q_\xi{}^*, M_\xi{}^*)$. In view of Eq. (2.18) this makes both $j_1(Q,M)$ and $j_1(Q^*,M^*)$ into fiber bundles over the same base manifold $\mathcal{S}$. On this basis, we state the following.

Theorem 2.2: *There exists a unique diffeomorphism $\psi: j_1(Q,M) \to j_1(Q^*,M^*)$ making the diagram*

$$\begin{array}{ccc} j_1(Q,M) & \xrightarrow{\ \psi\ } & j_1(Q^*,M^*) \\ \downarrow & & \downarrow \\ \mathcal{S} & = & \mathcal{S} \end{array} \tag{2.22}$$

commutative, and satisfying $\psi^*(\Theta_2) = \Theta_1$.

Proof: In coordinates, on account Eqs. (2.18), (2.19), the requirement of commutativity of the diagram (2.22) is expressed by the relations

$$\psi^*(\xi^\alpha) = \xi^\alpha, \quad \psi^*(y_i) = u_i \ , \quad \psi^*(v^i) = -x^i, \quad \psi^*(v) = u - x^i\, \psi^*(y_i) = u - x^i u_i\,.$$

Comparison with Eqs. (2.21a) and (2.21b) provides the evaluation

$$\psi^*(\Theta_2) = d(u - x^i u_i) - \psi^*(v_\alpha)\, d\xi^\alpha + x^i\, du_i = \Theta_1 + [u_\alpha - \psi^*(v_\alpha)]\, d\xi^\alpha,$$

showing that the condition $\psi^*(\Theta_2) = \Theta_1$ requires the further identification

$$\psi^*(v_\alpha) = u_\alpha\,.$$

This establishes at one time the existence and the uniqueness of a diffeomorphism $\psi: j_1(Q,M) \to j_1(Q^*,M^*)$ satisfying all stated requirements. □

In view of Theorem 2.2, the bundles $j_1(Q,M) \to B$ and $j_1(Q^*,M^*) \to B^*$ may be regarded as different copies of the same abstract bundle, henceforth denoted by $\mathcal{J} \to \mathcal{B}$. Depending on the context, we shall refer the latter to fibered coordinates $\xi^\alpha, x^i, \eta_\alpha, y_i, u$ or $\xi^\alpha, x^i, \eta_\alpha, y_i, v$, related to each other by the transformation law

$$u - v - x^i y_i = 0 \tag{2.23a}$$

and to the ordinary jet coordinates $\xi^\alpha, x^i, u, u_\alpha, u_i$ on $j_1(Q,M)$ and $\xi^\alpha, y_i, v, v_\alpha, v^i$ on $j_1(Q^*,M^*)$ by the further identifications

$$u_i = y_i \ , \quad v^i = -x^i \ , \quad u_\alpha = v_\alpha = \eta_\alpha\,. \tag{2.23b}$$

As a result, the fundamental vector fields $\partial/\partial u$ and $\partial/\partial v$ get identified. In a similar way, the Liouville one-forms (2.21a) and (2.21b) collapse into a single geometrical object, henceforth denoted by Θ, expressed in coordinates as

$$\Theta = du - \eta_\alpha\, d\xi^\alpha - y_i\, dx^i = dv - \eta_\alpha\, d\xi^\alpha + x^i\, dy_i\,. \tag{2.24}$$

The two-form

$$\Omega := -d\Theta = d\eta_\alpha \wedge d\xi^\alpha + dy_i \wedge dx^i \tag{2.25}$$

endows the base manifold $\mathcal{B}$ with a canonical symplectic structure.

The previous arguments, summarized into the diagram

$$\begin{array}{ccccc} j_1(Q,M) & = & \mathcal{J} & = & j_1(Q^*,M^*) \\ \downarrow & & \downarrow & & \downarrow \\ Q & & \mathcal{B} & & Q^* \\ \downarrow & & & & \downarrow \\ M & & & & M^* \end{array} \tag{2.26}$$

allow the construction of a completely involutory *Legendre transformation* between the bundles $Q \to M$ and $Q^* \to M^*$. The line of approach, similar to the one exploited in Sec. II A, may be traced as follows: every section $\varphi: M \to Q$ may be lifted to a map $j_1(\varphi): M \to j_1(Q,M)$, thereby giving rise, through the diagram (2.26), to correspondences $\Lambda_\varphi: M \to Q^*$, $\lambda_\varphi: M \to M^*$, and $\kappa_\varphi: M \to \mathcal{B}$.

In coordinates, expressing φ as $u = \varphi(\xi^1,\ldots,\xi^r,x^1,\ldots,x^n)$, and recalling Eq. (2.23a), as well as the definition of $j_1(\varphi)$, we get the representations

$$\Lambda_\varphi: \quad y_i = \frac{\partial \varphi}{\partial x^i} \quad , \quad v = \varphi - x^i \frac{\partial \varphi}{\partial x^i}; \tag{2.27a}$$

$$\lambda_\varphi: \quad y_i = \frac{\partial \varphi}{\partial x^i}; \tag{2.27b}$$

$$\kappa_\varphi: \quad y_i = \frac{\partial \varphi}{\partial x^i} \quad , \quad \eta_\alpha = \frac{\partial \varphi}{\partial \xi^\alpha}. \tag{2.27c}$$

In view of Eqs. (2.25) and (2.27c), the map κ_φ satisfies the identity

$$\kappa_\varphi^*(\Omega) = \kappa_\varphi^*(d\eta_\alpha \wedge d\xi^\alpha + dy_i \wedge dx^i) = d\left(\frac{\partial \varphi}{\partial \xi^\alpha} d\xi^\alpha + \frac{\partial \varphi}{\partial x^i} dx^i\right) = 0 \tag{2.28}$$

showing that the image $\kappa_\varphi(M)$ is a *Lagrangian submanifold* of $\mathcal{B}$.

In a perfectly symmetric way, every section $\psi: M^* \to Q^*$, lifted to a map $j_1(\psi): M^* \to j_1(Q^*,M^*)$, induces correspondences $\Lambda_\psi: M^* \to Q$, $\lambda_\psi: M^* \to M$, and $\kappa_\psi: M^* \to \mathcal{B}$. The implementation in coordinates is entirely straightforward, and is left to the reader.

Finally, when the map λ_φ associated with the section $\varphi: M \to Q$ is a *diffeomorphism*, the correspondence $\psi := \Lambda_\varphi \cdot \lambda_\varphi^{-1}: M^* \to Q^*$ is a *section* of the bundle $Q^* \to M^*$, described in coordinates as

$$v = -y_i x^i + \varphi(\xi^1,\ldots,\xi^r,x^1,\ldots,x^n) := -\psi(\xi^1,\ldots,\xi^r,y_1,\ldots,y_n) \tag{2.29}$$

with the functions $x^i(\xi^1,\ldots,\xi^r,y_1,\ldots,y_n)$ defined implicitly by Eq. (2.27b).

From Eqs. (2.27b) and (2.29), by elementary computations, we get the identities

$$\frac{\partial \psi}{\partial y_i} = x^i - y_j \frac{\partial x^j}{\partial y_i} - \frac{\partial \varphi}{\partial x^j} \frac{\partial x^j}{\partial y_i} = x^i, \quad \varphi = -\psi + y_i \frac{\partial \psi}{\partial y_i}. \tag{2.30}$$

Comparison with Eqs. (2.27a) and (2.27b) provides the identifications

$$\lambda_\psi = \lambda_\varphi^{-1}, \quad \varphi = \Lambda_\psi \cdot \lambda_\varphi$$

pointing out once again the symmetric role played by the sections φ and ψ.

The previous arguments extend to jet bundles the classical approach to the Legendre transformation developed by Tulczyjew.[5,8] In this connection, see also Ref. 10.

III. CLASSICAL MECHANICS

A. Lagrangian and Hamiltonian bundles

A well-known feature of classical mechanics is the invariance of Lagrange's equations under gauge transformations of the form $L \to L + \dot{f}$ involving the total time derivative of an arbitrary smooth function over the configuration manifold. This fact is conveniently accounted for by working in an environment in which gauge equivalent Lagrangians may be thought of as different *representations* of the same geometrical object. The geometrical setup, worked out in detail in Refs. 1 and 2, relies on the introduction of a double fibration $P \xrightarrow{\pi} \mathcal{V}_{n+1} \xrightarrow{t} \mathfrak{R}$, in which $\mathcal{V}_{n+1}$ is the configuration space–time of the dynamical system in study, with the fibration $\mathcal{V}_{n+1} \xrightarrow{t} \mathfrak{R}$ representing *absolute time*; $P \xrightarrow{\pi} \mathcal{V}_{n+1}$ is a principal fiber bundle, with structural group $(\mathfrak{R}, +)$, called the bundle of *affine scalars* over $\mathcal{V}_{n+1}$.

In what follows, we shall refer the manifold $\mathcal{V}_{n+1}$ to local coordinates t, q^i, and P to fibered local coordinates $t, q^i, u \quad (i = 1, ..., n)$, u denoting any trivialization of $P \to \mathcal{V}_{n+1}$. The first jet bundles associated with the fibration $P \to^{\pi} \mathcal{V}_{n+1}$ and with the composite fibration $P \to^{t \cdot \pi} \mathfrak{R}$, respectively, denoted by $j_1(P, \mathcal{V}_{n+1})$ and $j_1(P, \mathfrak{R})$, will be referred to jet coordinates t, q^i, u, p_0, p_i and $t, q^i, u, \dot{q}^i, \dot{u}$.

The manifold $j_1(P, \mathfrak{R})$ provides the basic environment for the gauge-invariant *Lagrangian* formulation of mechanics. As illustrated in Refs. 1 and 2, the latter carries two mutually commuting actions of the group $(\mathfrak{R}, +)$, locally generated by the vector fields $\partial/\partial u$ and $\partial/\partial \dot{u}$, and giving rise to corresponding quotient spaces and quotient maps. The situation is summarized into the diagram

$$\begin{array}{ccc} j_1(P, \mathfrak{R}) & \longrightarrow & \mathcal{L}^c(\mathcal{V}_{n+1}) \\ \downarrow & & \downarrow \\ \mathcal{L}(\mathcal{V}_{n+1}) & \longrightarrow & j_1(\mathcal{V}_{n+1}) \end{array} \tag{3.1}$$

in which all arrows express principal fibrations with structural group $(\mathfrak{R}, +)$, while $j_1(\mathcal{V}_{n+1}) := j_1(\mathcal{V}_{n+1}, \mathfrak{R})$ denotes the velocity space of the system.

More specifically, the manifold $\mathcal{L}(\mathcal{V}_{n+1})$, with coordinates $t, q^i, \dot{q}^i, \dot{u}$, is the quotient of $j_1(P, \mathfrak{R})$ by the action generated by $\partial/\partial u$. The one-parameter group generated by $\partial/\partial \dot{u}$ makes $\mathcal{L}(\mathcal{V}_{n+1})$ into a principal fiber bundle over $j_1(\mathcal{V}_{n+1})$, known as the *Lagrangian bundle*. Every section $l: j_1(\mathcal{V}_{n+1}) \to \mathcal{L}(\mathcal{V}_{n+1})$, expressed locally as $\dot{u} = L(t, q^i, \dot{q}^i)$, is called a *Lagrangian section*.

In a similar way, the quotient of $j_1(P, \mathfrak{R})$ by the action generated by $\partial/\partial \dot{u}$ is denoted by $\mathcal{L}^c(\mathcal{V}_{n+1})$. The principal fiber bundle $\mathcal{L}^c(\mathcal{V}_{n+1}) \to j_1(\mathcal{V}_{n+1})$, with structural group generated by $\partial/\partial u$, is called the *co-Lagrangian bundle*.

As pointed out in Ref. 1, the use of Lagrangian *sections* in place of Lagrangian *functions* automatically embodies the gauge invariance of the theory under arbitrary transformations $L \to L + \dot{f}$, and establishes a natural interpretation of the Poincaré–Cartan one-form as a connection one-form over the co-Lagrangian bundle.

The Hamiltonian counterpart of the construction stems from an analysis of the fibration $P \to \mathcal{V}_{n+1}$. Once again, the first-jet space $j_1(P, \mathcal{V}_{n+1})$ is endowed with two mutually commuting actions of the group $(\mathfrak{R}, +)$, now generated by the vector fields $\partial/\partial u$, $\partial/\partial p_0$. These give rise to corresponding quotient spaces and quotient maps, summarized into the diagram

$$\begin{array}{ccc} j_1(P,\mathcal{V}_{n+1}) & \longrightarrow & \mathcal{H}^c(\mathcal{V}_{n+1}) \\ \downarrow & & \downarrow \\ \mathcal{H}(\mathcal{V}_{n+1}) & \longrightarrow & \Pi(\mathcal{V}_{n+1}) \end{array} \tag{3.2}$$

in which all arrows express principal fibrations with structural group $(\mathfrak{R},+)$. The double quotient $\Pi(\mathcal{V}_{n+1})$ is called the *phase space* of the system.

More specifically, the manifold $\mathcal{H}(\mathcal{V}_{n+1})$, with coordinates $t,q^i,p_0\,p_i$, is the quotient of $j_1(P,\mathcal{V}_{n+1})$ by the action generated by $\partial/\partial u$. The action generated by $\partial/\partial p_0$ makes $\mathcal{H}(\mathcal{V}_{n+1})$ into a principal fiber bundle over $\Pi(\mathcal{V}_{n+1})$, known as the *Hamiltonian bundle*. Every section $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$, described in coordinates as $p_0=-H(t,q^i,p_i)$ is called a *Hamiltonian section*.

In a similar way, the quotient of $j_1(P,\mathcal{V}_{n+1})$ by the action generated by $\partial/\partial p_0$ is denoted by $\mathcal{H}^c(\mathcal{V}_{n+1})$. The principal fiber bundle $\mathcal{H}^c(\mathcal{V}_{n+1})\to\Pi(\mathcal{V}_{n+1})$, with structural group generated by $\partial/\partial u$, is called the *co-Hamiltonian bundle*.

The geometrical environment described by diagram (3.2) provides the starting point for a gauge-invariant formulation of Hamiltonian mechanics. A thorough analysis of this point may be found in Refs. 1, 2, 3 and references therein. For the present purposes we simply remind that the Liouville one-form of $j_1(P,\mathcal{V}_{n+1})$, expressed in coordinates as

$$\vartheta := du - p_0\,dt - p_i\,dq^i \tag{3.3}$$

determines a *connection* over the principal fiber bundle $j_1(P,\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$. The curvature of ϑ, described, up to a sign, by the exterior two-form

$$\Omega := -d\vartheta = dp_0\wedge dt + dp_i\wedge dq^i \tag{3.4}$$

endows the base manifold $\mathcal{H}(\mathcal{V}_{n+1})$ with a canonical symplectic structure.

B. Higher jet spaces

The algorithm developed in Sec. II B applies in a natural way to the Lagrangian and Hamiltonian bundles described in Sec. III A, thereby providing a mathematical environment for a unified formulation of time-dependent Lagrangian and Hamiltonian dynamics.

To start with, let us focus on the commutative diagram

$$\begin{array}{ccc} \mathcal{L}(\mathcal{V}_{n+1}) & \longrightarrow & j_1(\mathcal{V}_{n+1}) \\ \downarrow & & \downarrow \\ \mathcal{V}_{n+1} & = & \mathcal{V}_{n+1} \end{array} \tag{3.5}$$

and observe that, by construction, both $j_1(\mathcal{V}_{n+1})\to\mathcal{V}_{n+1}$ and $\mathcal{L}(\mathcal{V}_{n+1})\to\mathcal{V}_{n+1}$ are affine bundles [the second one identical to the quotient of $j_1(P,\mathfrak{R})\to P$ by the action generated by the vector field $\partial/\partial u$], while the map $\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})$ is at the same time an affine bundle homomorphism, fibered over $\mathcal{V}_{n+1}$, and a principal fiber bundle, with structural group $(\mathfrak{R},+)$.

The diagram (3.5) is therefore an example of *affine principal fibration* in the sense described in Sec. II B.

In a perfectly symmetric way, the diagram

$$\begin{array}{ccc} \mathcal{H}(\mathcal{V}_{n+1}) & \longrightarrow & \Pi(\mathcal{V}_{n+1}) \\ \downarrow & & \downarrow \\ \mathcal{V}_{n+1} & = & \mathcal{V}_{n+1} \end{array} \tag{3.6}$$

defines another affine principal fibration over the same base space $\mathcal{V}_{n+1}$.

More specifically, from the discussion of Sec. III A we can draw the following conclusions.

The bundle $\mathcal{H}(\mathcal{V}_{n+1})\to\mathcal{V}_{n+1}$ is canonically isomorphic to the space of *connections* over the principal fiber bundle $P\to\mathcal{V}_{n+1}$. At each $x\in\mathcal{V}_{n+1}$, the elements of the fiber $\mathcal{H}(\mathcal{V}_{n+1})_{|x}$ are in fact equivalence classes of sections $\varrho:\mathcal{V}_{n+1}\to P$ related to each other by the condition [notice that, consistently with the definition of $\mathcal{H}(\mathcal{V}_{n+1})$, we are not requiring $\varrho(x)=\varrho'(x)$],

$$\varrho\sim\varrho'\Leftrightarrow d(\varrho-\varrho')_{|x}=0$$

and therefore defining one and the same horizontal distributions along the fiber P_x.

Every section $\varrho:\mathcal{V}_{n+1}\to P$ defined in a neighborhood of a point x and described in coordinates as $u=\varrho(t,q^1,\ldots,q^n)$ may be lifted to a section $j_1(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$, denoted symbolically by $\dot{\varrho}$, and expressed in coordinates as $\dot{u}=(\partial\varrho/\partial t)+(\partial\varrho/\partial q^k)\,\dot{q}^k$. The restriction of $\dot{\varrho}$ to the fiber $j_1(\mathcal{V}_{n+1})_{|x}$ is an affine section $\dot{\varrho}_{|x}:j_1(\mathcal{V}_{n+1})_{|x}\to\mathcal{L}(\mathcal{V}_{n+1})_{|x}$. Two sections ϱ,ϱ' satisfy $\dot{\varrho}_{|x}=\dot{\varrho}'_{|x}$ if and only if the differential $d(\varrho-\varrho')$ vanishes at x.

In view of the stated results, every element $\sigma\in\mathcal{H}(\mathcal{V}_{n+1})_{|x}$ is easily seen to determine an affine section $\dot{u}=p_0(\sigma)+p_i(\sigma)\,\dot{q}^i$ of the bundle $\mathcal{L}(\mathcal{V}_{n+1})_{|x}\to j_1(\mathcal{V}_{n+1})_{|x}$. With the terminology of Sec. II B we have thus proved the following.

Proposition 3.1: The affine principal fibrations (3.5), (3.6) are affine dual *of each other under the bi-affine map* $F:\mathcal{L}(\mathcal{V}_{n+1})\times_{\mathcal{V}_{n+1}}\mathcal{H}(\mathcal{V}_{n+1})\to\mathfrak{R}$ *expressed in coordinates as*

$$F(t,q^i,\dot{q}^i,\dot{u},p_0,p_i)=\dot{u}-p_0-p_i\,\dot{q}^i. \tag{3.7}$$

Together with Theorem 2.2, Proposition 3.1 gives rise to a canonical identification between the first-jet spaces $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ and $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$. In the present context, this result is further enhanced by considering the fibration $\mathcal{H}(\mathcal{V}_{n+1})\to\mathfrak{R}$ coming from the composition $\mathcal{H}(\mathcal{V}_{n+1})\to\mathcal{V}_{n+1}\to\mathfrak{R}$. Denoting by $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ the associated first jet space, and recalling that the manifold $\mathcal{H}(\mathcal{V}_{n+1})$ is canonically endowed with the symplectic structure (3.4), we have in fact the following.

Theorem 3.1: *The manifolds* $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$ *are canonically diffeomorphic*.

Proof: By definition, both manifolds may be regarded as affine sub-bundles, respectively, of the tangent space $T(\mathcal{H}(\mathcal{V}_{n+1}))$ and of the cotangent space $T^*(\mathcal{H}(\mathcal{V}_{n+1}))$, according to the identifications

$$j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})=\{X\mid X\in T(\mathcal{H}(\mathcal{V}_{n+1})),\quad\langle X,dt\rangle=1\}, \tag{3.8a}$$

$$j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))=\left\{\omega\;\middle|\;\omega\in T^*(\mathcal{H}(\mathcal{V}_{n+1})),\;\left\langle\frac{\partial}{\partial p_0},\omega\right\rangle=1\right\}. \tag{3.8b}$$

The conclusion then follows from the identity

$$\left\langle\frac{\partial}{\partial p_0},-X\lrcorner\Omega\right\rangle=\left\langle-X\wedge\frac{\partial}{\partial p_0}\;\middle|\;dp_0\wedge dt+dp_i\wedge dq^i\right\rangle=\langle X,dt\rangle$$

showing that the correspondence $X\to-X\lrcorner\Omega$ determines a diffeomorphism of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ onto $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$, fibered over $\mathcal{H}(\mathcal{V}_{n+1})$. □

In view of the previous results, all spaces $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$, and $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$ are canonically diffeomorphic, and may be identified. For definiteness, and without any loss in generality, we choose to regard all of them as different copies of the manifold $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$. Depending on the context, we shall refer $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ to ordinary jet coordinates $t,q^i,p_0,p_i,\dot{q}^i,\dot{p}_0,\dot{p}_i$, or to coordinates $t,q^i,\dot{u},p_i,\dot{q}^i,\dot{p}_0,\dot{p}_i$ related to the previous ones by the transformation [analogous to Eq. (2.23a)]

$$\dot{u}-p_0-p_i\,\dot{q}^i=0. \tag{3.9}$$

The relationships with the standard jet coordinates $t,q^i,\dot{q}^i,\dot{u},\dot{u}_t,\dot{u}_{q^i},\dot{u}_{\dot{q}^i}$ on $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ and $t,q^i,p_i,p_0,p_{0t},p_{0q^i},p_{0p_i}$ on $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$ are then expressed by the identifications

$$\dot{p}_0=\dot{u}_t=p_{0t}, \quad \dot{p}_i=\dot{u}_{q^i}=p_{0q^i}, \quad p_i=\dot{u}_{\dot{q}^i}, \quad \dot{q}^i=-p_{0p_i} \tag{3.10}$$

summarizing the content of Eqs. (2.23b) and (3.4), and of Theorem 3.1.

The quotient of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ by the action of the one-parameter group of diffeomorphisms generated by the vector field $\partial/\partial\dot{u}=\partial/\partial p_0$ will be denoted by $\mathcal{B}$, and will be referred to coordinates $t,q^i,\dot{q}^i,p_i,\dot{p}_0,\dot{p}_i$. The quotient map makes $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})\to\mathcal{B}$ into a principal fiber bundle. The Liouville one-forms of $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ and $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$, unified into the single expression

$$\Theta:=d\dot{u}-\dot{p}_0\,dt-\dot{p}_i\,dq^i-p_i\,d\dot{q}^i=dp_0-\dot{p}_0\,dt-\dot{p}_i\,dq^i+\dot{q}^i\,dp_i \tag{3.11}$$

endow $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})\to\mathcal{B}$ with a canonical connection. The exterior two-form

$$\Upsilon:=-d\,\Theta=d\dot{p}_0\wedge dt+d\dot{p}_i\wedge dq^i+dp_i\wedge d\dot{q}^i \tag{3.12}$$

makes the manifold $\mathcal{B}$ into a symplectic manifold.

The previous discussion, summarized into the commutative diagram,

$$\begin{array}{ccccc} j_1(\mathcal{L}(V_{n+1},j_1(\mathcal{V}_{n+1})) & = & j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R}) & = & j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1})) \\ \downarrow & & \downarrow & & \downarrow \\ \mathcal{L}(\mathcal{V}_{n+1}) & & \mathcal{B} & & \mathcal{H}(\mathcal{V}_{n+1}) \\ \downarrow & & & & \downarrow \\ j_1(\mathcal{V}_{n+1}) & & \swarrow & \searrow & \Pi(\mathcal{V}_{n+1}) \end{array} \tag{3.13}$$

provides the necessary tool for the application of the Legendre transformation in time dependent analytical mechanics, along the lines discussed in Sec. II. An alternative approach, leading to a construction bearing interesting analogies with diagram (3.13) may be found in Ref. 11.

C. Dynamics

As a final topic, we discuss the Lagrangian and Hamiltonian formulation of dynamics within the geometrical framework developed so far. The analysis will provide a gauge-invariant extension to nonautonomous systems of the classical results of Tulczyjew.[5–9]

Let $l:j_1(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$ denote a Lagrangian section, expressed in coordinates as $\dot{u}=L(t,q^i,\dot{q}^i)$. On account of the identifications (3.10), the first jet extension $j_1(l):j_1(\mathcal{V}_{n+1})\to j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ is described by the equations

$$\dot{u}=L(t,q^i,\dot{q}^i) \quad , \quad \dot{p}_0=\dot{u}_t=\frac{\partial L}{\partial t} \quad , \quad \dot{p}_i=\dot{u}_{q^i}=\frac{\partial L}{\partial q^i} \quad , \quad p_i=\dot{u}_{\dot{q}^i}=\frac{\partial L}{\partial \dot{q}^i}. \tag{3.14}$$

The map $j_1(l)$ carries a complete information on dynamics. Indeed, according to the diagram (3.13), the image space $\mathcal{E}:=j_1(l)(j_1(\mathcal{V}_{n+1}))$ may be viewed as a submanifold of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$. Switching to coordinates $t,q^i,p_0,p_i,\dot{q}^i,\dot{p}_0,\dot{p}_i$ through Eq. (3.9), let us accordingly rephrase Eqs. (3.14) in the equivalent form

$$p_0+\frac{\partial L}{\partial \dot{q}^i}\,\dot{q}^i-L(t,q^i,\dot{q}^i)=0 \quad , \quad \dot{p}_0=\frac{\partial L}{\partial t} \quad , \quad p_i=\frac{\partial L}{\partial \dot{q}^i} \quad , \quad \dot{p}_i=\frac{\partial L}{\partial q^i}. \tag{3.15}$$

By the very definition of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, Eqs. (3.15) provide a system of ordinary differential equations, not in normal form, for the determination of the family of sections $\gamma:\mathfrak{R}\to\mathcal{H}(\mathcal{V}_{n+1})$ $[\Leftrightarrow\gamma(t)\equiv(t,q^i(t),p_0(t),p_i(t))]$ whose jet extension $\dot\gamma:=j_1(\gamma)$ satisfies $\dot\gamma(t)\in\mathcal{E}\ \forall\ t$. In the resulting context, the last pair of relations (3.15) reproduce the content of Lagrange's equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q^i}\right)-\frac{\partial L}{\partial q^i}=0,\quad i=1,\ldots,n,$$

while the first pair describes the evolution of the Hamiltonian $H:=-L+(\partial L/\partial\dot q^i)\,\dot q^i$.

Precisely the same state of affairs occurs if one considers a Hamiltonian section $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$, expressed in coordinates as $p_0=-H(t,q^i,p_i)$. On account of Eqs. (3.10), the first jet extension $j_1(h):\Pi(\mathcal{V}_{n+1})\to j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$ is now described by the system

$$p_0=-H(t,q^i,p_i),\quad \dot p_0=-\frac{\partial H}{\partial t},\quad \dot p_i=-\frac{\partial H}{\partial q^i},\quad \dot q^i=\frac{\partial H}{\partial p_i}.\tag{3.16}$$

Once again, according to the diagram (3.13), the image space $\mathcal{E}:=j_1(h)(\Pi(\mathcal{V}_{n+1}))$ may be regarded as a $(2n+1)$-dimensional submanifold of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$.

Equations (3.16) play therefore the role of a system of ordinary differential equations, now in normal form, characterizing the totality of sections $\gamma:\mathfrak{R}\to\mathcal{H}(\mathcal{V}_{n+1})$ whose jet extension satisfies $\dot\gamma(t)\in\mathcal{E}\ \forall\ t$. More specifically, the last pair of equations (3.16) reproduces the content of Hamilton's equations, while the first pair describes the evolution of the Hamiltonian.

For completeness, let us also write down the *Legendre maps* associated with the sections $l:j_1(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$ and $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$ considered above. The argument is a replica of the one worked out in detail in Sec. II B, so that we shall merely state the results.

(i) Given any section $l:j_1(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$, consider the jet extension $j_1(l)$. Composing the latter with the (significant) vertical arrows of the diagram (3.13) generates three maps $\Lambda_l:j_1(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$, $\lambda_l:j_1(\mathcal{V}_{n+1})\to\Pi(\mathcal{V}_{n+1})$, and $\kappa_l:j_1(\mathcal{V}_{n+1})\to\mathcal{B}$.

In coordinates, expressing l as $\dot u=L(t,q^i,\dot q^i)$, we have the explicit representations [see Eqs. (2.27a)–(2.27c)]

$$\Lambda_l:\quad p_i=\frac{\partial L}{\partial\dot q^i},\quad p_0=L-\dot q^i\frac{\partial L}{\partial\dot q^i};\tag{3.17a}$$

$$\lambda_l:\quad p_i=\frac{\partial L}{\partial\dot q^i};\tag{3.17b}$$

$$\kappa_l:\quad p_i=\frac{\partial L}{\partial\dot q^i},\quad \dot p_0=\frac{\partial L}{\partial t},\quad \dot p_i=\frac{\partial L}{\partial q^i}.\tag{3.17c}$$

In view of Eqs. (3.12) and (3.17c), the map κ_l satisfies the identity

$$\kappa_l^*(\Upsilon)=\kappa_l^*(d\dot p_0\wedge dt+d\dot p_i\wedge dq^i+dp_i\wedge d\dot q^i)=d\left(\frac{\partial L}{\partial t}dt+\frac{\partial L}{\partial q^i}dq^i+\frac{\partial L}{\partial\dot q^i}d\dot q^i\right)\equiv 0\tag{3.18}$$

indicating that the image space $\kappa_l(j_1(\mathcal{V}_{n+1}))$ is a *Lagrangian submanifold* of $\mathcal{B}$.

Equations (3.17b) express the familiar Legendre transformation. Under the regularity assumption $\det\|\partial^2L/\partial\dot q^i\partial\dot q^j\|\neq 0$, the latter may be solved with respect to the variables $\dot q^i$. Substituting the result into the second equation (3.17a) one then gets the expression $p_0=-H(t,q^i,p_i)$, describing the *Hamiltonian section* $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$ associated with l.

A perfectly symmetric construction holds starting with a Hamiltonian section $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$. Once again the jet extension $j_1(h):\Pi(\mathcal{V}_{n+1})\to j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$, composed with the significant vertical arrows of diagram (3.13), gives rise to maps $\Lambda_h:\Pi(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$, $\lambda_h:\Pi(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})$ and $\kappa_h:\Pi(\mathcal{V}_{n+1})\to\mathcal{B}$, expressed in coordinates as

$$\Lambda_h: \quad \dot{q}^i=\frac{\partial H}{\partial p_i}, \quad \dot{u}=-H+\frac{\partial H}{\partial p_i}p_i; \tag{3.19a}$$

$$\lambda_h: \quad \dot{q}^i=\frac{\partial H}{\partial p_i}; \tag{3.19b}$$

$$\kappa_h: \quad \dot{q}^i=\frac{\partial H}{\partial p_i}, \quad \dot{p}_0=-\frac{\partial H}{\partial t} \quad , \quad \dot{p}_i=-\frac{\partial H}{\partial q^i}. \tag{3.19c}$$

$H(t,q^i,p_i)$ denoting the Hamiltonian function involved in the local representation of h. Exactly as above, Eqs. (3.12) and (3.17c) provide the identity

$$\kappa_h^*(\Upsilon)=\kappa_h^*(d\dot{p}_0\wedge dt+d\dot{p}_i\wedge dq^i+dp_i\wedge d\dot{q}^i)=d\left(-\frac{\partial H}{\partial t}dt-\frac{\partial H}{\partial q^i}dq^i-\frac{\partial H}{\partial p_i}dp_i\right)\equiv 0 \tag{3.20}$$

showing that the image space $\kappa_h(\mathcal{H}(\mathcal{V}_{n+1}))$ is a Lagrangian submanifold of $\mathcal{B}$. Under the further assumption $\det\|\partial^2 H/\partial p_i\partial p_j\|\neq 0$ Eqs. (3.19b) may be solved with respect to the variables p_i, in which case the second expression (3.19a) provides the representation of the Lagrangian section associated with h.

From a geometrical viewpoint, a significant implication of the previous discussion is the fact that, in the environment $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, the Lagrangian and Hamiltonian approaches to mechanics are nothing but different representations of the same $(2n+1)$-dimensional submanifold, described indifferently as $\mathcal{E}=j_1(l)(j_1(\mathcal{V}_{n+1}))=j_1(h)(\Pi(\mathcal{V}_{n+1}))$.

This aspect is further enhanced by observing that, according to Eqs. (3.11), (3.14), and (3.16), the embedding $\mathcal{E}\overset{i}{\to} j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ satisfies the identity

$$i^*(\Theta)=0, \tag{3.21}$$

showing that the hypersurface $\mathcal{E}$ is *horizontal* with respect to the canonical connection of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})\to\mathcal{B}$. Now, a straightforward argument indicates that *every* horizontal submanifold $i:\mathfrak{S}\to j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ has dimension $\leqslant 2n+1$. [Indeed, by Eq. (3.21), the projection $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})\overset{\pi}{\to}\mathcal{B}$ is locally injective on $\mathfrak{S}$, while Eq. (3.21) itself requires $i^*(d\Theta)=0$. Therefore, by the nonsingularity of the two-form (3.12) $\dim(\mathfrak{S})=\dim(\pi(\mathfrak{S}))\leqslant\frac{1}{2}\dim(\mathcal{B})=2n+1$.] Regular dynamical systems may therefore be viewed as *horizontal submanifolds of maximal dimension* in $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, projecting injectively onto both $j_1(\mathcal{V}_{n+1})$ and $\Pi(\mathcal{V}_{n+1})$.

The previous conclusion extends to the newer context the results originally established by Tulczyjew in the autonomous case[5–9] (in this connection see also Refs. 12, 13, and 10). The analogies are easily understood by observing that the projection $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})\overset{\pi}{\to}\mathcal{B}$ sets up a 1–1 correspondence between horizontal *slicings* of maximal dimension in $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ and Lagrangian submanifolds in $\mathcal{B}$. The details are straightforward, and are left to the reader. In coordinates, the previous assertions have their analytical counterpart in Eqs. (3.18) and (3.20).

ACKNOWLEDGMENT

Research partly supported by the National Group for Mathematical Physics (GNFM–INDAM).

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Asymptotic expansion of the quasiconfluent hypergeometric function

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(Received 28 November 2002; accepted 13 January 2003)

The asymptotic expansion of the hypergeometric function ${}_2F_1(a,b;c;z/b)$ in the case of quasiconfluence, i.e., for $|b|\to\infty$, is revised. A very simple expansion, in terms of a semiasymptotic sequence of polynomials, is presented. Some properties of those polynomials are discussed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1560551]

I. INTRODUCTION

In a series of recent papers,[1–3] Chidichimo and Thorsley have discussed several procedures for obtaining asymptotic expansions of the electric dipole (E1) differential excitation function in a treatment of the Coulomb excitation of positive ions by nuclei. As a complementary mathematical result, useful for their treatment of the physical problem, they have obtained the first three terms of an asymptotic expansion [Eq. (2.7) in Ref. 3] of the Gauss hypergeometric function, ${}_2F_1(a,b;c;z/b)$, in power series of $1/b$ with coefficients closely related to the confluent hypergeometric functions ${}_1F_1(a+k;c+k;z)$, k integer. That result is, in fact, a particularization of an expansion of the generalized hypergeometric function ${}_{p+1}F_q(a_1,\ldots,a_p,b;c_1,\ldots,c_q;z/b)$, in the case of quasiconfluence, i.e., $|b|$ large, in terms of generalized hypergeometric functions ${}_pF_q(a_1+k,\ldots,a_p+k;c_1+k,\ldots,c_q+k;z)$. Such expansion, whose first terms can be found in Sec. 3.5, Eq. (21), of a book by Luke,[4] reads (with a different but conventional notation)

$$
{}_{p+1}F_q\left(\begin{matrix}a_1,\ldots,a_p,b\\ c_1,\ldots,c_q\end{matrix}\middle|\,\frac{z}{b}\right)=A_0(z)+\frac{1}{b}\frac{1}{2}A_2(z)+\frac{1}{b^2}\left(\frac{1}{3}A_3(z)+\frac{1}{8}A_4(z)\right)
$$
$$
+\frac{1}{b^3}\left(\frac{1}{4}A_4(z)+\frac{1}{6}A_5(z)+\frac{1}{48}A_6(z)\right)
$$
$$
+\frac{1}{b^4}\left(\frac{1}{5}A_5(z)+\frac{13}{72}A_6(z)+\frac{1}{24}A_7(z)+\frac{1}{384}A_8(z)\right)+\cdots, \qquad (1)
$$

where it has been denoted

$$
A_k(z)=z^k\frac{d^k}{dz^k}\ {}_pF_q\left(\begin{matrix}a_1,\ldots,a_p\\ c_1,\ldots,c_q\end{matrix}\middle|\,z\right)\ =z^k\frac{(a_1)_k\ldots(a_p)_k}{(c_1)_k\ldots(c_q)_k}\ {}_pF_q\left(\begin{matrix}a_1+k,\ldots,a_p+k\\ c_1+k,\ldots,c_q+k\end{matrix}\middle|\,z\right). \qquad (2)
$$

The procedure followed in Refs. 3 and 4 to obtain the reported terms of the mentioned expansion consists in a judicious rearrangement of the series expansion of ${}_{p+1}F_q$. Obviously, the derivation of new terms of the expansion becomes more and more tedious. Here we suggest two alternative methods to complete the expansion (1). The first one makes use of the Barnes integral representation of the generalized hypergeometric functions and of an asymptotic expansion of the ratio of gamma functions. The second one, much more efficient, gives directly the result of grouping in (1) terms containing the same $A_k(z)$ and makes use only of the relation between the differential equations satisfied by ${}_{p+1}F_q$ and ${}_pF_q$.

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II. A PROCEDURE BASED ON INTEGRAL REPRESENTATIONS

The starting point is the Barnes integral representation of the generalized hypergeometric series,

$$ {}_{p+1}F_q\left(\begin{matrix} a_1,\ldots,a_p,b \\ c_1,\ldots,c_q \end{matrix}\middle| \frac{z}{b}\right)=\frac{\Pi_{j=1}^{q}\Gamma(c_j)}{2\pi i(\Pi_{j=1}^{p}\Gamma(a_j))\Gamma(b)}\int_{-i\infty}^{+i\infty}\frac{(\Pi_{j=1}^{p}\Gamma(a_j+s))\Gamma(b+s)\Gamma(-s)}{\Pi_{j=1}^{q}\Gamma(c_j+s)} \times\left(-\frac{z}{b}\right)^s \mathrm{d}s. \tag{3}$$

Here the integration path is such that it leaves all poles of $\Gamma(a_j+s)$, $\Gamma(b+s)$ and $\Gamma(c_j+s)$ to the left, and those of $\Gamma(-s)$ to the right. (See figures in Sec. 5.6 of Ref. 5 and in Sec. 8.6 of Ref. 6 illustrating the choice of the path in the particular case $p=q=1$.) Now, we can make use of a well-known asymptotic expansion [Eq. (3.31) of Ref. 5 and also Eq. (12) in Sec. 2.11 of Ref. 4] of the ratio of gamma functions

$$ \frac{\Gamma(b+\alpha)}{\Gamma(b+\beta)}\sim b^{\alpha-\beta}\sum_{k=0}^{\infty}\frac{(-)^k B_k^{(\alpha-\beta+1)}(\alpha)\,(\beta-\alpha)_k}{k!}b^{-k}, \tag{4}$$

where $B_k^{(\gamma)}(x)$ are the generalized Bernoulli polynomials,[4,5] defined by the generating formula

$$ \frac{t^\gamma e^{xt}}{(e^t-1)^\gamma}=\sum_{k=0}^{\infty}\frac{t^k}{k!}B_k^{(\gamma)}(x),\quad |t|<2\pi. \tag{5}$$

To our purposes, (4) can be reduced to

$$ \frac{\Gamma(b+s)}{\Gamma(b)\,b^s}\sim\sum_{k=0}^{\infty}\frac{(-)^k B_k^{(s+1)}(s)\,(-s)_k}{k!}b^{-k}. \tag{6}$$

The $B_k^{(s+1)}(s)$ turn out to be polynomials of degree k in the variable s. They satisfy the relation[4]

$$ (-)^k B_k^{(s+1)}(s)=\frac{s-k}{s}B_k^{(s)}, \tag{7}$$

the $B_k^{(s)}\equiv B_k^{(s)}(0)$ being obtained directly, by means of

$$ B_k^{(s)}=\frac{\mathrm{d}^k}{\mathrm{d}t^k}\left(\frac{t}{e^t-1}\right)^s\Bigg|_{t=0}, \tag{8}$$

or successively, through the recurrence relation

$$ B_0^{(s)}=1,\quad \frac{B_k^{(s)}}{k!}=-\frac{s}{k}\left(\frac{1}{2}\frac{B_{k-1}^{(s)}}{(k-1)!}+\sum_{j=2}^{k}\frac{B_j}{j!}\frac{B_{k-j}^{(s)}}{(k-j)!}\right). \tag{9}$$

Here, B_j are the Bernoulli numbers. (Notice that only even values of j are effective in the sum.) Obviously, the $B_k^{(s)}$ can be written as linear combination of the polynomials $(-s+k+1)_j$ in the form

$$ \frac{B_k^{(s)}}{k!}=s\sum_{l=1}^{k}(-)^{k+l-1}\alpha_{k,l}(-s+k+1)_{l-1},\quad k=1,2,\ldots. \tag{10}$$

Comparison of equal powers of s in the two sides of this equation would allow one to determine the coefficients $\alpha_{k,l}$. Nevertheless, we will see in Sec. IV that they can be more trivially obtained by using the recurrence

$$(k+l)\alpha_{k,l}=(k-1+l)\alpha_{k-1,l}+\alpha_{k-1,l-1}, \tag{11}$$

understanding that

$$\alpha_{0,0}=1, \quad \alpha_{k,0}=0 \quad \text{for } k>0, \tag{12}$$

$$\alpha_{k,l}=0 \quad \text{if } l>k. \tag{13}$$

For $l=1$ and for $l=k$ the recurrence (11) reduces to a two-term one and can be easily solved to give

$$\alpha_{k,1}=\frac{1}{k+1}, \quad \alpha_{k,k}=\frac{1}{2^k k!}, \quad k=1,2,\ldots. \tag{14}$$

Here is a table of the first coefficients:

$$\alpha_{0,0}=1,$$

$$\alpha_{1,1}=\tfrac{1}{2},$$

$$\alpha_{2,1}=\tfrac{1}{3}, \quad \alpha_{2,2}=\tfrac{1}{8},$$

$$\alpha_{3,1}=\tfrac{1}{4}, \quad \alpha_{3,2}=\tfrac{1}{6}, \quad \alpha_{3,3}=\tfrac{1}{48},$$

$$\alpha_{4,1}=\tfrac{1}{5}, \quad \alpha_{4,2}=\tfrac{13}{72}, \quad \alpha_{4,3}=\tfrac{1}{24}, \quad \alpha_{4,4}=\tfrac{1}{384},$$

$$\alpha_{5,1}=\tfrac{1}{6}, \quad \alpha_{5,2}=\tfrac{11}{60}, \quad \alpha_{5,3}=\tfrac{17}{288}, \quad \alpha_{5,4}=\tfrac{1}{144}, \quad \alpha_{5,5}=\tfrac{1}{3840}.$$

In view of (7) and (10), the asymptotic expansion (6) can be written in the form

$$\frac{\Gamma(b+s)}{\Gamma(b)\,b^s}\sim\sum_{k=0}^{\infty}\frac{1}{b^k}\sum_{l=1}^{k}(-)^{k+l}\alpha_{k,l}(-s)_{k+l}, \tag{15}$$

with the convention that, here and in what follows, the empty sum on the index l (for $k=0$) is to be replaced by the expression resulting by taking $l=0$ and $\alpha_{0,0}=1$. By substituting the expansion (15) in the right-hand side of (3) and interchanging sums and integration, one obtains the formal expansion

$${}_{p+1}F_q\left(\begin{matrix}a_1,\ldots,a_p,b\\ c_1,\ldots,c_q\end{matrix}\middle|\,\frac{z}{b}\right)\sim\sum_{k=0}^{\infty}\frac{1}{b^k}\sum_{l=1}^{k}(-)^{k+l}\alpha_{k,l}\frac{\Pi_{j=1}^{q}\Gamma(c_j)}{2\pi i\Pi_{j=1}^{p}\Gamma(a_j)}$$
$$\times\int_{-i\infty}^{+i\infty}\frac{(\Pi_{j=1}^{p}\Gamma(a_j+s))\Gamma(-s+k+l)}{\Pi_{j=1}^{q}\Gamma(c_j+s)}(-z)^s\,ds. \tag{16}$$

Replacement, in each integral, of the variable of integration s by $v=s-(k+l)$ leads to

$$ {}_{p+1}F_q\left(\begin{matrix}a_1,\ldots,a_p,b\\ c_1,\ldots,c_q\end{matrix}\middle|\frac{z}{b}\right)\sim\sum_{k=0}^{\infty}\frac{1}{b^k}\sum_{l=1}^{k}\alpha_{k,l}\frac{\Pi_{j=1}^{q}\Gamma(c_j)}{2\pi i\Pi_{j=1}^{p}\Gamma(a_j)}z^{k+l} $$

$$ \times\int_{-i\infty}^{+i\infty}\frac{(\Pi_{j=1}^{p}\Gamma(a_j+k+l+v))\Gamma(-v)}{\Pi_{j=1}^{q}\Gamma(c_j+k+l+v)}(-z)^v\,\mathrm{d}v. \tag{17} $$

Notice that the integration path in the complex v plane leaves the poles of $\Gamma(a_j+k+l+v)$ and $\Gamma(c_j+k+l+v)$ to the left and those of $\Gamma(-v)$ to the right. Recalling the Barnes integral representation of the generalized hypergeometric functions, already used in (3), and the notation (2), we obtain, finally, the expansion

$$ {}_{p+1}F_q\left(\begin{matrix}a_1,\ldots,a_p,b\\ c_1,\ldots,c_q\end{matrix}\middle|\frac{z}{b}\right)\sim A_0(z)+\sum_{k=1}^{\infty}\frac{1}{b^k}\sum_{l=1}^{k}\alpha_{k,l}A_{k+l}(z). \tag{18} $$

III. A SEMIASYMPTOTIC EXPANSION

Computational use of the expansion (18) would recommend to rearrange its terms in the form

$$ {}_{p+1}F_q\left(\begin{matrix}a_1,\ldots,a_p,b\\ c_1,\ldots,c_q\end{matrix}\middle|\frac{z}{b}\right)\sim\sum_{j=0}^{\infty}\mathcal{P}_j(1/b)\,A_j(z), \tag{19} $$

where the $\mathcal{P}_j(1/b)$ stand for the resulting polynomials in the variable $1/b$. Obviously,

$$ \mathcal{P}_0(1/b)=1,\quad \mathcal{P}_1(1/b)=0,\quad \mathcal{P}_j(1/b)=\sum_{k=[(j+1)/2]}^{j-1}\alpha_{k,j-k}\left(\frac{1}{b}\right)^k. \tag{20} $$

It is not difficult to find those polynomials without need of obtaining and rearranging the expansion (18). Since they do not depend on the numbers p and q of parameters, we can refer to the particular case $p=q=1$. Then, (19) becomes

$$ {}_2F_1\left(a,b;c;\frac{z}{b}\right)\sim\sum_{j=0}^{\infty}\mathcal{P}_j(1/b)\,A_j(z), \tag{21} $$

where now

$$ A_j(z)=z^j\frac{(a)_j}{(c)_j}\;{}_1F_1(a+j;c+j;z). \tag{22} $$

Since the expansion (21) must obey the hypergeometric equation

$$ \left(\left(\frac{z}{b}-\frac{z^2}{b^2}\right)\frac{\mathrm{d}^2}{\mathrm{d}\left(\frac{z}{b}\right)^2}+\left(c-(a+b+1)\frac{z}{b}\right)\frac{\mathrm{d}}{\mathrm{d}\left(\frac{z}{b}\right)}-ab\right)\;{}_2F_1\left(a,b;c;\frac{z}{b}\right)=0, \tag{23} $$

one has the condition

$$ \sum_{n=0}^{\infty}\mathcal{P}_n(1/b)\left(z(b-z)\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(bc-(a+b+1)z)\frac{\mathrm{d}}{\mathrm{d}z}-ab\right)A_n(z)=0, \tag{24} $$

to be satisfied by the polynomials $\mathcal{P}_n$. From the definition (22) and the relation [Eq. (13.4.9) of Ref. 7]

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k}\ {}_1F_1(a;c;z)=\frac{(a)_k}{(c)_k}\ {}_1F_1(a+k;c+k;z) \tag{25}$$

one obtains immediately

$$\frac{\mathrm{d}}{\mathrm{d}z}A_n(z)=z^{-1}(nA_n(z)+A_{n+1}(z)), \tag{26}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}A_n(z)=z^{-2}(n(n-1)A_n(z)+2nA_{n+1}(z)+A_{n+2}(z)). \tag{27}$$

Therefore, (24) can be written

$$\sum_{n=0}^{\infty}\mathcal{P}_n(1/b)\left(\left(\frac{b}{z}-1\right)(n(n-1)A_n(z)+2nA_{n+1}(z)+A_{n+2}(z))\right.$$
$$\left.+\left(\frac{bc}{z}-(a+b+1)\right)(nA_n(z)+A_{n+1}(z))-abA_n(z)\right)=0. \tag{28}$$

On the other hand, the confluent hypergeometric equation

$$\left(z\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c+n-z)\frac{\mathrm{d}}{\mathrm{d}z}-(a+n)\right)\ {}_1F_1(a+n;c+n;z)=0 \tag{29}$$

together with the relation

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k}\ {}_1F_1(a+n;c+n;z)=\frac{(c)_n}{(a)_n}z^{-n-k}A_{n+k}(z), \tag{30}$$

trivially deduced from (25), provides us with the recurrence relation

$$A_{n+2}(z)+(c+n-z)A_{n+1}(z)-(a+n)zA_n(z)=0, \tag{31}$$

which allows us to write the condition (28) in the form

$$\sum_{n=0}^{\infty}\mathcal{P}_n(1/b)(bn(a+n-1)A_{n-1}(z)-n(a+n-b)A_n(z)-(2n+a+1)A_{n+1}(z)-A_{n+2}(z))=0 \tag{32}$$

or, equivalently,

$$\sum_{n=0}^{\infty}A_n(z)((a+n)(b(n+1)\mathcal{P}_{n+1}(1/b)-n\mathcal{P}_n(1/b)-\mathcal{P}_{n-1}(1/b))$$
$$+(bn\mathcal{P}_n(1/b)-(n-1)\mathcal{P}_{n-1}(1/b)-\mathcal{P}_{n-2}(1/b)))=0, \tag{33}$$

which obviously is satisfied if the polynomials $\mathcal{P}_n(1/b)$ obey the three-term relation

$$bn\mathcal{P}_n(1/b)=(n-1)\mathcal{P}_{n-1}(1/b)+\mathcal{P}_{n-2}(1/b). \tag{34}$$

This condition and the starting value of $\mathcal{P}_0(1/b)$ allow one to obtain the polynomials very easily. The first ones are

$$\mathcal{P}_0\left(\frac{1}{b}\right)=1,$$

$$\mathcal{P}_1\left(\frac{1}{b}\right)=0,$$

$$\mathcal{P}_2\left(\frac{1}{b}\right)=\frac{1}{2}\frac{1}{b},$$

$$\mathcal{P}_3\left(\frac{1}{b}\right)=\frac{1}{3}\left(\frac{1}{b}\right)^2,$$

$$\mathcal{P}_4\left(\frac{1}{b}\right)=\frac{1}{8}\left(\frac{1}{b}\right)^2+\frac{1}{4}\left(\frac{1}{b}\right)^3,$$

$$\mathcal{P}_5\left(\frac{1}{b}\right)=\frac{1}{6}\left(\frac{1}{b}\right)^3+\frac{1}{5}\left(\frac{1}{b}\right)^4,$$

$$\mathcal{P}_6\left(\frac{1}{b}\right)=\frac{1}{48}\left(\frac{1}{b}\right)^3+\frac{13}{72}\left(\frac{1}{b}\right)^4+\frac{1}{6}\left(\frac{1}{b}\right)^5.$$

The sequence of polynomials $\{\mathcal{P}_n(t)\}$ does not constitute an asymptotic one for $t\to 0$, since

$$\mathcal{P}_{2k}(t)=O(\mathcal{P}_{2k-1}(t)), \quad \text{as } t\to 0.$$

However, we can say that it is a semiasymptotic sequence to refer to the fact that, for $t\to 0$,

$$\mathcal{P}_{n+1}(t)= \text{ either } O(\mathcal{P}_n(t)) \text{ or } o(\mathcal{P}_n(t))$$

whereas

$$\mathcal{P}_{n+2}(t)=o(\mathcal{P}_n(t)).$$

In this sense, the expansion (19) is a semiasymptotic one.

IV. SOME PROPERTIES OF THE POLYNOMIALS $\mathcal{P}_n(z)$

We have seen in Sec. III that the polynomials $\mathcal{P}_n(z)$, defined by

$$\mathcal{P}_0(z)=1, \quad \mathcal{P}_1(z)=0, \quad \mathcal{P}_n(z)=\sum_{k=[(n+1)/2]}^{n-1}\alpha_{k,n-k}\,z^k, \tag{35}$$

can be determined by means of the recurrence

$$n\mathcal{P}_n(z)=z((n-1)\mathcal{P}_{n-1}(z)+\mathcal{P}_{n-2}(z)). \tag{36}$$

This relation allows us to obtain a recurrence for the coefficients $\alpha_{k,l}$ entering in the expansion (18). By substituting in (36) the polynomials $\mathcal{P}$ by their definition (35) and comparing equal powers of z, one obtains

$$n\alpha_{k,n-k}=(n-1)\alpha_{k-1,n-k}+\alpha_{k-1,n-k-1}, \tag{37}$$

the recurrence anticipated in (11).

It is not difficult to find a generating function for the polynomials $\mathcal{P}$. Let us denote

$$\Phi(z,t)\equiv\sum_{n=0}^{\infty}\mathcal{P}_n(z)\,t^n. \tag{38}$$

By multiplying both sides of the recurrence (36) by t^{n-1} and summing for n from 1 to ∞, it becomes

$$\frac{\partial}{\partial t}\Phi(z,t)=zt\left(\frac{\partial}{\partial t}\Phi(z,t)+\Phi(z,t)\right), \tag{39}$$

which, solved, gives

$$\Phi(z,t)=(1-zt)^{-1/z}e^{-t}. \tag{40}$$

From (38), it is immediate to see that

$$\mathcal{P}_n(z)=\frac{1}{n!}\frac{\partial^n}{\partial t^n}((1-zt)^{-1/z}e^{-t})\bigg|_{t=0}, \tag{41}$$

or, equivalently,

$$\mathcal{P}_n(z)=\frac{1}{2\pi i}\int^{(0+)}(1-zt)^{-1/z}e^{-t}\frac{\mathrm{d}t}{t^{n+1}}, \tag{42}$$

the closed integration contour in the complex t plane leaving the point $1/z$ in the external region. The representation (41) leads to an explicit expression of the polynomials,

$$\mathcal{P}_n(z)=\frac{1}{n!}\sum_{j=0}^{n}(-1)^{n-j}\binom{n}{j}\left(\frac{1}{z}\right)_j z^j, \tag{43}$$

or, more concisely,

$$\mathcal{P}_n(z)=\frac{(-1)^n}{n!}\ {}_2F_0\left(-n,\frac{1}{z};;z\right), \tag{44}$$

understanding that

$${}_2F_0\left(-0,\frac{1}{z};;z\right)\equiv 1. \tag{45}$$

Nevertheless, the recurrence (36) is preferable for the computation of the $\mathcal{P}_n(z)$.

ACKNOWLEDGMENT

This work has been supported by Comisión Interministerial de Ciencia y Tecnología.

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Noncommutative phase and unitarization of $GL_{p,q}(2)$

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(Received 23 October 2002; accepted 21 November 2002)

In this article, imposing Hermitian conjugate relations on the two-parameter deformed quantum group $GL_{p,q}(2)$ is studied. This results in a noncommutative phase associated with the unitarization of the quantum group. After the achievement of the quantum group $U_{p,q}(2)$ with pq real via a noncommutative phase, the representation of the algebra is built by means of the action of the operators constituting the $U_{p,q}(2)$ matrix on states. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556552]

I. INTRODUCTION

The mathematical construction of a quantum group G_q pertaining to a given Lie group G is simply a deformation of a commutative Poisson–Hopf algebra defined over G. The structure of a deformation is not only a Hopf algebra but characteristically a noncommutative algebra as well. The notion of quantum groups in physics is widely known to be the generalization of the symmetry properties of both classical Lie groups and Lie algebras, where two different mathematical blocks, namely deformation and co-multiplication, are simultaneously imposed either on the related Lie group or on the related Lie algebra.

A quantum group is defined algebraically as a quasi-triangular Hopf algebra. It can be either noncommutative or commutative. It is fundamentally a bi-algebra with an antipode so as to consist of either the q-deformed universal enveloping algebra of the classical Lie algebra or its dual, called the matrix quantum group, which can be understood as the q-analog of a classical matrix group.[1] One needs four axioms, namely morphisms, in order to define a bi-algebraic structure: associativity, co-associativity, unit and co-unit. There is an additional structure, called the connecting axiom, which is needed to link the algebra to its dual one.

Although the applications of quantum groups mainly concentrate on the studies of quantum integrable models using the quantum inverse scattering method and noncommutative geometry, there have been many phenomenological applications of quantum algebras in nuclear physics, condensed matter physics, molecular physics, quantum optics and elementary particle physics. The most important and remarkable application arose from the q-deformation of the known quantum mechanical harmonic oscillator algebra. The algebraic approaches to the oscillator algebras involve the known creation, annihilation and number operators. It is worth emphasizing the importance of the algebra possessing Hermitian operators, giving rise to the ability of representing the physical observables. An algebra, therefore, needs to have a $*$ structure to be interpreted as an algebra of observables. The simplest matrix quantum group with such a structure is $SU_q(2)$.[2]

Let us now review the quantum group $GL_{p,q}(2)$ and then its unitary form $U_{q,\bar{q}}(\mathrm{gl}(2))$.[3] The representation matrix and the algebra of the two-parameter deformed quantum group $GL_{p,q}(2)$ are defined in the following way:[4,5]

$$A=\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{1}$$

$$ab=q^2ba, \quad ac=p^2ca, \quad bd=p^2db, \quad cd=q^2dc, \tag{2}$$

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$$ad-da=(q^2-p^{-2})bc, \quad bc=p^2q^{-2}cb.$$

The co-multiplication Δ, the co-unit ε, and the antipode (matrix inverse) S, whose bi-algebra is generated by the matrix elements a, b, c, and d, are given by

$$\Delta(A)=\begin{pmatrix} a\otimes a+b\otimes c & a\otimes b+b\otimes d \\ c\otimes a+d\otimes c & c\otimes b+d\otimes d \end{pmatrix}, \tag{3}$$

$$\varepsilon(A)=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4}$$

$$S(A)=\mathcal{D}^{-1}\begin{pmatrix} d & -p^{-2}b \\ -p^2c & a \end{pmatrix}=\begin{pmatrix} d & -q^{-2}b \\ -q^2c & a \end{pmatrix}\mathcal{D}^{-1}, \tag{5}$$

where the quantum determinant of A is defined by

$$\mathcal{D}\equiv \det_{p,q}A=ad-q^2bc=ad-p^2cb\,. \tag{6}$$

The co-product and the antipode of the quantum determinant are given by

$$\Delta(\mathcal{D})=\mathcal{D}\otimes\mathcal{D}, \tag{7}$$

$$S(\mathcal{D})=\mathcal{D}^{-1}. \tag{8}$$

A unitarized form of $\mathrm{GL}_{p,q}(2)$, named $\mathrm{U}_{\bar{q},q}(2)$, can be found in the work of Jagannathan and Van der Jeugt.[3] It is important to notice that our notation is different from the usual one as regards the usage of the deformation parameters p and q. The deformation parameters p and q should be replaced by $p^{1/2}$ and $q^{1/2}$ to obtain the usual convention in Ref. 3. The fundamental A-matrix of the quantum group is given by

$$A=\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} a & -\bar{q}^2\mathcal{D}c^* \\ c & \mathcal{D}a^* \end{pmatrix}=\begin{pmatrix} a & -q^2c^*\mathcal{D} \\ c & a^*\mathcal{D} \end{pmatrix}, \tag{9}$$

where the matrix elements satisfy

$$\begin{gathered} ac=\bar{q}^2ca, \quad a\mathcal{D}=\mathcal{D}a, \quad ac^*=q^2c^*a, \quad \mathcal{D}c^*=e^{4i\theta}c^*\mathcal{D}, \quad cc^*=c^*c\,, \\ \mathcal{D}^*\mathcal{D}=\mathcal{D}\mathcal{D}^*=1, \quad aa^*+|q|^4c^*c=1, \quad a^*a+c^*c=1\,. \end{gathered} \tag{10}$$

Here $q=|q|e^{i\theta}$, $p=\bar{q}$ and θ is a phase. The case $\mathcal{D}=1$ which also implies $\theta=0$ corresponds to $\mathrm{SU}_q(2)$.

In this article an algebra obtained by imposing $*$ relations on the operators a, b, c and d which are the matrix elements of the quantum group $\mathrm{GL}_{p,q}(2)$ will be considered. We are able to do this for pq real. In the limit $p=\bar{q}$, our algebra coincides with $\mathrm{U}_{q,\bar{q}}(2)$.[3] We thus name this algebra $\mathrm{U}_{p,q}(2)$. Representation of this algebra is constructed and the relationships of these representations to q-oscillators and to two-parameter coherent states are discussed.

II. THE UNITARIZATION OF THE QUANTUM GROUP $\mathrm{GL}_{p,q}(2)$ WITH $p\neq\bar{q}$

In order to obtain $\mathrm{SU}_q(2)$, elements of the fundamental A-matrix, $A\in\mathrm{GL}_q(2,\mathbb{C})$, are chosen in such a way that $A^*=A^{-1}$ and $\det_q(A)=1$. This choice brings about a restriction on the elements of the matrix such that $b=-qc^*$ and $d=a^*$. The procedure applied to the quantum group $\mathrm{GL}_{p,q}(2,\mathbb{C})$ to carry out the unitarization is similar to the one applied to the one-parameter deformed quantum group in order to transform $\mathrm{GL}_q(2,\mathbb{C})$ into $\mathrm{U}_q(2)$ but it is not completely the

same. The most important point of the procedure we have studied is that the matrix of the quantum group should be factorized into a product which consists of the square root of the quantum determinant and a new matrix whose determinant is unity:

$$\mathcal{D}=\delta^2\,, \tag{11}$$

$$A=\delta A_{\text{right}}\,. \tag{12}$$

The co-product and the antipode of δ are given by

$$\Delta(\delta)=\delta\otimes\delta\,, \tag{13}$$

$$S(\delta)=\delta^{-1}\,, \tag{14}$$

which are consistent with the equations (7) and (8). The next step is to impose the unitarity condition on the new matrix, resulting in finding the relation between the elements of this matrix as in the $\mathrm{U}_q(2)$ case. Therefore, the elements of the matrix A_{right} become the elements of $\mathrm{SU}_r(2)$ with $r\in\mathbb{R}$,

$$r=pq=\overline{pq}\,. \tag{15}$$

Lastly, the relations between the original matrix elements can be achieved through the relations between the new ones obtained after the unitarization of the matrix with the condition

$$\delta\delta^*=s^2\delta^*\delta\,, \tag{16}$$

where s is a central element of the resultant unitarized algebra of $\mathrm{GL}_{p,q}(2)$. It commutes with all elements in the algebra and is also Hermitian $s=s^*$. The co-product, co-unit and the antipode of the central element s are given by

$$\Delta(s)=s\otimes s\,, \tag{17}$$

$$\varepsilon(s)=1\,, \tag{18}$$

$$S(s)=s^{-1}\,. \tag{19}$$

This leads to the matrix elements b and d being respectively replaced by a combination of c^* and a^* multiplied by inverse of s and a unitary operator u. The new fundamental A-matrix of the unitary quantum group is given by

$$A=\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} a & -\overline{q}^2 s^{-1}uc^* \\ c & s^{-1}ua^* \end{pmatrix}\,. \tag{20}$$

It can be easily checked that with these relations a, c and b, d defined by (20) satisfy the commutation relations (2) of $\mathrm{GL}_{p,q}(2)$. The co-product, the co-unit and the antipode of the unitary operator u are given by

$$\Delta(u)=u\otimes u\,, \tag{21}$$

$$\varepsilon(u)=1\,, \tag{22}$$

$$S(u)=u^*\,. \tag{23}$$

The whole algebra of the unitarized two-parameter quantum group, which the matrix elements obey, is given by

$$
\begin{aligned}
&ac = p^2 ca, \quad a^* c^* = \bar{p}^{-2} c^* a^*, \\
&ac^* = q^2 s^2 c^* a, \quad a^* c = \bar{q}^{-2} s^{-2} c a^*, \\
&aa^* - s^2 a^* a = (1 - r^2) cc^*, \quad cc^* = \frac{q\bar{q}}{p\bar{p}} s^2 c^* c, \\
&ua = s^2 au, \quad u^* a^* = s^{-2} a^* u^*, \\
&ua^* = s^2 a^* u, \quad u^* a = s^{-2} a u^*, \\
&uc = \frac{p\bar{q}}{\bar{p}q} s^2 cu, \quad u^* c^* = \frac{p\bar{q}}{\bar{p}q} s^{-2} c^* u^*, \\
&uc^* = \frac{\bar{p}q}{p\bar{q}} s^2 c^* u, \quad u^* c = \frac{\bar{p}q}{p\bar{q}} s^{-2} c u^*, \\
&uu^* = u^* u = 1 .
\end{aligned}
\tag{24}
$$

It can be shown that the commutation relations (24) satisfy the co-product algebra homomorphism and the antipode algebra anti-homomorphism.

III. THE REPRESENTATION OF THE QUANTUM GROUP $U_{p,q}(2)$

The operators constituting an $SU_q(2)$ matrix which corresponds to $\mathcal{D}=1$, q real in (9) can be represented by their action on states $|n,m\rangle$ where n is non-negative integer corresponding to the particle number associated with the creation operator a^* and m is a positive or negative integer associated with the Fourier transform of c.[6] This serves two purposes. One is that it proves the algebra presented in the previous section is consistent. The second is that it gives physical insight on the oscillator properties of the operators. The action of the operators a, a^* and c, c^* of $SU_q(2)$ on the states $|n,m\rangle$ is given by

$$a|n,m\rangle = \sqrt{1-q^{2n}}\,|n-1,m\rangle\,, \tag{25}$$

$$a^*|n,m\rangle = \sqrt{1-q^{2n+2}}\,|n+1,m\rangle\,, \tag{26}$$

$$c|n,m\rangle = q^n|n,m-1\rangle\,, \tag{27}$$

$$c^*|n,m\rangle = q^n|n,m+1\rangle\,. \tag{28}$$

Here m is an integer and n is a non-negative integer. Motivated by this, we look for a representation of the algebra (24) on such states. The deformation parameters p and q are reparametrized in order to achieve a convenient form for the representation

$$p = \sqrt{\frac{r}{t}}\, e^{i\theta/2}, \quad q = \sqrt{rt}\, e^{-i\theta/2}, \tag{29}$$

where r, t and θ are real independent parameters. The parameters r and t are positive by definition and θ is a phase angle. The representation also depends on a real integer parameter k associated with the eigenvalue of the central element s. The special case where $t=1$, $\theta=0$, $k=0$, and therefore $p=q$, corresponds to the $SU_q(2)$ algebra for which it is necessary that $q \in (0,1)$ whereas the case $k=0$, $t=1$ corresponds to $U_{q,\bar{q}}(2)$ discussed in Sec. I. The operators c, c^*, a, a^*, u, u^* and s act on states

$$c|n,m\rangle = r^n (te^{-i\theta})^{m-1} |n,m-(k+1)\rangle\,, \tag{30}$$

$$c^*|n,m\rangle = r^n (te^{i\theta})^{m+k} |n,m+(k+1)\rangle\,, \tag{31}$$

$$a|n,m\rangle = \sqrt{1-r^{2n}}\,(te^{-i\theta})^m |n-1,m-k\rangle\,, \tag{32}$$

$$a^*|n,m\rangle = \sqrt{1-r^{2n+2}}\,(te^{i\theta})^{m+k} |n+1,m+k\rangle\,, \tag{33}$$

$$u|n,m\rangle = e^{i(k-2m)\theta} |n,m-2k\rangle\,, \tag{34}$$

$$u^*|n,m\rangle = e^{i(2m+3k)\theta} |n,m+2k\rangle\,, \tag{35}$$

$$s|n,m\rangle = t^k |n,m\rangle\,, \tag{36}$$

which explicitly shows that u is actually a noncommutative unitary phase operator. It can be easily seen that setting $t=1$, $\theta=0$, $k=0$ leads to $p=q$. The representation above then reduces to the representation (25)–(28) by the replacement of p and q by $p^{1/2}$ and $q^{1/2}$.

IV. CONCLUSION

The most interesting aspect of our construction is the appearance of the noncommutative phase described by the unitary operator u. The work of Ref. 6 was motivated by generalizing $\mathrm{SU}_q(2)$, resulting in introducing a parameter p and operator d satisfying

$$d|n,m\rangle = p^{1-m} |n,m-1\rangle\,. \tag{37}$$

The action of this operator has some resemblance to the action of the square root of the quantum determinant $\mathcal{D}$ which can be shown to be given by

$$\delta|n,m\rangle = (te^{-i\theta})^m |n,m-k\rangle\,. \tag{38}$$

Reference 6 claimed that the operator d can be interpreted as a deformation of a phase operator. The work of this article shows that a rigorous foundation for a noncommutative unitary phase operator lies in the two-parameter deformed quantum group.

Whether applications such as the quantum phase operator for a quantized boson can be incorporated into this formalism will be the subject of further research.

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The Balian–Low theorem for the symplectic form on $\mathbb{R}^{2d}$

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(Received 13 November 2002; accepted 7 January 2003)

In this paper we extend the Balian–Low theorem, which is a version of the uncertainty principle for Gabor (Weyl–Heisenberg) systems, to functions of several variables. In particular, we first prove the Balian–Low theorem for arbitrary quadratic forms. Then we generalize further and prove the Balian–Low theorem for differential operators associated with a symplectic basis for the symplectic form on $\mathbb{R}^{2d}$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1559415]

I. INTRODUCTION

For a given function $g \in L^2(\mathbb{R}^d)$ we define the following two unitary operators on $L^2(\mathbb{R}^d)$:

$$M_n(g)(x) = e^{2\pi i n \cdot x} g(x), \quad n \in \mathbb{R}^d$$

and

$$T_m(g)(x) = g(x-m), \quad m \in \mathbb{R}^d,$$

called *modulation* and *translation* operators, respectively. In 1946, Gabor[15] proposed to use these operators to define the collections of functions

$$g_{m,n}(x) = e^{2\pi i n \cdot x} g(x-m), \quad m, n \in \mathbb{Z},$$

to be used in the analysis of information conveyed by communications channels. These systems have been studied extensively in recent years. The edited books by Benedetto and Frazier[7] and by Feichtinger and Strohmer,[14] as well as Gröchenig's treatise,[17] provide detailed treatments of various issues of the theory. Gabor systems are especially interesting because of their effective role in the time-frequency analysis of a wide variety of signals.

Let us now introduce some terms and notation that will be used throughout this paper. We say that a collection $\{f_k : k = 1,\ldots\} \subset L^2(\mathbb{R}^d)$ of functions is a *frame* for $L^2(\mathbb{R}^d)$, with *frame bounds* A and B, if

$$\forall \quad f \in L^2(\mathbb{R}^d), \quad A\|f\|_2^2 \leqslant \sum_k |\langle f, f_k \rangle|^2 \leqslant B\|f\|_2^2.$$

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A frame is *tight* if $A=B$; and a frame is *exact* if it is no longer a frame after removal of any of its elements. For any frame $\{f_k:k=1,\ldots\}$ there exists a *dual frame* $\{\tilde{f}_k:k=1,\ldots\}$ such that

$$\forall \quad f\in L^2(\mathbb{R}^d), \quad f=\sum_k \langle f,f_k\rangle \tilde{f}_k=\sum_k \langle f,\tilde{f}_k\rangle f_k, \tag{1.1}$$

where the series converge in $L^2(\mathbb{R}^d)$. The choice of coefficients for expressing f in terms of $\{f_k:k=1,\ldots\}$ or $\{\tilde{f}_k:k=1,\ldots\}$ is not unique, unless the frame is a *basis. A frame is a basis if and only if it is exact*, e.g., Ref. 8.

For a frame $\{f_k:k=1,\ldots\}\subset L^2(\mathbb{R}^d)$ we define the associated *frame operator* S on $L^2(\mathbb{R}^d)$ by the rule,

$$\forall \quad f\in L^2(\mathbb{R}^d), \quad S(f)=\sum_k \langle f,f_k\rangle f_k.$$

S is a bounded and invertible map of $L^2(\mathbb{R}^d)$ onto itself. Given a frame $\{f_k:k=1,\ldots\}$, our canonical choice of the dual frame $\{\tilde{f}_k:k=1,\ldots\}$ will be defined by $\tilde{f}_k=S^{-1}(f_k)$. If a frame is exact then $\{f_k:k=1,\ldots\}$ and $\{\tilde{f}_k:k=1,\ldots\}$ are *biorthogonal*, that is,

$$\langle f_k,\tilde{f}_l\rangle=\delta_{k,l}, \quad k,l=1,\ldots,$$

where $\delta_{k,l}$ denotes the *Kronecker delta function*, i.e., it is 1 if $k=l$ and 0 otherwise. It is elementary to show that $S^{-1}(g_{m,n})=(S^{-1}(g))_{m,n}$ for Gabor frames $\{g_{m,n}\}$.

The *Fourier transform* is the unitary transformation $\mathcal{F}$ of $L^2(\mathbb{R}^d)$ onto itself, defined formally by

$$\hat{f}(\xi)=\mathcal{F}(f)(\xi)=\int_{\mathbb{R}^d} f(x)e^{2\pi i x\cdot\xi}\,dx.$$

We write $\mathbb{R}^d$ for arguments of a function $f\in L^2(\mathbb{R}^d)$ and $\hat{\mathbb{R}}^d$ for arguments of its Fourier transform.

We employ the standard notation in harmonic analysis, e.g., Ref. 28.

The following result is a version of the uncertainty principle for Gabor systems for the case $d=1$. It was first proved independently by Balian[3] and Low.[23] Both proofs contained a gap, which was corrected; and the result was generalized by Coifman, Daubechies, and Semmes from Gabor systems which form orthonormal bases to Gabor systems which form exact frames,[12] see also Refs. 6 and 8. A different proof of Theorem 1.1 was given by Battle.[4] Battle proved also an analogous result for wavelets.[5]

Theorem 1.1. Balian–Low theorem (BLT): *Let* $g\in L^2(\mathbb{R})$ *have the property that* $\{g_{m,n}: m,n\in\mathbb{Z}\}$ *is a Gabor orthonormal basis for* $L^2(\mathbb{R})$. *Then*

$$\left(\int_{\mathbb{R}}|g(x)|^2|x|^2\,dx\right)\left(\int_{\hat{\mathbb{R}}}|\hat{g}(\xi)|^2|\xi|^2\,d\xi\right)=\infty. \tag{1.2}$$

Remark: Our original goal in this paper was to obtain a generalization of Theorem 1.1 for functions of several variables. In the process, and after having obtained some of our main results, we became aware of the work of Gröchenig, Han, Heil, and Kutyniok,[18] in which the authors also extend the Balian–Low theorem to d-dimensions. Two of their fundamental results may be compared with our Theorem 2.1 and Theorem 2.5. In fact, Theorem 2.5 is identical with the BLT for nonlattices in Ref. 18 and Theorem 2.1 extends the weak BLT for lattices in Ref. 18 to more general position and momentum operators. Further, using techniques from the theory of metaplectic representations, the authors in Ref. 18 generalize Theorem 2.5 to a Balian–Low type theorem for exact frames on symplectic lattices; for their setting their assertion states that there exists $i\in\{1,\ldots,d\}$ such that (2.8) below holds.

We follow a different path and prove that the choice of coordinates in (2.8) is not canonical, i.e., there is no ''preference'' for the directional derivatives and for multiplications by the standard basis coordinates. This means that one can work in any representation of $\mathbb{R}^d$, e.g., Theorem 3.6.

In Sec. II we prove the generalization of the Balian–Low theorem to d-dimensions in the standard coordinate system; this is Theorem 2.1. As a corollary, we prove a Balian–Low theorem for arbitrary non-negative quadratic forms (Corollary 2.3). In Sec. III we state and prove our main results, Theorem 3.6 and Theorem 3.7, which assert a Balian–Low phenomenon (3.6) similar to but more far-reaching than (1.2). The proof depends on our definition of generalized Fourier transforms which, in turn, allows us to reduce a rather general and comprehensive problem to the Balian–Low theorem in the standard coordinates as formulated in Theorem 2.5.

Our approach is both straightforward and natural. This is an essential part of our contribution. It is also based on the quantum mechanical point of view.

II. BALIAN–LOW THEOREM IN STANDARD COORDINATES

Let $v,w\in\mathbb{R}^d$ be nonzero vectors. We define the following operators, wherever they make sense in $L^2(\mathbb{R}^d)$:

$$P_v(f)(x)=\left(\sum_{i=1}^{d} v^i x^i\right) f(x)$$

and

$$M_w(f)(x)=\mathcal{F}^{-1}\left(\left(\sum_{i=1}^{d} w^i \xi^i\right)\hat{f}(\xi)\right)(x)=\mathcal{F}^{-1}(P_w(\hat{f}))(x),$$

where $v=(v^1,\ldots,v^d)=\Sigma v^j u_j$, $u_j=(0,\ldots,0,1,0,\ldots,0)$ with 1 in the jth coordinate, and $v^j\in\mathbb{R}$. These unit vectors u_j define the *standard Euclidean basis* $\{u_j : j=1,\ldots,d\}$ of $\mathbb{R}^d$. If the vectors v and w in the definitions of P_v and M_w are elements of the standard basis, then we shall use the notation P_i and M_i for the operators induced by the ith basis vector u_i.

The following result is our first generalization of the Balian–Low theorem. The technique of proof is a well-known method for proving Balian–Low-type theorems. $\tilde{g}$ denotes the canonical dual defined in Sec. I.

Theorem 2.1: *Let* $\{g_{m,n} : m,n\in\mathbb{Z}^d\}$ *be an exact frame for* $L^2(\mathbb{R}^d)$. *If* $v, w\in\mathbb{R}^d$ *satisfy* $v\cdot w\neq 0$, *then*

$$\|P_v(g)\|_2\|M_w(g)\|_2\|P_v(\tilde{g})\|_2\|M_w(\tilde{g})\|_2=\infty. \tag{2.1}$$

Proof: We may assume without loss of generality that $|v|=|w|=1$, where $||$ denotes the Euclidean norm in $\mathbb{R}^d$. We shall proceed with a proof by contradiction; and so we assume that all four functions in (2.1) are elements of $L^2(\mathbb{R}^d)$. Because of the biorthogonality relations for g and $\tilde{g}$ we compute

$$\begin{aligned}\langle P_v(g),\tilde{g}_{m,n}\rangle&=\langle P_v(g),\tilde{g}_{m,n}\rangle-\left(\sum_{i=1}^{d} v^i m^i\right)\langle g,\tilde{g}_{m,n}\rangle\\&=\int_{\mathbb{R}^d}\left(\sum_{i=1}^{d} v^i(x^i-m^i)\right) g(x)\overline{\tilde{g}(x-m)}e^{-2\pi i n\cdot x}\,dx\\&=e^{-2\pi i m\cdot n}\int_{\mathbb{R}^d}\left(\sum_{i=1}^{d} v^i x^i\right)\overline{\tilde{g}(x)}g(x+m)e^{-2\pi i n\cdot x}\,dx\\&=e^{-2\pi i m\cdot n}\langle g_{-m,-n},P_v(\tilde{g})\rangle.\end{aligned} \tag{2.2}$$

From our assumption that $M_w(g) \in L^2(\mathbb{R}^d)$, it follows that the distributional partial derivative of g, $\partial_w g$, belongs to $L^2(\mathbb{R}^d)$. From a standard result about Sobolev spaces, see, e.g., Ref. 24, Theorem 1.1, there exists a function h such that $g=h$, a.e., and h is absolutely continuous on almost all straight lines parallel to the vector w. Thus the distributional directional derivative of g coincides with the classical directional derivative $D_w(g)$, a.e., and so

$$M_w(g)(x) = \frac{i}{2\pi} D_w(g)(x), \text{a.e.}$$

Moreover, our assumptions imply that $D_w(g)$, $D_w(\tilde{g}) \in L^2(\mathbb{R}^d)$. Therefore, using integration by parts, an appropriate change of variables, and the biorthogonality relations between g and $\tilde{g}$, we can compute

$$\begin{aligned}
\langle g_{m,n}, M_w(\tilde{g})\rangle &= \frac{1}{2\pi i}\int_{\mathbb{R}^d} g(x-m)e^{2\pi i n\cdot x}\overline{D_w(\tilde{g})(x)}\ dx \\
&= \frac{i}{2\pi}\int_{\mathbb{R}^d} D_w(g(x-m)e^{2\pi i n\cdot x})\overline{\tilde{g}(x)}\ dx \\
&= \frac{i}{2\pi}\int_{\mathbb{R}^d} (D_w(g)(x-m)e^{2\pi i n\cdot x} + (w\cdot n)g(x-m)e^{2\pi i n\cdot x})\overline{\tilde{g}(x)}\ dx \\
&= \frac{ie^{2\pi i m\cdot n}}{2\pi}\int_{\mathbb{R}^d} (D_w(g)(x) + 2\pi i(w\cdot n)g(x))e^{2\pi i n\cdot x}\overline{\tilde{g}(x+m)}\ dx \\
&= e^{2\pi i m\cdot n}(\langle M_w(g), \tilde{g}_{-m,-n}\rangle + (w\cdot n)\,\delta_{m,0}\delta_{n,0}) \\
&= e^{2\pi i m\cdot n}\langle M_w(g), \tilde{g}_{-m,-n}\rangle. \qquad (2.3)
\end{aligned}$$

Because of (2.2), (2.3), and the frame representation property (1.1), we have

$$\begin{aligned}
\langle P_v(g), M_w(\tilde{g})\rangle &= \sum_{m,n\in\mathbb{Z}^d} \langle P_v(g), \tilde{g}_{m,n}\rangle\langle g_{m,n}, M_w(\tilde{g})\rangle \\
&= \sum_{m,n\in\mathbb{Z}^d} \langle g_{-m,-n}, P_v(\tilde{g})\rangle\langle M_w(g), \tilde{g}_{-m,-n}\rangle \\
&= \sum_{m,n\in\mathbb{Z}^d} \langle M_w(g), \tilde{g}_{m,n}\rangle\langle g_{m,n}, P_v(\tilde{g})\rangle \\
&= \langle M_w(g), P_v(\tilde{g})\rangle. \qquad (2.4)
\end{aligned}$$

It is not difficult to verify that

$$[P_v, M_w] = \frac{1}{2\pi i}(v\cdot w)\ \ \mathrm{Id}, \qquad (2.5)$$

where the commutator $[P_v, M_w] = P_v M_w - M_w P_v$ and where Id denotes the identity operator, e.g., Ref. 25 where (2.5) appears for the position and momentum operators associated with the standard basis vectors; see also the trivial calculation in Ref. 8. Thus, for functions g, $\tilde{g} \in L^2(\mathbb{R}^d)$, such that $P_v(g)$, $P_v(\tilde{g}) \in L^2(\mathbb{R}^d)$ and $M_w(g)$, $M_w(\tilde{g}) \in L^2(\mathbb{R}^d)$, we have

$$\langle P_v(g), M_w(\tilde{g})\rangle = \langle M_w(g), P_v(\tilde{g})\rangle + \frac{1}{2\pi i}(v\cdot w)\langle g, \tilde{g}\rangle = \langle M_w(g), P_v(\tilde{g})\rangle + \frac{1}{2\pi i}(v\cdot w).$$

Since we have assumed that $v\cdot w \neq 0$, we obtain a contradiction with our calculation (2.4).■

Remark: The claim (2.1) is true if in Theorem 2.1 we consider the more general system $\{g_{m,n}:(m,n)\in\Lambda\}$, where Λ is an arbitraty lattice in $\mathbb{R}^{2d}$. For an analogous result for position and momentum operators associated with the integer lattice $\mathbb{Z}^{2d}$ see Theorem 8 in Ref. 18.

Corollary 2.2: Let $\{g_{m,n}:m,n\in\mathbb{Z}^d\}$ *be an exact frame for* $L^2(\mathbb{R}^d)$. *If* $v,w\in\mathbb{R}^d$ *satisfy* $v\cdot w\neq 0$, *then*

$$\|P_v(g)\|_2\|M_w(g)\|_2=\infty.$$

Proof: In view of Theorem 2.1, it is enough to show that $P_v(g)\in L^2(\mathbb{R}^d)$ if and only if $P_v(\tilde{g})\in L^2(\mathbb{R}^d)$, and that $M_w(g)\in L^2(\mathbb{R}^d)$ if and only if $M_w(\tilde{g})\in L^2(\mathbb{R}^d)$. This, in turn, was proved by Daubechies and Janssen[13] for the position and momentum operators associated with the standard basis vectors, see also Ref. 8, Theorem 7.7. The proof for arbitrary operators P_v and M_w is analogous, and it uses the d-dimensional Sobolev space argument which we have used in the proof of Theorem 2.1 instead of one-dimensional considerations. ■

Example: To show that the condition $v\cdot w\neq 0$ is necessary consider $L^2(\mathbb{R}^2)$ with the orthonormal Gabor basis generated by

$$g(x,y)=\chi_{[0,1]}(x)\quad\mathcal{F}^{-1}(\chi_{[0,1]})(y)$$

and the vectors $v=(1,0)$ and $w=(0,1)$. Then

$$\|P_v(g)\|_2^2=\int_{\mathbb{R}^2}|xg(x,y)|^2\,dx\,dy=\int_{\mathbb{R}}|x\chi_{[0,1]}(x)|^2\,dx\int_{\mathbb{R}}|\mathcal{F}^{-1}(\chi_{[0,1]})(y)|^2\,dy<\infty$$

and

$$\|M_w(g)\|_2^2=\int_{\mathbb{R}^2}|\eta\hat{g}(\xi,\eta)|^2\,d\xi\,d\eta=\int_{\mathbb{R}}|\mathcal{F}(\chi_{[0,1]})(\xi)|^2\,d\xi\int_{\mathbb{R}}|\eta(\chi_{[0,1]})(\eta)|^2\,d\eta<\infty.$$

Corollary 2.3: Let $\omega(x)$ *be any positive quadratic form on* $\mathbb{R}^d$ *and let* $\{g_{m,n}:m,n\in\mathbb{Z}^d\}$ *be an exact frame for* $L^2(\mathbb{R}^d)$. *Then*

$$\left(\int_{\mathbb{R}^d}\omega(x)|g(x)|^2\,dx\right)\left(\int_{\hat{\mathbb{R}}^d}\omega(\xi)|\hat{g}(\xi)|^2\,d\xi\right)=\infty.$$

Proof: Clearly, for any vector $v\neq 0$ we have $v\cdot v\neq 0$. Thus, from Corollary 2.2 it follows that for any $\alpha_k\geqslant 0$ and $v_k\in\mathbb{R}^d$, $k=1,\ldots,d$, where some $\alpha_k>0$, either

$$\left(\sum_{k=1}^{d}\alpha_k\int_{\mathbb{R}^d}\left(\sum_{i=1}^{d}v_k^i x^i\right)^2|g(x)|^2\,dx\right)=\infty$$

or

$$\left(\sum_{k=1}^{d}\alpha_k\int_{\hat{\mathbb{R}}^d}\left(\sum_{i=1}^{d}v_k^i\xi^i\right)^2|\hat{g}(\xi)|^2\,d\xi\right)=\infty.$$

The result follows since any quadratic form on $\mathbb{R}^d$ is of the form

$$\omega(x)=\sum_{k=1}^{d}\alpha_k\left(\sum_{i=1}^{d}v_k^i x^i\right)^2,$$

where the α_k's are non-negative. ■

We now consider a countable collection Λ of vectors in $\mathbb{R}^{2d}$. For any pair $(m,n)\in\Lambda$, $m,n\in\mathbb{R}^d$, we shall associate the *translation–modulation transformation* $T_{m,n}$ defined on $L^2(\mathbb{R}^d)$ as follows:

$$T_{m,n}(g)(x)=e^{2\pi in\cdot x}g(x+m).$$

From now on we shall write $g_{m,n}=T_{m,n}(g)$. The study of *nonuniform* Gabor systems, i.e., those Gabor systems which are associated with a set Λ which is not a lattice, has increased in recent years because of applications of such systems to problems in signal processing, e.g., Refs. 9, 10, 16, 21. Of course, not all Λ's generate orthonormal bases or even frames. In order for a Gabor system to have good signal representation properties, Λ must satisfy certain density conditions. The most general results so far in this direction were obtained by Ramanathan and Steger[26] and by Christensen, Deng, and Heil.[11]

Example: One easily constructs examples of uniform orthonormal Gabor bases for $L^2(\mathbb{R}^d)$. The most simple example is $g(x)=\chi_{[0,1]^d}$ with the lattice $\Lambda=\mathbb{Z}^{2d}$. More interestingly there is the work of Liu and Wang,[22] where the authors provide examples of nonuniform Gabor bases and frames, i.e., examples where Λ is not a lattice.

For $d=1$ let $\Omega=[0,1]\cup[3,4]$ and

$$\Lambda=\{6\mathbb{Z}+\{-1,0,1\}\}\times\{\tfrac{1}{2}\mathbb{Z}\}.$$

Then $g(x)=(1/\sqrt{2})\chi_\Omega(x)$ forms an orthonormal basis with translations and modulations in Λ. We would like to stress that although Λ is a periodic set it is not a lattice, since in general a sum of two vectors in Λ is not an element of Λ. We note that $\Lambda=-\Lambda$.

Reference 22 also provides an account of differences between nonuniform Gabor bases in one and higher dimensions.

To prove Theorem 2.5 we shall need the following lemma, the proof of which is similar to the proof of analogous statements in Theorem 2.1.

Lemma 2.4: Let $g\in L^2(\mathbb{R}^d)$, and let $\{g_{m,n}:(m,n)\in\Lambda\}$ be an orthonormal basis for $L^2(\mathbb{R}^d)$. If $P_i(g)$, $M_i(g)\in L^2(\mathbb{R}^d)$, then

$$\langle g_{m,n},P_i(g)\rangle=e^{2\pi im\cdot n}\langle P_i(g),g_{-m,-n}\rangle \tag{2.6}$$

and

$$\langle g_{m,n},M_i(g)\rangle=e^{2\pi im\cdot n}\langle M_i(g),g_{-m,-n}\rangle. \tag{2.7}$$

Proof: Since Λ does not posses a lattice structure we cannot use (2.2) and (2.3). Indeed, the fact that a dual to a Gabor frame is also a frame of Gabor type holds only for systems associated with lattices. However, the assumption that $\{g_{m,n}:(m,n)\in\Lambda\}$ is an orthonormal basis for $L^2(\mathbb{R}^d)$ compensates for this lack of structure in Λ,

$$\begin{aligned}\langle g_{m,n},P_i(g)\rangle&=\int_{\mathbb{R}^d}g(x-m)e^{2\pi in\cdot x}\overline{P_i(g)(x)}\;dx\\&=e^{2\pi im\cdot n}\int_{\mathbb{R}^d}g(x)e^{2\pi in\cdot x}\overline{(x_i+m_i)g(x+m)}\;dx\\&=e^{2\pi im\cdot n}(\langle P_i(g),g_{-m,-n}\rangle+m_i\langle g,g_{-m,-n}\rangle)\\&=e^{2\pi im\cdot n}\langle P_i(g),g_{-m,-n}\rangle.\end{aligned}$$

The last equality above follows from the orthogonality of $\{g_{m,n}:(m,n)\in\Lambda\}$. Similarly, using orthogonality and the integration by parts formula, we calculate

$$\begin{aligned}\langle g_{m,n}, M_i(g)\rangle &= -\frac{i}{2\pi}\int_{\mathbb{R}^d} g(x-m)e^{2\pi i n\cdot x}\overline{D_i(g)(x)}\ dx\\ &= \frac{i}{2\pi}\int_{\mathbb{R}^d} D_i(g(x-m)e^{2\pi i n\cdot x})\overline{g(x)}\ dx\\ &= \frac{ie^{2\pi i m\cdot n}}{2\pi}\int_{\mathbb{R}^d}(D_i(g)(x)+2\pi i m_i g(x))e^{2\pi i n\cdot x}\overline{g(x+m)}\ dx\\ &= e^{2\pi i m\cdot n}(\langle M_i(g), g_{-m,-n}\rangle + m_i\langle g, g_{-m,-n}\rangle)\\ &= e^{2\pi i m\cdot n}\langle M_i(g), g_{-m,-n}\rangle.\end{aligned}$$

■

Theorem 2.5: *Let $\Lambda\subset\mathbb{R}^{2d}$ be a countable sequence of vectors with the property that $\Lambda = -\Lambda$. Let $\{T_{m,n}:(m,n)\in\Lambda\}$ be the associated family of translation-modulation transformations, and assume $\{g_{m,n}:(m,n)\in\Lambda\}$ is an orthonormal basis for $L^2(\mathbb{R}^d)$ for some $g\in L^2(\mathbb{R}^d)$. For any $i=1,\ldots,d$,*

$$\|P_i(g)\|_2\|M_i(g)\|_2=\infty. \tag{2.8}$$

Proof: Because of (2.6) and (2.7), the representation property of bases, and the fact that $\Lambda = -\Lambda$, we obtain

$$\begin{aligned}\langle M_i(g), P_i(g)\rangle &= \sum_{(m,n)\in\Lambda}\langle M_i(g), g_{m,n}\rangle\langle g_{m,n}, P_i(g)\rangle\\ &= \sum_{(m,n)\in\Lambda}\langle g_{-m,-n}, M_i(g)\rangle\langle P_i(g), g_{-m,-n}\rangle\\ &= \langle P_i(g), M_i(g)\rangle.\end{aligned} \tag{2.9}$$

On the other hand, again using the classical result from Ref. 24 used in Theorem 2.1, we note that $M_i(g)\in L^2(\mathbb{R}^d)$ implies that $\partial g/\partial x^i$ exists a.e. Thus, integration by parts yields

$$\langle M_i(g), P_i(g)\rangle = \langle P_i(g), M_i(g)\rangle - \frac{1}{2\pi i},$$

which, in turn, leads to a contradiction with the calculation (2.9). ■

III. BALIAN–LOW THEOREM AND SYMPLECTIC FORMS

The standard *symplectic form* Ω on $\mathbb{R}^{2d}$ is defined as

$$\Omega((x,y),(\xi,\eta)) = x\cdot\eta - y\cdot\xi,$$

for any $x, y, \xi, \eta\in\mathbb{R}^d$. Note that $\Omega((x,0),(0,\xi)) = x\cdot\xi$. This observation, when compared to Theorem 2.1, suggests a direction which we are going to follow in this section, and which yields our main result, Theorem 3.6.

Definition: (a) A *symplectic basis* for $\mathbb{R}^{2d}$ with respect to the symplectic form Ω is a basis $\{a_j, b_j : j=1,\ldots,d\}\subset\mathbb{R}^{2d}$ for $\mathbb{R}^{2d}$ for which

$$\Omega(a_i, a_j) = \Omega(b_i, b_j) = 0$$

and

$$\Omega(a_i, b_j) = \delta_{i,j},$$

for all $i,j=1,\ldots,d$.

(b) If $\{\nu_i : i=1,\ldots,d\}\subset\mathbb{R}^d$ is any orthonormal basis for $\mathbb{R}^d$, then $a_i=(\nu_i,0)$, $b_i=(0,\nu_i)$, $i=1,\ldots,d$, is a symplectic basis for $\mathbb{R}^{2d}$. For a nontrivial example in $\mathbb{R}^4$ take the row vectors of the matrix

$$\begin{pmatrix} 1 & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{2} & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 1 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{6}}{2} & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}.$$

(c) Consider the space $\mathbb{R}^{2d}$ with coordinates $(x^1,\ldots,x^d,y^1,\ldots,y^d)$ and let Ω be the symplectic form on $\mathbb{R}^{2d}$. A *Lagrangian plane* Π in $\mathbb{R}^{2d}$ is a d-dimensional subspace with the property that

$$\Omega|_{\Pi}=0.$$

If Π is a Lagrangian plane in $\mathbb{R}^{2d}$ and if $v_1,\ldots,v_d\in\Pi\subset\mathbb{R}^{2d}$ is a basis for Π then, in particular, we have

$$\Omega(v_i,v_j)=0,$$

for all $i,j=1,\ldots,d$. For classical treatments of these and other related notions see, e.g., Refs. 1 and 2. A similar approach is used by Hörmander[20] to define Fourier integral operators, a special case of which we consider below. A recent exposition of related results in case of Hermitian symplectic geometry is due to Harmer.[19]

We now define the differential operators $\{Q_{v_j}, j=1,\ldots,d\}$ associated with a given basis $\{v_j : j=1,\ldots,d\}$ for a given Lagrangian plane Π. Each Q_{v_j} is defined by its action on a function h as follows:

$$Q_{v_j}(h)(x)=\frac{i}{2\pi}\nabla_j(h)(x)+f_j(x)h(x), \tag{3.1}$$

where

$$\nabla_j=\sum_{k=1}^{d} v_j^{k+d}\frac{\partial}{\partial x^k}$$

and

$$f_j(x)=\sum_{k=1}^{d} v_j^k x^k.$$

Recall that v_j^k is the kth coordinate of the vector $v_j\in\mathbb{R}^{2d}$ and that $x=\Sigma_{k=1}^{d}x^k u_k\in\mathbb{R}^d$.

The next result serves as the main motivation for our work. It is analogous to a similar observation about commutators of position and momentum operators that was asserted in Eq. (2.5). Its proof is also a straightforward calculation.

Proposition 3.1: For any two vectors $v,w\in\mathbb{R}^{2d}$

$$[Q_v, Q_w] = \frac{i}{2\pi}\Omega(v,w)\mathrm{Id},$$

where the commutator $[A,B]=AB-BA$.

For the purpose of the next definitions we shall make the following assumption: for given vectors $v_1,\ldots,v_d \in \mathbb{R}^{2d}$, define $B_v(j,k)=v_j^{k+d}$, $j,k=1,\ldots,d$, to be a $d\times d$ matrix, and assume that it is *nondegenerate*, i.e.,

$$\det B_v \neq 0.$$

As a consequence of Proposition 3.1 we observe that the Q_{v_j}'s commute with each other if the v_j's form a basis for Π. This commutativity implies, in particular, that $\nabla_k f_j = \nabla_j f_k$, and so we deduce that $f_j(x)=\nabla_j(xF_v x)$, for some quadratic form F_v. Thus the common eigenfunction for all the operators $\{Q_{v_j}\}$ has the form:

$$\psi_\xi(x) = \frac{1}{\sqrt{|\det B_v|}} e^{-2\pi i x^t B_v^{-1}\xi + 2\pi i x^t F_v x},$$

for any $\xi \in \mathbb{R}^d$. Moreover, let $A_v(j,k)=v_j^k$, $j,k=1,\ldots,d$. Then, the commutativity of the Q_{v_j}'s implies that

$$A_v B_v^t - B_v A_v^t = 0, \tag{3.2}$$

where A^t is the adjoint of A. It follows from (3.2) that $B_v^{-1}A_v$ is symmetric. It is also easy to see that

$$F_v = \tfrac{1}{2} B_v^{-1} A_v .$$

Let us now define the following *generalized Fourier transforms* $\mathcal{F}_v$ on the space of tempered distributions on $\mathbb{R}^d$, through their action on the space of Schwartz functions:

$$\mathcal{F}_v(h)(\xi) = \int_{\mathbb{R}^d} h(x)\overline{\psi_\xi(x)}\,dx = \int_{\mathbb{R}^d} h(x)\frac{1}{\sqrt{|\det B_v|}} e^{2\pi i x^t B_v^{-1}\xi - \pi i x^t B_v^{-1} A_v x}\,dx.$$

The operators $\mathcal{F}_v$ are unitary when restricted to $L^2(\mathbb{R}^d)$, since they are combinations of unitary transformations.

We shall now consider two different representations of functions or even distributions associated with two different Lagrangian planes: Π with the basis $v_1,\ldots,v_d$, and Γ with the basis $w_1,\ldots,w_d$. Assume that $\Pi\cap\Gamma=\{0\}$. Moreover, assume that B_v and B_w are nondegenerate. Define the $d\times d$ matrix $Y_{v,w}(i,j)=\Omega(v_i,w_j)$. Note that $Y_{v,w}=\mathrm{Id}$ if and only if $\{v_1,\ldots,v_d,w_1,\ldots,w_d\}$ forms a symplectic basis for $\mathbb{R}^{2d}$.

Lemma 3.2:

$$\det Y_{v,w} \neq 0.$$

Proof: Indeed, if $\Pi\cap\Gamma=\{0\}$, then $\{v_1,\ldots,v_d,w_1,\ldots,w_d\}$ forms a (not necessarily symplectic) basis for $\mathbb{R}^{2d}$. In this basis the matrix of Ω has the form

$$\begin{pmatrix} 0 & Y_{v,w} \\ -Y_{v,w} & 0 \end{pmatrix}$$

and so, $(\det Y_{v,w})^2 = \det\Omega \neq 0$. ∎

The matrix $Y_{v,w}$ can be represented, with the use of matrices A_v, A_w, B_v, B_w, as

$$Y_{v,w}=A_vB_w^t-B_vA_w^t.$$

As a consequence, we derive the following formula, which we shall use in the proof of Theorem 3.6:

$$F_v-F_w=\tfrac{1}{2}(B_v^{-1}A_v-B_w^{-1}A_w)=\tfrac{1}{2}B_v^{-1}Y_{v,w}(B_w^{-1})^t. \tag{3.3}$$

Lemma 3.3: For any tempered distribution h on $\mathbb{R}^d$, the relationship between its "v" and "w" generalized Fourier transform representations is

$$\mathcal{F}_w(h)(\eta)=\frac{1}{\sqrt{|\det Y_{v,w}|}}e^{-\pi i\eta^tY_{v,w}^{-1}B_vB_w^{-1}\eta+\pi i\sigma/4}\times\int_{\mathbb{R}^d}e^{\pi i\xi^t(Y_{v,w}^{-1})^t\eta+\pi i\eta^tY_{v,w}^{-1}\xi-\pi i\xi^t(B_v^{-1})^tB_w^tY_{v,w}^{-1}\xi}\mathcal{F}_v(h)(\xi)\ d\xi,$$

where σ is the difference between the positive and negative squares of the quadratic form F_v-F_w.

Proof: The expression in Lemma 3.3 is to be understood in the sense of distributions, and thus it is enough to check its validity on Schwartz functions. Note that the inverse of the generalized Fourier transform $\mathcal{F}_v$ has the form

$$h(x)=\frac{1}{\sqrt{|\det B_v|}}\int_{\mathbb{R}^d}e^{-2\pi ix^tB_v^{-1}\xi+2\pi ix^tF_vx}\mathcal{F}_v(h)(\xi)\ d\xi.$$

Taking the generalized Fourier transform $\mathcal{F}_w$ of this expression and using (3.3), we obtain

$$\begin{aligned}\mathcal{F}_w(h)(\eta)&=\frac{1}{\sqrt{|\det B_vB_w|}}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}e^{2\pi ix^t(B_w^{-1}\eta-B_v^{-1}\xi)+2\pi ix^t(F_v-F_w)x}\mathcal{F}_v(h)(\xi)\ dx\,d\xi\\&=\frac{e^{\pi i\sigma/4}}{\sqrt{|\det Y_{v,w}|}}\int_{\mathbb{R}^d}e^{-\pi i(B_w^{-1}\eta-B_v^{-1}\xi)^tB_w^tY_{v,w}^{-1}B_v(B_w^{-1}\eta-B_v^{-1}\xi)}\mathcal{F}_v(h)(\xi)\ d\xi\\&=\frac{1}{\sqrt{|\det Y_{v,w}|}}e^{\pi i\sigma/4-\pi i\eta^tY_{v,w}^{-1}B_vB_w^{-1}\eta}\\&\quad\times\int_{\mathbb{R}^d}e^{\pi i\xi^t(B_v^{-1})^tB_w^tY_{v,w}^{-1}B_vB_w^{-1}\eta+\pi i\eta^tY_{v,w}^{-1}\xi-\pi i\xi^t(B_v^{-1})^tB_w^tY_{v,w}^{-1}\xi}\mathcal{F}_v(h)(\xi)\ d\xi.\end{aligned}$$

In order to finish the proof, it is now enough to observe that

$$B_w^tY_{v,w}^{-1}B_v=B_v^t(Y_{v,w}^{-1})^tB_w,$$

due to (3.3), and that the above representation of $\mathcal{F}_w$ simplifies exactly to the formula in the statement of Lemma 3.3. ■

We shall now introduce two more representations of tempered distributions associated with a collection of vectors $\{v_1,\ldots,v_d,w_1,\ldots,w_d\}$:

$$\tilde{\mathcal{F}}_v(g)(\xi)=e^{-\pi i\xi^t(B_v^{-1})^tB_w^tY_{v,w}^{-1}\xi}\mathcal{F}_v(g)(\xi)$$

and

$$\tilde{\mathcal{F}}_w(g)(\eta)=e^{-\pi i\sigma/4}e^{-\pi i\eta^tY_{v,w}^{-1}B_vB_w^{-1}\eta}\mathcal{F}_w(g)(\eta).$$

Remark: In view of Steger's observation, these modifications of the generalized Fourier transforms may be compared to the metaplectic representations of symplectic transformations which send bases of Lagrangian planes into elements of the standard basis for $\mathbb{R}^{2d}$.

Proposition 3.4: If $\{v_1,\dots,v_d,w_1,\dots,w_d\}$ *forms a symplectic basis in* $\mathbb{R}^{2d}$, *i.e.*, $Y_{v,w}=\mathrm{Id}$, *then the relation between* $\widetilde{\mathcal{F}}_v$ *and* $\widetilde{\mathcal{F}}_w$ *takes the form of the standard Fourier transform:*

$$\widetilde{\mathcal{F}}_w(g)(\eta)=\int_{\mathbb{R}^d} e^{2\pi i\xi\cdot\eta}\widetilde{\mathcal{F}}_v(g)(\xi)\quad d\xi. \tag{3.4}$$

Proof: It follows easily from Lemma 3.3 that

$$\widetilde{\mathcal{F}}_w(g)(\eta)=\frac{1}{\sqrt{|\det Y_{v,w}|}}\int_{\mathbb{R}^d} e^{\pi i[\xi^t(Y_{v,w}^{-1})^t\eta+\eta^tY_{v,w}^{-1}\xi]}\widetilde{\mathcal{F}}_v(g)(\xi)\quad d\xi. \tag{3.5}$$

Since $\{v_1,\dots,v_d,w_1,\dots,w_d\}$ is a symplectic basis for $\mathbb{R}^{2d}$, we have $Y_{v,w}=\mathrm{Id}$, and so (3.5) reduces to (3.4). ∎

We can view (3.4) as a formal and general expression for the usual Fourier transform of distributions. We also note that $\widetilde{\mathcal{F}}_v$ and $\widetilde{\mathcal{F}}_w$ are unitary transformations when restricted to $L^2(\mathbb{R}^d)$.

It is evident that the operators $\mathcal{F}_v$ and $\mathcal{F}_w$ composed with operators Q_{v_j} and Q_{w_j}, respectively, become multiplications by jth coordinates. We use this fact to deduce the following lemma, which we shall use in the proof of our Theorem 3.6.

Lemma 3.5: For each $j=1,\dots,d$, *the operators* Q_{v_j} *are multiplications by* ξ_j *in the* $\widetilde{\mathcal{F}}_v$ *representation, and all operators* Q_{w_j} *are multiplications by* η_j *in the* $\widetilde{\mathcal{F}}_w$ *representation, i.e.*,

$$\widetilde{\mathcal{F}}_v(Q_{v_j}(g))(\xi)=\xi_j\widetilde{\mathcal{F}}_v(g)(\xi),$$

$$\widetilde{\mathcal{F}}_w(Q_{w_j}(g))(\eta)=\eta_j\widetilde{\mathcal{F}}_w(g)(\eta).$$

We can now formulate and prove our main results.

Theorem 3.6: *Let* $\Lambda\subset\mathbb{R}^{2d}$ *be a countable sequence of points with the property* $\Lambda=-\Lambda$. *Let* $\{T_{m,n}:(m,n)\in\Lambda\}$ *be the family of associated translation–modulation transformations* $T_{m,n}$. *For a function* $g\in L^2(\mathbb{R}^d)$, *assume that* $\{g_{m,n}=T_{m,n}(g):(m,n)\in\Lambda\}$ *forms an orthonormal basis for* $L^2(\mathbb{R}^d)$. *For any two vectors* $v,w\in\mathbb{R}^{2d}$ *for which the symplectic form is nonvanishing, i.e.*,

$$\Omega(v,w)\neq 0,$$

we have

$$\|Q_v(g)\|_2\|Q_w(g)\|_2=\infty. \tag{3.6}$$

Proof: (i) Without loss of generality we may assume that $\Omega(v,w)=1$. There exists a collection of vectors $\{v_2,\dots,v_d,w_2,\dots,w_d\}\subset\mathbb{R}^{2d}$ such that if we let $v_1=v$ and $w_1=w$, then $\{v_1,\dots,v_d,w_1,\dots,w_d\}$ forms a symplectic basis of $\mathbb{R}^{2d}$. (This result is a simple algebraic fact; for its Hermitian version see Ref. 19.) With these vectors we associate the corresponding differential operators $Q_{v_1},\dots,Q_{v_d}$, $Q_{w_1},\dots,Q_{w_d}$, and the induced $d\times d$ matrices A_v,A_w,B_v,B_w. For this part of the proof assume that

$$\det B_v\neq 0\quad\text{and}\quad\det B_w\neq 0.$$

Due to the assumption about the basis $\{v_1,\dots,v_d,w_1,\dots,w_d\}$, the matrix

$$\begin{pmatrix} A_v^t & B_v^t \\ A_w^t & B_w^t \end{pmatrix}$$

is symplectic, i.e.,

$$A_v B_v^t - B_v A_v^t = 0, \quad A_w B_w^t - B_w A_w^t = 0 \tag{3.7}$$

and

$$A_v B_w^t - B_v A_w^t = \mathrm{Id}, \quad A_w B_v^t - B_w A_v^t = -\mathrm{Id}. \tag{3.8}$$

Given a vector $(p,q) \in \mathbb{R}^{2d}$, we use translation by x and the symmetry of $B_v^{-1}A_v$ to calculate

$$\begin{aligned} \tilde{\mathcal{F}}_v(T_{p,q}(g))(\xi) &= \frac{1}{|\sqrt{\det B_v}|} e^{-\pi i \xi^t (B_v^{-1})^t B_w^t \xi} \int_{\mathbb{R}^d} g(x+p) e^{2\pi i x^t (B_v^{-1}\xi + q) - \pi i x^t B_v^{-1} A_v x}\, dx \\ &= c_{p,q} e^{-\pi i \xi^t (B_v^{-1})^t B_w^t \xi - 2\pi i p^t B_v^{-1} \xi} \mathcal{F}_v(g)(\xi + B_v q + A_v p), \end{aligned}$$

where $c_{p,q}$ is a complex constant of absolute value equal to 1. Recall that for a symplectic basis, $Y_{v,w} = \mathrm{Id}$. Because of this and the symmetry of $B_w B_v^{-1}$, which, in turn, follows from (3.3), we obtain

$$\tilde{\mathcal{F}}_v(T_{p,q}(g))(\xi) = c_{p,q} e^{2\pi i (-(B_v^{-1})^t p + B_w q + B_w B_v^{-1} A_v p)\cdot \xi} \tilde{\mathcal{F}}_v(g)(\xi + B_v q + A_v p).$$

Therefore we can write

$$\tilde{\mathcal{F}}_v(T_{p,q}(g))(\xi) = c_{p,q} T_{(p',q')}(\tilde{\mathcal{F}}_v(g))(\xi),$$

where

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \begin{pmatrix} A_v p + B_v q \\ -(B_v^{-1})^t p + B_w q + B_w B_v^{-1} A_v p \end{pmatrix}. \tag{3.9}$$

Equation (3.3) yields $A_w = -(B_v^{-1})^t + B_w (B_v^{-1} A_v)^t$. Thus, using the symmetry of $B_v^{-1}A_v$, we can write (3.9) in a more familar form

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \begin{pmatrix} A_v & B_v \\ A_w & B_w \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix}.$$

Overall, we obtain that in the $\tilde{\mathcal{F}}_v$ representation, a Gabor system remains a Gabor system, but associated with a new set Λ':

$$\tilde{\mathcal{F}}_v(T_{m,n}(g)) = c_{m',n'} (\tilde{\mathcal{F}}_v(g))_{m',n'},$$

where the primes indicate the elements of the new sequence. Since we know that $\tilde{\mathcal{F}}_v$ is unitary on $L^2(\mathbb{R}^d)$, if $\{g_{m,n} : (m,n) \in \Lambda\}$ is an orthonormal basis for $L^2(\mathbb{R}^d)$ then so is $\{c_{m',n'} (\tilde{\mathcal{F}}_v(g))_{m',n'} : (m',n') \in \Lambda'\}$, where $\Lambda' = -\Lambda'$. Thus, using Theorem 2.5 and invoking Proposition 3.4, we obtain that

$$\|\xi_1 \tilde{\mathcal{F}}_v(g)(\xi)\|_2 \| \eta_1 \tilde{\mathcal{F}}_w(g)(\eta)\|_2 = \infty. \tag{3.10}$$

Moreover, because of Lemma 3.5, we know that Q_{v_1} becomes multiplication by v_1 in the $\tilde{\mathcal{F}}_v$ representation, and similarly Q_{w_1} becomes multiplication by w_1 in the $\tilde{\mathcal{F}}_w$ representation, both in the sense of distributions. Thus (3.10) is equivalent to (3.6), since the generalized Fourier transforms are unitary on $L^2(\mathbb{R}^d)$ and because of Lemma 3.5.

(ii) First, let us observe that, since $\Omega(v,w)=1$, we cannot have both $(v^{1+d},\ldots,v^{2d})=0$ and $(w^{1+d},\ldots,w^{2d})=0$. Therefore, without loss of generality, we assume that $(v^{1+d},\ldots,v^{2d})\neq 0$.

Recall that according to (3.1) we write $Q_v=(i/2\pi)\nabla_v+f_v$. Thus we may always find a (nonunique) nondegenerate linear transformation of $\mathbb{R}^d$ such that the operator $(i/2\pi)\nabla_v$ becomes $(i/2\pi)(\partial/\partial\tilde{x}^1)$, in the new coordinates. The operator Q_v can be then written as

$$Q_v=\frac{i}{2\pi}\frac{\partial}{\partial\tilde{x}^1}+\tilde{a}_v^1\tilde{x}^1+\cdots+\tilde{a}_v^d\tilde{x}^d.$$

We also note that

$$\tilde{a}_v^1\tilde{x}^1+\cdots+\tilde{a}_v^d\tilde{x}^d=\frac{\partial}{\partial\tilde{x}^1}\left(\tilde{a}_v^1\frac{(\tilde{x}^1)^2}{2}+\tilde{a}_v^2\tilde{x}^1\tilde{x}^2+\cdots+\tilde{a}_v^d\tilde{x}^1\tilde{x}^d\right)=\frac{\partial}{\partial\tilde{x}^1}q(\tilde{x}).$$

We define a unitary transformation U of $L^2(\mathbb{R}^d)$ to be

$$U(g)(\tilde{x})=e^{-2\pi iq(\tilde{x})}g(\tilde{x}).$$

It is easy to verify that the operator Q_v takes the form $(i/2\pi)(\partial/\partial\tilde{x}^1)$ in this new representation, i.e.,

$$U(Q_v(g))(\tilde{x})=\frac{i}{2\pi}\frac{\partial}{\partial\tilde{x}^1}U(g)(\tilde{x}).$$

Also, the operator $U\circ Q_w\circ U^{-1}$ may be written in an analogous form

$$\tilde{b}_w^1\frac{i}{2\pi}\frac{\partial}{\partial\tilde{x}^1}+\cdots+\tilde{b}_w^d\frac{i}{2\pi}\frac{\partial}{\partial\tilde{x}^d}+\tilde{a}_w^1\tilde{x}^1+\cdots+\tilde{a}_w^d\tilde{x}^d.$$

We shall consider three different possibilities for the differential part of the operator $U\circ Q_w\circ U^{-1}$.

(iia) In case $\tilde{b}_w=(\tilde{b}_w^1,\ldots,\tilde{b}_w^d)=0$, $U\circ Q_w\circ U^{-1}$ has the form

$$\tilde{a}_w^1\tilde{x}^1+\cdots+\tilde{a}_w^d\tilde{x}^d.$$

Since $\Omega(v,w)=1$, we have $\tilde{a}_w^1=1$. We make the following nondegenerate linear transformation in $\mathbb{R}^d$:

$$z^1=\tilde{a}_w^1\tilde{x}^1+\cdots+\tilde{a}_w^d\tilde{x}^d,\quad z^2=\tilde{x}^2,\quad\ldots,\quad z^d=\tilde{x}^d. \tag{3.11}$$

Thus we obtain

$$U\circ Q_v\circ U^{-1}=\frac{i}{2\pi}\frac{\partial}{\partial z^1},\quad U\circ Q_w\circ U^{-1}=z^1,$$

and the problem reduces to the standard Balian–Low theorem, Theorem 2.1.

(iib) If $\tilde{b}_w=\alpha b_v=(\alpha,0,\ldots,0)$ and $\alpha\neq 0$ then, since we again have $\tilde{a}_w^1=1$, by making the same transformation (3.11) as in part (iia), we obtain

$$U\circ Q_v\circ U^{-1}=\frac{i}{2\pi}\frac{\partial}{\partial z^1},\quad U\circ Q_w\circ U^{-1}=\alpha\frac{i}{2\pi}\frac{\partial}{\partial z^1}+z^1.$$

It is again easy to see that our result follows from the standard Balian–Low theorem.

(iic) Finally we consider the case $\tilde{b}_w\neq\alpha b_v$ for all α. We can make a linear transformation in $\mathbb{R}^d$ such that $U\circ Q_v\circ U^{-1}$ remains the differentiation with respect to the first coordinate z^1, and the differential part of $U\circ Q_w\circ U^{-1}$ becomes the differentiation with respect to the second coordinate z^2, i.e.,

$$U\circ Q_v\circ U^{-1}=\frac{i}{2\pi}\frac{\partial}{\partial z^1},\quad U\circ Q_w\circ U^{-1}=\frac{i}{2\pi}\frac{\partial}{\partial z^2}+z^1+c_w^2z^2+\cdots+c_w^dz^d.$$

We now define the following two families of vectors in $\mathbb{R}^{2d}$:

$$v_1=(0,\ldots,0;1,0,\ldots,0),$$

$$v_2=(0,c_w^2,c_w^3,\ldots,c_w^d;0,1,0,\ldots,0),$$

$$v_3=(0,c_w^3,0,\ldots,0;0,0,1,0,\ldots,0),$$

$$\cdots,$$

$$v_d=(0,c_w^d,0,\ldots,0;0,\ldots,0,1),$$

and

$$w_1=(1,c_w^2,c_w^3,\ldots,c_w^d;0,1,0,\ldots,0),$$

$$w_2=(0,1,0,\ldots,0;1,0,\ldots,0),$$

$$w_3=(0,c_w^3,1,0,\ldots,0;0,0,1,0,\ldots,0),$$

$$\cdots,$$

$$w_d=(0,c_w^d,0,\ldots,0,1;0,\ldots,0,1),$$

and associated with them operators

$$Q_{v_1}=\frac{i}{2\pi}\frac{\partial}{\partial z^1},$$

$$Q_{v_2}=\frac{i}{2\pi}\frac{\partial}{\partial z^2}+c_w^2z^2+c_w^3z^3+\cdots+c_w^dz^d,$$

$$Q_{v_3}=\frac{i}{2\pi}\frac{\partial}{\partial z^3}+c_w^3z^2,$$

$$\cdots,$$

$$Q_{v_d}=\frac{i}{2\pi}\frac{\partial}{\partial z^3}+c_w^dz^2,$$

and

$$Q_{w_1}=\frac{i}{2\pi}\frac{\partial}{\partial z^2}+z^1+c_w^2z^2+c_w^3z^3+\cdots+c_w^dz^d,$$

$$Q_{w_2}=\frac{i}{2\pi}\frac{\partial}{\partial z^1}+z^2,$$

$$Q_{w_3}=\frac{i}{2\pi}\frac{\partial}{\partial z^3}+c_w^3z^2+z^3,$$

$$\cdots,$$

$$Q_{w_d}=\frac{i}{2\pi}\frac{\partial}{\partial z^d}+c_w^dz^2+z^d.$$

It is not difficult to verify that $\{v_1,\ldots,v_d;w_1,\ldots,w_d\}$ forms a symplectic basis in $\mathbb{R}^{2d}$ and that the matrices B_v and B_w are both nondegenerate. Thus we have reduced this situation to the case described in part (i). ■

Remark: We used the notion of a symplectic matrix in the proof of Theorem 3.6. A matrix M is *symplectic* if it preserves the symplectic form Ω, i.e., $\Omega(Mv,Mw)=\Omega(v,w)$, for all $v,w\in\mathbb{R}^{2d}$. The collection of all such matrices forms a group, the so-called *symplectic group*, which plays a significant role in the study of Hamiltonian systems. In fact, the symplectic matrices generate invertible transformations which take a Hamiltonian system into another such system of differential equations, see, e.g., Refs. 1, 2, and 27.

Following Ref. 18 we say that a lattice $\Lambda\subset\mathbb{R}^{2d}$ is *symplectic* if

$$\Lambda=rM(\mathbb{Z}^{2d})$$

for some $r\in\mathbb{R}\backslash\{0\}$ and M a symplectic matrix. A generalized Fourier transform $\widetilde{\mathcal{F}}_v$ maps a symplectic lattice Λ into another symplectic lattice Λ', according to the formula (3.9).

Theorem 3.7: *Let $\Lambda\subset\mathbb{R}^{2d}$ be a lattice. Let $\{T_{m,n}:(m,n)\in\Lambda\}$ be the family of associated translation–modulation transformations $T_{m,n}$. For a function $g\in L^2(\mathbb{R}^d)$, assume that $\{g_{m,n}=T_{m,n}(g):(m,n)\in\Lambda\}$ forms an exact frame for $L^2(\mathbb{R}^d)$ and let $\tilde{g}$ be the canonical dual to g. For any two vectors v, $w\in\mathbb{R}^{2d}$ for which the symplectic form is nonvanishing, i.e.,*

$$\Omega(v,w)\neq 0,$$

we have

$$\|Q_v(g)\|_2\|Q_w(g)\|_2\|Q_v(\tilde{g})\|_2\|Q_w(\tilde{g})\|_2=\infty. \tag{3.12}$$

Proof: The proof is analogous to the proof of Theorem 3.6. We start with the case where vectors $v=v_1,w=w_1$ allow an extension $\{v_1,\ldots,v_d,w_1,\ldots,w_d\}$ which forms a symplectic basis of $\mathbb{R}^{2d}$ and has nondegenerate associated matrices B_v and B_w. The generalized Fourier transforms $\widetilde{\mathcal{F}}_v$ and $\widetilde{\mathcal{F}}_w$ change the operators Q_v and Q_w into position and momentum operators, P_1 and M_1, in appropriate representations, respectively. Moreover, $\widetilde{\mathcal{F}}_v$ maps the lattice Λ into another lattice $\Lambda'\subset\mathbb{R}^{2d}$. Since generalized Fourier transforms are unitary in $L^2(\mathbb{R}^d)$, we finish by using, instead of Theorem 2.5, a version of Theorem 2.1 for general lattices, see the remark after the proof of Theorem 2.1.

The general case is reduced to the above situation analogously to the general case in Theorem 3.6. ■

ACKNOWLEDGMENTS

The second named author (W.C.) presented this work at the Analysis and Probability Related to Solvable Lie Groups conference in Zakopane in June 2002. Afterwards it was brought to our attention by Professor Tim Steger that Theorem 3.6 can also be proved using the theory of metaplectic representations. We gratefully acknowledge Professor Steger for his comments. We also gratefully acknowledge Professor Raymond Johnson for making us aware of the connection between the work of Hörmander and our results. The first named author (J.J.B.) was partially supported by NSF–DMS Grant No. 0139759 (2002–2005) and the General Research Board of the University of Maryland.

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First integrals of a generalized Darboux–Halphen system

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(Received 14 November 2002; accepted 20 December 2002)

A third-order system of nonlinear, ordinary differential equations depending on three arbitrary parameters is analyzed. The system arises in the study of SU(2)-invariant hypercomplex manifolds and is a dimensional reduction of the self-dual Yang–Mills equation. The general solution, first integrals, and the Nambu–Poisson structure of the system are explicitly derived. It is shown that the first integrals are multi-valued on the phase space even though the general solution of the system is single-valued for special choices of parameters. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1556194]

I. INTRODUCTION

The study of integrable or solvable nonlinear systems dates back to the fundamental works of Euler, Liouville, Riemann, Poincaré, and many others. Surprisingly (perhaps), there is still no single adequate definition of ''integrability.'' Certainly, nonlinear systems which can be explicitly solved by quadratures in the real domain should be considered as integrable, as should the Hamiltonian systems with action-angle variables (integrability in the Liouville sense). In contrast, the notion of integrability in the complex plane is still in its early stages of development. For example, if the general solution of a nonlinear ordinary differential equation is everywhere single-valued in its domain of existence, then we consider the equation to be integrable in the complex plane. Fundamental contributions of Kovalevskaya,[17] Painlevé,[24] and more recent work[27,28] have led to some progress toward the understanding of complex integrability (or nonintegrability). But the complex behavior of large classes of physically important nonlinear equations still remains to be completely understood. Some of these equations can be ''solved'' in terms of linear equations but are not single-valued in the complex plane.

In this article we consider the system of nonlinear ordinary differential equations

$$\dot{M} = (\text{adj } M)^T + M^T M - (\text{Tr } M) M, \tag{1}$$

for a 3×3 matrix valued function $M(t)$ where adj M is the adjoint matrix of M satisfying $(\text{adj } M)M = (\det M)I$, M^T is the transpose of M and the dot denotes differentiation with respect to t. The system (1) was obtained as a dimensional reduction of the self-dual Yang–Mills (SDYM) equations corresponding to an infinite-dimensional gauge group of diffeomorphisms Diff(S^3) of a three-sphere.[7] These equations were also derived in Ref. 16 where they were shown to represent an SU(2) invariant hypercomplex four-manifold. Since the Weyl curvature of a hypercomplex four-manifold is self-dual, Eq. (1) describes a class of self-dual Weyl Bianchi IX space–times with Euclidean signature.[6]

In the next section we will review the fact that Eq. (1) reduces to the system

$$\dot{\omega}_1 = \omega_2\omega_3 - \omega_1(\omega_2 + \omega_3) + \tau^2,$$

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$$\begin{aligned}\dot{\omega}_2 &= \omega_3\omega_1 - \omega_2(\omega_3+\omega_1) + \tau^2,\\ \dot{\omega}_3 &= \omega_1\omega_2 - \omega_3(\omega_1+\omega_2) + \tau^2,\\ \tau^2 &= \alpha_1^2(\omega_1-\omega_2)(\omega_3-\omega_1) + \alpha_2^2(\omega_2-\omega_3)(\omega_1-\omega_2) + \alpha_3^2(\omega_3-\omega_1)(\omega_2-\omega_3),\end{aligned} \tag{2}$$

for the functions $\omega_i(t)$, $i=1,2,3$, and where α_1, α_2, and α_3 are constants. We will refer to system (2) as the generalized Darboux–Halphen (DH) system, which will be the subject of our discussion for the remainder of this article. Equation (2) with $\tau\equiv 0$, becomes the classical DH system which first appeared in Darboux's work on triply orthogonal surfaces[8] and was later solved by Halphen.[15] In subsequent studies, the classical DH system has arisen as the vacuum Einstein equations for hyperkähler Bianchi-IX metrics[11,5] and in the similarity reductions of associativity equations on a three-dimensional Frobenius manifold.[9] Halphen showed that the general system (2) can be solved in terms of hypergeometric functions.[14] Special solutions have also been given in terms of theta functions and automorphic forms.[7,23,1] Special cases of Eq. (2) arise in the study of solvable models of spherically symmetric shear-free fluids in general relativity[13] as well.

As mentioned earlier, it was shown in Ref. 7 that Eq. (1) arises as a reduction of the SDYM equations. From the Lax pair for SDYM, it is possible to derive a linear problem (see, e.g., Ref. 2) which can be employed to solve the initial value problem for Eq. (1). This linear problem is related to the monodromy preserving deformations corresponding to the Riccati reduction of the Painlevé VI equation. Analysis of Eq. (1) using the associated linear problem was given in Refs. 6 and 16.

In Sec. II we outline the reduction of Eq. (1) to the generalized DH system (2) and derive its general solution. In Sec. III we discuss the first integrals and a set of ''action-angle'' variables for the DH system in terms of hypergeometric functions. We then analyze the behavior of the first integrals as functions of the dependent variables. In particular we find that the first integrals are transcendental and nonmeromorphic even though in certain cases, the general solution is single-valued in the complex t-plane. Indeed, the nonexistence of meromorphic first integrals for the classical DH equations was proved in Ref. 19. Finally, in Sec. IV we consider the dynamics of the DH system as a Nambu–Poisson flow in a three-dimensional manifold and investigate the algebraic properties of the underlying Nambu–Poisson structures.

II. SOLUTION OF THE DH SYSTEM

In this section we outline the procedure of constructing the general solution of Eq. (1) following the method discussed in Ref. 3. The matrix M in Eq. (1) is a complex-valued function of the (complex) independent variable t. In this article, we study the case where the symmetric part M_s of M has *distinct* eigenvalues. The degenerate cases corresponding to eigenvalues with higher multiplicities have been studied in Ref. 3.

The matrix M is first decomposed into symmetric and skew-symmetric parts and then the symmetric part M_s is diagonalized by a complex orthogonal matrix. (This is possible because of our assumption that the eigenvalues of M_s are distinct.) Thus we have

$$M = M_s + M_a = P(d+a)P^{-1},$$

$P\in \mathrm{SO}(3,\mathbf{C})$, $d := \mathrm{diag}(\omega_1,\omega_2,\omega_3)$ where the ω_i, $i=1,2,3$, are distinct, and the elements of the skew-symmetric matrix a are denoted as $a_{12}:=\tau_3$, $a_{23}:=\tau_1$, and $a_{31}:=\tau_2$. Using the above factorization of M, Eq. (1) can be transformed into Eq. (2) with $\tau^2:=\tau_1^2+\tau_2^2+\tau_3^2$, together with the linear equation: $\dot{P}=-Pa$ for the matrix P. The equations for the skew-symmetric part,

$$\dot{\tau}_1 = -\tau_1(\omega_2+\omega_3), \quad \dot{\tau}_2 = -\tau_2(\omega_3+\omega_1), \quad \dot{\tau}_3 = -\tau_3(\omega_1+\omega_2),$$

can be integrated to obtain

$$\tau_1^2=\alpha_1^2(\omega_1-\omega_2)(\omega_3-\omega_1),\quad \tau_2^2=\alpha_2^2(\omega_2-\omega_3)(\omega_1-\omega_2),\quad \tau_3^2=\alpha_3^2(\omega_3-\omega_1)(\omega_2-\omega_3),$$

where α_1, α_2, and α_3 are arbitrary constants. This defines τ^2 in terms of the ω_i in Eq. (2). Once a solution of the DH system (2) has been found, the matrix M can be reconstructed after solving the linear equation ($\dot{P}=-Pa$) for P.

In order to solve Eq. (2), we set

$$\omega_1=-\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s(s-1)},\quad \omega_2=-\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s-1},\quad \omega_3=-\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s}, \tag{3}$$

where the function $s(t)$ is given by the cross-ratio

$$s=\frac{\omega_1-\omega_3}{\omega_2-\omega_3}, \tag{4}$$

$\omega_i\neq\omega_j$ when $i\neq j$. Then it follows from Eq. (2) that $s(t)$ satisfies the Schwarzian equation

$$\frac{d}{dt}\left(\frac{\ddot{s}}{\dot{s}}\right)-\frac{1}{2}\left(\frac{\ddot{s}}{\dot{s}}\right)^2+\frac{\dot{s}^2}{2}V(s)=0, \tag{5}$$

with

$$V(s)=\frac{1-\alpha_2^2}{s^2}+\frac{1-\alpha_3^2}{(s-1)^2}+\frac{\alpha_2^2+\alpha_3^2-\alpha_1^2-1}{s(s-1)}.$$

The solution $s(t)$ of Eq. (5) is obtained implicitly by setting

$$t(s)=\frac{u_1(s)}{u_2(s)}, \tag{6}$$

where $u_1(s)$ and $u_2(s)$ are two independent solutions of the Fuchsian differential equation

$$\frac{d^2u}{ds^2}+\frac{1}{4}V(s)u=0 \tag{7}$$

with three regular singular points at 0, 1, and ∞. The transformation

$$u(s)=s^{c/2}(1-s)^{(a+b-c+1)/2}\chi(s) \tag{8}$$

maps Eq. (7) to the Gauss hypergeometric equation

$$s(1-s)\frac{d^2\chi}{ds^2}+[c-(a+b+1)s]\frac{d\chi}{ds}-ab\chi=0, \tag{9}$$

where $a=(1+\alpha_1-\alpha_2-\alpha_3)/2$, $b=(1-\alpha_1-\alpha_2-\alpha_3)/2$, and $c=1-\alpha_2$. Thus we have the following.

Proposition 1: The general solution of the DH system (2) is given by Eq. (3) where the function $s(t)$ is defined by the inverse of the ratio $t(s)=\chi_1(s)/\chi_2(s)$ of two linearly independent solutions of the hypergeometric equation (9).

Equation (6) describes the conformal mapping of the upper (or lower) half s-plane onto the interior of a triangular region T bounded by three circular arcs in the complex t-plane (see, e.g., Ref. 22). When the parameters α_1, α_2, α_3 are non-negative real numbers satisfying $\alpha_1+\alpha_2+\alpha_3<1$, the circular arcs of T form angles $\pi\alpha_1$, $\pi\alpha_2$, $\pi\alpha_3$ at the vertices which are the images of the singular points $s=0$, $s=1$, and $s=\infty$ of Eq. (7). The inverse map $s(t)$, which solves Eq. (5),

is analytic in the interior of T and can be analytically extended by inversions across its boundary. If the parameters assume the values $\alpha_1=1/p_1$, $\alpha_2=1/p_2$, $\alpha_3=1/p_3$, where p_1, p_2, p_3 are positive integers or ∞, then $s(t)$ can be extended to a single-valued, meromorphic function in a region D which is the uniform covering of an infinite number of nonoverlapping circular triangles obtained by inversions across the boundaries of T and its images. The boundary ∂D of D contains a dense set of essential singularities and forms a movable natural boundary. However, for general values of the parameters α_1, α_2, α_3 the function $s(t)$ is densely branched about the movable singularities at the vertices of T. The solutions $\omega_i(t)$ to the DH system given by Eq. (3) inherit the same singularity structure as $s(t)$ and are also branched in the complex t-plane for generic choices of α_1, α_2, α_3.

III. FIRST INTEGRALS AND ACTION-ANGLE VARIABLES

In the previous section we outlined a mechanism for expressing the general solution of the DH system via the solutions of a second-order, linear equation (7). This linearization scheme given by Eqs. (3)–(7) is implicit since the Schwarzian function $s(t)$ is the inverse of the ratio of the solutions of the linear equation. The first integrals of the DH system are determined by the arbitrary constants parametrizing the space of general solutions for the linear equation (7). However, these integrals do not have a simple dependence on the DH variables ω_i due to the implicit nature of the linearization process. In this section, we will discuss the properties of the first integrals as functions of the DH variables.

Let u_1 and u_2 be any two linearly independent solutions of Eq. (7) with Wronskian $W(u_1,u_2)=u_1u_2'-u_2u_1'=1$, where prime denotes differentiation with respect to s. The general solution of the Schwarzian equation (5) is given implicitly by [cf. Eq. (6)]

$$t(s)=\frac{J_2u_1(s)-J_1u_2(s)}{I_2u_1(s)-I_1u_2(s)}, \tag{10}$$

where I_α and J_α, $\alpha=1,2$, are constants satisfying $I_1J_2-I_2J_1\neq 0$. Only three of the four constants can be chosen independently because it is evident from Eq. (10) that only their ratios are related to $s(t)$ and its first two t-derivatives. Therefore, without loss of generality we take them to satisfy $I_1J_2-I_2J_1=1$. Differentiating Eq. (10) twice with respect to s we obtain two linear equations for I_1 and I_2:

$$I_2u_1-I_1u_2=\dot{s}^{1/2}, \quad I_2u_1'-I_1u_2'=\tfrac{1}{2}\dot{s}^{-3/2}\ddot{s},$$

whose solutions are

$$I_\alpha=\frac{d\phi_\alpha}{dt}, \quad \phi_\alpha=\dot{s}^{-1/2}u_\alpha(s), \quad \alpha=1,2. \tag{11}$$

The remaining two constants are then obtained from Eqs. (10) and (11) and the normalization $I_1J_2-I_2J_1=1$. They are given by

$$J_\alpha=tI_\alpha-\phi_\alpha, \quad \alpha=1,2.$$

Viewed as functions of t, s, $\dot{s}$ and $\ddot{s}$, the I_α and J_α are first integrals for the Schwarzian equation. This fact can be verified directly by differentiating the expressions for I_α and J_α with respect to t, and using Eq. (5). Moreover, by solving the functions s, $\dot{s}$ and $\ddot{s}$ from Eqs. (3) and (4), the I_α and J_α can be expressed in terms of the DH variables ω_i and t. Hence, they are also integrals of motion for the DH system. The explicit expressions for ϕ_α and I_α in terms of the DH variables are as follows:

$$\phi_\alpha = \sqrt{2r(\omega_i)}u_\alpha(s(\omega_i)), \quad I_\alpha = \sqrt{\frac{2}{r(\omega_i)}}u'_\alpha(s(\omega_i)) - (\omega_1-\omega_2-\omega_3)\sqrt{\frac{r(\omega_i)}{2}}u_\alpha(s(\omega_i)), \tag{12}$$

where $r(\omega_i)=\sqrt{(\omega_2-\omega_3)/(\omega_1-\omega_2)(\omega_1-\omega_3)}$ and $s(\omega_i)$ is given by Eq. (4). Equation (12) [equivalently, Eq. (11)] represents a nonalgebraic, transcendental transformation defined via the solution u_α of the Fuchsian equation (7), between the ω_i (or s, $\dot{s}$, $\ddot{s}$) and the variables $\{\phi_\alpha, I_\alpha\}$. In terms of these new variables, the nonlinear DH system (2) can be reformulated as a linear Hamiltonian system [cf. Eq. (11)]

$$\dot{\phi}_\alpha = \frac{\partial H}{\partial I_\alpha} = I_\alpha, \quad \dot{I}_\alpha = -\frac{\partial H}{\partial \phi_\alpha} = 0, \quad H = \frac{I_1^2+I_2^2}{2}, \quad \alpha = 1,2, \tag{13}$$

together with the algebraic constraint

$$\phi_1 I_2 - \phi_2 I_1 = W(u_1,u_2) = 1 \tag{14}$$

among the coordinates ϕ_α and the canonically conjugate "momenta" I_α. Since the latter system (13) can be integrated by quadratures, the canonical coordinates $\{I_\alpha, \phi_\alpha\}$ can be regarded as playing the role of the action-angle variables for the DH system. The dynamics in the four-dimensional phase space is restricted to the constraint subspace defined by Eq. (14). This represents an indefinite quadric which is a connected but noncompact, three-dimensional submanifold of the phase space. The flow is determined by a one-dimensional linear subspace: $c_1\phi_1 - c_2\phi_2 = 1$, obtained as the intersection of the constraint submanifold with the level sets of the first integrals $I_1 = c_1$, $I_2 = c_2$, where c_1, c_2 are constants determined by the initial conditions in (2).

The above results lead to the next proposition.

Proposition 2: Let ω_i, $i=1,2,3$, be a solution of the generalized DH system (2) and let u_1, u_2 be any two solutions of Eq. (7) with unit Wronskian. Then I_α and $J_\alpha = tI_\alpha - \phi_\alpha$, $\alpha=1,2$, are first integrals of the DH system, where ϕ_α and I_α are given by Eq. (12). Furthermore, the DH system are equivalent to a constrained Hamiltonian system given by Eqs. (13) and (14) with $\{\phi_\alpha, I_\alpha\}$ as the canonical variables. The associated Hamilton's equations (13) are linear and can be solved by quadratures.

The first integrals I_α, $\alpha=1,2$, are constant functions of t in the domain of analyticity of the $\omega_i(t)$, and their values are determined by the initial conditions. However, the I_α are not single-valued as functions of ω_i (or equivalently of the Schwarzian variables s, $\dot{s}$, $\ddot{s}$). The nonanalytic behavior is essentially due to the fact that in the complex s-plane, continuation along closed circuits around the branch points $s=0$, $s=1$, and $s=\infty$ transforms any two independent solutions of the Fuchsian equation (7) by the corresponding monodromy matrix. The branching properties of the I_α can be characterized explicitly by expressing them as functions of s, $\dot{s}$, and $\ddot{s}$ and the fundamental matrix of solutions of the hypergeometric equation (9). If the u_α in Eq. (11) are replaced by the solutions of the hypergeometric equation (9) by using the transformation (8), then this yields

$$[I_1 \quad I_2] = \sigma[\lambda \quad 1]\begin{bmatrix}\chi_1(s) & \chi_2(s)\\ \chi_1'(s) & \chi_2'(s)\end{bmatrix}, \tag{15}$$

where

$$\sigma(s,\dot{s}) = s^{c/2}(1-s)^{(a+b-c+1)/2}\dot{s}^{1/2} \quad \text{and} \quad \lambda(s,\dot{s},\ddot{s}) = \frac{a+b+1-cs}{2s(1-s)} - \frac{\ddot{s}}{2\dot{s}^2}.$$

It is clear from Eq. (15) that I_α are not branched as functions of $\ddot{s}$ and that they have square-root branch points as a function of $\dot{s}$ at $\dot{s}=0$ and $\dot{s}=\infty$ (in fact, I_α^2 are single-valued as functions of both $\dot{s}$ and $\ddot{s}$). When $\dot{s}$ and $\ddot{s}$ are held fixed, the only places where the I_α can be branched are at $s=0$, $s=1$, and $s=\infty$. Let γ_0 and γ_1 be two closed curves with a common base point in the finite

complex s-plane enclosing the points $s=0$ and $s=1$, respectively, and traversed once in the positive direction. Analytic continuation along γ_0 and γ_1 transforms the fundamental matrix of solutions of Eq. (9) according to

$$\gamma_\mu:\ \begin{pmatrix} \chi_1(s) & \chi_2(s) \\ \chi_1'(s) & \chi_2'(s) \end{pmatrix} \mapsto \begin{pmatrix} \chi_1(s) & \chi_2(s) \\ \chi_1'(s) & \chi_2'(s) \end{pmatrix} M_\mu, \quad \mu=0,1.$$

For generic values of a, b, c and for the choice of basis solutions, $\chi_1=F(a,b,c;s)$, $\chi_2=F(a,b,a+b-c+1;s)$ of the hypergeometric equation, the monodromy matrices M_μ are given by[25]

$$M_0=\begin{pmatrix} 1 & e^{-2\pi i b}-e^{-2\pi i c} \\ 0 & e^{-2\pi i c} \end{pmatrix} \quad \text{and} \quad M_1=\begin{pmatrix} e^{-2\pi i(a+b-c)} & 0 \\ 1-e^{-2\pi i(a-c)} & 1 \end{pmatrix}.$$

The only other source of branching in Eq. (15) arises from the analytic continuation of σ along γ_μ which yields

$$\gamma_0:\ \sigma\mapsto e^{i\pi c}\sigma, \quad \gamma_1:\ \sigma\mapsto e^{i\pi(a+b-c)}\sigma.$$

The branching at $s=\infty$ can be determined from the branching at $s=0$ and $s=1$. A closed circuit (defined in a similar way as for γ_0 and γ_1 above) around the point $s=\infty\in\mathcal{CP}^1$ is homotopic to $\gamma_0^{-1}\circ\gamma_1^{-1}$. The corresponding monodromy matrix is given by $M_\infty=(M_1M_0)^{-1}$. The monodromy matrix M for any closed circuit γ can be expressed in terms of the fundamental monodromy matrices M_0 and M_1 associated with γ_0 and γ_1, respectively. Finally, taking all the sources of branching into account in (15), we obtain the following result.

Proposition 3: The first integrals of the DH system given by (15) are multi-valued functions of s with branch points at $s=0$, $s=1$, and $s=\infty$. The multi-valued behavior can be expressed in terms of the fundamental determinations:

$$\gamma_0:\ [I_1 \quad I_2]\mapsto[I_1 \quad I_2]M_0e^{i\pi c}, \quad \gamma_1:\ [I_1 \quad I_2]\mapsto[I_1 \quad I_2]M_1e^{i\pi(a+b-c)},$$

where M_0 and M_1 are the monodromy associated with a fundamental matrix solution of the hypergeometric equation (9) around the closed curves γ_0 and γ_1, respectively.

Remark 1: The multi-valued behavior of the first integrals I_α may also be described in terms of the DH variables ω_i. It follows from Eq. (4) that the branch points $s=0$, $s=1$, and $s=\infty$ correspond to the complex diagonal hyperplanes $\omega_i=\omega_j$, $i\neq j$. The monodromy group generated by M_0 and M_1 determines a (complex) representation of the fundamental group $\pi_1(\mathcal{M}_3)$ on the complement $\mathcal{M}_3=C^3\backslash\cup\{\omega_i=\omega_j, i\neq j\}$ of the arrangement of the diagonal hyperplanes in C^3. Arnold,[4] in his study of pure braid groups, discussed the cohomology of the complement $\mathcal{M}_n$ of the diagonal hyperplane arrangement in C^n. In particular, he proved that the integral cohomology ring $H^*(\mathcal{M}_n,Z)$ is isomorphic to the algebra generated by the closed differential one-forms: $\omega_{jk}=(1/2\pi i)d\ln(\omega_j-\omega_k)$, $j\neq k$ which satisfy $\omega_{kl}\wedge\omega_{lm}+\omega_{lm}\wedge\omega_{mk}+\omega_{mk}\wedge\omega_{kl}\equiv 0$. Note that for $n=3$, there is only one independent relation: $\omega_{12}\wedge\omega_{23}+\omega_{23}\wedge\omega_{31}+\omega_{31}\wedge\omega_{12}\equiv 0$, which is indeed satisfied by the parametrization of the ω_i in Eq. (3).

Remark 2: The first integrals in Eq. (15) for the classical DH system ($\alpha_1=\alpha_2=\alpha_3=0$) are expressed in terms of the special hypergeometric Eq. (9) with $a=b=\frac{1}{2}$, $c=1$. In this case, the monodromy matrices with respect to the basis $\chi_1=F(\frac{1}{2},\frac{1}{2},1;s)$ and $\chi_2=iF(\frac{1}{2},\frac{1}{2},1;1-s)$, are given by

$$M_0=\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad M_1=\begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix}.$$

The corresponding monodromy group is the subgroup $\Gamma(2)$ (principal congruent subgroup of level 2) of the modular group $\mathrm{SL}(2,Z)$, defined as $\Gamma(2):=\{g\in\mathrm{SL}(2,Z)|g\equiv Id(\mathrm{mod}\ 2)\}$. When $a=b$

$=\frac{1}{12}$, $c=\frac{1}{2}$ in Eq. (9), the associated monodromy group is the full modular group SL(2,Z) which is isomorphic to the pure braid group B_3 of three colored strands. Similar representations of pure braid group B_n are given by the monodromy group associated with particular Picard–Fuchs equations with n regular singular points which arise in the theory of Frobenius manifolds.[9] This is related to Arnold's work[4] (see Remark 1) on the presentation of pure braid group as the fundamental group of the complement $\mathcal{M}_n$ under the action of the Coxeter group A_n.

It is important to note that the first integrals I_α, J_α remain multi-valued independent of the choice of parameters, even in the particular cases where the general solution is single-valued in its domain of existence. For instance, the classical DH system [Eq. (2) with $\tau\equiv 0$] can be solved in terms of the elliptic modular function and the general solution is analytic inside a circle D in the complex t-plane (see, e.g., Refs. 7 and 1). It was shown in Ref. 19 that the classical DH system does not possess a meromorphic first integral. This is consistent with our results that first integrals do indeed exist, but they are nonalgebraic and multi-valued functions of the ω_i. Thus there is no natural connection between the analyticity properties of the solution and the first integrals for the DH system. To establish such connection for nonlinear differential equations is a very delicate issue. For specific cases of Hamiltonian dynamical systems, it was proved under certain assumptions that if the system admits solutions that are branched, then the system can not possess analytic first integrals independent of the Hamiltonian.[18] Furthermore, Ziglin's work[27,28] reveals that branching of solutions and the absence of single-valued first integrals in certain Hamiltonian systems are *both* consequences of the same complex singularity structure of the solutions (although one does not necessarily imply the other). However, it should be noted that these results do not rule out the possibility that multi-valued first integrals may exist. Indeed this is the case for the DH system which serves as an important example of equations that are integrable in the sense that the general solutions can be expressed in terms of linear equations, yet the constants of integrations are not single-valued functions of the dependent variables.

IV. POISSON STRUCTURES

The DH equations (2) may be viewed as a complex dynamical system on a manifold $\mathcal{M}$ of (complex) dimension 3 where the DH variables ω^i, $i=1,2,3$, are local holomorphic coordinates on $\mathcal{M}$. (*Note:* In this section the standard notation for coordinate functions ω^i is used instead of ω_i to denote the DH variables.) Solutions of Eq. (2) determine a flow given by the integral curves of a holomorphic vector field $X\in\mathcal{TM}$ expressed in local coordinates ω^i as $X=X^i\partial_i$, $X^i:=\omega^j\omega^k-\omega^i(\omega^j+\omega^k)+\tau^2$, $i\neq j\neq k$, and cyclic. Here $\partial_i:=\partial/\partial\omega^i$, and summation over repeated indices is implied. Denote by $\Lambda^p(\mathcal{M})$ and $\Lambda_q(\mathcal{M})$ the respective spaces of (holomorphic) p-forms and q-vectors (contravariant, skew-symmetric q-tensor fields) on $\mathcal{M}$. Let $\nu\in\Lambda^3(\mathcal{M})$ be a nondegenerate three-form given in terms of local coordinates by

$$\nu=\frac{1}{\Delta(\omega^1,\omega^2,\omega^3)}d\omega^1\wedge d\omega^2\wedge d\omega^3, \tag{16}$$

for some function $\Delta\in C^\infty(\mathcal{M})$, $\Delta\neq 0$, which is to be determined later. Using the three-form ν we define the dual map $\Phi:\Lambda_q(\mathcal{M})\to\Lambda^{3-q}(\mathcal{M})$ and its inverse $\Phi^{-1}:\Lambda^p(\mathcal{M})\to\Lambda_{3-p}(\mathcal{M})$ by the inner products

$$\Phi(A):=i_A\nu,\quad \Phi^{-1}(\beta):=i_{\tilde{\nu}}\beta,$$

where $A\in\Lambda_q(\mathcal{M})$, $\beta\in\Lambda^p(\mathcal{M})$, and $\tilde{\nu}:=\Delta\partial_1\wedge\partial_2\wedge\partial_3\in\Lambda_3(\mathcal{M})$ is the inverse of the three-form ν. In particular, note that for β_1, $\beta_2\in\Lambda^1(\mathcal{M})$, the vector $v=\Phi^{-1}(\beta_1\wedge\beta_2)$ satisfies $i_v\beta_1=i_v\beta_2=0$.

Since the first integrals I_1 and I_2 of Eq. (2) are constant along the integral curves of X, it follows that $\dot{I}_\alpha=i_X(dI_\alpha)=0$, $\alpha=1,2$. The one-forms dI_1 and dI_2 span a two-dimensional, integrable (in the Frobenius sense) co-distribution of $\mathcal{T}^*\mathcal{M}$, dual to the vector field X. Hence the vector field can be expressed as $X=G\Phi^{-1}(dI_1\wedge dI_2)=Gi_{\tilde{\nu}}(dI_1\wedge dI_2)$ for some function G

$\in C^\infty(\mathcal{M})$. Without any loss of generality, we can set $G=1$ and thus determine the function Δ in Eq. (16). A straightforward calculation using the explicit forms of the I_α in Eq. (12) yields

$$\Delta(\omega^1,\omega^2,\omega^3)=4(\omega^2-\omega^3)(\omega^3-\omega^1)(\omega^1-\omega^2). \tag{17}$$

Therefore we have the following characterization of the DH vector field X.

Proposition 4: The DH system (2) defines a flow in a three-dimensional, complex manifold $\mathcal{M}$ equipped with a nondegenerate three-form ν given in terms of local coordinates by Eqs. (16) and (17). The flow is an integral submanifold of $\mathcal{M}$ generated by the vector field $X\in T\mathcal{M}$ which is dual to the integrable codistribution spanned by the one-forms dI_1 and dI_2. That is,

$$X=\Phi^{-1}(dI_1\wedge dI_2)=\tilde{\nu}(\cdot,dI_1,dI_2). \tag{18}$$

Let H denote the union of the complex hyperplanes given by $\omega^i=\omega^j$, $i\neq j$. It is evident from Eqs. (17) and (12) that the three-form ν and the one-forms dI_1, dI_2 are singular on H. Hence the manifold $\mathcal{M}$ is prescribed by $\mathcal{M}=\mathbf{C}^3\backslash H$ on which Eq. (18) is valid and defines the holomorphic vector field X. The flow defined by Eq. (18) on $\mathcal{M}$ corresponds to the functions $\omega^i(t)$ which remain distinct for all t in the domain of analyticity of the DH solutions. It should be noted, however, that the DH flow itself [given by Eq. (2)] is *not* singular on H, but the corresponding vector field can no longer be defined via Eq. (18). In fact, the complex planes $\omega^i=\omega^j$, $i\neq j$, are invariant manifolds of the DH flow. The flow restricted to these planes corresponds to the special cases of Eq. (2) which are solved either by quadratures or in terms of Bessel's equation.[3]

It follows from Proposition 4 that the intersection of the two-dimensional level sets of the first integrals I_1 and I_2 defines (locally) a unique solution curve for Eq. (2) on $\mathcal{M}$. We will next show that $\mathcal{M}$ is a Poisson manifold with a pair of Poisson structures defined in a natural way via the first integrals I_α. Furthermore, the DH vector field X is locally Hamiltonian with respect to both Poisson structures.

A Poisson structure on $\mathcal{M}$ is specified by a bi-vector $B\in\Lambda_2(\mathcal{M})$ whose Nijenhuis–Schouten bracket with itself, defined by the three-vector $[B,B]_S=0$. In terms of the coordinates ω^i,

$$B=B^{ij}\partial_i\wedge\partial_j, \quad [B,B]_S^{ijk}:=\partial_l(B^{ij})B^{lk}+\partial_l(B^{jk})B^{li}+\partial_l(B^{ki})B^{lj}=0.$$

The Poisson bracket of functions $f,\ g\in C^\infty(\mathcal{M})$ is the pairing defined by

$$\{f,g\}:=B(df,dg),$$

which is skew-symmetric and satisfies the Leibniz rule $\{fg,h\}=f\{g,h\}+g\{f,h\}$ and the Jacobi identity $\{\{f,g\},h\}+\{\{g,h\},f\}+\{\{h,f\},g\}=[B,B]_s(df,dg,dh)=0$, for all $f,g,h\in C^\infty(\mathcal{M})$. A Hamiltonian vector field X_H with respect to a Poisson structure B is defined as $X_H:=B(\cdot,dH)$ where $H(\omega^i)$ is the Hamiltonian function on $\mathcal{M}$. The Hamiltonian flow given by the integral curves of X_H corresponds to the solution of the system

$$\dot{\omega}^i=X_H(\omega^i)=\{\omega^i,H\}, \quad i=1,2,3.$$

In three dimensions it is convenient to introduce the Poisson one-form $\theta\in\Lambda^1(\mathcal{M})$ (see, e.g., Ref. 12) by $\theta=\Phi(B)=i_B\nu$, which is the dual of the Poisson bi-vector. The Jacobi identity can be reformulated as the Frobenius integrability condition for the Poisson one-form θ. Specifically, we have the following.

Lemma 1. $B\in\Lambda_2(\mathcal{M})$ is a Poisson bi-vector if and only if the dual one-form $\Phi(B):=\theta\in\Lambda^1(\mathcal{M})$ satisfies $\theta\wedge d\theta=0$.

Proof: If $B\in\Lambda_2(\mathcal{M})$ and $\nu\in\Lambda^3(\mathcal{M})$, then we have the contraction formula (see, e.g., Ref. 20)

$$\nu([B,B]_s)=2i_Bdi_B\nu-i_Bi_Bd\nu.$$

Since ν is a top-degree holomorphic form, $d\nu=0$. Furthermore, we have $B=\Phi^{-1}(\theta)=\tilde{\nu}(\theta)$. Hence

$$\nu([B,B]_s)=2i_B d\theta=2\tilde{\nu}(\theta\wedge d\theta)$$

and the result follows.

In terms of the functions I_1 and I_2, define the bi-vectors

$$B_\alpha:=\Phi^{-1}(dI_\alpha)=\tilde{\nu}(\cdot,\cdot,dI_\alpha),\quad \alpha=1,2, \tag{19}$$

on $\mathcal{M}$. The corresponding dual one-forms $\Phi(B_\alpha)=dI_\alpha$ are exact. Therefore it follows immediately from Lemma 1 that the B_α are Poisson bi-vectors. The DH vector field X in Eq. (18) can be expressed as

$$X=-B_1(\cdot,dI_2)=B_2(\cdot,dI_1), \tag{20}$$

which is a Hamiltonian vector field with respect to both Poisson structures B_α. As a result, the DH equations (2) satisfy the Poisson bracket formulations

$$\dot{\omega}^i=X(\omega^i)=\{\omega^i,I_1\}_2=\{\omega^i,-I_2\}_1,$$

where $\{g,h\}_\alpha=B_\alpha(dg,dh)$, $\alpha=1$, 2. Moreover, B_1 and B_2 are compatible Poisson structures, namely, there exist functions λ_1, λ_2 such that the linear combination $B=\lambda_1 B_1+\lambda_2 B_2$ is also a Poisson bi-vector. It is easy to verify that the corresponding dual one-form $\theta=\Phi(B)=\lambda_1 dI_1+\lambda_2 dI_2$ satisfies Lemma 1 when λ_1, λ_2 are arbitrary differentiable functions of I_1 and I_2. For a given Poisson structure B, it is also possible to find a corresponding Hamiltonian function $H(I_1,I_2)$ such that $X=B(\cdot,dH)=\mu^{-1}(dH\wedge\theta)$ gives the DH vector field as in Eq. (18). This is equivalent to the first-order, linear partial differential equation $\lambda_2(\partial H/\partial I_1)-\lambda_1(\partial H/\partial I_2)=1$, which can be solved by the method of characteristics. Thus X does not have a unique representation as a Hamiltonian vector field; the simplest forms are the ones given in Eq. (20). A Hamiltonian system with compatible Poisson structures is called a bi-Hamiltonian system. The DH vector field X in Eq. (20) is therefore a bi-Hamiltonian vector field with respect to the pair of compatible Hamiltonian structures $\{(B_1,-I_2),(B_2,I_1)\}$.

Remark 3: Since $\mathcal{M}$ is odd-dimensional [$\dim(\mathcal{M})=3$], the B_α are degenerate (rank 2) bi-vector fields on $\mathcal{M}$. It follows from Eq. (19) that $B_1(\cdot,dI_1)=B_2(\cdot,dI_2)=0$. Therefore, I_1 and I_2 are the Casimir functions for the Poisson structures B_1 and B_2 respectively, and satisfy $\{g,I_\alpha\}_\alpha=0$, $\alpha=1,2$, for any $g\in C^\infty(\mathcal{M})$. Furthermore, since $B_\alpha(dI_1,dI_2)=\{I_1,I_2\}_\alpha=0$, the first integrals I_1 and I_2 are in involution.

Remark 4: The flow associated with the vector field X preserves the three-form ν on $\mathcal{M}$. Indeed we have

$$\mathcal{L}_X\nu=d\Phi(X)=d[\Phi\circ\Phi^{-1}(dI_1\wedge dI_2)]=d(dI_1\wedge dI_2)=0.$$

Note that on a three-dimensional *real* phase space, ν would be phase volume element that is invariant along the flow of X. Thus the condition $\mathcal{L}_X\nu=0$ on the DH phase space $\mathcal{M}$ can be regarded as the holomorphic extension of the Liouville theorem on an odd-dimensional (complex) phase space.

We summarize the results discussed above.

Proposition 5: The DH system (2) represents a bi-Hamiltonian flow on $\mathcal{M}$ corresponding to the Poisson structures $B_1=\Phi^{-1}(dI_1)$, $B_2=\Phi^{-1}(dI_2)$; and Hamiltonians $-I_2$, I_1 respectively. The DH vector field X is Hamiltonian with respect to both Poisson structures as given by Eq. (20). Furthermore, the first integrals I_1 and I_2 are in involution with respect to both Poisson structures.

The local expressions for the Poisson structures B_k are considerably simple in terms of the "action-angle" variables $\{I_\alpha,\phi_\alpha,\alpha=1,2\}$ introduced via Eqs. (13) and (14) in Sec. II. Any three of the four variables can be taken to form a natural set of local coordinates on $\mathcal{M}$ while the

remaining variable is solved algebraically using the constraint equation (14). For example, if we take $\{\phi_1, I_1, I_2\}$ as new local coordinates on $\mathcal{M}$ and use the relations between the ω_i and $\{I_\alpha, \phi_\alpha\}$ from Eq. (12), then in the new coordinates the three-vector $\tilde{\nu}$ [inverse of ν in Eq. (16)] takes the form

$$\tilde{\nu} = I_1 \frac{\partial}{\partial \phi_1} \wedge \frac{\partial}{\partial I_1} \wedge \frac{\partial}{\partial I_2}.$$

Furthermore, from Eqs. (19) and (20) we have the following expressions for the Poisson bi-vectors and the DH vector field:

$$B_1 = -I_1 \frac{\partial}{\partial \phi_1} \wedge \frac{\partial}{\partial I_2}, \quad B_2 = I_1 \frac{\partial}{\partial \phi_1} \wedge \frac{\partial}{\partial I_1}, \quad X = I_1 \frac{\partial}{\partial \phi_1}.$$

Both Hamiltonian structures $(B_1, -I_2)$ or (B_2, I_1) yield the same dynamical equations: $\dot{\phi}_1 = I_1$, $\dot{I}_1 = \dot{I}_2 = 0$ which together with the algebraic constraint [Eq. (14)] are then equivalent to the DH dynamics given by Eqs. (13).

Note that the two sets of fundamental Poisson brackets,

$$\begin{aligned} &\{\phi_1, I_1\}_1 = 0, \quad \{I_2, \phi_1\}_1 = I_1, \quad \{I_1, I_2\}_1 = 0, \\ &\{\phi_1, I_1\}_2 = I_1, \quad \{I_2, \phi_1\}_2 = 0, \quad \{I_1, I_2\}_2 = 0, \end{aligned} \tag{21}$$

with respect to the respective Poisson structures B_1 and B_2, are *linear* in the coordinate I_1. Each set corresponds to a Lie–Poisson bracket on $\mathcal{M}$ induced by certain three-dimensional Lie algebra **g**. The Lie–Poisson structure can be defined by identifying $\mathcal{M}$ with the dual **g*** of **g**, and the linear coordinate functions $\{y_k, k = 1,2,3\}$ on **g*** with the coordinates $\{\phi_1, I_1, I_2\}$. Then the fundamental Lie–Poisson brackets induced by **g** on $\mathcal{M}$ are defined as $\{y_i, y_j\} := c_{ij}{}^k y_k$, where c_{ij}^k are the structure constants associated with the Lie algebra bracket $[e_i, e_j] = c_{ij}^k e_k$ with respect to a basis $\{e_i, i = 1,2,3\}$ of **g**. Let $\mathbf{g_1}$ and $\mathbf{g_2}$ denote the Lie algebras corresponding to the first and second set of fundamental Poisson brackets, respectively. Then it is evident from Eq. (21) that both $\mathbf{g_1}$ and $\mathbf{g_2}$ are solvable Lie algebras with one-dimensional centers corresponding to the respective Casimir functions I_1 and I_2. However, $\mathbf{g_1}$ is nilpotent of degree 2, whereas $\mathbf{g_2}$ contains a one-dimensional ideal generated by the element corresponding to I_1 whose normalizer is $\mathbf{g_2}$ itself. In fact, it is easy to verify that choosing *any* three of the four "action-angle" variables as local coordinates on $\mathcal{M}$ yields two distinct, canonical Lie–Poisson structures which correspond to solvable Lie algebras, moreover, one of the Lie algebras is nilpotent.

The volume form ν together with the Hamiltonians I_1 and $-I_2$ induce a Nambu–Poisson structure on the manifold $\mathcal{M}$. Nambu[21] proposed a generalization of the Poisson bracket to study the dynamics of a "canonical triplet" of variables in a three-dimensional real phase space. In its simplest form, the canonical Nambu bracket of functions $g_i \in C^\infty(R^3)$, $i = 1,2,3$, is given by the Jacobian

$$\{g_1, g_2, g_3\} = \frac{\partial(g_1, g_2, g_3)}{\partial(x^1, x^2, x^3)} = \tilde{\epsilon}(dg_1, dg_2, dg_3),$$

where x^i, $i = 1,2,3$, are local coordinates and $\tilde{\epsilon}$ is the inverse of the standard volume form $\epsilon = dx^1 \wedge dx^2 \wedge dx^3$ on R^3. The Nambu dynamics is prescribed as $\dot{x}^i = \{x^i, H_1, H_2\}$ in terms of two "Hamiltonian" functions H_1 and H_2. Takhtajan[26] extended the Nambu formalism to higher dimensions and introduced the analog of the Jacobi identity for Nambu brackets—the so-called "fundamental identity." An example of a Nambu–Poisson structure (of order n) on an n-dimensional manifold $\mathcal{N}$ with a volume form $\nu_{\mathcal{N}} \in \Lambda^n(\mathcal{N})$ is the n-linear map $\{\cdot,\ldots,\cdot\}$: $\underbrace{C^\infty(\mathcal{N}) \otimes \ldots \otimes C^\infty(\mathcal{N})}_{n \text{ factors}} \mapsto C^\infty(\mathcal{N})$ defined as

$$dg_1 \wedge dg_2 \wedge \cdots \wedge dg_n := \{g_1, g_2, \ldots, g_n\} \nu_{\mathcal{N}},$$

for functions $g_j \in C^\infty(\mathcal{N})$, $j = 1,2,\ldots,n$. It can be shown that the bracket defined above is a Nambu–Poisson bracket,[10] namely, it is skew-symmetric, a derivation, and satisfies the "fundamental identity"

$$\{f_1, \ldots, f_{n-1}, \{g_1, \ldots, g_n\}\} = \sum_{i=1}^{n} \{g_1, \ldots, g_{i-1}, \{f_1, \ldots, f_{n-1}, g_i\}, g_{i+1}, \ldots, g_n\}.$$

The Nambu formulation of the DH system arises as a special case ($n = 3$) of the above example with a Nambu–Poisson structure on $\mathcal{M}$ prescribed by

$$\{g_1, g_2, g_3\} := \Phi^{-1}(dg_1 \wedge dg_2 \wedge dg_3) = \tilde{\nu}(dg_1, dg_2, dg_3). \tag{22}$$

Then from Eq. (18), the vector field X is the generator of a Nambu–Hamilton flow on the DH phase space $\mathcal{M}$ given by the action $\dot{g} = X(g) = \{g, I_1, I_2\}$ on functions $g \in C^\infty(\mathcal{M})$. Therefore, we have the following.

Proposition 6: The DH system (2) is equivalent to the Nambu–Hamilton equation of motions $\dot{\omega}^i = \{\omega^i, I_1, I_2\}$, $i = 1,2,3$, *with respect to the Nambu–Poisson bracket defined by Eq. (22) together with the "Hamiltonians"* I_1 *and* I_2. *The vector field X in Eq. (18) is a Nambu–Hamiltonian vector field.*

Remark 5: The essential difference between the DH bracket and the canonical Nambu bracket is the "discriminant" function $\Delta(\omega_1, \omega_2, \omega_3)$. In the DH case, Δ is given by Eq. (17), whereas $\Delta \equiv 1$ for the canonical Nambu bracket.

Remark 6: It is possible to construct an infinite family of Poisson brackets characterized by functions $I \in C^\infty(\mathcal{M})$ as $\{f,g\}_I = \{f,g,I\}$, from the Nambu–Poisson bracket in Eq. (22). The brackets defined by the Poisson bi-vectors B_α in Eq. (19) are in fact induced in this way from Eq. (22) with $I = I_\alpha$, $\alpha = 1,2$. In general, a Nambu bracket of order $n > 2$ on a manifold of dimension $k \geqslant n$ can induce infinite families of lower order Nambu structures, including families of Poisson brackets.[26]

Remark 7: The "fundamental identity" for the bracket defined by Eq. (22) is equivalent to the statement that any Nambu–Hamiltonian vector field is a derivation of the Nambu bracket. Indeed, consider the vector field $Y = \tilde{\nu}(\cdot, df_1, df_2)$ where f_1, $f_2 \in C^\infty(\mathcal{M})$ are the "Hamiltonians." Clearly from Eq. (22), $Y(g) = \{g, f_1, f_2\}$ for all $g \in C^\infty(\mathcal{M})$. Y also preserves the volume form (and its inverse $\tilde{\nu}$), since $\mathcal{L}_Y \nu = d i_Y \nu = d(df_1 \wedge df_2) = 0$. Now taking the Lie derivative of Eq. (22) with respect to Y and using the Leibniz rule to expand the right-hand side gives the "fundamental identity" for the bracket in Eq. (22).

V. CONCLUSION

In this article, we studied the general solution and first integrals of the generalized DH system (2). We showed that the integral curves of the solution are locally defined by the intersection of the level sets of the first integrals in a three-dimensional phase space $\mathcal{M}$ which is a Nambu–Poisson manifold. In order to study the global dynamics, it is necessary to consider the phase flow on the covering manifolds associated with the multi-valued first integrals. The covering manifolds are generally densely branched for the DH system, although it is possible to obtain finite or denumerable infinite sheeted covering of $\mathcal{M}$ corresponding to particular choices of the DH parameters. In these latter cases, there may be several interesting avenues of investigation including the topological properties of the DH phase space as well as the conformal class of SU(2)-invariant hypercomplex manifolds which correspond to these special DH solutions.

It is also worth mentioning that the DH system can be regarded as a gradient flow: $X = \eta(\cdot, dV)$ for some flat, indefinite metric η^{-1}. The potential function V is a homogeneous polynomial of degree 3 in the ω_i, invariant under cyclic permutation of $(\omega_1, \omega_2, \omega_3)$. It is conceivable

that further insights into the complex dynamics of the DH system may be gained by considering it as a gradient flow with a polynomial potential rather than a Nambu–Poisson flow with multi-valued Hamiltonians.

ACKNOWLEDGMENTS

The authors acknowledge useful discussions with Mark Ablowitz and Alexander Veselov. S.C. would especially like to thank Leon Takhtajan for his valuable comments and encouragement during early stages of this work. This work has been partially supported by Grant No. NAL/00344/G from the Nuffield Foundation and a Grigsby-Sensenbaugh foundation grant from the University of Colorado.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

Darboux covariant equations of von Neumann type and their generalizations

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(Received 30 May 2002; accepted 11 December 2002)

Lax pairs with operator valued coefficients, which are explicitly connected by means of an additional condition, are considered. This condition is proved to be covariant with respect to the Darboux transformation of a general form. Nonlinear equations arising from the compatibility condition of the Lax pairs in the matrix case include, in particular, Nahm equations, and Volterra, Bogoyavlenskii and Toda lattices. The examples of other one-, two- and multi-field lattice equations are also presented. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1554762]

I. INTRODUCTION

In the present article we consider a large class of the integrable systems of nonlinear equations taking values on an associative ring of noncommutative operators. They are defined as the compatibility condition of Lax pairs characterized by the property that the equation for the time evolution of the wave function is explicitly determined (in a local way) by the coefficients of the spectral problem. There exist different types of Lax pairs, whose coefficients are connected explicitly. Lax pairs with coefficients defined on an associative algebra of scalar pseudo-differential operators were introduced in Refs. 1 and 2 (see also Ref. 3 and references therein). These Lax pairs play an important role in the Sato theory[4] and in constructing the modifications of KP hierarchy.[5,6] The case of the shift operators and associated lattice equations were discussed in Ref. 7. The approach, which is applied below to connect the coefficients of the Lax pairs, differs from known ones. The hierarchy of Darboux covariant nonlinear ''multi-field'' equations we describe in this article contains, as the simplest case, the ''one-field'' equations of von Neumann type,

$$i\dot{\rho}=[H(\rho),\rho], \quad i\dot{\rho}=[H,f(\rho)]. \tag{1}$$

These equations and their solutions were investigated in the context of the density matrices and Hamiltonians in Refs. 8–10, where, for instance, the formulas of the Darboux transformation were constructed. In the matrix case, the multi-field equations we derive here admit the reductions leading to known and new integrable nonlinear lattice systems.

The technique exploited in this article combines and develops the approaches of Refs. 11 and 12. In Sec. II we show that the relations between the coefficients of the equations forming the Lax

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pair, i.e., necessary conditions for the Lax pair compatibility, are identically satisfied if an additional condition on the coefficients is imposed. This condition connects explicitly the coefficients of the equations of the Lax pair and allows us to write in a closed form the nonlinear equations, which follow the compatibility condition. A theorem establishing the Darboux covariance of the Lax pair with the additional condition and, consequently, of the corresponding nonlinear equations is proved in Sec. III. This theorem gives an effective tool of producing the infinite hierarchies of solutions, including the multi-soliton solutions, for nonlinear equations and their reductions. The equations of von Neumann type and associated lattice equations are considered in Sec. IV. The next two sections are devoted to two- and multi-field generalizations of the von Neumann type equations. The examples presented include known lattice equations as well as some new ones. Particular cases of the Darboux transformation satisfying the conditions of the theorem of Sec. III are discussed in the Appendix.

II. LAX PAIR AND MULTI-FIELD EQUATIONS

Let us begin with the overdetermined system of linear equations (Lax pair)

$$\begin{aligned} -i\dot{\psi} &= \psi A(\lambda), \\ z_\lambda \psi &= \psi H(\lambda). \end{aligned} \tag{2}$$

Here λ and z_λ are complex numbers, ψ takes values in a given linear space $\mathcal{L}$, $A(\lambda)$ and $H(\lambda)$ are linear operators $\mathcal{L}\mapsto\mathcal{L}$ belonging to an associative ring, and the dot denotes a derivative (i.e., an operator satisfying the Leibnitz rule). The compatibility condition of Eqs. (2) is

$$i\dot{H}(\lambda)=[A(\lambda),H(\lambda)]. \tag{3}$$

If we assume that the operators entering the Lax pair are rational functions of λ with operator valued coefficients of the form

$$A(\lambda)=\sum_{k=0}^{L}\lambda^k B_k+\sum_{k=1}^{M}\frac{1}{\lambda^k}C_k, \tag{4}$$

$$H(\lambda)=\sum_{k=0}^{N}\lambda^k H_k, \tag{5}$$

then Eq. (3) becomes equivalent to the following system of algebraic and differential relations between operators B_k, C_k, and H_k:

$$\sum_{k=\max\{0,m-L\}}^{N}[B_{m-k},H_k]=0 \quad (N<m\leqslant L+N), \tag{6}$$

$$\sum_{k=0}^{\min\{N,m+M\}}[C_{k-m},H_k]=0 \quad (-M\leqslant m<0), \tag{7}$$

$$i\dot{H}_m=\sum_{k=\max\{0,m-L\}}^{m}[B_{m-k},H_k]+\sum_{k=m+1}^{\min\{N,m+M\}}[C_{k-m},H_k] \quad (0\leqslant m\leqslant N). \tag{8}$$

The connection between operators B_k, C_k, and H_k, which is implied by Eqs. (6) and (7), is implicit. It is possible to express B_k and C_k explicitly in terms of the operators H_k in order to satisfy Eqs. (6) and (7) *identically*. Indeed, let us put

$$B_k=\frac{1}{(L-k)!}\left(\frac{d^{L-k}}{d\varsigma^{L-k}}f(\varsigma^N H(\varsigma^{-1}),\varsigma^{-1})\right)\Big|_{\varsigma=0}, \tag{9}$$

$$C_k=\frac{1}{(M-k)!}\left(\frac{d^{M-k}}{d\varepsilon^{M-k}}g(H(\varepsilon),\varepsilon)\right)\Big|_{\varepsilon=0}, \tag{10}$$

where $f(X,\lambda)$ and $g(X,\lambda)$ are well defined functions of an operator X and parameter λ. We assume hereafter that for any operator $X(\lambda)$, which is analytic in the neighborhood of the point $\lambda=\infty$, the function $f(X(\lambda),\lambda)$ is also analytic and the condition

$$[f(X(\lambda),\lambda),X(\lambda)]=0 \tag{11}$$

is valid in this neighborhood as well. In the case of the function $g(X,\lambda)$, analogous properties have to take place in the neighborhood of the point $\lambda=0$. In particular we have

$$[g(X(\lambda),\lambda),X(\lambda)]=0. \tag{12}$$

Equations (6) and (7) are fulfilled for any B_k and C_k defined by Eqs. (9) and (10) as a consequence of the following identities:

$$\frac{d^{N+L-m}}{d\varsigma^{N+L-m}}[f(\varsigma^N H(\varsigma^{-1}),\varsigma^{-1}),\varsigma^N H(\varsigma^{-1})]\big|_{\varsigma=0}\equiv 0 \quad (N<m\leqslant L+N),$$

$$\frac{d^{M+m}}{d\varepsilon^{M+m}}[g(H(\varepsilon),\varepsilon),H(\varepsilon)]\big|_{\varepsilon=0}\equiv 0 \quad (-M\leqslant m<0).$$

Using Eqs. (6) and (7) we can rewrite Eqs. (8) as

$$-i\dot{H}_m=\sum_{k=m+1}^{N}[B_{m-k},H_k]+\sum_{k=0}^{m}[C_{k-m},H_k], \tag{13}$$

where the coefficients B_k and C_k for $k<0$ are calculated accordingly to Eqs. (9) and (10). The operator $A(\lambda)$ given by (4), (9), and (10) is conveniently represented in the following equivalent way:

$$A(\lambda)=[F(H(\lambda),\lambda)]_\infty+[G(H(\lambda),\lambda)]_0. \tag{14}$$

Here

$$F(H(\lambda),\lambda)=\lambda^L f(H(\lambda)/\lambda^N,\lambda), \tag{15}$$

$$G(H(\lambda),\lambda)=\lambda^{-M}g(H(\lambda),\lambda), \tag{16}$$

symbols $[\cdots]_\infty$ and $[\cdots]_0$ denote the parts of the power expansions in λ that contain non-negative and negative powers, respectively. These equations establish a connection between the coefficients of Lax pair (2).

In what follows we restrict our consideration to functions $f(X,\lambda)$ and $g(X,\lambda)$, which possess an additional property, namely they are covariant with respect to a similarity transformation T:

$$f(T^{-1}XT,\lambda)=T^{-1}f(X,\lambda)T,\quad g(T^{-1}XT,\lambda)=T^{-1}g(X,\lambda)T. \tag{17}$$

Conditions (11), (12), and (17) are not very restrictive and are satisfied, for example, by polynomials in X and sums of negative powers of polynomials in X with scalar coefficients. If X is a self-adjoint operator, then these conditions are valid for all $f(X,\lambda)$ and $g(X,\lambda)$ determined via the spectral theorem.

III. DARBOUX COVARIANCE

Let us consider the transformation

$$\psi[1]=\psi D(\lambda), \tag{18}$$

where $\cdots[1]$ denotes the image under the transformation, and $D(\lambda)$ is an invertible linear operator depending on λ. We say that the Lax pair (2) is Darboux covariant with respect to transformation $\{\psi,A(\lambda),H(\lambda)\}\rightarrow\{\psi[1],A[1](\lambda),H[1](\lambda)\}$ if the following equations hold

$$\begin{aligned} -i\dot{\psi}[1]&=\psi[1]A[1](\lambda),\\ z_\lambda\psi[1]&=\psi[1]H[1](\lambda), \end{aligned} \tag{19}$$

and the structure of $A[1](\lambda)$ and $H[1](\lambda)$ is the same as the structure of $A(\lambda)$ and $H(\lambda)$. The notion of ''structure'' means that the shapes of the coefficients of Lax pairs (2) and (19) are the same. The most important point is that the locations of singularities of $A(\lambda)$ and $A[1](\lambda)$, $H(\lambda)$ and $H[1](\lambda)$ and their types should coincide. The transformations of the form (18) that satisfy these conditions are called Darboux transformations.[13] These transformations allow one to generate the hierarchies of solutions of nonlinear equations admitting the compatibility condition representation and of associated Lax pairs. In finite dimensional (matrix) cases $D(\lambda)$ is termed the Darboux matrix.[14]

Substituting (18) into (19) we obtain expressions for the coefficients of the transformed Lax pair

$$A[1](\lambda)=-iD(\lambda)^{-1}\dot{D}(\lambda)+D(\lambda)^{-1}A(\lambda)D(\lambda), \tag{20}$$

$$H[1](\lambda)=D(\lambda)^{-1}H(\lambda)D(\lambda). \tag{21}$$

If $D(\lambda)$ and $D(\lambda)^{-1}$ are regular on the plane of parameter λ at singular points of the coefficients of Lax pair, then the sufficient condition for $D(\lambda)$ to define the Darboux transformation comes from the requirement that the right-hand sides in Eqs. (20) and (21) have no the singularities at the points, which are the singular point of $D(\lambda)$ and $D^{-1}(\lambda)$. We refer the reader to the Appendix, where the examples of such transformation are presented.

The following theorem gives sufficient conditions of covariance of Eq. (14), which explicitly connects the coefficients of the Lax pair (2), with respect to the Darboux transformation (18), (20), and (21).

Theorem: *If $D(\lambda)$ and $D(\lambda)^{-1}$ are rational functions in λ that have poles at finite points $\mu_1,\ldots,\mu_s$ and $\mu_{s+1},\ldots,\mu_S$, respectively, $\mu_k\neq 0$ $(k=1,\ldots,S)$ and $[D(\lambda)^{-1}\dot{D}(\lambda)]_\infty=0$, then Eq. (14) is Darboux covariant.*

Proof: Substituting (14) into (20) yields

$$A[1](\lambda)=-iD(\lambda)^{-1}\dot{D}+D(\lambda)^{-1}[F(H(\lambda),\lambda)]_\infty D(\lambda)+D(\lambda)^{-1}[G(H(\lambda),\lambda)]_0 D(\lambda). \tag{22}$$

It is enough to show that

$$A[1](\lambda)=[F(H[1](\lambda),\lambda)]_\infty+[G(H[1](\lambda),\lambda)]_0. \tag{23}$$

The right-hand side of (22) is a rational function of λ with poles at most at $\mu_1,\ldots,\mu_S$ and 0, ∞. Therefore the following decomposition holds

$$A[1](\lambda)=\sum_{k=1}^{S}[A[1](\lambda)]_{\mu_k}+[A[1](\lambda)]_\infty+[A[1](\lambda)]_0, \tag{24}$$

where $[A[1](\lambda)]_{\mu_k}$ is the principal part of the Laurent expansion of $A[1](\lambda)$ at the point $\lambda=\mu_k$. Since the first term in formula (22) can have poles at most at $\mu_1,\ldots,\mu_S$ and vanishes as $\lambda\to\infty$, we obtain

$$[A[1](\lambda)]_\infty=[D(\lambda)^{-1}[F(H(\lambda),\lambda)]_\infty D(\lambda)]_\infty+[D(\lambda)^{-1}[G(H(\lambda),\lambda)]_0 D(\lambda)]_\infty,$$

$$[A[1](\lambda)]_0=[D(\lambda)^{-1}[F(H(\lambda),\lambda)]_\infty D(\lambda)]_0+[D(\lambda)^{-1}[G(H(\lambda),\lambda)]_0 D(\lambda)]_0.$$

Using equalities

$$[D(\lambda)^{-1}[F(H(\lambda),\lambda)]_\infty D(\lambda)]_\infty=[D(\lambda)^{-1}F(H(\lambda),\lambda)D(\lambda)]_\infty,$$

$$[D(\lambda)^{-1}[F(H(\lambda),\lambda)]_\infty D(\lambda)]_0=[[D(\lambda)^{-1}F(H(\lambda),\lambda)D(\lambda)]_\infty]_0=0,$$

$$[D(\lambda)^{-1}[G(H(\lambda),\lambda)]_0 D(\lambda)]_\infty=[[D(\lambda)^{-1}G(H(\lambda),\lambda)D(\lambda)]_0]_\infty=0,$$

$$[D(\lambda)^{-1}[G(H(\lambda),\lambda)]_0 D(\lambda)]_0=[D(\lambda)^{-1}G(H(\lambda),\lambda)D(\lambda)]_0,$$

we have

$$[A[1](\lambda)]_\infty=[D(\lambda)^{-1}F(H(\lambda),\lambda)D(\lambda)]_\infty, \tag{25}$$

$$[A[1](\lambda)]_0=[D(\lambda)^{-1}G(H(\lambda),\lambda)D(\lambda)]_0. \tag{26}$$

It follows from the definition of the Darboux transformation that for $k=1,\ldots,S$,

$$[A[1](\lambda)]_{\mu_k}\equiv 0. \tag{27}$$

Combining (24)–(27) and taking into account (21) and (15)–(17), we get (23). ■

It is well known that the conditions (27) can be solved resulting in an explicit expression for $D(\lambda)$ in terms of solutions of the Lax pair (2) and a dual pair, which belong to the kernel of this operator or its inverse one. For this reason, we prefer to use the name of the Darboux transformation technique instead of the dressing method. In the Appendix we give examples of the Darboux transformations, which satisfy the conditions of our theorem and can be used to construct the hierarchies of solutions of nonlinear equations (8) under constraints (9) and (10). The applications of the Darboux transformation technique to certain nonlinear equations of von Neumann type, including an equation in the infinite dimensional case, which are of interest in connection with quantum mechanics and statistical physics, can be found in Refs. 8–10.

If operator T in Eqs. (17) is independent of λ, then the expressions on the right-hand sides of these formulas correspond to so-called gauge transformations of wave functions,

$$\psi\to\tilde{\psi}=\psi T.$$

The case of the Lax pairs with $g(X,\lambda)\equiv 0$ is gauge equivalent to the case $f(X,\lambda)\equiv 0$ if T solves the equation

$$i\dot{T}=B_0 T.$$

Some of the lattice equations presented in the next sections are the compatibility condition of gauge equivalent Lax pairs.

IV. EQUATIONS OF VON NEUMANN TYPE (ONE-FIELD EQUATIONS)

In this section we consider the case $N=1$, i.e.,

$$H(\lambda)=\lambda H_1+H_0.$$

The compatibility condition of the Lax pair gives us the equation

$$\begin{aligned} i\dot{H}_0&=[B_0,H_0]+[C_1,H_1],\\ \dot{H}_1&=0, \end{aligned} \tag{28}$$

where

$$B_0=\frac{1}{L!}\left(\frac{d^L}{d\varsigma^L}f(H_1+\varsigma H_0),\varsigma^{-1})\right)\Big|_{\varsigma=0}, \tag{29}$$

$$C_1=\frac{1}{(M-1)!}\left(\frac{d^{M-1}}{d\varepsilon^{M-1}}g(\varepsilon H_1+H_0,\varepsilon)\right)\Big|_{\varepsilon=0}. \tag{30}$$

We refer to this case as "one-field" because H_1 is the constant operator. The right-hand side of Eq. (28) combines both types of the nonlinearities as in the equations of von Neumann type (1). The nonlinear equations corresponding to simplest choices of functions $f(X,\lambda)$ and $g(X,\lambda)$ are presented below. We also obtain the equations that follow them if the matrix coefficients H_1 and H_0 are defined in a special manner.

A. $f(X,\lambda)=iX^l$ $(l\in\mathbf{N})$, $g(X,\lambda)=0$, $L=1$

The compatibility condition leads to the equation

$$\dot{H}_0=\sum_{m=1}^{l}[H_1^{m-1}H_0H_1^{l-m},H_0]. \tag{31}$$

This equation with $l=2$ is a multi-dimensional Euler's top equation.[15–17] Darboux covariance of Eq. (31) and associated Lax pair was proved in Ref. 9.

Let matrices H_1 and H_0 have the form

$$H_{1,kj}=\delta_{k,j-1},\quad H_{0,kj}=\rho_k\delta_{k,j+l-1}. \tag{32}$$

Then Eq. (31) yields

$$\dot{\rho}_k=\rho_k\sum_{m=1}^{l-1}(\rho_{k+m}-\rho_{k-m}). \tag{33}$$

These equations are known as the Bogoyavlenskii lattice.[18] In the case $l=2$ Eqs. (33) coincide with the Volterra system[19]

$$\dot{\rho}_k=\rho_k(\rho_{k+1}-\rho_{k-1}), \tag{34}$$

which describes stimulated scattering of plasma oscillations by ions.[20]

B. $f(X,\lambda)=iX^{-n}$ $(n\in\mathbf{N})$, $g(X,\lambda)=0$, $L=1$

In this case Eq. (28) is written as given

$$\dot{H}_0=-\sum_{m=1}^{n}[H_1^{-m}H_0H_1^{m-n-1},H_0]. \tag{35}$$

The Bogoyavlenskii lattice (33) with $l=n+1$ follows this equation if matrices H_1 and H_0 are chosen in the form

$$H_{1,kj}=\delta_{k,j-1},\quad H_{0,kj}=\rho_k\delta_{k,j-n-1}. \tag{36}$$

C. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{l}$ $(l\in\mathbf{N})$, $M=1$

From Eq. (28) we have

$$\dot{H}_0=[H_0^l,H_1]. \tag{37}$$

Assuming that matrices H_1 and H_0 are represented in the following manner,

$$H_{1,kj}=\delta_{k,j-l+1},\quad H_{0,kj}=\rho_k\delta_{k,j+1}, \tag{38}$$

we obtain the well known lattice[18]

$$\dot{\rho}_k=\prod_{m=0}^{l-1}\rho_{k-m}-\prod_{m=0}^{l-1}\rho_{k+m}. \tag{39}$$

These equations with $l=2$ are obviously reduced to the Volterra system (34). If we put

$$\rho_k=\exp(u_k),$$

then Eqs. (39) read as

$$\dot{u}_k=\exp\left(\sum_{m=1}^{l-1}u_{k-m}\right)-\exp\left(\sum_{m=1}^{l-1}u_{k+m}\right). \tag{40}$$

As it was noted at the end of Sec. III, this case is gauge equivalent to the case in Sec. IV A.

D. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{l}$ $(l\in\mathbf{N})$, $M=2$

Equation (28) yields

$$\dot{H}_0=\sum_{m=0}^{l-1}[H_0^mH_1H_0^{l-m-1},H_1]. \tag{41}$$

Supposing

$$H_{1,kj}=\delta_{k,j-l+2},\quad H_{0,kj}=\rho_k\delta_{k,j+2}, \tag{42}$$

we have

$$\dot{\rho}_k=\sum_{m=0}^{l-1}\left(\prod_{i=0}^{m-1}\rho_{k-2i}\prod_{i=0}^{l-m-2}\rho_{k+2i-l+2}-\prod_{i=0}^{m-1}\rho_{k-2i+l-2}\prod_{i=0}^{l-m-2}\rho_{k+2i}\right). \tag{43}$$

(It is assumed hereafter that $\Pi_{i=0}^{m}\ldots_i=1$ if $m<0$.) In the case $l=3$ these equations are equivalent to the Volterra system (34).

E. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{-l}$ $(l\in\mathbb{N})$, $M=1$

Equation (28) takes the form

$$\dot{H}_0=[H_0^{-l},H_1]. \tag{44}$$

If matrices H_1 and H_0 are defined as follows,

$$H_{1,kj}=\delta_{k,j+l+1},\quad H_{0,kj}=\rho_k\delta_{k,j+1}, \tag{45}$$

then the compatibility condition implies

$$\dot{\rho}_k=\prod_{m=1}^{l}\rho_{k+m}^{-1}-\prod_{m=1}^{l}\rho_{k-m}^{-1}. \tag{46}$$

Introducing two sets of new dependent variables,

$$\rho_k=\exp(-u_k),$$

$$v_k=\rho_k^{-1},$$

we obtain equivalent representations of Eqs. (46):

$$\dot{u}_k=\exp\left(\sum_{m=0}^{l}u_{k-m}\right)-\exp\left(\sum_{m=0}^{l}u_{k+m}\right) \tag{47}$$

and

$$\dot{v}_k=v_k^2\left(\prod_{m=1}^{l}v_{k-m}-\prod_{m=1}^{l}v_{k+m}\right). \tag{48}$$

Equations (47) with $l=2$ were studied in Ref. 21. A Lax pair for Eqs. (48) was found in Ref. 18. These equations in the case $l=1$ obey a symmetry $v_k\to -v_k$ and look like a natural generalization of the Volterra system (34).

F. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{-l}$ $(l\in\mathbb{N})$, $M=2$

In this case Eq. (28) is written in the next manner

$$\dot{H}_0=-\sum_{m=1}^{l}[H_0^{-m}H_1H_0^{m-l-1},H_1]. \tag{49}$$

If matrices H_1 and H_0 are defined as follows,

$$H_{1,kj}=\delta_{k,j+l+2},\quad H_{0,kj}=\rho_k\delta_{k,j+2}, \tag{50}$$

then we come to equations

$$\dot{\rho}_k=\sum_{m=1}^{l}\left(\prod_{i=1}^{m}\rho_{k+2i-l-2}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i-2}^{-1}-\prod_{i=1}^{m}\rho_{k+2i}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i+l}^{-1}\right). \tag{51}$$

G. $f(X,\lambda)=0$, $g(X,\lambda)=g(X)$, $M=1$

Here we have

$$i\dot{H}_0=[g(H_0),H_1]. \tag{52}$$

By construction, $g(H_0)$ commutes with H_0. The Lax representation and Darboux covariance properties of Eq. (52) with arbitrary well-defined function $g(X)$ were established in Ref. 10. The cases $g(X)=iX^3$ and $g(X)=iX^{-1}$ were considered in Ref. 22 in the framework of the symmetry approach to the classification problem of integrable equations on free associative rings. The Lax representation for the equations in these cases seems to be new.

H. $f(X,\lambda)=X^4$, $g(X,\lambda)=0$, $L=2$

The compatibility condition (28) becomes

$$i\dot{H}_0=[h(H_0),H_0]=[H_1,F(H_0)] \tag{53}$$

[compare with Eqs. (1)], where

$$h(H_0)=H_0^2H_1^2+H_0H_1H_0H_1+H_0H_1^2H_0+H_1H_0^2H_1+H_1H_0H_1H_0+H_1^2H_0^2,$$

$$F(H_0)=H_0^3H_1+H_0^2H_1H_0+H_0H_1H_0^2+H_1H_0^3.$$

Let us note that, contrary to the previous example, $[F(H_0),H_0]\neq 0$. We refer to the maps $H_0\mapsto F(H_0)$ of such a kind as *non-Abelian functions*, or *non-Abelian nonlinearities*.[12] This example is a particular case of the equations (41).

V. TWO-FIELD EQUATIONS

A few examples of systems appearing if $N=2$ are considered in this section.

A. $f(X,\lambda)=iX$, $g(X,\lambda)=0$, $L=1$

The compatibility condition (8) leads to equations

$$\dot{H}_0=[H_1,H_0],$$

$$\dot{H}_1=[H_2,H_0],$$

$$\dot{H}_2=0.$$

It is checked immediately that functions

$$F_1=(H_2-\sigma H_0)/(2i),$$

$$F_2=(H_2+\sigma H_0)/2,$$

$$F_3=H_1/(2i),$$

where σ is a parameter ($\sigma\neq 0$), satisfy equations

$$\dot{F}_1=[F_2,F_3]+i[F_3,F_1], \tag{54}$$

$$\dot{F}_2=[F_3,F_1]+i[F_3,F_2], \tag{55}$$

$$\dot{F}_3=\sigma[F_1,F_2]. \tag{56}$$

In terms of new dependent variables

$$f_k = gF_k g^{-1} \quad (k=1,2,3),$$

where g solves equation

$$\dot{g} = -igF_3,$$

Eqs. (54)–(56) are rewritten as

$$\dot{f}_1 = [f_2, f_3],$$

$$\dot{f}_2 = [f_3, f_1],$$

$$\dot{f}_3 = \sigma[f_1, f_2].$$

If we impose condition $f_k^+ = -f_k$, then σ has to be real. This system with $\sigma = 1$ is known as Nahm equations.[23,24] It will be shown in the next subsection that this case is also connected with Toda lattice equation.

B. $f(X,\lambda) = iX^l$ $(l \in \mathbf{N})$, $g(X,\lambda) = 0$, $L = 1$

From Eqs. (8) we have

$$\dot{H}_0 = \sum_{m=1}^{l} [H_2^{m-1} H_1 H_2^{l-m}, H_0], \tag{57}$$

$$\dot{H}_1 = [H_2^l, H_0] + \sum_{m=1}^{l} [H_2^{m-1} H_1 H_2^{l-m}, H_1], \tag{58}$$

$$\dot{H}_2 = 0.$$

If we put

$$H_{2,kj} = \delta_{k,j-1}, \quad H_{1,kj} = h_k \delta_{k,j+l-1}, \quad H_{0,kj} = \rho_k \delta_{k,j+2l-1}, \tag{59}$$

then Eqs. (57) and (58) read as

$$\begin{aligned} \dot{h}_k &= \rho_{k+l} - \rho_k + h_k \sum_{m=1}^{l-1} (h_{k+m} - h_{k-m}), \\ \dot{\rho}_k &= \rho_k \sum_{m=0}^{l-1} (h_{k+m} - h_{k-l-m}). \end{aligned} \tag{60}$$

Let

$$h_k = \dot{\sigma}_k.$$

If coefficients ρ_k are chosen as given,

$$\rho_k = C e^{\sum_{m=0}^{l-1} (\sigma_{k+m} - \sigma_{k-l-m})}$$

(C is arbitrary constant), then system (60) is equivalent to the following equations:

$$\ddot{\sigma}_k = C(e^{\sum_{m=0}^{l-1}(\sigma_{k+m+l}-\sigma_{k-m})} - e^{\sum_{m=0}^{l-1}(\sigma_{k+m}-\sigma_{k-l-m})}) + \dot{\sigma}_k \sum_{m=1}^{l-1} (\dot{\sigma}_{k+m} - \dot{\sigma}_{k-m}). \tag{61}$$

Assuming $l=1$ and $C=1$ we come to the Toda lattice equation[25–27]

$$\ddot{\sigma}_k = e^{\sigma_{k+1}-\sigma_k} - e^{\sigma_k-\sigma_{k-1}}. \tag{62}$$

Equations (61) can be viewed as a generalization of the Toda lattice on the systems of particles interacting with a finite number of nearest neighborhoods. For $n\times n$ matrices, these equations admit additional reductions

$$\sigma_{m+1+k} = -\sigma_{m+1-k} \quad \text{if} \quad n=2m+1,$$

$$\sigma_{m+k} = -\sigma_{m+1-k} \quad \text{if} \quad n=2m,$$

or

$$\sigma_{m+k} = -\sigma_{m-k} \quad \text{if} \quad n=2m$$

$(k=0,\ldots,m)$. In the case $l=1$, these reductions lead to generalized periodic Toda lattices, whose connection with the root systems of semisimple Lie algebras was established in Ref. 28.

C. $f(X,\lambda)=iX^{-l}$ $(l\in\mathbb{N})$, $g(X,\lambda)=0$, $L=1$

The compatibility condition in this case yields

$$\dot{H}_0 = -\sum_{m=1}^{l} [H_2^{-m} H_1 H_2^{m-l-1}, H_0], \tag{63}$$

$$\dot{H}_1 = [H_2^{-l}, H_0] - \sum_{m=1}^{l} [H_2^{-m} H_1 H_2^{m-l-1}, H_1], \tag{64}$$

$$\dot{H}_2 = 0.$$

If H_2, H_1 and H_0 are defined in the following manner,

$$H_{2,kj} = \delta_{k,j+1}, \quad H_{1,kj} = h_k \delta_{k,j+l+1}, \quad H_{0,kj} = \rho_k \delta_{k,j+2l+1}, \tag{65}$$

then Eqs. (63) and (64) are written as

$$\begin{aligned} \dot{h}_k &= \rho_{k+l} - \rho_k - h_k \sum_{m=1}^{l} (h_{k+m} - h_{k-m}), \\ \dot{\rho}_k &= \rho_k \sum_{m=1}^{l} (h_{k-l-m} - h_{k+m}). \end{aligned} \tag{66}$$

In the case $l=1$ these equations are the so-called Belov–Chaltikian lattice.[29] The bilinear approach was applied to the Belov–Chaltikian lattice in Ref. 30.

Expressing dependent variables in terms of the new ones,

$$h_k = \dot{\sigma}_k,$$

$$\rho_k = C e^{\sum_{m=1}^{l}(\sigma_{k-l-m}-\sigma_{k+m})}$$

(C is a constant), we reduce Eqs. (66) to the Toda-type lattice equations

$$\ddot{\sigma}_k = C(\mathrm{e}^{\sum_{m=1}^{l}(\sigma_{k-m}-\sigma_{k+l+m})} - \mathrm{e}^{\sum_{m=1}^{l}(\sigma_{k-l-m}-\sigma_{k+m})}) - \dot{\sigma}_k \sum_{m=1}^{l} (\dot{\sigma}_{k+m} - \dot{\sigma}_{k-m}). \tag{67}$$

D. $f(X,\lambda)=0$, $g(X,\lambda)=iX^l$ $(l\in\mathbb{N})$, $M=1$

In this case Eqs. (8) are rewritten as given:

$$\dot{H}_0 = [H_0^l, H_1], \tag{68}$$

$$\dot{H}_1 = [H_0^l, H_2], \tag{69}$$

$$\dot{H}_2 = 0.$$

If matrices H_2, H_1 and H_0 have the form

$$H_{2,kj} = \delta_{k,j-2l+1}, \quad H_{1,kj} = h_k \delta_{k,j-l+1}, \quad H_{0,kj} = \rho_k \delta_{k,j+1}, \tag{70}$$

then Eqs. (68) and (69) yield

$$\begin{aligned} \dot{h}_k &= \prod_{m=0}^{l-1} \rho_{k-m} - \prod_{m=0}^{l-1} \rho_{k+l+m}, \\ \dot{\rho}_k &= h_{k-l} \prod_{m=0}^{l-1} \rho_{k-m} - h_k \prod_{m=0}^{l-1} \rho_{k+m}. \end{aligned} \tag{71}$$

These equations with $l=1$ are equivalent to the Toda lattice (62).

E. $f(X,\lambda)=0$, $g(X,\lambda)=iX^l$ $(l\in\mathbb{N})$, $M=2$

From Eqs. (8) we have

$$\dot{H}_0 = [H_0^l, H_2] + \sum_{m=0}^{l-1} [H_0^m H_1 H_0^{l-m-1}, H_1], \tag{72}$$

$$\dot{H}_1 = \sum_{m=0}^{l-1} [H_0^m H_1 H_0^{l-m-1}, H_2], \tag{73}$$

$$\dot{H}_2 = 0.$$

Taking matrices H_2, H_1 and H_0 as given,

$$H_{2,kj} = \delta_{k,j-2l+2}, \quad H_{1,kj} = h_k \delta_{k,j-l+2}, \quad H_{0,kj} = \rho_k \delta_{k,j+2}, \tag{74}$$

we put compatibility condition into the form

$$\dot{h}_k=\sum_{m=0}^{l-1}\left(h_{k-2m}\prod_{i=0}^{m-1}\rho_{k-2i}\prod_{i=0}^{l-m-2}\rho_{k+2i-l+2}-h_{k-2m+l-2}\prod_{i=0}^{m-1}\rho_{k-2i+l-2}\prod_{i=0}^{l-m-2}\rho_{k+2i}\right),$$

$$\dot{\rho}_k=h_{k-l}\sum_{m=0}^{l-1}h_{k-2m}\prod_{i=0}^{m-1}\rho_{k-2i}\prod_{i=0}^{l-m-2}\rho_{k+2i-l+2}$$

$$-h_k\sum_{m=0}^{l-1}h_{k-2m-2}\prod_{i=0}^{m-1}\rho_{k-2i-2}\prod_{i=0}^{l-m-2}\rho_{k+2i-l}+\prod_{i=0}^{l-1}\rho_{k-2i}-\prod_{i=0}^{l-1}\rho_{k+2i}. \tag{75}$$

In the case $l=2$ and $h_k=0$ these equations coincide with the Volterra system (34).

F. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{-l}$ $(l\in\mathbf{N})$, $M=1$

In this case Eqs. (8) yield

$$\dot{H}_0=[H_0^{-l},H_1], \tag{76}$$

$$\dot{H}_1=[H_0^{-l},H_2], \tag{77}$$

$$\dot{H}_2=0.$$

Let the matrices H_2, H_1, and H_0 be represented in the following manner:

$$H_{2,kj}=\delta_{k,j+2l+1},\quad H_{1,kj}=h_k\delta_{k,j+l+1},\quad H_{0,kj}=\rho_k\delta_{k,j+1}. \tag{78}$$

The compatibility condition leads to the system

$$\dot{h}_k=\prod_{m=1}^{l}\rho_{k+m}^{-l}-\prod_{m=1}^{l}\rho_{k-l-m}^{-l},$$

$$\dot{\rho}_k=h_{k+l}\prod_{m=1}^{l}\rho_{k+m}^{-l}-h_k\prod_{m=1}^{l}\rho_{k-m}^{-l}. \tag{79}$$

G. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{-l}$ $(l\in\mathbf{N})$, $M=2$

Equations (8) give

$$\dot{H}_0=[H_0^{-l},H_2]-\sum_{m=1}^{l}[H_0^{-m}H_1H_0^{m-l-1},H_1], \tag{80}$$

$$\dot{H}_1=-\sum_{m=1}^{l}[H_0^{-m}H_1H_0^{m-l-1},H_2], \tag{81}$$

$$\dot{H}_2=0.$$

Supposing

$$H_{2,kj}=\delta_{k,j+2l+2},\quad H_{1,kj}=h_k\delta_{k,j+l+2},\quad H_{0,kj}=\rho_k\delta_{k,j+2}, \tag{82}$$

we have

$$\dot{h}_k=\sum_{m=1}^{l}\left(h_{k+2m-2l-2}\prod_{i=1}^{m}\rho_{k+2i-2l-2}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i-l-2}^{-1}-h_{k+2m}\prod_{i=1}^{m}\rho_{k+2i}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i+l}^{-1}\right),$$
$$\dot{\rho}_k=h_k\sum_{m=1}^{l}h_{k+2m-l-2}\prod_{i=1}^{m}\rho_{k+2i-l-2}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i-2}^{-1}-h_{k+l}\sum_{m=1}^{l}h_{k+2m}\prod_{i=1}^{m}\rho_{k+2i}^{-1}\prod_{i=0}^{l-m}\rho_{k-2i+l}^{-1}$$
$$+\prod_{i=1}^{l}\rho_{k+2i}^{-1}-\prod_{i=1}^{l}\rho_{k-2i}^{-1}. \tag{83}$$

H. $f(X,\lambda)=iX^2$, $g(X,\lambda)=0$, $L=2$

The compatibility condition (8) in this case is written as

$$\dot{H}_0=[H_1^2,H_0]+[H_2,H_0^2],$$
$$\dot{H}_1=[H_2,H_0H_1+H_1H_0],$$
$$\dot{H}_2=0.$$

Taking matrices H_2, H_1, and H_0 as follows,

$$H_{2,kj}=\delta_{k,j-1},\quad H_{1,kj}=h_k\delta_{k,j},\quad H_{0,kj}=\rho_k\delta_{k,j+1}, \tag{84}$$

we obtain

$$\dot{h}_k=\rho_{k+1}(h_{k+1}+h_k)-\rho_k(h_k+h_{k-1}),$$
$$\dot{\rho}_k=\rho_k(\rho_{k+1}-\rho_{k-1}+h_k^2-h_{k-1}^2). \tag{85}$$

This system is the first member of the hierarchy of higher Toda lattices.[31,32] In the case $h_k=0$ this system is nothing but the Volterra system (34).

VI. MULTI-FIELD EQUATIONS

In this section we present nonlinear equations that follow Eq. (8) with positive integer N for special choices of functions $f(X,\lambda)$ and $g(X,\lambda)$.

A. $f(X,\lambda)=iX^l$ $(l\in\mathbb{N})$, $g(X,\lambda)=0$, $L=1$

The compatibility condition is

$$\dot{H}_i=[H_N^l,H_{i-1}]+\sum_{m=1}^{l}[H_N^{m-1}H_{N-1}N_N^{l-m},H_i] \tag{86}$$

$(i=0,\ldots,N)$. If we put

$$H_{i,kj}=\rho_k^{(i)}\delta_{k,j+(N-i)l-1} \tag{87}$$

$(\rho_k^{(N)}=1)$, then Eqs. (86) give

$$\dot{\rho}_k^{(i)}=\rho_{k+l}^{(i-1)}-\rho_k^{(i-1)}+\rho_k^{(i)}\sum_{m=0}^{l-1}(\rho_{k+m}^{(N-1)}-\rho_{k+(i-N+1)l-m}^{(N-1)}). \tag{88}$$

B. $f(X,\lambda)=iX^{-l}$ $(l\in\mathbf{N})$, $g(X,\lambda)=0$, $L=1$

In this case Eqs. (8) are written in the following way:

$$\dot{H}_i=[H_N^{-l},H_{i-1}]-\sum_{m=1}^{l}[H_N^{-m}H_{N-1}N_N^{m-l-1},H_i] \tag{89}$$

$(i=0,\ldots,N)$. Assuming

$$H_{i,kj}=\rho_k^{(i)}\delta_{k,j-(N-i)l-1},\quad \rho_k^{(N)}=1, \tag{90}$$

we obtain

$$\dot{\rho}_k^{(i)}=\rho_{k-l}^{(i-1)}-\rho_k^{(i-1)}+\rho_k^{(i)}\sum_{m=1}^{l}(\rho_{k+(N-i-1)l+m}^{(N-1)}-\rho_{k-m}^{(N-1)}). \tag{91}$$

C. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{l}$ $(l\in\mathbf{N})$, $M=1$

The compatibility condition (8) yields

$$\dot{H}_i=[H_0^{l},H_{i+1}] \tag{92}$$

$(i=0,\ldots,N)$. Let matrices H_i have the form

$$H_{i,kj}=\rho_k^{(i)}\delta_{k,j-il+1}, \tag{93}$$

where $\rho_k^{(N)}=1$. In this case Eqs. (92) lead to the following lattice equations:

$$\dot{\rho}_k^{(i)}=\rho_{k-l}^{(i+1)}\prod_{m=0}^{l-1}\rho_{k-m}^{(0)}-\rho_k^{(i+1)}\prod_{m=0}^{l-1}\rho_{k+il+m}^{(0)}. \tag{94}$$

The case $l=1$ was studied in Refs. 33 and 34.

D. $f(X,\lambda)=0$, $g(X,\lambda)=iX^{-l}$ $(l\in\mathbf{N})$, $M=1$

From Eqs. (8) we have

$$\dot{H}_i=[H_0^{-l},H_{i+1}] \tag{95}$$

$(i=0,\ldots,N)$. If matrices H_i are defined as follows

$$H_{i,kj}=\rho_k^{(i)}\delta_{k,j+il+1}, \tag{96}$$

then Eqs. (95) give

$$\dot{\rho}_k^{(i)}=\rho_{k+l}^{(i+1)}\prod_{m=1}^{l}\rho_{k+m}^{-1}-\rho_k^{(i+1)}\prod_{m=1}^{l}\rho_{k-il-m}^{-1}, \tag{97}$$

where we use the notation

$$\rho_k^{(0)}=\rho_k.$$

VII. CONCLUSION

In future we will continue the study of the von Neumann type equations and their generalizations presented in the previous sections. The integrals and the multi-soliton solutions will be

considered. An investigation of the hierarchies of symmetries and compatible flows for these equations can lead to new hierarchies of integrable equations.[22,35–37] The results will be of special interest in the case of integrable lattice equations. It should be also mentioned that discretizations of the lattice equations have attracted much attention in recent years (see, e.g., Ref. 38 and references therein).

ACKNOWLEDGMENTS

N.V.U. is grateful to Jan L. Cieśliński and Marek Czachor for hospitality. This research was supported in part by KBN Grant No. 2 P03B 126 22 (J.L.C.), KBN Grant No. 5 P03B 040 20 (M.C.), the Alexander von Humboldt foundation (M.C.) and Nokia–Poland (N.V.U.).

APPENDIX: DARBOUX TRANSFORMATIONS

Here we discuss briefly some particular cases of the Darboux transformation, which satisfy the conditions of the theorem in Sec. III. Let the operator $D(\lambda)$ in (18) be represented as given,

$$D(\lambda)=\mathbf{1}+\frac{\nu-\mu}{\mu-\lambda}P, \tag{A1}$$

where

$$P=\frac{\varphi\chi}{(\chi,\varphi)},$$

χ is a solution of the Lax pair (2) with parameter ν,

$$-i\dot{\chi}=\chi A(\nu),$$

$$z_\nu\chi=\chi H(\nu),$$

φ is a solution of the dual Lax pair with parameter μ,

$$i\dot{\varphi}=A(\mu)\varphi,$$

$$z_\mu\varphi=H(\mu)\varphi,$$

and (χ,φ) is a scalar product. It is obvious that $P^2=P$ and

$$-i\dot{P}=PA(\nu)P_\perp-P_\perp A(\mu)P$$

$(P_\perp=\mathbf{1}-P)$. If coefficients of the transformed Lax pair (19) are defined by

$$\begin{aligned}A(\lambda)[1]&=\sum_{k=0}^{L}\lambda^k B_k[1]+\sum_{k=1}^{M}\frac{1}{\lambda^k}C_k[1],\\ H(\lambda)[1]&=\sum_{k=0}^{N}\lambda^k H_k[1],\end{aligned} \tag{A2}$$

where

$$B_k[1]=B_k+(\mu-\nu)\sum_{m=k+1}^{L}(\mu^{m-k-1}P_\perp B_m P-\nu^{m-k-1}PB_mP_\perp),$$

$$C_k[1]=C_k-(\mu-\nu)\sum_{m=k}^{M}(\mu^{k-m-1}P_\perp C_m P-\nu^{k-m-1}PC_mP_\perp),$$

$$H_k[1]=H_k+(\mu-\nu)\sum_{m=k+1}^{N}(\mu^{m-k-1}P_\perp H_m P-\nu^{m-k-1}PH_mP_\perp),$$

then Eqs. (19) are identically fulfilled. This statement can be proved by direct computation. Since

$$D(\lambda)^{-1}=\mathbf{1}+\frac{\mu-\nu}{\nu-\lambda}P,$$

operators $D(\lambda)$ and $D(\lambda)^{-1}$ have poles in points μ and ν. It is seen from Eq. (A2) that Eq. (27) is valid.

The formulas written above form the so-called binary Darboux transformation. The corresponding Darboux transformation for an n-dimensional matrix case is produced from them if we assume in (A1) that

$$P=\varphi(\chi\varphi)^{-1}\chi,$$

where χ and φ are, respectively, $m\times n$ and $n\times m$ matrix solutions of direct and dual Lax pairs. Some examples of Darboux transformations in the infinite dimensional case, which are suitable for integrable lattice equations, were given in Ref. 13. Very recently a new construction of the Darboux transformation in terms of Clifford numbers was described in Ref. 39.

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Differential geometry of group lattices

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(Received 11 July 2002; accepted 22 November 2002)

In a series of publications we developed ''differential geometry'' on discrete sets based on concepts of noncommutative geometry. In particular, it turned out that first-order differential calculi (over the algebra of functions) on a discrete set are in bijective correspondence with digraph structures where the vertices are given by the elements of the set. A particular class of digraphs are Cayley graphs, also known as group lattices. They are determined by a discrete group G and a finite subset S. There is a distinguished subclass of ''bicovariant'' Cayley graphs with the property $\mathrm{ad}(S)S \subset S$. We explore the properties of differential calculi which arise from Cayley graphs via the above correspondence. The first-order calculi extend to higher orders and then allow us to introduce further differential geometric structures. Furthermore, we explore the properties of ''discrete'' vector fields which describe deterministic flows on group lattices. A Lie derivative with respect to a discrete vector field and an inner product with forms is defined. The Lie–Cartan identity then holds on all forms for a certain subclass of discrete vector fields. We develop elements of gauge theory and construct an analog of the lattice gauge theory (Yang–Mills) action on an arbitrary group lattice. Also linear connections are considered and a simple geometric interpretation of the torsion is established. By taking a quotient with respect to some subgroup of the discrete group, generalized differential calculi associated with so-called Schreier diagrams are obtained. [DOI: 10.1063/1.1540713]

CONTENTS

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I. INTRODUCTION

In a series of papers[1–7] we developed differential geometry on discrete sets (see also Refs. 8–14 for related work). A key concept is a differential calculus (over the algebra $\mathcal{A}$ of functions) on a set. First-order differential calculi on discrete sets were found to be in bijective correspondence with digraph structures,[3] where the vertices of the digraph are given by the elements of the set and neither multiple arrows nor loops are admitted. In particular, this supplies the elements of the set with neighborhood relations. An important example is a differential calculus which corresponds to the hypercubic lattice and which leads to an elegant formulation of lattice gauge theory.[1]

A special class of digraphs are *Cayley graphs*[15] (see Refs. 16 and 17, for example), which are also known as *group lattices* in the physics literature. These are determined by a discrete group G and a subset S. The elements of G are the vertices of the digraph and the elements of S determine (via right action) arrows from a vertex g to ''neighboring'' vertices. Hypercubic lattices, on which the usual lattice (gauge) theories are built, are special Cayley graphs. Another example of importance for physics is the truncated icosahedron which models the C_{60} Fullerene.[18] Physical models on group lattices have also been considered in Refs. 19–22, in particular. Furthermore, Cayley graphs play a role in the study of connectivity and routing problems in communication networks (see Ref. 23 for a review).

The above-mentioned correspondence between digraphs and first-order differential calculi suggests to explore those calculi which correspond to Cayley graphs. Moreover, given a first-order differential calculus which corresponds to a Cayley graph, it naturally extends to higher orders so that we have a notion of r-forms, $r>1$. This provides the basis for introducing further differential geometric structures, following general recipes of noncommutative geometry.

In Sec. II we introduce first-order differential calculi associated with group lattices. Our approach very much parallels standard constructions in ordinary differential geometry. In particular, we first introduce vector fields on a group lattice and then 1-forms as duals of these. Section III concerns maps between group lattices which are ''differentiable'' in an algebraic sense.[4] Of special importance for us are ''bicovariant'' group lattices (G,S) with the property that the left and right actions on G with respect to all elements of S are differentiable.

A first-order differential calculus naturally extends to higher orders, i.e., to a full differential calculus. The structure of differential calculi obtained from group lattices is the subject of Sec. IV.

Geometric relations are often more conveniently expressed in terms of vector fields than forms. In Sec. V we introduce a special class of vector fields which we call ''discrete'' and a subclass of ''basic'' vector fields and explore their properties. A Lie derivative with respect to a discrete vector field and an inner product of discrete vector fields and forms is defined. For basic vector fields with differentiable flow the Lie–Cartan formula holds.

Section VI treats connections on (left or right) $\mathcal{A}$-modules over differential calculi associated with group lattices. In particular, Yang–Mills fields are considered and an analog of the lattice gauge theory action on an arbitrary group lattice is constructed.

If the module is the space of 1-forms, we are dealing with linear connections. This is the subject of Sec. VII. In particular, we find that the condition of vanishing torsion of a linear connection has a simple geometric meaning.

A differential calculus on a group lattice induces a "generalized differential calculus" on a coset space. The resulting differential calculus is generalized in the sense that the space of 1-forms is, in general, larger than the $\mathcal{A}$-bimodule generated by the image of the space of functions under the action of the exterior derivative. There is a generalized digraph ("Schreier diagram" [16]) associated with such a first-order differential calculus which in general has multiple links and also loops. Some further remarks are collected in Sec. IX.

Most of the material of Sec. II already appeared in earlier work (see Refs. 2, 6, and 10, in particular), but the results in Secs. III–VIII are new to the best of our knowledge.

II. FIRST-ORDER DIFFERENTIAL CALCULUS ASSOCIATED WITH A GROUP LATTICE

Let G be a discrete group and $\mathcal{A}$ the algebra of complex-valued functions $f: G\to\mathbb{C}$.[24] With $g\in G$ we associate $e^g\in\mathcal{A}$ such that $e^g(g')=\delta_{g,g'}$ for all $g'\in G$. The set of e^g, $g\in G$, forms a linear basis of $\mathcal{A}$ over $\mathbb{C}$, since every function f can be written in the form $f=\Sigma_{g\in G}f(g)e^g$. In particular, we have $e^g e^{g'}=\delta^{g,g'}e^g$ and $\Sigma_{g\in G}e^g=\mathbf{1}$, where $\mathbf{1}$ denotes the constant function which is the unit of $\mathcal{A}$.

The left and right translations by a group element g, $L_g(g')=gg'$ and $R_g(g')=g'g$, induce automorphisms of $\mathcal{A}$ via the pull-backs $(L_g^*f)(g')=f(L_g g')=f(gg')$ and $(R_g^*f)(g')=f(R_g g')=f(g'g)$. In particular, we obtain

$$L_g^* e^{g'}=e^{g^{-1}g'},\quad R_g^* e^{g'}=e^{g'g^{-1}} \tag{2.1}$$

for all g, $g'\in G$. Introducing[25]

$$\ell_g f=R_g^* f-f \tag{2.2}$$

so that $(\ell_g f)(g')=f(g'g)-f(g')$, we find the modified Leibniz rule

$$\ell_g(ff')=(\ell_g f)(R_g^* f')+f(\ell_g f'). \tag{2.3}$$

The maps $\ell_g:\mathcal{A}\to\mathcal{A}$, $g\in G$, generate an $\mathcal{A}$-bimodule via

$$(f\cdot\ell_g)f':=f\ell_g f',\quad (\ell_g\cdot f)f':=(\ell_g f')(R_g^* f) \tag{2.4}$$

so that

$$\ell_g\cdot f=(R_g^* f)\cdot\ell_g. \tag{2.5}$$

Indeed, one easily verifies that

$$(ff')\cdot\ell_g=f\cdot(f'\cdot\ell_g),\quad \ell_g\cdot(ff')=(\ell_g\cdot f)\cdot f'. \tag{2.6}$$

The modified Leibniz rule can now be written as

$$\ell_g(ff')=(\ell_g\cdot f')f+(f\cdot\ell_g)f'. \tag{2.7}$$

Let S be a *finite* subset of G which does not contain the unit e of G. From G and S we construct a directed graph as follows. The vertices of the digraph represent the elements of G and there is an arrow from the site (vertex) representing g to the one representing gh if and only if $h\in S$. In other words, there is an arrow from g to g' iff $g^{-1}g'\in S$. A digraph obtained in this way is called a *Cayley graph* or a *group lattice*.[26]

Lemma 2.1: The connected component of the unit e in the group lattice is the subgroup of G generated by S.

Proof: Let H be the subgroup of G generated by S. Every element $g\in H$ can be written as a finite product $g=h_1^{k_1}\cdots h_r^{k_r}$ with $h_i\in S$ and $k_i\in\{\pm 1\}$. If $k_r=1$, there is an arrow from $h_1^{k_1}\cdots h_{r-1}^{k_{r-1}}$

to g. If $k_r=-1$, there is an arrow from g to $h_1^{k_1}\cdots h_{r-1}^{k_{r-1}}$. By iteration, g is connected to e. Hence H is contained in the connected component $\mathcal{C}_e$ of e. Because of the group property, every element connected to an element of H must itself be an element of H. Hence $\mathcal{C}_e=H$. ■

It follows that the group lattice (G,S) is connected if and only if S generates G (see also Ref. 27, p. 17). If the subgroup H generated by S is smaller than G, the group lattice consists of a set of disjoint but isomorphic parts corresponding to the set of left cosets gH, $g\in G$.

For $h\in S$, the maps $\ell_h:\mathcal{A}\to\mathcal{A}$ are naturally associated with the arrows of the digraph since $(\ell_h f)(g)=f(gh)-f(g)$ is the difference of the values of a function f at two connected "neighboring" points of the digraph. The maps ℓ_h generate an $\mathcal{A}$-bimodule $\mathcal{X}$.[28] At each $g\in G$, they span a linear space which we call the *tangent space* at g.

Let Ω^1 be the $\mathcal{A}$-bimodule dual to $\mathcal{X}$ such that

$$\langle f\cdot X,\alpha\rangle=\langle X,f\alpha\rangle=f\langle X,\alpha\rangle,\quad \langle X\cdot f,\alpha\rangle=\langle X,\alpha f\rangle \tag{2.8}$$

for all $X\in\mathcal{X}$, $f\in\mathcal{A}$ and $\alpha\in\Omega^1$. If $\{\theta^h|h\in S\}$ denotes the set of elements of Ω^1 dual to $\{\ell_h|h\in S\}$, so that $\langle \ell_{h'},\theta^h\rangle=\delta^h_{h'}$, then

$$\langle \ell_{h'},\theta^h f\rangle=\langle \ell_{h'}\cdot f,\theta^h\rangle=\langle (R^*_{h'}f)\cdot\ell_{h'},\theta^h\rangle=R^*_{h'}f\,\delta^h_{h'}=\langle \ell_{h'},(R^*_h f)\,\theta^h\rangle \tag{2.9}$$

for all h, $h'\in S$. Hence

$$\theta^h f=R^*_h f\,\theta^h. \tag{2.10}$$

The space of 1-forms Ω^1 is a free $\mathcal{A}$-bimodule and $\{\theta^h|h\in S\}$ is a basis. A linear map $\mathrm{d}:\mathcal{A}\to\Omega^1$ can now be introduced by

$$\mathrm{d}f=\sum_{h\in S}(\ell_h f)\,\theta^h. \tag{2.11}$$

It satisfies the Leibniz rule $\mathrm{d}(ff')=(\mathrm{d}f)f'+f(\mathrm{d}f')$. In particular, we obtain

$$\mathrm{d}e^g=\sum_{h\in S}(\ell_h e^g)\,\theta^h=\sum_{h\in S}(e^{gh^{-1}}-e^g)\,\theta^h. \tag{2.12}$$

Now we multiply both sides from the left by $e^{gh^{-1}}$ with some fixed $h\in S$. Since h is different from the unit element of G, we obtain $e^{gh^{-1}}\mathrm{d}e^g=e^{gh^{-1}}\theta^h$. From this we find[29]

$$\theta^h=\sum_{g\in G}e^{gh^{-1}}\mathrm{d}e^g=\sum_{g\in G}e^g\mathrm{d}e^{gh}. \tag{2.13}$$

Furthermore,

$$\theta:=\sum_{h\in S}\theta^h=\sum_{g\in G,h\in S}e^g\mathrm{d}e^{gh} \tag{2.14}$$

satisfies

$$\mathrm{d}f=\theta f-f\theta=[\theta,f]. \tag{2.15}$$

Moreover, we obtain

$$\langle X,\mathrm{d}f\rangle=Xf. \tag{2.16}$$

Let us introduce

$$\mathcal{I}=\{(g,g')\in G\times G | g^{-1}g'\notin S_e\}, \tag{2.17}$$

where $S_e=S\cup\{e\}$. This is the set of pairs (g,g') for which $e^g\mathrm{d}e^{g'}=0$. Note that $e^g\mathrm{d}e^g=-e^g\theta\neq 0$.

The first-order differential calculus $(\mathcal{A},\Omega^1,\mathrm{d})$ constructed above is also obtained from the universal first-order differential calculus $(\mathcal{A},\Omega_u^1,\mathrm{d}_u)$ as the quotient $\Omega^1=\Omega_u^1/\mathcal{J}^1$ with respect to the submodule $\mathcal{J}^1$ of Ω_u^1 generated by all elements of the form $e^g\mathrm{d}_u e^{g'}$ with $(g,g')\in\mathcal{I}$. If $\pi_u:\Omega_u^1\to\Omega^1$ denotes the corresponding projection, then we have $\mathrm{d}=\pi_u\mathrm{d}_u$.

Lemma 2.2: If S_e is a subgroup of G, the corresponding first-order differential calculus on the component connected to the unit is the universal one.

Proof: According to Lemma 2.1, the e-component is S_e. Since for every pair $(h,h')\in S_e\times S_e$, $h\neq h'$, there is an element $h''\in S$ such that $h=h'h''$, there is an arrow from h' to h in the associated digraph. Hence all pairs of different elements of S_e are connected by a pair of antiparallel arrows. This characterizes the universal differential calculus. ■

Example 2.1: One of the simplest examples is obtained as follows. Let $G=\mathbb{Z}$, the additive group of integers, and $S=\{1\}$. Then we have $(\ell_1 f)(k)=f(k+1)-f(k)$ and $\theta^1=\Sigma_{k\in\mathbb{Z}}e^k\mathrm{d}e^{k+1}$. Introducing the coordinate function $t=\Sigma_{k\in\mathbb{Z}}ke^k$, we find $\theta^1=\mathrm{d}t$ and $\ell_1 f=\partial_{+t}f$ with the discrete derivative $\partial_{+t}f(t)=f(t+1)-f(t)$. Hence

$$\mathrm{d}f=(\partial_{+t}f)\mathrm{d}t. \tag{2.18}$$

This example is important as a model for a discrete parameter space, and in particular as a model for discrete time. A generalization is obtained by taking the additive group $G=\mathbb{Z}^n$ and $S=\{(1,0,...,0),(0,1,0,...,0),\ldots,(0,...,0,1)\}=:\{\hat{m}|1\leqslant m\leqslant n\}$ which generates G. This leads to an oriented hypercubic lattice digraph. Then $(\ell_{\hat{m}}f)(k)=f(k+\hat{m})-f(k)=:(\partial_{+\hat{m}}f)(k)$ and $\theta^{\hat{m}}=\Sigma_{k\in\mathbb{Z}^n}e^k\mathrm{d}e^{k+\hat{m}}$. Introducing coordinates via $x=\Sigma_{k\in\mathbb{Z}^n}ke^k=(x^1,\ldots,x^n)$, we find

$$\mathrm{d}f=\sum_{m=1}^{n}(\partial_{+\hat{m}}f)\mathrm{d}x^m,\quad \theta^{\hat{m}}=\mathrm{d}x^m. \tag{2.19}$$

This differential calculus appeared first in Ref. 1 (see also Ref. 30) and turned out to be useful, in particular, in the context of lattice gauge theory[31] and completely integrable lattice models.[5] ■

Example 2.2: Let $G=\mathbb{Z}_m$ $(m=2,3,...)$, the finite additive group of elements 0, 1, 2, ..., $m-1$ with composition law addition modulo m. The unit element is $e=0$. Choosing $S=\{1\}$, we have a single basis 1-form θ^1. In contrast to example 2.1, here θ^1 is not exact. Indeed, suppose that $\theta^1=\mathrm{d}f$ for some function f. This is equivalent to $\ell_1 f=\mathbf{1}$ which leads to the contradiction $m=\Sigma_g(\ell_1 f)(g)=0$. By taking direct products of this lattice, a group lattice structure for $G=\mathbb{Z}_m^n$ is obtained. ■

Example 2.3: For $G=\mathbb{Z}_2$, the only group lattice is the complete digraph corresponding to the universal first-order differential calculus on the two elements $\{0,1\}$. For $G=\mathbb{Z}_3$, one has to distinguish two cases. If S contains a single element only, the group lattice is a closed linear chain of arrows (cf. example 2.2). The choice $S=\{1,2\}$ leads to the complete digraph on the three elements and thus to the universal differential calculus. Less simple structures appear for $G=\mathbb{Z}_m$, $m>3$. For example, choosing $G=\mathbb{Z}_4$ and $S=\{1,2\}$, we obtain the group lattice drawn in Fig. 1. ■

Example 2.4: The permutation group $\mathcal{S}_3$ has the six elements

$$e,\quad (12),(13),(23),\quad (123),(132)$$

grouped into conjugacy classes. Choosing $S=\{(12),(13),(23)\}$, we have three left-invariant 1-forms $\theta^{(12)}$, $\theta^{(13)}$, $\theta^{(23)}$. The corresponding digraph is drawn on the left-hand side of Fig. 2. Here a line represents a double arrow.

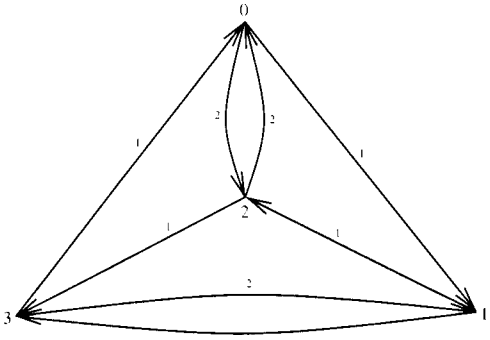

FIG. 1. The group lattice of $\mathbb{Z}_4$ with $S=\{1,2\}$.

If we choose $S=\{(123),(132)\}$, then S does not generate $\mathcal{S}_3$ and the digraph is disconnected. The two parts are drawn in the middle of Fig. 2. Since S_e is a subgroup, according to Lemma 2.2 we have the universal first-order differential calculus on the two disjoint parts of $\mathcal{S}_3$ in this case.

Another choice is $S=\{(12),(123)\}$. The corresponding digraph is shown on the right-hand side of Fig. 2 (see also Refs. 16 and 17). ■

We call a group lattice *bicovariant* if $\mathrm{ad}(S)S\subset S$. The significance of this definition will be made clear in Sec. III. Our previous examples of group lattices are indeed bicovariant, except for $(\mathcal{S}_3, S=\{(12),(123)\})$. Since S is assumed to be a *finite* set, we have the following result.

Lemma 2.3:

$$\mathrm{ad}(g)S\subset S \;\Rightarrow\; \mathrm{ad}(g^{-1})S\subset S. \tag{2.20}$$

Proof: By assumption, $\mathrm{ad}(g)$ is a map $S\to S$ which is clearly injective. Since S is a finite set, it is then also surjective. As a consequence, $\mathrm{ad}(g^{-1})S=\mathrm{ad}(g)^{-1}S=S$. ■

Example 2.5: Let $G=A_5$, the alternating group consisting of the even permutations of five objects. It is generated by the two permutations $a=(12345)$ and $b=(12)(34)$ which satisfy $a^5=e$, $b^2=e$, and $(ab)^3=e$. Let $S=\{a,a^{-1},b\}$. Then the group lattice is a truncated icosahedron, obtained from the icosahedron by replacing each of the 12 sites by a pentagon. The result is a group lattice structure for the C_{60} Fullerene.[18] This group lattice is not bicovariant. ■

In the following we refer to a pair of elements $h_1, h_2\in S$ such that $h_1h_2=e$ as a "biangle," to a triple h_0, h_1, $h_2\in S$ such that $h_1h_2=h_0$ as a "triangle," and to a quadruple of elements h_1, h_2, h_3, $h_4\in S$ such that $h_1h_2=h_3h_4\notin S_e$ as a "quadrangle" (see Fig. 3).[32] In particular, each pair h_1, h_2 of commuting elements of S with $h_1h_2\notin S_e$ determines a quadrangle.

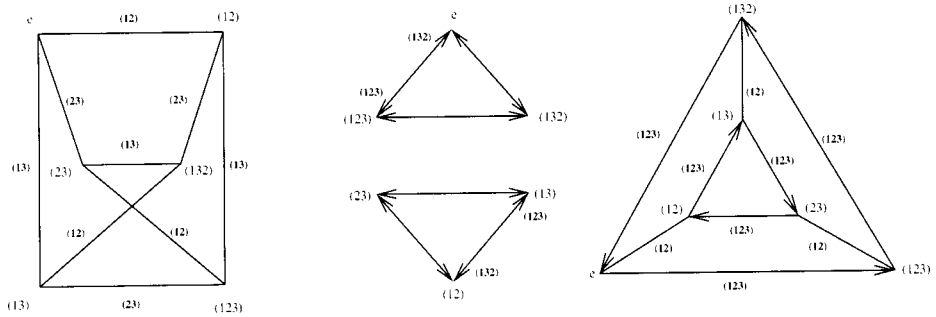

FIG. 2. Digraphs corresponding to the three different choices {(12),(13),(23)}, {(123),(132)}, and {(12),(123)} of $S\subset\mathcal{S}_3$.

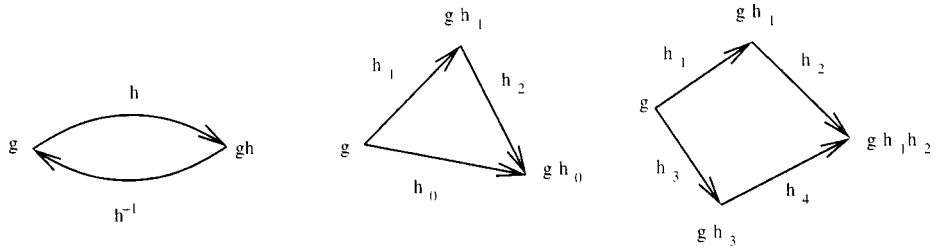

FIG. 3. Group lattice parts corresponding to a biangle, a triangle, and a quadrangle, respectively.

III. DIFFERENTIABLE MAPS BETWEEN GROUP LATTICES

Let (G_i, S_i), $i=1,2$, be two group lattices. A map $\phi: G_1 \to G_2$ induces an algebra homomorphism $\phi^*: \mathcal{A}_2 \to \mathcal{A}_1$ where $\phi^* f_2 = f_2 \circ \phi$. In particular,

$$\phi^* e^{g_2} = e^{\phi^{-1}\{g_2\}}, \tag{3.1}$$

where we introduced the notation

$$e^K := \sum_{g \in K} e^g \tag{3.2}$$

for $K \subset G$, and $e^{\varnothing} := 0$. The following result shows that every homomorphism between algebras of functions on group lattices is realized by a pull-back map (see also Ref. 33).

Theorem 3.1: *If $\Phi: \mathcal{A}_2 \to \mathcal{A}_1$ in an algebra homomorphism, then there is a map $\phi: G_1 \to G_2$, such that $\Phi = \phi^*$.*

Proof: If $f \in \mathcal{A}_1$ is such that $f^2 = f$, then $f = e^K$ for some $K \subset G_1$. In fact, since $f = \Sigma_{g_1 \in G_1} f(g_1) e^{g_1}$, we find $f(g_1)(f(g_1)-1)=0$ for all $g_1 \in G_1$, so that $f(g_1) \in \{0,1\}$. Hence $f = \Sigma_{g_1 \in K} e^{g_1}$ with $K = \{g_1 \in G_1 | f(g_1) = 1\}$. From $e^{g_2} e^{g_2'} = \delta^{g_2, g_2'} e^{g_2}$ in $\mathcal{A}_2$ we find $\Phi(e^{g_2})\Phi(e^{g_2'}) = \delta^{g_2, g_2'} \Phi(e^{g_2})$. Hence $\Phi(e^{g_2}) = e^{K_{g_2}}$ for some $K_{g_2} \subset G_1$. Furthermore, from $\Phi(e^{g_2})\Phi(e^{g_2'}) = 0$ for $g_2 \neq g_2'$ we infer $K_{g_2} \cap K_{g_2'} = \varnothing$ and from $\Phi(\mathbf{1}_2) = \mathbf{1}_1$ we obtain $\bigcup_{g_2 \in G_2} K_{g_2} = G_1$. Hence we have a partition of G_1. Now we define $\phi: G_1 \to G_2$ by setting $\phi(g_1) = g_2$ for all $g_1 \in K_{g_2}$. Then ϕ is well defined and $\phi^*(e^{g_2}) = e^{K_{g_2}} = \Phi(e^{g_2})$. ■

Now we try to extend ϕ^* to 1-forms requiring

$$\phi^*(f \mathrm{d}_2 f') = (\phi^* f)\mathrm{d}_1(\phi^* f'). \tag{3.3}$$

However, this is not well defined unless it is guaranteed that the right side vanishes whenever the left side vanishes. By linearity, it is sufficient to consider

$$\phi^*(e^{g_2} \mathrm{d}_2 e^{g_2'}) = e^{\phi^{-1}\{g_2\}} \mathrm{d}_1 e^{\phi^{-1}\{g_2'\}} \tag{3.4}$$

for all g_2, $g_2' \in G_2$. The consistency condition now takes the form $\phi^{-1}\mathcal{I}_2 \subset \mathcal{I}_1$, so that $\phi(g_1)^{-1}\phi(g_1') \notin S_2 \cup \{e_2\}$ implies $g_1^{-1} g_1' \notin S_1$. Here e_1 and e_2 are the units of G_1 and G_2, respectively. For the corresponding digraphs this implies that if there is no arrow from an image point $\phi(g_1)$ to a different image point $\phi(g_1')$, then there is also no arrow from g_1 to g_1'. The above condition is equivalent to

$$g_1^{-1} g_1' \in S_1 \;\Rightarrow\; \phi(g_1)^{-1}\phi(g_1') \in S_2 \cup \{e_2\}, \tag{3.5}$$

which says that if there is an arrow from g_1 to g_1' and $\phi(g_1)\neq\phi(g_1')$, then there is also an arrow from $\phi(g_1)$ to $\phi(g_1')$. A map with this property will be called *differentiable* (see also Ref. 4). In this case we have more generally $\phi^*(f\alpha)=(\phi^*f)(\phi^*\alpha)$ for $f\in\mathcal{A}_2$ and $\alpha\in\Omega_2^1$.

In order to define a dual of ϕ^* on vector fields, ϕ has to be differentiable and a bijection. Then we set

$$\langle\phi_* X_1,\alpha_2\rangle=\langle X_1,\phi^*\alpha_2\rangle\circ\phi^{-1}, \tag{3.6}$$

where $X_1\in\mathcal{X}_1$ and $\alpha_2\in\Omega_2^1$. As a consequence, we obtain

$$\phi_*(f\cdot X)=(\phi^{-1*}f)\cdot\phi_* X \tag{3.7}$$

and, using (2.16), we find

$$\phi_* X=\phi^{-1*}X\phi^*. \tag{3.8}$$

In particular, for each $g\in G$ the left translation $L_g: G\to G$ is a differentiable map since if $g'^{-1}g''\in S$, then also $(gg')^{-1}(gg'')\in S$. The special basis of 1-forms $\{\theta^h|h\in S\}$ and the dual basis $\{\ell_h|h\in S\}$ of vector fields are left-invariant:

$$L_g^*\theta^h=\theta^h,\quad L_{g*}\ell_h=\ell_h\quad(\forall g\in G,h\in S). \tag{3.9}$$

Hence the differential calculus of a group lattice is *left covariant*.

The condition for the right translation $R_g: G\to G$ to be differentiable is that for $g'^{-1}g''\in S$ also $(g'g)^{-1}(g''g)=g^{-1}(g'^{-1}g'')g\in S$. This amounts to $\mathrm{ad}(g^{-1})h\in S$ for all $h\in S$. As a consequence of Lemma 2.3, differentiability of R_g implies differentiability of $R_{g^{-1}}$ and we obtain

$$R_g^*\theta^h=\sum_{g'\in G}(R_g^*e^{g'})\mathrm{d}R_g^*e^{g'h}=\sum_{g''\in G}e^{g''}\mathrm{d}e^{g''ghg^{-1}}=\theta^{\mathrm{ad}(g)h}. \tag{3.10}$$

Furthermore,

$$R_{g*}\ell_h=\ell_{\mathrm{ad}(g^{-1})h},\quad R_{g^{-1}*}\ell_h=\ell_{\mathrm{ad}(g)h}. \tag{3.11}$$

If R_g and $R_{g'}$ are both differentiable, so is $R_{gg'}$ and we have $R_{gg'}^*=R_g^*\circ R_{g'}^*$ on 1-forms.

If R_g is differentiable for all $g\in G$, then the differential calculus is called *right covariant*. A differential calculus which is both left and right covariant is called *bicovariant*.[34] Bicovariance of a group lattice, as defined in Sec. II, is the weaker condition $\mathrm{ad}(h)S\subset S$ [and then also $\mathrm{ad}(h^{-1})S\subset S$] for all $h\in S$. This means that for all $h\in S$ the maps R_h and $R_{h^{-1}}$ are differentiable. If S does not generate G, this condition is indeed weaker than bicovariance of the first-order differential calculus. But then the corresponding digraph is disconnected (cf. Lemma 2.1). So, if S generates G, the bicovariance conditions for the first-order differential calculus and the group lattice coincide.

IV. HIGHER-ORDER DIFFERENTIAL CALCULUS OF A GROUP LATTICE

Let (Ω_u,d_u) be the (full) universal differential calculus over $\mathcal{A}$. Then we have $\Omega_u=\bigoplus_{r=0}^{\infty}\Omega_u^r$ with $\Omega_u^0=\mathcal{A}$. Let $\mathcal{J}$ be the differential ideal of Ω_u generated by $\mathcal{J}^1$ where $\Omega^1=\Omega_u^1/\mathcal{J}^1$. Since $\mathcal{J}^1$ is homogeneous of grade 1, the differential ideal $\mathcal{J}$ is also graded, $\mathcal{J}=\bigoplus_{r=0}^{\infty}\mathcal{J}^r$ with $\mathcal{J}^0=\{0\}$. Then $\Omega=\Omega_u/\mathcal{J}$ inherits the grading, i.e., $\Omega=\bigoplus_{r=0}^{\infty}\Omega^r$ with $\Omega^0=\mathcal{A}$. The projection $\pi_u:\Omega_u\to\Omega$ is a graded algebra homomorphism and we have a differential map $\mathrm{d}:\Omega\to\Omega$ such that $\mathrm{d}\pi_u=\pi_u\mathrm{d}_u$. It satisfies $\mathrm{d}^2=0$ and has the graded derivation property (Leibniz rule)

$$\mathrm{d}(\omega\omega')=(\mathrm{d}\omega)\omega'+(-1)^r\omega\mathrm{d}\omega' \tag{4.1}$$

for all $\omega \in \Omega^r$ and $\omega' \in \Omega$. In this section we explore for group lattices the structure of Ω beyond 1-forms.

For $(g,g') \in \mathcal{I}$ we obtain $0=\pi_u \mathrm{d}_u(e^g \mathrm{d}_u e^{g'})=\pi_u(\mathrm{d}_u e^g)\pi_u(\mathrm{d}_u e^{g'})=\mathrm{d}e^g \mathrm{d}e^{g'}$. Using (2.12) and introducing $\tilde{g}=g^{-1}g'$, this results in the 2-form relations

$$\sum_{h,h' \in S} \delta^{\tilde{g}}_{hh'} \theta^h \theta^{h'} = 0 \quad \forall \tilde{g} \notin S_e . \tag{4.2}$$

If S_e is a subgroup of G, there are no such conditions. In this case, the group lattice is disconnected with components the left cosets of S_e in G and with the universal differential calculus on each component (see Lemma 2.2). If S_e is not a subgroup, then there are elements h, $h' \in S$ such that $hh' \notin S_e$ and therefore nontrivial relations of the form (4.2) appear.

The following well-known result implies that at the level of r-forms, $r>2$, no further relations appear which are not directly taken into account by the 2-form relations.

Lemma 4.1: Let $\alpha \in \Omega^1_u$. The two-sided ideal generated by α and $\mathrm{d}_u\alpha$ is a differential ideal in Ω_u.

Proof: This is an immediate consequence of the Leibniz rule for d_u and $\mathrm{d}_u^2=0$. ■

Remark: If for some $h \in S$ also $h^{-1} \in S$, then the 2-forms $\theta^h \theta^{h^{-1}}$, $\theta^{h^{-1}} \theta^h$ do not vanish. As a consequence, we have forms $\theta^h \theta^{h^{-1}} \theta^h \cdots$ of arbitrarily high order. This could be avoided by setting $\theta^h \theta^{h^{-1}} = \theta^{h^{-1}} \theta^h = 0$. However, such a restriction may exclude interesting cases. For example, one can formulate the Connes and Lott two-point space geometry[8] using $(\mathbb{Z}_2, \{1\})$. The only nonvanishing 2-form is then $\theta^1 \theta^1$. If we set this to zero, then every 2-form automatically vanishes, and thus in particular the curvature of a connection. Moreover, such 2-form relations imposed ''by hand'' in general induce higher form relations, which have to be elaborated and taken into account. The 2-form $\theta^h \theta^{h^{-1}}$ has the interesting property that it commutes with all functions.■

Applying d to $\theta^h = \Sigma_{g \in G} e^g \mathrm{d}e^{gh}$, using the Leibniz rule for d and formulas from Sec. II, we find

$$\mathrm{d}\theta^h = \theta\theta^h + \theta^h\theta - \Delta(\theta^h), \tag{4.3}$$

where

$$\Delta(\theta^h) = \sum_{h',h'' \in S} \delta^h_{h'h''} \theta^{h'} \theta^{h''} \tag{4.4}$$

determines an $\mathcal{A}$-bimodule morphism[35] $\Delta: \Omega^1 \to \Omega^2$. Using (2.15), we obtain[36]

$$\mathrm{d}\alpha = \theta\alpha + \alpha\theta - \Delta(\alpha) \tag{4.5}$$

for an arbitrary 1-form α. A special case of this formula is

$$\mathrm{d}\theta = 2\theta^2 - \Delta(\theta). \tag{4.6}$$

As the sum of all basic 2-forms, $\theta^2 = \Sigma_{h,h' \in S} \theta^h \theta^{h'}$ comprises all the 2-form relations. Since $\Delta(\theta)$ contains all ''triangular'' 2-forms, the difference $\theta^2 - \Delta(\theta)$ consists of the sum of all nonzero 2-forms of the form $\theta^h \theta^{h'}$ with $hh'=e$. Introducing

$$\Delta^e := \sum_{h \in S_{(0)}} \theta^h \theta^{h^{-1}} \tag{4.7}$$

where $S_{(0)} := \{h \in S \,|\, h^{-1} \in S\}$, we obtain

$$\theta^2 - \Delta(\theta) = \Delta^e \tag{4.8}$$

and thus

$$\mathrm{d}\theta = \theta^2 + \Delta^e = \Delta(\theta) + 2\Delta^e. \tag{4.9}$$

Let us extend the map Δ to Ω by requiring

$$\Delta(f) = 0 \tag{4.10}$$

for all $f \in \mathcal{A}$ and

$$\Delta(\omega\omega') = \Delta(\omega)\omega' + (-1)^r \omega\Delta(\omega') \tag{4.11}$$

for all $\omega \in \Omega^r$ and $\omega' \in \Omega$. This is just the (graded) Leibniz rule, hence Δ is a graded derivation.

Lemma 4.2:

$$\mathrm{d}\omega = [\theta, \omega] - \Delta(\omega) \quad \forall\, \omega \in \Omega, \tag{4.12}$$

where [,] *is the graded commutator*.

Proof: We use induction on the grade r of forms $\omega \in \Omega^r$. For 0-forms the formula is just (2.15), for 1-forms it coincides with (4.5). Let us now assume that it holds for forms of grade lower than r. For $\psi \in \Omega^k$, $k < r$, and $\omega \in \Omega^{<r}$ we then obtain

$$\mathrm{d}(\psi\omega) = (\mathrm{d}\psi)\omega + (-1)^r \psi \mathrm{d}\omega = ([\theta, \psi] - \Delta(\psi))\omega + (-1)^r \psi\ ([\theta, \omega] - \Delta(\omega)) = [\theta, \psi\omega] - \Delta(\psi\omega)$$

using the Leibniz rules for d and Δ. ■

Iterated application of (4.11) leads to

$$\Delta(\theta^{h_1} \cdots \theta^{h_r}) = \Delta(\theta^{h_1})\theta^{h_2} \cdots \theta^{h_r} - \theta^{h_1}\Delta(\theta^{h_2})\theta^{h_3} \cdots \theta^{h_r} + \cdots + (-1)^{r-1}\theta^{h_1} \cdots \theta^{h_{r-1}}\Delta(\theta^{h_r}). \tag{4.13}$$

Furthermore,

$$\begin{aligned} 0 = \mathrm{d}^2\omega &= [\theta, \mathrm{d}\omega] - \Delta(\mathrm{d}\omega) \\ &= [\theta, [\theta, \omega]] - [\theta, \Delta(\omega)] - \Delta([\theta, \omega]) + \Delta^2(\omega) \\ &= [\theta^2 - \Delta(\theta), \omega] + \Delta^2(\omega) \end{aligned} \tag{4.14}$$

shows that

$$\Delta^2(\omega) = -[\Delta^e, \omega]. \tag{4.15}$$

Acting with Δ on (4.8), using (4.11) and the last identity, we deduce

$$\Delta(\Delta^e) = 0. \tag{4.16}$$

Remark: The cohomology of the universal differential calculus is always trivial. But this does not hold for its reductions, in general. For example, for $m > 2$, the group lattice $(\mathbb{Z}_m, \{1\})$ has nontrivial cohomology. There is only a single basis 1-form θ^1 and the 2-form relations enforce $(\theta^1)^2 = 0$ so that there are no nonvanishing 2-forms. In particular, $\mathrm{d}\theta^1 = 0$. But we have seen in example 2.2 that θ^1 is not exact. The cohomology of the group lattice $(\mathbb{Z}_4, \{1,2\})$, for example, is trivial. ■

A. Action of differentiable maps on forms

According to Sec. III, a map $\phi: G \to G$ is differentiable (with respect to a group lattice structure determined by a choice $S \subset G$) if the pull-back ϕ^* extends from $\mathcal{A}$ to the first-order differ-

ential calculus, i.e., it also acts on Ω^1 as an $\mathcal{A}$-bimodule homomorphism and satisfies $\phi^*(\mathrm{d}f) = \mathrm{d}(\phi^* f)$. Moreover, we can extend it to the whole of Ω as an algebra homomorphism via

$$\phi^*(\omega\omega') = (\phi^*\omega)(\phi^*\omega'). \tag{4.17}$$

Lemma 4.3: For a differentiable map $\phi: G \to G$ we have

$$\phi^* \circ \mathrm{d} = \mathrm{d} \circ \phi^* \quad (on\ \ \Omega). \tag{4.18}$$

Proof: Since ϕ is differentiable, the formula holds on 0-forms. If it holds on r-forms, then

$$\phi^*\mathrm{d}(f\mathrm{d}\omega) = \phi^*(\mathrm{d}f\mathrm{d}\omega) = (\phi^*\mathrm{d}f)\phi^*\mathrm{d}\omega = (\mathrm{d}\phi^* f)\mathrm{d}\phi^*\omega = \mathrm{d}[(\phi^* f)\mathrm{d}\phi^*\omega] = \mathrm{d}\phi^*(f\mathrm{d}\omega).$$

Since every $(r+1)$-form can be written as a sum of terms like $f\mathrm{d}\omega$ with $f \in \mathcal{A}$ and $\omega \in \Omega^r$, the formula holds for $(r+1)$-forms and thus on Ω by induction. ■

By definition, a differentiable map $\phi: G \to G$ preserves the 1-form relations. Since ϕ^* commutes with d, it also preserves the 2-form relations.

Lemma 4.4: For a map $\phi: G \to G$, which is differentiable and a bijection, we have

$$\phi^* \theta = \theta, \tag{4.19}$$

$$\Delta \circ \phi^* = \phi^* \circ \Delta. \tag{4.20}$$

Proof: First we note that (2.14) can be written as

$$\theta = \sum_{(g,g') \notin \mathcal{I}} e^g \mathrm{d}e^{g'} - \sum_{g \in G} e^g \mathrm{d}e^g = \sum_{g,g' \in G} e^g \mathrm{d}e^{g'} - \sum_{g \in G} e^g \mathrm{d}e^g.$$

Then, using $\phi^* e^g = e^{\phi^{-1}(g)}$, we find

$$\phi^* \theta = \sum_{g,g' \in G} e^{\phi^{-1}(g)} \mathrm{d}e^{\phi^{-1}(g')} - \sum_{g \in G} e^{\phi^{-1}(g)} \mathrm{d}e^{\phi^{-1}(g)} = \theta$$

since ϕ is bijective. The second assertion now follows from

$$[\phi^*\theta, \phi^*\omega] - \phi^*\Delta(\omega) = \phi^*\mathrm{d}\omega = \mathrm{d}\phi^*\omega = [\theta, \phi^*\omega] - \Delta(\phi^*\omega).$$

■

B. The structure of the space of 2-forms

Let $S_{(1)}$ denote the subset of S, the elements of which can be written as products of two other elements of S, i.e., $S_{(1)} = S^2 \cap S$ where $S^2 = \{hh' | h, h' \in S\}$. Furthermore, let $S_{(2)}$ be the set of elements of G which do not belong to S_e, but can be written as a product hh' for some h, $h' \in S$. Hence $S_{(2)} = S^2 \backslash S_e$. Since for every element of $S_{(2)}$ there is a 2-form relation, the number of independent 2-forms is $|S|^2 - |S_{(2)}|$. Now we have a decomposition $S \times S = \{(h, h^{-1}) | h \in S_{(0)}\} \cup \{(h,h') | hh' \in S_{(1)}\} \cup \{(h,h') | hh' \in S_{(2)}\}$ which defines a direct sum decomposition of Ω^2. Introducing projections

$$p_{(e)}(\theta^{h_1}\theta^{h_2}) = \delta^e_{h_1 h_2} \theta^{h_1}\theta^{h_2}, \tag{4.21}$$

$$p_{(h)}(\theta^{h_1}\theta^{h_2}) = \delta^h_{h_1 h_2} \theta^{h_1}\theta^{h_2} \quad (h \in S_{(1)}), \tag{4.22}$$

$$p_{(g)}(\theta^{h_1}\theta^{h_2}) = \delta^g_{h_1 h_2} \theta^{h_1}\theta^{h_2} \quad (g \in S_{(2)}), \tag{4.23}$$

which extend to left $\mathcal{A}$-module homomorphisms $p_{(e)}, p_{(h)}, p_{(g)}: \Omega^2 \to \Omega^2$, every 2-form $\psi \in \Omega^2$ can be decomposed with the help of the identity

$$\psi = \left(p_{(e)} + \sum_{h \in S_{(1)}} p_{(h)} + \sum_{g \in S_{(2)}} p_{(g)} \right) \psi. \tag{4.24}$$

The three parts of this decomposition correspond, respectively, to biangles, triangles, and quadrangles, which we introduced in Sec. II.

A relation between elements of S which leads to a 2-form relation has the form $h_1 h_1' = h_2 h_2' = \cdots = h_k h_k' \notin S_e$. The latter then implies the 2-form relation

$$\theta^{h_1} \theta^{h_1'} + \theta^{h_2} \theta^{h_2'} + \cdots + \theta^{h_k} \theta^{h_k'} = 0. \tag{4.25}$$

Let us now assume that (G,S) is bicovariant. Given $h_1, h_2 \in S$ with $h_1 h_2 \notin S_e$, we then obtain a chain $\cdots = h_0 h_1 = h_1 h_2 = h_2 h_3 = \cdots$ where $h_0 = \mathrm{ad}(h_1) h_2$ and $h_3 = \mathrm{ad}(h_2^{-1}) h_1$, and so forth. Since S is assumed to be finite, only a finite part of the chain contains pairwise different members. This means that the chain must actually consist of "cycles," i.e., subchains of the form $h_1 h_2 = h_2 h_3 = \cdots = h_{r-1} h_r = h_r h_1$. A relation like $\theta^h \theta^{h'} = 0$, consisting of a single term, is only possible if $h' = h$ and $h^2 \notin S_e$.

Example 4.1: For the permutation group $\mathcal{S}_3$ and $S = \{(12),(13),(23)\}$ (see example 2.4) we have $S_{(0)} = S$ [since $(ij)^2 = e$], $S_{(1)} = \varnothing$, and $S_{(2)} = \{(123),(132)\}$. As a consequence of the cycles $(12)(13) = (13)(23) = (23)(12) = (123)$ and $(12)(23) = (23)(13) = (13)(12) = (132)$ the three basic 1-forms $\theta^{(12)}, \theta^{(13)}, \theta^{(23)}$ have to satisfy the two 2-form relations

$$\theta^{(12)} \theta^{(13)} + \theta^{(13)} \theta^{(23)} + \theta^{(23)} \theta^{(12)} = 0, \quad \theta^{(12)} \theta^{(23)} + \theta^{(23)} \theta^{(13)} + \theta^{(13)} \theta^{(12)} = 0.$$

Hence there are $3^2 - 2 = 7$ independent 2-forms: $\theta^{(12)} \theta^{(12)}$, $\theta^{(13)} \theta^{(13)}$, $\theta^{(23)} \theta^{(23)}$ and, say, $\theta^{(13)} \theta^{(23)}$, $\theta^{(23)} \theta^{(12)}$, $\theta^{(12)} \theta^{(23)}$, $\theta^{(23)} \theta^{(13)}$.

If we choose $S = \{(123),(132)\}$, then S_e is a subgroup and we have the universal calculus on the two cosets of S_e in $\mathcal{S}_3$. Then there are no 2-form relations. ■

Example 4.2: The alternating group A_4 has the following elements,

$$e, \quad (123),(243),(134),(142), \quad (132),(234),(143),(124), \quad (12)(34),(13)(24),(14)(23)$$

grouped into conjugacy classes. Choosing $S = \{(123),(243),(134),(142)\}$, the group lattice is connected. As a consequence of

$$(123)(134) = (134)(243) = (243)(123) = (124) = (142)^2,$$

$$(123)(243) = (243)(142) = (142)(123) = (143) = (134)^2,$$

$$(123)(142) = (142)(134) = (134)(123) = (234) = (243)^2,$$

$$(134)(142) = (142)(243) = (243)(134) = (132) = (123)^2,$$

we obtain four 2-form relations, so there are 12 independent 2-forms. Note that in this example there are two different cycles for each of the elements (124), (143), (234), (132) of $S_{(2)}$. ■

Remark: For a bicovariant differential calculus a bimodule isomorphism $\sigma: \Omega^1 \otimes_{\mathcal{A}} \Omega^1 \to \Omega^1 \otimes_{\mathcal{A}} \Omega^1$ exists[6,34] such that

$$\sigma(\theta^{h_1} \otimes_{\mathcal{A}} \theta^{h_2}) = \theta^{\mathrm{ad}(h_1) h_2} \otimes_{\mathcal{A}} \theta^{h_1} = \theta^{h_0} \otimes_{\mathcal{A}} \theta^{h_1} \tag{4.26}$$

with inverse

$$\sigma^{-1}(\theta^{h_1} \otimes_{\mathcal{A}} \theta^{h_2}) = \theta^{h_2} \otimes_{\mathcal{A}} \theta^{\mathrm{ad}(h_2^{-1}) h_1} = \theta^{h_2} \otimes_{\mathcal{A}} \theta^{h_3}. \tag{4.27}$$

These formulas show that the 2-form relations, and moreover each cycle, is invariant under σ. Woronowicz[34] introduced the wedge product

$$\theta^h \wedge \theta^{h'} = \tfrac{1}{2}(\mathrm{id} - \sigma)(\theta^h \otimes_{\mathcal{A}} \theta^{h'}). \tag{4.28}$$

A particular consequence is

$$\theta^h \wedge \theta^h = 0. \tag{4.29}$$

Furthermore, for every cycle there is a 2-form relation. For example,

$$\theta^{h_1} \wedge \theta^{h_2} + \cdots + \theta^{h_r} \wedge \theta^{h_1} = 0 \tag{4.30}$$

for the cycle $h_1 h_2 = h_2 h_3 = \cdots = h_r h_1$. This means that the Woronowicz wedge product refines our 2-form relations by decoupling cycles belonging to the same $g \in S_{(2)}$ and imposing a separate 2-form relation for each cycle. In the example of the alternating group A_4, this yields eight conditions from the previous four, e.g., instead of

$$\theta^{(123)}\theta^{(134)} + \theta^{(134)}\theta^{(243)} + \theta^{(243)}\theta^{(123)} + \theta^{(142)}\theta^{(142)} = 0 \tag{4.31}$$

we obtain

$$\theta^{(123)} \wedge \theta^{(134)} + \theta^{(134)} \wedge \theta^{(243)} + \theta^{(243)} \wedge \theta^{(123)} = 0 = \theta^{(142)} \wedge \theta^{(142)}. \tag{4.32}$$

■

Example 4.3: Besides the unit element e, the group $\mathcal{S}_4$ of permutations of four objects has the following 23 elements,

$$(12),(13),(14),(23),(24),(34),$$

$$(123),(124),(132),(134),(142),(143),(234),(243),$$

$$(12)(34),(13)(24),(14)(23),$$

$$(1234),(1243),(1324),(1342),(1423),(1432),$$

grouped into conjugacy classes. Choosing $S = \{(12),(13),(14),(23),(24),(34)\}$, we find $S_{(0)} = S$, $S_{(1)} = \varnothing$ and

$$S_{(2)} = \{(123),(132),(124),(142),(134),(143),(234),(243),(12)(34),(13)(24),(14)(23)\}.$$

Hence there are 11 2-form relations and thus $6^2 - 11 = 25$ independent products of two of the 1-forms θ^h, $h \in S$. Six of them are of the form $\theta^{(ij)}\theta^{(ij)}$, $i \neq j$. These would vanish if we required the Woronowicz wedge product. ■

Given a 2-form

$$\psi = \sum_{h,h' \in S} \psi_{h,h'} \theta^h \theta^{h'} \tag{4.33}$$

the biangle and triangle coefficient functions $\psi_{h,h'}$ are uniquely determined, but there is an ambiguity in the quadrangle coefficients due to the 2-form relations (4.2). As a consequence of the latter, writing

$$\psi_{(g)} = p_{(g)}\psi = \sum_{h,h' \in S} \check{\psi}_{(g)h,h'} \theta^h \theta^{h'} \tag{4.34}$$

for $g \in S_{(2)}$, there is a freedom of gauge transformations $\check{\psi}_{(g)h,h'} \mapsto \check{\psi}_{(g)h,h'} + \Psi_{(g)}\delta^g_{hh'}$ with an arbitrary function $\Psi_{(g)}$ on G. The differences

$$\psi_{(g)h,h';\hat{h},\hat{h}'} := \check{\psi}_{(g)h,h'} - \check{\psi}_{(g)\hat{h},\hat{h}'} \tag{4.35}$$

are gauge invariant for all pairs h, h' and $\hat{h}$, $\hat{h}'$ with $\hat{h}\hat{h}' = hh' = g$. As a consequence, the *quadrangle components* of ψ (with $hh' = g$) defined in a symmetric way by

$$\psi_{(g)h,h'} := \sum_{\hat{h},\hat{h}'} \delta^g_{\hat{h}\hat{h}'}\psi_{(g)h,h';\hat{h},\hat{h}'} = |g|\check{\psi}_{h,h'} - \sum_{\hat{h},\hat{h}'} \delta^g_{\hat{h}\hat{h}'}\check{\psi}_{\hat{h},\hat{h}'} \tag{4.36}$$

with $|g| := \Sigma_{h,h'}\delta^g_{hh'}$ are independent of the choice of the coefficient functions $\check{\psi}_{(g)h,h'}$ (from their gauge equivalence class). They satisfy $\Sigma_{h,h'}\delta^g_{hh'}\psi_{(g)h,h'} = 0$ and

$$\psi_{(g)} = \frac{1}{|g|}\sum_{h,h' \in S} \delta^g_{hh'}\psi_{(g)h,h'}\theta^h\theta^{h'}. \tag{4.37}$$

The equation $\psi_{(g)} = 0$ for a 2-form ψ is equivalent to the vanishing of all the differences $\psi_{(g)h,h';\hat{h},\hat{h}'}$ where $hh' = \hat{h}\hat{h}' = g$.

Example 4.4: Consider $G = \mathcal{S}_3$ with $S = \{(12),(13),(23)\}$ (see example 4.1). A 2-form

$$\psi = \sum_{(ij),(kl) \in S} \psi_{(ij),(kl)}\theta^{(ij)}\theta^{(kl)} = \sum_{(ij) \in S} \psi_{(e)(ij),(ij)}\theta^{(ij)}\theta^{(ij)} + \sum_{\substack{(ij),(kl) \in S \\ (ij)(kl) = (123)}} \check{\psi}_{((123))(ij),(kl)}\theta^{(ij)}\theta^{(kl)}$$

$$+ \sum_{\substack{(ij),(kl) \in S \\ (ij)(kl) = (132)}} \check{\psi}_{((132))(ij),(kl)}\theta^{(ij)}\theta^{(kl)} \tag{4.38}$$

then has biangle components $\psi_{(e)(ij),(ij)}$, $(ij) \in S$. The quadrangle components are

$$\begin{aligned}
\psi_{((123))(12),(13)} &= 2\check{\psi}_{((123))(12),(13)} - \check{\psi}_{((123))(13),(23)} - \check{\psi}_{((123))(23),(12)}, \\
\psi_{((123))(13),(23)} &= 2\check{\psi}_{((123))(13),(23)} - \check{\psi}_{((123))(12),(13)} - \check{\psi}_{((123))(23),(12)}, \\
\psi_{((123))(23),(12)} &= 2\check{\psi}_{((123))(23),(12)} - \check{\psi}_{((123))(12),(13)} - \check{\psi}_{((123))(13),(23)},
\end{aligned} \tag{4.39}$$

and similar expressions for $\psi_{((132))(ij),(kl)}$. ■

V. DISCRETE AND BASIC VECTOR FIELDS

A vector field is by definition an expression of the form $X = \Sigma_{h \in S}X^h \cdot \ell_h$ with $X^h \in \mathcal{A}$. In this section we explore the properties of special classes of vector fields.

A. Discrete vector fields

A vector field will be called *discrete* if it has the property

$$X(ff') = (Xf)f' + f(Xf') + (Xf)(Xf') \quad \forall f, f' \in \mathcal{A}. \tag{5.1}$$

As a consequence, its components satisfy

$$X^hX^{h'} = \delta^{h,h'}X^h \quad \forall h, h' \in S. \tag{5.2}$$

This implies that, at every site g, the components $X^h(g)$ all vanish except for at most one component which must then be equal to 1. In particular, the vector fields ℓ_h satisfy (5.1) and are therefore discrete.

Discrete vector fields are precisely those vector fields which describe a deterministic motion on a group lattice in the following way, where S specifies the possible "directions." A "particle" moving on a group lattice stops if it reaches a site g where $X^h(g)=0$ for all $h\in S$. It moves further to gh if $X^h(g)=1$ for some $h\in S$.

In the following, a visualization is helpful. If $X^h(g)=1$, we assign an "X-arrow" to the site g pointing to the site gh in the group lattice.

Remark: An important generalization of discrete vector fields is given by vector fields $P=\Sigma_{h\in S}P^h\cdot\ell_h$ satisfying $P^h\geqslant 0$ and $\Sigma_{h\in S}P^h\leqslant\mathbf{1}$. In the context of random walks, $P^h(g)$ may be interpreted as the probability for a move from g to gh. Then $P^e(g):=1-\Sigma_{h\in S}P^h(g)$ is the probability for a rest at the site g. See also Refs. 33 and 37. ■

It is convenient to introduce X^e such that $X^e(g)=1$ if $X^h(g)=0$ for all $h\in S$, and $X^e(g)=0$ otherwise. Then we have the useful formula

$$(I+X)f=\sum_{h\in S_e}X^hR_h^*f \tag{5.3}$$

where I is the identity on $\mathcal{A}$.

Lemma 5.1: If X is a discrete vector field, then $I+X$ is an endomorphism of $\mathcal{A}$ and there is a map $\phi_X:G\to G$ such that

$$I+X=\phi_X^* \quad \textit{on } \mathcal{A}. \tag{5.4}$$

Proof: Using (5.1), it is easily verified that $I+X$ is an algebra homomorphism $\mathcal{A}\to\mathcal{A}$. Then Theorem 3.1 ensures the existence of a map $\phi_X:G\to G$ with $I+X=\phi_X^*$. ■

A more concrete description of the map ϕ_X is obtained below. Since for each $g\in G$ there is precisely one $h\in S_e$ with $X^h(g)=1$, a discrete vector field X determines a map $s_X:G\to S_e$. Then

$$X=\sum_{h\in S}X^h\cdot\ell_h=\sum_{g\in G}e^g\cdot\ell_{s_X(g)}=:\ell_{s_X} \tag{5.5}$$

(where $\ell_e=0$). Conversely, every map $s:G\to S_e$ defines a discrete vector field via the last formula. In fact, this correspondence between discrete vector fields and maps $G\to S_e$ is easily seen to be bijective.

Let us now define

$$\phi_X(g):=gs_X(g). \tag{5.6}$$

Then we obtain

$$(\phi_X^*f)(g)=f(\phi_X(g))=f(gs_X(g))=\sum_{h\in S_e}X^h(g)(R_h^*f)(g) \tag{5.7}$$

so that

$$\phi_X^*=\sum_{h\in S_e}X^hR_h^* \quad \text{on } \mathcal{A}. \tag{5.8}$$

Now (5.3) shows that $I+X=\phi_X^*$ on functions, in accordance with Lemma 5.1.

For a map $\phi:G\to G$ the expression ϕ^*-I is in general not a vector field. For example, since $(X^2f)(g)$ in general also depends on the values of f at over-next neighbors, $\phi_X^2-I=2X+X^2$ is not a vector field.

Lemma 5.2: For a map $\phi: G \to G$ the expression $\phi^* - I$ is a discrete vector field if and only if $(g, \phi(g)) \notin \mathcal{I}$ for all $g \in G$.

Proof: If $(g, \phi(g)) \notin \mathcal{I}$, then $g^{-1}\phi(g) \in S_e$ and thus defines a map $s: G \to S_e$ such that $\phi(g) = gs(g)$. This map defines a discrete vector field X such that $\phi^* = \phi_X^* = I + X$. The converse is a simple consequence of (5.6). ■

Discrete vector fields need not generate differentiable maps. In fact, since $I + \ell_h = R_h^*$, the corresponding condition for the discrete vector fields ℓ_h is $\mathrm{ad}(h^{-1})h' \in S$ for all $h' \in S$ (see Sec. III). This condition is also needed for right covariance of the group lattice differential calculus, but is weaker than that.

Theorem 5.1: *For a discrete vector field X, the following conditions are equivalent.*

(1) ϕ_X is differentiable.
(2) $(gs_X(g))^{-1} g' s_X(g') \in S_e$ for all g, g' with $g^{-1}g' \in S$.
(3) For each discrete vector field Y there is a discrete vector field Z such that $\phi_Y^* \phi_X^* = \phi_X^* \phi_Z^*$.[38]

Proof: Using (5.6), the equivalence of (1) and (2) follows from (3.5). With $X = \Sigma_{h \in S_e} X^h \cdot \ell_h$, $Y = \Sigma_{h \in S_e} Y^h \cdot \ell_h$ and $Z = \Sigma_{h \in S_e} Z^h \cdot \ell_h$, the formula in (3) reads

$$\sum_{h_1, h \in S_e} Y^h (R_h^* X^{h_1}) R_{hh_1}^* = \sum_{h_1, h' \in S_e} X^{h_1} (R_{h_1}^* Z^{h'}) R_{h_1 h'}^* .$$

Hence, for all g, $g' \in G$ we obtain

$$\sum_{h_1, h \in S_e} Y^h(g) X^{h_1}(gh)\, \delta_{hh_1}^{g'} = \sum_{h_1, h' \in S_e} X^{h_1}(g) Z^{h'}(gh_1)\, \delta_{h_1 h'}^{g'} .$$

Since $X^h(g) = \delta^h_{s_X(g)}$, this becomes

$$\sum_{h_1, h \in S_e} \delta^h_{s_Y(g)} \delta^{h_1}_{s_X(gh)} \delta^{g'}_{hh_1} = \sum_{h_1, h' \in S_e} \delta^{h_1}_{s_X(g)} \delta^{h'}_{s_Z(gh_1)} \delta^{g'}_{h_1 h'}$$

and thus

$$s_X(g)^{-1} s_Y(g) s_X(g s_Y(g)) = s_Z(g s_X(g)) \in S_e . \tag{5.9}$$

Since for all g, g' with $g^{-1}g' \in S$ there is a discrete vector field Y such that $g^{-1}g' = s_Y(g)$, we have shown that (3) implies (2). Conversely, if (2) holds, then we define $s_Z(gs_X(g))$ by the left-hand side of the above formula. This determines a discrete vector field Z at all sites except those which have an outgoing X-arrow but no incoming one. At those sites g', we can choose arbitrary values of $s_Z(g')$. Then (3) holds. ■

Example 5.1: If $\mathrm{ad}(h^{-1})S \subset S$ for all $h \in S$, then a map $s: G \to S_e$, with the property that for all $g \in G$ we have $s(gh) = s(g)$ for all $h \in S_e$, solves condition (2) of Theorem 5.1 and thus defines a discrete vector field X for which ϕ_X is differentiable. But then $X = 0$ or $X = \ell_h$ for some $h \in S$ (on each connected component of the group lattice).

Another example, which trivially satisfies condition (2), is given by a map with $s(gh) = h^{-1}s(g)h$. ■

A discrete vector field X generates a discrete flow on $\mathcal{A}$ via $(I + X)^n$, $n = 0,1,2,...$ (see also the Appendix). We sometimes refer to $\phi_X^* = I + X$ as the *flow* of X. If the flow is differentiable, then it extends to Ω. Moreover, if ϕ_X is also invertible, it induces a map ϕ_{X*} on the space $\mathcal{X}$ of vector fields via (3.6).

B. Discrete vector fields with invertible flow

The following result characterizes discrete vector fields with invertible flow.

Theorem 5.2: *Let $X=\Sigma_{h\in S}X^h\cdot\ell_h$ be a discrete vector field. The following conditions are equivalent:*

(1) $I+X$ is an automorphism of $\mathcal{A}$.
(2) For every g with $X^h(g)=1$ for some $h\in S$, there is precisely one $h'\in S$ such that $X^{h'}(gh'^{-1})=1$. If $X^h(g)=0$ for all $h\in S$, then also $X^h(gh^{-1})=0$ for all $h\in S$.[39]
(3) $\Sigma_{h\in S_e}X^h(gh^{-1})=1$ for all $g\in G$.

Proof: We already know that $I+X$ is a homomorphism (Lemma 5.1). Hence $I+X$ is an automorphism if and only if it is bijective, which means that $(I+X)f'=f$ has a unique solution f' for each $f\in\mathcal{A}$. This equation reads

$$\sum_{h'\in S_e}X^{h'}(g)f'(gh')=f(g)\quad\forall g\in G. \tag{5.10}$$

"(1)⇒(2)": We assume that $I+X$ is an automorphism. Let g be such that $X^h(g)=0$ for all $h\in S$. Suppose that $X^{h'}(gh'^{-1})=1$ for some $h'\in S$. Then (5.10) implies $f'(g)=f(g)$ and also $f'(g)=f(gh'^{-1})$ in contradiction to $I+X$ being surjective. Hence the second part of condition (2) holds.

Let g be such that $X^h(g)=1$ for some $h\in S$. Suppose that $X^{h'}(gh'^{-1})=0$ for all $h'\in S$. Then (5.10) places no restrictions on $f'(g)$ which contradicts that $I+X$ is injective. Hence $X^{h_g}(gh_g^{-1})=1$ for some $h_g\in S$. Now suppose that there are two different elements h_g, h_g' with this property. Then (5.10) implies $f'(g)=f(gh_g^{-1})=f(gh_g'^{-1})$ which restricts f. This contradicts that $I+X$ is surjective. Hence the first part of condition (2) holds.
"(2)⇒(3)": This is easily verified.
"(3)⇒(1)": Multiplying (5.10) with $X^h(g)$, $h\in S_e$, and using (5.2) leads to $X^h(g)(f'(gh)-f(g))=0$ for all $g\in G$ and $h\in S_e$. Hence, for every $g'\in G$ such that $g'^{-1}g\in S_e$ we have

$$X^{g'^{-1}g}(g')[f'(g)-f(g')]=0.$$

Condition (3) implies that for each g there is exactly one g' such that $X^{g'^{-1}g}(g')=1$. The above equation then defines a function f' on G. In fact, the latter is given by

$$f'(g)=\sum_{h\in S_e}X^h(gh^{-1})f(gh^{-1}).$$

Hence $I+X$ is surjective. Furthermore, $f=0$ enforces $f'=0$ so that $I+X$ is also injective. ■

If $I+X$ is invertible, according to condition (2) of Theorem 5.2 there is a map $r_X:G\to S_e$ such that $X^h(gh^{-1})=\delta^{h,r_X(g)}$, i.e.,

$$R^*_{h^{-1}}X^h=\delta^{h,r_X}. \tag{5.11}$$

Whereas s_X determines the outgoing X-arrow at a site g with $s_X(g)\neq e$, the map r_X determines the corresponding incoming X-arrow.

Lemma 5.3: The components of a discrete vector field X with invertible flow satisfy

$$(R^*_{h^{-1}}X^h)(R^*_{h'^{-1}}X^{h'})=\delta^{h,h'}R^*_{h^{-1}}X^h\quad\forall h,h'\in S. \tag{5.12}$$

Proof: This follows immediately from (5.11). ■

As a consequence of (5.11), both maps are related by

$$s_X(gr_X(g)^{-1}) = r_X(g). \tag{5.13}$$

Since the incoming X-arrow at $gs_X(g)$ is the outgoing X-arrow at g, also the following relation holds:

$$r_X(gs_X(g)) = s_X(g). \tag{5.14}$$

In particular, these relations imply $r_X(g)=e$ if and only if $s_X(g)=e$.

Lemma 5.4: Let X be a discrete vector field with invertible flow. Then

$$\phi_X^{-1}(g) = gr_X(g)^{-1}. \tag{5.15}$$

Proof: Using (5.6), (5.13), and (5.14), we find

$$\phi_X(gr_X(g)^{-1}) = gr_X(g)^{-1}s_X(gr_X(g)^{-1}) = gr_X(g)^{-1}r_X(g) = g,$$

$$\phi_X(g)r_X(\phi_X(g))^{-1} = gs_X(g)r_X(gs_X(g))^{-1} = gs_X(g)s_X(g)^{-1} = g.$$

■

As a consequence of (5.15), on $\mathcal{A}$ we have

$$(\phi_X^{-1})^* = R^*_{r_X^{-1}} = \sum_{h\in S_e} \delta^{h,r_X} R^*_{h^{-1}} = \sum_{h\in S_e} (R^*_{h^{-1}}X^h) R^*_{h^{-1}}. \tag{5.16}$$

Lemma 5.5: If $I+X$ with a discrete vector field X is invertible on $\mathcal{A}$, its inverse is $I+\check{X}$ with[40] $\check{X} = \sum_{h\in S} \delta^{h,r_X}\cdot \ell_{h^{-1}}$.

Proof: This follows immediately from (5.11) and (5.16). ■

Theorem 5.3: *Let X be a discrete vector field with invertible flow. Then ϕ_X is differentiable if and only if $\phi_X^{*-1} Y \phi_X^*$ is a discrete vector field for all discrete vector fields Y.*

Proof: According to Theorem 5.1, ϕ_X is differentiable if and only if for each discrete vector field Y there is a discrete vector field Z such that $\phi_Y^*\phi_X^* = \phi_X^*\phi_Z^*$. Using

$$\phi_X^{*-1} Y \phi_X^* = \phi_X^{*-1}(\phi_Y^* - I)\phi_X^* = \phi_X^{*-1}\phi_Y^*\phi_X^* - I$$

the last condition translates to

$$\phi_X^{*-1} Y \phi_X^* = \phi_Z^* - I = Z.$$

■

Corollary: Let X be a discrete vector field with differentiable and invertible ϕ_X. Then ϕ_{X*} [*defined by* (3.6)] *maps discrete vector fields to discrete vector fields.*

Proof: This follows directly from (3.8) and Theorem 5.3. ■

C. Another extension of the flow to forms and vector fields on a bicovariant group lattice

In this subsection we assume that the group lattice is bicovariant, so that R_h is differentiable for all $h\in S$ (see Sec. III). Let X be a discrete vector field. Then

$$R_X\omega := \sum_{h\in S_e} X^h R_h^*\omega \tag{5.17}$$

directly extends (5.8) from functions to arbitrary forms.

Remark: Bicovariance does not imply that ϕ_X is differentiable. Even if ϕ_X is differentiable, we have in general $\phi_X^*\omega \neq R_X\omega$ (see example 5.2 below). Hence, there are two natural actions on forms, ϕ_X^* and R_X. They coincide on functions, but differ, in general, on forms. ■

Lemma 5.6: If X is a discrete vector field with invertible flow on a bicovariant group lattice, then R_X is invertible on Ω with

$$R_X^{-1}=\sum_{h\in S_e}(R^*_{h^{-1}}X^h)R^*_{h^{-1}}. \tag{5.18}$$

Proof: We have

$$\sum_{h\in S_e}(R^*_{h^{-1}}X^h)R^*_{h^{-1}}R_X=\sum_{h,h'\in S_e}(R^*_{h^{-1}}X^h)R^*_{h^{-1}}X^{h'}R^*_{h'}=\sum_{h,h'\in S_e}(R^*_{h^{-1}}X^hX^{h'})R^*_{h^{-1}h'}$$

$$=\sum_{h\in S_e}(R^*_{h^{-1}}X^h)I=I$$

where we used (5.2) and condition (3) of Theorem 5.2 in the last steps. In a similar way, $R_X\Sigma_{h\in S_e}(R^*_{h^{-1}}X^h)\ R^*_{h^{-1}}=I$ is obtained with the help of (5.12). ■

Assuming that R_X is invertible on $\mathcal{A}$, following (3.6) we define a map R_{X*} on vector fields $Y\in\mathcal{X}$ by

$$\langle R_{X*}Y,\alpha\rangle=R_X^{-1}\langle Y,R_X\alpha\rangle. \tag{5.19}$$

Lemma 5.7: Let X be a discrete vector field with invertible flow on a bicovariant group lattice. Then R_{X*} acts on $\mathcal{X}$ as follows,

$$R_{X*}Y=\sum_{h\in S_e}(R^*_{h^{-1}}X^h)\cdot R_{h*}Y. \tag{5.20}$$

Proof: This is obtained from (5.19) using $R_X^{-1}=\phi_X^{*-1}$ on functions, (5.16), (5.2), and (3.6) applied to the map R_h. ■

With the help of (3.8), (5.11), and $\mathrm{ad}(h)^{-1}S=S$ for $h\in S_e$, (5.20) reads

$$R_{X*}Y=\sum_{h\in S_e}(R^*_{h^{-1}}X^h)\cdot R^*_{h^{-1}}Y\ \ R^*_h=\sum_{h,h'\in S_e}(R^*_{h^{-1}}X^h)(R^*_{h^{-1}}Y^{\mathrm{ad}(h)h'})\cdot\ell_{h'}$$

$$=\sum_{h,h'\in S_e}\delta^{h,r_X}\ (R^*_{h^{-1}}Y^{\mathrm{ad}(h)h'})\cdot\ell_{h'}. \tag{5.21}$$

If Y is a discrete vector field, further evaluation leads to

$$R_{X*}Y=\sum_{h'\in S_e}\delta^{\mathrm{ad}(r_X)h',s_Y\circ R_{r_X^{-1}}}\cdot\ell_{h'}=\ell_{\mathrm{ad}(r_X^{-1})(s_Y\circ R_{r_X^{-1}})}=\sum_{g\in G}e^g\cdot\ell_{\mathrm{ad}(r_X(g)^{-1})s_Y(gr_X(g)^{-1})} \tag{5.22}$$

where $r_X^{-1}(g):=(r_X(g))^{-1}$.

Lemma 5.8: Let X be a discrete vector field on a bicovariant group lattice. If R_X is invertible on $\mathcal{A}$, then R_{X*} maps discrete vector fields to discrete vector fields.

Proof: This is a simple consequence of (5.22). ■

D. Basic vector fields

A discrete vector field X which at every site has exactly one outgoing and one incoming X-arrow will be called *basic*. This means that for each $g\in G$ there is precisely one $h\in S$ such that $X^h(g)=1$ and precisely one $h'\in S$ such that $X^{h'}(gh'^{-1})=1$. As a consequence, $\Sigma_{h\in S}X^h(g)=1$ (and thus $X^e=0$) and $\Sigma_{h\in S}X^h(gh^{-1})=1$.

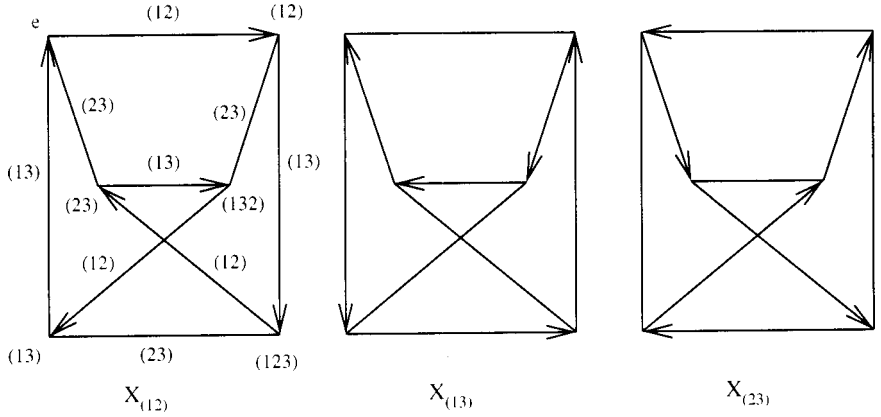

FIG. 4. A basis of basic vector fields on $\mathcal{S}_3$ with respect to $S=\{(12),(13),(23)\}$.

Lemma 5.9: A discrete vector field X is basic if and only if $I+X$ is invertible on $\mathcal{A}$ and s_X has values in S.

Proof: This is an immediate consequence of Theorem 5.2 and the definition of basic vector fields. ■

For a basic vector field, the bijection $\phi_X : G \to G$ given by $\phi_X(g) = g\, s_X(g)$ satisfies

$$\phi_X^* f = \sum_{h \in S} X^h R_h^* f \quad (\forall f \in \mathcal{A}). \tag{5.23}$$

In particular, the vector fields ℓ_h, $h \in S$, are basic and we have $\phi_{\ell_h} = R_h$.

A set of basic vector fields $\{X_h | h \in S\}$ forms a basis of $\mathcal{X}$ if for all $g \in G$ we have $e^g \cdot \{X_h | h \in S\} = e^g \cdot \{\ell_h | h \in S\}$. The elements of the dual basis of 1-forms are determined by $\langle X_h, \alpha^{h'} \rangle = \delta_h^{h'}$. The coefficient matrices in

$$X_h = \sum_{h' \in S} X_h^{h'} \cdot \ell_{h'}, \quad \alpha^h = \sum_{h' \in S} \alpha_{h'}^h \theta^{h'}, \tag{5.24}$$

which mediate the change of basis are inverse to one another. At each $g \in G$, these matrices act as permutations on S. The dual basis 1-forms satisfy $\alpha^h f = (\phi_{X_h}^* f)\alpha^h$. Furthermore, $\Sigma_h \alpha^h = \theta$ and

$$\mathrm{d}f = \sum_{h \in S} (X_h f)\alpha^h. \tag{5.25}$$

Example 5.2: Let us consider $\mathcal{S}_3$ with $S=\{(12),(13),(23)\}$ (see also example 2.4). Figure 4 shows three vector fields which form a basis of $\mathcal{X}$. For the basic vector field

$$X = (e^e + e^{(123)} + e^{(132)}) \cdot \ell_{(12)} + (e^{(12)} + e^{(13)} + e^{(23)}) \cdot \ell_{(13)}$$

we obtain $s_X(e) = s_X(123) = s_X(132) = (12)$ and $s_X(12) = s_X(13) = s_X(23) = (13)$, and ϕ_X is differentiable.[41] Since $\theta^h = \Sigma_g e^g \mathrm{d} e^{gh}$, we have $\phi_X^*(\theta^h) = \Sigma_g \phi_X^*(e^g)\mathrm{d}\phi_X^*(e^{gh})$. In this way we obtain $\phi_X^*(\theta^{(12)}) = \theta^{(13)}$. On the other hand, with

$$R_X = (e^e + e^{(123)} + e^{(132)})R_{(12)}^* + (e^{(12)} + e^{(13)} + e^{(23)})R_{(13)}^*,$$

we find

$$R_X(\theta^{(12)}) = (e^e + e^{(123)} + e^{(132)})\,\theta^{(12)} + (e^{(12)} + e^{(13)} + e^{(23)})\,\theta^{(23)},$$

which is different from $\phi_X^*(\theta^{(12)})$. Hence, in general we have $\phi_X^* \neq R_X$ on forms. ■

Example 5.3: Let us choose $G=\mathbb{Z}_3\times\mathbb{Z}_3$ with $S=\{(0,1),(1,0)\}$. Then

$$X^{(0,1)}=e^{(0,0)}+e^{(1,0)}+e^{(0,1)}+e^{(2,1)}+e^{(1,2)}+e^{(2,2)}, \quad X^{(1,0)}=e^{(2,0)}+e^{(1,1)}+e^{(0,2)}$$

are the components of a basic vector field. The corresponding map ϕ_X is *not* differentiable. Since $(1,0)^{-1}(2,0)=(1,0)\in S$ (using a multiplicative notation for the group operation), but $s_X((1,0))^{-1}(1,0)^{-1}(2,0)s_X((2,0))\notin S_e$, this follows using Theorem 5.1. We can also apply (3.5) directly: there is an arrow from (1, 0) to (2, 0) in the group lattice, but $\phi_X((1,0))=(1,1)$ is not connected with $\phi_X((2,0))=(0,0)$. ■

In the following we restrict our considerations to bicovariant group lattices [so that $\mathrm{ad}(S)S\subset S$ and $\mathrm{ad}(S)^{-1}S\subset S$].

Lemma 5.10: If X is a basic vector field, then R_X is invertible on Ω with

$$R_X^{-1}=\sum_{h\in S}(R^*_{h^{-1}}X^h)R^*_{h^{-1}}. \tag{5.26}$$

Furthermore, for $Y\in\mathcal{X}$ we have

$$R_{X*}Y=\sum_{h\in S}(R^*_{h^{-1}}X^h)R_{h*}Y. \tag{5.27}$$

Proof: Since a basic vector field has an invertible flow and $X^e=0$, the first equation follows directly from Lemma 5.6 and the second from Lemma 5.7. ■

Two basic vector fields *X,Y* form a *biangle* if $s_Y\cdot s_X=e$, which associates with each $g\in G$ a group lattice biangle.[42] Three basic vector fields *X,Y,Z* constitute a *triangle* if $s_Y\cdot s_X=s_Z$, which assigns to each $g\in G$ a group lattice triangle. Furthermore, four basic vector fields *X,Y,W,Z* make up a *quadrangle* if $s_Y\cdot s_X=s_W\cdot s_Z\notin S_e$. This maps a group lattice quadrangle to each *g*. Below we express these conditions more directly in terms of the vector fields with the help of the next result.

Lemma 5.11: For basic vector fields X and Y the following identity holds,

$$R_XR_{R_{X*}Y}=R^*_{s_Y\cdot s_X}. \tag{5.28}$$

Proof:

$$\begin{aligned}
R_XR_{R_{X*}Y}&=\sum_{h,h_1,h_2\in S}X^{h_1}(R^*_{h_1h^{-1}}X^h)(R^*_{h_1h^{-1}}Y^{\mathrm{ad}(h)h_2})R^*_{h_1h_2}\\
&=\sum_{h_1,h_2\in S}X^{h_1}Y^{\mathrm{ad}(h_1)h_2}R^*_{h_1h_2}\\
&=\sum_{g\in S^2}\left(\sum_{h_1,h_2\in S}\delta^g_{h_1h_2}X^{h_1}Y^{\mathrm{ad}(h_1)h_2}\right)R^*_g\\
&=\sum_{g\in S^2}\left(\sum_{h_1,h_2\in S}\delta^g_{h_2h_1}X^{h_1}Y^{h_2}\right)R^*_g=\sum_{g\in S^2}\delta^g_{s_Y\cdot s_X}R^*_g=R^*_{s_Y\cdot s_X}
\end{aligned}$$

using (5.21) and (5.12). ■

The above biangle condition is now seen to be equivalent to

$$R_XR_{R_{X*}Y}=I \tag{5.29}$$

and the triangle condition can be expressed as

$$R_X R_{R_X * Y} = R_Z \,. \tag{5.30}$$

Furthermore, the above quadrangle condition takes the form

$$R_X R_{R_X * Y} = R_Z R_{R_Z * W} \neq R_{X'} \tag{5.31}$$

for all discrete vector fields X'.

E. Lie derivative with respect to a discrete vector field

The notion of the Lie derivative is easily taken over from continuum differential geometry to the discrete framework of group lattices. Let X be a discrete vector field. On functions, the Lie derivative with respect to X is given by

$$\pounds_X f = \phi_X^* f - f = (I + X) f - f = Xf. \tag{5.32}$$

If ϕ_X is differentiable, we can extend the Lie derivative to forms $\omega \in \Omega$ via

$$\pounds_X \omega = \phi_X^* \omega - \omega \tag{5.33}$$

so that, in particular,

$$\pounds_{\ell_h} \omega = R_h^* \omega - \omega, \quad \pounds_{\ell_h} \theta^{h'} = \theta^{\mathrm{ad}(h) h'} - \theta^{h'}. \tag{5.34}$$

For ψ, $\omega \in \Omega$, we also have

$$\pounds_X (\psi \omega) = \phi_X^* (\psi \omega) - \psi \omega = (\pounds_X \psi)\, \omega + \psi \pounds_X \omega + (\pounds_X \psi) \pounds_X \omega. \tag{5.35}$$

Assuming ϕ_X to be differentiable and invertible, the Lie derivative acts on vector fields as follows,

$$\pounds_X Y = Y - \phi_{X*} Y = \phi_X^{*-1} \circ [X, Y] \tag{5.36}$$

using (3.8). In particular, with $I + \ell_h = R_h^*$ we obtain

$$\pounds_{\ell_h} \ell_{h'} = R_{h^{-1}}^* \circ [R_h^*, R_{h'}^*] = R_{h'}^* - R_{\mathrm{ad}(h^{-1}) h'}^* \,. \tag{5.37}$$

Since $\mathrm{ad}(h^{-1}) h' \in S$ for differentiable R_h, this can be written as

$$\pounds_{\ell_h} \ell_{h'} = \ell_{h'} - \ell_{\mathrm{ad}(h^{-1}) h'} \tag{5.38}$$

and also in the form

$$\pounds_{\ell_h} \ell_{h'} = \ell_h \ell_{\mathrm{ad}(h^{-1}) h'} - \ell_{h'} \ell_h \tag{5.39}$$

which involves a generalization of the ordinary commutator of vector fields.

F. Inner product of discrete vector fields and forms

In this subsection we extend the inner product (or contraction) $\langle X, \alpha \rangle$ of vector fields and 1-forms to forms of higher grade. More precisely, we restrict our considerations to *discrete* vector fields X with a *differentiable* flow, i.e., the associated map ϕ_X is assumed to be differentiable.

For all $f \in \mathcal{A}$ and $\alpha \in \Omega^1$ we require

$$X \lrcorner f = 0, \quad X \lrcorner \alpha = \langle X, \alpha \rangle. \tag{5.40}$$

Furthermore, for a discrete vector field X with differentiable map ϕ_X, we demand

$$X\lrcorner(\omega\omega')=(X\lrcorner\omega)\phi_X^*\omega'+(-1)^r\omega(X\lrcorner\omega') \tag{5.41}$$

for all $\omega\in\Omega^r$ and $\omega'\in\Omega$.[43] In particular, using (2.16) and the Leibniz rule for d, we obtain

$$X(ff')=X\lrcorner d(ff')=(Xf)\phi_X^*f'+fXf', \tag{5.42}$$

which is a reformulation of (5.1).

It is easily verified that (5.41) is compatible with the $\mathcal{A}$-bimodule structure of Ω, i.e., $X\lrcorner[(\omega f)\omega']=X\lrcorner[\omega(f\omega')]$. The consistency with the commutation relations (2.10) follows from

$$X\lrcorner(\theta^h f)=(X\lrcorner\theta^h)\phi_X^*f=X^h\sum_{h'}X^{h'}R_{h'}^*f=X^hR_h^*f=(R_h^*f)(X\lrcorner\theta^h)=X\lrcorner[(R_h^*f)\theta^h] \tag{5.43}$$

which holds for a discrete vector field X.

The definition (5.41) is also consistent with the 2-form relations. Let $(g,g')\in\mathcal{I}$, so that $0=e^g\mathrm{d}e^{g'}=-(\mathrm{d}e^g)e^{g'}$. The corresponding 2-form relation is $\mathrm{d}e^g\mathrm{d}e^{g'}=0$. Applying $X\lrcorner$ to the left hand side, we obtain

$$\begin{aligned}X\lrcorner(\mathrm{d}e^g\mathrm{d}e^{g'})&=(X\lrcorner\mathrm{d}e^g)\phi_X^*(\mathrm{d}e^{g'})-\mathrm{d}e^gX\lrcorner\mathrm{d}e^{g'}=(Xe^g)\mathrm{d}(\phi_X^*e^{g'})-\mathrm{d}e^g(Xe^{g'})\\&=(\phi_X^*e^g-e^g)\mathrm{d}(\phi_X^*e^{g'})-\mathrm{d}e^g(\phi_X^*e^{g'}-e^{g'})\\&=\phi_X^*(e^g\mathrm{d}e^{g'})-e^g\mathrm{d}(\phi_X^*e^{g'})-\mathrm{d}e^g\phi_X^*e^{g'}-(\mathrm{d}e^g)e^{g'}=-\mathrm{d}(e^g\phi_X^*e^{g'}).\end{aligned} \tag{5.44}$$

But the last expression vanishes since the function $e^g\phi_X^*e^{g'}$ vanishes identically. Indeed, it obviously vanishes at elements of G different from g. Evaluated at g, it yields $(\phi_X^*e^{g'})(g)=e^{g'}(\phi_X(g))=e^{g'}(gs(g))$ which vanishes since $(g,g')\in\mathcal{I}$.

Remark: Let $h_1h_2=h_2h_3=\cdots=h_rh_1$ be a cycle of a bicovariant group lattice. Then

$$\ell_h\lrcorner(\theta^{h_1}\theta^{h_2}+\theta^{h_2}\theta^{h_3}+\cdots)=\delta_h^{h_1}R_h^*\theta^{h_2}-\delta_h^{h_2}\theta^{h_1}+\delta_h^{h_2}R_h^*\theta^{h_3}-\delta_h^{h_3}\theta^{h_2}+\cdots,$$

where the second and third terms on the right-hand side cancel since $\mathrm{ad}(h_2)h_3=h_1$, and the same happens with the remaining terms. In particular, the first term cancels the last one. Since the 2-form relations are sums of cycles, this means that $\ell_h\lrcorner$ applied to a 2-form relation automatically vanishes. In fact, we have the stronger result that ℓ_h-contractions with any cycle vanish (which perfectly matches the Woronowicz wedge product). A particular consequence is that the condition $\psi=0$ for a 2-form $\psi=\psi_{h_1,h_2}\theta^{h_1}\theta^{h_2}$ is stronger than $\ell_h\lrcorner\psi=0$ for all $h\in S$. For example, the vanishing of $\ell_{h_1}\lrcorner\ell_{h_2}\lrcorner\psi=\psi_{h_2,\mathrm{ad}(h_2^{-1})h_1}-\psi_{h_1,h_2}$ obviously does not imply vanishing ψ. ■

Lemma 5.12: If X is a basic vector field with differentiable flow, then

$$X\lrcorner\Delta(\omega)+\Delta(X\lrcorner\omega)=0\quad(\forall\,\omega\in\Omega). \tag{5.45}$$

Proof: For functions the identity is trivially satisfied. Let us prove it first for 1-forms. A basic vector field satisfies $X\lrcorner\theta=\mathbf{1}$ and the flow map ϕ_X is a bijection. Since ϕ_X is assumed to be differentiable, we also have $\phi_X^*\theta=\theta$ according to (4.19). As a consequence, we find

$$X\lrcorner\theta^2=(X\lrcorner\theta)\phi_X^*\theta-\theta(X\lrcorner\theta)=0.$$

Using

$$\Delta([\theta,f])=[\Delta(\theta),f]=[\theta^2-\Delta^e,f]=[\theta^2,f]$$

for $f \in \mathcal{A}$, we thus obtain

$$X \lrcorner \Delta(\mathrm{d}f) + \Delta(X \lrcorner \mathrm{d}f) = X \lrcorner \Delta(\mathrm{d}f) = 0.$$

Since every 1-form α is a sum of terms like $f' \mathrm{d}f$ with $f, f' \in \mathcal{A}$, the last identity extends to

$$X \lrcorner \Delta(\alpha) + \Delta(X \lrcorner \alpha) = X \lrcorner \Delta(\alpha) = 0.$$

Let us now assume that our assertion holds for differential forms of grade $< k$. Then we find

$$\begin{aligned} X \lrcorner \Delta(\psi\omega) + \Delta(X \lrcorner (\psi\omega)) &= X \lrcorner (\Delta(\psi)\omega + (-1)^r \psi \Delta(\omega)) + \Delta((X \lrcorner \psi)\phi_X^* \omega + (-1)^r \psi X \lrcorner \omega) \\ &= X \lrcorner \Delta(\psi)\phi_X^* \omega - (-1)^r \Delta(\psi) X \lrcorner \omega + (-1)^r (X \lrcorner \psi)\phi_X^* \Delta(\omega) \\ &\quad + \psi X \lrcorner \Delta(\omega) + \Delta(X \lrcorner \psi)\phi_X^* \omega - (-1)^r (X \lrcorner \psi)\Delta(\phi_X^* \omega) \\ &\quad + (-1)^r \Delta(\psi) X \lrcorner \omega + \psi \Delta(X \lrcorner \omega) = 0 \end{aligned}$$

for $\psi \in \Omega^r$, $r < k$, and $\omega \in \Omega^{<k}$, using $\phi_X^* \circ \Delta = \Delta \circ \phi_X^*$ [see (4.20)]. By induction on the grade of the argument ω, the formula (5.45) is proven. ■

Theorem 5.4: *For a basic vector field X with differentiable flow the following (Lie–Cartan) identity holds,*

$$\mathcal{L}_X \omega = X \lrcorner \mathrm{d}\omega + \mathrm{d}(X \lrcorner \omega) \quad (\forall\, \omega \in \Omega). \tag{5.46}$$

Proof: With the help of (4.12) and (5.41), (5.45) can be reformulated as follows,

$$\begin{aligned} 0 &= X \lrcorner \Delta(\omega) + \Delta(X \lrcorner \omega) \\ &= X \lrcorner ([\theta, \omega] - \mathrm{d}\omega) + [\theta, X \lrcorner \omega] - \mathrm{d}(X \lrcorner \omega) \\ &= (X \lrcorner \theta)\phi_X^* \omega - (-1)^r (X \lrcorner \omega)\phi_X^* \theta - \omega X \lrcorner \theta - X \lrcorner \mathrm{d}\omega + (-1)^r (X \lrcorner \omega)\theta - \mathrm{d}(X \lrcorner \omega) \\ &= \phi_X^* \omega - \omega - X \lrcorner \mathrm{d}\omega - \mathrm{d}(X \lrcorner \omega) \end{aligned}$$

for $\omega \in \Omega^r$, using in the last step $X \lrcorner \theta = \mathbf{1}$ and $\phi_X^* \theta = \theta$, which hold for a basic vector field with differentiable flow. Now (5.46) is obtained recalling the definition (5.33). ■

Lemma 5.13: If $\phi: G \to G$ is an invertible differentiable map and X a discrete vector field with differentiable flow, then

$$\phi^*(X \lrcorner \omega) = (\phi_*^{-1} X) \lrcorner \phi^* \omega \quad (\forall\, \omega \in \Omega). \tag{5.47}$$

Proof: For a 1-form α the formula follows from (3.6) (even more generally for an arbitrary vector field X). Furthermore, we have

$$\phi^*[X \lrcorner (\psi\omega)] = \phi^*[(X \lrcorner \psi)\phi_X^* \omega + (-1)^r \psi X \lrcorner \omega] = \phi^*(X \lrcorner \psi)\phi^* \phi_X^* \omega + (-1)^r (\phi^* \psi)\phi^*(X \lrcorner \omega).$$

Let us assume that the identity holds for grades lower than k. For $\psi \in \Omega^r$, $r < k$, and ω of grade lower than k, we then obtain

$$\begin{aligned} \phi^*[X \lrcorner (\psi\omega)] &= [(\phi_*^{-1} X) \lrcorner \phi^* \psi]\phi^* \phi_X^* \phi^{*-1}(\phi^* \omega) + (-1)^r (\phi^* \psi)(\phi_*^{-1} X) \lrcorner \phi^* \omega \\ &= (\phi_*^{-1} X) \lrcorner \phi^*(\psi\omega) \end{aligned}$$

since

$$\phi^* \phi_X^* \phi^{*-1} = \phi^*(I + X)\phi^{*-1} = I + \phi_*^{-1} X = \phi_{\phi_*^{-1} X}^*$$

using (3.8). Now the identity follows by induction. ■

Lemma 5.14: A discrete vector field X with differentiable flow satisfies

$$X \lrcorner X \lrcorner \omega = 0 \quad (\forall\, \omega \in \Omega). \tag{5.48}$$

Proof: Again, we use induction with respect to the grade of ω. We have $X \lrcorner X \lrcorner \alpha = 0$ trivially for $\alpha \in \Omega^1$. Next we calculate

$$\begin{aligned} X \lrcorner X \lrcorner (\psi\omega) &= X \lrcorner [(X \lrcorner \psi)\phi_X^* \omega + (-1)^r \psi X \lrcorner \omega] \\ &= (X \lrcorner X \lrcorner \psi)\phi_X^{*2}\omega - (-1)^r (X \lrcorner \psi) X \lrcorner \phi_X^* \omega \\ &\quad + (-1)^r (X \lrcorner \psi)\phi_X^* (X \lrcorner \omega) + \psi (X \lrcorner X \lrcorner \omega) \end{aligned}$$

with the help of Lemma 5.13 and

$$\phi_{X*}^{-1} X = \phi_X^* X (\phi_X^{-1})^* = \phi_X^* (\phi_X^* - I)(\phi_X^{-1})^* = \phi_X^* - I = X.$$

This implies that if the assertion holds for ω of grade $< r$, then it also holds for grade r. ■

VI. CONNECTIONS AND PARALLEL TRANSPORTS

A *connection* on a left $\mathcal{A}$-module $\mathfrak{C}$ is a linear map $\nabla : \mathfrak{C} \to \Omega^1 \otimes_{\mathcal{A}} \mathfrak{C}$ such that

$$\nabla(fE) = \mathrm{d}f \otimes_{\mathcal{A}} E + f\nabla(E) \quad (\forall E \in \mathfrak{C}). \tag{6.1}$$

If (Ω, d) is the differential calculus of a group lattice, we have the following result.

Lemma 6.1: Every connection on $\mathfrak{C}$ is of the form

$$\nabla(E) = \theta \otimes_{\mathcal{A}} E - \mathcal{V}(E) \quad (\forall E \in \mathfrak{C}), \tag{6.2}$$

where $\mathcal{V} : \mathfrak{C} \to \Omega^1 \otimes_{\mathcal{A}} \mathfrak{C}$ satisfies

$$\mathcal{V}(fE) = f\mathcal{V}(E). \tag{6.3}$$

Conversely, every linear map $\mathcal{V}$ with this property defines a connection via the above formula.

Proof: This is easily verified using (2.15). ■

Writing

$$\mathcal{V} = \sum_{h \in S} \theta^h \otimes_{\mathcal{A}} \mathcal{V}_{\ell_h} \tag{6.4}$$

with *parallel transport operators* $\mathcal{V}_{\ell_h}$ in the ℓ_h direction, (6.3) leads to

$$\mathcal{V}_{\ell_h}(fE) = (R_{h^{-1}}^* f)\mathcal{V}_{\ell_h}(E) \tag{6.5}$$

using (2.10). In particular,

$$\mathcal{V}_{\ell_h}(e^g E) = e^{gh} \mathcal{V}_{\ell_h}(E), \tag{6.6}$$

which shows that we have a transport in the forward direction. We generalize it to a transport along an arbitrary vector field X by

$$\mathcal{V}_X = \sum_{h \in S} (R_{h^{-1}}^* X^h) \mathcal{V}_{\ell_h}. \tag{6.7}$$

Lemma 6.2: For a basic vector field X,

$$\mathcal{V}_X(fE)=(R_X^{-1}f)\mathcal{V}_XE. \tag{6.8}$$

Proof: Using (6.7), (6.5), (5.12), and (5.26) we obtain

$$\mathcal{V}_X(fE)=\sum_{h\in S}(R^*_{h^{-1}}X^h)(R^*_{h^{-1}}f)\mathcal{V}_{\ell_h}E$$

$$=\sum_{h,h'\in S}(R^*_{h^{-1}}X^h)(R^*_{h^{-1}}f)(R^*_{h'^{-1}}X^{h'})\mathcal{V}_{\ell_{h'}}E=(R_X^{-1}f)\mathcal{V}_XE.$$

■

A connection can be extended to a map $\nabla:\Omega\otimes_{\mathcal{A}}\mathfrak{C}\to\Omega\otimes_{\mathcal{A}}\mathfrak{C}$ via

$$\nabla(\omega\otimes_{\mathcal{A}}E)=\mathrm{d}\omega\otimes_{\mathcal{A}}E+(-1)^r\omega\nabla E\quad\forall\,\omega\in\Omega^r,E\in\mathfrak{C}. \tag{6.9}$$

The *curvature* of the connection ∇ is the left $\mathcal{A}$-module homomorphism $\mathcal{R}:\mathfrak{C}\to\Omega^2\otimes_{\mathcal{A}}\mathfrak{C}$ defined by

$$\mathcal{R}(E)=-\nabla^2E. \tag{6.10}$$

More generally, $\mathcal{R}=-\nabla^2$ is defined as a map $\Omega\otimes_{\mathcal{A}}\mathfrak{C}\to\Omega\otimes_{\mathcal{A}}\mathfrak{C}$. It has the property

$$\mathcal{R}(\omega\otimes_{\mathcal{A}}E)=\omega\mathcal{R}(E) \tag{6.11}$$

and satisfies the *second Bianchi identity*

$$(\nabla\mathcal{R})(E):=\nabla(\mathcal{R}(E))-\mathcal{R}(\nabla E)=0. \tag{6.12}$$

A. Gauge theory

Let $\mathfrak{C}$ be a right $\mathcal{A}$-module. Then $\mathfrak{C}e^g$, for fixed $g\in G$, is a complex vector space. Let $E_i(g)$, $i=1,...,m(g)$, be a basis of this vector space. In general, its dimension varies with g. In the following we assume, for simplicity, that $m(g)$ is independent of g and finite.[44] Choosing an order $E_1(g),\ldots,E_m(g)$ for all $g\in G$, we obtain a right $\mathcal{A}$-module basis of $\mathfrak{C}$ by setting $E_i:=\Sigma_{g\in G}E_i(g)$. Then $\mathfrak{C}$ is a free right $\mathcal{A}$-module.

An element $\Psi\in\mathfrak{C}\otimes_{\mathcal{A}}\Omega^r$ can be written as $\Psi=E_i\otimes_{\mathcal{A}}\psi^i$ (using the summation convention) with an r-form field $\psi:G\to(\Omega^r)^m$ transforming according to $\psi\mapsto\psi'=\gamma\psi$ under the action of a gauge group Γ, corresponding to changes of the basis of $\mathfrak{C}$. A *right* $\mathcal{A}$-module connection ∇ has to satisfy $\nabla(E\otimes_{\mathcal{A}}\omega)=\nabla(E)\omega+E\otimes_{\mathcal{A}}\mathrm{d}\omega$ for all $\omega\in\Omega$, so that

$$\nabla\Psi=\nabla(E_j)\psi^j+E_i\otimes_{\mathcal{A}}\mathrm{d}\psi^i=E_i\otimes_{\mathcal{A}}(\mathrm{d}\psi^i+A^i_j\psi^j)=E_i\otimes_{\mathcal{A}}\mathrm{D}\psi^i. \tag{6.13}$$

Here A is a gauge potential 1-form and

$$\mathrm{D}\psi:=\mathrm{d}\psi+A\psi \tag{6.14}$$

is the *exterior covariant derivative* of ψ with the transformation law $(\mathrm{D}\psi)'=\gamma\mathrm{D}\psi$.

Similarly, an r-form field φ transforming according to $\varphi\mapsto\varphi'=\varphi\gamma^{-1}$ under the action of the gauge group corresponds to an element of a *left* $\mathcal{A}$-module. Then

$$\mathrm{D}\varphi:=\mathrm{d}\varphi-(-1)^r\varphi A \tag{6.15}$$

defines a covariant exterior derivative, i.e., $(\mathrm{D}\varphi)'=(\mathrm{D}\varphi)\gamma^{-1}$. Furthermore, we have

$$(\mathrm{D}\varphi)\psi+(-1)^r\varphi\mathrm{D}\psi=\mathrm{d}(\varphi\psi). \tag{6.16}$$

Introducing

$$W := \theta + A = \sum_{h \in S} W_h \theta^h, \tag{6.17}$$

which obeys the transformation law

$$W \to W' = \gamma W \gamma^{-1}, \quad W'_h = \gamma W_h (R_h^* \gamma^{-1}), \tag{6.18}$$

under a gauge transformation, and using (4.12), we obtain

$$\mathrm{D}\psi = W\psi - (-1)^r \psi\theta - \Delta(\psi), \tag{6.19}$$

$$\mathrm{D}\varphi = \theta\varphi - (-1)^r \varphi W - \Delta(\varphi). \tag{6.20}$$

From $\nabla^2\Psi = E_i \otimes_{\mathcal{A}} \mathrm{D}^2\psi =: E_i \otimes_{\mathcal{A}} F_j^{\ i} \psi^j$ originates the curvature 2-form

$$F = \mathrm{d}A + A^2 = W^2 - \Delta(W) - \Delta^e = \sum_{h,h' \in S} F_{h,h'} \theta^h \theta^{h'}, \tag{6.21}$$

which satisfies the Bianchi identity

$$0 = \mathrm{D}F := \mathrm{d}F + [A,F] = [W,F] - \Delta(F). \tag{6.22}$$

The biangle, triangle, and quadrangle parts of the curvature 2-form are, respectively, given by

$$F_{(e)h,h'} = W_h R_h^* W_{h'} - I \quad \text{for a biangle } hh' = e, \tag{6.23}$$

$$F_{(h_0)h,h'} = W_h R_h^* W_{h'} - W_{h_0} \quad \text{for a triangle } hh' = h_0 \in S_{(1)}, \tag{6.24}$$

$$F_{(g)h,h';\hat{h},\hat{h}'} = W_h R_h^* W_{h'} - W_{\hat{h}} R_{\hat{h}}^* W_{\hat{h}'} \quad \text{for a quadrangle } hh' = \hat{h}\hat{h}' = g \in S_{(2)}. \tag{6.25}$$

For 0-form fields ψ and ϕ we write

$$\mathrm{D}\psi = \sum_{h \in S} \nabla_{\ell_h} \psi \theta^h, \quad \mathrm{D}_\varphi = \sum_{h \in S} (\nabla_{\ell_h} \varphi) W_h \theta^h. \tag{6.26}$$

Then

$$\nabla_{\ell_h} \psi = W_h R_h^* \psi - \psi. \tag{6.27}$$

If the group Γ is unitary and if $W_h^{-1} = W_h^\dagger$, (where $\dagger$ denotes Hermitian conjugation), then $\psi^\dagger \mapsto \psi^\dagger \gamma^{-1}$ and we obtain

$$\nabla_{\ell_h} \psi^\dagger = (R_h^* \psi^\dagger) W_h^{-1} - \psi^\dagger = (\nabla_{\ell_h} \psi)^\dagger. \tag{6.28}$$

An example of a Lagrangian for the 0-form field ψ is

$$\mathcal{L}_\psi = \sum_{h \in S} \frac{1}{2} \nabla_{\ell_h} \psi^\dagger \nabla_{\ell_h} \psi = \sum_{h \in S} \frac{1}{2} (R_h^*(\psi^\dagger \psi) + \psi^\dagger \psi - \psi^\dagger W_h R_h^* \psi - (R_h^* \psi^\dagger) W_h^\dagger \psi) \tag{6.29}$$

with corresponding action

$$\mathrm{S}_\psi = \sum_{g \in G} \mathcal{L}_\psi(g) = \sum_{g \in G} \sum_{h \in S} \frac{1}{2} (2\psi^\dagger \psi - \psi^\dagger W_h R_h^* \psi - \psi^\dagger (R_{h^{-1}}^* W_h^\dagger \psi))(g). \tag{6.30}$$

In order to build a Lagrangian from r-form fields, $r>0$, we need an inner product of r-forms. It should satisfy

$$(f\omega, f'\omega') = f^\dagger f'(\omega, \omega') \tag{6.31}$$

(where $f^\dagger$ is the complex conjugate of the function f). A natural choice of inner product of 1-forms is then determined by

$$(\theta^h, \theta^{h'}) = \delta^{h,h'}. \tag{6.32}$$

As a consequence, the above Lagrangian for a 0-form field ψ can be written as follows,

$$\mathcal{L}_\psi = \tfrac{1}{2}(\mathrm{D}\psi^\dagger, \mathrm{D}\psi). \tag{6.33}$$

For a biangle or triangle $h_1 h_2 \in S_e$, we set

$$(\theta^{h_1}\theta^{h_2}, \theta^h \theta^{h'}) = \delta^{h_1,h}\delta^{h_2,h'}. \tag{6.34}$$

For a quadrangle $h_1 h_2 = g \notin S_e$ and a 2-form ψ we define

$$(\theta^{h_1}\theta^{h_2}, \psi) = \psi_{(g)h_1,h_2} \tag{6.35}$$

where $\psi_{(g)h_1,h_2}$ are the quadrangle components of ψ as defined in (4.36). In particular,

$$(\theta^{h_1}\theta^{h_2}, \theta^h\theta^{h'}) = |g|\,\delta^{h_1,h}\delta^{h_2,h'} - \delta_g^{hh'} \quad \text{if } h_1 h_2 = g \in S_{(2)}. \tag{6.36}$$

As a consequence of these definitions, biangle, triangle, and quadrangle 2-forms are orthogonal to each other. The Yang–Mills Lagrangian for the gauge potential A then takes the form

$$\mathcal{L}_{YM} := \frac{1}{2m}\,\mathrm{tr}\left((p_{(e)}F, p_{(e)}F) + \sum_{h\in S_{(1)}} (p_{(h)}F, p_{(h)}F) + \sum_{g\in S_{(2)}} \frac{1}{|g|}(p_{(g)}F, p_{(g)}F) \right) \tag{6.37}$$

and the corresponding action is $\mathbb{S}_{\mathrm{YM}} = \Sigma_{g'\in G}\mathcal{L}_{\mathrm{YM}}(g')$. From biangles, triangles, and quadrangles, respectively, the following contributions arise:

$$\mathrm{tr}(p_{(e)}F, p_{(e)}F) = \sum_{h,h'\in S} \delta^e_{hh'}\,\mathrm{tr}(2I - W_h(R_h^* W_{h'}) - (R_h^* W_{h'}^\dagger)W_h^\dagger), \tag{6.38}$$

$$\mathrm{tr}(p_{(h_0)}F, p_{(h_0)}F) = \sum_{h,h'\in S} \delta^{h_0}_{hh'}\,\mathrm{tr}(2I - W_{h_0}^\dagger W_h(R_h^* W_{h'}) - (R_h^* W_{h'}^\dagger)W_h^\dagger W_{h_0}), \tag{6.39}$$

$$\mathrm{tr}(p_{(g)}F, p_{(g)}F) = \mathrm{tr}\left(3|g|I - \sum_{h_1,h_2,h_3,h_4\in S} \delta^g_{h_1h_2}\delta^g_{h_3h_4}(R_{h_1}^* W_{h_2}^\dagger)W_{h_1}^\dagger W_{h_3}(R_{h_3}^* W_{h_4}) \right). \tag{6.40}$$

These expressions are indeed gauge invariant and thus also $\mathcal{L}_{\mathrm{YM}}$. The latter generalizes the Lagrangian of lattice gauge theory to arbitrary group lattices. It involves parallel transports U_P around the special plaquettes P given by biangles, triangles, and quadrangles. Lattice gauge theory models on group lattices (G,S) with $S = S^{-1}$ have previously been considered in Ref. 20 with an action of the form $\Sigma_{P\in\mathcal{P}}\mathrm{tr}[U_P + U_P^{-1}]$ where the sum is over some choice of set $\mathcal{P}$ of plaquettes (not restricted to biangles, triangles, and quadrangles). In contrast, we have used the natural differential geometry of the group lattice in order to determine a direct analog of the Yang–Mills action.

VII. LINEAR CONNECTIONS

A connection on Ω^1, regarded as a left $\mathcal{A}$-module, is called a *linear connection*. We introduce matrices $V_h=(V_{h,h'}^{h''})$ with entries in $\mathcal{A}$ via

$$\mathcal{V}_{\ell_{h'}}(\theta^h)=\sum_{h''\in S}(R^*_{h'-1}V^h_{h',h''})\,\theta^{h''} \tag{7.1}$$

so that

$$\nabla\theta^h=\theta\otimes_{\mathcal{A}}\theta^h-\sum_{h'\in S}V^h_{h'}\otimes_{\mathcal{A}}\theta^{h'} \tag{7.2}$$

with

$$V^h_{h'}:=\sum_{h''\in S}V^h_{h'',h'}\,\theta^{h''}. \tag{7.3}$$

From the definition of the curvature we obtain

$$\mathcal{R}(\theta^h)=-\Delta^e\otimes_{\mathcal{A}}\theta^h-\sum_{h'\in S}\Delta(\theta^{h'})\otimes_{\mathcal{A}}\mathcal{V}_{\ell_{h'}}(\theta^h)+\sum_{h',h''\in S}\theta^{h'}\theta^{h''}\otimes_{\mathcal{A}}\mathcal{V}_{\ell_{h''}}\mathcal{V}_{\ell_{h'}}(\theta^h), \tag{7.4}$$

where we used (4.3), (4.9), (6.2), and (6.4).

The *torsion* of a linear connection is the left $\mathcal{A}$-module homomorphism $\Theta:\Omega^1\to\Omega^2$ defined by

$$\Theta(\alpha)=\mathrm{d}\alpha-\pi\circ\nabla\alpha\quad\forall\,\alpha\in\Omega^1, \tag{7.5}$$

where π is the canonical projection $\Omega^1\otimes_{\mathcal{A}}\Omega^1\to\Omega^2$. Then

$$\begin{aligned}\Theta^h:=\Theta(\theta^h)&=\theta^h\theta-\Delta(\theta^h)+\pi\mathcal{V}(\theta^h)\\&=\theta^h\theta-\Delta(\theta^h)+\sum_{h'\in S}\theta^{h'}\mathcal{V}_{\ell_{h'}}(\theta^h)\\&=\sum_{h_1,h_2\in S}(\delta^h_{h_1}-\delta^h_{h_1h_2}+V^h_{h_1,h_2})\,\theta^{h_1}\theta^{h_2}\end{aligned} \tag{7.6}$$

using (4.3), (4.4), (6.2), (6.4), and (7.1). The torsion extends to a map $\Theta:\Omega\otimes_{\mathcal{A}}\Omega^1\to\Omega$ via

$$\Theta=\mathrm{d}\circ\pi-\pi\circ\nabla, \tag{7.7}$$

where π now denotes more generally the canonical projection $\Omega\otimes_{\mathcal{A}}\Omega^1\to\Omega$. It has the property

$$\Theta(\omega\otimes_{\mathcal{A}}\alpha)=(-1)^r\omega\Theta(\alpha) \tag{7.8}$$

for all $\alpha\in\Omega^1$ and $\omega\in\Omega^r$. From (7.7) we obtain the *first Bianchi identity*

$$\mathrm{d}\circ\Theta+\Theta\circ\nabla=\pi\circ\mathcal{R} \tag{7.9}$$

and thus

$$\mathrm{d}\Theta^h-\theta\Theta^h+\sum_{h'\in S}V^h_{h'}\Theta^{h'}=\pi\mathcal{R}(\theta^h) \tag{7.10}$$

or, using (4.12),

$$\Theta^h\theta+\Delta(\Theta^h)-\sum_{h'\in S}V^h_{h'}\Theta^{h'}=-\pi\mathcal{R}(\theta^h). \tag{7.11}$$

Writing

$$\mathcal{R}(\theta^h)=\sum_{h'\in S}\mathcal{R}^h_{h'}\otimes_{\mathcal{A}}\theta^{h'} \tag{7.12}$$

with $\mathcal{R}^h_{h'}\in\Omega^2$, we find

$$\nabla(\mathcal{R}(\theta^h))=\sum_{h'\in S}\left(\theta\mathcal{R}^h_{h'}-\Delta(R^h_{h'})-\sum_{h''\in S}\mathcal{R}^h_{h''}V^{h''}_{h'}\right)\otimes_{\mathcal{A}}\theta^{h'} \tag{7.13}$$

using (6.9), (4.13), and (7.2). Furthermore,

$$\mathcal{R}(\nabla\theta^h)=\sum_{h'\in S}\left(\theta\mathcal{R}^h_{h'}-\sum_{h''\in S}V^h_{h''}\mathcal{R}^{h''}_{h'}\right)\otimes_{\mathcal{A}}\theta^{h'} \tag{7.14}$$

so that the second Bianchi identity (6.12) takes the form

$$\Delta(\mathcal{R}^h_{h'})=\sum_{h''\in S}(V^h_{h''}\mathcal{R}^{h''}_{h'}-\mathcal{R}^h_{h''}V^{h''}_{h'}). \tag{7.15}$$

A. A transport of vector fields

Let $\nabla:\Omega^1\to\Omega^1\otimes_{\mathcal{A}}\Omega^1$ be a linear connection with parallel transport operator $\mathcal{V}_X$. Via

$$\langle\tilde{\mathcal{V}}_{\ell_h}Y,\alpha\rangle=R^*_h\langle Y,\mathcal{V}_{\ell_h}\alpha\rangle \tag{7.16}$$

a dual of $\mathcal{V}_{\ell_h}$ is defined which acts on vector fields. From this definition we obtain

$$\tilde{\mathcal{V}}_{\ell_h}(f\cdot Y)=(R^*_h f)\cdot\tilde{\mathcal{V}}_{\ell_h}Y. \tag{7.17}$$

In particular,

$$\tilde{\mathcal{V}}_{\ell_h}(e^g\cdot Y)=e^{gh^{-1}}\cdot\tilde{\mathcal{V}}_{\ell_h}Y, \tag{7.18}$$

which shows that the transport acts in the backward direction $gh^{-1}\leftarrow g$. Furthermore, (7.1) leads to

$$\tilde{\mathcal{V}}_{\ell_h}\ell_{h'}=\sum_{h''\in S}V^{h''}_{h,h'}\cdot\ell_{h''}. \tag{7.19}$$

Defining

$$\tilde{\mathcal{V}}_X:=\sum_{h\in S}X^h\tilde{\mathcal{V}}_{\ell_h}\quad(\text{on }\mathcal{X}), \tag{7.20}$$

(7.16) and (7.17) generalize, respectively, to

$$\langle\tilde{\mathcal{V}}_X Y,\alpha\rangle=R_X\langle Y,\mathcal{V}_X\alpha\rangle \tag{7.21}$$

and

$$\tilde{\nabla}_X(f\cdot Y)=(R_X f)\cdot\tilde{\nabla}_X Y \tag{7.22}$$

for a basic vector field X, by use of (5.12) and (6.7). In Sec. VII C we will see that the inverse of $\tilde{\nabla}_X$, provided it exists, is the parallel transport of a linear connection on $\mathcal{X}$, associated with the linear connection on Ω^1 in a natural geometric way.

Remark: For a symmetric group lattice we may introduce $\hat{\nabla}_{\ell_h}:=\tilde{\nabla}_{\ell_{h-1}}$ which satisfies (6.5) and thus defines a connection on $\mathcal{X}$ according to Lemma 6.1. ■

B. The geometric meaning of (vanishing) torsion

For a biangle $h_1h_2=e$ the vanishing of the corresponding part of the torsion 2-form (7.6) means

$$V^h_{h_1,h_2}=-\delta^h_{h_1} \tag{7.23}$$

and thus

$$\tilde{\nabla}_{\ell_{h_1}}(\ell_{h_2})=-\ell_{h_1}. \tag{7.24}$$

We conclude that the transport $\tilde{\nabla}$ preserves a biangle if the corresponding biangle torsion vanishes.

For a triangle $h_1h_2=h_0$, the corresponding part of the torsion 2-form (7.6) vanishes if and only if

$$V^h_{h_1,h_2}=\delta^h_{h_0}-\delta^h_{h_1}, \tag{7.25}$$

which can be written as

$$\tilde{\nabla}_{\ell_{h_1}}(\ell_{h_2})=\ell_{h_0}-\ell_{h_1}. \tag{7.26}$$

Associated with the latter triangle, there is a triangle composed of the two vectors ℓ_{h_1} and ℓ_{h_0} at $g\in G$, and the vector ℓ_{h_2} at gh_1. The latter vector is backwards parallel transported by $\tilde{\nabla}_{\ell_{h_1}}$ to the tangent space at g. The condition of vanishing triangle torsion means that the three vectors at g then form a triangle. In this sense the transport preserves triangles if the triangle torsion vanishes.

A corresponding statement also holds for a quadrangle $h_1h_2=\hat{h}_1\hat{h}_2=g\notin S_e$. If we consider[45]

$$Q^h_{(g)h_1,h_2;\hat{h}_1,\hat{h}_2}=\check{Q}^h_{(g)h_1,h_2}-\check{Q}^h_{(g)\hat{h}_1,\hat{h}_2} \tag{7.27}$$

as the associated quadrangle torsion part, its vanishing means

$$V^h_{h_1,h_2}-V^h_{\hat{h}_1,\hat{h}_2}=\delta^h_{\hat{h}_1}-\delta^h_{h_1}, \tag{7.28}$$

which is equivalent to

$$\tilde{\nabla}_{\ell_{h_1}}(\ell_{h_2})-\tilde{\nabla}_{\ell_{\hat{h}_1}}(\ell_{\hat{h}_2})=\ell_{\hat{h}_1}-\ell_{h_1}. \tag{7.29}$$

There is a quadrangle composed of the two vectors ℓ_{h_1} and $\ell_{\hat{h}_1}$ at $g\in G$, the vector ℓ_{h_2} at gh_1, and the vector $\ell_{\hat{h}_2}$ at $g\hat{h}_1$. The latter two vectors are backwards parallel transported by $\tilde{\nabla}_{\ell_{h_1}}$ and $\tilde{\nabla}_{\ell_{\hat{h}_1}}$, respectively, to the tangent space at g. The condition of vanishing quadrangle torsion then has the effect that the resulting four vectors also form a quadrangle in the tangent space at g.

The presence of biangle, triangle, and quadrangle torsion thus means that a biangle, triangle, and quadrangle composed of vectors ℓ_h in the group lattice is, in general, not mapped by $\widetilde{\mathcal{V}}$ to a closed polygon in a tangent space.

C. Linear connections on vector fields

Again, let $\nabla:\Omega^1\to\Omega^1\otimes_{\mathcal{A}}\Omega^1$ be a linear connection with parallel transport operator $\mathcal{V}_X$. Then

$$\langle \mathcal{U}_X Y, \mathcal{V}_X \alpha\rangle = R_X^{-1}\langle Y,\alpha\rangle \tag{7.30}$$

for all basic vector fields X associates with $\mathcal{V}_X$ a linear operator $\mathcal{U}_X:\mathcal{X}\to\mathcal{X}$. This definition means that parallel transport preserves contractions of vector fields and 1-forms. Writing

$$\mathcal{U}_{\ell_h}\ell_{h'} = \sum_{h''\in S} R^*_{h^{-1}}(U_h)^{h''}_{h'}\cdot \ell_{h''} \tag{7.31}$$

with matrices U_h, we find from (7.30) and (7.1) that

$$U_h = V_h^{-1}. \tag{7.32}$$

In particular, we need the V_h to be invertible. Furthermore, from (6.7) we obtain

$$\mathcal{U}_X = \sum_{h\in S} (R^*_{h^{-1}}X^h)\cdot \mathcal{U}_{\ell_h}. \tag{7.33}$$

Lemma 7.1: For basic vector fields X,

$$\mathcal{U}_X(f\cdot Y) = (R_X^{-1}f)\cdot \mathcal{U}_X(Y). \tag{7.34}$$

Proof: Using (5.12) and (5.26) we obtain

$$\begin{aligned}\langle \mathcal{U}_X(f\cdot Y), \mathcal{V}_X\alpha\rangle &= R_X^{-1}\langle f\cdot Y,\alpha\rangle = (R_X^{-1}f)R_X^{-1}\langle Y,\alpha\rangle = (R_X^{-1}f)\langle \mathcal{U}_X Y, \mathcal{V}_X\alpha\rangle\\ &= \langle (R_X^{-1}f)\cdot \mathcal{U}_X Y, \mathcal{V}_X\alpha\rangle.\end{aligned}$$

■

In particular,

$$\mathcal{U}_{\ell_h}(f\cdot Y) = (R^*_{h^{-1}}f)\cdot \mathcal{U}_{\ell_h} Y \tag{7.35}$$

so that

$$\nabla Y := \theta\otimes_{\mathcal{A}} Y - \mathcal{U}(Y), \quad \mathcal{U}(Y) := \sum_{h\in S} \theta^h\otimes_{\mathcal{A}}\mathcal{U}_{\ell_h} Y \tag{7.36}$$

defines a connection on $\mathcal{X}$, i.e., a linear map $\nabla:\mathcal{X}\to\Omega^1\otimes_{\mathcal{A}}\mathcal{X}$ with the property $\nabla(f\cdot Y) = \mathrm{d}f\otimes_{\mathcal{A}} Y + f\nabla Y$ (see Sec. VI). Next we establish the relation with the transport $\widetilde{\mathcal{V}}_X$ introduced in the previous subsection.

Lemma 7.2: For basic vector fields X,

$$\mathcal{U}_X = \widetilde{\mathcal{V}}_X^{-1}. \tag{7.37}$$

Proof: With the help of (7.17), (7.19), (7.31), and (7.35) we find $\mathcal{U}_{\ell_h}\widetilde{\mathcal{V}}_{\ell_h} Y = Y$ for all vector fields Y. Using (5.12) for an arbitrary basic vector field X and $\Sigma_{h\in S}X^h = \mathbf{1}$, we obtain

$$\mathcal{U}_X\tilde{\mathcal{V}}_X=\sum_{h,h'\in S}(R^*_{h^{-1}}X^h)\cdot\mathcal{U}_{\ell_h}(X^{h'}\tilde{\mathcal{V}}_{\ell_{h'}})$$

$$=\sum_{h,h'\in S}(R^*_{h^{-1}}X^h)(R^*_{h^{-1}}X^{h'})\cdot\mathcal{U}_{\ell_h}\tilde{\mathcal{V}}_{\ell_{h'}}$$

$$=\sum_{h\in S}(R^*_{h^{-1}}X^h)\cdot\mathcal{U}_{\ell_h}\tilde{\mathcal{V}}_{\ell_h}=\sum_{h\in S}X^hI=I.$$

■

Let us also define

$$\nabla_{\ell_h}Y:=Y-\mathcal{U}_{\ell_h}Y,\quad \nabla_{\ell_h}\alpha:=\alpha-\mathcal{V}_{\ell_h}\alpha, \tag{7.38}$$

which satisfy

$$\nabla_{\ell_h}(f\alpha)=(\overline{\ell}_hf)\alpha+(R^*_{h^{-1}}f)\nabla_{\ell_h}\alpha,\quad \nabla_{\ell_h}(f\cdot Y)=(\overline{\ell}_hf)\cdot Y+(R^*_{h^{-1}}f)\cdot\nabla_{\ell_h}Y, \tag{7.39}$$

where

$$\overline{\ell}_h=\ell_hR^*_{h^{-1}}=I-R^*_{h^{-1}} \tag{7.40}$$

is the backward difference operator on $\mathcal{A}$. Then the following identity holds:

$$\overline{\ell}_h\langle Y,\alpha\rangle=\langle\nabla_{\ell_h}Y,\alpha\rangle+\langle Y,\nabla_{\ell_h}\alpha\rangle-\langle\nabla_{\ell_h}Y,\nabla_{\ell_h}\alpha\rangle. \tag{7.41}$$

In general, the parallel transport of a discrete vector field along a discrete vector field is not a discrete vector field. A parallel transport or connection which maps discrete vector fields into discrete vector fields will be called ''discrete.'' In this case, the matrices V_h represent permutations.

VIII. DIFFERENTIAL CALCULI ON COSET SPACES OF DISCRETE GROUPS

Let H be a subgroup of G and let G/H denote the set of right cosets of H in G, i.e., $K\in G/H$ has the form $K=Hg$ for some $g\in G$. The algebra $\mathcal{A}_{G/H}$ of complex valued functions $F:G/H\to\mathbb{C}$ can be naturally identified with a subalgebra of the algebra $\mathcal{A}=\mathcal{A}_G$ of functions on G. Since the cosets form a partition of G, using our notation (3.2) we find $e^Ke^{K'}=\delta^{K,K'}e^K$ and $\Sigma_{K\in G/H}e^K=\mathbf{1}$. As a consequence, each element $F\in\mathcal{A}_{G/H}$ has a unique decomposition $F=\Sigma_{K\in G/H}F(K)e^K$. The right action of G on G induces a right action on G/H:

$$R^*_gF=\sum_{K\in G/H}F(K)R^*_ge^K=\sum_{K\in G/H}F(K)e^{Kg^{-1}}. \tag{8.1}$$

Let (G,S) be a group lattice. The 1-forms $\{\theta^h|h\in S\}$ then generate an $\mathcal{A}_{G/H}$-bimodule $\Omega^1_{G/H}$ such that

$$\theta^he^K=(R^*_he^K)\theta^h=e^{Kh^{-1}}\theta^h \tag{8.2}$$

and

$$\mathrm{d}e^K=\sum_{h\in S}(e^{Kh^{-1}}-e^K)\theta^h \tag{8.3}$$

defines a linear map $\mathrm{d}:\mathcal{A}_{G/H}\to\Omega^1_{G/H}$ which satisfies

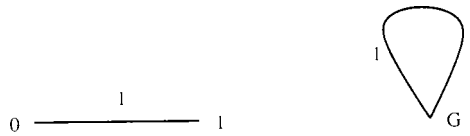

FIG. 5. The symmetric digraph of $(\mathbb{Z}_2,\{1\})$ and the corresponding coset graph corresponding to the choice $H=\mathbb{Z}_2$.

$$\mathrm{d}(FF')=(\mathrm{d}F)F'+F\mathrm{d}F' \tag{8.4}$$

for all F, $F'\in\mathcal{A}_{G/H}$, so that $(\Omega^1_{G/H},\mathrm{d})$ is a first-order differential calculus over $\mathcal{A}_{G/H}$. It is important to note, however, that $\Omega^1_{G/H}$ is not, in general, generated by $\mathcal{A}_{G/H}$, i.e., $\mathcal{A}_{G/H}(\mathrm{d}\mathcal{A}_{G/H})\mathcal{A}_{G/H}$ is smaller than $\Omega^1_{G/H}$.[46] In any case, the first-order differential calculus extends to a differential calculus $(\Omega_{G/H},\mathrm{d})$ over $\mathcal{A}_{G/H}$. A closer inspection shows that the latter is simply obtained from the group lattice differential calculus (Ω,d) by restricting $\mathcal{A}_G$ to the subalgebra of functions corresponding to $\mathcal{A}_{G/H}$.

Drawing an arrow from a point representing a coset K to a point representing a coset K' whenever there is an $h\in S$ such that $K'=Kh$, we obtain a digraph. This *coset digraph*[47] is also known as the *Schreier diagram* of the triple (G,S,H) (see Ref. 16, for example). In contrast to the digraphs (group lattices) considered in the previous sections, coset digraphs may have multiple arrows between two sites and even loops (i.e., arrows from a site to itself). Indeed, whenever we have different h, $h'\in S$ such that $Hh=Hh'$, then there are multiple arrows in a coset digraph. The resulting discrete geometry is therefore more complex than the one determined by (ordinary) differential calculi on the algebra of functions on the corresponding set of points. Such a generalization may prove to be relevant for the description of electric circuits, for example.

Example 8.1: Let $G=\mathbb{Z}_2=\{0,1\}$, the cyclic group of order 2 with group operation the addition modulo 2. With $S=\{1\}$, we have $S_{(0)}=S$, $S_{(1)}=S_{(2)}=\varnothing$. Choosing $H=G$, the coset space consists of a single element only and the algebra of functions on it is therefore $\mathbb{C}$. The 1-form θ^1 corresponds to a loop (see Fig. 5). Then we have $\Omega^r_{\mathbb{Z}_2/\mathbb{Z}_2}=\mathrm{span}_{\mathbb{C}}\{(\theta^1)^r\}$ for $r>0$. According to (4.3), the action of d on forms is determined by $\mathrm{d}\theta^1=2\,\theta^1\theta^1$ together with the Leibniz rule. As a consequence, $\mathrm{d}\theta^{2r}=0$ and $\mathrm{d}\theta^{2r+1}=2(\theta^1)^{2(r+1)}$. ■

Example 8.2: Choosing $\mathbb{Z}_3$ with $S=\{1,2\}$ and passing to the single point coset space $\mathbb{Z}_3/\mathbb{Z}_3$, one remains with two 1-forms θ^h, $h=1,2$. According to (4.3), the exterior derivative then acts as follows,

$$\mathrm{d}\theta^1=2(\theta^1)^2-(\theta^2)^2+\theta^1\theta^2+\theta^2\theta^1, \tag{8.5}$$

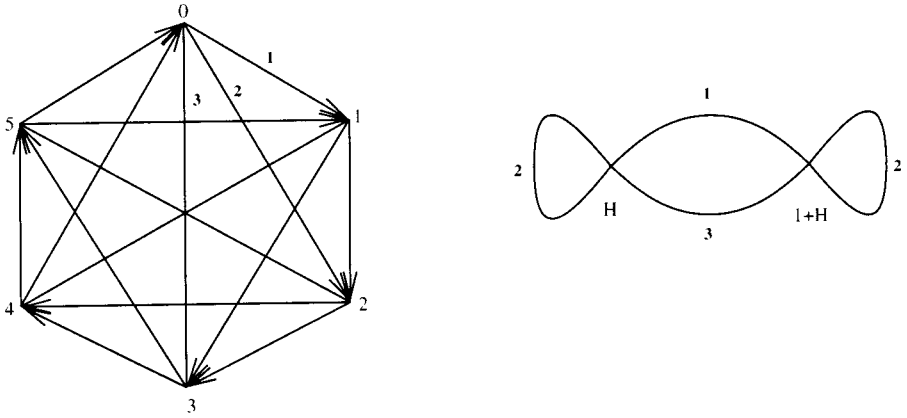

FIG. 6. Group lattice of $(\mathbb{Z}_6,\{1,2,3\})$ and the coset digraph for $H=\{0,2,4\}$.

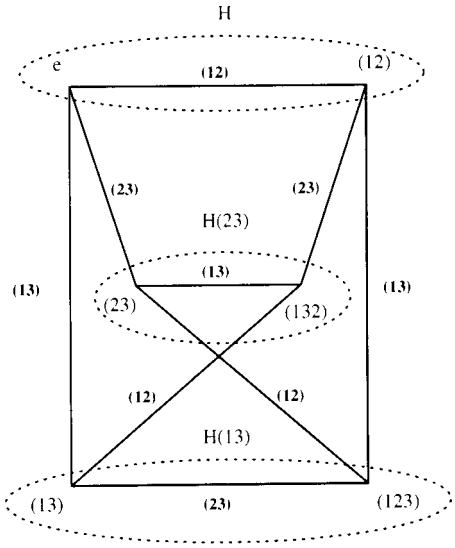

FIG. 7. The right cosets of $\mathcal{S}_3$ with respect to the subgroup $H=\{e,(12)\}$.

$$\mathrm{d}\theta^2=2(\theta^2)^2-(\theta^1)^2+\theta^1\theta^2+\theta^2\theta^1. \tag{8.6}$$

■

Example 8.3: An example of a coset digraph containing both loops and multiple links is given by $G=\mathbb{Z}_6$, the cyclic group of order 6 with group operation $\dot{+}$, addition modulo 6. With $S=\{1,2,3\}$ we find $S_{(0)}=\{3\}$, $S_{(1)}=\{2,3\}$, and $S_{(2)}=\{4,5\}$ which implies that we have two 2-form relations and consequently seven independent 2-forms. Choosing $H=\{0,2,4\}$, there are only two cosets, H and $1\dot{+}H$. Since $H\overset{1,3}{\leftrightarrow}1\dot{+}H$, $H\overset{2}{\leftrightarrow}H$ and $1\dot{+}H\overset{2}{\leftrightarrow}1\dot{+}H$, we obtain the graph in Fig. 6.■

Example 8.4: Let us consider the $\mathcal{S}_3$ group lattice of examples 2.4 and 4.1 with $S=\{(12),(13),(23)\}$. The following table expresses the action of R_h, $h\in S$, on G:

	(12)	(13)	(23)
e	(12)	(13)	(23)
(12)	e	(123)	(132)
(13)	(132)	e	(123)
(23)	(123)	(132)	e
(123)	(23)	(12)	(13)
(132)	(13)	(23)	(12)

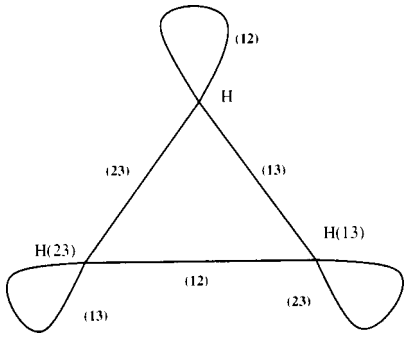

FIG. 8. Loops in the coset digraph of $\mathcal{S}_3$ with respect to the subgroup $H=\{e,(12)\}$ and $S=\{(12),(13),(23)\}$.

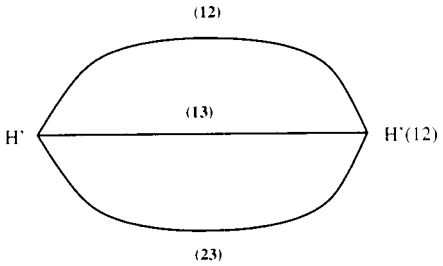

FIG. 9. An $\mathcal{S}_3$ coset digraph with multiple arrows.

Choosing the subgroup $H=\{e,(12)\}$, the corresponding right cosets are H, $H(13)=\{(13),(123)\}$, and $H(23)=\{(23),(132)\}$ (see Fig. 7).

The action of R_h, $h\in S$, on the cosets is given by the following table:

	(12)	(13)	(23)
H	H	$H(13)$	$H(23)$
$H(13)$	$H(23)$	H	$H(13)$
$H(23)$	$H(13)$	$H(23)$	H

Since $H\overset{(12)}{\mapsto}H$, $H(13)\overset{(23)}{\mapsto}H(13)$ and $H(23)\overset{(13)}{\mapsto}H(23)$, there are loops in the coset digraph (see Fig. 8). This has its origin in the fact that $S\cap H=\{(12)\}$ and thus $H(12)=H$.[48] The 1-forms $e^H\theta^{(12)}$, $e^{H(13)}\theta^{(23)}$, and $e^{H(23)}\theta^{(13)}$ are associated with the loops and therefore cannot be expressed in terms of functions and differentials. In order to eliminate the loops, one could set these 1-forms to zero. As a consequence of such additional relations, the resulting bimodule of 1-forms is no longer free.

As a further example, let us consider the subgroup $H'=\{e,(123),(132)\}$. The corresponding cosets are H' and $H'(12)=\{(12),(23),(13)\}$. The table of the right action R_h on these cosets is then

	(12)	(13)	(23)
H'	$H'(12)$	$H'(12)$	$H'(12)$
$H'(12)$	H'	H'	H'

In this case, we have multiple arrows in the coset digraph (see Fig. 9). By imposing the relations $\theta^{(12)}=\theta^{(13)}=\theta^{(23)}$ on the differential calculus, we could eliminate the multiple links. ■

Example 8.5: Let $G=S_4$ and $S=\{(12),(13),(14),(23),(24),(34)\}$, as in example 4.3. Furthermore, we choose a subgroup H of order 3 with eight cosets:

$$H=\{e,(123),(132)\},\quad H(12)=\{(12),(23),(13)\},$$

$$H(12)(34)=\{(12)(34),(243),(143)\},\quad H(14)=\{(14),(1234),(1324)\},$$

$$H(13)(24)=\{(142),(234),(13)(24)\},\quad H(24)=\{(24),(1423),(1342)\},$$

$$H(14)(23)=\{(124),(14)(23),(134)\},\quad H(34)=\{(34),(1243),(1432)\}.$$

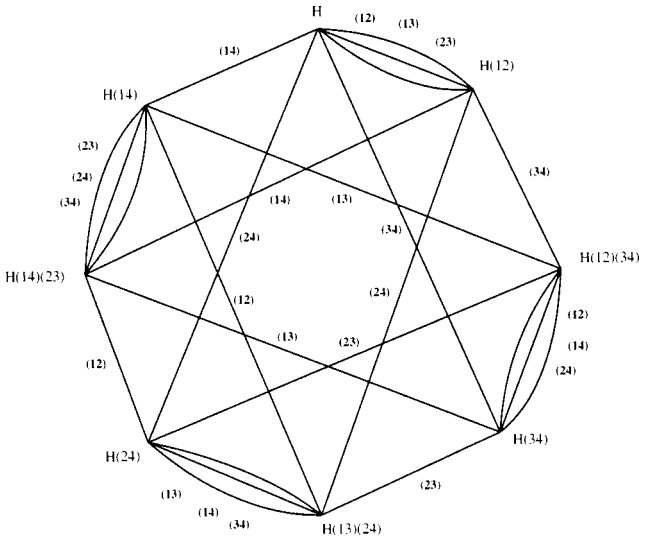

FIG. 10. Coset digraph of $\mathcal{S}_4$ with $S=\{(12),(13),(14),(23),(24),(34)\}$ and $H=\{e,(123),(132)\}$.

The table of right actions of the elements of S on G/H is

	(12)	(13)	(14)	(23)	(24)	(34)
H	$H(12)$	$H(12)$	$H(14)$	$H(12)$	$H(24)$	$H(34)$
$H(12)$	H	H	$H(14)(23)$	H	$H(13)(24)$	$H(12)(34)$
$H(14)$	$H(13)(24)$	$H(12)(34)$	H	$H(14)(23)$	$H(14)(23)$	$H(14)(23)$
$H(24)$	$H(14)(23)$	$H(13)(24)$	$H(13)(24)$	$H(12)(34)$	H	$H(13)(24)$
$H(34)$	$H(12)(34)$	$H(14)(23)$	$H(12)(34)$	$H(13)(24)$	$H(12)(34)$	H
$H(12)(34)$	$H(34)$	$H(14)$	$H(34)$	$H(24)$	$H(34)$	$H(12)$
$H(13)(24)$	$H(14)$	$H(24)$	$H(24)$	$H(34)$	$H(12)$	$H(24)$
$H(14)(23)$	$H(24)$	$H(34)$	$H(12)$	$H(14)$	$H(14)$	$H(14)$

and the coset digraph is drawn in Fig. 10. If we impose the relations

$$e^{H}\theta^{(12)}=e^{H}\theta^{(13)}=e^{H}\theta^{(23)},\quad e^{H(12)}\theta^{(12)}=e^{H(12)}\theta^{(13)}=e^{H(12)}\theta^{(23)},$$

$$e^{(12)(34)H}\theta^{(12)}=e^{H(12)(34)}\theta^{(14)}=e^{H(12)(34)}\theta^{(24)},\quad e^{H(34)}\theta^{(12)}=e^{H(34)}\theta^{(14)}=e^{H(34)}\theta^{(24)},$$

$$e^{(13)(24)H}\theta^{(13)}=e^{H(13)(24)}\theta^{(14)}=e^{H(13)(24)}\theta^{(34)},\quad e^{H(24)}\theta^{(13)}=e^{H(24)}\theta^{(24)}=e^{H(24)}\theta^{(34)},$$

$$e^{(14)(23)H}\theta^{(23)}=e^{H(14)(23)}\theta^{(24)}=e^{H(14)(23)}\theta^{(34)},\quad e^{H(14)}\theta^{(23)}=e^{H(14)}\theta^{(24)}=e^{H(14)}\theta^{(34)},$$

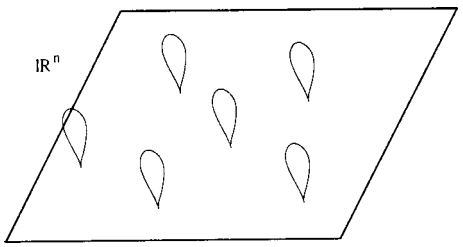

FIG. 11. Visualization of the geometry considered in Sec. VIII A.

then the multiple links are eliminated. The bimodules of differential forms are then no longer free. ■

The relations one has to impose on the 1-forms of a generalized differential calculus on a coset space in order to reduce it to an ordinary differential calculus (without loops or multiple links in the associated digraph) are of the form $e^K\theta^h=0$ or $e^K(\theta^{h_1}-\theta^{h_2})=0$. Such relations do not lead to additional higher form relations. For relations eliminating loops this follows from

$$\mathrm{d}(e^K\theta^h)=(\theta e^K-e^K\theta)\theta^h+e^K(\theta\theta^h+\theta^h\theta-\Delta(\theta^h))=-e^K\Delta(\theta^h)=-\Delta(e^K\theta^h).$$

A similar calculation applies to relations eliminating multiple links.

A. Higgs field from gauge theory with an internal coset lattice

Let (Ω, d) be the usual differential calculus over the algebra $\mathcal{A}$ of smooth functions on $\mathbb{R}^n$. Furthermore, let $(\tilde{\Omega},\tilde{\mathrm{d}})$ denote the "loop" differential calculus over the algebra $\tilde{\mathcal{A}}=\mathbb{C}$ of functions on the single point space $\mathbb{Z}_2/\mathbb{Z}_2$, see example 8.1. The skew-tensor product[49] $\hat{\Omega}=\Omega\hat{\otimes}\tilde{\Omega}$ of the two differential calculi then defines a new differential calculus $(\hat{\Omega},\hat{\mathrm{d}})$ over $\mathcal{A}$. Figure 11 visualizes the underlying geometry.

Let us introduce $\rho:=(1/c)\theta^1$ with a real constant c, so that $\tilde{\mathrm{d}}\rho=2c\rho^2$, $\tilde{\mathrm{d}}\rho^{2r}=0$ and $\tilde{\mathrm{d}}\rho^{2r+1}=2c\rho^{2r+2}$ (see example 8.1). Then $\hat{\mathrm{d}}f=\mathrm{d}f$ and $\hat{\mathrm{d}}(\omega\rho^r)=(\mathrm{d}\omega)\rho^r+(-1)^s\omega\tilde{\mathrm{d}}\rho^r$ for $\omega\in\Omega^s$. Let $\hat{A}$ be a gauge potential 1-form. With the decomposition $\hat{A}=A+\phi\rho$, the field strength $\hat{F}=\hat{\mathrm{d}}\hat{A}+\hat{A}^2$ becomes

$$\hat{F}=F+\mathrm{D}\phi\,\rho+(\phi^2+2c\phi)\rho^2, \tag{8.7}$$

where we used $A\rho=-\rho A$ and introduced the exterior covariant derivative $D\phi=\mathrm{d}\phi+[A,\phi]$. In terms of $\varphi:=\phi+cI$, this reads

$$\hat{F}=F+\mathrm{D}\varphi\rho+(\varphi^2-c^2I)\rho^2. \tag{8.8}$$

Let us now introduce an inner product on $\hat{\Omega}$ such that

$$(\omega\rho^r,\omega'\rho^s):=\delta_{rs}\lambda^r(\omega,\omega') \tag{8.9}$$

with a positive constant λ and the usual sesquilinear inner product[50] (ω,ω') of differential forms on $\mathbb{R}^n$ with respect to a (pseudo-) Riemannian metric. Then we find

$$(\hat{F},\hat{F})=\frac{1}{2}F^\dagger_{\mu\nu}F^{\mu\nu}+\lambda(\nabla_\mu\varphi)^\dagger\nabla^\mu\varphi+\lambda^2(\varphi^2-c^2I)^\dagger(\varphi^2-c^2I). \tag{8.10}$$

If we set

$$\varphi=\begin{pmatrix}0 & \chi^\dagger\\ \chi & 0\end{pmatrix} \tag{8.11}$$

then

$$\varphi^2=\begin{pmatrix}\chi^\dagger\chi & 0\\ 0 & \chi\chi^\dagger\end{pmatrix}. \tag{8.12}$$

Taking the trace of (8.10) results in

$$\mathrm{tr}(\hat{F},\hat{F})=\tfrac{1}{2}\mathrm{tr}(F^\dagger_{\mu\nu}F^{\mu\nu})+2\lambda\,\mathrm{tr}((\nabla_\mu\chi)^\dagger\nabla^\mu\chi)+2\lambda^2(\|\chi\|^2-c^2I)^2. \tag{8.13}$$

The constants can now be chosen in such a way that the usual Yang–Mills–Higgs Lagrangian is obtained. More complicated examples can be constructed by replacing $\mathbb{Z}_2$ with $\mathbb{Z}_N$, $N>2$ (see also example 8.2 and Ref. 51).

IX. CONCLUSIONS

With this work we have started to develop a formalism of differential geometry of group lattices, based on elementary concepts of noncommutative geometry. A group lattice (G,S) naturally determines a differential calculus over the algebra of functions on the discrete group G and we systematically explored the structure of differential calculi which emerge in this way.

Counterparts of the Yang–Mills action on arbitrary group lattices are obtained. They generalize the familiar action of lattice gauge theory. In particular, these can be further analyzed using the methods of Ref. 20.

Whereas noncommutative geometry conveniently defines general geometric structures in terms of differential forms, their geometric significance in special cases, like the group lattices under consideration, is often easier to understand when expressed in terms of vector fields. A large part of this work has therefore been devoted to the properties of a class of vector fields on group lattices, which we called ''discrete vector fields,'' and the subclass of ''basic vector fields.'' We also introduced an inner product of discrete vector fields (with differentiable flow) and forms. In particular, this opens the possibility to develop mechanics on group lattices using familiar formulas of symplectic geometry.

A linear connection (on the space of 1-forms) on a group lattice defines a parallel transport of vector fields along a vector field. We found a very simple geometric picture associated with the condition of vanishing torsion, which strongly corroborates the formalism.

Continuing this work, in a forthcoming paper we develop ''Riemannian geometry'' on group lattices. More precisely, for making contact with classical geometry, the subclass of *bicovariant* group lattices turns out to be distinguished. We introduced these lattices as those for which all the left and right actions, L_h, R_h, $h\in S$, are differentiable maps (in the sense of Sec. III).

The geometric framework presented in this work may also be helpful for the construction and analysis of completely integrable models on group lattices. The differential calculus associated with a linear or quadratic lattice (see example 2.1) has already been applied in this context.[5]

APPENDIX: INTEGRAL CURVES OF DISCRETE VECTOR FIELDS

Let (G,S) be a group lattice. A map $\gamma:\mathbb{Z}\to G$ which is a solution of the equation

$$\partial_{+t}(\gamma^* f)=\gamma^*(Xf) \quad (\forall f\in\mathcal{A}) \tag{A1}$$

for some discrete vector field $X=\Sigma_{h\in S}X^h\cdot\ell_h\in\mathcal{X}$ is called an *integral curve* of X. More explicitly, this reads

$$f(\gamma(t+1))-f(\gamma(t))=\sum_{h\in S}X^h(\gamma(t))[f(\gamma(t)h)-f(\gamma(t))], \tag{A2}$$

or

$$\begin{aligned} f(\gamma(t+1))&=\sum_{h\in S}X^h(\gamma(t))f(\gamma(t)h)+\left(1-\sum_{h\in S}X^h(\gamma(t))\right)f(\gamma(t))\\ &=\sum_{h\in S_e}X^h(\gamma(t))f(\gamma(t)h)=((I+X)f)(\gamma(t)) \end{aligned} \tag{A3}$$

(where $X^e(g)=1$ iff $X^h(g)=0$ for all $h\in S$). Since precisely one component $X^h(\gamma(t))$, $h\in S_e$, is different from zero and then equal to 1, we obtain $f(\gamma(t+1))=f(\Sigma_{h\in S_e}X^h(\gamma(t))\gamma(t)h)$ for all $f\in\mathcal{A}$ and thus

$$\gamma(t+1)=\sum_{h\in S_e} X^h(\gamma(t))\,\gamma(t)h. \tag{A4}$$

The flow $\phi_t: G\to G$ generated by X has to satisfy the same equation, so that

$$\phi_{t+1}=\sum_{h\in S_e}(X^h R_h)\circ\phi_t. \tag{A5}$$

Furthermore, $\phi_0=\mathrm{id}$, the identity on G. On functions, we have [cf. (A3)]

$$\phi^*_{t+1}f=\phi^*_t((I+X)f) \tag{A6}$$

with the solution

$$\phi^*_t=(I+X)^t \tag{A7}$$

as expected on the basis of our earlier considerations.

Let us supply $\mathbb{Z}$ with the first-order differential calculus of example 2.1, and G with the calculus associated with the subset $S\subset G\backslash\{e\}$. According to the criterium (3.5), the map γ is differentiable iff $\gamma(t)^{-1}\gamma(t+1)\in S_e$ for all $t\in\mathbb{Z}$. But this is automatically satisfied for an integral curve as a consequence of (A4). We have already learned, however, that the flow of X is not in general differentiable as a map $G\to G$ (with respect to the differential calculus induced by S).

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[24] The formalism developed in this work may be generalized by replacing $\mathbb{C}$ with an arbitrary field $\mathbb{K}$.
[25] Here and in the following we slightly depart from corresponding definitions used in Ref. 6. In particular, our definition of θ^h below corresponds to $\theta^{h^{-1}}$ in the latter work.
[26] One could think of extending the formalism to *infinite* subsets S of an infinite discrete group G. Then one has to find a way to make sense of infinite summations (over the elements of S, at $g\in G$) appearing in the following formulas.
[27] J.-P. Serre, *Trees* (Springer, Berlin, 1980).
[28] This is a sub-bimodule of the bimodule generated by all ℓ_g, $g\in G$. Of course, it depends on the choice of S and should therefore rather be denoted as $\mathcal{X}_S$, for example. Since in most parts of this article S is a fixed set, we simply write $\mathcal{X}$ instead of $\mathcal{X}_S$.

[29] If $|G|$ is infinite, the right side looks like an infinite sum. Note, however, that at each element $g \in G$ this reduces to $\theta^h|_g = \mathrm{d}e^{gh}|_g$.

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[39] These conditions mean that if there is an outgoing X-arrow at g, then there is also precisely one incoming X-arrow. If there is no outgoing arrow, then there is also no incoming arrow.

[40] This expression is not in general a vector field unless S is symmetric, i.e., $S = S^{-1}$. It is actually a vector field for the *opposite* group lattice (G, S^{-1}).

[41] In fact, all basic vector fields on S_3 with $S = \{(12),(13),(23)\}$ generate differentiable maps $G \to G$. This follows from $S^{-1} = S$ and $S^3 = S$, which implies that every expression of the form $s(g)^{-1} h s(gh)$ (for s with values in S) lies in S, so that condition (2) of Theorem 5.1 holds.

[42] Here we use the notation $(s_Y \cdot s_X)(g) = s_Y(g) s_X(g)$.

[43] Except for 1-forms, we have in general $X \lrcorner \omega \neq \Sigma_h X^h (\ell_h \lrcorner \omega)$ where $X = \Sigma_h X^h \cdot \ell_h$.

[44] Bundles over discrete spaces with varying dimension of the fibers have been considered in particular for particle physics model building. See, for example, A. Connes, "Essay on physics and non-commutative geometry," in *The Interface of Mathematics and Particle Physics*, edited by D. Quillen, G. Segal and S. Tsou (Oxford University Press, Oxford, 1990), p. 9.

[45] See the discussion of 2-form components at the end of Sec. IV B.

[46] Such generalized first-order differential calculi have already been considered in H. C. Baehr, A. Dimakis, and F. Müller-Hoissen, "Differential calculi on commutative algebras," preprint MPI-PhT/94-83, hep-th/9412069, Appendix A (1994). They cannot be obtained as a quotient of the universal first order differential calculus.

[47] This should not be confused with *Cayley coset digraphs* as considered, for example, in G. Sabidussi, Duke Math. J. **26**, 693 (1959); E. Knill, "Notes on the connectivity of Cayley coset diagraphs," math.CO/9411221.

[48] Note that $Hh = H$ implies $(Hg)\mathrm{ad}(g^{-1})h = Hg$, so we also have a loop at Hg and then at every coset. If $\mathrm{ad}(g)h \in H$ and thus $Hgh = Hg$ for all g, we can eliminate these loops by reducing S to $S \backslash \{h\}$. But if $\mathrm{ad}(g)h \notin H$ for some g, it will not be possible to get rid of the loops by choosing a smaller set S without simultaneously eliminating some arrows between different points.

[49] Given two spaces with differential calculi (Ω_i, d_i), $i = 1,2$, the skew tensor product $\Omega_1 \hat{\otimes} \Omega_2$ with $\mathrm{d}(\omega_1 \hat{\otimes} \omega_2) = (\mathrm{d}_1 \omega_1) \hat{\otimes} \omega_2 + (-1)^r \omega_1 \hat{\otimes} \mathrm{d}_2 \omega_2$ for $\omega_1 \in \Omega_1^r$ and $\omega_2 \in \Omega_2$ defines a differential calculus on their direct product. See Ref. 4 and D. Kastler, *Cyclic Cohomology Within the Differential Envelope* (Hermann, Paris, 1988), Appendix A, for example.

[50] It has the properties $(f\omega, f'\omega') = f^\dagger f' (\omega, \omega')$ and $(\omega, \omega')^\dagger = (\omega', \omega)$ where $\dagger$ denotes complex or Hermitian conjugation. Furthermore, $(\mathrm{d}x^{\mu_1} \cdots \mathrm{d}x^{\mu_r}, \mathrm{d}x^{\nu_1} \cdots \mathrm{d}x^{\nu_s}) = \delta_{r,s} g^{\mu_1 \rho_1} \cdots g^{\mu_r \rho_r} \delta^{[\nu_1}_{\rho_1} \cdots \delta^{\nu_r]}_{\rho_r}$.

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Cyclic identities for Jacobi elliptic and related functions

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(Received 15 July 2002; accepted 16 January 2003)

Identities involving cyclic sums of terms composed from Jacobi elliptic functions evaluated at p equally shifted points on the real axis were recently found. These identities played a crucial role in discovering linear superposition solutions of a large number of important nonlinear equations. We derive four master identities, from which the identities discussed earlier are derivable as special cases. Master identities are also obtained which lead to cyclic identities with alternating signs. We discuss an extension of our results to pure imaginary and complex shifts as well as to the ratio of Jacobi theta functions. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1560856]

I. INTRODUCTION

In a recent paper,[1] we have given many new mathematical identities involving the Jacobi elliptic functions sn (x,m), cn (x,m), and dn (x,m), where m is the elliptic modulus parameter $(0 \leqslant m \leqslant 1)$. The functions sn (x,m), cn (x,m), and dn (x,m) are doubly periodic functions with periods $(4K(m), i2K'(m))$, $(4K(m), i4K'(m))$, and $(2K(m), i4K'(m))$, respectively.[2] Here, $K(m)$ denotes the complete elliptic integral of the first kind, and $K'(m)=K(1-m)$. The $m=0$ limit gives $K(0)=\pi/2$ and trigonometric functions: $\mathrm{sn}(x,0)=\sin x$, $\mathrm{cn}(x,0)=\cos x$, and $\mathrm{dn}(x,0)=1$. The $m \to 1$ limit gives $K(1) \to \infty$ and hyperbolic functions: $\mathrm{sn}(x,1) \to \tanh x$, $\mathrm{cn}(x,1) \to \mathrm{sech}\, x$, and $\mathrm{dn}(x,1) \to \mathrm{sech}\, x$. For simplicity, from now on we will not explicitly display the modulus parameter m as an argument of the Jacobi elliptic functions.

The cyclic identities discussed in Ref. 1 play an important role in showing that a kind of linear superposition is valid for many nonlinear differential equations of physical interest.[3,4] In all identities, the arguments of the Jacobi functions in successive terms are separated by either $2K(m)/p$ or $4K(m)/p$, where p is an integer. Each p-point identity of rank r involves a cyclic homogeneous polynomial of degree r (in Jacobi elliptic functions with p equally spaced arguments) related to other cyclic homogeneous polynomials of degree $r-2$ or smaller. In Ref. 1, explicit algebraic proofs were given for specific small values of p and r by using standard properties of Jacobi elliptic functions. However, identities corresponding to higher values of p and r were only verified numerically using advanced mathematical software packages. In this article, we present rigorous mathematical proofs valid for arbitrary p and r. As a useful byproduct, we determine explicit forms for the constants appearing in various identities. All the identities in Ref. 1 corresponded to real shifts of multiples of $2K(m)/p$ or $4K(m)/p$. Here, we discuss how to obtain new identities corresponding to pure imaginary shifts by multiples of $i2K'(m)/p$ or $i4K'(m)/p$, as well as identities corresponding to complex shifts by multiples of $2[K(m)+iK'(m)]/p$ or $4[K(m)+iK'(m)]/p$. We also discuss the identities for the nine secondary Jacobi elliptic functions like cd (x,m), ns (x,m), and ds (x,m). Also, we give results for several identities involving Weier-

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strass elliptic functions and ratios of Jacobi theta functions, both of which are intimately related with the Jacobi elliptic functions.[2] In our proofs, we classify the identities into four types, each with its own ''master identity'' which we prove using a combination of the Poisson summation formula and the special properties of elliptic functions.

All our identities involve sums of the following generic form:

$$S_p(x_0)=\sum_{j=1}^{p} f(x_j), \tag{1}$$

where $f(x)$ is composed from Jacobi elliptic functions with arguments corresponding to p equally spaced points

$$x_j=x_0+(j-1)T/p, \quad j=1,\ldots,p \ ,$$

where T is a period of $f(x)$ and the base point x_0 is an arbitrary complex number. We define the quantities P,Q by

$$f(z+2iK')=(-1)^P f(z), \quad f(z+2K)=(-1)^Q f(z), \quad P,Q=0,1. \tag{2}$$

Note that $Q=0,1$ correspond to real periods $2K(m), 4K(m)$ and $P=0,1$ correspond to pure imaginary periods $i2K'(m), i4K'(m)$, respectively. We denote the four possibilities as $(+,+)$, $(-,+)$, $(+,-)$ and $(-,-)$, where the first sign refers to the sign of $(-1)^P$ and the second to that of $(-1)^Q$. We will derive master identities for each of these four possibilities.

For example, one of the simplest identities discussed in Ref. 1 reads

$$\sum_{j=1}^{p} \mathrm{dn}(x_j)\,\mathrm{dn}(x_{j+1})=A, \tag{3}$$

where A is a constant independent of the base point x_0, $T=2K$ and p is any integer. In this case, we have $f(z)=\mathrm{dn}(z)\ \mathrm{dn}(z+T/p)$ which corresponds to $P=0,Q=0$, since $\mathrm{dn}(z+2K)=\mathrm{dn}(z)$ and $\mathrm{dn}(z+2iK')=-\mathrm{dn}(z)$. Liouville's theorem can be used to prove the above identity, since $\mathrm{dn}(z)$ has simple poles within its fundamental region $(0,2K,2K+4iK',4iK')$ at iK' and $3iK'$ both of which we collectively refer to as z^*. The identity $\mathrm{dn}(z^*+u)+\mathrm{dn}(z^*-u)=0$ for arbitrary complex u then implies that every pole in the sum is cancelled exactly by a zero of the same order. Thus the sum is an analytic function without any poles in the finite part of the complex plane and by Liouville's theorem must be a constant.[5] This is an explicit illustration of the general principle underlying the identities, namely that the orders of poles in a higher order polynomial are reduced by some zeros leading to simpler sums. However, this method does not yield the constants like A explicitly. In fact, using the Poisson summation formula and special properties of Jacobi elliptic functions, we show below that the constant A in Eq. (3) is given by

$$A=\frac{p}{2K}\int_0^{2K}\mathrm{dn}(x)\,\mathrm{dn}(x+T/p)\,dx=p\left(\mathrm{dn}(2K/p)-\frac{\mathrm{cn}(2K/p)Z(\beta_{2K})}{\mathrm{sn}(2K/p)}\right), \tag{4}$$

where Z is the Jacobi zeta function $[Z\equiv Z(\beta_q,m)]$ (Ref. 2) with $\beta_q\equiv\arcsin(\mathrm{sn}(q/p,m))$.

Identities analogous to Eq. (3) also hold for sn and cn. For instance,

$$\sum_{j=1}^{p} \mathrm{sn}(x_j)\,\mathrm{sn}(x_{j+1})=\frac{pZ(\beta_{2K})}{m\,\mathrm{sn}(2K/p)}. \tag{5}$$

Here T is $2K$ as this is the periodicity of $f(z)=\mathrm{sn}(z)\ \mathrm{sn}(z+T/p)$. The expression as given above is valid for all integer values of $p>2$, with both sides vanishing when $p=2$.

A further generalization that can be easily treated with the techniques developed below is to sums that involve rth neighbors. We consider the case when r and p are coprime integers and

$1 \leqslant r < p-1$, the other cases being included since identities for any choice of p also include the identities for the factors of p. Such a generalization of say Eq. (4) above is

$$\sum_{j=1}^{p} \mathrm{dn}(x_j)\mathrm{dn}(x_{j+r}) = p\left(\mathrm{dn}(2rK/p) - \frac{\mathrm{cn}(2rK/p)Z(\beta_{2rK})}{\mathrm{sn}(2rK/p)} \right). \tag{6}$$

Another easy generalization is to identities involving terms consisting of a product of an arbitrary number of Jacobi elliptic functions.

The plan of this article is as follows. In Sec. II, we derive the master identities which form the basis for obtaining all the identities in this article, and are tabulated in Appendixes A and B. Section III contains a derivation of identities involving alternating signs. In Sec. IV, we present a collection of comments, including some which permit a generalization of all the identities to incorporate pure imaginary and complex shifts and to present the identities for Weierstrass functions as well as for ratios of Jacobi theta functions.

II. THE MASTER IDENTITIES

In this section, we derive the four master identities corresponding to Q,P taking on values 0,1, which effectively encompass most of the cyclic identities discussed in Ref. 1. The remaining identities in Ref. 1 correspond to master identities with alternating signs, and these are discussed in the next section.

For completeness we first derive the finite version of the Poisson summation formula[6] that fully exploits the equally spaced nature of the sampling points, and which plays a crucial role in subsequent derivations. Since $f(x)$ has a period T, we may expand it in a Fourier series:

$$f(x) = \frac{1}{T}\sum_{k=-\infty}^{\infty} a_k\, e(kx/T), \quad a_k = \int_0^T f(x)\, e(-kx/T)\, \mathrm{d}x, \tag{7}$$

where we have introduced the convenient notation $e(x) \equiv \exp(2\pi i x)$. The required sum may then be written as

$$S_p(x_0) = \sum_{j=1}^{p} f(x_j) = \frac{1}{T}\sum_{k=-\infty}^{\infty} a_k\, e(kx_0/T) \sum_{j=1}^{p} e(kj/p). \tag{8}$$

Using the simple identity

$$\sum_{j=1}^{p} e(kj/p) = \begin{cases} p & \text{if} \quad p|k \\ 0 & \text{otherwise,} \end{cases} \tag{9}$$

we get

$$S_p(x_0) = \frac{p}{T}\sum_{k,\ p|k} a_k\, e(kx_0/T). \tag{10}$$

Note that we need to evaluate only those Fourier coefficients a_k for which k is a multiple of p.

A. Cases corresponding to $Q=0$

We first derive the two master identities corresponding to $Q=0$ (or equivalently $T=2K$), allowing P to be either 1 or 0. Consider the rectangle $ABCD \equiv (-K, K, K+2iK', -K+2iK')$. We assume that $f(z)$ has a finite number of poles inside $ABCD$ situated at points $z_w^* = iK' + wT/p$, where $w = 0, \pm 1, \pm 2, \ldots$ and $|w| < p$. Let the principal part of $f(z)$ about the pole z_w^* be

$$\sum_{l=1}^{L_w} \frac{\alpha_l^{(w)}}{(z-z_w^*)^l}, \tag{11}$$

which makes this a pole of order L_w.

We now use the fact that $f(z)$ is composed of elliptic functions, and this essentially allows evaluation of a_k. To evaluate a_k, for $k\neq 0$, consider the integral over the rectangle $ABCD$:

$$\begin{aligned}\oint f(z)\, e(-kz/T)\, \mathrm{d}z &= a_k + \int_{K+2iK'}^{-K+2iK'} f(z)\, e(-kz/T)\, \mathrm{d}z \\ &= a_k + \int_{K}^{-K} f(z+2iK')\, e(-k[z+2iK']/T)\, \mathrm{d}z \\ &= a_k + (-1)^{P+1} q^{-2k} \int_{-K}^{K} f(z)\, e(-kz/T)\, \mathrm{d}z \\ &= a_k[1+(-1)^{P+1} q^{-2k}], \end{aligned} \tag{12}$$

where $q=\exp(-\pi K'/K)$ is the Jacobian nome.[2] The contributions of the vertical segments of the integration contour are equal and opposite, and cancel each other.

On the other hand, the sum of the residues of $f(z)\, e(-kz/T)$ may also be calculated. The residue at the pole z_w^* is

$$\begin{aligned}\mathrm{Res}[f(z)\, e(-kz/T)] &= \mathrm{Res}[f(z)\, e(-k[z-(iK'+wT/p)]/T) q^{-k} e(-kw/p)] \\ &= q^{-k}\mathrm{Res}\left[\left(\sum_{l=1}^{L_w} \frac{\alpha_l^{(w)}}{(z-z_w^*)^l}\right)\left(\sum_{n=0}^{\infty}\left(\frac{-2\pi i k}{T}\right)^n \frac{(z-z_w^*)^n}{n!}\right)\right] \\ &= q^{-k}\sum_{l=1}^{L_w}\left[\frac{\alpha_l^{(w)}}{(l-1)!}\left(\frac{-2\pi i}{T}\right)^{l-1} k^{l-1}\right]. \end{aligned} \tag{13}$$

For the second equality, we have made use of the fact that only those a_k for which k/p is an integer need to be evaluated, thanks to the Poisson summation formula Eq. (10).

Define $L' \equiv \mathrm{Max}\{L_1, L_2, \ldots, L_w\}$ and $\gamma_l = \Sigma_w \alpha_l^{(w)}$, $l=1,\ldots,L'$, where we set nonexistent $\alpha^{(w)}$ to be zero. We also set L to be the maximum integer such that γ_L is nonzero. If $L=0$, there are no nonvanishing γ and the function is regular. Using $T=2K$ the sum of the residues at all the interior poles may be written as

$$\mathrm{Res} = q^{-k}\sum_{l=1}^{L}\left[\frac{\gamma_l}{(l-1)!}\left(\frac{-2\pi i}{2K}\right)^{l-1} k^{l-1}\right]. \tag{14}$$

Thus

$$a_k = \frac{2\pi i q^{-k}}{1+(-1)^{P+1}q^{-2k}}\sum_{l=1}^{L}\left[\frac{\gamma_l}{(l-1)!}\left(\frac{-2\pi i}{2K}\right)^{l-1} k^{l-1}\right], \quad k\neq 0. \tag{15}$$

Therefore, Eq. (10) now becomes

$$S_p(x_0) = \frac{p}{2K}\left[a_0 + 2\pi i \sum_{l=1}^{L}\frac{\gamma_l}{(l-1)!}\left(\frac{-2\pi i}{2K}\right)^{l-1} \sum_{k\neq 0,\, p|k} \frac{k^{l-1} q^{-k}}{1+(-1)^{P+1}q^{-2k}} e\left(\frac{kx_0}{2K}\right)\right]. \tag{16}$$

We are in a position to derive two master identities (MI) corresponding to the $P=1$ and $P=0$ cases, which we call MI-I and MI-II, respectively. We state for convenience the following well-known symmetry properties:

$$\mathrm{sn}(z+2K)=-\mathrm{sn}(z),\quad \mathrm{cn}(z+2K)=-\mathrm{cn}(z),\quad \mathrm{dn}(z+2K)=\mathrm{dn}(z),$$

$$\mathrm{sn}(z+2iK')=\mathrm{sn}(z),\quad \mathrm{cn}(z+2iK')=-\mathrm{cn}(z),\quad \mathrm{dn}(z+2iK')=-\mathrm{dn}(z).$$

1. MI-I: Case $Q=0$, $P=1$

MI-I identities result if there are an odd total number of dn and cn, and an even total number of sn and cn functions in $f(z)$, i.e., if one considers terms of the form $\mathrm{dn}^a\ \mathrm{sn}^b\ \mathrm{cn}^c$, then $a+c$ is odd and $b+c$ is even. The primitive function of this type is $\mathrm{dn}(z)$ and we consider an "archetypal sum" σ_1 from which identities in this class can be derived:

$$\sigma_1(x_0)=\sum_{j=1}^{p}\mathrm{dn}(x_j), \tag{17}$$

where p is any (odd or even) integer. We note that in the case of MI-I

$$a_0=\int_0^{T=2K} f(x)\,dx=i\pi\gamma_1, \tag{18}$$

as can be seen on integrating $f(z)$ around $ABCD$, and making use of the antisymmetry about $2iK'$, since we are considering the case $P=1$.

Since $\mathrm{dn}(z)$ has a single simple pole at iK' interior to $ABCD$ with $\gamma_1=-i$, using the Poisson summation formula yields

$$\sigma_1(x_0)=\frac{p\pi}{2K}\left[1+2\sum_{k\neq 0,p|k}\frac{q^{-k}}{1+q^{-2k}}e\left(\frac{kx_0}{2K}\right)\right]. \tag{19}$$

The above expression for $\sigma_1(x_0)$ now allows us to rewrite $S_p(x_0)$ as given in Eq. (16), yielding our first master identity:

$$S_p(x_0)=i\sum_{l=1}^{L}\frac{(-1)^{l-1}\gamma_l}{(l-1)!}\frac{d^{l-1}}{dx_0^{l-1}}\sigma_1(x_0). \tag{20}$$

Thus all the sums in this class can be written as sums over the higher order derivatives of the function $\mathrm{dn}(z)$. The highest derivative order is one less than the maximum of the orders of the function $f(z)$ at all the interior poles. We see that the sums involving the Jacobi functions are intimately related to their singularity structure in the complex plane.

As an illustration, consider the sum

$$S_p(x_0)=\sum_{j=1}^{p}\mathrm{dn}(x_j)\mathrm{dn}(x_{j+1})\mathrm{dn}(x_{j+2}). \tag{21}$$

The relevant function is $f(z)=\mathrm{dn}(z)\mathrm{dn}(z+2K/p)\mathrm{dn}(z+4K/p)$, with poles at iK', $iK'-2K/p$, and $iK'-4K/p$ within $ABCD$. The principal part of the function $\mathrm{dn}(z)[\mathrm{dn}(z+2K/p)\mathrm{dn}(z+4K/p)+\mathrm{dn}(z-2K/p)\mathrm{dn}(z+2K/p)+\mathrm{dn}(z-4K/p)\mathrm{dn}(z-2K/p)]$ around $z=iK'$ determines the γ_l. The singularity of $\mathrm{dn}(z)$ is simple, therefore $L=1$. Using the identity $\mathrm{dn}(z+iK')=-i\,\mathrm{cs}(z)$ we get that $\gamma_1=-i[\mathrm{cs}^2(2K/p)-2\mathrm{cs}(2K/p)\mathrm{cs}(4K/p)]$. Substituting this result in Eq. (20) gives the identity

$$\sum_{j=1}^{p}\mathrm{dn}(x_j)\mathrm{dn}(x_{j+1})\mathrm{dn}(x_{j+2})=[\mathrm{cs}^2(2K/p)-2\mathrm{cs}(2K/p)\mathrm{cs}(4K/p)]\sum_{j=1}^{p}\mathrm{dn}(x_j). \tag{22}$$

As another example consider

$$S_p(x_0)=\sum_{j=1}^{p} \mathrm{sn}(x_j)\,\mathrm{cn}(x_j)\,\mathrm{dn}(x_j)[\mathrm{dn}(x_{j+1})+\mathrm{dn}(x_{j-1})]. \tag{23}$$

The relevant function now is $f(z)=\mathrm{sn}(z)\,\mathrm{cn}(z)\,\mathrm{dn}(z)[\mathrm{dn}(z+2K/p)+\mathrm{dn}(z-2K/p)]$. There are three poles, one at iK' and the others at $iK'\pm 2K/p$. To get the quantities γ_l, it is convenient to consider the principal part of $f(z)+f(z+2K/p)+f(z-2K/p)$ around $z=iK'$. At iK', while the product of the three functions sn, cn and dn gives an order three singularity, it is reduced by one due to the vanishing of a constant term in the expansion of $\mathrm{dn}(z+2K/p)+\mathrm{dn}(z-2K/p)$ around the same point. Thus we get that the maximum order of $f(z)$ is $L=2$ while $\gamma_1=0$ and $\gamma_2=(-2i/m)\mathrm{ds}(2K/p)\,\mathrm{ns}(2K/p)$. Substitution in Eq. (20) leads to the identity

$$\sum_{j=1}^{p} \mathrm{sn}(x_j)\,\mathrm{cn}(x_j)\,\mathrm{dn}(x_j)[\mathrm{dn}(x_{j+1})+\mathrm{dn}(x_{j-1})] = 2\mathrm{ds}(2K/p)\,\mathrm{ns}(2K/p)\sum_{j=1}^{p} \mathrm{cn}(x_j)\,\mathrm{sn}(x_j). \tag{24}$$

Several other identities of this type are given in Appendix A.

2. MI-II: Case $Q=0$, $P=0$

This case results when there are an even total number of dn and cn and an even total number of sn and cn, i.e., if one considers terms of the form $\mathrm{dn}^a\,\mathrm{sn}^b\,\mathrm{cn}^c$, then both $a+c$ and $b+c$ must be even. In this case the relevant primitive function can be taken as $\mathrm{dn}^2(z)$ and we define and evaluate the following archetypal sum:

$$\sigma_2(x_0)=\sum_{j=1}^{p} \mathrm{dn}^2(x_j)=\frac{pE}{K}+\frac{p\pi^2}{K^2}\sum_{k\neq 0,\, p|k}\frac{kq^k}{1-q^{2k}}e\left(\frac{kx_0}{2K}\right). \tag{25}$$

Here E is the complete elliptic integral of the second kind.[2] We note that in this case γ_1 is zero, as the integral of $f(z)$ around the rectangle $ABCD$ vanishes.

Substituting Eq. (25) in Eq. (16) yields the second master identity:

$$S_p(x_0)=\frac{p}{2K}\left[\int_0^{2K} f(x)\mathrm{d}x+2\gamma_2 E\right]+\sum_{l=2}^{L}\frac{(-1)^{l-1}\gamma_l}{(l-1)!}\frac{d^{l-2}}{dx_0^{l-2}}\sigma_2(x_0). \tag{26}$$

Thus all MI-II identities have derivatives of $\mathrm{dn}^2(z)$ upto order $L-2$. This is also the only master identity that has a nonvanishing ''constant'' (independent of x_0) term on the right hand side. The simplest member of this class has already been discussed in Eq. (3). We note that the relevant function for this identity is $f(z)=\mathrm{dn}(z)\mathrm{dn}(z+2K/p)$. There are two poles, one at iK' and the other at $iK'-2K/p$. Thus we can construct $\mathrm{dn}(z+iK')[\mathrm{dn}(z+iK'+2K/p)+\mathrm{dn}(z+iK'-2K/p)]=-\mathrm{cs}(z)[\mathrm{cs}(z+2K/p)+\mathrm{cs}(z-2K/p)]$ and its principal part around $z=0$ will give us the γ_l. The principal part of $\mathrm{cs}(z)$ around $z=0$ is $1/z$. Therefore the only relevant number is $\gamma_1=-[\mathrm{cs}(2K/p)+\mathrm{cs}(-2K/p)]=0$. Anyway we have already observed above that for this class $\gamma_1=0$ from the fact that $ABCD$ is a period parallelogram for $f(z)$. Thus the sum of the principal parts cancel and so do all the γ_l. Hence using Eq. (26), we obtain the identity (4). In fact, we can easily generalize using the same argument to a cyclic sum of any even number of dn or sn or cn. For instance,

$$\sum_{j=1}^{p} \mathrm{dn}(x_j)\mathrm{dn}(x_{j+r})\mathrm{dn}(x_{j+s})\mathrm{dn}(x_{j+t}) = \frac{p}{2K}\int_0^{2K} f(x)\mathrm{d}x, \tag{27}$$

where $f(x)=\mathrm{dn}(x)\mathrm{dn}(x+r2K/p)\mathrm{dn}(x+s2K/p)\mathrm{dn}(x+t2K/p)$.

As another example, we establish the identity

$$\sum_{j=1}^{p} \mathrm{dn}^2(x_j)\mathrm{dn}^2(x_{j+1}) = A \sum_{j=1}^{p} \mathrm{dn}^2(x_j) + B. \tag{28}$$

Writing $f(z) = \mathrm{dn}^2(z)\mathrm{dn}^2(z+2K/p)$, there are two poles of order 2 at iK' and $iK'-2K/p$ within $ABCD$. We find that $L=2$ and $\gamma_2 = 2\mathrm{cs}^2(2K/p)$. Thus applying the master identity leads to

$$A = -2\mathrm{cs}^2(2K/p), \quad B = \frac{p}{2K}\left(\int_0^{2K} \mathrm{dn}^2(t)\mathrm{dn}^2(t+2K/p)\, \mathrm{d}t + 4E\, \mathrm{cs}^2(2K/p) \right). \tag{29}$$

For an example of this class with $L=3$, we prove the identity

$$\sum_{j=1}^{p} \mathrm{cn}(x_j)\, \mathrm{sn}(x_j)[\mathrm{dn}^3(x_{j+1}) + \mathrm{dn}^3(x_{j-1})] = A \sum_{j=1}^{p} \mathrm{cn}(x_j)\, \mathrm{sn}(x_j)\, \mathrm{dn}(x_j). \tag{30}$$

We can derive this using the master identity with $f(z) = \mathrm{cn}(z)\, \mathrm{sn}(z)[\mathrm{dn}^3(z+2K/p) + \mathrm{dn}^3(z-2K/p)]$, and we find that $L=3$ with $\gamma_2 = 0$ and $\gamma_3 = (2/m)\, \mathrm{ds}(2K/p)\, \mathrm{ns}(2K/p)$. Thus the first derivative of $\mathrm{dn}^2(z)$ will appear on the RHS, which indeed leads to the above identity with the constant $A = -2\, \mathrm{ns}(2K/p)\, \mathrm{ds}(2K/p)$. Note that

$$\int_0^{2K} f(t)\, \mathrm{d}t = \int_0^{K} [f(t) + f(-t)]\, \mathrm{d}t = 0, \tag{31}$$

since $f(t)$ is an odd function of t.

B. Cases corresponding to $Q=1$

When $Q=1$, the function $f(z)$ has a real period $4K$. We consider the rectangle $ABCD \equiv (-\epsilon, 4K-\epsilon, 4K-\epsilon+2iK', -\epsilon+2iK')$, where ϵ is a small positive number, and integrate around this rectangle. Poles occur at $iK'+w4K/p$ and $iK'+2K+w4K/p$ inside the rectangle $ABCD$. If the principal part around $iK'+w4K/p$ is given by the set of coefficients $\{\gamma_l\}$, the set around $iK'+2K+w4K/p$ is $\{-\gamma_l\}$, since $f(z+2K) = -f(z)$. Also note that

$$a_0 = \int_0^{4K} f(x)\mathrm{d}x = 0, \tag{32}$$

due to antisymmetry about $2K$. Applying the Poisson summation formula and following the same procedures as for the previous cases, we get the equivalent of Eq. (16):

$$S_p(x_0) = \frac{2\pi i\, p}{4K} \sum_{l=1}^{L} \frac{\gamma_l}{(l-1)!} \left(\frac{-2\pi i}{4K} \right)^{l-1} \sum_{k \neq 0, p|k} \frac{k^{l-1}[1-(-1)^k]q^{-k/2}}{1+(-1)^{P+1}q^{-k}} e\left(\frac{kx_0}{4K} \right). \tag{33}$$

We note that $S_{2p}(x_0) = 0$, i.e., the sums in these cases vanish for even values of p. This is, however, a trivial identity since $f(x_j) = -f(x_{j+p/2})$ for $j = 1, \ldots, p/2$. Thus, for $Q=1$, it is sufficient to only consider identities where p is odd.

1. MI-III: Case $Q=1$, $P=0$

This case applies when $f(z)$ has an even total number of dn and cn and there are an odd total number of sn and cn, i.e., if one considers terms of the form $\mathrm{dn}^a\, \mathrm{sn}^b\, \mathrm{cn}^c$, then $a+c$ is even and $b+c$ is odd. The relevant primitive function here is $\mathrm{sn}(z)$ and the archetypal sum is

$$\sigma_3(x_0) = \sum_{i=j}^{p} \mathrm{sn}(x_j) = \frac{2\pi i\, p}{4K\sqrt{m}} \sum_{k \neq 0, p|k} \frac{[1-(-1)^k]q^{-k/2}}{1-q^{-k}} e\left(\frac{kx_0}{4K} \right). \tag{34}$$

Therefore, using Eq. (34) in Eq. (33), we get the third master identity:

$$S_p(x_0)=\sqrt{m}\sum_{l=1}^{L}\frac{(-1)^{l-1}\gamma_l}{(l-1)!}\frac{d^{l-1}}{dx_0^{l-1}}\sigma_3(x_0). \tag{35}$$

As an illustration take $f(z)=\mathrm{sn}^2(z)[\mathrm{sn}(z+4K/p)+\mathrm{sn}(z-4K/p)]$. This gives $L=1$ with $\gamma_1=(2/m^{3/2})[\mathrm{ns}^2(4K/p)-\mathrm{ds}(4K/p)\,\mathrm{cs}(4K/p)]$. The resulting identity is

$$\sum_{j=1}^{p}\mathrm{sn}^2(x_j)[\mathrm{sn}(x_{j+1})+\mathrm{sn}(x_{j-1})]=(2/m)[\mathrm{ns}^2(4K/p)-\mathrm{ds}(4K/p)\,\mathrm{cs}(4K/p)]\sum_{j=1}^{p}\mathrm{sn}(x_j). \tag{36}$$

An example with $L=2$ is provided by $f(z)=\mathrm{sn}(z)\,\mathrm{dn}(z)[\mathrm{sn}(z+4K/p)\,\mathrm{cn}(z+4K/p)+\mathrm{sn}(z-4K/p)\,\mathrm{cn}(z-4K/p)]$. This results in $\gamma_1=0$ while $\gamma_2=-(2/m^{3/2})\mathrm{ns}(4K/p)[\mathrm{cs}(4K/p)+\mathrm{ds}(4K/p)]$. Therefore the first derivative of sn will appear on the right hand side of the identity which we write as

$$\sum_{j=1}^{p}\mathrm{sn}(x_j)\,\mathrm{dn}(x_j)[\mathrm{sn}(x_{j+1})\,\mathrm{cn}(x_{j+1})+\mathrm{sn}(x_{j-1})\,\mathrm{cn}(x_{j-1})]$$

$$=(2/m)\mathrm{ns}(4K/p)[\mathrm{cs}(4K/p)+\mathrm{ds}(4K/p)]\sum_{j=1}^{p}\mathrm{cn}(x_j)\,\mathrm{dn}(x_j). \tag{37}$$

2. MI-IV: Case $Q=1$, $P=1$

This case applies when there are an odd total number of dn and cn and there are an odd total number of sn and cn in $f(z)$, i.e., if one considers terms of the form $\mathrm{dn}^a\,\mathrm{sn}^b\,\mathrm{cn}^c$, then both $a+c$ and $b+c$ must be odd. The relevant primitive function here is $\mathrm{cn}(z)$ and the archetypal sum is

$$\sigma_4(x_0)=\sum_{i=1}^{p}\mathrm{cn}(x_i)=\frac{2\pi p}{4K\sqrt{m}}\sum_{k\neq 0,\,p|k}\frac{[1-(-1)^k]q^{-k/2}}{1+q^{-k}}e\left(\frac{kx_0}{4K}\right). \tag{38}$$

Therefore, using Eq. (38) in Eq. (33), we get the fourth and final master identity:

$$S_p(x_0)=i\sqrt{m}\sum_{l=1}^{L}\frac{(-1)^{l-1}\gamma_l}{(l-1)!}\frac{d^{l-1}}{dx_0^{l-1}}\sigma_4(x_0). \tag{39}$$

As an illustration, consider $f(z)=\mathrm{cn}^2(z)[\mathrm{cn}(z+4K/p)+\mathrm{cn}(z-4K/p)]$. This gives $L=1$ with $\gamma_1=(2i/m^{3/2})[\mathrm{ds}^2(4K/p)-\mathrm{ns}(4K/p)\,\mathrm{cs}(4K/p)]$. The resulting identity is

$$\sum_{j=1}^{p}\mathrm{cn}^2(x_j)[\mathrm{cn}(x_{j+1})+\mathrm{cn}(x_{j-1})]=(2/m)[\mathrm{ns}(4K/p)\,\mathrm{cs}(4K/p)-\mathrm{ds}^2(4K/p)]\sum_{j=1}^{p}\mathrm{cn}(x_j). \tag{40}$$

For $f(z)=\mathrm{cn}^2(z)\,\mathrm{dn}(z)[\mathrm{sn}(z+4K/p)+\mathrm{sn}(z-4K/p)]$, we get $L=2$ and $\gamma_1=0$ while $\gamma_2=(-2i/m^{3/2})\,\mathrm{cs}(4K/p)\,\mathrm{ds}(4K/p)$. The resultant identity therefore involves the first derivative of cn:

$$\sum_{j=1}^{p}\mathrm{cn}^2(x_j)\,\mathrm{dn}(x_j)[\mathrm{sn}(x_{j+1})+\mathrm{sn}(x_{j-1})]=(2/m)\mathrm{cs}(4K/p)\mathrm{ds}(4K/p)\sum_{j=1}^{p}\mathrm{sn}(x_j)\mathrm{dn}(x_j). \tag{41}$$

This completes our enumeration of master identities for ordinary sums. Many additional examples are given in Appendix A.

III. MASTER IDENTITIES WITH ALTERNATING SIGNS

Alternating sums provide an immediate and important extension of the master identities discussed above. We consider sums of the form

$$S_p^A(x_0)=\sum_{j=1}^{p}(-1)^{j-1}f(x_j), \tag{42}$$

where again $f(x)$ has the properties discussed for the ordinary sums in Eq. (1). We are, however, forced to restrict p to be *even* in this section and as a result we only have MI-I and MI-II master identities with alternating signs. One of the consequences of having an alternating sum, as we will see below, is the appearance of the simply periodic Jacobi zeta function[7] as an important player.

To clarify the differences that arise between ordinary and alternating sums we first work out an example:

$$\begin{aligned}S_p^A(x_0)&=\sum_{j=1}^{p}(-1)^{j-1}\mathrm{dn}^2(x_j)[\mathrm{dn}(x_{j+r})+\mathrm{dn}(x_{j-r})]\\&=2[\mathrm{ds}(r2K/p)\,\mathrm{ns}(r2K/p)-(-1)^r\mathrm{cs}^2(r2K/p)]\sum_{j=1}^{p}(-1)^{j-1}\mathrm{dn}(x_j).\end{aligned} \tag{43}$$

Here the spacing is $r2K/p$. Since r and p are coprimes and p is restricted to be an even integer, hence for alternating sums r can only take odd integral values.

To prove the above identity, in the case $r=1$, consider the sums S_p^+ and S_p^-, corresponding to the positive and negative signed terms in S_p^A. We have to take $f(z)=\mathrm{dn}^2(z)[\mathrm{dn}(z+T/p)+\mathrm{dn}(z-T/p)]$ with $T=2K$,

$$\begin{aligned}S_p^+(x_0)&=\mathrm{dn}^2(x_1)[\mathrm{dn}(x_2)+\mathrm{dn}(x_p)]+\mathrm{dn}^2(x_3)[\mathrm{dn}(x_4)+\mathrm{dn}(x_2)]\\&\quad+\cdots+\mathrm{dn}^2(x_{p-1})[\mathrm{dn}(x_p)+\mathrm{dn}(x_{p-2})],\end{aligned} \tag{44}$$

and

$$\begin{aligned}S_p^-(x_0)&=\mathrm{dn}^2(x_2)[\mathrm{dn}(x_3)+\mathrm{dn}(x_1)]+\mathrm{dn}^2(x_4)[\mathrm{dn}(x_5)+\mathrm{dn}(x_3)]\\&\quad+\cdots+\mathrm{dn}^2(x_p)[\mathrm{dn}(x_1)+\mathrm{dn}(x_{p-1})].\end{aligned} \tag{45}$$

We see that

$$S_p^-(x_0)=S_p^+(x_0+T/p)$$

and

$$S_p^+(x_0)=\sum_{j=1}^{\tilde{p}}\mathrm{dn}^2[x_0+jT/\tilde{p}][\mathrm{dn}(x_0+jT/\tilde{p}+T/p)+\mathrm{dn}(x_0+jT/\tilde{p}-T/p)], \tag{46}$$

where we have defined $\tilde{p}=p/2$. The important point to note is that while the above sum appears to be in the form of an ordinary sum considered earlier by simply replacing p with $\tilde{p}$, it is not so, as the function $f(x)$ (which usually depends on p) has remained the same, or equivalently the position of the symmetric poles is still at $iK'\pm T/p$, rather than $iK'\pm T/\tilde{p}$.

Applying the Poisson summation formula we get

$$S_p^+(x_0)=\frac{\tilde{p}}{2K}\left[a_0+\sum_{k\neq 0,\tilde{p}|k} a_k\, e\left(\frac{kx_0}{2K}\right)\right]. \tag{47}$$

Note that we now need a_k for k that is a multiple of $\tilde{p}=p/2$ and not merely those that are multiples of p. For such k we get upon integrating over the same rectangle $ABCD$ that is relevant for type I ordinary identities,

$$a_k=4\pi[\mathrm{ns}(2K/p)\mathrm{ds}(2K/p)-(-1)^{k/\tilde{p}}\mathrm{cs}^2(2K/p)]\frac{q^k}{1+q^{2k}}. \tag{48}$$

This is because at the poles $iK'\pm 2K/p$, $f(x)\,e(kx/2K)$ has a residue of $2i\mathrm{cs}^2(2K/p)q^{-k}(-1)^{k/\tilde{p}}$. Now the negative signed sum S_p^- is related to the positive signed one, by merely a shift in the argument by an amount $2K/p$. Thus subtracting the two sums leads to a cancellation of the zero mode term involving a_0 and also restricts $k/\tilde{p}$ to be odd integers. We then finally get

$$S_p^A(x_0)=\frac{8\pi}{2K}[\mathrm{ns}(2K/p)\mathrm{ds}(2K/p)+\mathrm{cs}^2(2K/p)]\sum_{k/\tilde{p}=\mathrm{odd}}\frac{q^k}{1+q^{2k}}e\left(\frac{kx_0}{2K}\right). \tag{49}$$

A similar evaluation of the archetypal alternating sum can be done with $f(z)=\mathrm{dn}(z)$ which is simpler as there is only one pole at iK' within $ABCD$:

$$\sigma_1^A(x_0)=\sum_{j=1}^{p}(-1)^{j-1}\mathrm{dn}(x_j)=\frac{2\pi}{K}\sum_{k/\tilde{p}=\mathrm{odd}}\frac{q^k}{1+q^{2k}}e\left(\frac{kx_0}{2K}\right). \tag{50}$$

Therefore the stated alternating identity (43) follows.

We can now generalize these arguments and provide master identities for alternating sums. Consider an elliptic function $f(z)$ of real period T satisfying Eq. (1) that has poles at $iK'+wT/p$ where $w=0,\pm 1,\pm 2,\ldots$ and $|w|<p$. For both MI-I and MI-II classes we have

$$S_p^A(x_0)=\frac{\tilde{p}}{K}\sum_{k/\tilde{p}=\mathrm{odd}} a_k\, e\left(\frac{kx_0}{2K}\right), \tag{51}$$

thus there are no constant terms, even for type II alternating identities.

For type I and II identities we can write the a_k, the counterpart of Eq. (15), as

$$a_k=\frac{2\pi i q^{-k}}{1+(-1)^{P+1}q^{-2k}}\sum_{l=1}^{L}\left[\frac{\tilde{\gamma}_l}{(l-1)!}\left(\frac{-2\pi i}{2K}\right)^{l-1}k^{l-1}\right]. \tag{52}$$

The difference between the Eqs. (15) and (52) that is crucial is that $\tilde{\gamma}_l=\Sigma_w(-1)^w\alpha_l^{(w)}$. Thus at the pole wT/p, the coefficient of the order l principal part gets weighted by a factor of $(-1)^w$, as the residue calculation is restricted to those k where $k/\tilde{p}$ is an odd integer. Therefore, for instance, $\tilde{\gamma}_1$ *does not in general* have the meaning of sum of residues at all the poles. This in turn implies that it need not vanish for type II alternating identities.

Defining the first archetypal alternating sum as in Eq. (50), we then see that for type I identities,

$$S_p^A(x_0)=i\sum_{l=1}^{L}\frac{(-1)^{l-1}\tilde{\gamma}_l}{(l-1)!}\frac{d^{l-1}}{dx_0^{l-1}}\sigma_1^A(x_0). \tag{53}$$

Some alternating sum identities of type I are

$$\sum_{j=1}^{p}(-1)^{j-1}\mathrm{sn}(x_j)[\mathrm{cn}(x_{j+1})+\mathrm{cn}(x_{j-1})]=0, \tag{54}$$

$$\sum_{j=1}^{p}(-1)^{j-1}\mathrm{sn}(x_j)\,\mathrm{cn}(x_j)\,\mathrm{dn}(x_j)[\mathrm{dn}(x_{j+1})+\mathrm{dn}(x_{j-1})]$$

$$=2\,\mathrm{ns}(2K/p)\mathrm{ds}(2K/p)\sum_{j=1}^{p}(-1)^{j-1}\mathrm{sn}(x_j)\,\mathrm{cn}(x_j). \tag{55}$$

Turning to the type II alternating identities, it turns out that the primitive function in this case is Jacobi zeta function $Z(x)$ rather than $\mathrm{dn}^2(x)$. To see this, consider the second archetypal sum as

$$\sigma_2^A(x_0)=\sum_{j=1}^{p}(-1)^{j-1}Z(x_j). \tag{56}$$

On using the Fourier series expansion[8,9] and the Poisson summation formula for $Z(x)$ we get

$$\sum_{j=1}^{p}(-1)^{j-1}Z(x_j)=\frac{2\tilde{p}\pi i}{K}\sum_{k/\tilde{p}=\mathrm{odd}}\frac{q^{-k}}{1-q^{-2k}}e\left(\frac{kx_0}{2K}\right). \tag{57}$$

Following the steps carried out above then leads to the second master identity:

$$S_p^A(x_0)=\sum_{l=1}^{L}\frac{(-1)^{l-1}\tilde{\gamma}_l}{(l-1)!}\frac{d^{l-1}}{dx_0^{l-1}}\sigma_2^A(x_0). \tag{58}$$

Some alternating sum identities of type II are

$$\sum_{j=1}^{p}(-1)^{j-1}\mathrm{dn}(x_j)[\mathrm{cn}(x_{j+1})\,\mathrm{sn}(x_{j+1})+\mathrm{cn}(x_{j-1})\,\mathrm{sn}(x_{j-1})]$$

$$=-(4/m)\mathrm{ds}(2K/p)\,\mathrm{ns}(2K/p)\sum_{j=1}^{p}(-1)^{j-1}Z(x_j), \tag{59}$$

$$\sum_{j=1}^{p}(-1)^{j-1}\,\mathrm{cn}^3(x_j)[\mathrm{cn}(x_{j+1})+\mathrm{cn}(x_{j-1})]=(2/m^2)\mathrm{cs}(2K/p)\,\mathrm{ns}(2K/p)\sum_{j=1}^{p}(-1)^{j-1}\mathrm{dn}^2(x_j), \tag{60}$$

$$\sum_{j=1}^{p}(-1)^{j-1}\,\mathrm{cn}^2(x_j)\,\mathrm{sn}(x_j)\mathrm{dn}(x_j)[\mathrm{cn}(x_{j+1})+\mathrm{cn}(x_{j-1})]$$

$$=-(4/m^2)\mathrm{ds}^2(2K/p)\,\mathrm{cs}(2K/p)\,\mathrm{ns}(2K/p)\sum_{j=1}^{p}(-1)^{j-1}Z(x_j)$$

$$+(2/m)\,\mathrm{cs}(2K/p)\,\mathrm{ns}(2K/p)\sum_{j=1}^{p}(-1)^{j-1}\,\mathrm{cn}(x_j)\,\mathrm{sn}(x_j)\mathrm{dn}(x_j). \tag{61}$$

Summarizing, for functions of the form $f(z)=h(z)[g(z+T/p)+g(z-T/p)]$, which occur in ordinary sums, we may use the symmetrized form $h(z)[g(z+T/p)+g(z-T/p)]+g(z)[h(z+T/p)+h(z-T/p)]$ and evaluate its principal part at iK'. On the other hand, for alternating sums, we may use the antisymmetrized form $h(z)[g(z+T/p)+g(z-T/p)]-g(z)[h(z+T/p)+h(z-T/p)]$ and consider its principal part at iK'. Its generalization to more complex forms of $f(z)$ is straightforward. Using the master identities derived in this and the previous section and this methodology, we have obtained a large number of identities, some of which are given in Appendixes A and B.

IV. COMMENTS AND DISCUSSION

In this section, we give some general comments and extensions in several new directions.

(i) Identities for auxiliary functions: Until now, we have discussed identities for the three basic Jacobi elliptic functions sn, cn, and dn. However, nine auxiliary functions are also frequently found in the literature. They are

$$\begin{aligned} \mathrm{nd}\,u &\equiv \frac{1}{\mathrm{dn}\,u}; \quad \mathrm{cd}\,u \equiv \frac{\mathrm{cn}\,u}{\mathrm{dn}\,u}; \quad \mathrm{sd}\,u \equiv \frac{\mathrm{sn}\,u}{\mathrm{dn}\,u}; \\ \mathrm{ns}\,u &\equiv \frac{1}{\mathrm{sn}\,u}; \quad \mathrm{cs}\,u \equiv \frac{\mathrm{cn}\,u}{\mathrm{sn}\,u}; \quad \mathrm{ds}\,u \equiv \frac{\mathrm{dn}\,u}{\mathrm{sn}\,u}; \\ \mathrm{nc}\,u &\equiv \frac{1}{\mathrm{cn}\,u}; \quad \mathrm{dc}\,u \equiv \frac{\mathrm{dn}\,u}{\mathrm{cn}\,u}; \quad \mathrm{sc}\,u \equiv \frac{\mathrm{sn}\,u}{\mathrm{cn}\,u}. \end{aligned} \tag{62}$$

Identities for these auxiliary functions are readily obtained via the following relations:[2,8]

$$\mathrm{dn}(u,m) = \sqrt{1-m}\,\mathrm{nd}\,(u-K,m) = -i\,\mathrm{cs}\,(u-iK',m) = i\sqrt{1-m}\,\mathrm{sc}\,(u-K-iK',m), \tag{63}$$

$$\mathrm{sn}(u,m) = \mathrm{cd}\,(u-K,m) = \frac{1}{\sqrt{m}}\mathrm{ns}\,(u-iK',m) = \frac{1}{\sqrt{m}}\mathrm{dc}\,(u-K-iK',m), \tag{64}$$

$$\mathrm{cn}(u,m) = -\sqrt{1-m}\,\mathrm{sd}\,(u-K,m) = \frac{-i}{\sqrt{m}}\mathrm{ds}\,(u-iK',m) = \frac{-i\sqrt{1-m}}{\sqrt{m}}\mathrm{nc}\,(u-K-iK',m). \tag{65}$$

As an example, consider the identity $\mathrm{dn}(u,m)\,\mathrm{dn}(u+K,m) = \sqrt{1-m}$. Using Eq. (63), we obtain

$$\begin{aligned} \mathrm{nd}\,(x,m)\,\mathrm{nd}\,(x+K,m) &= \frac{1}{\sqrt{1-m}}, \\ \mathrm{cs}\,(x,m)\,\mathrm{cs}\,(x+K,m) &= -\sqrt{1-m}, \\ \mathrm{sc}\,(x,m)\,\mathrm{sc}\,(x+K,m) &= \frac{-1}{\sqrt{1-m}}. \end{aligned} \tag{66}$$

(ii) Identities for pure imaginary shifts: So far, we have focused our attention on identities involving Jacobi elliptic functions evaluated at points separated by real gaps T/p, with real T. As mentioned in Ref. 1, since Jacobi functions are doubly periodic, we can convert each identity to another one involving points separated by pure imaginary gaps iT'/p, with real T'. The procedure consists of taking any given identity, writing it for modulus $1-m$ [noting that $K(1-m) = K'(m)$], using the standard results[2,8]

$$\begin{aligned} \mathrm{sn}(x,1-m) &= \frac{-1}{\sqrt{1-m}}\mathrm{dn}(ix+K(m)+iK'(m),m), \\ \mathrm{cn}(x,1-m) &= \frac{i\sqrt{m}}{\sqrt{1-m}}\mathrm{cn}(ix+K(m)+iK'(m),m), \\ \mathrm{dn}(x,1-m) &= \sqrt{m}\,\mathrm{sn}(ix+K(m)+iK'(m),m), \end{aligned} \tag{67}$$

and changing to a new variable $u = ix+K(m)+iK'(m)$.

For instance, again consider the simple identity $\mathrm{dn}(x,m)\,\mathrm{dn}(x+K,m)=\sqrt{1-m}$. Rewriting with modulus $1-m$, using Eq. (67), and changing to the new variable $u=ix+K(m)+iK'(m)$ gives a simple identity involving a pure imaginary shift

$$\mathrm{sn}(u,m)\,\mathrm{sn}(u+iK'(m),m)=1/\sqrt{m}. \tag{68}$$

A more nontrivial example consists of identity (42) in Ref. 1:

$$\begin{aligned}&\mathrm{sn}(x,m)\,\mathrm{sn}(x+4K(m)/3,m)\,\mathrm{sn}(x+8K(m)/3,m)\\&\quad=\frac{-1}{1-q^2}[\mathrm{sn}(x,m)+\mathrm{sn}(x+4K(m)/3,m)+\mathrm{sn}(x+8K(m)/3,m)],\end{aligned} \tag{69}$$

where $q\equiv\mathrm{dn}(2K(m)/3,m)$.

The corresponding identity with pure imaginary shifts is

$$\begin{aligned}&\mathrm{dn}(u,m)\,\mathrm{dn}(u+4iK'(m)/3,m)\,\mathrm{dn}(u+8iK'(m)/3,m)\\&\quad=\frac{-(1-m)}{1-q'^2}[\mathrm{dn}(u,m)+\mathrm{dn}(u+4iK'(m)/3,m)+\mathrm{dn}(u+8iK'(m)/3,m)],\end{aligned} \tag{70}$$

where $q'\equiv\mathrm{dn}(2K'(m)/3,1-m)$.

(iii) Identities for complex shifts: Just as we have derived identities containing pure imaginary shifts, we can also derive new identities involving complex shifts. Here, the procedure consists of taking any given identity for real shifts, writing it for modulus $1/m$ (noting that $K(1/m)=\sqrt{m}[K(m)+iK'(m)],$),[2] using the standard results

$$\mathrm{sn}\left(x,\frac{1}{m}\right)=\sqrt{m}\ \mathrm{sn}\left(\frac{x}{\sqrt{m}},m\right);\quad \mathrm{cn}\left(x,\frac{1}{m}\right)=\mathrm{dn}\left(\frac{x}{\sqrt{m}},m\right);\quad \mathrm{dn}\left(x,\frac{1}{m}\right)=\mathrm{cn}\left(\frac{x}{\sqrt{m}},m\right), \tag{71}$$

and changing to a new variable $u=x/\sqrt{m}$.

As a simple example, let us once more take the simple identity $\mathrm{dn}(x,m)\,\mathrm{dn}(x+K,m)=\sqrt{1-m}$. It now transforms to

$$\mathrm{cn}(u,m)\,\mathrm{cn}(u+K(m)+iK'(m),m)=-i\frac{\sqrt{1-m}}{\sqrt{m}}. \tag{72}$$

As a second example, take identity (45) in Ref. 1:

$$\begin{aligned}&\mathrm{cn}(x,m)\,\mathrm{sn}(x+4K/3,m)\,\mathrm{sn}(x+8K/3,m)+\mathrm{cn}(x+4K/3,m)\,\mathrm{sn}(x+8K/3,m)\,\mathrm{sn}(x,m)\\&\quad+\mathrm{cn}(x+8K/3,m)\,\mathrm{sn}(x,m)\,\mathrm{sn}(x+4K/3,m)\\&\quad=\frac{-(1+q)^2}{m}[\mathrm{cn}(x,m)+\mathrm{cn}(x+4K/3,m)+\mathrm{cn}(x+8K/3,m)],\end{aligned} \tag{73}$$

where $q\equiv\mathrm{dn}(2K(m)/3,m)$.

The corresponding identity with complex shifts is

$$\begin{aligned}&\mathrm{dn}(u,m)\,\mathrm{sn}(u+4(K+iK')/3,m)\,\mathrm{sn}(u+8(K+iK')/3,m)+\ \mathrm{dn}(u+4(K+iK')/3,m)\,\mathrm{sn}(u+8(K\\&\quad+iK')/3,m)\,\mathrm{sn}(u,m)+\ \mathrm{dn}(u+8(K+iK')/3,m)\,\mathrm{sn}(u,m)\,\mathrm{sn}(u+4(K+iK')/3,m)\\&\quad=-(1+r)^2[\mathrm{dn}(u,m)+\mathrm{dn}(u+4(K+iK')/3,m)+\mathrm{dn}(u+8(K+iK')/3,m)],\end{aligned} \tag{74}$$

where $r\equiv q(1/m)=\mathrm{cn}(2\{K(m)+iK'(m)\}/3,m)$.

(iv) Identities for ratios of Jacobi elliptic functions: In applications involving linear superposition of solutions of nonlinear differential equations,[3,4] one often needs identities for ratios of Jacobi elliptic functions like cndn/sn. These can be obtained from the identities derived in this article. For example, noting that

$$\frac{\mathrm{cn}\,x\ \mathrm{dn}\,x}{\mathrm{sn}\,x}=\frac{\mathrm{dn}\,2x+\mathrm{cn}\,2x}{\mathrm{sn}\,2x}=i[\sqrt{m}\,\mathrm{cn}(2x+iK',m)+\mathrm{dn}(2x+iK',m)] \tag{75}$$

gives rise to

$$\begin{aligned}&\frac{\mathrm{cn}\,(x+2K/3)\ \mathrm{dn}\,(x+2K/3)}{\mathrm{sn}\,(x+2K/3)}\ \frac{\mathrm{cn}\,(x+4K/3)\ \mathrm{dn}\,(x+4K/3)}{\mathrm{sn}\,(x+4K/3)}\\&\quad+\frac{\mathrm{cn}\,(x+4K/3)\ \mathrm{dn}\,(x+4K/3)}{\mathrm{sn}\,(x+4K/3)}\ \frac{\mathrm{cn}\,x\ \mathrm{dn}\,x}{\mathrm{sn}\,x}+\frac{\mathrm{cn}\,x\ \mathrm{dn}\,x}{\mathrm{sn}\,x}\ \frac{\mathrm{cn}\,(x+2K/3)\ \mathrm{dn}\,(x+2K/3)}{\mathrm{sn}\,(x+2K/3)}\\&=-m[\mathrm{cn}(2u)\,\mathrm{cn}(2u+4K/3)+\mathrm{cn}(2u+4K/3)\,\mathrm{cn}(2u+8K/3)+\mathrm{cn}(2u+8K/3)\,\mathrm{cn}(2u)]\\&\quad-[\mathrm{dn}(2u)\,\mathrm{dn}(2u+4K/3)+\mathrm{dn}(2u+4K/3)\,\mathrm{dn}(2u+8K/3)+\mathrm{dn}(2u+8K/3)\,\mathrm{dn}(2u)],\end{aligned} \tag{76}$$

where $u=x+iK'(m)/2$. In the above derivation, the cn dn terms cancel in view of identity (33) in Ref. 1. Further, the right hand side of Eq. (76) has the constant value $q(2+q)[m-(1+q)^2]/(1+q)^2$, $q\equiv\mathrm{dn}(2K(m)/3,m)$, due to identities (32) in Ref. 1.

Other identities involving ratios follow from useful equations analogous to Eq. (75):

$$\begin{gathered}\frac{\mathrm{sn}\,x\ \mathrm{dn}\,x}{\mathrm{cn}\,x}=\frac{1-\mathrm{cn}\,2x}{\mathrm{sn}\,2x},\quad \frac{\mathrm{sn}\,x\ \mathrm{cn}\,x}{\mathrm{dn}\,x}=\frac{1-\mathrm{dn}\,2x}{m\,\mathrm{sn}\,2x},\quad \frac{\mathrm{cn}\,x}{\mathrm{sn}\,x\ \mathrm{dn}\,x}=\frac{1+\mathrm{cn}\,2x}{\mathrm{sn}\,2x},\\ \frac{\mathrm{sn}\,x}{\mathrm{cn}\,x\ \mathrm{dn}\,x}=\frac{\mathrm{dn}\,2x-\mathrm{cn}\,2x}{(1-m)\,\mathrm{sn}\,2x},\quad \frac{\mathrm{dn}\,x}{\mathrm{sn}\,x\ \mathrm{cn}\,x}=\frac{1+\mathrm{dn}\,2x}{\mathrm{sn}\,2x}.\end{gathered} \tag{77}$$

(v) Cyclic identities for Weierstrass functions: Jacobi elliptic functions are closely related with the Weierstrass function $\mathcal{P}(u)$,[2,7] the relations being

$$\mathrm{sn}\,u=[\mathcal{P}(u)-e_3]^{-1/2},\quad \mathrm{cn}\,u=\left[\frac{\mathcal{P}(u)-e_1}{\mathcal{P}(u)-e_3}\right]^{1/2},\quad \mathrm{dn}\,u=\left[\frac{\mathcal{P}(u)-e_2}{\mathcal{P}(u)-e_3}\right]^{1/2}, \tag{78}$$

where

$$e_1=(2-m)/3,\quad e_2=(2m-1)/3,\quad e_3=-(1+m)/3. \tag{79}$$

$\mathcal{P}(u)$ has implicit arguments corresponding to its two periods $2\omega_1=2K(m)$ and $2\omega_3=2iK'(m)$.[7] Using this relationship and identities obtained by us, we can immediately write down identities for the Weierstrass function for shifts in the units of ω_1/p, ω_3/p and ω_2/p where $\omega_2=-(\omega_1+\omega_3)$. For example, using identity (28), one gets

$$\begin{aligned}&\sum_{j=1}^{p}\mathcal{P}(u+2(j-1)\omega_1/p)\,\mathcal{P}(u+2j\omega_1/p)\\&\quad=(B+pAe_1-pe_1^2)-(A-2e_1)\sum_{j=1}^{p}\mathcal{P}(u+2(j-1)\omega_1/p),\end{aligned} \tag{80}$$

where A,B are the constants appearing in Eq. (28).

(vi) Cyclic identities for Jacobi theta functions: The connection between the four Jacobi theta functions $\theta_1(z),\theta_2(z),\theta_3(z),\theta_4(z)$ and the Jacobi elliptic functions is given by[7]

$$\mathrm{sn}\,u=\frac{1}{m^{1/4}}\frac{\theta_1(z)}{\theta_4(z)},\quad \mathrm{cn}\,u=\frac{(1-m)^{1/4}}{m^{1/4}}\frac{\theta_2(z)}{\theta_4(z)},\quad \mathrm{dn}\,u=(1-m)^{1/4}\frac{\theta_3(z)}{\theta_4(z)},\tag{81}$$

where $z\equiv u\pi/2K(m)$. Therefore, any of our cyclic identities for real, imaginary or complex shift can also be rewritten as identities for the ratios of Jacobi elliptic functions for shifts in units of π/p, $\pi\tau/p$ or $\pi(1+\tau)/p$, respectively, where $\tau=iK'/K$. As an illustration, we consider identity (A3). In terms of theta functions, one gets

$$\prod_{j=1}^{p}\frac{\theta_3(z+(j-1)\pi/p)}{\theta_4(z+(j-1)\pi/p)}=\left(\prod_{n=1}^{(p-1)/2}\frac{\theta_2^2(2nK/p)}{\theta_1^2(2nK/p)}\right)\sum_{j=1}^{p}\frac{\theta_3(z+(j-1)\pi/p)}{\theta_4(z+(j-1)\pi/p)}.\tag{82}$$

ACKNOWLEDGMENTS

It is a pleasure to thank Professor Henry McKean and Professor Ashok Raina for insightful comments and suggestions. The work of A.K. and U.S. was supported in part by Grant No. FGO2-84ER40173 from the U.S. Department of Energy.

APPENDIX A: EXAMPLES USING THE MASTER IDENTITIES

In this appendix, we present a collection of identities involving cyclic combinations of Jacobi elliptic functions (excluding those that are already mentioned in the text). These identities are derived by using various choices of $f(x)$ in the four master identities [Eqs. (20), (26), (35), and (39)] developed in the text. We use the notation $a\equiv r2K/p$ and $b\equiv r4K/p$, where $1\leqslant r<p-1$ and $(r,p)=1$. We also use $a'=s2K/p$, $a''=t2K/p$ and $b'=s4K/p$, where s,r,t are all distinct. Also we use $s_j\equiv\mathrm{sn}(x_j)$, etc., where $x_j=x_0+(j-1)T/p$. Note that $T=2K$ for the first two master identities, while it is $4K$ for the remaining two. It may be noted here that for every identity of class MI-I, there are analogous identities of classes MI-III and MI-IV and therefore we give only a few distinct identities of each of these class. In any case, these identities are not exhaustive (as indeed they cannot be) but are meant to be representative low L identities. A more exhaustive collection of identities can be found in Ref. 10.

1. Examples belonging to the class MI-I

$$\sum_{j=1}^{p}s_j(c_{j+r}+c_{j-r})=(p/2K)\int_0^{2K}f(x)\mathrm{d}x=0.\tag{A1}$$

$$\sum_{j=1}^{p}d_jd_{j+r}\cdots d_{j+(l-1)r}=\left[\prod_{k=1}^{(l-1)/2}\mathrm{cs}^2(ka)+2(-1)^{(l-1)/2}\sum_{k=1}^{(l-1)/2}\prod_{n=1,n\neq k}^{l}\mathrm{cs}([n-k]a)\right]\sum_{j=1}^{p}d_j.\quad(l\leqslant p).\tag{A2}$$

For the special case $l=p$, this identity takes the simpler form

$$\prod_{j=1}^{p}d_j=\prod_{n=1}^{(p-1)/2}\mathrm{cs}^2\left(\frac{2Kn}{p}\right)\sum_{j=1}^{p}d_j.\tag{A3}$$

$$\sum_{j=1}^{p}d_j^2(d_{j+r}+d_{j-r})=2[\mathrm{ds}(a)\,\mathrm{ns}(a)-\mathrm{cs}^2(a)]\sum_{j=1}^{p}d_j.\tag{A4}$$

$$\sum_{j=1}^{p} c_j(c_{j+r}d_{j+r}+c_{j-r}d_{j-r})=(-2/m)\mathrm{cs}(a)[\mathrm{ds}(a)-\mathrm{ns}(a)]\sum_{j=1}^{p} d_j. \tag{A5}$$

$$\sum_{j=1}^{p} d_j(d_{j+s}d_{j+r}+d_{j-s}d_{j-r})=-2[\mathrm{cs}(a)\mathrm{cs}(a')+\mathrm{cs}(a-a')\{\mathrm{cs}(a)-\mathrm{cs}(a')\}\ ]\ \sum_{j=1}^{p} d_j. \tag{A6}$$

$$\begin{aligned}\sum_{j=1}^{p} s_j^2(c_{j+r}c_{j+s}d_{j+t}+c_{j-r}c_{j-s}d_{j-t})&\\ =(2/m^2)[\mathrm{cs}(a)\mathrm{cs}(a'')\mathrm{ds}(a')\,\mathrm{ns}(a)+\mathrm{cs}(a')\mathrm{cs}(a'')\mathrm{ds}(a)\,\mathrm{ns}(a')&\\ +\mathrm{ds}(a)\mathrm{ds}(a')\mathrm{ds}(a'')\,\mathrm{ns}(a'')-\mathrm{cs}(a-a'')\mathrm{ds}(a-a')\,\mathrm{ns}^2(a)&\\ -\mathrm{cs}(a''-a')\,\mathrm{ds}(a-a')\,\mathrm{ns}^2(a')-\mathrm{ds}(a-a'')\mathrm{ds}(a'-a'')\,\mathrm{ns}^2(a')]\ \sum_{j=1}^{p} d_j.&\end{aligned} \tag{A7}$$

$$\sum_{j=1}^{p} d_j^2(c_{j+r}s_{j+r}+c_{j-r}s_{j-r})=-2[\mathrm{cs}^2(a)+\mathrm{ds}(a)\,\mathrm{ns}(a)]\ \sum_{j=1}^{p} c_js_j. \tag{A8}$$

$$\sum_{j=1}^{p} s_jc_j(d_{j+r}d_{j+s}+d_{j-r}d_{j-s})=-2\mathrm{cs}(a)\mathrm{cs}(a')\sum_{j=1}^{p} c_js_j. \tag{A9}$$

$$\begin{aligned}\sum_{j=1}^{p} d_jc_js_j(d_{j+r}^3+d_{j-r}^3)=-2[\mathrm{cs}^2(a)\,\mathrm{ns}^2(a)+\mathrm{ns}^2(a)\mathrm{ds}^2(a)&\\ +\mathrm{ds}^2(a)\mathrm{cs}^2(a)+3\mathrm{cs}^2(a)\,\mathrm{ns}(a)\mathrm{ds}(a)]\sum_{j=1}^{p} c_js_j.&\end{aligned} \tag{A10}$$

$$\begin{aligned}\sum_{j=1}^{p} d_j^3(d_{j+r}^2+d_{j-r}^2)=-2\mathrm{cs}^2(a)\sum_{j=1}^{p} d_j^3+2[\mathrm{cs}^2(a)\,\mathrm{ns}^2(a)+\mathrm{ns}^2(a)\mathrm{ds}^2(a)&\\ +\mathrm{ds}^2(a)\mathrm{cs}^2(a)-3\mathrm{cs}^2(a)\,\mathrm{ns}(a)\mathrm{ds}(a)]\sum_{j=1}^{p} d_j.&\end{aligned} \tag{A11}$$

2. Examples belonging to the class MI-II

$$\sum_{j=1}^{p} c_jc_{j+r}=p\,\mathrm{cn}(a)\left(1-\frac{\mathrm{dn}(a)Z(\beta_{2rK})}{m\mathrm{sn}(a)\,\mathrm{cn}(a)}\right). \tag{A12}$$

$$\sum_{j=1}^{p} d_jd_{j+1}\cdots d_{j+r-1}=(p/2K)\int_0^{2K}\prod_{j=0}^{r-1}\mathrm{dn}(x+(j2K/p)\,\mathrm{d}x,\quad (r\ \text{even}). \tag{A13}$$

$$d_1d_2\cdots d_p=(1-m)^{p/4},\quad (p\ \text{even}). \tag{A14}$$

$$\sum_{j=1}^{p} c_j d_j (s_{j+r} + s_{j-r}) = 0. \tag{A15}$$

$$\sum_{j=1}^{p} c_j d_j (c_{j+r} d_{j+r} + c_{j-r} d_{j-r}) = -\gamma_2 \sum_{j=1}^{p} d_j^2 + (p/2K)\left(\int_0^{2K} f(x)\mathrm{d}x + 2\gamma_2 E \right),$$

$$f(x) = \mathrm{cn}(x)\mathrm{dn}(x)[\mathrm{cn}(x+a)\mathrm{dn}(x+a) + \mathrm{cn}(x-a)\mathrm{dn}(x-a)], \quad \gamma_2 = \frac{4}{m}\mathrm{cs}(a)\mathrm{ds}(a). \tag{A16}$$

$$\sum_{j=1}^{p} d_j^3 (d_{j+r} + d_{j-r}) = -\gamma_2 \sum_{j=1}^{p} d_j^2 + (p/2K)\left(\int_0^{2K} f(x)dx + 2\gamma_2 E \right),$$

$$f(x) = \mathrm{dn}^3(x)[\mathrm{dn}(x+a) + \mathrm{dn}(x-a)], \quad \gamma_2 = -2\,\mathrm{ns}(a)\mathrm{ds}(a). \tag{A17}$$

$$\sum_{j=1}^{p} d_j^3 (d_{j+r}^3 + d_{j-r}^3) = -\gamma_2 \sum_{j=1}^{p} d_j^2 + (p/2K)\left(\int_0^{2K} f(x)dx + 2\gamma_2 E \right),$$

$$f(x) = \mathrm{dn}^3(x)[\mathrm{dn}^3(x+a) + \mathrm{dn}^3(x-a)], \quad \gamma_2 = 12\mathrm{cs}^2(a)\,\mathrm{ns}(a)\mathrm{ds}(a). \tag{A18}$$

$$\sum_{j=1}^{p} c_j s_j d_j (d_{j+r}^2 + d_{j-r}^2) = -2\mathrm{cs}^2(a) \sum_{i=1}^{p} c_j s_j d_j . \tag{A19}$$

$$\sum_{j=1}^{p} s_j c_j^2 d_j (c_{j+r} + c_{j-r}) = (2/m)\,\mathrm{cs}(a)\,\mathrm{ns}(a) \sum_{j=1}^{p} c_j s_j d_j . \tag{A20}$$

$$\sum_{j=1}^{p} s_j c_j d_j^2 (d_{j+r}^3 + d_{j-r}^3) = -4\,\mathrm{cs}^2(a)\,\mathrm{ns}(a)\mathrm{ds}(a) \sum_{j=1}^{p} c_j s_j d_j . \tag{A21}$$

3. Examples belonging to the class MI-III

$$\sum_{j=1}^{p} s_j s_{j+r} \cdots s_{j+(l-1)r} = \frac{1}{m^{(l-1)/2}} \left(\prod_{k=1}^{(l-1)/2} (-)\mathrm{ns}^2(kb) + 2 \sum_{k=1}^{(l-1)/2} \prod_{n=1, n\neq k}^{l} \mathrm{ns}(nb - kb) \right) \sum_{j=1}^{p} s_j \tag{A22}$$

for odd $l \leqslant p$. When $l = p$, the resulting identity takes the simpler form

$$\prod_{j=1}^{p} s_j = \left(\prod_{n=1}^{(p-1)/2} \left(\frac{-1}{m} \right) \mathrm{ns}^2\left(\frac{4Kn}{p} \right) \right) \sum_{j=1}^{p} s_j . \tag{A23}$$

$$\sum_{j=1}^{p} s_j (c_{j+s} c_{j+r} + c_{j-s} c_{j-r}) = -\frac{2}{m}[\mathrm{ds}(b)\mathrm{ds}(b') + \mathrm{ds}(b-b')\{\mathrm{ns}(b) - \mathrm{ns}(b')\}] \sum_{j=1}^{p} s_j . \tag{A24}$$

$$\sum_{j=1}^{p} c_j d_j (s_{j+r}^2 + s_{j-r}^2) = (2/m)[\mathrm{ns}^2(b) + \mathrm{ds}(b)\mathrm{cs}(b)] \sum_{j=1}^{p} c_j d_j . \tag{A25}$$

$$\sum_{j=1}^{p} d_j c_j (s_{j+r} s_{j+s} + s_{j-r} s_{j-s}) = (2/m)\,\mathrm{ns}(b)\,\mathrm{ns}(b') \sum_{j=1}^{p} c_j d_j . \tag{A26}$$

$$\sum_{j=1}^{p} s_j^4(s_{j+r}+s_{j-r}) = -(2/m)\,\mathrm{cs}(b)\mathrm{ds}(b)\sum_{j=1}^{p} s_j^3 + (2/m^2)\mathrm{ns}^2(b)[\mathrm{ns}^2(b)-\mathrm{cs}(b)\mathrm{ds}(b)]\sum_{j=1}^{p} s_j\,. \tag{A27}$$

$$\sum_{j=1}^{p} s_j^4(d_{j+r}c_{j+s}+d_{j-r}c_{j-s}) = (2/m)\mathrm{cs}(b)\mathrm{ds}(b')\sum_{j=1}^{p} c_j d_j s_j^2 + (2/m^2)[\mathrm{ns}(b)\mathrm{ds}(b)\,\mathrm{ns}(b')\mathrm{cs}(b') + \mathrm{cs}(b)\mathrm{ds}(b')\{\mathrm{ns}^2(b)+\mathrm{ns}^2(b')\}]\sum_{j=1}^{p} c_j d_j\,. \tag{A28}$$

4. Examples belonging to the class MI-IV

$$\sum_{j=1}^{p} d_j(s_{j+r}+s_{j-r}) = 0. \tag{A29}$$

$$\sum_{j=1}^{p} c_j c_{j+r}\cdots c_{j+(l-1)r} = \frac{1}{m^{(l-1)/2}}\left(\prod_{k=1}^{(l-1)/2}\mathrm{ds}^2(kb) + 2(-1)^{(l-1)/2}\sum_{k=1}^{(l-1)/2}\prod_{n=1,n\neq k}^{l}\mathrm{ds}(nb-kb)\right)\sum_{j=1}^{p} c_j \tag{A30}$$

for l odd, and $l\leqslant p$. When $l=p$, the resulting identity takes the simpler form

$$\prod_{j=1}^{p} c_j = \prod_{n=1}^{(p-1)/2}\frac{1}{m}\mathrm{ds}^2\left(\frac{4Kn}{p}\right)\sum_{j=1}^{p} c_j\,. \tag{A31}$$

$$\sum_{j=1}^{p} d_j(d_{j+r}c_{j+r}+d_{j-r}c_{j-r}) = -2\mathrm{ds}(b)[\mathrm{cs}(b)-\mathrm{ns}(b)]\sum_{j=1}^{p} c_j\,. \tag{A32}$$

$$\sum_{j=1}^{p} d_j(c_{j+r}d_{j+s}+c_{j-r}d_{j-s}) = -2[\{\mathrm{ds}(b)-\mathrm{ds}(b-b')\}\mathrm{cs}(b')+\mathrm{cs}(b-b')\mathrm{cs}(b)]\sum_{j=1}^{p} c_j\,. \tag{A33}$$

$$\sum_{j=1}^{p} c_j^2(d_{j+r}s_{j+r}+d_{j-r}s_{j-r}) = (-2/m)[\mathrm{ds}^2(b)+\mathrm{cs}(b)\mathrm{ns}(b)]\sum_{j=1}^{p} s_j d_j\,. \tag{A34}$$

$$\sum_{j=1}^{p} s_j d_j(c_{j+r}c_{j+s}+c_{j-r}c_{j-s}) = (-2/m)\mathrm{ds}(b)\mathrm{ds}(b')\sum_{j=1}^{p} s_j d_j\,. \tag{A35}$$

$$\sum_{j=1}^{p} s_j^2 d_j^2(c_{j+r}+c_{j-r}) = -2\mathrm{ns}(b)\mathrm{cs}(b)\sum_{j=1}^{p} c_j^3 + \frac{2}{m}\mathrm{cs}(b)\mathrm{ns}^3(b)[m\,\mathrm{sn}^2(b)+\mathrm{cn}^2(b)-\mathrm{cn}(b)]\sum_{j=1}^{p} c_j\,. \tag{A36}$$

APPENDIX B: EXAMPLES USING MASTER IDENTITIES WITH ALTERNATING SIGNS

The identities in this appendix are only valid when p is an even integer. Since r and p are coprime, r is necessarily odd. We use the notation

$$\sum_{j=1}^{p}(-1)^{j-1}\equiv\sum_{A}\ .$$

1. Examples belonging to the class MI-I

$$\sum_{A} d_j d_{j+r} d_{j+2r} = -[\mathrm{cs}^2(a)+2\mathrm{cs}(a)\mathrm{cs}(2a)]\sum_{A} d_j\,. \tag{B1}$$

$$\sum_{A} d_j d_{j+r} d_{j+s} = -[\mathrm{cs}(a)\mathrm{cs}(a')+\mathrm{cs}(a)\mathrm{cs}(a'-a)-\mathrm{cs}(a')\mathrm{cs}(a'-a)]\sum_{A} d_j\,. \tag{B2}$$

$$\sum_{A} s_j d_j (c_{j+r}d_{j+r}+c_{j-r}d_{j-r}) = -2\mathrm{cs}(a)[-\mathrm{ns}(a)+\mathrm{ds}(a)]\sum_{A} c_j s_j\,. \tag{B3}$$

2. Examples belonging to the class MI-II

While there are no ordinary identities of this class with $L=1$, alternating identities abound. They are therefore unique and characterized by the appearance of the Jacobian zeta function. Also they have helped us in finding identities for the product of p sn's as well as of p cn's:

$$\sum_{A} d_j d_{j+r} = -2\mathrm{cs}(a)\sum_{A} Z_j \qquad (p\geqslant 4). \tag{B4}$$

$$\sum_{A} s_j s_{j+r} = (2/m)\mathrm{ns}(a)\sum_{A} Z_j \qquad (p\geqslant 4). \tag{B5}$$

$$\sum_{A} c_j c_{j+r} = -(2/m)\mathrm{ds}(a)\sum_{A} Z_j \qquad (p\geqslant 4). \tag{B6}$$

$$\sum_{A} d_j d_{j+r} d_{j+2r} d_{j+3r} = 2[\mathrm{cs}(a)\mathrm{cs}(2a)\mathrm{cs}(3a)+\mathrm{cs}^2(a)\mathrm{cs}(2a)]\ \sum_{A} Z_j\,. \tag{B7}$$

This generalizes for any even number $l<p$ to

$$\sum_{A} d_j d_{j+r}\cdots d_{j+(l-1)r} = 2(-1)^{l/2}\left(\sum_{k=1}^{l/2}(-1)^{k-1}\prod_{n=1,n\neq k}^{l}\mathrm{cs}([n-k]a)\right)\sum_{A} Z_j\,. \tag{B8}$$

Similarly, for any even number $l\leqslant p$, $p\geqslant 4$, we get

$$\sum_{A} s_j s_{j+r}\cdots s_{j+(l-1)r} = (2/m^{l/2})\left(\sum_{k=1}^{l/2}(-1)^{k-1}\prod_{n=1,n\neq k}^{l}\mathrm{ns}([n-k]a)\right)\sum_{A} Z_j\,. \tag{B9}$$

$$\sum_{A} c_j c_{j+r}\cdots c_{j+(l-1)r} = 2(-1/m)^{l/2}\left(\sum_{k=1}^{l/2}(-1)^{k-1}\prod_{n=1,n\neq k}^{l}\mathrm{ds}([n-k]a)\right)\sum_{A} Z_j\,. \tag{B10}$$

When $l=p$ $(p\geqslant 4)$ the last two identities reduce to

$$m^{p/2}\prod_{j=1}^{p} s_j = \left(\prod_{n=1}^{p/2-1}\mathrm{ns}^2\left(\frac{2Kn}{p}\right)\right)\sum_{A} Z_j\,. \tag{B11}$$

$$m^{p/2}\prod_{j=1}^{p} c_j = \sqrt{1-m}(-1)^{p/2}\left(\prod_{n=1}^{p/2-1} \mathrm{ds}^2\left(\frac{2Kn}{p}\right)\right)\sum_A Z_j . \tag{B12}$$

$$\sum_A d_j^3(d_{j+r}+d_{j-r}) = 2\,\mathrm{ns}(a)\mathrm{ds}(a)\sum_A d_j^2 . \tag{B13}$$

$$\sum_A d_j^3[c_{j+r}s_{j+r}+c_{j-r}s_{j-r}] = -(12/m)\mathrm{cs}^2(a)\,\mathrm{ds}(a)\,\mathrm{ns}(a)\sum_A Z_j$$
$$-2\mathrm{ns}(a)\,\mathrm{ds}(a)\sum_A c_j s_j d_j . \tag{B14}$$

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Lifshitz tails for random acoustic operators

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(Received 20 June 2002; accepted 29 December 2002)

This paper is devoted to the study of Lifshitz tails for random acoustic operators of the form $A_\omega = -\nabla (1/\varrho_\omega) \nabla$. We prove that the integrated density of states of A_ω has a Lifshitz behavior at the edges of internal spectral gaps if and only if the integrated density of states of a well-chosen periodic operator is nondegenerate at the same edges. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1558902]

I. INTRODUCTION

We consider A_ω, the self-adjoint operator on $L^2(\mathbb{R}^d)$ formally defined by

$$A_\omega = A(\varrho_\omega) = -\nabla \frac{1}{\varrho_\omega} \nabla = -\sum_{i=1}^{d} \partial_{x_i} \frac{1}{\varrho_\omega} \partial_{x_i}, \tag{1}$$

where ϱ_ω is a positive and bounded function.

A_ω is called the acoustic operator, see Ref. 4 for the physicals interpretations. Let us start by defining the main object of our study, the integrated density of states. For this we consider Λ a cube of $\mathbb{R}^d$. We note by $A_{\omega,\Lambda}$ the restriction of A_ω to Λ with self-adjoint boundary conditions. As A_ω is elliptic, the resolvent of $A_{\omega,\Lambda}$ is compact and, consequently, the spectrum of $A_{\omega,\Lambda}$ is discrete and is made of isolated eigenvalues of finite multiplicity.[21] We define

$$N_\Lambda(E) = \frac{1}{\mathrm{vol}(\Lambda)} \cdot \#\{\text{eigenvalues of } A_{\omega,\Lambda} \leqslant E\}. \tag{2}$$

Here $\mathrm{vol}(\Lambda)$ is the volume of Λ in the Lebesgue sense and $\#E$ is the cardinal of E.

It is shown that the limit of $N_\Lambda(E)$ when Λ tends to $\mathbb{R}^d$ exists almost surely and is independent of the boundary conditions. It is called the integrated density of states of A_ω (IDS for the short form). See Ref. 7.

The question we are interested in here regards the behavior of N at the edges of the spectrum of A_ω.

A. The behavior of the IDS

We give a brief history of the subject. In 1964, Lifshitz[16] argued that, for a Schrödinger operator of the form $H_\omega = -\Delta + V_\omega$, there exists $c_1, c_2 > 0$ such that $N(E)$ satisfies the asymptotic:

$$N(E) \simeq c_1 \exp(-c_2 (E - E_0)^{-d/2}), \quad E \to E_0. \tag{3}$$

Here E_0 is the bottom of the spectrum of H_ω. The behavior (3) is known as Lifshitz tails (for more details see part IV.9.A of Ref. 20). Lifshitz predicted (3) also at fluctuating edges inside the spectrum. We refer to this asymptotic by ''internal Lifshitz tails.''

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The principal results known on Lifshitz tails are mainly shown for Schrödinger operators (for continuous and discrete cases). (See Refs. 6, 8, 12, 18, 19, and 22 and others.[13])

Lifshitz tails for an operator of type (1), to our knowledge, has never been studied so far. However, Kozlov in Ref. 11 gives the Weyl asymptotic of $N(E)$ in the neighborhood of 0.

B. The result

The essential goal of this work is to study internal Lifshitz tails for the operator defined by (1). Using the technique of periodic approximation, we prove that the IDS exhibits internal Lifshitz tails at the edges of the spectral gaps if and only if the IDS of some periodic operator is non degenerate at the same edges.

To present our result let us consider the following plan.

In Sec. II, we define the model to be studied and specify various assumptions. We introduce a periodic reference operator A_{ω^+}. We state the principal theorem (Theorem 2.2) which gives the Lifshitz tails.

To prove Theorem 2.2, we start by locating the integrated density of states of our random operator in the neighborhood of an energy E_+. This will be done in Secs. III and IV.

Section V is devoted to the proof of Theorem 2.2.

II. THE MODEL

Let us start this section by giving the expression of ϱ_ω. We assume that ϱ_ω is a function which satisfies the following.

(H.0)

$$\varrho_\omega = \varrho_0\left(1+\sum_{\gamma\in\Gamma}\omega_\gamma u_\gamma\right),$$

where

(i) ϱ_0 is measurable with real values and $\mathbb{Z}^d$-periodic function, i.e.,

$$\varrho_0(x)=\varrho_0(x+\gamma), \quad \forall x\in\mathbb{R}^d, \quad \gamma\in\mathbb{Z}^d.$$

(ii) There exists constants $\varrho_{0,+}>\varrho_{0,-}>0$ such that for almost all $x\in\mathbb{R}^d$, we have

$$0<\varrho_{0,-}\leqslant\varrho_0(x)\leqslant\varrho_{0,+}. \tag{4}$$

(iii) For $\gamma\in\mathbb{Z}^d$, we set $u_\gamma(\cdot)=u(\cdot-\gamma)$. We suppose that u is a function with real values such that there exists $U_+>0$: such that for almost all $x\in\mathbb{R}^d$,

$$0\leqslant U(x)\equiv\sum_{\gamma\in\mathbb{Z}^d}u_\gamma(x)\leqslant U_+<\infty. \tag{5}$$

(iv) $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ is a family of nonconstant and positive, independent identically distributed random variables whose common probability measure is noted by $\mathbb{P}_{\omega_0}$. We note the probability space by $(\Omega,\mathcal{F},\mathbb{P})$. We assume that $\mathbb{P}_{\omega_0}$ is compactly supported.

Let $\mathcal{A}(\varrho_\omega)$ be the quadratic form defined as follows: for $u\in H^1(\mathbb{R}^d)=\mathcal{D}(\mathcal{A}(\varrho_\omega))$,

$$\mathcal{A}(\varrho_\omega)[u,u]=\int_{\mathbb{R}^d}\frac{1}{\varrho_\omega(x)}\nabla u(x)\overline{\nabla u(x)}dx.$$

$\mathcal{A}(\varrho_\omega)$ is a symmetrical, closed, and positive quadratic form. A_ω given by (1) is defined to be the self-adjoint operator associated to $\mathcal{A}(\varrho_\omega)$.[21]

Assumption (H.0) ensures that A_ω is a measurable family of self-adjoint operators and ergodic.[6,20] Indeed, if τ_γ refers to the translation by γ, then $(\tau_\gamma)_{\gamma\in\mathbb{Z}^d}$ is a group of unitary operators on $L^2(\mathbb{R}^d)$ and for $\gamma\in\mathbb{Z}^d$ we have

$$\tau_\gamma A_\omega \tau_{-\gamma}=A_{\tau_\gamma\omega}.$$

According to Refs. 6 and 20 we know that there exists Σ, Σ_{pp}, Σ_{ac}, and Σ_{sc} closed and nonrandom sets of $\mathbb{R}$ such that Σ is the spectrum of A_ω with probability one and such that if σ_{pp} (respectively, σ_{ac} and σ_{sc}) design the pure point spectrum (respectively, the absolutely continuous and singular continuous spectrum) of A_ω, then $\Sigma_{pp}=\sigma_{pp}$, $\Sigma_{ac}=\sigma_{ac}$, and $\Sigma_{sc}=\sigma_{sc}$ with probability one.

A. Reference operator

It is convenient to consider A_ω as a perturbation of some periodic operator A_{ω^+}. More precisely, for $\varrho_{\omega^+}=\varrho_0(1+\omega^+\Sigma_{\gamma\in\mathbb{Z}^d}u_\gamma)$, where $\omega^+=\sup(\operatorname{supp}\mathbb{P}_{\omega_0})$ we write

$$A_\omega=A_{\omega^+}+\Delta A_\omega,$$

with

$$A_{\omega^+}=A(\varrho_{\omega^+})$$

and

$$\Delta A_\omega=A_\omega-A_{\omega^+}=-\nabla\frac{\varrho_{\omega^+}-\varrho_\omega}{\varrho_{\omega^+}\varrho_\omega}\nabla\geqslant 0.$$

1. Some Floquet theory

Now we review some standard facts from the Floquet theory for periodic operators. Basic references for this material are Refs. 15, 21, and 23.

As ϱ_{ω^+} is $\mathbb{Z}^d$-periodic, for any $\gamma\in\mathbb{Z}^d$, we have

$$\tau_\gamma A_{\omega^+}\tau_\gamma^*=\tau_\gamma A_{\omega^+}\tau_{-\gamma}=A_{\omega^+}.$$

Let $\mathbb{T}^*=\mathbb{R}^d/(2\pi\mathbb{Z}^d)$. We define $\mathcal{H}$ by

$$\mathcal{H}=\{u(x,\theta)\in L^2_{loc}(\mathbb{R}^d)\otimes L^2(\mathbb{T}^*);\forall(x,\theta,\gamma)\in\mathbb{R}^d\times\mathbb{T}^*\times\mathbb{Z}^d;\ u(x+\gamma,\theta)=e^{i\gamma\theta}u(x,\theta)\}.$$

There exists U a unitary isometry from $L^2(\mathbb{R}^d)$ to $\mathcal{H}$ such that A_{ω^+} admits the Floquet decomposition[15,23]

$$UA_{\omega^+}U^*=\int_{\mathbb{T}^*}^{\oplus}A_{\omega^+}(\theta)d\theta.$$

Here $A_{\omega^+}(\theta)$ is the operator A_{ω^+} acting on $\mathcal{H}_\theta$, defined by

$$\mathcal{H}_\theta=\{u\in L^2_{loc}(\mathbb{R}^d);\forall\gamma\in\mathbb{Z}^d,u(x+\gamma)=e^{i\gamma\theta}u(x)\}.$$

As A_{ω^+} is elliptic, we know that, $A_{\omega^+}(\theta)$ has a compact resolvent; hence its spectrum is discrete.[21] We denote its eigenvalues, called Floquet eigenvalues of A_{ω^+}, by

$$E_0(\theta)\leqslant E_1(\theta)\leqslant\cdots\leqslant E_n(\theta)\leqslant\cdots.$$

The corresponding eigenfunctions are denoted by $(w(x,\cdot)_j)_{j\in\mathbb{N}}$. The functions $(\theta\to E_n(\theta))_{n\in\mathbb{N}}$ are Lipshitz-continuous, and we have

$$E_n(\theta)\to+\infty \quad \text{as} \quad n\to+\infty \quad \text{uniformly in} \quad \theta.$$

The spectrum $\sigma(A_{\omega^+})$ of A_{ω^+} is made of bands [i.e., $\sigma(A_{\omega^+})=\cup_{n\in\mathbb{N}}E_n(\mathbb{T}^*)$]. The periodic operator A_{ω^+} has an IDS which will be denoted by n. The behavior of n at a band edge E_+, is said to be nondegenerate if

$$\lim_{\varepsilon\to 0^+}\frac{\log|n(E_+ +\varepsilon)-n(E_+)|}{\log\varepsilon}=\frac{d}{2}. \tag{6}$$

Remark 2.1: (1) It is proven in Ref. 12 that (6) is equivalent to say that the floquet eigenvalues reaching the band edge E_+ has only nondegenerate quadratic extrima at that edge, i.e., if θ^0 is such that $E_n(\theta^0)=E_+$ then θ^0 is a nondegenerate quadratic extrumum of E_n.

(2) In Ref. 10, (6) is established for the bottom of the spectrum of Schrödinger operators. For acoustic operators we expect (6) at internal edges of the spectrum for $d=1$.[21]

2. Main assumptions

We assume the following.

(H.1)

There exists E_+ and $\delta>0$ such that $\sigma(A_{\omega^+})\cap[E_+,E_+ +\delta)=[E_+,E_+ +\delta)$ and $\sigma(A_{\omega^+})\cap(E_+ -\delta,E_+]=\varnothing$.

To prove our result, we will need the following assumptions.

(H.2)

There exists $g_+(x)\in L^p(C_0)$ with $C_0=\{x\in\mathbb{R}^d;\forall 1\leqslant j\leqslant d;-\frac{1}{2}<x_j\leqslant\frac{1}{2}\}$ and ($p=2$, if $d\leqslant 3$,$p>2$, if $d=4$ and $p>d/2$ if $d\geqslant 5$) such that for some $\nu>d+2$, for all $\gamma\in\Gamma$ and a.e., $x\in C_0$ we have

$$0\leqslant u(x+\gamma)\cdot(1+|\gamma|)^{\nu}\leqslant g_+(x),$$

and for all $1\leqslant i\leqslant d$,

$$0\leqslant|(\partial_{x_i}u)(x+\gamma)|\cdot(1+|\gamma|)^{\nu}\leqslant g_+(x).$$

(H.3)

$$\limsup_{\varepsilon\to 0^+}\frac{\log|\log\mathbb{P}_{\omega^0}([\omega^+-\varepsilon,\omega^+])|}{|\log\varepsilon|}=0.$$

As, $\Delta A_\omega\geqslant 0$ and ω^+ is in the support of $\mathbb{P}_{\omega_0}$, Σ contains an interval of the form $[E_+,E_+ +a](a>0)$ (see Ref. 9).

As we are interested in the behavior of the IDS in the neighborhood of E_+, we require that E_+ remains always the edge of a gap for Σ, when the perturbation is turned on. More precisely, if for all $t\in[0,1]$, we define $A_{\omega,t}=A_{\omega^+}+t\Delta A_\omega$ and Σ_t is the almost sure spectrum of $A_{\omega,t}$, then one requires that the following assumption holds.

(H.4)

There exists $\delta'>0$ such that for all $t\in[0,1]$, $\Sigma_t\cap[E_+-\delta',E_+)=\varnothing$.

3. The main result

The main result of this work is as follows.

Theorem 2.2: *Let A_ω be the operator defined by (1), and assume that (H.1), (H.2), (H.3), and (H.4) hold, then E_+ is a continuity point for N and we have*

$$\liminf_{\varepsilon\to 0^+}\frac{\log|\log(N(E_+ +\varepsilon)-N(E_+))|}{\log\varepsilon}\geqslant -\frac{d}{2},$$

$$\lim_{\varepsilon\to 0^+}\frac{\log|\log(N(E_+ +\varepsilon)-N(E_+))|}{\log\varepsilon}=-\frac{d}{2}\Leftrightarrow \lim_{\varepsilon\to 0^+}\frac{\log(n(E_+ +\varepsilon)-n(E_+))}{\log\varepsilon}=\frac{d}{2}.$$

Remark 2.3: The result of Theorem 2.2 is stated for lower band edges. Under adequate assumptions the corresponding result can be proved for upper band edges.

Outline of the proof: To prove Theorem 2.2, we use periodic approximations. We prove a lower and an upper bounds on $N(E_+ +\varepsilon)-N(E_+)$. The upper and lower bounds are proven separately.

To prove the upper bound, we compare $N(E_+ +\varepsilon)-N(E)$ to the IDS of well chosen Anderson discrete model. More precisely, we prove that for an energy E close to E_+, $N(E)-N(E_+)$ can be upper bounded by $N_{\mathcal{E}_0}(E)$, the IDS of the bounded random operator $A_\omega^0=\Pi_0 A_\omega \Pi_0$. Here Π_0, is the spectral projection for A_{ω^+} on the band starting at E_+. So to study the behavior of $N(E)-N(E_+)$, we study the behavior of $N_{\mathcal{E}_0}(E)$. This represents several advantages: first, A_ω^0 is equivalent to a random Jacobi matrix acting on $L^2(\mathbb{T}^*)\otimes\mathbb{C}^n$. The second advantage is that while E_+ is an interior edge of a gap for A_ω, it becomes the bottom of the spectrum for A_ω^0. We prove that, when n, the IDS of the periodic operator is nondegenerate at E_+, A_ω^0 is lower bounded by the usual discrete random operator whose behavior of the IDS at the edges of the spectral gaps is already known. This lower bound on the operator immediately yields an upper bound on the density of states. The lower bound is proved by constructing a large enough number of orthogonal approximate eigenfunctions of $A_{\omega,\Lambda}$ associated with approximate eigenvalues in $[E_+-\varepsilon,E_+ +\varepsilon]$. This will enable us to lower bound the number of the eigenvalues of $A_{\omega,\Lambda}$ in the interval $[E_+-\varepsilon,E_+ +\varepsilon]$.

Now we make some remarks about our assumptions. Let us start with (H.1). Figotin and Kuchment in Ref. 5 studied the existence of open spectral gaps in the spectrum of certain periodic acoustic operators for $d=2$ and 3. In assumption (H.1) we asked that $E_+>0$ which excludes the spectral gap $(-\infty,0)$. Lifshitz tails are likely to occur at the neighborhood of the fluctuating edges. See Ref. 20. It should be noted that 0 is not a fluctuating edge of the spectrum. It belongs to the spectrum of A_ω independently of the choice of $\varrho_\omega(x)$.

If the support of $\mathbb{P}_{\omega_0}$ is connected, the assumption (H.4) can be replaced by (H.4.bis). There exists $\delta'>0$ such that $\Sigma\cap[E_+-\delta',E_+)=\varnothing$.

By adding a disorder parameter g in the equation which defines ϱ_ω, i.e.,

$$\varrho_\omega=\varrho_0\left(1+g\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma u_\gamma\right),$$

we can choose g small enough so that the spectral gap in $\sigma(A_{\omega^+})$ will not be closed after the perturbation.[4]

Remark 2.4: As it is already mentioned in remark 11 of Ref. 4, one can use the result of Theorem 2.2 to show either Anderson localization[4] *or dynamical localization*[2] *under assumptions on the distribution of the random variables weaker than those required in these references. This was done in the Schrödinger case by Veselić.*[24]

III. LOCALIZATION IN ENERGY FOR THE DENSITY OF STATES

The goal of this part is to give an estimate of $N(E)-N(E_+)$ for an energy E close to E_+. This will be accomplished by means of the IDS of certain reference operators.

A. Wannier basis

We recall concepts used in Ref. 12. Let $\mathcal{E}\subset L^2(\mathbb{R}^d)$ a closed subspace invariant by the $\mathbb{Z}^d$ translations, i.e., such that $\Pi^{\mathcal{E}}$, the orthogonal projection on $\mathcal{E}$, satisfies

$$\forall\,\gamma\in\mathbb{Z}^d,\quad \Pi^{\mathcal{E}}=\tau_\gamma^*\Pi^{\mathcal{E}}\tau_\gamma.$$

Following the computations done in Sec. 1.2 of Ref. 12, we see that there exists an orthonormal system of vectors $(\tilde{w}_{n,0})_{n\in N}$ such that for $\tilde{w}_{n,\gamma}=\tau_\gamma(\tilde{w}_{n,0})$; $(\tilde{w}_{n,\gamma})_{(n\in N;\gamma\in\mathbb{Z}^d)}$ is an orthonormal basis of $\mathcal{E}$. Such system is called *Wannier basis* of $\mathcal{E}$. The vectors $(\tilde{w}_{n,0})_{n\in N}$ are called *Wannier generators* of $\mathcal{E}$.

Let $\mathcal{E}\subset L^2(\mathbb{R}^d)$ be a space which is translation invariant. $\mathcal{E}$ is said to be of finite energy for A_ω if $\Pi^{\mathcal{E}}A_\omega\Pi^{\mathcal{E}}$ is a bounded operator. In this case, $\mathcal{E}$ admits a finite set of Wannier generators.

Let J_0 be the set of indices of the Floquet eigenvalues of A_{ω^+} which take the value E_+ in certain points $\theta\in\mathbb{T}^*$. We identify J_0 to $\{1,\ldots,n_0\}$. Let Z be the set of $\theta\in\mathbb{T}^*$ for which there exists $j\in J_0$ such that $E_j(\theta)=E_+$. When n has a nondegenerate behavior at E_+, Z is a set of isolated points.[11] For $j\in J_0$ we define $Z_j=\{\theta\in\mathbb{T}^*;E_j(\theta)=E_+\}$. The sequence $(Z_j)_{j\in J_0}$ is decreasing and $Z_1=Z$. For $\theta^0\in Z$, N_{θ^0} is the set of indices such that, $E_j(\theta^0)=E_+$. We recall that the Floquet eigenvector associated with the eigenvalue $E_j(\theta)$ is denoted by $w_j(\cdot,\theta)$.

Lemma 3.1 (Ref. 12): There exists $(v_j(\cdot,\theta))_{j\in J_0}$ functions in $\mathcal{H}_\theta$ such that:

(1) for $\theta^0\in Z$ and $j\in N_{\theta^0}$, there exists V_{θ^0} a neighborhood of V_{θ^0} (in $\mathbb{T}^*$) such that,

the map $\theta\in V_{\theta^0}\mapsto v_j(\cdot,\theta)\in\mathcal{H}_\theta$ is real analytic [i.e., $\theta\to T_{\theta\to\theta^0}v_j(\cdot,\theta)$ is analytic of V_{θ^0} in $\mathcal{H}_{\theta^0}$],

For $\theta\in V_{\theta^0}$, $span\langle((v_j(\cdot,\theta))_{j\in N_{\theta^0}})\rangle=span\langle((w_j(\cdot,\theta))_{j\in N_{\theta^0}})\rangle$.

(2) For $\theta\in\mathbb{T}^*$, we have

the system $((v_j(\cdot,\theta))_{j\in N_{\theta^0}})$ is orthonormal in $\mathcal{H}_\theta$.

$span\langle(w_j(\cdot,\theta)_{j\in J_0})\rangle=span\langle(v_j(\cdot,\theta))_{j\in J_0}\rangle$.

For $(\theta,\theta')\in(\mathbb{T}^*)^2$, we define $T_{\theta\to\theta'}:\mathcal{H}_\theta\mapsto\mathcal{H}_{\theta'}$ by $(T_{\theta\to\theta'}v)(x)=e^{ix\cdot(\theta'-\theta)}v(x)$.

B. Reduction to discrete problem

The reduction procedure consists in decomposing the operator A_ω according to various translation-invariants subspaces. The random operators thus obtained are reference operators. They will be used for the upper bound on the IDS.

Let

J_- be the set of indices smaller than $\inf J_0$;

J_+ be the set of the indices greater than $\sup J_0$.

We denote by $\Pi_0(\theta)$ [respectively, $\Pi_-(\theta)$ and $\Pi_+(\theta)$] the orthogonal projections in $\mathcal{H}_\theta$ on the vector space generated by $(w_j(\cdot,\theta))_{j\in J_0}$ [respectively, by $(w_j(\cdot,\theta))_{j\in J_-}$ and $(w_j(\cdot,\theta))_{j\in J_+}$]. These three projections are two-by-two orthogonal and their sum is the identity for all $\theta\in\mathbb{T}^*$.

One defines

$$\Pi_\alpha=U^{-1}\left(\int_{\mathbb{T}^*}\Pi_\alpha(\theta)\,d\theta\right)U:L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d),$$

where $\alpha\in\{-,0,+\}$. Π_α is an orthogonal projection on $L^2(\mathbb{R}^d)$ and for all $\gamma\in\mathbb{Z}^d$, we have $\tau_\gamma^*\Pi_\alpha\tau_\gamma=\Pi_\alpha$. Note that Π_-, Π_0, and Π_+ are mutually orthogonal and that $\Pi_-+\Pi_0+\Pi_+=Id_{L^2(\mathbb{R}^d)}$. For $\alpha\in\{-,0,+\}$, we set $\mathcal{E}_\alpha=\Pi_\alpha(L^2(\mathbb{R}^d))$. These spaces are translation invariant. Moreover $\mathcal{E}_-$ and $\mathcal{E}_0$ are of finished energies for A_{ω^-}. We prove the following.

Theorem 3.2: *Let A_ω be defined by (1). We assume that (H.1), (H.2), (H.3), and (H.4) hold. There exists $E_0>E_+$ and $C>1$ such that, for $E_+\leqslant E\leqslant E_0$ we have*

$$0 \leqslant N(E) - N(E_+) \leqslant N_{\mathcal{E}_0}(C \cdot (E - E_+) + E_+), \tag{7}$$

where $N_{\mathcal{E}_0}$ *is the IDS of* $A_\omega^0 = \Pi_0 A_\omega \Pi_0$.

Theorem 3.2 immediately gives the following corollary.

Corollary 3.3: Under the assumptions of the last theorem, E_+ *is a continuity point for* N. *More precisely, there exists* $C > 1$ *and* $E_0 > E_+$ *such that, for* $E_+ \leqslant E \leqslant E_0$ *we have*

$$0 \leqslant N(E) - N(E_+) \leqslant n(C \cdot (E - E_+) + E_+) - n(E_+).$$

Proof: As $\Delta A_\omega \geqslant 0$, this implies $\Pi_0 A_\omega \Pi_0 \geqslant \Pi_0 A_{\omega^+} \Pi_0$. Thus, if $n_{\mathcal{E}_0}$ is the integrated density of states $\Pi_0 A_{\omega^+} \Pi_0$, we have

$$N_{\mathcal{E}_0}(E) \leqslant n_{\mathcal{E}_0}(E).$$

As Π_0 commutes with A_{ω^+}, if E is close enough to E_+ such that $E \geqslant E_+$, then we have

$$n_{\mathcal{E}_0}(E) = n(E) - n(E_+).$$

The continuity of N in E_+ is an immediate consequence of the continuity of n. □

IV. THE PROOF OF THEOREM 3.2

To prove Theorem 3.2, we will approach the density of states of A_ω by the density of states of periodic approximations. In a neighborhood of E_+, we will control the behavior of the density of states of periodic approximations via the density of states of periodic approximations of the reference operators. We then compute the limit for the density of states of the reference operators and we obtain the sought for result.

A. The periodic approximations

Let $k \in \mathbb{N}^*$. We define the following periodic operator:

$$A_{\omega,k} = -\nabla \frac{1}{\varrho_{\omega,k}} \nabla,$$

where the function $\varrho_{\omega,k}$ is defined by

$$\varrho_{\omega,k} = \varrho_0 \left(1 + \sum_{\gamma \in C_k \cap \mathbb{Z}^d} \omega_\gamma \sum_{\beta \in (2k+1)\mathbb{Z}^d} u_{\gamma+\beta} \right),$$

C_k is the cube

$$C_k = \left\{ x \in \mathbb{R}^d; \forall 1 \leqslant j \leqslant d, \ -\frac{2k+1}{2} < x_j \leqslant \frac{2k+1}{2} \right\}.$$

$A_{\omega,k}$ is $(2k+1)\mathbb{Z}^d$-periodic and essentially self-adjoint operator. Let $\mathbb{T}_k^* = (\mathbb{R}^d)/[2\pi/(2k+1)]\mathbb{Z}^d$. We define $N_{\omega,k}$ the IDS of $A_{\omega,k}$ by

$$N_{\omega,k}(E) = \frac{1}{(2\pi)^d} \sum_{n \in \mathbb{N}} \int_{\{\theta \in \mathbb{T}_k^*, \ E_{\omega,k,n}(\theta) \leqslant E\}} d\theta. \tag{8}$$

Let $dN_{\omega,k}$ be the derivative of $N_{\omega,k}$ in the distribution sense. As $N_{\omega,k}$ is increasing, $dN_{\omega,k}$ is a positive measure; it is the density of states of $A_{\omega,k}$. We denote by dN the density of states of A_ω. For all $\varphi \in C_0^\infty(\mathbb{R})$, $dN_{\omega,k}$ verifies (see Refs. 12 and 21)

$$\langle \varphi, dN_{\omega,k}\rangle = \frac{1}{(2\pi)^d}\int_{\theta\in \mathbb{T}_k^*} \mathrm{tr}_{\mathcal{H}_\theta}(\varphi(A_{\omega,k,\theta}))d\theta = \frac{1}{\mathrm{vol}(C_k)}\mathrm{tr}(\chi_{C_k}\varphi(A_{\omega,k})\chi_{C_k}), \tag{9}$$

where for $\Lambda\subset\mathbb{R}^d$, χ_Λ will design the characteristic function of Λ and $\mathrm{tr}(A)$ is the trace of A (we index by $\mathcal{H}_\theta$ if the trace is taken in $\mathcal{H}_\theta$). The proof of (9) is given in Ref. 12.

Theorem 4.1: *(1) For any $\varphi\in C_0^\infty(\mathbb{R})$ and for almost all $\omega\in\Omega$ we have*

$$\lim_{k\to\infty}\langle \varphi, dN_{\omega,k}\rangle = \langle \varphi, dN\rangle.$$

(2) For any $\lambda\in\mathbb{R}$ a continuity point for N, we have $\lim_{k\to\infty}\mathbb{E}(N_{\omega,k}(\lambda)) = N(\lambda)$.

Remark 4.2: The result of Theorem 4.1 is close to that of Theorem 5.1 of Ref. 12. The proof is also similar and is based on functional analysis. The unique difference in the proof comes from the control of the behavior of the resolvent. In Ref. 12, the perturbation was a potential; in our case, it is a differential operator of the same order as the background operator. We will give a sketch of the proof.

Proof: Let $\varphi\in C_0^\infty(\mathbb{R})$. From Refs. 1 and 20, we know that

$$\langle \varphi, dN\rangle = \int_{\mathbb{R}}\varphi(\lambda)dN = \mathbb{E}\left(\frac{1}{\mathrm{vol}(C_0)}\mathrm{tr}(\chi_{C_0}\varphi(A_\omega)\chi_{C_0})\right).$$

By writing $\chi_{C_k} = \Sigma_{\gamma\in C_k\cap\mathbb{Z}^d}\tau_\gamma(\chi_{C_0})$, we have

$$\mathbb{E}(\mathrm{tr}(\chi_{C_k}\varphi(A_{\omega,k})\chi_{C_k})) = \sum_{\gamma\in C_k\cap\mathbb{Z}^d}\mathbb{E}[\mathrm{tr}(\tau_\gamma(\chi_{C_0})\varphi(A_{\omega,k}))].$$

As the family of random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ is independent and identically distributed, we compute

$$\mathbb{E}(\mathrm{tr}(\chi_{C_k}\varphi(A_{\omega,k})\chi_{C_k})) = \#(C_k\cap\mathbb{Z}^d)\mathbb{E}(\mathrm{tr}(\chi_{\Lambda_0}\varphi(A_{\omega,k}))).$$

So from (9), we obtain

$$\mathbb{E}(\langle \varphi, dN_{\omega,k}\rangle) = \frac{1}{\mathrm{vol}(C_0)}\mathbb{E}(\mathrm{tr}(\chi_{C_0}\varphi(A_{\omega,k})\chi_{C_0})).$$

The random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ and the functions ϱ_0 and u are bounded; hence, $A_{\omega,k}$ is lower bounded uniformly in ω and k. Let $\lambda_0\in\mathbb{R}^*$ such that $I\leqslant\lambda_0+A_{\omega,k}$ and $I\leqslant\lambda_0+A_\omega$, for all $\omega\in\Omega$ and $k\in\mathbb{N}^*$.

Let $\varphi\in C_0^\infty(\mathbb{R})$ and $\tilde{\varphi}$ be an almost analytic extension of $(\lambda_0+x)^{-q}\varphi(x)$, where $q>2d+1$. The Helffer–Sjöstrand formula[14] gives

$$\varphi(A_{\omega,k}) = \frac{i}{2\pi}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)(\lambda_0+A_{\omega,k})^{-q}(z-A_{\omega,k})^{-1}\,dz\wedge d\bar{z}.$$

We have the following.

Lemma 4.3 (Ref. 3): For $q>d/2$, $\chi_{C_0}(\lambda_0+A_{\omega,k})^{-q}(z-A_{\omega,k})^{-1}\chi_{C_0}$ is trace class.

So, we can write that

$$\mathrm{tr}(\chi_{C_0}\varphi(A_{\omega,k})\chi_{C_0}) = \frac{i}{2\pi}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)\mathrm{tr}(\chi_{C_0}(\lambda_0+A_{\omega,k})^{-q}(z-A_{\omega,k})^{-1}\chi_{C_0})dz\wedge d\bar{z}.$$

This implies that

$$|\mathbb{E}(\langle\varphi,dN_{\omega,k}\rangle)-\langle\varphi,dN\rangle|=|\mathbb{E}(\mathrm{tr}(\chi_{C_0}\varphi(A_{\omega,k})))-\mathbb{E}(\mathrm{tr}(\chi_{C_0}\varphi(A_\omega)))|$$

$$\leqslant\mathbb{E}\left(\frac{1}{\pi}\int_{\mathbb{C}}\left|\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)\right|\|\mathrm{tr}[\chi_{C_0}\{(\lambda_0+A_{\omega,k})^{-q}(z-A_{\omega,k})^{-1}\right.$$

$$\left.-(\lambda_0+A_\omega)^{-q}(z-A_\omega)^{-1}\}]\|dx\,dy\right). \tag{10}$$

Now we state a lemma which will be proven later.

Lemma 4.4: Let I be a relatively compact open interval in $\mathbb{R}$. There exists $K>0$, such that $\forall\varphi\in C_0^\infty(I)$,

$$(10)\leqslant\mathbb{E}\left(K\int_{\mathbb{R}^2}\left|\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)\right|\cdot\sum_{\beta,\gamma\in\mathbb{Z}^d,|\gamma|>k}\frac{e^{-|\mathrm{Im}(z)||\beta|/K}}{|\mathrm{Im}(z)|^2}\|\tau_{\beta+\gamma}u\|_{L^2(C_0)}\,dx\,dy\right).$$

From Lemma 4.4 and the fact that $\Sigma_{\gamma\in\mathbb{Z}^d}\|\tau_\gamma u\|_{L^p(C_0)}<\infty$, we obtain that there exists $K>0$ such that for any $\varphi\in C_0^\infty(\mathbb{R})$ we have

$$|\mathbb{E}(\langle\varphi,dN_{\omega,k}\rangle)-\langle\varphi,dN\rangle|\leqslant\mathbb{E}\left(K\int_{\mathbb{R}^2}\left|\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)\right|\sum_{\beta,\gamma^d\in\mathbb{Z}^d,|\gamma|>k}\frac{e^{-|\mathrm{Im}(z)||\beta|/K}}{|\mathrm{Im}(z)|^2}\|\tau_{\beta+\gamma}u\|_{L^p(C_0)}dx\,dy\right)$$

$$<+\infty.$$

As for any $M\in\mathbb{N}$; $|(\partial\tilde{\varphi}/\partial\bar{z})(z)|=O(|\mathrm{Im}(z)|^M)$, Lebesgue's dominated convergence theorem applied to (10) implies that

$$\lim_{k\to\infty}|\mathbb{E}(\langle\varphi,dN_{\omega,k}\rangle)-\langle\varphi,dN\rangle|=0.$$

So the first assertion of Theorem 4.1.

The proof of the second assertion is given in Ref. 12.

B. Localization in energy

In this section we prove a result similar to Theorem 3.2 for the counting functions of the periodic approximations of reference operators.

Let $k\in\mathbb{N}^*$. We define the operators

$$A_{\omega^+,0}=\Pi_0A_{\omega^+}\Pi_0$$

and

$$A_{\omega,k,-}=\Pi_-A_{\omega,k}\Pi_-=\Pi_-A_{\omega^+}\Pi_-+\Pi_-\Delta A_{\omega,k}\Pi_-.$$

In an analogous way, we define, $\Delta A_{\omega,k,0}$, $\Delta A_{\omega,k,+}$, $A_{\omega,k,+}$, $A_{\omega^+,+}$, and $A_{\omega,k,0}$. According to the assumption (H.1) and as $\Delta A_\omega\geqslant 0$, we know that there exists $a>0$ such that, for any $k\in\mathbb{N}$, we have

$$A_{\omega,k,+}\geqslant A_{\omega^+,+}\geqslant(E_++a)\Pi_+. \tag{11}$$

The projector Π_- is $\mathbb{Z}^d$-periodic, hence it is $(2k+1)\mathbb{Z}^d$-periodic. So, according to the Floquet theory, we decompose it jointly with $A_{\omega,k}$:

$$\Pi_-=\int_{\mathbb{T}_k^*}^{\oplus}\Pi_{k,-}(\theta)d\theta.$$

For $\theta \in \mathbb{T}^*_k$, the operator $\Pi_{k,-}(\theta)$ is an orthogonal projection in $\mathcal{H}_\theta$; the same for $\Pi_{k,+}(\theta)$ and $\Pi_{k,0}(\theta)$. Finally one defines the operator

$$A_{\omega,k,-}(\theta) = \Pi_{k,-}(\theta) A_{\omega,k}(\theta) \Pi_{k,-}(\theta),$$

and in an analogous way, we define the operators $A_{\omega,k,0}(\theta)$ and $A_{\omega,k,+}(\theta)$. From (11), we get that

$$A_{\omega,k,+}(\theta) \geqslant (E_+ + a)\Pi_{k,+}(\theta). \tag{12}$$

For an operator H with a discrete spectrum, we note his counting function by

$$\mathcal{V}(H,E) = \#\{\text{eigenvalues of } H \leqslant E\}.$$

One, then, shows the following lemma.

Lemma 4.5: We assume that (H.1), (H.2), (H.3), and (H.4) hold. There exists $E_0 > E_+$ *and* $C > 1$ *such that for* $E_+ \leqslant E \leqslant E_0$ *we have*

$$0 \leqslant \mathcal{V}(A_{\omega,k}(\theta),E) - \mathcal{V}(A_{\omega,k}(\theta),E_+) \leqslant \mathcal{V}(A_{\omega,k,0}(\theta), C\cdot(E-E_+)+E_+). \tag{13}$$

Proof: We define $\tilde{A}_{\omega,k} = A_{\omega,k} - E_+$ and $\tilde{A}_{\omega^+} = A_{\omega^+} - E_+$. As we did previously we define $\tilde{A}_{\omega,k,-}(\theta)$, $\tilde{A}_{\omega,k,+}(\theta)$, and $\tilde{A}_{\omega,k,0}(\theta)$, i.e.,

$$\tilde{A}_{\omega,k,-}(\theta) = \Pi_{k,-}(\theta)\tilde{A}_{\omega,k}(\theta)\Pi_{k,-}(\theta).$$

To prove Lemma 4.5, it is enough to prove the following.

Lemma 4.6: We assume that (H.1), (H.2), (H.3), and (H.4) hold. There exists $\tilde{E}_0 > 0$ *and* $C > 1$ *such that for* $0 \leqslant \tilde{E} \leqslant \tilde{E}_0$, *we have*

$$0 \leqslant \mathcal{V}(\tilde{A}_{\omega,k}(\theta),\tilde{E}) - \mathcal{V}(\tilde{A}_{\omega,k}(\theta),0) \leqslant \mathcal{V}(\tilde{A}_{\omega,k,0}(\theta), C\tilde{E}).$$

Proof: If (H.4) holds, then for any $t \in [0,1]$ and any $k \in \mathbb{N}^*$, we have $[-\delta,0) \cap \sigma(\tilde{A}_{\omega,k,t}) = \varnothing$ where $\tilde{A}_{\omega,k,t} = \tilde{A}_{\omega^+} + t\Delta A_{\omega,k}$.[9] Thus, for any $t \in [0,1]$ and $\tilde{E} \in [-\delta',0)$, we have

$$\mathcal{V}(\tilde{A}_{\omega,k,t}(\theta),\tilde{E}) = \mathcal{V}(\tilde{A}_{\omega,k,t}(\theta),0^-).$$

Here $\tilde{A}_{\omega,k,t}(\theta) = \Pi_k(\theta)\tilde{A}_{\omega^+}(\theta)\Pi_k(\theta) + t\Delta A_{\omega,k}(\theta)$. But the function $t \mapsto \mathcal{V}(\tilde{A}_{\omega,k,t}(\theta),\tilde{E})$ is continuous for $t \in [0,1]$ and $\tilde{E} \in [-\delta',0[$. It is integer valued and hence, constant. Thus, for $\tilde{E} \in [-\delta',0[$, we have

$$\begin{aligned}\mathcal{V}(\tilde{A}_{\omega,k}(\theta),\tilde{E}) &= \mathcal{V}(\tilde{A}_{\omega,k,t}(\theta),\tilde{E}) = \mathcal{V}(\tilde{A}_{\omega,k,t=0}(\theta),\tilde{E}) \\ &= \mathcal{V}(\tilde{A}_{\omega^+,k}(\theta),\tilde{E}) = (2k+1)^d \mathcal{V}(\tilde{A}_{\omega^+}(\theta),\tilde{E}) = (2k+1)^d \#J_-.\end{aligned}$$

Here J_- is the set of indices of the Floquet eigenvalues of $\tilde{A}_{\omega^+}(\theta)$ smaller than 0.

We decompose $\mathcal{H}$ in the following way:

$$\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}^+, \quad \mathcal{H}_- = \Pi_{k,-}(\theta)\mathcal{H} \quad \text{and} \quad \mathcal{H}^+ = \Pi_k^+(\theta)\mathcal{H} = (\Pi_{k,0}(\theta) + \Pi_{k,+}(\theta))\mathcal{H}.$$

So we write $\tilde{A}_{\omega,k}(\theta)$ in the following matrix form:

$$\begin{pmatrix} \tilde{A}_{\omega,k,-}(\theta) & \tilde{A}^{-,+}_{\omega,k}(\theta) \\ \tilde{A}^{+,-}_{\omega,k}(\theta) & \tilde{A}^{+}_{\omega,k}(\theta) \end{pmatrix},$$

where $\tilde{A}_{\omega,k,-}(\theta)=\Pi_{k,-}(\theta)\tilde{A}_{\omega,k}\Pi_{k,-}(\theta)$, $\tilde{A}^{+}_{\omega,k}(\theta)=\Pi^{+}_{k}(\theta)\tilde{A}_{\omega,k}(\theta)\Pi^{+}_{k}(\theta)$, $\tilde{A}^{+,-}_{\omega,k}(\theta)=\Pi^{+}_{k}(\theta)\tilde{A}_{\omega,k}(\theta)\Pi_{k,-}(\theta)$, and $\tilde{A}^{-,+}_{\omega,k}(\theta)$ is the adjoint of $\tilde{A}^{+,-}_{\omega,k}(\theta)$. From (14), we can see that the number of the Floquet eigenvalues of $\tilde{A}_{\omega,k}(\theta)$ less than 0 is equal to the rank of $\Pi_{k,-}(\theta)$. Then, one proves the following.

Lemma 4.7 (Ref. 12): For $\tilde{E}\geqslant 0$,

$$0\leqslant \mathcal{V}(\tilde{A}_{\omega,k}(\theta),\tilde{E})-\mathcal{V}(\tilde{A}_{\omega,k}(\theta),0)\leqslant \mathcal{V}(\tilde{A}^{+}_{\omega,k}(\theta),\tilde{E}). \tag{14}$$

Proof: The proof of this lemma is based on the min–max principle and is given in Ref. 12.□

We recall that $\mathcal{H}^{+}$ is decomposed into two orthogonal spaces, $\mathcal{H}^{+}=\mathcal{H}_0\oplus\mathcal{H}_{+}$; this gives the following matrix:

$$\tilde{A}^{+}_{\omega,k}(\theta)=\begin{pmatrix}\tilde{A}_{\omega,k,0}(\theta) & \tilde{A}_{\omega,k,0,+}(\theta)\\ \tilde{A}_{\omega,k,+,0}(\theta) & \tilde{A}_{\omega,k,+}(\theta)\end{pmatrix}.$$

Here $\tilde{A}_{\omega,k,0}(\theta)=\Pi_{k,0}(\theta)\tilde{A}_{\omega,k}(\theta)\Pi_{k,0}(\theta)$, $\tilde{A}_{\omega,k,+}(\theta)=\Pi_{k,+}(\theta)\tilde{A}_{\omega}\Pi_{k,+}(\theta)$, $\tilde{A}_{\omega,k,+,0}(\theta)=\Pi_{k,+}(\theta)\tilde{A}_{\omega,k}(\theta)\Pi_{k,0}(\theta)$, and $\tilde{A}_{\omega,k,0,+}(\theta)$ is the adjoint of $\tilde{A}_{\omega,k,+,0}(\theta)$. As $\tilde{A}_{\omega^{+},k,+}(\theta)\geqslant a\Pi_{k,+}(\theta)$ and $\Delta A_{\omega,k}(\theta)\geqslant 0$, to prove Lemma 4.6, it is enough to show the following lemma.

Lemma 4.8: There exists $C>1$ *such that*

$$\begin{pmatrix}\tilde{A}_{\omega,k,0}(\theta) & \tilde{A}_{\omega,k,0,+}(\theta)\\ \tilde{A}_{\omega,k,+,0}(\theta) & \tilde{A}_{\omega,k,+}(\theta)\end{pmatrix}\geqslant\frac{1}{C}\begin{pmatrix}\tilde{A}_{\omega,k,0}(\theta) & 0\\ 0 & \tilde{A}_{\omega,k,+}(\theta)\end{pmatrix}.$$

Proof: Let $\varphi\in\mathcal{H}^{+}\cap\mathcal{D}(\tilde{A}^{+}_{\omega})$. We set $\varphi=\varphi_{+}+\varphi_0$. As $\mathcal{H}_0$ and $\mathcal{H}_{+}$ are orthogonal and invariant by $\tilde{A}_{\omega^{+}}$, there exists $C>1$ such that

$$\langle\tilde{A}_{\omega,k,+}(\theta)\varphi_{+},\varphi_{+}\rangle\leqslant C\langle\tilde{A}_{\omega^{+},k,+}(\theta)\varphi_{+},\varphi_{+}\rangle\leqslant C\langle\tilde{A}^{+}_{\omega,k}(\theta)\varphi,\varphi\rangle. \tag{15}$$

We know that

$$\langle\tilde{A}^{+}_{\omega}(\theta)\varphi,\varphi\rangle=\langle\tilde{A}_{\omega,k,+}(\theta)\varphi_{+},\varphi_{+}\rangle+\langle\tilde{A}_{\omega,k,0}(\theta)\varphi_0,\varphi_0\rangle+2\,\mathrm{Re}(\langle\tilde{A}_{\omega,k,+,0}(\theta)\varphi_0,\varphi_{+}\rangle).$$

This leads to

$$\langle\tilde{A}_{\omega,k,+}(\theta)\varphi_{+},\varphi_{+}\rangle+\langle\tilde{A}_{\omega,k,0}(\theta)\varphi_0,\varphi_0\rangle\leqslant\langle\tilde{A}^{+}_{\omega}(\theta)\varphi,\varphi\rangle+2|\langle\tilde{A}_{\omega,k,+,0}(\theta)\varphi_0,\varphi_{+}\rangle|. \tag{16}$$

As $\tilde{A}^{+}_{\omega}$ is positive we write

$$\begin{aligned}|\langle\tilde{A}_{\omega,k,+,0}(\theta)\varphi_0,\varphi_{+}\rangle|&\leqslant|\langle(\tilde{A}^{+}_{\omega,k}(\theta))^{1/2}\varphi,(\tilde{A}^{+}_{\omega,k})^{1/2}\varphi_{+}\rangle|+|\langle\tilde{A}_{\omega,k,+}(\theta)\varphi_{+},\varphi_{+}\rangle|\\&\leqslant\|(\tilde{A}^{+}_{\omega,k}(\theta))^{1/2}\varphi\|\cdot\|(\tilde{A}^{+}_{\omega,k}(\theta))^{1/2}\varphi_{+}\|+|\langle\tilde{A}_{\omega,k,+}(\theta)\varphi_{+},\varphi_{+}\rangle|.\end{aligned}$$

Taking (15) into account, we get that there exists $C>1$ such that

$$|\langle\tilde{A}_{\omega,k,+,0}(\theta)\varphi_0,\varphi_{+}\rangle|\leqslant C\langle\tilde{A}^{+}_{\omega,k}(\theta)\varphi,\varphi\rangle. \tag{17}$$

The proof of Lemma 4.8 is ended by taking (16) and (17) into account. □

To finish the proof of Lemma 4.6 we use (14). As $\tilde{A}_{\omega,k,+}(\theta)\geqslant a\Pi_{+,k}(\theta)$ and $\Delta A_{\omega,k}(\theta)>0$, in the neighborhood of 0 the non-negative eigenvalues of $\tilde{A}^{+}_{\omega,k}(\theta)$ are lower bounded by the eigenvalues of $(1/C)(\tilde{A}_{\omega,k,0}(\theta))$; we obtain thus the estimate of Lemma 4.6. □

Now, we have all the necessary tools to prove Theorem 3.2. We note by $N(A_{\omega,k,0},E)$ the IDS of $A_{\omega,k,0}$ and by $N(A_{\omega,k},E)$ that of $A_{\omega,k}$. By definition we have

$$N(A_{\omega,k},E)=\frac{1}{(2\pi)^d}\int_{\mathbb{T}_k^*}\mathcal{V}(A_{\omega,k}(\theta),E)d\theta$$

and

$$N(A_{\omega,k,0},E)=\frac{1}{(2\pi)^d}\int_{\mathbb{T}_k^*}\mathcal{V}(A_{\omega,k,0}(\theta),E)d\theta.$$

As in Ref. 12, for any $\varphi\in C_0^\infty(\mathbb{R})$, we have

$$\lim_{k\to\infty}\mathbb{E}\left(\int_{\mathbb{R}}\varphi(\lambda)dN(A_{\omega,k,0},\lambda)\right)=\int_{\mathbb{R}}\varphi(\lambda)dN_{\mathcal{E}_0}(\lambda). \tag{18}$$

Here $dN_{\mathcal{E}_0}$ is the density of states of $A_{\omega,k,0}$. According to this, one can see that to prove Theorem 3.2, it is enough to integrate Eq. (13), use Proposition 4.1 of Ref. 12 and Theorem 4.1. For E close to E_+, a continuity point for $N(E)$ and $N_{\mathcal{E}_0}(C\cdot E)$, we obtain

$$0\leqslant N(E)-N(E_+)\leqslant N_{\mathcal{E}_0}(C\cdot(E-E_+)+E_+).$$

So the proof of Theorem 3.2. □

V. THE PROOF OF THEOREM 2.2

For $v\in\mathcal{H}^2$ one defines the following norm:

$$\sup_{\theta\in\mathbb{T}^*}\left(|\langle v(.,\theta),A_{\omega^+}(\theta)v(.,\theta)\rangle_{L^2(C_0)}|+\|v(.,\theta)\|^2_{L^2(C_0)}\right)=\|v\|_{A_{\omega^+},\infty}.$$

Let $L^2_{\text{unif}}(\mathbb{R}^d)$ be the space defined by

$$L^p_{\text{loc,unif}}(\mathbb{R}^d)=\{u \text{ measurable};\ \sup_{\gamma\in\mathbb{Z}^d}\|u\|_{L^p(\gamma+C_0)}<\infty\}$$

endowed with the norm $\sup_{\gamma\in\mathbb{Z}^d}\|u\|_{L^p(\gamma+C_0)}$.

Let $0\leqslant V\in L^p_{\text{loc,unif}}(\mathbb{R}^d)$ where p is taken as in the assumption (H.2). We define the operator $Op_{V,v}:L^2(\mathbb{T}^*)\to L^2(\mathbb{R}^d)$ by

$$\forall t\in L^2(\mathbb{T}^*),\quad Op_{V,v}(t)=\sqrt{V(x)}\int_{\mathbb{T}^*}v(x,\theta)t(\theta)d\theta.$$

The following lemma is of use.

Lemma 5.1 (Ref. 12): Let $v\in\mathcal{H}^2_\theta$. If $\|v\|_{A_{\omega^+},\infty}<+\infty$, then $Op_{V,v}$ is bounded, precisely there exists $C>0$ such that,

$$\|Op_{V,v}\|_{\mathcal{L}(L^2(\mathbb{T}^*),L^2(\mathbb{R}^d))}\leqslant C\|v\|_{A_{\omega^+},\infty}\sqrt{\|V\|_{L^p_{\text{loc,unif}}}}.$$

We set $f(x,\theta)=v_1(x,\theta)$ [$v_1(x,\theta)$ is one of the vectors constructed in Lemma 3.1]. Let us remark on the following.

Remark 5.2: For any $1\leqslant i\leqslant d$, we have $\|\partial_{x_i}f(x,\theta)\|_{A_{\omega^+},\infty}<+\infty$.

A. The upper bound

We start this section by recalling that the integrated density of states n of the background operator A_{ω^+}, is said to be nondegenerate at a band edge E_+ if

$$\lim_{\varepsilon\to 0^+}\frac{\log|n(E_+ +\varepsilon)-n(E_+)|}{\log\varepsilon}=\frac{d}{2}.$$

We prove the following theorem.

Theorem 5.3: *Let A_ω the operator defined by (1). We assume that (H.1), (H.2), (H.3), and (H.4) hold and n is nondegenerate at E_+, then*

$$\limsup_{\varepsilon\to 0^+}\frac{\log|\log(N(E_+ +\varepsilon)-N(E_+))|}{\log\varepsilon}\leqslant -\frac{d}{2}.$$

Proof: To prove the upper bound, it is enough to prove the same upper bound on $N_{\mathcal{E}_0}$ (defined in Theorem 3.2). To do this, we show that when n has a nondegenerate behavior at energy E_+, then $N_{\mathcal{E}_0}$ (and so N) may be compared to the IDS of some well chosen, discrete Andreson model (whose behavior of its IDS is already known).

As $\Delta A_\omega\geqslant 0$, if a vector minimizes $A^0_\omega=\Pi_0 A_\omega\Pi_0$, it necessarily minimizes $A^0_{\omega^+}=\Pi_0 A_{\omega^+}\Pi_0$; hence, it has to be concentrated in the quasimomentum θ near the zeros of $(E_j(\theta)-E_+)_{1\leqslant j\leqslant n_0}$. For this we have to take into account all the points where the Floquet eigenvalues reach E_+.

So we begin by isolating the contributions from the various points for which $E_1(\theta)$ take the value E_+.

We recall that the band at E_+ is generated by $(E_j(\theta))_{1\leqslant j\leqslant n_0}$. For $1\leqslant j\leqslant n_0$, $Z_j=\{\theta\in\mathbb{T}^*;E_j(\theta)=E_+\}$. The sequence $(Z_j)_{1\leqslant j\leqslant n_0}$ is decreasing $(Z_{j+1}\subset Z_j)$. Let $\theta^0\in Z$. We set $j(\theta^0)=\sup N_{\theta^0}$ with $N_{\theta^0}=\{j,1\leqslant j\leqslant n_0;E_j(\theta^0)=E_+\}$. Let $m=\#Z$. We replace the Floquet eigenvectors $(w_j(\cdot,\theta))_{1\leqslant j\leqslant j(\theta^0)}$ associated to $(E_j(\theta))_{1\leqslant j\leqslant j(\theta^0)}$ by the vectors $(v_j(\cdot,\theta))_{1\leqslant j\leqslant j(\theta^0)}$ constructed in Lemma 3.1. They are analytic in a neighborhood V_{θ^0} of θ^0. Let θ be close to θ^0. The operator $A^0_{\omega^+}=\Pi_0 A_{\omega^+}\Pi_0$ is unitarily equivalent to the multiplication by a matrix-valued function on $\mathbb{T}^*$. This matrix-valued function takes the following block diagonal form:

$$A^0_{\omega^+}(\theta)=\begin{pmatrix} B_{j(\theta^0)}(\theta) & 0 & 0 & \dots & 0\\ 0 & E_{j(\theta^0)+1}(\theta) & 0 & \dots & 0\\ 0 & 0 & \ddots & \ddots & \vdots\\ 0 & 0 & \dots & 0 & E_{n_0}(\theta)\end{pmatrix},$$

where the matrix $B_{j(\theta^0)}(\theta)$ is $j(\theta^0)\times j(\theta^0)$ blocks given by

$$\begin{pmatrix} \langle v_1(\cdot,\theta),A_{\omega^+}(\theta)v_1(\cdot,\theta)\rangle_{L^2(C_0)} & \dots & \langle v_1(\cdot,\theta),A_{\omega^+}(\theta)v_{j(\theta^0)}(\cdot,\theta)\rangle_{L^2(C_0)}\\ \vdots & \ddots & \vdots\\ \langle v_{j(\theta^0)}(\cdot,\theta),A_{\omega^+}(\theta)v_1(\cdot,\theta)\rangle_{L^2(C_0)} & \dots & \langle v_{j(\theta^0)}(\cdot,\theta),A_{\omega^+}(\theta)v_{j(\theta^0)}(\cdot,\theta)\rangle_{L^2(C_0)}\end{pmatrix}.$$

The matrix $B_{j(\theta^0)}(\theta)$ have eigenvalues $(E_j(\theta))_{1\leqslant j\leqslant j(\theta^0)}$.

For $\theta^0\in Z$, we define

$$\overline{\omega}_{\theta^0}(\theta)=\sum_{j=1}^{d}(1-\cos(\theta_j-\theta_j^0)).$$

We recall (see remark 2.1) that the nondegeneracy of n implies that the eigenvalues $(E_j(\theta))_{1\leqslant j\leqslant j(\theta^0)}$ are nondegenerate at E_+. So there exists $\widetilde{V}_{\theta^0}$ (an open neighborhood of θ^0) and $C>1$ such that, for $\theta\in\widetilde{V}_{\theta^0}$ we have the following:

for $1\leqslant j\leqslant j(\theta^0)$, $C(E_j(\theta)-E_+)\geqslant\overline{\omega}_{\theta^0}(\theta)$,

for $j \geqslant j(\theta^0)$, $C(E_j(\theta)-E_+) \geqslant 2$.

Remark 5.4: The neighborhood $\tilde{V}_{\theta^0}$ can be chosen such that $V_{\theta^0} \subset \tilde{V}_{\theta^0}$, where V_{θ^0} was defined in Lemma 3.1.

Let $A^b_{\omega^+,\theta^0}(\theta)$ the $n_0 \times n_0$ diagonal matrix with identical diagonal entries equal to $\overline{\omega}_{\theta^0}$. For $\theta \in \tilde{V}_{\theta^0}$, we have

$$A^b_{\omega^+,\theta^0}(\theta) \leqslant C(\cdot A^0_{\omega^+}(\theta) - E_+ I_d). \tag{19}$$

Here I_d is the identity matrix.

Finally, we note that $(\tilde{V}_{\theta^0})_{\theta^0 \in Z}$ can be chosen so that they cover $\mathbb{T}^*$ (i.e., $\cup_{\theta^0 \in Z} \tilde{V}_{\theta^0} = \mathbb{T}^*$,) and such that each one of them contains only one point of Z (i.e., for $\theta \in Z, \theta' \in Z$ such that $\theta \neq \theta'$, we have $\theta' \notin \overline{\tilde{V}}_\theta$). We order the points in $Z = \{\theta^k; 1 \leqslant k \leqslant m\}$. Let $(\chi_k)_{1 \leqslant k \leqslant m}$ be $C_0^\infty(\mathbb{T}^*)$ functions which form a partition of the unity on $\mathbb{T}^*$ such that

for $1 \leqslant k \leqslant m$, $\mathrm{supp}(\chi_k) \subset \tilde{V}_{\theta^k}$,
for $1 \leqslant k \leqslant m$, $0 \leqslant \chi_k \leqslant 1$,
for $1 \leqslant k \leqslant m$, $\chi_k \equiv 1$ in a neighborhood of θ^k.
So there exists $C > 1$ such that for any $\theta \in \mathbb{T}^*$, we have

$$\frac{1}{m} \leqslant \sum_{k=1}^m \chi_k^2 \leqslant 1 \quad \text{and} \quad \sum_{k=1}^m A^b_{\omega^+,\theta^k}(\theta)\chi_k^2 \leqslant C A^0_{\omega^+}(\theta). \tag{20}$$

For $t \in L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m$, we note $t = (t_{j,k})_{1 \leqslant j \leqslant n_0; 1 \leqslant k \leqslant m}$. We consider t as a system of m columns denoted by $(t_{\cdot,k})_{1 \leqslant k \leqslant m}$. Each component belongs to $\mathbb{C}^{n_0}$. We endow $L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m$ with the scalar product generating the following Euclidean norm:

$$\|t\|^2_{L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}\otimes\mathbb{C}^m} = \sum_{k=1}^m \|t_{\cdot,k}\|^2_{L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}} = \sum_{1 \leqslant j \leqslant n_0, 1 \leqslant k \leqslant m} \|t_{j,k}\|^2_{L^2(\mathbb{T}^*)}.$$

We define the mapping $S: L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \to L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m$ by

$$S(t) = (\chi_k t)_{1 \leqslant k \leqslant m} = (\chi_k t_j)_{1 \leqslant j \leqslant n_0; 1 \leqslant k \leqslant m}, \quad \text{if} \quad t = (t_j)_{1 \leqslant j \leqslant n_0} \in L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0}.$$

The adjoint of S, $S^*: L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m \to L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0}$ is defined by

$$S^*(t) = \left(\sum_{1 \leqslant k \leqslant m} \chi_k t_{j,k} \right)_{1 \leqslant j \leqslant n_0} \quad \text{for} \quad t = (t_{j,k})_{1 \leqslant j \leqslant n_0; 1 \leqslant k \leqslant m} \in L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m.$$

According to Eq. (20) we have $(1/m) I_d \leqslant S^* \circ S \leqslant I_d$ [here I_d is the identity in $L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0}$], thus S is one to one. One shows the following lemma.

Lemma 5.5: There exists $C > 1$ such that, for $t \in L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0}$, we have

$$\langle A^a_\omega St, St \rangle_{L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}\otimes\mathbb{C}^m} \leqslant C \langle (A^0_\omega - E_+ I_d)t, t \rangle_{L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}},$$

where the operator A^a_ω acting on $L^2(\mathbb{T}^*) \otimes \mathbb{C}^{n_0} \otimes \mathbb{C}^m$ is defined by

$$A^a_\omega t = A^a_{\omega^+} t + \Delta A^a_{\omega^+,\omega} t = (A^a_{j,k} t_{j,k} + \Delta A^a_\omega t_{j,k})_{1 \leqslant j \leqslant n_0; 1 \leqslant k \leqslant m}.$$

Here

$A^a_{j,k}$ is the multiplication by ϖ_{θ^k} acting as a multiplication on $L^2(\mathbb{T}^*)$,
$\Delta A^a_\omega = \Sigma_{\gamma \in \mathbb{Z}^d} \omega^+_\gamma \Pi_\gamma$,
Π_γ is the orthogonal projection on the vector $\theta \mapsto e^{i\gamma\theta}$ in $L^2(\mathbb{T}^*)$.

Before proving this lemma let us use it to end the proof of Theorem 5.3. By Proposition 4.1 of Ref. 12, we know that A^a_ω and A^0_ω both have an IDS which we will denote, respectively, by $N^a(E)$ and $N_{\mathcal{E}_0}(E)$. Moreover, for E, a continuity point for $N_{\mathcal{E}_0}$, we have

$$N_{\mathcal{E}_0}(E)=\lim_{q\to+\infty}\frac{1}{\Lambda_q}\{\text{eigenvalues of } A^0_{\omega,q}\leqslant E\},$$

where

$$A^0_{\omega,q}=\Pi^0_q A^0_\omega \Pi^0_q,$$

and for $t=(t_j)_{1\leqslant j\leqslant n_0}\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}$,

$$\Pi^0_q t=\left(\sum_{\gamma\in\Lambda_q} e^{i\gamma\theta}\int_{\mathbb{T}^*} e^{-i\gamma\theta}t_{j(\theta)}d\theta\right)_{1\leqslant j\leqslant n_0}$$

with $\Lambda_q=\{\gamma\in\mathbb{Z}^d;|\gamma|\leqslant q\}$.

$N^a(E)$ is given by

$$N^a(E)=\lim_{q\to+\infty}\frac{1}{\Lambda_q}\{\text{eigenvalues of } A^a_{\omega^+,q}\leqslant E\},$$

where

$$A^a_{\omega,q}=\Pi^a_q A^a_\omega \Pi^a_q$$

and for $t=(t_j)_{1\leqslant j\leqslant n_0}\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}$,

$$\Pi^a_q t=\left(\sum_{\gamma\in\Lambda_q} e^{i\gamma\theta}\int_{\mathbb{T}^*} e^{-i\gamma\theta}t_{j,k}(\theta)d\theta\right)_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m}.$$

Let us compare $N_{\mathcal{E}_0}$ and N^a.

Lemma 5.6 (Ref. 12): For any $\delta>0$ and any $l\in\mathbb{N}$, there exists $C_l(\delta)>0$ such that, for $q\geqslant 1$,

$$\|\Pi^a_{(1+\delta)q}\circ S\circ\Pi^0_q - S\circ\Pi^0_q\|_{\mathcal{L}(L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0},L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}\otimes\mathbb{C}^m)}\leqslant C_l(\delta)q^{-l}.$$

Let $\varepsilon>0$ and $t\in\Pi^0_q(L^2(\mathbb{T}^*)\otimes\mathbb{C}^n)$; such that $\langle(A^0_\omega-E_+Id)t,t\rangle\leqslant\varepsilon\|t\|^2$. Lemma 5.5 says that there exists $C>1$ such that

$$\langle A^a_\omega St,St\rangle\leqslant C\cdot\varepsilon\|t\|^2. \tag{21}$$

So by Lemma 5.6, we know that

$$\begin{aligned}\langle A^a_\omega(\Pi^a_{(1+\delta)q}S)t,(\Pi^a_{(1+\delta)q}S)t\rangle&\leqslant C\cdot\varepsilon\|t\|^2+2|\langle A^a_\omega(1-\Pi^a_{(1+\delta)q})St,(\Pi^a_{(1+\delta)q})St\rangle|\\&\quad+|\langle A^a_\omega(1-\Pi^a_{(1+\delta)q})St,(1-\Pi^a_{(1+\delta)q})St\rangle|\leqslant(C\cdot\varepsilon+C_\delta q^{-1})\|t\|^2.\end{aligned} \tag{22}$$

As $(1/m)\,I_d\leqslant S^*\circ S\leqslant I_d$, we have

$$\|t\|^2\leqslant\frac{m}{1-C_\delta q^{-1}}\|(\Pi^a_{(1+\delta)q}S)t\|^2. \tag{23}$$

Thus $\Pi^a_{(1+\delta)q}S$ is one to one from $\Pi^0_q(L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0})$ to $\Pi^0_q(L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}\otimes\mathbb{C}^m)$ and for q large enough (dependent on δ and ε), we have

$$\langle A^a_\omega(\Pi^a_{(1+\delta)q}S)t,(\Pi^a_{(1+\delta)q}S)t\rangle\leqslant C\cdot m(1+\delta)\varepsilon\|(\Pi^a_{(1+\delta)q}S)t\|^2. \tag{24}$$

Moreover, we have

$$\#\{\text{eigenvalues of } A^0_{\omega,q}\leqslant(E_+ +\varepsilon)\}=\sup\{\dim(\mathfrak{N}),\mathfrak{N} \text{ is a linearsubspace of } \Pi^0_q(L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}) \text{ such that for all } t\in\mathfrak{N},\ \langle A^0_\omega t,t\rangle\leqslant(E_+ +\varepsilon)\cdot\|t\|^2\}.$$

There is a similar characterization for the counting function of A^a_ω. Using (21) and (24) for q large enough, we obtain

$$\#\{\text{eigenvalues of } A^0_{\omega,q}\leqslant E_+ +\varepsilon\}\leqslant\#\{\text{eigenvalues of } A^a_{\omega,(1+\delta)q}\leqslant C\cdot(1+\delta)\cdot m\cdot\varepsilon\}.$$

We divide by the volume of Λ_q then we take $q\to+\infty$. We get that, for ε small such that $E_+ +\varepsilon$ is a continuity point of $N_{\mathcal{E}_0}(E)$, we have

$$N_{\mathcal{E}_0}(E_+ +\varepsilon)\leqslant(1+\delta)^d N^a(C(1+\delta)m\cdot\varepsilon). \tag{25}$$

Using the right continuity of $N_{\mathcal{E}_0}(E)$ and its most denumerable number of discontinuity points, we extend the estimate (25), to some interval of the form $[E_+,E_+ +E]$. When δ goes to 0, we get

$$N_{\mathcal{E}_0}(E_+ +\varepsilon)\leqslant N^a(C\cdot m\cdot\varepsilon).$$

To complete the proof of Theorem 5.3, we use Theorem 3.2 and the fact that N^a admits Lifshits tails at 0. See Ref. 12.

$$\limsup_{\varepsilon\to0^+}\frac{\log|\log(N(E_+ +\varepsilon)-N(E_+))|}{\log\varepsilon}\leqslant-\frac{d}{2}.$$

This ends the proof of the Theorem 5.3. □

The proof of Lemma 5.5: The proof of this lemma is similar to the one given in Ref. 12. For this we will not give all details. We recall the following notation:

$$\Delta A_\omega=-\nabla\frac{\varrho_{\omega^+}-\varrho_\omega}{\varrho_{\omega^+}\varrho_\omega}\nabla=-\nabla V_\omega\nabla,$$

where $V_\omega=\Sigma_{\gamma\in\mathbb{Z}^d}(\omega^+-\omega_\gamma)(u_\gamma/D_\omega)$ and $D_\omega=\varrho_{\omega^+}(1+\Sigma_{\gamma\in\mathbb{Z}^d}\omega_\gamma u_\gamma)$. Let $t=(t_j)_{1\leqslant j\leqslant n_0}\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}$; we compute

$$\langle\Delta A^0_\omega t,t\rangle=\sum_{i=1}^d\left\|\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m}Op_{V_\omega,\partial_{x_i}v_j(\cdot,\theta)}(\chi_k t_j)\right\|^2_{L^2(\mathbb{R}^d)}$$

changing $v_j(x,\theta^k)$ in Ref. 12 by $\partial_{x_i}v_j(x,\theta^k)$, following the same steps and taking (19) into account we get that there exists $C>1$ such that

$$\langle A^b_\omega St,St\rangle\leqslant C\langle(A^0_\omega-E_+I_d)t,t\rangle, \tag{26}$$

where

$A^b_\omega=A^a_{\omega^+}+\Delta A^b_\omega$,

$A^a_{\omega^+}$ is defined in Lemma 5.5,

ΔA^b_ω is the operator defined by, for $t\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}\otimes\mathbb{C}^m$,

$$\langle \Delta A_\omega^b t,t\rangle = \sum_{\gamma\in\mathbb{Z}^d} \omega_\gamma^+ \langle V_\gamma^b t,t\rangle,$$

where V_γ^b is an operator matrix whose coefficients are operators with the following kernels:

$$\int_{\mathbb{R}^d} \frac{u_\gamma(x)}{D_\omega(x)} \nabla v_j(x,\theta^k)\overline{\nabla v_{j'}(x,\theta^{k'})} e^{i((\theta-\theta^k)-(\theta'-\theta^{k'}))x}\,dx.$$

We set

$$e^{i(\theta-\theta^k)x} = \left(\frac{e^{i(\theta-\theta^k)x}-1}{\sqrt{\omega_k}}\right)\cdot\sqrt{\omega_k}+1$$

and

$$g_k(x,\theta) = \frac{e^{i(\theta-\theta^k)x}-1}{\sqrt{\overline{\omega_k}(\theta)}}.$$

As θ^k is the single zero of $\overline{\omega_k}(\theta)$ and it is nondegenerate, there exists $C>0$, such that for $x\in\mathbb{R}^d$, $\theta\in\mathbb{T}^*$ and $1\leqslant k\leqslant m$, we have

$$|g_k(x,\theta)|\leqslant C(1+|x|). \tag{27}$$

We set

$$A_\gamma = \int_{\mathbb{R}^d} u(x)\left|\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m} \nabla v_j(x,\theta^k)\int_{\mathbb{T}^*} e^{-i\theta\gamma} t_{j,k}(\theta)\,d\theta\right|^2_{\mathbb{C}^d} dx$$

and

$$B_\gamma = \int_{\mathbb{R}^d} u(x)\left|\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m} \nabla v_j(x,\theta^k)\int_{\mathbb{T}^*} g_k(x,\theta)e^{-i\theta\gamma}\sqrt{\overline{\omega_k}(\theta)}\,t_{j,k}(\theta)\,d\theta\right|^2_{\mathbb{C}^d} dx.$$

Developing $\langle V_\gamma^b t,t\rangle$ and using the Cauchy–Schwartz inequality, we get

$$\langle V_\gamma^b t,t\rangle \geqslant (\sqrt{A_\gamma}-\sqrt{B_\gamma})^2 \geqslant (1-\alpha)A_\gamma + \left(1-\frac{1}{\alpha}\right)B_\gamma,$$

for any $0<\alpha<1$.

For α, small, we obtain that there exists $C>0$ such that

$$A_\gamma \leqslant 2(B_\gamma + C\langle V_\gamma^b t,t\rangle). \tag{28}$$

Developing the sum in A_γ, we get

$$A_\gamma = \sum_{1\leqslant j,j'\leqslant n_0;1\leqslant k,k'\leqslant m} v_{jk,j'k'}\hat{t}_{j,k}(\gamma)\overline{\hat{t}_{j',k'}(\gamma)},$$

where

$$\hat{t}_{j,k}(\gamma) = \int_{\mathbb{T}^*} e^{-i\theta\gamma} t_{j,k}(\theta)\,d\theta,$$

$$v_{jk,j'k'}=\int_{\mathbb{R}^d}u_\gamma(x)\nabla v_j(x,\theta^k)\overline{\nabla v_{j'}(x,\theta^{k'})}dx=\sum_{i=1}^{d}\int_{\mathbb{R}^d}u_\gamma(x)\partial_{x_i}v_j(x,\theta^k)\overline{\partial_{x_i}v_{j'}(x,\theta^{k'})}dx.$$

By Ref. 17 it is proved that the matrix $V=(v_{jkj'k'})_{1\leqslant j,j'\leqslant n_0;1\leqslant k,k'\leqslant m}$ is defined positive. So we get that there exists $C>0$ such that we have

$$\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m}\left|\int_{\mathbb{T}^*}e^{-i\theta\gamma}t_{j,k}(\theta)d\theta\right|^2\leqslant CA_\gamma. \tag{29}$$

We multiply by $\omega_\gamma^+=\omega^+-\omega_\gamma$ the two members of (29) then we sum on $\gamma\in\mathbb{Z}^d$,

$$\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma^+\sum_{1\leqslant j\leqslant n;1\leqslant k\leqslant m}\left|\int_{\mathbb{T}^*}e^{-i\theta\gamma}t_{j,k}(\theta)d\theta\right|^2\leqslant C\left(\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma^+A_\gamma\right).$$

By taking (28) into account and using assumption (H.2), we get that

$$\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma^+\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m}\left|\int_{\mathbb{T}^*}e^{-i\theta\gamma}t_{j,k}(\theta)d\theta\right|^2$$
$$\leqslant C\left(\sum_{1\leqslant j\leqslant n_0;1\leqslant k\leqslant m}\int_{\mathbb{T}^*}\overline{\omega_k}(\theta)|t_{j,k}(\theta)|^2d\theta+\langle\Delta A_\omega^b t,t\rangle\right).$$

Using the last inequality and the definition of A_ω^a and ΔA_ω^a one gets that there exists $C>0$ such that, $\forall t\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}$, we have

$$\langle\Delta A_\omega^a St,St\rangle\leqslant C(\langle A_{\omega^+}^a St,St\rangle+\langle\Delta A_\omega^b St,St\rangle). \tag{30}$$

As $\Delta A_\omega^b\geqslant 0$, we know that

$$\langle A_{\omega^+}^a St,St\rangle\leqslant(\langle A_{\omega^+}^a St,St\rangle+\langle\Delta A_\omega^b St,St\rangle). \tag{31}$$

From (26), (30), and (31), we deduce that $\forall t\in L^2(\mathbb{T}^*)\otimes\mathbb{C}^{n_0}$,

$$\langle A_\omega^a St,St\rangle\leqslant C\cdot\langle A_\omega^b St,St\rangle\leqslant C\cdot\langle(A_\omega^0-E_+I_d)t,t\rangle.$$

This ends the proof of Lemma 5.5. □

B. The lower bound

We set

$\kappa=1/2$ (respectively, 1/3) if n is degenerate (respectively, non degenerate) at E_+.

$s=2/(\nu-d)$ (respectively, 1) if n is degenerate (respectively, nondegenerate) at E_+.

Theorem 5.7: *Let A_ω, the operator defined by* (1). *We assume that (H.1), (H.2), (H.3), and (H.4) hold. Then, we have*

$$\liminf_{\varepsilon\to 0^+}\frac{\log|\log(N(E_++\varepsilon)-N(E_+))|}{\log\varepsilon}\geqslant -s\frac{d}{2}. \tag{32}$$

The proof of Theorem 5.7: By assumption, there is a spectral gap below E_+ of length at least $\delta'>0$. Thus, for $\varepsilon<\delta'$ we have

$$N(E_++\varepsilon)-N(E_+)=N(E_++\varepsilon)-N(E_+-\varepsilon).$$

To prove Theorem 5.7, we will lower bound $N(E_+ + \varepsilon) - N(E_+ - \varepsilon)$. Then, for N large, we will show that A_{ω,Λ_N} (A_{ω,Λ_N} is A_ω restricted to Λ_N with Dirichlet boundary conditions) has a large number of eigenvalues in $(E_+ - \varepsilon, E_+ + \varepsilon)$ with large probability. For this we will construct a family of approximate eigenvectors associated to approximate eigenvalues of A_{ω,Λ_N} in $[E_+ - \varepsilon, E_+ + \varepsilon]$. These functions will be constructed from an eigenvector of A_{ω^+} associated with E_+. Locating this eigenvector in θ and imposing to $\omega^+_\gamma = \omega^+ - \omega_\gamma$ to be small for γ in some well chosen box, one obtains an approximate eigenfunction of A_{ω,Λ_N}. Locating the eigenfunction in x in several disjointed places, we get several eigenfunctions two-by-two orthogonal. In order to simplify the notations, we assume in what follows that $\theta^0 = 0$ is a point where $E_1(\theta)$ reaches E_+ in nondegenerate (respectively, degenerate) way if n is nondegenerate (respectively, degenerate). For the same arguments as in Ref. 12, there exists $C > 0$ such that, we have the following.

If n is nondegenerate at E_+, we set $f(\cdot,\theta) = v_1(\cdot,\theta)$ (v_1 is the vector constructed in Lemma 3.1) one has

$$\|(A_{\omega^+}(\theta) - E_+) f(\cdot,\theta)\|_{L^2(C_0)} \leqslant C|\theta|^2. \tag{33}$$

If n is degenerate at E_+, in an analogous way as in the Lemma 3.1, one can construct functions $(v_j)_{1\leqslant j\leqslant q}$ which are analytical in θ in a neighborhood of θ^0 and which generate the same vector space as $(w_j)_{1\leqslant j\leqslant q}$. From Ref. 12 we know that there exits $(f_j(\theta))_{1\leqslant j\leqslant q}$ such that for $\theta = (\theta_1, \theta')$ the function $\vec{f}(\cdot,\theta) = \Sigma_{1\leqslant j\leqslant q} f_j(\theta) v_j(\cdot,\theta)$ verifies

$$|\theta_1| \leqslant \|\vec{f}(\cdot,\theta)\|_{L^2(C_0)} = \|f(\theta)\|_{\mathbb{C}^q}$$

and

$$\|(A_{\omega^+}(\theta) - E_+)\vec{f}(\cdot,\theta)\|_{L^2(C_0)} \leqslant C(|\theta_1|\cdot|\theta'|^2 + |\theta'|^3 + |\theta|^4). \tag{34}$$

We set

$$f(\cdot,\theta) = \frac{\vec{f}(\cdot,\theta)}{|\theta_1|}. \tag{35}$$

Let $0 < \xi < 1$ be a small constant. Let $\chi \in C_0^\infty(\mathbb{R})$ such that it is positif, supported in $[\xi/2, \xi]$ and $\int_{[\xi/2,\xi]} \chi(t)^2\, dt = 2$.
For $\varepsilon > 0$, we define

$$\mathcal{W}_\varepsilon(\theta) = \varepsilon^{-(d-1+2\kappa)/4} \chi(\varepsilon^{-\kappa}\theta_1) \prod_{j=2}^{d} \chi(\varepsilon^{-1/2}\theta_j) \in L^2(\mathbb{T}^*)$$

and

$$\mathcal{W}^f_\varepsilon(\cdot,\theta) = \mathcal{W}_\varepsilon(\theta)\cdot f(\cdot,\theta).$$

Now let us estimate $\|(A_{\omega^+} - E_+)\mathcal{W}^f_\varepsilon\|^2$; we have

$$\|(A_{\omega^+} - E_+)\mathcal{W}^f_\varepsilon\|^2 = \frac{1}{\mathrm{vol}(\mathbb{T}^*)} \int_{\mathbb{T}^*} \|(A_{\omega^+}(\theta) - E_+) f(\cdot,\theta)\|^2_{L^2(C_0)} |\mathcal{W}_\varepsilon(\theta)|^2\, d\theta.$$

If n is nondegenerate at E_+, from Eq. (33), we get

$$\|(A_{\omega^+}-E_+)\mathcal{W}_\varepsilon^f\|_{\mathcal{H}}^2 \leqslant C^2 \int_{\mathbb{T}^*} |\theta|^4 |\mathcal{W}_\varepsilon(\theta)|^2 \, d\theta$$
$$\leqslant C^2\varepsilon^2 \int_{[\xi/2,\xi]^d} |\theta|^4 \prod_{j=1}^{d} \chi^2(\theta_j) d\theta$$
$$\leqslant \frac{\varepsilon^2}{8} \quad \text{if } \xi \text{ is small enough.} \tag{36}$$

If n is degenerate at E_+, we use Eq. (34) to get that

$$\|(A_{\omega^+}-E_+)\mathcal{W}_\varepsilon^f\|_{\mathcal{H}}^2 \leqslant C^2 \int_{\mathbb{T}^*} (|\theta'|^2+|\theta'|^3/|\theta_1|+|\theta|^4/|\theta_1|)^2 |\mathcal{W}_\varepsilon(\theta)|^2 \, d\theta$$
$$\leqslant C^2\varepsilon^2 \int_{[\xi/2,\xi]^d} (|\theta'|^2+\varepsilon^{1/6}|\theta'|^3/|\theta_1|+|\theta|^4/|\theta_1|)^2 \prod_{j=1}^{d} \chi^2(\theta_j) d\theta$$
$$\leqslant \frac{\varepsilon^2}{8} \quad \text{if } \xi \text{ is small enough.} \tag{37}$$

For $\beta \in \mathbb{Z}^d$, we define

$$\mathcal{W}_{\varepsilon,\beta}^f(\cdot,\theta) = e^{-i\beta\cdot\theta}\mathcal{W}_\varepsilon^f(\cdot,\theta) \quad \text{and} \quad \mathcal{W}_{\alpha,\varepsilon,\beta,\zeta}^f(\cdot,\theta) = e^{-i\beta\cdot\theta}(\Pi_{\Lambda_\alpha(\zeta)}\mathcal{W}_\varepsilon^f)(\cdot,\theta),$$

where $\Lambda_\alpha(\zeta)$ is the cube defined by

$$\Lambda_\alpha(\zeta) = \{\gamma \in \mathbb{Z}^d; \text{ for } 1 \leqslant j \leqslant d; |\gamma_j| \leqslant \zeta^{-(1/2+\alpha)}\}$$

and $\Pi_{\Lambda_\alpha(\zeta)}$ is the orthogonal projection on $\Lambda_\alpha(\zeta)$.

We set

$$\mathcal{U}_{\varepsilon,\beta}^f(x) = \int_{\mathbb{T}^*} \mathcal{W}_{\varepsilon,\beta}^f(x,\theta) d\theta \quad \text{and} \quad \mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f(x) = \int_{\mathbb{T}^*} \mathcal{W}_{\alpha,\varepsilon,\beta,\zeta}^f(x,\theta) d\theta.$$

For N large and β well chosen $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$, $\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f$ will be an approximate eigenfunction of A_{ω,Λ_N} associated to an approximate eigenvalue in the interval $[E_+-\varepsilon, E_++\varepsilon]$.

We show initially that $\|\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f\|_{L^2(\mathbb{R}^d)} > C > 0$. Note that

$$(\mathrm{vol}(\mathbb{T}^*))\|\mathcal{U}_{\varepsilon,\beta}^f\|_{L^2(\mathbb{R}^d)}^2 = \|\mathcal{W}_{\varepsilon,\beta}^f\|_{\mathcal{H}}^2 = \int_{\mathbb{T}^*} \|f(\cdot,\theta)\|_{L^2(C_0)}^2 |\mathcal{W}_\varepsilon(\theta)|^2 \, d\theta \geqslant 2^d.$$

As in Ref. 12 we remark that $\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f$ and $\mathcal{U}_{\varepsilon,\beta}^f$ are close to each other. More precisely, for any $n \in \mathbb{N}$ and $\beta \in \mathbb{Z}^d$, there exists $C_n > 0$ such that

$$(\mathrm{vol}(\mathbb{T}^*)) \cdot \|\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f - \mathcal{U}_{\varepsilon,\beta}^f\|_{L^2(\mathbb{R})} = \|\mathcal{W}_{\alpha,\varepsilon,\beta,\zeta}^f - \mathcal{W}_{\varepsilon,\beta}^f\|_{\mathcal{H}} \leqslant C_n \varepsilon^{-n\kappa} \zeta^{n(1/2+\alpha)}. \tag{38}$$

So, if $\zeta = \varepsilon^s$ (s was defined in the beginning of this section), for ε small enough, we get

$$\|\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f\|_{L^2(\mathbb{R}^d)} \geqslant 1.$$

Now we have to look to the conditions under which we have

$$\|(A_\omega - E_+)\mathcal{U}_{\alpha,\varepsilon,\beta,\zeta}^f\|^2 \leqslant \varepsilon^2.$$

Note that

$$\|(A_{\omega,\Lambda_N}-E_+)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2\leqslant\|(A_\omega-E_+)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2\leqslant 2\|(A_{\omega^+}-E_+)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2+2\|\Delta A_\omega\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2. \tag{39}$$

Equations (36) and (37) give the bound on the first member of (39), it just remains to us to control the second term of (39). We have

$$\|(\Delta A_\omega)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2\leqslant 2\|(\nabla V_\omega)\cdot(\nabla\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta})\|^2+2\|V_\omega\Delta\mathcal{U}^f_{\alpha,\varepsilon,\beta,\zeta}\|^2. \tag{40}$$

We recall that $\omega^+_\gamma=\omega^+-\omega_\gamma$. To estimate (40), one needs the following lemmas.

Lemma 5.8: There exists $K>0$, such that

$$\|(\nabla V_\omega)\cdot(\nabla\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s})\|^2\leqslant\varepsilon^4+K(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma)^2. \tag{41}$$

Lemma 5.9: There exists $K>0$, such that

$$\|V_\omega\Delta\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s}\|^2\leqslant\varepsilon^4+K(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma)^2. \tag{42}$$

Before showing these two lemmas let us use them to finish the proof of Theorem 5.7.

Combining (41) and (42) and taking (40) into account we get $K>0$, such as

$$\|(\Delta A_\omega)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s}\|^2\leqslant\varepsilon^3+K(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma)^2. \tag{43}$$

By (36), (37), and (43), it follows that

$$\|(A_\omega-E_+)\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s}\|^2\leqslant\frac{\varepsilon^2}{2}+K(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma)^2. \tag{44}$$

Now, for N large, we may divide Λ_N into $N(\varepsilon)$ disjoints cubes of size $2\Lambda_\alpha(\varepsilon^s)$. For $\alpha<\frac{1}{2}$, there exists $C>0$ such as $N(\varepsilon)$ satisfies

$$N(\varepsilon)\simeq\frac{(2N)^d}{\varepsilon^{-sd(1/2+\alpha)}}\geqslant\frac{(N\varepsilon^s)^d}{C}. \tag{45}$$

We have

$$\cup_{j=1}^{N(\varepsilon)}(\beta_j+\Lambda_\alpha(\varepsilon^s))\subset\Lambda_N \quad\text{and for } j\neq j';(\beta_j+2\Lambda_\alpha(\varepsilon^s))\cap(\beta_{j'}+2\Lambda_\alpha(\varepsilon^s))=\varnothing.$$

This implies that for $j\neq j'$, $\mathcal{U}^f_{\alpha,\varepsilon,\beta_j,\varepsilon^s}$ and $\mathcal{U}^f_{\alpha,\varepsilon,\beta_{j'},\varepsilon^s}$ are orthogonal.

We denote the counting function of the eigenvalues of A_{ω,Λ_N} below E by $\Theta_{\Lambda_N}(E)$, then

$$\begin{aligned}\mathbb{E}(\Theta_{\Lambda_N}(E+\varepsilon)-\Theta_{\Lambda_N}(E-\varepsilon))&=\mathbb{E}(\#\{\text{eigenvalues of }\Pi_N A_\omega\Pi_N\text{ in }[E_+-\varepsilon,E_++\varepsilon]\})\\&\geqslant\mathbb{E}(\#\{1\leqslant j\leqslant N(\varepsilon);\|(A_\omega-E_+)\mathcal{U}^f_{\alpha,\varepsilon,\beta_j,\varepsilon^s}\|_{L^2(\mathbb{R}^d)}\leqslant\varepsilon\})\\&\geqslant\mathbb{E}\left(\sum_{j=1}^{N(\varepsilon)}B_j(\omega)\right),\end{aligned} \tag{46}$$

where

$$B_j(\omega)=\begin{cases}1 & \text{if } K(\varepsilon^{s\alpha(\nu-\mathrm{d})}\cdot\varepsilon+\sup_{\gamma\in\beta_j+2\Lambda_\alpha(\varepsilon^s)}\omega_\gamma^+)^2\leqslant\dfrac{\varepsilon^2}{2},\\ 0 & \text{if not.}\end{cases}$$

The $(B_j)_{1\leqslant j\leqslant N(\varepsilon)}$ are independent, identically distributed, Bernoulli random variables. So Eqs. (46) and (45), imply that there exists $C>0$, such that one has

$$N_{\Lambda_N}(E+\varepsilon)-N_{\Lambda_N}(E-\varepsilon)=\frac{1}{((2N+1))^d}\mathbb{E}(\#\{\text{eigenvalues of } \Pi_N A_\omega \Pi_N \text{ in } [E_+-\varepsilon,E_++\varepsilon]\})$$
$$\geqslant\frac{N(\varepsilon)}{(2N+1)^d}\mathbb{P}(B_1=1)\geqslant\frac{1}{C}\varepsilon^{sd}\mathbb{P}(B_1=1).$$

Hence, taking the limit $N\to\infty$, we get that, for $\varepsilon>0$ small, we obtain

$$N(E_++\varepsilon)-N(E_+-\varepsilon)\geqslant\frac{1}{C}\varepsilon^{sd}\mathbb{P}(B_1=1). \tag{47}$$

It just remains to estimate $\mathbb{P}(B_1=1)$. If for $1\leqslant j\leqslant N(\varepsilon)$, and $\gamma\in\beta_j+2\Lambda_\alpha(\varepsilon)$, one has $\omega_\gamma^+\leqslant\varepsilon/2K$, then for ε rather small

$$K(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sup_{\gamma\in\beta_j+2\Lambda_\alpha(\varepsilon^s)}\omega_\gamma^+)^2\leqslant\varepsilon^2\cdot K\left(\varepsilon^{\alpha(\nu-d)}+\frac{1}{2K}\right)^2\leqslant\frac{\varepsilon^2}{2}.$$

As the random variables are independent identically distributed, one has the estimate

$$\mathbb{P}(B_j=1)\geqslant\left(\mathbb{P}\left(\omega_0^+\leqslant\frac{\varepsilon}{2K}\right)\right)^{2\#\Lambda_\alpha(\varepsilon^s)}.$$

Hence, taking the double logarithm of (47), using assumption (H.3) and the fact that $\#\Lambda_\alpha(\varepsilon^s)=\varepsilon^{-sd[(1/2)+\alpha]}$, we get that

$$\lim_{\varepsilon\to0^+}\frac{\log|\log(N(E_++\varepsilon)-N(E_+))|}{\log\varepsilon}\geqslant-s\frac{d}{2}-s\,d\alpha. \tag{48}$$

Equation (48) is true for any $\alpha>0$, by taking α small we end the proof of Theorem 5.7. □

The proof of Lemma 5.8:

$$\|(\nabla V_\omega)\cdot(\nabla\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s})\|^2\leqslant2^d\sum_{i=1}^d\|(\partial_{x_i}V_\omega)(\partial_{x_i}\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s})\|^2. \tag{49}$$

We recall that

$$\omega_\gamma^+=\omega^+-\omega_\gamma\quad\text{and}\quad V_\omega=\frac{\varrho_{\omega^+}-\varrho_\omega}{\varrho_{\omega^+}\cdot\varrho_\omega}=\frac{1}{D_\omega}\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma^+u_\gamma,$$

here $D_\omega=\varrho_{\omega^+}\cdot(1+\Sigma_{\gamma\in\mathbb{Z}^d}\omega_\gamma u_\gamma)$. We compute

$$\partial_{x_i}V_\omega=\frac{1}{D_\omega}\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma^+\partial_{x_i}u_\gamma-\frac{1}{D_\omega^2}\sum_{\gamma\in\mathbb{Z}^d}(\omega^+-\omega_\gamma)u_\gamma\partial_{x_i}D_\omega.$$

So,

$$\|(\partial_{x_i}V_\omega)(\partial_{x_i}\mathcal{U}^f_{\alpha,\varepsilon,\beta,\varepsilon^s})\|^2 \leqslant 2\left\| \frac{1}{D_\omega}\sum_{\gamma\in\mathbb{Z}^d}\omega^+_\gamma \partial_{x_i}u_\gamma(\mathcal{U}^{\partial_{x_i}f}_{\alpha,\varepsilon,\beta,\varepsilon^s})\right\|^2 + 2\left\|\left(\frac{\partial_{x_i}D_\omega}{D^2_\omega}\right)\sum_{\gamma\in\mathbb{Z}^d}\omega^+_\gamma u_\gamma(\mathcal{U}^{\partial_{x_i}f}_{\alpha,\varepsilon,\beta,\varepsilon^s})\right\|^2. \tag{50}$$

We study the behavior of the quantity on the right-hand side of Eq. (50). Using the fact that $\|D_\omega\|_\infty > 1/C > 0$, we obtain that

$$\left\| \frac{1}{D_\omega}\sum_{\gamma\in\mathbb{Z}^d}\omega^+_\gamma \partial_{x_i}u_\gamma(\mathcal{U}^{\partial_{x_i}f}_{\alpha,\varepsilon,\beta,\varepsilon^s})\right\|^2 \leqslant \varepsilon^5 + \int_{\mathbb{R}^d}\left(\sum_{\gamma\in\mathbb{Z}^d}\omega^+_\gamma\partial_{x_i}u_\gamma(x)\right)^2|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\beta}(x)|^2\,dx. \tag{51}$$

We used an estimate like (38) to replace $\mathcal{U}^{\partial_{x_i}f}_{\alpha,\varepsilon,\beta,\varepsilon^s}$ with $\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\beta}$.

We set

$$S_{\beta,\varepsilon} = \int_{\mathbb{R}^d}\left(\sum_{\gamma\in\mathbb{Z}^d}\omega^+_\gamma\partial_{x_i}u_\gamma\right)^2|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\beta}(x)|^2\,dx.$$

By the use of assumption (H.2), we get that

$$S_{\beta,\varepsilon} \leqslant \sum_{\eta\in\mathbb{Z}^d}\left(\sum_{\gamma\in\mathbb{Z}^d}(1+|\eta-\gamma|)^{-\nu}\omega^+_\gamma\right)^2\cdot\int_{C_0}g^2_+(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta-\beta}(x)|^2\,dx. \tag{52}$$

There exists $B>0$ such that

$$\sum_{\eta\notin\Lambda_\alpha(\varepsilon^s)}(1+|\eta|)^{-\nu} \leqslant B\cdot\varepsilon^{\alpha s(\nu-d)}\cdot\varepsilon^{(s/2)(\nu-d)} \leqslant B\cdot\varepsilon^{\alpha s(\nu-d)}\cdot\varepsilon.$$

Using the fact that the random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ are bounded, we obtain that there exists $B'>0$ such that

$$S_{\beta,\varepsilon} \leqslant \sum_{\eta\in\mathbb{Z}^d}\left(B'\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon + \sum_{\gamma\in\eta+\Lambda_\alpha(\varepsilon^s)}(1+|\eta-\gamma|)^{-\nu}\omega^+_\gamma\right)^2\cdot\int_{C_0}g^2_+(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta-\beta}(x)|^2\,dx.$$

One splits the sum on $\eta\in\mathbb{Z}^d$ in two parts according to whether η belongs to $\beta+\Lambda_\alpha(\varepsilon^s)$ or not.

For the sum on $\eta\notin\beta+\Lambda_\alpha(\varepsilon^s)$, there exists $C>0$ such that

$$\sum_{\eta\notin\beta+\Lambda_{\alpha(\varepsilon^s)}}\left(C\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon + \sum_{\gamma\in\eta+\Lambda_\alpha(\varepsilon^s)}(1+|\eta-\gamma|)^{-\nu}\omega^+_\gamma\right)^2\cdot\left(\int_{C_0}g^2_+(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta-\beta}(x)|^2\,dx\right)$$
$$\leqslant C\sum_{\eta\notin\Lambda_\alpha(\varepsilon)}\int_{C_0}g^2_+(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta}(x)|^2\,dx. \tag{53}$$

By the use of the nonstationary phase and following the same computation done in Ref. 12 one proves that, for n entire, there exists $C_n>0$ such that

$$\sum_{\eta\notin\Lambda_\alpha(\varepsilon^s)}\left(\int_{C_0}g^2_+(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta}(x)|^2\,dx\right)\leqslant C_n\varepsilon^{\alpha sn}. \tag{54}$$

For the sum on η in $\beta+\Lambda_\alpha(\varepsilon^s)$, one gets

$$\sum_{\eta\in\beta+\Lambda_\alpha(\varepsilon^s)}\left(C\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sum_{\gamma\in\Lambda_\alpha(\varepsilon^s)}(1+|\gamma|)^{-\nu}\omega^+_{\gamma+\eta}\right)^2\cdot\int_{C_0}g_+^2(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta}(x)|^2\,dx$$
$$\leqslant\left(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\left[\sum_{\gamma\in\Lambda_\alpha(\varepsilon^s)}(1+|\gamma|)^{-\nu}\right]\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma\right)^2$$
$$\times\sum_{\eta\in\Lambda_\alpha(\varepsilon^s)}\int_{C_0}g_+^2(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta}(x)|^2\,dx. \tag{55}$$

Using the fact that $(\partial_{x_i}f)(x,\theta)$ verifies assumptions of Lemma 5.1 (see Remark 5.2) and $g_+(x)\in L^p(C_0)$, we see that there exists $K>0$ such that

$$\sum_{\eta\in\Lambda_\alpha(\varepsilon^s)}\int_{C_0}g_+^2(x)|\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\eta}(x)|^2\,dx=\sum_{\eta\in\Lambda_\alpha(\varepsilon^s)}\int_{C_0}g_+^2(x)\left|\int_{\mathbb{T}^*}e^{i\eta\cdot\theta}\mathcal{W}_\varepsilon(\theta)(\partial_{x_i}f)(x,\theta)d\theta\right|^2dx$$
$$\leqslant K. \tag{56}$$

So we use (51), (52), (53), (54), (55), and (56), to get that

$$\left\|\frac{1}{D_\omega}\sum_{\gamma\in\mathbb{Z}^d}(\omega^+-\omega_\gamma)(\partial_{x_i}u_\gamma)(\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\beta})\right\|^2$$
$$\leqslant\varepsilon^5+K\left(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sum_{\gamma\in\Lambda_\alpha(\varepsilon^s)}(1+|\gamma|)^{-\nu}\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma\right)^2.$$

We can use the same idea to prove that there exists $K>0$, such that

$$\left\|\left(\frac{\partial_{x_i}D_\omega(x)}{D^2_\omega(x)}\right)\sum_{\gamma\in\mathbb{Z}^d}(\omega^+-\omega_\gamma)u_\gamma\mathcal{U}^{\partial_{x_i}f}_{\varepsilon,\beta}\right\|^2$$
$$\leqslant\varepsilon^5+K\left(\varepsilon^{s\alpha(\nu-d)}\cdot\varepsilon+\sum_{\gamma\in\Lambda_\alpha(\varepsilon^s)}(1+|\gamma|)^{-\nu}\sup_{\gamma\in\beta+2\Lambda_\alpha(\varepsilon^s)}\omega^+_\gamma\right)^2.$$

By taking the last estimates and Eqs. (49) into account we obtain Lemma 5.8. □

The proof of Lemma 5.9: The proof of Lemma 5.9 is similar to that of Lemma 5.9. Indeed $(\partial^2_{x_i}f)(x,\theta)$ verifies the same properties which are useful as $(\partial_{x_i}f)(x,\theta)$ and following the same step as for the proof of (41), we prove (42). □

ACKNOWLEDGMENT

The author would like to thank Frédéric Klopp under whose guidance this research was undertaken and for valuable comments.

APPENDIX

The proof of Lemma 4.4: The proof is based on Lemma 4.3 and on the Combes–Thomas argument (see Ref. 4) to obtain the exponential decreasing of the resolvent. To estimate the right-hand side of Eq. (10), we write that

$$\|\mathrm{tr}[\chi_{C_0}((\lambda_0+A_{\omega,k})^{-q}(z-A_{\omega,k})^{-1}-(\lambda_0+A_\omega)^{-q}(z-A_\omega)^{-1})]\|_{\mathrm{tr}}\leqslant A+B$$

with

$$A=\|\mathrm{tr}(\chi_{C_0}[(z-A_{\omega,k})^{-1}-(z-A_\omega)^{-1}](\lambda_0+A_\omega)^{-q}\chi_{C_0})\|$$

and

$$B=\|\mathrm{tr}(\chi_{C_0}(z-A_{\omega,k})^{-1}[(\lambda_0+A_{\omega,k})^{-q}-(\lambda_0+A_\omega)^{-q}]\chi_{C_0})\|.$$

We control separately A and B. For A, we get

$$\begin{aligned}A&\leqslant\|\mathrm{tr}(\chi_{C_0}(z-A_{\omega,k})^{-1}(A_\omega-A_{\omega,k})(z-A_\omega)^{-1}(\lambda_0+A_\omega)^{-q}\chi_{C_0})\|\\&\leqslant\left\|\chi_{C_0}(z-A_{\omega,k})^{-1}\left(\nabla\frac{1}{\varrho_\omega\varrho_{\omega,k}}\left(\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma u_\gamma-\sum_{\gamma\in C_k\cap\mathbb{Z}^d}\omega_\gamma\sum_{\beta\in(2k+1)\mathbb{Z}^d}u_{\gamma+\beta}\right)\nabla\right)\right.\\&\quad\left.\cdot(z-A_\omega)^{-1}(\lambda_0+A_\omega)^{-q}\chi_{C_0}\right\|_{\mathrm{tr}}.\end{aligned}$$

As

$$\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma u_\gamma-\sum_{\gamma\in C_k\cap\mathbb{Z}^d}\omega_\gamma\sum_{\beta\in(2k+1)\mathbb{Z}^d}u_{\gamma+\beta}=\sum_{\gamma\in\mathbb{Z}^d,|\gamma|>k}(\omega_{\tilde\gamma}-\omega_\gamma)u_\gamma,$$

where $\tilde\gamma=\gamma\ [\mathrm{mod}\ (2k+1)\mathbb{Z}^d]$, we get that

$$A\leqslant\left\|\chi_{C_0}(z-A_{\omega,k})^{-1}\left(\nabla\frac{1}{\varrho_\omega\varrho_{\omega,k}}\left(\sum_{\gamma\in\mathbb{Z}^d,|\gamma|>k}(\omega_{\tilde\gamma}-\omega_\gamma)u_\gamma\right)\nabla\right)\times(z-A_\omega)^{-1}(\lambda_0+A_\omega)^{-q}\chi_{C_0}\right\|_{\mathrm{tr}}.$$

As the random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ are bounded, we get that there exists $M>0$, such that

$$\begin{aligned}A&\leqslant M\sum_{\gamma\in\mathbb{Z}^d,|\gamma|>k}\left\|\chi_{C_0}(z-A_{\omega,k})^{-1}\left(\nabla\frac{1}{\varrho_\omega\varrho_{\omega,k}}u_\gamma\nabla\right)(z-A_\omega)^{-1}(\lambda_0+A_\omega)^{-q}\chi_{C_0}\right\|_{\mathrm{tr}}\\&\quad\times\sum_{\beta\in\mathbb{Z}^d,\gamma\in\mathbb{Z}^d,|\gamma|>k}\left\|\chi_{C_0}(z-A_{\omega,k})^{-1}\left(\nabla\frac{1}{\varrho_\omega(x)\varrho_{\omega,k}(x)}u_\gamma\nabla\right)(z-A_\omega)^{-1}\chi_{\beta+C_0}\right\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\\&\quad\cdot\|\chi_{\beta+C_0}(\lambda_0+A_\omega)^{-q}\chi_{C_0}\|_{\mathrm{tr}}.\end{aligned}$$

By the use of Combes–Thomas argument, see Ref. 4, we get that there exists $K>0$ such that

$$\begin{aligned}&\left\|\chi_{C_0}(z-A_{\omega,k})^{-1}\left(\nabla\frac{1}{\varrho_\omega\varrho_{\omega,k}}u_\gamma\nabla\right)\times(z-A_\omega)^{-1}\chi_{\alpha+C_0}\right\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\\&\qquad\leqslant\frac{K}{|\mathrm{Im}(z)|^2}e^{-|\mathrm{Im}(z)||\beta|/K}\|\tau_{\beta+\gamma}u\|_{L^p(C_0)},\end{aligned}$$

thus from Lemma 4.3 we get

$$A\leqslant K\sum_{\beta,\gamma\in\mathbb{Z}^d,|\gamma|>k}\frac{e^{-|\mathrm{Im}(z)||\beta|/K}}{|\mathrm{Im}(z)|^2}\|\tau_{\beta+\gamma}u\|_{L^p(C_0)}.$$

We can proceed in the same manner to estimate B. Finally, we obtain

$$|\mathbb{E}(\langle\varphi,dN_{\omega,k}\rangle)-\langle\varphi,dN\rangle|\leqslant\mathbb{E}\Bigg(\frac{K}{\pi}\int_{\mathbb{R}^2}\left|\frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)\right| \times K\sum_{\alpha,\gamma\in\mathbb{Z}^d,|\gamma|>k}\frac{e^{-|\mathrm{Im}(z)||\beta|/K}}{|\mathrm{Im}(z)|^2}\|\tau_{\beta+\gamma}u\|_{L^p(C_0)}dx\,dy\Bigg).$$

This ends the proof of Lemma 4.4. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 4 APRIL 2003

$\mathcal{N}$-point and higher-genus osp(1|2) fusion

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(Received 12 June 2002; accepted 16 December 2002)

We study affine osp(1|2) fusion, the fusion in osp(1|2) conformal field theory, for example. Higher-point and higher-genus fusion is discussed. The fusion multiplicities are characterized as discretized volumes of certain convex polytopes, and are written explicitly as multiple sums measuring those volumes. We extend recent methods developed to treat affine su(2) fusion. They are based on the concept of generalized Berenstein–Zelevinsky triangles and virtual couplings. Higher-point tensor products of finite-dimensional irreducible osp(1|2) representations are also considered. The associated multiplicities are computed and written as multiple sums. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1557913]

I. INTRODUCTION

The representation theory of finite-dimensional irreducible representations of the Lie superalgebra osp(1|2) is well-known.[1] That includes the decomposition of ordinary three-point tensor products. However, to the best of our knowledge, the literature does not offer discussions of general $\mathcal{N}$-point couplings. Here we shall consider those and compute the associated tensor product multiplicities. They are characterized as discretized volumes of certain convex polytopes (i.e., the number of integer points bounded by the polytope), and are written explicitly as multiple sums measuring those volumes. The results are obtained by extending recent methods developed to treat su(N) tensor products, and are based on the concept of generalized Berenstein–Zelevinsky (BZ) triangles and virtual couplings.[2,3]

The seminal work by Berenstein and Zelevinsky[4] shows how one may represent ordinary su(N) three-point couplings by triangular arrangements of non-negative integers. Their results were extended in Ref. 3 to higher-point couplings, by gluing such triangles together. Here we shall associate two types of triangles to osp(1|2) three-point couplings. We denote them osp(1|2) BZ triangles, and ''super-triangles,'' respectively. The gluing method of Ref. 3 is then applied to treat higher-point osp(1|2) couplings.

We then turn to our second objective: affine osp(1|2) fusion, the fusion in osp(1|2) conformal field theory, for example. Ordinary three-point fusion has been studied from various points of view.[5–7] For integer level, k, and associated admissible (or integrable) representations,[8,5] we show that the level dependence of a fusion may be incorporated in the osp(1|2) BZ triangles or super-triangles. That allows us to discuss higher-point fusion along the lines of Ref. 9 on higher-point su(2) fusion. As for the tensor products above, the $\mathcal{N}$-point osp(1|2) fusion multiplicities are characterized by level-dependent convex polytopes, and written explicitly as multiple sums.

Our approach admits also an extension to higher-genus, h, fusion. The associated fusion multiplicities are characterized as discretized volumes of certain convex polytopes, and are written explicitly as multiple sums. To illustrate and demonstrate consistency, we consider in detail the genus-one one- and two-point fusions.

This work presents the first general results on $\mathcal{N}$-point osp(1|2) tensor products, and on $\mathcal{N}$-point and higher-genus osp(1|2) fusion. The results are general as they cover all integer $\mathcal{N}$, k and h. They are also very explicit and should therefore be easy to use in applications. Implementation in computer programming is also straightforward.

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A. osp(1|2) representation theory

Here we recall some basic facts on the Lie superalgebra osp(1|2) and its irreducible representations.[1] A "physicist-friendly" review may be found in Ref. 10, while general Lie superalgebra theory is considered in Refs. 11 and 12.

The Lie superalgebra osp(1|2) is a five-dimensional graded extension of the three-dimensional Lie algebra su(2):

$$\begin{aligned} &[J^3,J^\pm]=\pm J^\pm,\quad [J^3,j^\pm]=\pm\tfrac{1}{2}j^\pm,\quad [J^+,J^-]=2J^3,\\ &\{j^+,j^-\}=2J^3,\quad \{j^\pm,j^\pm\}=\pm 2J^\pm,\quad [J^\pm,j^\mp]=-j^\pm. \end{aligned} \tag{1}$$

All other (anti-)commutators vanish. The three even generators J^+, J^- and J^3 generate an su(2) subalgebra of osp(1|2), while j^+ and j^- are two odd generators. They comprise a spin-$\frac{1}{2}$ representation of the su(2) subalgebra in the adjoint representation.

Every finite-dimensional irreducible representation has an isospin j associated to it, where

$$2j\in\mathbb{Z}_{\geqslant}. \tag{2}$$

Such a representation $\mathcal{R}_j$ has dimension $4j+1$:

$$\mathcal{R}_j:\quad |j,j\rangle,\ |j,j-\tfrac{1}{2}\rangle,\ldots,\ |j,0\rangle,\ldots,\ |j,-j+\tfrac{1}{2}\rangle,\ |j,-j\rangle. \tag{3}$$

The states $|j,m\rangle$ and $|j,m'\rangle$ have the same parity if and only if $m-m'\in\mathbb{Z}$. The parity $p(\mathcal{R}_j)$ of the representation $\mathcal{R}_j$ is defined as the parity of the state $|j,j\rangle$. The mode m is the eigenvalue of J^3: $J^3|j,m\rangle=m|j,m\rangle$. It is observed that the representation (3) splits into two su(2) representations—one of spin j and one of spin $j-\frac{1}{2}$. The former consists of the states $|j,m\rangle$ with $j-m\in\mathbb{Z}_{\geqslant}$, while the latter consists of the states with $j-m\in\mathbb{Z}_{\geqslant}+\frac{1}{2}$. Disregarding the notion of parity, the osp(1|2) representation space (3) becomes analogous to a single su(2) representation space of spin $2j$. That observation will turn out to be useful in the following.

We shall use the same notation j for an osp(1|2) isospin as for an su(2) spin, but refer to them as indicated. An su(2) representation of spin j is indicated by $\mathcal{R}_j^{\mathrm{su}(2)}$.

II. TENSOR PRODUCTS

Decompositions of ordinary tensor products of finite-dimensional irreducible representations are easily computed:

$$\mathcal{R}_{j_1}\otimes\mathcal{R}_{j_2}=\mathcal{R}_{|j_1-j_2|}\oplus\mathcal{R}_{|j_1-j_2|+1/2}\oplus\cdots\oplus\mathcal{R}_{j_1+j_2-1/2}\oplus\mathcal{R}_{j_1+j_2}. \tag{4}$$

Note the resemblance to tensor products of integer-spin su(2) representations:

$$\mathcal{R}^{\mathrm{su}(2)}_{2j_1}\otimes\mathcal{R}^{\mathrm{su}(2)}_{2j_2}=\mathcal{R}^{\mathrm{su}(2)}_{2|j_1-j_2|}\oplus\mathcal{R}^{\mathrm{su}(2)}_{2|j_1-j_2|+1}\oplus\cdots\oplus\mathcal{R}^{\mathrm{su}(2)}_{2(j_1+j_2)-1}\oplus\mathcal{R}^{\mathrm{su}(2)}_{2(j_1+j_2)}. \tag{5}$$

Instead of considering a tensor product of the form

$$\mathcal{R}_{j_1}\otimes\mathcal{R}_{j_2}\supset\mathcal{R}_{j_3} \tag{6}$$

we may equivalently consider the symmetric three-point coupling to the singlet:

$$\mathcal{R}_{j_1}\otimes\mathcal{R}_{j_2}\otimes\mathcal{R}_{j_3}\supset\mathcal{R}_0. \tag{7}$$

Similar couplings of su(N) representations are neatly described by Berenstein–Zelevinsky (BZ) triangles.[4] In the case of su(2) the BZ triangle is trivial but has led to characterizations of higher-point and higher-genus couplings and fusions as discretized volumes of certain polytopes.[9] Here we shall discuss the generalization to osp(1|2).

A. Berenstein–Zelevinsky super-triangle

An su(2) BZ triangle is a triangular arrangement of three non-negative integer entries a, b and c:

$$\mathcal{R}_{j_1}^{\mathrm{su}(2)}\otimes\mathcal{R}_{j_2}^{\mathrm{su}(2)}\otimes\mathcal{R}_{j_3}^{\mathrm{su}(2)}\supset\mathcal{R}_0^{\mathrm{su}(2)}\leftrightarrow\begin{array}{ccc} & b & \\ c & & a \end{array} \tag{8}$$

subject to the spin constraints

$$a=-j_1+j_2+j_3\in\mathbb{Z}_{\geqslant},\qquad b=j_1-j_2+j_3\in\mathbb{Z}_{\geqslant},\qquad c=j_1+j_2-j_3\in\mathbb{Z}_{\geqslant}, \tag{9}$$

and hence

$$2j_1=b+c,\quad 2j_2=c+a,\qquad 2j_3=a+b. \tag{10}$$

When all three spins are integer, either a, b and c must all be even or all be odd. Exploring the similarity between (4) and (5) we see that we may describe three-point couplings of osp(1|2) representations by standard BZ triangles,

$$\mathcal{R}_{j_1}\otimes\mathcal{R}_{j_2}\otimes\mathcal{R}_{j_3}\supset\mathcal{R}_0\leftrightarrow\begin{array}{ccc} & B & \\ C & & A \end{array} \tag{11}$$

with isospins

$$4j_1=B+C,\quad 4j_2=C+A,\qquad 4j_3=A+B,\qquad A,\ B,\ C\in\mathbb{Z}_{\geqslant}, \tag{12}$$

or equivalently by BZ *super-triangles*

$$\mathcal{R}_{j_1}\otimes\mathcal{R}_{j_2}\otimes\mathcal{R}_{j_3}\supset\mathcal{R}_0\leftrightarrow\begin{array}{ccc} & b & \\ & \epsilon & \\ c & & a \end{array} \tag{13}$$

with isospins

$$2j_1=\mathrm{b}+\mathrm{c}+\epsilon,\qquad 2j_2=\mathrm{c}+\mathrm{a}+\epsilon,\qquad 2j_3=\mathrm{a}+\mathrm{b}+\epsilon,\qquad \mathrm{a},\ \mathrm{b},\ \mathrm{c}\in\mathbb{Z}_{\geqslant},\qquad \epsilon\in\{0,1\}. \tag{14}$$

The *super-entry* ϵ measures the ''parity violation'' of the coupling:

$$\begin{aligned}\epsilon&=p(\mathcal{R}_{j_1})+p(\mathcal{R}_{j_2})+p(\mathcal{R}_{j_3})\mod(2)\\&=2(j_1+j_2+j_3)\mod(2).\end{aligned} \tag{15}$$

Relaxing the isospin-independent constraints on the entries (thereby allowing a, b, c, $\epsilon\in\mathbb{Z}$), there are infinitely many *generalized* super-triangles associated to a three-point coupling. They are all related through additions of integer multiples of the (basis) *virtual* super-triangle

$$\mathcal{V}=\begin{array}{ccc} & \overline{1} & \\ 1 & & 1 \end{array} \tag{16}$$

where $\overline{n}\equiv -n$. Given an initial generalized super-triangle $\mathcal{T}_0$ [see (31) for a choice when extended to higher-point couplings], all other generalized super-triangles are of the form

$$\mathcal{T}=\mathcal{T}_0+\sum_{v\in\mathbb{Z}} v\,\mathcal{V}. \tag{17}$$

However, due to the constraint on ϵ, only one super-triangle in this infinite chain of generalized super-triangles will satisfy all the requirements. We shall call it a *true* super-triangle. By construction, if a coupling of three isospins (j_1, j_2, j_3) to the singlet is not possible, there will be no true super-triangle associated to that isospin triplet.

A motivation for introducing super-triangles is that they seem to indicate how one may generalize the representation of su(N) couplings by BZ triangles to a representation of Lie superalgebra couplings by (extended) super-triangles. Even though the osp(1|2) super-triangles are slightly more complicated to work with than the osp(1|2) BZ triangles, we shall consider them throughout this article alongside the BZ triangles. They provide us with alternative characterizations of tensor product couplings and fusions—representations that are more ''supersymmetric.'' Furthermore, in Sec. V we will indicate how super-triangles appear natural from the point of view of three-point functions in osp(1|2) conformal field theory.

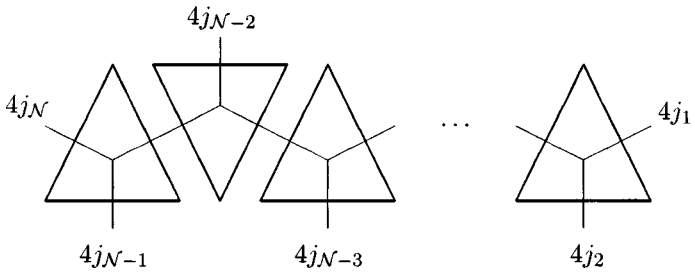
B. Higher-point couplings

In a decomposition of a higher-point tensor product, the singlet may occur more than once, i.e., the associated tensor product multiplicity, $T_{j_1,\ldots,j_{\mathcal{N}}}$, may be greater than one:

$$\mathcal{R}_{j_1}\otimes\cdots\otimes\mathcal{R}_{j_{\mathcal{N}}}\supset T_{j_1,\ldots,j_{\mathcal{N}}}\mathcal{R}_0\,. \tag{18}$$

The similar situation for su(2) couplings is described in Refs. 3 and 9 [Ref. 3 covers all su(N) but does not discuss fusion]. There it is discussed how BZ triangles may be glued together to form $\mathcal{N}$-sided diagrams representing the $T^{\mathrm{su}(2)}_{j_1,\ldots,j_{\mathcal{N}}}$ different su(2) couplings. Likewise, we can associate an $\mathcal{N}$-sided diagram to each of the $T_{j_1,\ldots,j_{\mathcal{N}}}$ different osp(1|2) $\mathcal{N}$-point couplings. Due to the existence of two types of triangles (11) and (13), we may represent an osp(1|2) $\mathcal{N}$-point coupling by two different types of diagrams. We shall call the ones based on super-triangles *super-diagrams*.

The general method for computing higher-point su(N) tensor product multiplicities outlined in Ref. 3, is based on gluing BZ triangles together using *gluing* diagrams (we refer to Ref. 3 for details). This idea extends readily to osp(1|2) tensor products (18). To be explicit, let us consider the following $\mathcal{N}$-point diagram (in this example $\mathcal{N}$ is assumed odd):



(19)

The role of the gluing is to take care of the summation over internal isospins in a tractable way. The dual picture of ordinary (Feynman tree-) graphs is shown in thinner lines. Along a gluing, the opposite isospins must be identified.

Let us begin by considering the diagrams obtained by extending (11). The starting point in Ref. 3 and here is to relax the constraint that the entries should be *non-negative* integers. As for the super-triangles above, a diagram of that kind is called a *generalized* diagram. Any such generalized diagram, respecting the gluing constraints and the outer isospin constraints (19), will suffice as an initial diagram. All other diagrams that are associated to the same outer isospins may then be obtained by adding integer linear combinations of so-called *virtual* diagrams: adding a basis

virtual diagram changes the value of $4j$ of a given internal isospin by two, leaving all other internal isospins and all outer isospins unchanged. Thus, the basis virtual diagram associated to a particular gluing is of the form:

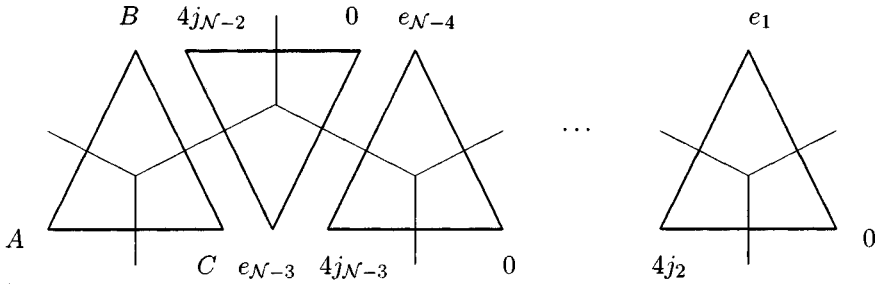
$$\mathcal{G}= \quad \begin{array}{ccccc} & & \overline{1} & & 1 \\ & \iddots & & & \\ \overline{1} & & & & \overline{1} \\ & & \iddots & & \\ 1 & & \overline{1} & & \end{array} \quad . \tag{20}$$

Enumerating the gluing diagrams (20) in (19) from right to left, the associated integer coefficients in the linear combinations are $g_1,\ldots,g_{\mathcal{N}-3}$. If $\mathcal{D}_0$ denotes an initial diagram, all generalized diagrams will then be of the form

$$\mathcal{D}=\mathcal{D}_0+\sum_{l=1}^{\mathcal{N}-3}\sum_{g_l\in\mathbb{Z}} g_l\mathcal{G}_l\,. \tag{21}$$

It remains to be accounted for how to write down an initial diagram $\mathcal{D}_0$. However, that is straightforward:

$\mathcal{D}_0 \;=$



(22)

with

$$\begin{gathered} e_l=4(j_1+\ldots+j_l),\quad 1\leqslant l\leqslant\mathcal{N}-3,\\ A=-S+4j_{\mathcal{N}-1}+4j_{\mathcal{N}},\quad B=S-4j_{\mathcal{N}-1},\quad C=S-4j_{\mathcal{N}}, \end{gathered} \tag{23}$$

and

$$S\equiv 2(j_1+\ldots+j_{\mathcal{N}}). \tag{24}$$

Reimposing the condition that all the entries in $\mathcal{D}$ (21) must be *non-negative* results in a set of inequalities defining a convex polytope in the Euclidean space $\mathbb{R}^{\mathcal{N}-3}$:

$$
\begin{gathered}
0 \leqslant g_1,\ 4j_1 - g_1,\ 4j_2 - g_1, \\
0 \leqslant g_2 - g_1,\ 4j_3 - g_2 + g_1,\ 4(j_1 + j_2) - g_2 - g_1, \\
\vdots \\
0 \leqslant g_{\mathcal{N}-3} - g_{\mathcal{N}-4},\ 4j_{\mathcal{N}-2} - g_{\mathcal{N}-3} + g_{\mathcal{N}-4},\ 4(j_1 + \ldots + j_{\mathcal{N}-3}) - g_{\mathcal{N}-3} - g_{\mathcal{N}-4}, \\
0 \leqslant S - 4j_{\mathcal{N}-1} - g_{\mathcal{N}-3},\ S - 4j_{\mathcal{N}} - g_{\mathcal{N}-3},\ -S + 4(j_{\mathcal{N}-1} + j_{\mathcal{N}}) + g_{\mathcal{N}-3}.
\end{gathered}
\tag{25}
$$

By construction, its discretized volume is the tensor product multiplicity $T_{j_1,\ldots,j_{\mathcal{N}}}$. The volume may be measured explicitly, expressing the multiplicity as a multiple sum. In order to avoid discussing intersection of faces we have to choose an "appropriate order" of summation (see Refs. 2, 3, and 9). Making such a choice is straightforward, and we find that the osp(1|2) tensor product multiplicity $T_{j_1,\ldots,j_{\mathcal{N}}}$ may be written as

$$
\begin{aligned}
T_{j_1,\ldots,j_{\mathcal{N}}} = & \sum_{g_{\mathcal{N}-3}=S-4(j_{\mathcal{N}-1}+j_{\mathcal{N}})}^{\min\{S-4j_{\mathcal{N}-1},\ S-4j_{\mathcal{N}}\}} \quad \sum_{g_{\mathcal{N}-4}=-4j_{\mathcal{N}-2}+g_{\mathcal{N}-3}}^{\min\{g_{\mathcal{N}-3},\ 4(j_1+\ldots+j_{\mathcal{N}-3})-g_{\mathcal{N}-3}\}} \\
& \times \cdots \times \sum_{g_2=-4j_4+g_3}^{\min\{g_3,\ 4(j_1+\ldots+j_3)-g_3\}} \quad \sum_{g_1=\max\{0,\ -4j_3+g_2\}}^{\min\{4j_1,\ 4j_2,\ g_2,\ 4(j_1+j_2)-g_2\}} 1.
\end{aligned}
\tag{26}
$$

This is the first general result for higher-point osp(1|2) tensor product multiplicities.

Following methods discussed in Refs. 2, 3, and 9, it is not difficult to derive necessary and sufficient conditions determining when an osp(1|2) $\mathcal{N}$-point tensor product multiplicity is nonvanishing. The conditions are

$$
2j_l,\ S - 4j_l \in \mathbb{Z}_{\geqslant}, \qquad l = 1,\ldots,\mathcal{N}
\tag{27}
$$

with S defined in (24).

Gluing super-triangles together to represent higher-point couplings is not a lucrative alternative to the method above. Nevertheless, we give here the associated gluing super-diagram:

$$
\mathcal{G} = \begin{array}{ccccc}
 & & & 0 & 1 \\
 & & \iddots & & \overline{1} \\
 & 0 & & & 0 \\
 & \overline{1} & & \iddots & \\
1 & & 0 & &
\end{array}
\,.
\tag{28}
$$

There is a virtual super-triangle associated to each of the glued super-triangles, i.e., there are $\mathcal{N}-2$ (basis) virtual super-diagrams associated to an $\mathcal{N}$-point super-diagram. In a self-explaining notation we then have that any generalized super-diagram may be written

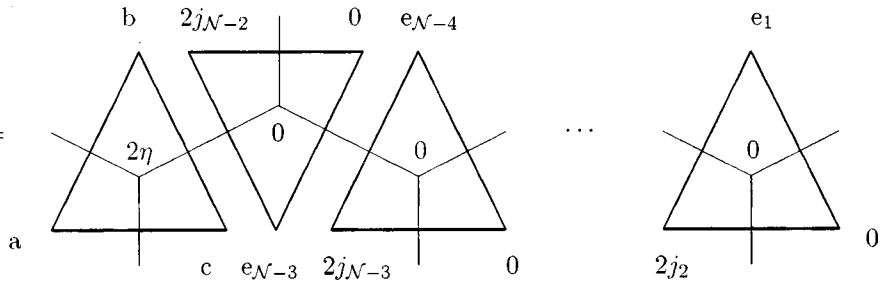
$$
\mathcal{D} = \mathcal{D}_0 + \sum_{l=1}^{\mathcal{N}-2} \sum_{v_l \in \mathbb{Z}} v_l \mathcal{V}_l + \sum_{l=1}^{\mathcal{N}-3} \sum_{g_l \in \mathbb{Z}} g_l \mathcal{G}_l .
\tag{29}
$$

Now, recall that the super-entry measures the parity violation as indicated in (15). For $\mathcal{N}$-point couplings it is the sum of the $\mathcal{N}-2$ super-entries that measures the parity violation. It is therefore natural to introduce the *parity parameter* η,

$$
2\eta = \left(\sum_{l=1}^{\mathcal{N}-2} \epsilon_l \right) \bmod (2) = \begin{cases} 0 & \text{for } S \in 2\mathbb{Z}_{\geqslant}, \\ 1 & \text{for } S \in 2\mathbb{Z}_{\geqslant} + 1, \end{cases}
\tag{30}
$$

which of course must depend only on the outer isospins [through S (24)]. We may now write down an initial super-diagram:

$\mathcal{D}_0$ =



(31)

with

$$e_l = 2(j_1 + \cdots + j_l), \quad 1 \leqslant l \leqslant \mathcal{N}-3,$$

$$a = -\frac{S}{2} - \eta + 2(j_{\mathcal{N}-1} + j_{\mathcal{N}}), \quad b = \frac{S}{2} - \eta - 2j_{\mathcal{N}-1}, \quad c = \frac{S}{2} - \eta - 2j_{\mathcal{N}}. \tag{32}$$

Since $S/2 - \eta = [S/2]$ ($[x]$ denotes the integer value of x, i.e., the greatest integer less than or equal to x), the entries a, b and c are integers. Imposing the condition that the diagram (29) must be true leads to a set of inequalities in the parameters v and g defining a convex polytope as (25). This polytope is embedded in the Euclidean space $\mathbb{R}^{2\mathcal{N}-5}$. The inequalities are straightforward to write down, but are not given here.

C. Four-point couplings

To illustrate the results above we shall compute the osp(1|2) four-point tensor product multiplicity T_{j_1,j_2,j_3,j_4}. We shall do it in two ways: first by reducing the general result (25) and (26) to $\mathcal{N}=4$, and then by gluing super-triangles together.

It follows from (25) that

$$0 \leqslant g,\ 4j_1 - g,\ 4j_2 - g,\ S - 4j_3 - g,\ S - 4j_4 - g,\ -S + 4(j_3 + j_4) + g \tag{33}$$

and therefore

$$\begin{aligned} T_{j_1,j_2,j_3,j_4} &= \sum_{g = \max\{0,\ 2(j_1+j_2-j_3-j_4)\}}^{\min\{2(j_1+j_2+j_3-j_4),\ 2(j_1+j_2-j_3+j_4),\ 4j_1,\ 4j_2\}} 1 \\ &= 1 + \min\{4j_1,\ \ldots,\ 4j_4,\ S - 4j_1,\ \ldots,\ S - 4j_4\}, \end{aligned} \tag{34}$$

provided the conditions (27) are satisfied.

Now we turn to the super-triangle approach. For $\mathcal{N}=4$, the convex polytope defined by (29) and (31) becomes

$$\begin{gathered} 0 \leqslant v_1 + g,\ 2j_1 + v_1,\ 2j_2 + v_1, \\ 0 \leqslant -g - 2v_1 \leqslant 1, \\ 0 \leqslant -\left[\frac{S+1}{2}\right] + 2(j_3 + j_4) + v_2 + g,\ \left[\frac{S}{2}\right] - 2j_3 + v_2,\ \left[\frac{S}{2}\right] - 2j_4 + v_2, \\ 0 \leqslant 2\eta - g - 2v_2 \leqslant 1. \end{gathered} \tag{35}$$

Note that the inequalities $0 \leqslant \epsilon_1, \epsilon_2 \leqslant 1$ fix v_1 and v_2 in terms of g:

$$v_1 = -\left[\frac{g+1}{2}\right], \qquad v_2 = -\left[\frac{g+1-2\eta}{2}\right]. \tag{36}$$

That means that the set of inequalities in g, v_1 and v_2 reduces to a set of inequalities in the gluing coordinate g alone. It is not hard to verify that the associated (one-dimensional) polytope is identical to (33). Thus, the two ways of counting the tensor product multiplicity T_{j_1,j_2,j_3,j_4} are essentially equivalent. That generalizes to $\mathcal{N}$-point couplings.

III. FUSION

Here we shall extend the above discussion on tensor products to affine fusion, fusion in osp(1|2) conformal field theory, for example. To distinguish this consideration from the similar one concerning tensor products, we denote finite-dimensional irreducible affine modules of isospin j by M_j. The fusion of three such modules to the singlet is written [cf. the analogous three-point coupling (7)]

$$M_{j_1} \times M_{j_2} \times M_{j_3} \supset N^{(k)}_{j_1,j_2,j_3} M_0 . \tag{37}$$

The fusion multiplicity $N^{(k)}_{j_1,j_2,j_3}$ depends on the level k, where k characterizes the affine extension of osp(1|2) that turns it into a level-k affine Lie superalgebra. We shall consider only k a positive integer, and the so-called admissible (or integrable) representations.[8,5] They are (for k a positive integer) characterized by

$$2j \in \mathbb{Z}_{\geqslant}, \qquad 2j \leqslant k. \tag{38}$$

The ordinary fusion multiplicities are well-known in that case:[5,6]

$$N^{(k \geqslant j_1+j_2+j_3-1/2)}_{j_1,j_2,j_3} = T_{j_1,j_2,j_3}, \qquad N^{(k<j_1+j_2+j_3-1/2)}_{j_1,j_2,j_3} = 0. \tag{39}$$

We recall that a nonvanishing three-point tensor product multiplicity is one. The nonvanishing conditions follow immediately from (4).

The threshold level, t, of a three-point coupling is the minimum level at which the coupling appears in fusion.[13] This means, in particular, that t is integer and that $t \leqslant k$ for the coupling to appear. From (39), it is straightforward to determine the threshold level of an osp(1|2) coupling of three isospins (j_1, j_2, j_3):

$$t = \left[\frac{S}{2}\right]. \tag{40}$$

One may also assign a threshold level to an osp(1|2) BZ triangle or super-triangle. It is known how to do that for su($N \leqslant 4$)[14,15] and has been explored further in Ref. 16. To the BZ osp(1|2) triangle (11) we may assign the threshold level

$$t = \left[\frac{A+B+C}{2}\right] \tag{41}$$

and to the super-triangle (13) we may assign the threshold level

$$t = \mathrm{a} + \mathrm{b} + \mathrm{c} + \epsilon. \tag{42}$$

Since t is integer, the condition $t \leqslant k$ on (41) is equivalent to

$$A + B + C - 1 \leqslant 2k. \tag{43}$$

A higher-point coupling can also be assigned a threshold level.[9] It is defined in the same way as for three-point couplings.

Recently, efforts have been made to characterize fusion multiplicities in terms of polytopes. Most results so far pertain to three-point fusion,[16,17] but also higher-genus and higher-point su(2) fusions have been discussed.[9] Below we shall extend the latter results to osp(1|2).

A. Higher-point fusion

We are now in a position to discuss $\mathcal{N}$-point fusion. Using osp(1|2) BZ triangles, we see that fusion is described by supplementing the set of inequalities (25) by $\mathcal{N}-2$ conditions like (43)—a condition associated to each of the $\mathcal{N}-2$ participating triangles. Thus, an $\mathcal{N}$-point fusion is characterized by the inequalities

$$\begin{gathered}
0\leqslant g_1,\ 4j_1-g_1,\ 4j_2-g_1,\ 2k-4(j_1+j_2)+g_1+1,\\
0\leqslant g_2-g_1,\ 4j_3-g_2+g_1,\ 4(j_1+j_2)-g_2-g_1,\ 2k-4(j_1+j_2+j_3)+g_1+g_2+1,\\
\vdots\\
0\leqslant g_{\mathcal{N}-3}-g_{\mathcal{N}-4},\ 4j_{\mathcal{N}-2}-g_{\mathcal{N}-3}+g_{\mathcal{N}-4},\ 4(j_1+\cdots+j_{\mathcal{N}-3})\\
\quad -g_{\mathcal{N}-3}-g_{\mathcal{N}-4},\quad 2k-4(j_1+\ldots+j_{\mathcal{N}-2})+g_{\mathcal{N}-3}+g_{\mathcal{N}-4}+1,\\
0\leqslant S-4j_{\mathcal{N}-1}-g_{\mathcal{N}-3},\ S-4j_{\mathcal{N}}-g_{\mathcal{N}-3},\ -S+4(j_{\mathcal{N}-1}+j_{\mathcal{N}})+g_{\mathcal{N}-3},\quad 2k-S+g_{\mathcal{N}-3}+1,
\end{gathered} \tag{44}$$

defining a convex polytope embedded in $\mathbb{R}^{\mathcal{N}-3}$. Its discretized volume is the fusion multiplicity $N^{(k)}_{j_1,\ldots,j_{\mathcal{N}}}$. It may be measured explicitly, expressing the multiplicity as a multiple sum:

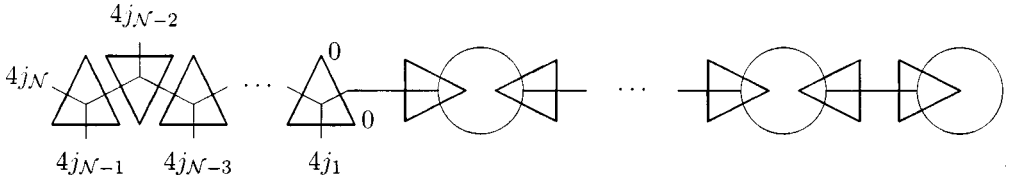
$$\begin{aligned}
N^{(k)}_{j_1,\ldots,j_{\mathcal{N}}}=&\sum_{g_{\mathcal{N}-3}=\max\{S-4(j_{\mathcal{N}-1}+j_{\mathcal{N}}),\ -2k+S-1\}}^{\min\{S-4j_{\mathcal{N}-1},\ S-4j_{\mathcal{N}}\}}\\
&\times\sum_{g_{\mathcal{N}-4}=\max\{-4j_{\mathcal{N}-2}+g_{\mathcal{N}-3},-2k+4(j_1+\ldots+j_{\mathcal{N}-2})-g_{\mathcal{N}-3}-1\}}^{\min\{g_{\mathcal{N}-3},\ 4(j_1+\ldots+j_{\mathcal{N}-3})-g_{\mathcal{N}-3}\}}\\
&\vdots\\
&\times\sum_{g_2=\max\{-4j_4+g_3,\ -2k+4(j_1+\ldots+j_4)-g_3-1\}}^{\min\{g_3,\ 4(j_1+\ldots+j_3)-g_3\}}\\
&\times\sum_{g_1=\max\{0,\ -4j_3+g_2,\ -2k+4(j_1+j_2+j_3)-g_2-1\}}^{\min\{4j_1,\ 4j_2,\ g_2,\ 4(j_1+j_2)-g_2\}}1.
\end{aligned} \tag{45}$$

This is a new result.

IV. HIGHER-GENUS FUSION

Here we will discuss the extension of our results above on genus-zero fusion to generic genus-h fusion. The results here generalize the similar ones in Ref. 9 on higher-genus su(2) fusion. $N^{(k,h)}_{j_1,\ldots,j_{\mathcal{N}}}$ denotes the genus-h $\mathcal{N}$-point fusion multiplicity.

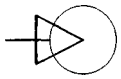
A simple extension of (19) is the following genus-h $\mathcal{N}$-point diagram (in this example $\mathcal{N}$ is assumed even, while h is arbitrary):



(46)

The dual trivalent fusion graph is represented by thinner lines and loops. h is the number of such loops or handles. The role of the two zeros in (46) will be discussed below. The number of internal isospins or gluings is $\mathcal{N}+3(h-1)$, while the number of vertices or triangles is $\mathcal{N}+2(h-1)$.

First we consider the tadpole diagram



(47)

In terms of osp(1|2) BZ triangles the basis diagram associated to it is

$$\begin{matrix} 0 \\ 0 \end{matrix} \quad 2. \tag{48}$$

We call (48) a *loop-gluing* diagram. Since we are gluing over even integers, the initial tadpole diagram will depend on $2j$ being even (indicated by $p=0$) or odd (indicated by $p=1$). With l being the coefficient to (48), the polytope is defined by

$$0 \leqslant 2j,\ 2j,\ p+2l,\ 2k-4j-p-2l+1. \tag{49}$$

Thus, the genus-one one-point fusion multiplicity becomes

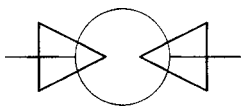
$$N_j^{(k,1)} = \sum_{l=[-p+1/2]}^{[2k-4j-p+1/2]} 1 = k-2j+1 \tag{50}$$

irrespective of $2j$ being even or odd. That independence is novel compared to the similar situation for su(2).[9]

The basis loop-gluing super-diagram associated to (47) is

$$\begin{matrix} 0 & & \\ & 0 & 1. \\ 0 & & \end{matrix} \tag{51}$$

Let us also describe the basis loop-gluing diagrams associated to the genus-one two-point fusion



(52)

In terms of osp(1|2) BZ diagrams there are two basis loop-gluings associated to this fusion. They may be represented by the diagrams

$$\mathcal{L} = \begin{matrix} \overline{1} & & \overline{1} \\ & 1 \quad 1 & \\ 1 & & 1 \end{matrix}, \qquad \mathcal{L}' = \begin{matrix} 1 & & 1 \\ & \overline{1} \quad 1 \quad 1 & \\ & & \overline{1} \end{matrix}. \tag{53}$$

They differ significantly from the su(2) basis loop-gluing diagrams,[9] as they do not constitute a basis of su(2) loop-gluing diagrams. Similarly, the two loop-gluing super-diagrams are

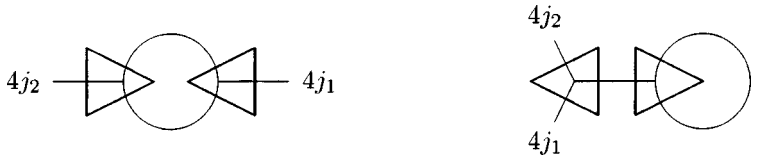
$$\mathcal{L} = \begin{array}{ccccccc} \overline{1} & & & & & \overline{1} \\ & 1 & 0 & & 0 & 1 & \\ 0 & & & & & 0 \end{array}, \qquad \mathcal{L}' = \begin{array}{ccccccc} 0 & & & & & 0 \\ & 1 & 0 & & 0 & 1 & \\ \overline{1} & & & & & \overline{1} \end{array}. \tag{54}$$

It is noted that the choice of loop-gluing basis (53) is not a convenient one. Had we only been interested in the polytope characterization of the fusion multiplicity and not an explicit measure of its discretized volume, this symmetric basis would suffice. But in order to be able to choose an appropriate order of summation (i.e., avoid discussing intersection of faces), we can not allow both diagrams to affect all the entries of the two triangles. A good but less symmetric basis is

$$\mathcal{L} = \begin{array}{ccccc} \overline{1} & & & & \overline{1} \\ & 1 & 1 & & \\ 1 & & & & 1 \end{array}, \qquad \mathcal{L}^+ = \begin{array}{ccccc} 0 & & & & 0 \\ & 2 & 2 & & \\ 0 & & & & 0 \end{array}, \tag{55}$$

where $\mathcal{L}^+ = \mathcal{L} + \mathcal{L}'$.

As a nontrivial check of our procedure, we now consider the genus-one two-point fusion in detail using the two different channels



(56)

Consistency requires the associated fusion multiplicities to coincide. To ensure that we are gluing over even integers, an initial diagram associated to the channel on the left depends on $2j_1+2j_2$ being even (indicated by $p=0$) or odd (indicated by $p=1$). Using the loop-gluing diagrams (55), and writing the inequalities associated to the rightmost triangle first, we find the polytope defined by

$$\begin{aligned} &0 \leqslant 2j_1-l,\ 2j_1+l,\ 2j_2+l+2l^++p,\ 2k-4j_1-2j_2-l-2l^+-p+1, \\ &0 \leqslant 2j_2-l,\ \ 2j_2+l,\ \ 2j_1+l+2l^++p,\ \ 2k-2j_1-4j_2-l-2l^+-p+1. \end{aligned} \tag{57}$$

It follows that the genus-one two-point fusion multiplicity is in fact independent of p, and is given by

$$N^{(k,1)}_{j_1,j_2} = (k-2\max\{j_1,\ j_2\}+1)(4\min\{j_1,\ j_2\}+1). \tag{58}$$

It is straightforward to choose an initial diagram associated to the channel on the right (56) that is independent of p. Using the gluing diagram (20) and the loop-gluing diagram (48), we are led to consider the polytope defined by

$$\begin{aligned} &0 \leqslant 2l+g,\ \ -g,\ \ -g,\ \ 2k-2l+g+1, \\ &0 \leqslant 2j_1+2j_2+g,\ \ 2j_1-2j_2-g,\ \ -2j_1+2j_2-g,\ \ 2k-2j_1-2j_2+g+1. \end{aligned} \tag{59}$$

Its discretized volume is seen to be (58), as desired. This result resembles the similar one for su(2),[9] but differs by involving the two *different* factors 2 and 4.

Note that (58) reduces correctly to (50) for $\min\{j_1, j_2\}=0$. In fact, it is a general feature of fusion that the $\mathcal{N}$-point fusion multiplicity $N^{(k,h)}_{j_1,\ldots,j_{\mathcal{N}}}$ is equal to the $(\mathcal{N}+1)$-point fusion multiplicity $N^{(k,h)}_{j_1,\ldots,j_{\mathcal{N}},0}$ (it is further recalled that a fusion multiplicity is symmetric under permutations

of its lower indices). That is not an obvious property of our construction, but will be used below. There we shall restrict to $\mathcal{N}\geqslant 3$ which accordingly is not a real restriction. The rationale for doing it, though, is that it allows us to make a universal choice of initial diagram associated to the fusion (46). On the other hand, in the case of zero-, one- or two-point fusion it results in unnecessarily complicated polytopes and multiple sums. For the benefit of the presentation here, we are not including other specific results than (50) and (58) for such lower-point fusions. However, they are easily obtained following our general procedure.

A. General result

It is now straightforward to write down the inequalities defining the convex polytope associated to (46). Here we focus on the osp(1|2) BZ triangle approach using (20) and (55), in particular. Our choice of initial diagram is indicated in (46) by the two zeros: all entries of the higher-genus part to the right of them are zero, while the $\mathcal{N}$-point part follows the pattern of the initial diagram (22) (assuming $\mathcal{N}\geqslant 3$, see the comments above). Enumerating the gluings from right to left (and $\mathcal{L}^+$ before $\mathcal{L}$), the integer coefficients in the linear combinations are $-g_1,\ldots,-g_h,g_{h+1},\ldots,g_{\mathcal{N}+h-2}$ (the sign convention is merely for convenience), and $l_1^+,l_1,\ldots,l_{h-1}^+,l_{h-1}$, while l is associated to the tadpole at the extreme right. Listing the inequalities associated to the triangles from right to left, we have the following convex polytope (assuming $h\geqslant 1$):

$$
\begin{gathered}
0\leqslant g_1,\ g_1,\ 2l-g_1,\ 2k-g_1-2l+1,\\
0\leqslant g_1-l_1,\ g_1+l_1,\ -g_1+2l_1^++l_1,\ 2k-g_1-2l_1^+-l_1+1,\\
0\leqslant g_2-l_1,\ g_2+l_1,\ -g_2+2l_1^++l_1,\ 2k-g_2-2l_1^+-l_1+1,\\
\vdots\\
0\leqslant g_{h-1}-l_{h-1},\ g_{h-1}+l_{h-1},\ -g_{h-1}+2l_{h-1}^++l_{h-1},\ 2k-g_{h-1}-2l_{h-1}^+-l_{h-1}+1,\\
0\leqslant g_h-l_{h-1},\ g_h+l_{h-1},\ -g_h+2l_{h-1}^++l_{h-1},\ 2k-g_h-2l_{h-1}^+-l_{h-1}+1,\\
0\leqslant g_{h+1}+g_h,\ -g_{h+1}+g_h,\ 4j_1-g_{h+1}-g_h,\ 2k-4j_1+g_{h+1}-g_h+1,\\
0\leqslant g_{h+2}-g_{h+1},\ 4j_1-g_{h+2}-g_{h+1},\ 4j_2-g_{h+2}+g_{h+1},2k-4(j_1+j_2)+g_{h+2}+g_{h+1}+1,\\
\vdots\\
0\leqslant g_{\mathcal{N}+h-2}-g_{\mathcal{N}+h-3},\ 4(j_1+\ldots+j_{\mathcal{N}-3})-g_{\mathcal{N}+h-2}-g_{\mathcal{N}+h-3},\ 4j_{\mathcal{N}-2}-g_{\mathcal{N}+h-2}\\
+g_{\mathcal{N}+h-3},\ 2k-4(j_1+\ldots+j_{\mathcal{N}-2})+g_{\mathcal{N}+h-2}+g_{\mathcal{N}+h-3}+1,\\
0\leqslant S-4j_{\mathcal{N}-1}-g_{\mathcal{N}+h-2},\ S-4j_{\mathcal{N}}-g_{\mathcal{N}+h-2},\ -S+4(j_{\mathcal{N}-1}+j_{\mathcal{N}})\\
+g_{\mathcal{N}+h-2},\ 2k-S+g_{\mathcal{N}+h-2}+1.
\end{gathered}
\tag{60}
$$

By construction, its discretized volume is the fusion multiplicity $N_{j_1,\ldots,j_{\mathcal{N}}}^{(k,h)}$, which then provides the first characterization of general osp(1|2) fusion multiplicities. The volume may be measured explicitly expressing $N_{j_1,\ldots,j_{\mathcal{N}}}^{(k,h)}$ as a multiple sum:

$$
N_{j_1,\ldots,j_{\mathcal{N}}}^{(k,h)}=\sum_{g_{\mathcal{N}+h-2}}\ldots\sum_{g_h}\left(\sum_{l_{h-1}}\sum_{l_{h-1}^+}\sum_{g_{h-1}}\right)\ldots\left(\sum_{l_1}\sum_{l_1^+}\sum_{g_1}\right)\sum_{l}1\ . \tag{61}
$$

The integer summation variables are bounded according to

$$\left[\frac{g_1+1}{2}\right]\leqslant l\leqslant\left[\frac{2k-g_1+1}{2}\right],$$

$$|l_1|\leqslant g_1\leqslant\min\{2l_1^+ + l_1,\ 2k-2l_1^+ - l_1+1\},$$

$$\left[\frac{g_2-l_1+1}{2}\right]\leqslant l_1^+\leqslant\left[\frac{2k-g_2-l_1+1}{2}\right],$$

$$-g_2\leqslant l_1\leqslant g_2,$$

$$\vdots$$

$$|l_{h-1}|\leqslant g_{h-1}\leqslant\min\{2l_{h-1}^+ + l_{h-1},\quad 2k-2l_{h-1}^+ - l_{h-1}+1\},$$

$$\left[\frac{g_h-l_{h-1}+1}{2}\right]\leqslant l_{h-1}^+\leqslant\left[\frac{2k-g_h-l_{h-1}+1}{2}\right], \tag{62}$$

$$-g_h\leqslant l_{h-1}\leqslant g_h,$$

$$|g_{h+1}|\leqslant g_h\leqslant\min\{4j_1-g_{h+1},\ 2k-4j_1+g_{h+1}+1\}$$

$$\max\{-4j_2+g_{h+2},\quad -2k+4(j_1+j_2)-g_{h+2}-1\}\leqslant g_{h+1}\leqslant\min\{g_{h+2},\ 4j_1-g_{h+2}\}$$

$$\vdots$$

$$\max\{-4j_{\mathcal{N}-2}+g_{\mathcal{N}+h-2},\quad -2k+4(j_1+\cdots+j_{\mathcal{N}-2})-g_{\mathcal{N}+h-2}-1\}$$
$$\leqslant g_{\mathcal{N}+h-3}\leqslant\min\{g_{\mathcal{N}+h-2},\quad 4(j_1+\cdots+j_{\mathcal{N}-3})-g_{\mathcal{N}+h-2}\}$$

$$\max\{S-4(j_{\mathcal{N}-1}+j_{\mathcal{N}}),\ -2k+S-1\}\leqslant g_{\mathcal{N}+h-2}\leqslant\min\{S-4j_{\mathcal{N}-1},\ S-4j_{\mathcal{N}}\}.$$

This constitutes the first explicit result for the general genus-h $\mathcal{N}$-point fusion multiplicities.

An advantage of using super-triangles instead of the osp(1|2) BZ triangles employed above, is that the variables v, g and l all appear with unit coefficients in the polytope-defining inequalities similar to (60). However, it is not straightforward to measure the discretized volume of that polytope. The reason is similar to the one excluding the basis (53) as a "good basis."

V. CONCLUSION

We have considered higher-point couplings of finite-dimensional irreducible representations of osp(1|2). The associated tensor product multiplicities were characterized as discretized volumes of certain convex polytopes, and written explicitly as multiple sums. The results are general.

We have also considered affine osp(1|2) fusion. By extending the results on tensor products, we characterized a general genus-h $\mathcal{N}$-point fusion multiplicity as a discretized volume of a certain convex polytope, and wrote down an explicit multiple sum measuring that volume. This result is also general.

It has been demonstrated, though not emphasized explicitly, that a fusion polytope may be embedded in the associated tensor product polytope. The reason is that the set of defining inequalities of a fusion polytope is obtained by supplementing the set of defining inequalities of the associated tensor product polytope by level-dependent inequalities. That offers a geometric interpretation of affine fusion being a truncated tensor product.

In the derivation of our results we have described three-point couplings by triangular arrangements of non-negative integers similar to the su(2) BZ triangles. We introduced two types. We based most of our results on a direct adaption of the ordinary su(2) BZ triangle. However, we also

introduced a super-triangle and discussed some of its alternative features. Here we will indicate how it appears natural from the point of view of correlators in osp(1|2) conformal field theory. Three-point functions in conformal field theory with affine Lie group symmetry have been considered in Ref. 18. Their level-dependence was subsequently addressed in Ref. 19. The idea is to associate so-called elementary polynomials to the elementary couplings appearing in an expansion of a three-point coupling. The three-point functions are then constructed as (linear combinations of) products of those polynomials. The algebraic relations (syzygies) among the elementary couplings complicate the construction. In some cases they may be taken into account at the level of BZ triangles by forbidding certain configurations. In terms of polynomials that amounts to forbidding certain products, as there is a correspondence between BZ triangles and polynomials. As we will show elsewhere,[7] the situation for osp(1|2) is most easily handled using our super-triangles. The constraint on the super-entry ϵ (14) is neatly encoded by associating a Grassmann odd polynomial to a super-triangle with $\epsilon=1$. This also introduces a natural way of implementing the osp(1|2) syzygy.[20,21]

ACKNOWLEDGMENTS

The author thanks Chris Cummins and Pierre Mathieu for helpful comments.

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On the asymptotic distribution of the commutator and anticommutator of random matrices

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(Received 22 May 2001; accepted 15 November 2002)

We study in the limit of infinite matrix order the normalized eigenvalue counting measures of the commutator and anticommutator of two Hermitian (or real symmetric) matrices rotated independently one respect to another by the random unitary (or orthogonal) Haar distributed matrix. We establish the convergence with probability 1 to a limiting nonrandom measure. We obtain and analyze the functional equations for the Stieltjes transforms of the limiting measures. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1557329]

I. INTRODUCTION

We consider two ensembles: commutator and anticommutator of n-dimensional Hermitian (or real symmetric) random matrices H_n of the form

$$H_n = i[H_{1,n}, H_{2,n}] \equiv i(H_{1,n}H_{2,n} - H_{2,n}H_{1,n}) \tag{1.1}$$

and of the form

$$\tilde{H}_n = H_{1,n}H_{2,n} + H_{2,n}H_{1,n}, \tag{1.2}$$

where

$$H_{1,n} = V_n^* A_n V_n, \quad H_{2,n} = U_n^* B_n U_n.$$

We assume that A_n and B_n are nonrandom Hermitian (or real symmetric for the second ensemble) matrices, and V_n and U_n are unitary (or orthogonal) independent random matrices uniformly distributed over the unitary group $\mathrm{U}(n)$ [or over the orthogonal group $\mathrm{O}(n)$] with respect to the Haar measure. For the sake of definiteness we will restrict ourself to the case of Hermitian matrices and the group $\mathrm{U}(n)$, respectively. The results for symmetric matrices and for the group $\mathrm{O}(n)$ have the same form, although their proof is more difficult.

We are interested in the asymptotic behavior as $n \to \infty$ of the *normalized eigenvalue counting measure* (NCM) N_n of the ensemble (1.1), defined for any Borel set $\Delta \subset \mathbf{R}$ by the formula

$$N_n(\Delta) = \frac{\#\{\lambda_i \in \Delta\}}{n}, \tag{1.3}$$

where λ_i, $i = 1, \ldots, n$ are the eigenvalues of H_n. The NCM $\tilde{N}_n$ of the ensemble (1.2) is defined analogously.

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The ensemble (1.1) was studied recently in Ref. 3 in the context of free (noncommutative) probability. In particular, it follows from results of Ref. 5 that if the norms of matrices A_n and B_n are uniformly in n bounded, i.e., their NCM $N_{1,n}$ and $N_{2,n}$ have uniformly in n compact supports, and if these measures have weak limits as $n\to\infty$,

$$N_{1,n}\to N_1, \quad N_{2,n}\to N_2, \tag{1.4}$$

then the NCM (1.3) of random matrix (1.1) converges weakly with probability 1 to a nonrandom measure N. Besides, if

$$f(z)=\int_{-\infty}^{\infty}\frac{N(\mathrm{d}\lambda)}{\lambda-z}, \quad \mathrm{Im}\, z\neq 0, \tag{1.5}$$

is the *Stieltjes transform* of this limiting measure and

$$f_r(z)=\int_{-\infty}^{\infty}\frac{N_r(\mathrm{d}\lambda)}{\lambda-z}, \quad r=1,2, \tag{1.6}$$

are the Stieltjes transforms of N_r, $r=1,2$ of (1.4) having all moments finite and if

$$m_r^{(2)}-m_r^2>0, \;\; m_r^{(2)}=\int_{-\infty}^{+\infty}\lambda^2 N_r(\mathrm{d}\lambda), \quad m_r=\int_{-\infty}^{+\infty}\lambda N_r(\mathrm{d}\lambda), \;\; r=1,2, \tag{1.7}$$

then according to Ref. 3 $f(z)$ satisfies the following relation (this relation is understood in Ref. 3 as an equality of formal power series):

$$-(1+z^{-1}f(z^{-1}))=\left(\frac{2}{w(1+w/2)(1+w)^2}\cdot[R_{E,1}]^{\langle -1\rangle}\left(\frac{w}{2}\right)\cdot[R_{E,2}]^{\langle -1\rangle}\left(\frac{w}{2}\right)\right)^{\langle -1\rangle}(z^2), \tag{1.8}$$

where "$h^{\langle -1\rangle}$" denotes the functional inverse and $R_{E,r}(w)$, $r=1,2$, denotes the even part of the corresponding modified R-transforms

$$R_{E,r}(w)=(wR_r(w)-wR_r(-w))/2, \;\; r=1,2. \tag{1.9}$$

Here $R_r(w)$, $r=1,2$, denote Voiculescu's R-transforms[9,10] of the measures N_r, $r=1,2$, of (1.4) defined by the relations

$$z=-\frac{1}{f_r(z)}+R_r(-f_r(z)), \;\; r=1,2, \tag{1.10}$$

where $f_r(z)$, $r=1,2$, are Stieltjes transforms of the measures N_r, $r=1,2$.

Here and below the convergence with probability 1 is understood as that in the natural probability space

$$\Omega=\prod_n \Omega_n, \tag{1.11}$$

where Ω_n is the probability space of matrices (1.1) that is the product of two copies of the group $\mathrm{U}(n)$ for U_n and V_n.

In this article we obtain the analogous results for ensembles (1.1) and (1.2) under weaker assumptions and by using a method that does not involve combinatorics. This is because we work with the Stieltjes transforms of measures (1.3) and (1.4) and derive directly the functional equations for their limits.

We list below the properties of the Stieltjes transform that we will need (see e.g., Ref. 1).

Proposition 1.1: Let m be a non-negative and normalized to unity measure and

$$s(z)=\int_{-\infty}^{+\infty}\frac{m(d\lambda)}{\lambda-z},\quad \mathrm{Im}\quad z\neq 0,$$

be the Stieltjes transform of m (here and below integrals without limits denote the integrals over the whole axis). Then

(i) $s(z)$ *is analytic in* $\mathbf{C}\backslash\mathbf{R}$ *and*

$$|s(z)|\leqslant|\mathrm{Im}\, z|^{-1}; \tag{1.12}$$

(ii)

$$\mathrm{Im}\, s(z)\mathrm{Im}\, z>0,\ \ \mathrm{Im}\, z\neq 0; \tag{1.13}$$

(iii)

$$\lim_{y\to\infty} y|s(iy)|=1; \tag{1.14}$$

(iv) for any continuous function φ *with a compact support we have the inversion (Frobenius-Perron) formula*

$$\int_{-\infty}^{+\infty}\phi(\lambda)m(d\lambda)=\lim_{\varepsilon\to 0}\frac{1}{\pi}\int_{-\infty}^{+\infty}\phi(\lambda)\,\mathrm{Im}\, s(\lambda+i\varepsilon). \tag{1.15}$$

(v) Conversely, any function verifying (1.12)–(1.14) is the Stieltjes transform of a non-negative and normalized to unity measure and this one-to-one correspondence between measures and their Stieltjes transforms is continuous if one will use the topology of weak convergence for measures and the topology of convergence on compact sets of $\mathbf{C}\backslash\mathbf{R}$ *for the Stieltjes transforms.*

II. MAIN RESULTS

We formulate now our main results. Since eigenvalues of a Hermitian matrix are unitary invariant we can replace matrices (1.1) and (1.2) by

$$H_n=i[A_n, U_n^* B_n U_n],\ \ \tilde{H}_n=A_n U_n^* B_n U_n+U_n^* B_n U_n A_n, \tag{2.1}$$

where A_n, B_n and U_n are the same as in (1.1) and (1.2). However, it is useful to keep in mind that the problem is symmetric in A_n and B_n. We prove the following theorems.

Theorem 2.1: *Let* H_n *be the random* $n\times n$ *matrix of the form (1.1). Assume that the normalized eigenvalue counting measures* $N_{r,n}, r=1,2$, *of matrices* A_n *and* B_n *converge weakly as* $n\to\infty$ *to the non-negative and normalized to 1 measures* N_r, $r=1,2$, *satisfying conditions (1.7) respectively and that*

$$\sup_n\int_{-\infty}^{+\infty}|\lambda|^6 N_{r,n}(d\lambda)\leqslant m_6<\infty,\ \ r=1,2.$$

Let also $f_r(z)$, $r=1,2$, *be the Stieltjes transforms of the measures* N_r, $r=1,2$.

Then the normalized eigenvalue counting measure N_n *of* H_n *converges with probability 1 to a nonrandom non-negative and normalized to 1 measure N whose Stieltjes transform (1.5) is a unique solution of the system of functional equations*

$$\Gamma_1(z)=f_2\left(\frac{\Delta_2(z)}{f(z)}-\frac{1-zf(z)}{2\Gamma_1(z)}\right),$$

$$-\Gamma_1(z)=f_2\left(\frac{\Delta_2(z)}{f(z)}+\frac{1-zf(z)}{2\Gamma_1(z)}\right),$$

$$f^2(z)\frac{1-z^2f^2(z)}{4}=-\Gamma_1^2(z)\Gamma_2^2(z), \tag{2.2}$$

$$\Gamma_2(z)=f_1\left(\frac{\Delta_1(z)}{f(z)}-\frac{1-zf(z)}{2\Gamma_2(z)}\right),$$

$$-\Gamma_2(z)=f_1\left(\frac{\Delta_1(z)}{f(z)}+\frac{1-zf(z)}{2\Gamma_2(z)}\right)$$

in the class of functions $f(z)$ *satisfying (1.13) and (1.14) and functions* $\Delta_r(z)$, $\Gamma_r(z)$, $r=1,2$, *analytic for* $\operatorname{Im} z\neq 0$ *and satisfying conditions*

$$z\Delta_r(z)=-m_r+O(|\operatorname{Im} z|^{-2}),\quad r=1,2,\quad |\operatorname{Re} z|\leqslant|\operatorname{Im} z|,\ z\to\infty, \tag{2.3}$$

$$z\Gamma_r(z)=\sqrt{m_r^{(2)}-m_r^2}+O(|\operatorname{Im} z|^{-1}),\quad r=1,2,\quad |\operatorname{Re} z|\leqslant|\operatorname{Im} z|,\ z\to\infty. \tag{2.4}$$

Theorem 2.2: *Let* $\tilde{H}_n$ *be the random* $n\times n$ *matrix of the form (1.2) and let the conditions of Theorem 1 be satisfied.*

Then the normalized eigenvalue counting measure $\tilde{N}_n$ *of* $\tilde{H}_n$ *converges with probability 1 to a nonrandom non-negative and normalized to 1 measure* $\tilde{N}$ *whose Stieltjes transform (1.5) is a unique solution of the system of functional equations*

$$\Omega_1(z)+\Delta_1(z)=f_2\left(\frac{\Delta_2(z)}{f(z)}\frac{\Omega_1(z)}{\Omega_1(z)+\Delta_1(z)}-\frac{1-zf(z)}{2(\Omega_1(z)+\Delta_1(z))}\right),$$

$$-(\Omega_1(z)-\Delta_1(z))=f_2\left(\frac{\Delta_2(z)}{f(z)}\frac{\Omega_1(z)}{\Omega_1(z)-\Delta_1(z)}+\frac{1-zf(z)}{2(\Omega_1(z)-\Delta_1(z))}\right),$$

$$f^2(z)\left(\frac{1-z^2f^2(z)}{4}+z\Delta_1(z)\Delta_2(z)\right)=-(\Omega_1^2(z)-\Delta_1^2(z))(\Omega_2^2(z)-\Delta_2^2(z))+\Delta_1^2(z)\Delta_2^2(z), \tag{2.5}$$

$$\Omega_2(z)+\Delta_2(z)=f_1\left(\frac{\Delta_1(z)}{f(z)}\frac{\Omega_2(z)}{\Omega_2(z)+\Delta_2(z)}-\frac{1-zf(z)}{2(\Omega_2(z)+\Delta_2(z))}\right),$$

$$-(\Omega_2(z)-\Delta_2(z))=f_1\left(\frac{\Delta_1(z)}{f(z)}\frac{\Omega_2(z)}{\Omega_2(z)-\Delta_2(z)}+\frac{1-zf(z)}{2(\Omega_2(z)-\Delta_2(z))}\right)$$

in the class of functions $f(z)$ *satisfying (1.13) and (1.14) and functions* $\Delta_r(z)$, $\Omega_r(z)$, $r=1,2$, *analytic for* $\operatorname{Im} z\neq 0$ *and satisfying conditions*

$$z\Delta_r(z)=-m_r+O(|\operatorname{Im} z|^{-1}),\quad r=1,2,\quad |\operatorname{Re} z|\leqslant|\operatorname{Im} z|,\ z\to\infty, \tag{2.6}$$

$$z\Omega_r(z)=\sqrt{m_r^{(2)}}+O(|\operatorname{Im} z|^{-1}),\quad r=1,2,\quad |\operatorname{Re} z|\leqslant|\operatorname{Im} z|,\ z\to\infty. \tag{2.7}$$

Remark 2.1: Its easy to see that in the case of symmetric limiting measures N_1 *and* N_2 *one can reduce the systems (2.2) and (2.5) setting* $\Delta_r(z)\equiv 0$, $r=1,2$, *to the following system:*

$$\Gamma_1(z)=f_2\left(-\frac{1-zf(z)}{2\Gamma_1(z)}\right),$$

$$f^2(z)\frac{1-z^2f^2(z)}{4}=-\Gamma_1^2(z)\Gamma_2^2(z), \tag{2.8}$$

$$\Gamma_2(z)=f_1\left(-\frac{1-zf(z)}{2\Gamma_2(z)}\right).$$

Moreover, since in this case $m_r=0$, $r=1,2$, *the functions* $\Gamma_r(z)$ *and* $\Omega_r(z)$, $r=1,2$, *will have the same asymptotics. Hence, the limiting NCM* N *of ensemble (1.1) will be equal to the limiting NCM* $\widetilde{N}$ *of ensemble (1.2).*

Remark 2.2: The system (2.2) and relation (1.8) are equivalent.

Indeed, suppose that the limiting measures N_r, $r=1,2$, are symmetric and denote by $N_r^{(2)}$, $r=1,2$, the probability measures uniquely defined by its Stieltjes transforms:

$$f_r^{(2)}(z)=\int_0^{+\infty}\frac{N_r^{(2)}(d\lambda)}{\lambda-z}=\int_{-\infty}^{+\infty}\frac{N_r(d\lambda)}{\lambda^2-z},\quad r=1,2. \tag{2.9}$$

In this case, according to Remark 2.1 the system (2.2) can be reduced to the system (2.8). The measures $N_r^{(2)}$, $r=1,2$, will be supported on the non-negative real semi-axis and its first moments will be equal to the second moments of N_r, $r=1,2$,

$$\int_0^{+\infty}\lambda N_r^{(2)}(d\lambda)=m_r^{(2)},\quad r=1,2. \tag{2.10}$$

Consider the functions

$$\varphi_r^{(2)}(z)=-(1+z^{-1}f_r^{(2)}(z^{-1})),\quad r=1,2.$$

Since $(\varphi_r^{(2)})'(0)=m_r^{(2)}\neq 0$, $r=1,2$, then, according to the local inversion theorem, the functions $\varphi_r^{(2)}(z)$, $r=1,2$, also have the unique functional inverses $\chi_r^{(2)}(\varphi)$, $r=1,2$, defined and analytic in a neighborhood of zero and assuming its values in a neighborhood of zero. Denote

$$S_r^{(2)}(\varphi)=\chi_r^{(2)}(\varphi)\varphi^{-1}(1+\varphi),\quad r=1,2,$$

and following Voiculescu[8,10,2] call $S_r^{(2)}(\varphi)$, $r=1,2$, the S-transform of the probability measures $N_r^{(2)}$, $r=1,2$, on the real non-negative semi-axis. Besides, using the relation (2.9) and the symmetry of measures N_r, $r=1,2$, we obtain

$$\varphi_r^{(2)}(z^2)=\varphi_r(z),\varphi_r(z)=-(1+z^{-1}f_r(z^{-1})),\quad r=1,2.$$

Using this relation we rewrite the system (2.8) in the following form:

$$\begin{aligned}&\frac{\psi(z)}{2}=\varphi_r^{(2)}\left(\left(\frac{\Gamma_{3-r}(z)}{1+\psi(z)/2}\right)^2\right),\quad r=1,2,\\&\frac{(1+\psi(z))^2}{z^2}\,\frac{\psi(z)}{2}\left(1+\frac{\psi(z)}{2}\right)=\Gamma_1^2(z)\Gamma_2^2(z),\end{aligned} \tag{2.11}$$

where

$$\psi(z)=-(1+zf(z))\equiv\varphi(z^{-1})=\varphi^{(2)}(z^{-2}),\quad \varphi^{(2)}(z)=-(1+z^{-1}f^{(2)}(z^{-1})),$$

$$f^{(2)}(z)=\int_{-\infty}^{+\infty}\frac{N(d\lambda)}{\lambda^2-z}.$$

By using the S-transforms $S_r^{(2)}(\varphi)$, $r=1,2$, we can rewrite two first equations of the system (2.11) in the form

$$\Gamma_{3-r}^2(z)=\frac{\psi(z)}{2}\left(1+\frac{\psi(z)}{2}\right)S_r^{(2)}\left(\frac{\psi(z)}{2}\right),\quad r=1,2.$$

Using this relations and the last equation of system (2.11) we obtain

$$S^{(2)}(\psi)=\frac{1}{2}\,\frac{1+\psi/2}{1+\psi}S_1^{(2)}\left(\frac{\psi}{2}\right)S_2^{(2)}\left(\frac{\psi}{2}\right), \tag{2.12}$$

where $S^{(2)}(\psi)$ denotes S-transform of probability measure $N^{(2)}$ defined by its Stieltjes transform $f^{(2)}(z)$. This measure will be also supported on the non-negative real semi-axis and will have non zero first moment $2m_1^{(2)}m_2^{(2)}$. The relation (2.12) was obtained by Nica and Speicher in Ref. 3 in the case of measures N_r, $r-1,2$, having all moments finite and proved to be equivalent to the relation (1.8).

As for the general case, we can apply the R-transforms (1.10) of the measures N_r, $r=1,2$, to the two first and two last equations of the system (2.2) and obtain the following relations.

$$\frac{1}{\Gamma_{3-r}(z)}+\hat{R}_r(\Gamma_{3-r}(z))=\frac{1-zf(z)}{2\Gamma_{3-r}(z)},\quad r=1,2, \tag{2.13}$$

where

$$\hat{R}_r(w)=\frac{R_r(w)-R_r(-w)}{2},\quad r=1,2. \tag{2.14}$$

As was shown in Ref. 3 there exist the probability measures $\hat{N}_r$, $r=1,2$, whose R-transforms are $\hat{R}_r(w)$, $r=1,2$. According to (2.14) these measures are symmetric and their second moments are equal to $m_r^{(2)}-m_r$, $r=1,2$. Thus, applying to the relation (2.13) the Stieltjes transforms $\hat{f}_r(z)$ of measures $\hat{N}_r$, $r=1,2$, we obtain the first and last equations of the system (2.8). As was shown above, this system will be equivalent to the relation (1.8), where $R_{E,r}(w)=w\hat{R}_r(w)$, $r=1,2$.

III. PROOF OF THE THEOREMS

We use the technique introduced in Ref. 4 and developed in Refs. 7 and 6. Let us recall its basic means. First, it is a resolvent identity

$$G_2(z)=G_1(z)-G_1(z)(M_2-M_1)G_2(z),\mathrm{Im}\,z\neq 0, \tag{3.1}$$

valid for any Hermitian M_1 and M_2 and their resolvents $G_1(z)$ and $G_2(z)$. Our main tool as is follows.

Proposition 3.1:[4] *Let $\Phi:\mathbf{M}_n\to\mathbf{C}$ be a continuously differentiable function. Then the following relation hold for any $M\in\mathbf{M}_n$ and any Hermitian element $X\in\mathbf{M}_n$:*

$$\int_{\mathbf{U}(n)}\Phi'(U^*MU)\cdot[X,U^*MU]\mathrm{d}U=0, \tag{3.2}$$

where Φ' is derivative of Φ, $[M_1,M_2]=M_1M_2-M_1M_2$ and $\int_{\mathbf{U}(n)}\cdots\mathrm{d}U$ denotes the integration over $U(n)$ with respect to the normalized Haar measure.

Proof: To prove (3.2) we use the right shift invariance of the Haar measure: $\mathrm{d}U=\mathrm{d}(UU_0)$, $\forall U_0\in U(n)$ according to which the integral

$$\int_{U(n)} \Phi(e^{-i\varepsilon X} U^* M U e^{i\varepsilon X}) \mathrm{d}U$$

is independent of ε for any Hermitian $X \in \mathbf{M}_n$. Thus its derivative with respect to ε at $\varepsilon = 0$ is zero. This derivative is the lhs of (3.2). ■

Remark 3.1: Due to the linearity on X the relation (3.2) is true for arbitrary X, not only for Hermitian ones.

Proposition 3.2: System (2.2) has not two different solutions in the class of functions $f(z)$, $\Delta_r(z)$, $\Gamma_r(z)$, $r=1,2$, *analytic for* $\operatorname{Im} z \neq 0$ *and satisfying conditions (1.13), (1.14) and (2.3), (2.4).*

Proof: Assume that there exist two solutions $(f', \Delta_r', \Gamma_r', r=1,2)$ and $(f'', \Delta_r'', \Gamma_r'', r=1,2)$ of the system. Denote $\delta f = f' - f''$, $\delta\Delta_r = \Delta_r' - \Delta_r''$, $\delta\Gamma_r = \Gamma_r' - \Gamma_r''$, $r=1,2$. Then, by using (2.2) and the following relation,

$$f_r(z) = -(z-m_r)^{-1} + z^{-1}(z-m_r)^{-1} \int_{-\infty}^{+\infty} \frac{\lambda(\lambda - m_r) N_r(\mathrm{d}\lambda)}{\lambda - z}, \quad r=1,2,$$

we obtain the linear system for $\delta\Gamma_r$, $\delta\Delta_r$, $r=1,2$, and δf:

$$\begin{aligned}
&a_1(z)\,\delta\Delta_2 + b_1(z)\,\delta\Gamma_1 + c_1(z)\,\delta f = 0,\\
&a_2(z)\,\delta\Delta_2 + b_2(z)\,\delta\Gamma_1 + c_2(z)\,\delta f = 0,\\
&b_3(z)\,\delta\Gamma_1 + c_3(z)\,\delta f + d_3(z)\,\delta\Gamma_2 = 0,\\
&c_4(z)\,\delta f + d_1(z))\,\delta\Gamma_2 + e_1(z)\,\delta\Delta_1 = 0,\\
&c_5(z)\,\delta f + d_2(z))\,\delta\Gamma_2 + e_2(z)\,\delta\Delta_1 = 0,
\end{aligned} \tag{3.3}$$

where

$$a_1 = \frac{\Gamma'}{f'} - \left(J_2(x_-', x_-'') - \frac{I_2(x_-')}{x_-'} \right) \frac{1}{x_-'' f'}, \qquad b_1 = s_2'' - m_2 - \left(J_2(x_-', x_-'') - \frac{I_2(x_-')}{x_-'} \right) \frac{t_1''}{x_-'' \Gamma_1'},$$

$$a_2 = -\frac{\Gamma'}{f'} - \left(J_2(x_+', x_+'') - \frac{I_2(x_+')}{x_+'} \right) \frac{1}{x_+'' f'}, \qquad b_2 = -(s_2'' - m_2) + \left(J_2(x_+', x_+'') - \frac{I_2(x_+')}{x_+'} \right) \frac{t_1''}{x_+'' \Gamma_1'},$$

$$c_1 = \frac{z}{2} - \frac{\Gamma'}{f'} s_2'' + \left(J_2(x_-', x_-'') - \frac{I_2(x_-')}{x_-'} \right) \frac{1}{x_-''} \left(\frac{s_2''}{f'} + \frac{z}{2\Gamma_1'} \right),$$

$$c_2 = \frac{z}{2} + \frac{\Gamma'}{f'} s_2'' + \left(J_2(x_+', x_+'') - \frac{I_2(x_+')}{x_+'} \right) \frac{1}{x_+''} \left(\frac{s_2''}{f'} - \frac{z}{2\Gamma_1'} \right),$$

$$b_3 = z^3(\Gamma_1' + \Gamma_1'')(\Gamma_2')^2, \quad c_3 = z^3(f' + f'') \frac{1 - z((f')^2 + (f'')^2)}{4}, \quad d_3 = z^3(\Gamma_2' + \Gamma_2'')(\Gamma_1'')^2,$$

$$x_\pm^{\prime,\prime\prime} = s_2^{\prime,\prime\prime} \pm t_1^{\prime,\prime\prime}, \quad s_2^{\prime,\prime\prime} = \frac{\Delta_2^{\prime,\prime\prime}}{f^{\prime,\prime\prime}}, t_1^{\prime,\prime\prime} = \frac{1 + z f^{\prime,\prime\prime}}{2\Gamma_1^{\prime,\prime\prime}}, \tag{3.4}$$

$$I_2(z) = \int_{-\infty}^{+\infty} \frac{\lambda(\lambda - m_2) N_2(\mathrm{d}\lambda)}{\lambda - z}, \quad J_2(z', z'') = \int_{-\infty}^{+\infty} \frac{\lambda(\lambda - m_2) N_2(\mathrm{d}\lambda)}{(\lambda - z')(\lambda - z'')}, \tag{3.5}$$

and d_r, e_r, c_{3+r}, $r=1,2$, can be obtained from a_r, b_r, c_r, $r=1,2$, by replacing N_2, $\Delta_2^{\prime,\prime\prime}$ and $\Gamma_1^{\prime,\prime\prime}$ by N_1, $\Delta_1^{\prime,\prime\prime}$ and $\Gamma_2^{\prime,\prime\prime}$ in above formulas.

For any $y_0>0$ consider the domain

$$E(y_0)=\{z\in\mathbf{C}:|\mathrm{Im}\,z|\geqslant y_0,|\mathrm{Re}\,z|\leqslant|\mathrm{Im}\,z|\}. \tag{3.6}$$

Due to the conditions (2.4) and the third equation of the system (2.2) we have for $z\in E(y_0)$

$$1+zf^{\prime,\prime\prime}(z)=-2z^{-2}((m_1^{(2)}-m_1^2)(m_2^{(2)}-m_2^2)+O(|\mathrm{Im}\,z|^{-1})),\quad z\to\infty. \tag{3.7}$$

Besides, if

$$k(z)=\int_{-\infty}^{+\infty}\frac{\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)}{\lambda-z},\quad l(z',z'')=\int_{-\infty}^{+\infty}\frac{\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)}{(\lambda-z')(\lambda-z'')},$$

where

$$\mu_1=\int_{-\infty}^{+\infty}\lambda\mu(\mathrm{d}\lambda)$$

and μ is non-negative and normalized to the 1 measure having finite sixth moment, then we have for $z,z',z''\in E(y_0)$,

$$\left|zk(z)+\int_{-\infty}^{+\infty}\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)\right|=\left|\int_{-\infty}^{+\infty}\frac{\lambda^2(\lambda-\mu_1)\mu(\mathrm{d}\lambda)}{\lambda-z}\right|\leqslant 6y_0^{-1}\int_{-\infty}^{+\infty}|\lambda|^3\mu(\mathrm{d}\lambda),$$

$$\left|z'z''l(z',z'')-\int_{-\infty}^{+\infty}\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)\right|=\left|\int_{-\infty}^{+\infty}\frac{\lambda^2(\lambda-\mu_1)(z'+z''-\lambda)\mu(\mathrm{d}\lambda)}{(\lambda-z')(\lambda-z'')}\right|$$

$$\leqslant 6y_0^{-1}\int_{-\infty}^{+\infty}|\lambda|^3\mu(\mathrm{d}\lambda),$$

i.e.,

$$zk(z)=-\int_{-\infty}^{+\infty}\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)+O(|\mathrm{Im}\,z|^{-1}),\quad z\to\infty,\ z\in E(y_0),$$

$$z'z''l(z',z'')=\int_{-\infty}^{+\infty}\lambda(\lambda-\mu_1)\mu(\mathrm{d}\lambda)+O(|\mathrm{Im}\,z|^{-1}),\quad z',z''\to\infty,\ z',z''\in E(y_0).$$

Thus, we obtain from the relation above, (3.4), (3.5), (3.7) and conditions (2.3), (2.4) that for $z\to\infty$, $z\in E(y_0)$

$$s_r^{\prime,\prime\prime}(z)=m_r+o(1),\ t_r^{\prime,\prime\prime}(z)=z(\sqrt{m_r^{(2)}-m_r^2}+o(1)),\ x_\pm^{\prime,\prime\prime}(z)=\pm z(\sqrt{m_1^{(2)}-m_1^2}+o(1)),\ r=1,2,$$

and, e.g.,

$$x_\pm'x_\pm''(z)J_2(x_\pm',x_\pm'')=m_1^{(2)}-m_1^2+o(1).$$

Hence we have

$$a_1(z)=-\alpha+o(1),\quad a_2(z)=\alpha+o(1),\quad b_{1,2}(z)=-2z^{-1}\beta^2\alpha+o(1),$$

$$c_r(z)=z/2+o(1),\quad r=1,2,4,5,\quad c_3(z)=z^2/2+o(1),\quad b_3(z)=2\beta^2\alpha+o(1),$$

$$d_3(z)=2\beta\alpha^2+o(1),\quad d_{1,2}(z)=-2z^{-1}\beta\alpha^2+o(1),\quad e_1(z)=-\beta+o(1),\quad e_2(z)=\beta+o(1),$$

where $\alpha=\sqrt{m_1^{(2)}-m_1^2}$, $\beta=\sqrt{m_2^{(2)}-m_2^2}$. Thus the determinant of system (3.3) is equal asymptotically to $2\alpha^4\beta^4>0$. We conclude that if y_0 in (3.6) is big enough, then system (3.3) has only trivial solution, thus solutions $(f',\ \Delta_r',\ \Gamma_r',\ r=1,2)$ and $(f'',\ \Delta_r'',\ \Gamma_r'',\ r=1,2)$ of the system (2.2) coincide. ■

Proof of Theorem 2.1: Because of unitary invariance of eigenvalues of Hermitian matrices we can assume without loss of generality that the unitary matrix V in (1.1) is set to unity, i.e., we can work with the random matrix (2.1). We will omit below the subindex n in all cases when it will not lead to confusion. C will denote the n-independent constant that may be different in different bounds.

Write the resolvent identity (3.1) for the pair $(H,0)$:

$$zG(z)+I=i(H_1H_2G(z)-H_2H_1G(z)). \tag{3.8}$$

By using Proposition 3.1 with the matrix element $\Phi(M)=(G(z))_{ab}=((i[H_1,M]-z)^{-1})_{ab}$ as $\Phi(M)$, we have

$$\langle (GH_1[X,H_2]G)_{ab}\rangle=\langle (G[X,H_2]H_1G)_{ab}\rangle. \tag{3.9}$$

Choosing the matrix X with only (a,b)-th nonzero entries, we obtain

$$2\langle (G(z)H_1)_{aa}(H_2G(z))_{bb}\rangle=\langle (G(z)H_1H_2)_{aa}G_{bb}(z)\rangle+\langle G_{aa}(z)(H_2H_1G(z))_{bb}\rangle. \tag{3.10}$$

Applying to this quantity $n^{-2}\Sigma_{a,b=1}^n$ and taking into account the identity (3.8) we obtain the relation

$$2\langle \delta_{1,n}(z)\,\delta_{2,n}(z)\rangle=\langle g_n(z)(k_{1,n}(z)+k_{2,n}(z))\rangle, \tag{3.11}$$

where

$$\delta_{r,n}(z)=n^{-1}\mathrm{Tr}G(z)H_r,\ \ r=1,2,\quad g(z)=n^{-1}\mathrm{Tr}G(z)=\int_{-\infty}^{+\infty}\frac{N_n(\mathrm{d}\lambda)}{\lambda-z},$$
$$k_{1,n}(z)=n^{-1}\mathrm{Tr}G(z)H_1H_2, k_{2,n}(z)=n^{-1}\mathrm{Tr}G(z)H_2H_1. \tag{3.12}$$

Introduce now the centralized quantities

$$g_n^o(z)=g_n(z)-f_n(z),\quad \delta_{r,n}^o(z)=\delta_{2,n}(z)-\Delta_{2,n}(z),\quad k_{r,n}^o(z)=k_{r,n}(z)-\langle k_{r,n}(z)\rangle,\ \ r=1,2, \tag{3.13}$$

where

$$f_n(z)=\langle g_n(z)\rangle,\quad \Delta_{2,n}(z)=\langle \delta_{2,n}(z)\rangle. \tag{3.14}$$

With these notations (3.11) becomes

$$2\Delta_{1,n}(z)\Delta_{2,n}(z)=f_n(z)(\langle k_{1,n}(z)\rangle+\langle k_{2,n}(z)\rangle)+r_n(z), \tag{3.15}$$

where

$$r_n(z)=-2\langle \delta_{1,n}^o(z)\,\delta_{2,n}(z)\rangle+\langle g_n^o(z)(k_{1,n}(z)+k_{2,n}(z))\rangle. \tag{3.16}$$

Besides, applying to the relation (3.8) the operation $n^{-1}\mathrm{Tr}$, we obtain

$$zf_n(z)+1=i\{\langle k_{1,n}(z)\rangle-\langle k_{2,n}(z)\rangle\}. \tag{3.17}$$

Using previous relation we obtain from (3.15) and (3.17)

$$\begin{aligned}\langle k_{1,n}(z)\rangle &= \frac{\Delta_{1,n}(z)\Delta_{2,n}(z)}{f_n(z)} - i\,\frac{1+zf_n(z)}{2} - \frac{r_n(z)}{2\,f_n(z)},\\ \langle k_{2,n}(z)\rangle &= \frac{\Delta_{1,n}(z)\Delta_{2,n}(z)}{f_n(z)} + i\,\frac{1+zf_n(z)}{2} - \frac{r_n(z)}{2\,f_n(z)}.\end{aligned} \tag{3.18}$$

On the other hand, choosing in (3.9) the matrix X with only (a,c)-th nonzero entries and applying $n^{-1}\Sigma_{a=1}^{n}$, we obtain the following matrix relation:

$$\langle\{\delta_{2,n}(z)A - k_{1,n}(z)I\}G(z)\rangle - \langle g_n(z)H_2H_1G(z)\rangle + \langle\delta_{1,n}(z)H_2G(z)\rangle = 0.$$

Using relations (3.8), (3.13), (3.17) and (3.18), we obtain from the previous relation

$$\begin{aligned}&\left(-i\,\frac{1-zf_n(z)}{2}I + \Delta_{2,n}(z)\left(\frac{\Delta_{1,n}(z)}{f_n(z)}I - A\right)\right)\langle G(z)\rangle - (\Delta_{1,n}(z)I - f_n(z)A)\langle H_2G(z)\rangle\\ &\quad = -if_n(z)I + R_{1,n}(z),\end{aligned} \tag{3.19}$$

where

$$\begin{aligned}R_{1,n}(z) = \frac{r_n(z)}{2\,f_n(z)}\langle G(z)\rangle &+ \langle\delta^o_{2,n}(z)H_1G(z)\rangle + \langle\delta^o_{1,n}(z)H_2G(z)\rangle\\ &- \langle g^o_n(z)H_2H_1G(z)\rangle - \langle k^o_{1,n}(z)G(z)\rangle.\end{aligned} \tag{3.20}$$

Multiplying the relation (3.19) by A from the left and applying the operation $n^{-1}\mathrm{Tr}$, we obtain

$$\begin{aligned}&f_n(z)\langle p_{1,n}(z)\rangle - \Delta_{1,n}(z)\left(i\,\frac{1-zf_n(z)}{2} + \langle k_{1,n}(z)\rangle\right) - \Delta_{2,n}(z)\left(\Delta_{1^{(2)},n}(z) - \frac{\Delta^2_{1,n}(z)}{f_n(z)}\right)\\ &\quad = -if_n(z)m_{1,n} + n^{-1}\mathrm{Tr}H_1R_{1,n}(z),\end{aligned} \tag{3.21}$$

where

$$p_{1,n}(z) = n^{-1}\mathrm{Tr}H_1^2H_2G(z),\quad \Delta_{1^{(2)},n}(z) = \langle n^{-1}\mathrm{Tr}H_1^2G(z)\rangle,\quad m_{1,n} = n^{-1}\mathrm{Tr}H_1 = \int_{-\infty}^{\infty} N_{1,n}(\mathrm{d}\lambda). \tag{3.22}$$

Using relation (3.18), we obtain from (3.21)

$$\langle p_{1,n}(z)\rangle = \frac{\Delta_{1^{(2)},n}(z)\Delta_{2,n}(z)}{f_n(z)} - iz\Delta_{1,n}(z) - m_{1,n} + \hat{r}_n(z), \tag{3.23}$$

where

$$\hat{r}_n(z) = -\frac{\Delta_{1,n}(z)r_n(z)}{2\,f_n^2(z)} + \frac{n^{-1}\mathrm{Tr}H_1R_{1,n}(z)}{f_n(z)}. \tag{3.24}$$

Consider now the matrix

$$Y_1(z) = H_2G(z). \tag{3.25}$$

Its clear that $\delta_{2,n}(z) = n^{-1}\mathrm{Tr}Y_1(z)$. On other hand, using to the $Y_1(z)$ the Proposition 3.1, we obtain

$$\langle([X,H_2]G)_{ab}\rangle - i\langle(H_2GH_1[X,H_2]G)_{ab}\rangle = -i\langle(H_2G[X,H_2]H_1G)_{ab}\rangle. \tag{3.26}$$

Choosing in (3.26) the matrix X with only (a,c)-th nonzero entries and applying $n^{-1}\Sigma_{a=1}^{n}$, we obtain the following matrix relation:

$$\begin{aligned}\langle Y_1(z)\rangle - i\langle k_{1,n}(z)Y_1(z)\rangle + i\langle \delta_{2,n}(z)H_2H_1G(z)\rangle \\ + \langle (i\{p_{2,n}(z)I - \delta_{2^{(2)},n}(z)A\} - m_{2,n}I)G(z)\rangle = 0,\end{aligned} \tag{3.27}$$

where

$$p_{2,n}(z) = n^{-1}\mathrm{Tr}H_2^2H_1G(z), \quad \delta_{2^{(2)},n}(z) = n^{-1}\mathrm{Tr}H_2^2G(z), \quad m_{2,n} = n^{-1}\mathrm{Tr}H_2 = \int_{-\infty}^{\infty} N_{2,n}(\mathrm{d}\lambda). \tag{3.28}$$

Introduce the centralized quantities

$$p^o_{2,n}(z) = p_{2,n}(z) - \langle p_{2,n}(z)\rangle, \quad \delta^o_{2^{(2)},n}(z) = \delta_{2^{(2)},n}(z) - \Delta_{2^{(2)},n}(z), \quad \Delta_{2^{(2)},n}(z) = \langle \delta_{2^{(2)},n}(z)\rangle. \tag{3.29}$$

Besides, applying to (3.27) $n^{-1}\mathrm{Tr}$ and using relations (3.13), (3.17) and (3.29), we obtain

$$\langle p_{2,n}(z)\rangle = \frac{\Delta_{2^{(2)},n}(z)\Delta_{1,n}(z)}{f_n(z)} - iz\Delta_{2,n}(z) - im_{2,n} + \tilde{r}_n(z), \tag{3.30}$$

where

$$\tilde{r}_n(z) = f_n^{-1}(z)(\langle \delta^o_{2,n}(z)(k_{1,n}(z) + k_{2,n}(z))\rangle - \langle p^o_{2,n}(z)g_n(z)\rangle + \langle \delta^o_{2^{(2)},n}(z)\delta_{1,n}(z)\rangle). \tag{3.31}$$

On other hand, using relations (3.8), (3.13), (3.18) and (3.29), we obtain from (3.27)

$$\begin{aligned}\Delta_{2^{(2)},n}(z)\left(\frac{\Delta_{1,n}(z)}{f_n(z)}I - A\right)\langle G(z)\rangle + \left(-i\frac{1 - zf_n(z)}{2}I - \Delta_{2,n}(z)\left(\frac{\Delta_{1,n}(z)}{f_n(z)}I - A\right)\right)\langle Y_1(z)\rangle \\ = -i\Delta_{2,n}(z)I + R_{2,n}(z),\end{aligned} \tag{3.32}$$

where

$$\begin{aligned}R_{2,n}(z) = -i\frac{r_n(z)}{2f_n(z)}\langle Y_1(z)\rangle - i\tilde{r}_n(z)\langle G(z)\rangle - \langle k^o_{1,n}(z)Y_1(z)\rangle + \langle \delta^o_{2,n}(z)H_2H_1G(z)\rangle \\ - \langle p^o_{2,n}(z)G(z)\rangle + \langle \delta^o_{2^{(2)},n}(z)H_1G(z)\rangle.\end{aligned} \tag{3.33}$$

Multiplying the relation (3.32) by A from the left and applying the operation $n^{-1}\mathrm{Tr}$, we obtain

$$\begin{aligned}\Delta_{2^{(2)},n}(z)\left(\frac{\Delta^2_{1,n}(z)}{f_n(z)} - \Delta_{1^{(2)},n}(z)\right) - \left(i\frac{1 - zf_n(z)}{2} + \frac{\Delta_{1,n}(z)\Delta_{2,n}(z)}{f_n(z)}\right)\langle k_{1,n}(z)\rangle + \Delta_{2,n}(z)\langle p_{1,n}(z)\rangle \\ = -i\Delta_{2,n}(z)m_{1,n} + n^{-1}\mathrm{Tr}H_1R_{2,n}(z).\end{aligned} \tag{3.34}$$

Using relations (3.18) and (3.23) we obtain from (3.34)

$$f_n^2(z)\frac{1 - z^2f_n^2(z)}{4} = -\Gamma^2_{1,n}(z)\Gamma^2_{2,n}(z) + \hat{r}_{2,n}(z), \tag{3.35}$$

where

$$\Gamma_{r,n}(z)=\sqrt{\Delta_{r^{(2)},n}(z)f_n(z)-\Delta_{r,n}^2(z)},\quad r=1,2, \tag{3.36}$$

and

$$\hat{r}_{2,n}(z)=-f_n^2(z)\left(\frac{r_n(z)}{2f_n(z)}\left(\langle k_{1,n}(z)\rangle+\frac{r_n(z)}{2f_n(z)}\right)+\Delta_{2,n}(z)\tilde{r}_n(z)+n^{-1}\mathrm{Tr}H_1R_{2,n}(z)\right). \tag{3.37}$$

We show in Theorem 3.1 that there exist y_0 and $C(y_0)$, both positive and independent of n and such that the variances of random variables $g_n(z)$, $\delta_{r,n}(z)$, $\delta_{r^{(2)},n}(z)$, $k_{r,n}(z)$, $p_{r,n}(z)$, $r=1,2$, admit the following bounds for $z\in E(y_0)$:

$$v_1=\langle|g_n(z)-\langle g_n(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},$$

$$v_{1+r}=\langle|\delta_{r,n}(z)-\langle\delta_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad v_{3+r}=\langle|\delta_{r^{(2)},n}(z)-\langle\delta_{r^{(2)},n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2}, \tag{3.38}$$

$$v_{5+r}=\langle|k_{r,n}(z)-\langle k_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad v_{7+r}=\langle|p_{r,n}(z)-\langle p_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad r=1,2.$$

Besides, using Cauchy–Schwarz and Holder inequalities and conditions of the theorem, we obtain the following bounds:

$$|\delta_{r,n}(z)|=|n^{-1}\mathrm{Tr}H_rG(z)|\leqslant\frac{(n^{-1}\mathrm{Tr}H_r^2)^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{m_6^{1/6}}{|\mathrm{Im}\,z|},\quad r=1,2, \tag{3.39}$$

$$|\delta_{r^{(2)},n}(z)|=|n^{-1}\mathrm{Tr}H_r^2G(z)|\leqslant\frac{(n^{-1}\mathrm{Tr}H_r^4)^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{m_6^{1/3}}{|\mathrm{Im}\,z|},\quad r=1,2, \tag{3.40}$$

$$\begin{aligned}|k_{r,n}(z)|&=|n^{-1}\mathrm{Tr}H_rH_{3-r}G(z)|\\&\leqslant\frac{(n^{-1}\mathrm{Tr}H_r^2H_{3-r}^2)^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{(n^{-1}\mathrm{Tr}H_r^4)^{1/4}(n^{-1}\mathrm{Tr}H_{3-r}^4)^{1/4}}{|\mathrm{Im}\,z|}\leqslant\frac{m_6^{1/3}}{|\mathrm{Im}\,z|},\quad r=1,2.\end{aligned} \tag{3.41}$$

These inequalities and relation (3.17) imply that uniformly in n

$$zg_n(z)=-1+O(|\mathrm{Im}\,z|^{-1}),\quad zf_n(z)=-1+O(|\mathrm{Im}\,z|^{-1}). \tag{3.42}$$

In addition using Proposition 1.1, relation (3.38) and the Cauchy–Schwarz inequality, we obtain, e.g.,

$$\begin{aligned}|\langle g_n^o n^{-1}\mathrm{Tr}H_1H_2H_1G(z)\rangle|&\leqslant v_1^{1/2}\frac{\langle(n^{-1}\mathrm{Tr}H_1^2H_2H_1^2H_2)^{1/2}\rangle}{|\mathrm{Im}\,z|}\\&\leqslant v_1^{1/2}\frac{\langle n^{-1}\mathrm{Tr}H_1^2H_2H_1^2H_2\rangle^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{2C^{1/2}(y_0)m_6^{1/2}}{n|\mathrm{Im}\,z|}.\end{aligned} \tag{3.43}$$

As a result of inequalities (3.39)–(3.41) and (3.43), Cauchy–Schwarz inequality, bounds for corresponding variances (3.38) and relations (3.42), we obtain that for $z\in E(y_0)$ the terms $r_n(z)$, $\hat{r}_n(z)$, $\tilde{r}_n(z)$ and $\hat{r}_{2,n}(z)$ in the previous formulas are of the order $O(n^{-1})$:

$$|r_n(z)|\leqslant\frac{C(y_0)}{n|\mathrm{Im}\,z|},\quad \hat{r}_n(z)\leqslant\frac{C(y_0)}{n},\quad \tilde{r}_n(z)\leqslant\frac{C(y_0)}{n},\quad \hat{r}_{2,n}(z)\leqslant\frac{C(y_0)}{n|\mathrm{Im}\,z|}. \tag{3.44}$$

Thus the relation (3.35) implies the third equation of the system (2.2).

Besides, we have obtained [(3.19) and (3.32)] the following linear system with matrix coefficients of matrix variables $\langle G(z)\rangle$ and $\langle Y_1(z)\rangle$:

$$\begin{aligned}(-i\alpha_n(z)I+\Delta_{2,n}(z)P)\langle G(z)\rangle - f_n(z)P\langle Y_1(z)\rangle = -if_n(z)I+R_{1,n},\\ \Delta_{2^{(2)},n}(z)P\langle G(z)\rangle +(-i\alpha_n(z)I-\Delta_{2,n}(z)P)\langle Y_1(z)\rangle = -i\Delta_{2,n}(z)I+R_{2,n},\end{aligned} \tag{3.45}$$

where

$$\alpha_n(z)=\frac{1-zf_n(z)}{2},\quad P=\frac{\Delta_{1,n}(z)}{f_n(z)}I-A. \tag{3.46}$$

The "determinant" D of this system is equal to

$$\begin{aligned}D&=-\alpha_n^2(z)I+\Gamma_{2,n}^2(z)P^2\\ &=\Gamma_{2,n}^2(z)\left(A-\left(\frac{\Delta_{1,n}(z)}{f_n(z)}-\frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right)I\right)\left(A-\left(\frac{\Delta_{1,n}(z)}{f_n(z)}+\frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right)I\right).\end{aligned} \tag{3.47}$$

Besides, using the resolvent identity (3.8) and the trace property, we obtain

$$z\Delta_{r,n}(z)=-n^{-1}\mathrm{Tr}H_r+z^{-1}\langle n^{-1}\mathrm{Tr}H_r[H_1,H_2]^2G(z)\rangle,\quad r=1,2,$$

$$z\Delta_{r^{(2)},n}(z)=-n^{-1}\mathrm{Tr}H_r^2+\langle n^{-1}\mathrm{Tr}H_r^2[H_1,H_2]G(z)\rangle,\quad r=1,2,$$

and

$$1+zf_n(z)=z^{-1}\langle n^{-1}\mathrm{Tr}[H_1,H_2]^2G(z)\rangle.$$

In addition, using 1.1, we obtain

$$|\langle n^{-1}\mathrm{Tr}H_r[H_1,H_2]^2G(z)\rangle|\leqslant\frac{\langle n^{-1}\mathrm{Tr}H_r[H_1,H_2]^4H_r\rangle^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{Cm_6^{5/6}}{|\mathrm{Im}\,z|},\quad r=1,2,$$

$$|\langle n^{-1}\mathrm{Tr}H_r^2[H_1,H_2]G(z)\rangle|\leqslant\frac{\langle n^{-1}\mathrm{Tr}H_r^2[H_1,H_2]^2H_r^2\rangle^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{Cm_6^{1/3}}{|\mathrm{Im}\,z|},\quad r=1,2,$$

and

$$|\langle n^{-1}\mathrm{Tr}[H_1,H_2]^2G(z)\rangle|\leqslant\frac{\langle n^{-1}\mathrm{Tr}[H_1,H_2]^4\rangle^{1/2}}{|\mathrm{Im}\,z|}\leqslant\frac{Cm_6^{2/3}}{|\mathrm{Im}\,z|}.$$

As a result of the bounds above we have for z belonging to the domain $E(y_0)$ and y_0 sufficiently large uniformly in n

$$zf_n(z)=-1+O(|\mathrm{Im}\,z|^{-2}),\quad \alpha_n(z)=1+O(|\mathrm{Im}\,z|^{-2}), \tag{3.48}$$

$$z\Delta_{r,n}(z)=-n^{-1}\mathrm{Tr}H_r+O(|\mathrm{Im}\,z|^{-2}),\quad r=1,2, \tag{3.49}$$

$$z\Gamma_{r,n}(z)=\sqrt{n^{-1}\mathrm{Tr}H_r^2-(n^{-1}\mathrm{Tr}H_r)^2}+O(|\mathrm{Im}\,z|^{-1}),\quad r=1,2. \tag{3.50}$$

According to the conditions of the theorem there exists n' sufficiently large and such that for all $n\geqslant n'$ we have

$$0<(m_r^{(2)}-m_r^2)/2\leqslant n^{-1}\mathrm{Tr}H_r^2-(n^{-1}\mathrm{Tr}H_r)^2\leqslant 2(m_r^{(2)}-m_r^2),\quad r=1,2.$$

Thus, the matrix D is uniformly in n invertible for $n \geqslant n'$ and $z \in E(y_0)$,

$$\|D^{-1}\| \leqslant C, \tag{3.51}$$

and its inverse is equal to

$$D^{-1} = \Gamma_{2,n}^{-2}(z) G_1\left(\frac{\Delta_{1,n}(z)}{f_n(z)} - \frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right) G_1\left(\frac{\Delta_{1,n}(z)}{f_n(z)} + \frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right), \tag{3.52}$$

where $G_1(z) = (H_1 - z)^{-1} = (A - z)^{-1}$. Hence the system (3.45) has the solution

$$\begin{aligned} \langle G(z) \rangle &= -\alpha_n(z) f_n(z) D^{-1} + \tilde{R}_{1,n}, \\ \langle Y_1(z) \rangle &= (-\alpha_n(z) \Delta_{2,n}(z) I + i \Gamma_{2,n}^2(z) P) D^{-1} + \tilde{R}_{2,n}, \end{aligned} \tag{3.53}$$

where

$$\tilde{R}_{1,n} = D^{-1}(P(f_n(z) R_{2,n} - \Delta_{2,n}(z) R_{1,n}) - i \alpha_n(z) R_{1,n}),$$

$$\tilde{R}_{2,n} = D^{-1}(P(\Delta_{2,n}(z) R_{2,n} - \Delta_{2^{(2)},n}(z) R_{1,n}) - i \alpha_n(z) R_{2,n}).$$

Applying to the relations (3.53) the operation $n^{-1}\mathrm{Tr}$ and using relation (3.52) and the resolvent identity, we obtain

$$\begin{aligned} \Gamma_{2,n}(z) &= f_{1,n}\left(\frac{\Delta_{1,n}(z)}{f_n(z)} - \frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right) + r_{1,n}(z), \\ -\Gamma_{2,n}(z) &= f_{1,n}\left(\frac{\Delta_{1,n}(z)}{f_n(z)} + \frac{\alpha_n(z)}{\Gamma_{2,n}(z)}\right) + r_{2,n}(z), \end{aligned} \tag{3.54}$$

where

$$f_{1,n}(z) = \int_{-\infty}^{+\infty} \frac{N_{1,n}(\mathrm{d}\lambda)}{\lambda - z}, \tag{3.55}$$

$$\begin{aligned} r_{1,n}(z) &= \left(\frac{\Gamma_{2,n}(z)}{f_n(z)} - i \frac{\Delta_{2,n}(z)}{2\Gamma_{2,n}(z)}\right) n^{-1}\mathrm{Tr}\tilde{R}_{1,n} + i n^{-1}\mathrm{Tr}\tilde{R}_{2,n}, \\ r_{2,n}(z) &= -\left(\frac{\Gamma_{2,n}(z)}{f_n(z)} + i \frac{\Delta_{2,n}(z)}{2\Gamma_{2,n}(z)}\right) n^{-1}\mathrm{Tr}\tilde{R}_{1,n} + i n^{-1}\mathrm{Tr}\tilde{R}_{2,n}. \end{aligned} \tag{3.56}$$

Besides, using Proposition 1.1, Cauchy–Schwarz and Holder inequalities and the bound (3.51), we obtain for $z \in E(y_0)$ the following bounds:

$$|n^{-1}\mathrm{Tr}D^{-1}PG(z)| \leqslant \frac{C}{|\mathrm{Im}\, z|}\left(\frac{m_6^{1/6}}{1 + m_6^{1/3}/|\mathrm{Im}\, z|} + (n^{-1}\mathrm{Tr}H_r^2)^{1/2}\right) \leqslant \frac{C m_6^{1/6}}{|\mathrm{Im}\, z|}\left(\frac{1}{1 + m_6^{1/3}/|\mathrm{Im}\, z|} + 1\right),$$

$$|n^{-1}\mathrm{Tr}D^{-1}PH_1G(z)| \leqslant \frac{C m_6^{1/3}}{|\mathrm{Im}\, z|}\left(\frac{1}{1 + m_6^{1/3}/|\mathrm{Im}\, z|} + 1\right),$$

$$|\langle(n^{-1}\mathrm{Tr}D^{-1}PH_2G(z)\rangle| \leqslant \frac{C}{|\mathrm{Im}\, z|}\left(\frac{m_6^{1/3}}{1+m_6^{1/3}/|\mathrm{Im}\, z|}+(n^{-1}\mathrm{Tr}H_1^2H_2^2)^{1/2}\right)$$
$$\leqslant \frac{Cm_6^{1/3}}{|\mathrm{Im}\, z|}\left(\frac{1}{1+m_6^{1/3}/|\mathrm{Im}\, z|}+1\right).$$

Using, in addition, Proposition 1.1, we obtain

$$|\langle g_n^o(n^{-1}\mathrm{Tr}D^{-1}PH_2H_1G(z)\rangle| \leqslant \frac{v_1^{1/2}C}{|\mathrm{Im}\, z|}\left(\frac{m_6^{1/6}\langle(n^{-1}\mathrm{Tr}H_1^2H_2^2)^{1/2}\rangle}{1+m_6^{1/3}/|\mathrm{Im}\, z|}+\langle(n^{-1}\mathrm{Tr}H_1^2H_2H_1^2H_2)^{1/2}\rangle\right)$$
$$\leqslant \frac{2C(y_0)m_6^{1/2}}{n|\mathrm{Im}\, z|}\left(\frac{1}{1+m_6^{1/3}/|\mathrm{Im}\, z|}+1\right).$$

These inequalities imply that for $z\in E(y_0)$ the terms $r_{1,n}(z)$ and $r_{2,n}(z)$ are of the order $O(n^{-1})$.

Using the arguments above in which the roles of H_1 and H_2 are interchanged, we obtain

$$\Gamma_{1,n}(z)=f_{2,n}\left(\frac{\Delta_{2,n}(z)}{f_n(z)}-\frac{\alpha_n(z)}{\Gamma_{1,n}(z)}\right)+r'_{1,n}(z),$$
$$-\Gamma_{1,n}(z)=f_{2,n}\left(\frac{\Delta_{2,n}(z)}{f_n(z)}+\frac{\alpha_n(z)}{\Gamma_{1,n}(z)}\right)+r'_{2,n}(z), \tag{3.57}$$

where

$$f_{2,n}(z)=\int_{-\infty}^{+\infty}\frac{N_{2,n}(\mathrm{d}\lambda)}{\lambda-z} \tag{3.58}$$

and where the terms $r_{1,n}(z)$ and $r_{2,n}(z)$ are of the order $O(n^{-1})$. Thus, the relations (3.57) and (3.54) lead to the first and to the last pairs of equations of the system (2.2).

Besides, for $z\in\mathbf{C}\backslash\mathbf{R}$ we have the following bounds:

$$|f_n(z)|\leqslant|\mathrm{Im}\, z|^{-1},\quad |\Delta_{r,n}(z)|\leqslant m_6^{1/6}|\mathrm{Im}\, z|^{-1},\quad |\Gamma_{r,n}(z)|\leqslant 4m_6^{1/6}|\mathrm{Im}\, z|^{-1},\ \ r=1,2.$$

These bounds imply that sequences $\{f_n(z)\}$, $\{\Delta_{r,n}(z)\}$, $\{\Gamma_{r,n}(z)\}$, $r=1,2$, are analytic and uniformly in n bounded for $z\in\mathbf{C}\backslash\mathbf{R}$. Thus the sequences are compact with respect to uniform convergence on any compacts of this domain. In addition, according to the hypothesis of the theorem, the normalized counting measures $N_{r,n}$ of matrices $H_{r,n}$, $r=1,2$, converge weakly to a limiting measures N_r, $r=1,2$. Thus their Stieltjes transforms (3.55) and (3.58) converge uniformly on compacts of $E(y_0)$, $y_0>|\mathrm{Im}z|$ to the Stieltjes transforms $f_{1,2}(z)$ of $N_{1,2}$. Hence, if y_0 is large enough, there exist five analytic in $E(y_0)$ functions f and Δ_r,Γ_r, $r=1,2$ verifying for $z\in E(y_0)$ the limiting system (2.5). Its unique solubility in domain (3.6) where y_0 is large enough is proved in Proposition 3.2. Besides, all five functions f_n, $\Delta_{r,n}$, $r=1,2$, are *a priori* analytic for $z\in\mathbf{C}\backslash\mathbf{R}$. Thus, their limits f,Δ_r,Γ_r, $r=1,2$, are also analytic for $z\in\mathbf{C}\backslash\mathbf{R}$. In view of the weak compactness of probability measures and the continuity of the one-to-one correspondence between non-negative measures and their Stieltjes transforms [see Proposition 1.1(v)] there exists a unique non-negative measure N such that f admits the representation (1.5). The measure N is a normalized to 1 measure in view of (3.48).

We conclude that the whole sequence $\{f_n(z)\}$ converges uniformly on compacts of $z\in\mathbf{C}\backslash\mathbf{R}$ to the limiting function $f(z)$ verifying (2.5). This result, Theorem 3.1 and the Borel–Cantelli lemma imply that the sequence $\{g_n(z)\}$ where $g_n(z)$ is defined in (3.12) converges with probability 1 to $f(z)$ for any fixed $z\in E(y_0)$. Since the convergence of a sequence of analytical functions on any countable set having an accumulation point in their common domain of definition implies the

uniform convergence of the sequence on any compact of the domain we obtain the convergence $g_n(z)$ to $f(z)$ with probability 1 on any compact of $\mathbf{C}\backslash\mathbf{R}$. Due to the continuity of the one-to-one correspondence between probability measures and their Stieltjes transforms the normalized counting measure (NCM) of the eigenvalues of random matrix (1.1) converge weakly with probability 1 to the nonrandom measure N whose Stieltjes transform (1.5) satisfies (2.5). Theorem 2.1 is proved. ■

Theorem 3.1: *Let H_n be the random matrix of the form (1.1) satisfying the conditions of Theorem 2.1. Then there exist y_0 and $C(y_0)$, both positive and independent of n and such that the variances of random variables $g_n(z)$, $\delta_{r,n}(z)$, $\delta_{r^{(2)},n}(z)$, $k_{r,n}(z)$, $p_{r,n}(z)$, $r=1,2$, admit the bounds for $z\in E(y_0)$:*

$$v_1=\langle|g_n(z)-\langle g_n(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},$$

$$v_{1+r}=\langle|\delta_{r,n}(z)-\langle\delta_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad v_{3+r}=\langle|\delta_{r^{(2)},n}(z)-\langle\delta_{r^{(2)},n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\tag{3.59}$$

$$v_{5+r}=\langle|k_{r,n}(z)-\langle k_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad v_{7+r}=\langle|p_{r,n}(z)-\langle p_{r,n}(z)\rangle|^2\rangle\leqslant\frac{C(y_0)}{n^2},\quad r=1,2.$$

Proof: We will obtain the bounds (3.59) following the scheme used in Refs. 4, 7, and 6 for the estimates of corresponding variances in the cases of additive and multiplicative ensembles. Namely, using Proposition 3.1 and the resolvent identity we will derive and analyze the system of inequalities

$$v_i\leqslant\sum_{j=1,j\neq i}^{9}\alpha_{ij}(y_0)v_i^{1/2}v_j^{1/2}+\frac{\beta_i(y_0)}{n^2},\quad i=1,\ldots,9.\tag{3.60}$$

After the proper rescaling the coefficients $\alpha_{ij}(y_0)$ and $\beta_i(y_0)$, $i,j=1,\ldots,9$, of this system will admit the following relations for some $\nu>0$ and $C>0$ both independent of y_0:

$$|\alpha_{ij}(y_0)|\leqslant\frac{C}{y_0^{\nu}},\quad |\beta_i(y_0)|\leqslant C.$$

Thus, choosing y_0 sufficiently large and then fixing it, we will obtain from the system (3.60) the bounds (3.59).

We will use below the notations $g(z)$, $\delta_r(z)$, $\delta_{r^{(2)}}(z)$, $k_r(z)$, $p_r(z)$, $r=1,2$, for $g_n(z)$, $\delta_{r,n}(z)$, $\delta_{r^{(2)},n}(z)$, $k_{r,n}(z)$, $p_{r,n}(z)$, $r=1,2$, correspondently. Besides, because of the symmetry of the problem with respect to H_1 and H_2 it suffices to prove only odd relations of the system (3.60). The first inequality of the system (3.60) follows from the resolvent identity (3.8). Indeed, using the Cauchy–Schwarz inequality, we obtain for $z\in E(y_0)$ [cf. (3.17)]

$$v_1=\langle g^o(\overline{z})g(z)\rangle=\frac{i}{z}(\langle g^o(\overline{z})k_1(z)\rangle-\langle g^o(\overline{z})k_1(z)\rangle)\leqslant\frac{1}{y_0}(v_1^{1/2}v_6^{1/2}+v_1^{1/2}v_7^{1/2}).$$

Hence, we have

$$\alpha_{1p}(y_0)\equiv\frac{1}{y_0},\quad p=6,7,\quad \alpha_{1q}(y_0)\equiv 0,q=2,\ldots,5,8,9,\quad \beta_1(y_0)\equiv 0.\tag{3.61}$$

To get the third inequality of the system (3.60) consider the matrix $V_1=\langle\delta_2^o(\overline{z})UGU^*\rangle$. It is clear that $n^{-1}\mathrm{Tr}BV_1$ is the variance v_3:

$$\langle|\delta_2^o(z)|^2\rangle=\langle\delta_2^o(\overline{z})n^{-1}\mathrm{Tr}U^*BUG\rangle=\langle\delta_2^o(\overline{z})n^{-1}\mathrm{Tr}BUGU^*\rangle=n^{-1}\mathrm{Tr}BV_1.$$

Applying to the function $\Phi(M)=(MUG(\overline{z})U^*)^o_{aa}(UG(z)U^*)_{bd}$ the analog of Proposition 3.1 obtained from the left shift invariance of the Haar measure, we obtain

$$\langle\{(B[X,U\overline{G}U^*])_{aa}-i(BU\overline{G}[A,U^*[B,X]U]\overline{G}U^*)_{aa}\}(UGU^*)_{bd}\rangle$$
$$+\langle(BU\overline{G}U^*)^o_{aa}\{([X,UGU^*])_{bd}-i(UG[A,U^*[B,X]U]GU^*)_{bd}\}\rangle=0.$$

Choosing the matrix X with only (b,c)-th nonzero entries, applying $n^{-2}\Sigma_{a,b=1}^n$ and using the trace property, we obtain the relation

$$V_1-\langle\delta_2^o(\overline{z})g(z)\rangle+i\langle\delta_2^o(\overline{z})U\{\delta_2(z)A-k_1(z)I\}G(z)U^*\rangle-i\langle\delta_2^o(\overline{z})g(z)BUAG(z)U^*\rangle$$
$$+i\langle\delta_2^o(\overline{z})\delta_1(z)BUG(z)U^*\rangle+n^{-2}\Psi=0, \tag{3.62}$$

where

$$\Psi=\langle[U\overline{G}U^*,B]UGU^*\rangle-i\langle[U[U\overline{G}U^*BU\overline{G},A]U^*,B]UGU^*\rangle. \tag{3.63}$$

Multiplying the relation (3.62) by B from the left and applying the operation $n^{-1}\mathrm{Tr}$, we obtain

$$v_3=m_{2,n}\langle\delta_2^o(\overline{z})g(z)\rangle-i\langle\delta_2^o(\overline{z})\delta_2(z)k_2(z)\rangle+i\langle\delta_2^o(\overline{z})\delta_2(z)k_1(z)\rangle+i\langle\delta_2^o(\overline{z})g(z)p_2(z)\rangle$$
$$-i\langle\delta_2^o(\overline{z})\delta_1(z)\delta_{2^{(2)}}(z)\rangle+n^{-3}\mathrm{Tr}B\Psi. \tag{3.64}$$

Using the centralized quantities (3.13) and (3.29) we can write

$$\langle\delta_2^o(\overline{z})\delta_2(z)k_r(z)\rangle=v_3\langle k_r(z)\rangle+\langle\delta_2^o(\overline{z})k_r(z)\rangle\langle\delta_2(z)\rangle,\quad r=1,2,$$

$$\langle\delta_2^o(\overline{z})g(z)p_2(z)\rangle=\langle\delta_2^o(\overline{z})g(z)\rangle\langle p_2(z)\rangle+\langle\delta_2^o(\overline{z})p_2(z)\rangle\langle g(z)\rangle,$$

$$\langle\delta_2^o(\overline{z})\delta_1(z)\delta_{2^{(2)}}(z)\rangle=\langle\delta_2^o(\overline{z})\delta_1(z)\rangle\langle\delta_{2^{(2)}}(z)\rangle+\langle\delta_2^o(\overline{z})\delta_{2^{(2)}}(z)\rangle\langle\delta_1(z)\rangle.$$

Besides, using Proposition 1.1, the Holder inequality and relation (3.63), we obtain

$$|n^{-1}\mathrm{Tr}B\Psi|\leqslant 2\frac{n^{-1}\mathrm{Tr}B^2}{|\mathrm{Im}\,z|^2}+8\frac{(n^{-1}\mathrm{Tr}B^6)^{1/2}(n^{-1}\mathrm{Tr}A^2)^{1/2}}{|\mathrm{Im}\,z|^3}.$$

Thus, in view of the relations above and the Cauchy–Schwarz inequality, we have the bounds

$$|\langle\delta_2^o(\overline{z})\delta_2(z)k_r(z)\rangle|\leqslant\frac{m_{1,n}m_{2,n}}{y_0}v_3+\frac{m_{2,n}}{y_0}v_3^{1/2}v_{5+r}^{1/2},\quad r=1,2,$$

$$|\langle\delta_2^o(\overline{z})g(z)p_2(z)\rangle|\leqslant\frac{(m_{1,n}^{(2)})^{1/2}(n^{-1}\mathrm{Tr}B^4)^{1/2}}{y_0}v_3^{1/2}v_1^{1/2}+\frac{1}{y_0}v_3^{1/2}v_9^{1/2},$$

$$|\langle\delta_2^o(\overline{z})\delta_1(z)\delta_{2^{(2)}}(z)\rangle|\leqslant\frac{m_{2,n}^{(2)}}{y_0}v_3^{1/2}v_2^{1/2}+\frac{m_{1,n}}{y_0}v_3^{1/2}v_5^{1/2}.$$

These bounds and relation (3.64) lead for $m_6^{1/3}y_0^{-1}\leqslant\frac{1}{2}$ to the third inequality of the system (3.60), in which

$$\alpha_{31}(y_0)\equiv 2\left(m_6^{1/6}+\frac{m_6^{1/2}}{y_0}\right),\quad \alpha_{32}(y_0)\equiv 2\frac{m_6^{1/3}}{y_0},\quad \alpha_{35}(y_0)\equiv\alpha_{3r}(y_0)\equiv 2\frac{m_6^{1/6}}{y_0},\quad r=6,7,$$
$$\alpha_{39}(y_0)\equiv\frac{2}{y_0},\quad \beta_3(y_0)\equiv\frac{4m_6^{1/3}}{y_0^2}\left(1+\frac{4}{y_0}\right). \tag{3.65}$$

To get the fives inequality of the system (3.60) consider the matrices $V_2=\langle\delta^o_{2(2)}(\overline{z})UGU^*\rangle$ and $W_2=\langle\delta^o_{2(2)}(\overline{z})UAGU^*\rangle$. It is clear that $n^{-1}\mathrm{Tr}B^2V_2$ is the variance v_5. Besides, applying to the function $\Phi(M)=(M^2UG(\overline{z})U^*)^o_{aa}(UG(z)U^*)_{bd}$ the analog of Proposition 3.1 obtained from the left shift invariance of the Haar measure, we obtain after the procedure similar to that used above the following relation:

$$\begin{aligned}V_2-\langle\delta^o_{2(2)}(\overline{z})g(z)\rangle I+i\langle\delta^o_{2(2)}(\overline{z})\{\delta_1(z)B-k_1(z)I\}UG(z)U^*\rangle\\ -i\langle\delta^o_{2(2)}(\overline{z})(g(z)B-\delta_2(z))UAG(z)U^*\rangle+n^{-2}\Psi_1=0,\end{aligned} \tag{3.66}$$

where

$$\Psi_1=\langle[U\overline{G}U^*,B^2]UGU^*\rangle-i\langle[U[U\overline{G}U^*B^2U\overline{G},A]U^*,B]UGU^*\rangle.$$

On the other hand, applying the same procedure to the function $\Phi(M)=(M^2UG(\overline{z})U^*)^o_{aa}(UAG(z)U^*)_{bd}$, we obtain

$$\begin{aligned}W_2-\langle\delta^o_{2(2)}(\overline{z})\delta_1(z)\rangle I+i\langle\delta^o_{2(2)}(\overline{z})\{\delta_{1(2)}(z)B-(p_1(z)-iz\delta_1-im_{1,n})I\}UG(z)U^*\rangle\\ -i\langle\delta^o_{2(2)}(\overline{z})(\delta_1(z)B-k_2(z)I)UAG(z)U^*\rangle+n^{-2}\Psi_2=0,\\ \Psi_2=\langle[U\overline{G}U^*,B^2]UAGU^*\rangle-i\langle[U[U\overline{G}U^*B^2U\overline{G},A]U^*,B]UAGU^*\rangle.\end{aligned} \tag{3.67}$$

Multiplying relations (3.66) and (3.67) by B^2 from the left and regrouping terms, we obtain the following linear system of the matrix variables $Q_1=B^2V_2$ and $Q_2=B^2W_2$:

$$\begin{aligned}(I+i\{\Delta_1(z)B-\langle k_1(z)\rangle I\})Q_1-i(f(z)B-\Delta_2(z)I)Q_2=P_1-n^{-2}B^2\Psi_1,\\ i(\Delta_{1(2)}(z)B-(\langle p_1(z)\rangle-iz\Delta_1-im_{1,n})I)Q_1+(I-i\{\Delta_1(z)B-\langle k_2(z)\rangle I\})Q_2=P_2-n^{-2}B^2\Psi_2,\end{aligned} \tag{3.68}$$

where

$$\begin{aligned}P_1=\langle\delta^o_{2(2)}(\overline{z})g(z)\rangle B^2-i\langle\delta^o_{2(2)}(\overline{z})\delta^o_1(z)B^3UG(z)U^*\rangle+i\langle\delta^o_{2(2)}(\overline{z})k^o_1(z)B^2UG(z)U^*\rangle\\ +i\langle\delta^o_{2(2)}(\overline{z})g^\circ(z)B^3UAG(z)U^*\rangle-i\langle\delta^o_{2(2)}(\overline{z})\delta^o_2(z)B^2UAG(z)U^*\rangle,\end{aligned}$$

$$\begin{aligned}P_2=\langle\delta^o_{2(2)}(\overline{z})\delta_1(z)\rangle B^2-i\langle\delta^o_{2(2)}(\overline{z})\delta^o_{1(2)}(z)B^3UG(z)U^*\rangle+i\langle\delta^o_{2(2)}(\overline{z})p^o_1(z)B^2UG(z)U^*\rangle\\ +i\langle\delta^o_{2(2)}(\overline{z})\delta^o_1(z)B^2UG(z)U^*\rangle-z\langle\delta^o_{2(2)}(\overline{z})\delta^o_1(z)B^3UAG(z)U^*\rangle\\ -i\langle\delta^o_{2(2)}(\overline{z})k^o_2(z)B^2UAG(z)U^*\rangle.\end{aligned}$$

The "determinant" $\hat{D}$ of the system (3.68) is equal to

$$\hat{D}=-\Gamma_1(z)(B^2+a(z)B+c(z)I)=-\Gamma_1(z)(B-b_+(z))(B-b_-(z)),$$

where

$$a(z)=\Gamma_1^{-1}(z)(\Delta_1(z)(\langle k_1(z)\rangle+\langle k_2(z)\rangle)-\Delta_{1(2)}(z)\Delta_2(z)-f(z)(\langle p_1(z)\rangle-i(z\Delta_1(z)+m_{1,n})),$$

$$c(z)=-\Gamma_1^{-1}(z)(1-i(\langle k_1(z)\rangle-\langle k_2(z)\rangle)+\langle k_1(z)\rangle\langle k_2(z)\rangle-\Delta_2(z)(\langle p_1(z)\rangle-i(z\Delta_1(z)+m_{1,n}))),$$

$$b_{\pm}(z)=(-a(z)\pm\sqrt{a^2(z)-4c(z)})/2.$$

Besides, using the resolvent identity (3.8), Proposition 1.1 and the trace property, we obtain

$$z\langle k_r(z)\rangle=-n^{-1}\mathrm{Tr}H_1n^{-1}\mathrm{Tr}H_2+iz^{-1}\langle n^{-1}\mathrm{Tr}H_rH_{3-r}[H_1,H_2]G(z)\rangle,\quad r=1,2,$$

$$z\langle p_1(z)\rangle=-n^{-1}\mathrm{Tr}H_1^2n^{-1}\mathrm{Tr}H_2+iz^{-1}\langle n^{-1}\mathrm{Tr}H_1^2H_2[H_1,H_2]G(z)\rangle.$$

These relations imply that for z belonging to the domain $E(y_0)$ and y_0 sufficiently large uniformly in n we have

$$k_r(z)=-n^{-1}\mathrm{Tr}H_1n^{-1}\mathrm{Tr}H_2+O(|\mathrm{Im}\,z|^{-1}),\quad r=1,2,$$

$$p_1(z)=-n^{-1}\mathrm{Tr}H_1^2n^{-1}\mathrm{Tr}H_2+O(|\mathrm{Im}\,z|^{-1}).$$

As result of the relations above and (3.48)–(3.50), we obtain that for $z\to\infty$, $z\in E(y_0)$,

$$a(z)=O(1),\quad c(z)=-z^2((m_{1,n}^{(2)}-m_{1,n}^2)^{-1}+O(|\mathrm{Im}\,z|^{-1}))$$

and hence

$$b_{\pm}=\pm z((m_{1,n}^{(2)}-m_{1,n}^2)^{-1/2}+O(|\mathrm{Im}\,z|^{-1})).$$

Thus, the matrix $\hat{D}$ is unifomly in n invertible for all $n\geqslant n'$ and we have for y_0 sufficiently large and $z\in E(y_0)$

$$\|\hat{D}^{-1}\|\leqslant C.$$

Solving the system (3.68), we obtain

$$Q_1=\hat{D}^{-1}((I-i\{\Delta_1(z)B-\langle k_2(z)\rangle I\})(P_1-n^{-2}B^2\Psi_1)-i(f(z)B-\Delta_2(z))(P_2-n^{-2}B^2\Psi_2)).$$

Applying to this relation the operation $n^{-1}\mathrm{Tr}$, we obtain on the lhs the variance v_5. Using Proposition 1.1, we obtain the following bound for the rhs:

$$\sum_{j=1,j\neq5}^{8}\alpha_{ij}(y_0)v_5^{1/2}v_j^{1/2}+n^{-2}\beta_5(y_0),$$

where

$$\alpha_{51}(y_0)\equiv C\left(m_6^{1/3}+2\frac{m_6^{2/3}}{y_0}\right),\quad \alpha_{52}(y_0)\equiv 2C\frac{m_6^{1/6}}{y_0}\left(m_6^{1/3}+2m_6^{2/3}+\frac{3m_6^{2/3}+4m_6+4y_0^{-1}m_6^{2/3}}{y_0}\right),$$

$$\alpha_{53}(y_0)\equiv\alpha_{57}(y_0)\equiv 2C\frac{m_6^{2/3}}{y_0^2},\quad \alpha_{34}(y_0)\equiv 2\frac{m_6^{1/6}}{y_0},\quad \alpha_{56}(y_0)\equiv\frac{C}{y_0}\left(m_6^{1/3}+2\frac{m_6^{2/3}}{y_0}\right),\quad (3.69)$$

$$\alpha_{58}(y_0)\equiv 2C\frac{m_6^{1/2}}{y_0^2},\quad \beta_5(y_0)\equiv 2C\frac{m_6^{2/3}}{y_0^2}\left(1+\frac{4m_6^{1/3}}{y_0}\right)\left(1+2\frac{m_6^{1/3}+m_6^{1/6}}{y_0}\right).$$

Repeating the procedure analogous to that used above for the matrices $V_3=\langle k_2^o(\overline{z})UGU^*\rangle$, $W_3=\langle k_2^o(\overline{z})UAGU^*\rangle$ and $V_4=\langle p_2^o(\overline{z})UGU^*\rangle$, $W_4=\langle p_2^o(\overline{z})UAGU^*\rangle$, we obtain the sevens and nines inequalities of the system (3.60), in which

$$\alpha_{72}(y_0)=O(1),\quad \alpha_{92}(y_0)=O(1),\quad \alpha_{7r}(y_0)=O(y_0^{-1}),$$
$$\alpha_{9q}(y_0)=O(y_0^{-1}),\quad r=1,3,\ldots,6,8,\ q=1,3,\ldots,7,\quad \beta_s(y_0)=O(y_0^{-2}),\ s=7,9. \tag{3.70}$$

Using the symmetry of ensemble, we obtain the remaining even inequalities of the system (3.60).

Let us introduce new variables

$$u_1=y_0^{1/2}v_1^{1/2},\quad u_{1+r}=y_0^{1/4}v_{1+r}^{1/2},\quad u_{3+r}=v_{3+r}^{1/2},\quad u_{5+r}=v_{5+r}^{1/2},\quad u_{7+r}=v_{7+r}^{1/2},\quad r=1,2. \tag{3.71}$$

Then we obtain from (3.60), (3.61), (3.65), (3.69) and (3.70) the following system,

$$u_i^2\leqslant \sum_{j=1,j\neq i}^{9} a_{ij}u_iu_j+\frac{\gamma_i}{n^2},\quad i=1,\ldots,9. \tag{3.72}$$

in which the coefficients $\{a_{ij},\ i\neq j\}$ have the form $a_{ij}=y_0^{-1/4}b_{ij}$, where b_{ij} are bounded in y_0 and in n as $y_0\to\infty$ and $n\to\infty$. By choosing y_0 sufficiently big (and then fixing it), we can guarantee that $0<a_{ij}<\frac{1}{10}$, $i\neq j$. Thus, summing the nine relations (3.72), we can write the result in the form $(\hat{a}u,u)\leqslant\gamma/n^2$, where $\gamma=\gamma_1+\cdots+\gamma_9$ and $(\hat{a})_{ij}=\delta_{ij}-(1-\delta_{ij})/10$, $i,j=1,\ldots,9$. Since the minimum eigenvalue of matrix $\hat{a}$ is $\frac{1}{5}$, we obtain from (3.71) bounds (3.59). ■

Proof of Theorem 2.2: The proof of Theorem 2.2 follows the proof of Theorem 2.1 line by line. Indeed, using Proposition 3.1 with the matrix element $\Phi(M)=(G(z))_{ab}=((H_1M+MH_1-z)^{-1})_{ab}$ as $\Phi(M)$, we obtain [cf. (3.9)]

$$\langle (GH_1[X,H_2]G)_{ab}\rangle+\langle (G[X,H_2]H_1G)_{ab}\rangle=0. \tag{3.73}$$

Choosing in this relation the matrix X with only (a,b)-th nonzero entries and applying to the result $n^{-2}\Sigma_{a,b=1}^{n}$, we obtain

$$\langle g_n(z)(k_{1,n}(z)-k_{2,n}(z))\rangle=0, \tag{3.74}$$

where $g(z)$ and $k_r(z)$, $r=1,2$, are defined in (3.12). Besides, using the resolvent identity (3.1) for the pair $(\tilde{H},0)$,

$$zG(z)+I=H_1H_2G(z)+H_2H_1G(z), \tag{3.75}$$

and centralized quantities (3.13), we obtain from (3.74) [cf. (3.18)]

$$\langle k_{1,n}(z)\rangle=\langle k_{2,n}(z)\rangle-\frac{r_n(z)}{f_n(z)},$$
$$1+zf_n(z)=2\langle k_{2,n}(z)\rangle-\frac{r_n(z)}{f_n(z)}, \tag{3.76}$$

where $f_n(z)$ is defined in (3.14) and

$$r_n(z)=\langle g_n^o(z)(k_{1,n}(z)-k_{2,n}(z))\rangle. \tag{3.77}$$

On the other hand, choosing in (3.73) the matrix X with only (a,c)-th nonzero entries, applying $n^{-1}\Sigma_{a=1}^{n}$ and using relations (3.75), (3.13) and (3.76) we obtain the following matrix relation [cf. (3.19)]:

$$\left(\frac{1-zf_n(z)}{2}I+\Delta_{2,n}(z)A\right)\langle G(z)\rangle-(\Delta_{1,n}(z)I-f_n(z)A)\langle H_2G(z)\rangle=f_n(z)I-R_{1,n}(z), \tag{3.78}$$

where $R_{1,n}(z)$ is defined in (3.20). Multiplying the relation (3.78) by A from the left and applying the operation $n^{-1}\mathrm{Tr}$ we obtain

$$f_n(z)\langle p_{1,n}(z)\rangle+\Delta_{1,n}(z)\left(\frac{1-zf_n(z)}{2}-\langle k_{1,n}(z)\rangle\right)+\Delta_{2,n}(z)\Delta_{1^{(2)},n}(z)$$
$$=f_n(z)m_{1,n}-n^{-1}\mathrm{Tr}H_1R_{1,n}(z), \tag{3.79}$$

where $p_{1,n}(z)$ and $m_{1,n}$ are defined in (3.22). Using relation (3.76) we obtain from (3.79)

$$\langle p_{1,n}(z)\rangle=\frac{\Delta_{1^{(2)},n}(z)\Delta_{2,n}(z)}{f_n(z)}+z\Delta_{1,n}(z)+m_{1,n}-\hat{r}_n(z), \tag{3.80}$$

where $\hat{r}_n(z)$ is defined in (3.24). Besides, applying to the matrix $Y_1(z)$ (3.25) the Proposition 3.1 and performing a procedure analogous to that used above we obtain the following matrix relation [cf. (3.27)]:

$$\langle Y_1(z)\rangle-\langle k_{1,n}(z)Y_1(z)\rangle-\langle\delta_{2,n}(z)H_2H_1G(z)\rangle+\langle(\{p_{2,n}(z)I+\delta_{2^{(2)},n}(z)A\}-m_{2,n}I)G(z)\rangle=0, \tag{3.81}$$

where $p_{2,n}(z)$ and $m_{2,n}$ are defined in (3.28). Applying to (3.81) $n^{-1}\mathrm{Tr}$, introducing the centralized quantities (3.29) and using relation (3.13) we obtain [cf. (3.30)]

$$\langle p_{2,n}(z)\rangle=\frac{\Delta_{2^{(2)},n}(z)\Delta_{1,n}(z)}{f_n(z)}+z\Delta_{2,n}(z)+m_{2,n}+\tilde{r}_n(z),$$

where $\tilde{r}_n(z)$ is defined in (3.31). On the other hand, using relations (3.75), (3.13), (3.76) and (3.29), we obtain from (3.81) [cf. (3.32)]

$$-\Delta_{2^{(2)},n}(z)\left(\frac{\Delta_{1,n}(z)}{f_n(z)}I-A\right)\langle G(z)\rangle+\left(\frac{1-zf_n(z)}{2}I+\Delta_{2,n}(z)A\right)\langle Y_1(z)\rangle$$
$$=\Delta_{2,n}(z)I-R_{2,n}(z), \tag{3.82}$$

where $R_{2,n}(z)$ is defined in (3.33). Multiplying the relation (3.82) by A from the left and then applying the operation $n^{-1}\mathrm{Tr}$, we obtain [cf. (3.34)]

$$-\Delta_{2^{(2)},n}(z)\left(\frac{\Delta_{1,n}^2(z)}{f_n(z)}-\Delta_{1^{(2)},n}(z)\right)+\frac{1-zf_n(z)}{2}\langle k_{1,n}(z)\rangle++\Delta_{2,n}(z)\langle p_{1,n}(z)\rangle$$
$$=\Delta_{2,n}(z)m_{1,n}-n^{-1}\mathrm{Tr}H_1R_{2,n}(z). \tag{3.83}$$

Using relations (3.76) and (3.80) we obtain from (3.83) [cf. (3.35)]

$$f_n^2(z)\left(\frac{1-z^2f_n^2(z)}{4}+z\Delta_{1,n}(z)\Delta_{2,n}(z)\right)$$
$$=-(\Omega_{1,n}^2(z)-\Delta_{1,n}^2(z))(\Omega_{2,n}^2(z)-\Delta_{2,n}^2(z))++\Delta_{1,n}^2(z)\Delta_{2,n}^2(z)-\hat{r}_{2,n}(z), \tag{3.84}$$

where

$$\Omega_{r,n}(z)=\sqrt{\Delta_{r^{(2)},n}(z)f_n(z)},\quad r=1,2 \tag{3.85}$$

and $\hat{r}_{2,n}(z)$ is defined in (3.37).

Mimicking the proof of Theorem 3.1 one can obtain that there exists positive constant y_0 independent of n and such that the variances of random variables $g_n(z)$, $\delta_{r,n}(z)$, $\delta_{r^{(2)},n}(z)$,

$k_{r,n}(z)$, $p_{r,n}(z)$, $r=1,2$, admit bounds (3.38) for $z\in E(y_0)$, i.e., they are of the order $O(n^{-2})$. Hence, the terms $r_n(z)$, $\hat{r}_n(z)$, $\tilde{r}_n(z)$ and $\hat{r}_{2,n}(z)$ in the previous formulas are of the order $O(n^{-1})$.

Thus the relation (3.84) implies the third equation of the system (2.5).

Besides, we have obtained [(3.78) and (3.82)] the following linear system with matrix coefficients of matrix variables $\langle G(z)\rangle$ and $\langle Y_1(z)\rangle$ [cf. (3.45)]

$$\begin{aligned}(\alpha_n(z)I+\Delta_{2,n}(z)A)\langle G(z)\rangle - f_n(z)P\langle Y_1(z)\rangle = f_n(z)I-R_{1,n},\\ -\Delta_{2^{(2)},n}(z)P\langle G(z)\rangle+(\alpha_n(z)I+\Delta_{2,n}(z)A)\langle Y_1(z)\rangle=\Delta_{2,n}(z)I-R_{2,n},\end{aligned} \tag{3.86}$$

where $\alpha_n(z)$ and P are defined in (3.46). The "determinant" $\tilde{D}$ of this system is equal to [cf. (3.47)]

$$\begin{aligned}\tilde{D}&=(\alpha_n(z)+\Delta_{2,n}(z)A)^2I-\Omega_{2,n}^2(z)P^2\\ &=-(\Omega_{2,n}^2(z)-\Delta_{2,n}^2(z))\left(A-\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)-\alpha_n(z)}{\Omega_{2,n}(z)+\Delta_{2,n}(z)}I\right)\\ &\quad\times\left(A-\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)+\alpha_n(z)}{\Omega_{2,n}(z)-\Delta_{2,n}(z)}I\right).\end{aligned} \tag{3.87}$$

In addition, we have for z belonging to the domain $E(y_0)$ and y_0 sufficiently large uniformly in n the followings analogs of the asymptotics (3.48)–(3.50):

$$\begin{aligned}zf_n(z)&=-1+O(|\mathrm{Im}\,z|^{-1}),\quad \alpha_n(z)=1+O(|\mathrm{Im}\,z|^{-1}),\\ z\Delta_{r,n}(z)&=-n^{-1}\mathrm{Tr}H_r+O(|\mathrm{Im}\,z|^{-1}),\quad r=1,2,\\ z\Omega_{r,n}(z)&=\sqrt{n^{-1}\mathrm{Tr}H_r^2}+O(|\mathrm{Im}\,z|^{-1}),\quad r=1,2.\end{aligned}$$

Thus, the matrix D is uniformly in n invertible for $n\geqslant n'$ and $z\in E(y_0)$ and its inverse is equal to [cf. (3.52)]

$$\begin{aligned}\tilde{D}^{-1}&=-(\Omega_{2,n}^2(z)-\Delta_{2,n}^2(z))^{-2}G_1\left(\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)-\alpha_n(z)}{\Omega_{2,n}(z)+\Delta_{2,n}(z)}\right)\\ &\quad\times G_1\left(\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)+\alpha_n(z)}{\Omega_{2,n}(z)-\Delta_{2,n}(z)}\right).\end{aligned} \tag{3.88}$$

Hence the system (3.45) has the solution

$$\begin{aligned}\langle G(z)\rangle&=f_n(z)(\alpha_n(z)+\Delta_{2,n}(z)A)D^{-1}+f_n(z)\Delta_{2,n}(z)PD^{-1}+\tilde{R}_{1,n},\\ \langle Y_1(z)\rangle&=\Delta_{2,n}(z)(\alpha_n(z)+\Delta_{2,n}(z)A)D^{-1}+\Omega_{2,n}^2(z)PD^{-1}+\tilde{R}_{2,n},\end{aligned} \tag{3.89}$$

where

$$\begin{aligned}\tilde{R}_{1,n}&=-D^{-1}(P(\Delta_{2,n}(z)A+\alpha_n(z)I)R_{1,n}+f_n(z)PR_{2,n}),\\ \tilde{R}_{2,n}&=-D^{-1}(P(\Delta_{2,n}(z)A+\alpha_n(z)I)R_{2,n}-\Delta_{2^{(2)},n}(z)PR_{1,n}).\end{aligned} \tag{3.90}$$

Applying to the relations (3.89) the operation $n^{-1}\mathrm{Tr}$ and using relation (3.88) and the resolvent identity, we obtain

$$\Omega_{2,n}(z)+\Delta_{2,n}(z)=f_{1,n}\left(\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)-\alpha_n(z)}{\Omega_{2,n}(z)+\Delta_{2,n}(z)}\right)+r_{1,n}(z),$$
$$-\Omega_{2,n}(z)+\Delta_{2,n}(z)=f_{1,n}\left(\frac{\Omega_{2,n}(z)\Delta_{1,n}(z)f_n^{-1}(z)+\alpha_n(z)}{\Omega_{2,n}(z)-\Delta_{2,n}(z)}\right)+r_{2,n}(z), \tag{3.91}$$

where

$$r_{1,n}(z)=\frac{\Omega_{2,n}(z)}{f_n(z)}n^{-1}\mathrm{Tr}\tilde{R}_{1,n}+n^{-1}\mathrm{Tr}\tilde{R}_{2,n},$$
$$r_{2,n}(z)=-\frac{\Omega_{2,n}(z)}{f_n(z)}n^{-1}\mathrm{Tr}\tilde{R}_{1,n}+n^{-1}\mathrm{Tr}\tilde{R}_{2,n}. \tag{3.92}$$

The arguments analogous to those used above imply that for $z\in E(y_0)$ the terms $r_{1,n}(z)$ and $r_{2,n}(z)$ are of the order $O(n^{-1})$. Thus, the relations (3.91) lead to the last pair of equations of the system (2.5). Using the arguments above in which the roles of H_1 and H_2 are interchanged, we obtain the first pair of equations of the system (2.5).

Thus, to complete the proof we have to use the compactness of the uniformly in n bounded sequences of analytics functions $\{f_n(z)\}$, $\{\Delta_{r,n}(z)\}$, $\{\Omega_{r,n}(z)\}$, $r=1,2$, and one-to-one correspondence between probability measures and their Stieljes transforms. ■

IV. EXAMPLES

(1) Consider the case when $N_2=(\delta_{-1}+\delta_1)/2$ and N_1 is arbitrary.

(a) In the case of measure N_1 having all moments finite this example for the commutator was calculated in Ref. 3. In our case the system (2.2) reduces to

$$f(z)=f_1\left(z-\frac{1+zf(z)-2\Delta_1(z)}{2f(z)}\right),$$
$$f(z)=f_{-1}\left(z-\frac{1+zf(z)+2\Delta_1(z)}{2f(z)}\right), \tag{4.1}$$

where

$$f_{-1}(z)=\int_{-\infty}^{+\infty}\frac{N_1(d\lambda)}{-\lambda-z}.$$

Setting in (4.1)

$$\hat{\Delta}_1(z)=1+zf(z)+2\Delta_1(z),\quad \hat{\Delta}_{-1}(z)=1+zf(z)-2\Delta_1(z),$$

we rewrite the system (4.1) in the form

$$f(z)=f_1\left(z-\frac{\hat{\Delta}_{-1}(z)}{f(z)}\right),$$
$$f(z)=f_{-1}\left(z-\frac{\hat{\Delta}_1(z)}{f(z)}\right),$$
$$f(z)=\frac{1-\hat{\Delta}_1(z)-\hat{\Delta}_{-1}(z)}{-z}.$$

Thus, according to Ref. 4, the limiting measure N of ensemble (1.1) in this case will be equal to the limiting NCM of the ensemble $A_n - U_n^* A_n U_n$.

(b) On other hand, in this case the system (2.5) will have the form

$$\begin{aligned} f(z)+\Delta_2(z) &= f_1\left(\frac{z}{2}-\frac{1}{2(f(z)+\Delta_2(z))}\right), \\ f(z)-\Delta_2(z) &= f_{-1}\left(\frac{z}{2}-\frac{1}{2(f(z)-\Delta_2(z))}\right). \end{aligned} \tag{4.2}$$

Setting

$$f_+(z)=f(z)+\Delta_2(z), \quad f_-(z)=f(z)-\Delta_2(z),$$

we split the system (4.2) into two equations,

$$f_+(z)=f_1\left(\frac{z}{2}-\frac{1}{2\,f_+(z)}\right),$$

$$f_-(z)=f_{-1}\left(\frac{z}{2}-\frac{1}{2\,f_-(z)}\right).$$

Thus, according to Ref. 4, the limiting measure $\widetilde{N}$ of ensemble (1.2) in this case will be equal to $\widetilde{N}=(N_+ + N_-)/2$, where the measures $N_\pm$ are the limiting NCMs of the ensembles $\pm(A_n + U_n^* A_n U_n)$.

(2) Consider the case when $N_1=\alpha\delta_a+\beta\delta_b$, $a<b$, $\alpha+\beta=1$, $\alpha,\beta>0$ and N_2 is semi-circular distribution

$$N_2(\mathrm{d}\lambda)=\frac{\sqrt{4w^2-\lambda^2}}{2\pi w^2}\,\mathrm{d}\lambda.$$

(a) In the special case this example was calculated also in Ref. 3. In our case the system (2.2) reduces to the equation

$$2w^2l^2z^2f^2(z)+z^3f(z)+z^2-2w^2l^2(\alpha-\beta)^2=0,$$

where $l=(b-a)/2$. Solving this equation we obtain

$$N(\mathrm{d}\lambda)=|\alpha-\beta|\,\delta_0+\frac{\sqrt{\lambda^2(8w^2l^2-\lambda^2)-16w^4l^4(\alpha-\beta)^2}}{4\pi w^2l^2|\lambda|}\chi_{[-\lambda_+,-\lambda_-]\cup[\lambda_-,\lambda_+]}(\lambda)\mathrm{d}\lambda,$$

where $\lambda_\pm=2wl\sqrt{1\pm\sqrt{1-(\alpha-\beta)^2}}$. In the case $\alpha=\beta$, N is semi-circular.

(b) Let us set $b=-a=l$. In this case the system (2.5) reduces to the equation

$$(2w^2l^2f^2(z)+zf(z)+1)(4w^2l^2f(z)+z)^2+2w^2l^2(\alpha-\beta)^2=0.$$

Solving this equation we obtain

$$\widetilde{N}(\mathrm{d}\lambda)=\left\{\frac{\sqrt{8w^2l^2-\lambda^2+\sqrt{(8w^2l^2-\lambda^2)^2-(\alpha-\beta)^2(8w^2l^2)^2}}}{4\sqrt{2}\pi w^2l^2}\chi_{[-\lambda_-,\lambda_-]}(\lambda)\right.$$
$$\left.+\frac{\sqrt{8w^2l^2(1+|\alpha-\beta|)-\lambda^2}}{8\pi w^2l^2}\chi_{[-\lambda_+,-\lambda_-]\cup[\lambda_-,\lambda_+]}(\lambda)\right\}\mathrm{d}\lambda,$$

where $\lambda_{\pm}=2wl\sqrt{2(1\pm|\alpha-\beta|)}$. In the case $\alpha=\beta$, N is semi-circular with parameter $2w^2l^2$; in the case $|\alpha-\beta|=1$, N is semi-circular with parameter $4w^2l^2$.

ACKNOWLEDGMENTS

The author is thankful to Professor Anne Boutet de Monvel and Professor L. Pastur for numerous helpful discussions. Thanks also to Ministère des Affaires Etrangères de France for financial support.

APPENDIX

Let us denote for any $q,r\in\mathbf{N}$, $\alpha=(\alpha_1,\ldots,\alpha_p)$, $\beta=(\beta_1,\ldots,\beta_p)$, $p=(p_1,\ldots,p_r)$, $\alpha_i,\beta_i,p_j\in\mathbf{N}$,

$$P_q\{\alpha,\beta\}\equiv\{\alpha_1,\beta_1\}\cdots\{\alpha_q,\beta_q\}=A_n^{\alpha_1}U_n^*B_n^{\beta_1}U_n\cdots A_n^{\alpha_q}U_n^*B_n^{\beta_q}U_n,$$

$$M_r^{(p)}(\alpha,\beta)\equiv M_r^{(p)}(P_{p_1}^{(1)}\{\alpha^{(1)},\beta^{(1)}\},\ldots,P_{p_r}^{(r)}\{\alpha^{(r)},\beta^{(r)}\})$$
$$=\langle n^{-1}\mathrm{Tr}P_{p_1}^{(1)}\{\alpha^{(1)},\beta^{(1)}\}\cdots n^{-1}\mathrm{Tr}P_{p_r}^{(r)}\{\alpha^{(r)},\beta^{(r)}\}\rangle,$$

where A_n and B_n are nonrandom $n\times n$ Hermitian matrices, U_n is a unitary random random matrix uniformly distributed over the unitary group $U(n)$ with respect to the Haar measure and $\langle\cdot\rangle$ denotes the average over unitary group.

Proposition A.1: For any n, r, p_j, $\alpha_i^{(j)}$, $\beta_i^{(j)}\in\mathbf{N}$ we have the following identity:

$$\begin{aligned}
M_r^{(p)}(\alpha,\beta)=\delta_{p_1,1}m_1^{(\alpha_1^{(1)})}m_2^{(\beta_1^{(1)})}M_{r-1}^{(p')}(\alpha',\beta')+(1-\delta_{p_1,1})&\\
\times\Bigg(m_1^{(\alpha_1^{(1)})}M_r^{(p_1-1,p')}(\{\alpha_2^{(1)},\beta_2^{(1)}\}\cdots\{\alpha_{p_1}^{(1)},\beta_{p_1}^{(1)}+\beta_1^{(1)}\},Q_{r-1}^{(p')}(\alpha',\beta'))&\\
+m_2^{(\beta_{p_1}^{(1)})}M_r^{(p_1-1,p')}(\{\alpha_1^{(1)}+\alpha_{p_1}^{(1)},\beta_1^{(1)}\}\cdots\{\alpha_{p_1-1}^{(1)},\beta_{p_1-1}^{(1)}\},Q_{r-1}^{(p')}(\alpha',\beta'))&\\
+\sum_{l=2}^{p_1-1}M_{r+1}^{(l-1,p_1-l,p')}(\{\alpha_1^{(1)}+\alpha_l^{(1)},\beta_1^{(1)}\}\cdots\{\alpha_{l-1}^{(1)},\beta_{l-1}^{(1)}\},&\qquad\text{(A1)}\\
\{\alpha_{l+1}^{(1)},\beta_{l+1}^{(1)}\}\cdots\{\alpha_{p_1}^{(1)},\beta_{p_1}^{(1)}+\beta_l^{(1)}\},Q_{r-1}^{(p')}(\alpha',\beta'))&\\
-\sum_{m=1}^{p_1-1}M_{r+1}^{(m,p_1-m,p')}(P_m^{(1)}\{\alpha^{(1)'},\beta^{(1)'}\},P_{p_1-m}^{(1)}\{\alpha^{(1)''},\beta^{(1)''}\},Q_{r-1}^{(p')}(\alpha',\beta')))&\\
+\frac{1-\delta_{r,1}}{n^2}\sum_{l=2}^{r}\sum_{m=1}^{p_l}(M_{r-1}^{(\hat{p},p_1+p_l-1,\tilde{p})}(Q_{l-2}^{(\hat{p})}(\hat{\alpha},\hat{\beta}),\{\alpha_1^{(l)},\beta_1^{(l)}\}\cdots\{\alpha_m^{(l)}&\\
+\alpha_1^{(1)},\beta_1^{(1)}\}\cdots\{\alpha_{p_1}^{(1)},\beta_{p_1}^{(1)}+\beta_m^{(l)}\}\cdots\{\alpha_{p_l}^{(l)},\beta_{p_l}^{(l)}\},Q_{r-l}^{(\tilde{p})}(\tilde{\alpha},\tilde{\beta}))&\\
-M_{r-1}^{(\hat{p},p_1+p_l,\tilde{p})}(Q_{l-2}^{(\hat{p})}(\hat{\alpha},\hat{\beta}),P_m^{(l)}\{\alpha^{(l)'},\beta^{(l)'}\}&\\
\times P_{p_1}^{(1)}\{\alpha^{(1)},\beta^{(1)}\}P_{p_l-m}^{(l)}\{\alpha^{(l)''},\beta^{(l)''}\},Q_{r-l}^{(\tilde{p})}(\tilde{\alpha},\tilde{\beta}))),&
\end{aligned}$$

where

$$m_1^{(\tau)}=n^{-1}\mathrm{Tr}A_n^{\tau},\quad m_2^{(\tau)}=n^{-1}\mathrm{Tr}B_n^{\tau},$$

$$p'=(p_2,\ldots,p_r),\quad Q_{r-1}^{(p')}(\alpha',\beta')=(P_{p_2}^{(2)}\{\alpha^{(2)},\beta^{(2)}\},\ldots,P_{p_r}^{(r)}\{\alpha^{(r)},\beta^{(r)}\}),$$

$$M_{r-1}^{(p')}(\alpha',\beta')=M_{r-1}^{(p')}(Q_{r-1}^{(p')}(\alpha',\beta')),$$

$$P_m^{(t)}\{\alpha^{(t)'},\beta^{(t)'}\}=\{\alpha_1^{(t)},\beta_1^{(t)}\}\cdots\{\alpha_m^{(t)},\beta_m^{(t)}\},\quad P_{p_t-m}^{(t)}\{\alpha^{(t)''},\beta^{(t)''}\}=\{\alpha_{m+1}^{(t)},\beta_{m+1}^{(t)}\}\cdots\{\alpha_{p_1}^{(t)},\beta_{p_t}^{(t)}\},$$

$$\hat{p}=(p_2,\ldots,p_{l-1}),\ \tilde{p}=(p_{l+1},\ldots,p_r),\quad Q_{l-2}^{(\hat{p})}=(P_2^{(2)}\{\alpha^{(2)},\beta^{(2)}\},\ldots,P_{p_{l-1}}^{(l-1)}\{\alpha^{(l-1)},\beta^{(l-1)}\}),$$

$$Q_{l-2}^{(\tilde{p})}=(P_{p_{l+1}}^{(l+1)}\{\alpha^{(l+1)},\beta^{(l+1)}\},\ldots,P_{p_r}^{(r)}\{\alpha^{(r)},\beta^{(r)}\}).$$

Proof: Consider the function

$$\Phi(U_n^*B_n^{\beta_1}U_n)=\langle(P_{p_1}^{(1)}\{\alpha^{(1)},\beta^{(1)}\})_{a,b}\,n^{-1}\mathrm{Tr}P_{p_1}^{(2)}\{\alpha^{(2)},\beta^{(2)}\}\cdots n^{-1}\mathrm{Tr}P_{p_r}^{(r)}\{\alpha^{(r)},\beta^{(r)}\}\rangle.$$

Using for this function Proposition 3.1, choosing the matrix X with only (a,b)-th nonzero entries and then applying $n^{-2}\Sigma_{a,b=1}^{n}$ we obtain the relation (A1). ■

Corollary: It follows from relation (A1) that any mixed moment $M_r^{(p)}(\alpha,\beta)$ can be represented as follows:

$$M_r^{(p)}(\alpha,\beta)=\sum_{a_i\geqslant 0,a_1+\cdots+a_{|\alpha|}=|\alpha|}\ \sum_{b_i\geqslant 0,b_1+\cdots+b_{|\beta|}=|\beta|}C_n(r;a,b)\prod_{i=1}^{|\alpha|}\prod_{j=1}^{|\beta|}m_1^{(a_i)}m_2^{(b_j)},$$

where $a=(a_1,\ldots,a_{|\alpha|})$ and $b=(b_1,\ldots,b_{|\beta|})$ are multi-indexes,

$$|\alpha|=\sum_{i=1}^{r}\sum_{j=1}^{p_i}\alpha_j^{(i)},\quad |\beta|=\sum_{i=1}^{r}\sum_{j=1}^{p_i}\beta_j^{(i)},$$

and the coefficients $C_n(r;a,b)$ are uniformly in n bounded as $n\to\infty$.

Remark A.1: In this article we deal with unitary and Hermitian matrices, i.e., we assume that the matrices U_n and V_n in (1.1) are unitary and A_n and B_n in (1.2) are Hermitian. It is natural also to consider the case of orthogonal U_n and W_n and real symmetric A_n and B_n. This case can be handled by using the analog of formula (3.2) of the orthogonal group $\mathrm{O}(n)$. Indeed, it is easy to see that this analog has the form

$$\int_{\mathbf{O}(n)}\Phi'(O^TMO)\cdot[X,O^TMO]\mathrm{d}O=0,$$

where O^T is the transposed to O and X is a real antisymmetric matrix. By using this formula, we obtain, e.g., instead of (3.10),

$$\begin{aligned}&2\langle(G(z)H_1)_{aa}(H_2G(z))_{bb}\rangle+\langle(G(z)H_1)_{ab}(H_2G(z))_{ab}\rangle+\langle(G(z)H_2)_{ab}(H_1G(z))_{ab}\rangle\\&\quad=\langle(G(z)H_1H_2)_{aa}G_{bb}(z)\rangle+\langle G_{aa}(z)(H_2H_1G(z))_{bb}\rangle+\langle(G(z)H_1H_2)_{ab}G_{ab}(z)\rangle\\&\qquad+\langle G_{ab}(z)(H_2H_1G(z))_{ab}\rangle.\end{aligned}$$

The last two terms on both sides of this formula give four additional terms in (3.16):

$$\langle-n^{-2}\mathrm{Tr}(H_1G)^TH_2G\rangle-\langle n^{-2}\mathrm{Tr}(H_2G)^TH_1G\rangle+\langle n^{-2}\mathrm{Tr}(H_1H_2G)^TG\rangle+\langle G^TH_2H_1G\rangle.$$

These terms, however, produce the asymptotically vanishing contribution to the remainder (3.16), because we have

$$\left|\langle -n^{-2}\mathrm{Tr}(H_1G)^TH_2G\rangle - \langle n^{-2}\mathrm{Tr}(H_2G)^TH_1G\rangle + \langle n^{-2}\mathrm{Tr}(H_1H_2G)^TG\rangle + \langle G^TH_2H_1G\rangle\right| \leqslant \frac{4}{ny_0^2}m_6^{1/3}.$$

Similar, and also negligible as $n\to\infty$, terms appear in formulas (3.20), (3.24), (3.56) and (3.92) in the proofs of Theorems 2.2 and 3.1. As a result, we obtain in this case the same systems (2.2) and (2.5), defining the Stieltjes transforms of the limiting eigenvalue counting measures of the analogs of ensembles (1.1) and (1.2) with the real symmetric A_n and B_n and orthogonal Haar-distributed U_n and V_n.

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Erratum: "*N* coupled nonlinear Schrödinger equations: Special set and applications to *N*=3" [J. Math. Phys. 43, 6325 (2002)]

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[DOI: 10.1063/1.1560857]

1. On page 6326, 3rd line below Eq.(6), $\phi_m(t-z/v)\exp\{i[t-z/(2v)]/(2v)\}$ should read $\phi_m(t-z/v)\exp\{\pm i\beta_m[t-z/(2v)]/(2v)\}$.
2. On page 6329, 3rd line should read $C_j=\{\pm 2[(N-j+1)!][c_1-2(j-1)^2\alpha^2]/(N+j-1)!\}^{1/2}$, for $j>1$.
3. On page 6333, 7th line from bottom should read $C_1=(D_1/D)^{1/2}$, $C_2=(D_2/D+6\beta_2 k^4\alpha^2)^{1/2}$, $C_3=(D_3/D+6\beta_3 k^2\alpha^2)^{1/2}$.
4. On page 6334, C_1 on the 2nd line should be replaced by C_1^2.
5. On page 6335:

(i) For $N=2$ interaction type $(++)$, the following solution should be added after the solutions $(2, 3)_2$ and $(1, 2)_1$:

$(2, 2)_1 \quad C_1^2+C_2^2=2\alpha^2, \quad c_1=c_2=-\alpha^2$.

(ii) For $N=3$, interaction type $(---)$ solution $(1, 2, 3)_2$, the inequality for c_1 should read $c_1>8\alpha^2$.

6. On page 6336, for interaction type $(-+-)$ solution $(1, 1, 2)_1$, the first equality should read $-C_1^2+C_2^2=-c_1$.
7. On page 6337, for interaction type $(++-)$:

(i) $(2, 2, 3)_2$ should be replaced by $(2, 3, 3)_2$.

(ii) The last equality for solution $(1, 2, 2)_1$ should read $c_2=c_3$.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

The discretized harmonic oscillator: Mathieu functions and a new class of generalized Hermite polynomials

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(Received 5 August 2002; accepted 21 January 2003)

We present a general, asymptotical solution for the discretized harmonic oscillator. The corresponding Schrödinger equation is canonically conjugate to the Mathieu differential equation, the Schrödinger equation of the quantum pendulum. Thus, in addition to giving an explicit solution for the Hamiltonian of an isolated Josephon junction or a superconducting single-electron transistor (SSET), we obtain an asymptotical representation of Mathieu functions. We solve the discretized harmonic oscillator by transforming the infinite-dimensional matrix-eigenvalue problem into an infinite set of algebraic equations which are later shown to be satisfied by the obtained solution. The proposed ansatz defines a new class of generalized Hermite polynomials which are explicit functions of the coupling parameter and tend to ordinary Hermite polynomials in the limit of vanishing coupling constant. The polynomials become orthogonal as parts of the eigenvectors of a Hermitian matrix and, consequently, the exponential part of the solution can not be excluded. We have conjectured the general structure of the solution, both with respect to the quantum number and the order of the expansion. An explicit proof is given for the three leading orders of the asymptotical solution and we sketch a proof for the asymptotical convergence of eigenvectors with respect to norm. From a more practical point of view, we can estimate the required effort for improving the known solution and the accuracy of the eigenvectors. The applied method can be generalized in order to accommodate several variables. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1561156]

I. INTRODUCTION

This paper is closely related to one of the famous eigenvalue problems, namely that of a one-dimensional harmonic oscillator. It is common knowledge that if the eigenvectors are required to have continuous second-order derivatives, each eigenvector is expressible as a product of a Hermite polynomial and an exponential term. The corresponding eigenvalues are equidistantly spaced and bounded from below. Another way to state the problem is given by the annihilation and creation operators which directly diagonalize the Hamiltonian. In comparison, the quartic anharmonic oscillator was solved by Bender and Wu in Ref. 1. A method for finding eigenvalues for anharmonic oscillators was created by Meißner and Steinborn in Ref. 2. A general method for polynomial potentials was introduced recently by Meurice.[3,4]

Instead of continuous functions, we consider functions defined only on a discrete, equidistantly-spaced and countable set on $\mathbb{R}$. The obvious advantage of this approach is that it transforms the problem into an eigenvalue problem of an infinite-dimensional, tri-diagonal matrix. The corresponding Schrödinger equation is canonically conjugate to the Mathieu differential equation.[5] Numerical solutions for noninteger orders are naturally obtained by diagonalizing the very same matrix, see Ref. 6 and the references therein for applications.

In physics, the discretized harmonic oscillator is manifestly realized by the Hamiltonian of an

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isolated Josephson junction[7,8] and the Hamiltonian of the, slightly misleadingly named, superconducting single-electron transistor (SSET).[8,9] Presently, excited states are seldom considered because of the radical approximations under which the Hamiltonian is solved. Even if the excited states are numerically obtained, it is not immediately evident, what happens when the coupling is changed. In this paper we give an explicit, asymptotical solution for the discretized harmonic oscillator which corresponds to strong Josephson coupling in case of the SSET. The same Hamiltonian also describes the so-called quantum pendulum, or a particle in a periodic potential.[10,11]

The corresponding asymptotical eigenvalues have been available for almost 50 years due to the work of Meixner and Schäfke on Mathieu functions in Ref. 12. First, by calculating the determinant of the matrix representation accurately enough, we continue this expansion by several orders in the coupling parameter. Then we propose an ansatz that transforms the matrix equation into an infinite set of algebraic equations and proceed by recursively solving these equations. The general properties of the coefficients in the ansatz can be obtained by studying any occurring regularities and reinserting these into the solution. Thus, in addition to the eigenvalues, we have successfully conjuctured the general form of the asymptotical eigenvectors. In each order of the expansion, the expressions are quoted in terms of an arbitrary quantum number, n, whenever possible. The leading terms have been determined and rephrased in terms of an arbitrary order, m, too. We find that the eigenvectors are asymptotical solutions of certain differential equations, which enables us to obtain further orders in their expansions.

The only real-valued parameter in the solution is the coupling constant, because all coefficients, both in the eigenvalues and in the ansatz are rational numbers. As a practical application, the rate of convergence of the solution towards numerically obtained, ''exact,'' solution, can be reliably estimated. In the asymptotical limit, the dependence in terms of n and m assumes the form of a simple monomial, at least down to the limits of numerical precision.

The solutions of order $m \leqslant 5$ are very simple to program and directly apply as numerical solutions of the discretized harmonic oscillator. For sufficiently small values of the coupling constant the eigenvectors are practically exact and thus they facilitate studies which require the structure of the excited states. We have proven, with the help of recursion relations of Hermite polynomials, that the first three leading orders of the obtained solution are correct. The calculation up to the seventh order should be performed in the future. We also outline an explicit proof concerning the normwise convergence of the eigenvectors. The asymptotical nature of the solutions must be stressed. A very thorough introduction on the subject has been given been given by Boyd in Ref. 13.

It is justified to ask, is the proposed solution completely new. The answer is, naturally, yes and no. Both discretized and discrete harmonic oscillators have been widely studied before. Both cases are related to orthogonal polynomials, so the work of Kravchuk[14] and Hahn[15] must be mentioned. The discrete harmonic oscillator, where the position coordinate is restricted to a finite number of values, is explicitly solved by Kravchuk polynomials as shown by Lorente in Ref. 16. Several discretizations of the harmonic oscillator have been previously solved, each giving rise to a specific class of generalized Hermite polynomials. Discretization by an exponential lattice $\{-q^n, q^n | n \in \mathbb{Z}\}$, where $0<q<1$, defines the so-called q-deformed harmonic oscillator and generalized q-Hermite polynomials which are rigorously discussed by Berg and Ruffing in Ref. 17. For other applications of the q-deformed harmonic oscillators, see, e.g., Refs. 18 and 19, where other discretizations are reviewed, too. Borzov, in Ref. 20, considers generalized derivation operators as generators of Hermite polynomials and states that the generalized Hermite polynomials either satisfy a second-order differential operator or there is no differential equation of finite order for these polynomials. Many other types of generalizations are also known, see e.g., the multidimensional Hermite polynomials of Rösler,[21] Hermite polynomials orthogonal with respect to the measure $|\xi|^{\gamma} \exp(-\xi^2) d\xi$, where $\gamma > -1$,[22,23] and parabosonic Hermite polynomials.[24] In the future, it must be established whether the presented class of Hermite polynomials is related to the q-Hermite polynomials, if it results from some other discretization or is it an explicit example of the second group of Borzov's categorization. Complementary results concerning the introduction of distant boundaries for the continuous problem are also known.[25,26] Finally, it should be empha-

sized that instead of deforming the harmonic oscillator, we solve its common-sense discretization, used especially in numerical calculations. The asymptotical effects of the discretization are explicitly calculated.

We also briefly consider the abruptly changing nature of the solutions when the coupling constant vanishes. This behavior is evident for both versions of the harmonic oscillator and the Mathieu differential equation. The asymptotical nature of the solutions and the eigenvalues is caused by this divergence. For the Mathieu equation this has been well documented, see, e.g., Refs. 5, 12, and 27. A more physically motivated approach is given by Bender, Pelster, and Weissbach in Ref. 28, where, e.g., the instanton equation and the Blasius equation are examined. The present methods are closely related to these, although we can not carry the calculation as far in the perturbative expansion. This is explained by the necessity of obtaining the expansion for the eigenvalues which makes the present problem technically more demanding.

The present method can be generalized in a fairly obvious manner. Other differential equations with analytical solutions can be discretized in the same manner if the correct expansions are found for all parts of the solution. An easier generalization is related to multi-dimensional difference equations with harmonic (quadratic) potential terms. The existing solution[29] for Hamiltonians of one-dimensional arrays of Josephson junctions become more transparent with the help of present formalism.

The paper is organized as follows. In Sec. II we define the discretized harmonic oscillator and connect it to the Mathieu differential equation as well as the continuous case. The solution ansatz and the resulting set of equations are reviewed. In Sec. III we quote our conjectures for the general form of the coefficients in the ansatz. We also present the explicit values of the leading coefficients. In Sec. IV we study solving the set of equations which yields the asymptotical eigenvectors. Efficient truncations of the set of equations are explained. The effort for improving the obtained results with the present method is estimated. In Sec. V we prove that the solution satisfies the difference equations, at least for the three leading orders. The rate of convergence and the induced asymptotical orthonormality are also reviewed. Finally, in Sec. VI the conclusions are drawn and an outlook of future possibilities is given.

A final note for those that are only interested in applying these results in numerical and/or theoretical analysis. Please review the beginning of Sec. II in order to find the correct parameters for the discretized harmonic or Mathieu equation. Then proceed to Sec. III and use the given expressions as approximate solutions in Eq. (30).

II. THE DISCRETIZED HARMONIC OSCILLATOR

The eigenvalue problem corresponding to the harmonic oscillator is the differential equation for $\psi(x)$,

$$-\frac{1}{2}\frac{d^2\psi}{dx^2}+\frac{\omega^2x^2}{2}\psi=\lambda\psi. \tag{1}$$

The eigenvectors corresponding to the well-known eigenvalues,

$$\lambda_n=\omega(n+1/2), \tag{2}$$

where $n=0,1,2,\ldots$, are given by

$$\psi_n(x)=A_nH_n(\xi)e^{-\xi^2/2}. \tag{3}$$

Here $\xi=\sqrt{\omega}\,x$, A_n is a normalization factor, and H_n is the Hermite polynomial of order n. The Hermite polynomials are solutions of the Hermite differential equation

$$y''-2xy'+2ny=0, \tag{4}$$

where $n=0,1,2,\ldots$. For our convenience, we write the polynomials, given by Rodrigues' formula, as

$$H_n(\xi)=(-1)^n \exp(\xi^2)\frac{d^n}{d\xi^n}\exp(-\xi^2)=\sum_{k=0}^{k'} h_k^{(n)}\xi^{n+2(k-k')}, \tag{5}$$

where $k':=\lfloor n/2\rfloor$, i.e., $k'=n/2$ if n is even and $k'=(n-1)/2$ if n is odd. The quantity k' proves to be extremely useful in further analysis. The Hermite polynomials satisfy the recursion relation

$$H_{n+1}(\xi)=2\xi H_n(\xi)-2nH_{n-1}(\xi). \tag{6}$$

Many of the generalizations of the Hermite polynomials boil down to a generalization of this recursion relation.[16,17,19,24]

The discretized version of Eq. (1) is obtained by restricting the values of x onto an evenly spaced, countable subset of $\mathbb{R}$. This corresponds e.g., to the discretization of charge in case of a Josephson junction or a SSET. Only the constant nearest-neighbor coupling is retained which yields a tri-diagonal matrix $H(x_0)$ with nonzero matrix elements

$$H_{jj}(x_0)=\tfrac{1}{2}\omega^2(j-x_0)^2, \quad H_{j+1,j}(x_0)=H_{j,j+1}(x_0)=-\tfrac{1}{2}. \tag{7}$$

Here the parameter $x_0\in[-\frac{1}{2},\frac{1}{2}]$ is the displacement of the origin with respect to the matrix element $j=0$. All eigenvalues of $H(x_0)$ have been translated by -1 in order to simplify the diagonal matrix elements. The standard way to write the Hamiltonian of an inhomogeneous SSET is obtained from Eqs. (7.36) and (7.39) of Ref. 8 and rephrasing it in terms of the number operator for Cooper pairs yields the matrix

$$H_{jj}^{(\mathrm{SSET})}(N_0)=E_C(j-N_0)^2, \quad H_{j+1,j}^{(\mathrm{SSET})}(N_0)=H_{j,j+1}^{(\mathrm{SSET})}(x_0)=-\tfrac{1}{2}E_J(\theta), \tag{8}$$

where N_0 is the number of Cooper pairs which minimizes the charging energy, $E_C=(2e)^2/2C_\Sigma$ is the unit of charging energy, and $E_J(\theta)$ is the effective Josephson energy which depends on the total phase θ across the SSET. Consequently, we solve the Hamiltonian of SSET if we find the eigenenergies and eigenvector for the discretized harmonic oscillator with $\omega=(2E_C/E_J(\theta))^{1/2}$.

In the following, we are searching for eigenvectors with finite Euclidean norm, i.e.,

$$\|\psi\|^2=\sum_{j=-\infty}^{\infty}|\psi_j|^2<\infty. \tag{9}$$

The existence and uniqueness of such solutions follows from the generalization of the Gershgorin eigenvalue theory by Shivakumar, Rudraiah, and Williams in Ref. 30. First the number of eigenvalues of $H(x_0)$ on a given interval can be shown to coincide with number of eigenvalues for a finite-dimensional truncation of the matrix, $H^{(N)}(x_0)$, if the dimension N is sufficiently large. A sufficient condition for this is that, in the ordered sequence of diagonal matrix elements, the difference between two consecutive values exceeds $4\times|-1/2|=2$. Furthermore, they prove that, for finite values of n, the eigenvector $\psi_n^{(N)}$ of $H^{(N)}(x_0)$ tends to the corresponding eigenvector of $H(x_0)$ when $N\to\infty$.

We now establish the connection between the $H(x_0)$ and the Mathieu differential equation[5]

$$\frac{d^2y}{dv^2}+(a-2q\cos(2v))y=0, \tag{10}$$

where a is the eigenvalue, also known as the characteristic value when the solution y has period of π or 2π. We follow the derivation of Shirts in Ref. 6 and use Floquet's theorem to obtain

$$y=\exp(i\nu v)P(v)=\exp(i\nu v)\sum_k c_{2k}\exp(2ikv), \tag{11}$$

where the Fourier expansion of $P(v)$ has been inserted. This corresponds to the matrix equation for the coefficients c_{2k} compactly written as

$$c_{2k-2}-V_{2k}c_{2k}+c_{2k+2}=0, \tag{12}$$

where $V_{2k}=[a-(\nu+2k)^2]/q$. This is identical to the discretized harmonic oscillator Hamiltonian $H(x_0)$ with an eigenvalue λ after identifications

$$\nu=-2x_0, \quad k=j, \quad q=4/\omega^2, \quad a=8\lambda/\omega^2, \tag{13}$$

where elements are identified according to $2k\leftrightarrow j$. Thus all results obtained for the discretized harmonic oscillator also hold for Mathieu functions (11) with parameters given in Eq. (13). For $x_0=0$ and $x_0=\pm\frac{1}{2}$ the solutions of $H(x_0)$ can be chosen to be even or odd with respect to j. This corresponds to writing $P(v)$ in terms of sines and cosines. Special attention must be given to the even solutions of $H(x_0=0)$, where the resulting equations in the matrix representation read

$$-\psi_1/\sqrt{2}=\lambda_{2n}\psi_0, \tag{14}$$

$$-\psi_0/\sqrt{2}+\omega^2\psi_1/2-\psi_2/2=\lambda_{2n}\psi_1, \tag{15}$$

$$-\psi_{j-1}/2+\omega^2 j^2\psi_j/2-\psi_{j+1}/2=\lambda_{2n}\psi_j, \quad j\geqslant 2. \tag{16}$$

The eigenvalues for $x_0=0$ correspond to characteristic values $\{a_{2n}(q),b_{2n}(q)\}$, while the case $x_0=\pm\frac{1}{2}$ is linked to $\{a_{2n+1}(q),b_{2n+1}(q)\}$ as defined in Ref. 5.

The asymptotical expansion of the eigenvalues corresponding to the limit $q\to\infty$ or $\omega\to 0$ was obtained by Meixner and Schäfke in Ref. 12. The derivation of the eigenvalues is based on the three-term recurrence relations for the Mathieu functions and the requirement that the norm of the error in the eigenvalue equation vanishes faster than a specific power of ω. Meixner and Schäfke quote the asymptotical characteristic values of the Mathieu equation up to and including the order ω^7 in Theorem 7 in Sec. 2.3. Some error estimates for asymptotical expansions of Mathieu functions by Kurz are given in Ref. 27. Because the Mathieu equation is also the Schrödinger equation of the quantum pendulum or a particle in a periodic potential, it has been studied independently in physics, too.[10,11,31] Especially, the same general expansion for eigenvalues and several further terms for the ground state energy were obtained by Stone and Reeve in Ref. 11.

In this limit, we can write the eigenvalues of $H(x_0)$ as

$$\lambda_n\sim\sum_{m=0}^{\infty}\lambda_n^{(m)}\omega^m, \tag{17}$$

where $\omega\to 0$, and

$$\lambda_n^{(m)}=\sum_{k=0}^{m'}\lambda_{n,k}^{(m)}\hat{n}^{m+2(k-m')} \tag{18}$$

with $\hat{n}:=2n+1$ and $m'=\lfloor m/2\rfloor$. This structure is identical to that of the Hermite polynomials (5), if one identifies $\hat{n}$ with ξ. By Ref. 12, the eigenvalues (20) do depend on x_0, but this dependence decreases exponentially as $\omega\to 0$. The maximal difference is given by[12]

$$\lambda_n(x_0=\pm\tfrac{1}{2})-\lambda_n(x_0=0)\sim(-1)^n B_0(1-B_1\omega)\omega^{-n-3/2}\exp(-8/\omega), \tag{19}$$

where B_0 and B_1 depend on n but not on ω.

This allows us to write the eigenvalues of $H(x_0)$ as

$$\lambda_n \sim -1+\frac{\omega\hat{n}}{2}-\frac{\omega^2 d_2}{2^6}-\frac{\omega^3 d_3}{2^{11}}-\frac{\omega^4 d_4}{2^{17}}-\frac{\omega^5 d_5}{2^{23}}-\frac{\omega^6 d_6}{2^{27}}-\frac{\omega^7 d_7}{2^{33}}-\frac{\omega^8 d_8}{2^{40}}-\frac{\omega^9 d_9}{2^{47}}-\frac{\omega^{10} d_{10}}{2^{51}}$$
$$-\frac{\omega^{11} d_{11}}{2^{57}}-\frac{\omega^{12} d_{12}}{2^{61}}-\frac{\omega^{13} d_{13}}{2^{69}}-\frac{\omega^{14} d_{14}}{2^{72}}-\frac{\omega^{15} d_{15}}{2^{79}}-\frac{\omega^{16} d_{16}}{2^{87}}+\mathcal{O}(\omega^{17}), \tag{20}$$

where the coefficients d_k read

$$d_2=\hat{n}^2+1,$$

$$d_3=\hat{n}^3+3\hat{n},$$

$$d_4=5\hat{n}^4+34\hat{n}^2+9,$$

$$d_5=33\hat{n}^5+410\hat{n}^3+405\hat{n},$$

$$d_6=63\hat{n}^6+1260\hat{n}^4+2943\hat{n}^2+486,$$

$$d_7=527\hat{n}^7+15617\hat{n}^5+69001\hat{n}^3+41607\hat{n},$$

$$d_8=9387\hat{n}^8+388780\hat{n}^6+2845898\hat{n}^4+4021884\hat{n}^2+506979,$$

$$d_9=175045\hat{n}^9+9702612\hat{n}^7+107798166\hat{n}^5+288161796\hat{n}^3+130610637\hat{n},$$

$$d_{10}=422565\hat{n}^{10}+30315780\hat{n}^8+480439190\hat{n}^6+2135766820\hat{n}^4+2249346285\hat{n}^2+238353840,$$

$$d_{11}=4194753\hat{n}^{11}+379291385\hat{n}^9+8186829426\hat{n}^7+55529955498\hat{n}^5+110241863469\hat{n}^3$$
$$+41540033277\hat{n},$$

$$d_{12}=10645960\hat{n}^{12}+1187264199\hat{n}^{10}+33678377895\hat{n}^8+327725946398\hat{n}^6+1081358909790\hat{n}^4$$
$$+940077055035\hat{n}^2+88258370067,$$

$$d_{13}=440374207\hat{n}^{13}+59495737574\hat{n}^{11}+2155821044201\hat{n}^9+28738150160500\hat{n}^7$$
$$+1448212492647 69\hat{n}^5+236410740537606\hat{n}^3+78243613727607\hat{n},$$

$$d_{14}=578183175\hat{n}^{14}+93209584104\hat{n}^{12}+4215683624295\hat{n}^{10}+74269604367684\hat{n}^8$$
$$+537905750769429\hat{n}^6+1456767306013752\hat{n}^4+1105711550410653\hat{n}^2$$
$$+94839535889532,$$

$$d_{15}=12308013927\hat{n}^{15}+2337227706555\hat{n}^{13}+129437253243675\hat{n}^{11}+2928506455684095\hat{n}^9$$
$$+29119560960614085\hat{n}^7+120372998803922241\hat{n}^5+170921920649402745\hat{n}^3$$
$$+51316344023990085\hat{n},$$

$$d_{16}=530039126159\hat{n}^{16}+117243302735480\hat{n}^{14}+7823093961425652\hat{n}^{12}$$
$$+222043810819026856\hat{n}^{10}+2924952921130025194\hat{n}^8+17380315268028265224\hat{n}^6$$
$$+40851669411526600980\hat{n}^4+27983551470330365784\hat{n}^2+2235152520630714879.$$

We obtain the terms for orders $8 \leqslant m \leqslant 11$ by exploiting Eq. (18) when explicitly evaluating the determinant of Eq. (7). As a first step, setting $x_0 = 0$ halves the dimension of the tri-diagonal matrix. Next, by translating one of the eigenvalues close to zero by substracting the known expansion of this eigenvalue, the determinant becomes an essentially linear function of the chosen, translated eigenvalue. The next unknown term is inserted as a parameter and the determinant is calculated for several values of ω, preferably in the form $\{2^{-k}\omega_0\}_{k=0}^{3-5}$. This choice lets us separate the leading correction and the subsequent corrections. In order to obtain the terms d_{2k} and d_{2k+1}, we must correctly determine all eigenvalues λ_n when $n \leqslant k$. Sufficient accuracy is guaranteed by using the high-precision numerics of MATHEMATICA software. The method for obtaining the orders $m > 11$ requires explicit knowledge on the properties of the eigenvectors and the discussion is postponed until the end of Sec. III.

The asymptotical nature of the expansion means that for each value of ω and n, there exists and optimal order m which minimizes the error in the eigenvalue, i.e., the function

$$\Delta\lambda(\omega,n,m) := \left| \lambda_n - \sum_{m'=0}^{m} \lambda_n^{(m')} \omega^{m'} \right|, \tag{21}$$

with respect to m. The exact eigenvalue λ_n exists and is finite for all nonzero values of ω according to the Sturmian theory of second-order linear differential equations, see e.g., Ref. 5. In other words, for sufficiently small values of ω the error is dominated by the first omitted term, i.e., $\Delta\lambda(\omega,n,m) \sim |\lambda_n^{(m+1)}| \omega^{m+1}$. Because the asymptotical eigenvalue is divergent, it surely crosses the exact eigenvalue when ω is increased, but this occurs outside the range of asymptotical convergence. Similar asymptotical convergence should be observed for the asymptotical eigenvectors, too. Assuming $\psi_n^{(m,x_0)}$ corresponds to the asymptotical expansion of the eigenvalues up to and including order ω^m, we expect error in the norm to behave as

$$\| \psi_n^{(m,x_0)} - \psi_n^{(x_0)} \| \sim C(n,m) \omega^m, \tag{22}$$

where $\omega \to 0$ and $C(n,m)$ is a simple function of n and m. Although this has not been proven, Eq. (22) appears to be correct and we will ultimately give an approximate expression for $C(n,m)$, too. Outside the regime of asymptotical convergence the error (22) approaches $\sqrt{2}$ as the asymptotical solution becomes orthogonal to the exact one.

Next we show that the discrete eigenvalue problem Eq. (7) is a meaningful asymptotical limit of the continuous harmonic oscillator equation (1). The problems are identical in the leading infinitesimal order when ω is infinitesimal, but the limit $\omega \to 0$ is subtle. As long as $\omega > 0$, both the eigenvalues and eigenvectors of the discretized problem tend to those of the continuous harmonic oscillator with this ω. For $\omega = 0$ the continuous problem becomes abruptly the free particle Hamiltonian with solutions

$$\psi_{\omega=0}(x) = e^{ikx}, \quad \lambda_{\omega=0} = k^2/2, \tag{23}$$

where k is the standard name for the wave number. Simultaneously the discretized problem becomes the well-known nearest-neighbor chain with eigenvectors and eigenvalues,

$$\psi_k = \{e^{ik(j-x_0)}\}_j, \quad \lambda_{\omega=0} = -\cos(k). \tag{24}$$

For sufficiently small values of k we have $\lambda_{\omega=0} \approx -1 + k^2/2$, in agreement with Eq. (23). In contrast, we are interested in the bound-state solutions of Eq. (1) and those eigenvectors of the discretized problem that can be uniquely related to these continuous solutions for $\omega > 0$.

The harmonic oscillator is discretized by restricting the values of x onto a countable and evenly spaced subset of $\mathbb{R}$. The lowest-order central approximation for a second-order derivative is simply

$$\psi''(x)=\frac{\psi(x-h)-2\psi(x)+\psi(x+h)}{h^2}[+\mathcal{O}(h^4)]. \tag{25}$$

Assuming $\psi(x)$ to be real analytic allows us to write the numerator of the right-hand side as a Taylor series

$$\psi(x+h)-2\psi(x)+\psi(x-h)=\sum_{k=1}^{\infty}\frac{2h^{2k}}{(2k)!}\frac{d^{2k}\psi(x)}{dx^{2k}}. \tag{26}$$

If h is infinitesimal and as the derivatives of ψ are finite in all orders, the only remaining term is $h^2\psi''(x)$. Thus, in the lowest infinitesimal order the discretized eigenvalue problem gives a second-order differential equation

$$-\frac{1}{2}\frac{d^2\psi_x}{dx^2}+\frac{\omega^2x^2}{2h^2}\psi_x=h^{-2}(-1+\lambda)\psi_x \tag{27}$$

which is identical to Eq. (1) apart from the constant $-h^{-2}$ and the redefinitions $\omega\mapsto\omega/h$ and $\lambda\mapsto\lambda/h^2$. The discreteness of the problem can also be varied by rescaling the value of ω. Thus, instead of decreasing the size h of the steps, we set $h=1$ and let $\omega\to0$. From Eq. (27) we see that asymptotically the eigenvalues and eigenvectors have the form $\lambda_n\sim-1+\omega(n+1/2)$ and $\psi_x\sim\psi(x)$, as expected.

We have already pointed out that the matrix $H(x_0)$ in Eq. (7) can be derived from the Mathieu equation. The underlying reason for this is that the problems are canonically conjugate. Inserting the full expansion Eq. (26) into Eq. (27) yields an obvious differential equation in ψ_x with respect to x. The canonical transformation $id/dx\to\tilde{v}$ and $x\to-id/d\tilde{v}$ preserves the eigenvalues and produces the differential equation

$$-\frac{\omega^2}{2}\frac{d^2\psi_{\tilde{v}}}{d\tilde{v}^2}-\left(\sum_{k=0}^{\infty}\frac{(-1)^k\tilde{v}^{2k}}{(2k)!}\right)\psi_{\tilde{v}}=\lambda\psi_{\tilde{v}}. \tag{28}$$

Noticing that the sum is equal to $\cos(\tilde{v})$ and setting $v:=(\tilde{v}+\pi)/2$, we obtain the canonical form of the Mathieu equation with parameters given in Eq. (13).

After these important preliminaries, we are able to proceed towards the actual solution for the discretized harmonic oscillator. In order to treat eigenvectors of all matrices $H(x_0)$ on an equal footing, we replace the index j by $x:=j-x_0$. For arbitrary values of x_0 and j the new index x becomes a continuous one on $\mathbb{R}$. We thus obtain functions $\psi_x^{(n)}$, where n is the state index. We propose that these functions $\psi_x^{(n)}$ are real-analytic and that they give the eigenvectors of $H(x_0)$ asymptotically, i.e.,

$$\psi_n^{(x_0)}\sim\{\psi_{j-x_0}^{(n)}\}_{j=-\infty}^{\infty} \tag{29}$$

when $\omega\to0$. The problem tends to the continuous one in the lowest (infinitesimal) approximation in ω. Thus it is reasonable to assume that the lowest-order approximation for the solution functions is given by $\psi_x^{(n)}\sim\psi_n(x)$ as $\omega\to0$.

The general form of the asymptotical solution of the discretized harmonic oscillator now reads

$$\psi_x^{(n)}\propto\exp\left(\sum_{k=1}^{\infty}\sum_{l=k}^{\infty}\alpha_{kl}^{(n)}\omega^{l-1}\xi^{2k}\right)\sum_{k=0}^{k'}\sum_{l=1}^{\infty}(h_k^{(n)}\omega^{l-1}\beta_{kl}^{(n)}\xi^{n+2(k-k')}), \tag{30}$$

where $\alpha_{kl}^{(n)}$ and $\beta_{kl}^{(n)}$ are constants to be determined. The solution to the continuous case yields $\alpha_{1,1}^{(n)}=-1/2$ and $\beta_{k,1}^{(n)}=1$. We are free to normalize the solution so we can choose $\beta_{0,l}^{(n)}=0$ for $l>1$.

The main point of introducing the functions $\psi_x^{(n)}$ is that they transform the difference-equation-type eigenvalue problem corresponding to the discretized harmonic oscillator into an infinite set of algebraic equations for each value of n. The eigenvalues (20) appear as parameters and they are required in order to solve the equations for the sets of coefficients $\{\alpha_{kl}^{(n)}\}$ and $\{\beta_{kl}^{(n)}\}$. Fortunately, the equations uniquely determine every single coefficient. Because the expansion of the eigenvalues is asymptotical, the meaning of the full solution to these equations must be determined later.

In practice, we need a suitable truncation of Eq. (30) and thus we define an (un-normalized) approximate eigenvector

$$\psi_n^{(m,x_0)} := \{\psi_{j-x_0}^{(n,m)}\}_{j=-\infty}^{\infty}, \tag{31}$$

where $\psi_x^{(n,m)}$ contains only those terms with $l \leqslant m$. The definition of $\psi_n^{(1,x_0)}$ obviously coincides with the continuous solution at x_0. In numerical calculations, and always for even values of m, we must truncate the eigenvector with respect to j, by setting $(\psi_n^{(m,x_0)})_j = 0$ for components $|j| > j_0$ with a sufficiently large value of j_0.

We now give the infinite set of algebraic equations corresponding to the transformation of the difference equation when the solution functions $\psi_x^{(n)}$ are substituted into the eigenvalue equation. Rearranging the terms, we find that each equation can be written in the form

$$\frac{\psi_{x-1}^{(n)} + \psi_{x+1}^{(n)}}{2} = \psi_x^{(n)}(-\lambda_n + \omega^2 x^2/2), \tag{32}$$

where $x = j - x_0$. Inserting the general ansatz (30) into Eq. (32) expresses the equation in terms of ξ and ω. The exponential part of the ansatz on the right-hand side canceled simply by substracting the corresponding exponent from those on the left-hand side. This yields an equation

$$\begin{aligned}
&\frac{1}{2}\Bigg[\exp\Bigg(\sum_{k=1}^{\infty} \sum_{l=k}^{\infty} \alpha_{kl}^{(n)} \omega^{k+l-1} [(x-1)^{2k} - x^{2k}] \Bigg) \sum_{k=0}^{k'} \sum_{l=1}^{\infty} (h_k^{(n)} \omega^{l-1} \beta_{kl}^{(n)} [\sqrt{\omega}(x-1)]^{n+2(k-k')}) \\
&\quad + \exp\Bigg(\sum_{k=1}^{\infty} \sum_{l=k}^{\infty} \alpha_{kl}^{(n)} \omega^{k+l-1} [(x+1)^{2k} - x^{2k}] \Bigg) \sum_{k=0}^{k'} \sum_{l=1}^{\infty} (h_k^{(n)} \omega^{l-1} \beta_{kl}^{(n)} [\sqrt{\omega}(x+1)]^{n+2(k-k')}) \Bigg] \\
&\quad = \Bigg[-\sum_{m=0}^{\infty} \lambda_{n(m)} \omega^m + \frac{\omega^2 x^2}{2} \Bigg] \sum_{k=0}^{k'} \sum_{l=1}^{\infty} (h_k^{(n)} \omega^{l-1} \beta_{kl}^{(n)} [\sqrt{\omega}\, x]^{n+2(k-k')}).
\end{aligned} \tag{33}$$

These equations are then expanded as functions of x and ω as the resulting equations are easier to solve. The equations must hold for all values of the linearly independent variables x and ω so each equation must be solved separately. For the purposes of generality, it would be preferable to expand with respect to ξ, but the resulting equations are much more difficult, both to obtain and to solve. Nevertheless, the obtained solution can be inserted into to these equations in order to show that the results are correct. This will be done in Sec. V.

In order to obtain the eigenvector $\psi_n^{(m,x_0)}$ we must solve and satisfy all equations corresponding to

$$\{\{\omega^{m'} \xi^{n+2m'-2l'}\}_{l'=0}^{m'+k'}\}_{m'=0}^{m}. \tag{34}$$

This is of course done recursively, by inserting the known part of the solution and solving for the next level. In order to connect Eq. (34) with the order of the solution, we state that the equations corresponding to a fixed value of m' uniquely determines the coefficients with $l = m'$.

After a while, one starts to see regularities in the coefficients and attempts to express these in a functional form. We have been able to find rather general expressions for the coefficients. This

means that the coefficients have been expressed in terms of n and the order of the expansion, whenever this is possible. We have conjectured the general form of the terms which means that we know how far away we are from obtaining further terms.

We have found that the functions $\psi_x^{(n,m)}(\xi)$ are asymptotical solutions of the differential equation

$$\left(-\sum_{k=0}^{m} \frac{\omega^k}{(2k)!} \frac{d^{2k}}{d\xi^{2k}} + \frac{\omega\xi^2}{2} \right) \psi_x^{(n,m)} = \sum_{k=0}^{m} \lambda_n^{(k)} \omega^k \psi_x^{(n,m)} \tag{35}$$

in a specific sense. After all derivatives have been carried out, the terms multiplying the common exponential factor cancel up to and including the order ω^m. If the solution $\psi_x^{(n,m-1)}$ is known, we obtain an explicit differential equation for the exponential part $\omega^{m-1} f_m(\xi)$, the correction to the Hermite polynomial $\omega^{m-1} g_m(\xi)$ and the energy eigenvalue $\lambda_n^{(m)}$. In case of the ground state and the first excited state $(n=1)$, the condition, $g_m(\xi)=0$ for $m>1$, renders the problem solvable. For $n \geqslant 2$ we must insert the ansatz (30) in order to obtain the solution.

The results are, naturally, in complete agreement with those obtained by using the difference equation. We are using just another representation of the original problem. Equation (35) enables us to obtain the solutions for fixed values of n up to relatively high orders with respect to powers of ω. Thus we can both extend the general expression for the eigenenergies in Eq. (20) and those for the coefficients in the exponential part of the solutions. For the ground state energy, we find the terms beyond order ω^{16} to be

$$\begin{aligned}
&- \frac{363372562420411197\,\omega^{17}}{2^{79}} - \frac{6258692522467212813\,\omega^{18}}{2^{83}} - \frac{227867608383920243815\,\omega^{19}}{2^{88}} \\
&- \frac{4372199488222446620121\,\omega^{20}}{2^{92}} - \frac{3528079925224487409071 63\,\omega^{21}}{2^{98}} \\
&- \frac{7465886451386334274097895\,\omega^{22}}{2^{102}} - \frac{3307527354378972602024109 59\,\omega^{23}}{2^{107}} \\
&- \frac{765423730757089866585192 7581\,\omega^{24}}{2^{111}} - \frac{1477812451863756884805687589129\,\omega^{25}}{2^{118}} \\
&- \frac{3713271881925876341845235739 0369\,\omega^{26}}{2^{122}} \\
&- \frac{1939848955425261040700592191917783\,\omega^{27}}{2^{128}} \\
&- \frac{5259857310102927552686981463533 6865\,\omega^{28}}{2^{131}} \\
&- \frac{5914101566562517015636997146651378649\,\omega^{29}}{2^{137}} \\
&- \frac{1721293554549854866839521988306985061 49\,\omega^{30}}{2^{141}} \\
&- \frac{1036239234300373834418904578648469718 2753\,\omega^{31}}{2^{146}} + \mathcal{O}(\omega^{32}).
\end{aligned} \tag{36}$$

The corresponding asymptotical eigenvector contains $31(1+31)/2=496$ linearly independent terms. The coefficient of $\omega^{30}\xi^2$ in the exponential part reads

$$-\frac{52073289804594394288581898717780194255195675647281 93}{27652924046177972695504290658083968267415715 84}. \tag{37}$$

The general solution is given in the next section.

III. THE GENERAL SOLUTION OF THE DISCRETIZED HARMONIC OSCILLATOR

For reasons of completeness and easy accessibility some of the definitions will be repeated in this section. The mth order solution function $\psi_x^{(n,m)}$, corresponds all terms up to and including $l=m$ in Eq. (30). The asymptotical expansion of the eigenvalues λ_n is given in Eq. (20). The state index n determines two expansion parameters,

$$\hat{n} := 2n+1 \quad \text{and} \quad k' := \lfloor n/2 \rfloor, \tag{38}$$

where $k'=n/2$ if n is even and $k'=(n-1)/2$ if n is odd. The gamma function $\Gamma(x)$ is the generalized factorial with the defining property $x\Gamma(x)=\Gamma(x+1)$. We need the values for integer and half-integer values which read

$$\Gamma(k)=(k-1)!, \quad \Gamma(k+\tfrac{1}{2})=2^{-k}\sqrt{\pi}(2k-1)!!, \tag{39}$$

where the double factorial $k!!$ for integer values of k is given by $k(k-2)\times\cdots\times(1 \text{ or } 2)$. The coefficients in the Hermite polynomials simplify to

$$h_k^{(n)}=\frac{(-1)^{k'+k}2^{2k+(1-(-1)^n)/2}n!}{(2k+(1-(-1)^n)/2)!(k'-k)!}. \tag{40}$$

A convenient normalization for the eigenvectors is obtained by requiring that

$$\psi_x^{(n)} \sim \xi^{(1-(-1)^n)/2}, \quad x \to 0, \tag{41}$$

i.e., ~ 1 for even values of n and $\sim \xi$ for odd values of n. Also bear in mind that

$$\alpha_{1,1}^{(n)}=-1/2, \quad \beta_{k,1}^{(n)}=1, \text{ and } \beta_{0,l(>1)}^{(n)}=0. \tag{42}$$

Under these constraints we have conjectured that the general form of the coefficients. In the exponential part,

$$\exp\left(\sum_{k=1}^{\infty}\sum_{l=k}^{\infty}\alpha_{kl}^{(n)}\omega^{l-1}\xi^{2k}\right), \tag{43}$$

the coefficients can be written as

$$\alpha_{k,k+l}^{(n)}=\sum_{l'=0}^{l}\alpha_{k,k+l}^{[l']}\hat{n}^{l'}. \tag{44}$$

Please note that if the coefficient $\alpha_{kl}^{(n)}$ are written as polynomials in n instead of $\hat{n}$, the signs of the corresponding expansion coefficients $\tilde{\alpha}_{k,k+l}^{[l']}$ appear to be given by $(-1)^k$. An efficient way to write these coefficients is given by

$$\alpha_{k,k+l}^{(n)}=(-1)^k 2^{-2k}\left(\sum_{l'=0}^{\lfloor l/2\rfloor}\frac{\Gamma(k+1/2)Q(k,l,2k-5+l')\hat{n}^{l-2l'}}{\Gamma(k+l)\sqrt{\pi}} + \sum_{l'=0}^{\lfloor (l-1)/2\rfloor}\overline{Q}(k,l,k-2+l')\hat{n}^{l-1-2l'}\right), \tag{45}$$

where $Q(k,l,2k-5+l')$ and $\overline{Q}(k,l,k-2+l')$ are polynomials in k of orders $2k-5+l'$ and $k-2+l'$, respectively. An important consequence of Eq. (45) is that regardless of the values of l and n we have

$$\lim_{k\to\infty} \alpha^{(n)}_{k+1,k+1+l}/\alpha^{(n)}_{k,k+l} = -1/4. \tag{46}$$

The explicit expressions for the seven leading coefficients have been obtained and they read

$$\alpha^{(n)}_{kk} = \frac{(-1)^k 2^{2-2k}\Gamma(k+1/2)}{k(2k-1)^2\Gamma(k)\sqrt{\pi}},$$

$$\alpha^{(n)}_{k,k+1} = (-1)^k 2^{-2-2k}\left(\frac{1}{k} + \frac{\Gamma(k+1/2)}{\Gamma(k+1)\sqrt{\pi}}\frac{\hat{n}}{k}\right),$$

$$\alpha^{(n)}_{k,k+2} = (-1)^k 2^{-4-2k}\left(\hat{n} + \frac{\Gamma(k+1/2)}{24\Gamma(k+2)\sqrt{\pi}}[(3+52k+40k^2)+(9+12k)\hat{n}^2]\right),$$

$$\alpha^{(n)}_{k,k+3} = (-1)^k 2^{-9-2k}\Bigg\{(-1+7k+5k^2)+(3+4k)\hat{n}^2 + \frac{\Gamma(k+1/2)}{24\Gamma(k+3)\sqrt{\pi}}\times[(243+1119k + 1928k^2+1376k^3+320k^4)\hat{n}+(33+101k+104k^2+32k^3)\hat{n}^3]\Bigg\},$$

$$\begin{aligned}\alpha^{(n)}_{k,k+4} = (-1)^k 2^{-14-2k}\Bigg\{&(53+120k+136k^2+40k^3)\hat{n}+(37+72k+32k^2)\hat{n}^3/3 + \frac{\Gamma(k+1/2)}{48\Gamma(k+4)\sqrt{\pi}}\\ &\times[(-2612925-5292132k+10675063k^2+36766856k^3+40148416k^4+21300608k^5\\ &+5544448k^6+565760k^7)/315+(11070+60044k+130810k^2+142112k^3+81280k^4\\ &+23168k^5+2560k^6)\hat{n}^2+(585+2288k+3585k^2+2696k^3+960k^4+128k^5)\hat{n}^4]\Bigg\},\end{aligned}$$

$$\begin{aligned}\alpha^{(n)}_{k,k+5} = (-1)^k 2^{-20-2k}\Bigg\{&(-5187-672k+6580k^2+7684k^3+3164k^4+452k^5)/3+(1214+3744k\\ &+4080k^2+1968k^3+320k^4)\hat{n}^2+(345+808k+576k^2+128k^3)\hat{n}^4/3+\frac{\Gamma(k+1/2)}{48\Gamma(k+5)\sqrt{\pi}}\\ &\times[(740893230+3944788389k+9627147810k^2+14943869467k^3+15287941200k^4\\ &+10116675072k^5+4238798592k^6+1079918592k^7+152076288k^8+9052160k^9)\hat{n}/315\\ &+(1825740+11037114k+27955236k^2+37919062k^3+30169312k^4+14491648k^5\\ &+4122880k^6+636928k^7+40960k^8)\hat{n}^3/3+(85050+381087k+729798k^2+752369k^3\\ &+447024k^4+152576k^5+27648k^6+2048k^7)\hat{n}^5/5]\Bigg\},\end{aligned}$$

$$\alpha_{k,k+6}^{(n)}=(-1)^k 2^{-26-2k}\Big\{(378033+496368k+786528k^2+710816k^3+339904k^4+79552k^5$$
$$+7232k^6)\hat{n}/3+(69714+241312k+303392k^2+177696k^3+49408k^4+5120k^5)\hat{n}^3/3$$
$$+(17217+45360k+40960k^2+15360k^3+2048k^4)\hat{n}^5/15+\frac{\Gamma(k+1/2)}{180\Gamma(k+6)\sqrt{\pi}}$$
$$\times[(-24640192386810-105728184475128k-155775948330744k^2$$
$$-74654535511116k^3+74660144680858k^4+156803802177352k^5$$
$$+134434233033760k^6+70722102090816k^7+24590691451392k^8+5680345583616k^9$$
$$+839668527104k^{10}+71921254400k^{11}+2714009600k^{12})/9009+(22093103970$$
$$+162201234402k+504160865145k^2+882850470198k^3+986932878421k^4$$
$$+745434338828k^5+388089936864k^6+138972684672k^7+33504543744k^8$$
$$+5179637760k^9+462565376k^{10}+18104320k^{11})\hat{n}^2/21+(152041050+991922940k$$
$$+2784482730k^2+4353707520k^3+4203836660k^4+2632731680k^5+1088777440k^6$$
$$+294912320k^7+50245120k^8+4874240k^9+204800k^{10})\hat{n}^4+(2606310+12799746k$$
$$+27798345k^2+34245070k^3+26181505k^4+12857468k^5+4055200k^6+792320k^7$$
$$+87040k^8+4096k^9)\hat{n}^6]\Big\}.$$

Thus, for an arbitrary order m, we can obtain the expressions for coefficients corresponding to $\{\omega^{m-1}\xi^{2(m-l')}\}_{l'=0}^{6}$. Furthermore we find

$$\alpha_{1,8}^{(n)}=-(505549159\hat{n}+177209155\hat{n}^3+8289645\hat{n}^5+40329\hat{n}^7)/2^{37}$$
$$-(-2741702+12248825\hat{n}^2+1518052\hat{n}^4+26073\hat{n}^6)/2^{32},$$

$$\alpha_{1,9}^{(n)}=-(-840819020949+1419128841068\hat{n}^2+221074444682\hat{n}^4+6195597884\hat{n}^6$$
$$+21259875\hat{n}^8)/(3\times 2^{47})-(1318785849\hat{n}+459389255\hat{n}^3+29718111\hat{n}^5+335617\hat{n}^7)/2^{38},$$

$$\alpha_{2,9}^{(n)}=(131257276187\hat{n}+37843099187\hat{n}^3+1323046497\hat{n}^5+4456305\hat{n}^7)/2^{44}$$
$$+(48228434+93959845\hat{n}^2+8787700\hat{n}^4+110661\hat{n}^6)/2^{34}.$$

The exponential part (43) is now completely determined up to the ninth order, i.e., known for arbitrary values of n for terms with $l\leqslant 9$.

If we exclude the dependence on 2^{-2k} and also that given by the gamma functions in the coefficients, we observe a very distinct regularity. The dependence of the leading power k in each polynomial sequence starting from $\hat{n}^0$ for a fixed value l in $\alpha_{k,k+l}^{(n)}$ and going upwards by one both for l and the power of $\hat{n}$ is so far always given by

$$\{\tilde{\alpha}_{(l,l')}\}_{l'}=\{\tilde{\alpha}_{(l,0)}/(4^{l'}(l')!)\}. \tag{47}$$

The initial values in cases $l'\leqslant 5$ are given by

$$\{\tilde{\alpha}_{(l,0)}\}_{l=0}^{5}=\{1,1/4,5/48,5/512,221/96768,113/786432\}. \tag{48}$$

This dependence is by no means proven but it corroborates our choice for the prefactors in Eq. (45). A bit surprisingly, we find that the coefficients $\alpha_{k,k+l}^{(n)}$ in Eq. (44) contain information about the energy eigenvalues in cases $n=0$ and $n=1$, i.e.,

$$\alpha_{-1,m}^{(n=0 \text{ or } 1)} = -\lambda_{n=0 \text{ or } 1}^{(m)}. \tag{49}$$

The right-hand side is taken from Eq. (20) and it is correctly reproduced for $m \leqslant 6$.

The coefficients $\{\beta_{kl}^{(n)}\}$ determine a set of new polynomials, where the coefficients multiplying the powers of ξ depend on ω. In the limit $\omega \to 0$ these polynomials tend to the Hermite polynomials. They are, unquestionably, a new class of generalized Hermite polynomials. They are defined as parts of the eigenvectors of a Hermitian matrix. Because the exponential part is rather complicated, the measure, with respect to which they become asymptotically orthogonal, is necessarily a complicated one. It depends on both of the eigenvectors, i.e., it is not a measure in the classical sense at all. No simple recursion relation for the polynomials is yet known, and we do not know, whether they satisfy any differential equation of finite order. This means that they could be an example of the second category of generalized Hermite polynomials as defined by Borzov in Ref. 20. Such discussion is beyond the scope of the present study and we will concentrate on simpler properties of the polynomials.

Our generalized Hermite polynomials are defined as

$$H_n^{\omega}(\xi) := \sum_{k=0}^{k'} \tilde{h}_k^{(n)} \xi^{n+2(k-k')}, \tag{50}$$

where the modified coefficients are given by

$$\tilde{h}_k^{(n)} := h_k^{(n)} \sum_{l=1}^{\infty} (\omega^{l-1} \beta_{kl}^{(n)}). \tag{51}$$

Because the generalized Hermite polynomials $H_n^{\omega}(\xi)$ fix the nodes (zeroes) of the functions $\psi_x^{(n)}$, it is equally important to obtain correct polynomials as it is to obtain the correct exponential factors.

We conjecture that the general form of the coefficients $\{\beta_{kl}^{(n)}\}$ reads

$$\beta_{kl}^{(n)} = \sum_{l'=0}^{l-1} \left(\sum_{\bar{l}=1}^{2(l-1)-l'} (\rho_{l'\bar{l}}^{(l)} + [(1-(-1)^n)/2] \bar{\rho}_{l'\bar{l}}^{(l)}) k^{\bar{l}} \right) (k')^{l'}, \tag{52}$$

where $\rho_{l'\bar{l}}^{(l)}$ and $\bar{\rho}_{l'\bar{l}}^{(l)}$ are constants. Additionally, $\bar{\rho}_{l'\bar{l}}^{(l)} = 0$ when $\bar{l} = 2(l-1)-l'$ or $l' = l-1$. This expansion with respect to k and k' shows that even and odd values of n should be treated separately.

Some general properties of the coefficients $\rho_{l'\bar{l}}^{(l)}$ and $\bar{\rho}_{l'\bar{l}}^{(l)}$ have been gleaned. The recurring appearance of the factor $(10k'-k)$ is by far the most striking of the observed regularities. This factor may, in time, explain some properties generalized Hermite polynomials. We conjecture that

$$\sum_{l'=0}^{l-1} (\rho_{l',2(l-1)-m_0-l'}^{(l)} k^{2(l-1)-m_0-l'} n^{l'}) = k^{l-1-m_0} (10k'-k)^{l-1-2m_0} P(2m_0, l), \tag{53}$$

where $2m_0 < l$ and $P(2m_0, l)$ denotes a $(2m_0)$th order polynomial in k and k'. Similarly, the difference between even and odd values of n corresponds to

$$\sum_{l'=0}^{l-2} (\bar{\rho}_{l',2l-3-m_0-l'}^{(l)} k^{2l-3-m_0-l'} n^{l'}) = k^{l-1-m_0} (10k'-k)^{l-2-2m_0} \bar{P}(2m_0, l), \tag{54}$$

where $2m_0<l-1$ and $\overline{P}(2m_0,l)$ again denotes a $(2m_0)$th order polynomial in k and k'.

In the leading and next-to-leading orders the polynomials $P(0,l)$, $P(2,l)$, $\overline{P}(0,l)$, and $\overline{P}(2,l)$ have been explicitly evaluated. Thus, we define the quantities

$$B(l,2l-2):=\frac{k^{l-1}(10k'-k)^{l-1}}{48^{l-1}(l-1)!} \tag{55}$$

and

$$B(l,2l-3):=\frac{k^{l-2}(10k'-k)^{l-3}}{5\times 48^{l-1}(l-2)!}[(l-2)658(k')^2+(402-126l)k'k+(8l-31)k^2], \tag{56}$$

which has been confirmed up to the sixth order, i.e., $l=6$. Similarly, the leading differences give rise to the quantities

$$\overline{B}(l,2l-3):=\frac{4k^{l-1}(10k'-k)^{l-2}}{48^{l-2}(l-2)!} \tag{57}$$

and

$$\overline{B}(l,2l-4):=\frac{k^{l-2}(10k'-k)^{l-4}}{5\times 48^{l-1}(l-3)!}[(2632l-2576)(k')^2+(1470-504l)k'k+(32l-145)k^2]. \tag{58}$$

The leading terms are very similar, but also the next-to-leading terms $B(l,2l-3)$ and $\overline{B}(l,2l-4)$ share several common features. Most importantly, the l-dependence in the polynomial section is identical, apart from a factor of 4.

Below, we give the explicit values of the coefficients $\beta_{kl}^{(n)}$ in cases $2\leqslant l\leqslant 7$. It is convenient to separate the even and odd values of n, because the correct expansion parameter appears to be k'. Please note that these expressions automatically yield $\beta_{0,l}^{(n)}=0$ for $l>1$,

$$\beta_{k,2}^{(2k')}=[(3k-k^2)+(10k)k']/48,$$

$$\beta_{k,2}^{(2k'+1)}=\beta_{k,2}^{(2k')}+k/12,$$

$$\beta_{k,3}^{(2k')}=[(855k-64k^2-14k^3+5k^4)+(784k+48k^2-100k^3)k'+(1316k+500k^2)(k')^2]/23040,$$

$$\beta_{k,3}^{(2k'+1)}=\beta_{k,3}^{(2k')}+[(249k+49k^2-20k^3)+(532k+200k^2)k']/11520,$$

$$\beta_{k,4}^{(2k')}=B(4,6)+B(4,5)+[(371385k-203498k^2-12129k^3+1438k^4)+(1110698k+102042k^2-26252k^3)k'+(496932k+93984k^2)(k')^2+560200k(k')^3]/23224320,$$

$$\beta_{k,4}^{(2k'+1)}=\beta_{k,4}^{(2k')}+\overline{B}(4,5)+\overline{B}(4,4)+[(67680k+12347k^2-2602k^3)+(108544k+33762k^2)k'+114456k(k')^2]/3870720,$$

$$\beta_{k,5}^{(2k')}=B(5,8)+B(5,7)+[(278751375k-202014918k^2+35222268k^3+4026748k^4+28158k^5-9944k^6)+(713250468k-281790420k^2-61452368k^3-196176k^4+209856k^5)k'+(1105743252k+198178852k^2-10630680k^3-275344k^4)(k')^2+(319197168k+81282336k^2-22799744k^3)(k')^3+(271672512k+148408976k^2)(k')^4]/22295347200,$$

$$\beta_{k,5}^{(2k'+1)}=\beta_{k,5}^{(2k')}+\overline{B}(5,7)+\overline{B}(5,6)+[(119817225k-23468037k^2-12060122k^3-330312k^4+100198k^5)+\ (436319556k+103769756k^2-5886336k^3-1921112k^4)k'+(321608148k+118383396k^2-904080k^3)(k')^2+(224147856k+120486304k^2)\times(k')^3]/11147673600,$$

$$\beta_{k,6}^{(2k')}=B(6,10)+B(6,9)+[(134035780725k-166751340588k^2+39327194883k^3-2269605874k^4-477614210k^5-19226552k^6+221782k^7+484k^8)+(413990823078k-217584747090k^2+22678956764k^3+8841166604k^4+479019924k^5-6549884k^6+566984k^7)k'+(526339688532k-155591533528k^2-55003198072k^3-3518713436k^4+85514000k^5-24903296k^6)(k')^2+(556945898088k+131085561976k^2+2790556248k^3-280060176k^4+424040144k^5)(k')^3+(116760015552k+34523271136k^2-5865150192k^3-3338174576k^4)(k')^4+(79966766400k+46102886720k^2+10162787360k^3)(k')^5]/11771943321600,$$

$$\beta_{k,6}^{(2k'+1)}=\beta_{k,6}^{(2k')}+\overline{B}(6,9)+\overline{B}(6,8)+[(34460588160k-26910050283k^2+72069996k^3+1282383895k^4+103465570k^5-948002k^6-316976k^7)+(216801198648k-21671791146k^2-18471533106k^3-1699322576k^4+78651584k^5+5865684k^6)k'+(345295895928k+96181762100k^2+1478206984k^3-1409258180k^4+60822872k^5)\times(k')^2+(160052617776k+64547633160k^2+3204992824k^3-1898232512k^4)(k')^3+(83156900448k+47130830560k^2+10276562912k^3)(k')^4]/5885971660800,$$

$$\beta_{k,7}^{(2k')}=B(7,12)+B(7,11)+[(2116744695077512 5k-3431804636834514 0k^2+13674300462898392k^3-1352901404372446k^4-2843855572731k^5+113118751597906k^6+704407032828k^7+12949326156k^8-177366189k^9+37677640k^{10})+(59570630372492640k-60644270495554704k^2+10066261151648252k^3+1046023367606 52k^4-246415137367020k^5-202073627715 48k^6-460168946016k^7+2604105504k^8-2483040560k^9)k'+(99669485611466412k-39020273844707836k^2+2200698814542984k^3+2070713072954600+212428368788100k^5+5622413614220k^6+82814211480k^7+70784553840k^8)(k')^2+(82488078028378080k-18442822328400480k^2-9100818756007520k^3-964844434165920k^4-24156442527360k^5-3013682511840k^6-1116228072960k^7)(k')^3+(66588038149135200k+18345507366303440k^2+1191268975557840k^3+10518809509520k^4+424741146429 60k^5+10244315921840k^6)(k')^4+(10839030004200960k+3516288982521792k^2-3638959534104 96k^3-304221200739456k^4-516106679088 00k^5)(k')^5$$

$$+(6218212960526208k+3705496740373376k^2+898601964676416k^3$$
$$+1106840374640000k^4)(k')^6]/1542595452862464000,$$

$$\beta_{k,7}^{(2k'+1)}=\beta_{k,7}^{(2k')}+\overline{B}(7,11)+\overline{B}(7,10)+[(-460686821541975k-1941941074537755k^2$$
$$+366877584331212k^3+41494582964306k^4-9965970910165k^5-1112954021925k^6$$
$$-34972438722k^7+958101144k^8+3798795k^9)+(9145976126266080k$$
$$-3823250702059872k^2-191143081971676k^3+173415983605096k^4$$
$$+24948282593576k^5+815890000796k^6-41300603344k^7+1974092120k^8)k'$$
$$+(19045045703842332k-607795420829248k^2-1422456568355676k^3$$
$$-195873935369616k^4-2655255816252k^5+611948653316k^6-98001423520k^7)$$
$$\times(k')^2+(18941405236672032k+5863460843089248k^2+345511721120640k^3$$
$$-55753844615456k^4-6547232531184k^5+1792716525600k^6)(k')^3$$
$$+(6296099301099168k+2692631923242160k^2+232744611197904k^3$$
$$-59049744898144k^4-14606140268720k^5)(k')^4+(2605202959125888k$$
$$+1525593370591680k^2+365590616623232k^3+44670372947200k^4)$$
$$\times(k')^5]/257099242143744000.$$

In combination with the exponential parts these coefficients determine explicit, analytical expressions for solution function $\psi_x^{(n,7)}$ for arbitrary values of n.[32]

It must be re-emphasized that Eq. (30) is an asymptotical solution. Two partially overlapping reasons for this behavior must be stated. First, the solution depends on two independent length scales, i.e., x and ω, and second, the coordinate transformation $x\mapsto\xi=\sqrt{\omega}x$ is singular at $\omega=0$. These points are rather extensively covered in Ref. 13. The eigenvalues are asymptotically exact for even values of n at $x_0=0$ and, probably, for odd values of n at $x_0=\pm\frac{1}{2}$. Because the error decays exponentially in $1/\omega$, this dependence on x_0 vanishes much before the asymptotical behavior of Eq. (22), i.e., $\|\psi_n^{(m,x_0)}-\psi_n^{(x_0)}\|\sim C(n,m)\omega^m$, appears.

Comparison against numerically obtained eigenstates allows us to give an approximate expression for the function $C(n,m)$. The validity of the calculations is limited by the numerical precision, i.e., to norms of the order of 10^{-11}–10^{-12}. We have employed the reliable diagonalization routines of MATLAB software for this purpose. We have studied eigenvectors up to $n\approx 40$–50 and the corresponding asymptotical solutions $\psi_n^{(m,x_0)}$ up to the fifth order. A reasonable, order-of-magnitude estimate for the error in the Euclidean norm, when $n\leqslant 40$, is given by

$$C(n,m)\approx c_m\hat{n}^{2m}, \tag{59}$$

where

$$c_1=0.03,\quad c_2=0.002,\quad c_3=0.0006,\quad c_4=1.5\times 10^{-6},\quad \text{and}\quad c_5=3\times 10^{-8}. \tag{60}$$

There is a slight difference between even and odd cases, but this is insignificant in an estimate like this. The value of c_5 is set to fit the observed trend in the other coefficients as the asymptotical behavior is only glimpsed. In cases $m=2$ and $m=4$, it is vitally important to remember to truncate the asymptotical eigenvector $\psi_n^{(m,x_0)}$ correctly.

For larger values of n, one needs very small values of ω in order to obtain accurate or even reasonable results. But for relatively small values of n, say $n\leqslant 10$, the error is extremely small at

$\omega \approx 0.01$. The strong dependence on n means that the first few states can be obtained to a high precision even for quite strong couplings in the neighborhood of $\omega \approx 0.1$. We have determined the ground state $n=0$ up to the 31st order and numerical comparison strongly supports the asymptotical behavior ω^m for $m \leqslant 13$.

In order to make the above discussion more concrete, we explicitly give the second-order solutions as functions of ω, $\xi = \sqrt{\omega}\, x$, n (not $\hat{n}$) and k'. For even values of n we find the solution function

$$\psi_x^{(n,2)} = A_{n,x_0} \exp(-(\tfrac{1}{2} + (3+2n)\omega/32)\xi^2 + (\omega/96)\xi^4) \sum_{k=0}^{k'} (h_k^{(n)} \xi^{2k} (1 + (3k - k^2 + 10kk')\omega/48)), \tag{61}$$

where A_{n,x_0} is a normalization factor which ensures that $\|\psi_n^{(2,x_0)}\| = 1$. For odd values of n the result is nearly identical, i.e.,

$$\psi_x^{(n,2)} = A_{n,x_0} \exp(-(\tfrac{1}{2} + (3+2n)\omega/32)\xi^2 + (\omega/96)\xi^4) \sum_{k=0}^{k'} (h_k^{(n)} \xi^{2k} (1 + (7k - k^2 + 10kk')\omega/48)). \tag{62}$$

The tiny difference $3k \to 7k$ in the generalized Hermite polynomial is very important, because otherwise the asymptotical convergence $\|\psi_n^{(m,x_0)} - \psi_n^{(x_0)}\| \sim \omega^2$ does not appear. The common exponential part in the third order solution function $\psi_x^{(n,3)}$ reads

$$\exp(-(\tfrac{1}{2} + (3+2n)\omega/32 + (53 + 69n + 21n^2)\omega^2/1536)\xi^2 + (\omega/96 + (11+6n)\omega^2/1024)\xi^4 - (\omega^2/1280)\xi^6)). \tag{63}$$

The explicit solution function $\psi_x^{(n,m)}$ solves the asymptotical eigenvalue equation up to the order ω^m and yields a normwise convergence of $\sim \omega^m$.

When employing these asymptotical solutions, one should first study, how accurate eigenvectors are required for the problem at hand. The next step is to choose the order of the solution and the correct truncation with respect to x. Then, the calculations are performed and the results are obtained, hopefully faster than with the conventional approach of numerical diagonalization.[6]

IV. COMMENTS ON SOLVING THE ANSATZ

In this section we discuss how to solve the set of algebraic equations resulting from Eq. (33) as effectively as possible. First we observe that the zeroth order, i.e., terms proportional to arbitrary powers of ξ are satisfied by the fact $\exp(0)=1$. Next, all equations related to terms

$$\{\omega \xi^{n+2-2l'}\}_{l'=0}^{1+k'} \tag{64}$$

are identically satisfied because of the recursion relation (6) rewritten in terms of the coefficients $h_k^{(n)}$. A careful reader notices that terms proportional to $\beta_{k,l=2}^{(n)}$ do appear, but they identically cancel and thus they are not constrained in this order.

From here on, we proceed by recursively solving the coefficients for the next order and also for sufficiently many values of n so that all coefficients in the expansions of $\{\alpha_{kl}^{(n)}\}$ and $\{\beta_{kl}^{(n)}\}$ have been constrained. In reality, we first obtained the solution function $\psi_x^{(n=0,m=6)}$ and a poorly formulated expression for arbitrary second-order solution, i.e., $\psi_x^{(n,m=2)}$, but let us proceed in the way this should be done. Because the equation are quite difficult to handle with pen and paper, we chose to write and simplify the equations with MATHEMATICA software.[33]

We first consider the cases $n=0$ and $n=2$ as simple examples. For $n=0$ we expand Eq. (33) up to and including order ω^3 to find

$$\left\{1-\frac{\omega}{2}+\omega^2\left(\alpha_{1,2}^{(0)}+\frac{1}{8}+\frac{x^2}{2}\right)+\omega^3\left[-\frac{1}{48}+\frac{\alpha_{1,2}^{(0)}}{2}+\alpha_{1,3}+\alpha_{2,2}^{(0)}+x^2\left(-\frac{1}{4}-2\alpha_{1,2}^{(0)}+6\alpha_{2,2}^{(0)}\right)\right]\right\}$$
$$=\left[1-\frac{\omega}{2}+\frac{\omega^2(x^2+1/16)}{2}+\frac{\omega^3}{512}\right]. \tag{65}$$

Immediately, we obtain

$$\alpha_{1,2}^{(0)}=-3/32 \quad \text{and} \quad \alpha_{2,2}^{(0)}=1/96. \tag{66}$$

Inserting these into Eq. (65) gives $\alpha_{1,3}^{(0)}=-53/1536$.

In the case $n=2$ and we examine all terms below the order of ω^4. The generalized Hermite polynomial now reads

$$H_2^{\omega}(\xi)=-2+4\omega x^2(1+\beta_{1,1}^{(2)}\omega+\beta_{1,2}^{(2)}\omega^2+\beta_{1,3}^{(2)}\omega^3)+\mathcal{O}(\omega^5). \tag{67}$$

Expanding all terms and moving them onto the same side yields the equation

$$0=\omega^2\left(\frac{23}{32}+\alpha_{1,2}^{(2)}-2\beta_{1,1}^{(2)}\right)+\omega^3\left[-\frac{521}{1536}-\frac{5\alpha_{1,2}^{(2)}}{2}+\alpha_{1,3}^{(2)}+\alpha_{2,2}^{(2)}+\beta_{1,1}^{(2)}-2\beta_{1,2}^{(2)}\right.$$
$$+x^2\left(-\frac{43}{16}-12\alpha_{1,2}^{(2)}+6\alpha_{2,2}^{(2)}\right)\Big]+\omega^4\left[\frac{341}{24576}+\frac{(\alpha_{1,2}^{(2)})^2}{2}-\frac{5\alpha_{1,3}^{(2)}}{2}+\alpha_{1,4}^{(2)}+\alpha_{1,2}^{(2)}\left(\frac{9}{8}-2\beta_{1,1}^{(2)}\right)\right.$$
$$-\frac{\beta_{1,1}^{(2)}}{4}+\beta_{1,2}^{(2)}-2\beta_{1,3}^{(2)}+x^2\left(\frac{953}{768}+2(\alpha_{1,2}^{(2)})^2-12\alpha_{1,3}^{(2)}-37\alpha_{2,2}^{(2)}+6\alpha_{2,3}^{(2)}+\alpha_{1,2}^{(2)}\left(\frac{29}{2}-10\beta_{1,1}^{(2)}\right)\right.$$
$$\left.\left.-\frac{39\beta_{1,1}^{(2)}}{16}\right)+x^4\left(\frac{29}{24}+4\alpha_{1,2}^{(2)}-32\alpha_{1,3}^{(2)}\right)\right]. \tag{68}$$

Notice that all terms proportional to ω^0 and ω^1 have canceled out, which again shows that the lowest-order approximation for the eigenvalue and eigenstate are already correct and agree with the results for the continuous case. The three coefficients related to the $\psi^{(2,2)}$ can be solved from the coefficients of ω^2, ω^3x^2, and ω^4x^4 and they read

$$\alpha_{1,2}^{(2)}=-7/32, \quad \alpha_{2,2}^{(2)}=1/96, \quad \text{and} \quad \beta_{1,1}^{(2)}=1/4. \tag{69}$$

Substituting these into the set of equations and extending the calculation to order ω^6 we find the subsequent coefficients to be

$$\alpha_{1,3}^{(2)}=-275/1536, \quad \alpha_{2,3}^{(2)}=23/1024, \quad \alpha_{3,3}^{(2)}=-1/1280, \quad \text{and} \quad \beta_{1,2}^{(2)}=37/256. \tag{70}$$

After solving a sufficient number of coefficients $\alpha_{kl}^{(n)}$ and $\beta_{kl}^{(n)}$ one should start searching for regularities in the solution.

Almost immediately we guessed the polynomial character of $\alpha_{kl}^{(n)}$, first in terms of n and later noticing that they should be written in terms of $\hat{n}$ as in Eq. (44). This considerably helps solving the coefficients $\beta_{kl}^{(n)}$ as for larger values of n the coefficients $\alpha_{kl}^{(n)}$ appear as constants, not unknowns.

In the beginning, we tried to solve all possible terms up to a given order in ω. First one should notice that only terms with $l\leqslant m$ are required for the solution function $\psi_x^{(n,m)}$. Assuming that the previous orders have been explicitly obtained, means that only the equations corresponding to $m'=m$ in Eq. (34) have to be solved. In addition, generally known coefficients $\alpha_{k,m}^{(n)}$ identically satisfy equations corresponding to the highest powers of ξ. Explicitly, if we assume that coefficients $\{\alpha_{k,m}^{(n)}\}_{k=k_0}^{m}$ are known, only the equations for

$$\{\omega^m \xi^{n+2k_0-2l'}\}_{l'=0}^{k_0+k'} \tag{71}$$

are required and the expansion of Eq. (33) has to be carried out up to and including the order $\omega^{m+k_0+n/2}$ for coefficients $l \leqslant m$.

After obtaining a rather complicated expression for the coefficients $\beta_{k,l=3}^{(n)}$, we happened to transform it into form equivalent to the present form and conjecture the general form of $\beta_{kl}^{(n)}$ in Eq. (52). The most important lesson taught by the discretized harmonic oscillator when solving the coefficients is that your numbers may be wrong, but the general forms usually are not. On several occasions, this became painfully obvious when the numbers did not check. Each and every time the general forms were correct, but the used expansion of Eq. (33) or the numbers inserted into it were not.

Later on, we started to study the regularities in the general expressions. The polynomial structure of the coefficients $\alpha_{kl}^{[l']}$ that do not contain any gamma functions was relatively easy obtain, but the other set required a real stroke of luck. We managed to write some of these coefficients $\alpha_{kl}^{[l']}$ as explicit products. After being pointed out, by MATHEMATICA, that the first two could be written in terms of gamma functions, it was only a question of finding the correct gammas before Eq. (45) was written. In order to appreciate the technical part of obtaining the general form of the coefficients we point out that the coefficient $\alpha_{k,k+4}^{(n)}$ was completed by solving the 12th order solution $\psi_{n=0}^{(m=12,x_0)}$ and confirmed by the case $n=1$. Further terms have been obtained by solving the asymptotical differential equations (35).

The regularities in the coefficients $\{\beta_{kl}^{(n)}\}$ have been found out using by studying the expansions with respect to k and k'. By conjecturing the recurring appearance of $(10k'-k)$ in Eqs. (53) and (54) it becomes possible to solve the quantities defined in Eqs. (55)–(58). In addition to these, the general expression for $\rho_{k,l-3}^{(l)}$ can be obtained from the known coefficients.

Finally, we will estimate the difficulty of obtaining the explicit asymptotical solution $\psi_n^{(m,x_0)}$. We assume that both the expansion of the eigenvalues up to the required order and the solution $\psi_n^{(m-1,x_0)}$ have been obtained in advance. The coefficients $\alpha_{km}^{(n)}$ can be determined from the exponential parts of the eigenvectors up to and including the case $n=m-1$. The completely general expressions in Eq. (45) are finished at much slower a pace. The asymptotically satisfied differential equations (35) speed up this process considerably.

Obtaining the coefficients $\beta_{km}^{(n)}$ is more difficult. The general form (52) shows that all states up to $n=4m-3$ must be solved. The explicit expressions for the leading parts, i.e., $B(l,2l-2)$, $B(l,2l-3)$, $\overline{B}(l,2l-3)$, and $\overline{B}(l,2l-4)$ make this task easier by five states. Thus all states up to $n=4l-8$ must be found, unless further general properties are found.

Regardless of these simplifications, the number of required terms and participating equations grows quite fast. Obviously, the general form of the coefficients in the exponential factor is much easier to obtain and thus they should be applied as early as possible. It is also possible that considerable simplifications or generalizations for the known coefficients lurk just around the corner. This has already happened on several occasions so far. We still choose to pause here, as the given general expressions have been validated rather convincingly and it not obvious, how, if at all, the next orders in the expansion would improve the results qualitatively. We hope a solid foundation has been laid for those striving towards the complete, asymptotical solution for the discretized harmonic oscillator.

V. PROVING THE SOLUTION AND SOME GENERAL PROPERTIES

Finally, we attack the difficult problem of actually showing that the solution is a general one. Thus far we have solved the equations for an increasing number of eigenstates using Eq. (33). This formulation is the best if actual numerical values of the coefficients $\alpha_{kl}^{(n)}$ and $\beta_{kl}^{(n)}$ are sought after. This is explained by symbolic math being most effective when the number of unknowns and symbols is as small as possible. In principle, the process explained below could be used for

obtaining recursion relations between the coefficients of the solution and, subsequently, the full solution. Presently, we only show that the equations corresponding to leading orders up to ω^3 are satisfied identically.

We have to solve the equations corresponding to $\{\omega^m \xi^{n+m-2l'}\}_{l'=0}^{k'+m}$ in order to obtain the mth order solution. We have now obtained the explicit solution up to the seventh order so we can check if it is correct. For this purpose, we must write Eq. (33) explicitly in terms of $u := \sqrt{\omega}$ and ξ, although odd powers of u eventually cancel. Multipliers of $\alpha_{kl}^{(n)}$ and $\beta_{kl}^{(n)}$ now read

$$u^{2(l-1)}[(\xi \pm u)^{2k} - \xi^{2k}] \quad \text{and} \quad (\xi \pm u)^{n+2(k-k')}, \tag{72}$$

respectively. On the right-hand side the nontrivial term is given by $\omega\xi^2/2$. Expanding all terms multiplying a fixed term $h_k^{(n)}$ up to the order yields terms

$$h_k^{(n)}\left[1+u^2\left(2(k-k')-\hat{n}/2+\frac{\xi^2}{2}+\frac{(n-1+2(k-k'))(n+2(k-k'))}{\xi^2}\right)\right]$$
$$= h_k^{(n)}\left(1+u^2\left(-\hat{n}/2+\frac{\xi^2}{2}\right)\right). \tag{73}$$

The terms proportional to ξ^2 cancel and equating each power of ξ separately yields an equation

$$h_k^{(n)} 2(k'-k) + [2(k+1)^2 \mp (k+1)] h_{k+1}^{(n)} = 0, \tag{74}$$

where the signs $+$ and $-$ corresponds the even and odd values of n, respectively. The above equation is identically satisfied by the Hermite polynomials, which proves that the first-order solution $\psi_n^{(1,x_0)}$ is correct. A careful observer immediately asks about the second order corrections $\beta_{k,2}^{(n)}$ which also yield terms proportional to u^2. However, these coefficients are not fixed at all by Eq. (33) in the order u^2. The only term that is easily solvable from this relation in the dominant coefficient $\alpha_{1,1}^{(n)} = -1/2$ which removes $h_{k-1}^{(n)}$ from the recursion relations. Later on, the dominant coefficients $\{\alpha_{kk}^{(n)}\}_{k=1}^{m}$ cancel the term $h_{k-m}^{(n)}$ in the order ω^m.

In the next order ω^2 we insert the solved coefficients and obtain for even values of a recursion relation

$$6(n+2-2k)h_{k-1}^{(n)} + [(2k^3+k^2(42-11n)-6n-3n^2-k(-6+9n-5n^2)]h_k^{(n)} - (1+k)(1+2k)$$
$$\times(22+31k+k^2-5n-5kn)h_{k+1}^{(n)} + 2(2k+4)(2k+3)(2k+2)(2k+1)h_{k+2}^{(n)} = 0, \tag{75}$$

which is again identically satisfied by the Hermite polynomials. For odd values of n, we find a similar recursion relation, once we replace $k' = n/2$ by $k' = (n-1)/2$. This completes the proof in order ω^2 and validates the second-order eigenvectors $\psi_n^{(2,x_0)}$.

In the third order the recursion relation for even values of n reads

$$180(-4+2k-n)h_{k-2}^{(n)} + 30(62-42k-24k^2+4k^3+74n-10kn-22k^2n+17n^2+10kn^2)h_{k-1}^{(n)}$$
$$+[-450n-450n^2-90n^3-10k^5+k^4(-452+105n)+k^3(-2332+2458n-300n^2)$$
$$+k^2(4230+4912n-1204n^2+125n^3)+k(-300-585n-1258n^2+179n^3)]h_k^{(n)}$$
$$+(1+k)(1+2k)(1022+2705k+3684k^2+326k^3+5k^4-2274n-4430kn-1726k^2n$$
$$-50k^3n+454n^2+579kn^2+125k^2n^2)h_{k+1}^{(n)} - 16(1+k)(2+k)(1+2k)(3+2k)(110+101k$$
$$+5k^2-50n-25kn)h_{k+2}^{(n)} + 256(1+k)(2+k)(3+k)(1+2k)(3+2k)(5+2k)h_{k+3}^{(n)} = 0. \tag{76}$$

Because the Hermite polynomials satisfy this and the corresponding relation for odd values of n the solution $\psi_n^{(3,x_0)}$ has been rigorously proven as correct.

The eigenvectors $\psi_n^{(m,x_0)}$ tend to the eigenvectors $\psi_n^{(x_0)}$ of $H(x_0)$ at an asymptotical rate proportional to ω^m. The exact eigenvectors are orthogonal as eigenvectors of a Hermitian matrix and by their closure relation we can write

$$\psi_n^{(m,x_0)} \sim \psi_n^{(x_0)} + \omega^m \sum_{n'} b_{n'} \psi_{n'}^{(x_0)}, \tag{77}$$

where $b_{n'}$ are finite constants such that $\Sigma_n |b_n|^2 < \infty$ in the limit $\omega \to 0$. The orthonormality relation for the asymptotical solutions thus reads

$$\langle \psi_n^{(m,x_0)} | \psi_{n'}^{(m,x_0)} \rangle = \delta_{nn'} + \mathcal{O}(\omega^m), \tag{78}$$

provided that the sum $\Sigma_n |b_n|$ is finite for both states. In other words, the eigenvectors $\psi_n^{(m,x_0)}$ become orthonormal at the rate of ω^m. Numerical checks seem to confirm this, at least for relatively small values of n.

As a final effort, we outline a plausible ''proof'' for the asymptotical convergence. As a first step, we show that without loss of generality we can examine a finite truncation of the eigenvector $\psi_n^{(n,x_0)}$, the vector $\psi_{n,j_0}^{(x_0)} := \{\psi_{j-x_0}^{(n)}\}_{j=-j_0}^{j_0}$ for sufficiently large j_0. For sufficiently large values of $|j|$ the eigenvalue λ_n becomes insignificant in Eq. (32) and we write an approximate equation

$$(\psi_{x-1}^{(n)} - 2\psi_x^{(n)} + \psi_{x+1}^{(n)})/(x^2) = \omega^2. \tag{79}$$

For sufficiently large values of x and/or j the sign of $\psi_x^{(n)}$ is constant and this equation shows that the function $\tilde{\psi}_x = \psi_{j_0-x_0}^{(n)} \exp(-\omega(x^2 - j_0^2)/(2+\varepsilon))$, for some small $\varepsilon > 0$, is a dominant sequence for $\psi_x^{(n)}$. Now, the limiting sequence of norms

$$\lim_{j_0 \to \infty} \| \psi_n^{(x_0)} - \psi_{n,j_0}^{(x_0)} \| \tag{80}$$

vanishes exponentially with respect to j_0. In other words, we can always find a finite j_0 such that the error in the norm is sufficiently small.

Next we use the fact that solution $\psi_n^{(m,x_0)}$ satisfies the eigenvalue equation (32) up to the order ω^m when written in terms of ξ. Thus we can write

$$\frac{\psi_{x-1}^{(n,m)} + \psi_{x+1}^{(n,m)}}{2\psi_x^{(n,m)}(-\lambda_n + \omega\xi^2/2)} = 1 + \mathcal{O}(\omega^{m+1}). \tag{81}$$

We fix the scales of the eigenvectors by setting $(\psi_n^{(m,x_0)})_j = (\psi_n^{(x_0)})_j$ for an arbitrary j. It would be very tempting to say that Eq. (81) implies $(\psi_n^{(m,x_0)})_{j+1} = (\psi_n^{(x_0)})_{j+1}(1 + \mathcal{O}(\omega^{m+1}))$ and then wonder why convergence is not asymptotically proportional to ω^{m+1}. As already explained the solution $\psi_n^{(m,x_0)}$ does not fix the coefficients $\beta_{k,m+1}^{(n)}$ which most definitely yield terms proportional to ω^m. Thus we obtain a relation

$$(\psi_n^{(m,x_0)})_{j+1} = (\psi_n^{(x_0)})_{j+1}(1 + \mathcal{O}(\omega^m)). \tag{82}$$

By matching the eigenvectors at $j = 0$, and expanding the components to the finite values $\pm j_0$ shows that the order of error is ω^m for all components with $|j| \leqslant j_0$. Becase the error caused by the truncation is insignificant the result holds for the full eigenvectors and we obtain the desired result

$$\|\psi_n^{(m,x_0)} - \psi_n^{(x_0)}\| \sim \omega^m, \tag{83}$$

or at least show that the result is quite plausible.

VI. CONCLUSIONS

We have obtained an explicit, asymptotical solution for the discretized harmonic oscillator. Both the eigenvalues and eigenvectors have been obtained and we can choose a prespecified rate of convergence towards the exact solutions. This is done by truncating the ansatz solution accordingly. Because the problem can be mapped onto the Mathieu differential equation, we simultaneously provide asymptotical expressions for the Mathieu functions. The Schrödinger equation of the quantum pendulum corresponds to the Mathieu equation, which yields immediate applications for the results.

The method described above can be generalized to accommodate several coordinate dimensions with only minor changes. This should make the results of Ref. 29 both more transparent and more rigorous. The tunnelling–charging Hamiltonian of a Cooper pair pump corresponds to a modified multidimensional Mathieu equation.

Alternatively, ansatzes similar to Eq. (30) could be constructed in case of difference equations that become identical to analytically solvable differential equations in some asymptotical limit. Initially, the problem assumes the form of an infinite-dimensional, two-parameter (eigenvalue) problem, where the asymptotical solutions (eigenvalues and eigenvectors) must be obtained. The ansatz maps the problem onto an infinite set of algebraic equations that must solved. If the form of the ansatz is correct, one may determine some general properties of the exact solution.

ACKNOWLEDGMENTS

This work has been supported by the Academy of Finland under the Finnish Center of Excellence Programme 2000–2005 (Project No. 44875, Nuclear and Condensed Matter Program at JYFL). Dr. L. Kahanpää is acknowledged for insightful discussions and suggestions. The author thanks Professor J. Timonen for valuable references added to the final draft of the paper.

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[33] Many MATHEMATICA notebooks containing much of the data used in calculations is available at http://www.cc.jyu.fi/~mimaau/harmonic. The general results have been compiled into Mathieunewgen.nb, where the eigenvalue is given up to 19th order as a well as the general expression for the coefficient $\alpha_{k,k+7}^{(n)}$.

Perturbative analysis of dynamical localization

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(Received 6 January 2003; accepted 25 January 2003)

In this paper we present a mathematical investigation of the phenomenon of dynamical localization in a class of quasi-periodically and periodically time-dependent two-level systems. Our results are based on a sort of ''renormalization'' procedure, which is developed here in a systematic way in order to adapt it to the case of dynamical localization. In the quasi-periodic case this procedure leads to a formal perturbative expansion free of secular terms. In the periodic case a convergent perturbative solution is obtained and, in particular, a convergent perturbative expansion for the secular frequency is presented. The case of ac–dc fields is discussed in some detail, leading to the conclusion that the phenomenon of dynamical localization is not exact in that situation. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1562750]

I. GENERAL DESCRIPTION AND PREVIOUS RESULTS

The study of periodically or quasi-periodically time-dependent two-level systems is of basic importance for many physical applications, ranging from condensed matter physics to quantum optics, as in problems of the theory of spin resonance, in problems of quantum tunnelling, in the semi-classical theory of the laser and, more recently, in BEC's, in quantum computation and spintronics. They can be used to describe the behavior of a spin 1/2 system in a time-dependent magnetic field, in which case the Schrödinger equation takes the simplified form (we adopt $\hbar = 1$)

$$i\partial_t \Psi = H(t)\Psi\,, \quad \text{with} \quad H(t) = -\frac{1}{2}\vec{B}(t)\cdot\vec{\sigma}, \tag{1.1}$$

where $\Psi(t) = \binom{\psi_1(t)}{\psi_2(t)} \in \mathbb{C}^2$, $\vec{B}(t) = (B_1(t), B_2(t), B_3(t))$ and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices. These systems have been analyzed in various approximations since the pioneering works of Rabi,[1] Bloch and Siegert, [2] and Autler and Townes[3] (see also Refs. 4, 5, 6 for more recent discussions). Of particular interest is the situation where (1.1) takes the form

$$i\partial_t \Psi(t) = H_1(t)\Psi(t), \quad \text{with} \quad H_1(t) := \epsilon\sigma_3 - f(t)\sigma_1\,, \tag{1.2}$$

where $f(t)$ is a function of time t and $\epsilon \in \mathbb{R}$ is constant. By a $\pi/2$-rotation around the 2-axis, we get the equivalent system

$$i\partial_t \Phi(t) = H_2(t)\Phi(t), \quad \text{with} \quad H_2(t) := \epsilon\sigma_1 + f(t)\sigma_3\,, \tag{1.3}$$

where $\Phi(t) := \exp(-i\pi\sigma_2/4)\Psi(t)$ and $H_2(t) := \exp(-i\pi\sigma_2/4)\, H_1(t)\exp(i\pi\sigma_2/4)$.

One can either interpret the system (1.2) as describing a spin 1/2 system as (1.1) under a magnetic field $\vec{B} = (2f(t), 0, -2\epsilon)$, or as a system with an unperturbed diagonal Hamiltonian $H_0 := \epsilon\sigma_3$, representing a two-level system with energy levels $\pm\epsilon$, subjected to a time-dependent

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perturbation $H_I(t) := -f(t)\sigma_1$, inducing a time-depending transition between the unperturbed eigenstates of H_0. The equivalent system (1.3), in turn, represents either a spin 1/2 system as (1.1) under a magnetic field $\vec{B}=(-2\epsilon, 0, -2f(t))$, or a two-level system composed by two uncoupled (for $\epsilon=0$) orthogonal time-dependent states $\exp(-i\int_0^t f(\tau)d\tau)\binom{1}{0}$ and $\exp(+i\int_0^t f(\tau)d\tau)\binom{0}{1}$, subjected to a constant perturbation $\epsilon\sigma_1$ inducing a transition between them.

Let $\Phi_+=\binom{1}{0}$ and $\Phi_-=\binom{0}{1}$ be two orthogonal states corresponding to $\Psi_+=(1/\sqrt{2})\binom{1}{1}$ and $\Psi_-=(1/\sqrt{2})\binom{1}{-1}$. Denoting by $U(t)=U(t, 0)$ the family of unitary operators implementing the time-evolution associated to $H_2(t)$, the probability of transition from Φ_+ at $t=0$ to Φ_- at time t is $P(t) := |(\Phi_+, U(t)\Phi_-)|^2 = |U_{12}(t)|^2$. For $f(t)\equiv 0$ one has, as well known, $P(t)=\sin(\Omega t)^2$, with $\Omega=\epsilon$, and the transition probability transits between 0 and the maximal value 1 within a period π/ϵ. For $f(t)=F_0$, a nonzero constant (dc-field), one has $P(t)=(\epsilon/\Omega)^2\sin(\Omega t)^2$, with $\Omega=\sqrt{\epsilon^2+F_0^2}$ and the situation changes compared to the $f(t)\equiv 0$ case in that the transition probability is suppressed by a factor ϵ^2.

Much more interesting is the situation when the interaction f is periodically varying in time. For the simplest case of a monochromatic interaction $f(t)=\varphi\cos(\omega t)$ (ac-field), it was first shown in Refs. 7 and 8 that one has $\Omega_1=\epsilon J_0(2\varphi/\omega)$ as the first order of approximation in ϵ for the transition frequency, where J_0 is the Bessel function of the first kind and order zero. Hence, if the field strength φ and the frequency ω are chosen such that $\chi_1=2\varphi/\omega$ is a zero of J_0, then $\Omega\approx 0$, which implies long transition times. This phenomenon became known as *coherent destruction of tunnelling* or *dynamical localization effect*.

The effect of dynamical localization, first pointed in Refs. 7 and 8, indicates the possibility of approximately freezing the initial state of a quantum system through the action of a suitable *external* time-dependent interaction. This effect may play an important role in manipulation of q-bits, in connection with the so-called Zeno's effect and in the phenomenon of induced transparency. It has been the object of various recent investigations. In Ref. 10, for instance, a rigorous general criterion for the occurrence of dynamical localization was established and applied to interesting situations, like the ac–dc field and the bichromatic field. Some of the conclusions of Ref. 10 on the ac–dc field are indirectly reproduced in Sec. V. For an extensive review on dynamical localization, see Ref. 9. We also refer the reader to Refs. 10, 13, 14, 17, and 18 for more references on this subject.

For a two-level system with $\epsilon\neq 0$ and for arbitrary f, the transition probability $P(t)$ cannot be identically zero, for that would imply that the unitary evolution $U(t)$ is diagonal, and this contradicts the Schrödinger equation $i\partial_t U(t)=H_2(t)U(t)$, as one easily checks. Hence, the freezing effect cannot be exact. Therefore, a more detailed analysis of the complete series expansion for the transition frequency Ω in terms of ϵ is required.

The aim of this paper is twofold. From one side we intend to systematize the methods of Ref. 15 and the convergence proofs of Ref. 16. From the other side, our goal is to develop, in a mathematically complete way, the perturbation theory required for the analysis of the dynamical localization effect in two-level systems with periodic f.

To explain the purpose, the strategy and the results of the present paper, we have to describe some of our previous results. In Refs. 15 and 16 we studied the system described by (1.2) or (1.3) in the situation where f is a periodic or quasi-periodic function of time and ϵ is "small." It is well known that the usual perturbative approach leads to difficulties involving secular terms (i.e., polynomials in t that appear order by order in perturbation theory and spoil the uniform convergence (in t) of the perturbative series) and, for quasi-periodic interactions, small denominators.

In Refs. 15 and 16, a special perturbative expansion (power series expansion in ϵ) was developed, whose main virtue is to be free of secular terms. The algorithm employed involves an inductive "renormalization" of a sort of effective field introduced through an exponential Ansatz (the function g, to be introduced below). For the sake of the reader we will shortly recall our method of elimination of secular terms in Sec. II. This method is further developed and systematized in Sec. III. The elimination of the secular terms resembles the treatment of "zero modes," discussed, i.e., in Ref. 11.

In the general case where f is *quasi-periodic*, it was established in Ref. 15 that the coefficients

of the expansion are also well-defined quasi-periodic functions of time but, due mainly to the presence of small denominators, we were not able to prove convergence of our ϵ-expansion. Actually, a convergent power expansion in ϵ is not expected without further assumptions (for a detailed analysis of these issues in related systems, see Ref. 12).

Less problematic is the case when f is *periodic*, since small denominators are absent. In Ref. 16, we showed how the difficulties analyzed in Ref. 15 can be circumvented in the case of *periodic* f and we were able to establish the convergence of our perturbative ϵ-expansion uniformly in $t\in\mathbb{R}$. As discussed in Ref. 16, our method not only recovers the Floquet form of the solution of the time-dependent Schrödinger equation [see (1.6)–(1.7) below], but also allows the computation of the secular frequency and of the Fourier coefficients in terms of explicit *convergent* ϵ-expansions, which constitutes a feature of our algorithm, compared to other expansion methods.

Due to the technical difficulties involved, we restricted our analysis in Ref. 16 to two classes of periodic functions, namely those satisfying the conditions (I) or (II) presented in Theorem 1.1, below (see also Ref. 16). In the present paper we extend the results of Ref. 16 to an additional class of periodic functions. As we will discuss in detail, it turns out that the situation we treat here is precisely the relevant one for the rigorous discussion of the phenomenon of dynamical localization. The inclusion of this new class of periodic functions leads to an essentially complete perturbative solution for some simple periodic functions, as $f(t)=F_0+\varphi\cos(\omega t)$ (ac–dc fields), representing a physically relevant situation.

The main result of Ref. 16 can be captured in the next theorem, for whose statement we need a definition we will repeatedly use in this work: for an almost periodic function h we denote by $M(h)$ the "mean value" of h, defined as $M(h):=\lim_{T\to\infty}(1/2T)\int_{-T}^{T}h(t)dt$. The mean value $M(h)$ equals the constant term in the Fourier expansion of h.

Theorem 1.1: *Let f be a real T_ω-periodic function of time ($T_\omega:=2\pi/\omega$ with $\omega>0$) whose Fourier decomposition $f(t)=\Sigma_{n\in\mathbb{Z}}F_n e^{in\omega t}$, contains only a finite number of terms, i.e., the set of integers $\{n\in\mathbb{Z}|F_n\neq 0\}$ is a finite set. Let $\Phi(t)=\binom{\phi_+(t)}{\phi_-(t)}=U(t)\Phi(0)=U(t,0)\Phi(0)$ be the solution of Eq. (1.3). Consider the two following distinct conditions on f:* **(I)** *$M(\mathcal{Q}_0)\neq 0$.* **(II)** *$M(\mathcal{Q}_0)=0$ but $M(\mathcal{Q}_1)\neq 0$, where*

$$q(t) \;:=\; \exp\left(i\int_0^t f(\tau)d\tau\right),\quad \mathcal{Q}_0(t) \;:=\; q(t)^2 \;=\; \exp\left(2i\int_0^t f(\tau)d\tau\right) \tag{1.4}$$

and

$$\mathcal{Q}_1(t) \;:=\; \mathcal{Q}_0(t)\int_0^t(\mathcal{Q}_0(\tau)^{-1}-M(\mathcal{Q}_0^{-1}))d\tau. \tag{1.5}$$

Then, for each f as above, satisfying condition (I) or (II), there exists a constant $K>0$ (depending on the Fourier coefficients $\{F_n, n\in\mathbb{Z}, n\neq 0\}$ and on ω) so that, for each ϵ with $|\epsilon|<K$, there are $\Omega\in\mathbb{R}$ and T_ω-periodic functions $u_{11}^{\pm}$ and $u_{12}^{\pm}$ such that the propagator $U(t)$ can be written as

$$U(t)=\begin{pmatrix} U_{11}(t) & U_{12}(t)\\ U_{21}(t) & U_{22}(t)\end{pmatrix}=\begin{pmatrix} U_{11}(t) & U_{12}(t)\\ -\overline{U_{12}(t)} & \overline{U_{11}(t)}\end{pmatrix},$$

with

$$U_{11}(t) \;=\; e^{-i\Omega t}u_{11}^{-}(t)+e^{i\Omega t}u_{11}^{+}(t),\quad U_{12}(t) \;=\; e^{-i\Omega t}u_{12}^{-}(t)+e^{i\Omega t}u_{12}^{+}(t). \tag{1.6}$$

The functions $u_{11}^{\pm}$ and $u_{12}^{\pm}$ have absolutely and uniformly converging Fourier expansions,

$$u_{11}^{\pm}(t) \;=\; \sum_{n\in\mathbb{Z}}\mathcal{U}_{11}^{\pm}(n)e^{in\omega t},\quad u_{12}^{\pm}(t) \;=\; \sum_{n\in\mathbb{Z}}\mathcal{U}_{12}^{\pm}(n)e^{in\omega t}. \tag{1.7}$$

Moreover, under the same assumptions, Ω and the Fourier coefficients $\mathcal{U}_{11}^{\pm}(n)$ and $\mathcal{U}_{12}^{\pm}(n)$ can be expressed in terms of absolutely converging power series on ϵ. □

Let us now discuss the conditions (I) and (II) of Theorem 1.1. Writing the Fourier decomposition of f as $f(t)=F_0+\Sigma_{n=1}^{J}[\varphi_1^{(n)}\cos(n\omega t)+\varphi_2^{(n)}\sin(n\omega t)]$ the set $\mathfrak{F}_{J,\omega}$ of all possible functions f with a given J and ω can be identified with the parameter space $\mathbb{R}^{2J+1}$ of all real coefficients F_0, $\varphi_{1,2}^{(n)}$, $1\leqslant n\leqslant J$. The (complex) condition $M(\mathcal{Q}_0)=0$ determines a $(2J)$- or $(2J-1)$-dimensional subset of $\mathfrak{F}_{J,\omega}$, where condition (II) eventually applies. It is also on this subset that the more restrictive condition $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=0$ should hold, restricting the parameter space of f to a $(2J-1)$-, $(2J-2)$- or $(2J-3)$-dimensional subset, if it is nontrivial. One should, therefore, expect that successive conditions like (I) and (II) would eventually exhaust completely the set $\mathfrak{F}_{J,\omega}$.

To illustrate all this, let us consider the simplest example, when f represents a monochromatic interaction: $f(t)=\varphi\cos(\omega t)$. A simple computation shows that $M(\mathcal{Q}_0)=J_0(2\varphi/\omega)$. Hence, condition (I) is satisfied, except when $\varphi=\omega x_a/2$, $a=1,2,\ldots$, where x_a is the a-th zero of J_0 in $\mathbb{R}_+$. Condition (II), however, is never fulfilled because $M(\mathcal{Q}_1)$ vanishes identically in this case (see Ref. 16 or below for details). To achieve a complete solution we have, therefore, to extend Theorem 1.1 to include further conditions beyond (I) and (II), holding when $\varphi=\omega x_a/2$.

It is important to note that the condition $M(\mathcal{Q}_0)=J_0(2\varphi/\omega)=0$ coincides with the condition for dynamical localization pointed in Refs. 7 and 8, mentioned above. Hence, at least in this case, the situation where (I) and (II) are violated is precisely the relevant one for the rigorous treatment of dynamical localization. In fact, due to the general form of the ϵ-expansion for the secular frequency Ω, it turns out that this is true for general quasi-periodic f, not only for the monochromatic situation.

In this paper we identify the first condition following (I) and (II), which we call condition (III), and show that the method of elimination of secular terms holds in this case as well, two highly nontrivial tasks. For periodic interactions, we show that the expansion (2.4) converges for $|\epsilon|$ sufficiently small, uniformly for all $t\in\mathbb{R}$. As we will discuss, this leads to a complete perturbative solution for the ac–dc field.

Concerning the dynamical localization effect, our results can be summarized as follows. We establish for periodic f that the secular frequency Ω is an analytic function of ϵ (for $|\epsilon|$ small) and express each term of the perturbative series in a closed form. We establish that, in the situation of approximate dynamical localization, not only the first order term of the perturbative expansion of Ω is zero, but also the second order term. We establish in the monochromatic case that the third order term of the perturbative expansion of Ω is nonzero. This proves that the effect is a third order one, and that the dynamical localization is not exact. In Sec. V we analyze in detail the case of ac–dc fields and point to other situations where approximate dynamical localization can be seen. As far as we know these results are new, since they require a detailed knowledge of the expansion series. Note also that our expansion is very general, in the sense that it is not limited to monochromatic interactions, or ac–dc fields.

In this paper, $\mathbb{Z}_+$ will denote the set of all non-negative integers (zero included) and $\mathbb{Z}_*$ the set of all integers, excluding zero. $\mathbb{Z}_{*+}$ is the set of all positive integers. These notations are also applied to $\mathbb{Z}^A$ and to the real line $\mathbb{R}$. Vectors in $\mathbb{Z}^A$ (or $\mathbb{R}^A$) will be written as $\underline{v}$. The operation $\underline{v}\cdot\underline{u}$ will denote the scalar product in $\mathbb{Z}^A$ (or $\mathbb{R}^A$), defined as $\underline{v}\cdot\underline{u}:=v_1u_1+\cdots+v_Au_A$.

For a quasi-periodic function $h:\mathbb{R}\to\mathbb{C}$, we write its Fourier decomposition as $h(t)=\Sigma_{\underline{m}\in\mathbb{Z}^A}H_{\underline{m}}e^{i\underline{m}\cdot\underline{\omega}_h t}$, where A is some positive integer and $\underline{\omega}_h\in\mathbb{R}_+^A$. The Fourier coefficient $H_{\underline{0}}$ will be denoted simply as H_0. For $m\in\mathbb{Z}$ we denote by $\langle\langle m\rangle\rangle$ the following function:

$$\langle\langle m\rangle\rangle := \begin{cases} |m|, & \text{for } m\neq 0, \\ 1, & \text{for } m=0. \end{cases} \tag{1.8}$$

Beyond the functions $\mathcal{Q}_0$ and $\mathcal{Q}_1$ defined in (1.4)–(1.5) we will often use the following functions:

$$\mathcal{Q}_2(t) \;:=\; \mathcal{Q}_0(t)\int_0^t (\mathcal{Q}_0(\tau)-M(\mathcal{Q}_0))d\tau, \quad \mathcal{Q}_3(t) \;:=\; \mathcal{Q}_0(t)\int_0^t (\mathcal{Q}_1(\tau)-M(\mathcal{Q}_1))d\tau. \tag{1.9}$$

Note that, by their definitions, the functions $\mathcal{Q}_i$, $i=0,\ldots,3$, are quasi-periodic if f is quasi-periodic. We will have more to say about their properties below.

II. ELIMINATION OF SECULAR TERMS. THE MAIN RESULTS

We recall in this section some of the methods and techniques developed in the previous works.[15,16] A key result for our method is the theorem below, proven in Ref. 15, which presents the solution of Eq. (1.3) in terms of particular solutions of a generalized Riccati equation.

Theorem 2.1: *Let $f:\mathbb{R}\to\mathbb{R}$, $f\in C^1(\mathbb{R})$ and $\epsilon\in\mathbb{R}$ and let $g:\mathbb{R}\to\mathbb{C}$, $g\in C^1(\mathbb{R})$, be a particular solution of the generalized Riccati equation,*

$$\dot{G}-iG^2-2ifG+i\epsilon^2 \;=\; 0. \tag{2.1}$$

Then, the function $\Phi:\mathbb{R}\to\mathbb{C}^2$ given by $\Phi(t)=\binom{\phi_+(t)}{\phi_-(t)}=U(t)\Phi(0)=U(t,0)\Phi(0)$, where

$$U(t):=\begin{pmatrix} R(t)(1+ig(0)S(t)) & -i\epsilon R(t)S(t) \\ -i\epsilon\overline{R(t)}\;\overline{S(t)} & \overline{R(t)}(1-i\overline{g(0)}\;\overline{S(t)}) \end{pmatrix},$$

with $R(t):=\exp(-i\int_0^t(f(\tau)+g(\tau))\,d\tau)$ and $S(t):=\int_0^t R(\tau)^{-2}\,d\tau$, is a solution of (1.3) with initial value $\Phi(0)=\binom{\phi_+(0)}{\phi_-(0)}\in\mathbb{C}^2$. □

Let us briefly describe some of the ideas leading to Theorem 2.1 and to other results of Ref. 15. As we saw in Ref. 15, the solutions of Eq. (1.3) can be studied in terms of the solutions of a particular complex version of Hill's equation:

$$\ddot{\phi}(t)+(i\dot{f}(t)+\epsilon^2+f(t)^2)\phi(t) \;=\; 0. \tag{2.2}$$

In fact, a simple computation shows that the components $\Phi(t)$ satisfy $\ddot{\phi}_\pm+(\pm i\dot{f}+\epsilon^2+f^2)\phi_+=0$. If we attempt to solve (2.2) using the Ansatz,

$$\phi(t)=\exp\left(-i\int_0^t (f(\tau)+g(\tau))d\tau\right), \tag{2.3}$$

it follows that g has to satisfy the generalized Riccati equation (2.1). We then try to find solutions for g in terms of a power expansion in ϵ (vanishing for $\epsilon=0$) like

$$g(t) \;=\; q(t)\sum_{n=1}^{\infty} v_n(t)\,\epsilon^n, \tag{2.4}$$

where the function q was defined in (1.4) and is of central importance in this work.

The heuristic idea behind the Ansätze (2.3) and (2.4) is the following. For $\epsilon\equiv 0$ a solution for (2.2) is given by $\exp(-i\int_0^t f(\tau)d\tau)$. Thus, in (2.3) and (2.4) we are searching for solutions in terms of an "effective external field" of the form $f+g$, with g given in terms of a convergent power series expansion in ϵ, vanishing for $\epsilon=0$. A solution of the form (2.3) leads to one of the two independent solutions of (2.2). The full solution of (1.3) in terms of solutions of Eq. (2.1) is that described in Theorem 2.1 (see the discussion of Ref. 15).

We proceed inserting (2.4) into (2.1). The result is a set of recursive first order linear differential equations for the functions v_n that can be easily integrated. The solutions are

$$v_1(t)=\kappa_1 q(t)\,, \qquad v_2(t) \;=\; q(t)\left[i\int_0^t (\kappa_1^2 \mathcal{Q}_0(\tau)-\mathcal{Q}_0(\tau)^{-1})\,d\tau+\kappa_2\right], \tag{2.5}$$

$$v_n(t)=q(t)\left[i\left(\int_0^t \sum_{p=1}^{n-1} v_p(\tau) v_{n-p}(\tau)\,d\tau\right)+\kappa_n\right], \qquad \text{for } n\geqslant 3\,, \tag{2.6}$$

where the κ_n's above, $n=1,2,\ldots,$ are *arbitrary* integration constants. Defining

$$\mathcal{I}_2(t) \;:=\; \kappa_1^2\mathcal{Q}_0(t)-\mathcal{Q}_0(t)^{-1}, \;\; \mathcal{I}_n(t) \;:=\sum_{p=1}^{n-1} v_p(t)v_{n-p}(t), \;\; n\geqslant 3,$$

we can write (2.5)–(2.6) as $v_1(t)=\kappa_1 q(t)$, $v_n(t)=iq(t)\int_0^t \mathcal{I}_n(\tau)d\tau+\kappa_n q(t)$, $n\geqslant 2$. Observe that, in particular, we could just set all the κ_n's equal to zero. However, this is not a clever choice, since it would result in polynomial terms on t (the so-called *secular terms*) for the series expansion (2.4). This, of course, would restrict the convergence of the series to short times. As noticed in Ref. 15, there is a choice of the κ_n for which one can eliminate all polynomial terms on t. This procedure, which we call the *elimination of secular terms*, will be briefly described now.

First of all, assuming that $f:\mathbb{R}\to\mathbb{R}$ is quasi-periodic, then q, defined in (2.4), is also quasi-periodic and so is v_1 in (2.5). The same is true for the integrand $\mathcal{I}_2$ which appears in v_2, Eq. (2.5). Recalling that $\mathcal{I}_2$ depends on the free integration constant κ_1, the key idea is to fix κ_1 in such a way that the mean value of $\mathcal{I}_2$ is equal to zero, that is $M(\mathcal{I}_2)=M(\kappa_1^2\mathcal{Q}_0-\mathcal{Q}_0^{-1})=0$. Since $\mathcal{Q}_0$ is a quasi-periodic function, it readily follows from this that

$$\kappa_1^2 \;=\; \frac{\overline{M(\mathcal{Q}_0)}}{M(\mathcal{Q}_0)}. \tag{2.7}$$

With this choice of κ_1 one guarantees the absence of a constant term in the Fourier expansion of $\mathcal{I}_2$. Since $\mathcal{I}_2$ is being integrated in time, this would imply the absence of a linear term on t in the final expression for v_1. An important remark is that (2.7) will only make sense if we assume $M(\mathcal{Q}_0)\neq 0$.

Under this assumption we can now proceed and fix recursively all integration constants κ_m by *imposing* a zero mean value for the integrands $\mathcal{I}_n$'s, $n=3,4,\ldots,$ which appear in (2.6). This procedure removes, order by order in ϵ, the presence of the secular terms in the series expansion (2.4) for g and recursively implies that all functions v_n are quasi-periodic. Once all secular terms have been removed, we may write $v_n(t)=\Sigma_{\underline{m}\in\mathbb{Z}^A} V_{\underline{m}}^{(n)} e^{i\underline{m}\cdot\omega t}$, provided the sum converges absolutely. This was proven as follows:[15] first it was shown that the Fourier coefficients $Q_{\underline{m}}$ of q satisfy $|Q_{\underline{m}}|\leqslant \mathcal{Q}e^{-\chi|\underline{m}|}$, for some $\chi>0$. Then, the method of elimination of secular terms described above was applied to fix the integration constants κ_n, leading to inductive bounds of the form $|V_{\underline{m}}^{(n)}|\leqslant \mathcal{K}_n e^{-\chi|\underline{m}|}$ for all $n=1,2,\ldots,$ thus proving convergence of the Fourier expansion. Due to the bad behavior of $\mathcal{K}_n$ for $n\to\infty$, it was not possible to prove convergence of the ϵ-expansion (2.4), and that might be seen as a formal quasi-periodic power series solution of (2.1).

The reason for the bad behavior of $\mathcal{K}_n$ is the presence of *small denominators* in the recursive relations for the coefficients $V_{\underline{m}}^{(n)}$. A general discussion of these problems is found in Ref. 15. However, in the case where f is *periodic*, stronger results are possible. In Ref. 16, where this case was studied, it was possible to prove the convergence of the power series (2.4) and uniform convergence of the Fourier series involved in the computation of the wave functions. Moreover, absolute convergence of the ϵ-expansions leading to the *secular frequency* and to the coefficients of the Fourier expansion of the wave functions was also proven.

All the work done in Refs. 15 and 16 was restricted to the conditions (I) and (II) of Theorem 1.1. These conditions are consequences of the method of elimination of secular terms. Clearly, (I) is vital for (2.7). Both cases were studied in Refs. 15 and 16. In the present work, we study a more restrictive condition than those represented by (I) and (II). Namely, we are concerned here with the

situation where $M(\mathcal{Q}_0)=0$ and also $M(\mathcal{Q}_1)=0$. In this case, the complexity of the calculations needed to find the proper choice of the constants κ_n grows very much in comparison with the cases (I) and (II). The reason is that, due to the hypothesis $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=0$, one needs to work with higher order terms in the expansion (2.4). This will become more clear in Sec. IV.

We are ready now to state the two main theorems of this work.

Theorem 2.2: *Let $f:\mathbb{R}\to\mathbb{R}$ be a real quasi-periodic function satisfying*

$$\text{(III) } M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=0, \ \ but \ \ M(\mathcal{Q}_3)\neq 0.$$

Then, there are constants $\kappa_n, n\geqslant 1$, such that all functions v_n given in (2.5)–(2.6) are quasi-periodic. The explicit recursive expressions for the constants κ_n are found in (4.42)–(4.43). □

The proof of this theorem is the content of Sec. IV. This theorem states that the procedure of elimination of secular terms outlined above also works under (III). When f is quasi-periodic this does not imply, however, that the formal solution (2.4) of (2.1) converges, since we have the same difficulties discussed in detail in Ref. 15.

For *periodic* f, the situation is different and stronger results can be proven. Let $f(t)=\Sigma_{m\in\mathbb{Z}}F_m e^{im\omega t}$ be a real periodic function with frequency ω. If $F_0=M(f)=0$, q and $\mathcal{Q}_0=q^2$ are also periodic and their spectra of frequencies are subsets of $\{n\omega, n\in\mathbb{Z}\}$. Following the notation employed in Ref. 16, we write the Fourier expansions of q and $\mathcal{Q}_0$ as

$$q(t) \ = \ \sum_{m\in\mathbb{Z}} Q_m e^{im\omega t}, \quad \mathcal{Q}_0(t) \ = \ q(t)^2 \ = \ \sum_{m\in\mathbb{Z}} Q_m^{(2)} e^{im\omega t}. \tag{2.8}$$

By relations (2.5)–(2.6) and with the choice of constants κ_n mentioned in Theorem 2.2 [see (4.42)–(4.43)], the functions v_n are also periodic and their spectra of frequencies are also subsets of $\{n\omega, n\in\mathbb{Z}\}$. We write their Fourier expansions as $v_n(t)=\Sigma_{m\in\mathbb{Z}}V_m^{(n)}e^{im\omega t}$.

In Appendix B we prove the theorem below, which justifies our whole procedure for the case of *periodic* interactions and establishes the convergence of (2.4).

Theorem 2.3: *Let $f(t)$ be as above with $F_0=M(f)=0$ and such that condition (III) of Theorem 2.2 is satisfied. Moreover, assume that the coefficients Q_m and $Q_m^{(2)}$ above satisfy the following: for any $\chi>0$ there is a positive constant $\mathcal{Q}\equiv\mathcal{Q}(\chi)$ such that*

$$|Q_m| \ \leqslant \ \mathcal{Q}\frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2} \quad \text{and} \quad |Q_m^{(2)}| \ \leqslant \ \mathcal{Q}\frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2}, \tag{2.9}$$

for all $m\in\mathbb{Z}$, where the symbol $\langle\langle m\rangle\rangle$ was defined in (1.8). Then, with the constants κ_n fixed as in Theorem 2.2, the Fourier coefficients of the functions v_n given in (2.5)–(2.6) satisfy

$$|V_m^{(n)}| \ \leqslant \ M_0(M_1)^n \ \frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2} \ , \quad \forall m\in\mathbb{Z}, \ \ n\geqslant 1,$$

for some positive constants M_0, M_1. As a consequence, the power series expansion (2.4), representing a solution of Eq. (2.1), converges uniformly for all $t\in\mathbb{R}$, provided $|\epsilon|<1/M_1$. □

It follows from this theorem that the main consequences of Theorem 1.1 are valid under condition (III) as well. In particular, the Floquet form (1.6) holds and the secular frequency Ω and the Fourier coefficients of (1.7) are analytic functions of ϵ for $|\epsilon|$ small enough. We remark that (2.9) was established in Ref. 15 for f periodic and represented by a *finite* Fourier series. The condition $F_0=M(f)=0$ above is not crucial and can be eliminated following the procedure described in Ref. 16.

A. The secular frequency

A feature of our method is that it allows us to present the complete ϵ-expansion for the secular frequency Ω (also known as Rabi frequency) associated to the solutions of (1.2)–(1.3) [see (1.6)]. One has (see Refs. 15, 16, and 17)

$$\Omega \;=\; M(f)+M(g)=F_0+\sum_{n=1}^{\infty}\epsilon^n M(qv_n)\,.$$

By Theorem 2.3 above, this expansion is convergent for $|\epsilon|$ small enough. The knowledge of the complete expansion is particularly important for the qualitative investigation of the long-time behavior of the solutions. After some simple calculations using (2.5)–(2.6) one gets

$$\Omega=F_0+\epsilon\kappa_1 M(\mathcal{Q}_0)+\epsilon^2[i\kappa_1^2 M(\mathcal{Q}_2)-iM(\mathcal{Q}_1)+\kappa_2 M(\mathcal{Q}_0)]+\epsilon^3[2\kappa_1 M(\mathcal{Q}_3)+\kappa_3 M(\mathcal{Q}_0)]$$
$$+O(\epsilon^4)\,. \tag{2.10}$$

As we will show in Corollary 3.2, $M(\mathcal{Q}_0)=0$ implies $M(\mathcal{Q}_2)=0$. Hence, for case (II),

$$\Omega \;=\; F_0-i\epsilon^2 M(\mathcal{Q}_1)+2\kappa_1\epsilon^3 M(\mathcal{Q}_3)+O(\epsilon^4)\,, \tag{2.11}$$

and for case (III),

$$\Omega \;=\; F_0+2\kappa_1\epsilon^3 M(\mathcal{Q}_3)+O(\epsilon^4)\,. \tag{2.12}$$

Actually, after fixing κ_1 in Sec. IV A, we will see that $\Omega=F_0+2\epsilon^3|M(\mathcal{Q}_3)|+O(\epsilon^4)$.

In this case (III), if one additionally has $F_0=0$, then $\Omega=O(\epsilon^3)$, a fact first pointed in Ref. 17. This implies long transition times for certain probability amplitudes, a phenomenon known as dynamical localization (see Ref. 10 and other references therein). In Sec. V we discuss this situation for f describing a monochromatic interaction.

III. SPECIAL PROPERTIES. THE RENORMALIZATION OPERATION

Let us now introduce some notations and techniques that will be useful below. Since expressions as $f(\xi)\int_0^{\xi}d\xi' g(\xi')$ will often appear throughout our calculations, we define a shorthand notation,

$$(f\,|\,g)_{\xi} \;:=\; f(\xi)\int_0^{\xi}d\xi'\,g(\xi')\,. \tag{3.1}$$

Moreover, if $(f\,|\,g)_t$ is quasi-periodic function on t, then $M(f\,|\,g)$ will denote its mean value. We also define $(f\,|\,g\,|\,h)_{\xi}:=(f\,|\,(g\,|\,h)_{\xi'})_{\xi}=f(\xi)\int_0^{\xi}d\xi' g(\xi')\int_0^{\xi'}d\xi'' h(\xi'')$. Further compositions like $(f_1\,|f_2\,|\cdots|\,f_n)_{\xi}$ are defined in an analogous way, so that, for $n>2$, $(f_1\,|f_2\,|\cdots|\,f_n)_{\xi}$ $:=(f_1\,|\,(f_2\,|\cdots|\,f_n)_{\xi'})_{\xi}$.

A. Properties of the mean value

The following general results on the mean value of some quasi-periodic functions will be used for many purposes in the present work.

Proposition 3.1: Let a, b and $c:\mathbb{R}\to\mathbb{C}$ be quasi-periodic functions with Fourier components denoted by $A_{\underline{m}}$, $B_{\underline{m}}$ and $C_{\underline{m}}$, $\underline{m}\in\mathbb{Z}^A$, respectively. We have the following statements:

(1) If $M(c)=0$, then the Fourier components of the function $h(t):=(b\,|\,c)_t$ are given by

$$H_{\underline{n}} \;=\; \sum_{\underline{m}\neq\underline{0}}\frac{i\,C_{\underline{m}}(B_{\underline{n}}-B_{\underline{n}-\underline{m}})}{\underline{m}\cdot\underline{\omega}}, \tag{3.2}$$

for all $\underline{n}\in\mathbb{Z}^A$. Moreover, if $M(b)=0$ and $C_{\underline{m}}B_{-\underline{m}}=C_{-\underline{m}}B_{\underline{m}}$ for all $\underline{m}\neq\underline{0}$, then $M(h)=0$.

(2) If $M(b)=0$ and $M(c)=0$, then $M(b\,|\,c)=-M(c\,|\,b)$.
(3) If $M(c)=0$, then $M(c\,|\,c)=0$.
(4) If $M(a)=M(c)=M(b\,|\,c)=0$, then

$$M(a\,|\,b\,|\,c) \;=\; -M\left[\,b(t)\left(\int_0^t a(\tau)\,d\tau\right)\left(\int_0^t c(\tau)\,d\tau\right)\right]. \tag{3.3}$$

Moreover, if also $M(b\,|\,a)=0$, *then* $M(a\,|\,b\,|\,c)=M(c\,|\,b\,|\,a)$.

(5) *If* $M(a)=M(b)=M(c)=0$ *and* $M(b\,|\,c)=M(c\,|\,a)=M(a\,|\,b)=0$, *then*

$$M(a\,|\,b\,|\,c)+M(b\,|\,c\,|\,a)+M(c\,|\,a\,|\,b) \;=\; 0\,. \tag{3.4}$$

(6) If $M(a)=0$, *it follows from (3) and (5) that* $M(a\,|\,a\,|\,a)=0$. □

Proof: We can prove (3.2) by explicitly computing the Fourier decomposition of $h(t)$. Now, if $M(b)=B_0=0$ and $C_{\underline{m}}B_{-\underline{m}}=C_{-\underline{m}}B_{\underline{m}}$ for all $\underline{m}\in\mathbb{Z}^A_*$, then

$$H_0 \;=\; \sum_{\underline{m}\neq\underline{0}} \frac{-i\,C_{\underline{m}}B_{-\underline{m}}}{\underline{m}\cdot\underline{\omega}} \;=\; \frac{-i}{2}\sum_{\underline{m}\neq\underline{0}} \frac{(C_{\underline{m}}B_{-\underline{m}}-C_{-\underline{m}}B_{\underline{m}})}{\underline{m}\cdot\underline{\omega}} \;=\; 0\,. \tag{3.5}$$

Since $M(h)=H_0$, we completed the proof of (1). To demonstrate (2) we simply use the first equality of (3.5) to write $M(b\,|\,c)=\Sigma_{\underline{m}\neq\underline{0}}(-i\,C_{\underline{m}}B_{-\underline{m}}/(\underline{m}\cdot\underline{\omega}))$ and $M(c\,|\,b)=\Sigma_{\underline{m}\neq\underline{0}}(-i\,B_{\underline{m}}C_{-\underline{m}}/(\underline{m}\cdot\underline{\omega}))$. Changing $\underline{m}\to-\underline{m}$ the statement follows. Statement (3) is a mere consequence of (2) when we take $b=c$. The first statement (4) can be proven using (2), taking $h(t):=(b\,|\,c)_t$, noticing that $M(h)=M(b\,|\,c)=0$ and $M(a)=0$ and using (2). To prove the second statement in (4), all we need to do is to interchange the roles of c and a (note that since $M(b\,|\,a)=0$, the mean value of $(c\,|\,b\,|\,a)_t$ is well defined). Finally, statement (5) can be easily obtained writing $b(t)=(d/dt)\int_0^t b(\tau)d\tau$ and using integration by parts, together with (3.3). ■

The following trivial corollary is of crucial importance for some of our calculations.

Corollary 3.2: For $M(\mathcal{Q}_0)=0$ *one always has* $M(\mathcal{Q}_2)=0$. □

Proof: If $M(\mathcal{Q}_0)=0$ then, by (1.9), $\mathcal{Q}_2(t)=(\mathcal{Q}_0\,|\,\mathcal{Q}_0)_t$. Hence, from statement (3) of Proposition 3.1, it follows that $M(\mathcal{Q}_2)=0$. ■

B. The Renormalization Operation

For general quasi-periodic functions $a_1,\ldots,a_n$, the function $(a_1\,|\cdots|\,a_n)_t$ is not always quasi-periodic, since an integration performed on a quasi-periodic function with a nonzero mean value would produce a (linear in t) secular term, which would eventually become a higher degree polynomial after further integrations. Here we will describe an operation designed to produce a quasi-periodic function out of $(a_1\,|\cdots|\,a_n)_t$ through interactive subtractions of the mean value of the functions being integrated, a procedure we call ''renormalization'' due to some analogy with the procedure of perturbative renormalization in quantum field theory. We will use this procedure of renormalization in the following sections and here we present its definition and basic properties.

Let $a_1,\ldots,a_n$ be quasi-periodic functions. We define inductively the *renormalization operation* $\mathscr{R}_n$ acting on $(a_1\,|\cdots|\,a_n)$ by

$$\mathscr{R}_1 a_1(t):=a_1(t),$$

$$\mathscr{R}_2(a_1\,|\,a_2)_t:=(a_1\,|\,\mathscr{R}_1(a_2)-M(\mathscr{R}_1(a_2)))_t \;=\; (a_1\,|\,a_2-M(a_2))_t,$$

$$\mathscr{R}_n(a_1\,|\cdots|\,a_n)_t:=(a_1\,|\,\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n)-M(\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n)))_t,$$

for $n>2$. We will now prove some elementary facts on $\mathscr{R}_n$ which will be used below. The first important observation is that if $a_1,\ldots,a_n$ are quasi-periodic functions, then $\mathscr{R}_n(a_1\,|\cdots|\,a_n)$ is also quasi-periodic. This can be easily seen by induction, through the obvious remark that the mean value of $\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n)-M(\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n))$ is zero. Note also that, trivially,

$$a_0\,\mathscr{R}_n(a_1\,|\cdots|\,a_n) \;=\; \mathscr{R}_n(a_0a_1\,|\cdots|\,a_n)\,. \tag{3.6}$$

The following proposition is a trivial but useful restatement of the definition of the $\mathscr{R}_n$'s

Proposition 3.3: For all $n\geqslant 2$ the following statement holds: if $a_1,\ldots,a_n$ are quasi-periodic functions, then $\mathscr{R}_n(a_1\,|\cdots|\,a_n)=\mathscr{R}_2(a_1\,|\,\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n))$. Consequently, for $n>2$,

$$\mathscr{R}_n(a_1\,|\cdots|\,a_n) \;=\; \mathscr{R}_2(a_1\,|\;\mathscr{R}_2(a_2\,|\;\mathscr{R}_2(\cdots|\,\mathscr{R}_2(a_{n-1}\,|\,a_n))\cdots)\,). \tag{3.7}$$

□

Proof: By the definition of $\mathscr{R}_2$,

$$\begin{aligned}\mathscr{R}_2(a_1\,|\,\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n))&=(a_1\,|\,\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n)-M(\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_n)))\\&=\mathscr{R}_n(a_1\,|\cdots|\,a_n).\end{aligned}$$

■

Relation (3.7) shows that the operation $\mathscr{R}_n$ can be obtained by iteration of the operation $\mathscr{R}_2$. One also has the following useful proposition.

Proposition 3.4: For all $n\geqslant 1$ the following statement holds: if $a_1,\ldots,a_n$ are quasi-periodic functions and $a_n=\mathscr{R}_2(b\,|\,c)$ for quasi-periodic functions b,c, then $\mathscr{R}_n(a_1\,|\cdots|\,a_{n-1}\,|\,a_n)=\mathscr{R}_{n+1}(a_1\,|\cdots|\,a_{n-1}\,|\,b\,|\,c)$. □

Proof: For $n=1$, let $a_1=\mathscr{R}_2(b\,|\,c)$. Then $\mathscr{R}_1a_1=a_1=\mathscr{R}_2(b\,|\,c)$, trivially. For $n=2$, let $a_2=\mathscr{R}_2(b\,|\,c)$. Then, $\mathscr{R}_2(a_1\,|\,a_2)=(a_1\,|\,a_2-M(a_2))=(a_1\,|\,\mathscr{R}_2(b\,|\,c)-M(\mathscr{R}_2(b\,|\,c)))$, but, by definition, $\mathscr{R}_3(a_1\,|\,b\,|\,c)=(a_1\,|\,\mathscr{R}_2(b\,|\,c)-M(\mathscr{R}_2(b\,|\,c)))$ and the statement holds again. For $n>2$, let $a_n=\mathscr{R}_2(b\,|\,c)$. Then, by induction,

$$\begin{aligned}\mathscr{R}_{n+1}(a_1\,|\cdots|\,a_{n-1}\,|\,b\,|\,c)&=(a_1\,|\quad\mathscr{R}_n(a_2\,|\cdots|\,a_{n-1}\,|\,b\,|\,c)-M(\mathscr{R}_n(a_2\,|\cdots|\,a_{n-1}\,|\,b\,|\,c)))\\&=(a_1\,|\quad\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_{n-1}\,|\,a_n)-M(\mathscr{R}_{n-1}(a_2\,|\cdots|\,a_{n-1}\,|\,a_n)))\\&=\mathscr{R}_n(a_1\,|\cdots|\,a_{n-1}\,|\,a_n).\end{aligned}$$

■

If a and $b_1,\ldots,b_m$ are quasi-periodic, a function like $\Sigma_{k=1}^m(a\,|\,b_k)$ may not be a sum of quasi-periodic functions, even when $(a\,|\,\Sigma_{k=1}^m b_k)=\Sigma_{k=1}^m(a\,|\,b_k)$ is quasi-periodic, since we are not assuming that $M(b_k)=0$ for each individual k. This fact notwithstanding, the following simple statement holds and will be repeatedly used.

Proposition 3.5: Let a and $b_1,\ldots,b_m$ be quasi-periodic functions. Then $\mathscr{R}_2(a\,|\,\Sigma_{k=1}^m b_k)=\Sigma_{k=1}^m\mathscr{R}_2(a\,|\,b_k)$. Consequently, $\mathscr{R}_n(a_1\,|\cdots|\,a_{n-1}\,|\,\Sigma_{k=1}^m b_k)=\Sigma_{k=1}^m\mathscr{R}_n(a_1\,|\cdots|\,a_{n-1}\,|\,b_k)$ for quasi-periodic functions $a_1,\ldots,a_{n-1}$ and $b_1,\ldots,b_m$. □

Proof: We have

$$\mathscr{R}_2\left(a\,\middle|\,\sum_{k=1}^m b_k\right) \;=\; \left(a\,\middle|\,\sum_{k=1}^m b_k-M\left(\sum_{k=1}^m b_k\right)\right) \;=\; \sum_{k=1}^m(a\,|\,b_k-M(b_k)) \;=\; \sum_{k=1}^m\mathscr{R}_2(a\,|\,b_k).$$

The general case follows this and from (3.7). ■

The following corollary follows from Propositions 3.4 and 3.5.

Corollary 3.6: Let $a_1,\ldots,a_{n-1}$, $b_1,\ldots,b_m$ and $c_1,\ldots,c_m$ be quasi-periodic functions. Then,

$$\mathscr{R}_n\left(a_1\,\middle|\cdots|a_{n-1}|\sum_{k=1}^m\mathscr{R}_2(b_k|c_k)\right)=\sum_{k=1}^m\mathscr{R}_{n+1}(a_1|\cdots|a_{n-1}|b_k|c_k).$$

□

With the shorthand notation introduced in (3.1) and the definition of $\mathcal{Q}_0$ in (1.4), we see from (1.5), (1.9) that $\mathcal{Q}_1(t)=\mathscr{R}_2(\mathcal{Q}_0\,|\,\overline{\mathcal{Q}_0})_t$, $\mathcal{Q}_2(t)=\mathscr{R}_2(\mathcal{Q}_0\,|\,\mathcal{Q}_0)_t$, $\mathcal{Q}_3(t)=\mathscr{R}_2(\mathcal{Q}_0\,|\,\mathcal{Q}_1)_t$. Below, we will often use the following compact notation:

$$(i\,|\,j)_t:=(\mathcal{Q}_i\,|\,\mathcal{Q}_j)_t,\quad (i\,|\,\overline{j})_t:=(\mathcal{Q}_i\,|\,\overline{\mathcal{Q}_j})_t,\quad (i\,|\,j\,|\,k)_t:=(\mathcal{Q}_i\,|\,\mathcal{Q}_j\,|\,\mathcal{Q}_k)_t,$$

etc, for $i,j,k=0,\ldots,3$. In other words, we simply use the index n of $\mathcal{Q}_n$ to denote $\mathcal{Q}_n$ itself. Moreover, by $M(i\,|\,j)$ we will denote the mean value of $(i\,|\,j)_t$, etc. Note that for $M(\mathcal{Q}_0)=0$ one has with this notation $\mathcal{Q}_1(t)=(0\,|\,\overline{0})_t$ and $\mathcal{Q}_2(t)=(0\,|\,0)_t$ and for $M(\mathcal{Q}_1)=0$ one has $\mathcal{Q}_3(t)=(0\,|\,1)_t$. We will often write $\mathcal{Q}_3$ this way. For $M(\mathcal{Q}_0)=0$, other identities will also be at hand. For instance, one has

$$(0\,|\,0\,|\,0)_t \;=\; (0\,|\,(0\,|\,0)_{t'})_t \;=\; (0\,|\,2)_t \;\text{ and }\; (1\,|\,0)_t \;=\; (2\,|\,\overline{0})_t, \tag{3.8}$$

since $M(0\,|\,0)=0$, by item (3) of Proposition 3.1. Relations like these will be often employed.

IV. THE CASE $M(\mathcal{Q}_0)=0$ AND $M(\mathcal{Q}_1)=0$

In this section we will prove the Theorem 2.2. Our interest is to study the situation complementary to cases (I) and (II), i.e., the situation where one has the condition

$$(\mathrm{III}_0)\; M(\mathcal{Q}_0)=0 \;\text{ and }\; M(\mathcal{Q}_1)=0.$$

To remove the secular terms from g, applying the method described in the previous section, we will be forced to add a further restriction to (III_0), namely the condition $M(0\,|\,1)\neq 0$.

Recall that the functions q and $\mathcal{Q}_1$ depend primordially on the interaction f [see the definitions (1.4)–(1.5)], so conditions (I), (II) or (III_0) apply upon the properties of f. As we already saw in Sec. (I), the function $f(t)=\varphi\cos(\omega t)$ only satisfies condition (I) or (III_0), depending on the particular choice of the parameters φ,ω. We will have more to say about this example later on in Sec. V. Now, let us work with the expansion for g in order to remove all of its secular terms.

Again, our Ansatz to solve (2.1) is (2.4). The solutions for v_n are (2.5)–(2.6). One sees immediately from condition (III_0) that v_1 and v_2 do not suffer from secular terms. Indeed, since $M(\mathcal{Q}_0^{-1})=\overline{M(\mathcal{Q}_0)}=0$, we conclude that the mean value of the integrand $\mathcal{I}_2$ in (2.5) is zero. Therefore, the integration occurring in the expression for v_2 in (2.5) does not produce a linear term in t. These facts imply that v_1 and v_2 are quasi-periodic under (III_0). From these considerations we see that the condition $M(\mathcal{I}_n)=0$, $n\geqslant 3$, becomes recursively identical to $\Sigma_{p=1}^{n-1}M(v_p v_{n-p})$, $n\geqslant 3$, since the v_n's become successively quasi-periodic when the interactive procedure is run.

If we succeed in fixing $M(\mathcal{I}_n)=0$ for all n, we may rewrite (2.5)–(2.6) in a "renormalized" form:

$$v_1(t)=\kappa_1 q(t), \qquad v_2(t) \;=\; q(t)^{-1}(i\kappa_1^2\mathcal{Q}_2(t)-i\mathcal{Q}_1(t)+\kappa_2\mathcal{Q}_0(t)), \tag{4.1}$$

$$v_n(t)=q(t)^{-1}\left\{ i\sum_{p=1}^{n-1} \mathscr{R}_2(0\,|\,v_p v_{n-p})_t+\kappa_n\mathcal{Q}_0(t)\right\}, \quad n\geqslant 3, \tag{4.2}$$

where $\mathcal{Q}_0$, $\mathcal{Q}_1$ and $\mathcal{Q}_2$ were defined in (1.4), (1.5) and (1.9), respectively.

Let us move on and analyze the third order term. According to (2.6) the integrand $\mathcal{I}_3$ which appears in the definition of v_3 is given by $2v_1v_2$. Using (4.1) we have

$$v_1v_2 \;=\; i\kappa_1^3\mathcal{Q}_2-i\kappa_1\mathcal{Q}_1+\kappa_1\kappa_2\mathcal{Q}_0\,. \tag{4.3}$$

From Corollary 3.2, we readily see that $M(\mathcal{I}_3)=2M(v_1v_2)=0$, implying that v_3 is quasi-periodic.

Until now we have verified the absence of secular terms in the series expansion of g up to order three in ϵ. As we shall see next, for the same to be true up to order four, we have to make a special choice for the value of the constant κ_1.

A. The absence of secular terms in v_4. Fixing κ_1

As one sees from (2.6), the integrand in v_4 is $\mathcal{I}_4 := 2v_1v_3+v_2^2$. Since v_1, v_2, v_3 are quasi-periodic, the mean value of $\mathcal{I}_4$ is well defined. Let us explicitly evaluate $\mathcal{I}_4$. Using (2.5)–(2.6) one gets

$$\mathcal{I}_4 = -4\kappa_1^4(0\,|\,2)+4\kappa_1^2(0\,|\,1)+6i\kappa_1^2\kappa_2\mathcal{Q}_2+(2\kappa_1\kappa_3+\kappa_2^2)\mathcal{Q}_0 \\ -2i\kappa_2\mathcal{Q}_1-\kappa_1^4(2\,|\,0)+2\kappa_1^2(2\,|\,\overline{0})-(1\,|\,\overline{0})\,. \tag{4.4}$$

The functions on the r.h.s. of (4.4) are all quasi-periodic, since $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$. Therefore, we are allowed to take the mean value of each individual term above. The result is

$$M(\mathcal{I}_4) = -4\kappa_1^4M(0\,|\,2)+4\kappa_1^2M(0\,|\,1)-\kappa_1^4M(2\,|\,0)+2\kappa_1^2M(2\,|\,\overline{0})-M(1\,|\,\overline{0}).$$

By statements (2) and (6) of Proposition 3.1 and by (3.8) we have

$$M(2\,|\,0)=-M(0\,|\,2) = -M(0\,|\,0\,|\,0)=0\,, \tag{4.5}$$

$$M(2\,|\,\overline{0})=M(1\,|\,0) = -M(0\,|\,1)\,. \tag{4.6}$$

Hence,

$$M(\mathcal{I}_4) = 2\kappa_1^2M(0\,|\,1)-M(1\,|\,\overline{0})\,. \tag{4.7}$$

We have the following.

Proposition 4.1: Under $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=0$, one has $M(1\,|\,\overline{0})=2\overline{M(0\,|\,1)}$. □

Proof: By the definition of $\mathcal{Q}_1$, $M(0\,|\,1)=M(0\,|\,0\,|\,\overline{0})$ and

$$M(1\,|\,\overline{0})=M\left(\mathcal{Q}_0(t)\left(\int_0^t\mathcal{Q}_0(\tau)^{-1}\,d\tau\right)\left(\int_0^t\mathcal{Q}_0(\tau)^{-1}\,d\tau\right)\right)=-M(\overline{0}\,|\,0\,|\,\overline{0})\,, \tag{4.8}$$

where, in the last equality, we have used statement (4) of Proposition 3.1. Now, by statement (5) of the same proposition, we can write

$$M(0\,|\,0\,|\,\overline{0})+M(0\,|\,\overline{0}\,|\,0)+M(\overline{0}\,|\,0\,|\,0) = 0 \tag{4.9}$$

[recall that $M(0\,|\,\overline{0})=M(\overline{0}\,|\,0)=M(0\,|\,0)=0$]. Once again, by statement (4) of Proposition 3.1, $M(0\,|\,0\,|\,\overline{0})=M(\overline{0}\,|\,0\,|\,0)$. Thus, (4.9) reads as $2M(0\,|\,0\,|\,\overline{0})+M(0\,|\,\overline{0}\,|\,0)=0$. Taking the complex conjugate yields $2\overline{M(0\,|\,0\,|\,\overline{0})}+M(\overline{0}\,|\,0\,|\,\overline{0})=0$. Finally, using $M(0\,|\,1)=M(0\,|\,0\,|\,\overline{0})$ and (4.8), we get $M(1\,|\,\overline{0})=2\overline{M(0\,|\,1)}$. ■

We have just proven that $M(\mathcal{I}_4)=2(\kappa_1^2M(0\,|\,1)-\overline{M(0\,|\,1)})$. Now we impose $M(\mathcal{I}_4)=0$. Of course, this will be the case if $M(0\,|\,1)=0$ but, in the situation where $M(0\,|\,1)\neq 0$ this can be achieved by fixing κ_1 as [see (4.7)]

$$\kappa_1 = \left(\frac{\overline{M(0\,|\,1)}}{M(0\,|\,1)}\right)^{1/2} = \left(\frac{\overline{M(\mathcal{Q}_3)}}{M(\mathcal{Q}_3)}\right)^{1/2}. \tag{4.10}$$

Thus, κ_1 is a phase: $|\kappa_1|=1$. It will be henceforth assumed that $M(0\,|\,1)\neq 0$. If $M(0\,|\,1)=0$, κ_1 has to be fixed by $M(\mathcal{I}_5)=0$. We shall not treat this more restrictive case here.

So far, we have verified the absence of secular terms in the series expansion (2.4) for g up to order three in ϵ and we have eliminated them from v_4 by making a special choice for the value of κ_1 [given by (4.10)]. At this point we would like to proceed recursively by imposing

$M(\mathcal{I}_n)=0$, for all $n\geqslant 5$. This would give the correct values for the constants κ_p, $p\geqslant 2$, and guarantee the absence of secular terms in all v_n, $n\geqslant 5$. This recursive procedure was used in Ref. 15 to eliminate the secular terms from g in cases (I) and (II). Here, we still have to determine the constants κ_2 and κ_3 explicitly (not recursively) before running the recursive procedure.

B. The absence of secular terms in v_5. Fixing κ_2

Let us begin by calculating the integrand $\mathcal{I}_5$ which appears in v_5. Taking $n=5$ in (2.6) we get $\mathcal{I}_5=2v_1v_4+2v_2v_3$. We first evaluate v_1v_4 explicitly and then v_2v_3.

Since we have $M(\mathcal{I}_3)=0$ and since with the choice of κ_1 in (4.10) we imposed $M(\mathcal{I}_4)=0$, we have by the recursive relations (4.1)–(4.2),

$$v_1v_3=2i\kappa_1\,\mathscr{R}_2(0\,|\,v_1v_2)+\kappa_1\kappa_3\mathcal{Q}_0\,, \tag{4.11}$$

$$v_1v_4=2i\kappa_1\,\mathscr{R}_2(0\,|\,v_1v_3)+i\kappa_1\,\mathscr{R}_2(0\,|\,v_2^2)+\kappa_1\kappa_4\mathcal{Q}_0\,. \tag{4.12}$$

Inserting (4.3) onto the r.h.s. of (4.11) we get

$$v_1v_3 \;=\; -2\kappa_1^4\,\mathscr{R}_2(0\,|\,2)+2\kappa_1^2\,\mathscr{R}_2(0\,|\,1)+2i\kappa_1^2\kappa_2\,\mathscr{R}_2(0\,|\,0)+\kappa_1\kappa_3\,\mathcal{Q}_0\,. \tag{4.13}$$

Inserting this onto the r.h.s. of (4.12) gives

$$\begin{aligned}v_1v_4=&-4i\kappa_1^5\,\mathscr{R}_3(0\,|\,0\,|\,2)+4i\kappa_1^3\,\mathscr{R}_3(0\,|\,0\,|\,1)-4\kappa_1^3\kappa_2\,\mathscr{R}_3(0\,|\,0\,|\,0)+2i\kappa_1^2\kappa_3\,\mathscr{R}_2(0\,|\,0)\\&+i\kappa_1\,\mathscr{R}_2(0\,|\,v_2^2)+\kappa_1\kappa_4\mathcal{Q}_0\,.\end{aligned} \tag{4.14}$$

Let us now compute v_2^2. Since $v_2=\kappa_2 q+iq^{-1}(\kappa_1^2\mathcal{Q}_2-\mathcal{Q}_1)$, we have

$$v_2^2 \;=\; \kappa_2^2\mathcal{Q}_0+2i\kappa_1^2\kappa_2\mathcal{Q}_2-2i\kappa_2\mathcal{Q}_1+s\,, \tag{4.15}$$

where $s:=-\mathcal{Q}_0^{-1}(\kappa_1\mathcal{Q}_2-\mathcal{Q}_1)^2$ and κ_1 alone. Now, we insert this into (4.14) and get

$$\begin{aligned}v_1v_4=&-4i\kappa_1^5\,\mathscr{R}_3(0\,|\,0\,|\,2)+4i\kappa_1^3\,\mathscr{R}_3(0\,|\,0\,|\,1)-6\kappa_1^3\kappa_2\,\mathscr{R}_2(0\,|\,2)+2i\kappa_1^2\kappa_3\,\mathscr{R}_2(0\,|\,0)\\&+i\kappa_1\kappa_2^2\,\mathscr{R}_2(0\,|\,0)+2\kappa_1\kappa_2\,\mathscr{R}_2(0\,|\,1)+i\kappa_1\,\mathscr{R}_2(0\,|\,s)+\kappa_1\kappa_4\mathcal{Q}_0\,,\end{aligned} \tag{4.16}$$

where we used the fact that $\mathscr{R}_3(0\,|\,0\,|\,0)=\mathscr{R}_2(0\,|\,2)$. Collecting in (4.16) the terms depending only on κ_1, and defining

$$\mathcal{A}_1 \;:=\; -4\kappa_1^4\,\mathscr{R}_3(0\,|\,0\,|\,2)+4\kappa_1^2\,\mathscr{R}_3(0\,|\,0\,|\,1)+\mathscr{R}_2(0\,|\,s), \tag{4.17}$$

expression (4.16) becomes

$$v_1v_4 \;=\; -6\kappa_1^3\kappa_2\,\mathscr{R}_2(0\,|\,2)+2\kappa_1\kappa_2\,\mathscr{R}_2(0\,|\,1)+i\kappa_1(2\kappa_1\kappa_3+\kappa_2^2)\,\mathcal{Q}_2+\kappa_1\kappa_4\mathcal{Q}_0+i\kappa_1\mathcal{A}_1\,. \tag{4.18}$$

From definition (4.17), it is evident that $\mathcal{A}_1$ is quasi-periodic, since it is a sum of quasi-periodic functions. Note that (4.17) depends only on the constant κ_1. Since we are working under the condition $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$, we can drop the symbol $\mathscr{R}_2$ above. From this fact and from relation (4.5), we conclude that $M(v_1v_4)=2\kappa_1\kappa_2\,M(0\,|\,1)+i\kappa_1M(\mathcal{A}_1)$.

Let us now calculate the second term in $\mathcal{I}_5$, namely, v_2v_3. A lengthy computation, analogous to the one above, gives

$$v_2v_3=-2i\kappa_1^5\mathscr{R}_2(2\,|\,2)+2i\kappa_1^3\mathscr{R}_2(2\,|\,1)-2\kappa_1^3\kappa_2\mathscr{R}_2(2\,|\,0)+2i\kappa_1^3\mathscr{R}_2(1\,|\,2)-2i\kappa_1\mathscr{R}_2(1\,|\,1)$$
$$+2\kappa_1\kappa_2\mathscr{R}_2(1\,|\,0)-2\kappa_1^3\kappa_2\mathscr{R}_2(0\,|\,2)+2\kappa_1\kappa_2\mathscr{R}_2(0\,|\,1)+i(2\kappa_1\kappa_2^2+\kappa_1^2\kappa_3)\mathcal{Q}_2-i\kappa_3\mathcal{Q}_1$$
$$+\kappa_2\kappa_3\mathcal{Q}_0\,. \tag{4.19}$$

Clearly the r.h.s. of (4.19) is quasi-periodic. Since we are working under the condition $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$, we can drop the symbol $\mathscr{R}_2$ above and reorder (4.19) in the form

$$v_2v_3=i(2\kappa_1\kappa_2^2+\kappa_1^2\kappa_3)\mathcal{Q}_2-i\kappa_3\mathcal{Q}_1+\kappa_2\kappa_3\mathcal{Q}_0-2i\kappa_1^5(2\,|\,2)-2i\kappa_1(1\,|\,1)+2i\kappa_1^3[(2\,|\,1)$$
$$+(1\,|\,2)]-2\kappa_1^3\kappa_2[(2\,|\,0)+(0\,|\,2)]+2\kappa_1\kappa_2[(1\,|\,0)+(0\,|\,1)]\,. \tag{4.20}$$

Above, we also used $\mathscr{R}_2(0\,|\,0)=\mathcal{Q}_2$. From (4.20), from the fact that $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$ and from statements (2) and (3) of Proposition 3.1, we see immediately that $M(v_2v_3)=0$.

We are now ready to find the value of κ_2 by imposing the condition $M(\mathcal{I}_5)=0$, which guarantees the absence of secular terms in v_5. Since $M(\mathcal{I}_5)=2M(v_1v_4)+2M(v_2v_3)=4\kappa_1\kappa_2M(0\,|\,1)+2i\kappa_1M(\mathcal{A}_1)$, we conclude that

$$\kappa_2 \;=\; -\frac{iM(\mathcal{A}_1)}{2M(0\,|\,1)}. \tag{4.21}$$

Note that the r.h.s. of (4.21) depends on the previously fixed κ_1.

C. The absence of secular terms in v_6. Fixing κ_3

We still have to find κ_3 in order to fix recursively all κ_n's for $n\geqslant 4$. κ_3 will be fixed by eliminating the secular terms from v_6, that is, by imposing $M(\mathcal{I}_6)=0$. First of all, we need to write $\mathcal{I}_6$. Using relation (2.6) for $n=6$ we find that $\mathcal{I}_6=2v_1v_5+2v_2v_4+v_3^2$. Let us calculate $2v_1v_5$. Another lengthy computation gives

$$2v_1v_5 \;=\; \mathcal{A}_2-12\kappa_1^3\kappa_3\mathscr{R}_2(0\,|\,2)+4\kappa_1\kappa_3\mathscr{R}_2(0\,|\,1)+4i\kappa_1(\kappa_2\kappa_3+\kappa_1\kappa_4)\mathcal{Q}_2+2\kappa_1\kappa_5\mathcal{Q}_0\,, \tag{4.22}$$

where $\mathcal{A}_2$ is the quasi-periodic function defined by

$$\mathcal{A}_2:=8\kappa_1^6\mathscr{R}_3(0\,|\,2\,|\,2)-8i\kappa_1^4\mathscr{R}_3(0\,|\,2\,|\,1)-8i\kappa_1^4\kappa_2\mathscr{R}_3(0\,|\,2\,|\,0)-8\kappa_1^4\mathscr{R}_3(0\,|\,1\,|\,2)$$
$$+8\kappa_1^2\mathscr{R}_3(0\,|\,1\,|\,1)+8i\kappa_1^2\kappa_2\mathscr{R}_3(0\,|\,1\,|\,0)+16i\kappa_1^2\kappa_2\mathscr{R}_3(0\,|\,0\,|\,1)-32i\kappa_1^4\kappa_2\mathscr{R}_3(0\,|\,0\,|\,2)$$
$$-12\kappa_1^2\kappa_2^2\mathscr{R}_2(0\,|\,2)-4\kappa_1^2\mathscr{R}_2(0\,|\,\mathcal{A}_1)\,, \tag{4.23}$$

which depends only on the constants κ_1 and κ_2. Since $2v_1v_5$ given above is a sum of quasi-periodic functions we can take the mean value of each individual term which appears on the r.h.s. of (4.22) and write

$$2M(v_1v_5) \;=\; M(\mathcal{A}_2)+4\kappa_3\kappa_1M(0\,|\,1)\,, \tag{4.24}$$

where, once again, we have used $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$ and the identity (4.5).

The second term of $\mathcal{I}_5$, namely $2v_2v_4$, is given by

$$2v_2v_4=\mathcal{A}_3-4\kappa_1^3\kappa_3\mathscr{R}_2(2\,|\,0)+4\kappa_1\kappa_3\mathscr{R}_2(1\,|\,0)+2i(\kappa_1^2\kappa_4+2\kappa_1\kappa_2\kappa_3)\mathcal{Q}_2-2i\kappa_4\mathcal{Q}_1$$
$$+2\kappa_2\kappa_4\mathcal{Q}_0 \tag{4.25}$$

where $\mathcal{A}_3$ is given by

$$\mathcal{A}_3 := 8\kappa_1^6 \mathscr{R}_3(2\,|\,0\,|\,2) - 8\kappa_1^4 \mathscr{R}_3(2\,|\,0\,|\,1) - 8i\kappa_1^4\kappa_2 \mathscr{R}_3(2\,|\,0\,|\,0) - 8\kappa_1^4 \mathscr{R}_3(1\,|\,0\,|\,2)$$
$$+ 8\kappa_1^2 \mathscr{R}_3(1\,|\,0\,|\,1) + 8i\kappa_1^2\kappa_2 \mathscr{R}_3(1\,|\,0\,|\,0) - 8i\kappa_1^4\kappa_2 \mathscr{R}_3(0\,|\,0\,|\,2) + 8i\kappa_1^2\kappa_2 \mathscr{R}_3(0\,|\,0\,|\,1)$$
$$- 8\kappa_1^2\kappa_2^2 \mathscr{R}_3(0\,|\,0\,|\,0) - 2\kappa_1^2 \mathscr{R}_2(2\,|\,v_2^2) + 2\,\mathscr{R}_2(1\,|\,v_2^2) + 2i\kappa_2\,\mathscr{R}_2(0\,|\,v_2^2), \tag{4.26}$$

which is quasi-periodic and depends only on the constants κ_1 and κ_2.

We can now proceed and take the mean value of $2v_2v_4$ from (4.25). Using $M(\mathcal{Q}_0) = M(\mathcal{Q}_1) = M(\mathcal{Q}_2) = 0$ and (4.5), we get

$$2M(v_2v_4) \;=\; M(\mathcal{A}_3) + 4\kappa_1\kappa_3 M(0\,|\,1)\,. \tag{4.27}$$

We are almost through with the calculation of $\mathcal{I}_6$. We still need v_3^2. Using relations (4.1)–(4.3),

$$\begin{aligned} v_3 &= q^{-1}\{2i\,\mathscr{R}_2(0\,|\,v_1v_2) + \kappa_3\mathcal{Q}_0\} \\ &= q^{-1}\{-2\kappa_1^3\,\mathscr{R}_2(0\,|\,2) + 2\kappa_1\,\mathscr{R}_2(0\,|\,1) + 2i\kappa_1\kappa_2\mathcal{Q}_2 + \kappa_3\mathcal{Q}_0\}. \end{aligned} \tag{4.28}$$

Hence, $v_3^2 = \kappa_3^2\mathcal{Q}_0 + 4\kappa_1\kappa_3[-\kappa_1^2\,\mathscr{R}_2(0\,|\,2) + \mathscr{R}_2(0\,|\,1) + i\kappa_2\mathcal{Q}_2] - 4\mathcal{A}_4$, where $\mathcal{A}_4$ and depends only on the already fixed constants κ_1 and κ_2: $\mathcal{A}_4 := \mathcal{Q}_0^{-1}[i\kappa_1^3\,\mathscr{R}_2(0\,|\,2) - i\kappa_1\,\mathscr{R}_2(0\,|\,1) + \kappa_1\kappa_2\mathcal{Q}_2]^2$. Therefore, using once more $M(\mathcal{Q}_0) = M(\mathcal{Q}_2) = 0$ and (4.5), we get $M(v_3^2) = 4\kappa_3\kappa_1 M(0\,|\,1) - 4M(\mathcal{A}_4)$. Finally, imposing $M(\mathcal{I}_6) = 0$, i.e., $2M(v_1v_5) + 2M(v_2v_4) + M(v_3^2) = 0$, we obtain from our previous calculations,

$$\kappa_3 \;=\; \frac{4M(\mathcal{A}_4) - M(\mathcal{A}_3) - M(\mathcal{A}_2)}{4\kappa_1 M(0\,|\,1)}. \tag{4.29}$$

Note that the r.h.s. of (4.29) depends on the previously fixed κ_1 and κ_2.

D. The absence of secular terms in v_n, $n \geqslant 7$. Fixing κ_{n-3} recursively

So far, we have fixed the constants κ_1, κ_2 and κ_3 individually. Now we proceed to fix recursively all other κ_{n-3} for all $n \geqslant 7$. We have to impose

$$M(\mathcal{I}_n) \;=\; 0 \;\Rightarrow\; M\left(\sum_{p=1}^{n-1} v_p v_{n-p}\right) \;=\; 0, \tag{4.30}$$

for all $n \geqslant 7$. Condition (4.30) guarantees the absence of secular terms in all v_n, $n \geqslant 7$.

The idea now is to use (4.30) to calculate recursively the constants κ_{n-3}, for all $n \geqslant 7$, that is, κ_4, κ_5, … . Of course, we already have κ_1, κ_2 and κ_3 and, hence, we completely know v_1, v_2 and v_3. We also know that all functions from v_1 to v_6 are quasi-periodic. From now on we will work inductively: we assume for each $n \geqslant 7$ that we fixed $\kappa_1, \ldots, \kappa_{n-4}$ by imposing $M(\mathcal{I}_m) = 0$ for all $m = 2, \ldots, n-1$ and that, as a consequence, all functions $v_1, \ldots, v_{n-1}$ are quasi-periodic. This is already known for $n = 7$. By our inductive hypothesis, we are allowed to take the summation out of the mean value M in (4.30) and write

$$2[M(v_1v_{n-1}) + M(v_2v_{n-2}) + M(v_3v_{n-3})] + \sum_{p=4}^{n-4} M(v_p v_{n-p}) \;=\; 0\,, \tag{4.31}$$

where, by convention, $\Sigma_{p=4}^{n-4} M(v_p v_{n-p}) = 0$ for $n = 7$. Let us introduce now the following definition:

$$l_m(t) \;=\; q(t)(v_m(t) - \kappa_m q(t))\,, \tag{4.32}$$

for all $m \geqslant 4$. Note that, by relation (2.6), the functions l_m's above can also be written as

$$l_m(t) \;=\; i\,q(t)^2\left(\int_0^t \sum_{p=1}^{m-1} v_p(\tau)v_{m-p}(\tau)\,d\tau\right). \tag{4.33}$$

For $m<n$ we are allowed to write

$$l_m(t) \;=\; i\,q(t)^2\left(\int_0^t \sum_{p=1}^{m-1} [v_p(\tau)v_{m-p}(\tau)-M(v_pv_{m-p})]\,d\tau\right) \;=\; i\sum_{p=1}^{m-1} \mathscr{R}_2(0\,|\,v_pv_{m-p})_t\,, \tag{4.34}$$

since we assumed $M(\Sigma_{p=1}^{m-1}v_pv_{m-p})=M(\mathcal{I}_m)=0$ for all $m<n$, by the inductive hypothesis. Hence, l_m are quasi-periodic for all $m<n$, by the inductive hypothesis.

Let us use the definition given in (4.32) and evaluate the first three terms which appear in (4.31). Beginning with the first one, we have

$$M(v_1v_{n-1}) \;=\; M(v_1(q^{-1}l_{n-1}+\kappa_{n-1}q)) \;=\; \kappa_1 M(l_{n-1})\,, \tag{4.35}$$

where we have used (2.5) and the fact that $M(\mathcal{Q}_0)=0$. Using (4.32), the second term of (4.31) can be evaluated as

$$M(v_2v_{n-2}) \;=\; M(v_2(q^{-1}l_{n-2}+\kappa_{n-2}q)) \;=\; M(q^{-1}v_2l_{n-2})\,, \tag{4.36}$$

where we have used (4.1) to express qv_2 and the fact that $M(\mathcal{Q}_0)=M(\mathcal{Q}_1)=M(\mathcal{Q}_2)=0$. Finally, for the third term of (4.31), we have

$$M(v_3v_{n-3}) \;=\; M(v_3(q^{-1}l_{n-3}+\kappa_{n-3}q)) \;=\; M(q^{-1}v_3l_{n-3})+\kappa_{n-3}M(qv_3)\,. \tag{4.37}$$

The product qv_3 can be obtained from (4.28), from which we conclude that $M(qv_3)=2\kappa_1M(0\,|\,1)$. Inserting this into (4.37) gives

$$M(v_3v_{n-3}) \;=\; M(q^{-1}v_3l_{n-3})+2\kappa_1\kappa_{n-3}M(0\,|\,1)\,. \tag{4.38}$$

The substitution of (4.35), (4.36) and (4.38) into (4.31), gives us

$$2\left\{\underbrace{\kappa_1M(l_{n-1})}_{\text{(i)}}+\underbrace{M(q^{-1}v_2l_{n-2})}_{\text{(ii)}}+\underbrace{M(q^{-1}v_3l_{n-3})}_{\text{(iii)}}+\underbrace{2\kappa_{n-3}\kappa_1M(0\,|\,1)}_{\text{(iv)}}\right\}+\underbrace{\sum_{p=4}^{n-4}M(v_pv_{n-p})}_{\text{(v)}}$$
$$=\;0\,. \tag{4.39}$$

Before we proceed, let us make some comments on our strategy. Equation (4.39) is a direct consequence of (4.30) and, thus, is being imposed for each $n\geqslant 7$, leading to the values of κ_4, κ_5 and so on. By our induction hypothesis, we have fixed the constants $\kappa_1,\ldots,\kappa_{n-4}$ and, hence, we completely know $v_1,\ldots,v_{n-4}$. For this reason the terms (iii) and (v) are known by assumption [by (4.34), the evaluation of l_{n-3} requires the knowledge of $v_1,\ldots,v_{n-4}$]. Our aim is to use (4.39) as a condition to fix κ_{n-3} and we, therefore, have to isolate the dependence of (4.39) on κ_{n-3}. The function l_{n-2}, in term (ii), depends implicitly on v_{n-3} and, hence, on κ_{n-3} [see, again, relation (4.34)]. The term (i), however, depends implicitly on κ_{n-2} and κ_{n-3}. This dependence on κ_{n-2} could be a problem, since we are still working to fix κ_{n-3}. Nevertheless, as will be shown, the conditions $M(\mathcal{Q}_1)=0$ and $M(\mathcal{Q}_2)=0$ fortunately eliminate κ_{n-2} from the final expression, and we will be led to a condition expressing κ_{n-3} in terms of known quantities.

Let us now compute terms (i) and (ii). After a long computation, found in Appendix A 1, we get

$$\kappa_1M(l_{n-1}) \;=\; 2\kappa_1\kappa_{n-3}M(0\,|\,1)+\mathcal{R}_n^{(1)}\,, \tag{4.40}$$

where $\mathcal{R}_n^{(1)}$ is defined in (A6) and depends on constants $\kappa_1, \ldots, \kappa_{n-4}$ only. For term (ii) of (4.39) we get, after another long computation presented in Appendix A 2,

$$M(q^{-1}v_2 l_{n-2}) = -2\kappa_1\kappa_{n-3}M(0\,|\,1)+\mathcal{R}_n^{(2)}, \tag{4.41}$$

where $\mathcal{R}_n^{(2)}$ is defined in (A7). We again stress that $\mathcal{R}_n^{(2)}$ depends on $\kappa_1, \ldots, \kappa_{n-4}$ only.

We are now ready to give the precise value of κ_{n-3} in order to satisfy (4.30). Collecting (4.40) and (4.41) and inserting them into (4.39), we obtain

$$\kappa_{n-3} = \frac{-1}{4\kappa_1 M(0\,|\,1)}\left\{\sum_{p=4}^{n-4} M(v_p v_{n-p})+2\mathcal{R}_n^{(1)}+2\mathcal{R}_n^{(2)}+2M(q^{-1}v_3 l_{n-3})\right\},$$

for all $n\geqslant 7$. Note that $\mathcal{R}_n^{(1)}$ and $\mathcal{R}_n^{(2)}$ can be recursively computed for all n [see Eqs. (A6)–(A7)]. The functions l_{n-3} can also be recursively computed for all n by means of (4.34).

Summarizing our conclusions, under conditions (III_0) and $M(0\,|\,1)\neq 0$, i.e., under condition (III) of Theorem 2.2, and with the constants κ_n recursively chosen as

$$\kappa_1=\left(\frac{\overline{M(0\,|\,1)}}{M(0\,|\,1)}\right)^{1/2}, \quad \kappa_2 = -\frac{iM(\mathcal{A}_1)}{2M(0\,|\,1)}, \quad \kappa_3 = \frac{4M(\mathcal{A}_4)-M(\mathcal{A}_3)-M(\mathcal{A}_2)}{4\kappa_1 M(0\,|\,1)}, \tag{4.42}$$

$$\kappa_{n-3}=\frac{-1}{4\kappa_1 M(0\,|\,1)}\left\{\sum_{p=4}^{n-4} M(v_p v_{n-p})+2\mathcal{R}_n^{(1)}+2\mathcal{R}_n^{(2)}+2M(q^{-1}v_3 l_{n-3})\right\}, \quad n\geqslant 7, \tag{4.43}$$

all secular terms are eliminated from (2.4). Note that hypothesis $M(0\,|\,1)\neq 0$ is the *only* additional restriction needed to (4.42)–(4.43). The proof of Theorem 2.2 is thus complete. ■

V. MONOCHROMATIC FIELDS. Ac–dc FIELDS

We illustrate our method and our results considering the simplest case of monochromatic interactions (ac–dc field) $f(t)=F_0+\varphi\cos(\omega t)$, important in physical applications. We want to show that with conditions (I)–(III) we obtain with our method convergent perturbative solutions of this problems for all parameters F_0 and φ, except perhaps for spurious situations. For the ac–dc field one has $\mathcal{Q}_0(t)=\Sigma_{n\in\mathbb{Z}}J_n(\chi_1)e^{i(n+\chi_2)\omega t}$, where J_n are the Bessel function of the first kind and where we defined $\chi_1:=2\varphi/\omega$ and $\chi_2:=2F_0/\omega$. Hence, condition (I) (treated in detail in Ref. 16) holds provided $\chi_2=-m$, with m integer, and provided χ_1 is not a zero of J_m. By (2.10),

$$\Omega = -\frac{m\omega}{2}+\epsilon J_m(\chi_1)+O(\epsilon^2).$$

See also the discussion in Ref. 10. Let us consider the complementary situations.

(i). Consider $\chi_2=-m$, a nonzero integer, and χ_1 is a zero of J_m. One has $M(\mathcal{Q}_0)=0$ and we have to look first at $M(\mathcal{Q}_1)$. We get, $M(\mathcal{Q}_1)=\Sigma_{k\in\mathbb{Z}_*}(J_{k+m}(\chi_1)^2/ik\omega)$. For integer m one has the identity

$$\sum_{k\in\mathbb{Z}_*}\frac{J_{k+m}(x)^2}{k} = J_m(x)\left[-2\frac{\partial}{\partial\nu}J_\nu(x)\bigg|_{\nu=m}+\pi Y_m(x)\right], \tag{5.1}$$

where $\pi Y_m(x):=((\partial/\partial\nu)J_\nu(x)-(-1)^m(\partial/\partial\nu)J_{-\nu}(x))|_{\nu=m}$ are Bessel functions of the second kind. Because χ_1 is bound to be a zero of J_m, one concludes that $M(\mathcal{Q}_1)=0$ in this case. A direct computation shows that $M(0\,|\,1)=(1/\omega^2)\mathcal{T}_m(\chi_1)$, where $\mathcal{T}_m(x):=-\Sigma_{k,\,p\,\in\,\mathbb{Z}_*}(J_{m+p}(x)J_{m+p-k}(x)J_{m+k}(x)/kp)$. Numerical calculations indicate that $\mathcal{T}_m(x)$ does

not vanish at the zeros of J_m. We conclude that condition (III) holds in case **i**, except, perhaps, for spurious zeros of J_m for which $\mathcal{T}_m$ eventually vanishes, and whose existence could not be ruled out numerically. By (2.11),

$$\Omega = -\frac{m\omega}{2}+\frac{2\epsilon^3}{\omega^2}\mathcal{T}_m(\chi_1)+O(\epsilon^4).$$

(ii). Consider χ_2 noninteger (see also the discussion in Ref. 10). One has $M(\mathcal{Q}_0)=0$, and we have to look at $M(\mathcal{Q}_1)$. We get, $M(\mathcal{Q}_1)=(i/\omega\chi_2)[J_0(\chi_1)^2+2\chi_2^2\Sigma_{k=1}^{\infty}(J_k(\chi_1)^2/(\chi_2^2-k^2)]$. Generally, the r.h.s is non-zero and we have condition (II). Hence, by (2.11),

$$\Omega = F_0+\frac{\epsilon^2}{\omega\chi_2}\left[J_0(\chi_1)^2+2\chi_2^2\sum_{k=1}^{\infty}\frac{J_k(\chi_1)^2}{\chi_2^2-k^2}\right]+O(\epsilon^3). \tag{5.2}$$

Note, however, that on each interval $\chi_2\in(k,k+1)$, $k=1,2,\ldots$, the terms $J_k(\chi_1)^2/(\chi_2^2-k^2)$ $+J_{k+1}(\chi_1)^2/(\chi_2^2-(k+1)^2)$ vary continuously from $+\infty$ to $-\infty$. Hence, there is on each interval $(k,k+1)$, $k=0,1,2,\ldots$, a special value χ_2^s of χ_2 (depending on χ_1) for which $M(\mathcal{Q}_1)=0$, and we would be out of case (II). But when $2\chi_2$ is a noninteger, one has $M(\mathcal{Q}_3)=0$. Hence, except for the very unlikely case where $2\chi_2^s$ is an integer, we would be out of condition (III) as well, and $\Omega=F_0+O(\epsilon^4)$.

Another special situation would occur when χ_2 is chosen to satisfy $F_0-i\epsilon^2M(\mathcal{Q}_1)=0$. By the argument above, this is possible, but χ_2 will depend on ϵ. It is therefore unclear if Ω will be just $O(\epsilon^4)$ or "small" [eventually leading to an even stronger dynamical localization than we have in case (III)]. It is not even clear if we would be in a situation where our series converge, and we left this other special situation without more comments.

It is interesting to compare the expressions for the secular frequency Ω in the three situations above (for $F_0\neq 0$) with the situation where $\varphi=0$, where the secular frequency Ω_0 is Ω_0 $:=F_0\sqrt{1+(\epsilon/F_0)^2}=F_0+(\epsilon^2/2F_0)+O(\epsilon^4)$. This reveals the effect of the ac-field $\varphi\cos(\omega t)$ on the secular frequency. Taking $\chi_1\to 0$ in (5.2) we recover Ω_0.

(iii) Consider $\chi_2=0$, i.e., $F_0=0$, and $\chi_1=x_a$, the a-th zero of J_0 on $\mathbb{R}_+$. This case is interesting in connection with the issue of dynamical localization, as discussed in Refs. 7, 8, 9, 10, and 17. Here $M(\mathcal{Q}_0)=0$ and $M(\mathcal{Q}_1)=(i/\omega)\,\Sigma_{m=1}^{\infty}(J_m(\chi_1)^2-J_{-m}(\chi_1)^2)/m=0$, since $J_k(x)$ $=(-1)^kJ_{-k}(x)$. Thus, condition (II) does not apply and we have to look at $M(0\,|\,1)$. We obtain $M(0\,|\,1)=(1/\omega^2)\mathcal{T}(x_a)$, with $\mathcal{T}(x_a):=-\Sigma_{n,m\in\mathbb{Z}_*}[J_n(x_a)J_{n-m}(x_a)J_m(x_a)/n\,m]$. We conclude that condition (III) will be valid, except perhaps for spurious zeros of J_0 for which $\mathcal{T}(x_a)$ eventually vanishes. Numerical computations, though, indicate that such zeros may not exist.

We conclude that condition (III) is suitable for studying the monochromatic field when χ_1 lies over the "resonant" points x_a, leading, together with condition (I), to a complete solution for the ac–dc field except, perhaps, for some rather spurious situations. Note, finally, that in case (iii) we have $\Omega=O(\epsilon^3)$ [see (2.12)]. In fact, the first contribution to Ω is $2(\epsilon^3/\omega^2)\mathcal{T}(x_a)$. This weak dependence on ϵ implies long transition times for certain probability amplitudes.

To test our algorithm and to extract more information from our solutions, we computed numerically the propagator $U(t)$ given in (1.6) for the case (iii) described above. The results are excellent and are reported in Ref. 18.

APPENDIX A: SOME SPECIAL RELATIONS

Here we prove some of the relations used in Sec. IV. Since they involve a somewhat large amount of algebraic manipulations we prefer to separate them from the main text. We will, often without explicit mention, make repeated use of the propositions and corollaries of Secs. III A and III B.

1. Obtaining relation (4.40)

Let us explicitly write $\kappa_1 l_{n-1}$ in term (i) of (4.39) using Eq. (4.33). We have $\kappa_1 l_{n-1}(t) = A(t) + B(t)$, where

$$A(t) \;:=\; 2i\,\kappa_1 \mathscr{R}_2(0 \mid v_1 v_{n-2}), \quad B(t) \;:=\; i\kappa_1 \sum_{p=2}^{n-3} \mathscr{R}_2(0 \mid v_p v_{n-1-p})\,. \tag{A1}$$

The above expressions for $A(t)$ and $B(t)$ will now be worked individually. Let us start with $A(t)$. By the inductive hypothesis, we are allowed to use (4.1)–(4.2). We write

$$\begin{aligned} A(t) &= 2\,i\,\kappa_1^2 \mathscr{R}_2\left(0 \;\middle|\; i\sum_{p=1}^{n-3} \mathscr{R}_2(0 \mid v_p v_{n-2-p}) + \kappa_{n-2}\mathcal{Q}_0\right) \\ &= -2\,\kappa_1^2 \sum_{p=1}^{n-3} \mathscr{R}_3(0 \mid 0 \mid v_p v_{n-2-p}) + 2\,i\,\kappa_1^2 \kappa_{n-2}\mathscr{R}_2(0 \mid 0)\,. \end{aligned}$$

Note that $A(t)$ is implicitly dependent on κ_{n-3}, namely through v_{n-3}. To make this dependence explicit we have to split the sum containing v_{n-3} and write v_{n-3} with the use of (4.2):

$$\begin{aligned} A(t) &= -2\,\kappa_1^2 \sum_{p=2}^{n-4} \mathscr{R}_3(0 \mid 0 \mid v_p v_{n-2-p}) - 4\,\kappa_1^2 \mathscr{R}_3(0 \mid 0 \mid v_1 v_{n-3}) + 2\,i\,\kappa_1^2 \kappa_{n-2}\mathscr{R}_2(0 \mid 0) \\ &= -2\,\kappa_1^2 \sum_{p=2}^{n-4} \mathscr{R}_3(0 \mid 0 \mid v_p v_{n-2-p}) - 4i\,\kappa_1^3 \sum_{p=1}^{n-4} \mathscr{R}_4(0 \mid 0 \mid 0 \mid v_p v_{n-3-p}) \\ &\quad - 4\,\kappa_1^3 \kappa_{n-3}\mathscr{R}_3(0 \mid 0 \mid 0) + 2\,i\,\kappa_1^2 \kappa_{n-2}\mathscr{R}_2(0 \mid 0)\,. \end{aligned} \tag{A2}$$

We will now work on $B(t)$, Eq. (A1). Using (4.1)–(4.2), we have

$$B(t) = 2i\kappa_1\,\mathscr{R}_2(0 \mid v_2 v_{n-3}) + i\kappa_1 \sum_{p=3}^{n-4} \mathscr{R}_2(0 \mid v_p v_{n-1-p})\,. \tag{A3}$$

Next, we have to compute separately $v_2 v_{n-3}$. Using once more (4.1), (4.2) and (3.6) [which implies $\mathcal{Q}_0^{-1}\mathcal{Q}_i \mathscr{R}_2(0 \mid a) = \mathscr{R}_2(i \mid a)$], we get

$$\begin{aligned} v_2 v_{n-3} &= -\kappa_1^2 \sum_{p=1}^{n-4} \mathscr{R}_2(2 \mid v_p v_{n-3-p}) + \sum_{p=1}^{n-4} \mathscr{R}_2(1 \mid v_p v_{n-3-p}) + i\kappa_2 \sum_{p=1}^{n-4} \mathscr{R}_2(0 \mid v_p v_{n-3-p}) \\ &\quad + \kappa_{n-3}(i\kappa_1^2 \mathcal{Q}_2 - i\mathcal{Q}_1 + \kappa_2 \mathcal{Q}_0)\,. \end{aligned}$$

This expression for $v_2 v_{n-3}$ has to be introduced into the first term of (A3). The result is

$$\begin{aligned} B(t) &= 2i\kappa_1 \sum_{p=1}^{n-4} \{-\kappa_1^2 \mathscr{R}_3(0 \mid 2 \mid v_p v_{n-3-p}) + \mathscr{R}_3(0 \mid 1 \mid v_p v_{n-3-p}) + i\kappa_2 \mathscr{R}_3(0 \mid 0 \mid v_p v_{n-3-p})\} \\ &\quad + i\kappa_1 \sum_{p=3}^{n-4} \mathscr{R}_2(0 \mid v_p v_{n-1-p}) + 2i\kappa_1\kappa_{n-3}[i\kappa_1^2 \mathscr{R}_2(0 \mid 2) - i\,\mathscr{R}_2(0 \mid 1) + \kappa_2 \mathscr{R}_2(0 \mid 0)]\,. \end{aligned} \tag{A4}$$

Since both A and B are quasi-periodic, we can now compute $\kappa_1 M(l_{n-1}) = M(A) + M(B)$. Using (A2), (A4), (4.5) and the already proven fact that $M(0 \mid 0) = 0$, we get

$$\kappa_1 M(l_{n-1}) \;=\; 2\kappa_1\kappa_{n-3} M(0\,|\,1)+\mathcal{R}_n^{(1)}, \tag{A5}$$

where

$$\begin{aligned}\mathcal{R}_n^{(1)} :=& 2i\kappa_1 \sum_{p=1}^{n-4} \{-2\kappa_1^2 M(\mathscr{R}_4(0\,|\,0\,|\,0\,|\,v_p v_{n-3-p}))+M(\mathscr{R}_3(0\,|\,1\,|\,v_p v_{n-3-p}))\\ &-\kappa_1^2 M(\mathscr{R}_3(0\,|\,2\,|\,v_p v_{n-3-p}))+i\kappa_2 M(\mathscr{R}_3(0\,|\,0\,|\,v_p v_{n-3-p}))\}\\ &-2\,\kappa_1^2 \sum_{p=2}^{n-4} M(\mathscr{R}_3(0\,|\,0\,|\,v_p v_{n-2-p}))+i\kappa_1 \sum_{p=3}^{n-4} M(\mathscr{R}_2(0\,|\,v_p v_{n-1-p})).\end{aligned} \tag{A6}$$

This is the desired relation (4.40). By inspection, one verifies that $\mathcal{R}_n^{(1)}$ depends on the constants $\kappa_1, \ldots, \kappa_{n-4}$ only. Note that the constant κ_{n-2} disappeared completely when we took the mean value of $A(t)+B(t)$, due to the crucial fact that $M(\mathcal{Q}_2)=0$. This is very important, otherwise we would have in (A5) an equation for *two* unknowns κ_{n-3} and κ_{n-2}.

2. Obtaining relation (4.41)

The main point is to make the κ_{n-3} dependence of $l_{n-2}(t)$ explicit. Using (4.34) and (4.2) for $v_{n-3}(t)$, we can write

$$\begin{aligned}q^{-1}v_2 l_{n-2} =& i\sum_{p=1}^{n-3} \mathscr{R}_2(qv_2\,|\,v_p v_{n-2-p}) \;=\; 2i\,\mathscr{R}_2(qv_2\,|\,v_1 v_{n-3})+i\sum_{p=2}^{n-4} \mathscr{R}_2(qv_2\,|\,v_p v_{n-2-p})\\ =& 2i\kappa_1 \mathscr{R}_2\left(qv_2 \,\middle|\, i\sum_{p=1}^{n-4} \mathscr{R}_2(0\,|\,v_p v_{n-3-p})+\kappa_{n-3}\mathcal{Q}_0\right)+i\sum_{p=2}^{n-4} \mathscr{R}_2(qv_2\,|\,v_p v_{n-2-p})\\ =& -2\kappa_1 \sum_{p=1}^{n-4} \mathscr{R}_3(qv_2\,|\,0\,|\,v_p v_{n-3-p})+i\sum_{p=2}^{n-4} \mathscr{R}_2(qv_2\,|\,v_p v_{n-2-p})\\ &+2i\kappa_1\kappa_{n-3}\mathscr{R}_2(qv_2\,|\,0).\end{aligned}$$

By (4.1), $\mathscr{R}_2(qv_2\,|\,0)=i\kappa_1^2\mathscr{R}_2(2\,|\,0)-i\,\mathscr{R}_2(1\,|\,0)+\kappa_2\mathscr{R}_2(0\,|\,0)$. Hence, $M(\mathscr{R}_2(qv_2\,|\,0))=iM(0\,|\,1)$. Therefore, $M(q^{-1}v_2 l_{n-2})=-2\kappa_1\kappa_{n-3}M(0\,|\,1)+\mathcal{R}_n^{(2)}$, where

$$\mathcal{R}_n^{(2)} \;:=\; -2\kappa_1 \sum_{p=1}^{n-4} M(\mathscr{R}_3(qv_2\,|\,0\,|\,v_p v_{n-3-p}))+i\sum_{p=2}^{n-4} M(\mathscr{R}_2(qv_2\,|\,v_p v_{n-2-p})). \tag{A7}$$

This is the desired equation (4.41). By inspection, one verifies that $\mathcal{R}_n^{(2)}$ depends on the constants $\kappa_1, \ldots, \kappa_{n-4}$ only.

APPENDIX B: PROOF OF CONVERGENCE OF THE ϵ EXPANSION

Here we will present the proof of Theorem 2.3, i.e., the proof of convergence of the ϵ expansion of (2.4) for periodic f. It follows the ideas of Ref. 16, but technical adaptations are necessary. For the sake of simplification we shall consider here only the case where $F_0=M(f)=0$. The general case $F_0\neq 0$ can be treated following the lines described in detail in Ref. 16.

In terms of the Fourier coefficients Q_m and $Q_m^{(2)}$, appearing in (2.8), of the Fourier coefficients $V_m^{(n)}$ of v_n and in terms of the constants κ_n, relations (4.1)–(4.2) become

$$V_m^{(1)}=\kappa_1 Q_m, \quad V_m^{(2)} \;=\; \sum_{\substack{n_1\in\mathbb{Z}\\ n_1\neq 0}} \frac{Q_{m-n_1}(\kappa_1^2 Q_{n_1}^{(2)}-\overline{Q_{-n_1}^{(2)}})}{n_1\omega}+\kappa_2 Q_m, \tag{B1}$$

$$V_m^{(n)} = \sum_{\substack{n_1,\, n_2 \in \mathbb{Z} \\ n_1+n_2 \neq 0}} \frac{Q_{m-(n_1+n_2)}}{(n_1+n_2)\omega} \left(\sum_{p=1}^{n-1} V_{n_1}^{(p)} V_{n_2}^{(n-p)} \right) + \kappa_n Q_m, \quad \text{for } n \geqslant 3. \tag{B2}$$

Of course, due to the choices of the constants κ_n described before, no secular terms appear.

By (2.9) and by an inductive argument, we will prove the following statement: for all $p \in \mathbb{N}$ and all $m \in \mathbb{Z}$ there are constants $K_p > 0$ such that

$$|V_m^{(p)}| \leqslant K_p \frac{e^{-\chi|m|}}{\langle\langle m \rangle\rangle^2}. \tag{B3}$$

To show this, let us first recall the following result, proven in:[16]

Lemma B.1: For $\chi > 0$ *and* $m \in \mathbb{Z}$ *define* $\mathcal{B}(m) \equiv \mathcal{B}(m, \chi) := \Sigma_{n \in \mathbb{Z}} (e^{-\chi(|m-n|+|n|)} / \langle\langle m-n \rangle\rangle^2 \langle\langle n \rangle\rangle^2$. *Then one has* $\mathcal{B}(m) \leqslant B_0 (e^{-\chi|m|} / \langle\langle m \rangle\rangle^2)$, *for some constant* $B_0 \equiv B_0(\chi) > 0$ *and for all* $m \in \mathbb{Z}$. □

From (B1) and (2.9), we have

$$|V_m^{(1)}| \leqslant \mathcal{Q} \frac{e^{-\chi|m|}}{\langle\langle m \rangle\rangle^2}, \quad |V_m^{(2)}| \leqslant \frac{2\mathcal{Q}^2}{\omega} \sum_{n_1 \in \mathbb{Z}_*} \frac{e^{-\chi(|m-n_1|+|n_1|)}}{\langle\langle m-n_1 \rangle\rangle^2 \langle\langle n_1 \rangle\rangle^2} \frac{1}{|n_1|} + |\kappa_2| \mathcal{Q} \frac{e^{-\chi|m|}}{\langle\langle m \rangle\rangle^2},$$

where we used $|\kappa_1| = 1$. By Lemma B.1, the sum over n_1 can be bounded by $B_0(e^{-\chi|m|}/\langle\langle m \rangle\rangle^2)$. Hence, $|V_m^{(1)}| \leqslant K_1 (e^{-\chi|m|}/\langle\langle m \rangle\rangle^2)$ and $|V_m^{(2)}| \leqslant K_2 (e^{-\chi|m|}/\langle\langle m \rangle\rangle^2)$, for all $m \in \mathbb{Z}$, by choosing $K_1 := \mathcal{Q}$ and $K_2 := (2\mathcal{Q}^2 B_0/\omega) + |\kappa_2| \mathcal{Q}$.

To proceed, let us assume (B3) for all $p = 1, \ldots, n-1$. By (B2) and (2.9), we have

$$|V_m^{(n)}| \leqslant \frac{\mathcal{Q}}{\omega} \left(\sum_{\substack{n_1,\, n_2 \in \mathbb{Z} \\ n_1+n_2 \neq 0}} \frac{e^{-\chi(|m-n_1-n_2|+|n_1|+|n_2|)}}{\langle\langle m-n_1-n_2 \rangle\rangle^2 \langle\langle n_1 \rangle\rangle^2 \langle\langle n_2 \rangle\rangle^2} \frac{1}{|n_1+n_2|} \right) \left(\sum_{p=1}^{n-1} K_p K_{n-p} \right)$$
$$+ |\kappa_n| \mathcal{Q} \frac{e^{-\chi|m|}}{\langle\langle m \rangle\rangle^2}, \quad \text{for } n \geqslant 3.$$

Applying twice Lemma B.1, the sums over n_1, n_2 can be bounded by $(B_0)^2 (e^{-\chi|m|}/\langle\langle m \rangle\rangle^2)$. Therefore, $|V_m^{(n)}| \leqslant K_n (e^{-\chi|m|}/\langle\langle m \rangle\rangle^2)$ for all $m \in \mathbb{Z}$, by choosing

$$K_n := \frac{(B_0)^2 \mathcal{Q}}{\omega} \left(\sum_{p=1}^{n-1} K_p K_{n-p} \right) + \kappa_n^0 \mathcal{Q}, \tag{B4}$$

where κ_n^0 is some suitably chosen upper bound for $|\kappa_n|$. We now turn our attention to $|\kappa_n|$, for which we have to find estimates using again the inductive hypothesis (B3) for all $p = 1, \ldots, n-1$. Now, κ_1, κ_2 and κ_3 are fixed by (4.42) and κ_n, $n \geqslant 4$, are given by (4.43), from which we get

$$|\kappa_n| \leqslant \frac{1}{4|M(0\,|\,1)|} \left[\underbrace{\sum_{p=4}^{n-1} |M(v_p v_{n+3-p})|}_{T_1} + 2\underbrace{|\mathcal{R}_{n+3}^{(1)}|}_{T_2} + 2\underbrace{|\mathcal{R}_{n+3}^{(2)}|}_{T_3} + 2\underbrace{|M(q^{-1} v_3 l_n)|}_{T_4} \right], \tag{B5}$$

for $n \geqslant 4$. We have to bound each of the terms T_i indicated above. Let us start with T_1.

Bound for T_1: We have $M(v_p v_{n+3-p}) = \Sigma_{m \in \mathbb{Z}} V_m^{(p)} V_{-m}^{(n+3-p)}$. Hence, by the inductive hypothesis (B3), assumed for $p = 1, \ldots, n-1$, we get

$$T_1 = \sum_{p=4}^{n-1} |M(v_p v_{n+3-p})| \leqslant \eta_1 \sum_{p=4}^{n-1} K_p K_{n+3-p}, \tag{B6}$$

where $\eta_1 := \Sigma_{m\in\mathbb{Z}}(e^{-2\chi|m|}/\langle\langle m\rangle\rangle^2)$.

Bound for T_2: Eq. (A6) involves sums of the mean value of functions like $\mathscr{R}_k(a_1\,|\cdots|\,a_k)$. Let us prove a general statement about such functions.

Proposition B.2: For $k\geqslant 2$, let $a_1,\ldots,a_k$ be periodic functions with the same frequency ω, and such that $a_l(t)=\Sigma_{m\in\mathbb{Z}}A^{(l)}(m)e^{im\omega t}$, where the Fourier coefficients $A^{(l)}(m)$ satisfy

$$|A^{(l)}(m)| \leqslant \alpha_l \frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2}, \tag{B7}$$

for all $m\in\mathbb{Z}$ and all $l=1,\ldots,k$, where $\alpha_l>0$ and $\chi>0$. Then, there is a positive constant β_k such that the Fourier coefficients $\mathscr{R}_k(a_1\,|\cdots|\,a_k)(m)$, $m\in\mathbb{Z}$, of $\mathscr{R}_k(a_1\,|\cdots|\,a_k)_t$ are bounded by

$$|\,\mathscr{R}_k(a_1\,|\cdots|\,a_k)(m)| \leqslant \beta_k\,\alpha_1\cdots\alpha_k\,\frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2}. \tag{B8}$$

□

Proof: Let us first consider the case $k=2$. The Fourier coefficients of $\mathscr{R}_2(a_1\,|\,a_2)_t$ are given by

$$\mathscr{R}_2(a_1\,|\,a_2)(m) = \sum_{n\in\mathbb{Z}} A^{(1)}(m-n)\tilde{A}^{(2)}(n), \tag{B9}$$

where

$$\tilde{A}^{(2)}(m) := \begin{cases} \dfrac{A^{(2)}(m)}{im\omega}, & \text{for } m\neq 0, \\ -\dfrac{1}{i\omega}\displaystyle\sum_{k\in\mathbb{Z}_*}\frac{A^{(2)}(k)}{k}, & \text{for } m=0. \end{cases}.$$

From (B7), it follows that $|A^{(2)}_l(m)|\leqslant\alpha_2\,(D_0/\omega)\,(e^{-\chi|m|}/\langle\langle m\rangle\rangle^2)$, where $D_0 := \Sigma_{m\in\mathbb{Z}}(e^{-\chi|m|}/\langle\langle m\rangle\rangle^2)$. Therefore, $|\,\mathscr{R}_2(a_1\,|\,a_2)(m)|\leqslant\alpha_1\alpha_2\,(B_0D_0/\omega)\;e^{-\chi|m|}/\langle\langle m\rangle\rangle^2)$, from (B9), by (B7) and by Lemma *B.1*. This proves the statement for $k=2$. The general case follows from (3.7), by induction. ■

As a corollary, one sees from (2.9) that the functions $\mathcal{Q}_0$, $\mathcal{Q}_1$ and $\mathcal{Q}_2$ have Fourier coefficients bounded as $|\,\mathcal{Q}_i(m)|\leqslant\gamma_i\,(e^{-\chi|m|}/\langle\langle m\rangle\rangle^2)$ for some positive γ_i. Moreover, by the inductive hypothesis (B3) and by Lemma B.1, the Fourier coefficients $(v_pv_q)(m)$ of product functions like $v_p(t)v_q(t)$, with $p,q=1,\ldots,n-1$, are also bounded as

$$|(v_pv_q)(m)| \leqslant B_0\,K_p\,K_q\frac{e^{-\chi|m|}}{\langle\langle m\rangle\rangle^2} \tag{B10}$$

for all $m\in\mathbb{Z}$. The consequence of all this is that for $i_j\in\{0,1,2\}$ and $p,\ q=1,\ldots,n-1$ one has $|\,\mathscr{R}_k(i_1|i_2|\cdots|i_{k-1}|v_pv_q)(m)|\leqslant\gamma_{i_1,i_2,\cdots,i_{k-1}}\;K_p\,K_q\;\,(e^{-\chi|m|}/\langle\langle m\rangle\rangle^2)$, $\forall m\in\mathbb{Z}$, with some positive constants $\gamma_{i_1,i_2,\cdots,i_{k-1}}$, depending on the indices i_j. Turning our attention back to (A6), we conclude

$$|\mathcal{R}^{(1)}_{n+3}| \leqslant \eta_2\sum_{p=1}^{n-1}K_pK_{n-p}+\eta_3\sum_{p=2}^{n-1}K_pK_{n+1-p}+\eta_4\sum_{p=3}^{n-1}K_pK_{n+2-p}, \tag{B11}$$

for certain positive constants η_2,η_3,η_4.

Bound for T_3: Since qv_2 is a linear combination of the functions $\mathcal{Q}_0$, $\mathcal{Q}_1$ and $\mathcal{Q}_2$, we conclude from (A7) and from the previous arguments that

$$|\mathcal{R}^{(2)}_{n+3}| \leqslant \eta_5 \sum_{p=1}^{n-1} K_p K_{n-p} + \eta_6 \sum_{p=2}^{n-1} K_p K_{n+1-p}, \tag{B12}$$

for certain positive constants η_5, η_6.

Bound for T_4: By (4.34), one has $M(q^{-1}v_3 l_n) = i\Sigma_{p=1}^{n-1} M(\mathscr{R}_2(qv_3 \,|\, v_p v_{n-p}))$. From (4.28) and (B10), we see that both qv_3 and $v_p v_{n-p}$ satisfy the conditions of Proposition B.2. Hence, by (B8), $M(\mathscr{R}_2(qv_3 \,|\, v_p v_{n-p})) \leqslant \eta_7 K_p K_{n-p}$ for some positive constant η_7 and

$$M(q^{-1}v_3 l_n) \leqslant \eta_7 \sum_{p=1}^{n-1} K_p K_{n-p}. \tag{B13}$$

We are finished with the bounds for the terms T_i of (B5). If we collect (B6), (B11), (B12) and (B13) and return to (B4), we conclude that we can find positive constants Γ such that we can recursively define

$$K_n := \Gamma\left[\sum_{p=1}^{n-1} K_p K_{n-p} + \sum_{p=2}^{n-1} K_p K_{n+1-p} + \sum_{p=3}^{n-1} K_p K_{n+2-p} + \sum_{p=4}^{n-1} K_p K_{n+3-p}\right]. \tag{B14}$$

for $n>4$, after fixing the convenient values for K_1, K_2, K_3 and K_4. Note that we can choose $K_1=K_2=K_3=K_4$ taking $K_i=\max\{K_1,K_2,K_3,K_4\}$ for all $i=1,\ldots,4$.

Expression (B14) has an analogous one in Ref. 16, with the distinction that only the two first sums above occurred in the corresponding expression for K_n. From now on, we follow closely the steps of Ref. 16. The first one is to show that K_n is a *nondecreasing* sequence. We have

$$K_{n+1}-K_n := \Gamma\left[\left(\sum_{a=1}^{4} K_a\right)K_n + \left(\sum_{a=1}^{3} K_a\right)(K_n - K_{n-a}) + \sum_{p=4}^{n-1} K_p (K_{n+4-p} - K_{n-p})\right].$$

Therefore, assuming inductively $K_1=K_2=K_3=K_4\leqslant\ldots\leqslant K_n$ implies $K_n \leqslant K_{n+1}$, thus proving that the sequence is nondecreasing. Next, we write (B14) as

$$K_n = \Gamma\left[\sum_{a=1}^{3}\left(\sum_{b=a}^{3} K_b\right)K_{n-a} + \sum_{p=4}^{n-1} K_p (K_{n-p}+K_{n+1-p}+K_{n+2-p}+K_{n+3-p})\right].$$

Since the sequence is nondecreasing, we have $K_{n-p}+K_{n+1-p}+K_{n+2-p}+K_{n+3-p} \leqslant 4K_{n+3-p}$ and $K_{n-a} \leqslant K_{n-1}$ for $a=1,2,3$. Hence, we may say that

$$K_n \leqslant \Gamma\sum_{a=1}^{3}\left(\sum_{b=a}^{3} K_b\right)K_{n-1} + 4\Gamma\sum_{p=4}^{n-1} K_p K_{n+3-p} = \tilde{\Gamma} K_{n-1} K_4 + 4\Gamma\sum_{p=4}^{n-1} K_p K_{n+3-p}, \tag{B15}$$

where $\tilde{\Gamma} := (\Gamma/K_4)\,\Sigma_{a=1}^{3}(\Sigma_{b=a}^{3} K_b)$ is a positive constant. Adding up the positive quantity $\tilde{\Gamma}\Sigma_{p=4}^{n-2} K_p K_{n+3-p}$ to (B15) and setting $\Lambda := \max\{\tilde{\Gamma}, 4\Gamma\}$, we get $K_n \leqslant \Lambda\Sigma_{p=4}^{n-1} K_p K_{n+3-p}$. Let us now define another auxiliary sequence by $J_n := \Lambda\Sigma_{p=4}^{n-1} J_p J_{n+3-p}$ for $n>4$, with $J_l = K_l$ for $l=1,2,3,4$. It is a simple exercise to show that $K_n \leqslant J_n$ for all n. Now, let us consider the translated sequence $L_n = J_{n+2}$, $n \geqslant 1$. We have

$$L_n = \Lambda\sum_{p=4}^{n+1} J_p J_{n+5-p} = \Lambda\sum_{p=4}^{n+1} L_{p-2} L_{n+3-p} = \Lambda\sum_{p=2}^{n-1} L_p L_{n+1-p}. \tag{B16}$$

The sequence $\mathbf{c}_n$ defined by $\mathbf{c}_n = \Sigma_{p=2}^{n-1} \mathbf{c}_p \mathbf{c}_{n-p+1}$ for $n \geqslant 3$, with $\mathbf{c}_1 = \mathbf{c}_2 = 1$, defines the so-called "Catalan numbers," which can be expressed in a closed form as $\mathbf{c}_n = (2n-4)!/(n-1)!(n-2)!$, $n \geqslant 2$. By Stirling's formula, the $\mathbf{c}_n$'s have the following asymptotic behavior:

$\mathbf{c}_n \approx (1/16\sqrt{\pi})(4^n/n^{3/2})$, for n large. The existence of a connection between the Catalan numbers and the sequence L_n is evident from (B16). Two distinctions are the factor Λ appearing in (B16) and the fact that $L_1=L_2=K_3=K_4$ are not necessarily equal to 1. One can, however, easily show that $L_n=(K_3)^{n-1}\Lambda^{n-2}\mathbf{c}_n$, $n\geqslant 2$. Hence, the following asymptotic behavior can be established:

$$L_n \approx \frac{1}{16\sqrt{\pi}K_3\Lambda^2} \frac{(4K_3\Lambda)^n}{n^{3/2}}, \quad n \text{ large.}$$

Since $K_n \leqslant J_n = L_{n-2}$, we conclude that for n large $K_n \leqslant M_0(M_1)^n$, for some positive constants M_0, M_1. This completes the proof of Theorem 2.3. ■

ACKNOWLEDGMENTS

J.C.A.B. is partially supported by CNPq. The work of D.A.C. is supported by FAPESP.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

The increase of binding energy and enhanced binding in nonrelativistic QED

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(Received 4 November 2002; accepted 22 January 2003)

We consider a Pauli–Fierz Hamiltonian for a particle coupled to a photon field. We discuss the effects of the increase of the binding energy and enhanced binding through coupling to a photon field, and prove that both effects are the results of the existence of the ground state of the self-energy operator with total momentum $P=0$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1562007]

I. INTRODUCTION

We consider a charged particle coupled to a photon field that interacts with an external potential in nonrelativistic QED. This system will be described by a Pauli–Fierz Hamiltonian, whereas neglecting the radiation effects, one obtains a corresponding Schrödinger operator. In the present article, we discuss two closely related questions:

(1) Does the interaction with a quantized radiation field increase binding abilities of a potential (whether the Pauli–Fierz Hamiltonian can have a ground state if the Schrödinger operator with the same potential does not)?
(2) If the corresponding Schrödinger operator has discrete spectrum, should the binding energy (the difference between the infimum of the energy with and without potential, measured in units mc^2, where m is the bare electron mass) increase if the interaction with the radiation field is considered?

We emphasize here that the asserted increase of binding energy holds with respect to the bare electron mass. In physical experiments, the binding energy is usually measured in units $m_{phys}c^2$, where m_{phys} is the rest mass of the free infraparticle (comprising the free electron together with a cloud of low-energetic photons that it binds). In these units, the binding energy decreases.

Physical intuition suggests that the answer to both (1) and (2) should be in the affirmative. The free infraparticle binds a larger quantity of low-energetic photons than the confined particle, and thus possesses a larger effective mass. In order for the particle to leave the potential well, an additional energetic effort, proportional to the difference of the two effective masses, is therefore necessitated, relative to the situation without coupling to the quantized electromagnetic field.

Recently, problems 1 and 2 were actively studied in the mathematical literature. First, let us mention the paper by M. Griesemer, E. Lieb, and M. Loss,[7] where the authors proved that the binding energy cannot be decreased by the photon field. Another (and more important) achievement in Ref. 7 is a criterion for a Pauli–Fierz Hamiltonian to have a ground state. This criterion

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will be also used in the present article. The investigation of enhanced binding (problem 1) was started by F. Hiroshima and H. Spohn,[11] who considered the Pauli–Fierz Hamiltonian in the dipole approximation. In this approximation, the dependence of the magnetic vector potential on the coordinates of the particle is neglected. They proved the existence of enhanced binding for sufficiently large values of the coupling parameter α (which is the fine structure constant, $\alpha \approx 1/137$ in nature).

A different approach was implemented in Ref. 9. The Pauli-Fierz operator without spin term ($\sqrt{\alpha}\sigma \cdot B$) was studied with a potential, for which the corresponding Schrödinger operator does not have discrete eigenvalues, but which is very close to the appearance of the first eigenvalue. The first step was to estimate the self-energy for small α with an error of the order $o(\alpha^2)$, and then it was proved that by adding the potential, one gets a shift $C\alpha^2$ of the infimum of the spectrum, which for small α implies the existence of the ground state.[7] This approach was further developed in a recent preprint,[4] where the case of a particle with spin was considered.

The increase of the binding energy for the Coulomb potential $e|x|^{-1}$ in a model situation, where the electron charge e is constant, but α tends to zero, was proved by C. Hainzl,[8] by controlling the expansion of the ground state energy to order $o(\alpha^2)$. To establish the corresponding result for the physical case $e=-\sqrt{\alpha}$ by the methods of Ref. 8, one would have to control the expansion at least up to order $O(\alpha^3)$. On the other hand, simple physical arguments show that this effect is caused by the form of the self-energy operator and does not depend on the coefficient of the potential. For fixed α, the increase of the binding energy should exist for all values of $e<0$.

It is necessary to emphasize that the methods of Refs. 9 and 8 are asymptotic in α, and that they can hardly be generalized in a manner to cover the physical case, where α is a fixed constant. Studying this case requires a different strategy, which is not based on asymptotic expansions in α. The work at hand is the first attempt to develop such methods. We prove two very simple theorems, showing that both effects take place if the self-energy operator, restricted to the states with total momentum $P=0$ (operator T_0), has a ground state. The proof of these two statements is based on direct variational estimates of the binding energy, and the results are independent of α. Establishing the connection between the existence of the ground state of the operator T_0, and the existence of enhanced and increased binding is the main achievement of the present article.

The existence of the ground state of T_0 is a problem important for different aspects of nonrelativistic QED, and has been solved in Ref. 5 for small α. Applying the results of Ref. 5 and some generalizations thereof stated in the Appendix of the present article, we immediately obtain a new, very simple proof of enhanced binding for small α, in both the spin and spinless cases, as well as the proof of the increase of the binding energy for all potentials, for which the corresponding Schrödinger operator has a ground state. In particular, we prove the increase of binding energy for the Coulomb potential ($e|x|^{-1}$), for all $e<0$.

II. DEFINITIONS AND MAIN THEOREMS

The Hamiltonian for an electron interacting with the quantized radiation field and a given external potential $V(x)$, $x \in \mathbb{R}^3$, is

$$H = T + V(x), \tag{2.1}$$

where

$$T = (p + \sqrt{\alpha}A(x))^2 + g\sqrt{\alpha}\sigma \cdot B(x) + H_f. \tag{2.2}$$

We fix units such that $\hbar = c = 1$ and the electron mass $m = 1/2$, $\alpha = e^2$ is the ''fine structure'' constant, where e is the electron charge. The natural value of α is $\simeq 1/137$, however, as usual[1,11] we will think about α as a parameter in the operator T. The main results of this paper (Theorems 1 and 2) are true for all $\alpha > 0$. An artificial parameter g, which can attain the values of either 0 or

1, is introduced to describe both the spin ($g=1$) and the spinless ($g=0$) cases. As usual $\sigma=(\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices, $p=-i\nabla_x$, $B(x)=\operatorname{curl} A(x)$. The magnetic vector potential $A(x)$ is given by

$$A(x)=\sum_{\lambda=1,2}\int_{\mathbb{R}^3}\frac{\chi(|k|)}{2\pi|k|^{1/2}}\varepsilon_\lambda[a_\lambda(k)e^{ikx}+a_\lambda^*(k)e^{-ikx}]\mathrm{d}k, \tag{2.3}$$

where the operators a_λ, a_λ^* satisfy the usual commutation relations

$$[a_\nu(k),\ a_\lambda^*(q)]=\delta(k-q)\delta_{\lambda,\nu},\quad [a_\lambda(k),\ a_\nu(q)]=0.$$

The vectors $\varepsilon_\lambda(k)\in\mathbb{R}^3$ are the two possible orthonormal polarization vectors perpendicular to k.

The function $\chi(|k|)$ in (2.3) describes the ultraviolet cutoff on the wavenumbers $|k|$. The only restriction on $\chi(|k|)$, which we need at the moment, is $\chi(|k|)\equiv 0$ for $|k|>\Lambda$ with some $\Lambda>0$.

The photon field energy H_f is given by

$$H_f=\sum_{\lambda=1,2}\int_{\mathbb{R}^3}|k|a_\lambda^*(k)a_\lambda(k)\mathrm{d}k.$$

Regarding the potential $V(x)$ we assume that $V(x)=V(|x|)$, $V(x)\in\mathcal{L}_{2,loc}(\mathbb{R}^3)$, $|V(x)|\leqslant C$ for $|x|\geqslant a$ with some constants $C>0$, $a>0$ and $|V(x)|\to 0$ as $|x|\to\infty$. For $g=1$ the operators T and H are considered on the space

$$\mathcal{H}=\mathcal{L}_2(\mathbb{R}^3;\ \mathbb{C}^2)\otimes\mathcal{F},$$

where $\mathcal{F}$ is the Fock space for the photon field.

If $g=0$, the corresponding space is

$$\mathcal{H}=\mathcal{L}_2(\mathbb{R}^3)\otimes\mathcal{F}.$$

According to Ref. 10, the operator H is semibounded from below and essentially self-adjoint.

For an arbitrary self-adjoint operator $\mathcal{A}$, let $s(\mathcal{A})$ and $s_{disc}(\mathcal{A})$ be the spectrum and the discrete spectrum of $\mathcal{A}$ and let

$$E_0=\inf s(T),\quad E_1=\inf s(H)\quad\text{and}\quad \Delta_E=E_0-E_1.$$

To compare the binding energy in the presence of the photon field (Δ_E) and the binding energy without photon field let us consider the Schrödinger operator

$$h=-\Delta+V(|x|) \tag{2.4}$$

with the same potential $V(|x|)$ as in (2.1). Denote by $-e_0$ the lowest eigenvalue of the operator h [if $s_{disc}(h)=\varnothing$, $e_0=0$]. Obviously e_0 is the binding energy for the Schrödinger operator. According to Ref. 7

$$\Delta_E\geqslant e_0. \tag{2.5}$$

In the present article it will be proved that, under some conditions, the strong inequality

$$\Delta_E>e_0 \tag{2.6}$$

holds.

Suppose now that the potential $V(|x|)$ is short-range, $|V(|x|)|\leqslant c(1+|x|)^{-2-\delta}$, $\delta>0$, and its negative part is nontrivial. We can write $V(|x|)$ as $\beta V_0(|x|)$, where $V_0(|x|)$ is a short-range potential, which we will keep fixed and $\beta>0$ is a coupling constant. Denote by β_0 the minimal

value of the coupling constant β, such that for $\beta>\beta_0$, the operator h with the potential $\beta V_0(|x|)$ has nonempty discrete spectrum, and by β_1 the minimal value of the coupling constant such that for all $\beta>\beta_1$ operator H with the same potential has a ground state.

It will be proved that under the same conditions as we need for (2.6)

$$\beta_1<\beta_0.$$

This means that the photon field increases the binding abilities of potentials. To formulate those conditions, we need to introduce some more definitions.

First, notice that the operator T is translationally invariant. It commutes with the operator of the total momentum

$$P_{\text{tot}}=p_{el}\otimes I_f+I_{el}\otimes P_f, \tag{2.7}$$

where p_{el} and $P_f=\Sigma_{\lambda=1,2}\int \mathrm{d}^3k\, k a_\lambda^*(k)a_\lambda(k)$ denote the electron and the photon momentum operators, respectively.

The Hilbert space $\mathcal{H}$ can be written as a direct integral

$$\mathcal{H}=\int^{\oplus}\mathrm{d}^3P\mathcal{H}_P, \tag{2.8}$$

where $\mathcal{H}_P$ are the fiber Hilbert spaces associated to the fixed values P of the conserved momentum, which are invariant under space and time translations. For any fixed value P of the total momentum the restriction of T to the fiber space $\mathcal{H}_P$ is given by the operator

$$T_P=(P-P_f+\sqrt{\alpha}A(0))^2+\sqrt{\alpha}g\sigma\cdot B(0)+H_f. \tag{2.9}$$

The operator T_P with $P=0$ (we will call it T_0) plays an especially important role.

The main theorems will be proved under the following assumption.

Condition 1: There is an element $\psi_0\in\mathcal{H}_0$, satisfying

$$T_0\psi_0=E_0\psi_0. \tag{2.10}$$

We note that Condition 1 contains two parts. For it to be satisfied, we must first have

$$E_0=\inf s(T)=\inf s(T_0),$$

and, second, E_0 has to be in the point spectrum of the operator T_0. These issues will be further addressed after the statements of the theorems.

Theorem 1 (The increase of the binding energy): *Let Condition 1 be satisfied and $s_{disc}(h)\neq\varnothing$. Then*

$$\Delta_E>e_0. \tag{2.11}$$

Theorem 2 (Enhanced binding): *Let Condition 1 be fulfilled, and let $V(|x|)=\beta V_0(|x|)$ be a short-range potential with the properties described above. Then*

$$\beta_1<\beta_0. \tag{2.12}$$

Remark: (1) Let us first discuss Theorems 1 and 2 for the spinless case $g=0$. The fact that $\inf s(T_0)=E_0$ was proved by J. Fröhlich for all α. Recently, it was proved in Ref. 5 that for small α, and an ultraviolet cutoff $\chi\in C^1(\mathbb{R}_+)$, E_0 is contained in the point spectrum of T_0. Thus, under these assumptions, the conditions of Theorems 1 and 2 are clearly fulfilled.

(2) If $g=1$ (inclusion of particle spin), both parts of condition 1 remain true for small α. This follows from the generalizations of Ref. 5 outlined in the Appendix of the present work.

(3) It may be useful to briefly comment on the case for models that include an infrared regularization. It follows from Ref. 5 that Condition 1 is satisfied by models that are infrared regularized by an infrared cutoff function in $A(0)$ that vanishes nowhere on $(0,\Lambda)$ (this technical requirement is used for the Ward-Takahashi identities within the operator-theoretic renormalization group scheme of Ref. 5). Consequently, Theorems 1 and 2 hold for these models. If the infrared cutoff vanishes in an open neighborhood of $\{0\}$, or if it is incorporated by adding a small photon mass, the methods of Ref. 6 can be applied to verify Condition 1.

Corollary 1: Let the ultraviolet cutoff $\chi(|k|)$ be fixed and have bounded first derivatives. Then one can find a number α_0 independent of the potential $V(|x|)$, such that for all $0<\alpha<\alpha_0$ the following two statements hold:

(i) If $e_0\neq 0$, then $\Delta_E>e_0$.

(ii) If $V(|x|)=\beta V_0(|x|)$ is a short-range potential satisfying the same condition as formulated above, then $\beta_1<\beta_0$.

III. PROOF OF THEOREM 1

To prove the theorem, we shall construct a trial function $\varphi\in\mathcal{H}$, such that

$$(H\varphi,\ \varphi)<(E_0-e_0)\|\varphi\|^2. \tag{3.1}$$

Let ψ_0 be the ground state of the operator T_0,

$$T_0\psi_0=E_0\psi_0,\quad \|\psi_0\|_{\mathcal{H}_0}=1. \tag{3.2}$$

We will need the following fact.

Lemma 1: Assume ψ_0 and E_0 as in Condition 1. Then, the relation

$$\|(P_f-\sqrt{\alpha}A(0))\psi_0\|\neq 0 \tag{3.3}$$

holds. [Notice that $(P_f-\sqrt{\alpha}A(0))\psi_0$ is a three-component vector with components $\psi_{0i}\in\mathcal{H}_0$ $i=1,2,3$. As usual $\|(P_f-\sqrt{\alpha}A(0))\psi_0\|=(\Sigma_{i=1}^3\|\psi_{0i}\|_{\mathcal{H}_0}^2)^{1/2}$.]

Proof: By contradiction. Assume that (3.3) is incorrect. Then,

$$P_f\psi_0=\sqrt{\alpha}A(0)\psi_0, \tag{3.4}$$

and the magnetic term yields

$$\sigma\cdot B_f(0)\psi_0=i\sigma(P_f\wedge A(0)+A(0)\wedge P_f)\psi_0=i\sigma\left(\frac{1}{\sqrt{\alpha}}P_f\wedge P_f+\sqrt{\alpha}A(0)\wedge A(0)\right)\psi_0=0.$$

Thus,

$$T_0\psi_0=H_f\psi_0=E_0\psi_0.$$

But this yields a contradiction, since the only eigenvector of H_f is the Fock vacuum, which fails to satisfy (3.4) if $\alpha\neq 0$. This establishes the lemma.

Thus,

$$(P_f-\sqrt{\alpha}A(0))\psi_0=\sum_{i=1}^{3}e_i\psi_{0i}\not\equiv 0,$$

where e_i is the orthonormal basis in $\mathbb{R}^3$. Without loss of generality, we assume $\psi_{01}\not\equiv 0$. Let $\tilde{\psi}_{01}$ be a fixed function in $D(T_0)$, such that $\|\tilde{\psi}_{01}\|_{\mathcal{H}_0}=1$ and

$$\Re(\tilde{\psi}_{01},\psi_{01})_{\mathcal{H}_0}\geq\tfrac{1}{2}\|\psi_{01}\|_{\mathcal{H}_0}. \tag{3.5}$$

For our estimates it is more convenient to consider the functions ψ_0 and $\tilde{\psi}_{01}$ in the coordinate (for photons) representation. Let $\xi_i\in\mathbb{R}^3$ be the position vectors of photons. A function $\psi\in\mathcal{H}_0$ can be written as

$$\psi=\bigoplus_n \psi_n(s,\ \xi_1,\ \ldots,\ \xi_n,\ \lambda_1,\ \ldots,\ \lambda_n), \tag{3.6}$$

where s is the electron spin and λ_i are the polarization vectors of photons.

For $x\in\mathbb{R}^3$ and an arbitrary element $\psi\in\mathcal{H}_0$ we define the operator S_x and the function $\psi_x\in\mathcal{H}_0$ by the formula

$$\psi_x=S_x\psi=\bigoplus_n \psi_n(s,\ \xi_1-x,\ldots,\ \xi_n-x,\ \lambda_1,\ \ldots,\ \lambda_n). \tag{3.7}$$

Denote by $f_0(|x|)$ the real normalized eigenfunction of the operator h corresponding to the lowest eigenvalue and let $f_1(x)\in C_0^2(\mathbb{R}^3)$ be the function with the following properties:

(i) $f_1(x)$ is real.

(ii) $\|f_1(x)\|=1$.

(iii) $f_1(x)$ is symmetric with respect to the reflections $x_2\leftrightarrow -x_2$ and $x_3\leftrightarrow -x_3$ and antisymmetric with respect to the reflection $x_1\leftrightarrow -x_1$. [Everywhere in the article $x=(x_1,\ x_2,x_3)\in\mathbb{R}^3$.]

(iv)

$$\left(\frac{\partial f_0(|x|)}{\partial x_1},\ f_1(x)\right)>\frac{1}{2}\left\|\frac{\partial f_0}{\partial x_1}\right\|.$$

Now we are ready to define the trial function φ. Let η be a real valued parameter, which will be specified later, and let

$$\varphi=f_0(x)\psi_{x0}+i\eta f_1(x)\tilde{\psi}_{x01}, \tag{3.8}$$

where the functions f_0, f_1, ψ_0, $\tilde{\psi}_{01}$ are defined above, $\psi_{x0}=S_x\psi_0$ and $\tilde{\psi}_{x01}=S_x\tilde{\psi}_{01}$. Our next goal is to prove (3.1) for η small and negative.

Obviously

$$(H\varphi,\varphi)=(Hf_0(x)\psi_{x0},f_0(x)\psi_{x0})-\eta^2(Hf_1(x)\tilde{\psi}_{x01},f_1(x)\tilde{\psi}_{x01})-2\eta\Im(Hf_0(x)\psi_{x0},f_1(x)\tilde{\psi}_{x01}). \tag{3.9}$$

The second term on the right side of (3.9) can be estimated from above as $c_0\eta^2$ with a constant c_0 independent of η. Let us evaluate the first term. Notice that

$$pf_0(x)\psi_{x0}=(pf_0(x))\psi_{x0}-f_0(x)P_f\psi_{x0}, \tag{3.10}$$

which implies

$$\begin{aligned}(Hf_0(x)\psi_{x0},f_0(x)\psi_{x0})&=\|pf_0(x)|^2\|\psi_{x0}\|^2_{\mathcal{H}_0}+(f_0(x)V(|x|),f_0(x))\|\psi_{x0}\|^2_{\mathcal{H}_0}\\&\quad+\|f_0(x)\|^2(T\psi_0,\psi_0)_{\mathcal{H}_0}=(E_0-e_0)\|f_0(x)\psi_0\|^2.\end{aligned} \tag{3.11}$$

Here we also used the orthogonality

$$\left(\frac{\partial f_0}{\partial x_i},\ f_0\right)=0,\quad i=1,\ 2,\ 3.$$

To estimate the last term in (3.9) recall that because of the symmetry

$$(f_0, f_1)=0,\ \ (V(|x|)f_0, f_1)=0,\ \ (\Delta f_0, f_1)=0,\quad \left(\frac{\partial f_0}{\partial x_i}, f_1\right)=0,\quad i=2,3.$$

Hence

$$-2\eta\Im(Hf_0(x)\psi_{x0}, f_1(x)\tilde{\psi}_{x01})=2\eta\left(\frac{\partial f_0}{\partial x_1}, f_1\right)\Re(\psi_{01}, \tilde{\psi}_{01})\leqslant\frac{\eta}{2}\|\psi_{01}\|_{\mathcal{H}_0}\left\|\frac{\partial f_0}{\partial x_1}\right\|^2 \tag{3.12}$$

for $\eta<0$.

Combining (3.12), (3.7) and (3.10) we arrive at

$$(H\varphi,\varphi)\leqslant(E_0-e_0)\|f_0\|^2+c_0\eta^2+\frac{\eta}{2}\left\|\frac{\partial f_0}{\partial x_1}\right\|^2\|\psi_{01}\|_{\mathcal{H}_0}\ . \tag{3.13}$$

To complete the proof of Theorem 1 notice that

$$\|\varphi\|_{\mathcal{H}}^2=\|f_0(x)\|^2+\eta^2\|f_1(x)\|^2=\|f_0(x)\|^2+\eta^2$$

and hence

$$(H\varphi,\varphi)\leqslant(E_0-e_0)\|\varphi\|_{\mathcal{H}}^2+\eta^2[|E_0-e_0|+c_0]+\frac{\eta}{6}\|\nabla f_0\|^2\|\psi_{01}\|_{\mathcal{H}_0}, \tag{3.14}$$

which for

$$0>\eta>-\tfrac{1}{6}\|\nabla f_0(x)\|^2\|\psi_{01}\|_{\mathcal{H}_0}[|E_0-e_0|+c_0]^{-1}$$

yields (3.1).

IV. PROOF OF THEOREM 2

We shall prove that for $\beta=\beta_0$

$$\inf s(H)<E_0\,. \tag{4.1}$$

The statement of the theorem follows from (4.1), Ref. 9, and variational arguments.

Let $0\leqslant\gamma<1$. $V_0(|x|)$ satisfies the conditions of the theorem,

$$h_{\gamma,\beta_0}=-(1-\gamma)\Delta+\beta_0V_0(|x|). \tag{4.2}$$

The operator h_{γ,β_0} does not have discrete eigenvalues for $\gamma=0$, but for all $0<\gamma<1$ it has at least one real spherically symmetric eigenfunction $f_\gamma(|x|)$.

Let φ be the function defined by (3.8) with $f_0(|x|)$ replaced by $f_\gamma(|x|)$ and $f_1(|x|)$ replaced by $f_{\gamma,1}(x)=(\partial/\partial x_1)\,f_\gamma(|x|)$. We shall prove that for $\gamma>0$, $|\eta|$ sufficiently small ($\eta<0$), the inequality

$$(H\varphi,\varphi)<E_0\|\varphi\|^2 \tag{4.3}$$

is true.

To this end, first let us recall some properties of the functions f_γ for small γ (see, for example, Ref. 13).

Let $\mathbb{B}$ be the closure of the space $C_0^\infty(\mathbb{R}^3)$ in the norm $\|\psi\|_{\mathbb{B}}=\|\nabla\psi\|$. The equation

$$-\Delta\psi+\beta_0V_0(x)\psi=0$$

has a unique spherically symmetric solution $\overline{\psi}\in\mathbb{B}$, $\|\overline{\psi}\|_{\mathbb{B}}=1$. This solution (which is called the virtual level or zero-resonance) satisfies $\Delta\overline{\psi}$, $V_0(|x|)\overline{\psi}\in\mathcal{L}^2(\mathbb{R}^3)$. Assume that the eigenfunctions $f_\gamma(x)$ are normalized by the condition $\|\nabla f_\gamma(x)\|=1$. Then[13]

$$\|\Delta f_\gamma-\Delta\overline{\psi}\|\to 0 \quad \text{as} \quad \gamma\to 0\,,$$

which implies the inequality

$$\|\Delta f_\gamma\|\leqslant 2\|\Delta\overline{\psi}\|\|\nabla f_\gamma\|=C_0\|\nabla f_\gamma\| \tag{4.4}$$

for all γ small and C_0 independent of γ. Let us turn directly to estimating the quadratic form $(H\varphi,\varphi)$.

Similarly to (3.10) we have

$$\begin{aligned}(H\varphi,\ \varphi)=&(Hf_\gamma(x)\psi_{x0},\ f_\gamma(x)\psi_{x0})-\eta^2(Hf_{\gamma,1}(x)\widetilde{\psi}_{x01},\ f_{\gamma,1}(x)\widetilde{\psi}_{x01})\\&-2\eta\Im(Hf_\gamma(x)\psi_{x0},\ \ f_{\gamma,1}(x)\widetilde{\psi}_{x01}).\end{aligned} \tag{4.5}$$

For the second term on the right side of (4.5) the bound holds:

$$|\eta^2(Hf_{\gamma,1}(x)\widetilde{\psi}_{x01},f_{\gamma,1}(x)\widetilde{\psi}_{x01})|\leqslant\eta^2\{C_1\|f_{\gamma,1}\|^2+C_2\|\nabla f_{\gamma,1}\|^2\}\leqslant\eta^2[C_1+2C_2C_0]\|\nabla f_\gamma\|^2, \tag{4.6}$$

where the constants C_1 and C_2 depend on $\widetilde{\psi}_{01}$, but do not depend on f_γ, and C_0 is the constant from (4.4).

Analogously to (3.12) and (4.2), respectively

$$(Hf_\gamma(x)\psi_{x0},f_\gamma(x)\psi_{x0})=E_0\|f_\gamma(x)\|^2+(h_{0,\beta_0}f_\gamma(x),f_\gamma(x)) \tag{4.7}$$

and

$$-2\eta\Im(Hf_\gamma(x)\psi_{x0},f_{\gamma,1}(x)\widetilde{\psi}_{x01})\leqslant-\frac{|\eta|}{2}\left\|\frac{\partial f_\gamma}{\partial x_1}\right\|^2\|\psi_{01}\|_{\mathcal{H}_0}=-\frac{|\eta|}{6}\|\psi_{01}\|_{\mathcal{H}_0}\|\nabla f_\gamma\|^2, \tag{4.8}$$

recalling that $\|\psi_0\|_{\mathcal{H}_0}=1$.

Combining (4.5) with (4.6)–(4.8) we obtain

$$\begin{aligned}(H\varphi,\ \varphi)\leqslant&E_0\|f_\gamma(x)\|^2+(h_{0,\beta_0}f_\gamma(x),\ f_\gamma(x))+\left\{\eta^2[C_1+2C_2C_0]-\frac{|\eta|}{6}\|\psi_{01}\|_{\mathcal{H}_0}\right\}\|\nabla f_\gamma(x)\|^2\\&\leqslant E_0\|\varphi\|^2+(1-\delta)\|\nabla f_\gamma\|^2+\beta_0(V_0f_\gamma(x),f_\gamma(x)),\end{aligned} \tag{4.9}$$

where

$$\delta=\frac{|\eta|}{6}\|\psi_{01}\|_{\mathcal{H}_0}-\eta^2\left[\frac{1}{3}|E_0|+C_1+2C_2C_0\right]. \tag{4.10}$$

Here we used the relation

$$\|\varphi\|_{\mathcal{H}}^2=\|f_\gamma(x)\|^2+\eta^2\|f_{\gamma,1}\|^2\|\widetilde{\psi}_{01}\|_{\mathcal{H}_0}^2=\|f_\gamma(x)\|^2+\tfrac{1}{3}\eta^2\|\nabla f_\gamma\|^2.$$

Notice that for $|\eta|$ small, $\delta>0$, and to complete the proof of the theorem it suffices to take $0<\gamma\leqslant\delta$.

ACKNOWLEDGMENTS

S.V. would like to thank H. Spohn for attracting his attention to the results of Ref. 6. T.C. is deeply indebted to J. Fröhlich for his advice and important comments. He also thanks H. Spohn for discussions. This work was partially supported by the European project HPRN-CT-2002-0027. T.C. was supported by a Courant Instructorship.

APPENDIX

In this Appendix, we comment on the following statements that were central for the applications of Theorems 1 and 2 in the case $g=1$. For α sufficiently small, we have the following.

(i) The global minimum of inf spec$\{T_P\}$ for $P\in\mathbb{R}^3$ is attained at $P=0$.

(ii) There exists a ground state $\psi_0\in\mathcal{H}_0$ of T_0 for $g=1$.

Let us comment on the proof. We recall that

$$T_P=(P-P_f-\sqrt{\alpha}A)^2+ig\sqrt{\alpha}\,\sigma\cdot(P_f\wedge A+A\wedge P_f)+H_f,$$

where $A\equiv A(0)$. Let us to begin with include an artificial infrared regularization in the quantized electromagnetic vector potential, which acts like a momentum cutoff at small $\rho>0$ (some requirements on its precise form are formulated in Ref. 5), by which we substitute $A\to A(\rho)$ (under a slight abuse of notation), and $T_P\to T_P(\rho)$. Then, in addition to (i) and (ii), we claim the following.

(iii) For all $\rho>0$, and $|P|\geqslant 0$ and α sufficiently small,

$$E(P,\rho):=\inf\ \mathrm{spec}\{T_P(\rho)\}$$

is an eigenvalue, whose eigenspace in $\mathcal{H}_P\cong\mathbb{C}^2\otimes\mathcal{F}$ has dimension 2. Assume $\psi_P(\rho)\in\mathbb{C}^2\otimes\mathcal{F}$ is an eigenvector. Then, if $P=0$, $\psi_0(\rho)$ tends to a ground state $\psi_0(0)\in\mathbb{C}^2\otimes\mathcal{F}$ in the limit $\rho\to 0$. We note that the last statement is false in the case $|P|>0$; if $|P|>0$, $T_P(0)$ fails to have a ground state in $\mathbb{C}^2\otimes\mathcal{F}$.

(iv) For some $\delta>0$, $0<P_c<1$ and α sufficiently small,

$$|\partial_P^b(E(P,\rho)-P^2)|\leqslant C\alpha^\delta \tag{A1}$$

uniformly for $\rho\geqslant 0$, with $b=0,1,2$, and all P, $|P|<P_c$.

The detailed proof of these results will be published separately. The degeneracy of the ground state energy has recently been proved by F. Hiroshima and H. Spohn,[12] for the case where the photons have a small mass. We will here briefly sketch the strategy, which is an extension of Ref. 5. It uses the operator-theoretic renormalization group based on the smooth Feshbach map,[2,3,5] and its framework can be roughly outlined as follows. One introduces a certain Banach space $\mathcal{W}$ of bounded operators acting on the Hilbert space $\mathbf{1}_2\otimes\chi(H_f<1)\mathcal{H}_P$ (more precisely, one considers a particular Banach space of generalized Wick kernels that parametrizes such operators, but for simplicity, we do not make this distinction here), and makes a careful choice of a small polydisc $\mathcal{P}\subset\mathcal{W}$. Furthermore, one introduces a renormalization map $\mathcal{R}:\mathcal{P}\to\mathcal{P}$, constructed by way of the isospectral smooth Feshbach map, and a rescaling transformation. The idea then is to focus on the dynamical system $(\mathcal{P},\mathcal{R})$. A key property of $\mathcal{R}$ is that it is contractive on a subspace of $\mathcal{P}$ of finite codimension. Using the smooth Feshbach map, one associates $T_P(\rho)$ to an element $H^{(0)}\in\mathcal{P}$, and considers the orbit $(H^{(n)})_{n\in\mathbb{N}_0}$ under $\mathcal{R}$ that emanates from this initial condition. The elements $H^{(n)}$ of this orbit are called *effective Hamiltonians*, where n is the *scale*, and, in particular, they are mutually isospectral in the sense of the Feshbach theorem.[2] The fixed point of $\mathcal{R}$ on this orbit corresponds to the effective Hamiltonian in the scaling limit, $H^{(\infty)}$, and by isospectrality of the smooth Feshbach map, its spectral properties are directly related to those of $T_P(\rho)$.

The main ingredients in this construction are, in addition to the arguments developed in Ref. 5, *parity invariance*, and *irrelevance* of the B-field operator in renormalization group terminology. (TC thanks J. Fröhlich for pointing out this key fact.) Indeed, under parity inversion, $x\to -x$, we have

$$P \to -P\ , \quad P_f \to -P_f\ , \quad A(\rho) \to -A(\rho),$$

with respect to which $T_P(\rho)$ is evidently invariant. The most general form of the effective Hamiltonian in the scaling limit is

$$H^{(\infty)} = \alpha^{(\infty)}(P,\rho)H_f + \beta^{(\infty)}(P,\rho)P\cdot P_f + \mu^{(\infty)}(P,\rho)\sigma\cdot P_f + \nu^{(\infty)}(P,\rho)\sigma\cdot P,$$

where the coefficients $\alpha^{(\infty)}(P,\rho)$, $\beta^{(\infty)}(P,\rho)$, $\mu^{(\infty)}(P,\rho)$, and $\nu^{(\infty)}(P,\rho)$ transform trivially under spatial rotations and reflections, and are uniformly bounded in $\rho \geqslant 0$. Uniform boundedness with respect to $\rho \geqslant 0$ is in part due to the irrelevance of the B-field operator, and absence of interactions is due to the infrared regularization.

The renormalization map $\mathcal{R}$ is constructed in a manner that it commutes with parity inversion, thus all $H^{(n)}$, $n \in \mathbb{N}_0$, and $H^{(\infty)}$ are parity invariant. However, under parity reversal, $\sigma\cdot P$ and $\sigma\cdot P_f$ change their signs. Therefore, $\nu(P,\rho) = \mu(P,\rho) = 0$, which implies that the ground state energy of $H^{(\infty)}(P,\rho)$, of value 0, is doubly degenerate. Owing to the isospectrality properties of the smooth Feshbach map, the same statement applies to $T_P(\rho)$. This proves (iii).

For the proof of (i) and (iv), we remark that combining parity invariance with the generalized Ward–Takahashi identities of Ref. 5, it can be shown that the σ^0-component of the interaction in $H^{(n)}$ is marginal, where $n \in \mathbb{N}_0$, while the σ^i-components, for $i = 1,2,3$, are irrelevant. Hence, the study of marginal operators in Ref. 5 can be straightforwardly adapted to the current problem, and the corresponding results are valid even for $g = 1$. This immediately implies (i) and (iv).

To prove (ii), we note that (iv) implies

$$|\partial_P E(P,\rho)| \geqslant (1 - C\alpha^{\delta})|P|,$$

which is bounded away from 0 for all $0 \leqslant |P| \leqslant P_c$, for C independent of $\rho \geqslant 0$. Thus, $E(P,\rho)$ has no minima away from 0 for $0 \leqslant |P| \leqslant P_c$. Furthermore, writing $H_0 := H_f + (P - P_f)^2$ and $T_P = H_0 + W$, we consider

$$T_P = H_0 + (H_0+\alpha)^{1/2}((H_0+\alpha)^{-1/2}W(H_0+\alpha)^{-1/2})(H_0+\alpha)^{1/2}.$$

From Refs. 5 and 7 follows that $\|(H_0+\alpha)^{-1/2}W(H_0+\alpha)^{-1/2}\| \leqslant C\sqrt{\alpha}$, hence $T_P \geqslant C(H_0 - \alpha)$ for $C \geqslant 1/2$, and α sufficiently small. Since $\inf \mathrm{spec}\{H_0\} \geqslant C_1 P_c^2$ for $|P| \geqslant P_c$ with some $C_1 > 0$, it is evident that for all $\rho \geqslant 0$, $|E(P,\rho)|$ has its global minimum at $P = 0$, such that (ii) follows.

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Breit–Wigner formula at barrier tops[a)]

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(Received 13 May 2002; accepted 19 January 2003)

For noncritical energies, the asymptotic behavior of the scattering phase and of the time-delay are known to be described by a Weyl type formula and the Breit–Wigner formula, respectively. We consider here the case of critical energy levels in dimension 1. We obtain the semiclassical asymptotics of the scattering phase and of the time-delay, uniformly with respect to the energy in a neighborhood of a critical value. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1562749]

I. INTRODUCTION

We study the asymptotic behavior in the semiclassical limit of the scattering phase and the time-delay for the one-dimensional Schrödinger operator,

$$P(x,hD)=h^2D^2+V(x), \quad D=\frac{1}{i}\frac{\partial}{\partial x}, \tag{1}$$

for energies close to a critical value V_0 of the potential $V(x)$. We will focus here on the case where V_0 is a nondegenerate, global maximum of the potential. We shall consider the two cases where $V(x)$ reaches its maximum at one point (case I) and at two points (case II). In case I, the underlying classical system presents a saddle point, whereas in case II it presents a heteroclinic orbit between the two saddle points associated to the points of maximum. (See Fig. 1.) The case where V_0 is a local maximum, more precisely the case of a homoclinic orbit for the associated Hamiltonian system, can be treated in the same way, and we also provide results in that case (cf. the discussion after Theorem 2.2).

The scattering phase $\theta(E,h)$ is *a priori* a very simple object, namely the argument [up to normalization; see (30) below] of the determinant of the scattering matrix (which is unitary) associated to P. The remarkable fact, proved by Birman and Krein (cf. Ref. 1), is that, under suitable assumptions on the potential V, in particular when $V\to 0$ when $x\to\infty$ fast enough, this quantity is strongly related to spectral properties of P. Indeed we have, for $E>0$,

$$\theta(E,h)=\pi s(E,h) \mod \pi\mathbb{Z}, \tag{2}$$

where $s(E,h)$ is the Spectral Shift Function (for short SSF), defined as a distribution in $\mathcal{S}'(\mathbb{R})$ by $s(E,h)=0$ for $E\ll 0$, and

$$\langle s',f\rangle=\mathrm{Tr}(f(P(x,hD))-f(h^2D^2)). \tag{3}$$

The SSF can be seen as an extension to the continuous spectrum of the counting function for the eigenvalues of P since, as one can see easily, for $E<0$,

$$\mathcal{N}(E,h)=s(E,h), \tag{4}$$

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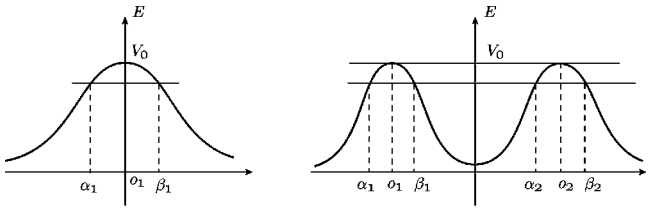

FIG. 1. Potentials.

where $\mathcal{N}(E,h)$ is the number of eigenvalues of $P(x,hD)$ not exceeding E.

As for the counting function $\mathcal{N}(E,h)$, the asymptotic behavior of $s(E,h)$ as $h\to 0$ has been shown to be of Weylian type, but only in certain particular circumstances. Let us be more precise. We denote by $s^{\mathrm{cl}}(E)$ the classical analog of the spectral shift function defined by

$$\langle s^{\mathrm{cl}}(E), f'(E)\rangle = -\int\int_{\mathbb{R}^{2n}} \{f(p(x,\xi)) - f(p_0(\xi))\}\,dx\,d\xi, \tag{5}$$

where $p(x,\xi)=\xi^2+V(x)$ and $p_0(\xi)=\xi^2$ are the semiclassical symbols of P and h^2D^2, respectively. Notice that

$$s^{\mathrm{cl}}(E) = \tau_n \int_{\mathbb{R}^n} \{(E-V(x))_+^{n/2} - E_+^{n/2}\}\,dx, \tag{6}$$

where $a_+ = \max(a,0)$ and τ_n is the volume of the unit sphere in $\mathbb{R}^n$. We recall also that an energy level E is said to be *nontrapping* for P if every trajectory of the Hamiltonian field H_p on $p^{-1}(E)$ escapes to infinity as time goes to both $+\infty$ and $-\infty$. Robert and Tamura (see Ref. 2) have proved the following.

Theorem 1.1: *If each $E\in[E_1,E_2]\subset\mathbb{R}^+$ is nontrapping, then $s(E,h)$ has a complete asymptotic expansion as $h\to 0$, uniform with respect to E in $[E_1,E_2]$. Moreover, at leading order we have*

$$s(E,h) = (2\pi h)^{-n} s^{\mathrm{cl}}(E) + O(h^{1-n}), \quad \text{as } h\to 0. \tag{7}$$

When the energy is trapping, however, it is believed that the scattering phase varies very rapidly because of the presence of poles of the scattering matrix called *resonances* close to the real axis.

The case of trapping energies which are regular values of p has already been investigated, and we would like to mention here two works on the scattering phase in such a situation. In Ref. 3, Gérard, Martinez and Robert have studied the scattering phase in the presence of shape resonances, that is, resonances generated by the presence of a well in an island (cf. Ref. 4), which are known to be exponentially (with respect to h) close to the real axis. They have proved that the scattering phase increases by π at the real part of such a resonance. More precisely, they obtain the so-called Breit–Wigner formula for the time-delay (the derivative of the scattering phase with respect to the energy). In the same situation, Nakamura[5] associates to P two Hamiltonians P_{int} and P_{ext}, corresponding to the bounded and unbounded component of $p^{-1}(E)$, respectively. He shows that if E is nontrapping in some interval for P_{ext}, the spectral shift function for P is approximated in that energy interval by the sum of the SSF for P_{ext}, the asymptotic behavior of which we know from Theorem 1.1, and the eigenvalue counting function for P_{int}. These eigenvalues are close to the shape resonances of P, and cause again rapid variations of the scattering phase.

As we have already said, our concern here is the behavior of the Spectral Shift Function for energies close to a critical value of the symbol p. We work here in the case of dimension 1, and

the methods we use can probably not be easily adapted to higher dimensional situations (see Ref. 6 for recent results concerning the Breit–Wigner formula in the n-dimensional, noncritical case). But we provide very precise results, which we think to be of interest for the understanding of the scattering phase in a general setting. In particular in our case II, the underlying mechanical system, though it is not chaotic, is highly unstable, and it is an important question to understand scattering data in such a situation.

In our settings, the barrier top energy $E=V_0$ is trapping since it takes infinite time for classical particles to arrive at a barrier top: it generates hyperbolic fixed points for the associated Hamiltonian flow. Notice also that in case I, $E\neq V_0$ is always nontrapping, but in case II, E is nontrapping above V_0 and trapping below V_0 because of the presence of a potential well.

Roughly speaking, we prove here that the Robert and Tamura formula (7) still holds in our case I, provided we replace $s^{\mathrm{cl}}(E)$ by $\sigma_{\mathrm{ext}}(E,h)$, the real part of a natural regularized classical action $s^{\mathrm{reg}}(E,h)$ [see (13) for the precise definition]. Indeed $s^{\mathrm{cl}}(E)$ presents a logarithmic singularity at $E=V_0$ (see Lemma 4.1), but from our computation emerges a purely quantum contribution, closely related to the tunneling phenomenon through the barrier, which cancels the singularity. In case II, the same phenomenon takes place, and we recover Nakamura's result replacing $s^{\mathrm{cl}}(E)$ by its regularization. More precisely, $s^{\mathrm{cl}}(E)$ is then the sum of two actions $s^{\mathrm{cl}}_{\mathrm{ext}}(E)$ and $s^{\mathrm{cl}}_{\mathrm{int}}(E)$ associated to the sea and the well, respectively, and these have to be replaced by $\sigma_{\mathrm{ext}}(E,h)$ and $\sigma_{\mathrm{int}}(E,h)$, respectively, the real part of the corresponding contributions in $s^{\mathrm{reg}}(E,h)$ (Theorem 2.1). Moreover, we are able to describe precisely the behavior of $s^{\mathrm{reg}}(E,h)$ in both cases I and II in a whole interval $]V_0-\delta,V_0+\delta[$. In case II, and when $E<V_0$, we recover the Breit–Wigner formula for the time-delay. Therefore we have extended the Breit–Wigner formula to a whole neighborhood of V_0 (Theorem 2.2).

Our starting point in this short paper is the asymptotic formulas for the scattering matrix obtained in Ref. 7 for the case I and in Ref. 10 for the case II. These formulas were obtained using the so-called *exact WKB analysis* (see Ref. 8), together with microlocal connection formulas obtained through a reduction to a normal form (see Ref. 9). In Sec. I we state our precise results. We recall briefly in Sec. II the basic facts in 1-dimensional scattering, and we present the results of Ref. 10. We prove our results in Sec. III.

II. PRELIMINARIES AND RESULTS

We consider the one-dimensional Schrödinger equation (1) where the potential V satisfies the following assumptions.

(H1) The function V is real on $\mathbb{R}$ and dilation analytic, that is, V is holomorphic in a sector $\mathcal{S}=\{x\in\mathbb{C};|\mathrm{Im}\,x|<\tan\theta_0|\mathrm{Re}\,x|\}\cup\{|\mathrm{Im}\,x|<\delta\}$ for some $0<\theta_0<\pi/2$ and $\delta>0$.

(H2) The potential V is short range, that is, there exist positive constants ϵ and C such that $|V(x)|\leqslant C(1+|x|)^{-1-\epsilon}$ in $\mathcal{S}$.

Let V_0 be the maximum of the potential on the real axis which we assume to be positive. We consider the two cases:

(Case I) $V^{-1}(V_0)=\{o_1\}$;

(Case II) $V^{-1}(V_0)=\{o_1,o_2\}$ $(o_1<o_2)$.

From now on, we will use the convention that $*$ stands for 1 in case I and 2 in case II.

In both cases, we assume furthermore that the curvature does not vanish at each critical point:

(H3) $V''(o_j)=-1/(2\rho_j^2)$, $\rho_j>0$, $j=1,*$.

If $E<V_0$ and is sufficiently close to V_0, say $|E-V_0|<\delta$, the equation $V(x)-E=0$ has 2 real roots $\alpha_1(E),\beta_1(E)$ near o_1 $(\alpha_1<o_1<\beta_1)$ in both cases and 2 other real roots $\alpha_2(E),\beta_2(E)$ near o_2 $(\alpha_2<o_2<\beta_2)$ in case II. We then define the action integrals between these turning points and $\pm\infty$ as follows:

$$s_j(E)=2\int_{\alpha_j(E)}^{\beta_j(E)}\sqrt{V(x)-E}\,dx,\quad j=1,*, \tag{8}$$

$$s^{\mathrm{cl}}_{\mathrm{ext}}(E)=2\left(\int_{-\infty}^{\alpha_1(E)}+\int_{\beta_*(E)}^{\infty}\right)\{\sqrt{E-V(x)}-\sqrt{E}\}dx-2\sqrt{E}(\beta_*(E)-\alpha_1(E)), \tag{9}$$

$$s^{\mathrm{cl}}_{\mathrm{int}}(E)=2\int_{\beta_1(E)}^{\alpha_2(E)}\sqrt{E-V(x)}dx \quad (\text{in case II}). \tag{10}$$

Let us remark here that the classical counterpart of the spectral shift function $s^{\mathrm{cl}}(E)$ [see (5)] is related with these actions by

$$s^{\mathrm{cl}}(E)=\begin{cases} s^{\mathrm{cl}}_{\mathrm{ext}}(E) & (\text{case I}),\\ s^{\mathrm{cl}}_{\mathrm{ext}}(E)+s^{\mathrm{cl}}_{\mathrm{int}}(E) & (\text{case II}).\end{cases} \tag{11}$$

In our results will also appear the Jost function N of the harmonic oscillator (see Remark 4.3). It is the analytic function in $\{z\in\mathbb{C}\backslash\{0\};|\arg z|<\pi\}$ defined by

$$N(z)=\frac{\sqrt{2\pi}}{\Gamma(z+1/2)}e^{z\log(z/e)}. \tag{12}$$

Instead of the classical actions given by (8), (9) and (10), the relevant quantities are going to be the *regularized* actions $s^{\mathrm{reg}}_{\mathrm{ext}}(E,h)$ and $s^{\mathrm{reg}}_{\mathrm{int}}(E,h)$, defined for $E<V_0$ and $|E-V_0|<\delta$ by

$$s^{\mathrm{reg}}_{\mathrm{ext,int}}(E,h)=s^{\mathrm{cl}}_{\mathrm{ext,int}}(E)+ih\log\left\{N\left(i\frac{s_1(E)}{2\pi h}\right)N\left(i\frac{s_*(E)}{2\pi h}\right)\right\}, \tag{13}$$

or their real parts,

$$\sigma_{\mathrm{ext,int}}(E,h)=s^{\mathrm{cl}}_{\mathrm{ext,int}}(E)-h\left\{\arg N\left(i\frac{s_1(E)}{2\pi h}\right)+\arg N\left(i\frac{s_*(E)}{2\pi h}\right)\right\}, \tag{14}$$

where $\arg(is_j(E)/(2\pi h))=\pi/2$ for $E<V_0$. We will see in Proposition 4.4 that these functions $\sigma_{\mathrm{ext,int}}(E,h)$ can be extended as holomorphic functions of E to a whole complex neighborhood of $E=V_0$, of course depending on h. It is also important to notice already that, far from the barrier top, the functions $\sigma_{\mathrm{ext,int}}(E,h)$ coincide with $s^{\mathrm{cl}}_{\mathrm{ext,int}}(E)$ [see (43)]. More precisely, in the region $|\arg(is_j(E)/2\pi h)|<\pi$, we have

$$\sigma_{\mathrm{ext,int}}(E,h)\to s^{\mathrm{cl}}_{\mathrm{ext,int}}(E), \quad \text{as} \quad |E-V_0|/h\to+\infty. \tag{15}$$

At last, we will need in case II another function γ, which gives the width of the resonances: again for $E<V_0$ and $|E-V_0|<\delta$, we put

$$\gamma(E,h)=\frac{\left|N\left(i\frac{s_1(E)}{2\pi h}\right)N\left(i\frac{s_2(E)}{2\pi h}\right)\right|-1}{\left|N\left(i\frac{s_1(E)}{2\pi h}\right)N\left(i\frac{s_2(E)}{2\pi h}\right)\right|+1}. \tag{16}$$

We will also show in Lemma 4.5 that this function γ extends holomorphically to a complex neighborhood of $E=V_0$.

We are now able to state our results. Let us first describe the asymptotic behavior of the scattering phase.

Theorem 2.1: *There exists $C>0$ such that if E is real and $|E-V_0|\leqslant Ch$; then we have in case I,*

$$\theta(E,h)=\frac{\sigma_{\text{ext}}(E,h)}{2h}+O(h\log(1/h)), \tag{17}$$

and in case II,

$$\theta(E,h)=\frac{\sigma_{\text{ext}}(E,h)}{2h}+\tan^{-1}\left\{\gamma(E,h)\tan\frac{\sigma_{\text{int}}(E,h)}{2h}\right\}+O(h\log(1/h)). \tag{18}$$

The asymptotic formulas (17) and (18) are analogous, respectively, to the results of Refs. 2 and 5. The second term in the right hand side of (18) is related to the presence of the potential well and causes rapid variations. It will be seen more clearly in the next result, describing the asymptotic behavior of the *time-delay*, which is the derivative of the scattering phase with respect to the energy E.

Theorem 2.2: *There exists $C>0$ such that if E is real and $|V_0-E|\leqslant Ch$; then we have in case I,*

$$\frac{d\theta}{dE}=\frac{\rho_1}{h}\log\frac{1}{h}+O\left(\frac{1}{h}\right). \tag{19}$$

In case II, if E is real and $|V_0-E|\leqslant Ch/\log(1/h)$, then we have

$$\frac{d\theta}{dE}=\frac{\rho_1+\rho_2}{2h}\left\{1+\frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\text{int}}/2h)+\gamma^2}\right\}\log\frac{1}{h}+O\left(\frac{1}{h}\right). \tag{20}$$

Notice that the energy interval in case II is smaller than in case I because of the presence of resonances closer to the real axis in that case (see Lemma 3.2 and the end of Sec. IV).

We have proved a similar formula in the homoclinic case (see the end of Sec. II). For example, suppose V has exactly two local maxima at o_1 and o_2, with $V(o_1)<V(o_2)$. For energies E close to $V_0=V(o_1)$, and assuming that the turning points α_2 and β_2 are simple, the formula (18) still holds, but with γ defined as

$$\gamma(E,h)=\frac{\left|N\left(i\frac{s_1(E)}{2\pi h}\right)\right|-1}{\left|N\left(i\frac{s_1(E)}{2\pi h}\right)\right|+1}. \tag{21}$$

Notice that this new definition for γ is what could be expected in view of (43). For the time-delay we obtain, with this new γ,

$$\frac{d\theta}{dE}=\frac{\rho_1}{2h}\left\{1+\frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\text{int}}/2h)+\gamma^2}\right\}\log\frac{1}{h}+O\left(\frac{1}{h}\right). \tag{22}$$

The reader may notice that, in each of these cases, the leading term is logarithmic with respect to h, hence one gets a non-Weylian asymptotic in these small neighborhoods of the potential maximum.

Let us add some comments about our formula (20), in particular, on the function

$$B(E,h)=\frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\text{int}}/2h)+\gamma^2}, \tag{23}$$

which is the contribution from the potential well. As $h\to 0$, the function $\gamma(E,h)$ tends to 0 for $E<V_0$ and to 1 for $E>V_0$. It also equals 1/3 for $E=V_0$. On the other hand, when γ is small, B

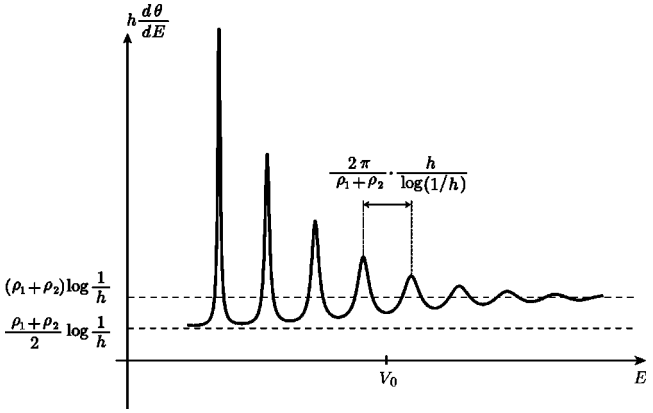

FIG. 2. The time-delay.

presents a spike at each zero of $\cos(\sigma_{\text{int}}/2h)$, whose height is $1/\gamma$ and width γ (see Lemma 4.5). These zeros of $\cos(\sigma_{\text{int}}/2h)$ (the real part of the resonances; see Ref. 10) are given by the Bohr–Sommerfeld type quantization condition,

$$\sigma_{\text{int}}(E,h)=(2n+1)\pi h, \tag{24}$$

and it follows from Proposition 4.4 that the distance between two such successive zeros in a complex disk centered at V_0 of radius $Ch/\log(1/h)$ is $2\pi(\rho_1+\rho_2)^{-1}h/\log(1/h)$.

Thus we have obtained an extension of the *Breit–Wigner formula* to a complete real neighborhood of the potential maximum.

At last, we would like to mention that the configuration of the graph of $B(E,h)$ (Fig. 2) can be understood in a more intuitive way. Let us denote

$$r(E,h)=\frac{1}{\left|N\left(i\frac{s_1(E)}{2\pi h}\right)N\left(i\frac{s_2(E)}{2\pi h}\right)\right|},\quad \theta(E,h)=\frac{\sigma_{\text{int}}}{h}-\pi.$$

Then

$$B(E,h)=\frac{1-r^2}{1-2r\cos\theta+r^2},$$

which is the Poisson kernel of the unit disk. More precisely, it is the harmonic function in the unit disk $\{z=re^{i\theta}\in\mathbb{C};|z|<1\}$ whose boundary value is the delta function supported at $z=1$. By (44), the function $r(E,h)$ is in fact

$$r(E,h)=\frac{1}{\sqrt{1+e^{-s_1(E)/h}}\sqrt{1+e^{-s_2(E)/h}}}.$$

It is a decreasing analytic function with respect to E, satisfying $0<r<1$ near V_0. As $h\to 0$, the function r tends to a Heaviside function which equals 1 in the trapping region $E<V_0$, and 0 in the nontrapping region $E>V_0$. The function $\theta(E,h)$ is also analytic near V_0, and it increases with rate $(\rho_1+\rho_2)\log(1/h)$ (see Proposition 4.4). Therefore, the point $z(E,h)=r(E,h)e^{i\theta(E,h)}$ spirals in the unit disk, near the boundary when $E<V_0$, and then B presents a spike each time θ vanishes because of the delta boundary value. When $E>V_0$, the point $z(E,h)=r(E,h)e^{i\theta(E,h)}$ spirals near the origin, and B varies slowly.

III. THE SCATTERING MATRIX

We recall here the definitions of the phase shift and of the time-delay in our one-dimensional setting. Under the assumptions (H1) and (H2) on the potential $V(x)$, and for E in $\Pi_{\theta_0}=\{E \in \mathbb{C}\backslash\{0\}; |\arg E|<2\theta_0\}$, there exists exactly one solution $f_r^{\pm}$ and exactly one solution $f_l^{\pm}$ of (1) such that

$$\begin{aligned} f_r^{\pm}(x) &\sim e^{\pm i\sqrt{E}x/h}, \quad \text{as} \quad \mathrm{Re}\, x \to +\infty \quad \text{in} \quad \mathcal{S}, \\ f_l^{\pm}(x) &\sim e^{\pm i\sqrt{E}x/h}, \quad \text{as} \quad \mathrm{Re}\, x \to -\infty \quad \text{in} \quad \mathcal{S}. \end{aligned} \tag{25}$$

These solutions (usually called Jost solutions) are holomorphic in $(x,E) \in \mathcal{S}\times\Pi_{\theta_0}$, and the two pairs (f_l^+, f_l^-) and (f_r^+, f_r^-) form two bases of the space of solutions of Eq. (1). These bases are related to each other by a constant matrix (the transmission matrix) $\mathbb{T}(E,h)$:

$$\begin{pmatrix} f_l^+ \\ f_l^- \end{pmatrix} = \mathbb{T}(E,h) \begin{pmatrix} f_r^+ \\ f_r^- \end{pmatrix}. \tag{26}$$

The determinant of this matrix is 1 since $[f_l^+, f_l^-] = \det \mathbb{T}\, [f_r^+, f_r^-]$, and the Wronskians $[f_l^+, f_l^-]$ and $[f_r^+, f_r^-]$ are both equal to $-2i\sqrt{E}/h$.

For a complex function $(x,E,h) \mapsto f(x,E,h)$, we will denote by f^* the function given by

$$f^*(x,E,h) = \overline{f(\overline{x},\overline{E},h)}.$$

It is easy to see that $f_{l,r}^- = (f_{l,r}^+)^*$, so that $\mathbb{T}$ is of the form

$$\mathbb{T} = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \quad aa^* - bb^* = 1. \tag{27}$$

Since the entries a and b can be written in terms of Jost solutions:

$$a(E,h) = \frac{ih}{2\sqrt{E}}[f_l^+, f_r^-], \quad b(E,h) = -\frac{ih}{2\sqrt{E}}[f_l^+, f_r^+], \tag{28}$$

they are holomorphic in $E \in \Pi_{\theta_0}$, as well as $a^*(E,h)$ and $b^*(E,h)$.

The scattering matrix is defined as the matrix associated with the change of basis between the outgoing pair of solutions (f_r^+, f_l^-) and the incoming pair of solutions (f_l^+, f_r^-): if

$$p_+ f_r^+ + p_- f_l^- = q_+ f_l^+ + q_- f_r^-,$$

then

$$\begin{pmatrix} p_+ \\ p_- \end{pmatrix} = \mathbb{S}(E,h) \begin{pmatrix} q_+ \\ q_- \end{pmatrix}.$$

In terms of a and b we immediately have

$$\mathbb{S} = \frac{1}{a^*} \begin{pmatrix} 1 & -b^* \\ b & 1 \end{pmatrix}. \tag{29}$$

Suppose now that E is a positive real number. Then $\mathbb{S}(E,h)$ is unitary by (27), and its determinant is a complex number of modulus 1. The scattering phase $\theta(E,h)$ is defined as half of the argument of $\det \mathbb{S}$:

$$\det \mathbb{S}(E,h) = e^{2i\theta(E,h)}. \tag{30}$$

The function θ is real, and it can be written as

$$\theta(E,h) = \arg a(E,h) = -\arg a^*(E,h). \tag{31}$$

Thus, what we have to do in order to prove our Theorem 2.1 is to examine the asymptotic behavior of $a^*(E,h)$ obtained in Refs. 7 and 10 (see also Ref. 11). Notice that, even if our results here concern only real values of the energy E, we shall need estimates in a complex neighborhood of V_0.

Let us recall now these estimates. For $E_0 \in \mathbb{C}$ and $r>0$ any real number, we denote by $D(E_0,r)$ the set of $E \in \mathbb{C}$ such that $|E-E_0|<r$.

Theorem 3.1: There exists $h_0>0$ and $C>0$ such that, for all $h \in]0,h_0]$ and all $E \in D(V_0,Ch)$, one has in case I:

$$a^*(E,h) = e^{(s_1(E)-is_{\mathrm{ext}}^{\mathrm{cl}}(E))/2h} N\left(i\frac{s_1(E)}{2\pi h}\right)(1+O(h\log h)), \tag{32}$$

whereas, in case II,

$$a^*(E,h) = e^{(s_1(E)+s_2(E)-is_{\mathrm{ext}}^{\mathrm{cl}}(E))/2h}\left(e^{is_{\mathrm{int}}^{\mathrm{cl}}(E)/2h} + N\left(i\frac{s_1(E)}{2\pi h}\right)N\left(i\frac{s_2(E)}{2\pi h}\right)e^{-is_{\mathrm{int}}^{\mathrm{cl}}(E)/2h}\right)$$
$$\times(1+O(h\log h)). \tag{33}$$

For later needs, we notice that $\theta(E,h)$ can also be defined as a complex-valued function of complex $E \in \Pi_{\theta_0}$ by

$$\theta(E,h) = \frac{1}{2i}\log\frac{a(E,h)}{a^*(E,h)}. \tag{34}$$

Indeed, since a and a^* are holomorphic in Π_{θ_0}, $\theta(E,h)$ is singular only at zeros of a and a^*. The zeros of a are complex conjugates of those of a^*, and it is enough to study the asymptotic distribution of zeros of a^*. This was done in Refs. 7 and 10 in cases I and II, respectively, through Theorem 3.1, using also Rouché's theorem. We obtain the following result.

Lemma 3.2: There exists $C>0$ such that $\theta(E,h)$ extends holomorphically to the disk $D(V_0,Ch)$ in case I, and to the disk $D(V_0,Ch/\log(1/h))$ in case II.

Let us explain briefly how we obtained Theorem 3.1. We use here the notations and conventions of Ref. 11 (in particular for the normalization of the solutions). We compute a transition matrix at each maximum T_j, $j=1,*$, the transition matrix T_l between $-\infty$ and α_1, and the transition matrix T_r between β_* and $+\infty$. In case II, we compute also a transition matrix T_{12} between β_1 and α_2. Then the transition matrix $\mathbb{T}$ can be written as

$$\mathbb{T} = T_l \cdot T_1 \cdot T_r, \tag{35}$$

in case I, and, in case II as

$$\mathbb{T} = T_l \cdot T_1 \cdot T_{12} \cdot T_2 \cdot T_r. \tag{36}$$

In Ref. 10 the following result is proved (see also Ref. 11, Proposition 3 for precise definitions of the transition matrices T_l, T_1, T_{12}, T_2, T_r and the classical actions S_l, S_r associated to $-\infty$ and $+\infty$, respectively).

Proposition 3.3: (1) There exist $R>0$ and $\epsilon>0$ such that

$$T_l=\sqrt[4]{E}\begin{pmatrix} e^{i\pi/4}e^{-iS_l(E)/h}(1+O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{-i\pi/4}e^{iS_l(E)/h}(1+O(h)) \end{pmatrix}, \tag{37}$$

$$T_r=\frac{1}{\sqrt[4]{E}}\begin{pmatrix} e^{-i\pi/4}e^{-iS_r(E)/h}(1+O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{i\pi/4}e^{iS_r(E)/h}(1+O(h)) \end{pmatrix}, \tag{38}$$

$$T_{1,2}=\begin{pmatrix} e^{is_{\mathrm{int}}(E)/2h}(1+O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{-is_{\mathrm{int}}(E)/2h}(1+O(h)) \end{pmatrix}, \tag{39}$$

uniformly with respect to E in every compact subset of $D(V_0,R)$.

(2) For any $r>0$, one has

$$T_j=e^{s_j(E)/2h}\begin{pmatrix} N\left(-\frac{is_j(E)}{2\pi h}\right)(1+O(h\log h)) & 1+O(h) \\ 1+O(h) & N\left(\frac{is_j(E)}{2\pi h}\right)(1+O(h\log h)) \end{pmatrix}, \tag{40}$$

uniformly with respect to E in every compact subset of $D(V_0,rh)$.

Theorem 3.1 follows immediately from this proposition. Notice also that we can obtain that way the scattering matrix in the homoclinic case. Then formula (36) still holds for the scattering matrix for these energies, but T_2 now reads as

$$T_2=e^{s_2(E)/2h}\begin{pmatrix} 1+O(h\log h) & 1+O(h) \\ 1+O(h) & 1+O(h\log h) \end{pmatrix}.$$

Thus, in this case, we get as in Theorem 3.1,

$$a^*(E,h)=e^{(s_1(E)+s_2(E)-is_{\mathrm{ext}}^{\mathrm{cl}}(E))/2h}\left(e^{is_{\mathrm{int}}^{\mathrm{cl}}(E)/2h}+N\left(i\frac{s_1(E)}{2\pi h}\right)e^{-is_{\mathrm{int}}^{\mathrm{cl}}(E)/2h}\right)(1+O(h\log h)). \tag{41}$$

IV. PROOFS

We proceed first to the proof of Theorem 2.1, that is, we calculate the argument of a^* through (32) and (33). For shorter expressions, we put

$$r_j(E,h)=\left|N\left(i\frac{s_j(E)}{2\pi h}\right)\right|,\quad \phi_j(E,h)=\arg N\left(i\frac{s_j(E)}{2\pi h}\right). \tag{42}$$

In case I, we get immediately

$$\theta(E,h)=\frac{s_{\mathrm{ext}}^{\mathrm{cl}}}{2h}-\phi_1+O(h\log h)=\frac{\sigma_{\mathrm{ext}}}{2h}+O(h\log h).$$

In case II, we have

$$\theta(E,h)=\frac{s_{\mathrm{ext}}^{\mathrm{cl}}}{2h}-\arg(e^{is_{\mathrm{int}}^{\mathrm{cl}}/2h}+r_1r_2e^{i(\phi_1+\phi_2)}e^{-is_{\mathrm{int}}^{\mathrm{cl}}/2h})+O(h\log h)$$

$$=\frac{\sigma_{\mathrm{ext}}}{2h}-\arg(e^{i\sigma_{\mathrm{int}}/2h}+r_1r_2e^{-i\sigma_{\mathrm{int}}/2h})+O(h\log h),$$

and since

$$\arg(e^{i\sigma_{\rm int}/2h}+r_1r_2e^{-i\sigma_{\rm int}/2h})=\arg\left\{(1+r_1r_2)\cos\frac{\sigma_{\rm int}}{2h}+i(1-r_1r_2)\sin\frac{\sigma_{\rm int}}{2h}\right\}$$
$$=\tan^{-1}\left(\frac{1-r_1r_2}{1+r_1r_2}\tan\frac{\sigma_{\rm int}}{2h}\right),$$

we get (18). This ends the proof of Theorem 2.1.

In order to prove our second result, we will have to investigate some analyticity properties of terms appearing on the rhs of (32) and (33). Let us begin with the action integrals $s_j(E)$, $s^{\rm cl}_{\rm ext}(E)$ and $s^{\rm cl}_{\rm int}(E)$: they were defined for $E<V_0$, $|E-V_0|<\delta$ in Sec. 1. See Ref. 10 for the proof of the following lemma (with slightly different notations).

Lemma 4.1: There exist a positive constant R and functions g_j, $j=1,2$, $g_{\rm ext}$ and $g_{\rm int}$ holomorphic in $D(0,R)$, such that $s_j(E)$, $s^{\rm cl}_{\rm ext}(E)$ and $s^{\rm cl}_{\rm int}(E)$ are all real for $0<V_0-E<R$ and

$$s_j(E)=2\pi\rho_j(V_0-E)(1+(V_0-E)g_j(V_0-E))\quad(j=1,2),$$

$$s^{\rm cl}_{\rm ext,int}(E)=s^{\rm cl}_{\rm ext,int}(V_0)+\frac{1}{2\pi}(s_1(E)+s_*(E))\log(V_0-E)+(V_0-E)g_{\rm ext,int}(V_0-E),$$

where $\log\lambda>0$ *when* $\arg\lambda=0$.

We also recall some properties of the function $N(z)$.

Lemma 4.2: $N(z)$ is holomorphic in $\{z\in\mathbb{C}\backslash\{0\};|\arg z|<\pi\}$ and in this domain,

$$\lim_{|z|\to\infty}N(z)=1. \tag{43}$$

In particular, on the positive imaginary axis $z=it$, $t>0$, we have

$$|N(it)|^2=1+e^{-2\pi t}, \tag{44}$$

$$\arg N(it)=t\log t+tg(t), \tag{45}$$

where g is a real and analytic function and extends holomorphically to a complex neighborhood of the origin.

Proof: The formula (43) is nothing else than Stirling formula, and (44) follows easily from the product formula of the Gamma function:

$$\left|\Gamma\left(\frac{1}{2}+it\right)\right|^2=\Gamma\left(\frac{1}{2}+it\right)\Gamma\left(\frac{1}{2}-it\right)=\frac{\pi}{\cosh\pi t}. \tag{46}$$

For (45), we have

$$\arg N(it)=t\log t-t-\arg\Gamma(1/2+it).$$

Using (46), we can rewrite the last term of the right hand side as

$$\arg\Gamma\left(\frac{1}{2}+it\right)=\frac{i}{2}\log\pi-i\log\Gamma\left(\frac{1}{2}+it\right)-\frac{i}{2}\log(\cosh\pi t).$$

This function can be extended analytically to $\mathbb{C}\backslash i(\mathbb{Z}+1/2)$ and equals 0 when $t=0$. Hence we can write $\arg N(it)$ in the form (45). □

Remark 4.3: The function $N(z)$ can be characterized as the Jost function of the harmonic oscillator (see Ref. 12). Let $\psi_\pm(x)$ be the solutions to (1) with $V(x)=x^2$ and $h=1$ whose asymptotic behavior at $\pm\infty$ is given by

$$\psi_{\pm}(x)\sim(x^2-E)^{-1/4}\exp\left(\pm\int_{x_0}^{x}(y^2-E)^{1/2}\,dy\right),\quad as\quad x\to\mp\infty.$$

It is possible to define these solutions for arbitrary $x_0\in\mathbb{R}$ when E is negative. Then the Jost function of the harmonic oscillator, which is defined as the Wronskian of these solutions, is independent of x_0 and given by

$$\frac{1}{2}[\psi_+,\psi_-]=N\left(-\frac{E}{2}\right).$$

The following result justifies in particular the terminology *regularized* actions.

Proposition 4.4: There exists $C>0$ such that the functions $\sigma_{\mathrm{ext}}(E,h)$ and $\sigma_{\mathrm{int}}(E,h)$ can be extended as holomorphic functions with respect to E in $D(V_0,Ch)$. Moreover the following asymptotic formula holds in this domain:

$$\sigma_{\mathrm{ext,int}}(E,h)=s^{\mathrm{cl}}_{\mathrm{ext,int}}(V_0)-(\rho_1+\rho_*)(V_0-E)\log\frac{1}{h}+O(V_0-E),\quad as\quad h\to 0.$$

Proof: From Lemmas 4.1 and 4.2, we get

$$\sigma_{\mathrm{ext,int}}(E,h)=s^{\mathrm{cl}}_{\mathrm{ext,int}}(V_0)-(\rho_1+\rho_*)(V_0-E)\log\frac{1}{h}+G(E,h),$$

with

$$G(E,h)=(V_0-E)g_{\mathrm{ext,int}}(V_0-E)$$
$$-\sum_{j=1,*}\left[\frac{s_j}{2\pi}\left\{g\left(\frac{s_j}{2\pi h}\right)+\log(\rho_j(1+(V_0-E)g_j))\right\}+\rho_j(V_0-E)^2g_j\log\frac{1}{h}\right].$$

□

At last, let us observe some properties of the function $\gamma(E,h)$.

Lemma 4.5: There exist positive C and R such that the function $E\mapsto\gamma(E,h)$ is holomorphic in $(V_0-R,V_0+R)\times i(-Ch,Ch)$. Moreover, on (V_0-R,V_0+R) in particular, $0<\gamma<1$ and the following:

(i) if $\lambda=O(h)$, there exist $0<\gamma_0<\gamma_1<1$ independent of λ and of h such that $\gamma_0<\gamma(E,h)<\gamma_1$ and in particular $\gamma(V_0,h)=1/3$;

(ii) if $|(V_0-E)/h|\to\infty$,

$$\gamma(E,h)=\begin{cases}O(e^{-s_1(E)/h}+e^{-s_2(E)/h}) & (E<V_0),\\ 1-O(e^{(s_1(E)+s_2(E))/2h}) & (E>V_0).\end{cases}$$

Proof: With (44), one obtains

$$\gamma(E,h)=\frac{\sqrt{1+e^{-s_1(E)/h}}\sqrt{1+e^{-s_2(E)/h}}-1}{\sqrt{1+e^{-s_1(E)/h}}\sqrt{1+e^{-s_2(E)/h}}+1},$$

and the lemma follows easily. In particular this function has singularities at the points satisfying $s_j(E)=(2n+1)\pi ih$ $(j=1,2)$. □

Now we can deduce Theorem 2.2 from Theorem 2.1, making use of the analyticity of the remainder terms. Indeed, let $R_I(E,h)$, $R_{II}(E,h)$ be the the remainder terms of (17), (18) respectively:

$$R_I(E,h)=\theta(E,h)-\frac{\sigma_{\rm ext}(E,h)}{2h},$$

$$R_{II}(E,h)=\theta(E,h)-\frac{\sigma_{\rm ext}(E,h)}{2h}-\tan^{-1}\left\{\gamma(E,h)\tan\frac{\sigma_{\rm int}(E,h)}{2h}\right\}.$$

We have the following key result.

Proposition 4.6: There exists $C>0$ such that $R_I(E,h)$ and $R_{II}(E,h)$ are holomorphic with respect to E in $D(V_0,Ch)$ and in $D(V_0,Ch/\log(1/h))$, respectively, for all sufficiently small h.

Proof: The functions $\theta(E,h)$ and $\sigma_{\rm ext}(E,h)$ are holomorphic in the required domain by Lemma 3.2 and Proposition 4.4. It remains to show that the last term of R_{II} is also holomorphic in $D(V_0,Ch/\log(1/h))$. Let us calculate the derivative:

$$\left\{\tan^{-1}\left(\gamma\tan\frac{\sigma_{\rm int}}{2h}\right)\right\}'=\frac{1}{2h}\,\frac{\gamma\sigma_{\rm int}'+2h\gamma'\cos(\sigma_{\rm int}/2h)\sin(\sigma_{\rm int}/2h)}{(1-\gamma^2)\cos^2(\sigma_{\rm int}/2h)+\gamma^2}. \tag{47}$$

Both γ and $\sigma_{\rm int}$ being holomorphic, it suffices to see that the denominator $d(E,h)=(1-\gamma^2)\cos^2(\sigma_{\rm int}/2h)+\gamma^2$ does not vanish in $D(V_0,Ch/\log(1/h))$. First we see that for real E in this domain, $d(E,h)$ is real and bounded from below by a positive constant independent of both E and h. Next for complex E, we see

$$\gamma(E,h)\to\frac{1}{3},\quad \left|\operatorname{Im}\frac{\sigma_{\rm int}}{2h}\right|\leqslant C(\rho_1+\rho_2)+O\left(\frac{1}{\log(1/h)}\right),$$

as h tends to 0. Hence, by continuity, $d(E,h)$ stays away from 0 for sufficiently small C and h.□

Proposition 4.6 enables us to estimate the derivatives of R_I and R_{II} in terms of themselves by Cauchy's integral formula; if a function $R(E)$ is holomorphic in $\overline{D(V_0,r)}$, then its derivative is bounded from above in $D(V_0,r/2)$ by $2\sup_{D(V_0,r)}|R(E)|/r$. We recall that $R_I=O(h\log(1/h))$ in $D(V_0,Ch)$, and that $R_{II}=O(h\log(1/h))$ in $D(V_0,Ch/\log(1/h))$. Thus we obtain

$$\frac{dR_I}{dE}=O(\log(1/h)),\quad \frac{dR_{II}}{dE}=O((\log h)^2).$$

On the other hand, we know from Proposition 4.4 that

$$\frac{d\sigma_{\rm ext,int}}{dE}=(\rho_1+\rho_*)\log\frac{1}{h}+O(1),$$

and since $hd\gamma/dE=O(1)$,

$$h\frac{d}{dE}\left\{\tan^{-1}\left(\gamma\tan\frac{\sigma_{\rm int}}{2h}\right)\right\}=(\rho_1+\rho_2)\,\frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\rm int}/2h)+\gamma^2}\log\frac{1}{h}+O(1).$$

This completes the proof of Theorem 2.2.

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Bi-Hamiltonian partially integrable systems

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(Received 5 December 2002; accepted 20 February 2003)

Given a first order dynamical system possessing a commutative algebra of dynamical symmetries, we show that, under certain conditions, there exists a Poisson structure on an open neighborhood of its regular (not necessarily compact) invariant manifold which makes this dynamical system into a partially integrable Hamiltonian system. This Poisson structure is by no means unique. Bi-Hamiltonian partially integrable systems are described in some detail. As an outcome, we state the conditions of quasiperiodic stability (the KAM theorem) for partially integrable Hamiltonian systems. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1566453]

I. INTRODUCTION

Given a smooth real manifold Z, let we have k mutually commutative vector fields $\{\vartheta_\lambda\}$ which are independent almost everywhere on Z, i.e., the set of points where the multivector field $\wedge^k \vartheta_\lambda$ vanishes is nowhere dense. We denote by $\mathcal{S}\subset C^\infty(Z)$ the $\mathbb{R}$-subring of smooth real functions f on Z whose derivations $\vartheta_\lambda \rfloor df$ vanish for all ϑ_λ. Let $\mathcal{A}$ be the k-dimensional $\mathcal{S}$-Lie algebra generated by the vector fields $\{\vartheta_\lambda\}$. One can think of one of its elements as being a first order dynamic equation on Z and of the other as being the dynamical symmetries. Accordingly, elements of $\mathcal{S}$ are regarded as integrals of motion. For the sake of brevity, we agree to call $\mathcal{A}$ a dynamical algebra.

Completely and partially integrable systems on symplectic manifolds[1] and broadly integrable dynamical systems of Bogoyavlenkij[2,3] exemplify finite-dimensional commutative dynamical algebras. Recall that, given a symplectic manifold (Z,Ω), we have a partially integrable system (henceforth PIS) if there exist $1\leqslant k\leqslant \dim Z/2$ smooth real functions $\{H_\lambda\}$ in involution which are independent almost everywhere on Z, i.e., the set of points where the k-form $\wedge^k dH_\lambda$ vanishes is nowhere dense. The Hamiltonian vector fields ϑ_λ of functions H_λ mutually commute and are independent almost everywhere. They make up a commutative dynamical algebra over the Poisson subalgebra $\mathcal{S}$ of elements of $C^\infty(Z)$ commuting with all the functions H_λ.

An important peculiarity of a finite-dimensional commutative dynamical algebra $\mathcal{A}$ is that its regular invariant manifolds are toroidal cylinders $\mathbb{R}^{k-m}\times T^m$. At the same time, no preferable Poisson structure is associated to a commutative Lie algebra $\mathcal{A}$ because its Lie–Poisson structure is zero. Therefore, we are free with analyzing different Poisson structures which make $\mathcal{A}$ into a Hamiltonian system. However, this analysis essentially differs from that of noncommutative integrable systems (see Ref. 4 for a survey). One has investigated different symplectic structures around invariant tori of commutative integrable systems.[2,3,5,6] For instance, the classical

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Liouville–Arnold theorem[1,7] and the Nekhoroshev theorem[8,9] state that, under certain conditions, every symplectic structure making a commutative dynamical algebra into a Hamiltonian system takes a canonical form around a compact invariant manifold.

Our goal is to describe all Poisson structures bringing a commutative dynamical algebra into a PIS near its regular invariant manifold, which need not be compact.

Definition 1: A k-dimensional commutative dynamical algebra on a regular Poisson manifold (Z, w) is said to be a PIS if (a) $\mathcal{A}$ is generated by Hamiltonian vector fields of k almost everywhere independent integrals of motion $H_\lambda \in C^\infty(Z)$ in involution; (b) all elements of $\mathcal{S} \subset C^\infty(Z)$ are mutually in involution.

It follows at once from this definition that the Poisson structure w is at least of rank $2k$ and $\mathcal{S}$ is a commutative Poisson algebra. If $2k = \dim Z$, we have a completely integrable system on a symplectic manifold.

Theorem 1 below states the following.

(i) Under certain conditions, an open neighborhood U of a regular invariant manifold M of the dynamical system $\mathcal{A}$ is a trivial principal bundle,

$$U = N \times (\mathbb{R}^{k-m} \times T^m) \stackrel{\pi}{\to} N \tag{1}$$

over a domain $N \subset \mathbb{R}^{\dim Z - k}$ with the structure group $\mathbb{R}^{k-m} \times T^m$;

(ii) The toroidal domain (1) is provided with a Poisson structure w such that $(w, \mathcal{A})$ is a PIS in accordance with Definition 1.

Note that a trivial fibration in invariant manifolds is a standard property of integrable systems.[1–3,8–12] However, there exists a well-known obstruction to its global extension in the case of compact invariant manifolds,[13] and there is an additional obstruction similar to that in Ref. 3 if invariant manifolds are noncompact.

A Poisson structure in Theorem 1 is by no means unique. Let the toroidal domain (1) be provided with bundle coordinates (r^A, y^λ), where (r^A) are coordinates on N and $(y^\lambda) = (t^a, \varphi^i)$ are standard coordinates on the toroidal cylinder $\mathbb{R}^{k-m} \times T^m$. It is readily observed that, if a Poisson bivector field on the toroidal domain U satisfies Definition 1, it takes the form

$$w = w_1 + w_2 = w^{A\lambda}(r^B)\partial_A \wedge \partial_\lambda + w^{\mu\nu}(r^B, y^\lambda)\partial_\mu \wedge \partial_\nu. \tag{2}$$

The converse also holds (see Theorem 2 below). For any Poisson bivector field w (2) of rank $2k$ on U, there exists a toroidal domain $U' \subset U$ such that $(w, \mathcal{A})$ is a PIS on U'. Moreover, Theorem 3 in Sec. III states that there is a toroidal domain U' such that, restricted to U', this Poisson bivector field takes the canonical form (16).

Now, let w and w' be two different Poisson structures (2) which make a commutative dynamical algebra $\mathcal{A}$ into the different PISs $(w, \mathcal{A})$ and $(w', \mathcal{A})$.

Definition 2: We agree to call the triple $(w, w', \mathcal{A})$ a bi-Hamiltonian PIS if any Hamiltonian vector field $\vartheta \in \mathcal{A}$ with respect to w possesses the same Hamilton representation

$$\vartheta = -w \rfloor df = -w' \rfloor df, \quad f \in \mathcal{S}, \tag{3}$$

relative to w', and *vice versa*.

Definition 2 establishes a *sui generis* equivalence between the PISs $(w, \mathcal{A})$ and $(w', \mathcal{A})$. Theorem 4 below states that the triple $(w, w', \mathcal{A})$ is a bi-Hamiltonian PIS in accordance with Definition 2 iff. the Poisson bivector fields w and w' (2) differ only in the second terms w_2 and w_2'. Moreover, these Poisson bivector fields admit a recursion operator.

Let now $\mathcal{A}$ be a commutative dynamical algebra associated to a PIS on a symplectic manifold (Z, Ω). In this case, condition (b) in Definition 1 is not necessarily satisfied, unless it is a completely integrable system. Nevertheless, there exists a Poisson structure w of rank $2k$ on the toroidal domain (1) such that, with respect to w, all integrals of motion H_λ of the original PIS remain to be in involution, and they possess the same Hamiltonian vector fields ϑ_λ (see Theorem 6 below).

Therefore, one can think of the triple $(\Omega, w, \{H_\lambda\})$ as being a special bi-Hamiltonian system, though it fails to satisfy Definition 2. Conversely, if Z is even dimensional, any Poisson bivector field w (2) setting a PIS $(w, \mathcal{A})$ is extended to an appropriate symplectic structure Ω such that $(\Omega, \mathcal{A})$ is a PIS on the symplectic manifold (Z, Ω).

There are several reasons in order to make a commutative dynamical algebra $\mathcal{A}$ into a Hamiltonian one. For instance, one can quantize $\mathcal{A}$ around its invariant manifold by quantizing the Poisson algebra $\mathcal{S}$.[12,14] Of course, quantization of $\mathcal{A}$ with respect to different Poisson structures need not be equivalent. However, we focus on another result. In Sec. V, we show that, introducing an appropriate Poisson structure and using the methods in Ref. 10, one can extend the well-known KAM theorem to PISs.

II. SEMILOCAL GEOMETRY AROUND AN INVARIANT MANIFOLD

Given a k-dimensional commutative dynamical algebra $\mathcal{A}$ on a smooth manifold Z, let $\mathcal{V}$ be the smooth involutive distribution on Z spanned by the vector fields $\{\vartheta_\lambda\}$, and let G be the group of local diffeomorphisms of Z generated by the flows of these vector fields (we follow the terminology of Ref. 15). Maximal integral manifolds of $\mathcal{V}$ are the orbits of G, and are invariant manifolds of $\mathcal{A}$.[15] Let $z \in Z$ be a regular point of the distribution $\mathcal{V}$, i.e., $\wedge^k_k \vartheta_\lambda(z) \neq 0$. Since the group G preserves $\wedge^k \vartheta_\lambda$, the maximal integral manifold M of $\mathcal{V}$ through z is also regular. Furthermore, there exists an open neighborhood U of M such that, restricted to U, the distribution $\mathcal{V}$ is regular and yields a foliation $\mathfrak{F}$ of U.

Theorem 1: Let us suppose that: (i) the vector fields ϑ_λ on U are complete, (ii) the foliation $\mathfrak{F}$ of U admits a transversal manifold Σ and its holonomy pseudogroup on Σ is trivial, (iii) the leaves of this foliation are mutually diffeomorphic. Then the following hold.

(I) There exists an open neighborhood of M, say U again, which is the trivial principal bundle (1) over a domain $N \subset \mathbb{R}^{\dim Z - k}$ with the structure group $\mathbb{R}^{k-m} \times T^m$.

(II) If $2k \leqslant \dim Z$, there exists a Poisson structure w of rank $2k$ on U such that $(w, \mathcal{A})$ is a PIS in accordance with Definition 1.

Let us note the following. Condition (i) states that G is a group of diffeomorphisms of U. Condition (ii) is equivalent to the assumption that $U \to U/G$ is a fibered manifold.[16] Each fiber M_r, $r \in N$, of this fibered manifold admits a free transitive action of the group $G_r = G/K_r$, where K_r is the isotropy group of an arbitrary point of M_r. In accordance with condition (iii), all the groups G_r, $r \in N$, are isomorphic to the toroidal cylinder group $\mathbb{R}^{k-m} \times T^m$ for some $0 \leqslant m \leqslant k$. The goal is to define these isomorphisms so that they provide a smooth action of $\mathbb{R}^{k-m} \times T^m$ in U. We follow the proof in Refs. 7 and 17 generalized to noncompact invariant manifolds. We establish a particular trivialization (1) such that the generators ϑ_λ of the algebra $\mathcal{A}$ take the specific form (8). Part (II) of Theorem 1 is based on this trivialization

Proof: (I) By virtue of the condition (ii), the foliation $\mathfrak{F}$ of U is a fibered manifold

$$\pi: U \to N, \tag{4}$$

admitting a section σ such that and $\Sigma = \sigma(N)$.[16] Since the vector fields ϑ_λ on U are complete and mutually commutative, the group G of their flows is an additive Lie group of diffeomorphism of U. Its group space is a vector space $\mathbb{R}^k$ coordinated by parameters (s^λ) of the flows with respect to the basis $\{e_\lambda = \vartheta_\lambda\}$. Since vector fields ϑ_λ are independent everywhere on U, the action of $\mathbb{R}^k$ in U is locally free, i.e., isotropy groups of points of U are discrete subgroups of the group $\mathbb{R}^k$. Its orbits are fibers of the fibered manifold (4). Given a point $r \in N$, the action of $\mathbb{R}^k$ in the fiber $M_r = \pi^{-1}(r)$ factorizes as

$$\mathbb{R}^k \times M_r \to G_r \times M_r \to M_r \tag{5}$$

through the free transitive action in M_r of the factor group $G_r = \mathbb{R}^k/K_r$, where K_r is the isotropy group of an arbitrary point of M_r. It is the same group for all points of M_r because $\mathbb{R}^k$ is a commutative group. Since the fibers M_r are mutually diffeomorphic, all isotropy groups K_r are

isomorphic to the group $\mathbb{Z}^m$ for some fixed $0\leqslant m\leqslant k$. Accordingly, the groups G_r are isomorphic to the additive group $\mathbb{R}^{k-m}\times T^m$. Let us bring the fibered manifold $U\to N$ (4) into a principal bundle with the structure group G_0, where we denote $\{0\}=\pi(M)$. For this purpose, let us determine isomorphisms $\rho_r: G_0\to G_r$ of the group G_0 to the groups G_r, $r\in N$. Then, a desired fiberwise action of G_0 in U is defined by the law

$$G_0\times M_r\to\rho_r(G_0)\times M_r\to M_r. \tag{6}$$

Generators of each isotropy subgroup K_r of $\mathbb{R}^k$ are given by m linearly independent vectors of the group space $\mathbb{R}^k$. One can show that there exist ordered collections of generators $(v_1(r),\ldots,v_m(r))$ of the groups K_r such that $r\mapsto v_i(r)$ are smooth $\mathbb{R}^k$-valued fields on N. Indeed, given a vector $v_i(0)$ and a section σ of the fibered manifold (4), each field $v_i(r)=(s^\alpha(r))$ is the unique smooth solution of the equation

$$g(s^\alpha)\sigma(r)=\sigma(r),\quad (s^\alpha(0))=v_i(0),$$

on an open neighborhood of $\{0\}$. Let us consider the decomposition

$$v_i(0)=B_i^a(0)e_a+C_i^j(0)e_j,\quad a=1,\ldots,k-m,\quad j=1,\ldots,m,$$

where $C_i^j(0)$ is a nondegenerate matrix. Since the fields $v_i(r)$ are smooth, there exists an open neighborhood of $\{0\}$, say N again, where the matrices $C_i^j(r)$ are nondegenerate. Then,

$$A_r=\begin{pmatrix}\mathrm{Id} & (B(r)-B(0))C^{-1}(0)\\ 0 & C(r)C^{-1}(0)\end{pmatrix} \tag{7}$$

is a unique linear morphism of the vector space $\mathbb{R}^k$ which transforms the frame $v_\lambda(0)=\{e_a,v_i(0)\}$ into the frame $v_\lambda(r)=\{e_a,v_i(r)\}$. Since it is also an automorphism of the group $\mathbb{R}^k$ sending K_0 onto K_r, we obtain a desired isomorphism ρ_r of the group G_0 to the group G_r. Let an element g of the group G_0 be the coset of an element $g(s^\lambda)$ of the group $\mathbb{R}^k$. Then, it acts in M_r by the rule (6) just as the element $g((A_r^{-1})^\lambda_\beta s^\beta)$ of the group $\mathbb{R}^k$ does. Since entries of the matrix A (7) are smooth functions on N, this action of the group G_0 in U is smooth. It is free, and $U/G_0=N$. Then, the fibered manifold $U\to N$ is a trivial principal bundle with the structure group G_0. Given a section σ of the principal bundle $U\to N$, its trivialization $U=N\times G_0$ is defined by assigning the points $\rho^{-1}(g_r)$ of the group space G_0 to the points $g_r\sigma(r)$, $g_r\in G_r$, of a fiber M_r. Let us endow G_0 with the standard coordinate atlas $(y^\lambda)=(t^a,\varphi^i)$ of the group $\mathbb{R}^{k-m}\times T^m$. Then, we provide U with the trivialization (1) with respect to the coordinates (r^A,t^a,φ^i), where (r^A), $A=1,\ldots,\dim Z-k$, are coordinates on the base N. The vector fields ϑ_λ on U relative to these coordinates read

$$\vartheta_a=\partial_a,\quad \vartheta_i=-(BC^{-1})_i^a(r)\partial_a+(C^{-1})_i^k(r)\partial_k. \tag{8}$$

Accordingly, the subring $\mathcal{S}$ restricted to U is the pull-back $\pi^*C^\infty(N)$ onto U of the ring of smooth functions on N.

(II) Let us split the coordinates (r^A) into some k coordinates (I_λ) and $\dim Z-2k$ coordinates (z^A). Then, we can provide the toroidal domain U (1) with the Poisson bivector field

$$w=\partial^\lambda\wedge\partial_\lambda \tag{9}$$

of rank $2k$. The independent complete vector fields ∂_a and ∂_i are Hamiltonian vector fields of the functions $H_a=I_a$ and $H_i=I_i$ on U which are in involution with respect to the Poisson bracket

$$\{f,f'\}=\partial^\lambda f\partial_\lambda f'-\partial_\lambda f\partial^\lambda f' \tag{10}$$

defined by the bivector field (9). By virtue of the expression (8), the Hamiltonian vector fields $\{\partial_\lambda\}$ generate the $\mathcal{S}$-algebra $\mathcal{A}$.

III. POISSON STRUCTURES AROUND AN INVARIANT MANIFOLD

Theorem 2: For any Poisson bivector field w (2) of rank $2k$ on U, there exists a toroidal domain $U' \subset U$ such that $(w, \mathcal{A})$ is a PIS on U'.

It is readily observed that any Poisson bivector field w (2) fulfills condition (b) in Definition 1, but condition (a) imposes a restriction on the toroidal domain U. The key point is that the characteristic foliation $\mathcal{F}$ of U yielded by the Poisson bivector fields w (2) is the pull-back of a k-dimensional foliation $\mathcal{F}_N$ of the base N, which is defined by the first summand w_1 (2) of w. With respect to the adapted coordinates (J_λ, z^A), $\lambda = 1,...,k$, on the foliated manifold $(N, \mathcal{F}_N)$, the Poisson bivector field w reads

$$w = w^\mu_\nu(J_\lambda, z^A)\partial^\nu \wedge \partial_\mu + w^{\mu\nu}(J_\lambda, z^A, y^\lambda)\partial_\mu \wedge \partial_\nu. \tag{11}$$

Then, condition (a) in Definition 1 is satisfied if $N' \subset N$ is a domain of a coordinate chart (J_λ, z^A) of the foliation $\mathcal{F}_N$. In this case, the dynamical algebra $\mathcal{A}$ on the toroidal domain $U' = \pi^{-1}(N')$ is generated by the Hamiltonian vector fields

$$\vartheta_\lambda = -w \rfloor dJ_\lambda = w^\mu_\lambda \partial_\mu \tag{12}$$

of the k independent functions $H_\lambda = J_\lambda$.

Proof: The characteristic distribution of the Poisson bivector field w (2) is spanned by the Hamiltonian vector fields

$$v^A = -w \rfloor dr^A = w^{A\mu}\partial_\mu \tag{13}$$

and the vector fields

$$w \rfloor dy^\lambda = w^{A\lambda}\partial_A + 2w^{\mu\lambda}\partial_\mu.$$

Since w is of rank $2k$, the vector fields ∂_μ can be expressed into the vector fields v^A (13). Hence, the characteristic distribution of w is spanned by the Hamiltonian vector fields v^A (13) and the vector fields

$$v^\lambda = w^{A\lambda}\partial_A. \tag{14}$$

The vector fields (14) are projected onto N. Moreover, one can derive from the relation $[w,w] = 0$ that they generate a Lie algebra and, consequently, span an involutive distribution $\mathcal{V}_N$ of rank k on N. Let $\mathcal{F}_N$ denote the corresponding foliation of N. We consider the pull-back $\mathcal{F} = \pi^*\mathcal{F}_N$ of this foliation onto U by the trivial fibration π.[16] Its leaves are the inverse images $\pi^{-1}(F_N)$ of leaves F_N of the foliation $\mathcal{F}_N$, and so is its characteristic distribution $T\mathcal{F} = (T\pi)^{-1}(\mathcal{V}_N)$. This distribution is spanned by the vector fields v^λ (14) on U and the vertical vector fields on $U \to N$, namely, the vector fields v^A (13) generating the algebra $\mathcal{A}$. Hence, $T\mathcal{F}$ is the characteristic distribution of the Poisson bivector field w. Furthermore, since $U \to N$ is a trivial bundle, each leaf $\pi^{-1}(F_N)$ of the pull-back foliation $\mathcal{F}$ is the manifold product of a leaf F_N of N and the toroidal cylinder $\mathbb{R}^{k-m} \times T^m$. It follows that the foliated manifold $(U, \mathcal{F})$ can be provided with an adapted coordinate atlas

$$\{(U_\iota, J_\lambda, z^A, y^\lambda)\}, \quad \lambda = 1,..,k, \quad A = 1,...,\dim Z - 2k, \tag{15}$$

such that (J_λ, z^A) are adapted coordinates on the foliated manifold $(N, \mathcal{F}_N)$, i.e., transition functions of coordinates z^A are independent of J_λ, while transition functions of coordinates $(y^\lambda) = (t^a, \varphi^\lambda)$ on the toroidal cylinder $\mathbb{R}^{k-m} \times T^m$ are independent of coordinates J_λ and z^A. With respect to these coordinates, the Poisson bivector field (2) takes the form (11). Let N' be the

domain of a coordinate chart (15). Then, the dynamical algebra $\mathcal{A}$ on the toroidal domain $U'=\pi^{-1}(N')$ is generated by the Hamiltonian vector fields ϑ_λ (12) of functions $H_\lambda=J_\lambda$.

Note that the coefficients $w^{\mu\nu}$ in the expressions (2) and (11) are affine in coordinates y^λ because of the relation $[w,w]=0$ and, consequently, are constant on tori. Furthermore, one can improve the expression (11) as follows.

Theorem 3: Given a PIS $(w,\mathcal{A})$ on a Poisson manifold (w,U), there exists a toroidal domain $U'\subset U$ equipped with partial action-angle coordinates (I_a,I_i,z^A,x^a,ϕ^i) such that, restricted to U', a Poisson bivector field takes the canonical form

$$w=\partial^a\wedge\partial_a+\partial^i\wedge\partial_i, \tag{16}$$

while the dynamical algebra $\mathcal{A}$ is generated by Hamiltonian vector fields of the action coordinate functions $H_a=I_a$, $H_i=I_i$.

Theorem 3 extends the Liouville–Arnold theorem to the case of a Poisson structure and a noncompact invariant manifold. To prove it (see Appendix A), we reformulate the proof of the Liouville–Arnold theorem for noncompact invariant manifolds in Refs. 11 and 12 in terms of a leafwise symplectic structure.

Given a dynamic equation $\xi\in\mathcal{A}$, it may happen that no Poisson bivector field (2) makes ξ into a Hamilton equation. If ξ is a nowhere vanishing complete vector field whose trajectories are not located in tori, one can choose ξ as one of the generators, e.g., $\xi=\vartheta_1$ in Theorem 1 so that U can be provided with a trivialization such that $\xi=\vartheta_1=\partial_1$ in the expression (8). Then, the Poisson structure (9) brings ξ into a Hamilton equation. This improves the well-known result of Hojman[18] that, under certain conditions, a first order dynamic equation can be brought into a Hamilton one with respect to a Poisson structure of rank 2. Moreover, any dynamic equation ξ on U gives rise to an equivalent Hamilton equation $\partial_t+\xi$ of time-dependent mechanics on $\mathbb{R}^2\times U$.[11,12]

IV. BI-HAMILTONIAN STRUCTURES

Now, let w and w' be two different Poisson structures (2) on the toroidal domain (1) which make a commutative dynamical algebra $\mathcal{A}$ into two different PISs $(w,\mathcal{A})$ and $(w',\mathcal{A})$.

Theorem 4: (I) The triple $(w,w',\mathcal{A})$ is a bi-Hamiltonian system PIS in accordance with Definition 2 iff the Poisson bivector fields w and w' (2) differ only in the second terms w_2 and w_2'. (II) These Poisson bivector fields admit a recursion operator.

Proof: (I) It is easily justified that, if Poisson bivector fields w (2) fulfill Definition 2, they are distinguished only by the second summand w_2. Conversely, as follows from the proof of Theorem 2, the characteristic distribution of a Poisson bivector field w (2) is spanned by the vector fields (13) and (14). Hence, all Poisson bivector fields w (2) distinguished only by the second summand w_2 have the same characteristic distribution, and they bring $\mathcal{A}$ into a PIS on the same toroidal domain U'. Then, the condition in Definition 2 is easily justified.

(II) The result follows from the forthcoming Lemma 5.

Given a smooth real manifold X, let w and w' be Poisson bivector fields of rank $2k$ on X, and let

$$w^\sharp: T^*X\to TX, \quad w'^\sharp: T^*X\to TX \tag{17}$$

be the corresponding bundle homomorphisms. A tangent-valued one-form R on X yields bundle endomorphisms

$$R: TX\to TX, \quad R^*: T^*X\to T^*X. \tag{18}$$

It is called a recursion operator if

$$w'^\sharp=R\circ w^\sharp=w^\sharp\circ R^*. \tag{19}$$

Given a Poisson bivector field w and a tangent valued one-form R such that $R\circ w^\sharp = w^\sharp \circ R^*$, the well-known sufficient condition for $R\circ w^\sharp$ to be a Poisson bivector field is that the Nijenhuis torsion of R and the Magri–Morosi concomitant of R and w vanish.[19,20] However, as we will see later, recursion operators between Poisson bivector fields in Theorem 4 need not satisfy these conditions.

Lemma 5: A recursion operator between Poisson structures of the same rank exists iff their characteristic distributions coincide.

Proof: It follows from the equalities (19) that a recursion operator R sends the characteristic distribution of w to that of w', and these distributions coincide if w and w' are of the same rank. Conversely, let regular Poisson structures w and w' possess the same characteristic distribution $T\mathcal{F}\to TX$ tangent to a foliation $\mathcal{F}$ of X. Let $T\mathcal{F}^*\to X$ be the dual of $T\mathcal{F}\to X$, and let

$$0\to T\mathcal{F}\xrightarrow{i_\mathcal{F}} TX\to TX/T\mathcal{F}\to 0, \tag{20}$$

$$0\to \operatorname{Ann} T\mathcal{F}\xrightarrow{i^*_\mathcal{F}} T^*X\to T\mathcal{F}^*\to 0, \tag{21}$$

be the corresponding exact sequences. The bundle homomorphisms $w^\sharp$ and $w'^\sharp$ (17) factorize in a unique fashion

$$w^\sharp: T^*X\xrightarrow{i^*_\mathcal{F}} T\mathcal{F}^*\xrightarrow{w^\sharp_\mathcal{F}} T\mathcal{F}\xrightarrow{i_\mathcal{F}} TX,$$

$$w'^\sharp: T^*X\xrightarrow{i^*_\mathcal{F}} T\mathcal{F}^*\xrightarrow{w'^\sharp_\mathcal{F}} T\mathcal{F}\xrightarrow{i_\mathcal{F}} TX$$

through the bundle isomorphisms

$$w^\sharp_\mathcal{F}: T\mathcal{F}^*\to T\mathcal{F}, \quad w'^\sharp_\mathcal{F}: T\mathcal{F}^*\to T\mathcal{F}.$$

Let us consider the inverse isomorphisms

$$w^\flat_\mathcal{F}: T\mathcal{F}\to T\mathcal{F}^*, \quad w'^\flat_\mathcal{F}: T\mathcal{F}\to T\mathcal{F}^*, \tag{22}$$

and the compositions

$$R_\mathcal{F} = w'^\sharp_\mathcal{F}\circ w^\flat_\mathcal{F}: T\mathcal{F}\to T\mathcal{F}, \quad R^*_\mathcal{F} = w^\flat_\mathcal{F}\circ w'^\sharp_\mathcal{F}: T\mathcal{F}^*\to T\mathcal{F}^*. \tag{23}$$

There is the obvious relation

$$w'^\sharp_\mathcal{F} = R_\mathcal{F}\circ w^\sharp_\mathcal{F} = w^\sharp_\mathcal{F}\circ R^*_\mathcal{F}.$$

In order to obtain a recursion operator (19), it suffices to extend the morphisms $R_\mathcal{F}$ and $R^*_\mathcal{F}$ (23) onto TX and T^*X, respectively. For this purpose, let us consider a splitting

$$\zeta: TX\to T\mathcal{F}, \quad TX = T\mathcal{F}\oplus(\mathrm{Id} - i_\mathcal{F}\circ\zeta)TX = T\mathcal{F}\oplus E,$$

of the exact sequence (20) and the dual splitting

$$\zeta^*: T\mathcal{F}^*\to T^*X, \quad T^*X = \zeta^*(T\mathcal{F}^*)\oplus(\mathrm{Id} - \zeta^*\circ i^*_\mathcal{F})T^*X = \zeta^*(T\mathcal{F}^*)\oplus E'$$

of the exact sequence (21). Then, the desired extensions are

$$R := R_\mathcal{F}\times \mathrm{Id}\, E, \quad R^* := (\zeta\circ R^*_\mathcal{F})\times \mathrm{Id}\, E'.$$

This recursion operator is invertible, i.e., the morphisms (18) are bundle isomorphisms.

For instance, the Poisson bivector field w (2) and the Poisson bivector field

$$w_0 = w^{A\lambda}(r)\,\partial_A \wedge \partial_\lambda \tag{24}$$

admit a recursion operator $w_0^\sharp = R \circ w^\sharp$ whose entries are given by the equalities

$$R^A_B = \delta^A_B, \quad R^\mu_\nu = \delta^\mu_\nu, \quad R^A_\lambda = 0, \quad w^{\mu\lambda} = R^\lambda_B w^{B\mu}. \tag{25}$$

Its Nijenhuis torsion fails to vanish, unless coefficients $w^{\mu\lambda}$ are independent of coordinates y^λ.

Turn now to the case of a commutative dynamical algebra $\mathcal{A}$ defined by a PIS on a symplectic manifold (Z,Ω). The following generalization of the Nekhoroshev theorem to noncompact invariant manifolds addresses such a system.

Theorem 6: Let $(\Omega,\{H_\lambda\},\vartheta_\lambda)$ be a k-dimensional PIS on a $2n$-dimensional symplectic manifold (Z,Ω). Let the distribution $\mathcal{V}$, its regular integral manifold M, an open neighborhood U of M, and the foliation $\mathfrak{F}$ of U be as those in Theorem 1. Under conditions (i)–(iii) of Theorem 1, the following hold.

(I) There exists an open neighborhood of M, say U again, which is the trivial bundle (1) in toroidal cylinders $\mathbb{R}^{k-m}\times T^m$ over a domain $N\subset\mathbb{R}^{2n-k}$.

(II) It is provided with the partial action-angle coordinates $(I_\lambda, z^A, y^\lambda)$ such that the functions H_λ depend only on the action coordinates I_λ and the symplectic form Ω on U reads

$$\Omega = dI_\lambda \wedge dy^\lambda + \Omega_{AB}(I_\mu, z^C)\,dz^A \wedge dz^B + \Omega^\lambda_A(I_\mu, z^C)\,dI_\lambda \wedge dz^A. \tag{26}$$

(III) There exists a Darboux coordinate chart $Q\times\mathbb{R}^{k-m}\times T^m \subset U$, foliated in toroidal cylinders $\mathbb{R}^{k-m}\times T^m$ and provided with coordinates $(I_\lambda, p_s, q^s, \overline{y}^\lambda)$ such that the symplectic form Ω (26) on this chart takes the canonical form

$$\Omega = dI_\lambda \wedge d\overline{y}^\lambda + dp_s \wedge dq^s. \tag{27}$$

This theorem is proved in Appendix B. Part (I) repeats exactly that of Theorem 1, while the proof of part (II) follows that of Theorem 3. The proof of part (III) is a generalization of that of Proposition 1 in Ref. 21 to noncompact invariant manifolds. As follows from the expression (27), the PIS in Theorem 6 can be extended to a completely integrable system on some open neighborhood of M, but Hamiltonian vector field of its additional local integrals of motion fail to be complete.

A glance at the symplectic form Ω (26) shows that there exists a Poisson structure w of rank $2k$, e.g., $w=\partial^\lambda\wedge\partial_\lambda$ on U such that, with respect to w, the integrals of motion H_λ of the original PIS remain to be in involution, and they possess the same Hamiltonian vector fields ϑ_λ. Hence, $(\Omega,w,\{H_\lambda\})$ is the above-mentioned bi-Hamiltonian system. Conversely, if Z is even dimensional, any Poisson bivector field w (11) is extended to an appropriate symplectic structure Ω as follows.

Proposition 7: The Poisson bivector field w (11) on a toroidal domain U' in Theorem 2 is extended to a symplectic structure Ω on U' such that integrals of motion $H_\lambda = J_\lambda$ remain in involution and their Hamiltonian vector fields with respect to w and Ω coincide.

Proof: The Poisson bivector field w (11) on the foliated manifold $(U,\mathcal{F})$ defines a leafwise symplectic form $\Omega_\mathcal{F}$ (A3). Restricted to the toroidal domain U' in Theorem 2 where coordinates J_λ have trivial transition functions, the exact sequence (A2) admits the splitting

$$\zeta^*: T\mathcal{F}^* \to T^*U', \quad \zeta^*(\overline{d}J_\mu) = dJ_\mu, \quad \zeta^*(\overline{dy}^\mu) = dy^\mu$$

such that $\zeta^*\circ\Omega_\mathcal{F}$ is a presymplectic form on U'. Let $\Omega_Z = \Omega_{AB}(z^C)\,dz^A\wedge dz^B$ be also a presymplectic form on U'. It always exists. Then, $\Omega = \zeta^*\circ\Omega_\mathcal{F} + \Omega_Z$ is a desired symplectic form on U'.

V. KAM THEOREM FOR PARTIALLY INTEGRABLE SYSTEMS

Let $\{\mathcal{H}_i\}$, $i=1,...,k$, be a partially integrable system on a $2n$-dimensional symplectic manifold (Z,Ω). Let M be its regular connected compact invariant manifold which admits an open neighborhood satisfying Theorem 6. In this case, Theorem 6 comes to the above-mentioned Nekhoroshev theorem. By virtue of this theorem, there exists an open neighborhood of M which is a trivial composite bundle

$$\pi: U = V \times W \times T^k \to V \times W \to V \tag{28}$$

[cf. (B2)] over domains $W \subset \mathbb{R}^{2(n-k)}$ and $V \subset \mathbb{R}^k$. It is provided with the partial action-angle coordinates (I_i, z^A, ϕ^i), $i=1,...,k$, $A=1,...,2(n-k)$, such that the symplectic form Ω on U reads

$$\Omega = dI_i \wedge d\phi^i + \Omega_{AB}(I_j, z^C) dz^A \wedge dz^B + \Omega^i_A(I_j, z^C) dI_i \wedge dz^A \tag{29}$$

[cf. (26)], while integrals of motion H_i depend only on the action coordinates I_j.

Note that, in accordance with part (III) of Theorem 6, one can always restrict U to a Darboux coordinate chart provided with coordinates $(I_i, p_s, q^s; \varphi^i)$ such that the symplectic form Ω (29) takes the canonical form

$$\Omega = dI_i \wedge d\varphi^i + dp_s \wedge dq^s.$$

Then, the PIS $\{H_i\}$ on this chart can be extended to a completely integrable system, e.g., $\{H_i, p_s\}$, but its invariant manifolds fail to be compact. Therefore, this is not the case of the KAM theorem.

Let $\mathcal{H}(I_j)$ be a Hamiltonian of a PIS on U (28). Its Hamiltonian vector field

$$\xi = \partial^i \mathcal{H}(I_J) \partial_i \tag{30}$$

with respect to the symplectic form Ω (29) yields the Hamilton equation

$$\dot{I}_i = 0, \quad \dot{z}^A = 0, \quad \dot{\phi}^i = \partial^i \mathcal{H}(I_j) \tag{31}$$

on U. Let us consider perturbations

$$\mathcal{H}' = \mathcal{H} + \mathcal{H}_1(I_j, z^A, \phi^j). \tag{32}$$

We assume the following. (i) The Hamiltonian $\mathcal{H}$ and its perturbations (32) are real analytic, although generalizations to the case of infinite and finite order of differentiability are possible.[10,22] (ii) The Hamiltonian $\mathcal{H}$ is nondegenerate, i.e., the frequency map

$$\omega: V \times W \ni (I_j, z^A) \mapsto \xi^i(I_j) \in \mathbb{R}^k$$

is of rank k.

Note that $\omega(V \times W) \subset \mathbb{R}^k$ is open and bounded. As usual, given $\gamma > 0$, let

$$\Omega_\gamma = \left\{ \omega \in \mathbb{R}^k : |\omega^i a_i| \geqslant \gamma \left(\sum_{j=1}^k |a_j| \right)^{-k-1}, \quad \forall a \in \mathbb{Z}^k \backslash 0 \right\}$$

denote the Cantor set of nonresonant frequencies. The complement of $\Omega_\gamma \cap \omega(V \times W)$ in $\omega(V \times W)$ is dense and open, but its relative Lebesgue measure tends to zero with γ. Let us denote $\Gamma_\gamma = \omega^{-1}(\Omega_\gamma)$, also called the Cantor set.

A problem is that the Hamiltonian vector field of the perturbed Hamiltonian (32) with respect to the symplectic form Ω (29) leads to the Hamilton equation $\dot{z}^A \neq 0$ and, therefore, no torus (31) persists.

To overcome this difficulty, let us provide the toroidal domain U (28) with the degenerate Poisson structure given by the Poisson bivector field

$$w=\partial^i\wedge\partial_i \tag{33}$$

of rank $2k$. It is readily observed that, relative to w, all integrals of motion of the original PIS $(\Omega,\{H_i\})$ remain in involution and, moreover, they possess the same Hamiltonian vector fields ϑ_i. In particular, a Hamiltonian $\mathcal{H}$ with respect to the Poisson structure (33) leads to the same Hamilton equation (31). Thus, we can think of the pair $(w,\{H_i\})$ as being a PIS on the Poisson manifold (U, w). The key point is that, with respect to the Poisson bivector field w (33), the Hamiltonian vector field of the perturbed Hamiltonian $\mathcal{H}'$ (32) is

$$\xi'=\partial^i\mathcal{H}'\partial_i-\partial_i\mathcal{H}'\partial^i, \tag{34}$$

and the corresponding first order dynamic equation on U reads

$$\dot I_i=-\partial_i\mathcal{H}'(I_j,z^B,\phi^j),\quad \dot z^A=0,\quad \dot\phi^i=\partial^i\mathcal{H}'(I_j,z^B,\phi^j). \tag{35}$$

This is a Hamilton equation with respect to the Poisson structure w (33), but is not so relative to the original symplectic form Ω. Since $\dot z^A=0$ and the toroidal domain U (28) is a trivial bundle over W, one can think of the dynamic equation (35) as being a perturbation of the dynamic equation (31) depending on parameters z^A. Furthermore, the Poisson manifold (U, w) is the product of symplectic manifold $(V\times T^k,\Omega')$ with the symplectic form

$$\Omega'=dI_i\wedge d\phi^i \tag{36}$$

and the Poisson manifold $(W,w=0)$ with the zero Poisson structure. Therefore, the equation (35) can be seen as a Hamilton equation on the symplectic manifold $(V\times T^k,\Omega')$ depending on parameters. Then, one can apply the conditions of quasiperiodic stability of symplectic Hamiltonian systems depending on parameters[10] to the perturbation (35).

In a more general setting, these conditions can be formulated as follows. Let $(w,\{H_i\})$, $i=2,...,k$, be a PIS on a regular Poisson manifold (Z, w) of rank $2k$. Let M be its regular connected compact invariant manifold, and let U be its toroidal neighborhood U (28) in Theorem 3 provided with the partial action-angle coordinates (I_i,z^A,ϕ^i) such that the Poisson bivector w on U takes the canonical form (33). The following result is a reformulation of that in Ref. 10 (Sec. 5c), where $P=W$ is a parameter space and σ is the symplectic form (36) on $V\times T^k$.

Theorem 8: Given a torus $\{0\}\times T^k$, let

$$\xi=\xi^i(I_j,z^A)\partial_i \tag{37}$$

[cf. (30)] be a real analytic Hamiltonian vector field whose frequency map

$$\omega: V\times W\ni(I_j,z^A)\mapsto\xi^i(I_j,z^A)\in\mathbb{R}^k$$

is of maximal rank at $\{0\}$. Then, there exists a neighborhood $N_0\subset V\times W$ of $\{0\}$ such that, for any real analytic Hamiltonian vector field

$$\widetilde\xi=\widetilde\xi_i(I_j,z^A,\phi^j)\partial^i+\widetilde\xi^i(I_j,z^A,\phi^j)\partial_i$$

[cf. (34)] sufficiently near ξ (37) in the real analytic topology, the following holds. Given the Cantor set $\Gamma_\gamma\subset N_0$, there exists the $\widetilde\xi$-invariant Cantor set $\widetilde\Gamma\subset N_0\times T^k$ which is a C^∞-near-identity diffeomorphic image of $\Gamma_\gamma\times T^k$.

Theorem 8 is an extension of the KAM theorem to PISs on Poisson manifolds (Z, w). Given a PIS $(\Omega,\{H_i\})$ on a symplectic manifold (Z,Ω), Theorem 8 enables one to obtain its perturbations (34) possessing a large number of invariant tori, though these perturbations are not Hamiltonian.

APPENDIX A

Proof of Theorem 3: First, let us employ Theorem 2 and restrict U to the toroidal domain, say U again, equipped with coordinates $(J_\lambda, z^A, y^\lambda)$ such that the Poisson bivector field w takes the form (11) and the algebra $\mathcal{A}$ is generated by the Hamiltonian vector fields ϑ_λ (12) of k independent functions $H_\lambda = J_\lambda$ in involution. Let us choose these vector fields as new generators of the group G and return to Theorem 1. In accordance with this theorem, there exists a toroidal domain $U' \subset U$ provided with another trivialization $U' \to N' \subset N$ in toroidal cylinders $\mathbb{R}^{k-m} \times T^m$ and endowed with bundle coordinates $(J_\lambda, z^A, y'^\lambda)$ such that the vector fields ϑ_λ (12) take the form (8). For the sake of simplicity, let U', N', and y' be denoted U, N, and $y = (t^a, \varphi^i)$ again. Herewith, the Poisson bivector field w is given by the expression (11) with new coefficients.

Let $w^\sharp : T^*U \to TU$ be the corresponding bundle homomorphism, and let $T\mathcal{F}^* \to U$ denote the dual of the characteristic distribution $T\mathcal{F} \to U$. We have the exact sequences

$$0 \to T\mathcal{F} \xrightarrow{i_\mathcal{F}} TU \to TU/T\mathcal{F} \to 0, \tag{A1}$$

$$0 \to \operatorname{Ann} T\mathcal{F} \to T^*U \xrightarrow{i^*_\mathcal{F}} T\mathcal{F}^* \to 0. \tag{A2}$$

The bundle homomorphism $w^\sharp$ factorizes in a unique fashion,

$$w^\sharp : T^*U \xrightarrow{i^*_\mathcal{F}} T\mathcal{F}^* \xrightarrow{w^\sharp_\mathcal{F}} T\mathcal{F} \xrightarrow{i_\mathcal{F}} TU$$

through the bundle isomorphism

$$w^\sharp_\mathcal{F} : T\mathcal{F}^* \to T\mathcal{F}, \quad w^\sharp_\mathcal{F} : \alpha \mapsto -w(x) \rfloor \alpha.$$

Then, the inverse isomorphisms $w^\flat_\mathcal{F} : T\mathcal{F} \to T\mathcal{F}^*$ provides the foliated manifold $(U, \mathcal{F})$ with the leafwise symplectic form

$$\Omega_\mathcal{F} = \Omega^{\mu\nu}(J_\lambda, z^A, t^a)\overline{d}J_\mu \wedge \overline{d}J_\nu + \Omega^\nu_\mu(J_\lambda, z^A)\overline{d}J_\nu \wedge \overline{d}y^\mu, \tag{A3}$$

$$\Omega^\alpha_\mu w^\mu_\beta = \delta^\alpha_\beta, \quad \Omega^{\alpha\beta} = -\Omega^\alpha_\mu \Omega^\beta_\nu w^{\mu\nu}, \tag{A4}$$

where $\{\overline{d}J_\mu, \overline{d}y^\mu\}$ is the dual of the basis $\{\partial^\mu, \partial_\mu\}$ for the characteristic distribution $T\mathcal{F}$. Recall that leafwise (or tangential) exterior forms are defined as sections of the exterior bundle $\wedge T\mathcal{F}^* \to U$, while the leafwise exterior differential $\overline{d}$ acts on them by the law

$$\overline{d}\psi = \overline{d}J_\lambda \wedge \partial^\lambda \psi + \overline{d}y^\lambda \wedge \partial_\lambda \psi$$

(see, e.g., Refs. 23 and 24). The leafwise symplectic form $\Omega_\mathcal{F}$ is nondegenerate and $\overline{d}$-closed, i.e., $\overline{d}\Omega_\mathcal{F} = 0$. Let us show that it is $\overline{d}$-exact.

Let F be a leaf of the foliation $\mathcal{F}$ of U. There is a homomorphism of the de Rham cohomology $H^*(U)$ of U to the de Rham cohomology of $H^*(F)$ of F. One can show that this homomorphism factorizes through the leafwise cohomology[24]

$$H^*(U) \to H^*_\mathcal{F}(U) \to H^*(F). \tag{A5}$$

Since N is a domain of an adapted coordinate chart of the foliation $\mathcal{F}_N$, the foliation $\mathcal{F}_N$ of N is a trivial fiber bundle $N = V \times W \to W$. Since $\mathcal{F}$ is the pull-back onto U of the foliation $\mathcal{F}_N$ of N, it is also a trivial fiber bundle

$$U = V \times W \times (\mathbb{R}^{k-m} \times T^m) \to W \tag{A6}$$

over a domain $W \subset \mathbb{R}^{\dim Z - 2k}$. It follows that

$$H^*(U) = H^*(T^m) = H^*_{\mathcal{F}}(U).$$

Then, the closed leafwise two-form $\Omega_{\mathcal{F}}$ (A3) is exact due to the absence of the term $\Omega_{\mu\nu} dy^\mu \wedge dy^\nu$. Moreover, $\Omega_{\mathcal{F}} = \overline{d}\Xi$ where Ξ reads

$$\Xi = \Xi^\alpha(J_\lambda, z^A, y^\lambda)\overline{d}J_\alpha + \Xi_i(J_\lambda, z^A)\overline{d}\varphi^i$$

up to a $\overline{d}$-exact leafwise form.

The Hamiltonian vector fields $\vartheta_\lambda = \vartheta^\mu_\lambda \partial_\mu$ (8) obey the relation

$$\vartheta_\lambda \rfloor \Omega_{\mathcal{F}} = -\overline{d}J_\lambda, \quad \Omega^\alpha_\beta \vartheta^\beta_\lambda = \delta^\alpha_\lambda, \tag{A7}$$

which falls into the following conditions:

$$\Omega^\lambda_i = \partial^\lambda \Xi_i - \partial_i \Xi^\lambda, \tag{A8}$$

$$\Omega^\lambda_\alpha = -\partial_a \Xi^\lambda = \delta^\lambda_a. \tag{A9}$$

The first of the relations (A4) shows that Ω^α_β is a nondegenerate matrix independent of coordinates y^λ. Then, the condition (A8) implies that $\partial_i \Xi^\lambda$ are independent of φ^i, and so are Ξ^λ since φ^i are cyclic coordinates. Hence,

$$\Omega^\lambda_i = \partial^\lambda \Xi_i, \tag{A10}$$

$$\partial_i \rfloor \Omega_{\mathcal{F}} = -\overline{d}\Xi_i. \tag{A11}$$

Let us introduce new coordinates $I_a = J_a$, $I_i = \Xi_i(J_\lambda)$. By virtue of the equalities (A9) and (A10), the Jacobian of this coordinate transformation is regular. The relation (A11) shows that ∂_i are Hamiltonian vector fields of the functions $H_i = I_i$. Consequently, we can choose vector fields ∂_λ as generators of the algebra $\mathcal{A}$. One obtains from the equality (A9) that $\Xi^a = -t^a + E^a(J_\lambda, z^A)$ and Ξ^i are independent of t^a. Then, the leafwise Liouville form Ξ reads

$$\Xi = (-t^a + E^a(I_\lambda, z^A))\overline{d}I_a + E^i(I_\lambda, z^A)\overline{d}I_i + I_i\overline{d}\varphi^i.$$

The coordinate shifts

$$x^a = -t^a + E^a(I_\lambda, z^A), \quad \phi^i = \varphi^i - E^i(I_\lambda, z^A)$$

bring the leafwise form $\Omega_{\mathcal{F}}$ (A3) into the canonical form

$$\Omega_{\mathcal{F}} = \overline{d}I_\alpha \wedge \overline{d}x^a + \overline{d}I_i \wedge \overline{d}\phi^i$$

which ensures the canonical form (16) of the Poisson bivector field w.

APPENDIX B

Proof of Theorem 6: (I). See the proof of part (I) of Theorem 1.

(II). One can specify the coordinates on the base N of the trivial bundle $U \to N$ as follows. Let us consider the morphism

$$\pi' = \overset{\lambda}{\times} H_\lambda : U \to V \tag{B1}$$

of U onto a domain $V\subset\mathbb{R}^k$. It is of constant rank and, consequently, is a fibered manifold. The fibration π' factorizes as

$$\pi': U \overset{\pi}{\to} N \overset{\pi''}{\to} V$$

through the fiber bundle π. The map $\pi''=\pi'\circ\sigma$ is also a fibered manifold. One can always restrict the domain N to a chart of the fibered manifold π''. Then, $N\to\pi''(N)=V$ is a trivial bundle, and so is $U\to V$. Thus, we have the composite fibration

$$U=V\times W\times(\mathbb{R}^{k-m}\times T^m)\to V\times W\to V. \tag{B2}$$

Let us provide its base V with the coordinates (J_λ) such that $J_\lambda(u)=H_\lambda(u)$, $u\in U$. Then N can be equipped with the bundle coordinates (J_λ,z^A), $A=1,...,2(n-k)$, and $(J_\lambda,z^A,t^a,\varphi^i)$ are coordinates on U (B2). Since fibers of $U\to N$ are isotropic, the symplectic form Ω on U relative to the coordinates $(J_\lambda,z^A,y^\lambda)$ reads

$$\Omega=\Omega^{\alpha\beta}\,dJ_\alpha\wedge dJ_\beta+\Omega^\alpha_\beta\,dJ_\alpha\wedge dy^\beta+\Omega_{AB}\,dz^A\wedge dz^B+\Omega^\lambda_A\,dJ_\lambda\wedge dz^A+\Omega_{AB}\,dz^A\wedge dy^\beta. \tag{B3}$$

The Hamiltonian vector fields $\vartheta_\lambda=\vartheta^\mu_\lambda\partial_\mu$ (8) obey the relations $\vartheta_\lambda\rfloor\Omega=-dJ_\lambda$, which give the coordinate conditions

$$\Omega^\alpha_\beta\vartheta^\beta_\lambda=\lambda^\alpha_\lambda,\quad \Omega_{A\beta}\vartheta^\beta_\lambda=0. \tag{B4}$$

The first of them shows that Ω^α_β is a nondegenerate matrix independent of coordinates y^λ. Then, the second one implies $\Omega_{A\beta}=0$.

By virtue of the well-known Künneth formula for the de Rham cohomology of manifold products, the closed form Ω (B3) is exact, i.e., $\Omega=d\Xi$ where the Liouville form Ξ is

$$\Xi=\Xi^\alpha(J_\lambda,z^B,y^\lambda)dJ_\alpha+\Xi_i(J_\lambda,z^B)d\varphi^i+\Xi_A(J_\lambda,z^B,y^\lambda)dz^A.$$

Since $\Xi_a=0$ and Ξ_i are independent of φ^i, it follows from the relations

$$\Omega_{A\beta}=\partial_A\Xi_\beta-\partial_\beta\Xi_A=0$$

that Ξ_A are independent of coordinates t^a and are at most affine in φ^i. Since φ^i are cyclic coordinates, Ξ_A are independent of φ^i. Hence, Ξ_i are independent of coordinates z^A, and the Liouville form reads

$$\Xi=\Xi^\alpha(J_\lambda,z^B,y^\lambda)dJ_\alpha+\Xi_i(J_\lambda)d\varphi^i+\Xi_A(J_\lambda,z^B)dz^A. \tag{B5}$$

Because entries Ω^α_β of $d\Xi=\Omega$ are independent of y^λ, we obtain the following.

(i) $\Omega^\lambda_i=\partial^\lambda\Xi_i-\partial_i\Xi^\lambda$. Consequently, $\partial_i\Xi^\lambda$ are independent of φ^i, and so are Ξ^λ since φ^i are cyclic coordinates. Hence, $\Omega^\lambda_i=\partial^\lambda\Xi_i$ and $\partial_i\rfloor\Omega=-d\Xi_i$. A glance at the last equality shows that ∂_i are Hamiltonian vector fields. It follows that, from the beginning, one can separate m integrals of motion, say H_i again, whose Hamiltonian vector fields are tangent to invariant tori. In this case, the matrix B in the expressions (7) and (8) vanishes, and the Hamiltonian vector fields ϑ_λ (8) read

$$\vartheta_a=\partial_a,\quad \vartheta_i=(C^{-1})^k_i\partial_k. \tag{B6}$$

Moreover, the coordinates t^a are exactly the flow parameters s^a. Substituting the expressions (B6) into the first condition (B4), we obtain

$$\Omega=\Omega^{\alpha\beta}\,dJ_\alpha\wedge dJ_\beta+dJ_a\wedge ds^a+C^i_k\,dJ_i\wedge d\varphi^k+\Omega_{AB}\,dz^A\wedge dz^B+\Omega^\lambda_A\,dJ_\lambda\wedge dz^A.$$

It follows that Ξ_i are independent of J_a, and so are $C^k_i=\partial^k\Xi_i$.

(ii) $\Omega^\lambda_a = -\partial_a \Xi^\lambda = \delta^\lambda_a$. Hence, $\Xi^a = -s^a + E^a(J_\lambda)$ and Ξ^i are independent of s^a.

In view of items (i)–(ii), the Liouville form Ξ (B5) reads

$$\Xi = (-s^a + E^a(J_\lambda, z^B))dJ_a + E^i(J_\lambda, z^B)dJ_i + \Xi_i(J_j)d\varphi^i + \Xi_A(J_\lambda, z^B)dz^A.$$

Since the matrix $\partial^k \Xi_i$ is nondegenerate, we can perform the coordinate transformation $I_a = J_a$, $I_i = \Xi_i(J_j)$ together with the coordinate shifts

$$x^a = -s^a + E^a(J_\lambda, z^B), \quad \phi^i = \varphi^i - E^j(J_\lambda, z^B)\frac{\partial J_j}{\partial I_i}.$$

These transformations bring Ω into the form (26).

(III) Since functions I_λ are in involution and their Hamiltonian vector fields ∂_λ mutually commute, a point $z \in M$ has an open neighborhood $Q \times O_z$, $O_z \in \mathbb{R}^{k-m} \times T^m$, endowed with the Darboux coordinates $(I_\lambda, p_s, q^s, \tilde{y}^\lambda)$ such that the symplectic form Ω (26) is given by the expression (27). Here, $\tilde{y}^\lambda(I_\lambda, z^A, y^\alpha)$ are local functions whose Hamiltonian vector fields are ∂^λ. They take the form

$$\tilde{y}^\lambda = y^\lambda + f^\lambda(I_\lambda, z^A). \tag{B7}$$

With the group G, one can extend these functions to the open neighborhood

$$\widetilde{U} = Q \times \mathbb{R}^{k-m} \times T^m$$

of M by the law

$$\tilde{y}^\lambda(I_\lambda, z^A, G(y)^a) = G(y)^\lambda + f^\lambda(I_\lambda, z^A).$$

Substituting the functions (B7) on $\widetilde{U}$ into the expression (26), one brings the symplectic form Ω into the canonical form (27) on $\widetilde{U}$.

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The norm-1-property of a quantum observable

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(Received 18 December 2002; accepted 10 February 2003)

A normalized positive operator measure $X \mapsto E(X)$ has the norm-1-property if $\|E(X)\| = 1$ whenever $E(X) \neq O$. This property reflects the fact that the measurement outcome probabilities for the values of such observables can be made arbitrarily close to one with suitable state preparations. Some general implications of the norm-1-property are investigated. As case studies, localization observables, phase observables, and phase space observables are considered. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1566454]

I. INTRODUCTION

Spectral measures possess many important properties which have a direct physical meaning for the quantum observables represented by such measures. Among them are the following properties: (1) the norm of any nonzero operator (projection) in the range of a spectral measure is one, (2) the range of a spectral measure is a Boolean σ-algebra with respect to the order structure of operators, (3) any coarse-graining of such a measure is a function of that measure. The first property allows one to decide (with probabilistic certainty) on the values of the corresponding observable and, for instance, to make the variance of such a quantity in a suitable state arbitrarily small. The Boolean structure of the range of a spectral measure allows one to combine, in a natural way, statements concerning the values (or measurement outcomes) of such observables. Finally, the third property is intimately related to the possibility of joint measurability of various coarse grainings of such observables. In representing a quantum observable as a semispectral measure, i.e., a normalized positive operator measure, one loses, in general, the above-mentioned properties of spectral measures, and thus also the physical interpretation of the relevant measurement context becomes somewhat obscure. In this paper we study these properties and their inter-relations for semispectral measures and we consider their realizations for the approximate localization, phase and the phase space observables.

II. THE NORM-1-PROPERTY AND ϵ-DECIDABILITY

Let $\mathcal{H}$ be a complex separable Hilbert space and $\mathcal{L}(\mathcal{H})$ the set of bounded operators on it. Let Ω be a nonempty set and $\mathcal{A}$ a σ-algebra of subsets of Ω. Consider a normalized positive operator measure $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$, for short, POM. Such operator measures represent physical quantities, observables, of a physical system described by the Hilbert space $\mathcal{H}$. The elements $E(X)$ in the

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range of E, ran(E), are positive operators bounded by the unit operator, that is, $O \leqslant E(X) \leqslant I$. Let $\mathcal{E}(\mathcal{H})$ denote the set of operators A with $O \leqslant A \leqslant I$. They are called effects. Clearly, for any $A \in \mathcal{E}(\mathcal{H})$, its square root $A^{1/2}$ is also an effect with $A \leqslant A^{1/2} \leqslant I$. In particular, the square root of an effect A is self-adjoint implying $\|A^{1/2}\|^2 = \|A\|$. From this equation one notices that $\|A\| = 1$ if and only if $\|A^{1/2}\| = 1$. Also, for any $A \in \mathcal{E}(\mathcal{H})$, the spectrum of A, $\sigma(A)$, is a subset of $[0,1]$, and A is a projection operator ($A^2 = A$) if and only if $\sigma(A) \subseteq \{0,1\}$.

We say that a POM $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ has the *norm-1-property* if the norm of any nonzero effect $E(X)$ equals one, that is, $\|E(X)\| = 1$, whenever $E(X) \neq O$. Clearly, if E is projection valued, that is, each $E(X)$ is a projection operator, then E has the norm-1-property.

Lemma 1: If E has the norm-1-property, then for any $O \neq E(X) \neq I$, *the spectrum of* $E(X)$ *contains* 0 *and* 1.

Proof: The norm of an effect $E(X)$ is equal to its spectral radius,

$$\|E(X)\| \;=\; \sup\{\lambda : \lambda \in \sigma(E(X))\}.$$

Let X' denote the complement of a set $X \subset \Omega$. If E has the norm-1-property, then $\|E(X)\| = 1$ as well as $\|E(X')\| = 1$ for any $O \neq E(X) \neq I$, so that by the closedness of the spectrum, 1 is contained both in $\sigma(E(X))$ and in $\sigma(E(X'))$. Since $E(X') = I - E(X)$ and $\sigma(I - E(X)) = 1 - \sigma(E(X))$, one has $0 \in \sigma(E(X))$. □

We say that a POM $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ has the *ϵ-decidability-property*, if for each $E(X) \neq O$ and for any $\epsilon > 0$ there is a unit vector φ such that $\langle \varphi \mid E(X)\varphi \rangle \geqslant 1 - \epsilon$.

Proposition 1: A POM $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ *has the norm-1-property if and only if it has the* ϵ*-decidability-property*.

Proof: For any effect $E(X)$, we have $\|E(X)\| = 1$ if and only if $\|E(X)^{1/2}\| = 1$. The latter equation can be written as

$$\sup\{\langle \varphi \mid E(X)\varphi \rangle \mid \varphi \in \mathcal{H}, \|\varphi\| = 1\} = 1.$$

□

If an observable (POM) $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ has the ϵ-decidability-property, then for each $X \in \mathcal{A}$ for which $E(X) \neq O$ and for each $\epsilon > 0$ there is a vector state φ ($\|\varphi\| = 1$) such that the probability for a measurement of E to lead to a result in X in that state φ is greater than $1 - \epsilon$. Since probability one and probability almost one are operationally indistinguishable such observables resemble sharp observables, that is, projection valued observables. The following result, known to be valid for sharp observables (spectral measures), exhibits this similarity.

Proposition 2: Consider a bounded real POM $E: \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ *and assume that it has the norm-1-property. Then for each* $\epsilon > 0$ *there is a vector state* $\varphi \in \mathcal{H}$ *such that* $\mathrm{Var}(E, \varphi) < \epsilon$.

Proof: For any $x \in \mathbb{R}$, $x \in \mathrm{supp}(E)$ if and only if for each $\eta > 0$, $E((x - \eta, x + \eta)) \neq O$. Since $E((x - \eta, x + \eta)) \neq O$ implies $\|E((x - \eta, x + \eta))\| = 1$, there is a unit vector $\varphi_\eta \in \mathcal{H}$ such that $\langle \varphi_\eta \mid E((x - \eta, x + \eta))\varphi_\eta \rangle \geqslant 1 - \eta$. Since $\mathrm{supp}(E) \subset [-\alpha, \alpha]$ for some $\alpha > 0$, we now get

$$\mathrm{Var}(E, \varphi_\eta) = \int_{\mathbb{R}} x^2 \, dE_{\varphi_\eta, \varphi_\eta}(x) - \left[\int_{\mathbb{R}} x \, dE_{\varphi_\eta, \varphi_\eta}(x) \right]^2 \leqslant 15 \eta \alpha^3,$$

which tends to zero with $\eta \to 0$. □

III. REGULAR OBSERVABLES AND THEIR COARSE-GRAININGS

For any $A \in \mathcal{E}(\mathcal{H})$ we denote $A' := I - A$ and call it the complement effect of A. If $O \neq A \neq I$, we say that A is *regular* if neither $A \leqslant A'$ nor $A' \leqslant A$. A nontrivial effect A ($\neq O, I$) is regular if and only if $A \not\leqslant \frac{1}{2} I$ and $A \not\geqslant \frac{1}{2} I$; equivalently, if and only if its spectrum extends both below and above $\frac{1}{2}$. Similarly, an observable $E: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ is *regular* if any of its nontrivial effects $E(X)$ is regular.

Proposition 3: If a POM E has the norm-1-property, then it is regular.

Proof: Assume that $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ has the norm-1-property. Then for any $X\in\mathcal{A}$, if $O\neq E(X)\neq I$, we have $0,1\in\sigma(E(X))$, showing that $E(X)$ is regular. □

The converse statement would be false. As a simple example consider a two-valued POM defined as follows: fix a $\lambda\neq\frac{1}{2}$, $0<\lambda<1$, fix also two mutually orthogonal unit vectors φ,ψ and set $A:=\lambda P[\varphi]+(1-\lambda)P[\psi]$. Then A and its complement $A':=I-A$ constitute a regular POM but $\|A\|=\max\{\lambda,1-\lambda\}<1$.

Assume that a POM $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ has an effect $E(X)\neq O$ whose norm is strictly less than 1. Then 1 is not in the spectrum of $E(X)$, that is, 0 is not in the spectrum of its complement effect $E(X')$. Therefore, $E(X')$ is invertible, $\mathrm{ran}(E(X'))=\mathcal{H}$, and for any one-dimensional projection operator P, the greatest lower bound of $E(X')$ and P exists and equals $E(X')\wedge P=\lambda P$, where $\lambda=\|E(X')^{-1/2}\varphi\|^{-2}\neq 0$, with φ being a unit vector such that $P\varphi=\varphi$.[1]

Denoting by $\mathcal{P}(\mathcal{H})_1$ the set of one-dimensional projections on $\mathcal{H}$ we may write any effect A as a join of the weak atoms contained in it, that is, in the form $A=\vee_{P\in\mathcal{P}(\mathcal{H})_1}(A\wedge P)$.[1] Therefore, we now have that the set of effects B which are below A and $E(X')$ is different from zero, that is,

$$lb\,(A,E(X')):=\{B\in\mathcal{E}(\mathcal{H}):B\leqslant A,B\leqslant E(X')\}\neq\{O\}.$$

Consider an arbitrary POM $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$. The range of E is closed under the mapping $E(X)\mapsto E(X)'$. Also the order of effects (as positive operators) may be restricted to $\mathrm{ran}(E)$. However, the map $\mathrm{ran}(E)\ni E(X)\mapsto E(X)'\in\mathrm{ran}(E)$ need not be an orthocomplementation, since $E(X)\wedge_{\mathrm{ran}(E)}E(X)'$ may fail to exist, and even if it does exist, it need not be the null effect O. Neither does it need to hold that $E(X\cap Y)=E(X)\wedge_{\mathrm{ran}(E)}E(Y)$. In particular, this oddity occurs if $\|E(X)\|<1$ for some $E(X)\neq O$. However, if E is regular, then $\mathrm{ran}(E)$ is a Boolean lattice with respect to the order and the complement restricted to $\mathrm{ran}(E)$. The converse is also true: if $(\mathrm{ran}(E),\leqslant,')$ is Boolean, then E is regular.[2] In particular, in that case we have $E(X)\wedge_{\mathrm{ran}(E)}E(X)'=O$ for any $X\in\mathcal{A}$. Any (nonzero) lower bound of $E(X)$ and $E(X)'$ [in $\mathcal{E}(\mathcal{H})$] is necessarily irregular, and as such cannot be contained in the range of E, which is Boolean.

Consider next two POMs E and E_1 defined on the Borel sigma algebras $(\Omega,\mathcal{B}(\Omega))$ and $(\Omega_1,\mathcal{B}(\Omega_1))$ of some complete, separable, metric spaces Ω and Ω_1. We say that E_1 is a coarse-graining of E if $\mathrm{ran}(E_1)\subseteq\mathrm{ran}(E)$. If E is regular, then there is a Borel function $f:\Omega\to\Omega_1$ such that $E_1=E^f$, that is, $E_1(Y)=E(f^{-1}(Y))$ for all $Y\in\mathcal{B}(\Omega_1)$.[3] The converse statement would be false: there are irregular observables, e.g., observables with the $\vee$-property (or strong observables) such that their coarse grainings are functions.[4]

We close this section with a result concerning finite coarse-grainings of an observable having the norm-1-property.

Proposition 4: Let $E:\mathcal{B}(\Omega)\to\mathcal{E}(\mathcal{H})$ be an observable with the norm-1-property. Let $\mathcal{C}=(A_i)_{i=1}^n$ be a partition of unity in $\mathrm{ran}(E)$. *Define a mapping $u_{\mathcal{C}}:\mathcal{E}(\mathcal{H})\to\mathcal{E}(\mathcal{H})$ by $B\mapsto\Sigma_{i=1}^n A_i^{1/2}BA_i^{1/2}$. Then for every $1\leqslant i\leqslant n$ there is a sequence $(\psi_k^i)_{k\in\mathbb{N}}$ of unit vectors in $\mathcal{H}$ such that*

$$\lim_{k\to\infty}\langle\,\psi_k^i\,|\,u_{\mathcal{C}}(B)\psi_k^i\,\rangle=\lim_{k\to\infty}\langle\,\psi_k^i\,|\,A_i^{1/2}BA_i^{1/2}\psi_k^i\,\rangle$$

for all $B\in\mathcal{E}(\mathcal{H})$.

Proof: Owing to the norm-1-property, we can find a sequence of unit vectors $(\psi_k^i)_{k\in\mathbb{N}}$ such that $\langle\,\psi_k^i\,|\,A_i\psi_k^i\,\rangle\to 1$, $k\to\infty$. Since $(A_i)_{i=1}^n$ is a partition of unity, it follows that $\Sigma_{j\neq i}\langle\,\psi_k^i\,|\,A_j\psi_k^i\,\rangle\to 0$. From

$$0\leqslant\langle\,\psi_k^i\,|\,A_j^{1/2}BA_j^{1/2}\psi_k^i\,\rangle\leqslant\|B\|\|A_j^{1/2}\psi_k^i\|\to 0,\quad j\neq i,$$

the desired statement follows. □

IV. LOWER BOUNDS FOR PAIRS OF EFFECTS

The norm-1-property of an observable $E:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ is closely related to the set of lower bounds of an effect and its complement. Indeed, if E does not have the norm-1-property, then $lb\,(E(X),E(X'))\neq\{O\}$ for some $O\neq E(X)\neq I$. On the other hand, if E has the norm-1-property, then $E(X)\wedge_{\mathrm{ran}(E)}E(X')=O$ for any $X\in\mathcal{A}$, and any lower bound of $E(X)$ and $E(X')$ [in $\mathcal{E}(\mathcal{H})$] is necessarily irregular, and as such cannot be contained in the range of E. These observations call for a further study of the set of lower bounds of an effect and its complement.

Let $A,B\in\mathcal{E}(\mathcal{H})$, and let $A=\vee_{P\in\mathcal{P}(\mathcal{H})_1}\lambda(A,P)P$ and $B=\vee_{P\in\mathcal{P}(\mathcal{H})_1}\lambda(B,P)P$. If $\mathrm{ran}(A^{1/2})\cap\mathrm{ran}(B^{1/2})=\{0\}$, then $A\wedge B=O$, and if $\mathrm{ran}\,(A^{1/2})\cap\mathrm{ran}\,(B^{1/2})\neq\{0\}$, then $lb\,(A,B)\neq\{O\}$. In the latter case, the greatest lower bound $A\wedge B$ may or may not exist. In any case, there is always a maximal lower bound.

Proposition 5 (Ref. 5): Let $A,B\in\mathcal{E}(\mathcal{H})$. There is a maximal $C\in\mathcal{E}(\mathcal{H})$ such that $C\leqslant A,B$.

Proof: The set of lower bounds $lb\,(A,B)$ of A and B is a nonempty partially ordered set in $\mathcal{E}(\mathcal{H})$. Let $K\subset lb\,(A,B)$ be a chain. K is a directed set, and by indexing its elements by themselves, K becomes an increasing net in $\mathcal{E}(\mathcal{H})$. Applying known results (e.g., Ref. 6, Lemma 1), one obtains $C\in\mathcal{E}(\mathcal{H})$ such that

$$\lim_{D\in K}\langle\, D\varphi\,|\,\varphi\,\rangle=\langle\, C\varphi\,|\,\varphi\,\rangle$$

for all $\varphi\in\mathcal{H}$. It follows that $C\in lb\,(A,B)$ and that $D\leqslant C$ for all $D\in K$. By Zorn's lemma, $lb\,(A,B)$ has a maximal element. □

Corollary 1: Let $A,B\in\mathcal{E}(\mathcal{H})$. Then every lower bound of A,B lies under a maximal lower bound.

Proof: For every $D_0\in lb\,(A,B)$, set $S(D_0)=\{D\in lb\,(A,B):D_0\leqslant D\}$. Then $S(D_0)$ is partially ordered and nonempty, because $D_0\in S(D_0)$. By the same arguments as above, there is a maximal element in $S(D_0)$. □

For any $A\in\mathcal{E}(\mathcal{H})$, let E^A denote its spectral measure, so that $A=\int_0^1\lambda\,dE^A(\lambda)$. Consider the reduced operators

$$\tilde{A}:=A[I-E^A(\{1\})-E^A(\{0\})]=\int_{0+}^{1-}\lambda\,dE^A(\lambda),$$

$$\widetilde{I-A}:=(I-A)[I-E^A(\{0\})-E^A(\{1\})]=\int_{0+}^{1-}(1-\lambda)\,dE^A(\lambda),$$

where the spectral projections $E^A(\{0\})$ and $E^A(\{1\})$ are nonzero exactly when 0 and 1 are eigenvalues of A.

Proposition 6 (Ref. 7): The infimum $A\wedge A'$ in $\mathcal{E}(\mathcal{H})$ exists if and only if the reduced operators $\tilde{A}$ and $\widetilde{I-A}$ are comparable. In each case, the infimum coincides with the smaller of the above two and is equal to

$$\int_0^1\min(\lambda,1-\lambda)dE^A(\lambda).$$

Corollary 2: Let $A\in\mathcal{E}(\mathcal{H})$. If 0,1 are not eigenvalues of A, then $A\wedge A'$ exists if and only if $A\leqslant I-A$ or $A\geqslant I-A$, that is, A is irregular.

Example 1: Let P_0,P_1,P_2,P_3 be four mutually orthogonal projections which sum up to the unit operator, and let $0<\lambda,\mu<1,\lambda\neq\mu$. Then $A=0P_0+1P_1+\lambda P_2+\mu P_3$ is an effect with $0,1,\lambda,\mu$ as the eigenvalues. Then A and $I-A$ are of norm one, both having 0 and 1 as eigenvalues, and they constitute a simple observable with the range $\{O,A,I-A,I\}$. Now $A\wedge(I-A)$ exists in $\mathcal{E}(\mathcal{H})$ if and only if the reduced operators $\tilde{A}=\lambda P_2+\mu P_3$ and $\widetilde{I-A}=(1-\lambda)P_2+(1-\mu)P_3$ are comparable. This is the case exactly when either $\lambda\leqslant\frac{1}{2},\mu\leqslant\frac{1}{2}$ or $\lambda\geqslant\frac{1}{2},\mu\geqslant\frac{1}{2}$. In that case $A\wedge(I$

$-A$) is the smaller of the two effects $\widetilde{A}$ and $\widetilde{I-A}$. Clearly, $A\wedge(I-A)$, when it exists, is irregular and is therefore not contained in the range of the regular observable in question.

V. EXAMPLES

In this section properties discussed above are considered for the localization observables, the phase observables, and the phase space observables together with their polar and Cartesian marginal measures.

A. Approximate localization

Massless relativistic particles are known to be approximately localizable in the sense that they admit localization observables $E:\mathcal{B}(\mathbb{R}^3)\to\mathcal{L}(\mathcal{H})$, that is, POMs which are covariant under Euclidean motions and dilations, having the norm-1-property for (nonempty) open sets $U\subset\mathbb{R}^3$, see Refs. 8–10. For any nonempty open set $U\subset\mathbb{R}^3$ there is thus a sequence of unit vectors $(\psi_n)_{n\in\mathbb{N}}$ such that

$$\lim_{n\to\infty}\langle\,\psi_n\,|\,E(U)\psi_n\,\rangle=1. \tag{1}$$

Example 2 below shows that there are (non-normalized) positive operator measures which do have the norm-1-property for open sets but not for all Borel sets. Therefore, we shall take a closer look at the norm-1-property.

Example 2: Let $C\subset[0,1]$ be a Cantor set with positive Lebesgue measure. It is well-known that C is compact and nowhere dense. Define a function $f:\mathbb{R}\to\mathbb{R}$ with $f(x)=\frac{1}{2}$ for $x\in C$ and $f(x)=1$ otherwise, and define a (non-normalized) positive operator measure $E:\mathcal{B}(\mathbb{R})\to L^2(\mathbb{R})$ via the equation

$$(E(X)\psi)(x)=\chi_X(x)f(x)\psi(x).$$

For any nonempty open set $U\subset\mathbb{R}$, the intersection $U\cap C'$ is an open set with positive Lebesgue measure. Since $E(U\cap C')\leqslant E(U)$, and, by definition, $\|E(U\cap C')\|=1$, it follows that $\|E(U)\|=1$ for all open set $U\subset\mathbb{R}$. However, it lacks the norm-1-property, since $\|E(C)\|=\frac{1}{2}$.

Let now Ω be a locally compact second countable topological space and $\mathcal{B}(\Omega)$ the Borel σ-algebra of Ω. In this case every finite Borel measure is a Radon measure.

Proposition 7: A POM $E:\mathcal{B}(\Omega)\to\mathcal{L}(\mathcal{H})$ has the norm-1-property if and only if $\|E(K)\|=1$ for all compact sets $K\subset\Omega$ such that $E(K)\neq O$.

Proof: Assume that E has the norm-1-property for compact sets K for which $E(K)\neq O$ and let $X\in\mathcal{B}(\Omega)$. If X contains a compact set K such that $E(K)\neq O$, then from $E(K)\leqslant E(X)$ one gets $\|E(X)\|=1$. On the other hand, if $E(K)=O$ for all compact sets $K\subset X$, then for any unit vector $\varphi\in\mathcal{H}$,

$$\langle\,\varphi\,|\,E(X)\varphi\,\rangle=\sup\{\langle\,\varphi\,|\,E(K)\varphi\,\rangle\,|\,K\subset X,K\text{ compact }\}=0,$$

showing that also $E(X)=O$. □

Compact sets are closed. Therefore, we may replace ''compact'' with ''closed'' in the previous Proposition. This gives us the following formulation, which should be compared with Eq. (1).

Corollary 3: If for any open set U, $E(U)\neq I$, there is a sequence $(\psi_n)_{n\in\mathbb{N}}$ of unit vectors such that

$$\lim_{n\to\infty}\langle\,\psi_n\,|\,E(U)\psi_n\,\rangle=0, \tag{2}$$

then E has the norm-1-property.

Condition (2) means that with a suitable preparation of the state of the system, the probability for a measurement result to be in the set U can be made arbitrarily small. It appears reasonable to expect that an approximate localization observable should fulfill also this condition.

Let G be a locally compact second countable group, H a closed and normal subgroup, and Ω the quotient group G/H. The Haar measure of Ω is denoted by μ_Ω. Assume that (U,E) is a transitive system of covariance, where U is a unitary representation of G in a Hilbert space $\mathcal{H}$ and $E:\mathcal{B}(\Omega)\to\mathcal{L}(\mathcal{H})$ is a POM such that $U(g)E(X)U(g)^*=E(g\cdot X)$ for all $g\in G, X\in\mathcal{B}(\Omega)$.

Lemma 2 below is part of Lemma 3.3 in Ref. 11, and Proposition 8 is a slight modification of Theorem 1 of Ref. 12. We find it useful to give the proofs of these statements here.

Lemma 2: Let α be a finite nonzero measure on $\mathcal{B}(\Omega)$. Then for all $X\in\mathcal{B}(\Omega)$,

$$\mu_\Omega(X)=\frac{1}{\alpha(\Omega)}\int_\Omega \alpha(\omega X^{-1})\,d\mu_\Omega(\omega). \tag{3}$$

Proof: Let $X\in\mathcal{B}(\Omega)$. The set $\tilde{X}:=\{(\omega,\eta)\in\Omega\times\Omega\,|\,\eta^{-1}\omega\in X\}$ is a Borel subset of $\Omega\times\Omega$. Clearly, $\chi_{\tilde{X}}(\omega,\eta)=\chi_X(\eta^{-1}\omega)$. Applying the Fubini theorem to $\chi_{\tilde{X}}$ one gets

$$\int_\Omega\left(\int_\Omega \chi_X(\eta^{-1}\omega)\,d\mu_\Omega(\omega)\right)d\alpha(\eta)=\int_\Omega\left(\int_\Omega \chi_X(\eta^{-1}\omega)\,d\alpha(\eta)\right)d\mu_\Omega(\omega).$$

By the left invariance of the Haar measure μ_Ω, the value of the left-hand side of this equality is just $\mu_\Omega(X)\alpha(\Omega)$. On the right-hand side we can write $\chi_X(\eta^{-1}\omega)=\chi_{\omega X^{-1}}(\eta)$. Now Eq. (3) follows. □

Proposition 8: For any $X\in\mathcal{B}(\Omega)$, $E(X)=O$ if and only if $\mu_\Omega(X)=0$.

Proof: For any $\psi\in\mathcal{H}$ and $X\in\mathcal{B}(\Omega)$, denote $p_\psi(X)=\langle\,\psi\,|\,E(X)\psi\,\rangle$. By lemma 2, we have

$$\mu_\Omega(X)=\frac{1}{p_\psi(\Omega)}\int_\Omega p_\psi(\omega X^{-1})\,d\mu_\Omega(\omega). \tag{4}$$

Assume that $E(X)=O$. Then $p_\psi(X)=0$ for all $\psi\in\mathcal{H}$. Let $\omega\in\Omega$. Because E is covariant, there is a $g\in G$ such that $p_\psi(\omega X)=p_{U(g)^*\psi}(X)$ for all $\psi\in\mathcal{H}$. Hence $p_\psi(\omega X)=0$ and

$$\mu_\Omega(X^{-1})=\frac{1}{p_\psi(\Omega)}\int_\Omega p_\psi(\omega X)\,d\mu_\Omega(\omega)=0.$$

Since μ_Ω is the Haar measure, $\mu_\Omega(X)=0$ if and only if $\mu_\Omega(X^{-1})=0$.

Assume then that $\mu_\Omega(X)=0$. Using Eq. (4) we see that for any $\psi\in\mathcal{H}$, $p_\psi(\omega^{-1}X)=0$ for μ_Ω-almost all $\omega\in\Omega$. Let $\{\varphi_j\}_{j\in\mathbb{N}}$ be an orthonormal basis of $\mathcal{H}$ and let N_j be the set of those $\omega\in\Omega$ for which $p_{\varphi_j}(\omega^{-1}X)$ is not zero. Then every N_j as well as $N=\cup_{j\in\mathbb{N}}N_j$ are μ_Ω-null sets. Assume that $\omega\notin N$. Then for all $k,j\in\mathbb{N}$,

$$\begin{aligned}|\langle\,\varphi_k\,|\,E(\omega^{-1}X)\varphi_j\,\rangle| &= |\langle\,E(\omega^{-1}X)^{1/2}\varphi_k\,|\,E(\omega^{-1}X)^{1/2}\varphi_j\,\rangle|\\ &\le \|E(\omega^{-1}X)^{1/2}\varphi_k\|\cdot\|E(\omega^{-1}X)^{1/2}\varphi_j\|\\ &= p_{\varphi_k}(\omega^{-1}X)\cdot p_{\varphi_k}(\omega^{-1}X)=0.\end{aligned}$$

From this it follows that for each $j\in\mathbb{N}$, $E(\omega^{-1}X)\varphi_j=0$, and thus $E(\omega^{-1}X)=O$. For a fixed $\omega\in N'$ we can take $g\in G$ such that $E(\omega^{-1}X)=U(g)E(X)U(g)^*$. This means that $E(X)=O$. □

Setting Propositions 7 and 8 together we get the following statement.

Proposition 9: A covariant POM E has the norm-1-property if and only if $\|E(K)\|=1$ for any compact set K with positive Haar measure.

We wish to emphasize that it remains an open question if condition (1) implies the norm-1-property for covariant observables.

B. Phase observables

Phase observables are an important class of physical quantities which can be represented only in terms of POMs, since there are no phase shift covariant projection valued measures. Such observables can be characterized in various equivalent ways, the most direct being as follows. Let $(|n\rangle)_{n\in\mathbb{N}}\subset\mathcal{H}$ be an orthonormal basis (number basis) of $\mathcal{H}$. Then any sequence of unit vectors $(\xi_n)_{n\in\mathbb{N}}\subset\mathcal{H}$ defines a (phase shift covariant) POM $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ through

$$E(X)=\sum_{n,m\in\mathbb{N}}\langle\,\xi_n\,|\,\xi_m\,\rangle\frac{1}{2\pi}\int_X e^{i(n-m)x}\,dx\,|n\,\rangle\langle\,m|,\quad X\in\mathcal{B}([0,2\pi)),$$

with the (covariance) property

$$e^{ixN}E(X)e^{-ixN}=E(X\dot{+}x),$$

where $N=\Sigma_{n\in\mathbb{N}}n|n\,\rangle\langle\,n|$ and $\dot{+}$ denotes addition modulo 2π. Conversely, any phase observable is of that form for some sequence of unit vectors $(\xi_n)_{n\in\mathbb{N}}\subset\mathcal{H}$, see, e.g., Ref. 13. Apart from the trivial phase [for which $(\xi_n)_{n\in\mathbb{N}}$ is orthonormal], the simplest among them are the elementary phase observables E_{el}, defined by sequences $(\xi_n)_{n\in\mathbb{N}}$ such that $\langle\,\xi_n\,|\,\xi_m\,\rangle=\delta_{nm}$, except for $n=s,m=t,s\neq t$, in which case $\langle\,\xi_s\,|\,\xi_t\,\rangle=z$, $0<|z|<1$. Such a phase observable has both regular and irregular elements in its range but none of them, except $E_{\mathrm{el}}(X)=I$, has norm one. Indeed, the eigenvalues of its effects $E_{\mathrm{el}}(X)$ satisfy $0\leqslant e_-(X)\leqslant e_0(X)=\ell(X)/2\pi\leqslant e_+(X)$, with

$$e_\pm(X)=\frac{\ell(X)}{2\pi}\pm|z|\left|\frac{1}{2\pi}\int_X e^{i(s-t)x}\,dx\right|.$$

Varying X we get both regular and irregular effects. But always $\|E_{\mathrm{el}}(X)\|=e_+(X)<1$. Thus $\mathrm{ran}(E_{\mathrm{el}})$ is not Boolean and E_{el} does not have the ϵ-decidability property.

The canonical phase observable $E_{\mathrm{can}}:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ is defined by a constant sequence $\xi_n=\xi$ for all n. The Hilbert space $L^2([0,2\pi))$ has an orthonormal basis $\{e_n\}_{n\in\mathbb{Z}}$, where e_n is the function $x\mapsto(1/\sqrt{2\pi})\,e^{inx}$. Let $V:\mathcal{H}\to L^2([0,2\pi)]$ be the isometric linear mapping satisfying $V|n\rangle=e_n$ for all $n\in\mathbb{N}$. The Hilbert space $\mathcal{H}$ can be identified via V with the Hardy subspace H^2 of $L^2([0,2\pi)]$. With this identification, $P:=VV^*$ is the orthogonal projection of $L^2([0,2\pi)]$ onto H^2. Let for $X\in\mathcal{B}([0,2\pi))$, M_{χ_X} be the multiplication operator acting on $L^2([0,2\pi)]$, $M_{\chi_X}f=\chi_X f$. It is easy to see that

$$E_{\mathrm{can}}(X)=V^*M_{\chi_X}V=V^*PM_{\chi_X}V.$$

The spectra of the operators $E_{\mathrm{can}}(X)$ and PM_{χ_X} are therefore the same. On the other hand, by the Hartman–Wintner theorem (Ref. 14, p. 183) the spectrum of the Toeplitz operator PM_{χ_X} is the closed interval $[\mathrm{ess\,inf}\,\chi_X,\mathrm{ess\,sup}\,\chi_X]$. Hence the following proposition is obtained.

Proposition 10: For any $X\in\mathcal{B}([0,2\pi))$ of nonzero Lebesgue measure the norm $\|E_{can}(X)\|=1$. Moreover, if also the complement set X' has nonzero measure, then the spectrum of $E_{can}(X)$ is the whole interval $[0,1]$.

The norm-1-property of E_{can} implies that E_{can} is regular. While $0,1\in\sigma(E_{\mathrm{can}}(X))$ for any $O\neq E_{\mathrm{can}}(X)\neq I$, it is well known that they are not eigenvalues of $E_{\mathrm{can}}(X)$, see e.g., Ref. 15, p. 5929. Therefore $E_{\mathrm{can}}(X)\wedge E_{\mathrm{can}}(X')$ does not exist in $\mathcal{E}(\mathcal{H})$. It follows that there exist at least two incomparable lower bounds of $E_{\mathrm{can}}(X)$ and $E_{\mathrm{can}}(X')$ in $\mathcal{E}(\mathcal{H})$. Apart from that, $(\mathrm{ran}(E_{\mathrm{can}}),\leqslant,')$ is Boolean and E_{can} has the ϵ-decidability property.

The norm-1-property of the canonical phase observable has been obtained by elementary methods already in Ref. 15. These methods were needed to study also some properties of the phase space observables, see below. For the present purpose we find it useful to give an independent proof for Proposition 10.

C. The phase space observable $A_{|0\rangle}$

As another physically relevant example, consider the two-dimensional phase space observable $A_{|0\rangle}$ generated by the ground state $|0\rangle$ of the number operator $N=\Sigma_{n=0}^{\infty} n|n\rangle\langle n|$. As is well known, the phase space observable $A_{|0\rangle}$ has the structure

$$A_{|0\rangle}(Z)=\frac{1}{\pi}\int_Z |z\rangle\langle z|\, d\lambda(z), \quad Z\in\mathcal{B}(\mathbb{C}),$$

where $|z\rangle=e^{-|z|^2/2}\Sigma_{n=0}^{\infty}(z^n/\sqrt{n!})\,|n\rangle$ is a coherent state (for each $z\in\mathbb{C}$) and $\lambda:\mathcal{B}(\mathbb{C})\to[0,\infty]$ the two-dimensional Lebesgue measure. For any $Z\in\mathcal{B}(\mathbb{C})$ of finite measure one has $A_{|0\rangle}(Z)\leqslant[\lambda(Z)/\pi]I$, showing that there are effects $A_{|0\rangle}(Z)$ with norm strictly less than one, even less than $\frac{1}{2}$. Therefore, the phase space observable $A_{|0\rangle}$ does not have the norm-1-property and is irregular. Its range is not Boolean.

1. Polar coordinate marginal measures

Using the polar decomposition of complex numbers ($z=re^{i\theta}$), consider a set of the form $Z=[0,r)\times[0,2\pi)$, so that $\lambda(Z)=\pi r^2$ and thus $\|A_{|0\rangle}(Z)\|\leqslant r^2$. This shows that not only the phase space observable $A_{|0\rangle}$ but also its number margin

$$\mathcal{B}([0,\infty))\ni R\mapsto A_{|0\rangle}(R\times[0,2\pi))=:A^r_{|0\rangle}(R)\in\mathcal{L}(\mathcal{H})$$

fails to have the norm-1-property and is irregular. On the other hand, if we consider sets of the form $Z=[0,\infty)\times\Theta$, with $\Theta\in\mathcal{B}([0,2\pi))$, the estimate $\langle\varphi\,|\,A_{|0\rangle}(Z)\varphi\rangle\leqslant\lambda(Z)/\pi,\varphi\in\mathcal{H},\|\varphi\|=1$, does not help to bound the norm of the effect $A_{|0\rangle}(Z)$. However, it can be shown[15] that the angle margin of $A_{|0\rangle}$, that is, the POM,

$$\mathcal{B}([0,2\pi))\ni\Theta\mapsto A_{|0\rangle}([0,\infty))\times\Theta)=:A^{\theta}_{|0\rangle}(\Theta)\in\mathcal{L}(\mathcal{H})$$

has the norm-1-property: for any $\Theta\in\mathcal{B}([0,2\pi))$ of nonzero Lebesgue measure,

$$\|A^{\theta}_{|0\rangle}(\Theta)\|=1.$$

Therefore, $A^{\theta}_{|0\rangle}$ is regular and it has the ϵ-decidability property.

2. Cartesian marginal measures

Consider next the norm properties of the Cartesian marginal (with respect to $z=x+iy$) measures

$$\mathcal{B}(\mathbb{R})\ni X\mapsto A_{|0\rangle}(X\times\mathbb{R})=:A^x_{|0\rangle}(X)\in\mathcal{L}(\mathcal{H}),$$

$$\mathcal{B}(\mathbb{R})\ni Y\mapsto A_{|0\rangle}(\mathbb{R}\times Y)=:A^y_{|0\rangle}(Y)\in\mathcal{L}(\mathcal{H}).$$

This is most readily done by using the $L^2(\mathbb{R})$-realization of $A_{|0\rangle}$ [obtained via the isometry $\mathcal{H}\ni|n\rangle\mapsto f_n\in L^2(\mathbb{R})$, where f_n is the nth Hermite function]. In that representation the marginal measures are identified, respectively, as unsharp position and unsharp momentum with the effects $A^x_{|0\rangle}(X)\equiv(|f_0|^2*\chi_X)[(1/\sqrt{2})\,Q]$ and $A^y_{|0\rangle}(Y)\equiv(|\hat{f}_0|^2*\chi_X)[(1/\sqrt{2})\,P]$, where Q and P are the usual position and momentum operators and $\hat{f}_0$ is the Fourier transform of f_0.[16] (We recall that it is customary to use the coordinates $q=x/\sqrt{2},p=y/\sqrt{2}$ for position and momentum observables.) Using the spectral calculus one gets the norm estimates

$$\|A^x_{|0\rangle}(X)\|=\left\|(|f_0|^2*\chi_X)\left(\frac{1}{\sqrt{2}}Q\right)\right\| \leqslant\sup_{x\in\mathbb{R}}\left|(|f_0|^2*\chi_X)\left(\frac{1}{\sqrt{2}}x\right)\right|,$$

$$\|A^{\gamma}_{|0\rangle}(Y)\| = \left\| (|\hat{f}_0|^2 * \chi_Y)\left(\frac{1}{\sqrt{2}}P\right)\right\| \leqslant \sup_{y\in\mathbb{R}}\left|(|\hat{f}_0|^2 * \chi_Y)\left(\frac{1}{\sqrt{2}}y\right)\right|.$$

This shows that, e.g., $\|A^{x}_{|0\rangle}((-\epsilon,\epsilon))\| \leqslant 2\epsilon/\sqrt{\pi}$, which is less than $\frac{1}{2}$ whenever $\epsilon < \sqrt{\pi}/4$. An immediate computation also shows that for any bounded $X\in\mathbb{R}$, $\sup_{x\in\mathbb{R}}|(|f_0|^2 * \chi_X)[(1/\sqrt{2})\,x]| < 1$ and thus $\|A^{x}_{|0\rangle}(X)\| < 1$, whereas for complements of bounded sets X one gets $\|A^{x}_{|0\rangle}(X')\| = 1$. Finally, we observe that for any regular effect $A^{x}_{|0\rangle}(X)$, the meet $A^{x}_{|0\rangle}(X) \wedge A^{x}_{|0\rangle}(X)'$ does not exist in $\mathcal{E}(\mathcal{H})$. On the other hand, if $A^{x}_{|0\rangle}(X)$ is irregular, then $\{O, A^{x}_{|0\rangle}(X), A^{x}_{|0\rangle}(X)', I\}$ is non-Boolean.

3. Two-photon coherent state probability measures

The fact that the angle margin $A^{\theta}_{|0\rangle}$ has the norm-1-property means that for any $\Theta \in \mathcal{B}([0,2\pi))$ (of nonzero measure) there is a sequence of unit vectors $\varphi_n \in \mathcal{H}$ such that the probabilities $\langle\, \varphi_n \,|\, A^{\theta}_{|0\rangle}(\Theta)\varphi_n \,\rangle$ tend to one with growing n. In fact, choosing a coherent state $|\alpha\rangle$, $\alpha\in\mathbb{C}$, such that $\arg\alpha \in \Theta$ is a Lebesgue point of Θ, then $\lim_{|\alpha|\to\infty}\langle\, \alpha \,|\, A^{\theta}_{|0\rangle}(\Theta)|\alpha\,\rangle = 1$, see Ref. 15. On the other hand, our investigations of Cartesian marginal measures show that for no bounded $X\in\mathcal{B}(\mathbb{R})$, is there a sequence (φ_n) of unit vectors for which the probabilities $\langle\, \varphi_k \,|\, A^{x}_{|0\rangle}(X)\varphi_k\,\rangle$ would tend to one. We state this obvious fact since one might expect that, for instance, squeezing the vacuum state $|0\rangle$, $S(r)|0\rangle = e^{ra^2 - ra^{*2}}|0\rangle$, and rotating and displacing it appropriately, the probability $\langle\, 0 \,|\, S(r)^* A^{x}_{|0\rangle}(X) S(r)|0\,\rangle$ would tend to one (with growing squeeze parameter r). That this is not the case is seen directly from these probabilities. Instead of considering coherent and squeezed states we study directly the more general case of two-photon coherent states.[17]

Let $|\beta;\mu,\nu\rangle$, $\beta,\ \mu,\ \nu\in\mathbb{C}$, $|\mu|^2 - |\nu|^2 = 1$, be a two-photon coherent state (TCS), that is, it satisfies the following eigenvalue equation:

$$(\mu a + \nu a^*)|\beta;\mu,\nu\rangle = \beta|\beta;\mu,\nu\rangle.$$

An arbitrary TCS $|\beta;\mu,\nu\rangle$ can be written in the form

$$e^{-i\theta/2}R(\theta)D(z)S(\epsilon)|0\rangle,$$

where $R(\theta) := e^{i\theta N}$, $\theta\in[0,2\pi)$, $D(z) := e^{za^* - \bar{z}a}$, $z\in\mathbb{C}$, $S(\epsilon) := e^{1/2\bar{\epsilon}a^2 - 1/2\epsilon a^{*2}}$, $\epsilon\in\mathbb{C}$, are the rotation, displacement, and squeezing operators, respectively. Note that $|\mu|^2 - |\nu|^2 = 1$ implies that $|\mu| \geqslant 1$ and $|\nu/\mu| \in [0,1)$. We go on to determine the density of the probability measure $Z \mapsto \langle\beta;\mu,\nu|A_{|0\rangle}(Z)|\beta;\mu,\nu\rangle$.

Let μ, ν, and β be fixed. From Ref. 17 Eq. (3.20), one gets

$$\langle z|\beta;\mu,\nu\rangle = \frac{1}{\sqrt{\mu}}\exp\left(-\frac{1}{2}|z|^2 - \frac{1}{2}|\beta|^2 - \frac{\nu}{2\mu}\bar{z}^2 + \frac{\bar{\nu}}{2\mu}\beta^2 + \frac{1}{\mu}\bar{z}\beta\right)$$

for all $z,\ \beta\in\mathbb{C}$. Denote $\gamma = \bar{\mu}\beta - \nu\bar{\beta}$. Then $\beta = \gamma\mu + \bar{\gamma}\nu$. Defining $z' := z - \gamma$ one gets

$$\langle z|\beta;\mu,\nu\rangle = \frac{1}{\sqrt{\mu}}\exp\left(-\frac{1}{2}|z'|^2 - \frac{\nu}{2\mu}\bar{z'}^2 + \frac{1}{2}\bar{z'}\gamma - \frac{1}{2}z'\bar{\gamma}\right)$$

and, thus,

$$|\langle z|\beta;\mu,\nu\rangle|^2 = \frac{1}{|\mu|}\exp\left[-|z'|^2 - \mathrm{Re}\left(\frac{\nu}{\mu}\bar{z'}^2\right)\right] = |\langle z'|0;\mu,\nu\rangle|^2.$$

Using the above equation one easily sees that

$$\langle\beta;\mu,\nu|A_{|0\rangle}(Z)|\beta;\mu,\nu\rangle=\frac{1}{\pi}\int_Z|\langle z|\beta;\mu,\nu\rangle|^2d\lambda(z)=\langle 0;\mu,\nu|A_{|0\rangle}(Z-\gamma)|0;\mu,\nu\rangle$$

for all $Z\in\mathcal{B}(\mathbb{C})$.

Next we calculate the Cartesian margins of the probability measure

$$Z\mapsto\langle\beta;\mu,\nu|A_{|0\rangle}(Z)|\beta;\mu,\nu\rangle.$$

Now for all $X,\ Y\in\mathcal{B}(\mathbb{R})$,

$$\langle\beta;\mu,\nu|A^x_{|0\rangle}(X)|\beta;\mu,\nu\rangle=\frac{1}{\sqrt{\pi}|\mu|\sqrt{1-\mathrm{Re}(\nu/\mu)}}\int_{X-\mathrm{Re}\,\gamma}\exp\left\{-x^2\left[\frac{1-|\nu/\mu|^2}{1-\mathrm{Re}(\nu/\mu)}\right]\right\}dx,$$

$$\langle\beta;\mu,\nu|A^y_{|0\rangle}(Y)|\beta;\mu,\nu\rangle=\frac{1}{\sqrt{\pi}|\mu|\sqrt{1+\mathrm{Re}(\nu/\mu)}}\int_{Y-\mathrm{Im}\,\gamma}\exp\left\{-y^2\left[\frac{1-|\nu/\mu|^2}{1+\mathrm{Re}(\nu/\mu)}\right]\right\}dy,$$

so that the variances of these probability measures are

$$\mathrm{Var}\,(A^x_{|0\rangle},|\beta;\mu,\nu\rangle)=\frac{1}{2}\cdot\frac{1-\mathrm{Re}(\nu/\mu)}{1-|\nu/\mu|^2}\geqslant\frac{1}{2},$$

$$\mathrm{Var}\,(A^y_{|0\rangle},|\beta;\mu,\nu\rangle)=\frac{1}{2}\cdot\frac{1+\mathrm{Re}(\nu/\mu)}{1-|\nu/\mu|^2}\geqslant\frac{1}{2}.$$

Thus, there is no sequence of TCS's for which the limit measure of corresponding Cartesian marginal probability measures is concentrated on a point. The uncertainty product, the product of the variances of the marginal measures is

$$\mathrm{Var}\,(A^x_{|0\rangle},|\beta;\mu,\nu\rangle)\cdot\mathrm{Var}\,(A^y_{|0\rangle},|\beta;\mu,\nu\rangle)=\frac{1-(\mathrm{Re}(\nu/\mu))^2}{4(1-|\nu/\mu|^2)^2}\geqslant\frac{1}{4}$$

and the lower bound is attained if and only if $\nu=0$ ($|\mu|=1$), that is, the corresponding TCS is a coherent state (up to a physically irrelevant phase factor).

When we denote $\beta\equiv se^{i\varphi}$, $s\in[0,\infty)$, $\varphi\in[0,2\pi)$, $\theta_\mu:=\arg\mu$, $\theta_\nu:=\arg\nu$, the probability density of the angle margin $A^\theta_{|0\rangle}$ in the state $|\beta;\mu,\nu\rangle$ gets the form

$$\begin{aligned}g_{|\beta;\mu,\nu\rangle}(\theta)&:=\frac{1}{\pi}\int_0^\infty|\langle re^{i\theta}|se^{i\varphi};\mu,\nu\rangle|^2r\,dr\\&=\frac{1}{|\mu|}\exp\left\{-\left[1-\left|\frac{\nu}{\mu}\right|\cos(2\varphi-\theta_\mu-\theta_\nu)\right]s^2\right\}\times\left\{\frac{1}{2\pi[1+|\nu/\mu|\cos(2\theta-\theta_\mu+\theta_\nu)]}\right.\\&\quad+\frac{s\cos(\theta+\theta_\mu-\varphi)\exp\{s^2\cos^2(\theta+\theta_\mu-\varphi)/[|\mu|^2+|\nu\mu|\cos(2\theta-\theta_\mu+\theta_\nu)]\}}{2\sqrt{\pi}|\mu|[1+|\nu/\mu|\cos(2\theta-\theta_\mu+\theta_\nu)]^{3/2}}\\&\quad\left.\times\left\{1+\mathrm{erf}\left[\frac{s\cos(\theta+\theta_\mu-\varphi)}{|\mu|\sqrt{1+|\nu/\mu|\cos(2\theta-\theta_\mu+\theta_\nu)}}\right]\right\}\right\}.\end{aligned}$$

When $|\beta;\mu,\nu\rangle$ is a coherent state $|\beta\rangle$ ($\mu=1$ and $\nu=0$) then

$$g_{|\beta\rangle}(\theta)\to\delta_{2\pi}(\theta-\varphi)$$

when $s\to\infty$. Also if s is fixed and $\varphi=(\theta_\mu+\theta_\nu)/2$ then if $|\nu|\to\infty$,

$$g_{|\beta;\mu,\nu\rangle}(\theta) \sim \frac{1}{2\pi} \frac{1}{|\mu| + |\nu| \cos(2\theta - \theta_\mu + \theta_\nu)} \to \delta_\pi(\theta - \theta_\mu/2 + \theta_\nu/2 + \pi/2)/2$$

(π-periodic Dirac delta). In particular, this holds for a squeezed and rotated vacuum ($s=0$).

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Rigorous proof of isotope effect by Bardeen–Cooper–Schrieffer theory

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(Received 27 February 2002; accepted 31 January 2003)

In this article, we present a rigorous proof of the isotope effect within the theory of Bardeen–Cooper–Schrieffer for isotropic superconductors. We show that, when the interaction kernel is a positive constant, the isotope effect is exact; when the interaction kernel is a positive function depending on the energies of the pairing electrons, the isotope effect is no longer exact but lies within a sharp range determined by the varying kernel function. Moreover, we show that our method here may be extended to establish an existence and uniqueness theorem for the transition temperature in the Bogoliubov–Tolmachev–Shirkov model which allows separate phonon and Coulomb dominance in their respective energy regimes. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1565831]

I. INTRODUCTION

It is well known that the modern theory of superconductivity is based on a mechanism that allows electrons to form bosonic pairs. In a conductive metal, an electron first polarizes the medium by attracting positively charged ions; these excess positive ions in turn attract a neighboring electron, giving an effective attractive interaction between the two electrons. If this attraction is strong enough to override the repulsive screened Coulomb interaction, it gives rise to a net attractive interaction, and superconductivity happens.[35] Historically, the importance of such an electron-lattice ion interaction mechanism in explaining superconductivity was first explored in 1950 by Fröhlich[10] and confirmed shortly afterwards by Maxwell[22] and Reynolds *et al.*[27] through their discovery of the isotope effect in mercury. They found that the superconductive-normal phase transition temperature T_c depends on the isotope mass M of the mercury ions forming the crystal lattices they had tested according to the law

$$T_c M^{1/2} = C, \tag{1.1}$$

where C is a constant. This discovery indicates through the manifestation of the mass of the solid lattice ions that lattice vibrations are indeed essential for electrons to acquire attraction by the exchange of virtual phonons through the electron and crystal lattice ion interactions.[10,11,4] In 1956, Cooper[7] demonstrated that however weak the interelectron attraction may be, two electrons just above the Fermi sea could be bound (the Cooper pairing). In 1957, Bardeen, Cooper, and Schrieffer (BCS) published their monumental work[5] on a microscopic theory of superconductivity based on the Cooper pairing theory. Therefore, the isotope effect is one of the most important physical effects that unveiled to the physicists about 50 years ago the correct way to solve the mystery of superconductivity.

In fact, using the BCS theory, the isotope effect can be established as follows.

Consider the BCS gap equation

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$$\Delta(x)=\int_I K(x,y)\frac{\tanh((1/2T)\sqrt{y^2+\Delta^2(y)})}{\sqrt{y^2+\Delta^2(y)}}\Delta(y)\,dy, \tag{1.2}$$

where $I=[-a,a]$ is a finite interval, $T\geqslant 0$ is the absolute temperature, $\Delta(x)$ is the energy gap function which is proportional to the Landau order parameter so that $\Delta(x)=0$ corresponds to the normal phase and $\Delta(x)\neq 0$ corresponds to the superconducting phase, and $K(x,y)$ is the negative of the interaction matrix elements for the transition of a pair of electrons, of spin up and spin down, with momentum vectors $\mathbf{p}$ and $-\mathbf{p}$ to a pair with momentum vectors $\mathbf{q}$ and $-\mathbf{q}$, so that $x=|\mathbf{p}|^2-\varepsilon_F$ and $y=|\mathbf{q}|^2-\varepsilon_F$ denote the corresponding energy fluctuations around the Fermi energy ε_F. In general, $K(x,y)$ is the sum of two terms. The first term, negative, arises from the repulsive Coulomb force, while the second term, positive, arises from the attractive phonon force. Thus, if the phonon interaction is dominant in a band near the Fermi shell $|\mathbf{p}|^2=\varepsilon_F, |\mathbf{q}|^2=\varepsilon_F$, we will have $K(x,y)>0$. This idealistic assumption, as well as the assumption that $K(x,y)$ is continuous for $-a\leqslant x,y\leqslant a$, will be observed throughout the article (except in Sec. VI). Physicists expect the existence of a unique transition temperature $T_c>0$ so that, when $T<T_c$, (1.2) has a positive solution representing the superconducting phase, but when $T>T_c$, the only solution is the trivial zero solution, representing the normal phase. Besides, as $T\to T_c$, the positive solution goes to zero.

Therefore, when one takes the BCS over-simplified assumption that the integral kernel $K(x,y)$ is a constant, $K(x,y)=K$, one arrives at

$$1=2K\int_0^a \frac{\tanh(y/2T_c)}{y}\,dy \tag{1.3}$$

in the subcritical limit $T\to T_c$. In this equation, one has by using an integration by parts the relation

$$1=2K\tanh\frac{a}{2T_c}\ln\frac{a}{T_c}-K\int_0^{a/T_c}\ln x\,\mathrm{sech}^2\left(\frac{x}{2}\right)dx. \tag{1.4}$$

In the weak coupling limit, the ratio a/T_c is assumed to be sufficiently large and K sufficiently small. Thus

$$K\int_0^{a/T_c}\ln x\,\mathrm{sech}^2\left(\frac{x}{2}\right)dx\approx K\int_0^{\infty}\ln x\,\mathrm{sech}^2\left(\frac{x}{2}\right)dx. \tag{1.5}$$

The value of the integral J on the right-hand side of (1.5) is known[28] to be related to Euler's number γ, $J=-2\ln(2\gamma/\pi)$. Since the ratio $2\gamma/\pi$ is about 1.13 and $\tanh(a/2T_c)\approx 1$, one obtains in view of (1.4) and (1.5) the well-known BCS formula

$$T_c\approx 1.13ae^{-1/2K}. \tag{1.6}$$

However, since the truncation upper limit a is normally taken to be $\hbar\omega_D$ (the Planck constant times the Debye frequency), which is proportional to $M^{-1/2}$ for a single-element solid,[28] one has thus arrived at (1.1) in approximation under the weak coupling limit assumption.

The above approach in proving the isotope effect has been exclusively adopted in literature and texts.[3,5,16,18,25,26,28–30,34–36]

The importance of the isotope effect motivates our rigorous study in the present article. There are several mathematical questions involved in the calculation of the transition temperature T_c and its dependence on other quantities. First, one asks whether there exists a unique transition temperature T_c for the BCS equation (1.2). Second, one wonders whether the positive gap solution is unique and continuously depends on T when $T<T_c$ and whether the solution really goes to zero as $T\to T_c$ from below. Third, one wants to know whether (1.1) holds exactly or approximately as

stated in (1.5) when the integral kernel $K(x,y)$ is a constant. Lastly, one hopes to know what one can say for the isotope effect when $K(x,y)$ is not a constant. The purpose of this article is to answer these questions.

As an application of our method, we shall also present an existence and uniqueness theorem for the transition temperature in the Bogoliubov–Tolmachev–Shirkov model where the interaction kernel may change sign reflecting the phonon attraction and Coulomb repulsion in their respective energy regimes.

II. EXISTENCE OF TRANSITION TEMPERATURE

We first show that, when T is sufficiently large, the only solution of (1.2) is the zero solution. For convenience, we use the notation $\beta=1/T$ and rewrite (1.2) as

$$\Delta(x)=\int_I K(x,y)f_\beta(\sqrt{\Delta^2(y)+y^2})\Delta(y)\,dy\equiv\mathcal{M}(\Delta)(x), \tag{2.1}$$

where

$$f_\beta(t)=\frac{\tanh\frac{1}{2}\beta t}{t},\quad t>0;\quad f_\beta(0)=\lim_{t\to 0^+}f_\beta(t)=\frac{1}{2}\beta. \tag{2.2}$$

It is easily checked that f decreases in the variable $t\geqslant 0$. In particular, we have

$$f_\beta(t)\leqslant \tfrac{1}{2}\beta,\quad t\geqslant 0. \tag{2.3}$$

Let Δ be a non-negative fixed point of the operator $\mathcal{M}$ and set

$$\Delta_0=\sup_{x\in I}\Delta(x). \tag{2.4}$$

Since the nonlinearity function of the equation (2.1), namely,

$$f_\beta(\sqrt{u^2+x^2})u, \tag{2.5}$$

increases when $u\geqslant 0$, we have in view of (2.3)

$$\Delta_0\leqslant\int_I K(x,y)f_\beta(\sqrt{\Delta_0^2+y^2})\Delta_0\,dy\leqslant\left(\frac{1}{2}\beta\int_I K(x,y)\,dy\right)\Delta_0. \tag{2.6}$$

Hence, as expected, $\Delta_0=0$ when $\beta>0$ is sufficiently small.

Next, we show that, when β is sufficiently large, (2.1) has a positive solution.

As a preparation, we show that there is a constant $\delta_0>0$ independent of $\beta>0$ such that

$$\delta>\mathcal{M}(\delta),\quad \forall\,\delta>\delta_0. \tag{2.7}$$

In other words, (2.1) has a family of β-independent constant supersolutions which may assume arbitrarily large values.

In fact, since $\tanh\frac{1}{2}\beta t\leqslant 1$, we have

$$\int_I K(x,y)f_\beta(\sqrt{\delta^2+y^2})\,dy\leqslant\int_I K(x,y)\frac{1}{\sqrt{\delta^2+y^2}}\,dy. \tag{2.8}$$

However, as the right-hand side of (2.8) goes to zero uniformly as $\delta\to\infty$, we see that we have arrived at the desired conclusion, (2.7).

The above simple observation about the supersolutions of (2.1) implies the important conclusion that the existence of a positive solution is equivalent to the existence of a nontrivial subsolution, say Δ_0, of the equation (2.1), satisfying

$$\Delta_0\leqslant\mathcal{M}(\Delta_0). \tag{2.9}$$

To see this, choose $\delta>\delta_0$ sufficiently large so that

$$\sup_{x\in I}\Delta(x)\leqslant\delta. \tag{2.10}$$

Then we obtain a pair of sub- and supersolutions, Δ_0 and $\Delta^0=\delta$, satisfying $\Delta_0(x)\leqslant\Delta^0(x)$, $x\in I$. Since the nonlinearity function (2.5) is monotone, it is standard that the iterative algorithm,

$$\Delta_n=\mathcal{M}(\Delta_{n-1}),\quad n=2,3,\ldots;\quad \Delta_1=\Delta_0\ \text{ or }\ \Delta_1=\Delta^0, \tag{2.11}$$

converges to a nontrivial fixed point, say Δ, of $\mathcal{M}$. It is clear that this fixed point is a positive solution of (2.1) satisfying $\Delta_0\leqslant\Delta\leqslant\Delta^0$.

We now show that, when β is sufficiently large, (2.1) has a nontrivial subsolution.

To see this, we use the fact $K(x,y)>0$ for $-a\leqslant x,y\leqslant 0$ to observe that there holds the uniform limit

$$\lim_{\varepsilon\to 0}\int_I K(x,y)\,\frac{1}{\sqrt{\varepsilon^2+y^2}}\,dy=\infty. \tag{2.12}$$

Since for fixed $\varepsilon>0$ there also holds the uniform limit

$$\lim_{\beta\to\infty}\tanh\left(\tfrac{1}{2}\beta\sqrt{\varepsilon^2+x^2}\right)=1, \tag{2.13}$$

we can combine (2.12) and (2.13) to obtain

$$\inf_{x\in I}\int_I K(x,y)f_\beta\left(\sqrt{\varepsilon^2+y^2}\right)dy>1 \tag{2.14}$$

when $\beta>0$ is large and $\varepsilon>0$ is small. In this situation, we may set $\Delta_0=\varepsilon$ and conclude that Δ_0 is a positive subsolution of (2.1).

Set

$$\Lambda=\{\beta>0\,|\,(2.1)\ \text{ has a positive solution}\}. \tag{2.15}$$

We claim that Λ is connected. Indeed, we show that whenever $\beta\in\Lambda$, there holds $[\beta,\infty)\subset\Lambda$. For convenience, we rewrite (2.1) as

$$\Delta=\mathcal{M}_\beta(\Delta) \tag{2.16}$$

to emphasize the dependence of the operator $\mathcal{M}$ on β explicitly.

If Δ_β is a positive solution of (2.16), then $\Delta_\beta=\mathcal{M}_\beta(\Delta_\beta)<\Delta_\alpha(\Delta_\beta)$ for $\alpha>\beta$. Hence Δ_β is a nontrivial subsolution of the equation $\Delta=\mathcal{M}_\alpha(\Delta)$. Therefore $\alpha\in\Lambda$ as expected.

We already proved that $\Lambda\neq\varnothing$. Now define

$$\beta_c=\inf\{\beta\,|\,\beta\in\Lambda\}. \tag{2.17}$$

We can conclude that $\beta_c>0$. Thus, for $0<\beta<\beta_c$, (2.1) has no positive solution; for $\beta>\beta_c$, (2.1) has a positive solution. In other words, the existence and uniqueness of a positive transition temperature $T_c=1/\beta_c$ follows.

III. TEMPERATURE DEPENDENCE OF GAP FUNCTION

We first show that (2.1) may have only one positive solution for any given $\beta>0$.

Let Δ be a positive solution of (2.1). Choose the number δ in (2.7) to be sufficiently large so that $\delta>\Delta$. Then we can invoke the iterative algorithm (2.11) with $\Delta_1=\Delta^0=\delta$ and obtain another solution, say Δ', satisfying $\Delta'\geqslant\Delta$. We prove that $\Delta'=\Delta$.

Suppose otherwise that $\Delta'\neq\Delta$. Then define

$$\mathcal{A}=\left\{\alpha\geqslant 0 \;\middle|\; \inf_{x\in I}(\Delta(x)-\alpha\Delta'(x))\geqslant 0\right\}. \tag{3.1}$$

Since Δ and Δ' are positive over $I=[-a,a]$, $\mathcal{A}$ contains a small interval near the origin. Besides, we claim that $\mathcal{A}\cap[1,\infty)=\varnothing$. To see this, suppose that there is an $\alpha\geqslant 1$ in $\mathcal{A}$. Then $\Delta(x)-\alpha\Delta'(x)\geqslant 0$. In particular, $\Delta(x)\geqslant\Delta'(x)$. Hence $\Delta=\Delta'$, which contradicts our assumption.

Define $\alpha_0=\sup\{\alpha\mid\alpha\in\mathcal{A}\}$. Then $0<\alpha_0\leqslant 1$. Since it is obvious that $\mathcal{A}$ is closed, we see that α_0 cannot be equal to 1. That is, $0<\alpha_0<1$.

We record here our observation above,

$$\Delta(x)\geqslant\alpha_0\Delta'(x),\quad x\in I. \tag{3.2}$$

Since $f_\beta(t)$ decreases in $t>0$, we have

$$f_\beta(\sqrt{(\Delta')^2+x^2})<f_\beta(\sqrt{(\alpha_0\Delta')^2+x^2}). \tag{3.3}$$

In view of the form of the nonlinear function (2.5) and the property (3.3), we have

$$\mathcal{M}(\alpha_0\Delta')>\alpha_0\mathcal{M}(\Delta'). \tag{3.4}$$

As a consequence of (3.2) and (3.4), we have

$$\Delta=\mathcal{M}(\Delta)\geqslant\mathcal{M}(\alpha_0\Delta')>\alpha_0\mathcal{M}(\Delta')=\alpha_0\Delta' \tag{3.5}$$

everywhere in I. Define

$$\varepsilon=\inf_{x\in I}(\Delta(x)-\alpha_0\Delta'(x))/\sup_{x\in I}\Delta'(x). \tag{3.6}$$

Then $\varepsilon>0$ and $\alpha_0+\varepsilon\in\mathcal{A}$. This violates the definition of α_0. Hence $\Delta=\Delta'$ and (2.1) may have only one positive solution.

The above uniqueness result allows us to write the positive solution of (2.1) for given $\beta\in\Lambda$ as Δ_β. For $\beta',\beta''\in\Lambda$ with $\beta'<\beta''$, since

$$\Delta_{\beta'}=\mathcal{M}_{\beta'}(\Delta_{\beta'})<\mathcal{M}_{\beta''}(\Delta_{\beta'}),$$

we see that $\Delta_{\beta'}$ is a subsolution of (2.1) at $\beta=\beta''$. Hence $\Delta_{\beta'}<\Delta_{\beta''}$.

Let $\{\beta_n\}$ be a decreasing sequence satisfying

$$\lim_{n\to\infty}\beta_n=\beta_0. \tag{3.7}$$

If $\beta_0 > \beta_c$, then $\beta_0 \in \Lambda$ and $\Delta_{\beta_n} > \Delta_{\beta_0} > 0$. Taking the limit as $n \to \infty$ with $\beta = \beta_n$ in (2.1), we see that the sequence $\{\Delta_{\beta_n}\}$ converges to a positive solution bounded from below by Δ_{β_0}. The uniqueness result at $\beta = \beta_0$ indicates that this positive solution can only be Δ_{β_0} itself.

Similarly, we can show that an increasing (convergent) sequence $\{\beta_n\}$ leads to the corresponding convergence of the solution sequence $\{\Delta_{\beta_n}\}$.

The above discussion shows that, above β_c, the positive solution Δ_β depends continuously and monotonically on its parameter β.

To conclude this section, we study what happens when $\beta_0 = \beta_c$ in (3.6).

In fact, the monotonicity

$$\Delta_{\beta_1} > \Delta_{\beta_2} > \cdots > \Delta_{\beta_n} > \cdots \geqslant 0 \tag{3.8}$$

implies that the limit

$$\Delta_{\beta_c}(x) = \lim_{n \to \infty} \Delta_{\beta_n}(x) \tag{3.9}$$

exists and is a non-negative solution of the equation (2.1) for $\beta = \beta_c$.

We now prove that the equation (2.1) at $\beta = \beta_c$ does not have any non-negative solution except the zero solution.

Otherwise suppose that Δ is a non-negative solution of (2.1) which is positive somewhere. The structure of the equation (2.1) says that Δ is positive everywhere because $\beta = \beta_c > 0$ and $K(x,y) > 0$ for $-a \leqslant x, y \leqslant a$. Let $\alpha \in (0,1)$ be an arbitrary constant. Then, similar to (3.4), we have

$$\mathcal{M}_{\beta_c}(\alpha\Delta) > \alpha \mathcal{M}_{\beta_c}(\Delta) = \alpha\Delta. \tag{3.10}$$

Using the continuous dependence of the operator $\mathcal{M}_\beta$ on the parameter $\beta > 0$ in (3.10), we see that

$$\mathcal{M}_{\beta_c - \varepsilon}(\alpha\Delta)(x) \geqslant \alpha\Delta(x), \quad x \in I, \tag{3.11}$$

when $\varepsilon > 0$ is sufficiently small. In other words, $\Delta_0 \equiv \alpha\Delta$ is a positive subsolution of the equation (2.1) at $\beta = \beta_c - \varepsilon$. Hence (2.1) has a positive solution at $\beta = \beta_c - \varepsilon$ which contradicts the definition of β_c stated in (2.17).

In conclusion, we have obtained the desired limit

$$\lim_{\beta \to \beta_c^+} \Delta_\beta = 0. \tag{3.12}$$

IV. LIMITING QUOTIENT

In order to formulate a rigorous way to determine the critical number β_c (namely, T_c), we need another piece of preparation.

Let us consider the simplest situation when the kernel function $K(x,y) = K$ in the equation (2.1) is a constant. For $\beta > \beta_c$, the positive constant solution of (2.1) is now denoted by $\Delta(\beta)$. We have

$$1 = 2K \int_0^a \frac{\tanh(\frac{1}{2}\beta\sqrt{\Delta^2(\beta) + x^2})}{\sqrt{\Delta^2(\beta) + x^2}}\, dx. \tag{4.1}$$

Now taking $\beta \to \beta_c^+$ in (4.1), we see in view of the conclusion (3.12) the validity of the equation

$$1 = 2K \int_0^a \frac{\tanh(\frac{1}{2}\beta_c x)}{x}\, dx, \tag{4.2}$$

which determines the critical number β_c implicitly and is the basis for the derivation of the isotope effect in the BCS theory (see Sec. I).

When the kernel function $K(x,y)$ is not constant, one is tempted to go through the same procedure and to formulate the equation

$$1=\int_I K(x,y)\frac{\tanh(\frac{1}{2}\beta\sqrt{\Delta^2(\beta;y)+y^2})}{\sqrt{\Delta^2(\beta;y)+y^2}}\frac{\Delta(\beta;y)}{\Delta(\beta;x)}\mathrm{d}y,\quad \beta>\beta_c, \tag{4.3}$$

where $\Delta(\beta;x)=\Delta_\beta(x)$ is the unique positive solution of (2.1) already obtained in Secs. 2 and 3.

In order to determine β_c, we may take the limit $\beta\to\beta_c^+$ as before and arrive formally at

$$1=\int_I K(x,y)\frac{\tanh(\frac{1}{2}\beta_c|y|)}{|y|}\left\{\lim_{\beta\to\beta_c^+}\frac{\Delta(\beta;y)}{\Delta(\beta;x)}\right\}\mathrm{d}y. \tag{4.4}$$

It is clear that the existence of the limit of the quotient of $\Delta(\beta;y)$ and $\Delta(\beta,x)$ as $\beta\to\beta_c^+$ under the integral in (4.4) becomes a legitimate question.

For this purpose, define

$$Q(\beta;x,y)=\frac{\Delta(\beta;x)}{\Delta(\beta;y)},\quad \beta>\beta_c,\quad x,y\in I. \tag{4.5}$$

We ask whether the limit

$$\lim_{\beta\to\beta^+} Q(\beta;x,y),\quad x,y\in I, \tag{4.6}$$

exists which guarantees the legitimacy of (4.4). At this time, we may only answer this question in a weak sense, that is, in the sense of subsequences.

To see this, we rewrite Q as

$$Q(\beta;x,y)=\frac{\int_I K(x,\xi)f_\beta(\sqrt{\Delta^2(\xi)+\xi^2})\Delta(\xi)\,\mathrm{d}\xi}{\int_I K(y,\zeta)f_\beta(\sqrt{\Delta^2(\zeta)+\zeta^2})\Delta(\zeta)\,\mathrm{d}\zeta}\equiv\frac{\int_I K(x,\xi)\varphi(\xi)\,\mathrm{d}\xi}{\int_I K(y,\zeta)\varphi(\zeta)\,\mathrm{d}\zeta}. \tag{4.7}$$

Set

$$q_1=\min\{K(x,y)\mid -a\leqslant x,y\leqslant a\}, \tag{4.8}$$

$$q_2=\max\{K(x,y)\mid -a\leqslant x,y\leqslant a\}. \tag{4.9}$$

Then $q_2\geqslant q_1>0$ and it is clear that the function Q has the upper and lower bounds

$$\frac{q_1}{q_2}\leqslant Q(\beta;x,y)\leqslant\frac{q_2}{q_1},\quad x,y\in I. \tag{4.10}$$

Besides, for any $\varepsilon>0$, there is a $\delta>0$, so that

$$|K(x,\xi)-K(x',\xi)|<\varepsilon,\quad |K(y,\zeta)-K(y',\zeta)|<\varepsilon$$

whenever $x,x',y,y'\in I$ satisfy $|x-x'|<\delta,|y-y'|<\delta$. Hence

$$|Q(x,y)-Q(x',y)|\leqslant\frac{\int_I|K(x,\xi)-K(x',\xi)|\varphi(\xi)\,\mathrm{d}\xi}{\int_I K(y,\zeta)\varphi(\zeta)\,\mathrm{d}\zeta}<\frac{\varepsilon}{q_1},$$

$$|Q(x,y)-Q(x,y')|\leqslant\frac{(\int_I K(x,\xi)\varphi(\xi)\,\mathrm{d}\xi)\int_I|K(y,\zeta)-K(y',\zeta)|\varphi(\zeta)\,\mathrm{d}\zeta}{(\int_I K(y,\zeta)\varphi(\zeta)\,\mathrm{d}\zeta)(\int_I K(y',\eta)\varphi(\eta)\,\mathrm{d}\eta)}<\frac{q_2\varepsilon}{q_1^2},$$

which implies that $Q(\beta;x,y)$ is uniformly continuous for $x,y\in I$ with respect to the parameter $\beta>\beta_c$. Consequently, the set $\{Q(\beta;x,y)\}_{\beta>\beta_c}$ is precompact in the space $C(I\times I)$ and for any sequence labeled by $\beta>\beta_c$ with $\beta\to\beta_c$, there is a convergent subsequence. The limit of any of such convergent sequence lies in $C(I\times I)$, of course. Therefore, in sense of subsequence convergence, the limit (4.6) is well defined, although it may not be unique.

Let $Q(\beta_c;x,y)$ denote any limit of (4.6) (in the sense of subseqeunce convergence). Inserting $Q(\beta_c;x,y)$ into (4.4), we obtain the equation

$$1=\int_I K(x,y)Q(\beta_c;y,x)\frac{\tanh(\frac{1}{2}\beta_c|y|)}{|y|}\,\mathrm{d}y, \tag{4.11}$$

which determines the critical number β_c implicitly and extends the classic equation (4.2).

In the next section, we estimate β_c.

V. PROOF OF ISOTOPE EFFECT

From (4.10), we see that the (subsequential or weak) limit $Q(\beta_c;x,y)$ of $Q(\beta_c;x,y)$ as $\beta\to\beta_c^+$ satisfies the same bounds,

$$\frac{q_1}{q_2}\leqslant Q(\beta_c;x,y)\leqslant\frac{q_2}{q_1},\quad x,y\in I. \tag{5.1}$$

Hence, inserting (5.1) into (4.11), we have

$$\frac{1}{2}\geqslant\frac{q_1^2}{q_2}\int_0^a\frac{\tanh(\frac{1}{2}\beta_c y)}{y}\,\mathrm{d}y, \tag{5.2}$$

$$\frac{1}{2}\leqslant\frac{q_2^2}{q_1}\int_0^a\frac{\tanh(\frac{1}{2}\beta_c y)}{y}\,\mathrm{d}y. \tag{5.3}$$

Set the function

$$F(t)=\int_0^t\frac{\tanh y}{y}\,\mathrm{d}y. \tag{5.4}$$

Then F is continuous, strictly increases, $F(0)=0$, and $F(\infty)=\infty$. With this function, we may rewrite (5.2) and (5.3) as

$$1\geqslant\frac{2q_1^2}{q_2}F(\tfrac{1}{2}\beta_c a), \tag{5.5}$$

$$1\leqslant\frac{2q_2^2}{q_1}F\left(\frac{1}{2}\beta_c a\right). \tag{5.6}$$

Let $x_1>0$ and $x_2>0$ be the unique points such that

$$F(x_1)=\frac{q_2}{2q_1^2},\quad F(x_2)=\frac{q_1}{2q_2^2}.$$

Then (5.5) and (5.6) give us

$$x_2 \leqslant \tfrac{1}{2}\beta_c a \leqslant x_1 .$$

In other words, the critical number β_c lies in the range

$$\frac{2x_2}{a} \leqslant \beta_c \leqslant \frac{2x_1}{a}. \tag{5.7}$$

Of course, when $K(x,y)$ is a constant, $q_1 = q_2 \equiv K_0$ and $x_1 = x_2 \equiv x_0$ and (5.7) becomes an equality,

$$\beta_c = \frac{2x_0}{a}. \tag{5.8}$$

Thus we have proved the original isotope effect (1.1) in an exact form (without assuming any approximation limit).

In fact, (5.7) may still be improved in some restrictive situations. For example, an interesting case is that $K(x,y)$ is separable and symmetric,

$$K(x,y) = B(x)B(y), \quad x,y \in I. \tag{5.9}$$

Denote the (positive) minimum and maximum values of B over the interval I by b_1 and b_2, respectively. Then $b_1^2 = q_1$ and $b_2^2 = q_2$. Since the solution of (2.1) is proportional to $B(x)$, letting $\beta \to \beta_c^+$ in (2.1) gives us

$$1 = \int_I B^2(y) \frac{\tanh(\tfrac{1}{2}\beta_c |y|)}{|y|} \mathrm{d}y, \tag{5.10}$$

which leads to the following improved bounds for β_c,

$$\frac{1}{2q_2} \leqslant F\left(\frac{1}{2}\beta_c a\right) \leqslant \frac{1}{2q_1}. \tag{5.11}$$

VI. APPLICATION TO A MODEL OF BOGOLIUBOV *et al.*

In the previous sections, we have taken the original BCS assumption that the interaction kernel $K(x,y)$ is positive throughout the cut-off range from the Fermi surface up to a level $a > 0$ (the cut-off energy is often taken to be $\hbar\omega_D$), which implies that the attractive phonon interaction is everywhere dominant. However, this assumption is only a simplified one. In order to make the model more realistic, Bogoliubov, Tolmachev, and Shirkov[6,18,28] considered a model in which the interaction kernel function $K(x,y)$ assumes the form

$$K(x,y) = K_{\text{phonon}}(x,y) + K_{\text{Coulomb}}(x,y), \tag{6.1}$$

where

$$K_{\text{phonon}}(x,y) \equiv \frac{K_1}{2} > 0, \quad |x|,|y| < a; \quad K_{\text{phonon}}(x,y) = 0 \quad \text{otherwise}, \tag{6.2}$$

$$K_{\text{Coulomb}}(x,y) \equiv -\frac{K_2}{2} < 0, \quad |x|,|y| < b; \quad K_{\text{Coulomb}}(x,y) = 0 \quad \text{otherwise}, \tag{6.3}$$

K_1, K_2 are constants, $a > 0$ is normally taken to be the Debye energy, $a = \hbar\omega_D$, as before, and $b > a$ is a cut-off energy for the range of the screened Coulomb repulsion. With this form of the

interaction kernel reflecting the mixed interaction of the phonon attraction and the Coulomb repulsion, one seeks[6,18,28] a piecewise constant solution of (1.1) of the form

$$\Delta(x)=\Delta_1, \quad |x|<a; \quad \Delta(x)=\Delta_2, \quad a<|x|<b; \quad \Delta(x)=0 \ \text{ otherwise.} \tag{6.4}$$

Hence, inserting (6.1)–(6.4) into (1.1), we arrive at the coupled system

$$\begin{aligned} \Delta_1&=(K_1-K_2)A_\beta(\Delta_1)-K_2B_\beta(\Delta_2),\\ \Delta_2&=-K_2(A_\beta(\Delta_1)+B_\beta(\Delta_2)), \end{aligned} \tag{6.5}$$

where A_β and B_β are the nonlinear transformations defined by

$$\begin{aligned} A_\beta(\Delta)&=\Delta\int_0^a f_\beta(\sqrt{\Delta^2+x^2})\,dx=\Delta\int_0^a \frac{\tanh(\frac{1}{2}\beta\sqrt{\Delta^2+x^2})}{\sqrt{\Delta^2+x^2}}\,dx,\\ B_\beta(\Delta)&=\Delta\int_a^b f_\beta(\sqrt{\Delta^2+x^2})\,dx=\Delta\int_a^b \frac{\tanh(\frac{1}{2}\beta\sqrt{\Delta^2+x^2})}{\sqrt{\Delta^2+x^2}}\,dx. \end{aligned} \tag{6.6}$$

The normal phase is characterized by the trivial solution of (6.5): $\Delta_1=0$, $\Delta_2=0$, and the superconducting phase is characterized by any nontrivial solution of (6.5) of the form

$$\Delta_1>0, \quad \Delta_2<0. \tag{6.7}$$

See Ref. 28 for some calculations in the zero temperature limit, $\beta=\infty$. Our purpose of the present section is to apply the method in the previous sections to study the system (6.5) at any arbitrary temperature. Our main result below is a proof of the existence and uniqueness of a positive transition temperature, $T_c=1/\beta_c$, so that when $T<T_c$, the system (6.5) has a nontrivial solution of the form (6.7), and, when $T>T_c$, the only solution of (6.5) is the trivial solution, $\Delta_1=\Delta_2=0$. In other words, we shall establish rigorously a superconducting-normal phase transition theorem for the phonon-Coulomb interaction model of Bogoliubov–Tolmachev–Shirkov[6,18,28] within the BCS theory.

For convenience, we introduce the new variables $u=\Delta_1$ and $v=-\Delta_2$. Then (6.5) becomes

$$\begin{aligned} u&=(K_1-K_2)A_\beta(u)+K_2B_\beta(v),\\ v&=K_2A_\beta(u)-K_2B_\beta(v). \end{aligned} \tag{6.8}$$

It is seen that the superconducting phase is given by any positive solution of (6.8): $u>0$, $v>0$.

From (2.3), we see that $A_\beta(u)\leqslant\frac{1}{2}\beta a u$ and $B_\beta(v)\leqslant\frac{1}{2}\beta(b-a)v$. Therefore, when β is small, the only non-negative solution of (6.8) is the trivial solution $u=0$, $v=0$.

We now consider the case when β is large.

There are two cases.

Case 1: $K_1>K_2$. We first show that (6.5) has a positive solution if and only if it has a subsolution (u_0,v_0) satisfying $u_0>0$, $v_0\geqslant 0$, and

$$\begin{aligned} u_0&\leqslant(K_1-K_2)A_\beta(u_0)+K_2B_\beta(v_0),\\ v_0&\leqslant K_2A_\beta(u_0)-K_2B_\beta(v_0). \end{aligned} \tag{6.9}$$

To this end, we define the iterative scheme

$$\begin{aligned} u_{n+1}&=(K_1-K_2)A_\beta(u_{n+1})+K_2B_\beta(v_n),\\ v_{n+1}+K_2B_\beta(v_{n+1})&=K_2A_\beta(u_{n+1}), \end{aligned} \tag{6.10}$$

$$n=1,2,\ldots; \quad v_1=v_0.$$

We first consider the function

$$H(u)=u-(K_1-K_2)A_\beta(u). \tag{6.11}$$

Since $H(0)=0$ and $H(\infty)=\infty$, the equation

$$H(u)=s \tag{6.12}$$

has at least one positive solution for any number $s>0$. We show that, in fact, (6.12) can only have one positive solution.

In fact, let u_1 and u_2 be two positive solutions of (6.12) with $s>0$ and $u_1<u_2$. Then $r=u_1/u_2<1$. Again, since $f_\beta(\sqrt{(ru)^2+x^2})>f_\beta(\sqrt{u^2+x^2})$ for $r\in(0,1)$ and $u>0$, A_β and B_β satisfy

$$rA_\beta(u)<A_\beta(ru), \quad rB_\beta(v)<B_\beta(rv), \quad r\in(0,1), \quad u,v>0. \tag{6.13}$$

In view of (6.13), we have, for $r\in(0,1)$,

$$\begin{aligned} u_1&=(K_1-K_2)A_\beta(u_1)+s\\ &=(K_1-K_2)A_\beta(ru_2)+s\\ &>(K_1-K_2)rA_\beta(u_2)+s\\ &=r(u_2-s)+s\\ &=ru_2+(1-r)s, \end{aligned}$$

which is false. Thus uniqueness follows.

We next show that, whenever $u^0>0$ is a number so that

$$H(u^0)\geqslant s \tag{6.14}$$

holds, then the solution u of (6.12) satisfies $u\leqslant u^0$. To this end, define the sequence

$$u_{n+1}=(K_1-K_2)A_\beta(u_n)+s, \quad n=1,2,\ldots; \quad u_1=u^0. \tag{6.15}$$

Then

$$u_2=(K_1-K_2)A_\beta(u^0)+s. \tag{6.16}$$

Comparing (6.16) with (6.14), we have $u_2\leqslant u^0$. Assume that

$$u^0=u_1\geqslant u_2\geqslant\cdots\geqslant u_k\geqslant 0 \tag{6.17}$$

at some step k. It can be shown by the monotonicity of $A_\beta(\cdot)$ that $u_k\geqslant u_{k+1}\geqslant 0$. Hence (6.17) is valid in general. Since the sequence $\{u_n\}$ is non-negative and decreases, we can take the $n\to\infty$ limit in (6.16) to get the unique solution u of (6.12). In particular, $u^0\geqslant u$ as claimed.

As a direct corollary of the above observation, it can be seen that the solution u of (6.12) increases as s increases. Indeed, let $0<s_1<s_2$ be two numbers and u_1 and u_2 be the two corresponding solutions of (6.12) when $s=s_1$ and $s=s_2$, respectively. Thus $H(u_2)>s_1$. Therefore, $u_1<u_2$.

Similarly, if $u_0\geqslant 0$ is such that

$$H(u_0)\leqslant s, \tag{6.18}$$

then the unique solution u of (6.12) satisfies $u_0 \leqslant u$. In fact, this fact is trivially true when $u_0 = 0$. If $u_0 > 0$, we define an iterative sequence $\{u_n\}$ according to (6.15) with $u_1 = u_0$. It is straightforward to see that there holds $u_1 \leqslant u_2 \leqslant \cdots \leqslant u_n \leqslant \cdots$. Using (6.15) and the property of $A_\beta(\cdot)$, we see that $\{u_n\}$ is bounded. Hence $\{u_n\}$ converges to the unique positive solution u of (6.12). In particular, $u_0 \leqslant u$.

We are now prepared to prove the convergence of the sequence $\{(u_n, v_n)\}$ defined by (6.10).

Since the functions $A_\beta(u)$ and $B_\beta(v)$ are bounded uniformly with respect to the parameter β, namely,

$$A_\beta(u) \leqslant C, \quad B_\beta(v) \leqslant C$$

for some absolute constant $C > 0$, there is an absolute constant $u^0 > 0$ so that

$$H(u^0) = u^0 - (K_1 - K_2) A_\beta(u^0) \geqslant K_2 B_\beta(v), \quad \forall v. \tag{6.19}$$

In the sequel, we always assume that u^0 is so chosen unless otherwise stated.

In the iterative scheme (6.10), if $v_1 = v_0 > 0$, then $u_2 > 0$ and $u_0 \leqslant u_2 \leqslant u^0$ by

$$H(u_0) = u_0 - (K_1 - K_2) A_\beta(u_0) \leqslant K_2 B_\beta(v_0)$$

and (6.19). Since the function

$$J(v) = v + K_2 B_\beta(v) \tag{6.20}$$

strictly increases with $J(0) = 0$ and $J(\infty) = \infty$, the equation

$$J(v) = s \tag{6.21}$$

has a unique solution, say v, in $[0, \infty)$ for each $s \in [0, \infty)$ and v increases as s increases. Hence, in (6.10), $v_2 > 0$ is well defined and $v_2 \geqslant v_1 = v_0$.

Assume that the inequalities

$$0 < u_0 = u_1 \leqslant u_2 \leqslant \cdots \leqslant u_k \leqslant u^0, \tag{6.22}$$

$$0 \leqslant v_0 = v_1 \leqslant v_2 \leqslant \cdots \leqslant v_k \tag{6.23}$$

hold at some step k. Then, in view of (6.22) and (6.23), u_k and v_k satisfy

$$H(u_k) = K_2 B_\beta(v_{k-1}) \leqslant K_2 B_\beta(v_k). \tag{6.24}$$

Hence we arrive at $u_{k+1} \geqslant u_k$ after comparing (6.24) with (6.14) and reviewing the definition of u_{k+1}. Thus

$$J(v_k) = K_2 A_\beta(u_k) \leqslant K_2 A_\beta(u_{k+1}). \tag{6.25}$$

Obviously, $v_{k+1} \leqslant v_k$ in view of (6.25) and the definition of v_{k+1} by (6.10). Of course, $u_{k+1} \leqslant u^0$ because u^0 has been chosen to be a (universal) supersolution [see (6.19)].

Therefore, we have shown that (6.22) and (6.23) are valid in general.

The boundedness of the sequence $\{v_n\}$ follows from the boundedness of the sequence $\{u_n\}$ and the second equation in (6.10). In fact, $v_n \leqslant K_2 A_\beta(u^0)$, $n = 1, 2, \ldots$.

Now, taking the $n \to \infty$ limit in the scheme (6.10), we obtain a solution pair (u, v) of the system (6.8) of Bogoliubov–Tolmachev–Shirkov.[6,18,28] Since $u > 0$ in view of (6.22), we see that $v > 0$ as well.

In order to prove the existence of a positive critical temperature T_c, we claim that the system (6.8) has a positive solution when $\beta = 1/T$ is sufficiently large.

Indeed, we may start from the simple BCS equation

$$u=(K_1-K_2)A_\beta(u), \tag{6.26}$$

which may be obtained by setting $v=0$ in the first equation in (6.8). Since $K_1>K_2$, we may use our study in Sec. II to see that when β is large, (6.26) has a positive solution, say u_0. Let $v_0=0$. Then the pair (u_0,v_0) satisfies (6.9). Hence, by virtue of the above discussion, the existence of a positive solution pair of the system (6.8) follows.

As in Sec. III, define

$$\Lambda=\{\beta>0 \mid (6.8) \text{ has a positive solution pair}\}. \tag{6.27}$$

We can prove that Λ is connected. To see this, we show that, if $\beta\in\Lambda$, then $\beta+\varepsilon\in\Lambda$ for any $\varepsilon>0$.

In fact, for $\beta\in\Lambda$, let (u,v) be a positive solution pair of the system (6.8). We rewrite (6.8) as

$$\begin{aligned} u&=(K_1-K_2)A_\beta(u)+K_2B_\beta(v),\\ v+K_2B_\beta(v)&=K_2A_\beta(u). \end{aligned} \tag{6.28}$$

Since $v>0$, we may choose $r\in(0,1)$ so that

$$B_{\beta+\varepsilon}(rv)=B_\beta(v). \tag{6.29}$$

However, from (6.28), we have

$$\begin{aligned} u&<(K_1-K_2)A_{\beta+\varepsilon}(u)+K_2B_\beta(v),\\ rv+K_2B_\beta(v)&<K_2A_{\beta+\varepsilon}(u). \end{aligned} \tag{6.30}$$

Combining (6.29) and (6.30), we obtain

$$\begin{aligned} u&<(K_1-K_2)A_{\beta+\varepsilon}(u)+K_2B_{\beta+\varepsilon}(rv),\\ rv+K_2B_{\beta+\varepsilon}(rv)&<K_2A_{\beta+\varepsilon}(u). \end{aligned} \tag{6.31}$$

In other words, we have recovered (6.9) with $u_0=u$, $v_0=rv$, and β being replaced by $\beta+\varepsilon$. Consequently, $\beta+\varepsilon\in\Lambda$.

Now define β_c as in (2.17). Then, again, $\beta_c>0$. We have just established the relations $(\beta_c,\infty)\subset\Lambda$ and $[0,\beta_c)\cap\Lambda=\varnothing$.

Case 2: $K_1\leqslant K_2$. We rewrite (6.8) as

$$\begin{aligned} u+(K_2-K_1)A_\beta(u)&=K_2B_\beta(v),\\ v+K_2B_\beta(v)&=K_2A_\beta(u), \end{aligned} \tag{6.32}$$

where $0<\beta\leqslant\infty$ with

$$\begin{aligned} A_\infty(u)&=u\int_0^a\frac{dx}{\sqrt{u^2+x^2}}=u\ln\left(\frac{a}{u}+\sqrt{\left(\frac{a}{u}\right)^2+1}\right),\\ B_\infty(v)&=v\int_a^b\frac{dx}{\sqrt{v^2+x^2}}=v\ln\left(\frac{b+\sqrt{v^2+b^2}}{a+\sqrt{v^2+a^2}}\right). \end{aligned} \tag{6.33}$$

As before, we can show that the system (6.32) has a positive solution pair if and only if there exists a nontrivial subsolution, (u_0,v_0), satisfying

$$u_0+(K_2-K_1)A_\beta(u_0)\leqslant K_2B_\beta(v_0),$$
$$v_0+K_2B_\beta(v_0)\leqslant K_2A_\beta(u_0), \tag{6.34}$$

where at least one of two numbers, u_0 and v_0, is positive, and the other may or may not be zero.

In fact, assume that $u_0>0$ and $v_0\geqslant 0$ satisfy (6.34). Define

$$u_{n+1}+(K_2-K_1)A_\beta(u_{n+1})=K_2B_\beta(v_n),$$
$$v_{n+1}+K_2B_\beta(v_{n+1})=K_2A_\beta(u_{n+1}), \tag{6.35}$$
$$n=1,2,\ldots;\quad v_1=v_0.$$

Using the monotonicity of the functions $P(u)=u+(K_2-K_1)A_\beta(u)$ and $Q(v)=v+K_2B_\beta(v)$, we see that the sequences $\{u_n\}$ and $\{v_n\}$ are well defined and that

$$u_0=u_1\leqslant u_2\leqslant\cdots\leqslant u_n\leqslant\cdots,\quad v_0=v_1\leqslant v_2\leqslant\cdots\leqslant v_n\leqslant\cdots. \tag{6.36}$$

Since the functions $A_\beta(\cdot)$ and $B_\beta(\cdot)$ are bounded, it follows from (6.35) that $\{u_n\}$ and $\{v_n\}$ are bounded sequences. Taking the limit $n\to\infty$ in (6.35), we see that $u=\lim_{n\to\infty}u_n$ and $v=\lim_{n\to\infty}v_n$ make a solution pair to the system (6.32). Since $u_0>0$, (6.36) implies that $u>0$. It follows from (6.32) that $v>0$ as well.

The case that $u_0\geqslant 0$, $v_0>0$ is similar.

In order to obtain a positive transition temperature for the system (6.32), it is a basic requirement that (6.32) has a positive solution pair at the zero temperature, $\beta=\infty$.

Inserting (6.33) into (6.32) with $\beta=\infty$, we have

$$u+(K_2-K_1)u\ln\left(\frac{a}{u}+\sqrt{\left(\frac{a}{u}\right)^2+1}\right)=K_2v\ln\left(\frac{b+\sqrt{v^2+b^2}}{a+\sqrt{v^2+a^2}}\right),$$
$$v+K_2v\ln\left(\frac{b+\sqrt{v^2+b^2}}{a+\sqrt{v^2+a^2}}\right)=K_2u\ln\left(\frac{a}{u}+\sqrt{\left(\frac{a}{u}\right)^2+1}\right). \tag{6.37}$$

We may choose the parameters a,b,K_1,K_2 suitably so that (6.37) has a positive solution. For some of the limiting cases about this existence problem, see Ref. 28. We will not pursue it further here. Instead, we are interested in the more general problem of the existence of a positive transition temperature T_c and we need some sufficient conditions under which the system (6.32) admits a positive solution pair at finite values of β. It is clear that one of the simplest of such sufficient conditions is the existence of a subsolution to (6.32) of the form

$$u_0=\varepsilon,\quad v_0=\varepsilon, \tag{6.38}$$

where $\varepsilon>0$ is small enough. However, in order to ensure the existence of such a subsolution, we may impose the condition

$$1+(K_2-K_1)\int_0^a\frac{\tanh(\frac{1}{2}\beta x)}{x}\,dx<K_2\int_a^b\frac{\tanh(\frac{1}{2}\beta x)}{x}\,dx,$$
$$1+K_2\int_a^b\frac{\tanh(\frac{1}{2}\beta x)}{x}\,dx<K_2\int_0^a\frac{\tanh(\frac{1}{2}\beta x)}{x}\,dx. \tag{6.39}$$

It is seen that, when (6.39) holds, the inequalities

$$\varepsilon+(K_2-K_1)A_\beta(\varepsilon)<K_2B_\beta(\varepsilon), \tag{6.40}$$

$$\varepsilon + K_2 B_\beta(\varepsilon) < K_2 A_\beta(\varepsilon)$$

can be achieved whenever ε is sufficiently small. That is, we have arrived at (6.34) with the pair of subsolution (u_0, v_0) defined in (6.38). Hence, in this situation, (6.32) has a positive solution. In other words, under the condition (6.39), the set Λ defined in (6.27) is not empty.

We next show that Λ is in fact an interval. To this end, assume $\beta \in \Lambda$ and $\varepsilon > 0$. We prove as before that $\beta + \varepsilon \in \Lambda$.

Let (u,v) be a positive solution of (6.32). We can find a pair of numbers $s,t \in (0,1)$ such that

$$A_{\beta+\varepsilon}(su) = A_\beta(u), \quad B_{\beta+\varepsilon}(tv) = B_\beta(v). \tag{6.41}$$

Inserting (6.41) into (6.32), we obtain

$$\begin{aligned} u + (K_2 - K_1) A_{\beta+\varepsilon}(su) &= K_2 B_{\beta+\varepsilon}(tv), \\ v + K_2 B_{\beta+\varepsilon}(tv) &= K_2 A_{\beta+\varepsilon}(su). \end{aligned} \tag{6.42}$$

Consequently, we are led to

$$\begin{aligned} su + (K_2 - K_1) A_{\beta+\varepsilon}(su) &< K_2 B_{\beta+\varepsilon}(tv), \\ tv + K_2 B_{\beta+\varepsilon}(tv) &< K_2 A_{\beta+\varepsilon}(su). \end{aligned} \tag{6.43}$$

In other words, $u_0 = su$, $v_0 = tv$ satisfy (6.34) when β is replaced by $\beta + \varepsilon$. Hence $\beta + \varepsilon \in \Lambda$.

Define β_c as in (2.17). Then $\beta_c > 0$ and the existence and uniqueness of a transition temperature T_c are again established as before.

VII. CONCLUSIONS

Returning to the original representation in terms of the absolute temperature, $T = 1/\beta$, we can summarize our study as follows: For the BCS equation (1.2), there exists a unique transition temperature T_c so that, when $0 \leqslant T < T_c$, the equation has a unique positive solution, say $\Delta(T;x)$. However, for $T \geqslant T_c$, the only non-negative solution of the equation is the zero solution. For $T < T_c$ the solution $\Delta(T;x)$ depends on T continuously and decreases as T increases so that

$$\lim_{T \to T_c^-} \Delta(T;x) = 0. \tag{7.1}$$

In general, the transition temperature $T_c = 1/\beta_c$ is implicitly determined by the equation (4.11). With the numbers q_1 and q_2 defined in (4.8) and (4.9), respectively, the transition temperature T_c has the lower and upper estimates

$$\frac{1}{2G(q_2/2q_1^2)} \leqslant \frac{T_c}{a} \leqslant \frac{1}{2G(q_1/2q_2^2)}, \tag{7.2}$$

where G is the inverse function of F defined in (5.4). In particular, when the kernel function is a constant, say K_0, (7.2) becomes an exact result,

$$\frac{T_c}{a} = \frac{1}{2G(1/2K_0)}. \tag{7.3}$$

If the superconductor is a single-element solid so that the integral upper limit a in (1.2) is such that a^{-2} is proportional to the isotope mass of the solid lattice ions, then (7.3) expresses exactly the isotope effect (1.1) but (7.2) gives us a slightly relaxed one,

$$C_1 \leqslant T_c M^{1/2} \leqslant C_2, \tag{7.4}$$

where the constants C_1 and C_2 depend on the range of the kernel function $K(x,y)$ so that $C_1 = C_2$ when $K(x,y)$ is a constant. We have seen through a study of the Bogoliubov–Tolmachev–Shirkov model that our method also applies to the situation when the kernel function is not positive definite.

As is well known now, the isotope effect in its most general form reads

$$T_c M^{\alpha} = C, \tag{7.5}$$

where the exponent α has the upper bound

$$\alpha \leqslant \tfrac{1}{2}. \tag{7.6}$$

The BCS proof of (1.1) through their formula (1.6) is based on a somewhat artificial single cutoff at the energy $\hbar\omega_D$ which leads to an exact value of α equal to $\frac{1}{2}$ as seen in the present article. In the work of Swihart,[32,33] it is shown that one may obtain values of α smaller than the BCS value of $\frac{1}{2}$, within the BCS theory, by assuming that the cutoff energy in the Coulomb part of the electron-electron interaction in the same sense of the Bogoliubov–Tolmachev–Shirkov model is independent of the isotope mass of the lattice ions. See also the works of Morel and Anderson[24] and Garland.[12–14] For some calculations involving multiband models, see Refs. 15, 17, 21, and 31.

A more general treatment of the isotope effect may be formulated in the Eliashberg theory.[8,9] See Refs. 1, 3, 17, 19, 20, and 36 for some updated reviews. However, mathematically, the Eliashberg equations are rather difficult and a rigorous understanding is yet to be achieved, although people have gained some knowledge on various limiting situations. For example, McMillan[23] and Allen and Dynes[2] have calculated T_c and confirmed the bound (7.6) in the real-axis limit of the Eliashberg equations. See also Ref. 36 for an elegant expression for α. Thus, it will be important to carry out a rigorous study of these equations.

ACKNOWLEDGMENTS

The author's research was supported partially by NSF under Grant Nos. DMS-9972300 and DMS-9729992 through the Institute for Advanced Study.

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Distributional Borel summability for vacuum polarization by an external electric field

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(Received 9 October 2002; accepted 4 February 2003)

It is proved that the divergent perturbation expansion for the vacuum polarization by an external constant electric field in the pair production sector is Borel summable in the distributional sense. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1565833]

I. INTRODUCTION AND STATEMENT OF THE RESULTS

Since 1970 the standard method to deal with divergent perturbation theory in quantum mechanics (QM) and quantum field theory (QFT) has been Borel summability.[1] For convenience of exposition, let us first recall its definition (Ref. 2; a classical reference is Ref. 3; general references especially dealing with QM and QFT are, e.g., Refs. 4–6).

Definition 1.1: Consider the formal power series $\Sigma_{n=0}^{\infty} a_n z^n$. *The series*

$$B(t) := \sum_{n=0}^{\infty} \frac{a_n}{n!} t^n \tag{1.1}$$

is called Borel transform of $\Sigma_{n=0}^{\infty} a_n z^n$. *Assume the following.*

(1) B(t) has a positive radius of convergence $C>0$.
(2) B(t), a priori holomorphic for $|t|<C$, *admits analytic continuation at least to a neighborhood of the positive real axis.*
(3) There is $R>0$ *such that the Laplace–Borel integral*

$$f(z) := \int_0^{\infty} B(zu)\, e^{-u}\, \mathrm{d}u \tag{1.2}$$

converges for $z \in C_R$ *and defines an analytic function therein. Here* C_R *is the disk of radius* $R/2$ *tangent to the imaginary axis at the origin, defined by* $C_R := \{z \in \mathbf{C}: \mathrm{Re}\, z^{-1} > R^{-1}\}$.

Then we say that $\Sigma_{n=0}^{\infty} a_n z^n$ *is Borel summable to* $f(z)$ *for* $z \in C_R$.

Remarks:

(1) If (1.1) is inserted into (1.2), and summation is formally interchanged with integration, we see that $f(z)$ admits the given formal power series as an asymptotic expansion as $z \to 0_+$. An expression equivalent to (1.2) is

$$\frac{1}{z} \int_0^{\infty} B(t)\, e^{-t/z}\, \mathrm{d}t. \tag{1.3}$$

(2) When the series $\Sigma_{n=0}^{\infty} a_n z^n$ has a positive radius of convergence the Laplace–Borel integral converges in the Borel polygon and yields therefore the analytic continuation of the sum $f(z)$ outside the circle of convergence if this is strictly contained in the Borel polygon;

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(3) In most applications, given a formal power series (example: a perturbation expansion) there is a natural candidate to the sum (example: the physical solution). A criterion is thus needed to check whether a formal power series representing the asymptotic expansion of a function is actually Borel summable to that function. The standard one is the Watson–Nevanlinna theorem (see Ref. 3, and also Ref. 7 for a new presentation in full generality of the original paper by Nevanlinna).

The vacuum polarization by a constant, external (i.e., non quantized) electromagnetic field admits a well known exact solution (Ref. 8; see also Ref. 5) which generates a divergent power series if expanded in powers of the fine structure constant. Historically, the pure magnetic case has been the first example where the Borel summability (of order 2) has been proved[9] (see also Ref. 10) through a direct verification of Properties 1–3 above. (Here also the Stieltjes summability holds;[11] it entails the convergence of the Padé approximants.) It is interesting to remark that the pure electric case, which has been recently reconsidered also to discuss this point,[10] represents instead a typical example where Borel summability cannot hold, because the Borel transform has singularities along the positive real axis.

To better clarify this point, consider the formal expansion $\Sigma_{n=0}^{\infty} n! z^n$. Its Borel transform is

$$B(t)=\sum_{n=0}^{\infty} t^n=\frac{1}{1-t}.$$

$B(t)$ is analytic on the whole of $\mathbf{C}$ except for the simple pole at $t=1$. Consider now the function

$$F(z):=\int_0^{\infty} \frac{e^{-t}}{1-zt}\,\mathrm{d}t, \quad z\in\mathbf{C}, \quad z\notin]0,+\infty[. \tag{1.4}$$

$F(z)$ is clearly holomorphic in $\{z\in\mathbf{C}:0<|z|;\ 0<\arg z<2\pi\}$ and its formal expansion at $z=0$ is $\Sigma_{n=0}^{\infty} n! z^n$. The nonexistence of the integral (1.4) for $z\in]0,+\infty[$ is due to the pole of the Borel transform $B(t)$ at $t=1$. Indeed this phenomenon occurs whenever the coefficients a_n have a constant sign, because in that case $B(t)$ has a singularity at $t=C$, where C is the radius of convergence of $B(t)$ (see, e.g., Ref. 12).

If we could perform the change of variable (1.3) for $F(z)$, as we can when the conditions of Definition 1.1 are satisfied, we could write

$$F(z)=\frac{1}{z}\int_0^{\infty}\frac{1}{1-t}e^{-(t/z)}\,\mathrm{d}t. \tag{1.5}$$

However (1.5) is only a formal writing because the integral on the rhs diverges for all $z\in\mathbf{C}$. Nevertheless, (1.5) could make sense if the Borel transform $B(t)=(1-t)^{-1}$ is regarded as an object more general than a function, for example a distribution. More precisely, in this case we can look at the boundary values $B(t\pm i0)=1/(1-t\pm i0)$, $t\geqslant 0$, of the holomorphic function $B(t)$, as tempered distributions:

$$B(t\pm i0)=\frac{1}{1-t\pm i0}:=\lim_{\epsilon\to 0_+}\frac{1}{1-t\pm i\epsilon}=PP\left(\frac{1}{1-t}\right)\pm i\,\delta(t-1). \tag{1.6}$$

Here $PP(1/(1-t))$ is the Cauchy principal-value distribution supported at 1. Note that $B(t-i0)=\overline{B(t+i0)}$. Next remark that the function

$$\Phi(z):=\frac{1}{z}\int_0^{\infty} B(t+i0)e^{-t/z}\,\mathrm{d}t \tag{1.7}$$

exists, is analytic for $z \in C_R \ \forall R>0$, i.e., in the half-plane $\mathrm{Re}\, z>0$, concides with $F(z)$ for $z \in \{z \in \mathbf{C}: \mathrm{Im}\, z>0; \mathrm{Re}\, z>0\}$, and admits $\Sigma_{n=0}^{\infty} n! z^n$ as a formal expansion at $z=0$. It is called the *upper sum* of the series (see also the remarks after Definition 1.2 below). Since the divergent series is real for $z \in [0,+\infty[$, so must be its sum provided it exists in any sense. Therefore the natural candidate for the Borel sum is

$$f(z) := \frac{1}{z} \int_0^{\infty} PP\left(\frac{1}{1-t}\right) e^{-t/z}\, \mathrm{d}t = \frac{1}{z} \int_0^{\infty} \frac{1}{2} \{B(t+i0) + \overline{B(t+i0)}\} e^{-t/z}\, \mathrm{d}t. \tag{1.8}$$

In other words $f(z) = \frac{1}{2}\{\Phi(z) + \overline{\Phi(\overline{z})}\} \forall\, z$, $\mathrm{Re}\, z>0$. In particular, $f(z) = \mathrm{Re}\, \Phi(z)$ for $z \in [0,+\infty[$.

This example shows that an extension of the Borel method to the case where the Borel transform admits singularities along the positive real axis has to allow for Borel transforms in the sense of distributions. In turn, distributions are particular cases of the hyperfunctions, defined as boundary values of holomorphic functions. The extension, called distributional Borel summability, has been developed in Ref. 13. Let us recall here the definition and some of the main results.

Definition 1.2: Consider again the formal power series $\Sigma_{n=0}^{\infty} a_n z^n$ and its Borel transform $B(t)$ as in Definition 1.1, with radius of convergence $C>0$. Assume the following:

(1) $B(t)$ admits analytic continuation to the intersection of some neighborhood of $\mathbf{R}_+$ with $\mathbf{C}_+ := \{t \in \mathbf{C}:\ \mathrm{Im}\, t>0\}$.
(2) The boundary value distribution $B(t+i0)$ exists $\forall\, t \geqslant 0$.
(3) Let $PP(B(t)) := \frac{1}{2}\{B(t+i0) + \overline{B(t+i0)}\}$, $t \geqslant 0$. Then there exists $R>0$ such that the Laplace–Borel integral

$$f(z) := \frac{1}{z} \int_0^{\infty} PP(B(t)) e^{-t/z}\, \mathrm{d}t \tag{1.9}$$

converges for $z \in C_R$, C_R as in Definition 1.1.

Then we say that the formal power series $\Sigma_{n=0}^{\infty} a_n z^n$ is Borel summable in the distributional sense to $f(z)$ for $z \in C_R$. The distribution $PP(B(t)): t \in \mathbf{R}_+$ is called distributional Borel transform of $\Sigma_{n=0}^{\infty} a_n t^n$.

Remarks:

(1) The distribution $PP(B(t))$ coincides with the holomorphic function $B(t)$, the Borel transform, for $0 \leqslant t < C$.
(2) The Laplace–Borel integrals

$$\Phi(z) := \frac{1}{z} \int_0^{\infty} B(t+i0) e^{-t/z}\, \mathrm{d}t, \tag{1.10}$$

$$\overline{\Phi(\overline{z})} := \int_0^{\infty} \overline{B(t+i0)} e^{-t/z}\, \mathrm{d}t \tag{1.11}$$

exist separately in C_R as analytic functions and uniquely define the ''upper'' and ''lower'' sums, respectively. Then $f(z) = \{\Phi(z) + \overline{\Phi(\overline{z})}\}/2$ for all $z \in C_R$. In particular, $f(z) = \mathrm{Re}\, \Phi(z)$, $\forall\, z \in C_R \cap \mathbf{R}_+$.

(3) As the ordinary Borel sum, the distributional Borel one is unique. We note for further reference that this method singles out also a unique function with zero asymptotic power series expansion, the so-called ''discontinuity,'' uniquely defined by

$$d(z) := \Phi(z) - \overline{\Phi(\overline{z})} = \frac{1}{z} \int_0^{\infty} \{B(t+i0) - \overline{B(t+i0)}\} e^{-t/z}\, \mathrm{d}t, \quad \forall\, z \in C_R.$$

In particular $d(z) = 2i\, \mathrm{Im}\, \Phi(z)$, $\forall\, z \in C_R \cap \mathbf{R}_+$.

In the above example we have

$$d(z)=\frac{1}{z}\int_0^\infty 2i\delta(t-1)e^{-t/z}\,\mathrm{d}t, \quad =\frac{2i}{z}e^{-1/z}.$$

(4) The analog of the Watson–Nevanlinna criterion has also been established.[13] Its conditions have been verified to prove the distributional Borel summability in a number of physically interesting cases which generate constant sign divergent perturbation expansions. Examples include the Rayleigh–Schrödinger perturbation theory for Stark effect[14] and the odd anharmonic oscillators,[15] which are summable to the resonances, and a variant of the bound state perturbation theory for the double well quartic oscillator.[16]

Let us now proceed to state the result of this article. Its proof is to be described in the next section.

The effective action for the vacuum polarization by a uniform electric field can be obtained as a particular case from the Schwinger solution[8,5] valid for a general external constant electromagnetic field, and reads

$$S(\alpha)=-\frac{1}{8\pi^2}\int_0^\infty \frac{e^{-is}}{s^3}\left\{(2\sqrt{\pi\alpha}s)\coth(2\sqrt{\pi\alpha}s)-1-\frac{4\pi\alpha s^2}{3}\right\}\mathrm{d}s. \tag{1.12}$$

Here α is the fine structure constant, and without loss the electron mass m and the strength E of the field are set equal to 1. Notice that (1.12) defines an analytic function of α for $-\pi<\arg\alpha<\pi$. It can be easily checked (see also Lemma 2.2 below) that $S(\alpha)$ admits the following formal expansion in power series of α:

$$S(\alpha)\sim-\frac{1}{8\pi^2}\sum_{n=2}^\infty (16\pi)^n B_{2n}\frac{(2n-3)!}{(2n)!}(-\alpha)^n=\sum_{n=2}^\infty a_n\alpha^n, \tag{1.13}$$

$$a_n:=-\frac{(-1)^n}{8\pi^2}(16\pi)^n B_{2n}\frac{(2n-3)!}{(2n)!}, \tag{1.14}$$

where $\{B_{2n}\}$, $n=0,1,\ldots$, is the sequence of the Bernoulli numbers. Now (see, e.g., Ref. 17)

$$B_0=1,\ B_{2n}=2(-1)^{n+1}\frac{(2n)!}{(2\pi)^{2n}}\sum_{m=1}^\infty m^{-2n},\ n=1,2,,\ldots. \tag{1.15}$$

Hence $a_n>0$ for all $n\in\mathbf{N}$ and $a_n\sim(2n)!$ as $n\to\infty$. Then we can state the main result of this article:

Theorem 1.3: *The perturbation expansion (1.13) is Borel summable in the distributional sense to* $\frac{1}{2}\{S(\alpha)+\overline{S}(\alpha)\}=\mathrm{Re}\,S(\alpha)$ *for any* $0\leqslant\alpha<+\infty$. *More precisely* $S(\alpha)$ *and* $\overline{S}(\overline{\alpha})$ *are the upper and lower sum of* $\Sigma_{n=0}^\infty a_n\alpha^n$ *for* $\mathrm{Re}\,\alpha>0$, *respectively*.

(1) The effective action $S(\alpha)$ is complex-valued, while the perturbation expansion is real. As already remarked (and will become evident in the course of the proof) the distributional Borel sum uniquely determines also the imaginary part $\mathrm{Im}\,S(\alpha)=-(i/2)\,d(\alpha)$, which has zero power series expansion in α. This is a point of some importance because the imaginary part is proportional to the pair creation rate.

(2) The numerical resummation procedure recently introduced by Ref. 18, which also yields the imaginary part, admits a rigorous justification within the present method if the convergence (in measure) can be proved of the Padé approximants for the distributional Borel transform.

II. PROOF OF THE DISTRIBUTIONAL SUMMABILITY

Consider the effective action (1.12). First of all notice that for $0<\arg\alpha<\pi$ we can rotate the integration path in (1.12) and choose the half-line $\Gamma:=\{s\in\mathbf{C}: s=-it, 0\leqslant t<+\infty\}$, i.e., the negative imaginary axis. Now $\coth(ix)=-i\cot(x), \forall\, x\in A:=\{x\in\mathbf{C}: x\neq k\pi\,; \forall\, k\in\mathbf{Z}\}$. Hence,

$$S(\alpha)=\frac{1}{8\pi^2}\int_0^\infty \frac{e^{-t}}{t^3}\left\{2\sqrt{\pi\alpha}t\cot(2\sqrt{\pi\alpha}t)-1+\frac{4\pi\alpha t^2}{3}\right\}\mathrm{d}t. \tag{2.1}$$

The proof of Theorem 1.3 is based on the fundamental criterion for distributional Borel summability (see Ref. 13, Theorem 1). Let us report here the part relevant to our purpose.

Theorem 2.1: *Let $\Sigma_{n-0}^{\infty}a_n z^n$ be a formal power series and $B(t)=\Sigma_{n-0}^{\infty}(a_n/n!)\,t^n$ its Borel transform. Assume the following.*

(1) $B(t)$ is convergent for $|t|<\rho$ for some $\rho>0$.
(2) $B(t)$ admits an analytic continuation to the region $\Omega_\rho:=\{t\in\mathbf{C}:\mathrm{Im}\,t>0;\mathrm{Re}\,t>-\rho\}$.
(3) There are $A>0$, $R>0$ such that

$$|B(t+i\eta_0)|\leqslant A\eta_0^{-1}\exp[t/R],\quad \forall\, t>0,\quad \forall\,\eta_0\in\,]0,\rho[. \tag{2.2}$$

Then the boundary value distributions $B(t+i0)$ and $PP(B(t))=\frac{1}{2}\{B(t+i0)+\overline{B(t+i0)}\}$ exist for all $t\geqslant 0$ and the integral

$$\frac{1}{z}\int_0^\infty PP(B(t))e^{-t/z}\,\mathrm{d}t \tag{2.3}$$

defines a real-analytic function $f(z)$ in C_R. Moreover,

$$\Phi(z):=\frac{1}{z}\int_0^\infty B(t+i0)e^{-t/z}\,\mathrm{d}t \tag{2.4}$$

is analytic in C_R and fulfills the estimates

$$\left|\Phi(z)-\sum_{n=0}^{N-1}a_n z^n\right|\leqslant C_0 c(\epsilon)^N N!|z|^N,\quad N=1,2,\ldots, \tag{2.5}$$

uniformly in $C_{R,\epsilon}:=\{z\in C_R:\arg z\geqslant -\pi/2+\epsilon\}$.

Remarks:

(1) $f(z)$ is the distributional Borel sum, and $\Phi(z)$ the upper sum of $\Sigma_{n-0}^{\infty}a_n z^n$. They are both uniquely determined by conditions 1 and 2, together with the imaginary part $[\Phi(z)-\overline{\Phi(\overline{z})}]/2i$.
(2) The estimate (2.2) makes the distribution $B(t)$ locally of order 1. However, it is not *a priori* tempered because it might grow faster than any polynomial at infinity.

Let us now proceed to apply this theorem to our case.

Lemma 2.2: For any α such that $0<\arg\alpha<\pi$ set $\beta=\sqrt{\alpha}$ and

$$\Phi(\beta):=S(\beta^2)=\frac{1}{8\pi^2}\int_0^\infty\frac{e^{-t}}{t^3}\left[2\sqrt{\pi}\beta t\cot(2\sqrt{\pi}\beta t)-1+\frac{4\pi\beta^2t^2}{3}\right]\mathrm{d}t. \tag{2.6}$$

Then $\Phi(\beta)$ is analytic for $0<\arg\beta<\pi/2$ and admits the following formal expansion in powers of β:

$$\Phi(\beta)\sim\frac{1}{8\pi^2}\sum_{n=2}^{\infty}(-16\pi)^n B_{2n}\frac{(2n-3)!}{(2n)!}\beta^{2n}=\sum_{n=2}^{\infty}a_n\beta^{2n}, \tag{2.7}$$

where $\{B_{2n}\}$ *is the sequence of the Bernoulli numbers defined by (1.15).*

Proof: Equation (2.7) corresponds to (1.13) with $\alpha=\beta^2$. Let us work it out for the sake of completeness. First recall that

$$x\cot x=\sum_{n=0}^{\infty}(-1)^n\frac{2^{2n}}{(2n)!}B_{2n}x^{2n},\quad |x|<\pi, \tag{2.8}$$

where $B_0=1$ and B_{2n} is given by the expression (1.15) (see, e.g., Ref. 17). Then

$$2\sqrt{\pi}\beta t\cot(2\sqrt{\pi}\beta t)=\sum_{n=0}^{\infty}(-1)^n\frac{2^{2n}}{(2n)!}B_{2n}2^{2n}\pi^n\beta^{2n}t^{2n}. \tag{2.9}$$

Since $B_0=1$ and $B_2=\frac{1}{6}$ we have

$$2\sqrt{\pi}\beta t\cot(2\sqrt{\pi}\beta t)-1+\frac{4}{3}\pi\beta^2t^2=\sum_{n=2}^{\infty}(-1)^n\frac{(16\pi)^n}{(2n!)}B_{2n}\beta^{2n}t^{2n}. \tag{2.10}$$

Hence

$$\begin{aligned}\Phi(\beta)&=\frac{1}{8\pi^2}\int_0^{\infty}e^{-t}\sum_{n=2}^{\infty}(-1)^n\frac{(16\pi)^n}{(2n!)}B_{2n}\beta^{2n}t^{2n-3}\,\mathrm{d}t\\&=\frac{1}{8\pi^2}\sum_{n=2}^{\infty}(-1)^n\frac{(16\pi)^n}{(2n!)}B_{2n}\beta^{2n}\int_0^{\infty}e^{-t}t^{2n-3}\,\mathrm{d}t\\&=\frac{1}{8\pi^2}\sum_{n=2}^{\infty}(-1)^n\frac{(16\pi)^n(2n-3)!}{(2n!)}B_{2n}\beta^{2n},\end{aligned}$$

and this concludes the proof of the lemma.

Lemma 2.3: Let $D:=\{t\in\mathbf{C}: t\neq k\sqrt{\pi}/2, \forall\, k\in\mathbf{Z}\}$, *and set*

$$B(t):=\frac{2\sqrt{\pi}t\cot(2\sqrt{\pi}t)-1+4\pi t^2/3}{8\pi^2t^3},\quad \forall\, t\in D. \tag{2.11}$$

Then $B(t)$ *is clearly analytic in* D *with simple poles at* $t=k\sqrt{\pi}/2$, $k\in\mathbf{Z}$. *Moreover,*

$$B(t)=\sum_{n=2}^{\infty}\frac{a_n}{(2n-3)!}t^{2n-3},\quad \forall\, t:|t|<\frac{\sqrt{\pi}}{2}, \tag{2.12}$$

i.e., B(t) is the Borel transform of $\Sigma_{n=2}^{\infty}a_n\beta^{2n-3}$.

Proof: To obtain (2.12) we proceed as in the previous lemma using (2.8). More precisely,

$$B(t)=\frac{1}{8\pi^2}\sum_{n=2}^{\infty}(-1)^n\frac{2^{2n}}{(2n!)}B_{2n}2^{2n}\pi^nt^{2n-3}=\sum_{n=2}^{\infty}\frac{a_n}{(2n-3)!}t^{2n-3},\quad |t|<\sqrt{\pi}/2.$$

Proposition 2.4: Let $\Sigma_{n=2}^{\infty}a_n\beta^{2n-3}$ *be the formal power series whose coefficients* a_n *are defined by (1.13) and (1.14) [see also (2.7)], and let B(t) be its Borel transform (2.11) with the expansion (2.12). Then B(t) satisfies the hypotheses of Theorem 2.1.*

Proof: By Lemma 2.3 Conditions 1 and 2 of Theorem 2.1 are satisfied with $\rho=\sqrt{\pi}/2$. As far as Condition 3 is concerned, we will prove it in the following stronger version: for any $R>0$ there is $A>0$ such that

$$|B(t+i\eta_0)|\leqslant A\,\eta_0^{-1}\exp(t/R),\quad \forall\, t>0,\quad \forall\,\eta_0\in\,]0,\sqrt{\pi}/2[. \tag{2.13}$$

To this end first let $0<\delta<\sqrt{\pi}/2$ be fixed. Then the function $B(t+i\eta_0)$ is continuous on the compact set $K:=\{z=t+i\eta_0\in\mathbf{C}:|t|\leqslant\delta;0\leqslant\eta_0\leqslant\sqrt{\pi}/2\}$. Hence $B(t+i\eta_0)$ is bounded in K by some constant $c>0$ and we can write

$$|B(t+i\eta_0)|\leqslant c\leqslant c\,\frac{\sqrt{\pi}}{2}\,\eta_0^{-1}\exp(t/R),$$

where the second inequality holds because $(\sqrt{\pi}/2)\,\eta_0^{-1}\geqslant 1$ and obviously we can choose R as large as we like. Hence it suffices to prove (2.13) for $t>\delta$ and $\eta_0\in\,]0,\sqrt{\pi}/2[$. Now for $t>\delta$ the term $1/6\pi|t+i\eta_0|$, which comes from the third summand in (2.11) where we have replaced t by $t+i\eta_0$, can be estimated as follows:

$$\frac{1}{6\pi|t+i\eta_0|}=\frac{1}{6\pi\sqrt{t^2+\eta_0^2}}\leqslant\frac{1}{6\pi\delta}$$

for $t>\delta$. Thus, this term trivially fulfills (2.13) with R as large as we like. Therefore we can restrict our attention to the term

$$B_1(t+i\eta_0):=2\sqrt{\pi}(t+i\eta_0)\cot\{2\sqrt{\pi}(t+i\eta_0)\}-1 \tag{2.14}$$

because the denominator $1/8\pi^2|t+i\eta_0|^3$ is bounded by $(1/8\pi^2)\,\delta^{-3}$ for $t>\delta$. Consider now the well known expansion (see, e.g., Ref. 17)

$$x\cot x=1+2x^2\sum_{n=1}^{\infty}\frac{1}{x^2-n^2\pi^2}. \tag{2.15}$$

Then, for any $R>0$, we have to find $A>0$ such that

$$|B_1(t+i\eta_0)|=4\pi|t+i\eta_0|^2\left|\sum_{n=1}^{\infty}\frac{1}{4\pi(t+i\eta_0)^2-n^2\pi^2}\right|\leqslant A\,\eta_0^{-1}\exp(t/R) \tag{2.16}$$

$\forall\, t>\delta,\ \eta_0\in\,]0,\sqrt{\pi}/2[$. First remark that

$$4\pi|t+i\eta_0|^2=4\pi(t^2+\eta_0^2)\leqslant 4\pi(t^2+1)\leqslant C_1\exp(t/R)$$

for a suitable constant $C_1>$ and $R>0$ arbitrarily large. Moreover, one has

$$\left|\sum_{n=1}^{\infty}\frac{1}{4(t+i\eta_0)^2/\pi-n^2}\right|\leqslant\sum_{n=1}^{\infty}\frac{1}{\sqrt{\{n^2-4(t^2-\eta_0^2)/\pi\}^2+64\eta_0^2t^2/\pi^2}}. \tag{2.17}$$

If $t\leqslant\eta_0$, the right hand side of Eq. (2.17) can be bounded by $\Sigma_{n=0}^{\infty}1/n^2=\pi^2/6$. Thus (2.16) holds for $R>0$ arbitrarily large by suitably choosing $A>0$. We are thus left with the case $t>\eta_0$, $t>\delta$, $\eta_0\in\,]0,\sqrt{\pi}/2[$. In this case, setting $Q(t,\eta_0):=[2\sqrt{t^2-\eta_0^2}]/\sqrt{\pi}]+1$ ($[x]=$greatest integer $\leqslant x$, $x\in\mathbf{R}$) we can estimate the rhs of (2.17) as follows:

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt{\{n^2-4(t^2-\eta_0^2)/\pi\}^2+64\eta_0^2t^2/\pi^2}}$$
$$\leqslant \sum_{n=1}^{Q(t,\eta_0)} \frac{1}{\sqrt{\{n^2-4(t^2-\eta_0^2)/\pi\}^2+64\eta_0^2t^2/\pi^2}}$$
$$+ \sum_{n=Q(t,\eta_0)+1}^{\infty} \frac{1}{\sqrt{\{n^2-4(t^2-\eta_0^2)/\pi\}^2+64\eta_0^2t^2/\pi^2}}$$
$$\leqslant \sum_{n=1}^{Q(t,\eta_0)} \frac{\pi}{8t\eta_0} + \sum_{n=Q(t,\eta_0)+1}^{\infty} \frac{1}{n^2-4(t^2-\eta_0^2)/\pi}. \tag{2.18}$$

The last inequality is a consequence of the positivity of $n^2-4(t^2-\eta_0^2)/\pi$ for $n\geqslant Q(t,\eta_0)+1$. Now the first summand in (2.18) can be bounded by

$$\frac{\pi}{8t\eta_0}\left(\frac{2}{\sqrt{\pi}}\sqrt{t^2-\eta_0^2}+1\right)\leqslant \frac{\sqrt{\pi}}{4}\eta_0^{-1}+\frac{\pi}{8t\eta_0} \tag{2.19}$$

and clearly satisfies (2.13) recalling that $t>\delta$. Concerning the second term in (2.18) we have

$$\sum_{Q(t,\eta_0)+1}^{\infty} \frac{1}{n^2-4(t^2-\eta_0^2)/\pi}\leqslant \int_{Q(t,\eta_0)+1}^{\infty}\frac{dx}{x^2-4(t^2-\eta_0^2)/\pi}+\frac{1}{(Q(t,\eta_0)+1)^2-4(t^2-\eta_0^2)/\pi}, \tag{2.20}$$

where the inequality follows by the well known comparison theorem between series with positive terms and generalized integrals. Since $[x]\leqslant x\ \forall\, x\geqslant 0$, recalling the definition of $Q(t,\eta_0)$, we can write

$$\sum_{Q(t,\eta_0)+1}^{\infty} \frac{1}{n^2-4(t^2-\eta_0^2)/\pi}\leqslant \int_{(2/\sqrt{\pi})\sqrt{t^2-\eta_0^2}+2}^{\infty}\frac{dx}{x^2-4(t^2-\eta_0^2)/\pi}+\frac{1}{3} \tag{2.21}$$

because $[x]^2=[x^2]$ and $[x]+1-x>0$, $\forall\, x>0$. Since the additive factor $\frac{1}{3}$ can be trivially absorbed in the constants, it is enough to estimate the integral in (2.21). One has

$$\int_{(2/\sqrt{\pi})\sqrt{t^2-\eta_0^2}+2}^{\infty}\frac{dx}{x^2-4(t^2-\eta_0^2)/\pi}=\frac{1}{4}\sqrt{\frac{\pi}{t^2-\eta_0^2}}\ln\left(1+\frac{2}{\sqrt{\pi}}\sqrt{t^2-\eta_0^2}\right).$$

Given $R>0$ arbitrarily large the existence of a constant $A>0$ such that

$$\frac{1}{4}\sqrt{\frac{\pi}{t^2-\eta_0^2}}\ln\left(1+\frac{2}{\sqrt{\pi}}\sqrt{t^2-\eta_0^2}\right)\leqslant A\,\eta_0^{-1}e^{t/R}$$

$\forall\, t>\delta$, $t>\eta_0$, $\forall\ \eta_0\in\,]0,\sqrt{\pi}/2[$ is now obvious. This concludes the proof of the proposition.

Corollary 2.5: In the notation of Lemmas 2.2 and 2.3 and Proposition 2.4 the boundary value distributions $B(t+i0)$ and $PP(B(t))$ exist for all $t\geqslant 0$. Moreover, the integral

$$\frac{1}{\beta}\int_0^{\infty} B(t+i0)e^{-t/\beta}\,dt \tag{2.22}$$

defines an analytic function on $D_1:=\{\beta\in\mathbf{C}:\mathrm{Re}\,\beta>0\}$, coinciding with $F(\beta):=\beta^{-3}\Phi(\beta)$ $\forall\ \beta:0<\arg\beta<\pi/2$. Equivalently, $\Sigma_{n=0}^{\infty}a_n\beta^{2n-3}$ is Borel summable in the distributional sense; its upper sum is $\beta^{-3}\Phi(\beta)$ while the distributional sum is

$$f(\beta) := \frac{1}{\beta}\int_0^\infty PP(B(t))e^{-t/\beta}\,dt \tag{2.23}$$

$\forall\ \beta \in D_1$; *moreover*,

$$f(\beta) = \tfrac{1}{2}\{\beta^{-3}\Phi(\beta) + (\overline{\beta})^{-3}\overline{\Phi}(\overline{\beta})\},\quad \beta \notin \mathbf{R}_+ . \tag{2.24}$$

Proof: The first assertion follows from Theorem 2.1 in view of Proposition 2.4, which also guarantees the existence of (2.22) in $C_R = \{\beta \in \mathbf{C}: \mathrm{Re}\,\beta^{-1} > R^{-1}\}\ \forall\ R > 0$. By the same results it suffices now to show that (2.22) coincides with $\beta^{-3}\Phi(\beta)$ for $0 < \arg\beta < \pi/2$. Indeed we have

$$\begin{aligned}\frac{1}{\beta}\int_0^\infty B(t+i0)e^{-t/\beta}\,dt &= \frac{1}{\beta}\lim_{\epsilon\to 0_+}\int_0^\infty B(t+i\epsilon)e^{-t/\beta}\,dt \\ &= \frac{1}{8\pi^2\beta}\lim_{\epsilon\to 0_+}\int_0^\infty e^{-t/\beta}(t+i\epsilon)^{-3} \\ &\quad\times\left\{2\sqrt{\pi}(t+i\epsilon)\cot(2\sqrt{\pi}(t+i\epsilon)) - 1 + \frac{4}{3}\pi(t+i\epsilon)^2\right\}dt.\end{aligned}$$

Now, performing the change of variables $t = s\beta$, $s \in \Gamma_1 := \{s: s = t/\beta, 0 \leqslant t < \infty\}$ we obtain

$$\begin{aligned}\frac{1}{\beta}\int_0^\infty B(t+i0)e^{-t/\beta}\,dt &= \frac{1}{8\pi^2\beta^3}\int_{\Gamma_1} s^{-3}e^{-s}\left\{(2\sqrt{\pi}\beta s)\cot(2\sqrt{\pi}\beta s) - 1 + \frac{4}{3}\pi\beta^2 s^2\right\}ds \\ &= \frac{1}{8\pi^2\beta^3}\int_0^\infty t^{-3}e^{-t}\left\{(2\sqrt{\pi}\beta t)\cot(2\sqrt{\pi}\beta t) - 1 + \frac{4}{3}\pi\beta^2 t^2\right\}dt,\end{aligned} \tag{2.25}$$

where the last equality follows from the analyticity of the integrand (in the variable s) in a sector containing $\mathbf{R}_+$, if $\beta \notin \mathbf{R}_+$. Now by (2.6) the integral (2.25) is precisely $\beta^{-3}\Phi(\beta)$, and this concludes the proof of the Corollary.

Remark: Notice that in the representations (2.23 and 2.24) we had to exclude $\beta \in \mathbf{R}$ because by (2.6) $\Phi(\beta)$ is not defined for $\beta \in \mathbf{R}$.

Now, multiplying by β^3 the functions $F(\beta) = \beta^{-3}\Phi(\beta)$ and $f(\beta)$ as well as the formal series $\Sigma_{n=2}^\infty a_n\beta^{2n-3}$ we immediately conclude the following.

Corollary 2.6: The formal power series $\Sigma_{n=2}^\infty a_n\beta^{2n}$ is Borel summable in the distributional sense $\forall\ \beta$:$\mathrm{Re}\,\beta > 0$. *Its upper sum is $\Phi(\beta)$, $\forall\ \beta \notin \mathbf{R}_+$, and its distributional sum is $\beta^3 f(\beta)$. For $\beta \notin \mathbf{R}_+$ one has $\beta^3 f(\beta) = \frac{1}{2}\{\Phi(\beta) + \overline{\Phi}(\overline{\beta})\}$.*

Proof of Theorem 1.3: From Corollary 2.6 we obtain

$$\Phi(\beta) = \beta^2\int_0^\infty B(t+i0)e^{-t/\beta}\,dt,\quad \forall\ \beta: 0 < \arg\beta < \frac{\pi}{2}, \tag{2.26}$$

where the rhs is the upper sum of $\Sigma_{n=2}^\infty a_n\beta^{2n}$, $\forall\ \beta: -\pi/2 < \arg\beta < \pi/2$. Now, setting $\beta = \sqrt{\alpha}$ and using (2.1) to represent $S(\alpha)$, we have

$$S(\alpha) = \sqrt{\alpha}\int_0^\infty B(t+i0)e^{-t/\sqrt{\alpha}}\,dt \tag{2.27}$$

and

$$\overline{S}(\overline{\alpha})=\sqrt{\alpha}\int_0^\infty \overline{B(t+i0)}e^{-t/\sqrt{\alpha}}\,dt$$

$\forall\ \alpha: 0<\arg\alpha<\pi$ [notice that (2.1) actually defines S as a holomorphic function of α for $0<\arg\alpha<\pi$]. On the other hand, the original representation (1.12) for $S(\alpha)$, namely

$$S(\alpha)=-\frac{1}{8\pi^2}\int_0^\infty \frac{e^{-is}}{s^3}\left\{(2\sqrt{\pi\alpha}s)\coth(2\sqrt{\pi\alpha}s)-1-\frac{4\pi\alpha s^2}{3}\right\}ds,$$

defines S as a holomorphic function of α for $-\pi<\arg\alpha<\pi$. Thus, it represents an analytic continuation of the lhs of (2.27) across the positive real axis because $S(\alpha)$ as represented by (2.27) and (2.1) coincide for $0<\arg\alpha<\pi$. Since the rhs of (2.27) is also an analytic function of α for $-\pi<\arg\alpha<\pi$ we can write

$$\begin{aligned}S(\alpha)&=-\frac{1}{8\pi^2}\int_0^\infty \frac{e^{-is}}{s^3}\left\{(2\sqrt{\pi\alpha}s)\coth(2\sqrt{\pi\alpha}s)-1-\frac{4\pi\alpha s^2}{3}\right\}ds\\&=\sqrt{\alpha}\int_0^\infty B(t+i0)e^{-t/\sqrt{\alpha}}\,dt,\quad \forall\ \alpha: -\pi<\arg\alpha<\pi.\end{aligned}\tag{2.28}$$

Thus $S(\alpha)$ is the upper sum of $\Sigma_{n=2}^\infty a_n\alpha^n$ and the distributional Borel sum is given by

$$\frac{1}{2}\{S(\alpha)+\overline{S}(\overline{\alpha})\}=\sqrt{\alpha}\int_0^\infty PP(B(t))e^{-t/\sqrt{\alpha}}\,dt,\quad \forall\ \alpha: -\pi<\arg\alpha<\pi.\tag{2.29}$$

In particular, the distributional Borel sum is $\mathrm{Re}\,S(\alpha)$ for $\alpha>0$. This concludes the proof of Theorem 1.3.

Remarks:

(1) It follows by the above theorem that the distributional Borel summability uniquely determines also

$$\mathrm{Im}\,S(\alpha)=\frac{1}{2i}[S(\alpha)-\overline{S}(\alpha)],\ \ \alpha\in\mathbf{R}_+.$$

Moreover, $\mathrm{Im}\,S(\alpha)$ is proportional to the pair-production rate. Its explicit expression is[5]

$$\mathrm{Im}\,S(\alpha)=\frac{1}{8\pi^3}\sum_{n=1}^\infty \frac{1}{n^2}\exp\left(-\frac{n\pi}{\alpha}\right)$$

and has zero asymptotic expansion in α.

(2) Strictly speaking, the representations (2.28) and (2.29) yield the distributional Borel–Leroy sum of order 2 (see Ref. 13, Theorem 3) of the divergent perturbation expansion (1.13). That definition is completely equivalent[13] to ordinary summability in the variable $\beta=\sqrt{\alpha}$. We have preferred to proceed in this last way for convenience of exposition.

ACKNOWLEDGMENT

This work was partially supported by Università di Bologna funds for selected research topics.

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Modular localization of massive particles with "any" spin in $d=2+1$[a)]

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(Received 30 August 2002; accepted 23 January 2003)

We discuss a concept of particle localization which is motivated from quantum field theory, and has been proposed by Brunetti, Guido and Longo and by Schroer. It endows the single-particle Hilbert space with a family of real subspaces indexed by the space–time regions, with certain specific properties reflecting the principles of locality and covariance. We show by construction that such a localization structure exists also in the case of massive anyons in $d=2+1$, i.e., for particles with positive mass and with arbitrary spin $s\in\mathbb{R}$. The construction is completely intrinsic to the corresponding ray representation of the (proper orthochronous) Poincaré group. Our result is of particular interest since there are no free fields for anyons, which would fix a localization structure in a straightforward way. We present explicit formulas for the real subspaces, expected to turn out useful for the construction of a quantum field theory for anyons. In accord with well-known results, only localization in string-like, instead of point-like or bounded, regions is achieved. We also prove a single-particle PCT theorem, exhibiting a PCT operator which acts geometrically correctly on the family of real subspaces. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1561592]

I. INTRODUCTION

Following Wigner,[1] the state space of an elementary relativistic particle corresponds to an irreducible ray representation of the Poincaré group. In three as well as in four dimensional space–time, the physically relevant representations—and hence the conceivable particle types—are classified by the mass m and the spin s which labels a representation of the covering of the rotation subgroup (if $m>0$). In three-dimensional space–time the latter is isomorphic to the group of reals, hence the spin may take *any* real value—in contrast to the four-dimensional situation where it is quantized, $s\in\frac{1}{2}\mathbb{N}_0$. Thus, in three-dimensional space–time there are more particle types; the exotic ones with non-half-integer spin are called *anyons*.

By modular localization of particles we mean a concept which has been advocated in recent years by Brunetti, Guido and Longo[2] and by Schroer:[3,4] Suppose there is a quantum field for the particle type at hand, and consider the single-particle states which are, together with a polarization cloud, created from the vacuum in a given space–time region. Thus the single-particle space gets equipped with a family of subspaces indexed by the space–time regions, with certain specific properties reflecting the localization properties of the underlying quantum field; cf. Definition 2.1 below. This will be a sufficient motivation for us to call a family of subspaces of the single-particle space with such properties a *localization structure* for the particle type at hand.

The question arises as to whether such a structure can be constructed for any given particle type (m,s) intrinsically within the single-particle theory—that is to say, without referring to a quantum field, but using as input only the corresponding ray representation of the Poincaré group. This has been achieved for spin zero and positive mass by Ramacher,[5] and for all positive energy

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representations of the Poincaré group by Brunetti, Guido and Longo.[2] The latter analysis includes reducible representations, but restricts to proper (not ray) representations, i.e., only the case of bosons and not the case of fermions or anyons is covered.

In the present article, this construction is performed for the case of massive anyons in $d=3$. The purpose of this construction is twofold: First, it shows that a localization structure indeed exists for all $m>0, s\in\mathbb{R}$. This is of particular interest because there are no free relativistic fields for anyons,[10] which would of course allow for a straightforward construction of the localization structure. (We mean fields creating finitely many copies of the irreducible representation from the vacuum. Grigore has constructed free fields in $d=2+1$ for any spin,[6] but in contradiction to the generalized spin statistics connection holding in algebraic quantum field theory[7–9] they have bosonic statistics. Presumably, this is due to the fields having infinitely many components.) Even worse, none of the hitherto proposed models of relativistic quantum fields for anyons in (continuous) three-dimensional space–time[11–17] has been worked out to the extent that the localization structure could be readily constructed from them. Second, our analysis is intended to be a step in the construction of a model which resembles as closely as possible a free field for anyons, in the sense of a ''second quantization functor'' from the single particle theories to field algebras. To this end it is gratifying that we have found explicit formulas for the real subspaces of localized states.

The article is organized as follows. In Sec. II, we make precise our definition of a localization structure for anyons; cf. Definition 2.1. In Sec. III, we construct a localization structure for any given particle type $m>0, s\in\mathbb{R}$, intrinsically within the corresponding Wigner space. The result is summarized in the main Theorem 3.2, which also contains a PCT theorem. All relevant properties can be shown, via modular theory along the lines of,[2] without reference to the specific irreducible representation (m,s)—except for the the so-called standard property, which guarantees that the constructed structure is nontrivial. This is the content of Sec. IV, where we explicitly exhibit sufficiently many ''localized states'' (Proposition 4.2). These are represented as families of functions which transform covariantly under the Poincaré group (Corollary 4.3). In Sec. V, we finally prove that the Bisognano–Wichmann property essentially fixes the localization structure and also implies a single-particle version of the spin-statistics connection.

II. DEFINITION OF A LOCALIZATION STRUCTURE FOR ANYONS

Let $\mathcal{H}$ be a Hilbert space describing anyons of the type (m,s). We define a localization structure as a family of subspaces of $\mathcal{H}$ with certain specific properties reflecting the localization properties of a hypothetical underlying quantum field.

Let us first describe the index set for this family. Each subspace is labeled by a space–time region belonging to a specific class $\mathcal{C}$, together with some additional information, which is needed to endow the index set with a partial order relation and with a nontrivial action of the 2π-rotation. In accord with the well-known result[7,8] that anyons cannot be localized in point-like, but only in string-like regions, each localization region $C\in\mathcal{C}$ must extend to infinity in some space-like direction e, $e^2=-1$. More specifically, we say that a space–time region C *contains a space-like direction* e if

$$C+e\subset C\,. \tag{1}$$

We take $\mathcal{C}$ to be the set of convex, causally complete regions which contain some space-like direction in this sense. (A region C is called causally complete if it contains all points x such that every inextendible causal curve through x passes through C.) Typical examples of regions in $\mathcal{C}$ are space-like cones and *wedge* regions, i.e., Poincaré transforms of the standard wedge,

$$W_1\doteq\{\,x\in\mathbb{R}^3\colon |x^0|<x^1\ \}\,. \tag{2}$$

Wedges are the largest regions in the class $\mathcal{C}$, in the sense that every $C\in\mathcal{C}$ is contained in some wedge.[2]

The additional information indicated above, which has to be specified along with each localization region $C\in\mathcal{C}$, is a path in the set of space-like directions. We denote the latter by

$$H\doteq\{e\in\mathbb{R}^3:e^2=-1\}\,, \tag{3}$$

and consider paths in H starting at a reference direction e_0, which we fix, once and for all, to be

$$e_0\doteq(0,0,-1)\,. \tag{4}$$

Given a region $C\in\mathcal{C}$, we shall say that a path $\tilde{e}$ *ends in* C if its endpoint is contained in C in the sense of Eq. (1). Two paths $\tilde{e}_1$ and $\tilde{e}_2$ starting at e_0 and ending in C will be called *equivalent w.r.t.* C iff the path $\tilde{e}_1^{-1}*\tilde{e}_2$ (the inverse of $\tilde{e}_1$ followed by $\tilde{e}_2$) is fixed-endpoint homotopic to a path which is contained in C. Now the index set for our localization structure, denoted by $\tilde{\mathcal{C}}$, is the set of pairs

$$(C,\tilde{e})\,, \tag{5}$$

where $C\in\mathcal{C}$ and $\tilde{e}$ is the equivalence class w.r.t. C of a path in H starting at e_0 and ending in C. For fixed $C\in\mathcal{C}$, we shall use the notation $\tilde{C}$ for an element of the form $(C,\tilde{e})$. To see what is involved, suppose C is a space-like cone or a wedge. Then the set of directions contained in C is a connected and simply connected subset of H (denoted C_H in Fig. 1), and different elements $(C,\tilde{e}_1)$ and $(C,\tilde{e}_3)$ differ just by a winding number; cf. Fig. 1. Consider now two such pairs $\tilde{C}_1\doteq(C_1,\tilde{e}_1)$ and $\tilde{C}_2\doteq(C_2,\tilde{e}_2)$. If $C_1\subset C_2$ and the corresponding paths $\tilde{e}_1$, $\tilde{e}_2$ are equivalent w.r.t. C_2, then we shall write

$$\tilde{C}_1\subset\tilde{C}_2\,. \tag{6}$$

If C_1 and C_2 are causally separated, then $\tilde{C}_1$ and $\tilde{C}_2$ determine a *relative winding number*,

$$N(\tilde{C}_1,\tilde{C}_2)\doteq\text{winding number of}\quad\tilde{e}_2^{-1}*\tilde{e}_1*\tilde{e}_{12}\,, \tag{7}$$

where $\tilde{e}_{12}$ is the "direct" path from e_1 to e_2 in clockwise direction. Finally, we note that the universal covering $\tilde{P}_+^\uparrow$ of the Poincaré group naturally acts on $\tilde{\mathcal{C}}$ as explained in Appendix B, cf. Eq. (B21), such that a 2π-rotation acts nontrivial—it maps, for example, $(C,\tilde{e}_3)$ in Fig. 1 onto $(C,\tilde{e}_1)$.

We now turn to the definition of a localization structure. We admit the case of several particle species of the same type (m,s), for example, a particle and its anti-particle.

Definition 2.1: Let U be a finite direct sum of copies of the irreducible representation of $\tilde{P}_+^\uparrow$ for mass $m>0$ and spin $s\in\mathbb{R}$, acting in a Hilbert space $\mathcal{H}$. A family of closed real subspaces $K(\tilde{C})$, $\tilde{C}\in\tilde{\mathcal{C}}$, of $\mathcal{H}$ is called a localization structure *for (m,s) if it has the following properties:*

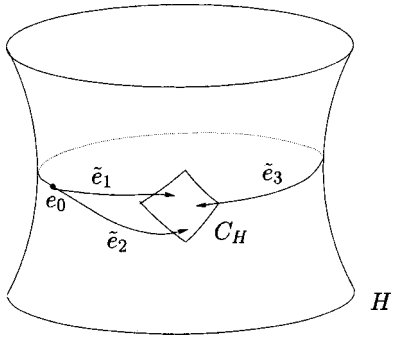

FIG. 1. $(C_1\tilde{e}_1)=(C_2\tilde{e}_2)\neq(C_3\tilde{e}_3)$.

(1) Isotony: *Let* $\tilde{C}_1 \subset \tilde{C}_2$ *in the sense of Eq. (6). Then*

$$K(\tilde{C}_1) \subset K(\tilde{C}_2) \ .$$

(2) Twisted locality: *There is a complex number* Z *of modulus one, such that for any pair* $\tilde{C}_1, \tilde{C}_2 \in \tilde{\mathcal{C}}$ *with* C_1 *causally separated from* C_2,

$$Z(\tilde{C}_1, \tilde{C}_2)\, K(\tilde{C}_2) \subset K(\tilde{C}_1)' \ . \tag{8}$$

Here, $Z(\tilde{C}_1, \tilde{C}_2) \doteq Z^{2N+1}$, *with* $N = N(\tilde{C}_1, \tilde{C}_2)$, *cf. (7), and the prime denotes the symplectic complement*. (The relevant notions referring to real subspaces of a Hilbert space are recalled in Appendix A.)

(3) Poincaré covariance: *For all* $\tilde{C} \in \tilde{\mathcal{C}}$ *and* $\tilde{g} \in \tilde{P}_+^{\uparrow}$,

$$U(\tilde{g})\, K(\tilde{C}) = K(\tilde{g} \cdot \tilde{C}) \ .$$

(4) Standardness: $K(\tilde{C})$ *is standard for all* $\tilde{C} \in \tilde{\mathcal{C}}$.

Remark: (*i*) Covariance implies that $K(\tilde{r}(2\pi) \cdot \tilde{C}) = e^{2\pi i s} K(\tilde{C})$, where $\tilde{r}(\cdot)$ denotes rotation. Therefore $K(\tilde{r}(2\pi) \cdot \tilde{C})$ coincides with $K(\tilde{C})$ if, and only if, $s \in \frac{1}{2}\mathbb{Z}$. Hence $K(\tilde{C})$ is independent of the path $\tilde{e}$, but only depends on C, iff $s \in \frac{1}{2}\mathbb{Z}$. Further, it can be shown using the free field formalism (or along the same lines as in the present analysis; cf. the remark after Proposition C.2), that in this case the localization structure can be extended to bounded regions.

(*ii*) In the framework of algebraic quantum field theory, a field algebra for anyons[18] is a family of operator algebras $\{\mathcal{F}(\tilde{C})\}_{\tilde{C} \in \tilde{\mathcal{C}}}$, indexed by the same class $\tilde{\mathcal{C}}$ (except that in general, each C must contain some space-like cone[19]). Suppose there are finitely many particle species of the type (m,s) and that $\{m\}$ is isolated from the rest of the spectrum, and denote by $E^{m,s}$ the projection onto the corresponding single-particle space. Then

$$K(\tilde{C}) \doteq E^{m,s} \mathcal{F}(\tilde{C})^{\mathrm{sa}}\, \Omega^{-} \quad (\text{norm closure}) , \tag{9}$$

$\tilde{C} \in \tilde{\mathcal{C}}$, is a localization structure. This is in fact the motivation for our definition. As an illustration, we show that twisted locality (8) holds in the case of bosons or fermions. In these cases field operators φ_1 and φ_2 localized in causally separated regions commute or anti-commute, respectively. These relations have been shown in Ref. 9, Sec. 2 to survive the projection $E^{m,s}$ in the sense that

$$(\, \varphi_1 \Omega, E^{m,s} \varphi_2 \Omega \,) = \pm (\, \varphi_2^* \Omega, E^{m,s} \varphi_1^* \Omega \,) , \tag{10}$$

respectively. Hence, putting $Z \doteq 1$ for bosons and $Z \doteq i$ for fermions, the imaginary part of $(\, Z\varphi_1 \Omega, E^{m,s} \varphi_2 \Omega \,)$ is zero if φ_1 and φ_2 are self-adjoint. This is twisted locality. In the general case of anyons, analogous considerations hold, with Z being defined as a root of the statistics phase.

We finally recall the definition of a certain maximality property called twisted Haag duality. Let $\tilde{C} = (C, \tilde{e})$ and $\tilde{C}' = (C', \tilde{e}')$, where C' is the causal complement of C and $\tilde{e}'$ is the equivalence class of a path ending in C' in the same sense as in Eq. (1). If C is not a wedge, then the region C' is not contained in any wedge region. In this case we define a real subspace corresponding to $\tilde{C}'$ via

$$K(\tilde{C}') \doteq \bigvee_{\tilde{C}_0 \subset \tilde{C}', \tilde{C}_0 \in \tilde{\mathcal{C}}} K(\tilde{C}_0) \, . \tag{11}$$

Definition 2.2: A localization structure is said to satisfy twisted Haag duality *if for every pair* $\tilde{C}, \tilde{C}'$ *as above the identity*

$$Z(\tilde{C},\tilde{C}')\,K(\tilde{C}')=K(\tilde{C})' \tag{12}$$

holds.

III. CONSTRUCTION OF THE LOCALIZATION STRUCTURE

Let U be a finite direct sum of copies of the irreducible representation of $\tilde{P}_+^\uparrow$ for mass $m>0$ and spin $s\in\mathbb{R}$. We now construct a corresponding localization structure along the same lines as in Ref. 2.

We start with the definition of the localization space associated with the standard wedge W_1; cf. Eq. (2). Associated with this wedge are the Lorentz boosts $\lambda_1(t)$ leaving W_1 invariant and acting on the coordinates x^0,x^1 as

$$\begin{pmatrix}\cosh(t) & \sinh(t)\\ \sinh(t) & \cosh(t)\end{pmatrix}, \tag{13}$$

and the reflection j about the edge of W_1,

$$j\colon (x^0,x^1,x^2)\mapsto(-x^0,-x^1,x^2)\,. \tag{14}$$

We define Δ to be the unique positive operator satisfying

$$\Delta^{it}=U(\tilde{\lambda}_1(-2\pi t))\quad,\quad t\in\mathbb{R}\,, \tag{15}$$

where $\tilde{\lambda}_1(\cdot)$ denotes the lift of $\lambda_1(\cdot)$ to the covering group $\tilde{P}_+^\uparrow$. We further pick an anti-unitary involution J satisfying

$$JU(\tilde{g})J=U(\tilde{j}\tilde{g}\tilde{j})\,,\quad \tilde{g}\in\tilde{P}_+^\uparrow\,, \tag{16}$$

where $\tilde{j}\cdot\tilde{j}$ denotes the lift of the adjoint action of j to the covering group $\tilde{P}_+^\uparrow$ [See (B17)]. Lemma B.3 asserts that such an involution exists. We mention as an aside, that the localization structure which we now construct is independent of the particular choice; cf. Proposition 5.2. We then define a closed operator S by

$$S\doteq J\,\Delta^{1/2}\,. \tag{17}$$

This operator is densely defined, antilinear and involutive due to the group relation $\tilde{j}\tilde{\lambda}_1(t)\tilde{j}=\tilde{\lambda}_1(t)$; cf. Ref. 2. Hence, the eigenspace of S for the eigenvalue 1 is a standard real subspace; cf. Appendix A. We take this subspace as our localization space for

$$\tilde{W}_1\doteq(W_1,\tilde{e}_{W_1})\,, \tag{18}$$

where $\tilde{e}_{W_1}$ is the equivalence class of a path starting from e_0 and staying within W_1 [in the sense of (1)]; in other words, we put

$$K(\tilde{W}_1)\doteq\{\phi\in\mathrm{dom}\ S\colon\ S\phi=\phi\}\,. \tag{19}$$

The motivation for this definition will become clear after Definition 5.1. Covariance forces us to define the real subspaces corresponding to arbitrary wedges $\tilde{W}=\tilde{g}\cdot\tilde{W}_1$ by

$$K(\tilde{g}\cdot\tilde{W}_1)\doteq U(\tilde{g})\,K(\tilde{W}_1),\quad \text{for } \tilde{g}\in\tilde{P}_+^\uparrow\,. \tag{20}$$

The following lemma asserts that this is well-defined.

Lemma 3.1: Let $\tilde{g}\in\tilde{P}_+^\uparrow$ satisfy $\tilde{g}\cdot\tilde{W}_1=\tilde{W}_1$. Then $U(\tilde{g})\,K(\tilde{W}_1)=K(\tilde{W}_1)$.

Proof: The set of Poincaré transformations $\tilde{g} \in \tilde{P}_+^\uparrow$ which map $\tilde{W}_1$ onto itself is the Abelian group generated by the one-parameter subgroups of the translations along the 2-axes and of the 1-boosts $\tilde{\lambda}_1(t)$. Both of these subgroups commute with $\tilde{j}$ and with the 1-boosts, hence their representers commute with S, which implies the claim. □

Next we associate real closed subspaces $K(\tilde{C})$ to arbitrary regions $\tilde{C} \in \tilde{\mathcal{C}}$ by intersections:

$$K(\tilde{C}) \doteq \bigcap_{\tilde{W} \supset \tilde{C}} K(\tilde{W}), \tag{21}$$

where the intersection goes over all wedge regions which contain $\tilde{C}$ in the sense of (6). If C is a wedge, this is consistent with (20) as a consequence of the positivity of the energy.[2] Note that if C is not a wedge, then (21) is the maximal subspace one can associate with C in view of locality.

We now state our main result.

Theorem 3.2: *The family* $\{K(\tilde{C})\}_{\tilde{C} \in \tilde{\mathcal{C}}}$ *constructed above is a localization structure for* (m,s), *cf. Definition* 2.1, *with* $Z = e^{i\pi s}$. *It also satisfies twisted Haag duality; cf. Eq. (12). Further, the anti-unitary involution* $U(\tilde{j})$ *defined by* $U(\tilde{j}) \doteq Z^{-1}J$ *is a PCT operator, that is, a representer of* $\tilde{j}$ *in the sense of Eq. (16), which acts geometrically correctly on the localization structure*:

$$U(\tilde{j})\, K(\tilde{C}) = K(\tilde{j} \cdot \tilde{C}), \quad \tilde{C} \in \tilde{\mathcal{C}}. \tag{22}$$

[The action of $\tilde{j}$ on $\tilde{C} \in \tilde{\mathcal{C}}$, denoted $\tilde{j} \cdot \tilde{C}$, is explained in Appendix B, cf. (B22).] It is noteworthy that the "spin-statistics connection" $Z^2 = e^{2\pi i s}$ necessarily holds as a consequence of the definition (19), as we show in Proposition 5.3.

Proof: Isotony and Poincaré covariance, i.e. properties (1) and (3) of Definition 2.1, follow immediately by construction. We next prove Eq. (22). From the group relations $\tilde{\lambda}_1(t)\tilde{j} = \tilde{j}\tilde{\lambda}_1(t)$, $\tilde{\lambda}_1(t)\tilde{r}(\pi) = \tilde{r}(\pi)\tilde{\lambda}_1(-t)$ and $\tilde{r}(\pi)\tilde{j} = \tilde{j}\tilde{r}(-\pi)$, and the fact that $Z^2 = e^{2i\pi s} = U(\tilde{r}(2\pi))$, it follows that the operator $U(\tilde{r}(\pi))U(\tilde{j})$ commutes with S. But this implies that

$$U(\tilde{j})\, K(\tilde{W}_1) = U(\tilde{r}(-\pi))\, K(\tilde{W}_1) = K(\tilde{j} \cdot \tilde{W}_1), \tag{23}$$

where we have used that $\tilde{j} \cdot \tilde{W}_1 = \tilde{r}(-\pi) \cdot \tilde{W}_1$. Hence, Eq. (22) holds for $\tilde{C} = \tilde{W}_1$. By covariance, it holds for all wedge regions, and by the intersection property (21) it holds for all $\tilde{C} \in \tilde{\mathcal{C}}$.

We next prove twisted Haag duality (12). Equation (23) implies that $JK(\tilde{W}_1) = ZK(\tilde{j} \cdot \tilde{W}_1)$. Now according to a general result about Tomita operators, see, e.g., Ref. 20, Prop. 2.3, the anti-unitary part J in the polar decomposition of S maps $K(\tilde{W}_1)$ onto its symplectic complement:

$$JK(\tilde{W}_1) = K(\tilde{W}_1)'. \tag{24}$$

Further, $Z = Z(\tilde{W}_1, \tilde{j} \cdot \tilde{W}_1)$ since the relative winding number $N(\tilde{W}_1, \tilde{j} \cdot \tilde{W}_1)$ is zero. We therefore have

$$Z(\tilde{W}_1, \tilde{j} \cdot \tilde{W}_1)\, K(\tilde{j} \cdot \tilde{W}_1) = K(\tilde{W}_1)'. \tag{25}$$

Now any $\tilde{W}_1' = (W_1', \tilde{e})$ differs from $\tilde{j} \cdot \tilde{W}_1$ by a rotation about a multiple of 2π. Replacing $\tilde{j} \cdot \tilde{W}_1$ by such $\tilde{W}_1'$, the above equation is still valid because $Z(\tilde{W}_1, \tilde{r}(2\pi N) \cdot \tilde{j} \cdot \tilde{W}_1)$ picks up a factor $e^{-2\pi i s N}$ which is compensated by the factor picked up by $K(\tilde{r}(2\pi N) \cdot \tilde{j} \cdot \tilde{W}_1)$. By covariance and the fact that $Z(\tilde{g} \cdot \tilde{C}_1, \tilde{g} \cdot \tilde{C}_2)$ is independent of $\tilde{g} \in \tilde{P}_+^\uparrow$, we get twisted Haag duality for wedge regions, i.e., for every pair $\tilde{W}, \tilde{W}'$ the identity

$$Z(\tilde{W}, \tilde{W}')\, K(\tilde{W}') = K(\tilde{W})', \tag{26}$$

holds. For smaller regions we use a chain of equalities similar to the proof of Corollary 3.4 of Ref. 2. Let $\tilde{C}$ and $\tilde{C}'$ be as in Definition 2.2. Then

$$Z(\tilde{C},\tilde{C}')\,K(\tilde{C}')=Z(\tilde{C},\tilde{C}')\bigvee_{\tilde{C}_0\subset\tilde{C}'}K(\tilde{C}_0)=Z(\tilde{C},\tilde{C}')\bigvee_{\tilde{W}'\subset\tilde{C}'}K(\tilde{W}')=\bigvee_{\tilde{W}'\subset\tilde{C}'}Z(\tilde{C},\tilde{W}')K(\tilde{W}')$$

$$=\bigvee_{\tilde{W}\supset\tilde{C}}K(\tilde{W})'=\left(\bigcap_{\tilde{W}\supset\tilde{C}}K(\tilde{W})\right)'=K(\tilde{C})'\,. \tag{27}$$

In the second equation we have used the fact that for any pair of causally separated regions $C,C_0\in\mathcal{C}$ there is a wedge W such that $C_0\subset W'\subset C'$, cf. Ref. 2; and also that

$$K(\tilde{W}_1)=\bigvee_{\tilde{C}\subset\tilde{W}_1}K(\tilde{C})\,. \tag{28}$$

This fact is asserted by Takesaki's theorem because the r.h.s. is a standard space contained in $K(\tilde{W}_1)$ and is, by Eq. (15) and covariance, invariant under the modular group of $K(\tilde{W}_1)$. The fourth equation follows from Eq. (26). We have also used the fact that $Z(\tilde{C}_1,\tilde{C}_2)$ is insensitive to making the regions C_1, C_2 smaller. We have thus proved twisted Haag duality, which obviously implies twisted locality, so we have shown property (2) of Definition 2.1.

It remains to prove property (4) of Definition 2.1, namely that $K(\tilde{C})$ is standard for each $\tilde{C}$. The real subspace associated to $\tilde{W}_1$ (and hence to any other wedge region $\tilde{W}$) has this property by construction; cf. Eq. (19) and Appendix A. The property that $K(\tilde{W})\cap iK(\tilde{W})=\{0\}$ transfers to the smaller spaces $K(\tilde{C})$. It remains to show that $K(\tilde{C})+iK(\tilde{C})$ is dense for all $\tilde{C}$. But this follows from Corollary 4.3 in the next section, bearing in mind the following consequence of the Reeh–Schlieder theorem for the free scalar massive field: Consider the set of Schwartz functions with compact support contained in a fixed open space–time region. The restrictions to the mass shell of the Fourier transforms of these functions are dense in the space of square-integrable functions on the mass shell. □

IV. STANDARDNESS OF THE REAL SUBSPACES

To prove that $K(\tilde{C})+iK(\tilde{C})$ is dense, we will explicitly exhibit sufficiently many elements in $K(\tilde{C})$. This will be the only place in our analysis where we make explicit use of the representation U of $\tilde{P}_+^\uparrow$. It suffices to consider U to be irreducible. For if U is reducible, we may take the involution J, cf. Eq. (16), as a direct sum of suitable involutions. We then obviously end up with a localization structure which is the direct sum of irreducible localization structures.

We recall the relevant irreducible representations, starting with some notational remarks. Let $L_+^\uparrow$ be the Lorentz group in $d=2+1$ and $\tilde{L}_+^\uparrow$ its universal covering group. (The relevant facts concerning $\tilde{L}_+^\uparrow$ and the covering $\tilde{L}_+^\uparrow\to L_+^\uparrow$ are recalled in Appendix B.) We denote elements of $\tilde{L}_+^\uparrow$ generically by $\tilde{\lambda}$, and the covering homomorphism $\tilde{L}_+^\uparrow\to L_+^\uparrow$ by

$$\tilde{\lambda}\mapsto\lambda\,. \tag{29}$$

The group $\tilde{P}_+^\uparrow$ is the semidirect product of $\tilde{L}_+^\uparrow$ with the translation group $\mathbb{R}^3$. Thus, elements of $\tilde{P}_+^\uparrow$ will be denoted by $\tilde{g}=(a,\tilde{\lambda})$, and the group multiplication is given by

$$(a,\tilde{\lambda})(a',\tilde{\lambda}')=(a+\lambda a',\tilde{\lambda}\tilde{\lambda}')\,. \tag{30}$$

We occasionally denote $(0,\tilde{\Lambda})$ simply by $\tilde{\Lambda}$. The irreducible representation of $\tilde{P}_+^\uparrow$ for $m>0$ and $s\in\mathbb{R}$, denoted by U in the sequel, is given as follows. Let H_m denote the positive mass shell $\{p\cdot p=m^2, p_0>0\}$ and $d\mu$ the Lorentz invariant measure on H_m. Then U acts on $\mathcal{H}\doteq L^2(H_m,d\mu)$ according to

$$(U(a,\tilde{\Lambda})\phi)(p)=e^{is\Omega(\tilde{\Lambda},p)}\,e^{ia\cdot p}\,\phi(\Lambda^{-1}p)\,, \tag{31}$$

where $\Omega(\tilde{\Lambda},p)\in\mathbb{R}$ is the Wigner rotation; cf. Eq. (76). To this representation a unique, up to a phase factor, anti-unitary involution J can be adjoined satisfying Eq. (16), thus extending U to $\tilde{P}_+$ within the same Hilbert space:

$$(J\phi)(p)\doteq e^{i\pi s}\,\overline{\phi(-jp)}\,; \tag{32}$$

cf. Lemma B.3. Let $\{K(\tilde{C})\}_{\tilde{C}\in\tilde{\mathcal{C}}}$ be the resulting localization structure as in Theorem 3.2.

We now calculate elements in $K(\tilde{C})$ for given $\tilde{C}\in\tilde{\mathcal{C}}$. By construction, $\phi\in K(\tilde{C})$ if and only if for all $\tilde{g}\in\tilde{P}_+^\uparrow$ which map $\tilde{C}$ into $\tilde{W}_1$, the vector $U(\tilde{g})\phi$ is in $K(\tilde{W}_1)$. [$\tilde{W}_1$ has been defined in Eq. (18).] In particular, it must be in the domain of $\Delta^{1/2}$. As is well-known,[21] this implies that the map

$$t\mapsto U(\tilde{\Lambda}_1(t))\,U(\tilde{g})\,\phi\quad,\quad t\in\mathbb{R}, \tag{33}$$

is the boundary value of an analytic $\mathcal{H}$-valued function on the strip $\mathbb{R}+i\,(0,\pi)$. But a complication arises from the Wigner rotation factor. Namely, the function $t\mapsto\exp(is\Omega(\tilde{\Lambda}_1(t)\tilde{\Lambda},p))$ has singularities in the strip for any fixed $p\in H_m$ and $\tilde{\Lambda}\in\tilde{L}_+^\uparrow$ in a neighborhood of the unit, which are branch points if s is not an integer (see Lemma C.1). Our strategy is to consider wave functions of the form $\phi=u\cdot\psi$ (point-wise multiplication), where u is a fixed nonvanishing function on the mass shell, suitably chosen as to compensate the singularities of the Wigner rotation factor. The action of $U(\tilde{g})$, according to Eq. (31), on wave functions of the form $(u\cdot\psi)(p)\doteq u(p)\psi(p)$ can be written as

$$(U(a,\tilde{\Lambda})\,u\cdot\psi)(p)=u(p)\,c(\tilde{\Lambda},p)\quad e^{ia\cdot p}\quad\psi(\Lambda^{-1}p)\,, \tag{34}$$

with

$$c(\tilde{\Lambda},p)\doteq u(p)^{-1}\quad e^{is\Omega(\tilde{\Lambda},p)}\quad u(\tilde{\Lambda}^{-1}p)\,. \tag{35}$$

In group theoretical terms, the map $c(\cdot,\cdot):\tilde{L}_+^\uparrow\times H_m\to\mathbb{C}\backslash\{0\}$ is a cocycle which is equivalent to the Wigner rotation factor. As indicated above, our strategy is to choose u such that $c(\tilde{\Lambda},p)$ has the desired analyticity properties. This will succeed only for certain $\tilde{\Lambda}\in\tilde{L}_+^\uparrow$ or, stated differently, for a certain $\tilde{C}\in\tilde{\mathcal{C}}$. We shall consider, as a first step, $\tilde{C}$ of the form $(C,\tilde{e}_0)$, with C containing the reference direction e_0, cf. Eq. (4), and where $\tilde{e}_0$ denotes the constant path at e_0. Stated differently, we consider elements $\tilde{\Lambda}\in\tilde{L}_+^\uparrow$ which satisfy

$$\tilde{\Lambda}\cdot\tilde{e}_0\in\tilde{W}_1\,. \tag{36}$$

By this we mean that W_1 contains the direction $\Lambda\cdot e_0$ in the sense of Eq. (1), and that the paths $\tilde{\Lambda}\cdot\tilde{e}_0$ and $\tilde{e}_{W_1}$, cf. Eq. (18), are equivalent w.r.t. W_1. The following function is suitable for this purpose, and in the sequel the cocycle c will be defined as in Eq. (35) above with this choice of u:

$$u(p)\doteq\left(\frac{p_0-p_1}{m}\cdot\frac{p_0-p_1+m-ip_2}{p_0-p_1+m+ip_2}\right)^s\quad,\quad p_0\doteq(p_1^2+p_2^2+m^2)^{1/2}\,. \tag{37}$$

Note that p_0-p_1 is strictly positive for all $p\in H_m$, hence the argument in brackets lies in the cut complex plane $\mathbb{C}\backslash\mathbb{R}_0^-$. Thus, taking it to the power of $s\in\mathbb{R}$ can be defined via the branch of the logarithm on $\mathbb{C}\backslash\mathbb{R}_0^-$ with $\ln 1=0$. This will always be understood in the sequel and will be called the power of s *within* $\mathbb{C}\backslash\mathbb{R}_0^-$.

Lemma 4.1: Let $\tilde{\Lambda}$ be an element of $\tilde{L}_+^\uparrow$ such that $\tilde{\Lambda}\cdot\tilde{e}_0\in\tilde{W}_1$ in the sense of equation (36). Then for all $p\in H_m$ the function

$$t\mapsto c(\tilde{\Lambda}_1(t)\tilde{\Lambda},p)$$

has an analytic extension into the strip $\mathbb{R}+i(0,\pi)$. This extension satisfies the boundary condition

$$c(\tilde{\Lambda}_1(t+i\pi)\tilde{\Lambda},p)=e^{i\pi s}\overline{c(\tilde{\Lambda}_1(t)\tilde{\Lambda},-jp)},\quad t\in\mathbb{R}. \tag{38}$$

Proof: As we show in Lemma B.1, $\tilde{\Lambda}$ can be decomposed into boosts and rotations as $\tilde{\Lambda}=\tilde{\Lambda}_1(t)\ \tilde{\Lambda}_2(t')\ \tilde{r}(\omega)$ for some unique $t,t',\omega\in\mathbb{R}$. We then denote $\omega'\doteq\omega-\pi/2$. Then $\tilde{\Lambda}\cdot\tilde{e}_0\in\tilde{W}_1$ if and only if

$$\Lambda_2(t')\,r(\omega')\,(0,1,0)\in W_1^-\quad\text{and}\quad\omega'\in(-\pi,\pi), \tag{39}$$

the latter condition singling out the correct leaf of the covering $\tilde{r}(\omega')\mapsto r(\omega')$. As the vector in Eq. (39) is equal to

$$(\sinh t'\sin\omega',\cos\omega',\cosh t'\sin\omega'),$$

condition (39) is equivalent to

$$|\sinh t'\sin\omega'|\leqslant\cos\omega'\quad\text{and}\quad\omega'\in\left[-\frac{\pi}{2},\frac{\pi}{2}\right]. \tag{40}$$

This implies condition (C8) of Proposition C.2 in Appendix C, which now asserts the claimed analyticity property and the correct boundary value of the cocycle. □

We denote by $C_0^\infty(\mathbb{R}^3)$ the C^∞-functions on $\mathbb{R}^3$ with compact support, and, for $f\in C_0^\infty(\mathbb{R}^3)$, by E_mf the restriction of the Fourier transform of f to the mass shell H_m. Our main result is the following proposition.

Proposition 4.2: Let C be a region in $\mathcal{C}$ containing the reference direction e_0 in the sense of Eq. (1), and let $\tilde{C}=(C,\tilde{e}_0)$. Then

$$K(\tilde{C})\ \supset\ \{u\cdot E_mf\ \mid\ f\in C_0^\infty(C),\ \textit{real valued}\}.$$

Before proving the proposition, we point out that the local subspaces for regions containing directions other than e_0 are obtained via covariance, and can be nicely characterized as follows. Define, for each $\tilde{\Lambda}\in\tilde{L}_+^\uparrow$, a function $u_{\tilde{\Lambda}}$ on the mass shell by

$$u_{\tilde{\Lambda}}(p)\doteq u(p)\,c(\tilde{\Lambda},p). \tag{41}$$

This is an ''intertwiner function'' for those single-particle vectors which are localized in regions extending to infinity in the direction $\tilde{\Lambda}\cdot\tilde{e}_0$.

Corollary 4.3: (i) Let $\tilde{\Lambda}\in\tilde{L}_+^\uparrow$ and $\tilde{C}\in\tilde{\mathcal{C}}$. If $\tilde{C}$ contains $\tilde{\Lambda}\cdot\tilde{e}_0$ in the sense of Eq. (36), then

$$K(\tilde{C})\ \supset\ \{u_{\tilde{\Lambda}}\cdot E_mf\ \mid\ f\in C_0^\infty(C),\ \textit{real valued}\}.$$

(ii) The wave functions $u_{\tilde{\Lambda}}\cdot E_mf$ transform covariantly in the sense that

$$U(a,\tilde{\lambda})\, u_{\tilde{\lambda}'}\cdot E_m f = u_{\tilde{\lambda}\tilde{\lambda}'}\cdot E_m(a,\lambda)_* f\,, \tag{42}$$

where the star denotes the push-forward, $(g_* f)(x) \doteq f(g^{-1}x)$.

Proof: (i) is an immediate consequence of Proposition 4.2, and (ii) follows from the cocycle relation (C10) below. □

It is noteworthy that the function $u_{\tilde{\lambda}}$ only depends on the path $\tilde{\lambda}\cdot\tilde{e}_0$ up to a multiplicative constant. For the stabilizer subgroup of $\tilde{e}_0$, namely the group of 1-boosts, modifies $u_{\tilde{\lambda}}$ only by a factor $c(\tilde{\lambda}_1(t),p) = e^{st}$.

Proof of Proposition 4.2: Let f be a smooth function with compact support in C, and let $\tilde{g} = (a,\tilde{\lambda})$ be such that $\tilde{g}\tilde{C} \subset \tilde{W}_1$. Note that then $\tilde{\lambda}\tilde{e}_0 \in \tilde{W}_1$ and $\mathrm{supp}\, g_* f \subset W_1$, where $g_* f$ denotes the push-forward as above. We have to show that $U(\tilde{g})\, u\cdot E_m f \in K(\tilde{W}_1)$. To this end we prove that the $\mathcal{H}$-valued function

$$t \mapsto \phi(t) \doteq U(\tilde{\lambda}_1(t)) U(\tilde{g})\, u\cdot E_m f\,, \quad t\in\mathbb{R}, \tag{43}$$

is the boundary value of an analytic function $\phi(\cdot)$ on the strip $G \doteq \mathbb{R} + i\,(0,\pi)$ which is continuous and bounded on its closure G^- and that the boundary values are related by

$$\phi(t+i\pi) = J\,\phi(t)\,, \quad t\in\mathbb{R}\,. \tag{44}$$

Using the push-forward to write $e^{ia\cdot p}(E_m f)(\lambda^{-1}p) = (E_m(a,\lambda)_* f)(p)$, we have

$$\phi(t) = U(\tilde{\lambda}_1(t)a, \tilde{\lambda}_1(t)\tilde{\lambda})\, u\cdot E_m f = v(t)\cdot\psi(t), \tag{45}$$

where we have written

$$v(t)(p) \doteq u(p)\, c(\tilde{\lambda}_1(t)\tilde{\lambda}, p)\,, \tag{46}$$

$$\psi(t)(p) \doteq (E_m \lambda_1(t)_* g_* f)(p)\,. \tag{47}$$

It follows from Lemma 4.1 that for fixed $p\in H_m$, $v(\cdot)(p)$ extends to an analytic function $v(\cdot,p)$ on the strip G, continuous on its closure, and that

$$v(t+i\pi,p) = e^{i\pi s} u(p)\, \overline{c(\tilde{\lambda}_1(t)\tilde{\lambda}, -jp)}\,. \tag{48}$$

Let us discuss the analyticity properties of $\psi(t)$. The matrix-valued function $t\mapsto\lambda_1(t)$ extends to an entire analytic function satisfying

$$\lambda_1(t+it') = \lambda_1(t)(j_{t'} + i\sin(t')\,\sigma)\,, \tag{49}$$

where $j_{t'}$ acts as multiplication by $\cos t'$ on the coordinates x^0 and x^1 and leaves the other coordinates unchanged, and σ acts as the Pauli matrix σ_1 on (x^0,x^1) and as zero on x^2.[22] Hence $\psi(\cdot)(p)$ extends, for fixed $p\in H_m$, to a function $\psi(\cdot,p)$ on G^- as follows:

$$\psi(t+it',p) \doteq (2\pi)^{-3/2} \int_{W_1} \mathrm{d}^3x\;\; e^{i\,p\cdot\lambda_1(t) j_{t'} x}\, e^{-\sin t'\; p\cdot\lambda_1(t)\sigma x}\;\; (g_* f)(x)\,. \tag{50}$$

Now for $x\in W_1$, the vector σx lies in the forward light cone, hence $p\cdot\lambda_1(t)\sigma x > 0$ for $p\in H_m$. Thus the second exponential term in Eq. (50) is a damping factor, and for fixed $\tau\in G^-$ the function $(p_1,p_2)\mapsto\psi(\tau,p)$ is of fast decrease. Further, due to the damping factor the function $\tau\mapsto\psi(\tau,p)$ is analytic on the strip G for fixed $p\in H_m$. Thus our function $t\mapsto\phi(t) = v(t)\psi(t)$ extends, point-wise in p, to a function $\phi(\tau,p) \doteq v(\tau,p)\psi(\tau,p)$ on G^-, analytic on the interior, and in addition $\phi(\tau,\cdot)\in L^2(H_m, d\mu)$ for each $\tau\in G^-$. By Eqs. (48) and (49) the analytic continuation satisfies, since $j_\pi = j$,

$$\phi(t+i\pi,p)=e^{i\pi s}u(p)\,\overline{c(\tilde{\lambda}_1(t)\tilde{\lambda},-jp)}\,(E_m j_* g_* f)(p)\,. \tag{51}$$

On the other hand, using $u(-jp)=\overline{u(p)}$, one calculates

$$(J\,\phi(t))(p)=e^{i\pi s}u(p)\,\overline{c(\tilde{\lambda}_1(t)\tilde{\lambda},-jp)}\,(E_m j_* g_* \overline{f})(p)\,. \tag{52}$$

Thus for real valued f, the Hilbert space valued function $\tau\mapsto\phi(\tau)$ defined by $\phi(\tau)\times(p)\doteq\phi(\tau,p)$ satisfies the desired equation (44). It remains to show that $\phi(\tau)$ is in fact analytic as a Hilbert space-valued function.

To this end let, for $x\in W_1$, $t_x\doteq\operatorname{arctanh}(x_0/x_1)$. Then $\sigma x=|\sigma x|\,\lambda_1(t_x)(1,0,0)$ and

$$p\cdot\lambda_1(t)\sigma x=|\sigma x|\,\{\cosh(t+t_x)p_0-\sinh(t+t_x)p_1\}\,. \tag{53}$$

Note that the argument in curly brackets is strictly larger than $|p_2|$ and than $|p_1|\times\exp(-|t+t_x|)$. Let $t+it'$ be contained in some compact subset $G_0\subset G$ of the strip. Then

$$|t|\leqslant T \quad \text{and}\ \sin t'\geqslant\varepsilon \quad \text{for some } T>0,\ \ \varepsilon>0\ . \tag{54}$$

Then the above estimates imply, using that $\exp(-|t_x|)=((x_1+|x_0|)/(x_1-|x_0|))^{1/2}$, that

$$\sin t'\ p\cdot\lambda_1(t)\sigma x>\alpha_1(x)|p_1|+\alpha_2(x)|p_2|, \tag{55}$$

where

$$\alpha_1(x)\doteq\frac{\varepsilon}{2}e^{-T}(x_1-|x_0|)>0\,, \tag{56}$$

$$\alpha_2(x)\doteq\frac{\varepsilon}{2}(x_1^2-x_0^2)^{1/2}>0\,. \tag{57}$$

This estimate implies that

$$\Psi(p_1,p_2)\doteq\int_{W_1}d^3x\,|g_* f(x)|\,e^{-\alpha_1(x)|p_1|-\alpha_2(x)|p_2|} \tag{58}$$

is a dominating function for $\psi(\tau,\cdot)$ for all τ in the compact subset G_0 of the strip, in the sense that $|\psi(\tau,p)|<\Psi(p_1,p_2)$ for all $\tau\in G_0$. This function is decreasing fast enough such that

$$\int d^2p\,|p_1|^n|p_2|^m\,|\Psi(p_1,p_2)|^2\ <\infty, \qquad \text{for all}\ \ n,m\in\mathbb{N}_0\,. \tag{59}$$

Namely, the integral coincides with $4n!m!$ times the integral of $|g_* f(x)g_* f(y)|\ (\alpha_1(x)+\alpha_1(y))^{-n-1}\ (\alpha_2(x)+\alpha_2(y))^{-m-1}$ over x and y in W_1, which is finite since α_1,α_2 are strictly positive functions on W_1 and $\operatorname{supp}(g_* f)$ is compactly contained in W_1. By similar considerations one gets a dominating function for $(\mathrm{d}/\mathrm{d}\tau)\,\psi(\tau,p)$, which we denote by Ψ' and which satisfies the analog of Eq. (59).

Next, we establish bounds for $v(\tau,p)$: We claim that $v(\tau,p)$ and $(\mathrm{d}/\mathrm{d}\tau)\,v(\tau,p)$ are bounded, uniformly in $\tau\in G_0$, by polynomials in $|p_1|$ and $|p_2|$ which we denote by V and V', respectively. We demonstrate here the case of non-negative spin s, the other case working analogously. One has the inequality $0<p_0\pm p_1\leqslant 2|p_1|+|p_2|+m$ and, using the identity $(-p_2+im)/(p_0-p_1)=i\,(p_0+p_1+m+ip_2)/(p_0-p_1+m-ip_2)$, the inequality $|(-p_2+im)(p_0-p_1)^{-1}|\leqslant 2(|p_1|+|p_2|+m)/m$. These imply, for $\tau\in G_0$, the estimate

$$v(\tau,p)\leqslant c_0(2|p_1|+|p_2|+m)^n(c_1+c_2(|p_1|+|p_2|+m))^{2n}\doteq V(|p_1|,|p_2|)\,,$$

where n is any integer $\geqslant s$, $c_1=|a-b|$ and $c_2=(2/m)\,e^{T-t}|a+b|$ with a and b as in Proposition C.2. Similar considerations hold for $s<0$, and for $(\mathrm{d}/\mathrm{d}\tau)\,v(\tau,p)$.

We have now established the following facts: $\phi(t)$ extends to a family $\phi(\tau)\in L^2(H_m,d\mu)$, $\tau\in G^-$, such that $\phi(\tau)(p)$ depends analytically on τ for each $p\in H_m$. Further, for τ in any fixed compact subset of the strip G, the p-point-wise derivative w.r.t. τ is dominated by a function $\Phi\in L^2(H_m,d\mu)$:

$$\left|\frac{\mathrm{d}}{\mathrm{d}\tau}\phi(\tau)(p)\right|\leqslant\Phi(p)\doteq V(\mathbf{p})\Psi'(\mathbf{p})+V'(\mathbf{p})\Psi(\mathbf{p}),\quad p=(\omega(\mathbf{p}),\mathbf{p}). \tag{60}$$

That Φ is in $L^2(H_m,d\mu)$ follows from Eq. (59) and the corresponding equation for Ψ'.

These facts imply, by the Lebesgue lemma on dominated convergence, that for arbitrary $\chi\in L^2(H_m,d\mu)$, the function

$$\tau\mapsto(\chi,\phi(\tau))$$

is analytic on the strip G, with a derivative being calculated via the p-point-wise derivative $(\mathrm{d}/\mathrm{d}\tau\,\phi(\tau)(p)$. Since weak and strong analyticity are equivalent, this implies that $\tau\mapsto\phi(\tau)$ is an analytic Hilbert space-valued function. This concludes the proof. □

V. IMPLICATIONS OF THE BISOGNANO–WICHMANN PROPERTY

In this section we show that the Bisognano–Wichmann property, defined below, essentially fixes the localization structure, and that it implies the spin-statistics connection as mentioned after Theorem 3.2.

Given a localization structure $K(\tilde{C})$, $\tilde{C}\in\tilde{\mathcal{C}}$, denote by S the canonical involution corresponding to $K(\tilde{W}_1)$, cf. Appendix A. Since S is a closed antilinear involution, it has a polar decomposition $S=:J\Delta^{1/2}$ with J being an anti-unitary involution and Δ a positive operator.

Definition 5.1: A localization structure satisfies the Bisognano–Wichmann property *if Δ^{it} and J satisfy Eqs. (15) and (16), thus representing the boosts and the reflection $\tilde{j}$, respectively.*

It is noteworthy that this property in fact *follows* from Definition 2.1 of a localization structure. This has been established by the author in Ref. 23 in the case of four-dimensional theories, and will be published elsewhere for anyons in $d=3$. Because of this fact we have been forced to take Eqs. (15) to (19) as the starting point of our construction.

We shall now see that the Bisognano–Wichmann property fixes uniquely a certain extension of the localization structure which is maximal in the sense that it satisfies twisted Haag duality, cf. (12).

Proposition 5.2: There is up to equivalence only one localization structure which satisfies the Bisognano–Wichmann property and twisted Haag duality.

By equivalent localization structure we mean a family $\hat{K}(\tilde{C})$, $\tilde{C}\in\tilde{\mathcal{C}}$, of closed real subspaces of a Hilbert space $\hat{\mathcal{H}}$ such that there is a unitary map $V:\mathcal{H}\to\hat{\mathcal{H}}$ satisfying $\hat{K}(\tilde{C})=V\,K(\tilde{C})$ for all $\tilde{C}\in\tilde{\mathcal{C}}$.

Proof: Let $K(\tilde{C})$, $\tilde{C}\in\tilde{\mathcal{C}}$, be a localization structure as in the proposition. With the same argument as in the proof of Theorem 3.2, Eq. (28) must hold for $K(\tilde{W}_1)$. Hence, the chain of equations (27) is valid, the last equation of which shows that, under the assumption of twisted Haag duality, $K(\tilde{C})$ is maximal in the sense that it satisfies Eq. (21). But this implies that the localization structure is fixed by the real subspaces associated to wedge regions, which in turn are fixed, due to the Bisognano–Wichmann property and covariance, by the real subspace $K(\tilde{W}_1)$ associated to $\tilde{W}_1$ and the representation U. Hence the localization structure is fixed by $K(\tilde{W}_1)$ or, equivalently, by the corresponding involution S. The positive part of the latter is fixed by the representation U; cf. Eq. (15), hence the only remaining freedom is the anti-unitary part J. But it turns out that J, and hence the entire localization structure, is fixed up to equivalence. More

precisely, let $\hat{K}(\tilde{C})$, $\tilde{C}\in\tilde{\mathcal{C}}$, be another localization structure as in the proposition, with $\hat{J}$ the anti-unitary part of the canonical involution corresponding to $\hat{K}(\tilde{W}_1)$. Then, as we show in Lemma B.3, there is a unitary V commuting with the representation U such that $\hat{J}=VJV^{-1}$. This implies that $\hat{K}(\tilde{C})=VK(\tilde{C})$ for all $C\in\tilde{\mathcal{C}}$, as claimed. □

We finally prove a single-particle version of the spin-statistics theorem.

Proposition 5.3: Let $\{K(\tilde{C})\}_{\tilde{C}\in\tilde{\mathcal{C}}}$ *be a localization structure for* (m,s) *satisfying the Bisognano–Wichmann property. Then the spin-statistics connection holds:*

$$Z^2=e^{2\pi is}. \tag{61}$$

Proof: We use the one-to-one correspondence between closed real standard subspaces K and densely defined anti-linear involutive operators S; cf. Appendix A. Let S' be the canonical involution corresponding to $K(\tilde{r}(\pi)\tilde{W}_1)$. Twisted locality (8) implies that

$$Z(\tilde{W}_1,\tilde{r}(\pi)\tilde{W}_1)\,S'\,Z(\tilde{W}_1,\tilde{r}(\pi)\tilde{W}_1)^*\subset S^*.$$

Now the relative winding number $N(\tilde{W}_1,\tilde{r}(\pi)\tilde{W}_1)$ is -1, hence

$$Z(\tilde{W}_1,\tilde{r}(\pi)\tilde{W}_1)=Z^{-1},$$

and we have $S'\subset Z^2\,S^*$. On the other hand,

$$S'=U(\tilde{r}(\pi))\,S\,U(\tilde{r}(-\pi)),$$

by covariance. But the group relations imply[2] that $S\;U(\tilde{r}(-\pi))=U(\tilde{r}(\pi))\;S^*$, hence $Z^2=U(\tilde{r}(2\pi))\equiv e^{2\pi is}$, which proves the claim. □

ACKNOWLEDGMENTS

I thank B. Schroer, H.-W. Wiesbrock, D. Guido, and R. Longo for stimulating discussions and D. Buchholz for valuable hints concerning the manuscript. Further, I gratefully acknowledge the hospitality extended to me by the Universities of Rome I and II, and financial support by the SFB 288 (Berlin), the EU (via TMR networks in Rome), the Graduiertenkolleg ''Theoretische Elementarteilchenphysik'' (Hamburg), and the DFG (Göttingen).

APPENDIX A: BASIC NOTIONS FROM THE TOMITA–TAKESAKI THEORY OF REAL SPACES

For a review of this theory, the reader is referred to one of the Refs. 2, 20, 24. Here we recall the relevant notions.

Let $\mathcal{H}$ be a (complex) Hilbert space with scalar product $(\,\cdot\,,\cdot\,)$. If K is a real subspace of $\mathcal{H}$, then its *symplectic complement* is the set of vectors $\psi\in\mathcal{H}$ such that the imaginary part of (ϕ,ψ) vanishes for all $\phi\in K$. It is a closed real subspace and is denoted by K'. If K_α, $\alpha\in I$, is a family of closed real subspaces, then the closed real span of these subspaces is denoted by $\vee_{\alpha\in I}K_\alpha$. Its symplectic complement is given by $(\vee_{\alpha\in I}K_\alpha)'=\cap_{\alpha\in I}K'_\alpha$.

A real closed subspace K of $\mathcal{H}$ is called *standard* if $K+iK$ is dense in $\mathcal{H}$ and $K\cap iK=\{0\}$. Real closed standard subspaces K of $\mathcal{H}$ are in one-to-one correspondence with antilinear, densely defined, closed operators S acting on $\mathcal{H}$ which are involutive (i.e., satisfy $S^2\subset\mathbf{1}$): Given S, let

$$K\doteq\{\,\phi\in\mathrm{dom}S\colon S\,\phi=\phi\,\}. \tag{A1}$$

Then every vector in the domain of S may be uniquely written as $\psi=\phi_1+i\phi_2$ with $\phi_1,\phi_2\in K$, namely $\phi_1\doteq\frac{1}{2}(\psi+S\psi)$ and $\phi_2\doteq(1/2i)\,(\psi-S\psi)$. Hence K is standard. It is called the real space corresponding to S. Conversely, a real closed standard subspace K defines an antilinear,

densely defined, closed involution S, by putting $S(\phi_1+i\phi_2)\doteq\phi_1-i\phi_2$ for $\phi_1,\phi_2\in K$. S is then called the *canonical involution* corresponding to K. If S corresponds to K and U is unitary, then USU^* corresponds to UK, and further S^* corresponds to K'.

APPENDIX B: THE UNIVERSAL COVERING GROUP OF THE POINCARÉ GROUP

1. Covering of the Lorentz group

The universal covering group $\tilde{L}_+^\uparrow$ of the proper orthochronous Lorentz group $L_+^\uparrow$ in three dimensions can be identified with the set

$$\{(\gamma,\omega)\,|\,\gamma\in\mathbb{C},\,|\gamma|<1,\,\omega\in\mathbb{R}\}\,, \tag{B1}$$

the group multiplication $(\gamma,\omega)(\gamma',\omega')=(\gamma'',\omega'')$ being given by (Ref. 25, p. 594)

$$\gamma''=(\gamma'+\gamma e^{-i\omega'})(1+\gamma\overline{\gamma'}e^{-i\omega'})^{-1},$$

$$\omega''=\omega+\omega'+\frac{1}{i}\log\{(1+\gamma\overline{\gamma'}e^{-i\omega'})(\text{c.c.})^{-1}\}. \tag{B2}$$

Here (c.c.) denotes the complex conjugate of the preceding factor and log is the branch of the logarithm on $\mathbb{C}\backslash\mathbb{R}_0^-$ with $\log 1=0$.

The covering homomorphism $\tilde{L}_+^\uparrow\to L_+^\uparrow$ is conveniently described via the double covering $SU(1,1)$ of $L_+^\uparrow$, which is the subgroup of $SL(2,\mathbb{C})$ [conjugate to $SL(2,\mathbb{R})$] consisting of elements of the form

$$\begin{pmatrix}\alpha & \beta\\ \overline{\beta} & \overline{\alpha}\end{pmatrix},\quad \alpha\overline{\alpha}-\beta\overline{\beta}=1. \tag{B3}$$

The covering homomorphism $\tilde{L}_+^\uparrow\to SU(1,1)$ associates to each (γ,ω) the $SU(1,1)$-matrix,

$$(1-|\gamma|^2)^{-1/2}\begin{pmatrix}e^{-i\,\omega/2} & \overline{\gamma}e^{-i\,\omega/2}\\ \gamma e^{i\omega/2} & e^{i\omega/2}\end{pmatrix}. \tag{B4}$$

The double covering $SU(1,1)\to L_+^\uparrow$ is given as follows. For $a=(a^0,a^1,a^2)\in\mathbb{R}^3$ we set

$$\underline{a}=\begin{pmatrix}a^0 & a^1-ia^2\\ a^1+ia^2 & a^0\end{pmatrix}. \tag{B5}$$

Then the double covering $SU(1,1)\to L_+^\uparrow$ associates to $A\in SU(1,1)$ the unique $\lambda\in L_+^\uparrow$ satisfying

$$\underline{\lambda a}=A\underline{a}A^*,\quad a\in\mathbb{R}^3. \tag{B6}$$

Let us determine the lifts of the one-parameter subgroups of boosts and rotations. Denote the boosts in the k-direction ($k=1,2$) by $\lambda_k(\cdot)$ and the rotations in the 1–2 plane by $r(\cdot)$. Explicitly, $\lambda_k(t)$ acts on the 0- and k-coordinates as the matrix (13), and $r(\omega)$ acts on the 1- and 2-coordinates as

$$\begin{pmatrix}\cos(\omega) & -\sin(\omega)\\ \sin(\omega) & \cos(\omega)\end{pmatrix}. \tag{B7}$$

We denote by $\tilde{\lambda}_1(\cdot)$, $\tilde{\lambda}_2(\cdot)$ and $\tilde{r}(\cdot)$ the unique lifts of these one-parameter groups to $\tilde{L}_+^\uparrow$.

Lemma B.1: (i) The lifts of the one-parameter groups are given by

$$\tilde{\lambda}_1(t)=(\tanh(t/2),0)\quad,\quad \tilde{\lambda}_2(t)=(i\tanh(t/2),0)\quad and\quad \tilde{r}(\omega)=(0,\omega). \tag{B8}$$

(ii) Every element $\tilde{\lambda}\in\tilde{L}_+^{\uparrow}$ *has a unique decomposition,*

$$\tilde{\lambda}=\tilde{\lambda}_1(t)\ \ \tilde{\lambda}_2(t')\ \ \tilde{r}(\omega),\qquad t,t',\omega\in\mathbb{R}. \tag{B9}$$

Proof: (i) One verifies that the three one-parameter maps are continuous and have the correct images under the covering projection (B4) and (B6).

(ii) Consider the action of the Lorentz transformation λ, corresponding to $\tilde{\lambda}$, on the point $(1,0,0)$. Define t' as the arcsinh of the 2-component of $\lambda\cdot(1,0,0)$, and t as the unique real number such that $\sinh(t)\cosh(t')$ is the 1-component of $\lambda\cdot(1,0,0)$. One then checks that the actions of λ and $\lambda_1(t)\lambda_2(t')$ on the point $(1,0,0)$ coincide. This implies that there is a unique $\omega\in\mathbb{R}$ such that Eq. (B9) holds. □

2. Wigner rotation

Let, for $p\in H_m$,

$$\gamma(p)\doteq\frac{p_1+ip_2}{p_0+m}\quad,\quad \tilde{h}(p)\doteq(\gamma(p),0), \tag{B10}$$

and denote by $h(p)$ the corresponding element in $L_+^{\uparrow}$. Then

$$h(p):(m,0,0)\mapsto p. \tag{B11}$$

This implies that for arbitrary $p\in H_m$ and $\tilde{\lambda}\in\tilde{L}_3^{\uparrow}$, the element

$$t(\tilde{\lambda},p)\doteq\tilde{h}(p)^{-1}\tilde{\lambda}\ \ \tilde{h}(\lambda^{-1}p) \tag{B12}$$

leaves $(m,0,0)$ invariant, hence is a rotation and may be written in the form

$$t(\tilde{\lambda},p)=(0,\Omega(\tilde{\lambda},p)), \tag{B13}$$

where $\Omega(\cdot,\cdot)$ is the so-called Wigner rotation. In fact, Eqs. (B12) and (B2) imply that, for $\tilde{\lambda}=(\gamma,\omega)$,

$$\Omega(\tilde{\lambda},p)=\omega+\frac{1}{i}\log\{(1-\gamma(p)\overline{\gamma e^{-i\omega}})(\text{c.c.})^{-1}\}$$
$$+\frac{1}{i}\log\left\{\left(1+\frac{\gamma-\gamma(p)e^{-i\omega}}{1-\gamma(p)\overline{\gamma e^{-i\omega}}}\,\overline{\gamma}(\lambda^{-1}p)\right)(\text{c.c.})^{-1}\right\}\quad. \tag{B14}$$

Note that $\Omega((0,\omega),p)=\omega$ for all ω and p, and that Ω satisfies the cocycle condition

$$\Omega(\tilde{\lambda}\tilde{\lambda}',p)=\Omega(\tilde{\lambda},p)+\Omega(\tilde{\lambda}',\lambda^{-1}p), \tag{B15}$$

for all $\tilde{\lambda},\tilde{\lambda}'\in\tilde{L}_+^{\uparrow}$ and $p\in H_m$.

3. Proper Poincaré group

The proper Poincaré group P_+ can be obtained from the proper orthochronous Poincaré group by adjoining the reflection j at the x^2-axis; cf. Eq. (14), with the appropriate relations:

$$j^2=\mathbb{1},\quad j(a,\mathbb{1})j=(j\cdot a,\mathbb{1}),$$

$$j\,\lambda_1(t)\,j=\lambda_1(t),\quad j\,r(\omega)\,j=r(-\omega). \tag{B16}$$

[Note that the last equations imply $j\lambda_2(t)j=\lambda_2(-t)$.] Correspondingly, the universal covering group $\tilde{P}_+$ of this (disconnected) group may be defined by adjoining an element $\tilde{j}$ to $\tilde{P}_+^\uparrow$ satisfying the relations

$$\tilde{j}^2=\mathbb{1}\quad\text{and}\quad \tilde{j}\,(a,(\gamma,\omega))\,\tilde{j}=(ja,(\overline{\gamma},-\omega))\,. \tag{B17}$$

In fact, the map $\tilde{j}\mapsto j$, $\tilde{\lambda}\mapsto\lambda$ is a homomorphism and hence a covering projection. Finally, we prove an important cocycle relation of the Wigner rotation (B13) with respect to $\tilde{j}$.

Lemma B.2: For all $\tilde{\lambda}\in\tilde{L}_+^\uparrow$ and $p\in H_m$ the following relation holds:

$$\Omega(\tilde{j}\tilde{\lambda}\tilde{j}\,,p)=-\Omega(\tilde{\lambda}\,,-j\cdot p)\,. \tag{B18}$$

Proof: From the definition of $\tilde{h}(p)$ via equation (B10) and the group relations (B17) satisfied by $\tilde{j}$ we get

$$\tilde{h}(-j\cdot p)=\tilde{j}\,\tilde{h}(p)\,\tilde{j}\quad. \tag{B19}$$

This implies $t(\tilde{\lambda},-j\cdot p)=\tilde{j}\,t(\tilde{j}\tilde{\lambda}\tilde{j},p)\,\tilde{j}$ and hence the claim. □

Lemma B.3: (i) Let U be the irreducible representation of $\tilde{P}_+^\uparrow$ for mass $m>0$ and spin $s\in\mathbb{R}$ defined in Eq. (31), and let J be the operator defined in Eq. (32). Then J is an anti-unitary involution satisfying the representation property

$$JU(\tilde{g})J=U(\tilde{j}\tilde{g}\tilde{j})\quad. \tag{B20}$$

(ii) Let U be a finite direct sum of copies of the irreducible representation of $\tilde{P}_+^\uparrow$ for mass $m>0$ and spin $s\in\mathbb{R}$, acting on a Hilbert space $\mathcal{H}$. Then there is a unique, up to equivalence, extension of U *from $\tilde{P}_+^\uparrow$ to $\tilde{P}_+$ in $\mathcal{H}$. Uniqueness means that if J and $\hat{J}$ are anti-unitary involutions satisfying the representation property (B20), then there is a unitary V commuting with $U(\tilde{P}_+^\uparrow)$ and satisfying $VJ=\hat{J}V$.*

Proof: (i) follows immediately from Lemma B.2. *(ii)* The existence of J follows from (i) by taking direct sums. To see uniqueness, let $C\doteq\hat{J}J$. It is a unitary operator commuting with the representation U and satisfying $CJ=JC^{-1}$. Using spectral calculus in the same way as in the proof of Proposition 3.1 in Ref. 26, we define a unitary root V of C, $V^2=C$, which still commutes with the representation U and satisfies $VJ=JV^{-1}$. Then V has the properties claimed in the lemma. □

4. Action of $\tilde{P}_+$ on $\tilde{\mathcal{C}}$

The universal covering group $\tilde{P}_+$ of the proper Poincaré group acts on $\tilde{\mathcal{C}}$ in the following way. Let $\tilde{C}=(C,\tilde{e})\in\tilde{\mathcal{C}}$ where $\tilde{e}$ is the equivalence class w.r.t. C of a path $t\mapsto\tilde{e}(t)$ in H starting at e_0 and ending in C. Identifying $\tilde{L}_+^\uparrow$ with the set of homotopy classes of paths in $L_+^\uparrow$ starting at the unit, an element $\tilde{g}=(a,\tilde{\lambda})\in\tilde{P}_+^\uparrow$ acts on $\tilde{C}$ as follows. Let $t\mapsto\tilde{\lambda}(t)$ be any path in $L_+^\uparrow$ which represents $\tilde{\lambda}$. Then we define

$$\tilde{g}\cdot\tilde{C}\doteq(g\cdot C,\tilde{\lambda}\cdot\tilde{e})\,, \tag{B21}$$

where $\tilde{\lambda}\cdot\tilde{e}$ is the equivalence class w.r.t. $\lambda\cdot C$ of the path $t\mapsto\tilde{\lambda}(t)\cdot\tilde{e}(t)$ in H. Further, the element $\tilde{j}\in\tilde{P}_+$ acts on $\tilde{C}$ as

$$\tilde{j}\cdot\tilde{C}\doteq(j\cdot C,\tilde{j}\cdot\tilde{e})\,, \tag{B22}$$

where $\tilde{j}\cdot\tilde{e}$ is the equivalence class w.r.t. $j\cdot C$ of the path $t\mapsto j\cdot\tilde{e}(t)$. Note that this path also starts at e_0 since we have chosen the reference direction e_0 so as to be invariant under j.

APPENDIX C: PROOF OF ANALYTICITY OF THE COCYCLE

We establish the required analyticity properties of the cocycle $c(\tilde{\Lambda},p)$, cf. Eq. (35), starting with the Wigner rotation factor for the 1-boosts. Let

$$l(p)\doteq p_0-p_1+m-ip_2 \tag{C1}$$

and

$$v(p)\doteq l(p)\,\overline{l(p)}^{-1}. \tag{C2}$$

Note that for all $p\in H_m$, the number $v(p)$ lies in the cut complex plane $\mathbb{C}\backslash\mathbb{R}_0^-$, allowing for our definition of the power $v(p)^s$ given before Lemma 4.1. We have the following lemma.

Lemma C.1: The Wigner rotation factor for the 1-boosts is given by

$$e^{is\Omega(\tilde{\Lambda}_1(t),p)}=v(p)^s\,v(\tilde{\Lambda}_1(-t)p)^{-s}\quad. \tag{C3}$$

As a function of t, it has branch points in the strip $\mathbb{R}+i(0,\pi)$ for any $p\in H_m$ if s is not an integer.

Proof: Equation (C3) is verified by direct calculation. But using

$$(\Lambda_1(t)p)_0-(\Lambda_1(t)p)_1=e^t(p_0-p_1)\,, \tag{C4}$$

we get

$$v(\Lambda_1(-t)\,p)=\frac{e^t(p_0-p_1)+m-ip_2}{e^t(p_0-p_1)+m+ip_2}. \tag{C5}$$

For any fixed $p\in H_m$, this function has zeros in the strip, which proves the claim. □

In the next proposition, we give an explicit expression for the cocycle $c(\tilde{\Lambda},p)$, exhibiting its analyticity properties.

Proposition C.2: Let $\tilde{\Lambda}=\tilde{\Lambda}_1(t)\;\;\tilde{\Lambda}_2(t')\;\;\tilde{r}(\omega)$, with $t,t',\omega\in\mathbb{R}$, and let $\omega'\doteq\omega-\pi/2$. Further, let $p\in H_m$ be arbitrary.

(i) Denote by ω_0' the representative of $\omega'+2\pi\mathbb{Z}$ in the interval $(-2\pi,0]$. Then

$$c(\tilde{\Lambda},p)=2^{-s}\,e^{s(t+t')}\,e^{is(\omega'-\omega_0')}\left(a-b+e^{-t}(a+b)\,\frac{-p_2+im}{p_0-p_1}\right)^{2s}\quad, \tag{C6}$$

where

$$a\doteq\cos\frac{\omega_0'}{2}\qquad and\qquad b\doteq e^{-t'}\sin\frac{\omega_0'}{2}\leqslant 0\,. \tag{C7}$$

The power of $2s$ is understood within $\mathbb{C}\backslash\mathbb{R}_0^-$.

(ii) Let $s\notin\frac{1}{2}\mathbb{N}_0$. The function $\tau\mapsto c(\tilde{\Lambda}_1(\tau)\tilde{\Lambda},p)$ is analytic in the strip $\mathbb{R}+i(0,\pi)$ if and only if the parameters t' and ω' satisfy the relation

$$-\sinh t'\,|\sin\omega'|\leqslant\cos\omega'\,. \tag{C8}$$

In this case, the upper and lower boundary values are related by

$$c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)|_{\tau=i\pi}=e^{i\pi s}\,e^{4\pi i s n(\omega')}\,\overline{c(\tilde{\lambda},-jp)}\,, \tag{C9}$$

where $n(\omega')$ *is the unique integer such that* $\omega'-2\pi n(\omega')\in(-\pi,\pi]$.

(iii) For $s\in\frac{1}{2}\mathbb{N}_0$, *the function* $\tau\mapsto c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)$ *is analytic in the strip* $\mathbb{R}+i(0,\pi)$ *and satisfies the boundary condition (C9) for* all $\tilde{\lambda}\in\tilde{L}_+^\uparrow$.

Remark: From *(iii)* it follows that for $s\in\frac{1}{2}\mathbb{N}_0$ the localization structure can be nontrivially extended to bounded regions as in Proposition 4.2. The same can be shown for $s\in-\frac{1}{2}\mathbb{N}$ if one uses, instead of our intertwining function $u=:u_s$ the function $u_s^-(p):=\overline{u_{|s|}(p)}$.

Proof: In the following, p denotes an arbitrary point on the mass shell. We will use the cocycle identity

$$c(\tilde{\lambda}\tilde{\lambda}',p)=c(\tilde{\lambda},p)\;\;c(\tilde{\lambda}',\lambda^{-1}p)\,,\quad \tilde{\lambda},\tilde{\lambda}'\in\tilde{L}_+^\uparrow\,, \tag{C10}$$

satisfied by c as a consequence of Eq. (B15). Thus, we first calculate $c(\tilde{\lambda},p)$ if $\tilde{\lambda}$ is a boost in the 1-direction or a rotation, and then use the above cocycle property for a general element $\tilde{\lambda}$.

The function v from Lemma C.1 is related to u, defined in Eq. (37), by

$$u(p)=\left(\frac{p_0-p_1}{m}\right)^s v(p)^s.$$

Hence, in view of the identity (C4), Lemma C.1 implies that

$$c(\tilde{\lambda}_1(t),p)=e^{st},\quad \text{for all } t\in\mathbb{R},p\in H_m\;\;. \tag{C11}$$

In order to calculate the cocycle for rotations, let us see how the function u transforms under rotations. Writing u as

$$u(p)=\left(\frac{p_0-p_1}{m}\right)^s (l(p)/\overline{l(p)})^s\,,$$

and using the identity

$$l(p)\cdot\overline{l(p)}=2(p_0+m)(p_0-p_1)\,,$$

we get

$$u(p)=(2m(p_0+m))^{-s}\;\;l(p)^{2s}.$$

Here we have used the fact that Re $l(p)>0$ to identify $(l(p)^2)^s$ with $l(p)^{2s}$. A straightforward calculation shows that l transforms under rotations as follows: For $\omega\in\mathbb{R}$,

$$l(r(-\omega)p)=l(p)\cdot l_\omega(p), \tag{C12}$$

where

$$l_\omega(p)\doteq e^{-i\omega/2}\left(\cos\frac{\omega}{2}+\sin\frac{\omega}{2}\,\frac{-p_2+im}{p_0-p_1}\right). \tag{C13}$$

Note that $l(p)$ and $l_\omega(p)$ are, as well as the l.h.s. of Eq. (C12), in $\mathbb{C}\backslash\mathbb{R}_0^-$ for all ω and p. Hence, we may take them to the power of $2s$ (within $\mathbb{C}\backslash\mathbb{R}_0^-$) separately, i.e., $(l(p)\,l_\omega(p))^{2s}=l(p)^{2s}l_\omega(p)^{2s}$. We thus have

$$u(r(-\omega)p)=u(p)\cdot l_\omega(p)^{2s}, \tag{C14}$$

and hence the cocycle for rotations is given by

$$c(\tilde{r}(\omega),p)=e^{is\omega}\,l_\omega(p)^{2s}. \tag{C15}$$

Now our results (C11) and (C15) imply, by the cocycle relation (C10), that for all $t,\omega\in\mathbb{R}$,

$$c(\tilde{\lambda}_1(t)\tilde{r}(\omega),p)=e^{st}\,e^{is\omega}l_\omega(\lambda_1(-t)p)^{2s}. \tag{C16}$$

Let us discuss how to take $l_\omega(p)$, see Eq. (C13), to the power of $2s$. As is clear from the construction, the dependence of l_ω on ω is 2π-periodic. Choosing a representative ω_0 of $\omega+2\pi\mathbb{Z}$ in the interval $(-2\pi,0]$, we may extract a factor $e^{-is\omega_0}$ from $l_{\omega_0}(p)^{2s}$. That is to say, we have

$$l_\omega(p)^{2s}=l_{\omega_0}(p)^{2s}=e^{-is\omega_0}\left(\cos\frac{\omega_0}{2}+\sin\frac{\omega_0}{2}\,\frac{-p_2+im}{p_0-p_1}\right)^{2s},\quad \omega_0\in(-2\pi,0]. \tag{C17}$$

[For $\omega_0\neq 0$ this is so because then the imaginary parts of the two factors on the r.h.s. of Eq. (C13) have opposite sign, while for $\omega_0=0$ both factors equal one.] Using this and Eq. (C4), we arrive at the expression

$$c(\tilde{\lambda}_1(t)\tilde{r}(\omega),p)=e^{st}\,e^{is(\omega-\omega_0)}\left\{\cos\frac{\omega_0}{2}+e^{-t}\sin\frac{\omega_0}{2}\,\frac{-p_2+im}{p_0-p_1}\right\}^{2s}, \tag{C18}$$

where ω_0 is the representative of $\omega+2\pi\mathbb{Z}$ in the interval $(-2\pi,0]$.

We are now prepared to prove Eq. (C6). Let $\tilde{\lambda}\in\tilde{L}_+^\uparrow$ be as in the proposition. Using $\tilde{\lambda}_2(t')=\tilde{r}(\pi/2)\,\tilde{\lambda}_1(t')\,\tilde{r}(-\pi/2)$, we rewrite $\tilde{\lambda}$ as

$$\tilde{\lambda}=\tilde{\lambda}_1(t)\,\tilde{r}\left(\frac{\pi}{2}\right)\tilde{\lambda}_1(t')\,\tilde{r}(\omega'),\quad \text{with}\quad \omega'\doteq\omega-\frac{\pi}{2}. \tag{C19}$$

Due to the cocycle relation (C10), $c(\tilde{\lambda},p)$ consists of two factors of the form calculated in Eq. (C18):

$$\begin{aligned}c(\tilde{\lambda},p)&=c\left(\tilde{\lambda}_1(t)\,\tilde{r}\left(\frac{\pi}{2}\right),p\right)\cdot c\left(\tilde{\lambda}_1(t')\,\tilde{r}(\omega'),r\left(-\frac{\pi}{2}\right)\lambda_1(-t)\;p\right)\\&=2^{-s}\,e^{st}\left\{1+e^{-t}\frac{-p_2+im}{p_0-p_1}\right\}^{2s}\cdot e^{st'}e^{is(\omega'-\omega_0')}\left\{a+b\;\frac{-q_2+im}{q_0-q_1}\right\}^{2s},\end{aligned} \tag{C20}$$

where ω_0' is the representant of $\omega'+2\pi\mathbb{Z}$ in $(-2\pi,0]$, and we have written a and b as in Eq. (C7) of the proposition and $q\doteq r(-\pi/2)\lambda_1(-t)\,p$. Explicitly, q reads as

$$q=(\cosh t\,p_0-\sinh t\,p_1,\,p_2,\,\sinh t\,p_0-\cosh t\,p_1),$$

and we calculate

$$\frac{-q_2+im}{q_0-q_1}=\frac{-e^tp_-+e^{-t}p_++2im}{e^tp_-+e^{-t}p_+-2p_2}=-\frac{e^tp_-+p_2-im}{e^tp_--p_2+im},$$

where $p_\pm\doteq p_0\pm p_1$. Then the product of the two curly brackets in (C20) yields

$$\left\{1+e^{-t}\frac{-p_2+im}{p_0-p_1}\right\}\left\{a+b\ \ \frac{-q_2+im}{q_0-q_1}\right\}=a-b+e^{-t}(a+b)\frac{-p_2+im}{p_0-p_1}. \tag{C21}$$

Having chosen $\omega_0'\in(-2\pi,0]$, we observe that $b\leqslant 0$, and equality holds only if $\omega_0'=0$. Hence $a+b=0$ implies $a-b=1$. Thus the r.h.s. is in $\mathbb{C}\setminus\mathbb{R}_0^-$. The same holds for the two factors on the l.h.s., hence we may take them to the power of $2s$ (within $\mathbb{C}\setminus\mathbb{R}_0^-$) separately. We therefore have

$$c(\tilde{\lambda},p)=2^{-s}\,e^{s(t+t')}\,e^{is(\omega'-\omega_0')}\,f(t,p)^{2s}, \tag{C22}$$

where

$$f(t,p)\doteq a-b+e^{-t}(a+b)\frac{-p_2+im}{p_0-p_1}. \tag{C23}$$

This proves part (i) of the Proposition.

We now discuss the analyticity properties of the function $c(\tilde{\lambda}_1(\cdot)\tilde{\lambda},p)$. If $\tilde{\lambda}$ is parametrized by $t,t',\omega\in\mathbb{R}$ as in the proposition, then $\tilde{\lambda}_1(\tau)\tilde{\lambda}=\tilde{\lambda}_1(\tau+t)\,\tilde{\lambda}_2(t')\,\tilde{r}(\omega)$ and we may write

$$c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)=2^{-s}\,e^{s(\tau+t+t')}\,e^{is(\omega'-\omega_0')}\,f(\tau+t,p)^{2s}\ \ , \tag{C24}$$

with $f(\cdot,p)$ as in Eq. (C23). Note that $f(\cdot,p)$ is an entire analytic function and satisfies

$$f(t+i\pi,p)=\overline{f(t,-jp)}\ \ . \tag{C25}$$

For $s\in\frac{1}{2}\mathbb{N}_0$ (iii), the claimed analyticity and boundary conditions follow. To prove (ii), let $s\notin\frac{1}{2}\mathbb{N}_0$. Then the function $\tau\mapsto c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)$ has an analytic extension into the strip $\mathbb{C}+i(0,\pi)$ if and only if $f(\cdot,p)$ has no zeros in the strip. This can be decided by looking at the definition (C23), taking into consideration that $(-p_2+im)(p_0-p_1)^{-1}$ takes all values in the upper half plane $\mathbb{R}+i\mathbb{R}^+$ if p runs through H_m.

In the following, z_+^{2s} will denote z to the power of $2s$ defined via the branch of the logarithm on $\mathbb{C}\setminus\mathbb{R}_0^+$ satisfying $\log(-1)=i\pi$, if $z\in\mathbb{C}\setminus\mathbb{R}_0^+$. For $z\in\mathbb{C}\setminus\mathbb{R}_0^-$, z to the power of $2s$ defined via the branch of the logarithm on $\mathbb{C}\setminus\mathbb{R}_0^-$ satisfying $\log(1)=0$ will now be denoted by z_-^{2s}, instead of z^{2s} as before. We will use the following rules: **(1)** If z is in the upper complex half plane, then $z_-^{2s}=z_+^{2s}$, while for z in the lower half plane, $z_-^{2s}=e^{-4\pi is}z_+^{2s}$. **(2)** Complex conjugation commutes with taking powers within $z\in\mathbb{C}\setminus\mathbb{R}_0^-$: $(\overline{z})_-^{2s}=\overline{z_-^{2s}}$. **(3)** If $f(\tau,p)$ is contained in $\mathbb{C}\setminus\mathbb{R}_0^\pm$ for all τ in the strip $\mathbb{R}+i[0,\pi]$, then analytic continuation in τ commutes with taking powers within $\mathbb{C}\setminus\mathbb{R}_0^\pm$, respectively. That means, in particular, $f(\tau,p)_\pm^{2s}|_{\tau=i\pi}=f(i\pi,p)_\pm^{2s}$, where the l.h.s. denotes the analytic continuation of $f(\cdot,p)_\pm^{2s}$ from the real line to $i\pi$.

Case 1: $|b|>|a|$. Then $(a+b)(a-b)<0$, hence $a+b$ and $a-b$ have a different sign. Then $f(\cdot,p)$ has zeros in the strip and hence the cocycle has, for $s\notin\frac{1}{2}\mathbb{Z}$, no analytic continuation into the strip.

Case 2: $|b|\leqslant|a|$, i.e., $(a+b)(a-b)\geqslant 0$. We observe first that $a=0$ implies $\omega_0'=-\pi$, hence $b=-e^{-t'}<0$, contradicting the assumption. Hence $a\neq 0$ in the present case.

Case 2.1: Both $a+b$ and $a-b$ are greater than or equal to zero. Since $a\neq 0$ (as observed above), this implies that $a>0$ and consequently, b being nonpositive [cf. (C7)] that $a-b>0$. Hence $f(\tau,p)$ is contained in $\mathbb{C}\setminus\mathbb{R}_0^-$ for all τ in the strip, and our rules above, together with Eq. (C25), imply that $f(\tau,p)_-^{2s}|_{\tau=i\pi}=\overline{f(0,-jp)_-^{2s}}$. Hence we have

$$c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)|_{\tau=i\pi}=e^{i\pi s}\,e^{2is(\omega'-\omega_0')}\,\overline{c(\tilde{\lambda},-jp)}. \tag{C26}$$

In the case at hand, $a>0$ and consequently $\omega_0'\in(-\pi,0]$. Hence $(\omega'-\omega_0')/2\pi$ is just the integer $n(\omega')$ defined in the proposition, and the above equation coincides with Eq. (C9).

Case 2.2: Both $a+b$ and $a-b$ are less than or equal to zero. Similarly as in Case 2.1, this implies that $a+b<0$. Hence $f(\tau,p)$ is in the lower half plane for real τ, and is contained in $\mathbb{C}\backslash\mathbb{R}_0^+$ for all τ in the strip. Hence our three rules above imply that $f(\tau,p)^{2s}_-|_{\tau=i\pi}=e^{-4\pi i s}\overline{f(0,-jp)^{2s}_-}$. We thus have

$$c(\tilde{\lambda}_1(\tau)\tilde{\lambda},p)|_{\tau=i\pi}=e^{i\pi s}\,e^{2is(\omega'-\omega_0'-2\pi)}\,\overline{c(\tilde{\lambda},-jp)}\,. \tag{C27}$$

In the case at hand, $a<0$ and consequently $\omega_0'\in(-2\pi,-\pi)$. Hence $(\omega'-\omega_0'-2\pi)/2\pi$ is just the integer $n(\omega')$ defined in the proposition, and the above equation again coincides with Eq. (C9).

We have now shown that the cocycle has an analytic continuation into the strip if and only if $|b|\leqslant|a|$, and that the continuation satisfies Eq. (C9). It remains to show that $|b|\leqslant|a|$ is equivalent to the condition (C8). Both conditions are true for $\omega'\in 2\pi\mathbb{Z}$ and false for $\omega'\in\pi+2\pi\mathbb{Z}$, hence they coincide if $\omega'\in\pi\mathbb{Z}$. If $\omega'\notin\pi\mathbb{Z}$, then $|b|\leqslant|a|$ is equivalent to

$$e^{-t'}-e^{t'}\leqslant\left|\cot\frac{\omega_0'}{2}\right|-\left|\tan\frac{\omega_0'}{2}\right|=2\cos\omega_0'\,|\sin\omega_0'|^{-1}=2\cos\omega'\,|\sin\omega'|^{-1}\,,$$

hence to condition (C8). We have thus shown part *(ii)* of the proposition. □

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Towards Euclidean theory of infrared singular quantum fields

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(Received 6 December 2002; accepted 30 January 2003)

A new generalized formulation of the spectral condition is proposed for quantum fields with highly singular infrared behavior whose vacuum correlation functions are well defined only under smearing with analytic test functions in momentum space. The Euclidean formulation of QFT developed by Osterwalder and Schrader is extended to theories with infrared singular indefinite metric. The corresponding generalization of the reconstruction theorem is obtained. The fulfilment of the generalized spectral condition is verified for quantum fields representable by infinite series in the Wick powers of indefinite metric free fields. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1563734]

I. INTRODUCTION

The Euclidean methods are central to the rigorous construction of quantum field models with polynomial interaction in lower dimensions, see Ref. 1. This construction heavily relies on the use of Osterwalder-Schrader reconstruction theorem[2,3] which allows to pass from Euclidean Green's functions to quantum field theory in the Minkowski spacetime. However, the results of Refs. 2, 3 in their initial form are inapplicable to models with a singular infrared behavior violating the positivity condition and, in particular, to gauge theories. The problem of the Euclidean formulation of QFT in the case of pseudo-Wightman axioms with an indefinite metric[4,5] was considered in Ref. 6 within the traditional framework of tempered Schwartz distributions. However, as shown, in particular, by the example of the Schwinger model in an arbitrary α-gauge,[7] the exact operator solutions of gauge models can be much more singular and, in general, are well defined only under smearing with analytic test functions in momentum space. In this work, we study the possibility of extending the Euclidean theory to the fields whose vacuum expectation values are analytic functionals in momentum representation.

One of the main difficulties is connected with the adequate generalization of the spectral condition, which determines the analyticity properties of the Wightman functions. In indefinite metric field theories, the space-time translations are implemented by pseudo-unitary (in general, unbounded) operators in the state space and, therefore, the spectral condition can be formulated only in the weak form, i.e., as a restriction on the n-point Wightman functions w_n. When w_n are tempered distributions, it is of the same form as in the ordinary Wightman theory:[8]

$$\operatorname{supp} \hat{W}_n \subset \overline{\mathbb{V}}_+^n, \quad \hat{W}_n(p_1,\ldots,p_n) = \int W_n(\xi_1,\ldots,\xi_n) e^{ip_1\xi_1+\ldots+ip_n\xi_n} \mathrm{d}p_1 \ldots \mathrm{d}p_n, \tag{1}$$

where $\overline{\mathbb{V}}_+$ is the closed upper light cone and $W_n(\xi)$ is the Wightman function w_{n+1} expressed in terms of the difference variables $\xi_j = x_j - x_{j+1}$:

$$w_{n+1}(x_1,\ldots,x_{n+1}) = W_n(x_1-x_2,\ldots,x_n-x_{n+1}). \tag{2}$$

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If $\hat{W}_n$ are analytic functionals, then the condition (1) becomes inapplicable because of the lack of test functions with compact support. The problem of the appropriate generalization of the spectral condition was raised by Moschella and Strocchi.[9] In Ref. 10, it was suggested to overcome this difficulty using the notion of carrier cone which replaces the notion of support for analytic functionals and whose existence for a wide class of functionals was proved in Refs. 11 and 12. The generalized spectral condition which is obtained from (1) by replacing the support with a carrier cone is sufficient for deriving the usual analyticity properties of the Wightman functions[10] and is fulfilled for the sums of infinite series in the Wick powers of indefinite metric free fields.[13] Moreover, fields representable by such series satisfy even stronger condition stated in terms of the notion of *strong carrier cone* which is introduced by Definition 2 below. The latter arises naturally when one tries to bring the definition of carrier cone into line with the operation of tensor product of functionals, which plays an important role in the problem under consideration. The use of the generalized spectral condition in such a stronger form yields simple and effective estimates for the Schwinger functions which allow developing the Euclidean formulation in complete analogy with the case of tempered fields.[3] In this paper, the analysis of the Euclidean formulation of QFT is performed at the level of the Wightman functions of the theory. At the same time, we believe that the developed approach provides a basis for considering more subtle questions connected with finding the Hilbert majorant of an indefinite metric.[4]

As in Refs. 9–12, we use the Gelfand–Shilov spaces S^{α}_{β} as the functional domain of definition of fields in momentum space. The generalized functions belonging to S'^{α}_{β} (Ref. 14) grow at infinity like $\exp(|p|^{1/\beta})$ and their Fourier-transforms like $\exp(|x|^{1/\alpha})$. Thus, the indices α and β control, respectively, the possible infrared and ultraviolet singularities. If $0 \leqslant \alpha < 1$, then the elements of S^{α}_{β} are entire analytic functions. It is important that our treatment covers the case $\alpha = 0$ which corresponds to an arbitrary singular infrared behavior.

In Sec. II, we introduce the definition of strong carrier cone and prove that the intersection of strong carrier cones of a functional is again its strong carrier cone. Analogous result for carrier cones ensuring, in particular, the existence of the smallest carrier cone was established in Ref. 11. In Sec. III, we prove that the definition of strong carrier cone is compatible with the operation of tensor product of functionals. In Sec. IV, the theory of Laplace transformation is extended to functionals with convex strong carrier cones. In particular, we prove a Paley–Wiener–Schwartz-type theorem characterizing those analytic functions that are Laplace transforms of such functionals. In Sec. V, this theorem is applied to derive estimates for the Schwinger functions. In the same section the main result of the paper is presented, namely, the generalized Euclidean reconstruction theorem which covers field theories with arbitrarily singular infrared behavior. In Sec. VI, we check that the generalized spectral condition is satisfied for normally ordered entire functions of indefinite metric free fields. Section VII is devoted to concluding remarks. Some details of proofs are given in Appendixes A and B.

II. STRONG CARRIER CONES

The space $S^{\alpha}_{\beta}(\mathbb{R}^k)$ is by definition[15] the union (inductive limit) with respect to $A, B > 0$ of the Banach spaces composed of smooth functions on $\mathbb{R}^k$ with the finite norm

$$\|\!|f|\!\|_{A,B} = \sup_{p \in \mathbb{R}^k, \lambda, \mu} \frac{|p^{\mu} \partial^{\lambda} f(p)|}{A^{|\lambda|} B^{|\mu|} |\lambda|^{\alpha|\lambda|} |\mu|^{\beta|\mu|}}, \tag{3}$$

where λ and μ run over all multi-indices and the standard multi-index notation is used. The spaces S^{α}_{β} are nontrivial if $\alpha + \beta > 1$ or if $\alpha > 0$ and $\alpha + \beta = 1$. From now on, we assume that one of these conditions is satisfied. If $0 \leqslant \alpha < 1$, then S^{α}_{β} consists of (the restrictions to $\mathbb{R}^k$ of) entire analytic functions and an alternative description of these spaces in terms of complex variables is possible.[15] Namely, an analytic function f on $\mathbb{C}^k$ belongs to the class S^{α}_{β} if and only if

$$|f(w)| \leqslant C \exp(-|p/B|^{1/\beta} + |Aq|^{1/(1-\alpha)}), \quad w = p + iq \in \mathbb{C}^k,$$

for some A, $B>0$ depending on f. For definiteness, we assume the norm $|\cdot|$ on $\mathbb{R}^k$ to be uniform, i.e., $|p|=\sup_{1\leqslant j\leqslant k}|p_j|$. The main element of the approach developed in Refs. 11 and 12 is the employment, in addition to the spaces S^α_β, of analogous spaces associated with cones.

Definition 1: Let U be a nonempty cone in $\mathbb{R}^k$. The Banach space $S^{\alpha,A}_{\beta,B}(U)$, $0\leqslant\alpha<1$, consists of entire analytic functions on $\mathbb{C}^k$ with the finite norm

$$\|f\|_{U,A,B}=\sup_{w\in\mathbb{C}^k}|f(w)|\exp(|p/B|^{1/\beta}-|Aq|^{1/(1-\alpha)}-\delta_U(Ap)^{1/(1-\alpha)}), \tag{4}$$

where $\delta_U(p)=\inf_{p'\in U}|p-p'|$. The space $S^\alpha_\beta(U)$ is defined to be the inductive limit $\lim_{A,B>0}\limits{\rightarrow} S^{\alpha,A}_{\beta,B}(U)$.

A nonempty closed cone K is called a carrier cone of the functional $u\in S'^{\alpha}_{\beta}(\mathbb{R}^k)$ if u extends continuously to every space $S^\alpha_\beta(U)$, where U is a cone with an open projection[16] such that $K\subset U$. As shown in Refs. 11 and 12, the space $S^\alpha_\beta(\mathbb{R}^k)$ is dense in each space $S^\alpha_\beta(U)$. The space of the functionals carried by the cone K is therefore identified with $s'^{\alpha}_{\beta}(K)$, where $s^\alpha_\beta(K)=\lim_{U}\limits{\rightarrow} S^\alpha_\beta(U)$.

It should be mentioned that in Refs. 11 and 12, the spaces $S^\alpha_\beta(U)$ are defined for open cones U and a closed cone K is said to be a carrier cone of u if this functional has a continuous extension to every $S^\alpha_\beta(U)$, where $K\setminus\{0\}\subset U$. This definition is equivalent to the one given here. It is easy to see that all results of Refs. 11 and 12 concerning the spaces $S^\alpha_\beta(U)$ remain true for any nonempty cone U. In what follows, we find it convenient to use the spaces $S^\alpha_\beta(U)$ associated with arbitrary nonempty cones because this allows handling the degenerate cone $\{0\}$ on the same footing as nondegenerate closed carrier cones. We also note that in Refs. 11 and 12, the space $s^\alpha_\beta(K)$ was denoted by $S^\alpha_\beta(K)$. Here, such notation might lead to confusion because the spaces $S^\alpha_\beta(K)$ and $S^\alpha_\beta(U)$ are no longer distinguished by the type of the cone.

The following result established in Ref. 11 shows that every functional of the class $S'^{\alpha}_{\beta}(\mathbb{R}^k)$ has a uniquely defined minimal carrier cone.

Theorem 1: *If both K_1 and K_2 are carrier cones of $u\in S'^{\alpha}_{\beta}(\mathbb{R}^n)$, then so is $K_1\cap K_2$.*

The cone $\overline{\mathbb{V}}^n_+$, which enters into the formulation (1) of the spectral condition, has a natural direct product structure and the following definition turns out to be useful for generalizing the spectral condition.

Definition 2: Let $K_1,\ldots,K_n$ be nonempty closed cones in $\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_n}$ respectively. The cone $K_1\times\cdots\times K_n$ is called a strong carrier cone of the functional $u\in S'^{\alpha}_{\beta}(\mathbb{R}^{k_1+\ldots+k_n})$ if u allows a continuous extension to the space $s^\alpha_\beta(K_1,\ldots,K_n)=\lim_{U_1,\ldots,U_n}\limits{\rightarrow} S^\alpha_\beta(U_1\times\cdots\times U_n)$, where the inductive limit is taken over all cones $U_1,\ldots,U_n$ with open projections such that $K_j\subset U_j$ for all $j=1,\ldots,n$.

The meaning of the spaces $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$ is clarified by Lemma 5 below. If $n=1$, then we recover the definition of carrier cone. As shown in Ref. 12, the natural embeddings $S^{\alpha,A}_{\beta,B}(U)\to S^{\alpha,A'}_{\beta,B'}(U)$ are compact for $A'>A$, $B'>B$ sufficiently large. Therefore, $S^\alpha_\beta(U)$ and $s^\alpha_\beta(K_1,\ldots,K_n)$ are DFS spaces (we recall that DFS spaces are, by definition, the inductive limits of injective compact sequences of locally convex spaces). In particular, they (and their duals) are reflexive, complete, and Montel spaces.[17]

Clearly, $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)\subset s'^{\alpha}_{\beta}(K_1\times\cdots\times K_n)$, but the following example shows that the condition $u\in s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$ is, in general, stronger than the condition $u\in s'^{\alpha}_{\beta}(K_1\times\cdots\times K_n)$.

Example 1: Let $u(p)$ be the function equal to unity on the set $\{p\in\mathbb{R}^2|p_2\geqslant-|p_1|^{2/3}\}$ and zero outside this set. As a generalized function, u obviously belongs to $s'^{\alpha}_{\beta}(\mathbb{R}\times\overline{\mathbb{R}}_+)$ for all $0\leqslant\alpha<1$ and $\beta>1-\alpha$. Let us show that $u\notin s'^{2/3}_{1/2}(\mathbb{R},\overline{\mathbb{R}}_+)=S'^{2/3}_{1/2}(\mathbb{R}\times\mathbb{R}_+)$. Use the test function $f(w)=\exp(-w_1^2-w_2^3)$ belonging to $S^{2/3}_{1/2}(\mathbb{R}\times\mathbb{R}_+)$ and define $g(w)$ by the same formula as f but with the twice less exponent. By the above-mentioned density property, there exists a sequence $g_\nu\in S^{2/3}_{1/2}(\mathbb{R}^2)$ converging to g in $S^{2/3}_{1/2}(\mathbb{R}\times\mathbb{R}_+)$. Set $f_\nu(w)=g_\nu(w)\overline{g_\nu(\overline{w})}$ (bar means complex conju-

gation). Obviously, $f_\nu(p)\geqslant 0$ and $f_\nu \to f$ in $S^{2/3}_{1/2}(\mathbb{R}\times\mathbb{R}_+)$. Since the integral $\int u(p)f(p)\mathrm{d}p$ is divergent, we conclude by the monotonic convergence theorem that $\int u(p)f_\nu(p)\mathrm{d}p\to\infty$ as $\nu\to\infty$.

The following analogue of Theorem 1 is valid.

Theorem 2: *Let $K_1^{(1,2)},\ldots,K_n^{(1,2)}$ be nonempty closed cones in $\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_n}$ respectively. If both $K_1^{(1)}\times\cdots\times K_n^{(1)}$ and $K_1^{(2)}\times\cdots\times K_n^{(2)}$ are strong carrier cones of $u\in S'^{\alpha}_{\beta}(\mathbb{R}^{k_1+\ldots+k_n})$, then so is $(K_1^{(1)}\cap K_1^{(2)})\times\cdots\times(K_n^{(1)}\cap K_n^{(2)})$.*

Before we pass to the proof, let us set up the notation and recall some facts concerning cones in $\mathbb{R}^k$. Let $\mathcal{C}(\mathbb{R}^k)$ denote the set of all cones in $\mathbb{R}^k$ containing the origin and let $\mathcal{O}(\mathbb{R}^k)$ be the subset of $\mathcal{C}(\mathbb{R}^k)$ consisting of cones with open projections (or, which is the same, of those cones whose intersection with $\mathbb{R}^k\backslash\{0\}$ is open). We note that the cones U_j in Definition 2 belong to $\mathcal{O}(\mathbb{R}^{k_j})$. Obviously, for any (open) subset O of the unit sphere there is a unique cone $U\in\mathcal{C}(\mathbb{R}^k)$ [respectively, $U\in\mathcal{O}(\mathbb{R}^k)$] such that O is the projection of U. Using this one-to-one correspondence, one can apply standard compactness arguments to cones in $\mathcal{C}(\mathbb{R}^k)$ to obtain:

(i) if $U\in\mathcal{C}(\mathbb{R}^k)$, $V\in\mathcal{O}(\mathbb{R}^k)$, and $U\Subset V$,[18] then there exists $W\in\mathcal{O}(\mathbb{R}^k)$ such that $U\Subset W\Subset V$;

(ii) if $U_1,U_2\in\mathcal{C}(\mathbb{R}^k)$ and $\overline{U_1}\cap\overline{U_2}=\{0\}$, then there exist V_1, $V_2\in\mathcal{O}(\mathbb{R}^k)$ such that $U_{1,2}\Subset V_{1,2}$ and $\overline{V_1}\cap\overline{V_2}=\{0\}$;

(iii) if $V\in\mathcal{C}(\mathbb{R}^k)$, $U\in\mathcal{O}(\mathbb{R}^k)$, and $V\Subset U$, then $\overline{V}\cap\Delta U=\{0\}$, where $\Delta U=(\mathbb{R}^k\backslash U)\cup\{0\}$ corresponds to the complement of the projection of U in the unit sphere.

Proof of Theorem 2: Let $u_{1,2}$ be the extensions of u to the spaces $s^{\alpha}_{\beta}(K_1^{(1,2)},\ldots,K_n^{(1,2)})$ which exist by the hypothesis and let $f\in s^{\alpha}_{\beta}(K_1^{(1)},\ldots,K_n^{(1)})\cap s^{\alpha}_{\beta}(K_1^{(2)},\ldots,K_n^{(2)})$. By Definition 2, there are cones $U_1^{(1,2)}\in\mathcal{O}(\mathbb{R}^{k_1}),\ldots,U_n^{(1,2)}\in\mathcal{O}(\mathbb{R}^{k_n})$ such that $K_1^{(1,2)}\times\cdots\times K_n^{(1,2)}\subset V^{(1,2)}=U_1^{(1,2)}\times\cdots\times U_n^{(1,2)}$ and $f\in S^{\alpha}_{\beta}(V^{(1)})\cap S^{\alpha}_{\beta}(V^{(2)})=S^{\alpha}_{\beta}(V^{(1)}\cup V^{(2)})$. The existence of continuous dense embeddings $S^{\alpha}_{\beta}(\mathbb{R}^{k_1+\ldots+k_n})\to S^{\alpha}_{\beta}(V^{(1)}\cup V^{(2)})\to s^{\alpha}_{\beta}(K_1^{(1,2)},\ldots,K_n^{(1,2)})$ implies that u_1 and u_2 coincide on $S^{\alpha}_{\beta}(V^{(1)}\cup V^{(2)})$ and, consequently,

$$u_1(f)=u_2(f)\quad\text{for every}\quad f\in s^{\alpha}_{\beta}(K_1^{(1)},\ldots,K_n^{(1)})\cap s^{\alpha}_{\beta}(K_1^{(2)},\ldots,K_n^{(2)}). \tag{5}$$

Let us consider the mapping

$$j:\ s^{\alpha}_{\beta}(K_1^{(1)},\ldots,K_n^{(1)})\times s^{\alpha}_{\beta}(K_1^{(2)},\ldots,K_n^{(2)})\to s^{\alpha}_{\beta}(K_1^{(1)}\cap K_1^{(2)},\ldots,K_n^{(1)}\cap K_n^{(2)})$$

taking (f_1,f_2) to f_1-f_2. If j is subjective, then $s^{\alpha}_{\beta}(K_1^{(1)}\cap K_1^{(2)},\ldots,K_n^{(1)}\cap K_n^{(2)})$ is topologically isomorphic to the quotient space $[s^{\alpha}_{\beta}(K_1^{(1)},\ldots,K_n^{(1)})\times s^{\alpha}_{\beta}(K_1^{(2)},\ldots,K_n^{(2)})]/\ker j$ by the open mapping theorem (see Ref. 19, Theorem IV.8.3), which is applicable because all spaces under consideration are DFS. From (5), it follows that $\ker j$ is contained in the kernel of the functional $(f_1,f_2)\to u_1(f_1)+u_2(f_2)$. As a consequence, the latter allows a canonical decomposition of the form $\tilde{u}\circ j$, where $\tilde{u}$ belongs to $s'^{\alpha}_{\beta}(K_1^{(1)}\cap K_1^{(2)},\ldots,K_n^{(1)}\cap K_n^{(2)})$ and, as one can easily see, is the extension of u. Thus, it remains to prove the subjectivity of j. It is ensured by the following decomposition theorem for test functions.

Theorem 3: *If $f\in s^{\alpha}_{\beta}(K_1^{(1)}\cap K_1^{(2)},\ldots,K_n^{(1)}\cap K_n^{(2)})$ then $f=f^{(1)}+f^{(2)}$ with $f^{(1,2)}\in s^{\alpha}_{\beta}(K_1^{(1,2)},\ldots,K_n^{(1,2)})$.*

To prove Theorem 3, we need three lemmas.

Lemma 1: Let $U\in\mathcal{C}(\mathbb{R}^{k_1})$, $V\in\mathcal{C}(\mathbb{R}^{k_2})$, and let U_1, $U_2\in\mathcal{C}(\mathbb{R}^{k_1})$ be such that $\overline{U_1}\cap\overline{U_2}=\{0\}$. Then for every $f\in S^{\alpha}_{\beta}(U\times V)$ one can find $f_{1,2}\in S^{\alpha}_{\beta}((U\cup U_{1,2})\times V)$ such that $f=f_1+f_2$. If $U\in\mathcal{O}(\mathbb{R}^{k_1})$, then the condition $\overline{U_1}\cap\overline{U_2}=\{0\}$ can be replaced by $\overline{U_1}\cap\overline{U_2}\subset U$.

Proof will be given for $0<\alpha<1$, when the space $S^{\alpha}_{1-\alpha}$ is nontrivial. The more difficult case $\alpha=0$ is considered in Appendix A. By (II), there exist cones $Q_1,Q_2\in\mathcal{O}(\mathbb{R}^{k_1})$ such that $U_{1,2}\Subset Q_{1,2}$

and $\overline{Q}_1\cap\overline{Q}_2=\{0\}$, and in view of (I) one can find cones V_1, $V_2\in\mathcal{O}(\mathbb{R}^{k_1})$ such that $U_{1,2}\Subset V_{1,2}\Subset Q_{1,2}$. Set $W_1=Q_1$ and $W_2=\Delta Q_1$. By (III) we have $\overline{W}_1\cap\overline{V}_2=\overline{V}_1\cap\overline{W}_2=\{0\}$. Let $g_0\in S^{\alpha,A_0}_{1-\alpha,B_0}(\mathbb{R}^{k_1})$ and $\int_{\mathbb{R}^{k_1}}g_0(p')\mathrm{d}p'=1$. We set

$$g_{1,2}(w)=\int_{W_{2,1}}g_0(w'-\eta)\mathrm{d}\eta,\quad w=(w',w'')\in\mathbb{C}^{k_1}\times\mathbb{C}^{k_2}. \tag{6}$$

Obviously, g_1, g_2 are entire analytic functions on $\mathbb{C}^{k_1}\times\mathbb{C}^{k}{}_2$ and $g_1+g_2=1$. If $\eta\in W_{1,2}$, then $|p'-\eta|\geqslant\delta_{W_{1,2}}(p')$ and in view of (4) we have

$$|g_{1,2}(w)|\leqslant C\exp\left[(A_0|q'|)^{1/(1-\alpha)}-\delta_{W_{2,1}}\left(\frac{p'}{2B_0}\right)^{1/(1-\alpha)}\right]. \tag{7}$$

Set $f_{1,2}=fg_{1,2}$ and fix A, $B>0$ such that $f\in S^{\alpha,A}_{\beta,B}(U\times V)$. If $p'\notin V_1$, then $\delta_{U_1}(p')\geqslant\theta|p'|$ for some $0<\theta<1$ and in view of the inequality $|p'|\geqslant\delta_U(p')$ we have $\delta_U(p')\leqslant\delta_{U_1\cup U}(p'/\theta)$. Hence, taking (4), (7) and the relation $\delta_{U\times V}(p)=\max[\delta_U(p'),\delta_V(p'')]$ into account, we find that

$$|f_1(w)|\leqslant C\|f\|_{A,B}\exp[(2(A_0+A)|q|)^{1/(1-\alpha)}+\delta_{(U_1\cup U)\times V}(Ap/\theta)^{1/(1-\alpha)}-(|p|/B)^{1/\beta}] \tag{8}$$

for $p'\notin V_1$. Further, there is $\theta_1>0$ such that $\delta_{W_2}(p')\geqslant\theta_1|p'|$ for $p'\in V_1$. Therefore, for $A\leqslant\theta_1/2B_0$, using (4) and (7), we obtain

$$|f_1(w)|\leqslant C\|f\|_{A,B}\exp[(2(A_0+A)|q|)^{1/(1-\alpha)}+\delta_V(Ap'')^{1/(1-\alpha)}-(|p|/B)^{1/\beta}] \tag{9}$$

for $p'\in V_1$. Comparing (8) and (9), we conclude that $f_1\in S^{\alpha,A'}_{\beta,B}((U\cup U_1)\times V)$ for $A'\geqslant 2(A_0+A)+A/\theta$. Analogous arguments show that $f_2\in S^{\alpha}_{\beta}((U\cup U_2)\times V)$ for B_0 sufficiently large.

If $U\in\mathcal{O}(\mathbb{R}^{k_1})$, then $K_1\cap K_2=\{0\}$ for the nonempty closed cones $K_{1,2}=\overline{U}_{1,2}\cap\Delta U$, and according to the above we have a decomposition $f=f_1+f_2$, where $f_{1,2}\in S^{\alpha}_{\beta}((U\cup K_{1,2})\times V)$. To complete the proof, it remains to note that $K_{1,2}\cup U\supset U_{1,2}\cup U$.

Lemma 2: Let $U_1\in\mathcal{O}(\mathbb{R}^{k_1})$, $U_2\in\mathcal{O}(\mathbb{R}^{k_2})$, $U\in\mathcal{C}(\mathbb{R}^{k})$, *and* $V_{1,2}\in\mathcal{C}(\mathbb{R}^{k_{1,2}})$ *be such that* $V_{1,2}\Subset U_{1,2}$. *Then for every* $f\in S^{\alpha}_{\beta}(U_1\times U_2\times U)$, *there is a decomposition* $f=f_1+f_2$, *where* $f_1\in S^{\alpha}_{\beta}(V_1\times\mathbb{R}^{k_2}\times U)$ *and* $f_2\in S^{\alpha}_{\beta}(\mathbb{R}^{k_1}\times V_2\times U)$.

Proof: By (I), one can find $W_{1,2}\in\mathcal{O}(\mathbb{R}^{k_{1,2}})$ such that $V_{1,2}\Subset W_{1,2}\Subset U_{1,2}$. Set $Q_1=\overline{V}_1\times\Delta W_2$ and $Q_2=\Delta W_1\times\overline{V}_2$. According to (III) we have $\overline{Q}_1\cap\overline{Q}_2=\{0\}$ and by Lemma 1, $f=f_1+f_2$, where $f_{1,2}\in S^{\alpha}_{\beta}([(U_1\times U_2)\cup Q_{1,2}]\times U)$. It remains to note that $(U_1\times U_2)\cup Q_1\supset V_1\times\mathbb{R}^{k_2}$ and $(U_1\times U_2)\cup Q_2\supset\mathbb{R}^{k_1}\times V_2$.

Lemma 3: Let V_1, $U_1,\ldots,V_n$, U_n *be cones in* $\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_n}$ *such that* $V_j\in\mathcal{C}(\mathbb{R}^{k_j})$, $U_j\in\mathcal{O}(\mathbb{R}^{k_j})$, *and* $V_j\Subset U_j$ *for all* $j=1,\ldots,n$. *If* $f\in S^{\alpha}_{\beta}(U_1\times\cdots\times U_n)$, *then* $f=f_1+\cdots+f_n$ *with* $f_j\in S^{\alpha}_{\beta}(\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_{j-1}}\times V_j\times\mathbb{R}^{k_{j+1}}\times\cdots\times\mathbb{R}^{k_n})$.

Proof: We shall prove the following stronger statement. Let the cones V_1, $U_1,\ldots,V_n$, U_n satisfy the conditions of the lemma and let $U\in\mathcal{C}(\mathbb{R}^{k})$. Then for every $f\in S^{\alpha}_{\beta}(U_1\times\cdots\times U_n\times U)$ there exists a decomposition $f=f_1+\cdots+f_n$, where $f_j\in S^{\alpha}_{\beta}(\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_{j-1}}\times V_j\times\mathbb{R}^{k_{j+1}}\times\cdots\times\mathbb{R}^{k_n}\times U)$. The statement of the lemma corresponds to the particular case $\mathbb{R}^{k}=U=\{0\}$. For $n=2$, the proof is reduced to applying Lemma 2. For $n>2$, we proceed by induction on n. Supposing the statement to hold up to $n-1$, we choose the cones $W_{1,2}\in\mathcal{O}(\mathbb{R}^{k_{1,2}})$ such that $V_{1,2}\Subset W_{1,2}\Subset U_{1,2}$. By Lemma 2, $f=\tilde{f}_1+\tilde{f}_2$, where $\tilde{f}_1\in S^{\alpha}_{\beta}(W_1\times\mathbb{R}^{k_2}\times U_3\times\cdots\times U_n\times U)$ and $\tilde{f}_2\in S^{\alpha}_{\beta}(\mathbb{R}^{k_1}\times W_2\times U_3\times\cdots\times U_n\times U)$, and in view of the natural isomorphisms $W_1\times\mathbb{R}^{k_2}\times U_3\times\cdots\times U_n\times U\cong W_1\times U_3\times\cdots\times U_n\times(\mathbb{R}^{k_2}\times U)$ and $\mathbb{R}^{k_1}\times W_2\times U_3\times\cdots\times U_n\times U\cong W_2\times U_3\times\cdots\times U_n\times(\mathbb{R}^{k_1}\times U)$ we obtain the desired decompositions of $\tilde{f}_1$ and $\tilde{f}_2$. The lemma is proved.

We now prove Theorem 3. By Lemma 3, we have a decomposition $f=f_1+\cdots+f_n$, where $f_j\in s^{\alpha}_{\beta}(\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_{j-1}},K^{(1)}_j\cap K^{(2)}_j,\mathbb{R}^{k_{j+1}},\ldots,\mathbb{R}^{k_n})$, $j=1,\ldots,n$. Let the cones $U^{(1)}_j$, $U^{(2)}_j$, U_j

$\in \mathcal{O}(\mathbb{R}^{k_j})$ be such that $f_j \in S^\alpha_\beta(\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_{j-1}},U_j,\mathbb{R}^{k_{j+1}},\ldots,\mathbb{R}^{k_n})$, $K_j^{(1,2)} \Subset U_j^{(1,2)}$ and $\overline{U_j^{(1)}} \cap \overline{U_j^{(2)}} \subset U_j$. By Lemma 1 there is a decomposition $f_j = f_j^{(1)} + f_j^{(2)}$, where $f_j^{(1,2)} \in S^\alpha_\beta(\mathbb{R}^{k_1} \times \ldots \times \mathbb{R}^{k_{j-1}} \times U_j^{(1,2)} \times \mathbb{R}^{k_{j+1}} \times \ldots \times \mathbb{R}^{k_n})$. Setting $f^{(1,2)} = f_1^{(1,2)} + \ldots + f_n^{(1,2)}$, we arrive at the desired result.

III. TENSOR PRODUCTS

We refer the reader to Ref. 19 for the definition and properties of the inductive topology (*i*-topology), projective topology (π-topology), and the topology of equicontinuous convergence (*e*-topology) on tensor products of locally convex spaces. Recall that π- and *e*-topologies coincide on the tensor products of nuclear spaces, while *i*- and π-topologies coincide on the tensor products of Fréchet spaces.

Lemma 4: Let $L^{(1)}$ and $L^{(2)}$ be DFS*-spaces. Then $L^{(1)} \otimes_i L^{(2)} = L^{(1)} \otimes_\pi L^{(2)}$. If $L^{(1)}$ is nuclear, then $(L^{(1)} \hat{\otimes}_i L^{(2)})' = L^{(1)\prime} \hat{\otimes}_i L^{(2)\prime}$, where the hat means completion and the prime denotes the strong dual space.*

The proof is given in Appendix B. In Ref. 20, it was shown that if $L^{(1)}$, $L^{(2)}$, and L are the strong duals of reflexive Fréchet spaces, then every separately continuous bilinear map of $L^{(1)} \times L^{(2)}$ into L is continuous. From Lemma 4, it follows that if $L^{(1)}$ and $L^{(2)}$ are DFS spaces, then an analogous statement holds for any locally convex space L.

Let $L^{(1)},\ldots,L^{(n)}$ be locally convex spaces. We denote by $L^{(1)} \hat{\otimes}_i \cdots \hat{\otimes}_i L^{(n)}$ the completion of $L^{(1)} \otimes \cdots \otimes L^{(n)}$ relative to *i*-topology. If L_n is a barrelled space, then there is the canonical identification

$$L^{(1)} \hat{\otimes}_i \cdots \hat{\otimes}_i L^{(n)} = (L^{(1)} \hat{\otimes}_i \cdots \hat{\otimes}_i L^{(n-1)}) \hat{\otimes}_i L^{(n)} \tag{10}$$

(to construct this isomorphism, one can use Theorems III.5.2 and III.5.4 of Ref. 19).

Lemma 5: Let $K_1,\ldots,K_n$ be nonempty closed cones in $\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_n}$, respectively, and let $0 \leqslant \alpha < 1$. *Then we have the isomorphisms*

$$s^\alpha_{gb}(K_1,\ldots,K_n) = s^\alpha_\beta(K_1,\ldots,K_{n-1}) \hat{\otimes}_i s^\alpha_\beta(K_n),$$

$$s'^\alpha_\beta(K_1,\ldots,K_n) = s'^\alpha_\beta(K_1) \hat{\otimes}_i \cdots \hat{\otimes}_i s'^\alpha_\beta(K_n).$$

Proof: As we have already mentioned above, the spaces introduced by Definition 2 are DFS. Moreover, they are nuclear as countable inductive limits of the spaces $S^\alpha_\beta(U)$, whose nuclearity was established in Ref. 12. Since $s^\alpha_\beta(K_1,\ldots,K_n)$ is Hausdorff and complete, the first isomorphism follows immediately from Definition 2 and the existence of the natural identification $S^\alpha_\beta(U_1 \times U_2) = S^\alpha_\beta(U_1) \hat{\otimes}_i S^\alpha_\beta(U_2)$ for any nonempty cones U_1, U_2, see Ref. 12, Theorem 3. The second isomorphism is obtained by induction from the first one using (10) and Lemma 4.

Lemma 6: Let G_1 and G_2 be subspaces of locally convex spaces L_1 and L_2 respectively. Then the topology of equicontinuous convergence on $G_1 \otimes G_2$ coincides with that induced from $L_1 \otimes_e L_2$.

Proof: Let $j_{1,2}$ be the natural injections of $G_{1,2}$ into $L_{1,2}$ and let $j = j_1 \otimes j_2$. We denote by $\mathcal{E}_{1,2}$ ($\widetilde{\mathcal{E}}_{1,2}$) the families of equicontinuous subsets of $L'_{1,2}$ (respectively, of $G'_{1,2}$). The polar sets of $(S_1 \otimes S_2)^o$, $S_{1,2} \in \mathcal{E}_{1,2}$ form the basis of neighborhoods of the origin for *e*-topology on $L_1 \otimes L_2$. Since $j'_{1,2}(\mathcal{E}_{1,2}) = \widetilde{\mathcal{E}}_{1,2}$ according to Ref. 19, Theorem IV.4.1, the sets $[j'_1(S_1) \otimes j'_2(S_2)]^o$, $S_{1,2} \in \mathcal{E}_{1,2}$, form the basis of neighborhoods of the origin for *e*-topology on $G_1 \otimes G_2$. It remains to note that in view of Proposition IV.2.3a of Ref. 19 and the equality $j' = j'_1 \otimes j'_2$ these sets coincide with $j^{-1}[(S_1 \otimes S_2)^o]$.

IV. LAPLACE TRANSFORMATION

Definition 3: Let $\beta>1$, let $V_1,\dots,V_n$ be nonempty open connected cones in $\mathbb{R}^{k_1},\dots,\mathbb{R}^{k_n}$, respectively, and let $V=V_1\times\cdots\times V_n$. The space $\mathcal{A}_\alpha^\beta(V_1,\dots,V_n)$ with $0<\alpha<1$ (with $\alpha=0$) consists of analytic functions in $T^V=\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_n}+iV$ that have, for any $\epsilon>0$ (respectively, for any R, $\epsilon>0$), the finite norms

$$\|\mathbf{v}\|_{\epsilon,V_1',\dots,V_n'}=\sup_{z\in T^{V'}}|\mathbf{v}(z)|\prod_{j=1}^{n}\exp(-\epsilon|z_j|^{1/\alpha}-\epsilon|y_j|^{-1/(\beta-1)})$$

$$\left(\text{respectively, }\ \|\mathbf{v}\|_{\epsilon,R,V_1',\dots,V_n'}=\sup_{z\in T^{V'},|z_j|\leqslant R}|\mathbf{v}(z)|\prod_{j=1}^{n}\exp(-\epsilon|y_j|^{-1/(\beta-1)})\right),\quad y_j=\operatorname{Im}z_j,$$

where $V_1',\dots,V_n'$ are arbitrary cones compact in $V_1,\dots,V_n$ and $V'=V_1'\times\cdots\times V_n'$.

If a nondegenerate bilinear form $\langle\cdot,\cdot\rangle$ is fixed on $\mathbb{R}^k$, then the Fourier transform of a test function $f(x)\in S_\alpha^\beta(\mathbb{R}^k)$ is defined by $\hat f(p)=\int f(x)e^{i\langle p,x\rangle}\,dx$. The mapping $f\to\hat f$ is a topological isomorphism of $S_\alpha^\beta(\mathbb{R}^k)$ onto $S_\beta^\alpha(\mathbb{R}^k)$. If $\beta>1$, V is an open connected cone in $\mathbb{R}^k$, and $K=V^*=\{p:\langle p,y\rangle\geqslant 0\,\forall y\in V\}$, then, as one can easily see, $e^{i\langle\cdot,z\rangle}\in s_\beta^\alpha(K)$ for any $z\in T^V$. The Laplace transform $\mathcal{L}_Vu$ of a functional $u\in s_\beta'^{\alpha}(K)$ is defined by $(\mathcal{L}_Vu)(z)=u(e^{i\langle\cdot,z\rangle})$, $z\in T^V$. As shown in Ref. 12, the Laplace operator $\mathcal{L}_V$ is a topological isomorphism of $s_\beta'^{\alpha}(K)$ onto $\mathcal{A}_\alpha^\beta(V)$ and hence $\mathcal{A}_\alpha^\beta(V)$ is a reflexive Fréchet space.

For $\mathbb{R}^k=\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_n}$, we assume that $\langle p,x\rangle=\Sigma_{j=0}^n\langle p_j,x_j\rangle_j$, where $\langle\cdot,\cdot\rangle_j$ is a nondegenerate bilinear form on $\mathbb{R}^{k_j}$.

Lemma 7: Let $\beta>1$, $0\leqslant\alpha<1$, and $\mathbf{v}\in\mathcal{A}_\alpha^\beta(V_1,\dots,V_n)$, where $V_1,\dots,V_n$ are nonempty open connected cones in $\mathbb{R}^{k_1},\dots,\mathbb{R}^{k_n}$, respectively. Then $\mathbf{v}(z_1,\dots,z_{n-1},\cdot)\in\mathcal{A}_\alpha^\beta(V_n)$ for any $z_1\in T^{V_1},\dots,z_{n-1}\in T^{V_{n-1}}$ and $\mathbf{v}_u(z_1,\dots,z_{n-1})=u(\mathbf{v}(z_1,\dots,z_{n-1},\cdot))$ belongs to $\mathcal{A}_\alpha^\beta(V_1,\dots,V_{n-1})$ for all $u\in\mathcal{A}_\alpha'^{\beta}(V_n)$. The mapping $u\to\mathbf{v}_u$ from $\mathcal{A}_\alpha'^{\beta}(V_n)$ into $\mathcal{A}_\alpha^\beta(V_1,\dots,V_{n-1})$ is continuous.

Proof: We define the space $A_\alpha^\beta(V_1,\dots,V_n)$ in the same way as $\mathcal{A}_\alpha^\beta(V_1,\dots,V_n)$ with the only difference that the elements of A_α^β need not be analytic functions. $\mathcal{A}_\alpha^\beta(V_1,\dots,V_n)$ is a closed subspace of $A_\alpha^\beta(V_1,\dots,V_n)$. Let $0<\alpha<1$, let $\epsilon>0$, and let $V_1',\dots,V_n'$ be closed subcones of $V_1,\dots,V_n$. Set $B_{\epsilon,V_n'}=\{u\in\mathcal{A}_\alpha'^{\beta}(V_n):|u(\mathbf{w})|\leqslant\|\mathbf{w}\|_{\epsilon,V_n'}\forall\mathbf{w}\in\mathcal{A}_\alpha^\beta(V_n)\}$. Using Definition 3, we obtain

$$|u(\mathbf{v}(z_1,\dots,z_{n-1}\cdot))|\leqslant\|\mathbf{v}(z_1,\dots,z_{n-1},\cdot)\|_{\epsilon,V_n'}\leqslant\|\mathbf{v}\|_{\epsilon,V_1',\dots,V_n'}\prod_{j=1}^{n-1}\exp(\epsilon|z_j|^{1/\alpha}+\epsilon|y_j|^{-1/(\beta-1)})$$

for every $u\in B_{\epsilon,V_n'}$ and every $z_j\in T^{V_j'}$, $1\leqslant j\leqslant n-1$. Consequently, $\|\mathbf{v}_u\|_{\epsilon,V_1',\dots,V_{n-1}'}\leqslant\|\mathbf{v}\|_{\epsilon,V_1',\dots,V_n'}$ for $u\in B_{\epsilon,V_n'}$. Thus, $\mathbf{v}_u$ belongs to the space $A_\alpha^\beta(V_1,\dots,V_{n-1})$ for any $u\in\mathcal{A}_\alpha'^{\beta}(V_n)$ and the image of $B_{\epsilon,V_n'}$ under the mapping $u\to\mathbf{v}_u$ is bounded in this space. The scalar multiples of $B_{\epsilon,V_n'}$ form a fundamental system of bounded subsets in the space $\mathcal{A}_\alpha'^{\beta}(V_n)$, which is bornologic as the strong dual of a Fréchet space, see Ref. 19, Sec. IV.6.6. Consequently, the mapping $u\to\mathbf{v}_u$ from $\mathcal{A}_\alpha'^{\beta}(V_n)$ to $A_\alpha^\beta(V_1,\dots,V_{n-1})$ is continuous. Let δ_z, $z\in T^{V_n}$, be the functional in $\mathcal{A}_\alpha'^{\beta}(V_n)$ which is equal to $\mathbf{w}(z)$ on the test function $\mathbf{w}\in\mathcal{A}_\alpha^\beta(V_n)$. Since $\mathcal{A}_\alpha^\beta(V_n)$ is a reflexive space, the linear span L of such functionals is dense in $\mathcal{A}_\alpha'^{\beta}(V_n)$. It is clear that $\mathbf{v}_u\in\mathcal{A}_\alpha^\beta(V_1,\dots,V_{n-1})$ for any $u\in L$ and, since $\mathcal{A}_\alpha^\beta$ is closed in A_α^β, we have $\mathbf{v}_u\in\mathcal{A}_\alpha^\beta(V_1,\dots,V_{n-1})$ for any $u\in\overline{L}=\mathcal{A}_\alpha'^{\beta}(V_n)$. The changes in the proof for the case $\alpha=0$ are obvious. The lemma is proved.

Let $V_1,\dots,V_n$ be nonempty open connected cones in $\mathbb{R}^{k_1},\dots,\mathbb{R}^{k_n}$, respectively, and let $K_j=V_j^*$, $j=1,\dots,n$. The product $\mathcal{A}_\alpha^\beta(V_1)\otimes_i\dots\otimes_i\mathcal{A}_\alpha^\beta(V_n)$ is continuously embedded into $\mathcal{A}_\alpha^\beta(V_1,\dots,V_n)$ by of the ordinary identification

$$(\mathbf{v}_1\otimes\cdots\otimes\mathbf{v}_n)(z_1,\ldots,z_n)=\mathbf{v}_1(z_1)\cdots\mathbf{v}_n(z_n),\quad \mathbf{v}_j\in\mathcal{A}'^{\beta}_{\alpha}(V_j).$$

We define the operator $\mathcal{L}_{V_1,\ldots,V_n}$: $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)\to\mathcal{A}'^{\beta}_{\alpha}(V_1,\ldots,V_n)$ as the continuous extension of $\mathcal{L}_{V_1}\otimes_i\cdots\otimes_i\mathcal{L}_{V_n}$ to $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$. By Lemma 5 and in view of the completeness of $\mathcal{A}'^{\beta}_{\alpha}$, such an extension exists and is uniquely defined. For any $u\in s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$, we have

$$(\mathcal{L}_{V_1,\ldots,V_n}u)(z)=u(e^{i\langle\cdot,z\rangle}),\quad z\in T^V, \tag{11}$$

where $V=V_1\times\cdots\times V_n$. Thus, $\mathcal{L}_{V_1,\ldots,V_n}$ is the restriction of the Laplace operator $\mathcal{L}_{V_1\times\ldots\times V_n}$ to $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$. To prove formula (11), it suffices to note that it holds for $u\in s'^{\alpha}_{\beta}(K_1)\otimes\cdots\otimes s'^{\alpha}_{\beta}(K_n)$ and next to make use of Lemma 5 and the continuity of both sides of the equality in u.

Theorem 4: *Let $\beta>1$, $0\leqslant\alpha<1$, let $V_1,\ldots,V_n$ be nonempty open connected cones in $\mathbb{R}^{k_1},\ldots,\mathbb{R}^{k_n}$, respectively, and let $K_j=V_j^*$, $j=1,\ldots,n$. The Laplace transformation $\mathcal{L}_{V_1,\ldots,V_n}$ is a topological isomorphism of $s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$ onto $\mathcal{A}'^{\beta}_{\alpha}(V_1,\ldots,V_n)$. If $u\in s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$, then $(\mathcal{L}_{V_1,\ldots,V_n}u)(\cdot+iy)$ tends to the Fourier transform of u in the strong topology of $S'^{\beta}_{\alpha}(\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_n})$ as $y\to0$ inside any cone $V_1'\times\cdots\times V_n'$, where $V_j'\Subset V_j$, $j=1,\ldots,n$.*

Proof: In Ref. 12 the statement was established for $n=1$ and it is sufficient to prove the theorem supposing it holds for the spaces over $n-1$ cones. The mapping $\mathcal{L}_{V_1,\ldots,V_n}$ is injective as the restriction of the injective operator $\mathcal{L}_{V_1\times\cdots\times V_n}$. Let $\mathbf{v}\in\mathcal{A}'^{\beta}_{\alpha}(V_1,\ldots,V_n)$. We define the bilinear form $b_{\mathbf{v}}$ on $\mathcal{A}'^{\beta}_{\alpha}(V_1,\ldots,V_{n-1})\times\mathcal{A}'^{\beta}_{\alpha}(V_n)$ by $b_{\mathbf{v}}(u_1,u_2)=u_1(\mathbf{v}_{u_2})$. By Lemma 7, the form $b_{\mathbf{v}}$ is separately continuous. Let $T_1:s^{\alpha}_{\beta}(K_1,\ldots,K_{n-1})\to\mathcal{A}'^{\beta}_{\alpha}(V_1,\ldots,V_{n-1})$ ($T_2:s^{\alpha}_{\beta}(K_n)\to\mathcal{A}'^{\beta}_{\alpha}(V_n)$) be the dual[21] mapping of $\mathcal{L}^{-1}_{V_1,\ldots,V_{n-1}}$ (respectively, of $\mathcal{L}^{-1}_{V_n}$). By Lemma 5, the separately continuous bilinear form $B_{\mathbf{v}}(f_1,f_2)=b_{\mathbf{v}}(T_1f_1,T_2f_2)$ on $s^{\alpha}_{\beta}(K_1,\ldots,K_{n-1})\times s^{\alpha}_{\beta}(K_n)$ uniquely determines a functional $u\in s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$ such that $u(f_1\otimes f_2)=B_{\mathbf{v}}(f_1,f_2)$. If $z=(z_1,\ldots,z_n)$, $\tilde{z}=(z_1,\ldots,z_{n-1})$, and $z_j\in T^{V_j}$, $j=1,\ldots,n$, then

$$u(e^{\langle\cdot,z\rangle})=B_{\mathbf{v}}(e^{\langle\cdot,\tilde{z}\rangle'},e^{\langle\cdot,z_n\rangle_n})=b_{\mathbf{v}}(\delta_{\tilde{z}},\delta_{z_n})=\mathbf{v}(z),$$

where $\langle p,\tilde{z}\rangle'=\sum_{j=1}^{n-1}\langle p_j,z_j\rangle_j$, $p\in\mathbb{R}^{k_1}\times\cdots\times\mathbb{R}^{k_{n-1}}$. Thus, $\mathbf{v}$ is the Laplace transform of u, i.e., the operator $\mathcal{L}_{V_1,\ldots,V_n}$ is bijective. The open mapping theorem shows that $\mathcal{L}_{V_1,\ldots,V_n}$ is a topological isomorphism. If $u\in s'^{\alpha}_{\beta}(K_1,\ldots,K_n)$ and $f\in S^{\beta}_{\alpha}(\mathbb{R}^{k_1+\ldots+k_n})$, then

$$\int(\mathcal{L}_{V_1,\ldots,V_n}u)(x+iy)f(x)\mathrm{d}x=u(e^{-\langle\cdot,y\rangle}\hat{f}),\quad y\in V_1\times\cdots\times V_n. \tag{12}$$

Indeed, the formula holds for $n=1$, see Ref. 12, and $\mathcal{L}_{V_1,\ldots,V_n}u$ coincides with $\mathcal{L}_{V_1\times\ldots\times V_n}u$. The direct check shows that $e^{-\langle\cdot,y\rangle}\hat{f}\to\hat{f}$ in the topology of $s^{\alpha}_{\beta}(K_1,\ldots,K_n)$ as $y\to0$ inside $V_1'\times\cdots\times V_n'$. Therefore, to prove the last statement of the theorem, it suffices to apply (12) and to take into account that in the Montel space S'^{β}_{α}, weak convergence and strong convergence are equivalent.

V. EUCLIDEAN RECONSTRUCTION THEOREM

From now on, the Lorentz product $p^0x^0-p^1x^1-\cdots-p^{d-1}x^{d-1}$ of p, $x\in\mathbb{R}^d$ will be denoted by px.

All requirements of the Wightman formalism except for the spectral condition are formulated in the usual way for the fields of the class S'^{β}_{α}, $0\leqslant\alpha<1$, $\beta>1$ (under the condition $\beta>1$, the local commutativity is formulated as usual). As we have already noted in Introduction, the spectral condition in standard form (1) is inapplicable in this case because of the lack of test functions of compact support in p-space. To obtain an appropriate generalization of the spectral condition, one can use the notion of strong carrier cone introduced in Sec. II. As a result, we come to the following set of axioms for the Wightman functions:

W1 (Growth and singularity) $w_n \in S'^{\beta}_{\alpha}(\mathbb{R}^{dn})0 \leqslant \alpha < 1,\ \beta > 1$;

W2 (Relativistic invariance) $w_n(\Lambda x_1 + a, \ldots, \Lambda x_n + a) = w_n(x_1, \ldots, x_n)$ for any proper Lorentz transformation Λ and vector $a \in \mathbb{R}^d$;

W3 (Generalized spectral condition) $\overline{\mathbb{V}}^n_+$ is a strong carrier cone of $\hat{W}_n$, i.e., $\hat{W}_n \in s'^{\alpha}_{\beta}(\overline{\mathbb{V}}_+, \ldots, \overline{\mathbb{V}}_+)$;

W4 (Locality) $w_n(x_1, \ldots, x_j, x_{j+1}, x_n) - w_n(x_1, \ldots, x_{j+1}, x_j, \ldots, x_n) = 0$ if $x_j - x_{j+1}$ is spacelike.

We do not impose the positivity condition on w_n, which corresponds to the case of an indefinite metric in the state space. Besides, we do not require the fulfillment of the cluster property which is not equivalent to the uniqueness of the vacuum in indefinite metric theories, see Ref. 4.

It should be noted that in the indefinite metric case, theory is not determined uniquely by its Wightman functions and to obtain its complete operator realization, it is necessary to specify, in addition to the sequence w_n, the Hilbert majorant of the indefinite metric which determines the convergence in the state space.[4] For simplicity, we restrict our consideration to Wightman functions and do not touch here more subtle questions concerning the construction of the Hilbert majorant.

Using Theorem 4 and condition W3, we conclude[22] that $W_n(\xi)$ is the boundary value of the function $\mathbf{W}_n(\zeta) = (2\pi)^{-dn}\mathcal{L}_{\mathbb{V}_-, \ldots, \mathbb{V}_-}\hat{W}_n$ holomorphic in the past tube $\mathbb{R}^{dn} + i\mathbb{V}^n_-$. Correspondingly, w_n is the boundary value of the function $\mathbf{w}_n(z_1, \ldots, z_n) = \mathbf{W}_{n-1}(z_1 - z_2, \ldots, z_{n-1} - z_n)$ holomorphic in the domain $\{z : z_j - z_{j+1} \in \mathbb{R}^d + i\mathbb{V}_-\}$. Standard analysis[23] based on the relativistic invariance and locality shows that $\mathbf{w}_n$ can be continued analytically to the extended domain O_n^{ext} which is invariant under the complex Lorentz transformations and the permutations of arguments. For $x = (x_1, \ldots, x_n) \in \mathbb{R}^{dn}$, we set $\iota x = (\iota x_1, \ldots, \iota x_n)$, where $\iota x_j = (ix_j^0, x_j^1, \ldots, x_j^{d-1})$. Then $\iota x \in O_n^{\mathrm{ext}}$ if and only if $x \in \mathbb{R}^{dn}_{\neq} = \{x \in \mathbb{R}^{dn} : x_i \neq x_j, 1 \leqslant i < j \leqslant n\}$, see Refs. 2 and 5. The Schwinger functions s_n are defined by the relation $s_n(x) = \mathbf{w}_n(\iota x)$, $x \in \mathbb{R}^{dn}_{\neq}$. In the same way as in the ordinary theory,[2,5] we establish that s_n are rotationally invariant and symmetric with respect to the permutations of arguments. Let $S_n(\xi)$ be the Schwinger function s_{n+1} expressed in terms of the difference variables $\xi_j = x_j - x_{j+1}$, and let $\mathbb{R}^{dn}_- = \{x \in \mathbb{R}^{dn} : x_j^0 < 0, j = 1, \ldots, n\}$. If $\xi \in \mathbb{R}^{dn}_-$, then $\iota\xi$ lies in the past tube and by Theorem 4, the function $S_n(\xi) = \mathbf{W}_n(\iota\xi)$ satisfies, for $0 < \alpha < 1$ (for $\alpha = 0$), the bound

$$
\begin{aligned}
&|S_n(\xi)| \leqslant C_\epsilon \exp[\epsilon|\xi|^{1/\alpha} + \epsilon(\min_{1 \leqslant j \leqslant n}|\xi_j^0|)^{-1/(\beta-1)}], \quad \xi \in \mathbb{R}^{dn}_-, \\
&(\text{respectively, } |S_n(\xi)| \leqslant C_{\epsilon,R} \exp[\epsilon(\min_{1 \leqslant j \leqslant n}|\xi_j^0|)^{-1/(\beta-1)}], \quad \xi \in \mathbb{R}^{dn}_-, \ |\xi| \leqslant R)
\end{aligned}
\tag{13}
$$

for any $\epsilon > 0$ (respectively, for any $\epsilon, R > 0$). As shown in Ref. 5 (see the proof of Theorem 9.30), for any $x \in \mathbb{R}^{dn}_{\neq}$ there exist a rotation T and a permutation π of the set $[1..n]$ such that

$$
\min_{1 \leqslant j \leqslant n-1}[(Tx_{\pi(j+1)})^0 - (Tx_{\pi(j)})^0] \geqslant c \min_{j \neq k}|x_j - x_k|, \tag{14}
$$

where c is a positive constant depending only on n. In view of the invariance of the Schwinger functions under rotations and permutations of arguments, (13) and (14) imply the inequality

$$
\begin{aligned}
&|s_n(x)| \leqslant C_\epsilon \exp[\epsilon|x|^{1/\alpha} + \epsilon(\min_{j \neq k}|x_j - x_k|)^{-1/(\beta-1)}], \quad x \in \mathbb{R}^{dn}_{\neq}, \\
&(\text{respectively, } |s_n(x)| \leqslant C_{\epsilon,R} \exp[\epsilon(\min_{j \neq k}|x_j - x_k|)^{-1/(\beta-1)}], \quad x \in \mathbb{R}^{dn}_{\neq}, \ |x| \leqslant R),
\end{aligned}
\tag{15}
$$

for any $\epsilon > 0$ (respectively, for any $\epsilon, R > 0$). The obtained estimates allow interpreting s_n as generalized functions defined under smearing with suitable test functions. The relevant test function spaces are introduced by the following definition:

Definition 4: Let $\alpha \geqslant 0$, $\beta > 1$ and let O be an open set in $\mathbb{R}^k$. We denote by $\Sigma_\alpha^\beta(O)$ the subspace of $S_\alpha^\beta(\mathbb{R}^k)$ consisting of those functions that are identically zero on the complement $\mathsf{C}O$ of O together with all their derivatives.

$\Sigma_\alpha^\beta(O)$ is a closed subspace of $S_\alpha^\beta(\mathbb{R}^k)$. Therefore, by Theorem 7′ of Ref. 17, we have $\Sigma_\alpha^\beta(O) = \varinjlim_{A,B>0} \Sigma_{\alpha,A}^{\beta,B}(O)$, where $\Sigma_{\alpha,A}^{\beta,B}(O)$ is the Banach space consisting of the functions $f \in \Sigma_\alpha^\beta(O)$ such that $\||f|\|_{B,A} < \infty$ [see formula (3)].

Lemma 8: Let O be an open set in $\mathbb{R}^k$. If $\alpha > 0$ (if $\alpha = 0$), then for any $A, B > 0$ there is $A' > 0$ such that for all $x \in O$ and $f \in \Sigma_{\alpha,A}^{\beta,B}(O)$ the inequality

$$|f(x)| \leqslant C \||f|\|_{B,A} \exp[-A'|x|^{1/\alpha} - A'(\delta_{\mathsf{C}O}(x))^{-1/(\beta-1)}]$$

$$\text{(respectively, } |f(x)| \leqslant C \||f|\|_{B,A} \exp[-A'(\delta_{\mathsf{C}O}(x))^{-1/(\beta-1)}] \quad \text{and} \quad f(x) = 0 \quad \text{for} \quad |x| \leqslant A),$$

is valid, where $\delta_{\mathsf{C}}O(x)$ is the distance from x to $\mathsf{C}O$.

Proof: Let $f \in \Sigma_{\alpha,A}^{\beta,B}(O)$, $x \in O$ and x_0 be a point in $\mathsf{C}O$ such that $|x - x_0| = \delta_{\mathsf{C}}O(x)$. By Taylor's formula, for every $m \in \mathbb{N} = 0,1,...$ we have $f(x) = \Sigma_{|\lambda|=m} \partial^\lambda f(x_0 + th) h^\lambda / \lambda!$, where $0 < t < 1$, $h = x - x_0$, and the standard multi-index notation is used. From (3) it follows that $|\partial^\lambda f(x)| \leqslant \||f|\|_{B,A} B^{|\lambda|} |\lambda|^{\beta|\lambda|}$. Since $|h^\lambda| \leqslant |h|^{|\lambda|}$, we get $|f(x)| \leqslant \||f|\|_{B,A} (B|h|)^m m^{\beta m} \Sigma_{|\lambda|=m} 1/\lambda! = \||f|\|_{B,A} (B|h|k)^m m^{\beta m}/m!$ and using the inequality $m! \geqslant (m/e)^m$, we find that $|f(x)| \leqslant \||f|\|_{B,A} \inf_{m \in \mathbb{N}} (B|h|ke)^m m^{(\beta-1)m}$. As shown in Ref. 15, Sec. IV.2, $\inf_m \xi^{-m} m^{\alpha m} \leqslant \exp(-\alpha/e\xi^{1/\alpha} + \alpha e/2)$ for any ξ, $\alpha > 0$. Replacing α and ξ with $\beta - 1$ and $1/B|h|ke$, respectively, we obtain

$$|f(x)| \leqslant C_1 \||f|\|_{B,A} \exp\left(-\frac{(\beta-1)}{e} (Bke\, \delta_{\mathsf{C}O}(x))^{-1/(\beta-1)} \right). \tag{16}$$

On the other hand, by (3) we have $|f(x)| \leqslant \||f|\|_{B,A} \inf_{m \in \mathbb{N}} (A/|x|)^m m^{\alpha m}$. For $\alpha = 0$, this implies that $f(x) = 0$ for $|x| > A$. If $\alpha > 0$, then an analogous estimation of the infimum shows that $|f(x)| \leqslant C_2 \||f|\|_{B,A} \exp(-\alpha/e(|x|/A)^{1/\alpha})$. Multiplying the last estimate and inequality (16) and taking the square root of the left- and right-hand sides, we arrive at the statement of the lemma.

Since $\delta_{\mathsf{C}\mathbb{R}^{dn}_{\neq}}(x) \leqslant \min_{j \neq k} |x_j - x_k|$ for $x \in \mathbb{R}^{dn}_{\neq}$, Lemma 8 and the estimate (15) imply that $s_n \in \Sigma'^\beta_\alpha(\mathbb{R}^{dn}_{\neq})$. Analogously, from (13) it follows that $S_n \in \Sigma'^\beta_\alpha(\mathbb{R}^{dn}_-)$.

For $\mathbf{v} \in \mathcal{A}_\alpha^\beta(\mathbb{V}_-, ..., \mathbb{V}_-)$, we set $l_{\mathbf{v}}(f) = (2\pi)^{-dn} \int_{\mathbb{R}^{dn}_-} \mathbf{v}(\iota x) f(x) dx$, $f \in \Sigma_\alpha^\beta(\mathbb{R}^{dn}_-)$. By Lemma 8, the mapping $\mathbf{v} \to l_{\mathbf{v}}$ from $\mathcal{A}_\alpha^\beta(\mathbb{V}_-, ..., \mathbb{V}_-)$ into $\Sigma'^\beta_\alpha(\mathbb{R}^{dn}_-)$ is continuous. Consequently, for every fixed $f \in \Sigma_\alpha^\beta(\mathbb{R}^{dn}_-)$ the functional $u \to l_{\mathcal{L}_{V_- \ldots V_- u}}(f)$ is continuous on $s'^\alpha_\beta(\overline{\mathbb{V}}_+, ..., \overline{\mathbb{V}}_+)$ and because of the reflexivity of the latter space there is an element $\check{f} \in s^\alpha_\beta(\overline{\mathbb{V}}_+, ..., \overline{\mathbb{V}}_+)$ such that

$$(2\pi)^{-dn} \int_{\mathbb{R}^{dn}_-} (\mathcal{L}_{\mathbb{V}_-, ..., V_-} u)(\iota\xi) f(\xi) \mathrm{d}\xi = u(\check{f}), \quad u \in s'^\alpha_\beta(\overline{\mathbb{V}}_+, ..., \overline{\mathbb{V}}_+). \tag{17}$$

Taking $u = \delta_p$ [the value of δ_p on a test function g is equal to $g(p)$], we find that

$$\check{f}(p) = (2\pi)^{-dn} \int_{\mathbb{R}^{dn}_-} f(\xi) \exp\left[\sum_{j=1}^n (p_j^0 \xi_j^0 - i p_j^1 \xi_j^1 - \cdots - i p_j^{d-1} \xi_j^{d-1}) \right] \mathrm{d}\xi. \tag{18}$$

The mapping $f \to \check{f}$ from $\Sigma_\alpha^\beta(\mathbb{R}^{dn}_-)$ to $s^\alpha_\beta(\overline{\mathbb{V}}_+, ..., \overline{\mathbb{V}}_+)$ has the continuous injective mapping $u \to l_{\mathcal{L}_{V_- \ldots V_- u}}$ as its dual. As a consequence, it is a continuous mapping with dense image.

Lemma 9: The mapping $f \to \check{f}$ defined by (18) is a continuous dense embedding of $\Sigma_\alpha^\beta(\mathbb{R}^{dn}_-)$ into $S^\alpha_\beta(\mathbb{R}^{dn}_+)$, where $\mathbb{R}^{dn}_+ = -\mathbb{R}^{dn}_-$.

To prove the lemma, we need the following auxiliary statement.

Lemma 10: Let V_1 and V_2 be nonempty open convex cones in $\mathbb{R}^{k_1}$ and $\mathbb{R}^{k_2}$, respectively. Then $\Sigma_\alpha^\beta(V_1\times V_2)=\Sigma_\alpha^\beta(V_1)\hat{\otimes}_i\Sigma_\alpha^\beta(V_2)$.

Proof: Applying Lemma 4 to the nuclear DFS-spaces $\Sigma_\alpha^\beta(V_{1,2})$, we obtain $\Sigma_\alpha^\beta(V_1)\otimes_i\Sigma_\alpha^\beta(V_2)=\Sigma_\alpha^\beta(V_1)\otimes_e\Sigma_\alpha^\beta(V_2)$ and by Lemma 6, it suffices to show that the tensor product $\Sigma_\alpha^\beta(V_1)\otimes\Sigma_\alpha^\beta(V_2)$ is dense in $\Sigma_\alpha^\beta(V_1\times V_2)$. In other words, we have to demonstrate that if a functional $u\in S_\alpha'^\beta(\mathbb{R}^{k_1+k_2})$ vanishes on $\Sigma_\alpha^\beta(V_1)\otimes\Sigma_\alpha^\beta(V_2)$, then it also vanishes on $\Sigma_\alpha^\beta(V_1\times V_2)$. To this end, we take $\psi_{1,2}\in\Sigma_\alpha^\beta(-V_{1,2})$ such that $\int_{\mathbb{R}^{k_{1,2}}}\psi_{1,2}\,dx=1$ and set $\Psi_\varepsilon(x_1,x_2)=\varepsilon^{-k_1-k_2}\psi_1(x_1/\varepsilon)\psi_2(x_2/\varepsilon)$. If $x\in\overline{V_1}\times\overline{V_2}$, then $\Psi_\varepsilon(x-\cdot)\in\Sigma_\alpha^\beta(V_1)\otimes\Sigma_\alpha^\beta(V_2)$ and, consequently, $(u*\Psi_\varepsilon)(x)=0$. Hence, for $f\in\Sigma_\alpha^\beta(V_1\times V_2)$, we have $u(f)=\lim_{\varepsilon\to 0}\int_{\overline{V_1}\times\overline{V_2}}(u*\Psi_\varepsilon(x)f(x)\,dx=0$. The lemma is proved.

Proof of Lemma 9: If $\check{f}=0$, then setting $u=\delta_{ip}$ in (17), we see that the Fourier transform of f vanishes and hence $f=0$. Thus, the mapping $f\to\check{f}$ is injective. For $f\in\Sigma_\alpha^\beta(\mathbb{R}_-)$, we set $\tilde{f}(p)=(2\pi)^{-1}\int_{\mathbb{R}_-}f(\xi)e^{\xi p}\,d\xi$. In the same way as above (see the paragraph preceding the formulation of Lemma 9), we establish that $\tilde{f}\in s_\beta^\alpha(\mathbb{R}_+)=S_\beta^\alpha(\mathbb{R}_+)$ and that the mapping P taking f to $\tilde{f}$ is a continuous dense embedding of $\Sigma_\alpha^\beta(\mathbb{R}_-)$ into $S_\beta^\alpha(\mathbb{R}_+)$. By Lemma 10, we have $\Sigma_\alpha^\beta(\mathbb{R}_-^d)=\Sigma_\alpha^\beta(\mathbb{R}_-)\hat{\otimes}_i\Sigma_\alpha^\beta(\mathbb{R}^{d-1})$ and Theorem 3 of Ref. 12 ensures that $S_\beta^\alpha(\mathbb{R}_+^d)=S_\beta^\alpha(\mathbb{R}_+)\hat{\otimes}_iS_\beta^\alpha(\mathbb{R}^{d-1})$. Let $L_1=P\hat{\otimes}_i\mathcal{F}$, where $\mathcal{F}$ is the (inverse) Fourier transformation on $\mathbb{R}^{d-1}$:

$$(\mathcal{F}f)(p^1,\ldots,p^{d-1})=(2\pi)^{-(d-1)}\int_{\mathbb{R}^{d-1}}f(\xi)e^{-i\xi^1p^1-\ldots-i\xi^{d-1}p^{d-1}}\,d\xi.$$

Obviously, L_1 is a continuous operator from $\Sigma_\alpha^\beta(\mathbb{R}_-^d)$ to $S_\beta^\alpha(\mathbb{R}_+^d)$ with a dense image. Besides, $(L_1f)(p)=\check{f}(p)$ for all $f\in\Sigma_\alpha^\beta(\mathbb{R}_-^d)$. Indeed, this equality holds for $f\in\Sigma_\alpha^\beta(\mathbb{R}_-)\otimes\Sigma_\alpha^\beta(\mathbb{R}^{d-1})$, and since both sides of the equality are continuous in f, it is valid everywhere on $\Sigma_\alpha^\beta(\mathbb{R}_-^d)$. Thus, the lemma is proved for $n=1$. For $n>1$, we make use of the representations $\Sigma_\alpha^\beta(\mathbb{R}_-^{dn})=\Sigma_\alpha^\beta(\mathbb{R}_-^d)\hat{\otimes}_i\cdots\hat{\otimes}_i\Sigma_\alpha^\beta(\mathbb{R}_-^d)$ and $S_\beta^\alpha(\mathbb{R}_+^{dn})=S_\beta^\alpha(\mathbb{R}_+^d)\hat{\otimes}_i\cdots\hat{\otimes}_iS_\beta^\alpha(\mathbb{R}_+^d)$ which follow by induction from (10), Lemma 10 and Theorem 3 of Ref. 12. Setting $L_n=L_1\hat{\otimes}_i\cdots\hat{\otimes}_iL_1$ and arguing as above, we make sure that L_n is a continuous operator from $\Sigma_\alpha^\beta(\mathbb{R}_-^{dn})$ to $S_\beta^\alpha(\mathbb{R}_+^{dn})$ with dense image and such that $(L_nf)(p)=\check{f}(p)$. The lemma is proved.

Substituting $u=\hat{W}_n$ in (17) yields

$$\int_{\mathbb{R}_-^{dn}}S_n(x)f(x)dx=\hat{W}_n(\check{f}),\quad f\in\Sigma_\alpha^\beta(\mathbb{R}_-^{dn}).\tag{19}$$

By condition (W3), there is a continuous seminorm P on $S_\beta^\alpha(\mathbb{R}_+^{dn})$ such that $|\hat{W}_n(f)|\leqslant P(f)$ for every test function in $S_\beta^\alpha(\mathbb{R}_+^{dn})$. By Lemma 9 and equality (19), it hence follows that $|S_n(f)|\leqslant P(\check{f})$, $f\in\Sigma_\alpha^\beta(\mathbb{R}_-^{dn})$.

Summarizing the above discussion, we obtain the following set of conditions on the Schwinger functions:

S1 (Growth and singularity) $s_n\in\Sigma_\alpha'^\beta(\mathbb{R}_{\neq}^{dn})$;

S2 (Euclidean invariance) $s_n(Tx_1+a,\ldots,Tx_n+a)=s_n(x_1,\ldots,x_n)$ for any rotation T and any $a\in\mathbb{R}^d$;

S3 (Laplace transform condition) There is a continuous seminorm P on $S_\beta^\alpha(\mathbb{R}_+^{dn})$ such that for every $f\in\Sigma_\alpha^\beta(\mathbb{R}_-^{dn})$ the inequality $|S_n(f)|\leqslant P(\check{f})$ holds, where $\check{f}$ is the function defined by formula (18);

S4 (Symmetry) $s_n(x_{\pi(1)},\ldots,x_{\pi(n)})=s_n(x_1,\ldots,x_n)$ for all permutations π of the indices.

We now can formulate the main result.

Theorem 5: *For a given sequence of Wightman functions w_n satisfying W1–W4, the corresponding sequence of the Schwinger functions s_n satisfies S1–S4. Conversely, generalized functions satisfying S1–S4 are the Schwinger functions corresponding to a uniquely determined sequence of Wightman functions satisfying W1–W4.*

Proof: The construction of the Schwinger functions corresponding to given Wightman functions and the derivation of the properties S1–S4 are given above and we only need to prove the converse statement. Let the sequence s_n satisfy S1–S4 and let L denote the image of $\mathbb{R}^{dn}_-$ under the mapping $f\to\check{f}$. By S3, the linear functional $\check{f}\to S_n(f)$ defined on L is continuous in the topology of $S^{\alpha}_{\beta}(\mathbb{R}^{dn}_+)$ and in view of Lemma 9 there is a uniquely determined generalized function $\hat{W}_n \in S'^{\alpha}_{\beta}(\mathbb{R}^{dn}_+)$ such that $\hat{W}_n(\check{f})=S_n(f)$, $f\in\Sigma^{\beta}_{\alpha}(\mathbb{R}^{dn}_-)$. The invariance of $\hat{W}_n$ under spatial rotations follows immediately from S2. To prove the invariance of $\hat{W}_n$ under pure Lorentz transformations, it suffices to show that $X_{0l}\hat{W}_n=0$, where $l=1,\ 2,\ 3$, $X_{0l}=\Sigma_{k=0}^{n}(p_k^0\partial/\partial p_k^l+p_k^l\partial/\partial p_k^0)$ are the infinitesimal generators of boosts. Let $Y_{0l}=\Sigma_{k=0}^{n}(\xi_k^0\partial/\partial\xi_k'-\xi_k^l\partial/\partial\xi_k^0)$ be the infinitesimal generators of Euclidean rotations. It is easy to see that $Y_{0l}f$ is taken to $X_{0l}\check{f}$ by the mapping $f\to\check{f}$ and hence $X_{0l}\hat{W}_n$ vanishes on L:

$$(X_{0l}\hat{W}_n)(\check{f})=-W_n(X_{0l}\check{f})=-S_n(Y_{0l}f)=(Y_{0l}S_n)(f)=0,\quad f\in\Sigma^{\beta}_{\alpha}(\mathbb{R}^{dn}_-).$$

Using Lemma 9 and the continuity of $\hat{W}_n$, we conclude that $X_{0l}\hat{W}_n=0$. By the proven Lorentz invariance, $\hat{W}_n$ belongs not only to $S'^{\alpha}_{\beta}(\mathbb{R}^{dn}_+)$, but also to every space $S'^{\alpha}_{\beta}((\Lambda\mathbb{R}^d_+)^n)$, where Λ is a proper Lorentz transformation, and, moreover, to every space $s'^{\alpha}_{\beta}(\Lambda\overline{\mathbb{R}}^d_+,\ldots,\Lambda\overline{\mathbb{R}}^d_+)$. Applying Theorem 2 and using the equality $\cap_{\Lambda}\Lambda\overline{\mathbb{R}}^d_+=\overline{\mathbb{V}}_+$, we conclude that $\overline{\mathbb{V}}^n_+$ is a strong carrier cone of $\hat{W}_n$. We now define the Wightman functions w_n by formula (2) and the second relation in (1). Obviously, w_n satisfy conditions W1, W2, and W3. Substituting $u=\hat{W}_n$ in (17) shows that s_n are indeed the Schwinger functions corresponding to w_n. The symmetry of s_n implies the symmetry of the Wightman functions w_n in their ordinary analyticity domain, whence property W4 is derived by the standard arguments.[23] The theorem is proved.

VI. WICK POWER SERIES

In this section, we show that the generalized spectral condition formulated in the preceding section is satisfied for the simplest examples of quantum fields with highly singular infrared behavior, namely, for the fields representable by infinite series in the Wick powers of an indefinite metric free field ϕ, i.e., by series of the form

$$\sum_{k=0}^{\infty} d_k:\phi^k:(x). \tag{20}$$

We assume that ϕ is a tempered operator-valued distribution acting in a Hilbert–Krein state space $\mathcal{H}$ (see Ref. 4 for the role of this condition). This means that $\mathcal{H}$ is endowed, in addition to an indefinite metric $\langle\cdot,\ \cdot\rangle$, by an auxiliary positive scalar product $(\cdot,\ \cdot)$ connected with $\langle\cdot,\ \cdot\rangle$ by the relation $\langle\Phi,\Psi\rangle=(\Phi,\theta\Psi)$, where $\Phi,\ \Psi\in\mathcal{H}$ and θ is a bounded self-adjoint operator such that $\theta^2=1$. The scalar product $(\cdot,\ \cdot)$ determines a distribution w_{maj}, which is called the majorant of the two-point vacuum average $w(x-x')=\langle\Psi_0,\phi(x)\phi(x')\Psi_0\rangle$, by the relation

$$(\phi(f)\Psi_0,\phi(g)\Psi_0)=\int w_{\mathrm{maj}}(x,x')\overline{f}(x)g(x')\mathrm{d}x\,\mathrm{d}x',$$

where Ψ_0 is the vacuum and f, g are test functions in the Schwartz space $S(\mathbb{R}^d)$. The the Krein structure implies[24] that $w_{\mathrm{maj}}(x,x')$ is the boundary value of a function $\mathbf{w}_{\mathrm{maj}}(z,z')$ holomorphic in the tubular domain $\{(z,z')\in\mathbb{C}^{2d}:\ y=\mathrm{Im}\,z\in\mathbb{V}_-,\ y'=\mathrm{Im}\,z'\in\mathbb{V}_+\}$. As in Ref. 25, we find it conve-

nient to characterize the infrared and ultraviolet behavior of the majorant by a pair of monotone nonnegative functions w_{IR} and w_{UV} increasing as their arguments tend to infinity and to zero, respectively, and satisfying the estimate

$$|\mathbf{w}_{\mathrm{maj}}(z,z')|\leqslant C(1+w_{\mathrm{IR}}(|z|+|z'|)+w_{\mathrm{UV}}(|y|+|y'|)),\quad (y,y')\in V\times V', \tag{21}$$

for any compact subcones V and V' of $\mathbb{V}_-$ and $\mathbb{V}_+$ (with constant C depending on V and V'). Formula (21) also allows to estimate the analytic two-point Wightman function $\mathbf{w}(z)$ because

$$|\mathbf{w}(x-x'-2iy)|^2\leqslant|\mathbf{w}_{\mathrm{maj}}(x-iy,x+iy)||\mathbf{w}_{\mathrm{maj}}(x'-iy,x'+iy)| \tag{22}$$

for all $y\in\mathbb{V}_+$. Indeed, as $\theta^2=1$, we have

$$|\langle\phi(f)\Psi_0,\phi(g)\Psi_0\rangle|\leqslant\|\phi(f)\Psi_0\|\|\phi(g)\Psi_0\|.$$

Taking $f(\xi)=(\nu/\sqrt{\pi})^{\mathrm{d}}e^{-\nu^2(\xi-x-iy)^2}$ and $g(\xi)=(\nu/\sqrt{\pi})^{\mathrm{d}}e^{-\nu^2(\xi-x'-iy)^2}$ and writing the left- and right-hand sides in this inequality as integrals over a plane in the analyticity domain and passing to the limit as $\nu\to\infty$, we immediately obtain (22). Choosing $V'=-V$ in (21) and substituting (21) in (22) yield

$$|\mathbf{w}(\zeta)|\leqslant C(1+w_{\mathrm{IR}}(2|\zeta|)+w_{\mathrm{UV}}(|\eta|)),\quad \eta=\mathrm{Im}\,\zeta\in V, \tag{23}$$

for any compact subcone V of $\mathbb{V}_-$ with C depending on V.

The following criterion allows finding the adequate test function space on which the series (20) is convergent.

Theorem 6: *Let ϕ be a free field acting in a Hilbert–Krein space $\mathcal{H}$, and let the positive majorant of its two-point Wightman function satisfy the inequality (21) with monotonic w_{IR} and w_{UV}. Let the coefficients d_k satisfy the condition*

$$|d_kd_l|\leqslant Ah^{k+l}|d_{k+l}| \tag{24}$$

with some A, $h>0$. Then the series (20) is well defined as an operator-valued generalized function on every space S_α^β such that $\alpha>0$, $\beta>1$, and the relations

$$\sum_k L^kk!|d_{2k}|w_{\mathrm{IR}}(r)^k\leqslant C_{L,\epsilon}e^{\epsilon r^{1/\alpha}},\quad \sum_k L^kk!|d_{2k}|w_{\mathrm{UV}}(t)^k\leqslant C_{L,\epsilon}e^{\epsilon l^{-1/(\beta-1)}} \tag{25}$$

hold for an arbitrarily large $L>0$ and an arbitrarily small $\epsilon>0$.

This theorem follows immediately from Theorem 3 of Ref. 25 because (25) implies the inequality

$$\inf_{t>0}e^{st}\sum_k L^kk!|d_{2k}|w_{\mathrm{UV}}(t)^k\leqslant C_{L,\epsilon}\exp[\beta(\epsilon/(\beta-1))^{(\beta-1)/\beta}s^{1/\beta}].$$

It is straightforward to verify that in the case $\alpha>1$, the sum of the series (20) satisfies the usual Wightman axioms (except positivity). For $0<\alpha<1$, we have the following theorem strengthening the results of Ref. 13.

Theorem 7: *Under the conditions of Theorem 6, the Wightman functions of the field $\varphi(x)=\Sigma_{k=0}^\infty d_k{:}\phi^k{:}(x)$ satisfy the requirements* W1–W4 *including the generalized spectral condition.*

Proof: The only nontrivial point is to check the fulfilment of the generalized spectral condition. The expression for the n-point vacuum expectation value of the field φ given by the Wick theorem is a power series in $n(n-1)/2$ variables $w(x_j-x_m)$ and can be written as

$$\langle\Psi_0,\varphi(x_1)\cdots\varphi(x_n)\Psi_0\rangle=\sum_K D_Kw^K,$$

where K is an integer-valued vector with nonnegative components k_{jm}, $1\leqslant j<m\leqslant n$, and $w^K(x)$ is the boundary value of the function $\mathbf{w}^K(z)=\Pi_{j<m}\mathbf{w}(z_j-z_m)^{k_{jm}}$ analytic in the tubular domain $\{z\in\mathbb{C}^{dn}: z_j-z_m\in\mathbb{R}^d+i\mathbb{V}_-, 1\leqslant j<m\leqslant n\}$. The usual combinatorial analysis related to the Wick theorem shows that

$$D_K=\frac{\kappa!}{K!}\prod_{1\leqslant j\leqslant n} d_{\kappa_j},$$

where $\kappa_j=k_{1j}+\cdots+k_{j-1,j}+k_{j,j+1}+\cdots+k_{jn}$ is the total number of pairings in the given term of the series that involve the argument x_j, and we follow the usual convention

$$K!=\prod_{j<m} k_{jm}!\,,\quad \kappa!=\prod_{1\leqslant j\leqslant n}\kappa_j!\,.$$

Correspondingly, the n-point Wightman function expressed in terms of the difference variables is given by

$$W_{n-1}(\xi)=\sum_K D_K W^K(\xi), \tag{26}$$

where $W^K(\xi)$ is the boundary value of the function $\mathbf{W}^K(\zeta)=\Pi_{j<m}\mathbf{w}(\zeta_j+\cdots+\zeta_{m-1})^{k_{jm}}$ analytic in the domain $\mathbb{R}^{d(n-1)}+i\mathbb{V}_-^{n-1}$. To prove the theorem, it is sufficient to establish that the series $\Sigma_K D_K\mathbf{W}^K$ converges unconditionally in $\mathcal{A}^\beta_\alpha(\mathbb{V}_-,\ldots,V_-)$. Indeed, in this case, Theorem 4 shows that $\hat{W}_{n-1}$, which is the inverse Laplace transform of the sum of this series, belongs to $s'^\alpha_\beta(\mathbb{V}_+,\ldots,\mathbb{V}_+)$, i.e., the generalized spectral condition is satisfied. Since $\mathcal{A}^\beta_\alpha$ is complete, it suffices to verify that

$$\sum_K |D_K|\|\mathbf{W}^K\|_{\epsilon,V_1,\ldots,V_{n-1}}<\infty \tag{27}$$

for any $\epsilon>0$ and any cones $V_1,\ldots,V_{n-1}$ compact in $\mathbb{V}_-$. Let V be the closed convex hull of the union $V_1\cup\cdots\cup V_{n-1}$. The cone V is the second dual cone of $V_1\cup\cdots\cup V_{n-1}$ and, therefore, is a compact subcone of $\mathbb{V}_-$ (because if $V\Subset U$ and U is an open cone, then $U^*\subset\operatorname{int}V^*$). Obviously, $\eta_j+\cdots+\eta_{m-1}\in V$ for any $\eta=(\eta_1,\ldots,\eta_{n-1})\in V_1\times\cdots\times V_{n-1}$ and for any $1\leqslant j<m\leqslant n$. Further, there is a $\lambda>0$ such that

$$|\eta_j+\cdots+\eta_{m-1}|\geqslant\lambda(|\eta_j|+\cdots+|\eta_{m-1}|) \tag{28}$$

for all $\eta\in\overline{\mathbb{V}_-}$ and $j<m$. Indeed, for fixed j and m, (28) is fulfilled if we take

$$\lambda=\lambda_{jm}=\inf_{(\eta_j,\ldots,\eta_{m-1})\in\overline{\mathbb{V}}_-^{m-j},\,|\eta_j|+\ldots+|\eta_{m-1}|=1}|\eta_j+\cdots+\eta_{m-1}|.$$

By the convexity of $\overline{\mathbb{V}_-}$, we have $\eta_j+\cdots+\eta_{m-1}=0$ if and only if $\eta_j=\cdots=\eta_{m-1}=0$. This implies that $\lambda_{jm}>0$ because the infimum is taken over a compact set. So we can set $\lambda=\min_{j<m}\lambda_{jm}$. By (23), (28), and the monotonicity of w_{IR} and w_{UV}, for $\zeta\in\mathbb{R}^{d(n-1)}+iV_1\times\cdots\times V_{n-1}$ we have

$$|\mathbf{W}^K(\zeta)|\leqslant(n+1)^{|K|}C^{|K|}\left(1+w_{\mathrm{IR}}(2n|\zeta|)^{|K|}+\sum_{i=1}^{n-1} w_{\mathrm{UV}}(\lambda|\eta_i|)^{|K|}\right), \tag{29}$$

where $|K|=\Sigma_{j<m}k_{jm}$. The condition (24) and the inequalities $|K|!/K!\leqslant(n(2n-1))^{|K|}$ and $\kappa!\leqslant|\kappa|!\leqslant 4^{|K|}(|K|!)^2$ following from the well-known properties of polynomial coefficients yield

$$|D_K| \leqslant A' h'^{|K|} |K|! |d_{2|K|}|, \tag{30}$$

where the constant h' depends on n. If w_{IR} and w_{UV} are not both identically zero (which is assumed), then (25) implies that for any $L>0$, there is a $\tilde{C}_L$ such that

$$k! |d_{2k}| \leqslant \tilde{C}_L L^{-k}, \quad k=0,1,\ldots. \tag{31}$$

Using (25), (29), (30), (31), and Definition 3, we obtain

$$|D_K| \|\mathbf{W}^K\|_{\epsilon, V_1, \ldots, V_{n-1}} \leqslant C'_{L,\epsilon} ((n+1) C h'/L)^{|K|}.$$

This proves (27) because the number of multi-indices K with fixed $|K|$ depends polynomially on $|K|$ and L is arbitrarily large. The theorem is proved.

VII. CONCLUSION

We see that the proposed formulation of the spectral condition offers a means for a reasonable generalization of a considerable part of the Wightman-type formalism to quantum fields with highly singular infrared behavior. In particular, gauge-dependent quark fields, which were claimed in Ref. 26 to be ill-defined mathematical objects, can be treated in this enlarged axiomatic framework. This situation is somewhat analagous to that in nonlocal QFT, where the corresponding generalization of local commutativity ensures the preservation of the PCT-symmetry[27] and the spin-statistics relation,[28] i.e., those basic physical results that are commonly believed to be consequences of locality.

In this paper, we have made no attempt to derive an appropriate extension to infrared singular fields of the Osterwalder–Schrader linear growth estimates which also ensure the reconstruction of Wightman functions from Schwinger functions and which proved to be effective in constructive QFT. At first glance, there are no obstacles for obtaining such a generalization provided the positivity condition is kept. However, this condition is violated for all relevant examples of infrared singular quantum fields. For this reason, we confined our consideration to the indefinite metric case.

We conclude by a remark on how a notion analogous to that of a strong carrier cone of an analytic functional can be introduced in the framework of Fourier hyperfunctions (i.e., functionals defined on S_1^1) which is universal for local QFT.[29,30] The construction given below is parallel to that of Sec. II.

Definition 1′: Let U be an open set in $\mathbb{R}^k$. The Banach space $S_{1,B}^{1,A}(U)$ consists of functions analytic in the $1/A$-neighborhood $U_{1/A}$ of U in $\mathbb{C}^k$ and having the finite norm

$$\|f\|_{U,A,B} = \sup_{w \in U_{1/A}} |f(w)| \exp(|p/B|).$$

The space $S_1^1(U)$ is defined to be the inductive limit $\lim_{\rightarrow A,B>0} S_{1,B}^{1,A}(U)$.

Let $\mathcal{R}^k$ be the radial compactification of $\mathbb{R}^k$. For $\mathcal{U} \subset \mathcal{R}^k$, we denote by $\tilde{\mathcal{U}}$ the set $\mathcal{U} \cap \mathbb{R}^k$. A compact set $\mathcal{K} \subset \mathcal{R}^k$ is said to be a carrier of a functional $u \in S_1'^1(\mathbb{R}^k)$ if u has a continuous extension to the space $s_1^1(\mathcal{K}) = \lim_{\rightarrow \mathcal{U}} S_1^1(\tilde{\mathcal{U}})$, where $\mathcal{U}$ runs over all open neighborhoods of $\mathcal{K}$ in $\mathcal{R}^k$.

The following definition is an analogue of Definition 2.

Definition 2′: Let $\mathcal{K}_1, \ldots, \mathcal{K}_n$ be compact sets in $\mathcal{R}^{k_1}, \ldots, \mathcal{R}^{k_n}$, respectively. The functional $u \in S_1'^1(\mathbb{R}^{k_1+\ldots+k_n})$ is said to be carried by the family of sets $\mathcal{K}_1, \ldots, \mathcal{K}_n$ if u has a continuous extension to the space $s_1^1(\mathcal{K}_1, \ldots, \mathcal{K}_n) = \lim_{\rightarrow \mathcal{U}_1, \ldots, \mathcal{U}_n} S_1^1(\tilde{\mathcal{U}}_1 \times \cdots \times \tilde{\mathcal{U}}_n)$, where the inductive limit is taken over all open neighborhoods $\mathcal{U}_1, \ldots, \mathcal{U}_n$ of the sets $\mathcal{K}_1, \ldots, \mathcal{K}_n$, respectively.

For $K\subset\mathbb{R}^k$, we denote by $\hat{K}$ the closure of K in $\mathcal{R}^k$. Let $K_1,\dots K_n$ be closed sets in $\mathbb{R}^{k_1},\dots,\mathbb{R}^{k_n}$, respectively, and let $K=K_1\times\cdots\times K_n$. The following example shows that the space $s_1'^1(\hat{K})$ is, in general, different from $s_1'^1(\hat{K}_1,\dots,\hat{K}_n)$.

Example 1′: Let $k_1=k_2=1$, $K_1=\overline{\mathbb{R}}_+$, $K_2=\{0\}$, and $K=\overline{\mathbb{R}}_+\times\{0\}$. Clearly, $s_1'^1(\hat{K}_1,\hat{K}_2)\subset s_1'^1(\hat{K})$. In this case, we can assume that $\tilde{\mathcal{U}}_{1,2}$ in Definition 2′ are just the ε-neighborhoods of $\mathbb{R}_+$ and $\{0\}$, respectively. If $\varepsilon<1/2$, then the sequence $g_n(p)=p_2^n e^{-p_1}$ converges to zero in every space $S^{1,A}_{1,B}(\tilde{\mathcal{U}}_1\times\tilde{\mathcal{U}}_2)$ with $A>2$ and $B>1$ and therefore is bounded in $s_1'(\hat{K}_1,\hat{K}_2)$. If the sequence g_n were bounded in the DFS-space $s_1^1(\hat{K})$, then it would be bounded in some space $S^{1,A}_{1,B}(\tilde{\mathcal{U}})$, where $\mathcal{U}$ is an open neighborhood of $\hat{K}$. However, any such $\mathcal{U}$ contains the ray $r_\lambda=\{(p_1,p_2):p_1\geqslant 0,p_2=\lambda p_1\}$ with some $\lambda>0$ and, therefore, we have $\|g_n\|_{\tilde{\mathcal{U}},A,B}\geqslant\sup_{p\in r_\lambda}|g_n(p)|=\lambda^n n^n e^{-n}$. Thus, the sequence g_n is unbounded in $s_1^1(\hat{K})$ and there is an $u\in s_1'^1(\hat{K})$ such that the number sequence $|u(g_n)|$ is unbounded (because any weakly bounded set in a locally convex space is bounded). Obviously, u does not belong to $s_1'^1(\hat{K}_1,\hat{K}_2)$ and so the latter is different from $s_1'^1(\hat{K})$.

This distinction may be essential for hyperfunction QFT, where the spectral condition can be formulated in two alternative ways. One can require either that $\hat{W}_n\in s_1'^1(\hat{\mathbb{V}}_+^n)$ as in Refs. 29 and 30 or that $\hat{W}_n\in s_1'^1(\hat{\mathbb{V}}_+,\dots,\hat{\mathbb{V}}_+)$. It would be worthwhile to examine the second condition from the viewpoint of the Euclidean formulation of hyperfunction QFT, but this is beyond the scope of the present paper.

ACKNOWLEDGMENTS

The author is grateful to M. A. Soloviev for helpful and stimulating discussions. This research was supported by the Russian Foundation for Basic Research (Grants Nos. 02-01-00556 and 00-15-96566) and INTAS (Grant No. 99-1-590).

APPENDIX A: PROOF OF LEMMA 1 FOR $\alpha=0$

Lemma 11: Let Q_1, Q_2 be nonempty cones in $\mathbb{R}^k$ and let h_1, h_2 be C^∞-functions on $\mathbb{C}^k$ such that $f=h_1+h_2$ is analytic in $\mathbb{C}^k$. If the norms $\|h_1\|_{Q_1,A,B}$, $\|h_2\|_{Q_2,A,B}$, and $\|\partial h_1/\partial\overline{w}_j\|_{Q_1\cup Q_2,A,B}$ [given by (4) with $\alpha=0$] are finite for some $A, B>0$, then one can find $f_{1,2}\in S^0_\beta(Q_{1,2})$ such that $f=f_1+f_2$.

Let us derive Lemma 1 from Lemma 11. Let $\chi\in C_0^\infty(\mathbb{R}^{k_1})$ satisfy $\int_{\mathbb{R}^{k_1}}\chi(p')\mathrm{d}p'=1$. We set $g_0(w')=\chi(\mathrm{Re}\,w')$ and define $g_{1,2}$ by (6). The functions $g_{1,2}(w)$ as well as their derivatives $\partial g_{1,2}/\partial\overline{w}_j$, $j=1,...,k_1+k_2$, satisfy the estimate (7) with $\alpha=0$ for any A_0, $B_0>0$. Therefore, setting $Q_{1,2}=(U\cup U_{1,2})\times V$ and repeating the proof for nonzero α, we conclude that the norms $\|fg_2\|_{Q_1,A,B}$, $\|fg_1\|_{Q_2,A,B}$, $\|f\partial g_2/\partial\overline{w}_j\|_{Q_1,A,B}$, and $\|f\partial g_1/\partial\overline{w}_j\|_{Q_2,A,B}$ are finite for A, B sufficiently large. Moreover, since $g_1+g_2=1$ and $\partial g_1/\partial\overline{w}_j=-\partial g_2/\partial\overline{w}_j$, we have $\|f\partial g_2/\partial\overline{w}_j\|_{Q_1\cup Q_2,A,B}<\infty$. Thus, $h_{1,2}=fg_{2,1}$ satisfy the conditions of Lemma 11 because $\partial h_1/\partial\overline{w}_j=f\partial g_2/\partial\overline{w}_j$ in view of the analyticity of f. Lemma 1 is proved.

Proof of Lemma 11: Let h be a measurable function on $\mathbb{C}^k$ and U be a nonempty cone in $\mathbb{R}^k$. For a, $b>0$ sufficiently large, from Definition (4) it follows that

$$C\|h\|_{U,A,B}\geqslant\|h\|'_{U,a,b}=\left[\int_{\mathbb{C}^k}|h(w)|^2\exp(-\rho_{U,a,b}(w))\mathrm{d}\lambda(w)\right]^{1/2},\tag{A1}$$

where $\rho_{U,a,b}(p+iq)=-\Sigma_{j=1}^k|p_j/b|^{1/\beta}+a\inf_{p'\in U}\Sigma_{j=1}^k|p_j-p'_j|+a\Sigma_{j=1}^k|q_j|$, $\mathrm{d}\lambda$ is the Lebesgue measure on $\mathbb{C}^k$, and C is a constant independent of h. If h is analytic, then using Cauchy's integral formula, one can prove[11] the converse statement, i.e., if $\|h\|'_{U,a,b}<\infty$ for some a, $b>0$, then $h\in S^0_\beta(U)$.

Suppose there is a locally integrable function ψ on $\mathbb{C}^k$ which has the finite norm $\|\psi\|'_{Q_1\cup Q_2,a_1,b_1}$ for some a_1, $b_1>0$ and satisfies, as a generalized function, the inhomogeneous Cauchy-Riemann equations

$$\frac{\partial\psi}{\partial\overline{w}_j}=\eta_j, \quad j=1,...,k, \tag{A2}$$

where $\eta_j=\partial h_1/\partial\overline{w}_j$. Then $f_1=h_1-\psi$ and $f_2=h_2+\psi$ satisfy, as generalized functions, the homogeneous equations $\partial f_{1,2}/\partial\overline{w}_j=0$ and, consequently, are ordinary analytic functions. Moreover, in view of (A1) we have $\|f_{1,2}\|'_{Q_{1,2},a,b}<\infty$ for $a\geqslant a_1$, $b>b_1$ sufficiently large, i.e., $f_{1.2}\in S^0_\beta(Q_{1.2})$. The following lemma allows to apply the Hörmander's L_2-estimates[31] to prove of the existence of a function ψ with the specified properties.

Lemma 12: For any a, $b>0$ and any nonempty cone $U\subset\mathbb{R}^k$ there are a plurisubharmonic function ρ on $\mathbb{C}^k$, positive numbers a', b', and a constant H such that $\rho_{U,a,b}-H\leqslant\rho\leqslant\rho_{U,a',b'}$.

Supposing Lemma 12 is proved, we finish the derivation of Lemma 11. Let $U=Q_1\cup Q_2$. By (A1) and the condition of Lemma 11, there are a, $b>0$ such that $\|\eta_j\|'_{U,a,b}<\infty$. According to Theorem 4.4.2 of Ref. 31 there exists a solution ψ of equations (A2) such that

$$2\int_{\mathbb{C}^k}|\psi|^2e^{-\rho}(1+\|w\|^2)^{-2}\mathrm{d}\lambda(w)\leqslant\sum_{j=1}^{k}\int_{\mathbb{C}^k}|\eta_j|^2e^{-\rho}\mathrm{d}\lambda(w), \tag{A3}$$

where $\|w\|=(|w_1|^2+\ldots+|w_k|^2)^{1/2}$. By Lemma 12, the integrals in the right-hand side are bounded by $e^H(\|\eta_j\|'_{U,a,b})^2$ and, therefore, are convergent. Estimating $e^{-\rho}$ in the left-hand side of (A3) from below by the function $e^{-\rho_{U,a',b'}}$, we conclude that $\|\tilde{\psi}\|'_{U,a',b'}<\infty$, where $\tilde{\psi}=(1+\|w\|^2)^{-1}\psi$. To complete the proof, it remains to note that $\|\psi\|'_{U,a_1,b_1}\leqslant C\|\tilde{\psi}\|'_{U,a',b'}$ for $a_1>a'$, $b_1>b'$.

Proof of Lemma 12 is essentially contained in the derivation of Theorem 5 of Ref. 12. We assume $0<a<1/2ek$; to pass to the general case, it suffices to make a rescaling of the arguments. Let $\sigma=eka$. By Lemma 4 of Ref. 12, there are a sequence $\varphi_N(w)\in S^0_\beta(\mathbb{R})$ and constants A, $B>0$ independent of N such that

$$|\varphi_N(w)|\leqslant A\exp(|q|-|p/b|^{1/\beta}), \quad w=p+iq\in\mathbb{C}, \tag{A4}$$

$$\ln|\varphi_N(iq)|\geqslant\sigma|q|, \tag{A5}$$

$$\ln|\varphi_N(w)|\leqslant|q|-N\ln^+(\sigma|p|/N)+B, \tag{A6}$$

where $\ln^+ r=\max(0,\ln r)$. Let $a'\geqslant 2$ and let

$$\tilde{\rho}(w)=\sup_{\kappa\in\mathbb{R}^k,N}\{\Phi_N(w-\kappa)+M_N(\kappa)\}, \quad M_N(\kappa)=\inf_{w\in\mathbb{C}^k}\{-\Phi_N(w-\kappa)+p_{U,a',b}(w)\}, \tag{A7}$$

where $\Phi_N(w)=2\Sigma_{j=1}^k\ln|\underline{\varphi_N}(w_j)|$. Obviously, we have $\tilde{\rho}\leqslant\rho_{U,a',b}$. Since functions Φ_N are plurisubharmonic, $\rho(w)=\lim_{w'\to w}\tilde{\rho}(w)$ is also a plurisubharmonic function, see Ref. 32, Sec. II.10.3. In view of the continuity of $\rho_{U,a',b}$ we have $\tilde{\rho}\leqslant\rho\leqslant\rho_{U,a',b}$ and it remains to show that $\tilde{\rho}\geqslant\rho_{U,a,b}-H$. From (A4) and the inequality $|p_j-\kappa_j|^{1/\beta}\geqslant|p_j|^{1/\beta}-|\kappa_j|^{1/\beta}$, it follows that

$$-\Phi_N(w-\kappa)/2-\sum_j|p_j/b|^{1/\beta}+\sum_j|q_j|\geqslant-k\ln A-\sum_j|k_j/b|^{1/\beta},$$

and hence $M_N(\kappa)\geqslant-k\ln A-\Sigma_j|\kappa_j/b|^{1/\beta}+L_N(\kappa)$, where

$$L_N(\kappa)=\inf_{w\in\mathbb{C}^k}\left\{-\Phi_N(w-\kappa)/2+\inf_{p'\in U}\sum_j|p_j-p'_j|+\sum_j|q_j|\right\}.$$

Therefore, estimating the supermum in (A7) from below by the value of the function at $\kappa=p=\mathrm{Re}\,w$ and taking (A5) and the inequality $2\sigma>a$ into account, we find that

$$\tilde{p}(w)\geqslant a\sum_j |q_j|-\sum_j |p_j/b|^{1/\beta}+\sup_N L_N(p)-k\ln A.$$

Thus, it suffices to show that $\sup_N L_N(p)\geqslant a\inf_{p'\in U}\Sigma_j|p_j-p'_j|-C$. Passing to the Euclidean norm $\|p\|$, using the elementary inequalities $\Sigma_j \ln^+|p_j|\geqslant\ln^+(\|p\|/\sqrt{k})$ and $\|p\|\leqslant\Sigma_j|p_j|$, and estimating Φ_N by (A6), we conclude that

$$L_N(p)\geqslant -kB+\inf_{\lambda\in\mathbb{R}^k}\{N\ln^+(\sigma\|\lambda\|/N\sqrt{k})+\delta_U(p+\lambda)\},$$

where $\delta_U(p)=\inf_{p'\in U}\|p-p'\|$. Estimating $\delta_U(p+\lambda)$ from below by $\max(\delta_U(p)-\|\lambda\|,0)$ and calculating the infimum with respect to λ yield $L_N(p)\geqslant N\ln^+(\sigma\delta_U(p)/N\sqrt{k})-kB$. Let $\delta_U(p)\geqslant e\sqrt{k}/\sigma$ and let N_0 be the integer part of $\sigma\delta_U(p)/e\sqrt{k}$. In view of the inequality $\Sigma_j|p_j|\leqslant\sqrt{k}\|p\|$ we find that

$$\sup_N L_N(p)\geqslant L_{N_0}\geqslant\frac{\sigma\delta_U(p)}{e\sqrt{k}}-1-kB\geqslant a\inf_{p'\in U}\sum_j|p_j-p'_j|-C.$$

Since $L_N(p)\geqslant -k\ln A$ by (A4), this inequality holds for all $p\in\mathbb{R}^k$ with a new constant C. The lemma is proved.

APPENDIX B: PROOF OF LEMMA 4

By Lemma 2 of Ref. 17, the spaces $L^{(1,2)}$ are representable as inductive limits of sequences of Banach spaces $L_k^{(1,2)}$ with injective connecting mappings $u_{km}^{(1,2)}:L_k^{(1,2)}\to L_m^{(1,2)}$, $1\leqslant k\leqslant m$, which take unit balls in $L_k^{(1,2)}$ to compact subsets of $L_m^{(1,2)}$. Let $M_k=L_k^{(1)}\otimes_i L_k^{(2)}=L_k^{(1)}\otimes_\pi L_k^{(2)}$ and $M=\varinjlim_k M_k$. We denote by $u_k^{(1,2)}$ and u_k the canonical embeddings of $L_k^{(1,2)}$ into $L^{(1,2)}$ and of M_k into M, respectively. One can identify the space M with $L^{(1)}\otimes_i L^{(2)}$ using the canonical separately continuous bilinear mapping from $L^{(1)}\times L^{(2)}$ into M which is uniquely determined by the relations

$$u_k^{(1)}(x_1)\otimes u_k^{(2)}(x_2)=u_k(x_1\otimes x_2),\quad x_{1,2}\in L_k^{(1,2)}. \tag{B1}$$

To prove the lemma, it suffices to show that this mapping is continuous. Let V be an absolutely convex neighborhood of the origin in M. Set $V_k=u_k^{-1}(V)$. We shall construct sequences of absolutely convex neighborhoods $V_k^{(1,2)}$ of the origin in $L_k^{(1,2)}$ such that

(i) $u_{km}^{(1,2)}(V_k^{(1,2)})\subset V_m^{(1,2)}$ for $m>k$;
(ii) $V_k^{(1)}\otimes V_k^{(2)}\subset V_k$, $k=1,2,\ldots$;
(iii) the set $u_{km}^{(1,2)}(V_k^{(1,2)})$ is compact in $L_m^{(1,2)}$ for $m>k$.

The sets $V^{(1,2)}=\cup_{k=1}^\infty u_k^{(1,2)}(V_k^{(1,2)})$ are neighborhoods of the origin in $L^{(1,2)}$ because they are absolutely convex [in view of (i)] and $[u_k^{(1,2)}]^{-1}(V^{(1,2)})$ contain $V_k^{(1,2)}$. Moreover, by (B1) and property (ii), we have $V^{(1)}\otimes V^{(2)}\subset V$, i.e., the mapping $(x,y)\to x\otimes y$ from $L^{(1)}\times L^{(2)}$ to M is continuous.

We construct the sequences $V_k^{(1,2)}$ by induction. Let $\tilde{V}_k$ denote the inverse image of V_k under the canonical bilinear mapping from $L_k^{(1)}\times L_k^{(2)}$ to M_k. Let $V_1^{(1,2)}$ be closed balls in $L_1^{(1,2)}$ such that $V_1^{(1)}\times V_1^{(2)}\subset\tilde{V}_1$. Suppose $V_1^{(1,2)},\ldots,V_k^{(1,2)}$ satisfying (i)–(iii) are constructed. The compactum $u_{k,k+1}^{(1)}(V_k^{(1)})\times u_{k,k+1}^{(2)}(V_k^{(2)})$ is contained in the open neighborhood of the origin $\tilde{V}_{k+1}$. Hence, there are closed balls $B^{(1,2)}$ in $L_{k+1}^{(1,2)}$ such that $[u_{k,k+1}^{(1)}(V_k^{(1)})+B^{(1)}]\times[u_{k,k+1}^{(2)}(V_k^{(2)})$

$+B^{(2)}]\subset\widetilde{V}_{k+1}$. Set $V_{k+1}^{(1,2)}=u_{k,k+1}^{(1,2)}(V_k^{(1,2)})+B^{(1,2)}$. Conditions (i) and (ii) are obviously satisfied. If $m>k+1$, then $u_{k+1,m}^{(1,2)}(V_{k+1}^{(1,2)})$ is the sum of the compact sets $u_{k,m}^{(1,2)}(V_k^{(1,2)})$ and $u_{k+1,m}^{(1,2)}(B^{(1,2)})$ and, therefore, is also compact.

To prove the second statement of the lemma it suffices to note that i- and π-topologies coincide on the tensor product of the Fréchet spaces $L^{(1)\prime}$ and $L^{(2)\prime}$ and that $(L^{(1)}\hat{\otimes}_\pi L^{(2)})'=L^{(1)\prime}\hat{\otimes}_\pi L^{(2)\prime}$ for arbitrary DF-spaces $L^{(1,2)}$ one of which is nuclear (see Ref. 19, Chap. IV, Problem 32). The lemma is proved.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

A symplectic framework for multiplane gravitational lensing

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(Received 16 October 2002; accepted 24 January 2003)

We construct a new framework for the study of multiplane gravitational lensing from the view point of symplectic geometry. Symplectic relations are used to compose the systems and weaker Lagrangian equivalence is applied for classifying the caustics of multiplane gravitational lensing. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1563042]

I. INTRODUCTION

Recently there appeared several articles considering gravitational lensing systems as applications of the theory of singularities for smooth mappings. The gravitational lensing is the deflection of light from a distant source (e.g., quasar) by an intervening matter distribution (e.g., a galaxy or a cluster of galaxies). The first gravitational lensed quasar was detected only in 1979. By now gravitational lensing is quite an active field in astrophysics.[1–3]

On the other hand, singularity theory of Lagrangian varieties[4,5] is the best natural setting for discussing optical systems. In fact, Petters and his collaborators[6,1] pointed out that a single gravitational lensing can be described in the framework of symplectic geometry. Especially the caustics in a single gravitational lensing system coincide with caustics in the theory of Lagrangian singularities. Moreover, they also investigate multiplane gravitational lensing as an application of singularity theory.[7,1] The standard treatment of gravitational lensing uses a notion of equivalence that yields either folds or cusps as the locally stable caustics for a k-plane lensing map (e.g., in Ref. 1). On the other hand, Levine and Petters[8] speculated that under a weaker notion of equivalence, some caustics other than folds and cusps would appear stable for lens systems exposed to a more restricted family of perturbations. However, in their framework for multiplane gravitation lensing generic caustics are the same as those for the single gravitational lensing. Current observed lensed systems fit with the standard notion of equivalence used in the lensing literature (where only folds or cusps appear). However, as instruments discover more and more lens systems, it may be possible to find a system that is exposed to more limited family of perturbations and for which caustics like handkerchief, etc., appear stable possibly for a ''short'' time period. Note that on cosmic time scales (i.e., of the order billions of years) events that last months or a few years are quite short, though such time periods are long enough on human time scales for us to carry out observations.

In this paper we propose the symplectic framework for multiplane gravitational lensing based on the notion of symplectic relation, which is a natural generalization of the notion of symplectic transformation (cf. Ref. 9). The original motivation for the paper was an attempt to describe expected nonstandard caustics in gravitational lensing using the weaker versions of Lagrangian equivalence acting on composite symplectic relations. These composites correspond to images of

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systems of gravitational rays by the subsequent gravitational lens, and their generic forms, described in the paper, reflect the complexity of composition.

In Sec. II we introduce the gravitational lensing problem and in Sec. III the problem is formulated in the language of Lagrangian stability and versality adapted to the product symplectic space of incoming and outgoing rays. The precise meaning of the composition of systems and their actions on the subsequent wave fronts represented by generating functions was introduced in Sec. IV. In Sec. V the local stability of double lensing systems was investigated and it is continued in Sec. VI by classification of the normal forms of generating pairs with respect to the natural groups of equivalences.

All manifolds and maps considered here are of class C^∞ unless stated otherwise.

II. GRAVITATIONAL LENSING

In this section we give a quick review of the basic concepts from the theory of gravitational lensing discussed already in Refs. 8, 7, 6, 10, 1, and 3.

(1) Single lensing (*cf., Refs. 6, 1, and 3*). Consider the typical single lens plane gravitational lensing as follows: We assume that the deflector is thin and apply the small angle approximation (cf., Ref. 6). The extra time with respect to the unperturbed ray is giving *the time-delay map*; $T_{\mathbf{s}}:\mathbb{R}^2\supset U\to\mathbb{R}$ defined by

$$T_{\mathbf{s}}(\mathbf{r})=(1+z_L)\left[\frac{d_{OL}d_{OS}}{2d_{LS}}\left\|\frac{\mathbf{s}}{d_{OS}}-\frac{\mathbf{r}}{d_{OL}}\right\|^2-\Psi(\mathbf{r})\right].$$

Here, z_L is the redshift of the lens plane, d_{OL},d_{OS},d_{LS} are angular diameter distances, $\mathbf{r}$ is the position on the lens plane where the ray hits, $\mathbf{s}$ is the position of the source, and $\Psi(\mathbf{r})$ is the two-dimensional potential of the deflector on the lens plane. *The deflector potentials* Ψ occurring in the time-delay map are given by

$$\Psi(\mathbf{r})=4\int_{\mathbb{R}^n}\sigma(\mathbf{r}')\ln\left\|\frac{\mathbf{r}'-\mathbf{r}}{d_{OL}}\right\|.$$

They are solutions of two-dimensional Poisson equation $\Delta\Psi(\mathbf{r})=8\pi\sigma(\mathbf{r})$, where $\sigma(\mathbf{r})$ is the surface mass density (cf., Fig. 1).

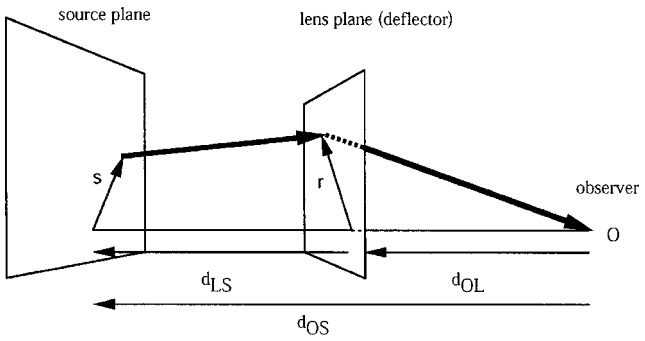

FIG. 1. A single lensing diagram. Angles are exaggerated. The distances are significantly larger than the diameter of the lens.

By suitable coordinate transformations, we can express the time-delay map in the convenient form:

$$T_{\mathbf{y}}(\mathbf{x}) = \Theta_L\left[\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2} - \psi(\mathbf{x})\right] \quad (\mathbf{x},\mathbf{y}\in\mathbb{R}^2).$$

Here **y** corresponds to the point on the source **s** plane and **x** corresponds to the point on the lens plane **r**.

Fermat's principle yields the critical points of the time delay map $T_{\mathbf{y}}(\mathbf{x})$ with respect to variations in **x** determining those rays that are real light rays (cf., Ref. 6). For this reason, a critical point of $T_{\mathbf{y}}(\mathbf{x})$ relative to **x** is called *an image* of the point source at **y**. *The magnification* of an image **x** of a source at **y** is defined by

$$A_{\mathbf{y}}(\mathbf{x}) = \frac{1}{\|\det T_{\mathbf{xx}}(\mathbf{x};\mathbf{y})\|},$$

where $T(\mathbf{x};\mathbf{y}) = T_{\mathbf{y}}(\mathbf{x})$ and $T_{\mathbf{xx}}(\mathbf{x};\mathbf{y})$ is the Hessian matrix with respect to **x**. *A caustic point* in gravitational lensing is a position $\mathbf{y}\in\mathbb{R}^2$ for which a source at **y** will have at least one image of infinite magnification. In other words, caustics are source positions $\mathbf{y}\in\mathbb{R}^2$ for which the time-delay map $T_{\mathbf{y}}(\mathbf{x})$ has at least one degenerate critical point (i.e., $\det T_{\mathbf{xx}}(\mathbf{x};\mathbf{y}) = 0$). So, we may consider that the time-delay map is *the generating family* of a certain Lagrangian submanifold in $T^*\mathbb{R}^2$ (cf., Sec. III).

(2) Multiplane gravitational lensing (cf., Refs. 8, 10, 1, and 3). Although we can consider a general k-planes gravitational lensing, we now only consider the case when $k=2$ (i.e, *a double plane gravitational lensing*) for convenience.

The typical double lens plane gravitational lensing situation is given as follows: There are two lens planes with ''thin'' deflectors in each plane. The deflectors are assumed to be independent, that is, the lens planes are sufficiently spaced so that they do not interact. Furthermore, the small angle approximation is assumed. We also parametrize all rays originating from the point source at **s**, deflected by two gravitational lens, using the four-dimensional vectors $(\mathbf{r}_1,\mathbf{r}_2)$. Relative to these approximations the extra time $T_{\mathbf{s}}$ to reach the indicated observer from **s** is given by the *time-delay map*. It is the function $T_{\mathbf{s}}: U_1\times U_2\subset\mathbb{R}^4\to\mathbb{R}$ with each domain $U_i\subset\mathbb{R}^2$ being an open subset, defined by

$$T_{\mathbf{s}}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{i=1}^{2}(1+z_i)\left[\frac{d_i d_{i+1}}{2d_{i,i+1}}\left\|\frac{\mathbf{r}_{i+1}}{d_{i+1}} - \frac{\mathbf{r}_i}{d_i}\right\|^2 - \Psi_i(\mathbf{r}_i)\right].$$

Here, z_i is the redshift of the ith lens plane, d_{ij} is the angular diameter distance separating the ith and jth lens planes, d_i is the angular diameter distance from the observer to the ith lens plane with $d_{k+1}\equiv d_S$ the distance to the source plane, $\mathbf{r}_i$ is the position on the ith plane where the ray hits, $\mathbf{r}_{k+1}\equiv\mathbf{s}$, and $\Psi_i(\mathbf{r}_i)$ is the two-dimensional potential of the deflector on the ith lens plane (cf., Fig. 2).

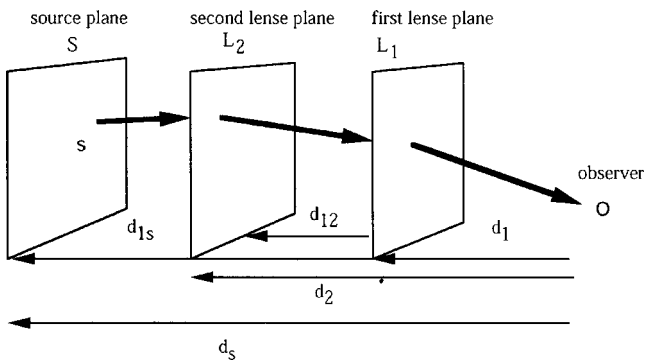

FIG. 2. A ray diagram for double plane gravitational lensing.

By suitable coordinate transformations, the double plane time-delay map can be expressed conveniently as follows:

$$T_{\mathbf{y}}(\mathbf{x}_1,\mathbf{x}_2)=\Theta_1\left[\frac{\|\mathbf{x}_2-\mathbf{x}_1\|^2}{2}-\beta_{1,2}\psi_1(\mathbf{x}_1)\right]+\Theta_2\left[\frac{\|\mathbf{x}_2-\mathbf{y}\|^2}{2}-\beta_{2,3}\psi_2(\mathbf{x}_2)\right],\quad (\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}\in\mathbb{R}^2).$$

In Ref. 10, Fermat's principle has been adapted exactly in the same way as it was used already for the single lens plane case, so that the *image* of a gravitational lensed point like light source at position $\mathbf{y}$ are identified to the critical points of $T_{\mathbf{y}}$, e.g., the set of images is given as follows:

$$\{(\mathbf{x}_1,\mathbf{x}_2)\,|\,\mathrm{grad}_{\mathbf{x}_i}\,T_{\mathbf{y}}(\mathbf{x}_1,\mathbf{x}_2)=\mathbf{0},\ \ i=1,2\}.$$

If we adapt this principle, then the classification of caustics for single and multiple lens planes is the same, namely, folds and cusps. It is, however, pointed out in Ref. 8 that double folds or handkerchiefs might appear as the stable caustics for double plane lensing under a more restricted family of perturbations. These singularities do not appear as generic caustics under the above-mentioned construction. Therefore, our opinion is that we need to have another interpretation of Fermat's principle.

III. A SYMPLECTIC FRAMEWORK FOR SINGLE GRAVITATIONAL LENSING

In Ref. 6 Petters pointed out that single gravitational lensing can be described in the framework of symplectic geometry (i.e, Lagrangian singularity theory). In the first place we briefly review the Lagrangian singularity theory.[4] Let $\pi:T^*\mathbb{R}^n\to\mathbb{R}^n$ be the cotangent bundle over $\mathbb{R}^n$. We may consider that $T^*\mathbb{R}^n=\mathbb{R}^{2n}$ and $\pi(q_1,\ldots,q_n;p_1,\ldots,p_n)=(q_1,\ldots,q_n)$, where $(q_1,\ldots,q_n;p_1,\ldots,p_n)$ are the canonical coordinates on $T^*\mathbb{R}^n$. There exits *the Liouville one-form* $\alpha=\Sigma_{i=1}^n p_i dq_i$ on $T^*\mathbb{R}^n$. We call the two-form $\omega=d\alpha=\Sigma_{i=1}^n dp_i\wedge dq_i$ *the canonical symplectic structure* on $T^*\mathbb{R}^n$. A *Lagrangian submanifold* $\iota:L\subset T^*\mathbb{R}^n$ is a submanifold with $L=n$ and $\iota^*\omega=0$. We call a map $\pi\circ\iota:L\to\mathbb{R}^n$ a *Lagrangian map*.

There is the notion of generating families for Lagrangian immersion germs as follows: Define an n-parameter family of function germs $F:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ to be a *Morse family* if the map germ

$$\frac{\partial F}{\partial\lambda}:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R}^k,0)$$

is nonsingular, where $\partial F/\partial\lambda(\lambda,q)=(\partial F/\partial\lambda_1(\lambda,q),\ldots,\partial F/\partial\lambda_k(\lambda,q))$. It follows that $\Sigma(F)=(\partial F/\partial\lambda)^{-1}(0)$ is a smooth submanifold germ in $(\mathbb{R}^k\times\mathbb{R}^n,0)$. For a Morse family F, we define a map germ

$$\Phi_F:\Sigma(F)\to T^*\mathbb{R}^n,\quad F_F(\lambda,q)=\left(q,\frac{\partial F}{\partial q}(\lambda,q)\right).$$

Then it is easy to see that Φ_F is a Lagrangian immersion germ. We also have the following well-known result:[4]

Proposition 3.1: All Lagrangian immersion germs are constructed by the above-presented method.

We call *F a generating family of* the Lagrangian submanifold germ $\Phi_F(\Sigma(F))$. By Proposition 3.1, we can interpret the local property of Lagrangian immersions by using the notion of generating family, so that the singularity theory of function germs has been applied.[4]

There is a natural equivalence among Lagrangian map germs. Let $\pi\circ\iota_i:(L_i,z_i)\to(R^n,\pi(z_i))$ $(i=1,2)$ be Lagrangian map germs. We say that $\pi\circ\iota_1:(L_1,z_1)\to(\mathbb{R}^n,\pi(z_1))$ and $\pi\circ\iota_2:(L_2,z_2)\to(\mathbb{R}^n,\pi(z_2))$ are *Lagrangian equivalent* if there exists a symplectic diffeomorphism germ $\Phi:(T^*\mathbb{R}^n,z_1)\to(T^*\mathbb{R}^n,z_2)$ with the form $\Phi(q,p)=(\phi_2(q),\phi_1(q,p))$ and a diffeomorphism germ $\phi:(L_1,z_1)\to(L_2,z_2)$ such that $\Phi\circ\iota_1=\iota_2\circ\phi$.

We also have natural corresponding equivalences among the Morse families. Let $F_i:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ $(i=1,2)$ be two Morse families. We say that F_1 and F_2 are R^+*-equivalent*

(respectively, *R-equivalent*) if there exists a diffeomorphism germ $\Psi:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R}^k\times\mathbb{R}^n,0)$ with the form $\Psi(\lambda,q)=(\psi_1(\lambda,q),\psi_2(q))$ and a function germ $\alpha:(\mathbb{R}^n,0)\to\mathbb{R}$ such that $F_1(\lambda,q)=F_2\circ\Psi(\lambda,q)+\alpha(q)$ (respectively, $F_1(\lambda,q)=F_2\circ\Psi(\lambda,q)$, i.e., α is constantly equal to 0). We also need the following generalized equivalence relation: For two Morse families $F_i:(\mathbb{R}^{k_i}\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ $(i=1,2)$, we say that F_1 and F_2 are *stably R^+-equivalent* if there exist nondegenerate quadratic forms $Q_1(\overline{\lambda}),Q_2(\tilde{\lambda})$, $(\overline{\lambda}\in\mathbb{R}^{k_3},\tilde{\lambda}\in\mathbb{R}^{k_4})$ with $k_1+k_3=k_2+k_4$ such that F_1+Q_1 and F_2+Q_2 are R^+-equivalent.

The following theorem is the principal result of the Lagrangian singularity theory:[4,5]

Theorem 3.2: *Let $F_i:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ $(i=1,2)$ be two Morse families.*

(1) If F_1 and F_2 induce the same Lagrangian submanifold germ, then F_1 and F_2 are R-equivalent.
(2) Lagrangian manifold germs $\Phi_{F_1}(\Sigma(F_1))$ and $\Phi_{F_2}(\Sigma(F_2))$ are Lagrangian equivalent if and only if F_1 and F_2 are stably R^+-equivalent.

We define the notion of stability of Lagrangian map germs as follows: A Lagrangian map germ is said to be *Lagrangian stable* if for every map representing the given map-germ there is a neighborhood $\mathcal{V}$ in the space of Lagrangian maps (in the C^∞-topology) and a neighborhood $\mathcal{U}$ of the source point of the germ, such that for each Lagrangian map belonging to $\mathcal{V}$ there is a point in $\mathcal{U}$ at which the germ of Lagrangian map-germ is Lagrangian equivalent to the original germ. The corresponding infinitesimal notion for generating family is given as follows: Let $F:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ be a Morse family. We say that F is *infinitesimally R^+-versal* if

$$\mathcal{E}_\lambda=\left\langle \frac{\partial f}{\partial\lambda_1},\ldots,\frac{\partial f}{\partial\lambda_k}\right\rangle_{\mathcal{E}_\lambda}+\left\langle \frac{\partial F}{\partial q_1}\middle|\mathbb{R}^k\times\{0\},\ldots,\frac{\partial F}{\partial q_n}|\mathbb{R}^k\times\{0\},1\right\rangle_{\mathbb{R}},$$

where $f(q)=F(q,0)$ and $\mathcal{E}_\lambda$ is the local ring of function germs $(\mathbb{R}^k,0)\to\mathbb{R}$. Then we have the following theorem (cf. Ref. 4).

Theorem 3.3: *Let $F:(\mathbb{R}^k\times\mathbb{R}^n,0)\to(\mathbb{R},0)$ be a Morse family. Then the Lagrangian map germ $\pi\circ\Phi_F$ is Lagrangian stable if and only if F is infinitesimally R^+-versal.*

Now let us recall the time-delay map $T_{\mathbf{y}}(\mathbf{x})$. If we consider the family of functions $F:\mathbb{R}^2\times\mathbb{R}^2\to\mathbb{R}$ given by

$$F(\lambda_1,\lambda_2,q_1,q_2)=\Theta\left[\frac{\|(\lambda_1,\lambda_2)-(q_1,q_2)\|^2}{2}-\psi(\lambda_1,\lambda_2)\right]=T_q(\lambda),$$

we can easily verify that F is a Morse family, so $\Phi_F:\Sigma(F)\to T^*\mathbb{R}^2$ is a Lagrangian immersion. Here, we have

$$\Sigma(F)=\{(\mathbf{x},\mathbf{y})|\operatorname{grad}_{\mathbf{x}}T=\mathbf{0}\},$$

so that the Lagrangian immersion is corresponding to those rays that are actual light rays. The set of critical values of the Lagrangian map $\pi\circ\Phi_F$ is the caustic.

On the other hand, we present another symplectic framework for single gravitational lensing, which is essentially the same as the above-mentioned framework. Our framework will be, however, very useful when we try to generalize this framework to the case of multiple planes gravitational lensing (cf., Sec. IV).

We consider the *product symplectic space*

$$\mathcal{M}_{(x,y)}=(T^*M_x\times T^*M_y,\omega_{M_y}\ominus\omega_{M_x}),$$

where ω_{M_y} and ω_{M_x} are the corresponding canonical symplectic forms, and $\Omega_{(x,y)}=\omega_{M_y}\ominus\omega_{M_x}=\pi_{M_y}^*\omega_{M_y}-\pi_{M_x}^*\omega_{M_x}$, where π_{M_x},π_{M_y} are the canonical projections of the product

$T^*M_x \times T^*M_y$. The corresponding phase spaces (T^*M_x, ω_{M_x}) and (T^*M_y, ω_{M_y}) are called the *observer space* and the *source space*, respectively. In our two-dimensional case $M_x = \mathbb{R}^2$ and $M_y = \mathbb{R}^2$. The concrete realized single lensing system is represented (following Ref. 6) by the Lagrangian submanifold

$$L_\psi = \{((\mathbf{x}, \mathrm{grad}_{\mathbf{x}} T), (\mathbf{y}, \mathrm{grad}_{\mathbf{y}} T)) \mid (\mathbf{x}, \mathbf{y}) \in M_x \times M_y\}.$$

This means that the generating function of L_ψ is the time-delay map

$$T(\mathbf{x}; \mathbf{y}) = \Theta_L \left[\frac{\|\mathbf{x} - \mathbf{y}\|^2}{2} - \psi(\mathbf{x}) \right] \quad (\mathbf{x}, \mathbf{y} \in \mathbb{R}^2).$$

By the previous arguments, light rays are given by $\{(\mathbf{x}, \mathbf{y}) \mid \mathrm{grad}_{\mathbf{x}} T = \mathbf{0}\}$ and the set of point sources for light rays is the Lagrangian submanifold

$$L_S = \{(\mathbf{y}, \mathrm{grad}_{\mathbf{y}} T) \in T^*M_y \mid (\mathbf{x}, \mathbf{y}) \in M_x \times M_y, \mathrm{grad}_{\mathbf{x}} T = \mathbf{0}\}$$

of T^*M_y. Then we have

$$\pi_{M_y}(L_\psi \cap ((M_x \times \{\mathbf{0}\}) \times T^*M_y)) = L_S.$$

Let us recall the basic notions of the theory of symplectic relations (Ref. 11). Let X_1, X_2 be smooth manifolds with the same dimension. We consider the product symplectic manifold

$$(T^*X_1 \times T^*X_2, \omega_{X_2} \ominus \omega_{X_1}),$$

where $\omega_{X_2} \ominus \omega_{X_1} = \pi_2^* \omega_{X_2} - \pi_1^* \omega_{X_1}$. We define a symplectic relation from T^*X_1 to T^*X_2 as a Lagrangian submanifold R of $(T^*X_1 \times T^*X_2, \omega_{X_2} \ominus \omega_{X_1})$. If the restriction of the projection

$$\pi_{X_1} \times \pi_{X_2} : T^*X_1 \times T^*X_2 \to X_1 \times X_2$$

to R is always nonsingular, we call R the *elementary symplectic relation*. Let R be a symplectic relation in $(T^*X_1 \times T^*X_2, \omega_{X_2} \ominus \omega_{X_1})$ and S be a subset of T^*X_1, then the symplectic image of S by R is defined as

$$R(S) = \{p_2 \in T^*X_2 : \exists_{p_1 \in S} (p_1, p_2) \in R\}.$$

If S is Lagrangian submanifold in (T^*X_1, ω_{X_1}), then $R(S)$ is a Lagrangian subset in (T^*X_2, ω_{X_2}).

Since both S and R are Lagrangian submanifolds, we have their generating families at least locally. We only consider the local situation here, so that we assume that $X_1 = X_2 = \mathbb{R}^n$. Let $F_1 : (\mathbb{R}^{k_1} \times X_1, 0) \to \mathbb{R}$ be a generating family of a Lagrangian submanifold germ $S \subset T^*X_1$ and $F_2 : (\mathbb{R}^{k_2} \times (X_1 \times X_2), 0) \to \mathbb{R}$ be a generating family of a symplectic relation $R \subset T^*X_1 \times T^*X_2$. Then we have a function germ

$$F : ((\mathbb{R}^{k_1} \times X_1 \times \mathbb{R}^{k_2}) \times X_2, 0) \to \mathbb{R}$$

defined by

$$F((\lambda_1, q_1, \lambda_2), q_2) = F_1(\lambda_1, q_1) + F_2(\lambda_2, q_1, q_2).$$

Hence we have the following lemma:

Lemma 3.4: If F is a Morse family, then F is a generating family of the Lagrangian submanifold $R(S) \subset T^*X_2$.

Proof: By definition, we have

$$S=\left\{\left(q_1,\frac{\partial F_1}{\partial q_1}(\lambda_1,q_1)\right)\middle|\frac{\partial F_1}{\partial \lambda_1}=0\right\},$$

$$R=\left\{\left(q_1,q_2,-\frac{\partial F_2}{\partial q_1}(\lambda_2,q_1),\frac{\partial F_2}{\partial q_2}(\lambda_2,q_2)\right)\middle|\frac{\partial F_2}{\partial \lambda_2}=0\right\}.$$

Therefore we have

$$R(S)=\left\{\left(q_2,\frac{\partial F_2}{\partial q_2}(\lambda_2,q_1,q_2)\right)\middle|\frac{\partial F_1}{\partial \lambda_1}=\frac{\partial F_2}{\partial \lambda_2}=0\,\frac{\partial F_1}{\partial q_1}=-\frac{\partial F_2}{\partial q_1}\right\}.$$

Since $\partial F/\partial\lambda_1=\partial F_1/\partial\lambda_1$, $\partial F/\partial\lambda_2=\partial F_2/\partial\lambda_2$, $\partial F/\partial q_1=\partial F_1/\partial q_1+\partial F_2/\partial q_2$ and $\partial F/\partial q_2=\partial F_2/\partial q_2$, we have

$$R(S)=\left\{\left(q_2,\frac{\partial F}{\partial q_2}((\lambda_1,q_1,\lambda_2),q_2)\right)\middle|\frac{\partial F}{\partial \lambda_1}=\frac{\partial F}{\partial \lambda_2}=\frac{\partial F}{\partial q_1}=0\right\},$$

so that F is a generating family of $R(S)$. Q.E.D.

In the case of single gravitational lensing, if S_0 denotes the observer Lagrangian submanifold of system of gravitational rays then the source Lagrangian submanifold of rays is an image

$$L_\psi(S_0)\subset T^*M_y.$$

In the standard setting (cf. Ref. 6 and the previous arguments) S_0 is the zero section of the cotangent bundle T^*M_x. Therefore we have

$$L_\psi(S_0)=\{(\mathbf{y},\mathrm{grad}_{\mathbf{y}}\,T)\,|\,\mathrm{grad}_{\mathbf{x}}\,T=\mathbf{0}\},$$

so that the generating family for $L_\psi(S_0)$ is given by

$$F(\lambda_1,\lambda_2,q_1,q_2)=\Theta\left[\frac{\|(\lambda_1,\lambda_2)-(q_1,q_2)\|^2}{2}-\psi(\lambda_1,\lambda_2)\right],$$

which is the same generating family as that of the source Lagrangian submanifold in the previous framework in Ref. 6. We call the pair (S,R) a (*single*) *lensing system* if S is a Lagrangian submanifold of T^*X_1 and R is a symplectic relation from T^*X_1 to T^*X_2. If the projection $\pi_1|_R:R\to T^*X_1$ is nonsingular, R is the graph of a symplectomorphism $H:T^*M_x\to T^*M_y$. In this case we say that (S,R) is *regular*. Moreover, if S is the zero section of T^*X_1, we call (S,R) a *special lensing system*. Therefore, the single gravitational lensing is a regular special lensing system.

IV. A SYMPLECTIC FRAMEWORK FOR MULTIPLANE GRAVITATIONAL LENSING

In this section we will construct the intrinsic framework for the study of gravitational lensing.

We can summarize the main problem in this paper as follows:

Problem: How can we construct the intrinsic framework for the study of double planes gravitational lensing?

In order to tackle this problem, we now interpret the Fermat's principle from another view point. We define

$$T_{\beta_{23}}(\mathbf{x}_2;\mathbf{y})=\Theta_2\left[\frac{\|\mathbf{y}-\mathbf{x}_2\|^2}{2}-\beta_{23}(\mathbf{x}_2)\right],$$

$$T_{\beta_{12}}(\mathbf{x}_1;\mathbf{x}_2)=\Theta_1\left[\frac{\|\mathbf{x}_2-\mathbf{x}_1\|^2}{2}-\beta_{12}(\mathbf{x}_1)\right].$$

Then $T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=T_{\beta_{12}}(\mathbf{x}_1,\mathbf{x}_2)+T_{\beta_{23}}(\mathbf{x}_2,\mathbf{y})$. We may consider that $T_{\beta_{23}}(\mathbf{x}_1,\mathbf{x}_2)$ and $T_{\beta_{12}}(\mathbf{x}_1;\mathbf{y})$ are, respectively, single time-delay maps. It is clear that

$$\mathrm{grad}_{\mathbf{x}_1} T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathrm{grad}_{\mathbf{x}_1} T_{\beta_{12}}(\mathbf{x}_1;\mathbf{x}_2),$$

$$\mathrm{grad}_{\mathbf{x}_2} T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathrm{grad}_{\mathbf{x}_2} T_{\beta_{12}}(\mathbf{x}_1;\mathbf{x}_2)+\mathrm{grad}_{\mathbf{x}_2} T_{\beta_{23}}(\mathbf{x}_2;\mathbf{y}).$$

These formulas suggest to us that the Fermat's principle can be interpreted as

$$\begin{cases}\mathrm{grad}_{\mathbf{x}_1} T_{\beta_{23}}(\mathbf{x}_1,\mathbf{x}_2)=\mathbf{0},\\ \mathrm{grad}_{\mathbf{x}_2} T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathbf{0}.\end{cases}$$

It follows that we consider the following families of functions: $F_1(\mathbf{x}_1,\mathbf{x}_2)=T_{\beta_{12}}(\mathbf{x}_1,\mathbf{x}_2)$, $F_2(\mathbf{x}_2,\mathbf{y})=T_{\beta_{23}}(\mathbf{x}_2,\mathbf{y})$ and $F(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=F_1(\mathbf{x}_1,\mathbf{x}_2)+F_2(\mathbf{x}_2,\mathbf{y})$. By Fermat's principle, we have two submanifolds:

$$\Sigma(F_1)=\{(\mathbf{x}_1,\mathbf{x}_2)\in\mathbb{R}^4 \mid \mathrm{grad}_{\mathbf{x}_1} F_1(\mathbf{x}_1,\mathbf{x}_2)=\mathbf{0}\},$$

$$\Sigma(F)=\{(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})\in\mathbb{R}^6 \mid \mathrm{grad}_{\mathbf{x}_1} F_1(\mathbf{x}_1;\mathbf{x}_2)=\mathrm{grad}_{\mathbf{x}_2} F(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathbf{0}\}.$$

Dimensions of both submanifolds are two. Moreover, we define the following mappings:

$$\Phi_{F_1}:\Sigma(F_1)\to T^*\mathbb{R}^2$$

by $\Phi_{F_1}(\mathbf{x}_1,\mathbf{x}_2)=(\mathbf{x}_2,\mathrm{grad}_{\mathbf{x}_2} F_1(\mathbf{x}_1,\mathbf{x}_2))$ and

$$\Phi_F:\Sigma(F)\to T^*\mathbb{R}^2$$

by $\Phi_F(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=(\mathbf{y},\mathrm{grad}_{\mathbf{y}} F(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}))$. By the previous arguments, images of both mappings are Lagrangian submanifolds. The later Lagrangian submanifold corresponds to the light source. The first Lagrangian submanifold corresponds to the light ray image on the second lens, since the distance between the first lens and the second lens is so long that there might be no interactions between these lenses. So we have to consider the stability of light ray under the independent perturbations of each lens planes.

On the other hand, we might consider that $F_2(\mathbf{x}_2,\mathbf{y})$ is a generating function of the graph of a certain symplectomorphism $H:T^*\mathbb{R}^2\to T^*\mathbb{R}^2$ (cf., Ref. 11). In this case, the Lagrangian submanifold $\Phi_F(\Sigma(F))$ can be considered as the image $H(\Phi_{F_1}(\Sigma(F_1)))$.

Since the single lensing system can be described under the framework of symplectic relations, we might construct the framework for the double gravitation lensing by using the composition of two symplectic relations.

The composition $R_2\circ R_1\subset(T^*X_1\times T^*X_3,\omega_{X_3}\ominus\omega_{X_1})$ of two symplectic relations $R_1\subset(T^*X_1\times T^*X_2,\omega_{X_2}\ominus\omega_{X_1})$, $R_2\subset(T^*X_2\times T^*X_3,\omega_{X_3}\ominus\omega_{X_2})$ is defined as follows:

$$R_2\circ R_1=\{(p_1,p_3)\in T^*X_1\times T^*X_3;\exists_{p_2\in T^*X_2}(p_1,p_2)\in R_1 \text{and } (p_2,p_3)\in R_2\}.$$

If S is Lagrangian submanifold in T^*X_1, then we have two symplectic images

$$R_1(S) \text{ and } R_2\circ R_1(S).$$

By the previous arguments, a double gravitational lensing is represented by the pair of symplectic relations $(L_{\beta_{12}},L_{\beta_{23}})$,

$$L_{\beta_{12}}\subset(T^*M_{x_1}\times T^*M_{x_2},\omega_{M_{r_2}}\ominus\omega_{M_{x_1}}),$$

$$L_{\beta_{23}}\subset(T^*M_{x_2}\times T^*M_y,\omega_{M_y}\ominus\omega_{M_{x_2}}).$$

Now the source Lagrangian subspace of the system is the image by the composition; $L_{\beta_{23}}\circ L_{\beta_{12}}(S_0)$, where S_0 is the zero section of $T^*M_{x_1}$. Since $T_{\beta_{12}}(\mathbf{x}_1,\mathbf{x}_2)$ and $T_{\beta_{23}}(\mathbf{x}_2,\mathbf{y})$ are the corresponding generating functions for the symplectic relations (the graphs of symplectomorphism) $L_{\beta_{12}}$ and $L_{\beta_{23}}$, then the configurational positions of rays emitted from the source at a point $\mathbf{y}$ are the points $((\mathbf{x}_1,\mathbf{x}_2),(\mathbf{x}_2,\mathbf{y}))\in L_{\beta_{12}}\times L_{\beta_{23}}$ given by the solutions $(\mathbf{x}_1,\mathbf{x}_2)$ of the system of equations

$$\mathrm{grad}_{\mathbf{x}_1}T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathbf{0}, \tag{1}$$

$$\mathrm{grad}_{\mathbf{x}_2}T_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y})=\mathbf{0}. \tag{2}$$

If we now consider a family of functions $F:\mathbb{R}^2\times\mathbb{R}^2\times M_y\to\mathbb{R}$ defined by

$$F(q,\lambda,\mu)=T_2(q,\lambda,\mu)=T_{\beta_{12}}(q,\lambda)+T_{\beta_{23}}(\lambda,\mu),$$

then F is a generating family for the image Lagrangian subspace

$$L_{\beta_{23}}\circ L_{\beta_{12}}(S_0)\subset T^*M_y.$$

According to the above-given arguments, we say that (S,R_1,R_2) is a *double lensing system* if S is a Lagrangian submanifold of T^*X_1 and R_i is a symplectic relation from T^*X_i to T^*X_{i+1}, where $i=1,2$. We also say that the double lensing system (S,R_1,R_2) is *regular* if both of R_i $(i=1,2)$ are graphs of symplectomorphisms. Moreover, we say that a double lensing system (S,R_1,R_2) is *special* if S is the zero section of T^*X_1. Therefore, a double gravitation lensing is a regular special double lensing system.

We now define a natural equivalence relation among double lensing system germs. Let $(S,R_1,R_2),(S',R_1',R_2')$ be double lensing system germs. We say that (S,R_1,R_2), (S',R_1',R_2') are *Lagrangian equivalent* if there exist a symplectic diffeomorphism germ and

$$\Phi_1:(T^*X_1,z_1)\to(T^*X_1,z_1'),$$

Lagrangian equivalence germs (symplectic diffeomorphisms preserving the cotangent bundle fibration)

$$\Phi_2:(T^*X_2,z_2)\to(T^*X_2,z_2'),\quad \Phi_3:(T^*X_3,z_3)\to(T^*X_3,z_3')$$

such that $\Phi_1(S)=S'$, $(\Phi_1\times\Phi_2)(R_1)=R_1'$ and $(\Phi_2\times\Phi_3)(R_2)=R_2'$.

Since there always exists a symplectic diffeomorphism germ $\Phi_1:(T^*X_1,z_1)\to(T^*X_1,z_1')$ such that $\Phi_1(S)=S'$, we may assume that $S=S'$ are equal to the zero section of T^*X_1. Therefore, without the loss of generality, we stick to special double lensing. In this case we say that (S,R_1,R_2), (S,R_1',R_2') are *strictly Lagrangian equivalent* if there exist Lagrangian equivalence germs

$$\Phi_2:(T^*X_2,z_2)\to(T^*X_2,z_2'),\quad \Phi_3:(T^*X_3,z_3)\to(T^*X_3,z_3')$$

such that $(\mathrm{id}_{T^*X_1}\times\Phi_2)(R_1)=R_1'$ and $(\Phi_2\times\Phi_3)(R_2)=R_2'$. This equivalence relation might be, however, too strong to give a classification of double lensing system germs. Therefore, we need an appropriate equivalence relation among special double lensing system germs.

Now we give a candidate of such a natural equivalence. We say that the special double lensing system germs (S,R_1,R_2), (S,R_1',R_2') are *weakly Lagrangian equivalent* if there exist Lagrangian equivalence germs

$$\tilde{\Phi}_3:(T^*X_3,z_3)\to(T^*X_3,z_3'),\quad \tilde{\Phi}:((T^*X_2\times T^*X_3,(z_2,z_3))\to(T^*X_2\times T^*X_3,(z_2',z_3'))$$

such that $\pi_{X_3}\circ\tilde{\Phi}=\tilde{\Phi}_3\circ\pi_{X_3}$ and $\tilde{\Phi}(R_1(S)\times R_2\circ R_1(S))=R_1'(S)\times R_2'\circ R_1'(S)$.

We have the following proposition.

Proposition 4.1: Suppose that (S,R_1,R_2), (S,R_1',R_2') *are weakly Lagrangian equivalent, then both of the Lagrangian submanifolds* $R_1(S)$, $R_1'(S)$ *and* $R_2\circ R_1(S)$, $R_2'\circ R_2'(S)$ *are Lagrangian equivalent*.

Proof: By definition we have a diffeomorphism germ $\Phi:(X_2\times X_3,(\pi_2(z_2),\pi_3(z_3)))\to(X_2\times X_3,(\pi_2(z_2'),\pi_3(z_3')))$ of the form $\Phi(x_2,x_3)=(\phi_2(x_2,x_3),\phi_3(x_3))$ and a symplectic diffeomorphism $\tilde{\Phi}:((T^*X_2\times T^*X_3,(z_2,z_3))\to(T^*X_2\times T^*X_3,(z_2',z_3'))$ of the form

$$\tilde{\Phi}((x_2,p_2),(x_3,p_3))=((\phi_2(x_2,x_3),\psi_2(x_2,x_3,p_2,p_3)),\phi_3(x_3),\psi_3(x_3,p_3))$$

such that $\tilde{\Phi}(R_1(S)\times R_2\circ R_3(S))=R_1'(S)\times R_2'\circ R_1'(S)$. Therefore we have $\tilde{\Phi}(R_1(S)\times\{z_3\})=(R_1'(S)\times\{z_3'\})$. We identify symplectic manifolds: $T^*X_2=T^*X_2\times\{z_3\}=T^*X_2\times\{z_3'\}$. Under this identification, the above-mentioned equality means that $R_1(S)$ and $R_1'(S)$ are Lagrangian equivalent.

By definition, we have $\tilde{\Phi}_3(R_2\circ R_1(S))=R_2'\circ R_1'(S)$. This fact means that $R_2\circ R_1(S)$, $R_2'\circ R_2'(S)$ are Lagrangian equivalent. Q.E.D.

By the above-given proposition, the weak Lagrangian equivalence among double lensing system germs preserve both caustics of the first and the second deflectors. It is the caustic equivalence already introduced in the classification of coisotropic varieties in Ref. 12.

V. GENERATING PAIRS FOR DOUBLE LENSING SYSTEMS

In this section we consider the problem how to construct a kind of the notion of generating families for double lensing systems. We already have a solution because a double plane gravitational lensing is described by the pair of time-delay maps. We only consider local properties, so that we assume that $X_1=X_2=X_3=\mathbb{R}^n$.

For any double lensing system germ (S,R_1,R_2), we have generating families $F_0:(\mathbb{R}^{k_0}\times X_1,0)\to\mathbb{R}$ of S, $F_1:(\mathbb{R}^{k_1}\times(X_1\times X_2),0)\to\mathbb{R}$ of R_1 and $F_2:(\mathbb{R}^{k_2}\times(X_2\times X_3),0)\to\mathbb{R}$ of R_2.

On the other hand, there always exists a symplectomorphism germ $\Phi_1:(T^*X_1,z_1)\to(T^*X_1,0)$ such that $\Phi_1(S)$ is a zero section germ of T^*X_1, so that we might assume that S is a zero section germ of T^*X_1 under the Lagrangian equivalence among double lensing system germs. In other words, it is enough to investigate special double lensing system germs. In this case F_0 can be chosen as a constant function. We call (F_1,F_2) a *generating pair* of the special lensing system germ (S,R_1,R_2) if F_i is a generating family of R_i $(i=1,2)$. Then F_1 can be regarded as a generating family of $R_1(S)\subset T^*X_2$ and $F=F_1+F_2$ is a generating family of $R_2\circ R_1(S)\subset T^*X_3$ (cf., Ref. 11).

Since a double gravitation lensing is a regular double lensing system, we now pay attention to regular special double lensing systems here. In this case $F_1:(X_1\times X_2,0)\to\mathbb{R}$ is a generating function of R_1 and $F_2:(X_2\times X_3,0)\to\mathbb{R}$ is a generating function of R_2. By the arguments in the previous paragraph, F_1 is a generating family of the Lagrangian submanifold germ $R_1(S)\subset T^*X_2$ and a map germ $F:((X_1\times X_2)\times X_3,0)\to\mathbb{R}$ defined by

$$F((x_1,x_2),x_3)=F_1(x_1,x_2)+F_2(x_2,x_3)$$

is a generating family of the Lagrangian submanifold germ $R_2 \circ R_1(S) \subset T^*X_3$. In other words, (F_1,F_2) is a *generating pair* of a regular special double lensing system germ (S,R_1,R_2) if $(dF_1(X_1\times X_2),(z_1,z_2))=(R_1,(z_1,z_2))$ and $(dF_2(X_2\times X_3),(z_2,z_3))=(R_2,(z_2,z_3))$.

Since any elementary symplectic relation has a generating function at least locally, we have the following fundamental proposition:

Proposition 5.1: All regular special double lensing system germs are constructed by the above-mentioned method.

We can translate equivalence relations among double lensing systems into those of corresponding generating pairs. We consider the ambiguity of the choice for generating pairs of a double lensing system.

Proposition 5.2: Let (F_1,F_2) *and* (G_1,G_2) *be generating pairs of a common regular special double lensing system germ. Then* $F_1=G_1+\text{constant}$ *and* $F_2=G_2+\text{constant}$.

For our purpose, we introduce equivalence relations among generating pairs for double lensing system germs. Let $F_1,G_1,(X_1\times X_2,0)\to\mathbb{R}$ and $F_2,G_2,(X_2\times X_3,0)\to\mathbb{R}$ be function germs. We say that (F_1,F_2) and (G_1,G_2) are $(R,L)^+$*-equivalent* if there exist diffeomorphism germs $\Phi_1:(X_1\times X_2,0)\to(X_1\times X_2,0)$ of the form $\Phi_1(x_1,x_2)=(\phi_1(x_1,x_2),\phi_2(x_2))$, and $\Phi_2:(X_2\times X_3,0)\to(X_2\times X_3,0)$ of the form $\Phi_2(x_2,x_3)=(\phi_2(x_2),\phi_3(x_3))$ and function germs $\alpha:(X_2,0)\to\mathbb{R}$, $\beta:(X_3,0)\to\mathbb{R}$ such that

$$\begin{cases} F_1(x_1,x_2)=G_1\circ\Phi_1(x_1,x_2)+\alpha(x_2), \\ F_2(x_2,x_3)=G_2\circ\Phi_2(x_2,x_3)+\beta(x_3). \end{cases}$$

Proposition 5.3: Let (F_1,F_2) *and* (G_1,G_2) *be, respectively, generating pairs of special regular double lensing system germs* (S_0,R_1,R_2) *and* $(S_0,R_1',R_2'))$. *Then* (S_0,R_1,R_2) *and* $(S_0,R_1',R_2'))$ *are strictly Lagrangian equivalent if and only if* (F_1,F_2) *and* (G_1,G_2) *are* $(R,L)^+$*-equivalent.*

We also say that (F_1,F_2) and (G_1,G_2) are $R\times L^+$*-equivalent* if there exists a diffeomorphism germ

$$\Phi:(X_1\times X_2\times X_3,0)\to(X_1\times X_2\times X_3,0)$$

of the form $\Phi(x_1,x_2,x_3)=(\phi_1(x_1,x_2,x_3),\phi_2(x_2,x_3),\phi(x_3))$ and a function germ $\alpha:(X_3,0)\to\mathbb{R}$ such that

$$F_1(x_1,x_2)+F_2(x_2,x_3)=G_1(\phi_1(x_1,x_2,x_3),\phi_2(x_2,x_3))+G_2(\phi_2(x_2,x_3),\phi(x_3))+\alpha(x_3).$$

Suppose that (F_1,F_2) and (G_1,G_2) are $R\times L^+$*-equivalent.* If we substitute $x_3=0$ into the both sides of the above-given equality, then we have

$$F_1(x_1,x_2)+F_2(x_2,0)=G_1(\phi_1(x_1,x_2,0),\phi_2(x_2,0))+G_2(\phi_2(x_2,0),0)+\alpha(0).$$

Therefore, F_1 and G_1 are R^+-equivalent.

By the general theory for Lagrangian singularities (cf., Ref. 4), we can show the following proposition:

Proposition 5.4: Let (F_1,F_2) *and* (G_1,G_2) *be, respectively, generating pairs of special regular double lensing system germs* (S_0,R_1,R_2) *and* $(S_0,R_1',R_2'))$. *Then* (S_0,R_1,R_2) *and* $(S_0,R_1',R_2'))$ *are weakly Lagrangian equivalent if and only if* (F_1,F_2) *and* (G_1,G_2) *are* $R\times L^+$*-equivalent.*

We say that (F_1,F_2) is *infinitesimally* $R\times L^+$*-stable* if

$$\mathcal{E}_{(x_1,x_2)}+\mathcal{E}_{(x_2,x_3)}\subset\left\langle\frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2,x_3)}}+\left\langle\frac{\partial(F_1+F_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{(x_2,x_3)}}+\left\langle\frac{\partial F_2}{\partial x_3},1\right\rangle_{\mathcal{E}_{x_3}}.$$

In this case, for F_1 we have

$$\mathcal{E}_{x_1}=\left\langle \frac{\partial f_1}{\partial x_1}\right\rangle_{\mathcal{E}_{x_1}}+\left\langle \left.\frac{\partial F_1}{\partial x_2}\right|_{x_2=0},1\right\rangle_{\mathbb{R}},$$

where $f_1(x_1)=F_1(x_1,0)$.

Now we have the following proposition:

Proposition 5.5: Let (F_1,F_2) *be a generating pair of a special regular double lensing system germ* (S_0,R_1,R_2). *Then the following are equivalent:*

(1) (F_1,F_2) *is infinitesimally* $R\times L^+$*-stable.*

(2) (F_1,F_2) *satisfies the following condition:*

$$\mathcal{E}_{(x_1,x_2)}=\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2)}}+\left\langle \frac{\partial (F_1+f_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{x_2}}+\left\langle \left.\frac{\partial F_2}{\partial x_3}\right|_{x_3=0},1\right\rangle_{\mathbb{R}},$$

where $f_2(x_2)=F_2(x_2,0)$.

(3) (F_1,F_2) *satisfies the following condition:*

$$\mathcal{E}_{(x_1,x_2)}+\mathcal{E}_{(x_2,x_3)}=\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2,x_3)}}+\left\langle \frac{\partial (F_1+F_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{(x_2,x_3)}}+\left\langle \frac{\partial F_2}{\partial x_3},1\right\rangle_{\mathcal{E}_{x_3}}.$$

(4) F_1 is *infinitesimally* R^+*-versal and*

$$\mathcal{E}_{x_2}\subset\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2)}}+\left\langle \frac{\partial (F_1+f_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{x_2}}+\left\langle \left.\frac{\partial F_2}{\partial x_3}\right|_{x_3=0},1\right\rangle_{\mathbb{R}}.$$

Proof: We assume that the condition (4) holds. Since F_1 is infinitesimally R^+-versal deformation of f_1, we can show that

$$\mathcal{E}_{(x_1,x_2)}=\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2)}}+\left\langle \frac{\partial F_1}{\partial x_2},1\right\rangle_{\mathcal{E}_{x_2}}.$$

We remark that

$$\frac{\partial F_1}{\partial x_2}=\frac{\partial (F_1+f_2)}{\partial x_2}-\frac{\partial f_2}{\partial x_2},$$

so that we have

$$\mathcal{E}_{(x_1,x_2)}=\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2)}}+\left\langle \frac{\partial (F_1+f_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{x_2}}+\left\langle \left.\frac{\partial F_2}{\partial x_3}\right|_{x_3=0},1\right\rangle_{\mathbb{R}}+\mathcal{E}_{x_2}.$$

It follows from the assumption that

$$\mathcal{E}_{(x_1,x_2)}=\left\langle \frac{\partial F_1}{\partial x_1}\right\rangle_{\mathcal{E}_{(x_1,x_2)}}+\left\langle \frac{\partial (F_1+f_2)}{\partial x_2}\right\rangle_{\mathcal{E}_{x_2}}+\left\langle \left.\frac{\partial F_2}{\partial x_3}\right|_{x_3=0},1\right\rangle_{\mathbb{R}}.$$

This means that the condition (2) holds. The converse assertion is trivial by definition.

By the Malgrange preparation theorem (cf., Ref. 13), we can easily show that the condition (3) is equivalent to the condition (2). Since $\mathcal{E}_{(x_1,x_2)}+\mathcal{E}_{x_2}=\mathcal{E}_{(x_1,x_2)}$, condition (1) implies condition (2). It follows from the inclusion $\mathcal{E}_{(x_1,x_2)}+\mathcal{E}_{(x_2,x_3)}\subset\mathcal{E}_{(x_1,x_2,x_3)}$ that condition (3) implies condition (1). This completes the proof.[14]

VI. CLASSIFICATION OF LENSING SYSTEMS AND CAUSTICS

We recall that the family of functions

$$F(x_1,x_2,x_3)=F_1(x_1,x_2)+F_2(x_2,x_3)$$

is a generating family for the Lagrangian submanifold-germ $R_2\circ R_1(S)\subset T^*X_3$ with (x_1,x_2) being the Morse parameters auxiliary in the reduction process (cf. Ref. 15). A *caustic* of the time-delay map in the case of the double lensing system is defined to be the set of source positions $x_3\in\mathbb{R}^2$, which are critical values of the projection

$$T^*X_3\ni R_2\circ R_1(S)\to X_3,$$

or the function $(x_1,x_2)\to F(x_1,x_2,x_3)$ has at least one degenerate critical point.

Using the $R\times L^+$ equivalency group and infinitesimal stability conditions obtained in Propositions 5.4 and 5.5 we can construct normal and prenormal forms of infinitesimally stable generating pairs (F_1,F_2), or equivalently the functions $F(x_1,x_2,x_3)=F_1(x_1,x_2)+F_2(x_2,x_3)$, which belong to the space of additively composed functions on $\Delta=\{(x_1,x_2,\tilde{x}_2,x_3)\in X_1\times X_2\times X_2\times X_3: x_2=\tilde{x}_2\}$, i.e.,

$$F(x_1,x_2,x_3)=\pi_{12}^*F_1(x_1,x_2)+\pi_{23}^*F_2(\tilde{x}_2,x_3)|_\Delta,$$

where π_{12},π_{23} are the canonical projections

$$\pi_{ij}:X_1\times X_2\times X_2\times X_3\to X_i\times X_j,\quad (ij)=(12),(23).$$

If (F_1,F_2) is an infinitesimally $R\times L^+$-stable generating pair, then by Proposition 5.5 (4) F_1 is infinitesimally versal. Now we define the subgroup of $R\times L^+$-equivalency group prescribed to F_1 and acting on F_2. We say that F_2 and G_2 are $(R\times L^+)_{F_1}$ equivalent if there exists $\Phi(x_1,x_2,x_3)=(\phi_1(x_1,x_2,x_3),\phi_2(x_2,x_3),\phi(x_3))$ and a function-germ $\alpha:(X_3,0)\to R$ such that F_1 is preserved, $F_1\circ(\phi_1,\phi_2)=F_1$ and (F_1,F_2) and (F_1,G_2) are $R\times L^+$-equivalent by Φ. Now we can formulate the following result.

Proposition 6.1: Any infinitesimally $R\times L^+$-stable pair is $R\times L^+$-equivalent to the pair (F_1,F_2), where F_1 is a versal unfolding of $F_1(x_1,0)$ and F_2 belongs to an open orbit of $(R\times L^+)_{F_1}$-action.

In the two-dimensional case we simplify the notation and write

$$F(x,u,v)=F_1(x,u)+F_2(u,v),\quad x,u,v\in\mathbb{R}^2.$$

Proposition 6.2: Let us assume that F_1 is an infinitesimally R^+-versal Morse family. Then the generic generating pair-germs (F_1,F_2) are $R\times L^+$-equivalent to one of the following normal forms:

$$(A_1A_1):\quad (F_1(x,u),F_2(u,v))=(\pm x_1^2\pm x_2^2,\pm u_1^2\pm u_2^2),$$

$$(A_1A_2):\quad (F_1(x,u),F_2(u,v))=(\pm x_1^2\pm x_2^2,u_1^3\pm u_2^2+v_1u_1),$$

$$(A_1A_3):\quad (F_1(x,u),F_2(u,v))=(\pm x_1^2\pm x_2^2,\pm u_1^4\pm u_2^2+v_1u_1^2+v_2u_1),$$

$$(A_2B_2):\quad (F_1(x,u),F_2(u,v))=(x_1^3\pm x_2^2+x_1u_1,\pm u_1^2\pm u_2^2+v_1u_1),$$

$$(A_2B_3):\quad (F_1(x,u),F_2(u,v))=(x_1^3\pm x_2^2+x_1u_1,u_1^3\pm u_2^2+v_1u_1+v_2u_1^2),$$

$$(A_2C_2):\quad (F_1(x,u),F_2(u,v))=(x_1^3\pm x_2^2+x_1u_1,u_1u_2\pm u_2^2+v_1u_2),$$

FIG. 3. The standard plane gravitational lensing.

$$(A_2C_3): \quad (F_1(x,u),F_2(u,v))=(x_1^3\pm x_2^2+x_1u_1,u_1u_2+u_2^3+v_1u_2+v_2u_2^2),$$

$$(A_3X): \quad (F_1(x,u),F_2(u,v))=(\pm x_1^4\pm x_2^2+x_1^2u_1+x_1u_2,\xi(u,v)),$$

where ξ is a smooth function-germ.

The first three cases (AA) give the standard plane caustics (i.e., nonsingular, folds and cusps).

The four cases (AB), (AC) are the composed A, B, and C boundary type caustics. However, only the case (A_2C_3) has the caustics at the origin as a composition. In this case we can calculate that (Fig. 3)

$$R_2\circ R_1(s)=\{(-2xy,y,x,x^2) \mid (x,y)\in(\mathbb{R}^2,0)\}\subset T^*X_3.$$

Therefore the projection onto X_3 is locally represented by $f:(\mathbb{R}^2,0)\to(\mathbb{R}^2,0)$; $f(x,y)=(-2xy,y)$ This map-germ is called the *pinch map* (cf., Fig. 4). This is a famous example which does not admit a Thom stratification (Ref. 16, p. 24).

The last case gives other possibilities of compositions with A_3-caustic. There might appear several complicated singularities.

An equivalence $R\times L^+$-group acting on $X_1\times X_2\times X_3$ is a subgroup of the (r,s)-equivalences introduced in Ref. 17, where $r=\dim X_2$ and $s=\dim X_3$. We recall that (r,s)-infinitesimal stability condition

$$\mathcal{E}_{(x,u)}=\left\langle\frac{\partial F_0}{\partial x}\right\rangle_{\mathcal{E}_{(x,u)}}+\left\langle\frac{\partial(F_0)}{\partial u}\right\rangle_{\mathcal{E}_{(u)}}+\left\langle\left.\frac{\partial F}{\partial v}\right|_{v=0},1\right\rangle_{\mathbb{R}}+\tilde{F}_0^*\mathcal{E}_{(\lambda,\mu)},$$

where $\tilde{F}_0=(F_0,u)$, $F_0(x,u)=F(x,u,0)$, $(\lambda,\mu)\in\mathbb{R}\times\mathbb{R}^2$, is weaker than the $R\times L^+$-infinitesimal stability condition.

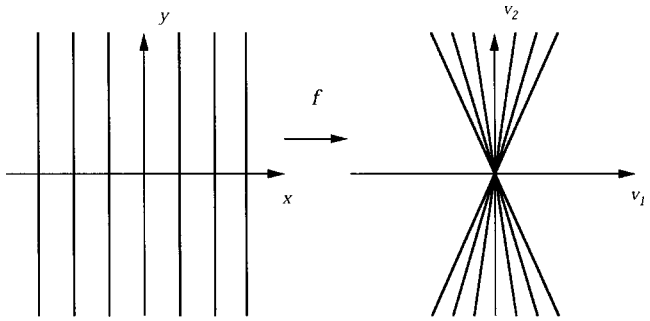

FIG. 4. The vertical lines are mapped onto the lines through the origin by the pinch map.

If $h(x,u,v)$ is an (r,s)-infinitesimally stable unfolding of $f_0(x)=F(x,0,0)$ then the prenormal form for infinitesimally $R\times L^+$-stable unfolding of f_0 is given in the form

$$F(x,u,v)=h(x,u,v)+\sum_{i=1}^{2} u_i g_i(u,v),$$

where $g_i\in\mathcal{E}_{(u,v)}$.

By (r,s)-stability theory (cf. Ref. 17), if $g\in\mathcal{E}_{(x,u,v)}$ is an (r,s)-stable unfolding of $\eta(x)=g(x,0,0)$, then g is (r,s)-equivalent to the function-germ

$$F(x,T_\sigma(u,v)),$$

where F is an $(r+s)$-stable unfolding of η and $T_\sigma(u,v)=T\circ W_\sigma$ is a composition of the polynomial mapping $T:(\mathbb{R}^2\times\mathbb{R}^2,0)\to(\mathbb{R}^2\times\mathbb{R}^2,0)$ and permutation of the variables W_σ. Here we have

$$T(u,v)=\left(u,v+p(u)+\sum_{i=1}^{s} v_i\xi_i(u)\right),$$

where $p(u)$ is a polynomial mapping $\mathbb{R}^r\to\mathbb{R}^s$ with zero constant term and degree at most $s+1$ and $\xi(u)$ are polynomial mappings $\mathbb{R}^r\to\mathbb{R}^s$ with zero constant terms and degree at most $s-1$. The permutation W_σ acting on u,v-variables, $W_\sigma(w_1,\ldots,w_{r+s})=(w_{\sigma(1)},\ldots,w_{\sigma(r+s)})$ is defined as one of the following permutations; Taking $k\leqslant\min\{r,s\}$ and integers $1\leqslant i_1<\cdots<i_k\leqslant r$, $1\leqslant j_1<\cdots<j_k\leqslant s$ we define σ as the product of the following transpositions: $\sigma=(i_1,r+j_1)(i_2,r+j_2)\cdots(i_k,r+j_k)$.

In our (2,2)-case all stable unfoldings are related to the corresponding strata of the family of mappings:

$$T(u,v)=\left(u_1,u_2,v_1+\sum_{1\leqslant i+j\leqslant 3} a_{ij}u_1^i u_2^j+\sum_{i,j=1}^{2} b_{ij}v_i u_j,\quad v_2+\sum_{1\leqslant i+j\leqslant 3} c_{ij}u_1^i u_2^j+\sum_{i,j=1}^{2} d_{ij}v_i u_j\right).$$

These unfoldings were classified in Refs. 18 and 19 and we may use them in our classification of gravitational caustics.

Remark 6.3: By the straightforward application of the classification theorem from Ref. 18 we find that the generic perturbations of the composed function-germs $F(x,u,v)=F_1(x,u)+F_2(u,v)$, *are* (2,2)*-equivalent to the following normal forms:*

$$F(x,u,v)=x_1^3\pm x_2^2+x_1u_1,$$

$$F(x,u,v)=x_1^3\pm x_2^2+x_1(v_1+u_1^2+\pm u_2^2),$$

$$F(x,u,v)=x_1^3\pm x_2^2+x_1(v_1-u_1^2-u_2^2),$$

$$F(x,u,v)=x_1^3\pm x_2^2+x_1(v_1+u_1^3+\pm u_2^2+u_1v_2),$$

$$F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2u_1+u_2x_1,$$

$$F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2(\pm u_1^2+u_2)+x_1(u_2+v_1),$$

$$F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2(u_1^3+u_1v_2+u_2)+x_1(u_2+v_1),$$

$$F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2(\pm u_1^2+u_2v_2+v_1)+x_1u_2,$$

$$F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2u_1+x_1(u_1^2\pm u_2^2+u_1v_1+v_2),$$

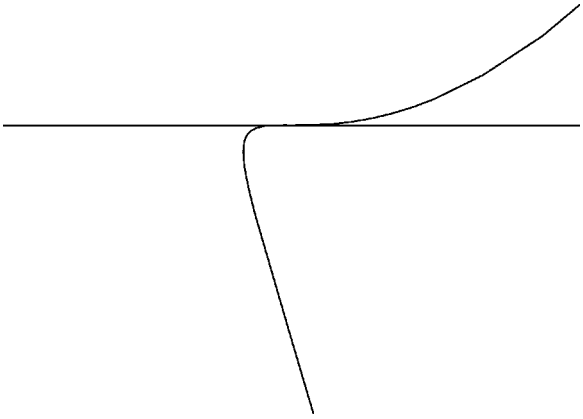

FIG. 5. The picture of the perturbed caustics of the original double lensing system. Twofold curves have order 3 contact at the origin.

$$F(x,u,v)=x_1^5\pm x_2^2+x_1^3u_1+x_1^2(u_2v_2+cu_2+u_1+v_1)+x_1u_2,(c\neq-\tfrac{2}{3}),$$

$$F(x,u,v)=x_1^3+x_2^3+x_1x_2u_1+x_1u_2+x_2(u_2v_2+u_1+cu_2+v_1),(c\neq 0),$$

$$F(x,u,v)=x_1^3-x_1x_2^2+x_1^2(u_1v_2+cu_1+u_2+v_1)+x_1u_2+x_2u_1,(c\in\mathbb{R}),$$

$$F(x,u,v)=x_1^3-x_1x_2^2+x_1^2(u_2v_2+u_1+v_1)+x_1u_2+x_2u_1.$$

By definition, (2,2)-equivalence destroys the exact structure of the composition of caustics. However the structure of generic perturbation of the caustics still remained. By the above list, we can calculate the discriminant set

$$\mathcal{D}_F=\left\{(v_1,v_2)\in X_3\left|\frac{\partial F}{\partial x_1}=\frac{\partial F}{\partial x_2}=\frac{\partial F}{\partial u_1}=\frac{\partial F}{\partial u_2}=0\right.\right\}.$$

Such sets are the perturbed caustics of the original double lensing systems. For the function germ $F(x,u,v)=\pm x_1^4\pm x_2^2+x_1^2u_1+x_1(u_1^2\pm u_2^2+u_1v_1+v_2)$ we have $\mathcal{D}_F=\{(t,0)\}\cup\{(6s^2\pm 2s, \pm 20s^3)\}$ which is depicted in Fig. 5. We can observe that two regular curves (i.e., folds) have order 3 contact at the origin. These two regular curves are the locus of fold points. Therefore, this is a double fold at the origin.

ACKNOWLEDGMENTS

S.I. partially supported by Grant-in-Aid for Scientific Research, JSPS, No. 14604003. S.J. partially supported by KBN Grant No. 2 P03A 020 17.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

Generalized forms and Einstein's equations

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(Received 26 July 2002; accepted 31 January 2003)

Generalized differential forms of different types are defined and their algebra and calculus are discussed. Complex generalized *p*-forms, a particular class of type two generalized forms, are considered in detail. It is shown that Einstein's vacuum field equations for Lorentzian four-metrics are satisfied if and only if a complex generalized one-form on the bundle of two component spinors is closed. A similar result for half-flat and anti self-dual holomorphic four-metrics is also presented. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1563846]

I. INTRODUCTION

Recently the algebra and calculus of generalized differential forms have been developed and examples of their physical application have been presented.[1,2] This paper contains a self-contained extension of this work and an application of it to Einstein's vacuum field equations. Earlier work concentrated on the presentation of generalized forms corresponding to ordered pairs of ordinary *p*- and $p+1$-forms. In this paper, a broader framework is introduced which includes those forms as a particular case. This new framework is constructed by introducing the concept of generalized *p*-forms of type *N* (*N* a non-negative integer) on an *n*-dimensional manifold M. Ordinary *p*-forms become generalized forms of type $N=0$, and the generalized forms corresponding to ordered pairs become generalized forms of type $N=1$. Forms of type *N* can be represented by 2^N-tuples of ordinary differential forms, where $-N\leqslant p\leqslant n$, and satisfy an exterior algebra and calculus which is a direct generalization of that satisfied by type $N=0$ and $N=1$ forms. As in the case of type 1 forms, forms of negative degree are admitted when *N* is positive.[3,4] The new framework naturally extends the one presented for type $N=1$ forms in Refs. 1 and 2. It encompasses the extension briefly mentioned in Ref. 1.

In Sec. II the algebra and calculus of generalized differential forms of type *N* are defined. The definitions are presented in a recursive fashion so that they are similar, in general form, to the definitions previously given for type $N=1$ generalized forms. Three different representations of generalized forms and their algebra and calculus are presented, including a matrix representation. While each of these representations has its uses, the main representation of type *N* forms used throughout the paper will be in terms of 2^N-tuples. Local definitions of generalized connections are presented, and on manifolds with metrics the Hodge (star) operator and duality, the codifferential and Laplacian for type *N* forms are defined. These definitions are the standard ones for $N=0$ (that is ordinary) forms,[5] and agree with the ones given in previous papers for $N=1$ forms.[1,2] Forms of type *N* can always be regarded as special cases of forms of type $\acute{N}$ where $N\leqslant\acute{N}$ but this may not always be the most efficient point of view. In Sec. III the basic algebra and calculus for the particular case of type $N=2$ generalized forms are presented in more detail and in terms of ordered quadruples of ordinary forms. The formulas here include results needed in the next section. They also illustrate in detail the difference between results for $N=2$ forms and results for $N=1$ forms obtained previously. The fourth section is devoted to a discussion of Lorentzian four-metrics and the condition of Ricci flatness. First the representation of the metric geometry via the Cartan structure equations for ordinary forms, including a two component spinor version, is

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reviewed. Then, by using that formalism, the condition for a four-metric to be Ricci flat is formulated as the requirement that a generalized one-form, defined on the bundle of two component spinors over a four dimensional manifold, be closed. Although the focus is on Lorentzian four-metrics it is clear that a similar result hold for four-metrics of all signatures. Half-flat four-metrics are also considered. The condition for a metric to be half-flat is reformulated as the requirement that a generalized one-form to be closed. The holomorphic anti-self-dual case is considered explicitly but Riemannian and ultrahyperbolic four-metrics can be dealt with in a similar way. These results can be viewed as giving a geometrical interpretation of Ricci flatness for four-metrics. They also provide an illustration of the relationship between half-flat metrics and Ricci flat, but not necessarily half-flat, metrics.

Most of the considerations in this paper are local in nature. Emphasis is placed on the algebra, calculus and local geometry rather than the global geometry. The letters over the forms indicate the degrees of the forms and whenever these degrees are obvious they will be omitted. By standard convention, ordinary p-forms (that is of type $N=0$) with p negative are zero. Where it is helpful a subscript will be used to denote the type of the form. Usually bold roman letters will be used for generalized forms and normal greek letters for ordinary forms.

II. GENERALIZED FORMS OF DIFFERENT TYPES

In this section generalized forms of different types will be defined and their exterior algebra and calculus will be discussed. The properties of generalized p-forms can be defined recursively (on N), using definitions which are formally similar to those for the special case, where $N=1$, discussed in Refs. 1 and 2. Here, using the terminology of Ref. 1, the *left* exterior product and *left* generalized derivative will always be used. While a few examples are given in this section a more extensive collection is presented in Sec. III.

The module of generalized p-forms of type $N=0$ is defined to be the module of ordinary p-forms on M, Λ_0^p, with the usual exterior product and exterior derivative. Then the module of generalized p-forms of type N, Λ_N^p, is defined as follows. For $N\geqslant 1$, a generalized p-form of type N, $\overset{p}{\mathbf{a}}_N\in\Lambda_N^p$, is defined to be ordered pairs of generalized p- and $p+1$-forms of type $N-1$,

$$\overset{p}{\mathbf{a}}_N\equiv(\overset{p}{\mathbf{a}}_{N-1},\ \overset{p+1}{\mathbf{a}}_{N-1}), \tag{1}$$

where N is any integer greater than or equal to 1.

Hence forms of type $N=1$ are ordered pairs of ordinary p- and $p+1$-forms, for example, $\overset{p}{\mathbf{a}}_1=(\overset{p}{\alpha},\ \overset{p+1}{\alpha})\in\Lambda_0^p\times\Lambda_0^{p+1}$, as in Refs. 1 and 2. Forms of type $N=2$ are ordered quadruples of ordinary p-, $p+1$-, $p+1$- and $p+2$-forms. For example, let $\overset{p}{\mathbf{a}}_2=(\overset{p}{\mathbf{a}}_1,\ \overset{p+1}{\mathbf{a}}_1)$ where $\overset{p}{\mathbf{a}}_1=(\overset{p}{\alpha},\ \overset{p+1}{\alpha})$, $\overset{p+1}{\mathbf{a}}_1=(\overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha})$, then $\overset{p}{\mathbf{a}}_2\in\Lambda_2^p$ is given by

$$\overset{p}{\mathbf{a}}_2=(\overset{p}{\alpha},\ \overset{p+1}{\alpha},\ \overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha})\in\Lambda_0^p\times\Lambda_0^{p+1}\times\Lambda_0^{p+1}\times\Lambda_0^{p+2}. \tag{2}$$

More generally, a p-form of type N will correspond to an ordered set of 2^N ordinary q-forms with $-N\leqslant p\leqslant q\leqq p+N$. Nonzero entries occur in the 2^N-tuple only when $0\leqslant q\leqslant n$ since, as mentioned above, any ordinary form, $\overset{q}{\alpha}$, with q negative is zero. Forms of type N_1 are naturally included in forms of type N_2 when $N_1<N_2$.

The exterior product is extended from ordinary forms to forms of type $N\geqslant 1$ as follows. Let $\overset{p}{\mathbf{a}}_N\equiv(\overset{p}{\mathbf{a}}_{N-1},\ \overset{p+1}{\mathbf{a}}_{N-1})$ and $\overset{q}{\mathbf{b}}_N\equiv(\overset{q}{\mathbf{b}}_{N-1},\ \overset{q+1}{\mathbf{b}}_{N-1})$ be a p-form and a q-form of type $N\geqslant 1$. Then the exterior product of $\overset{p}{\mathbf{a}}_N$ and $\overset{q}{\mathbf{b}}_N$ is the $p+q$-form of type N defined (recursively) by

$$\overset{p}{\mathbf{a}}_N\wedge\overset{q}{\mathbf{b}}_N=(\overset{p}{\mathbf{a}}_{N-1}\wedge\overset{q}{\mathbf{b}}_{N-1},\overset{p}{\mathbf{a}}_{N-1}\wedge\ \overset{q+1}{\mathbf{b}}_{N-1}+(-1)^q\ \overset{p+1}{\mathbf{a}}_{N-1}\wedge\overset{q}{\mathbf{b}}_{N-1}). \tag{3}$$

The exterior product satisfies all the usual rules, in particular $\overset{p}{\mathbf{a}}_N\wedge\overset{q}{\mathbf{b}}_N=(-1)^{pq}\overset{p}{\mathbf{b}}_N\wedge\overset{q}{\mathbf{a}}_N$. Furthermore, it follows that when $p+q<-N$, the exterior product is zero.

The exterior derivative, $d:\Lambda_N^p\to\Lambda_N^{p+1}$, is defined in the usual way for $N=0$ forms, and when $N\geqslant 1$ by

$$d\overset{p}{\mathbf{a}}_N=(d\overset{p}{\mathbf{a}}_{N-1}+(-1)^{p+1}k_N\ \overset{p+1}{\mathbf{a}}_{N-1},d\ \overset{p+1}{\mathbf{a}}_{N-1}), \tag{4}$$

where k_N is constant.

When $d\overset{p}{\mathbf{a}}_N$ is expressed in terms of ordinary forms it contains the constants $k_1,k_2,\ldots,k_N$. These will all be assumed to be nonzero unless it is stated otherwise. This exterior derivative also satisfies all the usual rules, in particular $d^2=0$, and $d(\overset{p}{\mathbf{a}}_N\wedge\overset{q}{\mathbf{b}}_N)=d\overset{p}{\mathbf{a}}_N\wedge\overset{q}{\mathbf{b}}_N+(-1)^p\overset{p}{\mathbf{a}}_N\wedge d\overset{q}{\mathbf{b}}_N$.

The above representation of the algebra and calculus of generalized forms will be the main one used in this paper. However it is appropriate to note here two alternative representations which can be useful. In the first of these type N forms of degree minus one, $\zeta_1,\ldots,\zeta_N$, which are required to satisfy all the usual rules of exterior algebra and calculus, together with the two conditions

$$\zeta_1\wedge\cdots\wedge\zeta_N\neq 0,\quad d\zeta_I=k_I,\quad I=1,...,N, \tag{5}$$

are introduced.[1] Then a generalized form of type N, $\overset{p}{\mathbf{a}}_N=(\overset{p}{\mathbf{a}}_{N-1},\ \overset{p+1}{\mathbf{a}}_{N-1})$, can be identified with

$$\overset{p}{\mathbf{a}}_N=\overset{p}{\mathbf{a}}_{N-1}+\ \overset{p+1}{\mathbf{a}}_{N-1}\wedge\zeta_N, \tag{6}$$

and it follows that the exterior product and derivative agree with Eqs. (3) and (4). For example, it follows from Eq. (5) that

$$d\overset{p}{\mathbf{a}}_N=d\overset{p}{\mathbf{a}}_{N-1}+(-1)^{p+1}k_N\ \overset{p+1}{\mathbf{a}}_{N-1}+d\ \overset{p+1}{\mathbf{a}}_{N-1}\wedge\zeta_N. \tag{7}$$

The recursive use of this identification can be illustrated by using the example of an $N=2$ form given above. In this case $\overset{p}{\mathbf{a}}_2=(\overset{p}{\alpha},\ \overset{p+1}{\alpha},\ \overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha})$ is identified with $\overset{p}{\mathbf{a}}_2=\overset{p}{\alpha}+\ \overset{p+1}{\alpha}\wedge\zeta_1+\ \overset{p+1}{\not{\alpha}}\wedge\ \zeta_2+\overset{p+2}{\alpha}\wedge\zeta_1\wedge\zeta_2$. It should be noted that while the identification continues to be unambiguous when $N\geqslant 3$ the relationship between the ordering of the forms in the two types of representations is not as simple as it is in the $N\leqslant 2$ cases.

The second of the alternative representation is in terms of matrix valued forms and is again defined recursively. Here the generalized form $\overset{p}{\mathbf{a}}_N=(\overset{p}{\mathbf{a}}_{N-1},\ \overset{p+1}{\mathbf{a}}_{N-1})$ is identified with a 2×2 matrix, $[\overset{p}{\mathbf{a}}_N]$, with entries that are forms of type $N-1$,

$$[\overset{p}{\mathbf{a}}_N]=\begin{bmatrix} \overset{p}{\mathbf{a}}_{N-1} & \overset{p+1}{\mathbf{a}}_{N-1} \\ 0 & (-1)^p\overset{p}{\mathbf{a}}_{N-1} \end{bmatrix}. \tag{8}$$

Exterior multiplication of generalized forms $\overset{p}{\mathbf{a}}_N$ and $\overset{q}{\mathbf{b}}_N$, as in Eq. (3), corresponds to matrix multiplication of $[\overset{p}{\mathbf{a}}_N]$ and $[\overset{q}{\mathbf{b}}_N]$. The matrix representation of the exterior derivative, given by Eq. (4), can be identified by using the 2×2 matrices

$$S=\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad K_N=\begin{bmatrix} 0 & 0 \\ k_N & 0 \end{bmatrix},$$

and the bracket, $\{A,B\}_r$, of 2×2 matrices defined by

$$\{A,B\}_r=AB+(-1)^rBA.$$

Then the matrix corresponding to $d\overset{p}{\mathbf{a}}_N$ is given by

$$[d\overset{p}{\mathbf{a}}_N]=Sd[\overset{p}{\mathbf{a}}_N]+\{K_N,[\overset{p}{\mathbf{a}}_N]\}_{p+1}. \tag{9}$$

Using the definitions recursively it follows that a generalized form of type N is identified with a $2^N\times 2^N$ matrix with entries which are ordinary forms. For example, if $\overset{p}{\mathbf{a}}_2=(\overset{p}{\alpha},\ \overset{p+1}{\alpha}\ ,\ \overset{p+1}{\not{\alpha}}\ ,\ \overset{p+2}{\alpha}\ )$, as above, then the 4×4 matrix representation of $\overset{p}{\mathbf{a}}_2$ is given by

$$[\overset{p}{\mathbf{a}}_2]=\begin{bmatrix} \overset{p}{\alpha} & \overset{p+1}{\alpha} & \overset{p+1}{\not{\alpha}} & \overset{p+2}{\alpha} \\ 0 & (-1)^p\overset{p}{\alpha} & 0 & (-1)^{p+1}\overset{p+1}{\not{\alpha}} \\ 0 & 0 & (-1)^p\overset{p}{\alpha} & (-1)^p\overset{p+1}{\alpha} \\ 0 & 0 & 0 & \overset{p}{\alpha} \end{bmatrix}. \tag{10}$$

The Poincaré lemma for generalized forms of type $N\geqq 1$ can be obtained by straightforward calculation.

Theorem 1: Let $\overset{p}{\mathbf{a}}_N=(\overset{p}{\mathbf{a}}_{N-1},\ \overset{p+1}{\mathbf{a}}_{N-1})$, with $N\geqq 1$, be nonzero and closed, so that $d\overset{p}{\mathbf{a}}_N=0$. Then

(a) $d\ \overset{-N}{\mathbf{a}}_N=0$ if and only if $k_I=0$ for all I, $1\leqslant I\leqslant N$, and $\overset{-N}{\mathbf{a}}_N=(0,...,0,c)$ where c is the nonzero constant;

(b) if $p\geqslant -N+1$, $d\overset{p}{\mathbf{a}}_N=0$ if and only if *either* $\overset{p}{\mathbf{a}}_N$ is exact *or* $k_I=0$ for all I, $1\leqslant I\leqslant N$, and all the ordinary forms in the 2^N-tuple are closed.

(c) When k_N is nonzero, $d\overset{p}{\mathbf{a}}_N=0$ if and only if $\overset{p}{\mathbf{a}}_N$ is exact.

Furthermore, $\overset{p+1}{\mathbf{a}}_{N-1}=(-1)^p k_N^{-1} d\overset{p}{\mathbf{a}}_{N-1}$ and $\overset{p}{\mathbf{a}}_N = d\,\overset{p-1}{\mathbf{b}}_N$ where $\overset{p-1}{\mathbf{b}}_N=(0,(-1)^p k_N^{-1}\overset{p}{\mathbf{a}}_{N-1}) + \overset{p-1}{\mathbf{c}}_N$ for any closed form $\overset{p-1}{\mathbf{c}}_N$.

Hence the de Rham cohomology determined by generalized forms is trivial unless *all* the constant k's are zero in which case the standard de Rham cohomology applies. These ideas can be straightforwardly extended to other differential operators. For example, suppose M is a complex manifold and ∂ and $\overline{\partial}$ are the usual Dolbeault differential operators on ordinary differential forms. These operators can be extended to operators acting on generalized forms by, for example, defining

$$\begin{gathered}\partial\zeta_I = l_I, \quad \overline{\partial}\zeta_I = m_I, \\ l_I + m_I = k_I, \quad I=1,\ldots,N,\end{gathered} \tag{11}$$

where l_I and m_I are constants, and replacing d and k_N in Eq. (5) by ∂ and l_N (respectively, $\overline{\partial}$ and m_N) in the obvious way. The nature of the Dolbeault cohomology determined by generalized forms, and the cohomology associated with the real operator $d^c = i(\overline{\partial}-\partial)$ will clearly be determined by the vanishing or nonvanishing of the constants m_I and $m_I - l_I$.

Let V be a vector field tangent to M. Then the inner product of V with a generalized p-form $\overset{p}{\mathbf{a}}_N \equiv (\overset{p}{\mathbf{a}}_{N-1}, \overset{p+1}{\mathbf{a}}_{N-1})$ is defined in the usual way for $N=0$ forms. For $N>0$ it is defined to be zero if $p=-N$ and if $p>-N$ it is defined to be the generalized $(p-1)$-form,

$$V\rfloor\overset{p}{\mathbf{a}}_N \equiv (V\rfloor\overset{p}{\mathbf{a}}_{N-1}, V\rfloor\overset{p+1}{\mathbf{a}}_{N-1}). \tag{12}$$

The Lie derivative of $\overset{p}{\mathbf{a}}_N$ is defined to be the p-form,

$$L_V\overset{p}{\mathbf{a}}_N \equiv V\rfloor d\overset{p}{\mathbf{a}}_N + d(V\rfloor\overset{p}{\mathbf{a}}_N). \tag{13}$$

It follows from this definition that

$$L_V\overset{p}{\mathbf{a}}_N = (L_V\overset{p}{\mathbf{a}}_{N-1}, L_V\overset{p+1}{\mathbf{a}}_{N-1}). \tag{14}$$

Let G be a Lie group and let $\mathcal{G}$ the Lie algebra of G. Generalized $\mathcal{G}$-valued connection one-forms and curvature two-forms of type N are defined in a similar manner to ordinary connection one-forms and curvature two-forms.[1,6] However the ordinary forms are replaced by generalized type-N forms. Here only the local definition of curvature is given. The appropriate geometrical setting for a global formulation needs further investigation. Let $\mathbf{A}_N$ be a generalized connection one-form, of type N, with values in $\mathcal{G}$. The curvature two-form of this connection is defined by the usual type of formula to be

$$\mathbf{F}_N = d\mathbf{A}_N + \tfrac{1}{2}[\mathbf{A}_N, \mathbf{A}_N]. \tag{15}$$

Hence if the commutation relations of the Lie algebra $\mathcal{G}$ are given by

$$[X_j, X_k] = C^i_{jk} X_i,$$

and if $\mathbf{A}_N = \mathbf{A}^i_N X_i$, where $\mathbf{A}^i_N$ are generalized one-forms, then if $\mathbf{F}_N = \mathbf{F}^i_N X_i$,

$$\mathbf{F}^i_N = d\mathbf{A}^i_N + \tfrac{1}{2} C^i_{jk}\mathbf{A}^j_N \wedge \mathbf{A}^k_N. \tag{16}$$

A generalized connection, $\mathbf{A}_N$, determines a generalized covariant exterior derivative, $\mathbf{D}$. Let $\overset{p}{\mathbf{b}}_N$ be any $\mathcal{G}$-valued generalized p-form of type N, then

$$\mathbf{D}\overset{p}{\mathbf{b}}_N = d\overset{p}{\mathbf{b}}_N + [\mathbf{A}_N, \overset{p}{\mathbf{b}}_N]. \tag{17}$$

As an example of a generalized connection, consider *affine* generalized connections with structure group $G=\mathrm{IGL}(n)$ and Lie algebra $\mathcal{G}$. The generators, X^b_a, of $\mathcal{G}$ satisfy the commutation relations

$$[X_a, X_b]=0,\ [X^a_b, X_c]=\delta^a_c X_b, [X^a_b, X^c_d]=(\delta^a_d X^c_b - \delta^c_b X^a_d).$$

The generalized connection one-form $\mathbf{A}_N$ and curvature two-form $\mathbf{F}_N$ are given by

$$\mathbf{A}_N = \mathbf{e}^a_N X_a + \mathbf{\Gamma}^a_{Nb} X^b_a, \quad \mathbf{F}_N = \mathbf{T}^a_N X_a + \mathbf{F}^a_{Nb} X^b_a, \tag{18}$$

where $\mathbf{e}^a_N$ is a moving co-frame of generalized one-forms on M, and Γ^a_{Nb} and the pair $\mathbf{T}^a_N$, $\mathbf{F}^a_{Nb}$ are, respectively, generalized one-forms and two-forms on M. The lower case italic indices range and sum over 1 to n. Computing the generalized curvature, as above, gives the Cartan structure equations. The first and second generalized Cartan structure equations are

$$\mathbf{T}^a_N = d\mathbf{e}^a_N - \mathbf{e}^b_N \wedge \mathbf{\Gamma}^a_{Nb}, \quad \mathbf{F}^a_{Nb} = d\mathbf{\Gamma}^a_{Nb} + \mathbf{\Gamma}^a_{Nc} \wedge \mathbf{\Gamma}^c_{Nb}, \tag{19}$$

where $\mathbf{T}^a_N$ is the generalized torsion and $\mathbf{F}^a_{Nb}$ is the generalized curvature of the generalized affine connection $\mathbf{\Gamma}^a_{Nb}$.

Next consider an oriented manifold M with a metric g of signature $(r, n\text{-}r)$ so that a Hodge star operator, duality, codifferential and Laplacian, etc., for generalized forms, $\overset{p}{\mathbf{a}}_N = (\overset{p}{\mathbf{a}}_{N-1}, \overset{p+1}{\mathbf{a}}_{N-1})$, of type N can be defined. The sign conventions of Ref. 2 are again used so the definitions and results below agree with the ones in that reference when $N=0$ and $N=1$. The definitions are again recursive in nature.

The (Hodge) star operator, $\star$: $\Lambda^p_N \to \Lambda^{n-p-N}_N$, and dual for generalized forms are defined as follows. For $N=0$, $\star\overset{p}{\mathbf{a}}_0 \equiv *\overset{p}{\alpha}$, where $*$ denotes the usual Hodge star operator on ordinary forms, and for $N \geqslant 1$,

$$\overset{p}{\mathbf{a}}_N \mapsto \star\overset{p}{\mathbf{a}}_N \equiv ([-1]^{n+p+N} \star \overset{p+1}{\mathbf{a}}_{N-1} \star \overset{p}{\mathbf{a}}_{N-1}). \tag{20}$$

This definition gives, as the dual to a type-N generalized p-form, a generalized $(n-p-N)$-form. It follows that if $\overset{p}{s} = (-1)^{np+p+n-r}$, then

$$\star\star\overset{p}{\mathbf{a}}_N = \overset{p}{s}(-1)^{Np}\overset{p}{\mathbf{a}}_N \equiv \lambda^2_N \overset{p}{\mathbf{a}}_N, \tag{21}$$

where λ_N depends on N and, as usual, n, p and the signature of the metric. The possible eigenvalues of $\star$ are $\pm\lambda_N$, where in fact $\lambda_N = 1$ or i. This agrees with the standard result for ordinary forms and the previously obtained expression for $N=1$ forms. With the above sign conventions, a generalized p-form is said to be self-dual if $\star\overset{p}{\mathbf{a}}_N = \lambda_N \overset{p}{\mathbf{a}}_N$, and anti-self-dual if $\star\overset{p}{\mathbf{a}}_N = -\lambda_N \overset{p}{\mathbf{a}}_N$. It is straightforward to see that necessary conditions for a generalized p-form to be either self-dual or anti-self-dual are that when N is zero or an even integer, the dimension of M, n, must be be even, when N is odd n must be odd, and that $p=(n-N)/2$. In fact $\star\overset{p}{\mathbf{a}}_N = \pm\lambda_N \overset{p}{\mathbf{a}}_N$ if and only if $\overset{p}{\mathbf{a}}_N = (\overset{(n-N)/2}{\mathbf{a}}_{N-1}, \pm\lambda^{-1}_N \star \overset{(n-N)/2}{\mathbf{a}}_{N-1})$.

Now

$$\overset{p}{\mathbf{a}}_N \wedge \star \overset{q}{\mathbf{b}}_N = ([-1]^{n+q+N} \overset{p}{\mathbf{a}}_{N-1} \wedge \star \overset{q+1}{\mathbf{b}}_{N-1}, \overset{p}{\mathbf{a}}_{N-1} \wedge \star \overset{q}{\mathbf{b}}_{N-1} + \overset{p+1}{\mathbf{a}}_{N-1} \wedge \star \overset{q+1}{\mathbf{b}}_{N-1}).$$

The simplest definition of a symmetric inner product of two generalized p-forms $\overset{p}{\mathbf{a}}_N$ and $\overset{p}{\mathbf{b}}_N$ is given by the usual expression for ordinary forms when $N=0$, $\langle \overset{p}{\alpha}, \overset{p}{\beta} \rangle$, and recursively, when $N \geqslant 1$, by

$$\langle \overset{p}{\mathbf{a}}_N, \overset{p}{\mathbf{b}}_N \rangle \equiv \langle \overset{p}{\mathbf{a}}_{N-1}, \overset{p}{\mathbf{b}}_{N-1} \rangle + \langle \overset{p+1}{\mathbf{a}}_{N-1}, \overset{p+1}{\mathbf{b}}_{N-1} \rangle. \tag{22}$$

This inner product is positive definite for a Riemannian manifold and can be used in the construction of Lagrangians. (As was noted in Ref. 2, alternative definitions may also be useful.)

A codifferential operator $\delta: \Lambda_N^p \to \Lambda_N^{p-1}$, by $\overset{p}{\mathbf{a}}_N \mapsto \delta \overset{p}{\mathbf{a}}_N$ is defined recursively as follows. If $\sigma^p = (-1)^{np-r+1}$, then

$$\delta \overset{p}{\mathbf{a}}_N = (-1)^{N(p+1)} \sigma^p \star d \star \overset{p}{\mathbf{a}}_N. \tag{23}$$

This definition agrees with the definition for ordinary forms, and the previously presented definition for $N=1$ forms, and implies that

$$\delta \overset{p}{\mathbf{a}}_N = (\delta \overset{p}{\mathbf{a}}_{N-1}, \delta \overset{p+1}{\mathbf{a}}_{N-1} + (-1)^p k_N \overset{p}{\mathbf{a}}_{N-1}). \tag{24}$$

From these definitions it follows that $\delta^2 = 0$, and $\delta \overset{-N}{\mathbf{a}}_N = 0$. If $\overset{p}{\mathbf{a}}_N$ is co-closed, that is $\delta \overset{p}{\mathbf{a}}_N = 0$, then in a result analogous to the Poincaré lemma above, it is co-exact, that is it is the codifferential of a generalized $(p+1)$-form.

Theorem 2: If $\overset{p}{\mathbf{a}}_N = (\overset{p}{\mathbf{a}}_{N-1}, \overset{p+1}{\mathbf{a}}_{N-1})$, and $\delta \overset{p}{\mathbf{a}}_N = 0$, then if $-N \leqslant p \leqslant n-1$, and k_N is nonzero, $\overset{p}{\mathbf{a}}_{N-1} = (-1)^{p+1} k_N^{-1} \delta \overset{p+1}{\mathbf{a}}_{N-1}$ and $\overset{p}{\mathbf{a}}_N = \delta \overset{p+1}{\mathbf{b}}_N$, where $\overset{p+1}{\mathbf{b}}_N = ((-1)^{p+1} k_N^{-1} \overset{p+1}{\mathbf{a}}_{N-1}, 0) + \overset{p+1}{\mathbf{c}}_N$, for any $\overset{p+1}{\mathbf{c}}_N$ which is co-closed. Furthermore, $\delta \overset{n}{\mathbf{a}}_N = 0$ if and only if $\overset{n}{\mathbf{a}}_N = 0$. Any type N form, with $p = -N$, is both co-closed and co-exact.

When M is compact without boundary, the condition, $\langle d\mathbf{a}_N, \mathbf{b}_N \rangle = \langle \mathbf{a}_N, \delta \mathbf{b}_N \rangle$, for this codifferential operator on generalized forms to be the adjoint of d, holds.

A Laplacian for generalized forms, $\Delta: \Lambda_N^p \to \Lambda_N^p$, is defined to be $\Delta = d\delta + \delta d$.

Computation, with the choice of signs made in this paper, gives the simple expression, in agreement with the previously presented $N=0$ and $N=1$ cases,

$$\Delta \overset{p}{\mathbf{a}}_N = (\Delta \overset{p}{\mathbf{a}}_{N-1} + k_N^2 \overset{p}{\mathbf{a}}_{N-1}, \Delta \overset{p+1}{\mathbf{a}}_{N-1} + k_N^2 \overset{p+1}{\mathbf{a}}_{N-1}). \tag{25}$$

It follows from this that $\overset{p}{\mathbf{a}}_N$ is a harmonic generalized form, that is $\Delta \overset{p}{\mathbf{a}}_N = 0$, if and only if $\Delta \overset{p}{\mathbf{a}}_{N-1} + k_N^2 \overset{p}{\mathbf{a}}_{N-1} = 0$, and $\Delta \overset{p+1}{\mathbf{a}}_{N-1} + k_N^2 \overset{p+1}{\mathbf{a}}_{N-1} = 0$. That is, a generalized form is harmonic only when its constituent ordinary forms satisfy a Klein–Gordon type of equation with a ''mass squared'' term given by k_N^2.

The choices of signs in the above definitions have been made in order to make generalized forms eigenforms of the operator $\star\star$, to give a definition of δ which was simply related to the

definition for ordinary forms and to ensure that the Laplacian on generalized forms was computable in terms of the Laplacian, not some other second order differential operator, acting on ordinary forms.

III. GENERALIZED FORMS OF TYPE $N=2$

In this section aspects of the algebra and calculus of generalized forms of type 2 will be considered in more detail and further applications of the results in Sec. II will be presented. Henceforth the generalized forms considered will be mainly of type $N=2$, so the subscript $N=2$ will be omitted in the remainder of the paper. As will be seen there is a loose analogy between going from real numbers to complex numbers to quaternions and going from ordinary forms to forms of type 1 and forms of type 2.

A. Basic algebra and calculus

As was noted in Sec. II, a generalized p-form of type 2, $\overset{p}{\mathbf{a}}$ $(-2\leqslant p\leqslant n)$, is an ordered quadruple of ordinary p-, $p+1$-, $p+1$-, and $p+2$- forms; that is since $\overset{p}{\mathbf{a}}$ is an ordered pair of the type 1 forms $\overset{p}{\mathbf{a}}_1=(\overset{p}{\alpha},\ \overset{p+1}{\alpha})$ and $\overset{p+1}{\mathbf{a}}_1=(\overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha})$

$$\overset{p}{\mathbf{a}}\equiv(\overset{p}{\alpha},\ \overset{p+1}{\alpha},\ \overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha}).$$

A minus two-form is an ordered quadruple $\overset{-2}{\mathbf{a}}=(0,0,0,\overset{0}{\alpha})$, where $\overset{0}{\alpha}$ is a function on M, and a minus one-form is an ordered quadruple $\overset{-1}{\mathbf{a}}=(0,\overset{0}{\alpha},\overset{0}{\not{\alpha}},\overset{1}{\alpha})$, where $\overset{1}{\alpha}$ is an ordinary one-form on M and $\overset{0}{\alpha}$, $\overset{0}{\not{\alpha}}$ are functions on M. A generalized p-form of type 2, given by a quadruple $(\overset{p}{\alpha},0,0,0)$, will be identified with the ordinary p-form $\overset{p}{\alpha}$. Consequently a function on M, $\overset{0}{\alpha}$, will be identified with the generalized 0-form $(\overset{0}{\alpha},0,0,0)$ while the quadruples $(0,\overset{0}{\alpha},0,0)$, $(0,0,\overset{0}{\alpha},0)$ and $(0,0,0,\overset{0}{\alpha})$, respectively, define two linearly independent generalized minus one-forms and a minus two-form. Just as an ordinary p-form $\overset{p}{\alpha}$ is naturally included in the generalized p-forms of type 2 as $(\overset{p}{\alpha},0,0,0)$, a generalized p-form of type 1, $(\overset{p}{\alpha},\ \overset{p+1}{\alpha})$, can be naturally included in the generalized p-forms of type 2 as $(\overset{p}{\alpha},\ \overset{p+1}{\alpha},0,0)$.

If $\overset{p}{\mathbf{a}}\equiv(\overset{p}{\alpha},\ \overset{p+1}{\alpha},\ \overset{p+1}{\not{\alpha}},\ \overset{p+2}{\alpha})$ and $\overset{q}{\mathbf{b}}\equiv(\overset{q}{\beta},\ \overset{q+1}{\beta},\ \overset{q+1}{\not{\beta}},\ \overset{q+2}{\beta})$, then the generalized exterior product and the generalized exterior derivative, d, defined in section two, are given in terms of ordinary forms by

$$\overset{p}{\mathbf{a}}\wedge\overset{q}{\mathbf{b}}=\overset{p+q}{\mathbf{c}}\equiv(\overset{p+q}{\gamma},\ \overset{p+q+1}{\gamma},\ \overset{p+q+1}{\not{\gamma}},\ \overset{p+q+2}{\gamma}),$$

$$\overset{p+q}{\gamma}=\overset{p}{\alpha}\wedge\overset{q}{\beta},$$

$$\overset{p+q+1}{\gamma}=\overset{p}{\alpha}\wedge\overset{q+1}{\beta}+(-1)^q\overset{p+1}{\alpha}\wedge\overset{q}{\beta}, \tag{26}$$

$$\overset{p+q+1}{\not\gamma} = \alpha \wedge \overset{q+1}{\not\beta} + (-1)^q \overset{p+1}{\not\alpha} \wedge \beta,$$

$$\overset{p+q+2}{\gamma} = \alpha \wedge \overset{q+2}{\beta} + (-1)^{q+1} \overset{p+1}{\alpha} \wedge \overset{q+1}{\beta} + (-1)^q \overset{p+1}{\not\alpha} \wedge \overset{q+1}{\beta} + (-1)^q \overset{p+2}{\alpha} \wedge \beta,$$

and

$$d\overset{p}{\mathbf{a}} \equiv \overset{p+1}{\mathbf{c}} \equiv (\overset{p+1}{\gamma}, \overset{p+2}{\gamma}, \overset{p+2}{\not\gamma}, \overset{p+3}{\gamma}),$$

$$\overset{p+1}{\gamma} = d\overset{p}{\alpha} + (-1)^{p+1} k_1 \overset{p+1}{\alpha} + (-1)^{p+1} k_2 \overset{p+1}{\not\alpha},$$

$$\overset{p+2}{\gamma} = d\overset{p+1}{\alpha} + (-1)^{p+1} k_2 \overset{p+2}{\alpha}, \tag{27}$$

$$\overset{p+2}{\not\gamma} = d\overset{p+1}{\not\alpha} + (-1)^p k_1 \overset{p+2}{\alpha},$$

$$\overset{p+3}{\gamma} = d\overset{p+2}{\alpha}.$$

The ordinary forms (and manifold) may be real or complex and a bar over ordinary forms denotes the usual complex conjugate.

The conjugate of $\overset{p}{\mathbf{a}}$, denoted $\overline{\overset{p}{\mathbf{a}}}$, is defined to be

$$(\overline{\overset{p}{\alpha}}, \overline{\overset{p+1}{\not\alpha}}, \overline{\overset{p+1}{\alpha}}, -\overline{\overset{p+2}{\alpha}}). \tag{28}$$

The generalized form is said to be self-conjugate, $\overset{p}{\mathbf{a}} = \overline{\overset{p}{\mathbf{a}}}$, when $\overset{p}{\alpha}$ is real, $\overset{p+1}{\not\alpha}$ is the complex conjugate of $\overset{p+1}{\alpha}$ and $\overset{p+2}{\alpha}$ is a purely imaginary ordinary one-form.

(Hence if $\overset{p}{\mathbf{a}} = \overset{p}{\alpha} + \overset{p+1}{\alpha} \wedge \zeta + \overset{p+1}{\not\alpha} \wedge \overline{\zeta} + \overset{p+2}{\alpha} \wedge \zeta \wedge \overline{\zeta}$, with $d\zeta = k$, $d\overline{\zeta} = \overline{k}$ the conjugate is just the obvious complex conjugate.)

The Poincare lemma of Sec. II can be written in the following way for type 2 forms.

Proposition 1: If $\overset{p}{\mathbf{a}} = (\overset{p}{\alpha}, \overset{p+1}{\alpha}, \overset{p+1}{\not\alpha}, \overset{p+2}{\alpha})$ is closed, so that $d\overset{p}{\mathbf{a}} = 0$, then

(a) $(-1)^p d\overset{p}{\alpha} = k_1 \overset{p+1}{\alpha} + k_2 \overset{p+1}{\not\alpha}$,

(b) $\overset{p}{\mathbf{a}}$ is exact, and $\overset{p}{\mathbf{a}} = d\overset{p-1}{\mathbf{b}} = d\overset{p-1}{\mathbf{c}}$, where $\overset{p-1}{\mathbf{b}} = (-1)^p k_2^{-1}(0,0,\overset{p}{\alpha}, \overset{p+1}{\alpha})$, and $\overset{p-1}{\mathbf{c}} = (-1)^p k_1^{-1}(0,\overset{p}{\alpha},0,-\overset{p+1}{\not\alpha})$.

The second equality in (b) illustrates a consequence of the freedom to add the exterior derivative of a complex generalized $(p-2)$-form to $\overset{p-1}{\mathbf{b}}$ or $\overset{p-1}{\mathbf{c}}$. If $\overset{p}{\mathbf{a}}$ is self-conjugate then $\overset{p-1}{\mathbf{b}}$ is the conjugate of $\overset{p-1}{\mathbf{c}}$.

B. Matrix Lie groups

Next consider Lie groups and Lie algebras, for simplicity matrix Lie groups. In the present context, and following Ref. 1, it is natural to associate with a Lie group G the semidirect product of G and Lie algebra-valued forms (viewed as the direct product of additive abelian groups). Define the (associated) Lie group $\mathbf{G}$ by

$$\mathbf{G}=\{\mathbf{a}|\mathbf{a}=\alpha(1,\overset{1}{A},\overset{1}{\mathbb{A}},\overset{2}{A})\},$$
$$\alpha(1,\overset{1}{A},\overset{1}{\mathbb{A}},\overset{2}{A})\equiv(\alpha,0,0,0)\wedge(1,\overset{1}{A},\overset{1}{\mathbb{A}},\overset{2}{A})=(\alpha,\alpha A,\alpha\overset{1}{\mathbb{A}},\alpha\overset{2}{A}), \tag{29}$$

where $\mathbf{a}$ is a complex generalized 0-form, α belongs to the Lie group G, with identity 1, and $\overset{1}{A},\overset{1}{\mathbb{A}},\overset{2}{A}$ are ordinary forms with values in the (matrix) Lie algebra of G (or more generally H, where G is a subgroup of H).

The product of two elements of $\mathbf{G}$, $\mathbf{a}=\alpha(1,\overset{1}{A},\overset{1}{\mathbb{A}},\overset{2}{A}))$ and $\mathbf{b}=\beta(1,\overset{1}{B},\overset{1}{\mathbb{B}},\overset{2}{B})$ is given by the above rules for exterior multiplication, and is $\mathbf{c}=\mathbf{a}\wedge\mathbf{b}=\alpha\beta(1,\overset{1}{C},\overset{1}{\mathbb{C}},\overset{2}{C})$, where

$$\overset{1}{C}=\overset{1}{B}+\beta^{-1}\overset{1}{A}\beta,$$
$$\overset{1}{\mathbb{C}}_1=\overset{1}{\mathbb{B}}+\beta^{-1}\overset{1}{\mathbb{A}}\beta,$$
$$\overset{2}{C}=\overset{2}{B}+\beta^{-1}\overset{2}{A}\beta+\overset{2}{L}, \tag{30}$$

where

$$\overset{2}{L}=\beta^{-1}\overset{1}{\mathbb{A}}\beta\wedge\overset{1}{B}-\beta^{-1}\overset{1}{A}\beta\wedge\overset{1}{\mathbb{B}}.$$

Here, in order to ensure that the ordinary forms take values in the Lie algebra of G, it is henceforth assumed that $\overset{1}{\mathbb{A}}=c\overset{1}{A},\overset{1}{\mathbb{B}}=c\overset{1}{B}$, where c equals one if necessary. Hence in the following, $L^2=0$.

The inverse of $\mathbf{a}$ is $\mathbf{a}^{-1}=\alpha^{-1}(1,-\alpha\overset{1}{A}\alpha^{-1},-c\alpha\overset{1}{A}\alpha^{-1},-\alpha\overset{2}{A}\alpha^{-1})$ and the identity is (1,0,0,0). Left fundamental one-forms, denoted $\mathbf{1}$, are formally defined by

$$\mathbf{l}=\mathbf{a}^{-1}\wedge d\mathbf{a}=(\overset{1}{\lambda},\overset{2}{\lambda},\overset{2}{\mathbb{\lambda}},\overset{3}{\lambda}),$$
$$\overset{1}{\lambda}=\alpha^{-1}d\alpha-(k_1+ck_2)\overset{1}{A},$$
$$\overset{2}{\lambda}=d\overset{1}{A}-(k_1+ck_2)\overset{1}{A}\wedge\overset{1}{A}-k_2\overset{2}{A}+\alpha^{-1}d\alpha\wedge\overset{1}{A}+\overset{1}{A}\wedge\alpha^{-1}d\alpha, \tag{31}$$
$$\overset{2}{\mathbb{\lambda}}=c(d\overset{1}{A}-(k_1+ck_2)\overset{1}{A}\wedge\overset{1}{A})+k_1\overset{2}{A}+c(\alpha^{-1}d\alpha\wedge\overset{1}{A}+\overset{1}{A}\wedge\alpha^{-1}d\alpha)+dc\wedge\overset{1}{A},$$
$$\overset{3}{\lambda}=d\overset{2}{A}+(k_1+ck_2)(\overset{2}{A}\wedge\overset{1}{A}-\overset{1}{A}\wedge\overset{2}{A})+\alpha^{-1}d\alpha\wedge\overset{2}{A}-\overset{2}{A}\wedge\alpha^{-1}d\alpha+dc\wedge\overset{1}{A}\wedge\overset{1}{A},$$

and $\mathbf{l}$ satisfies the Maurer–Cartan equation

$$d\mathbf{l}+\mathbf{l}\wedge\mathbf{l}=0. \tag{32}$$

In the special case where $\alpha=1$, $k_1+ck_2=-1$, and c is constant,

$$\mathbf{l}=a^{-1}\wedge d\mathbf{a}=(\overset{1}{A},F-k_2\overset{2}{A},c[F+c^{-1}k_1\overset{2}{A}],D\overset{2}{A}), \tag{33}$$

where here,

$$\begin{gathered} F\equiv d\overset{1}{A}+\overset{1}{A}\wedge\overset{1}{A}, \\ D\overset{2}{A}\equiv d\overset{2}{A}+\overset{1}{A}\wedge\overset{2}{A}-\overset{2}{A}\wedge\overset{1}{A}. \end{gathered} \tag{34}$$

C. Connections

The following is an outline of the basic formulas for type 2 connections and curvature. As in Sec. II, a discussion of connections in terms of bundles will be avoided here by working locally with type $N=2$ forms on M. Let the generalized connection and curvature forms on M be given by $\mathbf{A}^i=(\overset{1}{\alpha}{}^i,\overset{2}{\alpha}{}^i,\overset{2}{\not\alpha}{}^i,\overset{3}{\alpha}{}^i)$, $\mathbf{F}^i=(\overset{2}{\mathcal{F}}{}^i,\overset{3}{\mathcal{F}}{}^i,\overset{3}{\not{\mathcal{F}}}{}^i,\overset{4}{\mathcal{F}}{}^i)$. Then it follows from Eqs. (18) and (19) that

$$\begin{gathered} \overset{2}{\mathcal{F}}{}^i=d\overset{1}{\alpha}{}^i+\frac{1}{2}C^i_{jk}\overset{1}{\alpha}{}^j\wedge\overset{1}{\alpha}{}^k+k_1\overset{2}{\alpha}{}^i+k_2\overset{2}{\not\alpha}{}^i, \\ \overset{3}{\mathcal{F}}{}^i=D\overset{2}{\alpha}{}^i+k_2\overset{3}{\alpha}{}^i, \\ \overset{3}{\not{\mathcal{F}}}{}^i=D\overset{2}{\not\alpha}{}^i-k_1\overset{3}{\alpha}{}^i, \\ \overset{4}{\mathcal{F}}{}^i=D\overset{3}{\alpha}{}^i+C'^i_{jk}\overset{2}{\alpha}{}^j\wedge\overset{2}{\not\alpha}{}^k. \end{gathered} \tag{35}$$

Here D denotes the (formal) covariant exterior derivative of a $\mathcal{G}$-valued ordinary differential form with respect to the ordinary $\mathcal{G}$-valued 1-form $\overset{1}{\alpha}{}^i$;

$$D\overset{p}{\beta}{}^i\equiv d\overset{p}{\beta}{}^i+C^i_{jk}\overset{1}{\alpha}{}^j\wedge\overset{p}{\beta}{}^k.$$

Generalized gauge transformations, following Ref. 1, are determined by generalized 0-forms on M with values in the Lie group $\mathbf{G}$, as above. The gauge transformations determined by, $\mathbf{a}$, an element of $\mathbf{G}$, as in Eq. (29), are given by the standard formulas

$$\begin{gathered} \mathbf{A}\to(\mathbf{a}^{-1})d\mathbf{a}+(\mathbf{a}^{-1})\mathbf{A}\mathbf{a}, \\ \mathbf{F}\to(\mathbf{a}^{-1})\mathbf{F}\mathbf{a}. \end{gathered} \tag{36}$$

It should be noted, for example, that although it appears in the above expressions as if $\overset{1}{\alpha}$ in the above equations can be regarded as a connection one-form, it does not necessarily transform, under generalized gauge transformations in the same way as an ordinary connection transforms

under ordinary gauge transformations. Consequently the appropriate nonlocal geometrical formulation and application requires further investigation, possibly along lines similar to those referred to and discussed in, for example, Ref. 7.

Any ordinary connection $\overset{1}{\alpha}$ can determine flat (zero curvature) generalized connections. In this flat case it follows from Eq. (35) that the curvature of the connection $\overset{1}{\alpha}$ is given by $f^i = -(k_1\overset{2}{\alpha}^i + k_2\overset{2}{\not{\alpha}}^i)$. Further reference to Eq. (35), in the flat case, shows that the two-forms $\overset{2}{\alpha}^i$ (respectively, $\overset{2}{\not{\alpha}}^i = -k_2^{-1}(f^i - k_1\overset{2}{\alpha}^i)$) determine the three-forms $\overset{3}{\alpha}^i$ which automatically satisfies the fourth equation. Eq. (33) gives an alternative representation of a flat generalized connection.

D. Metric geometries, the codifferential and Laplacian

When M has a metric the dual of $\overset{p}{\mathbf{a}}$ is the n-p-2 form given by

$$\star\overset{p}{\mathbf{a}} \equiv (*\overset{p+2}{\alpha}, (-1)^{n+p} *\overset{p+1}{\not{\alpha}}, (-1)^{n+p+1} *\overset{p+1}{\alpha}, *\overset{p}{\alpha}). \tag{37}$$

If the dimension of M is even type 2 forms may be self-dual, or anti-self-dual, when $p = \frac{1}{2}(n-2)$. Such forms are given by

$$\overset{p}{\mathbf{a}} \equiv (\overset{p}{\alpha}, \overset{p+1}{\alpha}, \pm\lambda^{-1} *\overset{p+1}{\alpha}, \pm\lambda^{-1} *\overset{p}{\alpha}),$$

$$\overset{2}{\lambda} = \operatorname{sgn}(\det g).$$

For example, $N=2$ self/anti-self-dual forms on four manifolds are determined by a pair of one-forms and two-forms (or any one-form of type $N=1$).

The codifferential is given by

$$\delta\overset{p}{\mathbf{a}} = (\delta\overset{p}{\alpha}, \delta\overset{p+1}{\alpha} + (-1)^p k_1\overset{p}{\alpha}, \delta\overset{p+1}{\not{\alpha}} + (-1)^p k_2\overset{p}{\alpha}, \delta\overset{p+2}{\alpha} + (-1)^{p+1}k_1\overset{p+1}{\not{\alpha}} + (-1)^p k_2\overset{p+1}{\alpha}). \tag{38}$$

In the case of generalized forms of type 2, Theorem 2 implies the following.

Proposition 2: When k_2 is nonzero and the generalized form $\overset{p}{\mathbf{a}}$ is co-closed it must have the form

$$\overset{p}{\mathbf{a}} = ((-1)^{p+1}k_2^{-1}\delta\overset{p+1}{\not{\alpha}}, (-1)^{p+1}k_2^{-1}\delta\overset{p+2}{\alpha} + k_2^{-1}k_1\overset{p+1}{\not{\alpha}}, \overset{p+1}{\not{\alpha}}, \overset{p+2}{\alpha}) \tag{39}$$

and $\overset{p}{\mathbf{a}} = \delta\overset{p+1}{\mathbf{c}}$ where $\overset{p+1}{\mathbf{c}}$ may be chosen to be

$$\overset{p+1}{\mathbf{c}} = ((-1)^{p+1}k_2^{-1}\overset{p+1}{\not{\alpha}}, (-1)^{p+1}k_2^{-1}\overset{p+2}{\alpha}, 0, 0). \tag{40}$$

From Eq. (22), the inner product is given by

$$\langle \overset{p}{\mathbf{a}}, \overset{p}{\mathbf{b}} \rangle = \langle \overset{p}{\alpha}, \overset{p}{\beta} \rangle + \langle \overset{p+1}{\alpha}, \overset{p+1}{\beta} \rangle + \langle \overset{p+1}{\not{\alpha}}, \overset{p+1}{\not{\beta}} \rangle + \langle \overset{p+2}{\alpha}, \overset{p+2}{\beta} \rangle.$$

The Laplacian of $\overset{p}{\mathbf{a}}$ is given by

$$\overset{p}{\Delta}\mathbf{a}=(\overset{p}{\Delta}\alpha+c\overset{p}{\alpha},\overset{p+1}{\Delta}\overset{p+1}{\alpha}+c\overset{p+1}{\alpha},\overset{p+1}{\Delta}\overset{p+1}{\not{\alpha}}+c\overset{p+1}{\not{\alpha}},\overset{p+2}{\Delta}\overset{p+2}{\alpha}+c\overset{p+2}{\alpha}), \tag{41}$$

where $c=k_1^2+k_2^2$. Hence, unlike the case for $N=1$ forms in Ref. 2, the ''mass'' term c can be zero even if both (complex) k_1 and k_2 are non-zero.

IV. LORENTZIAN METRICS AND EINSTEIN'S EQUATIONS

The aim of this section is to consider Einstein's vacuum field equations on a four-manifold M. In order to fix notation, a standard formulation, which includes the use of two-component spinors, of the Cartan moving frame approach to four-metrics will be reviewed. Next a complex generalized one-form, $\mathbf{E}$, will be constructed on S, the total space of the bundle of two-component spinors over a four-manifold M with four-metric g. It will be shown that $\mathbf{E}$ is closed if and only if g is Ricci flat. Primary attention will be paid to Lorentzian four-metrics although similar results apply straightforwardly to other signatures and holomorphic four-metrics. Once again everything is local.

First, the Cartan approach to metrics can be summarized as follows. Let θ^a be a basis of ordinary one-forms, a Cartan co-frame for g, so that the line element for g is given by

$$ds^2=\eta_{ab}\theta^a\otimes\theta^b, \tag{42}$$

where, for 4-metrics

$$\eta_{ab}=\begin{bmatrix}0 & \epsilon_{AB}\\ -\epsilon_{AB} & 0\end{bmatrix}, \quad \text{and} \quad \epsilon_{AB}=\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix},$$

so that

$$ds^2=\theta^1\otimes\theta^4+\theta^4\otimes\theta^1-\theta^2\otimes\theta^3-\theta^3\otimes\theta^2. \tag{43}$$

In this section lower case italic indices sum and range over 1–4. Upper case italic indices sum and range over 0–1 and, as will be shown below, will be able to be interpreted as two-component spinor indices. Conventions include the standard two component spinor conventions.[8–10]

The orientation is such that, in the case of Lorentzian four-metrics, where θ^1 and θ^4 are real and θ^2 is the complex conjugate of θ^3, the volume element is given by $V=i\,\theta^1\wedge\theta^2\wedge\theta^3\wedge\theta^4$, and the structure group is S0(1,3) which is isomorphic to $\mathrm{SL}(2,\mathbb{C})/\mathbb{Z}_2$.

The Cartan structure equations are given by

$$\begin{gathered}D\theta^a\equiv d\theta^a-\theta^b\wedge\omega_b^a=0,\\ \omega_{ab}+\omega_{ba}=0,\\ d\omega_b^a+\omega_c^a\wedge\omega_b^c=\Omega_b^a=-\tfrac{1}{2}R_{bcd}^a\theta^c\wedge\theta^d,\end{gathered} \tag{44}$$

where ω_b^a denotes the Levi–Civita connection one-form, and R_{bcd}^a are the components of its curvature two-form Ω_b^a. Here, for any ordinary form the covariant exterior derivative is given by

$$D\alpha^a=d\alpha^a+\omega_{b\wedge}^a\alpha^b, \tag{45}$$

and the second covariant exterior derivative satisfies

$$D^2\alpha^a=\alpha^b\wedge\Omega_b^a.$$

The connection and curvature forms, which take values in the Lie algebra of the structure group, can be written as the sum of their self-dual and anti-self-dual parts on the algebra indices, ${}^+\omega_b^a$, ${}^-\omega_b^a$, ${}^+\Omega_b^a$, ${}^-\Omega_b^a$, respectively. Here, ${}^*{}^+\Omega_b^a=i\,{}^+\Omega_b^a$, ${}^*{}^-\Omega_b^a=-i\,{}^-\Omega_b^a$. In 4×4 matrix form

$$ {}^{+}\omega_b^a = \begin{bmatrix} \overline{\omega}_{0'}^{0'} 1 & \overline{\omega}_{1'}^{0'} 1 \\ \overline{\omega}_{0'}^{1'} 1 & -\overline{\omega}_{0'}^{0'} 1 \end{bmatrix}, \quad {}^{-}\omega_b^a = \begin{bmatrix} \omega_B^A & 0 \\ 0 & \omega_B^A \end{bmatrix}, \tag{46} $$

where 1 denotes the unit 2×2 matrix, $\overline{\omega}_{0'}^{0'}$, $\overline{\omega}_{1'}^{0'}$, $\overline{\omega}_{0'}^{1'}$ denote the independent components of ${}^{+}\omega_b^a$, the trace of the 2×2 matrix (ω_B^A) is zero and its entries are the complex conjugates of $\overline{\omega}_{B'}^{A'}$. Other self-dual and anti-self-dual objects can be written similarly, for instance,

$$ \begin{gathered} {}^{-}\Omega_b^a = \begin{bmatrix} \Omega_B^A & 0 \\ 0 & \Omega_B^A \end{bmatrix}, \\ \Omega_B^A = d\omega_B^A + \omega_C^A \wedge \omega_B^C . \end{gathered} \tag{47} $$

In the case of Lorentzian four-metrics, the self-dual connection and curvature are the complex conjugates of the anti-self-dual connection and curvature and take (complex conjugate) values in the Lie algebras $\mathrm{sl}(2,C)_R$ and $\mathrm{sl}(2,C)_L$.

The two-component spinor approach to the Cartan equations for 4-metrics can be summarized, using notation which is compatible with the above, as follows. The line element, given by Eqs. (42) and (43), can be written

$$ ds^2 = \epsilon_{AB}\epsilon_{A'B'}\theta^{AA'} \otimes \theta^{BB'}, \tag{48} $$

where the co-frame is represented by a 2×2 matrix $\theta^{AA'}$,

$$ \theta^{AA'} = \begin{bmatrix} \theta^{00'} & \theta^{01'} \\ \theta^{10'} & \theta^{11'} \end{bmatrix} = \begin{bmatrix} \theta^1 & \theta^3 \\ \theta^2 & \theta^4 \end{bmatrix}. \tag{49} $$

For Lorentzian four-metrics this is a Hermitian matrix valued one-form. By using the correspondences

$$ \begin{gathered} \theta^{AA'} \leftrightarrow \theta^a, \\ \delta_B^A \overline{\omega}_{B'}^{A'} \leftrightarrow {}^{+}\overline{\omega}_b^a, \delta_B^A \overline{\Omega}_{B'}^{A'} \leftrightarrow {}^{+}\overline{\Omega}_b^a, \\ \delta_{B'}^{A'} \omega_B^A \leftrightarrow {}^{-}\omega_b^a, \delta_{B'}^{A'} \Omega_B^A \leftrightarrow {}^{-}\Omega_b^a, \end{gathered} \tag{50} $$

the Cartan structure equations, Eq. (44), can be seen to take the spinorial form

$$ \begin{gathered} D\theta^{AA'} \equiv d\theta^{AA'} - \theta^{AB'} \wedge \omega_B^A - \theta^{BA'} \wedge \overline{\omega}_{B'}^{A'} = 0, \\ \Omega_B^A \equiv d\omega_B^A + \omega_C^A \wedge \omega_B^C, \\ \overline{\Omega}_{B'}^{A'} \equiv d\overline{\omega}_{B'}^{A'} + \overline{\omega}_{C'}^{A'} \wedge \overline{\omega}_{B'}^{C'} . \end{gathered} \tag{51} $$

The anti-self-dual and self-dual components of the Lorentzian Levi–Civita spin connection are given, respectively, by ω_B^A and $\overline{\omega}_{B'}^{A'}$, in agreement with Eq. (46). Unprimed upper case italic indices and primed upper case italic indices represent, respectively, transformation properties under $\mathrm{SL}(2,C)_L$ and $\mathrm{SL}(2,C)_R$. The components of the curvature two-forms are given by

$$\Omega^A_B = \Psi^A_{BCD}\Sigma^{CD} + 2\Lambda\Sigma^A_B + \Phi^A_{BC'D'}\Sigma^{C'D'},$$
$$\overline{\Omega}^{A'}_{B'} = \overline{\Psi}^{A'}_{B'C'D'}\overline{\Sigma}^{C'D'} + 2\Lambda\overline{\Sigma}^{A'}_{B'} + \Phi^{A'}_{B'CD}\Sigma^{CD}, \tag{52}$$

where $\Sigma^A_B = 1/2\,\theta^A_{A'} \wedge \theta^{A'}_B$ and $\overline{\Sigma}^{A'}_{B'} = 1/2\,\theta^{A'}_A \wedge \theta^A_{B'}$. The anti-self-dual and self-dual components of the Weyl spinor are given, respectively, by the totally symmetric spinors complex conjugate spinors Ψ_{ABCD} and $\Psi_{A'B'C'D'}$, and $-2\Phi^A_{BC'D'}$ and 24Λ correspond, respectively, to the trace free part of the Ricci tensor and the Ricci scalar.

Einstein's field equations, with cosmological constant λ, are given by

$$G_{ab} = -8\pi T_{ab} - \lambda g_{ab}, \tag{53}$$

and the spinor form of the Einstein tensor $G^{AA'}_{BB'} = -6(1/3\Phi^{AA'}_{BB'} + \Lambda\,\delta^A_B\delta^{A'}_{B'})$, is given by the three-form equation

$$(1/3\Phi^{AA'}_{BB'} + \Lambda\,\delta^A_B\delta^{A'}_{B'})\,\theta^{BC'} \wedge \theta^{CB'} \wedge \theta_{CC'} = \Omega^A_B \wedge \theta^{BA'} = -\overline{\Omega}^{A'}_{B'} \wedge \theta^{AB'}. \tag{54}$$

Hence the metric is Ricci-flat if and only if

$$\Omega^A_B \wedge \theta^{BA'} = \overline{\Omega}^{A'}_{B'} \wedge \theta^{AB'} = 0. \tag{55}$$

Consider now the two-component spinor bundle over M with fiber coordinates π_A and define on the total space, S, the *self-conjugate* generalized one-form $\mathbf{E}$ given by the quadruple

$$\mathbf{E} = (\pi_A\overline{\pi}_{A'}\theta^{AA'}, -k^{-1}\pi_A D\overline{\pi}_{A'} \wedge \theta^{AA'}, -\overline{k}^{-1} D\pi_A \wedge \overline{\pi}_{A'}\theta^{AA'}, (k\overline{k})^{-1} D\pi_A \wedge D\overline{\pi}_{A'} \wedge \theta^{AA'}), \tag{56}$$

where $\theta^{AA'}$ is a Hermitian matrix valued one-form on M, and ω^A_B and $\overline{\omega}^{A'}_{B'}$ are complex conjugate sl(2,C) valued connection one-forms on M. Here, D denotes a covariant exterior derivative, for example,

$$D\pi_A \equiv d\pi_A - \pi_B\omega^B_A, \tag{57}$$

and the choice $k_1 = k$, $k_2 = \overline{k}$ has been made.

By using the results above and the identities for the second derivative, such as

$$D^2\pi_A = -\pi_B\Omega^B_A, \tag{58}$$

it is a straightforward matter to show that

$$d\mathbf{E} = (\overset{2}{\varepsilon}, \overset{3}{\varepsilon}, \overset{3}{\not{\varepsilon}}, \overset{4}{\varepsilon}),$$

$$\overset{2}{\varepsilon} = \pi_A\overline{\pi}_{A'} D\theta^{AA'},$$

$$\overset{3}{\varepsilon} = k^{-1}[\pi_A\overline{\pi}_{A'}, \overline{\Omega}^{A'}_{B'} \wedge \theta^{AB'} + \pi_A D\overline{\pi}_{A'} \wedge D\theta^{AA'}], \tag{59}$$

$$\overset{3}{\not{\varepsilon}} = \overline{k}^{-1}[\pi_A\overline{\pi}_{A'}, \Omega^A_B \wedge \theta^{BA'} + D\pi_A \wedge \overline{\pi}_{A'} D\theta^{AA'}],$$

$$\overset{4}{\varepsilon} = (k\overline{k})^{-1}[D\pi_A \wedge D\overline{\pi}_{A'} \wedge D\theta^{AA'} - \pi_A D\overline{\pi}_{A'} \wedge \Omega^A_B \wedge \theta^{BA'} + D\pi_A \wedge \overline{\pi}_{A'}\overline{\Omega}^{A'}_{B'} \wedge \theta^{AB'}].$$

This leads immediately to the following theorem.

Theorem 3: The self-conjugate generalized one-form, **E**, on *S*, is closed if and only if

$$D\theta^{AA'}=0,$$
$$\Omega^{A}_{B}\wedge\theta^{BA'}=\overline{\Omega}^{A'}_{B'}\wedge\theta^{AB'}=0. \tag{60}$$

Consequently, when the four real one-forms defined by $\theta^{AA'}$ are linearly independent, and hence define a Lorentzian four-metric on M [as in Eq. (48)], the connection ω^{a}_{b} is the torsion free Levi-Civita connection, and the metric is Ricci flat, if and only if the complex generalized one-form **E** is closed.

The one form **E**, which is closed and hence exact when Einstein's vacuum field equations are satisfied, is not unique. For example $\mathbf{F}\wedge\mathbf{E}$, where **F** is a zero-form which is either closed or satisfies the condition $\mathbf{E}=d\mathbf{F}$, is also closed when Einstein's equations are satisfied. The generalized one-form **E** incorporates both the Witten–Nester two-form and the Sparling three-form which play an important role in the definitions of conserved quantities in general relativity. For a review of the latter and references to higher dimensions see, for example, Ref. 9. The generalized one-form **E** presented here effectively encodes the conditions that the one-forms $\theta^{AA'}$ must satisfy in order to determine a Ricci flat, Lorentzian, four-metric. By using Theorem 1, the following corollaries may be obtained. The first is a gauge noninvariant form, on *M*, of the gauge invariant result in the theorem.

Corollary 1: Einstein's vacuum field equations are satisfied if and only if

$$\mathbf{E}^{AA'}\equiv(\theta^{AA'},-k^{-1}\theta^{AB'}\wedge\overline{\omega}^{A'}_{B'},-\overline{k}^{-1}\theta^{BA'}\wedge\omega^{A}_{B},(k\overline{k})^{-1}\theta^{BB'}\wedge\omega^{A}_{B}\wedge\overline{\omega}^{A'}_{B'}), \tag{61}$$

is closed. In nonspinorial notation

$$\mathbf{E}^{a}=(\theta^{a},-k^{-1}\theta^{b}\wedge{}^{+}\omega^{a}_{b},-\overline{k}^{-1}\theta^{b}\wedge{}^{-}\omega^{a}_{b},(k\overline{k})^{-1}\theta^{c}\wedge{}^{-}\omega^{a}_{b}\wedge{}^{+}\omega^{b}_{c}),$$

$$d\mathbf{E}^{a}=(\overset{2}{\epsilon}{}^{a},\overset{3}{\epsilon}{}^{a},\overset{3}{\not\epsilon}{}^{a},\overset{4}{\epsilon}{}^{a}),$$

$$\overset{2}{\epsilon}{}^{a}=D\theta^{a},\ \overset{3}{\epsilon}{}^{a}=k^{-1}[\theta^{b}\wedge{}^{+}\Omega^{a}_{b}-D\theta^{b}\wedge{}^{+}\omega^{a}_{b}], \tag{62}$$

$$\overset{3}{\not\epsilon}{}^{a}=\overline{k}^{-1}[\theta^{b}\wedge{}^{-}\Omega^{a}_{b}-D\theta^{b}\wedge{}^{-}\omega^{a}_{b}],$$

$$\overset{4}{\epsilon}{}^{a}=(k\overline{k})^{-1}[{}^{+}\omega^{a}_{c}\wedge{}^{-}\Omega^{c}_{b}\wedge\theta^{b}-{}^{-}\omega^{a}_{c}\wedge{}^{+}\Omega^{c}_{b}\wedge\theta^{b}+{}^{-}\omega^{a}_{c}\wedge{}^{+}\omega^{c}_{b}\wedge D\theta^{b}].$$

Corollary 2: (a) **E** is closed if and only if

$$\mathbf{E}=d\mathbf{F}=d\overline{\mathbf{F}},\ \text{where}$$

$$\mathbf{F}=-(\overline{k})^{-1}(0,0,\pi_{A}\overline{\pi}_{A'},\theta^{AA'},-k^{-1}\pi_{A}D\overline{\pi}_{A'}\wedge\theta^{AA'}), \tag{63}$$

$$\overline{\mathbf{F}}=-(k)^{-1}(0,\pi_{A}\overline{\pi}_{A'},\theta^{AA'},0,\overline{k}^{-1}\pi_{A'}D\pi_{A}\wedge\theta^{AA'}).$$

(b) If **E** is closed then $\mathbf{F}-\overline{\mathbf{F}}$ is closed.

(c) Since

$$\mathbf{F}-\overline{\mathbf{F}}=(k\overline{k})^{-1}(0,\overline{k}\pi_{A}\overline{\pi}_{A'},\theta^{AA'},-k\pi_{A}\overline{\pi}_{A'},\theta^{AA'},D(\pi_{A}\overline{\pi}_{A'})\wedge\theta^{AA'}), \tag{64}$$

$\mathbf{F}-\overline{\mathbf{F}}$ is closed if and only if $D\theta^{AA'}=0$, that is the connection is torsion free.

In (a) use is made of the equation for the exterior derivative of the complex generalized zero-form $\mathbf{F}$,

$$d\mathbf{F}=\mathbf{E}-(k\overline{k})^{-1}(0,0,k\pi_A\overline{\pi}_{A'}D\theta^{AA'},\pi_A\overline{\pi}_{A'},\overline{\Omega}^{B'}_{A'}\wedge\theta^{AA'}+\pi_A D\overline{\pi}_{A'}\wedge D\theta^{AA'}).$$

(An unprimed connection one-form ω^A_B does not appear in $\mathbf{F}$, but $\mathbf{E}=d\mathbf{F}$ implies that the connection one-form ω^A_B appearing in the last equation is the anti-self-dual part of the Levi–Civita connection defined by $\theta^{AA'}$.)

It is a straightforward matter to construct, in a similar way, one-forms which are closed if and only if a 4-metric is half-flat. It suffices to demonstrate this here in the case of anti-self-dual half-flat holomorphic four-metrics.[9–11]

Theorem 4: Let g be a holomorphic four-metric on a four-manifold M given by $ds^2=\epsilon_{AB}\epsilon_{A'B'}\theta^{AA'}\otimes\theta^{BB'}$, and let $\mu_{A'}$ be any two-component spinor field with constant components. Consider the generalized one-form on the spin bundle over M given by

$$\mathbf{E}=(\pi_A\mu_{A'}\theta^{AA'},0,-\overline{k}^{-1}D\pi_A\wedge\mu_{A'}\theta^{AA'},0), \tag{65}$$

where π_A are fiber coordinates on the bundle. Then $\mathbf{E}$ is closed if and only if $d\theta^{AA'}-\theta^{AB'}\wedge\omega^A_B=0$; that is $\mathbf{E}$ is closed if and only if the self-dual part of the curvature of g is zero.

The formulation of this corollary emphasizes certain similarities and differences between the requirement that a metric be half-flat on the one hand and Ricci flat, but not necessarily half flat, on the other. However it can clearly be more economically expressed in terms of the closure of a generalized one-form of type $N=1$ given by $(\pi_A\mu_{A'}\theta^{AA'},-k_1^{-1}D\pi_A\wedge\mu_{A'}\theta^{AA'})$.

ACKNOWLEDGMENTS

I would like to thank Pawel Nurowski for helpful comments. I am also grateful to Chris Isham and the Theoretical Physics Group at Imperial College for hospitality while this research was being undertaken.

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Lie point symmetries and first integrals: The Kowalevski top

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(Received 29 August 2002; accepted 19 January 2003)

We show how the Lie group analysis method can be used in order to obtain first integrals of any system of ordinary differential equations. The method of reduction/increase of order developed by Nucci [J. Math. Phys. **37**, 1772–1775 (1996)] is essential. Noether's theorem is neither necessary nor considered. The most striking example we present is the relationship between Lie group analysis and the famous first integral of the Kowalevski top. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1561157]

I. INTRODUCTION

In January 2001, the first Whiteman prize for notable exposition on the history of mathematics was awarded to Thomas Hawkins by the American Mathematical Society. In the citation, published in the Notices of AMS **48**, 416–417 (2001), one reads that Thomas Hawkins "... has written extensively on the history of Lie groups. In particular, he has traced their origins to [Lie's] work in the 1870s on differential equations ... the *idée fixe* guiding Lie's work was the development of a Galois theory of differential equations ... [Hawkins's book[10]] highlights the fascinating interaction of geometry, analysis, mathematical physics, algebra, and topology ...."

In the Introduction of his book,[36] Olver wrote that "it is impossible to overestimate the importance of Lie's contribution to modern science and mathematics. Nevertheless, anyone who is already familiar with [it] ... is perhaps surprised to know that its original inspirational source was the field of differential equations."

Lie's monumental work on transformation groups,[20–22] and in particular contact transformations,[23] led him to achieve his goal.[24] Lie group analysis is indeed the most powerful tool to find the general solution of ordinary differential equations. Any known integration technique can be shown to be a particular case of a general integration method based on the derivation of the continuous group of symmetries admitted by the differential equation, i.e., the Lie symmetry algebra. In particular, Bianchi's theorem[2,36] states that if an admitted n-dimensional solvable Lie symmetry algebra is found, then the general solution of the corresponding n order system of ordinary differential equations can be obtained by quadratures. The admitted Lie symmetry algebra can be easily derived by a straightforward although lengthy procedure. As computer algebra softwares become widely used, the integration of systems of ordinary differential equations by means of Lie group analysis is getting easier to carry out.

A major drawback of Lie's method is that it is useless when applied to systems of n first order equations, because they admit an infinite number of symmetries, and there is no systematic way to find even one-dimensional Lie symmetry algebra, apart from trivial groups like translations in time admitted by autonomous systems. One may try to derive an admitted n-dimensional solvable Lie symmetry algebra by making an ansatz on the form of its generators.

However, Nucci[30] has remarked that any system of n first order equations could be transformed into an equivalent system where at least one of the equations is of second order. Then, the

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admitted Lie symmetry algebra is no longer infinite dimensional, and nontrivial symmetries of the original system could be retrieved.[30] This idea has been successfully applied in several instances.[30,43,5,40,32,33,35,31]

Here we show another striking application of such an idea. If we consider a system of first order equations, and by eliminating one of the dependent variables derive an equivalent system which has one equation of second order, then Lie group analysis applied to that equivalent system yields the first integral(s) of the original system which does not contain the eliminated dependent variable. Of course, if such first integrals exist. The procedure should be repeated on as many times as there are dependent variables in order to find all such first integrals. The first integrals correspond to the characteristic curves of determining equations of parabolic type[42] which are constructed by the method of Lie group analysis.

We would like to remark that interactive (not automatic) programs for calculating Lie point symmetries such as Refs. 28 and 29 are most appropriate for performing this task.

It is well known that if one finds a transformation which leaves invariant a functional describing a variational problem, then Noether's theorem[27] provides a first integral of the corresponding Euler–Lagrange system. Unfortunately, a general method for finding such a transformation does not exist. In addition, many equations of physical interest (e.g., Lorenz system in meteorology[25]) do not come from a variational problem. On the contrary, our method can be applied to any system of ordinary differential equations, even if they do not derive from a variational problem,[31] and we do not make any a priori hypothesis on the form of the first integrals, apart missing one of the unknowns.

In the next section, we describe the method in detail, in Secs. III and IV, we present the classical example of the Kowalevski top, and in Sec. V the three-dimensional Kepler problem in Cartesian coordinates. The last section contains some final comments.

II. OUTLINE OF THE METHOD

Let us consider the following autonomous (which could also be nonautonomous) system of N first order ordinary differential equations:

$$\begin{aligned} \dot{w}_1 &= F_1(w_1, w_2, \ldots, w_N), \\ \dot{w}_2 &= F_2(w_1, w_2, \ldots, w_N), \\ &\cdots, \\ \dot{w}_N &= F_N(w_1, w_2, \ldots, w_N). \end{aligned} \tag{1}$$

Let

$$I = I(w_1, w_2, \ldots, w_{s-1}, w_{s+1}, \ldots, w_N), \tag{2}$$

be a first integral which does not depend on w_s, and

$$X = V(t, w_1, \ldots, w_N)\partial_t + \sum_{k=1}^{N} G_k(t, w_1, \ldots, w_N)\partial_{w_k} \tag{3}$$

be a generator of a Lie point symmetry group for (1). If we derive w_s from one of the equations (1), say the first, then we obtain a system of $N-2$ equations of first order in $w_2, \ldots, w_{s-1}, w_{s+1}, \ldots, w_N$ and one of second order in w_1. We remark that the method does not depend on the equation we choose from (1) to derive w_s. After introducing the new notation u_j $(j = 1, \ldots, N-1)$, we can write the system we obtain as

$$\begin{aligned}
\ddot{u}_1 &= f_1(u_1,u_2,\ldots,u_{N-1},\dot{u}_1),\\
\dot{u}_2 &= f_2(u_1,u_2,\ldots,u_{N-1},\dot{u}_1),\\
&\cdots,\\
\dot{u}_{N-1} &= f_{N-1}(u_1,u_2,\ldots,u_{N-1},\dot{u}_1).
\end{aligned} \tag{4}$$

A generator of a Lie point symmetry group for (4) is

$$\overline{X} = \overline{V}(t,u_1,\ldots,u_{N-1})\partial_t + \sum_{j=1}^{N-1} \overline{G}_j(t,u_1,\ldots,u_{N-1})\partial_{u_j}. \tag{5}$$

If we apply Lie group analysis to system (4) using the interactive REDUCE programs developed by Nucci,[28,29] then we obtain a determining equation of parabolic type for V. Its characteristic curves will yield $m<N-1$ transformations, which eliminate $\dot{u}_1$ from all the first order equations in (4). Thus, we have obtained a system of $N-2$ equations of first order and one equation of second order in the new dependent variables $\tilde{u}_j$ such that $u_1=\tilde{u}_1$ and each of the other variables $\tilde{u}_j$ are either the original u_j itself, if $\dot{u}_1$ did not appear in the j-equation of system (4), or the corresponding characteristic curve. If we apply Lie group analysis to this final system, then again a determining equation of parabolic type will be derived, and its characteristic curve, when rewritten in the original variables, will be exactly the first integral (2).

Now let us consider a system of M second order ordinary differential equations

$$\ddot{x}_i = H_i(x_1,\ldots,x_M,\dot{x}_1,\ldots,\dot{x}_M) \quad (i=1,\ldots,M). \tag{6}$$

A generator of a Lie point symmetry group for this system has the form

$$\Gamma = \tau(t,x_1,\ldots,x_M)\partial_t + \sum_{i=1}^{M} \eta_i(t,x_1,\ldots,x_M)\partial_{x_i}. \tag{7}$$

System (6) can be converted into the following autonomous system of $2M$ first order ordinary differential equations:

$$\begin{aligned}
\dot{w}_i &= w_{M+i},\\
\dot{w}_{M+i} &= H_i(w_1,\ldots,w_M,w_{M+1},\ldots,w_{2M}).
\end{aligned} \tag{8}$$

At this point, we could either proceed as indicated above or choose one of the dependent variables to be the new independent variable y in order to reduce the order of system (8) by one.[30] For example, we could take $x_M \equiv w_M = y$. Then, system (8) becomes the following nonautonomous system of $2M-1$ first order ordinary differential equations with independent variable y:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}y} w_h &= w_{M+h}/w_{2M},\\
\frac{\mathrm{d}}{\mathrm{d}y} w_{M+h} &= H_h(w_1,\ldots,w_{M-1},y,w_{M+1},\ldots,w_{2M})/w_{2M},
\end{aligned} \tag{9}$$

where $h=1,\ldots,M-1$. Now, our method can be applied to this system as if it was system (1). The fact that system (9) is not autonomous does not effect the result, as we will show in the case of the three dimensional Kepler problem in Cartesian coordinates.

The same method can be applied to a single ordinary differential equation of order N which can be easily transformed into a system of N equations of first order. It should be noticed that there

could be several different ways of transforming an equation of order N into a system of N equations of first order. Then, the just described method may give different results, videlicet (*viz.*) no first integrals with certain reductions, all the first integrals with different reductions.

III. FINDING THE KOWALEVSKI TOP

The motion of a heavy rigid point about a fixed point is one of the most famous problems of classical mechanics.[7] In 1750, Euler[6] derived the equations of motion which now bear his name, and described what is nowadays known as the Euler–Poinsot case because of the geometrical description given by Poinsot about 100 years later.[38] It was Jacobi[13] who integrated this case by using the elliptic functions which he had developed (along with Legendre, Abel, and Gauss[26]) and mastered[14] (we have translated this fundamental text into Italian and extensively commented[41]). Another case was described by Lagrange,[19] and it is known as the Lagrange–Poisson case, due to the extensive study done later by Poisson.[39] This case can also be integrated by using Jacobi elliptic functions.[44] At the time, it seemed that other cases could easily be found and similarly integrated. In 1855, the Prussian Academy of Science proposed this topic for a competition, but nobody applied.[4] The problem was so elusive that the German mathematicians called it the mathematical mermaid (*die mathematische Nixe*).[17] More than 30 years elapsed before the Bordin prize was awarded to Kowalevski for finding and reducing to hyperelliptic quadratures the third case[16] which is since known as the Kowalevski top. She solved the problem by looking for solutions which are single-valued meromorphic functions in the entire complex plane of the variable t.[7] Her method became what is now known as the Painlevé–Kowalevski (or just Painlevé) method.[12] Hawkins had established "the nature and extent of Jacobi's influence upon Lie."[9] It is a remarkable coincidence that the mathematical mermaid can also be found by using Lie group analysis as we show in the following.

The Euler–Poisson equations describing the motion of a heavy rigid body about a fixed point are[16]

$$\begin{aligned}
\dot{p} &= ((B-C)rq + mg(\beta z_G - \gamma y_G))/A,\\
\dot{q} &= ((C-A)pr + mg(\gamma x_G - \alpha z_G))/B,\\
\dot{r} &= ((A-B)pq + mg(\alpha y_G - \beta x_G))/C,\\
\dot{\alpha} &= \beta r - \gamma q,\\
\dot{\beta} &= \gamma p - \alpha r,\\
\dot{\gamma} &= \alpha q - \beta p,
\end{aligned} \tag{10}$$

with A, B, C the principal moments of inertia, $p(t), q(t), r(t)$ the components of the angular velocity, m the mass of the body, g the acceleration of gravity, x_G, y_G, z_G the coordinates of the center of mass, and $\alpha(t), \beta(t), \gamma(t)$ the component of the unit vertical vector. There are three first integrals for system (10): conservation of energy, i.e.,

$$I_1 = \tfrac{1}{2}(Ap^2 + Bq^2 + cr^2) + mg\,(x_G\alpha + y_G\beta + z_G\gamma) \tag{11}$$

conservation of the vertical component of the angular momentum, i.e.,

$$I_2 = Ap\alpha + Bq\beta + Cr\gamma \tag{12}$$

the length of the unit vertical vector, i.e.,

$$I_3 = \alpha^2 + \beta^2 + \gamma^2 (= 1). \tag{13}$$

If we apply our method to system (10), then we find only the first integral of the unit vertical vector which has p,q,r as missing variables. Kowalevski found that if one imposes the following conditions on the parameters:

(1) $A=B=2C$,
(2) $z_G=0$, and either $x_G\neq 0$ or $y_G\neq 0$
then there exists a fourth integral, i.e.,

$$I_4=\left(p^2-q^2-mg\frac{x_G\alpha-y_G\beta}{C}\right)^2+\left(2pq-mg\frac{x_G\beta+y_G\alpha}{C}\right)^2. \tag{14}$$

We notice that γ and r are missing in (14). Thanks to our method, we can find the Kowalevski top by searching for a first integral which does not contain γ. First we derive γ from the second equation of system (10), i.e.,

$$\gamma=\frac{B\dot{q}+(A-C)pr+mgz_G\alpha}{mgx_G}$$

which implies that x_G must be different from zero. We obtain the following system of four equations of first order, and one of second order:

$$\begin{aligned}\ddot{u}_1=&\dot{u}_1(Au_1z_G+(A-C)u_3y_G)/Ax_G-(A-B)(A-C)u_1u_2^2/BC+(A-C)^2y_Gu_2u_3^2/ABx_G\\&+(A-C)u_1u_2u_3z_G/Bx_G-(A-C)(B-C)u_1u_3^2/AB-(Au_2x_G-Cu_3z_G)\\&\times(A-C)mgy_Gu_4/ABCx_G+(A(A-2C)u_2x_G+C(C-2A)u_3z_G)mgu_5/ABC\\&+(x_G^2+z_G^2)mgu_1u_4/Bx_G,\end{aligned} \tag{15}$$

$$\dot{u}_2=-\dot{u}_1By_G/Ax_G+u_3((C-A)y_Gu_2+(B-C)x_Gu_1)/Ax_G+mgz_G(-u_4y_G+u_5x_G)/Ax_G, \tag{16}$$

$$\dot{u}_3=((A-B)u_1u_2+mg(u_4y_G-u_5x_G))/C, \tag{17}$$

$$\dot{u}_4=-\dot{u}_1Bu_1/mgx_G+(C-A)u_1u_2u_3/mgx_G+(u_3u_5x_G-u_1u_4z_G)/x_G, \tag{18}$$

$$\dot{u}_5=\dot{u}_1Bu_2/mgx_G+(A-C)u_2^2u_3/mgx_G+z_Gu_2u_4/x_G-u_3u_4 \tag{19}$$

with

$$u_1=q,\quad u_2=p,\quad u_3=r,\quad u_4=\alpha,\quad u_5=\beta. \tag{20}$$

Now we apply Lie group analysis to system (15)–(19). An operator Γ

$$\Gamma=V(t,u_1,u_2,u_3,u_4,u_5)\partial_t+\sum_{k=1}^{5}G_k(t,u_1,u_2,u_3,u_4,u_5)\partial_{u_k} \tag{21}$$

is said to generate a Lie point symmetry group if its second prolongation

$$\underset{2}{\Gamma}=\Gamma+\sum_{k=1}^{5}\left(\frac{\mathrm{d}G_k}{\mathrm{d}t}-\dot{u}_k\frac{\mathrm{d}V}{\mathrm{d}t}\right)\partial_{\dot{u}_k}+\left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}G_1}{\mathrm{d}t}-\dot{u}_1\frac{\mathrm{d}V}{\mathrm{d}t}\right)-\ddot{u}_1\frac{\mathrm{d}V}{\mathrm{d}t}\right)\partial_{\ddot{u}_1}$$

applied to system (15)–(19), on their solutions, is identically equal to zero, i.e.,

$$\underset{2}{\Gamma}(15)|_{(15)-(19)}=0,$$

$$\underset{2}{\Gamma}(16)|_{(15)-(19)}=0,$$

$$\Gamma^{(17)}_{2}|_{(15)-(19)}=0, \tag{22}$$

$$\Gamma^{(18)}_{2}|_{(15)-(19)}=0,$$

$$\Gamma^{(19)}_{2}|_{(15)-(19)}=0.$$

The five determining equations (22) constitute an overdetermined system of linear partial differential equations in the unknowns $V, G_k (k=1,5)$ In fact, they are polynomials in $\dot{u}_1$, each coefficient of which must become identically equal to zero. In particular, the first determining equation in (22) is a polynomial of degree three for $\dot{u}_1$. The coefficient of highest degree yields an equation of parabolic type for V in four independent variables u_1, u_2, u_4, u_5, i.e.,

$$\begin{aligned}
&A^2mg^2x_G^2\frac{\partial^2 V}{\partial u_1^2}-2ABm^2g^2x_Gy_G\frac{\partial^2 V}{\partial u_1u_2}-2A^2Bmgu_1x_G\frac{\partial^2 V}{\partial u_1u_4}+2A^2Bmgu_2x_G\frac{\partial^2 V}{\partial u_1u_5}\\
&\quad+B^2m^2g^2y_G^2\frac{\partial^2 V}{\partial u_2^2}+2AB^2mgu_1y_G\frac{\partial^2 V}{\partial u_2u_4}-2AB^2mgu_2y_G\frac{\partial^2 V}{\partial u_2u_5}+A^2B^2u_1^2\frac{\partial^2 V}{\partial u_4^2}\\
&\quad-2A^2B^2u_1u_2\frac{\partial^2 V}{\partial u_4u_5}+A^2B^2u_2^2\frac{\partial^2 V}{\partial u_5^2}-A^2Bmgx_G\frac{\partial V}{\partial u_4}-AB^2mgy_G\frac{\partial V}{\partial u_5}=0.
\end{aligned} \tag{23}$$

Its three characteristic curves yield the following transformations:

$$\begin{aligned}
&u_2=s_2-\frac{Bu_1y_G}{Ax_G} \quad viz. \quad p=s_2-\frac{Bqy_G}{Ax_G},\\
&u_4=s_4-\frac{Bu_1^2}{2mgx_G} \quad viz. \quad \alpha=s_4-\frac{Bq^2}{2mgx_G},\\
&u_5=s_5+Bu_1\frac{By_Gu_1+2Ax_Gu_2}{2Amgx_G^2} \quad viz. \quad \beta=s_5+Bq\frac{By_Gq+2Ax_Gp}{2Amgx_G^2}
\end{aligned} \tag{24}$$

with s_2, s_4, and s_5 new unknown functions of t.

As outlined in Sec. II, transformations (24) eliminate $\dot{u}_1$ from all the first order equations in system (15)–(19).

In fact, system (15)–(19) becomes

$$\begin{aligned}
\ddot{u}_1=(&-6A^2BCu_1\tilde{u}_2^2x_G^2-4A^2BCu_1x_G\tilde{u}_2u_3z_G-2A^2Bmgu_1x_G^2y_G\tilde{u}_5-2A^2C^2u_3x_Gu_1\tilde{u}_2z_G\\
&+2A^2Bmgu_1x_Gy_G^2\tilde{u}_4-3A^2BCu_1^2y_Gu_3z_G+2A^2BC\dot{u}_1u_3x_Gy_G-5A^2BCu_1^2y_G\tilde{u}_2x_G\\
&+3AB^3u_1^3y_G^2-2A^2BCu_1u_3^2y_G^2-A^2BCu_1^3x_G^2-2A^2BCu_1u_3^2x_G^2-2AC^3u_3^2x_G^2u_1\\
&+2A^2Cmgx_Gu_1\tilde{u}_4z_G^2+2A^2Cmgx_G^3u_1\tilde{u}_4-4A^2Cmgx_G^2u_3z_G\tilde{u}_5-4A^2Cmgx_G^3\tilde{u}_2\tilde{u}_5\\
&+2A^2Cmgx_Gu_3z_G\tilde{u}_4y_G-7A^2B^2y_Gu_1^2\tilde{u}_2x_G+2A^2Cmgx_G^2\tilde{u}_2\tilde{u}_4y_G-4A^2C^2u_3^2x_G\tilde{u}_2y_G\\
&-3A^2B^2y_G^2u_1^3-B^2C^2y_Gu_1^2u_3z_G-2u_1A^4\tilde{u}_2^2x_G^2+2A^3\tilde{u}_2x_GCu_3^2y_G+2A^3\tilde{u}_2x_GCu_1u_3z_G\\
&+2A^3\tilde{u}_2^2x_G^2Cu_1-2u_1BC^3y_G^2u_3^2+5A^3\tilde{u}_2x_GBu_1^2y_G-2A^3\tilde{u}_2x_G^2mg\tilde{u}_4y_G+4A^3\tilde{u}_2^2x_G^2Bu_1\\
&+4ABCmgu_1x_G^2y_G\tilde{u}_5-2ABCmgu_1x_Gy_G^2\tilde{u}_4-2ABC^2\dot{u}_1u_3x_Gy_G+2ABC^2u_1x_G\tilde{u}_2u_3z_G\\
&+3ABC^2u_1^2y_Gu_3z_G+4ABC^2u_1u_3^2y_G^2+2ABC^2u_1u_3^2x_G^2+2AB^2Cu_1^2y_Gu_3z_G\\
&+10AB^2Cu_1^2y_G\tilde{u}_2x_G+2AC^3u_3^2x_G\tilde{u}_2y_G+2AC^2mgu_3x_G^2z_G\tilde{u}_5-4B^3Cy_G^2u_1^3
\end{aligned}$$

$$-2AC^2mgu_3x_Gz_G\tilde{u}_4y_G+2A^2C^2u_3^2x_G^2u_1-A^2BCu_1^3z_G^2+3AB^2Cu_1^3y_G^2$$
$$+2A^2BCu_1x_G\dot{u}_1z_G+2A^3\tilde{u}_2x_G^3mg\tilde{u}_5)/2A^2BCx_G^2, \tag{25}$$

$$\dot{\tilde{u}}_2=(-2A^2\tilde{u}_2u_3x_Gy_G+ABu_1^2y_Gz_G+2ABu_1\tilde{u}_2x_Gz_G+2ABu_1u_3x_G^2+2ABu_1u_3y_G^2-2ACu_1u_3x_G^2$$
$$+2AC\tilde{u}_2u_3x_Gy_G-2Amg\tilde{u}_4x_Gy_Gz_G+2Amg\tilde{u}_5x_G^2z_G-2BCu_1u_3y_G^2)/2A^2x_G^2, \tag{26}$$

$$\dot{u}_3=(2A^2u_1\tilde{u}_2x_G-3ABu_1^2y_G-4Bu_1\tilde{u}_2Ax_G+2Amg\tilde{u}_4x_Gy_G-2\tilde{u}_5x_G^2Amg+3B^2y_Gu_1^2)/2ACx_G, \tag{27}$$

$$\dot{\tilde{u}}_4=(-2A^2u_1\tilde{u}_2u_3x_G+ABu_1^3z_G+2ABu_1^2u_3y_G+2ABu_1\tilde{u}_2u_3x_G+2ACu_1\tilde{u}_2u_3x_G$$
$$-2Amgu_1\tilde{u}_4x_Gz_G+2Amgu_3\tilde{u}_5x_G^2-B^2u_1^2u_3y_G-2BCu_1^2u_3y_G)/2Amgx_G^2, \tag{28}$$

$$\dot{\tilde{u}}_5=(2A^2\tilde{u}_2^2u_3x_G-ABu_1^2\tilde{u}_2z_G+ABu_1^2u_3x_G-2ABu_1\tilde{u}_2u_3y_G-2AC\tilde{u}_2^2u_3x_G+2Amg\tilde{u}_2\tilde{u}_4x_Gz_G$$
$$-2Amgu_3\tilde{u}_4x_G^2-2B^2u_1^2\tilde{u}_2z_G-2B^2u_1^2u_3x_G+2BCu_1^2u_3x_G+2BCu_1\tilde{u}_2u_3y_G$$
$$-2Bmgu_1\tilde{u}_5x_Gz_G)/2Amgx_G^2, \tag{29}$$

with

$$\tilde{u}_2=s_2, \quad \tilde{u}_4=s_4, \quad \tilde{u}_5=s_5. \tag{30}$$

We now apply Lie group analysis to system (25)–(29). An operator $\tilde{\Gamma}$

$$\tilde{\Gamma}=\tilde{V}(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_t+\tilde{G}_1(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_{u_1}+\tilde{G}_2(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_{\tilde{u}_2}$$
$$+\tilde{G}_3(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_{u_3}+\tilde{G}_4(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_{\tilde{u}_4}+\tilde{G}_5(t,u_1,\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)\partial_{\tilde{u}_5} \tag{31}$$

is said to generate a Lie point symmetry group if its second prolongation $\tilde{\Gamma}_2$ applied to system (25)–(29), on their solutions, is identically equal to zero, i.e.,

$$\tilde{\Gamma}_2(25)|_{(25)-(29)}=0,$$
$$\tilde{\Gamma}_2(26)|_{(25)-(29)}=0,$$
$$\tilde{\Gamma}_2(27)|_{(25)-(29)}=0, \tag{32}$$
$$\tilde{\Gamma}_2(28)|_{(25)-(29)}=0,$$
$$\tilde{\Gamma}_2(29)|_{(25)-(29)}=0.$$

The five determining equations (32) constitute an overdetermined system of linear partial differential equations in the unknowns $\tilde{V}$, $\tilde{G}_k(k=1,5)$ In fact, they are polynomials in $\dot{u}_1$, each coefficient of which must become identically equal to zero. In particular, the fifth determining equation in (32) is a polynomial of degree one for $\dot{u}_1$. We call its two coefficients $c5k1$ and $c5k0$. For the sake of simplicity, we assume $\tilde{G}_k=0, \partial\tilde{V}/\partial t=0$. Then, the coefficient of degree one, i.e., $c5k1$, yields

$$\frac{\partial \widetilde{V}}{\partial u_1}=0.$$

Now, $c5k0$ is a polynomial of degree five in u_1. Therefore, its coefficients, call them $c5m5$,$c5m4$,$c5m3$,$c5m2$,$c5m1$,$c5m0$, must become identically equal to zero. The coefficient of degree five in u_1, i.e., $c5m5$, yields

$$\frac{\partial \widetilde{V}}{\partial \tilde{u}_4}A^2B^2Cz_G(-(A+2B)\tilde{u}_2z_G+(A-2B+2C)u_3x_G)=0 \tag{33}$$

which gives the condition on the parameter

$$z_G=0. \tag{34}$$

Then, the coefficient of degree four in u_1, i.e., $c5m4$, yields

$$-\left(3(A-B)\frac{\partial \widetilde{V}}{\partial u_3}mgy_Gx_G-(A-2B+2C)\frac{\partial \widetilde{V}}{\partial \tilde{u}_5}Cu_3x_G-(2A-B-2C)\frac{\partial \widetilde{V}}{\partial \tilde{u}_4}Cu_3y_G\right)$$
$$\times(A-2B+2C)AB^2u_3x_G=0 \tag{35}$$

which gives the condition on the parameters

$$A=2B-2C. \tag{36}$$

Then, the coefficient of degree three in u_1, i.e., $c5m3$, becomes

$$12\left(\frac{\partial \widetilde{V}}{\partial u_3}mgx_G-\frac{\partial \widetilde{V}}{\partial \tilde{u}_4}Cu_3\right)(2B-3C)(B-C)(B-2C)B^2\tilde{u}_2u_3y_G^2=0 \tag{37}$$

which gives the further condition on the parameters

$$B=2C. \tag{38}$$

Thus, we have found the Kowalevski top. We also notice that either condition $2B=3C$ or $B=C$ leads to the Lagrange top. Finally, we are left with two linear first order partial differential equations in $\widetilde{V}=\widetilde{V}(\tilde{u}_2,u_3,\tilde{u}_4,\tilde{u}_5)$, the coefficient of degree two in u_1, i.e., $c5m2$,

$$2\left(\frac{\partial \widetilde{V}}{\partial \tilde{u}_4}x_G-\frac{\partial \widetilde{V}}{\partial \tilde{u}_5}y_G\right)Cu_3\tilde{u}_2-4\frac{\partial \widetilde{V}}{\partial u_3}mgx_G^2\tilde{u}_2+(x_G{}^2+y_G{}^2)\frac{\partial \widetilde{V}}{\partial \tilde{u}_2}mgu_3=0 \tag{39}$$

and the coefficient of degree one in u_1, i.e., $c5m1$

$$\begin{aligned}&2C(C\tilde{u}_2^2-mg\tilde{u}_4x_G-mg\tilde{u}_5y_G)\frac{\partial \widetilde{V}}{\partial \tilde{u}_4}x_Gu_3\tilde{u}_2\\&-4C(C\tilde{u}_2^2-mg\tilde{u}_4x_G)\frac{\partial \widetilde{V}}{\partial \tilde{u}_5}y_Gu_3\tilde{u}_2\\&-2(2C\tilde{u}_2^2x_G-2mg\tilde{u}_4x_G^2+mg\tilde{u}_4y_G^2-mg\tilde{u}_5x_Gy_G)\frac{\partial \widetilde{V}}{\partial u_3}mgx_G\tilde{u}_2\end{aligned} \tag{40}$$

$$+(C\tilde{u}_2^2x_G^2+2C\tilde{u}_2^2y_G^2-mg\tilde{u}_4x_G^3-mg\tilde{u}_4x_Gy_G^2)\frac{\partial\tilde{V}}{\partial\tilde{u}_2}mgu_3=0.$$

If $\tilde{V}$ satisfies equations (39) and (40), then it is easy to prove that the determining equations (32) are identically satisfied by considering conditions (34), (36), (38) as well.

From (39) it is easy to obtain that $\tilde{V}=\tilde{V}(\eta_1,\eta_2,\eta_3)$ with

$$\eta_1=u_3^2+\frac{4x_G^2\tilde{u}_2^2}{x_G^2+y_G^2},\quad \eta_2=\tilde{u}_4-\frac{Cx_G\tilde{u}_2^2}{mg(x_G^2+y_G^2)},\quad \eta_3=\tilde{u}_5+\frac{Cy_G\tilde{u}_2^2}{mg(x_G^2+y_G^2)}. \tag{41}$$

Then, (40) becomes

$$2mg(y_G\eta_2-x_G\eta_3)\frac{\partial\tilde{V}}{\partial\eta_1}+C\frac{\partial\tilde{V}}{\partial\eta_2}\eta_3-C\frac{\partial\tilde{V}}{\partial\eta_3}\eta_2=0. \tag{42}$$

Its characteristic curves are

$$\xi_1=\eta_1+\frac{2mg}{C}(y_G\eta_3+x_G\eta_2),\quad \xi_2=\eta_2^2+\eta_3^2. \tag{43}$$

Finally, we have that $\tilde{V}=\Psi(\xi_1,\xi_2)$ with Ψ an arbitrary function of ξ_1,ξ_2, and consequently operator

$$\tilde{\Gamma}=\Psi(\xi_1,\xi_2)\partial_t \tag{44}$$

is a generator of a Lie point symmetry for system (25)–(29). Transforming (43) into the original unknown functions by using (41), (30), (24), and (20) yields

$$\xi_1=\frac{2}{C}\left(\frac{C}{2}(2p^2+2q^2+r^2)+mg\,(x_G\alpha+y_G\beta)\right),$$

$$\xi_2=C^2\frac{\left(p^2-q^2-mg\,\dfrac{x_G\alpha-y_G\beta}{C}\right)^2+\left(2pq-mg\,\dfrac{x_G\beta+y_G\alpha}{C}\right)^2}{m^2g^2(x_G^2+y_G^2)}$$

which correspond to the first integral of conservation of energy (11), and that derived by Kowalevski (14), respectively.

Can other cases of integrability (viz. integration by quadrature) be obtained by using our method? We leave the answer to a future paper. In Ref. 43, the application of our method led to an integrable case for a nonlinear system of three ordinary differential equations which does not possess the Painlevé property.

IV. FIRST INTEGRALS OF THE KOWALEVSKI TOP

We apply our method to the Kowalevski top itself which corresponds to the following conditions on the parameters:

(1) $A=B=2C$,
(2) $y_G=z_G=0,\quad x_G>0$.

The condition on y_G can be added without loss of generality. Then, system (10) become

$$\begin{aligned}
\dot{p} &= rq/2, \\
\dot{q} &= -pr/2 + mgx_G\gamma/2C, \\
\dot{r} &= -mgx_G\beta/C, \\
\dot{\alpha} &= \beta r - \gamma q, \\
\dot{\beta} &= \gamma p - \alpha r, \\
\dot{\gamma} &= \alpha q - \beta p.
\end{aligned} \tag{45}$$

The first integrals for the Kowalewski top are

(1) conservation of energy, i.e.,

$$I_1 = \frac{C}{2}(2p^2+2q^2+r^2) + mgx_G\alpha; \tag{46}$$

(2) conservation of the vertical component of the angular momentum, i.e.,

$$I_2 = C(2p\alpha + 2q\beta + r\gamma); \tag{47}$$

(3) the length of the unit vertical vector, i.e.,

$$I_3 = \alpha^2 + \beta^2 + \gamma^2 (=1); \tag{48}$$

(4) the first integral derived by Kowalevski, i.e.,

$$I_4 = \left(p^2 - q^2 - \frac{x_G\alpha mg}{C}\right)^2 + \left(2pq - \frac{x_G\beta mg}{C}\right)^2. \tag{49}$$

If our method is applied to (45), then all the first integrals can be obtained, apart from (47) which has all the unknown variables $p, q, r, \alpha, \beta, \gamma$ appearing in its expression. Let us observe that

β does not appear in I_1,

γ does not appear in both I_1 and I_4,

p does not appear in I_3.

In the following, we eliminate α, β, γ, p from system (45) one at a time.

A. Eliminating α

First we show a negative result: no first integral obtained. Let us assume that we do not know any of the first integrals. Therefore, we do not know *a priori* that none of the first integrals can be obtained by deriving α. We derive α from the fifth equation of system (45), i.e.,

$$\alpha = \frac{p\gamma - \dot{\beta}}{r}$$

and obtain the following system of four equations of first order, and one of second order:

$$\begin{aligned}
\ddot{u}_1 &= (-2Cu_1u_3^3 - 2Cu_1u_3u_4^2 - 2C\dot{u}_1u_2u_4 + 3Cu_2u_3^2u_5 \\
&\quad + 2Cu_2u_4^2u_5 - 2mgu_1\dot{u}_1x_G + 2mgu_1u_4u_5x_G)/2Cu_3, \\
\dot{u}_2 &= (-Cu_3u_4 + mgu_5x_G)/2C, \\
\dot{u}_3 &= (-mgu_1x_G)/C, \\
\dot{u}_4 &= (u_2u_3)/2, \\
\dot{u}_5 &= (-u_1u_3u_4 - \dot{u}_1u_2 + u_2u_4u_5)/u_3
\end{aligned} \tag{50}$$

with

$$u_1=\beta,\quad u_2=q,\quad u_3=r,\quad u_4=p,\quad u_5=\gamma. \tag{51}$$

If we apply Lie group analysis to system (50), then we obtain a determining equation of parabolic type for V in two independent variables. Its characteristic curve is

$$u_5u_3+u_1u_2$$

which yields the following transformation:

$$u_5=\frac{s_5-u_2u_1}{u_3}\quad viz.\quad \gamma=\frac{s_5-q\beta}{r} \tag{52}$$

with s_5 a new unknown function of t. Then, system (50) transforms into

$$\begin{aligned}
\ddot{u}_1&=(-3Cu_1u_2^2u_3^2-2Cu_1u_2^2u_4^2-2Cu_1u_3^4-2Cu_1u_3^2u_4^2-2C\dot{u}_1u_2u_3u_4+3Cu_2u_3^2\tilde{u}_5\\
&\quad+2Cu_2u_4^2\tilde{u}_5-2mgu_1^2u_2u_4x_G-2mgu_1\dot{u}_1u_3x_G+2mgu_1u_4\tilde{u}_5x_G)/2Cu_3^2,\\
\dot{u}_2&=(-Cu_3^2u_4-mgu_1u_2x_G+mg\tilde{u}_5x_G)/2Cu_3,\\
\dot{u}_3&=(-mgu_1x_G)/C,\\
\dot{u}_4&=u_2u_3/2,\\
\dot{\tilde{u}}_5&=(-2Cu_1u_2^2u_4-3Cu_1u_3^2u_4+2Cu_2u_4\tilde{u}_5+mgu_1^2u_2x_G-mgu_1\tilde{u}_5x_G)/2Cu_3,
\end{aligned} \tag{53}$$

with

$$\tilde{u}_5=s_5. \tag{54}$$

If we apply Lie group analysis to system (53), then we obtain a two dimensional Lie symmetry algebra generated by the following two operators:

$$\Gamma_1=\frac{\partial}{\partial t}, \tag{55}$$

$$\Gamma_2=-t\frac{\partial}{\partial t}+2u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}+u_3\frac{\partial}{\partial u_3}+u_4\frac{\partial}{\partial u_4}+3\tilde{u}_5\frac{\partial}{\partial\tilde{u}_5} \tag{56}$$

which in the original unknown functions correspond to

$$\Gamma_1=\frac{\partial}{\partial t}, \tag{57}$$

$$\Gamma_2=-t\frac{\partial}{\partial t}+p\frac{\partial}{\partial p}+q\frac{\partial}{\partial q}+r\frac{\partial}{\partial r}+2\alpha\frac{\partial}{\partial\alpha}+2\beta\frac{\partial}{\partial\beta}+2\gamma\frac{\partial}{\partial\gamma}. \tag{58}$$

This is a trivial finding.

B. Eliminating β

We derive β from the third equation of system (45), i.e.,

$$\beta = -\frac{C\dot{r}}{mgx_G}$$

and obtain the following system of four equations of first order, and one of second order:

$$\begin{aligned}
\ddot{u}_1 &= (mgx_G(u_1u_4 - u_3u_5)/C,\\
\dot{u}_2 &= (-Cu_1u_3 + mgx_Gu_5)/2C,\\
\dot{u}_3 &= u_1u_2/2,\\
\dot{u}_4 &= (-Cu_1\dot{u}_1 - mgx_Gu_2u_5)/mgx_G,\\
\dot{u}_5 &= (C\dot{u}_1u_3 + mgx_Gu_2u_4)/mgx_G
\end{aligned} \tag{59}$$

with

$$u_1 = r, \quad u_2 = q, \quad u_3 = p, \quad u_4 = \alpha, \quad u_5 = \gamma. \tag{60}$$

If we apply Lie group analysis to system (59), then we obtain a determining equation of parabolic type for V in three independent variables. Its two characteristic curves yield the following transformations:

$$\begin{aligned}
u_4 &= \frac{s_4 - Cu_1^2}{2mg\,x_G} \quad viz. \quad \alpha = \frac{s_4 - Cr^2}{2mg\,x_G},\\
u_5 &= \frac{Cu_3u_1 + s_6}{mg\,x_G} \quad viz. \quad \gamma = \frac{Cpr + s_6}{mg\,x_G}
\end{aligned} \tag{61}$$

with s_4 and s_6 new unknown functions of t. Then, system (50) transforms into

$$\begin{aligned}
\ddot{u}_1 &= (-Cu_1^3 - 2Cu_1u_3^2 + u_1\tilde{u}_4 - 2u_3\tilde{u}_5)/2C,\\
\dot{u}_2 &= \tilde{u}_5/2C,\\
\dot{u}_3 &= u_1u_2/2,\\
\dot{\tilde{u}}_4 &= -2u_2(Cu_1u_3 + \tilde{u}_5),\\
\dot{\tilde{u}}_5 &= u_2(-2Cu_1^2 + \tilde{u}_4)/2
\end{aligned} \tag{62}$$

with

$$\tilde{u}_4 = s_4, \quad \tilde{u}_5 = s_6. \tag{63}$$

If we apply Lie group analysis to system (62), then we obtain two first order partial differential equations for V:

$$\frac{\partial V}{\partial u_3} - 4Cu_3\frac{\partial V}{\partial \tilde{u}_4} = 0, \tag{64}$$

$$\frac{\partial V}{\partial u_2}-4Cu_2\frac{\partial V}{\partial \tilde{u}_4}=0, \tag{65}$$

with $V\equiv V(u_2,u_3,\tilde{u}_4)$. From (64) it is easy to obtain that $V\equiv V(\eta,u_2)$ with

$$\eta=2Cu_3^2+\tilde{u}_4. \tag{66}$$

Then, (65) becomes

$$\frac{\partial V}{\partial u_2}-4Cu_2\frac{\partial V}{\partial \eta}=0. \tag{67}$$

Its characteristic curve is

$$\xi_1=2Cu_2^2+\eta. \tag{68}$$

Finally, we have that $V=\psi(\xi_1)$ with ψ an arbitrary function of ξ, and consequently operator

$$\Gamma_1=\psi(\xi_1)\partial_t \tag{69}$$

is a generator of a Lie point symmetry for system (62). Transforming (68) into the original unknown functions by using (66), (63), (61), (60) yields

$$\xi_1=\frac{C}{2}(2p^2+2q^2+r^2)+mg\,x_G\alpha$$

which is exactly the first integral of conservation of energy (46). In addition, we have algorithmically derived that (69) is a generator of a Lie point symmetry for system (45).

C. Eliminating γ

We derive γ from the second equation of system (45), i.e.,

$$\gamma=\frac{C(2\dot{q}+pr)}{mgx_G}$$

and obtain the following system of four equations of first order, and one of second order:

$$\begin{gathered}\ddot{u}_1=u_1(-Cu_3^2+2mgu_4x_G)/4C,\\ \dot{u}_2=u_1u_3/2,\\ \dot{u}_3=-mgu_5x_G/C,\\ \dot{u}_4=(-2Cu_1\dot{u}_1-Cu_1u_2u_3+mgu_3u_5x_G)/mgx_G,\\ \dot{u}_5=(2C\dot{u}_1u_2+Cu_2^2u_3-mgu_3u_4x_G)/mgx_G\end{gathered} \tag{70}$$

with

$$u_1=q,\quad u_2=p,\quad u_3=r,\quad u_4=\alpha,\quad u_5=\beta. \tag{71}$$

If we apply Lie group analysis to system (70), then we obtain a determining equation of parabolic type for V in three independent variables. Its two characteristic curves yield the following transformations:

$$u_4=\frac{s_4-Cu_1^2}{mgx_G} \quad viz. \quad \alpha=\frac{s_4-Cq^2}{mgx_G},$$
$$u_5=\frac{2Cu_1u_2+s_5}{mgx_G} \quad viz. \quad \beta=\frac{2Cpq+s_5}{mgx_G} \tag{72}$$

with s_4 and s_5 new unknown functions of t. Then, system (70) transforms into

$$\begin{aligned}
\ddot{u}_1&=[u_1(-2Cu_1^2-Cu_3^2+2\tilde{u}_4)]/4C,\\
\dot{u}_2&=u_1u_3/2,\\
\dot{u}_3&=(-2Cu_1u_2-\tilde{u}_5)/C,\\
\dot{\tilde{u}}_4&=u_3(Cu_1u_2+\tilde{u}_5),\\
\dot{\tilde{u}}_5&=u_3(Cu_2^2-\tilde{u}_4)
\end{aligned} \tag{73}$$

with

$$\tilde{u}_4=s_4, \quad \tilde{u}_5=s_5. \tag{74}$$

If we apply Lie group analysis to system (73), then we obtain two first order partial differential equations for V:

$$u_3\frac{\partial V}{\partial u_2}-4u_2\frac{\partial V}{\partial u_3}+4Cu_2u_3\frac{\partial V}{\partial \tilde{u}_4}=0, \tag{75}$$

$$8Cu_2\tilde{u}_5\frac{\partial V}{\partial u_3}-Cu_3\tilde{u}_5\frac{\partial V}{\partial \tilde{u}_4}+Cu_3(\tilde{u}_4-Cu_2^2)\frac{\partial V}{\partial \tilde{u}_5}=0 \tag{76}$$

with $V\equiv V(u_2,u_3,\tilde{u}_4,\tilde{u}_5)$. From (75) it is easy to obtain that $V\equiv V(\eta_1,\eta_2,\tilde{u}_5)$ with

$$\eta_1=4u_2^2+u_3^2, \quad \eta_2=Cu_2^2-\tilde{u}_4. \tag{77}$$

Then, Eq. (76) becomes

$$2Cu_3\tilde{u}_5\frac{\partial V}{\partial \eta_1}+Cu_3\tilde{u}_5\frac{\partial V}{\partial \eta_2}-Cu_3(u_4-Cu_2^2)\frac{\partial V}{\partial \tilde{u}_5}=0. \tag{78}$$

Its characteristic curves are

$$\xi_1=C\eta_1-2\eta_2, \quad \xi_2=\eta_2^2+\tilde{u}_5^2. \tag{79}$$

Finally, we have that $V=\Psi(\xi_1,\xi_2)$ with Ψ an arbitrary function of ξ_1, ξ_2, and consequently operator

$$\Gamma_1=\Psi(\xi_1,\xi_2)\partial_t \tag{80}$$

is a generator of a Lie point symmetry for system (73). Transforming (79) into the original unknown functions by using (77), (74), (72), (71) yields

$$\xi_1=\frac{C}{2}(2p^2+2q^2+r^2)+mg\,x_G\alpha,$$

$$\xi_2=\left(p^2-q^2-\frac{x_G\alpha mg}{C}\right)^2+\left(2pq-\frac{x_G\beta mg}{C}\right)^2$$

which are exactly the first integral of conservation of energy (46), and that derived by Kowalevski (49), respectively. In addition, we have algorithmically derived that (80) is a generator of a Lie point symmetry for system (45).

D. Eliminating *p*

We derive p from the second equation of system (45), i.e.,

$$p=\frac{mg\gamma x_G-2C\dot{q}}{Cr}$$

and obtain the following system of four equations of first order, and one of second order:

$$\begin{gathered}\ddot{u}_1=u_1(-Cu_3^2+2mgu_4x_G)/4C,\\ \dot{u}_2=(Cu_1u_3u_4+2C\dot{u}_1u_5-mgu_2u_5x_G)/Cu_3,\\ \dot{u}_3=-mgu_5x_G/C,\\ \dot{u}_4=-u_1u_2+u_3u_5,\\ \dot{u}_5=(-2C\dot{u}_1u_2-Cu_3^2u_4+mgu_2^2x_G)/Cu_3\end{gathered}\tag{81}$$

with

$$u_1=q,\quad u_2=\gamma,\quad u_3=r,\quad u_4=\alpha,\quad u_5=\beta.\tag{82}$$

If we apply Lie group analysis to system (81), then we obtain a determining equation of parabolic type for V in three independent variables. Its two characteristic curves yield the following transformations:

$$\begin{gathered}u_2=\sqrt{s_6}\cos(2s_5-2u_3)\quad viz.\quad \gamma=\sqrt{s_6}\cos(2s_5-2r),\\ u_5=\sqrt{s_6}\sin(2s_5-2u_3)\quad viz.\quad \beta=\sqrt{s_6}\sin(2s_5-2r)\end{gathered}\tag{83}$$

with s_6 and s_5 new unknown functions of t. Then, system (81) transforms into

$$\begin{gathered}\ddot{u}_1=u_1(-Cu_3^2+2mgu_4x_G)/4C,\\ \dot{\tilde{u}}_2=2u_4\sqrt{\tilde{u}_2}\cos(2u_3-2\tilde{u}_5)[\tan(2u_3-2\tilde{u}_5)u_3+u_1],\\ \dot{u}_3=\sqrt{\tilde{u}_2}\sin(2u_3-2\tilde{u}_5)mgx_G/C,\\ \dot{u}_4=-\sqrt{\tilde{u}_2}\cos(2u_3-2\tilde{u}_5)[\tan(2u_3-2\tilde{u}_5)u_3+u_1],\\ \dot{\tilde{u}}_5=\sqrt{\tilde{u}_2}\cos(2u_3-2\tilde{u}_5)[-(Cu_3^2u_4-mg\tilde{u}_2x_G)-2C\dot{u}_1\tilde{u}_2\\ +(Cu_1u_4+2mg\tilde{u}_2x_G)\tan(2u_3-2\tilde{u}_5)u_3]/2C\tilde{u}_2u_3\end{gathered}\tag{84}$$

with

$$\tilde{u}_2=s_6,\quad \tilde{u}_5=s_5.\tag{85}$$

If we apply Lie group analysis to system (84), then we obtain a determining equation of parabolic type for V in two independent variables. Its characteristic curve yields the following transformation:

$$\tilde{u}_5=\frac{ss_5-u_1}{u_3} \quad viz. \quad \begin{aligned}\gamma&=\sqrt{s_6}\cos\left(2\,\frac{ss_5-q-r^2}{r}\right)\\ \beta&=\sqrt{s_6}\sin\left(2\,\frac{ss_5-q-r^2}{r}\right)\end{aligned}, \tag{86}$$

with ss_5 a new unknown function of t. Then, system (84) transforms into

$$\begin{aligned}\ddot{u}_1&=u_1(-Cu_3^2+2mgu_4x_G)/4C,\\ \dot{\tilde{u}}_2&=2u_4\sqrt{\tilde{u}_2}\cos((2u_1+2u_3^2-2\hat{u}_5)/u_3)[u_1+\tan((2u_1+2u_3^2-2\hat{u}_5)/u_3)u_3],\\ \dot{u}_3&=\sqrt{\tilde{u}_2}\sin((2u_1+2u_3^2-2\hat{u}_5)/u_3)mgx_G/C,\\ \dot{u}_4&=-\sqrt{\tilde{u}_2}\cos((2u_1+2u_3^2-2\hat{u}_5)/u_3)[u1+\tan((2u_1+2u_3^2-2\hat{u}_5)/u_3)u_3],\\ \dot{\hat{u}}_5&=\sqrt{\tilde{u}_2}\cos((2u_3^2-2\hat{u}_5+2u_1)/u_3)[[(2u_3^2+2\hat{u}_5-2u_1)mg\tilde{u}_2x_G+Cu_1u_3^2u_4]\\ &\quad\times\tan((2u_3^2-2\hat{u}_5+2u_1)/u_3)+(mg\tilde{u}_2x_G-cu_3^2u_4)u_3]/2c\tilde{u}_2u_3\end{aligned} \tag{87}$$

with

$$\hat{u}_5=ss_5. \tag{88}$$

If we apply Lie group analysis to system (87), then we obtain one first order partial differential equation for V:

$$\frac{\partial V}{\partial u_4}-2u_4\frac{\partial V}{\partial\tilde{u}_2}=0 \tag{89}$$

with $V\equiv V(\tilde{u}_2,u_4)$. Its characteristic curve is

$$\xi_1=\tilde{u}_2+u_4^2. \tag{90}$$

Finally, we have that $V=\psi(\xi_1)$ with ψ an arbitrary function of ξ_1, and consequently operator

$$\Gamma_1=\psi(\xi_1)\partial_t \tag{91}$$

is a generator of a Lie point symmetry for system (87). Transforming (90) into the original unknown functions by using (88), (86), (85), (83), (82) yields

$$\xi_1=\alpha^2+\beta^2+\gamma^2$$

which is exactly the first integral of the length of the unit vertical vector (48). In addition, we have algorithmically derived that (91) is a generator of a Lie point symmetry for system (45).

V. KEPLER PROBLEM

In Ref. 33, Nucci's method[30] was used to find symmetries additional to those reported by Krause[18] in his study of the complete symmetry group of the Kepler problem. A consequence of the application of Nucci's method was the demonstration of the group theoretical relationship between the simple harmonic oscillator and the Kepler problem. In Ref. 33, polar coordinates were

used, and Nucci's method was not applied to the three-dimensional case with the purpose of finding first integrals. We do it here by considering Cartesian coordinates.

The equations of motion of the Kepler problem are given by the following well-known three equations of second order:

$$\begin{aligned}\ddot{x}_1&=-\mu x_1/((x_1^2+x_2^2+x_3^2)^{3/2}),\\ \ddot{x}_2&=-\mu x_2/((x_1^2+x_2^2+x_3^2)^{3/2}),\\ \ddot{x}_3&=-\mu x_3/((x_1^2+x_2^2+x_3^2)^{3/2}).\end{aligned} \tag{92}$$

The first integrals for the Kepler problem are conservation of energy E, conservation of angular momentum $\mathbf{K}$, the Laplace–Runge–Lenz vector $\mathbf{L}$. None of the unknowns $x_1,x_2,x_3,\dot{x}_1,\dot{x}_2,\dot{x}_3$ are missing in the expression of E and the components of $\mathbf{L}$. This is not true for the three components of $\mathbf{K}$, i.e.,

$$K_1=x_3\dot{x}_2-\dot{x}_3x_2, \tag{93}$$

$$K_2=x_3\dot{x}_1-\dot{x}_3x_1, \tag{94}$$

$$K_3=x_1\dot{x}_2-\dot{x}_1x_2. \tag{95}$$

Therefore, we can only obtain the three components of $\mathbf{K}$ using our method. However, neither E nor $\mathbf{L}$ are needed to reduce system (92) to a linear oscillator, as we show in the following. Let us transform system (92) into a system of six equations of first order

$$\begin{aligned}\dot{w}_1&=w_4,\\ \dot{w}_2&=w_5,\\ \dot{w}_3&=w_6,\\ \dot{w}_4&=-\mu w_1/((w_1^2+w_2^2+w_3^2)^{3/2}),\\ \dot{w}_5&=-\mu w_2/((w_1^2+w_2^2+w_3^2)^{3/2}),\\ \dot{w}_6&=-\mu w_3/((w_1^2+w_2^2+w_3^2)^{3/2})\end{aligned} \tag{96}$$

with

$$w_1=x_1,\quad w_2=x_2,\quad w_3=x_3,\quad w_4=\dot{x}_1,\quad w_5=\dot{x}_2,\quad w_6=\dot{x}_3. \tag{97}$$

Consequently, the components of the angular momentum become

$$K_1=w_3w_5-w_6w_2, \tag{98}$$

$$K_2=w_3w_4-w_1w_6, \tag{99}$$

$$K_3=w_1w_5-w_4w_2. \tag{100}$$

We choose one of the dependent variables to be the new independent variable y in order to reduce the order of system (96) by one.[30] We take $w_3=y$. Then, system (96) becomes the following nonautonomous system of five first order ordinary differential equations:

$$w_1'=w_4/w_6,$$

$$
\begin{aligned}
w_2' &= w_5/w_6,\\
w_4' &= -\mu w_1/(w_6(w_1^2+w_2^2+y^2)^{3/2}),\\
w_5' &= -\mu w_2/(w_6(w_1^2+w_2^2+y^2)^{3/2}),\\
w_6' &= -\mu y/(w_6(w_1^2+w_2^2+y^2)^{3/2})
\end{aligned}
\tag{101}
$$

with prime denoting differentiation with respect to y. Let us observe that

w_4 does not appear in K_1,
w_5 does not appear in K_2,
w_6 does not appear in K_3,

We should remark that other variables are missing too. For example, w_1 is also missing in K_1. However, our method will yield the result whatever the choice of a missing variable. In the following, we eliminate w_4, w_5, w_6 from system (101) one at a time.

A. Eliminating w_4

We derive w_4 from the first equation of system (101), i.e.,

$$w_4 = w_1' w_6$$

and obtain the following nonautonomous system of three equations of first order, and one of second order:

$$
\begin{aligned}
u_4'' &= \mu(u_4' y - u_4)/(u_3^2(u_2^2+u_4^2+y^2)^{3/2}),\\
u_3' &= -\mu y/(u_3(u_2^2+u_4^2+y^2)^{3/2}),\\
u_2' &= u_1/u_3,\\
u_1' &= -\mu u_2/(u_3(u_2^2+u_4^2+y^2)^{3/2})
\end{aligned}
\tag{102}
$$

with

$$u_4 = w_1, \quad u_2 = w_2, \quad u_3 = w_6, \quad u_1 = w_5. \tag{103}$$

If we apply Lie group analysis to system (102), then after several reductions we obtain one first order partial differential equations for G_3,

$$u_1 \frac{\partial G_3}{\partial u_2} + u_3 \frac{\partial G_3}{\partial y} = 0 \tag{104}$$

with $G_3 \equiv G_3(u_1, u_2, u_3, y)$. Its solution is $G_3 = \psi(\xi_1)$ with ψ an arbitrary function of

$$\xi_1 = u_3 u_2 - y u_1. \tag{105}$$

Transforming (105) into the original unknown functions by using (97), (103) yields

$$\xi_1 = \dot{x}_3 x_2 - \dot{x}_2 x_3$$

which is exactly the first component of the angular momentum (93).

B. Eliminating w_5

We derive w_5 from the second equation of system (101), i.e.,

$$w_5 = w_2' w_6$$

and obtain the following nonautonomous system of three equations of first order, and one of second order:

$$\begin{aligned} u_4'' &= \mu(-u_4 + u_4' y)/(u_2(u_1^2 + u_4^2 + y^2)^{3/2}), \\ u_3' &= -\mu u_1/(u_2(u_1^2 + u_4^2 + y^2)^{3/2}), \\ u_2' &= -\mu y/((u_1^2 + u_4^2 + y^2)^{3/2}), \\ u_1' &= u_3/u_2 \end{aligned} \tag{106}$$

with

$$u_4 = w_2, \quad u_2 = w_6, \quad u_3 = w_4, \quad u_1 = w_1. \tag{107}$$

If we apply Lie group analysis to system (106), then after several reductions we obtain one first order partial differential equation for G_2,

$$u_3 \frac{\partial G_2}{\partial u_1} + u_2 \frac{\partial G_2}{\partial y} = 0 \tag{108}$$

with $G_2 \equiv G_2(u_1, u_2, u_3, y)$. Its solution is $G_2 = \phi(\xi_2)$ with ϕ an arbitrary function of

$$\xi_2 = y u_3 - u_1 u_2. \tag{109}$$

Transforming (109) into the original unknown functions by using (97), (107) yields

$$\xi_2 = x_3 \dot{x}_1 - \dot{x}_3 x_1$$

which is exactly the second component of the angular momentum (94).

C. Eliminating w_6

We derive w_6 from the first equation of system (101), i.e.,

$$w_6 = \frac{w_4}{w_1'}$$

and obtain the following nonautonomous system of three equations of first order, and one of second order:

$$\begin{aligned} u_4'' &= \mu u_4'^2(-u_4 + u_4' y)/(u_1^2(u_2^2 + u_4^2 + y^2)^{3/2}), \\ u_3' &= -\mu u_2 u_4'/(u_1(u_2^2 + u_4^2 + y^2)^{3/2}), \\ u_2' &= u_3 u_4'/u_1, \\ u_1' &= -\mu u_4 u_4'/(u_1(u_2^2 + u_4^2 + y^2)^{3/2}) \end{aligned} \tag{110}$$

with

$$u_4=w_1, \quad u_2=w_2, \quad u_3=w_5, \quad u_1=w_4. \tag{111}$$

If we apply Lie group analysis to system (110), then after several reductions we obtain one first order partial differential equation for G_3,

$$u_3\frac{\partial G_3}{\partial u_2}+u_1\frac{\partial G_3}{\partial u_1}=0 \tag{112}$$

with $G_3\equiv G_3(u_1,u_2,u_3,u_4)$ and with $G_3\equiv G_3(u_1,u_2,u_3,y)$. Its solution is $G_3=\varphi(\xi_3)$ with φ an arbitrary function of

$$\xi_3=u_1u_2-u_4u_3. \tag{113}$$

Transforming (113) into the original unknown functions by using (97), (111) yields

$$\xi_3=\dot{x}_2x_1-\dot{x}_1x_2$$

which is exactly the third component of the angular momentum (94).

Now let us derive w_5, w_4, and w_2 from (98), (99) and (100), i.e.,

$$w_5=\frac{-\xi_3w_6y+\xi_2\xi_1+\xi_1w_1w_6}{\xi_2y}, \tag{114}$$

$$w_4=\frac{\xi_2+w_1w_6}{y}, \tag{115}$$

$$w_2=\frac{-\xi_3y+\xi_1w_1}{\xi_2} \tag{116}$$

with ξ_1, ξ_2, ξ_3 new unknown functions of y. Substituting (114), (115), (116) into (101), and deriving w_6 from the first equation yields the following system of three equations of first order, and one of second order:

$$\begin{aligned} u_4''&=(\mu u_2(-u_4^3+3u_4^2u_4'y-3u_4u_4'^2y^2+u_4'^3y^3))/((u_1^2y^2-2u_3u_1u_4y+u_2^2u_4^2+u_2^2y^2+u_3^2u_4^2)^{3/2}),\\ u_3'&=0,\\ u_2'&=0,\\ u_1'&=0 \end{aligned} \tag{117}$$

with

$$u_4=w_1, \quad u_3=\xi_3, \quad u_2=\xi_2, \quad u_1=\xi_1.$$

It is easy to show that system (117) admits an eleven-dimensional Lie symmetry algebra. In fact, the first equation of (117) itself admits a Lie symmetry algebra of dimension eight, which means that it is is linearizable through a point transformation.[24] Thus, we have reduced the equations of motion of the Kepler problem to the harmonic oscillator[33,35] by using Lie group analysis.

VI. FINAL COMMENTS

We have found that Lie group analysis yields the first integrals admitted by any system of ordinary differential equations if the method developed by Nucci[30] is applied, the only limitation being the absence of at least one of the unknowns in each first integral.

Is it possible to obtain all of the first integrals by means of Lie group analysis? Also, what is the link between Painlevé method and Lie group analysis?[34] In addition, can Lax pairs be found by Lie group analysis? So far these are open questions that we hope to address in future work.

Let us conclude by underlining that the application of Nucci's method to the Kowalevski top have led us to understand how first integrals can be found by using Lie group analysis. In 1984, Cooke[4] wrote ''Kowalevskaya's work is an ingenious application of mathematics to a system of equations of great mathematical interest ... but since the case to which it applies is rather special, the details of her arguments are no longer worth troubling about.'' About the same time, a revival of interest into integrable problems of mechanics has led to numerous papers on the Kowalevski top. Just to cite a few, see Refs. 37, 11, 8, 1, 3, 15 and the entire No. 11 issue of J. Phys. A **34** (2001).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

Wave scattering in waveguides

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(Received 16 August 2002; accepted 30 January 2003)

The scattering of scalar waves by objects located inside a waveguide or a cavity is discussed using the method of pseudopotentials. Pseudopotentials were introduced to simulate short-range potentials in quantum mechanics and proved useful in many-body problems and in problems involving multicentered potentials. In this work it is shown that this approach can also be used to describe the scattering of classical scalar waves by objects confined to the interior of a waveguide or a cavity in terms of the scattering amplitudes of those objects in an extended medium.
 [DOI: 10.1063/1.1563847]

I. INTRODUCTION

In many areas of applied physics one encounters the problem of modeling the scattering of wave fields by objects in the interior of a spatially limited domain. For example, in underwater acoustics the active sonar detection of submerged objects depends on detecting the acoustic field scattered by the object. In general this problem cannot be reduced to just the problem of the scattering of a superposition of incident plane waves. One may have to include the scattering and rescattering of waves reflected from the surface and the bottom. One also would like to express this scattering process in terms of the plane wave scattering amplitudes computed in an unbounded, uniform, medium. These scattering amplitudes can be computed independently and used as inputs in one's calculations. What makes these problems difficult is the need to satisfy boundary conditions on the boundaries of the medium and on the surface of the scattering object. Even in the relatively simple case of a perfectly reflecting sphere in an uniform medium between two reflecting parallel planes the scattered field does not have a mathematically simple expression as it has in the case of the same sphere in an extended medium of similar physical properties.

The pseudopotential introduced by Huang and Yang[1] as a generalization of the Fermi pseudopotential, offers a convenient approach to this problem since from the start it separates the implementation of both sets of boundary conditions. The scattering properties of the object are subsumed in a series of field-dependent source terms added to the Helmholtz equation, the solution of this equation must then satisfy proper boundary conditions on the medium's boundaries. Besides its original use in obtaining thermodynamic properties of the hard-sphere Bose gas, recently the Huang and Yang pseudopotential has been used to discuss the properties of confined, low-density, atomic gases at very low temperature.[2]

An early application of the pseudopotential method to classical wave scattering can be found in a 1964 article by Chen.[3] In that article the pseudopotential of Liu and Wong[4] for a Dirichlet sphere (i.e., a hard sphere in quantum mechanics or a pressure release sphere in acoustics) is used to study scattering from such a sphere imbedded in a random medium. In this article the Liu and Wong pseudopotential is also discussed. It is shown that, despite it being formally distinct from the Huang and Yang pseudopotential, it does lead to the same equations for the problem of scattering in confined media.

In Sec. II of this article the pseudopotential of Huang and Yang is introduced and generalized to the case of arbitrary scattering objects. As an example this method is applied to the problem of scattering of waves generated by a point source from a perfectly reflecting sphere where both the

source and the scattering sphere are inside a larger sphere. A particular case of this problem is exactly solvable and can be used as a check on the applicability of the pseudopotential approach. In Sec. III the pseudopotential of Liu and Wong is introduced. Its generalization to arbitrary scattering objects is presented and it is applied to the same problem discussed in Sec. II to show that it leads to the same equations for the scattered field. It is shown in Sec. IV how to derive the scattering equations for the case of wave scattering by multiple objects using the Liu and Wong pseudopotential. In Sec. V the method of Sec. I is applied to the case of an object inside an ideal planar waveguide. Such waveguide, a uniform medium contained between two parallel planes, is an idealized version of the waveguides encountered in ocean acoustics. The physical implications of the equations obtained for the scattered field are discussed. In Sec. VI the results are summarized and compared with other works on similar problems.

II. THE GENERALIZED PSEUDOPOTENTIAL OF HUANG AND YANG

In a seminal article in 1957, Huang and Yang[1] showed that in the case of a scalar wave scattered by a Dirichlet sphere (i.e., the full wave field, incident plus scattered wave, vanishes on the surface of the sphere), the full wave field satisfies the following equation:

$$[\nabla^2+k^2]\psi(\mathbf{r})=-\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{[(2l+1)!!]^2}{k^{2l+1}[(2l+1)!]}\tan(\eta_l)Y_{lm}(\hat{\mathbf{r}})\frac{\delta(r)}{r^{l+2}}\left(\frac{\partial}{\partial r}\right)^{2l+1}[r^{l+1}\psi_{lm}(r)], \tag{2.1}$$

$$\psi_{lm}(r)=\int d\hat{\mathbf{r}}\,Y_{lm}(\hat{\mathbf{r}})^*\psi(\mathbf{r}). \tag{2.2}$$

In other words, Huang and Yang showed that the well-known expression for the full wave field in terms of the partial wave scattering phase shifts,

$$\psi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{lm}[j_l(kr)-\tan(\eta_l)n_l(kr)]Y_{lm}(\hat{\mathbf{r}}),\quad \tan(\eta_l)=\frac{j_l(ka)}{n_l(ka)} \tag{2.3}$$

satisfies Eq. (2.1), that is, the boundary conditions on the surface of the scattering sphere are implicit in the field-dependent source terms on the right-hand side of Eq. (2.1). In Eqs. (2.1)–(2.3), k is the wave number and a is the radius of the sphere. Standard notations are used for the spherical harmonics and the spherical Bessel and Neumann functions.

The wave equation with the pseudopotential is not a way of solving the problem of scattering by a single target. It is an identity satisfied by the solution to such a problem. Notice that the scattering phase shifts are inputs and not the final result of the calculation. However this equation can be used within any volume, bounded or not, as the pseudopotential vanishes away from the target's position. In the presence of boundaries this equation provides a way of including the effects of the volume's boundaries on the scattering by the target. To solve it the Green function for the Helmholtz equation (i.e., the equation without the pseudopotential) that satisfies appropriated boundary conditions at the volume's boundaries is needed.

It is clear from the article by Huang and Yang[1] that Eq. (2.1) can be generalized to the case of arbitrary scattering objects. For nonspherical objects one introduces the full wave field in terms of the scattering amplitude outside the circumscribing sphere. By circumscribing sphere it is meant the sphere with the shortest diameter that fully encases the object. Outside this sphere the wave field is a superposition of spherical harmonics and spherical Bessel and Hankel functions:

$$\psi(\mathbf{r})=\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l}\alpha_{l'm'}\left[j_{l'}(kr)Y_{l'm'}(\hat{\mathbf{r}})+i\sum_{l=0}^{\infty}\sum_{m=-l}^{l}T_{lm,l'm'}h_l^{(1)}(kr)Y_{lm}(\hat{\mathbf{r}})\right], \tag{2.4}$$

where

$$T_{lm,l'm'}=\frac{k}{4\pi}i^{l-l''}\int d\hat{\mathbf{p}}\,Y^*_{lm}(\hat{\mathbf{p}})\int d\hat{\mathbf{q}}\,Y_{l'm'}(\hat{\mathbf{q}})f(\hat{\mathbf{p}},\hat{\mathbf{q}}). \tag{2.5}$$

In Eq. (2.5) $f(\hat{\mathbf{p}},\hat{\mathbf{q}})$ is the scattering amplitude defined in the usual way in terms of the asymptotic limit for $r\to\infty$ of the full wave field created by the scattering of an incident plane wave by the object.[5]

In order to derive the wave equation with pseudopotential in the case of an arbitrary scattering object it is convenient to express Eq. (2.4) in terms of spherical Bessel and Neumann functions. From Eq. (2.4) one obtains

$$\psi(\mathbf{r})=\sum_{l'm'}\sum_{lm}Y_{lm}(\hat{\mathbf{r}})[j_l(kr)(I+iT)_{lm,l'm'}-n_l(kr)T_{lm,l'm'}]\alpha_{l'm'}. \tag{2.6}$$

Introducing now a new set of coefficients, $A_{lm}=\Sigma_{l'm'}(I+iT)_{lm,l'm'}\alpha_{l'm'}$ or, in operator notation, $A=(I+iT)\alpha$, one obtains a generalization of Eq. (4) in the article by Huang and Yang[1]

$$\psi(\mathbf{r})=\sum_{lm}Y_{lm}(\hat{\mathbf{r}})\left[j_l(kr)A_{lm}-n_l(kr)\left(T\frac{I}{I+iT}A\right)_{lm}\right]. \tag{2.7}$$

The same technique used by Huang and Yang to derive Eq. (2.1) for the sphere can be used to obtain from the expression in Eq. (2.7) the following equation in the case of an arbitrary scattering object:

$$[\nabla^2+k^2]\psi(\mathbf{r})=-\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(2l+1)!!}{k^{l+1}}Y_{lm}(\hat{\mathbf{r}})\frac{\delta(r)}{r^{l+2}}\left(T\frac{I}{I+iT}A\right)_{lm}, \tag{2.8}$$

where

$$A_{lm}=\frac{(2l+1)!!}{k^l(2l+1)!}\partial_r^{2l+1}[r^{l+1}\psi_{lm}(r)]_{r=0}. \tag{2.9}$$

The procedure to obtain equations describing scattering in a general case can be formulated without a specific expression for the Green function of the Helmholtz equation. This Green function for the cases of interest in this article, say a uniform fluid contained in a finite volume, or a uniform fluid inside an extended waveguide such as the planar one mentioned in the introduction and discussed in Sec. IV, obey the Helmholtz equation plus appropriate boundary conditions:

$$[\nabla^2+k^2]G_0(\mathbf{r},\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0). \tag{2.10}$$

In the case of a uniform medium $G_0(\mathbf{r},\mathbf{r}_0)$ can be written as

$$G_0(\mathbf{r},\mathbf{r}_0)=g(\mathbf{r}-\mathbf{r}_0)+G_0^{NS}(\mathbf{r},\mathbf{r}_0),\quad g(\mathbf{r})=-\frac{e^{ikr}}{4\pi r}. \tag{2.11}$$

That is, the Green function inside a confining volume or in a waveguide can be split into two parts, a singular one, which is just the Green function in the unbounded medium, and a nonsingular part enforcing the boundary conditions.

In the presence of a scattering object inside the confined spatial region, the Green function obeys a wave equation with pseudopotential and satisfies the same boundary conditions as $G_0(\mathbf{r},\mathbf{r}_0)$:

$$[\nabla^2+k^2]G(\mathbf{r},\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0)-\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\frac{(2l+1)!!}{k^{l+1}}\left[Y_{lm}(\hat{\mathbf{s}})\frac{\delta(s)}{s^{l+2}}\left(T\frac{I}{I+iT}A\right)_{lm}\right]_{\mathbf{s}=\mathbf{r}-\mathbf{r}_T}\right\}. \tag{2.12}$$

In the above equation $\mathbf{r}$ is the observation point, $\mathbf{r}_0$ is the position of the point source and $\mathbf{r}_T$ is the position of the scattering object. The A_{lm} are given by a generalization of Eq. (2.9):

$$A_{lm}=\frac{(2l+1)!!}{k^l(2l+1)!}\partial_s^{2l+1}\left[s^{l+1}\int d\hat{\mathbf{t}}\,Y_{lm}(\hat{\mathbf{t}})^*G(\mathbf{r}_T+s\hat{\mathbf{t}},\mathbf{r}_0)\right]_{s=0}. \tag{2.13}$$

The Green function of the Helmholtz equation, $G_0(\mathbf{r},\mathbf{r}_0)$, is now used to obtain a Lippmann–Schwinger integral equation:

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)-\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(2l+1)!!}{k^{l+1}}\int d\mathbf{r}'\,G_0(\mathbf{r},\mathbf{r}')\left\{Y_{lm}(\hat{\mathbf{s}})\frac{\delta(s)}{s^{l+2}}\left(T\frac{I}{I+iT}A\right)_{lm}\right\}_{\mathbf{s}=\mathbf{r}'-\mathbf{r}_T}. \tag{2.14}$$

The pseudopotential reduces this integral equation to a set of coupled linear algebraic equations by expressing the scattered field in terms of the A_{lm}. The full Green function is expressed in terms of the A_{lm} as follows:

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)-\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(2l+1)!!}{k^{l+1}}\left(T\frac{I}{I+iT}A\right)_{lm}\left\{\lim_{t\to 0}\left[\frac{1}{t^l}\int d\hat{\mathbf{r}}\,Y_{lm}(\hat{\mathbf{t}})G_0(\mathbf{r},\mathbf{r}_T+\mathbf{t})\right]\right\}. \tag{2.15}$$

The linear algebraic equations for the A_{lm} are obtained by inserting the expression for $G(\mathbf{r},\mathbf{r}_0)$ from Eq. (2.15) into Eq. (2.13). In order to obtain explicit expressions for these scattering equations one must compute the following quantities:

$$O_{lm}(\mathbf{r},\mathbf{r}_T)=\frac{i(2l+1)!!}{k^{l+1}}\left\{\lim_{t\to 0}\left[\frac{1}{t^l}\int d\hat{\mathbf{t}}\,Y_{lm}(\hat{\mathbf{t}})G_0(\mathbf{r},\mathbf{r}_T+\mathbf{t})\right]\right\}, \tag{2.16}$$

$$S_{lm}(\mathbf{r}_T,\mathbf{r}_0)=\frac{i(2l+1)!!}{k^{l+1}(2l+1)!}\left\{\lim_{s\to 0}\partial_s^{2l+1}\left[s^{l+1}\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*G_0(\mathbf{r}_T+\mathbf{s},\mathbf{r}_0)\right]\right\}. \tag{2.17}$$

$$K_{lm,l'm'}(\mathbf{r}_T)=\frac{i(2l+1)!!}{k^{l+1}(2l+1)!}\frac{(2l'+1)!!}{k^{l'}}\times\lim_{s\to 0}\partial_s^{2l+1}\left[s^{l+1}\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*\left(\lim_{t\to 0}\left[\frac{1}{t^{l'}}\int d\hat{\mathbf{t}}\,Y_{l'm'}(\hat{\mathbf{t}})G_0^{NS}(\mathbf{r}_T+\mathbf{s},\mathbf{r}_T+\mathbf{t})\right]\right)\right]. \tag{2.18}$$

One should also notice that the singular part of $G_0(\mathbf{r},\mathbf{r}_0)$, namely $g(\mathbf{r}-\mathbf{r}_0)$, the Green function of the Helmholtz equation in a unbounded and uniform fluid, yields the following result:

$$\lim_{s\to 0}\partial_s^{2l+1}\left\{s^{l+1}\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*\lim_{t\to 0}\left[\frac{1}{t^{l'}}\int d\hat{\mathbf{t}}\,Y_{l'm'}(\hat{\mathbf{t}})g(\mathbf{r}_T+\mathbf{s}-\mathbf{r}_T-\mathbf{t})\right]\right\}=\frac{k^{2l+1}(2l+1)!}{i[(2l+1)!!]^2}\delta_{ll'}\delta_{mm'}. \tag{2.19}$$

Thus for the A_{lm} one obtains the following equation:

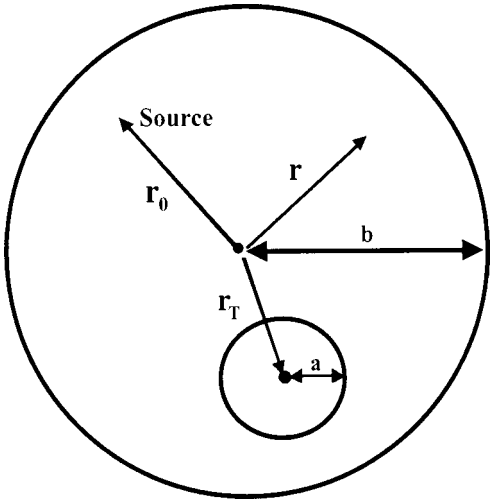

FIG. 1. The geometry of the sphere within a sphere scattering problem.

$$A_{lm}=-ikS_{lm}-\sum_{l'm'}\frac{(2l'+1)!!}{k^{l'+1}}\left(T\frac{I}{I+iT}A\right)_{l'm'}\frac{(2l+1)!!}{k^{l}(2l+1)!}\times\left[\frac{k^{2l+1}(2l+1)!}{i[(2l+1)!!]^2}\delta_{ll'}\delta_{mm'}\right.$$
$$\left.+\frac{k^{l}(2l+1)!}{(2l+1)!!}\frac{k^{l'+1}}{i(2l'+1)!!}K_{lm,l'm'}(\mathbf{r}_T)\right]. \tag{2.20}$$

The above equation can be simplified if one introduces a new variable, namely,

$$a_{lm}=\frac{i}{k}[(I+iT)^{-1}A]_{lm}. \tag{2.21}$$

From Eq. (2.20) one obtains the following equation for the new variable defined in Eq. (2.21):

$$a_{lm}=S_{lm}+i\sum_{l'm'}\sum_{l''m''}K_{lm,l'm'}(\mathbf{r}_T)T_{l'm',l''m'}a_{l''m''}. \tag{2.22}$$

The equation for the Green function can now be written as

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)+k\sum_{lm}\sum_{l'm'}O_{lm}(\mathbf{r},\mathbf{r}_T)T_{lm,l'm'}a_{l'm'}. \tag{2.23}$$

The resulting equations, Eqs. (2.22)–(2.23), show that, in the presence of boundaries, there is a coupling among the scattered partial waves. One should also notice that the only quantity related to the scattering target that appear in the coupling matrix, Eq. (2.18), is its position relative to the boundaries. This indicates that no matter what the nature of the target is, the coupling matrix given by Eq. (2.18) determines the coupling amongst the partial waves.

In order to illustrate the applicability of this formalism to scattering within a confined space an example introduced by Huang and Yang[1] will be discussed. These authors, in order to demonstrate the applicability of perturbation theory to the *s*-wave pseudopotential, considered the case of an scattering sphere within a larger, confining sphere with Dirichlet boundary conditions being satisfied on the surface of both spheres (see Fig. 1).

Thus it is desired to find the scattered field obtained when, for example, acoustic waves generated by a point source are scattered by a small sphere located inside a larger sphere. The interior surface of the larger sphere reflects both the sound coming directly from the source as well

as that scattered by the smaller sphere. Thus the total acoustic field inside the larger sphere when the smaller sphere is present is considerably more structurally complex than when that sphere is not there. Since this problem can be exactly solved when the spheres are concentric it provides a simple test regarding the use of the pseudopotential for scattering in a confined environment. In this case one wants to find the Green function that vanishes on the interior surface of the larger sphere and on the exterior surface of the smaller sphere. This Green function satisfies Eq. (2.12) with

$$T_{lm,l'm'}=kf_l\delta_{l,l'}\delta_{m,m'} \quad \text{and} \quad f_l=\frac{i}{k}\left[\frac{j_l(ka)}{h_l^{(1)}(ka)}\right]. \tag{2.24}$$

One notices that the scattering amplitudes due to the smaller sphere (of radius a) appear explicitly in the equation for the Green function. The Green function in the interior of the larger sphere (of radius b), in the absence of the smaller sphere, is

$$G_0(\mathbf{r},\mathbf{r}_0)=-ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)\left[h_l^{(1)}(kr_>)-\frac{h_l^{(1)}(kb)}{j_l(kb)}j_l(kr_>)\right]Y_{lm}(\hat{\mathbf{r}})Y_{lm}^*(\hat{\mathbf{r}}_0). \tag{2.25}$$

The quantities in Eqs. (2.16)–(2.18) can be explicitly computed in this case in terms of Bessel functions and spherical harmonics:

$$O_{lm}(\mathbf{r},\mathbf{r}_T)=h_l^{(1)}(ks)Y_{lm}(\hat{\mathbf{s}})\big|_{\mathbf{s}=\mathbf{r}-\mathbf{r}_T}-\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'}\frac{h_{l'}^{(1)}(kb)}{j_{l'}(kb)}j_{l'}(kr)Y_{l'm'}(\hat{\mathbf{r}})W_{lm,l'm'}(\mathbf{r}_T), \tag{2.26}$$

$$S_{lm}(\mathbf{r}_T,\mathbf{r}_0)=h_l^{(1)}(ks)Y_{lm}^*(\hat{\mathbf{s}})\big|_{\mathbf{s}=\mathbf{r}_0-\mathbf{r}_T}-\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'}\frac{h_{l'}^{(1)}(kb)}{j_{l'}(kb)}j_{l'}(kr_0)Y_{l'm'}^*(\hat{\mathbf{r}}_0)V_{lm,l'm'}(\mathbf{r}_T), \tag{2.27}$$

$$K_{lm,l'm'}(\mathbf{r}_T)=-\sum_{L=0}^{\infty}\sum_{M=-L}^{L}\frac{h_L^{(1)}(kb)}{j_L(kb)}V_{lm,LM}(\mathbf{r}_T)W_{l'm',LM}(\mathbf{r}_T), \tag{2.28}$$

$$W_{lm,l'm'}(\mathbf{r}_T)=4\pi(-1)^{l'}i^{l+l'}\sum_{L=0}^{\infty}\sum_{M=-L}^{L} i^L C_{LM,l'm'}^{lm}j_L(kr_T)Y_{LM}(\hat{\mathbf{r}}_T), \tag{2.29}$$

$$V_{lm,l'm'}(\mathbf{r}_T)=4\pi(-1)^{l'}i^{l+l'}\sum_{L=0}^{\infty}\sum_{M=-L}^{L} i^L C_{LM,lm}^{l'm'}j_L(kr_T)Y_{LM}(\hat{\mathbf{r}}_T), \tag{2.30}$$

$$C_{LMl'm'}^{lm}=\int d\hat{\mathbf{s}}\,Y_{l'm'}(\hat{\mathbf{s}})Y_{lm}^*(\hat{\mathbf{s}})Y_{LM}(\hat{\mathbf{s}}),$$

$$C_{LMl'm'}^{lm}=0$$

unless

$$M=m-m' \quad \text{and} \quad |l-l'|\leqslant L\leqslant l+l'. \tag{2.31}$$

The Gaunt numbers, the integral of three spherical harmonics [Eq. (2.31)], can be expressed in terms of the well-known Wigner's 3-j symbols.[6] This coupling among spherical harmonics appears because one has three distinct centers for the partial wave expansions, namely, the source position, the center of the target sphere and the center of the enclosing sphere. In the above equations one has an expression for the partial wave expansion of the full Green function (includ-

ing scattering by the smaller sphere) about the center of the enclosing sphere. In the algebraic manipulations the Gaunt numbers appear in the spherical harmonic expansion of a product of a spherical Bessel function and a spherical harmonic such as[7]

$$j_l(kt)Y_{lm}(\hat{\mathbf{t}})\big|_{\mathbf{t}=\mathbf{r}_T+\mathbf{s}}=4\pi(-i)^L\sum_{L'M'}\sum_{L''M''}i^{L'+L''}C^{LM}_{L'M',L''M''}j_{L'}(kr_T)Y_{L'M'}(\hat{\mathbf{r}}_T)j_{L''}(ks)Y_{L''M''}(\hat{\mathbf{s}}). \tag{2.32}$$

Now the case $\mathbf{r_T}=\mathbf{0}$ is considered. The Green function for this case can be expressed exactly in terms of Bessel functions and spherical harmonics since it is the Green function for the Helmholtz equation in the space bounded by two concentric spheres. Thus this case provides an algebraic test of the use of the pseudopotential to describe scattering in a confined medium. In the expressions for $V_{lm,l'm'}(\mathbf{0})$ and $W_{lm,l'm'}(\mathbf{0})$ only the term $L=0$ survives since $j_L(0)=0$ for $L>0$, then $V_{lm,l'm'}(\mathbf{0})=W_{lm,l'm'}(\mathbf{0})=\delta_{ll'}\delta_{mm'}$ since $C^{lm}_{00,l'm'}=C^{l'm'}_{00,lm}=(1/\sqrt{4\pi})\delta_{ll'}\delta_{mm'}$. Therefore $K_{lm,l'm'}(\mathbf{0})=-[h_l^{(1)}(kb)/j_l(kb)]\delta_{ll'}\delta_{mm'}$. One finds that

$$S_{lm}(\mathbf{0},\mathbf{r}_0)=\frac{i}{j_l(kb)}[j_l(kb)n_l(kr_0)-n_l(kb)j_l(kr_0)]Y^*_{lm}(\hat{\mathbf{r}}_0), \tag{2.33}$$

$$O_{lm}(\mathbf{r},\mathbf{0})=\frac{i}{j_l(kb)}[j_l(kb)n_l(kr)-n_l(kb)j_l(kr)]Y_{lm}(\hat{\mathbf{r}}) \tag{2.34}$$

and that

$$a_{lm}=\frac{h_l^{(1)}(ka)[j_l(kb)n_l(kr_0)-n_l(kb)j_l(kr_0)]Y^*_{lm}(\hat{\mathbf{r}}_0)}{j_l(kb)n_l(ka)-j_l(ka)n_l(kb)}, \tag{2.35}$$

thus

$$\begin{aligned}G(\mathbf{r},\mathbf{r}_0)=&-ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l}j_l(kr_<)\left[h_l^{(1)}(kr_>)-\frac{h_l^{(1)}(kb)}{j_l(kb)}j_l(kr_>)\right]Y_{lm}(\hat{\mathbf{r}})Y^*_{lm}(\hat{\mathbf{r}}_0)\\&-k\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{j_l(ka)}{j_l(kb)}\frac{[j_l(kb)n_l(kr)-n_l(kb)j_l(kr)][j_l(kb)n_l(kr_0)-n_l(kb)j_l(kr_0)]}{j_l(kb)n_l(ka)-j_l(ka)n_l(kb)}\\&\times Y_{lm}(\hat{\mathbf{r}})Y^*_{lm}(\hat{\mathbf{r}}_0)\end{aligned} \tag{2.36}$$

which can be shown to be the correct expression for the Green function in this case. A standard approach, using separation of variables, shows that, in the case of the concentric spheres, the Green function inside the larger sphere and outside the smaller one can be written as

$$\begin{aligned}G(\mathbf{r},\mathbf{r}_0)=&k\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{[j_l(kr_<)n_l(ka)-j_l(ka)n_l(kr_<)][j_l(kr_>)n_l(kb)-j_l(kb)n_l(kr_>)]}{[j_l(ka)n_l(kb)-j_l(kb)n_l(ka)]}\\&\times Y_{lm}(\hat{\mathbf{r}})Y^*_{lm}(\hat{\mathbf{r}}_0).\end{aligned} \tag{2.37}$$

It is straightforward to show that the expression in Eq. (2.36) reduces to the one in Eq. (2.37).

III. THE LIU AND WONG PSEUDOPOTENTIAL

Liu and Wong[4] showed that the wave function describing the scattering of a scalar wave by a Dirichlet sphere of radius a satisfies the following wave equation:

$$[\nabla^2+k^2]\psi(\mathbf{r})=\frac{1}{a}\,\delta(r-a)\,\frac{\partial}{\partial r}[r\psi(\mathbf{r})]. \tag{3.1}$$

Comparing with the pseudopotential of Huang and Yang, the simplicity of the pseudopotential of Liu and Wong is striking. In the above simple form the pseudopotential of Liu and Wong can be applied only to the case of scattering by a Dirichlet sphere.

In order to illustrate the applicability of the Liu and Wong pseudopotential to scattering in a confining environment it will be shown that using the Liu and Wong pseudopotential one can solve for the Green function of the Helmholtz equation in the space between two concentric spheres. The equation for the Green function in the interior space is

$$[\nabla^2+k^2]G(\mathbf{r},\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0)+\frac{1}{a}\,\delta(r-a)\,\frac{\partial}{\partial r}[rG(\mathbf{r},\mathbf{r}_0)]. \tag{3.2}$$

The above equation is solved by transforming it into a Lippmann–Schwinger integral equation using the Green function for the interior of the larger sphere given in Eq. (2.25) which is of the form

$$G_0(\mathbf{r},\mathbf{r}_0)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} g_l^0(r,r_0)Y_{lm}(\hat{\mathbf{r}})Y_{lm}^*(\hat{\mathbf{r}}_0). \tag{3.3}$$

Since in the concentric case the confined space has spherical symmetry one can also write

$$G(\mathbf{r},\mathbf{r}_0)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} g_l(r,r_0)Y_{lm}(\hat{\mathbf{r}})Y_{lm}^*(\hat{\mathbf{r}}_0). \tag{3.4}$$

The spherical harmonic expansion simplifies the Lippmann–Schwinger integral resulting in the equation:

$$g_l(r,r_0)=g_l^0(r,r_0)+ag_l^0(r,a)\,\frac{\partial}{\partial r'}[r'g_l(r',r_0]_{r'=a}. \tag{3.5}$$

From the above equation it follows that

$$\partial_r[rg_l(r,r_0)]_{r=a}=\frac{\partial_r[rg_l^0(r,r_0)]_{r=a}}{1-a\partial_r[rg_l^0(r,a)]_{r=a}}=-\frac{1}{a}\left[\frac{j_l(kr_0)n_l(kb)-j_l(kb)n_l(kr_0)}{j_l(ka)n_l(kb)-j_l(kb)n_l(ka)}\right]. \tag{3.6}$$

Thus one obtains for the radial Green function

$$g_l(r,r_0)=g_l^0(r,r_0)-\frac{j_l(kr_0)n_l(kb)-j_l(kb)n_l(kr_0)}{j_l(ka)n_l(kb)-j_l(kb)n_l(ka)}g_l^0(r,a). \tag{3.7}$$

It can be easily shown that the expression in Eq. (3.7) reproduces the result presented in Eq. (2.37).

The extension to the case of scattering by an arbitrary object is straightforward albeit being algebraically messy. For an arbitrary target one takes a to be the radius of the circumscribing sphere and use the previously mentioned form of the wave function for $r>a$, given by Eq. (2.4), as a reference. Then it is straightforward to show that the wave function describing the scattering of a scalar wave by an arbitrary target fulfills the following equation:

$$[\nabla^2+k^2]\psi(\mathbf{r})=\frac{1}{a}\,\delta(r-a)\,\frac{\partial}{\partial r}[rP\psi(\mathbf{r})], \tag{3.8}$$

where P is an operator such that

$$P\psi(\mathbf{r})=\sum_{lm}\sum_{l'm'}P_{lm,l'm'}Y_{lm}(\hat{\mathbf{r}})\int d\hat{\mathbf{s}}\,Y_{l'm'}(\hat{\mathbf{s}})^*\psi(r\hat{\mathbf{s}}). \tag{3.9}$$

In order to determine the operator P one must compare the solution of Eq. (3.8) in an extended medium with an arbitrary incident field with the wave function given by Eq. (2.4). First one transforms Eq. (3.8) into an equivalent Lippmann–Schwinger equation:

$$\begin{aligned}\psi(\mathbf{r})&=\psi_{\mathrm{inc}}(\mathbf{r})+\int d\mathbf{r}'\,g(\mathbf{r}-\mathbf{r}')\frac{1}{a}\delta(r'-a)\partial_{r'}[r'P\psi(\mathbf{r}')]\\&=\psi_{\mathrm{inc}}(\mathbf{r})+a\sum_{lm}\sum_{l'm'}\left[\int d\hat{\mathbf{t}}\,Y_{lm}(\hat{\mathbf{t}})g(\mathbf{r}-a\hat{\mathbf{t}})\right]P_{lm,l'm'}A_{l'm'},\end{aligned} \tag{3.10}$$

where

$$A_{lm}=\partial_s\left[s\int d\hat{\mathbf{s}}\,Y_{lm}^*(\hat{\mathbf{s}})\psi(\mathbf{s})\right]_{s=a}. \tag{3.11}$$

Using the multipole expansion of $g(\mathbf{r}-\mathbf{r}')$ one obtains

$$\psi(\mathbf{r})=\psi_{\mathrm{inc}}(\mathbf{r})+a\sum_{lm}\sum_{l'm'}[-ikj_l(ka)h_l^{(1)}(kr)Y_{lm}(\hat{\mathbf{r}})]P_{lm,l'm'}A_{l'm'}. \tag{3.12}$$

From the definition of A_{lm} in Eq. (3.11) and taking the limit of r approaching a from outside the circumscribing sphere one obtains an equation for the A_{lm}:

$$A_{lm}=A_{lm}^{\mathrm{inc}}-\sum_{l'm'}Q_{lm,l'm'}A_{l',m'},\quad A_{lm}^{\mathrm{inc}}=\partial_S\left[s\int d\hat{\mathbf{s}}\,Y_{lm}^*(\hat{\mathbf{s}})\psi_{\mathrm{inc}}(\mathbf{s})\right]_{s=a}. \tag{3.13}$$

The operator Q is related to the operator P through the following relation:

$$Q_{lm,l'm'}=[iksj_l(ks)\partial_s(sh_l^{(1)}(ks))]_{s=a}P_{lm,l'm'}. \tag{3.14}$$

Therefore one finds

$$A=(I+Q)^{-1}A^{\mathrm{inc}}. \tag{3.15}$$

Now let us compare the wave function in Eq. (3.12) with that in Eq. (2.4), they should be identical to each other. Using the definition of A_{lm} in Eq. (3.11) using the wave function in Eq. (2.4) one obtains

$$A=(I+U)A^{\mathrm{inc}},\quad U_{lm,l'm'}=[i\partial_s(sh_l^{(1)}(ks))]_{s=a}T_{lm,l'm'}\frac{1}{[\partial_s(sj_{l'}(ks))]_{s=a}}. \tag{3.16}$$

Comparing Eqs. (3.15) and (3.16) one finds that

$$Q=-U(I+U)^{-1},\quad P_{lm,l'm'}=\frac{1}{[iksj_l(ks)\partial_s(sh_l^{(1)}(ks))]_{s=a}}Q_{lm,l'm'}. \tag{3.17}$$

Equation (3.17) provides an expression for the operator P in terms of the transition matrix of the arbitrary scattering object.

As it was the case for the Huang and Yang pseudopotential one can also write down the general form of the equations describing scattering in a bounded volume or in a waveguide filled

with an uniform fluid using the Liu and Wong pseudopotential. In the case of sound generated by a point source the acoustic field satisfies the following equation for $r>a$:

$$[\nabla^2+k^2]G(\mathbf{r},\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0)+\frac{1}{a}\,\delta(|\mathbf{r}-\mathbf{r}_T|-a)\partial_S[sP_{\hat{s}}G(\mathbf{s}+\mathbf{r}_T,\mathbf{r}_0)]_{\mathbf{s}=\mathbf{r}-\mathbf{r}_T}. \tag{3.18}$$

Notice that in this formulation it is implicitly assumed that the origin is in the domain exterior to the circumscribing sphere, that is, it will be assumed that $r_T>a$. In this case the action of the projection operator can be described by the following equation:

$$P_{\hat{s}}G(\mathbf{s}+\mathbf{r}_T,\mathbf{r}_0)=\sum_{lm}\sum_{l'm'}P_{lm,l'm'}Y_{lm}(\hat{\mathbf{s}})\int d\hat{\mathbf{t}}\,Y^*_{l'm'}(\hat{\mathbf{t}})G(s\hat{\mathbf{t}}+\mathbf{r}_T,\mathbf{r}_0). \tag{3.19}$$

The above equation extends the definition of the operator P to the case in which the position of the scattering center does not coincide with the origin of the coordinate system.

The procedure for deriving the algebraic scattering equations starts with the use of $G_0(\mathbf{r},\mathbf{r}_0)$, the Green function in the absence of the scattering object, to obtain the Lippmann–Schwinger equation:

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)+\int d\mathbf{r}'\,G_0(\mathbf{r},\mathbf{r}')\frac{1}{a}\,\delta(|\mathbf{r}'-\mathbf{r}_T|-a)\partial_s[sP_{\hat{s}}G(\mathbf{s}+\mathbf{r}_T,\mathbf{r}_0)]_{\mathbf{s}=\mathbf{r}'-\mathbf{r}_T}. \tag{3.20}$$

Applying the definition of the P operator, Eq. (3.19), in the above equation yields

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)+a\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\alpha_{lm}A_{lm}\int d\hat{\mathbf{t}}\,G_0(\mathbf{r},\mathbf{r}_T+a\hat{\mathbf{t}})Y_{lm}(\hat{\mathbf{t}}), \tag{3.21}$$

$$A_{lm}=\partial_s\left[s\int d\hat{\mathbf{s}}\,Y^*_{lm}(\hat{\mathbf{s}})G(\mathbf{s}+\mathbf{r}_T,\mathbf{r}_0)\right]_{s=a}. \tag{3.22}$$

The equations for the A_{lm} are determined by using the expression for $G(\mathbf{r},\mathbf{r}_0)$, given by Eq. (3.21), into Eq. (3.22). Evidently the final equations will be just Eqs. (2.22) and (2.23). The several quantities appearing on those equations are obtained by evaluating the following expressions:

$$O_{lm}(\mathbf{r},\mathbf{r}_T)=\frac{i}{kj_l(ka)}\int d\hat{\mathbf{t}}\,Y_{lm}(\hat{\mathbf{t}})G_0(\mathbf{r},\mathbf{r}_T+a\hat{\mathbf{t}}),$$

$$S_{lm}(\mathbf{r}_T,\mathbf{r}_0)=\frac{i}{k(kaj_l'(ka)+j_l(ka))}\partial_s\left[s\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*G_0(\mathbf{r}_T+\mathbf{s},\mathbf{r}_0)\right]_{s=a}, \tag{3.23}$$

$$K_{lm,l'm'}(\mathbf{r}_T)=\frac{i}{k[j_{l'}(u)\partial_u(uj_l(u))]_{a=ka}}\partial_S\left[s\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*\int d\hat{\mathbf{t}}\,Y_{l'm'}(\hat{\mathbf{t}})G_0^{NS}(\mathbf{r}_T+\mathbf{s},\mathbf{r}_T+a\hat{\mathbf{t}})\right]_{s=a}.$$

The following result was useful to obtain the final expressions, identical to those in Eqs. (2.22) and (2.23), from Eqs. (3.21) and (3.22):

$$\partial_S\left[s\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*\int d\hat{\mathbf{t}}\,Y_{lm}(\hat{\mathbf{t}})g(\mathbf{r}_T+\mathbf{s}-(\mathbf{r}_T+a\hat{\mathbf{t}}))\right]_{s=a^+}=\{[-ikj_l(u)\partial_u h_l^{(1)}(u)]_{u=ka}\}\delta_{ll'}\delta_{mm'}. \tag{3.24}$$

The a_{lm} are related to the A_{lm} through the following relationship:

$$a_{lm}=\frac{1}{-ik\partial_s(sj_l(ks))_{s=a}}[(I+Q)A]_{lm}. \tag{3.25}$$

The following result was used to eliminate the A_{lm} in favor of the a_{lm}:

$$\sum_{l'm'} P_{lm,l'm'}A_{l'm'}=\frac{1}{iaj_l(ka)}\sum_{l'm'} T_{lm,l'm'}a_{l'm'}. \tag{3.26}$$

One notices that the expressions obtained using the Huang and Yang pseudopotential are just the limit $a\to 0$ of the above expressions. This is not surprising as the quantities on the right-hand side of Eqs. (3.21)–(3.23) are independent of a. This last statement can be proved by noticing that since the Green functions appearing in Eqs. (3.21)–(3.23) are evaluated away from the boundaries, in regions where the medium is uniform, they can be expressed in terms of multipole expansions:

$$G_0(\mathbf{r},\mathbf{r}')=\sum_{lm}\sum_{l'm'}\Gamma_{lm,l'm'}h_l^{(1)}(kr_>)Y_{lm}(\hat{\mathbf{r}}_>)j_{l'}(kr_<)Y_{l'm'}(\hat{\mathbf{r}}_<). \tag{3.27}$$

In the above equation $\mathbf{r}_>$ is the position vector with the larger magnitude and $\mathbf{r}_<$ is the position vector with the smaller magnitude. When either $\mathbf{r}$ or $\mathbf{r}'$ is a sum of two other vectors one should use either Eq. (2.32) or its equivalent for spherical Hankel functions[8] ($r_>>r_<$):

$$h_{LM}^{(1)}(ks)Y_{LM}(\hat{\mathbf{s}})|_{\mathbf{s}=\mathbf{r}_>+\mathbf{r}_<}=4\pi(-i)^L\sum_{L'M'}\sum_{L''M''}i^{L'+L''}C_{L'M',L''M''}^{LM}j_{L'}(kr_<)Y_{L'M'}(\hat{\mathbf{r}}_<)h_{L''}^{(1)}$$
$$\times(kr_>)Y_{L''M''}(\hat{\mathbf{r}}_>). \tag{3.28}$$

One finds then that after the angular integration the factors in the denominators cancel out a similar factor in the numerators rending the right-hand side of Eqs. (3.21)–(3.23) independent of a. This also shows that the functions and operators given by these equations are indeed the same ones defined before in Eqs. (2.16)–(2.18). Thus the equivalence of the Huang and Yang pseudopotential and that of Liu and Wong has been demonstrated in the general case of arbitrary scattering objects in arbitrary, bounded or unbounded, volumes.

IV. SCATTERING BY MULTIPLE OBJECTS

The problem of wave scattering by many objects, that is, the case of multicenter scattering, can also be formulated using pseudopotentials. The resulting equations coincide with those obtained using standard multiple scattering formulations. Nonetheless it is interesting to derive them using the pseudopotential, as there are some similarities with the problem of scattering in confined spaces that shed some light on the physics of this latter problem. In the following the multicenter scattering equations will be derived using the Liu and Wong pseudopotential. Of course the same result is obtained using the Huang and Yang pseudopotential as can be seen in a recent article by Baltenkov.[9]

Thus it is desired to obtain the equations describing the scattering of a scalar wave in a homogeneous medium by an assembly of objects. The objects may be all distinct from each other. A similar procedure could be applied for the case in which the objects and the medium are confined in a waveguide or in a cavity. The wave field generated by a point source and scattered by the collection of objects obeys the following equation:

$$[\nabla^2+k^2]G(\mathbf{r},\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0)+\sum_{j=1}^{n}\frac{1}{a_j}\delta(|\mathbf{r}-\mathbf{r}_j|-a_j)\frac{\partial}{\partial s}[sP_s^jG(\mathbf{s}+\mathbf{r}_j,\mathbf{r}_0)]_{\mathbf{s}=\mathbf{r}-\mathbf{r}_j}. \tag{4.1}$$

In this case the action of the operator P, allowing for distinct scattering objects, is given by

$$P_s^j G(\mathbf{s}+\mathbf{r}_j,\mathbf{r}_0)=\sum_{lm}\sum_{l'm'} P^j_{lm,l'm'}Y_{lm}(\hat{\mathbf{s}})\int d\hat{\mathbf{t}}\,Y^*_{l'm'}(\hat{\mathbf{t}})G(s\hat{\mathbf{t}}+\mathbf{r}_j,\mathbf{r}_0). \tag{4.2}$$

Using the Green function for the Helmholtz operator in an extended environment one obtains the following Lippmann–Schwinger equation:

$$G(\mathbf{r},\mathbf{r}_0)=g(\mathbf{r}-\mathbf{r}_0)+\sum_{j=1}^{n}\sum_{lm}\sum_{l'm'}\left[\frac{1}{a_j}\int d\mathbf{r}'\,g(\mathbf{r}'-\mathbf{r}_j)\delta(s-a_j)Y_{lm}(\hat{\mathbf{s}})|_{\mathbf{s}=\mathbf{r}'-\mathbf{r}_j}\right]P^j_{lm,l'm'}A^j_{l'm'}, \tag{4.3}$$

where

$$A^j_{lm}=\frac{\partial}{\partial s}\left[s\int d\hat{\mathbf{s}}\,Y^*_{lm}(\hat{\mathbf{s}})G(\mathbf{s}+\mathbf{r}_j,\mathbf{r}_0)\right]_{s=a_j}. \tag{4.4}$$

Expanding the Green function of the Helmholtz operator in Eq. (4.3) into spherical harmonics one obtains, after the angular integration, the following expression for the Green function in the multicenter scattering case:

$$G(\mathbf{r},\mathbf{r}_0)=g(\mathbf{r}-\mathbf{r}_0)+\sum_{j=1}^{n}\sum_{lm}\sum_{l'm'}[-ika_jj_l(ka_j)h_l^{(1)}(ks)Y_{lm}(\hat{\mathbf{s}})|_{\mathbf{s}=\mathbf{r}-\mathbf{r}_j}]P^j_{lm,l'm'}A^j_{l'm'}. \tag{4.5}$$

Now one inserts the Green function expression given by Eq. (4.5) into the right-hand side of Eq. (4.4) to obtain an equation for the A^i_{lm}. One has

$$\partial_s\left[s\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*g(\mathbf{r}_i+\mathbf{s}-\mathbf{r}_0)\right]_{s=a_i}=-ik[\partial_u(uj_l(u))]_{u=ka_j}[h^{(1)}_{lm}(ks)Y^*_{lm}(\hat{\mathbf{s}})]_{\mathbf{s}=\mathbf{r}_n-\mathbf{r}_i}. \tag{4.6}$$

For $i\neq j$ the following result holds:

$$\begin{aligned}\partial_s&\left[s\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*\int d\hat{\mathbf{t}}\,Y_{l'm'}(\hat{\mathbf{t}})g(\mathbf{r}_i+\mathbf{s}-\mathbf{r}_j-a_j\hat{\mathbf{t}})\right]_{s=a_j}\\&=-ikj_{l'}(ka_j)[\partial_u(uj_l(u))]_{u=ka_i}K_{lm,l'm'}(\mathbf{r}_i-\mathbf{r}_j),\end{aligned} \tag{4.7}$$

$$K_{lm,l'm'}(\mathbf{r}_i-\mathbf{r}_j)=4\pi(-i)^{l'}i^l\sum_{l''m''}i^{l''}C^{l'm'}_{lm,l''m''}h^{(1)}_{l''}(k\nu)Y_{l''m''}(\hat{\mathbf{v}})|_{\mathbf{v}=\mathbf{r}_i-\mathbf{r}_j}. \tag{4.8}$$

Thus one has

$$\begin{aligned}A^i_{lm}=&[-ik\partial_u(uj_l(u))]_{u=ka_j}[h_l^{(1)}(ks)Y^*_{lm}(\hat{\mathbf{s}})]_{\mathbf{s}=\mathbf{r}_0-\mathbf{r}_i}\\&+[-ikj_l(u)\partial_u(uh_l^{(1)}(u))]_{u=ka_i}\sum_{l'm'}P^i_{lm,l'm'}A^i_{l'm'}\\&+\sum_{j\neq i}^{n}\sum_{l'm'}\sum_{l'm'}[-ika_jj_{l'}(ka_j)\partial_n(uj_l(u))_{u=ka_i}]K_{lm,l'm'}(\mathbf{r}_i-\mathbf{r}_j)P^j_{l'm',l'm''}A^j_{l''m''}.\end{aligned} \tag{4.9}$$

Now, using the relationships in Eqs. (3.25) and (3.26) one finally obtains

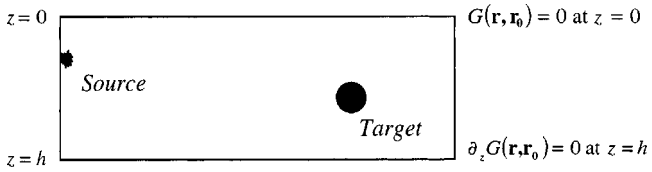

FIG. 2. Ideal waveguide with sound source and scattering object.

$$a^i_{lm}=h^{(1)}_l(ks)Y^*_{lm}(\hat{\mathbf{s}})\big|_{\mathbf{s}=\mathbf{r}_0-\mathbf{r}_i}+i\sum_{j\neq i}^{n}\sum_{l'm'}\sum_{l''m''}K_{lm,l'm'}(\mathbf{r}_i-\mathbf{r}_j)T^j_{l'm',l''m''}a^j_{l''m''}. \tag{4.10}$$

For the Green function one then has the following expression:

$$G(\mathbf{r},\mathbf{r}_0)=g(\mathbf{r}-\mathbf{r}_0)+ik\sum_{j=1}^{n}\sum_{lm}\sum_{l'm'}[h^{(1)}_l(ks)Y_{lm}(\hat{\mathbf{s}})]_{\mathbf{s}=\mathbf{r}-\mathbf{r}_j}T^j_{lm,l'm'}a^j_{l'm'}. \tag{4.11}$$

Equations (4.10)–(4.11) can also be obtained from the usual multiple scattering formalisms such as those of Foldy,[10] and of Twersky.[11] A recent review of multiple scattering can be found in an article by Tourin *et al.*,[12] where those approaches are discussed in an acoustic context. For example, one can compare Eqs. (4.10)–(4.11) with Eqs. (21) and (14) in a recent article by Wang and Ye[13] where the multiple scattering of sound by air bubbles in water is studied. Similar equations are obtained by Kafesaki and Economou[8] in a study of acoustic propagation in periodic composites consisting of solid spheres in a fluid host. As previously pointed out, the same results would be obtained had the Huang and Yang pseudopotential being used. In fact this pseudopotential has been used recently to derive expressions for the amplitudes of elastic electron scattering by multicentered targets in the presence of a background central atomic potential.[9] Obviously very similar equations are obtained in this case too.

V. SCATTERING IN AN IDEAL WAVEGUIDE

In this section the scattering problem in the interior of an ideal waveguide is discussed. The waveguide considered consists of two perfectly reflecting parallel planes encompassing an uniform fluid with the acoustic field obeying pressure release (Dirichlet) boundary conditions on the interior surface of one of the planes and acoustically hard (Neumann) boundary conditions on the interior surface of the other plane. This is an idealization of the type of acoustic waveguide found in ocean acoustics, the pressure release plane representing the air–sea interface and the hard plane representing the sea bottom. Accordingly the z axis is chosen pointing downwards with the plane $z=0$ being the air–sea interface and the plane $z=h$ being the bottom. The pseudopotential of Huang and Yang is employed to obtain equations describing the scattering of an acoustic field by an object in the waveguide (see Fig. 2).

The acoustic field in the waveguide is obtained by solving an equation like Eq. (2.12), the Green function solution to this equation, which includes waveguide and scattering effects, obeys Dirichlet boundary conditions at the plane $z=0$ and Neumann boundary conditions at the plane $z=h$. In order to solve it one needs the Green function for the Helmholtz equation in the waveguide. It satisfies the same boundary conditions as the solution at the waveguide boundaries. This Green function for the waveguide in the absence of the scattering object can be represented in several different ways. For this discussion it is convenient to use the representation obtained using the image method.[14]

$$G_0(\mathbf{r},\mathbf{r}_0)=\sum_{n=-\infty}^{\infty}(-1)^n[g(\mathbf{r}-\mathbf{r}_0^+-2nh\hat{\mathbf{e}}_z)-g(\mathbf{r}-\mathbf{r}_0^--2nh\hat{\mathbf{e}}_z)]. \tag{5.1}$$

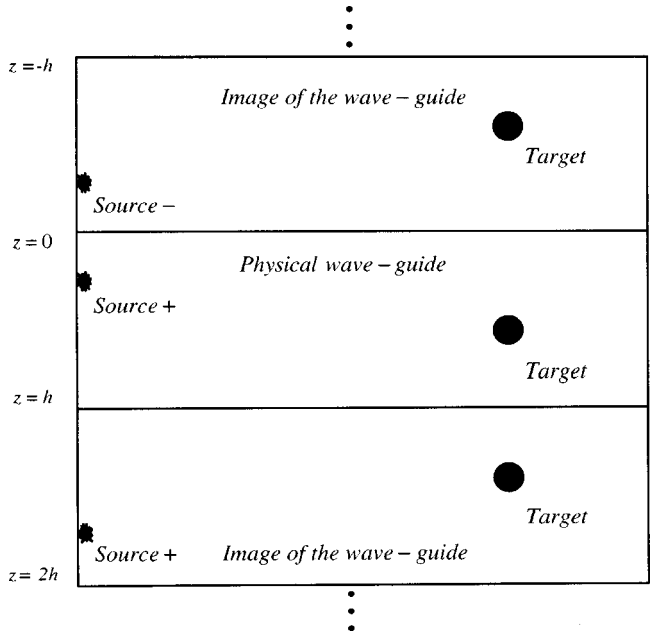

FIG. 3. Waveguide images with source and target images.

In the above equation, $\mathbf{r}_0^{\pm}=\mathbf{R}_0\pm z_0\hat{\mathbf{e}}_z$, and $g(\mathbf{r})=-\exp(ikr)/4\pi r$ is the usual Green function for the Helmholtz equation in an extended medium. It is worthwhile to explore a bit the physical picture provided by the image method by including the scattering object. In the image method the physical medium is extensive and unbounded, with the boundary conditions at the planes delimiting the waveguide being met by an infinite array of image sources with alternating signs. When reflected across a boundary where Dirichlet boundary conditions are to be satisfied the source image has the opposite sign while when reflected across a boundary where Neumann boundary conditions are to be obeyed the source image has the same sign as the source being reflected. Notice that one must take into account reflections of reflections, *ad infinitum*. There is also an infinite array of identical scattering objects as depicted in Fig. 3.

The image method shows that the problem of scattering by an object inside an ideal waveguide is equivalent to the problem of scattering by a linear periodic array of identical objects of the wave field created by a linear periodic array of sources. Thus the scattering problem in the waveguide is akin to a multitarget and multisource scattering problem. Since the sources and targets are distributed in a linear periodical array the matrix coupling the different targets in the multiscattering formulation can be made diagonal in its dependence on the target positions by a discrete Fourier transform. Thus one expects the final expression for the scattering field to include only the coupling of partial waves. The following detailed analysis based on the pseudopotential approach confirms this qualitative argument.

The equations describing scattering in the waveguide have the same form as Eqs. (2.22)–(2.23), for the quantities appearing in these equations, one finds

$$O_{lm}(\mathbf{r},\mathbf{r}_T)=\sum_{n=-\infty}^{\infty}(-1)^n\{h_l^{(1)}(k\nu)Y_{lm}(\hat{\mathbf{v}})|_{\mathbf{v}=\mathbf{r}-\mathbf{r}_T^{+}-2nh\hat{\mathbf{e}}_z}$$
$$-(-1)^{l+m}h_l^{(1)}(k\nu)Y_{lm}(\hat{\mathbf{v}})|_{\mathbf{v}=\mathbf{r}-\mathbf{r}_T^{-}-2nh\hat{\mathbf{e}}_z}\}, \tag{5.2}$$

$$S_{lm}(\mathbf{r}_T,\mathbf{r}_0)=(-1)^{l+m}\sum_{n=-\infty}^{\infty}(-1)^n\{h_l^{(1)}(k\nu)Y_{lm}(\hat{\mathbf{v}})|_{\mathbf{v}=\mathbf{r}_T-\mathbf{r}_0^+-2nh\hat{\mathbf{e}}_z}$$
$$-h_l^{(1)}(k\nu)Y_{lm}(\hat{\mathbf{v}})|_{\mathbf{v}=\mathbf{r}_T-\mathbf{r}_0^--2nh\hat{\mathbf{e}}_z}\}, \tag{5.3}$$

$$K_{lm,l'm'}(\mathbf{r}_T)=\delta_{mm'}\sqrt{4\pi}\sum_{L=|l-l'|}^{l+l'}(-1)^{L+l'}i^{L+l+l'}\sqrt{2L+1}C_{L0lm}^{l'm}\{(1+(-1)^L)R_L(0)$$
$$-(-1)^{l'+m}[(-1)^Lh_L^{(1)}(2kz_T)+R_L(-z_T)+(-1)^LR_L(z_T)]\}, \tag{5.4}$$

$$R_L(z)=\sum_{n=1}^{\infty}(-1)^nh_L^{(1)}(k(2nh+2z)),\quad -h<z<h. \tag{5.5}$$

One should notice that $K_{lm,l'm'}(\mathbf{r}_T)=0$ if $|m|>l$ or if $|m|>l'$. The coupling matrix depends only on z_T and is diagonal in m and m' due to the fact that the ideal waveguide has rotational symmetry for rotations around the z axis. Another property of the coupling matrix given by Eq. (5.4) is that it depends on $|m|$. Thus, even if the target has spherical symmetry, the scattered field will not have azimuthal symmetry. This is so because the line from the source to the target and the z axis define a preferred plane perpendicular to the boundaries of the waveguide. In the case of a point source and a spherically symmetric target the scattered field will have reflection symmetry across the preferred plane. This fact has an interesting physical consequence that is analogous to the well-known Zeeman effect in atomic physics. The scattering amplitudes are given now by the product $f_l\cdot a_{lm}$; thus even a spherical target will have scattering amplitudes that vary with the azimuthal index m in the waveguide. Instead of one lth partial wave scattering amplitude there will be $l+1$ amplitudes. If the target in the unbounded medium happens to exhibit a resonance in the lth partial wave, this resonance will be split into $l+1$ distinct resonances when the target is inside the waveguide. The shifts with respect to the original resonance frequency depend on the coupling matrix and all other partial wave amplitudes. The order of magnitude of any of the elements of the coupling matrix is, roughly, inversely proportional to the shortest distance from the target to the waveguide boundaries. Thus the resonance frequency shifts will also be inversely proportional to this distance. The farther the target is from any of the boundaries the more the scattering amplitudes will approach those at the unbounded medium.

VI. SUMMARY

The main point of this article is the application of the method of pseudopotentials to study the scattering of scalar waves in a confined medium. Along the way a generalization of the pseudopotential of Liu and Wong to arbitrary types of scattering objects was also developed. An application of particular interest deals with scattering in an ideal planar waveguide. This waveguide is an idealization of the waveguides found in ocean acoustics and, in particular, those in shallow coastal waters. It is possible to generalize the results of Sec. IV to the case of an inhomogeneous waveguide where the acoustical properties vary along the vertical direction, that is, are depth dependent in the ocean acoustics case.

Results similar to those in Eqs. (2.22)–(2.23) and Eqs. (5.2)–(5.4) were first obtained by the T-matrix method.[15] The T-matrix method is a technique to compute the scattering properties of objects in an extended medium when the incident field is a plane wave.[16] Using the T matrix in a confined medium involves decomposing the incident field into plane waves and then combining the outgoing spherical waves into a field that satisfies the boundary conditions in the waveguide. In the article by Sammelmann and Hackman[15] the T matrix for scattering in the waveguide is formally expressed as

$$T^{\mathrm{SH}}=-iT(1-iRT)^{-1}, \tag{6.1}$$

where T is the extended medium T matrix of the scattering object and R is an operator pertaining to the waveguide. Further examination shows that R is essentially the K operator in Eq. (2.22). It is clear that Eqs. (2.22)–(2.23) have the same formal structure as that implied in Eq. (6.1). In fact, in the notation used in Sec. II one can write

$$G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0)+k\sum_{lm}\sum_{l'm'}O_{lm}(\mathbf{r},\mathbf{r}_T)T^W_{lm,l'm'}S_{l'm'}(\mathbf{r}_T,\mathbf{r}_0),\quad T^W=T(I-iKT)^{-1}. \tag{6.2}$$

The pseudopotential approach is very flexible and is well suited for framing the discussion of the scattering in terms of the field generated by a point source, the Green function, which in confined environments is more useful than using a plane wave as the prototypical incident field. The confined medium does not have to be homogeneous but there must be a finite region around the target where the medium is homogeneous in order for the approach to work. This is so because the scattering properties of the target in a homogeneous and extended medium are inputs in the calculations. Applications to the cases of layered acoustical waveguides and acoustical waveguides with rough boundaries will be published elsewhere.

ACKNOWLEDGMENT

The Office of Naval Research supported this work at the Naval Research Laboratory.

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On harmonic oscillators on the two-dimensional sphere S^2 and the hyperbolic plane H^2. II.

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(Received 30 July 2002; accepted 13 January 2003)

The properties of several noncentral $n=2$ harmonic oscillators are examined on spaces of constant curvature. All the mathematical expressions are presented using the curvature κ as a parameter, in such a way that particularizing for $\kappa>0$, $\kappa=0$, or $\kappa<0$, the corresponding properties are obtained for the system on the sphere S^2, the Euclidean plane $\mathbb{E}^2$, or the hyperbolic plane H^2, respectively. First, the separability in several κ-dependent systems of coordinates, as well as the existence of four families of κ-dependent superintegrable potentials related with the harmonic oscillator, are studied. Then three harmonic oscillators (1:1, 2:1 and $\frac{1}{2}$:1) are studied by using two different methods: superseparability and complex factorization. The second part deals with the problem of the existence of superintegrable but not superseparable systems. Several κ-dependent superintegrable harmonic oscillators with higher-order constants of motion are studied. The constants of motion are obtained by making use of the method of the complex factorization. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1560552]

I. INTRODUCTION

The spherical version of the two-dimensional central harmonic oscillator, as well as the spherical Kepler potential, are superintegrable systems with quadratic constants of motion.[1–3] More recently, the theory of superintegrable systems[4–19] have been extended to the case of non-Euclidean configuration spaces and some new noncentral superintegrable potentials on constant curvature spaces have been obtained.[20–26]

In previous articles we have studied the existence[21] of superintegrable systems on two-dimensional (2-D) spaces of constant curvature (sphere S^2, Euclidean plane $\mathbb{E}^2$, and hyperbolic plane H^2), and then[24,25] the properties of two particular harmonic oscillators (isotropic and nonisotropic 2:1). From the viewpoint of integrability, these studies were focused on the quadratic superintegrability, that is, on the existence of systems that, besides the energy, admit two further independent constants of motion linear or quadratic in the velocities (quadratic superintegrability is a property closely related with superseparability). From the geometrical point of view, the idea was that, in the same way that the Euclidean plane $\mathbb{E}^2$ is a ''limiting particular case'' of constant curvature spaces, some classical and well known potentials (Kepler problem, harmonic oscillator, etc.) can also be considered as ''limiting particular cases'' of more general ''curved'' systems. If we introduce the curvature κ as a parameter, then the question will be the obtaining of κ-dependent functions with appropriate flat limit. Many different κ-dependent potentials will have the same flat limit, so we must require that certain fundamental properties of the Euclidean system continue to hold for the ''curved'' system. By fundamental properties we mean those related with

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superintegrability and, in the case of the harmonic oscillator, with the existence of a complex factorization.

At this point we quote a statement by Fronsdal in Ref. 27: "*A physical theory that treats space-time as Minkowskian flat must be obtainable as a well-defined limit of a more general physical theory, for which the assumption of flatness is not essential.*" Of course our study is not a relativistic one, but, in a sense, this statement can be considered as very similar (roughly speaking, changing Minkowskian by Euclidean and limiting the study to $n=2$ dimensions) to our assumption of considering the spherical and hyperbolic oscillators as κ-deformations of well known Euclidean systems, or conversely, the Euclidean oscillators as very particular cases of general "curved" systems.

In the following, all the mathematical expressions will depend of the curvature κ as a parameter, in such a way that for $\kappa>0$, $\kappa=0$, or $\kappa<0$, we will obtain the corresponding property particularized for the dynamical system on the sphere, on the Euclidean plane, or on the hyperbolic plane. In order to present these expressions in a form which holds simultaneously for any value of κ, we will make use[21,28] of the following "tagged" trigonometric functions,

$$\mathrm{C}_\kappa(x)=\begin{cases}\cos\sqrt{\kappa}\,x & \text{if} \quad \kappa>0,\\ 1 & \text{if} \quad \kappa=0,\\ \cosh\sqrt{-\kappa}\,x & \text{if} \quad \kappa<0,\end{cases} \qquad \mathrm{S}_\kappa(x)=\begin{cases}\dfrac{1}{\sqrt{\kappa}}\sin\sqrt{\kappa}\,x & \text{if} \quad \kappa>0,\\ x & \text{if} \quad \kappa=0,\\ \dfrac{1}{\sqrt{-\kappa}}\sinh\sqrt{-\kappa}\,x & \text{if} \quad \kappa<0,\end{cases} \tag{1}$$

and the κ-dependent tangent $\mathrm{T}_\kappa(x)$ defined in the natural way $\mathrm{T}_\kappa(x)=\mathrm{S}_\kappa(x)/\mathrm{C}_\kappa(x)$.

The main objective of this article is to develop a deeper analysis of the κ-dependent spherical (hyperbolic) oscillators going beyond of the two basic 1:1 and 2:1 cases (studied in Ref. 25). We will focus our attention on three fundamental questions: first, the κ-dependent versions of the two families of superintegrable Euclidean systems related with the harmonic oscillator (they will be denoted by U_a, U_b, U_{bb}, and U_e), second, the existence of two different curved versions of the nonisotropic rational 2:1 oscillator (they will be denoted by U_{21} and $U_{1/2,1}$), and, finally, the existence of other more general superintegrable κ-dependent oscillators (in these cases the superintegrability does not arise from superseparability).

In more detail, the plan of this article is as follows: In Secs. II and III we study the first question, making use of κ-dependent polar coordinates (this is a prolongation of Ref. 21; here we introduce some changes, rewrite the results in a different form and fill some gaps). In Sec. IV we study the three oscillators (1:1, 2:1, and $\frac{1}{2}$:1 that is a new one) endowed with quadratic superintegrability (superseparability) making use of κ-dependent parallel coordinates (this section is partially related to Ref. 25). In Sec. V we study other more general κ-dependent oscillators; we discuss two important points: the existence of superintegrability with higher-order integrals of motion, and the existence of a complex factorization. Finally, in Sec. VI we discuss the results and make some final comments.

II. GEODESIC MOTION, NOETHER SYMMETRIES AND CONSTANTS OF MOTION ON $(S^2,\mathbb{E}^2,H^2)$

In Ref. 25 we consider it convenient to start with polar (r,ϕ) coordinates (appropriate for central potentials) and then move to parallel coordinate systems. So we start with the following expression written in polar coordinates (r,ϕ),

$$ds^2=dr^2+\mathrm{S}_\kappa^2(r)\,d\phi^2, \tag{2}$$

that represents the differential element of distance on the spaces $(S^2,\mathbb{E}^2,H^2)$ with constant curvature κ. It reduces to

$$ds_1^2 = dr^2 + (\sin^2 r)\, d\phi^2, \quad ds_0^2 = dr^2 + r^2\, d\phi^2, \quad ds_{-1}^2 = dr^2 + (\sinh^2 r)\, d\phi^2,$$

in the three particular cases of the unit sphere, Euclidean plane, and "unit" Lobachewski plane. The three κ-dependent vector fields Y_1, Y_2, Y_J, with coordinate expressions given by

$$Y_1(\kappa) = (\cos\phi)\frac{\partial}{\partial r} - \left(\frac{C_\kappa(r)}{S_\kappa(r)}\sin\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_2(\kappa) = (\sin\phi)\frac{\partial}{\partial r} + \left(\frac{C_\kappa(r)}{S_\kappa(r)}\cos\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_J = \frac{\partial}{\partial\phi},$$

are generators of three different one-parameter groups of diffeomorphisms preserving the metric ds^2 (isometries of the Riemannian manifold). In fact they close the following Lie algebra,

$$[Y_1(\kappa), Y_2(\kappa)] = -\kappa Y_J, \quad [Y_1(\kappa), Y_J] = -Y_2(\kappa), \quad [Y_2(\kappa), Y_J] = Y_1(\kappa),$$

that represents the Lie algebra of the isometries of the spherical (Euclidean, hyperbolic) space. Notice that only if $\kappa = 0$ (Euclidean plane), Y_1 and Y_2 commute. Moreover, the Lagrangian for the geodesic (free) motion is given by the kinetic term arising from the metric

$$L(\kappa) = T(\kappa) = (\tfrac{1}{2})\,(v_r^2 + S_\kappa^2(r) v_\phi^2)$$

and is invariant under the actions of $Y_1(\kappa)$, $Y_2(\kappa)$, and $Y_J(\kappa)$,

A general standard Lagrangian (Riemmanian metric minus a potential) has the following form:

$$L(\kappa) = (\tfrac{1}{2})\,(v_r^2 + S_\kappa^2(r) v_\phi^2) - U(r,\phi,\kappa)$$

in such a way that for $\kappa = 0$ we recover a standard Euclidean system

$$\lim_{\kappa\to 0} L(\kappa) = (\tfrac{1}{2})\,(v_r^2 + r^2 v_\phi^2) - V(r,\phi), \quad V(r,\phi) = U(r,\phi,0).$$

In three particular cases this Lagrangian system possesses the vector fields Y_1, Y_2, or Y_J as exact Noether symmetries. If we denote by Y_s^t, $s = 1,2,J$, the natural lift to the tangent bundle (phase space) of the vector field Y_s, and by θ_L the Cartan semibasic one-form

$$\theta_L = v_r\, dr + S_\kappa^2(r) v_\phi\, d\phi,$$

then we have the following.

(1) If the potential U is of the form $U = U(z_2)$ with $z_2 = S_\kappa(r)\sin\phi$, then

$$P_1(\kappa) = i(Y_1^t(\kappa))\,\theta_L = (\cos\phi)\, v_r - (C_\kappa(r) S_\kappa(r)\sin\phi)\, v_\phi$$

is a constant of motion.

(2) If the potential U is of the form $U = U(z_1)$, $z_1 = S_\kappa(r)\cos\phi$, then

$$P_2(\kappa) = i(Y_2^t(\kappa))\,\theta_L = (\sin\phi)\, v_r + (C_\kappa(r) S_\kappa(r)\cos\phi)\, v_\phi$$

is a constant of motion.

(3) If the potential U depends only on the coordinate r (central potential), then

$$J(\kappa)=i(Y_J^t)\ \theta_L=\mathrm{S}_\kappa^2(r)\ v_\phi$$

is a constant of motion. Notice that the vector field Y_J is κ-independent but the integral of motion (angular momentun) $J(\kappa)$ is κ-dependent (we will return to this question in Sec. IV).

In these three very particular cases the corresponding system becomes integrable with a second integral, $P_1(\kappa)$, $P_2(\kappa)$, or $J(\kappa)$, arising from an exact symmetry. This Noether origin is the reason why this second integral is linear in the velocities (momenta).

Other not so simple integrable cases will have constants of motion quadratic, cubic, or of higher-order in the momenta. For example, the most general form of a quadratic constant is

$$I=I_{22}+I_{20}(r,\phi,\kappa)\,,\quad I_{22}=av_r^2+2bv_rv_\phi+cv_\phi^2,$$

where a, b, and c, are κ-dependent functions of r and ϕ. It can be proved that I_{22} turns out to be a linear combination of binary products of the above three linear functions

$$I_{22}(\kappa)=a_0P_1^2(\kappa)+b_0P_1(\kappa)P_2(\kappa)+c_0P_2^2(\kappa)+a_1P_2(\kappa)J(\kappa)+c_1P_1(\kappa)J(\kappa)+a_2J^2(\kappa)$$

where $(a_0,b_0,c_0;a_1,c_1;a_2)$ are real constants. A particular case is when the potential U is separable in the κ-dependent ''polar'' coordinate system (r,ϕ). Then it must have the following expression,

$$U=F(r)+\frac{G(\phi)}{\mathrm{S}_\kappa^2(r)}, \tag{3}$$

and be integrable with the following two quadratic integrals of motion:

$$I_1(\kappa)=P_1^2(\kappa)+P_2^2(\kappa)+2F(r)+\frac{2\,G(\phi)}{\mathrm{T}_\kappa^2(r)},$$

$$I_2(\kappa)=J^2(\kappa)+2\,G(\phi).$$

[If $G=0$, then U is a central potential and the function $I_2(\kappa)$ becomes $I_2=J^2(\kappa)$.]

Notice that in this separable case, as in other cases to be studied below, the constants of motion are nonlinear and arise from nonexact hidden symmetries of $L(\kappa)$ involving simultaneous transformations of coordinates and velocities.

III. SUPERINTEGRABILITY ON 2-D SPACES OF CONSTANT CURVATURE: SYSTEMS RELATED WITH THE HARMONIC OSCILLATOR

Fris, Mandrosov *et al.*[4] studied the Euclidean $n=2$ systems which admit separability in two different coordinate systems, and obtained four families V_r, $r=a,b,c,d$, of superintegrable potentials with constants of motion linear or quadratic in the momenta. In fact, if we call superseparable to a system that admits Hamilton–Jacobi separation of variables (Schroedinger in the quantum case) in more than one coordinate system, then quadratic superintegrability (superintegrability with linear or quadratic constants of motion) can be considered as a property arising from superseparability. The two first families, V_a and V_b, were directly related with the Harmonic oscillator,

$$V_a=\left(\frac{1}{2}\right)\omega_0^2(x^2+y^2)+\frac{k_2}{x^2}+\frac{k_3}{y^2}, \tag{4}$$

$$V_b=\left(\frac{1}{2}\right)\omega_0^2(4x^2+y^2)+k_2x+\frac{k_3}{y^2}, \tag{5}$$

and can be considered as the more general deformations of the 1:1 and 2:1 oscillators (k_2, k_3, representing the intensity of the deformation) preserving quadratic superintegrability (the three-dimensional generalizations of these potentials have been studied in Ref. 7).

We can consider every $n=2$ superintegrable system as described by the triple (I_1, I_2, I_3) of its three integrals. Then, if we identify the corresponding constant of motion by the dominant term in the momenta (i.e., the quadratic term for a quadratic integral), we have six posibilities in the Euclidean plane. The following three cases,

$$(p_x^2, p_y^2, J^2), \quad (p_x^2, p_y^2, Jp_y), \quad (p_x^2, p_y^2, Jp_x),$$

correspond to the families V_a (family of the oscillator x^2+y^2), V_b (oscillator $4x^2+y^2$), and $\tilde{V}_b$ (oscillator x^2+4y^2), where $\tilde{V}_b$ denotes the family obtained from V_b just by the change $(x,y)\leftrightarrow(y,x)$ that, in geometric terms, is a reflection in the line $x=y$ (of course V_a is invariant under this transformation and the pairs *with* and *without* a tilde must be considered as equivalent). The other two families, V_c ($\tilde{V}_c$) and V_d, that can be represented by the triples

$$(p_x^2+p_y^2, Jp_y, J^2), \quad (p_x^2+p_y^2, Jp_x, J^2), \quad (p_x^2+p_y^2, Jp_x, Jp_y)$$

are related with the Kepler problem.

Next, in the following two subsections, we will study the spherical and hyperbolic versions of potentials V_a and V_b.

A. Family U_a

The following spherical (hyperbolic) Lagrangian with curvature κ,

$$\begin{aligned} &U_a(r,\phi,\kappa)=k_1U_a^1+k_2U_a^2+k_3U_a^3+k_0, \quad k_1=(\tfrac{1}{2})\,\omega_0^2, \\ &U_a^1=U_{11}=\mathrm{T}_\kappa^2(r), \quad U_a^2=\frac{1}{(\mathrm{S}_\kappa(r)\cos\phi)^2}, \quad U_a^3=\frac{1}{(\mathrm{S}_\kappa(r)\sin\phi)^2}, \end{aligned} \tag{6}$$

is a superintegrable system endowed with the following three integrals of motion:

$$I_1(\kappa)=P_1^2(\kappa)+\omega_0^2\,(\mathrm{T}_\kappa(r)\cos\phi)^2+\frac{2\,k_2}{(\mathrm{T}_\kappa(r)\cos\phi)^2},$$

$$I_2(\kappa)=P_2^2(\kappa)+\omega_0^2\,(\mathrm{T}_\kappa(r)\sin\phi)^2+\frac{2\,k_3}{(\mathrm{T}_\kappa(r)\sin\phi)^2},$$

$$I_3(\kappa)=J^2(\kappa)+\frac{2\,k_2}{\cos^2\phi}+\frac{2\,k_3}{\sin^2\phi}.$$

Thus, this system is characterized by the triple (P_1^2, P_2^2, J^2), and must be interpreted as representing the spherical (hyperbolic) version of the Euclidean potential V_a.

B. Families U_b, U_{bb}, U_e, and the contribution of the angular momentum

The Euclidean family V_b admits two different κ-dependent versions that we will denote by U_b and U_{bb} (we have introduced some changes in the notation with repect to that of Ref. 25).

(*b*) *Family* U_b. The first κ-dependent family U_b is given by

$$U_b(r,\phi,\kappa)=k_1U_b^1+k_2U_b^2+k_3U_b^3+k_0, \quad k_1=(\tfrac{1}{2})\,\omega_0^2,$$

with

$$U_b^1 = U_{21} = \frac{1}{1-\kappa(\mathrm{S}_\kappa(r)\sin\phi)^2}[\,4A_b^2 + (\mathrm{S}_\kappa(r)\sin\phi)^2\,], \quad A_b = \frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2}$$
$$U_b^2 = \frac{\mathrm{T}_\kappa(r)\cos\phi}{\mathrm{C}_k^2(r)[\,1-\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2\,]^2}, \qquad U_b^3 = \frac{1}{(\mathrm{S}_\kappa(r)\sin\phi)^2}. \tag{7}$$

The total energy $I_0 = T + U_b$ splits in two independent constants of motion,

$$2I_0(\kappa) = I_1(\kappa) + I_2(\kappa),$$

with $I_1(\kappa)$ and $I_2(\kappa)$ given by

$$I_1(\kappa) = P_1^2(\kappa) + 4\,\omega_0^2 A_b^2 + 2k_2\,U_b^2\,(\cos^2 r)[1+\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2],$$

$$I_2(\kappa) = P_2^2(\kappa) + \kappa\,J^2(\kappa) + \omega_0^2\,(1+\kappa A_b^2)\,\frac{(\mathrm{S}_\kappa(r)\sin\phi)^2}{1-\kappa(\mathrm{S}_\kappa(r)\sin\phi)^2} + \quad 2k_2\,U_b^2\,(\mathrm{S}_\kappa(r)\sin\phi)^2$$
$$+ \frac{2k_3}{(\mathrm{S}_\kappa(r)\sin\phi)^2}.$$

The additional third integral is given by

$$I_3(\kappa) = J(\kappa)\,P_2(\kappa) + I_{30}(\kappa)$$

with

$$I_{30}(\kappa) = -\,\omega_0^2 \frac{\mathrm{T}_\kappa^3(r)\cos\phi\sin^2\phi}{[1-\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2]^2} - \frac{k_2\,[1+\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2](\mathrm{T}_\kappa(r)\sin\phi)^2}{2\,[1-\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2]^2} + \frac{2k_3\cos\phi}{\mathrm{T}_\kappa(r)\sin^2\phi}.$$

Thus the family U_b is characterized by the triple $(P_1^2, P_2^2 + \kappa J^2, JP_2)$ [and the associated family $\tilde{U}_b$ by the triple $(P_1^2 + \kappa J^2, P_2^2, JP_1)$] and satisfies the following Euclidean limit

$$\lim_{\kappa\to 0} U_b = \left(\frac{1}{2}\right)\omega_0^2\,r^2\,(4\cos^2\phi + \sin^2\phi) + k_2\,(r\cos\phi) + \frac{k_3}{(r\sin\phi)^2}.$$

(bb) *Family* U_{bb}. The second κ-dependent family U_{bb} is given by

$$U_{bb}(r,\phi,\kappa) = k_1 U_{bb}^1 + k_2 U_{bb}^2 + k_3 U_{bb}^3 + k_0, \quad k_1 = (\tfrac{1}{2})\,\omega_0^2,$$

$$U_{bb}^1 = \frac{1}{1-\kappa\,(\mathrm{S}_\kappa(r)\sin\phi)^2}[\,A_{bb}^2 + (\mathrm{S}_\kappa(r)\sin\phi)^2\,], \quad A_{bb} = \frac{\mathrm{T}_\kappa(r)\cos\phi}{1+\sqrt{1+\kappa\,(\mathrm{T}_\kappa(r)\cos\phi)^2}} \tag{8}$$

$$U_{bb}^2 = \frac{\mathrm{S}_\kappa(r)\sin\phi}{\sqrt{1-\kappa\,(\mathrm{S}_\kappa(r)\sin\phi)^2}}, \quad U_{bb}^3 = \frac{1}{(\mathrm{S}_\kappa(r)\cos\phi)^2}.$$

The total energy $I_0 = T + U_{bb}$ also splits as a sum of two independent constants of motion, $I_1(\kappa)$ and $I_2(\kappa)$, given by

$$I_1(\kappa) = P_1^2(\kappa) + 2w_0^2 A_{bb}^2 + \frac{2k_3}{(\mathrm{T}_\kappa(r)\cos\phi)^2},$$

$$I_2(\kappa) = P_2^2(\kappa) + \kappa\,J^2(\kappa) + 2w_0^2(1+\kappa A_{bb}^2)\,\frac{(\mathrm{S}_\kappa(r)\sin\phi)^2}{1-\kappa\,(\mathrm{S}_\kappa(r)\sin\phi)^2} + 2k_2 U_{bb}^2 + \frac{2k_3}{\cos^2\phi}.$$

The additional third integral is given by

$$I_3(\kappa)=J(\kappa)\,P_1(\kappa)+\omega_0^2\,I_{30}(\kappa)\,,$$

$$I_{30}(\kappa)=2w_0^2A_{bb}^2\frac{(\mathrm{S}_\kappa(r)\sin\phi)^2}{\sqrt{1-\kappa\,(\mathrm{S}_\kappa(r)\sin\phi)^2}}-\frac{k_2\mathrm{C}_\kappa(r)}{\sqrt{1-\kappa\,(\mathrm{S}_\kappa(r)\sin\phi)^2}}-2k_3\frac{\mathrm{T}_\kappa(r)\sin\phi}{\cos^2\phi}.$$

Thus the family U_{bb} is characterized by the triple $(P_1^2,P_2^2+\kappa J^2,JP_1)$ [and the associated family $\tilde{U}_{bb}$ by the triple $(P_1^2+\kappa J^2,P_2^2,JP_2)$] and satisfies the following Euclidean limit

$$\lim_{\kappa\to 0}U_{bb}=\left(\frac{1}{2}\right)\omega_0^2\,r^2\left[\left(\frac{1}{4}\right)\cos^2\phi+\sin^2\phi\right]+k_2\,(r\sin\phi)+\frac{k_3}{(r\cos\phi)^2}\,.$$

Notice that the Euclidean limit suggests the interpretation of U_{bb}^1 as a noncentral κ-dependent oscillator with $\frac{1}{2}$:1 as ratio of frequencies (but really different from the above $U_b^1=U_{21}$).

These three families of potentials, U_a, U_b, U_{bb}, can be considered from two different viewpoints; as a vector space or as a deformation. As a vector space because they were obtained[21] as solution of a system of two partial differential equations (quadratic integrability is related with a single equation and quadratic superintegrability with a system of two equations) and the solution of such a system turns out to be vector space of dimension four. As the equations depend on the derivatives of U but not on U itself, the solution is determined up to an additive constant k_0 (as expected for a potential); thus any solution can be written as a linear combination of four elements: three (r,ϕ)-dependent functions and a constant. We notice that in Ref. 21 the linear combination was given with another function U_{bb}^4 instead of U_{bb}^1; they are related by

$$U_{bb}^1=2U_{bb}^3-2U_{bb}^4-1\,,\quad U_{bb}^4=\frac{\cos r}{(\sin r\cos\phi)^2\,\sqrt{1-(\sin r\sin\phi)^2}}$$

(here we have particularized for $\kappa=1$ for ease of notation). By a deformation we mean that the linear combination is written in such a way that the first function U_r^1, $r=a,b,bb$, is considered as playing a much more important role that the other two potentials; that is, U_r^1 is important by itself but U_r^2 and U_r^3 must be interpreted as the only functions introducing a deformation of U_r^1 but preserving the existence of constants of motion (i.e., preserving the existence of symmetries). Notice that this is not a problem of perturbations since k_2, k_3, can take arbitrary values.

We close this section with the important question of the existence of the κ-dependent family U_{bb} different from U_b (i.e., $U_{bb}\neq U_b$). In spaces with $\kappa\neq 0$ the angular momentum J has a direct contribution to the energy since the kinetic term T can be written as $T=P_1^2+P_2^2+\kappa J^2$ (this contribution vanish in the limit $\kappa\to 0$). So if the total energy $I_0=T+U$ splits as a sum of two integrals of motion $I_0=I_1+I_2$, we then have two different ways for the place of J. This property can be considered as the reason for the existence of two different κ-dependent versions, U_b and U_{bb}, of V_b. Moreover, this very question is in fact related with the existence of a new family U_e.

(e) *Family* U_e. In the Euclidean case, there is also another superintegrable family

$$V_e=(\tfrac{1}{2})\,\omega_0^2(x^2+y^2)+k_2x+k_3y\,,\quad \tilde{V}_e=V_e \tag{9}$$

with associated triple (p_x^2,p_y^2,p_xp_y). It may be considered as a rather simple potential since it just reduces to the isotropic oscillator $V_{11}=V_a^1$ after a translation, i.e., center at an arbitrary point of the plane (in fact, this family was not considered in Ref. 4). Nevertheless, the κ-dependent version, which is given by

$$U_e(r,\phi,\kappa)=k_1U_e^1+k_2U_e^2+k_3U_e^3+k_0\,,\quad k_1=(\tfrac{1}{2})\,\omega_0^2\,,$$
$$U_e^1=\mathrm{T}_\kappa^2(r)\,,\quad U_e^2=\frac{\mathrm{T}_\kappa(r)\cos\phi}{\mathrm{C}_k(r)\sqrt{1-\kappa\,[\mathrm{S}_\kappa(r)\sin\phi]^2}}\,,\quad U_e^3=\frac{\mathrm{S}_\kappa(r)\sin\phi}{\sqrt{1-\kappa\,[\mathrm{S}_\kappa(r)\sin\phi]^2}}\,, \tag{10}$$

and is characterized by the triple $(P_1^2,P_2^2+\kappa J^2,P_1P_2)$, illustrates how ''curvature versions'' of simple Euclidean potentials can become quite interesting superintegrable functions on S^2 or H^2. Notice that, as U_e is not invariant under the change $\cos\phi\leftrightarrow\sin\phi$, it is not self-related for $\kappa\neq0$. There exists therefore another associated family $\widetilde{U}_e$ ($\widetilde{U}_e\neq U_e$) characterized by the triple $(P_1^2+\kappa J^2,P_2^2,P_1P_2)$. So, we can say that the deformation introduced by κ causes a splitting of V_e into U_e and $\widetilde{U}_e$; that is, $V_e\overset{\kappa}{\rightarrow}(U_e,\widetilde{U}_e)$.

We will see in the next section that the contribution of the angular momentum is a question closely related with the properties of the κ-dependent parallel coordinates.

IV. THREE HARMONIC OSCILLATORS (1:1, 2:1 AND $\frac{1}{2}$:1) ON 2-D CONSTANT CURVATURE SPACES: PARALLEL COORDINATES

In differential geometric terms, a ''geodesic parallel'' system of coordinates represents the Riemannian version of the Euclidean (x,y) system of Cartesian coordinates.[29] But one important property is that, when we introduce the curvature κ in the (x,y) system, we obtain not just one but two different systems that we denote by (u,y) and (x,v), respectively (a more detailed discussion of these properties is given in the appendix, see also Refs. 21 and 24). Moving from geometry to dynamics the important point is that, as we have two different ''parallel'' sytems, we then have two different ways of ''parallel'' Hamilton–Jacobi separability and, consequently, two different ways of obtaining κ-dependent integrable potentials.

In order to avoid complications with the use of different notations we will present (as far as possible) all the results in the (u,y) approach, and we will restrict the use of the (x,v) coordinates in some particular cases [the translation to the (x,v) notation of some of the results obtained is given in the Appendix].

A. Parallel coordinates and κ-dependent separability

The following expression written in (u,y) parallel coordinates

$$ds^2=\mathrm{C}_\kappa^2(y)du^2+dy^2 \tag{11}$$

represents the differential element of distance on the spaces $(S^2,\mathbb{E}^2,H^2)$ with constant curvature κ. So a standard Lagrangian (kinetic term minus potential function) has the following form:

$$L(\kappa)=(\tfrac{1}{2})(\,\mathrm{C}_\kappa^2(y)\,v_u^2+v_y^2\,)-U(u,y,\kappa),$$

in such a way that the Euclidean system is just given by the particular value of $L(\kappa)$ in $\kappa=0$:

$$\lim_{\kappa\to0}L(\kappa)=(\tfrac{1}{2})\,(v_x^2+v_y^2)-V(x,y)\,,\quad V(x,y)=U(x,y,0)\,.$$

The three κ-dependent vector fields, $Y_1(\kappa)$, $Y_2(\kappa)$, $Y_J(\kappa)$, have now the following expressions in parallel coordinates:

$$Y_1(\kappa)=\frac{\partial}{\partial u}\,,$$

$$Y_2(\kappa)=\kappa\,\mathrm{S}_\kappa(u)\mathrm{T}_\kappa(y)\,\frac{\partial}{\partial u}+\mathrm{C}_\kappa(u)\,\frac{\partial}{\partial y}\,,$$

$$Y_J(\kappa)=\mathrm{C}_\kappa(u)\mathrm{T}_\kappa(y)\frac{\partial}{\partial u}-\mathrm{S}_\kappa(u)\frac{\partial}{\partial y},$$

and the associated linear constants of motion are given by

$$P_1(\kappa)=\mathrm{C}_\kappa^2(y)\,v_u,$$

$$P_2(\kappa)=\kappa\,\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u+\mathrm{C}_\kappa(u)\,v_y,$$

$$J(\kappa)=\mathrm{C}_\kappa(u)\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u-\mathrm{S}_\kappa(u)\,v_y.$$

In contrast to the polar coordinates formalism, now the κ-dependence is present in both coordinates, u and y.

The particular expressions obtained for these three vector fields, $Y_s(\kappa)$, $s=1,2,J$, lead to a very interesting geometric question. According to the straightening-out theorem,[30] a vector field Y on an n-manifold M always admits a local coordinate system $\{x_1,\ldots,x_n\}$ in an appropriate neighborhood of a regular point m, $Y(m)\neq 0$, such that then it becomes $Y=\Sigma_k c_k(\partial/\partial x_k)$, with $c_{k_0}=1$, $c_k=0$, $k\neq k_0$. We have proven (at the beginning of Sec. II) that in the (r,ϕ) polar coordinates Y_J becomes $Y_J=\partial/\partial\phi$. Now we have obtained $Y_1=\partial/\partial u$. Similarly, in the (x,v) system, we will have $Y_2=\partial/\partial v$. So, these three coordinate systems, (r,ϕ), (u,y), and (x,v), are the three appropriated systems (via the straightening-out theorem) for obtaining the straight expressions of Y_J, Y_1, and Y_2, respectively.

Next we enumerate different possibilities for separability of κ-dependent potentials:

(i) A κ-dependent potential U, that in (u,y) ''parallel'' coordinates has an expression of the form

$$U=F(y)+\frac{G(u)}{\mathrm{C}_\kappa^2(y)},\tag{12}$$

is separable. It is therefore integrable with the following two quadratic integrals of motion:

$$I_1(\kappa)=P_1^2(\kappa)+2G(u),$$

$$I_2(\kappa)=P_2^2(\kappa)+\kappa J^2(\kappa)+2F(y)+2\kappa G(u)\,\mathrm{T}_\kappa^2(y).$$

Integrable potentials in this family are characterized by the pair $(P_1^2,P_2^2+\kappa J^2)$.

(ii) A potential U separable in (x,v) ''parallel'' coordinates is of the form

$$U=F(x)+\frac{G(v)}{\mathrm{C}_\kappa^2(x)},\tag{13}$$

and, when written in (u,y) ''parallel'' coordinates, it becomes

$$U=F[\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y)]+\frac{G[\mathrm{T}_\kappa(y)/\mathrm{C}_\kappa(u)]}{1-\kappa(\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y))^2}.\tag{14}$$

It is integrable with the following two integrals of motion:

$$I_1(\kappa)=P_1^2(\kappa)+\kappa J^2(\kappa)+2F[\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y)]+\kappa G[\mathrm{T}_\kappa(y)/\mathrm{C}_\kappa(u)]\left(\frac{(\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y))^2}{1-\kappa(\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y))^2}\right),$$

$$I_2(\kappa)=P_2^2(\kappa)+2G[\mathrm{T}_\kappa(y)/\mathrm{C}_\kappa(u)].$$

Integrable potentials in this family are characterized by the pair $(P_1^2+\kappa J^2,P_2^2)$.

At this point we wish to underline two properties directly related with the existence of these two different parallel systems of coordinates:

(a) The two expressions $z_1=\mathrm{S}_\kappa(r)\cos\phi$ and $z_2=\mathrm{S}_\kappa(r)\sin\phi$, arising in the study of the Noether theorem in polar (r,ϕ) coordinates, correspond to $z_1=\mathrm{S}_\kappa(x)$ and $z_2=\mathrm{S}_\kappa(y)$ when written in parallel coordinates.

(b) In spaces of constant curvature, the curvature κ and the angular momentum $J(\kappa)$ have a direct contribution to the energy in the sense that the kinetic term $T(\kappa)$ can be rewritten as follows:

$$\mathrm{C}_\kappa^2(y)\,v_u^2+v_y^2=P_1^2(\kappa)+P_2^2(\kappa)+\kappa J^2(\kappa).$$

In the particular case of the potential U being separable in "parallel" coordinates, then the total energy splits in two summands, $I_1(\kappa)$ and $I_2(\kappa)$, and both summands are integrals of motion. Then, if $\kappa\neq 0$, we have two alternatives for placing the contribution of the angular momentum: it can be present in the same term that $P_2^2(\kappa)$, as in (i), or in the same term that $P_1^2(\kappa)$, as in (ii) (an open question is the existence of a coordinate system in which the term κJ^2 splits in a different way).

Next we continue with the separability in other κ-dependent coordinate systems:

(iii) A potential U, when written in κ-dependent "parabolic" coordinates $(r+x,r-x)$, has the following expression:

$$U=\frac{1}{\mathrm{S}_\kappa(r)\mathrm{C}_\kappa(x)}[F(r+x)+G(r-x)], \tag{15}$$

is separable on S^2 (or H^2) with a second integral of motion given by

$$I_2(\kappa)=JP_2+W(r+x,r-x),$$

(the actual form of W depends on F and G). Separable potentials of this class are characterized by the pair $(P_1^2+P_2^2+\kappa J^2,JP_2)$.

(iv) A potential U, when written in κ-dependent "parabolic" coordinates $(r+y,r-y)$, has the following expression:

$$U=\frac{1}{\mathrm{S}_\kappa(r)\mathrm{C}_\kappa(y)}[F(r+y)+G(r-y)], \tag{16}$$

is separable on S^2 (or H^2) with a second integral of motion given by

$$I_2(\kappa)=JP_1+W(r+y,r-y).$$

Separable potentials of this class are characterized by the pair $(P_1^2+P_2^2+\kappa J^2,JP_1)$.

(v) A potential U can also be separable in the κ-dependent coordinates $z_+=x+y$ and $z_-=x-y$ (in the Euclidean plane these are just rotated Cartesian coordinates that correspond to the so-called light-cone coordinates in the Minkowskian plane). In this case it must take the form

$$U=\frac{1}{\mathrm{C}_\kappa(z_+)\mathrm{C}_\kappa(z_-)}[F(z_+)+G(z_-)], \tag{17}$$

with the second integral of motion given by

$$I_2(\kappa)=P_1P_2+W(z_+,z_-).$$

So these separable potentials are characterized by the pair $(P_1^2+P_2^2+\kappa J^2,P_1P_2)$. In the spherical case $\kappa>0$ the level curves, $z_+=\text{const}$ and $z_-=\text{const}$, are spherical parabolas with focus in the equator and the equator as axis (equator relative to the origin). Notice also that in S^2 (with κ

$=1$) the spherical parabolas can be identified with spherical elipses with $\pi/2$ as focal distance (this coordinate system is also well defined in the $\kappa<0$ case but then the geometric intepretation is not so simple).

The four superintegrable κ-dependent families U_a, U_b, U_{bb}, and U_e have the following expressions in (u,y) parallel coordinates:

$$
\begin{aligned}
U_a &= \left(\frac{1}{2}\right)\omega_0^2\, U_{11} + \frac{k_2}{(\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y))^2} + \frac{k_3}{(\mathrm{S}_\kappa(y))^2},\\
U_b &= \left(\frac{1}{2}\right)\omega_0^2\, U_{21} + \frac{k_2\,\mathrm{S}_\kappa(2\,u)}{(\mathrm{C}_\kappa(2\,u)\mathrm{C}_\kappa(y))^2} + \frac{k_3}{(\mathrm{S}_\kappa(y))^2},\\
U_{bb} &= \left(\frac{1}{2}\right)\omega_0^2\, U_{1/2,1} + k_2\mathrm{T}_k(y) + \frac{k_3}{(\mathrm{S}_\kappa(u/2)\mathrm{C}_\kappa(y))^2},\\
U_e &= \left(\frac{1}{2}\right)\omega_0^2\, U_{11} + \frac{k_2\mathrm{S}_\kappa(u)}{(\mathrm{C}_\kappa(u)\mathrm{C}_\kappa(y))^2} + k_3\mathrm{T}_\kappa(y),
\end{aligned}
\tag{18}
$$

where $U_{11}(u,y,\kappa)$, $U_{21}(u,y,\kappa)$, and $U_{1/2,1}(u,y,\kappa)$, are given by

$$
U_{m1} = \mathrm{T}_\kappa^2(y) + \frac{\mathrm{T}_\kappa^2(m\,u)}{\mathrm{C}_\kappa^2(y)}, \quad m = 1,2,\tfrac{1}{2}.
$$

All these systems are clearly separable in (u,y) parallel coordinates. In addition, U_a is separable in both polar (r,ϕ) and parallel (x,v) coordinates; U_b is separable in $(r+y,r-y)$ "parabolic" coordinates, U_{bb} is separable in $(r+x,r-x)$ "parabolic" coordinates, and, finally, U_e is separable in (z_+,z_-) "parabolic" coordinates.

Notice that (18) shows a high degree of simplicity since $U_a^1 = U_e^1 = U_{11}$, $U_b^1 = U_{21}$, and $U_{bb}^1 = U_{1/2,1}$, that in (r,ϕ) coordinates looked rather different, but now becomes very similar. Another remarkable result is the particular form obtained for U_{bb}^1 as the half-integer dependent function $U_{1/2,1}$. Next we will study in detail each one of these three U_{m1}, $m=1,2,\frac{1}{2}$, functions.

B. Isotropic 1:1 and nonisotropic 2:1 oscillators

The two potentials U_{11} and U_{21}, that can be considered as representing the κ-dependent versions of the Euclidean oscillators with ratio of frequencies given by 1:1 and 2:1, were studied in Ref. 25. It was proved that the superintegrability of these two systems is related to the existence of a complex factorization.

Let us first consider U_{11}. If we denote by K_1, K_2 the following two functions:

$$
K_1 = P_1(\kappa) + \mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(u)\,,
$$

$$
K_2 = P_2(\kappa) + \mathrm{i}\,\omega_0\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right),
$$

then the functions K_{ij}, $i,j=1,2$, defined as $K_{ij} = K_i K_j^*$ are constants of motion for U_{11}. Therefore the κ-dependent potential U_{11} is superintegrable with three integrals of motion given by

$$
I_1(\kappa) = |\,K_1\,|^2\,, \quad I_2(\kappa) = |\,K_2\,|^2\,, \quad I_3(\kappa) = \mathrm{Im}(K_{12}) = \omega_0\,J(\kappa)\,.
$$

The potential of the spherical (hyperbolic) 2:1 harmonic oscillator with curvature κ

$$U_{21}=\mathrm{T}_\kappa^2(y)+\frac{\mathrm{T}_\kappa^2(2\,u)}{\mathrm{C}_\kappa^2(y)} \tag{19}$$

is separable in (u,y) coordinates. The two constants of motion

$$I_1(\kappa)=P_1(\kappa)^2+\omega_0^2\,\mathrm{T}_\kappa^2(2\,u)\,,$$

$$I_2(\kappa)=P_2^2(\kappa)+\kappa\,J^2(\kappa)+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right)^2,$$

as well the additional third integral $I_3(\kappa)$, can also be obtained from a complex factorization. If we denote by K_1, K_2^+, K_2^- the following three complex functions,

$$K_1=P_1(\kappa)+\mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(2\,u)\,,$$

$$K_2^+=[P_2(\kappa)+\sqrt{\kappa}\,J(\kappa)]+\mathrm{i}\,\omega_0\,(\mathrm{C}_\kappa(u)+\sqrt{\kappa}\,\mathrm{S}_\kappa(u))\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right),$$

$$K_2^-=[P_2(\kappa)-\sqrt{\kappa}\,J(\kappa)]+\mathrm{i}\,\omega_0\,(\mathrm{C}_\kappa(u)-\sqrt{\kappa}\,\mathrm{S}_\kappa(u))\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right),$$

then we have the following. (i) The modulus of K_1 is the constant of motion $I_1(\kappa)$. (ii) The sum of the modulus of K_2^+ and K_2^- is also a constant of motion and coincides with $I_2(\kappa)$. (iii) The complex function K_{122}, defined as $K_{122}=K_1\,K_2^{(2)*}$ with $K_2^{(2)}=K_2^+\,K_2^-$, is a constant of motion. If we write $K_{122}=I_4(\kappa)+\mathrm{i}\,I_3(\kappa)$, then we obtain

$$I_3(\kappa)=J(\kappa)\,P_2(\kappa)+\omega_0^2\left(\frac{\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(u)}{\mathrm{C}_\kappa^2(2\,u)}\right)\mathrm{T}_\kappa^2(y)\,,$$

$$I_4(\kappa)=[P_2^2(\kappa)-\kappa\,J^2(\kappa)]P_1(\kappa)+\omega_0^2[2\,\mathrm{T}_\kappa(2\,u)\,v_y-\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u]\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right).$$

Therefore, the κ-dependent potential U_{21} is superintegrable with the following thre quadratic integrals of motion given by

$$I_1(\kappa)=|\,K_1\,|^2\,,\quad I_2(\kappa)=|\,K_2^+\,|^2+|\,K_2^-\,|^2\,,\quad I_3(\kappa)=\mathrm{Im}(K_{122})\,.$$

C. The nonisotropic $\frac{1}{2}$:1 oscillator

The noncentral oscillator U_{21} was already considered in Ref. 25 but the function

$$U_{1/2,1}=\mathrm{T}_\kappa^2(y)+\frac{\mathrm{T}_\kappa^2(u/2)}{\mathrm{C}_\kappa^2(y)} \tag{20}$$

is, in fact, a new one. It can be interpreted as representing the potential of the κ-dependent spherical (hyperbolic) version of the $\frac{1}{2}$:1 harmonic oscillator. In a similar way to the previous 2:1 case this system possesses two integrals of motion quadratic in the velocities:

$$I_1(\kappa)=P_1^2(\kappa)+\omega_0^2\,\mathrm{T}_\kappa^2(u/2)\,,$$

$$I_2(\kappa)=P_2^2(\kappa)+\kappa\,J^2(\kappa)+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u/2)}\right)^2.$$

Two questions immediately arise. First, does there exist a complex factorization for these integrals? Second, which is the relation of this potential with $\tilde{U}_{21}=U_{12}$ (in the Euclidean plane is the same system)?

The first question means that the additional integral $I_3(\kappa)$ must appear as the imaginary part of a certain complex function and that this complex function factors out in a similar way to the previous U_{11} and U_{21} cases. For the first function K_1 it is natural to propose

$$K_1=P_1(\kappa)+\mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(u/2)\,.$$

Concerning the second factor, we have obtained that if $K_2^{(1/2)}$ is given by

$$K_2^{(1/2)}=\mathrm{Re}[K_2^{(1/2)}]+\mathrm{i}\,\mathrm{Im}[K_2^{(1/2)}]\,,$$

$$\mathrm{Re}[K_2^{(1/2)}]=P_1P_2+\omega_0^2\,\mathrm{T}_\kappa(u/2)\tan y\,,$$

$$\mathrm{Im}[K_2^{(1/2)}]=\omega_0\,[\,\mathrm{S}_\kappa(y)\mathrm{C}_\kappa(y)\,v_u-\mathrm{T}_\kappa(u/2)v_y\,]\,,$$

then we have

$$\frac{d}{dt}\mathrm{Re}[K_2^{(1/2)}]=-\left(\frac{1}{2}\right)\left(\frac{\omega_0}{(\mathrm{C}_k(u/2)\mathrm{C}_\kappa(y))^2}\right)\mathrm{Im}[K_2^{(1/2)}]\,,$$

$$\frac{d}{dt}\mathrm{Im}[K_2^{(1/2)}]=\left(\frac{1}{2}\right)\left(\frac{\omega_0}{(\mathrm{C}_k(u/2)\mathrm{C}_\kappa(y))^2}\right)\mathrm{Re}[K_2^{(1/2)}]\,.$$

Hence

$$\frac{d}{dt}K_2^{(1/2)}=\left(\frac{\mathrm{i}}{2}\right)\left(\frac{\omega_0}{(\mathrm{C}_k(u/2)\mathrm{C}_\kappa(y))^2}\right)K_2^{(1/2)}$$

and consequently the function $K_1\,K_2^{(1/2)*}$ is a constant of motion. We have obtained that, if we write $K_1\,K_2^{(1/2)*}=I_4(\kappa)+\mathrm{i}\,I_3(\kappa)$, then $I_3(\kappa)$ and $I_4(\kappa)$ are given by

$$I_3=\mathrm{Im}(K_1\,K_2^*)=-\,\omega_0\,[\,JP_1-\omega_0^2\,\mathrm{T}_\kappa^2(u/2)\,\mathrm{T}_\kappa(y)\,]\,,$$

$$I_4=\mathrm{Re}(K_1\,K_2^*)=P_1^2P_2+\omega_0^2\,\mathrm{T}_\kappa(u/2)\,[\,2\,\mathrm{S}_\kappa(y)\mathrm{C}_\kappa(y)\,v_u-\mathrm{T}_\kappa(u/2)\,v_y\,]\,.$$

Concerning the second question, it is clear that, as far as $\kappa\neq 0$, we have different potentials, $U_{1/2,1}\neq U_{12}$, and also different complex factorizations. This is another example in which the deformation introduced by κ causes important qualitative changes.

We close this section with the following table that summarizes this κ-dependent situation:

Potential	Triple of quadratic constants	Euclidean limit
U_{21}	$(P_1^2,P_2^2+\kappa J^2,JP_2)$	$4\,x^2+y^2$
$U_{1/2,1}$	$(P_1^2,P_2^2+\kappa J^2,JP_1)$	$(\frac{1}{4})\,x^2+y^2$
$\tilde{U}_{21}=U_{12}$	$(P_1^2+\kappa J^2,P_2^2,JP_1)$	$x^2+4\,y^2$
$\tilde{U}_{1/2,1}=U_{1,1/2}$	$(P_1^2+\kappa J^2,P_2^2,JP_2)$	$x^2+(\frac{1}{4})\,y^2$

V. OTHER κ-DEPENDENT OSCILLATORS: SUPERINTEGRABILITY WITH HIGHER-ORDER CONSTANTS OF MOTION

The following function,

$$U_{m1}=\mathrm{T}_\kappa^2(y)+\frac{\mathrm{T}_\kappa^2(m\,u)}{\mathrm{C}_\kappa^2(y)}=\mathrm{T}_\kappa^2(m\,u)+\frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(m\,u)}, \tag{21}$$

is well defined for any value of m in the hyperbolic plane H^2 and for m integer or half-integer in the sphere S^2. As stated in point (i) of Sec. IV, this potential is separable in (u,y) parallel coordinates; therefore, it is integrable with quadratic constants of motion

$$I_1(\kappa)=P_1^2(\kappa)+\omega_0^2[\mathrm{T}_\kappa(m\,u)]^2,$$

$$I_2(\kappa)=[P_2^2(\kappa)+\kappa\,J^2(\kappa)]+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(m\,u)}\right)^2,$$

and satisfies the appropriate Euclidean limit

$$\lim_{\kappa\to 0}U_{m1}(\kappa)=(mx)^2+y^2$$

for representing the general non-isotropic m:1 oscillator on a 2-D manifold of constant curvature κ. Moreover, the integral $I_1(\kappa)$ is the sum of two squares (as in the Euclidean plane) and can be considered as the modulus of an appropriate complex function. In fact, it can also be obtained from the following property.

Proposition 1: Let K_1 be the following complex function:

$$K_1=P_1(\kappa)+\mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(m\,u).$$

Then the time evolution of K_1 is given by

$$\frac{d}{dt}K_1=\left(\frac{\mathrm{i}\,m\,\omega_0}{\mathrm{C}_\kappa^2(m\,u)\mathrm{C}_\kappa^2(y)}\right)K_1.$$

Proof: The proof follows by direct computation. Notice also that the appropriate Euclidean limit is satisfied:

$$\lim_{\kappa\to 0}K_1=J_x,\quad \frac{d}{dt}J_x=\mathrm{i}\,m\,\omega_0 J_x,\quad \text{with}\quad J_x=v_x+\mathrm{i}\,m\,\omega_0 x.$$

If we assume that the general U_{m1} potential generalizes the two particular superseparable cases, 2:1 and $\frac{1}{2}$:1, then it seems natural to suppose that, also in the general m case, the superintegrability of U_{m1} must arise from the existence of a certain complex function K_2 satisfying an appropriate time-evolution.

Next we consider the cases $m=3$ and $m=4$.

A. Nonisotropic 3:1 oscillator

The potential of the 3:1 oscillator is given by

$$U_{31}=\mathrm{T}_\kappa^2(y)+\frac{\mathrm{T}_\kappa^2(3u)}{\mathrm{C}_\kappa^2(y)}=\mathrm{T}_\kappa^2(3u)+\frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(3u)}. \tag{22}$$

We have obtained (we omit the details) that the following complex function $K_2^{(3)}$ defined as

$$K_2^{(3)} = \mathrm{Re}[K_2^{(3)}] + \mathrm{i}\,\mathrm{Im}[K_2^{(3)}],$$

with $\mathrm{Re}[K_2^{(3)}]$ and $\mathrm{Im}[K_2^{(3)}]$ given by

$$\mathrm{Re}[K_2^{(3)}] = P_2\,(P_2^2 - 3\,\kappa\,J^2) - \omega_0^2\,[3\mathrm{C}_\kappa(3u)\,v_y + \mathrm{S}_k(3u)\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u]\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(3u)}\right)^2,$$

$$\mathrm{Im}[K_2^{(3)}] = \omega_0\,[3\,v_y^2 - (\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)^2]\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(3u)}\right) - \omega_0^3\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(3u)}\right)^3,$$

satisfies the appropriate property

$$\frac{d}{dt}K_2^{(3)} = \left(\frac{3\,\mathrm{i}\,\omega_0}{\mathrm{C}_\kappa^2(3u)\mathrm{C}_\kappa^2(y)}\right)K_2^{(3)}.$$

Consequently, the complex function $\mathbb{K}$ defined as

$$\mathbb{K} = K_1\,K_2^{(3)*} \;=\; I_4 + \mathrm{i}\,I_3$$

is a constant of motion. Thus the potential U_{31} is superintegrable with the function I_3 as an additional constant of motion:

$$I_3 \;=\; I_{33} + \omega_0^2\,I_{31},$$

$$I_{33} \;=\; J\,(3\,P_2^2 - \kappa\,J^2),$$

$$I_{31} \;=\; [3\,\mathrm{S}_k(3u)\,v_y - \mathrm{C}_\kappa(3u)(\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)]\left[\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(3u)}\right]^2.$$

The Euclidean limit is given by

$$\lim_{\kappa\to 0} K_2^{(3)} = J_y^3, \quad \text{with} \quad J_y = v_y + \mathrm{i}\,\omega_0 y,$$

$$\lim_{\kappa\to 0} I_3 = 3(xv_y - yv_x)\,v_y^2 + \omega_0^2\,(yv_x - 9xv_y)\,y^2.$$

We notice that that the cubic character of the integral I_3 means that U_{31} is a superintegrable but not superseparable potential.

B. Nonisotropic 4:1 oscillator

The potential of the 4:1 oscillator is given by

$$U_{41} = \mathrm{T}_\kappa^2(y) + \frac{\mathrm{T}_\kappa^2(4u)}{\mathrm{C}_\kappa^2(y)} \;=\; \mathrm{T}_\kappa^2(4u) + \frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(4u)}. \tag{23}$$

We have obtained, also in this $m=4$ case, a complex factorization. The function $K_2^{(4)}$

$$K_2^{(4)} = \mathrm{Re}[K_2^{(4)}] + \mathrm{i}\,\mathrm{Im}[K_2^{(4)}],$$

with $\mathrm{Re}[K_2^{(4)}]$ and $\mathrm{Im}[K_2^{(4)}]$ given by

$$\mathrm{Re}[K_2^{(4)}]=P_2^4+\kappa^2J^4-6\kappa P_2^2J^2-2\,\omega_0^2[3v_y^2+2\kappa \mathrm{T}_\kappa(4u)\,(\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)\,v_y - \kappa(\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)^2]\left(\frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa(4u)}\right)+\omega_0^4\,\mathrm{T}_\kappa(y)\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(4u)}\right)^3,$$

$$\mathrm{Im}[K_2^{(4)}]=4\,\omega_0[\,v_y^2-\kappa\,(\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)^2\,]\,v_y\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(4u)}\right)-4\,\omega_0^3\,v_y\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(4u)}\right)^3,$$

satisfies the appropriate property

$$\frac{d}{dt}K_2^{(4)}=\left(\frac{4\,\mathrm{i}\,\omega_0}{\mathrm{C}_\kappa^2(4u)\mathrm{C}_\kappa^2(y)}\right)K_2^{(4)}.$$

Hence, the function $\mathbb{K}=K_1\,K_2^{(4)*}$ is a constant of motion for the potential U_{41}. If we write, as in previous cases, $\mathbb{K}=I_4+\mathrm{i}\,I_3$, then the superintegrability is given by $I_3=\mathrm{Im}[\mathbb{K}]$ that is an integral of fourth order in the momenta

$$I_3 = I_{34}+w_0^2\,I_{32}+w_0^4\,I_{30},$$

$$I_{34} = J\,P_2\,(P_2^2-\kappa\,J^2),$$

$$I_{32} = \left(\frac{1}{2}\right)[3\mathrm{S}_k(4u)\,v_y^2-2\mathrm{C}_\kappa(4u)\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_uv_y-\kappa\,\mathrm{S}_k(4u)(\mathrm{C}_\kappa(y)\mathrm{S}_k(y)\,v_u)^2]\left[\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(4u)}\right]^2,$$

$$I_{30}=-\left(\frac{1}{4}\right)\mathrm{S}_k(4u)\left[\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(4u)}\right]^4.$$

Finally, the Euclidean limit is given by

$$\lim_{\kappa\to0}K_2^{(4)}=J_y^4,\quad \lim_{\kappa\to0}I_3=\mathrm{Im}(J_xJ_y^4),$$

$$J_x=v_x+\mathrm{i}\,4\omega_0x,\quad J_y=v_y+\mathrm{i}\,\omega_0y.$$

We summarize the results obtained for $m=3$ and $m=4$ in the following table:

Potential	Triple of constants of motion	Euclidean limit
U_{31}	$P_1^2,\ P_2^2+\kappa\,J^2,\ J\,(3\,P_2^2-\kappa\,J^2)$	$9\,x^2+y^2$
U_{41}	$P_1^2,\ P_2^2+\kappa\,J^2,\ J\,P_2\,(P_2^2-\kappa\,J^2)$	$16\,x^2+y^2$

VI. FINAL COMMENTS AND OUTLOOK

We have discussed the properties of the different κ-dependent coordinate systems and the separability of κ-dependent potentials $U(\kappa)$ on 2-D spaces of constant curvature and then we have studied the superintegrabilty of the κ-dependent harmonic oscillators. We have started with the three quadratic superintegrable systems, U_{11}, U_{21}, and $U_{1/2,1}$ (U_{11} and U_{21} were studied in Refs. 24 and 25) and then we have analyzed the potentials U_{m1} with higher order constants of motion (superintegrable but not superseparable). Some interesting properties to be remarked are: the direct contribution to the energy of the curvature κ and the angular momentum $J(\kappa)$, the relation between the angular momentum $J(\kappa)$ and the two different separabilities in (u,y) and (x,v) ''parallel'' coordinates, the existence of a κ-dependent potential $U_{1/2,1}$ different from U_{21}, and the existence of a complex method for obtaining the superintegrability of the the potentials with nonquadratic constants of motion. Concerning this last point, we have proved by direct calculus

the existence of the complex functions $K_2^{(m)}$ for the values $m=3,4$ (in addition to the previous quadratic cases $m=1,2,\frac{1}{2}$), but it seems natural to assume that this procedure will also remain valid for other more general values of m (integer or half-integer). Hence, a question that remains open is the existence of a general algorithm for the complex factorization of U_{m1} in the general case (in the Euclidean case, discussed in Refs. 25 and 31, the function $K_2^{(m)}$ is just given by the mth power of the function J_y).

We have assumed, as a first step, that most of the fundamental properties of a κ-dependent system are common properties for the three particular cases ($\kappa>0$, $\kappa=0$, and $\kappa<0$). Nevertheless, it will also be convenient to study separately the spherical ($\kappa>0$) and the hyperbolic ($\kappa<0$) cases. As an example, in the spherical case, as S^2 is compact, there is only a small number of oscillators (U_{m1} with m integer or half-integer), but all of them are superintegrable. In the H^2 plane the potentials U_{m1} are well defined functions for arbitrary values of the parameter m. Therefore, the situation in H^2 looks rather similar to that of the Euclidean $\mathbb{E}^2$ plane, since all the oscillators U_{m1} are integrable and only in some particular cases do they become superintegrable. We have initiated in Ref. 32 a study of some properties that must be considered as intrinsically associated to the spherical $\kappa>0$ case.

We have proved that the assumption of considering the spherical and hyperbolic oscillators as κ-deformations of well known Euclidean systems (or conversely, the Euclidean oscillators as very particular cases of general ''curved'' systems) has been a successful idea when it is carried out by introducing formula (1) with the curvature κ as a parameter. Moreover, we think that this general idea and this particular technique can also be applied to other systems; not only to other superintegrable systems (e.g., systems related with the Kepler problem) but to integrable (or just separable) potentials. As an example, the integrability of a κ-dependent nonlinear Hénon–Heiles oscillator can be a matter to be studied from this geometric perspective.

ACKNOWLEDGMENTS

Support of Spanish projects, DGES-PB98-0370, BFM-2000-1066, and FPA-2000-1252 (Madrid), and CO2-399 (Castilla y Leon) is acknowledged.

APPENDIX: GEODESIC PARALLEL COORDINATES

Suppose M is a 2-D Riemannian manifold, O is a point on M and g_1, g_2, are two orthogonal geodesics by O. Let P be an arbitrary point (in some suitable neighborhood of O) and denote by P_1, P_2, the orthogonal projections of P on g_1, g_2. Then we can characterize the point P by

(1) the two distances (u,y) of O to P_1 (measured along g_1) and of P_1 to P (measured along the geodesic by P and P_1), respectively, and
(2) the two distances (x,v) of P_2 to P (measured along the geodesic by P and P_2) and of O to P_2 (measured along g_2), respectively.

In the first case we have the parallel coordinates of P relative to (O,g_1) and in the second case relative to (O,g_2). In the (u,y) system the curves ''$u=$const'' are geodesics and the curves ''$y=$const'' meet these geodesics orthogonally. In the (x,v) system the geodesics are the curves ''$v=$const.'' Notice that in the general case we have $u\neq x$ and $v\neq y$.

In the case of M being a space of costant curvature κ, the (u,y) and (x,v) expressions for the differential element of distance ds^2 are given by[29]

$$ds^2=\mathrm{C}_\kappa^2(y)\,du^2+dy^2 \quad \text{and} \quad ds^2=dx^2+\mathrm{C}_\kappa^2(x)\,dv^2\,, \tag{24}$$

so that in both cases we get $ds^2=dx^2+dy^2$ for the particular $\kappa=0$ Euclidean case. These two systems, although different for $\kappa\neq 0$, can be related by using formulas of spherical and hyperbolic trigonometry for $\kappa>0$ and for $\kappa<0$, respectively. Hence, all the κ-dependent formulas in this article, that have been written in the (u,y) language, can be translated into the (x,v) formalism.

We have made use of the (u,y) notation because it is in this notation in which the potentials U_{m1} are separable and become simpler in contrast with the (x,v) notation that becomes appropriate for the associated $\tilde{U}_{m1}$ potentials.

More concretely (and particularizing for $\kappa=1$ for ease of notation), the two oscillators U_{21} and $U_{1/2,1}$ that are separable in the (u,y) coordinate system, and so have rather simple expressions

$$U_{21}=\tan^2 y+\left(\frac{\tan 2u}{\cos y}\right)^2,$$

$$U_{1/2,1}=\tan^2 y+\left(\frac{\tan u/2}{\cos y}\right)^2,$$

become much more complicated when written in the (x,v) formalism:

$$U_{21}=\frac{1}{1-(\cos x\,\sin v)^2}[\,4A_b^2+(\cos x\,\sin v)^2\,],\quad A_b=\frac{\cos v\,\tan x}{\cos^2 v-\tan^2 x},$$

$$U_{1/2,1}=\frac{1}{1-(\cos x\,\sin v)^2}[\,A_{bb}^2+(\cos x\,\sin v)^2\,],\quad A_{bb}=\frac{\tan x}{\cos v+\sqrt{\cos^2 v+\tan^2 x}}.$$

Conversely, the two oscillators $U_{12}=\tilde{U}_{21}$ and $U_{1,1/2}=\tilde{U}_{1/2,1}$ that are given by

$$U_{12}=\frac{1}{1-(\sin u\,\cos y)^2}[\,(\sin u\,\cos y)^2+4B_b^2\,],\quad B_b=\frac{\cos u\,\tan y}{\cos^2 u-\tan^2 y},$$

$$U_{1,1/2}=\frac{1}{1-(\sin u\,\cos y)^2}[\,(\sin u\,\cos y)^2+B_{bb}^2\,],\quad B_{bb}=\frac{\tan y}{\cos u+\sqrt{\cos^2 u+\tan^2 y}},$$

become

$$U_{12}=\tilde{U}_{21}=\tan^2 x+\left(\frac{\tan 2v}{\cos x}\right)^2,$$

$$U_{1,1/2}=\tilde{U}_{1/2,1}=\tan^2 x+\left(\frac{\tan(v/2)}{\cos x}\right)^2$$

in the (x,v) system. This difference in the form of the potentials, which is clear for U_{21} and $U_{1/2,1}$, becomes much greater for U_{31}, U_{41}, and other more general oscillators.

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Stability of Beltrami flows

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(Received 21 February 2002; accepted 13 February 2003)

Stability of a special class of flows (which we call Beltrami flows) can be analyzed by invoking a constant of motion that bounds the energy of perturbations. This stability condition (a sufficient condition) suppresses any instability including non-exponential (secular) growth due to non-Hermiticity; it also prohibits nonlinear evolution to a large amplitude. The key to prove is the ''coerciveness'' of the constant of motion in the topology of the energy norm. The theory has been applied for an ideal (nondissipative) magnetized plasma. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1567798]

I. INTRODUCTION

Stability of a plasma with a flow constitutes a very challenging problem because the interaction between the perturbations and the ambient flow cannot generally be cast in an appropriate Hamiltonian form. The standard notion of ''energy,'' then, does not pertain and the energy may cease to be the basic determinant of the stability of the flow. The generators of flow dynamics become ''non-Hermitian'' due to the fact the energy (conjugate to ''time'') corresponds to the frequency of perturbations, and the frequency of perturbations in a flow may assume complex values. Consequently the spectral analysis (dispersion relation) of the generator to find ''mode'' frequencies does not lead to a complete understanding of stability because the modes are not necessarily independent; they compose a nonorthogonal set of elements of a Hilbert space. Interactions among different modes may bring about a variety of transient phenomena;[1] the existence of an algebraically growing instability in a system where the entire frequency spectrum is real is an example of the ''pathology'' in the system.

A system is defined to be stable if one can show that a norm of any possible perturbation is bounded. In the most familiar case when an appropriate ''energy'' of the perturbation is a constant of motion, and it consists of well-defined ''kinetic'' and ''potential'' parts, stability is insured for an equilibrium for which the potential energy is a minimum. The linear stability of magnetohydrodynamics (MHD) for a stationary (no flow) equilibrium falls in this category.

The stability argument finds a profound expression in the ''nonlinear stability'' of the so-called Taylor relaxed state[2] derived for ideal incompressible MHD as the minimizer of the magnetic energy for a given magnetic helicity. The ideal dynamics has two constants of motion: the magnetic helicity,[3] and the ''total energy,'' the sum of the magnetic and kinetic (flow) energies (the thermal energy is decoupled because of incompressibility). Any departure from the Taylor relaxed state, therefore, must increase the magnetic energy, resulting in a decrease of the remaining kinetic part of the total energy.

We note that the notion of ''relaxed states'' does not automatically warrant stability. For example the original idea behind Taylor relaxation was the search for a ''minimum energy state'' consistent with the helicity constraint. In this search the approximation of the total energy by magnetic energy happens to be rather fortuitous because the minimum magnetic energy state does

turn out to be demonstrably stable. This happy state does not persist when attempts are made to discover "relaxed states" in plasmas with flows and pressure gradients by the constrained minimization of the total energy including the kinetic and thermal components. If we find a relaxed state with a flow, we must separate the kinetic energies of the ambient flow and perturbations to study the stability; the criterion for stability, then, is the limit of the perturbation energy. Since a perturbation can grow by extracting energy from the ambient flow, the constancy of the total energy does not prevent the excitation of an instability. This process may be regarded as a negative energy perturbation in the flow. It is generally difficult to separate the perturbation energy from that of the ambient field, because their interaction is, often, very complicated. Even when we linearize the evolution equation, the representation of the energy (Hamiltonian) of the linearized dynamics is pathological as remarked above.

In this paper, we study the stability of a special class of states (with flows) that are derivable from variational principles, that is, the states obtained by the constrained minimization of a suitable target functional. For this special class of flows, we will show the existence of a constant of motion that, under some appropriate conditions, bounds the fluctuation energy ("coerciveness" in the topology of the energy norm).

The plan of the paper is to begin by analyzing a simple particular example [vortex dynamics in two dimensional space (Sec. II)] and then arrive at a general abstract theorem (Sec. III) for the stability criterion. Finally we shall apply the general result to study the stability of a relatively more complex physical system (Sec. IV). We consider an ideal magnetized plasma. The variational principle yields a Beltrami field that generalizes the Taylor state (force-free magnetic field) by endowing it with a flow in the direction parallel to the magnetic field, and a finite pressure. We obtain bounds for the flow velocity as well as for the Beltrami parameter—the measure of the shear of both magnetic and flow velocity fields. In Sec. V, we compare the derived stability condition (sufficient condition) with several of the previous results.[4–7]

II. TWO-DIMENSIONAL VORTEX DYNAMICS

A two-dimensional incompressible flow in a bounded domain Ω obeys the vortex dynamics

$$\partial_t W + \{\Phi, W\} = 0, \tag{1}$$

where the stream function Φ defined by $\mathbf{v} = (\partial_y \Phi, -\partial_x \Phi)$ acts as the effective Hamiltonian, W $(= -\Delta\Phi)$ is the flow vorticity, and the Poisson bracket has the standard form

$$\{a,b\} = (\partial_y a)(\partial_x b) - (\partial_x a)(\partial_y b) = -(\nabla a \times \nabla b)\cdot \mathbf{e}_z,$$

with $\mathbf{e}_z = \nabla x \times \nabla y$. The circulation of the flow must be conserved (Kelvin's theorem);

$$\oint_\Gamma \mathbf{n}\cdot\nabla\Phi \, d\gamma = K(\text{given constant}), \tag{2}$$

where $\mathbf{n}$ is the unit normal vector onto the boundary Γ. To confine the flow $\mathbf{v} = \nabla\Phi \times \mathbf{e}_z$ in Ω we demand

$$\Phi|_\Gamma = C(\text{unknown constant}), \tag{3}$$

where $|_\Gamma$ denotes the trace to the boundary value.

The general stationary solution (equilibrium flow) of this dynamics is given by $\{\Phi, W\} = 0$ implying $W = w(\Phi)$ with w being a certain smooth function. For the simplest nontrivial choice (w linear in Φ), the equilibrium condition yields what is called the "Beltrami flow,"

$$-\Delta\Phi (= W) = \mu\Phi \quad (\mu = \text{real constant}). \tag{4}$$

Remark 1: The Beltrami equation (4) with the circulation and boundary conditions (2) and (3) is equivalent to an inhomogeneous equation: writing $\Phi=\varphi+C$ (C is a constant), the transformed problem reads

$$(-\Delta-\mu)\varphi=\mu C,$$

$$\varphi|_\Gamma=0, \quad \oint_\Gamma \mathbf{n}\cdot\nabla\varphi\, d\gamma=K.$$

If μ is the eigenvalue of the Laplacian $-\Delta$ with the Dirichlet boundary condition, a solution may be obtained by demanding $C=0$. Otherwise, the system leads to $\varphi=-\mu(\Delta+\mu)^{-1}C$ with the constant C chosen to yield the prescribed K. We, thus, have a nontrivial solution for every complex number μ; the point spectrum of the Laplacian operator with the inhomogeneous circulation and boundary conditions (2) and (3) spans the totality of complex numbers. In what follows, we assume that μ is a real number (then φ is a real function).

The evolution equation (1), under the circulation and boundary conditions (2) and (3), has two essential integrals (constants of motion):

$$H_0=\|W\|^2\equiv\int_\Omega |W|^2\, dx \quad \text{(enstrophy)}, \tag{5}$$

$$H_1=\|\nabla\Phi\|^2=(W,\mathcal{P}\Phi)\equiv\int_\Omega W\cdot(\mathcal{P}\Phi)\ \ dx \quad \text{(energy)}, \tag{6}$$

where $\mathcal{P}\Phi=\Phi-C$ (C is chosen so that $\mathcal{P}\Phi|_\Gamma=0$) is a projection to homogenize the boundary condition (3). It is straightforward to see that the Beltrami equation (4) is reproduced as the Euler–Lagrange equation of the variational principle

$$\delta(H_0-\mu H_1)=0 \tag{7}$$

with the circulation and boundary conditions (2) and (3).

To study the stability of a Beltrami flow (denote the Hamiltonian by Φ_0), we linearize (1) with writing $\Phi=\Phi_0+\varphi$ and $-\Delta\varphi=\omega$ (the circulation $\int_\Omega\omega\, dx$ must be zero);

$$\partial_t\omega+\{\Phi_0,\omega\}+\{\varphi,-\Delta\Phi_0\}=0. \tag{8}$$

Using the equilibrium (4), we can write

$$\partial_t\omega+\{\Phi_0,\omega-\mu\varphi\}=0. \tag{9}$$

We easily verify that

$$G(\varphi)=(\omega,\omega-\mu\mathcal{P}\varphi)=\|\omega\|^2-\mu\|\nabla\varphi\|^2 \tag{10}$$

is a constant of motion [$dG(\varphi)/dt=0$] associated with the linearized dynamics (9). In a bounded domain, we have the inequality

$$\|-\Delta\varphi\|^2\geqslant\lambda\|\nabla\varphi\|^2 \tag{11}$$

with λ being the smallest eigenvalue of the Laplacian $-\Delta$ with the Dirichlet boundary condition (one easily finds $\lambda>0$). We, thus, have

$$G(\varphi)\geqslant\left(1-\frac{\mu}{\lambda}\right)\|-\Delta\varphi\|^2, \tag{12}$$

or

$$(\lambda-\mu)\|\nabla\varphi\|^2\leqslant G(\varphi) \tag{13}$$

implying that the energy $\|\nabla\varphi\|^2$ remains bounded for $\mu<\lambda$, because $G(\varphi)$ is a constant determined by the initial condition of the perturbation φ; the bound $\mu<\lambda$ on the Beltrami parameter gives a sufficient condition for the stability of the Beltrami flow.

We can generalize this argument to a variety of second-order nonlinear systems. We first cast the method in an abstract theorem.

III. VARIATIONAL PRINCIPLE AND CONSTANT OF MOTION

Let $f(a,b)$ be a bilinear map. We define $\mathcal{F}(u)=f(u,u)$, and consider an abstract nonlinear evolution equation

$$\partial_t u=\mathcal{F}(u). \tag{14}$$

We further suppose that there are symmetric bilinear forms $h_j(a,b)$ $(j=1,\ldots,\nu)$ such that

$$h_j(u,\mathcal{F}(u))=0 \quad (j=1,\ldots,\nu,\ \forall u). \tag{15}$$

It is now easy to show that $H_j(u)=h_j(u,u)$ [u is a solution of (14)] is a constant of motion for the evolution equation (14);

$$\frac{d}{dt}H_j(u)=2h_j(u,\partial_t u)=2h_j(u,\mathcal{F}(u))=0. \tag{16}$$

Let u_0 be a stationary point (equilibrium) of (14), i.e., $\mathcal{F}(u_0)=0$. We assume that u_0 solves

$$\delta\left[\sum_{j=1}^{\nu}\mu_j H_j(u)\right]=0 \tag{17}$$

with some fixed real numbers μ_j $(j=1,\ldots,\nu)$; cf. (7). We call such a u_0 as a ''Beltrami field.''

Remark 2: If (17) has a unique (or isolated) solution u_0, then this u_0 is an equilibrium of (14). Indeed, any departure from u_0 will change the value of $G(u)\equiv\Sigma_{j=1}^{\nu}\mu_j H_j(u)$, while $G(u)$ is a constant of motion.

To study the perturbations around u_0, the following theorem plays an essential role.

Theorem 1: *Suppose that $u=u_0+\tilde{u}$ (u_0 is a Beltrami field) satisfies either (14) or its "linearized" equation*

$$\partial_t\tilde{u}=f(u_0,\tilde{u})+f(\tilde{u},u_0). \tag{18}$$

Then,

$$G(\tilde{u})=\sum_{j=1}^{\nu}\mu_j H_j(\tilde{u}) \tag{19}$$

is a constant of motion.

Proof: Using (15), we observe

$$\begin{aligned}0&=\sum\ \mu_j h_j(u,\mathcal{F}(u))\\&=\sum\ \mu_j h_j(u_0+\tilde{u},\mathcal{F}(u_0+\tilde{u}))\\&=\sum\ \mu_j h_j(u_0,\mathcal{F}(u_0+\tilde{u}))+\sum\ \mu_j h_j(\tilde{u},\mathcal{F}(u_0+\tilde{u})).\end{aligned} \tag{20}$$

Since (17) implies $\Sigma \mu_j h_j(u_0,\delta)=0$ $(\forall \delta)$, the first sum in (20) vanishes. Hence, if u solves (14), we obtain

$$\frac{d}{dt}G(\tilde{u})=2\sum \mu_j h_j(\tilde{u},\partial_t\tilde{u})=2\sum \mu_j h_j(\tilde{u},\mathcal{F}(u_0+\tilde{u}))=0. \tag{21}$$

We can rewrite (20) as

$$0=\sum \mu_j h_j(\tilde{u},f(u_0,\tilde{u})+f(\tilde{u},u_0))+\sum \mu_j h_j(\tilde{u},\mathcal{F}(\tilde{u})). \tag{22}$$

By (15), the second term of (22) vanishes. If $\tilde{u}$ is a solution of (18), we obtain

$$\frac{d}{dt}G(\tilde{u})=2\sum \mu_j h_j(\tilde{u},f(u_0,\tilde{u})+f(\tilde{u},u_0))=0. \tag{23}$$

□

We note that although each functional H_j occurring in the sum that defines G is a constant of motion for the total field u, it is only the special linear combination (19) that is conserved for the perturbation, $\tilde{u}$. The coefficients μ_j included in G are the structure (Beltrami) parameters characterizing the equilibrium.

If a continuous quadratic form $F(v)$ satisfies (on a Hilbert space V)

$$F(v)\geqslant c\|v\|^2 \quad (\forall v\in V) \tag{24}$$

with some positive constant c ($\|v\|$ is the norm of v in V), $F(v)$ is said to be "coercive." The functional G of (12) for $\mu<\lambda$ is an example of a coercive form (we consider G as a continuous form in the topology of H^2 Sobolev space).

Obviously, we have the following Proposition.

Proposition 1: If $G(v)=\Sigma_{j=1}^{\nu}\mu_j H_j(v)$ *with given* μ_j *is a coercive form, then*

(1) $G(u)$ *has a unique "minimizer" that is given by the variational principle (17),*
(2) the minimizer u_0 *of* $G(u)$ *is a stationary point (equilibrium) of (14),*
(3) the minimizer u_0 *is "stable"; the norm of every perturbation* $\tilde{u}$ *is bounded by a constant that depends upon* $G(\tilde{u}|_{t=0})$.

IV. STABILITY OF MHD FLOW

We shall now put to work the general mathematical framework developed in the last section. We will apply Theorem 1 and Proposition 1 to investigate the stability of a three-dimensional plasma equilibrium with a flow. Let Ω be a bounded three-dimensional domain with a smooth boundary Γ. We assume that Ω is multiply connected with cuts Σ_ℓ $[\ell=1,\ldots,m$ (the first Betti number)], i.e., $\Omega\backslash\cup(\Sigma_\ell)$ is simply connected.

Remark 3: In a multiply connected domain $\Omega(\subset\mathbf{R}^3)$, the curl operator has a point spectrum that covers the entire complex plane.[8] This is because of the existence of a nonzero harmonic field ($\nabla\times\mathbf{h}=0$, $\nabla\cdot\mathbf{h}=0$ in Ω, and $\mathbf{n}\cdot\mathbf{h}=0$ on Γ), which plays the role of an inhomogeneous term in the eigenvalue problem

$$\nabla\times\mathbf{u}=\lambda\mathbf{u}.$$

We decompose the solenoidal field $\mathbf{u}$ into the harmonic component $\mathbf{h}$ and its orthogonal complement $\mathbf{u}_\Sigma$. We can show that the latter component is a member of the Hilbert space

$$L^2_\Sigma(\Omega)=\{\nabla\times\mathbf{a}\in L^2(\Omega);\ \ \mathbf{n}\times\mathbf{a}=0 \ \text{ on } \Gamma\}.$$

The eigenvalue problem now reads as

$$\nabla\times\mathbf{u}_\Sigma=\lambda(\mathbf{u}_\Sigma+\mathbf{h}).$$

If we take $\mathbf{h}=0$, we find a nontrivial solution only for $\lambda_j\in\sigma_p$, where σ_p is a countably infinite set of real numbers. The set σ_p constitutes the point spectrum of the self-adjoint curl operator that is defined in the Hilbert space $L^2_\Sigma(\Omega)$. For $\lambda'\notin\sigma_p$, we must invoke $\mathbf{h}\neq 0$ and find a solution $\mathbf{u}_\Sigma=(\mathrm{curl}-\lambda')^{-1}\lambda'\mathbf{h}$, where curl denotes the self-adjoint curl operator.[8] When the domain Ω is multiply connected, therefore, we can assume that the Beltrami parameters μ_j [to appear in (33)] are arbitrary real (and even complex) numbers; see (32). This fact is in analogy with the previous example (4); see *Remark 1*.

Ideal MHD description of a plasma is contained in the force equation

$$\partial_t\mathbf{v}+(\mathbf{v}\cdot\nabla)\mathbf{v}-(\nabla\times\mathbf{B})\times\mathbf{B}+\nabla p=0, \tag{25}$$

and the induction equation

$$\partial_t\mathbf{B}-\nabla\times(\mathbf{v}\times\mathbf{B})=0, \tag{26}$$

where $\mathbf{B}$ is the magnetic field, $\mathbf{v}$ is the incompressible flow velocity, and p is the pressure. We have normalized $\mathbf{B}$ by its representative value B^*, $\mathbf{v}$ by the Alfvén speed $c_A=B^*/\sqrt{\mu_0\rho}$ (ion mass density ρ is assumed to be a constant), p by B^{*2}/μ_0, and t by the Alfvén transit time ℓ/c_A. The length scale ℓ is arbitrary. We assume boundary conditions

$$\mathbf{n}\cdot\mathbf{v}=0,\quad \mathbf{n}\cdot\mathbf{B}=0\ \text{ on }\ \Gamma \tag{27}$$

and flux conditions

$$\int_{\Sigma_\ell}\mathbf{n}\cdot\mathbf{B}\,ds=K_\ell\quad(\ell=1,\ldots,m), \tag{28}$$

where the fluxes through the cuts are given constants. The dynamics allows three important constants of motion,

$$H_0=\|\mathbf{v}\|^2+\|\mathbf{B}\|^2\quad(\text{energy}), \tag{29}$$

$$H_1=(\mathbf{A},\mathbf{B})\quad(\text{magnetic helicity}), \tag{30}$$

$$H_2=2(\mathbf{v},\mathbf{B})\quad(\text{cross helicity}), \tag{31}$$

where $\mathbf{A}$ is the vector potential.

The variational principle

$$\delta(H_0-\mu_1H_1-\mu_2H_2)=0 \tag{32}$$

gives Beltrami fields defined by

$$(1-\mu_2^2)\nabla\times\mathbf{B}=\mu_1\mathbf{B}, \tag{33}$$

$$\mathbf{v}=\mu_2\mathbf{B}. \tag{34}$$

Remark 4: In standard literature, a solenoidal vector field obeying $\nabla\times\mathbf{u}=\alpha\mathbf{u}$ (with some scalar function α) is called a Beltrami field. For constant α, it is sometimes called a Trkal field. A ''force-free'' magnetic field satisfying $\nabla\times\mathbf{B}=\alpha\mathbf{B}$ with a constant α is the Taylor relaxed state, and is derived by a variational principle by minimizing the magnetic energy $H_m=\|\mathbf{B}\|^2$ subject to the constraint of constant magnetic helicity H_1.[2] The notion of ''relaxation'' assumes the selective dissipation of H_m with respect to the rugged invariant H_1 in a weakly dissipative turbulent plasma—the minimizer of H_m for a given (conserved) H_1 is the Taylor relaxed state. This model

is "unaware" of the flow velocity (that may, indeed, be small in some laboratory plasmas). Replacing H_m by H_0 in the variational principle, however, one obtains $\mathbf{v}=0$ in the relaxed state. It is through the constraint on the "cross helicity" H_2 that the relaxed states may acquire a finite flow. The extended variational principle (32) yields a Beltrami field that generalizes the Taylor state (force-free stationary equilibrium) imparting it with a field aligned flow $\mathbf{v}$ whose magnitude is scaled by μ_2 and a finite pressure ($p+v^2/2=$constant; a generalized Bernoulli law). The conditions for the variational principle to give a "minimizer" is related to the stability of the predicted state; see the Appendix.

Due to Theorem 1, the integral

$$G(\tilde{\mathbf{B}},\tilde{\mathbf{v}})=\|\tilde{\mathbf{v}}\|^2+\|\tilde{\mathbf{B}}\|^2-\mu_1(\tilde{\mathbf{A}},\tilde{\mathbf{B}})-2\mu_2(\tilde{\mathbf{v}},\tilde{\mathbf{B}}) \tag{35}$$

is a constant of motion for the perturbations $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{v}}$ satisfying the nonlinear equations (25) and (26), or their linearized equations. The flux condition (28) demands $\tilde{\mathbf{B}}\in L^2_\Sigma(\Omega)$.

We now prove the inequality

$$(\tilde{\mathbf{A}},\tilde{\mathbf{B}})\leqslant|\lambda|^{-1}\|\tilde{\mathbf{B}}\|^2, \tag{36}$$

where $|\lambda|=\min_j|\lambda_j|$ [λ_j ($j=1,2,\ldots$) are the eigenvalues of the self-adjoint curl operator]. Invoking the spectral resolution theorem due to Yoshida–Giga,[8] we expand $\mathbf{u}=\Sigma(\mathbf{u},\boldsymbol{\psi}_j)\boldsymbol{\psi}_j$ ($\forall\mathbf{u}\in L^2_\Sigma(\Omega)$), where $\boldsymbol{\psi}_j$ is the eigenfunction of the self-adjoint curl operator belonging to an eigenvalue λ_j, and write

$$\tilde{\mathbf{B}}=\sum\ (\tilde{\mathbf{B}},\boldsymbol{\psi}_j)\boldsymbol{\psi}_j$$

and

$$\mathcal{P}\tilde{\mathbf{A}}=\sum\ (\tilde{\mathbf{B}},\boldsymbol{\psi}_j)\boldsymbol{\psi}_j/\lambda_j,$$

where $\mathcal{P}$ is the orthogonal projection in $L^2(\Omega)$ onto $L^2_\Sigma(\Omega)$. We observe

$$\begin{aligned}(\tilde{\mathbf{A}},\tilde{\mathbf{B}})&=(\mathcal{P}\tilde{\mathbf{A}},\tilde{\mathbf{B}})\\&\leqslant\|\mathcal{P}\tilde{\mathbf{A}}\|\cdot\|\tilde{\mathbf{B}}\|=\left[\sum\ (\tilde{\mathbf{B}},\boldsymbol{\psi}_j)^2/\lambda_j^2\right]^{-1/2}\left[\sum\ (\tilde{\mathbf{B}},\boldsymbol{\psi}_j)^2\right]^{-1/2}\\&\leqslant|\lambda|^{-1}\sum\ (\tilde{\mathbf{B}},\boldsymbol{\psi}_j)^2\\&=|\lambda|^{-1}\|\tilde{\mathbf{B}}\|^2.\end{aligned}$$

Using

$$2(\tilde{\mathbf{v}},\tilde{\mathbf{B}})\leqslant\alpha\|\tilde{\mathbf{v}}\|^2+\alpha^{-1}\|\tilde{\mathbf{B}}\|^2\quad(\forall\alpha>0),$$

we obtain

$$G(\tilde{\mathbf{B}},\tilde{\mathbf{v}})\geqslant(1-\alpha|\mu_2|)\|\tilde{\mathbf{v}}\|^2+\left(1-\frac{|\mu_2|}{\alpha}-\frac{|\mu_1|}{|\lambda|}\right)\|\tilde{\mathbf{B}}\|^2. \tag{37}$$

The choices $\alpha=1/|\mu_2|$, and $\alpha=|\mu_2|/(1-|\mu_1|/|\lambda|)$ convert (37) to

$$G(\tilde{\mathbf{B}},\tilde{\mathbf{v}})\geqslant\left(1-\mu_2^2-\frac{|\mu_1|}{|\lambda|}\right)\|\tilde{\mathbf{B}}\|^2 \tag{38}$$

and

$$G(\tilde{\mathbf{B}},\tilde{\mathbf{v}}) \geqslant \left(1-\frac{\mu_2^2}{1-|\mu_1|/|\lambda|}\right)\|\tilde{\mathbf{v}}\|^2, \tag{39}$$

respectively. If $1-\mu_2^2-|\mu_1|/|\lambda|>0$, then (38) and (39) give bounds for the energy associated with the magnetic ($\tilde{\mathbf{B}}$) as well as the velocity ($\tilde{\mathbf{v}}$) fluctuations.

The ''sufficient condition'' for the stability, therefore, consists of the simultaneous inequalities

$$\mu_2^2<1, \tag{40}$$

$$\sigma \equiv \frac{|\mu_1|}{1-\mu_2^2} <|\lambda|, \tag{41}$$

where σ stands for the eigenvalue of the Beltrami equation (33) for $\mu_1>0$. The first stability condition requires that the flow velocity must not exceed the local Alfvén speed [see (34)], while the second condition demands that σ must not exceed the minimum of $|\lambda_j|$ (λ_j is the eigenvalue of the self-adjoint curl operator).

V. DISCUSSIONS

Combining a constant of motion and a coerciveness relation, we have derived a bound for the energy of perturbations yielding a sufficient condition for stability. The constant of motion (Theorem 1) is closely related to the variational principle characterizing the Beltrami equilibrium. Under appropriate boundary conditions, coerciveness is measured by the highest order of derivatives included in the functional, which is a consequence of a Poincaré-type inequality [the constant c in (24) is determined by the size of the domain]. In the inequalities (11) and (36), the constants are related to the eigenvalues of the self-adjoint operators assuming sufficiently smooth functions. These eigenvalues are compared with the Beltrami parameters to determine the stability.

The method developed here differs from the standard argument for stability based on the second variation of the target functional (constant of motion).[9,10] If an equilibrium is defined by a variational principle (first variation$=0$), the stability of the stationary point may be examined by analyzing the spectrum of the ''Hessian'' of the target functional on a function space. In general, this problem is highly nontrivial because the linearized operator describing the dynamics of perturbations may be non-Hermitian (see Sec. I). When the target functional of the variational principle is a symmetric quadratic form, however, the second variation yields a symmetric Hessian. This is an essential characteristic of the ''Beltrami'' class of equilibria, and it greatly simplifies the stability analysis. Our method does not invoke the second variation. Instead, we have found a constant of motion that is naturally deduced from the variational principle characterizing the stationary point. The success of this method is also primarily due to the assumption that the target functional ($G=$linear combination of constants of motion) is a symmetric quadratic form. The key of the stability theory is, then, the coerciveness of the constant of motion; it allows us to put a bound on the perturbation norm. The constant of motion of a perturbation is formally equivalent to the target functional G of the variational principle that determines the stationary point (Theorem 1). The coerciveness demands that the G is a convex form, and hence, the coerciveness condition may be related to the index of the Hessian. The former is, however, a more fundamental notion that is directly related to the ''topology'' of the function space. In the Appendix, we examine the relation between the coerciveness and the index of the Hessian.

The constant of motion may be regarded as a ''Lyapunov function.'' Tasso[5] developed a similar scheme for a dissipative system where the corresponding Lyapunov function may decay implying the damping of perturbations; see also Ref. 11. Following his idea, we can extend the stability regime by taking into account the resistive and viscous damping of energy. The key, again, is the ''coerciveness'' relation. We can apply (36) and similar inequalities to quantify the bound in terms of the eigenvalue of the self-adjoint curl operator.

If we consider only exponential instabilities (replacing ∂_t by $-i\omega$ and studying the dispersion relations), we can develop a more detailed analysis for special geometries. For example, in a 1D slab, the necessary and sufficient condition for stability against exponential growth is that either (40) or (41) is satisfied (not "and").[12] In this system the magnetic field curvature that may destabilize the Alfvén waves (kink modes) is absent, and only possible instabilities are of the Kelvin–Helmholtz type. Without the magnetic field, the well-known stability criterion for the Kelvin–Helmholtz mode is precisely our condition (41). The magnetic field, in this case, has a stabilizing effect (because of the absence of the kink modes), and hence, the stability condition (41) applies for any magnitude (μ_2) of the magnetic field. Moreover, the stabilization effect of the sheared magnetic field[7] can suppress the Kelvin–Helmholtz instability if the flow velocity is sufficiently small, i.e., the condition (40) is satisfied. We also remark that the stability region given by (40) is consistent to that predicted by assuming exponential growth and examining the quadratic integrals of the vortex dynamics equation.[4] Detailed analysis of the necessary and sufficient conditions for purely exponential instabilities will be discussed elsewhere.

ACKNOWLEDGMENTS

The work of Z.Y. was supported by Toray Science Foundation and of S.O. by Research Fellowships of the Japan Society for the Promotion of Science (JSPS) for Young Scientists. The work of S.M.M. was supported by The US Department of Energy Contract No. DE-FG03-96ER-54366.

APPENDIX: EIGENFUNCTION EXPANSION OF THE TARGET FUNCTIONAL

The relation between the coerciveness and the second variation of a functional can be clarified by resorting to an appropriate eigenfunction expansion. A detailed demonstration of this relationship will be worked out for MHD flows (Sec. IV).

We consider the target functional [see (29)–(32)]

$$G(\mathbf{B},\mathbf{v}) = H_0 - \mu_1 H_1 - \mu_2 H_2 = \|\mathbf{v}\|^2 + \|\mathbf{B}\|^2 - \mu_1(\mathbf{A},\mathbf{B}) - 2\mu_2(\mathbf{v},\mathbf{B}).$$

The simplest representation of the functional G and its Hessian operator (second variation of G) may be obtained in terms of the eigenfunction of the self-adjoint curl operator.[8] The complete orthogonal set $\boldsymbol{\psi}_j$ ($\nabla\times\boldsymbol{\psi}_j=\lambda_j\boldsymbol{\psi}_j$) spanning $L^2_\Sigma(\Omega)$ allows

$$\mathbf{B} = \sum_j b_j \boldsymbol{\psi}_j + \mathbf{B}_h,$$

$$\mathbf{v} = \sum_j v_j \boldsymbol{\psi}_j + \mathbf{v}_h,$$

where $\mathbf{B}_h$ and $\mathbf{v}_h$ are harmonic fields (see Remark 3). The flux condition (28) determines $\mathbf{B}_h$, while $\mathbf{v}_h$ is an unknown variable. Defining $\mathbf{B}-\mathbf{B}_h=\nabla\times\mathbf{A}_\sigma$ ($\mathbf{n}\times\mathbf{A}_\sigma=0$ on Γ) and $\mathbf{A}_g=\mathbf{A}-\mathbf{A}_\sigma$, we may write $\mathbf{B}_h=\nabla\times\mathbf{A}_g$. Using the definition

$$\Lambda_j = (\boldsymbol{\psi}_j, \mathbf{A}_g) \quad \text{(given constants)},$$

along with the other expansions, we obtain

$$H_0 = \|\mathbf{v}\|^2 + \|\mathbf{B}\|^2 = \sum_j (b_j^2 + v_j^2) + \|\mathbf{B}_h\|^2 + \|\mathbf{v}_h\|^2,$$

$$H_1 = (\mathbf{A},\mathbf{B}) = \sum_j (\lambda_j^{-1} b_j^2 + 2 b_j \Lambda_j) + (\mathbf{A}_g, \mathbf{B}_h),$$

$$H_2 = 2(\mathbf{v},\mathbf{B}) = 2\sum_j v_j b_j + 2(\mathbf{v}_h, \mathbf{B}_h),$$

and

$$G(\mathbf{B},\mathbf{v})=\sum_j\ (b_j^2+v_j^2-\mu_1\lambda_j^{-1}b_j^2-2\mu_1 b_j\Lambda_j-2\mu_2 b_j v_j)$$
$$+\|\mathbf{B}_h\|^2+\|\mathbf{v}_h\|^2-2\mu_2(\mathbf{B}_h,\mathbf{v}_h)-\mu_1(\mathbf{A}_g,\mathbf{B}_h).$$

We can now calculate the variations explicitly. The first variation (under $\delta\mathbf{A}_g=0$; gauge invariance)

$$\delta G=\sum_j\ [2(b_j-\mu_1\lambda_j^{-1}b_j-\mu_2 v_j-\mu_1\Lambda_j)\,\delta b_j+2(v_j-\mu_2 b_j)\,\delta v_j]+2(\mathbf{v}_h-\mu_2\mathbf{B}_h)\cdot\delta\mathbf{v}_h$$

determines the stationary point (equilibrium);

$$\mathbf{v}_{0h}=\mu_2\mathbf{B}_h,\quad v_{0j}=\mu_2 b_{0j},$$

$$b_{0j}=\frac{\mu_1\Lambda_j}{(1-\mu_2^2-\mu_1\lambda_j^{-1})},$$

where $\mathbf{B}_h$ and Λ_j are given constants.

Denoting

$$v_j=v_{0j}+\tilde{v}_j,\quad b_j=b_{0j}+\tilde{b}_j,$$

and defining the linear-transformed variables

$$\tilde{c}_j=\tilde{v}_j-\mu_2\tilde{b}_j,$$

we obtain

$$G=\sum_j\ (\tilde{b}_j^2+\tilde{v}_j^2-\mu_1\lambda_j^{-1}\tilde{b}_j^2-2\mu_2\tilde{b}_j\tilde{v}_j)+\|\tilde{\mathbf{v}}_h\|^2+G_0$$

$$=\sum_j\ [\tilde{c}_j^2+(1-\mu_2^2-\mu_1\lambda_j^{-1})\tilde{b}_j^2]+\|\tilde{\mathbf{v}}_h\|^2+G_0,$$

where

$$G_0=(1-\mu_2^2)\|\mathbf{B}_h\|^2-\mu_1(\mathbf{A}_g,\mathbf{B}_h)$$

is the minimum value of G. This expression of G gives the ''diagonalized'' Hessian evaluated at the stationary point. Let us write $\tilde{\mathbf{v}}_h=\tilde{v}_h\mathbf{h}$ ($\mathbf{h}$ is the normalized harmonic field) and define $\tilde{c}_h=\tilde{v}_h$ (the harmonic magnetic field $\mathbf{B}_h$ is fixed by the flux condition). The independent degrees of freedom associated with perturbations may be represented by an infinite dimension vector

$$\tilde{\mathbf{u}}=(\tilde{c}_h,\tilde{c}_1,\tilde{c}_2,\ldots,\tilde{b}_1,\tilde{b}_2,\ldots),$$

which lets us cast G in the canonical form

$$G=\tilde{\mathbf{u}}\mathcal{D}\tilde{\mathbf{u}}^T+G_0$$

with the diagonalized Hessian

$$\mathcal{D}_{j,k}=\begin{cases}\delta_{j,k} & \text{acting on } \tilde{c}_h,\tilde{c}_1,\tilde{c}_2,\dots,\\ (1-\mu_2^2-\mu_1\lambda_j^{-1})\,\delta_{j,k} & \text{acting on } \tilde{b}_1,\tilde{b}_2,\dots.\end{cases} \tag{A1}$$

The stationary point is stable if the index of the Hessian (the number of the negative eigenvalues of $\mathcal{D}$) is zero. The sufficient conditions for stability can be directly read off from (A1), and are

$$\mu_2^2<1 \tag{A2}$$

and

$$\begin{cases}\dfrac{\mu_1}{1-\mu_2^2}<\lambda_+ & \text{if } \mu_1>0,\\[2ex] \dfrac{|\mu_1|}{1-\mu_2^2}<|\lambda_-| & \text{if } \mu_1<0,\end{cases} \tag{A3}$$

with $\lambda_+=\min_{\lambda_j>0}\lambda_j$ and $\lambda_-=\max_{\lambda_j<0}\lambda_j$ [hence, $|\lambda|=\min(\lambda_+,|\lambda_-|)$]. Comparing (A2) and (A3) with (40) and (41), we find a slight improvement of the stability bound. This is due to the exact evaluation of the Hessian.

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Anomalous diffusion: Fractional Fokker–Planck equation and its solutions

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(Received 19 November 2002; accepted 23 January 2003)

We analyze a linear fractional Fokker–Planck equation for the case of an external force $F(x) \propto x|x|^{\alpha-1}$ and diffusion coefficient $D(x) \propto |x|^{-\theta}$ $(\alpha, \theta \in \mathcal{R})$. We also discuss the connection of the solutions found here with the Fox functions and the nonextensive statistics based on the Tsallis entropy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1566452]

I. INTRODUCTION

Anomalous diffusion is one of the most ubiquitous phenomena in nature.[1] It is present in a wide variety of physical situations. For instance, surface growth, transport of fluid in porous media,[2] two-dimensional rotating flow,[3] diffusion at liquid surfaces,[4] diffusion of plasma,[5] subrecoil laser cooling,[6] or even in multidisciplinary areas such as in analyzing the behavior of CTAB micelles dissolved in salted water[7] or econophysics.[8]

In a normal diffusion the second moment is given by $\langle x^2 \rangle \propto t$. On the other hand, when the second moment is finite and the diffusion is anomalous, we can have a correlated anomalous diffusion.[9] In general, this class of anomalous diffusive process is characterized by the power law pattern $\langle x^2 \rangle \propto t^{\alpha}$, where $\alpha > 1$ represents superdiffusion while $0 < \alpha < 1$ represents subdiffusion. Lévy anomalous diffusion,[10] in contrast to the correlated diffusion, does not have the second moment defined, i.e., $\langle x^2 \rangle$ diverges. Due to the broadness of the problems involving anomalous diffusion, one needs to apply different kinds of theoretical approaches such as nonlinear Fokker–Planck equation (or modified porous media equation),[11,12] fractional Fokker–Planck equation,[13] Fokker–Planck equation with spatial dependent diffusion coefficient, and generalized Langevin equations.

The fractional approach has been employed in a rich variety of scenarios such as continuous time random walk models,[13] generalized Langevin equations, or the generalized master equation. In particular, it can be used to model a great number of physical and biological systems. For instance, it can be used to describe relaxation to equilibrium in systems (such as polymers chains and membranes) with long temporal memory,[14] anomalous transport in disordered systems,[15] and to model non-Markovian dynamical processes in protein folding.[16] The advantage of the fractional model basically lies in the straightforward way of including external force terms and of calculating boundary value problems.

To investigate anomalous diffusion in a broad context, in general, is desirable since one can interpolate different models in a single scheme. In this direction, it would be useful to study a fractional (spatial and temporal) Fokker–Planck equation with a diffusion coefficient $D(x) \propto |x|^{-\theta}$. An equation of this type interpolates time and spatial (Lévy) fractional Fokker–Planck equation with diffusion on fractal medium in the sense of O'Shaughnessy and Procaccia

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($\theta \neq 0$).[17] A further ingredient to be incorporated in this equation is an external force (drift term). In this direction, the present work focuses attention on the discussion of

$$\frac{\partial}{\partial t}\rho(x,t) = {}_0D_t^{1-\gamma}\left\{\mathcal{D}\frac{\partial}{\partial |x|}\left[\ |x|^{-\theta}\frac{\partial^{\mu}}{\partial |x|^{\mu}}\rho(x,t)\right] - \frac{\partial}{\partial x}[F(x)\rho(x,t)]\right\}, \tag{1}$$

where $\gamma, \mu, \theta \in \mathcal{R}$, $F(x) \equiv -\mathrm{d}V(x)/\mathrm{d}x$ is a dimensionless external force associated with the potential $V(x)$, ${}_0D_t^{1-\gamma}$ is the fractional Riemann–Liouville derivative,[18] and $\partial^{\mu}/\partial|x|^{\mu}$ is also the fractional derivative. In particular, depending on the case we consider the fractional spatial derivative in the Riemann–Liouville approach[18] or in the Reiz approach.[13] For $(\gamma, \mu, \theta) = (1,1,0)$, Eq. (1) recovers the usual Fokker–Planck equation. Note that Eq. (1) is an integro-differential equation, and different from the diffusion wave equation[19] it is not necessary to use extra boundary conditions for $\gamma > 1$. It can be verified that $\int_{-\infty}^{\infty} \mathrm{d}x\ \ \rho(x,t)$ is time independent (hence, if ρ is normalized at $t=0$, it will remain so forever). Indeed, if we write the equation in the form $\partial_t \rho = \partial_x \mathcal{J}$ and assume the boundary conditions $\mathcal{J}(\pm\infty, t) \to 0$, it can be shown that $\int_{-\infty}^{\infty} \mathrm{d}x\ \ \rho(x,t)$ is a constant of motion.

In this work, we intend to investigate Eq. (1) by considering the external force $F(x) \propto x|x|^{\alpha-1}$. For this kind of external force one can obtain a new class of exact solutions in several intervals of the parameters θ, γ, and μ. Note that the external force can have short- or long-range behavior depending on the value of α. In addition, to perform our analysis we consider the boundary condition $\rho(x \to \pm\infty, t) \to 0$. By taking into account this requirement we employ, in particular, the initial condition $\rho(x,0) = \delta(x - x_0)$. We start by considering the case characterized by an arbitrary θ and $\mu = 1$ with $\alpha + \theta + 1 = 0$. In this case, the Rayleigh process[20] is included. Further, we investigate the case $\theta = 0$, $\alpha = 1$ and γ, μ arbitraries. In this last case, we have a mixing between the anomalous diffusion type correlated generated by the fractional derivative in time and Levy flights obtained with the spatial fractional derivative. We also investigate Eq. (1) by taking into account the parameters θ and μ for the following regions: (i) $\theta = 1$ and $-2 < \mu < 0$, (ii) $\theta = -1 - 2\mu$ with $-1 < \mu < 0$, and (iii) $\theta < 0$ for $\mu = -1$ by considering a linear drift ($\alpha = 1$). The remainder of this paper goes as follows. In Sec. II, we obtain the exact solutions for the previous cases. In Sec. III, we present our conclusion, giving a discussion about our results.

Thus, the results that emerge from Eq. (1) with the previous external force extend several cases present in the literature, such as that one obtained in Ref. 17, to discuss diffusion on fractals, for $\theta \neq 0$ and $(\mu, \gamma) = (1,1)$ without external force. The case $(\gamma, \mu) = (1,1)$, $\alpha = -2$ and $\theta = -3$ that has been applied to the fast electrons in a hot plasma in the presence of a dc electric field,[21] turbulent two particle diffusion in configuration space for $(\alpha, \theta) = (1/3, 1/3)$,[22] and the case $\theta \neq 0$ and $\gamma \neq 0$ that was addressed in Ref. 23 when the external force is absent.

II. FRACTIONAL FOKKER–PLANCK EQUATION

Let us start to analyze Eq. (1) with $\mu = 1$ and $\theta = 0$ in the presence of a drift force given by $F(x) = 2\mathcal{K}/x$, i.e., we consider $V(x) = -2\mathcal{K}\ln|x|$. In this case, applying the Laplace transform in Eq. (1), we obtain

$$s\rho(x,s) - \rho(x,0) = s^{1-\gamma}\left\{\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,s) - 2\mathcal{K}\frac{\partial}{\partial x}\left[\frac{1}{x}\ \ \rho(x,s)\right]\right\}, \tag{2}$$

where the initial condition $\rho(x,0) = \tilde{\rho}(x)$ and $\gamma > 0$ was used. This equation can be solved by the Green function method.[24] By substituting

$$\rho(x,s) = \int \mathrm{d}y \mathcal{G}(|x-y|, s)\tilde{\rho}(y) \tag{3}$$

into Eq. (2) what after some calculations gives

$$\mathcal{G}(x,s)=\frac{s^{\gamma(3/4+(1/2)(\mathcal{K}/\mathcal{D}))-1}}{\mathcal{D}^{1/2}\Gamma\left(\frac{\mathcal{K}}{\mathcal{D}}+\frac{1}{2}\right)}\left(\frac{x^2}{4\mathcal{D}}\right)^{1/4+\mathcal{K}/2\mathcal{D}}K_{\mathcal{K}/\mathcal{D}-1/2}\left(\frac{s^{\gamma/2}|x|}{\sqrt{\mathcal{D}}}\right),\tag{4}$$

where $K_n(x)$ is a modified Bessel function of third kind. Applying the inverse of Laplace transform we have that

$$\mathcal{G}(x,t)=\frac{1}{\Gamma\left(\frac{\mathcal{K}}{\mathcal{D}}+\frac{1}{2}\right)}\left(\frac{1}{4\mathcal{D}t^{\gamma}}\right)^{1/2}\mathrm{H}_{1\ 2}^{2\ 0}\left[\frac{x^2}{4\mathcal{D}t^{\gamma}}\middle|\begin{matrix}(1-\gamma/2,\gamma)\\ (1/2,1),\ (\mathcal{K}/\mathcal{D},1)\end{matrix}\right],\tag{5}$$

where

$$\mathrm{H}_{p\ q}^{m\ n}\left[x\middle|\begin{matrix}(a_1,A_1),(a_2,A_2),\ldots,(a_p,A_p)\\ (b_1,B_1),(b_2,B_2),\ldots,(b_q,B_q)\end{matrix}\right]=\frac{1}{2\pi i}\int_L ds\ \chi(s)x^s,$$

$$\chi(s)=\frac{\Pi_{i=1}^{m}\Gamma(b_i-B_is)\Pi_{i=1}^{n}\Gamma(1-a_i+A_is)}{\Pi_{i=m+1}^{q}\Gamma(1-b_i+B_is)\Pi_{i=1+n}^{p}\Gamma(a_i-A_is)},\tag{6}$$

is the Fox function.[13,25] Thus, we can find the solution by substituting Eq. (4) into Eq. (3), which yields

$$\rho(x,t)=\frac{1}{\Gamma\left(\frac{\mathcal{K}}{\mathcal{D}}+\frac{1}{2}\right)}\left(\frac{1}{4\mathcal{D}t^{\gamma}}\right)^{1/2}\int \mathrm{d}x'\tilde{\rho}(x')\mathrm{H}_{1\ 2}^{2\ 0}\left[\frac{(x-x')^2}{4\mathcal{D}t^{\gamma}}\middle|\begin{matrix}(1-\gamma/2,\gamma)\\ (1/2,1),\ (\mathcal{K}/\mathcal{D},1)\end{matrix}\right].\tag{7}$$

In Fig. 1 we show the behavior of Eq. (7) for typical values of γ for the initial condition $\tilde{\rho}(x)=\delta(x)$. It is interesting to note that the distribution, with the presence of this potential, is null at the origin (in contrast with the free case) and we do not have stationary solution for this case.

In order to analyze the Rayleigh process,[20] characterized by $F=-k_1x+k_2/x$, we may employ the procedure of separation of variables with the use of the following ansatz:

$$\rho_n(x,t)=\phi_n(t)\psi_n(x),\tag{8}$$

for a given eigenvalue λ_n. Now, introducing Eq. (8) into Eq. (1) with $\mu=1$ and $\theta=0$ one obtains

$$\begin{aligned}\frac{\mathrm{d}\phi_n(t)}{\mathrm{d}t}&=-\lambda_{n\ 0}D_t^{1-\gamma}\phi_n(t),\\ \mathcal{D}\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x^2}+\frac{\mathrm{d}}{\mathrm{d}x}\left[k_1x-\frac{k_2}{x}\right]\psi_n(x)&=-\lambda_n\psi_n(x).\end{aligned}\tag{9}$$

The solution for the temporal equation is given in terms of the Mittag–Leffter function

$$\phi_n(t)\propto \mathrm{E}_{\gamma}(-\lambda_nt^{\gamma})\equiv\sum_{j=0}^{\infty}\frac{(-\lambda_nt^{\gamma})^j}{\Gamma(1+\gamma j)}\tag{10}$$

and

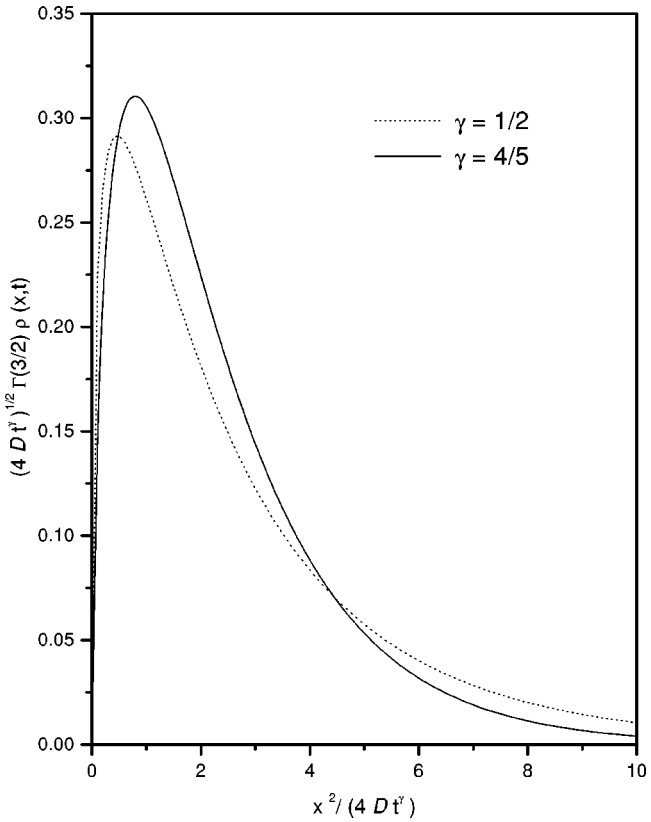

FIG. 1. $(4\mathcal{D}t^{\gamma})^{1/2}\Gamma(\frac{3}{2})\rho(x,t)$ vs $x^2/(4\mathcal{D}t^{\gamma})$ is plotted for typical values of γ. The initial condition is $\tilde{\rho}(x)=\delta(x)$ and $\mathcal{K}=\mathcal{D}$. We notice that the distribution vanishes for $x=0$ in contrast with the case where the external force (drift) is absent.

$$\rho(x,t)=\left(\frac{k_1}{2\mathcal{D}}\right)^{k_2/2\mathcal{D}+1/2}\frac{|x|^{k_2/\mathcal{D}}e^{-(k_1/2\mathcal{D})x^2}}{\Gamma\left(\frac{k_2}{2\mathcal{D}}+\frac{1}{2}\right)}\sum_{n=0}^{\infty}\left(\begin{array}{c} n \\ n+\frac{k_2}{2\mathcal{D}}-\frac{1}{2}\end{array}\right)\mathrm{L}_n^{(k_2/2\mathcal{D}-1/2)}\left(\frac{k_1x^2}{2\mathcal{D}}\right)$$

$$\times\mathrm{L}_n^{(k_2/2\mathcal{D}-1/2)}\left(\frac{k_1x_0^2}{2\mathcal{D}}\right)\mathrm{E}_{\gamma}(-\lambda_n t^{\gamma}), \tag{11}$$

with the initial condition $\rho(x,0)=\delta(x-x_0)$, $\lambda_n=2nk_1$ and $\mathrm{L}_n^{(\alpha)}(x)$ is the associated Laguerre polynomial. Equation (11) contains the usual Ornstein–Uhlenbeck process[26] and the usual Rayleigh process[20] as particular cases, and it extends the result obtained in Ref. 27.

Let us go back to Eq. (1) and consider the force $F(x)\propto x|x|^{\alpha-1}$, $\mathcal{D}(x)\propto|x|^{-\theta}$ and $\mu=1$. In this case, an analytical solution cannot easily be obtained for a generic α and θ. However, for $\theta\neq 0$ and $\alpha+\theta+1=0$ an exact solution can be obtained and it is given by

$$\rho(x,t)=\frac{2+\theta}{2\Gamma\left(\frac{\mathcal{K}}{\mathcal{D}}+\frac{1}{2+\theta}\right)}\left(\frac{1}{\mathcal{D}(2+\theta)^2t^{\gamma}}\right)^{1/(2+\theta)}\mathrm{H}_1^{2\ 0}{}_{2}\left[\frac{x^{2+\theta}}{\mathcal{D}(2+\theta)^2t^{\gamma}}\middle|\begin{array}{c}(1-\gamma/(2+\theta),\gamma) \\ (1-1/(2+\theta),1)\ ,\ (\mathcal{K}/\mathcal{D},1)\end{array}\right], \tag{12}$$

where, for simplicity, we are considering $\rho(x,0)=\delta(x)$ and the external force (drift) $F(x)=(2+\theta)\mathcal{K}/x^{1+\theta}$. In particular, Eq. (12) extends the results found in Ref. 28. The second moment is

given by $\langle x^2\rangle \propto t^{2\gamma/(2+\theta)}$ which scales with the exponent $2\gamma/(2+\theta)$ and clearly depends only on γ and θ. It also defines if the system exhibits a normal, super- or subdiffusion.

Let us now discuss Eq. (1) by considering a mixing between the spatial and temporal fractional derivatives, i.e., the case $\theta=0$ with arbitrary values of γ and μ. We also employ $\alpha=1$, i.e., $F(x)=-\mathcal{K}x$ to assure a stationary solution. Applying the Fourier transform in Eq. (1) and employing the Reiz representation for the spatial fractional derivative, we have

$$\frac{\partial}{\partial t}\rho(k,t) = -\ {}_0D_t^{1-\gamma}\left[\mathcal{D}|k|^{\overline{\mu}}\rho(k,t) + \mathcal{K}k\frac{\partial}{\partial k}\rho(k,t)\right], \tag{13}$$

where $\overline{\mu}=1+\mu$. The solution for Eq. (13) is given by

$$\rho(k,t) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\mathcal{D}|k|^{\overline{\mu}}}{\overline{\mu}\mathcal{K}}\right)^n \exp\left(\frac{-\mathcal{D}|k|^{\overline{\mu}}}{\mathcal{K}\overline{\mu}}\right)\mathrm{E}_\gamma(-\overline{\mu}n\mathcal{K}t^\gamma), \tag{14}$$

This solution recovers the usual one for $\gamma=1$ and $\overline{\mu}=2$ and it extends for $\overline{\mu}\neq 2$ the result found in Ref. 27. By using the inverse of Fourier transform, we obtain

$$\rho(x,t) = \frac{1}{\pi\overline{\mu}}\sum_{n,j=0}^{\infty}\frac{(-1)^j}{n!(2j)!}x^{2j}\,\Gamma\left(n+\frac{1}{\overline{\mu}}+\frac{2j}{\overline{\mu}}\right)\left(\frac{\overline{\mu}\mathcal{K}}{\mathcal{D}}\right)^{1/\overline{\mu}+2j/\overline{\mu}}\mathrm{E}_\gamma(-\overline{\mu}n\mathcal{K}t^\gamma)\ . \tag{15}$$

The stationary solution that emerges from this process is a Levy distribution.

Now, we consider some particular cases of Eq. (1) for $\gamma=1$ and nonzero values of μ and θ, and considering a linear drift, i.e., $\alpha=1$ and $F(x)=-2\mathcal{K}x$, too. For simplicity, we employ $\mathcal{D}=1$ and also assume that the function ρ has a scaling form given by

$$\rho(x,t) = \frac{1}{\Phi(t)}\mathcal{P}\left(\frac{x}{\Phi(t)}\right). \tag{16}$$

Substituting Eq. (16) into Eq. (1) and considering the drift $F=-2\mathcal{K}x$, we obtain

$$-k\frac{\mathrm{d}}{\mathrm{d}z}[z\mathcal{P}(z)] = \frac{\mathrm{d}}{\mathrm{d}z}\left[z^{-\theta}\frac{\mathrm{d}^\mu}{\mathrm{d}z^\mu}\mathcal{P}(z)\right] \tag{17}$$

and

$$\frac{\dot{\Phi}(t)}{\Phi(t)^2}+2\mathcal{K}\frac{1}{\Phi(t)} = k\left(\frac{1}{\Phi(t)}\right)^{2+\theta+\mu}, \tag{18}$$

where $z=|x|/\Phi(t)$ and k is an arbitrary constant introduced to decouple Eq. (1) in two ordinary differential equations, and it is determined by the normalization condition. By solving Eq. (18) we have that

$$\Phi(t) = \left[(\Phi(0))^{1+\theta+\mu}e^{-2(1+\theta+\mu)\mathcal{K}t} + \frac{k}{2\mathcal{K}}\,(1-e^{-2(1+\theta+\mu)\mathcal{K}t}\right)^{1/(1+\theta+\mu)}. \tag{19}$$

In order to obtain the solutions of Eq. (17), we perform one integration and the result is

$$z^{-\theta}\frac{\mathrm{d}^\mu}{\mathrm{d}z^\mu}\mathcal{P}(z) = -kz\mathcal{P}(z)+\mathcal{C}, \tag{20}$$

where $\mathcal{C}$ is an arbitrary constant. We use the Riemann–Liouville operator[18] for the spatial derivative, and we work with the *positive* x axis and, later on, we shall use the symmetry of the differential equation with respect to the spatial coordinate to extend the results to the entire real

axis (we are working, in other words, with $\partial^{\mu}/\partial|x|^{\mu}$). A complete analysis of Eq. (20) considering $\mu,\theta\neq 0$ is a hard task, thus, we restrict ourselves to the analysis of some particular situations.

We start by considering $\theta=1$ and $-2<\mu<0$. Applying the Laplace transform in Eq. (20) we obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}\overline{s}^2}\mathcal{P}(\overline{s})-\frac{1}{k}\overline{s}^{\mu}\mathcal{P}(\overline{s})=0, \tag{21}$$

where $\overline{s}$ is the conjugate variable of z in the Laplace transform. Solving this equation one obtains

$$\mathcal{P}(\overline{s})=\overline{s}^{1/2}\mathrm{K}_{1/(2+\mu)}\left(\frac{2\overline{s}^{(2+\mu/2)}}{k^{1/2}(2+\mu)}\right). \tag{22}$$

Inverting this expression yields

$$\mathcal{P}(z)=\frac{1}{2}[k^{3/2}(2+\mu)^{1-\mu}]^{1/(2+\mu)}\mathrm{H}_{1}^{2\ 0}{}_{2}\left[\frac{1}{z}(k^{1/2}(2+\mu))^{-2/(2+\mu)}\middle|\begin{matrix}(1,1)\\(1/(2+\mu),1/(2+\mu))\ ,\ (2/(2+\mu),1/(2+\mu))\end{matrix}\right]. \tag{23}$$

Next, we obtain the solution for the case $-1<\mu<0$ and $\theta=-1-2\mu$. Thus, going back to Eq. (20) and employing these last considerations, we have

$$\mathcal{P}(z)=\frac{1}{z^{1-\mu}}\exp\left[-\frac{\overline{k}}{z}\right], \tag{24}$$

where $\overline{k}$ is a constant. We notice that Eqs. (5) and (12) present the stretched exponential behavior for $|x|\to\infty$, in contrast with Eqs. (23) and (24) which exhibit the power law behavior in this asymptotic limit.

The case $\mu=-1$ and $\theta<0$ arbitrary lead us to

$$z^{-\theta}\int_0^z \mathrm{d}\overline{z}\,\mathcal{P}(\overline{z})=-kz\mathcal{P}(z)+\mathcal{C}, \tag{25}$$

whose solution for $\mathcal{C}=0$ is given by

$$\mathcal{P}(z)=\frac{1}{z^{1+\theta}}\exp\left[\frac{z^{-\theta}}{k\theta}\right]. \tag{26}$$

Similar distribution has essentially been obtained in stochastic models for the volatility in financial markets.[29]

The connection of the results obtained here with the nonextensive statistics[11] cannot be established for the case $\mu=1$ and θ arbitrary, since the asymptotic limit for large x gives a stretched exponential behavior. For the case in which μ is different from unity, it is possible, for some cases, to establish a connection between the solutions obtained here and the nonextensive statistics. This connection may be done in the asymptotic limit $|x|\to\infty$ that gives a power law behavior. Indeed, the functional form of $\rho(x,t)$ does not coincide for arbitrary value of x. However, the comparison of these expressions in the asymptotic limit $|x|\to\infty$ enables us to identify the type of tails which can be represented by the expression $1/|x|^{2/(q-1)}$ given in Ref. 11 for the entropic problem in this asymptotic behavior. For instance, for Eq. (24) we have that

$$q=\frac{3-\mu}{1-\mu}\,. \tag{27}$$

A similar result was found in Ref. 30 by considering a nonlinear fractional Fokker–Planck equation.

III. SUMMARY AND CONCLUSIONS

We have analyzed the fractional Fokker–Planck equations by considering an external force $F \propto x|x|^{\alpha-1}$ and the diffusion coefficient $\mathcal{D} \propto |x|^{-\theta}$. By using the Green function method and normalized scaled functions we were able to find explicit solutions for $\rho(x,t)$. In particular, we have extended the Rayleigh process by considering the fractional derivative in time. Similar solutions could be established for the halved diffusion equation by incorporating an adequate external force. Whenever appropriate we have also discussed the connection with nonextensive statistics, providing (through identification of the exact or at least asymptotic behaviors) the relation between the entropic index q and the exponents appearing in the Fokker–Planck equation. Finally, we expect that the results obtained here may be useful to the discussion of the anomalous diffusion systems where fractional diffusion equations play an important role.

ACKNOWLEDGMENTS

We thank Marcia C. Barbosa and L. A. N. Amaral for reading the manuscript. We also thank CNPq and Fundação Araucária (Brazilian agencies) for partial financial support.

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Wigner's theorem in a class of Hilbert C^*-modules

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(Received 12 November 2002; accepted 16 December 2002)

Let H be a complex Hilbert space, $\dim H>1$, and let $\mathcal{A}\subseteq\mathbf{B}(H)$ be a C^*-algebra such that the ideal $\mathbf{K}(H)$ of all compact operators on H is contained in $\mathcal{A}$. Let X be a Hilbert C^*-module over $\mathcal{A}$. We prove that any function $F:X\to X$ which preserves the absolute value of the $\mathcal{A}$-valued inner product on X is of the form $F(x)=\varphi(x)Ux$, $x\in X$, where φ is a phase function and U is an $\mathcal{A}$-linear isometry. The result generalizes Wigner's classical unitary-antiunitary theorem and its extension to Hilbert $\mathbf{K}(H)$-modules. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1556553]

I. INTRODUCTION AND STATEMENT OF THE RESULT

Wigner's unitary-antiunitary theorem states that each bijective function $F:H\to H$ acting on a complex Hilbert space $(H,(\cdot,\cdot))$ which satisfies $|(Fx,Fy)|=|(x,y)|$, $x,y\in H$, must be of the form $F(x)=\varphi(x)Ux$, $x\in H$, where $U:H\to H$ is either unitary or antiunitary operator and $\varphi:H\to\mathbf{C}$ is a phase function (i.e., its values are of modulus 1).

Wigner's theorem was first published in 1931.[16] We refer to Ref. 13 (see also references therein) for an exposition concerned with various aspects of the theorem.

Recently, Wigner's theorem has been generalized to Hilbert C^*-modules over matrix algebras M_d (Ref. 10) and over the elementary C^*-algebra $\mathbf{K}(H)$ of all compact operators on a Hilbert space H of arbitrary dimension.[4]

In the present article we extend Wigner's theorem to a broader class of Hilbert C^*-modules over concrete C^*-algebras of bounded operators on a Hilbert space H which contain the elementary algebra $\mathbf{K}(H)$. The proof uses extensions of Hilbert C^*-modules investigated in Ref. 3.

A (right) Hilbert C^*-module over a C^*-algebra $\mathcal{A}$ is a right $\mathcal{A}$-module V equipped with an $\mathcal{A}$-valued inner product $\langle\cdot,\cdot\rangle$ which is linear over $\mathcal{A}$ in the second and conjugate linear in the first variable, such that V is a Banach space with the norm $\|v\|=\|\langle v,v\rangle\|^{1/2}$. (We observe that the results from Refs. 10 and 4 are stated for left Hilbert C^*-modules. On the other hand, extensions of Hilbert C^*-modules are discussed in Ref. 3 for right modules. Hence the ''right'' organization of the present article appears as the more convenient one.) Hilbert C^*-modules are introduced and first investigated in Refs. 6, 12 and 14.

A Hilbert $\mathcal{A}$-module V is said to be full if the two sided ideal generated by all products $\langle v,w\rangle$, $v,w\in V$, is dense in $\mathcal{A}$.

If V and W are Hilbert $\mathcal{A}$-modules, we denote by $\mathbf{B}(V,W)$ the Banach space of all adjointable operators from V to W (i.e., of all maps $T:V\to W$ such that there exists $T^*:W\to V$ with the property $\langle Tv,w\rangle=\langle v,T^*w\rangle$, $\forall v,w$). When $V=W$ we write $\mathbf{B}(V)$ instead of $\mathbf{B}(V,V)$. It is well known that each adjointable operator T is necessarily bounded and $\mathcal{A}$-linear in the sense $T(va)=(Tv)a$, $\forall a\in\mathcal{A},\forall v\in V$. We additionally denote by $L_b(V)$ the set of all bounded $\mathcal{A}$-linear operators on V. In general, bounded $\mathcal{A}$-linear operators may fail to possess an adjoint, so $\mathbf{B}(V)$ may properly be contained in $L_b(V)$. However, if V is a Hilbert C^*-module over the elementary C^*-algebra $\mathbf{K}(H)$ of all compact operators on a Hilbert space H, then it is known that each bounded $\mathbf{K}(H)$-linear operator on V is necessarily adjointable; this follows from Theorem 1 in

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Ref. 8 and Theorem 2.8.6 in Ref. 5 (or, alternatively, from Remark 5 in Ref. 1). We refer the reader to Refs. 7 or 15 for general facts about Hilbert C^*-modules.

Before stating the main result we fix the rest of our notation.

Throughout, if a is an element of a C^*-algebra, $|a|$ denotes the unique positive square root of a^*a.

We shall fix a complex Hilbert space H such that $\dim H>1$. The C^*-algebras of all compact and bounded operators on H will be denoted by $\mathbf{K}$ and $\mathbf{B}$, respectively. Let further $(e_j)_{j\in J}$ denote a fixed approximate unit for $\mathbf{K}$. The field of complex numbers is denoted by $\mathbf{C}$.

Theorem 1: Let X *be a full Hilbert* C^**-module over a* C^**-algebra* $\mathcal{A}$ *of operators on a complex Hilbert space* H *with* $\dim H>1$, *such that* $\mathbf{K}\subseteq\mathcal{A}\subseteq\mathbf{B}$. *Let* $F:X\to X$ *be a function satisfying*

$$|\langle F(x),F(y)\rangle|=|\langle x,y\rangle|,\ \forall x,y\in X. \tag{1}$$

Then there exist an $\mathcal{A}$*-linear isometry* $U:X\to X$ *and a phase function* $\varphi:X\to\mathbf{C}$ *such that*

$$F(x)=\varphi(x)Ux,\ \forall x\in X.$$

Observe that the corresponding result for the case $\dim H=1$ is the classical Wigner's theorem. In this situation one can not exclude the antilinear alternative from the assertion of the theorem. On the other hand, if $\dim H>1$, then, as noted in Ref. 9, the nonappearance of antilinear isometries is the consequence of the noncommutativity of the underlying C^*-algebra. We further note that in the case $\mathcal{A}=\mathbf{K}$ the above result is proved in Ref. 4; thus Theorem 1 serves as a generalization of Theorem 1 from Ref. 4.

Finally, we show by Example 5 below that one can not conclude that U is an adjointable operator. However, in either of the two boundary cases, namely if $\mathcal{A}=\mathbf{K}$ or if X is strictly complete with respect to the ideal submodule $X\mathbf{K}$, the operator U from Theorem 1 possesses an adjoint; cf. Corollary 4 below.

II. PROOFS

We first summarize necessary facts about extensions of Hilbert C^*-modules; for the details (and a general exposition) we refer to Ref. 3.

Suppose that X is a full Hilbert $\mathcal{A}$-module with $\mathbf{K}\subseteq\mathcal{A}\subseteq\mathbf{B}$. Consider the ideal submodule $V=X\mathbf{K}$ associated with the essential ideal $\mathbf{K}$ of $\mathcal{A}$. Denote by $V_d=\mathbf{B}(\mathbf{K},V)$ the Hilbert C^*-module over the multiplier algebra $M(\mathbf{K})=\mathbf{B}$ consisting of all adjointable maps from $\mathbf{K}$ to V with the inner product $\langle r,s\rangle=r^*s$. Now observe that V is embedded in V_d via the map $\Gamma:V\to V_d$, $\Gamma(v)=r_v$ where $r_v:\mathcal{A}\to V$ denotes the "multiplier" $r_v(a)=va$. In the sequel we shall identify v in V with r_v in V_d; in this way V_d becomes an extension of V containing V as the ideal submodule $V=V_d\mathbf{K}$. Now recall Theorem 1.1 from Ref. 3: since X is an essential extension of V, there exists an injective morphism $\Lambda:X\to V_d$ of Hilbert C^*-modules acting as the identity operator on V. Thus, after identifying X with $\Lambda(X)$, we may write $V\leqslant X\leqslant V_d$.

Further, one defines a (variant of) strict topology on V_d by the family of seminorms $w\mapsto\|\langle v,w\rangle\|$, $v\in V$ and $w\mapsto\|wb\|$, $b\in\mathbf{K}$. It is proved in Ref. 3 that V is strictly dense in V_d: if (e_j) is an approximate unit for $\mathbf{K}$, then each w in V_d satisfies $w=(\text{st.})\lim_j we_j$. Moreover, it turns out that V_d is the completion of V with respect to the strict topology.

Note that in the case $V=\mathbf{K}$ the extended module V_d is nothing else than the multiplier algebra $\mathbf{B}=M(\mathbf{K})$ with the usual (C^*) strict topology on $\mathbf{B}$.

Finally, since V is an ideal submodule, it remains invariant for each adjointable operator on V_d and restriction to V gives an isomorphism of C^*-algebras of adjointable operators on V_d and on V (cf. Theorem 2.2 from Ref. 3). It is also noted in Ref. 3 that each $T\in\mathbf{B}(V_d)$ is strictly continuous and serves as the strict continuation of its restriction to V.

Proof of Theorem 1: We assume that $\mathbf{K}$ is properly contained in $\mathcal{A}$, for otherwise the assertion of the theorem is proved in Ref. 4.

First observe that the assumed property (1) of F implies

$$\langle F(x),F(x)\rangle=\langle x,x\rangle,\ \forall x\in X. \tag{2}$$

Since $V=X\mathbf{K}$ is an ideal submodule we have $V=\{v\in X:\langle v,v\rangle\in\mathbf{K}\}$ (cf. Ref. 2). Now the above equality (2) shows that V is invariant for F; thus the generalized Wigner's theorem for Hilbert C^*-modules over $\mathbf{K}$ applies. By Theorem 1 from Ref. 4 there exist a phase function $\varphi_0:V\to\mathbf{C}$ and an isometry $U_0\in\mathbf{B}(V)$ such that

$$F(v)=\varphi_0(v)U_0v,\ \forall v\in V. \tag{3}$$

Using Theorem 2.2 from Ref. 3 we can extend U_0 to an isometry $U_d\in\mathbf{B}(V_d)$; remember that U_d is the strict continuation of U_0.

Let us now fix $x\in X$ and $b\in\mathbf{K}$. We would like to conclude that $F(x)b$ belongs to $\operatorname{Im}U_0$. Let (v_λ) be an orthonormal basis for a Hilbert $\mathbf{K}$-module V. Recall from Ref. 1 that (v_λ) is an orthogonal system generating a dense submodule such that each $\langle v_\lambda,v_\lambda\rangle$ is a minimal projection in $\mathbf{K}$. It is proved in Ref. 1 that each v in V satisfies $v=\Sigma_\lambda v_\lambda\langle v_\lambda,v\rangle$. In particular, since $xb\in V$, we have $xb=\Sigma_\lambda v_\lambda\langle v_\lambda,xb\rangle$. Now

$$\begin{aligned}\langle F(x)b,F(x)b\rangle&=b^*\langle F(x),F(x)\rangle b=b^*\langle x,x\rangle b=\langle xb,xb\rangle=\sum_\lambda\langle xb,v_\lambda\rangle\langle v_\lambda,xb\rangle\\&=\sum_\lambda b^*\langle x,v_\lambda\rangle\langle v_\lambda,x\rangle b\\&=\sum_\lambda b^*\langle F(x),F(v_\lambda)\rangle\langle F(v_\lambda),F(x)\rangle b\\&=\sum_\lambda\langle F(x)b,F(v_\lambda)\rangle\langle F(v_\lambda),F(x)b\rangle\\&=\sum_\lambda\langle F(x)b,U_0v_\lambda\rangle\varphi_0(v_\lambda)\overline{\varphi_0(v_\lambda)}\langle U_0v_\lambda,F(x)b\rangle\\&=\sum_\lambda\langle F(x)b,U_0v_\lambda\rangle\langle U_0v_\lambda,F(x)b\rangle.\end{aligned}$$

Since U_0 is an isometry (i.e., $U_0^*U_0=I$), (U_0v_λ) is also an orthonormal system in V. Therefore, the equality obtained above, namely $\langle F(x)b,F(x)b\rangle=\Sigma_\lambda\langle F(x)b,U_0v_\lambda\rangle\langle U_0v_\lambda,F(x)b\rangle$, implies

$$F(x)b=\sum_\lambda U_0v_\lambda\langle U_0v_\lambda,F(x)b\rangle. \tag{4}$$

As an isometry U_0 has a closed image, thus (4) shows $F(x)b\in\operatorname{Im}U_0$.

Further, for arbitrary v in V we find

$$\begin{aligned}\langle U_0^*(F(x)b),v\rangle\langle v,U_0^*(F(x)b)\rangle&=\langle F(x)b,U_0v\rangle\langle U_0v,F(x)b\rangle\\&=\langle F(x)b,\varphi_0(v)U_0v\rangle\langle\varphi_0(v)U_0v,F(x)b\rangle\\&=b^*\langle F(x),F(v)\rangle\langle F(v),F(x)\rangle b\\&=b^*\langle x,v\rangle\langle v,x\rangle b=\langle xb,v\rangle\langle v,xb\rangle.\end{aligned}$$

By Lemma 1 from Ref. 4 there exists $\varphi_b(x)\in\mathbf{C}$ such that $|\varphi_b(x)|=1$ and

$$U_0^*(F(x)b)=\varphi_b(x)xb. \tag{5}$$

Since $U_0U_0^*$ is the orthogonal projection to $\mathrm{Im}\,U_0$ and since this closed submodule contains $F(x)b$, the action of U_0 to (5) gives

$$F(x)b=\varphi_b(x)U_0(xb). \tag{6}$$

Observe that the above equality (6) is obtained for arbitrary x in X and b in $\mathbf{K}$. Now take $b=e_j$; note additionally that U_0 is the restriction of the isometry $U_d\in\mathbf{B}(V_d)$. Then, if we denote $\varphi_{e_j}=\varphi_j$, (6) becomes

$$F(x)e_j=\varphi_j(x)U_d(x)e_j,\ \forall x\in X,\ \forall j. \tag{7}$$

We may assume that $(\varphi_j(x))$ is a convergent net with the limit $\varphi(x)$, for otherwise, since $|\varphi_j(x)|=1$, one can replace $(\varphi_j(x))$ with an appropriate subnet $(\varphi_{j(p)}(x))$. Since each y in V_d satisfies $y=(\mathrm{st.})\lim_j ye_j$, we may take strict limits in (7) to obtain

$$F(x)=\varphi(x)U_d(x),\ \forall x\in X. \tag{8}$$

The last equality also shows that X is invariant for U_d. Denoting by U the operator on X induced by U_d we finally obtain

$$F(x)=\varphi(x)Ux,\ \forall x\in X. \tag{9}$$

This concludes the proof, since U, as a restriction of U_d, is also an $\mathcal{A}$-linear isometry. □

Remark 2: It should be noted that the operator U from Theorem 1 is not only an isometry, but has a stronger property of preserving the inner products. This is indeed a general property of operators on Hilbert C^*-modules: each $\mathcal{A}$-linear isometry of Hilbert $\mathcal{A}$-modules $U:X\to Y$, adjointable or not, satisfies $\langle Ux_1,Ux_2\rangle=\langle x_1,x_2\rangle$, $\forall x_1,x_2\in X$. This is proved exactly as Theorem 3.5 in Ref. 7.

On the other hand, one can not conclude that the operator U from Theorem 1 possesses an adjoint; see Example 5 below. However, if $X=V_d$, i.e., when X coincides with the strict completion of V the operator U must be adjointable. To see this we first prove an independent proposition.

Proposition 3: Let V be a full Hilbert $\mathbf{K}$-module. Then $L_b(V_d)=\mathbf{B}(V_d)$.

Proof: Take $T\in L_b(V_d)$ and denote by T_0 the restriction of T to V (it is already observed that V, as an ideal submodule of V_d, remains invariant under each $\mathbf{B}$-linear operator on V_d).

Since V is a Hilbert C^*-module over $\mathbf{K}$, T_0 has the adjoint operator T_0^* on V. Let S be the extension of T_0^* to an operator on V_d; we also know that S is in fact the strict continuation of T_0^* (cf. Theorem 2.2 from Ref. 3).

Now we would like to conclude

$$\langle x,Ty\rangle=\langle Sx,y\rangle,\ \forall x,y\in V_d. \tag{10}$$

First observe that the above equality holds true for all x and y in V. Therefore for a fixed $x\in V_d$ and arbitrary $v\in V$ we have

$$\langle xe_j,Tv\rangle=\langle S(xe_j),v\rangle,\ \forall j. \tag{11}$$

Since (xe_j) strictly converges to x, strict continuity of S implies

$$\langle x,Tv\rangle=\langle Sx,v\rangle,\ \forall x\in V_d,\forall v\in V. \tag{12}$$

Now take arbitrary $y\in V_d$ and observe that (12) ensures

$$\langle x,T(ye_j)\rangle=\langle Sx,ye_j\rangle,\ \forall j. \tag{13}$$

Passing to the strict limits we obtain (10). □

Corollary 4: Let X be a full Hilbert C^*-module over a C^*-algebra $\mathcal{A}\subseteq\mathbf{B}$ of operators on a complex Hilbert space H with $\dim H>1$, *such that $\mathbf{K}\subseteq\mathcal{A}$. Assume further that X is strictly complete with respect to the strict topology induced by the ideal submodule $X\mathbf{K}$. Let $F:X\to X$ be a function satisfying*

$$|\langle F(x),F(y)\rangle|=|\langle x,y\rangle|,\ \forall x,y\in X.$$

Then there exists an isometry $U\in\mathbf{B}(X)$ and a phase function $\varphi:X\to\mathbf{C}$ such that

$$F(x)=\varphi(x)Ux,\ \forall x\in X.$$

Proof: By assumption X is strictly complete with respect to $X\mathbf{K}$, thus, by Theorem 1.6 from Ref. 3, unitarily equivalent to $(X\mathbf{K})_d$. Now the assertion follows from Theorem 1 and the preceding proposition. □

Example 5: We provide an example of an $\mathcal{A}$-linear isometry $U\in L_b(X)$ on a Hilbert $\mathcal{A}$-module X with $\mathbf{K}\subseteq\mathcal{A}\subseteq\mathbf{B}$ which is not an adjointable operator on X. [It should be observed that examples of nonadjointable operators on Hilbert C^*-modules are well known from the literature; see, for instance, Refs. 12 or 7. But in our situation, namely $V=X\mathbf{K}$ and $V\leqslant X\leqslant V_d$, the underlying C^*-algebra $\mathcal{A}$ contains $\mathbf{K}$. Therefore by the observation from the introduction, Theorem 2.2 in Ref. 3 and the above Proposition 3, we know $L_b(V)=\mathbf{B}(V)\simeq\mathbf{B}(V_d)=L_b(V_d)$. Hence it makes sense to ask whether there are nonadjointable isometries on X.]

First observe the following general remark. Suppose we are given an operator $T\in L_b(X)$. Consider the restriction T_0 of T to V (V is invariant for T) and its extension $T_d\in\mathbf{B}(V_d)$ to V_d and note that T_d is the strict continuation of T_0. Assume that there exists the adjoint $S\in\mathbf{B}(X)$ of T, that is, an operator $S:X\to X$ satisfying $\langle S(x),y\rangle=\langle x,T(y)\rangle$, $\forall x,y\in X$. From this equality one concludes that $S(x)$ must be the strict limit of the net $(T_d^*(x)e_j)$. Since T_d^* is $\mathcal{A}$-linear and strictly continuous, this implies $S(x)=T_d(x)$. In conclusion, S must coincide with the restriction of T_d^* to X. In other words, an operator $T\in L_b(X)$ possesses an adjoint if and only if X is invariant for T_d^*.

To provide a concrete example we borrow Example from Ref. 11, p. 54.

Let S be a unilateral shift on a separable Hilbert space H of infinite multiplicity. Consider the $*$-algebra $\mathcal{A}_0=\mathbf{K}+S\mathbf{B}S^*$ and denote by $\mathcal{A}$ the closure of $\mathcal{A}_0$ in the operator norm. Clearly, $\mathcal{A}$ is a C^*-algebra such that $\mathbf{K}\subseteq\mathcal{A}\subseteq\mathbf{B}$. We shall regard $\mathbf{K}$, $\mathcal{A}$ and $\mathbf{B}$ as Hilbert C^*-modules in the standard way. Define the left translation $L_S:T\mapsto ST$. Observe that L_S is an isometry on $\mathbf{B}$ for which both $\mathbf{K}$ and $\mathcal{A}$ are invariant. In particular, L_S is an $\mathcal{A}$-linear isometry on $\mathcal{A}$. Now notice that the adjoint operator L_S^* on $\mathbf{B}$ is in fact the left translation by S^*, namely $L_{S^*}:T\mapsto S^*T$. We claim that $\mathcal{A}$ is not invariant for L_{S^*}. Indeed, $L_{S^*}\mathcal{A}\subseteq\mathcal{A}$ would imply $S^*\in\mathcal{A}$, hence also $S\in\mathcal{A}$. But, as it is demonstrated in Ref. 11, this is impossible.

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Representations of a symplectic type subalgebra of W_∞

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(Received 25 November 2002; accepted 5 January 2003)

We classify the irreducible quasifinite highest weight modules over the symplectic Lie subalgebra W_∞, and realize them in terms of irreducible highest weight representations of classical Lie subalgebras of infinite matrices with finitely many nonzero diagonals. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1560553]

I. INTRODUCTION

The W-infinity algebras naturally arise in various physical theories, such as conformal field theory, the theory of the quantum Hall effect, etc. The $W_{1+\infty}$ algebra, which is the central extension of the Lie algebra $\mathcal{D}$ of differential operators on the circle, is the most fundamental among these algebras.

When we study the representation theory of a Lie algebra of this kind, we encounter the difficulty that although it admits a $\mathbb{Z}$-gradation, each of the graded subspaces is still infinite dimensional, and therefore the study of highest weight modules which satisfy the quasi-finiteness condition that its graded subspaces have finite dimension, becomes a nontrivial problem.

The study of representations of the Lie algebra $W_{1+\infty}$ was initiated in Ref. 8, where a characterization of its irreducible quasifinite highest weight representations was given, these modules were constructed in terms of irreducible highest weight representations of the Lie algebra of infinite matrices, and the unitary ones were described. On the basis of this analysis, further studies were made in the framework of vertex algebra theory for the $W_{1+\infty}$ algebra,[5,9] and for its matrix version.[4] The case of orthogonal subalgebras of $W_{1+\infty}$ was studied in Ref. 10. The symplectic subalgebra of $W_{1+\infty}$ was considered in Ref. 2 in relation to number theory.

Reference 1 developed a theory of quasifinite highest weight representation of the subalgebras $W_{\infty,p}$ of $W_{1+\infty}$, where $W_{\infty,p}$ $(p\in\mathbb{C}[x])$ is the central extension of the Lie algebra $\mathcal{D}p(t\partial_t)$ of differential operators on the circle that are a multiple of $p(t\partial_t)$. The most important of these subalgebras is $W_\infty = W_{\infty,x}$ that is obtained by taking $p(x)=x$. Its unitary quasifinite representations were studied in Ref. 7. In the present article we classify all irreducible quasifinite highest weight modules of the symplectic subalgebra $\mathcal{D}_{x,\theta}$ of W_∞ given by the minus fixed points of the anti-involution θ introduced by Bloch in Ref. 2. This is strongly used in the recent study of finite growth modules over conformal algebras.[3]

II. LIE ALGEBRAS $\widehat{g\ell}_\infty^{[m]}$ AND $c_\infty^{[m]}$

Denote by $R_m=\mathbb{C}[u]/(u^{m+1})$ the quotient algebra of the polynomial algebra $\mathbb{C}[u]$ by the ideal generated by u^{m+1} $(m\in\mathbb{Z}_+)$. Let $\mathbf{1}$ be the identity element in R_m. Denote by $g\ell_\infty^{[m]}$ the complex Lie algebra of all infinite matrices $(a_{ij})_{i,j\in\mathbb{Z}}$ with only finitely many nonzero diagonals with entries in R_m. Denote by E_{ij} the infinite matrix with 1 at (i,j)-place and 0 elsewhere. There is a natural automorphism ν of $g\ell_\infty^{[m]}$ given by

$$\nu(E_{i,j})=E_{i+1,j+1}. \tag{2.1}$$

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Let the weight of $E_{i,j}$ be $j-i$. This defines the *principal* $\mathbb{Z}$-gradation $g\ell_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(g\ell_\infty^{[m]})_j$. Denote by $\widehat{g\ell}_\infty^{[m]}=g\ell_\infty^{[m]}\oplus R_m$ the cental extension of $g\ell_\infty^{[m]}$ given by the following two-cocycle with values in R_m:

$$C(A,B)=\mathrm{Tr}([J,A]B), \tag{2.2}$$

where $J=\Sigma_{i\leqslant 0}E_{ii}$. The $\mathbb{Z}$-gradation of the Lie algebra $g\ell_\infty^{[m]}$ extends to $\widehat{g\ell}_\infty^{[m]}$ by putting the weight of R_m to be 0. In particular we have the *triangular decomposition*

$$\widehat{g\ell}_\infty^{[m]}=(\widehat{g\ell}_\infty^{[m]})_+\oplus(\widehat{g\ell}_\infty^{[m]})_0\oplus(\widehat{g\ell}_\infty^{[m]})_-, \tag{2.3}$$

where

$$(\widehat{g\ell}_\infty^{[m]})_\pm=\bigoplus_{j\in\mathbb{N}}(\widehat{g\ell}_\infty^{[m]})_{\pm j} \quad \text{and} \quad (\widehat{g\ell}_\infty^{[m]})_0=(g\ell_\infty^{[m]})_0\oplus R_m.$$

Given $\lambda\in(\widehat{g\ell}_\infty^{[m]})_0^*$, we let

$$\begin{aligned} c_i&=\lambda(u^i),\\ {}^a\lambda_j^{(i)}&=\lambda(u^iE_{j,j}),\\ {}^ah_j^{(i)}&={}^a\lambda_j^{(i)}-{}^a\lambda_{1+j}^{(i)}+\delta_{j,0}c_i, \end{aligned} \tag{2.4}$$

where $j\in\mathbb{Z}$ and $i=0,\ldots,m$. Let $L(\widehat{g\ell}_\infty^{[m]},\lambda)$ be the irreducible highest weight $\widehat{g\ell}_\infty^{[m]}$-module with highest weight λ. The ${}^a\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(\widehat{g\ell}_\infty^{[m]},\lambda)$.

Consider the vector space $R_m[t,t^{-1}]$, and take the R_m-basis $v_i=t^{-i}$, $i\in\mathbb{Z}$. Now consider the following $\mathbb{C}$-bilinear form on $R_m[t,t^{-1}]$:

$$C(u^mv_i,u^nv_j)=u^m(-u^n)\delta_{i,1-j}. \tag{2.5}$$

Denote by $\overline{c}_\infty^{[m]}$ the Lie subalgebra of $g\ell_\infty^{[m]}$ which preserves the bilinear form $C(\,,\,)$. We have

$$\overline{c}_\infty^{[m]}=\{(a_{ij}(u))_{i,j\in\mathbb{Z}}\in g\ell_\infty^{[m]}\mid a_{ij}(u)=(-1)^{i+j+1}a_{1-j,1-i}(-u)\}.$$

Denote by $c_\infty^{[m]}=\overline{c}_\infty^{[m]}\oplus R_m$ the central extension of $\overline{c}_\infty^{[m]}$ given by the restriction of the two-cocycle (2.2), defined in $g\ell_\infty^{[m]}$. This subalgebra inherits from $\widehat{g\ell}_\infty^{[m]}$ the principal $\mathbb{Z}$-gradation and the triangular decomposition (see Refs. 10 and 6 for notation)

$$c_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(c_\infty^{[m]})_j, \quad c_\infty^{[m]}=(c_\infty^{[m]})_+\oplus(c_\infty^{[m]})_0\oplus(c_\infty^{[m]})_-.$$

In particular, when $m=0$, we have the usual Lie subalgebra of $g\ell_\infty$, denoted by c_∞.

Given $\lambda\in(c_\infty^{[m]})_0^*$, denote by $L(c_\infty^{[m]};\lambda)$ the irreducible highest weight module over $c_\infty^{[m]}$ with highest weight λ.

For each $\lambda\in(c_\infty^{[m]})_0^*$, we let

$$\begin{aligned} c_i&=\lambda(u^i),\\ {}^c\lambda_j^{(i)}&=\lambda(u^iE_{j,j}-(-u)^iE_{1-j,1-j}),\\ {}^ch_j^{(i)}&={}^c\lambda_j^{(i)}-{}^c\lambda_{1+j}^{(i)},\\ {}^ch_0^{(i)}&={}^c\lambda_1^{(i)}+c_i \quad (i \text{ even}), \end{aligned} \tag{2.6}$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m$. The ${}^{c}\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(c_\infty^{[m]},\lambda)$.

III. THE SUBALGEBRA $\mathcal{D}_{\theta,x}$ AND ITS STRUCTURE OF PARABOLIC SUBALGEBRAS

Let $\mathcal{D}$ be the Lie algebra of regular differential operators on the circle, i.e., the operators on $\mathbb{C}[t,t^{-1}]$ of the form

$$E=e_k(t)\partial_t^k+e_{k-1}(t)\partial_t^{k-1}+\cdots+e_0(t), \quad \text{where } e_i(t)\in\mathbb{C}[t,t^{-1}].$$

The elements $t^k(\partial_t)^l$ $(l\in\mathbb{Z}_+,\ k\in\mathbb{Z})$ form its basis, where ∂_t denotes d/dt. Another basis of $\mathcal{D}$ is

$$t^kD^l \quad (l\in\mathbb{Z}_+,\ k\in\mathbb{Z}),$$

where $D=t\partial_t$.

We have the following two-cocycle on $\mathcal{D}$, where $f(w),g(w)\in\mathbb{C}[w]$:[8]

$$\Psi(z^rf(D),z^sg(D))=\begin{cases}\displaystyle\sum_{-r\leqslant m\leqslant -1} f(m)g(m+r) & \text{if } r=-s\geqslant 0\\ 0 \quad \text{if } r+s\neq 0.\end{cases} \tag{3.1}$$

The central extension $\hat{\mathcal{D}}$ of $\mathcal{D}$ by a one-dimensional center $\mathbb{C}C$, corresponding to the two-cocycle Ψ, is also denoted by $W_{1+\infty}$. The bracket in $W_{1+\infty}$ is given by

$$[t^rf(D),t^sg(D)]=t^{r+s}(f(D+s)g(D)-f(D)g(D+r))+\Psi(t^rf(D),t^sg(D))C. \tag{3.2}$$

Consider the following Lie subalgebras of $\mathcal{D}$:

$$\mathcal{D}_x:=\mathcal{D}D.$$

Denote by $\hat{\mathcal{D}}_x$ the central extension of $\mathcal{D}_x$ by $\mathbb{C}C$ corresponding to the restriction of the two-cocycle Ψ. Observe that $\hat{\mathcal{D}}_x$ is the well-known W_∞ subalgebra of $W_{1+\infty}$.

Letting wt $t^kf(D)D=k$, wt $C=0$ defines the *principal gradation* of $\hat{\mathcal{D}}_x$:

$$\hat{\mathcal{D}}_x=\bigoplus_{j\in\mathbb{Z}}(\hat{\mathcal{D}}_x)_j,$$

where $(\hat{\mathcal{D}}_x)_j=\{t^jf(D)\ D \mid f(w)\in\mathbb{C}[w]\}+\delta_{j0}\mathbb{C}C$.

In Ref. 2, the anti-involution θ in $\mathcal{D}_x$ was introduced:

$$\theta(t^kD^n)=-t^k(-D-k)^{n-1}D, \tag{3.3}$$

where $k\in\mathbb{Z}$ and $n\in\mathbb{N}$. We denote by $\mathcal{D}_{\theta,x}$ the Lie subalgebra of $\mathcal{D}_x$ consisting of its minus θ-fixed points. It inherits the principal $\mathbb{Z}$-gradation of $\mathcal{D}_x$ since θ preserves the principal $\mathbb{Z}$-gradation of $\mathcal{D}_x$, namely $\mathcal{D}_{\theta,x}=\oplus_{k\in\mathbb{Z}}(\mathcal{D}_{\theta,x})_k$, where

$$\begin{aligned}(\mathcal{D}_{\theta,x})_k&=\{t^kf(D)D \mid f\in\mathbb{C}[x] \ \text{ and}\theta(t^kf(D)D)=-t^kf(D)D\}\\ &=\{t^kg(D+k/2)D \mid g \ \text{ even polynomial}\}.\end{aligned} \tag{3.4}$$

We denote again by Ψ the restriction of the two-cocycle in (3.1) to $\mathcal{D}_{\theta,x}$,

$$\Psi(z^r f(D+r/2)D, z^s g(D+s/2)D)$$
$$= \begin{cases} \sum_{-r\leqslant m\leqslant -1} f(m+r/2)\, m\, g(m+r/2)(m+r) & \text{if } r=-s\geqslant 0 \\ 0 \quad \text{if } r+s\neq 0, \end{cases} \tag{3.5}$$

where $f(w)$ and $g(w)$ are even polynomials. Denote by $\widehat{\mathcal{D}_{\theta,x}}$ the central extension of $\mathcal{D}_{\theta,x}$ by $\mathbb{C}C$ corresponding to the two-cocycle Ψ.

We define a *parabolic subalgebra* $\mathcal{P}$ of $\widehat{\mathcal{D}_{\theta,x}}$ as a subalgebra of the form $\mathcal{P}=\oplus_{j\in\mathbb{Z}}\mathcal{P}_j$ where $\mathcal{P}_j=(\widehat{\mathcal{D}_{\theta,x}})_j$ if $j\geqslant 0$, and $\mathcal{P}_j\neq 0$ for some $j<0$. For each positive integer k we have that $\mathcal{P}_{-k}=\{t^{-k}g(D-k/2)D \mid g\in I_{-k}\}$, where I_{-k} is some subspace of the ring of even polynomials. Given $g(w)$ and $h(w)$ even polynomials we have that $t^{-k}h(D-k/2)D$ and $g(D)D\in\widehat{\mathcal{D}_{\theta,x}}$. One can compute

$$[g(D)D\,,\, t^{-k}h(D-k/2)D]=t^{-k}f(D-k/2)h(D-k/2)D, \tag{3.6}$$

where $f(w-k/2)=g(w-k/2)(w-k/2)-g(w+k/2)(w+k/2)$. As $g(w)$ ranges over all even polynomials, $f(w)$ ranges over all even polynomials, too. Thus (3.6) implies that if $h(w)\in I_{-k}$, then $h(w)$ multiplied by any even polynomial, also belongs to I_{-k}. Let $b_k(w)$ $(k\in\mathbb{N})$ be the unique monic even polynomial in I_{-k} of minimal degree when $I_{-k}\neq 0$, and let $b_k(w)=0$ when $I_{-k}=0$. We call $b_k(w)$ $(k\in\mathbb{N})$ the *characteristic polynomials* of $\mathcal{P}$.

Lemma 3.1: Let $\{b_k, k\in\mathbb{N}\}$ *be the sequence of characteristic polynomials of a parabolic subalgebra* $\mathcal{P}$ of the Lie algebra $\widehat{\mathcal{D}_{\theta,x}}$. *Then*

(a) $b_k(z)$ *divides* $(z+k/2+1)\,(-2z)\,b_{k+1}(z+\frac{1}{2})$ *for all* $k\in\mathbb{N}$,
(b) $b_{k+l}(w)$ *divides* $w(w-(k-l)/2)b_k(w+l/2)b_l(w-k/2)$ *for all* $k\in\mathbb{N}$, *and*
(c) $\mathcal{P}_{-k}\neq 0$ *for all* $k\in\mathbb{N}$.

Proof: It follows from

$$[\,tD\,,\, t^{-k-1}b_{k+1}(D-(k+1)/2)D]$$
$$=t^{-k}((D-k-1)b_{k+1}((D-(k+1)/2)-b_{k+1}(D+1-(k+1)/2)(D+1))D$$

that $b_k(w-k/2)$ divides

$$((w-k-1)\,b_{k+1}(w-(k+1)/2)-b_{k+1}(w+1-(k+1)/2)\,(w+1))\,w. \tag{3.7}$$

Now, by computing

$$[\,tD, t^{-k-1}b_{k+1}(D-(k+1)/2)\,(D-(k+1)/2)^2\,D]$$
$$=t^{-k}((D-k-1)\,b_{k+1}((D-(k+1)/2)\,(D-(k+1)/2)^2$$
$$-b_{k+1}(D+1-(k+1)/2)\,(D+1-(k+1)/2)^2\,(D+1))D,$$

we have that $b_k(w-k/2)$ divides

$$((w-k-1)\,(w-(k+1)/2)^2 b_{k+1}(w-(k+1)/2)$$
$$-(w+1-(k+1)/2)^2\;b_{k+1}(w+1-(k+1)/2)\;(w+1))\,w. \tag{3.8}$$

Thus, $b_k(w-k/2)$ divides (3.8) subtracted from (3.7) multiplied by $(w-(k+1)/2)^2$, which is equal to $(w+1)\,(-2(w-(k+1)/2)-1)\;\;b_{k+1}(w+1-(k+1)/2)$. Therefore, putting $z=w-k/2$, we obtain (a). This computation shows that if $b_{k+1}(z)\neq 0$, then $b_k(z)\neq 0$.

Part (b) can be proved in a similar fashion by computing

$$[t^{-k} b_k(D-k/2)\, D\,,\, t^{-l} b_l(D-l/2)\, D\,],$$

and

$$[t^{-k} (D-k/2)^2\ b_k(D-k/2)\, D\,,\, t^{-l} b_l(D-l/2)\, D\,].$$

This computation shows that if $b_k(z)$ and $b_l(z)$ are nonzero, then $b_{k+l}(z)\neq 0$.

Part (c) follows from (a) and (b). □

Lemma 3.2:

$$[(\widehat{\mathcal{D}_{\theta,x}})_1\,,(\widehat{\mathcal{D}_{\theta,x}})_k]=(\widehat{\mathcal{D}_{\theta,x}})_{k+1}\quad (k>1),$$

and

$$(\widehat{\mathcal{D}_{\theta,x}})_2=[(\widehat{\mathcal{D}_{\theta,x}})_1\,,(\widehat{\mathcal{D}_{\theta,x}})_1]\oplus\mathbb{C}\,t^2D.$$

Proof: Same as Lemma 3.3 in Ref. 10, but computing

$$[t\,(D+1/2)^l\,D\,,\,t^m\,(D+m/2)^k\,D]$$

with l and k even non-negative integers, instead of formula (3.33) in Ref. 10. □

Denote by $(\widehat{\mathcal{D}_{\theta,x}})_0(b_1,b_2)$ the subspace of $(\widehat{\mathcal{D}_{\theta,x}})_0$ spanned by

$$(g(D-\tfrac{1}{2})b_1(D-\tfrac{1}{2})\,(D-1)-g(D+\tfrac{1}{2})\,b_1(D+\tfrac{1}{2})\,(D+1))\,D$$

and

$$(f(D-1)b_2(D-1)(D-2)-f(D+1)\,b_2(D+1)(D+2))\,D-f(0)b_2(0)\,C,$$

where f, g are even polynomials.

Proposition 3.3: Let $\mathcal{P}$ be a parabolic subalgebra of $\widehat{\mathcal{D}_{\theta,x}}$ and let $b_1(z)$ and $b_2(z)$ be its first and second characteristic polynomials. Then

$$[\mathcal{P},\mathcal{P}]=(\widehat{\mathcal{D}_{\theta,x}})_0(b_1,b_2)\oplus(\oplus_{k\neq 0}\mathcal{P}_k).$$

Proof: We omit this proof since it is completely analogous to the proof of Proposition 3.2 in Ref. 10. □

IV. CHARACTERIZATION OF QUASIFINITE HIGHEST WEIGHT MODULES OF $\widehat{\mathcal{D}_{\theta,x}}$

Now, we begin our study of quasifinite representations over $\widehat{\mathcal{D}_{\theta,x}}$. Let $\mathfrak{g}=\oplus_{j\in\mathbb{Z}}\mathfrak{g}_j$ be a $\mathbb{Z}$-graded Lie algebra over $\mathbb{C}$, and let $\mathfrak{g}_+=\oplus_{j>0}\mathfrak{g}_j$. A $\mathfrak{g}$-module V is called $\mathbb{Z}$-*graded* if $V=\oplus_{j\in\mathbb{Z}}V_j$ and $\mathfrak{g}_iV_j\subset V_{i+j}$. A $\mathbb{Z}$-graded $\mathfrak{g}$-module V is called *quasifinite* if $\dim V_j<\infty$ for all j.

Given $\lambda\in\mathfrak{g}_0^*$, a *highest weight module* is a $\mathbb{Z}$-graded $\mathfrak{g}$-module $V(\mathfrak{g},\lambda)$ generated by a highest weight vector $v_\lambda\in V(\mathfrak{g},\lambda)_0$ which satisfies

$$hv_\lambda=\lambda(h)v_\lambda\quad (h\in\mathfrak{g}_0),\quad \mathfrak{g}_+v_\lambda=0. \tag{4.1}$$

A nonzero vector $v\in V(\mathfrak{g},\lambda)$ is called *singular* if $\mathfrak{g}_+v=0$.

The *Verma module* over $\mathfrak{g}$ is defined as usual:

$$M(\mathfrak{g},\lambda)=\mathcal{U}(\mathfrak{g})\otimes_{\mathcal{U}(\mathfrak{g}_0\oplus\mathfrak{g}_+)}\mathbb{C}_\lambda\,, \tag{4.2}$$

where $\mathbb{C}_\lambda$ is the one-dimensional $(\mathfrak{g}_0\oplus\mathfrak{g}_+)$-module given by $h\mapsto\lambda(h)$ if $h\in\mathfrak{g}_0$, $\mathfrak{g}_+\mapsto 0$, and the action of $\mathfrak{g}$ is induced by the left multiplication in $\mathcal{U}(\mathfrak{g})$. Here and further $\mathcal{U}(\mathfrak{q})$ stands for the

universal enveloping algebra of the Lie algebra $\mathfrak{q}$. Any highest weight module $V(\mathfrak{g},\lambda)$ is a quotient module of $M(\mathfrak{g},\lambda)$. The irreducible module $L(\mathfrak{g},\lambda)$ is the quotient of $M(\mathfrak{g},\lambda)$ by the maximal proper graded submodule.

Consider a parabolic subalgebra $\mathcal{P}=\oplus_{j\in\mathbb{Z}}\mathcal{P}_j$ of $\mathfrak{g}$ and let $\lambda\in\mathfrak{g}_0^*$ be such that $\lambda|_{\mathfrak{g}_0\cap[\mathcal{P},\mathcal{P}]}=0$. Then the $(\mathfrak{g}_0\oplus\mathfrak{g}_+)$-module $\mathbb{C}_\lambda$ extends to a $\mathcal{P}$-module by letting $\mathcal{P}_j$ act as 0 for $j<0$, and we may construct the highest weight module

$$M(\mathfrak{g},\mathcal{P},\lambda)=\mathcal{U}(\mathfrak{g})\otimes_{\mathcal{U}(\mathcal{P})}\mathbb{C}_\lambda$$

called the *generalized Verma module*. Clearly all these highest weight modules are graded.

From now on we will consider $\mathfrak{g}=\widehat{D_{\theta,x}}$ and $\lambda\in(\widehat{D_{\theta,x}})_0^*$. Let $b_1(w)$ and $b_2(w)$ two monic even polynomials and let $\lambda\in(\widehat{D_{\theta,x}})_0^*$ be such that $\lambda|_{(\widehat{D_{\theta,x}})_0(b_1,b_2)}=0$. Consider a parabolic subalgebra $\mathcal{P}$ of $\widehat{D_{\theta,x}}$ whose first and second characteristic polynomials are b_1 and b_2. Denote by $M(\widehat{D_{\theta,x}});\lambda,b_1,b_2)$ the generalized Verma module $M(\widehat{D_{\theta,x}}),\mathcal{P},\lambda)$. The polynomials b_1 and b_2 do not determine $\mathcal{P}$ uniquely, but, for our need, any corresponding parabolic $\mathcal{P}$ will do.

We omit the proof of the following proposition since it is essentially the same as the proof of Proposition 4.1 in Ref. 10, replacing Lemma 3.1 by our Lemma 3.1.

Proposition 4.1: The following conditions on $\lambda\in(\widehat{\mathcal{D}_{\theta,x}})^*$ *are equivalent:*

(a) $M(\widehat{D_{\theta,x}};\lambda)$ *contains a singular vector in the first graded subspace.*
(b) $L(\widehat{D_{\theta,x}};\lambda)$ *is quasifinite.*
(c) *There exist monic even polynomials* b_1 *and* b_2 *such that* $L(\widehat{D_{\theta,x}};\lambda)$ *is a quotient of a generalized Verma module* $M(\widehat{D_{\theta,x}};\lambda,b_1,b_2)$.

We shall write $M(\lambda)$ and $L(\lambda)$ in place of $M(\widehat{\mathcal{D}_{\theta,x}},\lambda)$ and $L(\widehat{\mathcal{D}_{\theta,x}},\lambda)$ if no ambiguity may arise.

Let $L(\lambda)$ be an irreducible quasifinite highest weight module over $\widehat{\mathcal{D}_{\theta,x}}$. By Proposition 4.1, there exists a monic even polynomial $b(w)$ such that

$$(t^{-1}b(D-1/2)D)v_\lambda=0.$$

We shall call such monic polynomial of minimal degree, uniquely determined by the highest weight λ, the *characteristic* polynomial of $L(\lambda)$.

A functional $\lambda\in(\widehat{\mathcal{D}_{\theta,x}})_0^*$ is described by its *labels* $\Delta_l=-\lambda(D^l)$ with l an odd non-negative integer, and the *central charge* $c=\lambda(C)$. We shall consider the generating series

$$\Delta_\lambda(x)=\sum_{l\geq 0,\, l\ \text{odd}}^{\infty}\frac{x^l}{l!}\Delta_l=-\lambda(\sinh(xD)). \tag{4.3}$$

Recall that an *even quasipolynomial* is a solution of a nontrivial linear differential equation with constant coefficients $p(\partial_t)=0$, where $p(x)$ is an even polynomial. One has the following characterization of quasifinite highest weight modules over $\widehat{\mathcal{D}_{\theta,x}}$.

Theorem 4.2: *A* $\widehat{\mathcal{D}_{\theta,x}}$*-module* $L(\lambda)$ *is quasifinite if and only if there exists an even quasipolynomial* $\phi_\lambda(x)$ *with* $\phi_\lambda(0)=0$, *such that*

$$\Delta_\lambda(x)=\left(\frac{\phi_\lambda(x)}{\sinh(x/2)}\right). \tag{4.4}$$

Proof: From Propositions 3.3 and 4.1, we have that $L(\lambda)$ is quasifinite if and only if there exist two even monic polynomials $b_1(w)$ and $b_2(w)$ such that

$$\lambda((\cosh(D-\tfrac{1}{2})b_1(D-\tfrac{1}{2})(D-1)-\cosh(D+\tfrac{1}{2})b_1(D+\tfrac{1}{2})(D+1))\,D)=0 \tag{4.5}$$

and

$$\lambda((\cosh(D-1)b_2(D-1)(D-2)-\cosh(D+1)b_2(D+1)(D+2))D-f(0)b_2(0)C)=0. \tag{4.6}$$

Using (4.3) together with the identities

$$f(D)e^{xD}=f\left(\frac{d}{dx}\right)(e^{xD}),\quad p(D)e^{x(D+1)}=e^{x}p(D)e^{xD}=e^{x}p\left(\frac{d}{dx}\right)e^{xD},$$

$$e^{x}p\left(\frac{d}{dx}\right)f(x)=p\left(\frac{d}{dx}-1\right)e^{x}f(x)$$

and the fact that b_1 is even, condition (4.5) can be rewritten as follows:

$$\begin{aligned}
0=\lambda\ & (\cosh(D-\tfrac{1}{2})b_1(D-\tfrac{1}{2})(D-1)-\cosh(D+\tfrac{1}{2})b_1(D+\tfrac{1}{2})(D+1))\,D\\
&=\frac{1}{2}\lambda\left(b_1\left(\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}-\frac{1}{4}\right)e^{x(D-1/2)}+b_1\left(-\frac{d}{dx}\right)\left(-\frac{d}{dx}-\frac{1}{2}\right)\left(-\frac{d}{dx}+\frac{1}{2}\right)e^{-x(D-1/2)}\right.\\
&\quad\left.-b_1\left(\frac{d}{dx}\right)\left(\frac{d}{dx}-\frac{1}{2}\right)\left(\frac{d}{dx}+\frac{1}{2}\right)e^{x(D+1/2)}-b_1\left(-\frac{d}{dx}\right)\left(-\frac{d}{dx}-\frac{1}{2}\right)\left(-\frac{d}{dx}+\frac{1}{2}\right)e^{-x(D+1/2)}\right)\\
&=\frac{1}{2}\lambda\left(b_1\left(\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}-\frac{1}{4}\right)e^{x(D-1/2)}+b_1\left(\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}-\frac{1}{4}\right)e^{-x(D-1/2)}\right.\\
&\quad\left.-b_1\left(\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}-\frac{1}{4}\right)e^{x(D+1/2)}--b_1\left(\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}-\frac{1}{4}\right)e^{x(D+1/2)}\right)\\
&=\frac{1}{2}b_1\left(\frac{d}{dx}\right)\ \left(\frac{d^2}{dx^2}-\frac{1}{4}\right)\ \lambda\ (e^{x(D-1/2)}+e^{-x(D-1/2)}-e^{x(D+1/2)}-e^{-x(D+1/2)})\\
&=\frac{1}{2}b_1\left(\frac{d}{dx}\right)\ \left(\frac{d^2}{dx^2}-\frac{1}{4}\right)\ \lambda\ (e^{-x/2}(e^{xD}-e^{-xD})-e^{x/2}(e^{xD}-e^{-xD}))\\
&=\frac{1}{2}b_1\left(\frac{d}{dx}\right)\ \left(\frac{d^2}{dx^2}-\frac{1}{4}\right)\ \lambda\ \left(-\sinh\left(\frac{x}{2}\right)\sinh(xD)\right).
\end{aligned}\tag{4.7}$$

Then we have

$$0=b_1\left(\frac{d}{dx}\right)\ \left(\frac{d^2}{dx^2}-\frac{1}{4}\right)\ \sinh\left(\frac{x}{2}\right)\ \Delta_\lambda(x). \tag{4.8}$$

Therefore, we obtain that $F(x)=\Delta_\lambda(x)\ \sinh(x/2)$ is an even quasipolynomial. Similarly, one can show from (4.6) that

$$0=b_2\left(\frac{d}{dx}\right)\ \left(\frac{d^2}{dx^2}-1\right)\ (\sinh(x)\ \Delta_\lambda(x)-c). \tag{4.9}$$

Taking $G(x)=\sinh(x)\ \Delta_\lambda(x)-c$ and noting that $G(x)=2F(x)\cosh(x/2)-c$, we see that $L(\widehat{\mathcal{D}_{\theta,x}};\lambda)$ is quasifinite if and only if $F(x)$ is an even quasipolynomial. □

We have the following.

Corollary 4.3: Let $L(\lambda)$ be a quasifinite irreducible highest weight module over $\widehat{\mathcal{D}_{\theta,x}}$, and let $b_1(w)$ be its first characteristic polynomial. Then $F(x)=\Delta_\lambda(x)\sinh(x/2)$ is an even quasipolyno-

mial. Let $F^{(m)}+a_{m_1}F^{(m-1)}+\cdots+a_0=0$ *be the minimal order linear differential equation with constant coefficients satisfied by* $F(x)$ *with* $w^{(m)}+a_{m_1}w^{(m-1)}+\cdots+a_0$ *an even polynomial. Then* $b_1(w)(w^2-\frac{1}{4})=w^{(m)}+a_{m_1}w^{(m-1)}+\cdots+a_0$.

The even quasipolynomial $\phi_\lambda(x)+c$, where $\phi_\lambda(x)$ is from (4.4) and c is the central charge, can be written in the form

$$\sum_r p_r(x)\cosh(e_r^+x)+\sum_s q_s(x)\sinh(e_s^-x), \tag{4.10}$$

where $p_r(x)$ [resp., $q_s(x)$] are nonzero even (resp., odd) polynomials and $e_i^\pm$ are distinct complex numbers. Note that $\Sigma_r p_r(0)=c$. The expression above is unique up to a sign of e_r^+ or a simultaneous sign changes of e_s^- and $q_s(x)$. The numbers e_r^+ (resp., e_x^-) appearing in (4.10) are called *even exponents* (resp., *odd exponents*) of the $\widehat{\mathcal{D}_{\theta,x}}$-module $L(\lambda)$ with *multiplicity* $p_r(x)$ [resp., $q_s(x)$]. Then the pair (e^+,e^-) determines $L(\lambda)$ uniquely. We will denote this module by $L(\widehat{\mathcal{D}_{\theta,x}};e^+,e^-)$.

V. INTERPLAY BETWEEN $\widehat{\mathcal{D}_{\theta,x}}$ AND THE INFINITE RANK CLASSICAL LIE ALGEBRAS OF TYPE *A* AND *C*

Let $\mathcal{O}$ denote the algebra of all holomorphic functions on $\mathbb{C}$ with the topology of uniform convergence on compact sets and $\mathcal{O}_{\text{even}}$ the set of even holomorphic functions. We consider the vector space $\mathcal{D}^{\mathcal{O}}$ spanned by the differential operators (of infinite order) of the form $t^kf(D)$, where $f\in\mathcal{O}$. The bracket in $\mathcal{D}$ extends to $\mathcal{D}^{\mathcal{O}}$. Similarly, we define a completion $\mathcal{D}^{\mathcal{O}}_{\theta,x}$ of $\mathcal{D}_{\theta,x}$ consisting of all differential operators of the form $t^kg(D+k/2)D$ where $g\in\mathcal{O}_{\text{even}}$.

Then the two-cocycle Ψ on $\mathcal{D}_{\theta,x}$ extends to a two-cocycle on $\mathcal{D}^{\mathcal{O}}_{\theta,x}$. Let $\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}}=\mathcal{D}^{\mathcal{O}}_{\theta,x}+\mathbb{C}C$ be the corresponding central extension.

Given $s\in\mathbb{C}$, we will consider the natural action of the Lie algebra $\mathcal{D}_{\theta,x}$ (resp., $\mathcal{D}^{\mathcal{O}}_{\theta,x}$) on $t^sR_m[t,t^{-1}]$. Taking the R_m-basis $v_j=t^{-j+s}$ $(j\in\mathbb{Z})$ of this space, we obtain a family of homomorphism of Lie algebras $\varphi_s^{[m]}:\mathcal{D}_{\theta,x}\to g\ell_\infty^{[m]}$ (resp., $\varphi_s^{[m]}:\mathcal{D}^{\mathcal{O}}_{\theta,x}\to g\ell_\infty^{[m]}$):

$$\begin{aligned}\varphi_s^{[m]}(t^kf(D+k/2)D)&=\sum_{j\in\mathbb{Z}} f(-j+k/2+s+u)(-j+s+u)E_{j-k,j}\\&=\sum_{i=0}^m\sum_{j\in\mathbb{Z}}\frac{(f(-j+k/2+s)(-j+s))^{(i)}}{i!}u^iE_{j-k,j},\\&=\sum_{i=0}^m\sum_{j\in\mathbb{Z}}\frac{f^{(i)}(-j+k/2+s)}{i!}((-j+s)u^i+u^{i+1})E_{j-k,j},\end{aligned} \tag{5.1}$$

where f is even and $f^{(i)}$ denotes the ith derivative. Note that this is the restriction to $\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}}$ of the homomorphism (3.2.1) in Ref. 8. Let

$$I_{s,k}^{[m]}=\{f\in\mathcal{O}_{\text{even}}\ \mid\ (f(-j+k/2+s))^{(i)}=0\ \text{ for all }\ n\in\mathbb{Z},\ 0\leqslant i\leqslant m\} \tag{5.2}$$

and let

$$J_s^{[m]}=\oplus_{k\in\mathbb{Z}}\{t^kf(D+k/2)D\ \ /f\in I_{s,k}^{[m]}\}. \tag{5.3}$$

Fix $\vec{s}=(s_1,\ldots,s_N)\in\mathbb{C}^N$, such that $s_i-s_j\notin\mathbb{Z}$ if $i\neq j$ and $s_i+s_j\notin\mathbb{Z}$ for all i,j. Also fix $\vec{m}=(m_1,\ldots,m_N)\in\mathbb{Z}_+^N$. Let $g\ell_\infty^{[\vec{m}]}=\oplus_{i=1}^N g\ell_\infty^{[m_i]}$ and consider the homomorphism

$$\varphi_{\vec{s}}^{[\vec{m}]}=\oplus_{i=1}^N\varphi_{s_i}^{[m_i]}\ :\ \mathcal{D}^{\mathcal{O}}_{\theta,x}\to g\ell_\infty^{[m_i]}. \tag{5.4}$$

Proposition 5.1: Given $\vec{s}$ and $\vec{m}$ as above we have the following exact sequence of Lie algebras:

$$0 \to J_{\vec{s}}^{[\vec{m}]} \to \mathcal{D}_{\theta,x}^{\mathcal{O}} \xrightarrow{\varphi_s^{[\vec{m}]}} g\ell_\infty^{[\vec{m}]} \to 0,$$

where $J_{\vec{s}}^{[\vec{m}]} = \cap_{i=1}^{N} J_{s_i}^{[m_i]}$.

Proof: For simplicity we prove this in the case $N=1$. By the assumptions above we have that $\vec{m}=m\in\mathbb{Z}_+$ and $\vec{s}=s\notin\mathbb{Z}/2$. The general case is similar.

It is clear that $\ker\varphi_s^{[m]} = J_s^{[m]}$. For the surjectivity we recall the following well known fact: for every discrete sequence of points in $\mathbb{C}$ and a non-negative integer m there exists $a(w)\in\mathcal{O}$ having the prescribed values of its first m derivatives at these points. Since $s\notin\mathbb{Z}/2$ the sequences $\{-j+k/2+s\}_{j\in\mathbb{Z}}$ and $\{j-k/1-s\}_{j\in\mathbb{Z}}$ are disjoint, then it is enough to find the preimage of $u^{m-i}\ E_{j-k,j}\in g\ell_\infty^{[m]}$ for $i=1,\ldots,m$, $j\in\mathbb{Z}$ and a fixed $k\in\mathbb{Z}$.

Consider $i=0$. There exists $a(w)\in\mathcal{O}$ such that (fix $r\in\mathbb{Z}$)

$$a^{(m)}(-j+k/2+s) = a^{(m)}(j-k/2-s) = \delta_{rj}$$

and

$$a^{(m-i)}(-j+k/2+s) = 0 = a^{(m-i)}(j-k/2-s) \quad \text{for } i=1,\ldots,m.$$

Taking $g(w)=[a(w)+a(-w)]/2\in\mathcal{O}_{\text{even}}$ we see that $\varphi_s^{[m]}(t^k g(D+k/2)D) = (s-r)\,u^m/m!\,E_{r-k,r}$. Similarly, taking $i>0$, inductively one can show that $u^{m-i}\ E_{j-k,j}\in \operatorname{Im}\varphi_s^{[m]}$. □

Now we want to extend the homomorphism (5.1) to a homomorphism between the central extensions of the corresponding Lie algebras. Define

$$\eta_i(x,s) = \frac{e^{(s-1/2)x} - (-1)^i e^{-(s-1/2)x}}{2}\ \frac{x^i}{i!} \quad (i\in\mathbb{Z}_+,\ \ s\in\mathbb{C}). \tag{5.5}$$

The homomorphism (5.1) preserves gradation. We have the following.

Proposition 5.2: The homomorphism $\varphi_s^{[m]}$ lifts to a Lie algebra homomorphism $\hat{\varphi}_s^{[m]}$ of the corresponding central extensions as follows:

$$\hat{\varphi}_s^{[m]}|_{(\widehat{\mathcal{D}_{\theta,x}})_j} = \varphi_s^{[m]}|_{(\mathcal{D}_{\theta,x})_j} \quad \text{if } j\neq 0, \tag{5.6}$$

$$\hat{\varphi}_s^{[m]}(\sinh(xD)) = \frac{1}{2}\sum_{i=0}^{m}\sum_{j\in\mathbb{Z}} \frac{\eta_i(x,s-j+1)-\eta_i(x,s-j)}{\sinh(x/2)} u^i E_j j - \frac{1}{2}\ \frac{\cosh((s-\frac{1}{2})x)-\cosh(x/2)}{\sinh(x/2)} c_0$$
$$-\frac{1}{2}\sum_{i=1}^{m}\frac{\eta_i(x,s)}{\sinh(x/2)} u^i\, c_0, \tag{5.7}$$

$$\hat{\varphi}_s^{[m]}(C) = 1. \tag{5.8}$$

Proof: Straightforward using formulas (3.3.3) and (3.3.4) in Ref. 8 and (5.1) □

The homomorphism $\varphi_s^{[m]}$ is defined for any $s\in\mathbb{C}$. However, for $s\in\mathbb{Z}/2$, it is no longer surjective. These cases are described by the following.

Proposition 5.3: For $s=0$ and $s=\frac{1}{2}$, we have the following exact sequence of Lie algebras:

$$0 \to J_s^{[m]} \to \mathcal{D}_{\theta,x}^{\mathcal{O}} \xrightarrow{\varphi_s^{[m]}} C \to 0,$$

where $C \simeq \bar{c}_\infty^{[m]}$.

Proof: First consider $s=\frac{1}{2}$. The homomorphism $\phi_s^{[m]}:\mathcal{D}_x\to g\ell_\infty^{[m]}$ introduced in Sec. 6 in Ref. 7 is surjective. Recall that we defined in $\mathcal{D}_x$ the anti-involution θ given in (3.3). It is easy to see that it transfers, via the $\phi_s^{[m]}$, to an anti-involution $\omega: g\ell_\infty^{[m]}\to g\ell_\infty^{[m]}$ as follows:

$$\omega(u^k+(\tfrac{1}{2}-j)u^{k-1})E_{ij})=((-u)^k+(\tfrac{1}{2}-i)(-u)^{k-1})E_{1-j,1-i}) \quad \text{for} \quad k\geqslant 1. \tag{5.9}$$

Therefore, the Lie algebra of $-\theta$-fixed points in $\mathcal{D}_x$, namely $\mathcal{D}_{\theta,x}$, maps surjectively to the Lie algebra of $-\omega$ fixed points in $g\ell_\infty^{[m]}$. Then it is enough to show that ω is conjugated by an automorphism T of $g\ell_\infty^{[m]}$ to the anti-involution defining $\overline{c}_\infty^{[m]}$.

For this define

$$\begin{gathered}
T(u^m\ \ E_{i,i+1})=(i+\tfrac{1}{2})\ \ u^m\ \ E_{i,i+1},\\
T(u^l\ \ E_{i,i+1})=(u^{l+1}-(i+\tfrac{1}{2})\ \ u^l)\ \ E_{i,i+1} \quad \text{for} \quad 0\leqslant l\leqslant m-1,\\
T(u^m\ \ E_{i+1,i})=\frac{-1}{(i+\frac{1}{2})}(-u)^m\ \ E_{i+1,i},\\
T(u^l\ \ E_{i+1,i})=\frac{1}{u-(i+\frac{1}{2})}(-u)^l\ \ E_{i+1,i} \quad \text{for} \quad 0\leqslant l\leqslant m-1.
\end{gathered} \tag{5.10}$$

It is a straightforward verification that this extends to an automorphism of the associative algebra $g\ell_\infty^{[m]}$ that conjugates ω to the anti-involution defining $\overline{c}_\infty$.

Now, consider the case $s=0$. In this case, the homomorphism $\phi_0^{[m]}:\mathcal{D}_x\to g\ell_\infty^{[m]}$ introduced in Sec. 6 in Ref. 7 is no longer surjective. However, it is surjective if we restrict $\phi_0^{[m]}:\mathcal{D}_x\to\mathfrak{g}^{[m]}$, where $\mathfrak{g}^{[m]}$ is the subalgebra of $g\ell_\infty^{[m]}$ from which we remove both axes. We will call such a homomorphism also $\phi_0^{[m]}$. Now, as above, the anti-involution θ in (3.3) transfers to $\mathfrak{g}^{[m]}$ as follows:

$$\omega_0((u^k+(-j)u^{k-1})E_{ij})=((-u)^k-i(-u)^{k-1})E_{-j,-i} \quad \text{for} \quad 1\geqslant k. \tag{5.11}$$

As above, it is enough to show that ω_0 is conjugated by an isomorphism $T:\mathfrak{g}^{[m]}\to g\ell_\infty^{[m]}$ to the anti-involution defining $\overline{c}_\infty^{[m]}$.

One should take $T=\pi\circ T'$, where π is the natural projection of $\mathfrak{g}^{[m]}$ onto $g\ell_\infty^{[m]}$ and T' is the automorphism of $\mathfrak{g}^{[m]}$ defined by

$$\begin{gathered}
T'(u^m\ \ E_{i,i+1})=-(i+1)\ \ (-u)^m\ \ E_{i,i+1},\\
T'(u^l\ \ E_{i,i+1})=(-1)^l(u^{l+1}-(i+1)\ \ u^l)\ \ E_{i,i+1} \quad \text{for} \quad 0\leqslant l\leqslant m-1,\\
T'(u^m\ \ E_{i+1,i})=\frac{-1}{(i+1)}(-u)^m\ \ E_{i+1,i},\\
T'(u^l\ \ E_{i+1,i})=\frac{1}{u-(i+1)}(-u)^l\ \ E_{i+1,i} \quad \text{for} \quad 0\leqslant l\leqslant m-1,
\end{gathered} \tag{5.12}$$

finishing the proof. □

Remark 5.4: (a) For $s=0$ and $s=\frac{1}{2}$, in view of the proposition above, by an abuse of notation we will denote again $\varphi_s^{[m]}$ the surjective homomorphism $\mathcal{D}_{\theta,x}$ onto $\overline{c}_\infty^{[m]}$ given by the old $\varphi_s^{[m]}$ composed with the isomorphism $C\simeq\overline{c}_\infty^{[m]}$.

(b) For $s\in\mathbb{Z}/2$ the image of $\mathcal{D}_{\theta,x}$ under the homomorphism $\varphi_s^{[m]}$ is $\nu^{\tilde{s}}(\overline{c}_\infty^{[m]})$, where ν was defined in (2.1) and $\tilde{s}=s$ if $s\in\mathbb{Z}$ and $\tilde{s}=s-\frac{1}{2}$ if $s\in\mathbb{Z}+\frac{1}{2}$. Therefore, we will only consider $s=0,\ \frac{1}{2}$ throughout the article.

Given $\vec{m}=(m_1,\ldots,m_N)\in\mathbb{Z}_+^N$ and $\vec{s}=(s_1,\ldots,s_N)$ such that $s_i\in\mathbb{Z}$ implies $s_i=0$, $s_i\in\mathbb{Z}+\frac{1}{2}$ implies $s_i=\frac{1}{2}$, and $s_i\neq\pm s_j \mod\mathbb{Z}$ for $i\neq j$, and combining Propositions 5.1–5.3, we obtain a homomorphism of Lie algebras:

$$\hat{\varphi}_{\vec{s}}^{[\vec{m}]}=\bigoplus_{i=1}^{N}\varphi_{s_i}^{[m_i]}:\widehat{\mathcal{D}_{\theta,x}}\to\mathfrak{g}^{[\vec{m}]}:=\oplus_{i=1}^{N}\mathfrak{g}^{[m_i]}, \tag{5.13}$$

where

$$\mathfrak{g}^{[m]}=\begin{cases}\widehat{g\ell}_\infty^{[m]} & \text{if } s\notin\mathbb{Z}/2\\ c_\infty^{[m]} & \text{if } s=0 \text{ or } s=\frac{1}{2}.\end{cases} \tag{5.14}$$

We can prove the following proposition in the same way as Proposition 5.1.

Proposition 5.5: The homomorphism $\hat{\varphi}_{\vec{s}}^{[\vec{m}]}$ extends to a surjective homomorphism of Lie algebras which is denoted again by $\hat{\varphi}_{\vec{s}}^{[\vec{m}]}$:

$$\hat{\varphi}_{\vec{s}}^{[\vec{m}]}=\bigoplus_{i=1}^{N}\hat{\varphi}_{s_i}^{[m_i]}:\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}}\to\mathfrak{g}^{[\vec{m}]}.$$

VI. REALIZATION OF QUASIFINITE HIGHEST WEIGHT MODULES OF $\widehat{\mathcal{D}_{\theta,x}}$

Let $\mathfrak{g}^{[m]}$ stand for $\widehat{g\ell}_\infty^{[m]}$ or $c_\infty^{[m]}$. The proof of the following proposition is standard.

Proposition 6.1: The $\mathfrak{g}^{[m]}$-module $L(\mathfrak{g}^{[m]},\ \lambda)$ is quasifinite if and only if all but finitely many of the $*h_k^{(i)}$ are zero, where $*$ represents a or c depending on whether $\mathfrak{g}^{[m]}$ is $\widehat{g\ell}_\infty^{[m]}$ or $c_\infty^{[m]}$.

Given $\vec{m}=(m_1,\ldots,m_N)\in\mathbb{Z}_+^N$, take a quasifinite $\lambda_i\in(\mathfrak{g}^{[m_i]})_0^*$ for each $i=1,\ldots,N$ and let $L(\mathfrak{g}^{[m_i]},\ \lambda_i)$ be the corresponding irreducible $\mathfrak{g}^{[m_i]}$-module. Let $\vec{\lambda}=(\lambda_1,\ldots,\lambda_N)$. Then the tensor product

$$L(\mathfrak{g}^{[\vec{m}]},\vec{\lambda})=\otimes_{i=1}^{N}L(\mathfrak{g}^{[m_i]},\ \lambda_i) \tag{6.1}$$

is an irreducible $\mathfrak{g}^{[\vec{m}]}$-module, with $\mathfrak{g}^{[\vec{m}]}=\oplus_{i=1}^{N}\mathfrak{g}^{[m_i]}$. The module $L(\mathfrak{g}^{[\vec{m}]},\vec{\lambda})$ can be regarded as a $\widehat{\mathcal{D}_{\theta,x}}$-module via the homomorphism $\varphi_{\vec{s}}^{[\vec{m}]}$, and will be denoted by $L_{\vec{s}}^{[\vec{m}]}(\vec{\lambda})$. We shall need the following proposition. Its proof is analogous to that of Proposition 4.3 in Ref. 8.

Proposition 6.2: Let V be a quasifinite $\widehat{\mathcal{D}_{\theta,x}}$-module. Then the action of $\widehat{\mathcal{D}_{\theta,x}}$ on V naturally extends to the action of $(\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}})_k$ on V for any $k\neq0$.

Theorem 6.3: *Let V be a quasifinite $\mathfrak{g}^{[\vec{m}]}$-module, which is regarded as a $\widehat{\mathcal{D}_{\theta,x}}$-module via the homomorphism $\varphi_{\vec{s}}^{[\vec{m}]}$. Then any $\widehat{\mathcal{D}_{\theta,x}}$-submodule of V is also a $\mathfrak{g}^{[\vec{m}]}$-submodule. In particular, the $\widehat{\mathcal{D}_{\theta,x}}$-module $L_{\vec{s}}^{[\vec{m}]}(\vec{\lambda})$ are irreducible if $\vec{s}=(s_1,\ldots,s_N)$ is such that $s_i\in\mathbb{Z}$ implies $s_i=0$, $s_i\in\mathbb{Z}+\frac{1}{2}$ implies $s_i=\frac{1}{2}$, and $s_i\neq\pm s_j \mod\mathbb{Z}$ for $i\neq j$.*

Proof: Let U be a $\widehat{\mathcal{D}_{\theta,x}}$-submodule of V. U is a quasifinite $\widehat{\mathcal{D}_{\theta,x}}$-module as well, hence by Proposition 6.2 it can be extended to $(\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}})_k$ for any $k\neq0$. By Proposition 5.5, the map $\varphi_{\vec{s}}^{[\vec{m}]}:(\widehat{\mathcal{D}_{\theta,x}}^{\mathcal{O}})_k\to(\mathfrak{g}^{[\vec{m}]})_k$ is surjective for any $k\neq0$. Thus U is invariant with respect to all members of the principal gradation of $(\mathfrak{g}^{[\vec{m}]})_k$ with $k\neq0$. Since $\mathfrak{g}^{[\vec{m}]}$ coincides with its derived algebra, this proves the theorem. □

We will show that in fact all the quasifinite $\widehat{\mathcal{D}_{\theta,x}}$-modules can be realized as some $L_{\vec{s}}^{[\vec{m}]}(\vec{\lambda})$. But first we shall calculate the generating series $\Delta_{m,s,\lambda}(x)$ of the highest weight and central charge c of the $\widehat{\mathcal{D}_{\theta,x}}$-module $L_s^{[m]}(\lambda)$.

Let $s\notin\mathbb{Z}/2$. Using formula (5.7), the fact that $\Delta(x)=\sinh(xD)$, and formulas (2.4) we have that

$$\Delta_{m,s,\lambda}(x)=-\lambda(\hat{\varphi}_s^{[m]}(\sinh(xD)))=\frac{1}{2}\sum_{i=0}^{m}\sum_{j\in\mathbb{Z}}\frac{\eta_i(x,s-j)}{\sinh(x/2)}\ {}^{a}h_j^{(i)}\ -\ \frac{1}{2}\frac{\cosh(x/2)}{\sinh(x/2)}c_0. \quad (6.2)$$

Thus, we have the following proposition.

Proposition 6.4: Consider the embedding $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{D}_{\theta,x}}\to\widehat{g\ell_\infty^{[m]}}$ *with* $s\notin\mathbb{Z}/2$. *The* $\widehat{g\ell_\infty^{[m]}}$*-module* $L(\widehat{g\ell_\infty^{[m]}},\lambda)$ *regarded as a* $\widehat{\mathcal{D}_{\theta,x}}$*-module is isomorphic to* $L(\widehat{\mathcal{D}_{\theta,x}},e^+,e^-)$ *where* e^+ *and* e^- *consist of exponents* $s-j-\frac{1}{2}$ *with* $j\in\mathbb{Z}$ *with multiplicities*

$$\sum_{0\leqslant i\leqslant m,\ i\ \text{even}}\frac{{}^{a}h_j^{(i)}\ x^i}{i!}\quad and\quad \sum_{0\leqslant i\leqslant m,\ i\ \text{odd}}\frac{{}^{a}h_j^{(i)}\ x^i}{i!}, \quad (6.3)$$

respectively.

Now consider $s=\frac{1}{2}$. Recall that by Remark 5.4 (a), in this case we have that the embedding $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{D}_{\theta,x}}\to c_\infty^{[m]}$ is actually the embedding given by formula (5.7) composed with T^{-1}, where T was introduced in (5.10). Using this, and also $\Delta(x)=\sinh(xD)$, formulas (2.6) and the fact that by definition $\eta_i(x,\frac{1}{2})=(-1)^i\eta_i(x,\frac{1}{2})$, we have that

$$\begin{aligned}\Delta_{m,s,\lambda}(x)&=-\lambda(\hat{\varphi}_s^{[m]}(\sinh(xD)))\\&=\frac{1}{2}\sum_{i=0}^{m}\sum_{j>0}\frac{\eta_i(x,j+\frac{1}{2})}{\sinh(x/2)}\,{}^{c}h_j^{(i)}\\&\quad+\ \frac{1}{2}\sum_{0\leqslant i\leqslant m,\ i\ \text{even}}\frac{\eta_i(x,\frac{1}{2})}{\sinh(x/2)}\ {}^{c}h_0^{(i)}-1/2\,\frac{\cosh(x/2)}{\sinh(x/2)}c_0.\end{aligned} \quad (6.4)$$

We can establish the following proposition.

Proposition 6.5: Consider the embedding $\hat{\varphi}_{1/2}^{[m]}:\widehat{\mathcal{D}_{\theta,x}}\to c_\infty^{[m]}$. *The* $c_\infty^{[m]}$*-module* $L(c_\infty^{[m]},\lambda)$ *regarded as a* $\widehat{\mathcal{D}_{\theta,x}}$*-module is isomorphic to* $L(\widehat{\mathcal{D}_{\theta,x}},e^+,e^-)$, *where* e^+ *and* e^- *consist of exponents* j *with* $j\in\mathbb{Z}_+$ *with multiplicities*

$$\sum_{0\leqslant i\leqslant m,\ i\ \text{even}}\frac{{}^{c}h_j^{(i)}\ x^i}{i!}\quad and\quad \sum_{0\leqslant i\leqslant m,\ i\ \text{odd}}\frac{{}^{c}h_j^{(i)}\ x^i}{i!}, \quad (6.5)$$

respectively, where ${}^{c}h_0^{(i)}=0$ *for* i *odd*.

Finally, consider $s=0$. Recall that by Remark 5.4(a), in this case we have again that the embedding $\hat{\varphi}_0^{[m]}:\widehat{\mathcal{D}_{\theta,x}}\to c_\infty^{[m]}$ is actually the embedding given by formula (5.7) composed with T^{-1}, where T was introduced right before (5.12). Using this, and also $\Delta(x)=\sinh(xD)$ and formulas (2.6), we have that

$$\begin{aligned}\Delta_{m,s,\lambda}(x)&=-\lambda(\hat{\varphi}_s^{[m]}(\sinh(xD)))=\frac{1}{2}\sum_{i=0}^{m}\sum_{j>0}\frac{(-1)^i\eta_i(x,-j)}{\sinh(x/2)}\ {}^{c}h_j^{(i)}\\&\quad+\ \frac{1}{2}\sum_{0\leqslant i\leqslant m,\ i\ \text{even}}\frac{\eta_i(x,0)}{\sinh(x/2)}\ {}^{c}h_0^{(i)}-\frac{1}{2}\frac{\cosh(x/2)}{\sinh(x/2)}c_0.\end{aligned} \quad (6.6)$$

We can establish the following proposition.

Proposition 6.6: Consider the embedding $\hat{\varphi}_0^{[m]}:\widehat{\mathcal{D}_{\theta,x}}\to c_\infty^{[m]}$. *The* $c_\infty^{[m]}$*-module* $L(c_\infty^{[m]},\lambda)$ *regarded as a* $\widehat{\mathcal{D}_{\theta,x}}$*-module is isomorphic to* $L(\widehat{\mathcal{D}_{\theta,x}},e^+,e^-)$ *where* e^+ *and* e^- *consist of exponents* $-\frac{1}{2}-j$ *with* $j\in\mathbb{Z}_+$ *with multiplicities*

$$\sum_{0\leqslant i\leqslant m,\ i\ \text{even}} \frac{{}^{c}h_j^{(i)}\ x^i}{i!} \quad and \quad \sum_{0\leqslant i\leqslant m,\ i\ \text{odd}} \frac{{}^{c}h_j^{(i)}\ (-x)^i}{i!}, \tag{6.7}$$

respectively, where ${}^{c}h_0^{(i)}=0$ *for* i *odd.*

Take an irreducible quasifinite highest weight $\widehat{\mathcal{D}_{\theta,x}}$-module V with central charge c and

$$\Delta(x)=\frac{\phi_\lambda(x)}{\sinh(x/2)}$$

with $\phi_\lambda(x)$ an even quasipolynomial such that $\phi_\lambda(0)=0$. We will write

$$\phi_\lambda(x)+c=\sum_{s\in\mathbb{C}}\sum_{i=1}^{m_s} a_{s,i}\ \ \eta_i(x,s), \tag{6.8}$$

where $a_{s,i}\in\mathbb{C}$ and $a_{s,i}\neq 0$ for only finitely many $s\in\mathbb{C}$. Since, by definition of η_i, we have that $\eta_i(x,-s)=(-1)^i\eta_i(x,s+1)$, to avoid ambiguities in the expression of $\phi_\lambda(x)$ above, we will choose the parameter s following these rules: when $s\in\mathbb{Z}$ we require $s\leqslant 0$; when $s\in\mathbb{Z}+\frac{1}{2}$, we ask $s\leqslant\frac{1}{2}$; when $s\notin\mathbb{Z}/2$, we require that $\operatorname{Im}s>0$ if $\operatorname{Im}s\neq 0$ or $s-[s]<\frac{1}{2}$ if $s\in\mathbb{R}$, where $\operatorname{Im}s$ is the imaginary part of s, and $[s]$ denotes the biggest integer smaller than s.

Decompose the set $\{s\in\mathbb{C}\mid a_{s,i}\neq 0 \text{ for some } j\}$ into a disjoint union of equivalence classes under the equivalence relation $s\sim s'$ if and only if $s=\pm s'$ (mod$\mathbb{Z}$). Pick a representative s in an equivalence class S such that $s=0$ if the equivalence class is in $\mathbb{Z}$ and $s=\frac{1}{2}$ if the equivalence class is in $\mathbb{Z}+\frac{1}{2}$. Let $S=\{s, s-k_1, s-k_2, \dots\}$ be such an equivalence class and take $m=\max_{s\in S}m_s$. Put $k_0=0$. It is easy to see that if $s=0$ or $\frac{1}{2}$, then $k_i\in\mathbb{N}$.

We associate to S the $\mathfrak{g}^{[m]}$-module $L_S^{[m]}(\lambda_S)$ in the following way: If $s\notin\mathbb{Z}/2$, let ${}^{a}h_{k_r}^{(i)}=a_{s+k_r}$ with $i=0,\dots,m_s$ and $r=0,1,2,\dots$. We associate to S the $\widehat{g\ell}_\infty^{[m]}$-module $L_S^{[m]}(\lambda_S)$ with central charges and labels

$$c_i=\sum_{k_r}\ {}^{a}h_{k_r}^{(i)},\quad {}^{a}\lambda_j^{(i)}=\sum_{k\geqslant j}\ ({}^{a}h_k^{(i)}-c_i\delta_{k0}).$$

Similarly, if $s\in\mathbb{Z}/2$ (i.e., $s=0$ or $s=\frac{1}{2}$), let ${}^{c}h_{k_r}^{(i)}=a_{s+k_r}$ with $i=0,\dots,m_s$ and $r=0,1,2,\dots$. We associate to S the $c_\infty^{[m]}$-module $L_S^{[m]}(\lambda_S)$ with central charges and labels

$$c_i=\sum_{k_r}\ {}^{c}h_{k_r}^{(i)}\ \ (i\ \text{ even}),\quad c_i=0\ \ (i\ \text{ odd}),\quad {}^{c}\lambda_j^{(i)}=\sum_{k\geqslant j}\ {}^{c}h_k^{(i)},$$

where $j\in\mathbb{N}$ and $i=0,\dots,m_s$. Denote by $\{s_1, s_2, \dots, s_N\}$ a set of representatives of equivalence classes in the set $\{s\in\mathbb{C}\mid a_{s,i}\neq 0 \text{for some } j\}$. By Theorem 6.3, the $\widehat{\mathcal{D}_{\theta,x}}$-module $L_{\vec{s}}^{[\vec{m}]}(\vec{\lambda})$ is irreducible for $\vec{s}=(s_1, s_2, \dots, s_N)$ such that $s_i\in\mathbb{Z}$ implies $s_i=0$, $s_i\in\mathbb{Z}+\frac{1}{2}$ implies $s_i=\frac{1}{2}$, and $s_i\neq\pm s_j \ \text{mod}\mathbb{Z}$ for $i\neq j$. Then we have

$$\Delta_{\vec{m},\vec{s},\vec{\lambda}}(x)=\sum_i\ \Delta_{m_i,s_i,\lambda_i}(x),\quad c=\sum_i\ c_0(i).$$

Using Theorem 6.3 and Propositions 6.4–6.6, we have proved the following.

Theorem 6.7: *Let V be an irreducible quasifinite highest weight $\widehat{\mathcal{D}_{\theta,x}}$-module with central charge c and*

$$\Delta(x)=\frac{\phi_\lambda(x)}{\sinh(x/2)}$$

with $\phi_\lambda(x)$ *an even quasipolynomial such that* $\phi_\lambda(0)=0$, *written in the form (6.8). Then V is isomorphic to the tensor product of the modules* $L_S^{[m]}(\lambda_S)$ *with distinct equivalence classes S.*

Remark 6.8: A different choice of the representative $s \notin \mathbb{Z}/2$ in S has the effect of shifting $\widehat{g\ell}_\infty^{[m]}$ via the automorphism ν^i for some i. It is easy to see that any irreducible quasifinite highest weight module $L(\widehat{\mathcal{D}_{\theta,x}},\lambda)$ can be obtained as above as a unique way up to the shift ν.

ACKNOWLEDGMENTS

The authors were supported in part by Conicet, ANPCyT, Agencia Cba Ciencia, Secyt-UNC and Fomec (Argentina). Special thanks go to MSRI (Berkeley) for the hospitality during our stay there, where part of this work was done.

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A bicategorical approach to Morita equivalence for von Neumann algebras

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(Received 12 June 2002; accepted 29 January 2003)

We relate Morita equivalence for von Neumann algebras to the ''Connes fusion'' tensor product between correspondences. In the purely algebraic setting, it is well known that rings are Morita equivalent iff they are equivalent objects in a bicategory whose 1-cells are bimodules. We present a similar result for von Neumann algebras. We show that von Neumann algebras form a bicategory, having Connes's correspondences as 1-morphisms, and (bounded) intertwiners as 2-morphisms. Further, we prove that two von Neumann algebras are Morita equivalent iff they are equivalent objects in the bicategory. The proofs make extensive use of the Tomita–Takesaki modular theory. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1563733]

I. INTRODUCTION

A recent trend in the interaction between operator algebras and quantum physics is the appearance of the notion of Morita equivalence[17] in both string theory[20] and quantization theory.[18,13] Furthermore, the tensor product between so-called correspondences of von Neumann algebras constructed by Connes[7] and Sauvageot[19] has played a useful role in conformal field theory[24] as well as in the theory of constrained quantization.[15] This tensor product is defined through the modular theory of operator algebras due to Tomita and Takesaki,[21,11,7] whose importance in quantum field theory has been particularly emphasized by Borchers.[3]

The purpose of the present paper is to relate the Connes–Sauvageot tensor product to Morita equivalence for von Neumann algebras. This will be done in a certain categorical setting, which itself was inspired by quantum field theory.[14] Namely, we work in the framework of bicategories.[2,16] Introduced by Bénabou in 1967,[2] bicategories form a generalization of monoidal categories (a monoidal category is a bicategory with one object). Monoidal categories now form a standard tool in the analysis of superselection sectors.[8] Our main result is that von Neumann algebras form a bicategory in which the morphisms are correspondences composed by the above-mentioned tensor product, and that two von Neumann algebras are Morita equivalent iff they are equivalent objects in this bicategory. This insight should have important applications to all areas mentioned.

The notion of Morita equivalence was originally introduced for rings. Two rings R,S are called Morita equivalent when their respective categories of right modules, $\mathfrak{M}_R$ and $\mathfrak{M}_S$, are equivalent. Rieffel introduced the notion of Morita equivalence for von Neumann algebras.[17] He called two von Neumann algebras $\mathfrak{M}$, $\mathfrak{N}$ Morita equivalent when their categories of normal unital *-representations, Rep($\mathfrak{M}$) and Rep($\mathfrak{N}$), are equivalent, where the equivalence is implemented by a normal *-functor. In this paper we will use an equivalent definition: Two von Neumann algebras $\mathfrak{M}$, $\mathfrak{N}$ are Morita equivalent when a correspondence $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$ exists for which the representation of $\mathfrak{M}$ on $\mathcal{H}$ is faithful and $\mathfrak{M}'\simeq\mathfrak{N}^{op}$ holds. The goal of this paper is to show a similarity between Morita equivalence for rings and for von Neumann algebras.[1,9]

As a tool, we will use bicategories.[2,16] Bicategories allow a composition of arrows that is

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associative only up to a family of isomorphisms. Strictly associative bicategories are 2-categories. For instance, the class of categories as objects, functors as 1-morphisms and natural transformations as 2-morphisms form a 2-category. Another example is the 2-category of topological spaces as objects, continuous maps as 1-morphisms, and homotopy classes of continuous maps as 2-morphisms. Each (relaxed) monoidal category M forms a bicategory, which in general is not a 2-category. This bicategory consists of one object (M); the objects of the category M form 1-morphisms of the bicategory. A composition functor $M\times M\rightarrow M$ that is associative up to isomorphism exists, since M is monoidal. The arrows M_1 of the category M form the 2-morphisms of the bicategory. The natural isomorphisms that are associated to the monoidal category ascertain that the coherence axioms for a bicategory are satisfied.

Further instructive examples of bicategories are the bicategory [Rings] and the bicategory [W*]. The bicategory [Rings] consists of rings as objects, bimodules as 1-morphisms, and bimodule maps as 2-morphisms. Similarly, but adding the appropriate analytical structure, the bicategory [W*] consists of von Neumann algebras as objects, correspondences as 1-morphisms, and bounded intertwiners as 2-morphisms.

Although from a categorical point of view the fact that Morita equivalence for rings is equivalent to equivalence in the bicategory is straightforward[2,5,16] (and some would say tautological, see cf. Refs. 22 and 23), the corresponding situation for von Neumann algebras is highly nontrivial for analytical reasons. For example, the fact that the coherence axiom in the definition of a bicategory is satisfied in our case has to be proved with the aid of Tomita–Takesaki modular theory. The same is true for our second main result, which we have already mentioned: two von Neumann algebras are Morita equivalent iff they are equivalent objects in [W*].

This paper is an abbreviated version of Ref. 5. All routine calculations may be found there, including a simple account of the bicategorical approach to Morita theory for rings.

Section II discusses the case of von Neumann algebras. First, we will prepare for the construction of the bicategory [W*] of von Neumann algebras. We will use the concept of ''Connes fusion'' [7,19] for the composition functor in this bicategory. This terminology is due to Wasserman.[24] Second, we will show that von Neumann algebras indeed form a bicategory. Finally, we will prove that two von Neumann algebras are Morita equivalent iff they are equivalent objects in the bicategory [W*].

II. THE BICATEGORY OF VON NEUMANN ALGEBRAS

As a preparation for the main result of this paper, consider the following definition, due to Connes.[7]

Definition II.1: *Let $\mathfrak{M},\mathfrak{N}$ be von Neumann algebras, $\mathcal{H}$ a Hilbert space. Suppose π_l is a normal unital representation of $\mathfrak{M}$ on $\mathcal{H}$ and π_r is a normal unital representation of $\mathfrak{N}^{op}$ on $\mathcal{H}$ (or equivalently, an antirepresentation of $\mathfrak{N}$) such that the actions of $\pi_l(\mathfrak{M})$ and $\pi_r(\mathfrak{N})$ commute. The triple $[\pi_l,\pi_r,\mathcal{H}]$ is called a correspondence, denoted by $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$. We write $x\eta$ instead of $\pi_l(x)\eta$ and ηy instead of $\pi_r(y)\eta$, for $x\in\mathfrak{M}$, $\eta\in\mathcal{H}$, $y\in\mathfrak{N}$.*

Viewing a von Neumann algebra as a ring, a correspondence may be seen as a bimodule. Examples of correspondences are not difficult to find. Suppose we have a normal, unital representation of a von Neumann algebra $\mathfrak{M}$ on a Hilbert space $\mathcal{H}$. Then we immediately have a correspondence

$$\mathfrak{M}\rightarrow\mathcal{H}\leftarrow(\mathfrak{M}')^{op}. \tag{1}$$

We will use the following notation. Let ϕ be a faithful normal semifinite weight on a von Neumann algebra $\mathfrak{M}$. Let $\mathfrak{M}_\phi=\{x\in\mathfrak{M}\mid \phi(x^*x)<\infty\}$ and let $\mathcal{H}_\phi$ be the Hilbert space, formed by completion of $\mathfrak{M}_\phi$ in the inner product originating from ϕ. The canonical inclusion will be denoted by $\Lambda_\phi:\mathfrak{M}_\phi\rightarrow\mathcal{H}_\phi$. The associated modular conjugation and modular operator will be denoted by J_ϕ and Δ_ϕ, respectively. The specific choice of ϕ merely affects these data, known as a standard form of $\mathfrak{M}$, up to unitary equivalence.[10]

Definition II.2: *An* identity correspondence *of a von Neumann algebra $\mathfrak{M}$ is given by a Hilbert space $\mathcal{H}_\phi$ as above, with left representation π_l and right representation π_r defined on the dense subspace $\Lambda_\phi(\mathfrak{M}_\phi)\subset\mathcal{H}_\phi$ by* (2) *and* (3),

$$\begin{aligned}&\pi_l:\mathfrak{M}\to\mathcal{B}(\mathcal{H}_\phi),\\ &\pi_l(x)\Lambda_\phi(\eta)=\Lambda_\phi(x\eta),\end{aligned}\tag{2}$$

and

$$\begin{aligned}&\pi_r:\mathfrak{M}\to\mathcal{B}(\mathcal{H}_\phi),\\ &\pi_r(x)\Lambda_\phi(\eta)=J_\phi\pi_l(x^*)J_\phi\Lambda_\phi(\eta).\end{aligned}\tag{3}$$

We will subsequently omit Λ_ϕ when no confusion arises.

Note that an identity correspondence is a special case of (1), since we have $J_\phi\mathfrak{M}J_\phi\cong\mathfrak{M}'$ by Tomita–Takesaki theory. Since the standard form of a von Neumann algebra is unique up to unitary equivalence,[10] so is an identity correspondence. Hence we will often write

$$\mathfrak{M}\to\mathfrak{L}^2(\mathfrak{M})\leftarrow\mathfrak{M},$$

for an identity correspondence, suppressing the weight ϕ. The notation $\mathfrak{L}^2(\mathfrak{M})$ is chosen in analogy to measure theory; recall that the latter is considered to be the commutative version of von Neumann algebras. For $\mathfrak{M}=\mathfrak{L}^\infty(X,\mu)$ one has $\mathfrak{L}^2(\mathfrak{M})\simeq\mathfrak{L}^2(X,\mu)$.

As a preparation for the construction of the bicategory [W*], we will now review the concept of Connes fusion, or the relative tensor product, see Refs. 6, 7, and 19.

Let $\mathfrak{M}\to\mathcal{H}\leftarrow\mathfrak{N}$ and $\mathfrak{N}\to\mathcal{K}\leftarrow\mathfrak{P}$ be two correspondences. Let ϕ be an arbitrary faithful normal semifinite weight on $\mathfrak{N}$. To obtain the relative tensor product $\mathfrak{M}\to\mathcal{H}\boxtimes_{\mathfrak{N}}\mathcal{K}\leftarrow\mathfrak{P}$, one defines a form $(\ ,\ )_0$ on the algebraic tensor product $D(\mathcal{H},\phi)\otimes_{\mathbb{C}}\mathcal{K}$, quotients by the null space, and completes. Here $D(\mathcal{H},\phi)$ is the dense subspace of *ϕ-bounded vectors* of $\mathcal{H}$, defined by

$$D(\mathcal{H},\phi)=\{\eta\in\mathcal{H}\mid\exists c:\forall y\in\mathfrak{N}_\phi,\ \|\pi_r(y)\eta\|_{\mathcal{H}}\leqslant c\,\phi(y^*y)\}.$$

Equivalently, one can define $D(\mathcal{H},\phi)$ as the set of $\eta\in\mathcal{H}$ for which the operator $R_\eta^\phi:\mathcal{H}_\phi\to\mathcal{H}$, is bounded, where R_η^ϕ is defined on the dense subspace $\mathfrak{N}_\phi\subset\mathfrak{N}$ by

$$R_\eta^\phi(J_\phi\Lambda_\phi(y^*))=\pi_r(y)\eta,\quad\forall y\in\mathfrak{N}_\phi.$$

Recall that $\mathcal{H}_\phi$ is a standard Hilbert space of $\mathfrak{N}$.

For later use, we will state some properties of R_η. The proof is easy calculation. For all $\eta_1,\eta_2\in D(\mathcal{H},\phi),x\in\mathfrak{N}$, we have

$$R_{\eta_1}^*R_{\eta_2}\in\mathfrak{N},\tag{4}$$

$$\Delta^{-1/2}x^*\Delta^{1/2}R_{\eta_1}^*R_{\eta_2}=R_{\eta_1 x}^*R_{\eta_2}\ \text{ on }\ \mathfrak{L}^2(\mathfrak{N}),\tag{5}$$

$$R_{\eta_1}^*R_{\eta_2}\Delta^{1/2}x\Delta^{-1/2}=R_{\eta_1}^*R_{\eta_2 x}\ \text{ on }\ \mathfrak{L}^2(\mathfrak{N}).\tag{6}$$

Further, we need a subspace $\mathfrak{N}_0\subset\mathfrak{N}$ that will be used later (Remark II.4). $\mathfrak{N}_0$ is defined as follows. Let $\tau_t(x)=\Delta_\phi^{it}x\Delta_\phi^{-it}$, $x\in\mathfrak{N}$, be the modular automorphism group of $\mathfrak{N}$, let

$$x_n=\sqrt{n/\pi}\int dt\,e^{-nt^2}\tau_t(x),\quad n=1,2,\ldots$$

and finally set

$$\mathfrak{N}_0 = \mathrm{Span}\{x_n | x \in \mathfrak{N}_\phi, \quad n = 1,2,\ldots\}.$$

Lemma II.3: In the above notation, $x_n \to x$ σ-weakly. Moreover, $\mathfrak{N}_0$ is a σ-dense and norm-dense subspace of $\mathfrak{N}_\phi$. Further, for $\xi \in \mathfrak{N}_0$,

$$\Delta^{1/2} \xi \Delta^{-1/2} \in \mathfrak{N}_\phi.$$

Proof: Compare Ref. 5 for details. The proof follows from the analyticity of the elements of $\mathfrak{N}_0$, see Ref. 4, and positivity and modular invariance of the weight ϕ. See also Ref. 21. □

To detail, the sesquilinear form $(\ ,\ )_0$ on $D(\mathcal{H},\phi) \otimes_{\mathbb{C}} \mathcal{K}$ is defined by

$$(\eta_1 \otimes \zeta_1, \eta_2 \otimes \zeta_2)_0 := \langle \zeta_1, R^*_{\eta_1} R_{\eta_2} \zeta_2 \rangle_{\mathcal{K}},$$

where $\langle\ ,\ \rangle_{\mathcal{K}}$ is the inner product on the Hilbert space $\mathcal{K}$. Note that since $R^*_{\eta_1} R_{\eta_2}$ is an element of $\mathfrak{N}$ by (4), the second argument of the inner product is indeed an element of $\mathcal{K}$. It is easy to see that $(\ ,\ )_0$ is a pre-inner product. Hence, if we quotient by the null space $\mathcal{N}$ and complete, we obtain a Hilbert space, denoted by $\mathcal{H} \boxtimes_{\mathfrak{N}} \mathcal{K}$. This Hilbert space $\mathcal{H} \boxtimes_{\mathfrak{N}} \mathcal{K}$ is an $\mathfrak{M} \to \mathcal{H} \boxtimes_{\mathfrak{N}} \mathcal{K} \leftarrow \mathfrak{P}$ correspondence, so that we may regard the above construction as the fusion of correspondences rather than merely as Hilbert spaces. Namely, we let the representations of $\mathfrak{M}$ on $\mathcal{H}$ and of $\mathfrak{P}$ on $\mathcal{K}$ descend to the quotient. Routine verification will show that the null space is closed under the actions of $\mathfrak{M}$ and $\mathfrak{P}$.

Remark II.4: The relative tensor product $\boxtimes_{\mathfrak{N}}$ has a property analogous to the balancedness of the tensor product of bimodules over rings, but with a crucial and interesting modification. Balancedness for a ring R and bimodules ${}_R M_R N$ means we have $(mr \otimes_R n) = (m \otimes_R rn)$, for $m \in M_R, n \in {}_R N, r \in R$. However, for $\eta \in \mathcal{H}, n \in \mathfrak{N}_0$, and $\zeta \in \mathcal{K}$ we have

$$\eta n \boxtimes_{\mathfrak{N}} \zeta = \eta \boxtimes_{\mathfrak{N}} (\Delta^{1/2} n \Delta^{-1/2}) \zeta, \tag{7}$$

and

$$\eta \boxtimes_{\mathfrak{N}} n \zeta_1 = \eta (\Delta^{-1/2} n \Delta^{1/2}) \boxtimes_{\mathfrak{N}} \zeta. \tag{8}$$

Let $\eta_2 \in D(\mathcal{H},\phi), x \in \mathfrak{N}_0, \zeta_2 \in \mathcal{K}$; then

$$\begin{aligned}(\eta_1 x \otimes \zeta_1, \eta_2 \otimes \zeta_2)_0 &= \langle \zeta_1, R^*_{\eta_1 x} R_{\eta_2} \zeta_2 \rangle_{\mathcal{K}} \\ &= \langle \zeta_1, (\Delta^{-1/2} x^* \Delta^{1/2}) R^*_{\eta_1} R_{\eta_2} \zeta_2 \rangle_{\mathcal{K}} \\ &= \langle (\Delta^{1/2} x \Delta^{-1/2}) \zeta_1, R^*_{\eta_1} R_{\eta_2} \zeta_2 \rangle_{\mathcal{K}} \\ &= (\eta_1 \otimes (\Delta^{1/2} x \Delta^{-1/2}) \zeta_1, \eta_2 \otimes \zeta_2)_0, \end{aligned} \tag{9}$$

where the second equality holds because of (5). This implies that $(\eta_1 x \otimes \zeta_1) - (\eta_1 \otimes (\Delta^{1/2} x \Delta^{-1/2}) \zeta_1)$ belongs to the null space $\mathcal{N}$. Since $\mathfrak{N}_0$ is a dense subspace of $\mathfrak{N}_\phi$, (7) holds for the completion $\mathcal{H} \boxtimes_{\mathfrak{N}} \mathcal{K}$. Moreover, for $x \in \mathfrak{N}_0$, we have $\Delta^{1/2} x \Delta^{-1/2} \in \mathfrak{N}$ so that all expressions in (9) are defined. The proof of (8) follows by a similar argument.

Now, we will show that the collection of von Neumann algebras forms a bicategory. This result was already stated in Ref. 14 without proof.

Proposition II.5: For any two von Neumann algebra's $\mathfrak{M}$, $\mathfrak{N}$, let $(\mathfrak{M},\mathfrak{N})$ be the category of correspondences as objects, and bounded linear bimodule maps as arrows. Then there exists a bicategory $[\mathsf{W}^*]$ with von Neumann algebras as objects and correspondences as 1-morphisms. The composition functor $(\mathfrak{M},\mathfrak{N}) \times (\mathfrak{N},\mathfrak{P}) \to (\mathfrak{M},\mathfrak{P})$ is given by the relative tensor product $\boxtimes_{\mathfrak{N}}$, and the unit arrow in $(\mathfrak{M},\mathfrak{M})$ is given by $I_{\mathfrak{M}} = \mathfrak{M} \to \mathfrak{L}^2(\mathfrak{M}) \leftarrow \mathfrak{M}$.

Proof: Unlike the case of rings, a nontrivial issue arises in the verification, related to Remark II.4. We will only stress the points at which the verification is not straightforward. The natural

isomorphism to obtain associativity is defined element wise and hence the existence of associativity coherence is routine calculation. The difficulty lies in the construction of the left and right identities and identity coherence.

For each pair of von Neumann algebras $(\mathfrak{M},\mathfrak{N})$, the so-called left identity $L_{(\mathfrak{M},\mathfrak{N})}$ is a natural isomorphism between the functors $\mathfrak{L}^2(\mathfrak{M})\boxtimes_{\mathfrak{M}(-)}$ and the identity functor $Id(\mathfrak{M})$ from $(\mathfrak{M}\mathfrak{N})$ to $(\mathfrak{M},\mathfrak{N})$.

More concretely, recall that $\Lambda_\phi:\mathfrak{M}_\phi\to\mathfrak{L}^2(\mathfrak{M})$ denotes the inclusion map. It satisfies

$$\begin{aligned} x\Lambda_\phi(y)&=\Lambda_\phi(xy),\\ \Delta_\phi^{1/2}\Lambda_\phi(y)&=\Lambda_\phi(\Delta_\phi^{1/2}y\Delta_\phi^{-1/2}), \end{aligned} \tag{10}$$

for $x\in\mathfrak{M}, y\in\mathfrak{M}_0$. See Ref. 11.

Let $x\in\mathfrak{M}_0, \zeta\in\mathcal{K}$. Then, we define $L_{(\mathfrak{M},\mathfrak{N})}$ on the dense subspace $\mathfrak{M}_0\boxtimes_{\mathfrak{M}}\mathcal{K}$ by

$$L_{(\mathfrak{M},\mathfrak{N})}:\ \Lambda_\phi(x)\boxtimes_{\mathfrak{M}}\zeta\mapsto x\zeta. \tag{11}$$

We will show that the map (11) is continuous, so that we may extend it to $\mathfrak{L}^2(\mathfrak{M})\boxtimes_{\mathfrak{M}}\mathcal{K}$. Consider

$$\|\Lambda_\phi(x)\boxtimes_{\mathfrak{M}}\zeta\|^2=\langle\zeta,R^*_{\Lambda_\phi(x)}R_{\Lambda_\phi(x)}\zeta\rangle_{\mathcal{K}}.$$

Observe that in this case, by definition of the right representation of $\mathfrak{M}$ on $\mathfrak{L}^2(\mathfrak{M})$, the operator $R_{\Lambda_\phi(x)}:\mathfrak{L}^2(\mathfrak{M})\to\mathfrak{L}^2(\mathfrak{M})$ is given by

$$R_{\Lambda_\phi(x)}J_\phi\Lambda_\phi(y^*)=\pi_r(y)\Lambda_\phi(x)=J_\phi y^*J_\phi\Lambda_\phi(x),$$

on the dense subspace $\mathfrak{M}_0$.

The following claims lead to continuity of the map (11). The proofs are easy calculations.

For $x,z\in\mathfrak{M}_0$, we have $R_{\Lambda_\phi(x)}\Lambda_\phi(z)=\Lambda_\phi(xz)$.

For $x\in\mathfrak{M}_0$, the operator $R^*_{\Lambda_\phi(x)}R_{\Lambda_\phi(x)}$ equals $\Lambda_\phi(x^*x)$ as operators on $\mathfrak{L}^2(\mathfrak{M})$.

Combining the statements above we obtain

$$\|\Lambda_\phi(x)\boxtimes_{\mathfrak{M}}\zeta\|^2=\langle\zeta,R^*_{\Lambda_\phi(x)}R_{\Lambda_\phi(x)}\zeta\rangle_{\mathcal{K}}=\|x\zeta\|^2_{\mathcal{K}}. \tag{12}$$

Hence $\Lambda_\phi(x)\boxtimes_{\mathfrak{M}}\zeta\mapsto x\zeta$ is a continuous map. It remains to show that $L_{(\mathfrak{M},\mathfrak{N})}$ is unitary and hence a natural isomorphism. We know that it is isometric by (12). Hence it is sufficient to show that the image of $\mathfrak{M}_0\boxtimes\mathcal{K}$ is dense in $\mathcal{K}$. Generally, $\mathbb{1}\in\mathfrak{M}$ is not an element of $\mathfrak{M}_\phi$. But, since $\mathfrak{M}_0$ is norm-dense in $\mathfrak{M}$, we may find a net $\mathcal{E}_\alpha$ in $\mathfrak{M}_0$, converging in norm to 1. Let $\zeta\in\mathcal{K}$. Then

$$\|\mathcal{E}_\alpha\zeta-\mathbb{1}\zeta\|_{\mathcal{K}}\leqslant\|\mathcal{E}_\alpha-\mathbb{1}\|_{\mathfrak{M}}\cdot\|\zeta\|_{\mathcal{K}}\to 0,$$

where we used the fact that a representation is norm decreasing. Hence, $\mathfrak{M}_0\mathcal{K}$ is dense in $\mathcal{K}$.

In contrast to the case of rings, the right identity $R_{(\mathfrak{M},\mathfrak{N})}$ is defined differently from the left identity. The right identity should be a natural isomorphism between the functor $(-)\boxtimes_{\mathfrak{N}}\mathfrak{L}^2(\mathfrak{N})$ and the identity $Id(\mathfrak{M},\mathfrak{N})$. Let $\mathcal{H}\in(\mathfrak{M},\mathfrak{N})\ \eta\in D(\mathcal{H},\phi), y\in\mathfrak{N}_0$. Then we define $R_{(\mathfrak{M},\mathfrak{N})}$ on the dense subspace $D(\mathcal{H},\phi)\boxtimes_{\mathfrak{N}}\mathfrak{N}_0$ by

$$R_{(\mathfrak{M},\mathfrak{N})}:\ \eta\boxtimes_{\mathfrak{N}}\Lambda_\phi(y)\mapsto\eta(\Delta_\phi^{-1/2}y\Delta_\phi^{1/2}). \tag{13}$$

Note that $\Delta_\phi^{-1/2} y \Delta_\phi^{1/2} \in \mathfrak{N}$, for $y \in \mathfrak{N}_0$, so that $\eta(\Delta_\phi^{-1/2} y \Delta_\phi^{1/2})$ is defined by definition of the right representation of $\mathfrak{N}$ on $\mathcal{H}$. We will show next that the map (13) is continuous, so that we may extend it to $\mathcal{H} \boxtimes_{\mathfrak{N}} \mathfrak{L}^2(\mathfrak{N})$. Consider

$$\| \eta \boxtimes_{\mathfrak{N}} \Lambda_\phi(y) \|^2 = (\Lambda_\phi(y), R_\eta^* R_\eta \Lambda_\phi(y))_{\mathfrak{L}^2(\mathfrak{N})}.$$

In this case, the operator $R_\eta : \mathfrak{L}^2(\mathfrak{N}) \to \mathcal{H}$ is defined by

$$R_\eta J_\phi \Lambda_\phi(y^*) = \pi_r(y)\eta = \eta y,$$

on the dense subspace $\mathfrak{N}_0$.

We make use of the following fact, proven by Connes (Ref. 6 Lemma 4). For $\zeta \in D(\mathcal{H}, \phi)$, we have

$$\phi(R_\zeta^* R_\zeta) = \| \zeta \|_{\mathcal{H}}^2.$$

Hence, using (5) and (6), we obtain

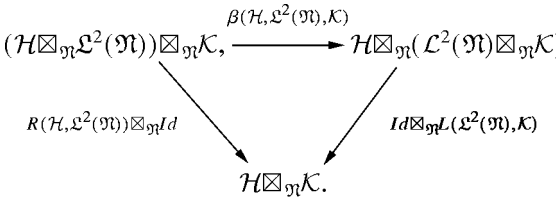
$$\begin{aligned} \| \eta \boxtimes_{\mathfrak{N}} \Lambda_\phi(y) \|^2 &= (\Lambda_\phi(y), R_\eta^* R_\eta \Lambda_\phi(y))_{\mathfrak{L}^2(\mathfrak{N})} \\ &= \phi(y^* R_\eta^* R_\eta y) \\ &= \phi(R^*_{\eta(\Delta_\phi^{-1/2} y \Delta_\phi^{1/2})} R_{\eta(\Delta_\phi^{-1/2} y \Delta_\phi^{1/2})}) \\ &= \| \eta(\Delta_\phi^{-1/2} y \Delta_\phi^{1/2}) \|_{\mathcal{H}}^2. \end{aligned} \tag{14}$$

Hence $\eta \boxtimes_{\mathfrak{N}} \Lambda_\phi(y) \mapsto \eta(\Delta_\phi^{1/2} y \Delta_\phi^{-1/2})$ is a continuous map. It is left to show that $R_{(\mathfrak{M},\mathfrak{N})}$ is unitary and hence a natural isomorphism. As above, (14) shows that it is isometric, hence it is sufficient to show that the image of $D(\mathcal{H}, \phi) \boxtimes \mathfrak{N}_0$ is dense in $\mathcal{H}$. As before, we have a net $\mathcal{E}_\alpha$ in $\mathfrak{N}_0$ converging to $\mathbb{1}$. Consider the net $\Delta_\phi^{1/2} \mathcal{E}_\alpha \Delta_\phi^{-1/2}$. This net is contained in $\mathfrak{N}_\phi$, as follows from Lemma II.3. By the inclusion $\mathfrak{N}_0 \subset \mathfrak{N}_\phi \subset \mathfrak{L}^2(\mathfrak{N})$ and the continuity just proven, we have

$$\Delta_\phi^{1/2} \mathcal{E}_\alpha \Delta_\phi^{-1/2} \boxtimes_{\mathfrak{N}} \eta \mapsto \eta \mathcal{E}_\alpha,$$

for $\eta \in D(\mathcal{H}, \phi)$. The right-hand side converges to η in norm. The observation that $D(\mathcal{H}, \phi) \subset \mathcal{H}$ is a dense subspace finishes the proof.

Finally, we need to prove identity coherence. Let $\mathfrak{M}$, $\mathfrak{N}$, $\mathfrak{P}$ be von Neumann algebras and ${}_{\mathfrak{M}}\mathcal{H}_{\mathfrak{N}}$ and ${}_{\mathfrak{N}}\mathcal{K}_{\mathfrak{P}}$ associated correspondences. It will be shown that the following diagram commutes:



Since the upper arrow $\beta(\mathcal{H}, \mathfrak{L}^2(\mathfrak{N}), \mathcal{K})$ is the associativity isomorphism, identity coherence boils down to

$$(\eta(\Delta_\phi^{-1/2} n \Delta_\phi^{1/2}) \boxtimes_{\mathfrak{N}} \zeta) \cong (\eta \boxtimes_{\mathfrak{N}} n\zeta),$$

for $\eta \in \mathcal{H}$, $n \in \mathfrak{L}^2(\mathfrak{N})$, $\zeta \in \mathcal{K}$. This follows immediately from Remark II.4. □

Note that the bicategory of von Neumann algebras, constructed as above, depends on the choice of a faithful normal semifinite weight for each von Neumann algebra, because the defini-

tion of the composition functor (i.e., the relative tensor product) depends on this choice. However, different weights lead to unitarily equivalent relative tensor products.[19] Hence the bicategory depends on the chosen weights only up to isomorphism.

III. MORITA THEORY FOR VON NEUMANN ALGEBRAS

The notion of Morita equivalence for von Neumann algebras was originally introduced by Rieffel. Two von Neumann algebras $\mathfrak{M}$, $\mathfrak{N}$ are said to be Morita equivalent if their representation categories Rep($\mathfrak{M}$) and Rep($\mathfrak{N}$) are equivalent, where the equivalence is implemented by a normal *-functor. Here Rep($\mathfrak{M}$) denotes the category of normal unital *-representations on Hilbert spaces as objects, and bounded linear intertwiners as arrows. For our purposes, we will use the following (equivalent) definition.

Definition III.1: Two von Neumann algebras $\mathfrak{M}$, $\mathfrak{N}$ *are called* Morita equivalent, *if a correspondence* $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$ *exists, where the representation of* $\mathfrak{M}$ *on* $\mathcal{H}$ *is faithful and for which*

$$\mathfrak{M}'\simeq\mathfrak{N}^{op}.$$

Note that faithfulness of $\mathfrak{M}$ directly implies faithfulness for $\mathfrak{N}$. Using somewhat different notation, Rieffel (Ref. 17, Theorem 8.5) proves equivalence between the definition above and his original definition. In this paper, we will not follow Rieffel's approach, which involves so-called normal $\mathfrak{N}$-rigged $\mathfrak{M}$-modules, and interior tensor products of these modules. Rieffel proves an Eilenberg–Watts-type theorem (Ref. 17, Theorem 5.5), which states that all functors of Rep($\mathfrak{N}$) to Rep($\mathfrak{M}$) are equivalent to taking the tensor product with such a normal $\mathfrak{N}$-rigged $\mathfrak{M}$-module. However, these modules are not Hilbert spaces, which is what we would like considering our definition of the tensor product and the bicategory of von Neumann algebras.

Now we are ready for the main theorem.

Theorem III.2: *Two von Neumann algebras are equivalent objects in the bicategory* [W*] *iff they are Morita equivalent.*

Proof: First, let us reformulate the first property in the theorem. The property that two von Neumann algebras $\mathfrak{M}$,$\mathfrak{N}$ are equivalent objects in the bicategory means that there must be an arrow in ($\mathfrak{M}$, $\mathfrak{N}$), i.e., a correspondence $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$ that is invertible up to isomorphism. In other words, there exists an arrow $\mathfrak{N}\rightarrow\mathcal{H}^{-1}\leftarrow\mathfrak{M}$ in ($\mathfrak{N}$, $\mathfrak{M}$), such that

$$\mathfrak{M}\rightarrow\mathcal{H}\boxtimes_{\mathfrak{N}}\mathcal{H}^{-1}\leftarrow\mathfrak{M}\cong\mathfrak{M}\rightarrow\mathfrak{L}^2(\mathfrak{M})\leftarrow\mathfrak{M}\quad\text{in}\quad(\mathfrak{M},\mathfrak{M}),\tag{16}$$

$$\mathfrak{N}\rightarrow\mathcal{H}^{-1}\boxtimes_{\mathfrak{M}}\mathcal{H}\leftarrow\mathfrak{N}\cong\mathfrak{N}\rightarrow\mathfrak{L}^2(\mathfrak{N})\leftarrow\mathfrak{N}\quad\text{in}\quad(\mathfrak{N},\mathfrak{N}).\tag{17}$$

"$\Leftarrow$:" Let $\mathfrak{M}$,$\mathfrak{N}$ be Morita equivalent. Then we have a correspondence $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$, where the representation of $\mathfrak{M}$ on $\mathcal{H}$ is faithful, and $\mathfrak{M}'\simeq\mathfrak{N}^{op}$. From $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$, we can define a correspondence $\mathfrak{N}\rightarrow\overline{\mathcal{H}}\leftarrow\mathfrak{M}$ by

$$n\,\overline{\eta}m:=m^*\eta n^*,\qquad\text{for}\quad n\in\mathfrak{N},m\in\mathfrak{M},\eta\in\mathcal{H},$$

where $\overline{\mathcal{H}}$ is $\mathcal{H}$ as a set, with the addition operator of $\mathcal{H}$ and conjugate scalar multiplication and inner product. Sauvageot (Ref. 19, Prop. 3.1) proves that the induced representation of $\mathfrak{M}$ on the relative tensor product $\mathcal{H}\boxtimes_{\mathfrak{N}}\overline{\mathcal{H}}$ is in standard form, hence

$$\mathfrak{M}\rightarrow\mathcal{H}\boxtimes_{\mathfrak{N}}\overline{\mathcal{H}}\leftarrow\mathfrak{M}\cong\mathfrak{M}\rightarrow\mathfrak{L}^2(\mathfrak{M})\leftarrow\mathfrak{M}.\tag{18}$$

Applying the same reasoning to $\mathfrak{N}\rightarrow\overline{\mathcal{H}}\leftarrow\mathfrak{M}$, we obtain $\mathfrak{M}\rightarrow\bar{\bar{\mathcal{H}}}\leftarrow\mathfrak{N}$ and clearly, we have $\bar{\bar{\mathcal{H}}}=\mathcal{H}$. Then

$$\mathfrak{N}\rightarrow\overline{\mathcal{H}}\boxtimes_{\mathfrak{M}}\bar{\bar{\mathcal{H}}}\leftarrow\mathfrak{N}=\mathfrak{N}\rightarrow\overline{\mathcal{H}}\boxtimes_{\mathfrak{M}}\mathcal{H}\leftarrow\mathfrak{N}\cong\mathfrak{N}\rightarrow\mathfrak{L}^2(\mathfrak{N})\leftarrow\mathfrak{N}.\tag{19}$$

Together, (18) and (19) prove that ${}_{\mathfrak{M}}\mathcal{H}_{\mathfrak{N}}$ is invertible, its inverse being ${}_{\mathfrak{N}}\overline{\mathcal{H}}_{\mathfrak{M}}$.

"$\Rightarrow$:" Suppose we have an invertible correspondence $\mathfrak{M}\rightarrow\mathcal{H}\leftarrow\mathfrak{N}$. We need to show that $\mathfrak{M}\simeq(\mathfrak{N}^{op})'$, and that the representation of $\mathfrak{M}$ is faithful. By definition of a correspondence, we have

$$\mathfrak{M}\subseteq(\mathfrak{N}^{op})', \tag{20}$$

so, considering the representation of $\mathfrak{M}$ on $\mathcal{H}\boxtimes_{\mathfrak{N}}\mathcal{H}^{-1}$, one has

$$\mathfrak{M}\boxtimes id_{\mathcal{H}^{-1}}\subseteq(\mathfrak{N}^{op})'\boxtimes id_{\mathcal{H}^{-1}}. \tag{21}$$

Now we will use a result from Sauvageot (Ref. 19, Prop. 3.3), who shows that for a von Neumann algebra $\mathfrak{P}$ and representations $\mathcal{K}_1\leftarrow\mathfrak{P}$ and $\mathfrak{P}\rightarrow\mathcal{K}_2$, one has

$$(\mathfrak{P}^{op})'\boxtimes_{\mathfrak{P}}id_{\mathcal{K}_2}=[id_{\mathcal{K}_1}\boxtimes_{\mathfrak{P}}\mathfrak{P}']' \tag{22}$$

in $\mathcal{K}_1\boxtimes_{\mathfrak{P}}\mathcal{K}_2$. Applying (22) to (21) we obtain

$$\mathfrak{M}\boxtimes_{\mathfrak{N}}id_{\mathcal{H}^{-1}}\subseteq(\mathfrak{N}^{op})'\boxtimes_{\mathfrak{N}}id_{\mathcal{H}^{-1}}=[id_{\mathcal{H}}\boxtimes_{\mathfrak{N}}\mathfrak{N}']',$$

hence, using the commutant of (22),

$$id_{\mathcal{H}}\boxtimes_{\mathfrak{N}}\mathfrak{N}'\subseteq[\mathfrak{M}\boxtimes_{\mathfrak{N}}id_{\mathcal{H}^{-1}}]'=id_{\mathcal{H}}\boxtimes_{\mathfrak{N}}\mathfrak{M}^{op}. \tag{23}$$

Now (23) implies that $\mathfrak{N}'\subseteq\mathfrak{M}^{op}$ by the definition of the representation of $\mathfrak{N}'$ on $\mathcal{H}\boxtimes_{\mathfrak{N}}\mathcal{H}^{-1}$. This, together with (20), proves $\mathfrak{M}\simeq(\mathfrak{N}^{op})'$. It remains to be shown that the representation of $\mathfrak{M}$ on $\mathcal{H}$ is faithful. However, this follows immediately from (16) and the fact that the standard representation of $\mathfrak{M}$ on $\mathfrak{L}^2(\mathfrak{M})$ is faithful. □

It is possible to restate Theorem III.2 in terms of representation categories. In the light of the remarks after Definition III.1, the proof follows from Rieffel,[17] but we prefer to prove the corollary directly.

Corollary III.3: Two von Neumann algebras are equivalent objects in the bicategory [W*] *iff their representation categories are equivalent, where the equivalence is implemented by a normal* *-*functor*.

Proof: "$\Rightarrow$:" The construction of the equivalence functor, given the invertible correspondence, is completely analogous to the case of rings, cf. Refs. 12 and 14. The fact that this construction yields a *-functor follows from a trivial computation. An application of (Ref. 17, Prop. 7.3) shows that this functor is normal.

"$\Leftarrow$:" Suppose F:Rep($\mathfrak{N}$)$\rightarrow$Rep($\mathfrak{M}$) is a normal *-functor, implementing the categorical equivalence. Consider $F(\mathfrak{L}^2(\mathfrak{M}))$, which has a left $\mathfrak{N}$-action by definition, and a right $\mathfrak{M}$-action through F. Applying the Eilenberg–Watts type theorem stated by Sauvageot (Ref. 19, Prop. 5.3), shows that $F(\mathfrak{L}^2(\mathfrak{M}))$ is invertible. Compare also Rieffel (Ref. 17, Prop. 5.4, Theorem 5.5). □

ACKNOWLEDGMENTS

This paper is based on a conjecture by N.P. Landsman. The author thanks him for his advice and helpful suggestions.

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A new realization for the $d=2$ topological algebra

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(Received 27 September 2002; accepted 31 January 2003)

We derive topological algebras for two-dimensional models admitting a $d=[\delta,b]$ decomposition (with b the BRST operator). In general, the topological algebra we obtain is not derived from the twisting of an $N=2$ supersymmetry algebra. We show, for the particular case of an Abelian model described by a ladder of matter, how to derive $N=2$ supersymmetry generators from the odd generators of the topological algebra. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1565832]

I. INTRODUCTION

Topological algebras appeared originally as a by-product of the twisting of two dimensional $N=2$ supersymmetric models,[1] a procedure that was employed in the description of topological field theories with matter fields. The main characteristic of such algebras lies on the existence of odd generators G_μ, Q $(Q^2=0)$ satisfying $[Q,G_\mu]=P_\mu$, which is an essential ingredient of topological quantum field theories (TQFT).[2] Since the generators Q and G_μ depend on the supersymmetry charge $Q_{\alpha a}$ $(\alpha,a\in\{1,2\};\ (1,2)\equiv(+,-))$ through the combinations $Q:=Q_{+-}+Q_{-+}$ and $G_\mu=(G_1,G_2):=(\frac{1}{2}(Q_{++}+Q_{--}), i/2\,(Q_{++}-Q_{--}))$, it is then clear that the topological algebras constructed in Refs. 1 and 3 arise as a direct consequence of an underlying $N=2$ supersymmetry algebra.

Here, we want to construct topological algebras that are not necessarily related to supersymmetry. Our strategy is to use the results of previous work[4–7] where we have studied the properties of models exhibiting the decomposition

$$d=[\delta,b]. \tag{1}$$

This is the starting point for our discussion of topological algebras. In fact, if we can identify the odd generators G_μ, Q with δ, b, then (1) becomes a natural realization of $[G_\mu,Q]=P_\mu$. Relation (1) has appeared in several different contexts. For example, in Ref. 4 it was applied to a D-dimensional model described by a generalized gauge ladder with zero curvature condition, e.g., $\mathcal{A}\equiv\Sigma_{i=0}^{D}\varphi_i^{1-i}:=c+A+\varphi_2^{-1}+\cdots+\varphi_D^{1-D}$, satisfying

$$\tilde{d}\mathcal{A}+\tfrac{1}{2}[\mathcal{A},\mathcal{A}]=0. \tag{2}$$

In Ref. 6 we have extended this model by introducing a curvature ladder $\mathcal{F}\equiv\Sigma_{i=0}^{D}\eta_i^{2-i}:=\phi+\psi+B+\cdots+\eta_D^{2-D}$ satisfying

$$\tilde{d}\mathcal{A}+\tfrac{1}{2}[\mathcal{A},\mathcal{A}]=\mathcal{F},\quad \tilde{d}\mathcal{F}+[\mathcal{A},\mathcal{F}]=0. \tag{3}$$

In both cases we have $\tilde{d}=b+d$ and δ is defined by the equations

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$$\mathcal{A}=e^{\delta}c, \quad \mathcal{F}=e^{\delta}\phi, \tag{4}$$

$$\tilde{d}=e^{\delta}be^{-\delta}. \tag{5}$$

Here, the space of fields and its derivatives $\mathcal{V}=\{\varphi_i^{1-i},\eta_i^{2-i},d\varphi_i^{1-i},d\eta_i^{2-i}\}$ is the ground space where we will construct a representation for the topological algebra (6)–(10). In this space we have automatically fulfilled the relation $[\delta,b]=d$ [this comes from the expansion of (5)] or its equivalent $[G_\mu,b]=-\partial_\mu$. We can then proceed to a full realization of the topological algebra by defining systematically on $\mathcal{V}$ the action of the other generators and ensuring their remaining algebraic relations are satisfied. In much the same way, we can introduce a matter ladder[4] $\mathcal{H}\equiv\Sigma_{i=0}^{D}h_i^{-i}$ with $\mathcal{H}=e^{\delta}h_0^0$ and extend the topological algebra to the space $\mathcal{V}$ defined by the component fields of $\mathcal{A}$, $\mathcal{F}$, $\mathcal{H}$ and their exterior derivatives. Depending on the way we define the relations among these ladders we will obtain distinct representations for the generators of the topological algebra. The introduction of the matter ladder $\mathcal{H}$ will allow us to describe topological matter in a different way than the one developed in Ref. 3.

In this work we will present a systematic procedure on how to obtain topological algebras for models admitting a $d=[\delta,b]$ decomposition. In order to relate our construction to the model described in Ref. 1 we will consider two-dimensional models defined in a Euclidean space $\mathcal{M}$. The fields are then considered as differential forms in $\mathcal{M}$ with values in a certain Lie algebra [that is not restricted to SO(2)]. With respect to the isometries of $\mathcal{M}$, $\mathrm{SO}(2)_{\mathcal{M}}$, the ladders $\mathcal{A}$, $\mathcal{F}$ and $\mathcal{H}$ carry no $\mathrm{SO}(2)_{\mathcal{M}}$ spinor field, therefore all fields in $\mathcal{V}$ will transform as $\mathrm{SO}(2)_{\mathcal{M}}$ tensors [even though $\mathcal{M}$ is a Euclidean space, we will use the terminology of Ref. 1 and sometimes we will refer to $\mathrm{SO}(2)_{\mathcal{M}}$ as "Lorentz" SO(2)]. We will see that the choice of a two-dimensional ladder of matter $\mathcal{H}$ together with the gauge ladder $\mathcal{A}$ will result in a model that contains all fields of the topological matter of Ref. 1. In this case, we will derive an action that is both BRST and M invariant but it is not included in the formalism of Ref. 1, which are not included in that formalism.

Our work is organized as follows. In Sec. II we introduce the topological algebra and set out our notation. In Sec. III we realize the topological algebra in the space $\mathcal{V}=\{\varphi_i^{1-i},d\varphi_i^{1-i},\eta_i^{2-i},d\eta_i^{2-i}\}$ determined by component fields of gauge and curvature ladders $\mathcal{A}=c+A+\varphi_2^{-1}$, $\mathcal{F}=\phi+\psi+B$. In Sec. IV we analyze a model defined by a ladder of matter $\mathcal{H}\equiv\Sigma_{i=0}^{2}h_i^{-i}:=h+\rho+\chi$ and a zero curvature condition. We restrict the fields to be Abelian, a condition that will allow us later on to derive an $N=2$ supersymmetry algebra from a (un)twisting procedure. We exhibit then an invariant action S ($bS=0\leftrightarrow QS=0$) by solving the descent equations associated to $bS=0$. In Sec. V we redo the same analysis of Sec. IV but relaxing the zero curvature condition. Section VI presents a model with zero curvature and $\tilde{d}$-closed gauge and matter ladders, i.e., $\tilde{d}\mathcal{A}=\tilde{d}\mathcal{H}=0$. In Sec. VII, having in mind the particular cases of Secs. IV and V, we show how to define supersymmetry generators from the odd generators of the topological algebra.

II. TOPOLOGICAL ALGEBRAS IN $D=2$

In this work fields and operators carry a bidegree (i,j). As a field, X_i^j means an i-form with ghost number j; as an operator, X_i^j means a superderivation which acts on a field with bidegree (m,n) producing another field with bidegree $(i+m,j+n)$. The total degree of X_i^j is $i+j$. Products of objects like $X_i^jX_k^l$ result in an object with bidegree $(i+k,j+l)$. We define $[X_i^j,X_k^l]:=X_i^jX_k^l-(-1)^{(i+j)(k+l)}X_k^lX_i^j$.

We deal with a two-dimensional Euclidean space with metric $g_{\mu\nu}=\delta_{\mu\nu}$. The antisymmetric symbol $\epsilon_{\mu\nu}$ has $\epsilon_{12}=1$. The gamma matrices are defined as in Ref. 1.

By a topological algebra we understand the algebra generated by the superderivations $\{P_\mu,\tilde{J},b,G_\mu,M\}$ with bidegrees (0,0), (0,0), (0,1), (0,−1), (0,1) and satisfying

$$[P_\mu,P_\nu]=[P_\mu,b]=[P_\mu,G_\nu]=[P_\mu,M]=b^2=M^2=0, \tag{6}$$

$$[\tilde{J},b]=[\tilde{J},M]=[b,M]=[G_\mu,G_\nu]=0, \tag{7}$$

$$[\tilde{J},P_\mu]=-i\epsilon_\mu{}^\nu P_\nu, \quad [\tilde{J},G_\mu]=-i\epsilon_\mu{}^\nu G_\nu, \tag{8}$$

$$[G_\mu,b]=-P_\mu, \tag{9}$$

$$[M,G_\mu]=-i\epsilon_\mu{}^\nu P_\nu. \tag{10}$$

Our $\tilde{J}$ generator corresponds in Ref. 1 to the twisting of internal and Lorentz SO(2) generators. Here, since we are not restricting the fields to be SO(2) valued, $\tilde{J}$ is related only to the generator of Lorentz SO(2) transformations and it acts on a vector field Ω_μ as $\tilde{J}\Omega_\mu:=-i\epsilon_\mu{}^\nu\Omega_\nu$. The generator of internal symmetry, at this point, does not enter the topological algebra. In what follows we will write $P_\mu=\partial_\mu$.

III. A MODEL WITH $\mathcal{A}$ AND $\mathcal{F}$

Let us consider a model defined by ladders

$$\mathcal{A}=c+A+\varphi, \quad \mathcal{F}=\phi+\psi+B, \tag{11}$$

where $c\equiv c_0^0$, $A\equiv A_1^0$, $\varphi\equiv\varphi_2^{-1}$, $\phi\equiv\phi_0^2$, $\psi\equiv\psi_1^1$, and $B\equiv B_2^0$. The field B is an arbitrary two form independent of A.

A. Defining G_μ, b, M

From (4) and (5) we obtain the following δ transformations:

$$\delta c=A, \quad \delta A=2\varphi, \quad \delta\varphi=0; \quad \delta\phi=\psi, \quad \delta\psi=2B, \quad \delta B=0, \quad [\delta,d]=0. \tag{12}$$

$\delta\equiv\delta_1^{-1}$ being a superderivation of bidegree $(1,-1)$ can be written as $\delta=G_\mu\otimes dx^\mu$. This together with $[\delta,d]=0$ determines G_μ as

$$G_\mu c=-A_\mu, \quad G_\mu A_\nu=\varphi_{\mu\nu}, \quad G_\mu\varphi_{\alpha\beta}=0, \quad G_\mu\partial_\nu=\partial_\nu G_\mu, \tag{13}$$

$$G_\mu\phi=\psi_\mu, \quad G_\mu\psi_\nu=-B_{\mu\nu}, \quad G_\mu B_{\alpha\beta}=0. \tag{14}$$

The BRST transformations arise from (3) and assume the form

$$bc=-c^2+\phi, \tag{15}$$

$$bA_\mu=\partial_\mu c-[c,A_\mu]+\psi_\mu, \tag{16}$$

$$b\varphi_{\mu\nu}=-F_{\mu\nu}-[c,\varphi_{\mu\nu}]+B_{\mu\nu}, \tag{17}$$

$$b\phi=-[c,\phi], \tag{18}$$

$$b\psi_\mu=-\partial_\mu\phi-[c,\psi_\mu]-[A_\mu,\phi], \tag{19}$$

$$bB_{\mu\nu}=\partial_\mu\psi_\nu-\partial_\nu\psi_\mu-[c,B_{\mu\nu}]+[A_\mu,\psi_\nu]-[A_\nu,\psi_\mu]-[\varphi_{\mu\nu},\phi], \tag{20}$$

with $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu+[A_\mu,A_\nu]$ and $b^2=0$.

$M\equiv M_0^1$ is a generator with bidegree (0,1), therefore we start defining it on c and ϕ as $Mc=a_1c^2+a_2\phi$ and $M\phi=a_3c^3+a_4c\phi+a_5\phi c$ with $a_1,\ldots,a_5$ arbitrary constants. Imposing (10), $[M,\partial_\mu]=0$ and $[M,b]=0$, we obtain $a_1=a_4=-a_5$, $a_3=0$ and

$$Mc = a_1 c^2 + a_2 \phi, \tag{21}$$

$$MA_\mu = a_1[c, A_\mu] + a_2 \psi_\mu + i\epsilon_\mu{}^\nu \partial_\nu c, \tag{22}$$

$$M\varphi_{\mu\nu} = a_1([A_\mu, A_\nu] + [c, \varphi_{\mu\nu}]) + a_2 B_{\mu\nu} + i\epsilon_\nu{}^\alpha \partial_\alpha A_\mu - i\epsilon_\mu{}^\alpha \partial_\alpha A_\nu, \tag{23}$$

$$M\phi = a_1[c, \phi], \tag{24}$$

$$M\psi_\mu = a_1([A_\mu, \phi] + [c, \psi_\mu]) - i\epsilon_\mu{}^\nu \partial_\nu \phi, \tag{25}$$

$$MB_{\mu\nu} = a_1([\varphi_{\mu\nu}, \phi] - [A_\mu, \psi_\nu] + [A_\nu, \psi_\mu] + [c, B_{\mu\nu}]) - i\epsilon_\nu{}^\alpha \partial_\alpha \psi_\mu + i\epsilon_\mu{}^\alpha \partial_\alpha \psi_\nu. \tag{26}$$

It is straightforward to verify that the set of generators $\{\partial_\mu, \tilde{J}, G_\mu, b, M\}$ satisfies the topological algebra (6) and (10). Since the constants appearing in the definition of M are not determined by the topological algebra, we have then established a family of topological algebras indexed by the values of (a_1, a_2).

IV. A MODEL WITH A MATTER LADDER AND A ZERO CURVATURE CONDITION (I)

Let us consider an Abelian model defined by ladders

$$\mathcal{A} = c + A + \varphi, \quad \mathcal{H} = h + \rho + \chi \tag{27}$$

with $h \equiv h_0^0$, $\rho \equiv \rho_1^{-1}$, $\chi \equiv \chi_2^{-2}$. We impose they obey equations

$$\tilde{d}\mathcal{H} = \mathcal{A}, \quad \tilde{d}\mathcal{A} = 0, \tag{28}$$

$$\mathcal{A} = e^\delta c, \quad \mathcal{H} = e^\delta h, \tag{29}$$

$$\tilde{d} = e^\delta b e^{-\delta}. \tag{30}$$

From (29) we obtain the δ-transformation as

$$\delta c = A, \quad \delta A = 2\varphi, \quad \delta\varphi = 0, \quad \delta h = \rho, \quad \delta\rho = 2\chi, \quad \delta\chi = 0, \tag{31}$$

which, in addition to (13), determines

$$G_\mu h = \rho_\mu, \quad G_\mu \rho_\nu = -\chi_{\mu\nu}, \quad G_\mu \chi_{\alpha\beta} = 0. \tag{32}$$

From (28) we have the following BRST transformations:

$$\begin{gathered} bc = 0, \quad bA_\mu = \partial_\mu c, \quad b\varphi_{\mu\nu} = -F_{\mu\nu}, \quad bh = c, \quad b\rho_\mu = -\partial_\mu h + A_\mu, \\ b\chi_{\mu\nu} = \partial_\mu \rho_\nu - \partial_\nu \rho_\mu + \varphi_{\mu\nu}. \end{gathered} \tag{33}$$

Since we are dealing with an Abelian model subjected to a zero curvature condition we write $Mc = 0$ and $Mh = a\,c$. Then (10) determines the M transformations as

$$\begin{gathered} Mc = 0, \quad MA_\mu = i\epsilon_\mu{}^\nu \partial_\nu c, \quad M\varphi_{\mu\nu} = i\epsilon_\nu{}^\alpha \partial_\alpha A_\mu - i\epsilon_\mu{}^\alpha \partial_\alpha A_\nu, \quad Mh = ac, \\ M\rho_\mu = aA_\mu - i\epsilon_\mu{}^\nu \partial_\nu h, \quad M\chi_{\mu\nu} = a\varphi_{\mu\nu} - i\epsilon_\nu{}^\alpha \partial_\alpha \rho_\mu + i\epsilon_\mu{}^\alpha \partial_\alpha \rho_\nu. \end{gathered} \tag{34}$$

G_μ, b, M given in (32)–(34) satisfy the topological algebra (6)–(10).

A. An invariant action

Let us consider $\mathcal{S}=\int\omega_2^0$ satisfying $b\mathcal{S}=\int b\,\omega_2^0$. This is equivalent to the system of descent equations

$$b\,\omega_2^0+d\,\omega_1^1=0,\quad b\,\omega_1^1+d\,\omega_0^2=0,\quad b\,\omega_0^2=0\,. \tag{35}$$

In order to solve (35) let us consider $b\,\omega_0^2=0$ with $\omega_0^2\in\mathcal{V}=\{c,A,\varphi,h,\rho,\chi,dc,dA,d\varphi,dh,\ d\rho,d\chi\}$. Here, since the fields are Abelian, we have $\omega_0^2(c,h)=0$. One possibility for obtaining a nontrivial solution is to consider a set of ladders $\mathcal{A}^I,\ \mathcal{H}^I,\ I=1,\ldots,2N$, where the index I splits as $I=(i,\hat{i}),\ i=1,\ldots,N$. We assume, for each value of I, the same set of equations as before, (32)–(34) for the Ith component of the ladders. It is possible to consider the splitting of I in such a way that the corresponding ladders are complex conjugates, i.e., $\mathcal{A}^{\hat{i}}:=\mathcal{A}^{*i},\ \mathcal{H}^{\hat{i}}:=\mathcal{H}^{*i}$, however, our discussion is not restricted by this choice.

Now we can write ω_0^2 as (we denote $c^{\hat{i}}\equiv\hat{c}^i$, etc.)

$$\omega_0^2=f_{ij}(h,\hat{h})c^ic^j+f_{i\hat{j}}(h,\hat{h})c^i\hat{c}^j+f_{\hat{i}\hat{j}}(h,\hat{h})\hat{c}^i\hat{c}^j \tag{36}$$

with $f_{ij}=-f_{ji},\ f_{\hat{i}\hat{j}}=-f_{\hat{j}\hat{i}}$. Then, $b\,\omega_0^2=0$ determines the following conditions on the functions $f_{ij},\ f_{i\hat{j}},\ f_{\hat{i}\hat{j}}$,

$$\begin{aligned}&\frac{\partial f_{ij}}{\partial\hat{h}^k}-\frac{1}{2}\frac{\partial f_{i\hat{k}}}{\partial h^j}+\frac{1}{2}\frac{\partial f_{j\hat{k}}}{\partial h^i}=0,\quad \frac{\partial f_{ij}}{\partial h^k}+\frac{\partial f_{jk}}{\partial h^i}+\frac{\partial f_{ki}}{\partial h^j}=0,\\ &\frac{\partial f_{\hat{i}\hat{j}}}{\partial h^k}-\frac{1}{2}\frac{\partial f_{k\hat{j}}}{\partial\hat{h}^i}+\frac{1}{2}\frac{\partial f_{k\hat{i}}}{\partial\hat{h}^j}=0,\quad \frac{\partial f_{\hat{i}\hat{j}}}{\partial\hat{h}^k}+\frac{\partial f_{\hat{j}\hat{k}}}{\partial\hat{h}^i}+\frac{\partial f_{\hat{k}\hat{i}}}{\partial\hat{h}^j}=0,\end{aligned} \tag{37}$$

which is solved by

$$f_{ij}=\frac{\partial K}{\partial h^i\partial\hat{h}^j}-\frac{\partial K}{\partial h^j\partial\hat{h}^i},\quad f_{i\hat{j}}=2\lambda\frac{\partial K}{\partial h^i\partial h^j}-2\frac{\partial K}{\partial\hat{h}^i\partial\hat{h}^j},\quad f_{\hat{i}\hat{j}}=-\lambda f_{ij} \tag{38}$$

with K an arbitrary function of $(h,\hat{h})$ and λ an arbitrary constant that should be made equal to 1 in case we describe our model by a pair of complex fields and their conjugates. Replacing (38) into (36) we obtain

$$\omega_0^2=2K_{i\hat{j}}c^ic^j+2K_{\hat{i}\hat{j}}\hat{c}^ic^j+2\lambda K_{ij}c^i\hat{c}^j+2\lambda K_{i\hat{j}}\hat{c}^i\hat{c}^j \tag{39}$$

with $K_{i\hat{j}}\equiv\partial K/\partial h^i\hat{h}^j$ etc. The use of the δ operator allows us to exhibit a particular solution to the descent equations.[4–9] In fact, in the case of $[\delta,d]=0$ we can write (35) in the form $\tilde{d}\tilde{\omega}=0$ for $\tilde{\omega}\equiv\omega_0^2+\omega_1^1+\omega_2^0:=e^{\delta}\omega_0^2$. Then from (39) and the definition of δ we obtain

$$\tilde{\omega}=2\tilde{K}_{i\hat{j}}\mathcal{A}^i\mathcal{A}^j+2\tilde{K}_{\hat{i}\hat{j}}\hat{\mathcal{A}}^i\mathcal{A}^j+2\lambda\tilde{K}_{ij}\mathcal{A}^i\hat{\mathcal{A}}^j+2\lambda\tilde{K}_{\hat{i}j}\hat{\mathcal{A}}^i\hat{\mathcal{A}}^j \tag{40}$$

with $\tilde{K}\equiv K(\mathcal{H},\hat{\mathcal{H}}):=e^{\delta}K(h,\hat{h})$ and $\tilde{K}_{i\hat{j}}\equiv\partial\tilde{K}/\partial\mathcal{H}^i\partial\hat{\mathcal{H}}^j$ etc. Writing $\mathcal{H}=h+\Theta,\ \hat{\mathcal{H}}=\hat{h}+\hat{\Theta}$ with $\Theta\equiv\rho+\chi$ and $\hat{\Theta}\equiv\hat{\rho}+\hat{\chi}$, we expand $\tilde{K}(\mathcal{H},\hat{\mathcal{H}})$ in a Taylor series around $(h,\hat{h})$,

$$\begin{aligned}\tilde{K}(\mathcal{H},\hat{\mathcal{H}})=&K(h,\hat{h})+\Theta^mK_m(h,\hat{h})+\hat{\Theta}^mK_{\hat{m}}(h,\hat{h})+\tfrac{1}{2}\Theta^m\Theta^nK_{mn}(h,\hat{h})\\&+\Theta^m\hat{\Theta}^nK_{m\hat{n}}(h,\hat{h})+\tfrac{1}{2}\hat{\Theta}^m\hat{\Theta}^nK_{\hat{m}\hat{n}}(h,\hat{h}),\end{aligned}$$

which gives the decompositions

$$\tilde{K}_{i\hat{j}}|_2^{-2}=\chi^m K_{mi\hat{j}}+\hat{\chi}^m K_{\hat{m}i\hat{j}}+\tfrac{1}{2}\rho^m\rho^n K_{mni\hat{j}}+\rho^m\hat{\rho}^n K_{m\hat{n}i\hat{j}}+\tfrac{1}{2}\hat{\rho}^m\hat{\rho}^n K_{\hat{m}\hat{n}i\hat{j}}, \tag{41}$$

$$\tilde{K}_{i\hat{j}}|_1^{-1}=\rho^m K_{mi\hat{j}}+\hat{\rho}^m K_{\hat{m}i\hat{j}}, \tag{42}$$

$$\tilde{K}_{i\hat{j}}|_0^0=K_{i\hat{j}}. \tag{43}$$

Here ω_2^0 is obtained by taking terms with bidegree (2,0) in $\tilde{\omega}$. Therefore, replacing (41)–(43) in (40) we obtain

$$\begin{aligned}
\omega_2^0&=\tilde{\omega}|_2^0\\
&=K_{mni\hat{j}}\rho^m\rho^n c^i c^j+2K_{mn\hat{i}\hat{j}}\rho^m\hat{\rho}^n c^i c^j+K_{\hat{m}\hat{n}i\hat{j}}\hat{\rho}^m\hat{\rho}^n c^i c^j+K_{mn\hat{i}\hat{j}}\rho^m\rho^n\hat{c}^i c^j+2K_{m\hat{n}\hat{i}\hat{j}}\rho^m\hat{\rho}^n\hat{c}^i c^j\\
&\quad+K_{\hat{m}\hat{n}\hat{i}\hat{j}}\hat{\rho}^m\hat{\rho}^n\hat{c}^i c^j+2K_{mi\hat{j}}\chi^m c^i c^j+2K_{\hat{m}i\hat{j}}\hat{\chi}^m c^i c^j+2K_{m\hat{i}\hat{j}}\chi^m\hat{c}^i c^j+2K_{\hat{m}\hat{i}\hat{j}}\hat{\chi}^m\hat{c}^i c^j\\
&\quad+2K_{mi\hat{j}}\rho^m c^i A^j+2K_{\hat{m}i\hat{j}}\hat{\rho}^m c^i A^j-2K_{mi\hat{j}}\rho^m c^j A^i-2K_{\hat{m}i\hat{j}}\hat{\rho}^m c^j A^i+2K_{m\hat{i}\hat{j}}\rho^m\hat{c}^i A^j\\
&\quad+2K_{\hat{m}\hat{i}\hat{j}}\hat{\rho}^m\hat{c}^i A^j-2K_{m\hat{i}\hat{j}}\rho^m c^j\hat{A}^i-2K_{\hat{m}\hat{i}\hat{j}}\hat{\rho}^m c^j\hat{A}^i+2K_{i\hat{j}}c^i\varphi^j-2K_{i\hat{j}}c^j\varphi^i+2K_{\hat{i}\hat{j}}\hat{c}^i\varphi^j-2K_{\hat{i}\hat{j}}c^j\hat{\varphi}^i\\
&\quad+2K_{i\hat{j}}A^i A^j+2K_{\hat{i}\hat{j}}\hat{A}^i A^j+\lambda(K_{mnij}\rho^m\rho^n c^i\hat{c}^j+2K_{m\hat{n}ij}\rho^m\hat{\rho}^n c^i\hat{c}^j+K_{\hat{m}\hat{n}ij}\hat{\rho}^m\hat{\rho}^n c^i\hat{c}^j\\
&\quad+K_{mn\hat{i}j}\rho^m\rho^n\hat{c}^i\hat{c}^j+2K_{m\hat{n}\hat{i}j}\rho^m\hat{\rho}^n\hat{c}^i\hat{c}^j+K_{\hat{m}\hat{n}\hat{i}j}\hat{\rho}^m\hat{\rho}^n\hat{c}^i\hat{c}^j+2K_{mij}\chi^m c^i\hat{c}^j+2K_{\hat{m}ij}\hat{\chi}^m c^i\hat{c}^j\\
&\quad+2K_{m\hat{i}j}\chi^m\hat{c}^i\hat{c}^j+2K_{\hat{m}\hat{i}j}\hat{\chi}^m\hat{c}^i\hat{c}^j+2K_{mij}\rho^m c^i\hat{A}^j+2K_{\hat{m}ij}\hat{\rho}^m c^i\hat{A}^j-2K_{mij}\rho^m\hat{c}^j A^i-2K_{\hat{m}ij}\hat{\rho}^m\hat{c}^j A^i\\
&\quad+2K_{m\hat{i}j}\rho^m\hat{c}^i\hat{A}^j+2K_{\hat{m}\hat{i}j}\hat{\rho}^m\hat{c}^i\hat{A}^j-2K_{m\hat{i}j}\rho^m\hat{c}^j\hat{A}^i-2K_{\hat{m}\hat{i}j}\hat{\rho}^m\hat{c}^j\hat{A}^i+2K_{ij}c^i\hat{\varphi}^j-2K_{ij}\hat{c}^j\varphi^i\\
&\quad+2K_{\hat{i}j}\hat{c}^i\hat{\varphi}^j-2K_{\hat{i}j}\hat{c}^j\hat{\varphi}^i+2K_{ij}A^i\hat{A}^j+2K_{\hat{i}j}\hat{A}^i\hat{A}^j).
\end{aligned} \tag{44}$$

From (28) we conclude that $\tilde{d}$ has trivial cohomology on $\mathcal{V}=\{\mathcal{A},\mathcal{H}\}$. Therefore any solution of $\tilde{d}\tilde{\omega}=0$ implies it exists $\hat{\omega}$ such that $\tilde{\omega}=\tilde{d}\hat{\omega}$. In particular $\omega_2^0=\tilde{\omega}|_2^0=(\tilde{d}\hat{\omega})|_2^0\equiv b\,\hat{\omega}|_2^{-1}+d\,\hat{\omega}|_1^0$. Explicitly

$$\begin{aligned}
\omega_2^0&=b\{K_{mn\hat{j}}\rho^m\rho^n c^j+2K_{m\hat{n}\hat{j}}\rho^m\hat{\rho}^n c^j+K_{\hat{m}\hat{n}\hat{j}}\hat{\rho}^m\hat{\rho}^n c^j+2K_{m\hat{j}}\rho^m A^j+2K_{\hat{m}\hat{j}}\hat{\rho}^m A^j+2K_{m\hat{j}}\chi^m c^j\\
&\quad+2K_{\hat{m}\hat{j}}\hat{\chi}^m c^j+2K_{\hat{j}}\varphi^j+\lambda(K_{mnj}\rho^m\rho^n\hat{c}^j+2K_{m\hat{n}j}\rho^m\hat{\rho}^n\hat{c}^j+K_{\hat{m}\hat{n}j}\hat{\rho}^m\hat{\rho}^n\hat{c}^j+2K_{mj}\rho^m\hat{A}^j\\
&\quad+2K_{\hat{m}j}\hat{\rho}^m\hat{A}^j+2K_{mj}\chi^m\hat{c}^j+2K_{\hat{m}j}\hat{\chi}^m\hat{c}^j+2K_j\hat{\varphi}^j)\}+d\{2K_{m\hat{j}}\rho^m c^j+2K_{\hat{m}\hat{j}}\hat{\rho}^m c^j+2K_{\hat{j}}A^j\\
&\quad+\lambda(2K_{mj}\rho^m\hat{c}^j+2K_{\hat{m}j}\hat{\rho}^m\hat{c}^j+2K_j\hat{A}^j)\}.
\end{aligned} \tag{45}$$

Then our action writes simply as a BRST variation $\mathcal{S}=b\int\hat{\omega}|_2^{-1}$.

We also have $[M,G_\mu]=-i\epsilon_\mu{}^\nu\partial_\nu\Rightarrow Me^\delta=e^\delta M-i\epsilon_\mu{}^\nu\partial_\nu\otimes dx^\mu e^\delta$. Therefore $M\omega_2^0=(M\tilde{\omega})|_2^1=(Me^\delta\omega_0^2)|_2^1=\frac{1}{2}\delta^2 M\omega_0^2-(i\epsilon_\mu{}^\nu\partial_\nu\otimes dx^\mu)\omega_1^1=i\epsilon_\mu{}^\nu\partial_\nu\omega_\alpha^1 dx^\mu dx^\alpha$ (we have $M\omega_0^2=0$ and $\omega_1^1\equiv\omega_\alpha^1 dx^\alpha$). Thus $M\mathcal{S}=\int dx^2(-i\partial^\mu\omega_\mu^1)=0$, i.e., the action is M-invariant.

V. A MODEL WITH MATTER, GAUGE AND CURVATURE LADDERS

Let us consider an Abelian model with ladders $\mathcal{A}$, $\mathcal{F}$, $\mathcal{H}$ which satisfy

$$\tilde{d}\mathcal{A}=\mathcal{F},\quad \tilde{d}\mathcal{F}=0\ \text{ and }\ \tilde{d}\mathcal{H}=0. \tag{46}$$

The G_μ transformations are given by (13), (14), and (32) and the BRST transformations assume the form

$$bc=\phi,\quad bA_\mu=\partial_\mu c+\psi_\mu,\quad b\varphi_{\mu\nu}=-F_{\mu\nu}+B_{\mu\nu},\quad b\phi=0,\ b\psi_\mu=-\partial_\mu\phi, \tag{47}$$

$$bB_{\mu\nu}=\partial_\mu\psi_\nu-\partial_\nu\psi_\mu,\quad bh=0,\quad b\rho_\mu=-\partial_\mu h,\quad b\chi_{\mu\nu}=\partial_\mu\rho_\nu-\partial_\nu\rho_\mu.$$

In order to determine the M transformation we assume that $Mc=a_1\phi$, $M\phi=a_2 c\,\phi$ and $Mh=a_3 c$. The algebraic relation (10) together with $[b,M]=0$ and $M^2=0$ impose $a_2=0$, $a_3=0$ and fix the M transformations as

$$\begin{aligned}&Mc=a_1\phi,\quad MA_\mu=a_1\psi_\mu+i\epsilon_\mu{}^\nu\partial_\nu c,\quad M\varphi_{\mu\nu}=a_1B_{\mu\nu}+i\epsilon_\nu{}^\alpha\partial_\alpha A_\mu-i\epsilon_\mu{}^\alpha\partial_\alpha A_\nu,\\&M\phi=0,\ M\psi_\mu=-i\epsilon_\mu{}^\nu\partial_\nu\phi,\quad MB_{\mu\nu}=-i\epsilon_\nu{}^\alpha\partial_\alpha\psi_\mu+i\epsilon_\mu{}^\alpha\partial_\alpha\psi_\nu,\quad Mh=0,\\&M\rho_\mu=-i\epsilon_\mu{}^\nu\partial_\nu h,\quad M\chi_{\mu\nu}=-i\epsilon_\nu{}^\alpha\partial_\alpha\rho_\mu+i\epsilon_\mu{}^\alpha\partial_\alpha\rho_\nu.\end{aligned}\tag{48}$$

Let us take ladders $\mathcal{A}^I$, $\mathcal{F}^I$, $\mathcal{H}^I$, $I=1,\ldots,2N$, $I=(i,\hat{i})$. Here, we write $\omega_0^2=F_{ij}(h,\hat{h})c^ic^j+F_{i\hat{j}}(h,\hat{h})c^i\hat{c}^j+F_{\hat{i}\hat{j}}(h,\hat{h})\hat{c}^i\hat{c}^j+G_i(h,\hat{h})\phi^i+G_{\hat{i}}(h,\hat{h})\hat{\phi}^i$. Then $b\omega_0^2=0$ gives

$$\omega_0^2=G_i(h,\hat{h})\phi^i+G_{\hat{i}}(h,\hat{h})\hat{\phi}^i.\tag{49}$$

An invariant action is given by $\mathcal{S}=\int\omega_2^0$ with

$$\begin{aligned}\omega_2^0&=(e^\delta\omega_0^2)|_2^0\\&=\tfrac{1}{2}G_{i,jk}\phi^i\rho^j\rho^k+G_{i,j\hat{k}}\phi^i\rho^j\hat{\rho}^k+\tfrac{1}{2}G_{i,\hat{j}\hat{k}}\phi^i\hat{\rho}^j\hat{\rho}^k+\tfrac{1}{2}G_{\hat{i},jk}\hat{\phi}^i\rho^j\rho^k\\&\quad+G_{\hat{i},j\hat{k}}\hat{\phi}^i\rho^j\hat{\rho}^k+\tfrac{1}{2}G_{\hat{i},\hat{j}\hat{k}}\hat{\phi}^i\hat{\rho}^j\hat{\rho}^k+G_{i,j}\phi^i\chi^j+G_{i,\hat{j}}\phi^i\hat{\chi}^j+G_{\hat{i},j}\hat{\phi^i}\chi^j\\&\quad+G_{\hat{i},\hat{j}}\hat{\phi}^i\hat{\chi}^j+G_{i,j}\psi^i\rho^j+G_{i,\hat{j}}\psi^i\hat{\rho}^j+G_{\hat{i},j}\hat{\psi}^i\rho^j+G_{\hat{i},\hat{j}}\hat{\psi}^i\hat{\rho}^j+G_iB^i+G_{\hat{i}}\hat{B}^i\end{aligned}\tag{50}$$

$$\begin{aligned}&=b\,(\tfrac{1}{2}G_{i,jk}c^i\rho^j\rho^k+G_{i,j\hat{k}}c^i\rho^j\hat{\rho}^k+\tfrac{1}{2}G_{i,\hat{j}\hat{k}}c^i\hat{\rho}^j\hat{\rho}^k+\tfrac{1}{2}G_{\hat{i},jk}\hat{c}^i\rho^j\rho^k\\&\quad+G_{\hat{i},j\hat{k}}\hat{c}^i\rho^j\hat{\rho}^k+\tfrac{1}{2}G_{\hat{i},\hat{j}\hat{k}}\hat{c}^i\hat{\rho}^j\hat{\rho}^k+G_{i,j}c^i\chi^j+G_{i,\hat{j}}c^i\hat{\chi}^j+G_{\hat{i},j}\hat{c}^i\chi^j+G_{\hat{i},\hat{j}}\hat{c}^i\hat{\chi}^j\\&\quad+G_{i,j}A^i\rho^j+G_{i,\hat{j}}A^i\hat{\rho}^j+G_{\hat{i},j}\hat{A}^i\rho^j+G_{\hat{i},\hat{j}}\hat{A}^i\hat{\rho}^j+G_i\varphi^i+G_{\hat{i}}\hat{\varphi}^i)+d\,(G_{i,j}c^i\rho^j\\&\quad+G_{i,\hat{j}}c^i\hat{\rho}^j+G_{\hat{i},j}\hat{c}^i\rho^j+G_{\hat{i},\hat{j}}\hat{c}^i\hat{\rho}^j+G_iA^i+G_{\hat{i}}\hat{A}^i)\end{aligned}\tag{51}$$

with G_i, $G_{\hat{i}}$ arbitrary functions of h, $\hat{h}$ and $G_{i,j}:=\partial G_i/\partial h^j$, etc. The expression given in (51) is essentially the same one given in (45) if we identify $G_i\leftrightarrow 2K_{\hat{i}}$, $G_{\hat{i}}\leftrightarrow 2K_i$ and take $\lambda=1$. Nonetheless, these models differ due to their different BRST transformations. Note that ω_0^2 given in (49) is M-invariant. Then, adopting the same procedure of the last section, we also obtain $M\mathcal{S}=0$.

This model admits a simpler form which consists in taking ladders $\mathcal{A}^i$, $\mathcal{F}^i$, $\mathcal{H}^i$, $i=1,\ldots,N$. Here the previous form for ω_2^0 becomes

$$\begin{aligned}\omega_2^0&=\tfrac{1}{2}G_{i,jk}\phi^i\rho^j\rho^k+G_{i,j}\psi^i\rho^j+G_iB^i\\&=b(\tfrac{1}{2}G_{i,jk}c^i\rho^j\rho^k+G_{i,j}c^i\chi^j+G_{i,j}A^i\rho^j+G_i\phi^i)+d(G_{i,j}c^i\rho^j+G_iA^i).\end{aligned}\tag{52}$$

In addition to the solution given in (52) we can also include in the action BRST-invariant terms involving derivates, for example,

$$b\int d^2xG_{i,j}(-\rho_\mu^i\partial^\mu h^j-\chi_{\mu\nu}^iB^{j\mu\nu})=\int d^2xG_{i,j}(\partial_\mu h^i\partial^\mu h^j+2\partial_\mu\rho_\nu^iB^{j\mu\nu}+2\chi_{\mu\nu}^i\partial^\mu\psi^{j\nu}).\tag{53}$$

These terms are not generated by the expansion of $e^\delta\omega_0^2$. This shows explicitly the particular character of our solution. The action determined by (52) and (53),

$$\int \mathrm{d}^2x \left(\epsilon^{\mu\nu}\left(-\frac{1}{2}G_{i,jk}\phi^i\rho^j_\mu\rho^k_\nu - G_{i,j}\psi^i_\mu\rho^j_\nu + \frac{1}{2}G_iB^i_{\mu\nu}\right) + G_{i,j}(\partial_\mu h^i\partial^\mu h^j + 2\partial_\mu\rho^i_\nu B^{j\mu\nu} + 2\chi^i_{\mu\nu}\partial^\mu\psi^{j\nu})\right),$$

contains component fields only from the curvature and matter ladders. It is, by construction, BRST-exact, therefore it determines an energy-momentum tensor BRST-exact. This action has no counterpart in the topological matter action found in Ref. 1.

VI. A MODEL WITH A MATTER LADDER AND A ZERO CURVATURE CONDITION (II)

Let us consider the previous model with a zero curvature condition

$$\tilde{d}\mathcal{H}=0, \quad \tilde{d}\mathcal{A}=0. \tag{54}$$

The set of transformations we obtain is

$$bc=0, \quad bA_\mu=\partial_\mu c, \quad b\varphi_{\mu\nu}=-F_{\mu\nu}, \quad bh=0, \quad b\rho_\mu=-\partial_\mu h, \quad b\chi_{\mu\nu}=\partial_\mu\rho_\nu-\partial_\nu\rho_\mu, \tag{55}$$

$$Mc=0, \quad MA_\mu=i\epsilon_\mu{}^\nu\partial_\nu c, \quad M\varphi_{\mu\nu}=i\epsilon_\nu{}^\alpha\partial_\alpha A_\mu - i\epsilon_\mu{}^\alpha\partial_\alpha A_\nu, \quad Mh=0, \tag{56}$$

$$M\rho_\mu=-i\epsilon_\mu{}^\nu\partial_\nu h, \quad M\chi_{\mu\nu}=-i\epsilon_\nu{}^\alpha\partial_\alpha\rho_\mu + i\epsilon_\mu{}^\alpha\partial_\alpha\rho_\nu. \tag{57}$$

Here, a BRST-invariant action writes as the integral of

$$\omega^0_2=G_{ij}(2c^i\varphi^j+A^iA^j)+G_{ij,k}(c^ic^j\chi^k+2c^iA^j\rho^k)+\tfrac{1}{2}G_{ij,kl}c^ic^j\rho^k\rho^l \tag{58}$$

with $G_{ij}=-G_{ji}$. Since we have $M\omega^0_2=\partial_\alpha(-2iG_{ij}\epsilon_\nu{}^\alpha c^iA^j_\mu - iG_{ij,k}\epsilon_\nu{}^\alpha c^ic^j\rho^k_\mu)dx^\mu dx^\nu$ we obtain $M\int\omega^0_2=0$. A possible kinetic term is

$$b\int G_{ij}(-\rho^i_\mu\partial^\mu h^j-\rho^i_\mu A^{\mu j})=\int \mathrm{d}^2x G_{ij}(\partial_\mu h^i\partial^\mu h^j+\partial_\mu h^iA^{\mu j}+\rho^i_\mu\partial^\mu c^j). \tag{59}$$

Once again, these previous terms determine an action

$$\int \mathrm{d}x^2\left(G_{ij}(\epsilon^{\mu\nu}c^i\varphi^j_{\mu\nu}+\epsilon^{\mu\nu}A^i_\mu A^j_\nu)+G_{ij,k}\left(\frac{1}{2}\epsilon^{\mu\nu}c^ic^j\chi^k_{\mu\nu}-2\epsilon^{\mu\nu}c^iA^j_\mu\rho^k_\nu\right) - \frac{1}{2}G_{ij,kl}\epsilon^{\mu\nu}c^ic^j\rho^k_\mu\rho^l_\nu+G_{ij}(\partial_\mu h^i\partial^\mu h^j+\partial_\mu h^iA^{\mu j}+\rho^i_\mu\partial^\mu c^j)\right), \tag{60}$$

which is BRST-exact.

VII. DERIVING A SUPERSYMMETRY FROM THE TOPOLOGICAL ALGEBRA

Let us now derive a realization of the $N=2$ supersymmetry generators in the space of Abelian fields $\mathcal{V}=\{c,A,\varphi,h,\rho,\chi,dc,dA,d\varphi,dh,d\rho,d\chi\}$ by following the procedure of Ref. 1. We define supersymmetry generators $Q_{\alpha a}\equiv(Q_{++},Q_{+-},Q_{-+},Q_{--})$ as $Q_{++}:=\gamma^\mu_{++}G_\mu$, $Q_{--}:=\gamma^\mu_{--}G_\mu$, $Q_{+-}:=\frac{1}{2}(-b+M)$, $Q_{-+}:=\frac{1}{2}(-b-M)$. Note that (9) differs by a minus sign to the corresponding relation $[Q,G_\mu]=\partial_\mu$ of Ref. 1. Then we have to consider here the association $-b\leftrightarrow Q$. The topological algebra (6)–(10) together with these definitions determines

$$\left.\begin{array}{c}[Q_{\alpha+},Q_{\beta+}]=0\\ [Q_{\alpha-},Q_{\beta-}]=0\\ [Q_{\alpha+},Q_{\beta-}]=\gamma^{\mu}_{\alpha\beta}\partial_{\mu}\end{array}\right\}\rightleftharpoons[Q_{\alpha a},Q_{\beta b}]=C_{ab}\gamma^{\mu}_{\alpha\beta}\partial_{\mu} \tag{61}$$

that corresponds to the algebra of the generators of $N=2$ supersymmetry. It should be noticed though that our model differs from the description of topological matter of Ref. 1, first, because we have extra fields $\varphi_2^{-1},\chi_2^{-2}$ and B that are necessary to guarantee $d=[\delta,b]$ (see Ref. 6), and, second, because our fields are not components of a pair of chiral and antichiral superfields. Also, the Lagrangians we obtained depend on arbitrary functions $K,G_i,G_{\hat{i}}$ of $(h,\hat{h})$. Contrarily to Ref. 1, the kinetic terms we introduce do not restrict $K_{i\hat{j}},G_{i\hat{j}}$ to be a Kähler metric.

VIII. CONCLUSION

All models exhibited here admit the decomposition $d=[\delta,b]$, which translates into the fundamental relation $[G_{\mu},b]=\partial_{\mu}$ of topological algebras. In addition, we also have $[d,\delta]=0$, which is equivalent to $[G_{\mu},\partial_{\nu}]=0$. As it was shown in Refs. 5 and 7, there are models where this relation does not hold and, as a result, a new operator $\Delta^{-1}_{\mu\nu}$ of bidegree $(0,-1)$ arises, i.e., $[G_{\mu},\partial_{\nu}]=\Delta^{-1}_{\mu\nu}$. In these cases there is no natural way to introduce the generator M in order to reproduce some of the relations of the topological algebra.

The same ideas presented here in the context of two dimensions also apply to four dimensions. However, what seems more significant is that they apply to any dimension and to any set of Lie algebra valued fields as far as they are components of ladders satisfying $d=[\delta,b]$. The special cases of two and four dimensions can be used to formulate an $N=2$ supersymmetric model provided we restrict the fields to be respectively SO(2) and SU(2) valued.[1,3] It becomes clear that the δ operator is not only a useful tool in the analysis of the descent equations,[4–9] or in the study of some aspects of topological Yang–Mills theories,[10,11] but it also allows us to represent topological algebras for a broader class of models.

ACKNOWLEDGMENTS

A.L.O. thanks Centro Brasileiro de Pesquisas Físicas (CBPF) for support. M.C. thanks Japanese monbusho for the scholarship and Professor T. Kori for many helpful discussions, and acknowledges the constant support from Aurelina Carvalho, Jose E. Carvalho, and Ying Chen, IC XC Nika.

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Solving simple quaternionic differential equations

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(Received 10 December 2002; accepted 27 January 2003)

The renewed interest in investigating quaternionic quantum mechanics, in particular tunneling effects, and the recent results on quaternionic differential operators motivate the study of resolution methods for quaternionic differential equations. In this paper, by using the real matrix representation of left/right acting quaternionic operators, we prove existence and uniqueness for quaternionic initial value problems, discuss the reduction of order for quaternionic homogeneous differential equations and extend to the noncommutative case the method of variation of parameters. We also show that the standard Wronskian cannot uniquely be extended to the quaternionic case. Nevertheless, the *absolute value* of the complex Wronskian admits a *noncommutative* extension for quaternionic functions of one real variable. Linear dependence and independence of solutions of homogeneous (right) H-linear differential equations is then related to this *new* functional. Our discussion is, for simplicity, presented for quaternionic second order differential equations. This involves no loss of generality. Definitions and results can be readily extended to the n-order case.
[DOI: 10.1063/1.1563735]

I. INTRODUCTION

Let $\mathbb{R}$, $\mathbb{C}\equiv\text{span}\{1,i\}$, and $\mathbb{H}\equiv\text{span}\{1,i,j,k\}$ be the real, complex, and quaternionic field,[3]

$$i^2=j^2=k^2=ijk=-1$$

and

$$\mathcal{F}:\mathbb{R}\to\mathbb{R}$$

be the set of real functions of real variable. Through the paper, quaternionic functions of real variable, $\Psi(x)\in\mathbb{H}\otimes\mathcal{F}$, will be denoted by greek letters and constant quaternionic coefficients by Roman letters. To shorten notation the prime and double prime in the quaternionic functions shall, respectively, indicate the first and second derivative of quaternionic functions with respect to the real variable x,

$$\Psi' := \frac{d\Psi}{dx} \quad \text{and} \quad \Psi'' := \frac{d^2\Psi}{dx^2}.$$

Due to the noncommutative nature of quaternions, it is convenient to distinguish between the left and right action of the quaternionic imaginary units i, j, and k by introducing the operators L_q and R_p whose action on quaternionic functions Ψ is given by

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$$L_q\Psi = q\,\Psi \quad \text{and} \quad R_p\Psi = \Psi\,p, \tag{1}$$

These (left/right acting) quaternionic operators satisfy

$$L_q\,L_p = L_{qp}, \quad R_q\,R_p = R_{pq}, \quad \text{and} \quad [\,L_q\,,R_p\,] = 0, \tag{2}$$

and admit for

$$q = q_0 + i\,q_1 + j\,q_2 + k\,q_3, \quad p = p_0 + i\,p_1 + j\,p_2 + k\,p_3, \quad \Psi = \Psi_0 + i\,\Psi_1 + j\,\Psi_2 + k\,\Psi_3,$$

the following *real* matrix representation[4–6]

$$L_q \leftrightarrow \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix}, \quad R_p \leftrightarrow \begin{pmatrix} p_0 & -p_1 & -p_2 & -p_3 \\ p_1 & p_0 & p_3 & -p_2 \\ p_2 & -p_3 & p_0 & p_1 \\ p_3 & p_2 & -p_1 & p_0 \end{pmatrix}, \quad \Psi \leftrightarrow \begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} \in \mathbb{R}^4 \otimes \mathcal{F}. \tag{3}$$

II. EXISTENCE AND UNIQUENESS

In this section we discuss existence and uniqueness for the quaternionic initial value problem

$$\Psi'' = \alpha\,\Psi' + \beta\,\Psi + \rho, \quad \Psi(x_0) = f, \quad \Psi'(x_0) = g, \tag{4}$$

with $\alpha(x)$, $\beta(x)$, $\rho(x) \in \mathbb{H} \otimes \mathcal{F}$, $x_0 \in I{:}(x_-, x_+)$ and $f, g \in \mathbb{H}$.

Theorem 1: Let α, β, and ρ in Eq. (4) be continuous functions of x on an open interval I containing the point $x = x_0$. Then, the initial value problem (4) has a solution Ψ on this interval and this solution is unique.

Proof: By using the real matrix representation (3), we can immediately rewrite the quaternionic initial value problem (4) in the following vector form:

$$\begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix}'' = \begin{pmatrix} \alpha_0 & -\alpha_1 & -\alpha_2 & -\alpha_3 \\ \alpha_1 & \alpha_0 & -\alpha_3 & \alpha_2 \\ \alpha_2 & \alpha_3 & \alpha_0 & -\alpha_1 \\ \alpha_3 & -\alpha_2 & \alpha_1 & \alpha_0 \end{pmatrix} \begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix}' + \begin{pmatrix} \beta_0 & -\beta_1 & -\beta_2 & -\beta_3 \\ \beta_1 & \beta_0 & -\beta_3 & \beta_2 \\ \beta_2 & \beta_3 & \beta_0 & -\beta_1 \\ \beta_3 & -\beta_2 & \beta_1 & \beta_0 \end{pmatrix} \begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} + \begin{bmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \rho_3 \end{bmatrix} \tag{5}$$

with

$$\begin{bmatrix} \Psi_0(x_0) \\ \Psi_1(x_0) \\ \Psi_2(x_0) \\ \Psi_3(x_0) \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \Psi_0'(x_0) \\ \Psi_1'(x_0) \\ \Psi_2'(x_0) \\ \Psi_3'(x_0) \end{bmatrix} = \begin{bmatrix} g_0 \\ g_1 \\ g_2 \\ g_3 \end{bmatrix}. \tag{6}$$

Equation (5) represents a (nonhomogeneous) linear system with $\alpha_m, \beta_m, \rho_m \in \mathbb{R} \otimes \mathcal{F}$, where $m = 0,1,2,3$. These functions are (see hypothesis of Theorem 1) continuous (real) functions of x on an open interval I containing the point $x = x_0$. Then, by a well-known theorem of analysis, see, for example, Ref. 7, the linear system (5) has a solution

$$\begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} \in \mathbb{R}^4 \otimes \mathcal{F}$$

on this interval satisfying (6), and this solution is unique. ■

III. LINEAR INDEPENDENCE AND DEPENDENCE OF SOLUTIONS

Let us now analyze the linear independence and dependence of the solutions of second order homogeneous differential equations

$$\Psi'' = \alpha\,\Psi' + \beta\,\Psi, \tag{7}$$

where α and β are (quaternionic) continuous functions of x on an open interval I. Equation (7) is linear over $\mathbb{H}$ from the right. Consequently, if φ is a solution of Eq. (7) only the function obtained by right multiplication by constant quaternionic coefficients, $\varphi\,u$, still represent a solution of such an equation. The general solution of Eq. (7) is given in terms of a pair of linearly independent solutions φ and ξ by

$$\Psi = \varphi\,u + \xi\,v, \tag{8}$$

where $\varphi = \varphi_0 + i\,\varphi_1 + j\,\varphi_2 + k\,\varphi_3$, $\xi = \xi_0 + i\,\xi_1 + j\,\xi_2 + k\,\xi_3 \in \mathbb{H}\otimes\mathcal{F}$, and $u, v \in \mathbb{H}$.

In the standard complex theory ($\varphi = \varphi_0 + i\,\varphi_1$ and $\xi = \xi_0 + i\,\xi_1 \in \mathbb{C}\otimes\mathcal{F}$) a useful criterion to establish linear independence and dependence of two solutions of homogeneous second order differential equation, uses the concept of *Wronskian* of these solutions defined by

$$W = \varphi\,\xi' - \varphi'\,\xi, \quad W \in \mathbb{C}\otimes\mathcal{F}. \tag{9}$$

This definition cannot be extended to quaternionic functions. Let us consider two linearly dependent solutions of Eq. (7),

$$\xi = \varphi\,q, \quad \varphi, \xi \in \mathbb{H}\otimes\mathcal{F}, \quad q \in \mathbb{H}. \tag{10}$$

By substituting $\xi = \varphi\,q$ and $\xi' = \varphi'\,q$ in the *Wronskian* (9), we find

$$\varphi\,\xi' - \varphi'\,\xi = \varphi\,\varphi'\,q - \varphi'\,\varphi\,q \neq 0.$$

Observe that a quaternionic function and its first derivative do not, in general, commute. Thus, the definition (9), and all its possible factor combinations cannot be extended to the quaternionic case.

Let us now use the linear dependence condition (10) to investigate the possibility to define a quaternionic functional which extends (in a nontrivial way) the standard (complex) *Wronskian* to the noncommutative case. From Eq. (10) and its derivative, we get

$$q = \varphi^{-1}\xi = (\varphi')^{-1}\xi',$$

where $\varphi^{-1} \equiv 1/\varphi$ and $(\varphi')^{-1} \equiv 1/\varphi'$. Consequently, for linearly dependent quaternionic solutions, we have

$$\xi' - \varphi'\,\varphi^{-1}\,\xi = 0. \tag{11}$$

To recover, in the complex limit, the standard definition (9) we multiply $\xi' - \varphi'\varphi^{-1}\xi$ by φ. Due to the noncommutative nature of quaternions, we have to consider the following possibilities:

$$W_L = \varphi\,(\,\xi' - \varphi'\,\varphi^{-1}\xi\,) \quad \text{and} \quad W_R = (\,\xi' - \varphi'\,\varphi^{-1}\xi\,)\,\varphi. \tag{12}$$

Obviously two other *similar* definitions can be obtained by $\varphi \leftrightarrow \xi$,

$$\tilde{W}_L = -\,\xi\,(\,\varphi' - \xi'\,\xi^{-1}\varphi\,) = -\,W_L[\varphi \leftrightarrow \xi] \quad \text{and} \quad \tilde{W}_R = -\,(\,\varphi' - \xi'\,\xi^{-1}\varphi\,)\,\xi = -\,W_R[\varphi \leftrightarrow \xi]. \tag{13}$$

The quaternionic functionals (12) and (13), which give in the complex limit the standard definition, extend a first important property of *Wronskian*. Two solutions of Eq. (7) are linearly dependent on I if $W_{L(R)}$ [$\tilde{W}_{L(R)}$] is zero on I. To avoid ambiguity in defining the *Wronskian*, we shall introduce a (real) functional,

$$|W|^2=|W_L|^2=|W_R|^2=|\tilde{W}_L|^2=|\tilde{W}_R|^2,$$

which extends the *squared absolute value* of the *Wronskian*. This *unique* functional is

$$|W|^2=|\varphi|^2\,|\xi'|^2+|\xi|^2\,|\varphi'|^2-\varphi'\,\varphi_c\,\xi\,\xi_c'-\xi'\,\xi_c\,\varphi\,\varphi_c' \qquad \in \mathbb{R}\otimes\mathcal{F}, \tag{14}$$

where $\varphi_c=\varphi_0-i\,\varphi_1-j\,\varphi_2-k\,\varphi_3$ and $\xi_c=\xi_0-i\,\xi_1-j\,\xi_2-k\,\xi_3$ are, respectively, the quaternionic conjugate functions of φ and ξ.

Observe that Eq. (14) can also be obtained as an application of the Dieudonné theory of quaternionic determinants.[8–12] In fact,

$$|W|^2=[\mathrm{Det}(M)]^2:=\det(M\,M^+), \tag{15}$$

where

$$M=\begin{pmatrix}\varphi & \xi\\ \varphi' & \xi'\end{pmatrix}.$$

Theorem 2: Let α and β in Eq. (7) be continuous functions of x on an open interval $I:(a,b)$. Then, two solutions φ and ξ of Eq. (7) on I are linearly dependent on I if and only if the *absolute value* of the Wronskian, $|W|$, is zero at some x_0 in I.

The proof will be divided into three steps:

(a) If φ and ξ are linearly dependent on I then $|W|=0$.
(b) If $|W|=0$ at some x_0 in I then $|W|=0$ on I.
(c) If $|W|=0$ at some x_0 in I then φ and ξ are linearly dependent on I.

Proof (a): If φ and ξ are linearly dependent on I, then Eq. (10) holds on I. From Eq. (10), we get

$$|W|^2=|\varphi|^2\,|\varphi'|^2\,|q|^2+|\varphi|^2\,|\varphi'|^2\,|q|^2-\varphi'\,\varphi_c\varphi\,|q|^2\,\varphi_c'-\varphi'\,|q|^2\,\varphi_c\varphi\varphi_c'=0,$$

then $|W|=0$.

Proof (b): Let us consider Eq. (14). By calculating the first derivative of the left-hand- and right-hand-side terms, we obtain

$$\begin{aligned}
2\,|W|\,|W|' &= \varphi'\,\varphi_c\xi'\,\xi_c'+\varphi\varphi_c'\xi'\,\xi_c'+\varphi\varphi_c\Psi_2''\xi_c'+\varphi\varphi_c\xi'\,\xi_c''+\xi'\,\xi_c\varphi'\,\varphi_c'+\xi\xi_c'\varphi'\,\varphi_c'\\
&\quad+\xi\xi_c\Psi_1''\varphi_c'+\xi\xi_c\varphi'\,\varphi_c''-\Psi_1''\varphi_c\xi\xi_c'-\varphi'\,\varphi_c'\xi\xi_c'-\varphi'\,\varphi_c\xi'\,\xi_c'-\varphi'\,\varphi_c\xi\xi_c''\\
&\quad-\Psi_2''\xi_c\varphi\varphi_c'-\xi'\,\xi_c'\varphi\varphi_c'-\xi'\,\xi_c\varphi'\,\varphi_c'-\xi'\,\xi_c\varphi\varphi_c''\\
&=|\varphi|^2(\Psi_2''\xi_c'+\xi'\,\xi_c'')+|\xi|^2(\Psi_1''\varphi_c'+\varphi'\,\varphi_c'')-\Psi_1''\varphi_c\xi\xi_c'-\varphi'\,\varphi_c\xi\xi_c''\\
&\quad-\Psi_2''\xi_c\varphi\varphi_c'-\xi'\,\xi_c\varphi\varphi_c''\\
&=|\varphi|^2(\alpha\,|\xi'|^2+\beta\,\xi\xi_c'+\mathrm{h.c.})+|\xi|^2(\alpha\,|\varphi'|^2+\beta\,\varphi\varphi_c'+\mathrm{h.c.})\\
&\quad-[(\alpha\,\varphi'\,\varphi_c+\beta\,|\varphi|^2)\,\xi\xi_c'+\mathrm{h.c.}]-[(\alpha\,\xi'\,\xi_c+\beta\,|\xi|^2)\,\varphi\varphi_c'+\mathrm{h.c.}]\\
&=2\,\mathrm{Re}[\alpha]\,(|\varphi|^2\,|\xi'|^2+|\xi|^2\,|\varphi'|^2-\varphi'\,\varphi_c\xi\xi_c'-\xi'\,\xi_c\varphi\varphi_c')=2\,\mathrm{Re}[\alpha]\,|W|^2.
\end{aligned}$$

By a simple integration, we find

$$|W(x)| = \exp\left[\int_{x_0}^{x} \mathrm{Re}[\alpha(y)]\,dy\right] |W(x_0)|. \tag{16}$$

This proves the statement (b).

Proof (c): From the statement (b), we have

$$|W(x_0)| = 0 \;\Rightarrow\; |W(x)| = 0, \quad x \in I.$$

This implies that the quaternionic matrix

$$\begin{pmatrix} \varphi & \xi \\ \varphi' & \xi' \end{pmatrix}$$

is not invertible on I.[12] Hence the linear system

$$\varphi\, q_1 + \xi\, q_2 = 0, \quad \varphi'\, q_1 + \xi'\, q_2 = 0,$$

in the unknowns $q_{1,2} \in \mathbb{H}$, has a solution (q_1, q_2) where q_1 and q_2 are not both zero. Recalling that φ and ξ are linearly independent on an interval I if

$$\varphi(x)\, q_1 + \xi(x)\, q_2 = 0 \;\Rightarrow\; q_1 = q_2 = 0,$$

the fact that q_1 and q_2 are not both zero guarantees the linear dependence of φ and ξ on I. ■

Example 1: Show that $\varphi = \exp[-ix]$ and $\xi = \exp[(i-j)x]$ form a basis of solutions of

$$\Psi'' + j\,\Psi' + (1-k)\,\Psi = 0, \tag{17}$$

on any interval.

Solution: Substitution shows that they are solutions,

$$[-1 + j(-i) + 1 - k]\exp[-ix] = 0,$$

$$[-2 + j(i-j) + 1 - k]\exp[(i-j)x] = 0,$$

and linear independence follows from Theorem 2, since

$$|W| = \sqrt{|i-j|^2 + |i|^2 + i(j-i) - (i-j)i} = \sqrt{5}.$$

IV. HOMOGENEOUS EQUATIONS: REDUCTION OF ORDER

Let φ be solution of Eq. (7) on some interval I. Looking for a solution in the form

$$\xi = \varphi\,\tau$$

and substituting ξ and its derivatives

$$\xi' = \varphi'\,\tau + \varphi\,\tau' \quad \text{and} \quad \xi'' = \varphi''\,\tau + 2\,\varphi'\,\tau' + \varphi\,\tau''$$

into Eq. (7), we obtain

$$\tau'' = (\varphi^{-1}\alpha\,\varphi - 2\,\varphi^{-1}\varphi')\,\tau'. \tag{18}$$

It is important to observe that, for quaternionic functions, we *cannot* give a formal solution of the previous equation. Only in particular cases, Eq. (18) can be immediately integrated. For example, for homogeneous second order equations with constant coefficients,

$$\alpha(x)\to a\in\mathbb{H} \quad \text{and} \quad \beta(x)\to b\in\mathbb{H},$$

at least one solution is in the form of a quaternionic exponential, $\varphi=\exp[qx]$, and consequently Eq. (18) reduces to

$$\varphi\tau''=(a-2\,q)\,\varphi\tau'. \tag{19}$$

Let us introduce the quaternionic function

$$\sigma=\varphi\tau'.$$

Observing that

$$\sigma'=\varphi'\,\tau'+\varphi\tau''=q\,\varphi\tau'+\varphi\tau'',$$

Eq. (19) can be rewritten as follows:

$$\sigma'=(a-q)\sigma. \tag{20}$$

This equation can be immediately integrated, its solution reads

$$\sigma=\exp[(a-q)x].$$

Thus, the second solution of the homogeneous second order differential equation with constant coefficients is given by

$$\xi=\exp[qx]\int \exp[-qx]\exp[(a-q)x]\,\mathrm{d}x. \tag{21}$$

In the complex limit ($a,q\in\mathbb{C}$) we find the well-known results $\xi\propto\exp[(a-q)x]$ if $2q\neq a$ and $\xi\propto x\exp[qx]$ if $2q=a$. In the quaternionic case ($a,q\in\mathbb{C}$), the integral which appears in (21) must be treated with care. The solution of this integral will give interesting information about the second solution of quaternionic differential equations with constant coefficients when the associated characteristic quadratic equation has a unique solution. To solve the integral in Eq. (21), we start by observing that

$$[e^{ux}e^{vx}]'=u\,e^{ux}e^{vx}+e^{ux}e^{vx}v=(L_u+R_v)\,e^{ux}e^{vx}.$$

If the operator L_u+R_v is invertible the previous equality implies

$$\int e^{ux}e^{vx}\,\mathrm{d}x=(L_u+R_v)^{-1}\,e^{ux}e^{vx}.$$

This result guarantees that, if the operator $L_{-q}-R_{a-q}$ is invertible the second solution can be written in the form

$$\begin{aligned}\xi&=\exp[qx]\,(L_{-q}+R_{a-q})^{-1}\exp[-qx]\exp[(a-q)x]\\&=\exp[qx]\,(R_{a-q}-L_q)^{-1}\exp[-qx]\exp[(a-q)x].\end{aligned} \tag{22}$$

If the operator $L_{-q}+R_{a-q}$ is *not* invertible, we need to solve the integral which appears in (21) by using the polar decomposition of quaternions (see example 3) and a term linearly dependent on x

will appear. In the complex case ($a,q\in\mathbb{C}$), the operator $L_{-q}+R_{a-q}$ is not invertible if and only if $2q=a$. In the quaternionic ($a,q\in\mathbb{H}$), the condition $2q\neq a$ does not guarantee that the operator is invertible.

Example 2: Knowing that $\varphi=\exp[-ix]$ is solution of the homogeneous second order equation (17), find (by using the method of reduction of order) a second independent solution, ξ.

Solution: We have $q=-i$ and $a=-j$. To use Eq. (22) we have to prove that the operator

$$L_{-q}+R_{a-q}=L_i+R_{i-j}$$

is invertible. A simple algebraic calculation shows that

$$(L_i-R_{i-j})(L_i+R_{i-j})=1.$$

Thus,

$$(L_{-q}+R_{a-q})^{-1}=L_i-R_{i-j}.$$

We are now ready to calculate ξ from Eq. (22),

$$\xi=\exp[-ix]\,(L_i-R_{i-j})\exp[ix]\exp[(i-j)x]=(L_i-R_{i-j})\exp[(i-j)x]=\exp[(i-j)x]\,j.$$

Due to the $\mathbb{H}$ linearity (from the right) of Eq. (17) the right factor j can be ignored recovering the solution of example 1.

Example 3: Inspection shows that

$$\Psi''+i\,\Psi'+\frac{k}{2}=0 \tag{23}$$

has $\varphi=\exp\{-[(i+j)/2]\,x\}$ as a first solution. Find the second linear independent solution.

Solution: We have $q=-(i+j)/2$ and $a=-i$. In this case, the operator

$$L_{-q}+R_{a-q}=L_{(i+j)/2}+R_{(j-i)/2}$$

is *not* invertible. This is easily seen by using, for example, the real matrix representation (3). Thus, the integral in Eq. (21) cannot be expressed in terms of an exponential product. Let us explicitly calculate ξ from Eq. (21). We find

$$\begin{aligned}\xi&=\exp\left[-\frac{i+j}{2}x\right]\int\exp\left[\frac{i+j}{2}x\right]\exp\left[\frac{j-i}{2}x\right]\mathrm{d}x\\&=\exp\left[-\frac{i+j}{2}x\right]\int\left(\cos\frac{x}{\sqrt{2}}+\frac{i+j}{\sqrt{2}}\sin\frac{x}{\sqrt{2}}\right)\left(\cos\frac{x}{\sqrt{2}}+\frac{j-i}{\sqrt{2}}\sin\frac{x}{\sqrt{2}}\right)\mathrm{d}x\\&=\exp\left[-\frac{i+j}{2}x\right]\int\{1-k\exp[-(i+j)x]\}\frac{1+k}{2}\,\mathrm{d}x.\end{aligned}$$

Due to the $\mathbb{H}$ linearity (from the right) of Eq. (23) the right factor $(1+k)/2$ can be removed. After integration, we find

$$\xi=\exp\left[-\frac{i+j}{2}x\right]\left\{x-k\frac{i+j}{2}\exp[-(i+j)x]\right\}=\left(x+\frac{i-j}{2}\right)\exp\left[-\frac{i+j}{2}x\right].$$

Observe that the quaternionic factor $(i-j)/2$ appears on the left of the quaternionic exponential and consequently *cannot* be removed. It is a fundamental part of the solution. Inspection shows that

$$\xi = x \exp\left[-\frac{i+j}{2} x \right]$$

is *not* the solution of Eq. (23).

V. NONHOMOGENEOUS EQUATIONS: VARIATION OF PARAMETERS

A general solution of the nonhomogeneous equation (4) is a solution of the form

$$\Psi = \Psi_h + \Psi_p, \tag{24}$$

where

$$\Psi_h = \varphi\, q_1 + \xi\, q_2$$

is a general solution of the homogeneous equation (7) and Ψ_p is any particular solution of (4) containing no arbitrary constants. In this section we discuss the so-called method of variation of parameters to find a particular solution for quaternionic nonhomogeneous differential equations.

A method to solve a homogeneous second order quaternionic differential equations with constant coefficients has been recently developed.[2] Quaternionic differential equations with nonconstant coefficients are under investigation. We suppose to know two independent solutions of the homogeneous equation associated with Eq. (7). We wish to investigate if the method of variation of parameters still works in the quaternionic case.

The method of variation of parameters involves replacing the constant q_1 and q_2 by quaternionic functions $\nu_1(x)$ and $\nu_2(x)$ to be determined so that the resulting function

$$\Psi_p = \varphi\, \nu_1 + \xi\, \nu_2$$

is a particular solution of Eq. (4). By differentiating Ψ_p we obtain

$$\Psi_p' = \varphi'\, \nu_1 + \xi'\, \nu_2 + \varphi\, \nu_1' + \xi\, \nu_2'.$$

The requirement that Ψ_p satisfies Eq. (4) imposes only *one* condition on ν_1 and ν_2. Hence, we can impose a second arbitrary condition, that is

$$\varphi\, \nu_1' + \xi\, \nu_2' = 0. \tag{25}$$

This reduces Ψ_p' to the form

$$\Psi_p' = \varphi'\, \nu_1 + \xi'\, \nu_2.$$

By differentiating this function we have

$$\Psi_p'' = \varphi''\, \nu_1 + \varphi'\, \nu_1' + \xi''\, \nu_2 + \xi'\, \nu_2'.$$

Substituting Ψ_p, Ψ_p', and Ψ_p'' in Eq. (4) we readily obtain

$$\varphi'\, \nu_1' + \xi'\, \nu_2' = \rho. \tag{26}$$

Collecting Eq. (25) and Eq. (26), we can construct the following matrix system:

$$\begin{pmatrix} \varphi & \xi \\ \varphi' & \xi' \end{pmatrix} \begin{bmatrix} \nu_1' \\ \nu_2' \end{bmatrix} = \begin{bmatrix} 0 \\ \rho \end{bmatrix}, \tag{27}$$

from which ($|W| \neq 0$) we obtain

$$\begin{bmatrix} \nu_1' \\ \nu_2' \end{bmatrix} = \begin{pmatrix} \varphi & \xi \\ \varphi' & \xi' \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ \rho \end{bmatrix} = \begin{pmatrix} [\varphi - \xi \xi'^{-1} \varphi']^{-1} & [\varphi' - \xi' \xi^{-1} \varphi]^{-1} \\ [\xi - \varphi \varphi'^{-1} \xi']^{-1} & [\xi' - \varphi' \varphi^{-1} \xi]^{-1} \end{pmatrix} \begin{bmatrix} 0 \\ \rho \end{bmatrix}. \tag{28}$$

Then,

$$\nu_1' = [\varphi' - \xi' \xi^{-1} \varphi]^{-1} \rho \quad \text{and} \quad \nu_2' = [\xi' - \varphi' \varphi^{-1} \xi]^{-1} \rho. \tag{29}$$

To find $\nu_1(x)$ and $\nu_2(x)$ we have to integrate the previous equations.

Example 4: Find a general solution of the nonhomogeneous quaternionic differential equation

$$\Psi'' + j\,\Psi' + (1-k)\,\Psi = i\,x. \tag{30}$$

Solution: The solution of the associated homogeneous equation (see example 1) is

$$\Psi_h = \exp[-ix]\,q_1 + \exp[-(i+j)x]\,q_2.$$

The particular solution is

$$\Psi_p = \exp[-ix]\,\nu_1 + \exp[-(i+j)x]\,\nu_2.$$

Consequently, from Eqs. (29) we find

$$\nu_1' = \exp[ix]\,x\,k \quad \text{and} \quad \nu_2' = -\exp[(i+j)x]\,x\,k$$

which after integration give

$$\nu_1(x) = (1-ix)\exp[ix]\,k \quad \text{and} \quad \nu_2(x) = -\tfrac{1}{2}[1-(i+j)x]\exp[(i+j)x]\,k.$$

Finally

$$\Psi_p = \tfrac{1}{2}[(i+j)\,x + k].$$

A general solution of Eq. (23) is

$$\Psi = \exp[-ix]\,q_1 + \exp[-(i+j)x]\,q_2 + \tfrac{1}{2}[(i+j)\,x + k].$$

VI. CONCLUSIONS AND OUTLOOKS

The recent results on violations of quantum mechanics by quaternionic potentials[1] and the possibility to get a better understanding of CP-violation phenomena within a quaternionic formulation of physical theories[1,13] stimulated the study of quaternionic differential operators.[2] In this paper, we have proved existence and uniqueness for quaternionic initial value problems and solved simple quaternionic differential equations by discussing the reduction of order for quaternionic homogeneous equations and by extending to the noncommutative case the method of variation of parameters and the definition of absolute value of the Wronskian functional.

In view of a more complete discussion of quantum dynamical systems using quaternionic wave packets, our next research (mathematical) interest will be the study of quaternionic integral transforms. The quaternionic formulation of Fourier transforms could find an immediate and interesting application in the study of delay time modifications of wave packets scattered by a quaternionic potential step.

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Geometric discretization of the Koenigs nets

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(Received 29 July 2002; accepted 28 January 2003)

We introduce the Koenigs lattice, which is a new integrable reduction of the quadrilateral lattice (discrete conjugate net) and provides natural integrable discrete analog of the Koenigs net. We construct the Darboux-type transformation of the Koenigs lattice and we show permutability of superpositions of such transformations, thus proving integrability of the Koenigs lattice. We also investigate the geometry of the discrete Koenigs transformation. In particular we characterize the Koenigs transformation in terms of an involution determined by a congruence conjugate to the lattice. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1563041]

I. INTRODUCTION

In the nineteenth century one of the most favorite subjects of the differential geometry[1,2] was investigation of special classes of surfaces (or, more appropriate, coordinate systems on surfaces and submanifolds) which allow for transformations exhibiting the so-called *permutability property*. Such transformations called, depending on the context, the Darboux, Bianchi, Bäcklund, Laplace, Moutard, Koenigs, Combescure, Lévy, Ribaucour or the fundamental transformation of Jonas, can be also described in terms of certain families of lines called line congruences.[3,4] It turns out that most of the ''interesting'' submanifolds is provided by reductions of conjugate nets, and the transformations between such submanifolds are the corresponding reductions of the fundamental (or Jonas) transformation of the conjugate nets.

From the other side such submanifolds are described by solutions of certain nonlinear partial differential equations, which turn out to be extensively studied in the modern theory of integrable systems; here also the existence of transformations (called in this context the Darboux transformations) appears to be essential. For example, the conjugate nets, their iso-conjugate deformations and transformations are described[5] by the so-called multicomponent Kadomtsev–Petviashvilii hierarchy, which is considered often as the basic system of equations of the soliton theory.[6,7]

Recently the integrable discrete (difference) versions of integrable differential equations attracted a lot of attention (see, for example, articles in Refs. 8, 9, 10, and 11). The interest in discrete integrable systems is stimulated from various directions, like numerical methods, theory of special functions, but also from statistical and quantum physics.[12,13] The discrete integrable systems are considered more fundamental then the corresponding differential systems. Discrete equations include the continuous theory as the result of a limiting procedure, moreover different limits may give from one discrete equation various differential ones. Furthermore, discrete equations reveal some symmetries lost in the continuous limit.

Some recent attempts to quantize the theory of gravity use approach of fluctuating geometries (see recent reviews[14,15]) based on the concept of discrete manifolds. During last few years the connection between geometry and integrability has been observed also at a discrete level. The present paper is the next one in the series of attempts to construct the integrable discrete geometry—the theory of lattice submanifolds described by integrable difference equations.

The natural discrete analogs of certain coordinate systems on surfaces were studied by

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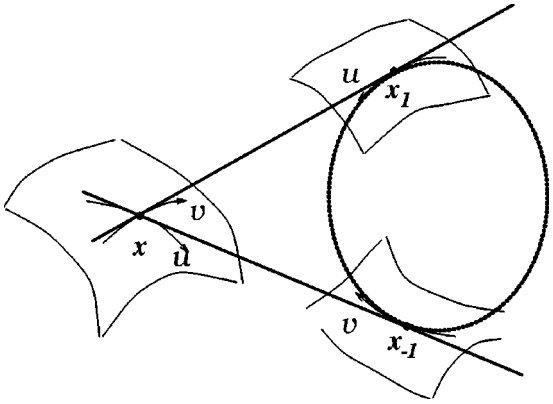

FIG. 1. The Koenigs net.

Sauer.[16] In particular, he introduced the discrete conjugate nets in $\mathbb{E}^3$ as lattices with planar elementary quadrilaterals. The importance of the discrete conjugate nets (the quadrilateral lattices) in the soliton theory was recognized recently in Refs. 17 and 18. The Darboux-type transformations of the quadrilateral lattices have been found in Ref. 19, and the geometry of these transformations was investigated in detail in Ref. 20. In the literature[21–25] there are known various integrable reductions of the quadrilateral lattices. We introduce here the discrete analogue of the Koenigs reduction of conjugate nets. Let us state briefly the main definitions, ideas and results of this paper.

Consider generic two-dimensional conjugate net[26] in M-dimensional projective space $\mathbb{P}^M$. The homogeneous coordinates $\boldsymbol{x}(u,v)\in\mathbb{R}^{M+1}_*$ of the net satisfy the Laplace equation

$$\boldsymbol{x}_{,uv}=a\boldsymbol{x}_{,u}+b\boldsymbol{x}_{,v}+c\boldsymbol{x}, \tag{1}$$

where comma denotes differentiation (e.g., $\boldsymbol{x}_{,u}=\partial\boldsymbol{x}/\partial u$), and a, b, c are functions of the conjugate parameters (u,v) of the net. Its Laplace transforms

$$\boldsymbol{x}_1=\boldsymbol{x}_{,v}-a\boldsymbol{x}, \quad \boldsymbol{x}_{-1}=\boldsymbol{x}_{,u}-b\boldsymbol{x}, \tag{2}$$

are another conjugate nets such that the v tangents of $\boldsymbol{x}$ coincide with the corresponding u-tangent lines of $\boldsymbol{x}_1$ and that the u tangents of $\boldsymbol{x}$ coincide with the corresponding v-tangent lines of $\boldsymbol{x}_{-1}$ (see Fig. 1). In the tangent plane at a point $\boldsymbol{x}$ there is a linear system (pencil) of conics tangent to the u-coordinate line at the point $\boldsymbol{x}_1$ and tangent to the v-curve at the point $\boldsymbol{x}_{-1}$. When there is one conic of this pencil with the second order contact with the u curve of $\boldsymbol{x}_1$ and with the second order contact with the v curve of $\boldsymbol{x}_{-1}$ then the net is called *the net of Koenigs*. It turns out that the Laplace equation (1) of the Koenigs net can be gauged into the form

$$\boldsymbol{x}_{,uv}=f\boldsymbol{x}. \tag{3}$$

The integrable discrete analog of two-dimensional conjugate net is a $\mathbb{Z}^2$-lattice made of planar quadrilaterals.[16,17] One can construct for such lattices[17] the analog of the Laplace transforms $\boldsymbol{x}_1$ and $\boldsymbol{x}_{-1}$. In the plane of the elementary quadrilateral at a point $\boldsymbol{x}(n_1,n_2)$ there is a pencil of conics passing through the points $\boldsymbol{x}_1(n_1,n_2)$ and $\boldsymbol{x}_1(n_1+1,n_2)$ of the Laplace transform $\boldsymbol{x}_1$ and passing through the points $\boldsymbol{x}_{-1}(n_1,n_2)$ and $\boldsymbol{x}_{-1}(n_1,n_2+1)$ of the Laplace transform $\boldsymbol{x}_{-1}$; we have replaced the tangency to a curve by its natural discrete analog of passing through two neighboring points of the discrete parametric curve. When there is one conic of this pencil passing through $\boldsymbol{x}_1(n_1+2,n_2)$ and passing through $\boldsymbol{x}_{-1}(n_1,n_2+2)$ then we call such a lattice *the Koenigs lattice*.

The reduction of the fundamental transformation of conjugate nets to the class of the Koenigs nets is called *the transformation of Koenigs*. Such transformation is determined only by the half of

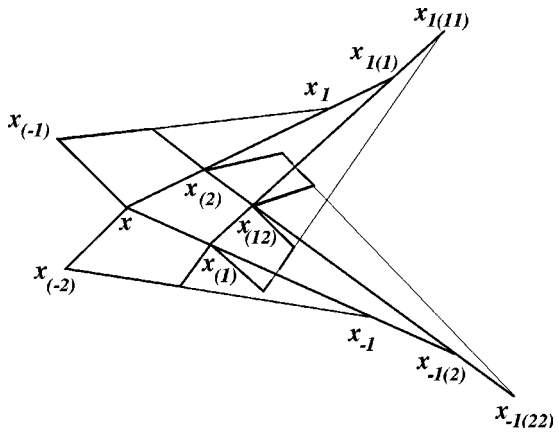

FIG. 2. The quadrilateral lattice and its Laplace transforms.

the data of the fundamental transformation: given congruence conjugate to the Koenigs net then the second Koenigs net $\boldsymbol{x}'$ is the harmonic conjugate of $\boldsymbol{x}$ with respect to the focal nets of the congruence. The discrete analogue of this construction is more subtle. One can show that $\boldsymbol{x}'$ is the image of $\boldsymbol{x}$ in an involution on the corresponding line of the congruence. This involution is uniquely defined by the focal nets of the congruence; in the continuous case the focal points are the double points of the involution.[3,26]

We have sketched the main ideas and results of the paper. The detailed presentation will be as follows. In Sec. II we define and study in detail the Koenigs lattice. In particular we discuss the integrability of the Koenigs lattice from the point of view of the Pascal theorem. In Sec. III we present the discrete analog of the Koenigs transformation and then in Sec. IV we investigate geometric properties of the Koenigs transformation. Finally, in Sec. V we investigate superpositions of the Koenigs transformation and prove their permutability, thus showing integrability of the Koenigs lattice.

It should be mentioned that the elliptic version of an integrable reduction (called the Bianchi system[27,28]) of Eq. (3) is equivalent to the Ernst equation describing axisymmetric stationary vacuum solutions of the Einstein equations[29–32] as well as the interaction of gravitational waves.[33] Results presented in this paper will be important[34] in geometric interpretation of the discrete version of the Bianchi system found recently in Refs. 35 and 36 (see also Ref. 37).

II. THE KOENIGS LATTICE

Consider a two-dimensional quadrilateral lattice in M-dimensional projective space $\mathbb{P}^M$, whose points labeled by two-dimensional integer lattice $\mathbb{Z}^2$, satisfy the property of planarity of elementary quadrilaterals.[16,17] In terms of the homogeneous coordinates such a lattice is described by solution of the discrete Laplace equation

$$\boldsymbol{x}_{(12)} = A_{(1)}\boldsymbol{x}_{(1)} + B_{(2)}\boldsymbol{x}_{(2)} + C\boldsymbol{x}, \tag{4}$$

where $\boldsymbol{x}:\mathbb{Z}^2 \to \mathbb{R}_*^{M+1}$ and subscripts in brackets mean shifts along the $\mathbb{Z}^2$ lattice, i.e., $\boldsymbol{x}_{(\pm 1)}(n_1,n_2) = \boldsymbol{x}(n_1 \pm 1, n_2)$, $\boldsymbol{x}_{(\pm 2)}(n_1,n_2) = \boldsymbol{x}(n_1,n_2 \pm 1)$, and $\boldsymbol{x}_{(\pm 1 \pm 2)}(n_1,n_2) = \boldsymbol{x}(n_1 \pm 1, n_2 \pm 1)$. Here also A, B, and C are functions on $\mathbb{Z}^2$ which characterize the lattice completely up to initial curves $\boldsymbol{x}(n_1,0)$ and $\boldsymbol{x}(0,n_2)$. Notice that multiplication of $\boldsymbol{x}$ by a nonzero function ρ implies the corresponding change of A, B, and C but does not change the lattice itself.

As it was shown in Ref. 17 because of the planarity of the elementary quadrilaterals of the lattice one can define its Laplace transforms $\boldsymbol{x}_1$ and $\boldsymbol{x}_{-1}$ (see Fig. 2)

$$\boldsymbol{x}_1 = \boldsymbol{x}_{(2)} - A\boldsymbol{x}, \quad \boldsymbol{x}_{-1} = \boldsymbol{x}_{(1)} - B\boldsymbol{x}.$$

Remark: Notice that our notation differs from that of Ref. 17 by opposite ordering of the transformations and by shifts in parameters. Moreover in Ref. 17 we used the affine gauge which made some formulas more complicated.

Using the discrete Laplace equation (4) one can show that $\boldsymbol{x}_{1(1)}$ is collinear with $\boldsymbol{x}$, $\boldsymbol{x}_{(2)}$ and $\boldsymbol{x}_1$,

$$\boldsymbol{x}_{1(1)}=B_{(2)}\boldsymbol{x}_{(2)}+C\boldsymbol{x}=B_{(2)}\boldsymbol{x}_1+(B_{(2)}A+C)\boldsymbol{x};$$

similarly $\boldsymbol{x}_{-1(2)}$ is collinear with $\boldsymbol{x}$, $\boldsymbol{x}_{(1)}$, and $\boldsymbol{x}_{-1}$,

$$\boldsymbol{x}_{-1(2)}=A_{(1)}\boldsymbol{x}_{(1)}+C\boldsymbol{x}=A_{(1)}\boldsymbol{x}_{-1}+(A_{(1)}B+C)\boldsymbol{x}.$$

Remark: Two functions H and K defined[17] as the cross ratios

$$H=\mathrm{cr}(\boldsymbol{x}_{(1)},\boldsymbol{x};\boldsymbol{x}_{-1},\boldsymbol{x}_{-1(2)})=-\frac{A_{(1)}B}{C},$$

$$K=\mathrm{cr}(\boldsymbol{x}_{(2)},\boldsymbol{x};\boldsymbol{x}_1,\boldsymbol{x}_{1(1)})=-\frac{B_{(2)}A}{C},$$

are gauge invariant and are called the invariants of the lattice $\boldsymbol{x}$. They are natural discrete analogs of the invariants,

$$h=c+ab-a_{,u},\quad k=c+ab-b_{,v},$$

of conjugate nets. In the continuous case the Koenigs nets have equal invariants, i.e., $h=k$. This property does not transfer to the discrete case.

It is well known (see, for example, Ref. 38) that five distinct points in a projective plane, no four of which are collinear, uniquely determine a conic. Moreover, a pencil of conics (one-dimensional linear subspace of the five-dimensional space of conics) is uniquely determined by four points (the base of the pencil) no three of which are collinear.

The four points $\boldsymbol{x}_1$, $\boldsymbol{x}_{1(1)}$, $\boldsymbol{x}_{-1}$, and $\boldsymbol{x}_{-1(2)}$ belong to the plane $P_{\boldsymbol{x}\boldsymbol{x}_{(1)}\boldsymbol{x}_{(2)}}$ of the elementary quadrilateral of $\boldsymbol{x}$ and define a linear system of conics. Let us choose the points $\boldsymbol{x}$, $\boldsymbol{x}_{-1(2)}$, $\boldsymbol{x}_{1(1)}$ as vertices of the local triangle of reference in that plane, i.e., a point $y_1\boldsymbol{x}+y_2\boldsymbol{x}_{-1(2)}+y_3\boldsymbol{x}_{1(1)}$ has coordinates proportional to (y_1,y_2,y_3). Then the equation of a general conic of the pencil is of the form

$$y_1^2+(A_{(1)}B+C)y_1y_2+(B_{(2)}A+C)y_1y_3+\lambda y_2y_3=0, \tag{5}$$

with λ being a parameter.

Definition 1: The Koenigs lattice is a two-dimensional quadrilateral lattice such that for every point $\boldsymbol{x}$ of the lattice there exist a conic passing through the six points $\boldsymbol{x}_1$, $\boldsymbol{x}_{1(1)}$, $\boldsymbol{x}_{1(11)}$, $\boldsymbol{x}_{-1}$, $\boldsymbol{x}_{-1(2)}$, and $\boldsymbol{x}_{-1(22)}$.

Proposition 1: The Laplace equation of the Koenigs lattice can be gauged into the canonical form

$$\boldsymbol{x}_{(12)}+\boldsymbol{x}=F_{(1)}\boldsymbol{x}_{(1)}+F_{(2)}\boldsymbol{x}_{(2)}. \tag{6}$$

Proof: The points $\boldsymbol{x}_{1(11)}$ and $\boldsymbol{x}_{-1(22)}$ also belong to the plane $P_{\boldsymbol{x}\boldsymbol{x}_{(1)}\boldsymbol{x}_{(2)}}=P_{\boldsymbol{x}\boldsymbol{x}_{-1(2)}\boldsymbol{x}_{1(1)}}$ and have the following decompositions:

$$\boldsymbol{x}_{1(11)}=-\left(CB_{(12)}+\frac{CC_{(1)}}{A_{(1)}}\right)\boldsymbol{x}+\left(B_{(12)}+\frac{C_{(1)}}{A_{(1)}}\right)\boldsymbol{x}_{-1(2)}+B_{(12)}\boldsymbol{x}_{1(1)},$$

$$\boldsymbol{x}_{-1(22)}=-\left(CA_{(12)}+\frac{CC_{(2)}}{B_{(2)}}\right)\boldsymbol{x}+A_{(12)}\boldsymbol{x}_{-1(2)}+\left(A_{(12)}+\frac{C_{(2)}}{B_{(2)}}\right)\boldsymbol{x}_{1(1)}.$$

In the pencil (5) there exist a conic passing through $\boldsymbol{x}_{1(11)}$ and $\boldsymbol{x}_{-1(22)}$ if and only if the coefficients of the Laplace equation (4) of the Koenigs lattice satisfy the constraint

$$\frac{AC_{(2)}}{A_{(12)}}=\frac{BC_{(1)}}{B_{(12)}}. \tag{7}$$

This constraint is the compatibility condition of the linear system for the unknown function ρ

$$\rho_{(12)}=-C\rho, \tag{8}$$

$$\rho_{(1)}A=\rho_{(2)}B. \tag{9}$$

Using solution of this system as the gauge function we obtain new representation

$$\tilde{\boldsymbol{x}}=\frac{1}{\rho}\boldsymbol{x},$$

of the Koenigs lattice which satisfies Eq. (6) with

$$F=\frac{A\rho}{\rho_{(2)}}=\frac{B\rho}{\rho_{(1)}}. \tag{10}$$

□

Remark: Equation (6), in a gauge equivalent form, appeared first in Refs. 35 and 36 in connection with the integrable discretization of the Bianchi–Ernst system.

Usually the integrability of a nonlinear problem is connected with its hidden linear structure. It turns out that, with the help of the celebrated Pascal theorem on six points on a conic, the discrete Koenigs constraint can be formulated in a linear way.

Proposition 2: The quadrilateral lattice $\boldsymbol{x}$ *is the Koenigs lattice if and only if the lines* $L_{\boldsymbol{x}_{-1}\boldsymbol{x}_{1(11)}}$, $L_{\boldsymbol{x}_1\boldsymbol{x}_{-1(22)}}$ *and* $L_{\boldsymbol{x}\boldsymbol{x}_{(12)}}$ *intersect in a single point.*

Proof: Recall that given six point 1, 2, 3, 4, 5, 6 belong to a conic if and only if the points $i=L_{12}\cap L_{45}$, $j=L_{23}\cap L_{56}$, and $k=L_{34}\cap L_{61}$ are collinear. We apply the Pascal theorem to the six points $\boldsymbol{x}_{-1}$, $\boldsymbol{x}_{-1(2)}$, $\boldsymbol{x}_{-1(22)}$, $\boldsymbol{x}_1$, $\boldsymbol{x}_{1(1)}$, and $\boldsymbol{x}_{1(11)}$. Because point $\boldsymbol{x}$ is the intersection of lines $L_{\boldsymbol{x}_{-1}\boldsymbol{x}_{-1(2)}}$ and $L_{\boldsymbol{x}_1\boldsymbol{x}_{1(1)}}$ and the point $\boldsymbol{x}_{(12)}$ is the intersection of lines $L_{\boldsymbol{x}_{-1(2)}\boldsymbol{x}_{-1(22)}}$ and $L_{\boldsymbol{x}_{1(1)}\boldsymbol{x}_{1(11)}}$ then there exists a conic passing through the six points if and only if the statement of the proposition holds. □

III. THE DISCRETE KOENIGS TRANSFORMATION

The Koenigs transformation is the reduction of the fundamental transformation to the class of the Koenigs nets and lattices. Let us first recall relevant definitions and results from the theory of transformations of quadrilateral lattices.[20] Then we present the algebraic definition of the Koenigs reduction of the fundamental transformation. We postpone to next section the discussion of the geometric interpretation of the Koenigs transformation.

A. The fundamental transformation of quadrilateral lattices

We recall the basic results from the theory of transformations of quadrilateral lattices.[20] The novelty here is the description of the theory in the homogeneous formalism (but the geometric content does not change). We constrain our presentation to two-dimensional lattices and congruences only.

Definition 2: The discrete two-dimensional line congruence L is a $\mathbb{Z}^2$ family of lines in $\mathbb{P}^M$ such that any two neighboring lines intersect. The intersection $\boldsymbol{y}_i = L \cap L_{(-i)}$, $i=1,2$, is called the ith focal lattice of the congruence.

Corollary 3: The focal lattices of discrete two-dimensional line congruences are quadrilateral lattices.

Definition 3: A two-dimensional quadrilateral lattice $\boldsymbol{x}$ and a two-dimensional congruence L are called conjugate when points of the lattice belong to the corresponding lines of the congruence, i.e., $\boldsymbol{x}(n_1,n_2) \in L(n_1,n_2)$ for all $(n_1,n_2) \in \mathbb{Z}^2$.

Definition 4: The quadrilateral lattice $\boldsymbol{x}'$ is a fundamental transform of $\boldsymbol{x}$ if there exists a congruence (called the congruence of the transformation) conjugate to both lattices.

Theorem 4: *Two quadrilateral lattices $\boldsymbol{x}$ and $\boldsymbol{x}'$ are fundamental transforms of each other if and only if there exist solutions ϕ and ϕ' of the Laplace equations of the lattices and there exist functions k and ℓ such that the system*

$$\Delta_1\left(\frac{\boldsymbol{x}'}{\phi'}\right) = k_{(1)}\Delta_1\left(\frac{\boldsymbol{x}}{\phi}\right), \tag{11}$$

$$\Delta_2\left(\frac{\boldsymbol{x}'}{\phi'}\right) = \ell_{(2)}\Delta_2\left(\frac{\boldsymbol{x}}{\phi}\right), \tag{12}$$

is satisfied.

Corollary 5: The system (11) *is compatible if and only if there exist a solution θ of the equation*

$$C\theta_{(12)} = -B\theta_{(1)} - A\theta_{(2)} + \theta, \tag{13}$$

called the adjoint of (4), *and the functions k and ℓ are solution of the following system*:

$$\begin{aligned} k - \ell &= \phi\theta, \\ \Delta_1\ell &= -(\phi_{(1)} - B\phi)\theta_{(1)}, \\ \Delta_2 k &= (\phi_{(2)} - A\phi)\theta_{(2)}. \end{aligned} \tag{14}$$

Corollary 6: The fundamental transformation of the given lattice $\boldsymbol{x}$ can be constructed when we are given a solution of its Laplace equation and a solution of its adjoint (both are given up to two functions of single variables). The next step is to find the functions k and ℓ (given up to a constant) by solving the system (14). *Finally, the transformed lattice in the gauge*

$$\hat{\boldsymbol{x}} = \frac{\boldsymbol{x}'}{\phi'},$$

is obtained (up to a constant vector) from the system (11). The coefficients of the Laplace equation of the lattice $\hat{\boldsymbol{x}}$ read

$$\hat{A} = A\frac{k_{(2)}\phi}{k\phi_{(2)}}, \quad \hat{B} = B\frac{\ell_{(1)}\phi}{\ell\phi_{(1)}}, \quad \hat{C} = 1 - \hat{A}_{(1)} - \hat{B}_{(2)}.$$

Remark: The corresponding tangent lines of $\boldsymbol{x}$ and $\boldsymbol{x}'$ intersect in points of the quadrilateral lattices

$$\mathcal{L}_1(\boldsymbol{x}) = \Delta_1\left(\frac{\boldsymbol{x}}{\phi}\right), \quad \mathcal{L}_2(\boldsymbol{x}) = \Delta_2\left(\frac{\boldsymbol{x}}{\phi}\right),$$

called the Lévy transforms[20] of $\boldsymbol{x}$.

Corollary 7: The focal lattices of the congruence of the transformation given by

$$\boldsymbol{y}_1 = k\frac{\boldsymbol{x}}{\phi} - \frac{\boldsymbol{x}'}{\phi'}, \quad \boldsymbol{y}_2 = \ell\frac{\boldsymbol{x}}{\phi} - \frac{\boldsymbol{x}'}{\phi'}, \tag{15}$$

satisfy equations

$$\begin{aligned} \boldsymbol{y}_1 - \boldsymbol{y}_2 &= \theta \boldsymbol{x}, \\ \Delta_1 \boldsymbol{y}_2 &= -(\boldsymbol{x}_{(1)} - B\boldsymbol{x})\,\theta_{(1)}, \\ \Delta_2 \boldsymbol{y}_1 &= (\boldsymbol{x}_{(2)} - A\boldsymbol{x})\,\theta_{(2)}, \end{aligned} \tag{16}$$

i.e., they can be found using the solution θ of the adjoint equation (13) only.

Remark: Equations (16) can be used to find congruences conjugate to the lattice $\boldsymbol{x}$. Notice that the role of the new solution ϕ of the Laplace equation (4) of the lattice $\boldsymbol{x}$ in equations (14) is taken in (16) by $\boldsymbol{x}$ itself.

Remark: The lattices $\boldsymbol{y}_1 = \mathcal{L}_1^*(\boldsymbol{x})$ and $\boldsymbol{y}_2 = \mathcal{L}_2^*(\boldsymbol{x})$ are also called the adjoint Lévy transforms[20] of $\boldsymbol{x}$.

B. The algebraic formulation of the discrete Koenigs transformation

Proposition 8: Given the Koenigs lattice $\boldsymbol{x}$ satisfying equation (6) and given a scalar solution θ of its adjoint equation (the Moutard equation)

$$\theta_{(12)} + \theta = F(\theta_{(1)} + \theta_{(2)}), \tag{17}$$

then the solution $\boldsymbol{x}'$ of the linear system

$$\begin{aligned} \Delta_1\left(\frac{\boldsymbol{x}'}{\phi'}\right) &= (\theta\theta_{(2)})_{(1)}\Delta_1\left(\frac{\boldsymbol{x}}{\phi}\right), \\ \Delta_2\left(\frac{\boldsymbol{x}'}{\phi'}\right) &= -(\theta\theta_{(1)})_{(2)}\Delta_2\left(\frac{\boldsymbol{x}}{\phi}\right), \end{aligned}$$

with

$$\phi = \theta_{(1)} + \theta_{(2)}, \quad \phi' = \frac{1}{\theta_{(1)}} + \frac{1}{\theta_{(2)}},$$

is a new Koenigs lattice satisfying equation (6) with

$$F' = F\frac{\theta_{(1)}\theta_{(2)}}{\theta\theta_{(12)}}. \tag{18}$$

Proof: First one should observe[35] that if θ satisfies the Moutard equation (17) then $\phi = \theta_{(1)} + \theta_{(2)}$ is a solution of the Koenigs lattice equation (6). Then the corresponding solutions of the system (14) are

$$k = \theta_{(2)}\theta, \quad \ell = -\theta_{(1)}\theta,$$

and the coefficients of the Laplace equation of the new quadrilateral lattice $\hat{\boldsymbol{x}}$ read

$$\hat{A} = F\frac{\theta_{(1)} + \theta_{(2)}}{\theta\theta_{(2)}}\left(\frac{\theta\theta_{(2)}}{\theta_{(1)} + \theta_{(2)}}\right)_{(2)},$$

$$\hat{B}=F\frac{\theta_{(1)}+\theta_{(2)}}{\theta\theta_{(1)}}\left(\frac{\theta\theta_{(1)}}{\theta_{(1)}+\theta_{(2)}}\right)_{(1)},$$

$$\hat{C}=1-\hat{A}_{(1)}-\hat{B}_{(2)}.$$

The function

$$\rho=\frac{\theta_{(1)}\theta_{(2)}}{\theta_{(1)}+\theta_{(2)}}=\frac{1}{\phi'},$$

is a solution of the system (8) and (9). This implies that

$$\boldsymbol{x}'=\phi'\hat{\boldsymbol{x}},$$

satisfies the Koenigs lattice equation (6), and the corresponding potential, according to Eq. (10), agrees with that given by (18). □

Corollary 9: The function ϕ' satisfies the Laplace equation of the lattice $\boldsymbol{x}'$.

Remark: The important observation that the adjoint of the Koenigs lattice equation is the Moutard equation is due to Nieszporski.[39]

IV. THE GEOMETRIC MEANING OF THE KOENIGS TRANSFORMATION

To present the geometric meaning of the discrete Koenigs transformation, introduced in the preceding section, we first recall standard results on involutions on a projective line L (see Ref. 38).

Theorem 10: *If a projective transformation $h:L\to L$ has two distinct fixed points $\boldsymbol{p}$ and $\boldsymbol{q}$ then h is an involution if and only if for any point $\boldsymbol{u}\in L$ its image $h(\boldsymbol{u})$ is the harmonic conjugate of $\boldsymbol{u}$ with respect to $\boldsymbol{p}$ and $\boldsymbol{q}$.*

Theorem 11: *A projective involution is uniquely determined giving two pairs of homologous points.*

A. The discrete Koenigs transformation as geometric reduction of the fundamental transformation

Proposition 12: Given Koenigs lattice $\boldsymbol{x}$ and its transform $\boldsymbol{x}'$, denote by $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ the focal lattices of the congruence of the transformation. The Koenigs transform $\boldsymbol{x}'$ is the image of $\boldsymbol{x}$ in the unique involution mapping $\boldsymbol{y}_1$ into $\boldsymbol{y}_{1(1)}$ and $\boldsymbol{y}_2$ into $\boldsymbol{y}_{2(2)}$.

Proof: In the gauge of Proposition 8 and due to Corollary 7 we have

$$\boldsymbol{x}=\frac{1}{\theta}(\boldsymbol{y}_1-\boldsymbol{y}_2),\quad \boldsymbol{x}'=-\frac{1}{\theta_{(1)}\theta_{(2)}}(\theta_{(1)}\boldsymbol{y}_1+\theta_{(2)}\boldsymbol{y}_2). \tag{19}$$

Equations (16) imply that

$$\boldsymbol{y}_{1(1)}=\frac{1}{\theta}(F\theta_1\boldsymbol{y}_1-(F\theta_1-\theta)\boldsymbol{y}_2),$$

$$\boldsymbol{y}_{2(2)}=\frac{1}{\theta}(F\theta_2\boldsymbol{y}_2-(F\theta_2-\theta)\boldsymbol{y}_1).$$

The unique involution mapping $\boldsymbol{y}_1$ into $\boldsymbol{y}_{1(1)}$ and $\boldsymbol{y}_2$ into $\boldsymbol{y}_{2(2)}$ is the projection of the linear map, which is convenient to choose in the form

$$\boldsymbol{y}_1\mapsto -F\boldsymbol{y}_1+\left(F-\frac{\theta}{\theta_1}\right)\boldsymbol{y}_2,$$

$$\boldsymbol{y}_2 \mapsto F\boldsymbol{y}_2 - \left(F - \frac{\theta}{\theta_2}\right)\boldsymbol{y}_1 .$$

As one can check directly the image of $\boldsymbol{x}$ in this mapping is $\boldsymbol{x}'$. □

Corollary 13: In the continuous limit the points of the focal lattices become the double points of the involution. This fact and Theorem 10 imply that $\boldsymbol{x}'$ becomes, in the limit, the harmonic conjugate of $\boldsymbol{x}$ with respect to the pair $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$.

It turns out that the property of the Koenigs transformation described in Proposition 12 holds exclusively for the Koenigs lattice and selects it from general quadrilateral lattices.

Proposition 14: Given two quadrilateral lattices $\boldsymbol{x}$ and $\boldsymbol{x}'$ related by the fundamental transformation such that the focal lattices $\boldsymbol{y}_1$, $\boldsymbol{y}_2$ of the congruence of the transformation do not degenerate to a single point. If $\boldsymbol{x}'$ is the image of $\boldsymbol{x}$ in the unique involution mapping $\boldsymbol{y}_1$ into $\boldsymbol{y}_{1(1)}$ and $\boldsymbol{y}_2$ into $\boldsymbol{y}_{2(2)}$ then $\boldsymbol{x}$ and $\boldsymbol{x}'$ are Koenigs lattices related by the Koenigs transformation.

Proof: Notice first that the excluded situation of the degenerated focal lattices corresponds to the trivial solution $\theta=0$ of the adjoint equation (13) of the lattice $\boldsymbol{x}$.

Formulas (15) and the assumption of the proposition imply the following constraint on the functions k and ℓ:

$$k_{(1)}k = \ell_{(2)}\ell .$$

This constraint allows to solve the system (14),

$$k = \frac{\phi\theta\theta_{(2)}A}{A\theta_{(2)} + B\theta_{(1)}}, \quad \ell = -\frac{\phi\theta\theta_{(1)}B}{A\theta_{(2)} + B\theta_{(1)}}, \tag{20}$$

and gives the following relation between the coefficients A and B of the Laplace equation (4):

$$kB\theta_{(1)} + \ell A\theta_{(2)} = 0.$$

In consequence we have also

$$k_{(1)} = -\frac{\phi\theta_{(1)}\theta_{(12)}BC}{A\theta_{(2)} + B\theta_{(1)}}, \quad \ell_{(2)} = \frac{\phi\theta_{(2)}\theta_{(12)}AC}{A\theta_{(2)} + B\theta_{(1)}}. \tag{21}$$

The above relations allow to check that the condition (7) holds for the lattice $\boldsymbol{x}$, which implies that $\boldsymbol{x}$ is the Koenigs lattice (notice that due to the symmetry between both lattices in the definition of the fundamental transformation and in the notion of the harmonic conjugate the analogous condition holds for the lattice $\boldsymbol{x}'$).

Assuming therefore that the function $\boldsymbol{x}$ of the first lattice is in the canonical gauge $A=B=F$, $C=-1$, one obtains from Eqs. (20) and (21) that

$$k = \theta\theta_{(2)}N_2(n_2), \quad \ell = \theta\theta_{(1)}N_1(n_1),$$

where $N_i(n_i), i=1,2,$ are functions (still to be determined) of single variables. Then the function

$$\phi = \theta_{(1)}N_1(n_1) - \theta_{(2)}N_2(n_2),$$

obtained using (14), satisfies equation (6) for generic F only if $N_1 = -N_2 = \text{const}$. Without loss of generality this constant can be put equal to 1. The rest of the proof is the same like the proof of Proposition 8. □

Remark: The above proposition in the continuous case was found by Koenigs.[40]

Remark: The excluded case $\theta=0$ corresponds to the reduction of the fundamental transformation to the radial transformation.[20]

Corollary 15: *For an arbitrary congruence conjugate to a quadrilateral lattice* $\boldsymbol{x}$ *its image* $\boldsymbol{x}'$ *with respect to the unique involution (defined on every line of the congruence) mapping* $\boldsymbol{y}_1$ *into* $\boldsymbol{y}_{1(1)}$ *and* $\boldsymbol{y}_2$ *into* $\boldsymbol{y}_{2(2)}$ *is a quadrilateral lattice if and only if* $\boldsymbol{x}$ *is a Koenigs lattice.*

B. Further geometric properties of the discrete Koenigs transformation

To understand more the relation between the Koenigs lattice, as defined in terms of conics, and the geometric description of the Koenigs transformation in terms of involutions on lines of the congruence, we will need the following result.

Theorem 16 (Desargues–Sturm): *A pencil of conics of a projective plane determines a projective involution on every line that does not intersect the base of the pencil.*

Remark: The results presented in this section are generalization to the discrete level of the results of Tzitzéica[41] and Eisenhart.[42]

It turns out that the Koenigs transformation defines certain family of quadrics. This family contains the pencils of conics of the both Koenigs lattices $\boldsymbol{x}$ and $\boldsymbol{x}'$.

Proposition 17: Given Koenigs lattice $\boldsymbol{x}$ *and its transform* $\boldsymbol{x}'$ *then the pencils of conics of both lattices determine the same involution on the intersection line of the planes of elementary quadrilaterals of* $\boldsymbol{x}$ *and* $\boldsymbol{x}'$.

Proof: In the gauge such that $\boldsymbol{x}$ satisfies Eq. (6), the equation of the pencil of conics (5) reads

$$y_1^2+(F_{(1)}F-1)y_1y_2+(F_{(2)}F-1)y_1y_3+\lambda y_2y_3=0. \tag{22}$$

When the parameter λ equals

$$\lambda_0=\frac{F}{F_{(12)}}+1-F_{(1)}F-F_{(2)}F, \tag{23}$$

the conic passes through $\boldsymbol{x}_{1(11)}$ and $\boldsymbol{x}_{-1(22)}$.

Instead of the basis $\boldsymbol{x}$, $\boldsymbol{x}_{-1(2)}$, and $\boldsymbol{x}_{1(1)}$ of the plane of the elementary quadrilateral of $\boldsymbol{x}$ let us choose points $\boldsymbol{x}$, $\boldsymbol{u}_1$, and $\boldsymbol{u}_2$, where

$$\boldsymbol{u}_1=\Delta_1\left(\frac{\boldsymbol{x}}{\phi}\right),\quad \boldsymbol{u}_2=\Delta_2\left(\frac{\boldsymbol{x}}{\phi}\right),$$

represent points of intersection of the tangent lines of $\boldsymbol{x}$ and $\boldsymbol{x}'$. Moreover the line $L_{\boldsymbol{u}_1\boldsymbol{u}_2}$ is the intersection of the planes of elementary quadrilaterals of $\boldsymbol{x}$ and $\boldsymbol{x}'$. The transition formulas read

$$\boldsymbol{x}_{-1(2)}=F_{(1)}\phi_{(1)}\boldsymbol{u}_1+\boldsymbol{x}\left(\frac{F_{(1)}\phi_{(1)}}{\phi}-1\right),$$

$$\boldsymbol{x}_{1(1)}=F_{(2)}\phi_{(2)}\boldsymbol{u}_2+\boldsymbol{x}\left(\frac{F_{(2)}\phi_{(2)}}{\phi}-1\right).$$

When (t_1,t_2,t_3) are coordinates of a point

$$\boldsymbol{y}=t_1\boldsymbol{x}+t_2\boldsymbol{u}_1+t_3\boldsymbol{u}_2,$$

then the equation of the pencil (23) is transformed into

$$t_1^2+a_1b_1t_2^2+a_2b_2t_3^2+t_1t_2(a_1+b_1)+t_1t_3(a_2+b_2)+t_2t_3(a_1b_2+a_2b_1+\mu)=0, \tag{24}$$

where

$$a_i=\frac{1}{F_{(i)}\phi_{(i)}}-\frac{1}{\phi},\quad b_i=\frac{F}{\phi_{(i)}}-\frac{1}{\phi},\quad i=1,2,$$

and

$$\mu=\frac{\lambda}{F_{(1)}F_{(2)}\phi_{(1)}\phi_{(2)}}. \tag{25}$$

The involution on the line $t_1=0$ is equivalent to the problem of finding the second root of the quadratic equation

$$a_1b_1t_2^2+a_2b_2t_3^2+t_2t_3(a_1b_2+a_2b_1+\mu)=0,$$

when the first root is given. The double points of the involution correspond to

$$\mu=-(a_1b_2+a_2b_1)\pm 2\sqrt{a_1b_1a_2b_2},$$

and their coordinates are solutions of the equation

$$(\sqrt{a_1b_1}t_2\pm\sqrt{a_2b_2}t_3)^2=0.$$

Finally, the double points are given by

$$\sqrt{a_1b_1}\boldsymbol{u}_2\pm\sqrt{a_2b_2}\boldsymbol{u}_1. \tag{26}$$

To find the equation of the second pencil of conics we take the primed version of Eq. (24) with

$$\boldsymbol{u}_1'=\Delta_1\left(\frac{\boldsymbol{x}'}{\phi'}\right)=\theta_{(1)}\theta_{(12)}\boldsymbol{u}_1,$$

$$\boldsymbol{u}_2'=-\Delta_2\left(\frac{\boldsymbol{x}'}{\phi'}\right)=\theta_{(2)}\theta_{(12)}\boldsymbol{u}_2,$$

and

$$a_i'=\frac{1}{F_{(i)}'\phi_{(i)}'}-\frac{1}{\phi'}=-\theta_i^2a_i,\quad b_i'=\frac{F'}{\phi_{(i)}'}-\frac{1}{\phi'}=-\frac{\theta_1\theta_2\theta_{12}}{\theta}b_i\quad i=1,2.$$

The double points on the line $t_1'=0$ of the second involution are given by

$$\sqrt{a_1'b_1'}\boldsymbol{u}_2'\pm\sqrt{a_2'b_2'}\boldsymbol{u}_1'=\frac{(\theta_{(1)}\theta_{(2)}\theta_{(12)})^{3/2}}{(\theta)^{1/2}}(\sqrt{a_1b_1}\boldsymbol{u}_2\pm\sqrt{a_2b_2}\boldsymbol{u}_1),$$

and due to Theorem 11, both evolutions are the same. □

Proposition 18: Given Koenigs lattice $\boldsymbol{x}$ and its transform $\boldsymbol{x}'$ then any pair of intersecting conics of two pencils determines a pencil of quadrics. Such a pencil defines on the line $L_{\boldsymbol{x}\boldsymbol{x}'}$ of the congruence the involution described in Proposition 12.

Proof: Let us choose points $\boldsymbol{x}$, $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, and $\boldsymbol{x}'$ as the vertices of the reference frame, then (t_1,t_2,t_3,t_4) are coordinates of a point

$$\boldsymbol{y}=t_1\boldsymbol{x}+t_2\boldsymbol{u}_1+t_3\boldsymbol{u}_2+t_4\boldsymbol{x}'.$$

Notice the following relation between these coordinates and the coordinates t_i' used in the last part of the proof above:

$$t_1'=t_4,\quad t_2'=\frac{t_2}{\theta_{(1)}\theta_{(12)}},\quad t_3'=-\frac{t_3}{\theta_{(2)}\theta_{(12)}}. \tag{27}$$

The transformation formulas (27) imply that the equation of the second pencil reads

$$\frac{\theta_{(1)}\theta_{(2)}}{\theta\theta_{(12)}}\left[a_1b_1t_2^2+a_2b_2t_3^2-t_2t_3\left(\frac{\theta_{(1)}}{\theta_{(2)}}a_1b_2+\frac{\theta_{(2)}}{\theta_{(1)}}a_2b_1+\frac{\mu'\theta}{\theta_{(1)}^2\theta_{(2)}^2\theta_{(12)}}\right)\right]-t_2t_4\left(\frac{\theta_{(1)}}{\theta_{(12)}}a_1+\frac{\theta_{(2)}}{\theta}b_1\right)$$
$$+t_3t_4\left(\frac{\theta_{(2)}}{\theta_{(12)}}a_2+\frac{\theta_{(1)}}{\theta}b_2\right)+t_4^2=0, \tag{28}$$

and, therefore, the relation between parameters of the corresponding conics in the pencils reads

$$\frac{\phi}{\theta_{(2)}}a_1b_2+\frac{\phi}{\theta_{(1)}}a_2b_1+\frac{\mu'\theta}{\theta_{(1)}^2\theta_{(2)}^2\theta_{(12)}}+\mu=0. \tag{29}$$

Any two corresponding conics of the pencils (24) and (28) define a pencil of quadrics and, finally, we obtain the following two-parameter linear system of quadrics:

$$t_1^2+a_1b_1t_2^2+a_2b_2t_3^2+t_1t_2(a_1+b_1)+t_1t_3(a_2+b_2)+t_2t_3(a_1b_2+a_2b_1+\mu)+\frac{\theta\theta_{(12)}}{\theta_{(1)}\theta_{(2)}}t_4^2+\nu t_1t_4$$
$$-t_2t_4\left(\frac{\theta}{\theta_{(2)}}a_1+\frac{\theta_{(12)}}{\theta_{(1)}}b_1\right)+t_3t_4\left(\frac{\theta}{\theta_{(1)}}a_2+\frac{\theta_{(12)}}{\theta_{(2)}}b_2\right)=0. \tag{30}$$

Notice that any pair of two conics of the pencils [i.e., an arbitrary fixed μ in Eq. (30)] determines the same involution on the line $t_2=t_3=0$ (the line of the congruence)

$$t_1^2+\nu t_1t_4+\frac{\theta\theta_{(12)}}{\theta_{(1)}\theta_{(2)}}t_4^2=0.$$

The fixed points of the involution correspond to

$$\nu=\pm\sqrt{\frac{\theta\theta_{(12)}}{\theta_{(1)}\theta_{(2)}}},$$

and read

$$\pm\sqrt{\theta\theta_{(12)}}\boldsymbol{x}+\sqrt{\theta_{(1)}\theta_{(2)}}\boldsymbol{x}'. \tag{31}$$

One can check using Eqs. (31) and (19) that the pairs $\boldsymbol{x}$ and $\boldsymbol{x}'$, $\boldsymbol{y}_1$ and $\boldsymbol{y}_{1(1)}$, and $\boldsymbol{y}_2$ and $\boldsymbol{y}_{2(2)}$ are harmonically conjugate with respect to the fixed points. □

Corollary 19: Equations (*23*) *and* (*25*)*, their primed versions, and Eq. (29) imply that the distinguished six-point conics of two pencils intersect.*

V. THE PERMUTABILITY OF SUPERPOSITIONS OF THE DISCRETE KOENIGS TRANSFORMATIONS

We show in this section that superpositions of the discrete Koenigs transformations satisfy the permutability property. We start with the relevant properties of the Moutard equation and then we present the permutability theorem for the discrete Koenigs transformation proving this way the integrability of the Koenigs lattice.

A. The discrete Moutard transformation and its permutability property

We recall the known material on the Darboux-type transformation for the Moutard equation[43,44] and the permutability theorem for this transformation.[25,45] The novelty here is the presentation of the Moutard transformation within the general setting of the fundamental transformation of quadrilateral lattices.

Consider the Moutard lattice, i.e., the quadrilateral lattice whose homogeneous coordinates $\boldsymbol{y}:\mathbb{Z}^2\to\mathbb{R}^{N+1}_*$ satisfy (up to a gauge) the discrete Moutard equation (17),

$$\boldsymbol{y}_{(12)}+\boldsymbol{y}=F(\boldsymbol{y}_{(1)}+\boldsymbol{y}_{(2)}). \tag{32}$$

Let θ be a scalar solution of this equation, linearly independent of the components of $\boldsymbol{y}$. One can check that the function $\psi=\theta_{(-1)}+\theta_{(-2)}$ satisfies the equation

$$\psi_{(12)}+\psi=F_{(-2)}\psi_{(1)}+F_{(-1)}\psi_{(2)}, \tag{33}$$

adjoint to the Moutard equation. Notice that, like in the Koenigs lattice case, to construct the fundamental transformation of the Moutard lattice we need only half of the data, but this time the solution of the Moutard equation gives a solution of its adjoint. The solution of the system (14) (with the change of notation $\phi\to\theta$ and $\theta\to\psi$) reads then

$$k=\theta\theta_{(-1)}, \quad \ell=-\theta\theta_{(-2)},$$

and the lattice $\hat{\boldsymbol{y}}$, the solution of the linear system

$$\Delta_1(\hat{\boldsymbol{y}})=\theta\theta_{(1)}\Delta_1\left(\frac{\boldsymbol{y}}{\theta}\right),$$

$$\Delta_2(\hat{\boldsymbol{y}})=-\theta\theta_{(2)}\Delta_2\left(\frac{\boldsymbol{y}}{\theta}\right),$$

satisfies the Laplace equation

$$\hat{\boldsymbol{y}}_{(12)}=F\frac{\theta_{(2)}}{\theta}\hat{\boldsymbol{y}}_{(1)}+F\frac{\theta_{(1)}}{\theta}\hat{\boldsymbol{y}}_{(2)}+\left(1-F\frac{\theta_{(2)}}{\theta}-F\frac{\theta_{(1)}}{\theta}\right)\hat{\boldsymbol{y}}.$$

Its gauge transform $\boldsymbol{y}'$ defined by

$$\hat{\boldsymbol{y}}=\boldsymbol{y}'\theta$$

satisfies the Moutard equation with the potential F' given by Eq. (18).

Finally, we obtain the known[44] formulas

$$\Delta_1(\theta\boldsymbol{y}')=\theta\theta_{(1)}\Delta_1\left(\frac{\boldsymbol{y}}{\theta}\right), \tag{34}$$

$$\Delta_2(\theta\boldsymbol{y}')=-\theta\theta_{(2)}\Delta_2\left(\frac{\boldsymbol{y}}{\theta}\right), \tag{35}$$

which allow to find the new Moutard lattice $\boldsymbol{y}'$ given the old Moutard lattice $\boldsymbol{y}$ and the scalar solution θ of the Moutard equation of $\boldsymbol{y}$. Notice that $\theta'=1/\theta$ satisfies the Moutard equation of $\boldsymbol{y}'$.

Let θ^1 and θ^2 be two solutions of the Moutard equation (17). Denote by $\boldsymbol{y}^{(1)}$ and $\theta^{2(1)}$ the transforms of $\boldsymbol{y}$ and θ^2 via θ^1 and denote by $\boldsymbol{y}^{(2)}$ and $\theta^{1(2)}$ the transforms of $\boldsymbol{y}$ and θ^1 via θ^2. Then $\boldsymbol{y}^{(1)}$, $\theta^{2(1)}$, and $\theta^{1(1)}=1/\theta^1$ satisfy the Moutard equation with the potential

$$F^{(1)}=F\frac{\theta^1_{(1)}\theta^1_{(2)}}{\theta^1\theta^1_{(12)}}, \tag{36}$$

and $\boldsymbol{y}^{(2)}$, $\theta^{1(2)}$, and $\theta^{2(2)}=1/\theta^2$ satisfy the Moutard equation with the potential

$$F^{(2)}=F\frac{\theta^2_{(1)}\theta^2_{(2)}}{\theta^2\theta^2_{(12)}}. \tag{37}$$

Notice[25,45] that the transformation formulas (34) give

$$\Delta_1(\theta^1\theta^{2(1)})=-\Delta_1(\theta^2\theta^{1(2)}), \tag{38}$$

$$\Delta_2(\theta^1\theta^{2(1)})=-\Delta_2(\theta^2\theta^{1(2)}), \tag{39}$$

which implies that fixing one of the two integration constants we have

$$\theta^1\theta^{2(1)}=-\theta^2\theta^{1(2)}=\Xi. \tag{40}$$

Then the lattices $\boldsymbol{y}^{(12)}$ of the one parameter family (due to the additive constant in Ξ) given by

$$\boldsymbol{y}^{(12)}=\boldsymbol{y}+\frac{\theta^1\theta^2}{\Xi}(\boldsymbol{y}^{(1)}-\boldsymbol{y}^{(2)}), \tag{41}$$

are simultaneously transforms of $\boldsymbol{y}^{(1)}$ via $\theta^{2(1)}$ and transforms of $\boldsymbol{y}^{(2)}$ via $\theta^{1(2)}$.

Remark: To obtain symmetric more form of the superposition formula (41) one can use the allowed gauge freedom in the transformation formulas.[25,45]

B. Superposition of the discrete Koenigs transformations

Let us use θ^1 and θ^2 to find two transforms of the Koenigs lattice $\boldsymbol{x}$ satisfying Eq. (6). According to notation of Proposition 8 denote by $\phi^1=\theta^1_{(1)}+\theta^1_{(2)}$ and $\phi^2=\theta^2_{(1)}+\theta^2_{(2)}$ the corresponding solutions of the Koenigs lattice equation. Denote by $\boldsymbol{x}^{(1)}$ and $\phi^{2(1)}$ the transforms of $\boldsymbol{x}$ and ϕ^2 with respect to θ^1, i.e.,

$$\Delta_1\left(\frac{1}{\phi^{1(1)}}\begin{pmatrix}\boldsymbol{x}^{(1)}\\ \phi^{2(1)}\end{pmatrix}\right)=(\theta^1\theta^1_{(2)})_{(1)}\Delta_1\left(\frac{1}{\phi^1}(\boldsymbol{x}\phi^2)\right), \tag{42}$$

$$\Delta_2\left(\frac{1}{\phi^{1(1)}}\begin{pmatrix}\boldsymbol{x}^{(1)}\\ \phi^{2(1)}\end{pmatrix}\right)=-(\theta^1\theta^1_{(1)})_{(2)}\Delta_2\left(\frac{1}{\phi^1}\begin{pmatrix}\boldsymbol{x}\\ \phi^2\end{pmatrix}\right), \tag{43}$$

where

$$\phi^{1(1)}=\frac{1}{\theta^1_{(1)}}+\frac{1}{\theta^1_{(2)}}.$$

According to Proposition 8 the functions $\boldsymbol{x}^{(1)}$, $\phi^{2(1)}$, and $\phi^{1(1)}$ satisfy the Koenigs lattice equation with the transformed potential $F^{(1)}$ given by (36). Similarly, by $\boldsymbol{x}^{(2)}$ and $\phi^{1(2)}$ denote the transforms of $\boldsymbol{x}$ and ϕ^1 with respect to θ^2, i.e.,

$$\Delta_1\left(\frac{1}{\phi^{2(2)}}\begin{pmatrix}\boldsymbol{x}^{(2)}\\ \phi^{1(2)}\end{pmatrix}\right)=(\theta^2\theta^2_{(2)})_{(1)}\Delta_1\left(\frac{1}{\phi^2}\begin{pmatrix}\boldsymbol{x}\\ \phi^1\end{pmatrix}\right), \tag{44}$$

$$\Delta_2\left(\frac{1}{\phi^{2(2)}}\begin{pmatrix}\boldsymbol{x}^{(2)}\\ \phi^{1(2)}\end{pmatrix}\right)=-(\theta^2\theta^2_{(1)})_{(2)}\Delta_2\left(\frac{1}{\phi^2}\begin{pmatrix}\boldsymbol{x}\\ \phi^1\end{pmatrix}\right), \tag{45}$$

where

$$\phi^{2(2)}=\frac{1}{\theta^2_{(1)}}+\frac{1}{\theta^2_{(2)}}, \tag{46}$$

and $\boldsymbol{x}^{(2)}$, $\phi^{1(2)}$, and $\phi^{2(2)}$ satisfy the Koenigs lattice equation with the transformed potential given by (37).

Proposition 20: The lattices $\boldsymbol{x}^{(12)}$ of the one parameter family (because of the free parameter in the definition of Ξ) given by

$$\boldsymbol{x}^{(12)}=-\frac{\Xi_{(1)}\Xi_{(2)}\phi^{1(21)}\phi^{2(12)}}{\phi^{1}\phi^{2}}\boldsymbol{x}+\frac{\phi^{1(21)}}{\phi^{1(1)}}\boldsymbol{x}^{(1)}+\frac{\phi^{2(12)}}{\phi^{2(2)}}\boldsymbol{x}^{(2)}, \tag{47}$$

where

$$\phi^{1(21)}=\frac{1}{\theta^{1(2)}_{(1)}}+\frac{1}{\theta^{1(2)}_{(2)}},\quad \phi^{2(12)}=\frac{1}{\theta^{2(1)}_{(1)}}+\frac{1}{\theta^{2(1)}_{(2)}}, \tag{48}$$

are simultaneously the Koenigs transforms of $\boldsymbol{x}^{(1)}$ via $\theta^{2(1)}$ and the Koenigs transforms of $\boldsymbol{x}^{(2)}$ via $\theta^{1(2)}$.

Proof: We have to check that $\boldsymbol{x}^{(12)}=\boldsymbol{x}^{(21)}$ defined in (47) satisfies equations

$$\Delta_1\left(\frac{\boldsymbol{x}^{(12)}}{\phi^{2(12)}}\right)=\ (\theta^{2(1)}\theta^{2(1)}_{(2)})_{(1)}\Delta_1\left(\frac{\boldsymbol{x}^{(1)}}{\phi^{2(1)}}\right), \tag{49}$$

$$\Delta_2\left(\frac{\boldsymbol{x}^{(12)}}{\phi^{2(12)}}\right)=-(\theta^{2(1)}\theta^{2(1)}_{(1)})_{(2)}\Delta_2\left(\frac{\boldsymbol{x}^{(1)}}{\phi^{2(1)}}\right), \tag{50}$$

which define the transform $\boldsymbol{x}^{(12)}=(\boldsymbol{x}^{(1)})^{(2)}$ of $\boldsymbol{x}^{(1)}$ via $\theta^{2(1)}$, and satisfies equations

$$\Delta_1\left(\frac{\boldsymbol{x}^{(21)}}{\phi^{1(21)}}\right)=\ (\theta^{1(2)}\theta^{1(2)}_{(2)})_{(1)}\Delta_1\left(\frac{\boldsymbol{x}^{(2)}}{\phi^{1(2)}}\right), \tag{51}$$

$$\Delta_2\left(\frac{\boldsymbol{x}^{(21)}}{\phi^{1(21)}}\right)=-(\theta^{1(2)}\theta^{2(2)}_{(1)})_{(2)}\Delta_2\left(\frac{\boldsymbol{x}^{(2)}}{\phi^{1(2)}}\right), \tag{52}$$

which define the transform $\boldsymbol{x}^{(21)}=(\boldsymbol{x}^{(2)})^{(1)}$ of $\boldsymbol{x}^{(2)}$ via $\theta^{1(2)}$. This can be done by direct verification using Eqs. (38)–(40) and (42)–(46). □

Remark: To obtain the superposition formula (47) we assume that $\boldsymbol{x}^{(21)}=\boldsymbol{x}^{(12)}$ and formulas (49)–(52) hold.

ACKNOWLEDGMENT

The author acknowledges partial support from KBN Grant No. 2P03B12622.

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Fractional operators and special functions. I. Bessel functions

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(Received 6 December 2002; accepted 3 January 2003)

Most of the special functions of mathematical physics are connected with the representation of Lie groups. The action of elements D of the associated Lie algebras as linear differential operators gives relations among the functions in a class, for example, their differential recurrence relations. In this paper, we define fractional generalizations D^{μ} of these operators in the context of Lie theory, determine their formal properties, and illustrate their use in obtaining interesting relations among the functions. We restrict our attention here to the Euclidean group E(2) and the Bessel functions. We show that the two-variable fractional operator relations lead directly to integral representations for the Bessel functions, reproduce known fractional integrals for those functions when reduced to one variable, and contribute to a coherent understanding of the connection of many properties of the functions to the underlying group structure. We extend the analysis to the associated Legendre functions in a following paper. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1561593]

I. INTRODUCTION

Most of the classical special functions are connected with the representation of Lie groups,[1–4] and appear as factors in multivariable functions on which the action of an associated Lie algebra is realized by linear differential operators. Many of the properties of the special functions are easily understood in this context. For example, the differential equations for the special functions are connected with the Casimir operator of the associated groups. The actions of appropriate elements D of the Lie algebra lead, when reduced to a single variable, to the standard differential recurrence relations for the functions, while the action of group elements e^{-tD} can be interpreted in terms of generalized generating functions when expressed using a Taylor series expansion in the group parameter t. Numerous examples are given in Refs. 1 and 3. In the present paper, we will define fractional generalizations D^{μ} of the D's in the context of Lie theory, determine their formal properties, and illustrate their usefulness in obtaining further interesting relations among the functions, including integral representations for the functions. Most of the specific results have been derived historically in other ways, but are unified here in a group setting.

Two examples of fractional operators in a single variable are provided by the fractional integrals of Riemann and Weyl (Ref. 5, Chap. 13). These give a useful way of changing the indices (degree or order) of the classical orthogonal functions (Jacobi, Gegenbauer, Legendre, Laguerre, Bessel, and Hermite functions). An example is Sonine's first integral for the Bessel functions,[6] 12.11.(1),

$$x^{\nu+\mu}J_{\nu+\mu}(x)=\frac{x^{\mu}}{2^{\mu-1}\Gamma(\mu)}\int_0^{\pi/2}J_{\nu}(x\sin\theta)\cos^{2\mu-1}\theta\sin^{\nu+1}\theta\,\mathrm{d}\theta \tag{1}$$

$$=\frac{1}{2^{\mu-1}\Gamma(\mu)}\int_0^{x}t^{\nu+1}J_{\nu}(t)(x^2-t^2)^{\mu-1}\,\mathrm{d}t. \tag{2}$$

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The expression on the second line is equivalent to the Riemann fractional integral $R_\mu x^{\nu/2} J_\nu(2\sqrt{x})$, where the integral operator R_μ is defined in general (Ref. 5, Chap. 13) as

$$(R_\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x f(t)(x-t)^{\alpha-1}\, dt. \tag{3}$$

Thus, with the replacement of t by $2\sqrt{t}$ and x by $2x$, (2) becomes

$$x^{(\nu+\mu)/2} J_{\nu+\mu}(2\sqrt{x}) = \frac{1}{\Gamma(\mu)} \int_0^x t^{\nu/2} J_\nu(2\sqrt{t})(x-t)^{\mu-1}\, dt = R_\mu x^{\nu/2} J_\nu(2\sqrt{x}). \tag{4}$$

A number of similar results are known for other special functions, for example,

$$2^{\lambda-\mu}(1-x^2)^{-(\lambda-\mu)/2} P_\nu^{\lambda-\mu}(x) = R_\mu 2^\lambda (1-x^2)^{-\lambda/2} P_\nu^\lambda(x) \tag{5}$$

for the associated Legendre functions with $\mathrm{Re}\,\lambda<1$, $\mathrm{Re}\,\mu>0$ [Ref. 5, 13.1(54)]. Askey (Ref. 7, Chap. 3) summarizes a number of results and gives some applications.

Other results are known with respect to the Weyl fractional integral W_μ (Ref. 5, Chap. 13) defined by

$$(W_\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_x^\infty f(t)(t-x)^{\alpha-1}\, dt. \tag{6}$$

Thus, from Ref. 5, 13.2(59),

$$x^{-(\nu-\mu)/2} K_{\nu-\mu}(2\sqrt{x}) = W_\mu x^{-\nu} K_\nu(2\sqrt{x}), \tag{7}$$

where K_ν is the hyperbolic Bessel or MacDonald function.

The simplicity of the results noted, and of many similar results,[7] is striking. The effect of the fractional integration is simply to change the indices on the special functions, while retaining the original functional form. There does not appear to be a systematic approach to the derivation of these results in the literature. Their form suggests that they must be associated with fractional generalizations of the stepping operators in the associated Lie algebra. In particular, the differential recurrence relations for the special functions are schematically of the form $DF_{\alpha,\ldots} = cF_{\alpha\pm1,\ldots}$, where D is a linear differential operator and the indices α label the functions in a realization of the algebra. This suggests that shifts of the indices by arbitrary amounts could be effected using fractional operators D^μ defined in analogy to the single-variable fractional derivatives defined in Ref. 5. This is the case, as we will see. The above-given fractional integrals are related, and simply give the action of the inverse multivariable operators $D^{-\mu}$ when reduced to a single variable.

We will define the fractional operators D^μ in the context of Lie theory and explore their general properties in Sec. II. We will then apply the results in a number of group settings in this and following papers to obtain generalized fractional-integral-type relations of the form $F_{\alpha+\mu,\ldots} = ND^\mu F_{\alpha,\ldots}$ for the special functions. Some are apparently new. We find that, with appropriate choices for the input functions, the fractional relations lead directly to known integral representations for the special functions, providing a group-theoretical setting for the latter.

In the present paper, we will restrict our attention to the development of our methods, and to applications to the Bessel functions. Our treatment is not exhaustive in either the theory or the applications considered.

II. FRACTIONAL OPERATORS

We will suppose that we have a Lie algebra which corresponds to one of the classical Lie groups, and is realized by the action of a set of linear differential operators $\{D(w,\partial_w)\}$ in a

collection of variables w acting on an appropriate set of functions. The exponentials e^{-tD} defined by Taylor series expansion in the group parameter t are elements of the Lie group taken to act on an appropriate class of functions F. We will assume that the group action $e^{-tD}F$ can be defined for all t, and will define a Weyl-type fractional operator D_W^μ as an integral over group elements by

$$D_W^\mu(w,\partial_w)F(w)=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\mathrm{d}t\,\frac{e^{-tD(w,\partial_w)}}{t^{\mu+1}}F(w). \tag{8}$$

The contour $C_W=(\infty,0+,\infty)$ in the complex t plane runs in from infinity, circles $t=0$ in the positive sense, and runs back to infinity. To define phases, we take the integrand as cut along the positive real axis with the phase of t taken as zero on the upper edge of the cut. The direction of the contour at infinity must be such that the integral converges. The above-given expression would be an identity for D a positive constant. Here, however, $D(w,\partial_w)$ is an operator which acts on functions F of the collection of variables w, and the existence of the integral depends on the functions as well as the contour.

Alternatively, D_W^μ can be defined as

$$D_W^\mu F=\frac{1}{\Gamma(-\mu+n)}D^n\int_0^\infty\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu-n+1}}F, \tag{9}$$

where $\mathrm{Re}\,\mu<n$ and end-point terms are assumed to vanish in the partial integrations which connect the two expressions.

It is straightforward using this expression to show that the fractional operators have the expected algebraic properties. Thus, for $\mathrm{Re}\,\mu<0$, $\mathrm{Re}\,\nu<0$, and $\mathrm{Re}(\mu+\nu)<0$,

$$\begin{aligned}D_W^\mu D_W^\nu F&=\frac{1}{\Gamma(-\mu)\Gamma(-\nu)}\int_0^\infty\mathrm{d}t\int_0^\infty\mathrm{d}u\,\frac{1}{t^{\mu+1}}\frac{1}{u^{\nu+1}}e^{-(t+u)D}F\\&=\frac{1}{\Gamma(-\mu)\Gamma(-\nu)}\int_0^\infty\mathrm{d}v\int_0^v\mathrm{d}t\,\frac{1}{t^{\mu+1}}\frac{1}{(v-t)^{\nu+1}}e^{-vD}F\\&=\frac{1}{\Gamma(-\mu)\Gamma(-\nu)}\int_0^\infty\mathrm{d}v\,\frac{e^{-vD}}{v^{\mu+\nu+1}}\cdot\int_0^1\mathrm{d}t'\,t'^{-\mu-1}(1-t')^{-\nu-1}\\&=\frac{1}{\Gamma(-\mu-\nu)}\int_0^\infty\mathrm{d}v\,\frac{e^{-vD}}{v^{\mu+\nu+1}}=D_W^{\mu+\nu}F.\end{aligned} \tag{10}$$

Exponents therefore add as we would expect, and the fractional operators of different orders commute,

$$D_W^\mu D_W^\nu=D_W^\nu D_W^\mu=D_W^{\mu+\nu},\quad [D_W^\mu,D_W^\nu]=0. \tag{11}$$

The result extends through (9) to general μ,ν for which the fractional operators are defined. By converting the integral in (10) back to a contour integral before taking the limit $\nu\to-\mu$, we find also that $D_W^\mu D_W^{-\mu}=\mathbf{1}$ where $\mathbf{1}$ is the unit operator, so $D_W^{-\mu}$ is the inverse of D_W^μ as implied by the group operations.

The fractional operator D_W^μ can also be defined in terms of the action of a generalized Weyl fractional integral $W_{-\mu}$ in the parameter x on the group operator $e^{-xD(w,\partial_w)}$. We will define $W_{-\mu}$ for general μ as

$$W_{-\mu}f(x)=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_x}\mathrm{d}t\,\frac{f(t)}{(t-x)^{\mu+1}}\,\mathrm{d}t, \tag{12}$$

where C_x is the contour $(\infty, x+, \infty)$. This definition is equivalent to (8) for $\mathrm{Re}\,\mu<0$. The action of $W_{-\mu}$ on f is just that of a fractional derivative,

$$(W_{-\mu}f)(x)=(-\mathrm{d}/\mathrm{d}x)^{\mu}f(x), \tag{13}$$

a result which is obvious for μ an integer so that the integration contour can be closed. In general, $W_{-\mu}$ gives the inverse of W_{μ} thought of as a repeated integral, $W_{-\mu}W_{\mu}=\mathbf{1}$.

D_W^{μ} can now be defined formally through the action of the fractional derivative $(-\mathrm{d}/\mathrm{d}x)^{\mu}$ on e^{-xD}, $(-\mathrm{d}/\mathrm{d}x)^{\mu}e^{-Dx}=D^{\mu}e^{-Dx}$. Multiplication by e^{xD} then gives $D_W^{\mu}F=e^{xD}(W_{-\mu}e^{-xD}F)$. This relation is easily checked by using $f(t)=e^{-tD}F$ in (12) and changing the integration variable from t to $t-x$. We find that

$$D_W^{\mu}F=e^{xD}(W_{-\mu}e^{-xD})F=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu+1}}F \tag{14}$$

in agreement with (8). That is, $D_W^{\mu}F=e^{xD}\,W_{-\mu}(e^{-xD}F)$ where $W_{-\mu}$ acts on the group parameter x and $D(w,\partial_w)$ acts on $F(w)$. The integrals in (8) and (14) can also be identified directly as $(-\mathrm{d}/\mathrm{d}x)^{\mu}e^{-xD}|_{x=0}=D_W^{\mu}$. The inverse of the fractional operator $D_W^{\mu}F$ is $D_W^{-\mu}F=e^{xD}\,W_{\mu}(e^{-xD}F)$.

We can define a second Riemann-type fractional operator by replacing the Weyl fractional integral by a Riemann fractional integral and noting the correspondence of $R_{-\alpha}$ to $(\mathrm{d}/\mathrm{d}x)^{\alpha}$, $R_{-\alpha}f(x)=(\mathrm{d}/\mathrm{d}x)^{\alpha}f(x)$. Thus, taking $f(t)=e^{tD}F$ and $\alpha=n-\mathrm{Re}\,\mu>0$ in (3) and following the above-given construction, we find

$$D_R^{\mu}F=e^{-xD}D^n(R_{n-\mu}e^{xD})F,\quad 0<n-\mathrm{Re}\,\mu. \tag{15}$$

By changing the integration variable from t to $x-t$ in (3), we then obtain the analog of (9),

$$(D_R^{\mu}F)(x)=\frac{1}{\Gamma(-\mu+n)}D^n\int_0^{x(w)}\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu-n+1}}F, \tag{16}$$

where we have noted the dependence of the final result on the value $x(w)$ of the group parameter t at the end point of the integration. As indicated, this will depend on the values of the variables w in F.

By going to a contour integral to handle the possible singularity at the lower limit of integration, we can write $D_R^{\mu}F$ in the more general form

$$D_R^{\mu}F=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_R}\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu+1}}F, \tag{17}$$

where C_R is the contour $C_R=(x(w),0+,x(w))$.

As we will see explicitly in later applications, the end point $x(w)$ of the contour must be chosen such that $D^{\mu}F$ satisfies a differential equation determined by the Casimir operators of the Lie algebra. This will require that a differential expression related to $e^{-tD}F$ vanishes for $t=x(w)$ for the given values of the variables w in F [see, for example, (85)].

The product of two Riemann fractional operators is given in the simple case $\mathrm{Re}\,\mu$, $\mathrm{Re}\,\nu<0$ by

$$D_R^{\mu}(D_R^{\nu}F)(x)=\frac{1}{\Gamma(-\mu)\Gamma(-\nu)}\int_0^x\mathrm{d}t\int_0^x\mathrm{d}u\,\frac{e^{-(t+u)D}}{t^{\mu+1}u^{\nu+1}}\,\theta(x-t-u). \tag{18}$$

$D^{\mu}(D^{\nu}F)$ will satisfy the expected differential equation for $D^{\mu}G$ provided $t+u=x$ on the boundary of the region of integration, a condition is enforced in (18) by the unit step function $\theta(z)$, $\theta(z)=1$ for $z>0$ and $\theta(z)=0$ for $z<0$. For an explicit example, see Sec. III D 1. The integral can be evaluated by shifting to $v=t+u$ as a new integration variable and identifying the remaining

integral with a beta function as in (10). The result is equal to $D_R^{\mu+\nu}F$. We therefore obtain the multiplication relation $D_R^\mu D_R^\nu = D_R^\nu D_R^\mu = D_R^{\mu+\nu}$ derived earlier for the Weyl fractional operators. This can be generalized to the contour integral representation (17).

Which expression for D^μ is appropriate in a particular setting, Weyl or Riemann, will depend on D and F. We will therefore simply denote the fractional operator as D^μ for formal purposes, and only specify the expression to be used in particular applications. The key restrictions will be the existence of a finite value of the group parameter $t=x(w)$ such that $e^{-xD}F=0$ in the Riemann case, and convergence of the integral for $t\to\infty$ in the Weyl case.

III. BESSEL FUNCTIONS AND E(2)

A. Algebraic considerations

As a first application of the fractional operators, we will consider the Bessel functions which we will denote generically as $Z_\nu(x)$. Bessel functions appear naturally in representations of E(2), the Euclidean group in two dimensions, and of E(1,1), the Poincaré group in two dimensions.[1,2] Both groups are real forms of SO(2,C), and the two are related to each other through the Weyl unitarity trick.[8] Since we are not concerned with unitary representations of the groups, it will be sufficient for our purposes to consider only the algebra of E(2).

The Lie algebra of E(2) is generated by three operators P_1, P_2, J_3 with the Lie products or commutation relations

$$[P_1,P_2]=0, \quad [J_3,P_1]=P_2, \quad [J_3,P_2]=-P_1. \tag{19}$$

There is one invariant operator, namely $P_1^2+P_2^2$, which commutes with all the generators.

The algebra can be realized by the action of differential operators on functions f of the coordinates (x_1, x_2) in the Euclidean plane. P_1 and P_2 correspond to the translation operators

$$P_1=\partial_1, \quad P_2=\partial_2 \tag{20}$$

and J_3, to a rotation in the plane,

$$J_3=-x_1\partial_2+x_2\partial_1. \tag{21}$$

The condition that the invariant operator $P_1^2+P_2^2$ be constant on the functions f gives the Helmholtz equation $(P_1^2+P_2^2)f=-k^2f$. In polar coordinates x, ϕ this becomes the differential equation

$$(P_1^2+P_2^2+k^2)f=\left[\frac{\partial^2}{\partial x^2}+\frac{1}{x}\frac{\partial}{\partial x}+\frac{1}{x^2}\frac{\partial^2}{\partial \phi^2}+k^2\right]f=0. \tag{22}$$

We can take $k^2=1$ by a scaling of the coordinates, and will do so. The rotation operator $J_3=-\partial_\phi$ commutes with the Helmholtz operator and may also be taken to have a constant value $-i\nu$ on the functions. The functions f in this realization of E(2) are then of the form

$$f_\nu(x,\phi)=e^{i\nu\phi}Z_\nu(x), \quad (P_1^2+P_2^2+1)f=0, \quad J_3f_\nu=-i\nu f_\nu \tag{23}$$

and involve Bessel functions Z_ν of order ν.

It is useful to change from the anti-Hermitian operator J_3 to the Hermitian operator iJ_3, and to introduce operators

$$P_+=-P_1-iP_2, \quad P_-=P_1-iP_2 \tag{24}$$

with the commutation relations

$$[P_+,P_-]=0, \quad [iJ_3,P_\pm]=\pm P_\pm. \tag{25}$$

The last relations imply that if f_ν is a solution of the Helmholtz equation with the index ν, then $P_\pm f_\nu$ is a solution with index $\nu\pm1$,

$$iJ_3(P_\pm f_\nu)=P_\pm(iJ_3\pm1)f_\nu=(\nu\pm1)(P_\pm f_\nu). \tag{26}$$

$P_\pm$ therefore act as stepping operators on the index.

The operators are given explicitly by

$$P_+=-e^{i\phi}\left(\frac{\partial}{\partial x}+\frac{i}{x}\frac{\partial}{\partial\phi}\right)=-t\partial_x+\frac{t^2}{x}\partial_t, \tag{27}$$

$$P_-=e^{-i\phi}\left(\frac{\partial}{\partial x}-\frac{i}{x}\frac{\partial}{\partial\phi}\right)=\frac{1}{t}\partial_x+\frac{1}{x}\partial_t, \tag{28}$$

where $t=e^{i\phi}$. In terms of that variable, $iJ_3=t\partial_t$. The Helmholtz operator is simply P_+P_-+1.

From (26), the action of $P_\pm$ on the functions $f_\nu(x,t)=t^\nu Z_\nu(x)$ must give constant multiples of $t^{\nu\pm1}Z_{\nu\pm1}(x)$. The constants of proportionality for the different Bessel functions are easily determined to be unity by using the behavior of the functions for $x\to0,\infty$. We therefore have the stepping relations

$$P_\pm t^\nu Z_\nu(x)=t^{\nu\pm1}Z_{\nu\pm1}(x), \tag{29}$$

which reduce to

$$\left(\mp\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\nu}{x}\right)Z_\nu(x)=Z_{\nu\pm1}(x) \tag{30}$$

once the t dependence is factored out. The latter are just the differential recurrence relations for the Bessel functions (Ref. 9, 7.2.8).

The relations in (29) suggest that

$$P_\pm^\mu t^\nu Z_\nu(x)=t^{\nu\pm\mu}Z_{\nu\pm\mu}(x) \tag{31}$$

for $P_\pm^\mu$ appropriately defined fractional operators such as the Weyl operators

$$P_\pm^\mu=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\mathrm{d}u\,\frac{e^{-uP_\pm}}{u^{\mu+1}}. \tag{32}$$

It is easily established that these operators have the expected properties. First, $P_\pm^\mu$ commute with the Helmholtz operator P_+P_-+1, so transform solutions of the Helmholtz equation to solutions. Further, from

$$[iJ_3,P_\pm^n]=\pm nP_\pm^n, \tag{33}$$

we find that

$$[iJ_3,e^{-uP_\pm}]=\pm\sum_{n=0}^{\infty}\frac{(-u)^n}{n!}nP_\pm^n \tag{34}$$

$$=\pm u\frac{\mathrm{d}}{\mathrm{d}u}e^{-uP_\pm}, \tag{35}$$

hence, after a partial integration in (32), that

$$[iJ_3, P_\pm^\mu] = \pm \mu P_\pm^\mu . \tag{36}$$

The action of $P_\pm^\mu$ on a solution f_ν therefore gives another solution with the index ν changed to $\nu \pm \mu$,

$$iJ_3(P_\pm^\mu f_\nu) = P_\pm^\mu (iJ_3 \pm \mu) f_\nu = (\nu \pm \mu)(P_\pm^\mu f). \tag{37}$$

This relation does not show directly that $P_\pm^\mu f_\nu = f_{\nu\pm\mu}$, but only that $P_\pm^\mu f_\nu$ is at most a linear combination of the two independent solutions of the Helmholtz equation with orders $\nu \pm \mu$. If the independent solutions are taken as the Hankel functions, the observation that the operators $P_\pm^\mu$ do not change the distinct asymptotic behaviors of those functions for $|x| \to \infty$ shows, in fact, that $P_\pm^\mu f_\nu = N(\nu,\mu) f_{\nu\pm\mu}$. The constant of proportionality will be found later by direct calculation to be unity, as in (52), establishing the validity of (31).

We can also define a fractional operator $(iJ_3)^\lambda$, and find after a brief calculation using the analog of (32) that

$$(iJ_3)^\lambda f_\nu = \nu^\lambda f_\nu . \tag{38}$$

$(iJ_3)^\lambda$ again satisfies the multiplication rule, $(iJ_3)^\lambda (iJ_3)^\mu = (iJ_3)^{\lambda+\mu}$.

The formal algebraic structure is completed by

$$(iJ_3)^\lambda P_\pm^\mu = P_\pm^\mu (iJ_3 \pm \mu)^\lambda, \quad P_\pm^\mu (iJ_3)^\lambda = (iJ_3 \mp \mu)^\lambda P_\pm^\mu . \tag{39}$$

These can be derived using the Baker–Hausdorff expansion of $e^A B e^{-A}$ as a series of n-fold commutators,

$$e^A B e^{-A} = B + \sum_{n=1}^{\infty} \frac{1}{n!} [A,[A,\ldots[A,B]\ldots]]. \tag{40}$$

Thus, choosing e^A as the exponential in the definition of $(iJ_3)^\lambda$, $e^A = e^{-itJ_3}$, B as $P_\pm^\mu$, and using (36) to evaluate the repeated commutators, we find that

$$\begin{aligned} e^{-itJ_3} P_\pm^\mu &= (e^{-itJ_3} P_\pm^\mu e^{itJ_3})\, e^{-itJ_3} = P_\pm^\mu + \sum_{n=1}^{\infty} \frac{(-t)^n}{n!} [iJ_3, iJ_3, \ldots [iJ_3, P_\pm^\mu]\ldots]\, e^{-itJ_3} \\ &= P_\pm^\mu e^{-t(iJ_3 \pm \mu)}. \end{aligned} \tag{41}$$

The first of the relations (39) then follows upon integration using the analog of (32). Application of this operator to a solution f_ν of the Helmholtz equation gives

$$(iJ_3)^\lambda P_\pm^\mu f_\nu = P_\pm^\mu (iJ_3 \pm \mu)^\lambda f_\nu = (\nu \pm \mu)^\lambda P_\pm^\mu f_\nu \tag{42}$$

The second of the relations (39) can be derived similarly. The complete algebraic structure defined by $(iJ_3)^\lambda$, $P_\pm^\mu$, the multiplication rules, and (39) is infinite, and has not been investigated except as applied to solutions of the Helmholtz equation.

B. Action of the group operators

The action of the exponential operators $e^{-uP_\pm} = e^{\pm uP_1 + iuP_2)}$ is easily determined and well known. P_1 and P_2 commute, and the exponentials e^{aP_1} and e^{aP_2} induce translations of the coordinates x_1, x_2 with $e^{aP_1} x_1 = x_1 + a$ and $e^{aP_2} x_2 = x_2 + a$. Thus, acting on functions analytic in the neighborhood of (x_1, x_2),

$$e^{-uP_+} F(x_1,x_2) = e^{uP_1} e^{iuP_2} F(x_1,x_2) = F(x_1 + u, x_2 + iu). \tag{43}$$

Applying this result to the functions $f_\nu = e^{i\nu\phi} Z_\nu(x)$ written in rectangular coordinates, we find that

$$e^{-uP_+} f_\nu = e^{u(P_1+iP_2)} \left(\frac{x_1+ix_2}{x_1-ix_2} \right)^{\nu/2} Z_\nu(\sqrt{x_1^2+x_2^2}) = t^\nu x^\nu (x^2+2uxt)^{-\nu/2} Z_\nu(\sqrt{x^2+2uxt}), \quad (44)$$

where $x = \sqrt{x_1^2+x_2^2}$ and $t = e^{i\phi} = \sqrt{(x_1+ix_2)/x}$. A similar calculation gives

$$e^{-uP_-} f_\nu = \left(\frac{t}{x} \right)^\nu \left(x^2 - \frac{2ux}{t} \right)^{\nu/2} Z_\nu\left(\sqrt{x^2 - \frac{2ux}{t}} \right). \quad (45)$$

We can also calculate directly in polar coordinates, a method which will be useful later. Thus, noting that $P_+ t^\nu x^\nu = (t/x)(t\partial_t - x\partial_x) t^\nu x^\nu = 0$ and using (30), we find that

$$P_+^n t^\nu Z_\nu(x) = (-2)^n t^{\nu+n} x^{\nu+n} \left(\frac{\mathrm{d}}{\mathrm{d}x^2} \right)^n (x^{-\nu} Z_\nu(x)). \quad (46)$$

The formal Taylor series expansion of e^{-uP_+} then gives

$$\begin{aligned} e^{-uP_+} t^\nu Z_\nu(x) &= \sum_{n=0}^\infty \frac{(2u)^n}{n!} (xt)^{\nu+n} \left(\frac{\mathrm{d}}{\mathrm{d}r^2} \right)^n (r^{-\nu} Z_\nu(r))\big|_{r=x} \\ &= t^\nu x^\nu \exp\left(2uxt \frac{\mathrm{d}}{\mathrm{d}w} \right) (w^{-\nu/2} Z_\nu(\sqrt{w}))\big|_{w=x^2} \\ &= t^\nu x^\nu (x^2+2uxt)^{-\nu/2} Z_\nu(\sqrt{x^2+2uxt}), \end{aligned} \quad (47)$$

where we have identified the exponential in the penultimate line as a translation operator. The result agrees with (44). A similar calculation for e^{-uP_-} reproduces (45).

Direct evaluations of $e^{-uP_\pm} f_\nu$ using the Taylor series for the exponentials and the relations $P_\pm^n t^\nu Z_\nu(x) = t^{\nu\pm n} Z_{\nu\pm n}(x)$, (29), give the generating functions

$$t^\nu x^\nu (x^2+2uxt)^{-\nu/2} Z_\nu(\sqrt{x^2+2uxt}) = \sum_{n=0}^\infty \frac{(-u)^n}{n!} t^{\nu+n} Z_{\nu+n}(x) \quad (48)$$

and

$$\left(\frac{t}{x} \right)^\nu \left(x^2 - \frac{2ux}{t} \right)^{\nu/2} Z_\nu\left(\sqrt{x^2 - \frac{2ux}{t}} \right) = \sum_{n=0}^\infty \frac{(-u)^n}{n!} t^{\nu-n} Z_{\nu-n}(x). \quad (49)$$

These equations give generalizations of Lommel's expansions for the Bessel functions (Ref. 6, Sec. 5.22). Thus, taking $x = \sqrt{z}$, $ut = h/2x = h/2\sqrt{z}$ in (48), and choosing Z_ν as the ordinary Bessel function J_ν, we obtain [Ref. 6, 5.22(1)]

$$(z+h)^{-\nu/2} J_\nu(\sqrt{z+h}) = \sum_{n=0}^\infty \frac{\left(-\frac{1}{2}h\right)^n}{n!} z^{-(\nu+n)/2} J_{\nu+n}(\sqrt{z}). \quad (50)$$

Similarly, for $x = \sqrt{z}$ and $u/t = -h/2\sqrt{z}$, (49) gives [Ref. 6, 5.22(2)]

$$(z+h)^{\nu/2} J_\nu(\sqrt{z+h}) = \sum_{n=0}^\infty \frac{(\frac{1}{2}h)^n}{n!} z^{(\nu-n)/2} J_{\nu-n}(\sqrt{z}). \quad (51)$$

The remaining Lommel-type formulas in Ref. 6, Sec. 5.22, follow from (48) and (49) for different choices of Z_ν. The present development provides a group-theoretical derivation of these results. See also Weisner.[10] Note the series (48) converges for $|u|<|x/2t|$, and that in (49), for $|u|<|xt/2|$, that is, for sufficiently small values of the group parameter u.

C. Weyl-type relations for Bessel functions

1. Relations using P_+^μ

The action of the Weyl-type operators P_+^μ on the Bessel functions is given by (8) and (44),

$$P_+^\mu t^\nu Z_\nu(x)=N(\nu,\mu)t^{\nu+\mu}Z'_{\nu+\mu}(x)$$
$$=\frac{1}{2\pi i}t^\nu x^\nu e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{du}{u^{\mu+1}}(x^2+2uxt)^{-\nu/2}Z_\nu(\sqrt{x^2+2uxt}\,). \tag{52}$$

C_W is a contour $(\infty,0+,\infty)$ in the complex u plane with the direction of approach to ∞ to be taken such that the integral converges. This will depend on the function Z_ν considered.

Proceeding formally, we can extract the expected factor $t^{\nu+\mu}$ from the integral by the change of variable $v=2uxt$. We will also replace x by $\sqrt{z}$, with the result

$$N(\nu,\mu)x^{-(\nu+\mu)/2}Z'_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^\mu e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+x)^{-\nu/2}Z_\nu(\sqrt{v+z}\,). \tag{53}$$

This result can also be obtained directly from the differential recurrence relations (30) by replacing x by $\sqrt{z}$, rewriting the resulting relation for P_+ in the form

$$-2\frac{d}{dz}(z^{-\nu/2}Z_\nu(\sqrt{z}))=z^{-(\nu+1)/2}Z_{\nu+1}(\sqrt{z}), \tag{54}$$

and determining the Weyl action of $(-2\,d/dz)^\mu$ on $z^{-\nu/2}Z_\nu(\sqrt{z})$.

The function $z^{-\lambda/2}Z_\lambda(\sqrt{z})$ satisfies the differential equation (Ref. 11, 9.1.53)

$$\left(\frac{d^2}{dz^2}+\frac{\lambda+1}{z}\frac{d}{dz}+\frac{1}{4z}\right)z^{-\lambda/2}Z_\lambda(\sqrt{z})=0. \tag{55}$$

Applying this operator with $\lambda=\nu+\mu$ to the integral in (53), converting the derivatives with respect to z to derivatives with respect to v, and using the differential equation for $\lambda=\nu$ to eliminate the derivative-free term proportional to $1/4z$ on the right-hand side, we find that the result vanishes provided

$$\int_{C_W}dv\,\frac{d}{dv}\left\{\frac{1}{v^\mu}\frac{d}{dv}[(v+z)^{-\nu/2}Z_\nu(\sqrt{v+z})]\right\}=0. \tag{56}$$

That is, the integral in (53) gives a Bessel function or combination of functions with argument $\sqrt{z}$ and order $\nu+\mu$ multiplied by $z^{-(\nu+\mu)/2}$ provided the function in curly braces vanishes at the end points of the integration.

When Z_ν is the Hankel function $H_\nu^{(1)}$, the condition in (56) is satisfied for contours that run to ∞ in the upper half plane, avoiding the possible singularity at $v=-z$ on the right. It also holds for a contour along the positive real axis for $\mathrm{Re}(\mu+\frac{1}{2}\nu+\frac{3}{4})>0$. In either case, an asymptotic argument shows that the Bessel function $Z'_{\nu+\mu}$ given by the integral is in fact $H^{(1)}_{\nu+\mu}(\sqrt{z})$ with coefficient $N(\nu,\mu)=1$ as expected. Thus,

$$z^{-(\nu+\mu)/2}H^{(1)}_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{(\infty e^{i\epsilon},0+,\infty e^{i\epsilon})}\frac{dv}{v^{\mu+1}}(v+z)^{-\nu/2}H^{(1)}_{\nu}(\sqrt{v+z}),\tag{57}$$

$\epsilon>0$. Tracing the calculation back, we find that the original expression (52) holds for $H^{(1)}_{\nu}$ for contours with $0\leqslant\arg(xtu)\leqslant 2\pi$ as $|u|\to\infty$.

A shift of the integration variable brings (57) to the form of a (generalized) Weyl fractional integral,

$$z^{-(\nu+\mu)/2}H^{(1)}_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{(\infty,z+,\infty)}\frac{dv}{(v-z)^{\mu+1}}v^{-\nu/2}H^{(1)}_{\nu}(\sqrt{v}).\tag{58}$$

The contour can be collapsed for $\mathrm{Re}\,\mu<0$, and (58) reduces to the known fractional integral [Ref. 5, 13.2(45)]. The latter can be written in the present notation as $z^{-(\nu-\mu)/2}H^{(1)}_{\nu-\mu}(\sqrt{z})=P^{-\mu}_{+}z^{-\nu}H^{(1)}_{\nu}(\sqrt{z})$, $\mathrm{Re}\,\mu>0$.

Similar considerations for the choice $Z_{\nu}=H^{(2)}_{\nu}$ in (52) show that that result holds for $0\geqslant\arg(xtu)>2\pi$, and that

$$z^{-(\nu+\mu)/2}H^{(2)}_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+z)^{-\nu/2}H^{(2)}_{\nu}(\sqrt{v+z}),\tag{59}$$

where v runs to ∞ in the lower half plane, avoiding the possible singularity at $v=-z$ on the right. The result also holds for a contour along the positive real axis for $\mathrm{Re}(\mu+\frac{1}{2}\nu+\frac{3}{4})>0$.

Combinations of $H^{(1)}_{\nu}$ and $H^{(2)}_{\nu}$ give the ordinary Bessel functions and the relations

$$z^{-(\nu+\mu)/2}J_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+z)^{-\nu/2}J_{\nu}(\sqrt{v+z}),\tag{60}$$

$$z^{-(\nu+\mu)/2}Y_{\nu+\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+z)^{-\nu/2}Y_{\nu}(\sqrt{v+z})\tag{61}$$

for $\mathrm{Re}(\mu+\frac{1}{2}\nu+\frac{3}{4})>0$. The contours in these cases must be taken parallel to the real axis for $v\to\infty$. The results reduce to the known fractional integrals [Ref. 5, 13.2(34) and 13.2(40)] for $\mathrm{Re}\,\mu<0$.

If we increase the phase of z by π and simultaneously rotate the contour C_W by π in the positive sense in expression (57), the substitutions $z=e^{i\pi}x$, $v=e^{i\pi}u$ restore the original contour while replacing $\sqrt{v+x}$ by $e^{i\pi/2}\sqrt{u+x}$. The definition of the MacDonald function K_{ν} in terms of the Hankel function $H^{(1)}_{\nu}$,

$$K_{\nu}(x)=\frac{i\pi}{2}e^{i\pi\nu/2}H^{(1)}_{\nu}(e^{i\pi/2}x),\tag{62}$$

then gives

$$x^{-(\nu+\mu)/2}K_{\nu+\mu}(\sqrt{x})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{du}{u^{\mu+1}}(u+x)^{-\nu/2}K_{\nu}(\sqrt{u+x}),\tag{63}$$

or, for $\mathrm{Re}\,\mu<0$,

$$x^{-(\nu+\mu)/2}K_{\nu+\mu}(\sqrt{x})=2^{\mu}\frac{1}{\Gamma(-\mu)}\int_0^{\infty}\frac{du}{u^{\mu+1}}(u+x)^{-\nu/2}K_{\nu}(\sqrt{u+x})$$

$$=2^{\mu}\frac{1}{\Gamma(-\mu)}\int_x^{\infty}\frac{dt}{(t-x)^{\mu+1}}K_{\nu}(\sqrt{t}) \tag{64}$$

in agreement with (7) or Ref. 5, 13.2(59).

2. Weyl-type relations from P_{-}^{μ}

The action of the Weyl-type operators P_{-}^{μ} on the Bessel functions is given by (8) and (45),

$$P_{-}^{\mu}t^{\nu}Z_{\nu}(x)=t^{\nu-\mu}Z_{\nu-\mu}(x)=\frac{1}{2\pi i}\left(\frac{t}{x}\right)^{\nu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{du}{u^{\mu+1}}\left(x^2-\frac{2ux}{t}\right)^{\nu/2}Z_{\nu}\left(\sqrt{x^2-\frac{2ux}{t}}\right). \tag{65}$$

C_W is again a contour $(\infty,0+,\infty)$ in the complex u plane with the direction of approach to ∞ to be taken such that the integral converges. We will scale out the t dependence through the substitutions $v=2ux/t$ and $x=\sqrt{z}$, and work with the reduced expression

$$z^{(\nu-\mu)/2}Z_{\nu-\mu}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(z-v)^{\nu/2}Z_{\nu}(\sqrt{z-v}). \tag{66}$$

We will suppose initially that $\arg z>0$. It is then possible for the choice $Z_{\nu}=H_{\nu}^{(1)}$ to rotate the integration contour into the lower half v plane. Then with v replaced by $e^{-i\pi}v$ and $z-v$ by $e^{i\pi}(v+z)$,

$$z^{(\nu-\mu)/2}H_{\nu-\mu}^{(1)}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}e^{2\pi i\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+z)^{\nu/2}H_{\nu}^{(1)}(\sqrt{v+z}), \tag{67}$$

where C_W is a contour $(\infty,0+,\infty)$ in the new variable v and $-\pi<\arg z<\pi$. By choosing $Z_{\nu}=H_{\nu}^{(2)}$ and $\mathrm{Im}\,z<0$ and rotating in the opposite sense, we obtain the second relation

$$z^{(\nu-\mu)/2}H_{\nu-\mu}^{(2)}(\sqrt{z})=\frac{1}{2\pi i}2^{\mu}\Gamma(\mu+1)\int_{C_W}\frac{dv}{v^{\mu+1}}(v+z)^{\nu/2}H_{\nu}^{(2)}(\sqrt{v+z}), \tag{68}$$

also valid for $-\pi<\arg z<\pi$. These results can also be obtained by considering $P_{+}^{-\mu}t^{\nu}Z_{\nu}$.

For $\mathrm{Re}\,\mu<0$, the contours can be collapsed, and

$$z^{(\nu-\mu)/2}H_{\nu-\mu}^{(1,2)}(\sqrt{z})=\frac{2^{\mu}}{\Gamma(-\mu)}e^{\pm i\pi\mu}\int_0^{\infty}\frac{dv}{v^{\mu+1}}(v+z)^{\nu/2}H_{\nu}^{(1,2)}(\sqrt{v+z}), \tag{69}$$

where $\mathrm{Im}\,v\to\pm\infty$ for $H^{(1)}$ and $H^{(2)}$. By considering the limiting behavior for $\mathrm{Im}\,v\to 0$ and combining the two functions, we obtain

$$\frac{2^{\mu}}{\Gamma(-\mu)}\int_0^{\infty}\frac{dv}{v^{\mu+1}}(v+z)^{\nu/2}J_{\nu}(\sqrt{v+z})=z^{(\nu-\mu)/2}[\cos\pi\mu J_{\nu-\mu}(\sqrt{z})+\sin\pi\mu Y_{\nu-\mu}(\sqrt{z})], \tag{70}$$

$$\frac{2^{\mu}}{\Gamma(-\mu)}\int_0^{\infty}\frac{dv}{v^{\mu+1}}(v+z)^{\nu/2}Y_{\nu}(\sqrt{v+z})=z^{(\nu-\mu)/2}[\cos\pi\mu Y_{\nu-\mu}(\sqrt{z})-\sin\pi\mu J_{\nu-\mu}(\sqrt{z})]. \tag{71}$$

These are equivalent to [Ref. 5, 13.2(35) and 13.2(39)] and are valid only for $\frac{1}{2}\operatorname{Re}\nu-\frac{3}{4}<\operatorname{Re}\mu<0$, with $\operatorname{Im}v\to 0$ for $\operatorname{Re}v\to\infty$.

3. Weyl-type integral representations for Bessel functions

We can use the above-given results to obtain integral representations for the Bessel functions. We begin with the observations that $t^{\mu}Z_{\mu}(x)=P_{+}^{\mu-1/2}t^{1/2}Z_{1/2}(x)$, and that $H_{1/2}^{(1)}(x)$ and $H_{1/2}^{(2)}(x)$ are elementary functions,

$$H_{1/2}^{(1)}(x)=\frac{1}{i}\left(\frac{2}{\pi x}\right)^{1/2}e^{ix},\quad H_{1/2}^{(2)}(x)=-\frac{1}{i}\left(\frac{2}{\pi x}\right)^{1/2}e^{-ix}. \tag{72}$$

The action of $P_{+}^{\mu-1/2}$ can be reduced as above, and we will begin with the expression in (53). This gives

$$\begin{aligned}x^{-\mu/2}H_{\mu}^{(1)}(\sqrt{x})&=\frac{1}{2\pi i}2^{\mu-1/2}e^{i(\mu-1/2)\pi}\Gamma\left(\mu+\frac{1}{2}\right)\int_{C_W}\frac{dv}{v^{\mu+1/2}}(v+x)^{-1/4}H_{1/2}^{(1)}(\sqrt{v+x})\\&=-\frac{1}{2\pi i}\frac{2^{\mu}}{\sqrt{\pi}}e^{i\pi\mu}\Gamma\left(\mu+\frac{1}{2}\right)\int_{C_W}\frac{dv}{v^{\mu+1/2}}(v+x)^{-1/2}e^{i\sqrt{v+x}}.\end{aligned} \tag{73}$$

Replacing x by x^2, letting $v=x^2(t^2-1)$, and removing a common factor of $x^{-\mu}$, we obtain

$$H_{\mu}^{(1)}(x)=-\frac{1}{2\pi i}\frac{2}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\mu}e^{i\pi\mu}\Gamma\left(\mu+\frac{1}{2}\right)\int_{(\infty,1+,\infty)}\frac{dt}{(t^2-1)^{\mu+1/2}}e^{ixt}. \tag{74}$$

This holds for general values of μ provided $\operatorname{Im}xt\to\infty$ for $|t|\to\infty$, and for $xt\to+\infty$ for $\operatorname{Re}\mu>\frac{1}{2}0$. The contour can be collapsed for $\operatorname{Re}\mu<\frac{1}{2}$ giving the generalized Mehler–Sonine integral representation for $H^{(1)}(x)$ [Ref. 6, 6.13(1)],

$$H_{\mu}^{(1)}(x)=-\frac{2i}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\mu}\frac{1}{\Gamma(\frac{1}{2}-\mu)}\int_{1}^{\infty}\frac{dt}{(t^2-1)^{\mu+1/2}}e^{ixt}. \tag{75}$$

The result satisfies the Bessel equation for $\operatorname{Im}xt\to\infty$ for $|t|\to\infty$.

A similar calculation for $H_{\mu}^{(2)}$ gives

$$H_{\mu}^{(2)}(x)=-\frac{1}{2\pi i}\frac{2}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\mu}e^{i\pi\mu}\Gamma\left(\mu+\frac{1}{2}\right)\int_{(\infty,1+,\infty)}\frac{dt}{(t^2-1)^{\mu+1/2}}e^{-ixt} \tag{76}$$

or, for $\operatorname{Re}\mu<\frac{1}{2}$,

$$H_{\mu}^{(1)}(x)=\frac{2i}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\mu}\frac{1}{\Gamma\left(\frac{1}{2}-\mu\right)}\int_{1}^{\infty}\frac{dt}{(t^2-1)^{\mu+1/2}}e^{-ixt}. \tag{77}$$

For x real and $-\frac{1}{2}<\operatorname{Re}\mu<\frac{1}{2}$, (75) and (77) can be combined to obtain the representations for J_{μ} and Y_{μ} noted in Ref. 6, 6.13(3) and (4),

$$J_{\mu}(x)=\frac{2}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\mu}\frac{1}{\Gamma(\frac{1}{2}-\mu)}\int_{1}^{\infty}dt\,\frac{\sin xt}{(t^2-1)^{\mu+1/2}}, \tag{78}$$

$$Y_\mu(x) = -\frac{2}{\sqrt{\pi}}\left(\frac{2}{x}\right)^\mu \frac{1}{\Gamma(\frac{1}{2}-\mu)} \int_1^\infty \mathrm{d}t \frac{\cos xt}{(t^2-1)^{\mu+1/2}}. \tag{79}$$

A different set of integral representations can be obtained by considering the action of the inverse operator $P_+^{-\mu-1/2}$ on $t^{1/2}H_{1/2}^{(1,2)}(x)$,

$$P_+^{-\mu-(1/2)}\, t^{1/2} H_{1/2}^{(1,2)}(x) = t^{-\mu} H_{-\mu}^{(1,2)}(x). \tag{80}$$

Using

$$H_{-\mu}^{(1)}(x) = e^{i\pi\mu} H_\mu^{(1)}(x), \quad H_{-\mu}^{(2)}(x) = e^{-i\pi\mu} H_\mu^{(2)}(x) \tag{81}$$

and following the above-presented manipulations, we obtain the integral representations

$$H_\mu^{(1)}(x) = \frac{i}{\pi}\frac{2}{\sqrt{\pi}}\left(\frac{x}{2}\right)^\mu e^{-2\pi i\mu}\Gamma\left(\frac{1}{2}-\mu\right)\int_{(\infty,1+,\infty)} \mathrm{d}t\,(t^2-1)^{\mu-(1/2)} e^{ixt}, \tag{82}$$

$$H_\mu^{(2)}(x) = \frac{i}{\pi}\frac{2}{\sqrt{\pi}}\left(\frac{x}{2}\right)^\mu \Gamma\left(\frac{1}{2}-\mu\right)\int_{(\infty,1+,\infty)} \mathrm{d}t\,(t^2-1)^{\mu-(1/2)} e^{-ixt}, \tag{83}$$

where, for convergence, t must approach ∞ on the contours in (82) and (83) with $\mathrm{Im}\, xt \to +\infty$ and $\mathrm{Im}\, xt \to -\infty$, respectively. These expressions are equivalent to the representations 6.11(4) and 6.11(5) in Ref. 6 obtained from Hankel's representation for the Bessel functions. [Watson uses a different phase convention in his 6.11(4) which is equivalent to replacing $t-1$ in (82) by $e^{2\pi i}(t-1)$. Watson's 6.11(5) is obtained from (83) by the substitutions $t-1 \to e^{i\pi}(u+1)$ and $t+1 \to e^{-i\pi}(u-1)$.] Other results, for example, Schäfli's integral for K_μ [Ref. 6, 6.15(4)], can be obtained from these. See Watson.[6]

D. Riemann-type relations for Bessel functions

1. Relations for $P_\pm^\mu$

For Riemann-type fractional operators, the roles of P_+^μ and P_-^μ are essentially reversed, and the relations apply to different Bessel functions. The action of the Riemann operator P_-^μ is given by (16) or (17) and (45). We will use the expression in (17) which gives

$$P_-^\mu t^\nu Z_\nu(x) = t^{\nu-\mu} Z_{\nu-\mu}(x) = \frac{1}{2\pi i} e^{i\pi\mu}\Gamma(\mu+1)\left(\frac{t}{x}\right)^\nu \times \int_{C_R} \frac{\mathrm{d}u}{u^{\mu+1}}\left(x^2 - \frac{2ux}{t}\right)^{\nu/2} Z_\nu\left(\sqrt{x^2-\frac{2ux}{t}}\right), \tag{84}$$

where $C_R = (u(x,t), 0+, u(x,t))$. The end points $u(x,t)$ of the integration must be chosen such that $t^{\mu-\nu}$ times the integral gives a solution $Z_{\nu-\mu}(x)$ of the Bessel equation. This requires that

$$\left(x^2 - \frac{2x}{t}u\right)^{\nu+1} \frac{\mathrm{d}}{\mathrm{d}u}\left[\left(x^2-\frac{2x}{t}u\right)^{-\nu/2} Z_\nu\left(\sqrt{x^2-\frac{2x}{t}u}\right)\right] = 0 \tag{85}$$

at the end points of the integration contour. [The integrand vanishes for $u = xt/2$, suggesting that value for $u(x,t)$. With that assumed, the precise condition for a solution of Bessel's equation follows by scaling the integration variable as in (86) to eliminate x and t from the limits of integration, applying the relevant operator, and then undoing the scaling in the resulting condi-

tion.] This condition can be satisfied for the Bessel functions $Z_\nu = J_\nu$, I_ν for end points $u(x,t) = xt/2$ in $C_R =$ provided $\mathrm{Re}\,\nu > -1$. The condition cannot be satisfied for other choices of the Bessel function Z_ν.

We can easily show that the Riemann operator defined by (84) satisfies the product rule $P_-^\lambda P_-^\mu = P_-^{\lambda+\mu}$ provided we choose the end points in the integrations properly. It is convenient in this to assume that $\mathrm{Re}\,\lambda < 0$ and $\mathrm{Re}\,\nu < 0$, conditions which can be attained using (16). The contour integrals can then be converted into ordinary integrals. The action of the group operator e^{-vP_-} on the integrand in (84) changes x^2 to $x^2 - 2vx/t$, but does not affect x/t since $P_-(x/t)^\sigma = 0$. As a result, the parameters u and v appear only in the sum $u+v$ as required by the operator relation $e^{-uP_-}e^{-vP_-} = e^{-(u+v)P_-}$. It is then straightforward to show that the double integral can be reduced to the product of a beta function and an integral of the form in (84), and gives a solution of the Bessel equation equal to $t^{\nu-\lambda-\mu}Z_{\nu-\lambda-\mu}(z)$, provided the end points in the successive integrations are taken as $v_0(x,t,u) = xt/2 - u$, $u_0(x,t) = xt/2$. The sublety is that the end point of the first integration depends on the variable in the second. The result gives an example of the formal relation in (18) which generalizes the product rule for Riemann fractional integrals.

A change of the integration variable to $v = 2u/xt$ converts (84) to the simpler form

$$Z_{\nu-\mu}(x) = \frac{1}{2\pi i} e^{i\pi\mu}\Gamma(\mu+1)\left(\frac{2}{x}\right)^\mu \int_{(1,0+,1)} \frac{dv}{v^{\mu+1}}(1-v)^{\nu/2} Z_\nu(x\sqrt{1-v}). \tag{86}$$

Alternatively, for $\mathrm{Re}\,\mu < 0$, we can collapse the integration contour in (84) and change to variables $z = x^2$, $v^2 = x^2 - 2ux/t$ to put the result in the form of a standard Riemann fractional integral,

$$z^{(\nu-\mu)/2} Z_{\nu-\mu}(\sqrt{z}) = \frac{2^\mu}{\Gamma(-\mu)} \int_0^z \frac{dv}{(z-v)^{\mu+1}} v^{\nu/2} Z_\nu(\sqrt{v}), \tag{87}$$

$\mathrm{Re}\,\mu < 0$, $\mathrm{Re}\,\nu > -1$. This reproduces Ref. 5, 13.1(63) and 13.1(83) for $Z_\nu = J_\nu$ and $Z_\nu = I_\nu$ when μ is replaced by $-\mu$ in accord with the convention used there.

For $Z_\nu = Y_\nu$, K_ν, the action of the Bessel operator in the variable $x = \sqrt{z}$ on the function "$Z_{\nu-\mu}$" defined by (86) leaves a term proportional to $x^{-\nu-\mu}$. The result is an inhomogeneous Bessel equation with a solution which involves a sum of a function $J_{\nu-\mu}$ or $I_{\nu-\mu}$ and the Lommel functions $s_{-\nu-\mu+1,\nu-\mu}(x)$ (Ref. 6, Sec. 10.7). The fractional integral Ref. 5, 13.1(73) is of this type.

An analysis similar to that above shows that the integral in (65), taken on a Riemann-type contour with end points at $u = -x/2t$ satisfies an inhomogeneous rather than homogeneous Bessel equation of order $\nu+\mu$. The general solution involves Lommel functions, and there is no Riemann definition for P_+^μ acting on Bessel functions alone.

2. Riemann-type integral representations for Bessel functions

The operator relation $P_-^\mu t^\nu Z_\nu(x) = t^{\nu-\mu} Z_{\nu-\mu}(x)$ immediately gives integral representations for J_ν and I_ν. We will start with the functions of order $\nu = -\frac{1}{2}$,

$$J_{-1/2}(x) = \frac{2}{\sqrt{\pi}}\frac{\cos x}{x^{1/2}}, \quad I_{-1/2}(x) = \frac{2}{\sqrt{\pi}}\frac{\cosh x}{x^{1/2}}. \tag{88}$$

Choosing $\mu = -\lambda - \frac{1}{2}$, (86) then gives

$$J_\lambda(x) = \frac{1}{2\pi i} e^{-i\pi(\lambda+1/2)}\Gamma\left(-\lambda+\frac{1}{2}\right)\frac{2}{\sqrt{\pi}}\left(\frac{x}{2}\right)^\lambda \int_{(1,0+,1)} dv\, v^{\lambda-(1/2)}(1-v)^{-1/2}\cos(x\sqrt{1-v}) \tag{89}$$

for general λ, or, replacing v by $1-t^2$,

$$J_\lambda(x)=\frac{\Gamma(\frac{1}{2}-\lambda)}{i\pi\Gamma(\frac{1}{2})}\int_{(0,1+,0)}dt\,(1-t^2)^{\lambda-(1/2)}\cos xt, \tag{90}$$

$$=\frac{2}{\sqrt{\pi}\Gamma\left(\lambda+\frac{1}{2}\right)}\left(\frac{x}{2}\right)^\lambda\int_0^1 dt\,(1-t^2)^{\lambda-(1/2)}\cos xt \tag{91}$$

for $\mathrm{Re}\,\lambda>-\frac{1}{2}$. The first is a standard Poisson-type integral representation for $J_\lambda(x)$ [Ref. 6, 3.3(2)]. The second gives the generalization of Ref. 6, 6.1(6).

Similarly, from $P_-^{-\lambda-(1/2)}t^{-1/2}I_{-1/2}(x)=t^\lambda I_\lambda(x)$,

$$I_\lambda(x)=\frac{1}{2\pi i}e^{-i\pi(\lambda+1/2)}\Gamma\left(-\lambda+\frac{1}{2}\right)$$
$$\times\left(\frac{x}{2}\right)^\lambda\int_{(1,0+,1)}dv\,v^{\lambda-(1/2)}(1-v)^{-1/2}\cosh(x\sqrt{1-v}), \tag{92}$$

$$=\frac{\Gamma(\frac{1}{2}-\lambda)}{i\pi\Gamma(\frac{1}{2})}\int_{(0,1+,0)}dt\,(1-t^2)^{\lambda-(1/2)}\cosh xt \tag{93}$$

$$=\frac{2}{\sqrt{\pi}\Gamma\left(\lambda+\frac{1}{2}\right)}\left(\frac{x}{2}\right)^\lambda\int_0^1 dt\,(1-t^2)^{\lambda-(1/2)}\cosh xt,\quad \mathrm{Re}\,\lambda>-\frac{1}{2}. \tag{94}$$

IV. SUMMARY

Many of the properties of the special functions arise from their connection to Lie groups.[1–3] Their differential recurrence relations, for example, reflect the action of particular multivariable operators D in the associated Lie algebra, the so-called stepping operators, on the functions in the relevant class. We have given general definitions of fractional operators D^λ in the context of Lie theory, and explored their formal properties. Our Weyl- and Riemann-type fractional operators generalize the single-variable Weyl and Riemann fractional integrals $W_{-\lambda}$ and $R_{-\lambda}$ (Ref. 5, Chap. 13). The operators D^λ change the indices on the special functions by fractional displacements related to λ, and provide useful connections between functions in different realizations of the Lie algebra.

We have illustrated the usefulness of the fractional operators in the case of the Euclidean group E(2) and the Bessel functions, and find that they contribute to a coherent overall picture of many relations among the Bessel functions as interpreted in the group context. For example, the formal relations $P_\pm^\lambda t^\mu Z_\mu(x)=t^{\mu\pm\lambda}Z_{\mu\pm\lambda}(x)$ give the integral relations connecting Bessel functions of different orders. When reduced to the single variable x, these generalize known fractional integral relations. Used with simple choices of μ and λ, with Z_μ an elementary function, they lead immediately to the standard integral representations for the various Bessel functions, representations which are derived in Ref. 6 from quite different starting points using different methods. In addition, the action of the elements $e^{-uP_\pm}$ on the functions $t^\mu Z_\mu(x)$ gives generating functions for the Bessel functions (the Lommel expansions), while the Bessel equation itself is the statement that the Casimir operator P_+P_- and the rotation operator iJ_3 have fixed values -1 and μ.

The applications of the fractional group operators will be extended in a following paper to the associated Legendre functions in the somewhat more complicated case of SO(2,1) and its conformal extension.

ACKNOWLEDGMENTS

This work was supported in part by the U. S. Department of Energy under Grant No. DE-FG02-95ER40896, and in part by the University of Wisconsin Graduate School with funds granted by the Wisconsin Alumni Reseach Foundation. The author would like to thank the faculty of the Institute for Advanced Study for their hospitality during the fall term of 1975 when the initial stages of this work were carried out, and the Aspen Center for Physics for its hospitality while parts of the final work were done.

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Fractional operators and special functions. II. Legendre functions

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(Received 6 December 2002; accepted 3 January 2003)

Most of the special functions of mathematical physics are connected with the representation of Lie groups. The action of elements D of the associated Lie algebras as linear differential operators gives relations among the functions in a class, for example, their differential recurrence relations. In this paper, we apply the fractional generalizations D^{μ} of these operators developed in an earlier paper in the context of Lie theory to the group SO(2,1) and its conformal extension. The fractional relations give a variety of interesting relations for the associated Legendre functions. We show that the two-variable fractional operator relations lead directly to integral relations among the Legendre functions and to one- and two-variable integral representations for those functions. Some of the relations reduce to known fractional integrals for the Legendre functions when reduced to one variable. The results enlarge the understanding of many properties of the associated Legendre functions on the basis of the underlying group structure. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1561594]

I. INTRODUCTION

The classical special functions (Jacobi, Gegenbauer, Legendre, Laguerre, Bessel, and Hermite functions) are all connected with the representation of Lie groups,[1–4] or more generally, to the realization of their Lie algebras by linear differential operators $D(w,\partial_w)$ acting on functions of the variables w. In particular, the special functions appear as factors in the multivariable functions on which the action of the Lie algebra is realized. Many of the properties of the special functions are easily understood in this context. For example, the differential equations for the special functions are connected with the Casimir operators of the associated groups. The actions of appropriate elements D of the Lie algebra lead, when reduced to a single variable, to the standard differential recurrence relations for the functions, while the action of group elements e^{-tD} can be interpreted in terms of generalized generating functions when expressed using a Taylor series expansion in the group parameter t. Numerous examples are given in Refs. 1 and 3.

The differential recurrence relations for the special functions are schematically of the form $DF_{\alpha,\ldots}=cF_{\alpha\pm1,\ldots}$ where the α's label the realization of the Lie algebra and D is a stepping operator. In a previous paper,[5] we defined fractional generalizations D^{μ} of the D's in the context of Lie theory, determined their formal properties, and illustrated their usefulness in obtaining further interesting relations among the functions using the group E(2) and the Bessel functions. We showed, for example, that shifts of the index ν of a Bessel function Z_{ν} by an arbitrary amount μ could be effected using D^{μ}. The resulting relations for the inverse operators $D^{-\mu}$, when reduced to a single variable, gave generalizations of known fractional integrals such as the Riemann integral

$$x^{(\nu+\mu)/2}J_{\nu+\mu}(2\sqrt{x})=\frac{1}{\Gamma(\mu)}\int_0^x t^{\nu/2}J_{\nu}(2\sqrt{t})(x-t)^{\mu-1}\,dt \tag{1}$$

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and the Weyl integral

$$x^{-(\nu-\mu)/2}K_{\nu-\mu}(2\sqrt{x})=\frac{1}{\Gamma(\mu)}\int_x^\infty t^{-\nu}K_\nu(2\sqrt{t})(t-x)^{\mu-1}, \tag{2}$$

Ref. 6, Chap. 13. Finally, we obtained integral representations for the Z's as the action of the D^μ's on appropriate input functions. While most of the specific results had been derived historically in other ways, the introduction of the fractional operators allowed them to be unified in a group setting.

We continue that program here for the associated Legendre functions, working in the context of the group SO(2,1) and its conformal extension. We find, in particular, fractional operators which raise or lower the order μ or degree ν of a general associated Legendre function F_ν^μ by arbitrary amounts, and use the results to unify and extend a number of known results for those functions.

We will summarize the definitions and properties of the fractional operators in Sec. II, and then apply the theory to derive a number of relations for the associated Legendre functions. These include generating functions, generalizations of known fraction integral relations, and some new integral relations. With appropriate choices for the input functions, the fractional operator relations give integral representations for the associated Legendre functions, and provide group-theoretical setting for those representations. We find, in particular, interesting double-integral representations.

II. FRACTIONAL OPERATORS

We will suppose that we have a Lie algebra which corresponds to one of the classical Lie groups, and is realized by the action of a set of linear differential operators $D(w,\partial_w)$ in variables w on an appropriate class of functions $F(w)$. The exponentials e^{-tD} defined by Taylor series expansion in the group parameter t are elements of the Lie group, and act on the same functions. We will suppose initially that $e^{-tD}F$ exists for all t, and define a Weyl-type fractional operator D_W^μ by an integral over group elements, with

$$D_W^\mu F(w)=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_W}\mathrm{d}t\,\frac{e^{-tD(w)}}{t^{\mu+1}}F(w). \tag{3}$$

The contour $C_W=(\infty,0+,\infty)$ in the complex t plane runs in from infinity, circles $t=0$ in the positive sense, and runs back to infinity. To define phases, we take the integrand as cut along the positive real axis with the phase of t taken as zero on the upper edge of the cut. The direction of the contour at infinity must be such that the integral converges.

The expression above would be an identity for D a positive constant. Here, however, $D(w,\partial_w)$ is an operator which acts on the functions $F(w)$, and the existence of the integral depends on the functions as well as the contour.

Alternatively, D_W^μ can be defined without the contour integral as

$$D_W^\mu F=\frac{1}{\Gamma(-\mu+n)}D^n\int_0^\infty\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu-n+1}}F, \tag{4}$$

where $\mathrm{Re}\,\mu<n$ and end point terms are assumed to vanish in the partial integrations which connect the two expressions.

We define a second Riemann-type fractional operator $D_R^\mu F$ by

$$D_R^\mu F=\frac{1}{2\pi i}e^{i\pi\mu}\Gamma(\mu+1)\int_{C_R}\mathrm{d}t\,\frac{e^{-tD}}{t^{\mu+1}}F, \tag{5}$$

where C_R is the contour $C_R=(x(w),0+,x(w))$. The end point $x(w)$ of the contour must be chosen such that $D^\mu F$ satisfies a differential equation determined by the Casimir operators of the Lie algebra. This will require that a differential expression related to $e^{-tD}F$ vanish at $t=x(w)$ for the given values of w (see, for example, Sec. VII C).

Which expression for D^μ is appropriate in a particular setting, Weyl or Riemann, will depend on D and F. We will therefore simply denote the fractional operator as D^μ for formal purposes, and only specify the expression to be used in connection with particular applications. The key restrictions will be the existence of a finite value of the group parameter $t=x(w)$ such that a differential expression related to $e^{-xD}F$ vanishes in the Riemann case, and the convergence of the integral for $t\to\infty$ in the Weyl case.

As shown in Ref. 5, the fractional operators satisfy the expected product rule for powers and commute,

$$D^\mu D^\nu = D^\nu D^\mu = D^{\mu+\nu}, \quad [D^\mu, D^\nu]=0. \tag{6}$$

The inverse of D^μ is just $D^{-\mu}$,

$$(D^\mu)^{-1}=D^{-\mu}, \quad D^{-\mu}D^\mu=\mathbf{1}. \tag{7}$$

III. LEGENDRE FUNCTIONS, SO(3), AND SO(2,1)

Legendre functions appear naturally in the representations of the rotation group SO(3) in three dimensions, the noncompact group SO(2,1), or of their covering group SU(2,C). See, for example, Refs. 1, 7, and 8. The Lie algebras so(3) $\simeq$ su(2) are defined by three elements J_1, J_2, J_3 with Lie products given by the commutator $[J_1,J_2]=J_3$ and its cyclic permutations. Thus, in a realization in which the Casimir operator $J_1^2+J_2^2+J_3^2$ has the fixed value $-\nu(\nu+1)$ and the commuting operator J_3 has the value $-i\mu$, the action of the so(3) algebra can be described in terms of coordinates $x_1=\sin\theta\cos\phi$, $x_2=\sin\theta\sin\phi$, $x_3=\cos\theta$ on the unit sphere S^2 by the action of the anti-Hermitian operators $J_1=-x_2\partial_3+x_3\partial_1$, $J_2=-x_3\partial_1+x_1\partial_3$, $J_3=-x_1\partial_2+x_2\partial_1$ on the functions $e^{i\mu\phi}\mathrm{P}_\nu^\mu(\cos\theta)$. Here $\mathrm{P}_\nu^\mu(\cos\theta)$ is the associated Legendre function "on the cut" $-1<\cos\theta<1$. This is defined in terms of the associated Legrendre function $P_\nu^\mu(z)$ for general complex z by

$$\mathrm{P}_\nu^\mu(\cos\theta)=\tfrac{1}{2}[e^{i\pi\mu/2}P_\nu^\mu(\cos\theta+i0)+e^{-i\pi\mu/2}P_\nu^\mu(\cos\theta-i0)], \tag{8}$$

where $P_\nu^\mu(z)$ is given in terms of the hypergeometric function ${}_2F_1$ by Ref. 9, Chap. 3,

$$P_\nu^\mu(x)=\frac{1}{\Gamma(1-\mu)}\left(\frac{z+1}{z-1}\right)^{\mu/2}{}_2F_1\left(-\nu,\nu+1;1-\nu;\frac{1-z}{2}\right), \tag{9}$$

and its analytic continuations. The values of ν and μ are arbitrary. There is no restriction to the integer values characteristic of the associated Legendre polynomials unless one insists on a unitary representation of the group SO(3). We will not, and will simply be concerned with realizations of the algebra so(3).

The algebra can also be realized on the functions $e^{i\mu\phi}\mathrm{Q}_\nu^\mu(\cos\theta)$, with $\mathrm{Q}_\nu^\mu(\cos\theta)$ a Legendre function of the second kind "on the cut,"

$$\mathrm{Q}_\nu^\mu(\cos\theta)=\tfrac{1}{2}e^{-i\pi\mu}[e^{-i\pi\mu/2}Q_\nu^\mu(\cos\theta+i0)+e^{-i\pi\mu/2}Q_\nu^\mu(\cos\theta-i0)], \tag{10}$$

with $Q_\nu^\mu(z)$ defined for general complex z by

$$Q_\nu^\mu(z)=e^{i\pi\mu}2^{-\nu-1}\frac{\Gamma(\frac{1}{2})\Gamma(\nu+\mu+1)}{\Gamma(\nu+\frac{3}{2})}z^{-\nu-\mu-1}(z^2-1)^{\mu/2}$$

$$\times {}_2F_1\left(1+\frac{\nu}{2}+\frac{\mu}{2},\frac{1}{2}+\frac{\nu}{2}+\frac{\mu}{2};\nu+\frac{3}{2};\frac{1}{z^2}\right). \tag{11}$$

The general forms of the P's and Q's appear naturally in representations of the noncompact group SO(2,1) on the unit hyperboloid H^2 with $x_1=\sinh\theta\cos\phi$, $x_2=\sinh\theta\sin\phi$, $x_3=\cosh\theta$, through the functions $e^{i\mu\phi}P_\nu^\mu(\cosh\theta)$ and $e^{i\mu\phi}Q_\nu^\mu(\cosh\theta)$, Ref. 1, Chap. VI. SO(3) and SO(2,1) are different real forms of the covering group SO(3,C), and the Lie algebras are related.[7] It will be most convenient for our purposes to work with the general forms of the functions, and with realizations of so(2,1).

The so(2,1) algebra is given in terms of three operators which we will take in the form

$$M_1=x_3\partial_1+x_1\partial_3,$$

$$M_2=x_3\partial_2+x_2\partial_3, \tag{12}$$

$$M_3=x_2\partial_1-x_1\partial_2.$$

These have the commutation relations

$$[M_1,M_2]=-M_3,\quad [M_2,M_3]=M_1,\quad [M_3,M_1]=M_2. \tag{13}$$

M_1 and M_1 generate Lorentz transformations in the 1 and 2 directions, equivalent to hyperbolic rotations on H^2, while M_3 generates rotations in the 1,2 plane.

The operator $-M_1^2-M_2^2+M_3^2$ is a Casimir invariant and may be taken to have fixed value on realizations of the algebra. We will also fix the value of the second commuting operator iM_3. When written in terms of the variables $z=\cosh\theta$ and $t=e^{i\phi}$, the relations $(-M_1^2-M_2^2+M_3^2)f=-\nu(\nu+1)f$, $iM_3f=\mu f$ imply that $f=f_\nu^\mu(z,t)=t^\mu F_\nu^\mu(z)$ where F_ν^μ is a solution of the associated Legendre equation

$$\left[(1-z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2}-2z\frac{\mathrm{d}}{\mathrm{d}z}-\frac{\mu^2}{1-z^2}+\nu(\nu+1)\right]F_\nu^\mu(z)=0 \tag{14}$$

with degree ν and order μ

The so(2,1) algebra can be put in a more useful form for our purposes by introducing operators $M_\pm$ defined by

$$M_\pm=\mp M_1-iM_2 \tag{15}$$

with the commutation relations

$$[iM_3,M_\pm]=\pm M_\pm,\quad [M_+,M_-]=-2iM_3. \tag{16}$$

In terms of the coordinates on H^2,

$$M_+=-e^{i\phi}(\partial_\theta+i\coth\theta\,\partial_\phi)=-t\sqrt{z^2-1}\,\partial_z+\frac{z}{\sqrt{z^2-1}}t^2\,\partial_t, \tag{17}$$

$$M_-=e^{-i\phi}(\partial_\theta-i\coth\theta\partial_\phi)=\frac{1}{t}\sqrt{z^2-1}\,\partial_z+\frac{z}{\sqrt{z^2-1}}\partial_t. \tag{18}$$

The commutation relations of $M_\pm$ with M_3 imply that $M_\pm t^\mu P_\nu^\mu(z) \propto t^{\mu\pm1} P_\nu^{\mu\pm1}(z)$ and $M_\pm t^\mu Q_\nu^\mu(z) \propto t^{\mu\pm1} Q_\nu^{\mu\pm1}(z)$. The constants of proportionality are easily determined and are the same for P_ν^μ and Q_ν^μ. After the t dependence is extracted, these relations reduce to the standard differential recurrence relations for the order μ,

$$-\sqrt{z^2-1}\frac{\mathrm{d}}{\mathrm{d}z}F_\nu^\mu(z)+\frac{\mu z}{\sqrt{z^2-1}}F_\nu^\mu(z)=-F_\nu^{\mu+1}(z), \tag{19}$$

$$\sqrt{z^2-1}\frac{\mathrm{d}}{\mathrm{d}z}F_\nu^\mu(z)+\frac{\mu z}{\sqrt{z^2-1}}F_\nu^\mu(z)=(\nu+\mu)(\nu-\mu+1)F_\nu^{\mu-1}(z), \tag{20}$$

where F_ν^μ is a general solution of the associated Legendre equation, Ref. 9, Sec. 3.8.

IV. CONFORMAL EXTENSION OF SO(2,1)

We have so far dealt with SO(3) and SO(2,1) considered as the groups of transformations on S^2 and H^2. These appear as subgroups of the group of Euclidean transformations E(3), and of the group of Poincaré or pseudo-Euclidean transformations E(2,1), obtained by adding the translation operators in 3 or $2+1$ dimensions to the original algebras. We will deal only with E(2,1). This is defined by the operators M_i in (12) and three translation operators $P_i=\partial_i$. We choose the metric such that $P^2=-P_1^2-P_2^2+P_3^2$, $M^2=-M_1^2-M_2^2+M_3^2$, and $x^2=-x_1^2-x_2^2+x_3^3$.

The P's commute,

$$[P_i,P_j]=0, \tag{21}$$

and transform as Lorentz vectors, with the commutation relations

$$\begin{aligned}
&[M_1,P_1]=-P_3, \quad [M_1,P_2]=0, \quad [M_1,P_3]=-P_1,\\
&[M_2,P_1]=0, \quad [M_2,P_2]=-P_3, \quad [M_2,P_3]=-P_2,\\
&[M_3,P_1]=P_2, \quad [M_3,P_2]=-P_1, \quad [M_3,P_3]=0,
\end{aligned} \tag{22}$$

with repect to the generators M_1, M_2 of Lorentz transformations, and the generator M_3 of rotations. P^2 commutes with the M's, and the solutions of the Klein–Gordon equation $P^2 f = m^2 f$ can be classified with respect to SO(2,1) by the values of M^2 and M_3.

In the special case that $P^2=0$, the symmetry group can be enlarged by the addition of a set of special conformal transformations with generators K_i and the dilatation operator D. See, for example, Ref. 4, Chap. 4. These are given in terms of the coordinates x_i by

$$\begin{aligned}
K_1&=2x_1\, x\cdot\partial+x^2\partial_1+x_1,\\
K_2&=2x_2\, x\cdot\partial+x^2\partial_2+x_2,\\
K_3&=-2x_3\, x\cdot\partial+x^2\partial_3-x_3,
\end{aligned} \tag{23}$$

$$D=x\cdot\partial+\tfrac{1}{2}=x_1\partial_1+x_2\partial_2+x_3\partial_3+\tfrac{1}{2}. \tag{24}$$

The K's commute,

$$[K_i,K_j]=0, \tag{25}$$

and transform as Lorentz vectors,

$$[M_1,K_1]=-K_3, \quad [M_1,K_2]=0, \quad [M_1,K_3]=-K_1,$$

$$[M_2,K_1]=0,\quad [M_2,K_2]=-K_3,\quad [M_2,K_3]=-K_2,$$
$$[M_3,K_1]=K_2,\quad [M_3,K_2]=-K_1,\quad [M_3,K_3]=0. \tag{26}$$

In addition,

$$[P_1,K_1]=[P_2,K_2]=2D,\quad [P_3,K_3]=-2D,$$
$$[P_1,K_2]=[K_1,P_2]=2M_3,\quad [P_3,K_i]=[K_3,P_i]=2M_i,\quad i=1,2. \tag{27}$$

Finally,

$$[D,P_i]=-P_i,\quad [D,K_i]=K_i,\quad [D,M_i]=0,\quad i=1,2,3. \tag{28}$$

Using the explicit realization of the above-given operators, we find also that

$$[K_i,P^2]=-4x_1P^2\simeq 0, \tag{29}$$

$$[D,P^2]=2P^2\simeq 0, \tag{30}$$

$$M^2+D^2-\tfrac{1}{4}=x^2P^2\simeq 0, \tag{31}$$

where the final weak equivalence in each relation holds for the action of the operator on solutions h of the wave equation $P^2h=0$.

We will deal with the solutions of the wave equation in terms of the homogeneous functions

$$h^\mu_\nu=x^\nu f^\mu_\nu(z,t)=x^\nu t^\mu F^\mu_\nu(z), \tag{32}$$

where $t^\mu F^\mu_\nu(z)$ is a solution of the associated Legendre equation on H^2 with $M^2=-\nu(\nu+1)$ and $iM_3=\mu$ as in (14), and x, t, and z are defined as

$$x=\sqrt{x^2},\quad z=x_3/x,\quad t=(x_1+ix_2)/\sqrt{x_1^2+x_2^2}. \tag{33}$$

In accord with the last two equations of (29), $Dh^\mu_\nu=(\nu+\frac{1}{2})h^\mu_\nu$, a relation which provides a geometric interpretation of the degree ν of the Legendre function.

The operators P_3 and K_3 act as stepping operators in ν. Thus, from the first two relations in (28),

$$D(P_3h^\mu_\nu)=P_3(D-1)h^\mu_\nu=(\nu-\tfrac{1}{2})P_3h^\mu_\nu, \tag{34}$$

$$D(K_3h^\mu_\nu)=K_3(D+1)h^\mu_\nu=(\nu+\tfrac{3}{2})K_3h^\mu_\nu, \tag{35}$$

so $P_3h^\mu_\nu\propto h^\mu_{\nu-1}$ and $K_3h^\mu_\nu\propto h^\mu_{\nu+1}$. In terms of our coordinates on H^2,

$$P_3=-\sinh^2\theta\frac{1}{x}\frac{\partial}{\partial\cosh\theta}+\cosh\theta\frac{\partial}{\partial x}=-(z^2-1)\frac{1}{x}\frac{\partial}{\partial z}+z\frac{\partial}{\partial x}, \tag{36}$$

while

$$K_3=-x\sinh^2\theta\frac{\partial}{\partial\cosh\theta}-x^2\cosh\theta\left(\frac{\partial}{\partial x}+\frac{1}{x}\right)=-x(z^2-1)\frac{\partial}{\partial z}-x^2z\left(\frac{\partial}{\partial x}+\frac{1}{x}\right). \tag{37}$$

Upon applying P_3 and K_3 to the functions h^μ_ν defined in (32), we find that

$$P_3 h_\nu^\mu(z) = x^{\nu-1} t^\mu \left[-(z^2-1)\frac{\partial}{\partial z} + \nu z \right] F_\nu^\mu(z) = x^{\nu-1} t^\mu (\nu+\mu) F_{\nu-1}^\mu(z), \tag{38}$$

$$K_3 h_\nu^\mu = x^{\nu+1} t^\mu \left[-(z^2-1)\frac{\partial}{\partial z} - (\nu+1) z \right] F_\nu^\mu(z) = -x^{\nu+1} t^\mu (\nu-\mu+1) F_{\nu+1}^\mu(z). \tag{39}$$

These relations give the standard differential recurrence relations in ν for the associated Legendre functions F_ν^μ after the dependence on x and t is removed. The indicated coefficients can be determined using the asymptotic behavior of those functions.

V. ACTION OF THE GROUP OPERATORS AND GENERATING FUNCTIONS

The action of the finite group operators $e^{-uM_\pm}$ on the functions f_ν^μ is easily determined. Thus, writing the stepping operation by M_+ in the form

$$M_+ f_\nu^\mu = \left[-t\sqrt{z^2-1}\,\partial_z + \frac{z}{\sqrt{z^2-1}} t^2 \partial_t \right] t^\mu F_\nu^\mu(z) = -t^{\mu+1}(z^2-1)^{(\mu+1)/2} \frac{d}{dz}[(z^2-1)^{-\mu/2} F_\nu^\mu(z)], \tag{40}$$

and noting that

$$M_+ t^\mu (z^2-1)^{\mu/2} = 0, \tag{41}$$

we can easily show that

$$\begin{aligned} e^{-uM_+} t^\mu F_\nu^\mu(z) &= t^\mu (z^2-1)^{\mu/2} e^{ut\sqrt{z^2-1}(\mathrm{d}/\mathrm{d}r)} (r^2-1)^{-\mu/2} F_\nu^\mu(r)\big|_{r=z} \\ &= t^\mu (z^2-1)^{\mu/2} [(z+ut\sqrt{z^2-1})^2-1]^{-\mu/2} F_\nu^\mu(z+ut\sqrt{z^2-1}). \end{aligned} \tag{42}$$

[This result is also easily obtained starting with the expression $t^\mu F_\nu^\mu(z) = (x_1+ix_2)^\mu \times (x_3^2 - x^2)^{-\mu/2} F_\nu^\mu(x_3/x)$, writing M_+ as $-x_3(\partial_1 + i\partial_2) - (x_1+ix_2)\partial_3$, and determining the action of e^{-uM_+} directly using the relations $M_+(x_1+ix_2)=0$ and $M_+ x^2 = 0$. See also Ref. 1, Chap. VI.]

Alternatively, by direct expansion of the exponential and the use of (19),

$$e^{-uM_+} t^\mu F_\nu^\mu(z) = \sum_{n=0}^{\infty} \frac{u^n}{n!} t^{\mu+n} F_\nu^{\mu+n}(z). \tag{43}$$

Comparison of the two expressions gives the generating function

$$t^\mu (z^2-1)^{\mu/2} [(z+ut\sqrt{z^2-1})^2-1]^{-\mu/2} F_\nu^\mu(z+ut\sqrt{z^2-1}) = \sum_{n=0}^{\infty} \frac{u^n}{n!} t^{\mu+n} F_\nu^{\mu+n}(z). \tag{44}$$

The series converges for $|u|$ sufficiently small as expected from Lie theory, with absolute convergence for either P_ν^μ or Q_ν^μ for

$$|u| < \frac{1}{|t|} \min \left| \sqrt{\frac{z\pm 1}{z\mp 1}} \right|. \tag{45}$$

The generating function for $F_\nu^\mu = P_\nu^\mu$ is known, Ref. 9, 19.10(4).

A similar calculation using M_- gives

$$e^{-uM_-}t^{\mu}F_{\nu}^{\mu}(z)=\sum_{n=0}^{\infty}\frac{(-u)^n}{n!}t^{\mu-n}\frac{\Gamma(\mu+\nu+1)\Gamma(\nu-\mu+n+1)}{\Gamma(\mu+\nu-n+1)\Gamma(\nu-\mu+1)}F_{\nu}^{\mu-n}(z)$$

$$=t^{\mu}(z^2-1)^{-\mu/2}\left[\left(z-\frac{u}{t}\sqrt{z^2-1}\right)^2-1\right]^{\mu/2}F_{\nu}^{\mu}\left(z-\frac{u}{t}\sqrt{z^2-1}\right), \tag{46}$$

with absolute convergence of the series for the condition in (45) with $1/t\to t$.

The action of the finite operators e^{-uP_3} and e^{-uK_3} in the conformal group on the functions h_{ν}^{μ} is well known,[4] but it is useful to determine it directly. In order to use the above-sketched method for $M_{\pm}$, we change from the variable $z=x_3/x$ to a new variable $y=x_3/(x_1^2+x_2^2)^{1/2}=z/\sqrt{z^2-1}=\coth\theta$ in terms of which

$$P_3=\sqrt{y^2-1}\left(\frac{1}{x}\frac{\partial}{\partial y}+\frac{y}{y^2-1}\frac{\partial}{\partial x}\right), \tag{47}$$

$$K_3=\sqrt{y^2-1}\left(x\frac{\partial}{\partial y}-\frac{y}{y^2-1}x\frac{\partial}{\partial x}x\right). \tag{48}$$

In this form,

$$P_3\,x^{\nu}(y^2-1)^{\nu/2}=0,\quad K_3\,x^{\nu}(y^2-1)^{(\nu+1)/2}=0, \tag{49}$$

for any ν. Extracting the relevant factors from the respective operands, we find that the actions of P_3 and K_3 can be written in terms of simple derivatives,

$$P_3\,x^{\nu}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)=P_3\,x^{\nu}(y^2-1)^{-\nu/2}\left[(y^2-1)^{\nu/2}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)\right]$$

$$=x^{\nu-1}(y^2-1)^{-(\nu-1)/2}\frac{\mathrm{d}}{\mathrm{d}y}\left[(y^2-1)^{\nu/2}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)\right], \tag{50}$$

$$K_3\,x^{\nu}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)=K_3\,x^{\nu}(y^2-1)^{(\nu+1)/2}\left[(y^2-1)^{-(\nu+1)/2}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)\right]$$

$$=x^{\nu+1}(y^2-1)^{(\nu+2)/2}\frac{\mathrm{d}}{\mathrm{d}y}\left[(y^2-1)^{-(\nu+1)/2}F_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right)\right]. \tag{51}$$

The use of y or $\coth\theta$ as the preferred variable is in this sense natural.

The above-given relations connect the action of e^{-uP_3} and e^{-uK_3} to Taylor series in y, and lead to

$$e^{-uP_3}x^{\nu}F_{\nu}^{\mu}=x^{\nu}\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}F_{\nu}^{\mu}\left(\frac{Y}{\sqrt{Y^2-1}}\right),\quad Y=y-\frac{u}{x}\sqrt{y^2-1}, \tag{52}$$

$$e^{-uK_3}x^{\nu}F_{\nu}^{\mu}=x^{\nu}\left(\frac{y^2-1}{Y^2-1}\right)^{(\nu+1)/2}F_{\nu}^{\mu}\left(\frac{Y}{\sqrt{Y^2-1}}\right),\quad Y=y-ux\sqrt{y^2-1}. \tag{53}$$

Equivalently, in terms of $z=\cosh\theta$ and the formal power series expansions of the exponentials,

$$e^{-uP_3}x^\nu F_\nu^\mu(z)=x^\nu\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{u}{x}\right)^n\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu+\mu-n+1)}F_{\nu-n}^\mu(z)$$

$$=x^\nu\left(1-2z\frac{u}{x}+\frac{u^2}{x^2}\right)^{\nu/2}F_\nu^\mu\left(\frac{z-\frac{u}{x}}{\sqrt{1-2z\frac{u}{x}+\frac{u^2}{x^2}}}\right), \tag{54}$$

$$e^{-uK_3}x^\nu F_\nu^\mu(z)=x^\nu\sum_{n=0}^{\infty}\frac{(ux)^n}{n!}\frac{\Gamma(\nu-\mu+n+1)}{\Gamma(\nu-\mu+1)}F_{\nu+n}^\mu(z)$$

$$=x^\nu(1-2zux+u^2x^2)^{-(\nu+1)/2}F_\nu^\mu\left(\frac{z-ux}{\sqrt{1-2zux+u^2x^2}}\right). \tag{55}$$

The series converge for $|h|<\min|z\pm\sqrt{z^2-1}|$, where $h=u/x$ for (54), and $h=ux$ for (55). The expressions (54) and (55) reproduce the known generating functions, Ref. 9, 19.10(3) and 19.10(2), respectively, for $F_\nu^\mu=P_\nu^\mu$, but hold also for the functions Q_ν^μ.

These relations give generating functions for the Legendre functions in terms of the degree ν. Thus, starting with $P_0^0(z)=1$ and using (55), we obtain the standard generating function for the Legendre polynomials,

$$e^{-uK_3}\cdot 1=(1-2zux+u^2x^2)^{-1/2}=\sum_{n=0}^{\infty}(ux)^nP_n(z). \tag{56}$$

The known generating function, Ref. 9, 3.7(34) for the Q_n follows from (55) with $Q_0^0\equiv Q_0=\frac{1}{2}\ln(z+1)/(z-1)$,

$$e^{-uK_3}\frac{1}{2}\ln\frac{z+1}{z-1}=(1-2zux+u^2x^2)^{-1/2}\ln\left(\frac{z-ux\sqrt{1-2zux+u^2x^2}}{\sqrt{z^2-1}}\right)=\sum_{n=0}^{\infty}(ux)^nQ_n(z). \tag{57}$$

Other simple generating functions can be obtained using different starting points. Thus, using

$$P_0^\mu(z)=\frac{1}{\Gamma(1-\mu)}\left(\frac{z+1}{z-1}\right)^{\mu/2} \tag{58}$$

in (55) gives

$$e^{-uK_3}P_0^\mu(z)=\frac{1}{\Gamma(1-\mu)}(1-2zux+u^2x^2)^{-1/2}\left(\frac{z-ux+\sqrt{1-2zux+u^2x^2}}{\sqrt{z^2-1}}\right)^\mu$$

$$=\sum_{n=0}^{\infty}\frac{(ux)^n}{n!}\frac{\Gamma(-\mu+n+1)}{\Gamma(-\mu+1)}P_n^\mu(z). \tag{59}$$

A similar generating function for the functions $Q_n^\lambda(z)$ follows from (55) and

$$Q_0^\mu(z)=\frac{1}{2}e^{i\pi\mu}\Gamma(\mu)\left[\left(\frac{z+1}{z-1}\right)^{\mu/2}-\left(\frac{z+1}{z-1}\right)^{-\mu/2}\right]. \tag{60}$$

Further results can be obtained using the known closed-form expressions for $Q_\nu^{1/2}$, $P_\nu^{1/2}$, $P_\nu^{-\nu}(z)$, and $Q_\nu^{\nu+1}(z)$, Ref. 9, Sec. 3.61.

We can also obtain interesting double series. Thus,

$$e^{-vM_+}e^{-uK_3}\cdot 1=[1-2ux(z+vt\sqrt{z^2-1})+u^2x^2]^{-1/2}=\sum_{n=0}^{\infty}(ux)^n\sum_{m=0}^{n}\frac{(vt)^m}{m!}P_n^m(z). \quad (61)$$

A series for Q_n^m with the same coefficients follows from (57) with the replacement of z by $z+vt\sqrt{v^2-1}$ in the function to be expanded. In that case, the sum on m does not terminate.

VI. FRACTIONAL STEPPING OPERATORS FROM SO(2,1)

We can define fractional stepping operators $M_\pm^\lambda$ as in Sec. II, with

$$M_\pm^\lambda=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\int_C du\,\frac{e^{-uM_\pm}}{u^{\lambda+1}}, \quad (62)$$

where C is an appropriately chosen contour in the complex u plane. The operator $(iM_3)^\sigma$ is defined similarly.

The formal properties of the operators are easily determined. $[M^2,M_\pm^\lambda]=0$, so $M_\pm^\lambda$ transform solutions $f_\nu^\mu(z,t)=t^\mu F_\nu^\mu(z)$ of the associated Legendre equation $[M^2+\nu(\nu+1)]f_\nu^\mu=0$ into solutions with the same degree ν. Further, from

$$[iM_3,M_\pm^n]=\pm nM_\pm^n, \quad (63)$$

we find that

$$[iM_3,e^{-uM_\pm}]=\pm\sum_{n=0}^{\infty}\frac{(-u)^n}{n!}nM_\pm^n=\pm u\frac{d}{du}e^{-uM_\pm}, \quad (64)$$

hence, after a partial integration in (62), that

$$[iM_3,M_\pm^\lambda]=\pm\lambda M_\pm^\lambda. \quad (65)$$

The operators $M_\pm^\lambda$ therefore increase or decrease the order μ by λ when applied to $f_\nu^\mu=t^\mu F_\nu^\mu(z)$,

$$iM_3(M_\pm^\lambda f_\nu^\mu)=M_\pm^\lambda(iM_3\pm\lambda)f_\nu^\mu=(\mu\pm\lambda)(M_\pm^\lambda f_\nu^\mu). \quad (66)$$

The new functions $M_\pm^\lambda f_\nu^\mu$ may involve a different combination of the fundamental solutions of the associated Legendre equation than appeared originally, with $(f')_\nu^{\mu\pm\lambda}=t^{\mu\pm\lambda}(F')_\nu^{\mu\pm\lambda}$. Furthermore, even when $F'=F$, the operations only give f' up to a constants of proportionality because of the sign and numerical factors in the recurrence relations (19) and (20). We will therefore write $M_\pm^\lambda f_\nu^\mu$ as

$$M_\pm^\lambda f_\nu^\mu=N_\pm(\nu,\mu,\lambda)(f')_\nu^{\mu\pm\lambda}, \quad (67)$$

where the functional form of F' and the constant N are to be determined.

The more general relations

$$(iM_3)^\sigma M_\pm^\lambda=M_\pm^\lambda(iM_3\pm\lambda)^\sigma, \quad M_\pm^\lambda(iM_3)^\sigma=(iM_3\mp\lambda)^\sigma M_\pm^\lambda, \quad (68)$$

can be derived using the Baker–Hausdorff expansion of $e^Ae^Be^{-A}$ as a series of n-fold commutators.[5] The operators $M_\pm$ are mixed with M_3 under commutation as in Eq. (13), with the result that there are apparently no simple expressions for commutators of the fractional operators M_+^λ and M_-^η for arbitrary values of λ and η. However,

$$[iM_3,M_+^\sigma M_-^\lambda]=(\sigma-\lambda)M_+^\sigma M_-^\lambda, \quad [iM_3,M_-^\lambda M_+^\sigma]=(\sigma-\lambda)M_-^\lambda M_+^\sigma, \quad (69)$$

so $M_+^\sigma M_-^\lambda$ and $M_-^\lambda M_+^\sigma$ both carry solutions f_ν^μ to solutions of the type $(f')_\nu^{\mu+\sigma-\lambda}$.

We can define fractional operators P_3^λ and K_3^λ as above. Since $[P^2,P_3^\lambda]=0$ and $[P^2,K_3^\lambda]\simeq 0$, these operators transform solutions $h_\nu^\mu(x,z,t)=x^\nu f_\nu^\mu(z,t)$ of $P^2h_\nu^\mu=0$ into solutions. Furthermore, $[M_3,P_3^\lambda]=[M_3,K_3^\lambda]=0$, so P_3^λ and K_3^λ do not change the value μ of iM_3.

Calculations similar to those which lead to (65) show that

$$[D,P_3^\lambda]=-\lambda P_3^\lambda, \quad [D,K_3^\lambda]=\lambda K_3^\lambda, \tag{70}$$

so these operators decrease or increase the value of ν by λ. Given the numerical factors in the recurrence relations (38) and (39), the transformed functions h' are determined only up to constants of proportionality,

$$P_3^\lambda h_\nu^\mu = N'_-(\nu,\mu,\lambda)\, h'^\mu_{\nu-\lambda}, \quad K_3^\lambda h_\nu^\mu = N'_+(\nu,\mu,\lambda)\, h'^\mu_{\nu+\lambda}. \tag{71}$$

Because

$$[M_\pm,P_3]=\pm P_\pm, \quad [M_\pm,K_3]=\pm K_\pm, \tag{72}$$

the operators $M_\pm^\sigma$ do not commute with P_3^λ and K_3^λ. However, it is easily shown that $M_\pm^\sigma P_3^\lambda$ and $P_3^\lambda M_\pm^\sigma$ both carry h_ν^μ to solutions of the type $(h')_{\nu-\lambda}^{\mu\pm\sigma}$. Similarly, $M_\pm^\sigma K_3^\lambda$ and $K_3^\lambda M_\pm^\sigma$ both carry h_ν^μ to solutions of the type $(h')_{\nu+\lambda}^{\mu\pm\sigma}$.

VII. CHANGE OF THE ORDER OF F_ν^μ USING $M_\pm^\lambda$

A. Weyl-type relations using M_+^λ

The action of the Weyl-type operator M_+^λ on the associated Legendre functions gives

$$\begin{aligned} M_+^\lambda t^\mu F_\nu^\mu(z) &= N_+(\nu,\mu,\lambda)\, t^{\mu+\lambda}(F')_\nu^{\mu+\lambda}(z) \\ &= \frac{1}{2\pi i} e^{i\pi\lambda}\Gamma(\lambda+1)t^\mu(z^2-1)^{\mu/2} \\ &\quad \times \int_{C_W} \frac{du}{u^{\lambda+1}}[(z+ut\sqrt{z^2-1})^2-1]^{-\mu/2}F_\nu^\mu(z+ut\sqrt{z^2-1}), \end{aligned} \tag{73}$$

where the direction of the contour C_W for $|u|\to\infty$ must be chosen to assure convergence of the integral.

It is easily shown that the integral converges and gives a solution of the associated Legendre equation for the choice $F_\nu^\mu=Q_\nu^\mu$ provided $\mathrm{Re}(\nu+\mu+\lambda+1)>0$. [It can be established that the integrals (74) and (79) in the following give solutions of the associated Legendre equation with the indicated indices by a calculation similar to that which leads to the condition (89) for the Riemann version of M_+^λ. The only change in the final condition is the replacement of v by $-v$ in (89), and the restrictions given on ν, μ, and λ follow.] The proportionality of the integral to $Q_\nu^{\mu+\lambda}$ and the value of the coefficient N_+ can be established using the asymptotic behavior of the two sides of (74) for $z\to\infty$, proportional in both cases to $z^{-\nu-1}$. We find that $N_+=e^{-i\pi\lambda}$, a result consistent with repeated application of the recurrence relation $M_+t^\mu F_\nu^\mu=-t^{\mu+1}F_\nu^{\mu+1}$.

After scaling out the variable t, (73) can be rewritten for $F_\nu^\mu=Q_\nu^\mu$ as

$$e^{-i\pi(\mu+\lambda)}Q_\nu^{\mu+\lambda}(z)=\frac{e^{i\pi\lambda}}{2\pi i}\Gamma(\lambda+1)\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{z^2-1}{Z^2-1}\right)^{\mu/2}e^{-i\pi\mu}Q_\nu^\mu(Z), \tag{74}$$

where $Z=z+u\sqrt{z^2-1}$ and $\mathrm{Re}(\nu+\mu+\lambda+1)>0$. That is,

$$M_+^\lambda t^\mu e^{-i\pi\mu} Q_\nu^\mu(z) = t^{\mu+\lambda} e^{-i\pi(\mu+\lambda)} Q_\nu^{\mu+\lambda}(z). \tag{75}$$

The expression in (74) can be put in the form of a generalized Weyl fractional integral by changing to Z as the integration variable

$$e^{-i\pi(\mu+\lambda)} Q_\nu^{\mu+\lambda}(z) = \frac{1}{2\pi i} e^{i\pi\lambda} \Gamma(\lambda+1)(z^2-1)^{(\nu+\lambda)/2} \times \int_{(\infty, z+, \infty)} \frac{dZ}{(Z-z)^{\lambda+1}} (Z^2-1)^{-\mu/2} e^{-i\pi\mu} Q_\nu^\mu(Z). \tag{76}$$

The contour can be collapsed for $\mathrm{Re}\,\lambda<0$, and (74) can then reduce to a form equivalent to the known fractional integral, Ref. 6, 13.2(30). However, the result in (74) is more general and has a clear connection with the underlying group theory.

The further substitutions $z=\cosh\theta$, $Z=\cosh\theta'$ convert (76) to an expression in terms of hyperbolic angles,

$$e^{-i\pi(\mu+\lambda)} Q_\nu^{\mu+\lambda}(\cosh\theta) = \frac{1}{2\pi i} e^{i\pi\lambda} \Gamma(\lambda+1) \sinh^{\mu+\lambda}\theta \int_{(\infty, \theta+, \infty)} \frac{d\theta'}{(\cosh\theta' - \cosh\theta)^{\lambda+1}} \times \sinh^{-\mu+1}\theta' e^{-i\pi\mu} Q_\nu^\mu(\theta'). \tag{77}$$

A different result holds for the Weyl action of M_+ on the functions $t^\mu P_\nu^\mu(z)$ as may be seen from the relation

$$P_\nu^\mu(z) = \frac{1}{\pi} e^{-i\pi\mu} \frac{1}{\cos\pi\nu} [\sin\pi(\nu+\mu) Q_\nu^\mu(z) - \sin\pi(\nu-\mu) Q_{-\nu-1}^\mu(z)]. \tag{78}$$

The operator M_+^λ acts on the Q's, but does not change the sine factors, with the result that, suppressing the dependence on t,

$$\begin{aligned} M_+^\lambda P_\nu^\mu(z) &= \frac{1}{2\pi i} e^{i\pi\lambda} \Gamma(\lambda+1) \int_{(\infty,0+,\infty)} \frac{du}{u^{\lambda+1}} \left(\frac{z^2-1}{Z^2-1}\right)^{\mu/2} P_\nu^\mu(Z) \\ &= \frac{1}{\pi} e^{-i\pi(\mu+\lambda)} \frac{1}{\cos\pi\nu} [\sin\pi(\nu+\mu) Q_\nu^{\mu+\lambda}(z) - \sin\pi(\nu-\mu) Q_{-\nu-1}^{\mu+\lambda}(z)] \\ &= \frac{\sin\pi(\nu-\mu)}{\sin\pi(\nu-\mu-\lambda)} P_\nu^{\mu+\lambda}(z) - \frac{2}{\pi} \sin\pi\nu \sin\pi\lambda\, e^{-i\pi(\mu+\lambda)} Q_\nu^{\mu+\lambda}(z) \end{aligned} \tag{79}$$

for $\mathrm{Re}(\pm(\nu+\frac{1}{2})+\mu+\lambda+\frac{1}{2})>0$ and $Z=z+\sqrt{z^2-1}$.

We emphasize that the different behavior of the Weyl-type operator M_+^λ on Q_ν^μ and P_ν^μ is associated with the fact that the integration contour runs to ∞. Q_ν^μ and $Q_{-\nu-1}^\mu$ have unique asymptotic limits for $z\to\infty$, behaving, respectively, as $z^{-\nu-1}$ and z^ν multiplied by series in $1/z^2$. The operator M_+^λ changes μ but does not affect ν. Since it carries solutions of the associated Legendre equation to solutions and, as is evident from (73), preserves the asymptotic behavior of the integrand for $z\to\infty$, it can only carry Q_ν^μ to a multiple of $Q_\nu^{\mu+\lambda}$ and $Q_{\nu-1}^\mu$ to a multiple of $Q_{-\nu-1}^{\mu+\lambda}$ with no mixing of the two functions. P_ν^μ, in contrast, involves both functions with different μ-dependent coefficients, and cannot be reproduced for general ν. It is useful in this respect to regard Q_ν^μ and $Q_{-\nu-1}^\mu$ as the fundamental solutions of the associated Legendre equation rather than P_ν^μ and Q_ν^μ. We will encounter similar situations later.

B. Weyl-type relations using M_-^λ

The action of the Weyl-type operators M_-^λ on the associated Legendre functions gives

$$\begin{aligned} M_-^\lambda t^\mu F_\nu^\mu(z) &= N_-(\nu,\mu,\lambda) t^{\mu-\lambda}(F')_\nu^{\mu-\lambda}(z) \\ &= \frac{1}{2\pi i}\Gamma(\lambda+1)e^{i\pi\lambda}t^\mu(z^2-1)^{-\mu/2} \\ &\quad\times\int_{C_W}\frac{du}{u^{\lambda+1}}\left[\left(z-\frac{u}{t}\sqrt{z^2-1}\right)^2-1\right]^{\mu/2}F_\nu^\mu\left(z-\frac{u}{t}\sqrt{z^2-1}\right). \end{aligned} \tag{80}$$

It can be established through a calculation equivalent to that which leads to condition (92) obtained later for the Riemann version of M_-^λ that this expression gives a solution of the associated Legendre equation provided the integral converges for $|u|\to\infty$.

The contour C_W must extend to $|u|\to\infty$, and must avoid the singularities of the integrand at $u/t=\sqrt{(z-1)/(z+1)}$, $\sqrt{(z+1)/(z-1)}$. The singularities are always in the right half of the u/t plane a finite distance from the origin for $|z\pm1|$ finite. For definiteness, we will consider the case in which, after scaling out the variable t, the initial contour is taken to run above both singularities. This allows us to rotate the contour in (80) counterclockwise by π, and then replace u by $e^{i\pi}u$, effectively returning to the expression in (80) with $-u$ replaced by u and with the acquisition of an extra phase $e^{-i\pi\lambda}$.

After identifying the constant of proportionality, we find for the choice $F_\nu^\mu=Q_\nu^\mu$ that

$$\begin{aligned} e^{-i\pi(\mu-\lambda)}Q_\nu^{\mu-\lambda}(z) &= \frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\frac{\Gamma(\nu+\mu-\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\mu+\nu+1)\Gamma(\nu-\mu+\lambda+1)} \\ &\quad\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{Z^2-1}{z^2-1}\right)^{\mu/2}e^{-i\pi\mu}Q_\nu^\mu(Z), \end{aligned} \tag{81}$$

$Z=z+u\sqrt{z^2-1}$. The integral converges and gives a solution $Q_\nu^{\nu-\lambda}$ of the associated Legendre equation for $\mathrm{Re}(\nu-\mu+\lambda+1)>0$.

The coefficient of the integral can be determined using the asymptotic behavior of the two sides of (81) for $z\to\infty$. It corresponds to a coefficient

$$N_-(\nu,\mu,\lambda)=e^{-i\pi\lambda}\frac{\Gamma(\nu+\mu+1)\Gamma(\nu-\mu+\lambda+1)}{\Gamma(\nu+\mu-\lambda+1)\Gamma(\nu-\mu+1)} \tag{82}$$

in the original expression (80), with the contour taken to run above the singularities of the integrand at $u/t=\sqrt{(z\pm1)/(z\mp1)}$. N_- is just the coefficient of the nth term in the generating function (46), up to the factor $1/n!$, but extended from integer n to noninteger values $n\to\lambda$ with the factor $(-1)^n\to e^{-i\pi\lambda}$. We note that the phase of the constant N_- defined through (80) depends on the choice of the original contour. The final result does not. [The contour rotation and substitution used above replace the factor $\exp(-uM_-)$ in the definition of M_-^λ by $\exp(-ue^{i\pi}M_-)$, effectively replacing $-u$ by u in the series (46). The resulting expression gives $(e^{i\pi}M_-)^\lambda$ when the integration in (62) is performed on the standard Weyl contour $(\infty,0+,\infty)$, hence the extra phase noted above in the expression for M_-^λ. Had we started instead with a contour that ran below both the singularities of the integrand, rotated the contour clockwise by π, and then replaced u by $e^{-i\pi}u$, the extra phase would have been $e^{i\pi\lambda}$, and the new N_- would be $e^{2i\pi\lambda}$ times the result in (82). The ultimate expression for $Q_\nu^{\mu-\lambda}$ does not change.] The contour in (81) can be closed for $\lambda=n$, one recovers the expression for $Q_\nu^{\mu-n}$ given by the generating function (46).

The above-mentioned results continue to hold for $Q^{\mu}_{-\nu-1}$ for $\mathrm{Re}(-\nu-\mu+\lambda)>0$, and (81) and (78) can be used to evaluate $M^{\lambda}_{-}P^{\mu}_{\nu}$. Remarkably, the coefficients $N_{-}(\nu,\mu,\lambda)$ and $N_{-}(-\nu-1,\mu,\lambda)$ are such that the sine functions in (78) are reproduced in the final result with $\mu\to\mu-\lambda$, and we find that

$$P^{\mu-\lambda}_{\nu}(z)=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\frac{\Gamma(-\nu-\mu)\Gamma(\nu-\mu+1)}{\Gamma(-\nu-\mu+\lambda)\Gamma(\nu-\mu+\lambda+1)}\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{Z^2-1}{z^2-1}\right)^{\mu/2}P^{\mu}_{\nu}(Z), \tag{83}$$

$\mathrm{Re}(\pm(\nu+\frac{1}{2})-\mu+\lambda+\frac{1}{2})>0$. This corresponds to a coefficient

$$\tilde{N}_{-}=e^{i\pi\lambda}\frac{\sin\pi(\nu+\mu)}{\sin\pi(\nu+\mu-\lambda)}N_{-}(\nu,\mu,\lambda)=\frac{\Gamma(-\nu-\mu+\lambda)\Gamma(\nu-\mu+\lambda+1)}{\Gamma(-\nu-\mu)\Gamma(\nu-\mu+1)} \tag{84}$$

in the relation $M^{\lambda}_{-}P^{\mu}_{\nu}=\tilde{N}_{-}(\nu,\mu,\lambda)P^{\mu-\lambda}_{\nu}$, with M^{λ}_{-} defined with the original contour in (80) taken above the singularities of the integrand. The change relative to (82) is in a different continuation of the alternating sign in the generating function (46), with the factor $e^{-i\pi\lambda}$ in N_{-} replaced by $\sin\pi(\nu+\mu)/\sin\pi(\nu+\mu-\lambda)$ in $\tilde{N}_{-}$. Because of the change in coefficients, it is again useful to regard Q^{μ}_{ν} and $Q^{\mu}_{-\nu-1}$ as the fundamental solutions rather than Q^{μ}_{ν} and P^{μ}_{ν}.

C. Riemann-type relations using $M^{\lambda}_{\pm}$

The action of the Riemann-type fractional operator M^{λ}_{+} is given by (73) on a finite contour $C_R=(u_0,0+,u_0)$ where the obvious choice of the end point u_0 is the point at which the argument of the Legendre function is $+1$,

$$u_0=e^{i\pi}\frac{1}{t}\left(\frac{z-1}{z+1}\right)^{1/2}. \tag{85}$$

Writing u as u_0v and factoring out the dependence on t, we obtain

$$N_{+}\left(\frac{z-1}{z+1}\right)^{(\mu+\lambda)/2}(F')^{\mu+\lambda}_{\nu}(z)=\frac{1}{2\pi i}\Gamma(\lambda+1)\int_{(1,0+,1)}\frac{dv}{v^{\lambda+1}}\frac{1}{(1-v)^{\mu}}\left(\frac{V-1}{V+1}\right)^{\mu/2}F^{\mu}_{\nu}(V), \tag{86}$$

where $V=z-(z-1)v$ and F and F' are possibly different associated Legendre functions. The last factor on the right-hand side has the same form as the function on the left, but with z replaced by V.

Defining

$$w^{\mu}_{\nu}(z)=\left(\frac{z-1}{z+1}\right)^{\mu/2}F^{\mu}_{\nu}(z) \tag{87}$$

and using the form of the associated Legendre equation satisfied by that function,

$$(z^2-1)w''+(2z-2\mu)w'-\nu(\nu+1)w=0, \tag{88}$$

with the replacement $\mu\to\mu+\lambda$, we find that (86) gives a solution of (88) provided

$$v^{-\lambda}(1-v)^{1-\mu}\frac{d}{dv}\left[\left(\frac{V-1}{V+1}\right)^{\mu/2}F^{\mu}_{\nu}(V)\right]=0 \tag{89}$$

at the end points of the integration contour. This condition is satisfied for P_ν^μ for $\mathrm{Re}\,\mu<1$ with the expected end points $v=1, e^{2\pi i}$. The expression in (89) does not vanish for Q_ν^μ, with the result that the right-hand side of (86) satisfies an inhomogenous version of the associated Legendre equation, so does not give $Q_\nu^{\mu+\lambda}$.

With the choice $F_\nu^\mu = P_\nu^\mu$ in (86), we find that $N_+ = e^{-i\pi\lambda}$ as before, and that

$$P_\nu^{\mu+\lambda}(z) = \frac{1}{2\pi i} e^{2i\pi\lambda}\Gamma(\lambda+1)\int_{(u_0,0+,u_0)} \frac{du}{u^{\lambda+1}}\left(\frac{z^2-1}{Z^2-1}\right)^{\mu/2} P_\nu^\mu(Z),$$

$$= \frac{1}{2\pi i} e^{i\pi\lambda}\Gamma(\lambda+1)\int_{(u_0',0+,u_0')} \frac{du}{u^{\lambda+1}}\left(\frac{z^2-1}{Z'^2-1}\right)^{\mu/2} P_\nu^\mu(Z'), \tag{90}$$

where $\mathrm{Re}\,\mu<1$, $Z' = z - u\sqrt{z^2-1}$, and $u_0' = \sqrt{(z-1)/(z+1)}$. Changing to Z' as the integration variable, we get the alternative form

$$P_\nu^{\mu+\lambda}(z) = \frac{1}{2\pi i}\Gamma(\lambda+1)(z^2-1)^{(\mu+\lambda)/2}\int_{(1,z+,1)} \frac{dZ'}{(Z'-z)^{\lambda+1}}(Z'^2-1)^{-\mu/2} P_\nu^\mu(Z'), \tag{91}$$

where $|\arg(Z'-z)| \leqslant \pi$. This result can be reduced in the case of real z with $-1<z<1$ to a known fractional integral, Ref. 6, 13.1(54).

A similar calculation for M_-^λ on the Riemann contour starting from (80) leads to the condition for a solution of the associated Legendre equation that the function

$$v^{-\lambda}(1-v)^{\mu+1}\frac{d}{dv}\left[\left(\frac{V+1}{V-1}\right)^{\mu/2} F_\nu^\mu(V)\right] \tag{92}$$

vanish at the end points. In fact, it has a finite value for $v=1, e^{2\pi i}$ for either P_ν^μ or Q_ν^μ. The functions defined by the integral satisfy inhomogeneous versions of the associated Legendre equation rather than the equation itself, and the Riemann version of M_-^λ appears not to be useful.

VIII. CHANGE OF THE DEGREE OF F_ν^μ USING K_3^λ AND P_3^λ

A. Relations for K_3^λ

The action of the operator K_3^λ on a function $x^\nu F_\nu^\mu$ increases the degree ν by λ as shown formally by the commutation relation (70). In particular, using the variable y and the expression in (53) for the action of e^{-uK_3}, we obtain a Weyl-type relation

$$K_3^\lambda x^\nu F_\nu^\mu\left(\frac{y}{\sqrt{y^2-1}}\right) = N_+'(\nu,\mu,\lambda)x^{\nu+\lambda}(F')_{\nu+\lambda}^\mu\left(\frac{y}{\sqrt{y^2-1}}\right)$$

$$= \frac{1}{2\pi i} e^{i\pi\lambda}\Gamma(\lambda+1)\int_{C_W} \frac{du}{u^{\lambda+1}}\left(\frac{y^2-1}{Y^2-1}\right)^{(\nu+1)/2} F_\nu^\mu\left(\frac{Y}{\sqrt{Y^2-1}}\right), \tag{93}$$

where $Y = y - xu\sqrt{y^2-1}$. The contour C_W must be chosen to run to $|u|\to\infty$, avoiding the singularities of the integrand at $Y=\pm 1$ or $xu = \sqrt{(y\pm 1)/(y\mp 1)}$. The singularities are both in the right-half xu plane a finite distance from the origin for $|y\pm 1|$ finite.

Following the procedure sketched in Sec. VII B, we change to xu as a new integration variable, pick an initial contour which runs above both singularities, rotate the contour counterclockwise by π, and replace u by $e^{i\pi}u$ to return to the standard contour. This gives

$$N'_+(\nu,\mu,\lambda)(F')^{\mu}_{\nu+\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}\Gamma(\lambda+1)\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{y^2-1}{Y^2-1}\right)^{(\nu+1)/2}F^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right),\tag{94}$$

where Y is now given by $Y=y+u\sqrt{y^2-1}$ and we have acquired an extra phase $e^{-i\pi\lambda}$. By considering the modified Legendre equation

$$(y^2-1)v''+(2y-\nu-\tfrac{1}{2})v'-(\mu^2-\tfrac{1}{4})v=0\tag{95}$$

satisfied by the function

$$v^{\mu}_{\nu}(y)=\left(\frac{y-1}{y+1}\right)^{(\nu+1)/2}(y^2-1)^{-1/4}F^{\mu}_{\nu}\left(\frac{y}{\sqrt{y^2-1}}\right),\tag{96}$$

we find that the right-hand side of (93) satisfies the associated Legendre equation for degree $\nu+\lambda$ and order μ provided that the function

$$u^{-\lambda}(1+u)^{-\lambda+(1/2)}\frac{d}{du}\left[\left(\frac{Y-1}{Y+1}\right)^{(\nu+1/2)/2}(Y^2-1)^{-1/4}F^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right)\right]\tag{97}$$

vanishes at the end points of the contour. This condition is satisfied for $F^{\mu}_{\nu}=P^{\mu}_{\nu}$ in (94) provided $\mathrm{Re}(\nu+\lambda-\mu+1)>0$, and for $F^{\mu}_{\nu}=Q^{\mu}_{\nu}$ provided $\mathrm{Re}(\nu+\lambda\pm\mu+1)>0$.

The form of the function in (96) is suggested by the Whipple transformation, Ref. 9, 3.3.2(13,14)

$$e^{-i\pi\mu}Q^{\mu}_{\nu}\left(\frac{y}{\sqrt{y^2-1}}\right)=\sqrt{\frac{\pi}{2}}\Gamma(\nu+\mu+1)(y^2-1)^{1/4}P^{-\nu-(1/2)}_{-\mu-(1/2)}(y)$$

which connects the actions of K_3^{λ} and M_-^{λ} and of P_3^{λ} and M_+^{λ}, and can be used to derive Eqs. (100) and (110) in the following from (83) and (74). The Whipple transformation is associated with the automorphism

$$D'=-iM_3,\quad iM'_3=-D,\quad M'_+=P_3,\quad M'_-=-K_3,$$

$$P'_+=-P_+,\quad P'_-=K_+,\quad P'_3=M_+,\quad K'_+=P_-,\quad K'_-=-K_-,\quad K'_3=-M_-$$

of the abstract conformal algebra. Using the explicit realizations of the operators given in Sec. IV, we find that

$$P'^2=x_+^2P^2\simeq 0\quad\text{and}\quad M'^2+D'^2-\tfrac{1}{4}=-\tfrac{1}{2}(P_3K_3+K_3P_3)-D^2-M_3^2-\tfrac{1}{4}=x_\perp^2P^2\simeq 0$$

when acting on solutions of the Laplace equation. These relations are only invariant under rotations about the 3 axis generated by M_3 and not under the full Lorentz group. The transformation maps realizations of the algebra to realizations, with $\nu'=-\mu-\frac{1}{2}$ $(iM'_3=-D)$ and $\mu'=-\nu-\frac{1}{2}$ $(D'=-iM_3)$. In terms of differential equations, the substitutions $z=y/\sqrt{y^2-1}$, $F^{\mu}_{\nu}(z)=(y^2-1)^{1/4}G^{\mu'}_{\nu'}(y)$ transform the associated Legendre equation satisfied by $F^{\mu}_{\nu}(z)$ into the same equation for $G^{\mu'}_{\nu'}(y)$. The specific connection of the functions can be established by matching their behavior for $z\to\infty$, $y\to 1$ and for $z\to 1$, $y\to\infty$.

The constant of proportionality N'_+ in (94) can be determined by changing to Y as the variable of integration in that equation, and then determining the asymptotic limits of the two sides for $y\to\infty$. We find that

$$N'_+(\nu,\mu,\lambda)=e^{-i\pi\lambda}\frac{\Gamma(\nu+\lambda-\mu+1)}{\Gamma(\nu-\mu+1)} \tag{98}$$

for both P^μ_ν and Q^μ_ν. The first can be established easily by identifying the characteristic power behavior $P^\mu_\nu(z)\propto[(z+1)/(z-1)]^{\mu/2}$ for $z\to 1$ on the two sides of the equation. The coefficient for Q^μ_ν follows from

$$e^{-i\pi\mu}Q^\mu_\nu(z)=\frac{\pi}{2\sin\pi\mu}\left[P^\mu_\nu(z)-\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu-\mu+1)}P^{-\mu}_\nu(z)\right]. \tag{99}$$

Using the result for N'_+ in (94), we find that

$$F^\mu_{\nu+\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1}\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{y^2-1}{Y^2-1}\right)^{(\nu+1)/2}F^\mu_\nu\left(\frac{Y}{\sqrt{Y^2-1}}\right), \tag{100}$$

where $\mathrm{Re}(\nu+\lambda-\mu+1)>0$ for P^μ_ν, and $\mathrm{Re}(\nu+\lambda\pm\mu+1)>0$ for Q^μ_ν. Alternatively, taking Y as the integration variable,

$$F^\mu_{\nu+\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1)}(y^2-1)^{(\nu+\lambda+1)/2}\times\int_{(\infty,y+,\infty)}\frac{dY}{(Y-y)^{\lambda+1}}(Y^2-1)^{-(\nu+1)/2}F^\mu_\nu\left(\frac{Y}{\sqrt{Y^2-1}}\right). \tag{101}$$

This expression has the form of a Weyl fractional integral, Ref. 6, Sec. 13.2, but is apparently not known in the general case.

The substitutions $Y=\coth\theta'$, $y=\coth\theta$ in (101) give

$$\begin{aligned}F^\mu_{\nu+\lambda}(\cosh\theta)&=-\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1}(\sinh\theta)^{\nu+\lambda+1}\\&\quad\times\int_{(0,\theta+,0)}\frac{d\theta'}{\sinh^2\theta'}\frac{1}{(\coth\theta'-\coth\theta)^{\lambda+1}}(\sinh\theta')^{\nu+1}F^\mu_\nu(\cosh\theta')\\&=-\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1}\\&\quad\times\int_{(0,\theta+,0)}\frac{d\theta'}{\sinh\theta'}\left(\frac{\sinh\theta'}{\sinh\theta}\right)^{\nu}\left(\frac{\sinh\theta'}{\sinh(\theta-\theta')}\right)^{\lambda+1}F^\mu_\nu(\cosh\theta'),\end{aligned} \tag{102}$$

while the substitutions $Y=\cosh\phi'$, $y=\cosh\phi$ give

$$F^\mu_{\nu+\lambda}(\coth\phi)=\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1}(\sinh\phi)^{\nu+\lambda+1}\times\int_{(\infty,\phi+,\infty)}\frac{\sinh\phi'\,d\phi'}{(\cosh\phi'-\cosh\phi)^{\lambda+1}}(\sinh\phi')^{-\nu-1}F^\mu_\nu(\coth\phi'). \tag{103}$$

Finally, with $y=z/\sqrt{z^2-1}$ and $Y=(z+u)/\sqrt{z^2-1}$ in (100),

$$F^{\mu}_{\nu+\lambda}(z)=\frac{1}{2\pi i}e^{i\pi\lambda}\frac{\Gamma(\lambda+1)\Gamma(\nu-\mu+1)}{\Gamma(\nu+\lambda-\mu+1}$$

$$\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}(u^2+2uz+1)^{-(\nu+1)/2}F^{\mu}_{\nu}\left(\frac{z+u}{\sqrt{u^2+2zu+1}}\right). \tag{104}$$

The foregoing relations for K^{λ}_3 are of the Weyl type. The natural end point for a Riemann-type contour for the original integrand in (93) is at $Y=1$ or $xu=\sqrt{(y-1)/(y+1)}$. x can again be scaled out, and the condition that the right-hand side of (93) define a solution of the associated Legendre equation reduces to the requirement that the function in (97), with $(1+u)^{-\lambda+(1/2)}$ replaced by $(1-u)^{-\lambda+(1/2)}$ and $Y=y-u\sqrt{y^2-1}$, vanish at the end points. It fails to vanish for F^{μ}_{ν} equal to either P^{μ}_{ν} or Q^{μ}_{ν}, and there is no Riemann-type expression for K^{λ}_3.

B. Relations for P^{λ}_3

The action of the operator P^{λ}_3 on $x^{\nu}F^{\mu}_{\nu}$ decreases ν by λ as shown by the commutation relation (70). Thus, using the variable $y=z/\sqrt{z^2-1}$ and the expression in (52) for the action of e^{-uP_3}, we obtain the Weyl-type relation

$$P^{\lambda}_3 x^{\nu}F^{\mu}_{\nu}\left(\frac{y}{\sqrt{y^2-1}}\right)=N'_{-}(\nu,\mu,\lambda)x^{\nu-\lambda}(F')^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)$$

$$=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\int_{C_W}\frac{du}{u^{\lambda+1}}\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}F^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right), \tag{105}$$

where $Y=y-u/x\sqrt{y^2-1}$. We will again take the initial integration contour to run to $|u|\to\infty$ above the singularities of the integrand at $u/x=\sqrt{(y\pm1)(y\mp1)}$, scale out the dependence on x, rotate the contour counterclockwise by π, and replace u by $e^{i\pi}u$ to reach the standard contour $(\infty,0+,\infty)$. This gives

$$N'_{-}(\nu,\mu,\lambda)(F')^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}\Gamma(\lambda+1)\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}F^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right), \tag{106}$$

where Y is now given by $Y=y+u\sqrt{y^2-1}$ and we have acquired an extra phase $e^{-i\pi\lambda}$. By considering the modified Legendre equation satisfied by the function[4]

$$\left(\frac{y+1}{y-1}\right)^{(\nu+1/2)/2}(y^2-1)^{-1/4}F^{\mu}_{\nu}\left(\frac{y}{\sqrt{y^2-1}}\right), \tag{107}$$

we find that the right-hand side of (105) satisfies the associated Legendre equation for degree $\nu-\lambda$ and order μ provided that the function

$$u^{-\lambda}(1+u)^{\nu+(3/2)}\frac{d}{du}\left[\left(\frac{Y+1}{Y-1}\right)^{(\nu+1/2)/2}(Y^2-1)^{-1/4}F^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right)\right] \tag{108}$$

vanishes at the end points of the contour. This condition is satisfied for $F^{\mu}_{\nu}=P^{\mu}_{\nu}$ in (106) provided $\mathrm{Re}(-\nu+\lambda-\mu)>0$. A comparison of the asymptotic limits of the two sides of (106) for $y\to\infty$ gives

$$N'_{-}(\nu,\mu,\lambda)=e^{-i\pi\lambda}\frac{\Gamma(-\nu+\lambda-\mu)}{\Gamma(-\nu-\mu)}, \tag{109}$$

and

$$P^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\frac{\Gamma(-\nu-\mu)}{\Gamma(-\nu+\lambda-\mu)}\int_{(\infty,0+,\infty}\frac{du}{u^{\lambda+1}}\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}P^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right). \tag{110}$$

The corresponding result for $F^{\mu}_{\nu}=Q^{\mu}_{\nu}$ involves an extra term related through the Whipple transformation, Ref. 9, 3.3.2(13,14) to that found for M^{λ}_{+} in Sec. VII A, and a different coefficient. We find that

$$\frac{e^{i\pi\lambda}}{2\pi i}\Gamma(\lambda+1)\frac{\Gamma(\nu-\lambda+\mu+1)}{\Gamma(\nu+\mu+1)}\int_{(\infty,0+,\infty)}\frac{du}{u^{\lambda+1}}\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}e^{-i\pi\mu}Q^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right)$$
$$=e^{-i\pi\mu}Q^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)-\pi\frac{\cos\pi\mu\sin\pi\lambda}{\sin\pi(\nu-\lambda+\mu)}P^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right), \tag{111}$$

$Y=y+u\sqrt{y^2-1}$, $\mathrm{Re}(\lambda-\nu\pm\mu)>0$.

The condition for there to be a Riemann-type representation for P^{λ}_{3} is given by (108) with $u+1$ replaced by $1-u$ and $Y=y-u(y-1)$. The result must vanish for $u=1$. This condition is satisfied for $F^{\mu}_{\nu}=Q^{\mu}_{\nu}$ for $\mathrm{Re}(\nu+\frac{3}{2})>0$, but is not satisfied for P^{μ}_{ν}. The Riemann integral for Q^{μ}_{ν} is

$$Q^{\mu}_{\nu-\lambda}\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\frac{\Gamma(\nu-\lambda+\mu+1}{\Gamma(\nu+\mu+1)}\int_{(u_0,0+,u_0)}\frac{du}{u^{\lambda+1}}$$
$$\times\left(\frac{Y^2-1}{y^2-1}\right)^{\nu/2}Q^{\mu}_{\nu}\left(\frac{Y}{\sqrt{Y^2-1}}\right), \tag{112}$$

where $Y=y-u\sqrt{y^2-1}$ and $u_0=\sqrt{(y-1)/(y+1)}$.

IX. INTEGRAL REPRESENTATIONS FOR ASSOCIATED LEGENDRE FUNCTIONS

A. Representations using $M^{\lambda}_{\pm}$

The fractional-operator relators $M^{\lambda}_{\pm}t^{\mu}F^{\mu}_{\nu}(z)=N_{\pm}t^{\mu\pm\lambda}F'^{\mu}_{\nu}(z)$ derived earlier can be converted into integral representations for the associated Legendre functions by a choice of μ for which the initial function is elementary. Thus, using M^{λ}_{+}, the choices

$$e^{-i\pi/2}Q^{1/2}_{\nu}(z)=\sqrt{\frac{\pi}{2}}(z^2-1)^{-1/4}[z+\sqrt{z^2-1}]^{-\nu-(1/2)} \tag{113}$$

in (76) and

$$e^{-i\pi/2}Q^{1/2}_{\nu}(\cosh\theta)=\sqrt{\frac{\pi}{2}}\sinh^{-1/2}\theta\, e^{-(\nu+1/2)\theta} \tag{114}$$

in (77) give simple Weyl-type integral representations for $Q^{\lambda+(1/2)}_{\nu}$. Choosing $\lambda=\mu-\frac{1}{2}$ in these expressions, we get, respectively,

$$(z^2-1)^{-\mu/2}e^{-i\pi\mu}Q^{\mu}_{\nu}(z)=\frac{1}{2\pi i}e^{i\pi(\mu-1/2)}\Gamma\left(\mu+\frac{1}{2}\right)\sqrt{\frac{\pi}{2}}\int_{(\infty,z+,\infty)}\frac{dZ}{(Z-z)^{\mu+1/2}}$$
$$\times(Z^2-1)^{-1/2}(Z+\sqrt{Z^2-1})^{-\nu-(1/2)} \tag{115}$$

and

$$e^{-i\pi\mu}Q_\nu^\mu(\cosh\theta)=\frac{1}{2\pi i}e^{i\pi(\mu-1/2)}\Gamma\left(\mu+\frac{1}{2}\right)\sqrt{\frac{\pi}{2}}\sinh^\mu\theta \times\int_{(\infty,\theta+,\infty)}\frac{d\theta'}{(\cosh\theta'-\cosh\theta)^{\mu+(1/2)}}e^{-(\nu+1/2)\theta'}, \tag{116}$$

for $\mathrm{Re}(\nu+\mu+1)>0$. If $\mathrm{Re}\,\mu<\frac{1}{2}$, the contour integrals can be collapsed, and the resulting form for (116) reduces to the standard integral representation, Ref. 9, 3.7(4). The fractional operator approach provides an interpretation of this result through its connection to the group SO(2,1).

The result in (116) can be transformed further by distorting the integration contour to $(\infty+i\pi,i\pi,-i\pi,\infty-i\pi)$, with $\theta'=0$ circumvented on the left. The result reduces for $\mathrm{Re}\,\mu<1/2$ to Ref. 9, 3.7(10). Similar manipulations are possible for the following expressions. For collections of known representations, see Refs. 9–11.

The use of (116) and

$$P_\nu^{1/2}(\cosh\theta)=\sqrt{\frac{2}{\pi}}\sinh^{-1/2}\theta\cosh\left(\nu+\frac{1}{2}\right)\theta \tag{117}$$

in the version of (79) obtained by the substitutions $z=\cosh\theta$, $z+u\sqrt{z^2-1}=\cosh\theta'$ in the integral on the first line gives a representation for $P_\nu^\mu(\cosh\theta)$ analogous to (116).

A second and more natural form of $M_+^\lambda P_\nu^\mu$ is given by the Riemann-type integral (90). Using $P_\nu^{1/2}$ as the input function, making the substitutions $z=\cosh\theta$, $Z'=\cosh\theta'$, and choosing $\lambda=\mu-\frac{1}{2}$, we obtain the integral representation

$$P_\nu^\mu(\cosh\theta)=\frac{1}{2\pi i}\Gamma\left(\mu+\frac{1}{2}\right)\sqrt{\frac{2}{\pi}}\sinh^\mu\theta\int_{(0,\theta+,0)}\frac{\mathrm{d}\theta'}{(\cosh\theta'-\cosh\theta)^{\mu+(1/2)}}\cosh\left(\nu+\frac{1}{2}\right)\theta', \tag{118}$$

where the denominator is now taken to have its principal phase, $-\pi\leqslant\arg(\cosh\theta'-\cosh\theta)\leqslant\pi$, and ν and μ are arbitrary. If $\mathrm{Re}\,\mu<1/2$, the contour can be collapsed and (118) reduces to Ref. 9, 3.7(9).

We can get alternative integral representations for Q_ν^μ and P_ν^μ by using

$$e^{-i\pi(\nu+1)}Q_\nu^{\nu+1}(z)=2^\nu\Gamma(\nu+1)(z^2-1)^{-(\nu+1)/2}, \tag{119}$$

$$P_\nu^{-\nu}(z)=\frac{2^{-\nu}}{\Gamma(\nu+1)}(z^2-1)^{\nu/2}. \tag{120}$$

Thus, from the Weyl-type integral (74),

$$e^{-i\pi(\nu+\lambda+1)}Q_\nu^{\nu+\lambda+1}(z)=\frac{1}{2\pi i}e^{i\pi\lambda}2^\nu\Gamma(\nu+1)\Gamma(\lambda+1)(z^2-1)^{(\nu+1)/2} \times\int_{(\infty,0+,\infty)}\frac{\mathrm{d}u}{u^{\lambda+1}}(Z^2-1)^{-\nu-1}, \tag{121}$$

$\mathrm{Re}(2\nu+\lambda+2)>0$, $Z=z+u\sqrt{z^2-1}$. The choice $\lambda=\mu-\nu-1$ then gives

$$e^{-i\pi\mu}Q_\nu^\mu(z)=\frac{1}{2\pi i}e^{i\pi(\mu-\nu-1)}2^\nu\Gamma(\nu+1)\Gamma(-\nu+\mu)(z^2-1)^{\mu/2}\int_{(\infty,0+,\infty)}\frac{\mathrm{d}u}{u^{\mu-\nu}}(Z^2-1)^{-\nu-1} \tag{122}$$

$$=\frac{1}{2\pi i}e^{i\pi(\mu-\nu-1)}2^{\nu}\Gamma(\nu+1)\Gamma(-\nu+\mu)(z^2-1)^{\mu/2}$$
$$\times\int_{(\infty,z+,\infty)}\frac{dZ}{(Z-z)^{\mu-\nu}}(Z^2-1)^{-\nu-1}, \tag{123}$$

$\mathrm{Re}(\nu+\mu+1)>0$. The substitutions $z=\cosh\theta$, $Z=\cosh\theta'$ in the second form gives an expression for $Q_\nu^\mu(\cosh\theta)$ different from (116),

$$e^{-i\pi\mu}Q_\nu^\mu(\cosh\theta)=\frac{1}{2\pi i}e^{i\pi(\mu-\nu-1)}2^{\nu}\Gamma(\nu+1)\Gamma(-\nu+\mu)\sinh^{\mu}\theta$$
$$\times\int_{(\infty,\theta_+,\infty)}\frac{d\theta'}{(\cosh\theta'-\cosh\theta)^{\mu-\nu}}\sinh^{-2\nu-1}\theta', \tag{124}$$

$\mathrm{Re}(\nu+\mu+1)>0$.

A similar construction starting from the Riemann-type integral (91) for M_+^λ with $\lambda=\nu+\mu$ and $P_\nu^{-\nu}$, (120), as the input gives

$$P_\nu^\mu(z)=\frac{1}{2\pi i}2^{-\nu}\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu+1)}(z^2-1)^{\mu/2}\int_{(1,z+,1)}\frac{dZ}{(Z-z)^{\nu+\mu+1}}(Z^2-1)^{\nu}, \tag{125}$$

$|\arg(Z-z)|\leqslant\pi$, $\mathrm{Re}(\nu+1)>0$. With $z=\cosh\theta$, $Z=\cosh\theta'$, this becomes

$$P_\nu^\mu(\cosh\theta)=\frac{1}{2\pi i}2^{-\nu}\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu+1)}\sinh^{\mu}\theta\int_{(0,\theta+,0)}\frac{d\theta'}{(\cosh\theta'-\cosh\theta)^{\nu+\mu+1}}\sinh^{2\nu+1}\theta', \tag{126}$$

where $-\pi\leqslant\arg(\cosh\theta'-\cosh\theta)\leqslant\pi$.

We can obtain further integral representations for Q_ν^μ and P_ν^μ using the Weyl-type integrals for M_-^λ in (81) and (83), respectively. Thus, using (81) with the input function $Q_\nu^{1/2}$, (113) and $\lambda=-\mu+\frac{1}{2}$, we find that

$$e^{-i\pi\mu}Q_\nu^\mu(z)=\frac{1}{2\pi i}e^{i\pi(-\mu+1/2)}\frac{\Gamma(-\mu+\frac{1}{2})}{(\nu+\frac{1}{2})}\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu-\mu+1)}\sqrt{\frac{\pi}{2}}$$
$$\times(z^2-1)^{-\mu/2}\int_{(\infty,0+,\infty)}\frac{dZ}{(Z-z)^{-\mu+(3/2)}}(Z+\sqrt{Z^2-1})^{-\nu-(1/2)}. \tag{127}$$

By changing to the angular variables $z=\cosh\theta$, $Z=\cosh\theta'$ and integrating once by parts, this can be rewritten as

$$e^{-i\pi\mu}Q_\nu^\mu(\cosh\theta)=\frac{1}{2\pi i}e^{-i\pi(\mu+1/2)}\frac{\Gamma(-\mu+\frac{1}{2})\Gamma(\nu+\mu+1)}{\Gamma(\nu-\mu+1)}\sqrt{\frac{\pi}{2}}$$
$$\times(\sinh\theta)^{-\mu}\int_{(\infty,\theta+,\infty)}d\theta'\,(\cosh\theta'-\cosh\theta)^{\mu-(1/2)}e^{-(\nu+1/2)\theta'} \tag{128}$$

$$= \frac{\Gamma(\nu+\mu+1)}{\Gamma(\mu+\frac{1}{2})\Gamma(\nu-\mu+1)}\sqrt{\frac{\pi}{2}}$$

$$\times(\sinh\theta)^{-\mu}\int_{\theta}^{\infty} d\theta'\,(\cosh\theta'-\cosh\theta)^{\mu-(1/2)}e^{-(\nu+1/2)\theta'}. \tag{129}$$

The first expression holds for $\mathrm{Re}(\nu-\mu+1)>0$, and the second with the additional constraint that $\mathrm{Re}\,\mu>-1/2$. The same results can be obtained without the partial integration by starting with $Q_\nu^{-1/2}$ and $\lambda=-\mu-\frac{1}{2}$.

Note that the integral in expression (128) for Q_ν^μ is the same as that in the expression for $Q_\nu^{-\mu}$ obtained from (116) with the replacement $\mu\to-\mu$. Comparison of the two results shows that

$$e^{-i\pi\mu}Q_\nu^\mu(z)=\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu-\mu+1)}e^{i\pi\mu}Q_\nu^{-\mu}(z) \tag{130}$$

as expected.

A similar calculation using (83) with the input function $P_\nu^{1/2}$ and $\lambda=\mu+\frac{1}{2}$ gives the integral representation

$$P_\nu^{-\mu}(\cosh\theta)=\frac{1}{2\pi i}e^{i\pi(\mu-1/2)}\frac{\sqrt{2\pi}}{\cos\pi\nu}\frac{\Gamma(\mu+\frac{1}{2})}{\Gamma(-\nu+\mu)\Gamma(\nu+\mu+1)}$$

$$\times\sinh^\mu\theta\int_{(\infty,\theta+,\infty)}\frac{d\theta'}{(\cosh\theta'-\cosh\theta)^{\mu+(1/2)}}\sinh\left(\nu+\frac{1}{2}\right)\theta', \tag{131}$$

valid for $\mathrm{Re}(\mu\pm(\nu+\frac{1}{2})+\frac{1}{2})>0$.

In contrast to the case of M_+^λ, the input functions $Q_\nu^{\nu+1}$ and $P_\nu^{-\nu}$, (119) and (120), do not give useful results for M_-^λ because of the appearance of infinite coefficients in (81) and (83). The problem arises from the recurrence relation connected with the action of M_-. The coefficient of $F_\nu^{\mu-1}$ in (20) vanishes for $\mu=-\nu$ or $\mu=\nu+1$, and all information about $F_\nu^{\mu-1}$ is lost for those values of μ.

There are no Riemann-type relations or corresponding integral representations involving M_-^λ.

B. Representations using K_3^λ and P_3^λ

The fractional operator relation $K_3^\lambda x^\nu F_\nu^\mu=N'_+x^{\nu+\lambda}F_{\nu+\lambda}^\mu$ gives integral representations for the associated Legendre functions when used with P_0^μ or Q_0^μ as the input function. Thus, using P_0^μ, (58), in (101) and replacing λ by ν in the result, we find that

$$P_\nu^\mu\left(\frac{y}{\sqrt{y^2-1}}\right)=\frac{1}{2\pi i}e^{i\pi\nu}\frac{\Gamma(\nu+1)}{\Gamma(\nu-\mu+1)}(y^2-1)^{(\nu+1)/2}$$

$$\times\int_{(\infty,y+,\infty)}\frac{dY}{(Y-y)^{\nu+1}}\frac{1}{\sqrt{Y^2-1}}(Y+\sqrt{Y^2-1})^\mu \tag{132}$$

for $\mathrm{Re}(\nu-\mu+1)>0$. A change to the angular variables $y=\cosh\phi$, $Y=\cosh\phi'$ gives

$$P_\nu^\mu(\coth\phi)=\frac{1}{2\pi i}e^{i\pi\nu}\frac{\Gamma(\nu+1)}{\Gamma(\nu-\mu+1)}(\sinh\phi)^{\nu+1}\int_{(\infty,\phi+,\infty)}\frac{d\phi'}{(\cosh\phi'-\cosh\phi)^{\nu+1}}e^{\mu\phi'}. \tag{133}$$

Finally, using P_0^μ, (58), in (104),

$$P_\nu^\mu(z)=\frac{1}{2\pi i}e^{i\pi\nu}\frac{\Gamma(\nu+1)}{\Gamma(\nu-\mu+1)}(z^2-1)^{-\mu/2}$$
$$\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\nu+1}}\frac{1}{\sqrt{u^2+2zu+1}}(z+u+\sqrt{u^2+2zu+1})^\mu, \tag{134}$$

which reduces for $\mu=0$ to

$$P_\nu(z)=\frac{1}{2\pi i}e^{i\pi\nu}\int_{(\infty,0+,\infty)}\frac{du}{u^{\nu+1}}\frac{1}{\sqrt{u^2+2zu+1}}, \tag{135}$$

$\mathrm{Re}(\nu+1)>0$.

We get similar integral representations for Q_ν^μ by using expression (60) in (100)–(104). Thus, in terms of the angular variable $z=\coth\phi$,

$$Q_\nu^\mu(\coth\phi)=\frac{1}{2\pi i}e^{i\pi\nu}\frac{\Gamma(\nu+1)}{\Gamma(\nu-\mu+1)}\frac{\pi}{\sin\pi\mu}(\sinh\phi)^{\nu+1}$$
$$\times\int_{(\infty,\phi+,\infty)}\frac{d\phi'}{(\cosh\phi'-\cosh\phi)^{\nu+1}}\sinh\mu\phi', \tag{136}$$

$\mathrm{Re}(\nu\pm\mu+1)>0$.

The Weyl-type relation (110) for $P_3^\lambda x^\nu P_\nu^\mu(z)$ with $\nu=0$ reduces after the use of the relation $P_0^\mu(\coth\phi')=e^{\mu\phi'}/\Gamma(1-\mu)$, the change of variables $y=\cosh\phi$, $Y=\cosh\phi'$, and a partial integration to

$$P_{-\lambda}^\mu(\coth\phi)=\frac{1}{2\pi i}e^{i\pi(\lambda-1)}\frac{\Gamma(\lambda)}{\Gamma(\lambda-\mu)}\sinh^\lambda\phi\int_{(\infty,\phi+,\infty)}\frac{d\phi'}{(\cosh\phi'-\cosh\phi)^\lambda}e^{\mu\phi'}, \tag{137}$$

$\mathrm{Re}(\lambda-\mu)>0$. The right-hand side of this expression is the same for the choice $\lambda=\nu+1$ as that in expression (133) for P_ν^μ, and we find that $P_{-\nu-1}^\mu(\coth\phi)=P_\nu^\mu(\coth\phi)$ as expected. This symmetry relation is a consequence of the relation

$$[K_3^\nu,P_3^{\nu+1}]h_0^\mu=[N_+'(-\nu-1,\mu,\nu)N_-'(0,\mu,\nu+1)-N_-'(\nu,\mu,\nu+1)N_+'(0,\mu,\nu)]h_0^\mu=0, \tag{138}$$

where the coefficients N_+' and N_-' given in (98) and (109) follow from the stepping relations in so(2,1).

The corresponding Weyl-type relation for $P_3^\lambda x^\nu Q_\nu^\mu(z)$ in (111) involves an extra term, and will not be given.

The Riemann-type relation for $P_3^\lambda x^\nu Q_\nu^\mu$ obtained by using (60) in (112) gives the further integral representation

$$Q_{-\lambda}^\mu(\coth\phi)=\frac{1}{2\pi i}\Gamma(\lambda)\frac{\Gamma(-\lambda+\mu+1)}{\Gamma(\mu)}\sinh^\lambda\phi\int_{(0,\phi+,0)}\frac{d\phi'}{(\cosh\phi'-\cosh\phi)^\lambda}\sinh\mu\phi', \tag{139}$$

where the phase of the denominator is to be taken between $-\pi$ and π. While the form of the integrands in (136) and (139) is the same for the choice $\lambda=\nu+1$ in the latter, the integration contours are different, and the difference between the Q_ν^μ and $Q_{-\nu-1}^\mu$ involves an admixture of P_ν^μ.

C. Double-integral representations

Combinations of the foregoing results give a number of double-integral representations for the associated Legendre functions according to the fractional relations

$$M_{\pm}^{\lambda'}K_3^{\lambda}x^{\nu}t^{\mu}F_{\nu}^{\mu}(z)=N_{\pm}(\nu+\lambda,\mu,\lambda')N'_{+}(\nu,\mu,\lambda)x^{\nu+\lambda}t^{\mu\pm\lambda'}F'^{\mu\pm\lambda'}_{\nu+\lambda}(z), \tag{140}$$

$$M_{\pm}^{\lambda'}P_3^{\lambda}x^{\nu}t^{\mu}F_{\nu}^{\mu}(z)=N_{\pm}(\nu-\lambda,\mu,\lambda')N'_{-}(\nu,\mu,\lambda)x^{\nu-\lambda}t^{\mu\pm\lambda'}F'^{\mu\pm\lambda'}_{\nu-\lambda}(z), \tag{141}$$

$$K_3^{\lambda}M_{\pm}^{\lambda'}x^{\nu}t^{\mu}F_{\nu}^{\mu}(z)=N'_{+}(\nu,\mu\pm\lambda',\lambda)N_{\pm}(\nu,\mu,\lambda')x^{\nu+\lambda}t^{\mu\pm\lambda'}F'^{\mu\pm\lambda'}_{\nu+\lambda}(z), \tag{142}$$

$$P_3^{\lambda}M_{\pm}^{\lambda'}x^{\nu}t^{\mu}F_{\nu}^{\mu}(z)=N'_{+}(\nu,\mu\pm\lambda',\lambda)N_{\pm}(\nu,\mu,\lambda')x^{\nu-\lambda}t^{\mu\pm\lambda'}F'^{\mu\pm\lambda'}_{\nu-\lambda}(z), \tag{143}$$

and similar relations for other products of the operators $M_{\pm}^{\lambda}$, K_3^{λ}, and P_3^{λ}. The appropriate definitions of the operators and the coefficients depend on the input functions. We will give only a few examples.

We first obtain a double integral for P_{ν}^{μ} using the operator $M_{+}^{\mu}K_3^{\nu}$. We start with (140) with $P_0^0=1$ as the input function. The action of K_3^{ν} gives P_{ν}^0, (135), where we have suppressed the factor x^{ν} in (140). Acting a second time with M_{+}^{μ} and suppressing the resulting factor t^{μ} gives, through (91),

$$P_{\nu}^{\mu}(z)=\frac{1}{(2\pi i)^2}e^{i\pi\nu}\Gamma(\mu+1)(z^2-1)^{\mu/2}$$
$$\times\int_{(1,z+,1)}\frac{dZ}{(Z-z)^{\mu+1}}\int_{(\infty,0+,\infty)}\frac{du}{u^{\nu+1}}\frac{1}{\sqrt{u^2+2Zu+1}} \tag{144}$$
$$=\frac{1}{(2\pi i)^2}e^{i\pi\nu}\Gamma(\mu+1)\left(\frac{z+1}{z-1}\right)^{\mu/2}$$
$$\times\int_{(0,1+,0)}\frac{dt}{(t-1)^{\mu+1}}\int_{(\infty,0+,\infty)}\frac{du}{u^{\nu+1}}\frac{1}{\sqrt{(u+1)^2+2tu(z-1)}}, \tag{145}$$

$\mathrm{Re}(\nu+1)>0$. The second form follows from the substitution $Z=1+(z-1)t$.

Note that the dependence of P_{ν}^{μ} on ν and μ is separated in the two integrals in (144) and (145). This will also be true in the following examples.

A similar calculation starting with $Q_0^0(z)$ and using (100) and (76) gives

$$Q_{\nu}^{\mu}(z)=\frac{1}{(2\pi i)^2}e^{i\pi(\nu+\mu)}\Gamma(\mu+1)(z^2-1)^{\mu/2}\int_{(\infty,z+,\infty)}\frac{dZ}{(Z-z)^{\mu+1}}$$
$$\times\int_{(\infty,0+,\infty)}\frac{du}{u^{\nu+1}}\frac{1}{\sqrt{u^2+2Zu+1}}\ln\frac{u+Z+\sqrt{u^2+2Zu+1}}{\sqrt{Z^2-1}}, \tag{146}$$

$\mathrm{Re}(\nu+1)>0$, $\mathrm{Re}(\nu+\mu+1)>0$.

If we consider $M_{+}^{\mu}M_{+}^{\nu}P_{\nu}^{-\nu}(z)$, use (120) and (91) to get an expression for P_{ν}^0 as in (125), and then use (91) again, we find that

$$P_{\nu}^{\mu}(z)=\frac{1}{(2\pi i)^2}2^{-\nu}\Gamma(\mu+1)(z^2-1)^{\mu/2}$$
$$\times\int_{(1,z+,1)}\frac{dZ'}{(Z'-z)^{\mu+1}}\int_{(1,Z'+,1)}\frac{dZ}{(Z-Z')^{\nu+1}}(Z^2-1)^{\nu} \tag{147}$$

$$= \frac{1}{(2\pi i)^2} 2^{-\nu}\Gamma(\mu+1)\left(\frac{z+1}{z-1}\right)^{\mu/2} \times \int_{(0,1+,0)} \frac{dt}{(t-1)^{\mu+1}} \int_{(0,1+,0)} \frac{du}{(u-1)^{\nu+1}} u^{\nu}\left(1+tu\frac{z-1}{2}\right)^{\nu}, \tag{148}$$

$\mathrm{Re}(\nu+1)>0$. Similarly, the expression for $M_+^{\mu} M_+^{-\nu-1} Q_{\nu}^{\nu+1}$ obtained by using (123) and (76) reduces to

$$e^{-i\pi\mu} Q_{\nu}^{\mu}(z) = \frac{1}{(2\pi i)^2} e^{i\pi(\mu-\nu)} 2^{\nu} \frac{\pi}{\sin\pi\nu} \Gamma(\mu+1)(z^2-1)^{\mu/2} \times \int_{(\infty,z+,\infty)} \frac{dZ}{(Z-z)^{\mu+1}} \int_{(\infty,Z+,\infty)} \frac{dZ'}{(Z'^2-1)^{\nu+1}} (Z'-Z)^{\nu} \tag{149}$$

$$= \frac{1}{2}\frac{1}{(2\pi i)^2} e^{i\pi(\mu-\nu)} \frac{\pi}{\sin\pi\nu} \Gamma(\mu+1)\left(\frac{z+1}{z-1}\right)^{\mu/2} \times \int_{(\infty,1+,\infty)} \frac{dt}{(t-1)^{\mu+1}} \int_{(\infty,1+,\infty)} \frac{du}{u^{\nu+1}} (u-1)^{\nu}\left(1+\frac{z-1}{2}tu\right)^{-\nu-1} \tag{150}$$

$$= -\frac{1}{2}\frac{1}{(2\pi i)^2} e^{i\pi(\mu-\nu)} \frac{\pi}{\sin\pi\nu} \Gamma(\mu+1)\left(\frac{z+1}{z-1}\right)^{\mu/2}\left(\frac{2}{z-1}\right)^{\nu+1} \times \int_{(0,1+,0)} dt \frac{t^{\nu+\mu}}{(t-1)^{\mu+1}} \int_{(0,1+,0)} du\, u^{\nu}(u-1)^{\nu}\left(1+\frac{2}{z-1}tu\right)^{-\nu-1}, \tag{151}$$

$\mathrm{Re}(\nu+\mu+1)>0$. The second expression follows from the first through the substitutions $Z'=1+u(Z-1)$, $Z=1+t(z-1)$. The last expression then follows from the replacements $u\to 1/u$, $t\to 1/t$, with a change in the phases so that $|\arg(t-1)|$, $|\arg(u-1)|\leqslant\pi$ in the final result.

As a final example, we obtain a double integral for Q_{ν}^{μ} using $K_3^{\nu} P_3^{\mu-1}$ and an input function $Q_{\mu-1}^{\mu}$, (119). Using (112) and (101), we find after some changes of variable that

$$e^{-i\pi\mu} Q_{\nu}^{\mu}\left(\frac{y}{\sqrt{y^2-1}}\right) = \frac{1}{(2\pi i)^2} e^{i\pi\nu}\sqrt{\pi}\frac{\pi}{\sin\pi\nu} \frac{\Gamma(\nu+1)\Gamma(\mu+1)}{\Gamma(\nu-\mu+1)\Gamma(\mu+\frac{1}{2})} 2^{-\nu-1}\left(\frac{2}{y-1}\right)^{-\nu} \times \int_{(\infty,1+,\infty)} \frac{dt}{(t-1)^{\nu+1}}\left(1+\frac{y-1}{2}t\right)^{-1/2} \times \int_{(0,1+,0)} \frac{du}{(u-1)^{\mu}} u^{\mu-1/2}\left(1+\frac{y-1}{2}tu\right)^{\mu-1/2}, \tag{152}$$

$\mathrm{Re}\,\mu>-\frac{1}{2}$.

X. REMARKS

The results obtained here demonstrate the utility of fractional operators in deriving relations for the associated Legendre functions F_{ν}^{μ}. Standard discussions[1–3] show that those functions give unitary representations of the Lie groups SO(2,1) or SO(3) for special values of ν and μ, with the groups typically acting as symmetry groups in applications where Legendre functions appear naturally. The operators $M_{\pm}$ in the Lie algebra of so(2,1) and K_3 and P_3 in its conformal extension generate changes in ν and μ in integer steps when acting on those representations. We have been concerned here only with realizations of the algebras through differential operators, and are able in

that context to define fractional operators which change ν and μ by arbitrary amounts. Thus, general functions P_ν^μ and Q_ν^μ can be constructed as in (144) and (146) starting with the trivial realizations $P_0^0=1$, $Q_0^0=\frac{1}{2}\ln[(z+1)/(z-1)]$ or from other special cases.

The results on Bessel functions derived in Ref. 5 using fractional operator methods can also be derived as limiting cases of results here. The connection occurs geometrically through a Wigner-Inönü contraction[7] in which we consider infinitesimal transformations in SO(2,1) near the apex of the hyperboloid H^2 at $z=\cosh\theta=1$. These are equivalent for θ sufficiently small to E(2) transformations in the tangent plane to H^2 at $\theta=0$. If we scale the angles with $\theta\to\vartheta/\nu$ and consider the limit $\nu\to\infty$, the associated Legendre equation (14), reduces to the hyperbolic Bessel equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\vartheta^2}+\frac{1}{\vartheta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}-\frac{\mu^2}{\vartheta^2}-1\right)Z_\mu(\vartheta)=0, \tag{153}$$

and the Bessel functions appear as confluent limits of the Legendre functions,

$$I_\mu(\vartheta)=\lim_{\nu\to\infty}\nu^\mu P_\nu^{-\mu}\left(\cosh\frac{\vartheta}{\nu}\right),\quad K_\mu(\vartheta)=\lim_{\nu\to\infty}\nu^{-\mu}e^{-i\pi\mu}Q_\nu^\mu\left(\cosh\frac{\vartheta}{\nu}\right), \tag{154}$$

Ref. 9, 7.8(1,4). In the same limit, the so(2,1) operators $M_\pm$ become multiples of the e(2) stepping operators $P_\pm$ used in Ref. 5,

$$M_+=-e^{i\phi}(\partial_\theta+i\coth\theta\,\partial_\phi)\to\nu\left(-t\partial_\vartheta+\frac{t^2}{\vartheta}\partial_t\right)=\nu P_+, \tag{155}$$

$$M_-=e^{-i\phi}(\partial_\theta-i\coth\theta\,\partial_\phi)\to\nu\left(\frac{1}{t}\partial_\theta+\frac{1}{\theta}\partial_t\right)=\nu P_-, \tag{156}$$

where $P=(P_1,P_2)$ is the translation operator in the plane. The generator M_3 of rotations around the axis of H^2 is the same as the generator J_3 of rotations in the tangent plane defined in Ref. 5, $M_3=J_3$. Upon scaling the group parameter or hyperbolic angle u in (62), with $u\to u/\nu$, we find that the fractional operators $M_\pm^\lambda$ transform as

$$M_\pm^\lambda=\frac{1}{2\pi i}e^{i\pi\lambda}\nu^\lambda\int_{(\infty,0+,\infty}\frac{\mathrm{d}u}{u^{\lambda+1}}e^{-uM_\pm/\nu}\xrightarrow[\nu\to\infty]{}\nu^\lambda P_\pm^\lambda. \tag{157}$$

The extra factors of ν are absorbed in the conformal limit, and relations given here for Legendre functions become relations for Bessel functions when the limit exists. As an example, the relation $M_+^\lambda t^\mu e^{-i\pi\mu}Q_\nu^\mu(\cosh\theta)=t^{\mu+1}e^{-i\pi(\mu+\lambda}Q_\nu^{\mu+\lambda}(\cosh\theta)$, which gives (74) for Legendre functions, becomes $P_+^\lambda t^\mu K_\mu(\vartheta)=t^{\mu+\lambda}K_{\mu+\lambda}(\vartheta)$ for $\theta=\vartheta/\nu$, $\nu\to\infty$, and gives

$$K_{\nu+\lambda}(\vartheta)=\frac{1}{2\pi i}e^{i\pi\lambda}\Gamma(\lambda+1)\int_{(\infty,0+,\infty)}\frac{\mathrm{d}u}{u^{\lambda+1}}\left(\frac{\vartheta^2}{\vartheta^2+2u\vartheta}\right)^{\mu/2}K_\mu(\sqrt{\vartheta^2+2u\vartheta}). \tag{158}$$

This is equivalent to Eq. 3.44 of Ref. 5 or, for $\mathrm{Re}\,\lambda<0$, to the known fractional integral, Ref. 6, 13.2(59).

The methods discussed here can clearly be generalized to other special functions and their associated groups,[1] for example, the Gegenbauer functions (this is where our development of the fractional operators actually started), Hermite or parabolic cylinder, Whittaker, Laguerre, and Jacobi functions. There are also intriguing second-order differential operators which have the properties of stepping operators in Lie algebras[4,12–15] and can be exponentiated and integrated formally to obtain fractional operators, but the explicit action of the exponentials is not known in general.

ACKNOWLEDGMENTS

This work was supported in part by the U. S. Department of Energy under Grant No. DE-FG02-95ER40896, and in part by the University of Wisconsin Graduate School with funds granted by the Wisconsin Alumni Reseach Foundation. The author would like to thank the faculty of the Institute for Advanced Study for their hospitality during the fall term of 1975 when the initial stages of this work were carried out, and the Aspen Center for Physics for its hospitality while parts of the final work were done.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 5 MAY 2003

On certain integrals that appear in conformal field theory

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(Received 26 January 2001; accepted 13 September 2001)

We consider several types of integrals that arise in the context of quantum field theory that factor into a holomorphic and antiholomorphic piece. This gives rise to a conformal block representations for some of the integrals. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1536020]

I. INTRODUCTION

In the framework of perturbative QCD at large Q^2 and low x, the conformal (global) group of transformations in the transverse coordinate space plays a crucial role. Indeed Lipatov and his collaborators[1] have derived the master equation for the derivative of the gluon structure function with respect to x by resuming the leading $(\alpha_s(\overline{Q^2})\log(1/x))^n$ terms at fixed $\alpha_s(\overline{Q^2})$. This derivative is a convolution in the transverse space of the gluon structure function times a conformal invariant kernel (BKKL kernel). All the relevant observables are then expressed as an expansion over the basis $E^{n,\nu}$ of the conformal eigenfunctions of this kernel. The integer n is the conformal spin and $i\nu$ corresponds to a continuous imaginary scaling dimension. In particular such expansions exist for the elastic off mass shell gluon-gluon amplitude corresponding to the exchange of the bare QCD hard Pomeron[1,2] and the conformal invariant triple Pomeron vertex.[3] For this purpose one is led following Ref. 1 to consider the eigenfunctions in a mixed representation which is obtained by a Fourier transform in two dimensions of $E^{n,\nu}$. To be more specific, these eigenfunctions in the coordinate space are the product of a holomorphic times an antiholomorphic function. Recently, it has been shown[2] that the answer is a sum of two products of a holomorphic times an antiholomorphic form. This was accomplished by noticing that the Fourier transform is the solution of a set of two linear differential equations one with respect to the complex variable and the other with respect to the complex conjugate variable. This structure of conformal blocks is already present in the computation of correlation functions in two dimensional conformal invariant quantum field theories.[4] Various theorems have been established for an integrand with integrable singularities at 0, 1 and ∞. In Ref. 2 a similar result seems to apply, as shown by the existence in this case of two differential equations. In the first part of this article we show that this is not a sheer coincidence but that similar theorems can apply for the bidimensional Fourier transform. As far as the triple conformal invariant Pomeron is concerned, specific analytic calculations have been done recently.[3] It turns out that this quantity is a peculiar case of a more general calculation involving a p-tuple conformally invariant integral in the complex space at a particular complex value of z (resp $\overline{z}$). The triple Pomeron corresponds to the case $z=1$ and $p=3$. Our second part is the derivation of this very general result. The key point is to find the set of two linear differential equations with respect to z and $\overline{z}$ of order $p+1$ which are obeyed by the p-tuple integral. The final answer will thus be a sum of conformal blocks, as expected, each block being the product of one of the $p+1$ solutions in z of the differential equation times the corresponding one in $\overline{z}$, in order to preserve the single valuedness of the solution. In our study, the system of

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linear equations is the one obeyed by the hypergeometric function ${}_{p+1}F_p(z)$. The case of degeneracy which is relevant for the calculation of the triple Pomeron vertex will be treated explicitly in a forthcoming paper.

II. BIDIMENSIONAL FOURIER TRANSFORMS

We begin this section with the following,

Lemma 1: For $0\leqslant x\leqslant y\leqslant \pi/2$, *let*

$$I_1=\int_0^{\pi/2}\left(\int_0^y e^{-R(\sin y-\sin x)}dx\right)dy.$$

Then $|I_1|\leqslant C_\epsilon R^{\epsilon-1}$, *for any* $0<\epsilon\leqslant 1$.

Proof: It follows from the mean value theorem and Jordan's lemma that for $0\leqslant x\leqslant y\leqslant \pi/2$, $\sin y-\sin x\geqslant(2/\pi)(\pi/2-y)(y-x)$, consequently,

$$\int_0^y e^{-R(\sin y-\sin x)}dx\leqslant\int_0^y e^{-R(2/\pi)(\pi/2-y)(y-x)}dx=\frac{\pi}{2R}\,\frac{1-e^{-(2R/\pi)(\pi/2-y)y}}{(\pi/2-y)}.$$

Substituting the above result into I_1 and then integrating by parts yields

$$I_1\leqslant\int_0^{\pi/2}\ln\left(\frac{\pi}{2}-y\right)e^{-(2R/\pi)(\pi/2-y)y}\left(\frac{\pi}{2}-2y\right)dy.$$

Since $|(\pi/2-y)^\epsilon\ln(\pi/2-y)|\leqslant K_\epsilon<\infty$ for $0\leqslant y\leqslant\pi/2$, $\epsilon>0$, we see that

$$\begin{aligned}I_1&\leqslant\frac{\pi}{2}K_\epsilon\int_0^{\pi/2}\left(\frac{\pi}{2}-y\right)^{-\epsilon}e^{-(2R/\pi)(\pi/2-y)y}dy\\&\leqslant\frac{\pi}{2}K_\epsilon\left(\frac{\pi}{4}\right)^{-\epsilon}\int_0^{\pi/4}e^{-(R/2)y}dy+\frac{\pi}{2}K_\epsilon\int_{\pi/4}^{\pi/2}\left(\frac{\pi}{2}-y\right)^{-\epsilon}e^{-(2R/\pi)(\pi/2-y)y}dy.\end{aligned}$$

Thus extending the region of integration in the first integral to the full semi-axis, then doing same thing to the second integral after replacing the second y in the exponential by $\pi/4$ and executing the change of variables $y_1=\pi/2-y$ yields

$$I_1\leqslant\frac{\pi}{2}\left(\frac{\pi}{4}\right)^{-\epsilon}\frac{2K_\epsilon}{R}+\frac{\pi}{2}K_\epsilon\left(\frac{2}{R}\right)^{1-\epsilon}\Gamma(1-\epsilon),$$

which gives the result.

With the above lemma we can now factorize certain double integrals. We will consider integrals of the form

$$I=\int\int_{\mathbb{C}\setminus[0,\infty)}f(t)\overline{g(t)}d^2t,$$

where $\mathbb{C}\setminus[0,\infty)$ is the complex plane cut along the real axis from zero to infinity. We will make the following assumptions about f and g.

(i) I converges.

(ii) $f(t)=\tilde f(t)e^{iqt}$, $g(t)=\tilde g(t)e^{iqt}$, $q\in\mathbb{R}$ where $\tilde f(t)$ and $\tilde g(t)$ are analytic for $t\in\mathbb{C}\setminus[0,\infty)$.

(iii) $k_f=|\int_0^\infty f(x)dx|<\infty$, $k_g=|\int_0^\infty g(x)dx|<\infty$.

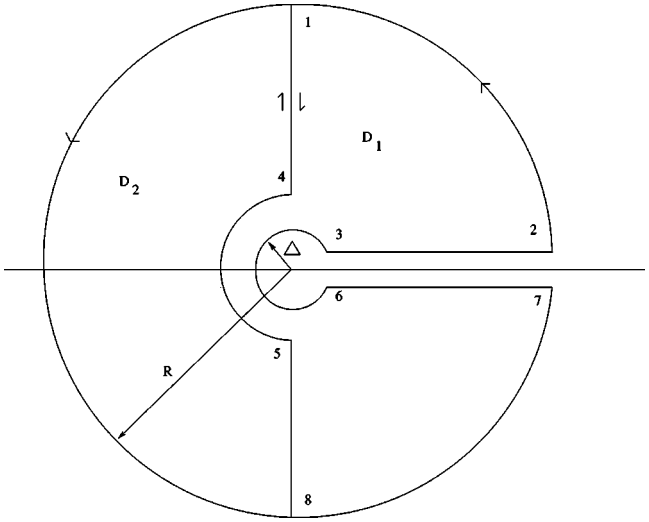

FIG. 1. Contour for $D_R\backslash[0,\infty)$.

(iv) $\lim_{R\to\infty} k_{\tilde{g}}(R)=0$, $\lim_{R\to\infty} k_{\tilde{f}}(R)=0$, and for ϵ small enough but positive $\lim_{R\to\infty} k_{\tilde{g}}(R)k_{\tilde{f}}(R)R^{1+\epsilon}=0$, where $k_{\tilde{g}}(R)=\max_{\theta\in[0,2\pi)}|\tilde{g}(\mathrm{Re}^{i\theta})|$ and $k_{\tilde{f}}(R)=\max_{\theta\in[0,2\pi]}|\tilde{f}(\mathrm{Re}^{i\theta})|$.

(v) Finally, $\lim_{r\to 0} k_{\tilde{f}}(r)r=0=\lim_{r\to 0} k_{\tilde{g}}(r)r$.

With the above assumptions $I=\lim_{R\to\infty} I_R$ where

$$I_R=\int\int_{D_R\backslash[0,R)} f(t)\overline{g(t)}d^2t,$$

with D_R being the disk of radius R. We proceed to cut $D_R\backslash[0,\infty)$ into the components indicated in Fig. 1. If we choose the point z_1 as the base point, then Stoke's Theorem implies that

$$I_R=\lim_{\Delta\to 0}\frac{i}{2}\int_{\partial D_1+\partial D_2} f_1(t)\overline{g(t)dt},$$

where ∂D_i, $i=1,2$, indicate the boundary of D_i, $i=1,2$, respectively, $f_1(t)=\int_{\Gamma_{1,t}} f(y)dy$, $\Gamma_{1,t}$ being the path followed from the point z_1 to t along the contour indicated on ∂D_1 or ∂D_2. Note that the contribution to I_R along Γ_{8541} on ∂D_2 cancels with the contribution of Γ_{1458} on ∂D_1. The integral

$$\left|\int_{\Gamma_{21}} f_1(t)\overline{g(t)}\ \overline{dt}\right|=\left|\int_0^{\pi/2} d\phi\int_{\phi}^{\pi/2} d\theta f(Re^{i\theta})\overline{g(Re^{i\phi})}\ e^{i(\theta-\phi)}R^2\right|$$

$$\leqslant k_{\tilde{g}}(R)k_{\tilde{f}}(R)R^2\int_0^{\pi/2} d\phi\int_{\phi}^{\pi/2} d\theta e^{-qR(\sin\theta-\sin\phi)},$$

which by Lemma 1 is bounded by

$$\leqslant k_{\tilde{g}}(R)k_{\tilde{f}}(R)R^{1+\epsilon}, \tag{1}$$

ϵ small but positive. Since

$$\int_{\Gamma_{18}} f_1(t)\overline{g(t)}\ \overline{dt} = \int_{\pi/2}^{3\pi/2} d\phi \int_{\pi/2}^{\phi} d\theta f(Re^{i\theta})\overline{g(Re^{i\phi})} e^{i(\theta-\phi)} R^2,$$

an argument similar to the one above results in a bound similar to (1). The integral

$$\left| \int_{\Gamma_{87}} f_1(t)\overline{g(t)}\ \overline{dt} \right| = \left| \int_{\Gamma_{87}} (f_7 + f_6 - f_7 + f_3 - f_6 + f_2 - f_3 + f_1 - f_2)\overline{g(t)dt} \right|,$$

where f_i means that the base point is a z_i, is bounded by

$$\leqslant c k_{\tilde{g}}(R) k_{\tilde{f}}(R) R^{1+\epsilon} + 2c k_f k_{\tilde{g}} + c r k_{\tilde{f}}(r) k_{\tilde{g}}(R) + c k_{\tilde{f}}(R) k_{\tilde{g}}(R).$$

The above inequalities also show that

$$\lim_{\Delta \to 0} \left| \int_{\Gamma_{63}} f_1(t)\overline{g(t)}\ \overline{dt} \right| = 0,$$

$$\left| \int_{\Gamma_{32}} (f_1 - f_2)\overline{g(t)}\ \overline{dt} \right| \leqslant c k_g k_{\tilde{f}}(R),$$

and

$$\lim_{\Delta \to 0} \left| \int_{\Gamma_{76}} f_1(t)\overline{g(t)}\ \overline{dt} - ((f_2 - f_3) + (f_6 - f_7) + f_7(t))\overline{g(t)}\ \overline{dt} \right| \leqslant c k_g k_{\tilde{f}}(R).$$

This leads to the following.

Lemma 2: Suppose f and g satisfy (i)–(v). Then,

$$\lim_{R \to \infty} \left| I_R - \lim_{\Delta \to 0} \left(\frac{i}{2} \int_{\Gamma_{76}} ((f_2 - f_3) + (f_6 - f_7))\overline{g(t)}\ \overline{dt} + \frac{i}{2} \int_{\Gamma_{32}} f_2(t)\overline{g(t)}\ \overline{dt} + \frac{i}{2} \int_{\Gamma_{76}} f_7(t)\overline{g(t)}\ \overline{dt} \right) \right| = 0.$$

We now consider the integral,

$$I = \int \int_{\hat{C}} t^{\gamma-1} \overline{t}^{\tilde{\gamma}-1} e^{i(\overline{q}t + q\overline{t})} d^2 t,$$

where $\hat{C}$ is the complex plane cut so as to make $\ln t$ well defined. By rotating and scaling the coordinate system we may write

$$I = q^{-\tilde{\gamma}} \overline{q}^{-\gamma} \hat{I},$$

where

$$\hat{I} = \int \int_{\mathbb{C} \setminus [0,\infty)} t^{\gamma-1} \overline{t}^{\tilde{\gamma}-1} e^{i(t + \overline{t})} d^2 t.$$

In the above integral the branch of the logarithm selected is such that $0 \leqslant \arg t < 2\pi$ and $\ln t$ is positive for $t > 1$. With $t = re^{i\theta}$ set

$$f(t) = t^{\gamma-1} e^{ir\cos\theta - r\sin\theta},$$

and

$$g(t)=t^{\bar{\tilde{\gamma}}-1}e^{-ir\cos\theta+r\sin\theta}.$$

Thus we find

$$\hat{I}=\int_0^\infty\int_0^{2\pi}r^{\gamma+\tilde{\gamma}-1}e^{i(\gamma-\tilde{\gamma})\theta}e^{2ri\cos\theta}dr\ d\theta,\quad q>0.$$

Since by stationary phase (Ref. 5, p. 101) $\int_0^{2\pi}e^{i(\gamma-\tilde{\gamma})\theta}e^{2ir\cos\theta}d\theta=O(1/\sqrt{r})$, we see that $\hat{I}$ converges uniformly for $0<\mathrm{Re}(\gamma+\tilde{\gamma})<\frac{1}{2}$ and thus defines, by Morera's theorem, an analytic function of γ and $\tilde{\gamma}$ for the values of these variables restricted to this domain.

We now consider the integral

$$I_R=\int\int_{D_R\setminus[0,R]}f(t)\overline{g(t)}d^2t,$$

with $0<\mathrm{Re}\ \gamma<\frac{1}{2}$, $0<\mathrm{Re}\,\tilde{\gamma}<\frac{1}{2}$ and $0<\mathrm{Re}(\gamma+\tilde{\gamma})<\frac{1}{2}$. If $\tilde{f}(t)=t^{\gamma-1}$ and $\tilde{g}(t)=t^{\bar{\tilde{\gamma}}-1}$, the conditions of Lemma 2 are satisfied and, taking into account the increment in the phase due to the cut, we find

$$\hat{I}=\lim_{R\to\infty}I_R=\frac{i}{2}(1-e^{2\pi i\gamma})e^{-2\pi i\tilde{\gamma}}\int_0^\infty x^{\gamma-1}e^{ix}dx\int_0^\infty y^{\tilde{\gamma}-1}e^{iy}dy+\frac{i}{2}(e^{2\pi i(\gamma-\tilde{\gamma})}-1)I(\gamma,\tilde{\gamma}),$$

where

$$I(\gamma,\tilde{\gamma})=\int_0^\infty dv\int_v^\infty du\,u^{\gamma-1}v^{\tilde{\gamma}-1}e^{i(u+v)}.$$

With the first two integrals replaced by their representation [Ref. 6, Formula (33), p. 12] in terms of gamma functions we find

$$\hat{I}=\frac{i}{2}(1-e^{2\pi i\gamma})e^{-2\pi i\tilde{\gamma}}e^{i(\gamma+\tilde{\gamma})\pi/2}\Gamma(\gamma)\Gamma(\tilde{\gamma})+\frac{i}{2}(e^{2\pi i(\gamma-\tilde{\gamma})}-1)I_1.$$

The first term can be analytically extended to $\gamma,\tilde{\gamma}\neq 0,-1,-2,\ldots$. To analyze the second term we break it up into three integrals over the following regions $R_1=\{(v,u),0\leqslant v<1,v\leqslant u<1\}$, $R_2=\{(u,v),0\leqslant v<1,1\leqslant u\leqslant\infty\}$ and $R_3=\{(u,v),1\leqslant v<\infty,v\leqslant u<\infty\}$. It is easy to see that I_1 can be analytically extended to $\gamma\neq 0,-1,-2,\ldots$, $\gamma+\tilde{\gamma}\neq 0,-1,-2,\ldots$, and $I_2=\int_0^1 v^{\tilde{\gamma}}e^{iv}\times du\int_1^\infty u^{\gamma-1}e^{iu}du$ can be extended to the region $\mathrm{Re}\,\gamma<1$, $\tilde{\gamma}\neq 0,-1,-2,\ldots$. For $\mathrm{Re}\,\gamma<1$,

$$|I_3|=\left|\int_1^\infty v^{\tilde{\gamma}-1}e^{iv}\int_v^\infty u^{\gamma-1}e^{iu}dudv\right|\leqslant C\int_1^\infty v^{\mathrm{Re}(\tilde{\gamma}+\gamma)-2}dv,$$

which converges uniformly for $\mathrm{Re}(\gamma+\tilde{\gamma})<1$. Consequently I_3 can be extended to $\mathrm{Re}\,\gamma<1$, $\mathrm{Re}(\gamma+\tilde{\gamma})<1$. This implies that $\hat{I}$ can be extended to the region $\mathrm{Re}(\gamma)<1$, $\mathrm{Re}(\gamma+\tilde{\gamma})<1$, $\gamma,\tilde{\gamma}\neq 0,-1,-2,\ldots$. For $\mathrm{Re}\,\gamma>0$ we can interchange the order of integration in $I(\gamma,\tilde{\gamma})$; then $\mathrm{Re}\,\gamma>0$, $0<\mathrm{Re}(\gamma+\tilde{\gamma})<1$, implies that $\mathrm{Re}\,\tilde{\gamma}<1$ so that the above arguments can be reapplied. Consequently we have shown the following

Theorem 1: *For* $0<\mathrm{Re}(\gamma+\tilde{\gamma})<1$, $\gamma,\tilde{\gamma}\neq 0,-1,-2,\ldots$, $q\neq 0$,

$$I=\frac{i}{2}(1-e^{2\pi i\gamma})e^{-2\pi i\tilde{\gamma}}q^{-\tilde{\gamma}}\bar{q}^{-\gamma}e^{i(\gamma+\tilde{\gamma})\pi/2}\Gamma(\gamma)\Gamma(\tilde{\gamma})+\frac{i}{2}(e^{2\pi i(\gamma-\tilde{\gamma})}-1)I(\gamma,\tilde{\gamma}).$$

In particular, if $\tilde{\gamma}-\gamma=n$, n an integer, the integral becomes

$$I=\sin(\pi\gamma)e^{in\pi/2}q^{-\tilde{\gamma}}\overline{q}^{-\gamma}\Gamma(\gamma)\Gamma(\tilde{\gamma}).$$

The next integral we will consider arises in the context of QCD and is given by

$$I=\int\int d^2z\,\frac{e^{i/2(q\overline{z}+\overline{q}z)}}{(z^2-\rho^2/4)^{u+1/2}(\overline{z}^2-\overline{\rho}^2/4)^{\hat{u}+1/2}},$$

where $u=-v_1+iv_2$, $\hat{u}=\hat{v}_1+i\hat{v}_2$, and $\mathrm{Re}(q\overline{\rho})\neq 0$. With an appropriate rotation and scaling the above integral becomes

$$I=\frac{1}{(\rho^2/4)^u(\overline{\rho}^2/4)^{\hat{u}}}I_1$$

with

$$I_1=\int_{\hat{C}}\int\frac{d^2z\;\; e^{i/2(q_1\overline{z}+\overline{q}_1z)}}{(z^2-1)^{u+1/2}(\overline{z}^2-1)^{\hat{u}+1/2}},$$

and $q_1=q\,\overline{\rho}/4$. With this notation $\hat{\mathbb{C}}$ in the above integral is the complex plane cut from $[1,\infty e^{i\phi})$ and from $(-\infty e^{-i\phi},-1]$ where $\phi=\arg(q_1)$. With the above cuts we use the branch of the logarithm so that the phase of z^2-1 is equal to zero for $z>1$ and π for $-1<z<1$ (see Ref. 7, p. 166). With $z=re^{i\theta}$ the argument of the exponential gives $(i/2)\,r|q_1|\cos(\theta-\phi)$. Thus elementary methods including stationary phase (Ref. 5, p. 101) shows that the above integral is uniformly convergent and defines by Morera's theorem an analytic function in the variables u and $\hat{u}$ for $-\frac{1}{4}<\mathrm{Re}(u+\hat{u})<1$ and $q_1\neq 0$. Furthermore, in this region the integral is also continuous in q_1. We restrict u, $\hat{u}$ and q_1 to the region $-\frac{1}{2}<\mathrm{Re}\;u,\mathrm{Re}\;\hat{u}<\frac{1}{2}$, $\mathrm{Re}q_1>0$ and consider the integral

$$I_R=\int_{\hat{D}_R}\int\frac{d^2ze^{i/2(\overline{q}_1z+q_1\overline{z})}}{(z^2-1)^{u+1/2}(\overline{z}^2-1)^{\hat{u}+1/2}}.$$

Using Stoke's theorem we integrate over ∂D_1 and ∂D_2 given in Fig. 2 with $\tilde{f}=(z^2-1)^{-(u+1/2)}$ and $\tilde{g}=(z^2-1)^{-(\hat{u}+1/2)}$ to find

$$I_R=\frac{i}{2}\oint_{\partial D_1+\partial D_2}f_1(z)\overline{g(z)}\;\overline{dz}.$$

The conditions on u and $\hat{u}$ are such that hypotheses (i), (ii), (iv), and (v) of Lemma 2 follow almost immediately. To verify (iii) for the above functions we begin by showing that $\left|\int_{\Gamma_{45}}\overline{g(z)dz}\right|$ where $z=1+re^{i\phi}$ is finite. Observe that

$$\left|\int_0^b\overline{g}\,\overline{dz}\right|<C_1\int_0^b r^{-\mathrm{Re}\,\hat{u}-1/2}dr<\infty,\;\;\mathrm{Re}\,\hat{u}<\frac{1}{2},$$

and using integration by parts that

$$\left|\int_b^\infty\overline{g(z)dz}\right|<C_2\frac{b^{-(2\mathrm{Re}\,\hat{u}+1)}}{|q_1|}<\infty,\;\;-\frac{1}{2}<\mathrm{Re}\,\hat{u},$$

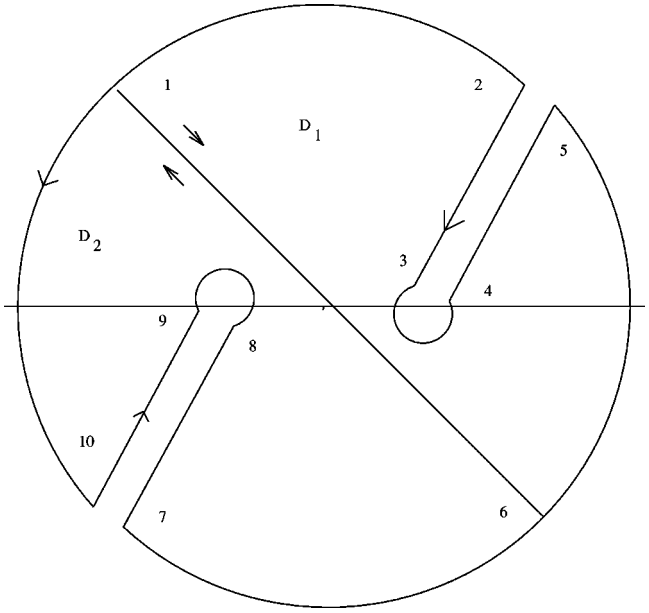

FIG. 2. Contour for Example 2.

for constants C_1 and C_2 independent of R. Applying the above reasoning to f on Γ_{45} shows that for $-\frac{1}{2}<\mathrm{Re}\ u$, $\mathrm{Re}\ \hat{u}<\frac{1}{2}$, (iii) is satisfied on this part of the contour. A similar argument and the fact that z appears as a single valued function in the exponential shows that $|\int_{\Gamma_{23}}\overline{g(z)dz}|$ and $|\int_{\Gamma_{23}}f(z)dz|$ are also finite. On Γ_{109}, with the phase of z^2-1 given as above, the previous arguments can be applied to show that the integrals $|\int_{\Gamma_{109)}}\overline{g(z)dz}|$ and $|\int_{\Gamma_{109}}f(z)dz|$ which are finite. Similar arguments can be applied to the integrals on Γ_{87}. Thus Lemma 2 implies that

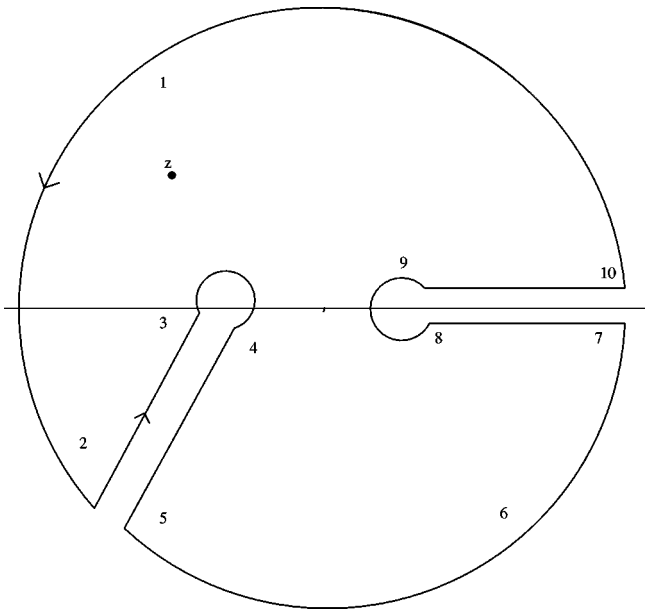

FIG. 3. Contour for Eq. (26).

$$I=\lim_{R\to\infty}\frac{i}{2}\left[\int_{\Gamma_{54}}(f_2-f_5)\overline{g(z)}d\overline{z}+\int_{\Gamma_{54}}f_5\overline{g(z)}d\overline{z}+\int_{\Gamma_{32}}f_2\overline{g(z)}d\overline{z}\right]$$
$$+\lim_{R\to\infty}\frac{i}{2}\left[\int_{\Gamma_{87}}(f_{10}-f_7)\overline{g(z)}d\overline{z}+\int_{\Gamma_{87}}f_7\overline{g(z)}d\overline{z}+\int_{\Gamma_{109}}f_{10}\overline{g(z)}d\overline{z}\right].$$

From Ref. 7, p. 167, Eq. (6), with $\overline{q_1}=|q_1|e^{-i\phi}$,

$$\lim_{R\to\infty}(f_5-f_2)=\frac{i\pi\Gamma\left(\frac{1}{2}\right)(\overline{q_1}/2)^u}{\Gamma\left(u+\frac{1}{2}\right)}H^{(1)}_{-u}(\overline{q_1}),$$

and

$$\lim_{R\to\infty}(f_7-f_{10})=\frac{i\pi\Gamma\left(\frac{1}{2}\right)(\overline{q_1}/2)^u}{\Gamma\left(u+\frac{1}{2}\right)}H^{(2)}_{-u}(\overline{q_1}).$$

Likewise, since $-\frac{1}{2}<\mathrm{Re}\,u,\ \mathrm{Re}\,\hat{u}<\frac{1}{2}$,

$$\lim_{R\to\infty}\int_{\Gamma_{45}}\overline{g(z)}d\overline{z}=\int_0^\infty\frac{e^{i\hat{q}_1e^{i\phi}(1+re^{-i\phi})}e^{-i\phi}}{(re^{-i\phi})^{\hat{u}+1/2}(2+re^{-i\phi})^{\hat{u}+1/2}}dr$$
$$=-\frac{e^{-i\pi/2}\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2}-\hat{u}\right)(q_1/2)^{\hat{u}}}{2}H^{(1)}_{\hat{u}}(q_1),$$

and

$$\lim_{R\to\infty}\int_{\Gamma_{87}}\overline{g(z)}d\overline{z}=\frac{e^{i\pi/2}\Gamma\left(\frac{1}{2}\right)(q_1/2)^{\hat{u}}\Gamma\left(\frac{1}{2}-\hat{u}\right)}{2}H^{(2)}_{\hat{u}}(q_1),$$

so that

$$I_1=\frac{i\pi}{4}\frac{\Gamma(1/2-\hat{u})}{\Gamma(1/2+u)}\left(\frac{q_1}{2}\right)^{\hat{u}}\left(\frac{\overline{q_1}}{2}\right)^u\times[H^{(1)}_{-u}(\overline{q_1})H^{(1)}_{\hat{u}}(q_1)-H^{(2)}_{-u}(\overline{q_1})H^{(2)}_{\hat{u}}(q_1)]$$
$$+4\sin\pi(\hat{u}-u)\sin(\pi(\hat{u}-u)-2|q_1|\cos\phi)e^{i\phi(\hat{u}-u)}I(|q_1|),\quad q_1\neq 0,\tag{2}$$

where

$$I(|q_1|)=\int_0^\infty\int_y^\infty\frac{e^{i|q_1|(r+y)}}{(r(re^{i\phi}+2)^{u+1/2})(y(ye^{-i\phi}+2)^{\hat{u}+1/2})}dr\ dy.$$

Using an argument similar to the one given above but more tedious it can be shown that $I(\hat{q}_1)$ has an analytic extension $-\frac{1}{4}<\mathrm{Re}\,u+\mathrm{Re}\,\hat{u}<1$, $u,\hat{u}\neq\frac{1}{2}+n,n=0,1,\ldots$. Thus we have shown the following.

Theorem 2: *For* $u=-v_1+iv_2$, $\hat{u}=v_1+iv_2$, $u,\hat{u}\neq\frac{1}{2}+n,n=0,1,\ldots$, I_1 *is given by Eq. (2). In particular, if* $v_1=n/2$, $v_2\neq 0$, *then*

$$I_1=\frac{i\pi}{4}\frac{\Gamma(\frac{1}{2}-\hat{u})}{\Gamma(\frac{1}{2}+u)}\left(\frac{q_1}{2}\right)^{\hat{u}}\left(\frac{\overline{q_1}}{2}\right)^{u}[H^{(1)}_{-u}(\overline{q_1})H^{(1)}_{\hat{u}}(q_1)-H^{(2)}_{-u}(\overline{q_1})H^{(2)}_{\hat{u}}(q_1)],\quad q_1\neq 0. \tag{3}$$

III. A p-UPLE CONFORMAL INTEGRAL AND APPLICATIONS

We now consider the integral

$$\begin{aligned}&I_{p+1}(a_0,\ a_i,\ b_i;\ \tilde{a}_0,\ \tilde{a}_i,\ \tilde{b}_i;\ z,\overline{z})\\&=\left(\frac{1}{2i}\right)^p\int\prod_{i=1}^{p}d^2z_i\ \ (z_i)^{a_i-1}(\overline{z_i})^{\tilde{a}_i-1}(1-z_i)^{b_i-a_i-1}(1-\overline{z_i})^{\tilde{b}_i-\tilde{a}_i-1}\\&\times\left(1-\left(\prod_{i=1}^{p}z_i\right)z\right)^{-a_0}\left(1-\left(\prod_{i=1}^{p}\overline{z_i}\right)\overline{z}\right)^{-\tilde{a}_0}.\end{aligned} \tag{4}$$

We will analyze the case when $a_i,\tilde{a}_i,b_i$ and $\tilde{b}_i$ obey the following conditions:

Condition C: For $i=0,...,p$ and $j=1,...,p$,

(a) $b_j,\tilde{b}_j,a_i,\tilde{a}_i\notin\mathbf{Z}$.
(b) $a_i-a_j,\tilde{a}_i-\tilde{a}_j,b_{i\neq 0}-b_j,\tilde{b}_{i\neq 0}-\tilde{b}_j,\ i\neq j\ \notin\mathbf{Z}$.
(c) $a_i-b_j,\tilde{a}_i-\tilde{b}_j\notin\mathbf{Z}$.
(d) $a_i-\tilde{a}_i,b_j-\tilde{b}_j\in Z$.

With $a^j=(a_1,...,a_j)$, $b^j=(b_1,...,b_j)$, $\tilde{a}^j=(\tilde{a}_1,...,\tilde{a}_j)$, $\tilde{b}^j=(\tilde{b}_1,...,\tilde{b}_j)$, and $I_1(a_0,\tilde{a}_0,z,\overline{z})=(1-z)^{-a_0}(1-\overline{z})^{-\tilde{a}_0}$ the above integral can be recast as the iterated integral,

$$\begin{aligned}&I_{p+1}(a_0,\ a^p,\ b^p;\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p;\ z,\overline{z})\\&=\left(\frac{1}{2i}\right)\int d^2z_p(z_p)^{a_p-1}(1-z_p)^{b_p-a_p-1}(\overline{z_p})^{\tilde{a}_p-1}\\&\times(1-\overline{z_p})^{\tilde{b}_p-\tilde{a}_p-1}I_p(a_0,\ a^{p-1},\ b^{p-1};\ \tilde{a}_0,\ \tilde{a}^{p-1},\tilde{b}^{p-1};\ z\ \ z_p,\overline{z}\ \overline{z_p}).\end{aligned} \tag{5}$$

The computation of this integral has already been done for $p=0$ and $p=1$ by various authors[4] in the case when $a_i=\tilde{a}_i$, $b_i=\tilde{b}_i$ and $a_0=\tilde{a}_0$. The result is a sum of a product of hypergeometric functions of z with its antiholomorphic part of argument $\overline{z}$ exhibiting the conformal block structure. Lipatov[1] has given the general form for $p=1$ without the restrictions on the $\tilde{a}_i$, $\tilde{a}_0$, $\tilde{b}_i$.

We propose to give the exact analytic structure of I_{p+1} for any positive integer value of p by showing that I_{p+1} obeys two linear differential equations of order $p+1$, namely,

$$O_z^{p+1}(a_0,\ a^p,\ b^p)I_{p+1}(a_0,\ a^p,\ b^p;\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p;\ z,\ \overline{z})=0,$$

and

$$O_{\overline{z}}^{p+1}(\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)I_{p+1}(a_0,\ a^p,\ b^p;\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p;\ z,\ \overline{z})=0,$$

where O_z^{p+1} (resp. $O_{\overline{z}}^{p+1}$) is the differential operator of order $p+1$ defining the hypergeometric function ${}_{p+1}F_p(a_0,\ a^p,\ b^p,\ z)$ [(resp.) ${}_{p+1}F_p(\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p,\ \overline{z})$]. In particular,

$$O_z^{p+1}=\frac{\partial}{\partial z}\prod_{i=1}^{p}\left(z\frac{\partial}{\partial z}+b_i-1\right)-\prod_{i=0}^{p}\left(z\frac{\partial}{\partial z}+a_i\right), \tag{6}$$

and

$$O_z^{p+1}=\frac{\partial}{\partial\overline{z}}\prod_{i=1}^{p}\left(\overline{z}\frac{\partial}{\partial\overline{z}}+\tilde{b}_i-1\right)-\prod_{i=0}^{p}\left(\overline{z}\frac{\partial}{\partial\overline{z}}+\tilde{a}_i\right). \tag{7}$$

The general solution of this system of differential equations is

$$I_{p+1}(z,\ \overline{z})=\sum_{i,j=0}^{p}\ \lambda_{ij}^{(p+1)}\ u_i^{p+1}\ (z)\ \tilde{u}_j^{p+1}\ (\overline{z}),$$

where $u_i^{p+1}(a_0,\ a^p,\ b^p,\ z)$ [resp. $\tilde{u}_j^{p+1}(\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p,\ \overline{z})$] is any of the $p+1$ independent solutions of the differential equation,

$$O_z^{p+1}\varphi_j(z)=0,\quad j=0,...,\ p,$$

namely,

$$u_0^{p+1}(a_0,\ a^p,\ b^p,\ z)={}_{p+1}F_p(a_0,\ a^p,\ b^p,\ z),$$

and

$$u_j^{p+1}(a_0,\ a^p,\ b^p,\ z)=z^{1-b_j}\,{}_{p+1}F_p(a_0-b_j+1,\ a_i-b_j+1,\ 1+b_i-b_j,\ 2-b_j;\ z). \tag{8}$$

Since the solution we are looking for has to be monovalued in $z\overline{z}$, the λ_{ij}'s have to be diagonal provided none of the differences b_i-b_j is an integer. Thus the general solution reduces to

$$\begin{aligned}&I_{p+1}(a_0,\ a^p,\ b^p;\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p;\ z,\overline{z})\\&\quad=\sum_{j=0}^{p}\lambda_j^{p+1}(a_0,\ a^p,\ b^p;\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)u_j^{p+1}(a_0,\ a^p,\ b^p;\ z)\tilde{u}_j^{p+1}(\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p;\ \overline{z})\end{aligned} \tag{9}$$

which exhibits a conformal block structure.

The $p+1$ unknown constants $\lambda_j(a_0,\ a^p,\ b^p,\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)$ are readily obtained by identifying the different behavior of the solution I_{p+1} near $z=0$.

At this stage we consider a generalized Euler function,[4]

$$B_{\alpha,\ \beta;\ \tilde{\alpha},\ \tilde{\beta}}=\frac{1}{2i}\int d^2t\ \ t^{\alpha-1}(1-t)^{\beta-1}(\overline{t})^{\tilde{\alpha}-1}(1-\overline{t})^{\tilde{\beta}-1},$$

which is defined and analytic for $\mathrm{Re}(\alpha+\tilde{\alpha})>0$, $\mathrm{Re}(\beta+\tilde{\beta})>0$, and $\mathrm{Re}(\alpha+\tilde{\alpha}+\beta+\tilde{\beta})<2$. Using arguments similar to those given in the previous section the above integral can be evaluated so that for $\alpha-\tilde{\alpha},\ \beta-\tilde{\beta}$ integer,

$$B_{\alpha,\ \beta;\ \tilde{\alpha},\ \tilde{\beta}}=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}\ \frac{\Gamma(\tilde{\alpha})\Gamma(\tilde{\beta})}{\Gamma(\tilde{\alpha}+\tilde{\beta})}\ \frac{\sin\pi\tilde{\alpha}\ \sin\pi\tilde{\beta}}{\sin\pi(\tilde{\alpha}+\tilde{\beta})}. \tag{10}$$

Note that since $\alpha-\tilde{\alpha}$ and $\beta-\tilde{\beta}$ are integer,

$$\frac{\sin\pi\tilde{\alpha}\ \sin\pi\tilde{\beta}}{\sin\pi(\tilde{\alpha}+\tilde{\beta})}\equiv\frac{\sin\pi\alpha\ \sin\pi\beta}{\sin\pi(\alpha+\beta)}.$$

To find λ_0^{p+1}, set $z=0$ in (4) in which case the integral is readily obtained since it factorizes. Thus,

$$\lambda_0^{p+1}(a_0,\ a^p,\ b^p,\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)=\prod_{i=1}^{p} B_{a_i,\ b_i-a_i;\ \tilde{a}_i,\ \tilde{b}_i-\tilde{a}_i}, \tag{11}$$

which is a_0, $\tilde{a}_0$ independent.

To find λ_j^{p+1}, set $z_j=[\Pi_{k=1,k\neq j}^{p} z_k z]^{-1} t$ and observe that

$$dz_j\ (z_j)^{a_j-1}(1-z_j)^{b_j-a_j-1}\left(1-\left(\prod_{i=1}^{p} z_i\right)z\right)^{-a_0}$$
$$=z^{1-b_j}(dt)\ t^{a_j-1}(1-t)^{-a_0}\left(\left(\prod_{k=1,k\neq j}^{p} z_k\right)z-t\right)^{b_j-a_j-1}\prod_{k=1,k\neq j}^{p}(z_k)^{1-b_j}.$$

In a neighborhood of $z=0$ we find

$$I_{p+1}\sim z^{1-b_j}(\overline{z})^{1-\tilde{b}_j}\left(\frac{1}{2i}\right)^p\int d^2t\ t^{b_j-2}(1-t)^{-a_0}\ \overline{t}^{\tilde{b}_j-2}(1-\overline{t})^{-\tilde{a}_0}$$
$$\times\prod_{k=1,k\neq j}^{p} d^2z_k(z_k)^{a_k-b_j}(1-z_k)^{b_k-a_k-1}(\overline{z_k})^{\tilde{a}_k-\tilde{b}_j}(1-\overline{z_k})^{\tilde{b}_k-\tilde{a}_k-1}(-1)^{b_j-\tilde{b}_j-a_j+\tilde{a}_j}.$$

Thus,

$$\lambda_j^{p+1}(a_0,a^p,b^p,\tilde{a}_0,\tilde{a}^p,\tilde{b}^p)=(-1)^{b_j-\tilde{b}_j-a_j+\tilde{a}_j}B_{b_j-1,\ -a_0+1;\tilde{b}_j-1,\ -\tilde{a}_0+1}$$
$$\times\prod_{i=1,i\neq j}^{p} B_{a_i-b_j+1,\ b_i-a_i;\tilde{a}_i-\tilde{b}_j+1,\tilde{b}_i-\tilde{a}_i}. \tag{12}$$

We now give some lemmas which will help prove that I_{p+1} has the form indicated above. Define

$$H_j^p(a_0,\ a^p,\ b^p,\ z,\ z_p)=(z_p)^{a_p-1}(1-z_p)^{b_p-a_p-1}u_j^p(a_0,\ a^{p-1},\ b^{p-1},\ zz_p),$$

and

$$K_j^p(a_0,\ a^p,\ b^p,\ z,\ z_p)=(z_p)^{a_p-1}(1-z_p)^{b_p-a_p+1}u_j^p(a_0,\ a^{p-1},\ b^{p-1},\ zz_p).$$

Lemma 3: Suppose condition C is satisfied. Then,

$$O_z^{p+1}\ H_0^{(p)}(a_0,\ a^p,\ b^p,\ z,\ z_p)=-\prod_{i=0}^{p-1}(a_i)\frac{\partial}{\partial z_p}K_0^p(a_0+1,\ a^p+1,\ b^p,\ z,\ z_p), \tag{13}$$

and for $j=1,...,p-1$,

$$O_z^{p+1}\ H_j^{(p)}(a_0,\ a^p,\ b^p,\ z,\ z_p)=-\prod_{i=0}^{p-1}(a_i-b_j+1)\frac{\partial}{\partial z_p}K_j^p(a_0+1,\ a^p+1,\ b^p,\ z,\ z_p). \tag{14}$$

Proof: Since

$$\left(z\frac{\partial}{\partial z}+a_i\right)\ {}_{p+1}F_p(a_i,\ b_i,\ z)=a_i\ {}_{p+1}F_p(a_i+1,\ b_i,\ z),$$

$$\left(z\frac{\partial}{\partial z}+b_i-1\right)\ {}_{p+1}F_p(a_i,\ b_i,\ z)=(b_i-1)\ {}_{p+1}F_p(a_i,\ b_i-1,\ z),$$

and

$$\frac{\partial}{\partial z}\,{}_{p+1}F_p(a_i,\ b_i,\ z)=a_0\prod_{k=1}^{p}\frac{a_k}{b_k}\,{}_{p+1}F_p(a_i+1,\ b_i+1,\ z),$$

Eq. (12) now follows after some algebra. Equation (13) similarly follows from the identities

$$\left(z\frac{\partial}{\partial z}+a_i\right)z^{1-b_j}\,{}_{p+1}F_p(a_i-b_j+1,\ 1+b_i-b_j,2-b_j\ \ z)$$
$$=(a_i-b_j+1)z^{1-b_j}\,{}_{p+1}F_p(a_i-b_j+2,\ 1+b_i-b_j,2-b_j,\ \ z),$$

$$\left(z\frac{\partial}{\partial z}+b_i-1\right)z^{1-b_j}\,{}_{p+1}F_p(a_i-b_j+1,\ 1+b_i-b_j,2-b_j,\ \ z)$$
$$=(b_i-b_j)z^{1-b_j}\,{}_{p+1}F_p(a_i-b_j+1,\ b_i-b_j,2-b_j\ \ z),$$

$$\left(z\frac{\partial}{\partial z}+b_j-1\right)z^{1-b_j}\,{}_{p+1}F_p\Big((a_i-b_j+1,\ 1+b_i-b_j,2-b_j,\ \ z)$$
$$=\left(\frac{(a_0-b_j+1)\Pi_{k=1}^{p}(a_i-b_j+1)}{(2-b_j)\Pi_{k=1}^{p}(b_i-b_j+1)}\right)z^{2-b_j}\,{}_{p+1}F_p(a_i-b_j+2,\ b_i-b_j+2,3-b_j\ \ z),$$

and

$$\frac{\partial}{\partial z}z^{1-b_j}\,{}_{p+1}F_p(a_i-b_j+1,\ b_i-b_j+1,2-b_j,\ \ z)$$
$$=(1-b_j)z^{-b_j}\,{}_{p+1}F_p(a_i-b_j+1,\ b_i-b_j+1,1-b_j\ \ z).$$

□

Let $\hat{I}_{p+1}$ be given for $0<|z|<1$ by Eqs. (9), (11), and (12) where we assume that a^p and b^p satisfy condition C. Since for $0<|z|<1$ the hypergeometric functions in $\hat{I}_{p+1}$ are defined by their series representation we seek a continuation of $\hat{I}_{p+1}$ to $|z|>1$. It follows from the Mellin-Barnes representation for ${}_{p+1}F_p(a_0,a^p,b^p,z)$ (Ref. 8, p. 149) that for $0<\arg\ z<2\pi$

$${}_{p+1}F_p(a_0,a^p,b^p,z)=\frac{\Pi_{i=1}^{p}\Gamma(b_i)}{\Pi_{i=0}^{p}\Gamma(a_i)}\sum_{j=0}^{p}\ \Gamma(a_j)\frac{\Pi_{\substack{k=0\\k\neq j}}^{p}\Gamma(a_k-a_j)}{\Pi_{k=1}^{p}\Gamma(b_k-a_j)}\left(\frac{e^{i\pi}}{z}\right)^{a_j}$$
$$\times\ {}_{p+1}F_p\left(a_j,1+a_j-b_i,1+a_j-a_i,\frac{1}{z}\right).\tag{15}$$

The following lemma will be useful in what follows:

Lemma 4: Suppose the points x_i and y_j, $i=0,...,p$, $j=1,\ldots p$, are distinct and none are equal to one. Then,

$$B_{n,k}=\prod_{i=1}^{p}\frac{1-x_i}{1-y_i}+\sum_{j=1}^{p}\frac{(1-x_n)(1-x_k)(x_0-y_j)(y_j-x_j)}{(1-y_j)(1-x_0)(y_j-x_n)(y_j-x_k)}\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{(x_i-y_j)}{(y_i-y_j)}=\frac{u_n\prod_{i=0}^{p}(u_k-u_i)}{u_0\prod_{i=1}^{p}(u_k-z_i)}\delta_{n,k}, \tag{16}$$

where $z_k=y_k-1$ *and* $u_i=x_i-1$.

Proof: $B_{n,k}$ is equal to

$$B_{n,k}=\prod_{i=1}^{p}\frac{u_i}{z_i}+\sum_{j=1}^{p}\frac{u_nu_k(u_0-z_j)(z_j-u_j)}{z_ju_0(z_j-u_n)(z_j-u_k)}\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{(u_i-z_j)}{(z_i-z_j)}.$$

Write $B_{n,k}\prod_1^p z_i/u_i=S_{n,k}$, where

$$S_{n,k}=1-\lambda\sum_{j=1}^{p}\frac{(z_j-u_0)(z_j-u_j)}{z_j(z_j-u_n)(z_j-u_k)}\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{(u_i-z_j)}{(z_i-z_j)},$$

and $\lambda=(u_ku_n/u_0)\prod_{i=1}^{p}z_i/u_i$. The function

$$f(z)=\lambda\frac{(z-u_0)}{z(z-u_n)(z-u_k)}\prod_{i=1}^{p}\frac{(z-u_i)}{(z-z_i)}$$

behaves as z^{-2} for large z, and by hypothesis has simple poles at $z=z_j$ and $z=0$. If $n=k$, then there is one extra simple pole at $z=u_k$. Cauchy's theorem says the sum of the residues is zero and the evaluation of the residues gives the result. □

With $s(a_i)=\sin\pi a_i$ we now prove the following.

Lemma 5: Suppose a_0, $\tilde{a}_0$, a^p, $\tilde{a}^p$, $\tilde{b}^p$ *and* b^p *satisfy condition* **C**. *Then*

$$\hat{I}_{p+1}(z,\overline{z})=\sum_{j=0}^{p}J_{jj}e^{i\pi(a_j-\tilde{a}_j)}z^{-a_j}\overline{z}^{-\tilde{a}_j}\,{}_{p+1}F_p\left(a_j,a_j-b_i+1,1+a_j-a_{l\neq j},\frac{1}{z}\right)$$
$$\times\ {}_{p+1}F_p\left(\tilde{a}_j,\tilde{a}_j-\tilde{b}_i+1,1+\tilde{a}_j-\tilde{a}_{l\neq j},\frac{1}{\overline{z}}\right),$$

where J_{jj} is given by

$$J_{jj}=\frac{s(\tilde{b}_j-\tilde{a}_j)}{s(\tilde{a}_0-\tilde{a}_j)}B_{a_j,a_0-a_j,\tilde{a}_j,\tilde{a}_0-a_j}\prod_{\substack{i=0\\ i\neq j}}^{p}B_{b_i-a_i,a_i-a_j,\tilde{b}_i-\tilde{a}_i,\tilde{a}_i-\tilde{a}_j},j\neq 0 \tag{17}$$

and

$$J_{00}=\prod_{i=1}^{p}B_{b_i-a_i,a_i-a_0,\tilde{b}_i-\tilde{a}_i,\tilde{a}_i-\tilde{a}_0}. \tag{18}$$

A heuristic argument for the above formula is given in Appendix A

Proof: From Eq. (15) it follows that

$$\lambda_0^{p+1}\,{}_{p+1}F_p(a_0,a^p,b^p,z)\;{}_{p+1}F_p(\tilde a_0,\tilde a^p,\tilde b^p;\overline{z})$$
$$=\prod_{i=1}^{p}\frac{s(\tilde a_i)s(\tilde b_i-\tilde a_i)}{s(\tilde b_i)}\left(\sum_{j=0}^{p}c_{0j}^{p}\left(\frac{e^{i\pi}}{z}\right)^{a_j}{}_{p+1}F_p\left(a_j,1+a_j-b_i,1+a_j-a_{l\neq j};\frac{1}{z}\right)\right)$$
$$\times\left(\sum_{j=0}^{p}\tilde c_{0j}^{p}\left(\frac{e^{-i\pi}}{\overline{z}}\right)^{\tilde a_j}{}_{p+1}F_p\left(\tilde a_j,1+\tilde a_j-\tilde b_i,1+\tilde a_j-\tilde a_{l\neq j};\frac{1}{\overline{z}}\right)\right),$$

where

$$c_{00}^{p}=\prod_{i=1}^{p}B(b_i-a_i,a_i-a_0)$$

and

$$c_{0j}^{p}=B(a_j,a_0-a_j)\prod_{\substack{i=1\\ i\neq j}}^{p}B(b_i-a_i,a_i-a_j),$$

with $B(a,b)=\Gamma(a)\Gamma(b)/\Gamma(a+b)$. The coefficient $\tilde c_{0k}^{p}$ is obtained from c_{0k}^{p} by replacing a_0, a^p and b^p by $\tilde a_0$, $\tilde a^p$ and $\tilde b^p$, respectively. Likewise, we find

$$\sum_{j=1}^{p}\lambda_j^{p+1}z^{1-b_j}\overline{z}^{1-\tilde b_j}\,{}_{p+1}F_p(a_l-b_j+1,1+b_i-b_j,2-b_j,z)$$
$$\times\;{}_{p+1}F_p\left(\tilde a_l-\tilde b_j+1,1+\tilde b_i-\tilde b_j,2-\tilde b_j;\frac{1}{\overline{z}}\right)$$
$$=\sum_{j=1}^{p}(-1)^{a_j-\tilde a_j}\frac{s(\tilde b_j-1)s(1-\tilde a_0)}{s(\tilde b_j-\tilde a_0)}\times\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{s(\tilde a_i-\tilde b_j+1)s(\tilde b_i-\tilde a_j)}{s(\tilde b_i-\tilde b_j+1)}$$
$$\times\left(\sum_{k=0}^{p}c_{jk}^{p}\left(\frac{e^{i\pi}}{z}\right)^{a_k}{}_{p+1}F_p\left(a_k,1+a_k-b_i,1+a_k-a_{l\neq k};\frac{1}{z}\right)\right)$$
$$\times\left(\left(\sum_{k=0}^{p}\tilde c_{jk}^{p}\left(\frac{e^{-i\pi}}{\overline{z}}\right)^{\tilde a_k}{}_{p+1}F_p\left(\tilde a_k,1+\tilde a_k-\tilde b_i1+\tilde a_k-\tilde a_{l\neq k};\frac{1}{\overline{z}}\right)\right)\right),$$

with

$$c_{j0}^{p}=\frac{\Gamma(2-b_j)\Gamma(b_j-1)}{\Gamma(b_j-a_j)\Gamma(a_j-b_j+1)}\prod_{i=1}^{p}B(b_i-a_i,a_i-a_0),$$

and

$$c_{jk}^{p}=\frac{\Gamma(2-b_j)\Gamma(b_j-1)}{\Gamma(b_j-a_0)\Gamma(a_0-b_j+1)}B(1-a_0,a_0-a_k)\prod_{\substack{i=1\\ i\neq k}}^{p}B(b_i-a_i,a_i-a_k)\frac{s(b_j-a_j)}{s(b_j-a_k)}.$$

With the simplifications

$$\frac{s(\tilde{a}_i-\tilde{b}_j+1)}{s(\tilde{b}_i-\tilde{b}_j+1)}=\frac{s(\tilde{a}_i-\tilde{b}_j)}{s(\tilde{b}_i-\tilde{b}_j)},$$

$$\frac{s(\tilde{b}_j-1)\Gamma(2-\tilde{b}_j)\Gamma(\tilde{b}_j-1)}{s(\tilde{b}_j-\tilde{a}_0)\Gamma(\tilde{b}_j-\tilde{a}_0)\Gamma(\tilde{a}_0-\tilde{b}_j+1)}=1,$$

$$\frac{s(1-\tilde{a}_0)}{s(b_j-1)}=-\frac{s(\tilde{a}_0)}{s(b_j)},$$

and

$$B(1-a_0,a_0-a_l)=B(a_l,a_0-a_l)\frac{s(a_l)}{s(a_0)},$$

the coefficient J_{nk}, $n\neq 0\neq k$, of

$$\left(\frac{e^{i\pi}}{z}\right)^{a_n}\left(\frac{e^{-i\pi}}{\bar{z}}\right)^{\tilde{a}_k}{}_{p+1}F_p\left(a_n,a_n-b_i+1,1+a_n-a_{l\neq n}\ \frac{1}{z}\right)$$
$$\times{}_{p+1}F_p\left(\tilde{a}_k,\tilde{a}_k-\tilde{b}_i+1,1+\tilde{a}_k-\tilde{a}_{l\neq k};\frac{1}{\bar{z}}\right)$$

becomes

$$J_{nk}=\prod_{\substack{i=0\\ i\neq n}}^{p}B(b_i-a_i,a_i-a_n)\prod_{\substack{i=0\\ i\neq k}}^{p}B(\tilde{b}_i-\tilde{a}_i,\tilde{a}_i-\tilde{a}_k)$$
$$\times\prod_{i=1}^{p}\sin\pi(\tilde{b}_i-\tilde{a}_i)B(a_n,a_0-a_n)B(\tilde{a}_k,\tilde{a}_0-\tilde{a}_k)\hat{J}_{nk},\tag{19}$$

where

$$\tilde{J}_{nk}=\prod_{i=1}^{p}\frac{s(\tilde{a}_i)}{s(\tilde{b}_i)}-\sum_{j=1}^{p}(-1)^{a_j-\tilde{a}_j}\frac{s(b_j-a_0)s(a_n)s(\tilde{a}_k)s(b_j-a_j)}{s(b_j)s(a_0)s(b_j-a_n)s(\tilde{b}_j-\tilde{a}_k)}\times\prod_{\substack{p=1\\ i\neq j}}^{p}\frac{s(\tilde{a}_i-\tilde{b}_j)}{s(\tilde{b}_i-\tilde{b}_j)}.\tag{20}$$

Now from the fact that $a_i-\tilde{a}_i$ and $b_i-\tilde{b}_i$ differ by integers we find

$$(-1)^{a_j-\tilde{a}_j}\frac{s(b_j-a_0)s(a_n)s(b_j-a_j)}{s(b_j)s(a_0)s(b_j-a_n)}=-\frac{s(\tilde{b}_j-\tilde{a}_0)s(\tilde{a}_0)s(\tilde{a}_n)s(\tilde{a}_j-\tilde{b}_j)}{s(\tilde{b}_j)s(\tilde{a}_0)s(\tilde{b}_j-\tilde{a}_n)}$$

so that

$$\tilde{J}_{nk}=\prod_{i=1}^{p}\frac{s(\tilde{a}_i)}{s(\tilde{b}_j)}+\sum_{j=1}^{p}\frac{s(\tilde{b}_j-\tilde{a}_0)s(\tilde{a}_n)s(\tilde{a}_k)s(\tilde{a}_j-\tilde{b}_j)}{s(\tilde{b}_j)s(\tilde{a}_0)s(\tilde{a}_n-\tilde{b}_j)s(\tilde{a}_k-\tilde{b}_j)}\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{s(\tilde{a}_i-\tilde{b}_j)}{s(\tilde{b}_i-\tilde{b}_j)}.\tag{21}$$

For $n=0\neq k$ the coefficient J_{0k} of

$$\left(\frac{e^{i\pi}}{z}\right)^{a_0}\left(\frac{e^{-i\pi}}{\bar{z}}\right)^{\tilde{a}_k}{}_{p+1}F_p\left(a_0,1+a_0-b_i,1+a_0-a_i,\frac{1}{z}\right)\ {}_{p+1}F_p\left(\tilde{a}_k,1+\tilde{a}_k-\tilde{b}_i,1+\tilde{a}_k-\tilde{a}_{l\neq k},\frac{1}{z}\right)$$

becomes, with the substitutions above,

$$J_{0,k}=\prod_{i=1}^{p} B(b_i-a_i,a_i-a_0)\prod_{\substack{i=1\\ i\neq k}}^{p} B(\tilde{b}_i-\tilde{a}_i,\tilde{a}_i-\tilde{a}_k)B(\tilde{a}_k,\tilde{a}_0-\tilde{a}_k)\hat{J}_{0,k},$$

where $\tilde{J}_{0,k}$ is given by (19) above with $n=k$. For $k=0$ we find

$$J_{0,0}=\prod_{i=1}^{p} B(b_i-a_i,a_i-a_0)\prod_{i=1}^{p} B(\tilde{b}_i-\tilde{a}_i,\tilde{a}_i-\tilde{a}_0)\prod_{i=1}^{p} s(\tilde{b}_i-\tilde{a}_i)$$
$$\times\left[\prod_{i=1}^{p}\frac{s(\tilde{a}_i)}{s(\tilde{b}_i)}-\sum_{j=1}^{p}\frac{s(\tilde{a}_0)s(\tilde{b}_j-\tilde{a}_j)}{s(\tilde{b}_j)s(\tilde{b}_j-\tilde{a}_0)}\prod_{\substack{i=1\\ i\neq j}}^{p}\frac{s(\tilde{a}_i-\tilde{b}_j)}{s(\tilde{b}_i-\tilde{b}_j)}\right]. \tag{22}$$

With the substitutions $y_j=\exp -2i\pi b_j$, $u_i=\exp -2i\pi a_i$ and $B_{n,k}=J_{n,k}\Pi_i^p(\exp i\pi a_i)/(\exp i\pi b_i)$ the result now follows from Lemma 4 and the symmetry between $J_{n,0}$ and $J_{0,n}$. □

Define

$$\psi_p=\sum_{i=1}^{p} b_i-\sum_{i=0}^{p} a_i,$$

and $\tilde{\psi}_p$ as above with b_i and a_i replaced by $\tilde{b}_i$ and $\tilde{a}_i$, respectively.

Lemma 6: Suppose condition C is satisfied, ψ_{p-1} is not an integer, $\mathrm{Re}(\psi_{p-1}+\tilde{\psi}_{p-1})>p-1$, $\mathrm{Re}(a_p+\tilde{a}_p)<0$, $\mathrm{Re}(b_p+\tilde{b}_p-a_p+\tilde{a}_p)<0$, $\mathrm{Re}(b_j+\tilde{b}_j-a_p-\tilde{a}_p)<2$, *and* $\mathrm{Re}(b_p+\tilde{b}_p-a_j-\tilde{a}_j)<2$. *Then for* $\arg z\neq 0$,

$$\int_\Gamma d\overline{z_p}\,a_0\prod_{i=0}^{p-1} a_i\,K_0^p(a_0+1,a^p+1,b^p,z,z_p)H_0^p(\tilde{a}_0,\tilde{a}^p,\overline{z,z_p})$$
$$+\sum_{j=1}^{p-1}\prod_{i=0}^{p-1}(a_i-b_j+1)\;K_j^p(a_0+1,a^p+1,b^p,z,z_p)H_j^p(\tilde{a}_0,\tilde{a}^p,\tilde{b}^p,\overline{z,z_p})=0, \tag{23}$$

where $\Gamma=[0,\infty\exp -i\phi)\cup[1,\infty)$, $\phi=\arg(z)$.

Proof: We use Γ (see Fig. 3) as cuts for z^α and $(1-z)^\alpha$ choosing the determination for both so that both give positive reals when their arguments are large positive real numbers. We begin by breaking up the above integral into pieces for which $|zz_p|<1$ and $|zz_p|>1$. For $|zz_p|>1$ we use the fact that

$$\prod_{i=0}^{p-1} a_i\lambda_0^{p-1}(a_0,a^{p-1},b^{p-1},\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1})$$
$$=\prod_{i=1}^{p-1}(b_i-a_i-1)\lambda_0^{p-1}(a_0+1,a^{p-1}+1,b^{p-1},\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1}), \tag{24}$$

and

$$\prod_{i=0}^{p-1}(a_i-b_j+1)\lambda_j^{p-1}(a_0,a^{p-1},b^{p-1},\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1})$$
$$=a_0\prod_{i=1}^{p-1}(b_i-a_i-1)\lambda_j^{p-1}(a_0+1,a^{p-1}+1,b^{p-1},\tilde{a}_0+1,\tilde{a}^{p-1}+1,\tilde{b}^{p-1}), \tag{25}$$

and Lemma 5 to represent the integrand in (22) for $|zz_p|>1$. The conditions on $a_0,\ldots,a_p$, $b_1,\ldots,a_p$, $\tilde{a}_0\ldots,\tilde{a}_p$, and $\tilde{b}_1,\ldots,\tilde{b}_p$ imply that the above integral is convergent for z_p in a neighborhood of ∞,0, and 1. Furthermore, with condition C and the condition on ψ_{p-1} the hypergeometric functions in the integrand behave as ${}_pF_{p-1}(a_0,a^p,b^p,z)\sim(1-z)^{\psi_{p-1}}$ (Ref. 9) so that the integral is convergent for $zz_p\sim 1$. The last part of condition C insures that the contributions along the two sides of each cut cancel out giving the result. □

We now prove our main result.

Theorem 3: *Suppose that condition C is satisfied,* ψ_{p-1} *is not an integer,* $\mathrm{Re}(\psi_{p-1}+\tilde{\psi}_{p-1})>p-1$, $\mathrm{Re}(a_p+\tilde{a}_p)>0$, $\mathrm{Re}(b_p+\tilde{b}_p-a_p-\tilde{a}_p)>0$, $\mathrm{Re}(b_j+\tilde{b}_j-a_p-\tilde{a}_p)<2$, *and* $\mathrm{Re}(b_p+\tilde{b}_p-a_j-\tilde{a}_j)<2$. *Then* I_{p+1} *is given by Eq. (8) with* λ_j^{p+1} *given by (9) and (10).* I_{p+1} *may be extended using the above representation so that only condition C is satisfied by the parameters.*

Proof: Consider I_{p+1} for $p=1$. The result is already known[4] and we will recover it. In this case,

$$I_2=\int\int_{\mathbb{C}\setminus\Gamma}\frac{d^2z_1}{2i}z_1^{a_1-1}(1-z_1)^{b_1-a_1-1}(1-zz_1)^{-a_0}\overline{z_1}^{\tilde{a}_1-1}(1-\overline{z_1})^{\tilde{b}_1-\tilde{a}_1-1}(1-\overline{zz_1})^{-\tilde{a}_0}$$

$$=\int\int_{\mathbb{C}\setminus\Gamma}\frac{d^2z_1}{2i}z_1^{a_1-1}(1-z_1)^{b_1-a_1-1}\overline{z_1}^{\tilde{a}_1-1}(1-\overline{z_1})^{\tilde{b}_1-\tilde{a}_1-1}I_1(a_0,\tilde{a}_0,zz_1,\overline{zz_1}),\tag{26}$$

where $\Gamma=[0,\infty\exp-i\phi)\cup[1,\infty)$, $\phi=\arg(z)$. (See Fig. 3.) We will use the determination given in the above lemma for z^α. We suppose that $\arg z\neq 0$. If $\mathrm{Re}(a_1+\tilde{a}_1)>0$, $\mathrm{Re}(b_1+\tilde{b}_1-a_1-\tilde{a}_1)>0$, $\mathrm{Re}(a_0+\tilde{a}_0)<0$, and $\mathrm{Re}(b_1+\tilde{b}_1-a_0-\tilde{a}_0)<2$, the above integral converges uniformly and absolutely on compact subsets of the z plane that exclude the real axis and defines an analytic function of the a and b variables. Utilizing the uniform convergence of the above integral and the continuity of the integrand it is not difficult to see that the integral is continuous in z. Furthermore, the integral with the integrand differentiated once and the integral with the integrand differentiated twice with respect to z also converge uniformly and absolutely, and are continuous functions in z. Switching to polar coordinates we find (suppressing the dependence on the parameters a and b)

$$I_2=\left(\int_0^{-\phi}+\int_{-\phi}^{2\pi}\right)\int_0^\infty\frac{r_1dr_1\,d\phi_1}{2i}f(re^{i\phi},re^{-i\phi},r_1e^{i\phi_1},r_1e^{-i\phi_1})$$

$$=\left(\int_0^{-\phi}+\int_{-\phi}^{2\pi}\right)F(re^{i\phi},re^{-i\phi},\phi_1)d\phi_1,$$

where $z=re^{i\phi}$ and $z_i=r_1e^{i\phi_1}$. Thus

$$\frac{\partial}{\partial z}I_2=\frac{1}{2}\left(\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\phi}\right)I_2=\frac{i}{2r}(F(re^{i\phi},re^{-i\phi},-\phi_-)-F(re^{i\phi},re^{-i\phi},-\phi_+))$$

$$+\left(\int_0^{-\phi}+\int_{-\phi}^{2\pi}\right)\frac{\partial}{\partial z}F(z,\overline{z},\phi_1)d\phi_1.\tag{27}$$

Here $F(re^{i\phi},re^{-i\phi},-\phi_-)=\lim_{\delta\to 0}F(re^{i\phi},re^{-i\phi},-\phi-\delta)$ and $F(re^{i\phi},re^{-i\phi},-\phi_+)=\lim_{\delta\to 0}F(re^{i\phi},re^{-i\phi},-\phi+\delta)$ where the limits exist due to the continuity properties discussed above. Part (d) of condition C shows that the first term on the right hand side of the second eqation in (27) is equal to zero. To justify the interchange of differentiation and integration we note that for ϕ_1 restricted so that $\epsilon\leqslant\phi_1\leqslant-\phi-\delta$, and $-\phi+\delta\leqslant\phi_1\leqslant 2\pi-\epsilon$, $\epsilon,\delta>0$, and $r_1>\epsilon$, $z^{a_1-1}\overline{z_1}^{\tilde{a}_1-1}(1-\overline{z_1})^{\tilde{b}_1-\tilde{a}_1-1}(1-z_1)^{b_1-a_1-1}I_1(a_0,\tilde{a}_0,zz_1,\overline{zz_1})$ is continuous and has a continuous partial with respect to z. Furthermore, from the uniform convergence of the integral

$$\int\int_{\mathbb{C}\setminus\Gamma} r_1 dr_1\, d\phi_1 z_1^{a_1-1}\overline{z}_1^{\tilde{a}_1-1}(1-\overline{z}_1)^{\tilde{b}_1-\tilde{a}_1-1}(1-z_1)^{b_1-a_1-1}\frac{\partial I_1}{\partial z}(a_0,\tilde{a}_0,zz_1,\overline{zz_1})$$

the standard theorem of interchanging integration and differentiation [Titchmarch, p. 59] may be applied. Thus

$$\frac{\partial}{\partial z}I_2=\frac{1}{2i}\int\int_{\mathbb{C}\setminus\Gamma} d^2z_1 z_1^{a_1-1}\overline{z}_1^{\tilde{a}_1-1}(1-\overline{z}_1)^{\tilde{b}_1-\tilde{a}_1-1}(1-z_1)^{b_1-a_1-1}\frac{\partial I_1}{\partial z}(a_0,\tilde{a}_0,zz_1,\overline{zz_1}).$$

The same reasoning may be applied to show that

$$\frac{\partial^2}{\partial z^2}I_2=\frac{1}{2i}\int\int_{\mathbb{C}\setminus\Gamma} d^2z_1 z_1^{a_1-1}\overline{z}_1^{\overline{a}_1-1}(1-\overline{z}_1)^{\overline{b}_1-\overline{a}_2-1}\frac{\partial^2}{\partial z^2}I_1(a_0,\overline{a}_0zz_1,\overline{zz_1}),$$

and from (12) above we find

$$O_z^2\ \ I_2(z,\ \overline{z})=-a_0\frac{1}{2i}\int d^2z_1\frac{\partial}{\partial z_1}K_0^{(1)}(a_0+1,\ a_1+1,\ b_1,\ z,\ z_1)H_0^{(1)}(\tilde{a}_0,\ \tilde{a}_1,\ \tilde{b}_1,\ \overline{z},\ \overline{z_1}).$$

Therefore Lemma 3, the Stoke's theorem and Lemma 6 imply

$$O_z^2 I_2=\frac{1}{4}\int_\Gamma K_0^{(1)}(z,z_1)H(\overline{z,z_1})d\overline{z_1}=0.$$

A similar discussion interchanging $z,a_0,\ a_1$, and b_1, with $\overline{z},\ \tilde{a}_0,\ \tilde{a}_1$, and $\tilde{b}_1$, respectively, shows that $O_z^2 I_2=0$ so that I_2 has the representation,

$$I_2=\sum_{i=0,j=0}^{1}\beta_{i,j}u_i^2(a_0,a_1,b_1,z)u_j^2(\tilde{a}_0,\tilde{a}_1,\tilde{b}_1,\overline{z}),$$

writing

$$\begin{aligned}I_2=&\int\int_{\substack{\mathbb{C}\setminus\Gamma\\ |z_1|\leqslant 1}}\frac{d^2z_1}{2i}z_1^{a_1-1}(1-z_1)^{b_1-a_1-1}(1-zz_1)^{-a_0}\overline{z}_1^{\tilde{a}_1-1}(1-\overline{z}_1)^{\tilde{b}_1-\tilde{a}_1-1}(1-\overline{zz_1})^{-\tilde{a}_0}\\&+\int\int_{\substack{\mathbb{C}\setminus\Gamma\\ |z_1|>1}}\frac{d^2z_1}{2i}z_1^{a_1-1}(1-z_1)^{b_1-a_1-1}(1-zz_1)^{-a_0}\overline{z}_1^{\tilde{a}_1-1}(1-\overline{z}_1)^{\tilde{b}_1-\tilde{a}_1-1}(1-\overline{zz_1})^{-\tilde{a}_0}=I_1^2+I_2^2.\end{aligned}\tag{28}$$

With the above constraints on the parameters we see that in a neighborhood of $z=0$, $I_2^1\sim K$ where K is a constant independent of z and $\overline{z}$. The change of variables $t=zz_1$ in the second integral yields

$$I_2^2=z^{1-b_1}\bar{z}^{1-\tilde{b}_1}(-1)^{b_1-\tilde{b}_1-a_1+\tilde{a}_1}\int\int_{\substack{\mathbb{C}\setminus[0\infty)\\ |t/z|>1}}\frac{d^2t}{2i}t^{b_1-2}\left(1-\frac{z}{t}\right)^{b_1-a_1-1}(1-t)^{-a_0}\bar{t}^{\tilde{b}_1-2}$$
$$\times\left(1-\frac{\bar{z}}{\bar{t}}\right)^{\tilde{b}_1-\tilde{a}_1-1}(1-\bar{t})^{-\tilde{a}_0}.$$

Consequently the dominated convergence theorem shows that

$$\lim_{z\to 0} z^{b_1-1}\bar{z}^{\tilde{b}_1-1}I_2^2=\lambda_1^2.$$

Since the only constraints on b_1 and $\tilde{b}_1$ are those given above and in condition C the previous discussion implies that $\beta_{0,1}^0=0=\beta_{1,0}^0$ and $\beta^{1,1}=\lambda_1^2$. We also find from the dominated convergence theorem that $\lim_{z\to 0} I_2=\lambda_0^2$. From the previous discussion the solution reads

$$I_2(a_0,\ a_1,\ b_1,\ \tilde{a}_0,\ \tilde{a}_1,\ \tilde{b}_1,\ z,\ \bar{z})$$
$$=\lambda_0^{(2)}(a_1,\ b_1;\ \tilde{a}_1,\ \tilde{b}_1)\ {}_2F_1(a_0,\ a_1,\ b_1;\ z)\ {}_2F_1(\tilde{a}_0,\ \tilde{a}_1,\ \tilde{b}_1;\ \bar{z})$$
$$+\lambda_1^{(2)}(a_0,\ a_1,\ b_1,\ \tilde{a}_0,\ \tilde{a}_1,\ \tilde{b}_1)(z)^{1-b_1}(\bar{z})^{1-\tilde{b}_1}\ {}_2F_1(a_0-b_1+1,\ a_1-b_1+1,\ 2$$
$$-b_1;\ z)\ {}_2F_1(\tilde{a}_0-\tilde{b}_1+1,\ \tilde{a}_1-\tilde{b}_1+1,\ 2-\tilde{b}_1;\ \bar{z}),$$

$$\lambda_0^{(2)}(a_1,\ b_1,\ \tilde{a}_1,\ \tilde{b}_1)=\frac{\Gamma(a_1)\Gamma(b_1-a_1)}{\Gamma(b_1)}\ \frac{\Gamma(\tilde{a}_1)\Gamma(\tilde{b}_1-\tilde{a}_1)}{\Gamma(\tilde{b}_1)}\ \frac{\sin\pi\tilde{a}_1\sin\pi(\tilde{b}_1-\tilde{a}_1)}{\sin\pi\tilde{b}_1}$$

and

$$\lambda_1^{(2)}(a_0,\ a_1,\ b_1,\ \tilde{a}_0,\ \tilde{a}_1,\ \tilde{b}_1)$$
$$=(-1)^{b_1-\tilde{b}_1+a_1-\tilde{a}_1}\frac{\Gamma(b_1-1)\Gamma(-a_0+1)}{\Gamma(-a_0+b_1)}\ \frac{\Gamma(\tilde{b}_1-1)\Gamma(-\tilde{a}_0+1)}{\Gamma(-\tilde{a}_0+\tilde{b}_1)}\ \frac{\sin\pi b_1\ \ \sin\pi(-a_0)}{\sin\pi(b_1-a_0)}$$

in agreement with previous results. This proves the result for $p=1$ with $\mathrm{Re}(a_1+\tilde{a}_1)>0$, $\mathrm{Re}(b_1+\tilde{b}_1-a_1-\tilde{a}_1)>0$, $\mathrm{Re}(a_0+\tilde{a}_0)<0$, $\mathrm{Re}(b_1+\tilde{b}_1-a_0-\tilde{a}_0)<2$ and $\arg z\neq 0$. We may now extend I_2 using the above representation so that only condition C is satisfied by the parameters.

Suppose now that

$$I_p(a_0,\ a^{p-1},\ b^{p-1},\ \tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1},\ z,\ \bar{z})$$
$$=\sum_{j=0}^{p-1}\lambda_j^{(p)}(a_0,\ a^{p-1},\ b^{p-1},\ \tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1})u_j^p(a_0,\ a^{p-1},\ b^{p-1},\ z)$$
$$\times\ \tilde{u}_j^p(\tilde{a}_0,\ \tilde{a}^{p-1}\ \tilde{b}^{p-1},\ \bar{z}).$$

Then

$$
\begin{aligned}
&I_{p+1}(a_0,\ a^p,\ b^p,\ \tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p,\ z,\ \overline{z})\\
&\quad=\sum_{j=0}^{p-1}\ \lambda_j^{(p)}(\tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1},\ \tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1})\frac{1}{2i}\\
&\quad\times\int\int_{\mathbb{C}\setminus\Gamma} d^2z_1(z_1)^{a_p-1}(1-z_1)^{b_p-a_p-1}u_j^p(a_0,\ a_i,\ b_i,\ zz_1)(\overline{z_1})^{\tilde{a}_p-1}\\
&\quad\times(1-\overline{z_1})^{\tilde{b}_p-\tilde{a}_p-1}u_j^p(\tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1},\ \overline{zz_1}).
\end{aligned}
$$

The conditions imposed above, Lemma 5, and the behavior of u_j^p in the neighborhood of 0, 1, and ∞ imply that the above integrals converge uniformly and absolutely on compact subsets of $\mathbb{C}\setminus[0,\infty)$. Thus by Morera's theorem I_{p+1} is analytic in the parameters $a_0,a^p,b^p,\ \tilde{a}_0,\tilde{a}^p$, and $\tilde{b}^p$ in the region specified. The same is true with u_j^p replaced by $(\partial/\partial z)\,u_j^p,\ \ldots,(\partial^{p+1}/\partial z^{p+1})\,u_j^p$. Repeating the argument above used for I_2 and using the last part of condition C yields

$$
\begin{aligned}
&\frac{\partial^i}{\partial\overline{z}^i}\frac{1}{2i}\int\int_{\mathbb{C}\setminus\Gamma} d^2z_1F_j^p(z,\overline{z},z_1,\overline{z_1},a_0,\ a^p,\ b^p,\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)\\
&\quad=\frac{1}{2i}\int\int_{\mathbb{C}\setminus\Gamma} d^2z_1\frac{\partial^i}{\partial z^i}F_j^p(z,\overline{z},z_1,\overline{z_1},a_0,\ a^p,\ b^p,\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p),
\end{aligned}
$$

where

$$
\begin{aligned}
&F_j^p(z,\overline{z},z_1,\overline{z_1},a_0,\ a^p,\ b^p,\tilde{a}_0,\ \tilde{a}^p,\ \tilde{b}^p)\\
&\quad=(z_1)^{a_p-1}(1-z_1)^{b_p-a_p-1}u_j^p(a_0,\ a_i,\ b_i,\ zz_1)\\
&\qquad\times(\overline{z_1})^{\tilde{a}_p-1}(1-\overline{z_1})^{\tilde{b}_p-\tilde{a}_p-1}u_j^p(\tilde{a}_0,\ \tilde{a}^{p-1},\ \tilde{b}^{p-1},\ \overline{zz_1}).
\end{aligned}
$$

Applying Lemma 3, Stoke's theorem, and Lemma 6 shows that

$$
O_z^{p+1}\ I_{p+1}(a_i,\ b_i,\ \tilde{a}_i,\ b_i,\ a_0,\ \tilde{a}_0,\ z,\ \overline{z})=0.
$$

A similar analysis can be applied to $O_{\overline{z}}^{p+1}$ and we are led to the solution

$$
I_{p+1}=\sum_{i,j=0}^{p}\beta_{i,j}u_i^{p+1}(a_0,a^p,b^p,z)u_j^{p+1}(\tilde{a}_0,\tilde{a}^p,\tilde{b}^p\overline{z}),
$$

where condition C insures that the $u_j^{p+1},j=0,\ldots,p$ are linearly independent. Write $I_{p+1}=\Sigma_{j=0}^pI_{p+1}^j$, where

$$
\begin{aligned}
I_{p+1}^j=&\frac{\lambda_j^p}{2i}\int\int_{\substack{\mathbb{C}\setminus\Gamma\\ |zz_1|<1}} d^2z_1z_1^{a_p-1}\overline{z_1}^{\tilde{a}_p-1}(1-z_1)^{b_p-a_p-1}(1-\overline{z_1})^{\tilde{b}_p-\tilde{a}_p-1}\\
&\times u_j^p(a_0,a^{p-1},b^{p-1},zz_1)u_j^p(\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1},\overline{zz_1}),
\end{aligned}
$$

for $j=0,\ldots,p-1$, and

$$I_{p+1}^{p}=\sum_{j=0}^{p-1}\frac{J_{jj}e^{i\pi(a_j-\tilde{a}_j)}}{2i}\int\int_{\substack{\mathbb{C}\setminus\Gamma\\ |zz_1|>1}} d^2z_1 z_1^{a_p-1}\overline{z}_1^{\tilde{a}_p-1}(1-z_1)^{b_p-a_p-1}(1-\overline{z}_1)^{\tilde{b}_p-\tilde{a}_p-1}(zz_1)^{-a_j}(\overline{zz_1})^{-\tilde{a}_j}$$

$$\times {}_pF_{p-1}\left(a_j,a_j-b_i+1,1+a_j-a_{i\neq j},\frac{1}{zz_1}\right)_p F_{p-1}\left(\tilde{a}_j,\tilde{a}_j-\tilde{b}_i+1,1+\tilde{a}_j-\tilde{a}_{i\neq j},\frac{1}{\overline{zz_1}}\right).$$

From the dominated convergence theorem we see that $\lim_{z\to 0} I_{p+1}^{0}=\lambda_0^{p+1}$ and $\lim_{z\to 0} z^{b_j-1}\overline{z}^{\tilde{b}_j-1}I_{p+1}^{j}=\lambda_j^{p+1}$. Furthermore, with the change of variables $t=zz_1$ it is not difficult to see that $\lim_{z\to 0} z^{b_p-1}\overline{z}^{\tilde{b}_p-1}I_{p+1}^{p}=K^{p+1}$, with K^{p+1} independent of z. Condition C and the above discussion shows that $\beta_{i,j}=0, i\neq j$ and $\beta_{i,i}=\lambda_i^{p+1}, i=0,\ldots,p-1$. In order to compute $\beta_{p,p}$ split I_{p+1} up into the pieces I_{p+1}^{a} for $|z_1|\leqslant 1$ and I_{p+1}^{b} for $|z_1|>1$. With the change of variables $t=zz_1$ the second integral becomes

$$I_{p+1}^{b}=z^{1-b_p}\overline{z}^{1-\tilde{b}_p}\int\int_{\mathbb{C}\setminus[0,\infty)} d^2t\,\chi_{|t|>|z|}(t)t^{2-b_p}\overline{t}^{2-\tilde{b}_p}\left(\frac{z}{t}-1\right)^{b_p-a_p-1}\left(\frac{\overline{z}}{\overline{t}}-1\right)^{\tilde{b}_p-\tilde{a}_p-1}$$

$$\times I_p(a_0,a^{p-1},b^{p-1},\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1},t,\overline{t}).$$

Using the dominated convergence theorem we see that

$$(-1)^{b_p-\tilde{b}_p-a_p+\tilde{a}_p}\lim_{z\to 0} z^{b_p-1}\overline{z}^{\tilde{b}_p-1}I_{p+1}^{b}$$

$$=\int\int_{\mathbb{C}\setminus[0,\infty)} d^2t\,t^{b_p-2}\overline{t}^{\tilde{b}_p-2}I_p(a_0,a^{p-1},b^{p-1},\tilde{a}_0,\tilde{a}^{p-1},\tilde{b}^{p-1},t,\overline{t}).$$

We now show that the above integral is equal to $(-1)^{b_p-\tilde{b}_p-a_p+\tilde{a}_p}\lambda_p^{p+1}$. Note that the result has been shown for $p=1$. Now suppose the result is true up to p. With the substitution of (5) for I_p we find

$$(-1)^{b_p-\tilde{b}_p-a_p+\tilde{a}_p}\lim_{z\to 0} z^{b_p-1}\overline{z}^{\tilde{b}_p-1}I_{p+1}^{b}$$

$$=\int\int_{\mathbb{C}\setminus[0,\infty)} d^2t\,t^{b_p-2}\overline{t}^{\tilde{b}_p-2}\int\int_{\mathbb{C}\setminus\Gamma} d^2z z^{a_{p-1}-1}\overline{z}^{\tilde{a}_{p-1}-1}(1-z)^{b_{p-1}-a_{p-1}-1}$$

$$\times(1-\overline{z})^{\tilde{b}_{p-1}-\tilde{a}_{p-1}-1}I_{p-1}(a_0,a^{p-2},b^{p-2},\tilde{a}_0,\tilde{a}^{p-2},\tilde{b}^{p-2},tz,\overline{tz}).$$

Since the above integral converges absolutely we can interchange the order of integration using Fubini's theorem, then set $u=zt$ to obtain

$$(-1)^{b_p-\tilde{b}_p-a_p+\tilde{a}_p}\lim_{z\to 0} z^{b_p-1}\overline{z}^{\tilde{b}_p-1}I_{p+1}^{b}$$

$$=\int\int_{\mathbb{C}\setminus[0,\infty)} d^2z z^{a_{p-1}-b_p}\overline{z}^{\tilde{a}_{p-1}-\tilde{b}_p}(1-z)^{b_{p-1}-a_{p-1}-1}(1-\overline{z})^{\tilde{b}_{p-1}-\tilde{a}_{p-1}-1}$$

$$\times\int\int_{\mathbb{C}\setminus\Gamma} d^2u u^{b_p-2}\overline{u}^{\tilde{b}_p-2}I_{p-1}(a_0,a^{p-2},b^{p-2},\tilde{a}_0,\tilde{a}^{p-2},\tilde{b}^{p-2},u,\overline{u}). \tag{29}$$

The claim now follows by induction. □

An alternative discussion to obtain (31) can be found in Appendix B.

We may now extend the result to the case when $\mathrm{Re}(\psi_{p-1}+\tilde{\psi}_{p-1})>-2$. The above representation may be used to define I_{p+1} when only condition C is imposed on the parameters which completes the proof.

ACKNOWLEDGMENTS

The authors would like to thank R. Peschanski, M. Bauer and R. Guida for useful discussions. We would also like to thank Ph. Di Fransesco for discussions leading to the use of Cauchy's theorem in Lemma 4. J.S.G. would like to thank the Service Physique Theorique at Saclay for their hospitality during his visit, especially P. Moussa. J.S.G. would also like to acknowledge useful discussions with Micheal Loss and Fernando Reitich. J.S.G. was supported in part by a grant from the Fullbright Foundation and NSF.

APPENDIX A

In this section we give a heuristic argument for Lemma 5. We begin by examining I_{p+1} for $|z|<1$ and switching to a new basis namely ${}_{p+1}G_p(a_i;b_i;z)$, which are nothing but the hypergeometric functions ${}_{p+1}F_p(a_i;b_i;z)$ up to a multiplicative factor, namely

$$ {}_{p+1}G_p(a_i;b_i;z)=\frac{\Pi_0^p\Gamma(a_i)}{\Pi_1^p\Gamma(b_i)}{}_{p+1}F_p(a_i;b_i;z). $$

The basis of the expansion is now $V_j(z),\tilde{V}_j(\bar{z})$ rather than $U_j(z)\tilde{U}_j(\bar{z})$ where

$$ V_j(z)=z^{1-b_j}\,{}_{p+1}G_p(a_i-b_j+1;b_k-b_j+1;z) $$

and

$$ \tilde{V}_j(\bar{z})=z^{1-\tilde{b}_j}\,{}_{p+1}\tilde{G}_p(\tilde{a}_i-\tilde{b}_j+1;\tilde{b}_k-\tilde{b}_j+1;\bar{z}). $$

In these formulas $k\neq j=0,p$ where by convention $b_0=\tilde{b}_0=1$.

In this basis the solution reads

$$ I_{p+1}=\sum_{j=0}^{p}\mu_j V_j(z)\tilde{V}(\bar{z}), $$

where the μ_j are obtained from the corresponding values of the λ_j.

It turns out that an obvious factorization does occur. Namely, by defining

$$ \mu_{p+1}=\frac{1}{\pi^2}(-1)^{a_0-\tilde{a}_0}\prod_{i=0}^{p}\Gamma(b_i-a_i)\Gamma(\tilde{b}_i-\tilde{a}_i)S(b_i-a_i) $$

we get

$$ \mu_j=\mu_{p+1}\,\frac{\Pi_{i=0}^{p}S(b_j-a_i)}{\Pi_{i=0\neq j}^{p}S(b_j-b_i)}. $$

To be more specific

$$\mu_0=\mu_{p+1}\ \frac{\Pi_{i=0}^{p}S(a_i)}{\Pi_{i=1}^{p}S(b_i)},$$

$$\mu_j=-\mu_{p+1}\frac{\Pi_{i=0}^{p}S(b_j-a_i)}{S(b_j)\Pi_{i=1\neq j}^{p}S(b_j-b_i)}.$$

Similarly, for $|z|>1$ it is useful to expand the integral as a combination of hypergeometric functions which are defined for $|z|>1$, namely

$$(z)^{-a_j}{}_{p+1}G_p\left(a_j,a_j-b_i+1;a_j-a_i+1;\frac{1}{z}\right),$$

or more specifically

$$W_j(z)=(z)^{-a_j}{}_{p+1}G_p\left(a_j,a_j-b_i+1;a_j-a_i+1;\frac{1}{z}\right),$$

the solution reads now

$$I_{p+1}=\sum_{j=0}^{p}\ \nu_j\ \ W_j(z)\tilde{W}_j(\overline{z}),$$

where the ν_j have to be determined from the value of the integral for $z\to\infty$.

We proceed as before and it turns out that the same factorization does occur, namely

$$\nu_j=(-1)^{s-\tilde{s}}\mu_{p+1}\frac{\Pi_{i=0}^{p}S(b_i-a_i)}{\Pi_{i=1\neq j}^{p}S(a_i-a_j)}.$$

Comparing μ_j and ν_j amounts but for a sign to interchange b_k and a_k as expected with the interchange of $z\to 1/z$. Indeed, if in the integrand of I_{p+1} we change $z_i\to 1/z_i$, the new integrand J reads

$$J=(-1)^{s-\tilde{s}}z^{-a_0}\overline{z}^{-\tilde{a}_0}\prod_{i=1}^{p}\ t_i^{a_0-b_i}(1-t_i)^{b_i-a_i-1}\left(1-\prod_{i=1}^{p}\ t_iz^{-1}\right)^{-a_0}$$
$$\times\prod_{i=1}^{p}\ \overline{t_i}^{\tilde{a}_0-\tilde{b}_i}(1-\overline{t_i})^{\tilde{b}_i-\tilde{a}_i-1}\left(1-\prod_{i=1}^{p}\ \overline{t_i}\overline{z}^{-1}\right)^{-\tilde{a}_0}.$$

It is now obvious that the result of the integral for $|z|>1$ is deduced from the result for $|z|<1$ by a simple change of the parameters of the hypergeometric functions of argument $1/z$ up to the multiplicative factor

$$(-1)^{s-\tilde{s}}z^{-a_0}\overline{z}^{-\tilde{a}_0},$$

namely, if we define α_i and β_i as the parameters, we get by simple identification

$$\alpha_0=a_0,$$

$$\alpha_i=a_0-b_i+1,$$

$$\beta_i=a_0-a_i+1,$$

which corresponds to the parameters of $W_0(z)$ and

$$\alpha_i-\beta_j+1=a_j-b_i+1,$$

$$\beta_i-\beta_j+1=a_j-a_i+1,$$

$$2-\beta_j=a_j-a_0+1,$$

which corresponds to the parameters of $W_j(z)$. The above argument can be made rigorous using (14).

APPENDIX B

In this appendix we give an alternative method to calculate λ_{p+1}^{p}. Besides the conditions imposed in the hypothesis of Theorem 3 it will assumed that $b_p-\tilde{b}_p-b_i+\tilde{b}_i\geqslant 0$, $i=0,\ldots,p-1$. We need to calculate

$$I=\sum_{i=0}^{p-1}\lambda_i^{p-1}\int t^{b_p-2}U_i(t)\overline{t^{\tilde{b}_p-2}}\tilde{U}_i(\overline{t})d^2t,$$

where

$$U_i(t)=t^{1-b_i}{}_pF_{p-1}(a_j-b_i+1;\ b_k-b_i+1;\ t),$$

where $j,k\neq i=0$, $p-1$, and λ_i^{p-1} is given in formula (11) and by convention $b_0=1$.

We split the domain of integration in two parts, and write $I=I_1+I_2$ where I_1 is the contribution for $|t|<1$ and I_2 for $|t|>1$. In the first domain the hypergeometric functions are convergent so that

$$I_1=\sum_{i=0}^{p-1}\lambda_i^{p-1}\int\int_{B/\Gamma} t^{b_p-2}U_i(t)\overline{t^{\tilde{b}_p-2}}\tilde{U}_i(\overline{t})d^2t,$$

where B is the unit disk in the complex plane and Γ is the contour used in the proof of Theorem 3. To calculate I_2, the other form of the solution which is valid for $|z|>1$ will be used, namely

$$I_2=\sum_{i=0}^{p-1}\nu_i^{p-1}\int\int_{B^c/\Gamma} t^{b_p-2}W_i(t)\overline{t^{\tilde{b}_p-2}}\tilde{W}_i(\overline{t})d^2t,$$

where

$$W_i(t)=t^{-a_i}{}_pF_{p-1}\left(a_i-b_j+1;a_i-a_k+1;\frac{1}{t}\right)$$

with the same convention for the indices j and k.

By definition

$$\lambda_i^{p-1}\frac{\prod_{j=0\neq i}^{p-1}\Gamma(b_j-b_i+1)\Gamma(\tilde{b}_j-\tilde{b}_i+1)}{\prod_{j=0}^{p-1}\Gamma(a_j-b_i+1)\Gamma(\tilde{a}_j-\tilde{b}_i+1)}=\mu_{p-1}\mu_i^{p-1},$$

$$\nu_i^{p-1}\frac{\prod_{j=0\neq i}^{p-1}\Gamma(a_i-a_j+1)\Gamma(\tilde{a}_i-\tilde{a}_j+1)}{\prod_{j=0}^{p-1}\Gamma(a_i-b_j+1)\Gamma(\tilde{a}_i-\tilde{b}_j+1)}=(-1)^{s-\tilde{s}}\mu_{p-1}\rho_i^{p-1},$$

$$s=\sum_{i=1}^{p-1} b_i-\sum_{i=0}^{p-1} a_i,$$

$$\mu_{p-1}=(-1)^{a_0-\tilde{a}_0}\frac{1}{\pi^2}\prod_{i=0}^{p-1}\Gamma(b_i-a_i)\Gamma(\tilde{b}_i-\tilde{a}_i)S(b_i-a_i),$$

$$\mu_i^{p-1}=\frac{\Pi_{j=0}^{p-1}S(b_i-a_j)}{\Pi_{j=0\neq i}^{p-1}S(b_i-b_j)},$$

and

$$\rho_i^{p-1}=\frac{\Pi_{j=0}^{p-1}S(b_j-a_i)}{\Pi_{j=0\neq i}^{p-1}S(a_j-a_i)}.$$

For w real and $|w|\leqslant r<1$ set

$$I_1^i(w)=\int\int_{B/\Gamma}(wt)^{b_p-2}U_i(wt)(\overline{wt})^{\tilde{b}_p-2}\tilde{U}_i(\overline{wt})d^2t$$

and expand $U_i(t)$ [resp. $\tilde{U}_i(\overline{t})$] as a series Σ_n (resp. Σ_m). The integration on the azimuthal angle ϕ yields at once

$$m=n+b_p-\tilde{b}_p-b_i+\tilde{b}_i.$$

The integral over the modulus of t is also straightforward and yields an additional factor

$$\frac{1}{2}\frac{\Gamma(n+b_p-b_i)}{\Gamma(n+b_p-b_i+1)}(w^2)^{n+b_p-b_i}.$$

Collecting all the pieces we get

$$I_1^i(w)=\pi\mu_{p-1}\mu_i^{p-1}w^{2(b_p-b_i-1)}\,{}_{2p+1}G_{2p}^i(w^2),$$

where ${}_{2p+1}G_{2p}^i(w^2)$ is the unrenormalized hyper geometric function the upper parameters of which are $a_j-b_i+1,\tilde{a}_j-b_i+1+b_p-\tilde{b}_p,b_p-b_i$ and the lower ones read $b_k-b_i+1,\tilde{b}_k-b_i+1+b_p-\tilde{b}_p,b_p-b_i+1,1+b_p-\tilde{b}_p-b_i+\tilde{b}_i$.

Now define

$$f_R(w)=\pi^2\mu_{p-1}\frac{1}{2i\pi}\int_{C_R}dt\prod_{j=0}^{p-1}\frac{\Gamma(1-b_j-t)\Gamma(b_p-\tilde{b}_p+\tilde{a}_j+t)}{\Gamma(1-a_j-t)\Gamma(b_p-\tilde{b}_p+\tilde{b}_j+t)}\frac{\Gamma(t+b_p-1)}{\Gamma(t+b_p)}w^{2(b_p-1+t)},$$

where C_R is a loop beginning and ending at $+\infty$ and encircling all poles of $\Gamma(\cdots-t)$ once in the negative direction but none of the poles of $\Gamma(\cdots+t)$. This yields at once

$$I_1(w)=f_R(w).$$

The same method holds for $I_2(w)$, w real and $|w|\geqslant r>1$, with the integration over the azimuthal angle yielding $n=m+b_p-\tilde{b}_p-a_i+\tilde{a}_i$ while the integration on the modulus of t gives

$$\frac{1}{2}\frac{\Gamma(\tilde{a}_i-\tilde{b}_p+1+m)}{\Gamma(\tilde{a}_i-\tilde{b}_p+2+m)}(w^2)^{-m-1+b_{\tilde{p}}-a_{\tilde{i}}}.$$

As before $I_2(w)$ is a complicated sum of G functions.

Now define

$$f_L(w)=(-1)^{s-\tilde{s}}\pi^2\mu_{p-1}\frac{1}{2i\pi}\int_{C_l}dt \times\prod_{j=0}^{p-1}\frac{\Gamma(1-b_j-t)\Gamma(b_p-\tilde{b}_p+\tilde{a}_j+t)}{\Gamma(1-a_j-t)\Gamma(b_p-\tilde{b}_p+\tilde{b}_j+t)}\frac{\Gamma(t+b_p-1)}{\Gamma(t+b_p)}w^{2(b_p-1+t)},$$

where C_L is a loop beginning and ending at $-\infty$ and encircling all poles of $\Gamma(\cdots+t)$ once in the positive direction but none of the poles of $\Gamma(\cdots-t)$.

It is easy to check that

$$f_L=-I_2(w)+\text{residus at}\quad t=1-b_p.$$

Indeed

$$\rho_i^{p-1}=(-1)^{s-\tilde{s}}\frac{\Pi_{j=0}^{p-1}S(\tilde{b}_j-\tilde{a}_i)}{\Pi_{j=0\neq i}^{p-1}S(\tilde{a}_j-\tilde{a}_i)}.$$

But Cauchy theorem implies that

$$f_L(w)=f_R(w),$$

so that in the limit $w\to 1$ we find

$$I=\pi^2\mu_{p-1}\prod_{j=0}^{p-1}\frac{\Gamma(b_p-b_j)\Gamma(1-\tilde{b}_p+\tilde{a}_j)}{\Gamma(b_p-a_j)\Gamma(1-\tilde{b}_p+\tilde{b}_j)}$$

or equivalently

$$I=\mu_{p-1}\prod_{j=0}^{p-1}\frac{S(b_p-a_j)}{S(b_p-b_j)}\prod_{j=0}^{p-1}\frac{\Gamma(1+a_j-b_p)\Gamma(1-\tilde{b}_p+\tilde{a}_j)}{\Gamma(1-b_p+b_j)\Gamma(1+\tilde{b}_j-\tilde{b}_p)}.$$

At this stage it is worth noticing that

$$\mu_p=\mu_{p-1}\Gamma(b_p-a_p)\Gamma(\tilde{b}_p-\tilde{a}_p)S(b_p-a_p),$$

which can be recast as

$$(-1)^{b_p-\tilde{b}_p-(a_p-\tilde{a}_p)}\mu_{p-1}\pi^2=\frac{\mu_p}{\Gamma(1+a_p-b_p)\Gamma(1+\tilde{a}_p-\tilde{b}_p)S(b_p-a_p)}.$$

This yields at once

$$I=(-1)^{b_p-\tilde{b}_p-(a_p-\tilde{a}_p)}\lambda_{p+1}^p.$$

This is the expected result.

As a nice application we may recover the generalized Euler formula, namely calculate

$$I=\int t^{a-1}U_0(t)\overline{t}^{\tilde{a}-1}\tilde{U}_0(\overline{t})d^2t,$$

where $U_0(t)=(1-t)^{b-1}={}_1F_0(b-1,t)$. If we follow the method presented above we are led to calculate

$$f_R=\frac{1}{2i\pi}\int_{C_R}dt\,\frac{\Gamma(-t)\Gamma(a-\tilde{a}+1-\tilde{b}+t)}{\Gamma(b-t)\Gamma(a-\tilde{a}+1+t)}\,\frac{\Gamma(t+a)}{\Gamma(t+a+1)}$$

since by identification $b_1=a-1$, $a_0=1-b$, it is easy to get that

$$f_R=IS(b)\Gamma(1-b)\Gamma(1-\tilde{b})\pi^2.$$

By picking the pole at $t=-a$, we get at once

$$f_L=\frac{\Gamma(a)\Gamma(1-\tilde{a}-\tilde{b})}{\Gamma(b+a)\Gamma(1-\tilde{a})}.$$

Collecting all the pieces the final result reads

$$I=\pi\frac{\Gamma(a)\Gamma(b)\Gamma(1-\tilde{a}-\tilde{b})}{\Gamma(1-\tilde{b})\Gamma(b+a)\Gamma(1-\tilde{a})}.$$

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On the uniform asymptotic expansion of the Legendre functions

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(Received 12 November 2002; accepted 22 November 2002)

A uniform expansion of the Legendre functions of large indices is considered by using the WKB approach. We obtain the recurrent formula for the coefficients of uniform expansion and compare them with the uniform expansion of the Bessel function. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1559414]

I. INTRODUCTION

A uniform expansion of special functions is a very useful representation of them which is used in many branches of science. It is well-known; an example is the Debay uniform expansion of the Bessel functions.[1] To obtain the uniform expansion one usually uses the complicated calculations which exploit a contour integral representation of the function (see, for example, Ref. 4). In this article we use the WKB approach to obtain a uniform expansion for the Legendre functions. Previously, this question was analyzed by Thorne in Ref. 8 by using a different approach and in Ref. 2 for the particular case of the Legendre equation. We would like to note that this special case of calculations plays an important role in the so called functional methods which are at present the most powerful method (see Ref. 7).

The organization of this article is as follows. First of all, in Sec. II we reobtain the Debay formulas for the uniform expansion of the Bessel function by using the WKB approach. In Sec. III, we apply the same method to the Legendre functions and their derivative. The Appendix contains the list of the first four coefficients in manifest form.

II. UNIFORM EXPANSION OF THE BESSEL FUNCTIONS

In this section we reobtain the well-known[1] uniform asymptotic expansion for the Bessel functions of the second kind, $I_n(n\lambda)$ and $K_n(n\lambda)$ for large value of n.

These functions obey the following differential equation,

$$W'' + \frac{1}{\lambda} W' = n^2 \left(1 + \frac{1}{\lambda^2} \right) W, \tag{1}$$

where the prime is the derivative with respect λ.

Let us represent the solution of the above equation as a series over small value of $1/n$:

$$W = C e^{nS_{-1} + S_0} \sum_{k=0}^{\infty} n^{-k} \omega_k \tag{2}$$

with $\omega_0 = 1$. Using this expression in Eq. (1) we obtain the chain of equations

$$S'_{-1} = \varepsilon \sqrt{1 + \frac{1}{\lambda^2}}, \tag{3a}$$

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$$S_0' = -\frac{1}{2S_{-1}'}\left\{S_{-1}'' + \frac{1}{\lambda}S_{-1}'\right\}, \tag{3b}$$

$$\omega_{k+1}' = -\frac{\varepsilon}{2}\left(\frac{\lambda\omega_k'}{\sqrt{1+\lambda^2}}\right)' - \frac{\varepsilon}{8}\frac{\lambda(\lambda^2-4)}{(1+\lambda^2)^{5/2}}\omega_k, \tag{3c}$$

where $\varepsilon=\pm 1$ and $k=0,1,\ldots$. With the new variable $t=1/\sqrt{1+\lambda^2}$, the last equation may be rewritten in more simple form,

$$\dot{\omega}_{k+1} = \frac{\varepsilon}{2}(t^2(1-t^2)\dot{\omega}_k)^{\cdot} + \frac{\varepsilon}{8}(1-5t^2)\omega_k, \tag{3d}$$

where the dot denotes the derivative with respect to t.

The first integral of Eqs. (3) has the following form,

$$\begin{aligned} S_{-1} &= \varepsilon(\eta(\lambda) + C_{-1}), \\ S_0 &= -\tfrac{1}{4}\ln(1+\lambda^2) + C_0, \\ \omega_{k+1} &= \frac{\varepsilon}{2}t^2(1-t^2)\dot{\omega}_k + \frac{\varepsilon}{8}\int_0^t (1-5t'^2)\omega_k(t')\,dt' + C_{k+1}, \end{aligned} \tag{4}$$

where

$$\eta(\lambda) = \sqrt{1+\lambda^2} + \ln\frac{\lambda}{1+\sqrt{1+\lambda^2}}. \tag{5}$$

To find the set of constants C_k, $k=-1,0,\ldots$, we take the limit $\lambda\to\infty$ in our expressions (2) and (4) and compare them with well-known asymptotic formulas[1]

$$I_n(n\lambda) \approx \frac{1}{\sqrt{2\pi n\lambda}}e^{n\lambda}\left(1+O\left(\frac{1}{\lambda}\right)\right), \quad K_n(n\lambda) \approx \sqrt{\frac{\pi}{2n\lambda}}e^{-n\lambda}\left(1+O\left(\frac{1}{\lambda}\right)\right). \tag{6}$$

Because the next term of expansion is $O(1/\lambda)$, we have to set $C_k=0$ for $k\geqslant 1$. Taking this into account we have the following expression for uniform expansion in the limit $\lambda\to\infty$:

$$W \approx \frac{1}{\sqrt{\lambda}}e^{\varepsilon n\lambda}Ce^{\varepsilon nC_{-1}+C_0}. \tag{7}$$

Therefore, $\varepsilon=1$ corresponds to the uniform expansion of $I_n(n\lambda)$ and $\varepsilon=-1$ to the $K_n(n\lambda)$. For coincidence of the expression (7) with the asymptotic expansions (6) we have to set $C_{-1}=C_0=0$ and $C=1/\sqrt{2\pi n}$ for $\varepsilon=1$, and $C=\sqrt{\pi/2n}$ for $\varepsilon=-1$.

Therefore, we arrive at the following well-known formulas for uniform expansion of the Bessel functions:

$$\begin{aligned} I_n(n\lambda) &= \sqrt{\frac{t}{2\pi n}}e^{n\eta(\lambda)}\sum_{k=0}^{\infty} n^{-k}\omega_k(t), \\ K_n(n\lambda) &= \sqrt{\frac{\pi t}{2n}}e^{-n\eta(\lambda)}\sum_{k=0}^{\infty} (-n)^{-k}\omega_k(t), \end{aligned} \tag{8}$$

where

$$\omega_{k+1}=\frac{1}{2}t^2(1-t^2)\dot{\omega}_k+\frac{1}{8}\int_0^t(1-5t'^2)\omega_k(t')\mathrm{d}t'. \tag{9}$$

In order to find formulas for the derivative of the Bessel functions we represent them in the following form:

$$\frac{1}{n}W'=\widetilde{C}e^{n\widetilde{S}_{-1}+\widetilde{S}_0}\sum_{k=0}^{\infty}n^{-k}\widetilde{\omega}_k. \tag{10}$$

Comparing the derivative of Eq. (2) with respect to λ with the above formula we obtain

$$\begin{gathered}\widetilde{S}_{-1}=S_{-1},\\ \widetilde{S}_0=S_0+\ln(\varepsilon S'_{-1}),\\ \widetilde{C}=\varepsilon C,\end{gathered} \tag{11}$$

$$\widetilde{\omega}_k=\omega_k+\frac{\varepsilon}{2}t(t^2-1)\omega_{k-1}+\varepsilon t^2(t^2-1)\dot{\omega}_{k-1}.$$

Therefore, with these expressions we arrive at the well-known formulas for uniform expansion of the derivative of the Bessel functions,

$$\begin{aligned}\frac{1}{n}I'_n(n\lambda)&=\frac{1}{\sqrt{2\pi nt}}\frac{1}{\lambda}e^{n\eta(\lambda)}\sum_{k=0}^{\infty}n^{-k}\overline{\omega}_k(t),\\ \frac{1}{n}K'_n(n\lambda)&=-\sqrt{\frac{\pi}{2nt}}\frac{1}{\lambda}e^{-n\eta(\lambda)}\sum_{k=0}^{\infty}(-n)^{-k}\overline{\omega}_k(t),\end{aligned} \tag{12}$$

where

$$\overline{\omega}_k=\omega_k+\tfrac{1}{2}t(t^2-1)\omega_{k-1}+t^2(t^2-1)\dot{\omega}_{k-1}. \tag{13}$$

III. UNIFORM EXPANSION OF THE LEGENDRE FUNCTIONS

In this section we employ the same approach for the Legendre functions. We consider the following equation,

$$(1-x^2)\Psi''-2x\Psi'-\left(n^2\gamma^2+\frac{n^2}{1-x^2}+2\xi\right)\Psi=0, \tag{14}$$

which has appeared in the context of quantum field theory in curved space–time.[5,6] Here $x\in(-1,1)$, n,γ and ξ are real numbers, and the prime is the derivative with respect to x. The particular case of this equation for $\xi=\frac{1}{8}$ has been considered in Ref. 2.

The solutions of this equation are the Legendre functions of the first and second kinds:

$$P^n_\mu[x],\quad Q^n_\mu[x] \tag{15}$$

with index

$$\mu=-\tfrac{1}{2}+\tfrac{1}{2}\sqrt{1-8\xi-4n^2\gamma^2}. \tag{16}$$

For $\xi=\frac{1}{8}$ these functions are called the cone functions.[1]

We assume $n>0$ and consider the following two independent solutions,

$$p_\mu^n[x]=P_\mu^{-n}[x],$$
$$q_\mu^n[x]=\frac{(-1)^n}{2}(Q_\mu^n[x]+Q_{-\mu-1}^n[x])=-\frac{\pi}{2\sin\pi\mu}P_\mu^n[-x]. \tag{17}$$

They are real functions for arbitrary μ and obey the following Wronskian condition:

$$W(p_\mu^n,q_\mu^n)=\frac{1}{1-x^2}.$$

To obtain the uniform expansion of functions (17) for large number n we represent the solution in the WKB form as follows:

$$\Psi=Ce^{nS_{-1}(x)+S_0(x)}\sum_{k=0}^{\infty}n^{-k}\psi_k(x) \tag{18}$$

with $\psi_0(x)=1$. We would like to note the difference of the uniform expansion in form (18), which is over inverse degree of n, with that considered by Thorne in Ref. 8. He obtained an expansion over inverse degree of $\mu+\frac{1}{2}=\sqrt{1-8\xi-4n^2\gamma^2}/2$.

Substituting the above expression in Eq. (14) we obtain the chain of equations

$$S_{-1}'=\varepsilon\sqrt{\frac{1}{(1-x^2)^2}+\frac{\gamma^2}{1-x^2}},$$
$$S_0'=-\frac{1}{2}\left\{\frac{S_{-1}''}{S_{-1}'}-\frac{2x}{1-x^2}\right\},$$
$$\psi_1'=-\frac{1}{2S_{-1}'}\left\{S_0'^2+S_0''-\frac{2x}{1-x^2}S_0'-\frac{2\xi}{1-x^2}\right\}, \tag{19}$$
$$\psi_{k+1}'=-\frac{\varepsilon}{2}\left\{\frac{(1-x^2)\psi_k'}{\sqrt{1+\gamma^2(1-x^2)}}\right\}'+\psi_1'\psi_k,\quad k\geqslant 1,$$

where $\varepsilon=\pm 1$.

The first integral of this chain has the following form:

$$S_{-1}(x)=\varepsilon\left[\gamma\arctan\frac{\gamma x}{\sqrt{1+\gamma^2(1-x^2)}}+\frac{1}{2}\ln\frac{(1+x)(1+\gamma^2(1-x)+\sqrt{1+\gamma^2(1-x^2)})}{(1-x)(1+\gamma^2(1+x)+\sqrt{1+\gamma^2(1-x^2)})}+C_{-1}\right],$$
$$S_0(x)=-\tfrac{1}{4}\ln(1+\gamma^2(1-x^2)), \tag{20}$$
$$\psi_{k+1}(x)=C_{k+1}(\varepsilon)-\frac{\varepsilon}{2}\frac{1-x^2}{\sqrt{1+\gamma^2(1-x^2)}}\psi_k'(x)+\varepsilon\int_0^x\left(-\frac{\gamma^2}{8}\left[\frac{2-x'^2}{(1+\gamma^2(1-x'^2))^{3/2}}\right.\right.$$
$$\left.\left.-\frac{5x'^2}{(1+\gamma^2(1-x'^2))^{5/2}}\right]+\frac{\xi}{(1+\gamma^2(1-x'^2))^{1/2}}\right)\psi_k(x')\,dx'.$$

We have already set the constant $C_0=0$. This leads to redefinition of the constant C only.

The formulas look simpler in terms of the new variable

$$v=\frac{x}{\sqrt{1+\gamma^2(1-x^2)}}, \tag{21}$$

instead of x. This quantity obeys the inequality: $|v|\leqslant|x|<1$. In terms of this variable we have

$$S_{-1}(v)=\varepsilon\left\{-\frac{1}{2}\ln\frac{1-v}{1+v}+\gamma\arctan\gamma v+C_{-1}\right\}, \tag{22a}$$

$$S_0(v)=\frac{1}{4}\ln\frac{1+\gamma^2v^2}{1+\gamma^2}, \tag{22b}$$

$$\begin{aligned}\psi_{k+1}(v)=C_{k+1}&-\frac{\varepsilon}{2}\frac{(1-v^2)(1+\gamma^2v^2)}{(1+\gamma^2)}\dot{\psi}_k(v)\\&+\frac{\varepsilon\gamma^2}{8(1+\gamma^2)}\int_0^v dv'\left\{5v'^2+\frac{1}{\gamma^2}-1+(8\xi-1)\frac{1+\gamma^2}{\gamma^2(1+\gamma^2v'^2)}\right\}\psi_k(v').\end{aligned} \tag{22c}$$

In the above formulas the dot denotes the derivative with respect to new variable v.

In order to find constants C_k we have to compare our formulas with exact expressions for the Legendre functions at a fixed point. For this reason we take the limit $x\to1$ in our formulas,

$$\Psi\approx C\left(\frac{1-x}{2}\right)^{-\varepsilon n/2}\exp\left[n\varepsilon\left(C_{-1}-\frac{1}{2}\ln(\gamma^2+1)+\gamma\arctan\gamma\right)\right], \tag{23}$$

and compare them with well-known expressions[3] for the Legendre functions at point $x=1$:

$$\begin{aligned}p^n_\mu[x]=P^{-n}_\mu[x]&\approx\frac{1}{n!}\left(\frac{1-x}{2}\right)^{n/2},\\q^n_\mu[x]=\frac{(-1)^n}{2}(Q^n_\mu[x]+Q^n_{-\mu-1}[x])&\approx\frac{(n-1)!}{2}\left(\frac{1-x}{2}\right)^{-n/2}.\end{aligned} \tag{24}$$

Therefore, from Eqs. (23) and (24) we observe that $\varepsilon=-1$ corresponds to $p^n_\mu[x]$ with $C=1/n!$, $\varepsilon=+1$ corresponds to $q^n_\mu[x]$ with $C=(n-1)!/2$, and

$$C_{-1}=\tfrac{1}{2}\ln(1+\gamma^2)-\gamma\arctan\gamma \tag{25}$$

for both signs of ε. Furthermore, the coefficients $\psi_k(v)$ must obey the following condition:

$$\psi_k(1)=0. \tag{26}$$

Taking into account the above formulas we arrive at the following expression for uniform expansion of the Legendre's functions,

$$p^n_\mu[x]=\frac{1}{n!}\left[\frac{1+\gamma^2v^2}{1+\gamma^2}\right]^{1/4}e^{nS_{-1}(v)}\sum_{k=0}^{\infty}n^{-k}\psi_k(v), \tag{27a}$$

$$q^n_\mu[x]=\frac{(n-1)!}{2}\left[\frac{1+\gamma^2v^2}{1+\gamma^2}\right]^{1/4}e^{-nS_{-1}(v)}\sum_{k=0}^{\infty}(-n)^{-k}\psi_k(v), \tag{27b}$$

where

$$S_{-1}(v)=\frac{1}{2}\ln\frac{1-v}{(1+v)(1+\gamma^2)}-\gamma[\arctan\gamma v-\arctan\gamma], \tag{27c}$$

$$\psi_{k+1}(v)=\frac{(1-v^2)(1+\gamma^2v^2)}{2(1+\gamma^2)}\dot{\psi}_k(v)-\frac{\gamma^2}{8(1+\gamma^2)}\times\int_1^v dv'\left\{5v'^2+\frac{1}{\gamma^2}-1+(8\xi-1)\frac{1+\gamma^2}{\gamma^2(1+\gamma^2v'^2)}\right\}\psi_k(v'). \tag{27d}$$

Taking into account the same procedure as we used above for the derivative of the Bessel functions we obtain the following formulas for uniform expansion of the derivative of functions p_μ^n and q_μ^n:

$$\frac{1}{n}\frac{d}{dx}p_\mu^n[x]=-\frac{1}{n!}\left[\frac{1+\gamma^2v^2}{1+\gamma^2}\right]^{3/4}\frac{1+\gamma^2}{1-v^2}e^{nS_{-1}(v)}\sum_{k=0}^{\infty}n^{-k}\overline{\psi}_k(v), \tag{28a}$$

$$\frac{1}{n}\frac{d}{dx}q_\mu^n[x]=\frac{(n-1)!}{2}\left[\frac{1+\gamma^2v^2}{1+\gamma^2}\right]^{3/4}\frac{1+\gamma^2}{1-v^2}e^{-nS_{-1}(v)}\sum_{k=0}^{\infty}(-n)^{-k}\overline{\psi}_k(v), \tag{28b}$$

$$\overline{\psi}_k(v)=\psi_k(v)-\frac{\gamma^2v(1-v^2)}{2(1+\gamma^2)}\psi_{k-1}(v)-\frac{(1-v^2)(1+\gamma^2v^2)}{1+\gamma^2}\dot{\psi}_{k-1}(v). \tag{28c}$$

The first four coefficients ψ_k and $\overline{\psi}_k$ are listed in the Appendix.

From the recurrent formula (27d) it is possible to find the value of the coefficients $\psi(v)$ for $\gamma\to\infty$. Indeed, comparing Eq. (27d) in the limit $v\to0$ and Eq. (9) in the limit $t\to1$ we obtain the following relation:

$$\psi_k(0)=(-1)^{k+1}\omega_k(1). \tag{29}$$

Now we represent formulas obtained in a slightly different form which is close to expansion of the Bessel functions. We set $x=\cos\epsilon$ and $\gamma=\lambda/\sin\epsilon$ and use the asymptotic expansion for the gamma function from Ref. 4:

$$\ln n!=\left(n+\frac{1}{2}\right)\ln n-n+\frac{1}{2}\ln2\pi+\sum_{k=1}^{\infty}\frac{B_{2k}}{2k(2k-1)}\frac{1}{n^{2k-1}},$$

$$\ln(n-1)!=\left(n-\frac{1}{2}\right)\ln n-n+\frac{1}{2}\ln2\pi+\sum_{k=1}^{\infty}\frac{B_{2k}}{2k(2k-1)}\frac{1}{n^{2k-1}},$$

where B_k are the Bernoulli numbers.

With these notations one has

$$p_\mu^n[\cos\epsilon]=\sqrt{\frac{t}{2\pi n}}e^{n\tilde{\eta}}\sum_{k=0}^{\infty}n^{-k}\psi_k^+(v)\left(\frac{\sin\epsilon}{\lambda n}\right)^n,$$

$$q_\mu^n[\cos\epsilon]=\sqrt{\frac{\pi t}{2n}}e^{-n\tilde{\eta}}\sum_{k=0}^{\infty}(-n)^{-k}\psi_k^+(v)\left(\frac{\sin\epsilon}{\lambda n}\right)^{-n}, \tag{30}$$

$$\frac{1}{n}\frac{dp_\mu^n[x]}{dx_{|x=\cos\epsilon}}=-\sqrt{\frac{1}{2\pi nt}}e^{n\tilde{\eta}}\sum_{k=1}^{\infty}n^{-k}\overline{\psi}_k^+(v)\left(\frac{\sin\epsilon}{\lambda n}\right)^n\frac{1}{\sin^2\epsilon},$$

$$\frac{1}{n}\frac{dq_\mu^n[x]}{dx}_{|x=\cos\epsilon}=\sqrt{\frac{\pi}{2nt}}e^{-n\tilde{\eta}}\sum_{k=1}^{\infty}(-n)^{-k}\overline{\psi}_k^+(v)\left(\frac{\sin\epsilon}{\lambda n}\right)^n\frac{1}{\sin^2\epsilon},$$

where

$$\tilde{\eta}=\ln\frac{\lambda}{\sqrt{1+\lambda^2}+\cos\epsilon}-\frac{\lambda}{\sin\epsilon}\left[\arctan\frac{\sin\epsilon}{\lambda}-\arctan\frac{\tan\epsilon}{\lambda t}\right]+1, \tag{31a}$$

$$t=\frac{1}{\sqrt{1+\lambda^2}},\quad v=t\cos\epsilon, \tag{31b}$$

$$\mu=-\frac{1}{2}+\frac{1}{2}\sqrt{1-8\xi-\frac{4n^2\lambda^2}{\sin^2\epsilon}}, \tag{31c}$$

and the coefficients ψ_k^+ are found from the relation

$$\sum_{k=0}^{\infty}n^{-k}\psi_k^+(v)=\exp\left(-\sum_{k=1}^{\infty}\frac{B_{2k}}{2k(2k-1)n^{2k-1}}\right)\sum_{k=0}^{\infty}n^{-k}\psi_k(v) \tag{31d}$$

by comparing the same degree of n in the left and right hand sides.

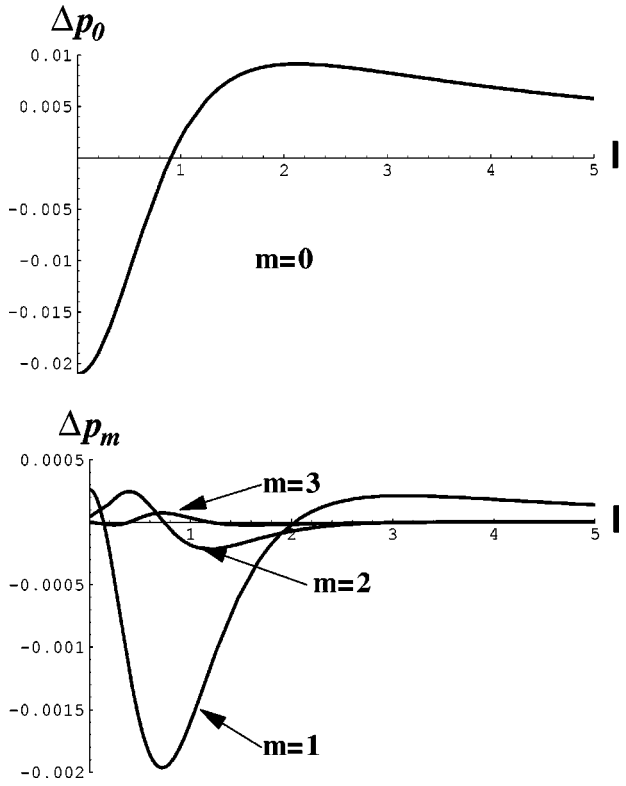

FIG. 1. The plot of the relative errors $\Delta p_m=(p_\mu^n-(p_\mu^n)_m)/p_\mu^n$ versus those of λ for $\epsilon=0.1$, $\xi=0$ and $n=4$. Here $(p_\mu^n)_m$ is the uniform expansion of the Legendre function p_μ^n up to degree m.

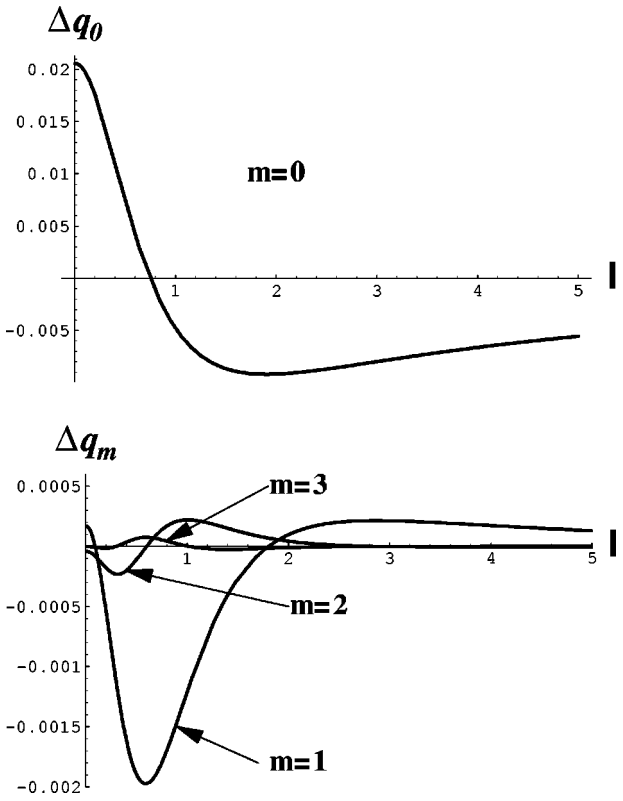

FIG. 2. The plot of the relative errors $\Delta q_m=(q_\mu^n-(q_\mu^n)_m)/q_\mu^n$ versus those of λ for $\epsilon=0.1$, $\xi=0$ and $n=4$. Here $(q_\mu^n)_m$ is the uniform expansion of the Legendre function q_μ^n up to degree m.

The expressions (30) have a form similar to that for the Bessel function expansion given by Eq. (8). Furthermore, it is easy to see that in the limit $\epsilon\to 0$ (the argument of the Legendre functions tends to unit and the lower index tends to infinity) the uniform expansion obtained is transformed to the uniform expansion of the Bessel functions below:

$$\lim_{\epsilon\to 0}\mu^n p_\mu^n[\cos\epsilon]=i^n I_n(n\lambda), \tag{32}$$

$$\lim_{\epsilon\to 0}\mu^{-n} q_\mu^n[\cos\epsilon]=i^{-n} K_n(n\lambda),$$

as it should be according to well-known formulas[3]

$$\lim_{z\to\infty} z^n P_z^{-n}\left[\cos\frac{x}{z}\right]=J_n(x), \tag{33}$$

$$\lim_{z\to\infty} z^n Q_z^{-n}\left[\cos\frac{x}{z}\right]=-\frac{\pi}{2}Y_n(x),$$

where $x=in\lambda$ and $z=in\lambda/\epsilon$. In this limit the function $\tilde{\eta}$ given by Eq. (31a) coincides with function η (5) in the uniform expansion of Bessel functions:

$$\lim_{\epsilon\to 0}\tilde{\eta}=\ln\frac{\lambda}{\sqrt{1+\lambda^2}+1}+\sqrt{1+\lambda^2}. \tag{34}$$

The numerical calculation of the relative errors $\Delta p_m=(p^n_\mu-(p^n_\mu)_m)/p^n_\mu$ and $\Delta q_m=(q^n_\mu-(q^n_\mu)_m)/q^n_\mu$ are plotted in Figs. 1 and 2 for different $m=0,1,2,3$ as a function of λ, where $(p^n_\mu)_m$ and $(q^n_\mu)_m$ are the uniform expansions of the Legendre functions p^n_μ and q^n_μ up to degree n^{-m}. The difference is smaller the greater λ.

In conclusion we would like to summarize the results. In this article we obtain the uniform expansion for the Legendre functions $p^n_\mu[x]$ and $q^n_\mu[x]$ given by Eq. (17) for large indices n and $\mu=-\frac{1}{2}+\frac{1}{2}\sqrt{1-8\xi-4n^2\gamma^2}$ as a series over inverse degree on n. These expansions of the functions are given by Eq. (27) and by Eq. (28) for their derivatives with respect to argument x. The coefficients of expansion may be found from recurrent chain of equations (27d) and (28c). The first four coefficients are listed in the Appendix.

ACKNOWLEDGMENTS

The author would like to thank Dr. M. Bordag for stimulation of this work and for reading this manuscript. The work was supported in part by the Russian Foundation for Basic Research Grant No. N 02-02-17177.

APPENDIX: MANIFEST FORM OF FIRST FOUR COEFFICIENTS

Below are the expressions for first four coefficients ψ_k and $\overline{\psi_k}$ in which we introduced for simplicity the following notations:

$$\delta=\arctan[\gamma]-\arctan[\gamma v],\quad \zeta=\xi-\frac{1}{8},\quad v=\frac{x}{\sqrt{1+\gamma^2(1-x^2)}},\tag{A1}$$

$$\begin{aligned}
\psi_0&=1,\\
\psi_1&=\frac{\delta\zeta}{\gamma}+\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}+\frac{v(\gamma^2-1)}{8}-\frac{5v^3\gamma^2}{24}\right],\\
\psi_2&=\frac{1}{2}\left(\frac{\delta\zeta}{\gamma}\right)^2+\frac{\delta\zeta}{\gamma}\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}+\frac{v(\gamma^2-1)}{8}-\frac{5v^3\gamma^2}{24}\right]+\frac{\zeta(-1+v^2)}{2(\gamma^2+1)}\\
&\quad+\frac{1}{(\gamma^2+1)^2}\left[\frac{4\gamma^4+84\gamma^2-63}{1152}+\frac{v(\gamma^2-1)(2\gamma^2+3)}{192}+\frac{v^2(9\gamma^4-58\gamma^2+9)}{128}\right.\\
&\quad\left.-\frac{5v^3\gamma^2(2\gamma^2+3)}{576}-\frac{77v^4\gamma^2(\gamma^2-1)}{192}+\frac{385v^6\gamma^4}{1152}\right],
\end{aligned}\tag{A2}$$

$$\begin{aligned}
\psi_3&=\frac{1}{6}\left(\frac{\delta\zeta}{\gamma}\right)^3+\frac{1}{2}\left(\frac{\delta\zeta}{\gamma}\right)^2\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}+\frac{v(\gamma^2-1)}{8}-\frac{5v^3\gamma^2}{24}\right]+\frac{\delta\zeta}{\gamma}\left[\frac{1}{(\gamma^2+1)^2}\right.\\
&\quad\times\left\{\frac{4\gamma^4+84\gamma^2-63}{1152}+\frac{v(\gamma^2-1)(2\gamma^2+3)}{192}+\frac{v^2(9\gamma^4-58\gamma^2+9)}{128}-\frac{5v^3\gamma^2(2\gamma^2+3)}{576}\right.\\
&\quad\left.\left.-\frac{77v^4\gamma^2(\gamma^2-1)}{192}+\frac{385v^6\gamma^4}{1152}\right\}+\frac{\zeta}{\gamma^2+1}\left\{-\frac{2\gamma^2+1}{2\gamma^2}+\frac{v^2}{2}\right\}\right]+\frac{\zeta^2(1-v)}{2\gamma^2(\gamma^2+1)}\\
&\quad+\frac{\zeta}{(\gamma^2+1)^2}\left[-\frac{2\gamma^2+7}{48}-\frac{v(3\gamma^2-11)}{16}+\frac{v^2(2\gamma^2+3)}{48}+\frac{v^3(44\gamma^2-29)}{48}-\frac{35v^5\gamma^2}{48}\right]\\
&\quad+\frac{1}{(\gamma^2+1)^3}\left[-\frac{1112\gamma^6+1116\gamma^4-918\gamma^2+5265}{414720}+\frac{v(4\gamma^6+728\gamma^4-4323\gamma^2+711)}{9216}\right.
\end{aligned}$$

$$+\frac{v^2(2\gamma^2+3)(9\gamma^4-58\gamma^2+9)}{3072}+\frac{v^3(2005\gamma^6-37671\gamma^4+37566\gamma^2-2025)}{27648}$$
$$-\frac{77v^4(\gamma^2-1)(2\gamma^2+3)}{4608}-\frac{13v^5\gamma^2(1053\gamma^4-3706\gamma^2+1053)}{15360}$$
$$+\frac{385v^6\gamma^4(2\gamma^2+3)}{27648}+\frac{17017v^7\gamma^4(\gamma^2-1)}{9216}-\frac{85085v^9\gamma^6}{82944}\Bigg];$$

$$\psi_0^+=\psi_0=1,$$
$$\psi_1^+=\psi_1-\frac{1}{12},$$
$$\psi_2^+=\psi_2-\frac{1}{12}\psi_1+\frac{1}{288}, \tag{A3}$$
$$\psi_3^+=\psi_3-\frac{1}{12}\psi_2+\frac{1}{288}\psi_1+\frac{139}{51840};$$

$$\overline{\psi_0}=1,$$
$$\overline{\psi_1}=\frac{\delta\zeta}{\gamma}+\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}-\frac{v(3\gamma^2+1)}{8}+\frac{7v^3\gamma^2}{24}\right],$$
$$\overline{\psi_2}=\frac{1}{2}\left(\frac{\delta\zeta}{\gamma}\right)^2+\frac{\delta\zeta}{\gamma}\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}-\frac{v(3\gamma^2+1)}{8}+\frac{7v^3\gamma^2}{24}\right]+\frac{\zeta(1-v^2)}{2(\gamma^2+1)} \tag{A4}$$
$$+\frac{1}{(\gamma^2+1)^2}\left[\frac{(2\gamma^2-27)(2\gamma^2-3)}{1152}-\frac{v(3\gamma^2+1)(2\gamma^2+3)}{192}-\frac{v^2(15\gamma^4-62\gamma^2+7)}{128}\right.$$
$$\left.+\frac{7v^3\gamma^2(2\gamma^2+3)}{576}+\frac{v^4\gamma^2(99\gamma^2-79)}{192}-\frac{455v^6\gamma^4}{1152}\right],$$
$$\overline{\psi_3}=\frac{1}{6}\left(\frac{\delta\zeta}{\gamma}\right)^3+\frac{1}{2}\left(\frac{\delta\zeta}{\gamma}\right)^2\frac{1}{\gamma^2+1}\left[\frac{2\gamma^2+3}{24}-\frac{v(3\gamma^2+1)}{8}+\frac{7v^3\gamma^2}{24}\right]$$
$$+\frac{\delta\zeta}{\gamma}\left[\frac{1}{(\gamma^2+1)^2}\times\left\{\frac{(2\gamma^2-3)(2\gamma^2-27)}{1152}-\frac{v(3\gamma^2+1)(2\gamma^2+3)}{192}-\frac{v^2(15\gamma^4-62\gamma^2+7)}{128}\right.\right.$$
$$\left.+\frac{7v^3\gamma^2(2\gamma^2+3)}{576}+\frac{v^4\gamma^2(99\gamma^2-79)}{192}-\frac{455v^6\gamma^4}{1152}\right\}-\frac{\zeta}{\gamma^2+1}\left\{\frac{1}{2\gamma^2}+\frac{v^2}{2}\right\}\Bigg]+\frac{\zeta^2(1-v)}{2\gamma^2(\gamma^2+1)}$$
$$+\frac{\zeta}{(\gamma^2+1)^2}\left[\frac{2\gamma^2-1}{48}+\frac{v(3\gamma^2-7)}{16}-\frac{v^2(2\gamma^2+3)}{48}-\frac{v^3(44\gamma^2-25)}{48}+\frac{35v^5\gamma^2}{48}\right]$$
$$+\frac{1}{(\gamma^2+1)^3}\left[-\frac{1112\gamma^6+5436\gamma^4+1242\gamma^2-1215}{414720}-\frac{v(12\gamma^6+904\gamma^4-4281\gamma^2+585)}{9216}\right.$$
$$-\frac{v^2(2\gamma^2+3)(15\gamma^4-62\gamma^2+7)}{3072}-\frac{v^3(2807\gamma^6-42897\gamma^4+37458\gamma^2-1863)}{27648}$$
$$+\frac{v^4(99\gamma^2-79)(2\gamma^2+3)}{4608}+\frac{11v^5\gamma^2(1521\gamma^4-4762\gamma^2+1241)}{15360}$$
$$\left.-\frac{455v^6\gamma^4(2\gamma^2+3)}{27648}-\frac{385v^7\gamma^4(51\gamma^2-47)}{9216}+\frac{95095v^9\gamma^6}{82944}\right].$$

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Toward solving the inhomogeneous Bloch equation

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(Received 16 June 2002; accepted 17 January 2003)

The homogeneous Bloch equation reduces to the Riccati equation. By linearizing the Riccati equation, a set of three solutions of the homogeneous Bloch equation is found. The fundamental matrix becomes singular. We clarify the utility and limitation of our approach to solve the homogeneous Bloch equation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1561155]

I. INTRODUCTION

Since the Bloch equation[1] was proposed in 1946, various workers have tried to solve it analytically. As yet few exact solutions are known.[2] Very recently, an interesting solution was found to the homogeneous Bloch equation.[3] This was done by solving the Riccati equation to which the homogeneous Bloch equation reduces. The reason why we persist in solving the homogeneous Bloch equation analytically is due to the fact that the inhomogeneous Bloch equation is uniquely solved by finding a fundamental system in terms of a set of three independent solutions of the homogeneous Bloch equation.

The homogeneous Bloch equation is the homogeneous system of first-order linear differential equations and able to reduce to the Riccati equation.[4] The Riccati equation can be cast into the second-order linear differential equation.[5] Thus we provide a set of solutions of the homogeneous Bloch equation. We have found a set of three solutions of the homogeneous Bloch equation. By using these solutions, we can define the 3×3 fundamental matrix. If the fundamental matrix is nonsingular, then we find the unique solution of the inhomogeneous Bloch equation. Unfortunately, the fundamental matrix becomes singular. This means two of them serve as independent solutions.

The purpose of this article is to clarify the utility and limitation of our approach to solving the homogeneous Bloch equation.

In Sec. II we show that the homogeneous Bloch equation reduces to the inhomogeneous system of four second-order linear differential equations. This has been done by linearizing the Riccati equation. Then in Sec. III we solve those differential equations and find the three solutions with the constraint. By using the three solutions above, we find the fundamental matrix in Sec. IV. The final section is devoted to our conclusions.

II. THE LINEARIZED RICCATI EQUATION

The Bloch equation for magnetization with infinite relaxation times is a homogeneous system of three first-order linear differential equations, and given by

$$\dot{\vec{M}} = -\gamma(\vec{B}\times\vec{M}), \tag{1}$$

where a dot means differentiation with respect to time. Here $\vec{M}$ and $\vec{B}$ are the magnetization vector and the applied magnetic field, respectively, and γ is the gyromagnetic ratio.

It immediately follows from Eq. (1) that the magnitude of the magnetization vector is preserved. Thus we can define $\vec{m}$ by

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$$\vec{m}=\frac{\vec{M}}{|\vec{M}|}, \tag{2}$$

which obeys the Bloch equation, i.e.,

$$\dot{\vec{m}}=-\gamma(\vec{B}\times\vec{m}), \tag{3}$$

with

$$\vec{m}\cdot\vec{m}=1. \tag{4}$$

Let us introduce the two variables, ξ and η, defined by

$$m_1+i\,m_2=\xi(1-m_3) \tag{5}$$

and

$$m_1-i\,m_2=\frac{1}{\eta}(m_3-1). \tag{6}$$

Then we find

$$\xi=\frac{m_1+i\,m_2}{1-m_3}=\frac{1+m_3}{m_1-i\,m_2} \tag{7}$$

and

$$\eta=-\frac{1-m_3}{m_1-i\,m_2}=-\frac{m_1+i\,m_2}{1+m_3}, \tag{8}$$

and the relationships between ξ and η such that

$$\xi\eta^*=\xi^*\eta=-1, \tag{9}$$

$$\xi\xi^*=\frac{1+m_3}{1-m_3}, \tag{10}$$

and

$$\eta=-\frac{1-m_3}{1+m_3}\xi. \tag{11}$$

Differentiating Eq. (7) with respect to time and substituting Eq. (3) into it, we find the Riccati equation

$$\dot{\xi}=\tfrac{1}{2}\gamma(B_2+i\,B_1)\,\xi^2-i\,\gamma B_3\,\xi+\tfrac{1}{2}\gamma(B_2-i\,B_1). \tag{12}$$

Similarly, we also find the same Riccati equation for η. Here use has been made of the relationship

$$B_1\,m_2-B_2\,m_1=-\tfrac{1}{2}(B_2+i\,B_1)(m_1+i\,m_2)-\tfrac{1}{2}(B_2-i\,B_1)(m_1-i\,m_2). \tag{13}$$

The Riccati equation (12) can be cast in the more convenient form

$$\dot{\xi}=i\,\dot{\chi}\,e^{-i\psi}\xi^2-i\,\dot{\chi}_3\,\xi-i\,\dot{\chi}\,e^{i\psi}, \tag{14}$$

where we have defined χ and χ_3 by

$$\chi=\frac{1}{2}\gamma\int_{t_0}^{t}B_0(\tau)\,\mathrm{d}\tau \tag{15}$$

and

$$\chi_3=\gamma\int_{t_0}^{t}B_3(\tau)\,\mathrm{d}\tau, \tag{16}$$

with

$$B_2\pm i\,B_1=\pm i\,B_0e^{\mp i\psi}, \tag{17}$$

$$B_0=\sqrt{B_1^2+B_2^2}, \tag{18}$$

and

$$\psi=\cos^{-1}\left(\frac{B_1}{B_0}\right)=\sin^{-1}\left(\frac{B_2}{B_0}\right)=\tan^{-1}\left(\frac{B_2}{B_1}\right). \tag{19}$$

The linearized Riccati equation has the form

$$\ddot{u}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-i(\dot{\psi}+\dot{\chi}_3)\right]\dot{u}+(\dot{\chi})^2u=0, \tag{20}$$

and an equation of this form results from the substitution

$$\xi=i\,\frac{1}{\dot{\chi}}\left(\frac{\dot{u}}{u}\right)e^{i\psi} \tag{21}$$

in the Riccati equation (14).

The linearized Riccati equation (20) yields

$$\mathrm{Re}\,\ddot{u}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\mathrm{Re}\,\dot{u}+(\dot{\chi})^2\,\mathrm{Re}\,u=(\dot{\psi}+\dot{\chi}_3)\,\mathrm{Im}\,\dot{u} \tag{22}$$

and

$$\mathrm{Im}\,\ddot{u}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\mathrm{Im}\,\dot{u}+(\dot{\chi})^2\,\mathrm{Im}\,u=-(\dot{\psi}+\dot{\chi}_3)\,\mathrm{Re}\,\dot{u}. \tag{23}$$

These are the inhomogeneous system of two second-order linear differential equations. The homogeneous second-order linear differential equations in Eqs. (22) and (23) can be solved and the general solutions are given by

$$\mathrm{Re}\,u=C_{11}\cos\chi+C_{12}\sin\chi \tag{24}$$

and

$$\mathrm{Im}\,u=C_{21}\cos\chi+C_{22}\sin\chi, \tag{25}$$

where C_{ij} $(i,j=1,2)$ are the constants of integration. By adapting Lagrange's method of variation of constants to the inhomogeneous system of second-order linear differential equations, Eqs. (22) and (23), we find

$$\ddot{C}_{11}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{11}+2\dot{\chi}\,\dot{C}_{12}=(\dot{\psi}+\dot{\chi}_3)(\dot{C}_{21}+\dot{\chi}\,C_{22})\,, \tag{26}$$

$$\ddot{C}_{12}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{12}-2\dot{\chi}\,\dot{C}_{11}=(\dot{\psi}+\dot{\chi}_3)(\dot{C}_{22}-\dot{\chi}\,C_{21})\,, \tag{27}$$

$$\ddot{C}_{21}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{21}+2\dot{\chi}\,\dot{C}_{22}=-(\dot{\psi}+\dot{\chi}_3)(\dot{C}_{11}+\dot{\chi}\,C_{12})\,, \tag{28}$$

and

$$\ddot{C}_{22}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{22}-2\dot{\chi}\,\dot{C}_{21}=-(\dot{\psi}+\dot{\chi}_3)(\dot{C}_{12}-\dot{\chi}\,C_{11})\,. \tag{29}$$

The linearized Riccati equation thus reduces to the inhomogeneous system of four second-order linear differential equations. These provide us with a set of solutions of the homogeneous Bloch equation. This is the utility of our approach.

III. A SET OF THREE SOLUTIONS

We solve the coupled differential equations (26)–(29) in this section.
From Eq. (26), we find

$$C_{22}=\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\left[\ddot{C}_{11}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{11}\right]+\frac{2}{\dot{\psi}+\dot{\chi}_3}\dot{C}_{12}-\frac{1}{\dot{\chi}}\dot{C}_{21}\,. \tag{30}$$

Substituting Eq. (30) back into Eqs. (27) and (28) and manipulating them, we obtain

$$\begin{aligned}C_{21}=&-\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\left\{3\,\ddot{C}_{12}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\dot{C}_{12}+(\dot{\psi}+\dot{\chi}_3)^2\,C_{12}\right\}\\&-\frac{1}{(\dot{\chi})^2(\dot{\psi}+\dot{\chi}_3)}\left\{C_{11}^{(3)}-\left[2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\ddot{C}_{11}\right.\\&\left.-\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^2-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)+2\,(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2\right]\dot{C}_{11}\right\}\end{aligned} \tag{31}$$

and

$$\begin{aligned}(\dot{\psi}+\dot{\chi}_3)\left[\ddot{C}_{21}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{21}+2(\dot{\chi})^2\,C_{21}\right]\quad&=-2\,\dot{\chi}\left[\ddot{C}_{12}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{12}+\frac{1}{2}(\dot{\psi}+\dot{\chi}_3)^2\,C_{12}\right]\\&\quad+[4\,(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2]\dot{C}_{11}\,.\end{aligned} \tag{32}$$

Again substituting Eqs. (30) and (31) back into Eq. (29), we find

$$\frac{4}{\dot{\psi}+\dot{\chi}_3}\left(C_{12}^{(3)}-\frac{3}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\dot{C}_{12}-\frac{1}{2}\left\{\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]^2 \right.\right.$$
$$\left.\left.-(\dot{\psi}+\dot{\chi}_3)^2\right\}\dot{C}_{12}-\frac{1}{4}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right](\dot{\psi}+\dot{\chi}_3)^2 C_{12}\right)$$
$$=-\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\left(C_{11}^{(4)}-2\left[2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]C_{11}^{(3)}\right.$$
$$-\left\{3\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-5\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]+\frac{d}{dt}\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)^2+4(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2\right\}\ddot{C}_{11}$$
$$-\left\{\frac{d^2}{dt^2}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-4\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\right]\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^3-2\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\right]\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)+3\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right.$$
$$-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\frac{d}{dt}\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)+\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)^2+2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)(\dot{\psi}+\dot{\chi}_3)^2-4(\dot{\chi})^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)$$
$$\left.\left.-(\dot{\psi}+\dot{\chi}_3)^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right\}\dot{C}_{11}-(\dot{\chi})^2(\dot{\psi}+\dot{\chi}_3)^2 C_{11}\right). \tag{33}$$

We thus postulate that

$$C_{12}^{(3)}-\frac{3}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\dot{C}_{12}-\frac{1}{2}\left\{\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]^2-(\dot{\psi}+\dot{\chi}_3)^2\right\}\dot{C}_{12}$$
$$-\frac{1}{4}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right](\dot{\psi}+\dot{\chi}_3)^2 C_{12}=0 \tag{34}$$

and

$$C_{11}^{(4)}-2\left[2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]C_{11}^{(3)}$$
$$-\left\{3\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-5\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]+\frac{d}{dt}\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)^2+4(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2\right\}\ddot{C}_{11}$$
$$-\left\{\frac{d^2}{dt^2}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-4\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\right]\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^3-2\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\right]\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)+3\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right.$$
$$-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\frac{d}{dt}\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)+\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)^2+2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)(\dot{\psi}+\dot{\chi}_3)^2-4(\dot{\chi})^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)$$
$$\left.-(\dot{\psi}+\dot{\chi}_3)^2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right\}\dot{C}_{11}-(\dot{\chi})^2(\dot{\psi}+\dot{\chi}_3)^2 C_{11}=0\,. \tag{35}$$

Here we have used the notations

$$C_{11}^{(3)}=\frac{d^3}{dt^3}C_{11},\quad C_{11}^{(4)}=\frac{d^4}{dt^4}C_{11},\quad \text{and}\quad C_{12}^{(3)}=\frac{d^3}{dt^3}C_{12}. \tag{36}$$

It is worth noticing that the general solution of Eq. (34) is given[6] by

$$C_{12}=C_1 v_1^2+C_2 v_1 v_2+C_3 v_2^2, \tag{37}$$

where C_i $(i=1,2,3)$ are constants of integration and v_1 and v_2 are linearly independent solutions of

$$\ddot{C}_{12}-\frac{1}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\dot{C}_{12}+\frac{1}{8}(\dot{\psi}+\dot{\chi}_3)^2 C_{12}=0. \tag{38}$$

After a rather tedious calculation using Eqs. (34) and (35) we find

$$\begin{aligned}\dot{C}_{21}=&-\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\frac{1}{2}\left(\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\ddot{C}_{12}+\left\{\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right.\\&\left.\times\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-(\dot{\psi}+\dot{\chi}_3)^2\right\}\dot{C}_{12}-\frac{1}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right](\dot{\psi}+\dot{\chi}_3)^2 C_{12}\Bigg)\\&-\frac{2}{\dot{\psi}+\dot{\chi}_3}\left[\ddot{C}_{11}-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\dot{C}_{11}+\frac{1}{2}(\dot{\psi}+\dot{\chi}_3)^2 C_{11}\right]\end{aligned} \tag{39}$$

and

$$\begin{aligned}C_{22}=&\frac{1}{(\dot{\chi})^2(\dot{\psi}+\dot{\chi}_3)}\frac{1}{2}\left(\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\ddot{C}_{12}+\left\{\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right.\\&\left.\times\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]+4(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2\right\}\dot{C}_{12}-\frac{1}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right](\dot{\psi}+\dot{\chi}_3)^2 C_{12}\Bigg)\\&+\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\left\{3\ddot{C}_{11}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\dot{C}_{11}+(\dot{\psi}+\dot{\chi}_3)^2 C_{11}\right\}.\end{aligned} \tag{40}$$

Having chosen

$$\ddot{C}_{11}-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\dot{C}_{11}+\frac{1}{2}(\dot{\psi}+\dot{\chi}_3)^2 C_{11}=0 \tag{41}$$

and

$$\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\ddot{C}_{12}+\left\{\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)+\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right.$$
$$\left.+4(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2\right\}\dot{C}_{12}-\frac{1}{2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right](\dot{\psi}+\dot{\chi}_3)^2 C_{12}=0\,, \tag{42}$$

we find

$$\dot{C}_{21}=\frac{2\dot{\chi}}{\dot{\psi}+\dot{\chi}_3}\dot{C}_{12}\,, \tag{43}$$

and

$$C_{22}=\frac{1}{\dot{\chi}(\dot{\psi}+\dot{\chi}_3)}\left[\ddot{C}_{11}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{11}\right]. \tag{44}$$

Differentiating Eq. (41) with respect to time once and twice and substituting them back into Eq. (35), we find the condition that Eq. (35) has the common solutions to Eq. (41):

$$\left\{\frac{d^2}{dt^2}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\right]\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-3\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right.$$
$$\left.+2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^2\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right\}\dot{C}_{11}-\frac{1}{2}\left\{3\frac{d}{dt}\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]-\left[5\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-2\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]\right.$$
$$\left.\times\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-\left(\frac{\ddot{\psi}+\ddot{\chi}_3}{\dot{\psi}+\dot{\chi}_3}\right)\right]+\frac{1}{2}[4(\dot{\chi})^2-(\dot{\psi}+\dot{\chi}_3)^2]\right\}(\dot{\psi}+\dot{\chi}_3)^2 C_{11}=0\,. \tag{45}$$

In order that C_{12} and C_{11} obey the differential equations (34) and (41), respectively, Eqs. (42) and (45) must be identical equations. This requirement creates a constraint. We thus require

$$\dot{\psi}+\dot{\chi}_3=C\dot{\chi}\,, \tag{46}$$

with

$$C=\pm 2\,. \tag{47}$$

It immediately follows from Eqs. (46) and (47) that Eqs. (42) and (45) are identically zero. Also from Eqs. (43) and (44), we find

$$\dot{C}_{21}=\pm\dot{C}_{12} \tag{48}$$

and

$$C_{22}=\mp C_{11}\,. \tag{49}$$

Thus Eqs. (34) and (41) yield

$$C_{12}^{(3)}-3\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\ddot{C}_{12}-\left[\frac{d}{dt}\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-2\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)^2-2(\dot{\chi})^2\right]\dot{C}_{12}=0 \tag{50}$$

and

$$\ddot{C}_{11}-\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)\dot{C}_{11}+2\,(\dot{\chi})^2\,C_{11}=0\,. \tag{51}$$

The general solution of Eq. (50) is easily found from Eqs. (37) and (38),

$$\begin{aligned}C_{12}&=C_1\cos^2\left(\frac{1}{\sqrt{2}}\chi\right)+C_2\cos\left(\frac{1}{\sqrt{2}}\chi\right)\sin\left(\frac{1}{\sqrt{2}}\chi\right)+C_3\sin^2\left(\frac{1}{\sqrt{2}}\chi\right)\\&=\frac{1}{2}(C_1+C_3)+\frac{1}{2}C_2\sin(\sqrt{2}\chi)+\frac{1}{2}(C_1-C_2)\cos(\sqrt{2}\chi)\,.\end{aligned} \tag{52}$$

Thus we have found the linearly independent solutions for C_{12} and C_{11};

$$C_{12}:\quad 1,\ \cos(\sqrt{2}\chi),\ \text{ and }\ \sin(\sqrt{2}\chi) \tag{53}$$

and

$$C_{11}:\quad \cos(\sqrt{2}\chi)\ \text{ and }\ \sin(\sqrt{2}\chi)\,. \tag{54}$$

The "solution" $C_{12}=1$ is spurious and arises from differentiating Eqs. (26)–(29). If it is substituted into the system of equations together with any of the solutions for C_{11}, they are not satisfied. Thus this solution should be discarded. The Wronskians of the solutions, Eqs. (53) and (54), do not vanish.

Using Eqs. (24) and (25) together with Eqs. (48) and (49), we find

$$u=(C_{11}\pm i\,C_{12})\,e^{\mp i\chi}\,. \tag{55}$$

Here we have assumed

$$C_{21}=\pm C_{12}\,. \tag{56}$$

With this choice there is no loss of generality.

Thus we have found the three types of solutions up to an overall factor:

$$u_1=\cos(\sqrt{2}\chi)\,e^{\mp i\chi}\,, \tag{57}$$

$$u_2=\sin(\sqrt{2}\chi)\,e^{\mp i\chi}\,, \tag{58}$$

and

$$u_3=e^{\mp i(1-\sqrt{2})\chi}\ \text{ or }\ e^{\mp i(1+\sqrt{2})\chi}\,. \tag{59}$$

They satisfy the differential equation

$$\ddot{u}-\left[\left(\frac{\ddot{\chi}}{\dot{\chi}}\right)-i(\pm 2\dot{\chi})\right]\dot{u}+(\dot{\chi})^2=0\,. \tag{60}$$

In terms of ξ defined by Eq. (21) we write out Eqs. (57)–(59) as

$$\xi_1=[\pm 1-i\sqrt{2}\tan(\sqrt{2}\chi)]\,e^{i\psi}\,, \tag{61}$$

$$\xi_2=[\pm 1+i\sqrt{2}\cot(\sqrt{2}\chi)]\,e^{i\psi}\,, \tag{62}$$

and

$$\xi_3 = \pm(1-\sqrt{2})\, e^{i\psi} \quad \text{or} \quad \pm(1+\sqrt{2})\, e^{i\psi}. \tag{63}$$

We thus have found a set of three solutions of the linearized Riccati equation with the constraint (46).

IV. THE FUNDAMENTAL MATRIX

A set of three solutions of the homogeneous Bloch equation is obtained from the solutions of the linearized Riccati equation corresponding to Eqs. (61)–(63).

Let $\vec{m}^{(i)}$ $(i=1,2,3)$ be

$$m_1^{(i)} = \frac{\xi_i + \xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{64}$$

$$m_2^{(i)} = -i\,\frac{\xi_i - \xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{65}$$

and

$$m_3^{(i)} = -\,\frac{1-\xi_i\,\xi_i^*}{1+\xi_i\,\xi_i^*}. \tag{66}$$

Then the fundamental matrix K is defined by

$$K_{ij} = (K)_{ij} = m_i^{(j)} \quad (i,j=1,2,3). \tag{67}$$

Here use has been made of the definitions of ξ and η, Eqs. (5) and (6), respectively, together with the relationship (9).

Substituting Eqs. (61)–(63) into Eqs. (64)–(66), we write out the elements of the fundamental matrix here:

$$K_{11} = \cos(\sqrt{2}\chi)[\pm\cos(\sqrt{2}\chi)\cos\psi + \sqrt{2}\sin(\sqrt{2}\chi)\sin\psi], \tag{68}$$

$$K_{21} = \cos(\sqrt{2}\chi)[\pm\cos(\sqrt{2}\chi)\sin\psi - \sqrt{2}\sin(\sqrt{2}\chi)\cos\psi], \tag{69}$$

$$K_{31} = \sin^2(\sqrt{2}\chi), \tag{70}$$

$$K_{12} = \sin(\sqrt{2}\chi)[\pm\sin(\sqrt{2}\chi)\cos\psi - \sqrt{2}\cos(\sqrt{2}\chi)\sin\psi], \tag{71}$$

$$K_{22} = \sin(\sqrt{2}\chi)[\pm\sin(\sqrt{2}\chi)\sin\psi + \sqrt{2}\cos(\sqrt{2}\chi)\cos\psi], \tag{72}$$

$$K_{32} = \cos^2(\sqrt{2}\chi), \tag{73}$$

$$K_{13} = \pm\frac{1}{\sqrt{2}}\cos\psi, \tag{74}$$

$$K_{23} = \pm\frac{1}{\sqrt{2}}\sin\psi, \tag{75}$$

and

$$K_{33} = \frac{1}{\sqrt{2}}. \tag{76}$$

First of all we have to calculate the determinant of the fundamental matrix. The result turns out to be

$$\det K = 0 \,. \tag{77}$$

This means that the fundamental matrix is singular and the three solutions are not linearly independent. It is obvious, because we can easily find the relationship

$$\vec{m}^{(1)} + \vec{m}^{(2)} = \sqrt{2}\, \vec{m}^{(3)} \,. \tag{78}$$

V. CONCLUSION

The homogeneous Bloch equation (3) can be written in a matrix form:

$$\dot{K} = A\, K \,, \tag{79}$$

where K is the fundamental matrix (the magnetization matrix) defined by Eq. (67) and a matrix A is given by

$$A = \begin{pmatrix} 0 & \gamma B_3 & -\gamma B_2 \\ -\gamma B_3 & 0 & \gamma B_1 \\ \gamma B_2 & -\gamma B_1 & 0 \end{pmatrix} , \tag{80}$$

which is antisymmetric and singular. Moreover, we find

$$\det \dot{K} = \mathrm{tr}\, A \det K = 0 \,. \tag{81}$$

We thus obtain from Eq. (81)

$$\det K = \det K(t_0) \,. \tag{82}$$

A key restriction to our treatment is to be imposed Eq. (46). This works as a constraint:

$$\gamma B_3 = \frac{\dot{B}_1 B_2 - B_1 \dot{B}_2}{B_1^2 + B_2^2} \pm \gamma \sqrt{B_1^2 + B_2^2} \,, \tag{83}$$

where the third component of the applied magnetic field is given by the remaining components which have no constraints.

We have found a set of three solutions of the homogeneous Bloch equation. These are not linearly independent, only two of them are linearly independent solutions. The first two solutions are unknown so far and the third solution is a generalized solution of the classical precession. The classical precession is given by choosing the applied magnetic field as

$$\vec{B} = \left(B_0 \cos \omega t,\, B_0 \sin \omega t,\, -\frac{\omega}{\gamma} \pm B_0 \right) , \tag{84}$$

where B_0 and ω are time-independent and then we find

$$\psi = \omega t \,. \tag{85}$$

In each solution the magnitude of the vector is preserved so that two variables are left to determine the system.

The linearized Riccati equation reduces to the inhomogeneous system of four second order linear differential equations, Eqs. (26)–(29). These provide us with a set of solutions of the homogeneous Bloch equation. This is the utility of our approach.

The reason why the third independent solution cannot be found in our approach is due to the fact that the constant solution of C_{12} is a spurious solution arising from differentiating the system of equations (26)–(29). This is a limitation of the method of linearizing the Riccati equation (12).

ACKNOWLEDGMENTS

I am indebted to Y. Takahashi for the discussions at earlier stages of this work. I thank M. Kawasaki and A. Z. Capri for continual discussions about solutions of the Bloch equation.

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Discrete transformation for the matrix three-wave problem in three dimensional space

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(Received 18 July 2002; accepted 6 December 2002)

Discrete transformation for three-wave problems is constructed in explicit form. Generalization of this system on the matrix case in three dimensional space together with corresponding discrete transformation is presented also. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1543636]

I. INTRODUCTION

The problem of three waves in two dimensions arises in different forms in many branches of the mathematical physics. Its application to problems of radiophysics and nonlinear optics can be found in Ref. 1. In connection with the inverse scattering method it was investigated in Ref. 2 and considered in detail in numerous further papers.

The goal of the present article is to generalize this system on the space of three dimensions while simultaneously exchanging the unknown scalar functions on the operator valued ones. The last generalization allows us to include into consideration the quantum region with the Heisenberg operators as unknown functions of the problem.

It is necessary to mention that numerous different (by the form) discrete transformations were used up to now with respect to two components hierarchies of integrable systems, which are connected with so called Darboux–Toda, Lotke–Volterra, and Heisenberg substitutions. In the present article we come to the substitutions which connect six independent functions, which corresponds to A_2 algebra but not to A_1 as it was in the case of the two component systems. This substitution may be considered as the integrable mapping, connecting six initial functions with the six final ones. Substitutions of the present article do not coincide with those recently introduced in Ref. 3, the so-called ultra-Toda mappings.

The method of this article without any difficulties can be generalized on the case of the nth wave problem. In this case the number of independent variables of substitution will be $(n\times(n+1))$, which coincides with the number of positive and negative roots of A_n algebra.

The traditional way for obtaining the system of equations for the three-wave problem in $(1+1)$ dimensions is the $L-A$ pair formalism

$$[\partial_x - u, \partial_t - v] = 0$$

with

$$u = \begin{pmatrix} c_1\lambda & (c_2-c_1)P & (c_3-c_1)Q \\ (c_1-c_2)B & c_2\lambda & (c_3-c_2)A \\ (c_1-c_3)D & (c_2-c_3)E & -(c_1+c_2)\lambda \end{pmatrix},$$

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$$v=\begin{pmatrix} d_1\lambda & (d_2-d_1)P & (d_3-d_1)Q \\ (d_1-d_2)B & d_2\lambda & (d_3-d_2)A \\ (d_1-d_3)D & (d_2-d_3)E & -(d_1+d_2)\lambda \end{pmatrix},$$

where c,d are four arbitrary numerical parameters ($\Sigma c_i=0,\Sigma d_i=0$) and (A,B,D,E,P,Q) are unknown functions of the problem. The system of equations for them has the form

$$\begin{aligned} &(d_2-d_1)P_x-(c_2-c_1)P_t+\nu EQ=0, \quad (d_3-d_1)Q_x-(c_3-c_1)Q_t-\nu PA=0, \\ &(d_3-d_2)A_x-(c_3-c_2)A_t+\nu QB=0, \quad (d_1-d_2)B_x-(c_1-c_2)B_t-\nu AD=0, \\ &(d_1-d_3)D_x-(c_1-c_3)D_t+\nu BE=0, \quad (d_2-d_3)E_x-(c_2-c_3)E_t-\nu DP=0, \end{aligned} \tag{1}$$

where $\nu=3(c_1d_2-c_2d_1)$. Solitonlike solution for the last system of equations may be easily found with the help of the technique of Ref. 4. From these results the first steps of the discrete transformation can be found, with respect to which the last system is invariant. In the present work the reader has to consider the form of the discrete transformation as a lucky guess.

II. DISCRETE TRANSFORMATION

We can assume (but this is a direct corollary of the results of Ref. 4) that the three ''new'' functions (Q,A,P), denoted by the bar symbols, connected with the old ones as following,

$$\overline{Q}=\frac{1}{D}, \quad \overline{A}=-\frac{B}{D}, \quad \overline{P}=\frac{E}{D},$$

satisfy the system (1). Then from the first and second equations of the first column it is possible to determine $\overline{E},\overline{B}$ functions with the result

$$\overline{E}=-\frac{1}{(c_1-c_3)}\frac{E}{D}(D_x-(c_2-c_1)BE)+\frac{1}{(c_2-c_3)}(E_x+(c_2-c_1)DP),$$

$$\overline{B}=\frac{1}{(c_1-c_3)}\frac{B}{D}(D_x-(c_2-c_1)BE)-\frac{1}{(c_1-c_2)}(B_x-(c_3-c_2)AD).$$

And in a self-consistent way we determine from the second and first equations of the second column $\overline{D}$. We will not present here this somewhat complex expression, because in a few lines below we will have an observable expression for this value. Straightforward but tedious calculations show that the third equation of the first column is also satisfied ($\overline{D}_3=-\overline{BE}$).

For further consideration it is more suitable to introduce three dependent variables ($\xi+\eta+\sigma=0$),

$$\xi=(d_2-d_1)t+(c_2-c_1)x, \quad \eta=(d_3-d_2)t+(c_3-c_2)x, \quad \sigma=(d_1-d_3)t+(c_1-c_3)x.$$

In each pair of variables $(\xi,\eta),(\xi,\sigma),(\eta,\sigma)$ the differentiation operators take the form

$$\begin{pmatrix} \partial_1\equiv\dfrac{(d_2-d_1)}{\nu}\partial_x-\dfrac{(c_2-c_1)}{\nu}\partial_t \\ \partial_2\equiv\dfrac{(d_3-d_2)}{\nu}\partial_x-\dfrac{(c_3-c_2)}{\nu}\partial_t \\ \partial_3\equiv\dfrac{(d_1-d_3)}{\nu}\partial_x-\dfrac{(c_1-c_3)}{\nu}\partial_t \end{pmatrix}=\begin{pmatrix} -\partial_\eta & \partial_\sigma & \partial_\sigma-\partial_\eta \\ \partial_\xi & \partial_\xi-\partial_\sigma & -\partial_\sigma \\ \partial_\eta-\partial_\sigma & -\partial_\xi & \partial_\eta \end{pmatrix}.$$

Really the explicit form of the generators of differentiation via (ξ,η,σ) variables will not be essential. Now the system (1) looks much more attractive:

$$P_1=-QE,\quad A_2=-BQ,\quad Q_3=-PA,$$
$$B_1=-AD,\quad E_2=-DP,\quad D_3=-EB. \tag{2}$$

In the last form the system is obviously invariant with respect to permutation of the indexes of differentiation with the simultaneous corresponding exchanging of unknown functions. The discrete transformation of the beginning of this section may be rewritten in more symmetrical form (we will denote it with the help of the symbol T_3):

$$\overline{Q}=\frac{1}{D},\quad \overline{A}=-\frac{B}{D},\quad \overline{P}=\frac{E}{D},$$

$$\overline{B}=D\left(\frac{B}{D}\right)_2,\quad \overline{E}=-D\left(\frac{E}{D}\right)_1,\quad \frac{\overline{D}}{D}=DQ-(\ln D)_{1,2}.$$

By the permutation indexes (1,3) (together with corresponding exchanging of unknown functions) it is possible to obtain the T_1 discrete transformation with respect to which the system (2) is also invariant:

$$\overline{P}=\frac{1}{B},\quad \overline{Q}=\frac{A}{B},\quad \overline{E}=-\frac{D}{B},$$

$$\overline{D}=B\left(\frac{D}{B}\right)_2,\quad \overline{A}=-B\left(\frac{A}{B}\right)_3,\quad \frac{\overline{B}}{B}=BP-(\ln B)_{2,3}.$$

And at last the discrete transformation T_2 has the form

$$\overline{A}=\frac{1}{E},\quad \overline{B}=\frac{D}{E},\quad \overline{Q}=-\frac{P}{E},$$

$$\overline{D}=-E\left(\frac{D}{E}\right)_1,\quad \overline{P}=E\left(\frac{P}{E}\right)_3,\quad \frac{\overline{E}}{E}=EA-(\ln E)_{1,3}.$$

In the form presented above substitutions T_i may be considered as a mapping, connected six initial (unbar) functions with six final (bar) ones. From the other side each substitution may be considered as the infinite dimensional chain of equations. For instance, the corresponding chain of equations in the case of T_1 substitution has the form

$$\frac{B^{n+1}}{B^n}-\frac{B^n}{B^{n-1}}=-(\ln B^n)_{2,3},\quad D^{n+1}=B^n\left(\frac{D^n}{B^n}\right)_2,\quad A^{n+1}=-B^n\left(\frac{A^n}{B^n}\right)_3,$$
$$E^{n+1}=-\frac{D^n}{B^n},\quad Q^{n+1}=\frac{A^n}{B^n}. \tag{3}$$

In the first row we have the latticelike system connecting three unknown functions (B,D,A) in each point of the lattice. The first chain for B functions is exactly the well known two dimensional Toda lattice.

III. SOME PROPERTIES OF THE DISCRETE TRANSFORMATIONS

All constructed above discrete transformations are invertible. This means that unbarred unknown functions may be presented in terms of the bar ones. For instance, T_3^{-1} looks like

$$D=\frac{1}{\overline{Q}},\quad B=-\frac{\overline{A}}{\overline{Q}},\quad E=\frac{\overline{P}}{\overline{Q}},$$

$$P=-\overline{Q}\left(\frac{\overline{P}}{\overline{Q}}\right)_2,\quad A=\overline{Q}\left(\frac{\overline{A}}{\overline{Q}}\right)_1,\quad \frac{Q}{\overline{Q}}=\overline{DQ}-(\ln\overline{Q})_{1,2}.$$

It is not difficult to check by direct computation that discrete transformations T_i are mutual commutative ($T_iT_j=T_jT_i$) on the solutions of the system (2).

We present below corresponding calculations to prove that $T_1T_2=T_2T_1=T_3$. Indeed, the result of the action of T_1 on some solution of the system (2) is the following:

$$P^1=\frac{1}{B},\quad Q^1=\frac{A}{B},\quad E^1=-\frac{D}{B},$$

$$D^1=B\left(\frac{D}{B}\right)_2,\quad A^1=-B\left(\frac{A}{B}\right)_3,\quad \frac{B^1}{B}=BP-(\ln B)_{2,3}.$$

Action of the T^2 transformation on this solution leads to

$$A^{21}=\frac{1}{E^1}=-\frac{B}{D},\quad B^{21}=\frac{D^1}{E^1}=D\left(\frac{B}{D}\right),$$

$$Q^{21}=-\frac{P^1}{E^1}=\frac{1}{D},\quad D^{21}=-E^1\left(\frac{D^1}{E^1}\right)_1=-\frac{D}{B}(B(\ln D)_2-B_2)_1=QD^2-D(\ln D)_{12},$$

$$P^{21}=E^1\left(\frac{P^1}{E^1}\right)_3=\frac{E}{D},\quad E^{21}=(E^1)^2A^1-E^1(\ln E^1)_{13}=-D\left(\frac{E}{D}\right)_1.$$

The same calculation repeated in the back direction shows that $W^{1,2}=W^{2,1}=W^3$—the result of application of the T_3 transformation to an initial solution W.

Thus from each given initial solution $W_0\equiv(A,P,Q,E,B,D)$ of the system (2) it is possible to obtain the chain of solutions labeled by two natural numbers $[l_1,l_2,$ or $(l_3)]$, the number of applications of the discrete transformations (T_1,T_2,T_3) to it (as it was shown above $T_1T_2=T_2T_1=T_3$).

The arising chain of equations with respect to (D,B,E) functions are exactly two dimensional Toda lattices. Their general solutions in the case of two fixed ends are well known.[5] As the reader will see shortly, this fact allows us to construct the many soliton solutions of the three-wave problem in the most straightforward way.

IV. RESOLVING DISCRETE TRANSFORMATION CHAINS

A. Two identities of Jacobi

We begin from the following obvious equalities for determinants of nth order,

$$\mathrm{Det}_n(T_n)\equiv D_n\begin{pmatrix}T_{n-1} & a\\ b & \tau\end{pmatrix}=D_{n-1}(T_{n-1})(\tau-bT_{n-1}^{-1}a)\equiv D_{n-1}(T_{n-1})\tilde{\tau},$$

where T_{n-1} is an $(n-1)\times(n-1)$ matrix, a,b are $(n-1)$ dimensional column (row) vectors, respectively, and τ is a scalar.

By the same reason the following formula takes place:

$$D_n\begin{pmatrix} T_{n-2} & a^1 & a^2 \\ b^1 & \tau_{11} & \tau_{12} \\ b^2 & \tau_{21} & \tau_{22} \end{pmatrix} = D_{n-2}(T_{n-2})D_2\begin{pmatrix} \tau_{11}-b^1T_{n-2}^{-1}a^1 & \tau_{12}-b^1T_{n-2}^{-1}a^2 \\ \tau_{21}-b^2T_{n-2}^{-1}a^1 & \tau_{11}-b^2T_{n-2}^{-1}a^2 \end{pmatrix},$$

where a^i,b^i are $(n-2)$ dimensional columns (rows) vectors and $\tau_{i,j}$ are components of a two-dimensional matrix. It is obvious how relations of these types may be continued.

Now, using results from above, let us transform the following expression:

$$D_n\begin{pmatrix} T_{n-1} & a^1 \\ b^1 & \tau_{11} \end{pmatrix}D_n\begin{pmatrix} T_{n-1} & a^2 \\ b^2 & \tau_{22} \end{pmatrix} - D_n\begin{pmatrix} T_{n-1} & a^2 \\ b^1 & \tau_{12} \end{pmatrix}D_n\begin{pmatrix} T_{n-1} & a^1 \\ b^2 & \tau_{21} \end{pmatrix}$$

$$= D_{n-1}^2(T_{n-1})D_2\begin{pmatrix} \tau_{11}-b^1T_{n-1}^{-1}a^1 & \tau_{12}-b^1T_{n-1}^{-1}a^2 \\ \tau_{21}-b^2T_{n-1}^{-1}a^1 & \tau_{11}-b^2T_{n-1}^{-1}a^2 \end{pmatrix} = D_{n-1}D_{n+1}\begin{pmatrix} T_{n-1} & a^1 & a^2 \\ b^1 & \tau_{11} & \tau_{12} \\ b^2 & \tau_{21} & \tau_{22} \end{pmatrix}.$$

We will treat the last equality as the first Jacobi identity. By the same technique it is not difficult to show that the following equality takes place:

$$D_n\begin{pmatrix} T_{n-1} & a^1 \\ b^1 & \tau \end{pmatrix}D_{n+1}\begin{pmatrix} T_{n-1} & a^1 & a^2 \\ d^1 & \nu & \mu \\ b^2 & \rho & \tau \end{pmatrix} - D_n\begin{pmatrix} T_{n-1} & a^1 \\ b^2 & \rho \end{pmatrix}D_{n+1}\begin{pmatrix} T_{n-1} & a^1 & a^2 \\ d^1 & \nu & \mu \\ b^1 & \tau & \sigma \end{pmatrix}$$

$$= D_n\begin{pmatrix} T_{n-1} & a^1 \\ d^1 & \nu \end{pmatrix}D_{n+1}\begin{pmatrix} T_{n-1} & a^1 & a^2 \\ b^2 & \rho & \tau \\ b^1 & \tau & \sigma \end{pmatrix}.$$

This equality will be used many times in what follows and will be called the second Jacobi identity. These identities can be generalized in the case of an arbitrary semi-simple group. The reader can find these results in Ref. 3.

B. Concrete calculations

Let us take an initial solution in the form

$$Q=A=P=0, \quad B\equiv B(2), \quad E\equiv E(1). \quad D_3=-BE. \tag{4}$$

Application to this solution by each inverse transformation T_i^{-1} means less via arising zeroes in the denominators. The chain of equations under such a boundary condition will be called the chain with the fixed end from the left (from one side).

The result of application to such initial solution l_3 times T_3 transformation looks like (for the checking of this fact only two Jacobi identities of the previous subsection are necessary)

$$Q^{(l_3}=(-1)^{l_3-1}\frac{\Delta_{l_3-1}}{\Delta_{l_3}}, \quad D^{(l_3}=(-1)^{l_3}\frac{\Delta_{l_3+1}}{\Delta_{l_3}}, \quad \Delta_0=1,$$

$$A^{(l_3}=(-1)^{l_3}\frac{\Delta_{l_3}^B}{\Delta_{l_3}}, \quad P^{(l_3}=\frac{\Delta_{l_3}^E}{\Delta_{l_3}}, \quad \Delta_0^B=\Delta_0^E=0, \tag{5}$$

$$B^{(l_3}=\frac{\Delta^B_{l_3+1}}{\Delta_{l_3}},\quad E^{(l_3}=(-1)^{l_3}\frac{\Delta^E_{l_3+1}}{\Delta_{l_3}},\quad \Delta_{-1}=0,$$

where Δ_n are minors of the nth order of infinite dimensional matrix

$$\Delta=\begin{pmatrix} D & D_2 & D_{22} & \dots \\ D_1 & D_{12} & D_{122} & \dots \\ D_{11} & D_{112} & D_{1122} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}, \tag{6}$$

and $\Delta^E_{l_3},\Delta^B_{l_3}$ are the minors of l_3 order in the matrices of which the last column (or row) is exchanged on the derivatives of the corresponding order on argument 1 of E function (on argument 2 of the B function in the second case).

In what follows the following notations will be used. W^{l_3,l_1} (W^{l_3,l_2}) is the result of application of discrete transformation $T^{l_3}T^{l_1}$ ($T^{l_3}T^{l_2}$) to the corresponding component of the three wave field. Δ^{l_3,l_1} (Δ^{l_3,l_2}) is the determinant of l_3+l_1 (l_3+l_2) orders, with the following structure of its determinant matrix. The first l_3 rows (columns) of it coincide with the matrix of (6) and the last l_1 (l_2) rows (columns) constructed from the derivatives of B (E) functions with respect argument 2 (1).

The result of additional application of l_1 times T_1 transformation to the solution (5) looks like

$$P^{(l_3,l_1}=\frac{\Delta_{l_3,l_1-1}}{\Delta_{l_3,l_1}},\quad B^{(l_3,l_1}=\frac{\Delta_{l_3,l_1+1}}{\Delta_{l_3,l_1}},\quad \Delta_0=1,\quad \Delta^{l_3,-1}\equiv\Delta^E_{l_3},$$

$$Q^{(l_3,l_1}=(-1)^{l_3+l_1-1}\frac{\Delta_{l_3-1,l_1}}{\Delta_{l_3,l_1}},\quad D^{(l_3,l_1}=(-1)^{l_3+l_1}\frac{\Delta_{l_3+1,l_1}}{\Delta_{l_3,l_1}}, \tag{7}$$

$$E^{(l_3,l_1}=(-1)^{l_3+l_1}\frac{\Delta_{l_3+1,l_1-1}}{\Delta_{l_3,l_1}},\quad A^{(l_3,l_1}=(-1)^{l_3+l_1}\frac{\Delta_{l_3-1,l_1+1}}{\Delta_{l_3,l_1}}.$$

We do not present the explicit form for components $W^{(l_3,l_2}$, which can be obtained without any difficulties from (7) by corresponding exchange of the arguments and unknown functions.

V. MANY-SOLITON SOLUTION OF THE SCALAR THREE-WAVE PROBLEM

The system (2) allows the following reduction (under the additional assumption that all operators of differentiation are the real ones $\partial_\alpha=\partial^*_\alpha$):

$$P=B^*,\quad A=E^*,\quad Q=D^*. \tag{8}$$

In this case the system (2) is reduced to three equations,

$$B_1=-DE^*,\quad E_2=-DB^*,\quad D_3=-BE, \tag{9}$$

for three complex valued unknown functions (E,B,D).

Now we would like to demonstrate how the multi-soliton solutions of the system (9) may be obtained with the help of the technique of discrete transformation in the most straightforward way.

With this aim let us consider the action of the direct and inverse T_i,T_i^{-1} transformations on the reduced solution of the system (9). The trick consists in the fact that discrete transformation does not conserve the condition of the reality (8) and, starting from the solution of the reduced system, we come back to the solution of the irreducible one and in some cases vice versa. We will

denote the three dimensional vector (Q,P,A) by the single symbol $\vec{Q}$ and by the symbol $\vec{D}$ three dimensional vector (D,B,E). Then the result of actions of direct and inverse transformations on the solution satisfying the condition of reality $\vec{Q}=\vec{D}^*$ is the following:

$$T_i^n(\vec{D},\vec{D}^*)=(t_i)^n(\vec{q},\vec{d}),\quad T_i^{-n}(\vec{D},\vec{D}^*)=(\vec{d}^*,\vec{Q}^*),$$

where t_i are pointlike symmetries of the system (2),

$$t_3(Q,P,A,D,B,E)=(Q,-P,-A,D,-B,-E),$$

$$t_2(Q,P,A,D,B,E)=(-Q,-P,A,-D,-B,E),$$

$$t_3(Q,P,A,D,B,E)=(-Q,P,-A,-D,B,-E).$$

It is obvious that t_i^2. Thus if we apply $2n$ times discrete transformation to the initial bad (nonreduced) solution $(0,\vec{D})$ and as a result obtain $(t^n\vec{D}^*,0)$, then in the middle of the chain we will have a solution satisfying the condition of reality, which coincides with the n soliton solution of the reduced system (9).

The solution of the chain with the boundary conditions $\vec{Q}=0$ on the left end of the chain and $\vec{D}=0$ on the right side we will call the chain with fixed ends. Really condition $\vec{D}=0$ is the system of equations from which initial functions D,B,E [see (9)] may be defined as the solutions of ordinary differential equations (see Appendix B).

VI. MATRIX THREE-WAVE PROBLEM IN THE SPACE OF THREE DIMENSIONS AND ITS DISCRETE TRANSFORMATION

In all calculations above we have never used (except for concrete resolving of discrete transformation chains) the condition that operators of differentiation are connected by the condition

$$\partial_1+\partial_2+\partial_3=0,$$

as it follows from the definition of this operators. So we can consider the system (2) where all three operators are independent from each other and correspond to differentiation with respect to one of the coordinates of three dimensional space. The second generalization consists in the possibility to consider the unknown function in (2) as the operator valued ones. Of course in this case the order of the multiplications is essential and exactly coincides with that fixed by the formula (2).

T_3 discrete transformation in this case looks like

$$\overline{Q}=D^{-1},\quad \overline{A}=-BD^{-1},\quad \overline{P}=D^{-1}E,$$

$$\overline{B}=-D(BD^{-1})_2,\quad \overline{E}=-D(D^{-1}E)_1,\quad D^{-1}\overline{D}=QD-(D^{-1}D_2)_1.$$

By the same technique for T_1 we have

$$\overline{P}=B^{-1},\quad \overline{Q}=B^{-1}A,\quad \overline{E}=-DB^{-1},$$

$$\overline{D}=(DB^{-1})_2B,\quad \overline{A}=-B(B^{-1}A)_3,\quad \overline{B}B^{-1}=BP-(B_3B^{-1})_2.$$

And at last the discrete transformation T_2 looks like

$$\overline{A}=E^{-1},\quad \overline{B}=E^{-1}D,\quad \overline{Q}=-PE^{-1},$$

$$\overline{D}=-E(E^{-1}D)_1,\quad \overline{P}=(PE^{-1})_3E,\quad E^{-1}\overline{E}=AE-(E^{-1}E_3)_1.$$

As in the scalar case the discrete transformations in the case under consideration are mutually commutative. The arising chains of equations for the (E,B,D) operator a valued function (the matrices of the finite dimensions, for instance) coincide with the previously investigated matrix Toda chain. Explicit solutions for this chain of equations with the fixed ends can be found in Ref. 6. Uniting these results it is possible to construct multi-soliton solutions of the matrix three-wave problem in three dimensions similar to way proposed in Ref. 7 for construction of multi-soliton solutions for the matrix Devay–Stewartson equation.

VII. OUTLOOK

The concrete results of the present article are concentrated in explicit formulas for discrete transformations for the three-wave problem of Sec. II and their generalization on the matrix case (Sec. VI).

But no less important is the understanding of how the method of the discrete transformation may be generalized in the case of multi-component systems, connected with the semi-simple algebras of the higher rank r. From results of the present article, it is clear that in the case of arbitrary semi-simple algebra there are r independent basis, mutually commutative discrete transformations. In what connection these commutative objects are with the main ingredients of the representation theory of the group is very interesting and an intriguing question for further investigation.

And, finally, the last comment. The chain with two fixed ends cannot be considered as the basis for some finite dimensional representation of the group of the discrete transformation, if it is at all possible to apply the term group for it in this case. On the function at the end point of chain it is impossible to act by direct transformation at the right side and inverse on the left end. What is discrete transformation from the group theoretical point of view in this case? We at this time have no answer on this question.

ACKNOWLEDGMENT

The authors are indebted to CONACYT for financial support.

APPENDIX A

In this appendix we would like to show how it is possible to construct two dimensional integrable systems connected with A_2 algebra.

Let us consider the following 3×3 polynomial matrix,

$$P(\lambda)=\begin{pmatrix} \tilde{P}^{11}_{n_1+1} & P^{12}_{n_2} & P^{13}_{n_3} \\ P^{21}_{n_1} & \tilde{P}^{22}_{n_2+1} & P^{23}_{n_3} \\ P^{31}_{n_1} & P^{32}_{n_2} & \tilde{P}^{33}_{n_3+1} \end{pmatrix}, \tag{A1}$$

where P^{ij}_k are the polynomials of degree k (with respect to parameter λ and sign $\tilde{P}$ means that coefficient function on the highest degree of the corresponding polynomial equal to unity).

Let us define the coefficient function of all polynomials from the condition that between the columns of the matrix

$$\overline{P}=P(\lambda)\exp(\tau_1 h_1+\tau_2 h_2).$$

The linear dependence takes place in $(n_1+n_2+n_3+3)$ points of the λ plane, h_1,h_2 are Cartan elements of A_2 algebra, and $\tau_i=\phi_i(t,\lambda)+f_i(x,\lambda)$. ϕ_i,f_i are arbitrary rational functions with respect to argument λ.

The last condition is equivalent to the following system of linear equations for defining the coefficient function (we present it here for elements of the first row):

$$\tilde{P}^{11}_{n_1+1}(\lambda_s)+c_s\exp(\tau_2^s-2\tau_1^s)P^{12}_{n_2}(\lambda_s)+d_s\exp-(\tau_2^s+\tau_1^s)P^{13}_{n_3}(\lambda_s)=0,$$
$$s=1,2,\ldots,(n_1+n_2+n_3+3),\tau_i^s\equiv\tau(\lambda_s). \tag{A2}$$

$(n_1+n_2+n_3+3)$ is exactly the number of coefficient functions of polynomials of the first row. Thus (A2) is the linear system of equations for their determination.

Let us now determine $\mathrm{Det}(P(\lambda))=\mathrm{Det}(\overline{P}(\lambda))$. From (A1) it follows that it is the polynomial of $(n_1+n_2+n_3+3)$ degree with unity coefficient before the highest term and from condition (A2) that it has zeroes in $(n_1+n_2+n_3+3)$ points λ_s of the λ plane. Thus

$$\mathrm{Det}(P(\lambda))=\mathrm{Det}(\overline{P}(\lambda))=\Pi_{k=1}^{(n_1+n_2+n_3+3)}(\lambda-\lambda_k). \tag{A3}$$

Now let us calculate the matrix $\dot{\tilde{P}}\overline{P}^{-1}$, where $\dot{f}$ means the differentiation with respect to one of two independent arguments of the problem x,t. From the definition of the inverse matrix it follows that matrix elements of this matrix are the following ones:

$$(\dot{\tilde{P}}\overline{P}^{-1})_{\alpha,\beta}=\frac{\mathrm{Det}(P_\beta\to\dot{P}_\alpha+P_\alpha(\dot{\tau}_{i+1}-\dot{\tau}_i)}{\Pi_{k=1}^{(n_1+n_2+n_3+3)}(\lambda-\lambda_k)},\quad \tau_0=\tau_3=0. \tag{A4}$$

This symbolical form means that the determinant matrix of the numerator arises after exchanging the β row of the P matrix on the α row of the matrix $\dot{\tilde{P}}\exp-(\tau_1h_1+\tau_2h_2)$.

It is not difficult to understand that matrix $\dot{\tilde{P}}\overline{P}^{-1}$ possesses all the same singularities as functions τ by themselves.

Now let us illustrate the situation on the example of three-wave interaction, choosing $\tau_1=\lambda(c_1t+c_2x)$, $\tau_2=\lambda(d_1t+d_2x)$. Let us calculate in this case, for instance, $(\overline{P}_t\overline{P}^{-1})_{11}$. In connection with (A4) the numerator determinant has

$$\mathrm{Det}\begin{pmatrix}\dot{\tilde{P}}_{n_1+1}+\tilde{P}_{n_1+1}c_1\lambda & \dot{P}_{n_2}+P_{n_2}(c_2-c_1)\lambda & \dot{P}_{n_3}-P_{n_3}c_2\lambda\\ P_{n_1} & \tilde{P}_{n_2+1} & P_{n_3}\\ P_{n_1} & P_{n_2} & \tilde{P}_{n_3+1}\end{pmatrix}.$$

It is obvious that between the columns of the matrix $\dot{\tilde{P}}$ the linear dependence takes place with the same coefficients and so the numerator determinant has zeroes in the same points as the determinant in the enumerator. Computation of the degrees of the numerator shows that it is a polynomial of the $(n_1+n_2+n_3+4)$ order and so the considered matrix element is the linear function of the λ parameter. From (A3) it follows that it equals exactly $c_1\lambda$. The same nonconversion calculations show that matrix $\overline{P}_t\overline{P}^{-1}$ coincides with the u matrix from the introduction after identification,

$$P=(P^{12})^{n_2}_{n_2},\quad Q=(P^{13})^{n_3}_{n_3},\quad B=(P^{21})^{n_1}_{n_1},$$
$$A=(P^{23})^{n_3}_{n_3},\quad D=(P^{31})^{n_1}_{n_1},\quad E=(P^{32})^{n_2}_{n_2},$$

where the values above are coefficients at the highest degree terms of the corresponding polynomial. These terms are known from the solution of the linear system (A2) and so we have explicit solution of the system (1).

APPENDIX B

In this appendix we would like to consider the simple example of soliton solution of the three-wave problem. We especially consider this simplest example in detail to give the reader the possibility to feel self-consistent of the whole construction of the present article.

In the notation of Sec. V, let $l_3=2, l_1=0$. We also have the condition that vector $D^{\vec{2,0}}=0$ is equivalent to the following system of equations,

$$\Delta_3=\Delta_3^B=\Delta_3^E=0. \tag{B1}$$

The first of these equations leads uniquely to the explicit form of the initial D function

$$D=\phi_1(1)f_1(2)+\phi_2(1)f_2(2), \quad \phi_1=\phi', \quad f_2=\dot{f}. \tag{B2}$$

Using the initial conditions (4), $\Delta_3^E=0$ may be rewritten consequently as

$$B\Delta_3^E=-\mathrm{Det}\begin{pmatrix} D & D_2 & D_1 \\ D_1 & D_{12} & D_{11} \\ D_{11} & D_{112} & D_{111} \end{pmatrix}=(\dot{f}_1f_2-\dot{f}_2f_1)\mathrm{Det}\begin{pmatrix} \phi_1 & \phi_2 & \phi_1'f_1+\phi_2'f_2 \\ \phi_1' & \phi_2' & \phi_1''f_1+\phi_2''f_2 \\ \phi_1'' & \phi_2'' & \phi_1'''f_1+\phi_2'''f_2 \end{pmatrix}.$$

Keeping in mind that ϕ, f are the functions of the different arguments, we conclude the last equation is equivalent to the zero of the two determinants of third order. The last condition in its turn can be rewritten as the system of equations

$$\begin{aligned} &\phi_1'=p\phi_1+q\phi_2, \quad \phi_2'=s\phi_1+t\phi_2, \\ &\phi_1''=p\phi_1'+q\phi_2', \quad \phi_2''=s\phi_1'+t\phi_2', \\ &\phi_1'''=p\phi_1''+q\phi_2'', \quad \phi_2'''=s\phi_1''+t\phi_2''. \end{aligned} \tag{B3}$$

From (B3) it follows immediately that $(\phi_2\neq c\phi_1)$ $p'=q'=s'=t'=0$ and functions $\phi_{1,2}$ are the solutions of the first row of (B3)—the linear system of equations with the constant coefficients. Solution of this system is obvious:

$$\phi_1=c_1\exp\lambda_1 1+c_2\exp\lambda_2 1, \quad \phi_2=c_3\exp\lambda_1 1+c_4\exp\lambda_2 1.$$

From the equation $E\Delta_3^B$ by the same way we obtain

$$f_1=d_1\exp\mu_1 2+d_2\exp\mu_2 2, \quad f_2=d_3\exp\mu_1 2+d_4\exp\mu_2 2,$$

where c, d, λ, μ are arbitrary numerical parameters.

The initial conditions

$$-D_3=D_1+D_2=BE\equiv(b_1\exp\mu_1 2+b_2\exp\mu_2 2)(e_1\exp\lambda_1 1+e_2\exp\lambda_2 1)$$

allow using (B2) to determine parameters b, e and find one relation connected parameters c, d, λ, μ. Now let us calculate vector $Q^{2,0}$ using explicit expressions for D, B, E functions. The last two we present in the following form $E=p\phi_1+q\phi_2$, $B=rf_1+sf_2$:

$$Q^{2,0}=-\frac{D}{D_2}=-\frac{\phi_1f_1+\phi_2f_2}{D\begin{pmatrix} \phi_1 & \phi_2 \\ \phi_1' & \phi_2' \end{pmatrix}D\begin{pmatrix} f_1 & \dot{f}_1 \\ f_2 & \dot{f}_2 \end{pmatrix}},$$

$$P^{2,0}=\frac{D\begin{pmatrix} f_1 & p \\ f_2 & q \end{pmatrix}}{D\begin{pmatrix} f_1 & \dot{f}_1 \\ f_2 & \dot{f}_2 \end{pmatrix}}, \quad A^{2,0}=\frac{D\begin{pmatrix} \phi_1 & \phi_2 \\ r & s \end{pmatrix}}{D\begin{pmatrix} \phi_1 & \phi_2 \\ \phi_1' & \phi_2' \end{pmatrix}}.$$

Conditions of reality lead to other restrictions on the parameters involved. It is clear that two possibilities in the choice of parameters λ and μ are $\lambda_2=-\lambda_1^*$, $\lambda_1=-\lambda_1{}^*$, and $\lambda_2=-\lambda_2{}^*$, with the same limitations on parameters μ_2. We do not present here explicit form for the other restrictions. This is pure algebraic manipulation.

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Erratum: A sum rule for associated Legendre polynomials with spherical triangles [J. Math. Phys. 44, 849 (2003)]

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[DOI: 10.1063/1.1562012]

We have corrected a few misprints in our article.

Immediately following Eq. (2), the sentence should read:

where $A^n_{j,m}=(-1)^m a_n^{j+2}K\int_0^{\pi}\int_0^{2\pi}\sigma_n(\theta,\phi)P_j^{-m}(\cos\theta)e^{-im\phi}d\phi\sin\theta d\theta$ and where $\sigma_n(\theta,\phi)$ is the electronic charge density on the surface of the nth sphere and where the first, second, and third terms are the contributions stemming from charges on sphere 1, sphere 2, and sphere 3, respectively.

Immediately following Eq. (10), the sentence should read:

where $P_\ell(\cos\beta')=\Sigma_{n=-\ell}^{\ell}(-1)^n P_\ell^{-n}(\cos\beta)P_\ell^n(\cos\lambda)e^{in(\phi_\lambda-\phi)}$ and is the sought-after sum rule for the associated Legendre polynomial with complex exponentials.

And Eq. (11) should read

$$V_1\delta_{\ell',0}\delta_{k,0}=(-1)^k\frac{A^1_{\ell',-k}}{a_1^{\ell'+1}}+(-1)^k\sum_{j=0}^{\infty}\frac{(\ell'+j)!}{(\ell'-k)!(j+k)!}\frac{a_1^{\ell'}}{{h_{12}}^{\ell'+j+1}}A^2_{j,-k}$$
$$+\sum_{j=0}^{\infty}(\ell'+j)!\frac{a_1^{\ell'}}{{h_{13}}^{\ell'+j+1}}\sum_{m=-\ell'}^{\ell'}\frac{g^m_{\ell',k}(-\cos\lambda_{13})}{(\ell'+m)!(j-m)!}(-1)^{m+\ell'+k}e^{i(k+m)\phi_{\lambda_{13}}}A^3_{j,m}$$

for $k\geqslant 0$, and

$$g^m_{\ell',k}(-\cos\lambda)=\sum_{n=0}^{\ell'}\frac{(-1)^n(\ell'+n)!}{2^n(n-m)!(n-k)!(\ell'-n)!}(1-\cos\lambda)^{(k+m)/2}(1+\cos\lambda)^{n-(k+m)/2}$$

and, importantly, be generalized to any number of spheres by cyclic permutation.

Erratum: The Hausdorff entropic moment problem [J. Math. Phys. 42, 2309 (2001)]

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[DOI: 10.1063/1.1555685]

The conditions of theorem 1 are only necessary due to the fact that the proof of sufficiency is based upon a wrong application of Hausdorff's theorem for the ordinary moment problem. To find the corresponding sufficient conditions is an open problem. The validity of the reconstruction method discussed in Sec. III remains because therein we do not use that theorem, although we assume the existence of the associated density.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

Controllability properties for finite dimensional quantum Markovian master equations

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(Received 3 December 2002; accepted 22 February 2003)

Various notions from geometric control theory are used to characterize the behavior of the Markovian master equation for N-level quantum mechanical systems driven by unitary control and to describe the structure of the sets of reachable states. It is shown that the system can be accessible but neither small-time controllable nor controllable in finite time. In particular, if the generators of quantum dynamical semigroups are unital, then the reachable sets admit easy characterizations as they monotonically grow in time. The two level case is treated in detail. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1571221]

I. INTRODUCTION

The main question that we discuss in this work is the following: to which density operators can we drive the quantum Markovian master equation by means of coherent control? This problem is of relevance whenever one is interested in quantum state manipulation in presence of nonunitary evolution, for example in the context of quantum information processing[5,16,18] and of molecular control.[22] The ultimate goal is obviously to know when and how the state of a quantum mechanical system can be arbitrarily manipulated by means of unitary (reversible) control operations or at least to what extent this is possible.

The viewpoint we take in this work is that of ''classical'' geometric control theory which provides us the tools to mathematically formalize and answer the questions posed. In classical control terms, the set of density operators to which we can steer the system is called the *reachable set* and the problem of arbitrary manipulability of the state can be formulated as a *controllability* problem.

The infinitesimal structure of the so-called quantum Markovian master equation, i.e., the ''axiomatic'' model for an open quantum system, is known since the works of Lindblad[15] and Gorini–Kossakowski–Sudarshan[8] and it is a prerequisite for the utilization of the Lie algebraic controllability methods developed below. We use the so-called *vector of coherences* formulation for the density matrix,[3] i.e., the expectation values corresponding to a complete set of Hermitian operators, here the Gell–Mann matrices. Such formulation allows to treat the master equation as a control system with affine vector fields or, geometrically, as a system living on a homogeneous space of a matrix Lie group and subordinated to an affine group action, plus constraints originating from the complete positivity of the quantum dynamical semigroup. If we drop these constraints, the system falls into a class of systems whose controllability properties were studied in detail in the past, see Refs. 10 and 19 for a general overview, and Refs. 6, 7, and 11 for the particular case of affine fields. Including the complete positivity requirements totally alter these results, because of the relaxation it induces.

The qualitative difference between studying the master equation and its controlled counterpart is that the master equation is an ODE whose solution, obtained integrating a single vector field, is a one parameter semigroup; the presence of control parameters in the controlled master equation implies that we have to consider a family of vector fields simultaneously, and therefore the

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admissible flow is a multiparameter semigroup or Lie semigroups.[9] Such a semigroup is the reachable set. When the reachable set is large enough to be a subgroup or at least to act transitively on the homogeneous space, then we have controllability. The problems arise when the reachable semigroup is not a group, as in the case of the controlled master equation. A novel element with respect to, for example, the control of Schrödinger equations[4] is that in the master equation one has to deal with a true *drift* term, i.e., a vector field which is both noncontrollable and nonrecurrent. Then it can happen that although it is (often) possible to generate motion in any direction (i.e., we have the accessibility property), the system in never controllable in finite time because the flow cannot be reversed. In other terms, the reachable set may be open and dense in the space of admissible density operators, but the initial condition of the controlled master equation always lies on the boundary of such set for any finite time and therefore it is not possible to reach arbitrary points in its neighborhoods. The vector of coherences representation is very useful in this respect, as it allows to explain the lack of controllability in terms of the trace of the dissipation/relaxation superoperator. In fact, the main reason for noncontrollability lies in the structure of the nonunitary operators given by complete positivity. When such infinitesimal generators is unital this is clearly visible: for the density operator ρ, $\mathrm{tr}(\rho)$ gives the level sets of a quadratic Lyapunov function centered in the origin. In this case, the controlled dynamics is stable and the control alone allows only to move within one of the level sets, not to pass from one level set to another. Since the nonunitary operator is pointing inward, as time passes also the controlled integral curves can move only inward and this establishes a monotonicity relation among the sets reachable at different time instants. As pointed out, for example, in Ref. 22, the presence of a dissipation (nonunitary) operator is essential for *any* motion not confined to a sphere in $\mathbb{R}^n$ to be accomplished. Notice that this holds regardless of the existence of a thermodynamic equilibrium, i.e., a fixed point for the original uncontrolled master equation. For affine dissipation operators, the situation is slightly more complicated and controllability may be recovered as a limit process. The atom with spontaneous emission is one such case and will be discussed in some detail. In this case, motion is not confined to the inward of spheres in $\mathbb{R}^n$ and ''purification'' processes are possible.

The organization of the paper is as follows: in Sec. II we review all the relevant notions concerning controllability of bilinear/affine systems on homogeneous spaces of a Lie group; in Sec. III the formalism of the vector of coherences parametrization is recalled and used to discuss controllability of Liouville dynamics; in Sec. IV the controllability of the master equation is treated and the main Theorem formulated. Finally, in Sec. V the two-level case is discussed in detail, first for general dissipation operators and then for few significant examples.

It is worth remarking that all our considerations make sense for finite dimensional quantum systems.

II. DRIFT AND CONTROLLABILITY FOR BILINEAR CONTROL SYSTEMS

All properties introduced in this section are standard in geometric control and are adequately surveyed for instance in Refs. 10 and 19. Consider the following bilinear control system:

$$\begin{aligned} \dot{x} &= B_0 x + \sum_{k=1}^{q} u_k B_k x, \\ x(0) &= x_i, \end{aligned} \tag{1}$$

where the controls $u_1,\ldots,u_q$ are real valued piecewise constant functions defined on $[0,\infty)$, $B_0,\ldots,B_q$ are square matrices and $x \in M$, an analytic manifold of real dimension n. In this work: M is $\mathbb{R}^n_0 = \mathbb{R}^n \backslash \{0\}$ or some n-dimensional homogeneous space (like a sphere) contained in $\mathbb{R}^r$, $r \geqslant n$, or some subset of $\mathbb{R}^n$ like a solid unit ball. The vector field $B_0 x$ is called the drift and $B_1 u_1 x,\ldots,B_q u_q x$ are the control vector fields.

Given $x_i \in M$, let us call $\mathcal{R}(x_i, T)$ the reachable set from x_i at time $T>0$ for the system (1):

$$\mathcal{R}(x_i, T) = \{x \in M \text{ s.t. } x(0)=x_i \text{ and } x(T)=x,\ T>0, \text{for some admissible control } u_1,\ldots,u_q\}.$$

If $\mathcal{R}(x_i, \leqslant T) = \cup_{0 \leqslant t \leqslant T} \mathcal{R}(x_i, t)$, then the *reachable set* from x_i is $\mathcal{R}(x_i) = \cup_{0 \leqslant t \leqslant \infty} \mathcal{R}(x_i, t)$. In correspondence of a given T_f and of $\mathcal{R}(x_i, \leqslant T_f)$, one can define the notions of finite time controllability as follows.

Definition 1: Given $T_f > 0$, *system (1) is* T_f-controllable *if* $\forall \; x_i, x_f \in M \exists$ *admissible control functions* $u_1, \ldots, u_q$ *such that the flow of (1) satisfies* $x(0) = x_i$ *and* $x(T_f) = x_f$.

The existence of a T_f finite is important for the application discussed in this work. When, instead, we are interested in controllability for any time in $\mathcal{R}(x_i)$, then we can use the following.

Definition 2: System (1) is controllable *if any* $x_f \in M$ *is reachable from any* $x_i \in M$ *for some admissible control function* $u_1, \ldots, u_q$.

Unlike the reachable set which accounts only for the positive time evolution of the trajectories of the system, the orbit $\mathcal{O}(x_i)$ requires to consider complete vector fields, i.e., defined on the whole time axis:

$$\mathcal{O}(x_i) = \cup_{t \in \mathbb{R}} \{x \in M \text{ s.t. } x(0) = x_i \text{ and } x(t) = x, t \in \mathbb{R}, \text{ for some admissible control } u_1, \ldots, u_q\}.$$

The difference between $\mathcal{O}(x_i)$ and $\mathcal{R}(x_i)$ corresponds to the difference between the accessibility and controllability properties.

Definition 3: System (1) is accessible *if* $\mathcal{R}(x_i, \leqslant T)$ *contains nonempty open sets of* M *for all* $T > 0$.

While accessibility guarantees the existence of open reachable sets, it does not say anything on x_i belonging to it.

Definition 4: System (1) is small-time controllable *if* x_i *belongs to the interior of the reachable set,* $\operatorname{int} \mathcal{R}(x_i, T)$, *for all* $T > 0$.

The accessibility property admits an algebraic characterization in terms of the Lie algebra generated by the vector fields $B_0 x, B_1 x, \ldots, B_q x$, call it $\mathrm{Lie}(B_0 x, B_1 x, \ldots, B_q x)$.

Theorem 1: (*Lie algebraic rank condition (LARC)): System (1) is accessible if and only if* $\dim(\mathrm{Lie}(B_0 x, B_1 x, \ldots, B_q x)) = \dim(M)$.

For bilinear systems, when accessibility holds there exists a Lie group of transformations, call it G, of (finite) dimension greater or equal than M acting transitively on M and to which we can lift the system. Invariance of the vector fields on a Lie group implies that the controllability conditions are global and independent of the point of application. For example, for both $\mathcal{R}(x_i)$ and $\mathcal{O}(x_i)$ we have $\mathcal{R}(x_i) = \mathcal{R}_G x_i$ and $\mathcal{O}(x_i) = \mathcal{O}_G x_i$, with $\mathcal{R}_G = \mathcal{R}(I)$ and $\mathcal{O}_G = \mathcal{O}(I)$ reachable set and orbit of the lifted system, where I is the identity matrix of G. Therefore we can work indifferently with vector fields on M $(B_0 x, B_1 u_1 x, \ldots, B_q u_q x)$ or with right invariant vector fields on the Lie group G (i.e., the matrices $B_0, B_1 u_1, \ldots, B_q u_q$ of $\mathfrak{g}$, the Lie algebra of G), to which we have lifted the system, starting from the identity of G:

$$\begin{aligned} \dot{g} &= B_0 g + \sum_{i=1}^{q} u_i(t) B_i g \quad g \in G, \\ g(0) &= I. \end{aligned} \tag{2}$$

In particular, the LARC condition and the so-called orbit theorem guarantee that $\mathcal{O}_G$ is the whole G and that M is nothing but a homogeneous space of G expressed in terms of equivalence classes as Gx, $x \in M$. The Lie algebra $\mathfrak{g}$ is therefore equal to $\mathrm{Lie}(B_0, \ldots, B_q)$ and the accessibility condition reformulates as transitivity of G (or of $\mathfrak{g}$, with a common abuse of terminology) on M.

Theorem 2: *System (1) is accessible if and only if* $\mathfrak{g}$ *is transitive on* M.

The LARC condition is only a necessary condition for controllability, even when it holds the reachable set needs not be the whole Lie group G. When $\mathcal{R}_G \subsetneq \mathcal{O}_G$ the lifted system is not controllable, the reason being that the drift is allowed to flow only along the time forward direction and may not be reversible by means of the control vector fields. In fact, the control vector fields are ''complete'' in the sense that, since u_k can assume both positive and negative values,

once exponentiated they generate a one parameter subgroup $\exp(tu_kB_k,\ t\geqslant 0)$. On the contrary, the drift produces only a subsemigroup $\exp(tB_0,\ t\geqslant 0)$ and thus $\mathcal{R}_G$ in general only has the structure of a *Lie semigroup* of G.[9]

The case of a compact group is exceptional, since compact Lie groups do not admit semigroups: $\exp(tB,\ t\geqslant 0)=\exp(tB,\ t\in\mathbb{R})$. Hence $\mathcal{R}_G$ collapses in $\mathcal{O}_G$ and the accessibility property collapses into (''long time'') controllability. The LARC condition then becomes necessary and sufficient for controllability: $\mathcal{R}(x_i)=\mathcal{O}_G x_i=Gx_i=M,\ \forall\ x_i\in M$.

In general, however, one has to deal with the case of $\mathcal{R}_G$ being only a Lie semigroup. Even if $\mathcal{R}_G$ is a proper semigroup, $\mathcal{R}_G\subsetneq G$, it may still happen that the action of $\mathcal{R}_G$ on M is transitive. In the literature, most results are in the form of sufficient conditions for controllability. For system (1), examples are

(1) $\mathcal{R}_G=G$ and G acts transitively on M,
(2) $\mathcal{R}_G$ acts transitively on M,
(3) $x_i\in \operatorname{int}\mathcal{R}(x_i, T)\ \forall\ T>0$.

For our case, none of these (or similar) conditions hold and ''negative'' results have to be established.

Affine vector fields case: The case of affine vector fields generalizes (1) to the following set of ODEs:

$$\begin{aligned}\dot{x}&=B_0x+b_0x_0+\sum_{k=1}^{q}\ (u_kB_kx+b_kx_0),\\ x(0)&=x_i,\end{aligned}\tag{3}$$

where x_0 is a real constant. It corresponds to a Lie group of transformations having the structure of a semidirect product $K\circledS V$ with V typically a n-dimensional real vector space and K a Lie group acting linearly on it. The dimension of $K\circledS V$ is $\dim(K)+n$. By choosing the following homogeneous coordinates for the state $\overline{x}=[x_0, x^T]^T$, the system (3) recovers the linear form of (1):

$$\dot{\overline{x}}=\overline{B}_0\overline{x}+\sum_{k=1}^{q}\ u_k\overline{B}_k\overline{x},$$

where $\overline{B}_k=\left[\begin{smallmatrix}0 & 0\\ b_k & B_k\end{smallmatrix}\right]$. The homogeneous coordinates allow to transform the affine action of $K\circledS V$ on x into linear action on $\overline{x}$. If $g=\left[\begin{smallmatrix}1 & 0\\ v & k\end{smallmatrix}\right]\in G=\left[\begin{smallmatrix}1 & 0\\ V & K\end{smallmatrix}\right]$, the action $\Phi: G\times M\to M$ is

$$\Phi(g)(\overline{x})=g\overline{x}=\begin{bmatrix}x_0\\ kx+vx_0\end{bmatrix}$$

so that the affine vector fields induced on $\overline{x}$ by Φ are

$$\Phi_*(\overline{B})(\overline{x})=\overline{B}\overline{x}=\begin{bmatrix}0\\ Bx+bx_0\end{bmatrix}$$

and the Lie bracket is

$$[\overline{A},\overline{B}]=\begin{bmatrix}0 & 0\\ Ab-Ba & [A,B]\end{bmatrix}.$$

Also for affine systems, special sufficient conditions for accessibility and controllability have been devised, see Refs. 6, 7, and 11 for details.

III. CONTROLLABILITY OF HAMILTONIAN DYNAMICS

To describe differential equations for density operators, we make use of the so-called vector of coherences formulation. A few essential facts about it are reported below; see, for example, Ref. 3 for a thorough description and further references.

A. Density operators and vectors of coherences

The state of a quantum mechanical system in an N-dimensional Hilbert space $\mathcal{H}^N$ can be described in terms of a trace 1 positive semidefinite Hermitian operator ρ called the density matrix. If the density operator is entirely characterized by a wave function $|\psi\rangle$, then the system is said to be in a pure state, ρ is defined as $\rho(t)=|\psi\rangle\langle\psi|$ and $\mathrm{tr}(\rho^2)=1$. If instead we have a statistical ensemble $\rho(t)=\Sigma_{i=1}^{N}p^{(i)}|\psi^{(i)}\rangle\langle\psi^{(i)}|$ for $p^{(i)}\geqslant 0$ and $\Sigma_{i=1}^{N}p^{(i)}=1$, then the system is said to be in a mixed state characterized by the pairs $\{p^{(i)},|\psi^{(i)}\rangle\}$ and $\mathrm{tr}(\rho^2)\leqslant 1$. In both cases, the properties of Hermitianity $\rho=\rho^{\dagger}$ and of unit trace $\mathrm{tr}(\rho)=1$ imply that the $N\times N$ matrix representing the density operator depends on $n=N^2-1$ real parameters. Up to the imaginary unit, $N\times N$ traceless Hermitian matrices form the Lie algebra $\mathfrak{su}(N)$ of dimension exactly n. If to it we add the (properly normalized) unit vector, then we obtain a complete basis for the density operator of an N-dimensional quantum mechanical system. In fact, the N-dimensional Pauli matrices λ_j, see, for example, Ref. 14 for their explicit expression, and the identity matrix $\lambda_0=N^{-1/2}I$, form a complete orthonormal set of basis operators for ρ (orthonormal in the sense that $\mathrm{tr}(\lambda_j\lambda_k)=\delta_{jk}$). In particular, then, $\rho=\Sigma_{j=0}^{n}\mathrm{tr}\,(\rho\lambda_j)\lambda_j=\Sigma_{j=0}^{n}\rho_j\lambda_j$, with $\rho_0=N^{-1/2}$ fixed constant and the n real parameters ρ_j giving the parametrization of ρ. Since the λ_k, $k=1,\ldots,n$, form a compete set of observable operators, the $\rho_j=\mathrm{tr}(\rho\lambda_j)$ are expectation values of ρ. Call $\boldsymbol{\rho}=[\rho_1\cdots\rho_n]^T$ such *vector of coherences* of ρ. Due to the constant component along λ_0, $\boldsymbol{\rho}$ is living on an affine space characterized by the extra fixed coordinate $\rho_0=N^{-1/2}$. Such n-dimensional Liouville space of vectors $\overline{\boldsymbol{\rho}}=[\rho_0\,\rho_1\cdots\rho_n]^T=[\rho_0\,\boldsymbol{\rho}^T]^T$ has Euclidean inner product given by the trace metric: $\|\overline{\boldsymbol{\rho}}\|=\sqrt{\langle\langle\overline{\boldsymbol{\rho}},\overline{\boldsymbol{\rho}}\rangle\rangle}=\sqrt{\mathrm{tr}(\rho^2)}$. The condition $\mathrm{tr}(\rho^2)\leqslant 1$ then translates in $\overline{\boldsymbol{\rho}}$-space as $\overline{\boldsymbol{\rho}}$ belonging to the solid affine ball of radius $1-(1/N)$ centered at $[\rho_0\,0\cdots 0]^T$, call it $\overline{\mathbb{B}}^n$, for all positive times. The surface of such ball generalizes the idea of Block sphere to N dimension and corresponds to pure states $\|\overline{\boldsymbol{\rho}}\|^2=1$. In terms of vector of coherences, the condition $\mathrm{tr}(\rho^2)\leqslant 1$ becomes the ball $\|\boldsymbol{\rho}\|^2\leqslant 1-(1/N)$ centered at the origin.

B. Hamiltonian dynamics

If H is a constant finite-dimensional Hamiltonian, for the density operator the Liouville equation is given by

$$\dot{\rho}(t)=-i[H,\rho]=-i\,\mathrm{ad}_H(\rho).$$

If $-iH\in\mathfrak{su}(N)$, then $-i\,\mathrm{ad}_H$ is a so-called commutator superoperator, i.e., a linear operator in the n-dimensional Liouville space of $\boldsymbol{\rho}$ vectors. In terms of $\boldsymbol{\rho}$, the action of $-i\,\mathrm{ad}_H$ is linear,

$$\dot{\boldsymbol{\rho}}=-i\,\mathrm{ad}_H\,\boldsymbol{\rho}, \tag{4}$$

H being traceless and Hermitian, in the $\{\lambda_j\}$ basis: $H=\Sigma_{l=1}^{n}h_l\lambda_l$. The process of passing from ρ to $\boldsymbol{\rho}$ is mathematically equivalent to passing to the adjoint representation of the Lie algebra $\mathfrak{su}(N)$. In fact, the corresponding basis in the adjoint representation is given by the $n\times n$ matrices $\mathrm{ad}_{\lambda_1},\ldots,\mathrm{ad}_{\lambda_n}$ of elements $(\mathrm{ad}_{\lambda_l})_{jk}=if_{ljk}$ with f_{ljk} real fully skew-symmetric (with respect to the permutation of any pair of indexes) tensor. Thus $-i\,\mathrm{ad}_H=-i\Sigma_{l=1}^{n}h_l\,\mathrm{ad}_{\lambda_l}$. The $n\times n$ matrices $-i\,\mathrm{ad}_{\lambda_1},\ldots,-i\,\mathrm{ad}_{\lambda_n}$ are real and skew symmetric and as such they are part of a basis of $\mathfrak{so}(n)$. Since

$$\dim\ (\mathfrak{so}(n))=\frac{n(n-1)}{2}=\frac{N^4-3N^2+2}{2},$$

for $N>2$ the n matrices $-i\,\mathrm{ad}_{\lambda_1},\ldots,-i\,\mathrm{ad}_{\lambda_n}$ span only a proper subalgebra $\mathrm{ad}_{\mathfrak{su}(N)}$ of $\mathfrak{so}(n)$. For example, for $N=3$, $n=\dim(\mathfrak{su}(3))=8$, while $\dim(\mathfrak{so}(8))=28$. In the Liouville equation (4), the propagator for $\boldsymbol{\rho}$ corresponding to the Hamiltonian H is an orthogonal matrix,

$$\boldsymbol{\rho}(t)=g(t)\boldsymbol{\rho}(0),\quad g(t)\in\exp(\mathrm{ad}_{\mathfrak{su}(N)})\subseteq\mathrm{SO}(n)$$

such that $\dot{g}(t)=-i\,\mathrm{ad}_H g(t)$, $g(0)=I$. The action of any $g\in\mathrm{SO}(n)$ on ρ is isometric and as such it preserves the inner product $\|\boldsymbol{\rho}\|$.

C. Coherent control of Hamiltonian dynamics

Assume that the Hamiltonian H is composed of a time-invariant part H_0 representing the free evolution of the system plus q time-varying forcing terms representing the interaction with q external fields, modeled semiclassically,

$$H(t)=H_0+\sum_{k=1}^{q}u_k(t)H_k,\quad -iH_0,-iH_k\in\mathfrak{su}(N),$$

with the parameters u_k representing the control fields. Consider a pure state of ket $|\psi\rangle\in\mathbb{S}\subset\mathcal{H}^N$ (where $\mathbb{S}$ is the sphere in N-dimensional Hilbert space) and its Schrödinger equation

$$i|\dot{\psi}\rangle=H_0|\psi\rangle+\sum_{k=1}^{q}u_kH_k|\psi\rangle,\quad |\psi(0)\rangle=|\psi_0\rangle. \tag{5}$$

The sphere $\mathbb{S}$ in $\mathcal{H}^N$ is a homogeneous space of $\mathrm{SU}(N)$. Compactness of $\mathrm{SU}(N)$ plus transitivity of the $\mathrm{SU}(N)$ action on $\mathbb{S}$ in this case guarantee the following (see Ref. 12 for the original formulation, Ref. 4 for a thorough discussion and Ref. 1 for more material on Lie algebras transitive on $\mathbb{S}$):

Theorem 3: *If* $\mathrm{Lie}(-iH_0,-iH_1,\ldots,-iH_q)=\mathfrak{su}(N)$ *then system (5) is controllable.* By computing the (real) dimension of such Lie algebra $\dim(\mathrm{Lie}(-iH_0,\ldots,-iH_q))=\dim(\mathfrak{su}(N))=n=\dim(\mathbb{S})$.

In the following we will always consider the controllable case for the wave function $|\psi\rangle$.

Assumption A1: System (5) is controllable.

Passing to density matrices, for a mixed state ρ driven by the same Hamiltonian $H(t)$ the corresponding forced Liouville equation written in terms of vector of coherences is

$$\dot{\boldsymbol{\rho}}=-i\,\mathrm{ad}_{H_0}\boldsymbol{\rho}-i\sum_{k=1}^{q}u_k\,\mathrm{ad}_{H_k}\boldsymbol{\rho}. \tag{6}$$

The vector fields $-i\,\mathrm{ad}_{H_0},\ldots,-i\,\mathrm{ad}_{H_q}$ corresponding to the Hamiltonian dynamics lack the translation component and belong to a subalgebra $\mathrm{ad}_{\mathfrak{su}(N)}$ of $\mathfrak{so}(n)$. Just like the Lie group $\mathrm{SU}(N)$ is acting transitively on the unit sphere on $\mathcal{H}^N$, so the orthogonal group $\mathrm{SO}(n)$ is acting transitively on a sphere $\|\boldsymbol{\rho}\|^2=\mathrm{const}\leqslant 1-(1/N)$. By dimension counting, $\exp(\mathrm{ad}_{\mathfrak{su}(N)})$ is not acting transitively on such sphere if $N>2$. In fact, it is well known that coherent control cannot modify the eigenvalues of ρ, and so controllability can occur only inside the leaf of the foliation of ρ (determined by the eigenvalues) that one starts with. See Ref. 20 for a description of the kinematic equivalence classes of density matrices in the context of dynamical control, or Ref. 13 for a complete description of the invariants of motion.

IV. CONTROLLABILITY OF MARKOVIAN MASTER EQUATIONS

The requirement of $\mathrm{tr}(\rho^2)\leqslant 1$ for the density operator is reformulated in the vector of coherences parametrization as $\|\overline{\boldsymbol{\rho}}\|^2\leqslant 1$. Thus $\overline{\mathbb{B}^n}$ has to be made invariant by the quantum dynamical

evolution. The main feature of the master equation is to capture all the possible infinitesimal generators that fulfill this condition. Obviously, also the driven master equation has to live on $\overline{\mathbb{B}}^n$, and all controllability questions have to be restricted to $\overline{\mathbb{B}}^n$.

A. Master equation

Calling $\mathcal{L}_D$ the superoperator representing the relaxing/dissipating part of the dynamics, in the basis $\{\lambda_j\}$ of traceless Hermitian matrices the Markovian master equation is expressed as[8]

$$\begin{aligned}\dot{\rho}=\mathcal{L}_H(\rho)+\mathcal{L}_D(\rho)&=-i\,\mathrm{ad}_H(\rho)+\frac{1}{2}\sum_{j,k=1}^{n}a_{jk}([\lambda_j,\rho\lambda_k]+[\lambda_j\rho,\lambda_k])\\&=-i[H,\rho]+\frac{1}{2}\sum_{j,k=1}^{n}a_{jk}(2\lambda_j\rho\lambda_k-\{\lambda_k\lambda_j,\rho\}),\end{aligned}\tag{7}$$

where the Hermitian matrix $A=(a_{jk})$ is positive semidefinite, $A\geqslant 0$, and $\{\cdot,\cdot\}$ is the anticommutator. For the basis $\{\lambda_j\}$, unlike a Lie bracket which is linear in the generators, the anticommutator has an affine structure: $\{\lambda_j,\lambda_k\}=(2\sqrt{2}/N)\,\delta_{jk}\lambda_0+\Sigma_{l=1}^{n}d_{jkl}\lambda_l$, with d_{jkl} the real and fully symmetric tensor. The expression of (7) in terms of vector of coherences is as follows:

$$\dot{\boldsymbol{\rho}}=-i\,\mathrm{ad}_H\boldsymbol{\rho}+\sum_{j,k=1}^{n}a_{jk}(L_{jk}\boldsymbol{\rho}+\mathbf{v}_{jk}\rho_0)\tag{8}$$

with L_{jk} $n\times n$ complex matrix of mixed symmetry and $\mathbf{v}_{jk}$ imaginary n vector given by

$$\begin{aligned}L_{jk}=(L_{jk})_{lr}&=-\frac{1}{4}\sum_{m=1}^{n}((f_{jmr}+id_{jmr})f_{kml}+(f_{kmr}-id_{kmr})f_{jml}),\\\mathbf{v}_{jk}&=\frac{i}{\sqrt{N}}[f_{jkl}\cdots f_{jkn}]^T.\end{aligned}\tag{9}$$

B. Coherent control of master equations

Under the assumption of weak and high frequency control fields, it is acceptable to assume that no time dependence is induced in the $\mathcal{L}_D$ term by the external fields. Adding the controls, Eq. (8) modifies as[23]

$$\dot{\boldsymbol{\rho}}=\mathcal{L}_{H_0}\boldsymbol{\rho}+\sum_{k=1}^{q}u_k\mathcal{L}_{H_k}\boldsymbol{\rho}+\mathcal{L}_D\boldsymbol{\rho}=-i\,\mathrm{ad}_{H_0}\boldsymbol{\rho}-i\sum_{k=1}^{q}u_k\,\mathrm{ad}_{H_k}\boldsymbol{\rho}+\sum_{j,k=1}^{n}a_{jk}(L_{jk}\boldsymbol{\rho}+\mathbf{v}_{jk}\rho_0)\tag{10}$$

or, in homogeneous coordinates and calling $\overline{L}_{jk}=\left[\begin{smallmatrix}0 & 0\\ \mathbf{v}_{jk} & L_{jk}\end{smallmatrix}\right]$, $j,k=1,\ldots,n$:

$$\begin{aligned}\dot{\overline{\boldsymbol{\rho}}}=\overline{\mathcal{L}}\overline{\boldsymbol{\rho}}&=\overline{\mathcal{L}}_{H_0}\overline{\boldsymbol{\rho}}+\sum_{k=1}^{q}u_k\overline{\mathcal{L}}_{H_k}\overline{\boldsymbol{\rho}}+\overline{\mathcal{L}}_D\overline{\boldsymbol{\rho}},\quad \overline{\boldsymbol{\rho}}\in\overline{\mathbb{B}}^n\\&=\begin{bmatrix}0 & 0\\ 0 & -i\,\mathrm{ad}_{H_0}\end{bmatrix}\overline{\boldsymbol{\rho}}+\sum_{k=1}^{q}u_k\begin{bmatrix}0 & 0\\ 0 & -i\,\mathrm{ad}_{H_k}\end{bmatrix}\overline{\boldsymbol{\rho}}+\sum_{j,k=1}^{n}a_{jk}\overline{L}_{jk}\overline{\boldsymbol{\rho}}.\end{aligned}\tag{11}$$

The state of (11) is living on $\mathbb{R}^{n+1}$ and is constrained by the positivity of ρ requirement to belong to $\overline{\mathbb{B}}^n$. However, the dissipation term $\mathcal{L}_D$ is not coherent and as such it enlarges the integral group of (11) from $\exp(\mathrm{ad}_{\mathfrak{su}(N)})$ to one of the Lie groups properly containing it. Examples are $\mathrm{SO}(n,\mathbb{R})$,

$\mathrm{SL}(n,\mathbb{R})$, $\mathrm{GL}^+(n,\mathbb{R})$, the connected component of $\mathrm{GL}(n,\mathbb{R})$ containing the identity, or their semidirect extensions $\mathrm{SO}(n,\mathbb{R})\circledS\mathbb{R}^n$, $\mathrm{SL}(n,\mathbb{R})\circledS\mathbb{R}^n$, and $\mathrm{GL}^+(n,\mathbb{R})\circledS\mathbb{R}^n$.

Since A is Hermitian, the number of independent parameters a_{jk} is n^2. It is convenient to rearrange the n^2 degrees of freedom in the following manner. From (9), it is straightforward to check that $\mathrm{Re}[(L_{kj})_{lr}]=\mathrm{Re}[(L_{jk})_{lr}]$, $\mathrm{Im}[(L_{kj})_{lr}]=-\mathrm{Im}[(L_{jk})_{lr}]$ and therefore $L_{kj}=L_{jk}^*$. If we call $L_{jk}^{\Re}=\mathrm{Re}[(L_{jk})_{lr}]$ and $L_{jk}^{\Im}=\mathrm{Im}[(L_{jk})_{lr}]$, then with respect to index permutation $L_{jk}^{\Re}$ is symmetric, $L_{kj}^{\Re}=L_{jk}^{\Re}$ while $L_{jk}^{\Im}$ is skew-symmetric, $L_{kj}^{\Im}=-L_{jk}^{\Im}$. Similarly, the Hermitianity of A implies $a_{kj}=a_{jk}^*$ or, if we write $a_{jk}^{\Re}=\mathrm{Re}[a_{jk}]$ and $a_{jk}^{\Im}=\mathrm{Im}[a_{jk}]$, $a_{kj}^{\Re}=a_{jk}^{\Re}$, $a_{kj}^{\Im}=-a_{jk}^{\Im}$. Therefore,

$$a_{jk}\overline{L}_{jk}+a_{kj}\overline{L}_{kj}=(2-\delta_{jk})a_{jk}^{\Re}\begin{bmatrix}0 & 0\\ 0 & L_{jk}^{\Re}\end{bmatrix}+2a_{jk}^{\Im}\begin{bmatrix}0 & 0\\ i\mathbf{v}_{jk} & -L_{jk}^{\Im}\end{bmatrix},\quad 1\leqslant j\leqslant k\leqslant n. \tag{12}$$

To have $A\geqslant 0$, a number of constraints among the a_{jk} must be imposed like, for example, $a_{jj}=a_{jj}^{\Re}\geqslant 0$ and $a_{jj}a_{kk}\geqslant(a_{jk}^{\Re})^2+(a_{jk}^{\Im})^2$ or $|a_{jk}|\leqslant(a_{jj}+a_{kk})/2$.

Our aim here is to draw conclusions about which $\overline{\boldsymbol{\rho}}$ can be reached by means of coherent control. In (11), unlike $\Sigma_{k=1}^q u_k\overline{\mathcal{L}}_{H_k}$, both $\overline{\mathcal{L}}_{H_0}$ and $\overline{\mathcal{L}}_D$ have integral curves that can flow only along the positive semiorbit and, in control terms, $\overline{\mathcal{L}}_{H_0}$ plays the role of the drift and $\overline{\mathcal{L}}_D$ that of a disturbance. Classically, a disturbance can be treated, for example, as a parametric family of vector fields with parameters belonging to admissible intervals (here a_{jk} such that $A\geqslant 0$). However, in the case of $\overline{\mathcal{L}}_D$ parametric the master equation becomes a differential inclusion and little can be said about its controllability properties. Therefore in this work we will assume to be dealing only with a precisely known value of A, hence of $\overline{\mathcal{L}}_D$.

Assumption A2: The parameters a_{jk}, $j,k=1,\ldots,n$ are fixed and known exactly.

Consequently we can treat $\overline{\mathcal{L}}_D$ as a part of the drift term (together with $\overline{\mathcal{L}}_{H_0}$) and use the tools of Sec. II.

Under the assumption of unitary controllability, the Lie algebra $\mathfrak{g}$ of interest here is the smallest Lie algebra of real matrices containing $\mathrm{ad}_{\mathfrak{su}(N)}$ and $\overline{\mathcal{L}}_{H_0}+\overline{\mathcal{L}}_D$ and closed with respect to the matrix commutation

$$\mathfrak{g}=\mathrm{Lie}(\overline{\mathcal{L}}_{H_0}+\overline{\mathcal{L}}_D,\overline{\mathcal{L}}_{H_1},\ldots,\overline{\mathcal{L}}_{H_q}).$$

Once $\mathfrak{g}$ is computed, the system can be lifted to G,

$$\dot{g}=\overline{\mathcal{L}}_{H_0}g+\sum_{k=1}^{q}u_k\overline{\mathcal{L}}_{H_k}g+\overline{\mathcal{L}}_Dg. \tag{13}$$

The following theorem gathers various results about accessibility and controllability for system (11). Concerning controllability, while for $\overline{\mathcal{L}}_D$ unital the results are sharp (and negative), the case of $\overline{\mathcal{L}}_D$ affine is more difficult to treat. In fact, in this case, in spite of the lack of small-time controllability it may happen that points that are not reachable in short time are reachable for T large enough and even that $\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i))=\overline{\mathbb{B}}^n$ asymptotically ($\mathrm{cl}(\cdot)$ means closure). The atom with spontaneous emission discussed in the examples of Sec. V is one such case. Essentially this fact depends on the existence of a fixed point for the master equation and on it being on the boundary of $\overline{\mathbb{B}}^n$, $\partial\overline{\mathbb{B}}^n$. However, even in this case $\partial\overline{\mathbb{B}}^n$ is reached only asymptotically and therefore the system fails to be controllable in finite time.

Theorem 4: *Under assumptions A1 and A2, we have the following:*

(1) System (11) is accessible in $\overline{\mathbb{B}}^n$ *if and only if* $\mathfrak{g}=\mathfrak{gl}(n,\mathbb{R})$ *or* $\mathfrak{g}=\mathfrak{gl}(n,\mathbb{R})\circledS\mathbb{R}^n$;
(2) System (11) is never small-time controllable in $\overline{\mathbb{B}}^n$ *for* $\overline{\mathcal{L}}_D\neq 0$;
(3) System (11) is never T_f*-controllable in* $\overline{\mathbb{B}}^n$ *for any* $T_f>0$ *and* $\overline{\mathcal{L}}_D\neq 0$;
(4) the system (11) is never controllable in $\overline{\mathbb{B}}^n$ *for* $\overline{\mathcal{L}}_D\neq 0$ *unital.*

Proof: The proof of Part (1) follows from Theorem 2. The only transitive Lie algebras on $\mathbb{R}^n_0$ (and thus on $\overline{\mathbb{B}}^n$) are $\mathfrak{sl}(n,\mathbb{R})$ and $\mathfrak{gl}(n,\mathbb{R})$ and their semidirect extensions $\mathfrak{sl}(n,\mathbb{R})\circledS\mathbb{R}^n$ and $\mathfrak{gl}(n,\mathbb{R})\circledS\mathbb{R}^n$. Recall that matrices in $\mathfrak{sl}(n,\mathbb{R})$ are traceless and that, using the decomposition $\mathfrak{gl}(n,\mathbb{R})=\mathfrak{sl}(n,\mathbb{R})\oplus\mathrm{span}(I_n)$ (I_n the $n\times n$ identity matrix), if $\mathrm{tr}(\overline{\mathcal{L}}_D)=n\alpha$ and $\overline{I}=\left[\begin{smallmatrix}0&0\\0&I_n\end{smallmatrix}\right]$, $\overline{\mathcal{L}}_D$ can be split as $\overline{\mathcal{L}}_D=\alpha\overline{I}+\tilde{\overline{\mathcal{L}}}_D$, $\alpha\in\mathbb{R}$, $\alpha<0$, $\tilde{\overline{\mathcal{L}}}_D\in\mathfrak{sl}(n,\mathbb{R})\circledS\mathbb{R}^n$. But since $a_{jj}\geqslant 0$, in order for $\overline{\mathcal{L}}_D$ to be traceless it must be $a_{jj}=0\ \forall\, j=1,\ldots,n$ and hence, from $|a_{jk}|\leqslant(a_{jj}+a_{kk})/2$ all $a_{jk}=0$. Therefore only $\mathfrak{gl}(n,\mathbb{R})$ and $\mathfrak{gl}(n,\mathbb{R})\circledS\mathbb{R}^n$ are compatible with $A\geqslant 0$.

To prove Part (2), one needs to show that the initial condition $\overline{\boldsymbol{\rho}}_i$ does not lie in $\mathrm{int}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i))$. It is quite easy to verify it for $\overline{\mathcal{L}}_D$ unital. In fact, if the initial state $\overline{\boldsymbol{\rho}}_i$ is such that $0<\|\overline{\boldsymbol{\rho}}_i\|=\delta\leqslant 1$, then for the Hamiltonian part $\langle\!\langle(\overline{\mathcal{L}}_{H_0}+\Sigma_{k=1}^q u_k\overline{\mathcal{L}}_{H_k})\overline{\boldsymbol{\rho}}_i,\overline{\boldsymbol{\rho}}_i\rangle\!\rangle=0$ while $\overline{\mathcal{L}}_D$ is pointing inward: $\langle\!\langle\overline{\mathcal{L}}_D\overline{\boldsymbol{\rho}}_i,\overline{\boldsymbol{\rho}}_i\rangle\!\rangle<0$. Therefore, the ball of radius δ is invariant for the flow of (11) and $\overline{\boldsymbol{\rho}}_i$ lies on the boundary of $\mathcal{R}(\overline{\boldsymbol{\rho}}_i)$. For $\overline{\mathcal{L}}_D$ affine, the lack of small-time local controllability is automatically verified for pure states $\|\overline{\boldsymbol{\rho}}_i\|=1$, because the physics of the problem imposes that $\overline{\boldsymbol{\rho}}$ such that $\|\overline{\boldsymbol{\rho}}\|=\sqrt{1+\epsilon}$, $\epsilon>0$ is not admissible. Writing the integral curves of the control system as $\overline{\boldsymbol{\rho}}(t)=\Phi(\mathcal{T}\exp\int_0^t\overline{\mathcal{L}}(\tau)\mathrm{d}\tau)(\overline{\boldsymbol{\rho}}_i)=g(t)\overline{\boldsymbol{\rho}}_i$ with $\mathcal{T}$ the Dyson operator, we can lift the dynamics to the system (13) with initial condition $g(0)=I$. $\overline{\boldsymbol{\rho}}_i\notin\mathrm{int}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i))$ for $\|\overline{\boldsymbol{\rho}}_i\|=1$ implies that the reachable set $\mathcal{R}(\overline{\boldsymbol{\rho}}_i)=\mathcal{R}_G\overline{\boldsymbol{\rho}}_i$ cannot be transitive on any neighborhood of $\overline{\boldsymbol{\rho}}_i$ and that for the lifted system $I\notin\mathrm{int}(\mathcal{R}_G)$. But, due to right invariance, the properties of accessibility, controllability, and transitivity have a global character and therefore $\mathcal{R}_G$ is not transitive for any neighborhood of any $\overline{\boldsymbol{\rho}}_i\in\overline{\mathbb{B}}^n$.

Concerning Part (3), if a finite time T_f is fixed, the reachable set $\mathcal{R}(\overline{\boldsymbol{\rho}}_i,\leqslant T_f)$ for the master equation is always only a Lie semigroup. In fact, if the fixed point of $\overline{\mathcal{L}}_D$ (when it exists) belongs to $\mathrm{int}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i,\leqslant T_f))$ then $\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i,\leqslant T_f))\subseteq\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i))\subsetneq\overline{\mathbb{B}}^n$; if instead it belongs to $\partial\,\overline{\mathbb{B}}^n$ then $\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i,\leqslant T_f))\subsetneq\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}_i))=\overline{\mathbb{B}}^n$. Even if a fixed point does not exist, we have that the norm of $\overline{\boldsymbol{\rho}}_i$ can grow only if $\langle\!\langle\overline{\mathcal{L}}_D\overline{\boldsymbol{\rho}}_i,\overline{\boldsymbol{\rho}}_i\rangle\!\rangle>0$ and that $\|\overline{\boldsymbol{\rho}}(t)\|$ can approach 1 at most as $t\to\infty$. Since $\overline{\mathcal{L}}_{H_0}$ and $\overline{\mathcal{L}}_{H_1},\ldots,\overline{\mathcal{L}}_{H_q}$ preserve the length, excluding the trivial cases the control cannot speed up the convergence to $\partial\,\overline{\mathbb{B}}^n$ from its "best" initial condition. But even in that case convergence is only asymptotic. Therefore, for any fixed T_f the open set $\mathcal{R}(\overline{\boldsymbol{\rho}}_i,\leqslant T_f)$ cannot be all of $\overline{\mathbb{B}}^n$ and neither can its closure.

Finally, the proof of noncontrollability in $\overline{\mathbb{B}}^n$ for $\overline{\mathcal{L}}_D$ unital follows from the same argument used above in Part (2). □

For the system lifted to its integral group, the small-time controllability property collapses into controllability and we have the following.

Corollary 1: The "lifted" system (13) is accessible for $G=\mathrm{GL}^+(n,\mathbb{R})$ *or* $G=\mathrm{GL}^+(n,\mathbb{R})\circledS\mathbb{R}^n$ *but it is never controllable on* G *for* $\overline{\mathcal{L}}_D\neq 0$.

Proof: The first part is obvious, since accessibility on the Lie group is a necessary condition for accessibility on the homogeneous space. Concerning controllability, from the proof of Theorem 4, Part (2), for the system (13), $I\notin\mathrm{int}(\mathcal{R}_G)$. But, for Lie groups, such property is a global one and therefore the system is never controllable. □

Another way to prove the previous corollary is via piecewise constant controls: in this case, $g(t)=\mathcal{T}\exp\int_0^t\overline{\mathcal{L}}(\tau)\mathrm{d}\tau=\Pi_{j=1}^r\exp((\overline{\mathcal{L}}_{H_0}+\overline{\mathcal{L}}_D+\Sigma_{k=1}^q u_{k_j}\overline{\mathcal{L}}_{H_k})(t_j-t_{j-1}))$ and using the formula $\det(\exp(\cdot))=\exp(\mathrm{tr}(\cdot))$ we have $\det(\Pi_{j=1}^r\exp((\overline{\mathcal{L}}_{H_0}+\overline{\mathcal{L}}_D+\Sigma_{k=1}^q u_{k_j}\overline{\mathcal{L}}_{H_k})(t_j-t_{j-1})))=\exp(\Sigma_{j=1}^r\mathrm{tr}((\overline{\mathcal{L}}_{H_0}+\overline{\mathcal{L}}_D+\Sigma_{k=1}^q u_{k_j}\overline{\mathcal{L}}_{H_k})(t_j-t_{j-1})))=\exp(\mathrm{tr}(\overline{\mathcal{L}}_D)t)\leqslant 1$. Therefore, $g(t)$

$\in \mathrm{GL}^+(n,\mathbb{R})$ or $g(t) \in \mathrm{GL}^+(n,\mathbb{R})\circledS\mathbb{R}^n$ (only in these cases (13) is accessible) must be such that $\det(g(t)) \leqslant 1$ and cannot generate the whole Lie group.

Yet another method to show the same thing is to use the necessary condition of Lemma 6.8 of Ref. 12. Write $\overline{\mathcal{L}_D} = \alpha \overline{I} + \tilde{\mathcal{L}}_D$, $\alpha \in \mathbb{R}$, $\alpha < 0$, $\tilde{\mathcal{L}}_D \in \mathfrak{sl}(n,\mathbb{R})\circledS\mathbb{R}^n$. Since $[\overline{I}, \overline{F}] = 0 \ \forall \ \overline{F} \in \mathfrak{gl}(n,\mathbb{R})\circledS\mathbb{R}^n$, under the assumption of accessibility the ideal in $\mathfrak{g}$ generated by the control vector fields coincides with the derived subalgebra $\mathfrak{g}_1 = [\mathfrak{g}, \mathfrak{g}]$ (and $\mathrm{span}(\overline{I})$ with the center of $\mathfrak{g}$) and it is contained in $\mathfrak{sl}(n,\mathbb{R})\circledS\mathbb{R}^n$. A necessary condition for $\mathcal{R}_G = G$ is that $\exp((\overline{\mathcal{L}_{H_0}} + \overline{\mathcal{L}_D})t) \in \exp(\mathfrak{g}_1)$ (i.e., to $\mathrm{SL}(n,\mathbb{R})$ or to $\mathrm{SL}(n,\mathbb{R})\circledS\mathbb{R}^n$) for some $t > 0$ which is obviously never true.

For $\overline{\mathcal{L}_D}$ unital, the reachable sets are balls in $\mathbb{R}^n$ (centered in 0) and are completely characterized by the following monotonicity property.

Corollary 2: If the system (11) is accessible and if $\overline{\mathcal{L}_D}$ unital then $\mathcal{R}(\overline{\boldsymbol{\rho}_i}, \leqslant T_1) \subsetneq \mathcal{R}(\overline{\boldsymbol{\rho}_i}, \leqslant T_2) \forall\ 0 < T_1 < T_2$ and $\mathcal{R}(\overline{\boldsymbol{\rho}_i})$ is the ball of radius $\|\overline{\boldsymbol{\rho}_i}\|$.

Proof: It follows from the observation above that $\overline{\boldsymbol{\rho}_\nu}$ of norm $\|\overline{\boldsymbol{\rho}_\nu}\|$ lies on the boundary of the set reachable from $\overline{\boldsymbol{\rho}_\nu}$ by the integral curves of (11). If $\overline{\boldsymbol{\rho}_\nu} = \overline{\boldsymbol{\rho}}(T_1) = \Phi(\mathcal{T} \exp \int_0^{T_1} \overline{\mathcal{L}}(\tau) d\tau)(\overline{\boldsymbol{\rho}_i})$, then $\mathcal{R}(\overline{\boldsymbol{\rho}_i}, \leqslant T_2) = \mathcal{R}(\overline{\boldsymbol{\rho}_i}, \leqslant T_1) \cup \mathcal{R}(\overline{\boldsymbol{\rho}}(T_1), \leqslant T_2 - T_1)$. Notice that this does not require $\overline{\mathcal{L}_D}$ to have a fixed point. Accessibility of (11), in fact, guarantees that $\overline{\boldsymbol{\rho}}(t)$ can be placed on any point of the sphere of radius $\|\overline{\boldsymbol{\rho}}(t)\|$ and therefore, as $t \to \infty$, (11) can be made to tend to the origin regardless of the existence of a fixed point for $\overline{\mathcal{L}_D}$. Hence $\mathcal{R}(\overline{\boldsymbol{\rho}_i})$ is anything inside the ball of radius $\|\overline{\boldsymbol{\rho}_i}\|$. □

V. TWO LEVEL SYSTEMS

For two level systems, $\boldsymbol{\rho}$ is the usual Bloch vector. Call $\lambda_k = (1/\sqrt{2})\,\sigma_k$, $k \in \{0, x, y, z\}$ the rescaled (identity and) Pauli matrices. Then in the $\{\lambda_k\}$ basis

$$\rho = \begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix} = \rho_0\lambda_0 + \rho_x\lambda_x + \rho_y\lambda_y + \rho_z\lambda_z = \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{2}} + \rho_z & \rho_x - i\rho_y \\ \rho_x + i\rho_y & \frac{1}{\sqrt{2}} - \rho_z \end{bmatrix} \tag{14}$$

and $\boldsymbol{\rho} = [\rho_x \ \rho_y \ \rho_z]^T$, where $\rho_k = \mathrm{tr}(\rho\lambda_k)$, i.e., $\rho_0 = (1/\sqrt{2})$, $\rho_x = \sqrt{2}\ \mathrm{Re}[\rho_{01}]$, $\rho_y = -\sqrt{2}\ \mathrm{Im}[\rho_{01}]$, and $\rho_z = (1/\sqrt{2})(\rho_{00} - \rho_{11})$. In our case, $\{\lambda_0, \lambda_k\} = \sqrt{2}\lambda_k$, $\{\lambda_j, \lambda_k\} = \sqrt{2}\,\delta_{jk}\lambda_0$, $\forall\ j,k \in \mathcal{I} = \{1, 2, 3\}$. Similarly to (14), the Hamiltonian H can be written as

$$H = \sum_{k \in \mathcal{I}} \sqrt{2} h_k \lambda_k = \begin{bmatrix} h_z & h_x - ih_y \\ h_x + ih_y & -h_z \end{bmatrix}$$

and, in the adjoint representation, from $-i\,\mathrm{ad}_H = (-i\,\mathrm{ad}_H)_{pm} = (\Sigma_{l \in \mathcal{I}} h_l f_{lpm})_{pm}$,

$$-i\,\mathrm{ad}_H = \begin{bmatrix} 0 & -h_z & h_y \\ h_z & 0 & -h_x \\ -h_y & h_x & 0 \end{bmatrix} = h_x \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} + h_y \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} + h_z \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{15}$$

Specifying the coherent controls: $h_k = (h_{0_k} + u_k)$, $k = 1, 2, 3$, where h_{0_k} are the basis components of the time-independent free Hamiltonian H_0 and $u_k = u_k(t)$, $k = 1, 2, 3$, the control parameters (some of the h_{0_k} or u_k may be 0). In the homogeneous coordinates, the vector field for the Hamiltonian acquires only a zero translation, and, from (15), the infinitesimal generators of the coherent rotations are

$$\overline{M}_1=\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&-1\\0&0&1&0\end{bmatrix},\quad \overline{M}_2=\begin{bmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&-1&0&0\end{bmatrix},\quad \overline{M}_3=\begin{bmatrix}0&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&0\end{bmatrix}.$$

Hence $\overline{\mathcal{L}}_{H_0}=\Sigma_{k=1}^{3}h_{0_k}\overline{M}_k$ and $\overline{\mathcal{L}}_{H_k}=\overline{M}_k$, $k=1,2,3$. In this case (12) simplifies to

$$a_{jk}\overline{L}_{jk}+a_{kj}\overline{L}_{kj}=\begin{bmatrix}0&0\\2ia_{jk}^{\mathfrak{I}}\mathbf{v}_{jk}&(2-\delta_{jk})a_{jk}^{\mathfrak{R}}L_{jk}\end{bmatrix}. \tag{16}$$

The nine degrees of freedom of A (constrained by the positive semidefiniteness requirement) are captured by the nine real parameters (reindexed cardinally),

$$\{a_4,a_5,\ldots,a_{12}\}=\{a_{xy}^{\mathfrak{R}},a_{xy}^{\mathfrak{I}},a_{xz}^{\mathfrak{R}},a_{xz}^{\mathfrak{I}},a_{yz}^{\mathfrak{R}},a_{yz}^{\mathfrak{I}},a_{xx}^{\mathfrak{R}},a_{yy}^{\mathfrak{R}},a_{zz}^{\mathfrak{R}}\}.$$

In terms of $a_4,\ldots,a_{12}$, the matrix A is

$$A=\begin{bmatrix}a_{10}&a_4+ia_5&a_6+ia_7\\a_4-ia_5&a_{11}&a_8+ia_9\\a_6-ia_7&a_8-ia_9&a_{12}\end{bmatrix}.$$

In order to impose the positive semidefiniteness of A, a sufficient condition is that all the principal minors have nonnegative determinant, i.e.,

$$a_{10}\geqslant 0,\quad a_{11}\geqslant 0,\quad a_{12}\geqslant 0, \tag{17}$$

$$a_{10}a_{11}\geqslant a_4^2+a_5^2,\quad a_{10}a_{12}\geqslant a_6^2+a_7^2,\quad a_{11}a_{12}\geqslant a_8^2+a_9^2, \tag{18}$$

$$a_{10}a_{11}a_{12}-a_{10}(a_8^2+a_9^2)-a_{11}(a_6^2+a_7^2)-a_{12}(a_4^2+a_5^2)+2a_4(a_6a_8+a_7a_9)-2a_5(a_6a_9-a_7a_8)\geqslant 0.$$

The infinitesimal generators corresponding to this parametrization are linear combinations of the $\overline{L}_{jk}$. Numbering in the same fashion as the $a_{jk}^{\mathfrak{R}},a_{jk}^{\mathfrak{I}}$ parameters, we obtain the nine linearly independent generators,

$$\overline{M}_4=\overline{L}_{xy}+\overline{L}_{yx}=\begin{bmatrix}0&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&0\end{bmatrix},\quad \overline{M}_5=i(\overline{L}_{xy}-\overline{L}_{yx})=\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\-2&0&0&0\end{bmatrix},$$

$$\overline{M}_6=\overline{L}_{xz}+\overline{L}_{zx}=\begin{bmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&1&0&0\end{bmatrix},\quad \overline{M}_7=i(\overline{L}_{xz}-\overline{L}_{zx})=\begin{bmatrix}0&0&0&0\\0&0&0&0\\2&0&0&0\\0&0&0&0\end{bmatrix},$$

$$\overline{M}_8=\overline{L}_{yz}+\overline{L}_{zy}=\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix},\quad \overline{M}_9=i(\overline{L}_{yz}-\overline{L}_{zy})=\begin{bmatrix}0&0&0&0\\-2&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix},$$

TABLE I. Examples of subalgebras of $\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3$ obtained for different A (not necessarily $A\geqslant 0$).

	Coefficients a_{jk}	$\mathfrak{g}$
case 1	$a_5=a_7=a_9=0$; a_{10}, a_{11}, a_{12} s.t. $\mathrm{tr}(\Sigma_{k=10}^{12}a_k\overline{M}_k)=0$	$\mathfrak{sl}(3,\mathbb{R})$
case 2	$a_5=a_7=a_9=0$; a_{10}, a_{11}, a_{12} s.t. $\mathrm{tr}(\Sigma_{k=10}^{12}a_k\overline{M}_k)\neq 0$	$\mathfrak{gl}(3,\mathbb{R})$
case 3	$a_4=a_6=a_8=a_{10}=a_{11}=a_{12}=0$	$\mathrm{ad}_{\mathfrak{su}(2)}\circledS\mathbb{R}^3$
case 4	a_{10}, a_{11}, a_{12} s.t. $\mathrm{tr}(\Sigma_{k=10}^{12}a_k\overline{M}_k)=0$	$\mathfrak{sl}(3,\mathbb{R})\circledS\mathbb{R}^3$
case 5	a_{10}, a_{11}, a_{12} s.t. $\mathrm{tr}(\Sigma_{k=10}^{12}a_k\overline{M}_k)\neq 0$	$\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3$
case 6	$a_4=\cdots=a_9=0$, $a_{10}=a_{11}=a_{12}$	$\mathrm{ad}_{\mathfrak{su}(2)}\oplus\mathrm{span}(\overline{I})$
case 7	$a_4=a_6=a_8=0$, $a_{10}=a_{11}=a_{12}$	$(\mathrm{ad}_{\mathfrak{su}(2)}\oplus\mathrm{span}(\overline{I}))\circledS\mathbb{R}^3$

$$\overline{M}_{10}=\overline{L}_{xx}=\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix},\quad \overline{M}_{11}=\overline{L}_{yy}=\begin{bmatrix}0&0&0&0\\0&-1&0&0\\0&0&0&0\\0&0&0&-1\end{bmatrix},$$

$$\overline{M}_{12}=\overline{L}_{zz}=\begin{bmatrix}0&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&0\end{bmatrix}.$$

The above expression of the matrix generators is very convenient for our purposes, because it splits the affine and linear parts of the action on $\boldsymbol{\rho}$. Furthermore, it makes it straightforward to check that $\mathrm{Lie}(\overline{M}_1,\ldots,\overline{M}_{12})=\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3$ (recall that $\dim(\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3)=12$). See Ref. 21 for a comparison.

In terms of the coherence vector and using homogeneous coordinates, Eq. (11) becomes

$$\dot{\overline{\boldsymbol{\rho}}}=\sum_{k=1}^{3}h_{0_k}\overline{M}_k\overline{\boldsymbol{\rho}}+\sum_{k=1}^{3}u_k\overline{M}_k\overline{\boldsymbol{\rho}}+\sum_{k=4}^{12}a_k\overline{M}_k\overline{\boldsymbol{\rho}},\quad \overline{\boldsymbol{\rho}}\in\overline{\mathbb{B}}^3. \tag{19}$$

Given $\overline{\mathcal{L}}_D$, the corresponding Lie algebra is

$$\mathfrak{g}=\mathrm{Lie}\left(\sum_{k=1}^{3}h_{0_k}\overline{M}_k+\sum_{k=4}^{12}a_k\overline{M}_k,\sum_{k=1}^{3}u_k\overline{M}_k\right)\subseteq\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3.$$

In general, $\mathfrak{g}$ varies with the values of a_k. A few prototypes of subalgebras obtained disregarding the assumption $A\geqslant 0$ are reported in Table I. Once $A\geqslant 0$ is imposed, case 1, case 3 and case 4 are not anymore admissible (the argument is the same as in the proof of Theorem 4, Part (1)).

The two level version of Theorem 4 is the following.

Theorem 5: *For a two-level master equation, under assumptions A1 and A2 we have*

(1) System (19) is accessible in $\overline{\mathbb{B}}^3$ *for* $\overline{\mathcal{L}}_D\neq\alpha\overline{I}+\Sigma_{k=5,7,9}a_k\overline{M}_k$, $\alpha\in\mathbb{R}$, $\alpha<0$.

(2) System (19) is never small-time nor finite-time controllable in $\overline{\mathbb{B}}^3$ *for* $\mathcal{L}_D\neq 0$.

Proof: The assumption $\overline{\mathcal{L}}_D\neq\alpha\overline{I}+\Sigma_{k=5,7,9}a_k\overline{M}_k$, $\alpha<0$, rules out case 6 and case 7 of Table I. By exclusion, or by exhaustive computation using the structure constant of the Appendix, any nonnull $\overline{\mathcal{L}}_D$ such that $\overline{\mathcal{L}}_D\neq\alpha\overline{I}+\Sigma_{k=5,7,9}a_k\overline{M}_k$ generates the Lie algebra of case 2 or case 5 as required by Theorem 4. □

Examples: In quantum information processing, some of the $\overline{M}_k$ admit well-known physical interpretations in terms of nonunitary quantum operations on a qubit normally used in the theory of error correction. For example $\overline{M}_{10}$, $\overline{M}_{11}$, and $\overline{M}_{12}$ are, respectively, the infinitesimal generators of the one-parameter semigroups corresponding to *bit flip*, *bit-phase flip*, and *phase flip* channels (see Ref. 17, Sec. 8.4) and so *a depolarizing channel* has a_{10}, a_{11}, and a_{12} all nonnull and equal.

(1) *Depolarizing channel ($\overline{\mathcal{L}}_D$ unital):* The depolarizing channel is given by $\overline{\mathcal{L}}_D=\alpha\overline{I}$, $\alpha<0$. Since $\overline{\mathcal{L}}_D$ commutes with everything, in this case the system is not accessible and furthermore its integral curves are not at all modified by coherent control. They will be pointing ''isotropically'' to the origin in $\mathbb{R}^3$.

(2) *Phase flip ($\overline{\mathcal{L}}_D$ unital):* The phase flip channel is also known as phase damping or pure coherence channel and it is given by $\overline{\mathcal{L}}_D$ aligned with $\overline{M}_{12}$. The effect of this one-parameter semigroup is to ''contract'' the Bloch sphere along the λ_x and λ_y directions, leaving it untouched along λ_z. As an example, check the accessibility property in correspondence of the following simple master equation:

$$\dot{\overline{\boldsymbol{\rho}}}=(u_1\overline{M}_1+u_2\overline{M}_2+u_3\overline{M}_3+a_{12}\overline{M}_{12})\overline{\boldsymbol{\rho}},$$

i.e., controls available along all the three directions and no free Hamiltonian. The Lie algebra $\mathrm{Lie}\{\overline{M}_1,\overline{M}_2,\overline{M}_3,\overline{M}_{12}\}$ is computed using the structure constants given in the Appendix and the Jacobi identity to eliminate terms not linearly independent.

First level Lie brackets,

$$[\overline{M}_1,\overline{M}_{12}]=-\overline{M}_8,\quad [\overline{M}_2,\overline{M}_{12}]=\overline{M}_6.$$

Second level Lie brackets,

$$[\overline{M}_1,\overline{M}_6]=-\overline{M}_4,\quad [\overline{M}_1,\overline{M}_8]=\overline{M}_{12}-\overline{M}_{11},\quad [\overline{M}_2,\overline{M}_6]=\overline{M}_{10}-\overline{M}_{11}.$$

Therefore

$$\mathfrak{g}=\{\overline{M}_1,\overline{M}_2,\overline{M}_3,\overline{M}_4,\overline{M}_6,\overline{M}_8,\overline{M}_{10}-\overline{M}_{12},\overline{M}_{12}-\overline{M}_{11},\overline{M}_{12}\}=\mathfrak{gl}(3,\mathbb{R})$$

and the process is accessible. Notice that $\overline{M}_{10}-\overline{M}_{12}$ and $\overline{M}_{12}-\overline{M}_{11}$ are *traceless*, i.e., they belong to $\mathfrak{sl}(3,\mathbb{R})$ (unlike $\overline{M}_{12}$) and therefore that $\mathfrak{g}_1=\mathfrak{sl}(3,\mathbb{R})$, as expected.

In this case, as it is easy to check (see also Ref. 3, Part 2, Sec. II.5) $\overline{\mathcal{L}}_D$ is not uniquely relaxing, i.e., a fixed point for the uncontrolled system does not exist. Thus the asymptotic value depends from the initial condition and $\lim_{t\to\infty}\overline{\boldsymbol{\rho}}=[\rho_0\ 0\ 0\ \rho_z(0)]^T$. Once the control is added, however, the controlled system can be made to converge to any $\tilde{\rho}_z$ in the interval $[-\rho_z(0),\rho_z(0)]$. In particular, if $\tilde{\rho}_z=0$ then $\mathcal{R}(\overline{\boldsymbol{\rho}}(0))=\{\overline{\boldsymbol{\rho}}\in\overline{\mathbb{B}}^n \text{ s.t. } \|\overline{\boldsymbol{\rho}}\|\leqslant\|\overline{\boldsymbol{\rho}}(0)\|\}$.

A Lie algebraic method *per se* is normally not constructive. However, what it tells in this case is that full accessibility is achieved only at the second level of brackets. Therefore a series expansion cannot be truncated before that, if one wants to assure the generation of group actions in arbitrary directions.

To understand what is happening to the integral curves of the system, it is convenient to split $\overline{\mathcal{L}}_D$ into part in $\mathfrak{sl}(3)$ and part in $\mathfrak{gl}(3)\backslash\mathfrak{sl}(3)$ as in the proof of Theorem 4: $\overline{\mathcal{L}}_D=\alpha\overline{I}+\tilde{\mathcal{L}}_D$, $\alpha<0$, $\tilde{\mathcal{L}}_D\in\mathfrak{sl}(3)$. For $\overline{\mathcal{L}}_D=a_{12}\overline{M}_{12}$,

$$\overline{\mathcal{L}}_D=a_{12}\overline{M}_{12}=\alpha\overline{I}+\tilde{\mathcal{L}}_D=-\frac{2a_{12}}{3}\overline{I}+\frac{a_{12}}{3}\begin{bmatrix}0&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&2\end{bmatrix}.$$

If $F(t)=\tilde{\mathcal{L}}_D+\Sigma_{k=1}^{3}(h_{0_k}+u_k(t))\overline{M}_k$, since $[\overline{I},F]=0\ \forall F\in\mathfrak{gl}(3,\mathbb{R})$, the flow of the system can be written as the exponential

$$g(t)=\mathcal{T}\exp\int_0^t(\alpha\overline{I}+F(\tau))\mathrm{d}\tau=\exp(t\alpha\overline{I})\,\mathcal{T}\exp\int_0^t F(\tau)\mathrm{d}\tau$$

and its action on $\overline{\boldsymbol{\rho}}$ as $\overline{\boldsymbol{\rho}}(t)=\exp(t\alpha\overline{I})\mathcal{T}\exp(\int_0^t F(\tau)\mathrm{d}\tau)\overline{\boldsymbol{\rho}}(0)$. The "isotropic" contraction $\exp(t\alpha\overline{I})$ corresponds to the depolarizing channel $\alpha/2(\overline{M}_{10}+\overline{M}_{11}+\overline{M}_{12})$ and cannot be reversed. Furthermore, the complete positivity constraint $A\geqslant 0$ imposes that the $\alpha\overline{I}$ part must be dominant with respect to the $F(t)$ part. Thus, regardless of the control action, the overall result is a contraction of the flow in $\overline{\mathbb{B}}^3$.

(3) *Amplitude damping ($\overline{\mathcal{L}}_D$ affine):* In terms of the master equation, the amplitude damping channel corresponds to an atomic system with spontaneous emission. In a two-level system, the excited state $|1\rangle$ can decay to ground state $|0\rangle$ while emitting a photon. The process of spontaneous emission is characterized in terms of the atomic ladder operators $\sigma_{\pm}=\sigma_x\pm i\sigma_y$ and of the damping coefficient $\gamma_{\downarrow}$ ($\gamma_{\downarrow}>0$) as (see, e.g., the survey in Refs. 2 and 17, Sec. 8.4.1)

$$\dot{\rho}=-i\,\mathrm{ad}_H(\rho)-\frac{\gamma_{\downarrow}}{2}(2\sigma_-\rho\sigma_+-\sigma_+\sigma_-\rho-\rho\sigma_+\sigma_-). \tag{20}$$

If, for example, $H=\sqrt{2}(h_{0_3}\lambda_3+\Sigma_{k=1}^{3}u_k\lambda_k)$ then

$$\dot{\overline{\boldsymbol{\rho}}}=\begin{bmatrix}0&0&0&0\\0&0&-h_{0_3}-u_3&u_2\\0&h_{0_3}+u_3&0&-u_1\\0&-u_2&u_1&0\end{bmatrix}\overline{\boldsymbol{\rho}}+\gamma_{\downarrow}\begin{bmatrix}0&0&0&0\\0&-\frac{1}{2}&0&0\\0&0&-\frac{1}{2}&0\\1&0&0&-1\end{bmatrix}\overline{\boldsymbol{\rho}}$$

$$=h_{0_3}\overline{M}_3\overline{\boldsymbol{\rho}}+\sum_{k=1}^{3}u_k\overline{M}_k\overline{\boldsymbol{\rho}}+\frac{\gamma_{\downarrow}}{2}(\overline{M}_{10}+\overline{M}_{11}-\overline{M}_5)\overline{\boldsymbol{\rho}}. \tag{21}$$

Since the unital part of $\overline{\mathcal{L}}_D$ is not proportional to the identity, by Theorem 5 spontaneous emission is an accessible process. From (16), the relaxation matrix is

$$A=\frac{\gamma_{\downarrow}}{2}\begin{bmatrix}1&-i&0\\i&1&0\\0&0&0\end{bmatrix}.$$

As the unital part of $\overline{\mathcal{L}}_D$ is invertible, (21) has a fixed point. Since $A\geqslant 0$ but not $A>0$, $\overline{\mathcal{L}}_D$ lies on an exposed face of the cone $A\geqslant 0$ and in correspondence the fixed point lies on $\partial\overline{\mathbb{B}}^3$, i.e., it is a pure state. Thus, asymptotically, $\overline{\mathcal{L}}_D$ admits a reachable set such that $\mathrm{cl}(\mathcal{R}(\overline{\boldsymbol{\rho}}(0)))=\overline{\mathbb{B}}^3$. As mentioned in the proof of Theorem 4, coherent control can speed up the "purification" of $\overline{\boldsymbol{\rho}}$ only for certain values of the initial condition. In fact, from

$$\frac{1}{2}\frac{d\|\overline{\boldsymbol{\rho}}\|^2}{dt}=\langle\langle\dot{\overline{\boldsymbol{\rho}}},\overline{\boldsymbol{\rho}}\rangle\rangle=\langle\langle h_{0_3}\overline{M}_3\overline{\boldsymbol{\rho}},\overline{\boldsymbol{\rho}}\rangle\rangle+\left\langle\left\langle\sum_{k=1}^{3}u_k\overline{M}_k\overline{\boldsymbol{\rho}},\overline{\boldsymbol{\rho}}\right\rangle\right\rangle+\frac{\gamma_{\downarrow}}{2}\langle\langle(\overline{M}_{10}+\overline{M}_{11}-\overline{M}_5)\overline{\boldsymbol{\rho}},\overline{\boldsymbol{\rho}}\rangle\rangle$$

only the last term gives a nontrivial contribution and can become positive, for example, in correspondence of ρ_z positive and ρ_x, ρ_y small enough,

$$\frac{\gamma_\downarrow}{2}\langle\langle(\overline{M}_{10}+\overline{M}_{11}-\overline{M}_5)\overline{\boldsymbol{\rho}},\overline{\boldsymbol{\rho}}\rangle\rangle=\frac{\gamma_\downarrow}{2}(2\rho_0\rho_z-(\rho_x^2+\rho_y^2+\rho_z^2)-\rho_z^2)=\frac{\gamma_\downarrow}{2}(2\rho_0\rho_z-\|\boldsymbol{\rho}\|^2-\rho_z^2).$$

However, the purification process remains an asymptotic process since as soon as coherent control has brought $\boldsymbol{\rho}$ to $[0\ 0\ +|\rho_z|]$, then purification can occur only because of $\overline{\mathcal{L}_D}$. Once again, notice how the role of $\overline{\mathcal{L}_D}$ is essential in moving around in the reachable set.

VI. CONCLUSION

The aim of this work is to shed light on the possibility and limits of coherent control of Markovian master equations using standard tools from geometric control theory. It turns out that there is a remarkable complementarity between admissible quantum dynamical semigroups and controllability: in the vector of coherences representation an admissible $\overline{\mathcal{L}_D}$ has to have a nonnull component along the nonzero-trace one-dimensional vector subspace of the Lie algebra of $n\times n$ matrices (or its semidirect extensions). A component in that direction guarantees noncontrollability in small and finite time. In the simple cases of unital dissipation operators, the fact that the ''uncontrollable'' direction has dimension 1 allows to obtain an order relation among the sets reachable at different times by means of arbitrary coherent controls.

APPENDIX: STRUCTURE CONSTANTS OF $\mathfrak{gl}(3,\mathbb{R})\circledS\mathbb{R}^3$

For the real Lie algebra $\mathfrak{gl}(3,\mathbb{R})$ in the basis $\overline{M}_1,\ldots,\overline{M}_{12}$, the structure constants, call them c_{jk}^l, are real but not totally skew symmetric,

$$c_{1,2}^3=c_{1,4}^6=c_{1,5}^7=c_{1,8}^{12}=c_{1,11}^8=c_{2,3}^1=c_{2,6}^{10}=c_{2,8}^4=c_{2,12}^6=c_{3,4}^{11}=c_{3,6}^8=c_{3,7}^9=c_{3,10}^4=c_{4,8}^2=1,$$

$$c_{4,10}^3=c_{5,8}^7=c_{5,10}^5=c_{5,11}^5=c_{6,9}^5=c_{6,12}^2=c_{7,8}^5=c_{7,10}^7=c_{7,12}^7=c_{8,11}^1=c_{9,11}^9=c_{9,12}^9=1,$$

$$c_{1,3}^2=c_{1,6}^4=c_{1,7}^5=c_{1,8}^{11}=c_{1,12}^8=c_{2,4}^8=c_{2,5}^9=c_{2,6}^{11}=c_{2,9}^5=c_{2,10}^6=c_{3,4}^{10}=c_{3,8}^6=-1,$$

$$c_{3,9}^7=c_{3,11}^4=c_{4,6}^1=c_{4,7}^9=c_{4,9}^7=c_{4,11}^3=c_{5,6}^9=c_{6,8}^3=c_{6,10}^2=c_{8,12}^1=-1.$$

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[23] In general, H_0 may not be the same as in (6), as is well known. This is irrelevant for our purposes.

Dissipative Schrödinger-type operators as a model for generation and recombination

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(Received 15 April 2002; accepted 15 January 2003)

Non-self-adjoint operators play an important role in the modeling of open quantum systems. We consider a one-dimensional Schrödinger-type operator of the form $-(1/2)(d/dx)(1/m)(d/dx)+V-\Sigma\kappa_j\delta(\cdot-x_j)$, $\mathrm{Im}(\kappa_j)>0$, with dissipative boundary conditions. An explicit description of the characteristic function, the minimal dilation and the generalized eigenfunctions of the dilation is given. The quantities of carrier and current densities are rigorously defined. Furthermore, we will show that the current is not constant and that the variation of the current depend essentially on the chosen density matrix and the imaginary parts of the delta potentials, i.e., $\mathrm{Im}(\kappa_j)$. This correspondence can be used to model a recombination-generation rate in the open quantum system. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1562748]

I. INTRODUCTION

To embed a quantum mechanically described structure into a macroscopic flow, one has to replace self-adjoint boundary conditions by non-self-adjoint ones [Ben Abdallah (1997, 1998); Frensley (1990); Kaiser (2001a)]. This leads to so-called open quantum systems. One-dimensional Schrödinger-type operators with dissipative boundary conditions have been intensely studied in Kaiser (2001b). We extend the model used there by adding dissipative delta perturbations, i.e., we consider an operator formally given by

$$H=-\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}+\tilde{V}, \tag{1.1}$$

where

$$\tilde{V}(\cdot)=V(\cdot)-\sum_{j=1}^{N}\kappa_j\delta(\cdot-x_j), \tag{1.2}$$

$x_j\in(a,b)$, $x_j\neq x_i$ for $i\neq j$, and $\kappa_j\in\mathbb{C}_+:=\{z\in\mathbb{C}|\mathrm{Im}(z)>0\}$. The potential V is assumed to be a real-valued $\mathsf{L}^2(a,b)$-function and the effective mass $m>0$ satisfies $m,(1/m)\in\mathsf{L}^\infty(a,b)$. Point interactions of this kind are extensively studied in the literature for self-adjoint boundary conditions and real coupling constants κ_j, cf. Albeverio (1988), Albeverio (2000) and references therein. Since the boundary conditions are not self-adjoint and the coupling constant are complex the expression (1.1)–(1.2) generates a maximal dissipative operator, see below. Such operators naturally arise if one is interested in mathematical models for semiconductor devices with recombination and generation processes of carriers which are embedded in a macrostructure. This case is not treated in Albeverio (1988) and Albeverio (2000). To analyze such operators it is fruitful to use the dilation theory for maximal dissipative operators [Foias (1970), Davies (1980)]. To Schrödinger operators this approach was specified in Pavlov (1977, 1981, 1984, 1996, 1999), see also Allakhverdiev (1987, 1988, 1989, 1990, 1993, 1997). In Kaiser (2002) this approach was used to

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define quantities such as steady states, carrier and current density for devices without recombination and generation. In the present article we modified this approach to fit our situation, i.e., where recombination and generation processes are included.

In a one-dimensional drift-diffusion model cf. Selberherr (1984), Markowich (1986), Markowich (1990), Jüngel (2001), the macroscopic flow is modeled by the continuity equations

$$\begin{aligned} \frac{\partial}{\partial t}n(x,t)-\frac{\partial}{\partial x}J_n(x,t)&=-R(n,p),\\ \frac{\partial}{\partial t}p(x,t)+\frac{\partial}{\partial x}J_p(x,t)&=-R(n,p), \end{aligned} \tag{1.3}$$

where n,p denote the electron and hole densities, J_n,J_p the corresponding currents and $R(n,p)$ the recombination-generation rate. The stationary continuity equation is given by Eq. (1.3), where $(\partial/\partial t)\,n(x,t)=(\partial/\partial t)\,p(x,t)=0$ and $J_k(x,t)=J_k(x)$, $k=n,p$. Replacing carrier densites n,p and current densities J_n,J_p by quantum mechanical expressions like Kaiser (2002) we are able to include recombination-generation effects into the open quantum system determined by (1.1) and (1.2) and to preserve the form of the continuity equations (1.3) for the quantum mechanically described structure. However, this implies that one has to choose the imaginary parts of the coupling constants κ_j in an appropriate manner. We outline how the imaginary parts have to be chosen. In forthcoming papers we have the aim to consider a dissipative Schrödinger–Poisson [Baro (2002)] system with recombination and generation effects.

The paper is organized as follows: In Sec. II we rigorously define the dissipative Schrödinger-type operator and show that the operator H is maximal dissipative. We use the well-known dilation theory as a main tool for our investigations. Therefore, the characteristic function and the minimal dilation corresponding to the maximal dissipative operator are the main objective in Secs. III and IV. Section V is devoted to the generalized eigenfunctions of the dilation operator. In Secs. VI and VII we give a definition of the density matrix and define the quantities of carrier and current densities in terms of the generalized eigenfunctions of the dilation [cf. Kaiser (2002)]. The motivation for this definition is, that the self-adjoint dilation is regarded as the Hamiltonian of a larger closed system which contains the open system given by the dissipative operator H. In Sec. VIII we show that, depending on the density matrix, loss and/or gain effect of the open system can be achieved. We close with some remarks and a discussion on how the imaginary parts of the delta potentials have to be chosen in order to include recombination-generation processes within the open quantum model.

II. DISSIPATIVE SCHRÖDINGER OPERATORS

Let x_j, $j=1,\ldots,N$, be numbers contained in the bounded interval $\Omega:=(a,b)\subset\mathbb{R}$, such that $a<x_1<x_2<\cdots<x_N<b$. Furthermore, let $V\in\mathsf{L}^2(a,b)$ be real-valued, and $m\in\mathsf{L}^\infty(a,b)$, with $m>0$ and $1/m\in\mathsf{L}^\infty(a,b)$. In accordance with Kaiser (2001b) we define the sesquilinear form

$$\begin{aligned} \mathfrak{t}[u,v]:=&\int_a^b\frac{1}{2}\,\frac{1}{m(x)}u'(x)\overline{v'(x)}+V(x)u(x)\overline{v(x)}dx-\kappa_a u(a)\overline{v(a)}\\ &-\sum_{j=1}^{N}\kappa_j u(x_j)\overline{v(x_j)}-\kappa_b u(b)\overline{v(b)}, \end{aligned}$$

for $u,v\in\mathsf{D}(\mathfrak{t})=\mathsf{W}^{1,2}(a,b)$ and $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+:=\{z\in\mathbb{C}|\mathrm{Im}(z)>0\}$. Mimicking the proof of Theorem 2.20 in Kaiser (2001a), we get that the form $\mathfrak{t}$ is closed on $\mathcal{H}=\mathsf{L}^2(a,b)$ and sectorial. Thus we get the existence of a maximal sectorial operator H, such that $(H\,f,v)=\mathfrak{t}[f,v]$ for all $f\in\mathsf{D}(H)$ and $v\in\mathsf{D}(\mathfrak{t})$. It can be shown that the operator H is given by

$$\mathsf{D}(H)=\left\{ f\in \mathsf{W}^{1,2}(a,b) \;\middle|\; \begin{array}{c} \frac{1}{m}f'\in \mathsf{W}^{1,2}(a,x_1)\oplus\bigoplus_{j=1}^{N-1}\mathsf{W}^{1,2}(x_j,x_{j+1})\oplus\mathsf{W}^{1,2}(x_N,b), \\ \frac{1}{2m(a)}f'(a)=-\kappa_a f(a),\ \frac{1}{2m(b)}f'(b)=\kappa_b f(b) \\ \frac{1}{2m(x_j+0)}f'(x_j+0)-\frac{1}{2m(x_j-0)}f'(x_j-0)=-\kappa_j f(x_j), \\ \forall j=1,\ldots,N \end{array} \right\},$$

and

$$(Hf)(x)=(l(f))(x),\quad f\in\mathsf{D}(H),$$

where

$$(l(f))(x):=-\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x)+V(x)f(x).$$

Since $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$, the operator H is dissipative, i.e., $\mathrm{Im}(Hf,f)\leqslant 0$, $f\in\mathsf{D}(H)$. This can be seen by

$$\mathrm{Im}(Hf,f)=\mathrm{Im}\,\mathfrak{t}[f,f]=-\frac{\alpha_a^2}{2}|f(a)|^2-\frac{\alpha_b^2}{2}|f(b)|^2-\sum_{j=1}^{N}\frac{\alpha_j^2}{2}|f(x_j)|^2,$$

where $\kappa_a=q_a+(i\alpha_a^2/2),\ldots,\kappa_b=q_b+(i\alpha_b^2/2)$, for some $q_a,\ldots,q_b,\alpha_a,\ldots,\alpha_b\in\mathbb{R}$, $\alpha_a,\ldots,\alpha_b>0$. A dissipative operator is called maximal dissipative, if it does not admit any proper dissipative extension. Since H is maximal sectorial it is also maximal dissipative. Furthermore, H is purely maximal dissipative [cf. Kaiser (2001a)], i.e., it has no self-adjoint part [Foias (1970)]. This implies that H has no real eigenvalues.

Let us introduce some notions. For simplicity we will occasional write $a=x_0$, $\kappa_a=\kappa_0$, $\alpha_a=\alpha_0$, $b=x_{N+1}$, $\kappa_b=\kappa_{N+1}$, and $\alpha_b=\alpha_{N+1}$. We set

$$\Delta(g,f)(x):=\frac{1}{2m(x+0)}g'(x+0)-\frac{1}{2m(x-0)}f'(x-0),\quad \Delta(g)(x):=\Delta(g,g)(x).$$

For a matrix $A=(a_{ij})$, with $a_{ij}\in\mathbb{C}$, $\overline{A}$ will denote the matrix in which every element is complex conjugated, i.e., $\overline{A}=(\overline{a}_{ij})$.

In order to get an explicit description of the resolvent of H we introduce the elementary solutions $v_a(x,z)$ and $v_b(x,z)$ defined by

$$l(v_a(\cdot,z))(x)-zv_a(x,z)=0,\quad v_a(a,z)=1,\quad \frac{1}{2m(a)}v_a'(a,z)=-\kappa_a,$$

$$\Delta(v_a(\cdot,z))(x_j)=-\kappa_j v_a(x_j,z),\qquad \forall j=1,\ldots,N,$$

$$l(v_b(\cdot,z))(x)-zv_b(x,z)=0,\ v_b(b,z)=1,\quad \frac{1}{2m(b)}v_b'(b,z)=\kappa_b,$$

$$\Delta(v_b(\cdot,z))(x_j)=-\kappa_j v_b(x_j,z),\qquad \forall j=1,\ldots,N.$$

The existence of these solutions can be proven as in Kaiser (2001b).

The Wronskian of $v_a(x,z)$ and $v_b(x,z)$ is defined by

$$W(v_a(\cdot,z),v_b(\cdot,z))(x):=v_a(x,z)\frac{1}{2m(x)}v_b'(x,z)-v_b(x,z)\frac{1}{2m(x)}v_a'(x,z).$$

We note that $W(v_a(\cdot,z),v_b(\cdot,z))(x)$ is constant for $x\in(x_i,x_{i+1})$. Furthermore, one easily checks that

$$W(v_a(\cdot,z),v_b(\cdot,z))(x_i-0)=W(v_a(\cdot,z),v_b(\cdot,z))(x_i+0).$$

Thus we write $W(z):=W(v_a(\cdot,z),v_b(\cdot,z))(x)$.

The functions defined by

$$v_{*a}(x,z):=\overline{v_a(x,\overline{z})},\quad \text{and}\quad v_{*b}(x,z):=\overline{v_b(x,\overline{z})},$$

are solutions of

$$l(v_{*a}(\cdot,z))(x)-zv_{*a}(x,z)=0,\quad v_{*a}(a,z)=1,\quad \frac{1}{2m(a)}v_{*a}'(a,z)=-\overline{\kappa_a},$$

$$\Delta(v_{*a}(\cdot,z))(x_j)=-\overline{\kappa_j}v_{*a}(x_j,z),\qquad \forall j=1,\ldots,N,$$

$$l(v_{*b}(\cdot,z))(x)-zv_{*b}(x,z)=0,\quad v_{*b}(b,z)=1,\quad \frac{1}{2m(b)}v_{*b}'(b,z)=\overline{\kappa_b},$$

$$\Delta(v_{*b}(\cdot,z))(x_j)=-\overline{\kappa_j}v_{*b}(x_j,z),\qquad \forall j=1,\ldots,N.$$

Obviously, the Wronskian $W_*(z):=W(v_{*a}(\cdot,z),v_{*b}(\cdot,z))(x)$ satisfies $W_*(z)=\overline{W(\overline{z})}$.

We are now able to write the resolvents of H and H^* as integral operators, where the kernels are given in terms of the elementary solutions (see also Kato (1980)).

Theorem 2.1: *Let $V\in\mathsf{L}^2(a,b)$ be real valued and $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$. Then the resolvent of the maximal dissipative operator H is given by*

$$((H-z)^{-1}f)(x)=-\frac{v_b(x,z)}{W(z)}\int_a^x v_a(y,z)f(y)\,dy-\frac{v_a(x,z)}{W(z)}\int_x^b v_b(y,z)f(y)\,dy,\qquad (2.1)$$

for $f\in\mathcal{H}$ and $z\in\varrho(H)$.

The resolvent of the adjoint operator H^* admits the representation

$$((H^*-z)^{-1}f)(x)=-\frac{v_{*b}(x,z)}{W_*(z)}\int_a^x v_{*a}(y,z)f(y)\,dy-\frac{v_{*a}(x,z)}{W_*(z)}\int_x^b v_{*b}(y,z)f(y)\,dy,\qquad (2.2)$$

for $f\in\mathcal{H}$ and $z\in\varrho(H^*)$.

We omit the proof, but note that $W(z)=0\Leftrightarrow z\in\sigma(H)$ and $W_*(z)=0\Leftrightarrow z\in\sigma(H^*)$, where $\sigma(\cdot)$ denotes the spectrum of the corresponding operator.

III. THE CHARACTERISTIC FUNCTION

We define the unclosed operator $\alpha:\mathcal{H}\to\mathbb{C}^{N+2}$ by

$$\alpha f=\begin{pmatrix}\alpha_b f(b)\\ -\alpha_N f(x_N)\\ \vdots\\ -\alpha_1 f(x_1)\\ -\alpha_a f(a)\end{pmatrix},\quad \mathsf{D}(\alpha)=\mathsf{C}(a,b).$$

Let us introduce the operator-valued function $T(z):\mathcal{H}\to\mathbb{C}^{N+2}$ given by

$$T(z)f:=\alpha(H-z)^{-1}f, \tag{3.1}$$

for $f\in\mathcal{H}$ and $z\in\varrho(H)$. Using the expression (2.1) we get

$$T(z)f=\frac{1}{W(z)}\begin{pmatrix} -\alpha_b\int_a^b v_a(y,z)f(y)\,dy \\ \alpha_N v_b(x_N,z)\int_a^{x_N} v_a(y,z)f(y)\,dy+\alpha_N v_a(x_N,z)\int_{x_N}^b v_b(y,z)\,dy \\ \vdots \\ \alpha_1 v_b(x_1,z)\int_a^{x_1} v_a(y,z)f(y)\,dy+\alpha_1 v_a(x_1,z)\int_{x_1}^b v_b(y,z)\,dy \\ \alpha_a\int_a^b v_b(y,z)f(y)\,dy \end{pmatrix}.$$

The adjoint operator $T(z)^*$ is given by

$$\begin{aligned}(T(z)^*\xi)(x)=\frac{1}{W_*(\overline{z})}\{&-\alpha_b v_{*a}(x,\overline{z})\xi^b+\alpha_N(v_{*b}(x_N,\overline{z})v_{*a}(x,\overline{z})\chi_{[a,x_1)}(x)\\ &+v_{*a}(x_N,\overline{z})v_{*b}(x,\overline{z})\chi_{[x_N,b]})\xi^N\\ &\vdots\\ &+\alpha_1(v_{*b}(x_1,\overline{z})v_{*a}(x,\overline{z})\chi_{[a,x_1)}(x)+v_{*a}(x_1,\overline{z})v_{*b}(x,\overline{z})\chi_{[x_1,b]})\xi^1\\ &+\alpha_a v_{*b}(x,\overline{z})\xi^a\},\end{aligned}$$

for $x\in[a,b]$, where

$$\xi=\begin{pmatrix}\xi^b\\ \xi^N\\ \vdots\\ \xi^1\\ \xi^a\end{pmatrix}\in\mathbb{C}^{N+2}. \tag{3.2}$$

Similarly, we define $T_*(z):\mathcal{H}\to\mathbb{C}^{N+2}$ by

$$T_*(z)f:=\alpha(H^*-z)^{-1}f,$$

for $f\in\mathcal{H}$ and $z\in\varrho(H)$. Using Eq. (2.2) one gets

$$T_*(z)f=\frac{1}{W(z)}\begin{pmatrix} -\alpha_b\int_a^b v_{*a}(y,z)f(y)\,dy \\ \alpha_N v_{*b}(x_N,z)\int_a^{x_N} v_{*a}(y,z)f(y)\,dy+\alpha_N v_{*a}(x_N,z)\int_{x_N}^b v_{*b}(y,z)\,dy \\ \vdots \\ \alpha_1 v_{*b}(x_1,z)\int_a^{x_1} v_{*a}(y,z)f(y)\,dy+\alpha_1 v_{*a}(x_1,z)\int_{x_1}^b v_{*b}(y,z)\,dy \\ \alpha_a\int_a^b v_{*b}(y,z)f(y)\,dy \end{pmatrix}.$$

The adjoint operator has the representation

$$\begin{aligned}(T_*(z)^*\xi)(x)=\frac{1}{W(\overline{z})}\{&-\alpha_b v_a(x,\overline{z})\xi^b+\alpha_N\big(v_b(x_N,\overline{z})v_a(x,\overline{z})\chi_{[a,x_N)}(x)\\&+v_a(x_N,\overline{z})v_b(x,\overline{z})\chi_{[x_N,b]}\big)\xi^N\\&\vdots\\&+\alpha_1\big(v_b(x_1,\overline{z})v_a(x,\overline{z})\chi_{[a,x_1)}(x)+v_a(x_1,\overline{z})v_b(x,\overline{z})\chi_{[x_1,b]}\big)\xi^1+\alpha_a v_b(x,\overline{z})\xi^a\},\end{aligned}$$

for $x\in[a,b]$.

Let us collect some properties of the above operators.

Lemma 3.1: Let $V\in\mathsf{L}^2(a,b)$ be real-valued, and $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$. Then we have

$$(H^*-z)^{-1}-(H-z)^{-1}=-iT_*(\overline{z})^*T_*(z)=-iT(\overline{z})^*T(z),\tag{3.3}$$

for $z\in\varrho(H)\cap\varrho(H^*)$.

Proof: A straightforward calculation shows that

$$(H^*f,g)-(f,H^*g)=i\sum_{j=0}^{N+1}\alpha_i^2 f(x_j)\overline{g(x_j)},$$

for $f,g\in\mathsf{D}(H^*)$. Setting $f=(H^*-z)^{-1}h$ and $g=(H^*-\overline{z})^{-1}k$ with $h,k\in\mathcal{H}$, $z,\overline{z}\in\varrho(H^*)$, we obtain

$$((H^*-z)^{-1}h,k)-(h,(H^*-\overline{z})^{-1}k)=-i\langle T_*(z)h,T_*(\overline{z})k\rangle_{\mathbb{C}^{N+2}},$$

and the first equality in (3.3) is proven. The second relation can be proven in the same fashion.□

The characteristic function $\Theta_H(\cdot)$ is a crucial element in the study of completely non-self-adjoint operators. It is a purely contractive valued and analytic function on $\overline{\mathbb{C}_-}$, where $\mathbb{C}_-:=\{z\in\mathbb{C}|\,\mathrm{Im}(z)<0\}$; cf. Foias (1970). The characteristic function $\Theta_H(\cdot)$ of the maximal dissipative operator H is a $(N+2)\times(N+2)$ matrix-valued function satisfying the relation

$$\Theta_H(z)T(z)f=T_*(z)f,\quad z\in\varrho(H)\cap\varrho(H^*),\quad f\in\mathcal{H}.\tag{3.4}$$

Let us compute the characteristic function $\Theta_H(\cdot)$ of H.

Theorem 3.2: *Let $V\in\mathsf{L}^2(a,b)$ be real-valued and $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_-$. Then the characteristic function of H is given by*

$$\Theta_H(z)=I_{\mathbb{C}^{N+2}}-\frac{i}{W_*(z)}\times\begin{pmatrix}-\alpha_b^2v_{*a}(b,z)&\alpha_b\alpha_Nv_{*a}(x_N,z)&\cdots&\alpha_b\alpha_1v_{*a}(x_1,z)&\alpha_b\alpha_a\\ \alpha_N\alpha_bv_{*a}(x_N,z)&-\alpha_N^2v_{*a}(x_N,z)v_{*b}(x_N,z)&\cdots&-\alpha_N\alpha_1v_{*a}(x_1,z)v_{*b}(x_N,z)&-\alpha_N\alpha_av_{*b}(x_N,z)\\ \vdots&\vdots&&\vdots&\cdots\\ \alpha_1\alpha_bv_{*a}(x_1,z)&-\alpha_1\alpha_Nv_{*a}(x_1,z)v_{*b}(x_N,z)&\cdots&-\alpha_1^2v_{*a}(x_1,z)v_{*b}(x_1,z)&-\alpha_1\alpha_av_{*b}(x_1,z)\\ \alpha_a\alpha_b&-\alpha_a\alpha_Nv_{*b}(x_N,z)&\cdots&-\alpha_a\alpha_1v_{*b}(x_1,z)&-\alpha_a^2v_{*b}(a,z)\end{pmatrix},\tag{3.5}$$

for $z\in\varrho(H)\cap\varrho(H^*)$.

Proof: It remains to verify that $\Theta_H(\cdot)$ given by (3.5) satisfies (3.4).

One easily checks, that Eq. (3.5) can be written as

$$\Theta_H(z)=I_{\mathbb{C}^{N+2}}-i\alpha T(\overline{z})^*.\tag{3.6}$$

Using Eq. (3.3) we get

$$\Theta_H(z)T(z)=T(z)-i\alpha T(\overline{z})^*T(z)=\alpha(H^*-z)^{-1}=T_*(z).$$

Thus Eq. (3.4) is verified.

Since

$$T(z)^*T(z)-T_*(z)^*T_*(z)=-2\,\mathrm{Im}(z)T(z)^*T(\overline{z})T(\overline{z})^*T(z),\quad \text{for } z\in\varrho(H)\cap\varrho(H^*),$$

we have for $z\in\mathbb{C}_-\cap\varrho(H)$ that

$$\|\Theta_H(z)T(z)f\|^2=\|T_*(z)f\|^2\leqslant\|T(z)f\|^2,\quad f\in\mathcal{H}.$$

Thus $\Theta_H(z)$ is a contraction for $z\in\mathbb{C}_-\cap\varrho(H)$. Since the spectrum of H consists of only isolated eigenvalues in $\mathbb{C}_-$, we get that the characteristic function $\Theta_H(z)$ admits a unique continuation to all $z\in\overline{\mathbb{C}_-}$; cf. (3.6). □

IV. DILATIONS

Since H is a maximal dissipative operator, there exists a larger Hilbert space $\mathcal{K}$ containing $\mathcal{H}$, i.e. $\mathcal{H}\subseteq\mathcal{K}$, and a self-adjoint operator K on $\mathcal{K}$ such that

$$P_{\mathcal{H}}^{\mathcal{K}}(K-z)^{-1}_{|\mathcal{H}}=(H-z)^{-1},\quad z\in\mathbb{C}_+,\tag{4.1}$$

[see Foias (1970)]. The operator K is called a dilation of H. K is said to be a minimal self-adjoint dilation, if

$$\operatorname*{clospan}_{z\in\mathbb{C}\setminus\mathbb{R}}(K-z)^{-1}\mathcal{H}=\mathcal{K}.\tag{4.2}$$

All minimal self-adjoint dilation of a maximal dissipative operator are isomorphic. In particular, all minimal self-adjoint dilation are unitarily equivalent.

The next step in our investigations is to obtain an explicit description of the self-adjoint dilation of H. Let us introduce the Hilbert space $\mathcal{K}$ defined by

$$\mathcal{K}:=\mathcal{D}_-\oplus\mathcal{H}\oplus\mathcal{D}_+,$$

with $\mathcal{D}_\pm:=\mathsf{L}^2(\mathbb{R}_\pm,\mathbb{C}^{N+2})$. Introducing the domain $\hat{\Omega}$,

$\mathbb{R}_-$		$\mathbb{R}_+$
$\mathbb{R}_-$	$[x_N,b]$	$\mathbb{R}_+$
$\mathbb{R}_-$	$\vdots$	$\mathbb{R}_+$
$\mathbb{R}_-$	$[x_i,x_{i+1}]$	$\mathbb{R}_+$
$\mathbb{R}_-$	$\vdots$	$\mathbb{R}_+$
$\mathbb{R}_-$	$[a,x_1]$	$\mathbb{R}_+$

we get $\mathcal{K}=\mathsf{L}^2(\hat{\Omega})$. For $\vec{g}\in\mathcal{K}$ we write

$$\vec{g}:=g_-\oplus g\oplus g_+,$$

where

$$g_- = \begin{pmatrix} g_-^b(x) \\ g_-^N(x) \\ \vdots \\ g_-^1(x) \\ g_-^a(x) \end{pmatrix} \quad \text{and} \quad g_+ = \begin{pmatrix} g_+^b(x) \\ g_+^N(x) \\ \vdots \\ g_+^1(x) \\ g_+^a(x) \end{pmatrix},$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Furthermore we will need the $(N+2)\times(N+2)$-matrices $K_\pm^b$, $K_\pm^a$, and $K_\pm^j$, $j=1,\ldots,N$, defined by

$$K_-^b := \frac{1}{\alpha_b}\begin{pmatrix} 1 & 0 & \cdots & 0 & -\kappa_b \\ 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \end{pmatrix}, \quad K_-^a := \frac{1}{\alpha_a}\begin{pmatrix} 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \\ 1 & 0 & \cdots & 0 & \kappa_a \end{pmatrix},$$

$$K_-^j := \frac{1}{\alpha_j}\begin{pmatrix} 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 1 & 0 & \cdots & 0 & \kappa_j \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \end{pmatrix} \leftarrow (j+1)\text{-th row},$$

and $K_+^b := \overline{K_-^b}$, $K_+^a := \overline{K_-^a}$, $K_+^j := \overline{K_-^j}$, as well as

$$E = \begin{pmatrix} 0 & \cdots & \cdots & 0 & 1 \\ 0 & \cdots & \cdots & 0 & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & \cdots & \cdots & 0 \\ -1 & 0 & \cdots & \cdots & 0 \end{pmatrix}.$$

We set

$$g_a = \begin{pmatrix} \frac{1}{2m(a)}g'(a) \\ 0 \\ \vdots \\ 0 \\ g(a) \end{pmatrix}, \quad g_b = \begin{pmatrix} \frac{1}{2m(b)}g'(b) \\ 0 \\ \vdots \\ 0 \\ g(b) \end{pmatrix}, \quad \text{and} \quad g_j = \begin{pmatrix} \Delta(g)(x_j) \\ 0 \\ \vdots \\ 0 \\ g(x_j) \end{pmatrix}.$$

Theorem 4.1: *Let* $V\in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V)=0$, $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$, *and* $x_1,\ldots,x_N\in(a,b)$, *such that* $x_1<x_2<\cdots<x_N$. *Then the operator K defined by*

$$\mathsf{D}(K):=\left\{\vec{g}\in\mathcal{K}\;\middle|\;\begin{array}{c} g_\pm\in \mathsf{W}^{1,2}(\mathbb{R}_\pm,\mathbb{C}^{N+2}),g\in \mathsf{W}^{1,2}(a,b),\\ \frac{1}{m}g'\in \mathsf{W}^{1,2}(a,x_1)\oplus\bigoplus_{j=1}^{N}\mathsf{W}^{1,2}(x_j,x_{j+1})\oplus \mathsf{W}^{1,2}(x_N,b)\\ K_-^a g_a+\sum_{j=1}^{N}K_-^j g_j+K_-^b g_b=g_-(0),\\ K_+^a g_a+\sum_{j=1}^{N}K_+^j g_j+K_+^b g_b=g_+(0)\end{array}\right\} \tag{4.3}$$

and

$$K\vec{g}:=-i\frac{d}{dx}g_-\oplus l(g)\oplus -i\frac{d}{dx}g_+,\quad \vec{g}\in\mathsf{D}(K),$$

is self-adjoint.

The proof is essentially the same as in Kaiser (2001b), so we omit it.

Figure 1 shows the boundary conditions of the operator K with respect to the domain $\hat{\Omega}$.

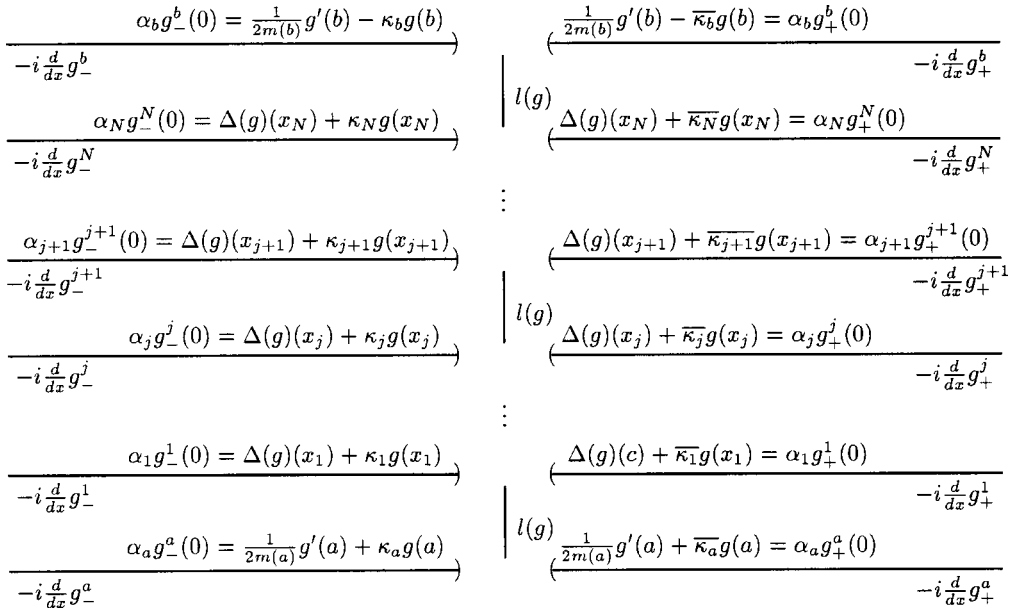

FIG. 1. Boundary conditions of the dilation K.

To show that K is the minimal dilation corresponding to H, let us compute the resolvent of K.

Theorem 4.2: *Assume that* $V\in \mathsf{L}^2(a,b)$ *is real-valued and* $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$. *Then the resolvent of* K *admits the representation*

$$\begin{aligned}(K-z)^{-1}(f_-\oplus f\oplus f_+)(x)&=i\int_{-\infty}^{x}e^{i(x-y)z}f_-(y)\,dy\oplus((H-z)^{-1}f)(x)\\&\quad+i\left(T_*(\overline{z})^*\int_{-\infty}^{0}e^{-iyz}f_-(y)\,dy\right)(x)\oplus i\int_0^x e^{i(x-y)z}f_+(y)\,dy\\&\quad+ie^{izx}T(z)f+i\Theta_H(\overline{z})^*\int_{-\infty}^{0}e^{i(x-y)z}f_-(y)\,dy,\end{aligned}\tag{4.4}$$

for $\mathrm{Im}(z)>0$ *and*

$$\begin{aligned}(K-z)^{-1}(f_-\oplus f\oplus f_+)(x)&=-i\int_x^0 e^{i(x-y)z}f_-(y)\,dy-ie^{izx}T_*(z)f-i\Theta_H(z)\int_0^\infty e^{i(x-y)z}f_+(y)\,dy\\&\quad\oplus((H^*-z)^{-1}f)(x)-i\left(T(\overline{z})^*\int_0^\infty e^{-iyz}f_+(y)\,dy\right)(x)\\&\quad\oplus-i\int_x^\infty e^{i(x-y)z}f_+(y)\,dy,\end{aligned}\tag{4.5}$$

for $\mathrm{Im}(z)<0$, *where* $\vec{f}=f_-\oplus f\oplus f_+\in\mathcal{K}$.

Proof: We will only prove Eq. (4.4) since the equality of (4.5) can be shown in the same fashion. Let $\mathrm{Im}(z)>0$, $\vec{f}\in\mathcal{K}$. We set

$$\begin{aligned}g_-(x)&:=i\int_{-\infty}^{x}e^{i(x-y)z}f_-(y)\,dy,\\g(x)&:=((H-z)^{-1}f)(x)+i\left(T_*(\overline{z})^*\int_{-\infty}^{0}e^{-iyz}f_-(y)\,dy\right)(x),\\g_+(x)&:=i\int_0^x e^{i(x-y)z}f_+(y)\,dy+ie^{izx}T(z)f+i\Theta_H(\overline{z})^*\int_{-\infty}^{0}e^{i(x-y)z}f_-(y)\,dy.\end{aligned}\tag{4.6}$$

One easily verifies that

$$(K-z)(g_-\oplus g\oplus g_+)=f_-\oplus f\oplus f_+.$$

Thus it remains to show that $\vec{g}$ satisfies the boundary conditions (4.3). We set $h=(H-z)^{-1}f$ and get

$$g_a=h_a+G_ag_-(0),\quad g_j=h_j+G_jg_-(0),\quad g_b=h_b+G_bg_-(0),\quad \forall j=1,\ldots,N,\tag{4.7}$$

where

$$G_a:=\begin{pmatrix}-\kappa_a(T_*(\overline{z})^*e_b)(a) & \cdots & -\kappa_a(T_*(\overline{z})^*e_1)(a) & \dfrac{1}{2m(a)}(T_*(\overline{z})^*e_a)(a)\\ 0 & \cdots & 0 & 0\\ \vdots & & \vdots & \vdots\\ 0 & \cdots & 0 & 0\\ (T_*(\overline{z})^*e_b)(a) & \cdots & (T_*(\overline{z})^*e_1)(a) & (T_*(\overline{z})^*e_a)(a)\end{pmatrix},$$

$$G_b := \begin{pmatrix} \frac{1}{2m(b)}(T_*(\overline{z})^* e_b)'(b) & \kappa_b(T_*(\overline{z})^* e_N)(b) & \cdots & \kappa_b(T_*(\overline{z})^* e_a)(b) \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \\ (T_*(\overline{z})^* e_b)(b) & (T_*(\overline{z})^* e_N)(b) & \cdots & (T_*(\overline{z})^* e_a)(b) \end{pmatrix},$$

and

$$G_j := \begin{pmatrix} -\kappa_j(T_*(\overline{z})^* e_b)(x_j) & \cdots & \Delta(T_*(\overline{z})^* e_j)(x_j) & \cdots & -\kappa_j(T^*(\overline{z})^* e_a)(x_j) \\ 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \\ (T_*(\overline{z})^* e_b)(x_j) & \cdots & (T_*(\overline{z})^* e_j)(x_j) & \cdots & (T^*(\overline{z})^* e_a)(x_j) \end{pmatrix},$$

where $e_a, e_j, e_b \in \mathbb{C}^{N+2}$ are given by

$$e_b = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad e_a = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad e_j = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}.$$

Since $h \in \mathsf{D}(H)$,

$$K_-^a h_a = K_-^j h_j = K_-^b h_b = 0, \ \ \forall j = 1,\ldots,N. \tag{4.8}$$

A straightforward calculation shows that

$$K_-^a G_a \xi = \xi^a e_a, \quad K_-^b G_b \xi = \xi^b e_b, \quad K_-^j G_j \xi = \xi^j e_j, \quad \forall j = 1,\ldots,N,$$

where $\xi \in \mathbb{C}^{N+2}$ [see (3.2)]. Therefore we get by (4.7) and (4.8),

$$K_-^a g_a + \sum_{j=1}^{N} K_-^j g_j + K_-^b g_b = g_-(0).$$

Using (4.6) we get

$$g_+(0) = iT(z)f + \Theta_H(\overline{z})^* g_-(0).$$

Since

$$K_+^a h_a = -i\alpha_a h(a) e_a, \quad K_+^b h_b = i\alpha_b h(b) e_b, \quad K_+^j h_j = -i\alpha_j h(x_j) e_j, \ \ \forall j = 1,\ldots,N,$$

we find by Eq. (3.1),

$$K_+^a h_a + \sum_{j=1}^{N} K_+^j h_j + K_+^b h_b = iT(z)f.$$

Note that

$$\Theta_H(\overline{z})^* = 1 + \alpha T_*(\overline{z})^*. \tag{4.9}$$

We have

$$K_+^a G_a = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \\ -i\alpha_a(T_*(\overline{z})^* e_b)(a) & \cdots & 1 - i\alpha_a(T_*(\overline{z})^* e_a)(a) \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \\ i\langle \alpha T_*(\overline{z})^* e_b, e_a \rangle_{\mathbb{C}^{N+2}} & \cdots & 1 + i\langle \alpha T_*(\overline{z})^* e_a, e_a \rangle_{\mathbb{C}^{N+2}} \end{pmatrix},$$

and similar

$$K_+^b G_b = \begin{pmatrix} 1 + i\langle \alpha T_*(\overline{z})^* e_b, e_b \rangle_{\mathbb{C}^{N+2}} & \cdots & i\langle \alpha T_*(\overline{z})^* e_a, e_b \rangle_{\mathbb{C}^{N+2}} \\ 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{pmatrix},$$

$K_+^j G_j =$

$$= \begin{pmatrix} 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \\ i\langle \alpha T_*(\overline{z})^* e_b, e_j \rangle_{\mathbb{C}^{N+2}} & \cdots & 1 + i\langle \alpha T_*(\overline{z})^* e_j, e_j \rangle_{\mathbb{C}^{N+2}} & \cdots & i\langle \alpha T_*(\overline{z})^* e_a, e_j \rangle_{\mathbb{C}^{N+2}} \\ 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \end{pmatrix},$$

for all $j = 1, \ldots, N$. Hence, we get by (4.9),

$$K_+^a G_a + \sum_{j=1}^N K_+ G_j + K_+ G_b = \Theta_H(\overline{z})^*$$

and, finally,

$$K_+ g_a + \sum_{j=1}^N K_+ g_j + K_+^b g_b = g_+(0),$$

which completes the proof. □

Using the expressions (4.4) and (4.5) for the resolvent of K, one easily verifies (4.1) and (4.2).

V. EIGENFUNCTION EXPANSION

The self-adjoint operator K is absolutely continuous and $\sigma(K) = \sigma_{\mathrm{ac}}(K) = \mathbb{R}$, i.e., the spectrum of K coincides with the real line. Its multiplicity is $N+2$. We are now going to compute the generalized eigenfunction $\vec{\phi}(\cdot, \lambda)$, $\lambda \in \mathbb{R}$, of K. We set

$$\vec{\phi}(x, \lambda) = \phi_-(x, \lambda) \oplus \phi(x, \lambda) \oplus \phi_+(x, \lambda),$$

for $x \in \hat{\Omega}$, where

$$\phi_-(x,\lambda)=\begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_-, \quad \phi_+(x,\lambda)=\begin{pmatrix} \phi_+^b(x,\lambda) \\ \phi_+^N(x,\lambda) \\ \vdots \\ \phi_+^1(x,\lambda) \\ \phi_+^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_+.$$

From

$$\begin{aligned}(K\vec{\phi})(x,\lambda) &= -i\frac{d}{dx}\phi_-(x,\lambda) \oplus l(\phi(\cdot,\lambda))(x) \oplus -i\frac{d}{dx}\phi_+(x,\lambda) \\ &= \lambda(\phi_-(x,\lambda) \oplus \phi(x,\lambda) \oplus \phi_+(x,\lambda)),\end{aligned}$$

$x \in \hat{\Omega}$, we find the equations

$$-i\frac{d}{dx}\begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix} = \lambda \begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_-, \tag{5.1}$$

$$l(\phi(\cdot,\lambda))(x) = \lambda\phi(x,\lambda), \quad x \in [a,b], \tag{5.2}$$

and

$$-i\frac{d}{dx}\begin{pmatrix} \phi_+^b(x,\lambda) \\ \phi_+^N(x,\lambda) \\ \vdots \\ \phi_+^1(x,\lambda) \\ \phi_+^a(x,\lambda) \end{pmatrix} = \lambda \begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_+. \tag{5.3}$$

The equations (5.1) and (5.3) have the solutions

$$\phi_-(x,\lambda) = C_- e^{ix\lambda}, \quad C_- \in \mathbb{C}^{N+2}, \quad x \in \mathbb{R}_-,$$

and

$$\phi_+(x,\lambda) = C_+ e^{ix\lambda}, \quad C_+ \in \mathbb{C}^{N+2}, \quad x \in \mathbb{R}_+.$$

The solution of (5.2) is given by a linear combination of the elementary solutions $v_a(x,\lambda)$ and $v_b(x,\lambda)$ on each interval $[x_j, x_{j+1})$, i.e.,

$$\phi(x,\lambda) = \sum_{j=0}^{N} (c_a^j v_a(x,\lambda) + c_b^j v_b(x,\lambda),)\chi_{[x_j,x_{j+1})}(x). \tag{5.4}$$

The eigenfunctions have to satisfy the boundary conditions, i.e.,

$$K_-^a \phi_a(\lambda) + \sum_{j=1}^{N} K_-^j \phi_j(\lambda) + K_-^b \phi_b(\lambda) = \phi_-(0,\lambda), \tag{5.5}$$

and

$$K_+^a \phi_a(\lambda) + \sum_{j=1}^{N} K_+^j \phi_j(\lambda) + K_+^b \phi_b(\lambda) = \phi_+(0,\lambda). \tag{5.6}$$

Furthermore, the condition

$$(c_a^{j+1} - c_a^j) v_a(x_j,\lambda) + (c_b^{j+1} - c_b^j) v_b(x_j,\lambda) = 0, \quad \forall j = 0,\ldots,N+1,$$

has to be satisfied. A straightforward calculation shows that

$$c_a^{N+1} = -\frac{\alpha_b}{W(z)} C_-^b, \quad c_a^j = c_a^{j+1} + \frac{\alpha_j v_b(x_j,\lambda)}{W(\lambda)} C_-^j, \quad j = 0,\ldots,N, \tag{5.7}$$

as well as

$$c_b^0 = \frac{\alpha_a}{W(z)} C_-^a, \quad c_b^j = c_b^{j+1} - \frac{\alpha_j v_a(x_j,\lambda)}{W(\lambda)} C_-^j, \quad j = 1,\ldots,N+1. \tag{5.8}$$

Inserting Eqs. (5.7) and (5.8) in (5.4) finally yields

$$\phi(x,\lambda) = (T_*(\lambda) * C_-)(x). \tag{5.9}$$

By inserting (5.9) in (5.6) we find

$$C_+ = \Theta_H(\lambda) * C_-, \quad \lambda \in \mathbb{R}.$$

Therefore we get

$$\vec{\phi}^{C_-}(x,\lambda) := e^{ix\lambda} C_- \oplus (T_*(\lambda) * C_-)(x) \oplus e^{ix\lambda} \Theta_H(\lambda) * C_-,$$

$x \in \hat{\Omega}$, $\lambda \in \mathbb{R}$.

A calculation as in Kaiser (2001b) shows that

$$\left(\frac{1}{\sqrt{2\pi}} \vec{\phi}^{C_-}(\cdot,\lambda), \frac{1}{\sqrt{2\pi}} \vec{\phi}^{C'_-}(\cdot,\lambda') \right)_{\mathcal{K}} = \delta(\lambda - \lambda') \langle C_-, C'_- \rangle.$$

Introducing the notions

$$\vec{\phi}(\cdot,\lambda,j) := \frac{1}{\sqrt{2\pi}} \vec{\phi}^{e_j}(\cdot,\lambda), \quad j = 0,\ldots,N+1, \tag{5.10}$$

where we have set $e_a = e_0$ and $e_b = e_{N+1}$, we get the following theorem.

Theorem 5.1: *Assume* $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, *and* $\kappa_a, \kappa_1, \ldots, \kappa_N, \kappa_b \in \mathbb{C}_+$. *Then the functions*

$$\{\vec{\phi}(\cdot,\lambda,a), \vec{\phi}(\cdot,\lambda,1), \ldots, \vec{\phi}(\cdot,\lambda,N), \vec{\phi}(\cdot,\lambda,b)\}_{\lambda \in \mathbb{R}},$$

perform a complete orthonormal system of generalized eigenfunctions of K, *i.e.*,

$$(\vec{\phi}(\cdot,\lambda,\tau), \vec{\phi}(\cdot,\lambda',\tau'))_{\mathcal{K}} = \delta(\lambda - \lambda')\, \delta_{\tau\tau'}, \quad \lambda,\lambda' \in \mathbb{R}, \quad \tau,\tau' = a,1,\ldots,N,b,$$

and their linear span, i.e., elements of the form

$$f(x) = \int_{\mathbb{R}} \sum_{\tau = a,1,\ldots,N,b} \vec{\phi}(x,\lambda,\tau) g^\tau(\lambda)\, d\lambda,$$

where g^τ, $\tau=a,1,\ldots,N,b$, *are smooth functions with compact support, is dense in* $\mathcal{K}$.

We say that $\{e^a(\lambda),e^1(\lambda),\ldots,e^N(\lambda),e^b(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of orthogonal bases in $\mathbb{C}^{N+2}$, if the components of the vectors $e^\tau(\lambda)$, $\tau=a,1,\ldots,N,b$, are Lebesgue measurable functions such that $\langle e^\tau(\lambda),e^\xi(\lambda)\rangle=\delta_{\tau,\xi}$ for *a.e.* $\lambda\in\mathbb{R}$. Thus we get the following.

Corollary 5.2: Suppose that $V\in\mathsf{L}^2(a,b)$, $\mathrm{Im}(V)=0$, $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$, *and* $x_1,\ldots,x_N\in(a,b)$ *with* $x_1<x_2<\cdots<x_N$. *If* $\{e^a(\lambda),e^1(\lambda),\ldots,e^N(\lambda),e^b(\lambda)\}_{\lambda\in\mathbb{R}}$ *is a measurable family of orthogonal bases in* $\mathbb{C}^{N+2}$, *then the system of eigenfunctions,*

$$\{\vec{\phi}(\cdot,\lambda,e^a(\lambda)),\vec{\phi}(\cdot,\lambda,e^1(\lambda)),\ldots,\vec{\phi}(\cdot,\lambda,e^N(\lambda)),\vec{\phi}(\cdot,\lambda,e^b(\lambda))\}_{\lambda\in\mathbb{R}},$$

where

$$\vec{\phi}(\cdot,\lambda,e^\tau(\lambda)):=\frac{1}{\sqrt{2\pi}}\vec{\phi}^{e^j(\lambda)}(\cdot,\lambda),\quad \tau=a,\ldots,b,$$

performs a complete orthonormal system of generalized eigenfunctions of K.

The generalized eigenfunctions $\phi(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. By the use of the incoming eigenfunctions, one defines a transform $\mathcal{F}:\mathcal{K}\to\hat{\mathcal{K}}:=\mathsf{L}^2(\mathbb{R},\mathbb{C}^{N+2})$ by

$$(\mathcal{F}\vec{g})(\lambda)=:\hat{g}(\lambda)=\begin{pmatrix}\hat{g}^b(\lambda)\\ \hat{g}^N(\lambda)\\ \vdots\\ \hat{g}^1(\lambda)\\ \hat{g}^a(\lambda)\end{pmatrix},$$

where

$$\hat{g}^\tau(\lambda):=\int_{\hat{\Omega}}\vec{g}(x),\overline{\vec{\phi}(x,\lambda,\tau)}dx\,.$$

$\mathcal{F}$ is a unitary operator and called the incomi ng Fourier transform. The inverse incoming Fourier transform $\mathcal{F}^{-1}$ is given by

$$(\mathcal{F}^{-1}\hat{g})(x)=\int_{\mathbb{R}}\sum_{\tau=a,1,\ldots,N,b}\vec{\phi}(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda)\,d\lambda,\quad \hat{g}\in\hat{\mathcal{K}}.$$

We note that

$$\mathcal{F}K\mathcal{F}^{-1}=M,\tag{5.11}$$

where M is the multiplication operator on $\hat{\mathcal{K}}$ given by

$$\mathsf{D}(M):=\{\hat{g}\in\hat{\mathcal{K}}\mid\lambda\hat{g}(\lambda)\in\hat{\mathcal{K}}\},$$

$$(M\hat{g})(\lambda):=\lambda\hat{g}(\lambda),\quad \hat{g}\in\mathsf{D}(M).$$

VI. CARRIER DENSITY

According to Kaiser (2002) we call $\varrho:\mathcal{K}\to\mathcal{K}$ a density matrix, if ϱ is a bounded, non-negative operator. A density matrix ϱ is called a steady state, if it commutes with K. For steady states ϱ there exists a function $\varrho(\cdot)\in\mathsf{L}^\infty(\mathbb{R},\mathfrak{B}(\mathbb{C}^{N+2}))$ such that the multiplication operator $\hat{\varrho}$, defined by

$$\mathsf{D}(\hat{\varrho}):=\{\hat{g}\in\hat{\mathcal{K}}\mid\varrho(\lambda)\hat{g}(\lambda)\in\hat{\mathcal{K}}\},$$

$$(\hat{\varrho}\hat{g})(\lambda) := \varrho(\lambda)\hat{g}(\lambda), \quad \hat{g} \in \mathsf{D}(\hat{\varrho}),$$

is unitarily equivalent to ϱ, i.e.,

$$\varrho = \mathcal{F}^{-1}\hat{\varrho}\mathcal{F}.$$

Since $\varrho \geqslant 0$ we get $\varrho(\lambda) \geqslant 0$ for *a.e.* $\lambda \in \mathbb{R}$.

The time evolution of a given density matrix ϱ is given by

$$\varrho(t) := e^{-itK}\varrho e^{itK}, \quad t \in \mathbb{R};$$

cf. Landau (1971). If ϱ commutes with K, we have $\varrho(t) = \varrho$ for all $t \in \mathbb{R}$. This justifies the definition of steady states.

Definition 6.1: A bounded self-adjoint operator A on a Hilbert space $\mathcal{K}$ is called an observable. We say that the observable A

(1) is admissible with respect to ϱ if ϱA is a trace class operator, i.e., $\varrho A \in \mathfrak{B}_1(\mathcal{K})$;
(2) is admissible with respect to K, if $E_K(\Delta)A \in \mathfrak{B}_1(\mathcal{K})$ for each bounded interval $\Delta \subset \mathbb{R}$, where $E_K(\Delta)$ denotes the spectral projection of K on Δ.

If the observable A is admissible with respect to ϱ, then its expectation value $\mathbb{E}_\varrho(A)$ with respect to the density matrix ϱ is defined by

$$\mathbb{E}_\varrho(A) := \mathrm{tr}(\varrho A).$$

To calculate the carrier density we consider the observable $U(\omega)$ given by

$$(U(\omega)\vec{f})(x) = 0 \oplus \chi_\omega(x) f(x) \oplus 0, \quad \vec{f} = f_- \oplus f \oplus f_+ \in \mathcal{K},$$

for any Borel subset $\omega \subseteq [a,b]$. We remark that $U(\omega)$ is a projection on $\mathcal{K}$ with $\mathrm{ran}(U(\omega)) \subseteq \mathcal{H}$.

Let us introduce some more notions: We set

$$\Phi(x,\lambda) = \begin{pmatrix} \phi(x,\lambda,N+1) \\ \vdots \\ \phi(x,\lambda,0) \end{pmatrix},$$

and $\overline{\Phi(x,\lambda)}$ denotes the vector $\Phi(x,\lambda)$ with each element complex conjugated.

As in Kaiser (2002), one proves the following lemma.

Lemma 6.2: Assume that $m + (1/m) \in \mathsf{L}^\infty(a,b)$, $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, $\kappa_a, \kappa_1, \ldots, \kappa_N, \kappa_b \in \mathbb{C}_+$, *and* $x_1, \ldots, x_n \in (a,b)$ *such that* $x_1 < x_2 < \cdots < x_N$.

(1) The observable $U(\omega)$ is admissible with respect to the minimal self-adjoint dilation K of the maximal dissipative operator H for any Borel set $\omega \subseteq [a,b]$. Furthermore, we get the representation

$$\mathrm{tr}(\varrho U(\omega)E_K(\Delta)) = \int_\Delta \mathrm{tr}(\varrho(\lambda)U(\omega)(\lambda))\, d\lambda,$$

for any bounded Borel set $\Delta \subset \mathbb{R}$ and any steady state ϱ, where

$$U(\omega)(\lambda) := \int_\omega D(x,\lambda)\, dx,$$

with

$$D(x,\lambda) := \overline{\Phi(x,\lambda)}\, \Phi(x,\lambda)^T.$$

(2) If the steady state ϱ satisfies the condition

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2+1}\, \|\varrho(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})} < \infty, \tag{6.1}$$

then the observable $U(\omega)$ is admissible with respect to ϱ for any Borel set $\omega \subseteq [a,b]$. Furthermore, we have

$$\operatorname{tr}(\varrho U(\omega)) = \int_{\mathbb{R}} \operatorname{tr}(\varrho(\lambda) U(\omega)(\lambda))\, d\lambda.$$

We set

$$u_\varrho(x,\lambda) := \operatorname{tr}(\varrho(\lambda) D(x,\lambda)),$$

for $x \in [a,b]$ and $\lambda \in \mathbb{R}$. Note that

$$u_\varrho(x,\lambda) = \langle \varrho(\lambda)^T \Phi(x,\lambda), \Phi(x,\lambda) \rangle, \tag{6.2}$$

where $\varrho(\lambda)^T$ denotes the transposed matrix of $\varrho(\lambda)$. Since $\varrho(\lambda)$ is non-negative, we get by the representation (6.2) that $u_\varrho(x,\lambda) \geqslant 0$ for $x \in [a,b]$ and *a.e.* $\lambda \in \mathbb{R}$. If the condition (6.1) is satisfied, we get by Lemma 6.2,

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} \int_\omega u_\varrho(x,\lambda)\, dx\, d\lambda,$$

for any Borel set $\omega \subseteq [a,b]$. Hence, by Fubini's Theorem we get

$$\mathbb{E}_\varrho(U(\omega)) = \int_\omega u_\varrho(x)\, dx, \tag{6.3}$$

where

$$u_\varrho(x) := \int_{\mathbb{R}} u_\varrho(x,\lambda)\, d\lambda \geqslant 0, \quad x \in [a,b]; \tag{6.4}$$

thus $u_\varrho \in \mathsf{L}^1(a,b)$. Clearly $\mathbb{E}_\varrho(U(\cdot))$ defines a measure which is absolutely continuous with respect to the Lebesgue measure. Since $\mathbb{E}_\varrho(U(\omega))$ can be interpreted as the number of carriers in $\omega \subseteq [a,b]$, its Radon–Nikodym derivative can be viewed as the carrier density of the system described by K. Since K is the dilation corresponding to the maximal dissipative operator H and $U(\omega)$ acts only on $\mathcal{H}$, we identify u_ϱ with the carrier density of the system described by H.

Note that

$$u_\varrho(x,\lambda) = \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \tag{6.5}$$

for $x \in [a,b]$ and $\lambda \in \mathbb{R}$. We call the matrix $D(x,\lambda)$ the carrier density observable and $u_\varrho(x,\lambda)$ the carrier density of the system described by H at point $x \in [a,b]$ and energy $\lambda \in \mathbb{R}$. This is justified since (6.5) can be seen as the expectation value of the carrier density observable.

Furthermore, we have

$$u_\varrho(x) = \int_{\mathbb{R}} \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \quad x \in [a,b],$$

i.e., the carrier density for each point x is the sum of the expectation values of the carrier density observable for the point x over all energies.

For real-valued $h \in \mathsf{L}^\infty(a,b)$ we define the multiplication operator $M(h)$ on the Hilbert space $\mathcal{K}$ by

$$(M(h)\vec{f})(x)=0\oplus h(x)f(x)\oplus 0,\quad \vec{f}=f_-\oplus f\oplus f_+\in\mathcal{K}.$$

We note that $M(\chi_\omega)=U(\omega)$, in particular $M(\chi_\Omega)=U(\Omega)=P_{\mathcal{H}}^{\mathcal{K}}$. Since

$$\varrho M(h)=\varrho U(\Omega)M(h),\quad h\in\mathsf{L}^\infty(a,b),$$

we get that the observable $M(h)$ is admissible with respect to ϱ.

Lemma 6.3: Assume that $m+(1/m)\in\mathsf{L}^\infty$, $V\in\mathsf{L}^2(a,b)$ *real-valued, and* $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$. *If the steady state* ϱ *satisfies the condition* (6.1), *then the carrier density* u_ϱ *defined by* (6.4) *is a non-negative* L^1*-function such that*

$$\mathrm{tr}(\varrho M(h))=\int_a^b u_\varrho(x)h(x)\,dx, \tag{6.6}$$

for any real-valued function $h\in\mathsf{L}^\infty(a,b)$. *In particular one has*

$$\|u_\varrho\|_{\mathsf{L}^1(\omega)}=\mathrm{tr}(\varrho U(\omega))\leqslant C_{\hat{\varrho}}\|(K-i)^{-1}P_{\mathcal{H}}^{\mathcal{K}}\|_{\mathfrak{B}_1}, \tag{6.7}$$

for each Borel set $\omega\subseteq[a,b]$.

Proof: By (6.3) we get that (6.6) holds for $h=\chi_\Omega$. By linearity (6.6) can be extended for arbitrary step functions h. Since u_ϱ is from $\mathsf{L}^1(a,b)$ and $\varrho U(\Omega)$ is of trace class, (6.6) admits a continuation to all L^∞-functions h, which proves the first part of the lemma.

Since $(K-i)^{-1}P_{\mathcal{H}}^{\mathcal{K}}$ is a trace class operator and since $\varrho(K-i)$ is a bounded operator whose norm can be estimated by $C_{\hat{\varrho}}$, we obtain

$$\mathrm{tr}(\varrho(K-i)(K-i)^{-1}U(\omega))\leqslant C_{\hat{\varrho}}\|(K-i)^{-1}P_{\mathcal{K}}^{\mathcal{H}}\|_{\mathfrak{B}_1}.$$

This verifies (6.7). □

Suppose that $\{\varrho(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of non-negative selfadjoint operators on $\mathbb{C}^{N+2}$. We can find a family of unitary operators $\{V(\lambda)\}_{\lambda\in\mathbb{R}}$ on $\mathbb{C}^{N+2}$ such that

$$\varrho(\lambda)=V(\lambda)\begin{pmatrix}\mu_b(\lambda)&0&\cdots&\cdots&0\\0&\mu_N(\lambda)&0&\cdots&0\\\vdots&&\ddots&&\vdots\\0&\cdots&0&\mu_1(\lambda)&0\\0&\cdots&\cdots&0&\mu_a(\lambda)\end{pmatrix}V(\lambda)^*,$$

for *a.e.* $\lambda\in\mathbb{R}$, where $\mu_\tau(\lambda)$, $\tau=a,1,\ldots,N,b$, are the non-negative eigenvalues of the matrix $\varrho(\lambda)$. Hence from Eq. (6.2) we obtain

$$u_\varrho(x,\lambda)=\left\langle\begin{pmatrix}\mu_b(\lambda)&\cdots&0\\\vdots&\ddots&\vdots\\0&\cdots&\mu_a(\lambda)\end{pmatrix}V(\lambda)^T\Phi(x,\lambda),V(\lambda)^T\Phi(x,\lambda)\right\rangle.$$

Introducing the measurable family of orthogonal bases $\{e^a(\lambda),\ldots,e^b(\lambda)\}_{\lambda\in\mathbb{R}}$, where $e^\tau(\lambda):=V(\lambda)e_\tau$, we find

$$u_\varrho(x,\lambda)=\sum_{\tau=a,\ldots,b}\mu_\tau(\lambda)|\phi(x,\lambda,e^\tau(\lambda))|^2,$$

for $x\in[a,b]$ and $\lambda\in\mathbb{R}$, where we used the fact that

$$V^T(\lambda)\Phi(x,\lambda)=\begin{pmatrix}\phi(x,\lambda,e_b(\lambda))\\ \vdots\\ \phi(x,\lambda,e_a(\lambda))\end{pmatrix}. \tag{6.8}$$

VII. CURRENT DENSITY

We define the current density $j_\varrho(x,\lambda)$ at point x and energy $\lambda\in\mathbb{R}$ of the system described by the dissipative operator H by

$$j_\varrho(x,\lambda):=\sum_{\tau=0}^{N+1}\mu_\tau(\lambda)\mathrm{Im}\left(\frac{1}{m(x)}\phi(x,\lambda,e^\tau(\lambda))'\overline{\phi(x,\lambda,e^\tau(\lambda))}\right). \tag{7.1}$$

See Landau (1971) for the motivation of this definition. We note that $\phi(x,\lambda,e^\tau(\lambda))'$ exists only for $x\neq x_j$, $j=1,\ldots,N$. Therefore, the definition (7.1) only makes sense for $x\in\cup_{j=0}^{N}(x_j,x_{j+1})$.

Equation (7.1) can be rewritten as

$$j_\varrho(x,\lambda)=\mathrm{Im}\left(\left\langle\varrho(\lambda)^T\frac{1}{m(x)}\Phi(x,\lambda)',\Phi(x,\lambda)\right\rangle\right). \tag{7.2}$$

Finally this can be expressed as

$$j_\varrho(x,\lambda)=\mathrm{tr}(\varrho(\lambda)C(x,\lambda)),$$

where

$$C(x,\lambda):=\mathrm{Im}\begin{pmatrix}\frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,N+1)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,N+1)}\\ \frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,N)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,N)}\\ \vdots & & \vdots\\ \frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,0)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,0)}\end{pmatrix}. \tag{7.3}$$

The current density is strongly related to the characteristic function of the operator H. This is shown in the next theorem.

Theorem 7.1: *Assume that* $m+(1/m)\in\mathsf{L}^\infty(a,b)$, $V\in\mathsf{L}^2(a,b)$, *with* $\mathrm{Im}(V)=0$, *and* $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$ *as well as* $x_1,\ldots,x_N\in(a,b)$ *such that* $x_1<x_2<\cdots<x_N$. *Let* ϱ *be a steady state. Then the current density* $j_\varrho(x,\lambda)$, $x\in[a,b]$, $x\neq x_j$, $\lambda\in\mathbb{R}$, *is independent of* x *for* $x\in(x_j,x_{j+1})$ *and admits the representation*

$$j_\varrho(x,\lambda)=\mathrm{tr}(\varrho(\lambda)C(x,\lambda)), \tag{7.4}$$

where

$$C(x,\lambda):=\sum_{j=0}^{N}E_j(\lambda)\Theta_H(\lambda)^*\chi_{(x_j,x_{j+1})}(x) \tag{7.5}$$

and

$$E_j(\lambda):=\frac{1}{2\pi}(P_-^j\Theta_H(\lambda)P_+^j-P_+^j\Theta_H(\lambda)P_-^j), \tag{7.6}$$

with

$$P^j_- := \sum_{z=0}^{j} P_z, \quad P^j_+ := \sum_{z=j+1}^{N+1} P_z, \quad P_z := \langle \cdot, e_z \rangle e_z .$$

Moreover, if $\mathrm{tr}(\varrho(\cdot)) \in \mathsf{L}^1(\mathbb{R})$, *then the total current* $j_\varrho(x)$ *at point* $x \in (x_j, x_{j+1})$,

$$j_\varrho(x) := \int_{\mathbb{R}} j_\varrho(x,\lambda)\, d\lambda,$$

is finite and can be estimated by

$$|j_\varrho(x)| \leqslant \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{tr}(\varrho(\lambda))\, d\lambda. \tag{7.7}$$

Proof: We have

$$j_\varrho(x,\lambda) = \mathrm{tr}(\varrho(\lambda) C(x,\lambda)), \tag{7.8}$$

where $C(x,\lambda)$ is given by (7.3). $C(x,\lambda)$ can be rewritten as

$$C(x,\lambda) = \frac{1}{i} \begin{pmatrix} W(\overline{\phi(\cdot,\lambda,N+1)}, \phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,N+1}, \phi(\cdot,\lambda,0))(x) \\ W(\overline{\phi(\cdot,\lambda,N)}, \phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,N)}, \phi(\cdot,\lambda,0))(x) \\ \vdots & & \vdots \\ W(\overline{\phi(\cdot,\lambda,0)}, \phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,0)}, \phi(\cdot,\lambda,0))(x) \end{pmatrix}. \tag{7.9}$$

Clearly, $W(\overline{\phi(\cdot,\lambda,l)}, \phi(\cdot,\lambda,m))(x)$ is constant for every x in each subinterval (x_j, x_{j+1}), for every $l,m = 0,\ldots,N+1$. Hence, $j_\varrho(x,\lambda)_{|(x_j,x_{j+1})}$ is constant.

Let us compute $C(x,\lambda)_{|(x_j,x_{j+1})}$. Since $\phi(x,\lambda,k)$ has to fulfill the boundary conditions (5.5) and (5.6) (see also Fig. 1), we get

$$\begin{aligned} W(\overline{\phi(\cdot,\lambda,l)}, \phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= W(\overline{\phi(\cdot,\lambda,l)}, \phi(\cdot,\lambda,m))(x_j+0) \\ &= W(\overline{\phi(\cdot,\lambda,l)}, \phi(\cdot,\lambda,m))(x_j-0) \\ &\quad - i\alpha_j^2 \overline{\phi(x_j,\lambda,l)}\, \phi(x_j,\lambda,m) + \delta_{jm} \frac{\alpha_m}{\sqrt{2\pi}} \overline{\phi(x_m,\lambda,l)} \\ &= W(\overline{\phi(\cdot,\lambda,l)}, \phi(\cdot,\lambda,m))(x_{j-1}+0) \\ &\quad - i\alpha_j^2 \overline{\phi(x_j,\lambda,l)}\, \phi(x_j,\lambda,m) + \delta_{jm} \frac{\alpha_m}{\sqrt{2\pi}} \overline{\phi(x_m,\lambda,l)} \\ &\quad \vdots \\ &= \sum_{\tau=0}^{j} \left\{ - i\alpha_\tau^2 \overline{\phi(x_\tau,\lambda,l)}\, \phi(x_\tau,\lambda,m) + \delta_{\tau,m} \frac{\alpha_\tau}{\sqrt{2\pi}} \overline{\phi(x_\tau,\lambda,l)} \right\}, \end{aligned}$$

for $l,m = 0,\ldots,N+1$ and $l > j$, where $\delta_{\tau,m} = \langle e_\tau, e_m \rangle$. Similarly, we obtain for all $l,m = 0,\ldots,N+1$, $l \leqslant j$,

$$
\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= W(\overline{\phi(x,\lambda,l)},\phi(x,\lambda,m))(x_{j+1}-0)\\
&= W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_{j+1}+0)\\
&\quad + i\alpha_{j+1}\overline{\phi(x_{j+1},\lambda,l)}\,\phi(x_{j+1},\lambda,m)\\
&\quad - \delta_{j+1,m}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_{j+1},\lambda,l)}\\
&= W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_{j+2}-0)\\
&\quad + i\alpha_{j+1}\overline{\phi(x_{j+1},\lambda,l)}\,\phi(x_{j+1},\lambda,m)\\
&\quad - \delta_{j+1,m}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_{j+1},\lambda,l)}\\
&\quad \vdots\\
&= \sum_{\tau=j+1}^{N+1}\left\{ i\alpha_\tau^2\overline{\phi(x_\tau,\lambda,l)}\,\phi(x_\tau,\lambda,m) - \delta_{\tau,m}\frac{\alpha_\tau}{\sqrt{2\pi}}\overline{\phi(x_\tau,\lambda,l)}\right\}.
\end{aligned}
$$

Note that

$$
\frac{1}{\sqrt{2\pi}}\langle \alpha T_*(\lambda)^* e_\xi, e_\tau\rangle = -\alpha_\tau\phi(x_\tau,\lambda,\xi),
$$

for all $\tau,\xi=0,\ldots,N+1$. Hence, we find

$$
\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= \frac{1}{\sqrt{2\pi}}\sum_{\tau=0}^{j}\{-i\sqrt{2\pi}\alpha_\tau\phi(x_\tau,\lambda,m)+\delta_{\tau,m}\}\alpha_\tau\overline{\phi(x_\tau,\lambda,l)}\\
&= -\frac{1}{2\pi}\sum_{\tau=0}^{j}\{i\langle \alpha T_*(\lambda)^* e_m, e_\tau\rangle + \langle e_m, e_\tau\rangle\}\overline{\langle \alpha T_*(\lambda)^* e_l, e_\tau\rangle},
\end{aligned}
\tag{7.10}
$$

for $l>j$. Using Eq. (4.9) we get

$$
\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= -\frac{1}{2\pi}\sum_{\tau=0}^{j}\langle \Theta_H(\lambda)^* e_m, e_\tau\rangle\overline{\langle \alpha T_*(\lambda)^* e_l, e_\tau\rangle}\\
&= -\frac{1}{2\pi}\langle P_-^j\Theta_H(\lambda)^* e_m, \alpha T_*(\lambda)^* e_l\rangle
\end{aligned}
\tag{7.11}
$$

or

$$
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} = -\frac{i}{2\pi}\langle P_-^j\Theta_H(\lambda)^* e_m, \Theta_H(\lambda)^* P_+^j\ \ e_l\rangle, \tag{7.12}
$$

for $l>j$. If $l\leqslant j$, then

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})}=\frac{1}{\sqrt{2\pi}}\sum_{\tau=j+1}^{N+1}\{i\sqrt{2\pi}\alpha_\tau\phi(x_\tau,\lambda,m)-\delta_{\tau,m}\}\alpha_\tau\overline{\phi(x_\tau,\lambda,l)}$$

$$=\frac{1}{2\pi}\sum_{\tau=j+1}^{N+1}\{i\langle T_*(\lambda)^*e_m,e_\tau\rangle+\langle e_m,e_\tau\rangle\}\overline{\langle\alpha T_*(\lambda)^*e_l,e_\tau\rangle}. \tag{7.13}$$

Using again (4.9) we obtain

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})}=\frac{1}{2\pi}\sum_{\tau=j+1}^{N+1}\langle\Theta_H(\lambda)^*e_m,e_\tau\rangle\overline{\langle\alpha T_*(\lambda)^*e_l,e_\tau\rangle}$$

$$=\frac{i}{2\pi}\langle P_+^j\Theta_H(\lambda)^*e_m,\Theta_H(\lambda)^*e_l\rangle, \tag{7.14}$$

which yields

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})}=\frac{i}{2\pi}\langle P_+^j\Theta_H(\lambda)^*e_m,\Theta_H(\lambda)^*P_-^j\quad e_l\rangle, \tag{7.15}$$

for $l\leqslant j$. Taking into account (7.9), (7.12) and (7.15) we find

$$\langle C(x,\lambda)e_m,e_l)\rangle_{|(x_j,x_{j+1})}=\frac{1}{2\pi}\langle\{P_-^j\Theta_H(\lambda)P_+^j-P_+^j\Theta_H(\lambda)P_-^j\}\Theta_H(\lambda)^*e_m,e_l\rangle, \tag{7.16}$$

for $m,l=0,1,\ldots,N+1$. Using notation (7.5) and (7.6) we immediately obtain (7.4).

From the above calculations we get for the total current $j_\varrho(x)$, $x\in(x_j,x_{j+1})$,

$$|j_\varrho(x)|\leqslant\|\varrho(\lambda)C(x,\lambda)\|_{\mathfrak{B}_1(\mathbb{C}^{N+2})}\leqslant\frac{1}{2\pi}\|\varrho(\lambda)\|_{\mathfrak{B}_1(\mathbb{C}^{N+2})}\|E_j(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})}.$$

By (7.6) one gets

$$E_j(\lambda)^*E_j(\lambda)=P_+^j\Theta_H(\lambda)^*P_-^j\Theta_H(\lambda)P_+^j+P_-^j\Theta_H(\lambda)^*P_+^j\Theta_H(\lambda)P_-^j,$$

which yields

$$E_j(\lambda)^*E_j(\lambda)\leqslant I.$$

Hence, $\|E_j(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})}\leqslant 1$ which verifies (7.7). □

Let us show that piecewise constant matrix-valued function $C(x,\lambda)$ is self-adjoint for each $x\neq x_j$. If $x\in(x_j,x_{j+1})$, then one gets

$$C(x,\lambda)^*=\Theta_H(\lambda)E_j(\lambda)^*=\frac{1}{2\pi}\Theta_H(\lambda)\{P_-^j\Theta_H(\lambda)^*P_+^j-P_+^j\Theta_H(\lambda)^*P_-^j\}.$$

One has

$$C(x,\lambda)^*=\frac{1}{2\pi}\{P_+^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j+P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j$$

$$-P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j-P_-^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j\}.$$

Since $P_+^j+P_-^j=I$ and $\Theta_H(\lambda)\Theta_H(\lambda)^*=I$ we find

$$C(x,\lambda)^* = \frac{1}{2\pi}\{-P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_-^j + P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j$$
$$-P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j + P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_+^j\},$$

which yields

$$C(x,\lambda)^* = \frac{1}{2\pi}\{P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)P_-^j\}\Theta_H(\lambda)^* = C(x,\lambda).$$

Since $C(x,\lambda)$ is self-adjoint it is useful, in correspondence to the carrier density, to make the following definition.

Definition 7.2: The piecewise constant matrix $C(\cdot,\lambda)$ defined by (7.5) is called the current density observable, and the piecewise constant function,

$$j_\varrho(x,\lambda) = \mathrm{tr}(\varrho(\lambda)C(x,\lambda)),$$

is called the current density at point $x\in[a,b]$, $x\neq x_j$, and energy $\lambda\in\mathbb{R}$.

The definition is justified by the fact that the current density is the expectation value of the current density observable at energy $\lambda\in\mathbb{R}$ and point $x\in\mathbb{R}$, i.e., $j_\varrho(x,\lambda)=\mathbb{E}_{\varrho(\lambda)}(C(x,\lambda))$. Using this notion we get

$$j_\varrho(x) = \int_{\mathbb{R}} \mathbb{E}_{\varrho(\lambda)}(C(x,\lambda))\,d\lambda.$$

Let us consider the special case, where the steady state ϱ is a function of K, i.e., $\varrho=f(K)$, for some $f\in\mathsf{L}^\infty(\mathbb{R})$, $f\geqslant 0$. In this case ϱ belong to the bicommutant of K. As in Kaiser (2002) we get that in this case the current density is zero. This fact is proven by the following corollary.

Corollary 7.3: Suppose that $m+(1/m)\in\mathsf{L}^\infty(a,b)$, $V\in\mathsf{L}^2(a,b)$, *such that* $\mathrm{Im}(V)=0$, $\kappa_a,\kappa_1,\ldots,\kappa_N,\kappa_b\in\mathbb{C}_+$, *as well as* $x_1,\ldots,x_N\in(a,b)$, *with* $x_1<x_2<\cdots<x_N$. *Furthermore, assume that the steady state* ϱ *is of the form* $\varrho=f(K)$, *where* $f\in\mathsf{L}^1(\mathbb{R})$ *is non-negative. Then* $j_\varrho(x,\lambda)=0$ *for* $x\neq x_\tau$, $\tau=a,x_1,\ldots,x_N,b$, *and a.e.* $\lambda\in\mathbb{R}$.

Proof: Clearly we have $\varrho(\lambda)=f(\lambda)I_{\mathbb{C}^{N+2}}$, $\lambda\in\mathbb{R}$. Thus we get for $x\in(x_j,x_{j+1})$,

$$j_\varrho(x,\lambda) = f(\lambda)\mathrm{tr}_{\mathbb{C}^{N+2}}(C(x,\lambda)).$$

Using (7.5) and (7.6) we obtain

$$j_\varrho(x,\lambda) = f(\lambda)\mathrm{tr}(E_j(x,\lambda)\Theta_H(\lambda)^*) = f(\lambda)\mathrm{tr}((P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)P_-^j)\Theta_H(\lambda)^*).$$

Since

$$\mathrm{tr}(P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*) = \mathrm{tr}(P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j) = \mathrm{tr}(P_-^j\Theta_H(\lambda)^*P_+^j\Theta_H(\lambda)P_-^j)$$

and

$$\mathrm{tr}(P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*) = \mathrm{tr}(P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j)$$

we have

$$\mathrm{tr}((P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)p_-^J)\Theta_H(\lambda)^*) = 0,$$

which proves $j_\varrho(x,\lambda)=0$. □

VIII. CURRENT VARIATIONS

In Theorem 7.1 we showed that the current density $j_\varrho(x,\lambda)$ is piecewise constant in x. Let us calculate the current difference for some $\tilde{a}\in(x_j,x_{j+1})$ and $\tilde{b}\in(x_{j+1},x_{j+2})$:

$$\begin{aligned} j_\varrho(\tilde{b},\lambda)-j_\varrho(\tilde{a},\lambda) &= \frac{1}{2\pi}\operatorname{tr}(\varrho(\lambda)\{C_{j+1}(\lambda)-C_j(\lambda)\}) \\ &= \frac{1}{2\pi}\operatorname{tr}(\varrho(\lambda)\{P_-^{j+1}\Theta_H(\lambda)P_-^{j+1}-P_-^j\Theta_H(\lambda)P_-^j\}\Theta_H^*(\lambda)) \\ &= \frac{1}{2\pi}\operatorname{tr}(\varrho(\lambda)\{P_{j+1}\Theta_H(\lambda)-\Theta_H(\lambda)P_{j+1}\}\Theta_H^*(\lambda)) \\ &= \frac{1}{2\pi}\operatorname{tr}(P_{j+1}\{\varrho(\lambda)-\Theta_H{}^*(\lambda)\varrho(\lambda)\Theta_H(\lambda)\}P_{j+1}). \end{aligned} \tag{8.1}$$

More general, we get for $\hat{a}\in(x_j,x_{j+1})$ and $\hat{b}\in(x_{j+k+1},x_{j+k+2})$

$$j_\varrho(\hat{b},\lambda)-j_\varrho(\hat{a},\lambda)=\frac{1}{2\pi}\operatorname{tr}(Q\{\varrho(\lambda)-\Theta_H(\lambda)\varrho(\lambda)\Theta_H^*(\lambda)\}Q), \tag{8.2}$$

where $Q=\Sigma_{\tau=j}^{j+k}P_\tau$.

From Eq. (8.2) we see that the current difference depends essentially on the density matrix $\varrho(\lambda)$. For example, if $\varrho(\lambda)$ commutes with $\Theta_H(\lambda)$ we get that the difference is zero. Hence, the current is constant. In the case that the difference in (8.2) is positive; the system is ''losing'' electrons between the points $\tilde{a}$ and $\tilde{b}$. If the difference in (8.2) is negative, the system ''gains'' electrons. The effect of losing and gaining electrons is closely related to a recombination–generation process.

In the following we are going to construct a density matrix $\varrho(\cdot)$, such that the r.h.s. of (8.2) is expressed in terms of the density $u_\varrho(x_\xi,\lambda)$ and the α_j's.

Let $\mathcal{R}_{\lambda_0},\mathcal{G}_{\lambda_0}\subseteq\{1,\ldots,N\}:=\mathcal{T}$ such that $\mathcal{R}_{\lambda_0}\cap\mathcal{G}_{\lambda_0}=\varnothing$, $\mathcal{R}_{\lambda_0}\cup\mathcal{G}_{\lambda_0}=\mathcal{T}$, and $u(\lambda_0)\in\mathbb{C}^{N+2}$ with

$$\langle u(\lambda_0),e_\tau\rangle=0,\quad \forall\,\tau\in\mathcal{R}_{\lambda_0},\ \text{and}\ \langle u(\lambda_0),\Theta_H(\lambda_0)e_\tau\rangle=0,\quad \forall\,\tau\in\mathcal{G}_{\lambda_0}, \tag{8.3}$$

where $\lambda_0\in\mathbb{R}$ is fixed. We define the operator $\varrho(\lambda_0)$ by

$$\varrho(\lambda_0)^T:=\overline{u(\lambda_0)}u(\lambda_0)^T.$$

The function $f(x,\lambda_0)$ given by

$$\begin{pmatrix} 0 \\ \vdots \\ 0 \\ f(x,\lambda_0) \end{pmatrix}=u(\lambda_0)^T\Phi(x,\lambda),$$

satisfies the following boundary conditions:

$$\Delta(f(\cdot,\lambda_0))(x_\tau)=-\kappa_\tau f(x_\tau,\lambda_0),\quad \forall\,\tau\in\mathcal{R}_{\lambda_0}, \tag{8.4}$$

$$\Delta(f(\cdot,\lambda_0))(x_\xi)=-\overline{\kappa_\xi}f(x_\xi,\lambda_0),\quad \forall\,\xi\in\mathcal{G}_{\lambda_0}. \tag{8.5}$$

Let $\omega=[\tilde{a},\tilde{b}]\subseteq\Omega$ be a given interval and $\mathcal{T}_\omega:=\{j\in\mathcal{T}\,|\,x_j\in\omega\}$. The current difference is then given by

$$j_\varrho(\tilde{b},\lambda_0)-j_\varrho(\tilde{a},\lambda_0)=\mathrm{Im}\left(\left\langle u(\lambda_0)^T\frac{1}{m(\tilde{b})}\Phi(\tilde{b},\lambda_0)',u(\lambda_0)^T\Phi(\tilde{b},\lambda_0)\right\rangle\right)$$
$$-\mathrm{Im}\left(\left\langle u(\lambda_0)^T\frac{1}{m(\tilde{a})}\Phi(\tilde{a},\lambda_0)',u(\lambda_0)^T\Phi(\tilde{a},\lambda_0)\right\rangle\right)$$
$$=\frac{1}{i}\sum_{\tau\in\mathcal{T}_\omega}\{W(\overline{f(\cdot,\lambda_0)},f(\cdot,\lambda_0))(x_\tau+0)-W(\overline{f(\cdot,\lambda_0)},f(\cdot,\lambda_0))(x_\tau-0)\}.$$

Using the boundary conditions (8.4) and (8.5) we obtain

$$j_\varrho(\tilde{b},\lambda_0)-j_\varrho(\tilde{a},\lambda_0)=\sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}}\alpha_\tau^2|f(x_\tau,\lambda_0)|^2-\sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}}\alpha_\xi^2|f(x_\xi,\lambda_0)|^2$$
$$=\sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}}\alpha_\tau^2\langle V(\lambda_0)\Phi(x_\tau,\lambda_0),V(\lambda_0)\Phi(x_\tau,\lambda_0)\rangle$$
$$-\sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}}\alpha_\xi^2\langle V(\lambda_0)\Phi(x_\xi,\lambda_0),V(\lambda_0)\Phi(x_\xi,\lambda_0)\rangle$$
$$=\sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}}\alpha_\tau^2u_\varrho(x_\tau,\lambda_0)-\sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}}\alpha_\xi^2u_\varrho(x_\xi,\lambda_0).$$

Clearly a vector $u(\lambda_0)$ with the properties (8.3) always exists. In the following we will construct a vector $u(\lambda_0)$ for almost every $\lambda_0\in\mathbb{R}$, such that $u(\lambda_0)$ is determined up to two given parameters. Let $u_a(\lambda_0),u_b(\lambda_0)\in\mathbb{C}$ be arbitrary. We are now going to construct the vector $u(\lambda_0)=(u^a(\lambda_0),\ldots,u^b(\lambda_0))^T$.

We set $P_{\mathcal{G}_{\lambda_0}}:=\Sigma_{j\in\mathcal{G}_{\lambda_0}}P_j$ and $m_{\mathcal{G}_{\lambda_0}}:=\#\mathcal{G}_{\lambda_0}$, i.e., the number of elements in $\mathcal{G}_{\lambda_0}$.

The first condition in (8.3) implies that $u^j(\lambda_0)=0$ for $j\in\mathcal{R}_{\lambda_0}$. Furthermore we set $u^a(\lambda_0)=u_a(\lambda_0)$ and $u^b(\lambda_0)=u_b(\lambda_0)$. The second condition in (8.3) can be rewritten as

$$P_{\mathcal{G}_{\lambda_0}}\Theta_H(\lambda_0)^*P_{\mathcal{G}_{\lambda_0}}u=-(u_b(\lambda_0)P_{\mathcal{G}_{\lambda_0}}\Theta_H(\lambda_0)^*e_b+u_a(\lambda_0)P_{\mathcal{G}_{\lambda_0}}\Theta_H(\lambda_0)^*e_a). \tag{8.6}$$

Since $P_{\mathcal{G}_{\lambda_0}}\Theta_H(\lambda_0)^*P_{\mathcal{G}_{\lambda_0}}$ can be seen as a $m_{\mathcal{G}_{\lambda_0}}\times m_{\mathcal{G}_{\lambda_0}}$-matrix, the equation (8.6) has a solution for *a.e.* λ_0 if

$$\det_{m_{\mathcal{G}_{\lambda_0}}}(P_{\mathcal{G}_{\lambda_0}}\Theta_H(\lambda_0)^*P_{\mathcal{G}_{\lambda_0}})\neq 0,$$

where $\det_{m_{\mathcal{G}_{\lambda_0}}}(\cdot)$ denotes the determinant in the vector space $\mathbb{C}^{m_{\mathcal{G}_{\lambda_0}}}$.

Since $\langle\Theta_H(\cdot)e_j,e_k\rangle$ is a bounded analytic function on $\overline{\mathbb{C}_-}$ [cf. Foias (1970)], we get that $\det_{m_{\mathcal{G}_{\lambda_0}}}(\cdot)$ is also a bounded analytic function on $\overline{\mathbb{C}_-}$. Hence $\det_{m_{\mathcal{G}_{\lambda_0}}}(\Theta_H(\lambda))\neq 0$ for *a.e.* λ_0.

The remaining components of u, i.e., u^j, $j\in\mathcal{G}_{\lambda_0}$, are then determined as the solution of the linear equation (8.6).

Thus we proved that we can construct a density matrix $\varrho(\lambda_0)$ for *a.e.* λ_0, such that we obtain a loss and gain effect at predefined points x_j. Furthermore, we showed that one has two degrees of freedom in the choice of $\varrho(\lambda_0)$, namely $u^b(\lambda_0)$ and $u^a(\lambda_0)$.

By repeating the above procedure for every $\lambda\in\mathbb{R}$ we can construct a density matrix $\varrho(\lambda)$ for every $\lambda\in\mathbb{R}$. It can easily be seen that the condition (6.1) is satisfied if $u^a(\lambda)$ and $u^b(\lambda)$ decay sufficiently fast, e.g., $u^a(\lambda),u^b(\lambda)$ have compact support.

We will give some examples: Assume that $u^b(\lambda_0), u^a(\lambda_0) \in \mathbb{C}$ are given and let $\mathcal{R}_{\lambda_0} = \{1,\dots,N\}$, $\mathcal{G}_{\lambda_0} = \varnothing$. Clearly the vector

$$u_R(\lambda_0) := (u^b(\lambda_0), 0, \cdots, 0, u^a(\lambda_0))^T$$

satisfies equation (8.3). Introducing the density matrix by

$$\varrho_R(\lambda_0)^T := \overline{u_R(\lambda_0)} u_R(\lambda_0)^T,$$

we get

$$j_{\varrho_R}(\tilde{b}, \lambda_0) - j_{\varrho_R}(\tilde{a}, \lambda_0) = -\sum_{\tau=1}^{N} \alpha_\tau^2 u_{\varrho_R}(x_\tau, \lambda_0),$$

i.e., the density matrix $\varrho_R(\lambda_0)$ is purely recombinative.

To obtain a density matrix which is purely generative we introduce the vector

$$u_G(\lambda_0) := \Theta_H(\lambda_0) u_R(\lambda_0),$$

which satisfies Eq. (8.3) with $\mathcal{R}_{\lambda_0} = \varnothing$ and $\mathcal{G}_{\lambda_0} = \{1,\dots,N\}$. As above we define the density matrix by $\varrho_G(\lambda_0)^T := \overline{u_G(\lambda_0)} u_G(\lambda_0)^T$ and get

$$j_{\varrho_G}(\tilde{b}, \lambda_0) - j_{\varrho_G}(\tilde{a}, \lambda_0) = \sum_{\tau=1}^{N} \alpha_\tau^2 u_{\varrho_G}(x_\tau, \lambda_0).$$

Thus $\varrho_G(\lambda_0)$ is purely generative. We note that

$$\varrho_G(\lambda_0) = \Theta_H(\lambda_0) \varrho_R(\lambda_0) \Theta_H(\lambda_0)^*. \tag{8.7}$$

IX. REMARKS

The definition of carrier and current density was formulated in terms of the complete orthonormal system of eigenfunctions $\{\vec{\phi}(\cdot, \lambda, a), \dots, \vec{\phi}(\cdot, \lambda, b)\}_{\lambda \in \mathbb{R}}$. Since the eigenfunctions behave on $\mathbb{R}_-$ like a free wave, they are called the incoming eigenfunctions. By Eq. (5.10) we can define another system of orthogonal eigenfunctions by

$$\vec{\phi}_{\text{out}}(\cdot, \lambda, j) := \frac{1}{\sqrt{2\pi}} \vec{\phi}^{\Theta(\lambda) e_j}(\cdot, \lambda), \quad j = 0, \dots, N+1,$$

which are called the outgoing eigenfunctions. By Eq. (6.8) the following relation holds:

$$\Theta_H(\lambda) \Phi_{\text{in}}(x, \lambda) = \begin{pmatrix} \phi_{\text{out}}(x, \lambda, b) \\ \vdots \\ \phi_{\text{out}}(x, \lambda, a) \end{pmatrix} := \Phi_{\text{out}}(x, \lambda), \tag{9.1}$$

where we have set $\Phi_{\text{in}}(x, \lambda) = \Phi(x, \lambda)$.

Using the outgoing eigenfunction we define the "outgoing" carrier and current density by

$$u_\varrho^{\text{out}}(x, \lambda) := \langle \varrho(\lambda)^T \Phi_{\text{out}}(x, \lambda), \Phi_{\text{out}}(x, \lambda) \rangle,$$

$$j_\varrho^{\text{out}}(x, \lambda) := \text{Im} \left\langle \varrho(\lambda)^T \frac{1}{m(x)} \Phi_{\text{out}}(x, \lambda)', \Phi_{\text{out}}(x, \lambda) \right\rangle.$$

Using (9.1) we get

$$u_{\varrho}^{\mathrm{out}}(x,\lambda)=u^{\mathrm{in}}_{\Theta_H\varrho\Theta_H^*}(x,\lambda),\quad j_{\varrho}^{\mathrm{out}}(x,\lambda)=j^{\mathrm{in}}_{\Theta_H\varrho\Theta_H^*}(x,\lambda),$$

where $u_{\varrho}^{\mathrm{in}}(x,\lambda)$, $j_{\varrho}^{\mathrm{in}}(x,\lambda)$ denotes the carrier, respectively current, density defined in the previous sections.

The incoming and the outgoing carrier and current densities coincide, if $\varrho(\lambda)$ commutes with the characteristic function $\Theta_H(\lambda)$. As already mentioned above in this case neither loss nor gain effects will occur.

In the previous section we gave an example for a purely recombinative density matrix $\varrho_R(\lambda)$ and an example for a strict generative matrix $\varrho_G(\lambda)$. Using the relations (9.1) and (8.7) we get

$$j^{\mathrm{in}}_{\varrho_G}(x,\lambda)=j^{\mathrm{out}}_{\varrho_R}(x,\lambda),$$

i.e., the generative matrix ϱ_G in the incoming representation becomes a recombinative matrix in the outgoing representation.

Introducing the notions $P_j^{\mathrm{in}}=\langle\cdot,e_j\rangle e_j$ and $P_j^{\mathrm{out}}=\langle\cdot,E_j\rangle E_j$, where $E_j=\Theta_H^*(\lambda)e_j$, we can rewrite (8.1) as follows:

$$j_{\varrho}(\tilde{b},\lambda)-j_{\varrho}(\tilde{a},\lambda)=\frac{1}{2\pi}\mathrm{tr}(\varrho(\lambda)\{P_j^{\mathrm{in}}-P_j^{\mathrm{out}}\}).$$

Let us consider two different dissipative Schrödinger operator H_n and H_p for the two different species of particles (electron and holes), with m_n, m_p, V_n, V_p, $\kappa_{j,n}$, $\kappa_{j,p}$, $j=1,\ldots,N$, and let x_j, $j=1,\ldots,N$, be numbers within the interval (a,b) such that $a<x_1<\cdots<x_N<b$. We denote by $u_{\varrho_k}(x,\lambda)$, respectively $j_{\varrho_k}(x,\lambda)$, the carrier density, respectively current density, corresponding to the density matrix ϱ_k and the operator H_k, $k=n,p$.

Assume that the sets $\mathcal{G}_\lambda=\mathcal{G}$ and $\mathcal{R}_\lambda=\mathcal{R}$ are given. Let $\varrho_n(\lambda)$ and $\varrho_p(\lambda)$ density matrices satisfying Eq. (6.1) such that

$$j_{\varrho_n}(\tilde{b},\lambda)-j_{\varrho_n}(\tilde{a},\lambda)=\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega}\alpha^2_{\tau,n}u_{\varrho_n}(x_\tau,\lambda)-\sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega}\alpha^2_{\xi,n}u_{\varrho_n}(x_\xi,\lambda),\quad \text{for } a.e.\quad \lambda\in\mathbb{R};\tag{9.2}$$

$$j_{\varrho_p}(\tilde{b},\lambda)-j_{\varrho_p}(\tilde{a},\lambda)=-\left(\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega}\alpha^2_{\tau,p}u_{\varrho_p}(x_\tau,\lambda)-\sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega}\alpha^2_{\xi,p}u_{\varrho_p}(x_\xi,\lambda)\right),\quad \text{for } a.e.\quad \lambda\in\mathbb{R}.\tag{9.3}$$

By the consideration of Sec. VIII, such density matrices exists. Integrating (9.2) and (9.3) with respect to λ yields

$$j_{\varrho_n}(\tilde{b})-j_{\varrho_n}(\tilde{a})=\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega}\alpha^2_{\tau,n}u_{\varrho_n}(x_\tau)-\sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega}\alpha^2_{\xi,n}u_{\varrho_n}(x_\xi,),\tag{9.4}$$

$$j_{\varrho_p}(\tilde{b})-j_{\varrho_p}(\tilde{a})=-\left(\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega}\alpha^2_{\tau,p}u_{\varrho_p}(x_\tau)-\sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega}\alpha^2_{\xi,p}u_{\varrho_p}(x_\xi)\right).\tag{9.5}$$

Integrating the stationary continuity equation [cf. (1.3)] over ω gives

$$j_{\varrho_n}(\tilde{b})-j_{\varrho_n}(\tilde{a})=-(j_{\varrho_p}(\tilde{b})-j_{\varrho_p}(\tilde{a})).\tag{9.6}$$

Matching Eq. (9.6) with (9.4) and (9.5) leads to a condition on the $\alpha^2_{j,n}$'s and $\alpha^2_{j,p}$'s, i.e.,

$$\alpha^2_{j,n}=u_{\varrho_p}(x_j,\lambda)\quad\text{and}\quad\alpha^2_{j,p}=u_{\varrho_n}(x_j,\lambda),\quad j=1,\ldots,N.\tag{9.7}$$

The equations (9.4), (9.5) can now be viewed as a stationary continuity equation with the recombination–generation term given by

$$\int_\omega R(u_{\varrho_n}(x),u_{\varrho_p}(x))\,dx=\sum_{j\in\mathcal{T}_\omega\cap\mathcal{R}} u_{\varrho_n}(x_j)u_{\varrho_p}(x_j)-\sum_{j\in\mathcal{T}_\omega\cap\mathcal{G}} u_{\varrho_n}(x_j)u_{\varrho_p}(x_j).$$

To solve the nonlinear equation given by (9.7) we introduce the operators $\mathcal{N}_k:\mathbb{R}_+^N\to\mathbb{R}_+^N$, given by

$$\mathcal{N}_k(\alpha_{1,k}^2,\ldots,\alpha_{N,k}^2)=(u_{\varrho_k}(x_1),\ldots,u_{\varrho_k}(x_N)),$$

where $k=n,p$.

A solution of (9.7) is thus given by a fixed point of the operator $\mathcal{E}$ defined by

$$\mathcal{E}(\alpha_{1,n}^2,\ldots,\alpha_{N,n}^2):=\mathcal{N}_p(\mathcal{N}_n(\alpha_{1,n}^2,\ldots,\alpha_{N,n}^2)).$$

As in Kaiser (2002) and Baro (2002) one can set up a dissipative Schrödinger–Poisson system using the definition of carrier densities introduced in this article. In addition to the Schrödinger–Poisson system considered in Baro (2002) the current is not constant. This system will be discussed in a forthcoming paper.

In Sec. VIII we constructed explicitly a density matrix $\varrho(\cdot)$ such that loss and gain effects occur at predefined points. Furthermore, we showed that one has two free parameters in the choice of $\varrho(\cdot)$, i.e., $u_b(\lambda)$ and $u_a(\lambda)$. These two parameters give the possibility to couple (for example) a drift diffusion model to the open quantum system. We intend to investigate this coupled system in a forthcoming paper.

For simplicity we considered imaginary potentials of the form $-(\alpha^2/2)\,\delta(\cdot-x_j)$. A further step in order to include recombination and generation into the model is to allow complex potentials, i.e., $\mathrm{Im}(V)=-\alpha^2/2$, where $\alpha=\alpha(x)\in L^p$ for some $p>1$. This would give the possibility of modeling recombination–generation rates on the whole interval Ω.

ACKNOWLEDGMENTS

The authors would like to thank Professor P. Degond, H.-Ch. Kaiser, and J. Rehberg for fruitful discussions. The financial support of the DFG (Grant No. RE 1480/1-2) is also gratefully acknowledged.

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Broken symmetries in the entanglement of formation

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(Received 12 September 2002; accepted 17 February 2003)

We compare some recent computations of the entanglement of formation in quantum information theory and of the entropy of a subalgebra in quantum ergodic theory. Both notions require optimization over decompositions of quantum states. We show that both functionals are strongly related for some highly symmetric density matrices. Indeed, for certain interesting regions the entanglement of formation can be expressed by the entropy of a commuting subalgebra, and the corresponding optimal decompositions can be obtained one from the other. We discuss the presence of broken symmetries in relation with the structure of the optimal decompositions. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1570509]

I. INTRODUCTION

Entanglement, always one of the most intriguing among quantum marvels, has lately become a powerful resource in prospective quantum information technologies;[1] measuring the entanglement content of states of multipartite quantum systems is thus of great practical importance. If a bipartite system $A+B$ is described by a density matrix ρ_{AB}, the so-called entanglement of formation[2] is measured by

$$E(\rho_{AB}) := \inf\left\{ \sum_j \lambda_j S(\mathrm{Tr}_B\, \pi_j) : \rho_{AB} = \sum_j \lambda_j \pi_j \right\}. \tag{1}$$

In the above expression, $S(\rho) := -\mathrm{Tr}\,\rho\log\rho$ denotes the von Neumann entropy of the state obtained by partial trace over B and the infimum is computed over all possible decompositions of ρ as convexly linear combinations, that is $\lambda_j > 0$, $\Sigma\lambda_j = 1$, of one-dimensional projections π_j of $A+B$. In the following we call such decompositions *extremal convex decompositions of* ρ to be distinguished from generic convex decompositions into mixed states.

When $\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$, the entanglement of formation gives the asymptotic ratio between the number of singlet states necessary to construct $N \gg 1$ copies of ρ_{AB}.[3] In the following, we will compare the entanglement of formation with a particular case of a more general quantity, the ''entanglement with respect to a subalgebra'' or ''entanglement,'' for short. This latter concept is related to the so-called ''entropy of a subalgebra'' $\mathcal{A}$ contained in a reference algebra $\mathcal{M}$, relative to a state ρ on $\mathcal{M}$,[4]

$$H_\rho(\mathcal{A}) := S(\rho\restriction\mathcal{A}) - \inf\left\{ \sum_j \lambda_j S(\rho_j\restriction\mathcal{A}) : \rho = \sum_j \lambda_j \rho_j \right\}. \tag{2}$$

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In the above expression, $S(\rho_j\restriction\mathcal{A})$ is the von Neumann entropy of the state ρ_j restricted to the subalgebra $\mathcal{A}$ and the infimum is calculated over all convexly linear decompositions of ρ into other states on $\mathcal{M}$. It plays a key role in extending the classical dynamical entropy of Kolmogorov to quantum systems.[5–7] The entanglement of formation (1) can be considered a special case of (3), as explained in Remark 2.1.ii below.

We shall call ''optimal'' those decompositions achieving the extremum in (1) and (2). Calculating either $E(\rho_{AB})$ or $H_\rho(\mathcal{A})$ is particularly complicated. The problem has been completely solved for the entanglement of formation if $\mathcal{H}_A=\mathcal{H}_B=\mathbf{C}^2$,[8] and for the entropy of a subalgebra if $\mathcal{M}=M_2(\mathbf{C})$.[17,9,10] So far, all other available results concern states ρ_{AB} and ρ that are highly symmetric, isotropic in Ref. 11, respectively, permutation-invariant in Ref. 13.

In this paper we will discuss the previously mentioned results by comparing the two notions of entanglement sketched above. We show, that some of them are one-to-one related. To do so, we shall focus on the structure of optimal decompositions in relation to the symmetries existing in the problem and show possible ways of breaking them. These symmetries form a group G and leave invariant both the state ρ and, as a set, the subalgebra $\mathcal{A}$. Given extremal optimal decompositions, the G-orbits of each of their pure states consist of optimal decomposers, too. We will study the dependence of either entanglements upon the number of different orbits.[12]

II. ENTANGLEMENT

In the following, we shall consider quantum systems described by algebras of operators, $\mathcal{M}$, acting on finite or infinite dimensional Hilbert spaces $\mathcal{H}$, with states, $\mathcal{M}\ni X\mapsto\mathrm{Tr}(\rho X)$, represented by density matrices which we shall denote by greek letters.

Definition 2.1: Given a finite dimensional subalgebra $\mathcal{A}\subseteq\mathcal{M}$, we define the entanglement of the state ρ with respect to $\mathcal{A}$ by

$$E(\rho;\mathcal{M},\mathcal{A}):=\inf\left\{\sum_j \lambda_j S(\rho_j\restriction\mathcal{A}) : \rho=\sum_j \lambda_j\rho_j\right\}, \tag{3}$$

where $\rho=\Sigma_j\lambda_j\rho_j$ runs through all convexly linear decompositions of ρ with states of $\mathcal{M}$, and $S(\rho_j\restriction\mathcal{A})$ is the von Neumann entropy of the state ρ_j restricted to the subalgebra $\mathcal{A}$.

Remarks 2.1:

(i) The entanglement (3) is a convex functional over the states,

$$E\left(\sum_j \mu_j\rho_j;\mathcal{M},\mathcal{A}\right)\leqslant\sum_j \mu_j E(\rho_j;\mathcal{M},\mathcal{A}),\quad \sum_j \mu_j=1,\quad \mu_j\geqslant 0. \tag{4}$$

This follows by choosing optimal decompositions for the ρ_j's, which together provide a decomposition, not necessarily optimal, for $\Sigma_j\mu_j\rho_j$.

(ii) The entanglement of formation in equation (1) can be obtained from equation (3) as follows: set $\mathcal{M}=\mathcal{A}\otimes\mathcal{B}$, where $\mathcal{A}$ and $\mathcal{B}$ are the algebras of observables of the systems $\mathcal{A}$ and $\mathcal{B}$. With $\rho=\rho_{AB}$ it turns out that $\rho_{AB}\mathcal{A}=\mathrm{Tr}_B\,\rho_{AB}$.

(iii) The entanglement (3) is related with the entropy of a subalgebra (2) by

$$E(\rho_{AB})=S(\rho_{AB}\restriction\mathcal{A}\otimes\mathbf{1}_B)-H_{\rho_{AB}}(\mathcal{A}\otimes\mathbf{1}_B). \tag{5}$$

Indeed, as we shall see below in Proposition 2.1, the infimum is achieved at decompositions using pure states of $\mathcal{M}$ only, and it enjoys some further remarkable properties.

The quantity in (5) and some techniques[13,14] that were developed for computing (2), have recently been used to attack the question whether the entanglement of formation is additive.[15] Among them, a useful result is contained in the following proposition. The idea is in Ref. 13 and, slightly extended, in Ref. 19. We include a proof for the benefit of the reader.

Proposition 2.1: If the algebra $\mathcal{M}$ is finite dimensional, then

(1) the entanglement $E(\rho;\mathcal{M},\mathcal{A})$ is achieved at certain extremal convex decompositions $\rho=\Sigma_j\lambda_j\pi_j$, $\lambda_j>0$ which saturate (3). Such decompositions are called *optimal*. Every pure state, π, which appears in at least one optimal decomposition of ρ is called *ρ-optimal* or an *optimal decomposer* of ρ.
(2) For every ρ there is an optimal decomposition with a length not exceeding the linear dimension of $\mathcal{M}$.
(3) The functional $E(\,.\,;\mathcal{M},\mathcal{A})$ is convexly linear on the convex hull $\mathcal{R}(\rho)$ of all ρ-optimal pure states: Let $\omega=\Sigma_i\alpha_i\pi_i$, $\alpha_i>0$, $\Sigma_i\alpha_i=1$ be any extremal convex decomposition where the π_j are some optimal decomposers of ρ. Then,

$$E(\omega;\mathcal{M},\mathcal{A})=\sum_i\ \alpha_i S(\pi_i\restriction\mathcal{A}). \tag{6}$$

Proof: Any mixed state ρ can be decomposed and, since the von Neumann entropy is concave on convex combinations, mixed states cannot improve (3) with respect to pure states. If $\mathcal{M}$ is d dimensional, compactness of the state space, extremality and compactness of the set of pure states ensure by a theorem of Caratheodory that we need not less than d and not more than d^2 decomposers.[10,16] Because of convexity (4), the functional $E(\,.\,;\mathcal{M},\mathcal{A})$ is the supremum over affine functionals. Thus, for every ρ there are functionals ℓ such that $E(\rho;\mathcal{M},\mathcal{A})=\ell(\rho)$, while, on generic states σ, $E(\sigma;\mathcal{M},\mathcal{A})\geqslant\ell(\sigma)$. Given an optimal decomposition $\rho=\Sigma_j\lambda_j\pi_j$ it follows

$$E(\rho;\mathcal{M},\mathcal{A})=\sum_j\ \lambda_j E(\pi_j;\mathcal{M},\mathcal{A})\geqslant\sum_j\ \lambda_j\ell(\pi_j)=\ell(\rho)=E(\rho;\mathcal{M},\mathcal{A}). \tag{7}$$

Since equality must hold in (7) and because $\lambda_j>0$, while $E(\pi_j;\mathcal{M},\mathcal{A})\geqslant\ell(\rho)$ by assumption, we conclude $E(\pi_j;\mathcal{M},\mathcal{A})=\ell(\pi_j)$ for all j. With $\omega\in\mathcal{R}(\rho)$, let us now fix this affine functional ℓ and consider the extremal decomposition $\omega=\Sigma\alpha_k\pi_k'$ such that all the π_i' are optimal decomposers of ρ. By convexity and the preceding argument we deduce

$$E(\omega;\mathcal{M},\mathcal{A})\leqslant\sum_k\ \alpha_k E(\pi_k';\mathcal{M},\mathcal{A})=\sum_k\ \alpha_k\ell(\pi_k')=\ell(\omega). \tag{8}$$

However, $\ell(\omega)\leqslant E(\omega;\mathcal{M},\mathcal{A})$ by our choice of ℓ, and equality holds in (8). Thus, $E(\cdot\,;\mathcal{M},\mathcal{A})$ is convexly linear on $\mathcal{R}(\rho)$. ■

Definition 2.2: We shall call the convex hull $\mathcal{R}(\rho)$ of the optimal decomposers of ρ a *leaf* with respect to the entanglement $E(\rho;\mathcal{M},\mathcal{A})$. Then, the state space appears as covered by leaves, and the entanglement itself is convexly linear above every leaf. That effect is referred to as the *roof property* of $E(\,\cdot\,;\mathcal{M},\mathcal{A})$,[10] i.e., $E(\,\cdot\,;\mathcal{M},\mathcal{A})$ is a convex roof.

Definition 2.3: Given ρ on $\mathcal{M}$, we shall call a group G a symmetry group with respect to $E(\rho;\mathcal{M},\mathcal{A})$, if for all $g\in G$ there exists a linear map $\gamma_g:\mathcal{M}\mapsto\mathcal{M}$ such that the state and the subalgebra $\mathcal{A}$ (as a set) are left invariant by γ_g, namely, $\gamma_g^*[\rho]=\rho$, where $\gamma_g^*[\rho](m)=\mathrm{Tr}(\rho\,\gamma_g(m))$.

Proposition 2.2: If G is a symmetry group with respect to $E(\rho;\mathcal{M},\mathcal{A})$, the leaf $\mathcal{R}(\rho)$ is G-invariant as a set. In particular, the action of G permutes the optimal decomposers of ρ.

Proof: Let $\rho=\Sigma_{j\in J}\lambda_j\rho_j$ be an optimal decomposition with respect to $E(\rho;\mathcal{M},\mathcal{A})$. Then, since $\gamma_g^*[\rho]=\rho$ and $\gamma(\mathcal{A})=\mathcal{A}$ for $g\in G$, the decomposition $\rho=\Sigma_{j\in J}\lambda_j\gamma_g^*(\rho_j)$ is also optimal. Therefore, its leaf $\mathcal{R}(\rho)$ must contain both the ρ_j's and the $\gamma_g^*(\rho_j)$'s. ■

Based on the previous two propositions, the entropy $H_\rho(\mathcal{A})$ has explicitly been computed in the following cases:

Case 1: (Refs. 17, 9, 10) Let $\mathcal{M}$ be the full 2×2 matrix algebra $M_2(\mathbf{C})$, $\mathcal{A}$ the subalgebra of all 2×2 matrices diagonal with respect to a given basis $|1\rangle$, $|2\rangle$, and $\rho=\left(\begin{smallmatrix}a & b\\ b^* & 1-a\end{smallmatrix}\right)$, $0\leqslant a\leqslant1$, $|b|^2\leqslant a(1-a)$, any density matrix.

Case 2: (Ref. 13) Let $\mathcal{M}=M_3(\mathbf{C})$, $\mathcal{A}$ the subalgebra of all 3×3 diagonal matrices with respect to the basis $|1\rangle$, $|2\rangle$, $|3\rangle$ and

$$\rho(x)=\frac{1}{3}\begin{pmatrix} 1 & x & x \\ x & 1 & x \\ x & x & 1 \end{pmatrix}, \quad -1/2\leqslant x\leqslant 1, \tag{9}$$

any density matrix invariant under the group of permutations of {1,2,3}.

For future comparison with the entanglement of formation of isotropic states of d-dimensional bipartite systems studied in Ref. 11, we fix an orthonormal basis $|j\rangle\in\mathbf{C}^d$ and consider the group G of permutations of $\{1,2,\ldots,d\}$. It turns out that any G-invariant density matrix $\rho(x)$ over $\mathcal{M}=M_d(\mathbf{C})$ can be written as

$$\rho_F=\frac{1-F}{d-1}(\mathbf{1}-|\psi\rangle\langle\psi|)+F|\psi\rangle\langle\psi|, \tag{10}$$

where $|\psi\rangle=(1/\sqrt{d})\,\Sigma_{j=1}^{d}|j\rangle$ and F is the fidelity parameter

$$0\leqslant F:=\langle\psi|\rho(x)|\psi\rangle=\frac{(d-1)x+1}{d-1}\leqslant 1. \tag{11}$$

Setting $s(t):=-t\log t$, we have

Case 1: For all ρ, the optimal decompositions are

$$\rho=\lambda|w_1\rangle\langle w_1|+(1-\lambda)|w_2\rangle\langle w_2|, \tag{12}$$

$$|w_1\rangle=\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad |w_2\rangle=\begin{pmatrix} z_2^* \\ z_1^* \end{pmatrix}, \quad b=z_1z_2^*, \tag{13}$$

$$|z_1|^2=(1+\sqrt{1-4|b|^2})/2=1-|z_2|^2, \quad \lambda=\frac{1}{2}\left(1+\frac{2a-1}{\sqrt{1-4|b|^2}}\right). \tag{14}$$

The corresponding entanglement is $E(\rho;M_2(\mathbf{C}),\mathcal{A})=s(|z_1|^2)+s(|z_2|^2)$.

If $\rho=\rho_F$ is permutation-invariant, that is, if $a=1/2$, $b=x/2$ $F=(1+x)/2$, the entanglement reads

$$E(\rho_F;M_2(\mathbf{C}),\mathcal{A})=s\left(\frac{1+2\sqrt{F(1-F)}}{2}\right)+s\left(\frac{1-2\sqrt{F(1-F)}}{2}\right). \tag{15}$$

Case 2: Given the group G of permutations of {1,2,3}, let V, V^2 implement unitarily the subgroup G_0 of cyclic permutations. Then, any G-invariant state ρ_F can be written

$$\rho_F=\tfrac{1}{3}|w\rangle\langle w|+\tfrac{1}{3}V|w\rangle\langle w|V^{-1}+\tfrac{1}{3}V^2|w\rangle\langle w|V^{-2}, \tag{16}$$

where

$$|w\rangle=\frac{1}{3}\begin{pmatrix} a+2b\cos\theta \\ a-2b\cos(\theta-\pi/3) \\ a-2b\cos(\theta+\pi/3) \end{pmatrix}, \quad a=\sqrt{3F}, \quad b=\sqrt{\frac{3}{2}(1-F)}. \tag{17}$$

The structure of optimal decompositions depends on the convexity of

$$\mathcal{S}(F) := \min_{\theta \in [0,2\pi]^3} \sum_{j=1}^{3} s(|w_j(F;\theta)|^2). \tag{18}$$

For $F \geqslant F^* := (2x^*+1)/3$, $x^* = -0.415\,023\,4$, the minimum is achieved at a single extremal G_0-orbit generated by the vectors

$$|w\rangle = \frac{1}{3}\begin{pmatrix} a+2b \\ a-b \\ a-b \end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix} \sqrt{F}+\sqrt{2(1-F)} \\ \sqrt{F}-\sqrt{(1-F)/2} \\ \sqrt{F}-\sqrt{(1-F)/2} \end{pmatrix}. \tag{19}$$

For each $0<F<F^*$, there are two different orbit-generating vectors, $|w_\pm(F)\rangle$, whose G_0-orbits provide different optimal decomposers for (18), and which form together one orbit of the full permutation group G. They are

$$|w_\pm(F)\rangle = \frac{1}{3}\begin{pmatrix} a+2b\cos\alpha_F \\ a-2b\cos(\pi/3 \mp \alpha_F) \\ a-2b\cos(\pi/3 \pm \alpha_F) \end{pmatrix}, \tag{20}$$

where the angle α_F varies with $0<F<F^*$.

Finally, for $F=0$, $\alpha_F = -\pi/6$, the minimum is achieved again at a single G-orbit containing the vector, $|w_0\rangle = (1/\sqrt{2})\,(1,0,-1)$. As the 6 vectors coincide pairwise up to a sign, the states form a single optimal decomposition of length 3.

In Ref. 13, it is shown that the above vectors give optimal decompositions as long as the function $\mathcal{S}(F)$ is convex. Numerically, this is the case for all $F \leqslant 8/9$. The corresponding entanglement is

$$E(\rho_F; M_3(\mathbf{C}), \mathcal{A}) = s\left(\frac{2-F+2\sqrt{2F(1-F)}}{3}\right) + 2\,s\left(\frac{1+F-2\sqrt{2F(1-F)}}{6}\right) \tag{21}$$

for fidelities $F^* \leqslant F \leqslant 8/9$. For $F=0$ the entanglement equals $\log 2$. We have only numerical results within the interval $0<F<F^*$,[14] reflecting that the exact dependence of the angle α_F in (20) as a function of F is unknown.

Remark 2.2: Permutation-invariant states as in (10) can be written as averages over the unitaries U_π implementing the permutation group G,

$$\rho_F = \frac{1}{d!}\sum_\pi U_\pi^{-1}|\phi\rangle\langle\phi|U_\pi, \tag{22}$$

if and only if $|\langle\psi|\phi\rangle|^2 = F$, where $|\psi\rangle$ is the vector in (11). Necessity comes from the fact that $U_\pi|\psi\rangle = |\psi\rangle$. Sufficiency: The identity $\mathbf{1}$ and $|\psi\rangle\langle\psi|$ form a basis for all possible contributions to the averages (22).

In view of the structure of the optimal decomposers discussed above, we introduce a notion of regularity with respect to a subgroup of a symmetry group, as follows:

Definition 2.4: Given a symmetry group G with respect to $E(\rho;\mathcal{M},\mathcal{A})$, we shall call a leaf $\mathcal{R}(\rho)$ regular of order n with respect to a subgroup $H \subset G$, if there exists n pure states $\overline{\rho_j} \in \mathcal{R}(\rho)$ such that $\gamma_h^*[\overline{\rho_j}] = \overline{\rho_j}$ for all $h \in H$, whereas the convex span of the orbits $\{\gamma_g^*[\overline{\rho_j}]\}_{g\in G}$ is the whole of $\mathcal{R}(\rho)$.

We illustrate the previous definitions with some examples.

Example 2.1: Let $\mathcal{M}$ be a full $d\times d$ matrix algebra on $\mathbf{C}^d$ and $\mathcal{A}\subset\mathcal{M}$ diagonal with respect to a chosen orthonormal basis $\{|j\rangle\}_{j=1}^d$ in $\mathbf{C}^d$. Let ρ be a symmetric density matrix, $\langle j|\rho|k\rangle = \langle k|\rho|j\rangle$. Then, with respect to the chosen representation, the transposition $\mathcal{T}$ respects both the state and the subalgebra $\mathcal{A}$. Also, $\mathcal{R}(\rho)$ is regular with respect to $G=H=\{\mathrm{id},\mathcal{T}\}$, the order of

regularity depending on the state ρ. In fact, let $\pi=|\psi\rangle\langle\psi|\in\mathcal{R}(\rho)$, then, because of Proposition 2.2, $\mathcal{T}(\pi)=\pi'=|\psi'\rangle\langle\psi'|\in\mathcal{R}(\rho)$, too. If $\pi\neq\pi'$, we may consider the state $\omega=\pi/2+\pi'/2$. which, by Proposition 2.1, is already optimally decomposed. Also,

$$E(\omega;\mathcal{M},\mathcal{A})=S(\pi\restriction\mathcal{A})=S(\omega\restriction\mathcal{A}). \tag{23}$$

Instead, the decomposition

$$\omega=\frac{1+\mathrm{Re}(\langle\psi|\psi'\rangle)}{2}\pi_+ + \frac{1-\mathrm{Re}(\langle\psi|\psi'\rangle)}{2}\pi_-, \tag{24}$$

where

$$\pi_\pm=\frac{|\psi\pm\psi'\rangle\langle\psi\pm\psi'|}{2(1\pm\mathrm{Re}(\langle\psi|\psi'\rangle)} \tag{25}$$

need not be optimal. However, the concavity of the von Neumann entropy yields

$$E(\omega;\mathcal{M},\mathcal{A})\leqslant\frac{1+\mathrm{Re}(\langle\psi|\psi'\rangle)}{2}S(\pi_+\restriction\mathcal{A})+\frac{1-\mathrm{Re}(\langle\psi|\psi'\rangle)}{2}S(\pi_-\restriction\mathcal{A})\leqslant(S(\omega\restriction\mathcal{A}). \tag{26}$$

It thus follows from (23) that $\pi\restriction\mathcal{A}=\pi_\pm\restriction\mathcal{A}$, whence the components $\psi(i)$, $\psi'(i)$ of ψ and ψ' must coincide apart from an overall phase. Thus, $\pi=\pi'$ and the $\mathcal{T}$-symmetry cannot be broken.

Example 2.2: Let $\mathcal{M}=\mathcal{A}\otimes\mathcal{B}$, with $\mathcal{A}$ and $\mathcal{B}$ isomorphic and $\sigma:\mathcal{A}\mapsto\mathcal{B}$ the algebraic exchange of the two of them. If ρ is a state on $\mathcal{M}$ such that $\rho\circ(\sigma^{-1}\otimes\sigma)=\rho$, in general, $\sigma^{-1}\otimes\sigma$ does not belong to any subgroup of regularity of ρ; indeed, if $\mathcal{A}$ (and thus $\mathcal{B}$) is a d-dimensional matrix algebra and $\{|\ell\rangle\}$ is an orthonormal basis in the corresponding Hilbert space $\mathcal{H}_A$ (and thus also in $\mathcal{H}_B$), the density matrix

$$\rho_{AB}:=\tfrac{1}{2}|1\rangle\langle1|\otimes|2\rangle\langle2|+\tfrac{1}{2}|2\rangle\langle2|\otimes|1\rangle\langle1|, \tag{27}$$

is such that $\mathrm{Tr}(\rho(\sigma^{-1}\otimes\sigma)(X\otimes Y))=\mathrm{Tr}(\rho(X\otimes Y))$. Also, ρ_{AB} is already optimally decomposed, $E(\rho_{AB};\mathcal{A},\mathcal{M})=0$ is achieved with the decomposers $|1\rangle\langle1|\otimes|2\rangle\langle2|$ and $|2\rangle\langle2|\otimes|1\rangle\langle1|$, which, however, are not invariant under $\sigma^{-1}\otimes\sigma$.

Example 2.3: Let $\mathcal{M}=\mathcal{A}\otimes\mathcal{B}$, with $\mathcal{A}$ and $\mathcal{B}$ both $d\times d$ full matrix algebras. We fix the same orthonormal basis $\{|\ell\rangle\}$ in both Hilbert spaces $\mathcal{H}_{A,B}$ and consider the one-parameter group U of unitaries

$$U_t:=\sum_{j,k}\mathrm{e}^{it(h_j-h_k)}|j\rangle\langle j|\otimes|k\rangle\langle k|. \tag{28}$$

The density matrix $\rho_{AB}:=\Sigma_{j,k}R_{jk}|j\rangle\langle k|\otimes|j\rangle\langle k|$, , $R=[R_{jk}]\geqslant0$, $\mathrm{Tr}\,R=1$, is U-invariant; moreover, $\sqrt{\rho_{AB}}=\Sigma_{j,k}(\sqrt{R})_{jk}|j\rangle\langle k|\otimes|j\rangle\langle k|$, so that the operators $\sqrt{\rho_{AB}}M\sqrt{\rho_{AB}}$, $M\in\mathcal{M}$, have the same matrix structure as ρ_{AB}. Choosing positive $M_j\geqslant0$, $j\in J$, such that $\Sigma_{j\in J}M_j=1$, ρ_{AB} decomposes into

$$\rho_{AB}=\sum_{j\in J}(\mathrm{Tr}(\rho_{AB}M_j))\frac{\sqrt{\rho_{AB}}M_j\sqrt{\rho_{AB}}}{\mathrm{Tr}(\rho_{AB}M_j)}. \tag{29}$$

Since it is also true that every mixed state ρ on $\mathcal{M}$ can be written as in (29) by means of a suitable positive M_j, (29) indeed exhausts all possible decompositions of ρ_{AB}. Thus, the decomposers π_j of ρ_{AB} which are optimal with respect to $E(\rho_{AB};\mathcal{M},\mathcal{A})$, have the same structure of ρ_{AB} and are

then U-invariant. Hence, the group U is a group of symmetries of ρ_{AB} with respect to entanglement and the leaf $\mathcal{R}(\rho_{AB})$ is regular with respect to $H \equiv U$, its order depending on which further symmetries are enjoyed by ρ_{AB}.

Example 2.4: Let $\mathcal{M}=M_2(\mathbf{C}),\mathcal{A}$ as in Case 1, and ρ_F a permutation-invariant state. The leaf $\mathcal{R}(\rho_F)$ is the orbit of the group G of permutations of $\{1,2\}$. This follows from the form of the optimal vectors (12) in such a case: $|w_1\rangle=\binom{z_1}{z_2}$, $|w_2\rangle=\binom{z_2}{z_1}$, with $z_{1,2}=\sqrt{1/2(1\pm 2\sqrt{F(1-F)})}$. It is regular of order 1 with respect to rotations with elements from $\mathcal{A}$.

Example 2.5: Let $\mathcal{M}=M_3(\mathbf{C})$ and ρ_F a permutation-invariant state. Then, for $F^* \leqslant F$ and F belonging to the convexity region of $\mathcal{S}(F)$ in (18), the structure of the optimal vectors (19) ensures that the leaf $\mathcal{R}(\rho_F)$ is regular of order 1 for the subgroup H of permutations $\{2,3\} \mapsto \{3,2\}$. However, at the point $F=F^*$ such a H-invariant vector bifurcates into the two optimal ones (20). Thus regularity with respect to the subgroup H is broken and remains broken for $0<F<F^*$. At $F=0$ optimal vector states of different G_0 orbits degenerate pairwise into a single one, and one of them is H-invariant, while the corresponding vector changes its sign.

In the last two examples, for all F when $d=2$, and for F greater than the bifurcation values F^* in the convexity region of $\mathcal{S}(F)$ in (18), when $d=3$, the leaf $\mathcal{R}(\rho_F)$ of a permutation-invariant ρ_F is generated by the orbit under the subgroup G_0 of cyclic permutations $V^j|w\rangle$, $j=0,1,2$. The vector $|w\rangle$ is invariant under a unique transposition out of G. This structure is indeed more general as will be shown in the next two propositions.

Proposition 2.3: Let $\mathcal{A}\subset\mathcal{M}=M_d(\mathbf{C})$ be chosen as in Example 2.1 and the density matrix ρ_F be invariant with respect to the permutation group G. If the leaf $\mathcal{R}(\rho_F)$ with respect to $\mathcal{A}$ is generated by exactly one G_0-orbit of a normalized vector state $|w\rangle \in \mathbf{C}^d$, with $G_0 \subset G$ the subgroup of cyclic permutations, then the entanglement is

$$E(\rho_F;M_d(\mathbf{C},\mathcal{A}))=s(p_F)+(d-1)s\left(\frac{1-p_F}{d-1}\right), \tag{30}$$

$$p_F := \frac{|\sqrt{F}+\sqrt{(d-1)(1-F)}|^2}{d}. \tag{31}$$

Remarks 2.3:

(i) The assumption of the previous proposition amounts to ask $\mathcal{R}(\rho_F)$ to be regular of order 1 with respect to the subgroup $H\subset G$ of permutations on $\{2,3,\ldots,d\}$. Indeed, the leaf is G-invariant, so that the d states $|\phi_j\rangle=V^j|w\rangle$, $j=0,1,\ldots,d-1$, obtained via cyclic permutations, must be invariant under the remaining $(d-1)!$ permutations This is possible only if $d-1$ of the d components of the optimal vector $|w\rangle$ are equal.

(ii) If $|w\rangle$ has three different components, then the decompositions (22) contain at least $d(d-1)$ different terms.

(iii) In Sec. III we will show that, upon identification of p_F with the quantity $\gamma(F)$ in Ref. 11, the entanglement of formation calculated there is given by (31) and (30) in a range $F^{**} \geqslant F > 1/d$. The upper limit F^{**} is a particular bifurcation point which was discovered in Ref. 11 and that will be reinterpreted accordingly within the framework of this work.

Proof: By hypothesis, $\rho_F=1/d\,\Sigma_{j=0}^{d-1}V^j|w\rangle\langle w|V^{-j}$ is an optimal decomposition with entanglement

$$E(\rho_F;M_d(\mathbf{C}),\mathcal{A})=\sum_{j=1}^{d} s(|\langle j|w\rangle|^2). \tag{32}$$

Also, taking into account Remarks 2.2 and 2.3, and decomposing

$$|w\rangle=\sqrt{F}|\psi\rangle+\varepsilon\sqrt{1-F}|w_1^{\perp}\rangle=\alpha|1\rangle+\beta\sum_{j=2}^{d}|j\rangle,$$

where ε is a pure phase, it follows that $|w_1^{\perp}\rangle=(\sqrt{d}|1\rangle-|\psi\rangle)/\sqrt{d-1}$ and

$$|w\rangle=\frac{1}{\sqrt{d}}\left[(\sqrt{F}+\varepsilon\sqrt{(1-F)(d-1)})|1\rangle+\left(\sqrt{F}-\varepsilon\sqrt{\frac{1-F}{d-1}}\right)\sum_{j=2}^{d}|j\rangle\right].$$

With $\xi:=2\,\mathrm{Re}(\varepsilon)$, the right-hand side of (32) reads

$$\mathcal{S}(\xi)=s(p(\xi))+(d-1)s\left(\frac{1-p(\xi)}{d-1}\right),$$

$$p(\xi)=\frac{F+(1-F)(d-1)+\xi\sqrt{F(1-F)(d-1)}}{d}.$$

It achieves its minimum at the maximum value of p that is for $\varepsilon=1$, from which the result follows. Indeed, as we show below, $|w\rangle$ must be real. If remark 2.3(i) applies we always get a local extremum. Either by direct calculation or relying on Ref. 13 one concludes $\epsilon=1$. ■

We now relax the hypothesis of the previous proposition and allow for more than one G_0-orbit to be optimal for the entanglement of ρ_F with respect to the subalgebra $\mathcal{A}$, that is we allow the leaf $\mathcal{R}(\rho_F)$ to be generated by more than one G_0-orbit.

Proposition 2.4: Let $\mathcal{A}\subset\mathcal{M}=M_d(\mathbf{C})$ be chosen as in Example 2.1. If the density matrix ρ_F is invariant with respect to the permutation group G and its entanglement with respect to $\mathcal{A}$ can be achieved at an optimal decomposition consisting of one G_0-orbit of normalized vector states $|w\rangle\in\mathbf{C}^d$, with $G_0\subset G$ the subgroup of cyclic permutations, then we have three possibilities:

(1) $|w\rangle=1/\sqrt{d}\,\Sigma_{k=1}^{d}|k\rangle$ in which case $F=1$ and $\rho_F=|\psi\rangle\langle\psi|$;
(2) $|w\rangle$ is real with 1 component equal to a_1 and $d-1$ real components all equal to $a_2\neq a_1$;
(3) $|w\rangle$ is real with 2 components $a_1\neq a_3$ and $d-2$ components all equal to a_3 different from both a_1 and a_2.

To prove the result we need a preliminary

Lemma 2.1: The vector $|w\rangle$ whose G_0-orbit is optimal can be chosen real.

Proof: Let v_k, $k=1,2,\ldots,d$, be the components of $|w\rangle$ with respect to the chosen orthonormal basis $\{|k\rangle\}$ and $|\psi\rangle=(1/\sqrt{d})\,\Sigma_{k=1}^{d}|k\rangle$. The assumption is that $\rho_F=1/d\,\Sigma_{j=0}^{d-1}V^j|w\rangle\langle w|V^{-j}$; from normalization it follows that the components of $|w\rangle$ must satisfy

$$\sum_{k=1}^{d}|w_k|^2=1\quad,\quad\left|\sum_{k=1}^{d}w_k\right|^2=1-\sum_{\ell\neq k=1}^{d}w_\ell^*w_j=dF. \tag{33}$$

Further, in order to implement optimality and achieve $E(\rho_F;\mathcal{M},\mathcal{A})$, we minimize

$$\mathcal{S}(w,\lambda,\mu):=-\sum_{k=1}^{d}|w_k|^2\log|w_k|^2+\lambda\sum_{k=1}^{d}|w_k|^2+\mu\sum_{\ell\neq k}w_\ell w_k^*, \tag{34}$$

with Lagrange multipliers λ, μ. Setting $v:=\Sigma_{k=1}^{d}w_k=\sqrt{dF}\,e^{i\theta}$, equating to zero the derivative of (34) with respect to w_j and multiplying by w_j we get

$$-|w_j|^2\log|w_j|^2+(\lambda-1)|w_k|^2+\mu(v^*w_j-|w_j|^2)=0.$$

Therefore, the quantity $v^*w_j\mu$ and thus, after summing over j, also μ, must be real, whence, necessarily $w_j=e^{i\theta}v_j$, with $v_j\in\mathbf{R}$, for all j. The result follows by eliminating the overall phase. ■

Proof: (Proposition 2.4) According to the previous Lemma, we choose $|w\rangle$ real and proceed to minimize

$$\mathcal{S}(w,\lambda,\mu) := -\sum_{k=1}^{d} w_k^2 \log w_k^2 + \lambda \sum_{k=1}^{d} w_k^2 + \mu \sum_{k=1}^{d} w_k. \tag{35}$$

Because of convexity, the function $g(x) := -x \log x^2$ intersects the straight line $f(x) := 2(1-\lambda)x - \mu$ in at most three points on $[-1,1]$. Therefore, the d solutions to

$$-2w_k \log w_k^2 - 2w_k + 2\lambda w_k + \mu = 0,$$

can have at most three different real values, a_i, $i=1,2,3$. We denote by n_i the number of times they appear among the components and consider the functional

$$\mathcal{S}(\vec{a};\vec{n};\lambda,\mu,\nu) := -\sum_{i=1}^{3} n_i a_i^2 \log a_i^2 + \lambda \sum_{i=1}^{3} n_i a_i^2 + \mu \sum_{i=1}^{3} n_i a_i, \tag{36}$$

where we treat the n_i's as continuous variables constrained by $n_1+n_2+n_3=d$. Minimizing (36) yields the following equations:

$$n_i(a_i \log a_i^2 + a_i - \lambda a_i - \mu) = 0, \quad i=1,2,3, \tag{37}$$

$$-a_i^2 \log a_i^2 + \lambda a_i^2 + \mu a_i + \nu, \quad i=1,2,3. \tag{38}$$

It follows that, if $n_i > 0$, $i=1,2,3$, then $\Sigma_{i=1}^{3}(\mu a_i + 2\nu + 2a_i^2) = 0$, $i=1,2,3$, and thus $a=b=c$. This case corresponds to $\rho_{F=1} = |\psi\rangle\langle\psi|$, a pure state, with null entanglement with respect to $\mathcal{A}$. Therefore, if there are three different intersections, the minimum entanglement is reached at the boundary values of n_i, $i=1,2,3$, that is, without loss of generality, at $n_1=n_2=1$ and $n_3=d-2$. If there are two intersections, that is, if, without loss of generality, $n_3=0$ and $a_1 \neq a_2 = a_3$, then, from (37) and (38), we calculate $\mu = -2(a_1+a_2)$, $\mu = a_1 a_2$ and deduce the equality

$$a_1^2 - a_2^2 + a_1 a_2 \log \frac{a_2^2}{a_1^2} = 0 \quad .$$

For fixed a_1, because of their convexity properties, the two functions $f(x) := \log(a_1^2/x^2)$ and $g(x) := (a_1/x) - (x/a_1)$ intersect at $x=a_1$, but, at no other points. Therefore, the entanglement is again minimal at the boundary, that is at, say $n_1=1$ and $n_2=d-1$. ■

Remark 2.4: Lagrange multipliers have been used in Ref. 11 in order to calculate the entanglement of formation of isotropic states of bipartite quantum systems, where it is shown that, when $F > 1/d$, the optimal decomposers have only two different components. We shall relate those results to ours in the following section, where we also discuss the fact, discovered in Ref. 11, stating there is a bifurcation point F^{**} such that the entanglement of formation is linear in F between F^{**} and $F=1$.

Proposition 2.4 shows that when the vector $|w\rangle$ has only two different components, then we reduce to the case discussed in Proposition 2.3. Instead, when $|w\rangle$ has three different components, which is possible in a range of values of F, then we have more than one optimal decomposition. If $d=3$ one gets at least two. Notice that these results are obtained under the hypothesis that G_0-orbits of vectors $|w\rangle$ provide optimal decompositions for the entanglement of ρ_F with respect to the subalgebra $\mathcal{A}$.

This fact is linked to the convexity of the function (18), which, as observed in the discussion of Case 2, fails in a neighborhood of $F=1$: If $F \geqslant F^{**}$ one needs two orbits: the optimal orbit for $F=F^{**}$ and the singlet for $F=1$, just as observed in Ref. 11. Consequently, for $F^{**} < F < 1$ no G_0-orbits can be optimal.

III. ENTANGLEMENT AND ENTANGLEMENT OF FORMATION

In this section we establish a one-to-one correspondence between the results of the previous section, in particular proposition 2.3, and the entanglement of formation of highly symmetric states as examined in Ref. 11. This concerns mainly the region $(1/d)\leqslant F$. From Ref. 11 we learned the existence of the bifurcation point F^{**}. On the other hand, our results in the region $(1/d)<F\leqslant F^{**}$ can be converted into those found by Terhal and Volbrecht. Indeed, the value of the entanglement of formation will be proved to be just (30).

To this end we consider the tensor product $\mathcal{M}:=\mathcal{A}\otimes\mathcal{B}$ of the full $d\times d$ matrix algebra, denoted by $\mathcal{A}$, with a copy, $\mathcal{B}$, of itself. We fix an orthonormal basis $\{|j\rangle\}$ of $\mathbf{C}^d$ and given any density matrix, that is a state on $\mathcal{A}$,

$$\rho_A=\sum_{j,k} R_{jk}|j\rangle\langle k|, \quad R=[R_{jk}]\geqslant 0, \quad \mathrm{Tr}\,R=1, \tag{39}$$

we embed it as $D[\rho_A]$ into the state space of $\mathcal{M}$ according to the following:

Definition 3.1: Let D be the linear map associating matrix units $|j\rangle\langle k|$ of $\mathcal{A}$ with matrix units $\{|j\rangle\langle k|\otimes|j\rangle\langle k|\}$ of $\mathcal{M}$. We shall refer to it as the *doubling map*. It transforms states ρ_A on $\mathcal{A}$ into states on $\mathcal{M}=\mathcal{A}\otimes\mathcal{B}$ of the form

$$\rho_A\mapsto D[\rho_A]:=\sum_{j,k} R_{jk}|j\rangle\langle k|\otimes|j\rangle\langle k|. \tag{40}$$

Remark 3.1: This yields the class of density matrices in Example 2.3, which we shall refer to as diagonal class (with respect to the chosen basis). On the given diagonal class the doubling map can be inverted

$$D^{-1}:\rho_{AB}=\sum_{j,k} R_{j,k}|j\rangle\langle k|\otimes|j\rangle\langle k|\mapsto\rho_A=\sum_{j,k} R_{j,k}|j\rangle\langle k|. \tag{41}$$

The argument developed in Example 2.3 ensures that decompositions of ρ_A can be mapped onto decompositions of $D[\rho_A]$. Vice versa, decompositions of ρ_{AB} provide decompositions for the diagonal class of ρ_A by applying D^{-1}. Moreover, if $\mathcal{A}_0\subset\mathcal{A}$ denotes the subalgebra of diagonal matrices in the given, fixed representation, then $S(\rho\restriction\mathcal{A}_0)=S(D[\rho_A]\restriction\mathcal{A})$. Therefore: *The entanglement is preserved by D*, in the sense that

$$E(\rho_A;\mathcal{A},\mathcal{A}_0)=E(D[\rho_A];\mathcal{A}\otimes\mathcal{B},\mathcal{A}). \tag{42}$$

In Ref. 11 the entanglement of formation has been calculated for the isotropic states

$$\omega_F=\frac{1-F}{d^2-1}(\mathbf{1}_{AB}-|\Psi\rangle\langle\Psi|)+F|\Psi\rangle\langle\Psi|. \tag{43}$$

In the above expression $\mathbf{1}_{AB}$ is the identity for the algebra $\mathcal{A}\otimes\mathcal{B}$ and

$$|\Psi\rangle=\frac{1}{\sqrt{d}}\sum_{j=1} |j\rangle\otimes|j\rangle. \tag{44}$$

Remark 3.2: The isotropic states are invariant under the group $\mathcal{G}$ of all unitaries of the form $U\otimes\tilde{U}$ where $\langle a|U|b\rangle=\langle a|\tilde{U}|b\rangle^*$,

$$U\otimes\tilde{U}\,\omega_F U^{-1}\otimes\tilde{U}^{-1}=\omega_F. \tag{45}$$

As in Remark 2.2, it follows that ω_F can be expressed as the following average with respect to the Haar measure $\mathrm{d}_G U$,

$$\omega_F = \int_{\mathcal{G}} \mathrm{d}_{\mathcal{G}} U \, U \otimes \tilde{U} |\Phi\rangle\langle\Phi| U^{-1} \otimes \tilde{U}^{-1}, \tag{46}$$

if and only if $F = \langle\Psi|\omega_F|\Psi\rangle = |\langle\Psi|\Phi\rangle|^2$.

We compare the isotropic state ω_F with the doubling of ρ_F in (10),

$$\begin{aligned} D[\rho_F] &= \frac{1-F}{d-1}(D[\mathbf{1}_A] - D[|\psi\rangle\langle\psi|]) + FD[|\psi\rangle\langle\psi|] \\ &= \frac{1-F}{d-1}\left(\sum_{j=1}^{d} |j\rangle\langle j| \otimes |j\rangle\langle j| - |\Psi\rangle\langle\Psi|\right) + F|\Psi\rangle\langle\Psi|. \end{aligned} \tag{47}$$

Proposition 3.1: Let $F > 1/d$ and consider the decomposition

$$\omega_F = \frac{1}{d!} \sum_{\pi} U_\pi^{-1} \otimes U_\pi^{-1} |\Phi\rangle\langle\Phi| U_\pi \otimes U_\pi$$

by means of the unitaries U_π that implement the permutation group G. If the latter is optimal for the entanglement of formation $E(\omega_F)$ with $|\Phi\rangle\langle\Phi|$ in the diagonal space, then $E(\omega_F) = E(\rho_F, \mathcal{A}, \mathcal{A}_0)$.

Proof: The $d!$ unitaries U_π form a subgroup $G \otimes G$ of the group of unitaries in Remark 3.2; they implement the permutation of the chosen basis $\{|j\rangle \otimes |j\rangle\}$ of the diagonal space. Then, $\langle\Psi|\omega_F|\Psi\rangle = \langle\Psi|D[\rho_F]|\Psi\rangle = F$ and

$$D[\rho_F] = \frac{1}{d!} \sum_{\pi} U_\pi^{-1} \otimes U_\pi^{-1} |\Phi\rangle\langle\Phi| U_\pi \otimes U_\pi.$$

If $|\Phi\rangle\langle\Phi|$ is optimal for ω_F, it turns out from Proposition 2.2 that the decomposeres $U \otimes \tilde{U} |\Phi\rangle\langle\Phi| U^{-1} \otimes \tilde{U}^{-1}$ are optimal, too. Thus the result follows from Proposition 2.1. ■

Remarks 3.3:

(i) If $F > 1/d$ the isotropic state ω_F is entangled. When $F \leqslant 1/d$ it becomes separable. There exist several proofs of this fact, e.g., Ref. 18.

(ii) In view of Remark 2.3(ii), the previous proposition establishes a link between our results and those of Ref. 11. In Ref. 11 a new symmetry breaking bifurcation point was observed at $F = 8/9$ when $d = 3$. The doubling map makes it correspond to a bifurcation point within case 2 of the previous section at the same value of F. The numerical analysis in Ref. 14 missed it, the needed accuracy being of the order of 10^{-4}. In both cases the leaves $\mathcal{R}(\omega_F)$, respectively, $\mathcal{R}(\rho_F)$, are identical for all F within $F^{**} = 8/9 < F < 1$. This unique leaf is generated by the optimal decompositions of $\omega_{8/9}$ which form one orbit, and by the pure state ω_1 given by (44). The same is true of $\rho_{8/9}$ and ρ_1. The latter orbits are singlets.

(iii) The entanglement of ρ_1 and $\rho_{8/9}$ that generate the leaf discussed in the previous remark do not coincide,[19]

$$E(\rho_1; \mathcal{M}, \mathcal{A}) = \ln 3, \quad E(\rho_{8/9}; \mathcal{M}, \mathcal{A}) = \ln 3 - \tfrac{1}{3} \ln 2. \tag{48}$$

We shall now relate the remark above to another observation which again relates entanglement of different algebras with one another.

From Case 1 in Sec. II, we know that vectors of the form $\binom{x}{y}$ and $\binom{y}{x}$, with $x^2 + y^2 = 1$ generate the leaf of some state ρ_2 on $M_2(\mathbf{C})$. These two-dimensional vectors can be embedded in $\mathbf{C}^3$ as follows:

$$|w_1\rangle=\begin{pmatrix} x \\ y/\sqrt{2} \\ y/\sqrt{2} \end{pmatrix}, \quad |w_2\rangle=\begin{pmatrix} y \\ x/\sqrt{2} \\ x/\sqrt{2} \end{pmatrix}. \tag{49}$$

With them we construct the density matrix in $M_3(\mathbf{C})$ of the form

$$\tilde{\rho}_3=\lambda|w_1\rangle\langle w_1|+(1-\lambda)|w_2\rangle\langle w_2|=\begin{pmatrix} a & b & b \\ b & c & c \\ b & c & c \end{pmatrix}. \tag{50}$$

It is easy to check that powers of $\tilde{\rho}_3$ have the same structure which is thus inherited by $\sqrt{\tilde{\rho}_3}$. It thus follows that

$$\sqrt{\tilde{\rho}_3}|\phi\rangle=\begin{pmatrix} u \\ v \\ v \end{pmatrix}$$

for any $|\phi\rangle$. The discussion of Example 2.3 assures that the optimal decomposers of $\tilde{\rho}_3$ with respect to the entanglement $E(\tilde{\rho};M_3(\mathbf{C}),\mathcal{A}_3)$, with $\mathcal{A}_3$ the maximally Abelian subalgebra in the chosen representation, have again the same form. But then, $\binom{x}{y}$ and $\binom{y}{x}$ being optimal with respect to $E(\rho_2;M_2(\mathbf{C}),\mathcal{A}_2)$, (50) is itself an optimal decomposition of $\tilde{\rho}_3$ with respect to $E(\tilde{\rho}_3;M_3(\mathbf{C}),\mathcal{A}_3)$.

According to the discussion at the beginning of this section, it also follows that the doubling map,

$$|w_1\rangle\mapsto|W_1\rangle=x|1\rangle\otimes|1\rangle+\frac{y}{\sqrt{2}}(|2\rangle\otimes|2\rangle+|3\rangle\otimes|3\rangle), \tag{51}$$

$$|w_2\rangle\mapsto|W_2\rangle=y|1\rangle\otimes|1\rangle+\frac{x}{\sqrt{2}}(|2\rangle\otimes|2\rangle+|3\rangle\otimes|3\rangle), \tag{52}$$

provides optimal decomposers, too. In particular, for given x,y on the unit circle the pure states $|W_j\rangle\langle W_j|$, $j=1,2$, generate a leaf of the entanglement of formation functional on which it is convexly linear.

Moreover, for $x=1/\sqrt{3}$ and $y=\sqrt{2/3}$, we get $|W_1\rangle=|\Psi\rangle$, with fidelity $F=|\langle\Psi|W_1\rangle|^2=1$, and $|W_2\rangle=|\Phi_{8/9}\rangle$ with fidelity $F=|\langle\Psi|W_2\rangle|^2=8/9$, indicating a reason for the bifurcation value $F=8/9$.

One observes that (51) and (52) become identical for $x=y=1/\sqrt{2}$ so that the doubling map gets the vector,

$$|W_3\rangle=\frac{1}{\sqrt{2}}|1\rangle\otimes|1\rangle+\frac{1}{2}(|2\rangle\otimes|2\rangle+|3\rangle\otimes|3\rangle), \tag{53}$$

which has fidelity

$$F=|\langle\Psi|W_3\rangle|^2=\tfrac{1}{2}+\sqrt{\tfrac{2}{3}}=p+(1-p)\,\tfrac{8}{9}\ , \quad 0<p=3\sqrt{6}-\tfrac{7}{2}<1. \tag{54}$$

Let us now consider the state

$$\rho_F=p|\Psi\rangle\langle\Psi|+(1-p)|\Phi_{8/9}\rangle\langle\Phi_{8/9}|. \tag{55}$$

By using (48), it can be shown that its entanglement $E(\rho_F)$ is larger than $pE(\rho(1))+(1-p)E(\rho(8/9))$ for $0<p<1$. This implies that convexity of $\mathcal{S}(F)$ in (32) is lost for $F>F^{**}$ in accordance with the discussion above.

We finally note that one can extend (49) to all dimensions larger than two. Indeed, let z_1,z_2 denote the components of a unit vector in two dimensions. By similar arguments one proves that the leaves of case 1 of the previous section are mapped onto certain leaves belonging to the entanglement of formation in $d+1$ dimensions by the embeddings

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to z_1|00\rangle + (z_2/\sqrt{d}) \sum_{j=2}^{d+1} |jj\rangle. \tag{56}$$

In particular, the embeddings of $\{z_1, z_2\}$ and $\{z_2^*, z_1^*\}$ form an optimal pair with respect to the entanglement of formation. One further observes in the special case $z_1 = 1/\sqrt{d+1}$ the embeddings (56) are the totally symmetric vector Ψ in $d+1$ dimensions and

$$\sqrt{\frac{d}{d+1}}|11\rangle + \sqrt{\frac{1}{d(d+1)}} \sum_{j=2}^{d+1} |jj\rangle. \tag{57}$$

Its fidelity reads $F = 4d/(1+d)^2$, and we see as above

$$F^{**}_{d+1} = 4d(d+1)^{-2}, \tag{58}$$

i.e., the bifurcation value given in Ref. 11 for $d+1 > 2$.

IV. CONCLUSIONS

We have studied in several examples the entanglement defined by a maximal commuting subalgebra of a full matrix algebra, and its relation to the entanglement of formation. Apart from its actual numerical value, what is interesting is the structure of both entanglement functionals upon the space of states, and their separation into different leaves. To some extent these leaves can be found by applying group theoretical considerations. They show a rich structure with varying stability under the groups under consideration. Since the same group appears in different algebraic contexts, it can be shown that the decompositions of states on different algebras can be related. This helps to control the optimal decompositions and to understand their variety. This new technique is shown at work in several examples: The doubling map relates two quite different lines of research which had been considered almost independently up to now. In particular we have a further proof of the entanglement of formation results for isotropic states of Terhal and Volbrecht in the region $(1/n) \leqslant F \leqslant F^{**}$.[11] Another embedding map verifies their bifurcation point F^{**} close to $F = 1$ as a footprint of a symmetry-breaking in two dimensions. It belongs to a class of maps which change entanglement but not the leaves. The leaves are respected because the entanglements differ just by a convexly linear function.

We have provided some examples of embedding procedures which allow to connect various entanglement problems not only with each other, but also with problems involving other quantities based on convex or concave roofs, for example general entanglement monotones or Holevo (1-shot) capacities.

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Lower bound for the superheating field in the weak-κ limit: The general case

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(Received 30 July 2002; accepted 23 February 2003)

We have constructed asymptotic matched solutions for the one dimensionnal Ginzburg–Landau system when κ is small [Math. Model. Num. Anal. **36**, 971–993 (2002)]. We have deduced an expansion in powers of $\kappa^{1/2}$ at all orders for the superheating field. In this paper, using these constructions, we propose to show that the superheating field admits for lower bound the expansion of the formal superheating field truncated at order n, for all $n \in \mathbb{N}$. We generalize the proof given in Eur. J. Appl. Math. **13**, 519–547 (2002), where this result is obtained for $n=1$. Then, we construct solutions of the Ginzburg–Landau system when the exterior magnetic field is near to the superheating field, and we give a localization of these solutions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1570944]

I. INTRODUCTION

The states of a superconducting material in an exterior magnetic field are described by the Ginzburg–Landau theory which introduces a functional ε depending in particular on a complex wave function and on the magnetic potential A. When the sample is a film and the exterior magnetic field is parallel to the surface, the Ginzburg–Landau model reduces to a one-dimensional problem where the wave function is real (and denoted by f) and where the functional is the following:

$$\varepsilon_d(f,A;h)=\int_{-d/2}^{d/2}\left[\frac{1}{2}(1-f(x)^2)^2-\frac{1}{2}+\kappa^{-2}f'(x)^2+f(x)^2A(x)^2+(A'(x)-h)^2\right]\mathrm{d}x, \quad (1.1)$$

with $(f,A)\in(H^1(]-d/2,d/2[))^2$. Here, d is proportional to the thickness of the film, h is proportional to the exterior magnetic field and κ is the Ginzburg–Landau parameter. We restrict ourselves to the study of symmetric solutions (f even and A odd) and consider a new normalization of the functional where ε_d is replaced by $(\varepsilon_d-(h^2-\frac{1}{2})d)$. We then restrict the problem to the interval $]-d/2,0]$, and translate it to $]0,d/2[$. We get formally, by taking the limit $d=+\infty$, the second functional

$$\varepsilon_\infty(f,A)=\int_0^{+\infty}\left[\frac{1}{2}(1-f(x)^2)^2+\kappa^{-2}f'(x)^2+f(x)^2A(x)^2+A'(x)^2\right]\mathrm{d}x+2\,h\,A(0), \quad (1.2)$$

defined for $(f,A)\in E_\infty=\{(f,A);\ (1-f)\in H^1(]0,+\infty[),A\in H^1(]0,+\infty[)\}$. If we introduce the new variable $H=A'$, the corresponding Ginzburg–Landau equations expressing the necessary conditions for minima are then

$$(\mathrm{GL})_\infty \quad \begin{cases} -\kappa^{-2}f''-f+f^3+fA^2=0 & \text{on }]0,+\infty[,\\ -A''+Af^2=0 & \text{on } 0,+\infty[,\\ H=A' & \text{on } 0,+\infty[\end{cases} \quad (1.3)$$

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with the boundary conditions

$$f'(0)=0, \quad H(0)=h. \tag{1.4}$$

The problem $(\mathrm{GL})_\infty$ is called the half-space model and was studied in Refs. 12 and 13 where computational solutions are given.

We consider the set $\mathcal{H}_\infty \subset \mathbb{R}^+$ of the h's such that there exist solutions of the (GL) system with $f>0$. We know that $\mathcal{H}_\infty$ is a bounded interval $[0,h^+)$ (see Ref. 3, Proposition 2.1) and we then introduce the following definition.

Definition 1.1: The superheating field $h^{sh}(\kappa)$ is defined as the supremum of the interval $\mathcal{H}_\infty$.

In Ref. 7 (see also Ref. 5), extending a work due to Dorsey, Dolgert, and Di Bartolo,[10] we have constructed a formal solution of the Ginzburg–Landau system, defined as a pair composed by a formal outer solution and a formal inner solution, matched in the Kaplun's sense[14] (see also Refs. 11 and 16). Then, as consequence of this construction, we have proved the existence of a formal expansion in powers of $\kappa^{1/2}$ at all orders for the superheating field denoted by $h^{sh,f}(\kappa) := \kappa^{-1/2}\Sigma_{i=0}^{+\infty} h_i \kappa^i$. We have shown how to compute the coefficients of this expansion in Proposition 4.6. in Ref. 7. Let us recall that the first coefficient is given by $h_0 = 2^{-3/4}$ and the second coefficient by $h_1 = 2^{-1/4}\frac{15}{32}$.

In an other hand, in Ref. 6, we have proved that there exist $\kappa_0>0$ and C such that, for all $\kappa \leqslant \kappa_0$, we have the inequality

$$\kappa^{1/2} h^{sh}(\kappa) \geqslant 2^{-3/4}\left(1+\tfrac{15}{32}\sqrt{2}\kappa + C\kappa^2\right). \tag{1.5}$$

In this paper, using the construction of a matched asymptotic solution of the Ginzburg–Landau system obtained in Ref. 7, we propose to establish the following theorem.

Theorem 1.2: *Let $n \in \mathbb{N}$. There exist C and $\kappa_0>0$ such that, for all $\kappa \leqslant \kappa_0$, we have the inequality*

$$\kappa^{1/2} h^{sh}(\kappa) \geqslant \sum_{i=0}^{n} h_i \kappa^i + C\kappa^{n+1}. \tag{1.6}$$

The plan is the following. In Sec. II, we expose the construction of formal solutions of $(\mathrm{GL})_\infty$ obtained by a matching procedure in Ref. 7. We recall the procedure that we have used to get a formal expansion in powers of $\kappa^{1/2}$ for the superheating field. In Sec. III, we construct an asymptotic matched solution for the Ginzburg–Landau system at order n. In Sec. IV, we present the construction of the subsolution (f,A). As in Ref. 6, the wave function f is obtained by modifying some coefficients of order $\mathcal{O}(\kappa)$ in the sense of Ref. 4 in the matched solution and by adding an exponential polynomial to control the sign of the remaining coefficients. This function only depends on two parameters, α and β. The potential A is obtained as the exact solution of the second equation of the Ginzburg–Landau system (1.3). To control the remaining coefficients in the region $[-\ln\kappa,+\infty[$, we make a good choice for the parameter β to get a negative sign for the expression $-\kappa^{-2}f''-f+f^3+A^2f$ for all value of α. Then, the pair (f,A) only depends on α and we denote it by (f_α,A_α). In some region $[0,\kappa^{-\rho}]$, $\rho>0$, we follow Ref. 6. Using a maximum principle, we get a lower bound for A_α by comparison with the formal solution presented in Sec. II. In Sec. V, we show under the condition (1.4) on $A'_\alpha(0)=h$ that (f_α,A_α) is a subsolution of $(\mathrm{GL})_\infty$ for a good choice of α. This implies the existence of a solution of $(\mathrm{GL})_\infty$, and we deduce the proof of Theorem 1.2. In Sec. VI, following the previous method, we construct a supersolution at order n of the (GL) equations. We deduce a localization of solutions of $(\mathrm{GL})_\infty$ for h near to the superheating field.

II. FORMAL SOLUTION OF $(GL)_\infty$

In the following sections, for $i=(i_0,\ldots,i_n)\in\mathbb{N}^{n+1}$, we set

$$|i|_{0,n}=i_0+i_1+\cdots+i_n,\quad |i|_{1,n}=i_1+i_2+\cdots+i_n,\quad |i|_{2,n}=i_1+2i_2+\cdots+ni_n. \tag{2.1}$$

Recall that in Ref. 7, we have constructed a formal solution of $(GL)_\infty$ as a pair composed by a formal outer solution, and a formal inner solution, matched in the Kaplun sense.[14]

An outer formal solution is a triplet of formal series (F^e,A^e,H^e), where

$$F^e(x;\kappa)=\tilde{F}^e(\kappa x;\kappa),\quad A^e(x;\kappa)=\tilde{A}^e(\kappa x;\kappa),\quad H^e(x;\kappa)=\tilde{H}^e(\kappa x;\kappa),$$

with

$$\tilde{F}^e(x';\kappa)=\sum_0^\infty \tilde{f}_i(x')\kappa^i,\quad \tilde{A}^e(x';\kappa)=\sum_0^\infty \tilde{A}_i(x')\kappa^i,\quad \tilde{H}^e(x';\kappa)=\sum_0^\infty \tilde{H}_i(x')\kappa^i,$$

satisfying the (GL) obtained after the scaling $x'=\kappa x$ in (1.3). Let us introduce $C(\kappa)$ the formal series defined by

$$C(\kappa)\sim\sum_{n=0}^{\infty} C_n\kappa^n,\quad C_j\in\mathbb{R}. \tag{2.2}$$

We denote by $\tilde{f}_0^{(m)}$ the derivative at order m of the function $\tilde{f}_0$. We have shown in Ref. 5 (see also Ref. 10) that the outer solution is described in the following way.

Proposition 2.1: All formal outer solutions are equal to

$$\tilde{F}^e(x',\kappa)\sim\tanh\left(\frac{x'+C(\kappa)}{\sqrt{2}}\right),$$

$$\tilde{A}^e(x',\kappa)\sim 0, \tag{2.3}$$

$$\tilde{H}^e(x',\kappa)\sim 0.$$

Furthermore, for all $n\geqslant 1$,

$$\tilde{f}_n=\sum_{m=1}^{n}\sum_{\substack{|i|_{2,n}=n\\ |i|_{1,n}=m}}\frac{m!}{i_1!\ \cdots\ i_n!}\prod_{k=1}^{n}(C_k)^{i_k}\ \tilde{f}_0^{(m)}, \tag{2.4}$$

$$|i|_{2,n}=n,$$

$$|i|_{1,n}=m,$$

where $\tilde{f}_0$ *is defined by*

$$\tilde{f}_0(x')=\tanh\left(\frac{x'+C_0}{\sqrt{2}}\right). \tag{2.5}$$

Let $(A(\kappa),B(\kappa),D(\kappa))$ three formal series in powers of κ. A formal inner solution, with initial data at zero $(A(\kappa),B(\kappa),D(\kappa))$ is a triplet (F^i,Q^i,H^i) such that

$$F^i(.,\kappa)=\sum_0^\infty F_k(.)\,\kappa^k,\quad Q^i(.,\kappa)=\sum_0^\infty Q_k(.)\,\kappa^k,\quad H^i(.,\kappa)=\kappa^{-1/2}\sum_0^\infty H_k(.)\,\kappa^k, \tag{2.6}$$

is a formal solution of the (GL) and satisfies the boundary conditions at zero

$$F^i(0,\kappa)=A(\kappa),\quad Q^i(0,\kappa)=B(\kappa),\quad H^i(0,\kappa)=D(\kappa),\quad (F^i)'(0,\kappa)=0,\quad (Q^i)'(0,\kappa)=\kappa^{1/2}h. \tag{2.7}$$

We set

$$\overline{A_n}=(A_0,\ldots,A_n),\quad \overline{B_n}=(B_0,\ldots,B_n),\quad \text{and } \overline{C_n}=(C_0,\ldots,C_n). \tag{2.8}$$

We have described in Ref. 7 (see Proposition 2.5) all the inner solutions in the following proposition.

Proposition 2.2: For all $n\geqslant 2$, the function F_n defined in (2.6) is equal to a sum of exponential polynomials. More precisely,

$$F_n=F_n^{\mathrm{pol}}+\psi(.)P_n(.,\psi(.)), \tag{2.9}$$

where F_n^{pol} is a polynomial of degree n, $P_n\in\mathbb{R}[X,Y]$ and $\psi(x):=\exp(-2A_0x)$, $A_0\in]0,1[$. Furthermore, for $n\geqslant 2$, $U_n(x):=P_n(x,0)$ is of degree $2n-2$.
For all $n\in\mathbb{N}$, the function Q_n, defined in (2.6) satisfies

$$Q_n=\phi(.)R_n(.,\phi(.)), \tag{2.10}$$

where $R_n\in\mathbb{R}[X,Y]$ and $\phi(x)=\exp(-A_0\ x)$.

Moreover, the polynomial $V_n(x):=R_n(x,0)$ is of degree $2n$.

Remark 2.3: In Ref. 7, we make explicit the dependency of the functions F_n, Q_n and H_n with respect to the constants $\overline{A_n}$, $\overline{B_n}$. In this paper, we have shown in Proposition 2.6 that for $n\geqslant 1$, F_n depends on $2n+1$ parameters $\overline{A_n}$ and $\overline{B_{n-1}}$. More precisely,

$$F_n^{\mathrm{pol}}(.;\overline{A_n};\overline{B_{n-1}})=A_n+\tilde{P}_n(.;\overline{A_{n-1}};\overline{B_{n-1}}),\quad \tilde{P}_n\in C^\infty(\mathbb{R}\times]0,\ 1[\times\mathbb{R}^{2n-1}),$$

and P_n defined in (2.9), depends only on $\overline{A_{n-1}};\overline{B_{n-1}}$. Moreover,

$$Q_n(.;\overline{A_n};\overline{B_n})=\phi(.)(B_n+\tilde{R}_n(.,\phi(.);\overline{A_n},\overline{B_{n-1}}),\quad \tilde{R}_n\in C^\infty(\mathbb{R}^2\times]0,\ 1[\times\mathbb{R}^{2n}).$$

Let us introduce the following definition.

Definition 2.4: Let $n\in\mathbb{N}^*$. The truncated inner solution at order n is defined by $(\Sigma_0^n F_i\kappa^i,\Sigma_0^n Q_i\kappa^i)$ and denoted by $(F^{i,(n)},Q^{i,(n)})$. The truncated outer solution at order n is defined by $(\Sigma_0^n\tilde{f}_i(x')\kappa^i,\Sigma_0^n\tilde{q}_i(x')\kappa^i)$ and denoted by $(\tilde{F}^{e,(n)},\tilde{Q}^{e,(n)})$. We introduce $F^{e,(n)}(x;\kappa)=\tilde{F}^{e,(n)}(\kappa x)$ and $Q^{e,(n)}(x;\kappa)=\tilde{Q}^{e,(n)}(\kappa x)$. We denote by $F^{\mathrm{pol},(n)}$ the polynomial part of $F^{i,(n)}$.

In order to clarify a more formal matching condition proposed by Van Dyke in Ref. 16, we have introduced in Ref. 7 the following definition.

Definition 2.5: Let $n\in\mathbb{N}$, $(F^{i,(n)},Q^{i,(n)})$ and $(F^{e,(n)},Q^{e,(n)})$ the triplets of functions introduced in Definition 2.4. We say that the inner and outer solutions are matched at order n on the interval $I_n(\delta_1,\delta_2,\kappa):=[\delta_1\kappa^{-1/(n+1)},\delta_2\kappa^{-1/(n+1)}]$ if and only if

$$\begin{aligned} F^{i,(n)}(x,\kappa)-F^{e,(n-1)}(x,\kappa)&=\mathcal{O}(\kappa^n),\\ Q^{i,(n)}(x,\kappa)-Q^{e,(n-1)}(\kappa x,\kappa)&=\mathcal{O}(\kappa^n). \end{aligned} \tag{2.11}$$

Let us write, for any $j\in\mathbb{N}$,

$$F_j^{\mathrm{pol}}(x)=\sum_{i=0}^{j}\alpha_{i,j}x^i, \tag{2.12}$$

and let

$$\beta_{i,j}=\frac{\tilde{f}_{j-i}^{(i)}(0)}{i!}, \tag{2.13}$$

where $\tilde{f}_i$ is defined in (2.4) and (2.5). The conditions of matching modulo $\mathcal{O}(\kappa^n)$ for outer and inner solutions are given by the following proposition (see Ref. 7 for a proof).

Proposition 2.6: Let $n\in\mathbb{N}$. The inner and outer solution are matched modulo $\mathcal{O}(\kappa^n)$ if and only if

$$\alpha_{i,j}=\beta_{i,j},\ \forall\ (i,j)\ \ such\ \ that\quad 0\leqslant i\leqslant j\leqslant n\quad (i,j)\neq(0,n). \tag{2.14}$$

Moreover, for all $\overline{C_n}\in\mathbb{R}^{n+1}$ such that $C_0>0$, the system of $2n+2$ equations with $2n+2$ unknowns $\overline{A_n}$ and $\overline{B_n}$ (2.14) admits a unique solution with $B_0<0$ and $A_0\in\,]0,1[$.

In all the following sections, we assume that (2.14) is satisfied for all $n\in\mathbb{N}$. Using Proposition 2.6, we suppose that the functions $F_n(x,\overline{A_n},\overline{B_{n-1}})$, $Q_n(x,\overline{A_n},\overline{B_n})$, and $H_n(x,\overline{A_n},\overline{B_n})$ are expressed in terms of the parameters C_i, for $i\in\{0,\ldots,n\}$.

We introduce then the following notations:

$$\begin{gathered}\check{F}_n(x;\overline{C_n}):=F_n(x;\overline{A_n}(\overline{C_n}),\ \overline{B_{n-1}}(\overline{C_{n-1}})),\quad \check{Q}_n(x;\overline{C_n}):=Q_n(x;\overline{A_n}(\overline{C_n}),\ \overline{B_n}(\overline{C_n})),\\ \check{H}_n(x;\overline{C_n}):=H_n(x;\overline{A_n}(\overline{C_n}),\ \overline{B_n}(\overline{C_n})).\end{gathered} \tag{2.15}$$

III. CONSTRUCTION OF ASYMPTOTIC MATCHED SOLUTIONS

A. Presentation of asymptotic matched solutions

Let us recall that in Ref. 7, we have introduced matched asymptotic solutions.

Definition 3.1: Let $n\in\mathbb{N}^*$, $F^{e,(n)}(x;\kappa)$, $F^{i,(n+1)}(x;\kappa)$, $F^{\mathrm{pol},(n+1)}(x;\kappa)$ and $Q^{i,(n)}$ be the functions introduced in Definition 2.4. We call asymptotic matched solution of $(\mathrm{GL})_\infty$ at order n, a pair $(f^{vd,(n)},A^{vd,(n)})$ defined by

$$f^{vd,(n)}(x;\kappa)=F^{e,(n)}(x;\kappa)+F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa) \tag{3.1}$$

and

$$A^{vd,(n)}(x,\kappa)=\kappa^{-1/2}Q^{i,(n)}. \tag{3.2}$$

Remark 3.2: From Propositions 2.1, 2.2, and 2.6, let us remark that $(f^{vd,(n)},A^{vd,(n)})$ is completely defined by the data of $\overline{C_n}\in\mathbb{R}^{n+1}$, $C_0>0$ and (2.14).

We have proved in Lemma 3.8 in Ref. 7 that $f^{vd,(n)}$ satisfies the Neumann condition at zero. In the following lemmas, we show that in the region $[0,\kappa^{-\rho}]$, $\rho>0$, the function $f^{vd,(n)}$ is equal to $F^{i,(n+1)}(x;\kappa)$ modulo $\mathcal{O}(\kappa^{n+1})$, and in the region $[\kappa^{-\rho},+\infty[$, equal to $F^{e,(n)}(x;\kappa)$ modulo $\mathcal{O}(\kappa^{n+1})$. First, let us estimate the difference $F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)$.

Lemma 3.3: Let $n\in\mathbb{N}$, $F^{i,(n)}$ and $F^{\mathrm{pol},(n)}$ be the functions introduced in Definition 2.4.

For $x\in\mathbb{R}^+$, we have the estimate

$$F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)=\mathcal{O}(\kappa)(x^{2n}+1)\exp(-2A_0x).$$

Proof: From Proposition 2.2 [see (2.9)], we have the equality

$$F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)=\exp(-2A_0\ \ x)\sum_{i=1}^{n+1}P_i(x,\exp(-2A_0\ \ x))\kappa^i, \tag{3.3}$$

where P_i is a polynomial with $\deg_x P_i(X,0)=2i-2$. The proof of Lemma 3.3 follows.

In the same way, following Ref. 6 (see also Ref. 5), one can estimate the difference $F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)$ in the interval $[0,\kappa^{-1/(n+2)}]$ and prove the following proposition.

Lemma 3.4: Let $F^{e,(n)}$ and $F^{\mathrm{pol},(n+1)}$ be introduced in Definition 2.4. For all $x \in [0,\kappa^{-1/(n+2)}]$, we have the estimates

$$-\kappa^{-2}(F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa))''=\sum_{\substack{2\leqslant j-n\leqslant i\leqslant j\\ n+2\leqslant j\leqslant n+3}} i(i-1)\beta_{i,j}\kappa^{j-2}x^{i-2}+\mathcal{O}(\kappa^{n+1}), \quad (3.4)$$

and

$$F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)=\mathcal{O}(\kappa^{n+1}). \quad (3.5)$$

B. Properties of the function $f^{vd,(n)}$

In all the following, we use the lemma (see Ref. 5 for a proof).

Lemma 3.5: Let $(\rho,\gamma)\in\mathbb{N}^2$, and $\delta\in\mathbb{R}$. Let g_1 and g_2 be the functions defined on $\mathbb{R}^+$ by

$$g_1(x):=\exp(-\delta\kappa x), \quad g_2(x):=\kappa^{-\rho}(x^{\gamma}+1)\exp(-\sqrt{2}x).$$

Then there exist $\kappa_0>0$, and $c>0$, such that, for all $\kappa\leqslant\kappa_0$, for all $x\in[-c\ln\kappa,+\infty[$,

$$g_2(x)\leqslant g_1(x).$$

Let us first analyze the decay of the functions $\tilde{f}_i$, $i\in\mathbb{N}^*$.

Lemma 3.6: For $i\in\mathbb{N}^*$, let $\tilde{f}_i$ be the function defined in (2.4). For $x'\in[\kappa^{-1/(n+2)},+\infty[$, we have the estimate

$$\tilde{f}_i(x';\kappa)=\mathcal{O}(\exp(-\sqrt{2}x')). \quad (3.6)$$

Proof: From Proposition 2.1, for $i\geqslant 1$, the function $\tilde{f}_i$ is equal to

$$\tilde{f}_i=P(\tilde{f}_0',\ldots,\tilde{f}_0^{(i)}),$$

where $\tilde{f}_0$ is defined in (2.5) and P is a polynomial. As $\tilde{f}_0'=(1/\sqrt{2})(1-\tilde{f}_0^2)$, it results that

$$\tilde{f}_i=\tilde{f}_0'\tilde{P}(\tilde{f}_0,\tilde{f}_0'), \quad (3.7)$$

where $\tilde{P}$ is a polynomial. Moreover, from (2.5), we get

$$\tilde{f}_0'(x')=\frac{1}{\sqrt{2}}\frac{1}{\cosh^2\left(\dfrac{x'+C_0}{\sqrt{2}}\right)}=\mathcal{O}(\exp(-\sqrt{2}x')).$$

Then, from (3.7), the proof of Lemma 3.6 follows.

Let us recall (see Ref. 6 and Ref. 10) that, at the "formal" superheating field, A_0, B_0, A_1, B_1, and C_1 are equal to

$$A_0=\frac{1}{\sqrt{2}}, \quad B_0=-2^{-1/4}, \quad A_1=-\frac{7}{32}, \quad B_1=-\frac{9}{16}2^{-1/4}, \quad C_1=-\frac{15}{16}2^{-1/2}. \quad (3.8)$$

We assume that (3.8) is satisfied in the following sections.

Proposition 3.7: Let $f^{vd,(n)}$ be the function introduced in (3.1). There exists $\kappa_0>0$ such that, for all $\kappa\leqslant\kappa_0$, for all $x\in\mathbb{R}^+$, we have the inequality

$$0<f^{vd,(n)}(x)\leqslant 1. \tag{3.9}$$

Proof: The function $\tilde{f}_1(x')$, equal to

$$\frac{C_1}{\sqrt{2}}\frac{1}{\cosh^2\left(\dfrac{x'+C_0}{\sqrt{2}}\right)}$$

is negative because $C_1<0$ [see (3.8)]. Consequently, from Lemma 3.6 and the fact that the sign of $\tilde{f}_1(x')$ is negative, we get the inequality

$$\sum_1^n \kappa^i \tilde{f}_i(\kappa x;\kappa)<0,$$

for κ small enough. From (3.1), we deduce the inequality

$$f^{vd,(n)}(x;\kappa)\leqslant \tanh\left(\frac{\kappa x+C_0}{\sqrt{2}}\right)+\sum_{i=0}^{n+1}\kappa^i\hat{F}_i(x), \quad \forall \quad x\in\mathbb{R}^+, \tag{3.10}$$

where

$$\hat{F}_i := F_i - F_i^{\text{pol}}. \tag{3.11}$$

From Proposition 2.2 [see (2.9)], we have the inequality

$$\sum_{i=0}^{n+1}\kappa^i\hat{F}_i(x)\leqslant \kappa\exp\left(-\frac{1}{\sqrt{2}}x\right)\left(\frac{B_0^2}{4A_0}\exp\left(-\frac{1}{\sqrt{2}}x\right)+\kappa P\left[x,\ \exp\left(-\frac{1}{\sqrt{2}}x\right),\ \kappa\right]\exp\left(-\frac{1}{\sqrt{2}}x\right)\right),$$

where P is a polynomial. On the other hand, from (3.8), $B_0^2/4A_0=\frac{1}{4}$; then, for κ small enough and for all $x\in\mathbb{R}^+$, we have the inequality

$$\frac{B_0^2}{4A_0}\exp\left(-\frac{1}{\sqrt{2}}x\right)+\kappa\exp\left(-\frac{1}{\sqrt{2}}x\right)P\left[x,\ \exp\left(-\frac{1}{\sqrt{2}}x\right),\ \kappa\right]\leqslant\frac{1}{2}.$$

We deduce the inequality

$$\sum_{i=0}^{n+1}\kappa^i\hat{F}_i(x)\leqslant\frac{\kappa}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{3.12}$$

According to (3.10) and (3.12), for all $x\in\mathbb{R}^+$, we get the inequality

$$f^{vd,(n)}(x;\kappa)\leqslant\tanh\left(\frac{\kappa x+C_0}{\sqrt{2}}\right)+\frac{\kappa}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

From Lemma 8.3 in Ref. 3, we get

$$\tanh\left(\frac{\kappa x+C_0}{\sqrt{2}}\right)+\frac{\kappa}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right)\leqslant 1.$$

The proof of Proposition 3.7 follows.

C. Estimate of the remaining term

To generalize the proof of Theorem 1.3 in Ref. 6, we must estimate the remainder obtained substituting f and A by $f^{vd,(n)}$ and $A^{vd,(n)}$ in the (GL) equations. First, we show the following proposition.

Proposition 3.8: Let $n\geqslant 2$. Let $f^{vd,(n)}$ and $A^{vd,(n)}$ be the functions defined in (3.1) and (3.2). We get the estimate

$$-(A^{vd,(n)})''+(f^{vd,(n)})^2A^{vd,(n)}=\mathcal{O}(\kappa^{n+1/2})(x^{2n+1}+1)\exp(-A_0x),\quad \forall x\in[0,\kappa^{-1/(n+2)}]. \tag{3.13}$$

Proof: In this proof, we denote $f^{vd,(n)}$ and $A^{vd,(n)}$ simply by f and A. In the interval $[0,\kappa^{-1/(n+2)}]$, in order to use Lemma 3.4, we can write f in the form of

$$f(x)=F^{i,(n+1)}(x)+[F^{e,(n)}(x)-F^{\mathrm{pol},(n+1)}(x)]. \tag{3.14}$$

By construction of the formal inner solution, we have the equality

$$-A''+A(F^{i,(n+1)})^2=\kappa^{-1/2}\sum_{m=n+1}^{3n+2}\kappa^m\sum_{\substack{\ell+|i|_{1,n+1}=m,\ \ell\leqslant n\\ |i|_{0,n+1}=2}}\frac{2!}{i_0!\cdots i_{n+1}!}Q_\ell\prod_{k=0}^{n+1}F_k^{i_k}. \tag{3.15}$$

Let $m\in\{n+1,\ldots,3n+2\}$, and let $(\ell,i)\in\{0,\ldots,n\}\times\mathbb{N}^{n+1}$ be a pair such that $\ell+|i|_{1,n+1}=m$. From Proposition 2.2, the polynomial associated with the function $Q_\ell\Pi_{k=0}^{n+1}F_k^{i_k}$ is of degree $2\ell+|i|_{1,n+1}$. The pairs $(\ell,i)\in\{0,\ldots,n\}\times\mathbb{N}^{n+1}$ such that $\ell+|i|_{1,n+1}=m$ and $2\ell+|i|_{1,n+1}$ is maximum are such that $\ell=n$ and $|i|_{1,n+1}=m-n$. For these pairs, the degree of the associated polynomial is equal to $m+n$. Then, we get the estimate

$$\sum_{\substack{\ell+|i|_{1,n+1}=m,\ \ell\leqslant n\\ |i|_{0,n+1}=2}}\frac{2!}{i_0!\cdots i_{n+1}!}Q_\ell\prod_{k=0}^{n+1}F_k^{i_k}=\mathcal{O}(x^{m+n}+1)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{3.16}$$

For $m>n+1$, for $x\in[0,\kappa^{-1/(n+2)}]$, we have the estimate

$$\kappa^m(x^{m+n}+1)=\mathcal{O}(\kappa^{n+1})(x^{2n+1}+1).$$

From (3.14), (3.15), and (3.16), we get then

$$\begin{aligned}(-A''+f^2A)(x)=&A((F^{e,(n)}(x)-F^{\mathrm{pol},(n+1)}(x))^2+2F^{i,(n+1)}(x)(F^{e,(n)}(x)-F^{\mathrm{pol},(n+1)}))(x)\\&+\mathcal{O}(\kappa^{n+1/2})(x^{2n+1}+1)\exp(-A_0x).\end{aligned} \tag{3.17}$$

From Lemma 3.4 and the fact that $F^{i,(n)}$ is bounded independently of κ on $\mathbb{R}^+$, we deduce the estimate

$$(F^{e,(n)}(x)-F^{\mathrm{pol},(n)}(x))^2+2F^{i,(n+1)}(x)(F^{e,(n)}(x)-F^{\mathrm{pol},(n)}(x))=\mathcal{O}(\kappa^{n+1}). \tag{3.18}$$

From Proposition 2.2, more precisely the expression (2.10) and the fact that V_n has for degree $2n$, we have the estimate

$$A(x)=\mathcal{O}(\kappa^{-1/2})\exp(-A_0x). \tag{3.19}$$

Thus, from Lemma 3.4, the fact that $F^{i,(n)}$ is bounded independently of κ on $\mathbb{R}^+$ and from (3.19), we deduce the estimate

$$A((F^{e,(n)}(x)-F^{\mathrm{pol},(n+1)}(x))^2+2F^{i,(n)}(x)(F^{e,(n)}(x)-F^{\mathrm{pol},(n+1)}(x)))=\mathcal{O}(\kappa^{n+1/2})\exp(-A_0x). \tag{3.20}$$

Then, using (3.17) and (3.20), the proof of Proposition 3.8 follows.

To simplify the notations, we set

$$f_i(x;\kappa)=\tilde{f}_i(\kappa x), \quad \forall \ \ i \ \ \in \mathbb{N}. \tag{3.21}$$

In the goal to control the sign of the remainder, we establish the following proposition.

Proposition 3.9: Let $n\geqslant 2$ and $f^{vd,(n)}$ be the function defined in (3.1). For $x\in[-c\ln\kappa,+\infty[$, $c>0$, we have the estimate

$$-\kappa^{-2}(f^{vd,(n)})''(x)-f^{vd,(n)}(x)+(f^{vd,(n)}(x))^3=\kappa^{n+1}\tilde{R}_n+\mathcal{O}(\kappa^{n+2})\exp(-2\sqrt{2}\kappa x), \tag{3.22}$$

where

$$\tilde{R}_n=\sum_{\substack{|i|_{0,n}=3\\ |i|_{1,n}=n+1}}\frac{3!}{i_0!..i_n!}\prod_{k=0}^{n}f_k^{i_k}. \tag{3.23}$$

Proof: We denote $f^{vd,(n)}$ simply by f. In the outer region, we may write, using Lemma 3.3, f in the form of

$$f=[F^{i,(n+1)}-F^{\mathrm{pol},(n+1)}]+F^{e,(n)}. \tag{3.24}$$

By construction of the outer solution, we have the equality

$$-\kappa^{-2}(F^{e,(n)})''-F^{e,(n)}+(F^{e,(n)})^3=\overline{R}_n, \tag{3.25}$$

where $\overline{R}_n$ is defined by

$$\overline{R}_n=\sum_{\substack{|i|_{0,n}=3\\ n+1\leqslant|i|_{1,n}\leqslant 3n}}\frac{3!}{i_0!i_1!\cdots i_n!}\prod_{k=0}^{n}f_k^{i_k}\kappa^{|i|_{1,n}}.$$

Using (3.24) and (3.25), we can write

$$\begin{aligned}-\kappa^{-2}f''-f+f^3=&-\kappa^{-2}(F^{i,(n+1)}-F^{\mathrm{pol},(n+1)})''-F^{i,(n+1)}+F^{\mathrm{pol},(n+1)}\\&+(F^{e,(n)}+(F^{i,(n+1)}-F^{\mathrm{pol},(n+1)}))^3-(F^{e,(n)})^3+\overline{R}_n.\end{aligned} \tag{3.26}$$

For $i\in\{1,\ldots,n+1\}$, we get from Proposition 2.2 [see (2.9)] the estimate

$$(F_i-F_i^{\mathrm{pol}})(x)=\mathcal{O}(x^{2i-2}+1)\exp(-2A_0x). \tag{3.27}$$

From Proposition 2.2, we have the estimates

$$-\kappa^{-2}(F^{i,(n+1)}-F^{\mathrm{pol},(n+1)})''=\mathcal{O}(\kappa^{-1})(x^{2n}+1)\exp(-2A_0x) \tag{3.28}$$

and

$$\begin{aligned}f^3(x)-(F^{e,(n)}(x))^3=&3(F^{e,(n)}(x))^2(F^{i,(n+1)}(x)-F^{\mathrm{pol},(n+1)}(x))+3F^{e,(n)}(x)(F^{i,(n+1)}(x)\\&-F^{\mathrm{pol},(n+1)}(x))^2+(F^{i,(n+1)}(x)-F^{\mathrm{pol},(n+1)}(x))^3\\=&\mathcal{O}(\kappa)(x^{2n}+1)\exp(-2A_0x),\end{aligned} \tag{3.29}$$

where $F^{i,(n+1)}$ is introduced in Definition 2.4. According to (3.27), (3.28), and (3.29), and from Lemma 3.5, we get the estimate, for $x\in[-c\ln\kappa,+\infty[$, $c>0$,

$$-\kappa^{-2}(F^{i,(n+1)}-F^{\mathrm{pol},(n+1)})''-F^{i,(n+1)}+F^{\mathrm{pol},(n+1)}+f^3(x)-(F^{e,(n)}(x))^3$$
$$=\mathcal{O}(\kappa^{n+2})\exp(-2\sqrt{2}\kappa x). \tag{3.30}$$

Let $i=(i_0,\ldots,i_n)\in\mathbb{N}^{n+1}$, such that $|i|_{0,n}=3$ and $n+2\leqslant|i|_{1,n}$. Then, either there exists $k\in\{0,\ldots,n\}$ such that $i_k=2$, or there exists (i_j,i_k), $j\neq0$, $k\neq0$, and $j\neq k$, such that $i_j\neq0$ and $i_k\neq0$. Then, from Lemma 3.6, we get the estimate

$$\overline{R_n}=\kappa^{n+1}\tilde{R}_n+\mathcal{O}(\kappa^{n+2})\exp(-2\sqrt{2}\kappa x), \tag{3.31}$$

where $\tilde{R}_n$ is defined by

$$\tilde{R}_n=\sum_{\substack{|i|_{0,n}=3\\|i|_{1,n}=n+1}}\frac{3!}{i_0!\cdots i_n!}\prod_{k=0}^{n}f_k^{i_k}.$$

According to (3.26) and (3.30), the proof of Proposition 3.9 follows.

Now, we can show the following proposition which generalizes Lemma 6.2 in Ref. 6, with $\alpha=0$.

Proposition 3.10: Let $n\geqslant2$. We have the estimate

$$-\kappa^{-2}(f^{vd,(n)})''-f^{vd,(n)}+(f^{vd,(n)})^3+(A^{vd,(n)})^2f^{vd,(n)}$$
$$=\mathcal{O}(\kappa^{n+1})+\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x),\quad\forall x\in[0,\kappa^{-1/(n+2)}]. \tag{3.32}$$

To simplify the notation, we introduce the following functions:

$$\tilde{B}_n=\sum_{\substack{\ell+|i|_{1,n}\leqslant n\\|i|_{0,n}=2}}\frac{2!}{i_0!\cdots i_n!}F_\ell\prod_{k=0}^{n}Q_k^{i_k}\kappa^{\ell+|i|_{1,n}}, \tag{3.33}$$

$$\tilde{C}_n=\sum_{\substack{|i|_{0,n}=3\\|i|_{1,n}\leqslant n}}\frac{3!}{i_0!\cdots i_n!}\prod_{k=0}^{n}F_k^{i_k}\kappa^{|i|_{1,n}}, \tag{3.34}$$

$$\tilde{H}_{n,m}=\sum_{\substack{\ell+|i|_{1,n}=m\\|i|_{0,n}=2}}\frac{2!}{i_0!\cdots i_n!}F_\ell\prod_{k=0}^{n}Q_k^{i_k}\kappa^{\ell+|i|_{1,n}}, \tag{3.35}$$

$$\tilde{E}_{n,m}=\sum_{\substack{|i|_{0,n}=3\\|i|_{1,n}=m}}\frac{3!}{i_0!\cdots i_n!}\prod_{k=0}^{n}F_k{}^{i_k}\kappa^{|i|_{1,n}}. \tag{3.36}$$

To prove Proposition 3.10, we establish the following lemma.

Lemma 3.11: Let $n\geqslant2$. Let $\tilde{E}_{n,m}$ be the function defined in (3.36) and $\beta_{i,j}$ defined in (2.13). We have the estimates

$$-F_n+\kappa^{-n}\tilde{E}_{n,n}+\sum_{i=2}^{n+2}i(i-1)\beta_{i,n+2}x^{i-2}=\mathcal{O}(x^{2n-2}+1)\exp(-2A_0x) \tag{3.37}$$

and

$$-F_{n+1}+\kappa^{-(n+1)}\tilde{E}_{n+1,n+1}+\sum_{i=3}^{n+3} i(i-1)\beta_{i,n+3}x^{i-2}=\mathcal{O}(1)+\mathcal{O}(x^{2n}+1)\exp(-2A_0x). \tag{3.38}$$

Proof: From Proposition 2.6 [see (2.14)],

$$(F_{n+2}^{\mathrm{pol}})''=\sum_{i=2}^{n+2} i(i-1)\alpha_{i,n+2}x^{i-2}=\sum_{i=2}^{n+2} i(i-1)\beta_{i,n+2}x^{i-2}.$$

By construction of the inner solution we have $(F_{n+2})''=-F_n+\kappa^{-n}\tilde{E}_{n,n}$, modulo a sum of exponential polynomials. Consequently, the expression

$$-F_n+\kappa^{-n}\tilde{E}_{n,n}-\sum_{i=2}^{n+2} i(i-1)\beta_{i,n+2}x^{i-2}$$

is a sum of exponential polynomials, and more precisely, using Proposition 2.2, is equal to $\mathcal{O}(|P|)\exp(-2A_0x)$ where P is a polynomial. We want to show that the degree of P is equal to $2n-2$. Let us consider $i=(i_0,\ldots,i_n)\in\mathbb{N}^{n+1}$ such that $|i|_{0,n}=3$ and $|i|_{1,n}=n$.

There are three cases to consider.

(1) There exists $(i_k,i_\ell)\in\mathbb{N}^2$, such that $(i_k,i_\ell)=(2,1)$, and then $i_j=0$ for all $j\neq k$ and $j\neq\ell$, $j\in\{0,\ldots,n\}$.

Let us determine the degree of the polynomial in the polynomial exponential part of $3F_\ell F_k^2$ with $2k+\ell=n$.

From Proposition 2.2, we have the equality

$$F_\ell F_k^2=(F_\ell^{\mathrm{pol}}+\exp(-2A_0x)P_\ell(x,\exp(-2A_0x)))(F_k^{\mathrm{pol}}+\exp(-2A_0x)P_k(x,\exp(-2A_0x)))^2.$$

From Proposition 2.2, the degree of the polynomial $2F_\ell^{\mathrm{pol}}F_k^{\mathrm{pol}}P_k(x,0)$ is equal to $\ell+k+2k-2=n+k-2<2n-2$.

The degree of $(F_k^{\mathrm{pol}})^2P_\ell(x,0)$ is equal to $2k+2\ell-2=n+\ell-2\leqslant 2n-2$.

(2) There exists $i_\ell\in\mathbb{N}$, such that $i_\ell=3$, and then $i_j=0$ for $j\neq\ell$, $j\in\{0,\ldots,n\}$. Let us consider ${F_\ell}^3$. The dominant term of $(F_\ell)^3$ is $(F_\ell^{\mathrm{pol}})^2P_\ell(x,\exp(-2A_0x))$. The degree of its polynomial part is equal to $4\ell-2<2n-2$.

(3) There exists $(i_j,i_k,i_\ell)\in\mathbb{N}^3$, such that $i_j=i_k=i_\ell=1$, and then $i_m=0$ for $m\neq j$, $m\neq k$, $m\neq\ell$, $m\in\{0,\ldots,n\}$.

Let us consider the term $F_jF_kF_\ell$ with $j+k+\ell=n$. The degree of the polynomial in the polynomial exponential part of $F_jF_kF_\ell$ is equal to $\ell+k+2(n-\ell-k)-2=2n-\ell-k-2<2n-2$. The proof of (3.37) follows.

Moreover,

$$(F_{n+3}^{\mathrm{pol}})''=\sum_{i=2}^{n+3} i(i-1)\alpha_{i,n+3}x^{i-2}=\sum_{i=2}^{n+3} i(i-1)\beta_{i,n+3}x^{i-2}.$$

By construction of the inner solution we have $(F_{n+3})''=-F_{n+1}+\kappa^{-(n+1)}\tilde{E}_{n+1,n+1}$, modulo a sum of exponential polynomials. Consequently, the expression

$$-F_{n+1}+\kappa^{-(n+1)}\tilde{E}_{n+1,n+1}-\sum_{i=3}^{n+3} i(i-1)\beta_{i,n+3}x^{i-2}$$

is equal to $2\beta_{2,n+3}+\mathcal{O}(|P|)\exp(-2A_0x)$ where P is a polynomial. Then we can conclude as previously. The proof of Lemma 3.11 follows.

Proof of Proposition 3.10: We continue to denote $f^{vd,(n)}$ and $A^{vd,(n)}$ by f and A. By construction of the inner solution, we have the equality

$$-\kappa^{-2}(F^{i,(n+1)})''-\sum_{0}^{n-1} F_i\kappa^i+\tilde{C}_n+\kappa^{-1}\tilde{B}_n=0, \tag{3.39}$$

where $\tilde{B}_n$ and $\tilde{C}_n$ are defined in (3.33) and (3.34).

With the aim to use Lemma 3.4, we write f in the form of

$$f=[F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)]+F^{i,(n+1)}(x;\kappa). \tag{3.40}$$

Using (3.39) and (3.40), we get the equality

$$\begin{aligned}-\kappa^{-2}f''-f+f^3+A^2f=&-\kappa^{-2}(F^{e,(n)}-F^{\mathrm{pol},(n+1)})''-\kappa^nF_n-\kappa^{n+1}F_{n+1}\\&-(F^{e,(n)}-F^{\mathrm{pol},(n+1)})+f^3-\tilde{C}_{n-1}+A^2f-\kappa^{-1}\tilde{B}_n.\end{aligned} \tag{3.41}$$

Estimate for the expression $A^2f-\kappa^{-1}\tilde{B}_n$: From Lemma 3.4 [see (3.5)] and (3.2), we get the equality

$$A^2f=\left(\kappa^{-1/2}\sum_{0}^{n} Q_i\kappa^i\right)^2(F^{i,(n+1)}+\mathcal{O}(\kappa^{n+1})). \tag{3.42}$$

Let us evaluate the difference $A^2F^{i,(n+1)}-\kappa^{-1}\tilde{B}_n$. We have the equality $A^2F^{i,(n+1)}=A^2F^{i,(n)}+A^2\kappa^{n+1}F_{n+1}$.

Now, from Proposition 2.2 [see (2.9)], for $x\in[0,\kappa^{-1/(n+2)}]$, we have the estimates

$$F_{n+1}=\mathcal{O}(x^{n+1}+1)\quad\text{and}\quad A^2=\mathcal{O}(\kappa^{-1})\exp(-2A_0x).$$

We deduce the estimate

$$A^2\kappa^{n+1}F_{n+1}=\mathcal{O}(\kappa^n)(x^{n+1}+1)\exp(-2A_0x).$$

The term $A^2F^{i,(n+1)}-\kappa^{-1}\tilde{B}_n$ consequently satisfies

$$\begin{aligned}A^2F^{i,(n+1)}-\kappa^{-1}\tilde{B}_n&=A^2F^{i,(n)}-\kappa^{-1}\tilde{B}_n+\mathcal{O}(\kappa^n)(x^{n+1}+1)\exp(-2A_0x)\\&=\kappa^{-1}\sum_{k=n+1}^{3n+1}\tilde{H}_{n,k}+\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x),\end{aligned} \tag{3.43}$$

where $\tilde{H}_{n,k}$ is defined in (3.35).

The dominant term of the expression $\Sigma_{k=n+1}^{3n+1}\tilde{H}_{n,k}$ is obtained for the values $\ell=1$, $i_0=1$ and $i_n=1$. Its expression is $2\kappa^nF_1Q_0Q_n$. From the structure of F_1 and Q_n [see (2.9) and (2.10)], we get the estimate

$$2\kappa^nF_1Q_0Q_n=\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x).$$

From (3.43), we deduce the estimate

$$A^2F^{i,(n+1)}-\kappa^{-1}\tilde{B}_n=\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x). \tag{3.44}$$

From (3.42) and (3.44), we get the estimate

$$A^2f-\kappa^{-1}\tilde{B}_n=\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x). \tag{3.45}$$

Estimate of the expression $f^3-\tilde{C}_{n-1}$*:* We have the equality

$$f^3-\tilde{C}_{n-1}=(F^{i,(n+1)})^3+3(F^{i,(n+1)})^2(F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x))+3F^{i,(n+1)}(F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x))^2+(F^{e,(n)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x))^3-\tilde{C}_{n-1}. \tag{3.46}$$

Moreover, using (3.34), we get

$$(F^{i,(n+1)})^3=\tilde{C}_{n+1}+\sum_{k=n+2}^{3n+3}\tilde{E}_{n+1,k}$$

Now, for $x\in[0,\kappa^{-1/(n+2)}]$, we have the estimate $\Sigma_{k=n+2}^{3n+3}\tilde{E}_{n+1,k}=\mathcal{O}(\kappa^{n+1})$. Moreover, we have the equality

$$\tilde{C}_{n+1}=\tilde{E}_{n+1,n+1}+\tilde{E}_{n,n}+\tilde{C}_{n-1}. \tag{3.47}$$

From (3.47), we get the estimate

$$(F^{i,(n+1)})^3-\tilde{C}_{n-1}=\tilde{E}_{n,n}+\tilde{E}_{n+1,n+1}+\mathcal{O}(\kappa^{n+1}). \tag{3.48}$$

Otherwise, from (2.9), and precisely from the fact that F_n^{pol} is of degree n, in the inner region, we have for $k\in\{0,\ldots,n+1\}$ the estimate $\kappa^k F_k=\mathcal{O}(1)$.

This implies

$$F^{i,(n+1)}=\mathcal{O}(1). \tag{3.49}$$

From (3.49) and Lemma 3.4, we obtain that

$$3F^{i,(n+1)^2}(F^{e,(n)}(\kappa x;\kappa)-F^{\mathrm{pol},(n)}(x))+3F^{i,(n+1)}(F^{e,(n)}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x))^2+(F^{e,(n)}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x))^3=\mathcal{O}(\kappa^{n+1}). \tag{3.50}$$

From (3.46), (3.48), and (3.50), we deduce the equality

$$f^3-\tilde{C}_{n-1}=\tilde{E}_{n,n}+\tilde{E}_{n+1,n+1}+\mathcal{O}(\kappa^{n+1}). \tag{3.51}$$

Simplifications of (3.41): From Lemma 3.4, (3.45) and (3.51), we can write (3.41) in the form of

$$-\kappa^{-2}f''-f+f^3+A^2f=\sum_{\substack{2\leqslant j-n\leqslant i\leqslant j\\ n+2\leqslant j\leqslant n+3}} i(i-1)\beta_{i,j}\kappa^{j-2}x^{i-2}+\mathcal{O}(\kappa^{n+1})-\kappa^n F_n-\kappa^{n+1}F_{n+1}+\tilde{E}_{n,n}+\tilde{E}_{n+1,n+1}+\mathcal{O}(\kappa^{n+1})+\mathcal{O}(\kappa^n)(x^{2n+1}+1)\exp(-2A_0x). \tag{3.52}$$

From Lemma 3.11 [see (3.37) and (3.38)], we deduce the estimates

$$-\kappa^n F_n+\tilde{E}_{n,n}+\kappa^n\sum_{i=2}^{n+2} i(i-1)\beta_{i,n+2}x^{i-2}=\mathcal{O}(\kappa^n)(x^{2n-2}+1)\exp(-2A_0x)$$

and

$$-\kappa^{n+1}F_{n+1}+\tilde{E}_{n+1,n+1}+\kappa^{n+1}\sum_{i=3}^{n+3} i(i-1)\beta_{i,n+3}x^{i-2}$$
$$=\mathcal{O}(\kappa^{n+1})+\mathcal{O}(\kappa^{n+1})(x^{2n}+1)\exp(-2A_0x).$$

These estimates and (3.52) complete the proof of Proposition 3.10.

IV. CONSTRUCTION OF A SUBSOLUTION

A. Presentation of a subsolution

We first recall the definition of a subsolution.

Definition 4.1: A triplet (f,A,h) *is a subsolution of* $(\mathrm{GL})_\infty$ *if*

$$-\kappa^{-2}f''+f(-1+f^2+A^2)\leqslant 0, \quad \forall \quad x\in\mathbb{R}^+,$$
$$(1-f)\in H^2(]0,\infty[), \quad f'(0)=0, \tag{4.1}$$

where A *is the unique solution in* $H^2(]0,+\infty[)$ *of*

$$-A''+f^2A=0,$$
$$A'(0)=h. \tag{4.2}$$

However, we shall say more briefly that f *is a subsolution for* $(\mathrm{GL})_\infty$. *Similarly, we say that* $(f,A;h)$ *is a supersolution if it satisfies the inverse inequality in (4.1).*

To construct a subsolution, we proceed as in Ref. 10. The parameter A_{n+1} is determined by the equality

$$F_{n+1}^{\mathrm{pol}}(0)=0, \tag{4.3}$$

where F_{n+1}^{pol} is defined in Proposition 2.2. From Proposition 2.6, for $k\in\{0,\ldots,n\}$, we have chosen to express A_k and B_k as functions of $C_0,\ldots,C_k$. It results from Proposition 2.2 and (4.3) that A_{n+1} is a function of $\overline{C_n}$. In the next sections, for $n\geqslant 1$, we assume that the constants $\overline{A_{n-1}}$, $\overline{B_{n-1}}$, and $\overline{C_{n-1}}$ are computed following the procedure exposed in Proposition 4.6 in Ref. 7, at order $2n-2$. Then, the function $f^{vd,(n)}$ only depends on the parameter C_n which remains "free" for the moment. In the following sections, we denote it by β. To get a negative sign of the expression $-\kappa^{-2}f''+f(-1+f^2+A^2)$ in the region $[-\ln\kappa,+\infty[$, we modify modulo $\mathcal{O}(\kappa)$ some coefficients in the outer solution, and more precisely in the function $\tilde{f}_n$. From (2.4), for $n\geqslant 2$, the function $\tilde{f}_n$ is equal to

$$\tilde{f}_n=\beta\tilde{f}_0'+\tilde{D}_n, \tag{4.4}$$

where

$$\tilde{D}_n=\sum_{m=2}^{n}\sum_{\substack{|i|_{2,n-1}=n\\ |i|_{1,n-1}=m}}\frac{m!}{i_1!\cdots i_{n-1}!}\prod_{k=1}^{n-1}(C_k)^{i_k}\ \tilde{f}_0^{(m)}. \tag{4.5}$$

From (4.4) and (4.5), let us remark that the reals $\tilde{f}_n'(0)$ and $\tilde{f}_n''(0)$ are affine functions of β. In the following, for $i\in\{0,\ldots,n\}$, the function $\overline{f_i}$ is defined by

$$x'\mapsto\overline{f_i}(x')=\tilde{f}_i((1+\alpha\kappa)x'), \tag{4.6}$$

where α is a parameter, which is assumed to satisfy

$$\alpha<0. \tag{4.7}$$

Remark 4.2: When we prove Theorem 1.2 in the case $n=1$ (see Ref. 6), we know the sign of the function $\tilde{f}_1$ on $\overline{\mathbb{R}^+}$, of $\tilde{f}_1'(0)$ and $\tilde{f}_1''(0)$ which play an important role in the proof of this theorem. In the general case ($n\geqslant 1$), we do not know a priori the sign of $\tilde{f}_n$ on $\overline{\mathbb{R}^+}$, and the signs of $\tilde{f}_n'(0)$ and $\tilde{f}_n''(0)$. To get a suitable sign of the function $\tilde{f}_n$ on $\overline{\mathbb{R}^+}$ and $\tilde{f}_n'(0)$ and $\tilde{f}_n''(0)$, we use the parameter β appearing in (4.4). Precisely, we will show that β can be chosen such that $\tilde{f}_n<0$ on $\overline{\mathbb{R}^+}$, $\tilde{f}_n'(0)>0$ and $\tilde{f}_n''(0)<0$.

For $i\in\{0,\ldots,n\}$, we denote by

$$\hat{f}_i(x;\kappa)=\overline{f_i}(\kappa x) \quad \text{and} \quad \hat{D}_i(x)=\tilde{D}_i((1+\alpha\kappa)\kappa x). \tag{4.8}$$

For $i\in\mathbb{N}$, we have an analogous conclusion to (3.6) replacing the function $\tilde{f}_i$ by the function $\hat{f}_i$.

Lemma 4.3: For $i\in\mathbb{N}^*$, let $\hat{f}_i$ be the function defined in (4.8). For all $\alpha<0$, for κ small enough, we have the estimate, for $x\in[-\ln\kappa,+\infty[$,

$$\hat{f}_i(x;\kappa)=\mathcal{O}(\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)). \tag{4.9}$$

By construction of the outer solution and expanding in powers of κ the first equation in (1.3), we get that the function $\tilde{f}_n$ satisfies the equation

$$-\tilde{f}_n''-\tilde{f}_n+\sum_{\substack{|i|_{0,n}=3\\ |i|_{1,n}=n}}\frac{3!}{i_0!\cdots i_n!}\prod_{k=0}^{n}\tilde{f}_k^{\,i_k}=0, \quad \text{on } \mathbb{R}^+.$$

From (4.4) and (4.8), for $n\geqslant 2$, it results that the function $\hat{f}_n$ satisfies the equation

$$-\kappa^{-2}\hat{f}_n''-\hat{f}_n+\sum_{\substack{|i|_{0,n}=3\\ |i|_{1,n}=n}}\frac{3!}{i_0!\cdots i_n!}\prod_{k=0}^{n}\hat{f}_k^{\,i_k}=\kappa\alpha(2+\kappa\alpha)(\hat{f}_n(1-3\hat{f}_0^2)+\hat{R}_{n-1}), \tag{4.10}$$

where the function $\hat{R}_{n-1}$ is defined by

$$\hat{R}_{n-1}=\sum_{\substack{|i|_{0,n-1}=3\\ |i|_{1,n-1}=n}}\frac{3!}{i_0!\cdots i_{n-1}!}\prod_{k=0}^{n-1}\hat{f}_k^{\,i_k}. \tag{4.11}$$

The function $\hat{R}_n$ does not depend on the parameter β, and moreover, from Lemma 4.3, for all α, there exists κ_0 such that, for all $\kappa\leqslant\kappa_0$, we have the estimates

$$\hat{D}_n=\mathcal{O}(\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)), \quad \hat{R}_{n-1}=\mathcal{O}(\exp(-2\sqrt{2}(1+\alpha\kappa)\kappa x)), \quad \forall \ n\geqslant 2. \tag{4.12}$$

Now, we can choose the parameter β as announced in Remark 4.2.

Lemma 4.4: For $n\geqslant 2$, let $\tilde{f}_n$, $\hat{f}_n$ and $\hat{R}_{n-1}$ be the functions defined respectively in (4.4), (4.8), and (4.11). There exist $\tilde{C}_1<0$ and $\tilde{C}_2>0$, such that, for all $\beta<\tilde{C}_1$, for all $\alpha<0$, we have the following properties:

$$\text{(a)} \ \ \hat{f}_n\leqslant 0, \quad \forall x\in\mathbb{R}^+,$$

$$\text{(b)} \ \ \tilde{f}_n'(0)>0, \quad \tilde{f}_n''(0)<0, \tag{4.13}$$

$$\text{(c)} \ \ \hat{f}_n(1-3\hat{f}_0^3)+\hat{R}_{n-1}\geqslant-\tilde{C}_2\hat{f}_n, \quad \forall x\in\mathbb{R}^+.$$

Proof: We have from (2.5) the inequalities

$$\tilde{f}_0''(0)<0 \quad \text{and} \quad \tilde{f}_0^{(3)}(0)>0. \tag{4.14}$$

According to (4.5), the reals $\tilde{D}_n'(0)$ and $\tilde{D}_n''(0)$ do not depend on β, because $\tilde{D}_n$ is independent of β. From (4.4) and (4.14), there exists $c<0$, such that, for all $\beta<c$, we have

$$\tilde{f}_n''(0)=\beta\tilde{f}_0'''(0)+\tilde{D}_n''(0)>0, \quad \tilde{f}_n'(0)=\beta\tilde{f}_0''(0)+\tilde{D}_n'(0)<0.$$

We deduce $(4.13)_b$.

According to (4.4), (4.8), the hypothesis $\beta<0$ and the fact that $\tilde{f}_0'>1-\tanh^2(C_0/\sqrt{2})\geqslant\frac{1}{2}$ on $\mathbb{R}^+$, we have the inequality, for all α and for $|\beta|$ large enough

$$\hat{f}_n\leqslant\beta\min_{x\in\mathbb{R}^+}\tilde{f}_0'+\max_{x\in\mathbb{R}^+}\hat{D}.$$

It results that, for $|\beta|$ large enough and for all $\alpha<0$, we get

$$\hat{f}_n\leqslant 0, \quad \forall\, x\in\mathbb{R}^+.$$

Property $(4.13)_a$ follows.

For $x\in\mathbb{R}^+$, as $\hat{f}_0(0)=\tilde{f}_0(0)=1/\sqrt{2}$, we get the inequality

$$3\hat{f}_0^2-1\geqslant 3\hat{f}_0^2(0)-1>\tfrac{1}{4}.$$

From Lemma 4.3, we have the estimate

$$\hat{f}_n=\mathcal{O}(\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)).$$

Using then (4.12), we deduce that there exists $\tilde{c}>0$ such that, for all $x\in\mathbb{R}^+$,

$$\hat{f}_n\geqslant-\tilde{c}|\hat{R}_{n-1}|.$$

We deduce that for $\tilde{C}_2=\frac{1}{4}+(1/\tilde{c})$, we have for all $x\in\mathbb{R}^+$,

$$-\hat{f}_n(-1+3\hat{f}_0^3)+\hat{R}_{n-1}\geqslant-\tilde{C}_2\hat{f}_n.$$

We get Inequality $(4.13)_c$. The proof of Lemma 4.4 follows.

In the following sections, we assume that the conclusion of Lemma 4.4 is verified.

Now, we follow Ref. 6. We denote by $\tilde{F}^{e,(n),m}$ the outer solution modified

$$\tilde{F}^{e,(n),m}=\sum_0^{n-1}\tilde{f}_i\kappa^i+\kappa^n\overline{f_n}. \tag{4.15}$$

In order to obtain the Neumann condition and control the sign in the interval $[0,\kappa^{-\rho}]$, $\rho>0$, we add to $f^{vd,(n)}$ modified a function $\kappa^{n+2}G$. The function G is assumed to have the form

$$G(x)=P(x)\exp(-2A_0x), \tag{4.16}$$

where P is a polynomial function, of degree $2n+2$ and where $A_0=1/\sqrt{2}$. This choice of P is motived by the structure of the formal solution. We look for a function P in the form of

$$P(x)=a(x^{2n+2}+x), \tag{4.17}$$

where a is a parameter. In the following sections, the function $f^{vdm,(n)}$ represents the function obtained after the modifications of the function $f^{vd,(n)}$ defined in (3.1). Precisely, it is given by

$$f^{vdm,(n)}(x;\kappa)=\tilde{F}^{e,(n),m}(\kappa x;\kappa)+F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)+\kappa^{n+2}G. \tag{4.18}$$

Let us express the condition $(f^{vdm,(n)})'(0;\kappa)=0$. By construction, we get

$$(f^{vdm,(n)})'(0;\kappa)=\sum_{j=0}^{n}\tilde{f}_j'(0)\kappa^{j+1}+\alpha\kappa^{n+2}\tilde{f}_n'(0)-\sum_{j=1}^{n+1}\alpha_{1,j}\kappa^j+a\kappa^{n+2}.$$

Using the matching conditions (2.14) for $i=1$, we get

$$(f^{vdm,(n)})'(0;\kappa)=\sum_{j=1}^{n+1}(\beta_{1,j}-\alpha_{1,j})\kappa^j+\alpha\kappa^{n+2}\tilde{f}_n'(0)+a\kappa^{n+2}=\kappa^{n+2}(\alpha\tilde{f}_n'(0)+a).$$

Finally, we obtain

$$a=-\alpha\tilde{f}_n'(0). \tag{4.19}$$

Using the relation (4.19), the parameter a becomes a function of the parameters α and β. As in Ref. 6, we use the following conventions. Let g be a function defined on $\mathbb{R}\times\mathbb{R}^+$, $(\alpha,\kappa)\to g(\alpha,\kappa)$. We will write $g(\alpha,\kappa)=\mathcal{O}_\alpha^{un}(\kappa^n)$, if there exists C, such that, for all α, there exists $\kappa_0(\alpha)$ such that, for all $\kappa\leqslant\kappa_0(\alpha)$, $|g(\alpha,\kappa)|\leqslant C\kappa^n$. Similarly, we will write $g(\alpha,\kappa)=\mathcal{O}(\kappa^n)$, if there exist C and κ_0, such that, for all α, for all $\kappa\leqslant\kappa_0$, $|g(\alpha,\kappa)|\leqslant C\kappa^n$.

We can show that $f^{vdm,(n)}$ satisfies the following property.

Proposition 4.5: Let $f^{vdm,(n)}$ be the function defined in (4.18). For all $\alpha<0$, there exists $\kappa_0>0$ such that, for all $\kappa\leqslant\kappa_0$, for all $x\in\mathbb{R}^+$, we have the inequalities

$$0<f^{vdm,(n)}(x)\leqslant 1. \tag{4.20}$$

Proof: From Proposition 3.7, when κ is small enough,

$$f^{vd,(n)}\leqslant 1,\quad \forall\ \ x\in\mathbb{R}^+.$$

According to (4.19), as $\alpha<0$ and $\tilde{f}_n'(0)>0$, we get $a>0$. Then, from (4.16) and (4.17), we get $G\geqslant 0$ for all $x\in\mathbb{R}^+$. Moreover, as $\alpha<0$, we have $\hat{f}_0(x)\leqslant\tilde{f}_0(\kappa x)$.

From (3.1) and (4.18), it results that there exists κ_0 such that, for all $\kappa\leqslant\kappa_0$, we have the inequalities, for all $\alpha<0$, for all $x\in\mathbb{R}^+$,

$$f^{vdm,(n)}(x)\leqslant f^{vd,(n)}(x)\leqslant 1.$$

Moreover, from (4.18), there exist κ_0 and $\hat{c}>0$ such that, for all $\alpha<0$, for all $\kappa\leqslant\kappa_0$, we have the inequalities

$$f^{vdm,(n)}(x)\geqslant\tilde{f}_0(0)-\hat{c}\kappa>0,\quad \forall\, x\in\mathbb{R}^+.$$

The proof of Proposition 4.5 follows.

The proof of Theorem 1.2 is a direct consequence of the following theorem:

Theorem 4.6: *Let $n\geqslant 2$. There exist $\tilde{C}$, $\alpha<0$ and $\kappa_0>0$ such that, for $\kappa\leqslant\kappa_0$ and for h,*

$$\kappa^{1/2}h=\sum_{0}^{n}h_i\kappa^i+\tilde{C}\kappa^{n+1}, \tag{4.21}$$

the function $f^{vdm,(n)}$ satisfies

$$(f^{vdm,(n)})'(0)=0,$$

and

$$\begin{gathered}-\kappa^{-2}(f^{vdm,(n)})''+f^{vdm,(n)}(-1+(f^{vdm,(n)})^2+(A^{vdm,(n)})^2)\leqslant 0,\\ (1-f^{vdm,(n)})\in H^2(]0,+\infty[),\end{gathered} \tag{4.22}$$

where $A^{vdm,(n)}$ *is the unique solution in* $H^2(]0,+\infty[)$ *of*

$$\begin{gathered}-(A^{vdm,(n)})''+(f^{vdm,(n)})^2A^{vdm,(n)}=0,\\ (A^{vdm,(n)})'(0)=h.\end{gathered} \tag{4.23}$$

In the next sections, we will prove Theorem 4.6. We set

$$R^{(n)}:=-\kappa^{-2}(f^{vdm,(n)})''+f^{vdm,(n)}(-1+(f^{vdm,(n)})^2+(A^{vdm,(n)})^2). \tag{4.24}$$

B. Control of the sign of $R^{(n)}$ in the outer region

In this section, we control the sign of $R^{(n)}$ in the interval $[-\ln\kappa,+\infty[$.

Proposition 4.7: There exist $\alpha_0<0$ *and* $\hat{C}>0$, *such that, for all* $\alpha<\alpha_0$, *for all* $\beta\leqslant-\hat{C}$, *there exists* κ_0 *such that, for all* $\kappa\leqslant\kappa_0$, *for all* $x\in[-\ln\kappa,+\infty[$, *we have the inequality*

$$R^{(n)}(x)\leqslant 0,\quad \forall x\in[-\ln\kappa,+\infty[. \tag{4.25}$$

Proof: Using (4.18), we write $f^{vdm,(n)}$ in the form of

$$f^{vdm,(n)}=f^{vd,(n-1)}+\kappa^n\hat{f}_n+\kappa^{n+1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})+\kappa^{n+2}G. \tag{4.26}$$

From Proposition 3.7, we have $0<f^{vdm,(n)}\leqslant 1$. Then, as in Ref. 6 (Proposition 6.4), we get the upper bound, for all $x\in\mathbb{R}^+$, for any $\delta\in]0,1/\sqrt{2}[$

$$(A^{vdm,(n)})^2(x)f^{vdm,(n)}(x)\leqslant\frac{h^2}{\delta^2}\exp(-2\delta x). \tag{4.27}$$

From Lemma 4.3, we have

$$\hat{f}_n=\mathcal{O}(\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)). \tag{4.28}$$

From (4.26), and by construction of the inner solution, we get

$$\begin{aligned}&-\kappa^{-2}(f^{vdm,(n)})''+f^{vdm,(n)}(-1+(f^{vdm,(n)})^2+(A^{vdm,(n)})^2)\\ &\quad=-\kappa^{-2}(f^{vd,(n-1)})''-\kappa^{n-2}\hat{f}_n''-\kappa^{n-1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})''-\kappa^nG''-f^{vd,(n-1)}\\ &\qquad-\kappa^n\hat{f}_n-\kappa^{n+1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})-\kappa^{n+2}G+(f^{vdm,(n)})^3+(A^{vdm,(n)})^2f^{vdm,(n)}.\end{aligned}$$

Using (4.16), (4.17), and (4.19), we express the function G in the form of

$$G(x)=-\alpha\tilde{f}_n'(0)(x^{2n+2}+x)\exp(-\sqrt{2}x).$$

From (4.27), (4.28), Proposition 2.2 and using Lemma 3.5, we deduce that there exists for all $\alpha<0$ a real κ_0, such that, for all $\kappa\leqslant\kappa_0$, for $x\in[-\ln\kappa,+\infty[$, we have the estimates

$$-\kappa^{n-1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})''-\kappa^nG''=\mathcal{O}_\alpha^{un}(\kappa^{n+1})|\hat{f}_n|,\quad (A^{vdm,(n)})^2f^{vdm,(n)}=\mathcal{O}(\kappa^{n+1})|\hat{f}_n| \tag{4.29}$$

and

$$-\kappa^{n+1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})-\kappa^{n+2}G=\mathcal{O}_{\alpha}^{un}(\kappa^{n+1})|\hat{f}_n|. \tag{4.30}$$

According to (4.29) and (4.30), Proposition 3.9 [see (3.22)], and using the equation satisfied by $\hat{f}_n$ in (4.10), we get the equality, for $x\in[-c\ln\kappa,+\infty[$,

$$\begin{aligned}-\kappa^{-2}(f^{vdm,(n)})''+f^{vdm,(n)}(-1+(f^{vdm,(n)})^2+(A^{vdm,(n)})^2)\\ =f^{vdm,(n)3}-(f^{vd,(n-1)})^3+\kappa^{n+1}\alpha(2+\alpha\kappa)(\hat{f}_n(1-3\hat{f}_0^2)+\hat{R}_{n-1})+\kappa^n\tilde{R}_{n-1}\\ -\kappa^n(3\hat{f}_0^2\hat{f}_n+\hat{R}_{n-1})+\mathcal{O}_{\alpha}^{un}(\kappa^{n+1})|\hat{f}_n|.\end{aligned} \tag{4.31}$$

Moreover, using (4.26), we get

$$f^{vdm,(n)3}-(f^{vd,(n-1)})^3=3(f^{vd,(n-1)})^2K_n+3f^{vd,(n-1)}K_n^2+K_n^3, \tag{4.32}$$

where

$$K_n:=\kappa^n\hat{f}_n+\kappa^{n+1}(F_{n+1}-F_{n+1}^{\mathrm{pol}})+\kappa^{n+2}G.$$

We have the estimates

$$3(f^{vd,(n-1)})^2K_n=3\kappa^n\hat{f}_nf_0^2+\mathcal{O}_{\alpha}^{un}(\kappa^{n+1})|\hat{f}_n|,\quad 3(f^{vd,(n-1)})K_n^2=\mathcal{O}_{\alpha}^{un}(\kappa^{2n})\hat{f}_n^2,$$

$$K_n^3=\mathcal{O}_{\alpha}^{un}(\kappa^{3n})|\hat{f}_n|^3.$$

We deduce the estimate

$$(f^{vdm,(n)})^3-(f^{vd,(n-1)})^3=3\kappa^n\hat{f}_nf_0^2+\mathcal{O}_{\alpha}^{un}(\kappa^{n+1})|\hat{f}_n|. \tag{4.33}$$

From Lemmas 3.6 and 4.3 (4.12), there exists κ_0 such that, for all $\alpha<0$, for all $\kappa\leqslant\kappa_0$, we get the estimate

$$\hat{R}_{n-1}-\tilde{R}_{n-1}=\mathcal{O}(\exp(-2\sqrt{2}(1+\alpha\kappa)\kappa x)). \tag{4.34}$$

From Lemma 4.4 [see $(4.13)_c$], for all $\alpha<0$, there exists κ_0 such that, for all $\kappa\leqslant\kappa_0$, we get the inequality,

$$\alpha(2+\alpha\kappa)(\hat{f}_n(1-3\hat{f}_0^2)+\hat{R}_{n-1})\leqslant-\overline{C}\alpha\hat{f}_n,\quad \overline{C}>0. \tag{4.35}$$

Using (4.33) and (4.35), Inequality (4.31) becomes

$$R^{(n)}\leqslant 3(f_0^2-\hat{f}_0^2)\kappa^n\hat{f}_n+\kappa^n(\hat{R}_{n-1}-\tilde{R}_{n-1})+\mathcal{O}_{\alpha}^{un}(\kappa^{n+1})|\hat{f}_n|-\overline{C}\alpha\kappa^{n+1}\hat{f}_n. \tag{4.36}$$

Moreover, we have the estimate

$$f_0^2-\hat{f}_0^2=\tanh\left(\frac{\kappa x+x_0}{\sqrt{2}}\right)-\tanh\left(\frac{(1+\alpha\kappa)\kappa x+x_0}{\sqrt{2}}\right)=\mathcal{O}(\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)).$$

As $\alpha<0$, we have $f_0^2-\hat{f}_0^2>0$. Otherwise, from (4.28) and the fact that $\hat{f}_n<0$, we have the inequality

$$(f_0^2-\hat{f}_0^2)\hat{f}_n\leqslant 0,\quad \forall\ \ x\in\mathbb{R}^+.$$

According to (4.4), (4.8), and (4.34), it results that there exists $\hat{C}>0$ such that, for all $\beta\leqslant-\hat{C}$, for all $\alpha<0$, we get

$$3(f_0^2-\hat{f}_0^2)\hat{f}_n+\hat{R}_{n-1}-\tilde{R}_{n-1}<0, \quad \forall \quad x\in\mathbb{R}^+. \tag{4.37}$$

Then, from (4.36) and (4.37), for $x\in[-c\ln\kappa,+\infty[$, we get

$$R^{(n)}\leqslant(\mathcal{O}_\alpha^{un}(\kappa^{n+1})-\overline{C}\alpha\kappa^{n+1})\hat{f}_n. \tag{4.38}$$

There exists $\alpha_0<0$ such that, for all $\alpha\leqslant\alpha_0$, we have the inequality

$$\mathcal{O}_\alpha^{un}(\kappa^{n+1})-\overline{C}\alpha\kappa^{n+1}>0.$$

As $\hat{f}_n<0$, we deduce that, there exists $\alpha_0<0$ such that, for all $\alpha<\alpha_0$, there exists $\kappa_0>0$ such that, for all $\kappa\leqslant\kappa_0$, for all $x\in[-c\ln\kappa,+\infty[$, $c>0$, the right-hand side of (4.38) is negative. The proof of Proposition 4.7 follows.

Remark 4.8: In the following sections, we choice the parameter β in such a way that Proposition 4.7 is satisfied. Now, the pair $(f^{vdm,(n)},A^{vdm,(n)})$ only depends on the parameter α. We express the dependency on α of the functions G, $f^{vdm,(n)}$, $A^{vdm,(n)}$, and $R^{(n)}$ by writing G_α, $f_\alpha^{(n)}$, $A_\alpha^{(n)}$, and $R_\alpha^{(n)}$.

C. Lower bound for $A_\alpha^{(n)}$

1. Presentation of the problem

In order to construct a subsolution, we must obtain a lower bound for the function $A_\alpha^{(n)}$. We first show that the function $A^{vd,(n)}$ defined in (3.2) is a good approximation for the function $A_\alpha^{(n)}$ in the interval $[0,\kappa^{-\rho}]$, $\rho>0$. In the same spirit of Ref. 6, we establish the following proposition.

Proposition 4.9: There exists $r_{j(j\in\{1,\ldots,2n+2\})}$, such that, for all $r_0\in\mathbb{R}$, there exists a constant $\tilde{C}(r_0)$ and a function $J(x)$ defined on $\mathbb{R}^+$, by

$$J(x)=R(x)\exp\left(-\frac{1}{\sqrt{2}}x\right), \tag{4.39}$$

where

$$R(x)=\sum_{j=1}^{2n+2} r_j x^j+r_0,$$

such that, for all α, there exists $\kappa_0>0$, such that, for all $\kappa\leqslant\kappa_0$ and with

$$\kappa^{1/2}h=\sum_{i=0}^{n} h_i\kappa^i+\tilde{C}(r_0)\kappa^{n+1}, \tag{4.40}$$

the solution of (4.23) satisfies the inequality

$$A^{vd,(n)}(x)+\kappa^{n+1/2}J(x)\leqslant A_\alpha^{(n)}(x)<0, \quad \forall \quad x\in\mathbb{R}^+, \tag{4.41}$$

where $A^{vd,(n)}$ is defined in (3.1).

2. Approximation in the inner region

The proof of Proposition 4.9 is similar to the proof of Proposition 5.1 in Ref. 6. Let us introduce the function Z_α defined by

$$Z_\alpha(x)=(A^{vd,(n)}-A_\alpha^{(n)})(x). \tag{4.42}$$

First, we establish the following lemma.

Lemma 4.10: There exists a polynomial of degree $2n+1$, $R_1(x)$, *such that, for all* $\alpha<0$, *there exists* $\kappa_0>0$ *such that, for all* $\kappa\leqslant\kappa_0$, *we have on the interval* $[0,\kappa^{-1/(n+2)}]$, *the inequality*

$$-Z_\alpha''+f_\alpha^{(n)2}Z_\alpha\leqslant\kappa^{n+1/2}R_1(x)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.43}$$

To establish Lemma 4.10, we evaluate the difference $\tilde{F}^{e,(n),m}(\kappa x)-F^{\mathrm{pol},(n+1)}(x;\kappa)$ on the interval $[0,\kappa^{-1/(n+2)}]$. Using Lemma 3.4 and the proof of Lemma 5.5 in Ref. 6, we can prove the following lemma.

Lemma 4.11: For all $\alpha<0$, *there exists* $\kappa_0>0$ *such that, for all* $\kappa\leqslant\kappa_0$, *for all* $x\in[0,\kappa^{-1/(n+2)}]$, *we have the estimate*

$$\tilde{F}^{e,(n),m}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)=\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{4.44}$$

Proof of Lemma 4.10: We have the equality

$$\begin{aligned}-Z_\alpha''+f_\alpha^{(n)2}Z_\alpha=&-(A^{vd,(n)}(x))''+(F^{i,(n)}+\kappa^{n+2}G_\alpha)^2A^{vd,(n)}(x)\\&+2(F^{i,n+1}+\kappa^{n+2}G_\alpha)(\tilde{F}^{e,(n),m}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa))A^{vd,(n)}(x)\\&+A^{vd,(n)}(x)(\tilde{F}^{e,(n),m}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa))^2.\end{aligned} \tag{4.45}$$

As in Ref. 6, let us introduce

$$B(x)=-(A^{vd,(n)}(x))''+(F^{i,(n+1)}+\kappa^{n+2}G_\alpha)^2(x)A^{vd,(n)}(x), \tag{4.46}$$

$$C(x)=2(F^{i,n+1}+\kappa^{n+2}G_\alpha)(x)(\tilde{F}^{e,(n),m}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa))A^{vd,(n)}(x), \tag{4.47}$$

and

$$D(x)=A^{vd,(n)}(x)(\tilde{F}^{e,(n),m}(\kappa x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa))^2. \tag{4.48}$$

From (4.16), (4.17), and (4.19), we get, for κ small enough

$$\kappa^{n+2}G_\alpha=\mathcal{O}_\alpha^{un}(\kappa^{n+1})(x^{2n+1}+1)\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

From Proposition 3.8, we get then the estimate

$$B(x)=\mathcal{O}_\alpha^{un}(\kappa^{n+1/2})(x^{2n+1}+1)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.49}$$

We deduce, using (4.49), the existence of $\kappa_0>0$ and $\overline{p}$, such that, for all $\kappa\leqslant\kappa_0$, for $x\in[0,\kappa^{-1/(n+2)}]$

$$B(x)\leqslant\kappa^{n+1/2}\overline{p}(x^{2n+1}+1)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.50}$$

From Lemma 4.11, for all $\alpha<0$, there exists κ_0 such that, for $\kappa\leqslant\kappa_0$, for $x\in[0,\kappa^{-1/(n+2)}]$, we have the estimates

$$F^{i,(n+1)}+\kappa^{n+2}G_\alpha=F_0+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)}),\quad A^{vd,(n)}=(\kappa^{-1/2}B_0+\mathcal{O}(\kappa^{1/2}))\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.51}$$

Using (4.47), (4.48), and (4.51), and following Ref. 6, we deduce that there exist some constants $\overline{p}$ and $\overline{q}$ such that

$$C(x)\leqslant\kappa^{n+1/2}\tilde{p}\exp\left(-\frac{1}{\sqrt{2}}x\right)\quad\text{and}\quad D(x)\leqslant\kappa^{n+1/2}\overline{q}\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.52}$$

From (4.36), (4.50), and (4.52), there exists a polynomial R_1 of degree $2n+1$ and κ_0 such that, for $\kappa\leqslant\kappa_0$, we get the inequality

$$-Z_\alpha''+(f_\alpha^{(n)})^2Z_\alpha\leqslant\kappa^{n+1/2}R_1(x)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.53}$$

We can choose

$$R_1(x)=\overline{p}x^{2n+1}+\overline{r},$$

where

$$\overline{r}=\overline{p}+\tilde{p}+\overline{q}. \tag{4.54}$$

The proof of Lemma 4.10 follows.

Using Lemmas 4.10 and 4.11, and following Ref. 6, we can state the following lemma.

Lemma 4.12: For $R_2(x)=\Sigma_1^{2n+2}r_ix^i$, let $J_2(x)=R_2(x)\exp[-(1/\sqrt{2})x]$. For $r_0\in\mathbb{R}$, let J be the function defined by

$$J=J_2+r_0\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.55}$$

There exists a polynomial R_2 such that, for all r_0, for all $\alpha<0$, there exists $\kappa_0>0$ such that, for all $\kappa\leqslant\kappa_0$, for all $x\in[0,\kappa^{-1/(n+2)}]$, we have the inequality

$$-(Z_\alpha''+(f_\alpha^{(n)})^2Z_\alpha)-\kappa^{n+1/2}(J''-(f_\alpha^{(n)})^2J)\leqslant-\kappa^{n+1/2}\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.56}$$

Proof: From the conclusion of Lemma 4.10, we get the inequality

$$-Z_\alpha''+f_\alpha^2Z_\alpha-\kappa^{n+1/2}(J''-f_\alpha^2J)\leqslant\kappa^{n+1/2}\left(R_1-R_2''+\sqrt{2}R_2'+\left(f_\alpha^2-\frac{1}{2}\right)(R_2+r_0)\right)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.57}$$

For $x\in\mathbb{R}$, we have

$$F^{i,(n+1)}-F^{\mathrm{pol},(n+1)}+\kappa^{n+1}G_\alpha=\mathcal{O}_\alpha^{un}(\kappa). \tag{4.58}$$

For $x\in[0,\kappa^{-1/(n+2)}]$, we have the estimate

$$\tilde{f}_0(\kappa x)=\tilde{f}_0(0)+\mathcal{O}(\kappa x). \tag{4.59}$$

From (4.15) and (4.59), we get

$$\tilde{F}^{e,(1),m}(\kappa x;\kappa)=\tilde{f}_0(0)+\mathcal{O}_\alpha(\kappa^{(n+1)/(n+2)}),\quad \forall\ x\in[0,\kappa^{-1/(n+2)}]. \tag{4.60}$$

From (4.18), (4.58), and (4.60), we get

$$f_\alpha(x)^2-\tfrac{1}{2}=\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)}). \tag{4.61}$$

Using (4.61), we have

$$\begin{aligned}
&R_1-R_2''+\sqrt{2}R_2'+(f_\alpha^2-\tfrac{1}{2})R_2\\
&\quad=(\sqrt{2}(2n+2)r_{2,2n+2}+\overline{p}+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_{2,2n+2}x)x^{2n+1}\\
&\qquad+\sum_{i=1}^{2n}(-i(i+1)r_{2,i+1}+\sqrt{2}ir_{2,i}+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_{2,i}x)x^i\\
&\qquad+\sqrt{2}r_{2,1}-2r_{2,2}+\overline{r}+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_{2,1}x+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_0.
\end{aligned} \tag{4.62}$$

To get a negative sign for the expression $R_1-R_2''+\sqrt{2}R_2'+(f_\alpha^2-\frac{1}{2})R_2$, we impose that

$$\begin{gathered}
\sqrt{2}(2n+2)r_{2,2n+2}+\overline{p}<-2,\\
\forall\ \ i\in\{1,\ldots,2n\},\quad i(i+1)r_{2,i+1}+\sqrt{2}\,i\,r_{2,i}<-2,\\
-2r_{2,2}+\overline{r}+\sqrt{2}r_{2,1}<-2,
\end{gathered} \tag{4.63}$$

where $\overline{p}$ and $\overline{r}$ are defined in (4.54). The system (4.63) admits solutions. We can indeed choose successively the constants $r_{2,2n+2}$, $r_{2,2n+1}$, ..., $r_{2,1}$ in (4.63). For all $\alpha<0$, there exists $\kappa_0(\alpha,r_0)>0$ such that, for all $\kappa\leqslant\kappa_0$, and for all $x\in[0,\kappa^{-1/(n+2)}]$,

$$\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_{2,i}x\leqslant 1,\quad \text{for all}\quad i\in\{1,\ldots,2n+2\}\quad\text{and}\quad \mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)})r_0<1. \tag{4.64}$$

According to (4.63) and (4.64), we deduce that, for all $\alpha<0$, there exists κ_0 such that, for $\kappa\leqslant\kappa_0$ and for all $x\in[0,\kappa^{-1/(n+2)}]$,

$$R_1-R_2''+\sqrt{2}R_2'+\left(f_\alpha^2-\frac{1}{2}\right)R_2\leqslant-\kappa^{n+1/2}\left(\sum_0^{2n+1}x^i\right). \tag{4.65}$$

Using (4.65), the inequality (4.57) becomes

$$-Z_\alpha''+f_\alpha^2Z_\alpha-\kappa^{n+1/2}(J_2''-f_\alpha^2J_2)\leqslant-\kappa^{n+1/2}\left(\sum_0^{2n+1}x^i\right)\exp\left(-\frac{1}{\sqrt{2}}x\right)\leqslant-\kappa^{n+1/2}\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

The proof of Lemma 4.12 follows.

3. Approximation in the outer region

Lemma 4.13: For $(r_{3,j})_{j\in\{0,\ldots,2n+2\}}\in\mathbb{R}^{2n+3}$, *let* R_3 *be a polynomial of degree* $2n+2$, *defined by*

$$R_3(x)=\sum_{j=0}^{2n+2}r_{3,j}x^j. \tag{4.66}$$

Let J_3 *be the function defined by*

$$J_3(x)=R_3(x)\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

Then, for all $r_{3,j}\,(j=0,\ldots,2n+1)$, *there exists* $\tilde{C}_3<0$ *such that, for all* $r_{3,2n+2}<\tilde{C}_3$, *for all* $\alpha<0$, *there exists* $\kappa_0>0$ *such that, for all* $\kappa\leqslant\kappa_0$, *we have*

$$-(Z_\alpha+\kappa^{n+1/2}J_3)''+f_\alpha^2(Z_\alpha+\kappa^{n+1/2}J_3)<0,\quad \forall\quad x\in[\kappa^{-1/(n+2)},+\infty[. \tag{4.67}$$

Proof: Step 1. Control in the interval $[\kappa^{-1/(n+2)},\kappa^{-1/2}]$. In this region, we write $f_\alpha^{(n)}$ in the form of

$$f_\alpha^{(n)}(x)=F^{e,(n),m}(x;\kappa)+[F^{i,(n+1)}(x;\kappa)-F^{\mathrm{pol},(n+1)}(x;\kappa)]+\kappa^{n+2}G_\alpha.$$

In the interval $[\kappa^{-1/(n+2)},\kappa^{-1/2}[$, from the structure of F_i and G_α, we get the estimate

$$\sum_{i=0}^{n+1}F_i\kappa^i+\kappa^{n+2}G_\alpha-F^{\mathrm{pol},(n+1)}=\mathcal{O}_\alpha^{un}(\kappa)(x^{2n+1}+1)\exp(-\sqrt{2}x).$$

For $\ell\in\{0,\ldots,n-1\}$, we have, for all $x\in[\kappa^{-1/(n+2)},\kappa^{-1/2}]$,

$$\kappa^\ell\tilde{f}_\ell(x)=\sum_{k=0}^{n+2-\ell}\frac{\tilde{f}_\ell^{(k)}(0)}{k!}\kappa^{k+\ell}x^k+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{4.68}$$

Furthermore, for all $x\in[\kappa^{-1/(n+2)},\kappa^{-1/2}]$,

$$\kappa^n\overline{f}_n(x)=\sum_{k=0}^{2}\frac{\tilde{f}_n^{(k)}(0)}{k!}\kappa^{k+n}x^k+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{4.69}$$

For $x\in[\kappa^{-1/(n+2)},\kappa^{-1/2}]$, from (4.18), (4.68), and (4.69), we can write

$$f_\alpha^{(n)}(x)=\sum_{j-n\leqslant i\leqslant j\leqslant n+1}\beta_{i,j}\kappa^jx^i+\frac{\tilde{f}_0^{(n+2)}(0)}{(n+2)!}\kappa^{n+2}x^{n+2}+o(\kappa^{n+2}x^{n+2})+\mathcal{O}_\alpha^{un}(\kappa^{n+1}).$$

From Proposition 2.2, Proposition 2.6 [see (2.14)], and the fact that $F_{n+1}^{\mathrm{pol}}(0)=0$, we can write this equality in the form of

$$f_\alpha^{(n)}(x)=\sum_{k=0}^{n+1}\kappa^kF_k^{\mathrm{pol}}+\frac{\tilde{f}_0^{(n+2)}(0)}{(n+2)!}\kappa^{n+2}x^{n+2}+o(\kappa^{n+2}x^{n+2})+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{4.70}$$

Using this expression to represent the function $f_\alpha^{(n)}$, we get

$$\begin{aligned}-Z_\alpha''+(f_\alpha^{(n)})^2Z_\alpha=&-(A^{vd,(n)})''\\&+A^{vd,(n)}\left(\sum_{k=0}^{n+1}\kappa^kF_k^{\mathrm{pol}}+\frac{\tilde{f}_0^{(n+2)}(0)}{(n+2)!}\kappa^{n+2}x^{n+2}+o(\kappa^{n+2}x^{n+2})+\mathcal{O}_\alpha(\kappa^{n+1})\right)^2.\end{aligned} \tag{4.71}$$

Using the equation verified by Q_j for $j\in\{1,\ldots,n\}$ and Proposition 2.2, we get the estimate on $[\kappa^{-1/(n+2)},\kappa^{-1/2}]$

$$Q_j'' - \sum_{\substack{\ell+|i|_{1,j}=j,\ \ell\in\mathbb{N} \\ |i|_{0,j}=2}} \frac{2!}{i_0!\cdots i_j!} Q_\ell \prod_{k=0}^{j} (F_k^{\mathrm{pol}})^{i_k} = \mathcal{O}(x^{2j-2}) \exp\left(-\frac{1}{\sqrt{2}}x\right).$$

For $j\in\{1,\ldots,n\}$, using the previous equality and from (4.71), we get

$$-Z_\alpha'' + f_\alpha^{(n)2} Z_\alpha = \kappa^{n+1} W A^{vd,(n)}, \tag{4.72}$$

where

$$W := \sum_{\substack{|i|_{1,n+1}=n+1 \\ |i|_{0,n+1}=2}} \prod_{k=0}^{n+1} (F_k^{\mathrm{pol}})^{i_k} + 2\frac{F_0}{(n+2)!} \tilde{f}_0^{(n+2)}(0)\kappa x^{n+2}. \tag{4.73}$$

From (4.72), it results the equality

$$\begin{aligned} &-(Z_\alpha + \kappa^{n+1/2} J_3)'' + (f_\alpha^{(n)})^2 (Z_\alpha + \kappa^{n+1/2} J_3) \\ &\quad = \kappa^{n+1} W.A^{vd,(n)} + \kappa^{n+1/2}((f_\alpha^{(n)2} - 1/2)R_3 - R_3'' + \sqrt{2}R_3') \exp\left(-\frac{1}{\sqrt{2}}x\right). \end{aligned} \tag{4.74}$$

As in Ref. 6 Lemma 5.7, we can prove that $(f_\alpha^{(n)})^2 - \frac{1}{2} > 0$ on $[\kappa^{-1/(n+1)}, \kappa^{-1/2}[$ and $(f_\alpha^{(n)})^2 - \frac{1}{2} = \mathcal{O}_\alpha^{un}(\kappa^{1/2})$.

Let us assume that

$$r_{3,2n+2} < 0. \tag{4.75}$$

Then, from (4.66) and (4.75), we deduce the upper bound, for some C, for $x \in [\kappa^{-1/(n+1)}, \kappa^{-1/2}[$ and for κ small enough

$$(f_\alpha^{(n)2} - \tfrac{1}{2})R_3 - R_3'' + \sqrt{2}R_3') \leqslant -R_3'' + \sqrt{2}R_3' \leqslant C r_{3,2n+2}\, x^{2n+1}. \tag{4.76}$$

Furthermore, as $A^{vd,(n)} = \mathcal{O}(\kappa^{-1/2})\exp(-(1/\sqrt{2})x)$ and $\deg F_n^{\mathrm{pol}} = n$ (see Proposition 2.2), and from (3.48), there exist $d>0$ and κ_0 such that, for all $\kappa \leqslant \kappa_0$, for all $x \in [\kappa^{-1/(n+2)}, \kappa^{-1/2}[$, we have the inequality

$$W A^{vd,(n)} \leqslant \mathrm{d}\kappa^{-1/2} x^{n+1} \exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.77}$$

Consequently, from (4.76) and (4.77), when κ is small enough, the right-hand side of (4.74) is negative on $[\kappa^{-1/(n+2)}, \kappa^{-1/2}[$.

Step 2. Control in the interval $[\kappa^{-1/2}, +\infty[$. In this region, from the structure of Q_i [see Proposition 2.2, (2.10)], we get for $i\in\{0,\ldots,n\}$, the estimate

$$Q_i = \left(\tilde{P}_i + \mathcal{O}\left(x^{m_i}\exp\left(-\frac{1}{\sqrt{2}}x\right)\right)\right)\exp\left(-\frac{1}{\sqrt{2}}x\right), \quad m_i\in\mathbb{N},$$

where $\tilde{P}_i$ is the polynomial part of R_n in the variable x. Let us recall that the degree of $\tilde{P}_i$ is equal to $2i$. We have the equality

$$-Q_i'' + f_\alpha^{(n)2} Q_i = \left(\left((f_\alpha^{(n)})^2 - \frac{1}{2}\right)\tilde{P}_i - \sqrt{2}\tilde{P}_i' + \tilde{P}_i'' + \mathcal{O}\left(\exp\left(-\frac{1}{\sqrt{2}}x\right)\right)\right)\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

Then, we can write

$$-(Z_\alpha+\kappa^{n+1/2}J_3)''+f_\alpha^{(n)2}(Z_\alpha+\kappa^{n+1/2}J_3)$$
$$=\left[\left(f_\alpha^{(n)2}-\frac{1}{2}\right)\kappa^{-1/2}\left(\sum_{i=0}^{n}(\kappa^i\tilde{P}_i)+\kappa^{n+1}R_3\right)\right.$$
$$\left.+\kappa^{1/2}\left(\sum_{i=1}^{n}(\sqrt{2}\tilde{P}_i'-\tilde{P}_i'')\kappa^{i-1}+\kappa^n(\sqrt{2}R_3'-R_3'')+\mathcal{O}\left(\exp\left(-\frac{1}{\sqrt{2}}x\right)\right)\right)\right]\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{4.78}$$

Let us denote by d_i, the coefficient of the monom of highest degree of $\tilde{P}_i$.

We set

$$\gamma_i=0 \quad \text{if } d_i<0, \quad \gamma_i=2d_i \quad \text{if } d_i>0.$$

As $r_{3,2n+2}<0$ and $\deg\tilde{P}_i=2i$, we have the inequality, for κ small enough and for $x\in[\kappa^{-1/2}, +\infty[$,

$$\sum_{i=0}^{n}\kappa^i\tilde{P}_i+\kappa^{n+1}R_3\leqslant\sum_{i=0}^{n}\gamma_i\kappa^i x^{2i}+\frac{\kappa^{n+1}}{2}r_{3,2n+2}x^{2n+2}.$$

The polynomial

$$\sum_{i=0}^{n}\gamma_i\kappa^i x^{2i}+\frac{\kappa^{n+1}}{2}r_{3,2n+2}x^{2n+2}$$

is negative on $[\kappa^{-1/2},+\infty[$ under the condition

$$r_{3,2n+2}<-2\sum_{i=0}^{n}\gamma_i. \tag{4.79}$$

Let us control the term $\Sigma_{i=1}^{n}(\sqrt{2}\tilde{P}_i'-\tilde{P}_i'')\kappa^{i-1}+\kappa^n(\sqrt{2}R_3'-R_3'')$. We have the inequality, for some C

$$\sum_{i=1}^{n}(\sqrt{2}\tilde{P}_i'-\tilde{P}_i'')\kappa^{i-1}+\kappa^n(\sqrt{2}R_3'-R_3'')\leqslant C\left(\sum_{i=1}^{n}\sqrt{2}i\,\gamma_i\kappa^{i-1}x^{2i-1}+\kappa^n(2n+2)r_{3,2n+2}x^{2n+1}\right).$$

The polynomial $\Sigma_{i=1}^{n}\sqrt{2}i\,\gamma_i\kappa^{i-1}x^{2i-1}+\kappa^n(2n+2)r_{3,2n+2}x^{2n+1}$ is negative on $[\kappa^{-1/2},+\infty[$ under the condition

$$r_{3,2n+2}<-\frac{1}{2n+2}\sum_{i=1}^{n}i.\gamma_i. \tag{4.80}$$

In conclusion, Inequality (4.67) is verified under conditions (4.75), (4.79), and (4.80), then under the unique condition

$$r_{3,2n+2}<\tilde{C}_3, \tag{4.81}$$

where $\tilde{C}_3$ is defined in the following way:

$$\tilde{C}_3 < \inf\left\{ -2\sum_{i=1}^{n} \gamma_i, -\frac{1}{2n+2}\sum_{i=1}^{n} i\gamma_i, 0 \right\}. \tag{4.82}$$

D. Proof of Proposition 4.9

This proof is similar to the proof of Proposition 5.1 in Ref. 6. We apply the maximum principle (see Lemma 5.2 in Ref. 6) to the function $Z_\alpha + \kappa^{n+1/2} J$. From Lemmas 4.12 and 4.13, we get for some $R(x)$

$$-(Z_\alpha + \kappa^{n+1/2} J)'' + f_\alpha^{(n)2}(Z_\alpha + \kappa^{n+1/2}) J \leqslant 0, \quad \forall \quad x \in \mathbb{R}^+.$$

According to (3.2) and (4.23), the condition $(Z_\alpha + \kappa^{n+1/2} J)'(0) \geqslant 0$ is satisfied if

$$\tilde{C} \leqslant J_2'(0) - \frac{r_0}{\sqrt{2}}. \tag{4.83}$$

If we assume (4.83), the proof of Proposition 4.9 follows.

V. THE FUNCTION $f_\alpha^{(n)}$ IS A SUBSOLUTION

Control of the sign of the function $R_\alpha^{(n)}$ in the inner region: We want to get an analogous estimate to (3.32) replacing the pair $(f^{vd,(n)}, A^{vd,(n)})$ by the pair $(f_\alpha^{(n)}, A_\alpha^{(n)})$.

Lemma 5.1: There exist some constants p_0 and p_1, and for all $r_0 > 0$, a constant $C(r_0)$ such that, for all $\alpha < 0$, there exists $\kappa_0 > 0$, such that, for all $\kappa \leqslant \kappa_0$ and for $h > 0$ such that

$$\kappa^{1/2} h = \sum_{i=0}^{n} h_i \kappa^i + \tilde{C}\kappa^{n+1}, \tag{5.1}$$

the pair $(f_\alpha^{(n)}, A_\alpha^{(n)})$ satisfies, for all $x \in [0, \kappa^{-1/(n+2)}]$, the estimate

$$R_\alpha^{(n)} \leqslant (-2\alpha \tilde{f}_n''(0) + p_0)\kappa^{n+1} + \kappa^n (p_1(1 + x^{2n+2}) - r_0)\exp(-\sqrt{2}x) - \kappa^n G_\alpha''. \tag{5.2}$$

Proof: In view to use Proposition 3.10, we write $f_\alpha^{(n)}$ in the form

$$f_\alpha^{(n)} = f^{vd,(n-1)} + \kappa^n \overline{f}_n(\kappa x) + \kappa^{n+1}(F_{n+1} - F_{n+1}^{\mathrm{pol}}) + \kappa^{n+2} G_\alpha. \tag{5.3}$$

For all $x \in [0, \kappa^{-1/(n+2)}]$, we have the equality

$$\overline{f}_n(\kappa x) = \tilde{f}_n((1 + \alpha\kappa)\kappa x) = \tilde{f}_n(\kappa x) + \alpha\kappa^2 x \int_0^1 \tilde{f}_n'(\kappa x + \alpha\kappa^2 x\, t)\, \mathrm{d}t. \tag{5.4}$$

Using (5.3) and (5.4), we get the equality

$$f_\alpha^{(n)} = f^{vd,(n)} + \alpha\kappa^{n+2} x \int_0^1 \tilde{f}_n'(\kappa x + \alpha\kappa^2 x\, t)\, \mathrm{d}t + \kappa^{n+2} G_\alpha. \tag{5.5}$$

According to (4.16) and (4.19), for all $\alpha < 0$, there exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, we have for $x \in [0, \kappa^{-1/(n+2)}]$, the estimate

$$\alpha\kappa^{n+2} x \int_0^1 \tilde{f}_n'(\kappa x + \alpha\kappa^2 x\, t)\, \mathrm{d}t + \kappa^{n+2} G_\alpha = \mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{5.6}$$

From (5.5), we get the estimate

$$-\kappa^{-2}(f_\alpha^{(n)})'' = -\kappa^{-2}(f^{vd,(n)})'' - 2\kappa^{n+1}\alpha \tilde{f}_n''(0) - \kappa^n G_\alpha'' + \mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{5.7}$$

According to (5.5) and (5.6), we deduce the equality

$$-f_\alpha^{(n)}=-f^{vd,(n)}+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{5.8}$$

From Proposition 4.9, we get

$$A_\alpha^{(n)2}f_\alpha^{(n)}\leqslant(A^{vd,(n)}+\kappa^{n+1/2}J)^2f_\alpha^{(n)}. \tag{5.9}$$

From (3.1), (3.2), (4.18), and (4.39), for $x\in[0,\kappa^{-1/(n+2)}]$, for κ small enough, we have the estimates

$$\begin{aligned} &f_\alpha^{(n)}=F_0+\mathcal{O}_\alpha^{un}(\kappa^{(n+1)/(n+2)}),\quad f^{vd,(n)}=F_0+\mathcal{O}(\kappa^{(n+1)/(n+2)}),\\ &A^{vd,(n)}=(\kappa^{-1/2}B_0+\mathcal{O}(k^{1/2}))\exp\left(-\frac{1}{\sqrt{2}}x\right),\quad J=(\mathcal{O}(x^{2n+2}+1)+r_0)\exp\left(-\frac{1}{\sqrt{2}}x\right). \end{aligned} \tag{5.10}$$

From (5.5), we have

$$(f_\alpha^{(n)})^3=(f^{vd,(n)})^3+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \tag{5.11}$$

Moreover from (3.8), we have $2F_0B_0=-2^{1/4}$. Then, following Ref. 6 (see Lemma 6.2), and from (5.7), (5.8), (5.10), and (5.11), we obtain that for all $\alpha<0$ and $r_0>0$, there exists κ_0 such that, for all $\kappa\leqslant\kappa_0$, we have the inequality

$$\begin{aligned} R_\alpha^{(n)}\leqslant&-\kappa^{-2}(f^{vd,(n)})''-f^{vd,(n)}+(f^{vd,(n)})^3+(A^{vd,(n)})^2f^{vd,(n)}-2\kappa^{n+1}\alpha\tilde{f}_n''(0)-\kappa^nG_\alpha''-\kappa^{n+2}G_\alpha\\ &-2^{1/4}r_0\kappa^n\exp(-\sqrt{2}x)+\mathcal{O}_{r_0}^{un}(\kappa^n)(x^{2n+2}+1)\exp(-\sqrt{2}x). \end{aligned} \tag{5.12}$$

Then, using Proposition 3.10 [see (3.32)], Inequality (5.12) becomes

$$\begin{aligned} R_\alpha^{(n)}\leqslant&-2\kappa^{n+1}\alpha\tilde{f}_n''(0)-\kappa^nG_\alpha''-\kappa^nr_0\exp(-\sqrt{2}x)+\mathcal{O}_{r_0}^{un}(\kappa^n)(x^{2n+1}+1)\exp(-\sqrt{2}x)\\ &+\mathcal{O}_\alpha^{un}(\kappa^{n+1}). \end{aligned}$$

The proof of Lemma 5.1 follows.

Then, we can express the following proposition, which can be proven as Proposition 6.3 in Ref. 10

Proposition 5.2: There exist $\tilde{C}$ and $\theta>0$, such that, for all $\alpha\in]-\infty,-\theta]$, there exist $\kappa_0>0$ and r_0, such that, for all $\kappa\leqslant\kappa_0$ and for $h>0$ such that

$$\kappa^{1/2}h=\sum_{i=0}^{n}h_i\kappa^i+\bar{C}\kappa^{n+1}, \tag{5.13}$$

the pair $(f_\alpha^{(n)},A_\alpha^{(n)})$ satisfies for all $x\in[0,\kappa^{-1/(n+2)}]$, the inequality

$$R_\alpha^{(n)}\leqslant 0. \tag{5.14}$$

Proof of Theorems 4.6 and 1.2: Theorem 4.6 follows immediately from Propositions 4.7 and 5.2. The proof of Theorem 1.2 is similar to the proof of Theorem 1.2 in Ref. 6 replacing the condition

$$\kappa^{1/2}h=h_0+h_1\kappa+C\kappa^2 \text{ with the formula } \kappa^{1/2}h=\sum_{i=0}^{n}h_i\kappa^i+\tilde{C}\kappa^{n+1}.$$

VI. CONSTRUCTION OF A SOLUTION OF $(GL)_\infty$

A. Construction of a supersolution

In this section, in order to construct a supersolution, we start with the function defined in (4.18). Let us recall that this function depends on two parameters that we denote by $\overline{\alpha}$ and $\overline{\beta}$. Here, we suppose that

$$\overline{\alpha}>0.$$

We prove the following theorem.

Theorem 6.1: *Let $n\geqslant 2$. There exist $\hat{C}$, $\overline{\alpha}>0$ and $\kappa_0>0$ such that, for $\kappa\leqslant\kappa_0$ and for*

$$\kappa^{1/2}h=\sum_0^n h_i\kappa^i+\hat{C}\kappa^{n+1}, \tag{6.1}$$

the function $f^{vdm,(n)}$ defined in (4.18) is a supersolution of $(GL)_\infty$.

Proof: Let us remark that some relations like (4.12) and $(4.13)_{(a,b)}$ are still true when $\overline{\alpha}>0$.

Step 1. Estimate in the region $[-\ln\kappa,+\infty[$. As $f^{vdm,(n)}>0$, $(A^{vdm,(n)})^2 f^{vdm,(n)}\geqslant 0$. Then, following the proof of Proposition 4.7, we get the inequality

$$\begin{aligned}
&-\kappa^{-2}(f^{vdm,(n)})''+f^{vdm,(n)}(-1+(f^{vdm,(n)})^2+(A^{vdm,(n)})^2)\\
&\quad\geqslant f^{vdm,(n)3}-(f^{vd,(n-1)})^3+\kappa^{n+1}\overline{\alpha}(2+\overline{\alpha}\kappa)(\hat{f}_n(1-3\hat{f}_0^2)+\hat{R}_{n-1})\\
&\qquad+\kappa^n\widetilde{R}_{n-1}-3\kappa^n\hat{f}_0^2\hat{f}_n+\kappa^n\hat{R}_{n-1}+\mathcal{O}_{\overline{\alpha}}^{un}(\kappa^{n+1})|\hat{f}_n|.
\end{aligned}\tag{6.2}$$

As $3\hat{f}_0^2-1\geqslant\frac{1}{4}$, there exists a constant $\widetilde{C}_3>0$ such that, for κ small enough

$$\overline{\alpha}(2+\overline{\alpha}\kappa)(\hat{f}_n(1-3\hat{f}_0^2)+\hat{R}_{n-1})\geqslant-\widetilde{C}_3\overline{\alpha}\hat{f}_n.$$

As $\overline{\alpha}>0$, we have $f_0^2-\hat{f}_0^2<0$. Otherwise, from (4.28) and the fact that $\hat{f}_n<0$, we get the inequality

$$(f_0^2-\hat{f}_0^2)\hat{f}_n\geqslant 0,\quad\forall\quad x\in\mathbb{R}^+.$$

According to (4.4), (4.8), and (4.34), it results that there exists $C_4>0$ such that, for all $\overline{\beta}\leqslant -C_4$, for all $\overline{\alpha}>0$, we get

$$3(f_0^2-\hat{f}_0^2)\hat{f}_n+\hat{R}_{n-1}-\widetilde{R}_{n-1}>0.$$

Then, according to (4.33) and (6.2), it results that

$$R^{(n)}\geqslant(\mathcal{O}_{\overline{\alpha}}^{un}(\kappa^{n+1})-C\overline{\alpha}\kappa^{n+1})\hat{f}_n. \tag{6.3}$$

The right-hand side of (6.3) is positive for $\overline{\alpha}$ large enough.

Step 2. Estimate in the region $[0,\kappa^{-1/(n+2)}]$. Following the proof of Proposition 4.9, and more precisely, replacing the function Z_α defined in (4.42) by the function $-Z_\alpha$, one can prove that there exists $\overline{r_j}$, $(j\in\{1,\ldots,2n+2\})$, such that, for all $\overline{r_0}\in\mathbb{R}$, there exists a constant $\hat{C}(\overline{r_0})$ and a function $\widetilde{J}$ defined on $\mathbb{R}^+$, by

$$\widetilde{J}(x)=R(x)\exp\left(-\frac{1}{\sqrt{2}}x\right), \tag{6.4}$$

where $R(x)=\Sigma_{j=1}^{2n+2}\overline{r}_j x^j+\overline{r}_0$, such that, for all $\overline{\alpha}>0$, there exists $\kappa_0>0$, such that, for all $\kappa \leqslant \kappa_0$ and with

$$\kappa^{1/2}h=\sum_{i=0}^{n} h_i\kappa^i+\hat{C}(\overline{r}_0)\kappa^{n+1}, \tag{6.5}$$

the solution of (4.23) satisfies the inequality

$$A^{vd,(n)}+\kappa^{n+1/2}\tilde{J}\geqslant A_\alpha^{(n)}, \quad \forall \quad x\in\mathbb{R}^+. \tag{6.6}$$

The condition on $\hat{C}$ is given by

$$\hat{C}\geqslant\tilde{J}'(0). \tag{6.7}$$

As $B_0<0$, let us remark that, from Proposition 2.2 ($\deg V_n=2n$), we have $A^{vd,(n)}+\kappa^{n+1}J\leqslant 0$, for $x\in[0,\kappa^{-1/(n+2)}]$ and κ small enough. Then, following the proof of Lemma 5.1, one can get the inequality

$$R_\alpha^{(n)}\geqslant -2\kappa^{n+1}(\overline{\alpha}\tilde{f}_n''(0)+p_0)-\kappa^n G_\alpha''+\kappa^n(p_1(1+x^{2n+2})-2^{1/4}\overline{r}_0)\exp(-\sqrt{2}x). \tag{6.8}$$

As $\tilde{f}_n''(0)<0$, for $\overline{\alpha}$ large enough, we have the inequality

$$-2\overline{\alpha}\tilde{f}_n''(0)-2p_0>0.$$

In another hand, according to (4.16) and (4.17), there exists $\rho>0$ such that

$$G_\alpha''\leqslant\tilde{f}_n'(0)\overline{\alpha}(1+x^{2n+2}-\rho)\exp(-\sqrt{2}x).$$

If we assume $\overline{r}_0\leqslant 2^{-1/4}\rho\tilde{f}_n'(0)\overline{\alpha}$ and if we choose $\overline{\alpha}$ large enough, we get

$$G_\alpha''\leqslant(p_1(1+x^{2n+2})-2^{1/4}\overline{r}_0)\exp(-\sqrt{2}x).$$

Thus, the right-hand side of inequality (6.8) is positive. The proof of Theorem 6.1 follows.

We denote by $(f_{\sup},A_{\sup})$ the supersolution obtained in Theorem 6.1.

B. Construction of solutions of $(GL)_\infty$

In this section, in order to simplify the computations, we set $n=2$ and we consider $f^{vd,(2)}$ and $A^{vd,(2)}$ introduced in Definition 3.1. These two functions only depend on the parameters C_0, C_1, and C_2 which are computed following Proposition 4.6 in Ref. 7. Let us recall that (see Ref. 5, p. 87 and Ref. 10)

$$C_0=\sqrt{2}\operatorname{arctanh}\left(\frac{1}{\sqrt{2}}\right), \quad C_1=-\tfrac{15}{16}\sqrt{2}, \quad C_2=\tfrac{429}{512}. \tag{6.9}$$

Using the construction of the subsolution and the supersolution exposed in the preceding sections, we get a localization of solutions of $(GL)_\infty$.

Theorem 6.2: *There exist C, $\tilde{C}_1>0$, $\tilde{C}_2>0$ and $\kappa_0>0$ such that, for all $\kappa\leqslant\kappa_0$ and $h>0$ such that*

$$\kappa^{1/2}h=\sum_{i=0}^{2} h_i\kappa^i+C\kappa^3, \tag{6.10}$$

there exists a pair (f,A) solution of $(GL)_\infty$ and satisfying the inequalities, for $x\in[0,+\infty[$

$$|f-f^{vd,(2)}|\leqslant \widetilde{C}_1\kappa^{3/2}\exp\left(-\frac{\sqrt{2}}{2}\kappa x\right), \tag{6.11}$$

and

$$|A-A^{vd,(2)}|\leqslant \widetilde{C}_2\kappa P(x)\exp\left(-\frac{\sqrt{2}}{2}x\right), \tag{6.12}$$

where P is a positive polynomial of degree 6.

Proof: Step 1. Construction of a solution. First, following Sects. IV and V, we construct a subsolution $(f_{\text{sub}},A_{\text{sub}})$ such that $A'_{\text{sub}}(0)=h$ where h satisfies (6.10) for some C. To express that the functions f_{sub} and $A^{vd,(2)}_{\text{sub}}$ defined in (3.2) and (4.18) depend on the parameters α and β, we set

$$f_{\text{sub}}(x;\kappa)=\sum_{k=0}^{1}\tilde{f}_k^{\text{sub}}(\kappa x)\kappa^k+\kappa^2\hat{f}_2^{\text{sub}}(x)+\sum_{k=0}^{3}\hat{F}_k^{\text{sub}}(x)\kappa^k+\kappa^4 G_\alpha(x) \tag{6.13}$$

and

$$A^{vd,(2)}_{\text{sub}}=\kappa^{-1/2}(Q_0^{\text{sub}}+\kappa Q_1^{\text{sub}}+\kappa^2 Q_2^{\text{sub}}). \tag{6.14}$$

The parameter β should satisfy the condition $\beta\leqslant -\hat{C}$ introduced in the proof of Proposition 4.7 and C should satisfy (4.83). Let us remark that we can choose $|\beta|$ arbitrarily large.

Now, in the same way, we want to construct a pair $(f_{\text{sup}},A_{\text{sup}})$ supersolution of (GL_∞) such that $A'_{\text{sup}}(0)=h$. In this goal, we modify the parameter C_1, and more precisely, we replace $(C_0,C_1,\overline{\beta})$ with $(C_0,C_1+\overline{\gamma}\kappa^\epsilon,\overline{\beta})$ in (2.14) (see Remark 3.2). ϵ and $\overline{\gamma}$ are parameters which will be determined later. Then, we introduce $(f_{\text{sup}},A^{vd,(2)}_{\text{sup}})$, the pair defined in (3.2) and (4.18) with this choice. To express that the functions f_{sup} and $A^{vd,(2)}_{\text{sup}}$ depend on the parameters $\overline{\alpha}$ and $\overline{\beta}$, we set

$$f_{\text{sup}}(x;\kappa)=\sum_{k=0}^{1}\tilde{f}_k^{\text{sup}}(\kappa x)\kappa^k+\kappa^2\hat{f}_2^{\text{sup}}(x)+\sum_{k=0}^{3}\hat{F}_k^{\text{sup}}(x)\kappa^k+\kappa^4 G_{\overline{\alpha}}(x) \tag{6.15}$$

and

$$A^{vd,(2)}_{\text{sup}}=\kappa^{-1/2}(Q_0^{\text{sup}}+\kappa Q_1^{\text{sup}}+\kappa^2 Q_2^{\text{sup}}). \tag{6.16}$$

From Ref. 5, p. 62, we have $A_1-(B_0^2/4A_0)=\tilde{f}'_0(0)C_1$. Otherwise, from Ref. 5, p. 86, for C_0 satisfying (6.9) and for all $(C_1,\beta)\in\mathbb{R}^2$, we get

$$\check{H}_2(0;C_0,C_1,\beta)=-2^{5/4}(\tilde{f}'_0(0)C_1+\tfrac{1}{4})^2-\tfrac{7}{8}2^{1/4}(\tilde{f}'_0(0)C_1+\tfrac{1}{4})-\tfrac{521}{2048}2^{1/4}. \tag{6.17}$$

From Ref. 7 (see Proposition 4.8 and Theorem 4.9), for C_0 and C_1 satisfying (6.9), we have

$$\frac{\partial\check{H}_2}{\partial C_1}(0;C_0,C_1,\overline{\beta})=0,$$

where $\check{H}_2$ is introduced in (2.15). For C_0 and C_1 satisfying (6.9), and for all $(\overline{\beta},\overline{\gamma})\in\mathbb{R}^2$, we have

$$\check{H}_2(0;C_0,C_1+\overline{\gamma}\kappa^\epsilon,\overline{\beta})=\check{H}_2(0;C_0,C_1,\overline{\beta})+\int_0^1\frac{\partial^2\check{H}_2}{\partial C_1^2}(0;C_0,C_1+\theta\overline{\gamma}\kappa^\epsilon,\overline{\beta})\,\mathrm{d}\theta\ \ \overline{\gamma}^2\kappa^{2\epsilon}. \tag{6.18}$$

From Theorem 4.9 in Ref. 7 (see also Ref. 5), for C_0 and C_1 satisfying (6.9) and for all $(\overline{\beta},\overline{\gamma}) \in \mathbb{R}^2$ and $\kappa>0$, we have

$$\check{H}_1(0;C_0,C_1+\overline{\gamma}\kappa^{\epsilon})=h_1, \quad \check{H}_2(0;C_0,C_1,\overline{\beta})=h_2. \tag{6.19}$$

From (6.17), we get the equality

$$\frac{\partial^2 \check{H}_2}{\partial C_1^2}(0;C_0,C_1+\theta\overline{\gamma}\kappa^{\epsilon},\overline{\beta})=-2^{9/4}\tilde{f}_0'(0)^2. \tag{6.20}$$

We remark that all the propositions in the preceding sections are still true when we replace $(C_0,C_1,\overline{\beta})$ with $(C_0,C_1+\overline{\gamma}\kappa^{\epsilon},\overline{\beta})$. It results that Theorem 6.1 is still true under two conditions satisfied by $\overline{\beta}$ and $\overline{\gamma}$. First, $\overline{\beta}$ should satisfy the condition $\overline{\beta}<-C_4$ which appears in the proof of Theorem 6.1. In order to satisfy the condition $(A_{\mathrm{sub}}-A_{\mathrm{sub}}^{vd,(2)})'(0)\geqslant 0$ [which corresponds to the condition (6.7)], from (6.10), (6.18), (6.19), and (6.20), we take $\epsilon=\frac{1}{2}$. Then, this condition is satisfied if we assume

$$C\geqslant \tilde{J}'(0)-2^{9/4}\tilde{f}_0'(0)^2\overline{\gamma}^2. \tag{6.21}$$

As the choice of β is independent of the choice of $\overline{\beta}$ and as we can choose β arbitrarly large, we choose β and $\overline{\beta}$ such that

$$4\overline{\beta}-\beta-2\sqrt{2}C_1^2>0. \tag{6.22}$$

This condition is introduced in order to get the inequality $f_{\mathrm{sub}}\leqslant f_{\mathrm{sup}}$. From (6.21), we remark that we can choose $\overline{\gamma}>0$.

Now, we compare f_{sub} and f_{sup}. From Proposition 2.1, we have

$$\tilde{f}_1=C_1\tilde{f}_0', \tag{6.23}$$

where

$$\tilde{f}_0'(x')=\cosh^{-2}\left(\frac{x'+C_0}{\sqrt{2}}\right). \tag{6.24}$$

According to (4.4), (4.5), and (4.8), we have

$$\hat{f}_2=C_2\hat{f}_0'+\hat{D}_2, \quad \text{with } \hat{D}_2=\frac{C_1^2}{2}\hat{f}_0''. \tag{6.25}$$

As $\tilde{f}_0^{\mathrm{sup}}=\tilde{f}_0^{\mathrm{sub}}$, from (6.13), (6.15), and (6.23), we have

$$\sum_{k=0}^{1}(\tilde{f}_i^{\mathrm{sup}}-\tilde{f}_i^{\mathrm{sub}})\kappa^i=\kappa^{3/2}\overline{\gamma}\tilde{f}_0'. \tag{6.26}$$

Moreover, from (6.13), (6.15), and (6.25), we have

$$\hat{f}_2^{\mathrm{sup}}-\hat{f}_2^{\mathrm{sub}}=\overline{\beta}\hat{f}_0'^{\mathrm{sup}}-\beta\hat{f}_0'^{\mathrm{sub}}+\hat{D}_2^{\mathrm{sup}}-\hat{D}_2^{\mathrm{sub}}. \tag{6.27}$$

According to (6.13),(6.15), (6.26), and (6.27), it results that

$$f_{\sup}-f_{\sub}=\kappa^2(\overline{\beta}\hat{f}_0'^{\sup}-\beta\hat{f}_0'^{\sub}+\hat{D}_2^{\sup}-\hat{D}_2^{\sub})+\kappa^{3/2}\overline{\gamma}f_0'^{\sup}+\sum_{k=1}^{3}(\hat{F}_k^{\sup}-\hat{F}_k^{\sub})\kappa^k+\kappa^4(G_{\overline{\alpha}}-G_\alpha). \tag{6.28}$$

Let us consider the term $\Sigma_{k=1}^{3}(\hat{F}_k^{\sup}-\hat{F}_k^{\sub})\kappa^k+\kappa^4(G_{\overline{\alpha}}-G_\alpha)$. In this sum, from Ref. 5, p. 52, the unique term depending on $\overline{\beta}$ and β is $\hat{F}_3^{\sup}-\hat{F}_3^{\sub}$. Moreover, we have

$$\hat{F}_1^{\sup}-\hat{F}_1^{\sub}=0, \tag{6.29}$$

and

$$\hat{F}_2^{\sup}-\hat{F}_2^{\sub}=\mathcal{O}(\kappa^{1/2})(x+1)\exp(-\sqrt{2}x). \tag{6.30}$$

According to (2.10) and (4.16), for $x\in\mathbb{R}^+$, we deduce that there exists $\overline{C}_{\overline{\beta},\beta}$ such that

$$\kappa^3(\hat{F}_3^{\sup}-\hat{F}_3^{\sub})+\kappa^4(G_{\overline{\alpha}}-G_\alpha)\geqslant\overline{C}_{\overline{\beta},\beta}\kappa^3(x^6+1)\exp(-\sqrt{2}x). \tag{6.31}$$

As $e^{-x}\leqslant\cosh^{-1}(x)\leqslant 2e^{-x}$, from (4.8) and (6.24), we get the inequalities

$$\overline{\beta}\hat{f}_0'^{\sup}\geqslant 4\overline{\beta}\exp(-\sqrt{2}((1+\overline{\alpha}\kappa)\kappa x+C_0)),\quad -\beta\hat{f}_0'^{\sub}\geqslant-\beta\exp(-\sqrt{2}((1+\alpha\kappa)\kappa x+C_0)), \tag{6.32}$$

and

$$\hat{D}_2^{\sup}-\hat{D}_2^{\sub}\geqslant-2\sqrt{2}C_1^2\exp(-\sqrt{2}((1+\alpha\kappa)\kappa x+C_0)). \tag{6.33}$$

According to (6.24), (6.25), (6.32), and (6.33), and as $\overline{\gamma}f_0'>0$, we get for $x\in\mathbb{R}^+$ and for $\hat{C}_{\overline{\beta},\beta}:=(4\overline{\beta}-\beta-2\sqrt{2}C_1^2)\exp(-\sqrt{2}C_0)$

$$\overline{\beta}\hat{f}_0'^{\sup}-\beta\hat{f}_0'^{\sub}+\hat{D}_2^{\sup}-\hat{D}_2^{\sub}\geqslant\hat{C}_{\overline{\beta},\beta}\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x). \tag{6.34}$$

From (6.22), it results that $C_{\overline{\beta},\beta}>0$. According to (6.28), (6.29), (6.30), (6.31), (6.34) and as $\overline{\gamma}f_0'^{\sup}>0$, we deduce that there exists $\tilde{C}$ such that

$$f_{\sup}-f_{\sub}\geqslant\hat{C}_{\overline{\beta},\beta}\kappa^2\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x)+(\kappa^{5/2}\tilde{C}(x+1)+\tilde{C}_{\overline{\beta},\beta}\kappa^3(x^6+1))\exp(-\sqrt{2}x).$$

It results that, for all $x\in\mathbb{R}^+$ and κ small enough, $f_{\sup}-f_{\sub}>0$. Then, using Proposition 6.5 in Ref. 3, we deduce that there exists a pair (f,A) solution of $(\mathrm{GL})_\infty$, such that

$$f_{\sub}\leqslant f\leqslant f_{\sup}. \tag{6.35}$$

Step 2. Estimates for $f-f^{vd,(2)}$ and $A-A^{vd,(2)}$. By definition of $f_{\sup}$ and $f^{vd,(2)}$, we have

$$f_{\sup}-f^{vd,(2)}=\kappa^2(\overline{\beta}\hat{f}_0'^{\sup}-C_2f_0'+\hat{D}_2^{\sup}-D_2)+\kappa^{3/2}\overline{\gamma}f_0'^{\sup}+\sum_{k=1}^{3}(\hat{F}_k^{\sup}-\hat{F}_k)\kappa^k+\kappa^4G_{\overline{\alpha}}. \tag{6.36}$$

Following the step 1, as $\overline{\alpha}>0$, we get

$$f_{\sup}-f^{vd,(2)}=\mathcal{O}(\kappa^{3/2})\exp(-\sqrt{2}\kappa x).$$

As $\alpha<0$, from (6.36) (replacing $f_{\sup}$ with $f_{\sub}$), we obtain

$$f_{\sub}-f^{vd,(2)}=\mathcal{O}(\kappa^{3/2})\exp(-\sqrt{2}(1+\alpha\kappa)\kappa x).$$

According to (6.35), we deduce that there exist $\tilde{C}_1>0$ and κ_0, such that, for all $\kappa\leqslant\kappa_0$, we get

$$|f-f^{vd,(2)}|\leqslant\tilde{C}_1\kappa^{3/2}\exp\left(-\frac{\sqrt{2}}{2}\kappa x\right),\quad \forall\, x\in\mathbb{R}^+.$$

Moreover, using Lemma 6.6 in Ref. 3, we know that the map defined on $C^0(\mathbb{R}^+)$ by $f\mapsto A(f)$, where $A(f)$ is the unique solution in $H^2(\mathbb{R}^+)$ of

$$-A''+f^2A=0,\quad A'(0)=h$$

is increasing. As $f_{\text{sub}}\leqslant f\leqslant f_{\text{sup}}$, it results that

$$A_{\text{sub}}\leqslant A\leqslant A_{\text{sup}}.$$

From Proposition 4.9 and (6.6), we get

$$A_{\text{sub}}^{vd,(2)}+\kappa^{5/2}J\leqslant A_{\text{sub}}\leqslant A\leqslant A_{\text{sup}}\leqslant A_{\text{sup}}^{vd,(2)}+\kappa^{5/2}\tilde{J}. \tag{6.37}$$

As $Q_0^{\text{sub}}=Q_0$ and $Q_1^{\text{sub}}=Q_1$, from (6.14), we get

$$A_{\text{sub}}^{vd,(2)}-A^{vd,(2)}=\kappa^{3/2}(Q_2^{\text{sub}}-Q_2).$$

From Proposition 2.2, we have the estimate

$$|Q_2^{\text{sub}}-Q_2|=\mathcal{O}(x^4+1)\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

Then, it results that

$$A_{\text{sub}}^{vd,(2)}-A^{vd,(2)}=\mathcal{O}(\kappa^{3/2})(x^4+1)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{6.38}$$

From Ref. 5, p. 52, we obtain $|Q_1^{\text{sup}}-Q_1|=\mathcal{O}(\kappa^{1/2})(x+1)\exp[-(1/\sqrt{2})\,x]$. As $|Q_2^{\text{sup}}-Q_2|=\mathcal{O}(x^4+1)\exp[-(1/\sqrt{2})\,x]$, we deduce that

$$A_{\text{sup}}^{vd,(2)}-A^{vd,(2)}=\mathcal{O}(\kappa)(x^4+1)\exp\left(-\frac{1}{\sqrt{2}}x\right). \tag{6.39}$$

Moreover, according to (4.39) and (6.4), we have the estimates

$$J=\mathcal{O}(x^6+1)\exp\left(-\frac{1}{\sqrt{2}}x\right),\quad \tilde{J}=\mathcal{O}(x^6+1)\exp\left(-\frac{1}{\sqrt{2}}x\right).$$

From (6.37), (6.38), and (6.39), it results that inequality (6.12) follows and this achieves the proof of Theorem 6.2.

VII. CONCLUSION

Theorem 1.2 leads one to express the following conjecture.

Conjecture 7.1: Let $h^{sh}(\kappa)$ be the superheating field, introduced in Definition 1.1 and $h^{sh,f}(\kappa):=\kappa^{-1/2}\Sigma_{i=0}^{+\infty}h_i\kappa^i$ be the formal superheating field.
For all $n\in\mathbb{N}$, there exist C and κ_0 such that, for all $\kappa\leqslant\kappa_0$ we have the inequality

$$\kappa^{1/2}h^{sh}(\kappa)\leqslant\sum_{i=0}^{n} h_i\kappa^i+C\kappa^{n+1}.$$

Let us recall that in Ref. 2, to get the DeGennes formula,[9] Bolley and Helffer have proved that

$$\kappa h^2\leqslant\frac{\sqrt{2}}{4}+\mathcal{O}(\kappa^{1/2}),$$

for all $h\in\mathcal{H}_\infty$ and for κ small enough. In Ref. 8, we improve this estimate and get

$$\kappa h^2\leqslant\frac{\sqrt{2}}{4}+\frac{15}{32}\kappa+\mathcal{O}(\kappa^{1+\rho})$$

for some $\rho>0$ and for all $h\in\mathcal{H}_\infty$. Taking account the lower bound for $h^{sh}(\kappa)$ obtained in Ref. 6, we deduce the Parr formula.[15] So, Conjecture 7.1 is an open problem for $n\geqslant 2$.

A second point is the study of the stability of the solutions of the (GL) equations constructed in Theorem 6.2. The goal is to prove that these solutions are stable.[1]

ACKNOWLEDGMENT

The author would like to thank B. Helffer for helpful discussions on the problem.

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Spectral properties of Pauli operators on the Poincaré upper-half plane

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(Received 14 December 2002; accepted 23 February 2003)

We investigate the essential spectrum of the Pauli operators (and the Dirac and the Schrödinger operators) with magnetic fields on the Poincaré upper-half plane. The magnetic fields under consideration are asymptotically constant (which may be equal to zero), or diverge at infinity. Moreover, the Aharonov–Casher type result is also considered. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1573742]

I. INTRODUCTION AND RESULT

In this article we study the spectral properties of the Pauli operator on the Poincaré upper-half plane $\mathbf{H}=\{(x,y)|x\in\mathbf{R},\ y>0\}$ endowed with the measure $dx\,dy/y^2$. The Pauli operator $P(\mathbf{a})$ is defined as the square of the Dirac operator $D(\mathbf{a})$ and has the physical interpretation as the Hamiltonian which governs a nonrelativistic spin 1/2 particle moving on $\mathbf{H}$. The following results (i)–(iii) are proved.

(i) The essential spectrum of $P(\mathbf{a})$ consists of the two parts; the continuous one and the (possibly empty) discrete Landau levels, if the magnetic field is asymptotically constant (Theorem 1.1 below).
(ii) If the magnetic field diverges at ''infinity,'' $P(\mathbf{a})$ has discrete spectrum (i.e., isolated eigenvalues of finite multiplicity), except for the ground state energy 0 which is an isolated eigenvalue of infinite multiplicity (Theorem 1.3 below).
(iii) For any compactly supported magnetic field, unlike the Euclidean case [Aharanov and Casher (1979)], the number of the zero-energy eigenstates of $P(\mathbf{a})$ is generically infinite (Theorem 1.6 below).

In the Euclidean case, Shigekawa (1991) studied the relation between the spectral properties of the Pauli operators and the asymptotic property of the magnetic fields in arbitrary space dimension [see also Ogurisu (1993)].

Fix some notation. For smooth manifolds Ω, we denote by $C_0^\infty(\Omega)$ the set of all complex valued, smooth functions on Ω with compact support and denote by $C(\Omega)$ the set of all complex valued, continuous functions on Ω. We denote by $C^k(\Omega;\mathbf{R}^n)$ the set of all k-times continuously differentiable maps from Ω to $\mathbf{R}^n$ and denote by $C(\Omega;\mathbf{R}^n)$ the set of all continuous maps from Ω to $\mathbf{R}^n$. We denote $\partial/\partial x$, $(1/i)(\partial/\partial x)$ by ∂_x, D_x, respectively. We denote L^2-norms on any function spaces by $\|\cdot\|$.

For a densely defined, closable linear operator A acting in a Hilbert space, we denote the domain of A by $D(A)$ and denote the operator closure of A by A. The notations $\ker(A)$ and $\mathrm{ran}(A)$ denote the kernel and the range of A, respectively. For any self-adjoint operator A, we denote the spectrum of A by $\sigma(A)$ and denote the essential spectrum of A by $\sigma_{\mathrm{ess}}(A)$ [e.g., Reed and Simon (1978), Vol. I].

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For a subset S of $\mathbf{R}$ and for a real number α, we denote by $S+\alpha$ the set $\{x+\alpha | x \in S\}$. If S is contained in the set of all positive real numbers, we denote by $\sqrt{S}$ the set $\{\sqrt{x} | x \in S\}$. If $S=\varnothing$, we set $S+\alpha=\varnothing$ and $\sqrt{S}=\varnothing$. For any family of sets $\{S_j\}_{j=0}^N$ with $N \geqslant 0$, we set $\cup_{j=0}^k S_j=\varnothing$ if $k<0$.

Throughout this article we always assume:

(B.0) The vector potential $\mathbf{a}=(a_1,a_2)$ belongs to $C^\infty(\mathbf{H};\mathbf{R}^2)$.

We introduce the differential operators $A(\mathbf{a})$ and $A^\dagger(\mathbf{a})$ with domain $C_0^\infty(\mathbf{H})$ as

$$A(\mathbf{a})=y(D_x-a_1(x,y))+iy(D_y-a_2(x,y)),$$

$$A^\dagger(\mathbf{a})=y(D_x-a_1(x,y))-iy(D_y-a_2(x,y))+1,$$

respectively. Note that $A^\dagger(\mathbf{a})$ is a formal adjoint operator of $A(\mathbf{a})$ with respect to the measure $dx\,dy/y^2$ and $A(\mathbf{a})$ is closable. The Dirac and the Pauli operators acting in $L^2(\mathbf{H}) \oplus L^2(\mathbf{H})$ are defined by

$$\mathcal{D}(\mathbf{a})=\begin{pmatrix} 0 & A^\dagger(\mathbf{a}) \\ A(\mathbf{a}) & 0 \end{pmatrix}, \tag{1.1}$$

and

$$P(\mathbf{a})=\mathcal{D}(\mathbf{a})^2=\begin{pmatrix} A^\dagger(\mathbf{a})A(\mathbf{a}) & 0 \\ 0 & A(\mathbf{a})A^\dagger(\mathbf{a}) \end{pmatrix}, \tag{1.2}$$

respectively. Under the condition (B.0), $P(\mathbf{a})$ is essentially self-adjoint on $C_0^\infty(\mathbf{H}) \oplus C_0^\infty(\mathbf{H})$ (see Lemma 2.1 in the next section). Hence, due to (1.1), so is $\mathcal{D}(\mathbf{a})$ [see Shubin (1976); see also Thaller (1992), Lemma 5.7]. The reason why we call $\mathcal{D}(\mathbf{a})$ by the name "Dirac operator" is explained in the Appendix. In what follows, for any closable operator T, we use the same symbol T for its closure, if there is no fear of confusion.

For any vector potential $\mathbf{a}$, we introduce the corresponding magnetic field B as

$$d\mathbf{a}(=\partial_x a_2-\partial_y a_1)=B/y^2.$$

In order to formulate our results, we introduce the following conditions for the magnetic fields.

(B.1) In addition to (B.0), there is a real number B_0 such that the perturbation

$$B_1=B-B_0 \tag{1.3}$$

decays at infinity, i.e., for any $\varepsilon>0$, there exists a compact subset K of $\mathbf{H}$ such that $|B_1(x,y)|<\varepsilon$ holds outside K.

(B.2) In addition to (B.0), the magnetic field B diverges at infinity, i.e., for any $N>0$ there exists a compact subset K of $\mathbf{H}$ such that $B(x,y) \geqslant N$ holds outside K.

Theorem 1.1: *Assume (B.1). Then we have*

$$\sigma_{\mathrm{ess}}(P(\mathbf{a}))=L(B_0) \cup [|B_0-1/2|^2,\ \infty),$$

where

$$L(B_0)=\begin{cases} \cup_{l=0}^{N(|B_0-1/2|)}\{l(|2B_0-1|-l)\}, & \text{if } B_0 \neq 1/2, \\ \varnothing, & \text{if } B_0=1/2, \end{cases} \tag{1.4}$$

and $N(x)$ denotes the largest integer less than x.

In particular, the ground state energy 0 belongs to $\sigma_{\mathrm{ess}}(P(\mathbf{a}))$ for all B_0 and, moreover, if $B_0 \neq 1/2$, it is an isolated eigenvalue of infinite multiplicity.

Remark 1.2: Let V belong to $C(\mathbf{H};\mathbf{R})$ *and decay at infinity. Then, using Lemma 2.1 in the next section, one can show the conclusion in Theorem 1.1 is still valid if we replace the operator* $P(\mathbf{a})$ *by* $P(\mathbf{a})+V$.

Theorem 1.3: *Assume (B.2). Then we have* $\sigma_{\mathrm{ess}}(P(\mathbf{a}))=\{0\}$ *and, moreover,* 0 *is an isolated eigenvalue of infinite multiplicity.*

Remark 1.4: Using the unitary transform $f(x,y)\mapsto f(-x,y)$, *one can show that the conclusion as in Theorem 1.3 is still valid in the case where B tends to* $-\infty$ *at infinity, instead of (B.2).*

The spectrum of the Dirac operator is known from the one of $P(\mathbf{a})$ because of the relation (1.2). In fact, if we introduce a slightly generalized form of the Dirac operator with non-negative constant mass m as

$$\mathcal{D}_m(\mathbf{a})=\mathcal{D}(\mathbf{a})+m\tau,\quad \tau=\begin{pmatrix}\mathrm{Id} & 0\\ 0 & -\mathrm{Id}\end{pmatrix}, \tag{1.5}$$

(the proof of) Proposition 2.5 in Shikegawa (1991) states that

$$\sigma(\mathcal{D}_m(\mathbf{a}))=\sqrt{\sigma(A(\mathbf{a})^*A(\mathbf{a}))+m^2}\cup(-\sqrt{\sigma(A(\mathbf{a})A(\mathbf{a})^*)+m^2}), \tag{1.6}$$

and the same equality replaced σ by σ_{ess} is valid. Here "Id" denotes the identity operator on $L^2(\mathbf{H})$.

For example, Theorem 1.1 yields the following

Corollary 1.5: Assume (B.1). Then we have

$$\sigma_{\mathrm{ess}}(\mathcal{D}_m(\mathbf{a}))=\begin{cases}(\sigma_-\backslash\{-m\})\cup\sigma_+\cup\sigma_c, & \text{if } B_0>1/2,\\ \sigma_c, & \text{if } B_0=1/2,\\ \sigma_-\cup(\sigma_+\backslash\{m\})\cup\sigma_c, & \text{if } B_0<1/2,\end{cases}$$

where we set

$$\sigma_-=-\sqrt{L(B_0)+m^2},$$

$$\sigma_+=\sqrt{L(B_0)+m^2},$$

$$\sigma_c=(-\infty,-\sqrt{|B_0-1/2|^2+m^2}]\cup[\sqrt{|B_0-1/2|^2+m^2},\ \infty).$$

Here $L(B_0)$ *is the set as in Theorem 1.1.*

Let T be a densely defined, closed operator acting in a Hilbert space. We say T *is semi-Fredholm* if the space $\mathrm{ran}(T)$ is closed and at least one of the dimensions of $\ker(T)$ and $\ker(T^*)$ is finite. Note that T is semi-Fredholm if and only if T^* is [Kato (1966), Chap. IV, Sec. 5, Corollary 5.14]. For any operator T, we define the index of T by

$$\mathrm{ind}(T)=\dim\ \ker(T)-\dim\ \ker(T^*),$$

which may take value $\pm\infty$, when either $\dim\ker(T)$ is finite or $\dim\ker(T^*)$ is.

Theorem 1.6: *Assume (B.1) and assume that the support of* B_1 *is compact. Then* $A(\mathbf{a})$ *is semi-Fredholm if and only if* $B_0\neq 1/2$. *Moreover, the index is given by*

$$\mathrm{ind}(A(\mathbf{a}))=\begin{cases}+\infty, & \text{if } B_0>1/2,\\ 0, & \text{if } B_0=1/2,\\ -\infty, & \text{if } B_0<1/2.\end{cases}$$

Remark 1.7: We recall the Aharonov–Casher (1979) theorem in the Euclidean setting, which corresponds to the case $B_0=1/2$ *in Theorem 1.6. Let* $\mathbf{a}=(a_1,a_2)\in C^\infty(\mathbf{R}^2;\mathbf{R}^2)$ *and assume that* $B_1=d\mathbf{a}$ *is compactly supported. Then the two-dimensional Pauli operator on* $\mathbf{R}^2$ *takes the form*

$$p(\mathbf{a})=\begin{pmatrix} a(\mathbf{a})^*a(\mathbf{a}) & 0 \\ 0 & a(\mathbf{a})a(\mathbf{a})^* \end{pmatrix}=\begin{pmatrix} \Sigma_{j=1}^2(D_{x_j}-a_j)^2+B_1 & 0 \\ 0 & \Sigma_{j=1}^2(D_{x_j}-a_j)^2-B_1 \end{pmatrix},$$

where $a(\mathbf{a})^*$ and $a(\mathbf{a})$ are the corresponding creation and annihilation operators. Then the zero-eigenspace of $p(\mathbf{a})$ is finite dimensional and the index can be described by the magnetic flux $F=(1/2\pi)\int_{R^2}B_1(z)dz$. Precisely,

$$\mathrm{ind}(a(\mathbf{a}))=\begin{cases} \mathrm{sgn}(F)\,|N(F)|, & \text{if } F\neq 0, \\ 0, & \text{if } F=0. \end{cases}$$

As for the proof [see Aharanov and Casher (1979) and the proof of Lemma 5.2 in Sec. V], the difference between the hyperbolic and Euclidean case is caused by the following two facts:

(1) There are many bounded, holomorphic functions on **H**, *unlike the Euclidean case*.
(2) Given $f\in C_0^\infty(\mathbf{H})$, there is a bounded solution to the Poisson–Dirichlét problem $(\partial_x^2+\partial_y^2)g=f$ on (any compact domain of) **H**. *In the Euclidean case, these solutions have logarithmic asymptotics at infinity*.

This article is organized as follows: In Sec. II, we introduce the auxiliary Schrödinger operator $H(\mathbf{a})$ and present some basic properties of $H(\mathbf{a})$. We prove Theorem 1.1 in Sec. III and prove Theorem 1.3 in Sec. IV. In Sec. V, we give a proof of Theorem 1.6. In the Appendix, we explain briefly that $\mathcal{D}(\mathbf{a})$ is a special case of the Dirac operator on a Clifford bundle over **H**.

II. THE SCHRÖDINGER OPERATOR ON THE UPPER-HALF PLANE

In this section we concern with the Schrödinger operator

$$H(\mathbf{a})=A^\dagger(\mathbf{a})A(\mathbf{a})+B=y^2(D_x-a_1)^2+y^2(D_y-a_2)^2$$

acting in $L^2(\mathbf{H})$. Initially we set the domain of $H(\mathbf{a})$ as $C_0^\infty(\mathbf{H})$.

Lemma 2.1: Assume (B.1) or (B.2). Then we have the following:

(i) The operator $A^\dagger(\mathbf{a})A(\mathbf{a})$ is essentially self-adjoint and its closure coincides with $A(\mathbf{a})^*\overline{A(\mathbf{a})}$.
(ii) The operator $A(\mathbf{a})A^\dagger(\mathbf{a})$ is essentially self-adjoint and its closure coincides with $\overline{A(\mathbf{a})}A(\mathbf{a})^*$.
(iii) $H(\mathbf{a})$ is essentially self-adjoint and, if (B.1) holds, then the operator equality,

$$\overline{H(\mathbf{a})}=A(a)^*(\mathbf{a})\overline{A(\mathbf{a})}+B,$$

holds.
(iv) Set $\mathbf{b}=(a_1-1/y,a_2)$, where $\mathbf{a}=(a_1,a_2)$. Then the operator $H(\mathbf{b})+B-1$ is essentially self-adjoint and the operator equality,

$$\overline{A(\mathbf{a})}A(\mathbf{a})^*=\overline{H(\mathbf{b})+B-1},$$

holds.
(v) Both $P(\mathbf{a})$ and $\mathcal{D}(\mathbf{a})$ are essentially self-adjoint.
(vi) Any $V\in C(\mathbf{H})$ which decays at infinity is relatively compact with respect to $\overline{H(\mathbf{a})}$.

Proof: We first consider the case of (B.1). The assertions (i)–(iv) and (vi) are known [Inahama and Shirai (2003), Lemmas 3.2 and 3.10]. Then (i) and (ii) imply that $P(\mathbf{a})$ is essentially self-adjoint, so is $\mathcal{D}(\mathbf{a})$ [Shubin (1976), Theorem 4.1; see also Thaller (1992), Lemma 5.7]. The essential self-adjointness of $H(\mathbf{a})$ is due to Shubin (1976).

Next we consider the case of (B.2). The proof of (vi) in Inahama and Shirai (2003) is still valid in this case. A direct calculation shows that

$$A(\mathbf{a})A^{\dagger}(\mathbf{a})=H(\mathbf{b})+B-1 \tag{2.1}$$

holds. It follows from the general result in Shubin (2001) that $H(\mathbf{a})$, $H(\mathbf{b})$ and the rhs of (2.1) are essentially self-adjoint, from which (iii) follows. Then (ii) and (iv) follows since the lhs of (2.1) has an extension $\overline{A(\mathbf{a})}A(\mathbf{a})^*$, which is self-adjoint (Reed and Simon, Vol. 2, Theorem X.25). We show (i). Set $(Vf)(x,y)=f(-x,y)$ for any $f\in L^2(\mathbf{H})$. Then V is a unitary operator and maps $C_0^{\infty}(\mathbf{H})$ to $C_0^{\infty}(\mathbf{H})$ surjectively. A direct calculation shows that

$$H(\mathbf{a})=A^{\dagger}(\mathbf{a})A(\mathbf{a})+B, \tag{2.2}$$

$$V^{-1}A(\mathbf{a})V=-A^{\dagger}(\tilde{\mathbf{a}}), \quad V^{-1}A^{\dagger}(\mathbf{a})V=-A(\tilde{\mathbf{a}}) \tag{2.3}$$

hold, where we set

$$\tilde{\mathbf{a}}(x,y)=(-a_1(-x,y)+1/y, a_2(-x,y)).$$

Then, by (2.3), we see that $V^{-1}A^{\dagger}(\mathbf{a})A(\mathbf{a})V=A(\tilde{\mathbf{a}})A^{\dagger}(\tilde{\mathbf{a}})$, so the assertion (i) follows from (ii) replaced $A^{\dagger}(\mathbf{a})$ and $A(\mathbf{a})$ by $A^{\dagger}(\tilde{\mathbf{a}})$ and $A(\tilde{\mathbf{a}})$, respectively. The rest of the assertion follows as in the case of (B.1). ■

The following result is due to Inahama and Shirai (2003):

Theorem 2.2: *Assume (B.1). Then we have*

$$\sigma_{\mathrm{ess}}(H(\mathbf{a}))=\sigma_L(B_0)\cup[1/4+B_0^2,\infty),$$

where

$$\sigma_L(B_0)=\begin{cases}\cup_{l=0}^{N(|B_0|-1/2)}\{(2l+1)|B_0|-l(l+1)\}, & \text{if } |B_0|>1/2,\\ \varnothing, & \text{if } |B_0|\leqslant 1/2,\end{cases}$$

and $N(x)$ denotes the largest integer less than x.

III. ASYMPTOTICALLY CONSTANT MAGNETIC FIELD CASE

In this section we give a proof of Theorem 1.1, which is essentially due to Theorem 2.2.

Lemma 3.1: Let $N(x)$ be the function as in Theorem 1.1. Then we have

$$(i)\quad N(|B_0|-1/2)=\begin{cases}N(|B_0-1/2|), & \text{if } B_0>1/2,\\ -1, & \text{if } -1/2\leqslant B_0\leqslant 1/2,\\ N(|B_0-1/2|)-1, & \text{if } B_0<-1/2,\end{cases}$$

$$(ii)\quad N(|B_0-1|-1/2)=\begin{cases}N(|B_0-1/2|)-1, & \text{if } B_0>3/2,\\ -1, & \text{if } 1/2\leqslant B_0\leqslant 3/2,\\ N(|B_0-1/2|), & \text{if } B_0<1/2.\end{cases}$$

Proof: It is easy to see that

$$N(|x|-1)+1=N(|x|) \tag{3.1}$$

holds for all $x\in\mathbf{R}$. First we show the assertion (i). If $B_0>1/2$, then $N(|B_0|-1/2)=N(B_0-1/2)=N(|B_0-1/2|)$. If $-1/2\leqslant B_0\leqslant 1/2$, then $-1/2\leqslant|B_0|-1/2\leqslant 0$, so we have $N(|B_0|-1/2)=-1$. If $B_0<-1/2$, then $|B_0|-1/2=-B_0-1/2=-(B_0-1/2)-1=|B_0-1/2|-1$, so we have $N(|B_0|-1/2)=N(|B_0-1/2|-1)=N(|B_0-1/2|)-1$ by (3.1).

Next we show (ii). If $B_0>3/2$, then $|B_0-1|-1/2=B_0-3/2=|B_0-1/2|-1$, so we have $N(|B_0-1|-1/2)=N(|B_0-1/2|-1)=N(|B_0-1/2|)-1$ by (3.1). If $1/2\leqslant B_0\leqslant 3/2$, then $-1/2$

$\leqslant |B_0-1|-1/2 \leqslant 0$, so we have $N(|B_0-1|-1/2)=-1$. If $B_0<1/2$, then $N(|B_0-1|-1/2)=N(-(B_0-1/2))=N(|B_0-1/2|)$. ■

Lemma 3.2: Let $L(B_0)$ be as in Theorem 1.1. Assume (B.1). Then it follows that

$$\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))=\begin{cases} L(B_0)\cup[|B_0-1/2|^2,\ \infty), & \text{if } B_0\geqslant 1/2,\\ (L(B_0)\backslash\{0\})\cup[|B_0-1/2|^2,\ \infty), & \text{if } B_0<1/2,\end{cases}$$

and

$$\sigma_{\mathrm{ess}}(A(\mathbf{a})A(\mathbf{a})^*)=\begin{cases} (L(B_0)\backslash\{0\})\cup[|B_0-1/2|^2,\ \infty), & \text{if } B_0>1/2,\\ L(B_0)\cup[|B_0-1/2|^2,\ \infty), & \text{if } B_0\leqslant 1/2.\end{cases}$$

Proof: It follows from Lemma 2.1 (iii) that

$$\begin{aligned}\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))&=\sigma_{\mathrm{ess}}(H(\mathbf{a})-B)\\ &=\sigma_{\mathrm{ess}}(H(\mathbf{a})-B_0)\\ &=(\sigma_L(B_0)-B_0)\cup[B_0^2+1/4-B_0,\infty)\\ &=(\sigma_L(B_0)-B_0)\cup[|B_0-1/2|^2,\ \infty),\end{aligned}\tag{3.2}$$

where we used Lemma 2.1 (vi) in the second equality and Theorem 2.2 in the third equality. By (2.4), we have

$$\sigma_L(B_0)-B_0=\bigcup_{l=0}^{N(|B_0|-1/2)}\{(2l+1)|B_0|-l(l+1)-B_0\}.\tag{3.3}$$

By Lemma 3.1 (i), if $B_0>1/2$, we have

$$\begin{aligned}\text{the rhs of (3.3)}&=\bigcup_{l=0}^{N(|B_0-1/2|)}\{(2l+1)B_0-l(l+1)-B_0\}\\ &=\bigcup_{l=0}^{N(|B_0-1/2|)}\{l((2B_0-1)-l)\}=L(B_0).\end{aligned}\tag{3.4}$$

Similarly, if $-1/2\leqslant B_0\leqslant 1/2$, we have

$$\text{the rhs of (3.3)}=\varnothing=L(B_0)\backslash\{0\},\tag{3.5}$$

and, if $B_0<-1/2$, we have

$$\begin{aligned}\text{the rhs of (3.3)}&=\bigcup_{l=0}^{N(|B_0-1/2|-1)}\{(2l+1)(-B_0)-l(l+1)-B_0\}\\ &=\bigcup_{l=0}^{N(|B_0-1/2|-1)}\{-2(l+1)B_0-l(l+1)\}\\ &=\bigcup_{k=1}^{N(|B_0-1/2|)}\{k((-2B_0+1)-k)\}=L(B_0)\backslash\{0\},\end{aligned}\tag{3.6}$$

where we changed the variable $l=k-1$ in the second equality. Then the first assertion in the lemma follows from (3.2)–(3.6).

As for the second assertion, using Lemma 2.1 (iv), we have

$$\sigma_{\mathrm{ess}}(A(\mathbf{a})A(\mathbf{a})^*)=\sigma_{\mathrm{ess}}(H(\mathbf{b})+B_0-1)$$
$$=\bigcup_{l=0}^{N(|B_0-1|-1/2)}\{(2l+1)|B_0-1|-l(l+1)+B_0-1\}\cup[|B_0-1/2|^2,\ \infty),$$

where $\mathbf{b}$ is as in Lemma 2.1. Then the result follows from Lemma 3.1 (ii) in a similar way. ■

Now, by Lemma 3.2, we complete the proof of Theorem 1.1, since the form (1.2) implies that $\sigma_{\mathrm{ess}}(P(\mathbf{a}))=\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))\cup\sigma_{\mathrm{ess}}(A(\mathbf{a})A(\mathbf{a})^*)$. Due to (1.6), Corollary 1.5 follows immediately.

IV. DIVERGING MAGNETIC FIELD CASE

In this section we give a proof of Theorem 1.3 following the same line of the argument as in Shikegawa (1991), Example 4.1. We assume (B.2) to the end of this section.

Lemma 4.1: Let A be a densely defined, closed operator acting in a separable Hilbert space. Then we have the following:

(i) *A^*A and AA^* have the same essential spectrum except perhaps at the point 0.*
(ii) *In addition, if 0 belongs to $\sigma_{\mathrm{ess}}(A^*A)$ but not to $\sigma_{\mathrm{ess}}(AA^*)$, the ground state energy 0 must be an isolated eigenvalue of A^*A of infinite multiplicity.*

Proof: The assertion (i) is well known as the spectral supersymmetry [see, e.g., Cycon *et al.* (1987), Theorem 6.3, Thaller (1992), Corollary 5.6]. The assertion (ii) immediately follows from (i). ■

The essential spectrum of $A(\mathbf{a})A(\mathbf{a})^*=H(\mathbf{b})+B-1$ is empty [Kondrat'ev and Shubin (2002)], hence Lemma 4.1 (i) implies that $\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))\subset\{0\}$. Then it follows that

$$\sigma_{\mathrm{ess}}(P(\mathbf{a}))=\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))\cup\sigma_{\mathrm{ess}}(A(\mathbf{a})A(\mathbf{a})^*)=\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))\subset\{0\}.$$

This shows the discreteness of the spectrum of $P(\mathbf{a})$, except for 0.

Next, we complete the proof of Theorem 1.3 by showing that 0 is an isolated eigenvalue of $A(\mathbf{a})^*A(\mathbf{a})$ of infinite multiplicity. Let D denote the Poincaré disk $\{w=re^{i\theta}=u+iv|0\leqslant r<1,0\leqslant\theta<2\pi\}$ endowed with the canonical measure $d\mu_D=4rdrd\theta/(1-r^2)^2$ and let E denote the Cayley transform from $\mathbf{H}$ to D defined by $Ez=(z-i)(z+i)^{-1}$. In what follows, for any function f on $\mathbf{H}$, we denote the function $f(E^{-1}\cdot)$ on D by $\tilde{f}$ for simplicity. For notational convenience, when we denote a function on D by $\tilde{f}$, we always assume that the inverse image of $\tilde{f}$ by E is some function f on $\mathbf{H}$. Note that E induces a unitary equivalence between $L^2(\mathbf{H})$ and $L^2(D)$: and transforms the hyperbolic Laplacian $y^2(\partial_x^2+\partial_y^2)$ to $\frac{1}{4}(1-r^2)^2(\partial_u^2+\partial_v^2)$.

Lemma 4.2: Assume (B.2). Then $\dim\ker(A(\mathbf{a}))=\infty$.

Proof: We write $B=B_1+B_2$ so that $\inf B_1>1$, $B_j\in C^2(\mathbf{H};\mathbf{R})$ for $j=1,2$ and B_2 is compactly supported. Then we can find a C^2-solution g_j which solves the equation $y^2(\partial_x^2+\partial_y^2)g_j=B_j$ on $\mathbf{H}$ for $j=1,2$ [see, Hormander (1963), Theorem 3.6.4 and Corollary 3.7.1]. Owing to the compactness of the support of B_2, we may assume that g_2 is bounded on $\mathbf{H}$. In fact, we can take g_2 as the solution to the Dirichlet problem $(\partial_u^2+\partial_v^2)\widetilde{g_1}=4\tilde{B}_2/(1-r^2)^2$ on (the closure of) D. We set $g=g_1+g_2$.

Owing to the gauge transform, we may assume that $\mathbf{a}=(-\partial_y g,\partial_x g)$ since g satisfies $y^2(\partial_x^2+\partial_y^2)g=B$. Then, using the form

$$A(\mathbf{a})=-2iy\overline{\partial_z}-y(a_1+ia_2),\quad \overline{\partial_z}=\tfrac{1}{2}(\partial_x+i\partial_y),\tag{4.1}$$

we can find that he^{-g} belongs to $\ker(A(\mathbf{a}))$ for any holomorphic function h, provided that he^{-g} belongs to $L^2(\mathbf{H})$.

We introduce the weight function on D as $\tilde{\varphi}=2\tilde{g}_1+2\log(1-r^2)$. Then $(\partial_u^2+\partial_v^2)\tilde{\varphi}=(B_1-1)/(1-r^2)^2\geqslant 0$, so $\tilde{\varphi}$ is sub-harmonic on D. Using Lemma 4.4.4 in Hormander (1966), we can deduce that the space

$$\mathcal{A}=\{\tilde{h}\,|\,\tilde{h}e^{-\tilde{\varphi}/2}\in L^2(D),\ \tilde{h}\ \text{is holomorphic on}\ D\}$$

has infinite dimension. Then, by the boundedness of g_2, we conclude that the map

$$\mathcal{A}\ni\tilde{h}\mapsto he^{-g}\in\ker(A(\mathbf{a}))$$

is well-defined, from which the lemma follows. ■

Remark 4.3: The above proof shows that the conclusion in Lemma 4.2 is still valid whenever

$$\liminf\{B(x,y)\,|\,d_{\mathbf{H}}((x,y),(0,1))\to\infty\}>1.$$

Here, $d_{\mathbf{H}}$ is the distance function on $\mathbf{H}$ induced by the standard metric. Explicitly,

$$\cosh d_{\mathbf{H}}(z_1,z_2)=\frac{(x_1-x_2)^2+y_1^2+y_2^2}{2y_1y_2}$$

for any $z_1=(x_1,y_1)$, $z_2=(x_2,y_2)\in\mathbf{H}$.

The condition (B.2) implies that 0 is an eigenvalue of $A(\mathbf{a})$, so of $A(\mathbf{a})^*A(\mathbf{a})$, of infinite multiplicity. We deduce that 0 is an isolated point of $\sigma(P(\mathbf{a}))$ by Lemma 4.1 (ii). This completes the proof.

V. AHARONOV–CASHER TYPE ARGUMENT

In this section we give a proof of Theorem 1.6. To the end of this section, in addition to (B.1), we assume that B_1 is compactly supported on $\mathbf{H}$. We use the same notation $\tilde{f}$ for the function $f(E^{-1}\cdot)$ on the Poincaré disk D as in the previous section.

Lemma 5.1: There exists $\tilde{g}\in C^2(D;\mathbf{R})$ which solves the equation

$$\tfrac{1}{4}(1-r^2)^2(\partial_u^2+\partial_v^2)\tilde{g}=\tilde{B}$$

on D. Moreover, the function

$$\tilde{g}_1=\tilde{g}+B_0\log(1-r^2)$$

is bounded on D.

Proof: Due to the compactness of the support of B_1, we can find the solution $\tilde{g}_1$ which solves the equation

$$\tfrac{1}{4}(1-r^2)^2(\partial_x^2+\partial_y^2)\tilde{g}_1=\tilde{B}_1$$

with the Dirichlét boundary condition on (the closure of) D. Then the lemma follows from the fact that $(\partial_u^2+\partial_v^2)\log(1-r^2)=-4(1-r^2)^{-2}$. ■

Lemma 5.2: Let $\tilde{g}$ be as in Lemma 5.1. Introduce the space

$$\tilde{\mathcal{A}}(\tilde{g})=\{\tilde{h}\,|\,\tilde{h}e^{-\tilde{g}}\in L^2(D),\ \tilde{h}\ \text{is holomorphic on}\ D\}.$$

Then we have

$$\dim \tilde{\mathcal{A}}(\tilde{g}) = \begin{cases} \infty, & \text{if } B_0 > 1/2, \\ 0, & \text{if } B_0 \leqslant 1/2. \end{cases}$$

Proof: Set $h_n(w) = w^n$ for each non-negative integer n. Then it follows from Lemma 5.1 that

$$\begin{aligned} \|h_n e^{-\tilde{g}}\|^2_{L^2(D)} &= \int_D |h_n|^2 e^{-2\tilde{g}} d\mu_D \\ &= 4 \int_0^{2\pi} d\theta \int_0^1 e^{-2\tilde{g}_1} (1-r^2)^{2(B_0-1)} r^{2n+1}\, dr \\ &\leqslant \int_0^{2\pi} d\theta 4 \int_0^1 e^{-2\tilde{g}_1} (1-r^2)^{2(B_0-1)} r\, dr \leqslant C \int_0^1 (1-r^2)^{2(B_0-1)} r\, dr, \end{aligned} \tag{5.1}$$

holds for some $C > 0$ and the rhs of (5.1) is finite if $2(B_0-1) > -1$, i.e., $B_0 > 1/2$. This shows that $\tilde{\mathcal{A}}(\tilde{g})$ has infinite dimension.

Next, we show the latter half of the assertion. For each $\tilde{h} \in \tilde{\mathcal{A}}(\tilde{g}) \backslash \{0\}$, we set

$$H(r) = \int_0^{2\pi} |\tilde{h}(re^{i\theta})|^2\, d\theta. \tag{5.2}$$

It is easy to see that H is increasing in r since $\tilde{h}$ is holomorphic. Then, by (5.2) and the second line of (5.1) replacing h_n by $\tilde{h}$, there exist C, $C' > 0$ such that

$$\|\tilde{h} e^{-\tilde{g}}\|^2_{L^2(D)} \geqslant C \int_0^1 H(r)(1-r^2)^{2(B_0-1)} r\, dr \geqslant C' \int_0^1 (1-r^2)^{2(B_0-1)} r\, dr, \tag{5.3}$$

where we used the boundedness of $\tilde{g}_1$ in the first inequality. The assertion (ii) follows since the rhs of (5.3) diverges if $B_0 \leqslant 1/2$. ■

Lemma 5.3: We have

$$\dim \ \ker(A(\mathbf{a})) = \begin{cases} \infty, & \text{if } B_0 > 1/2, \\ 0, & \text{if } B_0 \leqslant 1/2, \end{cases}$$

and

$$\dim \ \ker(A(\mathbf{a})^*) = \begin{cases} 0, & \text{if } B_0 \geqslant 1/2, \\ \infty, & \text{if } B_0 < 1/2. \end{cases}$$

Proof: We first show that $\dim \ker(A(\mathbf{a})) = \dim \tilde{\mathcal{A}}(\tilde{g})$. Let $\mathcal{A}(g)$ denote the space $\{h | \tilde{h} \in \tilde{\mathcal{A}}(\tilde{g})\}$. Owing to the gauge transform, we may assume that $\mathbf{a} = (-\partial_y g, \partial_x g)$ without loss of generality. By (4.1), we see that if $h \in \mathcal{A}(g)$ then $he^{-g} \in \ker(A(\mathbf{a}))$. This shows that $\dim \ker(A(\mathbf{a})) \geqslant \dim \mathcal{A}(g)$.

We show the converse inequality. Let $g \in C^2(\mathbf{H}; \mathbf{R})$ be any solution which solves the equation

$$y^2(\partial_x^2 + \partial_y^2) g = B$$

on $\mathbf{H}$. Assume that $f \in \ker(A(\mathbf{a}))$. Then fe^g satisfies $(\partial_x + i\partial_y)(fe^g) = 0$, so is holomorphic on $\mathbf{H}$, hence $f \in \mathcal{A}(g)$. This shows that $\dim \ker(A(\mathbf{a})) \leqslant \dim \mathcal{A}(g)$. Then the statements for $A(\mathbf{a})$ follow immediately from Lemma 5.2.

As for $A(\mathbf{a})^*$, taking the form

$$A(\mathbf{a})^* = -iy((\partial_x - i\partial_y) - i(a_1 - ia_2) + i/y)$$

into account, we can show, as in the case of $A(\mathbf{a})$, that

$$\ker (A(\mathbf{a})^*) \cong \{h | he^{-g'} \in L^2(\mathbf{H}), h \text{ is anti-holomorphic on } \mathbf{H}\},$$

where g' solves $y^2(\partial_x^2+\partial_y^2)g'=1-B$. Then the result follows from the argument above and the proof of Lemma 5.2 replaced "B_0" and "holomorphic" by "$1-B_0$" and "anti-holomorphic," respectively. ■

Lemma 5.4: Let T be a densely defined, closed operator acting in a Hilbert space. Then the following two conditions are equivalent:

(i) The subspace $\mathrm{ran}(T)$ *is closed and* $\dim\ker(T)$ is finite.

(ii) The infimum of the set $\sigma_{\mathrm{ess}}(T^*T)$ *is positive.*

In particular, the condition (ii) implies that T is semi-Fredholm.

Proof: This basic fact follows immediately from the closed graph theorem [see Kato (1966), Chap. IV, Theorem 5.2.]. ■

If $B_0<1/2$, Lemma 3.2 implies that $\inf\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))>0$. Then we deduce from Lemma 5.4 that $A(\mathbf{a})$ is semi-Fredholm and so is $A(\mathbf{a})^*$. If $B_0<1/2$, replacing $A(\mathbf{a})$ by $A(\mathbf{a})^*$, we have the same conclusion.

If $B_0=1/2$, Lemma 3.2 implies that $\inf\sigma_{\mathrm{ess}}(A(\mathbf{a})^*A(\mathbf{a}))=0$. Then we deduce from Lemma 5.3 that $\mathrm{ran}(A(\mathbf{a}))$ is not closed since $\dim\ker(A(\mathbf{a}))=0$ by Lemma 5.3 (ii). Thus $A(\mathbf{a})$ is not semi-Fredholm. This completes the proof of Theorem 1.6.

Let τ be the operator as in (1.5). The argument above also shows that $\ker(P(\mathbf{a}))$ is contained in the "spin-up" subspace $\{f\in L^2(\mathbf{H})\oplus L^2(\mathbf{H}) | \tau f=f\}$ if $B_0>1/2$, and contained in the "spin-down" subspace $\{f\in L^2(\mathbf{H})\oplus L^2(\mathbf{H}) | \tau f=-f\}$ if $B_0<1/2$.

APPENDIX: DIRAC OPERATORS ON CLIFFORD BUNDLES

In this appendix it is briefly explained that the operator $\mathcal{D}(\mathbf{a})$ is a special case of the geometric Dirac operators on a Clifford bundle. However, there is nothing new. As for a physical point of view, see Pnueli (1994), Pnueli (1994) and Pnueli (1995).

As for the language of Riemannian geometry, we refer to Roe (1988). Let M be an n-dimensional Riemannian manifold. We denote the (complexified) tangent and cotangent bundles over M by TM and T^*M, respectively, and denote by $\mathrm{Cl}(TM)$ the (bundle of complexified) Clifford algebra generated by TM. Let ∇^{LC} denote the Levi-Civita connection on TM. Let S be a Hermitian vector bundle of rank r over M. We denote the Hermitian metric on S by $(\cdot,\cdot)$, the fiber of S at $m\in M$ by S_m and the space of all smooth sections with compact support by $\Gamma_0(S)$. A connection ∇ on S is defined as a linear map from $\Gamma_0(S)$ to $\Gamma_0(T^*M\otimes S)$ which satisfies the Leibniz rule $\nabla(fs)=df\otimes s+f\nabla s$ for all $f\in C^\infty(M)$ and for all $s\in\Gamma_0(S)$. We assume that the connection ∇ is compatible with the metric, i.e., the condition $d(s_1,s_2)=(\nabla s_1,s_2)+(s_1,\nabla s_2)$ holds for all s_1, $s_2\in\Gamma_0(S)$, where d is the exterior derivative.

We say *S is a Clifford bundle over M* if it is a bundle of Clifford modules over M satisfying the following two conditions:

(i) The Clifford action of each vector in T_mM on S_m is skew-adjoint with respect to the Hermitian metric,

(ii) The connection ∇ is compatible with the Levi-Civita connection ∇^{LC} in the sense that $\nabla_X(Ys)=(\nabla^{\mathrm{LC}}_X Y)s+Y\nabla_X s$ holds for all vector fields X,Y and for all $s\in\Gamma_0(S)$.

For any local orthonormal frame $\{e_j\}_{j=1}^n$ of TM, *the Dirac operator $\mathcal{D}$ over S* is defined locally by $\Sigma_{j=1}^n e_j\nabla_{e_j}$. Note that the definition is independent of a choice of such frame and of local coordinate system of M.

In our case, set $M=\mathbf{H}$ and $S=\mathbf{H}\times\mathbf{C}^2$, the trivial Hermitian vector bundle of rank two over $\mathbf{H}$. In what follows we fix the standard (global) coordinate (x,y) of $\mathbf{H}$. Let f_1 and f_2 denote the standard orthonormal frame over $\mathbf{H}$, i.e.,

$$f_1=\begin{pmatrix}1\\0\end{pmatrix},\quad f_2=\begin{pmatrix}0\\1\end{pmatrix}.$$

If we choose $e_1=y\partial_x$, $e_2=y\partial_y$, then $\{e_j\}_{j=1}^2$ is an orthonormal frame over $T\mathbf{H}$ with respect to the Riemannian metric

$$g=(g_{jk})_{j,k=1}^2=\begin{pmatrix} y^{-2} & 0 \\ 0 & y^{-2} \end{pmatrix}.$$

Let $\{\omega_{ij}^k\}_{i,j,k=1}^2$ be the Christoffel symbol with respect to $\{e_j\}_{j=1}^2$ and $\{f_j\}_{j=1}^2$, i.e., $\{\omega_{ij}^k\}$ satisfies

$$\nabla_{e_i}f_j=\sum_{k=1}^2 \omega_{ij}^k f_k$$

for all $i,j=1,2$. If we choose

$$\gamma_1=\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \quad \gamma_2=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

then we can find that the Clifford relations $\gamma_j\gamma_k+\gamma_k\gamma_j=-2\delta_{jk}$ holds for all $j,k=1,2$, where δ_{jk} denotes the Kronecker delta. Hence $\{\gamma_j\}_{j=1}^2$ generates the matrix Clifford algebra. We can define the representation c of the Clifford algebra $\mathrm{Cl}(T\mathbf{H})$ uniquely by associating $c(e_j)$ to γ_j for $j=1,2$. This representation c defines a Clifford module structure over S.

We derive the expression of the Dirac operator in this case. By a long but straightforward calculation, we can find that the condition (i) in the definition of the Clifford bundle above is equivalent to the conditions $\omega_{ij}^k=\overline{\omega_{ik}^j}$ for all $i,j,k=1,2$, where $\overline{\cdot}$ denotes the complex conjugate and that the condition (ii) is equivalent to the conditions $\omega_{12}^1=\omega_{11}^2=\omega_{22}^1=\omega_{21}^2=0$, $i\omega_{11}^1=1+i\omega_{12}^2$ and $\omega_{21}^1=\omega_{22}^2$. Then, by the definition of D, we see that

$$\begin{aligned}\mathcal{D}&=\sum_{j=1}^2 c(e_j)\nabla_{e_j}\\ &=\sum_{j=1}^2 \gamma_j\nabla_{e_j}\\ &=\begin{pmatrix} 0 & (yD_x-i\omega_{11}^1)-i(yD_y-i\omega_{21}^1)+1 \\ (yD_x-i\omega_{11}^1)+i(yD_y-i\omega_{21}^1) & 0 \end{pmatrix},\end{aligned}$$

holds on $\Gamma_0(S)\cong C_0^\infty(\mathbf{H})\oplus C_0^\infty(\mathbf{H})$. Thus $\mathcal{D}$ coincides with the operator $\mathcal{D}(\mathbf{a})$ if we set $\omega_{11}^1=-iya_1$ and $\omega_{21}^1=-iya_2$, i.e., the admissible Dirac operators are of the form (1.1) in our case. This is the reason why we call $\mathcal{D}(\mathbf{a})$ by the name "Dirac operator."

Next, we clarify the relation between the Pauli operator $P(\mathbf{a})$ and the Clifford curvature on S. Let $R(X,Y)=[\nabla_X^{\mathrm{LC}},\nabla_Y^{\mathrm{LC}}]-\nabla_{[X,Y]}^{\mathrm{LC}}$ be the Riemann curvature operator and $K(X,Y)=[\nabla_X,\nabla_Y]-\nabla_{[X,Y]}$ the curvature operator of S. We introduce the Clifford contraction of K and the Riemann endomorphism as

$$\mathcal{K}=\sum_{j<k} \gamma_j\gamma_k K(e_j,e_k),$$

$$\mathcal{R}^S(X,Y)=\frac{1}{4}\sum_{j,k=1}^2 \gamma_j\gamma_k g(R(X,Y)e_j,e_k),$$

respectively, where $g(\cdot,\cdot)$ is the Riemannian metric on $T\mathbf{H}$. We define the twisting curvature of S by $F^S=K-\mathcal{R}^S$ and set

$$\mathcal{F}^S=\sum_{j<k}\gamma_j\gamma_k F^S(e_j,e_k).$$

Then we have

$$\mathcal{R}^S(e_1,e_2)=\begin{pmatrix}-i/2 & 0\\ 0 & i/2\end{pmatrix},\quad K(e_1,e_2)=\begin{pmatrix}-iB & 0\\ 0 & -i(B-1)\end{pmatrix},$$

$$\mathcal{K}=\begin{pmatrix}-B & 0\\ 0 & B-1\end{pmatrix},$$

where $B=y^2(\partial_x a_2-\partial_y a_1)$. Thus the Lichnerowicz formula reads as

$$\begin{aligned}P(\mathbf{a})=\mathcal{D}(\mathbf{a})^2&=\begin{pmatrix}A^*(\mathbf{a})A(\mathbf{a}) & 0\\ 0 & A(\mathbf{a})A^*(\mathbf{a})\end{pmatrix}=\begin{pmatrix}H(\mathbf{a}) & 0\\ 0 & H(\mathbf{b})\end{pmatrix}+\begin{pmatrix}-B & 0\\ 0 & B-1\end{pmatrix}\\ &=\nabla^*\nabla+\mathcal{K}=\nabla^*\nabla+\mathcal{F}^S+(-2)/4,\end{aligned}\tag{A1}$$

where $\mathbf{b}=\mathbf{a}+(-1/y,0)$ be as in Lemma 2.1 (iv) and ∇^* denotes the adjoint operator of ∇ from $\Gamma_0(T^*\mathbf{H}\otimes S)$ to $\Gamma_0(S)$. Here the factor -2 on the rhs of (6.1) is the scalar curvature of $\mathbf{H}$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

Geometrical phases for the $G(4,2)$ Grassmannian manifold

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(Received 24 January 2003; accepted 10 March 2003)

We generalize the usual Abelian Berry phase generated for example in a system with two nondegenerate states to the case of a system with two doubly degenerate energy eigenspaces. The parametric manifold describing the space of states of the first case is formally given by the $G(2,1)$ Grassmannian manifold, while for the generalized system it is given by the $G(4,2)$ one. For the latter manifold which exhibits a much richer structure than its Abelian counterpart we calculate the connection components, the field strength and the associated geometrical phases that evolve nontrivially both of the degenerate eigenspaces. A simple atomic model is proposed for their physical implementation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1572551]

I. INTRODUCTION

Geometrical phases have attracted much interest since the seminal work by Berry.[1] The simple example of the Abelian Berry phase produced, e.g., by the adiabatic transition of a spin-1/2 particle that follows a rotating magnetic field, has found many applications in quantum optics, molecular physics and so on. Theoretically, it was extended to non-Abelian phases by Wilczek and Zee[2] by additionally employing to the setup of the usual Berry phase a degenerate structure that allows geometrical unitary evolutions of higher dimensionality describing transitions of population within the degenerate eigenspace. There are different applications of geometrical evolutions in the literature[3] and in particular related to quantum information. Special attention has been given to the evolutions that are parametrized by the n-dimensional complex projective manifold, CP^n. It corresponds to the parametric manifold $\mathcal{M}$ of a physical model where n states out of $n+1$ are preserved degenerate at all times.[4] For this case the parametric space $\mathcal{M}$ is given by

$$CP^n \approx \frac{U(n+1)}{U(n)\times U(1)},$$

where the dictated control transformations are between the nondegenerate state and each degenerate one. By performing adiabatically closed paths in this parametric space geometrical unitary operators are generated, called holonomies, Γ, acting solely on the degenerate states. Their relevance for performing quantum computation was first demonstrated in Ref. 5. Since then they enjoyed theoretical applications in quantum optical models with laser beams,[6] trapped ions,[7] optical cavities[8] or quantum dots.[9]

A further generalization of the parametric control space is realized by employing the Grassmannian manifolds. They are given by the coset space structure,

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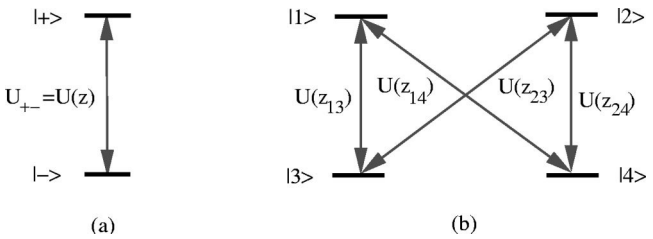

FIG. 1. Schematic state-structure and interactions parametrized by (a) the $G(2,1)$ and for (b) the $G(4,2)$ Grassmannian manifolds. The arrows represent $U(2)$ transformations between the connected states implemented e.g., by Raman transitions, while due to the coset structure there are no transformations between the degenerate states of (b).

$$G(m,n)\approx \frac{U(m)}{U(n)\times U(m-n)}\ .$$

The complex projective manifolds can be considered as a special case of the Grassmannian ones. In particular, for $m=2$ and $n=1$ we obtain the CP^1 space where the Berry phases are defined, while for $m=n+1$ we have the identity $G(n+1,n)\approx CP^n$. There are two degenerate eigenspaces corresponding to the $G(m,n)$ model that are n and $m-n$ dimensional. With the same adiabatic control procedure in the parametric space $\mathcal{M}=G(m,n)$ nontrivial holonomies are generated in both of them, contrary to all previously studied examples. Here, we shall restrict to the $G(4,2)$ case, where the connection components, the corresponding field strengths and a set of holonomies will be explicitly given.

II. HOLONOMIES AND PHYSICAL MODELS

A. Berry phases

The well known Berry phase can be produced by performing loops in the $G(2,1)\approx CP^1$ parametric space of external control parameters that determine the unitary evolution of two level system as sketched in Fig. 1(a). Let us present one possible Berry phase implementation in atomic physics.

Consider the case of an atom with two nondegenerate ground levels $|+\rangle$ and $|-\rangle$, with corresponding eigenvalues $E_+=\omega/2$ and $E_-=-\omega/2$, and an excited one $|e\rangle$. By performing a Raman adiabatic transfer[10] between levels $|+\rangle$, $|-\rangle$ with the help of two detuned laser fields with Rabi frequencies Ω_+ and Ω_- and common detuning Δ it is possible to adiabatically eliminate level $|e\rangle$ and create in the basis $\{|+\rangle,|-\rangle\}$ the following unitary transformation:

$$\mathcal{U}(\theta,\phi)=\begin{pmatrix} \cos\dfrac{\theta}{2} & ie^{i\phi}\sin\dfrac{\theta}{2} \\ ie^{-i\phi}\sin\dfrac{\theta}{2} & \cos\dfrac{\theta}{2} \end{pmatrix},$$

where $\theta=2|\Omega_{\text{eff}}|t$, $\phi=\arg\{\Omega_{\text{eff}}\}$ and $\Omega_{\text{eff}}=\Omega_+\Omega_-^*/(4\Delta)$. In the above evolution we have neglected the Stark shift effect which can be compensated with properly detuned lasers. In accordance the initial free Hamiltonian of the $|+\rangle$ and $|-\rangle$ states, given by $H_0=(\omega/2)\,\sigma_z$, is transformed as

$$H=\frac{\omega}{2}\mathcal{U}(\theta,\phi)\sigma_z\mathcal{U}^\dagger(\theta,\phi).$$

Assume that at time $t=0$ we have $\theta=\phi=0$ and the initial state of the system is given by $|\Psi_\pm(0)\rangle=|\pm\rangle$. Let us consider the evolution resulting when a closed path C is spanned very slowly in the parametric plane (θ,ϕ) in time interval T. Due to cyclicity and adiabaticity no population has moved from one state to the other at the end of the loop, that is, the energy of the

system has not changed. Still the states are allowed to obtain a geometrical phase factor at the end of this evolution, which can be calculated from the time evolution operator of the system given by the Schrödinger equation. A dynamical phase does not appear due to the geodesic character of Raman evolutions. In particular, we obtain that $|\Psi_+(T)\rangle=\Gamma_A^+(C)|+\rangle$ and $|\Psi_-(T)\rangle=\Gamma_A^-(C)|-\rangle$, that is, the states acquire a geometrical phase factor that depend on the spanned loop C, and a connection A. The components of the latter are defined, and analytically given for this case, by

$$A_\theta^\pm=\langle\pm|\mathcal{U}^\dagger\frac{\partial}{\partial\theta}\mathcal{U}|\pm\rangle=0 \qquad \text{and} \qquad A_\phi^\pm=\langle\pm|\mathcal{U}^\dagger\frac{\partial}{\partial\phi}\mathcal{U}|\pm\rangle=\pm i\sin^2\theta.$$

In terms of the connection A the phase factors $\Gamma_A^\pm(C)\equiv e^{i\varphi_\pm}$ are given by

$$\Gamma_A^\pm(C)=\exp\oint_C A^\pm=\exp\int\int_{\Sigma(C)} d\theta\, d\phi\; F_{\theta\phi}^\pm(\theta,\phi), \tag{1}$$

where $F_{\theta\phi}^\pm(\theta,\phi)=\partial_\theta A_\phi^\pm-\partial_\phi A_\theta^\pm=\pm i\sin 2\theta$ is the nonzero component of the field strength associated with A and $\Sigma(C)$ is the surface on the plane (θ,ϕ) bounded by the loop C. The second step in (1) is due to Stokes' theorem. For any C we obtain the relation $\varphi_+=-\varphi_-=\int\int_{\Sigma(C)}d\theta\, d\phi\,\sin 2\theta$ between the two Berry phases. Note that $\varphi_+=\Omega/2$ where Ω is the solid angle spanned by the circulation of a unit vector with directions given by the (θ,ϕ) angles. The half factor reflects the spin-1/2 transformation properties of the employed two atomic levels. This physical evolution produces a measurable Abelian Berry phase. Their generalization to unitary matrices (holonomies) with the employment of degenerate structures is given in the following for the case of the Grassmannian manifold $G(4,2)$.

B. Holonomies for the Grassmannian manifold $G(4,2)$

The Grassmannian manifold $G(4,2)$ corresponds to the parametric space of the Hamiltonian $H=\mathcal{U}H_0\mathcal{U}^\dagger$ where $H_0=\omega/2\,\mathrm{diag}(1,1,-1,-1)$ and $\mathcal{U}$ are $U(4)$ unitary transformations that act nontrivially on the Hamiltonian H_0. Clearly, H_0 has the following eigenvectors: $|+_1\rangle\equiv|1\rangle=(1,0,0,0)$, $|+_2\rangle\equiv|2\rangle=(0,1,0,0)$, $|-_1\rangle\equiv|3\rangle=(0,0,1,0)$ and $|-_2\rangle\equiv|4\rangle=(0,0,0,1)$. The first two states span the degenerate eigenspace S_+ with eigenvalue $E_+=\omega/2$, while the last two span the eigenspace S_- with eigenvalue $E_-=-\omega/2$. The schematic representation of this model is given in Fig. 1(b), where the eligible transformations are depicted by arrows. Each arrow corresponds to a $U(2)$ transformation $U(z_{ij})$ parametrized by a complex number $z_{ij}=\theta_{ij}\exp i\phi_{ij}$ for $i=1,2$ and $j=3,4$. Hence, the real decomposition of the parametric space $G(4,2)$ is given by $\mathcal{M}\equiv\{\theta_{ij},\phi_{ij}\}\equiv\{\sigma_{ij}\}$. Here we adopt the following ordering for the general unitary transformation, $\mathcal{U}(\sigma)=U(z_{13})U(z_{14})U(z_{23})U(z_{24})$.

Now we can define the connection components for each degenerate eigenspace. They are given from the following equation:

$$(A_\sigma^\pm)_{\alpha\beta}\equiv\langle\alpha|\mathcal{U}^\dagger(\sigma)\frac{\partial}{\partial\sigma}\mathcal{U}(\sigma)|\beta\rangle, \tag{2}$$

where the basis vector $|\alpha\rangle$ and $|\beta\rangle$ belong in the same degenerate eigenspace of H_0. From (2) we see that the matrix $A_\sigma^\pm$ is anti-Hermitian. For $\{\alpha,\beta\}=\{1,2\}$ we obtain the elements of the 2×2 matrix A^+, while for $\{\alpha,\beta\}=\{3,4\}$ we obtain the elements of A^-. The holonomic unitary operator, generated when a closed path, C, is spanned adiabatically in the space of the control parameters $\mathcal{M}$, is defined by

$$\Gamma_A^\pm(C)\equiv\mathbf{P}\exp\oint_C A^\pm.$$

The path ordering symbol does not allow us to calculate the path integral first and then to exponentiate the result as the different components of the connection A do not commute in general. For those cases the simple form of Stokes theorem does not apply.[11] Still it is possible to analytically calculate the holonomies which result from the commuting components of the connection A in the same way as we did for the Abelian case. Alternatively, the non-Abelian version of Stokes' theorem can be employed as in Refs. 6 and 12.

Before moving to the analytic calculation of the holonomies, let us see how the transformations $\mathcal{U}(\sigma)$ can be physically realized, for example, by an atomic system. According to Fig. 1(b) we can generalize the model of the two level atom with four levels, pair-wise degenerate and apply laser beams connecting these states via additional exciting states by Raman adiabatic transfers. As in the case of the two-level system presented in the previous subsection, a $U(2)$ unitary transformation results from each Raman transition. Successive applications of those unitaries are able to construct the general unitary transformation $\mathcal{U}(\sigma)$ parametrized by the $G(4,2)$ manifold. A detailed study of the generation of the Berry phases with $\mathcal{M}=CP^2$ control manifold with an atomic system manipulated by Raman transitions is given in Refs. 13–15.

III. CONNECTION AND FIELD STRENGTH COMPONENTS

A. Connection *A*

In this subsection we shall present the connection components related to the parametric space $G(4,2)$ by employing definition (2). In particular, they are 2×2 matrices paired in the following with respect to the S_+ and S_- degenerate eigenspaces they act on. Thus, we obtain

$$A^+_{\theta_{13}}=\sin\theta_{23}\cos\theta_{14}\cos\theta_{24}\begin{pmatrix}0 & -e^{i(\phi_{13}-\phi_{23})}\\ e^{-i(\phi_{13}-\phi_{23})} & 2i\sin(\phi_{13}-\phi_{14}+\phi_{24}-\phi_{23})\tan\theta_{14}\sin\theta_{24}\end{pmatrix},$$

$$A^-_{\theta_{13}}=\sin\theta_{14}\cos\theta_{23}\cos\theta_{24}\begin{pmatrix}0 & -e^{i(\phi_{14}-\phi_{13})}\\ e^{-i(\phi_{14}-\phi_{13})} & 2i\sin(\phi_{14}+\phi_{23}-\phi_{13}-\phi_{24})\tan\theta_{23}\sin\theta_{24}\end{pmatrix},$$

$$A^+_{\theta_{14}}=\sin\theta_{24}\begin{pmatrix}0 & -e^{i(\phi_{14}-\phi_{24})}\\ e^{-i(\phi_{14}-\phi_{24})} & 0\end{pmatrix},\qquad A^-_{\theta_{14}}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},$$

$$A^+_{\theta_{23}}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},\qquad A^-_{\theta_{23}}=\sin\theta_{24}\begin{pmatrix}0 & -e^{i(\phi_{24}-\phi_{23})}\\ e^{-i(\phi_{24}-\phi_{23})} & 0\end{pmatrix},$$

$$A^+_{\theta_{24}}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},\qquad A^-_{\theta_{24}}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}.$$

The matrix elements of $A_{\phi_{13}}$ are given by

$$(A^+_{\phi_{13}})_{11}=-i\sin^2\theta_{13}\cos^2\theta_{14},$$

$$(A^+_{\phi_{13}})_{12}=-\tfrac{1}{2}ie^{i(\phi_{13}-\phi_{23})}\sin 2\theta_{13}\sin\theta_{23}\cos\theta_{14}\cos\theta_{24}+\tfrac{1}{2}ie^{-i(\phi_{14}-\phi_{24})}\sin^2\theta_{13}\sin 2\theta_{14}\sin\theta_{24},$$

$$(A^+_{\phi_{13}})_{21}=(A^+_{\phi_{13}})^*_{12},$$

$$(A^+_{\phi_{13}})_{22}=i\sin^2\theta_{13}\sin^2\theta_{23}\cos^2\theta_{24}-i\sin^2\theta_{13}\sin^2\theta_{24}\sin^2\theta_{14}$$
$$+\tfrac{1}{2}i\cos(\phi_{23}-\phi_{13}+\phi_{14}-\phi_{24})\sin 2\theta_{13}\sin\theta_{14}\sin\theta_{23}\sin 2\theta_{24},$$

$$(A^-_{\phi_{13}})_{11}=i\sin^2\theta_{13}\cos^2\theta_{23},$$

$$(A^-_{\phi_{13}})_{12}=-\tfrac{1}{2}ie^{-i(\phi_{23}-\phi_{24})}\sin^2\theta_{13}\sin 2\theta_{23}\sin\theta_{24}$$
$$+\tfrac{1}{2}ie^{-i(\phi_{13}-\phi_{14})}\sin 2\theta_{13}\sin\theta_{14}\cos\theta_{23}\cos\theta_{24},$$

$$(A^-_{\phi_{13}})_{21}=(A^-_{\phi_{13}})^*_{12},$$

$$(A^-_{\phi_{13}})_{22}=i\sin^2\theta_{13}\sin^2\theta_{23}\sin^2\theta_{24}-i\sin^2\theta_{13}\sin^2\theta_{14}\cos^2\theta_{24}$$
$$-\tfrac{1}{2}i\cos(-\phi_{14}+\phi_{13}+\phi_{24}-\phi_{23})\sin 2\theta_{13}\sin\theta_{14}\sin\theta_{23}\sin 2\theta_{24},$$

$$A^+_{\phi_{14}}=i\sin^2\theta_{14}\begin{pmatrix}-1 & -e^{i(\phi_{14}-\phi_{24})}\cot\theta_{14}\sin\theta_{24}\\ -e^{-i(\phi_{14}-\phi_{24})}\cot\theta_{14}\sin\theta_{24} & \sin^2\theta_{24}\end{pmatrix},$$

$$A^-_{\phi_{14}}=i\sin^2\theta_{14}\cos^2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

$$A^+_{\phi_{23}}=i\sin^2\theta_{23}\cos^2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & -1\end{pmatrix},$$

$$A^-_{\phi_{23}}=i\sin^2\theta_{23}\begin{pmatrix}1 & e^{i(\phi_{24}-\phi_{23})}\cot\theta_{23}\sin\theta_{24}\\ e^{-i(\phi_{24}-\phi_{23})}\cot\theta_{23}\sin\theta_{24} & -\sin^2\theta_{24}\end{pmatrix},$$

$$A^+_{\phi_{24}}=i\sin^2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & -1\end{pmatrix},\qquad A^-_{\phi_{24}}=i\sin^2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

B. Field strength *F*

In this subsection we shall calculate the field strength F associated with the previous connections A. Its components are given by $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu+[A_\mu,A_\nu]$. Here, we shall restrict on the field strength components for which the commutator part $[A_\mu,A_\nu]$ is zero for all values of the parameters θ_{ij} and ϕ_{ij}. For them the computation of their holonomies is straightforward, as we shall see in the following subsection. Let us present first the (θ,ϕ) field strength components. The ones that are obtained from commuting connection components acting on the S_+ and S_- eigenspaces are given by

$$(F^+_{\theta_{24}\phi_{13}})_{11}=0,$$

$$(F^+_{\theta_{24}\phi_{13}})_{12}=\frac{i}{2}e^{i(\phi_{13}-\phi_{23})}\sin 2\theta_{13}\sin\theta_{23}\cos\theta_{14}\sin\theta_{24}+\frac{i}{2}e^{-i(\phi_{14}-\phi_{24})}\sin 2\theta_{14}\sin^2\theta_{13}\cos\theta_{24},$$

$$(F^+_{\theta_{24}\phi_{13}})_{21}=(F^+_{\theta_{24}\phi_{13}})^*_{12},$$

$$(F^+_{\theta_{24}\phi_{13}})_{22}=-i\sin\theta_{13}\sin 2\theta_{24}(\sin^2\theta_{14}+\sin^2\theta_{23})$$
$$+i\cos(\phi_{23}-\phi_{13}+\phi_{14}-\phi_{24})\sin 2\theta_{13}\sin\theta_{14}\sin\theta_{23}\cos 2\theta_{24},$$

$$(F^-_{\theta_{24}\phi_{13}})_{11}=0,$$

$$(F^-_{\theta_{24}\phi_{13}})_{12}=-\frac{i}{2}e^{i(\phi_{23}-\phi_{24})}\sin^2\theta_{13}\sin 2\theta_{23}\cos\theta_{24}-\frac{i}{2}e^{i(\phi_{13}-\phi_{14})}\sin 2\theta_{13}\sin\theta_{14}\cos\theta_{23}\sin\theta_{24},$$

$$(F^{-}_{\theta_{24}\phi_{13}})_{21}=(F^{-}_{\theta_{24}\phi_{13}})^{*}_{12},$$

$$(F^{-}_{\theta_{24}\phi_{13}})_{22}=i\sin^2\theta_{13}\sin 2\theta_{24}(\sin^2\theta_{23}+\sin^2\theta_{14})-i\cos(\phi_{13}-\phi_{14}+\phi_{24}-\phi_{23})\times\sin 2\theta_{13}\sin\theta_{14}\sin\theta_{23}\cos 2\theta_{24},$$

$$F^{+}_{\theta_{24}\phi_{14}}=\begin{pmatrix}0 & -\frac{1}{2}ie^{i(\phi_{14}-\phi_{24})}\sin 2\theta_{14}\cos\theta_{24}\\ -\frac{1}{2}ie^{-i(\phi_{14}-\phi_{24})}\sin 2\theta_{14}\cos\theta_{24} & i\sin^2\theta_{14}\sin 2\theta_{24}\end{pmatrix},$$

$$F^{-}_{\theta_{24}\phi_{14}}=-i\sin^2\theta_{14}\sin 2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

$$F^{+}_{\theta_{24}\phi_{23}}=i\sin^2\theta_{23}\sin 2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

$$F^{-}_{\theta_{24}\phi_{23}}=\begin{pmatrix}0 & \frac{1}{2}ie^{i(\phi_{24}-\phi_{23})}\sin 2\theta_{23}\cos\theta_{24}\\ \frac{1}{2}ie^{i(-\phi_{24}+\phi_{23})}\sin 2\theta_{23}\cos\theta_{24} & -i\sin^2\theta_{23}\sin 2\theta_{24}\end{pmatrix},$$

$$F^{+}_{\theta_{24}\phi_{24}}=-i\sin 2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},\qquad F^{-}_{\theta_{24}\phi_{24}}=i\sin 2\theta_{24}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

From the connection components where only the ones that act on S_+ commute we obtain the following field strength components:

$$F^{+}_{\theta_{23}\phi_{13}}=\frac{i}{2}\cos\theta_{24}\cos\theta_{23}\sin 2\theta_{13}\times\begin{pmatrix}0 & -e^{i(\phi_{13}-\phi_{23})}\cos\theta_{14}\\ -e^{-i(\phi_{13}-\phi_{23})}\cos\theta_{14} & 2\tan\theta_{13}\sin\theta_{23}+2\cos(\phi_{23}-\phi_{13}+\phi_{14}-\phi_{24})\sin\theta_{14}\sin\theta_{24}\end{pmatrix},$$

$$F^{+}_{\theta_{23}\phi_{23}}=-i\cos^2\theta_{24}\sin 2\theta_{23}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

while $F^{+}_{\theta_{23}\phi_{14}}=F^{+}_{\theta_{23}\phi_{24}}=0$. From the connection components where only the ones that act on S_- commute, we obtain the following field strength components:

$$F^{-}_{\theta_{14}\phi_{13}}=-\frac{i}{2}\sin 2\theta_{13}\cos\theta_{14}\cos\theta_{24}\times\begin{pmatrix}0 & -e^{-i(\phi_{13}-\phi_{14})}\cos\theta_{23}\\ -e^{i(\phi_{13}-\phi_{14})}\cos\theta_{23} & 2\tan\theta_{13}\sin\theta_{14}\cos\theta_{24}+2\cos(\phi_{13}-\phi_{14}+\phi_{24}-\phi_{23})\sin\theta_{23}\sin\theta_{24}\end{pmatrix},$$

$$F^{-}_{\theta_{14}\phi_{14}}=i\cos^2\theta_{24}\sin 2\theta_{14}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

while $F^{-}_{\theta_{14}\phi_{23}}=F^{-}_{\theta_{14}\phi_{24}}=0$. Finally, the (θ,θ) field strength components are given by

$$F^{+}_{\theta_{13}\theta_{24}} = \sin\theta_{23}\cos\theta_{14}\begin{pmatrix} 0 & -e^{i(\phi_{13}-\phi_{23})}\sin\theta_{24} \\ e^{-i(\phi_{13}-\phi_{23})}\sin\theta_{24} & -2i\sin(\phi_{13}-\phi_{14}+\phi_{24}-\phi_{23})\tan\theta_{14}\cos 2\theta_{24} \end{pmatrix},$$

$$F^{-}_{\theta_{13}\theta_{24}} = \sin\theta_{14}\cos\theta_{23}\begin{pmatrix} 0 & -e^{i(\phi_{14}-\phi_{13})}\sin\theta_{24} \\ e^{-i(\phi_{14}-\phi_{13})}\sin\theta_{24} & -2i\sin(\phi_{14}+\phi_{23}-\phi_{13}-\phi_{24})\tan\theta_{23}\cos 2\theta_{24} \end{pmatrix},$$

$$F^{+}_{\theta_{14}\theta_{23}} = F^{-}_{\theta_{14}\theta_{23}} = 0,$$

$$F^{+}_{\theta_{14}\theta_{24}} = -\cos\theta_{24}\begin{pmatrix} 0 & -e^{i(\phi_{14}-\phi_{24})} \\ e^{-i(\phi_{14}-\phi_{24})} & 0 \end{pmatrix}, \qquad F^{-}_{\theta_{14}\theta_{13}} = 0,$$

$$F^{+}_{\theta_{23}\theta_{24}} = 0 \qquad F^{-}_{\theta_{23}\theta_{24}} = -\cos\theta_{24}\begin{pmatrix} 0 & -e^{i(\phi_{24}-\phi_{23})} \\ e^{-i(\phi_{24}-\phi_{23})} & 0 \end{pmatrix},$$

$$F^{+}_{\theta_{13}\theta_{23}} = -\cos\theta_{23}\cos\theta_{14}\cos\theta_{24}\begin{pmatrix} 0 & -e^{i(\phi_{13}-\phi_{23})} \\ e^{-i(\phi_{13}-\phi_{23})} & 2i\sin(\phi_{13}-\phi_{14}+\phi_{24}-\phi_{23})\tan\theta_{14}\sin\theta_{24} \end{pmatrix},$$

$$F^{-}_{\theta_{13}\theta_{14}} = -\cos\theta_{14}\cos\theta_{23}\cos\theta_{24}\begin{pmatrix} 0 & -e^{i(\phi_{14}-\phi_{13})} \\ e^{-i(\phi_{14}-\phi_{13})} & 2i\sin(\phi_{14}+\phi_{23}-\phi_{13}-\phi_{24})\tan\theta_{23}\sin\theta_{24} \end{pmatrix}.$$

C. Holonomies Γ

In general, the explicit calculation of the Holonomies of matrix connections A is nonstraightforward as they involve the path ordering procedure when exponentiating their loop integral. On the other hand, it is possible to restrict our cyclic evolutions to specific planes (σ,σ') that correspond to commuting components A_σ and $A_{\sigma'}$. For those loops we can employ Stokes theorem for the Abelian theories and obtain

$$\Gamma^{\pm}_{A}(C) \equiv \mathbf{P}\exp\oint_C A^{\pm} = \exp\oint_C A^{\pm} = \exp\int\int_{\Sigma(C)} d\sigma\, d\sigma'\; F^{\pm}_{\sigma\sigma'}(\sigma,\sigma')\ , \tag{3}$$

where the rest of the variables are considered constant. The path ordering symbol has been taken out at the second step as the connection components on the (σ,σ') commute with each other. Hence, Stokes theorem can be applied straightforwardly as presented in the previous section for the Abelian Berry phase. An analytic expression for the holonomies can be obtained by exponentiating the 2×2 matrices resulting from the surface integral of the field strength components presented in the previous subsection.

IV. DISCUSSION

A theoretical model has been presented for the construction of non-Abelian holonomies for the $G(4,2)$ Grassmannian manifold. This is the generalization of the usual Abelian Berry phase to the case of a quantum system consisting of a doubly degenerate energy eigenspace. The evolution of both degenerate spaces has been presented that are produced from the same cyclic adiabatic evolution. The main difference with the Abelian case is that it is possible to have manipulations of state population in each degenerate space rather than just the generation of overall phase factors. This can be achieved, for example, by spanning loops C on the (θ_{24},ϕ_{13}) plane where the population can be interchanged in a well defined way between the states $|1\rangle$ and $|2\rangle$ as well as between $|3\rangle$ and $|4\rangle$. In contrast, loops on the (θ_{24},ϕ_{24}) plane contribute only Berry-like phases on the conjugate states $|2\rangle$ and $|4\rangle$ (see Fig. 1). It is worth noticing that the holonomic evolution is not producing any correlations between the two different eigenspaces S_+ and S_- due to the cyclicity of the adiabatic procedure. Even though it is possible to have each degenerate eigenspace evolving with a different holonomy there is a correspondence between the evolutions as can be easily seen

in the previous section facilitating eventually their detection in a physical system and the verification of the above results. Indeed, the components F^+ and F^- of the field strength have a similar functional dependence on the variables (θ_{ij}, ϕ_{ij}) and their surface integral in (3) bears a common dependence in the area $\Sigma(C)$. These holonomic characteristics can be verified in the laboratory with present technology by employing an atomic cloud and manipulating the atomic states with external laser beams.

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Contextual viewpoint to quantum stochastics

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(Received 21 January 2002; accepted 4 March 2003)

We study the role of context, complex of physical conditions, in quantum as well as classical experiments. It is shown that by taking into account contextual dependence of experimental probabilities we can derive the quantum rule for the addition of probabilities of alternatives. Thus we obtain quantum interference without applying the wave or Hilbert space approach. The Hilbert space representation of contextual probabilities is obtained as a consequence of the elementary geometric fact: cos-theorem. By using another fact from elementary algebra we obtain complex-amplitude representation of probabilities. Finally, we found contextual origin of noncommutativity of incompatible observables. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1570952]

I. INTRODUCTION

It is well known that the classical rule for the addition of probabilistic alternatives:

$$P = P_1 + P_2 \tag{1}$$

does not work in experiments with elementary particles. Instead of this rule, we have to use quantum rule:

$$P = P_1 + P_2 + 2\sqrt{P_1 P_2}\cos\theta. \tag{2}$$

The classical rule for the addition of probabilistic alternatives is perturbed by the so-called interference term. The difference between ''classical'' and ''quantum'' rules was (and is) the source of permanent discussions as well as various misunderstandings and mystifications, see, e.g., Refs. 1–23. We just note that the appearance of the interference term was the source of the wave-viewpoint to the theory of elementary particles. At least the notion of *superposition* of quantum states was proposed as an attempt to explain the appearance of a new probabilistic calculus in the two slit experiment, see, for example, Dirac's book[1] on historical analysis of the origin of quantum formalism. We also mention that Feynman interpreted (2) as evidence of the violation of the additivity postulate for ''quantum probabilities,'' see Ref. 5:

> ''From about the beginning of the twentieth century experimental physics amassed an impressive array of strange phenomena which demonstrated the inadequacy of classical physics. … The new theory asserts that there are experiments for which the exact outcome is fundamentally unpredictable and that in these cases one has to be satisfied with computing probabilities of various outcomes. But far more fundamental was the discovery that in nature the laws of combining probabilities were *not* those of classical probability theory of Laplace. The quantum mechanical laws of the physical world approach very closely the laws of Laplace as the size of the objects involved in the experiments increases. Therefore the laws of probabilities which are conventionally applied are quite satisfactory in analyzing the behavior of the roulette wheel but not the behavior of a single electron or a photon of light.''

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We underline that the detailed analysis of the origin of ''quantum probabilities'' was performed by Accardi in Ref. 10. In those papers there was investigated the role of *Bayes' formula* for conditional probabilities. This formula was automatically incorporated in conventional probability theory (Kolmogorov, 1933, see Ref. 24). It was pointed out that the use of this formula for statistical data obtained in quantum experiments is not really justified. It was proposed to modify Kolmogorov's axiomatics and consider non-Kolmogorovian probabilistic models without Bayes' formula. There was also introduced the notion of *statistical invariant*. By using statistical invariants there was investigated the problem of the existence of a Kolmogorov model describing given statistical data.

Recently the author demonstrated, see Refs. 22 and 23, that taking into account dependence of probabilities on complexes of physical conditions it is possible to obtain quantum rule for the addition of probabilistic alternatives (2) without having to apply to the Hilbert space formalism. Derivation of (2) in Refs. 22 and 23 was based on the use of the frequency theory of probability (von Mises, 1919, see, e.g., Ref. 24). That frequency derivation had two main disadvantages: (a) the frequency approach to probability was strongly criticized in mathematical literature; (b) frequency calculations obscured physical roots of the appearance of the intereference term in (2). In the present paper we are not rigidly coupled to some special approach to probability (frequency, measure-theoretical, axiomatic). Primary attention is paid to dependence of probability on the complex of experimental physical conditions—*context*, see Ref. 25. We demonstrated that by taking into account context-dependence of probabilities we can derive quantum rule for the addition of probabilistic alternatives (2). In this derivation we do not use linear algebra or complex numbers.

We also mention other fundamental investigations on the role of conditional probabilities in quantum theory: Gudder[15]—theory of probability manifolds and Ballentine[19]—axiomatic approach to conditional probability and quantum mechanics.

II. THE ROLE OF A COMPLEX OF PHYSICAL CONDITIONS

In fact, probabilities in (2) in quantum experiments are determined by at least three different contexts, $\mathcal{S},\mathcal{S}_1,\mathcal{S}_2$. We illustrate this situation by the following fundamental example.

Example (two slit experiment): In the two slit experiment rule (2) is induced by combining of statistical data obtained in three different experiments: both slits are open; only the jth slit is open, $j=1,2$. The main distinguishing feature of statistical data obtained in these three experiments is as follows. By combining by (1) data obtained in experiments in which only one of the slits is open we do not get the probability distribution for data obtained in the experiment in which both slits are open. On the other hand, we never observe a particle that passes through both slits simultaneously—it would be observed passing the first or second slit. There is no direct observation of particle splitting. As each particle passes only one of the slits, we have the standard case of alternatives. Thus we should use the conventional rule (1) for the addition of probabilities of alternatives. This disagreement between experimental statistical data and the rule of conventional probability theory looks like a kind of paradox. The traditional solution of this paradox is the use of the wave model for elementary particles.

We now perform detailed contextual analysis for the two slit experiment. We consider the following complexes of physical conditions, contexts:

$\mathcal{S}=$ both slits are open, $\mathcal{S}_j=$ only jth slit is open, $j=1,2$.

In fact, probabilities in (2) are related to these three contexts (see Accardi[10] or Ballentine[19]). Thus $P=P_{\mathcal{S}}(A)$ and $P_j=P_{\mathcal{S}_j/\mathcal{S}}P_{\mathcal{S}_j}(A)$, $j=1,2$.

Here we use various context-indexes. The $P_{\mathcal{S}}(A),P_{\mathcal{S}_j}(A)$ denote probabilities of an event A with respect to various contexts. The coefficients $P_{\mathcal{S}_j/\mathcal{S}}$, $j=1,2$, have another meaning. In general these are not probabilities of $\mathcal{S}_j$ with respect to the context $\mathcal{S}$ (besides some very special, ''classical,'' situations), because the context $\mathcal{S}_j$ in general is not an event for the context $\mathcal{S}$. The $P_{\mathcal{S}_j/\mathcal{S}}$, $j=1,2$, are kinds of *balance probabilities*. These are proportion coefficients for filtrations induced by contexts $\mathcal{S}$ and $\mathcal{S}_j$.

We explain how we can find balance probabilities in the frequency framework. Let $\mathcal{O}$ be a source of particles. Suppose that $\mathcal{O}$ produced M particles. They interacted with the context $\mathcal{S}$ and on the registration screen there were found N dots. Suppose that $\mathcal{O}$ again produced M particles. They interacted with the context $\mathcal{S}_1$ and on the registration screen there were found N_1 dots. In the same way we find the number N_2. We set

$$P_{\mathcal{S}_j/\mathcal{S}}=\frac{N_j}{N}. \tag{3}$$

Of course, (3) is just frequencies and to define probabilities we should consider the limit when $M\to\infty$, see Refs. 22 and 23 for detail.

However, we need not use only the frequency approach to define balance probabilities. In many cases these probabilities could be defined *a priori* by taking into account the geometry of the experiment, namely the location of the source of particles with respect to the screen with two slits.

We remark (and it is important for our further considerations) that we have the following balance condition:

$$P_{\mathcal{S}_1/\mathcal{S}}+P_{\mathcal{S}_2/\mathcal{S}}=1. \tag{4}$$

The balance condition has the following meaning: the total number of particles that arrives to the registration screen when both slits are open equals (on average) the sum of the corresponding numbers when only one of the slits is open. So by closing, for example, the first slit we do not change the number of particles that pass the second slit (on average). In fact, (4) gives the right description of the alternative situation in the two slit experiment. It is not related to alternative passing of slits by a particle in the experiment when both slits are open. This equation describes alternative sharing of particles between two preparation procedures: jth slit is open, $j=1,2$.

However, the balance probabilities $P_{\mathcal{S}_j/\mathcal{S}}$ would not play so important a role in our considerations. The crucial role will be played by contextual probabilities $P_{\mathcal{S}}(A), P_{\mathcal{S}_j}(A)$.

In many considerations (including works by the fathers of quantum mechanics, see e.g., Dirac,[1] see also Feynman[5]) people set $P=P(A)$ and $P_j=P_{\mathcal{S}_j/\mathcal{S}}P_{\mathcal{S}_j}(A)$. Finally, they get the contradiction between conventional probabilistic rule (1) and statistical data obtained in the interference experiments and described by quantum rule (2), see Refs. 10 and 13 for the detailed analysis of this ''contradiction.''

In Sec. III we derive quantum rule (2) in the contextual probabilistic framework.

III. INTERFERENCE TERM AS THE MEASURE OF STATISTICAL DEVIATIONS DUE TO THE CONTEXT TRANSITION

The following simple considerations give us the derivation of quantum probabilistic transformation (2) in the classical probabilistic framework.

Let $\mathcal{S}$ and $\mathcal{S}_j$, $j=1,2$, be three different complexes of conditions. We consider the transformation of probabilities induced by transitions from one complex of conditions to others:

$$\mathcal{S}\to\mathcal{S}_1, \quad \mathcal{S}\to\mathcal{S}_2. \tag{5}$$

We start by introducing balance probabilities, $P_{\mathcal{S}_j/\mathcal{S}}$. These are proportional coefficients for numbers of physical systems obtained after preparations under the complexes of physical conditions $\mathcal{S}$ and $\mathcal{S}_j$. If (starting with the same number of particles) we get N and N_j systems after $\mathcal{S}$ and $\mathcal{S}_j$ preparations, respectively, then $P_{\mathcal{S}_j/\mathcal{S}}$ are defined by (3). We assume that balance probabilities satisfy the balance equation (4). This is a quite natural condition: splitting (5) of the context $\mathcal{S}$ induces just sharing of physical systems produced by a source. We have already discussed this balance in the two slit experiment. We have the same situation in neutron interferometry for the balance between the number of particles coming to detectors when both paths are open and when just one of the paths is open.

We introduce the *measure of statistical perturbations* δ induced by context transitions:

$$\delta(A;\mathcal{S};\mathcal{S}_j)=P_{\mathcal{S}_1/\mathcal{S}}[P_{\mathcal{S}}(A)-P_{\mathcal{S}_1}(A)]+P_{\mathcal{S}_2/\mathcal{S}}[P_{\mathcal{S}}(A)-P_{\mathcal{S}_2}(A)].$$

This quantity describes the deformation of probability distribution $P_{\mathcal{S}}$ due to context transitions.

By using balance equation (4) we get

$$P_{\mathcal{S}}(A)=P_{\mathcal{S}}(A)P_{\mathcal{S}_1/\mathcal{S}}+P_{\mathcal{S}}(A)P_{\mathcal{S}_2/\mathcal{S}}.$$

Thus we get

$$P_{\mathcal{S}}(A)=P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)+P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)+\delta(A;\mathcal{S},\mathcal{S}_j). \tag{6}$$

Transformation (6) is the most general form of probabilistic transformations due to context transitions.

There is *the correspondence principle* between context unstable and (''classical'') context stable transformations: If $\mathcal{S}_j\to\mathcal{S}$, $j=1,2$, i.e., $\delta(A;\mathcal{S},\mathcal{S}_j)\to 0$, then contextual probabilistic transformation (6) coincides (in the limit) with the conventional formula of total probability, see Ref. 25.

The perturbation term $\delta(A;\mathcal{S},\mathcal{S}_j)$ depends on absolute magnitudes of probabilities. It would be natural to introduce normalized coefficient of the context transition

$$\lambda(A;\mathcal{S},\mathcal{S}_j)=\frac{\delta(A;\mathcal{S},\mathcal{S}_j)}{2\sqrt{P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)}},$$

which gives the relative measure of statistical deviations due to the transition from one complex of conditions, $\mathcal{S}$, to others, $\mathcal{S}_j$. Transformation (6) can be written in the following form:

$$P_{\mathcal{S}}(A)=\sum_{j=1,2}P_{\mathcal{S}_j/\mathcal{S}}P_{\mathcal{S}_j}(A)+2\sqrt{P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)}\lambda(A;\mathcal{S},\mathcal{S}_j). \tag{7}$$

In fact, there are two possibilities:

(1) $|\lambda(A;\mathcal{S},\mathcal{S}_j)|\leqslant 1$;

(2) $|\lambda(A;\mathcal{S},\mathcal{S}_j)|\geqslant 1$.

In both cases it is convenient to introduce a new context transition parameter $\theta=\theta(A;\mathcal{S},\mathcal{S}_j)$ and represent the context transition coefficient in the form:

$$\lambda(A;\mathcal{S},\mathcal{S}_j)=\cos\theta(A;\mathcal{S},\mathcal{S}_j),\ \theta\in[0,\pi];$$

and

$$\lambda(A;\mathcal{S},\mathcal{S}_j)=\pm\cosh\theta(A;\mathcal{S},\mathcal{S}_j),\ \theta\in[0,\infty),$$

respectively.

We have two types of probabilistic transformations induced by the transition from one complex of conditions to another:

$$P_{\mathcal{S}}(A)=\sum_{j=1,2}P_{\mathcal{S}_j/\mathcal{S}}P_{\mathcal{S}_j}(A)+2\sqrt{P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)}\cos\theta(A;\mathcal{S},\mathcal{S}_j), \tag{8}$$

$$P_{\mathcal{S}}(A)=\sum_{j=1,2}P_{\mathcal{S}_j/\mathcal{S}}P_{\mathcal{S}_j}(A)\pm 2\sqrt{P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)}\cosh\theta(A;\mathcal{S},\mathcal{S}_j). \tag{9}$$

We derived quantum probabilistic rule (2) in the classical probabilistic framework (in particular, without any reference to superposition of states) by taking into account the context dependence of probabilities.

Remark: Reference 10 was the first publication in which violation of the classical rule for the addition of probabilistic alternatives in the two slit experiment was coupled with the violation of Bayes' formula for conditional probabilities. The present paper undertakes the next important step—deriving the quantum rule for the addition of probabilistic alternatives in the two slit experiment by using the contextual approach to probability. One of the main differences between the contextual probabilistic approach used here and Accardi's conditional probability approach is that here the measure of statistical perturbations δ (or corresponding coefficient λ) is used instead of statistical invariants. Finally, we remark that, in fact, we studied the case that is trivial from the viewpoint of the theory of statistical invariants—two dichotomic variables. There always exists (under very natural restrictions of symmetry of matrixes of transition probabilities, see Ref. 10) Kolmogorovian model reproducing transition probabilities. However, in our approach even such models could demonstrate ''interference'' of probabilities, i.e., violation of the classical formula of total probability, cf. Refs. 24, 26, 27.

Relatively large statistical deviations are described by transformation (9). Such transformations do not appear in the conventional formalism of quantum mechanics. In principle, they could be described by so-called *hyperbolic quantum mechanics*, Refs. 28, 29.

Conclusion: For each fixed context (experimental arrangement), we have *classical statistics*. *Context transition* induces interference perturbation of the conventional rule for the addition of probabilistic alternatives.

IV. LINEAR ALGEBRA FOR PROBABILITIES, COMPLEX AMPLITUDES

One of the main distinguishing features of quantum theory is the Hilbert space calculus for probabilistic amplitudes. As we have already discussed, this calculus is typically associated with wavelike (superposition) features of quantum particles. We shall show that, in fact, the Hilbert space representation of probabilities was merely a mathematical discovery. Of course, this discovery simplifies essential calculations. However, this is pure mathematics; physics is related merely to the derivation of quantum interference rule (2).

The crucial point was the derivation (at the beginning purely experimental) of transformation (2) connecting probabilities with respect to three different contexts. In fact, linear algebra can be easily derived from this transformation. Everybody familiar with the elementary geometry will see that (2) is just the well known cos-theorem. This is the rule to find the third side in a triangle if we know the lengths of two other sides and the angle θ between them:

$$c^2 = a^2 + b^2 - 2ab\cos\theta$$

or if we want to have ''+'' before cos we use the so-called *parallelogram law*:

$$c^2 = a^2 + b^2 + 2ab\cos\theta. \tag{10}$$

Here c is the diagonal of the parallelogram with sides a and b and the angle θ between these sides. Of course, the parallelogram law is just the law of linear (two-dimensional Hilbert space) algebra: for finding the length c of the sum $\mathbf{c}$ of vectors $\mathbf{a}$ and $\mathbf{b}$ having lengths a and b and the angle θ between them.

We also can introduce complex waves by using the following elementary formula:

$$a^2 + b^2 + 2ab\cos\theta = |a + be^{i\theta}|^2. \tag{11}$$

Thus the context transitions $\mathcal{S}\rightarrow\mathcal{S}_j$ can be described by the wave:

$$\varphi = \sqrt{P_{\mathcal{S}_1/\mathcal{S}}P_{\mathcal{S}_1}(A)} + \sqrt{P_{\mathcal{S}_2/\mathcal{S}}P_{\mathcal{S}_2}(A)}e^{i\theta(A;\mathcal{S},\mathcal{S}_j)}.$$

V. "CLASSICAL" PROBABILISTIC DERIVATION OF THE SUPERPOSITION PRINCIPLE FOR WAVE FUNCTIONS IN THE TWO SLIT EXPERIMENT

We shall study in more detail the possibility of contextual (purely classical) derivation of the superposition principle for complex probability amplitudes, "waves," in the two slit experiment. We consider a one-dimensional model. It could be obtained by considering the distribution of particles on one fixed straight line, very thin strip. It is supposed that the source of particles is symmetric with respect to slits and the straight line (on the registration screen) passes through the center of the screen. This geometry implies that $P_{\mathcal{S}_j/\mathcal{S}}=1/2$, $j=1,2$. The symbol $A_x, x\in\mathbf{R}$, denotes the event of the registration of a particle at the point x of the straight line. We set:

$$p(x)=P_{\mathcal{S}}(A_x), \quad p_j(x)=P_{\mathcal{S}_j}(A_x), \quad j=1,2,$$

where contexts $\mathcal{S}$ and $\mathcal{S}_j$ were defined in Example 1. By using (8) we get

$$p(x)=\tfrac{1}{2}[p_1(x)+p_2(x)+2\sqrt{p_1(x)p_2(x)}\cos\theta(x)].$$

By using (11) we represent this probability as the square of a complex amplitude, $p(x)=|\phi(x)|^2$,

where

$$\phi(x)=\frac{1}{\sqrt{2}}(e^{i\theta_1(x)}\sqrt{p_1(x)}+e^{i\theta_2(x)}\sqrt{p_2(x)}) \tag{12}$$

and phases $\theta_j(x)$ are chosen in such a way that the phase shift $\theta_1(x)-\theta_2(x)=\theta(x)$. We also introduce complex amplitudes for probabilities $p_j(x)$: $\phi_j(x)=(1/\sqrt{2})\,e^{i\theta_j(x)}\sqrt{p_j(x)}$. Here $p_j(x)=|\phi_j(x)|^2$. The complex amplitudes are said to be *wave functions*: $\phi(x)$ is the wave function on (the straight line of) the registration screen when both slits are open; $\phi_j(x)$ is the wave function on (the straight line of) the registration screen when jth slit is open.

Let us set $\xi(x)=(\theta(x)/h)$, where $h>0$ is some scaling factor. We have

$$\phi(x)=\frac{1}{\sqrt{2}}\left(\exp\left(\frac{i\xi_1(x)}{h}\right)\sqrt{p_1(x)}+\exp\left(\frac{i\xi_2(x)}{h}\right)\sqrt{p_2(x)}\right), \quad \phi_j(x)=\frac{1}{\sqrt{2}}\exp\left(\frac{i\xi_j(x)}{h}\right)\sqrt{p_j(x)}.$$

By choosing h as the Planck constant we get a quantum-like representation of probabilities. We recall that we did not use any kind of wave argument. Superposition rule (12) was obtained in a purely classical probabilistic (but contextual!) framework.

Suppose now that ξ depends linearly on x: $\xi_j(x)=\mathbf{p}_j x/h$, $\xi(x)=\mathbf{p}x/h$, $\mathbf{p}=\mathbf{p}_1-\mathbf{p}_2$. Under such an assumption we shall get interference of two "free-waves" corresponding to momentums $\mathbf{p}_1$ and $\mathbf{p}_2$. Of course, this linearity could not be extracted from our general probabilistic considerations. This is a consequence of the concrete geometry of the experiment.[29]

VI. THE COEFFICIENT OF CONTEXT TRANSITION AS THE MEASURE OF INCOMPATIBILITY OF PHYSICAL OBSERVABLES

We now consider the relation between the coefficient of context transition (the measure of statistical deviations due to the change of complex of physical conditions) and incompatibility of physical observables in quantum mechanics (noncommutativity of corresponding operators). As everywhere in this paper, we consider dichotomic observables. Each event A generates the dichotomic variable a: $a=a_1$ if A occurs and $a=a_2$ if A does not occur. Values a_1 and a_2 do not play any role in our considerations; in principle, we can consider the case $a_1=0$ and $a_2=1$.

Definition: A physical observable a is incompatible with a pair $\mathcal{S}_1,\mathcal{S}_2$ of contexts if there exists a context $\mathcal{S}$ such that $\delta(a=a_i;\mathcal{S};\mathcal{S}_j)\neq 0$.

In such a case a transition from the complex of physical conditions $\mathcal{S}$ to complexes $\mathcal{S}_j$ induces non-negligible statistical deviations for a-measurements. It is not the same to measure a under the complex of conditions $\mathcal{S}$ or $\mathcal{S}_j$.

In fact, we need to consider two complexes $\mathcal{S}_1$ and $\mathcal{S}_2$, because we would like to consider another dichotomic variable b connected to these contexts.

We shall demonstrate that the incompatibility of physical observables in quantum mechanics is just a particular case of contextual incompatibility.

Let $\mathcal{H}$ be the two-dimensional Hilbert space. Rays of this space represent some class of complexes of physical conditions. Let the dichotomic variable a be represented by a self-adjoint operator (symmetric matrix) $\hat{a}$. We remark that we can associate with any physical observable a two complexes of conditions $\mathcal{S}_1^a, \mathcal{S}_2^a$, namely contexts corresponding to eigenvectors ϕ_1^a, ϕ_2^a of $\hat{a}$. The $\mathcal{S}_j^a$ describes the filter with respect to the value $a = a_j$.

Let us consider an other dichotomic physical observable $b = b_1, b_2$. It is represented by a self-adjoint operator $\hat{b}$ with eigenvectors ϕ_1^b, ϕ_2^b. These eigenvectors represent contexts $\mathcal{S}_1^b, \mathcal{S}_2^b$ (filtrations corresponding to $b = b_1$ and $b = b_2$, respectively).

Theorem: *Quantum physical observables a and b are incompatible (i.e., corresponding operators do not commute) iff the observable a is incompatible with the contexts $\mathcal{S}_j^b$ or vice versa*:

$$\delta(a = a_i; \mathcal{S}; \mathcal{S}_j^b) \neq 0 \quad \text{or} \quad \delta(b = b_i; \mathcal{S}; \mathcal{S}_j^a) \neq 0.$$

Proof: Let $\mathcal{S}$ be an arbitrary quantum context. Thus it can be represented by a normalized vector $\phi \in \mathcal{H}$. We have:

$$\delta(a = a_i; \mathcal{S}; \mathcal{S}_j^b) = P_{\mathcal{S}_1/\mathcal{S}}[P_{\mathcal{S}}(a = a_i) - P_{\mathcal{S}_1}(a = a_i)] + P_{\mathcal{S}_2/\mathcal{S}}[P_{\mathcal{S}}(a = a_i) - P_{\mathcal{S}_2}(a = a_i)]$$

$$= |(\phi, \phi_1^b)|^2 (|(\phi, \phi_i^a)|^2 - |(\phi_i^a, \phi_1^b)|^2) + |(\phi, \phi_2^b)|^2 (|(\phi, \phi_i^a)|^2 - |(\phi_i^a, \phi_2^b)|^2).$$

We have $(\phi, \phi_j^b) = k_j e^{i\xi_j}, (\phi_j^b, \phi_i^a) = k_{ji} e^{i\xi_{ji}}$, where $k_j, k_{ij} \geqslant 0$. We get

$$\delta(a = a_i; \mathcal{S}; \mathcal{S}_j^b) = 2k_1 k_2 k_{1i} k_{2i} \cos\theta_i,$$

where $\theta_i = \xi_2 - \xi_1 + \xi_{2i} - \xi_{1i}$.

(a) Let $[\hat{a}, \hat{b}] = 0$. Then $k_{12} = k_{21} = 0$. Hence $\delta(a = a_i; \mathcal{S}; \mathcal{S}_j^b) = 0$.

(b) Let $[\hat{a}, \hat{b}] \neq = 0$. Then $k_{12}, k_{21} \neq 0$. Let $k_1, k_2 > 0$ be arbitrary constants such that $k_1^2 + k_2^2 = 1$. We choose a context $\mathcal{S}$ that is described by the state:

$$\phi = \sqrt{k_1} e^{i\xi_{21}} \phi_1^b + \sqrt{k_2} e^{i\xi_{11}} \phi_2^b.$$

Here $\theta = 0$ and, hence,

$$\delta(a = a_i; \mathcal{S}; \mathcal{S}_j^b) = 2k_1 k_2 k_{i1} k_{i2} > 0.$$

Remark: Mathematically a fixed context can be described by, e.g., a Kolmogorov probability space. A *contextual probability model* is mathematically represented by a family of Kolmogorov probability spaces and transformations connecting probabilities belonging to different Kolmogorov spaces. We remark that families of Kolmogorov probability spaces are usually considered in mathematical statistics. However, in statistics people are interested in a totally different problem. They are interested in finding a parameter describing a probability space on the basis of results of measurement of some random variables. Statisticians have never tried to investigate transformations of probabilities corresponding to different values of the statistical parameter. In particular, interference of probabilities was not discovered in ordinary mathematical statistics. Another possibility is to describe contexts by using von Mises collectives. The corresponding contextual model is given by a family of collectives and transformations connecting probabilities corresponding to different collectives.

Conclusion: We demonstrated that a few elements of quantum formalismism which were commonly considered as essentially "quantum" can, in fact, be reproduced by using the contextual approach[22,23] to theory of statistical measurement. In particular, we obtain intereference of probabilities, complex probability amplitudes, Born's rule, Hilbert space structure, and noncommutative observables without having to refer to special quantum behavior of physical systems (see also Ref. 28), but only to context dependence of probabilities.

ACKNOWLEDGMENTS

I would like to thank L. Ballentine, W. De Myunck, L. Accardi, J. Summhammer, C. Fuchs, D. Mermin, A. Peres, I. Volovich, A. Holevo, S. Gudder, K. Gustafson, K. Hess, R. Gill, P. Lahti, J. Bub, T. Maudlin, B. Hiley, W. Philipp, H. Rauch, G. Emch, V. Belavkin, I. Helland, L. Hardy, S. Molotkov, and K. Valiev for fruitful (and sometimes rather critical) discussions.

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Generalized coherent states and the diagonal representation for operators

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(Received 3 December 2002; accepted 8 January 2003)

We consider the problem of existence of the diagonal representation for operators in the space of a family of generalized coherent states associated with a unitary irreducible representation of a (compact) Lie group. We show that necessary and sufficient conditions for the possibility of such a representation can be obtained by combining Clebsch–Gordan theory and the reciprocity theorem associated with induced unitary group representations. Applications to several examples involving SU(2), SU(3), and the Heisenberg–Weyl group are presented, showing that there are simple examples of generalized coherent states which do not meet these conditions. Our results are relevant for phase–space description of quantum mechanics and quantum state reconstruction problems. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1559416]

I. INTRODUCTION

There is a long history of attempts to express the basic structure of quantum mechanics, both kinematics and dynamics, in the *c*-number phase space language of classical mechanics. The first major step in this direction was taken by Wigner[1] very early in the development of quantum mechanics, during a study of quantum corrections to classical statistical mechanics. This led to the definition of a real phase space distribution[2]—now called the Wigner distribution—faithfully representing any pure or mixed state of a quantum system whose kinematics is governed by Heisenberg commutation relations for any number of Cartesian degrees of freedom. It was soon realized that this construction is dual to a rule proposed earlier by Weyl[3] to map classical dynamical variables onto quantum mechanical operators in an unambiguous way, in the sense that the expectation value of any quantum operator in any quantum state can be rewritten in a completely *c*-number form on the corresponding classical phase space.

The general possibilities of expressing quantum mechanical operators in classical *c*-number forms were later examined by Dirac[4] while developing the analogies between classical and quantum mechanics. The specific case of the Weyl–Wigner correspondence was carried further in important work by Groenewold and by Moyal.[5]

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Inspired by the needs of quantum optics, the general problem of setting up different classical variable–quantum operator correspondences has received enormous attention.[6] It has thus been appreciated that the Weyl–Wigner choice is just one of many possibilities, two other important ones being (in the language of photon annihilation and creation operators) the normal ordering[7] and the antinormal ordering[8] choices.

While the harmonic oscillator coherent states, with their remarkable properties, have played a crucial role in all these developments, the idea of coherent states itself has been extended, in two slightly different ways, by Klauder[9] and by Perelomov,[10] to the notion of *generalized coherent states*. A very interesting case is the family of coherent states in the context of an unitary irreducible representation (UIR) of any Lie group G on a Hilbert space $\mathcal{H}$. In particular, the generalized coherent states associated with the group SU(2)—the atomic coherent states[11]—have received enormous attention. A satisfactory generalization of the concept of Wigner distribution has also been achieved for the irreducible representations of SU(2).[12]

For the purpose of the present work *two different levels of completeness* exhibited by the harmonic oscillator coherent states should be highlighted:

(i) *Completeness at the state vector level:* This refers to the fact that every state vector can be written as a linear combination of the coherent states. In terms of the (rank-one) operators corresponding to projections onto the coherent states, this property is expressed by saying that the identity operator can be expressed as a linear combination of these one-dimensional projection operators. This aspect is sometimes known as *resolution of unity*.

(ii) *Completeness at the operator level:* This refers to the remarkable fact that every operator can be realized as a linear combination of projections onto coherent states. This property is often known as the *diagonal representation theorem*.[7] (The accompanying coefficient function of the linear expansion can in general be a very singular distribution.[13]) This diagonal representation of operators is dual to the normal ordering rule in the same sense as the Wigner and Weyl rules are dual to one another. We may note in passing that the diagonal representation has been central to many developments in quantum optics and laser physics. It also plays an important role in defining what is known as the $*$-product for operators.[14]

In view of the interest in generalized coherent states, it is important to know if these two levels of completeness apply to a given system of generalized coherent states or not. The (over) completeness property of the generalized coherent states at the state vector level usually (but not always) follows as a direct consequence of Schur's lemma: completeness at this level depends on whether the group representation under consideration possesses the square integrability property or not.

Completeness at the operator level—namely the question of whether the diagonal representation theorem applies to a given system of generalized coherent states—turns out to be considerably more subtle. In our opinion this question has hitherto not received the direct attention that it deserves (we should, however, invite the reader's attention to some very insightful remarks by Klauder and Skagerstam on this question[15]).

In an important recent work, Brif and Mann[16] have carried out extensive harmonic analysis in the space of rank-one projections onto a system of generalized coherent states. However, they do not study the question of which systems of generalized coherent states admit a diagonal representation for operators and which do not. Indeed, they give no indication that there can be fairly simple systems of generalized coherent states for which the diagonal representation theorem does not apply—in the sense that there exist operators which cannot be written as linear combinations of rank-one projection operators over these coherent states.

The main aim of the present paper is to examine in detail the question of completeness at the operator level and to develop necessary and sufficient conditions which will ensure that all operators on the (relevant) Hilbert space can indeed be expanded in terms of projections onto the generalized coherent states. The non-triviality of this question renders some amount of careful and delicate analysis indispensable, but we would like to assure the reader that the effort is so rewarding as to give a complete answer to an issue of considerable physical importance.

For definiteness we deal with the situation where the group G is compact, so that its chosen

UIR acts on a Hilbert space $\mathcal{H}$ of finite dimension. (However in some of the examples we formally extend our methods to certain noncompact G.) The important tools in our analysis are the well-known reciprocity theorem when one examines an induced representation of G[17] arising from some UIR of a subgroup $H \subset G$ and asks for the occurrence and multiplicity of various UIR's of G itself; and the structure of the Clebsch–Gordan series and coefficients for direct products of UIR's of G, in a form adapted to H. We will show that while the necessary and sufficient conditions mentioned above are met in certain cases of SU(2) and the Heisenberg–Weyl (HW) group, there are quite simple examples in the cases of SU(2) and SU(3) where they are not satisfied. This will attest to the necessity and significance of the conditions that we develop.

The contents of this paper are organized as follows. In Sec. II we set up the basic notations and definitions of generalized coherent states within a UIR of a general compact Lie group G, the two associated stability groups and coset spaces, and carry out the harmonic analysis at the vector level. The two distinct kinds of relationships between the stability groups are also carefully defined. Section III discusses the detailed properties of the projection operators onto the generalized coherent states, and performs the corresponding harmonic analysis. Using these and other results pertaining to the Clebsch–Gordan problem, we are able to obtain explicit necessary and sufficient conditions for existence of the diagonal representation in any given situation. In Sec. IV we consider applications to both SU(2) and SU(3), taking three examples in each case. The aim is to show how to check our conditions in practical cases, and to exhibit some simple situations where the diagonal representation exists, and other equally simple ones where it does not. Section V analyzes the Heisenberg–Weyl group in a heuristic way, to display how our conditions work and lead to expected results. Section VI contains concluding remarks. Appendixes A and B gather material on general Clebsch–Gordan series and coefficients, unit tensor operators, induced representation theory and the reciprocity theorem, for the convenience of the reader and to set up notations.

II. HARMONIC ANALYSIS ON COSET SPACES—THE VECTOR LEVEL

Let G be an n-dimensional compact Lie group. As described in Appendix A, we denote the various UIR's (upto equivalence) of G by a symbol J; within a UIR we denote a complete set of orthonormal basis labels (magnetic quantum numbers) by M. Both J and M stand in general for sets of several independent indices. Certain specific choices of the latter will be indicated later.

Let the Hilbert space $\mathcal{H}^{(J_0)}$ carry the N_{J_0}-dimensional UIR $\mathcal{D}^{(J_0)}(\cdot)$ of G. Choose and keep fixed some fiducial unit vector $\psi_0 \in \mathcal{H}^{(J_0)}$. The orbit of ψ_0 is the collection of vectors—generalized coherent states—$\psi(g) \in \mathcal{H}^{(J_0)}$ obtained by acting on ψ_0 with all $g \in G$:

$$\vartheta(\psi_0) = \{\psi(g) = \mathcal{D}^{(J_0)}(g)\psi_0 \mid g \in G\} \subset \mathcal{H}^{(J_0)}. \tag{2.1}$$

Similarly, if $\rho_0 = \psi_0 \psi_0^\dagger$ is the pure state density matrix corresponding to ψ_0, its orbit in the space of all density matrices is

$$\vartheta(\rho_0) = \{\rho(g) = \mathcal{D}^{(J_0)}(g)\rho_0 \;\; \mathcal{D}^{(J_0)}(g)^\dagger = \psi(g)\psi(g)^\dagger \mid g \in G\}. \tag{2.2}$$

Two important subgroups H_0, H in G are now defined

$$\begin{aligned} H_0 &= \{g \in G \mid \mathcal{D}^{(J_0)}(g)\psi_0 = \psi_0\} \subset G, \\ H &= \{g \in G \mid \mathcal{D}^{(J_0)}(g)\psi_0 = (\text{phase}) \;\; \psi_0\} \subset G. \end{aligned} \tag{2.3}$$

The dependences of H_0, H on ψ_0 are left implicit. The subgroup H_0 is the stability group of ψ_0 in the strict sense, while H is the stability group of ψ_0 upto phase factors. On the other hand, H is the stability group of ρ_0 in the strict sense:

$$H = \{g \in G \mid \rho(g) = \rho_0\} \subset G. \tag{2.4}$$

By standard arguments one has the identifications of the two orbits with corresponding coset spaces of G:

$$\vartheta(\psi_0) \simeq G/H_0 = \Sigma_0, \qquad \vartheta(\rho_0) \simeq G/H = \Sigma. \tag{2.5}$$

For definiteness we always take coset spaces to be made up of right cosets gH_0, gH in the two cases.

It is evident that H_0 is an invariant subgroup of H, and we can distinguish two qualitatively different situations depending on the nature of the quotient H/H_0:

$$\textbf{case A:} \quad H/H_0 = \text{trivial or discrete}, \qquad \textbf{case B:} \quad H/H_0 = \mathrm{U}(1). \tag{2.6}$$

These two possibilities can be pictured as follows: There is an obvious and natural projection map $\pi: \vartheta(\psi_0) \to \vartheta(\rho_0)$ or $\pi: \Sigma_0 \to \Sigma$. (Since H_0 is a subgroup of H, every H_0-coset lies within some H-coset.) With respect to this projection map, in case A for each $\rho \in \vartheta(\rho_0)$, there is just one or a discrete set of vectors $\psi \in \pi^{-1}(\rho) \subset \vartheta(\psi_0)$; while in case B $\pi^{-1}(\rho)$ consists of all vectors $\{e^{i\alpha}\psi\}$ for some fixed ψ and $0 \leqslant \alpha < 2\pi$. Stated in yet another manner: in case A with the help of action by elements in G the phase of ψ_0 [and so of any $\psi(g)$] can be altered in only a discrete set of ways or not at all; and in case B these phases can be altered in a continuous manner, so that each $\pi^{-1}(\rho)$ contains a "U(1)-worth of vectors."

We now wish to exploit the results of harmonic analysis arising from the natural UR's of G acting on square integrable functions on the two coset spaces Σ_0, Σ in order to extract the G representation contents of $\psi(g), \rho(g)$, respectively. The key point is that while both $\psi(g)$ and $\rho(g)$ have already known dependences on g, since they are obtained from ψ_0 and ρ_0, respectively, by actions via the given UIR $\mathcal{D}^{(J_0)}$ of G [and in particular $\psi(g)$ for different g may not be orthogonal, $\rho(g)$ for different g may not be trace orthogonal], they are linear quantities. Namely each of them belongs to a corresponding linear space. Therefore natural complete orthonormal sets of functions on Σ_0, Σ can be profitably used to project out the irreducible Fourier components of $\psi(g), \rho(g)$, respectively, with well defined irreducible behaviors under G, and then to resynthesize them. In the remainder of this section we look at the case of $\psi(g)$, i.e., we consider the situation at the vector level. In the following section we take up the case of $\rho(g)$ at the operator level.

We have seen that the two distinct possibilities for the quotient H/H_0 are given by Eq. (2.6). For simplicity in case A we limit ourselves to $H = H_0$, i.e., we will hereafter consider just two possibilities:

$$\textbf{case (a):} \quad H = H_0; \qquad \textbf{case (b):} \quad H/H_0 = \mathrm{U}(1). \tag{2.7}$$

In case (b) we have $H \simeq H_0 \times \mathrm{U}(1)$ apart possibly for some global identification rules. The intermediate case of H/H_0 discrete nontrivial can be handled by straightforward modifications of the analysis to follow. In case (a) the coset spaces Σ_0, Σ coincide; and the harmonic analysis to be now developed for functions on Σ to study $\psi(g)$ can later be used to study $\rho(g)$. In case (b), since H is larger than H_0 by exactly one U(1) angle, the coset space Σ_0 is also larger than Σ by (locally) one angle variable in the range $(0, 2\pi)$. Whereas for $\psi(g)$ we can use the results of harmonic analysis arising from appropriate UR's of G on Σ_0 or on Σ, for $\rho(g)$ we have to use the results on Σ alone. At this point, focusing on $\psi(g)$ we divide the discussion into cases (a) and (b).

A. Harmonic analysis in case (a): $H=H_0$

With respect to $H\subset G$ the significant information available about the properties of the generalized coherent state vectors $\psi(g)\in\vartheta(\psi_0)$ can be summarized as follows:

$$\begin{gathered} h\in H:\quad \mathcal{D}^{(J_0)}(h)\psi_0=\psi_0\,,\\ \psi(g)=\mathcal{D}^{(J_0)}(g)\psi_0\,,\\ \psi(gh)=\psi(g)\,,\\ \mathcal{D}^{(J_0)}(g')\psi(g)=\psi(g'g)\,. \end{gathered} \tag{2.8}$$

Let us denote a general point on Σ, a general H-coset, by $q=gH$. The identity coset $eH=H$ is the distinguished origin $q_0\in\Sigma$. A general $g'\in G$ maps q to $q'=g'q$. Also denote by $\ell(q)\in G$ a (local) choice of coset representatives $\Sigma\to G$:

$$q\in\Sigma\to\ell(q)\in G:\quad \ell(q)q_0=q\,. \tag{2.9}$$

(In general, considering that G is a principal fiber bundle over Σ as base and H as fiber and structure group, such coset representatives are definable only locally, and not in a globally smooth way; however these aspects involving domains of definition and overlap transition functions can be taken care of suitably.) Then the independent information contained in the vectors $\psi(g)$ can be reexpressed as follows:

$$\begin{gathered} \psi_0(q)=\psi(\ell(q))\,,\qquad \psi_0(q_0)=\psi_0\,,\\ \mathcal{D}^{(J_0)}(g)\psi_0(q)=\psi(g\quad \ell(q))=\psi(\ell(gq))=\psi_0(gq)\,. \end{gathered} \tag{2.10}$$

Based on these relationships we set up a UR of G on functions on Σ in this manner. The Hilbert space of the UR is

$$L^2(\Sigma,C)=\left\{ f(q)\in C \;\middle|\; \int_\Sigma d\mu(q)|f(q)|^2<\infty \right\}. \tag{2.11}$$

Here $d\mu(q)$ is the G-invariant integration volume element on $\Sigma, d\mu(gq)=d\mu(q)$; in the case of compact G and H we assume it is normalized to unit total volume for Σ. On these (scalar valued) functions $f(q)$ we define the action of G by unitary operators $\mathcal{U}(g)$:

$$(\mathcal{U}(g)f)(q)=f(g^{-1}q)\,. \tag{2.12}$$

It is now recognized that we have here the UR $\mathcal{D}^{(\mathrm{ind},0)}$ of G induced from the identity or trivial one-dimensional UIR of H, as described in Appendix B, Eq. (B4). (The superscript 0 is a reminder that the induction is from the trivial representation of H.) As explained there, by the well-known reciprocity theorem this UR $\mathcal{D}^{(\mathrm{ind},0)}$ of G contains a general UIR $\mathcal{D}^{(J)}$ of G as many times as the latter contains the trivial one-dimensional UIR of H. To make this quite explicit, at this point we choose the magnetic quantum number M within UIR's of G to consist of a triple $M=\mu\;\; j\;\; m$: here μ is a multiplicity label for UIR's of H, j is a label for UIR's of H, and m is a magnetic quantum number within the jth UIR of H. (As with J and M, here too j and m in general stand for sets of several quantum numbers each.) Then the general matrix element within the Jth UIR of G appears, adapted to H, as

$$\mathcal{D}^{(J)}_{MM'}(g)=\mathcal{D}^{(J)}_{\mu jm,\mu' j' m'}(g)\,. \tag{2.13}$$

With this information we have the result that a complete orthonormal basis for the Hilbert space $L^2(\Sigma,C)$ is given by

$$Y^{(J\lambda)}_{\mu jm}(q)=N_J^{1/2}\mathcal{D}^{(J)}_{\mu jm,\lambda 00}(\ell(q)),$$
$$Y^{(J\lambda)}_{\mu jm}(q_0)=N_J^{1/2}\delta_{\lambda\mu}\delta_{j0}\delta_{m0}. \tag{2.14}$$

(Here again $j=m=0$ corresponds to the identity UIR of H.) We can say that there are as many independent spherical harmonics on Σ of representation type J as $\mathcal{D}^{(J)}$ contains H-scalar states, and λ counts this multiplicity. The basic properties of these functions are

$$Y^{(J\lambda)}_{\mu jm}(gq)=\sum_{\mu' j' m'}\mathcal{D}^{(J)}_{\mu jm,\mu' j' m'}(g)Y^{(J\lambda)}_{\mu' j' m'}(q),$$
$$\int_\Sigma d\mu(q)Y^{(J'\lambda')}_{\mu' j' m'}(q)^*Y^{(J\lambda)}_{\mu jm}(q)=\delta_{J'J}\delta_{\lambda'\lambda}\delta_{\mu'\mu}\delta_{j'j}\delta_{m'm}, \tag{2.15}$$
$$\sum_{J\lambda\mu jm}Y^{(J\lambda)}_{\mu jm}(q)Y^{(J\lambda)}_{\mu jm}(q')^*=\delta(q',q)\,.$$

In the last completeness relation we have the Dirac delta function on Σ with respect to the volume element $d\mu(q)$.

Now we use the above tools to perform the harmonic analysis of $\psi_0(q)$. The results, as may be expected, will be simple, but the pattern for the later treatment of $\rho(g)$ will be set. Let us denote an orthonormal basis for $\mathcal{H}^{(J_0)}$, adapted to H, by $\Psi^{(J_0)}_{\mu jm}$,

$$\mathcal{D}^{(J_0)}(g)\Psi^{(J_0)}_{\mu jm}=\sum_{\mu' j' m'}\mathcal{D}^{(J_0)}_{\mu' j' m',\mu jm}(g)\Psi^{(J_0)}_{\mu' j' m'},$$
$$\Psi^{(J_0)\dagger}_{\mu' j' m'}\Psi^{(J_0)}_{\mu jm}=\delta_{\mu'\mu}\delta_{j'j}\delta_{m'm}. \tag{2.16}$$

Since ψ_0 is an H-invariant vector in $\mathcal{H}^{(J_0)}$, it follows that the UIR $\mathcal{D}^{(J_0)}$ of G contains at least one H-scalar state. Let us for simplicity choose ψ_0 to be the one corresponding to the multiplicity label μ having the value unity

$$\psi_0=\Psi^{(J_0)}_{100}\,. \tag{2.17}$$

Then the generalized coherent states $\psi(g)$, and hence $\psi_0(q)$, can be written out in explicit detail,

$$\psi(g)=\mathcal{D}^{(J_0)}(g)\psi_0=\sum_{\mu jm}\mathcal{D}^{(J_0)}_{\mu jm,100}(g)\Psi^{(J_0)}_{\mu jm},$$
$$\psi_0(q)=\psi(\ell(q))=N_{J_0}^{-1/2}\sum_{\mu jm}Y^{(J_0,1)}_{\mu jm}(q)\Psi^{(J_0)}_{\mu jm}. \tag{2.18}$$

We see that the Fourier coefficients of $\psi_0(q)$ are very simple:

$$\int_\Sigma d\mu(q)Y^{(J\lambda)}_{\mu jm}(q)^*\psi_0(q)=N_{J_0}^{-1/2}\delta_{JJ_0}\delta_{\lambda,1}\Psi^{(J_0)}_{\mu jm}. \tag{2.19}$$

This is as expected, and the expansion of $\psi_0(q)$ in the complete set $\{Y^{(J\lambda)}_{\mu jm}(q)\}$ gives back the second of Eq. (2.18).

B. Harmonic analysis in case (b): $H \simeq H_0 \times U(1)$

Now H_0 and H are distinct. The results expressed in Eqs. (2.18) and (2.19) remain valid and adequate as far as the harmonic analysis of $\psi(g)$ or $\psi_0(q)$ is concerned; we must just imagine H and Σ replaced throughout by H_0 and Σ_0 in the case (a) analysis. However since the larger subgroup H is now available, we outline the kind of induced UR of G we would have to set up on functions on the smaller coset space $\Sigma = G/H$, suitable for the harmonic analysis of $\psi(g)$ if one so wished.

With respect to $H \simeq H_0 \times U(1) \subset G$, in contrast to the previous Eq. (2.8), we can now say the following about the family of generalized coherent states:

$$\begin{gathered} h \in H: \qquad \mathcal{D}^{(0)}(h)\psi_0 = e^{i\varphi(h)}\psi_0, \\ \varphi(h^{-1}) = -\varphi(h), \\ \varphi(h) = 0 \quad \text{for} \quad h \in H_0, \\ \psi(gh) = e^{i\varphi(h)}\psi(g), \\ \mathcal{D}^{(J_0)}(g')\psi(g) = \psi(g'g). \end{gathered} \tag{2.20}$$

(The last statement here is the same as before.) Now let us denote a general H-coset, a point of Σ, by $r = gH$. (Since $H_0 \neq H$, the symbol q has been used up to label points of Σ_0.) The identity coset $eH = H$ is the distinguished origin $r_0 \in \Sigma$; and $g' \in G$ maps r to $r' = g'r$. In local coordinates, the point $q \in \Sigma_0$ (the larger coset space) is a pair, $q = (r, \alpha)$ where $r \in \Sigma$ and $\alpha \in [0, 2\pi)$ is the U(1) angle. Now let $\ell(r) \in G$ be a choice of (local) coset representatives $\Sigma \to G$:

$$r \in \Sigma \to \ell(r) \in G: \qquad \ell(r) r_0 = r\,. \tag{2.21}$$

Then the information (2.20) about the generalized coherent states $\psi(g)$ gets expressed in this way:

$$\begin{gathered} \tilde{\psi}_0(r) = \psi(\ell(r))\,, \qquad \tilde{\psi}_0(r_0) = \psi_0, \\ \mathcal{D}^{(J_0)}(g)\tilde{\psi}_0(r) = \mathcal{D}^{(J_0)}(g\ell(r))\psi_0 = \mathcal{D}^{(J_0)}(\ell(gr)\ell(gr)^{-1}g\ell(r))\psi_0 = e^{i\varphi(\ell(gr)^{-1}g\ell(r))}\tilde{\psi}_0(gr). \end{gathered} \tag{2.22}$$

The characteristic difference compared to Eq. (2.10), namely the presence of the nontrivial phase factor, is to be noted. This means that for analyzing $\psi(g)$ in this setting we must construct a UR of G on square integrable functions over Σ *involving a nontrivial multiplier*. The Hilbert space of this representation is [for simplicity we use the same symbol f as in Eq. (2.11)]:

$$L^2(\Sigma, C) = \left\{ f(r) \in C \;\middle|\; \int_\Sigma d\nu(r) |f(r)|^2 < \infty \right\}, \tag{2.23}$$

where $d\nu(r) = d\nu(gr)$ is the G-invariant normalized volume element on Σ. [Therefore locally $d\mu(q) = (1/2\pi)\, d\nu(r) d\alpha$.] On such $f(r)$ we set up a UR $\tilde{\mathcal{U}}(g)$ of G as follows:

$$(\tilde{\mathcal{U}}(g)f)(r) = e^{i\varphi(\ell(r)^{-1}g\ \ell(g^{-1}r))} f(g^{-1}r)\,. \tag{2.24}$$

This is recognized to be the UR of G induced from the nontrivial one-dimensional UIR $e^{i\varphi(h)}$ of H, in which H_0 is represented trivially. One can now proceed with the harmonic analysis of $\psi(g)$ in which the subgroup H plays the key role, by starting from an orthonormal basis for $\mathcal{H}^{(J_0)}$ adapted to H rather than merely to H_0. However as we have already performed the harmonic

analysis of $\psi(g)$ with respect to its strict stability subgroup H_0, we do not pursue case (b) for $\psi(g)$ any further; these additional details will become relevant in the next section, and will be spelt out there.

III. HARMONIC ANALYSIS FOR THE PROJECTIONS

When we turn to an analysis of the projection operators $\rho(g)=\psi(g)\psi(g)^\dagger$ we see that in both cases (a) and (b) the analysis must be based on the strict stability group H of ρ_0, and therefore with the appropriate induced UR of G on functions over Σ. (Thus uniformly the vector level analysis is better done using H_0, and the operator level analysis using H, whatever the relationship between H_0 and H may be.) The results of the harmonic analysis are now not as simple as for $\psi(g)$ in Eqs. (2.18) and (2.19). We now treat the details as far as possible parallel to the discussions in the preceding section, first for case (a) and then for case (b).

A. Projection operators in case (a)

The basic facts about the family of projection operators $\rho(g)$ are, in the pattern of Eqs. (2.8) and (2.20),

$$\begin{gathered} h\in H: \qquad \mathcal{D}^{(J_0)}(h)\rho_0\mathcal{D}^{(J_0)}(h)^\dagger=\rho_0, \\ \rho(g)=\mathcal{D}^{(J_0)}(g)\rho_0\mathcal{D}^{(J_0)}(g)^\dagger, \\ \rho(gh)=\rho(g), \\ \mathcal{D}^{(J_0)}(g')\rho(g)\mathcal{D}^{(J_0)}(g')^\dagger=\rho(g'g). \end{gathered} \tag{3.1}$$

Using the notations for the coset space $\Sigma=G/H$ already introduced in the preceding section under case (a), and the coset representatives $\ell(q)$ in Eq. (2.9), we can express the content of Eqs. (3.1) as follows:

$$\begin{gathered} \rho_0(q)=\rho(\ell(q)), \qquad \rho_0(q_0)=\rho_0, \\ \mathcal{D}^{(J_0)}(g)\rho_0(q)\mathcal{D}^{(J_0)}(g)^\dagger=\rho(g\ell(q))=\rho(\ell(gq))=\rho_0(gq). \end{gathered} \tag{3.2}$$

For the harmonic analysis of $\rho(g)$ or $\rho_0(q)$ we therefore set up on $L^2(\Sigma,C)$, by Eq. (2.12), the induced UR $\mathcal{D}^{(\mathrm{ind},0)}(g)=\mathcal{U}(g)$ of G just as was done for $\psi(g)$ in case (a). The UIR contents of this UR are as described in the preceding section. A complete orthonormal basis is provided by Eqs. (2.14) with the properties (2.15); so the UIR $\mathcal{D}^{(J)}$ of G is present as many times as it contains H-scalar states, and the index λ counts this multiplicity.

We can now project out the Fourier coefficients $\rho^{J\lambda}_{\mu jm}$ of $\rho(g)$ as operators acting on $\mathcal{H}^{(J_0)}$:

$$\rho^{J\lambda}_{\mu jm}=\int_\Sigma d\mu(q)Y^{(J\lambda)}_{\mu jm}(q)^*\rho_0(q). \tag{3.3}$$

On the one hand, combined use of Eqs. (2.15) and (3.2) and unitarity of $\mathcal{D}^{(J)}$ leads to the expected tensor operator behavior:

$$\mathcal{D}^{(J_0)}(g)\rho^{J\lambda}_{\mu jm}\mathcal{D}^{(J_0)}(g)^\dagger=\sum_{\mu' j' m'}\mathcal{D}^{(J)}_{\mu' j' m',\mu jm}(g)\rho^{J\lambda}_{\mu' j' m'}. \tag{3.4}$$

On the other hand, the completeness relation in Eq. (2.15) gives

$$\rho_0(q)=\sum_{J\lambda\mu jm}Y^{(J\lambda)}_{\mu jm}(q)\rho^{J\lambda}_{\mu jm}, \tag{3.5}$$

while of course $\rho(g)$ for general g is obtained by going to the H coset of g:

$$g=\ell(q)h, \quad q\in\Sigma, \quad h\in H: \quad \rho(g)=\rho_0(q). \tag{3.6}$$

However all this by no means implies that all the operators $\rho^{J\lambda}_{\mu jm}$ are nonvanishing. What is clear is that the UIR's J of G that appear as tensor operators in the harmonic analysis of $\rho(g)$ (and their corresponding multiplicities) must be some subset of the spectrum of UIR's of G that are known to be contained in the induced UR $\mathcal{D}^{(\mathrm{ind},0)}\equiv\mathcal{U}(\cdot)$, as dictated by the reciprocity theorem. Indeed one can see immediately that, when G and H are both compact and G/H is nontrivial, $\mathcal{H}^{(J_0)}$ is finite dimensional whereas $\mathcal{D}^{(\mathrm{ind},0)}$ is infinite dimensional; therefore only a finite subset of the $\rho^{J\lambda}_{\mu jm}$ can be nonzero.

To pin down further the tensor operators $\rho^{J\lambda}_{\mu jm}$ we relate them directly to the fiducial vector $\psi_0\in\mathcal{H}^{(J_0)}$ and to the generalized coherent states $\psi(g)$. We have introduced in Eq. (2.16) the orthonormal basis $\Psi^{(J_0)}_{\mu jm}$ for $\mathcal{H}^{(J_0)}$ adapted to H, and in Eq. (2.17) we have identified ψ_0 to be $\Psi^{(J_0)}_{100}$. This has given the explicit expressions (2.18) for $\psi(g)$ and $\psi_0(q)$. Combining these various results and also using Eq. (2.14) we see that the integrand on the right-hand side in Eq. (3.3) is

$$\begin{aligned} Y^{(J\lambda)}_{\mu jm}(q)^*\rho_0(q)=N_J^{1/2}\sum_{\substack{\mu' j' m'\\ \mu'' j'' m''}} & \Psi^{(J_0)}_{\mu' j' m'}\Psi^{(J_0)^\dagger}_{\mu'' j'' m''} \\ \times\ & \mathcal{D}^{(J_0)}_{\mu' j' m',100}(\ell(q))\,\mathcal{D}^{(J_0)}_{\mu'' j'' m'',100}(\ell(q))^*\,\mathcal{D}^{(J)}_{\mu jm,\lambda 00}(\ell(q))^*. \end{aligned} \tag{3.7}$$

For the product of the two $\mathcal{D}^*$ matrix elements we have the Clebsch–Gordan decomposition given in Eq. (A7) involving the Clebsch–Gordan coefficients of G adapted to H:

$$\begin{aligned} &\mathcal{D}^{(J_0)}_{\mu'' j'' m'',100}(\ell(q))^*\mathcal{D}^{(J)}_{\mu jm,\lambda 00}(\ell(q))^* \\ &\quad=\sum_{\substack{J'\Lambda\\ \nu kn\\ \nu' k' n'}} \mathcal{D}^{(J')}_{\nu' k' n',\nu kn}(\ell(q))^*\, C^{J_0}_{\mu'' j'' m''\ \ \mu jm\ \ \nu' k' n'}{}^*\ \ C^{J_0}_{100\ \ \lambda 00\ \ \nu kn} \\ &\quad=\sum_{\substack{J'\Lambda\nu\\ \nu' k' n'}} N_{J'}^{-1/2}\ C^{J_0}_{\mu'' j'' m''\ \ \mu jm\ \ \nu' k' n'}{}^*\ \ C^{J_0}_{100\ \ \lambda 00\ \ \nu 00}\ Y^{(J'\nu)}_{\nu' k' n'}(q)^*, \end{aligned} \tag{3.8}$$

since the second Clebsch–Gordan coefficient shows that in the sums over k and n only $k=n=0$ survives. Putting (3.8) into (3.3) and carrying out the integration we get the result

$$\rho^{J\lambda}_{\mu jm}=\frac{N_J^{1/2}}{N_{J_0}}\sum_{\Lambda}\ C^{J_0}_{100\ \ \lambda 00\ \ 100}\ \sum_{\substack{\mu' j' m'\\ \mu'' j'' m''}} C^{J_0}_{\mu'' j'' m''\ \ \mu jm\ \ \mu' j' m'}{}^*\,\Psi^{(J_0)}_{\mu' j' m'}\ \Psi^{(J_0)^\dagger}_{\mu'' j'' m''}. \tag{3.9}$$

The sum over the outer products of the elements of the basis for $\mathcal{H}^{(J_0)}$ reproduces exactly the Λth unit tensor of rank J on $\mathcal{H}^{(J_0)}$, as given in Eq. (A.12). Thus we have the final result

$$\rho^{J\lambda}_{\mu jm}=\frac{N_J^{1/2}}{N_{J_0}}\ \sum_{\Lambda}\ C^{J_0}_{100\ \ \lambda 00\ \ 100}\ U^{J\Lambda}_{\mu jm}\ . \tag{3.10}$$

We immediately see that a necessary condition for $\rho^{J\lambda}_{\mu jm}$ to be nonzero is that the UIR $\mathcal{D}^{(J)}$ must occur in the direct product $\mathcal{D}^{J_0}\times\mathcal{D}^{(J_0)^*}$, which is of course reasonable.

It is also evident that a certain rectangular matrix for each J, made up of specific Clebsch–Gordan coefficients, plays an important role here. We may write (3.10) as

$$\rho^{J\lambda}_{\mu jm}=\sum_{\Lambda} \quad \pi^{(J)}_{\lambda\Lambda} \quad U^{J\Lambda}_{\mu jm} \quad ,$$
$$\pi^{(J)}_{\lambda\Lambda}=\frac{N_J^{1/2}}{N_{J_0}} \quad C^{J_0 \quad J \quad J_0\Lambda}_{100 \quad \lambda 00 \quad 100} \quad . \tag{3.11}$$

The row index λ gives the multiplicity of occurrence of H-scalar states within the UIR $\mathcal{D}^{(J)}$ of G, while the column index Λ (which has no reference to H) gives the multiplicity of occurrence of $\mathcal{D}^{(J_0)}$ in the decomposition of the product $\mathcal{D}^{(J_0)}\times\mathcal{D}^{(J)}$. The necessary and sufficient conditions, in case (a), for being able to express every operator A on $\mathcal{H}^{(J_0)}$ as an integral over the projections $\rho(g)$ or $\rho_0(q)$, namely, as

$$A=\int_{\Sigma} d\mu(q) \quad a(q) \quad \rho_0(q)\,, \tag{3.12}$$

for some c-number function $a(q)$ depending linearly on A, are now clear. We know in advance that the set of unit tensor operators $U^{J\Lambda}_{\mu jm}$, with spectrum of $J\Lambda$ values completely and directly determined by $\mathcal{D}^{(J_0)}$ with no reference to the subgroup H, form a complete trace orthogonal set of operators on $\mathcal{H}^{(J_0)}$. Given the relations (3.11) for each J expressing the Fourier coefficients of $\rho_0(q)$ in terms of these unit tensors, we must be able to invert these relations and express each $U^{J\Lambda}_{\mu jm}$ as a Λ-dependent linear combination over λ of the $\rho^{J\lambda}_{\mu jm}$. Thus the necessary and sufficient conditions are as follows.

(i) Each UIR $\mathcal{D}^{(J)}$ of G contained in the product UR $\mathcal{D}^{(J_0)}\times\mathcal{D}^{(J_0)*}$ with some multiplicity must also occur in the UR $\mathcal{D}^{(\mathrm{ind},0)}$ of G induced from the identity UIR of H, with the same or higher multiplicity.

(ii) For each such $\mathcal{D}^{(J)}$, the rectangular matrix $\pi^{(J)}$ in (3.11) must have at least as many rows as it has columns, and it must be of maximal rank, namely equal to the number of columns.

B. Projection operators in case (b)

The main complication now is that ψ_0 and ρ_0 have different strict stability groups. We therefore have to unavoidably introduce extra quantum numbers in the state labels to take account of the structure $H\simeq \mathrm{U}(1)\times H_0$. Further in carrying out harmonic analyses over $\Sigma=G/H$, we must use two different sets of complete orthonormal spherical harmonics, one appropriate for $\psi(g)$ and another (simpler) one for $\rho(g)$. The increase in index structure in $\mathcal{D}$-functions, Y-functions, and Clebsch–Gordan coefficients are all inevitable.

A general element $h\in H$ is a pair $h=(e^{i\alpha},h_0)$ where $\alpha \in[0,2\pi)$ and $h_0\in H_0$ (subject possibly to some global identification rules). The label j for a general UIR of H is also a pair $j=(y,j_0)$ where $y\in\mathcal{Z}$ is the U(1) quantum number and j_0 labels a UIR of H_0 (again here y and j_0 may be constrained in some way). Within the UIR j_0 of H_0 we have as before an internal magnetic quantum number m. Therefore in a basis adapted to H the matrix elements in the UIR $\mathcal{D}^{(J)}$ of G look like

$$\mathcal{D}^{(J)}_{MM'}(g)=\mathcal{D}^{(J)}_{\mu y j_0 m,\mu' y' j_0' m'}(g)\,, \tag{3.13}$$

with the index μ counting the number of times the UIR $j\equiv(y,j_0)$ of H is present, etc. Correspondingly we have an orthonormal basis $\Psi^{(J_0)}_{\mu y j_0 m}$ for $\mathcal{H}^{(J_0)}$ with the transformation law

$$\mathcal{D}^{(J_0)}(g)\Psi^{(J_0)}_{\mu y j_0 m}=\sum_{\mu' y' j_0' m'} \quad \mathcal{D}^{(J_0)}_{\mu' y' j_0' m',\mu y j_0 m}(g) \quad \Psi^{(J_0)}_{\mu' y' j_0' m'}\,. \tag{3.14}$$

With no loss of generality we can assume that the fiducial vector ψ_0, invariant under H_0 but changing under the U(1) part of H, carries the U(1) quantum number $y=1$, and is the first such state in the case of multiplicity,

$$\psi_0 = \Psi^{(J_0)}_{1100}. \tag{3.15}$$

This replaces Eq. (2.17). For the generalized coherent state we have from Eq. (3.14) and (3.15), as replacement for Eq. (2.18):

$$\psi(g) = \mathcal{D}^{(J_0)}(g)\Psi^{(J_0)}_{1100} = \sum_{\mu y j_0 m} \mathcal{D}^{(J_0)}_{\mu y j_0 m,1100}(g) \quad \Psi^{(J_0)}_{\mu y j_0 m}. \tag{3.16}$$

For points of the coset space Σ and coset representatives we use the notations $r, \ell(r)$ already introduced in Sec. II under case (b). Now as was mentioned earlier, on Σ we have to employ two different complete orthonormal sets of functions, one to handle $\psi_0(r)$ and the other to handle $\rho_0(r)$. This is because two different induced UR's of G are involved—in the ψ case it is the UR $\mathcal{D}^{(\mathrm{ind},10)}$ induced from the nontrivial one-dimensional UIR $j=(1,0)$ of H as described in Eq. (2.24); in the ρ case it is the UR $\mathcal{D}^{(\mathrm{ind},00)}$ induced from the trivial one-dimensional UIR $j=(00)$ of H, analogous to Eq. (2.12). The two systems of complete orthonormal spherical harmonics on Σ are

$$\mathcal{D}^{(\mathrm{ind},10)}: \qquad \tilde{Y}^{(J,\lambda)}_{\mu y j_0 m}(r) = N_J^{1/2} \quad \mathcal{D}^{(J)}_{\mu y j_0 m,\lambda 100}(\ell(r)) \quad , \tag{3.17a}$$

$$\mathcal{D}^{(\mathrm{ind},00)}: \qquad Y^{(J,\lambda)}_{\mu y j_0 m}(r) = N_J^{1/2} \quad \mathcal{D}^{(J)}_{\mu y j_0 m,\lambda 000}(\ell(r)) \quad . \tag{3.17b}$$

We must appreciate that the spectrum of (J,λ) values present in the two cases may be different, even though each set by itself is orthonormal and complete over Σ with respect to the measure $d\ \nu(r)$. The transformation properties under G action, orthonormality and completeness relations in each case are analogous to Eq. (2.15) and need not be repeated.

Equations (3.1) continue to hold, while we replace Eq. (3.2) and the second of Eq. (2.18) by

$$\begin{gathered} \rho_0(r) = \rho(\ell(r)) = \tilde{\psi}_0(r)\tilde{\psi}_0(r)^\dagger, \\ \rho_0(r_0) = \rho_0\,, \\ \mathcal{D}^{(J_0)}(g)\rho_0(r)\mathcal{D}^{(J_0)}(g)^\dagger = \rho_0(gr)\,, \end{gathered} \tag{3.18}$$

$$\tilde{\psi}_0(r) = \psi(\ell(r)) = \sum_{\mu y j_0 m} \quad \mathcal{D}^{(J_0)}_{\mu y j_0 m,1100}(\ell(r)) \quad \Psi^{(J_0)}_{\mu y j_0 m} = N_{J_0}^{-1/2} \sum_{\mu y j_0 m} \quad \tilde{Y}^{(J_0,1)}_{\mu y j_0 m}(r)\Psi^{(J_0)}_{\mu y j_0 m}.$$

The pattern of calculations from here onwards is similar to case (a). We define the Fourier coefficients of the projection operators $\rho_0(r)$ with respect to the basis (3.17b) as

$$\begin{gathered} \rho^{J\lambda}_{\mu y j_0 m} = \int_\Sigma d\,\nu(r) \quad Y^{(J,\lambda)}_{\mu y j_0 m}(r)^* \quad \rho_0(r)\,, \\ \rho_0(r) = \sum_{J\lambda \mu y j_0 m} \quad Y^{(J,\lambda)}_{\mu y j_0 m}(r) \quad \rho^{J\lambda}_{\mu y j_0 m}\,, \end{gathered} \tag{3.19}$$

$$\mathcal{D}^{(J_0)}(g) \quad \rho^{J\lambda}_{\mu y j_0 m} \quad \mathcal{D}^{(J_0)}(g)^\dagger = \sum_{\mu' y' j_0' m'} \quad \mathcal{D}^{(J)}_{\mu' y' j_0' m',\mu y j_0 m}(g) \quad \rho^{J\lambda}_{\mu' y' j_0' m'}.$$

We then use Eq. (3.18) to directly relate $\rho^{J\lambda}_{\mu y j_0 m}$ to outer products of the basis vectors of $\mathcal{H}^{(J_0)}$, and then to the complete set of unit tensors on $\mathcal{H}^{(J_0)}$. Skipping the intermediate steps, the final result replacing Eq. (3.11) in case (a) is

$$\rho^{J\lambda}_{\mu y j_0 m} = \sum_{\Lambda} \quad \pi^{(J)}_{\lambda\Lambda} \quad U^{J\Lambda}_{\mu y j_0 m},$$

$$\pi^{(J)}_{\lambda\Lambda} = \frac{N_J^{1/2}}{N_{J_0}} \; C^{J_0 \quad J \quad J_0\Lambda}_{1100 \quad \lambda 000 \quad 1100}, \tag{3.20}$$

$$U^{J\Lambda}_{\mu y j_0 m} = \sum_{\substack{\mu' y' j_0' m' \\ \mu'' y'' j_0'' m''}} \quad C^{J_0 \quad J \quad J_0\Lambda}_{\mu'' y'' j_0'' m'' \quad \mu y j_0 m \quad \mu' y' j_0' m'} \; {}^{*} \quad \Psi^{(J_0)}_{\mu' y' j_0' m'} \quad \Psi^{(J_0)^{\dagger}}_{\mu'' y'' j_0'' m''}.$$

[For simplicity we have used the same symbols π, U here as in case (a)]. The necessary and sufficient conditions to be able to express any operator A on $\mathcal{H}^{(J_0)}$ as an integral over the projections $\rho(g) = \psi(g)\psi(g)^{\dagger}$ are now seen to read the same as in case (a), except that the family of rectangular matrices $\pi^{(J)}$ is specified in a different manner, and in condition (i) we have to read $\mathcal{D}^{(\mathrm{ind},00)}$ in place of $\mathcal{D}^{(\mathrm{ind},0)}$. For complete clarity, we state the two conditions explicitly: (i) Each UIR $\mathcal{D}^{(J)}$ of G contained in the product UR $\mathcal{D}^{(J_0)} \times \mathcal{D}^{(J_0)*}$ of G with some multiplicity must also occur in the UR $\mathcal{D}^{(\mathrm{ind},00)}$ of G induced from the identity UIR of $H \simeq U(1) \times H_0$, with the same or higher multiplicity. (ii) For each such $\mathcal{D}^{(J)}$, the rectangular matrix $\pi^{(J)}$ in (3.20) must have at least as many rows as it has columns, and it must be of maximal rank, namely equal to the number of columns.

In concluding this section we point out that we have made convenient choices of the vector ψ_0 in terms of a basis in $\mathcal{H}^{(J_0)}$, and this must be kept in mind since expressions for standard Clebsch–Gordan coefficients where available may differ from the ones needed in (3.11) and (3.20).

IV. APPLICATIONS TO SU(2) AND SU(3)

As examples of the criteria developed in the last section for the existence of the diagonal coherent state representation for operators (in short, diagonal representation), we consider here some illustrative instances involving the simplest compact groups SU(2) and SU(3). Since the representation theory of these groups, their Clebsch–Gordan series and [at least for SU(2)] the Clebsch–Gordan coefficients are all well known, we describe very briefly the main features of each case considered. One point worth repeating is that the Clebsch–Gordan coefficients which appear in the criteria for existence of the diagonal representation through the matrices $\pi^{(J)}$ are generally noncanonical. We must bear in mind the use of bases for UIR's of G adapted to the subgroup H determined by ψ_0, and the identifications of ψ_0 in Eqs. (3.15) and (2.17). We look at three SU(2) cases and three SU(3) cases to illustrate the ideas.

A. SU(2) Examples

With $G = \mathrm{SU}(2)$, the Clebsch–Gordan series multiplicity label Λ is absent, so we can set $\Lambda = 1$ everywhere. The UIR label J has values 0,1/2,1,… with $\mathcal{H}^{(J)}$ being of dimension $N_J = (2J+1)$. We denote the generators by T_1, T_2, T_3. In discussing stability subgroups we pay attention only to the components continuously connected to the identity.

Example 1: Assume $J_0 \geqslant 1$, and take ψ_0 to be a generic vector in $\mathcal{H}^{(J_0)}$, not an eigenvector of $\hat{n} \cdot T$ for any $\hat{n} \in S^2$. Independently of ψ_0, the spectrum of unit tensor operators on $\mathcal{H}^{(J_0)}$ is $J = 0,1,2,\ldots,2J_0$, once each. The stability groups are $H_0 = H = \{e\}$, so we have case (a). The orbits $\vartheta(\psi_0), \vartheta(\rho_0)$ and the two coset spaces Σ_0, Σ all coincide with SU(2) [or may be S0(3)] and are all three dimensional. Since H is trivial, it has only the trivial one-dimensional UIR, so the induced representation $\mathcal{D}^{(\mathrm{ind},0)}$ of SU(2) is the regular representation $\mathcal{D}^{(\mathrm{reg})}$. The spectrum and

multiplicity of UIR's present here is $J=0,1/2,1,\ldots,\infty$, $\mathcal{D}^{(J)}$ occurring $(2J+1)$ times. Therefore condition (i) for case (a) is obeyed. Turning to condition (ii), any basis $\Psi_{\mu}^{(J)}, \mu=1,2,\ldots,2J+1$, in $\mathcal{H}^{(J)}$ is an H-adapted basis and μ is a multiplicity label. We take $\psi_0=\Psi_1^{(J_0)}$ in $\mathcal{H}^{(J)}$, assuming for definiteness that in each $\mathcal{H}^{(J)}$ we have a noncanonical basis (not eigenvectors of T_3). The matrices $\pi_{\lambda\Lambda}^{(J)}$ of Eq. (3.11) are column vectors with $(2J+1)$ rows:

$$\pi_{\lambda 1}^{(J)}=\frac{\sqrt{2J+1}}{2J_0+1}\ C_{1\ \lambda\ 1}^{J_0\ J\ J_0}, \qquad \lambda=1,2,\ldots,2J+1. \tag{4.1}$$

(We emphasize these are not the usual Clebsch–Gordan coefficients.) For each $J=0,1,\ldots,2J_0$ in the generic case we can expect this to be nonzero at least for one value of λ, as no particular symmetries or selection rules are operative. So condition (ii) also holds, and the diagonal representation exists.

Example 2: Assume J_0 is an integer $\geqslant 1$, and take ψ_0 to be the eigenvector of T_3 with eigenvalue $M_0=0$, i.e., in the canonical basis, $\psi_0=\Psi_0^{(J_0)}$. Again the spectrum of unit tensor operators on $\mathcal{H}^{(J_0)}$ is $J=0,1,2,\ldots,2J_0$, once each. The stability groups are $H_0=H=\mathrm{U}(1)$ generated by T_3, so we have case (a) again. Now we use the canonical basis $\Psi_M^{(J)}$ in every $\mathcal{H}^{(J)}$, as it is adapted to H; the multiplicity labels λ, μ are not needed, and can all be set equal to unity. The orbits $\vartheta(\psi_0), \vartheta(\rho_0)$ and the coset spaces Σ_0, Σ all coincide with $\mathrm{SU}(2)/\mathrm{U}(1)=S^2$, and are all two dimensional. The induced UR $\mathcal{D}^{(\mathrm{ind},0)}$ of SU(2) is the helicity zero UR acting on functions on S^2, and this contains the UIR's $J=0,1,2,\ldots,\infty$, once each; thus condition (i) is obeyed. Turning to condition (ii), for each $J=0,1,\ldots,2J_0$ we have a single number $\pi_{11}^{(J)}$ to examine, and it is the canonical Clebsch–Gordan coefficient

$$\pi_{11}^{(J)}=\frac{\sqrt{2J+1}}{2J_0+1}\ C_{0\ 0\ 0}^{J_0\ J\ J_0}. \tag{4.2}$$

But it is known that this vanishes for $J=1,3,\ldots,2J_0-1$, hence condition (ii) is not obeyed, and the diagonal representation does not exist. This interesting situation was indeed noted by Klauder and Skagerstam a long time ago,[15] for the case $J_0=1$.

Example 3: Take any $J_0\geqslant 1/2$, and ψ_0 to be an eigenvector of T_3 in $\mathcal{H}^{(J_0)}$ with eigenvalue $M_0\neq 0$. Thus in the canonical basis we have $\psi_0=\Psi_{M_0}^{(J_0)}$, $|M_0|>0$. The spectrum of unit tensors on $\mathcal{H}^{(J_0)}$ is $J=0,1,\ldots,2J_0$; while the stability subgroups are $H_0=\{e\}, H=\mathrm{U}(1)$ generated by T_3, leading to case (b). In each $\mathcal{H}^{(J)}$ we can use the canonical basis, and the labels λ, μ, are not needed. The orbit $\vartheta(\psi_0)$ and the coset space Σ_0 are three dimensional, while $\vartheta(\rho_0)$ and Σ are S^2 as in example 2. The induced UR of SU(2) to be used for $\rho(g), \mathcal{D}^{(\mathrm{ind},00)}$ is again the helicity zero UR on functions on S^2, with the UIR spectrum $J=0,1,2,\ldots,\infty$, once each. So condition (i) of case (b) is obeyed. For $J=0,1,\ldots,2J_0$ we have to now examine the canonical Clebsch-Gordan coefficient [see Eq. (3.20)],

$$\pi_{11}^{(J)}=\frac{\sqrt{2J+1}}{2J_0+1}\ C_{M_0\ 0\ M_0}^{J_0\ J\ J_0}, \tag{4.3}$$

and as this is nonzero if $M_0\neq 0$, condition (ii) is obeyed and the diagonal representation exists.

In these three SU(2) examples, condition (i) was always obeyed; while in example 2 alone condition (ii) was violated. Now we look at three SU(3) examples, in one of which even condition (i) fails.

B. SU(3) Examples

With $G=\mathrm{SU}(3)$, the Clebsch–Gordan series multiplicity label Λ is generally necessary. The UIR's are labeled by a pair of independent integers, $J=(p,q)$, with $\mathcal{H}^{(p,q)}$, having dimension $N_{(p,q)}=\frac{1}{2}(p+1)(q+1)(p+q+2)$. We will throughout use the canonical basis within each

$\mathcal{H}^{(p,q)}$, labeled by the quantum numbers I, I_3, Y of the isospin SU(2) and hypercharge U(1) subgroups of SU(3). We will be using two subgroups, namely $\mathrm{U}(1)\times\mathrm{U}(1)$ and U(2). The corresponding induced UIR's of SU(3), arising from the trivial UIR's of these subgroups, have the following contents as deduced from the reciprocity theorem:

$$\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{U}(1)\times\mathrm{U}(1)} = \sum_{\substack{p,q=0 \\ p=q \bmod 3}}^{\infty} \oplus \; n_{p,q} \; \mathcal{D}^{(p,q)},$$

$$n_{p,q} = (p+1, q+1)_{<}; \tag{4.4a}$$

$$\mathcal{D}^{(\mathrm{ind},0)}_{U(2)} = \sum_{p=0}^{\infty} \oplus \; \mathcal{D}^{(p,p)}. \tag{4.4b}$$

We take $J_0 = (1,1)$ corresponding to the eight-dimensional octet or adjoint representation for the first two examples. The spectrum of unit tensor operators on $\mathcal{H}^{(1,1)}$ is known to be

$$(p,q) = (0,0), \quad (1,1), \quad (1,1), \quad (3,0), \quad (0,3), \quad (2,2). \tag{4.5}$$

We look at two choices of ψ_0.

Example 4: Take $\psi_0 = \Psi^{(1,1)}_{100}$. Then $H_0 = H = \mathrm{U}(1)\times\mathrm{U}(1)$ and we have case (a). In the canonical basis $\Psi^{(p,q)}_{I\ I_3 Y}$ for UIR's of SU(3), I_3 and Y determine a (one-dimensional) UIR of H, so I is the multiplicity label λ, μ,... of the general formalism. From Eq. (4.4a) we see that $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{U}(1)\times\mathrm{U}(1)}$ contains (0,0) once, (1,1) twice, (3,0) and (0,3) once each, and (2,2) three times. Condition (i) is then obeyed. Turning to condition (ii), for each of the (p,q) pairs listed in Eq. (4.5) we must examine the matrix $\pi^{(J)}_{\lambda\Lambda} = \pi^{(p,q)}_{I\Lambda}$. These involve quite simple Clebsch–Gordan coefficients of SU(3), which in turn are Clebsch–Gordan coefficients of SU(2) times so-called isoscalar factors. We have the following results:

$$(p,q) = (0,0): \qquad \pi^{(0,0)}_{0,1} = 1/8, \tag{4.6a}$$

$$(p,q) = (1,1): \qquad \pi^{(1,1)} = \frac{1}{\sqrt{8}} \begin{pmatrix} C^{8}_{100\ 000\ 100} & C^{8}_{100\ 000\ 100}{}^{8,1} & C^{8}_{100\ 000\ 100}{}^{8,2} \\ C^{8}_{100\ 100\ 100} & C^{8}_{100\ 100\ 100}{}^{8,1} & C^{8}_{100\ 100\ 100}{}^{8,2} \end{pmatrix} = \frac{1}{\sqrt{8}} \begin{pmatrix} 1/\sqrt{5} & 0 \\ 0 & 0 \end{pmatrix}, \tag{4.6b}$$

$$(p,q) = (3,0) \ \text{ or } \ (0,3): \qquad \pi^{(3,0) \text{ or } (0,3)}_{1,1} = \frac{\sqrt{10}}{8} \; C^{8}_{100\ 100}{}^{10 \text{ or } 10^*}_{100} = \frac{\sqrt{10}}{8} \frac{\sqrt{30}}{15} \; C^{1\ 1\ 1}_{0\ 0\ 0} = 0, \tag{4.6c}$$

$$(p,q) = (2,2): \qquad \pi^{(2,2)} = (\pi^{(2,2)}_{I,1}) = \frac{\sqrt{27}}{8} \begin{pmatrix} C^{8}_{100\ 000\ 100}{}^{27\ 8} \\ C^{8}_{100\ 100\ 100}{}^{27\ 8} \\ C^{8}_{100\ 200\ 100}{}^{27\ 8} \end{pmatrix} = \frac{\sqrt{27}}{8} \begin{pmatrix} -\sqrt{5}/45 \\ 0 \\ \dfrac{2\sqrt{10}}{9} \quad C^{1\ 2\ 1}_{0\ 0\ 0} \end{pmatrix}. \tag{4.6d}$$

We see that condition (ii) fails for $(p,q) = (1,1),(3,0),(0,3)$, so the diagonal representation does not exist. It is noteworthy that in some cases we have the vanishing of the iso-scalar factor, and in other cases of the multiplying SU(2) coefficient.

Example 5: Take $\psi_0 = \Psi^{(1,1)}_{000}$. Again, as $H_0 = H = U(2)$, we have case (a). But now when we examine the contents of $\mathcal{D}^{(\mathrm{ind},0)}_{U(2)}$ in Eq. (4.4b), we see that the UIR(1,1) occurs just once, while (3,0) and (0,3) are both absent. This means that even condition (i) is not satisfied, and so the diagonal representation does not exist.

Example 6: For the final SU(3) example, we choose the UIR $J_0=(3,0)$ with $N_{J_0}=10$. The fiducial state ψ_0 is taken to be the SU(2) scalar state with canonical quantum numbers $I\ I_3\ Y = 0,0,-2$:

$$\psi_0=\Psi^{(3,0)}_{00-2}. \tag{4.7}$$

[This is equivalent via an SU(3) transformation to choosing the highest weight state $\Psi^{(3,0)}_{3/2\ 3/2\ 1}$.] The corresponding stability groups are

$$H_0 \ = \ \mathrm{SU}(2)\,, \quad H \ = \ \mathrm{U}(2), \tag{4.8}$$

so this is an instance of case (b). The spectrum of unit tensors on $\mathcal{H}^{(3,0)}$ is determined by the Clebsch–Gordan series for the product $(3,0)\times(0,3)$:

$$(p,p)=(0,0),\ \ (1,1),\ \ (2,2),\ \ (3,3), \tag{4.9}$$

of dimensions 1, 8, 27, and 64, respectively. Combining this with Eq. (4.4b) we see that in this example both kinds of multiplicity labels μ, $\lambda,\ldots$ and Λ are not needed, so all the relevant matrices $(\pi^{(J)}_{\lambda\Lambda})$ reduce to single numbers. Comparing Eq. (4.9) with Eq. (4.4b) we see that condition (i) for existence of the diagonal representation is satisfied. Furthermore, since $I=I_3=0$ for the fiducial vector ψ_0 in Eq. (4.7), the relevant Clebsch–Gordan coefficients reduce to just the isoscalar factors. The necessary coefficients are tabulated in closed form in Ref. 18 and we read off the values needed,

$$\begin{aligned}
\pi^{(3,3)}&=\frac{8}{10}\ \ C^{10\ \ 64\ \ 10}_{00-2\ \ 000\ \ 00-2}=\frac{\sqrt{2}}{5\sqrt{7}},\\
\pi^{(2,2)}&=\frac{3\sqrt{3}}{10}\ \ C^{10\ \ 27\ \ 10}_{00-2\ \ 000\ \ 00-2}=\frac{3\sqrt{3}}{10\sqrt{7}},\\
\pi^{(1,1)}&=\frac{2\sqrt{2}}{10}\ \ C^{10\ \ 8\ \ 10}_{00-2\ \ 000\ \ 00-2}=\frac{1}{5},\\
\pi^{(0,0)}&=\frac{1}{10}\ \ C^{10\ \ 1\ \ 10}_{00-2\ \ 000\ \ 00-2}=\frac{1}{10}.
\end{aligned} \tag{4.10}$$

[For simplicity, as in Eq. (4.6), we have again indicated the relevant SU(3) UIR's by their dimensionalities, the 10 referring to (3,0)]. As these are all nonzero, condition (ii) is also satisfied, so we conclude that in this example the diagonal representation exists.

V. THE HEISENBERG–WEYL GROUP

The last application of our formalism is to the noncompact Heisenberg–Weyl (HW) group, denoted in this section by G. This will be somewhat heuristic as we shall often use Hilbert space vectors subject to delta-function normalization, induced representations whose reduction into UIR's involves continuous integrals, etc. The main aim is to show the relevance of the necessary and sufficient conditions of Sec. III for existence of the diagonal representation in this situation which underlies the very important case of ordinary coherent states. While the structure of G (recalled below) is quite simple, its UIR's and the various Clebsch–Gordan series have quite delicate properties. We give a brief account of all these aspects.

Topologically G has the structure of $\mathcal{R}^3$. Its Lie algebra $\underline{G}$ is spanned by three elements $t_j, j=1,2,3$, with the Lie bracket relations

$$[t_1,t_2]=t_3\,, \qquad [t_1 \ \text{ or } \ t_2,t_3]=0\,. \tag{5.1}$$

Finite group elements and the composition law and inverses are

$$\underline{\alpha},\underline{\beta}\in\mathcal{R}^3: \qquad g(\underline{\alpha})=\exp(\alpha_2 t_1-\alpha_1 t_2+\alpha_3 t_3)\,,$$

$$g(\underline{\alpha})^{-1}=g(-\underline{\alpha})\,, \tag{5.2}$$

$$g(\underline{\alpha})g(\underline{\beta})=g(\alpha_1+\beta_1,\alpha_2+\beta_2,\alpha_3+\beta_3+\tfrac{1}{2}(\alpha_1\beta_2-\alpha_2\beta_1))\,.$$

In a UR or UIR we will write $-iT_j, T_j$ Hermitian, for t_j, so the generator commutation relations and unitary operators for finite group elements are

$$[T_1,T_2]=i\,T_3\,, \quad [T_1 \text{ or } T_2,\ T_3]=0\,, \tag{5.3a}$$

$$g(\underline{\alpha})\to\mathcal{D}(\underline{\alpha})=\exp(i(\alpha_1 T_2-\alpha_2 T_1-\alpha_3 T_3))\,. \tag{5.3b}$$

The adjoint action on the generators is

$$\mathcal{D}(\underline{\alpha})\,(T_1,T_2,T_3)\,\mathcal{D}(\underline{\alpha})^{-1}=(T_1+\alpha_1 T_3,T_2+\alpha_2 T_3,T_3)\,. \tag{5.4}$$

The UIR's of G are of two types, depending on whether T_3 (which in any case is a scalar in a UIR) is zero or nonzero. If $T_3=0$, the UIR is one dimensional and is determined by choices of numerical values for T_1, T_2:

$$\mathcal{D}^{(q_0,p_0)}, \quad (q_0,p_0)\in\mathcal{R}^2: \qquad T_1^{(q_0,p_0)}=q_0\,, \quad T_2^{(q_0,p_0)}=p_0\,, \quad T_3^{(q_0,p_0)}=0\,. \tag{5.5}$$

On the other hand, for $T_3=c\neq 0$, by the Stone–von Neumann theorem we have an infinite-dimensional UIR on $L^2(\mathcal{R})$, acting on Schrödinger wave functions $\psi(q)$ of a real variable $q\in\mathcal{R}$ as follows:

$$\mathcal{D}^{(c)}, \quad c\neq 0: \quad \mathcal{H}^{(c)}=L^2(\mathcal{R})\,,$$

$$T_1^{(c)}=\hat{q}=q\,, \quad T_2^{(c)}=\hat{p}=-i\ c\frac{\partial}{\partial q}, \quad T_3^{(c)}=c\,. \tag{5.6}$$

Thus there is an $\mathcal{R}^2$-worth collection of inequivalent one-dimensional UIR's $\mathcal{D}^{(q_0,p_0)}$, $\dim\mathcal{H}^{(q_0,p_0)}=1$; and an $\mathcal{R}$-$\{0\}$-worth collection of inequivalent infinite-dimensional UIR's $\mathcal{D}^{(c)}$, $\dim\mathcal{H}^{(c)}=\infty$. Every UIR is nonfaithful.

In the sequel, whenever there is no danger of confusion, we omit the UIR labels (q_0,p_0) or c on the generators T_j.

Turning to the Clebsch–Gordan problem, this is easily analyzed by examining the sums of the individual generators of any two UIR's. There are three cases to consider. The following two results are obvious:

$$\mathcal{D}^{(q_0,p_0)}\times\mathcal{D}^{(q_0',p_0')}=\mathcal{D}^{(q_0+q_0',p_0+p_0')}, \tag{5.7a}$$

$$\mathcal{D}^{(q_0,p_0)}\times\mathcal{D}^{(c)}=\mathcal{D}^{(c)}. \tag{5.7b}$$

[In the latter case we may in fact appeal to Eq. (5.4)]. In the case of $\mathcal{D}^{(c)}\times\mathcal{D}^{(c')}$ we must distinguish between $c+c'=0$ and $c+c'\neq 0$. In either case the generators of the product, acting on $L^2(\mathcal{R}^2)$, are

$$T_1=q+q'\,, \quad T_2=-i\ c\frac{\partial}{\partial q}-i\ c'\frac{\partial}{\partial q'}, \quad T_3=c+c'\,. \tag{5.8}$$

For $c+c'\neq 0$ we switch to the independent variables $Q=q+q'$, $Q'=cq'-c'q$, so

$$T_1 = Q\,, \quad T_2 = -i(c+c')\frac{\partial}{\partial Q}\,, \quad T_3 = c+c'\,. \tag{5.9}$$

We see that Q' is totally absent and commutes with all the T_j. In case $c+c'=0$ we have

$$T_1 = q+q'\,, \quad T_2 = -i\,c\left(\frac{\partial}{\partial q}-\frac{\partial}{\partial q'}\right), \quad T_3 = 0\,, \tag{5.10}$$

(reminiscent of the EPR situation), and T_1 and T_2 form a complete commuting set. From all these results we see that

$$\mathcal{D}^{(c)}\times\mathcal{D}^{(-c)} = \iint_{\mathcal{R}^2}^{\oplus} dq_0\, dp_0\, \mathcal{D}^{(q_0,p_0)}, \tag{5.11a}$$

$$\mathcal{D}^{(c)}\times\mathcal{D}^{(c')} = \int_{\mathcal{R}}^{\oplus} dQ'\cdot\mathcal{D}^{(c+c')}\,, \quad c+c'\neq 0. \tag{5.11b}$$

In (5.11a) each one-dimensional UIR $\mathcal{D}^{(q_0,p_0)}$ appears once in a continuous fashion; while in (5.11b) the single infinite-dimensional UIR $\mathcal{D}^{(c+c')}$ appears infinitely often in a continuous sense, with Q' being a continuous multiplicity label. The full set of results for the Clebsch–Gordan problem is thus contained in Eqs. (5.7) and (5.11).

Now let us work within a particular UIR $\mathcal{D}^{(c)}$ acting on $\mathcal{H}^{(c)}$. From the results of the Clebsch–Gordan problem we see that the spectrum of irreducible unit tensors definable on $\mathcal{H}^{(c)}$ consists only of tensors belonging to the one-dimensional UIR's $\mathcal{D}^{(q_0,p_0)}$, once each in a continuous sense for every $(q_0,p_0)\in\mathcal{R}^2$. This is because $\mathcal{D}^{(c)}\times\mathcal{D}^{(c')}$ never contains $\mathcal{D}^{(c)}$, and $\mathcal{D}^{(c)}\times\mathcal{D}^{(q_0,p_0)}$ is exactly $\mathcal{D}^{(c)}$. These unit tensors are the familiar HW displacement operators which are a subset of the unitary $\mathcal{D}^{(c)}(\underline{\alpha})$ themselves. The displacement operators are

$$D^{(c)}(\alpha_\perp) = \mathcal{D}^{(c)}(\alpha_\perp,0) = \exp(i\ \ \alpha_1\hat{p} - i\ \ \alpha_2\hat{q}), \tag{5.12}$$

and for them the (finite form of the) adjoint action is

$$\mathcal{D}^{(c)}(\underline{\beta})D^{(c)}(\alpha_\perp)\mathcal{D}^{(c)}(\underline{\beta})^{-1} = e^{ic(\alpha_1\beta_2-\alpha_2\beta_1)}D^{(c)}(\underline{\alpha}_\perp)\,. \tag{5.13}$$

Therefore for each $(q_0,p_0)\in\mathcal{R}^2$ we define the (unitary) unit tensor operator

$$U^{(q_0,p_0)} = D^{(c)}\left(\frac{q_0}{c},\frac{p_0}{c}\right). \tag{5.14}$$

(For simplicity we avoid the label c on these operators.) Then from (5.13) we see that they have the correct transformation property, i.e., they belong to the one-dimensional UIR's $\mathcal{D}^{(q_0,p_0)}$:

$$\mathcal{D}^{(c)}(\underline{\alpha})U^{(q_0,p_0)}\mathcal{D}^{(c)}(\underline{\alpha})^{-1} = e^{i(\alpha_1p_0-\alpha_2q_0)}\ \ U^{(q_0,p_0)} = \mathcal{D}^{(q_0,p_0)}(\underline{\alpha})\ \ U^{(q_0,p_0)}. \tag{5.15}$$

Moreover by familiar calculations, say in a basis of eigenvectors of $\hat{q}$, we can verify the trace orthonormality property in the delta function sense:

$$\mathrm{Tr}(U^{(q_0',p_0')^\dagger}U^{(q_0,p_0)}) = 2\,\pi\,c\,\delta(q_0'-q_0)\,\delta(p_0'-p_0). \tag{5.16}$$

A general Hilbert–Schmidt operator A on $\mathcal{H}^{(c)}$ can then be expanded as an integral over these unit tensors:

$$A = \iint_{\mathcal{R}^2} dq_0\ \ dp_0\ \ a(q_0,p_0)\ \ U^{(q_0,p_0)},$$

$$a(q_0,p_0)=\frac{1}{2\pi c}\mathrm{Tr}\ \ (U^{(q_0,p_0)^\dagger}A), \tag{5.17}$$

$$\mathrm{Tr}(A^\dagger A)=2\pi c\iint_{\mathcal{R}^2}\ dq_0\,dp_0|a(q_0,p_0)|^2\,.$$

This is the Weyl representation for operators, and Eqs. (5.15)–(5.17) are the analogs in the present case for Eqs. (A13)–(A15) of the compact group case. All these results are available in advance of the choice of a fiducial vector, construction of its generalized coherent states, etc.

Now choose a fiducial unit vector $\psi_0\in\mathcal{H}^{(c)}$. From elementary quantum mechanics it is known that every real linear combination of $\hat{q}$ and $\hat{p}$ has a continuous spectrum and hence no normalizable eigenvectors. Therefore the stability group H_0 of ψ_0 is trivial. On the other hand, H is $\mathcal{R}$ [but effectively just U(1)] with generator T_3,

$$\psi_0\in\mathcal{H}^{(c)}\,,\quad \|\psi_0\|=1:\qquad H_0=\{e\}\,,\quad H=\{e^{-i\alpha_3 c},\ \ \alpha_3\in\mathcal{R}\}\,. \tag{5.18}$$

Thus for any ψ_0 we have case (b), and we have to examine the UIR content of the UR $\mathcal{D}^{(\mathrm{ind},00)}$ of G induced from the trivial one-dimensional UIR of H (namely, $T_3=0$). To apply the reciprocity theorem, we have to ask how often each UIR of G contains the trivial UIR of H. Clearly each $\mathcal{D}^{(q_0,p_0)}$ contains it once, while each $\mathcal{D}^{(c)}$ does not contain it at all. In other words,

$$\mathcal{D}^{(\mathrm{ind},00)}=\iint_{\mathcal{R}^2}\oplus\ \ dq_0\,dp_0\,\mathcal{D}^{(q_0,p_0)}, \tag{5.19}$$

which matches exactly with the spectrum and multiplicity of irreducible tensor operators $U^{(q_0,p_0)}$ definable on $\mathcal{H}^{(c)}$, so condition (i) is satisfied. As for condition (ii), since $\mathcal{D}^{(c)}\times\mathcal{D}^{(q_0,p_0)}=\mathcal{D}^{(c)}$, the quantity $\pi^{(q_0,p_0)}$ of Eq. (3.20) is just one number (disregarding the N_{J_0} in the denominator), and the question is whether it is always nonvanishing—we examine this more directly as follows.

The generalized coherent states and projection operators arising from ψ_0 are

$$\begin{aligned}\psi(\underline{\alpha})&=\mathcal{D}^{(c)}(\underline{\alpha})\psi_0=e^{-ic\alpha_3}D^{(c)}(\alpha_\perp)\psi_0,\\ \rho(\alpha_\perp)&=\psi(\underline{\alpha})\psi(\underline{\alpha})^\dagger=D^{(c)}(\alpha_\perp)\rho_0 D^{(c)}(\alpha_\perp)^\dagger\,,\\ \rho_0&=\psi_0\ \ \psi_0^\dagger.\end{aligned} \tag{5.20}$$

Under adjoint action we have

$$\mathcal{D}^{(c)}(\beta)\ \rho(\alpha_\perp)\ \mathcal{D}^{(c)}(\beta)^{-1}=\rho(\alpha_\perp+\beta_\perp), \tag{5.21}$$

and β_3 is absent on the right. If we denote the Fourier transform of $\rho(\alpha_\perp)$ by

$$\tilde{\rho}(q_0,p_0)=\frac{1}{2\pi}\iint_{\mathcal{R}^2}\ d^2\alpha\ \ e^{-i(\alpha_1 p_0-\alpha_2 q_0)}\rho(\alpha_\perp), \tag{5.22}$$

then (5.21) becomes

$$\mathcal{D}^{(c)}(\beta)\ \ \tilde{\rho}(q_0,p_0)\mathcal{D}^{(c)}(\beta)^{-1}=e^{i(\beta_1 p_0-\beta_2 q_0)}\ \ \tilde{\rho}(q_0,p_0)=\mathcal{D}^{(q_0,p_0)}(\beta)\ \ \tilde{\rho}(q_0,p_0). \tag{5.23}$$

Thus each $\tilde{\rho}(q_0,p_0)$ is a tensor operator of type $\mathcal{D}^{(q_0,p_0)}$, consisting of just one component, so it must be a scalar multiple of the unit tensor $U^{(q_0,p_0)}$. This factor is easily computed by a trace calculation since by (5.17) the unit tensors are a complete orthonormal (in the continuous sense) set. An elementary calculation shows that

$$\mathrm{Tr}(U^{(q_0',p_0')\dagger}\tilde{\rho}(q_0,p_0)) = 2\pi(\psi_0, U^{(q_0,p_0)}\psi_0)^*\,\delta(q_0-q_0')\,\delta(p_0-p_0'), \tag{5.24}$$

which gives the result

$$\tilde{\rho}(q_0,p_0) = \frac{1}{c}(\psi_0, U^{(q_0,p_0)}\psi_0)^* U^{(q_0,p_0)}. \tag{5.25}$$

The necessary and sufficient condition for the existence of the diagonal representation in terms of the projections $\rho(\alpha_\perp)$ of Eq. (5.20) is now clear: the fiducial vector ψ_0 must be chosen so that for all $(q_0,p_0)\in\mathcal{R}^2$,

$$\begin{aligned}(\psi_0, U^{(q_0,p_0)}\psi_0) &= \left(\psi_0, D^{(c)}\left(\frac{q_0}{c},\frac{p_0}{c}\right)\psi_0\right)\neq 0,\\ (\psi_0, D^{(c)}(q_0,p_0)\psi_0) &= (\psi_0, e^{i(q_0\hat{p}-p_0\hat{q})}\psi_0)\neq 0.\end{aligned} \tag{5.26}$$

Assuming this condition is satisfied, we can start from the Weyl representation (5.17) for any (Hilbert–Schmidt) operator A and obtain from it a diagonal coherent state representation:

$$\begin{aligned}A &= \iint_{\mathcal{R}^2} dq_0\,dp_0\,a(q_0,p_0)\quad U^{(q_0,p_0)} = \iint_{\mathcal{R}^2} dq_0\,dp_0\,a(q_0,p_0)\quad c(\psi_0, U^{(q_0,p_0)^\dagger}\psi_0)^{-1}\quad \tilde{\rho}(q_0,p_0)\\ &= \iint_{\mathcal{R}^2} d^2\alpha\quad \phi(\alpha_\perp)\rho(\alpha_\perp),\\ \phi(\alpha_\perp) &= \frac{c}{2\pi}\iint_{\mathcal{R}^2} dq_0\,dp_0\,e^{i(\alpha_2 q_0-\alpha_1 p_0)}\quad a(q_0,p_0)/(\psi_0, U^{(q_0,p_0)}\psi_0)^*.\end{aligned} \tag{5.27}$$

From Eq. (5.17) we know that for Hilbert–Schmidt A, the function $a(q_0,p_0)$ is square integrable over $\mathcal{R}^2$; in relation to this, the nature of the weight function $\phi(\alpha_\perp)$ in the diagonal representation is determined by the factor $(\psi_0, U^{(q_0,p_0)}\psi_0)^*$ in the denominator.

As an application we consider the case of the usual coherent states obtained when the fiducial vector ψ_0 is the Fock vacuum or the harmonic oscillator ground state. (Further, for simplicity we now set $c=1$.) The wave function is

$$\psi_0(q) = \pi^{-1/4}\quad e^{-q^2/2}, \tag{5.28}$$

and a simple calculation gives the displacement operator expectation value needed in Eqs. (5.26) and (5.27),

$$(\psi_0, U^{(q_0,p_0)}\psi_0) = (\psi_0, e^{i(q_0\hat{p}-p_0\hat{q})}\psi_0) = e^{-\frac{1}{4}(q_0^2+p_0^2)}. \tag{5.29}$$

This is indeed everywhere nonzero over $\mathcal{R}^2$, so the condition (5.26) for existence of the diagonal representation is, as expected, obeyed. The decaying exponential factor here means that the tensor operators $\tilde{\rho}^{(q_0,p_0)}$ provided by the projection operators $\rho(\alpha_\perp)$ differ from the normalized unit tensors $U^{(q_0,p_0)}$ by similarly decaying factors:

$$\tilde{\rho}(q_0,p_0) = e^{-\frac{1}{4}(q_0^2+p_0^2)}U^{(q_0,p_0)}. \tag{5.30}$$

It is to compensate for this diminishing norm of $\tilde{\rho}(q_0,p_0)$ as one goes towards infinity in the (q_0,p_0) phase plane that one finds that the weight function $\phi(\alpha_\perp)$, Eq. (5.27), has in general the character of a very singular distribution: the Fourier transform of $\phi(\alpha_\perp)$ is (essentially) the square integrable amplitude $a(q_0,p_0)$ times the exploding Gaussian $e^{\frac{1}{4}(q_0^2+q_0^2)}$.

Another interesting choice of fiducial state for diagonal representation has been considered by Haake and Wilkens,[19] namely the squeezed vacuum. The family of generalized coherent states in this case consists of Gaussian pure states squeezed by a fixed amount in a fixed direction in phase space, the center (q_0,p_0) of the Gaussian being allowed to be located at an arbitrary point in phase space. It is easy to see that in this case $\langle\psi_0|D(q_0,p_0)|\psi_0\rangle$ is nonvanishing, and the diagonal representation once again exists:

$$|\psi_0\rangle = S(\eta)|0\rangle, \quad S(\eta) = \exp\left(\frac{\eta}{2}\hat{a}^{\dagger 2} - \frac{\eta^*}{2}\hat{a}^2\right), \tag{5.31}$$

$$\langle\psi_0|D(q_0,p_0)|\psi_0\rangle = \langle 0|S(\eta)^{-1}D(q_0,p_0)S(\eta)|0\rangle$$
$$= \langle 0|D(e^{\eta}q_0, e^{-\eta}p_0)|0\rangle = \exp(-\tfrac{1}{4}(e^{2\eta}q_0^2 + e^{-2\eta}p_0^2)).$$

Returning to the general result (5.27) whenever ψ_0 is an acceptable fiducial vector, we can appeal to the fact that the Stone–von Neumann UIR of the HW group is square integrable and conclude that $(\psi_0, U^{(q_0,p_0)}\psi_0)$ is a square integrable function of (q_0,p_0). Thus this amplitude must approach zero as we move far away from the origin in $\mathcal{R}^2$. This has the consequence that, whatever the choice of ψ_0 [provided (5.26) holds], the weight function $\phi(\alpha_\perp)$ is in general a distribution, since in its Fourier representation (5.27) the square integrable amplitude $a(q_0,p_0)$ is *divided* by another square integrable amplitude.

We now make a series of statements which help in conveying the content of the condition (5.26) and in forming some (admittedly incomplete) idea of the set of fiducial vectors ψ_0 whose generalized coherent states are rich enough to allow for the diagonal representation:

(i) If $\psi_0(q)$ is any Gaussian wave function, then $(\psi_0, D^{(c)}(q_0,p_0)\psi_0)$ is clearly a complex Gaussian in (q_0,p_0), so condition (5.26) is satisfied.

(ii) If ψ_0 does/does not obey condition (5.26), then the transform of ψ_0 by the unitary operator representing any element of the metaplectic group $Mp(2)$ also does/does not obey condition (5.26). This is because under conjugation by such a unitary operator, $D^{(c)}(q_0,p_0)$ just becomes $D^{(c)}(q_0',p_0')$ for (q_0',p_0') some linear combinations of (q_0,p_0).

(iii) If either $\psi_0(q)$ or its Fourier transform $\tilde{\psi}_0(p)$ is a function of compact support, then condition (5.26) is definitely not obeyed, so the diagonal representation will not exist. This is because for such ψ_0, the quantity $(\psi_0, D^{(c)}(q_0,p_0)\psi_0)$ vanishes outside a finite strip parallel to the p_0 or to the q_0 axis. We can also see that as Fourier transforms of functions of compact support are entire functions of a certain class, wave functions $\psi_0(q)$ of this class violate condition (5.26) quite strongly—indeed their Fourier transforms $\tilde{\psi}_0(p)$ are of compact support.

In a purely qualitative manner we can appreciate now that Gaussian $\psi_0(q)$ and compact-supported $\psi_0(q)$ [or $\tilde{\psi}_0(p)$] are in some ways diametrically opposite from the point of view of condition (5.26). To conclude this section we consider a set of fiducial vector choices where condition (5.26) is violated, though only on a set of measure zero in the q_0–p_0 plane. This will then mean that in these cases for Hilbert–Schmidt operators A we do not have available the diagonal representation.

Consider the choice $|n\rangle$ for the fiducial vector ψ_0, this being the nth excited state of the harmonic oscillator, for $n \geqslant 1$. The resulting generalized coherent states are the *displaced Fock states*.[20] It is known that the matrix element (or better expectation value) needed in condition (5.26) is essentially a Laguerre polynomial, thus

$$|\psi_0\rangle = |n\rangle:$$

$$\langle\psi_0|D^{(c)}(q_0,p_0)|\psi_0\rangle = e^{-\frac{1}{4}(q_0^2+p_0^2)}L_n\left(\frac{q_0^2+p_0^2}{2}\right). \tag{5.32}$$

Now, as is well known, the polynomial $L_n(x)$ has exactly n distinct real zeroes in the semi-infinite interval $0<x<\infty$, hence the condition (5.26) is satisfied except on a discrete infinite sequence of circles in the q_0-p_0 plane. However, these singularities which are in the finite part of the (q_0,p_0) plane are not integrable. Therefore we do not have the possibility of the diagonal representation for the above choices of ψ_0.

Recalling condition (5.26) for the existence of the diagonal representation, and the various examples discussed above, we are led in the Heisenberg–Weyl case to the *conjecture* that condition (5.26) is obeyed if and only if the fiducial state ψ_0 has Gaussian Schrödinger wave function. This will then mean that apart from the traditional diagonal representation and the Haake–Wilkens diagonal representation there are no other ones for the Heisenberg–Weyl group.

VI. CONCLUDING REMARKS

We have developed necessary and sufficient conditions for a set of generalized coherent states, arising from a UIR of a compact Lie group to possess the property that a diagonal representation in terms of projections onto these states can be set up for any operator on the Hilbert space of the UIR. This has required combining several structures and properties—harmonic analysis on coset spaces, the theory of induced representations, the associated reciprocity theorem, and the Clebsch–Gordan problem and coefficients for the UIR's of the group under consideration. Each of these plays a crucial role in arriving at the complete set of conditions. The explicit examples involving SU(2), SU(3) and even the Heisenberg–Weyl group show how our conditions operate in practice, and how we cannot do without any of the ingredients mentioned above. In particular it is important to appreciate that the examples where the diagonal representation fails to exist are not particularly exotic or contrived; and we can often see in advance those cases where it is bound to be absent.

The comprehensive work of Brif and Mann[16] attempts also to exploit the methods of harmonic analysis on coset spaces to tackle the general closely related problems of Wigner distributions and state reconstruction problems. However, in the absence of detailed knowledge of the irreducible representation contents of various induced representations of G, it is easy to miss the fact that there are quite stringent conditions to be met before a diagonal representation can exist. The particular qualitative points to be made in connection with our approach are: for a given UIR of G, the complete set of irreducible unit tensor operators on the Hilbert space is immediately fixed, prior to construction of any set of generalized coherent states. As one then considers various choices of the fiducial vector ψ_0, one can see that for *larger* stability groups H_0 and H, the corresponding coset spaces Σ_0 and Σ are *smaller*, with the consequence that the set of projection operators onto the generalized coherent states also becomes *smaller*, and so the diagonal representation is less likely to exist.

Finally we may mention that the issue of reproducing various marginal probability distributions out of a Wigner-type distribution description of density operators has played no role in our considerations. This, the application of our methods to phase space description of quantum systems, quantum state reconstruction (tomography), and other aspects of Wigner distributions for quantum mechanics on Lie groups will be systematically studied elsewhere.

APPENDIX A: NOTATIONS FOR GROUP REPRESENTATIONS, CLEBSCH–GORDAN COEFFICIENTS, AND UNIT TENSORS

In this Appendix we collect some items of notation and familiar facts concerning the representation theory of compact groups, their Clebsch–Gordan series and coefficients in a general case involving multiplicity, and the definition and properties of unit tensors. All these are used in the main body of the paper.

We shall deal with a general compact semisimple Lie group G of dimension n [except that U(1) factors will be allowed], and a generic compact Lie subgroup H of dimension $k<n$. The various inequivalent UIR's of G will be labeled by a symbol J which in general comprises a collection of independent quantum numbers. The space of the Jth UIR, and its dimension, will be

written as $\mathcal{H}^{(J)}$ and N_J, respectively. Within the UIR we use the label M for a complete set of state labels for an orthonormal basis, denoting again several independent quantum numbers. The matrix elements of the UIR matrices $\mathcal{D}^{(J)}$ are written as $\mathcal{D}^{(J)}_{MM'}(g), g \in G$. We have

$$\begin{aligned} &\mathcal{D}^{(J)}(g)^{\dagger}\ \ \mathcal{D}^{(J)}(g)=1 \ \text{ on } \ \mathcal{H}^{(J)}, \\ &\mathcal{D}^{(J)}(g_1)\ \ \mathcal{D}^{(J)}(g_2)=\mathcal{D}^{(J)}(g_1 g_2). \end{aligned} \tag{A1}$$

The Peter–Weyl theorem gives us the orthogonality and completeness of these matrix elements taken from all UIR's of G. With respect to the translation invariant integration measure dg on G, normalized to unit total volume, these statements are expressed by

$$\begin{aligned} &\int_G dg\, \mathcal{D}^{(J')}_{M''M'''}(g)^{*}\mathcal{D}^{(J)}_{MM'}(g)=\delta_{J'J}\delta_{M''M}\delta_{M'''M'}/N_J, \\ &\sum_{JMM'} \ \ N_J\ \ \mathcal{D}^{(J)}_{MM'}(g)\mathcal{D}^{(J)}_{MM'}(g'^{*}=\delta(g^{-1}g'), \end{aligned} \tag{A2}$$

where $\delta(g)$ is the invariant Dirac delta function on G with respect to dg.

When we consider similarly the complete family of UIR's of the subgroup $H \subset G$, we replace the above symbols with the following:

$$g \to h\,, \quad J \to j\,, \quad M \to m\,, \quad \mathcal{D}^{(J)} \to D^{(j)}\,, \quad \mathcal{H}^{(J)} \to \mathcal{H}^{(j)}\,, \quad N_J \to N_j.$$

The relations (A2) corresponding to H hold with a normalized integration measure dh, and of course j,m are again in general sets of quantum numbers. In particular one may ask for the UIR's of G in a form, or in a basis, adapted to the reduction with respect to H. In that case, for each given UIR J of G, one has to ask which UIR's $D^{(j)}$ of H are contained within $\mathcal{D}^{(J)}$, and each one with what multiplicity. Then the state label M within $\mathcal{D}^{(J)}$ becomes a triple μjm: j and m are the UIR and internal state labels for H, while μ is an (orthonormal) multiplicity label which distinguishes the several occurrences of $D^{(j)}$ within $\mathcal{D}^{(J)}$. If in a particular case the multiplicity is unity, we just set $\mu=1$. Expressed in such a basis, the representation matrices of G appear as $\mathcal{D}^{(J)}_{\mu jm,\mu' j' m'}(g)$, and when $g \in H$ we have

$$\mathcal{D}^{(J)}_{\mu jm,\mu' j' m'}(h)=\delta_{\mu'\mu}\ \ \delta_{j'j}\ \ D^{(j)}_{mm'}(h)\,. \tag{A3}$$

Incidentally for the trivial or identity representations of G or of H we write $J=0, j=0$ respectively, with $M=m=0$ as well.

Now we set up a notation for Clebsch–Gordan coefficients and unit tensor operators, allowing for the possibility of multiplicity in the Clebsch–Gordan series, and for the coefficients to be complex in general. Considering the direct product $\mathcal{D}^{(J_1)} \times \mathcal{D}^{(J_2)}$ of two UIR's of G, let the UIR $\mathcal{D}^{(J_3)}$ be present upon reduction, possibly several times, and introduce an orthonormal label Λ to distinguish its several occurrences. Then, if $\Psi^{(J_1)}_{M_1}, \Psi^{(J_2)}_{M_2}$ are orthonormal bases for $\mathcal{H}^{(J_1)}, \mathcal{H}^{(J_2)}$, respectively, for each Λ the product vectors

$$\Psi^{(J_3,\Lambda)}_{M_3}=\sum_{M_1,M_2} \ \ C^{J_1\ \ J_2\ \ J_3\Lambda}_{M_1\ \ M_2\ \ M_3}\ \ \Psi^{(J_1)}_{M_1}\ \ \Psi^{(J_2)}_{M_2} \tag{A4}$$

transform by the UIR J_3 of G, and for different Λ they are orthogonal. Thus the orthonormality or unitarity and completeness relations for the Clebsch–Gordan coefficients are:

$$\sum_{M_1,M_2} C^{J_1\ J_2\ J_3\Lambda}_{M_1\ M_2\ M_3} C^{J_1\ J_2\ J_3'\Lambda'*}_{M_1\ M_2\ M_3'} = \delta_{\Lambda'\Lambda}\ \delta_{J_3'J_3}\ \delta_{M_3'M_3},$$
$$\sum_{\Lambda J_3,M_3} C^{J_1\ J_2\ J_3\Lambda}_{M_1\ M_2\ M_3} C^{J_1\ J_2\ J_3\Lambda*}_{M_1'\ M_2'\ M_3} = \delta_{M_1'M_1}\ \delta_{M_2'M_2}. \tag{A5}$$

The statement that for each $\Lambda, \Psi^{(J_3\Lambda)}_{M_3}$ transforms according to the UIR $\mathcal{D}^{(J_3)}$ of G leads to

$$\sum_{M_1,M_2} C^{J_1\ J_2\ J_3\Lambda}_{M_1\ M_2\ M_3}\ \mathcal{D}^{(J_1)}_{M_1'M_1}(g)\ \mathcal{D}^{(J_2)}_{M_2'M_2}(g) = \sum_{M_3'} C^{J_1\ J_2\ J_3\Lambda}_{M_1'\ M_2'\ M_3'}\ \mathcal{D}^{(J_3)}_{M_3'\ M_3}(g), \tag{A6}$$

from which follows, using (A5), the result for the product of any two $\mathcal{D}$ matrices:

$$\mathcal{D}^{(J_1)}_{M_1'M_1}(g)\ \mathcal{D}^{(J_2)}_{M_2'M_2}(g) = \sum_{\Lambda J_3 M_3'M_3} C^{J_1\ J_2\ J_3\Lambda}_{M_1'\ M_2'\ M_3'} C^{J_1\ J_2\ J_3\Lambda*}_{M_1\ M_2\ M_3}\ \mathcal{D}^{(J_3)}_{M_3'M_3}(g). \tag{A7}$$

Lastly we consider the Wigner–Eckart theorem, and the definition and properties of unit tensor operators within a UIR. A tensor operator of type J_2 connecting the two UIR's J_1 and J_3 is a collection of operators

$$T^{J_2}_{M_2}: \mathcal{H}^{(J_1)} \to \mathcal{H}^{(J_3)}, \tag{A8}$$

obeying the transformation rule

$$\mathcal{D}^{(J_3)}(g)\ T^{J_2}_{M_2} \mathcal{D}^{(J_1)}(g)^{-1} = \sum_{M_2'} \mathcal{D}^{(J_2)}_{M_2'M_2}(g)\ T^{J_2}_{M_2'}. \tag{A9}$$

The matrix elements of such a set of operators between the two sets of basis states involve a collection of reduced matrix elements labeled by the Clebsch−Gordan multiplicity label Λ and accompanied by corresponding Clebsch−Gordan coefficients:

$$(\Psi^{(J_3)}_{M_3},\ T^{J_2}_{M_2}\ \Psi^{(J_1)}_{M_1}) = \sum_{\Lambda} C^{J_1\ J_2\ J_3\Lambda*}_{M_1\ M_2\ M_3}\ \langle J_3 \| T^{J_2} \| J_1 \rangle_\Lambda. \tag{A10}$$

The occurrence of the complex conjugate of the Clebsch–Gordan coefficients is to be noted. One can then express $T^{J_2}_{M_2}$ explicitly as

$$T^{J_2}_{M_2} = \sum_{\Lambda M_1 M_3} C^{J_1\ J_2\ J_3\Lambda*}_{M_1\ M_2\ M_3}\ \langle J_3 \| T^{J_2} \| J_1 \rangle_\Lambda\ \Psi^{(J_3)}_{M_3}\ \Psi^{(J_1)\dagger}_{M_1}. \tag{A11}$$

Within a given UIR $\mathcal{D}^{(J_0)}$ of G on $\mathcal{H}^{(J_0)}$, Eq. (A11) leads to the definition of a complete set of unit tensor operators $U^{J\Lambda}_M$ as follows:

$$U^{J\Lambda}_M = \sum_{M_0 M_0'} C^{J_0\ J\ J_0\Lambda*}_{M_0\ M\ M_0'}\ \Psi^{(J_0)}_{M_0'}\ \Psi^{(J_0)\dagger}_{M_0}, \tag{A12}$$

where we have chosen specially simple values for the reduced matrix elements. These unit tensors obey, as a particular case of (A9):

$$\mathcal{D}^{(J_0)}(g)\ U^{J\Lambda}_M\ \mathcal{D}^{(J_0)}(g)^{-1} = \sum_{M'} \mathcal{D}^{(J)}_{M'M}(g)\ U^{J\Lambda}_{M'}. \tag{A13}$$

One can also easily establish their trace orthogonality:

$$\mathrm{Tr}(U^{J'\Lambda'\dagger}_{M'} \;\; U^{J\Lambda}_{M}) = \frac{N_{J_0}}{N_J} \;\; \delta_{\Lambda'\Lambda} \;\; \delta_{J'J} \;\; \delta_{M'M} \,. \tag{A14}$$

Therefore any operator A on $\mathcal{H}^{(J_0)}$ is uniquely expressible in the form

$$\begin{aligned} A &= \sum_{\Lambda JM} \;\; a^{J\Lambda}_{M} \;\; U^{J\Lambda}_{M} \,, \\ a^{J\Lambda}_{M} &= \frac{N_J}{N_{J_0}} \;\; \mathrm{Tr}(U^{J\Lambda\dagger}_{M} A) \,. \end{aligned} \tag{A15}$$

In Sec. III we have used such formulas in a basis adapted to H.

APPENDIX B: INDUCED REPRESENTATIONS ON COSET SPACES AND RECIPROCITY THEOREM

Here we outline the construction of induced UR's of G starting from UIR's of H, and the reciprocity theorem which tells us in detail the irreducible contents of such UR's of G. A direct construction of a class of UR's of a semidirect product of G by a certain Ábelian group (similar to the Euclidean and Poincaré groups) proves practically useful in this context.

1. The inducing construction

The UIR $D^{(j)}(h)$ of H is defined on the Hilbert space $\mathcal{H}^{(j)}$ of dimension N_j. Consider functions $\phi: G \to \mathcal{H}^{(j)}$ satisfying the following (right) covariance law under H:

$$\begin{aligned} & g \in G \to \phi(g) \in \mathcal{H}^{(j)} \,, \\ & \phi(gh) = D^{(j)}(h^{-1}) \;\; \phi(g), \\ & \phi_m(gh) = \sum_{m'} \;\; D^{(j)}_{m'm}(h)^* \;\; \phi_{m'}(g) \,. \end{aligned} \tag{B1}$$

(We avoid using letters ψ, Ψ for these vector valued functions on G since they have been used in the main text with specific meanings.) We now define an (left) action by G on such ϕ:

$$(\mathcal{U}(g)\phi)(g') = \phi(g^{-1}g') \,. \tag{B2}$$

The representation property is obvious, and so also the compatibility of the condition (B1) and the action (B2), i.e., the latter respects the former. Let $\Sigma = G/H$ be (as in the text) the space of right cosets in G with respect to H, and let $\ell(q)$ be a choice of (local) coset representatives $\Sigma \to G$. Then it is clear that the independent information in a ϕ obeying (B1) is contained in its values at coset representatives:

$$q \in \Sigma: \qquad \phi_0(q) = \phi(\ell(q)) \,. \tag{B3}$$

On these the action by G is easily computed

$$\mathcal{U}(g)\phi = \phi' :$$

$$\phi_0'(q)=\phi'(\ell(q))=\phi(g^{-1}\ell(q))=\phi(\ell(g^{-1}q)\ \ \ell(g^{-1}q)^{-1}\ \ g^{-1}\ell(q))$$
$$=D^{(j)}(\ell(q)^{-1}g\ \ \ell(g^{-1}q))\ \ \phi_0(g^{-1}q),$$

$$\phi_{0,m}'(q)=\sum_{m'}\ \ D^{(j)}_{mm'}\ \ (\ell(q)^{-1}\ \ g\ell(g^{-1}q))\ \ \phi_{0,m'}(g^{-1}q). \tag{B4}$$

We can now formally define the Hilbert space for these wave functions, in such a way that the operators $\mathcal{U}(g)$ are unitary. We use the following notation:

$$L^2(\Sigma,\mathcal{H}^{(j)})=\left\{\phi_0(q)\in\mathcal{H}^{(j)}\ \middle|\ q\in\Sigma,\ \|\phi_0\|^2=\int_\Sigma d\mu(q)(\phi_0(q),\phi_0(q))_{\mathcal{H}^{(j)}}<\infty\right\}. \tag{B5}$$

Here $d\mu(q)$ is the G-invariant normalized volume element on Σ, and it is obvious that unitarity of $D^{(j)}$ leads to unitarity of $\mathcal{U}(g)$. This UR of G is said to be induced from the UIR $D^{(j)}$ of H, and we will denote it as $\mathcal{D}^{(\mathrm{ind},j)}$ (the dependence on H being left implicit). Combining Eqs. (B4) and (B5) we see that we can introduce an (ideal) orthonormal basis $|q,m\rangle$ for $L^2(\Sigma,\mathcal{H}^{(j)})$ with these properties:

$$\phi_{0,m}(q)=\langle q,m|\phi_0\rangle\,,$$
$$\langle q',m'|q,m\rangle=\delta(q',q)\,\delta_{m'm}, \tag{B6}$$
$$\mathcal{U}(g)|q,m\rangle=\sum_{m'}\ \ D^{(j)}_{m'm}(\ell(gq)^{-1}g\ell(q))|gq,m'\rangle\,.$$

This can be viewed as a standard Wigner form for the UR $\mathcal{D}^{(\mathrm{ind},j)}$ of G.

Now the main question is: how often does the UIR $\mathcal{D}^{(J)}$ of G occur in the UR $\mathcal{D}^{(\mathrm{ind},j)}$ of G, and in case there is nontrivial multiplicity is there a natural way to choose a multiplicity label in an orthonormal manner? To answer these, we turn to a convenient construction of a Master UR of a certain semidirect product group $\mathcal{G}$ involving G, originally studied in the context of strong coupling theory.[21,22]

2. The group $\mathcal{G}$ and the *CGS* construction

Choose some UIR $\mathcal{D}^{(J_0)}$ of G (obeying a condition to be given later) and consider a group $\mathcal{G}$ defined as the semidirect product of G by an Ábelian part $P^{(J_0)}$ whose generators belong to $\mathcal{D}^{(J_0)}$. It is convenient to express the structure of $\mathcal{G}$ partly in finite form (the G part) and partly in terms of infinitesimal generators (the Ábelian part). Thus we look for unitary operators $\overline{U}(g),g\in G$, and additional (possibly non-Hermitian) operators $P^{(J_0)}_{M_0}$ obeying the relations

$$\overline{U}(g')\overline{U}(g)=\overline{U}(g'g),$$
$$\overline{U}(g)P^{(J_0)}_{M_0}\overline{U}(g)^{-1}=\sum_{M_0'}\ \mathcal{D}^{(J_0)}_{M_0'M_0}(g)P^{(J_0)}_{M_0'}, \tag{B7}$$
$$[P^{(J_0)}_{M_0},P^{(J_0)}_{M_0'}\ \text{ or }\ P^{(J_0)\dagger}_{M_0'}]=0.$$

These relations define $\mathcal{G}$, and the analogy to the structures of $E(3)$ or the Poincaré group is evident; therefore we can refer to the $P^{(J_0)}_{M_0}$ as momenta.

We now set up a solution to these relations on the space $\mathcal{H}^{(\mathrm{reg})}=L^2(G,\mathcal{C})$ of the regular representation $\mathcal{D}^{(\mathrm{reg})}$ of G. We introduce ideal basis vectors $|g\rangle$ obeying

$$\langle g'|g\rangle=\delta(g^{-1}g')\,. \tag{B8}$$

Choose now some numerical (possibly complex) values $p^{(J_0)}_{M_0}$ as possible eigenvalues of the $P^{(J_0)}_{M_0}$, and define $\overline{U}(g), P^{(J_0)}_{M_0}$ on the basis kets $|g\rangle\in\mathcal{H}^{(\mathrm{reg})}$ by

$$\begin{aligned}\overline{U}(g)|g'\rangle&=|gg'\rangle,\\ P^{(J_0)}_{M_0}|g'\rangle&=(\mathcal{D}^{(J_0)}(g')^{*}p^{(J_0)})_{M_0}|g'\rangle.\end{aligned} \tag{B9}$$

One can verify that $\overline{U}(g)$ are unitary, and that all the relations (B7) are obeyed, so we have here a certain master UR of $\mathcal{G}$ uniquely specified by the choice of $p^{(J_0)}$. The basis $|g\rangle$ is one in which the momenta are all simultaneously diagonal, and this is the essence of the *CGS* construction.

This UR of $\mathcal{G}$ can be analyzed in two interesting ways by using two separate bases for $\mathcal{H}^{(\mathrm{reg})}$. On the one hand, we can exploit the orthogonality and completeness of the UIR's of G as expressed by Eq. (A2), and so introduce a basis $|JMN\rangle$ defined and behaving as follows:

$$\begin{aligned}|JMN\rangle&=N_J^{1/2}\int_G dg\;\;\mathcal{D}^{(J)}_{MN}(g)^{*}|g\rangle,\\ \langle J'M'N'|JMN\rangle&=\delta_{J'J}\delta_{M'M}\delta_{N'N},\\ \overline{U}(g)|JMN\rangle&=\sum_{M'}\mathcal{D}^{(J)}_{M'M}(g)|JM'N\rangle.\end{aligned} \tag{B10}$$

In this basis in which the regular representation of G is fully reduced, we can exploit the information given in Appendix A to show that the matrix elements of the momenta $P^{(J_0)}_{M_0}$ have the following form:

$$\langle J'M'N'|\;\;P^{(J_0)}_{M_0}\;\;|JMN\rangle=\sqrt{\frac{N_J}{N_{J'}}}\sum_{\Lambda N_0}\;\;p^{(J_0)}_{N_0}C^{J\;\;J_0\;\;J'\Lambda *}_{M\;\;M_0\;\;M'}\;\;C^{J\;\;J_0\;\;J'\Lambda}_{N\;\;N_0\;\;N'}. \tag{B11}$$

This means that the reduced matrix element of $P^{(J_0)}$ with multiplicity label Λ is [see Eq. (A10)].

$$\langle J'N'\|P^{(J_0)}\|JN\rangle_\Lambda=\sqrt{\frac{N_J}{N_{J'}}}\sum_{N_0}\;\;p^{(J_0)}_{N_0}\;\;C^{J\;\;J_0\;\;J'\Lambda}_{N\;\;N_0\;\;N'}\,. \tag{B12}$$

We will use this in a moment.

The other way to exploit the CGS construction (B9) is to pass to a description in terms of a coset space. At this point we assume that the stability group of the numerical momentum $p^{(J_0)}_{M_0}$ is the subgroup $H\subset G$:

$$h\in H:\qquad \mathcal{D}^{(J_0)}(h)^{*}\;\;p^{(J_0)}=p^{(J_0)}\,. \tag{B13}$$

Thus the condition on the choice of the UIR J_0 of G while constructing $\mathcal{G}$ is that $\mathcal{H}^{(J_0)}$ must contain (at least) one H-scalar state. We then express a general $g'\in G$ as the product $g'=\ell(q)h$ of a coset representative and a subgroup element:

$$|g'\rangle = |q,h),$$
$$(q',h'|q,h) = \delta(q',q) \quad \delta(h^{-1}h'). \tag{B14}$$

Then Eq. (B9) appears as

$$\overline{U}(g)|q,h) = |g\ell(q)h\rangle = |\ell(gq)\ell(gq)^{-1}g\ell(q)h\rangle = |gq,\ell(gq)^{-1}g\ell(q)h),$$
$$P^{(J_0)}_{M_0}|q,h) = (\mathcal{D}^{(J_0)}(\ell(q))^* p^{(J_0)})_{M_0}|q,h). \tag{B15}$$

The key point is that in the last relation the eigenvalues of the momenta are independent of h, precisely because of Eq. (B13). To arrive at basic states behaving in the Wigner form (B6) under $\overline{U}(g)$ we just have to exploit the regular representation of H in the same way as we did for G in Eq. (B10). So from $|q,h)$ we pass to $|q,jmn\rangle$,

$$|q,jmn\rangle = N_j^{1/2}\int_H dh\, D^{(j)}_{mn}(h)^*|q,h),$$
$$\langle q',j'm'n'|q,jmn\rangle = \delta(q',q)\delta_{j'j}\delta_{m'm}\delta_{n'n}. \tag{B16}$$

In this basis we find

$$\overline{U}(g)|q,jmn\rangle = \sum_{m'} \quad D^{(j)}_{m'm}(\ell(gq)^{-1}g\ell(q))|gq,jm'n\rangle,$$
$$P^{(J_0)}_{M_0}|q,jmn\rangle = (\mathcal{D}^{(j_0)}(\ell(q))^* p^{(J_0)})_{M_0}|q,jmn\rangle. \tag{B17}$$

All the operators of $\mathcal{G}$, both $\overline{U}(g)$ and $P^{(J_0)}_{M_0}$, conserve the quantum numbers j and n. So if these are kept fixed, and only q and m are allowed to vary, we see that we have exactly recovered Eq. (B6). This shows that the *CGS* UR of $\mathcal{G}$ corresponding to a $p^{(J_0)}_{M_0}$ with stability group $H\subset G$ contains each induced UR $\mathcal{D}^{(\mathrm{ind},j)}$ of G exactly N_j times.

On the other hand, we can link up now to the results (B10) in the basis $|JMN\rangle$ by adapting the choice of labels $M,N,\ldots$ to reduction with respect to the subgroup H. As described in Appendix A, this makes $M,N\ldots$ into triples $\mu km,\nu jn,\ldots$, and then Eq. (B10) and (B12) become

$$\overline{U}(g)|J \quad \mu km \quad \nu jn\rangle = \sum_{\mu' k' m'} \quad \mathcal{D}^{(J)}_{\mu' k' m',\mu km}(g)|J \quad \mu' k' m' \quad \nu jn\rangle,$$
$$\langle J' \quad \nu' j' n'\|P^{(J_0)}\|J \quad \nu jn\rangle_\Lambda = \delta_{j'j}\delta_{n'n}\sqrt{\frac{N_J}{N_{J'}}}\sum_{\nu_0} \quad p^{(J_0)}_{\nu_0 00}\ C^{J\ \ J_0\ \ J'\Lambda}_{\nu jn\ \ \nu_0 00\ \ \nu' jn}. \tag{B18}$$

There are as many independent components to $p^{(J_0)}$ as there are H-scalar states in $\mathcal{D}^{(J_0)}$. So while $\overline{U}(g)$ conserve $\nu jn, P^{(J_0)}_{M_0}$ conserve only j and n, but not the multiplicity labels ν' and ν. Realizing that from the original basis $|g\rangle$ for $\mathcal{H}^{(\mathrm{reg})}$ we have arrived in two ways, via the sequences $|g\rangle\to|JMN\rangle\to|J \quad \mu km \quad \nu jn\rangle$ and $|g\rangle\to|q,h)\to|q,jmn\rangle$, at two alternative bases for the same UR of $\mathcal{G}$, in which the actions by $\overline{U}(g)$ and $P^{(J_0)}_{M_0}$ are, respectively, given by Eq. (B18) and Eq. (B17), we come to the following conclusions:

$$Sp(|J \quad \mu km \quad \nu jn\rangle|J \quad \mu km\nu \text{ varying, } jn \text{ fixed}) = Sp(|q,jmn\rangle|q,m \text{ varying, } jn \text{ fixed}), \tag{B19}$$

and the corresponding subspace of $\mathcal{H}^{(\mathrm{reg})}$ carries exactly once the induced UR $\mathcal{D}^{(\mathrm{ind},j)}$ of G. Comparing this with the reduced matrix element result (B18) we then see that this UR of G contains the UIR $\mathcal{D}^{(J)}$ of G as often as $\mathcal{D}^{(J)}$ contains the UIR $D^{(j)}$ of H, which is the reciprocity theorem; the index ν catalog (in an orthonormal way) these several occurrences of $\mathcal{D}^{(J)}$.

We appreciate that in the final statement of the reciprocity theorem the representation $\mathcal{D}^{(J_0)}$ and the momenta $P_{M_0}^{(J_0)}$ have disappeared; they play only an intermediate role in the CGS construction and in recognizing that we have two equally good bases for the Hilbert space carrying the UR $\mathcal{D}^{(\mathrm{ind},j)}$ of G.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

On noncommutative orbifolds of K3 surfaces

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(Received 11 November 2002; accepted 23 February 2003)

Using the algebraic geometry method of Berenstein and Leigh for the construction of the toroidal orbifold $(T^2\times T^2\times T^2)/(Z_2\times Z_2)$ with discrete torsion and considering local K3 surfaces, we present noncommutative aspects of the orbifolds of product of K3 surfaces. In this way, the ordinary complex deformation of K3 can be identified with the resolution of stringy singularities by noncommutative algebras using crossed products. We give representations and make some comments regarding the fractionation of branes. Illustrating examples are presented. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1572550]

I. INTRODUCTION

It has been known for a long time that noncommutative (NC) geometry plays an interesting role in the context of string theory[1] and, more recently, in certain compactifications of the matrix formulation of M-theory on NC torii,[2] which has opened new lines of research devoted, for example, to the study of solitons in connection with NC quantum field theories.[3]

In the context of superstring theory, NC geometry is involved whenever a B field is turned on. For example, in the study of $D(p-4)/Dp$ brane systems $(p>3)$ where, in particular, one can consider the ADHM construction of the $D0/D4$ system,[4] the NC version of the Nahm construction for monopoles,[5–7] the determination of the vacuum field solutions of the Higgs branch of supersymmetric gauge theories with eight supercharges[8–10] or in the study of tachyon condensation using the so-called GMS approach.[11]

However, most of the NC spaces considered in all these studies involve mainly NC $\mathbb{R}^d_\theta$ (Ref. 11), NC torii T^d_θ (Ref. 12), few cases of orbifolds of NC torii and some generalizations to NC higher dimensional cycles such as the NC Hizerbruch complex surface F_0 used in Ref. 13.

Recently some efforts have been devoted to go beyond these geometric spaces. In particular, a special interest has been given to build NC Calabi–Yau (NCCY) manifolds containing the commutative ones as subalgebras and, in the case of orbifolds of Calabi–Yau (CY) threefolds, an explicit construction has been given by means of the so-called the NC algebraic geometric method.[14] In that work, Berenstein and Leigh (BL) gave a realization of two NCCY three-folds with discrete torsion.

(1) The toroidal orbifolds $T^6/(Z_2\times Z_2)$, where T^6 is viewed as the product of three elliptic curves as $T^2\times T^2\times T^2$. This construction involves noncommuting variables satisfying the two-dimensional Clifford algebra.
(2) The orbifold of the quintic in the CP^4 projective space,

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$$P_5(z_j)=z_1^5+z_2^5+\cdots+z_5^5+\lambda\prod_{i=1}^{5} z_i=0, \tag{1}$$

by the Z_5^3 discrete torsion symmetry group. The quintic algebra $\mathcal{A}_\theta(5)$ reads as

$$\begin{gathered} z_1z_2=\alpha z_2z_1, \quad z_1z_3=\alpha^{-1}\beta z_3z_1, \\ z_1z_4=\beta^{-1}z_4z_1, \quad z_2z_3=\alpha\gamma z_3z_2, \\ z_2z_4=\gamma^{-1}z_4z_2, \quad z_3z_4=\beta\gamma z_4z_3, \\ z_iz_5=z_5z_i, \quad i=1,2,3,4, \end{gathered} \tag{2}$$

where α, β, and γ are fifth roots of the unity generating the Z_5^3 discrete group and where the z_i's are now the generators of the quintic algebra.

In this context, thinking of D-branes as coherent sheaves with support on a NC subvariety, they also explained the fractionation of branes by using a limit where the rank of the sheaf could jump at the singularity, leading to reducible matrix representations of the algebra.

Such formulation has been extended to higher dimensional orbifolds, understood as homogeneous hypersurfaces $P_{n+2}(z_1,z_2,\ldots,z_{n+2})$ in $\mathbf{CP^{n+1}}$ with some discrete group of isometries $\mathbf{Z_{n+2}^{n(n+1)/2}}$.[15] In all these works, the CY algebra has a typical form which reminds quantum groups and the Yang–Baxter equations.[16,17]

$$z_iz_j=\mathcal{R}_{ij}{}^{\alpha\beta}z_\alpha z_\beta, \tag{3}$$

where the four rank tensor $\mathcal{R}_{ij}{}^{\alpha\beta}$ was determined by the discrete torsion and the CY conditions. As we will see in this work, these $\mathcal{R}_{ij}{}^{\alpha\beta}$ can take the following form

$$\mathcal{R}_{ij}{}^{\alpha\beta}=\delta_i{}^\beta\delta_j{}^\alpha w^{\ell_{ij}}, \tag{4}$$

where w is an element of the discrete group G, which leaves invariant the CY algebraic equation, and ℓ_{ij} is an antisymmetric matrix satisfying the identity $\Sigma_i\ell_{ij}=0$ wich can be interpreted as the CY condition.

This analysis can also be adapted for lower dimensional CY manifolds.[18] In particular, we are interested in the case of the K3 surface. This is a very special surface because it is the only two-dimensional CY manifold. It can be represented in different ways depending on which property one is willing to study.

It can be easily seen to be related to the superconformal model corresponding to the polynomial constraint in $\mathrm{WCP}^3_{1,1,1,1}$ plus deformations[19,20] and so can be seen as a complex surface in this space. This representation makes very clear the complex structure of the surface. Another description is a local one in terms of the ADE classification of singularities near the singular loci of the orbifold T^4/Z_2. A third description is in terms of an elliptic fibration, which means that locally the surface could be seen as a two torus times a complex plane.

All along the paper we will be dealing with the two first descriptions, although the last one could be used to find a proper interpretation of the results we will find, as will be explained in the conclusions.

The aim of this work is to extend the results found in the case of the orbifold $T^6/(Z_2\times Z_2)$ to higher CY manifolds in terms of product of K3 surfaces and, as we are considering $Z_2\times Z_2$ orbifolds, which have $H^2(Z_2\times Z_2,\mathrm{U}(1))\simeq Z_2$, we can include the effect of discrete torsion.

It is known that when the discrete torsion is considered, the twisted sector modes are in $H^{2,1}$ and so act in the deformation of the complex structure of the orbifold.[20] However, there are not enough deformations available to resolve the singularities, because the discrete torsion is supported at them. In these cases, the only known way to resolve the singularities of the space is via NC geometry.

The outline of the paper is as follows. In Sec. II we review the basic facts of the construction of the K3 surfaces in terms of the ADE classification of singularities and study the deformations which can be made to the equations which define them. In Sec. III we will study how to construct

the NC algebra associated to the orbifolds of CY manifolds. In Sec. IV we specialize to the case of orbifolding the product of three K3 and construct the realization of the associated algebra. In Sec. V we extend the study to higher dimensional cases. We finish in Sec. VI with a discussion and some conclusions.

II. K3 SURFACES, WITH ADE SINGULARITIES, IN STRING THEORY COMPACTIFICATIONS

In this section we give certain essential aspects of K3 surfaces as well as methods for the resolution of ADE singularities. This study is based on the results of the geometric engineering of $D=4$ $N=2$ quantum field theory embedded in superstring theory compatifications.[21–23]

Roughly speaking, K3 is a two complex dimensional compact Kähler CY manifold with SU(2) holonomy group. It has many types of realizations, the simplest one is to consider the orbifold T^4/G, where T^4 is defined by the following complex identification equations:

$$\begin{aligned} z_j &\equiv z_j+1, \\ z_j &\equiv z_j+i, \quad j=1,2, \end{aligned} \tag{5}$$

and where G is a discrete subgroup of SU(2). For instance, if we consider $G=Z_2$, the K3 surface is obtained by imposing a extra constraint equations on T^4, namely

$$z_j \equiv -z_j, \quad j=1,2. \tag{6}$$

This symmetry has 16 singular fixed points. Near such points $(z_1,z_2)\equiv(-z_1,-z_2)$, the K3 surface looks like $\mathbb{C}^2/Z_2$ and can be determined algebraically in terms of the Z_2 invariant coordinates on $\mathbb{C}^2$, which are given by

$$\begin{aligned} x &= z_1^2, \\ y &= z_2^2, \\ z &= z_1 z_2, \end{aligned} \tag{7}$$

and give a map from $\mathbb{C}^2/Z_2$ to $\mathbb{C}^3$.

Locally, K3 can be viewed as a hypersurface in $\mathbb{C}^3$ defined by

$$z^2 = xy. \tag{8}$$

The equation (8), which is known by A_1 singularity, can be extended to the so-called A_{n-1} singularity having the following form:

$$A_{n-1}: z^n = xy. \tag{9}$$

Other singularities of local K3 surfaces are classified by the following equations:

$$\begin{aligned} D_n &: \ x^2+y^2z+z^{n-1}=0, \\ E_6 &: \ x^2+y^3+z^4=0, \\ E_7 &: \ x^2+y^3+yz^3=0, \\ E_8 &: \ x^2+y^3+z^5=0. \end{aligned} \tag{10}$$

Basically there are two ways for smoothing out the ADE singularities, either by deforming its Kähler or its complex structure. For later use we shall focus our attention on the resolution of the

A_{n-1} singularity, where the complex deformation deals with the left-hand side of Eq. (9), while the Kähler deformation, which consists in blowing up the singular point with the help of $(n-1)$ intersecting real S^2, treats the right-hand side of Eq. (9). In the case of K3 seen as an A_1 singularity these two operations are related, because the A_1 singularity can be seen as a vanishing 2-sphere, so either deforming the complex structure or making a blow-up consists in giving finite volume to it.

This method has a very nice interpretation in terms of the toric geometry realization of local K3 surfaces, where the Mori vectors are intimately related to the A_{n-1} Cartan subalgebra charges of the gauge symmetry involved in the geometric engineering method. Moreover, the corresponding toric graph looks similar to the A_{n-1} Dynkin diagram.

Since this method of doing is mirror to the complex deformation and, for latter use, we will only give the complex deformation of the A_{n-1} singularity. Indeed, Eq. (9) admits a discrete Z_n symmetry acting as follows:

$$\begin{aligned} z &\to wz, \quad w^n = 1, \\ x &\to x, \\ y &\to y, \end{aligned} \tag{11}$$

leaving x and y invariants. The deformation of the complex structure of the A_{n-1} singularity introduces extra terms breaking the Z_n symmetry as follows:

$$xy = z^n + P(z). \tag{12}$$

In this equation, the extra polynomial is given by

$$P(z) = \sum_{i=1}^{n-1} a_i z^{n-i-1}, \tag{13}$$

where the a_i's are complex parameters carrying the complex deformation of the A_{n-1} singularity. Their number is $(n-1)$ which is the rank of the A_{n-1} Lie algebra. These results have been used in many directions in string theory and F-theory compactifications, in particular, in the study of the quantum field theory using the geometric engineering method.

It should be interesting to note the following points for the A_{n-1} geometry:

(1) Since K3 is a self-mirror, Eq. (13) means that each monomial z^k is associated to a divisor of K3 explaining the monomial/divisor map involved in the mirror symmetry application in the toric geometry framework.
(2) The complex deformation acts only on the z variable, by introducing terms breaking the Z_n symmetry. The restoration of this symmetry leads to a limit where K3 develops the A_{n-1} singularity.
(3) The complex deformation of A_{n-1} singularity is similar to the resolution of stringy singularities by a NC algebra involved in the study of the orbifold C^2/Z_2 using the crossed product algebra.[24] Indeed, identifying the role of the Z_n symmetry involved in the complex deformation with the Z_n discrete torsion of the crossed product of C^2/Z_2, one can identify the complex deformation and the resolution of the stringy singularity of the orbifold C^2/Z_2.
This link can be understood by the fact the center of the algebras, being the singular geometry, is invariant under the Z_n symmetry corresponding to $P(z)=0$ in the commutative deformation. Taking into account this fact, one can see that the terms of the deformation, in the NC sense, must not be in the center of the algebra. By this argument, one can see that the complex deformation of C^2/Z_2, in the commutative sense, is similar to the stringy singularities by NC algebra involved in the study of the orbifold C^2/Z_2 using NC algebraic geometry method and the crossed product algebra.

III. NC ALGEBRAIC GEOMETRY METHOD

In this section, we will briefly review the NC algebraic geometry approach, introduced first in Ref. 14, for treating the NC aspects of orbifolds of the CY manifolds. In this method, the (singular) orbifold with discrete torsion can be viewed as a NC algebra. In other words, the algebraic realization of a commutative orbifold space with discrete torsion has a nice interpretation using NC algebra.

In this method ones proceeds following the next steps. First, one takes a d-dimensional (singular) complex CY manifold M^d defined by an equation of the form

$$f_j(u_i)=0, \quad i-j=d, \tag{14}$$

where the u_i are complex local coordinates. One looks for a discrete symmetry G,

$$G: \ u_i \to g u_i, \quad g \in G, \tag{15}$$

leaving $f_j(u_i)$ invariant

$$G: \ f_j(u_i) \to f_j(u_i), \tag{16}$$

and preserving the CY condition. After that, one considers the orbifold M^d/G which is constructed by identifying the points which are in the same orbit under the action of the group, i.e., $u_i \to g u_i$. The resulting space is smooth every where, except at the fixed points, which are invariant under nontrivial group elements.

Following Refs. 14, 15, 18, 24–26 and using the discrete symmetry group G, one can build the NC extensions of the above orbifold $(\mathcal{M}^d/G)_{nc}$. This procedure may be summarized as follows: the NC extension of this orbifold is obtained, as usual, by extending the commutative algebra $\mathcal{A}_c$ of functions on M^d/G to a NC one $\mathcal{A}_{nc} \sim (\mathcal{M}^d/G)_{nc}$. In this algebra, the coordinate functions u_i on the deformed geometry will obey the following constraint equations:

$$u_i u_j = \theta_{ij} u_j u_i, \tag{17}$$

where θ_{ij} are the NC parameters constrained by

$$\theta_{ij} \in G, \quad \theta_{ij}\theta_{ji}=1. \tag{18}$$

As we will see, the solution of these equations can take the following form:

$$\theta_{ij} = g^{\ell_{ij}}, \tag{19}$$

where g are the generators of G and ℓ_{ij} is an antisymmetric tensor. An explicit solution is obtained with the help of extra constraints on the θ_{ij}'s which can be easily specified once we know the elements of the center of the NC version of the orbifold, $\mathcal{Z}(\mathcal{A}_{nc})$.

The elements of $\mathcal{Z}(\mathcal{A}_{nc})$, which yield the commutative algebra, are the quantities invariant under the action of G. In this way, the algebraic geometry of $\mathcal{Z}(\mathcal{A}_\theta)$ is identified with the algebraic realization (13), which may be singular, while the algebraic geometry of the NC algebra will resolve the singularities. In other words, the commutative singularity can be deformed in a NC algebraic realization sense.

Since the deformation part is not invariant under G, one may say that this part resolving the singularity must be in $\mathcal{A}_\theta/\mathcal{Z}(\mathcal{A}_\theta)$ which may be a NC subspace algebra of $\mathcal{A}_{nc}$. By this argument, we think that the same feature appears in the ordinary complex deformation of A_{n-1} singularity of K3 surfaces where the extra terms solving the singularity are not invariant under the Z_n symmetry.

This important link between the complex deformations and the resolution of stringy singularities by the NC algebras push us to think about the extension of the result of BL concerning the orbifold of the torus $T^6/(Z_2 \times Z_2)$ in terms of K3 surfaces using NC algebraic geometry method.

Before doing this, let us first recall the BL work for $T^6/(Z_2\times Z_2)$. In this work, T^6 is viewed as the product of three elliptic curves as $T^2\times T^2\times T^2$, each given in the Weierstrass form

$$y_i^2=x_i(x_i-1)(x_i-a_i),\quad i=1,2,3, \tag{20}$$

for $i=1,2,3$, with a point added at infinity. The latter can be brought to a finite point by a change of variables

$$\begin{aligned} y_i\to y_i'&=\frac{y_i}{x_i^2},\\ x_i\to x_i'&=\frac{1}{x_i}. \end{aligned} \tag{21}$$

The $Z_2\times Z_2$ discrete symmetry acts by $y_i\to\pm y_i$ and $x_i\to x_i$ so that the holomorphic three form $dy_1\wedge dy_2\wedge dy_3$ is invariant under the orbifold action satisfying the CY condition. After introducing the discrete torsion, the constraints of the NC reads

$$\begin{aligned} &y_iy_j=-y_jy_i\quad \text{for } i\neq j,\\ &x_ix_j=x_jx_i\quad \text{for } i,j=1,2,3,\\ &x_iy_j=y_jx_i. \end{aligned} \tag{22}$$

and can be solved by

$$\begin{aligned} y_i&=a_i\sigma_i,\\ x_i&=b_iI_2. \end{aligned} \tag{23}$$

By this approach, the orbifold $T^6/(Z_2\times Z_2)$ with torsion defines a NCCY threefold, where the NC is carried by the discrete torsion phases and having a remarkable interpretation in terms of closed string states. On the fixed planes, the branes fractionate and local deformations are no more trivial. In what follows, we want to extend this result to higher dimensional CY manifolds. In particular we will consider CY's realized as orbifolds of K3 surfaces with discrete torsion. In other words, instead of having products of the T^2 elliptic curves, we will have products of K3 surfaces.

IV. NC ORBIFOLDS OF THE K3 SURFACES

In this section, we start by consider a general K3.[27] The latter are given by the following general form and with a point added at infinity:

$$z^2=f(x,y), \tag{24}$$

where f is obtained from a homogeneous function F with total degree 6 in complex variables u,v,w as follows:

$$F(u,v,w)=F_6(u,v,w). \tag{25}$$

Note that a special form which has been used in Ref. 27 for studying N-point deformation of algebraic K3 surfaces is given by

$$F(u,v,w)=u^2v^3w+u^4v^2. \tag{26}$$

However, in order to connect the algebraic geometry (24) to ones described in Sec. II, we will take here a special form of (25) as follows:

$$F(u,v,w)=u^4vw. \tag{27}$$

By this form, it is not difficult to see that (24) leads to the algebraic equation describing the A_1 singularity of $K3$ surfaces. Indeed, dividing Eq. (27) by u^6, one obtains

$$\frac{F(u,v,w)}{u^6}=\left(\frac{v}{u}\right)\left(\frac{w}{u}\right), \tag{28}$$

and so f is given by

$$f(x,y)=xy, \tag{29}$$

where

$$x=\frac{v}{u}, \quad y=\frac{w}{u}. \tag{30}$$

In this case, (24) looks like as the ALE space with A_1 singularity given by (7), and the analogue of the equations (21) reads now as

$$\begin{aligned} z\to z'&=\frac{z}{x^3},\\ x\to x'&=\frac{y}{x},\\ y\to y'&=\frac{1}{x}. \end{aligned} \tag{31}$$

By these equations, now we are in position to extend the results of the orbifold $T^6/(\mathbf{Z_2}\times\mathbf{Z_2})$ with discrete torsion. To start, we consider the following geometric realization of $\mathrm{K3}^{\otimes 3}/G$, that is, $\mathrm{K3}^{\otimes 3}$ is represented by the product of three K3 as follows:

$$z_i^2=x_iy_i, \quad i=1,2,3, \tag{32}$$

with an orbifold group G specified later on. *A priori* there are different symmetries leaving these equations invariant, but in order to keep the same analysis of Ref. 14, we will take G as Z_2^2 acting only on the z_i variables as follows:

$$z_i\to\pm z_i, \quad x_i\to x_i, \quad y_i\to y_i. \tag{33}$$

The reason behind choosing this symmetry is that the complex deformation of K3 surfaces acts only on the each z variable of K3 surfaces. The CY condition of this orbifold requires that the holomorphic six form,

$$\Omega_6=\mathrm{d}z_1\wedge\mathrm{d}z_2\wedge\mathrm{d}z_3\wedge\frac{\mathrm{d}x_1}{y_1}\wedge\frac{\mathrm{d}x_2}{y_2}\wedge\frac{\mathrm{d}x_3}{y_3}, \tag{34}$$

should be invariant under (33). Furthermore, since the $Z_2\times Z_2$ symmetry acts only on z_i, it follows that the invariance Ω_6 is reduced to the invariance of $\mathrm{d}z_1\wedge\mathrm{d}z_2\wedge\mathrm{d}z_3$. Having introduced these data, now we would like to introduce the discrete torsion. The orbifold $(K3\times K3\times K3)/Z_2^2$ with discrete torsion can be viewed as a NC hyper-Kahler CY manifold, where the $Z_2\times Z_2$ invariant terms are elements of the center of the algebra. Using this feature and the CY condition, the NC version of the orbifold $K3^3/Z_2^2$ is obtained by taking the coordinates functions as follows:

$$
\begin{aligned}
z_i z_j &= -z_j z_i\,,\\
z_i x_j &= x_j z_i\,,\\
y_i z_j &= z_j y_i\,,\\
x_i x_j &= x_j x_i\,,\\
y_i y_j &= y_j y_i\,,\\
y_i x_j &= x_j y_i\,,
\end{aligned}
\tag{35}
$$

with

$$
\begin{aligned}
z_i^2 z_j &= z_j z_i^2\,,\\
\left[z_i,\ \prod_{i=1}^{3} z_i\right] &= 0,
\end{aligned}
\tag{36}
$$

which means that the x_i, y_i, z_i^2, and $\Pi_i z_i$ are all in the center of the algebra. To find the points of the NC geometry, the algebra (35) and (36) can be represented in terms of the Pauli matrices as follows:

$$
z_i = a_i \sigma_i\,, \quad x_i = b_i I_2\,, \quad y_i = c_i I_2\,, \tag{37}
$$

where the a_i, b_i, c_i are complex scalars and I_2 is the two-dimensional identity matrix. Since the algebra (35) and (36) is very similar to the one describing the NC version of the orbifold torus, it follows that one should have the same interpretation in terms of resolution of singularities and reducibility of representations.

We can make the following remarks about the analysis made: the first one, which will be given in this section, is that we may find a Clifford algebra, in particular the Dirac algebra involved in the quantum field theory on Euclidean space. Another point is to consider the higher order of the discrete symmetries appearing in the geometry of ALE space, which will be treated in the next section.

Before going ahead, let us recall some useful properties of the Dirac algebra. The latter, which is involved in the study of fermions, is given by

$$
\{\gamma_i, \gamma_j\} = \delta_{ij}\,, \tag{38}
$$

where γ_i are complex matrices satisfying

$$
\gamma_0^\dagger = \gamma_0\,, \quad \gamma_i^\dagger = -\gamma_i\,, \quad \gamma_5^\dagger = \gamma_5\,. \tag{39}
$$

Note that the minus sign in (39) can be absorbed by transforming $\gamma_i \to i\gamma_i$, giving Hermitian Dirac matrices which will be useful for discussing the brane fractionation in this context.

As an illustrating application, we can consider the product of five K3 surfaces with Z_2^5 discrete symmetry. The latter acts on z_i, x_i, and y_i as

$$
\begin{aligned}
z_i \to z_i' &= z_i \omega^{q_i^a}, \quad a = 1,2,3,4\\
x_i \to x_i' &= x_i\,,\\
y_i \to y_i' &= y_i\,,
\end{aligned}
\tag{40}
$$

where $\omega = \pm 1$ and q_i^a are integer vectors satisfying the CY condition

$$\sum_{i=1}^{5} q_i^a = 0, \quad \mathrm{mod}\, 2; \quad a = 1, \ldots, 4. \tag{41}$$

Using the constraints on the θ parameters and the CY condition, one can write

$$\begin{gathered} \theta_{ij} = (-1)^{\ell_{ij}}, \\ \sum_{i=1}^{5} \ell_{ij} = 0, \ \mathrm{mod}\, 2, \end{gathered} \tag{42}$$

where ℓ_{ij} is an antisymmetric matrix of the following form:

$$\ell_{ij} = \Omega_{ab} q_i^a q_j^b, \tag{43}$$

where $\Omega_{ab} = -\Omega_{ba}$ and $\Omega_{ab} = 1$ for $a < b$.

Now, if we take $\ell_{ij} = 1$ that is

$$\theta_{ij} = -1 \quad \forall i \neq j \tag{44}$$

the NC algebra reduces to

$$z_i z_j = -z_j z_i, \quad \text{for } i \neq j \quad \text{for } i,j = 1,\ldots,5, \tag{45}$$

with all others commutations relations. Using the Dirac matrices, a four-dimensional realization of the algebra (45) can be written as follows:

$$z_i = a_i \gamma_i, \quad x_i = b_i I_4, \quad y_i = c_i I_4, \tag{46}$$

where now γ_i are given by

$$\gamma_1 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_{i+1} = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \quad i = 1,2,3, \quad \gamma_5 = -i \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}, \tag{47}$$

and where the σ_i are the Pauli matrices. At fixed locus, this representation becomes reducible as four out of the five variables z_i act by zero. Thus we get four distinct NC points, and so there four different irreducibles representations corresponding to the four eigenvalues of the nonzero z_i.

V. MORE ON THE ORBIFOLDS OF K3 SURFACES

As we have mentioned, the above geometry can be extended to ones with higher dimensional discrete symmetries. In this case, the analogue of Eq. (32) is

$$z_i^n = x_i y_i, \ \ i = 1, \ldots, m, \tag{48}$$

where m is an integer, which will be fixed later on. As in the previous examples, Eqs. (48) have a Z_n^{m-1} discrete group symmetry acting on the variables as follows:

$$\begin{gathered} z_i \to z_i' = \omega^{q_i^a} z_i, \quad a = 1, \ldots, m-1, \\ x_i \to x_i' = x_i, \\ y_i \to y_i' = y_i, \end{gathered} \tag{49}$$

so that $\mathrm{d}z_1 \wedge \mathrm{d}z_2 \wedge \cdots \wedge \mathrm{d}z_m$ is invariant. This satisfies the CY condition on the quotient space. In Eq. (45), ω is an element of the discrete group Z_n^{m-1} and where q_i^a are integers satisfying the follow-

ing condition: $\Sigma_{i=1}^{n+1} q_i^a = 0, \mod m$ which is also interpreted as the CY condition. Using the previous analysis, the NC version of the orbifold $K3 \otimes^m / Z_2^{m-1}$ is obtained by substituting the usual commutative algebra of the functions by the NC one. In this way, the coordinate functions x_i, y_i, and z_i on the deformed NC manifold obey the following identities:

$$\begin{aligned} z_i z_j &= \theta_{ij} z_j z_i, \\ z_i x_j &= x_j z_i, \\ y_i z_j &= z_j y_i, \\ x_i x_j &= x_j x_i, \\ y_i y_j &= y_j y_i, \\ y_i x_j &= x_j y_i, \end{aligned} \tag{50}$$

with

$$\begin{aligned} z_i^n z_j &= z_j z_i^n, \\ \left[z_i, \prod_{i=1}^{m} z_i \right] &= 0, \end{aligned} \tag{51}$$

which means that z_i^n and $\Pi_{i=1}^m z_i$ belong to the center of the NC algebra. Using all these identities, one can easily see that the θ_{ij} parameters must satisfy the following constraint equations:

$$\theta_{ij}^n = 1, \tag{52}$$

$$\prod_{i=1}^{m} \theta_{ij} = 1, \quad \forall i, \tag{53}$$

$$\theta_{ij} \theta_{ji} = 1. \tag{54}$$

These constraints can be solved as follows: First, Eqs. (52) show that

$$\theta_{ij} = \omega^{\ell_{ij}}, \quad \omega = \exp \frac{2i\pi}{n}, \tag{55}$$

where ℓ_{ij} is a $m \times m$ matrix. Second, putting this equation back into (52), one finds that ℓ_{ij} must satisfy

$$\begin{aligned} \ell_{ij} &= -\ell_{ji}, \\ \sum_{i=1}^{m} \ell_{ij} &= 0, \quad \mod n. \end{aligned} \tag{56}$$

Next we will build the irreducible representations of the NCCY algebra for a regular representation. Then we will give the representation for the fixed points (where becomes reducible). It turns out that the d dimension of the finite matrix representations of the orbifolds geometry algebra is a multiple of n. To see this property it is enough to take the determinant of both sides of NC variables, namely,

$$\det(z_i z_j) = (\theta_{ij})^d \det(z_j z_i) = \det(z_j z_i) \tag{57}$$

which constraint the dimension d of the representation to be such that

$$\theta_{ij}^{d}=1. \tag{58}$$

Using the identity (52), one discovers that d is a multiple of n.

We return to Eq. (48), the change of variables (31) takes now the following form:

$$\begin{aligned} z_i &\to \frac{z_i}{x_i^{6/n}}, \\ x_i &\to x_i'=\frac{y_i}{x_i}, \\ y_i &\to y_i'=\frac{1}{x_i}. \end{aligned} \tag{59}$$

If we require that $6/n$ must be integer, therefore one has only $n=2,3,6$.

(1) Case of n=2: we get the geometry related to A_1 singularity, described in Sec. IV.

(2) Case of n=3: Instead of being general, we give a concrete example corresponding to $m=3$. In this case the Eq. (48) reduces to

$$z_i^3=x_i y_i, \quad i=1,2,3, \tag{60}$$

being the A_2 singularity. Of course the NC version of this geometry is obtained from the one given in (50). In this case, the Eqs. (52) can be solved as follows:

$$\theta_{ij}=\omega^{\ell_{ij}}, \tag{61}$$

where ω is a phase so that $\omega^3=1$ and ℓ_{ij} is 3×3 antisymmetric matrix

$$\ell_{ij}=\begin{pmatrix} 0 & k & -k \\ -k & 0 & k \\ k & -k & 0 \end{pmatrix} \tag{62}$$

associated to the following commutations relations among z_i:

$$z_1 z_2=w^k z_2 z_1, \quad z_1 z_3=w^{-k} z_3 z_1, \quad z_2 z_3=w^k z_3 z_2. \tag{63}$$

Note that for $k=1$, this algebra has the same structures of the nonquartic K3 studied in Ref. 24 but with $\omega^4=1$. It is simple to see that there are three-dimensional representations. Indeed, we introduce the two following matrices:

$$P=\begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \quad Q=\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{64}$$

and so the algebra (50), for $k=1$, can be solved by taking the z_i variables matrices as

$$z_1=aP, \quad z_2=bQ, \quad z_3=cP^{-1}Q^{-1}. \tag{65}$$

Note that the only singularity in the commutative space happens when we take $b=c=0$. The representation theory on the NC algebra becomes reducible at that point. Therefore, we obtain three distinct irreducible representations.

(3) Case of n=6: Taking $m=6$, we have the algebraic geometry corresponding to the A_5 singularity,

$$z_i^6=x_iy_i, \quad i=1,\ldots,6. \tag{66}$$

This equation has Z_6^5 discrete symmetry, where in this case we have $\Sigma_{i=1}^6 q_i^a=0$, $a=1,\ldots,6$. The NC extension (57) is given by the following algebra:

$$z_iz_j=\omega^{\ell_{ij}}z_jz_i, \tag{67}$$

where ω is a phase such that, $\omega^6=1$, and ℓ_{ij} is 6×6 antisymmetric matrix given by

$$\ell_{ij}=\begin{pmatrix} 0 & \ell_{12} & \ell_{13} & \ell_{14} & \ell_{15} & \ell_{16} \\ -\ell_{12} & 0 & k_1 & k_2 & k_3 & k_4 \\ -\ell_{13} & -k_1 & 0 & k_5 & k_6 & k_7 \\ -\ell_{14} & -k_2 & -k_5 & 0 & k_8 & k_9 \\ -\ell_{15} & -k_3 & -k_6 & -k_8 & 0 & k_{10} \\ -\ell_{16} & -k_4 & -k_7 & -k_9 & -k_{10} & 0 \end{pmatrix}, \tag{68}$$

where

$$\begin{aligned} \ell_{12}&=k_1+k_2+k_3+k_4, \\ \ell_{13}&=-k_1+k_5+k_6+k_7, \\ \ell_{14}&=-k_2-k_5+k_8+k_9, \\ \ell_{15}&=-k_3-k_6-k_8+k_{10}, \\ \ell_{16}&=-k_4-k_7-k_9-k_{10}. \end{aligned} \tag{69}$$

In what follows we consider the fundamental 6×6 matrix representation obtained by using the following two matrices set Q, $P_{\eta_{\alpha\beta}};\alpha\beta=1,\ldots,6$ as follows:

$$P_{\eta_{\alpha\beta}}=\mathrm{diag}(1,\eta_{\alpha\beta},\eta_{\alpha\beta}^2,\ldots,\eta_{\alpha\beta}^5), \quad Q=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \tag{70}$$

where $\eta_{\alpha\beta}=w^{m_{\alpha\beta}}$ satisfying $\eta_{\alpha\beta}^6=1$. From these expressions, it is not difficult to see that the above matrices satisfy

$$P_\alpha P_\beta=P_{\alpha\beta}, \quad P_\alpha^6=1, \quad Q^6=1. \tag{71}$$

Using these identities and the CY condition, one can check that the z_i variables can be presented as

$$z_i=a_i\prod_{\alpha,\beta=1}^{6}(P_{\eta_{\alpha\beta}}^{q_i^\alpha}Q^{q_i^\beta}), \quad x_i=b_i\mathbf{I}_6, \quad y_i=c_i\mathbf{I}_6. \tag{72}$$

In the end of this section we would like to give a comment regarding the reducible representations for A_5 geometry. We will focus our attention on giving a particular solution. In this solution we will consider an algebra described by Z_6^2 orbifold with Z_6^3 discrete torsions and more general solutions can be given using similar analysis; more details can be found in Ref. 15. In this way, there exists situations where the representations are reducible. To see this, we start by recalling that the representation (72) corresponds to regular points of NC orbifolds of K3 CY surfaces. These solutions are irreducibles. However similar solutions may be worked out as well for orbifold points with the Z_6^3 discrete torsions. Indeed, choosing matrix coordinates z_5 and z_6 in the center of the algebra by setting

$$k_3=k_4=k_6=k_7=k_8=k_9=k_{10}=0, \tag{73}$$

the algebra reduces to

$$\begin{aligned} z_1z_2&=w^{k_1+k_2}z_2z_1,\\ z_1z_3&=w^{-k_1+k_5}z_3z_1,\\ z_1z_4&=w^{-k_2+k_5}z_4z_1,\\ z_2z_3&=w^{k_1}z_3z_2,\\ z_2z_4&=w^{k_2}z_4z_2,\\ z_3z_4&=w^{k_5}z_4z_3, \end{aligned} \tag{74}$$

and all remaining other relations are commuting. In this equation, the w are such that $w^6=1$; these are the phases of the Z_6^3 discrete torsions. In the singularity where the z_1, z_2, z_3, and z_4 moduli of Eq. (35) act by zero, the representation becomes reducible at $z_1=z_2=z_3=z_4=0$.

VI. CONCLUSION AND DISCUSSIONS

In this paper we have studied the NC version of orbifolds of product of K3 surfaces using the algebraic geometry approach of Refs. 14 and 25. In particular we have used a local description of K3 in terms of A_{n-1} geometry to extend the analysis on the NC orbifold torus with discrete torsion initiated in Ref. 14 and exposed explicitly the relation between NC data and the CY charges. Among our results, we have worked out several representations of the corresponding NC algebra by using generic CY charges and given comments regarding the fractionation of branes.

In this context, the ordinary complex deformation of K3 surfaces near an A_{n-1} singularity can be identified with the resolution of stringy singularities by NC algebras using crossed products in the $\mathbf{C^2/Z_n}$ orbifold space. This analysis can be generalized to D and E geometries by replacing the $\mathbf{Z_n}$ discrete symmetry by the corresponding ones.

On general grounds, it could be said that the appearance of NC geometry when considering discrete torsion is a natural thing. The first appearance of discrete torsion was related to some B-flux on a 2-cycle,[28] and a relation between the discrete torsion and the torsion part of the homology of the target space was carried in Ref. 29.

The implementation in the presence of D-branes[30,31] makes use of projective representations of the orbifold group, which are classified by $H^2(\Gamma,\mathrm{U}(1))$, in perfect correspondence with the previous arguments.

So there is an intimate relation between discrete torsion and the B-field and, in this way, with NC geometry. Even more interesting is the fact that is precisely the presence of this NC geometry which desingularizes the space.

This is important because could be applied to the resolution of singularities not only from a space–time point of view, but in the moduli space of certain theories. For example, a very close

case to the ones studied in this paper is that of a $D2$ brane wrapped n times over the fiber of an elliptic K3, which can be easily seen to have as moduli space the symmetric product[32]

$$\mathcal{M}_{1,n}=\mathrm{Sym}(\mathrm{K3})=\frac{\mathrm{K3}^{\otimes n}}{S_n}, \tag{75}$$

where $\mathcal{M}_{1,n}$ denotes the moduli space of a $D2$-brane with charges $(1,n)$ and S_n is the group of permutation of n elements.

On the other hand, the fact that it can be found a reducibility property in the representations of the algebras have lead previously, as we have already mentioned, to an interpretation in terms of the fractionation of branes. However, as we would interpret this configuration as arising as the moduli space of certain configurations, the precise meaning of this result is still not clear for us. However, all these facts will be explored in a future work.

ACKNOWLEDGMENTS

We thank C. Gómez, E.H. Saidi, and A. Uranga for useful conversations and encouragement. A. B. would like to thank Instituto de Física Teórica, Universidad Autónoma de Madrid for kind hospitality during the preparation of this work. He thanks M. Hssaini for discussions and for earlier collaboration on this subject. The work of A.B. is supported by SARS, Programme de Soutien à la Recherche Scientifique; Université Mohammed V-Agdal, Rabat. The work of P. R. is supported by an FPU/UAM grant.

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An algebraic method for solving the SU(3) Gauss law

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(Received 8 August 2002; accepted 7 March 2003)

A generalization of existing SU(2) results is obtained. In particular, the source-free Gauss law for SU(3)-valued gauge fields is solved using a non-Abelian analog of the Poincaré lemma. When sources are present, the color-electric field is divided into two parts in a way similar to the Hodge decomposition. Singularities due to coinciding eigenvalues of the color-magnetic field are also analyzed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1572198]

I. INTRODUCTION

Gaining knowledge about the solutions of Gauss's law is important in view of the central role that the law plays in quantizing Yang–Mills theory. Usually the Gauss law is ignored in the classical Hamiltonian formalism and then reintroduced at the quantum level as a condition on the physical states. Yet in order to remove the redundant degrees of freedom from the Hamiltonian we need a different approach. One way of addressing this problem is to search for a method to parametrize the dynamical variables of the theory so that Gauss's law is satisfied identically. The unconstrained variables thus obtained will then describe the physical degrees of freedom of Yang–Mills theory. In Refs. 1–12 a number of methods for working out parametrizations of this kind are presented, but yet another approach was proposed some years ago by Majumdar and Sharatchandra in Ref. 13. They parametrized the solutions of the SU(2) Gauss law

$$\sum_{k=1}^{3} \nabla_k(A) E_k = 0, \qquad \nabla_k(A) = \partial_k + ig[A_k(x), \cdot] \tag{1}$$

by expressing E_k as a sum of a covariant curl and a gradient thus obtaining an SU(2) generalization of the Poincaré lemma. In order to make use of this decomposition in QCD we need to generalize the results of Ref. 13 to SU(3), and it is the purpose of this paper to provide such an extension. Hopefully, the parametrization could then serve as a starting point for developing Hamiltonian formalism according to the lines sketched above. Besides Gauss's law, the decomposition might also be useful in parametrizing the non-Abelian generalization of the Coulomb gauge

$$\sum_{k=1}^{3} \nabla_k(A) \dot{A}_k = 0$$

proposed by Cronström.[14]

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II. SU(3) ALGEBRA

Write every element of the SU(3) algebra in the form

$$A=\tfrac{1}{2}A^a\lambda_a,$$

where the λ_a's stand for the Gell–Mann matrices

$$\lambda_a\lambda_b=\tfrac{2}{3}\delta_{ab}\mathbf{1}_{3\times3}+(d_{ab}{}^c+if_{ab}{}^c)\lambda_c.$$

Summation over repeated indices is implied. An inner product between two algebra elements is given by the Killing form

$$(A,B)=h_{ab}A^aB^b=6\,\mathrm{Tr}(AB),$$

$$h_{ab}=-f_{ac}{}^df_{bd}{}^c=3\delta_{ab}.$$

We have chosen the convention where the inner product is positive definite. This inner product defines a norm, which will be denoted by $|\cdot|$. The d tensor can be used to define a matrix-valued product

$$A*B=\tfrac{1}{2}d_{ab}{}^cA^aB^b\lambda_c=\{A,B\}-\tfrac{1}{9}(A,B)\mathbf{1}_{3\times3}.$$

In addition to the Jacobi identity there exist several other identities involving the structure constants of the algebra. They were worked out in Ref. 15,

$$f_{ea}{}^dd_{bc}{}^e+f_{eb}{}^dd_{ca}{}^e+f_{ec}{}^dd_{ab}{}^e=0, \tag{2a}$$

$$f_{ea}{}^bf_{cd}{}^e=\tfrac{2}{3}(\delta_{ac}\delta^b{}_d-\delta_{ad}\delta^b{}_c)+d_{ac}{}^ed_{ed}{}^b-d_{ec}{}^bd_{ad}{}^e, \tag{2b}$$

$$d_{ad}{}^ed_{eb}{}^c+d_{bd}{}^ed_{ea}{}^c+d_{ed}{}^cd_{ab}{}^e=\tfrac{1}{3}(\delta_{ab}\delta^c{}_d+\delta_b{}^c\delta_{ad}+\delta_a{}^c\delta_{bd}), \tag{2c}$$

$$3d_{ea}{}^bd_{cd}{}^e=\delta_{ac}\delta^b{}_d+\delta_{ad}\delta^b{}_c-\delta_a{}^b\delta_{cd}+f_{ac}{}^ef_{de}{}^b+f_{ad}{}^ef_{ce}{}^b. \tag{2d}$$

These relations correspond to the matrix identities

$$[A*B,C]+[B*C,A]+[C*A,B]=0, \tag{3a}$$

$$A*[B,C]+B*[A,C]+[C,A*B]=0, \tag{3b}$$

$$[A,[B,C]]=\tfrac{2}{9}(A,B)C-\tfrac{2}{9}(A,C)B+C*(A*B)-B*(A*C), \tag{3c}$$

$$A*(B*C)+B*(C*A)+C*(A*B)=\tfrac{1}{9}(A,B)C+\tfrac{1}{9}(B,C)A+\tfrac{1}{9}(A,C)B, \tag{3d}$$

$$3A*(B*C)=\tfrac{1}{3}(A,C)B+\tfrac{1}{3}(A,B)C-\tfrac{1}{3}(B,C)A+[[A,C],B]+[[A,B],C], \tag{3e}$$

Eq. (2a) giving rise to both of the relations (3a) and (3b). Modifying the conventions of Ref. 15 by some numerical factors, define two invariants of the algebra

$$I_2(A)=|A|^2, \tag{4a}$$

$$I_3(A)=(A,A*A)=36\det A. \tag{4b}$$

They remain unchanged under the adjoint action of the group

$$A\to\Omega^\dagger A\Omega,\quad \Omega\in\mathrm{SU}(3). \tag{5}$$

Given a matrix A one can define, following Ref. 15, another matrix $\hat{A}$

$$\hat{A} = I_3(A)A - I_2(A)A*A \tag{6}$$

with the properties

$$[A,\hat{A}] = 0, \quad (A,\hat{A}) = 0.$$

This suggests that we should define a third invariant by

$$I_8(A) = |\hat{A}|^2 = I_2(A)(\tfrac{1}{9}I_2(A)^3 - I_3(A)^2). \tag{7}$$

Diagonalizing A with a transformation of the form (5) one can see that I_8 vanishes if and only if A has two coinciding eigenvalues. In the generic case I_8 is strictly positive, though.

III. OUTLINE OF SOLUTION

In order to solve the Gauss law with sources

$$\sum_{k=1}^{3} \nabla_k(A)E_k = J_0, \tag{8}$$

take an ansatz of the form

$$E_k = \sum_{l,m=1}^{3} \epsilon_{klm}\nabla_l(A)C_m + \nabla_k(A)\phi, \tag{9}$$

with the covariant derivative $\nabla_k(A)$ defined in Eq. (1). Analogously with the ordinary Hodge decomposition, define ϕ as a solution to the covariant Poisson equation

$$\sum_{k=1}^{3} \nabla_k^2(A)\phi = J_0. \tag{10}$$

This equation has been analyzed in detail in Ref. 16 and it proves to be solvable for ϕ under certain fairly general conditions. Moreover, if ϕ is assumed to vanish sufficiently rapidly at infinity, the solution is also unique. Incidentally, Majumdar and Sharatchandra also included a covariant gradient term in their ansatz for the source-free Gauss law,[13] but their subsequent calculations[17] indicate that the gradient degrees of freedom are generically redundant. In the Appendix, the question whether the ansatz (9) contains enough degrees of freedom to cover the space of color-electric fields is discussed, however, for the moment take the ansatz (9) for granted. Combining now Gauss's law with the covariant divergence of Eq. (9) yields

$$\sum_{k=1}^{3} ig[B_k, C_k] = 0, \tag{11}$$

where B_k is the color-magnetic field

$$B_k = \sum_{l,m=1}^{3} \epsilon_{klm}\left(\partial_l A_m + \frac{1}{2}ig[A_l, A_m]\right).$$

Equation (11) could be solved by converting it into a system of real-valued equations and applying standard tools of linear algebra such as the Gauss elimination method. However, the elimination procedure would give very little insight into the algebraic nature of Eq. (11) and the solution obtained in this way would be complicated and formal. For this reason a less straightforward

method is preferred, which gives simpler solutions and makes algebraic features more transparent. To begin with, let us parametrize the images of the commutators appearing in Eq. (11). More precisely, each commutator takes a matrix value

$$ig[B_k,C_k]=F_k, \tag{12}$$

where F_k must satisfy certain consistency conditions so that Eq. (12) can be solved for C_k. Making use of the following property of the inner product,

$$(X,i[B_k,C_k])=-(i[B_k,X],C_k),$$

we see that F_k must be orthogonal to all matrices that commute with B_k. Equation (12) is properly solved in the next section, and it will turn out that in the generic case the solvability conditions read

$$(F_k,B_k)=0, \quad (F_k,\hat{B}_k)=0, \tag{13}$$

where $\hat{B}_k$ is defined according to Eq. (6). The geometric content of Eqs. (11)–(13) becomes clearer if we start regarding each matrix of the SU(3) algebra as an octet vector. The problem of parametrizing the solutions of Eq. (11) is then reduced to parametrizing all possible sets of three vectors F_k which satisfy the equation

$$\sum_{k=1}^{3} F_k=0 \tag{14}$$

and the orthogonality conditions (13). This task is simplified by a suitable choice of a basis for the SU(3) algebra. Generically, the following set of vectors will serve as a basis:

$$\begin{gathered} i[B_k,B_l], \quad k<l, \\ i[B_k,\hat{B}_l]+i[\hat{B}_k,B_l], \quad k<l, \\ \chi_1, \ \chi_2. \end{gathered} \tag{15}$$

Here χ_1 and χ_2 are some vectors which are orthogonal to all of the six vectors B_k and $\hat{B}_k$. We can define them as determinants

$$\chi_j=\tfrac{1}{2}\epsilon_{a_1\cdots a_6 b}{}^{c}B_1^{a_1}\hat{B}_1^{a_2}B_2^{a_3}\hat{B}_2^{a_4}B_3^{a_5}\hat{B}_3^{a_6}\eta_j^{b}\lambda_c, \quad j=1,2$$

where the η_j's are some constant octet vectors. Taking η_j parallel to some Gell–Mann matrix λ_a would reduce χ_j to a 7×7 determinant. To see the linear independence of the set (15) let us consider the equation

$$i\sum_{k<1} a_{kl}[B_k,B_l]+i\sum_{k<1}\hat{a}_{kl}([B_k,\hat{B}_l]+[\hat{B}_k,B_l])+b_1\chi_1+b_2\chi_2=0. \tag{16}$$

Taking the inner product with respect to B_m and $\hat{B}_m$ leads to the following pair of equations:

$$\begin{gathered} a_{kl}(B_m,i[B_k,B_l])+\hat{a}_{kl}(B_m,i[B_k,\hat{B}_l]+i[\hat{B}_k,B_l])=0, \\ a_{kl}(\hat{B}_m,i[B_k,B_l])+\hat{a}_{kl}(\hat{B}_m,i[B_k,\hat{B}_l]+i[\hat{B}_k,B_l])=0, \end{gathered}$$

with $m\neq k\neq l$. These equations have no nontrivial solutions if

$$((B_m, i[B_k, B_l])(\hat{B}_m, i[B_k, \hat{B}_l] + i[\hat{B}_k, B_l]) - (\hat{B}_m, i[B_k, B_l])(B_m, i[B_k, \hat{B}_l] + i[\hat{B}_k, B_l])) \neq 0. \tag{17}$$

Generically this condition is satisfied, since none of the identities (3) implies that the expression inside the parentheses should vanish. It is also possible to verify numerically, that is by assigning some test values to the vectors B_k, that this expression does not vanish identically. In the same way we see that the remaining coefficients b_1 and b_2 in Eq. (16) vanish if

$$(\chi_1, \chi_1)(\chi_2, \chi_2) - [(\chi_1, \chi_2)]^2 \neq 0. \tag{18}$$

As before, this is generically satisfied because the left-hand side does not vanish identically. The linear independence of the set (15) thus proven in the generic case, we use it as a basis for the vectors F_k,

$$F_k = i \sum_{\substack{l=1 \\ l \neq k}}^{3} (\alpha_{kl}[B_k, B_l] + \hat{\alpha}_{kl}([B_k, \hat{B}_l] + [\hat{B}_k, B_l])) + \beta_{1,k}\chi_1 + \beta_{2,k}\chi_2. \tag{19}$$

It should be noted that only six basis vectors are needed due to the orthogonality conditions (13). Substituting now these expansions into Eq. (14) gives the following relations:

$$\begin{aligned} &\alpha_{kl} - \alpha_{lk} = 0, \quad \hat{\alpha}_{kl} - \hat{\alpha}_{lk} = 0, \\ &\sum_{k=1}^{3} \beta_{1,k} = 0, \quad \sum_{k=1}^{3} \beta_{2,k} = 0. \end{aligned} \tag{20}$$

Let us finally count the number of degrees of freedom. Equation (20) states that the matrices α and $\hat{\alpha}$ are symmetric. Since four of the six coefficients $\beta_{i,k}$ are independent, the total number of free variables is $2\times3+2\times2=10$. This is the number of coordinates needed to parametrize three six-dimensional vectors F_k satisfying the eight-component equation (14). We have thus found all solutions to Eqs. (13) and (14) in the generic case, expressed in the form of expansion (19) satisfying the relations (20). Naturally there are nongeneric cases when either of the conditions (17) and (18) fails and the set (15) becomes linearly dependent. In those cases we must choose a different basis for the SU(3) algebra or at least replace the ill-behaved vectors of the set (15) with linearly independent ones. The method of solving Eq. (14) remains the same even if the basis is modified.

IV. INVERSE OF THE COMMUTATOR

The vectors F_k now known, it remains to solve Eq. (12) for the C_k's. Since the indices k are fixed at this stage, omit them for a moment and consider the equation

$$ig[B, C] = F. \tag{21}$$

To obtain the solvability conditions for F we must determine the zero modes of the commutator. For that purpose, let us express the left-hand side of Eq. (21) using octet vector notation

$$[B, C]^a = iM^a{}_c C^c,$$

where

$$M^a{}_c = f_{bc}{}^a B^b.$$

The characteristic polynomial of M becomes simpler to evaluate if we diagonalize B by a suitable unitary transformation of the form (5),

$$\Omega^\dagger B\Omega = \tfrac{1}{2}b^3\lambda_3 + \tfrac{1}{2}b^8\lambda_8, \quad \Omega \in \mathrm{SU}(3). \tag{22}$$

On the other hand, this transformation can equivalently be implemented by an orthogonal 8×8 matrix O

$$(\Omega^\dagger B\Omega)^a = O^a{}_b B^b.$$

Since the structure constants $f_{ab}{}^c$ transform as a tensor, we have

$$M^a{}_c = O_b{}^a O^d{}_c O^e{}_f f_{ed}{}^b (O_3{}^f b^3 + O_8{}^f b^8) = O_b{}^a \tilde{M}^b{}_d O^d{}_c,$$

$$\tilde{M}^b{}_d = b^3 f_{3d}{}^b + b^8 f_{8d}{}^b.$$

A straightforward calculation now gives

$$\det(M - x\mathbf{1}_{8\times 8}) = \det(\tilde{M} - x\mathbf{1}_{8\times 8}) = x^2\{x^6 + \tfrac{3}{2}[(b^3)^2 + (b^8)^2]x^4 + \tfrac{9}{16}[(b^3)^2 + (b^8)^2]^2 x^2 + \tfrac{1}{16}(b^3)^2[(b^3)^2 - 3(b^8)^2]^2\}.$$

With the help of the invariants (4a) and (7),

$$I_2(B) = 3[(b^3)^2 + (b^8)^2],$$

$$I_8(B) = 9(b^3)^2[(b^3)^2 + (b^8)^2][(b^3)^2 - 3(b^8)^2]^2,$$

the characteristic polynomial can be written as

$$\det(M - x\mathbf{1}_{8\times 8}) = x^2\left[x^2\left(x^2 + \frac{1}{4}I_2\right)^2 + \frac{1}{48}\frac{I_8}{I_2}\right].$$

The commutators thus fall into three classes according to the number of zero modes:

(1) $I_2 > 0$, $I_8 > 0$. This is the generic case, when all eigenvalues of B are distinct. The zero modes are given by B itself and the matrix $\hat{B}$ defined in Eq. (6).
(2) $I_2 > 0$, $I_8 = 0$. In this case B is nonvanishing but has two coinciding eigenvalues. One can conjugate B into the direction of λ_8,

$$B = \Omega(\tfrac{1}{2}b^8\lambda_8)\Omega^\dagger. \tag{23}$$

There are four zero modes, which are obtained by conjugating all the Gell–Mann matrices that commute with λ_8, i.e., they have the form

$$\Omega(\tfrac{1}{2}\lambda_a)\Omega^\dagger, \quad a = 1,2,3,8.$$

(3) $I_2 = 0$, $I_8 = 0$. This case is trivial, because B vanishes.

Let us now solve Eq. (21) in the generic case. There are solutions only if F is orthogonal to the zero modes of the commutator, i.e.,

$$(F,B) = 0, \quad (F,\hat{B}) = 0.$$

Introducing a projection operator

$$\Pi(F) = F - \frac{1}{I_2(B)}(B,F)B - \frac{1}{I_8(B)}(\hat{B},F)\hat{B}, \tag{24}$$

the conditions on F can also be expressed as a single equation

$$F=\Pi(F).$$

Equation (21) can thus be replaced by

$$ig[B,C]=\Pi(F). \tag{25}$$

The general form of the solution C is

$$C^a=t^a{}_bF^b, \tag{26}$$

where the tensor t depends only on B, because C must be linear in F. The basis for all such tensors was given in Ref. 15, and substituting it into Eq. (26) yields the following ansatz:

$$C=a_1F+a_2B*F+a_3\hat{B}*F+a_4[B,F]+a_5[\hat{B},F]+a_6B*[\hat{B},F]+a_7B+a_8\hat{B}.$$

Using identities (3) the commutator of this expression becomes

$$\begin{aligned}[B,C]=&\left(\frac{I_2}{6}a_4-\frac{I_8}{12I_2}a_6\right)F+\left(\frac{3I_3}{2I_2}a_4-\frac{3I_8}{2I_2^2}a_5\right)B*F-\left(\frac{3}{2I_2}a_4+\frac{3I_3}{2I_2}a_5+\frac{I_2}{12}a_6\right)\hat{B}*F\\&+\left(a_1+\frac{I_3}{2I_2}a_2-\frac{I_8}{I_2^2}a_3\right)[B,F]-\left(\frac{1}{2I_2}a_2+\frac{I_3}{I_2}a_3\right)[\hat{B},F]-a_3B*[\hat{B},F]\\&-\frac{1}{3}a_4(B,F)B+\frac{1}{6I_2}a_6(\hat{B},F)\hat{B}-\left(\frac{1}{6}a_5+\frac{I_3}{12I_2}a_6\right)((\hat{B},F)B+(B,F)\hat{B}).\end{aligned} \tag{27}$$

Inserting expansions (27) and (24) into Eq. (25) and equating terms of the same form determines six of the coefficients a_i,

$$a_1=0,\quad a_2=0,\quad a_3=0,$$

$$a_4=-\frac{i}{g}\frac{3}{I_2},\quad a_5=-\frac{i}{g}\frac{3I_3}{I_8},\quad a_6=\frac{i}{g}\frac{6I_2}{I_8}.$$

Hence, the solution to Eq. (25) is

$$C=-\frac{3i}{g}\left(\frac{1}{I_2}[B,F]+\frac{I_3}{I_8}[\hat{B},F]-\frac{2I_2}{I_8}B*[\hat{B},F]\right)+a_7B+a_8\hat{B}. \tag{28}$$

This formula becomes singular when I_8 tends to zero. In this limit B can be written in the form (23). The orthogonality conditions on F are

$$(\Omega(\tfrac{1}{2}\lambda_a)\Omega^\dagger,F)=0,\quad a=1,2,3,8. \tag{29}$$

When these requirements are fullfilled, it is straightforward to see that the following expression satisfies Eq. (21):

$$C=-\frac{4i}{g}\frac{1}{I_2}[B,F]+\Omega\left(\frac{1}{2}a^1\lambda_1+\frac{1}{2}a^2\lambda_2+\frac{1}{2}a^3\lambda_3+\frac{1}{2}a^8\lambda_8\right)\Omega^\dagger. \tag{30}$$

Formulas (28) and (30) thus solve the commutator equation (21) in the two nontrivial cases.

V. RESULTS

We are now ready to write down the general solution to Eq. (11). In the generic case the expansions (19) parametrize all possible values for the commutators (12). Substituting these expansions into Eq. (28) and simplifying the result with the identities (3) yields the solution

$$C_k=\frac{1}{g}\sum_{\substack{l=1\\ l\neq k}}^{3}[(\alpha_{kl}+I_3^{(k)}\hat{\alpha}_{kl})B_l+\hat{\alpha}_{kl}(\hat{B}_l-2I_2^{(k)}B_k*B_l)]+\frac{1}{g}\sum_{j=1}^{2}\beta_{j,k}\psi_{j,k}+\gamma_k B_k+\hat{\gamma}_k\hat{B}_k, \quad (31)$$

where

$$\Pi_k(\psi_{j,k})=-3i\left(\frac{1}{I_2^{(k)}}[B_k,\chi_j]+\frac{I_3^{(k)}}{I_8^{(k)}}[\hat{B}_k,\chi_j]-\frac{2I_2^{(k)}}{I_8^{(k)}}B_k*[\hat{B}_k,\chi_j]\right),$$
$$I_i^{(k)}\equiv I_i(B_k), \quad (32)$$

and Π_k stands for the projection operator of Eq. (24). The symmetry relations (20) must hold, while the zero mode coefficients γ_k and $\hat{\gamma}_k$ are arbitrary. Those parts of the solution corresponding to the two vectors χ_j have been left unsimplified. Of course, simplifications can be performed using the results of Ref. 18. In particular, it is shown there how the eighth rank permutation symbol can be expressed in a form involving only the structure constants $f_{ab}{}^c$ and $d_{ab}{}^c$. Constructing all possible sixth rank tensors that are antisymmetric in five indices and contracting them with the vectors B_l, $\hat{B}_l$ $(l\neq k)$, and η_j would give us the vectors needed to reduce the expression (32). Unfortunately there is such a large number of these tensors that the resulting formula would be unduly long. The unsimplified formula (32) seems to be the shortest expression that can be obtained. Still there is a relatively simple formula at hand if we diagonalize B_k with a transformation of the form (22). Making use of the fact that the eighth rank permutation symbol transforms as a tensor under the adjoint action (5) leads to

$$\Pi_k(\psi_{j,k})=\frac{1}{\sqrt{3}}I_2^{(k)}c_k^{ab}\Delta_{38b}^{(j,k)}\Omega_k\left(\frac{1}{2}\lambda_a\right)\Omega_k^\dagger, \quad (33)$$

where

$$\Delta_{abc}^{(j,k)}=\epsilon_{abd_1\cdots d_5c}(\Omega_k^\dagger B_l\Omega_k)^{d_1}(\Omega_k^\dagger\hat{B}_l\Omega_k)^{d_2}(\Omega_k^\dagger B_m\Omega_k)^{d_3}(\Omega_k^\dagger\hat{B}_m\Omega_k)^{d_4}(\Omega_k^\dagger\eta_j\Omega_k)^{d_5},$$

$$l\neq m\neq k,$$

$$c_k^{12}=-c_k^{21}=\tfrac{1}{3}[(b_k^3)^2-3(b_k^8)^2],$$

$$c_k^{45}=-c_k^{54}=\tfrac{2}{3}b_k^3(b_k^3-\sqrt{3}b_k^8),$$

$$c_k^{67}=-c_k^{76}=-\tfrac{2}{3}b_k^3(b_k^3+\sqrt{3}b_k^8),$$

and all the other components of the matrix c_k vanish.

In order to avoid singularities in the limit when two eigenvalues of B_k coincide we must find a way to regularize the vectors $\psi_{j,k}$. This singularity is present in Eq. (28), but it does not mean that the solution (31) would have to be singular. Actually, even the first six vectors of the basis (15), when inserted into Eq. (28), produced singular terms, but these terms were proportional to the zero modes B_k and $\hat{B}_k$. The singularities could then be removed by redefining the zero mode coefficients γ_k and $\hat{\gamma}_k$, and the same procedure can also be applied to the vectors $\psi_{j,k}$. Specifically, let us define

$$\psi_{j,k}=-\frac{1}{2\sqrt{3}}I_2^{(k)}\tilde{c}^a_{j,k}\Omega_k\left(\frac{1}{2}\lambda_a\right)\Omega_k^\dagger, \tag{34}$$

with

$$\tilde{c}^a_{j,k}=\frac{1}{3}[(b_k^3)^2-3(b_k^8)^2]\varepsilon^{abc}_{123}\Delta^{(j,k)}_{b8c}-\frac{2}{3}b_k^3(b_k^3-\sqrt{3}b_k^8)\left(\frac{1}{2}\varepsilon^{abc}_{453}+\frac{\sqrt{3}}{2}\varepsilon^{abc}_{458}\right)\left(\frac{\sqrt{3}}{2}\Delta^{(j,k)}_{b3c}-\frac{1}{2}\Delta^{(j,k)}_{b8c}\right)$$
$$-\frac{2}{3}b_k^3(b_k^3+\sqrt{3}b_k^8)\left(-\frac{1}{2}\varepsilon^{abc}_{673}+\frac{\sqrt{3}}{2}\varepsilon^{abc}_{678}\right)\left(-\frac{\sqrt{3}}{2}\Delta^{(j,k)}_{b3c}-\frac{1}{2}\Delta^{(j,k)}_{b8c}\right),$$

where ε^{abc}_{ijk} stands for the three-dimensional permutation symbol with indices taking the values i, j, and k. Equations (34) and (33) are equivalent apart from terms which are proportional to the zero modes. We can now pass to the limit when two eigenvalues of B_k coincide. Let us assume that the eigenvalues are ordered so that

$$b_k^3+\frac{1}{\sqrt{3}}b_k^8\geqslant -b_k^3+\frac{1}{\sqrt{3}}b_k^8\geqslant -\frac{2}{\sqrt{3}}b_k^8,$$

which means that the largest eigenvalues coincide in the limit $b_k^3\to 0$. In this limit the vectors $\psi_{j,k}$ are reduced to

$$\psi_{j,k}\to\frac{1}{6\sqrt{3}}(I_2^{(k)})^2\varepsilon^{abc}_{123}\Delta^{(j,k)}_{b8c}\Omega_k\left(\frac{1}{2}\lambda_a\right)\Omega_k^\dagger. \tag{35}$$

In order to show that this expression is single-valued we must verify that it is invariant under transformations which also leave B_k invariant. As B_k now takes the form (23), the transformations in question are the SU(2)×U(1) reparametrizations of the matrix Ω_k defined by

$$\Omega_k\to\Omega_k\omega,$$
$$\omega=\exp\left[\frac{i}{2}(\theta^1\lambda_1+\theta^2\lambda_2+\theta^3\lambda_3+\theta^8\lambda_8)\right]. \tag{36}$$

These transformations take

$$\lambda_a\to P_a{}^{a'}\lambda_{a'},$$
$$\Delta^{(j,k)}_{b8c}\to P_b{}^{b'}P_c{}^{c'}\Delta^{(j,k)}_{b'8c'},$$
$$P_a{}^{a'}=\left[\omega\left(\frac{1}{2}\lambda_a\right)\omega^\dagger\right]^{a'},$$

and as a result

$$\psi_{j,k}\to(\det_{3\times3}P)\psi_{j,k},$$
$$\det_{3\times3}P=\varepsilon^{abc}_{123}P_a{}^1P_b{}^2P_c{}^3.$$

Since $\det_{3\times3}P=1$ for transformations of the form (36), the solution (35) is invariant. Although this result was derived in the case when the largest eigenvalues of B_k coincide, the form of the solution

(34) makes it evident that $\psi_{j,k}$ is really single-valued regardless of which SU(2) subgroup survives in the limit of coinciding eigenvalues. So there will be no singularities in the fields C_k in Eq. (31).

So far we have found out that Eq. (11) possesses solutions which are regular everywhere in space. Yet it is possible that there might be some physically relevant degrees of freedom residing at points where two eigenvalues of B_k coincide and that we should search for singular solutions to Eq. (11) in order to detect these degrees of freedom. In fact, it is widely believed that there are singularities with local monopole-like behavior in the vicinity of points where two eigenvalues coincide. Usually these singularities arise as a result of gauge fixing,[19] but here they could emerge in connection with special solutions to Eq. (11). To determine such solutions we need to modify the basis (15) slightly. Consider the case when one component of the color-magnetic field, say B_3, has coinciding eigenvalues. B_3 takes the form (23) and in particular $\hat{B}_3=0$. (The eigenvalues of B_3 need not be ordered this time.) Yet the first six vectors of the set (15) remain generically independent while χ_1 and χ_2 vanish. Since F_3 in Eq. (12) now has to satisfy four orthogonality conditions according to Eq. (29), we see that the vectors χ_j should be replaced by two vectors $\tilde{\chi}_j$ which are orthogonal to the space spanned by the set $\{B_1,\hat{B}_1,B_2,\hat{B}_2\}$. We can take

$$\tilde{\chi}_1=i[\hat{B}_1,\hat{B}_2],$$

$$\tilde{\chi}_2=[B_1,B_2]*[\hat{B}_1,\hat{B}_2]-[B_1,\hat{B}_2]*[\hat{B}_1,B_2].$$

The expansion for F_k now takes the form of Eq. (19) satisfying the relations (20) with the obvious substitutions

$$\chi_j\rightarrow\tilde{\chi}_j,$$

$$\beta_{j,k}\rightarrow\tilde{\beta}_{j,k},\quad k=1,2,$$

$$\beta_{j,3}\rightarrow 0.$$

Inserting these expansions into Eqs. (28) and (30) leads to the solution

$$C_k=\frac{1}{g}\sum_{\substack{l=1\\ l\neq k}}^{3}[(\alpha_{kl}+I_3^{(k)}\hat{\alpha}_{kl})B_l+\hat{\alpha}_{kl}(\hat{B}_l-2I_2^{(k)}B_k*B_l)]+\frac{1}{g}\sum_{j=1}^{2}\tilde{\beta}_{j,k}\tilde{\psi}_{j,k}+\gamma_k B_k+\hat{\gamma}_k\hat{B}_k,\quad k=1,2, \tag{37}$$

$$C_3=\frac{1}{g}\sum_{l=1}^{2}(\alpha_{3l}B_l+\hat{\alpha}_{3l}\hat{B}_l)+\Omega_3\left(\frac{1}{2}\tilde{\gamma}_3^1\lambda_1+\frac{1}{2}\tilde{\gamma}_3^2\lambda_2+\frac{1}{2}\tilde{\gamma}_3^3\lambda_3+\frac{1}{2}\tilde{\gamma}_3^8\lambda_8\right)\Omega_3^{\dagger}.$$

Here the coefficients $\tilde{\gamma}_3^a$ are arbitrary and Ω_3 is a matrix which diagonalizes B_3. The vectors $\tilde{\psi}_{j,k}$ are defined as in Eq. (32), replacing only $\chi_j\rightarrow\tilde{\chi}_j$. Let us now compare the two solutions (31) and (37) at points where two eigenvalues of B_3 coincide. As 't Hooft mentioned in Ref. 19, this takes place at isolated points in three-dimensional space for generic magnetic fields. At such points the vectors $\psi_{j,1}$ and $\psi_{j,2}$ vanish, which corresponds to setting $\tilde{\beta}_{j,k}=0$ in Eq. (37). Equating the C_3 components of formulas (31) and (37) with the help of Eq. (35) determines the coefficients $\tilde{\gamma}_3^a$ as functions of $\beta_{j,3}$, γ_3, and $\hat{\alpha}_{3l}$. However, since $\hat{\alpha}_{3l}$ already appears in the first term of Eq. (37), there are effectively only three arbitrary parameters determining four unknown coefficients and accordingly, there is one more degree of freedom in the solution (37) which is not present in the formula (31). In all, there are thus three degrees of freedom in the exceptional solution (37) which cannot be obtained by taking the limit of Eq. (31). This leaves the door open for accepting singular solutions to Eq. (11). In that case, though, Eq. (10) should be replaced by

$$\sum_{k=1}^{3} \nabla_k^2(A)\,\phi = J_0 - \sum_{k,l,m=1}^{3} \varepsilon_{klm}\partial_k\partial_l C_m$$

to compensate for the possibility that the second weak derivatives of C_m do not commute.

VI. CONCLUSIONS

This paper presents a method by which the Gauss law (8) can be solved in the case of the SU(3) algebra using the ansatz (9). The fact that the left-hand side of the consistency equation (11) depends on the commutator properties of the color-magnetic field divides the solutions into different classes. This paper shows the source-free part of the solution explicitly in the generic case when the set (15) is linearly independent and in the case when one component of the color-magnetic field has coinciding eigenvalues. Although the SU(2) solution of Ref. 13 was simple, its SU(3) generalization (31) is much more complicated. The vectors χ_j of the basis (15) are mostly responsible for the complexity, and unfortunately we see no way out of this problem. We could replace the χ_j's by vectors which would be easier to invert with the formula (28), e.g., by

$$i[\hat{B}_1,\hat{B}_2], i[\hat{B}_1,\hat{B}_3],$$

but then the orthogonality conditions (13) for F_2 and F_3 would lead to complicated relations between the expansion coefficients. So there seems to be some kind of ''conservation of trouble'' inherent in this problem. Anyway, it is interesting that the fields C_k may have singularities at points where one component of the color-magnetic field possesses two coinciding eigenvalues. No explicit gauge fixing is needed to detect this singularity as it becomes apparent whenever one tries to solve Eq. (11). The method of solving this equation could also be generalized to higher dimensional SU(N) algebras in a straightforward manner, but the results would undoubtedly be even more complicated.

ACKNOWLEDGMENTS

The author would like to thank Professor C. Cronström for his guidance during the preparation of this paper. This research was supported by the Academy of Finland.

APPENDIX: MOTIVATION FOR THE GENERALIZED HODGE DECOMPOSITION

In order to prove that the space of color-electric fields can be parametrized with the ansatz (9) it is sufficient to show that the equations

$$\begin{aligned} E_k &= \sum_{l=1}^{3} (\nabla_l^2(A)\Phi_k - ig[G_{kl},\Phi_l]), \\ G_{kl} &= \partial_l A_k - \partial_k A_l - ig[A_k,A_l] = -\sum_{m=1}^{3} \varepsilon_{klm} B_m \end{aligned} \tag{A1}$$

can be solved for the field Φ_k. Making use of the identity

$$\sum_{l=1}^{3} (\nabla_l^2(A)\Phi_k - ig[G_{kl},\Phi_l]) = -\sum_{l,m=1}^{3} \varepsilon_{klm}\nabla_l(A) \sum_{p,q=1}^{3} \varepsilon_{mpq}\nabla_p(A)\Phi_q + \nabla_k(A)\sum_{l=1}^{3} \nabla_l(A)\Phi_l,$$

we see that Eq. (A1) then takes the form of Eq. (9) with

$$C_m = -\sum_{p,q=1}^{3} \varepsilon_{mpq}\nabla_p(A)\Phi_q, \quad \phi = \sum_{l=1}^{3} \nabla_l(A)\Phi_l. \tag{A2}$$

This paper does not attempt to solve Eq. (A1), but it seems fairly obvious that a solution exists. In a finite volume this equation can be converted into an integral equation after choosing suitable boundary conditions so that the ordinary Laplacian

$$\Delta = \sum_{l=1}^{3} \partial_l^2$$

has a unique inverse. The resulting integral equation can then be set into the form of a Fredholm equation and solved, at least formally, using the well-known Fredholm formulas. In infinite space this procedure would require that the fields E_k and the gauge potentials A_k decay sufficiently rapidly at infinity.

Equation (A1) shows that the ansatz (9) contains one redundant SU(3) algebra-valued field, because in general there are no relations like Eqs. (A2) among C_k and ϕ. This gives rise to a heuristic argument in favor of the choice (10) for the field ϕ, since we seem to be free to fix one field component at will. In order to be more exact we should investigate whether the space of color-electric fields with vanishing covariant divergences can be parametrized with the covariant curl ansatz

$$\tilde{E}_k = \sum_{l,m=1}^{3} \varepsilon_{klm} \nabla_l(A) C_m, \tag{A3}$$

where

$$\sum_{k=1}^{3} \nabla_k(A) \tilde{E}_k = 0,$$

$$\tilde{E}_k = E_k - \nabla_k(A)\phi.$$

In Ref. 17 Majumdar and Sharatchandra considered an SU(2) equation of the form (A3) with $\tilde{E}_k = 0$ and presented a method for obtaining a formal solution. Using the consistency condition (11) they eliminated C_3 and converted the remaining equations into the form of a Cauchy problem with initial data given on the plane $x_3 = 0$. They showed that a formal solution to the Cauchy problem can be constructed in a certain generic case as a power series near the initial plane $x_3 = 0$. Unfortunately there is an error in their reasoning concerning the convergence of the power series. Namely, they try to apply the Cauchy–Kovalevskaya theorem to equations of the form

$$\partial_3 C_j = G[C_1, C_2, \{A_k\}], \quad j = 1,2,$$

where the functional G depends on second order derivatives of C_1 and C_2 with respect to x_1 and x_2. In this case the Cauchy–Kovalevskaya theorem is not valid and the formal solution does not necessarily converge. The method of Ref. 17 would be easy to generalize to the case of Eq. (A3), but the formal solution might be mathematically meaningless. Anyway, this method hints that Eq. (A3) can generically be solved for the C_k's and accordingly, that the space of sufficiently regular color-electric fields with vanishing covariant divergences can be parametrized with the ansatz (A3). From the mathematical point of view this problem is still open.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

An invariant action for noncommutative gravity in four dimensions

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(Received 20 November 2002; accepted 5 March 2003)

Two main problems face the construction of noncommutative actions for gravity with star products: the complex metric and finding an invariant measure. The only gauge groups that could be used with star products are the unitary groups. I propose an invariant gravitational action in $D=4$ dimensions based on the constrained gauge group U(2,2) broken to U(1,1)×U(1,1). No metric is used, thus giving a naturally invariant measure. This action is generalized to the noncommutative case by replacing ordinary products with star products. The four-dimensional noncommutative action is studied and the deformed action to first order in deformation parameter is computed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1572199]

In noncommutative field theory based on the Moyal star product[1,2] the only gauge theories that can be used are based on unitary algebras. The presence of a constant background B-field for open or closed strings with D-branes lead to the noncommutativity of space–time coordinates. The Einstein–Hilbert action can be constructed either by insuring diffeomorphism invariance or local Lorentz invariance.[3,4] This program faces difficulties when ordinary products are replaced with star products. In this case, it is not an easy matter to define a generalization of Riemannian geometry. Noncommutative Riemannian geometry has been developed for noncommutative spaces based on the spectral triple.[5,6] The difficult part in applying this formalism is to determine the deformed spectral triple. In particular, the deformed Dirac operator is needed in order to apply this formalism to noncommutative spaces where the algebra is deformed with the star product. One must also find an invariant measure. There is, however, some recent progress on such formulation.[7] Recently, the effective action for gravity on noncommutative branes in presence of constant background B-field was derived and found to be noncovariant.[8] This conforms to the expectation that in this case space–time coordinates do not commute.

The approach based on gauging the Lorentz algebra also have problems, mainly that the metric becomes complex, and the antisymmetric part of the metric may have nonphysical propagating modes.[9] Finding an invariant measure is also problematic in this approach. One way to avoid the problem of finding an invariant measure is to require the action to be an invariant D-form in a D-dimensional space.[10,11] Experience with building gauge invariant actions which are also D-forms in a D-dimensional space tells us that these actions are usually topological, and therefore cannot describe gravity in dimensions of four or higher.[12] This is usually avoided by imposing constraints on some components of the gauge field strengths which, in some cases, is equivalent to a torsion free metric theory.[13] Constraints insure that the action, although metric independent, is not topological. The metric is then identified with some components of the gauge fields. Such constraints usually break the gauge group into a subgroup. In the noncommutative field theoretic approach to gravity this works after the constraints are imposed, provided that both the gauge group and the remaining subgroup are of the unitary type. There is a formulation of noncommutative gauge theories where the gauge group could also be of the orthogonal or symplectic type, but it turned out that there are problems associated with this formulation.[14–16] There

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is an alternative interpretation in the case where the constraints could be solved for some of the gauge fields in terms of the others. In this case one can insist on preserving gauge invariance in a nonlinear fashion, while changing the gauge transformations of those gauge fields that are now dependent in such a way as to preserve the constraints.[13] In this paper we give an invariant four-dimensional gravitational action and then generalize it to the noncommutative case. The action is based on gauging the group U(2,2) broken by constraints to $U(1,1)\times U(1,1)$. One obtains, depending on the constraints, topological gravity, Einstein gravity or conformal gravity. This construction can be extended to the noncommutative case by replacing ordinary products with star products. We derive the deformed curvatures, the deformed action and compute corrections to first order in the deformation parameter θ using the Seiberg–Witten map. We show that in this approach it is only possible to deform Gauss–Bonnet topological gravity, or conformal gravity but not Einstein gravity.

The noncommutative gravitational action was derived in dimensions two and three.[17–19] In four dimensions the smallest unitary group that contains both the spin-connection and the vierbein which spans the group SO(1,4) or SO(2,3) is U(2,2) or U(1,3). For definiteness we will consider the group U(2,2). The constraints should keep the SO(1,3) subgroup invariant. The appropriate subgroup is $U(1,1)\times U(1,1)$. To be precise we define the U(2,2) algebra as the set of 4×4 matrices M satisfying[20]

$$g^{\dagger}\Gamma_4 g=\Gamma_4,$$

where the 4×4 gamma matrices Γ_a, $a=1,2,3,4$ are the basis of a Clifford algebra

$$\{\Gamma_a,\Gamma_b\}=2\delta_{ab},$$

and where we have adopted the notation $\Gamma_4=i\Gamma_0$ and $x^4=ix^0$. The gauge fields A_μ satisfy

$$A_\mu^{\dagger}=-\Gamma_4 A_\mu \Gamma_4$$

and transform according to

$$A_\mu^g=g^{-1}A_\mu g+g^{-1}\partial_\mu g.$$

We can write

$$A=(ia_\mu+b_\mu\Gamma_5+e_\mu^a\Gamma_a+f_\mu^a\Gamma_a\Gamma_5+\tfrac{1}{4}\omega_\mu^{ab}\Gamma_{ab})\mathrm{d}x^\mu,$$

where

$$\Gamma_5=\Gamma_1\Gamma_2\Gamma_3\Gamma_4,\quad \Gamma_{ab}=\tfrac{1}{2}(\Gamma_a\Gamma_b-\Gamma_b\Gamma_a).$$

Let

$$D=\mathrm{d}+A,$$

$$D^2=F=(\mathrm{d}A+A^2),$$

so that F transforms covariantly $F^g=g^{-1}Fg$. Decomposing the field strength in terms of the Clifford algebra generators

$$F_{\mu\nu}=iF_{\mu\nu}^1+F_{\mu\nu}^5\Gamma_5+F_{\mu\nu}^a\Gamma_a+F_{\mu\nu}^{a5}\Gamma_a\Gamma_5+\tfrac{1}{4}F_{\mu\nu}^{ab}\Gamma_{ab},$$

where $F=\frac{1}{2}F_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu$, then the components are given by

$$F_{\mu\nu}^1=\partial_\mu a_\nu-\partial_\nu a_\mu,$$

$$F^5_{\mu\nu}=\partial_\mu b_\nu-\partial_\nu b_\mu+2e^a_\mu f_{\nu a}-2e^a_\nu f_{\mu a},$$

$$F^a_{\mu\nu}=\partial_\mu e^a_\nu-\partial_\nu e^a_\mu+\omega^{ab}_\mu e_{\nu b}-\omega^{ab}_\nu e_{\mu b}+2\,f^a_\mu b_\nu-2\,f^a_\nu b_\mu,$$

$$F^{a5}_{\mu\nu}=\partial_\mu f^a_\nu-\partial_\nu f^a_\mu+\omega^{ab}_\mu f_{\nu b}-\omega^{ab}_\nu f_{\mu b}+2e^a_\mu b_\nu-2e^a_\nu b_\mu,$$

$$F^{ab}_{\mu\nu}=\partial_\mu\omega^{ab}_\nu+\omega^{ac}_\mu\omega_{\nu c}{}^b+4(e^a_\mu e^b_\nu-f^a_\mu f^b_\nu)-\mu\leftrightarrow\nu.$$

We can impose the constraints

$$F^a_{\mu\nu}+F^{a5}_{\mu\nu}=0,\quad \text{or}\quad F^a_{\mu\nu}-F^{a5}_{\mu\nu}=0,$$

which break the gauge group U(2,2) to U(1,1)$\times$U(1,1) with generators

$$(1\pm\Gamma_5)\{1,\Gamma_{ab}\}.$$

One can solve the above constraints to determine ω^{ab}_μ in terms of $e^{a\pm}_\mu=e^a_\mu\pm f^a_\mu$ and b_μ. We can rewrite the constraints in the form

$$\partial_\mu e^{a+}_\nu-\partial_\nu e^{a+}_\mu+\omega^a_{\mu\,b}e^{b+}_\nu-\omega^a_{\nu\,b}e^{b+}_\mu+2e^{a+}_\mu b_\nu-2e^{a+}_\nu b_\mu=0$$

or

$$\partial_\mu e^{a-}_\nu-\partial_\nu e^{a-}_\mu+\omega^a_{\mu\,b}e^{b-}_\nu-\omega^a_{\nu\,b}e^{b-}_\mu-2e^{a-}_\mu b_\nu+2e^{a-}_\nu b_\mu=0,$$

which imply that $\omega^{ab}_\mu=\omega^{ab}_\mu(e^{a+}_\mu,b_\mu)$ or $\omega^{ab}_\mu=\omega^{ab}_\mu(e^{a-}_\mu,-b_\mu)$. The solutions which recover the Einstein action are obtained by imposing both sets of constraints simultaneously as these imply

$$f^a_\mu=\alpha e^a_\mu,\quad b_\mu=0,$$

where α is an arbitrary parameter.

The action which is invariant under the remaining U(1,1)$\times$U(1,1) group is given by,[21,22]

$$I=i\int_M \mathrm{Tr}(\Gamma_5 F\wedge F),$$

where $F=\frac{1}{2}F_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu$. Notice that Γ_5 commutes with the generators $\{1,\Gamma_5,\Gamma_{ab}\}$ of U(1,1) $\times$U(1,1) thus insuring the invariance of the action. This action is metric independent, and one expects the space–time metric to be generated from the gauge fields e^a_μ and f^a_μ. To see this we write the action when both sets of constraints are imposed simultaneously and the only independent field is e^a_μ. The action reduces to

$$I=\frac{i}{4}\int_M \mathrm{d}^4x\,\epsilon^{\mu\nu\rho\sigma}\epsilon_{abcd}(R^{ab}_{\mu\nu}+8(1-\alpha^2)e^a_\mu e^b_\nu)(R^{cd}_{\rho\sigma}+8(1-\alpha^2)e^c_\rho e^d_\sigma).$$

There are three possibilities $|\alpha|<1$, $|\alpha|=1$ and $|\alpha|>1$. The case $|\alpha|=1$ gives only the Gauss–Bonnet term and is topological. The cases with $|\alpha|<1$ and $|\alpha|>1$ give also the scalar curvature and cosmological constants with opposite signs. The Abelian gauge field a_μ decouples. This theory is different from the usual gauge formulations in that it has more vacua, and it allows for solutions with arbitrary cosmological constant. We could have restricted ourselves to SU(2,2) instead of U(2,2) as the gauge field a_μ decouples, but we did not do so because such a choice is not allowed in the noncommutative case. When only one of the constraints is imposed, then the form of the action does not change, where e^{a+}_μ is taken to be the independent field, we should solve for e^{a-}_μ from its equation of motion. It is known that the action in this case gives conformal supergravity.[20]

We are now ready to deal with formulating an action for gravity which is invariant under the star product. One of the main difficulties we mentioned in previous work is that the metric defined by $g_{\mu\nu}=e^a_\mu * e_{\nu a}$ is complex[9] and one has to obtain the correct action for the nonsymmetric part (or the complex part) of the metric.[23,24] The other problem is related to finding an invariant measure with respect to the star product.[25] Both of these problems could be solved by adopting the formalism given above. We shall show that the deformed vierbein $\hat{e}^a_\mu$ remains real. Gauge invariance with constraints eliminates some of the superfluous degrees of freedom. The constraints also make it possible to have nontopological actions with the advantage of not introducing a metric. The vierbeins are gauge fields corresponding to the broken generators. The action being a 4 form in $D=4$ dimensions is automatically invariant under the star product. The gauge fields transform according to

$$\tilde{A}^g=\tilde{g}^{-1}_*{*}\tilde{A}{*}\tilde{g}+\tilde{g}^{-1}_*{*}\mathrm{d}\tilde{g},$$

where $\tilde{g}$ satisfies

$$\tilde{g}^{-1}_*{*}\tilde{g}=1,\quad \tilde{g}^\dagger{*}\Gamma_4{*}\tilde{g}=\Gamma_4,$$

and the gauge field strength is

$$\tilde{F}=(\mathrm{d}\tilde{A}+\tilde{A}{*}\tilde{A}),$$

where

$$\tilde{A}=\tilde{A}_\mu\,\mathrm{d}x^\mu,\quad \tilde{F}=\tfrac{1}{2}\tilde{F}_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu,$$

and the coordinates x^μ satisfy

$$[x^\mu,x^\nu]=i\theta^{\mu\nu},\quad [\partial_\mu,\partial_\nu]=0,\quad \mathrm{d}x^\mu\wedge\mathrm{d}x^\nu=-\mathrm{d}x^\nu\wedge\mathrm{d}x^\mu,$$

which insures that $d^2=0$. We use the property

$$\tilde{A}{*}\tilde{A}=\tilde{A}^I_\mu{*}\tilde{A}^J_\nu T_I T_J\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu=\tfrac{1}{2}(\tilde{A}^I_\mu *_s\tilde{A}^J_\nu[T_I,T_J]+\tilde{A}^I_\mu *_a\tilde{A}^J_\nu\{T_I,T_J\})\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu,$$

where we have defined both the symmetric and antisymmetric star products by

$$f*_s g\equiv\frac{1}{2}(f*g+g*f)=fg+\left(\frac{i}{2}\right)^2\theta^{\mu\nu}\theta^{\kappa\lambda}\partial_\mu\partial_\kappa f\partial_\nu\partial_\lambda g+O(\theta^4),$$

$$f*_a g\equiv\frac{1}{2}(f*g-g*f)=\left(\frac{i}{2}\right)\theta^{\mu\nu}\partial_\mu f\partial_\nu g+\left(\frac{i}{2}\right)^3\theta^{\mu\nu}\theta^{\kappa\lambda}\theta^{\alpha\beta}\partial_\mu\partial_\kappa\partial_\alpha f\partial_\nu\partial_\lambda\partial_\beta g+O(\theta^5),$$

and T_I are the Lie algebra generators. Notice that both commutators and anticommutators appear in the products, making it necessary to consider only the unitary groups. The advantage in using the Dirac matrix representation is that all the generators corresponding to an even number of gamma matrices form the subgroup $\mathrm{U}(1,1)\times\mathrm{U}(1,1)$ of $\mathrm{U}(2,2)$ while the generators corresponding to an odd number of gamma matrices belong to the coset space $\mathrm{U}(2,2)/\mathrm{U}(1,1)\times\mathrm{U}(1,1)$. Therefore one can constrain some of the field strengths corresponding to the generators with an odd number of gamma matrices to zero thus breaking the symmetry. It is more difficult to solve the constraints in the noncommutative case. We shall make use of the Seiberg–Witten map to do this. The SW map is defined by the relation[2]

$$\tilde{g}^{-1}_*{*}\tilde{A}(A){*}\tilde{g}+\tilde{g}^{-1}_*{*}\mathrm{d}\tilde{g}=\tilde{A}(g^{-1}Ag+g^{-1}\,\mathrm{d}g),$$

and whose solution is equivalent to[2]

$$\delta\tilde{A}_\mu(\theta)=-\frac{i}{4}\delta\theta^{\nu\rho}\{\tilde{A}_\nu,(\partial_\rho\tilde{A}_\mu+\tilde{F}_{\rho\mu})\}_*,$$

$$\delta\tilde{\lambda}(\theta)=\frac{i}{4}\delta\theta^{\nu\rho}\{\partial_\nu\lambda,A_\rho\}_*,$$

where we have defined $\tilde{g}=e^{\tilde{\lambda}}$ and $g=e^{\lambda}$. These transformations do not preserve the constraints. To make these transformations compatible with the constraints one can follow the same procedure as in the commutative case. This is done by first solving the constraints and determining the dependent fields in terms of the independent ones and then modifying the transformations of these dependent fields in such a way as to preserve the constraints.

The constraints are given by

$$\tilde{F}^a_{\mu\nu}+\tilde{F}^{a5}_{\mu\nu}=0 \quad \text{or} \quad \tilde{F}^a_{\mu\nu}-\tilde{F}^{a5}_{\mu\nu}=0,$$

and the action invariant under $\mathrm{U}(1,1)\times\mathrm{U}(1,1)$ is

$$I=i\int_M \mathrm{Tr}(\Gamma_{D+1}\tilde{F}*\tilde{F}).$$

Notice that we can write $\tilde{F}=\frac{1}{2}\tilde{F}_{\mu\nu}\,\mathrm{d}x^\mu\wedge\mathrm{d}x^\nu$ and $\tilde{F}*\tilde{F}=(1/2^2)\tilde{F}_{\mu_1\mu_2}*\tilde{F}_{\mu_3\mu_4}\,\mathrm{d}x^{\mu_1}\wedge\mathrm{d}x^{\mu_2}\wedge\mathrm{d}x^{\mu_3}\wedge\mathrm{d}x^{\mu_4}$. The gauge fields $\tilde{A}_\mu$ are decomposed as in the commutative case. The field strengths are given by

$$\tilde{F}_{\mu\nu}(1)=i(\partial_\mu\tilde{a}_\nu-\partial_\nu\tilde{a}_\mu)+2(-\tilde{a}_\mu*_a\tilde{a}_\nu+\tilde{b}_\mu*_a\tilde{b}_\nu+\tilde{e}^a_\mu*_a\tilde{e}_{\nu a}-\tilde{f}^a_\mu*_a\tilde{f}_{\nu a}-\tfrac{1}{4}\tilde{\omega}^{ab}_\mu*_a\tilde{\omega}_{\nu ab}),$$

$$\tilde{F}_{\mu\nu}(\Gamma_5)=\partial_\mu\tilde{b}_\nu-\partial_\nu\tilde{b}_\mu+2(\tilde{e}^a_\mu*_s\tilde{f}_{\nu a}-\tilde{f}^a_\mu*_s\tilde{e}_{\nu a})+2(\tilde{b}_\mu*_a\tilde{a}_\nu+\tilde{a}_\mu*_a\tilde{b}_\nu)+\tfrac{1}{8}\epsilon_{abcd}\tilde{\omega}^{ab}_\mu*_a\tilde{\omega}^{cd}_\nu,$$

$$\begin{aligned}\tilde{F}_{\mu\nu}(\Gamma_{ab})=&\frac{1}{4}(\partial_\mu\tilde{\omega}^{ab}_\nu-\partial_\nu\tilde{\omega}^{ab}_\mu+\tilde{\omega}^{ac}_\mu*_s\tilde{\omega}_{\nu c}{}^b-\tilde{\omega}^{bc}_\mu*_s\tilde{\omega}_{\nu c}{}^a)+\frac{i}{2}(\tilde{a}_\mu*_a\tilde{\omega}^{ab}_\nu+\tilde{\omega}^{ab}_\mu*_a\tilde{a}_\nu)\\&-\tfrac{1}{4}\epsilon^{ab}{}_{cd}(\tilde{b}_\mu*_a\tilde{\omega}^{cd}_\nu+\tilde{\omega}^{cd}_\mu*_a\tilde{b}_\nu)-4\epsilon^{ab}{}_{cd}(\tilde{e}^c_\mu*_a\tilde{f}^d_\nu+\tilde{f}^d_\mu*_a\tilde{e}^c_\nu)\\&+(\tilde{e}^a_\mu*_s\tilde{e}^b_\nu-\tilde{e}^a_\nu*_s\tilde{e}^b_\mu-\tilde{f}^a_\mu*_s\tilde{f}^b_\nu+\tilde{f}^a_\nu*_s\tilde{f}^b_\mu),\end{aligned}$$

for the generators with an even number of gamma matrices, and by

$$\begin{aligned}\tilde{F}_{\mu\nu}(\Gamma_a)=&\partial_\mu\tilde{e}^a_\nu-\partial_\nu\tilde{e}^a_\mu+\tilde{\omega}^{ac}_\mu*_s\tilde{e}_{\nu c}+\tilde{e}^c_\mu*_s\tilde{\omega}_{\nu c}{}^a-2(\tilde{b}_\mu*_s\tilde{f}^a_v-\tilde{f}^a_\mu*_s\tilde{b}_\nu)\\&+2i(\tilde{a}_\mu*_a\tilde{e}^a_\nu+\tilde{e}^a_\mu*_a\tilde{a}_\nu)+\tfrac{1}{2}\epsilon^a{}_{bcd}(\tilde{f}^b_\mu*_a\tilde{\omega}^{cd}_\nu+\tilde{\omega}^{cd}_\mu*_a\tilde{f}^b_\nu),\end{aligned}$$

$$\begin{aligned}\tilde{F}_{\mu\nu}(\Gamma_a\Gamma_5)=&\partial_\mu\tilde{f}^a_\nu-\partial_\nu\tilde{f}^a_\mu+\tilde{\omega}^{ac}_\mu*_s\tilde{f}_{\nu c}+\tilde{f}^c_\mu*_s\tilde{\omega}_{\nu c}{}^a-2(\tilde{b}_\mu*_s\tilde{e}^a_v-\tilde{e}^a_\mu*_s\tilde{b}_\nu)\\&+2i(\tilde{a}_\mu*_a\tilde{f}^a_\nu+\tilde{f}^a_\mu*_a\tilde{a}_\nu)+\tfrac{1}{2}\epsilon^a{}_{bcd}(\tilde{e}^b_\mu*_a\tilde{\omega}^{cd}_\nu+\tilde{\omega}^{cd}_\mu*_a\tilde{e}^b_\nu),\end{aligned}$$

for the generators with an odd number of gamma matrices. In four dimensions, the action is

$$\begin{aligned}I=&i\int_M \mathrm{Tr}(\Gamma_5\tilde{F}*\tilde{F})=i\int_M \mathrm{d}^4x\,\epsilon^{\mu\nu\rho\sigma}\mathrm{Tr}(\Gamma_5\tilde{F}_{\mu\nu}*\tilde{F}_{\rho\sigma})\\=&i\int_M \mathrm{d}^4x\,\epsilon^{\mu\nu\rho\sigma}(2\tilde{F}^1_{\mu\nu}*_s\tilde{F}^5_{\rho\sigma}+\epsilon_{abcd}\tilde{F}^{ab}_{\mu\nu}*_s\tilde{F}^{cd}_{\rho\sigma}).\end{aligned}$$

Notice that although only the symmetric star product appears there are linear corrections in θ to the commutative action. As in the commutative case, the constraints have to be solved for $\tilde{\omega}_\mu^{ab}$ in terms of $\tilde{e}_\mu^{a+}$ or $\tilde{e}_\mu^{a-}$, $\tilde{b}_\mu$, and $\tilde{a}_\mu$. However, unlike the commutative case, it is not possible to impose both constraints simultaneously after setting $\tilde{b}_\mu=0$ because of the presence of the $\pm e^{\pm}\omega$ term in $\tilde{F}^a_{\mu\nu}\pm\tilde{F}^{a5}_{\mu\nu}$. These two constraints become incompatible except in the special case where $\tilde{e}_\mu^{a-}=0$, which corresponds to deforming the Gauss–Bonnet action. If only one constraint is imposed and $\tilde{\omega}_\mu^{ab}$ is determined from the constraint, the independent fields are $\tilde{e}_\mu^{a+}$, $\tilde{e}_\mu^{a-}$, $\tilde{b}_\mu$, and $\tilde{a}_\mu$ resulting in deformed conformal supergravity. It is not possible to obtain a deformation of Einstein gravity as the constraints could not be imposed simultaneously.

One can expand this action perturbatively in powers of θ. This can be done by using the Seiberg–Witten map for $\tilde{e}_\mu^{a+}$ $\tilde{e}_\mu^{a-}$, $\tilde{b}_\mu$ and $\tilde{a}_\mu$. These expressions are then used in the above constraint to determine $\tilde{\omega}_\mu^{ab}$. It is instructive to carry this procedure to first order in θ. Applying the Seiberg–Witten map, one gets

$$\tilde{e}_\mu^{a\pm}=e_\mu^{a\pm}+\frac{1}{2}\theta^{\kappa\rho}\left(a_\kappa\partial_\rho e_\mu^{a\pm}+e_\kappa^{a\pm}(2\partial_\rho a_\mu-\partial_\mu a_\rho)\mp\frac{i}{4}\epsilon_{abcd}(e_\kappa^{b\pm}(\partial_\rho\omega_\mu^{cd}+F_{\rho\mu}^{cd})+\omega_\kappa^{cd}\partial_\rho e_\mu^{b\pm})\right)$$

$$+O(\theta^2)\equiv e_\mu^{a\pm}+\frac{1}{2}\theta^{\kappa\rho}e_{\mu\kappa\rho}^{a\pm}+O(\theta^2),$$

$$\tilde{a}_\mu=a_\mu+\tfrac{1}{2}\theta^{\kappa\rho}(a_\kappa(2\partial_\rho a_\mu-\partial_\mu a_\rho)-b_\kappa(\partial_\rho b_\mu+F_{\rho\mu}^5)-e_\kappa^a(\partial_\rho e_\mu^a+F_{\rho\mu}^a)+f_\kappa^a(\partial_\rho f_\mu^a+F_{\rho\mu}^{a5})$$

$$+\tfrac{1}{8}\omega_\kappa^{ab}(\partial_\rho\omega_\mu^{ab}+F_{\rho\mu}^{ab}))+O(\theta^2)\equiv a_\mu+\tfrac{1}{2}\theta^{\kappa\rho}a_{\mu\kappa\rho}+O(\theta^2),$$

$$\tilde{b}_\mu=b_\mu+\tfrac{1}{2}\theta^{\kappa\rho}\left(b_\kappa(2\partial_\rho a_\mu-\partial_\mu a_\rho)+a_\kappa(\partial_\rho b_\mu+F_{\rho\mu}^5)-\frac{i}{8}\epsilon_{abcd}\omega_\kappa^{ab}(\partial_\rho\omega_\mu^{cd}+F_{\rho\mu}^{cd})\right)+O(\theta^2)$$

$$\equiv b_\mu+\tfrac{1}{2}\theta^{\kappa\rho}b_{\mu\kappa\rho}+O(\theta^2).$$

We do not take $\tilde{\omega}_\mu^{ab}$ as given by the SW map, but instead substitute the above expressions in the constraint equation to determine its value. First we write

$$\tilde{\omega}_\mu^{ab}=\omega_\mu^{ab}+\tfrac{1}{2}\theta^{\kappa\rho}\omega_{\mu\kappa\rho}^{ab}+O(\theta^2)$$

then the constraint becomes

$$\tilde{F}_{\mu\nu}^{a+}=F_{\mu\nu}^{a+}+\tfrac{1}{2}\theta^{\kappa\rho}(\partial_\mu e_{\nu\kappa\rho}^{a+}-\partial_\nu e_{\mu\kappa\rho}^{a+}+\omega_\mu^{ac}e_{\nu\kappa\rho}^{c+}-\omega_\nu^{ac}e_{\mu\kappa\rho}^{c+}+\omega_{\mu\kappa\rho}^{ac}e_\nu^{c+}-\omega_{\nu\kappa\rho}^{ac}e_\mu^{c+}$$

$$\mp 2(b_{\mu\kappa\rho}e_\nu^{a+}-b_{\nu\kappa\rho}e_\mu^{a+})-2(\partial_\kappa a_\mu\partial_\rho e_\nu^{a+}-\partial_\kappa a_\nu\partial_\rho e_\mu^{a+}))+O(\theta^2).$$

Substituting $\tilde{F}_{\mu\nu}^{a+}=0$, and $F_{\mu\nu}^{a+}=0$, we can solve for $\omega_{\mu\kappa\rho}^{ab}$ to obtain

$$\omega_{\mu\kappa\rho}^{ab}=\tfrac{1}{2}(e^{\nu b+}C_{\mu\nu\kappa\rho}^a-e^{\nu a+}C_{\mu\nu\kappa\rho}^b+e^{\sigma a+}e^{\nu b+}e_{\mu c}^{+}C_{\sigma\nu\kappa\rho}),$$

where

$$C_{\mu\nu\kappa\rho}^a=-(\partial_\mu e_{\nu\kappa\rho}^{a+}-\partial_\nu e_{\mu\kappa\rho}^{a+}+\omega_\mu^{ac}e_{\nu\kappa\rho}^{c+}-\omega_\nu^{ac}e_{\mu\kappa\rho}^{c+}-2(\partial_\kappa a_\mu\partial_\rho e_\nu^{a+}-\partial_\kappa a_\nu\partial_\rho e_\mu^{a+})).$$

To find the deformed action we first calculate

$$\tilde{F}_{\mu\nu}^1=F_{\mu\nu}^1+\tfrac{1}{2}\theta^{\kappa\rho}(\partial_\mu a_{\nu\kappa\rho}-\partial_\nu a_{\mu\kappa\rho}-\partial_\kappa a_\mu\partial_\rho a_\nu+\partial_\kappa b_\mu\partial_\rho b_\nu+\tfrac{1}{2}(\partial_\kappa e_\mu^{a+}\partial_\rho e_\nu^{a-}-\partial_\kappa e_\nu^{a+}\partial_\rho e_\mu^{a-})$$

$$-\tfrac{1}{4}\partial_\kappa\omega_\mu^{ab}\partial_\rho\omega_\nu^{ab})+O(\theta^2)\equiv F_{\mu\nu}^1+\tfrac{1}{2}\theta^{\kappa\rho}F_{\mu\nu\kappa\rho}^1+O(\theta^2),$$

$$\tilde{F}^{ab}_{\mu\nu}=F^{ab}_{\mu\nu}+\tfrac{1}{2}\theta^{\kappa\rho}(\partial_\mu\omega^{ab}_{\nu\kappa\rho}-\partial_\mu\omega^{ab}_{\nu\kappa\rho}+\omega^{ac}_{\mu}\omega^{cb}_{\nu\kappa\rho}-\omega^{ac}_{\nu}\omega^{cb}_{\mu\kappa\rho}-\omega^{bc}_{\mu}\omega^{ca}_{\nu\kappa\rho}+\omega^{bc}_{\nu}\omega^{ca}_{\mu\kappa\rho}$$
$$+4(e^{a+}_{\mu}e^{a-}_{\nu\kappa\rho}-e^{a+}_{\nu}e^{a-}_{\mu\kappa\rho}-e^{a-}_{\mu}e^{a+}_{\nu\kappa\rho}+e^{a-}_{\nu}e^{a+}_{\mu\kappa\rho})-8i\epsilon_{abcd}(\partial_\kappa e^{c+}_{\mu}\partial_\rho e^{d-}_{\nu}-\partial_\kappa e^{c+}_{\nu}\partial_\rho e^{d-}_{\mu})$$
$$-2(\partial_\kappa a_\mu\partial_\rho\omega^{ab}_{\nu}-\partial_\kappa a_\nu\partial_\rho\omega^{ab}_{\mu})-i\epsilon_{abcd}(\partial_\kappa b_\mu\partial_\rho\omega^{cd}_{\nu}-\partial_\kappa b_\nu\partial_\rho\omega^{cd}_{\mu}))+O(\theta^2)$$
$$\equiv F^{ab}_{\mu\nu}+\tfrac{1}{2}\theta^{\kappa\rho}F^{ab}_{\mu\nu\kappa\rho}+O(\theta^2).$$

Notice that all the above expressions are real. The appearance of $i\epsilon_{abcd}$ is due to the convention $x^4=ix^0$ so that $i\epsilon_{1234}=\epsilon_{1230}=1$. Therefore the conformal gravity action to first order in θ is given by

$$I=i\int \mathrm{d}^4x\,\epsilon^{\mu\nu\lambda\sigma}(\epsilon_{abcd}F^{ab}_{\mu\nu}F^{cd}_{\lambda\sigma}+\theta^{\kappa\rho}(2e^{a+}_{\mu}e^{a-}_{\nu}F^{1}_{\lambda\sigma\kappa\rho}+\epsilon_{abcd}F^{ab}_{\mu\nu}F^{cd}_{\lambda\sigma\kappa\rho}))+O(\theta^2),$$

where we have dropped total derivative terms. The deformation to the Gauss–Bonnet action is obtained from the above expression by setting $e^{a-}_{\mu}=0$. It would be instructive to compare this action with the one obtained from the Born–Infeld effective action in String theory where the field $B_{\mu\nu}$ has a constant background.[8] One can also compare these results by following the results of Jackiw–Pi[26] by defining covariant coordinate transformations on noncommutative spaces. More importantly is to compare this result with the spectral action for a deformed spectral triple $(\tilde{\mathcal{A}},\tilde{H},\tilde{D})$ where $\tilde{\mathcal{A}}=l(\mathcal{A})$, l is the left twist operator.[27] The difficult part is to obtain the deformed operator $\tilde{D}$ and it is hoped that the above formulation will give some hints on how to find the appropriate Dirac operator.

To summarize, we have proposed a four-dimensional gravitational action valid for both commutative and noncommutative field theories. This action differs from the familiar gravitational action in that it allows for other vacua besides those of the metric theory. The noncommutativity is obtained by replacing ordinary products with star products. The action is gauge invariant and do not involve explicit use of the metric. Only conformal gravity or Gauss–Bonnet topological gravity could be generalized to the noncommutative case as the constraints imposed on the gauge field strengths should be self-consistent. For some of the vacuum solutions, one of the gauge fields is identified with the vierbein, and the theory becomes metric. It will be interesting to study how to generalize this proposal to higher dimensions. There are no fundamental obstacles to this approach in even dimensions. In odd dimensions, however, it is not possible to impose constraints in such a way as to preserve a smaller unitary group including the spin-connection generators of $\mathrm{SO}(2n+1)$. It appears that in odd dimensions the only gravitational actions which are generalizable to the noncommutative case are of the Chern–Simons type,[28,29] and therefore must be topological. Finally, one can study the supersymmetric version of the four-dimensional gravitational action by considering the graded Lie-algebra $\mathrm{U}(2,2|1)$.

The author would like to thank the Alexander von Humboldt Foundation for support through a research award.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

Cubic algebraic equations in gravity theory, parametrization with the Weierstrass function and nonarithmetic theory of algebraic equations

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(Received 2 October 2001; accepted 20 January 2003)

A cubic algebraic equation for the effective parametrizations of the standard gravitational Lagrangian has been obtained without applying any variational principle. It was suggested that such an equation may find application in gravity theory, brane, string and Rundall–Sundrum theories. The obtained algebraic equation was brought by means of a linear-fractional transformation to a parametrizable form, expressed through the elliptic Weierstrass function, which was proved to satisfy the standard parametrizable form, but with g_2 and g_3 functions of a complex variable instead of the definite complex numbers [known from the usual (arithmetic) theory of elliptic functions and curves]. The generally divergent (two) infinite sums of the inverse first and second powers of the poles in the complex plane were shown to be convergent in the investigated particular case. Some relations were found, which ensure the parametrization of the cubic equation in its general form with the Weierstrass function. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1560855]

I. INTRODUCTION

The synthesis of algebraic geometry and physics has been known for a long time, beginning from the chiral Potts model, the algebraic Bethe ansatz (for a review of these aspects see Ref. 1) and ending up with orbifold models of string compactification.[2] In the context of string theories, the application of algebraic curves, related to Fermat's theorem, has also been pointed out.[3]

Concerning gravitational physics, which is an inherent constituent of any string, brane or ADS theories, any applications of the theory of algebraic curves are almost absent. In this aspect perhaps one of the most serious attempts was undertaken in the recent paper by Kraniotis and Whitehouse.[4] Based on a suitably chosen metric of an inhomogeneous cosmological model and introducing a pair of complex variables, the authors have succeeded in obtaining a *nonlinear partial differential equation,* parametrized by the well-known *Weierstrass function* (for a classical introduction in the theory of elliptic and Weierstrass functions, see Refs. 5–7). This convenient representation enabled the authors to express important physical quantities such as the Hubble constant and the scale factor through the Weierstrass and the Jacobi theta functions. In fact, an analogy has been used with the motion of a body in the field of a central force, depending on the inverse powers of the radial distance r. Then the solution of the trajectory equation is expressed in terms of elliptic and Weierstrass functions.[8]

Some important conclusions immediately follow from the paper by Kraniotis and Whitehouse,[4] and they provide an impetus towards further investigations. The first two conclusions are correctly noted by the authors themselves: (1) Other cases may exist, when solutions of nonlinear equations of general relativity might be expressed in terms of Weierstrass or theta functions,[9] associated with Riemann surfaces. (2) The differential equations of general relativity in a much broader context might be related to the mathematical theory of *elliptic curves and modular forms* (for an introduction, see Refs. 10–12) and even to the famous Taniyama–Shimura conjec-

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ture, stating that every elliptic curve over the field of rational numbers is a modular one. For a short review of some of the recent developments in the *arithmetic theory of elliptic curves*, the interested reader may consult also Ref. 13.

In this article an essential algebraic ''feature'' of the gravitational Lagrangian will be proved, which is inherent in its structure, mostly in its partial derivatives. This ''*algebraically inherent structure*'' represents the third conclusion, which in a sense may be related to the problems, discussed in Ref. 4.

However, this algebraic feature will become evident under some special assumptions. While in standard gravitational theory it is usually assumed that the metric tensor has an inverse one, in the so called *theories of spaces with covariant and contravariant metrics (and affine connections)*[14] instead of an inverse metric tensor one may have another contravariant tensor $\overline{g}^{jk}$, satisfying the relation $g_{ij}\overline{g}^{jk}\equiv l_i^k\neq\delta_i^k$. But then, since l_i^k cannot be determined from any physical considerations and at the same time the important mathematical structure from a physical point of view is the gravitational Lagrangian, a natural question arises: *Is it possible that in such a theory with a more general assumption with respect to the contravariant metric tensor, the gravitational Lagrangian is the same (scalar density) as in the usual case, provided also that the usual connection and the Ricci tensor are also given? From a physical point of view, this is the central problem, treated in this article, and the answer, which is given, is affirmative*. Namely, it has been shown that if e_i are the components of the covariant basic vectors, and dX^j are the components of a contravariant vector field (which, however, **are not** contravariant basic vectors and therefore $e_i dX^k\equiv\overline{l}_i^k\neq\delta_i^k$), then **they satisfy a cubic algebraic equation**. Of course, if dX^i are to be found from this equation, then it can be shown that $\overline{g}^{jk}$ will also be known because of the relation $\overline{g}^{jk}=dX^j dX^k$.

The obtained *cubic algebraic equation* can be expressed in a very simple form, but unfortunately it is not easy at all to solve it. That is why a mathematical approach for dealing with such an equation has been developed, on which any further physical application will be based. The equation has been derived in two cases—when $d^2X^i\equiv 0$ and when $d^2X^i\neq 0$. As will be shown, the first assumption means that dX has *zero-vorticity components* (and nonzero divergency, however), and in physical considerations this restriction can be imposed. The second assumption would mean that dX has both *nonzero divergency and nonzero vorticity* components. From the mathematical theory of cubic equations, the investigation of the two cases will not be different, because in the second case only the algebraic variety from the first case (with dX^i) will be supplemented with the components d^2X^i. The algebraic equation may enable one to make a kind of classification (from an algebraic point of view) of the contravariant tensors, satisfying the same gravitational Lagrangian.

So far, the problem investigated here may seem to be of pure ''mathematical'' interest, but it may also have numerous physical applications. In supergravity theories, ADS/CFT, five-dimensional and brane theories,[15–17] one deals with an action, consisting of a gravitational part, added to a (for example) string action of the kind $S_{\text{str.}}\equiv -T/2\int d^2\xi\sqrt{-h}h^{\alpha\beta}\partial_\alpha X^\mu\partial_\beta X_\mu$, where X^μ are the string coordinates, $h^{\alpha\beta}$ is the world sheet metric tensor, T is the string tension and the partial derivatives ∂_α are taken with respect to the world sheet coordinates $\xi^\alpha=(\tau,\sigma)$. One can easily guess that the above described methodology can easily be applied to the string part of the action. More concretely, $h^{\alpha\beta}$ may be expressed as $h^{\alpha\beta}=d\xi^\alpha d\xi^\beta$, the gravitational metric tensor may be assumed to depend on the string coordinates and the derivatives of the string coordinates will be taken with respect to the world sheet coordinates ξ^α. Also, the partial derivatives in the gravitational part of the action may also be taken with respect to the coordinates ξ^α. As a result, taking the gravitational and the string part of the action together and without applying any variational principle, one would get the same kind of cubic algebraic equation as the one which will be proposed in this article. In a sense, this dependence of g_{ij} on the string coordinates is a sort of coupling between the gravitational part of the action and the string one, and the resulting cubic equation may be called ''*an algebraic equation for the effective parametrization of the total Lagrangian in terms of the string coordinates*.'' Provided that the gravitational Lagrangian depends also on the *first* and *second differentials* of the metric tensor, the first variation of the

Lagrangian can be regarded also as a cubic algebraic equation with respect to the differentials of the vector field.[18]

There is also another interesting problem, which is related to the current trends in ADS/CFT correspondence[19] and the WZW theory of strings on a curved background.[20,21] For example, in WZW theory it is not clear how to relate the two-dimensional string worldsheet symmetries to the global symmetries (global coordinates) of the three-dimensional ADS space–time, in terms of which the parametrization of the group element is presented. If one has the ADS metric (and the ADS hyperboloid equation), then usually some parametrization of the global ADS coordinates is performed (usually from the viewpoint of maximum simplicity and convenience), which satisfies the hyperboloid equation. The formalism, developed in this article on the base of cubic algebraic equations, gives a possibility to find some other parametrizations. For example, the (three-dimensional) ADS space–time has a boundary which can be found when one of the (global) coordinates tends to infinity (for example $r\rightarrow\infty$), and thus a two-dimensional space is obtained, which can be identified with the one, on which the world-sheet coordinates are defined. By ''identification'' one may mean that not the two-dimensional coordinates, but only the Ricci tensors and the Christoffel connections of the two space–times can be identified. Then, and as will further be shown in the general case, the obtained in this article cubic algebraic equation will give an opportunity to relate one of the differentials with the Weierstrass function. In such a way, one obtains a system of two equations in partial derivatives, from where the parametrizations can be found. In principle, $2+1$ dimensional gravity and the WZW model of strings on an ADS background are very convenient for application of the algebro-geometric approach. Another interesting moment in these theories is that very often one has to deal with the ADS metric, written in different coordinates (including the two-dimensional coordinates of the world-sheet), and it may be supposed that the transition from one system of coordinates to another can probably be given by a linear-fractional transformation, which will be invesigated in this article. From this algebraic point of view, it is interesting to investigate the coordinate transformations in Ref. 22 and in Ref. 23.

Now some basic facts about the mathematical theory of cubic hypersurfaces[24] will be mentioned, which puts the emphasis especially on the classification of points on the cubic hypersurface, minimal cubic surfaces, two-dimensional birational geometry and quasi-groups. But no concrete applications of cubic curves are given. In well-known monographs,[25] the general theory of affine and projective varieties and algebraic and projective plane curves is exposed, and some examples are considered, too, but the theory of cubic forms is restricted only with Pascal's theorem. A more comprehensive introduction to the algebraic theory of second- and third-rank curves, their normal forms, turning points (where the second derivatives of the curve's equation equal zero), rational transformations, etc. are given in the book by Walker.[26] Of particular relevence to the present research will be the theorem[26] that if $f(x,y)=0$ is a nondegenerate cubic curve, then by introducing an affine set of coordinates $x_1=x/z$, $y_1=y/z$ and choosing the turning point at (0,0,1), the curve can be brought to the form $y^2=g(x)$, where $g(x)$ is a third-rank polynomial with different roots. However, the situation is much more interesting in the complex plane, where one may define the lattice $\Lambda=\{m\omega_1+n\omega_2|m,n\in Z;\ \omega_1,\omega_2\in C,\mathrm{Im}\,\omega_1/\omega_2>0\}$. Let a mapping f: $C/\Lambda\rightarrow CP^2$ be factorized along the points of the lattice part of the complex plane into the two-dimensional complex projective space CP^2. If under this mapping the complex coordinates z are mapped as $z\rightarrow(\rho(z),\rho'(z),1)$ when $z\neq 0$ and $z\rightarrow(0,1,0)$ when $z=0$ [$\rho(z)$ is the *Weierstrass elliptic function*], then the mapping f maps the torus C/Λ into the following *affine curve* $y^2=4x^3-g_2x-g_3$, where g_2 and g_3 are complex numbers.[13] The important meaning of this statement is that by excluding the points on the lattice which may be mapped into one point of the torus (where the Weierstrass function has real values), the mapping $z\rightarrow(x,y)=(\rho(z),\rho'(z))$ parametrizes the cubic curve. The consequence from that is also essential since the solution of the resulting differential equation can be obtained in terms of elliptic functions.[5,13,27] The parametrization is inherently connected to basic notions from algebraic geometry such as divisors and the Riemann–Roch theorem,[28] which reveals the dimension of the vector space of meromorphic functions, having a pole of order at most n at the point $z=0$. In the present article,

a more general parametrization of a cubic curve is considered, when g_2 and g_3 are not complex numbers (the so called *Eisenstein series* $g_2=60\Sigma_{\omega\subset\Gamma}1/\omega^4=\Sigma_{n,m}1/(n+m\tau)^4$; $g_3=140\Sigma_{\omega\subset\Gamma}1/\omega^6=\Sigma_{n,m}1/(n+m\tau)^6$), but complex functions. *It has been proved that if the Weierstrass function parametrizes again the cubic curve, then the infinite sums (in pole number terms)* $\Sigma_{\omega\subset\Gamma}1/\omega^n$ *for* $n=1$ *and* $n=2$ *turn out to be finite (convergent) ones, in spite of the fact that in the general case they might be infinite ones (divergent)*. The explanation of this fact from the point of view of algebraic geometry remains an open problem, but it can be supposed that standard *arithmetical theory* of elliptic functions and algebraic equations is contained in some other, more general theory, which may be called *nonarithmetical theory*, and from this theory the standard parametrization should also follow. The considered case of parametrization of a cubic curve with coefficient functions of a complex variable, although performed in this article in a trivial algebraic manner, is the first step towards constructing such a theory. At least, a certain motivation from a physical point of view is evident for constructing such a theory.

The above-presented outlook on standard parametrization implied the use of affine coordinates, which unfortunately exclude from consideration the infinity point. But the infinity point cannot be ruled out not only from mathematical grounds, but also from physical considerations. For example, in the five-dimensional Randall–Sundrum model,[29,30] one has to assume a compactification into a four-dimensional universe from an infinite extra dimension, containing also the infinity point. From this point of view, the more convenient transformation, chosen in the present article, which brings the cubic curve into a parametrizable form, is the *linear-fractional transformation*. This transformation allows one to parametrize with the Weierstrass function the ratio of two of the parameters entering the linear-fractional transformation and, in this case, the parameters in this transformation represent complex functions. Of course, the other parameters remain unfixed, leaving the opportunity to determine them in an appropriate way. In a sense, from most general grounds the appearance of the Weierstrass function in the linear-fractional transformation might be expected, since, according to a theorem in the well-known monograph of Courant and Hurwitz,[31] an algebraic curve of the kind $w^2=a_0v^4+a_1v^3+a_2v^2+a_1v+a_4$ can be parametrized as $v=[a\rho(z)+b]/[c\rho(z)+d]=\varphi(z)$ and $w=\varphi'(z)$ by means of the transformations $v=(av_1+b)/(cv_1+d)$ and $w=w_1(ad-bc)/(cv_1+d)^2$. In the case $a_0=0$ (which is the present case of a third-rank polynomial), $\varphi(z)$ will be a linear function of $\rho(z)$.

In the present article, however, the situation is quite different, since the linear-fractional transformation is applied only with respect to one of the variables (v), and in order to get the standard parametrizable form $w^2=4v^3-g_2v-g_3$ (with g_2 and g_3-complex functions), an additional quadratic algebraic equation has to be satisfied. What is more interesting is that after the parametrization is performed, the linear-fractional transformation turns out to be of a more general kind $v=[A(z)\rho(z)+(b/c)+B(z).(d/dt)(\rho^2(z))]/[C(z)\rho'(z)+D(z)+d/c]$, where A,B,C,D are functions of z, and the expression for v represents a *rational transformation of the kind* $v(z)=P(z)/Q(z)$. Now from another point of view it can also be understood why it is justifiable to apply the rational transformation only with respect to v and not with respect to w. The reason is in a well-known theorem[13] from algebraic geometry that "*each nondegenerate cubic curve does not admit a rational parametrization*." Since each nondegenerate cubic curve can be brought to the form $w^2=v(v-1)(v-\lambda)$ $(\lambda\neq0,1)$, the essence of the above theorem is that this (algebraic) form *cannot* be satisfied by a rational parametrization of **both** $v=P(z)/Q(z)$ and $w=T(z)/R(z)$.

The present article is organized as follows:

Section II gives some basic formulas about the so called gravitational theory with contravariant and covariant metric tensors. In Sec. III the third-rank algebraic equation has been derived, starting from the standard gravitational Lagrangian. Also, the effective parametrization problem has been formulated in an algebraic language. In Sec. IV the general mathematical setup for parametrization of the cubic equation has been discussed, and some physical motivation for the application of the linear-fractional transformation from the point of view of Randall–Sundrum theory has been presented. Section V shows how the cubic algebraic equation transforms under the action of the linear-fractional transformation. Section VI shows how from the transformed cubic

equation one can get the standard parametrizable form of the cubic equation (with g_2 and g_3-complex numbers) and also the *quadratic algebraic equation* is derived, which has to be fulfilled if the parametrizable form holds. The approach is valid also when $g_2(z)$ and $g_3(z)$ are complex functions. In Sec. VII it was proved that the nonlinear and nonpolynomial transformation from the ''unbar'' to the ''bar'' variables is also invertible, thus giving the opportunity to write down two of the additionally imposed equations in terms of the new ''bar'' variables. In Sec. VIII the Loran decomposition has been performed for the functions on both sides of the algebraic equation $(d\rho/dz)^2=M(z)\rho^3+N(z)\rho^2+P(z)\rho+E(z)$, where $\rho(z)$ is the Weierstrass function and M,N,P,E are functions of the complex variable z. A system of three iterative (depending on n) algebraic equations has been obtained, representing a necessary (but not sufficient!) condition for parametrization of a cubic equation of a general form with the Weierstrass function. It is not occasional that the condition is called ''a necessary, but not sufficient one,'' because in principle more algebraic equations have to be solved in order to prove the existence of such a parametrization. In Sec. IX the possible parametrization of the more simplified cubic equation $[\rho'(z)]^2=4\rho^3-g_2(z)\rho-g_3(z)$ has been considered, and of course the main motivation for considering such a case is the close analogy with the well-known case, when g_2 and g_3 are complex numbers. By calculating the coefficients in the negative power Loran expansion and combining them, it has been proved that the sums $\Sigma\,1/\omega$ and $\Sigma\,1/\omega^2$ represent finite (convergent) quantities. The other equations for the other values of $m=-3,-1$ have been presented in Appendix A; those for values of $m=2k$ are in Appendix B and those for $m=2k+1$ and $m=-k$ are in Appendix C. The equations in these appendices in fact complete the proof that all the Loran coefficient functions can be uniquely expressed through a combination of the finite sums G_n. The calculations are purely technical, but they serve as a strict mathematical motivation and a proof of the new and basic qualitative fact that the Weierstrass function can parametrize the simplified form of the cubic equation with coefficient functions $g_2(z)$ and $g_3(z)$. This fact probably might represent one of the starting points in the creation of the so called *nonarithmetical theory of algebraic equations*. In a future publication it will be shown also that in the case of poles at infinity ($\omega\to\infty$) the convergence of the infinite sums $\Sigma\,1/\omega$ and $\Sigma\,1/\omega^2$ [when the sum $\Sigma\,1/\omega^n$ tends to the Riemann zeta function $\xi(n)$ Ref. 40] can be proved after applying the Tauber theorem.[41]

II. COVARIANT AND CONTRAVARIANT METRIC TENSOR

Usually in gravitational theory it is assumed that a local coordinate system can be defined so that to each metric tensor g_{ij} an inverse one g^{jk} can be defined,

$$g_{ij}g^{jk}\equiv\delta_i^k=\{0 \text{ if } i\neq k \text{ and } 1 \text{ if } i=k\}. \tag{1}$$

However, the notion of a reference frame can be defined in different ways in Ref. 32—coordinate, tetrad and monad. In the last case the contravariant vector field dx^i of an observer, moving along a space–time trajectory, represents a reference system. In such a case one may have instead of (1)

$$e_i dx^j\equiv f_i^j\neq\delta_i^j=S(e_i,dx^j). \tag{2}$$

In the context of the so called dual algebraic spaces in Ref. 33, $S(e_i,dx^j)$ is called a *contraction operator*. Assuming that an inverse operator of contraction f_j^i exists, it can easily be obtained, as in Ref. 14:

$$e^j\equiv f_i^j dx^i. \tag{3}$$

Therefore, the metric tensor field g can be decomposed with respect to the contravariant basic eigenvectors in the following way:

$$g\equiv g_{ij}(e^i\otimes e^j)\equiv g_{ij}f_k^i f_l^j dx^k dx^l(e_k\otimes e_l)\equiv(dx^k dx^l)(e_k\otimes e_l), \tag{4}$$

and the contravariant components $\tilde{g}^{ij}$ of the tensor field g are represented as a contraction of the two vector fields dx^i and dx^j:

$$\tilde{g}^{ij} \equiv dx^i dx^j. \tag{5}$$

It is important to realize that this definition of a contravariant tensor field is not related to any notion of infinitesimality. In order to understand this, consider a set of global coordinates X^μ, defined on the given manifold and depending also on some other (local) coordinates. Then the set of global coordinates, regarded as functions of the local ones, can be considered as a system of equations, defining some algebraic surface. Provided that the partial derivatives of the global coordinates with respect to the local ones are nonzero, *at each point of this surface* the corresponding *tangent space* can be determined, and the differentials of the global coordinates are defined on this tangent space. If one assumes that the global differentials are infinitesimally small, then either the (partial) derivatives of the global coordinates or the ''local'' differentials should be small. However, the parial derivatives cannot be small, because one considers arbitrary global and local coordinates on the manifold. Also, if the local differentials are assumed to be small, then they will not be allowed to take arbitrary values. But this will mean that a large variety of integral curves on the manifold should be excluded from consideration. This will be unacceptable since one would like to define integral curves through each point of the manifold and, moreover, it would contradict our initial assumption about the existence of a tangent space at each point of the surface (or manifold). Therefore, as a partial case, each of the local differentials should be allowed to take arbitrary numerical values and, of course, they may be equal also to an arbitrary function of the local coordinates.

It might be concluded, therefore, that since the partial derivatives and the local differentials cannot be infinitesimally small, then the global differentials cannot also be infinitesimally small.

Apart from the definition (5) of a contravariant tensor field, we have also the definition of a length interval in Riemannian geometry

$$ds^2 \equiv l^2(\overline{r}) \equiv g_{ij} dx^i dx^j. \tag{6}$$

If we would like to ''incorporate'' in this definition the standard definition of an inverse metric tensor as $g_{ij}g^{jk} \equiv \delta_i^k$, we can set up for the ordinary inverse metric tensor

$$g^{ij} \equiv \frac{1}{l^2} dx^i dx^j. \tag{7}$$

Therefore, in terms of the differentials, the ordinary inverse tensor g^{ij} can be represented in the same way as in (5), but divided by the length interval. However, usually the length interval is not known, so from a physical point of view the definition (7) is undesirable and this is the motivation to deal further with the definition (5) of a contravariant tensor field. In order to distinguish the ''newly'' defined tensor in (5), a ''tilda'' sign has been placed.

From (3) and (7) it follows

$$\left[\frac{1}{l^2} - g_{kl} f_i^k f_j^l\right] dx^i dx^j \equiv 0. \tag{8}$$

Clearly, the requirement for existence of an inverse contraction operator is equivalent to putting $l=1$, i.e., assuming that there is a unit length interval, which is again physically unacceptable, and it is more natural to assume that the length interval is varying. Let us assume that l^2 and f_k^i are known in advance. Then it can be investigated which is the algebraic variety of values of dx^i, satisfying this quadratic form. The main difficulty in this approach is that f_k^i cannot be determined from physical considerations. That is why the aim in the next section will be to derive an algebraic equation, in which known physical quantities will enter—the metric tensor g_{ij}, the Christoffel connection Γ_{ij}^k and the Ricci tensor R_{ij}.

III. CUBIC ALGEBRAIC EQUATION NOT FOLLOWING FROM A VARIATIONAL PRINCIPLE

Further in this article it shall be assumed that if X^i are some generalized coordinates, defined on an n-dimensional manifold with coordinates on it $(x^1,x^2,\ldots,x^n)$, then the differential dX^i is defined in the corresponding tangent space T_X of the generalized coordinates $X^i \equiv X^i(x^1,x^2,x^3,\ldots,x^n)$. Even if written with a small letter, it shall be understood that x^i represent generalized coordinates.

Our starting point for the derivation of the cubic equation will be the assumption that *in spite of the choice for the contravariant metric tensor, the gravitational Lagrangian* $L=-\sqrt{-g}R$ *should be the same, provided also that the Ricci tensor does not change under the definition of the contravariant metric tensor*. The meaning of this statement is the following.

Essentially, the gravitational Lagrangian will have two representations. The **first representation** is based on the standardly defined Christoffell connection Γ^l_{ik},

$$\Gamma^l_{ik} \equiv \tfrac{1}{2} g^{ls}(g_{ks,i}+g_{is,k}-g_{ik,s}), \tag{9}$$

and the Ricci tensor,

$$R_{ik}=\frac{\partial \Gamma^l_{ik}}{\partial x^l}-\frac{\partial \Gamma^l_{il}}{\partial x^k}+\Gamma^l_{ik}\Gamma^m_{lm}-\Gamma^m_{il}\Gamma^l_{km}. \tag{10}$$

The **second representation** of the gravitational Lagrangian will be based on the definition (5) of the contravariant metric tensor $\tilde{g}^{jk}=dx^j dx^k$. Therefore, the Christoffell connection and the Ricci tensor will be different from the previous ones and will be denoted respectively by $\tilde{\Gamma}^l_{ik}$ and $\tilde{R}_{ik}$:

$$\tilde{\Gamma}^l_{ik} \equiv \tfrac{1}{2}\tilde{g}^{ls}(g_{ks,i}+g_{is,k}-g_{ik,s}) = \tfrac{1}{2} dx^l dx^s g_{ks,i} + \tfrac{1}{2} dx^l dx^s g_{is,k} - \tfrac{1}{2} dx^l dg_{ik}, \tag{11}$$

$$\tilde{R}_{ik}=\frac{\partial \tilde{\Gamma}^l_{ik}}{\partial x^l}-\frac{\partial \tilde{\Gamma}^l_{il}}{\partial x^k}+\tilde{\Gamma}^l_{ik}\tilde{\Gamma}^m_{lm}-\tilde{\Gamma}^m_{il}\tilde{\Gamma}^l_{km}. \tag{12}$$

The gravitational Lagrangian in this **second representation** is

$$L_2 \equiv -\sqrt{-g}R = -\sqrt{-g}\tilde{g}^{ik}\tilde{R}_{ik} = -\sqrt{-g}dx^i dx^k\left(\frac{\partial \tilde{\Gamma}^l_{ik}}{\partial x^l}-\frac{\partial \tilde{\Gamma}^l_{il}}{\partial x^k}\right)-\sqrt{-g}dx^i dx^k(\tilde{\Gamma}^l_{ik}\tilde{\Gamma}^m_{lm}-\tilde{\Gamma}^m_{il}\tilde{\Gamma}^l_{km}). \tag{13}$$

Note that physical meaning of this Lagrangian will depend not only on the properties of the (covariant) metric tensor, but also on the first and the second differentials dx^l and d^2x^l. It should be mentioned also that the notion of a metric tensor, depending on generalized coordinates, understood in the sense of a hypersurface (an infinite-dimensional manifold of all spacelike hypersurfaces, embedded in a given Riemannian space–time), has been introduced a long time ago by Kuchar in Ref. 34. In such an approach, the description of the gravitational field essentially depends on the *tangential and normal deformations* of the embedded hypersurface. In our case, we do not restrict to spacelike hypersurfaces, but the notion of the differentials begins to play a self-consistent role, similar to the dynamics and the deformations of the hypersurface in Kuchar's approach. Yet, the standard gravitational physics with the usual inverse metric tensor is contained in the approach proposed in this article, because one can identify the components of the usually known inverse metric tensor with the components of the contravariant metric tensor, defined in terms of the differentials. Thus one can obtain a *system of first-order nonlinear differential equations in partial derivatives*. The solution of this system may enable one to choose such global (generalized) coordinates, in terms of which the usual inverse tensor will be equivalent to the contravariant one in terms of the differentials.

Let us now use expressions (5) for the contravariant metric tensor $\tilde{g}^{ij}$ and (11) for the Christoffel connection $\tilde{\Gamma}^k_{ij}$ in order to rewrite the gravitational Lagrangian in the second representation. The first two terms in (13) can be calculated to be

$$-\sqrt{-g}dx^i dx^k\left(\frac{\partial\tilde{\Gamma}^l_{ik}}{\partial x^l}-\frac{\partial\tilde{\Gamma}^l_{il}}{\partial x^k}\right)=\sqrt{-g}dx^i dx^k dx^l\left\{g_{is,l}\frac{\partial(dx^s)}{\partial x^k}-\frac{1}{2}pg_{ik,l}+\frac{1}{2}g_{il,s}\frac{\partial(dx^s)}{\partial x^k}\right\}$$
$$=-\sqrt{-g}dx^i dx^l\{p\Gamma^r_{il}g_{kr}dx^k-\Gamma^r_{ik}g_{lr}d^2x^k-\Gamma^r_{l(i}g_{k)r}d^2x^k\}, \tag{14}$$

where p is the scalar quantity

$$p\equiv\mathrm{div}(dx)\equiv\frac{\partial(dx^l)}{\partial x^l}, \tag{15}$$

which "measures" the divergency of the vector field dx. It will be more interesting to calculate the contribution of the second term in (12),

$$-\sqrt{-g}dx^i dx^k(\tilde{\Gamma}^l_{ik}\tilde{\Gamma}^m_{lm}-\tilde{\Gamma}^m_{il}\tilde{\Gamma}^l_{km})=-\tfrac{1}{2}\sqrt{-g}dx^i dx^k dx^l dx^m(-dg_{lm}dx^s g_{ks,i}-dg_{ik}dx^r g_{mr,l}$$
$$+dg_{il}dx^r g_{mr,k}+dg_{km}dx^s g_{ls,i})$$
$$-\sqrt{-g}dx^i dx^k dx^l dx^m dx^s dx^r[g_{ks,i}g_{mr,l}-g_{ls,i}g_{mr,k}]=0, \tag{16}$$

and the *first differential* dg_{ij} is represented as $dg_{ij}\equiv(\partial g_{ij}/\partial x^s)\,dx^s\equiv\Gamma^r_{s(i}g_{j)r}dx^s$ and Γ^r_{si} is the standard Christoffell connection. Therefore, the second two terms in (13) give no contribution to the gravitational Lagrangian. This is not surprising, since the "factorization" of the contravariant metric tensor as $dx^i dx^j$ introduces an additional "symmetry," due to which all the terms in (16) cancel. That is why the **second representation** of the gravitational Lagrangian will be given only by the first two terms $-\sqrt{-g}dx^i dx^k(\partial\tilde{\Gamma}^l_{ik}/\partial x^l-\partial\tilde{\Gamma}^l_{il}/\partial x^k)$ in expression (13).

Concerning the **first representation** of the gravitational Lagrangian, it was based on the standard Christoffell connection Γ^k_{ij}, the Ricci tensor R_{ik} and the usual inverse metric tensor g^{ij}. The basic assumption at the beginning concerned the gravitational Lagrangian and the Ricci tensor, which means that together with the inverse metric tensor g^{ij}, **another contravariant tensor** $\tilde{g}^{ij}=dx^i dx^j$ exists, which enters the expression for the **first representation** of the gravitational Lagrangian

$$L_1=-\sqrt{-g}\tilde{g}^{ik}R_{ik}=-\sqrt{-g}dx^i dx^k R_{ik}. \tag{17}$$

Comparing this representation with the **second** one, given by expression (13),

$$L_2=-\sqrt{-g}\tilde{g}^{il}\tilde{R}_{il}=-\sqrt{-g}dx^i dx^l\{p\Gamma^r_{il}g_{kr}dx^k-\Gamma^r_{ik}g_{lr}d^2x^k-\Gamma^r_{l(i}g_{k)r}d^2x^k\}, \tag{18}$$

and remembering the initial assumption, acccording to which the Lagrangian should be **one and the same in both the representations (i.e.,** $L_1=L_2$**)**, one arrives at the following algebraic equation with respect to the first differential dx^k and the second differential d^2x^k:

$$dx^i dx^l(p\Gamma^r_{il}g_{kr}dx^k-\Gamma^r_{ik}g_{lr}d^2x^k-\Gamma^r_{l(i}g_{k)r}d^2x^k)-dx^i dx^l R_{il}=0. \tag{19}$$

In the limit $d^2x_k=0$ this equation assumes the form of a **manifestly cubic with respect to** dx^i **algebraic equation**

$$dx^i dx^j dx^k p\Gamma^r_{j(i}g_{k)r}-R_{ij}dx^i dx^j=0. \tag{20}$$

Equation (20) is the basic equation, which shall be investigated further in this article. Most importantly, it is manifestly cubic in the differentials dx^i. Due to this reason, one qualitative argument can be given in favor of such a Lagrangian. In 1988, Witten derived the Lagrangian for $2+1$-dimensional gravity in Ref. 35, which is also manifestly cubic in the chosen gauge variables A_μ. The Lagrangian was obtained under the assumption that there is an isomorphism between an abstractly introduced (d-dimensional) vector bundle with a structure group $\mathrm{SO}(d-1,d)$ and the tangent bundle of the given manifold, on which the metric is the induced one from the metric on the vector bundle. Besides, the verbein was assumed to be invertible, but as Witten remarks "permitting the verbein to not be invertible seems like a minor change." In the present case, we do not have at all any symmetry on the tangent bundle, nor is anything supposed about the dimensionality of space–time or even about the existence of the usual inverse tensor, but yet the Lagrangian exibits the same cubic structure. Therefore, it may be concluded that the cubic structure of Chern–Simons theory[35] is inherent in the structure of the gravitational Lagrangian itself, and not in the additional assumptions in Ref. 35, which affect the choice of the gauge variables. In view of this, it might be interesting to investigate whether there is a transition from the Lagrangian in our case to the Lagrangian for $2+1$-dimensional gravity, presented in Ref. 35.

Of course, one might slightly modify the basic assumption, concerning the first representation of the gravitational Lagrangian. For example, instead of assuming that the Ricci tensor will be the same in both representations, one might instead assume that the **Ricci tensor** should not change. In such a case again in the limit $d^2x^k=0$ the cubic algebraic equation will be in a form without the quadratic in dx^i term,

$$dx^i dx^j dx^k p\Gamma^r_{j(i}g_{k)r}-R=0. \tag{21}$$

One can write down also the vacuum Einstein equations when the contravariant tensor is defined as $\tilde{g}^{ij}=dx^i dx^j$:

$$\begin{aligned}0=\tilde{R}_{ij}-\tfrac{1}{2}g_{ij}\tilde{R}&=\tilde{R}_{ij}-\tfrac{1}{2}g_{ij}dx^m dx^n\tilde{R}_{mn}\\ &=-\tfrac{1}{2}pg_{ij}\Gamma^r_{mn}g_{kr}dx^k dx^m dx^n+\tfrac{1}{2}g_{ij}(\Gamma^r_{km}g_{nr}+\Gamma^r_{n(m}g_{k)r})d^2x^k dx^m dx^n\\ &\quad+p\Gamma^r_{ij}g_{kr}dx^k-(\Gamma^r_{ik}g_{jr}+\Gamma^r_{j(i}g_{k)r})d^2x^k.\end{aligned} \tag{22}$$

Note the following subtle moment: since we have an expression equal to zero, this time **it is not necessary** to assume that the above algebraic equation is valid under the assumption that the Ricci tensor does not change. Therefore, Eq. (22) provides the interesting possibility for classification of all solutions of the vacuum Einsteins equations with a given metric tensor g_{ij} and unknown contravariant tensor $\tilde{g}^{ij}=dx^i dx^j$. In spite of the presence of the second differentials d^2x^k, Eq. (22) can be treated on an equal footing as an algebraic equation simply by "extending" the algebraic variety for the $\{dx^k\}$ variables with the new variable $dy^k=d^2x^k$. However, if **additionally** it is assumed that the Ricci tensor does not change under the definition of the contravariant tensor (i.e., $\tilde{R}_{ij}=R_{ij}$), then one has

$$(\Gamma^r_{ik}g_{jr}+\Gamma^r_{j(i}g_{k)r})d^2x^k=p\Gamma^r_{ij}g_{kr}dx^k-R_{ij}, \tag{23}$$

and consequently all the terms with d^2x^k in the Einstein vacuum equations (22) drop out and the algebraic equation becomes a cubic one with respect to the variables dx^k only. The above analyses have the purpose to demonstrate that depending on the initial assumptions about the Ricci tensor or scalar curvature, the structure of the algebraic equation also changes.

In an algebraic language,[25,36,37] the investigated problem can be formulated in the following way:

Proposition 1: Let the differentials $dx^i(i=1,\ldots,n;n$ is the space–time dimension) represent elements of an algebraic variety $\overline{X}=(dx^1,dx^2\ldots,dx^n)$. For different metric tensors (and therefore different connections Γ^k_{ij} and Riemannian tensors R_{ik}), a set of polynomials (cubic algebraic

equations) $F(\overline{X})\equiv 0$ *may be obtained, which are defined on the algebraic variety* $\overline{X}$ *and belong to the ring* $R[dx^1,dx^2,\ldots,dx^n]$ *of all third-rank polynomials. Then finding all the possible parametrizations of some introduced generalized coordinates* $X^i(x^1,x^2,x^3,\ldots,x^n)$ *is equivalent to the following. (1) Finding all the elements* dX^i *of the algebraic variety* $\overline{X}$*, satisfying the equation* $F(\overline{X})\equiv 0$*. These elements will be represented in the following way:*

$$dx^i=\Phi^i(x^1,\ldots,x^n,g_{ij}(x^1,x^2,\ldots,x^n),\Gamma^k_{ij}(x^1,x^2,\ldots,x^n),R_{ij}(x^1,x^2,..,x^n)). \tag{24}$$

(2) Finding all the solutions of the above system of partial differential equations.

In the present case, the algebraic equation is obtained *before performing* the variation of the Lagrangian, unlike that considered in Ref. 18, when again a cubic algebraic equation had been obtained *after performing* a variation.

Let us comment briefly on the important from a physical point of view assumption $d^2x^i\equiv 0$, under which the cubic equation (20) was derived. Suppose that for the set of generalized coordinates $X^i\equiv X^i(x^1,x^2,\ldots,x^n)$ one has

$$dX\equiv a_i dx^i, \tag{25}$$

and let us assume that the Poincare theorem is fulfilled in respect to dx^i, i.e., $d^2x^i=0$. Then

$$d^2X=da_i dx^i+a_i d^2x^i=\frac{\partial a_i}{\partial x^j}dx^j\wedge dx^i=\left(\frac{\partial a_i}{\partial x^j}-\frac{\partial a_j}{\partial x^i}\right)dx^i dx^j. \tag{26}$$

Clearly, $d^2X=0$ only in the following two cases: (1) $a_i=\text{const}$, i.e., dX^i is a full differential, and

$$(2)\quad (rota)_{ij}\equiv \partial a_i/\partial xj-\partial a_j/\partial xi\equiv 0.$$

The last means that if dx^i are considered to be basic eigenvectors, then dX^i have *zero-vorticity components*. Throughout the whole article dX^i shall be considered as a vector field components in the tangent space T_X.

Note also that the algebraic equation (19) with first and second differentials dx^i and d^2x^i takes into account *two important physical characteristics of the vector field* dx^i*—the divergency p and the vorticity (through the term* d^2x^i*)*. It might be required that these characteristics vanish, i.e., $p=d^2x^i=0$. In such a case one is left only with the equation

$$R_{ik}dx^i dx^k\equiv 0. \tag{27}$$

If additionally the requirement for the existence of the (usual) inverse metric tensor is imposed, then the intersection variety of the quadratic form (27) with the quadratic forms (one when $\delta^j_i=0$ and the other when $\delta^i_i=1$)

$$g_{ik}dx^k dx^j\equiv\delta^j_i \tag{28}$$

has to be found. From the two last equations one easily obtains

$$(R_{ik}-\tfrac{1}{2}g_{ik}R)dx^k dx^j\equiv-\tfrac{1}{2}R\,\delta^j_i, \tag{29}$$

in which the left-hand side is identically zero for every dx^i in view of the Einstein equations $R_{ik}-\frac{1}{2}g_{ik}R\equiv 0$, but the right-hand side is zero only for $i\neq j$, but not also when $i=j$. Therefore, the Einstein equations are obtained only in one case and not in the other case. In fact, it should not be surprising that the Einstein equations cannot be obtained for both the cases $i\neq j$ and $i=j$. One should remember that the usual variational procedure in general relativity takes into account also the variation of the volume factor $\sqrt{-g}$, while in our purely algebraic treatment and without any variation this volume factor was not subjected to any changes at all. Moreover, it is one standard procedure to perform the variational procedure with the usual gravitational Lagrangian and the

inverse metric tensor (when the Einstein equations are obtained) and it is quite a different procedure to start from the other representation of the gravitational Lagrangian [where the variables to be variated are g_{ij}, Γ^k_{ij} (or $g_{ij,k}$) and dx^i and d^2x^i] and afterwards to impose the requirement for identification of the contravariant metric tensor with the inverse one in the form of another additional equation. So one should not even hope to obtain anything similar to the Einstein equations. However, as already shown, if one has the Einstein equations, one may still ask the question are they satisfied under the new definition of the contravariant tensor.

IV. PARAMETRIZATION OF THE CUBIC ALGEBRAIC EQUATION (20)—A GENERAL MATHEMATICAL SETUP

The aim of this section will be to provide some basic mathematical knowledge about parametrization of a cubic algebraic equation with the Weierstrass function. Also, some differences of the approach applied in this article from the standard one will be outlined.

In order to parametrize the obtained cubic algebraic equation (20), written in its most general form, one has to bring it to the so called parametrizable form, which in terms of the two variables $d\tilde{x}^4$ and $d\tilde{x}^5$ should be written as

$$(d\tilde{x}^5)^2 \equiv 4(d\tilde{x}^4)^3 - g_2(d\tilde{x}^4) - g_3, \tag{30}$$

where g_2 and g_3 are the complex numbers $g_2 = 60G_4 = 60\Sigma_\omega 1/\omega^4$ and $g_3 = 140G_6 = \Sigma_\omega 1/\omega^6$. Note that the variables in (30) are different from the original variables dx^4 and dx^5, since Eq. (30) has been obtained after applying the *linear-fractional transformation*

$$dx^5 \equiv \frac{a\widetilde{dx}^5 + b}{c\widetilde{dx}^5 + d}, \tag{31}$$

where a, b, c and d will be chosen to be functions of the complex variable z. This complex variable appears as a result of the parametrization of the algebraic equation with the *Weierstrass function*, which is the following complex meromorphic function:

$$\rho(z) \equiv \frac{1}{z^2} + \sum_{\varpi} \left[\frac{1}{(z-\varpi)^2} - \frac{1}{\varpi^2} \right]. \tag{32}$$

By parametrization it should be understood that if the variables $d\tilde{x}^4$ and $d\tilde{x}^5$ in Eq. (30) are identified with the Weierstrass function $\rho(z)$ and it derivative $\rho'(z)$, respectively,

$$d\tilde{x}^4 \equiv \rho(z), \quad d\tilde{x}^5 \equiv \rho'(z), \tag{33}$$

then these two functions satisfy the algebraic equation,[13] i.e.,

$$(\rho'(z))^2 \equiv 4(\rho(z))^3 - g_2(\rho(z)) - g_3. \tag{34}$$

Therefore, in terms of the algebro-geometric language, the Weierstrass function and its derivative should be considered as *uniformization functions* of the algebraic equation (30) and the complex variables z, on which they depend—a "*uniformization variable*." The properties of z are determined by the properties of the **elliptic Weierstrass function**. By definition a function f is an **elliptic**[13] if it is a **meromorphic** and a **double-periodic** one, which means the following.

(1) In a finite area of the complex plane there are no other points different from poles.

(2) For every number m and n there exist periods ω_1 and ω_2 of a two-dimensional lattice on the complex plane so that the values of the function f at the points z and $z + m\omega_1 + n\omega_2$ can be identified,

$$f(z) = f(z + m\omega_1 + n\omega_2), \tag{35}$$

where also $\mathrm{Im}(\omega_1/\omega_2)>0$ and $\omega=m\omega_1+n\omega_2$ is called the period of the lattice, based on the two elementary periods ω_1 and ω_2. The inequality means that the rotation from ω_1 to ω_2 should be performed in a clockwise direction. Therefore, the summation in formulas (32) for the Weierstrass function should be performed over all non-null elements of the two-dimensional lattice

$$\varpi\subset\Lambda=\{(m\varpi_1+n\varpi_2)|m,n\subset Z(\text{integer numbers}),\ \varpi_1,\varpi_2\subset C,\mathrm{Im}>0\}.$$

If the identification of the points on the lattice is performed along one direction (or axis), and moreover $m=1$, then this has the effect of rolling up the complex plane into a cylinder. If, further, an identification is performed along the points of the other direction (axis) and $\omega_2=\tau$, then the cylinder is rolled up to a torus.

The identification of the points on the complex plane in the definition of an elliptic function is similar to the identification of the complex coordinates of a cosmological space–time, which is frequently appplied in models of string null orbifold singularities and also the Randall–Sundrum (R-S) model.[29,30] The basic idea of the R-S model is that the process of compactification of the five-dimensional universe to our present four-dimensional universe is related to the existence of a *large extra dimension*. In the original R-S scenario the metric was chosen to be

$$ds^2=e^{-2kr_cr_5}\eta^{\mu\nu}dx^\mu dx^\nu+r_c^2dx_5^2, \tag{36}$$

where r_c is a compactification radius, $\eta^{\mu\nu}$ is the ordinary Minkowski metric, $x_5\subset[0,\pi]$ is a periodic coordinate, $\mu\nu$ are four-dimensional indices and k is a scale of order of the Planck scale. Instead of the coordinate x_5, one may chose for example a fifth coordinate $X_5=kr_cx_5$, which in view of the largeness of the scale factor k may be assumed to range to infinity. *But the infinity point, from a purely mathematical point of view, may be treated on an equal footing with all other points in the framework of projective geometry.*[7,26,38,39] In the present case the infinity point shall be realized at $dX^5\equiv-d/c$ after performing the *linear-fractional transformation*

$$dX^5\equiv\frac{ad\tilde{X}^5+b}{cd\tilde{X}^5+d}. \tag{37}$$

Also, the remaining four-dimensional space–time with coordinates (x^1,x^2,x^3,x^4) may be complexified in the following way:

$$z_1=x_1+ix_2;\quad z_2=x_3+ix_4. \tag{38}$$

The identification of points both in the definition of an elliptic function and in one of the space–time coordinates of the investigated cosmological space–time prompts the following question: is the complex (uniformization) variable z in the Weierstrass function an independent one or it is inherently related to the space–time coordinates? Further, in this article it will be shown that the parametrization will be performed with respect to the ratios a/c of the complex functions in the linear-fractional transformation (37) and also the differential $d\tilde{X}^5$, i.e.,

$$\frac{a}{c}\equiv\rho(z);\quad d\tilde{X}^5\equiv\rho'(z). \tag{39}$$

Since the variable z in the Weierstrass function is double periodic, it could be identified only with the complex periodic variable Z_3, obtained after the space–time complexification and containing X^5 as a real part. Taking into account (39) and assuming also that the complex functions b and d also depend on Z_3, one obtains the following differential equation for Z_3 from the expression (37) for the linear-fractional transformation (provided that it is the same for the complex differential dZ_3):

$$dZ_3=\frac{\rho(Z_3)\rho'(Z_3)+b/c}{\rho(Z_3)+d/c}\equiv F(Z_3). \tag{40}$$

If we assume that Z_3 depends on some (real or complex) variable λ and also that the ratios b/c and d/c are known, then after solving the differential equation (40)

$$\lambda=\int\frac{dZ_3}{F(Z_3)}+\text{const}=f(Z_3)+\text{const}. \tag{41}$$

Therefore, if λ represents another complex variable v, then all possible complex coordinate transformations $Z_3\rightarrow\lambda=v=f(Z_3)$ will be fixed (up to a numerical constant) by the requirement for identification of the complex variable in the Weierstrass function with one of the variables, describing the cosmological space–time. However, in this article the more general case of an independent variable z will be investigated.

Since further in the text the parametrization (33) will be repeatedly used, it is instructive to give just an idea of how in classical textbooks it is proved that the parametrization (33) satisfies Eq. (34). Let us take, for example, the proof, given in Ref. 13, where the basic idea is to compare the Loran expansions for the nonpositive degrees of z for the function $[\rho'(z)]^2$ and for the polynomial $a\rho^3(z)+b\rho^2(z)+c\rho(z)+d$, where a, b, c and d are complex numbers. If the corresponding coefficients in the Loran expansion of these two expressions are equal, this would mean that the expressions themselves are equal. Also, it should be accounted that the function $[\rho'(z)]^2$ is an *even one*, and consequently only the even (nonpositive) powers of z in the Loran decomposition of the two expressions should be taken into account. After performing the Loran decomposition, it becomes evident that equality of the two expressions is possible only if $a=4$, $b=0$, $c=-60G_4$, and $d=-140G_6$. Since these coefficients give exactly the algebraic equation (34), it follows that the Weierstrass function and its derivative (33) satisfy Eq. (34).

It is important to stress that the ''tilda'' differentials $d\tilde{x}^4$ and $d\tilde{x}^5$, which are related through the algebraic relation (30) and the parametrization (33) with the Weierstrass function, do not result in any dependence between the original differentials dx^4 and dx^5, which should remain independent since they are related to the independent coordinates in the gravitational Lagrangian. The reason for this independence between the tilda and the nontilda differentials is that the linear-fractional transformation (31), which relates $d\tilde{x}^5$ and dx^5, introduces an additional arbitrariness in the nontilda differentials due to the arbitrary complex functions a, b, c and d.

In the present case, however, there are some specific facts about the parametrization of the obtained cubic equation. After performing the transformation (31) with the purpose of choosing a, b, c and d to eliminate the highest (third) power of $\widetilde{dx}^5$, the obtained equation will be like Eq. (34), but with g_2 and g_3 functions and not complex numbers. On the other hand, the standard parametrization (33) with the Weierstrass function and its derivatives is valid *only* for g_2 and g_3 complex numbers. So basically there are two approaches to this problem. The first one is to assume that the obtained coefficient functions should equal the complex numbers g_2 and g_3. Then the standard parametrization is applied but there are additional equations that should be satisfied. This approach is worked out in Secs. V–VII. The second approach will be developed in Secs. VIII and IX and it is based again on the parametrizable form of the cubic algebraic equation but this time a Loran decomposition of the coefficient functions $g_2(z)$ and $g_3(z)$ is performed and subsequently the obtained system of linear equations is solved with respect to the coefficients of the Loran decomposition.

V. TRANSFORMED CUBIC EQUATION WITH THE HELP OF THE LINEAR-FRACTIONAL TRANSFORMATION

In order to derive this equation, all the terms with dx^5 in Eq. (20) shall be singled out and it can be written in the following way:

$$A(dx^5)^3+B(dx^5)^2+C(dx^5)+G^{(4)}(dx^4,\ldots,dx^1,g_{ij},\Gamma^k_{ij},R_{ik})\equiv 0, \tag{42}$$

where A, B and C are the following functions, depending on g_{ij}, Γ^k_{ij}, R_{ij} and the differentials dx^α, dx^β; the indices $\alpha,\beta=1,2,3,4;r=1,2,\ldots,5$.

$$A\equiv 2p\Gamma^r_{55}g_{5r}, \tag{43}$$

$$B\equiv 6p\Gamma^r_{\alpha 5}g_{5r}dx^\alpha, \tag{44}$$

and

$$C\equiv -2R_{\alpha 5}dx^\alpha+2p(2\Gamma^r_{\alpha\beta}g_{5r}+\Gamma^r_{5\alpha}g_{\beta r})dx^\alpha dx^\beta. \tag{45}$$

The function $G^{(4)}(\ldots)$ is of the following form:

$$G^{(4)}(dx^4,\ldots,dx^1,g_{ij},\Gamma^k_{ij},R_{ik})\equiv -R_{\alpha\beta}dx^\alpha dx^\beta+pdx^\gamma dx^\alpha dx^\beta\Gamma^r_{\gamma(\alpha}g_{\beta)r}. \tag{46}$$

In (46) the indice $\gamma=1,2,3,4$ and (α,β) means symmetrization with respect to the two indices. Further, after performing the linear-fractional transformation (31), one easily obtains the new cubic algebraic equation, written in terms of the new variables $\widetilde{dx}^5$:

$$\begin{aligned}(G^{(4)}c^3+aQ)(\widetilde{dx}^5)^3+(bQ+aT+3c^2dG^{(4)})(\widetilde{dx}^5)^2+(aS+bT+3cd^2G^{(4)})(\widetilde{dx}^5)\\ +(bS+G^{(4)}d^3)\equiv 0,\end{aligned} \tag{47}$$

where Q,T,S denote the following expressions:

$$Q\equiv Aa^2+Cc^2+Bac+2cdC, \tag{48}$$

$$T\equiv 2Aab+Bbc+Bad+2cdC, \tag{49}$$

$$S\equiv Ab^2+Bbd+Cd^2. \tag{50}$$

In fact, the linear-fractional transformation is performed with the purpose of setting up to zero the expression before $(\widetilde{dx}^5)^3$, from where $G^{(4)}$ is expressed as

$$G^{(4)}=-\frac{aQ}{c^3}. \tag{51}$$

This equation is the **first** additional equation, which is imposed in order to receive the parametrizable form of the cubic equation. Let us write down in more detail Eq. (51), in order to understand its meaning. Making use of the expressions for $G^{(4)}$ and Q, it can be written in the form again of a **cubic algebraic equation** with respect to the remaining four differentials

$$p\Gamma^r_{\gamma(\alpha}g_{\beta)r}dx^\gamma dx^\alpha dx^\beta+K^{(1)}_{\alpha\beta}dx^\alpha dx^\beta+K^{(2)}_\alpha dx^\alpha+2p\left(\frac{a}{c}\right)^3\Gamma^r_{55}g_{5r}=0, \tag{52}$$

where $K^{(1)}_{\alpha\beta}$ and $K^{(2)}_\alpha$ are the corresponding quantities

$$K^{(1)}_{\alpha\beta}\equiv -R_{\alpha\beta}+2p\frac{a}{c}\left(1+2\frac{d}{c}\right)(2\Gamma^r_{\alpha\beta}g_{5r}+\Gamma^r_{5\alpha}g_{\beta r}) \tag{53}$$

and

$$K^{(2)}_\alpha\equiv 2\frac{a}{c}\left[3p\frac{a}{c}\Gamma^r_{\alpha 5}g_{5r}-\left(1+2\frac{d}{c}\right)R_{\alpha 5}\right]. \tag{54}$$

The indices $\alpha,\beta,\gamma=1,2,3,4$ (but $r=1,2,\ldots,5$) and (α,β) mean symmetrization with respect to the two indices. In other words, the imposed (''by hand'') Eq. (51) *simply fixes the cubic algebraic equation with respect to the remaining four differentials, if one would like to parametrize the differential of the fifth coordinate with the Weierstrass function. No ratios* a/c and d/c are to be determined from this equation—later on from the equation with respect to the fifth coordinate they will be determined.

Using expression (51), the functions standing before $(\widetilde{dx}^5)^2$, $\widetilde{dx}^5$ in (47) and also the free term in the same equation can be written in a form of an algebraic expression with respect to a/c, b/c and b/d:

$$bQ+aT+3c^2dG^{(4)}=d^3\left\{-3A\frac{a}{c}\left(\frac{a}{d}\right)^2+C\frac{b}{d}\left(\frac{c}{d}\right)^2+2C\frac{b}{d}\frac{c}{d}-6C\frac{a}{d}+3A\frac{b}{d}\left(\frac{a}{d}\right)^2+B\frac{a}{d}\frac{b}{d}\frac{c}{d}-2B\left(\frac{a}{d}\right)^2-C\frac{a}{d}\frac{c}{d}\right\}, \tag{55}$$

$$aS+bT+3cd^2G^{(4)}=d^3\left\{-3A\left(\frac{a}{c}\right)^2\frac{a}{d}+B\frac{c}{d}\left(\frac{b}{d}\right)^2+2C\frac{c}{d}\frac{b}{d}-3B\frac{a}{c}\frac{a}{d}-6C\frac{a}{c}+2B\frac{a}{d}\frac{b}{d}+3A\frac{a}{d}\left(\frac{b}{d}\right)^2-C\frac{a}{d}\right\}, \tag{56}$$

and

$$bS+G^{(4)}d^3=d^3\left\{-A\left(\frac{a}{c}\right)^3+A\left(\frac{b}{d}\right)^3+B\left(\frac{b}{d}\right)^2-B\left(\frac{a}{c}\right)^2+C\frac{b}{d}-C\frac{a}{c}-2C\frac{a}{c}\frac{d}{c}\right\}. \tag{57}$$

Let us now introduce the notations

$$\frac{a}{c}\equiv m,\quad \widetilde{dx}^5\equiv n. \tag{58}$$

Equations (55)–(57) shall be rewritten in such a way so that the terms with powers of m will be singled out. The rest of the terms will be denoted by $\overline{F}$, $\overline{M}$ and $\overline{N}$ and they will contain powers of c/d and b/d only. The transformed equations (55)–(57), if substituted back in Eq. (47), allow one to write the equation in the following form:

$$\begin{aligned}&-3A\left(\frac{c}{d}\right)^2m^3n^2-3A\left(\frac{c}{d}\right)m^3n+\left[3A\left(\frac{c}{d}\right)^2\frac{b}{d}-2B\left(\frac{c}{d}\right)^2\right]m^2n^2-3B\frac{c}{d}m^2n\\&\quad+\left[-6C\frac{c}{d}+B\frac{b}{d}\left(\frac{c}{d}\right)^2-C\left(\frac{c}{d}\right)^2\right]mn^2+\left[-6C+2B\frac{c}{d}\frac{b}{d}+3A\frac{c}{d}\left(\frac{b}{d}\right)^2-C\frac{c}{d}\right]mn+\overline{F}n^2+\overline{N}n\\&\quad+\left[\overline{M}-Am^3-Bm^2-Cm-2\frac{d}{c}Cm\right]\equiv 0.\end{aligned} \tag{59}$$

The terms $\overline{F}$, $\overline{M}$ and $\overline{N}$ have the following forms:

$$\overline{F}\equiv C\frac{b}{d}\left(\frac{c}{d}\right)^2+2C\frac{b}{d}\frac{c}{d}, \tag{60}$$

$$\overline{M}=A\left(\frac{b}{d}\right)^3+B\left(\frac{b}{d}\right)^2+C\frac{b}{d}, \tag{61}$$

$$\overline{N}=B\frac{c}{d}\left(\frac{b}{d}\right)^2+2C\frac{c}{d}\frac{b}{d}, \tag{62}$$

In other words, we have transformed the original third-rank algebraic equation of five variables dx^1,dx^2,dx^3,dx^4,dx^5 into an algebraic equation of two variables only (m and n), but with a higher rank (in the case it is five).

VI. A PROPOSAL FOR STANDARD PARAMETRIZATION OF THE CUBIC ALGEBRAIC EQUATION WITH THE WEIERSTRASS FUNCTION

By standard parametrization it shall be meant that the cubic algebraic equation should be brought to its standard parametrizable form

$$\tilde{n}^2=4m^3-g_2m-g_3, \tag{63}$$

where g_2 and g_3 are the already known complex numbers. Then one has the right to set up

$$\tilde{n}=\rho'(z)=\frac{d\rho}{dz}. \qquad m=\rho(z). \tag{64}$$

In order to obtain the parametrizable form (63), it is instructive to write down the obtained algebraic equation in the form of a third-rank polynomial of m with coefficient functions $P_1(n)$, $P_2(n)$, $P_3(n)$ and $P_4(n)$, representing quadratic forms of n and at the same time cubic algebraic expressions with respect to c/d and b/d:

$$P_1(n)m^3+P_2(n)m^2+P_3(n)m+P_4(n)\equiv 0, \tag{65}$$

where

$$P_1(n)\equiv r_1n^2+r_2n+r_3=-3A\left(\frac{c}{d}\right)^2n^2-3A\frac{c}{d}n-A, \tag{66}$$

$$P_2(n)\equiv q_1n^2+q_2n+q_3=\left[3A\left(\frac{c}{d}\right)^2\frac{b}{d}-2B\left(\frac{c}{d}\right)^2\right]n^2-3B\frac{c}{d}n-B, \tag{67}$$

$$\begin{aligned}P_3(n)&\equiv p_1n^2+p_2n+p_3\\&=\left[-6C\frac{c}{d}+B\frac{b}{d}\frac{c}{d}-C\left(\frac{c}{d}\right)^2\right]n^2+\left[-6C+2B\frac{c}{d}\frac{b}{d}+3A\frac{c}{d}\left(\frac{b}{d}\right)^2-C\frac{c}{d}\right]n-C-2\frac{d}{c}C,\end{aligned} \tag{68}$$

$$P_4(n)\equiv\overline{F}n^2+\overline{N}n+\overline{M}. \tag{69}$$

Let us write down the last expression in the following form,

$$P_4(n)\equiv\overline{F}\left[\left(n+\frac{\overline{N}}{2\overline{F}}\right)^2+\frac{\overline{M}}{\overline{F}}-\left(\frac{\overline{N}}{2\overline{F}}\right)^2\right]\equiv\tilde{n}^2+\overline{M}-\frac{\overline{N}^2}{4\overline{F}}, \tag{70}$$

where $\tilde{n}$ denotes

$$\tilde{n}\equiv\sqrt{\overline{F}}\left(n+\frac{\overline{N}}{2\overline{F}}\right). \tag{71}$$

In terms of $\tilde{n}$, the transformed equation (65) can be written as

$$\tilde{n}^2=\overline{P}_1(\tilde{n})\,m^3+\overline{P}_2(\tilde{n})\,m^2+\overline{P}_3(\tilde{n})\,m+\overline{P}_4(\tilde{n}), \tag{72}$$

where the coefficient function $\overline{P}_1(\tilde{n})$ is

$$\overline{P}_1(\tilde{n})\equiv\overline{r}_1\tilde{n}^2+\overline{r}_2\tilde{n}+\overline{r}_3=-\frac{r_1}{\overline{F}}\tilde{n}^2+\left[\frac{\overline{N}}{\overline{F}^{3/2}}r_1-\frac{r_2}{\overline{F}^{1/2}}\right]\tilde{n}+\left[-r_1\frac{\overline{N}^2}{4\overline{F}^2}+r_2\frac{\overline{N}}{2\overline{F}}-r_3\right] \tag{73}$$

and

$$\overline{P}_4(\tilde{n})\equiv\frac{\overline{N}^2}{4\overline{F}}-\overline{M}. \tag{74}$$

The other coefficient functions $\overline{P}_2(\tilde{n})$ and $\overline{P}_3(\tilde{n})$ can be written analogously, but with (q_1,q_2,q_3) and (p_1,p_2,p_3) in (73) instead of (r_1,r_2,r_3). Note that unlike the expressions for r, q and p, representing cubic algebraic expressions with respect to b/d and c/d, the corresponding "bar" quantities represent more complicated expressions, which are no longer polynomials. It is also not correct to consider the transformation from (p,q,r) to $(\overline{p},\overline{q},\overline{r})$ as a linear affine transformation. The expressions $\overline{N}$ and $\overline{F}$ entering the coefficient functons of the transformation depend also on b/d and c/d, so presumably they could also be expressed through (p,q,r). The above transformation shall be investigated further.

Our purpose will be to identify the investigated Eq. (72) $\tilde{n}^2=\overline{P}_1(\tilde{n})m^3+\overline{P}_2(\tilde{n})m^2+\overline{P}_3(\tilde{n})m+\overline{P}_4(\tilde{n})$ **with Eq. (63)** $\tilde{n}^2=4m^3-g_2m-g_3$, **for which we already know that the substitution (64) can be performed**. In order to obtain the standard parametrizable form of the cubic equation, one has to require that the two equations are to be made equal, which means that the polynomials $\overline{P}_1(\tilde{n})$, $\overline{P}_2(\tilde{n})$, $\overline{P}_3(\tilde{n})$ and $\overline{P}_4(\tilde{n})$ (depending on the variable $\tilde{n}$) are to be made equal to the numerical coefficients 4, 0, $-g_2$, and $-g_3$, respectively. Therefore, the following system of equations should be fulfilled:

$$4=\overline{r}_1\tilde{n}^2+\overline{r}_2\tilde{n}+\overline{r}_3, \tag{75}$$

$$0=\overline{q}_1\tilde{n}^2+\overline{q}_2\tilde{n}+\overline{q}_3, \tag{76}$$

$$-g_2=\overline{p}_1\tilde{n}^2+\overline{p}_2\tilde{n}+\overline{p}_3, \tag{77}$$

$$-g_3=\frac{\overline{N}^2}{4\overline{F}}-\overline{M}. \tag{78}$$

The last equation (78) represents the **second** additional equation, imposed in order to obtain the parametrizable form of the cubic equation. Note that this equation has an extremely complicated structure: since $\overline{N}$, $\overline{F}$ and $\overline{M}$ are **third-rank polynomials with respect to** b/d and c/d, the equation will be of **sixth order**! This causes inconvenience in investigating such equations, therefore it is appropriate to search other variables, in terms of which the algebraic treatment will be comparatively more convenient.

Let us try to find such variables. From the first and the second equations (75) and (76) the terms with $\tilde{n}^2$ can be excluded, and also from the second and the third equations (76) and (77). The obtained equations are

$$4\overline{q}_1=(\overline{r}_2\overline{q}_1-\overline{r}_1\overline{q}_2)\tilde{n}+(\overline{r}_3\overline{q}_1-\overline{r}_1\overline{q}_3), \tag{79}$$

$$-g_2\overline{q_1}=(\overline{p_2}\overline{q_1}-\overline{p_1}\overline{q_2})\tilde{n}+(\overline{p_3}\overline{q_1}-\overline{p_1}\overline{q_3}). \tag{80}$$

From the last two equations the terms with $\tilde{n}$ can also be excluded and a fourth-rank algebraic equation is obtained with respect to p_i, q_i and r_i $(i=1,2,3)$:

$$(\overline{p_2}\overline{q_1}-\overline{p_1}\overline{q_2})(4\overline{q_1}-\overline{r_3}\overline{q_1}+\overline{r_1}\overline{q_3})+(\overline{r_2}\overline{q_1}-\overline{r_1}\overline{q_2})(g_2\overline{q_1}+\overline{p_3}\overline{q_1}-\overline{p_1}\overline{q_3})=0. \tag{81}$$

The above equation represents the **third** additional equation, imposed in order to obtain the parametrizable form of the cubic equation. This equation is difficult to deal with, but there is a way to rewrite it in a more convenient and simple form. Let us introduce the **"angular" type** variables l and f with the corresponding components:

$$l=(l^1,l^2,l^3)=(l_{12},l_{23},l_{31})=(\overline{p_1}\overline{q_2}-\overline{p_2}\overline{q_1},\overline{p_2}\overline{q_3}-\overline{p_3}\overline{q_2},\overline{p_3}\overline{q_1}-\overline{p_1}\overline{q_3}), \tag{82}$$

$$f=(f^1,f^2,f^3)=(f_{12},f_{23},f_{31})=(\overline{r_1}\overline{q_2}-\overline{r_2}\overline{q_1},\overline{r_2}\overline{q_3}-\overline{r_3}\overline{q_2},\overline{r_3}\overline{q_1}-\overline{r_1}\overline{q_3}). \tag{83}$$

In terms of these variables, the fourth-rank algebraic equation (81) will be reduced to the following quadratic equation:

$$4\overline{q_1}l^1+g_2f^1\overline{q_1}+l^1f^3+f^1l^3=0. \tag{84}$$

Having found the algebraic variety for $(\overline{q_1},l^1,l^3,f^1,f^3)$, one can go back to find the algebraic variety for $(\overline{p},\overline{q},\overline{r})$. From there by means of the inverse transformation of (73),

$$r_1=-\overline{F}\overline{r_1},\quad r_2=-\overline{F}^{1/2}\overline{r_2}-\overline{N}\overline{r_1}, \tag{85}$$

$$r_3=-\frac{\overline{N}^2}{4\overline{F}}\overline{r_1}-\frac{\overline{N}}{2\overline{F}^{1/2}}\overline{r_2}-\overline{r_3} \tag{86}$$

[the same for (p,q)], one can obtain the "nonbar" variables (p,q,r). As already mentioned, the coefficient functions of the above transformation depend in a complicated way on $\overline{N}$ and $\overline{F}$ and therefore on b/d and c/d. Therefore, if the dependence of b/d and c/d on the "bar" variables is known, one would have a well-determined transformation (although it is a nonpolynomial and nonlinear one) from the "nonbar" variables to the "bar" variables $(\overline{p},\overline{q},\overline{r})$. That is why the purpose in the next section will be to find this nonpolynomial transformation.

Finally, it may be noted that if the parametrization of (63) with the Weierstrass function is performed and $\tilde{n}=\rho'(z)=d\rho/dz$ and $m=\rho(z)$, then the parametrized cubic equation can be written in an integral form:

$$\int \frac{\mathrm{d}\rho(z)}{\sqrt{4\rho^3-g_2\rho-g_3\rho}}=\int \mathrm{d}z. \tag{87}$$

The variable z is a complex one and it may be different from the variables z_1 and z_2, "performing" the complexification of the four-dimensional manifold $(\alpha=1,...,4)$, and the integration is performed along some contour in the complex plane.

VII. FINDING THE NONLINEAR AND NONPOLYNOMIAL INVERTIBLE TRANSFORMATION

We shall start from expressions (66)–(68), from where one can find

$$r_3=-A,\quad r_2=3\frac{c}{d}r_3,\quad r_1=\frac{r_2^2}{3r_3}, \tag{88}$$

$$q_3=-B,\quad q_2=3\frac{c}{d}q_3,\quad q_1=-r_2\frac{q_2}{3q_3}\frac{b}{d}+2\frac{q_2^2}{9q_3},\tag{89}$$

where it has been used that $q_2/q_3=r_2/r_3$. If expressions (89) for $q=(q_1,q_2,q_3)$ are substituted into the expressions defined by (73) for $\overline{q_1}$, it can be obtained

$$\overline{q_1}=-\frac{q_1}{\overline{F}}=-\frac{1}{\overline{F}}\left(\frac{c}{d}\right)^2\left[2-3r_3\frac{b}{d}\right],\tag{90}$$

$$\overline{q_2}=\frac{\overline{N}}{\overline{F}^{3/2}}q_1-\frac{q_2}{\overline{F}^{1/2}}=\frac{\overline{N}}{\overline{F}^{3/2}}\left(\frac{c}{d}\right)^2\left[2-3r_3\frac{b}{d}\right]-3q_3\frac{c}{d}\frac{1}{\overline{F}^{1/2}},\tag{91}$$

$$\overline{q_3}=-q_1\frac{\overline{N}^2}{4\overline{F}^2}+q_2\frac{\overline{N}}{2\overline{F}}-q_3=q_3\left[\frac{3\overline{N}}{2\overline{F}}\frac{c}{d}-1\right]+r_3\left[\frac{3\overline{N}^2}{4\overline{F}^2}\left(\frac{c}{d}\right)^2\frac{b}{d}\right]-\frac{\overline{N}^2}{\overline{F}^2}\left(\frac{c}{d}\right)^2.\tag{92}$$

The corresponding equations for $r=(\overline{r_1},\overline{r_2},\overline{r_3})$ are

$$\overline{r_1}=-\frac{3r_3}{\overline{F}}\left(\frac{c}{d}\right)^2,\tag{93}$$

$$\overline{r_2}=\frac{\overline{N}}{\overline{F}^{3/2}}3r_3\left(\frac{c}{d}\right)^2-\frac{3r_3(c/d)}{\overline{F}^{1/2}},\tag{94}$$

$$\overline{r_3}=\overline{r_1}\left[-\frac{\overline{N}}{2(c/d)}+\frac{\overline{N}^2}{4\overline{F}}+\frac{\overline{F}}{3(c/d)^2}\right].\tag{95}$$

From the first and second two equations it can be obtained respectively

$$\overline{N}=\frac{1}{\overline{r_1}}\left[-\overline{r_2}\overline{F}^{1/2}+\overline{F}\frac{1}{c/d}\right]\tag{96}$$

and

$$\frac{(3+4\overline{r_1}^2-6\overline{r_1})}{12\overline{r_1}}Y^2+\frac{(\overline{r_1}-1)\overline{r_2}}{2\overline{r_1}}Y+\left(\frac{\overline{r_2}^2}{4\overline{r_1}^2}-\overline{r_3}\right)=0,\tag{97}$$

where $Y\equiv\overline{F}^{1/2}/(c/d)$. It is important to note that Y can be found as a solution of the above quadratic equation with coefficient functions, which consist only of $\overline{r}$. Therefore

$$\frac{c}{d}=\frac{1}{Y}\overline{F}^{1/2}=Z\overline{F}^{1/2},\quad \overline{N}=O\overline{F}^{1/2}=\left[\frac{1}{\overline{r_1}}\left(-\overline{r_2}+\frac{1}{Y}\right)\right]\overline{F}^{1/2}.\tag{98}$$

Now let us write down the corresponding equations for p from (68):

$$p_1=-6C\frac{c}{d}+B\frac{b}{d}\frac{c}{d}-C\left(\frac{c}{d}\right)^2,\tag{99}$$

$$p_2=-6C+\left(\frac{c}{d}\right)\left[2B\frac{b}{d}+3A\left(\frac{b}{d}\right)^2-C\right],\tag{100}$$

$$p_3 = -2C\frac{d}{c} - C. \tag{101}$$

If from the last expression C is expressed and is substituted into (99), an expression for b/d can be obtained in the form

$$\frac{b}{d} = -\frac{p_1}{q_3\overline{F}^{1/2}Z} + \frac{p_3 Z\overline{F}^{1/2}[6+Z\overline{F}^{1/2}]}{q_3[2+Z\overline{F}^{1/2}]}, \tag{102}$$

where the derived expressions (98) have also been used. In order to obtain an expression for b/d in terms of the "bar" variables $\overline{p}=(p_1,p_2,p_3)$, the "nonbar" variables p_1, p_2 and p_3 should be expressed from the system of equations for $\overline{p}$:

$$\overline{p_1} = -\frac{p_1}{\overline{F}}, \quad \overline{p_2} = \frac{\overline{N}}{\overline{F}^{3/2}}p_1 - \frac{p_2}{\overline{F}^{1/2}}, \tag{103}$$

$$\overline{p_3} = -p_1\frac{\overline{N}^2}{4\overline{F}^2} + p_2\frac{\overline{N}}{2\overline{F}} - p_3, \tag{104}$$

and substituted into (102). The result is

$$\frac{b}{d} = \frac{1}{q_3}\left[\frac{\overline{F}^{1/2}}{Z}\overline{p_1} - \frac{(6+Z\overline{F}^{1/2})}{(2+Z\overline{F}^{1/2})}\left(\frac{O^2\overline{F}^{1/2}}{4}Z\overline{p_1} + \frac{O\overline{F}^{1/2}Z}{2}\overline{p_2} + Z\overline{F}^{1/2}\overline{p_3}\right)\right]. \tag{105}$$

The only "unbar" variable q_3 can be expressed from the first two equations (90) and (91) for $\overline{q_1}$ and $\overline{q_2}$:

$$q_3 = -\frac{O\overline{q_1}+\overline{q_2}}{3Z}. \tag{106}$$

Also, from the third equation (92) for $\overline{q_3}$ it can be obtained

$$3r_3\frac{b}{d} = \frac{8[6Z\overline{q_3}+3O^2Z^3+(3OZ-2)(O\overline{q_1}+\overline{q_2})]}{3O^2Z^3}, \tag{107}$$

and from the first equation (90) the same expression can be found to be

$$3r_3\frac{b}{d} = \frac{2Z^2+\overline{q_1}}{Z^2}. \tag{108}$$

From the equality of the above two formulas one relation between the "bar" variables can be found. More concretely, since O and Z depend only on $\overline{r}$, the relation will concern how $\overline{q_3}$ can be expressed through O,Z and $\overline{q_1},\overline{q_2}$. This will not be used further in the text, since our main purpose will be to find the ratio $r_3\overline{F}/q_3^2$, which is to be used in the subsequent formulas

$$\frac{r_3\overline{F}}{q_3^2} = -\frac{\overline{F}^{1/2}(2Z^2+\overline{q_1})(2+Z\overline{F}^{1/2})}{(O\overline{q_1}+\overline{q_2})K_1}, \tag{109}$$

where K_1 is the expression

$$K_1 \equiv \overline{p}_1(2+Z\overline{F}^{1/2}) - Z^2(6+Z\overline{F}^{1/2})\left(\frac{O^2\overline{p}_1}{4} + \frac{O}{2}\overline{p}_2 + \overline{p}_3\right). \tag{110}$$

At this moment the only equation not yet used is the one which can be derived from (99)–(101) for p_2

$$p_2 = \frac{2p_3(c/d)(6+c/d)}{2+(c/d)}\left(-\frac{c}{d} + \frac{r_3}{q_3^2}3p_1 + \frac{1}{2}\right) + \left(2p_1 - \frac{r_3}{q_3^2}\frac{3p_1^2}{c/d}\right) - \frac{r_3}{q_3^2}\frac{3p_3^2(c/d)^3(6+c/d)^2}{(2+c/d)^2}. \tag{111}$$

If the p variables are expressed from (103) and (104) through their ''bar'' counterparts and all preceeding expressions are used, the following **cubic algebraic equation** with respect to $\overline{F}^{1/2} \equiv T$ is obtained,

$$N_1T^3 + N_2T^2 + N_3T + N_4 = 0, \tag{112}$$

where N_1, N_2, N_3 and N_4 are complicated expressions of the ''bar'' quantities only. These expressions will be presented in Appendix D. Therefore, the roots of this cubic equation with respect to T can be found and, consequently, the quantities $\overline{N},\overline{F},\overline{M}$ entering the second additional equation (78) also can be expressed in terms of the ''bar'' variables. This in fact proves the following. (1) The two additional equations (78) and (84), imposed in order to obtain the parametrizable form of the cubic equation, can be expressed in terms of the ''bar'' variables only. (2) The nonlinear and nonpolynomial transformation from the (r,q,p) to the $(\overline{r},\overline{q},\overline{p})$ variables is an invertible one. This is an important fact, since one first may study the properties of the algebraic equations, given by (78) and (84), and then choose the most convenient form for the ratios b/d and c/d.

VIII. PARAMETRIZATION OF A GENERAL CUBIC CURVE WITH COEFFICIENT FUNCTIONS OF A COMPLEX VARIABLE

In this section an attempt will be made to deal with a cubic curve of a more general kind,

$$\tilde{n}^2 = M(z)m^3 + N(z)m^2 + P(z)m + E(z), \tag{113}$$

where M, N, P and E are functions of the complex variable z and therefore **not complex numbers**, as usually accepted in standard complex analyses[5] and algebraic geometry.[13] In other words, the main problem is whether it is possible to parametrize with the Weierstrass function the above equation, i.e., when does the Weierstrass function satisfy the equation

$$\left(\frac{d\rho}{dz}\right)^2 = M(z)\rho^3 + N(z)\rho^2 + P(z)\rho + E(z)? \tag{114}$$

As already briefly discussed in Sec. IV for the standard and usually investigated case of M,N,P,E constants, the Weierstrass function parametrizes the cubic equation (113) *only if* $M=4$, $N=0$, $P=-60G_4$ and $Q=-140G_6$, but evidently in the present case of **functions**, the situation will be quite different.

Let us first decompose $\rho(z)$ into an infinite sum, assuming that $|\varpi|$ is a large number and therefore

$$\rho(z) = \frac{1}{z^2} + \sum\left[\frac{1}{\varpi^2(z/\varpi-1)^2} - \frac{1}{\varpi^2}\right] = \frac{1}{z^2} + \sum\frac{1}{\varpi^2}\left(2\frac{z}{\varpi} + 3\left(\frac{z}{\varpi}\right)^2 + \cdots + (n+1)\frac{z^n}{\varpi^n} + \cdots\right). \tag{115}$$

The first derivative of the Weierstrass function is

$$\rho'(z)=\frac{d\rho}{dz}=-\frac{2}{z^3}+\sum\frac{n(n+1)}{\varpi^{2+n}}z^{n-1} \tag{116}$$

and its square degree is

$$[\rho'(z)]^2=\frac{4}{z^6}-4\sum_{n=1}^{\infty}\frac{n(n+1)}{\varpi^{2+n}}z^{n-4}+\sum_{n=1}^{\infty}\frac{n^2(n+1)^2}{\varpi^{2(n+2)}}z^{2(n-1)}. \tag{117}$$

Note that in the strict mathematical sense, the second sum in the last expression is in fact a double sum over m and n,

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{mn(m+1)(n+1)}{\varpi^{m+n}}z^{m+n-2},$$

obtained as a result of the multiplication of the two infinite sums (116) for $\rho'(z)$ with different summation indices. Of course, since the two sums are equal and infinite ones, the representation in the form of a single sum is also correct. The appearence of the double sum should be kept in mind, since the idea further will be to compare the coefficient functions in the Loran power expansion of the functions on the left- and right-hand sides of (114), and naturally a double sum will appear on the R.H.S. of (114).

In reference to this, an important remark follows. Suppose one works in the framework of *standard arithmetical theory of elliptic functions*, when M, N, P and E are assumed to be just *number coefficients*. Since the Weierstrass functions $\rho(z)$ is an *even function of the complex variable z* (see Refs. 5 and 7), the whole expression on the right-hand side (R.H.S.) of (114) will be an *even* one, too. On the other hand, the function $\rho'(z)$ on the left-hand side (L.H.S.) of (114) is an *odd* one, but its square again gives an *even function*. Therefore, comparing the coefficients in front of the powers in z means that only the *even* powers should be included in the infinite sum decomposition,

$$[\rho'(z)]^2=\frac{4}{z^6}-76G_6-24G_4\frac{1}{z^2}+\ldots, \tag{118}$$

where G_n will denote the following infinite sum of the complex pole numbers:

$$G_n=\sum\frac{1}{\varpi^n}. \tag{119}$$

Note also another very important fact, the proof of which is given in Ref. 5: the infinite (in numbers of ϖ*) sum (119) is always convergent (i.e., finite) when* $n>2$*, but for* $n\leqslant 2$ *the finiteness is not guaranteed*! In the presently investigated case of M,N,P,E complex functions, no information is available whether the R.H.S. of (114) is an even or an odd function in z. Consequently, one should not use formulas (118), but just start with the more general expression (117) for $[\rho'(z)]^2$.

In order to find the Loran decomposition of the functions on the right-hand side of (114), one should first find second and the third powers of $\rho(z)$, which may be written as

$$\rho^2(z)=\frac{1}{z^4}+2\sum_{n=1}^{\infty}(n+1)\frac{z^{n-2}}{\varpi^n}+\sum_{n=1}^{\infty}(n+1)^2\frac{z^{2n}}{\varpi^{2n}}, \tag{120}$$

$$\rho^3(z)=\frac{1}{z^4}+2\sum_{n=1}^{\infty}(n+1)\frac{z^{n-4}}{\varpi^n}+\sum_{n=1}^{\infty}(n+1)^2\frac{z^{2n-2}}{\varpi^{2n}}+\sum_{n=1}^{\infty}(n+1)\frac{z^{n-2}}{\varpi^n}$$
$$+2\sum_{n=1}^{\infty}(n+1)\frac{z^{2n-2}}{\varpi^{2n}}+\sum_{n=1}^{\infty}(n+1)^2\frac{z^{3n}}{\varpi^{3n}}. \tag{121}$$

Since these two expressions are to be multiplied by another infinite sums, here in (120) and (121) we have retained the single-sum representaion.

The function $E(z)$ has the following Loran expansion around the zero point

$$E(z)=\sum_{m=-\infty}^{\infty}c_m^{(0)}z^m=\sum_{m=0}^{\infty}a_m^{(0)}z^m+\sum_{m=1}^{\infty}\frac{b_m^{(0)}}{z^m}, \tag{122}$$

where $a_m^{(0)}$ and $b_m^{(0)}$ can be represented as integrals along some contour in the complex plane (w is a complex integration variable)

$$a_m^{(0)}=\frac{1}{2\pi i}\int\frac{E(w)}{w^{m-1}\mathrm{d}w},\quad b_m^{(0)}=\frac{1}{2\pi i}\int E(w)w^{m-1}\mathrm{d}w. \tag{123}$$

The coefficient functions in the Loran expansion of the functions $N(z)$, $P(z)$ and $Q(z)$ will be denoted respectively by $c_m^{(1)}$, $c_m^{(2)}$ and $c_m^{(3)}$. Each term of the expression for the right-hand side of (114) is a product of two infinite sums, and the final result is

$$M(z)\rho^3+N(z)\rho^2+P(z)\rho+E(z)$$
$$=\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty}\{c_{m+4}^{(3)}+2(n+1)G_nc_{m+4-n}^{(3)}+(n+1)^2G_{2n}c_{m+2-2n}^{(3)}$$
$$+(n+1)G_nc_{m+2-n}^{(3)}+2(n+1)^2G_{2n}c_{m+2-2n}^{(3)}$$
$$+(n+1)^3G_{3n}c_{m-3n}^{(3)}+c_{m+4}^{(2)}+2(n+1)G_nc_{m-n+2}^{(2)}$$
$$+(n+1)^2G_{2n}c_{m-2n}^{(2)}+c_{m+2}^{(1)}+c_{m-n}^{(1)}G_n+c_m^{(0)}\}z^m. \tag{124}$$

In principle, the general case for an arbitrary m may also be considered. Then the above expression should be put equal to formulas (117) for $[\rho'(z)]^2$, where in the first sum one should set up $2(n-1)=m$ and in the second sum $n-4=m$. In the first sum in (117) the summation will be over values of $m=0,2,4,6,\ldots,2k,\ldots$, and in the second sum over $m=-3,-2,-1,0,1,2,\ldots$. In such a case and for a given n, one would have to consider a recurrent (in n) set of *seven algebraic equations* with respect to the *four Loran expansion coefficients* $c_n^{(0)},c_n^{(1)},c_n^{(2)},c_n^{(3)}$ and for the seven values of $m=-6,-3,-2,-1,0,2k,2k+1$ ($k=1,2,\ldots$). Therefore, the system of equations is predetermined, which enables one to find not only the unknown variables (the coefficient functions), but also certain relations about the ''coefficient'' expressions, represented in the case by the sums G_n. This is an important moment, which shall be worked out further in this article, and indeed certain interesting relations will be found. Moreover, since the summation over m on the R.H.S. of (124) ranges from $-\infty$ to $+\infty$, terms with values of m, different from the above written, shall be present also on the R.H.S. of (124), but not on the L.H.S. of (117). Therefore, *two additional algebraic equations* may be obtained by putting $m=-2k$ ($k\neq 0,1,3$) and then $m=-(2k+1)$ ($k\neq 0,1$) on the R.H.S. of (124) and then setting the whole expression equal to zero. In fact, effectively instead of two additional equations one may have just one additional equation by putting $m=-k$ ($k>3$ and $k\neq 6$), so the total number of equations will be *eight*. This complicated calculation for the general case has not been performed in the present article, because due to considerable technical difficulties it would be impossible to reconstruct analytically the whole set

of *Loran coefficients* $c_n^{(0)}, c_n^{(1)}, c_n^{(2)}, c_n^{(3)}$ as solutions of the above system of *eight algebraic equations*. However, the calculation will be performed in Appendix A for the simplified case, which will be described also below.

In this section we shall restrict ourselves to the case of negative-power expansion terms in the decomposition of $[\rho'(z)]^2$, obtained for values of $m=-6,-2,0$, and the main motivation for this is the analogy with the standard parametrization of the cubic curve. In the next sections the case of positive-power expansion will be considered, too. Unfortunately, even under this additional assumption it is impossible to resolve analytically the corresponding system of algebraic equations, if some other simplifying assumption is not added. This assumption will be given in the next section.

The first recurrent relation for $m=-6$ is

$$\begin{aligned}4=&c_{-2}^{(3)}+2(n+1)G_n c_{-n-2}^{(3)}+(n+1)^2 G_{2n} c_{-4-2n}^{(3)}+(n+1)G_n c_{-4-n}^{(3)}\\&+2(n+1)^2 G_{2n} c_{-4-2n}^{(3)}+(n+1)^3 G_{3n} c_{-6-3n}^{(3)}+c_{-2}^{(2)}+2(n+1)G_n c_{-n-4}^{(2)}\\&+(n+1)^2 G_{2n} c_{-6-2n}^{(2)}+c_{-4}^{(1)}+c_{-6-n}^{(1)} G_n+c_{-6}^{(0)}.\end{aligned} \tag{125}$$

For $m=-2$ the relation is

$$\begin{aligned}-76G_6=&c_4^{(3)}+2(n+1)G_n c_{4-n}^{(3)}+(n+1)^2 G_{2n} c_{2-2n}^{(3)}+(n+1)G_n c_{2-n}^{(3)}\\&+2(n+1)^2 G_{2n} c_{2-2n}^{(3)}+(n+1)^3 G_{3n} c_{-3n}^{(3)}+c_{-4}^{(2)}+2(n+1)G_n c_{-n+2}^{(2)}\\&+(n+1)^2 G_{2n} c_{-2n}^{(2)}+c_2^{(1)}+c_{-n}^{(1)} G_n+c_0^{(0)}.\end{aligned} \tag{126}$$

The last relation for $m=0$ is

$$\begin{aligned}-24G_4=&c_2^{(3)}+2(n+1)G_n c_{2-n}^{(3)}+(n+1)^2 G_{2n} c_{-2n}^{(3)}+(n+1)G_n c_{-n}^{(3)}\\&+2(n+1)^2 G_{2n} c_{-2n}^{(3)}+(n+1)^3 G_{3n} c_{-2-3n}^{(3)}+c_2^{(2)}+2(n+1)G_n c_{-n}^{(2)}\\&+(n+1)^2 G_{2n} c_{-2-2n}^{(2)}+c_0^{(1)}+c_{-2-n}^{(1)} G_n+c_{-2}^{(0)}.\end{aligned} \tag{127}$$

To avoid the possible confusion why n appears on the R.H.S of (125)–(127) but not on the L.H.S., let us remind the reader that the left-hand sides for $[\rho'(z)]^2$ in these three equations have been obtained by fixing both summation indices n $(n=m)$ and also m $(m=-6,-2,0)$, while on the right-hand sides only the indice m is fixed and *the indice n is left unfixed*! What will be performed in the next section will be for each value of $m=-6,-2,0$ to fix in an appropriate way the possible values of n. Therefore, more than three algebraic equations will be obtained, in which there will be no summation left.

From the above system of *three recurrent algebraic equations* (125)–(127), the infinite sequence of coefficient functions $c_n^{(0)}$, $c_n^{(1)}$, $c_n^{(2)}$ and $c_n^{(3)}$ should be found and, moreover, it should be proved that this sequence is convergent in the limit $n\to\pm\infty$. Still, because of the restriction to three values of m only, even if it is possible to find $c_n^{(0)}$, $c_n^{(1)}$, $c_n^{(2)}$, $c_n^{(3)}$, it would not be correct to assert that the Weierstrass function parametrizes an arbitrary cubic curve with coefficient functions of a complex variable. This problem probably may be resolved by means of computer simulations only.

In the next section the system of equations (125)–(127) shall be used for parametrizing a more simplified cubic curve [without the quadratic in $\rho(z)$ term].

IX. PARAMETRIZATION WITH THE WEIERSTRASS FUNCTION OF THE CUBIC CURVE $[\rho'(z)]^2=4\rho^3-g_2(z)\rho-g_3(z)$

The form of the cubic curve is the same as the parametrizable cubic curve in standard algebraic geometry,[5,10,11,13,31] but here it will be with g_2 and g_3 functions of a complex variable. The key problem which can be raised is *does there exist an algorithm for finding out the sequence*

of coefficient functions in the Loran decomposition of $g_2(z)$ and $g_3(z)$, satisfying the above algebraic equation, provided that its more simple form will result in the following restrictions on the coefficient functions of the already considered general cubic equation (114),

$$M(z)=4=\sum_{m=-\infty}^{m=+\infty} c_m^{(3)} z^m, \quad N(z)=\sum_{m=-\infty}^{m=+\infty} c_m^{(2)} z^m=0, \tag{128}$$

$$N(z)=-g_2(z)=-\sum_{m=-\infty}^{m=+\infty} c_m^{(1)} z^m, \quad E(z)=-g_3(z)=-\sum_{m=-\infty}^{m=+\infty} c_m^{(0)} z^m. \tag{129}$$

From the first sequence of equations one obtains for the coefficients $c_m^{(3)}$ and $c_m^{(2)}$,

$$c_0^{(3)}=4, \quad c_m^{(2)}=0 \quad \text{for all } m, \tag{130}$$

$$c_m^{(3)}=0 \quad \text{for all} \quad m\neq 0. \tag{131}$$

Taking the above relations into consideration, Eq. (126) for $m=-2$ can be written as

$$-24G_4=2(n+1)G_n c_{2-n}^{(3)}-c_0^{(1)}-G_n c_{-2-n}^{(1)}-c_{-2}^{(0)}. \tag{132}$$

For values of $n=2$ and $n=1$ from the above equation the following equations are obtained:

$$-24G_4=24G_2-c_0^{(1)}-c_0^{(1)}-c_{-4}^{(1)}G_2-c_{-2}^{(0)}, \tag{133}$$

$$24G_4=c_0^{(1)}+G_1 c_{-3}^{(1)}+c_{-2}^{(0)}. \tag{134}$$

From the above two equations $c_{-4}^{(1)}$ and $c_{-3}^{(1)}$ can be found:

$$c_{-4}^{(1)}=\frac{1}{G_2}[24G_4+24G_2-c_0^{(1)}-c_{-2}^{(0)}], \tag{135}$$

$$c_{-3}^{(1)}=\frac{1}{G_1}[c_0^{(1)}+c_{-2}^{(0)}-24G_4]. \tag{136}$$

From (132), the general recurrent relation for $n=p>2$ can be obtained:

$$c_{-2-p}^{(1)}=\frac{1}{G_p}[24G_4-c_0^{(1)}-c_{-2}^{(0)}]. \tag{137}$$

It is clear that for the determination of $c_{-4}^{(1)}, c_{-3}^{(1)}$ and $c_{-2-p}^{(1)}$ one has to know $c_{-2}^{(0)}$ and $c_0^{(1)}$. There is, however, one exception—in (135) $G_2=\Sigma\, 1/\varpi^2$ may be a divergent sum, so then one has $c_{-4}^{(1)}=24$ (since G_2 is in the denominator, when $G_2\to\infty$, the corresponding part of the expression will tend to zero).

Further, for $m=0$ and keeping in mind (130) and (131), Eq. (127) will give

$$\begin{aligned}-76G_6=&2(n+1)G_n c_{4-n}^{(3)}+(n+1)^2 G_{2n} c_{2-2n}^{(3)}+(n+1)G_n c_{2-n}^{(3)}\\&+2(n+1)^2 G_{2n} c_{2-2n}^{(3)}-c_2^{(1)}-c_{-n}^{(1)}G_n-c_0^{(0)}.\end{aligned} \tag{138}$$

For values of $n=4,2,1$, when there are nonvanishing values among the coefficients $c_m^{(3)}$, the corresponding equations are

$$-76G_6=40G_4-c_2^{(1)}-c_{-4}^{(1)}G_4-c_0^{(0)}, \tag{139}$$

$$-76G_6=12G_2-c_2^{(1)}-c_{-2}^{(1)}G_2-c_0^{(0)}, \tag{140}$$

$$-76G_6=48G_2-c_2^{(1)}-c_{-1}^{(1)}G_1-c_0^{(0)}. \tag{141}$$

The above linear algebraic equations can be solved trivially to find the coefficients $c_{-4}^{(1)}$, $c_{-2}^{(1)}$ and $c_2^{(1)}$, which depend on $c_{-1}^{(1)}$ and $c_0^{(0)}$:

$$c_{-4}^{(1)}=\frac{1}{G_4}[c_{-1}^{(1)}G_1-48G_2+40G_4], \tag{142}$$

$$c_{-2}^{(1)}=-36+\frac{G_1}{G_2}c_{-1}^{(1)}, \tag{143}$$

$$c_2^{(1)}=76G_6+48G_2-c_0^{(0)}-c_{-1}^{(1)}G_1. \tag{144}$$

Note that these coefficients can be divergent if G_2 and G_1 are divergent. Taking into account Eq. (144) and also (138) for the case $m=0$, but for a general value of $n=p\neq 1,2,4$, an expression for $c_{-k}^{(1)}$ can easily be found:

$$c_{-k}^{(1)}=\frac{1}{G_k}(-48G_2+c_{-1}^{(1)}G_1). \tag{145}$$

This formula should be compared to the previously derived formula (137), setting up $-2-p=-k$. From the two expressions $c_{-2}^{(0)}$ can be expressed

$$c_{-2}^{(0)}=24G_4-c_0^{(1)}-\frac{G_{k-2}}{G_k}(-48G_2+c_{-1}^{(1)}G_1). \tag{146}$$

However, $c_{-2}^{(0)}$ can be expressed also from the two formulas (135) and (142) for $c_{-4}^{(1)}$:

$$c_{-2}^{(0)}=24G_4+24G_2-c_0^{(1)}+\frac{G_2}{G_4}(48G_2-c_{-1}^{(1)}G_1-40G_4). \tag{147}$$

Comparing (146) and (147), an expression for $c_{-1}^{(1)}$ can be found, *which does not depend on any Loran coefficient functions*:

$$c_{-1}^{(1)}=\frac{16G_2}{G_1}\frac{[3G_2G_k-G_4G_k-3G_4G_{k-2}]}{[G_2G_k-G_4G_{k-2}]}. \tag{148}$$

Substituting this expression into the formula (145) for $c_{-k}^{(1)}$, one obtains the convergent expression $(k>2,k\neq 4)$:

$$c_{-k}^{(1)}=-\frac{16G_4}{G_k-(G_4/G_2)\,G_{k-2}}. \tag{149}$$

The obtained expression (148) for $c_{-1}^{(1)}$ can be substituted into (146) to find a formula for $c_{-2}^{(0)}$, which will depend on G_k and only on the Loran coeffficient function $c_0^{(1)}$.

$$c_{-2}^{(0)}=-c_0^{(1)}+24G_4+\frac{16G_{k-2}}{(G_k/G_4)-G_{k-2}/G_2}. \tag{150}$$

The above expression is well defined also when $G_2\to\infty$. It shall be proved subsequently that such a case will turn out to be impossible.

Further, from (150) and expression (136) for $c_{-3}^{(1)}$ it follows

$$c_{-3}^{(1)}=\frac{G_4}{G_2}\frac{16G_{k-2}}{[G_k-(G_4/G_2)G_{k-2}]}. \tag{151}$$

But since k in expression (149) can take a value $k=3$, it follows also

$$c_{-3}^{(1)}=-\frac{16G_4}{G_3-(G_4/G_2)G_1}. \tag{152}$$

The comparison of the two expressions gives the following formulas for the infinite sum G_k:

$$G_k=\gamma G_{k-2}=\gamma^s G_{k-2s}=\cdots=\gamma^{(2p-1/2)}G_1 \quad \text{for } k=2p=\gamma^p G_1 \quad \text{for } k=2p+1, \tag{153}$$

where

$$\gamma=2\frac{G_4}{G_2}-\frac{G_3}{G_1}. \tag{154}$$

Another recurrent relation for G_k can be found also from (151):

$$G_k=\frac{(G_{k-2})^2}{G_{k-4}}=\frac{(G_{k-4})^3}{(G_{k-6})^2}=\ldots=\frac{(G_{k-2s})^{s+1}}{(G_{k-2s-2)^2}}. \tag{155}$$

This formula for values of $k=2p$ and $k=2p+1$, combined with the previous formula (153), allows one to find an expression for G_1:

$$G_1=\frac{G_3^{(2p-1/2p-3)}}{G_{2p}^{2/(2p-3)}}=\frac{G_3^{p/(p-1)}}{G_{2p+1}^{1/(p-1)}}. \tag{156}$$

The last formula is interesting, because it shows that the divergent in the general case quantity G_1 in the present case is expressed through convergent quantities only—G_3 and G_{2p+1} (p is of course a finite number!). Substituting (156) into (155), one can get expressions for G_{2p} and G_{2p+1}:

$$G_{2p}=G_3\left(\frac{G_4}{G_2}\right)^{(2p-3)/2}; \quad G_{2p+1}=G_3\left(\frac{G_4}{G_2}\right)^{p-1}. \tag{157}$$

It is seen that G_2 is also expressed through convergent quantities.

From Eq. (125) for $m=-6$ one obtains

$$4=c_{-4}^{(1)}+c_{-6-n}^{(1)}G_n+c_{-6}^{(0)} \tag{158}$$

($n=1,\ldots,\infty$). Since $c_{-4}^{(1)}$ and $c_{-6-n}^{(1)}$ can be found, $c_{-6}^{(0)}$ can also be determined. It is clear that among the coefficients $c_m^{(0)}$ two of them, $c_{-6}^{(0)}$ and $c_{-2}^{(0)}$, can be determined from (158) and (150). The other coefficients will be determined in the Appendices.

Let us summarize the obtained results in this section and in Appendices A, B and C by formulating the following.

Proposition 2: Let $g_2(z)$ and $g_3(z)$ be functions of a complex variable, which have a Loran function decomposition $g_2(z)=\Sigma_{m=-\infty}^{\infty}c_m^{(1)}z^m$ and $g_3(z)=\Sigma_{m=-\infty}^{\infty}c_m^{(0)}z^m$ and satisfy the algebraic equation $[\rho'(z)]^2=4\rho^3-g_2(z)\rho-g_3(z)$, where $\rho(z)$ is the Weierstrass (elliptic) function. Then the following statements represent (only) necessary conditions for the fulfillment of the above equation:

(1) The poles of the Weierstrass function (even if they are infinite in number) must be situated in such a way so that the sums $G_1=\Sigma\,1/\varpi$ and $G_2=\Sigma\,1/\varpi^2$ are convergent (i.e., finite). The sum G_1 can be expressed through formula (156).

(2) All the coefficients $c_m^{(1)}$ and $c_m^{(0)}$ in the Loran positive- and negative-power expansion can be expressed uniquely from the finite sums G_n.
(3) The sum G_1 is proportional to the sum G_3 with a coefficient of proportionality, equal to the ratio of the sums G_2 and G_4, i.e., $G_1=(G_3/G_4)\,G_2$ [from (A22)]. This formula follows also from the more general one $G_{2p+1}=G_3(G_4/G_2)^{p-1}$ (157) for $p=0$.
(4) As a consequence from the above relation and formulas (153) and (154), the sum G_2 can be uniquely expressed as $G_2=\sqrt{G_1G_3}$.
(5) All the even-number sums $G_6, G_8, G_{10}, \ldots$ are equal to zero.
(6) The following relation is fulfilled, $G_k^2=20^2\,(G_{k-2}G_{k+2})/G_{2(k+1)}$, which can be obtained from (B15) and (B16). In order for this relation to comply with statement 5, additionally one should have that $G_5, G_7, G_{13}, G_{15}, G_{21}, G_{23}, \ldots$ should be zero. However, $G_9, G_{11}, G_{17}, G_{19}$ are different from zero.

Finally, with the help of (158), a check can also be made for the consistency of the obtained results. Substracting the two equations (158) for values of n and $n+l$, one obtains

$$\frac{G_n}{G_{n+6}-(G_4/G_2)\,G_{n+4}}-\frac{G_{n+l}}{G_{n+6+l}-(G_4/G_2)\,G_{n+4+l}}=0 \tag{159}$$

(it is more appropriate to divide everywhere by G_n). From (157) for values of $n=2p$ and $l=2q$, for example, it can be found

$$\frac{G_{n+l}}{G_n}=\left(\frac{G_4}{G_2}\right)^{2q}. \tag{160}$$

For other combinations (even and odd) of n and l the calculation is similar. Using the above formulas, it can easily be verified that Eq. (159) is *identically satisfied*. This confirms that the system of equations investigated in this paragraph gives consistent and noncontradictory results.

X. CONCLUSION

Let us summarize the obtained results.

In this article a cubic algebraic equation has been obtained with respect to the differentials dX^i of some generalized coordinates X^i. The derivation of the equation was possible due to the representation of the contravariant metric tensor in terms of a contraction of two differentials. Also, in Sec. III the equation was derived upon assuming that dX^i is either an exact differential, or that dX^i are **zero-helicity vector field components**.

The derived equation (20) clearly reflects the structure of the gravitational Lagrangian, and can be regarded as an equation for all its possible coordinate transformations (admissable parametrizations), provided that the Christoffell connection Γ_{ij}^k or the Ricci tensor R_{ij} is given.

The main problems, which one encounters when investigating such algebraic equations, are several, and in this article only one of them is resolved in more detail.

The **first** and most serious problem is that the equation is defined on an algebraic variety of several variables, since in gravity theory one usually deals with at least four-dimensional (and higher-dimensional also) manifolds. At the same time, the standard and known methods from algebraic geometry for parametrizing algebraic curves by means of the Weierstrass function concern only algebraic curves of two variables. That is why in the article one of the variables, dx^5, has been singled out on the basis of the physical consideration of the Randall–Sundrum models, and the other variable for convenience is chosen to be the ratio a/c of the functions $a(z)$ and $c(z)$, which enter in the **linear-fractional transformation** of dx^5. The rest of the variables dx^1, dx^2, dx^3, dx^4 enter the cubic equation in scalar quantities (functions). Of course, if a two-dimensional manifold is considered, then the algebraic equation will contain two variables only. Such an analysis of a two-dimensional algebraic equation and its parametrization may find application in string and brane theory (also in gravity theory).

For the purpose of higher-dimensional algebraic varieties and equations, probably methods from the theory of Abelian varieties and hyper-elliptical (Weierstrass) functions have to be applied.[42]

The **second problem** concerns the methods for bringing the algebraic equation to a parametrizable form. The standard approach of applying a **linear-fractional transformation** has been chosen for the purpose.

The advantages of the **linear-fractional transformation** are the following: (1) It contains more parameters (in the case, functions a,b,c,d of a complex variable) and it makes it possible to take account of the **point at infinity**. (2) In Sec. VI it was proved that by means of a suitable change of variables it is possible to derive a **second-order (quadratic) algebraic equation** in terms of ''angular''-type variables from the initial cubic algebraic equation. Since a quadratic equation is easier to deal with, this simplifies the analysis and, moreover, a transition to the original variables can also be performed.

The **third problem**, investigated in more detail in the present article, is the **form of the parametrizable cubic curve**. This was discussed in the Introduction, and evidently a concrete physical problem from gravity theory has shown the necessity to investigate the case when g_2 and g_3 are complex functions and not complex numbers, as it is in the standard theory of elliptic functions. In regard to this, in Secs. VIII and IX two mutually related problems for resolving are being stated: (1) Can the Weierstrass function $\rho(z)$ parametrize an **arbitrary cubic curve** with coefficient functions of a **complex variable**? (2) Can the Weierstrass function parametrize the well-known parametrizable form of the cubic equation, but again with coefficient functions depending on a complex variable? Although the explicit form of the equations for the Loran coefficient functions are presented in Sec. VIII, the first question still remains unanswered, and perhaps computer simulations only can help for its resolution. As for the second question, the answer is affirmative, and after solving a system of algebraic equations for various values of m and n, the explicit form of all the Loran coefficient functions $c_m^{(1)}$, $c_m^{(0)}$ was found, both from the negative-power and the positive-power expansion. A confirmation of the consistency of the derived equations is Eq. (159) for a value of $m=-6$, which is being satisfied by the previously derived equations. However, the values of the coefficient functions are perhaps not so important as the result, which follows from this calculation, namely: *The infinite sums G_1 and G_2, which in the general case might be divergent, in the particular case of the "parametrizable" form of the cubic algebraic equation with $g_2=g_2(z)$ and $g_3=g_3(z)$, should be convergent!* This fact, although of pure mathematical nature, probably deserves more attention and further elaboration from another point of view and by applying different mathematical approaches. The finiteness of G_1 and G_2 is not imposed ''by hand,'' but is obtained as a consequence of the fulfillment of the above mentioned equation, which is satisfied by the Weierstrass function.

ACKNOWLEDGMENTS

The author is greateful to Dr. L. Alexandrov and Dr. D. M. Mladenov (BLTP, Joint Institute for Nuclear Research, Dubna) for useful comments and their interest towards this work, to Professor N. A. Chernikov (BLTP, Joint Institute for Nuclear Research, Dubna) for his support and encouragement and to the Directorate of the Bogoliubov Laboratory for Theoretical Physics for the support during his stay in Dubna (Russia). The work on this article was supported also by a Shoumen University grant under Contract No. 005/2002. The author is grateful also to Dr. P. L. Bozhilov (Shoumen University, Bulgaria) for the possibility to participate in this grant.

APPENDIX A: ADDITIONAL SYSTEM OF EQUATIONS FOR $m=-3, -1$

In this Appendix the system of equations for $m=-3,-1$ will be presented, which were not investigated in Sec. IX. However, the method for their derivation is completely the same, but some new interesting consequences will appear.

For the purpose, let us first rewrite the two sums in expression (117) for $[\rho'(z)]^2$, putting in the first sum $2(n-1)=m$ and in the second term $n-4=m$. Then expression (117) acquires the form

$$[\rho'(z)]^2=\frac{4}{z^6}+\frac{1}{16}\sum_{m=0,2,4,\ldots}^{\infty} G_{m+6}(m+2)^2(m+4)^2z^m$$

$$-4\sum_{m=-3,-2,-1,0,1,..} G_{m+6}(m+4)(m+5)z^m. \tag{A1}$$

For $m=-3$ only the term from the second sum in (A1) will contribute. Putting also $m=-3$ in the R.H.S. of expression (124) for $M(z)\rho^3+N(z)\rho^2+P(z)\rho+E(z)$ for the case of $M=4$, $N=0$, $P(z)\equiv -g_2(z)$ and $E(z)\equiv -g_3(z)$ (i.e., $c_m^{(2)}=0$ for all m, $c_0^{(3)}\equiv 4$ and $c_m^{(3)}\equiv 0$ for $m\neq 0$), one has to take into account that terms with a "negative-valued" indice like $c^{(3)}_{-1-2n}, c^{(3)}_{-1-n}, c^{(3)}_{-3-3n} (n=1,2,\ldots.)$ are zero.

The obtained equation for $m=-3$ is

$$-8G_3=2(n+1)G_nc^{(3)}_{1-n}+c^{(1)}_{-1}+c^{(1)}_{-3-n}G_n+c^{(0)}_{-3}. \tag{A2}$$

For $n=1$, when the first term on the R.H.S. is nonzero, the equation is

$$-8G_3=16G_1+c^{(1)}_{-1}+c^{(1)}_{-4}G_1+c^{(0)}_{-3}. \tag{A3}$$

Since from expressions (151) and (142) from Sec. VII $c^{(1)}_{-3}$ and $c^{(1)}_{-4}$ can be found, from the above Eq. (A3) $c^{(0)}_{-3}$ can be expressed.

For $n=p>1$ Eq. (A2) is

$$-8G_3=c^{(1)}_{-1}+c^{(1)}_{-3-p}G_p+c^{(0)}_{-3}. \tag{A4}$$

Substracting the two equations (A3) and (A4), one can find the following expression for $c^{(1)}_{-3-p}$:

$$c^{(1)}_{-3-p}=\frac{G_1}{G_p}(16+c^{(1)}_{-4})=16\frac{G_1}{G_p}\frac{[(G_2/G_4)G_p+3(G_2/G_4)^2G_p-(3(G_2/G_4)+21)G_{p-2}]}{(G_2/G_4)G_p-G_{p-2}}. \tag{A5}$$

An expression for $c^{(1)}_{-3-p}$ can also be found from formulas (149) for $k=p+3$:

$$c^{(1)}_{-3-p}=-\frac{16G_4}{G_{p+3}-(G_4/G_3)G_{p+1}}. \tag{A6}$$

From the equality of the two expressions, G_1 can again be expressed as a convergent expression. Note also that the formulas $G_{2p}=G_3(G_4/G_2)^{(2p-3)/2}$ and $G_{2p+1}=G_3(G_4/G_2)^{p-1}$ from (157) satisfy the equality expression since then the denominators in (A5) and (A6) will be zero. This precludes the investigation of the system of equations for $m=-3$.

For $m=-1$, the general equation can be written as

$$-48G_5=2(n+1)G_nc^{(3)}_{3-n}+(n+1)G_nc^{(3)}_{1-n}+G_nc^{(1)}_{-1-n}+c^{(1)}_1+c^{(0)}_{-1}, \tag{A7}$$

and for $n=1$ and $n=2$ the corresponding equations are

$$-48G_5=8G_1+c^{(1)}_{-2}G_1+c^{(1)}_1+c^{(0)}_{-1}, \tag{A8}$$

$$-48G_5=G_2c^{(1)}_{-3}+c^{(1)}_1+c^{(0)}_{-1}. \tag{A9}$$

The coefficient $c^{(1)}_{-3}$ can also be found from (149) for $k=3$:

$$c_{-3}^{(1)} = -\frac{16G_4}{G_3 - (G_4/G_2)\,G_1}. \tag{A10}$$

Substituting (A10) into (A9) gives an opportunity to express $c_1^{(1)} + c_{-1}^{(0)}$ as

$$c_1^{(1)} + c_{-1}^{(0)} = -48G_5 + \frac{16G_2G_4}{G_3 - (G_4/G_2)\,G_1}. \tag{A11}$$

This expression, together with formulas (143) for $c_{-2}^{(1)}$ and (148) for $c_{-1}^{(1)}$, represented as $c_{-1}^{(1)} = F/G_1$, can be substituted into the first equation (A8) to obtain the following quadratic equation for G_1:

$$\left(G_3 - \frac{G_4}{G_2}G_1\right)\left(\frac{G_1}{G_2}F - 24G_1\right) + 16G_2G_4 = 0. \tag{A12}$$

In a similar way, one can write down the equation for $n=3$:

$$-48G_5 = 32G_3 + c_{-4}^{(1)}G_3 + c_1^{(1)} + c_{-1}^{(0)}. \tag{A13}$$

Substituting $c_{-4}^{(1)}$ and $c_1^{(1)} + c_{-1}^{(0)}$ from (142) and (A11), one can derive

$$2L = \frac{G_2}{G_3G_4}\frac{G_k}{G_{k-2}} - \frac{1}{G_3}, \tag{A14}$$

where

$$L = \frac{G_3 - (G_4/G_2)\,G_1}{7G_3(G_3 - (G_4/G_2)) + 2G_2G_4}. \tag{A15}$$

From the above two equations a relation, similar to (153), can be obtained,

$$G_k = \beta G_{k-2} = \beta^{(2p-1)/2}G_1 \quad \text{for } k=2p \quad = \beta^p G_1 \quad \text{for } k=2p+1, \tag{A16}$$

where

$$\beta = \frac{G_3G_4}{G_2}\left(2L + \frac{1}{G_3}\right). \tag{A17}$$

Of course, in order to have a unique determination of G_k, one has to require $\beta = \gamma$, where from (154) $\beta = 2(G_4/G_2) - G_3/G_1$. This will result again in a quadratic equation for G_1.

Much more important and informative in the investigated case, $m=-1$ turns out to be the equation for a general $n>3$:

$$-48G_5 = c_{-1-n}^{(1)}G_n + c_1^{(1)} + c_{-1}^{(0)}. \tag{A18}$$

Let us remind the reader that an expression for $c_{-1-n}^{(1)}$ can be written from (149):

$$c_{-n-1}^{(1)} = -\frac{16}{G_{n+1} - (G_4/G_2)\,G_{n-1}}. \tag{A19}$$

Also, from (A11) one has an expression for $c_1^{(1)} + c_{-1}^{(0)}$. These two expressions can be substituted into Eq. (A18), which acquires the form

$$G_n\left(G_3 - \frac{G_4}{G_2}G_1\right) = G_2G_4\left(G_{n+1} - \frac{G_2}{G_4}G_{n-1}\right). \tag{A20}$$

Now it is interesting to note that using the formulas

$$G_{n+1}=G_{2p+1}=G_3\left(\frac{G_4}{G_2}\right)^{p-1},\quad G_{n-1}=G_{2p-1}=G_3\left(\frac{G_4}{G_2}\right)^{p-2} \tag{A21}$$

from (157), it can easily be checked that the R.H.S. of (A20) is equal to zero for the case $n=2p$. The other case, $n=2p+1$, gives the same result. Therefore, from (A20) the following concise relation is obtained, expressing the proportionality of G_1 and G_2 with a coefficient of proportionality, the ratio G_3/G_4.

$$G_1=\frac{G_3}{G_4}G_2. \tag{A22}$$

APPENDIX B: ADDITIONAL SYSTEM OF EQUATIONS FOR $m=2k$

This appendix will preclude the proof, started in Sec. IX, that all the coefficient functions in the Loran function decomposition of the equation $[\rho'(z)]^2=4\rho^3-g_2(z)\rho-g_3(z)$ can be uniquely expressed, and especially those from the positive-power decomposition.

For $m=2k>0$, the corresponding equation is

$$\begin{aligned}(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}=&\,2(n+1)G_nc^{(3)}_{2(k+2)-n}+(n+1)^2G_{2n}c^{(3)}_{2(k+1)-2n}\\&+(n+1)G_nc^{(3)}_{2(k+1)-n}+2(n+1)^2G_{2n}c^{(3)}_{2(k+1)-2n}\\&+(n+1)^3G_{3n}c^{(3)}_{2k-3n}+c^{(1)}_{2(k+1)}+c^{(1)}_{2k-n}G_n+c^{(0)}_{2k}.\end{aligned} \tag{B1}$$

Additionally, fixing the value of $n=k+1$, one can obtain from (B1)

$$\begin{aligned}&(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}\\&\quad=12(k+2)^2G_{2(k+1)}+c^{(1)}_{2(k+1)}+G_{k+1}c^{(1)}_{k-1}+c^{(0)}_{2k}.\end{aligned} \tag{B2}$$

For $n=2(k+2)$ the equation is

$$\begin{aligned}&(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}\\&\quad=8(2k+5)G_{2(k+2)}+c^{(1)}_{2(k+1)}+c^{(1)}_{-4}G_{2(k+2)}+c^{(0)}_{2k}.\end{aligned} \tag{B3}$$

Subtracting the two equations, one can express $c^{(1)}_{k-1}$ as

$$c^{(1)}_{k-1}=\frac{1}{G_{k-1}}[-12(k+2)^2G_{2(k+1)}+8(2k+5)G_{2(k+2)}+c^{(1)}_{-4}G_{2(k+2)}]. \tag{B4}$$

Since $k\geqslant 1$, from this formula it is clear that all the Loran coefficients $c^{(1)}_m$ in the positive-power decomposition can be expressed, including the coefficient $c^{(1)}_0$, through which the coefficients from the negative-power decomposition in Sec. IX were expressed. Also, from (B4) $c^{(1)}_{2(k+1)}$ can be expressed (by performing the indice change $k-1\to 2(k+1)$.] If $c^{(1)}_{2(k+1)}$ is substituted back into Eq. (B3), one can express also the *even positive-power coefficients* $c^{(0)}_{2k}$ as

$$\begin{aligned}c^{(0)}_{2k}=&\,(k+2)[(k+1)^2(k+2)-16(k+3)]G_{2k+6}-[c^{(1)}_{-4}+8(2k+5)]G_{2(k+2)}\\&+\frac{1}{G_{2(k+2)}}[12(2k+5)^2G_{4(k+2)}-(32k+88+c^{(1)}_{-4})G_{2(2k+5)}].\end{aligned} \tag{B5}$$

Now let us write down Eq. (B1) for another possible value of $n=2(k+1)$:

$$(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}=4(2k+3)G_{2(k+1)}+c^{(1)}_{2(k+1)}+c^{(0)}_{2k}+c^{(1)}_{-2}G_{2(k+1)}. \tag{B6}$$

Combining (B3) and (B6), $c^{(1)}_{-2}$ can be expressed as

$$c^{(1)}_{-2}=\frac{1}{G_{2(k+1)}}[-4(2k+3)G_{2(k+1)}+8(2k+5)G_{2(k+2)}+c^{(1)}_{-4}G_{2(k+2)}]. \tag{B7}$$

The coefficient $c^{(1)}_{-4}$ can easily be calculated from (142) and (148) to be

$$c^{(1)}_{-4}=\frac{16[3(G_2/G_4)(G_2G_k-G_4G_{k-2})-20G_4G_{k-2}]}{G_2G_k-G_4G_{k-2}}. \tag{B8}$$

On the other hand, it is important to observe that $c^{(1)}_{-2}$ can be calculated independently also from Eq. (143) and (148):

$$c^{(1)}_{-2}=\frac{12(G_2G_k-G_4G_{k-2})-16G_4G_k}{G_2G_k-G_4G_{k-2}}. \tag{B9}$$

Note also that from relations (157) for G_{2p} and G_{2p+1} it follows

$$\frac{G_{k-2}}{G_k}=\frac{G_2}{G_4}\text{for}\ \ k=2p\ \ \text{and}\ \ k=2p+1 \tag{B10}$$

or, written in another way, $G_2G_k-G_4G_{k-2}=0$.

Setting up equal the two expressions (B7) and (B9) for $c^{(1)}_{-2}$, canceling the equal denominators and *subsequently* taking into account (B10), one can obtain the following concise recurrent relation,

$$G_k=\alpha(k)G_{k-2}, \tag{B11}$$

where $\alpha(k)$ denotes

$$\alpha(k)=20\frac{G_{2(k+2)}}{G_{2(k+1)}}. \tag{B12}$$

Continuing further the recurrent relation (B11), one can derive

$$G_k=\alpha(k)\alpha(k-2)\cdots\alpha(k-(k-3))G_{k-(k-1)}=\text{coeff}\cdot\frac{G_{2(k+2)}}{G_{2(k+1)}}\frac{G_{2k}}{G_{2(k-1)}}\frac{G_{2(k-2)}}{G_{2(k-3)}}\cdots\frac{G_{2.5}}{G_{2.4}}G_1. \tag{B13}$$

If $k=2p$, the numerical coefficient in (B13) will be 20^p.

A similar relation can be obtained by fixing $n=2(k+1)$. Then the corresponding equation is

$$(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}=4(2k+3)G_{2(k+1)}+c^{(1)}_{-1}G_{2(k+1)}+c^{(1)}_{2(k+1)}+c^{(0)}_{2k}. \tag{B14}$$

Substracting this equation from (B6) for $n=2(k+1)$ and taking into account expression (B4) for $c^{(1)}_{k-1}$, one can obtain

$$\frac{G_{k+1}}{G_{k-1}}[c^{(1)}_{-4}+8(2k+5)]G_{2(k+2)}=G_{2(k+1)}[c^{(1)}_{-2}+4(2k+3)+12(k+2)^2]\frac{(G_{k+1}-G_{k-1})}{G_{k-1}}, \tag{B15}$$

where $c_{-4}^{(1)}$ is given by (B8) and $c_{-2}^{(1)}$ by (B9). Substituting the above expressions into (B15) and again taking into account that $G_2G_k-G_4G_{k-2}=0$, one derives the following recurrent relation:

$$G_{2(k+1)}=20\frac{G_{k-1}}{G_{k+1}}. \tag{B16}$$

If this relation is substituted into (B11), then it can be derived that

$$G_k^2G_{k+1}=20G_{k-1}G_{k-2}G_{k+2}. \tag{B17}$$

This equality is valid for $k\geqslant 3$. For $k=3,5,7,9$ the above relation may be written as

$$G_3^2G_8=20G_1G_5, \quad G_5^2G_{12}=G_3G_7, \tag{B18}$$

$$G_7^2G_{16}=G_5G_9, \quad G_9^2G_{20}=G_7G_{11}. \tag{B19}$$

Since on the L.H.S. of (B18) and (B19) G_8, G_{12}, G_{16} and G_{20} are zero, the R.H.S. should also be zero. If $G_1\neq 0, G_3\neq 0$, the R.H.S. of the first pair of equations (B18) equals zero if $G_5=G_7=0$. But since G_5 and G_7 appear also on the R.H.S. of the second pair of equations (B19), the R.H.S. will be zero and therefore G_9 and G_{11} may be different from zero. The treatment of the subsequent equations is analogous. That is why one may conclude that a pair of even sums G_{2l+1}, G_{2l+3} $(l\geqslant 2)$ is zero, but the next pair G_{2l+5}, G_{2l+7} may be different from zero.

The last fixing of the value of $n=2k/3$ for the case $m=2k$ gives the equation

$$(k+2)[(k+1)^2(k+2)-8(2k+5)]G_{2k+6}=4\left(1+\frac{2k}{3}\right)^3G_{2k}+c_{2(k+1)}^{(1)}+c_{4k/3}^{(1)}G_{2k/3}+c_{2k}^{(0)}. \tag{B20}$$

Substracting from (B20) Eq. (B6) for $n=2(k+1)$ and setting up $2k/3=p$, one can derive

$$[12(p+1)+c_{-2}^{(1)}]G_{3p+2}-4(1+p)^3G_{3p}-c_{2p}^{(1)}G_p=0. \tag{B21}$$

Similarly, substracting from (B20) Eq. (B3) for $n=2(k+2)$, one obtains

$$4(1+p)^3G_{3p}+c_{2p}^{(1)}G_p-8(3p+5)G_{3p+4}-c_{-4}^{(1)}G_{3p+4}=0. \tag{B22}$$

From the two equations it follows

$$[12(p+1)+c_{-2}^{(1)}]G_{3p+2}=[8(3p+5)+c_{-4}^{(1)}]G_{3p+4}. \tag{B23}$$

Again taking into account (B7) for $c_{-2}^{(1)}$ and (B8) for $c_{-4}^{(1)}$ for the value of $k=3p$, one can obtain

$$G_{3p+4}=20\frac{G_{3p+2}}{G_{3p-2}}G_{3p}. \tag{B24}$$

However, in view of the relations (B18) and (B19) and the consequences from them, the last relation will make sense only when *each* of the indices $3p+4, 3p+2, 3p-2, 3p$ equals one of the indices $2l+5, 2l+7$ $(l\geqslant 2)$ and then the relation (B24) will be nonzero.

APPENDIX C: ADDITIONAL SYSTEM OF EQUATIONS FOR $m=2k+1$ AND $m=-k$

For $m=2k+1$ the corresponding equation is

$$-8(2k+5)(k+3)G_{2k+7}=c^{(3)}_{2k+5}+2(n+1)G_n c^{(3)}_{2k+5-n}+(n+1)^2 G_{2n}c^{(3)}_{2k+3-2n}$$
$$+(n+1)G_n c^{(3)}_{2k+3-n}+2(n+1)^2 G_{2n}c^{(3)}_{2k+3-2n}$$
$$+(n+1)^3 G_{3n}c^{(3)}_{2k+1-3n}+c^{(1)}_{2k+3}+c^{(1)}_{2k+1-n}G_n+c^{(0)}_{2k+1}. \quad \text{(C1)}$$

The important conclusion, which can be made from this equation, is the following: *if* $c^{(1)}_{2k+3}$ *is calculated from (B4) for value of* $k'-1=2k+3$, *then the odd number coefficients* $c^{(0)}_{2k+1}$ *can also be found!* Remember also that in Appendix B only the even number coefficients $c^{(0)}_{2k}$ were found [formula (B5)]. In order to express $c^{(0)}_{2k+1}$, it is enough to set up $n=2k+3$ in (C1), when from all the coefficients $c^{(3)}_m$ only the second term on the R.H.S. will be nonzero. Then

$$c^{(0)}_{2k+1}=-c^{(1)}_{2k+3}-c^{(1)}_{-4}G_{2k+5}-8(k+3)(2k+5)G_{2k+7}-16(k+3)G_{2k+5}. \quad \text{(C2)}$$

For another value of $n=(2k+3)/2$, Eq. (C1) acquires the following form:

$$-8((k+3)(2k+5)G_{2k+7})=3(2k+5)^2G_{2k+3}+c^{(1)}_{2k+3}+c^{(1)}_{(2k-1)/2}G_{(2k+3)/2}+c^{(0)}_{2k+1}. \quad \text{(C3)}$$

But since $c^{(1)}_{(2k-1)/2}$ and $G_{(2k+3)/2}$ have to be integers, this will be possible if for example $2k-1=2p$. For this value of k, one can express $c^{(0)}_{2p+2}$ from (C3):

$$c^{(0)}_{2p+2}=-c^{(1)}_{2p+4}-c^{(1)}_p G_{p+2}-12(p+3)^2G_{2p+4}-8(p+3)(2p+7)G_{2p+8}. \quad \text{(C4)}$$

However, $c^{(0)}_{2p+4}$ can be expressed also from Eq. (B2) for values of $m=2k$, $n=k+1$ and $k=p+2$:

$$c^{(0)}_{2p+2}=-c^{(1)}_{2p+4}-c^{(1)}_p G_{p+2}-12(p+3)^2G_{2p+4}$$
$$+(p+3)[(p+3)(p+2)^2-8(2p+7)]G_{2p+8}. \quad \text{(C5)}$$

From the two equations (C4) and (C5), one easily obtains

$$16(p+3)(2p+7)G_{2p+8}=0. \quad \text{(C6)}$$

Since the coefficient in front of G_{2p+8} is a positive one, (C6) will be fulfilled if

$$G_{2p+8}=G_{2k+6}=0. \quad \text{(C7)}$$

The last means that *the even-number sums* $G_6, G_8, G_{10}, \ldots$ *are zero!*

Again fixing the value of $n=2k+3$, one derives from (C1) the equation

$$-8(k+3)(2k+5)G_{2k+7}=[8(k+2)+c^{(1)}_{-2}]G_{2k+3}+c^{(1)}_{2k+3}+c^{(0)}_{2k+1}. \quad \text{(C8)}$$

Combining this equation with (C3), setting $2k-1=2p$, one can express $c^{(1)}_p$,

$$c^{(1)}_p=-\frac{(A(p)-c^{(1)}_{-2})G_{2p+4}}{G_{p+2}}, \quad \text{(C9)}$$

where

$$A(p)=3(2p+1)^2+26(2p+1)+59. \quad \text{(C10)}$$

Comparing this expression with formulas (B4) for $c^{(1)}_p$ and taking into account (B8) and (B9), one derives the following relation:

$$G_{2(p+3)}=\frac{1}{20}\frac{G_{2(p+2)}}{G_{2(p-2)}}. \quad \text{(C11)}$$

Expressing by means of (B15) $G_{2(p+2)}$ and $G_{2(p-2)}$ and substituting into (C11), one can obtain the relation also in another form,

$$G_{2(p+3)}=\frac{1}{20}\frac{G_{p+2}}{G_p}\frac{G_{p-4}}{G_{p-2}}. \tag{C12}$$

and from the two expressions one can obtain also the ratio $G_{2(p+2)}/G_{2(p-2)}$ without any numerical coefficients. Note also that (C11) and (C12) refer to nonzero even numbers of G_m since we have $2p=2k-1$, and the relations should be written in respect to k and not p.

The corresponding equation is

$$-8(k+3)(2k+5)G_{2k+7}=\tfrac{4}{27}(2k+4)^3G_{2k+1}+c^{(1)}_{2k+3}+G_{(2k+1)/3}c^{(1)}_{(4k+2)/3}+c^{(0)}_{2k+1}. \tag{C13}$$

Setting $2k+1=3p$ and keeping in mind that $c^{(1)}_{2p}$ and $c^{(1)}_{3p+2}$ can be found from (B4), one can express $c^{(0)}_{3p}$ as

$$c^{(0)}_{3p}=-\tfrac{4}{3}(3p+4)(3p+5)G_{3p+6}-4(p+1)^3G_{3p}-c^{(1)}_{3p+2}-G_pc^{(1)}_{2p}. \tag{C14}$$

The equation for the last case of $m=-k$ $(k>3,\ k\neq 6)$ is

$$\begin{aligned}&c^{(3)}_{4-k}+2(n+1)G_nc^{(3)}_{-k+4-n}+(n+1)^2G_{2n}c^{(3)}_{-k+2-2n}+(n+1)G_nc^{(3)}_{-k+2-n}\\&\quad+2(n+1)^2G_{2n}c^{(3)}_{-k+2-2n}+(n+1)^3G_{3n}c^{(3)}_{-k-3n}+c^{(1)}_{-k+2}+c^{(1)}_{-k-n}G_n+c^{(0)}_{-k}=0.\end{aligned} \tag{C15}$$

Since it has been shown already how all the Loran coefficient functions can be expressed and the treatment of this equation is completely analogous to the preceeding ones, Eq. (C15) shall not be considered.

APPENDIX D: COEFFICIENT FUNCTIONS N_1, N_2, N_3 AND N_4 DEPENDING ON THE "BAR" VARIABLES

The coefficient functions N_1, N_2, N_3 and N_4 in the cubic algebraic equation (112) for T in Sec. VII are the following:

$$\begin{aligned}N_1\equiv&2\,\overline{p}_1^2Z^2-2Z^4\overline{p}_1\left(\frac{O^2\overline{p}_1}{4}+\frac{O}{2}\overline{p}_2+\overline{p}_3\right)-Z^4\overline{p}_1(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3)\\&+Z^6(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3)\left(\frac{O^2\overline{p}_1}{4}+\frac{O\overline{p}_2}{2}+\overline{p}_3\right),\end{aligned} \tag{D1}$$

$$\begin{aligned}N_2\equiv&8Z\overline{p}_1^2-Z^2\overline{p}_1(\overline{p}_2+O\overline{p}_1)+[Z^4(\overline{p}_2+O\overline{p}_1)-16Z^3\overline{p}_1]\left(\frac{O^2}{4}\overline{p}_1+\frac{O}{2}\overline{p}_2+\overline{p}_3\right)\\&+(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3)\left[-\frac{15}{2}Z^3\overline{p}_1+\frac{23}{2}Z^5\left(\frac{O^2}{4}\overline{p}_1+\frac{O}{2}\overline{p}_2+\overline{p}_3\right)\right],\end{aligned} \tag{D2}$$

$$\begin{aligned}N_3\equiv&\left(\frac{O^2}{4}\overline{p}_1+\frac{O}{2}\overline{p}_2+\overline{p}_3\right)[30Z^4(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3)+8Z^3(\overline{p}_2+O\overline{p}_1)-24\overline{p}_1Z^2]+8\overline{p}_1^2\\&-4Z\overline{p}_1(\overline{p}_2+O\overline{p}_1)-8Z^2\overline{p}_1(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3),\end{aligned} \tag{D3}$$

$$N_4 \equiv -4\overline{p}_1(\overline{p}_2+O\overline{p}_1)+6Z\overline{p}_1(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3)+[-18Z^3(O^2\overline{p}_1+O\overline{p}_2+2\overline{p}_3) + 12Z^2(\overline{p}_2+O\overline{p}_1)]\left(\frac{O^2}{4}\overline{p}_1+\frac{O}{2}\overline{p}_2+\overline{p}_3\right). \tag{D4}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

Application of Poisson maps on coadjoint orbits of Sp(6,*R*) group to many body dynamics

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(Received 11 December 2002; accepted 20 February 2003)

The canonical transformation approach generated by the semisimple subgroup $GCM(3)\subset Sp(6,R)$ is applied to reduction of the Lie–Poisson bracket on coadjoint orbits of the $Sp(6,R)$ group and the Poisson coalgebra $sp_O^*(6)$ is determined. Investigating the construction of the N-particle phase, induced by this reduction, we identify the Poisson coalgebra $sp_O^*(6)$ as the algebra of quadratic $O(K)$, $K\equiv N-1$ invariant forms on symplectic $6K-12$ dimensional phase space $T^*[O(K-3)\backslash O(K)]$, $K\geqslant 3$. The general classification scheme of Poisson orbits for $sp_O^*(6)$ is found and applied to the classification of coadjoint orbits of the $Sp(6,R)$ group occurring in the decomposition of N-particle phase spaces. We show that the $sp_O^*(k)$, $k=4,6$ Poisson action on some class of surfaces determined by Casimir invariants is not transitive. The Poisson maps for all classes of orbits $sp_O^*(4)$ and $sp_O^*(6)$ are found. The quantum unitary irreducible representations of $sp_O^*(4)$ are obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1571222]

I. INTRODUCTION

As follows from the previous study to be presented in Secs. II and III, the total kinetic energy of a many-particle system can be separated into two terms. The microscopic formulation of the problem of extracting collective energy, by using the group theory method based on the semisimple GCM(3) subgroup of $Sp(6,R)$ group, has been studied in Refs. 1 and 2. The theoretical motivation for realization of this program was the Bohr–Mottelson unified model.[3,4] The microscopic group theoretical model based on GCM(3) with constrained kinetic energy[5] restates the classical fluid dynamics of Dedekind–Riemann ellipsoids.[6]

The $Sp(6,R)$ group was recognized as an appropriate group for the many-body theory of nuclear collective motion,[7–9] which establishes an important link between the collective dynamics and nuclear shell model. The mathematical methods have been developed for calculating the discrete infinite-dimensional unitary representations of $sp(6,R)$ algebra. In the cycle of papers (Refs. 10–12) the authors investigate the collective nuclear dynamics based on the $sp^*(4)$ dynamical coalgebra. Generalized vector coherent state theory,[13–17] the boson approach,[18] and the fermion realization[19] have been employed. The procedure for evaluating the matrix elements of general two-body interaction of the types used in the standard treatments of the nuclear many-body system[20,21] have been found.

A different approach,[22] closer to the original ideas,[1–5] as well to the theoretical methods developed on the basis of generalized hyperspherical coordinates,[23–25] which includes both parts of the kinetic energy and in which the role of the nuclear shell structure follows via effective cranked deformed harmonic potential obtained in the explicit form and depending on the $sp^*(6,R)$ Casimirs invariants, has been proposed. In this approach, the second term of the kinetic energy is described with the help of the six components of the symmetric three-dimensional matrix **Y** which augmented by an antisymmetric part, namely, the Kelvin circulation **J**, generates the nine-

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dimensional nonlinear Poisson coalgebra here denoted by $\mathrm{sp}_{\mathrm{O}}^{*}(6)$. The main aim of the paper is to obtain the classification scheme for the Poisson orbits of $\mathrm{sp}_{\mathrm{O}}^{*}(2\,p)$ in the cases $p=2$ and $p=3$ and to find Poisson maps for all classes of orbits of these structures.

In Secs. II and III we present the approach based on our earlier investigations,[22] which, via the theory of coadjoint transformations, separate the collective and the reduced single-particle kinetic energy and which give the physically important reduction for the Poisson brackets on coadjoint orbits of the $\mathrm{Sp}(6,R)$ group. The $\mathrm{sp}_{\mathrm{O}}^{*}(6)$ coalgebra is obtained, in the natural way, by introducing the symplectic space $T^{*}[\mathrm{SO}(N-4)\backslash\mathrm{SO}(N-1)]$, $N\geqslant 4$ essential for construction of many-particle phase spaces.

In Sec. IV we construct the Poisson representation for $\mathrm{sp}_{\mathrm{O}}^{*}(4)$ orbits. The classification scheme for the orbits of $\mathrm{sp}_{\mathrm{O}}^{*}(6)$ is presented in Sec. V and is applied for the $\mathrm{Sp}(6,R)$ group classification of many-particle phase spaces. Poisson maps for orbits of $\mathrm{sp}_{\mathrm{O}}^{*}(6)$ are found in Sec. VI. The singular classes of orbits, important for the introduced classification, are obtained in Sec. VII. The unitary irreducible finite dimensional representations of $\mathrm{sp}_{\mathrm{O}}^{*}(4)$ are found in Sec. VIII.

We hope that the result of this paper might also be useful as applied to few-particle dynamics. However, the presented material aims at application to the collective body dynamics ($N\gg 7$).

II. LIE–POISSON BRACKETS ON THE COADJOINT ORBITS OF THE Sp(6,*R*) GROUP

The physics interpretation of elements of the $\mathrm{sp}^{*}(6,R)$ coalgebra can be obtained by considering the $2N$-dimensional symplectic space. Let us introduce the points of this space with the help of the rectangular $6\times N$-dimensional matrix $\rho(\vec{r}_1,\ldots,\vec{r}_N)=(\vec{r}_1,\ldots,\vec{r}_N)$ $(\vec{r}_i)_\alpha=m_i^{1/2}\,(\vec{x}_{\alpha i}-\vec{\mathcal{X}}_\alpha)$, $(\vec{r}_i)_{3+\alpha}=m_i^{-1/2}\,(\vec{p}_i-m_i M^{-1}\,\vec{\mathcal{P}}_\alpha)$ where i is the particle number, $\vec{x}_i$, $\vec{p}_i$ are the spatial and the momentum coordinates of the ith particle obeying the canonical Poisson bracket relations: $\{x_{\alpha i},x_{\beta j}\}=\{p_{\alpha i},p_{\beta j}\}=0$, $\{x_{\alpha i},p_{\beta j}\}=\delta_{\alpha\beta}\,\delta_{ij}$, m_i are the masses of particles, M is the total mass, $(\vec{\mathcal{X}},\vec{\mathcal{P}})=(\Sigma m_i\,\vec{x}_i,M^{-1}\,\Sigma\vec{p}_i)$ are the vectors of coordinates and momenta of the center of mass motion.

Consider the following mapping:

$$\rho\mapsto x=\rho\cdot{}^{t}\rho\cdot K_6=\begin{pmatrix}\mathbf{U} & -\mathbf{Q}\\ \mathbf{P} & -{}^{t}\mathbf{U}\end{pmatrix},\quad K_6=\begin{pmatrix}\mathbf{0} & -\mathbf{1}\\ \mathbf{1} & \mathbf{0}\end{pmatrix},\tag{1}$$

$$U_{\alpha\beta}=\sum_i x_{\alpha i}\,p_{\beta i}-\mathcal{X}_\alpha\,\mathcal{P}_\beta,\quad Q_{\alpha\beta}=\sum_i m_i\,x_{\alpha i}\,x_{\beta i}-M\,\mathcal{X}_\alpha\,\mathcal{X}_\beta,\tag{2}$$

$$P_{\alpha\beta}=\sum_i m_i^{-1}\,p_{\alpha i}\,p_{\beta i}-M^{-1}\,\mathcal{P}_\alpha\,\mathcal{P}_\beta.\tag{3}$$

The elements of the matrices (**U**, **Q**, **P**) form a natural system of collective coordinates. The Poisson brackets for them follow from the canonical rules of particle coordinates and momenta: $\{X_{\alpha\beta},X'_{\gamma\delta}\}^{\mathrm{can}}_{x(\rho)}$, $X\in\{\mathbf{U},\mathbf{Q},\mathbf{P}\}$. The components of (**U**,**Q**,**P**) are scalars of the left translations generated by the coordinates of the center of mass motion: $\{X_{\alpha\beta},\mathcal{Y}_\gamma\}=0$ for $\vec{\mathcal{Y}}\in\{\vec{\mathcal{X}},\vec{\mathcal{P}}\}$.

There is another way of introducing the Poisson structure.[26–30] Using the standard notation for $\mathrm{gl}(3,R)$ generators $E_{ij}:(E_{ij})_{kl}=\delta_{ik}\,\delta_{jl}$, we introduce the base for the $\mathfrak{g}=\mathrm{sp}(6,R)$ algebra $\mathrm{sp}(6,R)=\{x\in\mathrm{gl}(6,R):\ x\cdot K+K\cdot{}^{t}x=\mathbf{0}_{6\times 6}\}$:

$$\hat{U}_{\alpha\beta}=E_{\beta\alpha}-E_{\alpha+3\beta+3},\quad \alpha,\beta=1,2,3,\tag{4}$$

$$\hat{Q}_{\alpha\beta}=-E_{\alpha+3\beta}-E_{\beta+3\alpha},\quad \hat{P}_{\alpha\beta}=E_{\alpha\beta+3}+E_{\beta\alpha+3},\quad 1\leqslant\alpha\leqslant\beta\leqslant 3.\tag{5}$$

With the help of x we define the mapping $\mathrm{sp}(6,R)$ algebra onto **R**, more precisely,

$$\mathfrak{g}^*\times\mathfrak{g}\mapsto\mathbf{R}: \quad \langle x,\hat{Y}\rangle=\tfrac{1}{2}\ \text{trace}\ \ x\cdot\hat{Y}, \quad X_{\alpha\beta}=\langle x,\hat{X}_{\alpha\beta}\rangle, \quad X=U,Q,P. \tag{6}$$

Then, the Lie–Poisson bracket[31] is defined as

$$\{X_{\alpha\beta},X'_{\gamma\delta}\}_x^{\mathrm{LP}}=\langle x,[\hat{X}_{\alpha\beta},\hat{X}'_{\gamma\delta}]\rangle. \tag{7}$$

The matrices x are identified with the points of dual space $\mathrm{sp}^*(6,R)$. In the case considered we have $\mathrm{sp}^*(6,R)=\mathrm{sp}(6,R)$. Both the brackets coincide: $\{.,.\}^{\mathrm{can}}=\{.,.\}^{\mathrm{LP}}=\{.,.\}$.

The $\mathrm{Sp}(6,R)$ group acts on the algebra by adjoint transformations $\hat{X}\mapsto\mathrm{Ad}_g(\hat{X})=g\cdot\hat{X}\cdot g^{-1}$. The coadjoint representation is the action of the group G on the real vector space $\mathfrak{g}^*$, $\mathrm{Ad}^*: G\mapsto\mathrm{End}(\mathfrak{g}^*)$, $\mathrm{Ad}^*_g(x)=x\circ\mathrm{Ad}_{g^{-1}}$; hence $(\mathrm{Ad}^*_g(x))(\hat{X}_{\alpha\beta})=\frac{1}{2}\,\mathrm{trace}\,x\cdot g^{-1}\cdot\hat{X}\cdot g=\frac{1}{2}\,\mathrm{trace}\,g\cdot x\cdot g^{-1}\cdot\hat{X}$, and we get: $\mathrm{Ad}^*_g(x)=g\cdot x\cdot g^{-1}$. The Lie–Poisson bracket is nondegenerated on coadjoint orbits.[32]

Taking into account that **Q** and **P** are positive definite let us decompose the matrices (**U**, **Q**, **P**) in the following way:

$$\mathbf{U}=\mathbf{d}\cdot\boldsymbol{\lambda}\cdot{}^t\mathbf{v}, \quad \mathbf{Q}=\langle m\rangle\,\mathbf{d}\cdot\boldsymbol{\lambda}^2\cdot{}^t\mathbf{d}, \quad \mathbf{P}=\langle m\rangle^{-1}\,\mathbf{d}\cdot[\,\mathbf{v}\cdot{}^t\mathbf{v}+\boldsymbol{\lambda}^{-1}\cdot\mathbf{Y}\cdot\boldsymbol{\lambda}^{-1}]\cdot{}^t\mathbf{d}, \tag{8}$$

where $\langle m\rangle=N^{-1}M$, $\mathbf{d}\in\mathrm{SO}(3)$ and $\boldsymbol{\lambda}$ is a diagonal matrix $\boldsymbol{\lambda}=\mathrm{diag}(\lambda_A,\lambda_B,\lambda_C)$, $\lambda_X\geqslant 0$, $\mathbf{v}\in\mathrm{gl}(3,R)$, **Y** is a positive definite and symmetric matrix. The representation in Eq. (8) results from the coadjoint transformation

$$\mathrm{sp}^*_{\mathrm{O}}(6)\ni\mathbf{a}(\mathbf{j},\mathbf{m})\mapsto x(\mathbf{d},\boldsymbol{\lambda},\mathbf{v},\mathbf{Y})=\mathrm{Ad}^*_{g(\sqrt{\langle m\rangle}\,\mathbf{d}\cdot\boldsymbol{\lambda},\,\mathbf{X})}(a(\mathbf{j},\mathbf{m})), \tag{9}$$

where

$$\mathrm{sp}^*_{\mathrm{O}}(6)=\left\{\,a(\mathbf{j},\mathbf{m})=\begin{pmatrix}-\frac{1}{2}\mathbf{j} & -1_{3\times3}\\ \mathbf{m} & -\frac{1}{2}\mathbf{j}\end{pmatrix}, \quad {}^t\mathbf{j}=-\mathbf{t}, \quad {}^t\mathbf{m}=\mathbf{m}\right\}, \tag{10}$$

under the substitutions

$$\mathbf{j}=\boldsymbol{\lambda}\cdot\mathbf{v}-{}^t\mathbf{v}\cdot\boldsymbol{\lambda}, \quad \mathbf{m}=\mathbf{Y}-\tfrac{1}{4}\mathbf{j}\cdot\mathbf{j}, \quad \mathbf{X}=\tfrac{1}{2}(\boldsymbol{\lambda}\cdot\mathbf{v}+{}^t\mathbf{v}\cdot\boldsymbol{\lambda}), \tag{11}$$

and where $g(a,u)$ are the elements of the fifteen–dimensional semidirect subgroup[2] $G=\mathrm{GCM}(3)\subset\mathrm{Sp}(6,R)$, $g(h,X)=\overline{h}(h)\cdot\overline{u}(u)$, $h\in\mathrm{GL}_+(3,R)$, $u={}^tu$. We denoted

$$\overline{h}(h)=\begin{pmatrix}h & \mathbf{0}\\ \mathbf{0} & {}^th^{-1}\end{pmatrix}, \quad \overline{u}(u)=\begin{pmatrix}\mathbf{1} & \mathbf{0}\\ u & \mathbf{1}\end{pmatrix}. \tag{12}$$

The group $\mathrm{CM}(3)\subset\mathrm{GCM}(3)$ obtained by the reduction: $\mathrm{GL}_+(3,R)\searrow\mathrm{SL}(3,R)$ has been applied to the collective nuclear dynamics in Ref. 1. The elements G obey the following rule of composition: $g(h,u)\cdot g(h',u')=g(h\cdot h',{}^th'\cdot u\cdot h'+u')$, hence $g^{-1}(h,u)=g(h^{-1},-{}^tg^{-1}\cdot u\cdot g^{-1})$.

The matrix **d** transforms the rest frame of references to the body frame. The solution to the matrix $\mathbf{v}=\mathbf{v}(\mathbf{l},\boldsymbol{\lambda},\mathbf{p}_\lambda,\mathbf{j})$ which regards the first relation in (11), suspended by the condition $\boldsymbol{\lambda}\cdot{}^t\mathbf{v}-\mathbf{v}\cdot\boldsymbol{\lambda}=\mathbf{l}$, where **l** is the antisymmetric angular momentum matrix, takes the following form:

$$\mathbf{v}=\mathbf{p}_\lambda+\hat{\mathbf{I}}\cdot\boldsymbol{\lambda}+\boldsymbol{\lambda}\cdot\hat{\mathbf{j}} \quad \text{where} \quad (\hat{\mathbf{x}})_{mn}=\begin{cases}0 & \text{if } m=n\\ (\lambda_m^2-\lambda_n^2)^{-1}x_{mn} & \text{if } m\neq n,\end{cases} \tag{13}$$

and then

$$\mathbf{X}=\boldsymbol{\lambda}\cdot\mathbf{p}_\lambda+\boldsymbol{\lambda}\cdot\hat{\mathbf{I}}\cdot\boldsymbol{\lambda}+\tfrac{1}{2}(\boldsymbol{\lambda}^2\cdot\hat{\mathbf{j}}+\hat{\mathbf{j}}\cdot\boldsymbol{\lambda}^2), \tag{14}$$

where the indices $X=\{A,B,C\}$ label the components of the matrices: $(\boldsymbol{\lambda},\mathbf{l},\mathbf{j},\mathbf{Y})$ and the right–hand side indices of the matrix $\mathbf{d}$.

If $\lambda_A\neq\lambda_B\neq\lambda_C$ [see Eq. (13)], i.e., if the eigenvalues of the matrix Q are nondegenerated, the formulas presented define the transformation $\boldsymbol{\tau}: W\ni\mathbf{w}=(\mathbf{d},\mathbf{l},\boldsymbol{\lambda},\mathbf{p}_\lambda,\mathbf{j},\mathbf{Y})\mapsto(\mathbf{U},\mathbf{Q},\mathbf{P})\in \mathrm{sp}^*(6,R)$ where $\mathbf{p}_\lambda=\mathrm{diag}(p^\lambda{}_A,p^\lambda{}_B,p^\lambda{}_C)$.

The transformation τ^{-1} is well definite as the mapping $\mathrm{sp}^*(6,R)\ni U\mapsto W/H_{\mathrm{oct}}$ where set U does not contain surfaces $\lambda_X=\lambda_Y$. Here $H_{\mathrm{oct}}\subset \mathrm{SO}(3)$ is the octahedral symmetry group consisting of 24 elements. The group H_{oct}, sometimes called the gauge symmetry group or the unambiguity group, is generated by the eigenvalue system: $\mathbf{Q}\cdot\mathbf{d}=\mathbf{d}\cdot\boldsymbol{\lambda}^2$ whose solutions to $\mathbf{d}$ are given modulo to the group transformations $H_{\mathrm{oct}}: \mathbf{d}\mapsto\mathbf{d_h}=\mathbf{d}\cdot\mathbf{h}$. This induces the action on W: $(H_{\mathrm{oct}},W)\ni(\mathbf{h},\mathbf{w})\mapsto\mathbf{w_h}=(\mathbf{d}\cdot\mathbf{h},\ \mathrm{Ad}_{\mathbf{h}^{-1}}(\mathbf{l}),\ldots,\mathrm{Ad}_{\mathbf{h}^{-1}}(\mathbf{Y}))$ and then the coset space W/H_{oct} is obtained from the formula

$$W/H_{\mathrm{oct}}=\{\mathbf{w}\in W,\ \ \mathbf{w}\equiv\mathbf{w}'\Leftrightarrow\mathbf{w}'=\mathbf{w_h},\ \mathbf{h}\in H_{\mathrm{oct}}\},\tag{15}$$

then $\mathrm{sp}^*(6,R)\equiv W/H$, which solves the problem of unique parametrization of orbit spaces.

Application of the transformation rules for the Poisson brackets $\{X_{\alpha\beta},X'_{\gamma\delta}\}_{\pi(\mathbf{w})}=(\partial_a\tau_{\alpha\beta})\times(\mathbf{w})\times(\partial_b\tau'_{\gamma\delta})(\mathbf{w})\times\{w_a,w_b\}_{\mathbf{w}}$, $(\mathbf{X},\mathbf{X}')\in(\mathbf{U},\mathbf{Q},\mathbf{P})$ lead to reduction of the Poisson structure. This reduction separates the orbit space into three commuting subspaces (see also the text in Sec. III):

$$\mathrm{sp}^*(6,R)\equiv(\mathrm{rot}^*(3),\ \ \mathrm{shape}^*(3),\ \ \mathrm{sp}^*_{\mathrm{O}}(6)).\tag{16}$$

For the space W we can rewrite the latter in the form $W=\mathrm{rot}^*(3)\times\mathrm{shape}^*(3)\times\mathrm{sp}^*_{\mathrm{O}}(6)$. Here $\mathrm{rot}^*(3)=(\mathbf{d},\mathbf{l})$ and $\mathrm{shape}^*(3)=(\boldsymbol{\lambda},\mathbf{p}_\lambda,1)\equiv\mathfrak{H}(3)$–is the Heisenberg algebra. The coordinates λ_X give the length of the principal axes for the ellipsoids of the density of the mass distribution. The Poisson brackets for nine elements of the $\mathrm{sp}^*_{\mathrm{O}}(6)$ coalgebra read[22]

$$\{J_X,J_Y\}=-\epsilon_{XYZ}J_Z,\quad \{J_X,Y_{YZ}\}=-\epsilon_{XYT}Y_{TZ}-\epsilon_{XZT}Y_{YT},\tag{17a}$$

$$\{Y_{XY},Y_{ZT}\}=-j_{XZ}Y_{YT}-j_{XT}Y_{YZ}-j_{YZ}Y_{XT}-j_{YT}Y_{XZ},\tag{17b}$$

where $\mathbf{J}=(J_A,J_B,J_C)$, $J_C=j_{AB}$, cycl C,A,B is the Kelvin circulation.

The traces of powers of matrices $a(\mathbf{j},\mathbf{m})=\overline{a}(\mathbf{J},\mathbf{Y})$ determine three independent invariants of the $\mathrm{sp}^*_{\mathrm{O}}(6)$ coalgebra. It is convenient to present the result by using the following invariants:

$$C_2(\overline{\mathbf{a}})=\sum_X\ (Y_{XX}+J_X{}^2),\quad \overline{C}_4(\overline{\mathbf{a}})=\sum_{X>Y}\ (Y_{XX}Y_{YY}-Y_{XY}{}^2)+\sum_{X,Y}\ J_XY_{XY}J_Y,\tag{18}$$

$$\overline{C}_6(\overline{\mathbf{a}})=\det\mathbf{Y},\tag{19}$$

whose values at the point $\overline{\mathbf{a}}_{\mathbf{f}}=\overline{\mathbf{a}}(\mathbf{J}=\mathbf{0},\mathbf{Y}=\mathrm{diag}(f_1^2,f_2^2,f_3^2))$ reads

$$C_2(\overline{\mathbf{a}}_{\mathbf{f}})=\sum_i\ f_i^2,\quad \overline{C}_4(\overline{\mathbf{a}}_{\mathbf{f}})=\sum_{i>j}\ f_i^2f_j^2,\quad \overline{C}_6(\overline{\mathbf{a}}_{\mathbf{f}})=(f_1f_2f_3)^2.\tag{20}$$

The families of surfaces

$$\langle f_1,f_2,f_3\rangle'=\left\{\overline{\mathbf{a}}(\mathbf{J},\mathbf{Y}):\ \ C_2(\overline{\mathbf{a}})=\sum_i\ f_i^2,\quad \overline{C}_4(\overline{\mathbf{a}})=\sum_{i>j}\ f_i^2f_j^2,\quad \overline{C}_6(\overline{\mathbf{a}})=(f_1f_2f_3)^2\ \right\}\tag{21}$$

are symplectic manifolds. However, as we will discuss further, in the cases $f_3=0$, they are not transitive $\mathrm{sp}^*_{\mathrm{O}}(6)$ spaces, i.e., they are not single orbits.

The definition of the orbit, which should be applied here, can be obtained with the help of the Poisson bracket: $\mathrm{A}^*_\psi:\mathfrak{h}^*\mapsto\mathfrak{h}^*$, $\mathfrak{h}^*\ni\varphi\mapsto\mathrm{A}^*_\psi(\varphi)(\mathbf{x})=(\exp\circ\mathrm{ad}^*{}_\psi)(\varphi)(\mathbf{x})$ where $(\mathrm{ad}^*{}_\psi(\varphi))(\mathbf{x})=\{\varphi,\psi\}_\mathbf{x}$, φ and ψ are functions on symplectic space $\langle f_1,f_2,f_3\rangle'\ni\mathbf{x}\mapsto\psi(\mathbf{x})\in R$. If $u^i(\mathbf{x})=x^i$, $i=1,\ldots,n$, $n\geqslant\dim\langle f_1,f_2,f_3\rangle'$ is some coordinates system, for example $(\mathbf{J},\mathbf{Y})$, we can define: $\mathcal{O}(\mathbf{x})=\{(y^1,\ldots,y^n),\ y^i=\mathrm{A}^*_\psi(u^i)(\mathbf{x}),\ i=1,\ldots,n\}$. For such orbits we have

$$\dim\mathcal{O}(\mathbf{x})=\mathrm{rank}\ \ |\mathbf{K}(\mathbf{x})|,\quad \mathbf{K}(\mathbf{x})=\{u^i,u^j\}_\mathbf{x}. \tag{22}$$

As will be discussed in Secs. V and VII, the six-dimensional surfaces $\langle f_1,f_2,0\rangle'$ contain two four-dimensional $\mathrm{sp}^*_\mathrm{O}(6)$ orbits.

III. REDUCTION OF *N*-PARTICLE PHASE SPACE

The expression for momentum of the ith particle which is consistent with the formula in (8) for the elements of matrix $\mathbf{P}$ has the form

$$\vec{p}_i=\frac{m_i}{M}\vec{\mathcal{P}}+\vec{P}\,(\vec{x})+\vec{p}\,'_i\,,\quad \vec{P}\,(\vec{x}_i)=m_i\,\vec{V}(\vec{x}),\quad \sum_i\,\vec{p}\,'_i\equiv 0,\quad \sum_i\,\vec{P}(\vec{x}_i)\cdot\,\vec{p}\,'_i=0, \tag{23}$$

where

$$\vec{V}(\vec{x})=\langle m\rangle^{-1}\,\mathbf{d}\cdot\mathbf{v}\cdot\boldsymbol{\lambda}^{-1}\cdot{}^t\mathbf{d}\cdot(\vec{x}-\vec{\mathcal{X}}) \tag{24}$$

defines the linear velocity field.

The Jacobi orthogonal N-dimensional matrices $\mathcal{J}=\mathcal{J}(\mathbf{m}):J_{Ni}=\sqrt{m_i/M}$ define the symplectic mapping of the "Jacobi+center of mass" space onto the original phase space: $(\overline{\mathbf{x}},\vec{\mathcal{X}},\overline{\mathbf{p}},\vec{\mathcal{P}})\mapsto(\mathbf{x},\mathbf{p})=(\mathcal{X}_\alpha+(\overline{\mathbf{x}}\cdot\mathcal{J})_{\alpha i}\,m_i^{-1/2},\ M^{-1}\,m_i\,\mathcal{P}_\alpha+(\overline{\mathbf{p}}\cdot\mathcal{J})_{\alpha i}\,m_i^{1/2})$. We have: $(\mathbf{U},\mathbf{Q},\mathbf{P})=(\overline{\mathbf{x}}\cdot{}^t\overline{\mathbf{p}},\ \overline{\mathbf{x}}\cdot{}^t\overline{\mathbf{x}},\ \overline{\mathbf{p}}\cdot{}^t\overline{\mathbf{p}})$. Taking into account the formulas in Eq. (23) we can write

$$\overline{\mathbf{x}}=\mathbf{d}\cdot\boldsymbol{\lambda}\cdot\mathbf{r},\quad \overline{\mathbf{p}}=\mathbf{d}\cdot(\mathbf{v}\cdot\mathbf{r}+\boldsymbol{\lambda}^{-1}\cdot\boldsymbol{\pi}), \tag{25a}$$

$$\mathbf{1}_{3\times 3}=\mathbf{r}\cdot{}^t\mathbf{r},\quad \mathbf{0}_{3\times 3}=\boldsymbol{\pi}\cdot{}^t\mathbf{r}, \tag{25b}$$

where $\mathbf{r}$ and $\boldsymbol{\pi}$ are the rectangular $3\times N-1$-dimensional matrices for which the constraining conditions result from the last relations in Eq. (23). The expression for the total kinetic energy takes the form

$$T=T_\mathrm{CM}+T_{\vec{V}}+T_\mathrm{rsp},\quad T_\mathrm{rsp}=(2\,\langle m\rangle)^{-1}\sum_X\,\lambda_X^{-2}\,Y_{XX}, \tag{26}$$

$$\mathbf{Y}=\boldsymbol{\pi}\cdot{}^t\boldsymbol{\pi},\quad T_{\vec{V}}=\frac{1}{2}\sum_i\,m_i\,{}^t\vec{V}(\vec{x}_i)\cdot\vec{V}(\vec{x}_i)=(2\,\langle m\rangle)^{-1}\,\mathrm{trace}\ \ \mathbf{v}\cdot{}^t\mathbf{v}, \tag{27}$$

where T_CM is the energy of center of mass motion, $T_{\vec{V}}$ is the energy of the Dedekind–Riemann model of ellipsoids. We will call T_rsp the reduced single-particle kinetic energy.

Interesting interpretation of coordinates $(\mathbf{r},\mathbf{j},\boldsymbol{\pi})$ is obtained by calculation of the pull back of the symplectic canonical two-form $\boldsymbol{\omega}(\overline{\mathbf{x}},\overline{\mathbf{p}})=\Sigma_{\alpha i}d\overline{x}_{\alpha i}\wedge d\overline{p}_{\alpha i}$. Applying the notation $\omega_\mathrm{r}={}^t\mathbf{d}\cdot d\,\mathbf{d}$, where $d\mathbf{x}$ is the matrix: $(d\mathbf{x})_{mn}=d\,x_{mn}$, dx_{mn} are one-forms, $\mathbf{x}\wedge\cdot\mathbf{y}$ denote the outer product contracted according to the rules of matrix multiplication, we find $(N\geqslant 4)$ the following formula:

$$\Omega=\Omega_{\mathrm{rot}*(3)}+\Omega_{\mathrm{shape}*(3)}+\Omega_{M_{(3,N-1)}}, \tag{28a}$$

$$\Omega_\mathrm{rot}=\tfrac{1}{2}\,\mathrm{trace}\ \boldsymbol{\omega}_\mathrm{r}\wedge\cdot(d\mathbf{l}-\mathbf{l}\cdot\boldsymbol{\omega}_\mathrm{r}),\quad \Omega_\mathrm{shape}=\sum_a\,d\lambda_a\wedge dp_a\,, \tag{28b}$$

$$\Omega_{\mathrm{M}_{(3,N-1)}}=\mathrm{trace}\,d\mathbf{r}\wedge\cdot\,d\,{}^t\mathbf{t},\quad \mathbf{t}=\boldsymbol{\pi}+\tfrac{1}{2}\,\mathbf{j}\cdot\mathbf{r}. \tag{28c}$$

Taking into consideration the constraints on $(\mathbf{r},\mathbf{t})$ in Eq. (25b) and the fact that $\mathbf{j}$ is antisymmetric, we get: $\mathbf{r}\cdot{}^t\mathbf{t}+\mathbf{t}\cdot{}^t\mathbf{r}=\mathbf{0}_{3\times 3}$. It is helpful to use the second formula in Eq. (28c) as a coordinate transformation $\sigma:(\mathbf{r},\mathbf{j},\boldsymbol{\pi})\mapsto(\mathbf{r},\mathbf{t}=\boldsymbol{\pi}+\frac{1}{2}\mathbf{j}\cdot\mathbf{r})$ and to define the $p\ \ (2K-p-1)$-dimensional symplectic manifold $M(2p,K),\ \ p\leqslant K$,

$$M(2p,K)=\left\{\hat{\rho}(\mathbf{r},\mathbf{t})=\begin{pmatrix}\mathbf{r}\\ \mathbf{t}\end{pmatrix}\in M_{2p,K},\ \ \mathbf{r}\cdot{}^t\mathbf{r}=\mathbf{1},\ \ \mathbf{r}\cdot{}^t\mathbf{t}+\mathbf{t}\cdot{}^t\mathbf{r}=\mathbf{0},\quad \Omega(\mathbf{r},\mathbf{t})=\sum_{\alpha,k} dr_{\alpha k}\wedge dt_{\alpha k}\right\}, \tag{29}$$

equivalent to $T^*[\mathrm{O}(K-p)\backslash\mathrm{O}(K)]$ $({}^t\hat{\rho}\in T^*[\mathrm{O}(K)/\mathrm{O}(K-p)])$. If $K=N-1\geqslant 3$, the calculation of inversion for σ gives

$$\sigma^{-1}:\quad \mathbf{j}(\mathbf{r},\mathbf{t})=\mathbf{t}\cdot{}^t\mathbf{r}-\mathbf{r}\cdot{}^t\mathbf{t},\quad \boldsymbol{\pi}(\mathbf{r},\mathbf{t})=\mathbf{t}\cdot\Pi(\mathbf{r}), \tag{30a}$$

$$\Pi(\mathbf{r})=\mathbf{1}_{N-1\times N-1}-{}^t\mathbf{r}\cdot\mathbf{r}. \tag{30b}$$

Defining the mapping $\hat{\rho}(\mathbf{r},\mathbf{t})\mapsto\hat{x}$ in the same way as $\rho\mapsto x$ in Eq. (1) i.e., $\hat{x}(\mathbf{r},\mathbf{t})=\hat{\rho}\cdot{}^t\hat{\rho}\cdot K_6$ and noticing the identities: $\mathbf{r}\cdot{}^t\mathbf{t}=-\frac{1}{2}\mathbf{j}$, $\mathbf{t}\cdot{}^t\mathbf{t}=\mathbf{Y}-\frac{1}{4}\mathbf{j}\cdot\mathbf{j}$, we get

$$M(6,N-1)\ni\hat{\rho}(\mathbf{r},\mathbf{t})\mapsto\hat{x}=\begin{pmatrix}-\frac{1}{2}\mathbf{j} & -\mathbf{1}\\ \mathbf{t}\cdot{}^t\mathbf{t} & -\frac{1}{2}\mathbf{j}\end{pmatrix}=\overline{\mathbf{a}}(\mathbf{j},\mathbf{Y}). \tag{31}$$

Hence, $\hat{\rho}(\mathbf{r},\mathbf{t})=\hat{\rho}(\mathbf{r}\cdot g,\mathbf{t}\cdot g)$, $g\in\mathrm{O}(N-1)$ and the symplectic space $M(6,N-1)$, in a natural way, defines the space $\mathrm{sp}^*_{\mathrm{O}}(6)=\{\overline{\mathbf{a}}(\mathbf{j},\mathbf{Y})\}\sim M(6,N-1)/\mathrm{O}(N-1)\equiv T^*[\mathrm{O}(N-4)\backslash\mathrm{O}(N-1)]/\mathrm{O}(N-1)$ as an algebra of the quadratic $\mathrm{O}(N-1)$ invariant forms on $M(6,N-1)$. The results of Sec. II give

$$\boldsymbol{\gamma}_{\mathbf{j}}:\quad [\mathrm{rot}^*(3),\mathrm{shape}^*(3)]\ni[(\mathbf{d},\mathbf{l}),(\boldsymbol{\lambda},\mathbf{p}_\lambda)]=\mathbf{w}\mapsto\boldsymbol{\gamma}_{\mathbf{j}}(\mathbf{w})\in\mathrm{GCM}(3), \tag{32}$$

where the mapping $\boldsymbol{\gamma}_{\mathbf{j}}(\mathbf{w})=\overline{g}(\mathbf{w},\mathbf{X}(\mathbf{w},\mathbf{j}))$ is defined by Eqs. (9) and (13) which enable one to rewrite the formulas in Eq. (25a) in the following form:

$$\Gamma:\quad [\mathrm{rot}^*(3),\mathrm{shape}^*(3),M(6,N-1)]\ni[\mathbf{w},\hat{\rho}(\mathbf{r},\mathbf{t})]\mapsto\begin{pmatrix}\mathbf{x}\\ \mathbf{p}\end{pmatrix}=\boldsymbol{\gamma}_{\mathbf{j}}(\mathbf{w})\cdot\begin{pmatrix}\mathbf{r}\\ \mathbf{t}\end{pmatrix}\in\mathcal{J}(3,N-1), \tag{33}$$

where $\mathcal{J}(3,N-1)$ denotes the Jacobi N-particle phase space. It establishes the physical role of the $6N-18$-dimensional manifold $M(6,N-1)$ which physically can be identified with $\mathfrak{H}_{\mathrm{c.m.}}(3)\times\mathrm{rot}^*(3)\times\mathrm{shape}^*(3)$ reduced phase space. Here, $\mathfrak{H}_{\mathrm{c.m.}}(3)$ denotes the Heisenberg coalgebra of the center of mass motion.

In the cases $N=2,3,4$, the matrix $\Pi(\mathbf{r})$ is the projection onto the null vector space: hence $\mathbf{Y}=\mathbf{0}$.

The obvious modification should be done in order to include the cases $N=2$ and $N=3$. Then, $(\mathbf{r},\mathbf{t})\in M(2N-2,N-1)$.

In the case $N=2$, $(\dim M(2,1)=0)$, $\boldsymbol{\lambda}=(\lambda_A)$ and the scheme leads to the spherical coordinates: $x_\alpha=x_\alpha(\theta,\varphi,\lambda_A)=d_{\alpha A}(\theta,\varphi)\,\lambda_A$, $p_\alpha=\Sigma_q x_{\alpha,q}(\theta,\varphi,\lambda_A)\,p_q$, $q\in\{\theta,\varphi,\lambda_A\}$, $d=d(\theta,\varphi)\in\mathrm{SO}(3)/\mathrm{SO}(2)$. The ambiguity group $H=H_{\mathrm{oct}}\to\mathrm{id}$.

For $N=3$, $\mathbf{d}\to\mathbf{d}'\in M_{3\times 2}$, ${}^t\mathbf{d}'\cdot\mathbf{d}'=\mathbf{1}_{2\times 2}$, $(\mathbf{d}',\mathbf{l}')\equiv T^*\mathrm{SO}(3)$, $\boldsymbol{\Lambda}'=\mathrm{diag}\,(\Lambda_A,\Lambda_B)$ for $\boldsymbol{\Lambda}=\boldsymbol{\lambda},\mathbf{p}_\lambda$, then $\mathbf{X}'\in M_{2\times 2}$ and $\boldsymbol{\gamma}(\mathbf{w})=\overline{\mathbf{d}'}(\mathbf{d}')\cdot\overline{\boldsymbol{\lambda}'}(\boldsymbol{\lambda}')\cdot\overline{X'}(\mathbf{w})\in M_{6\times 4}$. The space $M(4,2)$ is two dimensional:

$$M(4,2)=\left\{\begin{pmatrix}\mathbf{r}\\ \mathbf{t}\end{pmatrix},\ \mathbf{r}=\mathbf{r}(\varphi)=\begin{pmatrix}\cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi\end{pmatrix},\ \ \mathbf{t}=\frac{1}{2}\,\mathbf{r}_{,\varphi}\,p,\ \ \Omega(\varphi,p)=d\varphi\wedge dp\right\},\quad \mathbf{j}=p\,K_2. \tag{34}$$

The three-dimensional representation of the group $H_{\rm oct}$ reduces to the two-dimensional representation of the group: $H'=\{\mathbf{r}(0),\mathbf{r}(\pi/2),\mathbf{r}(\pi),\mathbf{r}(3\,\pi/2)\}$.

The case of four particles is determined by the representation of $M(6,3)$:

$$M(6,3)=\left\{\begin{pmatrix}\mathbf{r}\\ \mathbf{t}\end{pmatrix},\ \ \mathbf{r}=e^{\theta_3\hat{L}_3}\cdot e^{\theta_2\hat{L}_2}\cdot e^{\theta_1\hat{L}_3},\ \mathbf{t}=\frac{1}{2}\mathbf{j}\cdot\mathbf{r},\ \ \Omega=\sum\ d\theta_i\wedge dp_i\right\}. \tag{35}$$

Here $\mathbf{j}=\Sigma_X J_X(\boldsymbol{\theta},\mathbf{p})\,\hat{L}_X\cdot\mathbf{r}$, $(\hat{L}_Z)_{XY}=-\epsilon_{ZXY}$ and $(J_A\pm i\,J_B)(\boldsymbol{\theta},\mathbf{p})=-(\sin^{-1}\theta_2\,p_1+i\,p_2-\cot\theta_3\,p_3)\,e^{\pm i\,\theta_3}$, $J_C(\boldsymbol{\theta},\mathbf{p})=-p_3$ is the Poisson representation of the Kelvin circulation.

In all cases, we should extend the action of the transformation group $H_{\rm oct}$ (H') on the elements of $M(6,N-1)$. It is given by the left group translations: $(H_{\rm oct},M(6,N-1))\ni[h,\hat{\rho}(\mathbf{r},\mathbf{t})]\mapsto\hat{\rho}(h\cdot\mathbf{r},h\cdot\mathbf{t})\in M(6,N-1)$. This extension solves the problem of reversibility[22] of mapping Γ. Namely, the transformation Γ^{-1} should be considered as: $\mathcal{J}'(3,N-1)\mapsto[\mathrm{rot}^*(3),\mathrm{shape}^*(3),M(6,N-1)]/H$ where $H=H_{\rm oct},H'$ or $H=\mathrm{id}$, according to the particle number N. On $\mathcal{J}'(3,N-1)\subset\mathcal{J}(3,N-1)$ the eigenvalues of tensor $\mathbf{Q}$ have to be nondegenerated.

Taking into account these modifications we find the dimensions of phase spaces:

$$\dim\ \mathrm{rot}^*(3)+\dim\ \mathrm{shape}^*(3)=\begin{cases}6+6 & \text{if } N\geqslant 4\\ 6+4 & \text{if } N=3\\ 4+2 & \text{if } N=2.\end{cases} \tag{36}$$

Two representations of $\mathrm{so}^*(N-1)$ obtained by considering the mapping $\varrho\mapsto\mathbf{o}(\varrho)=-{}^t\varrho\cdot K_6\cdot\varrho\in\mathrm{so}^*(N-1)$, (a) for $\varrho=\overline{\rho}$ and (b) for $\varrho=\hat{\rho}$ are equal and we have: $\overline{\mathbf{o}}\equiv\hat{\mathbf{o}}=\vec{x}_n\cdot\vec{p}_m-\vec{x}_m\cdot\vec{p}_n$. The direct calculation gives: $\hat{\mathbf{o}}={}^t\mathbf{r}\cdot\mathbf{t}-{}^t\mathbf{t}\cdot\mathbf{r}$ and $\overline{\mathbf{o}}={}^t\mathbf{r}\cdot\boldsymbol{\pi}-{}^t\boldsymbol{\pi}\cdot\mathbf{r}+{}^t\mathbf{r}\cdot\mathbf{j}\cdot\mathbf{r}=\hat{\mathbf{o}}(\sigma(\mathbf{r},\mathbf{j},\boldsymbol{\pi}))$. The Poisson bracket on $M(6,K)$ has been obtained in Ref. 22 using, as the basis, the coordinates $(\mathbf{r},\mathbf{j},\boldsymbol{\pi})$.

IV. POISSON MAPS FOR $\mathrm{sp}^*_{\mathrm{O}}(4,R)$

The coadjoint transformation for $g=e^{i\pi\hat{J}_C}$ is the involution of $\mathrm{sp}^*_{\mathrm{O}}(6)$ which separates their elements into two classes, the even and the odd signature parity elements: $\mathrm{Ad}_g(X)=\pm X$ according to the sign. The even part consists of the four elements $\mathrm{sp}^*_{\mathrm{O}}(4):\mathrm{sp}^*_{\mathrm{O}}(4)=(J_C,Y_{AA},Y_{BB},Y_{AB})$ and Y_{CC}. The system of Poisson brackets for $\mathrm{sp}^*_{\mathrm{O}}(4)$ can be rewritten using the complex system of coordinates

$$\{J_0,Y^*_{\pm 2}\}=\mp i\,2\,Y^*_{\pm 2},\quad \{Y_0,Y^*_{\pm 2}\}=\pm\,i\,4\,J_0\,Y^*_{\pm 2},\quad \{Y^*_2,Y^*_{-2}\}=-i\ \ 8\,J_0\,Y_0, \tag{37a}$$

where

$$J_0=J_C,\quad Y_0=Y_{AA}+Y_{BB},\quad Y^*_{\pm 2}=Y_{AA}-Y_{BB}\pm 2\,i\,Y_{AB}. \tag{37b}$$

The Poisson rules in formula (37) are restated by considering the two-dimensional phase spaces $p_A>p_B\geqslant 0$,

$$\langle p_A,p_B\rangle'=\{(e^{i\,\varphi_C},p_C)\in\mathrm{S}^1\times[-p_A+p_B,p_A-p_B],\quad \{\varphi_C,p_C\}=1\ \}, \tag{38}$$

and by performing the following mapping:

$$J_0=p_C,\quad Y_0(\mathbf{p})=p_A^2+p_B^2-p_C^2,\quad Y^*_{\pm 2}=\sqrt{W}(\mathbf{p})\,e^{\pm i\varphi_C}, \tag{39a}$$

where

$$\sqrt{W}(\mathbf{p})=a_{-1,A}(\mathbf{p})\,a_{+1,A}(\mathbf{p})=a_{-1,B}(\mathbf{p})\,a_{+1,B}(\mathbf{p}), \tag{39b}$$

$$a_{\mu,m}(\mathbf{p})=\sqrt{p_A+p_B+\mu\, p_C}\,\sqrt{p_A-p_B+\mu\,\epsilon_m\, p_C},\quad \mu=\pm 1,\quad \epsilon_A=-\epsilon_B=1, \tag{39c}$$

and where p_m, $m=A,B$ are some new momenta which commute with all elements of $\mathrm{sp}^*_{\mathrm{O}}(4)$.

The domains of the given maps are open sets which we find noticing that the functions $Y^*_{\pm 2}$ are differentiable if $|p_C|\leqslant p_A-p_B$ only. The momenta p_A,p_B are the Poisson invariants. It is convenient to consider the following two invariant functions (Casimirs):

$$c_2(J,Y)=Y_0+J_0^2,\quad c_4(J,Y)=Y_{AA}\,Y_{BB}-Y_{AB}^2=\tfrac{1}{4}(Y_0^2+Y_2\,Y_{-2}). \tag{40}$$

On $\langle p_A,p_B\rangle'$ they take the following values:

$$c_2(p_A,p_B)=p_A^2+p_B^2,\quad c_4(p_A,p_B)=p_A^2\,p_B^2. \tag{41}$$

In the cases $p_B>0$ the values of Casimirs identify the orbits in a unique way; hence $\langle p_A,p_B\rangle=\langle p_A,p_B\rangle'$ where $\langle p_A,p_B\rangle$ denotes the orbit space.

In the cases $p_B=0$ it is not true. Namely, for two points $J_C=\pm p_A$, using the relations given in Eqs. (40) and (41) we find: $Y_{\pm 2}=Y_0=0$. Hence, all Poisson brackets in Eq. (37) vanish. Let $\mathcal{P}(X)$ denote the projection of X onto the momentum space. We have

$$\mathcal{P}(\langle p,0\rangle')=\mathcal{P}(\langle p,0\rangle)+\sum_{\sigma=\pm}\mathcal{P}(\langle f,\emptyset\rangle_{\pm}),\quad \langle f,0\rangle=\{(e^{i\,\varphi_C},p_C)\in \mathrm{S}^1\times(-f,f)\}, \tag{42}$$

where $\langle p_A,\emptyset\rangle_{\pm}$ are two zero-dimensional orbits represented by two single points $J_C=p_C=\pm p_A$, respectively. The class of zero-dimensional orbits include also the point: $\langle 0,0\rangle\equiv\langle 0,\emptyset\rangle_{\pm}\equiv(Y_\mu=0,J_0=0)$. The expressions $Y_\mu,\mu=\pm 2,0$ are even functions of momenta $\mathbf{p}$. It means that the conditions $p_A\geqslant p_B\geqslant 0$ wear out of all nonequivalent solutions.

The function $W(p_A,p_B,p_C)$ is positive if: (a) $|p_A-p_B|\leqslant p_C$ as well if (b) $J_0\geqslant p_A$.

The additional family of solutions could not be applied to the considered coalgebra. It results from the assumption $\mathrm{sp}^*_{\mathrm{O}}(4)\subset\mathrm{sp}^*_{\mathrm{O}}(6)$. The three-dimensional Kelvin circulation algebra $\mathrm{so}^*{}_J(3)\subset\mathrm{sp}^*_{\mathrm{O}}(6)$ is compact. Through the relation $J^2=\overline{G}^{XY}J_X\,J_X$, the Kelvin circulation defines the metric $\overline{\mathbf{G}}$ which is Euclidian $\overline{\mathbf{G}}={}^t\mathbf{d}\cdot\mathbf{E}\cdot\mathbf{d}=\mathbf{1},\mathbf{E}=\mathbf{1}$. The signature of the metric $\mathbf{E}$ has been established by the choice of the inertia tensor, and consequently, by the choice of the group $G=\mathrm{GCM}(3)$.

V. CLASSIFICATION SCHEME FOR $\mathrm{sp}^*_{\mathrm{O}}(6,R)$ ORBITS

In the next section we investigate the $\mathrm{sp}^*_{\mathrm{O}}(6)$ orbits considering the families of six-dimensional symplectic maps $M_{(f_1,f_2,f_3)},f_1>f_2>f_3>0$:

$$\mathcal{P}_{\mathbf{f}}=\{(p_A,p_B,p_C)\in(f_1,f_2)\times(f_2,f_3)\times(p_A,p_B)\}, \tag{43}$$

$$M_{\mathbf{f}}=\left\{(\mathbf{q},\mathbf{p}),\mathbf{q}=(\varphi_A,\varphi_B,\varphi_C)(\mathrm{mod}\,2\,\pi),\mathbf{p}\in\mathcal{P}_{\mathbf{f}},\quad \Omega(\mathbf{q},\mathbf{p})=\sum_X d\varphi_X\wedge dp_X\right\}, \tag{44}$$

and two four-dimensional ones $M_{(f,f,f_3)}$ and $M_{(f_1,f_3,f_3)}$, obtained by removing the canonical pairs (φ_A,p_A) and (φ_B,p_B), respectively.

The material of Sec. IV exhibits an important feature of the orbits $\mathrm{sp}^*_{\mathrm{O}}(4)$. There are surfaces distinguished by the $\mathrm{sp}^*_{\mathrm{O}}(4)$ values of Casimir functions which are not transitive subspaces: hence, Casimir functions do not specify the orbits uniquely. A similar effect of splitting out of orbits occurs for the coalgebra $\mathrm{sp}^*_{\mathrm{O}}(6)$ if $f_3=0$.

Theorem 1: $\mathrm{sp}^*_{\mathrm{O}}(6)$ *Poisson action on the* $d_{f_1f_2}=6-2\,\delta_{f_1f_2}-2\,\delta_{f_20}$*-dimensional manifold* $M_{(f_1,f_2,0)}$, $f_1>0$ *splits out* $M_{(f_1,f_2,0)}$ *onto the* $d_{f_1f_2}$*-dimensional orbit* $\langle f_1,f_2,0\rangle$ *and onto two* $d_{f_1f_2}-2$ *dimensional orbits* $\langle f_1,f_2,\emptyset\rangle_\pm$. *The orbits* $\langle f_10,\emptyset\rangle_\pm$ *are equivalent. For all orbits:* $f_3=0$ *the following formula holds*

$$\text{rank}\ \ \mathbf{Y}=2-\delta(f_2,0)-\delta(r,\emptyset),\quad r\in\{0,\emptyset\}. \tag{45}$$

The model of additional orbits $\langle f_1,f_2,\emptyset\rangle_\pm$, is easily obtained by considering the orbits of the SO(4) group. Let $\mathcal{O}_{(f,\pm g)}=\{(\mathbf{J},\mathbf{K}),\ \mathbf{J}^2+\mathbf{K}^2=f^2+g^2,\ \mathbf{J}\cdot\mathbf{K}=\pm f\,g\},\ 0\leqslant g\leqslant f$. Then, via the definition of the Poisson brackets: $\{J_X,J_Y\}=-\epsilon_{XYZ}J_Z$, $\{J_X,K_Y\}=-\epsilon_{XYZ}K_Z$, $\{K_X,K_Y\}=-\epsilon_{XYZ}J_Z$ and via the mapping: $Y_{XY}\mapsto K_XK_Y$ we get the $4-2\,(\delta_{fg}+\delta_{g0})$-dimensional models of the $\mathrm{sp}^*_{\mathrm{O}}(6)$ orbits

$$\mathcal{O}_{(f,\pm g)}\sim\langle f,g,\emptyset\rangle_\pm,\quad \mathcal{O}_{(f,0)}\sim\langle f,0,\emptyset\rangle,\quad \text{rank}\,\mathbf{Y}=1-\delta_{g0}, \tag{46}$$

for which $p_A\equiv0$ and $p_B\equiv0$ if $g=0$. The proof of the features of the classification scheme results from Eq. (46) and the formulas presented in Sec. VII.

The verification of these results can be examined in a simpler way. To this aim we can use formula (22). More precisely, let us consider the secular equation for the matrices $K^{ij}(\mathbf{a})=\{x^i,x^j\}_{\mathbf{a}}$, $i,j,\leqslant9, x^l\in\mathrm{sp}^*_{\mathrm{O}}(6)$ choosing the following four-dimensional set of points $\mathbf{a}_{\mathbf{f}\pm}(q)$:

$$\mathbf{J}_{\mathbf{f}\pm}(q)=(0,0,\pm f_{ac}\,h_q),\quad \mathbf{Y}_{\mathbf{f}\pm}(q)=\mathrm{diag}(\alpha+\beta,\alpha-\beta,f_2^2),\quad \alpha=f_a\,f_c-\tfrac{1}{2}(f_{ac}\,h_q)^2, \tag{47}$$

where $f_{ac}=f_a-f_c$, $h_q=(1-q^2)^{1/2}$, $\beta=q\,f_{ac}[(f_a+f_c)^2-(f_{ac}\,h_q)^2]^{1/2}$ and let (f_a,f_b,f_c), $f_a\geqslant f_c$ be received by a permutation of components f_i, $i\leqslant3$. We have: $c_2(\mathbf{x})=f_a^2+f_c^2$, $c_4(\mathbf{x})=(f_a\,f_c)^2$; hence, they belong to one $\mathrm{sp}^*_{\mathrm{O}}(4)$ orbit: $\langle p_A,p_B\rangle=\langle f_a,f_c\rangle$. We find

$$W(\lambda)=\det(K-\lambda\mathbf{1})=-\lambda^3\,w^{(2)}\times w^{(4)}, \tag{48a}$$

$$\begin{aligned}w^{(2)}=&-f_{ac}^2[-8\,f_a^2\,f_c^2-4\,f_a\,f_c\,(1+4\,f_a^2-10\,f_a\,f_c+4\,f_c^2)\,q^2\\&-f_{ac}^2\,(1+4\,(f_a^2-6\,f_a\,f_c+f_c^2))\,q^4+4\,f_{ac}^4\,q^6]+x^2,\end{aligned} \tag{48b}$$

$$\begin{aligned}w^{(4)}=&(f_a^2-f_b^2)^2\,(f_b^2-f_c^2)^2+[f_c^2-2\,f_a\,(1+f_b^2)^2\,f_c+f_b^4\,(2+f_c^2)+f_a^2\,(1+f_b^4+2\,f_c^2)\\&+f_{ac}^2[4\,f_a\,f_c-(1+f_b^2)^2]\,q^2+f_{ac}^4\,q^4\,]\,\lambda^2+\lambda^4,\end{aligned} \tag{48c}$$

where $f_{ac}=f_a-f_c$. The dimension of the orbit is equal to the number of nonvanishing roots of the polynomial $W(\lambda)$: $n=n_1+n_2$. Taking into account the relation $f_a=f_c\Rightarrow q=0$ we get the formulas: $n_1=2-2\,\max(\delta_{f_c0}\,\delta_{q0},\delta_{f_af_c})$, $n_2=4-2\,\delta_{f_bf_c}-2\,\delta_{f_bf_a}$ from which we can deduce the rules of dimensional space reduction. In particular, if $\mathbf{f}\neq(f,f,f)$, then the first polynomial leads to additional degeneracy if $f_c=q=0$, i.e., if $\alpha=\beta=0\Rightarrow\text{rank}\,\mathbf{Y}=1-\delta_{f_b0}$.

Taking into account Eq. (36) we can classify the coadjoint orbits of the group $\mathrm{Sp}(6,R)$ with the help of the $\mathrm{sp}^*_{\mathrm{O}}(6)$ orbits. The following formulas hold:

$$\dim\langle f_1,f_2,f_3\rangle^{\mathrm{sp}^*(6,R)}=18-2\,\delta_{f_1f_2}-2\,\delta_{f_2f_3}-8\,\delta_{f_1f_3}, \tag{49}$$

$$\dim\langle f_1,f_2,\varnothing\rangle_q^{\mathrm{sp}^*(6,R)}=16-2\,\delta_{f_1f_2}-2\,\delta_{f_20}-6\,\delta_{f_1f_2}\,\delta_{f_20}. \tag{50}$$

Using the above list it is interesting to construct the table presenting the $\mathrm{sp}^*(6,R)$ orbit classification of N-particle phase spaces

N:	2	3	4	5	6	$\geqslant 7$
$\langle \mathbf{f} \rangle$:	$\langle 0,0,0 \rangle$	$\langle f,0,\emptyset \rangle$	$\langle f,0,0 \rangle$	$\langle f_1,f_2,\emptyset \rangle_{\pm}$	$\langle f_1,f_2,0 \rangle$	$\langle f_1,f_2,f_3 \rangle$
Σd_i:	$6+0+0+0$	$10+2+2-2$	$12+4+2$	$12+4+4+4$	$12+6+4+8$	$18+6+6\,(N-5)$

In the third row of the table we display the dimensions of symplectic spaces that are important in the scheme considered: $d_1 = \dim \mathrm{rot}^*(3) + \dim \mathrm{shape}^*(3)$, $d_2 = \dim \mathrm{sp}^*_{\mathrm{O}}(6)$, $d_3 = 2q$, where q is the number of nonvanishing components of the vector $\mathbf{f}$ and d_4 suspend the result, so that $\Sigma_i d_i$ is the total dimension of Jacobi N-body phase space.

The values d_1 are valid only if all nonvanishing components of the weight vector $\mathbf{f}$ are different.

The case $N=3$ has been discussed earlier at the end of Sec. III. Two coordinates: (φ_f, f), $f^2 = \Sigma J_X^2$ are not physical in this case, so $q=2$ should by replaced by $q=0$, which improves the result.

The physics role of the dimension d_4 is elementary for the physics interpretation. Namely, d_4 is the dimension of the coadjoint orbits of group $\overline{G} = \mathrm{SO}(N-1)$; hence $d_4 = \dim \overline{G} - \dim H_{\mathbf{x}_0}$ where $\overline{G} = \mathrm{SO}(N-1)$ and $H_{\mathbf{x}_0} \subset \overline{G}$ is the stability subgroup of a point $\mathbf{x}_0 \in \mathcal{O}_{\mathbf{x}_0}$ where $\mathcal{O}^-_{\overline{x}_0} = \{\mathbf{o} \in \mathrm{so}^*(N-1), \mathbf{o} = \mathrm{Ad}^*_g(\overline{x}_0) = g \cdot \overline{x}_0 \cdot g^{-1}, g \in \overline{G}\}$. It results from the natural action of $\mathrm{SO}(N-1)$ on $M(6,N-1)$: $(\overline{G}, M(6,N-1)) \ni (g,(\mathbf{r},\mathbf{t})) \mapsto (\mathbf{r} \cdot g^{-1}, \mathbf{t} \cdot g^{-1})$. Since $\mathrm{trace}\,\mathbf{o}^{2p} = \mathrm{trace}\,\mathbf{a}^{2p}(\mathbf{j},\mathbf{m})$, so we can put: $\overline{x}_0 = \Sigma_{k \leqslant 3} f_k (E_{2k-1,2k} - E_{2k,2k-1})$. For the cases $f_1 > f_2 > f_3 > 0$; hence, if $N \geqslant 7$, the stability group $\overline{H}_{\overline{x}_0}$ is equal to: $\mathrm{SO}(2) \times \mathrm{SO}(2) \times \mathrm{SO}(2) \times \mathrm{SO}(N-7)$: thus, $d_4 = (N-1)(N-2)/2 - (N-7)(N-8)/2 - 3 = 6(N-5)$.

The assignation of the orbits in the two cases, for $N=5$ and for $N=6$, follows from the natural hierarchy of orbits determined by the rank of the matrix $\mathbf{Y}$. An independent proof of that result will not be presented here.

The above-presented discussion and the result of Sec. III enable us to assert that many particle phase spaces can be parametrized with the help of the maps

$$(\overline{\mathbf{x}},\overline{\mathbf{p}}) = (\overline{\mathbf{x}},\overline{\mathbf{p}})(q_{\mathrm{rot}\times\mathrm{shape}}, (\varphi_A,\varphi_B,\varphi_C,p_A,p_B,p_C), (f_1,f_2,f_3,\psi_1,\psi_2,\psi_3), \mathbf{q}^{(f_1,f_2,f_3)}_{\mathrm{so}^*(N-1)}), \quad (51)$$

where $\mathbf{f}$, $\boldsymbol{\psi}$ obey the canonical Poisson rules $\{\psi_i, f_j\} = \delta_{ij}$. Such maps have to be singular on the surfaces $f_i = f_j$ and $\lambda_X = \lambda_Y$.

VI. POISSON MAPS FOR $\mathrm{sp}^*_{\mathrm{O}}(6,R)$ ORBITS

In Sec. IV the orbits $\mathrm{sp}^*_{\mathrm{O}}(4)$ have been parametrized by a single canonical pair (φ_C, p_C) and two cyclic momenta p_A, p_B. Let $\psi(\mathbf{q}) = \psi'(p_A^2, p_B^2, p_A p_B, \varphi_C, p_C)$ denote the even signature parity function, $\boldsymbol{\varphi} = (\varphi_A,\varphi_B,\varphi_C)$, $\mathbf{p} = (p_A,p_B,p_C)$, $\mathbf{f} = (f_1,f_2,f_3)$ is the weight vector labeling the subspaces $\langle f_1,f_2,f_3 \rangle'$ [see Eqs. (18), (20)] and $\mathbf{z} = (J_A,J_B,J_{BC},Y_{AC})$ denote the vector of the odd parity signature coordinates. We will search for a Poisson map: $\Gamma: (\boldsymbol{\varphi},\mathbf{p},\mathbf{f}) \mapsto \mathbf{z}$ by assuming the validity of the canonical rules:

$$\{\varphi_m,\varphi_n\} = \{p_m,p_n\} = 0, \quad \{\varphi_m,p_n\} = \delta_{nm}, \quad (m,n) \in \{A,B\}. \quad (52)$$

Each Poisson bracket between a signature even and a signature odd parity elements of $\mathrm{sp}^*_{\mathrm{O}}(6)$ is linear function of the signature odd elements or it vanishes. Thus, for $H = H(\mathbf{q})$: $\{z_n, H\}_{\mathbf{q},z} = \Sigma_m z_m \mathcal{H}_{mn}(\mathbf{q}))$ and all coordinates $\mathbf{q}$ are constants of motion. The most important example is obtained for the following Hamiltonian function: $H(\mathbf{q}) = p_A^2 + p_B^2 = J_C^2 + Y_{AA} + Y_{BB}$. We get

$$\mathcal{H}\ (p_A^2+p_B^2)\ =2\begin{pmatrix} 0 & -J_C & Y_{BB} & Y_{AB} \\ J_C & 0 & -Y_{AB} & -Y_{AA} \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{53}$$

The eigensystem for this matrix determines two complex functions b_m, $m=A,B$,

$$b_m=U_m\,(p_m\,J_A+i\,Y_{BC})+i\,V_m\,(p_m\,J_B-i\,Y_{CA}), \tag{54a}$$

$$U_m=(p_C\,Y_{AA}+i\,p_m\,Y_{AB}),\quad V_m=(p_m\,\overline{p}_m^2-p_m\,Y_{AA}-i\,p_C\,Y_{AB}), \tag{54b}$$

where we used the notation: $\overline{p_A}=p_B$, $\overline{p_B}=p_A$. They obey the following Poisson relations:

$$\{b_m,H(\mathbf{p})\}=i\,2\,p_m\,b_m,\quad \{b_m^*,H(\mathbf{p})\}=-i\,2\,p_m\,b_m^*, \tag{55a}$$

$$\{b_m,\,Y_{AA}\,Y_{BB}-Y_{AB}^2\}=i\,2\,p_m\,\overline{p}_m^2, \tag{55b}$$

$$(b_m)_{,\varphi}=\hat{b}_m,\quad (\hat{b}_m)_{,\varphi}=-b_m,\quad \hat{b}_m=\gamma_m\,b_m=\gamma_m=\left(\frac{V_m}{U_m}\right)^*, \tag{55c}$$

valid for m equal to A and B. Above, for brevity, we used the notation: $\varphi_C\equiv\varphi$, $f_{,\varphi}=\{f,p_C\}$. For the functions γ_m we find the following expressions:

$$\gamma_m=\frac{-(p_m^2-p_C^2)\sqrt{W}(\mathbf{p})\cos 2\,\varphi+i\,p_m\,\overline{p}_m^2\,p_C}{h(p_m)}, \tag{55d}$$

$$h(x)=(x^2-J_C^2)\,Y_{AA}-Y_{AA}\,Y_{BB}+Y_{AB}^2 \tag{55e}$$

$$=-p_A^2\,p_B^2+\tfrac{1}{2}(x^2-p_C^2)\,(p_A^2+p_B^2-p_C^2+\sqrt{W}(\mathbf{p})\cos 2\varphi). \tag{55f}$$

Equations in (55c) say that in the Fourier decomposition of the complex functions $b_m(\varphi)$ there occur only components proportional to $e^{\pm i\,\varphi}$. Taking into account Eqs. (55a)–(55c) we write the expressions for the functions of canonical coordinates $b'_m(\boldsymbol{\varphi},\mathbf{p})=b'_\mu: b'_m=b_m\circ\Gamma$,

$$b'_m(\boldsymbol{\varphi},\mathbf{p})=e^{i\,\varphi_m}\sum_{\mu=\pm 1}R_{\mu m}(\mathbf{p})\,e^{i\,\mu\,\varphi}. \tag{56}$$

In order to find the functions $R_{\mu m}$ we use the relations (55c). The calculations give

$$\frac{R_{+m}}{R_{-m}}=e^{-i2\varphi}\,\frac{i+\gamma_m}{i-\gamma_m}=-\,\epsilon_m\,e^{-i2\varphi}\,\frac{(p_m-p_C)\,[a_{+1,m}^2-e^{i2\varphi}\,\sqrt{W}(\mathbf{p})]}{(p_m+p_C)\,[a_{-1,m}^2-e^{-i2\varphi}\,\sqrt{W}(\mathbf{p})]}=\epsilon_m\frac{(p_m-p_C)\,a_{+1,m}}{(p_m+p_C)\,a_{-1,m}}, \tag{57}$$

where $\sqrt{W}(\mathbf{p})$ and the functions $a_{\mu,m}$ have been defined in Eqs. (39b) and (39c). The result says that these ratios are real numbers. Using the previous result one also finds

$$|b'_m|^2=|R_{+m}|^2+|R_{-m}|^2+(R_{+m}\,R_{-m}^*+R_{+m}^*\,R_{-m})\cos 2\,\varphi=\frac{4\,\epsilon_m\,h(p_m)\,|R_-|^2}{a_{-1,m}^2\,(p_m+p_C)^2}. \tag{58}$$

It means that the functions $\epsilon_m\,h(p_m)$ are non-negative. Performing the calculations of the modulus of the functions b_m with the help of (54) one finds

$$b_m\, b_m^* = h(p_m)\, G(p_m), \tag{59}$$

$$G(x) = [\, Y_{BC}^2 + Y_{CA}^2 - J_A^2\, Y_{AA} - J_B^2\, Y_{BB} - 2\, J_B\, Y_{BC}\, J_C - 2\, J_A\, (J_B\, Y_{AB} + J_C\, Y_{CA})\,]\, x^2 + (J_A^2 + J_B^2)\, x^4 - Y_{AA}\, Y_{BC}^2 + 2\, Y_{AB}\, Y_{BC}\, Y_{CA} - Y_{BB}\, Y_{CA}^2 .$$

Considering the function defined by the Casimir invariants

$$\overline{G}(x) = \overline{C}_6 - \overline{C}_4\, x^2 + C_2\, x^4 - x^6, \tag{60}$$

one can show that $G - \overline{G}$ vanishes at p_m, $m = A, B$; hence, using the relations in Eq. (20)

$$G(p_m) = G_{\mathbf{f}}(p_m), \quad G_{\mathbf{f}}(x) = \prod_{i=1}^{3} (f_i^2 - x^2), \quad m = A, B, \tag{61}$$

and if we request that $(p_A, p_B) \in V_{\mathbf{f}}(p_A, p_B)$, where $V_{\mathbf{f}}(x,y)$, $(\overline{V}_{\mathbf{f}}(x,y))$ is an open set (closed),

$$V_{\mathbf{f}}(x,y): \qquad f_3 < y < f_2, \quad f_2 < x < f_1, \tag{62}$$

then, the factors $g^+(p_m) = \epsilon_m\, g(p_m)$, $g = (h, G_{\mathbf{f}})$, $\epsilon_A = -\epsilon_B = 1$ are non-negative. Comparing the result in Eq. (58) with the result in Eqs. (59) and (61) we get $R_{\mu m}$. The simplest choice of the phases leads to

$$R_{\mu m}(\mathbf{p}) = \frac{S_{\mu m}}{2}\ (p_m - \mu\, p_C)\, a_{\mu,m}(\mathbf{p})\, N_{\mathbf{f}}(p_m), \quad S_{\mu A} = 1, \quad S_{\mu B} = \mu, \tag{63}$$

$$N_{\mathbf{f}}(p_m) = \sqrt{\epsilon_m\, G_{\mathbf{f}}(p_m)} = \sqrt{p_m + f_2}\, \sqrt{\epsilon_m\, (p_m - f_2)} \prod_{\mu}\ \sqrt{f_1 + \mu p_m}\, \sqrt{p_m + \mu\, f_3}, \tag{64}$$

which lead to the final result on the functions b_m':

$$b_m'(\boldsymbol{\varphi}, \mathbf{p}) = e^{i\, \varphi_m}\, H_m(\varphi, \mathbf{p})\, N_{\mathbf{f}}(p_m), \tag{65}$$

where

$$H_m(\varphi, \mathbf{p}) = \frac{1}{2} \sum_{\mu}\ S_{\mu m}\, (p_m - \mu\, p_C)\, a_{\mu,m}(\mathbf{p})\, e^{i\, \mu\, \varphi}, \quad H_m\, H_m^* = \epsilon_m\, h_m(p_m). \tag{66}$$

Let us introduce a transformation to complex variables

$$Q_{\mu m}(J,Y) = p_m\, J_\mu + \mu\, Y_\mu, \quad J_\mu = J_A + i\, \mu\, J_B, \quad Y_\mu = Y_{CA} + i\, \mu\, Y_{BC}. \tag{67}$$

The application of the above to the functions b_m [see, Eq. (54)] leads to

$$b_m = H_m \sum_{\mu}\ U_{\mu m}\, Q_{\mu m}, \quad U_{\mu m} = -\tfrac{1}{2}\, \mu\, S_{\mu m}\, a_{-\mu,m}\, e^{i\, \mu\, x}, \tag{68}$$

where $\overline{A} = B$, $\overline{B} = A$. Comparing b_m with b_m' and removing the common factor H_m which follows from normalization, we get the linear system of equations for (J_μ, Y_μ),

$$\sum_{\mu}\ U_{\mu m}\, Q_{\mu m}(J,Y) - e^{i\, \varphi_m}\, N_{\mathbf{f}}(p_m) = 0, \quad \sum_{\mu}\ U_{\mu m}^*\, Q_{\mu m}^*(J,Y) - e^{-i\, \varphi_m}\, N_{\mathbf{f}}(p_m) = 0, \tag{69}$$

and that the solution X_μ', $X = (J,Y)$ defines mapping Γ. The solution takes the following form:

$$J'_\mu(\boldsymbol{\varphi}, \mathbf{f}, \mathbf{p}) = \sum_{\nu m} j_{\mu\nu m}\begin{pmatrix}\mathbf{f}\\ \mathbf{p}\end{pmatrix} e^{-i(\mu\varphi_C + \nu\varphi_m)}, \qquad Y'_\mu(\boldsymbol{\varphi}, \mathbf{f}, \mathbf{p}) = \sum_{\nu m} y_{\mu\nu m}\begin{pmatrix}\mathbf{f}\\ \mathbf{p}\end{pmatrix} e^{-i(\mu\varphi_C + \nu\varphi_m)}, \tag{70a}$$

where

$$j_{\mu\nu m}\begin{pmatrix}\mathbf{f}\\ \mathbf{p}\end{pmatrix} = -\mu S_{\mu m} S_{-\nu\bar{m}} a_{\nu\mu,m}(\mathbf{p}) \frac{N_{\mathbf{f}}(p_m)}{2p_m(p_A^2 - p_B^2)}, \tag{70b}$$

$$y_{\mu\nu m}\begin{pmatrix}\mathbf{f}\\ \mathbf{p}\end{pmatrix} = -S_{\mu m} S_{-\nu m} a_{\nu\mu,m}(\mathbf{p})(p_m - \mu\nu p_C) \frac{N_{\mathbf{f}}(p_m)}{2p_m(p_A^2 - p_B^2)}. \tag{70c}$$

An elementary calculation gives

$$J'_+ J'_- = [2(p_A^2 - p_B^2)^2]^{-1}\left(\sum_m (p_A^2 - p_B^2 + \epsilon_m(p_C^2 - \sqrt{W}(\mathbf{p})\cos 2\varphi_m))\left(\frac{N_{\mathbf{f}}(p_m)}{p_m}\right)^2 - 2p_C[\sqrt{(p_A - p_B)^2 - p_C^2}\, C_- + \sqrt{(p_A + p_B)^2 - p_C^2}\, C_+]\frac{N_{\mathbf{f}}(p_A) N_{\mathbf{f}}(p_B)}{p_A p_B}\right), \tag{71}$$

where we denoted $C_\pm = \cos(\varphi_A \pm \varphi_B)$. Rewriting relation (18) for invariant C_2 and using Eq. (20) we find the expression for the element Y_{CC},

$$Y'_{CC}(\boldsymbol{\varphi}, \mathbf{p}) = \sum_{i=1}^{3} f_i^2 - p_A^2 - p_B^2 - J'_- J'_+ . \tag{72}$$

The functions j and y in Eq. (70) are regular in all domain $V_{\mathbf{f}}$. The singularity of the expressions on the surface $p_B = 0$ is not essential. Indeed, the factor p_B^{-1} cancels with the numerator if the parameter f_3 is equal to zero.

VII. SINGULAR CASES OF $sp^*_O(6,R)$ ORBITS

The formulas obtained in Sec. VI are much simpler in two cases: (*a*) $f_1 = f_2 = p_A = f$ and (*b*) $f_2 = f_3 = p_B = f$. In case (*a*), the function $N_{ff_2f_2}(p_m)$ vanishes at $p_m = f = p_A$ while in the case (*b*), $N_{f_1ff}(p_m)$ vanishes at $p_m = f = p_B$. Thus, in both the cases we get the reduction of dimension of orbits by two units.

Let us, for example, consider case (*b*). For $\mathbf{f} = (f_1, f, f)$, $p_B \equiv f$, and we get

$$J'_\mu = \frac{\mu e^{-i\mu\varphi_C}}{2p_A}\sqrt{f_1^2 - p_A^2}\sum_{\nu=\pm 1} \nu a_{\mu\nu,A}(p_A, f, p_C) e^{-i\nu\varphi_A}, \tag{73a}$$

$$Y'_\mu = -\frac{e^{-i\mu\varphi_C}}{2p_A}\sqrt{f_1^2 - p_A^2}\sum_{\nu=\pm 1} a_{\mu\nu,A}(p_A, f, p_C)(p_A - \mu\nu p_C) e^{-i\nu\varphi_A}, \tag{73b}$$

$$Y'_{CC} = \frac{1}{2p_A^2}[f^2(f_1^2 + p_A^2) + (f_1^2 - p_A^2)(p_A^2 - p_C^2 + \sqrt{W}(p_A, f, p_C)\cos 2\varphi_A)], \tag{73c}$$

where $\mu = \pm 1$ and the $\sqrt{W}(\mathbf{p})$ is given in Eqs. (39b) and (39c). The components proportional to $e^{i\varphi_B}$ vanish. This decreases the number of modes and decreases the dimension of orbits $\langle f_1, f, f\rangle$.

If for $f = 0$ we put $p_C = \pm p_A$ and let $f_1 \to f$, then

$$Y'_\mu = 0, \quad Y_{CC} = 0, \quad J'_\mu|_{p_C = \pm p_A} = \mp e^{-i\mu(\varphi_C \mp \varphi_A)}\sqrt{f^2 - p_C^2}, \tag{74}$$

which leads to two equivalent, two-dimensional, orbits $\langle f,0,\emptyset\rangle$.

It is interesting to consider a more general type of configuration forming the surface $\Sigma_{f_1 f_2}:\langle f_1,f_2,0\rangle|_{p_B=0}$. Then, $|p_C|\leqslant p_A$, $p_A\in[f_2,f_1]$ and we get the following expressions:

$$X'_\mu|_{p_B=0}=\frac{e^{-i\mu\varphi_C}}{p_A^2}(h\,u_\mu(X)-f_1 f_2 p_{AC}\cos\varphi_B\, v_\mu(X)), \tag{75a}$$

$$[u_\mu(X),v_\mu(X)]=\begin{cases}[p_C\cos\varphi_A-i\mu p_A\sin\varphi_A,1] & \text{if } X=J,\\ [-p_{AC}^2\cos\varphi_A,p_C] & \text{if } X=Y,\end{cases} \tag{75b}$$

$$Y_{AB}=-\tfrac{1}{2}p_{AC}^2\sin 2\varphi_C,\quad Y_{mm}=\tfrac{1}{2}p_{AC}^2(1+\epsilon_m\cos 2\varphi_C),\qquad m=A,B, \tag{75c}$$

$$Y_{CC}=f_1^2+f_2^2-p_A^2-p_A^{-4}[(h\,p_C\cos\varphi_A-f_1 f_2 p_{AC}\cos\varphi_B)^2+p_A^2 h^2\sin^2\varphi_A], \tag{75d}$$

where $h=\sqrt{f_1^2-p_A^2}\,\sqrt{p_A^2-f_2^2}$ and $p_{AC}=\sqrt{p_A^2-p_C^2}$, for which we find

$$m_{XY}(\mathbf{Y})=\begin{vmatrix}Y_{XX} & Y_{XY}\\ Y_{XY} & Y_{XX}\end{vmatrix}=p_A^{-2}f_1^2 f_2^2 p_{AC}^2\sin^2\varphi_B\times\begin{cases}\sin^2\varphi_C & \text{if } X=B,\,Y=C\\ \cos^2\varphi_C & \text{if } X=C,\,Y=A\\ 0 & \text{if } X=A,\,Y=B.\end{cases} \tag{76}$$

The latter formulas establish the following rules:

$$\langle f_1,f_2,\emptyset\rangle_\pm=\{(\mathbf{q},\mathbf{p})\in M_{(f_1,f_2,0)},\ \ p_B=0,\ e^{i\varphi_B}=\pm 1\}. \tag{77}$$

All the presented equations provide the rules the reductions of the orbit dimensions, and they are in agreement with the material presented in Sec. V.

In Eq. (75) the dependence on φ_B occurs through the factor $f_1\ f_2\cos\varphi_B$ only: thus, in accordance with the so(4) model, we can fix the phase $\varphi_B=0$ and extend the range f_2: $|f_2|\leqslant f_1$.

VIII. FINITE DIMENSIONAL UIR OF $sp_O(4)$ ALGEBRA

The quantum form of the Poisson rules in Eq. (37) results from the relations

$$[\hat J_0,\hat Y^*_\mu]=\mu\,\hat Y^*_\mu,\quad [\hat Y^*_2,\hat Y^*_{-2}]=8\,\hat J_0\,\hat Y_0,\quad [\hat Y_0,\hat Y^*_{\pm 2}]=\mp 2\,(\hat J_0\,\hat Y^*_{\pm 2}+\hat Y^*_{\pm 2}\,\hat J_0). \tag{78}$$

For discussion of the above, let us introduce the following basis of the states:

$$|\mathbf{p}\rangle=|p_A,p_B,p_C\rangle,\quad \langle\boldsymbol{\varphi}|\mathbf{p}\rangle=(2\pi)^{-3/2}\exp\Big(i\hbar^{-1}\sum\varphi_X p_X\Big). \tag{79}$$

and consider the mapping

$$Y_0\mapsto\hat Y_0=\frac{1}{2}\sum_{r=\pm 1}Y_0(\hat p_A-\hat q,\hat p_B-\hat q-E,\hat p_C+r\,E)=(\hat p_A-q)^2+(\hat p_B-q-1)^2-\hat p_C^2-E, \tag{80a}$$

$$\hat Y^*_{\pm 2}=e^{\pm i2\hat\varphi_C}\sqrt{W(\hat p_A-\hat q,\hat p_B-\hat q-E,\hat p_C\pm E)},\quad (\hat Y^*_{\pm 2})^\dagger=\hat Y^*_{\mp 2}, \tag{80b}$$

$$J_0=p_C\mapsto\hat p_C. \tag{80c}$$

Here, E is the unit operator, $\hat q=q\,E$, and the parameter q fixes the beginning of the momentum scale. The function $\sqrt{W}$ is given in Eqs. (39b) and (39c). The application of the Schrödinger

quantization of coordinate and momentum operators: $\hat{\varphi}_X=\varphi_X$, $\hat{p}_X=-i\hbar\,\partial_{\varphi_X}$ to the given formulas restates the set of rules for the operator algebra in Eq. (78). Consider the action of the above-mentioned operators on the set of states: $|p_C\rangle=|p_A,p_B,p_C\rangle$,

$$\hat{J}_0\,|p_C\rangle=p_C\,|p_C\rangle,\quad \hat{Y}^*_{\pm 2}\,|p_C\rangle=\sqrt{W}(p_A-q,p_B-q-1,p_C\pm 1)\,|p_C\pm 2\rangle. \tag{81}$$

We find

$$0=\hat{Y}^*_{+2}\,|p_A-p_B\rangle=\hat{Y}^*_{-2}\,|-p_A+p_B\rangle, \tag{82}$$

so, if p_A-p_B is an integer number, while p_B is integer or half-integer number, then $|p_C\rangle=|\pm(p_A-p_B)\rangle$ are the highest and lowest states, respectively. It is convenient to rewrite the result using the Biedenharn pattern for carrier space of the algebra $u(2)$. Let $p_A=p_{21}$, $p_B=p_{22}$, and $p_{11}=\frac{1}{2}(p_A+p_B+p_C)$, then the set of states

$$\langle p_{12},p_{22}\rangle=\left\{|\mathrm{p}\rangle=\left|\begin{matrix}p_{21} & p_{22}\\ & p_{11}\end{matrix}\right\rangle,\quad p_{11}=p_{21},p_{21}-1,\ldots,p_{22}\right\},\qquad p_{11}\neq 1+q,\quad p_{22}\neq q, \tag{83}$$

spans the $p_{12}-p_{22}+1$ dimensional representation of the operators $\mathrm{sp}^*_{\mathrm{O}}(4)$. The conditions on the right-hand side of this formula will be discussed in the following.

Let us choose the value of the scale parameter q: $q=1$. Then, the explicit form of the expression for $Y_{\pm 2}$ is obtained from

$$\begin{aligned}H_{\pm 2}(\mathbf{p})=W(p_A-1,p_B-2,p_C\pm 1)&=(p_A-p_B\mp p_C)\,(p_A+p_B\pm p_C-2)\\ &\times(p_A-p_B\pm p_C+2)\times(p_A+p_B\mp p_C-4).\end{aligned} \tag{84}$$

Hence, $H_-|_{p_C=p_A-p_B}=H_+|_{p_C=-p_A+p_B}=2^4\,(p_A-p_B)\,(p_A-2)\,(p_B-1)$ from which we conclude that the states $p_A=m$, $p_B=1$, $p_C=\pm(p_A-p_B)$, as well as $p_A=2$, $p_B=m$, $p_C=\pm(p_A-p_B)$, are (additional) one-dimensional families of IUR,

$$|m,1\rangle_\pm=\left|\begin{matrix}m & 1\\ & p_\pm\end{matrix}\right\rangle=\left|\begin{matrix}2 & 3-m\\ & p_\pm\end{matrix}\right\rangle,\quad \begin{aligned}&Y_\mu\,|m,1\rangle_\pm=0,\quad \mu=0,\pm 2,\\ &\hat{J}_0\,|m,1\rangle_\pm=\pm(m-1)\,|m,1\rangle_\pm,\end{aligned} \tag{85}$$

where $p_+=m-1$ and $p_-=1$, and m is an odd integer number greater or equal to 2 (since, for $m=1$, dim$=1$ also results from the formula given below Eq. (83), this case is a regular one). In Eq. (85), we used the formula: $p_C=(2\,p_{11}-p_{21}-p_{22})$. These specific one-dimensional IUR results from the existence of the zero-dimensional orbits $\langle p,\emptyset\rangle_\pm$, $p>0$ for which $\mathbf{Y}=0$.

For the case $p_{22}=1$ we should modify the result in Eq. (83),

$$\langle p_{12},1\rangle=\left\{|\mathbf{p}\rangle=\left|\begin{matrix}p_{21} & 1\\ & p_{11}\end{matrix}\right\rangle,\quad p_{11}=p_{21}-1,\ldots,p_{22}-1\right\}. \tag{86}$$

The consistence of the choice of the scale parameter q with the sp$(6,R)$ IUR algebra classification should be proven. The coadjoint transformation in Eq. (9): $\mathrm{sp}^*_{\mathrm{O}}(6)\ni\mathbf{a}\mapsto x\in\mathrm{sp}^*(6,R)$ does not change the values of Casimirs C_2, $\overline{C}_4$, $\overline{C}_6$. Since the matrix $\mathbf{X}$ [see Eq. (14)] depends on $\mathbf{j}$, in the quantum theory we can conclude that they have to be mutually dependent, only. It is obvious that the same condition holds for the Casimirs of the sp$(4,R)$ and $\mathrm{sp}^*_{\mathrm{O}}(4)$. We will prove that such relations exist and just the value $q=1$ leads to the correct scaling of the components of weight vector $\vec{p}=(p_A,p_B)$.

The quantum $\mathrm{sp}^*_{\mathrm{O}}(4)$ algebra has two independent Casimir operators:

$$\hat{c}_2\,|\mathbf{p}\rangle=2\,(\hat{Y}_0+\hat{J}_0^2)\,|\mathbf{p}\rangle=c_2(p_A,p_B)\,|\mathbf{p}\rangle,\quad c_2(p_A,p_B)=8+2\,p_A\,(p_A-2)+2\,p_B\,(p_B-4). \tag{87}$$

The second invariant is slightly different than in the classic theory

$$\hat{c}_4'|\mathbf{p}\rangle=[\tfrac{1}{8}(2\hat{Y}_0^2-\hat{Y}_2\hat{Y}_{-2}-\hat{Y}_{-2}\hat{Y}_2)+\hbar^2\hat{J}_0^2]|\mathbf{p}\rangle=c_4'|\mathbf{p}\rangle,\quad c_4'=(p_A-1)^2(p_B-2)^2. \tag{88}$$

The eigenvalues of Casimir operators for the discrete series IUR of sp$(2m,R)$ are labeled by the lowest IUR of u(m) algebra $[p_1,\ldots,p_m]$ and we denote them by $\overline{c_m}(p_1,\ldots,p_m)$. In general, these eigenvalues can be obtained from the formula: $\overline{c_k}(p_1,\ldots,p_m)=(\overline{c_k})_{\mathfrak{h}}(-p_m,\ldots,-p_1)$, $\mathfrak{h}=\mathrm{sp}(2m)$, i.e., by modifying in this way the expressions for the compact sp$(2m)$ algebras. Taking into account the validity of the general formula:[32,33]

$$(\overline{c_k})_{\mathfrak{h}}(\mathbf{p})=\sum_{1\leqslant\alpha\leqslant m}[(m-\omega_\alpha)^k D_\alpha+(m+\omega_\alpha)^k D_{-\alpha}]D_0^{-1}, \tag{89}$$

where $\omega_\alpha=p_\alpha+m+1-\alpha$, $D_{\pm a}=\dim\langle p_1,\ldots,p_{\alpha-1},p_\alpha\pm1,p_{\alpha+1},\ldots,p_m\rangle_{\mathfrak{h}}$, $D_0=\dim\langle p_1,\ldots,p_m\rangle_{\mathfrak{h}}$, and noticing that $\hat{c}_4'=\frac{1}{8}\hat{c}_2^2-\hat{c}_4$ we find:

$$c_2(p_A,p_B)=\overline{c_2}(p_A,p_B)+8,\quad c_4'(p_A,p_B)=\overline{c_4'}+\tfrac{13}{4}\overline{c_2}+4. \tag{90}$$

This closes the proof of consistence for the scale parameter q. The meaning of the relations in Eq. (90) can be explained with the help of the Weil symmetry group $[W,\{\mathbf{p}\}]$. It consists of four elements $W=\{E_W,w_1,w_2,w_3\}$, $w_i\circ w_i=E$, $w_1\circ w_2=w_3$ where

$$\mathbf{p}_{w_1}=(-p_A+2,-p_B+4,p_C),\quad \mathbf{p}_{w_2}=(p_B-1,p_A+1,p_C),$$
$$(\mathbf{p})_{w_3}=(-p_B+3,-p_A+3,p_C), \tag{91}$$

which are the symmetries of algebra. In particular, we have $H_\mu(\mathbf{p}_{w_i})=H_\mu$. Both pairs of the functions (c_2,c_4') and $(\overline{c_2},\overline{c_4'})$ have the common Weil symmetry group.

The Weil symmetries reduce the number of nonequivalent UIR. The set P of nonequivalent finite dimensional UIR reads

$$P=\{\langle\tfrac{3}{2},\tfrac{3}{2}\rangle,\langle1,1\rangle,\langle2+m,1\rangle_\pm,\langle2+m,1+n\rangle,\ m=0,\tfrac{1}{2},\ldots,\ \ n=m+1,m,\ldots,0\text{ or }\tfrac{1}{2}\}. \tag{92}$$

The dimensions of these representations follow from the expression: $\dim\langle p_{21},p_{22}\rangle=p_{22}-p_{11}+1-2\,\delta_{p_{22}1}$ while $\langle p_{21},1\rangle_\pm$ are one-dimensional. The symmetry w_2 constrains the set P to two subsets: (a) $\langle p-1/2,p+1/2\rangle$ for which the finite dimensional representations do not exist, and to the set (b) $p_A-p_B=0,1,\ldots$ which we reduce with the help of the symmetry w_3 and using the unitarity condition $H_\mu\geqslant0\Rightarrow(p_A-2)(p_B-1)\geqslant0$.

Let us notice a few examples of application of the symmetry w_3 important for application to many-particle dynamics: $\langle1/2,1/2\rangle_{w_3}=\langle5/2,5/2\rangle$, $\langle3/2,1/2\rangle_{w_3}=\langle5/2,3/2\rangle$, $\langle1,1\rangle_{w_3}=\langle2,2\rangle$. As was discussed at the end of Sec. IV, $\mathrm{sp}_{\mathrm{O}}^*(4)$ also have noncompact orbits; hence for $\mathrm{sp}_{\mathrm{O}}(4)$ (operator) algebra exists a discrete series of infinite dimensional UIR. We will not discuss them here.

Summarizing the result, the finite dimensional IUR are obtained if $p_{11}-p_{22}\geqslant0$ are integer positive number, while p_{22} are integer or half-integer positive numbers. The eigenvalues of the operator $\hat{J}_0$ are integer numbers for all states.

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On the convergence to statistical equilibrium for harmonic crystals

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(Received 29 October 2002; accepted 2 January 2003)

We consider the dynamics of a harmonic crystal in d dimensions with n components, d,n arbitrary, $d,n\geqslant 1$, and study the distribution μ_t of the solution at time $t\in\mathbf{R}$. The initial measure μ_0 has a translation-invariant correlation matrix, zero mean, and finite mean energy density. It also satisfies a Rosenblatt—resp. Ibragimov–Linnik type mixing condition. The main result is the convergence of μ_t to a Gaussian measure as $t\to\infty$. The proof is based on the long time asymptotics of the Green's function and on Bernstein's ''room-corridors'' method. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1571658]

I. INTRODUCTION

Despite considerable efforts, the convergence to equilibrium for a mechanical system has remained as an extremely difficult problem. It has been recognized early on that for an infinitely extended system, possibly on top of local hyperbolicity, the flow of statistical information to infinity serves as a mechanism for relaxation. The two prime examples are the ideal gas and the harmonic crystal. We consider here the latter case. In the harmonic approximation the crystal is characterized by the displacement field $u(x)$, where $x\in\Gamma$, Γ is a regular lattice in $\mathbf{R}^d$, and $u(x)\in\mathbf{R}^n$ with n depending on the number of atoms in the unit cell. The field $u(x)$ is governed by a discrete wave equation. We will consider arbitrary d,n and for notational simplicity set $\Gamma=\mathbf{Z}^d$.

Our motivation to return to a well studied model is to a much wider class of initial measures than before. This project requires novel mathematical techniques. They have been developed for the wave and Klein–Gordon equation on $\mathbf{R}^d$ in Refs. 6–8, but the discrete structure poses extra difficulties.

Let us briefly comment on previous work. In Ref. 14 a general criterion is given which ensures mixing and Bernoulliness of the corresponding mechanical flow. Thereby the convergence to equilibrium is established for initial measures which are absolutely continuous with respect to the canonical Gaussian measure. In Ref. 14 moments of the displacement field are studied. This allows us to reduce the spectral analysis of the Liouvillian flow to the spectral properties of the dynamical group defined on solutions of finite energy. Since the crystal is assumed to be homogeneous, these spectral properties are determined by the dispersion relations $\omega_k(\theta)$, $k=1,\ldots,n$. The Liouvillian flow is mixing and even Bernoulli, if, except for crossing points, each $\omega_k(\theta)$ is a real-analytic function which is not identically constant. In particular, the Lebesgue measure of the set $\{\theta\in\mathbf{T}^d\colon \nabla\omega_k(\theta)=0\}$ is equal to zero. In Ref. 20, for the case $d=n=1$, initial

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measures are considered which have distinct temperatures to the left and to the right. In Ref. 2, again $d=n=1$, the convergence to equilibrium is proved for a more general class of initial measures characterized by a mixing condition of Rosenblatt—resp. Ibragimov–Linnik type and which are asymptotically translation-invariant to the left and to the right.

The detailed stationary phase analysis of Ref. 2 does not directly generalize to $d\geqslant 2$. Rather, we have to develop a novel ''cutoff strategy'' which more carefully exploits the mixing condition in Fourier space. This approach allows us to all d within essence the same conditions for the dispersion relations as in Ref. 14. Our extension requires the technique of holomorphic functions of several complex variables.

In parentheses we remark that, for the ideal gas, Dobrushin and Suhov[3] first realized the importance of a mixing condition on the initial measure. In Ref. 9 it is replaced by the condition of finite entropy per unit volume thus establishing convergence whenever the specific particle number, energy, and entropy are finite. No such general result seems to be available for the harmonic crystal.

We outline our main result and strategy of proof. The displacement field $u(x)$ is the deviation of the configuration of crystal atoms from their equilibrium positions. Assuming them to be small and expanding the forces to linear order yields the discrete linear wave equation,

$$\ddot{u}(x,t)=-\sum\nolimits_{y\in\mathbf{Z}^d}V(x-y)u(y,t);\qquad u|_{t=0}=u_0(x),\quad \dot{u}|_{t=0}=v_0(x),\quad x\in\mathbf{Z}^d. \tag{1.1}$$

Here $u(x,t)=(u_1(x,t),\ldots,u_n(x,t)),u_0=(u_{01},\ldots,u_{0n})\in\mathbf{R}^n$ and correspondingly for v_0. $V(x)$ is the interaction (or force) matrix, $(V_{kl}(x))$, $k,l=1,\ldots,n$. The dynamics (1.1) is invariant under lattice translations.

Let us denote by $Y(t)=(Y^0(t),Y^1(t))\equiv(u(\cdot,t),\dot{u}(\cdot,t))$, $Y_0=(Y_0^0,Y_0^1)\equiv(u_0(\cdot),v_0(\cdot))$. Then (1.1) takes the form of an evolution equation,

$$\dot{Y}(t)=\mathcal{A}Y(t),\quad t\in\mathbf{R};\quad Y(0)=Y_0. \tag{1.2}$$

Formally, this is the Hamiltonian system since

$$\mathcal{A}Y=J\begin{pmatrix}\mathcal{V}&0\\0&1\end{pmatrix}Y=J\nabla H(Y),\qquad J=\begin{pmatrix}0&1\\-1&0\end{pmatrix}. \tag{1.3}$$

Here $\mathcal{V}$ is a convolution operator with the matrix kernel V and H is the Hamiltonian functional,

$$H(Y)=\tfrac{1}{2}\langle v,v\rangle+\tfrac{1}{2}\langle\mathcal{V}u,u\rangle,\quad Y=(u,v), \tag{1.4}$$

where $\langle v,v\rangle=\Sigma_{x\in\mathbf{Z}^d}|v(x)|^2$ and $\langle\mathcal{V}u,u\rangle=\Sigma_{x,y\in\mathbf{Z}^d}(V(x-y)u(y),u(x))$,$(\cdot\,,\cdot)$ being the real scalar product in the Euclidean space $\mathbf{R}^n$.

We assume that the initial datum Y_0 is a random element of the Hilbert space $\mathcal{H}_\alpha$ of real sequences; see Definition 2.1. Y_0 is distributed according to the probability measure μ_0 of mean zero and satisfying the conditions **S1–S3** below. Given $t\in\mathbf{R}$, denote by μ_t the probability measure for $Y(t)$, the solution to (1.2) with random initial data Y_0. We study the asymptotics of μ_t as $t\to\pm\infty$.

The correlation matrices of the initial data are supposed to be translation-invariant, i.e., for $i,j=0,1$,

$$Q_0^{ij}(x,y):=E(Y_0^i(x)\otimes Y_0^j(y))=q_0^{ij}(x-y),\quad x,y\in\mathbf{Z}^d, \tag{1.5}$$

though our methods require in fact much weaker conditions. We also assume that the initial mean ''energy'' density is finite,

$$e_0:=E[|u_0(x)|^2+|v_0(x)|^2]=\operatorname{tr}q_0^{00}(0)+\operatorname{tr}q_0^{11}(0)<\infty,\quad x\in\mathbf{Z}^d. \tag{1.6}$$

Finally, it is assumed that the measure μ_0 satisfies a mixing condition of a Rosenblatt—resp. Ibragimov–Linnik type, which means that

$$Y_0(x) \text{ and } Y_0(y) \text{ are asymptotically independent as } |x-y|\to\infty. \tag{1.7}$$

Our main result is the (weak) convergence of the measures μ_t on the Hilbert space $\mathcal{H}_\alpha$ with $\alpha < -d/2$,

$$\mu_t \rightharpoonup \mu_\infty \text{ as } t\to\infty. \tag{1.8}$$

μ_∞ is a Gaussian measure on $\mathcal{H}_\alpha$. A similar convergence result holds for $t\to-\infty$. Explicit formulas for the correlation functions of the limit measure μ_∞ are given in (2.18)–(2.22). As an application of the results, we show that the initial ''white noise''-correlations provide the limit measure μ_∞ which coincides with the Gibbs canonical measure with the temperature $\sim e_0$. Respectively, μ_∞ is close to the canonical measure if the initial correlations are close to the white noise.

To prove the convergence (1.8) we follow general strategy.[2,4,6,7] There are three steps.

I. The family of measures μ_t, $t\geqslant 0$, is weakly compact in $\mathcal{H}_\alpha$ with $\alpha<-d/2$.

II. The correlation functions converge to a limit, for $i,j=0,1$,

$$Q_t^{ij}(x,y)=\int Y^i(x)\otimes Y^j(y)\,\mu_t(dY)\to Q_\infty^{ij}(x,y) \text{ as } t\to\infty. \tag{1.9}$$

III. The characteristic functionals converge to a Gaussian one,

$$\hat{\mu}_t(\Psi):=\int \exp(i\langle Y,\Psi\rangle)\mu_t(dY)\to\exp\left\{-\frac{1}{2}\mathcal{Q}_\infty(\Psi,\Psi)\right\} \text{ as } t\to\infty. \tag{1.10}$$

Here $\Psi=(\Psi^0,\Psi^1)\in\mathcal{D}=D\oplus D$, $D=C_0(\mathbf{Z}^d)\otimes\mathbf{R}^n$, where $C_0(\mathbf{Z}^d)$ denotes the space of the real sequences with finite support, $\langle Y,\Psi\rangle=\Sigma_{i=0,1}\Sigma_{x\in\mathbf{Z}^d}(Y^i(x),\Psi^i(x))$ and $\mathcal{Q}_\infty$ is the quadratic form with the matrix kernel $(Q_\infty^{ij}(x,y))_{i,j=0,1}$,

$$\mathcal{Q}_\infty(\Psi,\Psi)=\sum_{i,j=0,1}\ \sum_{x,y\in\mathbf{Z}^d}(Q_\infty^{ij}(x,y),\Psi^i(x)\otimes\Psi^j(y)). \tag{1.11}$$

Note that (1.1) is the translation-invariant convolution equation and admits a simple structure in the Fourier space. As a consequence, Fourier representation plays a central role in our proofs of properties **I** and **II**. On the other hand, Fourier transform alone does not suffice in proving **III**, since our main condition (1.7) is stated in the coordinate space and its equivalent interpretation in Fourier space is obscure.

Property **I** follows by the method:[22] we prove a uniform bound for the covariance of μ_t and refer to the Prokhorov Theorem. Property **II** is deduced from an analysis of the oscillatory integral representation of the correlation function in Fourier space. An important role is attributed to Lemma 3.1 reflecting the properties of the Fourier transformed correlation functions which is derived from the mixing condition. To prove **III** we exploit the dispersive properties of the dynamics (1.1) in coordinate space. The dispersion follows from a stationary phase method applied to the oscillatory integral representation of the Green's function in Fourier space. The dispersion allows us to represent the solution as a sum of weakly dependent random variables by the Bernstein-type ''room-corridor'' partition.

Let us explain in more detail the main idea for the proof of **III**. First let us consider the case $n=1$ and the nearest neighbor crystal for which the potential energy has the form

$$\frac{1}{2}\sum_{x,y\in\mathbf{Z}^d}(V(x-y)u(y),u(x))=\frac{1}{2}\sum_{x\in\mathbf{Z}^d}\left(\sum_{i=1}^{d}|u(x+e_i)-u(x)|^2+m^2|u(x)|^2\right),\qquad(1.12)$$

where $m\geqslant 0$ and $e_i=(\delta_{i1},\ldots,\delta_{id})$. The solution is represented through the Green's function, $\mathcal{G}(t,x)$,

$$Y(x,t)=\sum_{y\in\mathbf{Z}^d}\mathcal{G}(t,x-y)Y_0(y).\qquad(1.13)$$

The long-time asymptotics of the Green's function is analyzed by the stationary phase method based on the dispersion relation

$$\omega(\theta):=\hat{V}^{1/2}(\theta)=\left(2\sum_{j=1}^{d}(1-\cos\theta_j)+m^2\right)^{1/2},\quad\theta\in\mathbf{T}^d,\qquad(1.14)$$

where $\mathbf{T}^d$ is the real d-torus and $\hat{V}(\theta)$ stands for the Fourier transform of $V(x)$. The main features of ω for $m>0$ are

$$\text{(i)}\quad\omega(\theta)\neq 0,\quad\theta\in\mathbf{T}^d,\quad\text{and}\quad\text{(ii)}\quad\operatorname{mes}\mathcal{C}=0,\qquad(1.15)$$

where $\mathcal{C}$ is the *critical set* $\{\theta\in\mathbf{T}^d:\det\operatorname{Hess}\omega(\theta)=0\}$ and "mes" stands for the Lebesgue measure in $\mathbf{T}^d$. The Green's function has distinct asymptotic behavior in three zones of (x,t)-space: inside, resp., outside the light cone and in the "buffer zone," which is a small conical neighborhood of the boundary of the light cone. The light cone is determined by the group velocities $\nabla\omega(\theta)$ of the phonons, and its boundary is determined by the group velocities $\nabla\omega(\theta)$ with "critical" $\theta\in\mathcal{C}$, since they correspond to the maximal values of $|\nabla\omega(\theta)|$ with a fixed direction of $\nabla\omega(\theta)$ [cf. (1.16)]. Therefore, the buffer zone is determined by the velocities $\nabla\omega(\theta)$ with the θ from a small neighborhood of the critical set $\mathcal{C}$. The Green's function decays rapidly outside the light cone, as $t^{-d/2}$ inside the light cone except for the buffer zone, and more slowly in the buffer zone; cf. (1.18).

Now let us discuss the general case when $n\geqslant 1$. For $n>1$ an additional important feature occurs. In this case we have n dispersion relations $\omega_k(\theta)$, $k=1,\ldots,n$, which are the eigenvalues of the matrix $\hat{V}^{1/2}(\theta)$. Thus there can be "crossing points" where two or more dispersion relations $\omega_k(\theta)$ coincide which implies that they are not differentiable, in general. In this case the decay of the Green's function generally is slower than $t^{-d/2}$ everywhere in (x,t)-space. We estimate the decay by the stationary phase method, hence we need smooth branches of the dispersion relations $\omega_k(\theta)$ at least locally in θ. We establish the existence of the branches outside a set of the Lebesgue measure zero in $\mathbf{T}^d$ (see Lemma 2.2). For the proof we use the advanced variant of the Weierstrass Preparation Theorem from Ref. 15 and the analytic stratification of analytic sets.[12]

For $n\geqslant 1$ we define the critical set $\mathcal{C}$ as the subset of $\mathbf{T}^d$ which is the union over $k=1,\ldots,n$ of all the points θ either with a nondifferentiable $\omega_k(\theta)$, or with a degenerate Hessian of $\omega_k(\theta)$, or with $\omega_k(\theta)=0$. Lemmas 2.2, 2.3 imply that mes $\mathcal{C}=0$ which plays the central role in all proofs in the paper. The critical set is never empty. For example, let us fix $k=1,\ldots,n$ and consider the point $\theta\in\mathbf{T}^d$ with the maximal group velocity $|\nabla\omega_k(\theta)|>0$. Then $\det\operatorname{Hess}\omega_k(\theta)=0$ since $\operatorname{Hess}\omega_k(\theta)\,\nabla\omega_k(\theta)=0$:

$$(\operatorname{Hess}\omega_k(\theta)\,\nabla\omega_k(\theta))_i=\sum_j\frac{\partial^2\omega_k(\theta)}{\partial\theta_i\,\partial\theta_j}\frac{\partial\omega_k(\theta)}{\partial\theta_j}=\frac{1}{2}\frac{\partial}{\partial\theta_i}\sum_j\left|\frac{\partial\omega_k(\theta)}{\partial\theta_j}\right|^2=0,\quad i=1,\ldots,d,\qquad(1.16)$$

provided the derivatives exist. Thus even for $d=n=1$ the *uniform in* $x\in\mathbf{R}$ decay of the Green's function is slower than $t^{-1/2}$ since $\omega''(\theta)$ vanishes in some points. To overcome this difficulty, in Ref. 2 it is required that $\omega'''(\theta)\neq 0$ at points with $\omega''(\theta)=0$. Then the uniform decay of the Green's function is $t^{-1/3}$ which suffices in the case $d=1$ together with an additional assumption on

the higher moments of the initial measure. In contrast, the critical set and the slow decay of the Green's function do not occur for the Klein–Gordon equation analyzed in Refs. 4, 6.

For $d,n\geqslant 1$ Suhov and Shuhov have proved in Ref. 19 the convergence of the covariance, (1.9), for a *simple singularity* of $\omega_k(\theta)$ (in Arnold's terminology[1]) in the points $\theta\in\mathcal{C}$ with the degenerate Hessian. However, a similar detailed analysis of all degenerate points for $d,n\geqslant 1$ seems to be impossible. We avoid it by a novel "cutoff" strategy which allows us to cover the general case when the Lebesgue measure of the critical set $\mathcal{C}$ is zero. Namely, we choose an $\varepsilon>0$ and split the Fourier transform of the solution in two components $\hat{Y}(\theta,t)=\hat{Y}_f(\theta,t)+\hat{Y}_g(\theta,t)$ where $\hat{Y}_f(\theta,t)=0$ outside the ε-neighborhood of the critical set $\mathcal{C}$ while $\hat{Y}_g(\theta,t)=0$ inside the $\varepsilon/2$-neighborhood of $\mathcal{C}$. First, we use the mixing condition to estimate the contribution from the "critical" component $\hat{Y}_f$: we prove that it is small in the mean, i.e., its dispersion is negligible uniformly in $t\geqslant 0$, if $\varepsilon>0$ is sufficiently small. This follows from the identity mes $\mathcal{C}=0$ since the Fourier transforms of the initial correlation functions are absolutely continuous due to the mixing condition. A further step is to develop a Bernstein type argument to prove the Gaussian limit for the main "noncritical" component Y_g. We write it in the form (1.13):

$$Y_g(x,t)=\sum_{y\in\mathbf{Z}^d}\mathcal{G}_g(t,x-y)Y_0(y), \tag{1.17}$$

where $\mathcal{G}_g(t,x-y)$ is the "truncated" Green's function which is defined similarly to $Y_g(x,t)$: its Fourier transform $\hat{\mathcal{G}}_g(t,\theta)$ is zero inside the $\varepsilon/2$-neighborhood of $\mathcal{C}$. Then all the dispersion relations $\omega_k(\theta)$ are smooth and nondegenerate on the support of $\hat{\mathcal{G}}_g(t,\theta)$, hence the truncated Green's function has the standard decay,

$$\mathcal{G}_g(t,x-y)\leqslant\begin{cases}Ct^{-d/2}, & |y-x|\leqslant ct,\\ C_p(|t|+|x-y|+1)^{-p}, & |y-x|\geqslant ct,\end{cases} \tag{1.18}$$

with some $c>0$ and any $p>0$; cf. (5.2), (5.3). Therefore, the representation (1.17) demonstrates that for a fixed $x\in\mathbf{Z}^d$, the main contribution to $Y_g(x,t)$ comes from the section $B_t(x)=\{y\in\mathbf{Z}^d: |y-x|\leqslant ct\}$ of the light cone at time t. The "volume" of the section [i.e., the number of the points $y\in\mathbf{Z}^d\cap B_t(x)$] is $|B_t(x)|\sim t^d$. Therefore, (1.17) becomes, roughly speaking,

$$Y_g(x,t)\sim\frac{\Sigma_{y\in B_t(x)}Y_0(y)}{\sqrt{|B_t|}},\quad t\to\infty. \tag{1.19}$$

This implies the Gaussian limit by the Ibragimov–Linnik Central Limit Theorem,[13] since the random values $Y_0(y)$ are weakly dependent because of the mixing condition (1.7).

Remarks 1.1: (i) Physically, the asymptotics (1.18) reflects the isotropic propagation of phonons in the noncritical spectrum. The isotropy provides a "dynamical mixing" which leads to the Gaussian behavior by the statistical mixing condition (1.7). So the convergence to the statistical equilibrium (1.8) is provided by both kinds of the mixing simultaneously: the statistical mixing condition (1.7) and the dynamical mixing (1.18).

(ii) The degree $-d/2$ in (1.18) is related to the energy conservation since the Hamiltonian (1.4) is a quadratic form. Roughly speaking, (1.18) means the "energy diffusion," and the degree $-d/2$ resembles the diffusion kernel.

Finally, let us comment on our conditions concerning the interaction matrix $V(x)$. We assume the conditions **E1**–**E4** below which in a similar form appear also in Refs. 2, 14. **E1** means the exponential space-decay of the interaction in the crystal. **E2**, resp. **E3**, means that the potential energy is real, resp. non-negative. **E4** eliminates the constant part of the spectrum and ensures that mes $\mathcal{C}=0$ [cf. (1.15)]. We also introduce a new simple condition **E5** for the case $n>1$ which eliminates the *discrete* part of the spectrum for the covariance dynamics. It can be considerably weakened to the condition **E5′** from Remark 2.10 (iii). For example, the condition **E5′** holds for

the canonical Gaussian measures which are considered in Ref. 14. We show that the conditions **E4** and **E5** hold for "almost all" matrix-functions $V(\cdot)$ with the finite range of the interaction.

Furthermore, we do not require that $\omega_k(\theta)\neq 0$, $\theta\in\mathbf{T}^d$: note that $\omega(0)=0$ for the elastic lattice (1.14) in the case $m=0$. Our results hold whenever $\mathrm{mes}\{\theta\in\mathbf{T}^d:\omega_k(\theta)=0\}=0$. To cover this case we impose the new condition **ES** which is roughly speaking necessary and sufficient for the uniform bounds of the covariance. It can be simplified to the stronger condition

$$\|\hat{V}^{-1}(\theta)\|\in L^1(\mathbf{T}^d), \tag{1.20}$$

from Ref. 14, which holds for the elastic lattice (1.14) if either $d\geqslant 3$ or $m>0$. The condition (1.20) is equivalent to **ES** for the canonical Gibbs measures considered in Ref. 14. However, (1.20) does not hold in some particular interesting cases: for instance, for the elastic lattice (1.14) in the case $d=1,2$ and $m=0$, as it is pointed out in Ref. 14.

The main results of our paper are stated in Sec. II: Theorem *A* in Sec. II D, and its application in Sec. II E 4. The convergence (1.9) and the compactness **I** are established in Sec. III, and the convergence (1.10) in Secs. IV–VIII. Section IX concerns the ergodicity and the mixing properties of the limit measure. In the Appendix we analyze the crossing points of the dispersion relations.

II. MAIN RESULTS

A. Dynamics

We assume that the initial date Y_0 belongs to the phase space $\mathcal{H}_\alpha$, $\alpha\in\mathbf{R}$, defined below.

Definition 2.1: $\mathcal{H}_\alpha$ is the Hilbert space of pairs $Y=(u(x),v(x))$ of $\mathbf{R}^n$-valued functions of $x\in\mathbf{Z}^d$ endowed with the norm

$$\|Y\|_\alpha^2=\sum_{x\in\mathbf{Z}^d}(|u(x)|^2+|v(x)|^2)(1+|x|^2)^\alpha<\infty. \tag{2.1}$$

We impose the following conditions **E1**–**E5** on the matrix V.

E1 There exist constants $C,\alpha>0$ such that $|V_{kl}(z)|\leqslant Ce^{-\alpha|z|}$, $k,l\in\mathrm{I}_n:=\{1,\ldots,n\}$, $z\in\mathbf{Z}^d$.

Let us denote by $\hat{V}(\theta):=(\hat{V}_{kl}(\theta))_{k,\,l\in\mathrm{I}_n}$, where $\hat{V}_{kl}(\theta)\equiv\Sigma_{z\in\mathbf{Z}^d}V_{kl}(z)e^{iz\theta}$, $\theta\in\mathbf{T}^d$, and $\mathbf{T}^d$ denotes the d-torus $\mathbf{T}^d=\mathbf{R}^d/2\pi\mathbf{Z}^d$.

E2 V is real and symmetric, i.e., $V_{lk}(-z)=V_{kl}(z)\in\mathbf{R}$, $k,l\in\mathrm{I}_n$, $z\in\mathbf{Z}^d$.

The condition implies that $\hat{V}(\theta)$ is a real-analytic Hermitian matrix-function in $\theta\in\mathbf{T}^d$.

E3 The matrix $\hat{V}(\theta)$ is non-negative definite for each $\theta\in\mathbf{T}^d$.

The condition means that Eq. (1.1) is a hyperbolic like wave and Klein–Gordon equations considered in Refs. 6–8. Let us define the Hermitian non-negative definite matrix,

$$\Omega(\theta):=(\hat{V}(\theta))^{1/2}\geqslant 0, \tag{2.2}$$

with the eigenvalues $\omega_k(\theta)\geqslant 0$, $k\in\mathrm{I}_n$, the dispersion relations. For each $\theta\in\mathbf{T}^d$ the Hermitian matrix $\Omega(\theta)$ has the diagonal form in the basis of the orthogonal eigenvectors $\{e_k(\theta):k\in\mathrm{I}_n\}$:

$$\Omega(\theta)=B(\theta)\begin{pmatrix}\omega_1(\theta) & \cdots & 0\\ 0 & \ddots & 0\\ 0 & \cdots & \omega_n(\theta)\end{pmatrix}B^*(\theta), \tag{2.3}$$

where $B(\theta)$ is a unitary matrix. It is well known that the functions $\omega_k(\theta)$ and $B(\theta)$ are real-analytic outside the set of the "crossing" points θ_*: $\omega_k(\theta_*)=\omega_l(\theta_*)$ for some $l\neq k$. However, generally the functions are not smooth at the crossing points if $\omega_k(\theta)\not\equiv\omega_l(\theta)$. Therefore, we need the following lemma which we prove in the Appendix (cf. Ref. 21, Lemma 1.1).

Lemma 2.2: Let the conditions **E1**, **E2** *hold. Then there exists a closed subset* $\mathcal{C}_* \subset \mathbf{T}^d$ *such that we have the following:*

(i) the Lebesgue measure of $\mathcal{C}_*$ *is zero:*

$$\mathrm{mes}\mathcal{C}_* = 0. \tag{2.4}$$

(ii) *For any point* $\Theta \in \mathbf{T}^d \backslash \mathcal{C}_*$ *there exists a neighborhood* $\mathcal{O}(\Theta)$ *such that each dispersion relation* $\omega_k(\theta)$ *and the matrix* $B(\theta)$ *can be chosen as the real-analytic functions in* $\mathcal{O}(\Theta)$.

(iii) *The eigenvalues* $\omega_k(\theta)$ *have constant multiplicity in* $\mathbf{T}^d \backslash \mathcal{C}_*$, *i.e., it is possible to enumerate them so that we have for* $\theta \in \mathbf{T}^d \backslash \mathcal{C}_*$,

$$\omega_1(\theta) \equiv \cdots \equiv \omega_{r_1}(\theta), \ \ \omega_{r_1+1}(\theta) \equiv \cdots \equiv \omega_{r_2}(\theta), \ \ \ldots, \ \omega_{r_s+1}(\theta) \equiv \cdots \equiv \omega_n(\theta), \tag{2.5}$$

$$\omega_{r_\sigma}(\theta) \not\equiv \omega_{r_\nu}(\theta) \quad \text{if} \quad \sigma \neq \nu, \ \ 1 \leqslant r_\sigma, r_\nu \leqslant r_{s+1} := n. \tag{2.6}$$

(iv) *The spectral decomposition holds,*

$$\Omega(\theta) = \sum_1^{s+1} \omega_{r_\sigma}(\theta) \Pi_\sigma(\theta), \quad \theta \in \mathbf{T}^d \backslash \mathcal{C}_*, \tag{2.7}$$

where $\Pi_\sigma(\theta)$ *is the orthogonal projection in* $\mathbf{R}^n$ *which is real-analytic function of* $\theta \in \mathbf{T}^d \backslash \mathcal{C}_*$.

Below we denote by $\omega_k(\theta)$ the local real-analytic functions from Lemma 2.2 (ii). Our next condition is the following:

E4 $D_k(\theta) \not\equiv 0$, $\forall k \in \mathrm{I}_n$, where $D_k(\theta) := \det(\partial^2 \omega_k(\theta)/\partial\theta_i \, \partial\theta_j)_{i,j=1}^d$, $\theta \in \mathbf{T}^d \backslash \mathcal{C}_*$.

Let us denote $\mathcal{C}_0 := \{\theta \in \mathbf{T}^d : \det \hat{V}(\theta) = 0\}$ and $\mathcal{C}_k := \{\theta \in \mathbf{T}^d \backslash \mathcal{C}_* : D_k(\theta) = 0\}$, $k \in \mathrm{I}_n$. The following lemma is also proved in the Appendix.

Lemma 2.3: Let the conditions **E1**–**E4** *hold. Then* $\mathrm{mes}\, \mathcal{C}_k = 0$ *for* $k = 0, 1, \ldots, n$.

Our last condition on V is the following:

E5 For each $k \neq l$ the identity $\omega_k(\theta) - \omega_l(\theta) \equiv \mathrm{const}_-$, $\theta \in \mathbf{T}^d$ does not hold with $\mathrm{const}_- \neq 0$, and the identity $\omega_k(\theta) + \omega_l(\theta) \equiv \mathrm{const}_+$ does not hold with $\mathrm{const}_+ \neq 0$.

This condition holds trivially in the case $n = 1$.

We show that the conditions **E4** and **E5** hold for "almost all" functions V satisfying the conditions **E1**, **E2**. More precisely, let us fix an arbitrary $N \geqslant 1$ and denote by $\mathcal{R}_N$ the set of the "finite range" interaction matrices V with $V(x) = 0$ for $\max_i |x_i| > N$, and satisfying the condition **E2**. In the Appendix we prove the following lemma.

Lemma 2.4: For any $N \geqslant 1$ *the conditions* **E4** *and* **E5** *hold for the matrix-functions* V *from an open and dense subset of* $\mathcal{R}_N$.

The following proposition is proved in Ref. 14, p. 150 and Ref. 2, p. 128.

Proposition 2.5: Let **E1** *and* **E2** *hold, and* $\alpha \in \mathbf{R}$. *Then*

(i) *for any* $Y_0 \in \mathcal{H}_\alpha$ *there exists a unique solution* $Y(t) \in C(\mathbf{R}, \mathcal{H}_\alpha)$ *to the Cauchy problem (1.2).*

(ii) *The operator* $U(t): Y_0 \mapsto Y(t)$ *is continuous in* $\mathcal{H}_\alpha$.

Proof: Applying the Fourier transform to (1.2), we obtain

$$\dot{\hat{Y}}(\theta, t) = \hat{\mathcal{A}}(\theta) \hat{Y}(\theta, t), \ \ t \in \mathbf{R}, \quad \hat{Y}(0) = \hat{Y}_0, \tag{2.8}$$

where

$$\hat{\mathcal{A}}(\theta) = \begin{pmatrix} 0 & 1 \\ -\hat{V}(\theta) & 0 \end{pmatrix}, \quad \theta \in \mathbf{T}^d. \tag{2.9}$$

Note that $\hat{Y}(\cdot,t)\in D'(\mathbf{T}^d)$ for $t\in\mathbf{R}$. On the other hand, $\hat{V}(\theta)$ is a smooth function by **E1**. Therefore, the solution $\hat{Y}(\theta,t)$ of (2.8) exists, is unique and admits the representation $\hat{Y}(\theta,t)=\exp(\hat{\mathcal{A}}(\theta)t)\hat{Y}_0(\theta)$. It becomes (1.13) in the coordinate space, where the Green's function $\mathcal{G}(t,z)$ admits the Fourier representation

$$\mathcal{G}(t,z):=F^{-1}_{\theta\to z}[\exp(\hat{\mathcal{A}}(\theta)t)]=(2\pi)^{-d}\int_{\mathbf{T}^d}e^{-iz\theta}\exp(\hat{\mathcal{A}}(\theta)t)d\theta. \tag{2.10}$$

Hence, by the partial integration, $\mathcal{G}(t,z)\sim|z|^{-p}$ as $|z|\to\infty$ for any $p>0$ and bounded $|t|$ since $\hat{\mathcal{A}}(\theta)$ is the smooth function of $\theta\in\mathbf{T}^d$. Therefore, the convolution representation (1.13) implies $Y(t)\in\mathcal{H}_\alpha$. □

B. The convergence to statistical equilibrium

Let (Ω,Σ,P) be a probability space with expectation E and let $\mathcal{B}(\mathcal{H}_\alpha)$ denote the Borel σ-algebra in $\mathcal{H}_\alpha$. We assume that $Y_0=Y_0(\omega,\cdot)$ in (1.2) is a measurable random function with values in $(\mathcal{H}_\alpha,\mathcal{B}(\mathcal{H}_\alpha))$. In other words, for each $x\in\mathbf{Z}^d$ the map $\omega\mapsto Y_0(\omega,x)$ is a measurable map $\Omega\to\mathbf{R}^{2n}$ with respect to the (completed) σ-algebras Σ and $\mathcal{B}(\mathbf{R}^{2n})$. Then $Y(t)=U(t)Y_0$ is again a measurable random function with values in $(\mathcal{H}_\alpha,\mathcal{B}(\mathcal{H}_\alpha))$ owing to Proposition 2.5. We denote by $\mu_0(dY_0)$ a Borel probability measure on $\mathcal{H}_\alpha$ giving the distribution of the Y_0. Without loss of generality, we assume $(\Omega,\Sigma,P)=(\mathcal{H}_\alpha,\mathcal{B}(\mathcal{H}_\alpha),\mu_0)$ and $Y_0(\omega,x)=\omega(x)$ for $\mu_0(d\omega)$—almost all $\omega\in\mathcal{H}_\alpha$ and each $x\in\mathbf{Z}^d$.

Definition 2.6: μ_t is a Borel probability measure in $\mathcal{H}_\alpha$ which gives the distribution of Y(t):

$$\mu_t(B)=\mu_0(U(-t)B),\quad \forall B\in\mathcal{B}(\mathcal{H}_\alpha),\quad t\in\mathbf{R}. \tag{2.11}$$

Our main goal is to derive the convergence of the measures μ_t as $t\to\infty$. We establish the weak convergence of μ_t in the Hilbert spaces $\mathcal{H}_\alpha$ with $\alpha<-d/2$:

$$\mu_t \overset{\mathcal{H}_\alpha}{\rightharpoonup} \mu_\infty \quad \text{as} \quad t\to\infty, \tag{2.12}$$

where μ_∞ is a limit measure on the space $\mathcal{H}_\alpha$, $\alpha<-d/2$. This means the convergence

$$\int f(Y)\mu_t(dY)\to\int f(Y)\mu_\infty(dY),\quad t\to\infty, \tag{2.13}$$

for any bounded continuous functional f on $\mathcal{H}_\alpha$.

Definition 2.7: The correlation functions of the measure μ_t are defined by

$$Q^{ij}_t(x,y)=E(Y^i(x,t)\otimes Y^j(y,t)),\quad i,j=0,1,\quad x,y\in\mathbf{Z}^d, \tag{2.14}$$

if the expectations on the rhs are finite. Here $Y^i(x,t)$ are the components of the random solution $Y(t)=(Y^0(\cdot,t),Y^1(\cdot,t))$.

For a probability measure μ on $\mathcal{H}_\alpha$ we denote by $\hat{\mu}$ the characteristic functional (Fourier transform),

$$\hat{\mu}(\Psi)=\int \exp(i\langle Y,\Psi\rangle)\,\mu(dY),\quad \Psi\in\mathcal{D}.$$

A measure μ is called Gaussian (of zero mean) if its characteristic functional has the form

$$\hat{\mu}(\Psi)=\exp\{-\tfrac{1}{2}\mathcal{Q}(\Psi,\Psi)\},\quad \Psi\in\mathcal{D}, \tag{2.15}$$

where $\mathcal{Q}$ is a real non-negative quadratic form in $\mathcal{D}$. A measure μ is called translation-invariant if $\mu(T_hB)=\mu(B)$, $B\in\mathcal{B}(\mathcal{H}_\alpha)$, $h\in\mathbf{Z}^d$, where $T_hY(x)=Y(x-h)$, $x\in\mathbf{Z}^d$.

C. The mixing condition

Let $O(r)$ denote the set of all pairs of the subsets $\mathcal{A}$, $\mathcal{B}\subset\mathbf{Z}^d$ at distance $\mathrm{dist}(\mathcal{A},\mathcal{B})\geqslant r$ and $\sigma(\mathcal{A})$ be the σ-algebra in $\mathcal{H}_\alpha$ generated by $Y(x)$ with $x\in\mathcal{A}$. Define the Ibragimov–Linnik mixing coefficient of a probability measure μ_0 on $\mathcal{H}_\alpha$ by (cf. Ref. 13, Definition 17.2.2)

$$\varphi(r):=\sup_{(\mathcal{A},\mathcal{B})\in O(r)}\ \sup_{\substack{A\in\sigma(\mathcal{A}),B\in\sigma(\mathcal{B})\\ \mu_0(B)>0}}\frac{|\mu_0(A\cap B)-\mu_0(A)\mu_0(B)|}{\mu_0(B)}. \tag{2.16}$$

Definition 2.8: The measure μ_0 satisfies a strong, uniform Ibragimov–Linnik mixing condition if $\varphi(r)\to 0$ as $r\to\infty$.

Below, we specify the rate of decay of φ (see condition **S3**).

D. Statistical conditions and results

We assume that the initial measure μ_0 satisfies the following conditions **S0**–**S3**:

S0 μ_0 has zero expectation value, $EY_0(x)\equiv 0$, $x\in\mathbf{Z}^d$.

S1 μ_0 has translation-invariant correlation matrices, i.e., Eq. (1.5) holds for $x,y\in\mathbf{Z}^d$.

S2 μ_0 has a finite mean energy density, i.e., Eq. (1.6) holds.

S3 μ_0 satisfies the strong uniform Ibragimov–Linnik mixing condition with

$$\overline{\varphi}:=\int_0^{+\infty} r^{d-1}\varphi^{1/2}(r)\,dr<\infty. \tag{2.17}$$

We will deduce from **S0**–**S3** that $\hat{q}_0^{ij}\in C(\mathbf{T}^d)$, $i,j=0,1$ (see Lemma 3.1). This makes sense of our last condition **ES** concerning the initial covariance and the matrix $\Omega(\theta)$. We need it only in the case when $\mathcal{C}_0\neq\emptyset$, i.e., $\det V(\theta)=0$ for some points $\theta\in\mathbf{T}^d$:

ES $\|\Omega^{-i}(\theta)\hat{q}_0^{ij}(\theta)\Omega^{-j}(\theta)\|\in L^1(\mathbf{T}^d)$ for $i,j=0,1$.

This condition follows from **S0**–**S3** if $i=j=0$ or $\mathcal{C}_0=\emptyset$.

Next introduce the correlation matrix of the limit measure μ_∞. It is translation-invariant [cf. (1.5)]:

$$Q_\infty(x,y)=(q_\infty^{ij}(x-y))_{i,j=0,1}. \tag{2.18}$$

In the Fourier transform we have locally outside the critical set $\mathcal{C}_*$ (see Lemma 2.2),

$$\hat{q}_\infty^{ij}(\theta)=B(\theta)M_\infty^{ij}(\theta)B^*(\theta),\quad i,j=0,1, \tag{2.19}$$

where $B(\theta)$ is the smooth unitary matrix from Lemma 2.2 (ii) and $M_\infty^{ij}(\theta)$ is an $n\times n$-matrix with the smooth entries $(M_\infty^{ij}(\theta))_{kl}=\chi_{kl}(B^*(\theta)M_0^{ij}(\theta)B(\theta))_{kl}$. Here we set [see (2.5)]

$$\chi_{kl}=\begin{cases}1, & \text{if } k,l\in(r_{\sigma-1},r_\sigma],\ \sigma=1,\dots,s+1,\\ 0, & \text{otherwise,}\end{cases} \tag{2.20}$$

with $r_0:=0$, $r_{s+1}:=n$, and

$$M_0(\theta):=\frac{1}{2}\begin{pmatrix}\hat{q}_0^{00}(\theta)+\Omega^{-1}(\theta)\,\hat{q}_0^{11}(\theta)\,\Omega^{-1}(\theta) & \hat{q}_0^{01}(\theta)-\Omega^{-1}(\theta)\,\hat{q}_0^{10}(\theta)\,\Omega(\theta)\\ \hat{q}_0^{10}(\theta)-\Omega\,\hat{q}_0^{01}(\theta)\,\Omega^{-1}(\theta) & \hat{q}_0^{11}(\theta)+\Omega(\theta)\,\hat{q}_0^{00}(\theta)\,\Omega(\theta)\end{pmatrix}. \tag{2.21}$$

The local representation (2.19) can be expressed globally as

$$\hat{q}_\infty^{ij}(\theta)=\sum_{\sigma=1}^{s+1}\Pi_\sigma(\theta)M_0^{ij}(\theta)\Pi_\sigma(\theta),\quad \theta\in\mathbf{T}^d\backslash\mathcal{C}_*,\qquad i,j=0,1, \tag{2.22}$$

where $\Pi_\sigma(\theta)$ is the spectral projection from (2.7).

Remark 2.9: The condition **ES** implies that $(M_0^{ij})_{kl} \in L^1(\mathbf{T}^d)$, $k,l \in \mathrm{I}_n$. Therefore, (2.22) and (2.4) imply that also $(\hat{q}_\infty^{ij})_{kl} \in L^1(\mathbf{T}^d)$, $k,l \in \mathrm{I}_n$.

Theorem A: *Let $d,n \geqslant 1$, $\alpha < -d/2$ and assume that the conditions* **E1**–**E5**, **S0**–**S3** *hold. If $\mathcal{C}_0 \neq \emptyset$, then we assume also that* **ES** *holds. Then*

(i) *the convergence in (2.12) holds.*
(ii) *The limit measure μ_∞ is a Gaussian translation-invariant measure on $\mathcal{H}_\alpha$.*
(iii) *The characteristic functional of μ_∞ is the Gaussian,*

$$\hat{\mu}_\infty(\Psi) = \exp\{-\tfrac{1}{2}\mathcal{Q}_\infty(\Psi,\Psi)\}, \quad \Psi \in \mathcal{D}, \tag{2.23}$$

where $\mathcal{Q}_\infty$ is the quadratic form defined in (1.11).
(iv) *The measure μ_∞ is invariant, i.e., $[U(t)]^*\mu_\infty = \mu_\infty$, $t \in \mathbf{R}$.*

Remarks 2.10: (i) In the case $n=1$, the formulas (2.21), (2.22) become

$$\hat{q}_\infty = M_0 = \frac{1}{2}\begin{pmatrix} \hat{q}_0^{00} + \omega^{-2}\hat{q}_0^{11} & \hat{q}_0^{01} - \hat{q}_0^{10} \\ \hat{q}_0^{10} - \hat{q}_0^{01} & \hat{q}_0^{11} + \omega^2 \hat{q}_0^{00} \end{pmatrix}.$$

(ii) The *uniform* Rosenblatt mixing condition[18] also suffices, together with a higher power >2 in the bound (1.6): there exists $\delta > 0$ such that

$$E(|u_0(x)|^{2+\delta} + |v_0(x)|^{2+\delta}) < \infty.$$

Then (2.17) requires a modification: $\int_0^{+\infty} r^{d-1}\alpha^p(r)dr < \infty$, with $p = \min(\delta/(2+\delta), 1/2)$, where $\alpha(r)$ is the Rosenblatt mixing coefficient defined as in (2.16) but without $\mu_0(B)$ in the denominator. With these modifications, the statements of Theorem *A* and their proofs remain essentially unchanged.

(iii) The arguments with condition **E5** in Proposition 3.2 [see (3.7)–(3.13) below] demonstrate that the condition could be considerably weakened. Namely, it suffices to assume **E5′**. If for some $k \neq l$ we have either $\omega_k(\theta) + \omega_l(\theta) \equiv \mathrm{const}_+ \neq 0$ or $\omega_k(\theta) - \omega_l(\theta) \equiv \mathrm{const}_- \neq 0$, then

$$(B^*(\theta)\hat{q}_0^{ij}(\theta)B(\theta))_{kl} = 0, \quad \theta \in \mathbf{T}^d, \ i,j = 0,1. \tag{2.24}$$

The assertions (i)–(iii) of Theorem *A* follow from Propositions 2.11 and 2.12.

Proposition 2.11: The family of the measures $\{\mu_t, t \in \mathbf{R}\}$ is weakly compact in $\mathcal{H}_\alpha$ with any $\alpha < -d/2$, and the bounds hold:

$$\sup_{t \geqslant 0} E\|U(t)Y_0\|_\alpha^2 < \infty. \tag{2.25}$$

Proposition 2.12: For every $\Psi \in \mathcal{D}$, the convergence (1.10) holds.

Proposition 2.11 ensures the existence of the limit measures of the family $\{\mu_t, t \in \mathbf{R}\}$, while Proposition 2.12 provides the uniqueness. Propositions 2.11 and 2.12 are proved in Secs. III and IV–VIII, respectively.

Theorem A (iv) follows from (2.12) since the group $U(t)$ is continuous in $\mathcal{H}_\alpha$ by Proposition 2.5 (ii).

E. Examples and applications

Let us give the examples of the equations (1.1) and measures μ_0 which satisfy all conditions **E1**–**E5**, **S0**–**S3**, and **ES**.

1. Harmonic crystals

All conditions **E1**–**E5** hold for a one-dimensional (1-D) crystal with $n=1$ considered in Ref. 2. For any $d\geqslant 1$ and $n=1$ consider the simple elastic lattice corresponding to the quadratic form (1.12) with $m\neq 0$. Then $V(x)=F^{-1}_{\theta\to x}\omega^2(\theta)$ with $\omega(\theta)$ defined by (1.14), satisfies **E1**–**E4** with $\mathcal{C}_*=\emptyset$. In these examples the set $\mathcal{C}_0$ is empty, hence the condition **ES** is superfluous. Condition **E5** holds trivially since $n=1$.

2. Gaussian measures

We consider $n=1$ and construct Gaussian initial measures μ_0 satisfying **S0**–**S3**. We will define μ_0 by the correlation functions $q_0^{ij}(x-y)$ which are zero for $i\neq j$, while for $i=0,1$,

$$\hat{q}_0^{ii}(\theta):=F_{z\to\theta}q_0^{ii}(z)\in L^1(\mathbf{T}^d),\quad \hat{q}_0^{ii}(\theta)\geqslant 0. \tag{2.26}$$

Then by the Minlos theorem[11] there exists a unique Borel Gaussian measure μ_0 on $\mathcal{H}_\alpha$, $\alpha<-d/2$, with the correlation functions $q_0^{ij}(x-y)$. The measure μ_0 satisfies **S0**–**S2**. Further, let us provide, in addition to (2.26), that

$$q_0^{ii}(z)=0,\ |z|\geqslant r_0. \tag{2.27}$$

Then the mixing condition **S3** follows with $\varphi(r)=0$, $r\geqslant r_0$, since for Gaussian random values the orthogonality implies the independence. For example, (2.26) and (2.27) hold if we set $q_0^{ii}(z)=f(z_1)f(z_2)\cdot\cdots\cdot f(z_d)$, where $f(z)=\nu_0-|z|$ for $|z|\leqslant\nu_0$ and $f(z)=0$ for $|z|\geqslant\nu_0$ with $\nu_0:=[r_0/\sqrt{d}]$ (the integer part). Then by the direct calculation we obtain $\hat{f}(\theta)=(1-\cos\nu_0\theta)/(1-\cos\theta)$, $\theta\in\mathbf{T}^1$, and (2.26) holds. The measure μ_0 is nontrivial if $r_0\geqslant\sqrt{d}$: otherwise $\nu_0=0$, so $q_0^{ij}(z)\equiv 0$, and the measure $\mu_0(dY_0)$ is concentrated at the point $Y_0=0$.

3. Non-Gaussian measures

Let us choose some odd bounded nonconstant functions f^0, $f^1\in C(\mathbf{R})$ and consider a random function $(Y^0(x),Y^1(x))$ with the Gaussian distribution μ_0 from the previous example. Let us define μ_0^* as the distribution of the random function $(f^0(Y^0(x)),f^1(Y^1(x))$. Then **S0**–**S3** hold for μ_0^* with corresponding mixing coefficients $\varphi^*(r)=0$ for $r\geqslant r_0$. The measure μ_0^* is not Gaussian if the functions f^0, f^1 are bounded and nonconstant.

4. From statistical chaos to the Gibbs measure

Let us consider the initial measures which satisfy **S0**–**S3**, and with the correlation functions

$$(q_0^{ij})_{kl}(x-y):=E(Y_k^i(x,0)Y_l^j(y,0))=T_i\delta_{ij}\delta_{kl}\delta_{xy},\quad i,j=0,1,\ k,l\in\mathrm{I}_n,\quad x,y\in\mathbf{Z}^d, \tag{2.28}$$

where $T_{0,1}\geqslant 0$. These correlations correspond to the "chaos" with the zero correlation radius and uncorrelated components. Such measures exist on $\mathcal{H}_\alpha$ with $\alpha<-d/2$ by the Minlos Theorem:[11] for example, the "white noise" which is the corresponding Gaussian measure. Let us consider the crystal satisfying the conditions **E1**–**E4** and (1.20). Then also the conditions **E5′**, **ES** hold, so Theorem *A* is applicable [see Remark 2.10 (iii)]: it implies the convergence (2.12) to the Gaussian measure μ_∞ with the covariance (2.21), (2.22).

Additionally, let us assume that $T_0=0$ which physically means that only the initial velocities contribute, and initial deviations are adjusted to zero. Then the formulas (2.21), (2.22) become

$$\hat{q}_\infty(\theta)=M_0(\theta)=\frac{T_1}{2}\begin{pmatrix}\hat{V}^{-1}(\theta) & 0\\ 0 & (\delta_{kl})_{k,l\in\mathrm{I}_n}\end{pmatrix}. \tag{2.29}$$

According to (1.3), this means that the limit measure μ_∞ coincides with the *Gibbs canonical measure* corresponding to the temperature $\sim T_1$. In a more general framework, the limit measure is close to the Gibbs measure if the radius of the initial correlations is small in a suitable scaling limit (cf. Ref. 6, Proposition 4.2).

III. CONVERGENCE OF COVARIANCE AND COMPACTNESS

A. Mixing condition in terms of spectral density

The next Lemma reflects the mixing property in the Fourier transforms $\hat{q}_0^{ij}$ of initial correlation functions q_0^{ij}. Condition **S2** implies that $q_0^{ij}(z)$ is a bounded function. Therefore, its Fourier transform generally belongs to the Schwartz space of tempered distributions.

Lemma 3.1: Let the conditions **S0**–**S3** *hold. Then* $\hat{q}_0^{ij} \in C(\mathbf{T}^d)$, $i,j=0,1$.

Proof: It suffices to prove that

$$q_0^{ij}(z) \in l^1(\mathbf{Z}^d). \tag{3.1}$$

Conditions **S0**–**S3** imply by Ref. 13, Lemma 17.2.3 [or Lemma 8.2 (i) below]:

$$|q_0^{ij}(z)| \leqslant C e_0 \varphi^{1/2}(|z|), \quad z \in \mathbf{Z}^d, \tag{3.2}$$

where e_0 is defined by (1.6). Therefore, (2.17) implies (3.1):

$$\sum_{z \in \mathbf{Z}^d} |q_0^{ij}(z)| \leqslant C e_0 \sum_{z \in \mathbf{Z}^d} \varphi^{1/2}(|z|) < \infty.$$

□

B. Oscillatory integral arguments

In this section we uniformly estimate and check the convergence of the correlation matrices of measures μ_t with the help of the Fourier transform. The condition **S1** and the translation-invariant dynamics (1.1) imply that

$$Q_t^{ij}(x,y) \equiv \int Y^i(x) \otimes Y^j(y) \mu_t(dY) = q_t^{ij}(x-y), \quad x,y \in \mathbf{Z}^d. \tag{3.3}$$

Proposition 3.2: (i) The correlation matrices $q_t^{ij}(z)$, $i,j=0,1$, *are uniformly bounded,*

$$\sup_{t \geqslant 0} \sup_{z \in \mathbf{Z}^d} |q_t^{ij}(z)| < \infty. \tag{3.4}$$

(ii) The correlation matrices $q_t^{ij}(z)$, $i,j=0,1$, *converge for each* $z \in \mathbf{Z}^d$, *and*

$$q_t^{ij}(z) \to q_\infty^{ij}(z), \qquad t \to \infty, \tag{3.5}$$

where the functions $q_\infty^{ij}(z)$ *are defined above.*

Proof: For brevity, we prove (3.4) and (3.5) for $i=j=0$. In all other cases the proof of (3.5) is similar. The solution to the Cauchy problem (1.1) is

$$u(x,t) = (2\pi)^{-d} \int_{\mathbf{T}^d} e^{-ix\cdot\theta} (\cos \Omega t \ \hat{Y}_0^0(\theta) + \sin \Omega t \ \Omega^{-1} \hat{Y}_0^1(\theta)) d\theta,$$

where $\Omega \equiv \Omega(\theta)$ is the non-negative definite Hermitian matrix defined by (2.2). Furthermore, the translation invariance (1.5) implies that

$$E(\hat{Y}_0^i(\theta) \otimes \hat{Y}_0^j(\theta')) = (2\pi)^d \delta(\theta+\theta') \hat{q}_0^{ij}(\theta), \quad i,j=0,1. \tag{3.6}$$

Hence,

$$q_t^{00}(x-y) := E(u(x,t)\otimes u(y,t))$$
$$= (2\pi)^{-d}\int_{\mathbf{T}^d} e^{-i\theta(x-y)}[\cos\Omega t \;\; \hat{q}_0^{00}(\theta)\cos\Omega t$$
$$+ \sin\Omega t \;\; \Omega^{-1}\hat{q}_0^{10}(\theta)\cos\Omega t + \cos\Omega t \;\; \hat{q}_0^{01}(\theta)\Omega^{-1}\sin\Omega t$$
$$+ \sin\Omega t \;\; \Omega^{-1}\hat{q}_0^{11}(\theta)\Omega^{-1}\sin\Omega t]\,d\theta. \tag{3.7}$$

Therefore, the bound (3.4) with $i=j=0$ follows from Lemma 3.1 or condition **ES** if $\mathcal{C}_0\neq\emptyset$.

Let us check that the convergence (3.5) with $i=j=0$ also follows since the oscillatory integrals in (3.7) tend to zero. Consider for example the last term in the integrand of (3.7). We rewrite it using (2.3), in the form

$$L_0^{11}(\theta,t) := \sin\Omega t \;\; \Omega^{-1}\hat{q}_0^{11}(\theta) \;\; \Omega^{-1}\sin\Omega t = B(\theta)(\sin\omega_k t \;\; A_{kl}^{11}(\theta)\sin\omega_l t)_{k,l\in \mathrm{I}_n} B^*(\theta), \tag{3.8}$$

where $A^{11}(\theta) := B^*(\theta)\Omega^{-1}\hat{q}_0^{11}(\theta)\Omega^{-1}B(\theta)$. However, at this moment we have to choose certain smooth branches of the functions $B(\theta)$ and $\omega_k(\theta)$ since we are going to apply the stationary phase arguments which require a smoothness in θ. To make it correctly, we cut off all singularities. First, we define the combined *critical set*,

$$\mathcal{C} := \cup_k \mathcal{C}_k \cup \mathcal{C}_* \cup \mathcal{C}_0\,. \tag{3.9}$$

Then Lemmas 2.2, 2.3 imply the following lemma.

Lemma 3.3: Let conditions **E1**–**E4** *hold. Then* $\mathrm{mes}\,\mathcal{C}=0$.

Second, fix an $\varepsilon>0$ and choose a finite partition of unity,

$$f(\theta)+g(\theta)=1, \;\; g(\theta)=\sum_{m=1}^{M} g_m(\theta), \quad \theta\in\mathbf{T}^d, \tag{3.10}$$

where f, g_m are non-negative functions from $C_0^\infty(\mathbf{T}^d)$, the supports of g_m are sufficiently small and

$$\mathrm{supp} \;\; f\subset\{\theta\in\mathbf{T}^d\colon \mathrm{dist}(\theta,\mathcal{C})<\varepsilon\}, \;\; \mathrm{supp} g_m\subset\{\theta\in\mathbf{T}^d\colon \mathrm{dist}(\theta,\mathcal{C})\geqslant\varepsilon/2\}. \tag{3.11}$$

Now (3.8) can be rewritten as

$$L_0^{11}(\theta,t) = f(\theta)L_0^{11}(\theta,t) + \frac{1}{2}\sum_m g_m(\theta)B(\theta)((\cos(\omega_k-\omega_l)t$$
$$-\cos(\omega_k+\omega_l)t)A_{kl}^{11}(\theta))_{k,l\in\mathrm{I}_n} B^*(\theta). \tag{3.12}$$

By Lemma 2.2 and the compactness arguments, we can choose the supports of g_m so small that the eigenvalues $\omega_k(\theta)$ and the matrix $B(\theta)$ are real-analytic functions inside the $\mathrm{supp} g_m$ for every m: we do not mark the functions by the index m to not overburden the notations.

Let us substitute (3.12) into the last term of (3.7) and analyze the Fourier integrals with f and g_m separately. The integral with f converges to zero uniformly in $t\geqslant 0$, as $\varepsilon\to 0$. Indeed, by Lemma 3.3 we have

$$\left|\int_{\mathbf{T}^d} e^{-i\theta(x-y)} f(\theta)L_0^{11}(\theta,t)\,d\theta\right| \leqslant C\int_{\mathrm{dist}(\theta,\mathcal{C})<\varepsilon} \|\Omega^{-1}(\theta)\hat{q}_0^{11}(\theta)\Omega^{-1}(\theta)\|\,d\theta\to 0, \quad \varepsilon\to 0,$$

since the integrand is summable by Lemma 3.1 or condition **ES** if $\mathcal{C}_0\neq\emptyset$.

Below we will prove the convergence for the integrals with g_m. We will deduce the convergence from the fact that the identities $\omega_k(\theta)\pm\omega_l(\theta)\equiv\text{const}_\pm$ with the $\text{const}_\pm\neq 0$ are impossible by the condition **E5**. Furthermore, the oscillatory integrals with $\omega_k(\theta)\pm\omega_l(\theta)\not\equiv\text{const}$ vanish as $t\to\infty$. Hence, only the integrals with $\omega_k(\theta)-\omega_l(\theta)\equiv 0$ contribute to the limit since $\omega_k(\theta)+\omega_l(\theta)\equiv 0$ would imply $\omega_k(\theta)\equiv\omega_l(\theta)\equiv 0$ which is impossible by **E4**. A similar analysis of the three remaining terms in the integrand of (3.7) gives

$$\begin{aligned} q_t^{00}(x-y)&=(2\pi)^{-d}\int_{\mathbf{T}^d}e^{-i\theta(x-y)}f(\theta)L_0^{11}(\theta,t)\,d\theta+(2\pi)^{-d}\sum_m\ \int_{\mathbf{T}^d}g_m(\theta)\\ &\quad\times e^{-i\theta(x-y)}\left[\frac{1}{2}B(\theta)(\chi_{kl}(A_{kl}^{00}(\theta)+A_{kl}^{11}(\theta)))_{k,l\in\mathrm{I}_n}B^*(\theta)+\cdots\right]d\theta\\ &=(2\pi)^{-d}\int_{\mathbf{T}^d}e^{-i\theta(x-y)}f(\theta)L_0^{11}(\theta,t)\,d\theta+(2\pi)^{-d}\int_{\mathbf{T}^d}g(\theta)e^{-i\theta(x-y)}\hat{q}_\infty^{00}(\theta)\,d\theta+\cdots, \end{aligned} \tag{3.13}$$

according to the notations (2.18)–(2.21). Here $A^{00}(\theta):=B^*(\theta)\hat{q}_0^{00}(\theta)B(\theta)$ and "$\cdots$" stands for the oscillatory integrals which contain $\cos(\omega_k(\theta)\pm\omega_l(\theta))t$ and $\sin(\omega_k(\theta)\pm\omega_l(\theta))t$ with $\omega_k(\theta)\pm\omega_l(\theta)\not\equiv\text{const}$.

The oscillatory integrals converge to zero by the Lebesgue–Riemann Theorem since all the integrands in "$\cdots$" are summable and $\nabla(\omega_k(\theta)\pm\omega_l(\theta))=0$ only on the set of the Lebesgue measure zero. The summability follows from Lemma 3.1 or the condition **ES** since the matrices $B^*(\theta)$ are unitary. The zero measure follows similarly to (2.4) since $\omega_k(\theta)\pm\omega_l(\theta)\not\equiv\text{const}$.

At last, let us prove the convergence (3.5) with $i=j=0$. From the last line of (3.13) we know that $q_t^{00}(x-y)$ is close to the integral with g if ε is small and t is large. Therefore, the limit of $q_t^{00}(x-y)$ as $t\to\infty$ coincides with the limit of the integral as $\varepsilon\to 0$. Finally, this limit coincides with $q_\infty^{00}(x-y)$ since $\hat{q}_\infty^{00}\in L^1(\mathbf{T}^d)$ by Remark 2.9. □

C. Compactness of measures family

Proof of Proposition 2.11: The compactness of the measures family $\{\mu_t, t\in\mathbf{R}\}$ will follow from the bounds (2.25) by the Prokhorov Theorem (Ref. 22, Lemma II.3.1) using the method of Ref. 22, Theorem XII.5.2 since the embedding $\mathcal{H}_\alpha\subset\mathcal{H}_\beta$ is compact if $\alpha>\beta$.

First, the translation invariance (3.3) and Proposition 3.2 (i) imply that for $x\in\mathbf{Z}^d$ we have

$$e_t:=\int\left[|u_0(x)|^2+|v_0(x)|^2\right]\mu_t(dY_0)=\operatorname{tr}q_t^{00}(0)+\operatorname{tr}q_t^{11}(0)\leqslant\overline{e}<\infty,\quad t\geqslant 0. \tag{3.14}$$

Hence by the definition (2.1) we get for any $\alpha<-d/2$:

$$E\|U(t)Y_0\|_\alpha^2=e_t\sum_{x\in\mathbf{Z}^d}(1+|x|^2)^\alpha=C(\alpha)e_t\leqslant C(\alpha)\overline{e}<\infty,\quad t\geqslant 0.$$

□

IV. DUALITY ARGUMENT

To prove Theorem A, it remains to check Proposition 2.12. Let us rewrite (1.10) as follows:

$$E\exp\{i\langle Y(t),\Psi\rangle\}\to\hat{\mu}_\infty(\Psi),\quad t\to\infty. \tag{4.1}$$

We will prove it in Secs. V–VIII. In this section we evaluate $\langle Y(t),\Psi\rangle$ by using the following duality arguments. Remember that $Y_0\in\mathcal{H}_\alpha$ with $\alpha<-d/2$. For $t\in\mathbf{R}$ introduce a "formal adjoint" operator $U'(t)$ from space $\mathcal{D}$ to $\mathcal{H}_{-\alpha}$:

$$\langle Y, U'(t)\Psi\rangle = \langle U(t)Y, \Psi\rangle, \quad \Psi \in \mathcal{D}, \quad Y \in \mathcal{H}_\alpha. \tag{4.2}$$

Let us denote by $\Phi(\cdot,t) = U'(t)\Psi$. Then (4.2) can be rewritten as

$$\langle Y(t), \Psi\rangle = \langle Y_0, \Phi(\cdot,t)\rangle, \quad t \in \mathbf{R}. \tag{4.3}$$

The adjoint group $U'(t)$ admits the following convenient description. Lemma 4.1 below display that the action of group $U'(t)$ coincides with the action of $U(t)$, up to the order of the components.

Lemma 4.1: For $\Psi = (\Psi^0, \Psi^1) \in \mathcal{D}$ we have

$$\Phi(\cdot,t) := U'(t)\Psi = (\dot\psi(\cdot,t), \psi(\cdot,t)), \tag{4.4}$$

where $\psi(x,t)$ is the solution of Eq. (1.1) with the initial data $(u_0, v_0) = (\Psi^1, \Psi^0)$.

Proof: Differentiating (4.2) in t with $Y, \Psi \in \mathcal{D}$, we obtain that $\langle Y, \dot U'(t)\Psi\rangle = \langle \dot U(t)Y, \Psi\rangle$. The group $U(t)$ has the generator $\mathcal{A}$ from (1.3). The generator of $U'(t)$ is the conjugate operator to $\mathcal{A}$:

$$\mathcal{A}' = \begin{pmatrix} 0 & -\mathcal{V} \\ 1 & 0 \end{pmatrix}. \tag{4.5}$$

Hence, the representation (4.4) holds with $\ddot\psi(x,t) = -\Sigma_{y\in\mathbf{Z}^d} V(x-y)\psi(y,t)$. □

The lemma allows us to construct the oscillatory integral representation for $\Phi(x,t)$. Namely, (4.4), (4.5) imply that in the Fourier representation for $\Phi(\cdot,t) = U'(t)\Psi$ we have

$$\dot{\hat\Phi}(\theta,t) = \hat{\mathcal{A}}^*(\theta)\hat\Phi(\theta,t), \quad \hat\Phi(\theta,t) = \hat{\mathcal{G}}^*(t,\theta)\hat\Psi(\theta).$$

Here we denote [see (2.9)]

$$\hat{\mathcal{A}}^*(\theta) = \begin{pmatrix} 0 & -\hat V(\theta) \\ 1 & 0 \end{pmatrix}, \quad \hat{\mathcal{G}}^*(t,\theta) = e^{\hat{\mathcal{A}}^*(\theta)t} = \begin{pmatrix} \cos\Omega t & -\Omega\sin\Omega t \\ \Omega^{-1}\sin\Omega t & \cos\Omega t \end{pmatrix}, \tag{4.6}$$

with $\Omega \equiv \Omega(\theta) = \Omega^*(\theta)$. Therefore,

$$\Phi(x,t) = (2\pi)^{-d}\int_{\mathbf{T}^d} e^{-i\theta x}\hat{\mathcal{G}}^*(t,\theta)\hat\Psi(\theta)\,d\theta, \quad x \in \mathbf{Z}^d. \tag{4.7}$$

Since $f(\theta) + g(\theta) \equiv 1$ by (3.10), we can split Φ in two components:

$$\begin{aligned}\Phi(x,t) &= (2\pi)^{-d}\int_{\mathbf{T}^d} e^{-i\theta x}\hat{\mathcal{G}}^*(t,\theta)f(\theta)\hat\Psi(\theta)\,d\theta + (2\pi)^{-d}\int_{\mathbf{T}^d} e^{-i\theta x}\hat{\mathcal{G}}^*(t,\theta)g(\theta)\hat\Psi(\theta)\,d\theta \\ &= \Phi_f(x,t) + \Phi_g(x,t), \quad x \in \mathbf{Z}^d,\end{aligned} \tag{4.8}$$

where each function $\Phi_f(x,t)$ and $\Phi_g(x,t)$ admits the representation of type (4.4). By (3.11), the Fourier spectrum of Φ_f is concentrated near the critical set $\mathcal{C}$, while the spectrum of Φ_g is separated from $\mathcal{C}$.

V. STANDARD DECAY IN THE NONCRITICAL SPECTRUM

We prove the decay of type (1.18) for the "noncritical" component Φ_g. The function Φ_g can be expanded similarly to (3.12), in the form

$$\Phi_g(x,t) = \sum_m \sum_{\pm,\, k\in \mathrm{I}_n} \int_{\mathbf{T}^d} g_m(\theta) e^{-i(\theta x \pm \omega_k(\theta)t)} a_k^{\pm}(\theta)\hat\Psi(\theta)\,d\theta. \tag{5.1}$$

By Lemma 2.2 and the compactness arguments, we can choose the eigenvalues $\omega_k(\theta)$ and the matrices $a_k^{\pm}(\theta)$ as real-analytic functions inside the $\mathrm{supp} g_m$ for every m: we do not mark the functions by the index m to not overburden the notations.

Lemma 4.1 means that each component $\Phi_g^i(x,t)$, $i=0,1$, is a solution to Eq. (1.1). To prove (4.1), we analyze the radiative properties of $\Phi_g(x,t)$ in all directions. For this purpose, we apply the stationary phase method to the oscillatory integral (5.1) along the rays $x=vt$, $t>0$. Then the phase becomes $(\theta v \pm \omega_k(\theta))t$, and its stationary points are the solutions to the equations $v = \mp \nabla \omega_k(\theta)$. We collect all necessary asymptotics in the following lemma [cf. (1.18)].

Lemma 5.1: For any fixed $\Psi \in \mathcal{D}$ and $g(\theta) \in C_0^\infty(\mathbf{T}^d \backslash \mathcal{C})$ the following bounds hold:

(i)
$$\sup_{x \in \mathbf{Z}^d} |\Phi_g(x,t)| \leqslant C t^{-d/2}. \tag{5.2}$$

(ii) or any $p>0$ there exist $C_p, \gamma_g > 0$ such that

$$|\Phi_g(x,t)| \leqslant C_p (|t|+|x|+1)^{-p}, \quad |x| \geqslant \gamma_g t. \tag{5.3}$$

Proof: Consider $\Phi_g(x,t)$ along each ray $x=vt$ with arbitrary $v \in \mathbf{R}^d$. Substituting to (5.1), we get

$$\Phi_g(vt,t) = \sum_m \sum_{\pm,\, k \in \mathrm{I}_n} \int_{\mathbf{T}^d} g_m(\theta) e^{-i(\theta v \pm \omega_k(\theta))t} a_k^{\pm}(\theta) \hat{\Psi}(\theta) d\theta. \tag{5.4}$$

This is a sum of oscillatory integrals with the phase functions $\phi_k^{\pm}(\theta) = \theta v \pm \omega_k(\theta)$ and the amplitudes $a_k^{\pm}(\theta)$ which are real-analytic functions of the θ inside the $\mathrm{supp} g_m$. Since $\omega_k(\theta)$ is real-analytic, each function $\phi_k^{\pm}$ has no more than a finite number of stationary points $\theta \in \mathrm{supp} g_m$, solutions to the equation $v = \mp \nabla \omega_k(\theta)$. The stationary points are nondegenerate for $\theta \in \mathrm{supp} g_m$ by (3.11), (3.9), and **E4** since

$$\det\left(\frac{\partial^2 \phi_k^{\pm}}{\partial \theta_i \, \partial \theta_j} \right) = \pm D_k(\theta) \neq 0, \quad \theta \in \mathrm{supp} g_m. \tag{5.5}$$

At last, $\hat{\Psi}(\theta)$ is smooth since $\Psi \in \mathcal{D}$. Therefore, $\Phi_g(vt,t) = \mathcal{O}(t^{-d/2})$ according to the standard stationary phase method.[10,17] This implies the bounds (5.2) in each cone $|x| \leqslant ct$ with any finite c.

Further, denote by $\overline{v_g} := \max_m \max_{k \in \mathrm{I}_n} \max_{\theta \in \mathrm{supp} g_m} |\nabla \omega_k(\theta)|$. Then for $|v| > \overline{v_g}$ the stationary points do not exist on the $\mathrm{supp} g$. Hence, the integration by parts as in Ref. 17 yields $\Phi_g(vt,t) = \mathcal{O}(t^{-p})$ for any $p>0$. On the other hand, the integration by parts in (5.1) implies similar bound $\Phi_g(x,t) = \mathcal{O}((t/|x|)^l)$ for any $l>0$. Therefore, (5.3) follows with any $\gamma_g > \overline{v_g}$. Now the bounds (5.2) follow everywhere. □

VI. CONTRIBUTION OF CRITICAL SET

We are going to prove (4.1). Rewrite it using (4.3):

$$E \exp\{i\langle Y_0, \Phi(\cdot,t)\rangle\} - \hat{\mu}_\infty(\Psi) \to 0, \quad t \to \infty. \tag{6.1}$$

The splitting (4.8) gives $\langle Y_0, \Phi(\cdot,t)\rangle = \langle Y_0, \Phi_f(\cdot,t)\rangle + \langle Y_0, \Phi_g(\cdot,t)\rangle$. Our main argument is that the contribution of $\langle Y_0, \Phi_f(\cdot,t)\rangle$ to (6.1) has a small dispersion. We will deduce this from Lemmas 3.1, 3.3. At first, let us estimate the difference in (6.1) by the triangle inequality:

$$\begin{aligned} |E \exp\{i\langle Y_0, \Phi(\cdot,t)\rangle\} - \hat{\mu}_\infty(\Psi)| \leqslant |E \exp\{i\langle U(t) Y_0, \Psi\rangle\} - E \exp\{i\langle Y_0, \Phi_g(\cdot,t)\rangle\}| + |\hat{\mu}_\infty(\Psi_g) \\ - \hat{\mu}_\infty(\Psi)| + |E \exp\{i\langle Y_0, \Phi_g(\cdot,t)\rangle\} - \hat{\mu}_\infty(\Psi_g)| = I + II + III, \end{aligned} \tag{6.2}$$

where $\Psi_g := F^{-1}[g(\theta)\hat{\Psi}(\theta)] = \Phi_g(\cdot,0)$. Let us consider each of the three terms separately.

I. The first term $I=I(\varepsilon,t)$ represents the contribution of the neighborhood of the critical set $\{\theta\in\mathbf{T}^d\colon \mathrm{dist}(\theta,\mathcal{C})<\varepsilon\}$ and tends to zero as $\varepsilon\to 0$ uniformly in $t\geqslant 0$. Namely, by the Cauchy–Schwartz inequality,

$$I=|Ee^{i\langle Y_0,\Phi(\cdot,t)\rangle}-Ee^{i\langle Y_0,\Phi_g(\cdot,t)\rangle}|\leqslant E|e^{i\langle Y_0,\Phi_f(\cdot,t)\rangle}-1|\leqslant C(E|\langle Y_0,\Phi_f(\cdot,t)\rangle|^2)^{1/2}. \tag{6.3}$$

Using the Parseval identity and (4.8), we get

$$E|\langle Y_0,\Phi_f(\cdot,t)\rangle|^2=(2\pi)^{-2d}E|\langle \hat Y_0(\theta),f(\theta)\hat\Phi(\theta,t)\rangle|^2$$
$$=(2\pi)^{-2d}\langle E(\hat Y_0(\theta)\otimes\overline{\hat Y_0(\theta')}),\, f(\theta)f(\theta')\,\hat{\mathcal{G}}^*(t,\theta)\hat\Psi(\theta)\otimes\overline{\hat{\mathcal{G}}^*(t,\theta')\,\hat\Psi(\theta')}\,\rangle. \tag{6.4}$$

Now take into account that $E(\hat Y_0(\theta)\otimes\overline{\hat Y_0(\theta')})=(2\pi)^d\delta(\theta-\theta')\hat q_0(\theta)$ similarly to (3.6). Then (6.4), (4.6), (3.11) and the bounds $0\leqslant f(\theta)\leqslant 1$ imply

$$E|\langle Y_0,\Phi_f(\cdot,t)\rangle|^2\leqslant C_1\sum_{i,j=0,1}\int_{\mathrm{dist}(\theta,\mathcal{C})<\varepsilon}\|\Omega^{-i}(\theta)\hat q_0^{ij}(\theta)\Omega^{-j}(\theta)\|\,d\theta\to 0,\quad \varepsilon\to 0,$$

owing to Lemma 3.3 since the integrand is summable. The summability follows from Lemma 3.1 or condition **ES** if $\mathcal{C}_0\neq\emptyset$.

II. The second term $II=II(\varepsilon)$ tends to zero as $\varepsilon\to 0$. Indeed,

$$\mathcal{Q}_\infty(\Psi_g,\Psi_g)=(2\pi)^{-2d}\sum_{i,j=0}^{1}\int_{\mathbf{T}^d}(\hat q_\infty^{ij}(\theta),g(\theta)\hat\Psi^i(\theta)\otimes g(\theta)\overline{\hat\Psi^j(\theta)})\,d\theta\to\mathcal{Q}_\infty(\Psi,\Psi),$$
$$\varepsilon\to 0,$$

by the Lebesgue Dominated Convergence Theorem since $0\leqslant g(\theta)\leqslant 1$ and $\hat q_\infty^{ij}\in L^1(\mathbf{T}^d)$ by Remark 2.9. Hence for the Gaussian measure μ_∞, we get by (2.23),

$$|\hat\mu_\infty(\Psi_g)-\hat\mu_\infty(\Psi)|=|\exp\{-\tfrac{1}{2}\mathcal{Q}_\infty(\Psi_g,\Psi_g)\}-\exp\{-\tfrac{1}{2}\mathcal{Q}_\infty(\Psi,\Psi)\}|\to 0,\quad \varepsilon\to 0.$$

III. To prove Proposition 2.12, it remains to check that for any fixed $\varepsilon>0$, we have

$$III(\varepsilon,t)=|E\exp\{i\langle Y_0,\Phi_g(\cdot,t)\rangle\}-\hat\mu_\infty(\Psi_g)|\to 0,\quad t\to\infty. \tag{6.5}$$

We prove (6.5) in Sec. VIII using the Bernstein arguments of the next section.

VII. BERNSTEIN'S "ROOMS-CORRIDORS" PARTITION

Our proof of (6.5) is similar to the case of the continuous Klein–Gordon equation in $\mathbf{R}^d$:[6] all the integrals over $\mathbf{R}^d$ become the series over $\mathbf{Z}^d$, etc. Another novelty in the proofs is the following: in the case of the Klein–Gordon equation we have $\Phi(x,t)=0$ for $|x|\geqslant t+c(\Psi)$, while for the discrete crystal we have (5.3) instead.

Let us introduce a "room-corridor" partition of the ball $\{x\in\mathbf{Z}^d\colon |x|\leqslant\gamma_g t\}$ with γ_g from (5.3). For $t>0$ we choose below $\Delta_t,\rho_t\in\mathbf{N}$ (we will specify the asymptotic relations between t, Δ_t, and ρ_t). Let us set $h_t=\Delta_t+\rho_t$ and

$$a^j=jh_t,\ \ b^j=a^j+\Delta_t,\ \ j\in\mathbf{Z},\quad N_t=[(\gamma_g t)/h_t]. \tag{7.1}$$

We call the slabs $R_t^j=\{x\in\mathbf{Z}^d\colon |x|\leqslant N_t h_t,\ a^j\leqslant x_d<b^j\}$ the "rooms," $C_t^j=\{x\in\mathbf{Z}^d\colon |x|\leqslant N_t h_t,\ b^j\leqslant x_d<a^{j+1}\}$ the "corridors" and $L_t=\{x\in\mathbf{Z}^d\colon |x|>N_t h_t\}$ the "tails." Here $x=(x_1,\dots,x_d)$, Δ_t is the width of a room, and ρ_t is that of a corridor. Let us denote by χ_t^j the indicator of the room R_t^j, ξ_t^j that of the corridor C_t^j, and η_t that of the tail L_t. Then

$$\sum_t [\chi_t^j(x)+\xi_t^j(x)]+\eta_t(x)=1,\ x\in\mathbf{Z}^d, \tag{7.2}$$

where the sum Σ_t stands for $\Sigma_{j=-N_t}^{N_t-1}$. Hence we get the following Bernstein's type representation:

$$\langle Y_0,\Phi_g(\cdot,t)\rangle=\sum_t [\langle Y_0,\chi_t^j\Phi_g(\cdot,t)\rangle+\langle Y_0,\xi_t^j\Phi_g(\cdot,t)\rangle]+\langle Y_0,\eta_t\Phi_g(\cdot,t)\rangle. \tag{7.3}$$

Let us introduce the random variables $r_t^j,\ c_t^j,\ l_t$ by

$$r_t^j=\langle Y_0,\chi_t^j\Phi_g(\cdot,t)\rangle,\quad c_t^j=\langle Y_0,\xi_t^j\Phi_g(\cdot,t)\rangle,\ \ l_t=\langle Y_0,\eta_t\Phi_g(\cdot,t)\rangle. \tag{7.4}$$

Then (7.3) becomes

$$\langle Y_0,\Phi_g(\cdot,t)\rangle=\sum_t (r_t^j+c_t^j)+l_t. \tag{7.5}$$

Lemma 7.1: Let **S0**–**S3** *hold. The following bounds hold for* $t>1$:

$$E|r_t^j|^2\leqslant C(\Psi_g)\ \Delta_t/t,\ \ \forall j, \tag{7.6}$$

$$E|c_t^j|^2\leqslant C(\Psi_g)\ \ \rho_t/t,\ \ \forall j, \tag{7.7}$$

$$E|l_t|^2\leqslant C_p(\Psi_g)(1+t)^{-p},\quad \forall p>0. \tag{7.8}$$

Proof: We discuss (7.6), and (7.7), (7.8) can be done in a similar way [the proof of (7.8) additionally uses (5.3)]. Express $E|r_t^j|^2$ in the correlation matrices. Definition (7.4) implies that

$$E|r_t^j|^2=\langle\chi_t^j(x)\chi_t^j(y)q_0(x-y),\Phi_g(x,t)\otimes\Phi_g(y,t)\rangle. \tag{7.9}$$

According to (5.2), Eq. (7.9) implies that

$$E|r_t^j|^2\leqslant Ct^{-d}\sum_{x,y}\ \chi_t^j(x)\|q_0(x-y)\|=Ct^{-d}\sum_x\ \chi_t^j(x)\ \sum_z\ \|q_0(z)\|\leqslant C\Delta_t/t, \tag{7.10}$$

where $\|q_0(z)\|$ stands for the norm of a matrix $(q_0^{ij}(z))$. Therefore, (7.10) follows as $\|q_0(\cdot)\|\in l^1(\mathbf{Z}^d)$ by (3.1). □

VIII. IBRAGIMOV–LINNIK CENTRAL LIMIT THEOREM

In this section we prove the convergence (6.5). As was said, we use a version of the Central Limit Theorem developed by Ibragimov and Linnik.[13] If $\mathcal{Q}_\infty(\Psi_g,\Psi_g)=0$, (6.5) is obvious. Indeed, $|E\exp(i\langle Y_0,\Phi_g(\cdot,t)\rangle)-1|\leqslant E|\langle Y_0,\Phi_g(\cdot,t)\rangle|\leqslant(E\langle Y_0,\Phi_g(\cdot,t)\rangle^2)^{1/2}=(\mathcal{Q}_t(\Psi_g,\Psi_g))^{1/2}$, where $\mathcal{Q}_t(\Psi_g,\Psi_g)\to\mathcal{Q}_\infty(\Psi_g,\Psi_g)=0$, as $t\to\infty$. Thus, we may assume that for a given $\Psi\in\mathcal{D}$,

$$\mathcal{Q}_\infty(\Psi_g,\Psi_g)\neq 0. \tag{8.1}$$

Let us choose $0<\delta<1$ and

$$\rho_t\sim t^{1-\delta},\qquad \Delta_t\sim\frac{t}{\log t},\qquad t\to\infty. \tag{8.2}$$

Lemma 8.1: The following limit holds true:

$$N_t\left(\varphi(\rho_t)+\left(\frac{\rho_t}{t}\right)^{1/2}\right)+N_t^2\left(\varphi^{1/2}(\rho_t)+\frac{\rho_t}{t}\right)\to 0,\quad t\to\infty. \tag{8.3}$$

Proof: The function $\varphi(r)$ is nonincreasing; hence by (2.17),

$$r^d\varphi^{1/2}(r)=d\int_0^r s^{d-1}\varphi^{1/2}(r)\,ds\leqslant d\int_0^r s^{d-1}\varphi^{1/2}(s)\,ds\leqslant C\overline{\varphi}<\infty. \tag{8.4}$$

Furthermore, (8.2) implies that $h_t=\Delta_t+\rho_t\sim t/\log t$, $t\to\infty$. Therefore, $N_t\sim t/h_t\sim\log t$. Then (8.3) follows by (8.4) and (8.2). □

Proof of (6.5): By the triangle inequality,

$$\begin{aligned}|E\exp\{i\langle Y_0,\Phi_g(\cdot,t)\rangle\}-\hat{\mu}_\infty(\Psi_g)|&\leqslant\left|E\exp\{i\langle Y_0,\Phi_g(\cdot,t)\rangle\}-E\exp\left\{i\sum_t r_t^j\right\}\right|\\&+\left|\exp\left\{-\frac{1}{2}\sum_t E|r_t^j|^2\right\}-\exp\left\{-\frac{1}{2}\mathcal{Q}_\infty(\Psi_g,\Psi_g)\right\}\right|\\&+\left|E\exp\left\{i\sum_t r_t^j\right\}-\exp\left\{-\frac{1}{2}\sum_t E|r_t^j|^2\right\}\right|\\&\equiv I_1+I_2+I_3.\end{aligned} \tag{8.5}$$

We are going to show that all the summands I_1, I_2, I_3 tend to zero as $t\to\infty$.

Step (i): Equation (7.5) implies

$$I_1=\left|E\exp\left\{i\sum_t r_t^j\right\}\left(\exp\left\{i\sum_t c_t^j+il_t\right\}-1\right)\right|\leqslant C\sum_t E|c_t^j|+E|l_t|\leqslant C\sum_t (E|c_t^j|^2)^{1/2}+(E|l_t|^2)^{1/2}. \tag{8.6}$$

From (8.6), (7.7), (7.8), and (8.3) we obtain that

$$I_1\leqslant C_p t^{-p}+CN_t(\rho_t/t)^{1/2}\to 0,\quad t\to\infty. \tag{8.7}$$

Step (ii): By the triangle inequality,

$$\begin{aligned}I_2&\leqslant\frac{1}{2}\left|\sum_t E|r_t^j|^2-\mathcal{Q}_\infty(\Psi_g,\Psi_g)\right|\\&\leqslant\frac{1}{2}|\mathcal{Q}_t(\Psi_g,\Psi_g)-\mathcal{Q}_\infty(\Psi_g,\Psi_g)|\\&+\frac{1}{2}\left|E\left(\sum_t r_t^j\right)^2-\sum_t E|r_t^j|^2\right|+\frac{1}{2}\left|E\left(\sum_t r_t^j\right)^2-\mathcal{Q}_t(\Psi_g,\Psi_g)\right|\\&\equiv I_{21}+I_{22}+I_{23},\end{aligned} \tag{8.8}$$

where $\mathcal{Q}_t$ is the quadratic form with the matrix kernel $(Q_t^{ij}(x,y))$. (3.5) implies that $I_{21}\to 0$. As for I_{22}, we first obtain that

$$I_{22}\leqslant\sum_{\substack{j\neq k\\ |j|,|k|\leqslant N_t}}|Er_t^jr_t^k|. \tag{8.9}$$

The next lemma is the corollary of Ref. 13, Lemma 17.2.3.

Lemma 8.2: Let $\mathcal{A}$, $\mathcal{B}$ be the subsets of $\mathbf{Z}^d$ with the distance $\operatorname{dist}(\mathcal{A},\mathcal{B})\geqslant r>0$, *and let ξ, η be random variables on the probability space $(\mathcal{H}_\alpha,\mathcal{B}(\mathcal{H}_\alpha),\mu_0)$. Let ξ be measurable with respect to the σ-algebra $\sigma(\mathcal{A})$, and η with respect to the σ-algebra $\sigma(\mathcal{B})$. Then*

(i) $|E\xi\eta-E\xi E\eta|\leqslant Cab\ \varphi^{1/2}(r)$ *if* $(E|\xi|^2)^{1/2}\leqslant a$ *and* $(E|\eta|^2)^{1/2}\leqslant b$;

(ii) $|E\xi\eta-E\xi E\eta|\leqslant Cab\ \varphi(r)$ *if* $|\xi|\leqslant a$ *and* $|\eta|\leqslant b$, *a.s.*

We apply Lemma 8.2 to deduce that $I_{22}\to 0$ as $t\to\infty$. Note that $r_t^j=\langle Y_0(x),\chi_t^j(x)\Phi_g(\cdot,t)\rangle$ is measurable with respect to the σ-algebra $\sigma(R_t^j)$. The distance between the different rooms R_t^j is greater or equal to ρ_t according to (7.1). Then (8.9) and (7.6), **S3** imply by Lemma 8.2 (i), that

$$I_{22}\leqslant CN_t^2\varphi^{1/2}(\rho_t), \tag{8.10}$$

which tends to 0 as $t\to\infty$ by (8.3). Finally, it remains to check that $I_{23}\to 0$, $t\to\infty$. We have

$$\mathcal{Q}_t(\Psi_g,\Psi_g)=E\langle Y_0,\Phi_g(\cdot,t)\rangle^2=E\left(\sum_t\ (r_t^j+c_t^j)+l_t\right)^2,$$

according to (7.5). Therefore, by the Cauchy–Schwartz inequality,

$$\begin{aligned}I_{23}&\leqslant\left|E\left(\sum_t\ r_t^j\right)^2-E\left(\sum_t\ r_t^j+\sum_t\ c_t^j+l_t\right)^2\right|\\&\leqslant CN_t\sum_t\ E|c_t^j|^2+C_1\left(E\left(\sum_t\ r_t^j\right)^2\right)^{1/2}\\&\quad\times\left(N_t\sum_t\ E|c_t^j|^2+E|l_t|^2\right)^{1/2}+CE|l_t|^2.\end{aligned}\tag{8.11}$$

Then (7.6), (8.9), and (8.10) imply

$$E\left(\sum_t\ r_t^j\right)^2\leqslant\sum_t\ E|r_t^j|^2+\sum_{\substack{j\neq k\\ |j|,|k|\leqslant N_t}}|Er_t^jr_t^k|\leqslant CN_t\Delta_t/t+C_1N_t^2\varphi^{1/2}(\rho_t)\leqslant C_2<\infty.$$

Now (7.7), (7.8), (8.11), and (8.3) yield

$$I_{23}\leqslant C_1N_t^2\rho_t/t+C_2N_t(\rho_t/t)^{1/2}+C_3t^{-p}\to 0,\quad t\to\infty. \tag{8.12}$$

So, all the terms I_{21}, I_{22}, I_{23} in (8.8) tend to zero. Then (8.8) implies that

$$I_2\leqslant\frac{1}{2}\left|\sum_t\ E|r_t^j|^2-\mathcal{Q}_\infty(\Psi_g,\Psi_g)\right|\to 0,\quad t\to\infty. \tag{8.13}$$

Step (iii): It remains to verify that

$$I_3=\left|E\exp\left\{i\sum_t\ r_t^j\right\}-\exp\left\{-\frac{1}{2}E\left(\sum_t\ r_t^j\right)^2\right\}\right|\to 0,\quad t\to\infty. \tag{8.14}$$

Lemma 8.2, (ii) with $a=b=1$ yields

$$\left| E\exp\left\{ i\sum_t r_t^j \right\} - \prod_{-N_t}^{N_t-1} E\exp\{ir_t^j\} \right|$$

$$\leqslant \left| E\exp\{ir_t^{-N_t}\}\exp\left\{ i\sum_{-N_t+1}^{N_t-1} r_t^j \right\} - E\exp\{ir_t^{-N_t}\}E\exp\left\{ i\sum_{-N_t+1}^{N_t-1} r_t^j \right\} \right|$$

$$+ \left| E\exp\{ir_t^{-N_t}\}E\exp\left\{ i\sum_{-N_t+1}^{N_t-1} r_t^j \right\} - \prod_{-N_t}^{N_t-1} E\exp\{ir_t^j\} \right|$$

$$\leqslant C\varphi(\rho_t) + \left| E\exp\left\{ i\sum_{-N_t+1}^{N_t-1} r_t^j \right\} - \prod_{-N_t+1}^{N_t-1} E\exp\{ir_t^j\} \right|.$$

Then we apply Lemma 8.2, (ii) recursively and get, according to Lemma 8.1,

$$\left| E\exp\left\{ i\sum_t r_t^j \right\} - \prod_{-N_t}^{N_t-1} E\exp\{ir_t^j\} \right| \leqslant CN_t\varphi(\rho_t) \to 0, \quad t\to\infty. \tag{8.15}$$

It remains to check that

$$\left| \prod_{-N_t}^{N_t-1} E\exp\{ir_t^j\} - \exp\left\{ -\frac{1}{2}\sum_t E|r_t^j|^2 \right\} \right| \to 0, \quad t\to\infty. \tag{8.16}$$

According to the standard statement of the Lindeberg Central Limit Theorem (see, e.g., Ref. 16, Theorem 4.7) it suffices to verify the Lindeberg condition: $\forall\,\delta>0$,

$$\frac{1}{\sigma_t}\sum_t E_{\delta\sqrt{\sigma_t}}|r_t^j|^2 \to 0, \quad t\to\infty.$$

Here $\sigma_t \equiv \Sigma_t E|r_t^j|^2$, and $E_a f := E(X_a f)$, where X_a is the indicator of the event $|f|>a^2$. Note that (8.13) and (8.1) imply that $\sigma_t \to \mathcal{Q}_\infty(\Psi_g,\Psi_g)\neq 0$, $t\to\infty$. Hence it remains to verify that

$$\sum_t E_a|r_t^j|^2 \to 0, \quad t\to\infty, \quad \text{for any } a>0.$$

This follows from the bounds for the fourth order moments as in Ref. 6, Sec. IX. This completes the proof of Proposition 2.12. □

IX. ERGODICITY AND MIXING FOR THE LIMIT MEASURES

The limit measure μ_∞ is invariant by Theorem A (iv). Let E_∞ denote the integral over μ_∞.

Theorem 9.1: *Let all assumptions of Theorem A hold for the equation (1.1) and the initial measure μ_0. Then $U(t)$ is mixing with respect to the corresponding limit measure μ_∞, i.e., $\forall\, f,g\in L^2(\mathcal{H}_\alpha,\mu_\infty)$,*

$$\lim_{t\to\infty} E_\infty f(U(t)Y)g(Y) = E_\infty f(Y)E_\infty g(Y). \tag{9.1}$$

In particular, the group $U(t)$ is ergodic with respect to the measure μ_∞:

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T f(U(t)Y)dt = E_\infty f(Y) \quad (\text{mod } \mu_\infty). \tag{9.2}$$

Proof: Since μ_∞ is Gaussian, the proof of (9.1) reduces to the proof of the following convergence: $\forall \Psi_1, \Psi_2 \in \mathcal{D}$,

$$\lim_{t\to\infty} E_\infty \langle U(t)Y, \Psi_1\rangle\langle Y, \Psi_2\rangle = 0. \tag{9.3}$$

Using the Parseval identity and (4.8) we obtain similarly to (6.4) that

$$\begin{aligned} E_\infty \langle U(t)Y, \Psi_1\rangle\langle Y, \Psi_2\rangle &= (2\pi)^{-2d}\int_{\mathbf{T}^d} (\hat{\mathcal{G}}(t,\theta)\hat{q}_\infty(\theta), f(\theta)\hat{\Psi}_1(\theta)\otimes\overline{\hat{\Psi}_2}(\theta))\, d\theta \\ &\quad + (2\pi)^{-2d}\int_{\mathbf{T}^d} (\hat{\mathcal{G}}(t,\theta)\hat{q}_\infty(\theta), g(\theta)\hat{\Psi}_1(\theta)\otimes\overline{\hat{\Psi}_2}(\theta))\, d\theta \\ &= I_f(t) + I_g(t). \end{aligned} \tag{9.4}$$

Lemma 9.2: The uniform bound holds: $\|\hat{\mathcal{G}}(t,\theta)\hat{q}_\infty(\theta)\| \leqslant G(\theta)$, $t \geqslant 0$, *where* $G(\theta) \in L^1(\mathbf{T}^d)$.

Proof: (4.6) implies that

$$\hat{\mathcal{G}}(t,\theta)\hat{q}_\infty(\theta) = \begin{pmatrix} \cos\Omega t & \sin\Omega t \\ -\sin\Omega t\cdot\Omega & \cos\Omega t\cdot\Omega \end{pmatrix} \begin{pmatrix} \hat{q}_\infty^{00} & \hat{q}_\infty^{01} \\ \Omega^{-1}\hat{q}_\infty^{10} & \Omega^{-1}\hat{q}_\infty^{11} \end{pmatrix}. \tag{9.5}$$

Therefore,

$$\|\hat{\mathcal{G}}(t,\theta)\hat{q}_\infty(\theta)\| \leqslant C\sum_{i,j=0,1} \|\Omega^{-i}\hat{q}_\infty^{ij}(\theta)\|. \tag{9.6}$$

It remains to prove that $\Omega^{-i}\hat{q}_\infty^{ij}(\theta) \in L^1(\mathbf{T}^d)$. Since $\hat{q}_\infty(\theta) \in L^1(\mathbf{T}^d)$ by Remark 2.9, it suffices to verify that $\Omega^{-1}(\theta)\hat{q}_\infty^{1j}(\theta) \in L^1(\mathbf{T}^d)$, $j=0,1$. This also follows from Remark 2.9 if $\mathcal{C}_0 = \emptyset$. Otherwise, we will use the condition **ES**. Namely, owing to (2.22), we have

$$\Omega^{-1}(\theta)\hat{q}_\infty^{ij}(\theta) = \sum_{\sigma=1}^{s+1} \Pi_\sigma(\theta)\Omega^{-1}(\theta)M_0^{ij}(\theta)\Pi_\sigma(\theta), \tag{9.7}$$

since $\Omega^{-1}(\theta)$ commutes with its spectral projection $\Pi_\sigma(\theta)$. At last, (2.21) and **ES** imply

$$\Omega^{-1}M_0^{10} = \tfrac{1}{2}(\Omega^{-1}\hat{q}_0^{10} - \hat{q}_0^{01}\Omega^{-1}) \in L^1(\mathbf{T}^d),$$

$$\Omega^{-1}M_0^{11} = \tfrac{1}{2}(\Omega^{-1}\hat{q}_0^{11} + \hat{q}_0^{00}\Omega) \in L^1(\mathbf{T}^d).$$

□

The Lemma 9.2 together with (3.11) and Lemma 3.3 imply that $\forall \delta > 0$ $\exists \varepsilon > 0$ such that

$$|I_f(t)| \leqslant \delta, \qquad t \geqslant 0. \tag{9.8}$$

It remains to study the oscillatory integral $I_g(t)$. Rewrite it using (5.1), in the form

$$I_g(t) = \sum_m \sum_{\pm,\, k\in \mathrm{I}_n} \int_{\mathbf{T}^d} g_m(\theta) e^{\pm i\omega_k(\theta)t} a_k^{\pm}(\theta)(\hat{q}_\infty(\theta), \hat{\Psi}_1(\theta)\otimes\overline{\hat{\Psi}_2}(\theta))\, d\theta. \tag{9.9}$$

Here all phase functions $\omega_k(\theta)$ and the amplitudes $a_k^{\pm}(\theta)$ are smooth functions in the $\mathrm{supp} g_m$. Furthermore, $\nabla\omega_k(\theta) = 0$ only on the set of the Lebesgue measure zero. This follows similarly to (2.4) since $\nabla\omega_k(\theta) \not\equiv \mathrm{const}$ by the condition **E4**. Hence,

$$I_g(t) \to 0 \quad \text{as} \quad t\to\infty, \tag{9.10}$$

by the Lebesgue–Riemann Theorem since $\hat{q}_\infty \in L^1(\mathbf{T}^d)$. Finally, (9.4)–(9.10) imply (9.3) since $\delta > 0$ is arbitrary. □

Remark: A similar result for wave and Klein–Gordon equations has been proved in Refs. 4, 5.

ACKNOWLEDGMENTS

T. V. D. and A. I. K. were supported partly by the FWF-Project P16105-N05 of N. J. Mauser and research grants of DFG (436 RUS 113/615/0-1) and RFBR (01-01-04002). A. I. K. is also partly supported by the Max-Planck Institute for Mathematics in Sciences (Leipzig).

APPENDIX: CROSSING POINTS

1. Proof of Lemmas 2.2 and 2.3

Step 1: By the condition **E1** the matrix $\hat{V}(\theta)$ is an analytic function in a connected open (complex) neighborhood $\mathcal{O}_c(\mathbf{T}^d)$ of $\mathbf{T}^d$ in $\mathbf{T}^d_c := \mathbf{T}^d \oplus i\mathbf{R}^d$. Consider the analytic function $d(\theta,\omega) := \det(\hat{V}(\theta) - \omega^2)$ in $\mathcal{O}_c(\mathbf{T}^d) \times \mathbf{C}$ and the analytic subset defined by the equation $d(\theta,\omega) = 0$ in $\mathcal{O}_c(\mathbf{T}^d) \times \mathbf{C}$. The subset consists of the points $(\theta, \pm\omega_k(\theta))$, $k \in \mathrm{I}_n$. It is important that $d(\theta,\omega) \not\equiv 0$ for any fixed $\theta \in \mathcal{O}_c(\mathbf{T}^d)$, hence the function d satisfies the *Weierstrass condition* of Ref. 15, Section 2.1.1. Therefore, by the Weierstrass Preparation Theorem in Ref. 15, Thm 2.1, there exists a proper analytic *discriminant subset* $\Delta \subset \mathcal{O}_c(\mathbf{T}^d)$ s.t.: for $\Theta \in \mathcal{O}_c(\mathbf{T}^d) \setminus \Delta$ there exists a (complex) neighborhood $\mathcal{O}_c(\Theta)$ of Θ in $\mathcal{O}_c(\mathbf{T}^d)$ where each of $\omega_k(\theta)$ can be chosen as a holomorphic function. More precisely, this is established in the proof of Ref. 15, Proposition 2.1 which is the main step to the proof of the Weierstrass Theorem. We set $\mathcal{C}_* := \Delta \cap \mathbf{T}^d$ and $\mathcal{O}(\Theta) = \mathcal{O}_c(\Theta) \cap \mathbf{T}^d$ for $\Theta \in \mathbf{T}^d \setminus \mathcal{C}_*$. Then Lemma 2.2 (ii) follows for $\omega_k(\theta)$.

Step 2: The identity (2.4) will follow from the next general Proposition.

Proposition 10.1: Let $\mathcal{M}$ be a proper analytic subset of $\mathcal{O}_c(\mathbf{T}^d)$. Then the Lebesgue measure of the intersection $M = \mathcal{M} \cap \mathbf{T}^d$ is zero.

Proof: Let us use the analytic stratification of the analytic sets which is constructed in Ref. 12, Thm 19 of Chapter II.E and Thm 10 of Chapter III.A. Namely, for each $\Theta \in M$ there exists a complex neighborhood $\mathcal{O}_c(\Theta)$ s.t. $\mathcal{M} \cap \mathcal{O}_c(\Theta) = \cup_{0 \leqslant \delta \leqslant d-1} \mathcal{M}_\delta$, where each $\mathcal{M}_\delta$ is an analytic submanifold of the complex dimension $\delta \leqslant d-1$: here we use that $\mathcal{M}$ is the proper analytic subset in $\mathcal{O}_c(\Theta)$. Now

$$M \cap \mathcal{O}_c(\Theta) = \cup_{0 \leqslant \delta \leqslant d-1} (\mathcal{M}_\delta \cap \mathbf{T}^d).$$

Lemma 10.2: Let $\Theta \in M$ and $\delta = 0, \ldots, d-1$. Then there exists a (real) neighborhood $\mathcal{O}(\Theta)$ of Θ in $\mathbf{T}^d$ such that the intersection $\mathcal{M}_\delta \cap \mathcal{O}(\Theta)$ is contained in a smooth submanifold of $\mathbf{T}^d$ of the real dimension $d-1$.

Proof: We may assume that (i) $\mathcal{M}_\delta$ is defined by the equations $h_j(\theta) = 0$, $j = 1, \ldots, d-\delta$, with the holomorphic functions h_j in $\mathcal{O}_c(\Theta)$; and (ii) $\nabla_c h_j(\theta) \neq 0$, $\theta \in \mathcal{O}_c(\Theta)$, where ∇_c stands for the complex gradient. It is important that $d - \delta \geqslant 1$ so we have at least one function $h_1(\theta)$. Then $h_1(\theta) = f_1(\theta) + i g_1(\theta)$ with the real smooth functions f_1, g_1, and $f_1(\theta) = g_1(\theta) = 0$, $\theta \in M_\delta \cap \mathcal{O}_c(\Theta)$. However, $\nabla_c h_j(\theta) = \nabla_r f_1(\theta) + i \nabla_r g_1(\theta) \neq 0$, where ∇_r stands for the real gradient. Therefore, either $\nabla_r f_1(\Theta) \neq 0$ or $\nabla_r g_1(\Theta) \neq 0$. □

Now Proposition 10.1 obviously follows. □

This proposition implies (2.4) since Δ is a proper analytic subset of $\mathcal{O}_c(\mathbf{T}^d)$. Lemma 2.3 also follows from Proposition 10.1 since **E4** implies that $\det \hat{V}(\theta) \not\equiv 0$ in $\mathbf{T}^d$ and $D_k(\theta) \not\equiv 0$ in $\mathbf{T}^d \setminus \mathcal{C}_*$.

Step 3: Lemma 2.2 (iii) follows from the construction in Ref. 15, Sec. 2.1. Lemma 2.2 (iv) follows from (2.6) since the projection $\Pi_\sigma(\theta)$ can be expressed by the Cauchy integral over the contour surrounding the isolated eigenvalue $\omega_{r_\sigma}(\theta)$.

Step 4: It remains to prove Lemma 2.2 (ii). Let $\mathcal{O}(\Theta)$ denote a small real neighborhood of a point $\Theta \in \mathbf{T}^d \setminus \mathcal{C}_*$ and $E_\sigma(\theta) = \Pi_\sigma(\theta)\mathbf{R}^n$. It suffices to construct an orthonormal basis $\{e_k(\theta) : k \in (r_{\sigma-1}, r_\sigma]\}$ in $E_\sigma(\theta)$ which depends real-analytically on $\theta \in \mathcal{O}(\Theta)$.

Let us choose an arbitrary basis $\{b_k(\Theta): k \in (r_{\sigma-1}, r_\sigma]\}$ in $E_\sigma(\Theta)$. Then $\Pi_\sigma(\theta) b_k(\Theta)$ depend real-analytically on $\theta \in \mathcal{O}(\Theta)$, and $\{\Pi_\sigma(\theta) b_k(\Theta): k \in (r_{\sigma-1}, r_\sigma]\}$ is a basis of $E_\sigma(\theta)$ for θ from a reduced neighborhood $\mathcal{O}'(\Theta)$. Finally, construct the orthonormal basis $\{e_k(\theta): k \in (r_{\sigma-1}, r_\sigma]\}$ by the standard Hilbert–Schmidt orthogonalization process applied to $\{\Pi_\sigma(\theta) b_k(\Theta): k \in (r_{\sigma-1}, r_\sigma]\}$ for each $\theta \in \mathcal{O}'(\Theta)$. □

Remark 10.3: Lemma 2.2 (iii) also follows from Ref. 15, Sec. 2.1 since the enumeration (2.5), (2.6) corresponds to the factorization of the type in Ref. 15, Eq. (2.5) for the function $d(\theta, \omega)$, into the product of the irreducible factors, with the multiplicities $r_\sigma - r_{\sigma-1}$, which is constructed in Ref. 15, Thm 2.1.

2. Proof of Lemma 2.4

Step 1: Let us fix arbitrary $k, l \in \mathrm{I}_n$ and consider $\omega_k(\theta)$ as the functions of $V \in \mathcal{R}_N$ and of $\theta \in \mathbf{T}^d$. It suffices to prove that $D_k(\theta)$ and $\nabla(\omega_k(\theta) \pm \omega_l(\theta))$ are analytic and are not zero in an open dense subset in $\mathcal{R}_N \times \mathbf{T}^d$.

Let us consider $V_{k'l'}(x)$, $k', l' \in \mathrm{I}_n$, $|x_i| \leqslant N$, as the coordinates of the matrix-function V in the region $\mathcal{R}_N$. Condition **E2** allows us to consider $V_{k'l'}(x)$ as independent real variables for any $k', l' \in \mathrm{I}_n$ and the points x with either $x_1 > 0$, or $x_1 = 0$ and $x_2 > 0$, or $x_1 = x_2 = 0$ and $x_3 > 0$, etc. Let us identify $\mathcal{R}_N$ with corresponding range $\mathbf{R}^M$ of the independent real variables $V_{k'l'}(x)$.

Step 2: Consider $\omega_k(\theta)$ as the functions of $\{V_{k'l'}(x)\}$ and θ in $\mathbf{C}^M \times \mathbf{T}_c^d$. As above, each $\omega_k(\theta)$ can be chosen as a holomorphic function outside a proper analytic discriminant subset $\Delta \subset \mathbf{C}^M \times \mathbf{T}_c^d$. Lemma 10.2 implies that the region $O := (\mathbf{R}^M \times \mathbf{T}^d) \setminus \Delta$ is an open dense subset in $\mathbf{R}^M \times \mathbf{T}^d$. Therefore, it suffices to prove that the functions D_k and $\nabla(\omega_k \pm \omega_l)$ are not identically zero in each connected open component of O. However, the region of analyticity $\mathcal{O} := (\mathbf{C}^M \times \mathbf{T}_c^d) \setminus \Delta$ is connected. Hence, it remains to construct a point of $\mathbf{C}^M \times \mathbf{T}_c^d$ such that the functions D_k and $\nabla(\omega_k \pm \omega_l)$ are holomorphic and nonidentically zero in a neighborhood of the point. It is easy to construct such point for any $n \geqslant 1$: we can choose an arbitrary $\theta \in \mathbf{T}^d$ and the nearest neighbor crystal (1.12) repeated n times with distinct masses m_k, $k \in \mathrm{I}_n$. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 6 JUNE 2003

Hierarchy of equations for reduced density matrices at thermodynamic equilibrium with account taken of the spin of particles

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(Received 5 June 2002; accepted 17 January 2003)

The new approach in quantum statistical mechanics proposed by the author in previous publications is extended to systems of nonzero-spin particles. It is shown that properties of particles relevant to their spin can well be incorporated into the approach proposed. In so doing the principal ideas of the approach undergo no changes and lead to a hierarchy of equations for reduced density matrices at thermodynamic equilibrium that generalizes the hierarchy obtained earlier for spinless particles. Thermodynamics based on the hierarchy is worked out as well. The hierarchy and relevant thermodynamics enable one to calculate both thermodynamical properties of a system of particles and structural ones. With the help of perturbation expansions it is shown that the hierarchy has a solution and the solution is unique at least in the case of a weakly interacting system. Using the example of a hard-sphere system wherein triplet correlations are disregarded it is demonstrated that the hierarchy may serve as basis for deriving various results. Comparison of these results with results of other theoretical treatments evidences complete agreement within the limits allowed by the approximation used. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1562006]

I. INTRODUCTION

In a previous paper[1] (hereafter referred to as paper I) a new approach in equilibrium quantum statistical mechanics was proposed. The basic idea of the approach lies in obtaining a hierarchy of equations for s-particle reduced density matrices that corresponds to thermodynamic equilibrium, on the basis of most general assumptions by proceeding from the known fundamental equation for the time evolution of a density matrix. It turns out that, to this end, it is sufficient to make use of only one assumption according to which at thermodynamic equilibrium the reduced density matrices satisfy the principle of maximum statistical independence between quantities that determine the matrices. Moreover, in the course of deriving the hierarchy one is able to express all thermodynamic quantities in terms of functions that figure only in first equations of the hierarchy. Thus, it suffices to find those functions in order to attain a full thermodynamical and structural description of a system provided the interparticle potential is specified.

If $\hbar \to 0$, the hierarchy obtained goes over into the well-known equilibrium BBGKY hierarchy. This, on the one hand, enables one, when studying quantum systems, to employ methods and approximations that are developed for solution of the classical BBGKY hierarchy, and on the other hand this affords a possibility to elucidate the influence of quantum effects upon a system whose high-temperature behavior is described with the help of the BBGKY hierarchy. It should be emphasized that until the publication of paper I one did not succeed in obtaining a quantum analogue of the equilibrium BBGKY hierarchy (see the discussion in paper I of relevant difficulties, in particular, when one tries to use the Gibbs canonical or other similar ensembles), and the derivation of this analogue is due to the approach of paper I. To avoid any misunderstanding it is to be noted that in statistical mechanics there are different hierarchies. In order that a quantum hierarchy be an analogue of the classical BBGKY hierarchy the former must go over into the latter as $\hbar \to 0$.

In the event of a Bose system, special investigation is needed for the case of low temperatures when there appears a condensate analogous with that which forms at Bose condensation in an ideal gas. Extension of the above approach to this case was considered in a subsequent paper[2] (hereafter referred to as paper II). The condensate phase can be superfluid, and the phenomenon of superfluidity does not require, for its explanation, any additional hypotheses other than that used in paper I. It is worth adding that recently the hierarchy obtained in paper I was utilized for theoretical treatment of a quantum solid.[3]

However, solely spinless particles were implied in both the papers, I and II. Our aim in this paper is, by extending the approach proposed in paper I to systems containing particles with nonzero spin, to derive the corresponding hierarchy of equations for *s*-particle reduced density matrices. It will be shown that properties of particles relevant to their spin can, quite naturally, be incorporated into the approach proposed in paper I without any changes in the principal ideas of the approach. Thermodynamics based on the hierarchy will be constructed as well. All of this provides a means for calculating both thermodynamical properties of a system of nonzero-spin particles and structural ones, for example, spatial correlations. We shall also prove that the hierarchy has a solution and the solution is unique at least in the case of a weakly interacting system.

In the present paper we do not confine ourselves to obtaining general results but also we consider a method for solving the equations derived using, as an example, a system of hard spheres in which triplet correlations are neglected for the sake of simplicity. This simple example alleviates the problem of working out the method of solution while on the other hand the example makes it possible to elucidate whether the present theory reproduces well-established results seeing that hard-sphere systems are the objective of a great number of studies. We shall see that comparison of results given by the hierarchy with the results of other theoretical treatments evidences complete agreement within the limits allowed by the approximation used, namely, by the neglect of triplet correlations.

As mentioned above, in paper II it was demonstrated that the present approach permits one to treat the Bose condensation and, on this basis, superfluidity in Bose systems. At the same time from the results of paper II it follows that superfluidity cannot exist in systems of spinless fermions. Incorporation of the spin into the framework of the approach made in the present paper opens up possibilities of considering superfluidity in fermionic systems and thereupon superconductivity (in the case of charged fermions), which will provide a new method for studying these phenomena. Application of the results of the present paper together with, the ideas of paper II to treatment of superfluidity in fermionic systems will be the subject of a separate publication.

In the present paper for convenience sake, when referring to an equation of paper I, we shall place I in front; so we shall write, e.g., (I.2.7) implying Eq. (2.7) of paper I.

II. HIERARCHY OF EQUATIONS FOR REDUCED DENSITY MATRICES

We consider a system of N identical particles enclosed in a volume V. For convenience spin variables will be written as arguments of functions, and not as indices. So, the wave function of the system will be written in the form $\Psi=\Psi(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2,\ldots,\mathbf{r}_N,\sigma_N;t)$ where $\mathbf{r}_j$ are space coordinates and σ_j the spin variables. One may presume that each spin variable σ_j runs from 1 to κ upon setting, for instance, a correspondence of the type $\uparrow\rightarrow 1$ and $\downarrow\rightarrow 2$; here $\kappa=2S+1$ and S is the spin of a particle. The following abbreviated notation will be used:

$$\mathbf{x}_s=\mathbf{r}_1,\ldots,\mathbf{r}_s,\quad \mathbf{m}_s=\mathbf{p}_1,\ldots,p_s,\quad d\mathbf{x}_s=d\mathbf{r}_1\cdots d\mathbf{r}_s,\quad d\mathbf{m}_s=d\mathbf{p}_1\cdots d\mathbf{p}_s,$$
$$\mathbf{X}_s=\mathbf{r}_1,\sigma_1,\ldots,\mathbf{r}_s,\sigma_s,\quad \Sigma_s=\sigma_1,\ldots,\sigma_s,\quad \Gamma_s=\gamma_1,\ldots,\gamma_s. \tag{2.1}$$

In the present paper we shall consider pure states alone because the use of mixed states in the problem under study but complicates the notation without giving any advantage as it follows from paper I, and we define *s*-particle reduced density matrices by

$$R_s(\mathbf{X}_s,\mathbf{X}_s',t)=\frac{N!}{(N-s)!}\sum_{\sigma_{s+1},\ldots,\sigma_N=1}^{\kappa}\int \Psi(\mathbf{X}_s,\mathbf{r}_{s+1},\sigma_{s+1},\ldots,\mathbf{r}_N,\sigma_N;t)$$
$$\times\Psi^*(\mathbf{X}_s',\mathbf{r}_{s+1},\sigma_{s+1},\ldots,\mathbf{r}_N,\sigma_N;t)d\mathbf{r}_{s+1}\cdots d\mathbf{r}_N. \tag{2.2}$$

Since Ψ is assumed to be normalized to unity the normalization of R_s is

$$\sum_{\Sigma_s}\int R_s(\mathbf{X}_s,\mathbf{X}_s,t)d\mathbf{x}_s=\frac{N!}{(N-s)!}. \tag{2.3}$$

Here and henceforth, Σ_s (or Γ_s) under the summation sign means summation over all $\sigma_1,\ldots,\sigma_s$ (or $\gamma_1,\ldots,\gamma_s$) from 1 to κ. According to (2.2) the density matrices R_s and R_n with $n>s$ are interrelated by

$$R_s(\mathbf{X}_s,\mathbf{X}_s',t)=\frac{(N-n)!}{(N-s)!}\sum_{\sigma_{s+1},\ldots,\sigma_n=1}^{\kappa}\int R_n(\mathbf{X}_s,\mathbf{r}_{s+1},\sigma_{s+1},\ldots,\mathbf{r}_n,\sigma_n,$$
$$\mathbf{X}_s',\mathbf{r}_{s+1},\sigma_{s+1},\ldots,\mathbf{r}_n,\sigma_n,t)d\mathbf{r}_{s+1}\cdots d\mathbf{r}_n. \tag{2.4}$$

Note that (2.3) follows from (2.4) if one sets $s=0$ and assumes that $R_0=1$.

We introduce also diagonal elements of the density matrices summed up over the spin coordinates:

$$\rho_s(\mathbf{x}_s,t)=\sum_{\Sigma_s}R_s(\mathbf{X}_s,\mathbf{X}_s,t). \tag{2.5}$$

The quantity $\rho_1(\mathbf{r})$ is the spatial density of particles with the normalization as in paper I,

$$\int_V\rho_1(\mathbf{r},t)d\mathbf{r}=N. \tag{2.6}$$

From (2.4) it follows the relation

$$(N-s)\rho_s(\mathbf{x}_s,t)=\int_V\rho_{s+1}(\mathbf{x}_{s+1},t)d\mathbf{r}_{s+1}. \tag{2.7}$$

In this paper, studying symmetry or exchange effects we neglect direct interactions due to the spin of particles (such interactions are usually weak owing to their relativistic character[4] and are disregarded as a rule in statistical mechanics) and presume also that the external field does not act on the spins. For this reason we shall use a Hamiltonian of the form

$$\mathsf{H}=-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2+\sum_{j<k}^{N}K(|\mathbf{r}_j-\mathbf{r}_k|)+\sum_{j=1}^{N}V^{(e)}(\mathbf{r}_j), \tag{2.8}$$

upon assuming that the particles of mass m interact via a two-body potential $K(|\mathbf{r}_j-\mathbf{r}_k|)$ and are placed in an external field $V^{(e)}(\mathbf{r})$. Here and henceforth $\nabla_j=\partial/\partial\mathbf{r}_j$.

In a standard way[5,6] we get the hierarchy of equations for nonequilibrium density matrices [cf. Eq. (I.2.5)]

$$i\hbar\frac{\partial}{\partial t}R_s(\mathbf{X}_s,\mathbf{X}_s',t)=-\frac{\hbar^2}{2m}\sum_{j=1}^{s}[\nabla_j^2R_s(\mathbf{X}_s,\mathbf{X}_s',t)-\nabla_j'^2R_s(\mathbf{X}_s,\mathbf{x}_s',t)]+\sum_{j<k}^{s}[K(|\mathbf{r}_j-\mathbf{r}_k|)$$
$$-K(|\mathbf{r}_j'-\mathbf{r}_k'|)]R_s(\mathbf{X}_s,\mathbf{X}_s',t)+\sum_{j=1}^{s}[V^{(e)}(\mathbf{r}_j)-V^{(e)}(\mathbf{r}_j')]R_s(\mathbf{X}_s,\mathbf{X}_s',t)$$
$$+\sum_{j=1}^{s}\sum_{\sigma_{s+1}=1}^{\kappa}\int[K(|\mathbf{r}_j-\mathbf{r}_{s+1}|)-K(|\mathbf{r}_j'-\mathbf{r}_{s+1}|)]$$
$$\times R_{s+1}(\mathbf{X}_s,\mathbf{r}_{s+1},\sigma_{s+1},\mathbf{X}_s',\mathbf{r}_{s+1},\sigma_{s+1},t)d\mathbf{r}_{s+1}. \tag{2.9}$$

In a state of thermodynamic equilibrium the density matrices should have a form analogous to (I.2.7), so that

$$R_s=R_s(\mathbf{X}_s,\mathbf{X}_s')+R_s^{(t)}(\mathbf{X}_s,\mathbf{X}_s',t;N). \tag{2.10}$$

Here the time-dependent term $R_s^{(t)}$ is relevant to fluctuations. Henceforth we shall deal only with the term $R_s(\mathbf{X}_s,\mathbf{X}_s')$ that describes equilibrium properties. Following the procedure of paper I we introduce a complete orthonormal set of functions $\psi_\nu(\mathbf{x}_s)$ defined by

$$\mathsf{H}^{(s)}\psi_\nu(\mathbf{x}_s)=\varepsilon_\nu^{(s)}\psi_\nu(\mathbf{x}_s),\quad \mathsf{H}^{(s)}=-\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2+U_s(\mathbf{x}_s). \tag{2.11}$$

Note that the, yet to be determined, potentials $U_s(\mathbf{x}_s)$ supposed to be symmetric in $\mathbf{x}_s$ and real do not depend on the spins as long as we neglect direct spin-dependent interactions. The boundary conditions for the functions $\psi_\nu(\mathbf{x}_s)$ are the same as in paper I: the functions vanish at the boundary of the volume V. We do not presume any symmetry of $\psi_\nu(\mathbf{x}_s)$ (symmetric and antisymmetric functions will be set up below).

Inasmuch as the density matrices depend upon spin variables besides $\mathbf{r}_j$, it is necessary to introduce also an orthonormal basis relevant to the spin variables. For this purpose we can use the functions[7]

$$\chi_{\Gamma_s}(\Sigma_s)\equiv\chi_{\gamma_1,\ldots,\gamma_s}(\sigma_1,\ldots,\sigma_s)=\delta_{\gamma_1\sigma_1}\cdots\delta_{\gamma_s\sigma_s}. \tag{2.12}$$

Properties of these functions necessary for us are presented in Appendix A.

By analogy with (A9) the density matrices can always be expanded in a double series of the form

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\nu,\Gamma_s;\mu,\Delta_s}a^{(s)}_{\nu\Gamma_s\mu\Delta_s}\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\mu\Delta_s}(\mathbf{X}_s'). \tag{2.13}$$

Since, by (2.2),

$$R_s^*(\mathbf{X}_s,\mathbf{X}_s')=R_s(\mathbf{X}_s',\mathbf{X}_s), \tag{2.14}$$

one has

$$a^{(s)*}_{\nu\Gamma_s\mu\Delta_s}=a^{(s)}_{\mu\Delta_s\nu\Gamma_s}. \tag{2.15}$$

According to the principal idea of paper I we assume that at thermodynamic equilibrium the density matrices obey the principle of maximum statistical independence, that is to say, instead of the general form (2.13) they have the form

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=\sum_{\nu,\Gamma_s} n_s(\varepsilon_\nu^{(s)})\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\nu\Gamma_s}(\mathbf{X}_s'). \tag{2.16}$$

In order to avoid any misunderstanding a comment needs to be made as to Eq. (2.16) and the corresponding Eq. (I.2.11). Upon carrying out a linear transformation and introducing new functions $\Psi'_{\nu\Gamma_s}(\mathbf{X}_s)$ instead of $\Psi_{\nu\Gamma_s}(\mathbf{X}_s)$ the matrices $a^{(s)}_{\nu\Gamma_s\mu\Delta_s}$ can always be diagonalized because they are Hermitian according to (2.15). The relevant representation of the density matrices are often used in studies on reduced density matrices.[8,9] Equations (2.16) and (I.2.11) imply another thing. The new functions $\Psi'_{\nu\Gamma_s}(\mathbf{X}_s)$ will involve functions $\psi_\nu(\mathbf{x}_s)$ pertinent to different eigenvalues $\varepsilon_\nu^{(s)}$ and thereby the functions $\Psi'_{\nu\Gamma_s}(\mathbf{X}_s)$ will not satisfy equations of the type (2.11). We suppose that in a state of thermodynamic equilibrium the diagonalization as implied in (2.16) occurs if use is made of the functions $\psi_\nu(\mathbf{x}_s)$ which obey the Schrödinger-type equation of (2.11), and that the diagonal elements of $a^{(s)}_{\nu\Gamma_s\mu\Delta_s}$ denoted by n_s depend on $\varepsilon_\nu^{(s)}$ alone. In this case all the terms in (2.16) will be independent of one another as long as each of them will be relevant to only one eigenvalue $\varepsilon_\nu^{(s)}$. This corresponds with the principle of maximum statistical independence on which the approach of paper I is based.

It should be emphasized that the quantity $\varepsilon_\nu^{(s)}$ does not mean energy of a group of particles for there is no such energy independent of time in the case of interacting particles, and thereby the quantity $n_s(\varepsilon_\nu^{(s)})$ cannot be regarded as the occupation number of the νth state (see also paper I). It should be added that we assume $n_s(\varepsilon_\nu^{(s)})$ to be independent of Γ_s, that is, of the direction of the spin. It is worthy of note that introducing this last assumption excludes ferromagnetism from the present study.

As a matter of fact we look for a solution of the hierarchy (2.9) in the form (2.16), which will lead to equations for the potentials $U_s(\mathbf{x}_s)$ that determine $\psi_\nu(\mathbf{x}_s)$. We proceed in the same fashion as in paper I. By (2.11), from (2.16) it follows the equations

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2 R_s(\mathbf{X}_s,\mathbf{X}_s')=U_s(\mathbf{x}_s)R_s(\mathbf{X}_s,\mathbf{X}_s')-\sum_{\nu,\Gamma_s}\varepsilon_\nu^{(s)}n_s(\varepsilon_\nu^{(s)})\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\nu\Gamma_s}(\mathbf{X}_s'), \tag{2.17}$$

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j'^2 R_s(\mathbf{X}_s,\mathbf{X}_s')=U_s(\mathbf{x}_s')R_s(\mathbf{X}_s,\mathbf{X}_s')-\sum_{\nu,\Gamma_s}\varepsilon_\nu^{(s)}n_s(\varepsilon_\nu^{(s)})\Psi_{\nu\Gamma_s}(\mathbf{X}_s)\Psi^*_{\nu\Gamma_s}(\mathbf{X}_s'). \tag{2.18}$$

We insert (2.10) into (2.9) and neglect the time-dependent term $R_s^{(t)}$. Taking (2.17) and (2.18) into account then yields

$$\left\{U_s(\mathbf{x}_s)-U_s(\mathbf{x}_s')-\sum_{j<k}^{s}[K(|\mathbf{r}_j-\mathbf{r}_k|)-K(|\mathbf{r}_j'-\mathbf{r}_k'|)]-\sum_{j=1}^{s}[V^{(e)}(\mathbf{r}_j)-V^{(e)}(\mathbf{r}_j')]\right\}R_s(\mathbf{X}_s,\mathbf{X}_s')$$
$$=\sum_{j=1}^{s}\sum_{\sigma_{s+1}=1}^{\kappa}\int[K(|\mathbf{r}_j-\mathbf{r}_{s+1}|)-K(|\mathbf{r}_j'-\mathbf{r}_{s+1}|)]R_{s+1}(\mathbf{X}_s,\mathbf{r}_{s+1},\sigma_{s+1},\mathbf{X}_s',\mathbf{r}_{s+1},\sigma_{s+1})d\mathbf{r}_{s+1}. \tag{2.19}$$

Equation (2.19) represents a hierarchy of equations for the potentials $U_s(\mathbf{x}_s)$ because $R_s(\mathbf{X}_s,\mathbf{X}_s')$ are already determined by Eq. (2.16) according to which they are certain combinations of the functions $\psi_\nu(\mathbf{x}_s)$ while these last functions depend functionally on $U_s(\mathbf{x}_s)$ by virtue of (2.11). It should be observed that the last term in (2.17) and (2.18) that cannot be expressed in terms of $U_s(\mathbf{x}_s)$ and $R_s(\mathbf{X}_s,\mathbf{X}_s')$ has disappeared from (2.19). The equality of the last terms of (2.17) and (2.18) is due to the fact that the functions $\psi_\nu(\mathbf{x}_s)$ obey (2.11) [cf. the above comment upon (2.16)].

In contrast to (I.2.14), at a given s in (2.19) we have several equations because the arguments $\mathbf{X}_s$ and $\mathbf{X}_s'$ contain extra variables Σ_s and Σ_s' that do not figure in $U_s(\mathbf{x}_s)$. Consequently the

number of equations exceeds the number of unknowns. By rather a lengthy manipulation with the help of (A10) one can show that the left-hand side of (2.19) as well as the right-hand side have the structure

$$\sum_{P}^{(s)} (\pm)^p \delta(\Sigma_s, \mathsf{P}\Sigma_s') F(\mathbf{x}_s, \mathsf{P}\mathbf{x}_s'). \tag{2.20}$$

Here and in what follows the permutation operator P acts on the arguments in front of which it is placed, other symbols are defined in Appendix A. For this reason, in order that Eq. (2.19) be fulfilled at a given s it is sufficient to equate the corresponding functions $F(\mathbf{x}_s, \mathsf{P}\mathbf{x}_s')$ on the left and on the right, which will give only one equation for each s.

There is a more simple method of demonstrating that the equations of (2.19) with different Σ_s and Σ_s' are equivalent to one another at a given s. To this end we first expand $R_s(\mathbf{X}_s, \mathbf{X}_s')$ in terms of the functions of (A8) without taking account of the symmetry of $R_s(\mathbf{X}_s, \mathbf{X}_s')$. Then we shall see at once that the left-hand side of (2.19) and the right-hand side contain a factor $\delta(\Sigma_s, \Sigma_s')$ that cancels out, which gives an equation without Σ_s and Σ_s'. If one symmetrizes or antisymmetrizes the functions that enter into (2.19), this signifies that one forms combinations of the type (A10). Once corresponding terms of the combinations are equal to one another the whole combinations will be equal to each other as well.

Inasmuch as the equations of (2.19) with different Σ_s and Σ_s' are equivalent to one another at a given s, we may take only one of them. Instead of this it is convenient to take an equation that follows from (2.19) if one sets $\Sigma_s' = \Sigma_s$ and sums up over Σ_s. In order to write down the resulting equation let us introduce auxiliary functions defined by

$$\overline{R}_s(\mathbf{x}_s, \mathbf{x}_s') = \sum_{\Sigma_x} R_s(\mathbf{x}_s, \Sigma_s, \mathbf{x}_s', \Sigma_s), \tag{2.21}$$

wherein we write $\mathbf{x}_s$, Σ_s in place of $\mathbf{X}_s$. According to (2.5),

$$\rho_s(\mathbf{x}_s) = \overline{R}_s(\mathbf{x}_s, \mathbf{x}_s). \tag{2.22}$$

In terms of (2.21), Eq. (2.19) becomes

$$\left\{ U_s(\mathbf{x}_s) - U_s(\mathbf{x}_s') - \sum_{j<k}^{s} [K(|\mathbf{r}_j - \mathbf{r}_k|) - K(|\mathbf{r}_j' - \mathbf{r}_k'|)] - \sum_{j=1}^{s} [V^{(e)}(\mathbf{r}_j) - V^{(e)}(\mathbf{r}_j')] \right\} \overline{R}_s(\mathbf{x}_s, \mathbf{x}_s')$$
$$= \sum_{j=1}^{s} \int [K(|\mathbf{r}_j - \mathbf{r}_{s+1}|) - K(|\mathbf{r}_j' - \mathbf{r}_{s+1}|)] \overline{R}_{s+1}(\mathbf{x}_s, \mathbf{r}_{s+1}, \mathbf{x}_s', \mathbf{r}_{s+1}) d\mathbf{r}_{s+1}. \tag{2.23}$$

This hierarchy of equations for $U_s(\mathbf{x}_s)$ completely coincides with (I.2.14) if $R_s(\mathbf{x}_s, \mathbf{x}_s')$ is replaced by $\overline{R}_s(\mathbf{x}_s, \mathbf{x}_s')$. The question as to the solvability of the resultant hierarchy is equivalent to the same question concerning (I.2.14), and is discussed in paper I.

In fact we need not solve the hierarchy of (2.23) because in the approach used, only the limiting form of the hierarchy, as $\mathbf{x}_s' \to \mathbf{x}_s$, is required. Since Eq. (2.23) coincides with (I.2.14), and (2.22) is analogous with (I.2.2), we arrive at an equation wholly identical with (I.3.1), namely,

$$\rho_s(\mathbf{x}_s) \nabla_1 U_s(\mathbf{x}_s) = \rho_s(\mathbf{x}_s) \nabla_1 \left[\sum_{j=2}^{s} K(|\mathbf{r}_1 - \mathbf{r}_j|) + V^{(e)}(\mathbf{r}_1) \right] + \int \rho_{s+1}(\mathbf{x}_{s+1}) \nabla_1 K(|\mathbf{r}_1 - \mathbf{r}_{s+1}|) d\mathbf{r}_{s+1}. \tag{2.24}$$

Thus, the last equation is of the same form as in the case of spinless particles. It is apparent that this result stems from the fact that we discard direct spin interactions.

Let us now transform the expression of (2.16). We recast it in a form analogous to (I.2.16) upon introducing an operator $n_s(\mathsf{H}^{(s)})$ for which we take a representation of the type (I.2.19). Next we substitute (A10), expand $\psi_\nu(\mathbf{x}_s)$ in a Fourier integral, and make use of (A2) to (A4). As a result we get, in complete analogy with (I.2.20), that

$$R_s(\mathbf{X}_s,\mathbf{X}_s')=\frac{1}{2\pi i(2\pi\hbar)^{3s}s!}\int d\mathbf{m}_s\int_C dz\, n_s(z)\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$$
$$\times\sum_P^{(s)}(\pm)^p\delta(\mathsf{P}\Sigma_s,\Sigma_s')\exp\left[\frac{i}{\hbar}\sum_{k=1}^{s}(\mathbf{p}_k\mathbf{r}_k-\mathbf{r}_k'\mathsf{P}\mathbf{p}_k)\right] \tag{2.25}$$

with symbols defined in (2.1) and (2.20). The contour of integration C in the complex plane of z encloses all singularities of $\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$ (a possible form of C is shown in Fig. 1 of paper I). For the function $\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$ we shall obtain an equation identical to (I.2.22), namely,

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2\upsilon_s+\frac{i\hbar}{m}\sum_{i=1}^{s}\mathbf{p}_l\nabla_j\upsilon_s+\left[z-\frac{1}{2m}\sum_{k=1}^{s}\mathbf{p}_j^2-U_s(\mathbf{x}_s)\right]\upsilon_s=1. \tag{2.26}$$

It is worth remarking that (2.25) allows one to show, following the procedure of Appendix B of paper I, that the hierarchy of (2.23) is satisfied identically in the case of a spatially uniform medium if $s=1$.

From (2.25) we find the diagonal elements of the density matrices summed up over the spin projections defined in (2.5):

$$\rho_s(\mathbf{x}_s)=\frac{1}{2\pi i(2\pi\hbar)^{3s}s!}\int d\mathbf{m}_s\int_C dz\, n_s(z)\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)\sum_P^{(s)}(\pm)^p\kappa(P)\exp\left[\frac{i}{\hbar}\sum_{k=1}^{s}\mathbf{r}_k(\mathbf{p}_k-\mathsf{P}\mathbf{p}_k)\right], \tag{2.27}$$

wherein

$$\kappa(P)=\sum_{\Sigma_s}\delta(\mathsf{P}\Sigma_s,\Sigma_s). \tag{2.28}$$

It may be proven that $\kappa(P)=\kappa^\nu$ where ν is the number of cycles pertaining to the permutation P.

Thus, just as in paper I we have obtained a hierarchy of equations for $\rho_s(\mathbf{x}_s)$, $U_s(\mathbf{x}_s)$, and $\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)$ given by (2.24), (2.26), and (2.27). Equations (2.24) and (2.26) are identical with the ones for spinless particles, and are discussed in paper I. The spin manifests itself only in Eq. (2.27).

We turn now to the functions $n_s(z)$. In order to deduce a relationship between them we use (2.4) with $n=s+1$ upon substituting (2.25) there [the relation (2.4) will be satisfied for all n if it is satisfied for $n=s+1$]. By reasoning in the same way as in Sec. 4 of paper I with additional summation over the spin projections one will, instead of (I.4.12), arrive at

$$n_s(z)=\frac{4\pi\sqrt{2}s\hbar^3\rho}{\kappa m^{3/2}}\frac{d^2}{dz^2}\int_0^\infty n_{s-1}(z+x^2)dx, \tag{2.29}$$

where $\rho=N/V$. Here again in order to calculate all $n_s(z)$'s it is sufficient to know $n_1(z)$ or to resort to some argumentation. One may invoke the same argument as in Sec. 4 of paper I, which leads to (I.4.14). As a consequence, by making use of (2.29) one will, in complete parallel with (I.4.15) and (I.4.17), obtain

$$n_s(z)=A_se^{-z/\tau},\quad A_s=s!\left(\frac{\rho}{\kappa}\right)^{s-1}\left(\frac{2\pi\hbar^2}{m\tau}\right)^{3(s-1)/2}A. \tag{2.30}$$

In particular, for $n_1(z)\equiv n(z)$ one has

$$n(z)=Ae^{-z/\tau}. \tag{2.31}$$

Thus, the functions $n_s(z)$ depend upon two parameters A and τ, just as in the case of spinless particles. These parameters are connected by the normalization condition (2.6). In order to obtain a second equation for them it is necessary first to treat thermodynamics.

III. THERMODYNAMICS

Let us recall, in brief, the ideas of paper I as to constructing thermodynamics consistently with the equations for density matrices. At this stage of the theory it is possible to find the internal energy E and the pressure p. Leaning upon E, p and the second law of thermodynamics for quasistatic processes one is able to construct thermodynamics as a whole.

The energy of the system is given by the quantum mechanical formula

$$E=\sum_{\Sigma_s}\int \Psi^*(\mathbf{X}_N,t)\mathsf{H}\Psi(\mathbf{X}_N,t)d\mathbf{x}_N. \tag{3.1}$$

Henceforth we assume that the external field $V^{(e)}(\mathbf{r})$ is absent. By (2.2), (2.5), and (2.8) this last expression is reduced to

$$E=-\frac{\hbar^2}{2m}\sum_{\sigma=1}^{\kappa}\int [\nabla^2 R_1(\mathbf{r},\sigma,\mathbf{r}',\sigma)]_{\mathbf{r}'=\mathbf{r}}d\mathbf{r}+\frac{1}{2}\int K(|\mathbf{r}_1-\mathbf{r}_2|)\rho_2(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1\,d\mathbf{r}_2. \tag{3.2}$$

Then we take into account that, according to (2.25),

$$R_1(\mathbf{r},\sigma,\mathbf{r}',\sigma')=\frac{\delta_{\sigma\sigma'}}{2\pi i(2\pi\hbar)^3}\int d\mathbf{p}\int_C dz\, n_1(z)v_1(\mathbf{r},\mathbf{p},z)\exp\left[\frac{i}{\hbar}\mathbf{p}(\mathbf{r}-\mathbf{r}')\right]. \tag{3.3}$$

We restrict ourselves to consideration of spatially uniform systems, that is, of fluids. Then $\rho_2(\mathbf{r}_1,\mathbf{r}_2)=\rho_2(|\mathbf{r}_1-\mathbf{r}_2|)$, and substituting (3.3) into (3.2) gives

$$E=\frac{\kappa}{(2\pi)^4 i\hbar^3}\int d\mathbf{r}\,d\mathbf{p}\frac{\mathbf{p}^2}{2m}\int_C dz\, n_1(z)v_1(\mathbf{r},\mathbf{p},z)+\frac{V}{2}\int K(|\mathbf{r}|)\rho_2(|\mathbf{r}|)d\mathbf{r}. \tag{3.4}$$

The pressure p can be calculated with the help of the virial theorem, which gives, similarly to (I.3.7),

$$p=\frac{\kappa}{(2\pi)^4 i\hbar^3 V}\int d\mathbf{r}\,d\mathbf{p}\frac{\mathbf{p}^2}{3m}\int_C dz\, n_1(z)v_1(\mathbf{r},\mathbf{p},z)-\frac{1}{6}\int \rho_2(|\mathbf{r}|)\mathbf{r}\nabla K(|\mathbf{r}|)d\mathbf{r}. \tag{3.5}$$

Further calculations are analogous with those of Sec. 5 of paper I, and the dissimilarities in comparison with Sec. 5 of paper I come down to the appearance of an extra factor κ in some formulas. Equation (2.27) at $s=1$ with use made of (2.6), (2.31) and the average density $\rho=N/V$ leads to

$$\rho=\frac{\sqrt{\pi}}{2}A\kappa\omega\tau^{3/2}\quad\text{with}\quad\omega=\frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3}. \tag{3.6}$$

The first term in Eqs. (3.4) and (3.5) can readily be computed in the case of fluids to yield

$$E=\frac{3}{2}\tau N+2\pi N\rho\int_0^\infty r^2K(r)g(r)dr,\quad p=\rho\tau-\frac{2\pi}{3}\rho^2\int_0^\infty r^3\frac{dK}{dr}g(r)dr. \tag{3.7}$$

Here we have introduced the pair correlation function $g(r)$ according to the usual relation $\rho_2(r)=\rho^2 g(r)$ where $r=|\mathbf{r}|$. Note that E and p of (3.7) completely coincide with E and p as given by Eqs. (I.5.16) and (I.5.17) (the factor κ cancels out).

Next, we resort to the second law of thermodynamics for quasistatic processes embodied by the equation $\theta\, dS=dE+p\, dV$, θ being the temperature in units of energy ($\theta=k_BT$). The condition that the entropy S exists, namely the equality of the second derivatives $\partial^2 S/\partial V\partial\theta=\partial^2 S/\partial\theta\partial V$, entails

$$\frac{\rho^2}{N}\left(\frac{\partial E}{\partial\rho}\right)_\theta=p-\theta\left(\frac{\partial p}{\partial\theta}\right)_p, \tag{3.8}$$

where we differentiate with respect to $\rho=N/V$ instead of V, i.e., the arguments are taken to be θ and ρ, so that $E=E(\theta,\rho)$ and $p=p(\theta,\rho)$. We substitute (3.7) into (3.8) implying that $g(r)$ depends also on θ and ρ, that is, $g=g(r,\theta,\rho)$. There results

$$2\theta\frac{\partial\tau}{\partial\theta}+3\rho\frac{\partial\tau}{\partial\rho}-2\tau=\frac{4\pi\rho}{3}\int_0^\infty dr\, r^2\left(r\theta\frac{dK}{dr}\frac{\partial g}{\partial\theta}-3\rho K\frac{\partial g}{\partial\rho}+rK\frac{\partial g}{\partial r}\right). \tag{3.9}$$

Thus, we have two equations, (3.6) and (3.9), for the parameters A and τ that determine $n_s(z)$ of (2.30) and (2.31). It is worth remarking that the hierarchy (2.24), (2.26), and (2.27) does not contain the temperature θ explicitly. The hierarchy yields $g=g(r,\tau,\rho)$. The derivative $\partial g/\partial\theta$ that figures in (3.9) is to be understood as $\partial g/\partial\theta=(\partial g/\partial\tau)\cdot(\partial\tau/\partial\theta)$.

It remains to find conditions that should be imposed on solutions of the differential equation of (3.9). By proceeding from known properties of an ideal gas composed of particles with spin, one sees that the limiting condition at $K(r)\equiv 0$ now takes the parametric form, instead of (I.5.25),

$$\tau=\frac{2}{3}\left(\frac{\rho}{\kappa\omega}\right)^{2/3}\frac{G_1(\alpha)}{G_0^{5/3}(\alpha)},\quad \rho=\kappa\omega\theta^{3/2}G_0(\alpha), \tag{3.10}$$

in which α is the parameter and

$$G_k(\alpha)=\int_0^\infty\frac{x^{k+1/2}\,dx}{e^{x-\alpha}\mp 1}.$$

According to Appendix A the upper sign refers to bosons and the lower one to fermions.

In order to accomplish the construction of thermodynamics it is still necessary to find the Helmholtz free energy $F=E-\theta S$, for example. This can be done with the aid of the equations

$$E=-\theta^2\left(\frac{\partial}{\partial\theta}\frac{F}{\theta}\right)_\rho,\quad p=-\left(\frac{\partial F}{\partial V}\right)_\theta=\frac{\rho^2}{N}\left(\frac{\partial F}{\partial\rho}\right)_\theta. \tag{3.11}$$

It is important to note that these two simultaneous equations for F are compatible owing to the fulfilment of (3.8). Different forms for F obtained on the basis of (3.11) are adduced in Appendix B.

The above formulas show that to compute thermodynamic quantities one needs the pair correlation function. The formula for $g(\mathbf{r})$ follows from Eq. (2.27) at $s=2$ that can, analogously with (I.5.7), be reduced to the form

$$g(\mathbf{r})=\frac{1}{2\pi i(2\sqrt{2}\pi\hbar)^3\rho}\int d\mathbf{q}\int_C dz\, n(z)\upsilon(\mathbf{r},\mathbf{q},z)\left[\kappa\pm\exp\left(\frac{i}{\hbar}\mathbf{qr}\right)\right], \tag{3.12}$$

the function $\upsilon(\mathbf{r},\mathbf{q},z)$ being determined by Eq. (I.5.6), namely,

$$\frac{\hbar^2}{m}\nabla^2 v(\mathbf{r},\mathbf{q},z)+\frac{i\hbar}{m}\mathbf{q}\nabla v(\mathbf{r},\mathbf{q},z)+\left[z-\frac{\mathbf{q}^2}{4m}-U_2(|\mathbf{r}|)\right]v(\mathbf{r},\mathbf{q},z)=1. \tag{3.13}$$

Let us derive another formula for $g(\mathbf{r})$. Instead of $v(\mathbf{r},\mathbf{q},s)$ one may introduce $w(\mathbf{r},\mathbf{q},s)$ of (I.D.1), and moreover $\psi_\nu(\mathbf{r})$ as solutions of (I.D.3). Then the expression of (3.12) becomes

$$g(\mathbf{r})=\frac{1}{\rho}2\sqrt{2}\sum_\nu n(\varepsilon_\nu)\psi_\nu(\mathbf{r})[\kappa\psi_\nu^*(\mathbf{r})\pm\psi_\nu^*(-\mathbf{r})] \tag{3.14}$$

with $\psi_\nu(\mathbf{r})$ and ε_ν found from the Schrödinger-type equation

$$\frac{\hbar^2}{m}\nabla^2\psi_\nu(\mathbf{r})+[\varepsilon_\nu-U_2(|\mathbf{r}|)]\psi_\nu(\mathbf{r})=0. \tag{3.15}$$

For use later we need (3.14) and (3.15) for the case in which the potential $U_2(|\mathbf{r}|)$ is such that the spectrum is continuous. Following the procedure of Appendix D of paper I we transform (3.14) into the form

$$g(r)=\frac{1}{\pi\sqrt{2}\rho}\sum_{l=0}^{\infty}[\kappa\pm(-1)^l](2l+1)\int_0^\infty n\left(\frac{\hbar^2k^2}{m}\right)R_{kl}^2(r)dk. \tag{3.16}$$

The function R_{kl} obeys Eq. (I.D.8) in which $\varepsilon_{kl}=\hbar^2k^2/m$, namely,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{kl}}{dr}\right)-\frac{l(l+1)}{r^2}R_{kl}+\left[k^2-\frac{m}{\hbar^2}U_2(r)\right]R_{kl}=0 \tag{3.17}$$

with the following boundary condition as $r\to\infty$ [see (I.D.11)]

$$R_{kl}\to\frac{C_1}{r}\sin kr+\frac{C_2}{r}\cos kr,\quad C_1^2+C_2^2=\frac{2}{\pi}. \tag{3.18}$$

The formulas of the present section show that the spin affects the value of κ alone, the quantity κ being even absent from a number of formulas. However, one should not think that the existence of the spin manifests itself only in a trivial manner. If $\kappa>1$, Eq. (3.14) will contain the functions $\psi_\nu(\mathbf{r})$ of both parities. This will have an appreciable effect on the properties of $g(r)$ and thereupon on thermodynamic properties, which will be confirmed by an example considered in Sec. V.

IV. PERTURBATION EXPANSIONS

As shown in paper I the equations that determine the pair correlation function can be treated with the help of expansion in powers of the Fourier transform of the potential $U_2(\mathbf{r})$. The first term in the square brackets of the relevant equations of (I.5.14) and (I.5.15) will contain the factor κ now. However $U_2(\mathbf{r})$ itself is an unknown function determined by other equations of the hierarchy. In this section we shall show that one can look for a solution of the hierarchy equations directly in terms of expansions in powers of the interaction potential $K(r)$, which will permit us to answer some general questions. For convenience we introduce a dimensionless parameter λ, so that $K(r)=\lambda\tilde{K}(r)$, and shall speak of expansions in powers of λ.

We shall assume that the external potential $V^{(e)}=0$. By making use of (2.7) we recast (2.24) in the form

$$\nabla_1 U_s(\mathbf{x}_s)=\nabla_1\sum_{j=2}^{s} K(|\mathbf{r}_1-\mathbf{r}_j|)+\frac{\int \rho_{s+1}(\mathbf{x}_{s+1})\nabla_1 K(|\mathbf{r}_1-\mathbf{r}_{s+1}|)d\mathbf{r}_{s+1}}{\frac{1}{N-s}\int \rho_{s+1}(\mathbf{x}_{s+1})d\mathbf{r}_{s+1}}. \tag{4.1}$$

Let us choose a value of s and find ρ_{s+1} upon setting $U_{s+1}=0$. In the latter case, on account of the limiting condition of (I.2.23), Eq (2.26) yields

$$\upsilon_{s+1}(\mathbf{x}_{s+1},\mathbf{m}_{s+1},z)=\left(z-\frac{1}{2m}\sum_{j=1}^{s+1}\mathbf{p}_j^2\right)^{-1}.$$

Now by (2.27) we compute $\rho_{s+1}(\mathbf{x}_{s+1})$ in this case, which allows us to calculate the term of U_s proportional to λ with the aid of (4.1). It is to be emphasized that this term will be known exactly.

Next we rewrite (2.26) as

$$\frac{\hbar^2}{2m}\sum_{j=1}^{s}\nabla_j^2\upsilon_s+\frac{i\hbar}{m}\sum_{j=1}^{s}\mathbf{p}_j\nabla_j\upsilon_s+\left(z-\frac{1}{2m}\sum_{j=1}^{s}\mathbf{p}_j^2\right)\upsilon_s=1+U_s(\mathbf{x}_s)\upsilon_s. \tag{4.2}$$

Let us represent υ_s in terms of the Fourier integral

$$\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)=\int \gamma_s(\mathbf{q}_1,\ldots,\mathbf{q}_s;\mathbf{m}_s,z)\exp\left(\frac{i}{\hbar}\sum_{k=1}^{s}\mathbf{q}_k\mathbf{r}_k\right)d\mathbf{q}_{(s)}, \tag{4.3}$$

where $d\mathbf{q}_{(s)}=d\mathbf{q}_1\ldots d\mathbf{q}_s$. We substitute (4.3) into the left-hand side of (4.2) and find γ_s by using the inverse Fourier transform. Inserting this γ_s back into (4.3) yields

$$\upsilon_s(\mathbf{x}_s,\mathbf{m}_s,z)=\frac{1}{z-\frac{1}{2m}\sum_{j=1}^{s}\mathbf{p}_j^2}+\frac{1}{(2\pi\hbar)^{3s}}\int\frac{d\mathbf{q}_{(s)}}{z-\frac{1}{2m}\sum_{j=1}^{s}(\mathbf{p}_j+\mathbf{q}_j)^2}\exp\left(\frac{i}{\hbar}\sum_{k=1}^{s}\mathbf{q}_k\mathbf{r}_k\right)$$
$$\times\int d\mathbf{x}_s' U_s(\mathbf{x}_s')\upsilon_s(\mathbf{x}_s',\mathbf{m}_s,z)\exp\left(-\frac{i}{\hbar}\sum_{k=1}^{s}\mathbf{q}_k\mathbf{r}_k'\right). \tag{4.4}$$

Once the term of order λ in U_s is known Eq. (4.4) permits us to find terms of orders 1 and λ in υ_s. Therefore we are able to calculate $\rho_s(\mathbf{x}_s)$, too, by (2.27) to the same order in λ.

We substitute the expression obtained for $\rho_s(\mathbf{x}_s)$ into (4.1) written for U_{s-1} and calculate terms of orders λ and λ^2 in U_{s-1}, which will give terms of orders 1, λ, and λ^2 in υ_{s-1} and ρ_{s-1} by (4.4) and (2.27). Proceeding in the same manner we shall finally arrive at $g(\mathbf{r})=\rho_2(\mathbf{r})/\rho^2$ for which we shall know terms in $1,\lambda,\ldots,\lambda^{s-1}$. As to thermodynamic quantities we shall know terms in $1,\lambda,\ldots,\lambda^s$. according to (3.7) because Eq. (3.9) too can be solved by expanding in powers of λ analogously with Sec. 7 of paper I. It is important to stress that all those terms will be known exactly. Hence by starting from Eq. (4.1) with an appropriate number s we are able to calculate any term in the perturbation expansion of any quantity.

The method considered proves the existence of a solution to the hierarchy of the present paper as well as to the hierarchy of paper I. Of course, it is yet necessary to prove that the relevant series converge, which is not a simple matter. As is usual with perturbation expansions we suppose that they converge (perhaps asymptotically) at least for not too large λ, i.e., in the case of a weak coupling.

The result obtained shows also that the hierarchy of equations can be solved without any approximation introduced usually, when one deals with a hierarchy, to cut it off. An analogous result exists for the classical equilibrium BBGKY hierarchy as well (see, e.g., Ref. 10 and references therein). It is worthy of remark that the classical BBGKY hierarchy is equivalent to Eq. (4.1)

together with the relation $\rho(\mathbf{x}_s)=A_s\exp[-U(\mathbf{x}_s)/\theta]$ instead of (2.26) and (2.27) (see paper I). In practice however one is obliged to introduce some approximation or other inasmuch as the resulting series prove to be too cumbersome for practical use.

The method presented enables one also to demonstrate the uniqueness of solution. The functions ρ_s and U_s are determined uniquely by Eqs. (2.27) and (4.1) since the constant appearing when integrating (4.1) is found from the condition that $U_s=0$ at infinity (see paper I). So we need consider only (4.4). Since U_s always contains a factor λ in view of (4.1), terms of order λ^l in v_s when placed in the right-hand side of (4.4) permit one to calculate terms of order λ^{l+1}. The term of order $\lambda^0=1$ is given by (4.4) explicitly. Hence all terms of the expansions in powers of λ will be found uniquely.

V. HARD SPHERES UNDER THE NEGLECT OF TRIPLET CORRELATIONS

Having considered a weak interaction potential $K(r)$ we turn to the opposite case of an extremely singular potential, namely, the potential of hard spheres. This example will permit us, on the one hand, to verify the equations obtained by comparing results yielded by them with established results while on the other hand this simple example will enable us to work out a method for solving the equations and extracting concrete physical results from them.

In the case of hard spheres $K(r)=\infty$ if $r<a$ and $K(r)=0$ if $r>a$. To simplify the problem we shall disregard triplet correlations, in which case $U_2(r)=K(r)$ according to paper I [this may also be seen from (4.1) upon setting $s=2$ and taking into account that the last term vanishes if $\rho_3=$constant]. Note that the same example was considered in paper I as well, which will permit us to make a direct comparison of results for spinless particles and for particles with nonzero spin given by the present approach.

To begin with, let us examine the pair correlation function $g(r)$. It is apparent that $g(r)=0$ if $r<a$. If $r>a$ we set $U_2=K=0$ in Eq. (3.17), in which case the solution of the equation can be obtained in terms of Bessel functions. The constants of integration are found from the conditions: $R_{kl}=0$ at $r=a$ and (3.18). Upon inserting the result into (3.16) we shall arrive at an expression of the type (I.6.3):

$$g(r)=\frac{1}{\pi\sqrt{2}\rho r}\sum_{l=0}^{\infty}[\kappa\pm(-1)^l](2l+1)\int_0^{\infty}kn\left(\frac{\hbar^2k^2}{m}\right)\frac{[N_\nu(ka)J_\nu(kr)-J_\nu(ka)N_\nu(kr)]^2}{J_\nu^2(ka)+N_\nu^2(ka)}dk, \tag{5.1}$$

$J_\nu(x)$ and $N_\nu(x)$ being the Bessel and Neumann functions, respectively, with $\nu=l+\frac{1}{2}$. The function $n(z)$ is given by (2.31) with A from (3.6). The overall properties of $g(r)$ will be analogous with the ones presented in paper I when discussing (I.6.3).

We turn now to Eq. (3.9) that determines $\tau(\theta,\rho)$. The integrals in (3.9) that contain derivatives with respect to r require special treatment as long as the potential $K(r)$ of hard spheres has an infinite jump at $r=a$. One may resort to the procedure described when deriving (I.6.5),[11] which will yield the following result, on account of (5.1):

$$\int_0^{\infty}dr\,r^3K(r)\frac{\partial g}{\partial r}=\frac{a\hbar^2}{m}H_\kappa(\bar{\tau}) \tag{5.2}$$

with $\bar{\tau}=a^2m\tau/\hbar^2$ and

$$H_\kappa(\xi)=\frac{\kappa\pm1}{2\kappa}H^{(+)}(\xi)+\frac{\kappa\mp1}{2\kappa}H^{(-)}(\xi), \tag{5.3}$$

wherein

$$H^{(\pm)}(\xi)=\frac{8}{(\pi\xi)^{3/2}}\sum_{l=0}^{\infty}[1\pm(-1)^l](2l+1)\int_0^{\infty}\frac{\exp(-x^2/\xi)x\,dx}{J^2_{l+1/2}(x)+N^2_{l+1/2}(x)}. \tag{5.4}$$

It is not a simple matter to find out analytically the behavior of $H_\kappa(\xi)$ when $\xi\to\infty$. A numerical calculation permits one to suggest that, as $\xi\to\infty$,

$$H_\kappa(\xi)=\xi+\sqrt{\pi\xi}+2/3+O(1/\xi). \tag{5.5}$$

Note that the terms written down in (5.5) do not contain κ, which amounts to saying that $H^{(+)}(\xi)$ and $H^{(-)}(\xi)$ are also given by (5.5) in this approximation. If $\xi\to 0$, $H^{(+)}(\xi)$ is determined by the series of (I.6.7) while $H^{(-)}(\xi)$ by the series of (I.6.8). The most interesting case is that of spin-half fermions [$\kappa=2$ with the lower sign in (5.3)]. Then

$$H_2(\xi)=\tfrac{1}{4}H^{(+)}(\xi)+\tfrac{3}{4}H^{(-)}(\xi), \tag{5.6}$$

and, as $\xi\to 0$,

$$H_2(\xi)=\frac{1}{2}\left(1+\frac{27}{2}\xi-\frac{95}{3}\xi^2+\frac{42\,091}{360}\xi^3-\frac{1\,491\,327}{2800}\xi^4+\cdots\right). \tag{5.7}$$

With Eq. (5.2) at our disposal we can reduce Eq. (3.9) to a form analogous with (I.6.9):

$$2\left[1+\frac{2}{3}nH'_\kappa(\overline{\tau})\right]\theta\frac{\partial\overline{\tau}}{\partial\theta}+3n\frac{\partial\overline{\tau}}{\partial n}-2\overline{\tau}-\frac{4}{3}nH_\kappa(\overline{\tau})=0, \tag{5.8}$$

where $n=\pi a^3\rho$ and the prime over $H'_\kappa(\overline{\tau})$ denotes differentiation with respect to the argument. Referring to paper I for details let us outline key steps in integrating Eq. (5.8). At first, it is necessary to solve the ordinary differential equation

$$\frac{dt}{dn}=\frac{4}{9n^{2/3}}H_\kappa(n^{2/3}t) \tag{5.9}$$

with $t=\overline{\tau}/n^{2/3}$. Let the general solution of this equation be $t=f_1(n,t_0)$ where t_0 is the value of t at $n=0$. Then the solution of (5.8) satisfying the condition of (3.10) can be represented parametrically as [cf. (I.6.16) and (I.6.17)]

$$\tau=\left(\frac{\rho}{\pi\sqrt{2}\omega}\right)^{2/3}f_1(n,\gamma),\quad \gamma=\frac{(4\pi)^{2/3}G_1(\alpha)}{3\kappa^{2/3}G_0^{5/3}(\alpha)}, \tag{5.10}$$

$$\theta=\left(\frac{\rho}{\kappa\omega G_0(\alpha)}\right)^{2/3}\exp\left\{\frac{4}{9}\int_0^n H'_\kappa[x^{2/3}f_1(x,\gamma)]dx\right\}, \tag{5.11}$$

where α is the parameter and $\gamma=\gamma(\alpha)$ is an auxiliary function.

For high temperatures we have again the expressions of (I.6.19) with the results that follow from them. Disparity with paper I reveals itself only in the low-temperature region. This is natural, for the spin is manifested only at low temperatures. In the following we shall consider fermions alone. At $\theta=0$, (5.10) and (5.11) yield, analogously to (I.6.32),

$$\tau^{(0)}=\left(\frac{\rho}{\pi\sqrt{2}\omega}\right)^{2/3}f_1\left[n,\frac{1}{5}\left(\frac{6\pi}{\kappa}\right)^{2/3}\right], \tag{5.12}$$

while the derivative $\partial\tau/\partial\theta$ as $\theta\to 0$ is

$$\frac{\partial\tau}{\partial\theta}=\frac{\pi^2}{3}\left(\frac{2\kappa\omega}{3\rho}\right)^{2/3}\theta\exp\left\{-\frac{4}{9}\int_0^n H'_\kappa\left[x^{2/3}f_1\left(x,\frac{1}{5}\left(\frac{6\pi}{\kappa}\right)^{2/3}\right)\right]dx\right\}. \tag{5.13}$$

As a consequence, the $\tau(\theta)$ dependence is again represented schematically by curve 2 in Fig. 2 of paper I as in the case of spinless fermions.

Henceforth we confine ourselves to the case of spin-half fermions when $\kappa=2$. If $n=\pi a^3\rho$ is small we introduce (5.7) into (5.9) and look for a solution in terms of a series in powers of $n^{1/3}$. As a result, instead of (I.6.34) and (I.6.35) we have

$$\tau=\left(\frac{\rho}{\pi\sqrt{2}\omega}\right)^{2/3}\left[\gamma+\frac{2}{3}n^{1/3}+3\gamma n+\frac{3}{2}n^{4/3}-\frac{38}{9}\gamma^2n^{5/3}-\frac{31}{162}\gamma n^2+\frac{1}{54}\left(\frac{667}{21}+\frac{6013}{10}\gamma^3\right)n^{7/3}-\cdots\right], \tag{5.14}$$

$$\theta=\left(\frac{\rho}{2\omega G_0(\alpha)}\right)^{2/3}\left(1+3n-\frac{76}{9}\gamma n^{5/3}-\frac{31}{162}n^2+\frac{6013}{180}\gamma^2n^{7/3}-\cdots\right). \tag{5.15}$$

Here again α is the parameter, and $\gamma(\alpha)$ is defined in (5.10).

The expressions of (3.7) for the internal energy E and the pressure p assume the form

$$E=\tfrac{3}{2}\tau N,\quad p=\rho\tau+\frac{2\pi a\hbar^2}{3m}\rho^2H_\kappa(\overline{\tau}), \tag{5.16}$$

when use is made of (5.2). The free energy F and the chemical potential $\mu=(F+pV)/N$ can be found in complete parallel with (I.6.36) and (I.6.37):

$$F=N\theta\left\{\alpha-\frac{2G_1(\alpha)}{3G_0(\alpha)}+n^{1/3}\left(\frac{G_0(\alpha)}{2\pi}\right)^{2/3}\left[2-\frac{3}{2}n+\frac{38}{3}\gamma^2n^{4/3}+\frac{152}{9}\gamma n^{5/3}+\left(\frac{3769}{567}-\frac{6013}{90}\gamma^3\right)n^2+\cdots\right]\right\}, \tag{5.17}$$

$$\mu=\theta\left\{\alpha+n^{1/3}\left(\frac{G_0(\alpha)}{2\pi}\right)^{2/3}\left[4+9\gamma n^{2/3}+\frac{3}{2}n+\frac{152}{27}\gamma n^{5/3}+\left(\frac{3769}{1134}-\frac{6013}{180}\gamma^3\right)n^2+\cdots\right]\right\}. \tag{5.18}$$

These formulas together with (5.15) give parametric dependence of F and μ upon θ and ρ.

For low temperatures one may obtain expressions similar to (I.6.38) and (I.6.39), namely,

$$\tau=\frac{2}{5}\varepsilon_0\left\{1+\frac{10n^{1/3}}{3(3\pi)^{2/3}}+3n+\frac{15n^{4/3}}{2(3\pi)^{2/3}}-\frac{38}{45}(3\pi)^{2/3}n^{5/3}-\frac{31}{162}n^2+\cdots+\frac{5\pi^2\theta^2}{12\varepsilon_0^2}\left[1-3n+\frac{76}{45}(3\pi)^{2/3}n^{5/3}+\frac{1489}{162}n^2+\cdots\right]\right\}, \tag{5.19}$$

$$\mu=\varepsilon_0\left[1+\frac{4n^{1/3}}{(3\pi)^{2/3}}+\frac{24}{5}n+\frac{27n^{4/3}}{2(3\pi)^{2/3}}-\frac{76}{45}(3\pi)^{2/3}n^{5/3}-\cdots\right], \tag{5.20}$$

where $\varepsilon_0=(3\rho/4\omega)^{2/3}$ is the Fermi energy of the corresponding ideal gas at $\theta=0$.

Comparison of the above formulas with the corresponding formulas of paper I indicates that, owing to the spin, terms depending on n change the order of magnitude. For example, the leading correction to F and μ is now of the order $n^{1/3}\sim a$, while in I it was of the order $n^{5/3}\sim a^5$ for F and of the order $n\sim a^3$ for μ.

Let us compare our results with the ones of numerous studies on hard-sphere Fermi systems. In our formulas it is easy to obtain explicitly the correction of order $a\sim n^{1/3}$ to different quantities since, upon dropping terms of order $a^3\sim n$ and higher in (5.15), one is able to express $G_0(\alpha)$ in terms of θ while the term of order $n^{1/3}$ in (5.14) does not depend on α. Let us write down the resulting corrections to the quantities E_{id}, p_{id}, μ_{id} of an ideal gas:

$$E=E_{\mathrm{id}}+\frac{\pi a\hbar^2\rho}{m}N,\quad p=p_{\mathrm{id}}+\frac{\pi a\hbar^2\rho^2}{m},\quad \mu=\mu_{\mathrm{id}}+\frac{2\pi a\hbar^2\rho}{m}. \tag{5.21}$$

These expressions coincide exactly with the ones given by the method of pseudopotentials for spin-half fermions in the same approximation.[12]

In order to compare higher terms in a we consider virial coefficients. The coefficients are defined by (I.6.29), and the procedure of calculating them is described in paper I. Making use of (5.14), (5.15), (5.16), and (5.7) entails

$$a_2=\frac{1}{8\sqrt{2}}+\frac{a}{2\lambda}+\frac{9\pi}{2}\left(\frac{a}{\lambda}\right)^3-\frac{38}{3}\pi^2\left(\frac{a}{\lambda}\right)^5+\frac{6013}{90}\pi^3\left(\frac{a}{\lambda}\right)^7+O\left[\left(\frac{a}{\lambda}\right)^9\right], \tag{5.22}$$

$$a_3=\frac{1}{32}-\frac{1}{18\sqrt{3}}+\frac{9\pi}{8\sqrt{2}}\left(\frac{a}{\lambda}\right)^3+\frac{9\pi}{4}\left(\frac{a}{\lambda}\right)^4-\frac{19}{3\sqrt{2}}\pi^2\left(\frac{a}{\lambda}\right)^5-\frac{380}{27}\pi^2\left(\frac{a}{\lambda}\right)^6+O\left[\left(\frac{a}{\lambda}\right)^7\right]. \tag{5.23}$$

In Refs. 12 and 13 and other papers only virial coefficients for spinless particles are cited. Provided, however, one knows the second virial coefficient $a_{2F}^{(0)}$ for spinless fermions and the second virial coefficient $a_{2B}^{(0)}$ for spinless bosons, then for fermions of spin S,[12,14]

$$a_{2F}^{(S)}=\frac{S+1}{2S+1}a_{2F}^{(0)}+\frac{S}{2S+1}a_{2B}^{(0)}. \tag{5.24}$$

If one sets $S=1/2$ here and substitutes $a_{2F}^{(0)}$ and $a_{2B}^{(0)}$ given in Refs. 12 and 13, one will get an exact coincidence with the first four terms in (5.22). Terms of order $(a/\lambda)^7$ are not cited in Refs. 12 and 13. However, in case one takes such terms from (I.6.30) and (I.6.40), one will obtain the fifth term in (5.22). Terms of order $(a/\lambda)^7$ are cited in Ref. 14, but they do not coincide with those of (I.6.30) and (I.6.40). The formulas of Ref. 14 may however contain errors as was remarked when discussing (I.6.40). The first correction to a_3 is written down in Ref. 15. At $S=1/2$ it is $a^2/2\lambda^2$, whereas in (5.23) it is of the order $(a/\lambda)^3$ although the sign is the same. This discrepancy is not unexpected because the third virial coefficient is affected essentially by triplet correlations that were ignored.

Let us make a remark as to formula (5.24). The formula may readily be proven on condition one uses the canonical ensemble.[12,14] In our approach the formula is not at all trivial because τ is different for Bose and Fermi systems.

We may also make a comparison with known results at $\theta=0$. If, in (5.19) and (5.20), one discards all terms of higher order than the first in a one will again arrive at (5.21). The same result is given, at $\theta=0$, by other methods;[12] however the next term is of the order a^2 whereas on the grounds of (5.19) and (5.20) the corrections to (5.21) are of the order a^3. This points to the rather evident fact that the triplet correlations play a more essential role at $\theta=0$ (cf. the above discrepancies concerning a_3). At the same time the first corrections in a are given correctly by the approximation used in the present section even at $\theta=0$.

In conclusion, we see that the present theory reproduces the known results for hard spheres adequately although we have resorted to a rather simple approximation in order to facilitate the problem. At the same time the discrepancies that occur are physically understandable.

APPENDIX A: PROPERTIES OF THE FUNCTIONS $\chi_{\Gamma_s}(\Sigma_s)$

We shall use the following abbreviated notation for products of Kronecker's δ-symbols:

$$\delta_{\gamma_1\sigma_1}\delta_{\gamma_2\sigma_2}\cdots\delta_{\gamma_s\sigma_s}=\delta(\Gamma_s,\Sigma_s). \tag{A1}$$

From this we get the evident property

$$\delta(\mathsf{P}_1\Gamma_s,\mathsf{P}_2\Sigma_s)=\delta(\Gamma_s,\mathsf{P}_2\mathsf{P}_1^{-1}\Sigma_s)=\delta(\mathsf{P}_1\mathsf{P}_2^{-1}\Gamma_s,\Sigma_s), \tag{A2}$$

where P_1 and P_2 are operators that permute the quantities $\gamma_1,\ldots,\gamma_s$ or $\sigma_1,\ldots,\sigma_s$. In the notation (A1) the functions of (2.12) take the form

$$\chi_{\Gamma_s}(\Sigma_s)=\delta(\Gamma_s,\Sigma_s). \tag{A3}$$

These functions satisfy the orthogonality and completeness relations

$$\sum_{\Sigma_s}\chi_{\Gamma_s}(\Sigma_s)\chi_{\Gamma_s'}(\Sigma_s)=\delta(\Gamma_s,\Gamma_s'),\quad \sum_{\Gamma_s}\chi_{\Gamma_s}(\Sigma_s)\chi_{\Gamma_s}(\Sigma_s')=\delta(\Sigma_s,\Sigma_s'). \tag{A4}$$

Any function $\varphi(\Sigma_s)$ in a space of $\sigma_1,\ldots,\sigma_s$ can be expanded in terms of $\chi_{\Gamma_s}(\Sigma_s)$,

$$\varphi(\Sigma_s)=\sum_{\Gamma_s}a_{\Gamma_s}\chi_{\Gamma_s}(\Sigma_s), \tag{A5}$$

in which the coefficients a_{Γ_s} are given by

$$a_{\Gamma_s}\equiv a_{\gamma_1,\ldots,\gamma_s}=\sum_{\Sigma_s}\varphi(\Sigma_s)\chi_{\Gamma_s}(\Sigma_s). \tag{A6}$$

Now any function $f(\mathbf{X}_s)\equiv f(\mathbf{r}_1,\sigma_1,\ldots,\mathbf{r}_j,\sigma_j,\ldots,\mathbf{r}_s,\sigma_s)$ can be expanded as

$$f(\mathbf{X}_s)=\sum_{\nu,\Gamma_s}a_{\nu\Gamma_s}\tilde{\Psi}_{\nu\Gamma_s}(\mathbf{X}_s) \tag{A7}$$

in terms of the orthonormal functions

$$\tilde{\Psi}_{\nu\Gamma_s}(\mathbf{X}_s)=\chi_{\Gamma_s}(\Sigma_s)\psi_\nu(\mathbf{x}_s), \tag{A8}$$

wherein we imply that the functions $\psi_\nu(\mathbf{x}_s)$ are defined by (2.11). If the function $f(\mathbf{X}_s)$ is symmetric (for bosons) or antisymmetric (for fermions) under the interchange of any two out of the pairs $\mathbf{r}_j,\sigma_j(j=1,\ldots,s)$, the expression (A7) can be reformulated as

$$f(\mathbf{X}_s)=\sum_{\nu,\Gamma_s}a_{\nu\Gamma_s}\Psi_{\nu\Gamma_s}(\mathbf{X}_s), \tag{A9}$$

where

$$\Psi_{\nu\Gamma_s}(\mathbf{X}_s)=\frac{1}{s!}\sum_{P_{r\sigma}}^{(s)}(\pm)^p\mathsf{P}_{r\sigma}\chi_{\Gamma_s}(\Sigma_s)\psi_\nu(\mathbf{x}_s). \tag{A10}$$

Here $\mathsf{P}_{r\sigma}$ is an operator that permutes the pairs $\mathbf{r}_j,\sigma_j$; the summation is over all permutations $P_{r\sigma}$; the number of quantities permuted is parenthesized over the summation sign; the upper sign

refers to bosons and the lower one to fermions; and p is the parity of the permutation. As distinct from (A7), the expansion (A9) takes account of the symmetry of $f(\mathbf{X}_s)$ explicitly.

APPENDIX B: FREE ENERGY

The free energy can be calculated similarly to (I.5.28). Let us obtain a general formula. Integrating the first equation of (3.11) gives

$$F(\theta,\rho)=-\theta\int_{\theta_0}^{\theta}E(x,\rho)\frac{dx}{x^2}-\theta N s_0(\rho) \tag{B1}$$

with an arbitrary constant θ_0. In order to find the function $s_0(\rho)$ we differentiate (B1) with respect to ρ and take account of the second equation of (3.11) and also of (3.8) written as

$$\frac{\rho^2}{N}\left(\frac{\partial E}{\partial\rho}\right)_{\theta}=-\theta^2\left(\frac{\partial}{\partial\theta}\frac{p}{\theta}\right)_{\rho}. \tag{B2}$$

Then the integral containing $\partial E/\partial\rho$ is readily evaluated and we get

$$\frac{ds_0}{d\rho}=-\frac{1}{\theta_0\rho^2}p(\theta_0,\rho),\quad s_0(\rho)=-\frac{1}{\theta_0}\int_{\rho_0}^{\rho}p(\theta_0,y)\frac{dy}{y^2}+\overline{s_0}, \tag{B3}$$

where ρ_0 and $\overline{s_0}$ are arbitrary constants. The first equation of (B3) corresponds to (I.5.30) with reference to (I.5.17). The constant $\overline{s_0}$ is expressed via $F(\theta,\rho)$ at $\theta=\theta_0$ and $\rho=\rho_0$, which gives a formula for calculating F,

$$F(\theta,\rho)=-\theta\int_{\theta_0}^{\theta}E(x,\rho)\frac{dx}{x^2}+\frac{\theta}{\theta_0}N\int_{\rho_0}^{\rho}p(\theta_0,y)\frac{dy}{y^2}+\frac{\theta}{\theta_0}F(\theta_0,\rho_0). \tag{B4}$$

By integrating first the second equation of (3.11), likewise one can obtain another formula,

$$F(\theta,\rho)=N\int_{\rho_0}^{\rho}p(\theta,y)\frac{dy}{y^2}-\theta\int_{\theta_0}^{\theta}E(x,\rho_0)\frac{dx}{x^2}+\frac{\theta}{\theta_0}F(\theta_0,\rho_0). \tag{B5}$$

Note that this last formula may be also derived from (B4) if one interchanges ρ and ρ_0 as well as θ and θ_0.

Let us obtain still another formula for the free energy. To this end we eliminate τ between the equations of (3.7) with the result

$$\frac{2}{N}E-\frac{3}{\rho}p=2\pi\rho\int_0^{\infty}dr\,r^2\left[2K(r)+r\frac{dK}{dr}\right]g(r,\theta,\rho). \tag{B6}$$

Substituting (3.11) leads to an equation for F, namely,

$$2\theta\frac{\partial F}{\partial\theta}+3\rho\frac{\partial F}{\partial\rho}-2F=-2\pi\rho N\int_0^{\infty}dr\,r^2\left[2K(r)+r\frac{dK}{dr}\right]g(r,\theta,\rho). \tag{B7}$$

We integrate this quasilinear partial differential equation with the aid of the method of characteristics. If $I(\theta,\rho)$ denotes the integral in (B7) the characteristic equations may be written as

$$\frac{d\theta}{2\theta}=\frac{d\rho}{3\rho}=\frac{dF}{2F-2\pi\rho N I(\theta,\rho)}. \tag{B8}$$

Upon presuming θ to be an independent variable we solve these equations, which allows us to write the general solution of Eq. (B7) in the form

$$F(\theta,\rho)=-\pi N\frac{\rho}{\sqrt{\theta}}\int_{\theta_0}^{\theta} I\left(y,\rho\frac{y^{3/2}}{\theta^{3/2}}\right)\frac{dy}{\sqrt{y}}+\theta\Phi\left(\frac{\rho}{\theta^{3/2}}\right). \tag{B9}$$

Here $\Phi(x)$ is an arbitrary function and θ_0 is an arbitrary constant. Setting $\theta=\theta_0$ in (B9) yields

$$F(\theta_0,\rho)=\theta_0\Phi\left(\frac{\rho}{\theta_0^{3/2}}\right),$$

which permits one to find $\Phi(x)$. Inserting this $\Phi(x)$ and the integral $I(\theta,\rho)$ of (B7) into (B9) and making the replacement $y=\theta\xi^2$ leads to

$$F(\theta,\rho)=2\pi\rho N\int_0^{\infty} dr\, r^2\left(2K+r\frac{dK}{dr}\right)\int_1^{\sqrt{\theta_0/\theta}} d\xi\, g(r,\theta\xi^2,\rho\xi^3)+\frac{\theta}{\theta_0}F\left[\theta_0,\rho\left(\frac{\theta_0}{\theta}\right)^{3/2}\right]. \tag{B10}$$

Note that Eq. (3.14) of paper II may be reduced to a form similar to (B10) if use is made of the second equation of (3.11).

If one presumes ρ to be the independent variable in (B8), another formula results,

$$F(\theta,\rho)=2\pi\rho N\int_0^{\infty} dr\, r^2\left(2K+r\frac{dK}{dr}\right)\int_1^{(\rho_0/\rho)^{1/3}} d\xi\, g(r,\theta\xi^2,\rho\xi^3)+\frac{\rho^{2/3}}{\rho_0^{2/3}}F\left[\theta\left(\frac{\rho_0}{\rho}\right)^{2/3},\rho_0\right]. \tag{B11}$$

The last formulas express the free energy in terms of the pair correlation function if the free energy is known at $\theta=\theta_0$ or at $\rho=\rho_0$. If one follows the line $\rho=\rho_0(\theta/\theta_0)^{3/2}$ in the ρ–θ plane, Eqs. (B10) and (B11) coincide in form and the last terms will contain $F(\theta_0,\rho_0)$. In this case it is sufficient to know $F(\theta_0,\rho_0)$ and $g(r,\theta,\rho)$ in order to compute $F(\theta,\rho)$. In particular, the temperature θ_0 and the density ρ_0 may be chosen such that formulas of classical physics will be applicable for calculating $F(\theta_0,\rho_0)$.

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Superconductivity near critical temperature

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(Received 29 March 2002; accepted 21 February 2003)

In this paper we study the superconductivity for a sample subjected to an applied magnetic field and slightly below the critical temperature T_c. We use the Ginzburg–Landau functional to estimate the value of the critical field H_c, and examine the superconductivity when temperature is close to T_c and the applied field is below H_c. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1570508]

I. INTRODUCTION

According to the Ginzburg–Landau theory, superconductivity is described by a complex-valued function ψ (called an order parameter) and a real-valued vector field $\mathbb{A}$ (called a magnetic potential). $(\psi,\mathbb{A})$ is a minimizer of the energy functional (see Refs. 1–6):

$$\mathbb{G}[\psi,\mathbb{A}]=\int_\Omega\{|\xi\nabla\psi-i\gamma\lambda\mathbb{A}\psi|^2+\tfrac{1}{2}(1-|\psi|^2)^2\}\mathrm{d}x+\gamma^2\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbb{A}-\mathbb{H}_{\mathrm{appl}}|^2\,\mathrm{d}x,$$

where $\mathbb{H}_{\mathrm{appl}}$ is the applied field; λ (the penetration depth), ξ (the coherence length), and γ are positive parameters depending on materials and temperature. The following two numbers are important. The first one is μ,

$$\mu=\frac{1}{\xi^2}=\frac{4m\alpha^2l^2(T_c-T)}{\hbar^2T_c},\tag{1.1}$$

here T is the temperature, T_c is the critical temperature in zero field, $\hbar$ is the Planck's constant, l is a typical scale for the sample, m is the electron mass, and α is a material constant which is independent of temperature. Note that in (1.1) $T<T_c$, hence $\mu>0$. Another one is the Ginzburg–Landau parameter $\kappa=\lambda/\xi$. $\kappa>1/\sqrt{2}$ for type II superconductors, and $0<\kappa<1/\sqrt{2}$ for type I superconductors. Note that

$$\kappa=\lambda\sqrt{\mu}.\tag{1.2}$$

Let

$$\mathcal{A}=\frac{\gamma\lambda}{\xi}\mathbb{A},\quad \mathcal{H}_{\mathrm{appl}}=\frac{\gamma\lambda}{\xi}\mathbb{H}_{\mathrm{appl}}.$$

Then we can write $(1/\xi^2)\mathbb{G}[\psi,\mathbb{A}]$ as

$$\int_\Omega\{|\nabla\psi-i\mathcal{A}\psi|^2+(\mu/2)(1-|\psi|^2)^2\}\mathrm{d}x+\frac{\kappa^2}{\mu}\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathcal{A}-\mathcal{H}_{\mathrm{appl}}|^2\,\mathrm{d}x.\tag{1.3}$$

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Throughout this paper we assume that Ω is a bounded, smooth and simply connected domain in $\mathbb{R}^3$. We use the following notations:

$$\nabla_{\mathcal{A}}\psi=\nabla\psi-i\psi\mathcal{A},\quad \nabla^2_{\mathcal{A}}\psi=(\nabla-i\mathcal{A})^2\psi=\Delta\psi-i[2\mathcal{A}\cdot\nabla\psi+\psi\,\mathrm{div}\,\mathcal{A}]-|\mathcal{A}|^2\psi.$$

Our interest in this paper is the superconductivity under temperature T slightly below the critical temperature T_c. So we are led to investigate the minimizers of the Ginzburg–Landau functional where the value of μ is small. To understand the behavior of the minimizers under applied fields, let us consider an applied field of the form $\mathcal{H}_{\mathrm{appl}}=\sigma\mathbf{h}$, where $\mathbf{h}$ is a unit vector, and $\sigma>0$ is a parameter. Letting

$$\mathcal{A}=\sigma\mathbf{A},$$

the associated energy can be written as

$$\mathcal{G}[\psi,\mathbf{A}]=\int_\Omega\{|\nabla_{\sigma\mathbf{A}}\psi|^2+(\mu/2)(1-|\psi|^2)^2\}\mathrm{d}x+\frac{\kappa^2\sigma^2}{\mu}\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{A}-\mathbf{h}|^2\,\mathrm{d}x. \tag{1.4}$$

The (global) minimizers of the functional $\mathcal{G}$ [in the space $\mathcal{W}(\Omega)$, see Sec. III] satisfy the following Euler equations (called Ginzburg–Landau system):

$$\begin{gathered}-\nabla^2_{\sigma\mathbf{A}}\psi=\mu(1-|\psi|^2)\psi\quad\text{in }\Omega,\\ \mathrm{curl}^2\,\mathbf{A}=\frac{\mu}{\sigma\kappa^2}\Im\{\overline{\psi}\nabla_{\sigma\mathbf{A}}\psi\}\chi_\Omega\quad\text{in }\mathbb{R}^3,\\ (\nabla_{\sigma\mathbf{A}}\psi)\cdot\nu=0,\quad[\nu\cdot\mathbf{A}]=0,\quad[\nu\times\mathrm{curl}\,\mathbf{A}]=0\quad\text{on }\partial\Omega,\\ \mathrm{curl}\,\mathbf{A}\to\mathbf{h}\quad\text{as }|x|\to\infty.\end{gathered} \tag{1.5}$$

Here ν is the unit outer-normal vector at the boundary of Ω, $[\cdot]$ denotes the jump in the enclosed quantity across $\partial\Omega$, and χ_Ω is the characteristic function of Ω, namely, $\chi_\Omega(x)=1$ if $x\in\Omega$, and $\chi_\Omega(x)=0$ if $x\notin\Omega$. In this paper, the minimizers of $\mathcal{G}$ are called the *minimal solutions* of (1.5).

It is well known that, when the applied field is strong, the sample is in the normal state, namely, $\psi=0$. For a given unit vector $\mathbf{h}$, let $\mathbf{F_h}$ be a smooth vector field such that

$$\mathrm{curl}\,\mathbf{F_h}=\mathbf{h},\quad \mathrm{div}\,\mathbf{F_h}=0\quad\text{in }\mathbb{R}^3. \tag{1.6}$$

$(0,\mathbf{F_h})$ is a solution of (1.5) (which corresponds with the normal state) and is called a *trivial solution*. Note that $(0,\mathbf{F_h})$ is the only minimizer if σ is sufficiently large. We are interested in the existence of nontrivial minimizers and their behavior. Thus, with respect to the functional $\mathcal{G}$, we define a critical field by

$$H_c(\mathbf{h},\mu,\kappa)=\inf\{\sigma>0:\quad(0,\mathbf{F_h})\ \text{is a global minimizer of}\ \mathcal{G}\}. \tag{1.7}$$

If we fix κ and μ, and let the strength of the applied magnetic field increase to $H_c(\mathbf{h},\mu,\kappa)$, then the applied field completely penetrates the sample and destroys superconductivity. In Ref. 7 we gave a definition of the upper critical field H_{C_3} in the same manner. However, the scaling here is different to those used in Ref. 7.

Our first result is the estimate of the value of $H_c(\mathbf{h},\mu,\kappa)$ for a superconductor with small μ.

Theorem 1: *For any unit vector* $\mathbf{h}$ *there exist two positive constants* $a(\mathbf{h})$ *and* $\lambda(\mathbf{h})$ *depending only on* $\mathbf{h}$ *and* Ω *such that, for small* $\mu>0$ *and* $\kappa\geqslant\lambda(\mathbf{h})\sqrt{\mu}$,

$$H_c(\mathbf{h},\kappa,\mu)=a(\mathbf{h})\sqrt{\mu}+o(\sqrt{\mu}). \tag{1.8}$$

The numbers $a(\mathbf{h})$ and $\lambda(\mathbf{h})$ will be given in (2.4) and (3.10), respectively. Theorem 1 shows that, close to the critical temperature T_c, samples lose superconductivity under a very weak applied field.

Next we examine the behavior of the minimizers of $\mathcal{G}$ with μ tends to zero, which describes the superconductivity of a sample subjected to the applied field below $H_c(\mathbf{h},\mu,\kappa)$ and with temperature slightly below T_c. We shall see that the asymptotic behavior of the minimizers for small μ depends on the scale of κ.

Theorem 2: *Consider the applied field* $\mathbf{H}_{\text{appl}}=a\sqrt{\mu}\mathbf{h}$, *where* $\mathbf{h}$ *is a unit vector, and* a *is a fixed number,* $0<a<a(\mathbf{h})$. *Let* $(\psi_\mu,\mathbf{A}_\mu)$ *be a minimal solution of (1.5).*

(i) If $\kappa=\lambda\sqrt{\mu}$ *with* $\lambda\geqslant\lambda(\mathbf{h})$ *being fixed, then we have, as* $\mu\to 0$,

$$\begin{aligned}\psi_\mu&=c_\mu[1+ia\sqrt{\mu}w_a+a^2\mu(\mu_a+ib_av_a)+o(\mu)],\\ \mathbf{A}_\mu&=\mathbf{A}_a+ab_a\mathbf{B}_a\sqrt{\mu}+o(\sqrt{\mu}),\\ |c_\mu|^2&=c_a^2+ab_a\mu+o(\mu),\end{aligned}\tag{1.9}$$

where the constants b_a *and* c_a, *the vector fields* $\mathbf{A}_a$ *and* $\mathbf{B}_a$, *and the functions* w_a, u_a *and* v_a *are determined by* $\mathbf{h}$, a *and* Ω. $c_a\neq 0$ *and* $\mathbf{A}_a\neq\mathbf{F}_\mathbf{h}$ *for* $0<a<a(\mathbf{h})$, *and*

$$c_a\to 0 \quad \textit{and} \quad \mathbf{A}_a\to\mathbf{F}_\mathbf{h} \quad \textit{in} \quad C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3) \quad \textit{as} \quad a\to a(\mathbf{h}).$$

(ii) If $\kappa>0$ *is fixed, then we have, as* $\mu\to 0$,

$$\begin{aligned}\psi_\mu&=C_\mu[1+ia\sqrt{\mu}w_\mathbf{h}+a^2\mu\psi_\mathbf{h}+O(\mu^{3/2})],\\ \mathbf{A}_\mu&=\mathbf{F}_\mathbf{h}+\frac{\mu|C_\mu|^2}{\kappa^2}\mathbf{U}_\mathbf{h}+O(\mu^{3/2}),\\ |C_\mu|&=\sqrt{1-\left(\frac{a}{a(\mathbf{h})}\right)^2}+O(\sqrt{\mu}),\end{aligned}\tag{1.10}$$

where the functions $w_\mathbf{h}$ *and* $\psi_\mathbf{h}$ *and the vector field* $\mathbf{U}_\mathbf{h}$ *are determined by* $\mathbf{h}$ *and* Ω.

Remark 1.1: Theorem 1 and conclusion (i) of Theorem 2 together give a description of superconductivity near the critical temperature T_c for type I superconductors of size comparable with the penetration depth. When the temperature increases to T_c (so μ tends to zero), a very weak (but fixed) applied field penetrates the sample and destroys superconductivity. However, if the applied field is kept below from $H_c(\mathbf{h},\mu,\kappa)$ by a gap of scale $O(\sqrt{\mu})$, it partially penetrates the sample, and superconductivity persists.

Remark 1.2: Conclusion (ii) of Theorem 2 needs a careful explanation. It describes the behavior of a sample of size much smaller than the penetration depth, and subjected to the applied field below $H_c(\mathbf{h},\mu,\kappa)$. When the temperature increases to T_c, the applied field penetrates the sample almost completely (more precisely, the leading order magnetic field is the applied field), however, superconductivity may persist. We would like to mention that a similar phenomenon on thin films has been found by Chapman, Du, and Gunzburger in Ref. 8 (Sec. 2): For a very thin film, the applied field will penetrate the film almost completely but superconductivity may persist.

The expansions (1.10) also imply that, near the critical temperature T_c, type I behavior may be observed in a type II superconductor at certain scale. It will be interesting to compare this phenomenon with the observations in Refs. 8 and 9, where Chapman, Du, and Gunzburger observed that for any value of κ which can be small, a very thin film will behave as a type II superconductor [see Ref. 8 (Sec. 2)]; and Richardson and Rubinstein found that a material can exhibit both types of behavior depending upon its geometry [see Ref. 9 (p. 1288)].

Remark 1.3: Theorem 2 shows that, if μ is small, the minimizers have no vortices. A similar phenomenon on small samples has been found by Aftalion and Dancer[10] and Aftalion and Du:[11] A superconductor of very small size does not allow vortices to exist, no matter what the value of κ is. Let us remark that, the value of μ is small for a sample of small size, see (1.1).

Remark 1.4: The numbers $a(\mathbf{h})$ and $\lambda(\mathbf{h})$ are determined in terms of the solutions of some elliptic equations, see Secs. II and III. Our approach relies on understanding of these problems. It seems to us that $\kappa=\lambda(\mathbf{h})\sqrt{\mu}$ is a critical value, and it is interesting to investigate the behavior of superconductivity for $0<\kappa<\lambda(\mathbf{h})\sqrt{\mu}$.

Remark 1.5: It is well known that, the minimizers of the Ginzburg–Landau functional exhibit various phenomena for parameters of different scales. Therefore, to address different questions people use different scaling and reach the energy functionals in different forms. Especially if we choose the penetration length λ as the length unit, then we may take $\lambda=1$ and $\mu=\kappa^2$. In a rescaled domain (also denoted by Ω) we can rewrite the functional (1.3) in the following form (see Ref. 6, p. 562):

$$\int_\Omega \{|\nabla\psi-i\mathcal{A}\psi|^2+(\kappa^2/2)(1-|\psi|^2)^2\}\mathrm{d}x+\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathcal{A}-\mathcal{H}_{\mathrm{appl}}|^2\,\mathrm{d}x. \tag{1.11}$$

In recent years many authors have used the functional (1.11) to study the behavior of superconductors of large κ when the applied fields are close to the upper critical field H_{C_3} (see for instance Refs. 3, 7, and 12–25), or close to the first critical field H_{C_1} (see Refs. 26–28). Especially, the estimate of H_{C_3} for a superconducting cylinder with infinite height and constant cross section Ω_0 was carried out by Bauman–Phillips–Tang,[15] Bernoff–Sternberg,[16] Giorgi–Phillips,[17] Lu–Pan,[7,18,19] del Pino–Felmer–Sternberg,[20] Helffer–Morame,[21] and it was finally proved by Helffer–Pan[23] that, if κ is large,

$$H_{C_3}(\kappa)=\frac{\kappa}{\beta_0}+\frac{C_1}{\beta_0^{3/2}}\kappa_{\max}+O(\kappa^{-1/3}),$$

where β_0 is the lowest eigenvalue of the Schrödinger operator with a unit magnetic field on the half plane and $0.5<\beta_0<0.76$ (see Refs. 7 and 18), $\kappa_{\max}$ is the maximum value of the curvature of the boundary of Ω_0, and $C_1>0$ is a universal constant; moreover, as the applied field decreases from $H_{C_3}(\kappa)$, superconductivity nucleates at the maximum points of the curvature. Comparing these results with our Theorems 1 and 2 in this paper, we see that the behavior of the minimizers for small μ are quite different to those with large μ.

This paper is organized as follows. In Sec. II we study the eigenvalue problem of $-\nabla^2_{\epsilon\mathbf{F_h}}$ with ϵ being small. The proof is standard and lengthy, and is hence given in Appendix A. [Note that the study of the upper critical field $H_{C_3}(\kappa)$ for large κ has led to the estimate of the lowest eigenvalue of $-\nabla^2_{b\mathbf{F_h}}$ for large value of b, see the references quoted above.] In Sec. III we discuss the solutions of several elliptic equations in $\mathbb{R}^3$ which are needed to describe the behavior of the minimizers of the functional (1.4). In Sec. IV we estimate the value of $H_c(\mathbf{h},\mu,\kappa)$ for small μ, and study the behavior of the minimizers under an applied field below $H_c(\mathbf{h},\mu,\kappa)$. Theorem 4.1 concerns the case where $\kappa=\lambda\sqrt{\mu}$ with $\lambda\geqslant\lambda(\mathbf{h})$, and Theorem 4.2 concerns the case where κ is fixed. The proof of Theorem 4.1 is lengthy, and therefore some technical details will be given in Appendix B. Theorem 4.2 can be proved following the line of the proof of Theorem 4.1. However, since the conclusions are somewhat unexpected, we present the main part of the proof in Sec. IV, and include some technical details in Appendix C. Theorems 1 and 2 are consequences of Theorems 4.1 and 4.2.

II. ESTIMATE OF EIGENVALUE $\mu(\epsilon \mathbf{F_h})$ FOR SMALL PARAMETER ϵ

Given a unit vector $\mathbf{h}$, let $\mathbf{F_h}$ be the vector field satisfying (1.6), and for $\epsilon>0$ let $\mu(\epsilon \mathbf{F_h})$ be the lowest eigenvalue of the equation

$$-\nabla^2_{\epsilon \mathbf{F_h}} \phi = \mu \phi \quad \text{in } \Omega, \quad (\nabla_{\epsilon \mathbf{F_h}} \phi)\cdot \nu = 0 \quad \text{on } \partial\Omega. \tag{2.1}$$

We shall estimate the value $\mu(\epsilon \mathbf{F_h})$ for small ϵ. Let

$$\omega(\mathbf{h}) = \inf_{\phi \in W^{1,2}(\Omega)} \fint_\Omega |\nabla \phi - \mathbf{F_h}|^2 \, dx, \tag{2.2}$$

where $\fint_\Omega \phi \, dx = (1/|\Omega|)\int_\Omega \phi \, dx$. $\omega(\mathbf{h})$ is achieved by the unique (real) solution $w_{\mathbf{h}}$ of the equation

$$\Delta w_{\mathbf{h}} = 0 \quad \text{in } \Omega, \quad \frac{\partial w_{\mathbf{h}}}{\partial \nu} = \mathbf{F_h}\cdot \nu \quad \text{on } \partial\Omega, \quad \int_\Omega w_{\mathbf{h}} \, dx = 0. \tag{2.3}$$

Up to an additive constant, the minimizer is unique. Note that $\operatorname{div} \mathbf{F_h} = 0$. So

$$\int_\Omega |\nabla w_{\mathbf{h}}|^2 \, dx = \int_{\partial\Omega} w_{\mathbf{h}} \frac{\partial w_{\mathbf{h}}}{\partial \nu} \, dS = \int_{\partial\Omega} w_{\mathbf{h}} \mathbf{F_h}\cdot \nu \, dS = \int_\Omega \nabla w_{\mathbf{h}} \cdot \mathbf{F_h} \, dx.$$

Thus

$$\omega(\mathbf{h}) = \fint_\Omega |\nabla w_{\mathbf{h}} - \mathbf{F_h}|^2 \, dx = \fint_\Omega (|\mathbf{F_h}|^2 - |\nabla w_{\mathbf{h}}|^2) \, dx.$$

We define

$$a(\mathbf{h}) = \frac{1}{\sqrt{\omega(\mathbf{h})}}. \tag{2.4}$$

Lemma 2.1: Let $\mu(\epsilon \mathbf{F_h})$ be the lowest eigenvalue of (2.1). As $\epsilon \to 0$ we have

$$\mu(\epsilon \mathbf{F_h}) = \omega(\mathbf{h})\epsilon^2 + O(\epsilon^3). \tag{2.5}$$

Let ϕ_ϵ be the eigenfunction of (2.1) associated with $\mu(\epsilon \mathbf{F_h})$ such that $\|\phi_\epsilon\|_{L^\infty(\Omega)} = 1$. ϕ_ϵ has the expansion

$$\phi_\epsilon = \alpha_\epsilon + i\epsilon\beta_\epsilon w_{\mathbf{h}} + \epsilon^2 \phi_2 + o(\epsilon^2), \tag{2.6}$$

where α_ϵ and β_ϵ are constants, $|\alpha_\epsilon|$ and β_ϵ converge to 1 as $\epsilon \to 0$, and ϕ_2 is a smooth function depending on $\mathbf{h}$.

The proof of Lemma 2.1 is standard, and will be given in Appendix A for the reader's convenience.

III. SOME ELLIPTIC PROBLEMS IN THE SPACE $W^{1,2}(\Omega)\times \mathbf{D}^{1,2}(\mathbb{R}^3, \mathbf{div})$

In the first part of this section we derive the elliptic estimates of the minimal solutions of Ginzburg–Landau system (1.5), and in the second part we discuss the properties of the solutions of some elliptic equations in $\mathbb{R}^3$, which are needed in the description of the minimal solutions of (1.5) in Sec. IV.

Let us recall the definition of the minimizers of the Ginzburg–Landau functional $\mathcal{G}$. Let

$$D^{1,2}(\mathbb{R}^3) = \{\phi \in L^1_{\mathrm{loc}}(\mathbb{R}^3): \ |\nabla \phi| \in L^2(\mathbb{R}^3)\}.$$

Define $\|\phi\|_{1,2}=\|\nabla\phi\|_{L^2(\mathbb{R}^3)}$. After identifying two functions that differ by a constant, $(D^{1,2}(\mathbb{R}^3),\|\cdot\|_{1,2})$ is a Hilbert space (Ref. 29, Lemma II.5.1). Let $\mathbf{D}^{1,2}(\mathbb{R}^3)$ denote the corresponding space of vector fields. It follows from Theorem II.6.2 in Ref. 29 that for any $\mathbf{B}\in\mathbf{D}^{1,2}(\mathbb{R}^3)$, there exists a unique constant vector $\mathbf{B}_0$ such that $\mathbf{B}-\mathbf{B}_0$ can be approximated in the norm $\|\cdot\|_{1,2}$ by C_0^∞ vector fields. It is well known that, for any $\mathbf{B}\in\mathbf{D}^{1,2}(\mathbb{R}^3)$,

$$\|\mathbf{B}\|_{1,2}^2\equiv\int_{\mathbb{R}^3}|\nabla\mathbf{B}|^2\,dx=\int_{\mathbb{R}^3}\{|\mathrm{curl}\,\mathbf{B}|^2+|\mathrm{div}\,\mathbf{B}|^2\}dx, \tag{3.1}$$

see Ref. 30, also see Ref. 17 [(3.2)]. The following subspace of $\mathbf{D}^{1,2}(\mathbb{R}^3)$ is useful to us:

$$\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})=\{\mathbf{A}\in\mathbf{D}^{1,2}(\mathbb{R}^3):\ \mathrm{div}\,\mathbf{A}=0\ \text{ in }\ \mathbb{R}^3\}.$$

Let $W^{1,2}(\Omega,\mathbb{C})$ be the Sobolev space of all complex-valued functions defined on $\overline{\Omega}$, and

$$\mathcal{W}(\Omega)=\{(\psi,\mathbf{A}):\ \psi\in W^{1,2}(\Omega,\mathbb{C}),\quad \mathbf{A}-\mathbf{F_h}\in\mathbf{D}^{1,2}(\mathbb{R}^3)\}.$$

We consider the variational problem for the functional $\mathcal{G}$ on $\mathcal{W}(\Omega)$. Let

$$C(\mathbf{h},\mu,\kappa,\sigma)=\inf_{(\psi,\mathbf{A})\in\mathcal{W}(\Omega)}\mathcal{G}[\psi,\mathbf{A}].$$

It is easy to show that the (global) minimizers exist, and satisfy the Euler equations (1.5).

Remark 3.1: (i) Giorgi and Phillips[17] considered the solutions $(\psi,\mathbf{A})$ of (1.5) such that $\psi\in W^{1,2}(\Omega)$ and $\mathbf{A}-\mathbf{F_h}\in\hat{H}^1(\mathbb{R}^3)$, where $\hat{H}^1(\mathbb{R}^3)$ is the completion of $C_0^\infty(\mathbb{R}^3,\mathbb{R}^3)$ with respect to the norm $\|\mathbf{A}\|=\|\nabla\mathbf{A}\|_{L^2(\mathbb{R}^3)}$. Our setting is equivalent to theirs. In fact, for any solution $(\psi,\mathbf{A})\in\mathcal{W}(\Omega)$ of (1.5), there exists a unique constant vector $\mathbf{B}_0$ such that $\mathbf{A}-\mathbf{F_h}-\mathbf{B}_0\in\hat{H}^1(\mathbb{R}^3)$; and due to the gange invariance of (1.5) $(e^{-i\mathbf{B}_0\cdot x}\psi,\mathbf{A}-\mathbf{B}_0)$ is also a solution of (1.5). We choose the space $\mathbf{D}^{1,2}(\mathbb{R}^3)$ instead of $\hat{H}^1(\mathbb{R}^3)$ so that we are free to add a constant vector to the magnetic potential $\mathbf{A}$. It will be clear that such freedom is useful in our study.

Due to the gauge invariance of $\mathcal{G}$, we can replace $\mathbf{A}$ by $\hat{\mathbf{A}}$ that satisfies $\mathrm{curl}\,\hat{\mathbf{A}}=\mathrm{curl}\,\mathbf{A}$ and $\mathrm{div}\,\hat{\mathbf{A}}=0$ in $\mathbb{R}^3$, see Ref. 17 (Lemma 3.1). So we can restrict the functional $\mathcal{G}$ on a subspace

$$\mathcal{W}(\Omega,\mathrm{div})=\{(\psi,\mathbf{A})\in\mathcal{W}(\Omega):\ \mathrm{div}\,\mathbf{A}=0\ \text{ in }\ \mathbb{R}^3\}.$$

In the following we always assume that the solutions of (1.5) satisfy $\mathrm{div}\,\mathbf{A}=0$ in $\mathbb{R}^3$.

(ii) In (1.5) the boundary condition $[\mathbf{A}\cdot\nu]=0$ on $\partial\Omega$ is a consequence of the fact that $\mathbf{A}\in W^{1,2}(\mathbb{R}^3)$, and the boundary condition $[\mathrm{curl}\,\mathbf{A}\times\nu]=0$ on $\partial\Omega$ is a consequence of the fact that $(\psi,\mathbf{A})$ is a weak solution of the Euler equations, see Ref. 30 (Chap. 5, Sec. 4). Therefore when we consider the minimal solutions of (1.5) (they are weak solutions), we may write (1.5) as follows:

$$-\nabla_{\sigma\mathbf{A}}^2\psi=\mu(1-|\psi|^2)\psi\quad\text{ in }\ \Omega,$$

$$\mathrm{curl}^2\,\mathbf{A}=\frac{\mu}{\sigma\kappa^2}\Im\{\overline{\psi}\nabla_{\sigma\mathbf{A}}\psi\}\chi_\Omega\quad\text{ in }\ \mathbb{R}^3,\quad \mathbf{A}-\mathbf{F_h}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}),$$

$$(\nabla_{\sigma\mathbf{A}}\psi)\cdot\nu=0\quad\text{ on }\ \partial\Omega.$$

(iii) It has been proved by many authors that the solutions $(\psi,\mathbf{A})$ of (1.5) satisfy $\|\psi\|_{L^\infty(\Omega)}\leqslant 1$.

Now we can give a simple lower bound estimate on $H_c(\mathbf{h},\mu,\kappa)$ for small μ. The proof follows from Ref. 7 (Lemma 2.1).

Theorem 3.2: *Given a unit vector* $\mathbf{h}$ *we have, for small* $\mu>0$ *and for any* $\kappa>0$,

$$H_c(\mathbf{h},\kappa,\mu)\geqslant a(\mathbf{h})\sqrt{\mu}+o(\sqrt{\mu}). \tag{3.2}$$

Proof: If $\mu(\sigma\mathbf{F_h})<\mu$ and ϕ_σ is the associated eigenfunction of (2.1), we take $(t\phi_\sigma,\mathbf{F_h})$ as a test field, where

$$t=\frac{\sqrt{\mu-\mu(\sigma\mathbf{F_h})}\|\phi_\sigma\|_{L^2(\Omega)}}{\sqrt{\mu}\|\phi_\sigma\|^2_{L^4(\Omega)}}.$$

We have

$$\inf_{(\psi,\mathbf{A})\in\mathcal{W}(\Omega)}\mathcal{G}[\psi,\mathbf{A}]\leqslant\mathcal{G}[t\phi_\sigma,\mathbf{F_h}]\leqslant\frac{\mu}{2}|\Omega|-\frac{1}{2\mu}[\mu-\mu(\sigma\mathbf{F_h})]\frac{\|\phi_\sigma\|^4_{L^2(\Omega)}}{\|\phi_\sigma\|^4_{L^4(\Omega)}}<\frac{\mu}{2}|\Omega|.$$

So the minimizers are nontrivial. In order to obtain (3.2), we use Lemma 2.1 to estimate the largest value of σ such that $\mu(\sigma\mathbf{F_h})\leqslant\mu$. □

Now we consider the regularity of a minimal solution $(\psi,\mathbf{A})$ of (1.5). Obviously ψ is smooth in Ω and $\mathbf{A}$ is smooth in $\mathbb{R}^3\backslash\partial\Omega$. We shall discuss the regularity of ψ and $\mathbf{A}$ on $\partial\Omega$. In the following we always let C denote a generic positive constant that is independent of ϵ but may vary from line to line. Let B_r denote the open ball centered at the origin and with radius r.

Lemma 3.3: Let $(\psi,\mathbf{A})\in\mathcal{W}(\Omega,\mathrm{div})$ *be a minimal solution of (1.5). We have*

$$\|\nabla(\mathbf{A}-\mathbf{F_h})\|_{L^2(\mathbb{R}^3)}=\|\mathrm{curl}\,\mathbf{A}-\mathbf{h}\|_{L^2(\mathbb{R}^3)}\leqslant\frac{\mu}{\sqrt{2}\kappa\sigma}\|\psi\|^2_{L^4(\Omega)}. \tag{3.3}$$

For any $0<\alpha<1$, $\psi\in C^{2+\alpha}(\overline{\Omega})$ *and* $\mathbf{A}\in C^{1+\alpha}(\overline{\Omega})$; *and for any* $R>0$ *such that* $\overline{\Omega}\subset B_R$, *there exist* $C(\alpha,R)>0$ *and* $q=3/(1-\alpha)$ *such that, for all positive numbers* μ, κ, *and* σ,

$$\|\nabla(\mathbf{A}-\mathbf{F_h})\|_{C^\alpha(R_R)}\leqslant C(\alpha,R)\left\{\frac{\mu}{\sigma\kappa}\|\psi\|^2_{L^4(\Omega)}+\frac{\mu}{\sigma\kappa^2}\|\overline{\psi\nabla}_{\sigma\mathbf{A}}\psi\|_{L^q(\Omega)}\right\}. \tag{3.4}$$

Proof: Step 1. We prove (3.3). From the first equation in (1.5) we have

$$\int_\Omega|\nabla_{\sigma\mathbf{A}}\psi|^2\,\mathrm{d}x=\mu\int_\Omega(1-|\psi|^2)|\psi|^2\,\mathrm{d}x.$$

So

$$\mathcal{G}[\psi,\mathbf{A}]=\frac{\mu}{2}|\Omega|-\frac{\mu}{2}\int_\Omega|\psi|^4\,\mathrm{d}x+\frac{\kappa^2\sigma^2}{\mu}\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{A}-\mathbf{h}|^2\,\mathrm{d}x.$$

Since $C(\mathbf{h},\mu,\kappa,\sigma)\leqslant\mu|\Omega|/2$, we have

$$\frac{\kappa^2\sigma^2}{\mu}\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{A}-\mathbf{h}|^2\,\mathrm{d}x=C(\mathbf{h},\mu,\kappa,\sigma)-\frac{\mu}{2}|\Omega|+\frac{\mu}{2}\int_\Omega|\psi|^4\,\mathrm{d}x\leqslant\frac{\mu}{2}\int_\Omega|\psi|^4\,\mathrm{d}x.$$

So (3.3) is true.

Step 2. We prove (3.4). Let

$$\mathbf{f}=\frac{\mu}{\sigma\kappa^2}\Im\{\overline{\psi\nabla}_{\sigma\mathbf{A}}\psi\}\chi_\Omega.$$

Obviously $\mathbf{f}\in L^2(\mathbb{R}^3)$. Let $\mathbf{U}=\mathbf{A}-\mathbf{F_h}$. Since $[\mathrm{curl}\,\mathbf{A}\times\nu]=0$ on $\partial\Omega$, and from the second equation in (1.5), $\mathbf{U}$ is a weak solution of the equation $\mathrm{curl}^2\,\mathbf{U}=\mathbf{f}$ in $\mathbb{R}^3$. Since $\mathrm{div}\,\mathbf{U}=0$ in $\mathbb{R}^3$, this equation can be written as follows:

$$-\Delta \mathbf{U}=\mathbf{f} \quad \text{in } \mathbb{R}^3. \tag{3.5}$$

Applying the De Giorgi L^∞ estimate (Ref. 31, Theorem 8.18) to each component of (3.5), we find that, there exists $C>0$ such that, for any $0<r<R$,

$$\|\mathbf{U}\|_{L^\infty(B_r)}\leqslant C\{(R-r)^{-3/2}\|\mathbf{U}\|_{L^2(B_R)}+R^{1/2}\|\mathbf{f}\|_{L^2(B_R)}\}.$$

In order to prove (3.4), let us choose $\rho=\max_{x\in\Omega}|x|$ and fix $R>\rho$. From the above inequality, for any $\rho<r<R$ we can find a constant $C(r,R)>0$ such that

$$\|\mathbf{U}\|_{L^\infty(B_r)}\leqslant C(r,R)\{\|\mathbf{U}\|_{L^2(B_R)}+\|\mathbf{f}\|_{L^2(B_R)}\}. \tag{3.6}$$

Applying the Hölder estimate for weak solutions (Ref. 31, Theorem 8.24) to (3.5) we find that, for some $0<\alpha_0<1$ and $\rho<r<R$,

$$\|\mathbf{U}\|_{C^{\alpha_0}(B_r)}\leqslant C(r,R)\{\|\mathbf{U}\|_{L^2(B_R)}+\|\mathbf{f}\|_{L^2(B_R)}\}. \tag{3.7}$$

Hence $\mathbf{A}\in C^{\alpha_0}(\overline{\Omega})$. Next, since $\operatorname{div}\mathbf{A}=0$, we write the first and third equalities in (1.5) as follows:

$$\begin{aligned} -\Delta\psi+2i\sigma\mathbf{A}\cdot\nabla\psi+\sigma^2|\mathbf{A}|^2\psi&=\mu(1-|\psi|^2)\psi \quad \text{in } \Omega,\\ \frac{\partial\psi}{\partial\nu}&=i\sigma\mathbf{A}\cdot\nu\psi \quad \text{on } \partial\Omega. \end{aligned} \tag{3.8}$$

From the fact that $\mathbf{A}\in C^{\alpha_0}(\overline{\Omega})$, and applying the Hölder gradient estimate (see for instance Ref. 31, Theorem 8.33) to (3.8), we find that $\psi\in C^{1+\alpha_0}(\overline{\Omega})$. Therefore, $\mathbf{f}\in C^{\alpha_0}(\overline{\Omega})$, and hence $\mathbf{f}\in L^\infty(\mathbb{R}^3)$. Now we apply the Hölder gradient estimate to (3.5) again and find that, for any $0<\alpha<1$, $\mathbf{U}\in C^{1+\alpha}(B_R)$, and

$$\|\nabla\mathbf{U}\|_{C^\alpha(B_r)}\leqslant C(r,R,\alpha)\{\|\mathbf{f}\|_{L^q(B_R)}+\|\nabla\mathbf{U}\|_{L^2(B_R)}+\|\mathbf{U}\|_{L^2(B_R)}\},$$

where $q=3/(1-\alpha)$. Hence $\mathbf{A}\in C^{1+\alpha}(B_R)$. Since $\operatorname{div}\mathbf{U}=0$, from (3.1) we have

$$\|\nabla\mathbf{U}\|_{L^2(B_R)}\leqslant\|\nabla\mathbf{U}\|_{L^2(\mathbb{R}^3)}=\|\operatorname{curl}\mathbf{U}\|_{L^2(\mathbb{R}^3)},$$

$$\|\mathbf{U}\|_{L^2(B_R)}\leqslant C'R\|\mathbf{U}\|_{L^6(B_R)}\leqslant C'R\|\mathbf{U}\|_{L^6(\mathbb{R}^3)}\leqslant CR\|\nabla\mathbf{U}\|_{L^2(\mathbb{R}^3)}=CR\|\operatorname{curl}\mathbf{U}\|_{L^2(\mathbb{R}^3)}.$$

Using these inequalities together with (3.3), (3.6), and (3.7) we get (3.4).

For any $0<\alpha<1$, since $\mathbf{A}\in C^{1+\alpha}(\overline{\Omega})$, we apply the Hölder estimate to (3.8) again to conclude that $\psi\in C^{2+\alpha}(\overline{\Omega})$. □

The rest of this section is devoted to the discussions of some elliptic equations in $\mathbb{R}^3$. We begin with the equation

$$\operatorname{curl}^2\mathbf{U}=(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\chi_\Omega \quad \text{in } \mathbb{R}^3, \quad \mathbf{U}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div}), \tag{3.9}$$

where $\mathbf{h}$ is a unit vector, $\mathbf{F}_{\mathbf{h}}$ and $w_{\mathbf{h}}$ were given in (1.6) and (2.3), respectively. Now we choose $\mathbf{F}_{\mathbf{h}}$ such that $\int_\Omega\mathbf{F}_{\mathbf{h}}\,dx=\mathbf{0}$. If $\mathbf{U}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div})$ is a weak solution of (3.9), then $\mathbf{U}$ is called a finite energy solution.

Lemma 3.4: (3.9) has a finite energy solution $\mathbf{U}_{\mathbf{h}}$, *and* $\mathbf{U}_{\mathbf{h}}\in C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3)$ *for any* $0<\alpha<1$. *Moreover, the finite energy solutions of (3.9) are unique up to an additive constant vector.*

Proof: Consider a functional

$$J[\mathbf{A}]=\int_{\mathbb{R}^3}|\operatorname{curl}\mathbf{A}|^2\,dx-2\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\mathbf{A}\,dx.$$

J is a convex functional on the space

$$X=\left\{\mathbf{A}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div}):\ \int_\Omega\mathbf{A}\,dx=\mathbf{0}\right\}.$$

Using (3.1) and the Poincaré inequality we check

$$\lim_{\mathbf{A}\in X,\|\mathbf{A}\|_{1,2}\to\infty}J[\mathbf{A}]=+\infty.$$

Thus J has a minimizer $\mathbf{U}_{\mathbf{h}}$ in X, which is a finite energy solution of (3.9). As in the proof of Lemma 3.3 we can show that $\mathbf{U}_{\mathbf{h}}\in C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. If (3.9) has another finite energy solution $\mathbf{U}$, we let $\mathbf{B}=\mathbf{U}_{\mathbf{h}}-\mathbf{U}$. Then $\mathbf{B}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div})$ and $\mathbf{B}$ is a harmonic vector field. So $\mathbf{B}$ is a constant vector. □

In the following we always choose $\mathbf{U}_{\mathbf{h}}$ such that $\int_\Omega\mathbf{U}_{\mathbf{h}}\,dx=\mathbf{0}$. Now we can define

$$\lambda(\mathbf{h})=\sqrt{\frac{2}{\omega(\mathbf{h})|\Omega|}}\,\|\operatorname{curl}\mathbf{U}_{\mathbf{h}}\|_{L^2(\mathbb{R}^3)}. \tag{3.10}$$

Next, given a unit vector $\mathbf{h}$ and constants $\lambda>0$ and $\rho\geqslant 0$, we consider

$$\begin{gathered}\Delta w=0\quad\text{in }\Omega,\\ \lambda^2\operatorname{curl}^2\mathbf{A}=\rho(\nabla w-\mathbf{A})\chi_\Omega\quad\text{in }\mathbb{R}^3,\quad \mathbf{A}-\mathbf{F}_{\mathbf{h}}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div}),\\ \frac{\partial w}{\partial\nu}=\mathbf{A}\cdot\nu\quad\text{on }\partial\Omega.\end{gathered} \tag{3.11}$$

The weak solutions of (3.11) are critical points of the functional

$$\mathcal{J}_\rho[w,\mathbf{A}]=\lambda^2\int_{\mathbb{R}^3}|\operatorname{curl}\mathbf{A}-\mathbf{h}|^2\,dx+\rho\int_\Omega|\nabla w-\mathbf{A}|^2\,dx.$$

A solution $(w,\mathbf{A})$ of (3.11) is called a finite energy solution if $w\in W^{1,2}(\Omega)$ and $\mathbf{A}-\mathbf{F}_{\mathbf{h}}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div})$. Let us define

$$Y=\left\{(w,\mathbf{A}):\ w\in W^{1,2}(\Omega),\quad \mathbf{A}-\mathbf{F}_{\mathbf{h}}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div}),\quad \int_\Omega w\,dx=0,\quad \int_\Omega\mathbf{A}\,dx=\mathbf{0}\right\}.$$

We can show that Y contains exactly one finite energy solution of (3.11). In fact, as in Lemma 3.4 we can show that (3.11) has a finite energy solution. If $(w_1,\mathbf{A}_1)$ and $(w_2,\mathbf{A}_2)$ are finite energy solutions of (3.11), and let $v=w_1-w_2$ and $\mathbf{B}=\mathbf{A}_1-\mathbf{A}_2$, then we have

$$\begin{gathered}\Delta v=0\quad\text{in }\Omega,\\ \lambda^2\operatorname{curl}^2\mathbf{B}=\rho(\nabla v-\mathbf{B})\chi_\Omega\quad\text{in }\mathbb{R}^3,\quad \mathbf{B}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div}),\\ \frac{\partial v}{\partial\nu}=\mathbf{B}\cdot\nu\quad\text{on }\partial\Omega.\end{gathered}$$

As in Lemma 3.3 we can show that $\mathbf{B}\in C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. $\mathbf{D}=\operatorname{curl}\mathbf{B}$ is a weak solution of

$$\lambda^2 \operatorname{curl}^2 \mathbf{D} = -\rho \mathbf{D}_{\chi_\Omega} \quad \text{in } \mathbb{R}^3,$$

and hence $\operatorname{curl} \mathbf{B} = \mathbf{0}$. Since $\mathbf{B} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \operatorname{div})$, $\mathbf{B} = \mathbf{b}$, a constant vector. Using the equations for $(v, \mathbf{B})$ again we find that $\nabla v = \mathbf{b}$. Hence v is a linear function, $v = \mathbf{b} \cdot x + c$, and $(w_1, \mathbf{A}_1) = (w_2 + \mathbf{b} \cdot x + c, \mathbf{A}_2 + \mathbf{b})$.

Let $(w^\rho, \mathbf{A}^\rho)$ denote the unique finite energy solution of (3.9) in Y. Then

$$\mathcal{J}_\rho[w^\rho, \mathbf{A}^\rho] = \inf_{(w, \mathbf{A}) \in Y} \mathcal{J}_\rho[w, \mathbf{A}].$$

Note that $(w^0, \mathbf{A}^0) = (w_{\mathbf{h}}, \mathbf{F}_{\mathbf{h}})$.

Now we consider the following question: Given $a > 0$, look for all positive ρ's such that

$$a^2 \fint_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \, dx + \rho = 1. \tag{3.12}$$

Lemma 3.5: (i) For any $\lambda > 0$ *and* $0 < a < a(\mathbf{h})$, *there exists a unique positive number* $\rho = \rho(a)$ *such that (3.12) holds.* $\rho(a)$ *is strictly decreasing in a, and* $\lim_{a \to 0^+} \rho(a) = 1$.

(ii) If $\lambda \geqslant \lambda(\mathbf{h})$, *then*

$$(3.12) \text{ has} \begin{cases} \text{a unique positive solution } \rho(a) & \text{if } 0 < a < a(\mathbf{h}), \\ \text{a unique non-negative solution } \rho = 0 & \text{if } a = a(\mathbf{h}), \\ \text{no non-negative solutions} & \text{if } a > a(\mathbf{h}), \end{cases} \tag{3.13}$$

and $\lim_{a \to a(\mathbf{h})^-} \rho(a) = 0$.

(iii) If $0 < \lambda < \lambda(\mathbf{h})$, *then there exists* $C(\lambda) > 0$ *such that,*

$$(3.12) \text{ has} \begin{cases} \text{a unique positive solution } \rho(a) & \text{if } 0 < a < a(\mathbf{h}), \\ \text{a unique positive solution } \rho(a(\mathbf{h})) \text{ and } \rho = 0 & \text{if } a = a(\mathbf{h}), \\ \text{exactly two positive solutions } \rho_*(a) < \rho(a) & \text{if } a(\mathbf{h}) < a < C(\lambda), \\ \text{exactly one positive solution} & \text{if } a = C(\lambda), \\ \text{no non-negative solutions} & \text{if } a > C(\lambda), \end{cases} \tag{3.14}$$

and $\lim_{a \to a(\mathbf{h})} \rho(a) = \rho(a(\mathbf{h}))$.

Proof: Step 1. Fix $\lambda > 0$. For $a \geqslant 0$ and $\rho \geqslant 0$, we define a function

$$f(a, \rho) = a^2 \fint_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \, dx + \rho.$$

Using the uniqueness of the finite energy solutions of (3.11) in the set Y, we find that $f(a, \rho)$ is continuous for $\rho \geqslant 0$ and $a \geqslant 0$. We can show that f is twice differentiable for $a > 0$, $\rho > 0$. To prove this, we fix $a > 0$ and $\rho > 0$. Then, for small $t \neq 0$, we define

$$v^{\rho,t} = \frac{w^{\rho+t} - w^\rho}{t}, \quad \mathbf{B}^{\rho,t} = \frac{\mathbf{A}^{\rho+t} - \mathbf{A}^\rho}{t}.$$

We can show that, there exists $(v^\rho, \mathbf{B}^\rho) \in Y$ such that $v^{\rho,t} \to v^\rho$ in $C^{2+\alpha}(\overline{\Omega})$ and $\mathbf{B}^{\rho,t} \to \mathbf{B}^\rho$ in $C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3)$ as $t \to 0$, and $(v^\rho, \mathbf{B}^\rho)$ satisfies

$$\Delta v^\rho = 0 \quad \text{in } \Omega,$$

$$\lambda^2 \operatorname{curl}^2 \mathbf{B}^\rho = \{(\nabla w^\rho - \mathbf{A}^\rho) + \rho(\nabla v^\rho - \mathbf{B}^\rho)\} \chi_\Omega \quad \text{in } \mathbb{R}^3, \quad \mathbf{B}^\rho \in \mathbf{D}^{1,2}(\mathbb{R}^3, \operatorname{div}), \tag{3.15}$$

$$\frac{\partial v^\rho}{\partial \nu}=\mathbf{B}^\rho\cdot\nu \quad \text{on } \partial\Omega.$$

Similarly we define

$$z^{\rho,t}=\frac{v^{\rho+t}-v^\rho}{t}, \quad \mathbf{D}^{\rho,t}=\frac{\mathbf{B}^{\rho+t}-\mathbf{B}^\rho}{t}.$$

We can show that, there exists $(z^\rho,\mathbf{D}^\rho)\in Y$ such that $z^{\rho,t}\to z^\rho$ in $C^{2+\alpha}(\overline{\Omega})$ and $\mathbf{D}^{\rho,t}\to\mathbf{D}^\rho$ in $C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3)$ as $t\to 0$, and $(z^\rho,\mathbf{D}^\rho)$ satisfies

$$\Delta z^\rho=0 \quad \text{in } \Omega,$$

$$\lambda^2\,\text{curl}^2\,\mathbf{D}^\rho=\{2(\nabla v^\rho-\mathbf{B}^\rho)+\rho(\nabla z^\rho-\mathbf{D}^\rho)\}\chi_\Omega \quad \text{in } \mathbb{R}^3, \quad \mathbf{D}^\rho\in\mathbf{D}^{1,2}(\mathbb{R}^3,\text{div}), \tag{3.16}$$

$$\frac{\partial z^\rho}{\partial \nu}=\mathbf{D}^\rho\cdot\nu \quad \text{on } \partial\Omega.$$

We compute

$$\frac{\partial f}{\partial \rho}(a,\rho)=1+2a^2\fint_\Omega(\nabla w^\rho-\mathbf{A}^\rho)\cdot(\nabla v^\rho-\mathbf{B}^\rho)\,dx,$$

$$\frac{\partial^2 f}{\partial \rho^2}(a,\rho)=2a^2\fint_\Omega\{|\nabla v^\rho-\mathbf{B}^\rho|^2+(\nabla w^\rho-\mathbf{A}^\rho)\cdot(\nabla z^\rho-\mathbf{D}^\rho)\}\,dx.$$

Multiplying (3.15) and (3.16) by $\mathbf{D}^\rho$ and $\mathbf{B}^\rho$, respectively, and integrating, we find

$$\begin{aligned}0&=\int_\Omega\{\mathbf{D}^\rho[(\nabla w^\rho-\mathbf{A}^\rho)+\rho(\nabla v^\rho-\mathbf{B}^\rho)]-\mathbf{B}^\rho[2(\nabla v^\rho-\mathbf{B}^\rho)+\rho(\nabla z^\rho-\mathbf{D}^\rho)]\}dx\\&=\int_\Omega\{-(\nabla w^\rho-\mathbf{A}^\rho)\cdot(\nabla z^\rho-\mathbf{D}^\rho)+2|\nabla v^\rho-\mathbf{B}^\rho|^2+\rho(\mathbf{D}^\rho\cdot\nabla v^\rho-\mathbf{B}^\rho\cdot\nabla z^\rho)\}dx.\end{aligned}$$

Here we have used the fact

$$\int_\Omega\nabla z^\rho\cdot(\nabla w^\rho-\mathbf{A}^\rho)\,dx=0, \quad \int_\Omega\nabla v^\rho\cdot(\nabla v^\rho-\mathbf{B}^\rho)\,dx=0.$$

Now, since $\Delta v^\rho=0$, $\Delta z^\rho=0$, $\text{div}\,\mathbf{B}^\rho=0$ and $\text{div}\,\mathbf{D}^\rho=0$ in Ω, $\partial v^\rho/\partial\nu=\mathbf{B}^\rho\cdot\nu$ and $\partial z^\rho/\partial\nu=\mathbf{D}^\rho\cdot\nu$ on $\partial\Omega$, we have

$$\begin{aligned}\int_\Omega(\mathbf{D}^\rho\cdot\nabla v^\rho-\mathbf{B}^\rho\cdot\nabla z^\rho)\,dx&=\int_\Omega\text{div}(v^\rho\mathbf{D}^\rho-z^\rho\mathbf{B}^\rho)\,dx\\&=\int_{\partial\Omega}(v^\rho\mathbf{D}^\rho-z^\rho\mathbf{B}^\rho)\cdot\nu\,dS\\&=\int_{\partial\Omega}\left(v^\rho\frac{\partial z^\rho}{\partial\nu}-z^\rho\frac{\partial v^\rho}{\partial\nu}\right)dS\\&=\int_\Omega\text{div}(v^\rho\nabla z^\rho-z^\rho\nabla v^\rho)\,dx=0.\end{aligned}$$

Thus

$$\int_\Omega (\nabla w^\rho - \mathbf{A}^\rho)\cdot(\nabla z^\rho - \mathbf{D}^\rho)\,dx = 2\int_\Omega |\nabla v^\rho - \mathbf{B}^\rho|^2\,dx.$$

Also note that

$$\int_\Omega \nabla v^\rho \cdot (\nabla w^\rho - \mathbf{A}^\rho)\,dx = 0.$$

Hence $f(a,\rho)$ is a C^2 function for $a>0$ and $\rho>0$, and

$$\begin{aligned} \frac{\partial f}{\partial \rho}(a,\rho) &= 1 - 2a^2 \fint_\Omega (\nabla w^\rho - \mathbf{A}^\rho)\cdot \mathbf{B}^\rho\,dx, \\ \frac{\partial^2 f}{\partial \rho^2}(a,\rho) &= 6a^2 \fint_\Omega |\nabla v^\rho - \mathbf{B}^\rho|^2\,dx > 0. \end{aligned} \tag{3.17}$$

Recall that $\mathbf{A}^0 = \mathbf{F_h}$ and $w^0 = w_{\mathbf{h}}$. We can define $(v^0,\mathbf{B}^0)$ and $(z^0,\mathbf{D}^0)$ using the equations (3.15) and (3.16) for $\rho=0$. Then we have $\mathbf{B}^0 = (1/\lambda^2)\mathbf{U_h}$. We compute $f(a,0)$ and the one-sided derivatives at $\rho=0$,

$$\begin{aligned} f(a,0) &= a^2 \fint_\Omega |\nabla w_{\mathbf{h}} - \mathbf{F_h}|^2\,dx = a^2\omega(\mathbf{h}), \\ \frac{\partial f}{\partial \rho}(a,0^+) &= 1 - a^2\omega(\mathbf{h})\frac{\lambda(\mathbf{h})^2}{\lambda^2}, \\ \frac{\partial^2 f}{\partial \rho^2}(a,0^+) &= 6a^2 \fint_\Omega |\nabla v^0 - \mathbf{B}^0|^2\,dx > 0. \end{aligned} \tag{3.18}$$

In fact,

$$\begin{aligned} \frac{\partial f}{\partial \rho}(a,0^+) &= 1 + 2a^2 \fint_\Omega (\nabla w^0 - \mathbf{A}^0)\cdot(\nabla v^0 - \mathbf{B}^0)\,dx \\ &= 1 - \frac{2a^2}{\lambda^2|\Omega|}\int_\Omega (\nabla w_{\mathbf{h}} - \mathbf{F_h})\cdot \mathbf{U_h}\,dx \\ &= 1 - \frac{2a^2}{\lambda^2|\Omega|}\|\operatorname{curl}\mathbf{U_h}\|^2_{L^2(\mathbb{R}^3)} = 1 - a^2\omega(\mathbf{h})\frac{\lambda(\mathbf{h})^2}{\lambda^2}. \end{aligned}$$

Step 2. We show that, for any $\lambda>0$ and $0<a<a(\mathbf{h})$, there exists a unique ρ, $0<\rho<1$, such that (3.12) holds. Note that $f(a,1)>1$ for all $a>0$, and $f(a,0) = a^2\omega(\mathbf{h}) < 1$ for $0<a<a(\mathbf{h})$. Thus there exists $\rho=\rho(a)$, $0<\rho(a)<1$, such that $f(a,\rho(a))=1$. Suppose that for some $0<a<a(\mathbf{h})$, the equation $f(a,\rho)=1$ has two positive roots. Since $f(a,0)<1$ and $f(a,+\infty)=+\infty$, the equation must have one more root. Thus $f(a,\cdot)$ must have a local maximum point. But this is impossible since $(\partial^2 f/\partial\rho^2)(a,\rho)>0$ for all $\rho>0$. Thus (3.12) has exactly one positive root $\rho=\rho(a)$.

Obviously $\lim_{a\to 0^+}\rho(a)=1$. We prove

$$\frac{\partial f}{\partial \rho}(a,\rho(a)) > 0. \tag{3.19}$$

Since $f(a,0)<1$ and $f(a,\infty)=\infty$, the uniqueness of $\rho(a)$ implies that $(\partial f/\partial\rho)(a,\rho(a))\geqslant 0$. Suppose $(\partial f/\partial\rho)(a,\rho(a))=0$. Then (3.17) implies that $\rho(a)$ is a strictly local minimum point. So there exists a positive number $\rho_1<\rho(a)$ such that $f(a,\rho_1)>f(a,\rho(a))=1$. Since $f(a,0)<1$, there must exist another positive number $\rho_2<\rho_1$ such that $f(a,\rho_2)=1$, which contradicts the uniqueness of $\rho(a)$. So (3.19) is true.

Applying the implicit function theorem to the equation $f(a,\rho)=0$, we conclude that $\rho(a)$ is a differentiable function for $0<a<a(\mathbf{h})$, and

$$\frac{\partial f}{\partial a}(a,\rho(a))+\frac{\partial f}{\partial\rho}(a,\rho(a))\rho'(a)=0,$$

namely

$$2a\int_\Omega|\nabla w^{\rho(a)}-\mathbf{A}^{\rho(a)}|^2\,dx+\frac{\partial f}{\partial\rho}(a,\rho(a))\rho'(a)=0.$$

From this and (3.19) we see that $\rho'(a)<0$. Thus $\rho(a)$ is strictly decreasing for $a\in(0,a(\mathbf{h}))$.

Step 3. Assume $\lambda\geqslant\lambda(\mathbf{h})$. We prove (3.13).

Case 3.1: $0<a<a(\mathbf{h})$. The couclusion has been proved in step 2.

Case 3.2: $a=a(\mathbf{h})$. From (3.8), $f(a(\mathbf{h}),0)=1$, $(\partial f/\partial\rho)(a(\mathbf{h}),0^+)\geqslant 0$ and $(\partial^2 f/\partial\rho^2)\times(a(\mathbf{h}),\rho)>0$. Hence (3.12) has no positive solutions, and $\lim_{a\to a(\mathbf{h})^-}\rho(a)=\rho(a(\mathbf{h}))=0$. We define $\rho(a(\mathbf{h}))=0$.

Case 3.3: $\lambda>\lambda(\mathbf{h})$ and $a(\mathbf{h})<a\leqslant[\lambda/\lambda(\mathbf{h})]a(\mathbf{h})$. Then $f(a,0)>1$, $(\partial f/\partial\rho)(a,0^+)\geqslant 0$ and $(\partial^2 f/\partial\rho^2)(a,\rho)>0$. Hence (3.12) has no non-negative solutions.

Case 3.4: $a>[\lambda/\lambda(\mathbf{h})]a(\mathbf{h})$. Then $f(a,0)>1$, $(\partial f/\partial\rho)(a,0^+)<0$, $(\partial^2 f/\partial\rho^2)(a,\rho)>0$. To show that (3.12) has no non-negative solutions, we prove that

$$\min_{\rho\geqslant 0} f(a,\rho)>1.$$

Suppose the minimum is less than 1. Since $f(a,+\infty)=+\infty$, the minimum is achieved at $\rho_0\geqslant 0$, $f(a,\rho_0)\leqslant 1$. Then $\rho_0<1$. For $0<a'<a$ we have $f(a',\rho_0)<f(a,\rho_0)\leqslant 1$. Especially $f(a(\mathbf{h}),\rho_0)<f(a,\rho_0)\leqslant 1$, which is impossible. (3.13) is proved.

Step 4. Assume $0<\lambda<\lambda(\mathbf{h})$. We shall show that there exists $C(\lambda)>0$ such that (3.14) holds.

Case 4.1: $0<a<a(\mathbf{h})$. The conclusion has been proved in step 2.

Case 4.2: $a=a(\mathbf{h})$. From (3.18), $f(a(\mathbf{h}),0)=1$, $(\partial f/\partial\rho)(a(\mathbf{h}),0^+)<0$ and $(\partial^2 f/\partial\rho^2)\times(a(\mathbf{h}),\rho)>0$. Hence, beside the zero solution, (3.12) has a unique positive solution $\rho(a(\mathbf{h}))>0$.

Case 4.3: $a>a(\mathbf{h})$. Then $f(a,0)>1$ and $(\partial f/\partial\rho)(a,0^+)=1-a^2\omega(\mathbf{h})[\lambda(\mathbf{h})^2/\lambda^2]$. There exists $\delta>0$ sufficiently small such that, for $a(\mathbf{h})<a<a(\mathbf{h})+\delta$ and $0<\rho<\delta$:

$$f(a,\rho)=f(a,0)+\frac{\partial f}{\partial\rho}(a,0^+)\rho+O(\rho^2)=a^2\omega(\mathbf{h})+\left(1-a^2\omega(\mathbf{h})\frac{\lambda(\mathbf{h})^2}{\lambda^2}\right)\rho+O(\rho^2).$$

For small $\rho>0$, if we choose a_ρ such that $a_\rho^2\omega(\mathbf{h})=1+c\rho$, where $0<c<[\lambda(\mathbf{h})^2/\lambda^2]-1$, then

$$f(a_\rho,\rho)-1=-\left(\frac{\lambda_h^2}{\lambda^2}-1-c\right)\rho+O(\rho^2)<0.$$

Hence if a is sufficiently close to $a(\mathbf{h})$, we have $\min_{\rho\geqslant 0}f(a,\rho)<1$; and since $f(a,0)>1$ and $(\partial^2 f/\partial\rho^2)(a,\rho)>0$, (3.12) has exactly two positive solutions.

Note that if $\min_{\rho\geqslant 0}f(a_0,\rho)<1$ for some $a_0>0$, then $\min_{\rho\geqslant 0}f(a,\rho)<1$ for all $0<a<a_0$. Also note that

$$\min_{\rho\geqslant 0} f(a,\rho)\geqslant \min\{1,\ a^2 m_0\},\quad \text{where } m_0=\min_{0\leqslant\rho\leqslant 1}\int\!\!\!\!\!\!-_{\Omega}|\nabla w^{\rho}-\mathbf{A}^{\rho}|^2\,dx>0.$$

Thus there exists $C(\lambda)$, $a(\mathbf{h})<C(\lambda)<+\infty$, such that

$$\min_{\rho\geqslant 0} f(a,\rho)\begin{cases}<1 & \text{if } a(\mathbf{h})<a<C(\lambda),\\ =1 & \text{if } a=C(\lambda),\\ >1 & \text{if } a>C(\lambda).\end{cases}$$

So (3.14) is true. □

Remark 3.6: When $\lambda\geqslant\lambda(\mathbf{h})$ and $0<a<a(\mathbf{h})$, we write

$$\mathbf{A}_a=\mathbf{A}^{\rho(a)},\quad \mathbf{B}_a=\mathbf{B}^{\rho(a)},\quad c_a=\sqrt{\rho(a)},\quad v_a=v^{\rho(a)},\quad w_a=w^{\rho(a)}. \tag{3.20}$$

$(w_a,\mathbf{A}_a,c_a)$ satisfies

$$\begin{gathered}\Delta w_a=0\quad \text{in } \Omega,\\ \lambda^2\,\mathrm{curl}^2\,\mathbf{A}_a=c_a^2(\nabla w_a-\mathbf{A}_a)\chi_{\Omega}\quad \text{in } \mathbb{R}^3,\quad \mathbf{A}_a-\mathbf{F}_{\mathbf{h}}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}),\\ \frac{\partial w_a}{\partial\nu}=\mathbf{A}_a\cdot\nu\quad \text{on } \partial\Omega,\\ a^2\int\!\!\!\!\!\!-_{\Omega}|\nabla w_a-\mathbf{A}_a|^2\,dx+c_a^2=1,\end{gathered} \tag{3.21}$$

and $(v_a,\mathbf{B}_a)$ satisfies

$$\begin{gathered}\Delta v_a=0\quad \text{in } \Omega,\\ \lambda^2\,\mathrm{curl}^2\,\mathbf{B}_a=\{(\nabla w_a-\mathbf{A}_a)+c_a^2(\nabla v_a-\mathbf{B}_a)\}\chi_{\Omega}\quad \text{in } \mathbb{R}^3,\quad \mathbf{B}_a\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}),\\ \frac{\partial v_a}{\partial\nu}=\mathbf{B}_a\cdot\nu\quad \text{on } \partial\Omega.\end{gathered} \tag{3.22}$$

Using (3.17) and (3.19) we find

$$\int_{\Omega}(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{B}_a\,dx=\lambda^2\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{B}_a|^2\,dx+c_a^2\int_{\Omega}|\nabla v_a-\mathbf{B}_a|^2\,dx<\frac{|\Omega|}{2a^2}. \tag{3.23}$$

Lemma 3.7: (i) Fix $\lambda>\lambda(\mathbf{h})$. *We have, as* $a\to a(\mathbf{h})^-$,

$$c_a^2=\frac{\lambda^2}{\lambda^2-\lambda(\mathbf{h})^2}(1-a^2\omega(\mathbf{h}))+O((1-a^2\omega(\mathbf{h}))^2). \tag{3.24}$$

(ii) If $\lambda=\lambda(\mathbf{h})$, *we have, as* $a\to a(\mathbf{h})^-$,

$$c_a^2=\left\{\frac{\sqrt{\omega(\mathbf{h})|\Omega|}}{\sqrt{3}\left\|\nabla v^0-\dfrac{1}{\lambda^2}\mathbf{U}_{\mathbf{h}}\right\|_{L^2(\Omega)}}+o(1)\right\}\sqrt{1-a^2\omega(\mathbf{h})}. \tag{3.25}$$

Proof: From Lemma 3.5, for any $0<\rho<1$, (3.12) determines a unique number a such that $\rho=c_a^2$. Recall that $\mathbf{B}^0=(1/\lambda^2)\mathbf{U_h}$. As in the proof of Lemma 3.5 (Step 1), we compute the one-sided derivatives at $\rho=0$:

$$\begin{aligned}\left.\frac{d}{d\rho}\right|_{\rho=0^+}\int_\Omega|\nabla w^\rho-\mathbf{A}^\rho|^2\,dx&=-\frac{\lambda(\mathbf{h})^2}{\lambda^2}\omega(\mathbf{h})|\Omega|,\\ \left.\frac{d^2}{d\rho^2}\right|_{\rho=0^+}\int_\Omega|\nabla w^\rho-\mathbf{A}^\rho|^2\,dx&=6\int_\Omega\left|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U_h}\right|^2dx.\end{aligned}\tag{3.26}$$

Thus for $\rho>0$ small,

$$\int_\Omega|\nabla w^\rho-\mathbf{A}^\rho|^2\,dx=\omega(\mathbf{h})|\Omega|-\frac{\lambda(\mathbf{h})^2}{\lambda^2}\omega(\mathbf{h})|\Omega|\rho+3\rho^2\int_\Omega\left|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U_h}\right|^2dx+o(\rho^2).$$

Recall that, when $\lambda\geqslant\lambda(\mathbf{h})$, $\rho(a)\to0$ as $a\to a(\mathbf{h})^-$. Letting $\rho=\rho(a)$ and plugging it into (3.12) yields

$$\rho(a)=1-a^2\omega(\mathbf{h})+\frac{a^2\omega(\mathbf{h})\rho(a)\lambda(\mathbf{h})^2}{\lambda^2}-\frac{3a^2\rho(a)^2}{|\Omega|}\left\|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U_h}\right\|^2_{L^2(\Omega)}+o(\rho(a)^2).\tag{3.27}$$

When $\lambda>\lambda(\mathbf{h})$, (3.24) follows from (3.27). When $\lambda=\lambda(\mathbf{h})$, (3.27) reads

$$(1-\rho(a))(1-a^2\omega(\mathbf{h}))=\frac{3a^2\rho(a)^2}{|\Omega|}\left\|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U_h}\right\|^2_{L^2(\Omega)}+o(\rho(a)^2).$$

So

$$\rho(a)=\frac{\sqrt{\omega(\mathbf{h})|\Omega|}}{\sqrt{3}\left\|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U_h}\right\|_{L^2(\Omega)}}(1+o(1))\sqrt{1-a^2\omega(\mathbf{h})}.$$

□

Remark 3.8: For the functional $\mathcal{J}_\rho$ defined above, we have

$$\begin{aligned}\frac{d}{d\rho}\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]&=\int_\Omega|\nabla w^\rho-\mathbf{A}^\rho|^2\,dx+2\lambda^2\int_{\mathbb{R}^3}(\operatorname{curl}\mathbf{A}^\rho-\mathbf{h})\cdot\operatorname{curl}\mathbf{B}^\rho\,dx\\&\quad+2\rho\int_\Omega(\nabla w^\rho-\mathbf{A}^\rho)\cdot(\nabla v^\rho-\mathbf{B}^\rho)dx\\&=\int_\Omega|\nabla w^\rho-\mathbf{A}^\rho|^2\,dx.\end{aligned}$$

We compute the one-sided derivatives of $\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]$ at $\rho=0$,

$$\left.\frac{d}{d\rho}\right|_{\rho=0^+}\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]=\int_\Omega|\nabla w^0-\mathbf{A}^0|^2\,dx=\omega(\mathbf{h})|\Omega|,$$

$$\left.\frac{d^2}{d\rho^2}\right|_{\rho=0^+}\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]=-2\int_\Omega(\nabla w^0-\mathbf{A}^0)\cdot\mathbf{B}^0\,dx=-\frac{\lambda(\mathbf{h})^2}{\lambda^2}\omega(\mathbf{h})|\Omega|, \tag{3.28}$$

$$\left.\frac{d^3}{d\rho^3}\right|_{\rho=0^+}\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]=6\int_\Omega\left|\nabla v^0-\frac{1}{\lambda^2}\mathbf{U}_\mathbf{h}\right|^2 dx.$$

These results will be needed in Sec. IV.

IV. ASYMPTOTIC BEHAVIOR OF MINIMIZERS FOR SMALL μ

In this section we consider a superconductor with small μ, and subjected to an applied field $\mathbf{H}=\sigma\mathbf{h}$, where $\mathbf{h}$ is a unit vector. We shall estimate the value of $H_c(\mathbf{h},\mu,\kappa)$, and examine the behavior of the minimal solutions of (1.5).

We first consider the case where $\kappa=\lambda\sqrt{\mu}$. To describe the behavior of the minimizers we need $\mathbf{A}_a$, w_a, c_a [see (3.21)], $\mathbf{B}_a$, v_a [see (3.22)], and u_a which is the unique solution of the equation

$$\begin{aligned}&\Delta u=|\mathbf{A}_a|^2-2\mathbf{A}_a\cdot\nabla w_a-\frac{1}{a^2}(1-c_a^2)\quad\text{in }\Omega,\\ &\frac{\partial u}{\partial\nu}=-w_a\mathbf{A}_a\cdot\nu\quad\text{on }\partial\Omega,\qquad\int_\Omega u\,dx=0.\end{aligned} \tag{4.1}$$

Let

$$b_a=2a^2c_a^2\frac{\int_\Omega w_a\mathbf{A}_a\cdot(\nabla v_a-\mathbf{B}_a)dx}{1-2a^2\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{B}_a\,dx}.$$

Theorem 4.1: *Let* $\mathbf{h}$ *be a unit vector,* $\lambda\geqslant\lambda(\mathbf{h})$, *and* $\kappa=\lambda\sqrt{\mu}$.
(i) As $\mu\to0$,

$$H_c(\mathbf{h},\mu,\lambda\sqrt{\mu})=a(\mathbf{h})\sqrt{\mu}+\begin{cases}O(\mu^{3/2}) & \text{if } \lambda>\lambda(\mathbf{h}),\\ o(\sqrt{\mu}) & \text{if } \lambda=\lambda(\mathbf{h}).\end{cases}$$

(ii) Assume $\sigma=a\sqrt{\mu}$, *where* a *is fixed and* $0<a<a(\mathbf{h})$. *Let* $(\psi_\mu,\mathbf{A}_\mu)$ *be a minimal solution of (1.5) for* $\kappa=\lambda\sqrt{\mu}$. *Then we have, as* $\mu\to0$,

$$\begin{aligned}&\psi_\mu=c_\mu[1+ia\sqrt{\mu}w_a+a^2\mu(u_a+ib_av_a)+o(\mu)],\\ &\mathbf{A}_\mu=\mathbf{A}_a+ab_a\sqrt{\mu}\mathbf{B}_a+o(\sqrt{\mu}),\\ &|c_\mu|^2=c_a^2+ab_a\mu+o(\mu).\end{aligned} \tag{4.2}$$

(iii) Assume $\sigma=a_\mu\sqrt{\mu}<H_c(\mathbf{h},\mu,\lambda\sqrt{\mu})$, *where* $a_\mu\to a(\mathbf{h})$ *as* $\mu\to0$. *The minimizer* $(\psi_\mu,\mathbf{A}_\mu)$ *has the expansions*

$$\begin{aligned}&\psi_\mu=l_\mu[1+ia_\mu\sqrt{\mu}w_\mathbf{h}+a_\mu^2\mu(u_\mu+iv_\mu)],\\ &\mathbf{A}_\mu=\mathbf{F}_\mathbf{h}+\frac{|l_\mu|^2}{\lambda^2}[\mathbf{U}_\mathbf{h}+o(1)],\end{aligned} \tag{4.3}$$

where u_μ *and* v_μ *are real-valued functions,* $\|u_\mu\|_{C^{2+\alpha}(\bar{\Omega})}$ *is bounded, and* $l_\mu \to 0$ *as* $\mu \to 0$. *Moreover, if* $\lambda > \lambda(\mathbf{h})$, *there exists a constant* $c(\lambda) > 0$ *such that, for all small* μ,

$$c(\lambda)|l_\mu|^2 + \mu \|\nabla v_\mu\|^2_{L^2(\Omega)} \leqslant C\mu + \left[1 - \left(\frac{a_\mu}{a(\mathbf{h})}\right)^2\right]. \tag{4.4}$$

Proof: Write $\epsilon = \sqrt{\mu}$ and $\kappa = \lambda\epsilon$. Let $\sigma = a\sqrt{\mu} = a\epsilon$. The functional $\mathcal{G}$ is written as

$$\mathcal{G}[\psi, \mathbf{A}] = \int_\Omega \{|\nabla_{a\epsilon\mathbf{A}}\psi|^2 + (\epsilon^2/2)(1 - |\psi|^2)^2\} dx + a^2\lambda^2\epsilon^2 \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{A} - \mathbf{h}|^2 \, dx.$$

Rewrite (1.5) as follows:

$$\begin{gathered} -\nabla^2_{a\epsilon\mathbf{A}}\psi = \epsilon^2(1 - |\psi|^2)\psi \quad \text{in } \Omega, \\ a\epsilon\lambda^2 \operatorname{curl}^2 \mathbf{A} = \Im\{\bar{\psi}\nabla_{a\epsilon\mathbf{A}}\psi\}\chi_\Omega \quad \text{in } \mathbb{R}^3, \\ (\nabla_{a\epsilon\mathbf{A}}\psi)\cdot\nu = 0, \quad [\nu\cdot\mathbf{A}] = 0, \quad [\nu \times \operatorname{curl}\mathbf{A}] = 0 \quad \text{on } \partial\Omega, \\ \operatorname{curl}\mathbf{A} \to \mathbf{h} \quad \text{as } |x| \to \infty. \end{gathered} \tag{4.5}$$

Step 1. We shall show that there exists $L > 0$ independent of $\mathbf{h}$ such that

$$H_c(\mathbf{h}, \epsilon^2, \lambda\epsilon) \geqslant a(\mathbf{h})\epsilon - L\epsilon^2. \tag{4.6}$$

We shall also look for an estimate for the energy of the minimal solutions [see (4.9) below], which is useful in the proof of (4.2).

Step 1.1. Let a be fixed, $0 < a < a(\mathbf{h})$. Then $\mathbf{A}_a$, w_a, c_a, $\mathbf{B}_a$, u_a, v_a are well defined. Let us choose a test field $(\phi^\epsilon, \mathbf{A}^\epsilon)$ by

$$\phi^\epsilon = c_a[1 + ia\epsilon w_a + a^2\epsilon^2(u_a + ib_a v_a)], \quad \mathbf{A}^\epsilon = \mathbf{A}_a + ab_a\epsilon\mathbf{B}_a,$$

where b_a is the number given in the beginning of this section. Computations show that

$$\mathcal{G}[\phi^\epsilon, \mathbf{A}^\epsilon] \leqslant I_a\epsilon^2 + M_a\epsilon^4 + O(\epsilon^5),$$

where

$$I_a = \frac{|\Omega|}{2}(1 - c_a^2)^2 + a^2\{c_a^2\|\nabla w_a - \mathbf{A}_a\|^2_{L^2(\Omega)} + \lambda^2\|\operatorname{curl}\mathbf{A}_a - \mathbf{h}\|^2_{L^2(\mathbb{R}^3)}\},$$

$$\begin{aligned} M_a = {} & a^4c_a^2[\|\nabla u_a\|^2_{L^2(\Omega)} + \|w_a\mathbf{A}_a\|^2_{L^2(\Omega)}] - 2a^2c_a^2(1 - c_a^2)\|w_a\|^2_{L^2(\Omega)} \\ & - 2a^6c_a^4|\Omega| \frac{[\int_\Omega w_a\mathbf{A}_a\cdot(\nabla v_a - \mathbf{B}_a)dx]^2}{1 - 2a^2\int_\Omega(\nabla w_a - \mathbf{A}_a)\cdot\mathbf{B}_a \, dx}. \end{aligned}$$

We claim that

$$I_a < \frac{|\Omega|}{2} \quad \text{if } \lambda \geqslant \lambda(\mathbf{h}) \quad \text{and } 0 < a < a(\mathbf{h}). \tag{4.7}$$

To prove (4.7), we introduce

$$F(a, \rho) = \frac{|\Omega|}{2}(1 - \rho)^2 + a^2\mathcal{J}_\rho[w^\rho, \mathbf{A}^\rho].$$

Note that $I_a = F(a,\rho(a))$. When $\lambda \geqslant \lambda(\mathbf{h})$, $0<a<a(\mathbf{h})$, and $0<\rho<\rho(a)$, from Remark 3.8 we have

$$\frac{\partial F}{\partial \rho}(a,\rho) = |\Omega|\left\{ \rho - 1 + a^2 \fint_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \, dx \right\} = |\Omega|[f(a,\rho)-1] < 0.$$

Hence $I_a = F(a,\rho(a)) < F(a,0) = |\Omega|/2$, and (4.7) is true.

From (4.7) we find that, for fixed $0<a<a(\mathbf{h})$, $\mathcal{G}[\phi^\epsilon, \mathbf{A}^\epsilon] < |\Omega|\epsilon^2/2$ for all small ϵ, and hence the minimizers of $\mathcal{G}$ are nontrivial.

Step 1.2. Next we assume a depends on ϵ,

$$a = a(\mathbf{h}) - L\epsilon^2, \tag{4.8}$$

where $L>0$ is independent of ϵ. Then

$$1 - a^2\omega(\mathbf{h}) = 2L\sqrt{\omega(\mathbf{h})}\,\epsilon^2 + O(\epsilon^4).$$

Case 1: $\lambda > \lambda(\mathbf{h})$. For the function $F(a,\rho)$ given above, we compute the one-side derivatives, and use (3.18), (3.28) to get

$$\frac{\partial F}{\partial a}(a,\rho) = 2a\mathcal{J}_\rho[w^\rho, \mathbf{A}^\rho], \quad \frac{\partial F}{\partial \rho}(a,\rho) = |\Omega|[f(a,\rho)-1],$$

$$\frac{\partial F}{\partial a}(a(\mathbf{h}),0^+) = 0, \quad \frac{\partial F}{\partial \rho}(a(\mathbf{h}),0^+) = 0, \quad \frac{\partial^2 F}{\partial a^2}(a(\mathbf{h}),0^+) = 0,$$

$$\frac{\partial^2 F}{\partial a \partial \rho}(a(\mathbf{h}),0^+) = 2|\Omega|\sqrt{\omega(\mathbf{h})}, \quad \frac{\partial^2 F}{\partial \rho^2}(a(\mathbf{h}),0^+) = |\Omega|\left[1 - \left(\frac{\lambda(\mathbf{h})}{\lambda}\right)^2\right].$$

From (2.4) and (3.24) we have

$$\rho(a) = \frac{\lambda^2}{\lambda^2 - \lambda(\mathbf{h})^2}\left(1 - \frac{a^2}{a(\mathbf{h})^2}\right) + O((a(\mathbf{h})-a)^2) = \frac{2\lambda^2\sqrt{\omega(\mathbf{h})}(a(\mathbf{h})-a)}{\lambda^2 - \lambda(\mathbf{h})^2} + O((a(\mathbf{h})-a)^2).$$

Using the Taylor expansion we find that, for a slightly less that $a(\mathbf{h})$,

$$\begin{aligned} I_a - \frac{|\Omega|}{2} &= F(a,\rho(a)) - F(a(\mathbf{h}),0) \\ &= \frac{|\Omega|}{2}\rho(a)\left\{ 4\sqrt{\omega(\mathbf{h})}(a-a(\mathbf{h})) + \left[1 - \left(\frac{\lambda(\mathbf{h})}{\lambda}\right)^2\right]\rho(a)\right\} + o((a(\mathbf{h})-a)^2 + \rho(a)^2) \\ &= -|\Omega|\sqrt{\omega(\mathbf{h})}\rho(a)(a(\mathbf{h})-a) + o((a(\mathbf{h})-a)^2). \end{aligned}$$

Using this and (4.8), and noting that $M_a \leqslant M^0 c_a^2 = M^0\rho(a)$, we find

$$I_a + M_a\epsilon^2 \leqslant \frac{|\Omega|}{2} - \rho(a)\epsilon^2\{|\Omega|\sqrt{\omega(\mathbf{h})}L - M^0\} + o(\epsilon^2).$$

Choose L so that $|\Omega|\sqrt{\omega(\mathbf{h})}L > 3M^0$. Then for all small $\epsilon>0$ we have

$$\mathcal{G}[\phi^\epsilon, \mathbf{A}^\epsilon] \leqslant \frac{|\Omega|}{2}\epsilon^2 - \frac{|\Omega|}{2}\sqrt{\omega(\mathbf{h})}L\rho(a)\epsilon^4.$$

So the minimizers of $\mathcal{G}$ are nontrivial. Equation (4.6) is proved for $\lambda>\lambda(\mathbf{h})$.

Case 2: $\lambda=\lambda(\mathbf{h})$. From (3.28) we have, for small $\rho>0$,

$$\mathcal{J}_p[w^\rho,\mathbf{A}^\rho]=\omega(\mathbf{h})|\Omega|\rho-\frac{1}{2}\omega(\mathbf{h})|\Omega|\rho^2+\left\|\nabla v^0-\frac{1}{\lambda(\mathbf{h})^2}\mathbf{U}_\mathbf{h}\right\|^2_{L^2(\Omega)}\rho^3+o(\rho^3).$$

From this, (3.25) and (4.8),

$$\begin{aligned}I_a&=\frac{|\Omega|}{2}(1-\rho(a))^2+a^2\mathcal{J}_{\rho(a)}[w^{\rho(a)},\mathbf{A}^{\rho(a)}]\\&=|\Omega|\left\{\frac{1}{2}-(1-a^2\omega(\mathbf{h}))\rho(a)+\frac{\rho(a)^2}{2}(1-a^2\omega(\mathbf{h}))\right.\\&\quad\left.+\frac{a^2\omega(\mathbf{h})\rho(a)}{3}(1-a^2\omega(\mathbf{h}))\right\}+o(\rho(a)^3),\end{aligned}$$

$$\begin{aligned}\frac{I_a+M_a\epsilon^2-\frac{|\Omega|}{2}}{|\Omega|\rho(a)}&\leqslant-(1-a^2\omega(\mathbf{h}))\left(1-\frac{\rho(a)}{2}\right)+\frac{1}{3}(1-a^2\omega(\mathbf{h}))+\frac{M^0}{|\Omega|}\epsilon^2+o(1-a^2\omega(\mathbf{h}))\\&=-\left(\frac{2}{3}+o(1)\right)(1-a^2\omega(\mathbf{h}))+\frac{M^0}{|\Omega|}\epsilon^2=-\left(\frac{4}{3}L\sqrt{\omega(\mathbf{h})}-\frac{M^0}{|\Omega|}+o(1)\right)\epsilon^2.\end{aligned}$$

Choosing L large we find

$$I_a+M_a\epsilon^2\leqslant\frac{|\Omega|}{2}-\frac{|\Omega|}{2}L\sqrt{\omega(\mathbf{h})}\rho(a)\epsilon^2.$$

Thus $\mathcal{G}[\phi^\epsilon,\mathbf{A}^\epsilon]<|\Omega|\epsilon^2/2$ for all small ϵ, and hence the minimizers are nontrivial. Equation (4.6) is proved for $\lambda=\lambda(\mathbf{h})$.

Step 2. Proof of conclusion (ii): Fix a such that $0<a<a(\mathbf{h})$, and let $\sigma=a\epsilon$. From step 1 we know that (4.5) has a nontrivial minimal solution $(\psi_\epsilon,\mathbf{A}_\epsilon)$ satisfying $\operatorname{div}\mathbf{A}_\epsilon=0$ in $\mathbb{R}^3$ and $\int_\Omega\mathbf{A}_\epsilon\,dx=\mathbf{0}$, and we have an energy upper bound for small $\epsilon>0$:

$$C(\mathbf{h},\epsilon^2,\lambda\epsilon,a\epsilon)\leqslant I_a\epsilon^2+M_a\epsilon^4+C\epsilon^5,\tag{4.9}$$

where C is independent of ϵ. We shall show that ψ_ϵ and $\mathbf{A}_\epsilon$ have expansions as described in (4.2).

Step 2.1. Proof of the leading order terms: The energy estimate shows that $\{\mathbf{A}_\epsilon\}$ is bounded in $\mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div})$, and $\nabla\psi_\epsilon\to0$ as $\epsilon\to0$. Let $c_\epsilon=\fint_\Omega\psi_\epsilon\,dx$. Up to a gauge transform, we may assume that $c_\epsilon\to c^*$ as $\epsilon\to0$. Computing the energy $\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]$ and comparing it with the energy upper bound given in (4.9), we can show that $c^*\neq0$. Hence $c_\epsilon\neq0$ for all small ϵ, and thus we can write

$$\psi_\epsilon=c_\epsilon(1+a\epsilon\psi_{1,\epsilon}),\qquad\int_\Omega\psi_{1,\epsilon}\,dx=0.$$

From (4.5) we derive the equations for $(\psi_{1,\epsilon},\mathbf{A}_\epsilon)$,

$$-\Delta\psi_{1,\epsilon}+2ia\epsilon\mathbf{A}_\epsilon\cdot\nabla\psi_{1,\epsilon}+a\epsilon|\mathbf{A}_\epsilon|^2(1+a\epsilon\psi_{1,\epsilon})=\frac{\epsilon}{a}(1-|c_\epsilon(1+a\epsilon\psi_{1,\epsilon})|^2)(1+a\epsilon\psi_{1,\epsilon})\quad\text{in }\Omega,$$

$$\lambda^2\operatorname{curl}^2\mathbf{A}_\epsilon=|c_\epsilon|^2\Im\{\nabla\psi_{1,\epsilon}-i\mathbf{A}_\epsilon+\epsilon[a\overline{\psi}_{1,\epsilon}(\nabla\psi_{1,\epsilon}-i\mathbf{A}_\epsilon)-ia\psi_{1,\epsilon}\mathbf{A}_\epsilon]\}\chi_\Omega\quad\text{in }\mathbb{R}^3,$$

$$\frac{\partial \psi_{1,\epsilon}}{\partial \nu} = i(1 + a\epsilon\psi_{1,\epsilon})\mathbf{A}_\epsilon \cdot \nu \quad \text{on } \partial\Omega.$$

The equations are understood in the weak sense. As in Lemma 3.3 we can show that $\|\psi_{1,\epsilon}\|_{C^{2+\alpha}(\bar{\Omega})} \leqslant C$, $\|\mathbf{A}_\epsilon\|_{C^{1+\alpha}(\bar{\Omega})} \leqslant C$, and $\{\mathbf{A}_\epsilon\}$ is bounded in $C^{2+\alpha}_{\text{loc}}(\mathbb{R}^3 \backslash \partial\Omega)$. Thus we can pass to a subsequence and assume that

$$\psi_{1,\epsilon} \to \psi^* \quad \text{in } C^{2+\alpha}(\bar{\Omega}), \quad \mathbf{A}_\epsilon \to \mathbf{A}^* \quad \text{in } C^{2+\alpha}_{\text{loc}}(\mathbb{R}^3 \backslash \partial\Omega) \cap C^{1+\alpha}(\bar{\Omega}) \quad \text{as } \epsilon \to 0,$$

and $(\psi^*, \mathbf{A}^*, c^*)$ satisfies the equations

$$\Delta \psi^* = 0 \quad \text{in } \Omega,$$

$$\lambda^2 \operatorname{curl}^2 \mathbf{A}^* = |c^*|^2 \Im\{\nabla \psi^* - i\mathbf{A}^*\}\chi_\Omega \quad \text{in } \mathbb{R}^3, \quad \mathbf{A}^* - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \text{div}), \tag{4.10}$$

$$\frac{\partial \psi^*}{\partial \nu} = i\mathbf{A}^* \cdot \nu \quad \text{on } \partial\Omega.$$

Note that $\int_\Omega \psi^* \, dx = 0$. The uniqueness of the finite energy solutions of (4.10) implies that $\psi^* = iw^*$ for some real-valued function w^*.

Introduce $\psi_{2,\epsilon}$ and $\mathbf{A}_{1,\epsilon}$ by

$$\psi_{1,\epsilon} = iw^* + a\epsilon\psi_{2,\epsilon}, \quad \mathbf{A}_\epsilon = \mathbf{A}^* + a\epsilon\mathbf{A}_{1,\epsilon}.$$

The equations for $(\psi_{2,\epsilon}, \mathbf{A}_{1,\epsilon})$ are

$$\Delta \psi_{2,\epsilon} = |\mathbf{A}^*|^2 - 2\mathbf{A}^* \nabla w^* - \frac{1}{a^2}(1 - |c_\epsilon|^2) + p_\epsilon \quad \text{in } \Omega,$$

$$\lambda^2 \operatorname{curl}^2 \mathbf{A}_{1,\epsilon} = \{b_\epsilon(\nabla w^* - \mathbf{A}^*) + |c_\epsilon|^2 \Im(\nabla \psi_{2,\epsilon} - i\mathbf{A}_{2,\epsilon} + \mathbf{q}_\epsilon)\}\chi_\Omega \quad \text{in } \mathbb{R}^3, \tag{4.11}$$

$$\frac{\partial \psi_{2,\epsilon}}{\partial \nu} = i\mathbf{A}_{1,\epsilon} \cdot \nu - w^* \mathbf{A}^* \cdot \nu + r_\epsilon \quad \text{on } \partial\Omega,$$

where

$$b_\epsilon = \frac{|c_\epsilon|^2 - |c^*|^2}{a\epsilon}, \tag{4.12}$$

and we have

$$\|p_\epsilon\|_{C^{1+\alpha}(\bar{\Omega})} + \|\mathbf{q}_\epsilon\|_{C^{1+\alpha}(\bar{\Omega})} + \|r_\epsilon\|_{C^{1+\alpha}(\partial\Omega)} \leqslant C\epsilon[1 + \|\psi_{2,\epsilon}\|_{C^{1+\alpha}(\bar{\Omega})} + \|\mathbf{A}_{1,\epsilon}\|_{C^{1+\alpha}(\bar{\Omega})}] = o(1).$$

Using the equation for w^* we have

$$\int_{\partial\Omega} w^* \mathbf{A}^* \cdot \nu \, dS = \int_{\partial\Omega} w^* \frac{\partial w^*}{\partial \nu} dS = \int_\Omega \text{div}(w^* \nabla w^*) dx = \int_\Omega |\nabla w^*|^2 \, dx.$$

Integrating the first equation in (4.11) yields

$$\int_\Omega \left\{ |\mathbf{A}^*|^2 - 2\mathbf{A}^* \cdot \nabla w^* - \frac{1}{a^2}(1 - |c_\epsilon|^2) + p_\epsilon \right\} dx = \int_{\partial\Omega} \{i\mathbf{A}_{1,\epsilon} \cdot \nu - w^* \mathbf{A}^* \cdot \nu + r_\epsilon\} dS.$$

Taking the real part of the equality we find

$$1-|c_\epsilon|^2=a^2\fint_\Omega|\nabla w^*-\mathbf{A}^*|^2\,dx+o(1).$$

Sending ϵ to zero we get

$$|c^*|^2=1-a^2\fint_\Omega|\nabla w^*-\mathbf{A}^*|^2\,dx.$$

Comparing this and (4.10) with (3.21) we find that

$$w^*=w_a,\quad \mathbf{A}^*=\mathbf{A}_a,\quad |c^*|=c_a. \tag{4.13}$$

Step 2.2. Proof of the correction terms. We need

Claim 1: $\{b_\epsilon\}$ *is bounded.*

The proof will be given in Appendix B. So we can pass to a subsequence and assume that $\lim_{\epsilon\to 0} b_\epsilon=b$. Now write

$$\psi_\epsilon=c_\epsilon(1+ia\epsilon w_a+a^2\epsilon^2\psi_{2,\epsilon}),\quad \mathbf{A}_\epsilon=\mathbf{A}_a+a\epsilon\mathbf{A}_{1,\epsilon}. \tag{4.14}$$

Applying the elliptic estimates to (4.11), we can pass to a subsequence again and assume that

$$\psi_{2,\epsilon}\to\psi_2=u_a+bv_a\quad\text{in } C^{2+\alpha}(\overline{\Omega}),\quad \mathbf{A}_{1,\epsilon}\to b\mathbf{B}_a\quad\text{in } C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)\quad\text{as } \epsilon\to 0. \tag{4.15}$$

In order to show $b=b_a$, we compute the energy of $(\psi_\epsilon,\mathbf{A}_\epsilon)$,

$$\begin{aligned}
\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]&=I_a\epsilon^2+\frac{\epsilon^2}{2}(|c_\epsilon|^2-c_a^2)^2|\Omega|-2a^3\epsilon^3(|c_\epsilon|^2-c_a^2)\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{A}_{1,\epsilon}\,dx\\
&\quad+a^4\epsilon^4\Big\{|c_\epsilon|^2\|\Re(\nabla\psi_{2,\epsilon})\|^2_{L^2(\Omega)}+|c_\epsilon|^2\|\Im(\nabla\psi_{2,\epsilon})-w_a\mathbf{A}_a-\mathbf{A}_{1,\epsilon}\|^2_{L^2(\Omega)}\\
&\quad+\lambda^2\|\operatorname{curl}\mathbf{A}_{1,\epsilon}\|^2_{L^2(\mathbb{R}^3)}-\frac{2}{a^2}|c_\epsilon|^2(1-|c_\epsilon|^2)\|w_a\|^2_{L^2(\Omega)}\Big\}+O(\epsilon^5)\\
&=I_a\epsilon^2+a^4b^2\epsilon^4\Big\{\frac{|\Omega|}{2a^2}-2\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{A}_{1,\epsilon}\,dx\\
&\quad+\lambda^2\|\operatorname{curl}\mathbf{A}_{1,\epsilon}\|^2_{L^2(\mathbb{R}^3)}+c_a^2\|\nabla v_a-\mathbf{B}_a\|^2_{L^2(\Omega)}\|\Big\}\\
&\quad+a^4c_a^2\epsilon^4\Big\{\|\nabla u_a\|^2_{L^2(\Omega)}+\|w_a\mathbf{A}_a\|^2_{L^2(\Omega)}-2b\int_\Omega w_a\mathbf{A}_a\cdot(\nabla v_a-\mathbf{B}_a)dx\Big\}\\
&\quad-2a^2c_a^2(1-c_a^2)\epsilon^4\|w_a\|^2_{L^2(\Omega)}+o(\epsilon^4)\\
&=I_a\epsilon^2+a^4b^2\epsilon^4\Big\{\frac{|\Omega|}{2a^2}-\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{B}_a\,dx\Big\}\\
&\quad+a^4c_a^2\epsilon^4\Big\{\|\nabla u_a\|^2_{L^2(\Omega)}+\|w_a\mathbf{A}_a\|^2_{L^2(\Omega)}-2b\int_\Omega w_a\mathbf{A}_a\cdot(\nabla v_a-\mathbf{B}_a)dx\Big\}\\
&\quad-2a^2c_a^2(1-c_a^2)\epsilon^4\|w_a\|^2_{L^2(\Omega)}+o(\epsilon^4)\\
&=I_a\epsilon^2+a^4\epsilon^4(\alpha b^2-2\beta b)+\gamma\epsilon^4+o(\epsilon^4)
\end{aligned}$$

$$=I_a\epsilon^2+\epsilon^4\left(\gamma-\frac{a^4\beta^2}{\alpha}\right)+a^4\epsilon^4\alpha\left(b-\frac{\beta}{\alpha}\right)^2+o(\epsilon^4),$$

where

$$\alpha=\frac{|\Omega|}{2a^2}-\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{B}_a\,dx>0,$$

$$\beta=c_a^2\int_\Omega w_a\mathbf{A}_a\cdot(\nabla v_a-\mathbf{B}_a)dx,$$

$$\gamma=a^4c_a^2[\|\nabla u_a\|^2_{L^2(\Omega)}+\|w_a\mathbf{A}_a\|^2_{L^2(\Omega)}]-2a^2c_a^2(1-c_a^2)\|w_a\|^2_{L^2(\Omega)}.$$

Comparing it with the energy upper bound estimate (4.9) we find $b=\beta/\alpha=b_a$, hence

$$\lim_{\epsilon\to0}\frac{|c_\epsilon|^2-c_a^2}{\epsilon}=ab_a.$$

From this, (4.14) and (4.15), we get the expansion formulas in (4.2). Conclusion (ii) is proved. Moreover, we have

$$\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]=I_a\epsilon^2+\epsilon^4\left(\gamma-\frac{a^4\beta^2}{\alpha}\right)+o(\epsilon^4)=I_a\epsilon^2+M_a\epsilon^4+o(\epsilon^4).$$

Step 3. We show that, if $\lambda\geqslant\lambda(\mathbf{h})$,

$$H_c(\mathbf{h},\epsilon^2,\lambda\epsilon)\leqslant a(\mathbf{h})\epsilon+o(\epsilon). \tag{4.16}$$

Let us choose a sequence $\{a_\epsilon\}$ such that $\sigma=\epsilon a_\epsilon<H_c(\mathbf{h},\epsilon^2,\lambda\epsilon)$, $a_\epsilon\to a$ as $\epsilon\to0$, where

$$a\geqslant a(\mathbf{h}). \tag{4.17}$$

So the functional $\mathcal{G}$ has a nontrivial minimizer $(\phi_\epsilon,\mathbf{A}_\epsilon)$. We shall show that we must have $a=a(\mathbf{h})$. Then (4.16) follows. We shall also show that $(\phi_\epsilon,\mathbf{A}_\epsilon)$ has expansions as given in (4.3).

Step 3.1. As in step 2, we have $\nabla\phi_\epsilon\to0$ as $\epsilon\to0$. Let $l_\epsilon=\int_\Omega\phi_\epsilon\,dx$. At moment we do not know yet whether $l_\epsilon\neq0$, and hence we cannot write ϕ_ϵ in the form $l_\epsilon(1+a\epsilon\varphi_{1,\epsilon})$ as in step 2. Instead, let us write

$$\phi_\epsilon=l_\epsilon+\epsilon a_\epsilon m_\epsilon\phi_{1,\epsilon},\quad\text{where}\quad\int_\Omega\phi_{1,\epsilon}\,dx=0,\quad\|\phi_{1,\epsilon}\|_{L^\infty(\Omega)}=1,\quad m_\epsilon>0. \tag{4.18}$$

From (4.5) we get the following equations for $(\phi_{1,\epsilon},\mathbf{A}_\epsilon)$:

$$\begin{aligned}&-\Delta\phi_{1,\epsilon}+2i\epsilon a_\epsilon\mathbf{A}_\epsilon\cdot\nabla\phi_{1,\epsilon}+\epsilon a_\epsilon|\mathbf{A}_\epsilon|^2\left(\frac{l_\epsilon}{m_\epsilon}+\epsilon a_\epsilon\phi_{1,\epsilon}\right)\\&\quad=\epsilon(1-|l_\epsilon+\epsilon a_\epsilon m_\epsilon\phi_{1,\epsilon}|^2)\left(\frac{l_\epsilon}{a_\epsilon m_\epsilon}+\epsilon\phi_{1,\epsilon}\right)\quad\text{in }\Omega,\end{aligned}$$

$$\lambda^2\,\mathrm{curl}^2\,\mathbf{A}_\epsilon=m_\epsilon\Im\{\overline{l_\epsilon}+\epsilon a_\epsilon m_\epsilon\overline{\phi}_{1,\epsilon}\}\left[\nabla\phi_{1,\epsilon}-iA_\epsilon\left(\frac{l_\epsilon}{m_\epsilon}+\epsilon a_\epsilon\phi_{1,\epsilon}\right)\right]\chi_\Omega\quad\text{in }\mathbb{R}^3, \tag{4.19}$$

$$\frac{\partial \phi_{1,\epsilon}}{\partial \nu} = i\left(\frac{l_\epsilon}{m_\epsilon} + \epsilon a_\epsilon \phi_{1,\epsilon}\right)\mathbf{A}_\epsilon \cdot \nu \quad \text{on } \partial\Omega.$$

As in step 2 we find that $\|\mathbf{A}_\epsilon\|_{C^{1+\alpha}(\bar{\Omega})}$ is bounded. Making gauge transforms and passing to a subsequence if necessary, we may assume that

$$l_\epsilon \to l_0, \quad \mathbf{A}_\epsilon \to \mathbf{A}_* \quad \text{in } C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3) \quad \text{as } \epsilon \to 0, \quad \mathbf{A}_* - \mathbf{F}_\mathbf{h} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \text{div}). \tag{4.20}$$

Step 3.2. We show that $l_0 = 0$. We need the following conclusion.

Claim 2: $\{l_\epsilon/m_\epsilon\}$ is bounded.

The proof of claim 2 will be given in Appendix B. From claim 2, passing to a subsequence we may assume that

$$\lim_{\epsilon \to 0} \frac{l_\epsilon}{m_\epsilon} = b_*. \tag{4.21}$$

Applying the elliptic estimate to (4.19) we may assume that $\phi_{1,\epsilon} \to \phi_*$ in $C^{2+\alpha}(\bar{\Omega})$ as $\epsilon \to 0$, $\|\phi_*\|_{L^\infty(\Omega)} = 1$, $\int_\Omega \phi_* \, dx = 0$, and $(\phi_*, \mathbf{A}_*)$ satisfies

$$\begin{aligned} \Delta \phi_* &= 0 \quad \text{in } \Omega, \\ \lambda^2 \operatorname{curl} \mathbf{A}_* &= |l_0|^2 \Im\{\nabla \phi_* - i b_* \mathbf{A}_*\} \chi_\Omega \quad \text{in } \mathbb{R}^3, \\ \frac{\partial \phi_*}{\partial \nu} &= i b_* \mathbf{A}_* \cdot \nu \quad \text{on } \partial\Omega. \end{aligned} \tag{4.22}$$

Since $\phi_* \not\equiv 0$ we find that $b_* \neq 0$. Let $\phi_* = i b_* w_*$. Then w_* is a real-valued function.

Now we rewrite

$$\phi_\epsilon = l_\epsilon (1 + i \epsilon a_\epsilon w_* + \epsilon^2 a_\epsilon^2 \phi_{2,\epsilon}).$$

Then $\epsilon \phi_{2,\epsilon} \to 0$ in $C^{2+\alpha}(\bar{\Omega})$. From (4.5) we derive the equation of $\phi_{2,\epsilon}$,

$$\begin{aligned} \Delta \phi_{2,\epsilon} &= |\mathbf{A}_*|^2 - 2\mathbf{A}_* \nabla w_* - \frac{1}{a^2}(1 - |l_0|^2) + \tilde{p}_\epsilon \quad \text{in } \Omega, \\ \frac{\partial \phi_{2,\epsilon}}{\partial \nu} &= \frac{i}{\epsilon a_\epsilon}[\mathbf{A}_\epsilon \cdot \nu - \mathbf{A}_* \cdot \nu] - w_* \mathbf{A}_* \cdot \nu + \tilde{r}_\epsilon \quad \text{on } \partial\Omega, \end{aligned} \tag{4.23}$$

where $\tilde{p}_\epsilon \to 0$ in $C^{2+\alpha}(\bar{\Omega})$ and $\tilde{r}_\epsilon \to 0$ in $C^{1+\alpha}(\partial\Omega)$ as $\epsilon \to 0$. Integrating this equation, then taking the real part, and using the fact that $\int_{\partial\Omega} w_* \mathbf{A}_* \cdot \nu \, dS = \int_\Omega |\nabla w_*|^2 \, dx$, we find

$$1 - l_0^2 = a^2 \fint_\Omega |\nabla w_* - \mathbf{A}_*|^2 \, dx. \tag{4.24}$$

Suppose $\rho = |l_0|^2 > 0$. From (4.22), (3.21) and Lemma 3.5 we find that $(w_*, \mathbf{A}_*) = (w^\rho, \mathbf{A}^\rho)$, and

$$f(a, \rho) = 1, \tag{4.25}$$

where the function f was defined in the proof of Lemma 3.5. However, since $\lambda \geqslant \lambda(\mathbf{h})$ and $a \geqslant a(\mathbf{h})$, (4.25) holds only when $a = a(\mathbf{h})$ and $\rho = 0$. This contradiction shows that we must have $l_0 = 0$.

Step 3.3. Plugging $l_0 = 0$ into (4.22) we find that $\mathbf{A}_* = \mathbf{F}_\mathbf{h}$ and $w_* = w_\mathbf{h}$. From (4.24) we find

$$1=a^2\fint_\Omega|\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}}|^2\,dx=a^2\omega(\mathbf{h}).$$

Hence $a=a(\mathbf{h})$ and $a_\epsilon=a(\mathbf{h})+o(1)$. So (4.17) and hence (4.16) are proved.

Write

$$\mathbf{A}_\epsilon=\mathbf{F}_{\mathbf{h}}+|l_\epsilon|^2\mathbf{B}_\epsilon,\quad \psi_{2,\epsilon}=u_\epsilon+iv_\epsilon,\quad u_\epsilon \text{ and } v_\epsilon \text{ are real.} \tag{4.26}$$

From (4.5) and (4.23) we have

$$\Delta u_\epsilon=|\mathbf{F}_{\mathbf{h}}|^2-2\mathbf{F}_{\mathbf{h}}\nabla w_{\mathbf{h}}-\frac{1}{a^2}+p_{1,\epsilon},\quad \Delta v_\epsilon=p_{2,\epsilon}\quad \text{in } \Omega,$$

$$\lambda^2\,\mathrm{curl}^2\,\mathbf{B}_\epsilon=(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}}+\tilde{\mathbf{q}}_\epsilon)\chi_\Omega\quad \text{in } \mathbb{R}^3,$$

$$\frac{\partial u_\epsilon}{\partial\nu}=-w_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}\cdot\nu+r_{1,\epsilon},\quad \frac{\partial v_\epsilon}{\partial\nu}=\frac{|l_\epsilon|^2}{\epsilon a_\epsilon}\mathbf{B}_\epsilon\cdot\nu+r_{2,\epsilon}\quad \text{on } \partial\Omega.$$

Here $p_{1,\epsilon}$, $p_{2,\epsilon}\to 0$ in $C^{2+\alpha}(\overline{\Omega})$, $\tilde{\mathbf{q}}_\epsilon\to\mathbf{0}$ in $C^{1+\alpha}(\overline{\Omega})$, $r_{1,\epsilon}$, $r_{2,\epsilon}\to 0$ in $C^{1+\alpha}(\partial\Omega)$ as $\epsilon\to 0$. We find that $\mathbf{B}_\epsilon\to\mathbf{B}^0=(1/\lambda^2)\mathbf{U}_{\mathbf{h}}$ in $C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$, and $\|u_\epsilon\|_{C^{2+\alpha}(\overline{\Omega})}$ is bounded. Recall that $l_\epsilon\to 0$. So $(\phi_\epsilon,\mathbf{A}_\epsilon)$ has the expansions given in (4.3).

Step 3.4. Now assume $\lambda>\lambda(\mathbf{h})$ and prove (4.4). We shall use the energy estimate to obtain (4.4). Note that $\int_\Omega\phi_{2,\epsilon}\,dx=0$, $\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\nabla\phi_{2,\epsilon}\,dx=0$, and $\{\nabla u_\epsilon\}$ is bounded. As in step 2.2 we compute

$$\begin{aligned}
\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]&=\epsilon^2a_\epsilon^2|l_\epsilon|^2\Big\{\|\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}}\|^2_{L^2(\Omega)}-2|l_\epsilon|^2\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\mathbf{B}_\epsilon\,dx\\
&\quad-2\epsilon a_\epsilon|l_\epsilon|^2\int_\Omega\mathbf{B}_\epsilon\cdot\Im\{\nabla\phi_{2,\epsilon}\}dx\\
&\quad+|l_\epsilon|^4\|\mathbf{B}_\epsilon\|^2_{L^2(\Omega)}+\epsilon^2a_\epsilon^2\|\nabla\phi_{2,\epsilon}+w_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}+|l_\epsilon|^2w_{\mathbf{h}}\mathbf{B}_\epsilon\|^2_{L^2(\Omega)}\Big\}\\
&\quad+\frac{\epsilon^2}{2}(1-|l_\epsilon|^2)^2|\Omega|+\epsilon^2a_\epsilon^2\lambda^2|l_\epsilon|^4\|\mathrm{curl}\,\mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)}+O(\epsilon^4|l_\epsilon|^2)\\
&=\epsilon^2a_\epsilon^2|l_\epsilon|^2\Big\{\omega(\mathbf{h})|\Omega|+|l_\epsilon|^2\Big[\lambda^2\|\mathrm{curl}\,\mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)}-2\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\mathbf{B}_\epsilon\,dx\Big]\\
&\quad+\|\epsilon a_\epsilon\nabla v_\epsilon-|l_\epsilon|^2\mathbf{B}_\epsilon\|^2_{L^2(\Omega)}\Big\}+\frac{\epsilon^2}{2}(1-|l_\epsilon|^2)^2|\Omega|+O(\epsilon^4|l_\epsilon|^2)\\
&=\frac{|\Omega|\epsilon^2}{2}+\epsilon^2|l_\epsilon|^2\Big\{|\Omega|[a_\epsilon^2\omega(\mathbf{h})-1]+a_\epsilon^2|l_\epsilon|^2\Big[\frac{|\Omega|}{2a_\epsilon^2}\\
&\quad+\lambda^2\|\mathrm{curl}\,\mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)}-2\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\mathbf{B}_\epsilon\,dx\Big]+a_\epsilon^2\|\epsilon a_\epsilon\nabla v_\epsilon-|l_\epsilon|^2\mathbf{B}_\epsilon\|^2_{L^2(\Omega)}+O(\epsilon^2)\Big\}.
\end{aligned}$$

Since $\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]<|\Omega|\epsilon^2/2$, from the above computations we find

$$\begin{aligned}
&|\Omega|[a_\epsilon^2\omega(\mathbf{h})-1]+a_\epsilon^2|l_\epsilon|^2\Big[\frac{|\Omega|}{2a_\epsilon^2}+\lambda^2\|\mathrm{curl}\,\mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)}-2\int_\Omega(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\mathbf{B}_\epsilon\,dx\Big]\\
&+a_\epsilon^2\|\epsilon a_\epsilon\nabla v_\epsilon-|l_\epsilon|^2\mathbf{B}_\epsilon\|^2_{L^2(\Omega)}=O(\epsilon^2).
\end{aligned}$$

Since $a_\epsilon \to a = a(\mathbf{h})$ and $\mathbf{B}_\epsilon \to \mathbf{B}^0 = (1/\lambda^2)\mathbf{U}_\mathbf{h}$ weakly in $\mathbf{D}^{1,2}(\mathbb{R}^3, \mathrm{div})$ as $\epsilon \to 0$, we have

$$\begin{aligned}
&\frac{|\Omega|}{2a_\epsilon^2} + \lambda^2 \|\mathrm{curl}\, \mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)} - 2\int_\Omega (\nabla w_\mathbf{h} - \mathbf{F}_\mathbf{h}) \cdot \mathbf{B}_\epsilon \, dx \\
&\quad \geqslant \frac{|\Omega|}{2a^2} + \lambda^2 \|\mathrm{curl}\, \mathbf{B}^0\|^2_{L^2(\mathbb{R}^3)} - 2\int_\Omega (\nabla w_\mathbf{h} - \mathbf{F}_\mathbf{h}) \cdot \mathbf{B}^0 \, dx + o(1) \\
&\quad = \frac{|\Omega|\omega(\mathbf{h})}{2} - \frac{1}{\lambda^2} \|\mathrm{curl}\, \mathbf{U}_\mathbf{h}\|^2_{L^2(\mathbb{R}^3)} + o(1) \\
&\quad = \frac{|\Omega|\omega(\mathbf{h})}{2}\left(1 - \frac{\lambda(\mathbf{h})^2}{\lambda^2}\right) + o(1).
\end{aligned}$$

Thus

$$a_\epsilon^2 \omega(\mathbf{h}) - 1 + \frac{1}{2} a_\epsilon^2 |l_\epsilon|^2 \omega(\mathbf{h}) \left(1 - \frac{\lambda(\mathbf{h})^2}{\lambda^2} + o(1)\right) + \frac{a_\epsilon^2}{|\Omega|} \|\epsilon a_\epsilon \nabla v_\epsilon - |l_\epsilon|^2 \mathbf{B}_\epsilon\|^2_{L^2(\Omega)} = O(\epsilon^2).$$

When $\lambda > \lambda(\mathbf{h})$, we can find a constant $c(\lambda) > 0$ such that

$$a_\epsilon^2 \omega(\mathbf{h}) - 1 + c(\lambda)|l_\epsilon|^2 + \frac{a_\epsilon^2}{|\Omega|} \|\epsilon a_\epsilon \nabla v_\epsilon - |l_\epsilon|^2 \mathbf{B}_\epsilon\|^2_{L^2(\Omega)} = O(\epsilon^2).$$

Thus

$$\frac{a_\epsilon^2 \omega(\mathbf{h}) - 1}{\epsilon^2} + c(\lambda) \frac{|l_\epsilon|^2}{\epsilon^2} + \|\nabla v_\epsilon\|^2_{L^2(\Omega)} \leqslant C. \tag{4.27}$$

Equation (4.4) and hence conclusion (iii) are proved.

Step 3.5. Proof of conclusion (i): When $\lambda = \lambda(\mathbf{h})$, the conclusion follows from (4.6) and (4.16). When $\lambda > \lambda(\mathbf{h})$, (4.27) implies $a_\epsilon \leqslant a(\mathbf{h}) + O(\epsilon^2)$, from which we conclude

$$H_c(\mathbf{h}, \epsilon^2, \lambda\epsilon) \leqslant a(\mathbf{h})\epsilon + O(\epsilon^3). \tag{4.28}$$

From (4.6) and (4.28) we get conclusion (i). □

We next consider the case where κ is fixed. To describe the minimal solutions we need the vector field $\mathbf{F}_\mathbf{h}$ [see (1.6)], the function $w_\mathbf{h}$ [see (2.3)], and the function $\psi_\mathbf{h}$ which is the unique solution of the following equation:

$$\begin{aligned}
&-\Delta \psi = 2\mathbf{F}_\mathbf{h} \cdot \nabla w_\mathbf{h} - |\mathbf{F}_\mathbf{h}|^2 + \omega(\mathbf{h}) \quad \text{in } \Omega, \\
&\frac{\partial \psi}{\partial \nu} = -w_\mathbf{h} \mathbf{F}_\mathbf{h} \cdot \nu \quad \text{on } \partial\Omega, \quad \int_\Omega \psi \, dx = 0.
\end{aligned} \tag{4.29}$$

Note that $\psi_\mathbf{h}$ can be represented by

$$\psi_\mathbf{h} = \frac{w_\mathbf{h}^2}{2} + \frac{1}{2} \fint_\Omega w_\mathbf{h}^2 \, dx + \phi_\mathbf{h},$$

where $\phi_\mathbf{h}$ satisfies

$$\begin{aligned}
&-\Delta \phi_\mathbf{h} = \omega(\mathbf{h}) - |\mathbf{F}_\mathbf{h} - \nabla w_\mathbf{h}|^2 \quad \text{in } \Omega, \\
&\frac{\partial \phi_\mathbf{h}}{\partial \nu} = 0 \quad \text{on } \partial\Omega, \quad \int_\Omega \phi_\mathbf{h} \, dx = 0.
\end{aligned} \tag{4.30}$$

Theorem 4.2: *Let* $\mathbf{h}$ *be a unit vector and* $\kappa>0$ *be fixed.*

(i) As $\mu\to 0$,

$$H_c(\mathbf{h},\mu,\kappa)=a(\mathbf{h})\sqrt{\mu}+O(\mu^{3/2}). \tag{4.31}$$

(ii) Assume $\sigma=a\sqrt{\mu}$, *where* a *is fixed and* $0<a<a(\mathbf{h})$. *Let* $(\psi_\mu,\mathbf{A}_\mu)$ *be a minimal solution of (1.5). Then we have, as* $\mu\to 0$,

$$\begin{gathered}\psi_\mu=c_\mu[1+ia\sqrt{\mu}w_{\mathbf{h}}+a^2\mu\psi_{\mathbf{h}}+O(\mu^{3/2})],\\ \mathbf{A}_\mu=\mathbf{F}_{\mathbf{h}}+\frac{\mu|c_\mu|^2}{\kappa^2}\mathbf{U}_{\mathbf{h}}+O(\mu^{3/2}),\\ |c_\mu|=\sqrt{1-\left(\frac{a}{a(\mathbf{h})}\right)^2}+O(\sqrt{\mu}).\end{gathered} \tag{4.32}$$

(iii) Assume $\sigma=a_\mu\sqrt{\mu}<H_c(\mathbf{h},\mu,\kappa)$, *where* $a_\mu\to a(\mathbf{h})$ *as* $\mu\to 0$. *The minimizer* $(\psi_\mu,\mathbf{A}_\mu)$ *has the expansions*

$$\begin{gathered}\psi_\mu=l_\mu(1+ia_\mu\sqrt{\mu}w_{\mathbf{h}}+\mu v_\mu),\\ \mathbf{A}_\mu=\mathbf{F}_{\mathbf{h}}+\frac{\mu|l_\mu|^2}{\kappa^2}\mathbf{U}_{\mathbf{h}}+O(\mu^{3/2}|l_\mu|^2),\\ |l_\mu|^2+\mu\int_\Omega|\nabla v_\mu|^2\,dx\leqslant C\mu+2\left[1-\left(\frac{a_\mu}{a(\mathbf{h})}\right)^2\right].\end{gathered} \tag{4.33}$$

Proof: Write $\epsilon=\sqrt{\mu}$ and $\sigma=a\sqrt{\mu}=a\epsilon$. Then

$$\mathcal{G}[\psi,\mathbf{A}]=\int_\Omega\left\{|\nabla_{a\epsilon\mathbf{A}}\psi|^2+\frac{\epsilon^2}{2}(1-|\psi|^2)^2\right\}dx+a^2\kappa^2\int_{\mathbb{R}^3}|\operatorname{curl}\mathbf{A}-\mathbf{h}|^2\,dx,$$

and (1.5) is written as

$$\begin{gathered}-\nabla^2_{a\epsilon\mathbf{A}}\psi=\epsilon^2(1-|\psi|^2)\psi\quad\text{in }\Omega,\\ \operatorname{curl}^2\mathbf{A}=\frac{\epsilon}{a\kappa^2}\Im\{\overline{\psi}\nabla_{a\epsilon\mathbf{A}}\psi\}\chi_\Omega\quad\text{in }\mathbb{R}^3,\\ (\nabla_{a\epsilon\mathbf{A}}\psi)\cdot\nu=0,\quad[\nu\cdot\mathbf{A}]=0,\quad[\nu\times\operatorname{curl}\mathbf{A}]=0\quad\text{on }\partial\Omega,\\ \operatorname{curl}\mathbf{A}\to\mathbf{h}\quad\text{as }|x|\to\infty.\end{gathered} \tag{4.34}$$

Step 1. We show that there exists $L>0$ independent of $\mathbf{h}$ such that

$$H_c(\mathbf{h},\epsilon^2,\kappa)\geqslant a(\mathbf{h})\epsilon-L\epsilon^2. \tag{4.35}$$

Let $a_\epsilon=a(\mathbf{h})-L\epsilon^2$, and choose a test field $(\phi^\epsilon,\mathbf{A}^\epsilon)$ by

$$\begin{gathered}\phi^\epsilon=c(\epsilon)(1+ia_\epsilon\epsilon w_{\mathbf{h}}+a_\epsilon^2\epsilon^2\psi_{\mathbf{h}}),\\ \mathbf{A}^\epsilon=\mathbf{F}_{\mathbf{h}}+\frac{\epsilon^2|c(\epsilon)|^2}{\kappa^2}\mathbf{U}_{\mathbf{h}},\\ |c(\epsilon)|=\sqrt{1-a_\epsilon^2\omega(\mathbf{h})}.\end{gathered}$$

Computations show that

$$\mathcal{G}[\phi^\epsilon,\mathbf{A}^\epsilon]=\epsilon^2|\Omega|\left[\frac{1}{2}(1-|c(\epsilon)|^2)^2+a_\epsilon^2\omega(\mathbf{h})|c(\epsilon)|^2\right]+O(\epsilon^4)$$
$$=\frac{\epsilon^2|\Omega|}{2}[1-(1-a_\epsilon^2\omega(\mathbf{h}))^2]+O(\epsilon^4).$$

Choose L sufficiently large and we find $C(\mathbf{h},\epsilon^2,\kappa,a_\epsilon\epsilon)\leqslant G[\phi^\epsilon,\mathbf{A}^\epsilon]<|\Omega|\epsilon^2/2$ for small ϵ. So the minimizers are nontrivial. Therefore (4.35) holds.

Step 2. Proof of conclusion (ii): Fix a such that

$$0<a<a(\mathbf{h}). \tag{4.36}$$

Let $\sigma=a\epsilon$. From step 1 we know that (4.34) has a nontrivial minimal solution $(\psi_\epsilon,\mathbf{A}_\epsilon)$ satisfying $\operatorname{div}\mathbf{A}_\epsilon=0$ in $\mathbb{R}^3$, $\int_\Omega\mathbf{A}_\epsilon\,dx=\mathbf{0}$, and for small $\epsilon>0$ we have

$$\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]=C(\mathbf{h},\epsilon^2,\kappa,a\epsilon)\leqslant\frac{\epsilon^2|\Omega|}{2}[1-(1-a^2\omega(\mathbf{h}))^2]+O(\epsilon^4). \tag{4.37}$$

We shall show that ψ_ϵ and $\mathbf{A}_\epsilon$ have expansions as described in (4.32).

Step 2.1. Proof of the leading terms: The energy estimate (4.37) yields

$$\mathbf{A}_\epsilon\to\mathbf{F}_\mathbf{h}\ \text{ strongly in }\ \mathbf{D}^{1,2}(\mathbb{R}^3)\quad\text{and}\quad\nabla\psi_\epsilon\to0\ \text{ in }\ L^2(\Omega)\quad\text{as}\quad\epsilon\to0.$$

Recall that $|\psi_\epsilon|\leqslant1$. Replacing ψ_ϵ be $\psi_\epsilon e^{ic(\epsilon)}$ if necessary, we may assume that, for some constant c_0, $\psi_\epsilon\to c_0$ in $W^{1,2}(\Omega)$ as $\epsilon\to0$.

Set $\mathbf{A}_{1,\epsilon}=(1/\epsilon)(\mathbf{A}_\epsilon-\mathbf{F}_\mathbf{h})$. We claim that

$$\mathbf{A}_{1,\epsilon}\to\mathbf{0}\quad\text{in}\ \ C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)\quad\text{and weakly in}\ \ \mathbf{D}^{1,2}(\mathbb{R}^3)\quad\text{as}\quad\epsilon\to0. \tag{4.38}$$

To prove (4.38), note that $\mathbf{A}_{1,\epsilon}$ is a weak solution of

$$\operatorname{curl}^2\mathbf{A}_{1,\epsilon}=\mathbf{f}_{0,\epsilon}\quad\text{and}\ \ \operatorname{div}\mathbf{A}_{1,\epsilon}=0\quad\text{in}\ \ \mathbb{R}^3,$$

where $\mathbf{f}_{0,\epsilon}=(1/a\kappa^2)\Im\{\overline{\psi_\epsilon}\nabla_{a\epsilon\mathbf{A}_\epsilon}\psi_\epsilon\}\chi_\Omega$. Since $\|\mathbf{f}_{0,\epsilon}\|_{L^2(\mathbb{R}^3)}\to0$ as $\epsilon\to0$ and $\{\mathbf{A}_{1,\epsilon}\}$ is bounded in $\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$, as in the proof of Lemma 3.3 we can show that, $\{\mathbf{A}_{1,\epsilon}\}$ is bounded in $C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. Passing to a subsequence we have $\mathbf{A}_{1,\epsilon}\to\mathbf{A}_1$ in $C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ and weakly in $\mathbf{D}^{1,2}(\mathbb{R}^3)$ as $\epsilon\to0$, and $\mathbf{A}_1$ satisfies

$$\Delta\mathbf{A}_1=\mathbf{0},\quad\mathbf{A}_1\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}),\quad\int_\Omega\mathbf{A}_1\,dx=\mathbf{0}.$$

Since the only harmonic functions on $\mathbb{R}^3$ with their gradients in $L^2(\mathbb{R}^3)$ are constant, we must have $\mathbf{A}_1=\mathbf{0}$. Thus (4.38) is true.

Now we use (4.38) to compute the energy $\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]$, and compare it with the energy upper bound (4.37) to conclude that $c_0\neq0$. Let $c_\epsilon=\int_\Omega\psi_\epsilon\,dx$. $c_\epsilon\to c_0$ as $\epsilon\to0$, and thus $c_\epsilon\neq0$ for all small ϵ. So we can write

$$\psi_\epsilon=c_\epsilon(1+a\epsilon\psi_{1,\epsilon}),\quad\text{where}\ \int_\Omega\psi_{1,\epsilon}\,dx=0.$$

From the first equation in (4.34) we find an equation for $\psi_{1,\epsilon}$,

$$-\Delta\psi_{1,\epsilon}+2ia\epsilon\mathbf{A}_\epsilon\cdot\nabla\psi_{1,\epsilon}+a\epsilon|\mathbf{A}_\epsilon|^2(1+a\epsilon\psi_{1,\epsilon})=\epsilon(1-|c_\epsilon|^2|1+a\epsilon\psi_{1,\epsilon}|^2)(1+a\epsilon\psi_{1,\epsilon}) \quad \text{in } \Omega,$$
$$\frac{\partial\psi_{1,\epsilon}}{\partial\nu}=i(1+a\epsilon\psi_{1,\epsilon})\mathbf{A}_\epsilon\cdot\nu \quad \text{on } \partial\Omega. \tag{4.39}$$

Applying the elliptic estimate to (4.39), we can pass to a subsequence and find $\psi_{1,\epsilon}\to\psi_1$ in $C^{2+\alpha}(\bar{\Omega})$ as $\epsilon\to0$, where ψ_1 satisfies

$$\Delta\psi_1=0 \quad \text{in } \Omega, \quad \frac{\partial\psi_1}{\partial\nu}=i\mathbf{F}_\mathbf{h}\cdot\nu \quad \text{on } \partial\Omega, \quad \int_\Omega\psi_1\,dx=0.$$

Thus $\psi_1=iw_\mathbf{h}$. So $\psi_{1,\epsilon}\to iw_\mathbf{h}$ in $C^{2+\alpha}(\bar{\Omega})$ as $\epsilon\to0$.

Step 2.2. Proof of the correction terms: Write $\psi_{1,\epsilon}=iw_\mathbf{h}+\epsilon\psi_{2,\epsilon}$, $\mathbf{A}_{1,\epsilon}=(\epsilon/\kappa^2)|c_\epsilon|^2\mathbf{A}_{2,\epsilon}$. Then

$$\psi_\epsilon=c_\epsilon(1+ia\epsilon w_\mathbf{h}+a\epsilon^2\psi_{2,\epsilon}), \quad \mathbf{A}_\epsilon=\mathbf{F}_\mathbf{h}+\frac{\epsilon^2}{\kappa^2}|c_\epsilon|^2\mathbf{A}_{2,\epsilon}. \tag{4.40}$$

We can show

$$\|\mathbf{A}_{2,\epsilon}-\mathbf{U}_\mathbf{h}\|_{L^\infty(\mathbb{R}^3)}\leqslant C\epsilon,$$
$$\|\psi_{2,\epsilon}-a\psi_\mathbf{h}\|_{C^{2+\alpha}(\bar{\Omega})}\leqslant C\epsilon, \tag{4.41}$$
$$|c_\epsilon|^2=1-a^2\omega(\mathbf{h})+O(\epsilon).$$

Then (4.32) follows. The proof of (4.41) is lengthy and is in the same sprint as in step 2.2 of the proof of Theorem 4.1, and hence will be given in Appendix C. From (4.41) we get conclusion (ii).

Step 3. Proof of conclusions (i) and (iii): We first show that

$$H_c(\mathbf{h},\epsilon^2,\kappa)\leqslant a(\mathbf{h})\epsilon+o(\epsilon). \tag{4.42}$$

Let us choose a sequence $\{a_\epsilon\}$ such that $\sigma=\epsilon a_\epsilon<H_c(\mathbf{h},\epsilon^2,\kappa)$ and $a_\epsilon\to a$ as $\epsilon\to0$, where $a\geqslant a(\mathbf{h})$. So the functional $\mathcal{G}$ has a nontrivial minimizer $(\phi_\epsilon,\mathbf{A}_\epsilon)$. We shall show that $a=a(\mathbf{h})$. The proof is similar to step 3 in the proof of Theorem 4.1.

First we show that $\phi_\epsilon\to0$ in $C^{2+\alpha}(\bar{\Omega})$ and $\mathbf{A}_\epsilon\to\mathbf{F}_\mathbf{h}$ in $C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3)$ as $\epsilon\to0$. Write

$$\phi_\epsilon=l^\epsilon+\epsilon m^\epsilon\phi_{1,\epsilon}, \quad \mathbf{A}_\epsilon=\mathbf{F}_\mathbf{h}+\epsilon\mathbf{A}_{1,\epsilon},$$

where l^ϵ and m^ϵ are constants,

$$l^\epsilon\to0 \quad \text{as } \epsilon\to0, \quad m^\epsilon>0, \quad \int_\Omega\phi_{1,\epsilon}\,dx=0, \quad \|\phi_{1,\epsilon}\|_{L^\infty(\Omega)}=1. \tag{4.43}$$

As in step 2 we can show that $\mathbf{A}_{1,\epsilon}\to\mathbf{0}$ in $C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3)$ as $\epsilon\to0$.

We claim that

$$\left|\frac{l^\epsilon}{m^\epsilon}\right|\leqslant C. \tag{4.44}$$

The proof of (4.44) will be given in Appendix C. From (4.44) and passing to a subsequence if necessary, we may assume $\lim_{\epsilon\to0}(l^\epsilon/m^\epsilon)=b$. From (4.34) we get an equation of $\phi_{1,\epsilon}$,

$$
\begin{aligned}
&-\Delta\phi_{1,\epsilon}+2i\epsilon a_\epsilon(\mathbf{F_h}+\epsilon\mathbf{A}_{1,\epsilon})\cdot\nabla\phi_{1,\epsilon}+a_\epsilon^2\epsilon|\mathbf{F_h}+\epsilon\mathbf{A}_{1,\epsilon}|^2\left(\frac{l^\epsilon}{m^\epsilon}+\epsilon\phi_{1,\epsilon}\right)\\
&\quad=\epsilon(1-|l^\epsilon+\epsilon m^\epsilon\phi_{1,\epsilon}|^2)\left(\frac{l^\epsilon}{m^\epsilon}+\epsilon\phi_{1,\epsilon}\right)\quad\text{in }\ \Omega,\\
&\frac{\partial\phi_{1,\epsilon}}{\partial\nu}=ia_\epsilon\left(\frac{l^\epsilon}{m^\epsilon}+\epsilon\phi_{1,\epsilon}\right)(\mathbf{F_h}+\epsilon\mathbf{A}_{1,\epsilon})\cdot\nu\quad\text{on }\ \partial\Omega.
\end{aligned}
\tag{4.45}
$$

Using (4.44) and applying the elliptic estimate to (4.55) we know that $\{\phi_{1,\epsilon}\}$ is uniformly bounded in $C^{2+\alpha}(\bar{\Omega})$. Passing to a subsequence again we may assume that $\phi_{1,\epsilon}\to\phi_1$ in $C^{2+\alpha}(\bar{\Omega})$ as $\epsilon\to0$, $\|\phi_1\|_{L^\infty(\Omega)}=1$, $\int_\Omega\phi_1\,dx=0$, and ϕ_1 satisfies

$$
\Delta\phi=0\quad\text{in }\ \Omega,\quad\frac{\partial\phi}{\partial\nu}=iab\mathbf{F_h}\cdot\nu\quad\text{on }\ \partial\Omega.
$$

Therefore $\phi_1=iabw_\mathbf{h}$, which implies $b\neq0$ since $\phi_1\not\equiv0$. So we have

$$
m^\epsilon=\frac{l^\epsilon}{b}+o(l^\epsilon)\quad\text{and }\ \phi_{1,\epsilon}-ia_\epsilon bw_\mathbf{h}\to0\quad\text{in }\ C^{2+\alpha}(\bar{\Omega})\quad\text{as }\ \epsilon\to0.
$$

Thus we can write

$$
\phi_\epsilon=l^\epsilon(1+i\epsilon a_\epsilon w_\mathbf{h}+\epsilon^2v_\epsilon),\quad\mathbf{A}_\epsilon=\mathbf{F_h}+\epsilon^2\mathbf{B}_\epsilon,
\tag{4.46}
$$

where v_ϵ satisfies $\int_\Omega v_\epsilon\,dx=0$ and $\epsilon\|v_\epsilon\|_{C^{2+\alpha}(\bar{\Omega})}=o(1)$. We can apply the elliptic estimate to the equation of $\mathbf{B}_\epsilon$ to show that $\{\mathbf{B}_\epsilon\}$ is bounded in $C^{1+\alpha}(\bar{\Omega})$. Using this and (4.46) we compute

$$
\begin{aligned}
\int_\Omega|\nabla_{\epsilon a_\epsilon\mathbf{A}_\epsilon}\phi_\epsilon|^2\,dx=a_\epsilon^2\epsilon^2|l^\epsilon|^2\Bigg\{&\int_\Omega\left[|\nabla w_\mathbf{h}-\mathbf{F_h}|^2+a_\epsilon^2\epsilon^2|w_\mathbf{h}\mathbf{F_h}|^2+\frac{\epsilon^2}{a_\epsilon^2}|\nabla v_\epsilon+O(1)|^2\right]dx\\
&+\frac{2\epsilon}{a_\epsilon}\Im\int_\Omega(\nabla w_\mathbf{h}-\mathbf{F_h}+i\epsilon a_\epsilon w_\mathbf{h}\mathbf{F_h})\cdot\nabla v_\epsilon\,dx+O(\epsilon^2)\Bigg\}.
\end{aligned}
$$

Note that $\int_\Omega(\nabla w_\mathbf{h}-\mathbf{F_h})\cdot\nabla v_\epsilon\,dx=0$. We use Cauchy inequality to control the last term on the right-hand side (see step C2 in Appendix C for a similar computation) and get

$$
\int_\Omega|\nabla_{\epsilon a_\epsilon\mathbf{A}_\epsilon}\phi_\epsilon|^2\,dx\geqslant a_\epsilon^2\epsilon^2|l^\epsilon|^2\int_\Omega\left\{\left|\nabla w_\mathbf{h}-\mathbf{F_h}\right|^2+\frac{\epsilon^2}{2a_\epsilon^2}\left|\nabla v_\epsilon\right|^2\right\}dx-C\epsilon^4|l^\epsilon|^2.
$$

On the other hand, since

$$
(|\phi_\epsilon|^2-1)^2=(1-|l^\epsilon|^2)^2-4\epsilon^3|l^\epsilon|^2(1-|l^\epsilon|^2)\Re(v_\epsilon)+O(\epsilon^2|l^\epsilon|^2)
$$

and $\int_\Omega v_\epsilon\,dx=0$, we find

$$
\int_\Omega(|\phi_\epsilon|^2-1)^2\,dx=(1-|l^\epsilon|^2)^2|\Omega|+O(\epsilon^2|l^\epsilon|^2).
$$

Thus

$$\frac{\epsilon^2}{2}|\Omega| \geqslant \mathcal{G}[\phi_\epsilon, \mathbf{A}_\epsilon]$$

$$\geqslant \int_\Omega \left\{ \left| \nabla_{\epsilon a_\epsilon \mathbf{A}_\epsilon} \phi_\epsilon \right|^2 + \frac{\epsilon^2}{2}(|\phi_\epsilon|^2 - 1)^2 \right\} dx$$

$$\geqslant a_\epsilon^2 \epsilon^2 |l^\epsilon|^2 \int_\Omega \left\{ |\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}}|^2 + \frac{\epsilon^2}{2a_\epsilon^2} |\nabla v_\epsilon|^2 \right\} dx + \frac{\epsilon^2}{2}(1 - |l^\epsilon|^2)^2 |\Omega| - C\epsilon^4 |l^\epsilon|^2.$$

From these inequalities we find

$$a_\epsilon^2 \omega(\mathbf{h}) - 1 + \frac{|l^\epsilon|^2}{2} + \frac{\epsilon^2}{2} \fint_\Omega |\nabla v_\epsilon|^2 \, dx \leqslant C\epsilon^2.$$

Comparing this with the condition $a \geqslant a(\mathbf{h})$ we find $a = a(\mathbf{h})$. So (4.42) is proved.

Moreover, from the above inequality we get

$$\fint_\Omega |\nabla v_\epsilon|^2 + \frac{|l^\epsilon|^2}{\epsilon^2} \leqslant 2C + 2\omega(\mathbf{h}) \frac{a^2 - a_\epsilon^2}{\epsilon^2}. \tag{4.47}$$

On the other hand, we can show that

$$\mathbf{A}_\epsilon = \mathbf{F}_{\mathbf{h}} + \frac{\epsilon^2}{\kappa^2} |l^\epsilon|^2 \mathbf{U}_{\mathbf{h}} + O(\epsilon^3 |l^\epsilon|^2), \tag{4.48}$$

see step C2 in Appendix C for more details of the argument. From (4.46), (4.47), and (4.48) we get (4.33). Conclusion (iii) is proved.

Plugging $a = a(\mathbf{h})$ into (4.47) we also get $a_\epsilon \leqslant a(\mathbf{h})\sqrt{1 + C\epsilon^2}$, which implies that, the functional $\mathcal{G}$ has nontrivial minimizers only if

$$|\sigma| \leqslant a(\mathbf{h})\epsilon + M\epsilon^3.$$

We can show that M can be chosen independent of $\mathbf{h}$. Thus we find

$$H_c(\mathbf{h}, \epsilon^2, \kappa) \leqslant a(\mathbf{h})\epsilon + M\epsilon^3.$$

This and (4.35) together give (4.31). Conclusion (i) is proved. □

Proof of Theorems 1 and 2: Theorem 2 is a direct consequence of Theorems 4.1 and 4.2. To obtain Theorem 1 we need to show that the estimate (1.8) holds uniformly for all $\kappa \geqslant \lambda(\mathbf{h})\sqrt{\mu}$. Note that Theorem 3.2 gives a lower bound for $H_c(\mathbf{h}, \mu, \kappa)$ uniformly for all $\kappa > 0$. Also note that the functional $\mathcal{G}$ is increasing in κ and hence $H_c(\mathbf{h}, \mu, \kappa)$ is decreasing in κ. Thus the first conclusion of Theorem 4.1 gives a uniform upper bound of $H_c(\mathbf{h}, \mu, \kappa)$ for all $\kappa \geqslant \lambda(\mathbf{h})\sqrt{\mu}$. □

Note added in proof: During proofreading we learned from Professor B. Helffer that, the result of Lemma 2.1 can also be proved and improved by using the Kato's perturbation theory, see: T. Kato, *Perturbation Theory of Linear Operators* (Springer-Verlag, New York, 1966). For superconductivity in one dimensional slabs, various limiting cases $\kappa \to 0$ or size to the film tending to zero have been analyzed by C. Bolley and B. Helffer in their papers: Rigorous results on Ginzburg-Landau models in a film submitted to an exterior parallel magnetic field, I, II, Nonlinear Stud. **3**, 1–29, 121–152 (1996). We would like to thank Professor Helffer for giving the information.

ACKNOWLEDGMENTS

This work was partially supported by the National Natural Science Foundation of China, the Science Foundation of the Ministry of Education of China, the Zhejiang Provincial Natural Science Foundation of China, and the National University of Singapore Academic Research Grant No. R-146-000-033-112.

APPENDIX A: PROOF OF LEMMA 2.1

Without loss of generality we may assume that $\mathbf{h}=(0,0,1)$ and choose $\mathbf{F_h}=(0,x_3,0)$. For convenience, we write $\mu(\epsilon)=\mu(\epsilon\mathbf{F_h})$. From the variational characteristic of the lowest eigenvalue,

$$\mu(\epsilon)=\inf_{\phi\in W^{1,2}(\Omega)}\frac{\int_\Omega|\nabla_{\epsilon\mathbf{F_h}}\phi|^2\,dx}{\int_\Omega|\phi|^2\,dx}.$$

Taking a test function $\phi=1+i\epsilon w_{\mathbf{h}}$, where $w_{\mathbf{h}}$ is the solution of (2.3), we have

$$\mu(\epsilon)\leqslant\frac{\int_\Omega|\nabla_{\epsilon\mathbf{F_h}}\phi|^2\,dx}{\int_\Omega|\phi|^2\,dx}=\epsilon^2\frac{\int_\Omega(|\nabla w_{\mathbf{h}}-\mathbf{F_h}|^2+\epsilon^2|w_{\mathbf{h}}\mathbf{F_h}|^2)dx}{\int_\Omega(1+\epsilon^2|w_{\mathbf{h}}|^2)dx}=\omega(\mathbf{h})\epsilon^2+O(\epsilon^4).$$

So we can write $\mu(\epsilon)=\epsilon^2\lambda_\epsilon$, where $\{\lambda_\epsilon\}$ is bounded. Passing to a subsequence if necessary, we may assume that $\lim_{\epsilon-0}\lambda_\epsilon=\lambda_0$. We shall prove that $\lambda_0=\omega(\mathbf{h})$.

Let ϕ_ϵ be a normalized eigenfunction of (2.1), $\|\phi_\epsilon\|_{L^\infty(\Omega)}=1$. From the elliptic estimate we have $\|\phi_\epsilon\|_{C^{2+\alpha}(\Omega)}\leqslant C(\alpha)$ for all small ϵ. After passing to a subsequence we have $\phi_\epsilon\to\phi_0$ in $C^{2+\alpha}(\Omega)$ as $\epsilon\to0$, $\|\phi_0\|_{L^\infty(\Omega)}=1$, $\Delta\phi_0=0$ in Ω and $\partial\phi_0/\partial\nu=0$ on $\partial\Omega$. Thus $\phi_0\equiv$constant. We may assume $\phi_0=1$. So $\phi_\epsilon\to1$ in $C^{2+\alpha}(\Omega)$ as $\epsilon\to0$.

Let us write

$$\alpha_\epsilon=\fint_\Omega\phi_\epsilon\,dx,\quad \psi_\epsilon=\phi_\epsilon-\alpha_\epsilon.$$

Using (2.1) we find

$$\Delta\psi_\epsilon-2i\epsilon x_3\partial_{x_2}\psi_\epsilon-\epsilon^2x_3^2\psi_\epsilon+\epsilon^2\lambda_\epsilon\psi_\epsilon=\epsilon^2\alpha_\epsilon(x_3^2-\lambda_\epsilon)\quad\text{in }\Omega,$$

$$\frac{\partial\psi_\epsilon}{\partial\nu}-i\epsilon\mathbf{F_h}\cdot\nu\psi_\epsilon=i\epsilon\alpha_\epsilon\mathbf{F_h}\cdot\nu\quad\text{on }\partial\Omega.$$

Recall that $\|\nabla_{\epsilon\mathbf{F_h}}\phi_\epsilon\|^2_{L^2(\Omega)}=\epsilon^2\lambda_\epsilon\|\phi_\epsilon\|^2_{L^2(\Omega)}$. We have

$$\begin{aligned}\|\psi_\epsilon\|_{L^2(\Omega)}&=\|\phi_\epsilon-\alpha_\epsilon\|_{L^2(\Omega)}\\&\leqslant C\|\nabla\phi_\epsilon\|_{L^2(\Omega)}\\&=C\|\nabla_{\epsilon\mathbf{F_h}}\phi_\epsilon+i\epsilon\mathbf{F_h}\phi_\epsilon\|_{L^2(\Omega)}\\&\leqslant C\|\nabla_{\epsilon\mathbf{F_h}}\phi_\epsilon\|_{L^2(\Omega)}+C\epsilon\|\mathbf{F_h}\phi_\epsilon\|_{L^2(\Omega)}\\&\leqslant C\epsilon.\end{aligned}$$

We apply the elliptic estimate to get $\|\psi_\epsilon\|_{W^{k.2}(\Omega)}\leqslant C(k)\epsilon$, and then use the Sobolev imbedding theorem to find $\|\psi_\epsilon\|_{L^\infty(\Omega)}\leqslant C\epsilon$. Let

$$\phi_1^\epsilon=\frac{\psi_\epsilon}{\epsilon}=\frac{\phi_\epsilon-\alpha_\epsilon}{\epsilon}.$$

We have $\|\phi_1^\epsilon\|_{L^\infty(\Omega)}\leqslant C$, $\int_\Omega\phi_1^\epsilon\,dx=0$, and

$$\begin{aligned}&\Delta\phi_1^\epsilon-2i\epsilon x_3\partial_{x_2}\phi_1^\epsilon-\epsilon^2x_3^2\phi_1^\epsilon+\epsilon^2\lambda_\epsilon\phi_1^\epsilon=\epsilon\alpha_\epsilon(x_3^2-\lambda_\epsilon)\quad\text{in }\Omega,\\&\frac{\partial\phi_1^\epsilon}{\partial\nu}-i\epsilon\mathbf{F_h}\cdot\nu\phi_1^\epsilon=i\alpha_\epsilon\mathbf{F_h}\cdot\nu\quad\text{on }\partial\Omega.\end{aligned}\tag{A1}$$

Applying the elliptic estimate we find $\|\phi_1^\epsilon\|_{C^{2+\alpha}(\Omega)} \leqslant C(\alpha)$. After passing to a subsequence we have $\phi_1^\epsilon \to \phi_1$ in $C^{2+\alpha}(\Omega)$ as $\epsilon \to 0$. $\int_\Omega \phi_1 \, dx = 0$, $\Delta \phi_1 = 0$ in Ω and $\partial \phi_1 / \partial \nu = i \mathbf{F_h} \cdot \nu$ on $\partial\Omega$. Let $\phi_1 = iw$, then w solves (2.3). Thus $\phi_1 = i w_{\mathbf{h}}$.

Let us write

$$\phi_1^\epsilon = i \beta_\epsilon w_{\mathbf{h}} + \epsilon \phi_2^\epsilon, \quad \beta_\epsilon = -i \frac{\int_\Omega w_{\mathbf{h}} \phi_1^\epsilon \, dx}{\int_\Omega |w_{\mathbf{h}}|^2 \, dx}.$$

Note that $\int_\Omega w_{\mathbf{h}} \phi_2^\epsilon \, dx = 0$. Since $\int_\Omega \phi_1^\epsilon \, dx = 0$ and $\int_\Omega w_{\mathbf{h}} \, dx = 0$, we have $\int_\Omega \phi_2^\epsilon \, dx = 0$. From (A1) we find

$$\begin{aligned} &\Delta \phi_2^\epsilon - 2i\epsilon x_3 \partial_{x_2} \phi_2^\epsilon - \epsilon^2 x_3^2 \phi_2^\epsilon + \epsilon^2 \lambda_\epsilon \phi_2^\epsilon = f_\epsilon \quad \text{in } \Omega, \\ &\frac{\partial \phi_2^\epsilon}{\partial \nu} - i\epsilon \mathbf{F_h} \cdot \nu \phi_2^\epsilon = (i\delta_\epsilon - \beta_\epsilon w_{\mathbf{h}}) \mathbf{F_h} \cdot \nu \quad \text{on } \partial\Omega, \end{aligned} \tag{A2}$$

where

$$f_\epsilon = -2\beta_\epsilon x_3 \partial_{x_2} w_{\mathbf{h}} + i\epsilon \beta_\epsilon w_{\mathbf{h}} (x_3^2 - \lambda_\epsilon) + \alpha_\epsilon (x_3^2 - \lambda_\epsilon), \quad \delta_\epsilon = \frac{\alpha_\epsilon - \beta_\epsilon}{\epsilon}.$$

Since $\phi_1^\epsilon \to i w_{\mathbf{h}}$ in $C^{2+\alpha}(\Omega)$, we have $\beta_\epsilon \to 1$ as $\epsilon \to 0$. Recall that we have chosen a subsequence such that $\lambda_\epsilon \to \lambda_0$. Thus $f_\epsilon \to -2x_3 \partial_{x_2} w_{\mathbf{h}} + x_3^2 - \lambda_0$ uniformly as $\epsilon \to 0$.

Now we show that

$$|\delta_\epsilon| \leqslant C \quad \text{for all small } \epsilon. \tag{A3}$$

Suppose (A3) were not true. Passing to a subsequence we may assume that $\delta_\epsilon \to \infty$. Let $\xi_\epsilon = \phi_2^\epsilon / \delta_\epsilon$. Then we have

$$\int_\Omega \xi_\epsilon \, dx = 0, \quad \int_\Omega w_{\mathbf{h}} \xi_\epsilon \, dx = 0. \tag{A4}$$

From (A2) we have

$$-\nabla^2_{\epsilon \mathbf{F_h}} \xi_\epsilon - \epsilon^2 \lambda_\epsilon \xi_\epsilon = -\frac{f_\epsilon}{\delta_\epsilon} \quad \text{in } \Omega,$$

$$\nabla_{\epsilon \mathbf{F_h}} \xi_\epsilon \cdot \nu = \left(i - \frac{\beta_\epsilon}{\delta_\epsilon} w_{\mathbf{h}} \right) \mathbf{F_h} \cdot \nu \quad \text{on } \partial\Omega.$$

Case 1: $\|\xi_\epsilon\|_{L^2(\Omega)} \leqslant C$ for all small ϵ. Applying the elliptic estimate we find that $\|\xi_\epsilon\|_{W^{k.2}(\Omega)} \leqslant C(\kappa)$ and $\|\xi_\epsilon\|_{C^{2+\alpha}(\Omega)} \leqslant C(\alpha)$. So we can find a subsequence, still denoted by ξ_ϵ, such that $\xi_\epsilon \to \xi_0$ in $C^{2+\alpha}(\Omega)$ as $\epsilon \to 0$. $\int_\Omega \xi_0 \, dx = 0$, $\Delta \xi_0 = 0$ in Ω and $\partial \xi_0 / \partial \nu = i \mathbf{F_h} \cdot \nu$ on $\partial\Omega$. Hence $\xi_0 = i w_{\mathbf{h}}$. But this is impossible since, from the second equality of (A4), we have $\int_\Omega w_{\mathbf{h}} \xi_0 \, dx = 0$. So case 1 cannot happen.

Case 2: $\|\xi_\epsilon\|_{L^2(\Omega)}$ is not bounded. Passing to a subsequence we may assume that $c_\epsilon = \|\xi_\epsilon\|_{L^2(\Omega)} \to \infty$. Let $\tilde{\xi}_\epsilon = \xi_\epsilon / c_\epsilon$. Then $\tilde{\xi}_\epsilon$ satisfies the following equation:

$$-\nabla^2_{\epsilon \mathbf{F_h}} \tilde{\xi}_\epsilon - \epsilon^2 \lambda_\epsilon \tilde{\xi}_\epsilon = -\frac{f_\epsilon}{c_\epsilon \delta_\epsilon} \quad \text{in } \Omega,$$

$$\nabla_{\epsilon \mathbf{F_h}} \tilde{\xi}_\epsilon \cdot \nu = \left(\frac{i}{c_\epsilon} - \frac{\beta_\epsilon}{c_\epsilon \delta_\epsilon} w_{\mathbf{h}} \right) \mathbf{F_h} \cdot \nu \quad \text{on } \partial\Omega.$$

Again we can find a subsequence, still denoted by $\tilde{\xi}_\epsilon$, such that $\tilde{\xi}_\epsilon \to \tilde{\xi}_0$ in $C^{2+\alpha}(\Omega)$, $\|\tilde{\xi}_0\|_{L^2(\Omega)} = 1$, $\int_\Omega \tilde{\xi}_0 \, dx = 0$, $\Delta \tilde{\xi}_0 = 0$ in Ω and $\partial \tilde{\xi}_0 / \partial \nu = 0$ on $\partial\Omega$. Thus $\tilde{\xi}_0 = 0$. This contradicts the condition $\|\tilde{\xi}_0\|_{L^2(\Omega)} = 1$. Case 2 cannot happen.

We have proved that (A3) is true. We may assume that $\lim_{\epsilon \to 0} \delta_\epsilon = \delta_0$. Now we return to (A2). Repeating the argument used in case 2, we can show that $\|\phi_2^\epsilon\|_{L^2(\Omega)} \leqslant C$. Then we apply the elliptic estimate to show that $\|\phi_2^\epsilon\|_{C^{2+\alpha}(\Omega)}$ is bounded. Thus we can find a subsequence, still denoted by ϕ_2^ϵ, such that $\phi_2^\epsilon \to \phi_2$ in $C^{2+\alpha}(\Omega)$ as $\epsilon \to 0$. ϕ_2 satisfies

$$\begin{aligned} -\Delta \phi_2 &= 2x_3 \partial_{x_2} w_{\mathbf{h}} - x_3^2 + \lambda_0 \quad \text{in } \Omega, \\ \frac{\partial \phi_2}{\partial \nu} &= (i\delta_0 - w_{\mathbf{h}}) \mathbf{F_h} \cdot \nu \quad \text{on } \partial\Omega. \end{aligned} \tag{A5}$$

Integrating the equation we find

$$\begin{aligned} \lambda_0 |\Omega| &= \int_\Omega \{x_3^2 - 2x_3 \partial_{x_2} w_{\mathbf{h}} - \Delta \phi_2\} dx \\ &= \int_\Omega x_3^2 \, dx - \int_{\partial\Omega} \left\{ 2x_3 w_{\mathbf{h}} \mathbf{e}_2 \cdot \nu + \frac{\partial \phi_2}{\partial \nu} \right\} dS \\ &= \int_\Omega |\mathbf{F_h}|^2 \, dx - \int_{\partial\Omega} (w_{\mathbf{h}} + i\delta_0) \mathbf{F_h} \cdot \nu \, ds \\ &= \int_\Omega |\mathbf{F_h}|^2 \, dx - \int_{\partial\Omega} w_{\mathbf{h}} \mathbf{F_h} \cdot \nu \, dS \\ &= \int_\Omega (|\mathbf{F_h}|^2 - |\nabla w_{\mathbf{h}}|^2) dx \\ &= \omega(\mathbf{h}) |\Omega|. \end{aligned}$$

Thus $\lambda_0 = \omega(\mathbf{h})$, namely, $\lambda_\epsilon \to \omega(\mathbf{h})$ as $\epsilon \to 0$.

Furthermore, following the same spirit we can examine the higher order terms and show that $\lambda_\epsilon - \omega(\mathbf{h}) = O(\epsilon)$. Thus we have proved that, as $\epsilon \to 0$,

$$\mu(\epsilon) = \omega(\mathbf{h}) \epsilon^2 + O(\epsilon^3), \quad \phi_\epsilon = \alpha_\epsilon + i\epsilon \beta_\epsilon w_{\mathbf{h}} + \epsilon^2 \phi_2 + o(\epsilon^2), \tag{A6}$$

where $\alpha_\epsilon \to 1$, $\beta_\epsilon \to 1$, $w_{\mathbf{h}}$ is the unique real solution of (2.3), and ϕ_2 is a solution of (A5). Thus (2.5) and (2.6) are proved. □

APPENDIX B: PROOF OF CLAIMS 1 AND 2

In this section we keep the notations in the proof of Theorem 4.1.

Proof of claim 1: Step B1. We first show the following

Subclaim 1: If the condition $\lim_{\epsilon - 0} |b_\epsilon| = +\infty$ holds, then there exists a constant C independent of ϵ such that, for all small ϵ,

$$\|\psi_{2,\epsilon}\|_{L^\infty(\Omega)} \leqslant C |b_\epsilon|. \tag{B1}$$

Suppose (B1) were not true. We pass to a subsequence if necessary and assume that

$$d_\epsilon=\frac{\|\psi_{2,\epsilon}\|_{L^\infty(\Omega)}}{|b_\epsilon|}\to\infty \quad \text{as} \quad \epsilon\to 0.$$

Set

$$\phi_\epsilon=\frac{\psi_\epsilon}{b_\epsilon d_\epsilon}, \quad \mathbf{D}_\epsilon=\frac{\mathbf{A}_{1,\epsilon}}{b_\epsilon d_\epsilon}.$$

$(\phi_\epsilon,\mathbf{D}_\epsilon)$ satisfies

$$\Delta\phi_\epsilon=O\left(\frac{1}{b_\epsilon d_\epsilon}\right) \quad \text{in} \quad \Omega,$$

$$\lambda^2\,\mathrm{curl}^2\,\mathbf{D}_\epsilon=\left\{\frac{1}{d_\epsilon}(\nabla w_a-\mathbf{A}_a)+|c_\epsilon|^2\Im\left(\nabla\phi_\epsilon-i\mathbf{D}_\epsilon+\frac{\mathbf{q}_\epsilon}{b_\epsilon d_\epsilon}\right)\right\}\chi_\Omega \quad \text{in} \quad \mathbb{R}^3,$$

$$\frac{\partial\phi_\epsilon}{\partial\nu}=i\mathbf{D}_{1,\epsilon}\cdot\nu-\frac{1}{b_\epsilon d_\epsilon}w_a\mathbf{A}_a\cdot\nu+O\left(\frac{r_\epsilon}{b_\epsilon d_\epsilon}\right) \quad \text{on} \quad \partial\Omega.$$

Recall that $\int_\Omega\phi_\epsilon\,dx=0$, $\int_\Omega\mathbf{D}_\epsilon\,dx=\mathbf{0}$, and $\mathbf{D}_\epsilon\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$. From the second equation we get

$$\lambda^2\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{D}_\epsilon|^2\,dx+|c_\epsilon|^2\int_\Omega|\nabla\phi_\epsilon-i\mathbf{D}_\epsilon|^2\,dx=\int_\Omega\left\{\frac{1}{d_\epsilon}(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{D}_\epsilon+\frac{|c_\epsilon|^2}{b_\epsilon d_\epsilon}\mathbf{q}_\epsilon\cdot\mathbf{D}_\epsilon\right\}dx.$$

Thus we can pass to a subsequence again and assume that $\phi_\epsilon\to\phi$ in $C^{2+\alpha}(\overline{\Omega})$ and $\mathbf{D}_\epsilon\to\mathbf{D}$ in $C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ as $\epsilon\to 0$, $\mathbf{D}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$, $\int_\Omega\phi\,dx=0$, $\|\phi\|_{L^\infty(\Omega)}=1$, and $(\phi,\mathbf{D})$ satisfies

$$\Delta\phi=0 \quad \text{in} \quad \Omega,$$

$$\lambda^2\,\mathrm{curl}^2\,\mathbf{D}=c_\alpha^2\Im\{\nabla\phi-i\mathbf{D}\}\chi_\Omega \quad \text{in} \quad \mathbb{R}^3, \tag{B2}$$

$$\frac{\partial\phi}{\partial\nu}=i\mathbf{D}\cdot\nu \quad \text{on} \quad \partial\Omega.$$

From the proof of Lemma 3.4 we know that the only finite energy solution of (B2) is $\phi=$constant and $\mathbf{D}=$constant vector. The condition $\int_\Omega\phi\,dx=0$ implies that $\phi=0$, which contradicts the condition $\|\phi\|_{L^\infty(\Omega)}=1$. Hence (B1) is true.

Step B2. Now we show that $\{b_\epsilon\}$ is bounded. Suppose not. We may assume that $\lim_{\epsilon\to 0}|b_\epsilon|=\infty$. Let

$$\varphi_\epsilon=\frac{\psi_{1,\epsilon}}{b_\epsilon}, \quad \mathbf{B}_\epsilon=\frac{\mathbf{A}_{1,\epsilon}}{b_\epsilon}.$$

Then $(\varphi_\epsilon,\mathbf{B}_\epsilon)$ satisfies

$$\Delta\varphi_\epsilon=O\left(\frac{1}{b_\epsilon}\right) \quad \text{in} \quad \Omega,$$

$$\lambda^2\,\mathrm{curl}^2\,\mathbf{B}_\epsilon=\left\{(\nabla w_a-\mathbf{A}_a)+|c_\epsilon|^2\Im\left(\nabla\varphi_\epsilon-i\mathbf{B}_\epsilon+\frac{\mathbf{q}_\epsilon}{b_\epsilon}\right)\right\}\chi_\Omega \quad \text{in} \quad \mathbb{R}^3,$$

$$\frac{\partial\varphi_\epsilon}{\partial\nu}=i\mathbf{B}_{1,\epsilon}\cdot\nu-\frac{1}{b_\epsilon}w_a\mathbf{A}_a\cdot\nu+O\left(\frac{r_\epsilon}{b_\epsilon}\right) \quad \text{on} \quad \partial\Omega.$$

Using subclaim 1, we can pass to a subsequence and assume that $\varphi_\epsilon \to \varphi$ in $C^{2+\alpha}(\overline{\Omega})$ and $\mathbf{B}_\epsilon \to \mathbf{B}$ in $C^{1+\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ as $\epsilon \to 0$, $\mathbf{B} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \mathrm{div})$, $\int_\Omega \varphi \, dx = 0$, and $(\varphi, \mathbf{B})$ satisfies

$$\Delta \varphi = 0 \quad \text{in } \Omega,$$

$$\lambda^2 \operatorname{curl}^2 \mathbf{B} = \{\nabla w_a - \mathbf{A}_a + c_a^2 \Im(\nabla \varphi - i\mathbf{B})\}\chi_\Omega \quad \text{in } \mathbb{R}^3,$$

$$\frac{\partial \varphi}{\partial \nu} = i\mathbf{B} \cdot \nu - w_a \mathbf{A}_a \cdot \nu \quad \text{on } \partial\Omega.$$

Comparing this with (3.22) and (4.1) we find that

$$\varphi = u_a + i v_a, \quad \mathbf{B} = \mathbf{B}_a.$$

Next, to derive a contradiction we compute the energy $\mathcal{G}[\psi_\epsilon, \mathbf{A}_\epsilon]$. Write

$$\psi_\epsilon = c_\epsilon(1 + ia\epsilon w_a + a^2 \epsilon^2 b_\epsilon \varphi_\epsilon), \quad \mathbf{A}_\epsilon = \mathbf{A}_a + a\epsilon b_\epsilon \mathbf{B}_\epsilon.$$

Under the condition $\lim_{\epsilon \to 0} |b_\epsilon| = \infty$ we have,

$$\mathcal{G}[\psi_\epsilon, \mathbf{A}_\epsilon] = (I_{1,\epsilon} + I_{2,\epsilon} + I_{3,\epsilon})\epsilon^2,$$

where

$$I_{1,\epsilon} = a^2 |c_\epsilon|^2 \|\nabla w_a - \mathbf{A}_a\|^2_{L^2(\Omega)} + a^2 \lambda^2 \|\operatorname{curl} \mathbf{A}_a - \mathbf{h}\|^2_{L^2(\mathbb{R}^3)} + \frac{|\Omega|}{2}(1 - |c_\epsilon|^2)^2,$$

$$I_{2,\epsilon} = 2a^2 \epsilon b_\epsilon \left\{ \lambda^2 \int_{\mathbb{R}^3} (\operatorname{curl} \mathbf{A}_a - \mathbf{h}) \cdot \operatorname{curl} \mathbf{B}_\epsilon \, dx - |c_\epsilon|^2 \int_\Omega (\nabla w_a - \mathbf{A}_a) \cdot \mathbf{B}_\epsilon \, dx \right\},$$

$$I_{3,\epsilon} = a^4 \epsilon^2 b_\epsilon^2 \{ |c_\epsilon|^2 \|\nabla \varphi_\epsilon - i\mathbf{B}_\epsilon\|^2_{L^2(\Omega)} + \lambda^2 \|\operatorname{curl} \mathbf{B}_\epsilon\|^2_{L^2(\mathbb{R}^3)} \}$$
$$- a^2 \epsilon^2 |c_\epsilon|^2 (1 - |c_\epsilon|^2) \|w_a\|^2_{L^2(\Omega)} + O(\epsilon^2 b_\epsilon).$$

Using the last equality in (3.21) we find

$$I_{1,\epsilon} = I_a + \frac{|\Omega|}{2}(|c_\epsilon|^2 - c_a^2)^2,$$

where I_a was given in step 1.1 of the proof of Theorem 4.1. Using (3.22) we find

$$I_{2,\epsilon} = 2a^3 \epsilon b_\epsilon (c_a^2 - |c_\epsilon|^2) \int_\Omega (\nabla w_a - \mathbf{A}_a) \cdot \mathbf{B}_\epsilon \, dx$$

$$= -2a^2 (|c_\epsilon|^2 - c_a^2)^2 \left\{ \int_\Omega (\nabla w_a - \mathbf{A}_a) \cdot \mathbf{B}_a \, dx + o(1) \right\}.$$

We have assumed $|b_\epsilon| \to \infty$, hence $(|c_\epsilon|^2 - c_a^2)^2 \gg \epsilon^2$. Using (3.22) we have

$$I_{3,\epsilon} = a^2 (|c_\epsilon|^2 - c_a^2)^2 \{ \lambda^2 \|\operatorname{curl} \mathbf{B}_a\|^2_{L^2(\mathbb{R}^3)} + c_a^2 \|\nabla v_a - \mathbf{B}_a\|^2_{L^2(\Omega)} + o(1) \}$$

$$= a^2 (|c_\epsilon|^2 - c_a^2)^2 \left\{ \int_\Omega (\nabla w_a - \mathbf{A}_a) \cdot \mathbf{B}_a \, dx + o(1) \right\}.$$

From these and (3.23), we can find a positive constant C such that

$$\frac{\mathcal{G}[\psi_\epsilon,\mathbf{A}_\epsilon]}{\epsilon^2}-I_a=a^2(|c_\epsilon|^2-c_a^2)^2\left\{\frac{|\Omega|}{2a^2}-\int_\Omega(\nabla w_a-\mathbf{A}_a)\cdot\mathbf{B}_a\,dx+o(1)\right\}>C(|c_\epsilon|^2-c_a^2)^2\gg\epsilon^2,$$

which contradicts (4.9). Thus $\{b_\epsilon\}$ is bounded. □

Proof of claim 2: Suppose $\{l_\epsilon/m_\epsilon\}$ were not bounded. Passing to a subsequence we may assume $m_\epsilon\ll|l_\epsilon|$. Then we use (4.18) to get

$$\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]=\epsilon^2\left\{a_\epsilon^2|l_\epsilon|^2\|\mathbf{A}_\epsilon-\nabla\zeta_\epsilon\|^2_{L^2(\Omega)}+a_\epsilon^2\lambda^2\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}+\frac{|\Omega|}{2}(1-|l_\epsilon|^2)^2+o(\epsilon|l_\epsilon|^2)\right\},\tag{B3}$$

where $\zeta_\epsilon=-(im_\epsilon/l_\epsilon)\phi_{1,\epsilon}$.

Case 1: $l_0\neq0$. Since $a_\epsilon\to a$ as $\epsilon\to0$, from (B3) we have

$$\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]=\epsilon^2\left\{a^2l_0^2\|\mathbf{A}_\epsilon-\nabla\zeta_\epsilon\|^2_{L^2(\Omega)}+a^2\lambda^2\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}+\frac{|\Omega|}{2}(1-l_0^2)^2+o(1)\right\}.$$

On the other hand, if we let $\rho=l_0^2$ and choose a test field $(\psi,\mathbf{A})$, where $\psi=l_0(1+\epsilon a_\epsilon w^\rho)$ and $\mathbf{A}=\mathbf{A}^\rho$, we find an energy upper bound

$$\mathcal{G}[\psi,\mathbf{A}]=\epsilon^2\left\{a^2l_0^2\|\mathbf{A}^\rho-\nabla w^\rho\|^2_{L^2(\Omega)}+a^2\lambda^2\|\mathrm{curl}\,\mathbf{A}^\rho-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}+\frac{|\Omega|}{2}(1-l_0^2)^2+o(1)\right\}.$$

Since $(\phi_\epsilon,\mathbf{A}_\epsilon)$ is a minimizer, we have $\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]\leqslant\mathcal{G}[\psi,\mathbf{A}]$, from which we derive

$$\begin{aligned}\mathcal{J}_\rho[\zeta_\epsilon,\mathbf{A}_\epsilon]&=l_0^2\|\mathbf{A}_\epsilon-\nabla\zeta_\epsilon\|^2_{L^2(\Omega)}+\lambda^2\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}\\&\leqslant l_0^2\|\mathbf{A}^\rho-\nabla w^\rho\|^2_{L^2(\Omega)}+\lambda^2\|\mathrm{curl}\,\mathbf{A}^\rho-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}+o(1)\\&=\mathcal{J}_\rho[w^\rho,\mathbf{A}^\rho]+o(1).\end{aligned}$$

Thus $\{(\zeta_\epsilon,\mathbf{A}_\epsilon)\}$ is a minimizing sequence of the functional $\mathcal{J}_\rho$, hence contains a subsequence which converges to the minimizer $(w^\rho,\mathbf{A}^\rho)$. However, $|\zeta_\epsilon|=|(m_\epsilon/l_\epsilon)\phi_{1,\epsilon}|\to0$ as $\epsilon\to0$. This contradiction shows that case 1 cannot happen.

Case 2: $l_0=0$. Then $l_\epsilon\to0$ and $\|\zeta_\epsilon\|_{L^\infty(\Omega)}\to0$ as $\epsilon\to0$. Since $\mathcal{G}[\phi_\epsilon,\mathbf{A}_\epsilon]\leqslant|\Omega|\epsilon^2/2$, we have

$$a_\epsilon^2|l_\epsilon|^2\|\mathbf{A}_\epsilon-\nabla\zeta_\epsilon\|^2_{L^2(\Omega)}+a_\epsilon^2\lambda^2\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}+\frac{|\Omega|}{2}(1-|l_\epsilon|^2)^2+o(\epsilon|l_\epsilon|^2)\leqslant\frac{|\Omega|}{2},$$

so

$$a_\epsilon^2\|\mathbf{A}_\epsilon-\nabla\zeta_\epsilon\|^2_{L^2(\Omega)}+\frac{a_\epsilon^2\lambda^2}{|l_\epsilon|^2}\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}\leqslant|\Omega|-\frac{|\Omega|}{2}|l_\epsilon|^2+o(\epsilon).\tag{B4}$$

Especially we have $\|\mathrm{curl}\,\mathbf{A}_\epsilon-\mathbf{h}\|^2_{L^2(\mathbb{R}^3)}\leqslant C|l_\epsilon|^2\to0$. Thus $\mathbf{A}_\epsilon\to\mathbf{F}_\mathbf{h}$ in $L^2(\Omega)$ as $\epsilon\to0$. Plugging it back to (B4) and using the minimality of $w_\mathbf{h}$, we have

$$a^2\|\mathbf{F}_\mathbf{h}-\nabla w_\mathbf{h}\|^2_{L^2(\Omega)}\leqslant a^2\|\mathbf{F}_\mathbf{h}-\nabla\zeta_\epsilon\|_{L^2(\Omega)}\leqslant|\Omega|+o(1).$$

Hence $a^2\|\mathbf{F}_\mathbf{h}-\nabla w_\mathbf{h}\|^2_{L^2(\Omega)}\leqslant|\Omega|$. From this and (4.17) we conclude that $a=a(\mathbf{h})$, and $\nabla\zeta_\epsilon\to\nabla w_\mathbf{h}$ as $\epsilon\to0$. Then we apply the elliptic estimate to the equation of ζ_ϵ [which can be derived from (4.19)], and use the condition $\int_\Omega\zeta_\epsilon\,dx=0$ to conclude that $\zeta_\epsilon\to w_\mathbf{h}$ as $\epsilon\to0$, which contradicts the fact $\|\zeta_\epsilon\|_{L^\infty(\Omega)}\to0$ as $\epsilon\to0$. Case 2 cannot happen. Now claim 2 is proved. □

APPENDIX C: PROOF OF (4.41) AND (4.44)

In this section we keep the notations in the proof of Theorem 4.2.

Proof of (4.41): Step C1. Using (4.40) we compute

$$\nabla_{a\epsilon\mathbf{A}_\epsilon}\psi_\epsilon = a\epsilon c_\epsilon\Bigg[i(\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}}) + \epsilon(\nabla\psi_{2,\epsilon} + a w_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}) - i\epsilon^2\left(a\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}} + \frac{|c_\epsilon|^2}{\kappa^2}\mathbf{A}_{2,\epsilon}\right) + a\epsilon^3\frac{|c_\epsilon|^2}{\kappa^2}\mathbf{A}_{2,\epsilon}(i w_{\mathbf{h}} - \epsilon\psi_{2,\epsilon})\Bigg]. \tag{C1}$$

From step 2.1 of the proof of Theorem 4.2 we have $\epsilon\psi_{2,\epsilon}\to 0$ in $C^{2+\alpha}(\overline{\Omega})$ and $\epsilon\mathbf{A}_{2,\epsilon}\to\mathbf{0}$ in $C^{1+\alpha}(\overline{\Omega})$ as $\epsilon\to 0$. So we can write

$$\mathfrak{I}\{\overline{\psi_\epsilon}\nabla_{a\epsilon\mathbf{A}_\epsilon}\psi_\epsilon\} = a\epsilon|c_\epsilon|^2(\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}} + \epsilon\mathfrak{I}\{\nabla\psi_{2,\epsilon}\} + \epsilon\hat{\mathbf{q}}_\epsilon),$$

where $\|\hat{\mathbf{q}}_\epsilon\|_{C^{1+\alpha}(\overline{\Omega})}\leq C$ for some C independent of ϵ. $\mathbf{A}_{2,\epsilon}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$ and satisfies the equation

$$\mathrm{curl}^2\,\mathbf{A}_{2,\epsilon} = (\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}} + \epsilon\mathfrak{I}\{\nabla\psi_{2,\epsilon}\} + \epsilon\hat{\mathbf{q}}_\epsilon)\chi_\Omega \quad \text{in } \mathbb{R}^3,$$

and $\int_\Omega \mathbf{A}_{2,\epsilon}\,dx = \mathbf{0}$. Let

$$\mathbf{B}_\epsilon = \mathbf{A}_{2,\epsilon} - \mathbf{U}_{\mathbf{h}}, \quad \mathbf{f}_{1,\epsilon} = \epsilon(\mathfrak{I}\{\nabla\psi_{2,\epsilon}\} + \hat{\mathbf{q}}_\epsilon)\chi_\Omega\,.$$

Then $\int_\Omega \mathbf{B}_\epsilon\,dx = \mathbf{0}$, and

$$\mathrm{curl}^2\,\mathbf{B}_\epsilon = \mathbf{f}_{1,\epsilon} \quad \text{in } \mathbb{R}^3. \tag{C2}$$

As $\epsilon\to 0$ we have $\epsilon\psi_{2,\epsilon}\to 0$ in $C^{2+\alpha}(\overline{\Omega})$ and hence $\|\mathbf{f}_{1,\epsilon}\|_{C^{1+\alpha}(\overline{\Omega})}\to 0$. Although $\mathbf{f}_{1,\epsilon}$ depends on $\mathbf{A}_{2,\epsilon}$ and hence depends on $\mathbf{B}_\epsilon$, we treat it as a given vector field, and treat $\mathbf{B}_\epsilon$ as a solution of a linear system. Recall that $\mathbf{B}_\epsilon\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$, and hence $\mathbf{B}_\epsilon$ is a finite energy solution of (C2). Write (C2) as

$$-\Delta\mathbf{B}_\epsilon = \mathbf{f}_{1,\epsilon} \quad \text{in } \mathbb{R}^3. \tag{C3}$$

Using Newton potential we can show that (C3) has a finite energy solution $\mathbf{u}_\epsilon$ which decays to $\mathbf{0}$ as $|x|\to\infty$, and

$$\|\mathbf{u}_\epsilon\|_{L^\infty(\mathbb{R}^3)}\leq C'\|\mathbf{f}_\epsilon\|_{L^\infty(\mathbb{R}^3)} = C'\epsilon\|\mathfrak{I}\{\nabla\psi_{2,\epsilon}\} + \hat{\mathbf{q}}_\epsilon\|_{L^\infty(\Omega)},$$

where C' is independent of ϵ. On the other hand, as in the proof of Lemma 3.4 we can show that, up to an additive constant vector, $\mathbf{B}_\epsilon$ is the only solution of (C3) in $\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div})$. Therefore $\mathbf{B}_\epsilon = \mathbf{u}_\epsilon - \mathbf{c}_\epsilon$, where $\mathbf{c}_\epsilon = \fint_\Omega \mathbf{u}_\epsilon\,dx$. Hence we conclude that

$$\mathbf{A}_{2,\epsilon} = \mathbf{U}_{\mathbf{h}} + \mathbf{B}_\epsilon, \quad \|\mathbf{B}_\epsilon\|_{L^\infty(\mathbb{R}^3)}\leq C\epsilon\|\mathfrak{I}\{\nabla\psi_{2,\epsilon}\} + \hat{\mathbf{q}}_\epsilon\|_{L^\infty(\Omega)}, \tag{C4}$$

where C is independent of ϵ.

Step C2. Now we use the energy estimate to show that

$$|c_\epsilon|^2 = 1 - a^2\omega(\mathbf{h}) + O(\epsilon), \quad \int_\Omega |\nabla\psi_{2,\epsilon}|^2\,dx\leq C. \tag{C5}$$

Note that at moment we do not know yet whether $\psi_{2,\epsilon}$ is bounded in $W^{1,2}(\Omega)$, but we know that $\epsilon\psi_{2,\epsilon}\to 0$ in $C^{2+\alpha}(\overline{\Omega})$ as $\epsilon\to 0$. Using (C1) and (C4) we find

$$\int_\Omega |\nabla_{a\epsilon\mathbf{A}_\epsilon}\psi_\epsilon|^2\,dx = a^2\epsilon^2|c_\epsilon|^2\int_\Omega \{|\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}}|^2+\epsilon^2|\nabla\psi_{2,\epsilon}+aw_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}-ia\epsilon\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(\epsilon)|^2$$
$$+2\epsilon(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\Im[\nabla\psi_{2,\epsilon}+aw_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}-ia\epsilon\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(\epsilon)]\}dx.$$

Recall that

$$\int_\Omega (\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\nabla\psi_{2,\epsilon}\,dx=0.$$

Note that we always have

$$\int_\Omega \{|\nabla\psi_{2,\epsilon}+aw_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}-ia\epsilon\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(\epsilon)|^2+2a(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\Im[-i\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(1)]\}dx$$
$$\geqslant\frac{1}{2}\int_\Omega|\nabla\psi_{2,\epsilon}|^2\,dx-C, \tag{C6}$$

where C is independent of ϵ. In fact, since $\int_\Omega\psi_{1,\epsilon}\,dx=0$, (C6) is obviously true when $\|\psi_{2,\epsilon}\|_{L^2(\Omega)}$ is uniformly bounded. If $\|\psi_{2,\epsilon}\|_{L^2(\Omega)}\to\infty$, we have

$$\int_\Omega|\nabla\psi_{2,\epsilon}+aw_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}-ia\epsilon\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(\epsilon)|^2\,dx=(1+o(1))\int_\Omega|\nabla\psi_{2,\epsilon}|^2\,dx\geqslant C\int_\Omega|\psi_{2,\epsilon}|^2\,dx$$
$$\geqslant 4a\int_\Omega|(\nabla w_{\mathbf{h}}-\mathbf{F}_{\mathbf{h}})\cdot\Im[i\psi_{2,\epsilon}\mathbf{F}_{\mathbf{h}}+O(1)]|dx.$$

So (C6) is true. Using (C6) we find

$$\int_\Omega|\nabla_{a\epsilon\mathbf{A}_\epsilon}\psi_\epsilon|^2\,dx\geqslant a^2\epsilon^2|c_\epsilon|^2\left\{\omega(\mathbf{h})|\Omega|+\frac{\epsilon^2}{2}\int_\Omega|\nabla\psi_{2,\epsilon}|^2\,dx-C\epsilon^2\right\}. \tag{C7}$$

From (4.40) we have

$$|\psi_\epsilon|^2=|c_\epsilon|^2(1+a^2\epsilon^2g_\epsilon),$$

where

$$g_\epsilon=w_{\mathbf{h}}^2+\frac{2}{a}\Re(\psi_{2,\epsilon})+2\epsilon w_{\mathbf{h}}\Im(\psi_{2,\epsilon})+\epsilon^2|\psi_{2,\epsilon}|^2.$$

So

$$\int_\Omega(|\psi_\epsilon|^2-1)^2\,dx=(|c_\epsilon|^2-1)^2|\Omega|+2a^2\epsilon^2|c_\epsilon|^2(|c_\epsilon|^2-1)\int_\Omega g_\epsilon\,dx+a^4\epsilon^4|c_\epsilon|^4\int_\Omega g_\epsilon^2\,dx.$$

$\int_\Omega g_\epsilon\,dx=O(1)$ since $\int_\Omega\psi_{2,\epsilon}\,dx=0$, and $\epsilon^2g_\epsilon^2=o(1)$ since $\epsilon\psi_{2,\epsilon}=o(1)$. So

$$\int_\Omega(|\psi_\epsilon|^2-1)^2\,dx=(|c_\epsilon|^2-1)^2|\Omega|+O(\epsilon^2). \tag{C8}$$

From (C7) and (C8) we get

$$\int_\Omega \left\{ |\nabla_{a\epsilon \mathbf{A}_\epsilon} \psi_\epsilon|^2 + \frac{\epsilon^2}{2}(|\psi_\epsilon|^2-1)^2 \right\} dx$$
$$\geqslant \frac{\epsilon^2|\Omega|}{2}\left\{ 2a^2|c_\epsilon|^2\omega(\mathbf{h}) + \epsilon^2 \fint_\Omega |\nabla \psi_{2,\epsilon}|^2\, dx + (|c_\epsilon|^2-1)^2 - C\epsilon^2 \right\}.$$

Comparing this with (4.37) we find

$$a^2|c_\epsilon|^2\omega(\mathbf{h}) + \frac{1}{2}(|c_\epsilon|^2-1)^2 + \frac{\epsilon^2}{2}\fint_\Omega |\nabla \psi_{2,\epsilon}|^2\, dx \leqslant a^2\omega(\mathbf{h}) - \frac{1}{2}a^4\omega(\mathbf{h})^2 + C\epsilon^2.$$

Thus

$$[|c_\epsilon|^2 - 1 + a^2\omega(\mathbf{h})]^2 + \epsilon^2 \fint_\Omega |\nabla \psi_{2,\epsilon}|^2\, dx \leqslant C\epsilon^2.$$

(C5) is proved.

Step C3. Plugging $\psi_{1,\epsilon} = i w_{\mathbf{h}} + \epsilon \psi_{2,\epsilon}$ into (4.39) we find

$$\begin{aligned} &-\Delta \psi_{2,\epsilon} + 2ia(\mathbf{F_h} + \epsilon \mathbf{A}_{1,\epsilon})\cdot(i\nabla w_{\mathbf{h}} + \epsilon \nabla \psi_{2,\epsilon}) + a|\mathbf{F_h} + \epsilon \mathbf{A}_{1,\epsilon}|^2(1 + ia\epsilon w_{\mathbf{h}} + a\epsilon^2 \psi_{2,\epsilon}) \\ &\quad = (1-|c_\epsilon^2||1 + a\epsilon(i w_{\mathbf{h}} + \epsilon \psi_{2,\epsilon})|^2)\left(\frac{1}{a} + i\epsilon w_{\mathbf{h}} + \epsilon^2 \psi_{2,\epsilon}\right) \quad \text{in } \Omega, \\ &\frac{\partial \psi_{2,\epsilon}}{\partial \nu} = -a w_{\mathbf{h}} \mathbf{F_h}\cdot \nu + i\epsilon[a\psi_{2,\epsilon}\mathbf{F_h}\cdot\nu + (1 + a\epsilon(i w_{\mathbf{h}} + \epsilon \psi_{2,\epsilon}))\mathbf{A}_{1,\epsilon}\cdot \nu] \quad \text{on } \partial\Omega. \end{aligned} \tag{C9}$$

Recall that $\|\mathbf{A}_{1,\epsilon}\|_{C^{1+\alpha}(\Omega)} = O(\epsilon)$ and $\int_\Omega \psi_{2,\epsilon}\, dx = \underline{0}$. Using (C5) and applying the elliptic estimate to (C9) we see that $\{\psi_{2,\epsilon}\}$ is bounded in $C^{2+\alpha}(\overline{\Omega})$. Passing to a subsequence we find that $\psi_{2,\epsilon} \to \psi_2$ in $C^{2+\alpha}(\overline{\Omega})$ as $\epsilon \to 0$, and ψ_2 satisfies

$$-\Delta \psi_2 - 2a\mathbf{F_h}\cdot\nabla w_{\mathbf{h}} + a|\mathbf{F_h}|^2 = a\omega(\mathbf{h}) \quad \text{in } \Omega,$$

$$\frac{\partial \psi_2}{\partial \nu} = -a w_{\mathbf{h}} \mathbf{F_h}\cdot\nu \quad \text{on } \partial\Omega.$$

Moreover $\int_\Omega \psi_2\, dx = 0$. Comparing this equation with (4.29) we find that $\psi_2 = a\psi_{\mathbf{h}}$. Since the limit is independent of the choice of subsequences, we must have $\psi_{2,\epsilon} \to a\psi_{\mathbf{h}}$ in $C^{2+\alpha}(\Omega)$ as $\epsilon \to 0$. From this and (C4) we find $\|\mathbf{B}_\epsilon\|_{L^\infty(\mathbb{R}^3)} \leqslant C\epsilon$. This verifies the first inequality in (4.41). Using this, and applying the elliptic estimate to the equation of $\psi_{2,\epsilon} - a\psi_{\mathbf{h}}$ derived from (C9), we get the second inequality in (4.41). The third inequality in (4.41) has been proved in (C5). □

Proof of (4.44): Suppose (4.44) were not true. Passing to a subsequence we assume $m^\epsilon \ll |l^\epsilon|$. Let

$$\zeta^\epsilon = -\frac{i m^\epsilon}{a_\epsilon l^\epsilon}\phi_{1,\epsilon}.$$

Since $|\mathbf{A}_{1,\epsilon}| = o(\epsilon)$ and $m^\epsilon/l^\epsilon = o(1)$, we have

$$\frac{\epsilon^2}{2}|\Omega| \geqslant \mathcal{G}[\phi_\epsilon, \mathbf{A}_\epsilon] \geqslant \int_\Omega \left\{ |\nabla_{\epsilon a_\epsilon \mathbf{A}_\epsilon} \phi_\epsilon|^2 + \frac{\epsilon^2}{2}(1-|\phi_\epsilon|^2)^2 \right\} \mathrm{d}x$$
$$= \epsilon^2 \left\{ a_\epsilon^2 |l^\epsilon|^2 \int_\Omega |\mathbf{F_h} - \nabla \zeta^\epsilon|^2 \, \mathrm{d}x + \frac{1}{2}(1-|l^\epsilon|^2)^2 |\Omega| + o(\epsilon |l^\epsilon|^2) \right\}$$
$$= \epsilon^2 |\Omega| \left\{ \frac{1}{2} + a_\epsilon^2 |l^\epsilon|^2 \fint_\Omega |\mathbf{F_h} - \nabla \zeta^\epsilon|^2 \, \mathrm{d}x - |l^\epsilon|^2 + \frac{1}{2}|l^\epsilon|^4 + o(\epsilon |l^\epsilon|^2) \right\}.$$

Therefore

$$a_\epsilon^2 \fint_\Omega |\mathbf{F_h} - \nabla \zeta^\epsilon|^2 \, \mathrm{d}x \leqslant 1 + o(\epsilon).$$

From (4.17), $a_\epsilon \geqslant a(\mathbf{h}) + o(1)$. So we find

$$\fint_\Omega |\mathbf{F_h} - \nabla \zeta^\epsilon|^2 \, \mathrm{d}x \leqslant \omega(\mathbf{h}) + o(1).$$

It implies that $\{\zeta^\epsilon\}$ is a minimizing sequence of $\omega(\mathbf{h})$. Note that $\int_\Omega \zeta^\epsilon \, \mathrm{d}x = 0$. We can pass to a subsequence and assume that $\zeta^\epsilon \to w_\mathbf{h}$ weakly in $W^{1,2}(\Omega)$ and strongly in $L^2(\Omega)$ as $\epsilon \to 0$. However, using (4.43) we find

$$\|\zeta^\epsilon\|_{L^2(\Omega)} = \left\| \frac{m_\epsilon}{a_\epsilon l^\epsilon} \phi_{1,\epsilon} \right\|_{L^2(\Omega)} \to 0 \quad \text{as} \quad \epsilon \to 0.$$

This contradiction shows that (4.44) is true. □

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Tensor operators and constructing indecomposable representations of semidirect product groups

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(Received 28 November 2002; accepted 5 March 2003)

Consider a semidirect product group $G=H\ltimes V$, where H is reductive and V is a vector group. Two irreps π_1 and π_2 of H can be ''assembled'' into a representation of G if it is possible to construct an indecomposable representation Π of G whose restriction to H is $\pi_1\oplus\pi_2$. It is shown that this is equivalent to the existence of a tensor operator from π_2 to π_1 carrying a representation of H which is equivalent to a nontrivial quotient of the representation which defines the semidirect product. This provides a systematic method for deciding whether two irreps can be assembled, and, if so, in how many inequivalent ways. The method is applied in many of the standard examples that arise in physical questions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1571659]

I. INTRODUCTION

Cantoni[1] considered semidirect product groups $G=H\ltimes V$, where H is reductive and V is Abelian. Suppose π_1 and π_2 are finite-dimensional irreps of H. He asked whether it is possible to ''assemble'' them into an indecomposable representation of G, that is, to construct an indecomposable representation Π of G whose restriction to H is $\pi_1\oplus\pi_2$. By explicit calculation, he answered this question in a number of cases.

In the present work, we consider the special case in which V is a vector group, a case which includes many groups that are important in physics. From Proposition 3.1 below, it follows that any finite-dimensional irreducible representation of G is obtained by taking an irrep of H and extending it to G by letting V act trivially. The interest in indecomposable representations of the sort described above is that they show how the action of the Abelian subgroup V can couple different irreps of the reductive subgroup H.

After some preliminaries about the structure of an ''assembled'' representation, we show that the construction of such a representation Π amounts to specifying a ''tensor operator'' in the sense of Rowe and Repka.[3] This leads to a systematic approach which makes it possible to describe not only when such a construction is possible, but also to describe the number of mutually inequivalent constructions there are. For a given group G, the theory provides a straightforward method for deciding whether particular irreps π^λ and π^μ of H can be assembled into an indecomposable representation of G. For many of the groups of interest in physics, the representation of H which defines the semidirect product is sufficiently simple that it is possible to give an explicit description of all pairs π^λ and π^μ which can be assembled into indecomposable representations of G.

A number of examples are given, including the semidirect product of each of the groups $\mathrm{SU}(n)$, $\mathrm{Sp}(n)$, and $\mathrm{SO}(n)$ with its standard representation. In particular, we recover and extend most of the examples of Cantoni, with additional information about multiplicities.

II. PRELIMINARIES AND NOTATION

Let H be a reductive group, and π_0 a representation of H on a finite dimensional vector space V. Construct a semidirect product group, $G=H\ltimes V$, with the following multiplication: $\forall\ (g_1,v_1),\ (g_2,v_2)\in G,(g_1,v_1)(g_2,v_2)=(g_1g_2,\pi_0(g_2^{-1})v_1+v_2)$. We will consider the problem of constructing representations of G given representations of H.

For convenience, we will assume H is connected, as it usually is in the examples of interest. Also assume that π_0 does not contain the trivial representation of H. If V is a complex vector space, we will nonetheless consider it as a real vector space (i.e., by restricting to real scalars). We write π_0^c for the complexification of π_0.

We write $\{\alpha\}$ for the positive roots of H, $\{\beta_i\}$ for the simple roots, and $\{\beta_i^*\}$ for the corresponding fundamental weights. Though we will define the $\{\beta_i\}$ and $\{\beta_i^*\}$ as elements of the dual and co-dual spaces of the root space (respectively), we will also treat them as elements of the root space under the standard identification. As usual, $\delta=\frac{1}{2}\Sigma_{\alpha>0}\alpha$. If λ is a dominant integral weight and π^λ is a representation of G on a finite dimensional vector space with highest weight λ, then the dimension of π^λ is given by the Weyl dimension formula (cf., Humphreys[2]),

$$\dim(\pi^\lambda)=\frac{\Pi_{\alpha>0}(\lambda+\delta,\alpha)}{\Pi_{\alpha>0}(\delta,\alpha)}. \tag{1}$$

III. INDECOMPOSABLE REPRESENTATIONS

A. Structure of indecomposable representations

Proposition 3.1: Suppose Π *is a representation of* G *on a finite-dimensional (complex) Hilbert space* $\mathbb{H}$. *Then* $\mathbb{H}$ *contains a nonzero* G*-invariant subspace* $\mathbb{H}'$ *on which* V *acts trivially*.

Proof: Since V is Abelian, it is in particular solvable, so Lie's Theorem says that there exists a nonzero $\varphi\in\mathbb{H}$ which is a simultaneous eigenvector for the restriction of Π to V, i.e., for every $v\in V$, $\Pi(v)\varphi=\alpha_\varphi(v)\varphi$, for some $\alpha_\varphi(v)\in\mathbb{C}$.

Now, for any $v\in V$, $h\in H$, we have

$$\Pi(v)\Pi(h)\varphi=\Pi(h)\Pi(h^{-1}vh)\varphi=\Pi(h)\Pi(v^{h^{-1}})\varphi=\Pi(h)\alpha_\varphi(v^{h^{-1}})\varphi=\alpha_\varphi(v^{h^{-1}})\Pi(h)\varphi,$$

showing that not only φ, but also $\Pi(h)\varphi$, for any $h\in H$, is an eigenvector for $\Pi(v)$.

Let $\mathbb{H}'$ be the H-invariant subspace generated by φ. Since it is spanned by eigenvectors for V, it is in fact G-invariant. For fixed $v\in V$, note that the eigenvalue $\alpha_\varphi(v^{h^{-1}})$ is a continuous function of $h\in H$. Since there can be only finitely many distinct eigenvalues in a finite-dimensional space, the connectedness of H implies that it must be a constant function. In other words, for each $v\in V$, $\Pi(v)$ acts on $\mathbb{H}'$ as a scalar $\alpha(v)\cdot I$. In particular, on $\mathbb{H}'$, $\Pi(v)$ commutes with $\Pi(h)$, for all $v\in V$, $h\in H$.

The character α of V can be written as $\alpha(v)=e^{A(v)}$, for some $A\in V^*\otimes\mathbb{C}$, where V^* means the real dual of V, with V regarded as a real vector space. The action of $h\in H$ is given by $\alpha(v^h)=e^{A(v^h)}=e^{A(\pi_0(h)(v))}=e^{(\overline{\pi_0}(h^{-1})(A))(v)}$, where $\overline{\pi_0}$ is the contragredient to π_0, acting on $V^*\otimes\mathbb{C}$. But since $\alpha(v^h)=\alpha(v)$, for all $v\in V$, $h\in H$, we see that A is fixed by $\overline{\pi_0}$. Since π_0 is assumed not to contain the trivial representation of H, this is possible only if $A=0$. This shows that V acts trivially on $\mathbb{H}'$, completing the proof. ●

Theorem 3.2: *Suppose* Π *is an indecomposable representation of* G *on a finite-dimensional Hilbert space* $\mathbb{H}$, *which, when restricted to* H, *is the direct sum of two irreps. Then it is possible to find an* H*-decomposition* $\mathbb{H}=\mathbb{H}_1\oplus\mathbb{H}_2$, *such that* $\mathbb{H}_1$ *and* $\mathbb{H}_2$ *carry irreps of* H *and* $\mathbb{H}_1$ *is* G*-invariant. Moreover, the action of* V *is trivial on* $\mathbb{H}_1$ *and on* $\mathbb{H}/\mathbb{H}_1$.

Proof: Let $\mathbb{H}_1$ be the subspace $\mathbb{H}'$ defined in proposition 3.1. Applying the proposition again to $\mathbb{H}/\mathbb{H}_1$ shows that V acts trivially there (in this case, $\mathbb{H}'$ is the whole space). Define $\mathbb{H}_2$ as an H-complementary subspace to $\mathbb{H}_1$. ●

B. Assembling irreps

Suppose Π is an indecomposable representation of G and define $\mathbb{H}_i$, $i=1,2$, as in theorem 3.2. Let π_i be the representation of H on $\mathbb{H}_i$, $i=1,2$. In this situation, we will say that "π_1 and π_2 are assembled into the representation Π of G." Note that the first irrep mentioned, π_1, occurs as a G-subrepresentation of Π.

If a basis is chosen for $\mathbb{H}$ which consists of a basis for $\mathbb{H}_1$ followed by a basis for $\mathbb{H}_2$, then for any $h \in H$, $v \in V$, the corresponding operators have block upper triangular matrices of the following forms:

$$\Pi(h) = \begin{pmatrix} \pi_1(h) & 0 \\ 0 & \pi_2(h) \end{pmatrix}, \quad \Pi(v) = \begin{pmatrix} I & T(v) \\ 0 & I \end{pmatrix}. \tag{2}$$

The indecomposability of Π implies that $T(v)$ is not identically zero.

IV. TENSOR OPERATORS

Suppose Π is an indecomposable representation of G on a finite-dimensional Hilbert space $\mathbb{H}$, which, when restricted to H, is the direct sum of two irreps. Define subspaces $\mathbb{H}_1$ and $\mathbb{H}_2$ as in theorem 3.2 and, for each $v \in V$, define $T(v) \in \hom(\mathbb{H}_2, \mathbb{H}_1)$ as in (2). Then $\{T(v): v \in V\}$ is a tensor operator in the sense of Rowe and Repka.[3] It can be written as a sum of tensor operators, each of which has rank equal to the rank of one of the irreducible constituents of π_0^c. Specifically, for $v \in V$, $h \in H$, $\psi \in \mathbb{H}_2$, $\pi_1(h)T(v)\psi = \pi_1(h)T(v)\pi_2(h^{-1})\pi_2(h)\psi = T^h(v)\pi_2(h)\psi$, where

$$T^h(v) = T(v^h); \tag{3}$$

i.e., under the action $h: T \mapsto T^h = \pi_1(h)T\pi_2(h^{-1})$, the matrices $\{T(v): v \in V\}$ carry a representation of H which is isomorphic to a nontrivial quotient of π_0^c.

Conversely, suppose we are given such a tensor operator, i.e., a (nonzero) collection of linear maps $T(v) \in \hom(\mathbb{H}_2, \mathbb{H}_1)$ which satisfy (3) and which carry a representation of H which is isomorphic to a nontrivial quotient of π_0^c. Then Eq. (2) gives an indecomposable representation Π of G whose restriction to H is $\pi_1 \oplus \pi_2$, with π_1 acting on a G-invariant subspace.

Let us consider possible equivalences between such representations. Any operator which commutes with the action of G must be block upper triangular because of the invariance of $\mathbb{H}_1$. Because of the irreducibility of both π_1 and π_2, the diagonal blocks must be scalars. If π_1 and π_2 are inequivalent representations of H, then the top right block must be zero. If π_1 and π_2 are equivalent, then, choosing compatible bases for $\mathbb{H}_1$ and $\mathbb{H}_2$, we find that the top right block must be a scalar. In either case, the only representations equivalent to the representation Π constructed above are those constructed in the same way using scalar multiples of the tensor operator T.

We have proven the following:

Theorem 4.1: *Let π_1 and π_2 be irreducible finite-dimensional representations of H. Then, in the language of Cantoni,[1] π_1 and π_2 can be "assembled" into an indecomposable representation of G if and only if there is a tensor operator T from π_2 into π_1, with T carrying a representation of H which is isomorphic to some nontrivial quotient of π_0^c.*

Moreover, if, up to scalar multiples, there is only one such tensor operator T from π_2 into π_1, then there is only one such assemblage, up to equivalence. If there are more than one such tensor operator, then there are infinitely many inequivalent assemblages, indexed by tensor operators modulo nonzero scalar multiples.

One of the main results of Rowe and Repka[3] is that the existence of a tensor operator from π_2 into π_1 having the same rank as an irrep π is equivalent to the occurrence of π_1 in the tensor product $\pi_2 \otimes \pi$. Combining this result with theorem 4.1, we obtain the following theorem:

Theorem 4.2: *With π_1 and π_2 as above, π_1 and π_2 can be "assembled" into an indecomposable representation of G if and only if the tensor product $\pi_0^c \otimes \pi_2$ contains π_1. Moreover, the number of inequivalent such assemblages is determined by the multiplicity with which π_1 occurs in $\pi_0^c \otimes \pi_2$: if it occurs only once, then there is only one assemblage, up to equivalence. Otherwise, there are infinitely many inequivalent assemblages.*

V. EXAMPLE: THE EUCLIDEAN GROUP E(2)

The two-dimensional Euclidean group E(2) is the semidirect product of SO(2) and $\mathbb{R}^2$, the groups of rotations and translations of the plane, respectively. We write χ_n for the character of SO(2) given by

$$\chi_n\left(\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\right) = e^{in\theta}.$$

It is also possible to express E(2) as the semidirect product of the unit circle $S^1=\{e^{i\theta}\}$ and $\mathbb{C}$, using the matrix realization,

$$\mathrm{E}(2)=\left\{\begin{pmatrix} e^{i\theta} & z \\ 0 & 1 \end{pmatrix} : \theta\in\mathbb{R},\ \ z\in\mathbb{C}\right\}. \tag{4}$$

Here we could think of $V=\mathbb{C}$ as a one-dimensional complex vector space carrying the irrep χ_1 of $S^1\cong\mathrm{SO}(2)$, but as described above, it is necessary for present purposes to regard it as a two-dimensional real vector space on which $S^1\cong\mathrm{SO}(2)$ acts by rotations. In particular, the complexification $\mathbb{C}\otimes V$ is the direct sum $\chi_1\oplus\chi_{-1}$.

In this context, theorem 4.2 says that an irrep χ_n of $H=\mathrm{SO}(2)$ can be assembled into an indecomposable representation of G with either χ_{n+1} or χ_{n-1}, reproducing the result of Cantoni.[1] Explicitly, these representations are given as follows:

$$\begin{pmatrix} e^{i\theta} & z \\ 0 & 1 \end{pmatrix}\mapsto\begin{pmatrix} e^{in\,\theta} & e^{i(n+1)\theta}\overline{z} \\ 0 & e^{i(n+1)\theta} \end{pmatrix},\quad \begin{pmatrix} e^{i\theta} & z \\ 0 & 1 \end{pmatrix}\mapsto\begin{pmatrix} e^{in\theta} & e^{i(n-1)\theta}z \\ 0 & e^{i(n-1)\theta} \end{pmatrix}.$$

If we had worked with V as a complex vector space, we would have missed the first possibility.

VI. EXAMPLE: SU($N+1$)

Let $H=\mathrm{SU}(n+1)$; then the simple roots of H are $\beta_1,\ldots,\beta_n$, given by $\beta_i(u_0,\ldots,u_n)=u_{i-1}-u_i$. The fundamental weights are $\beta_1^*,\ldots,\beta_n^*$, given by $\beta_i^*(u_0,\ldots,u_n)=\Sigma_{j=0}^{i-1}u_j$. It follows that $\delta=\frac{1}{2}\Sigma_{\alpha>0}\alpha=\Sigma_{k=1}^n\beta_k^*$. Let $e_0=\beta_1^*, e_i=\beta_i^*-\beta_{i-1}^*$ $(2\leqslant i\leqslant n-1)$, and $e_n=-\beta_n^*$.

We shall consider the case where π_0 is the "standard" $(n+1)$-dimensional (complex) representation of SU$(n+1)$; its highest weight is e_0, and its weights e_i all have multiplicity one. The complexification of this $2(n+1)$-dimensional real vector space carries two irreps, π_0^1, which is the irrep just mentioned, with highest weight e_0, and its contragredient π_0^2, which has weights $-e_i$, $i=0,\ldots,n$, and highest weight $-e_n$.

We note that for $n=1$, i.e., for $H=\mathrm{SU}(2)$, these irreps π_0^1 and π_0^2 are equivalent, but for $n>1$, they are inequivalent, and the difference between their highest weights is e_0+e_n, which is not in the root lattice.

For any dominant integral weight λ, we write π^λ for the irrep with highest weight λ.

Proposition 6.1: For any dominant integral weight λ,

$$\sum_{\ell=0}^{n}\prod_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)=(n+1)\prod_{\alpha>0}(\delta+\lambda,\alpha).\ (*)$$

Proof: Write $\lambda=\Sigma_{k=1}^n c_k\beta_k^*$; then $\lambda+\delta=\Sigma_{k=1}^n(c_k+1)\beta_k^*=\Sigma_{k=1}^n x_k\beta_k^*$, where $x_k=c_k+1$.

Fix i and j with $1\leqslant i\leqslant j\leqslant n$; note that the right side of $(*)$ is a product of factors of the form $X_{ij}=\Sigma_{k=i}^j x_k$. Assume that $X_{ij}=0$; it follows that all products in $(*)$ are zero except for $\Pi_{\alpha>0}(e_{i-1}+\delta+\lambda,\alpha)$ and $\Pi_{\alpha>0}(e_j+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^j\beta_k=Y_{ij}$ is zero. Now, we shall show that $\Pi_{\alpha>0}(e_{i-1}+\delta+\lambda,\alpha)$

$=-\Pi_{\alpha>0}(e_j+\delta+\lambda,\alpha)$. To do this, still under the assumption that $X_{ij}=0$, we shall consider both of the remaining products as polynomials in $x_1,\ldots,x_n$, show that they have the same roots, and finally conclude that they differ by a sign.

Define a real-valued function m on the root space as follows: if $\alpha=\Sigma_{k=1}^n p_k\beta_k$, let $m(\alpha)=p_{j+1}-p_j-p_i+p_{i-1}$. Let $\gamma=\Sigma_{k=1}^n a_k\beta_k$ be a fixed positive root of H, and for convenience, let $a_0=a_{n+1}=0$ and $m=m(\gamma)$. Now, $(e_{i-1}+\delta+\lambda,\gamma)=(\delta+\lambda,\gamma)+a_i-a_{i-1}=(\delta+\lambda,\gamma)+a_i-a_{i-1}+mX_{ij}=(\delta+\lambda,\gamma)+a_{j+1}-a_j-m+mX_{ij}=(\delta+\lambda,\gamma)+(e_j,\gamma)+(e_j+\delta+\lambda,mY_{ij})=(e_j+\delta+\lambda,\gamma+mY_{ij})$. The map $T:\alpha\to\alpha+m(\alpha)Y_{ij}$ is the reflection in the hyperplane perpendicular to Y_{ij}, and thus $\gamma+mY_{ij}$ is a root of H. So, if $(e_{i-1}+\delta+\lambda,\gamma)=0$, then $(e_j+\delta+\lambda,\pm(\gamma+mY_{ij}))=0$, and since T is one-to-one, the two polynomials have exactly the same roots. Furthermore, as an element of the Weyl group, T has an odd length, so T maps an odd number of positive roots to negative roots. Hence the products differ by a minus sign.

Since each factor of $\Pi_{\alpha>0}(\delta+\lambda,\alpha)$ is equal to X_{ij} for some i and j, we have shown that the roots of the right side of $(*)$ are contained within the roots of the left side of $(*)$. Since the right side of $(*)$ is a product of distinct linear factors (in the x_i), then the left side of $(*)$ is divisible by each of these factors. But both sides of $(*)$ are of the same degree, hence it follows that they differ by a multiplicative constant. Substituting $\lambda=0$ shows that the constant must be $n+1$. ●

Proposition 6.2: Fix $j\in\{1,\ldots,n\}$ and consider a dominant integral weight $\lambda=\Sigma_{k=1}^n c_k\beta_k^*$ with $c_j=0$; then

$$\prod_{\alpha>0}(e_j+\delta+\lambda,\alpha)=0.$$

Proof: Let $\alpha=\beta_j>0$. Then, if $j\neq n$, $(e_j+\delta+\lambda,\alpha)=(\beta_{j+1}^*-\beta_j^*+\Sigma_{k=1}^n\beta_k^*+\Sigma_{k=1}^n c_k\beta_k^*,\beta_j)=-1+1+c_j=0$, so the product is zero. The proof is similar for $j=n$. ●

In the tensor product $\pi^\lambda\otimes\pi_0^1$, any irreducible representation that occurs must have highest weight $\lambda+e_i$, for some $i\in\{0,\ldots,n\}$, and cannot occur more than once. By the Weyl dimension formula (1), the sum of the dimensions of the irreducible representations with highest weights $\lambda+e_i$ is $\Sigma_{\ell=0}^n\Pi_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)$, and $\dim(\pi^\lambda\otimes\pi_0^1)=\dim(\pi_0^1)\dim(\pi^\lambda)=(n+1)\times[\Pi_{\alpha>0}(\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)]$. Now, we would like to show that the sum of the dimensions of the $\pi^{\lambda+e_i}$ $(i=0,\ldots,n)$ is equal to the dimension of the tensor product $\pi^\lambda\otimes\pi_0^1$; this follows immediately from proposition 6.1 if all the $\lambda+e_i$ are dominant integral weights.

Now $\mu=\Sigma_{i=1}^n z_i\beta_i^*$ is not a dominant integral weight if and only if $z_i<0$, for some $i\in\{1,\ldots,n\}$. Since $\lambda=\Sigma_{k=1}^n c_i\beta_i$ is the highest weight of π^λ, the one and only way that $\lambda+e_i$ would not be a dominant integral weight is if $c_i=0$. Thus, proposition 6.2 implies that if $\lambda+e_i$ is not a dominant integral weight, then the dimension formula gives a value of zero. Taken together, propositions 6.1 and 6.2 imply that the irreducible representations that occur in the tensor product $\pi^\lambda\otimes\pi_0^1$ are exactly the $\pi^{\lambda+e_i}$ for which $\lambda+e_i$ is a dominant integral weight. Taking contragredients, we also see that the irreducible representations that occur in the tensor product $\pi^\lambda\otimes\pi_0^2$ are exactly the $\pi^{\lambda-e_i}$ for which $\lambda-e_i$ is a dominant integral weight. Noting that $\lambda+e_i$ is never equal to $\lambda-e_j$, we have proved the following.

Theorem 6.3: *The irreducible representations π^λ and π^μ of $H=\mathrm{SU}(n+1)$ can be assembled into an indecomposable representation of $G=\mathrm{SU}(n+1)\ltimes\mathbb{C}^{n+1}$ if and only if $\mu=\lambda\pm e_i$, for some $i\in\{0,\ldots,n\}$.*

For $n=1$, i.e., for $H=\mathrm{SU}(2)$, each such assemblage can be constructed in infinitely many inequivalent ways. If $n>1$, for each of the possible pairs of representations, the assemblage is unique.

VII. EXAMPLE: SU(3)$\ltimes\mathbb{R}^8$

Let $H=\mathrm{SU}(3)$ and let π_0 be the eight-dimensional real (adjoint) representation of H; it has weights: $e_1=\beta_1^*+\beta_2^*$, $e_2=2\beta_1^*-\beta_2^*$, $e_3=2\beta_2^*-\beta_1^*$, $e_4=-\beta_1^*-\beta_2^*$, $e_5=-2\beta_1^*-\beta_2^*$, e_6

$=-2\beta_2^*-\beta_1^*$, $e_7=0$, and $e_8=0$. Now we will consider the case where $G=\mathrm{SU}(3)\ltimes\mathbb{R}^8$. If the highest weight of a representation π^λ of H is $\lambda=c_1\beta_1^*+c_2\beta_2^*$, then the dimension of π^λ is given by (1); it is $\dim(\pi^\lambda)=(c_1+1)(c_2+1)(c_1+c_2+2)/2$.

Lemma 7.1: $\Sigma_{k=1}^8\dim(\pi^{\lambda+e_k})=8\dim(\pi^\lambda)$.

Proof: A direct calculation gives the result. ●

In the tensor product $\pi^\lambda\otimes\pi_0$, any irreducible representation that occurs must have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,8\}$ and cannot occur more than once unless it has highest weight λ, in which case it cannot occur more than twice. We would like to show that the irreducible representation with highest weight $\lambda+e_i, i\in\{1,\ldots,6\}$ occurs exactly once in the tensor product, provided that $\lambda+e_i$ is a dominant integral weight, and that there are two copies of the irreducible representation with highest weight λ in the tensor product. This is easy to show if neither c_1 nor c_2 is equal to zero; the proof is as follows.

If $\lambda=c_1\beta_1^*+c_2\beta_2^*$ is the highest weight of an irreducible representation π^λ of H, and c_1 and c_2 are both not zero, then the weight $\lambda+e_1$ occurs in the tensor product $\pi^\lambda\otimes\pi_0$ with multiplicity one; $\lambda+e_2$ occurs with multiplicity two, as does $\lambda+e_3$; and λ occurs with multiplicity six. This implies that the irreducible representations with highest weights $\lambda+e_1,\lambda+e_2$, and $\lambda+e_3$ occur in the tensor product with multiplicity one, and the irreducible representation with highest weight λ occurs with multiplicity 2. This result, along with lemma 7.1 and the fact that if $\lambda+e_i$ is not a dominant integral weight and is substituted into (1), a value of zero is obtained (this can be verified by direct computation), shows that the irreducible representations with highest weights $\lambda+e_i$ for some $i\in\{1,\ldots,6\}$ appear exactly once in the tensor product, and the irreducible representation with highest weight λ occurs twice.

Now, suppose that $\lambda=c_1\beta_1^*+c_2\beta_2^*$ is the highest weight of an irreducible representation π^λ of H, with $c_1>1$ and $c_2=0$. Then the only possible irreducible representations that may occur in the tensor product are those with highest weight $\lambda+e_1$, $\lambda+e_3$, $\lambda+e_5$, or λ, since these are the only $\lambda+e_i$ that are dominant integral weights. In the tensor product $\pi^\lambda\otimes\pi_0$, the weight $\lambda+e_1$ occurs with multiplicity one; $\lambda+e_3$ occurs with multiplicity two; $\lambda+e_5$ occurs with multiplicity six; and λ occurs with multiplicity four. This implies that the irreducible representations that occur in the tensor product occur only once and are those with highest weights $\lambda+e_1$, $\lambda+e_3$, $\lambda+e_5$, and λ. If $c_1=1$ and $c_2=0$ then one can check that the irreducible representations that occur in the tensor product $\pi^\lambda\otimes\pi_0$ all have multiplicity one and are those with highest weights $\lambda+e_1$, $\lambda+e_3$, and λ. Similarly, one can show that if $c_1=0$ and $c_2>1$, then the irreducible representations that occur in the tensor product all have multiplicity one and are those with highest weights $\lambda+e_1$, $\lambda+e_2$, $\lambda+e_6$, and λ. Also, if $c_1=0$ and $c_2=1$ then the irreducible representations that occur in the tensor product all have multiplicity one and are those with highest weights $\lambda+e_1$, $\lambda+e_2$, and λ. If $c_1=c_2=0$ then all that appears in the tensor product is the adjoint representation, which has highest weight $\lambda+e_1=0+e_1=e_1$.

Thus, we have proven the following theorem:

Theorem 7.2: *The representations of $H=\mathrm{SU}(3)$ that may be assembled with π^λ into a representation of $G=\mathrm{SU}(3)\ltimes\mathbb{R}^8$ are those that have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,8\}$. Furthermore, if $\lambda=c_1\beta_1^*+c_2\beta_2^*$ and neither c_1 nor c_2 are zero, then there are infinitely many inequivalent ways of assembling π^λ with itself and exactly one way of assembling π^λ and $\pi^{\lambda+e_i}$, $i\in\{1,\ldots,6\}$. If either $c_1=0$ or $c_2=0$ and $\lambda+e_i$ is a dominant integral weight, then there is exactly one way of assembling π^λ and $\pi^{\lambda+e_i}$.*

VIII. EXAMPLE: Sp(*N*)

Let $H=\mathrm{Sp}(n)$; then the simple roots of H are $\beta_1,\ldots,\beta_n$, given by $\beta_i(u_1,\ldots,u_n)=u_i-u_{i+1}$ for $i=1,\ldots,n-1$, and $\beta_n(u_1,\ldots,u_n)=2u_n$. The fundamental weights are $\beta_i^*,\ldots,\beta_n^*$ given by $\beta_i^*(u_1,\ldots,u_n)=\Sigma_{k=1}^i u_k$. It follows that $\delta=\frac{1}{2}\Sigma_{\alpha>0}\alpha=\Sigma_{k=1}^n\beta_k^*$. Let $e_1=\beta_1^*$, $e_i=\beta_i^*-\beta_{i-1}^*(2\leqslant i\leqslant n)$, and $e_{n+j}=-e_j$ for $j=1,\ldots,n$. We shall consider the case where π_0 is the "standard" $2n$-dimensional (real) representation of $\mathrm{Sp}(n)$; its highest weight is e_1, and all its weights have multiplicity one.

Proposition 8.1: For any dominant integral weight λ,

$$\sum_{\ell=1}^{2n} \prod_{\alpha>0} (e_\ell+\delta+\lambda,\alpha)=2n\prod_{\alpha>0}(\delta+\lambda,\alpha). \quad (*)$$

Proof: Let $\lambda=\Sigma_{k=1}^{n} c_k\beta_k^*$; then $\lambda+\delta=\Sigma_{k=1}^{n}(c_k+1)\beta_k^*=\Sigma_{k=1}^{n}x_k\beta_k^*$, where $x_k=c_k+1$.

Fix i and j with $1\leqslant i\leqslant j\leqslant n$.

Case A: Suppose that $X_{ij}=\Sigma_{k=i}^{j}x_k=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{j}\beta_k=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$ is the same as that given for SU$(n+1)$ if one changes e_{i-1} to e_i and e_j to e_{j+1}. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ can be obtained by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{n+j+1}, and a_k to $-a_k$, for $k=i-1,i,j,j+1$.

Case B: Suppose that $X_{ij}=(\Sigma_{k=i}^{j}x_k)+(\Sigma_{k=j+1}^{n-1}2x_k)+x_n=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=(\Sigma_{k=i}^{j}\beta_k)+(\Sigma_{k=j+1}^{n-1}2\beta_k)+\beta_n=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ is similar to the one given for SU$(n+1)$; it may be obtained by making the following changes: e_{i-1} to e_i, e_j to e_{n+j+1}, a_{j+1} to $-a_{j+1}$, and a_j to $-a_j$. The proof that $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$ can be obtained from the proof for SU$(n+1)$ by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{j+1}, a_{i-1} to $-a_{i-1}$, a_i to $-a_i$.

Case C: Suppose that $X_{ij}=(2\Sigma_{k=i}^{n-1}x_k)+x_n=0$, $(i<n)$. Then all products in $(*)$ are zero except for $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=2\Sigma_{k=i}^{n-1}\beta_k+\beta_n=Y_{ij}$ is zero. Now, we will show that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$ by considering the two products as polynomials in $x_1,\ldots,x_n$, showing that they have the same roots, and then concluding that they must differ by a factor of -1.

Let γ be as in the proof for SU$(n+1)$, and let $m=m(\gamma)=a_i-a_{i-1}$. Now, $(e_i+\delta+\lambda,\gamma)=(\delta+\lambda,\gamma)+a_i-a_{i-1}=(\delta+\lambda,\gamma)+a_i-a_{i-1}+mX_{ij}=(\delta+\lambda,\gamma)+a_{i-1}-a_i-2m+mX_{ij}=(\delta+\lambda,\gamma)+(e_{n+i},\gamma)+(e_{n+i}+\delta+\lambda,mY_{ij})=(e_{n+i}+\delta+\lambda,\gamma+mY_{ij})$. Hence, by the same line of reasoning as in the proof for SU$(n+1)$, the products must differ by a sign.

Since each factor of $\Pi_{\alpha>0}(\delta+\lambda,\alpha)$ is covered by one of the above cases for some i and j, we have shown that the roots of the right side of $(*)$ are contained within the roots of the left side of $(*)$. By comparing degrees and substituting $\lambda=0$, we obtain the result. ●

Proposition 8.2: Fix $j\in\{1,\ldots,n\}$ *and consider a dominant integral weight* $\lambda=\Sigma_{k=1}^{n}c_k\beta_k^*$ *with* $c_j=0$; *then*

$$\prod_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=0, \quad \text{if } j\neq n,$$

and

$$\prod_{\alpha>0}(e_{n+j}+\delta+\lambda,\alpha)=0.$$

Proof: If $j\in\{1,\ldots,n-1\}$, then $(e_{j+1}+\delta+\lambda,\beta_j)=-1+1+c_j=0$ and $(e_{n+j}+\delta+\lambda,\beta_j)=-1+1+c_j=0$. If $j=n$, then $(e_{2n}+\delta+\lambda,\beta_j)=-2+2+c_j=0$. Thus, the proposition has been proven. ●

In the tensor product $\pi^\lambda\otimes\pi_0$, any irreducible representation that occurs must have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,2n\}$, and cannot occur more than once. By (1), the sum of the dimensions of the irreducible representations with highest weights $\lambda+e_i$ $(i=1,\ldots,2n)$ is $\Sigma_{\ell=1}^{2n}\Pi_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)$, and $\dim(\pi^\lambda\otimes\pi_0)=\dim(\pi_0)\dim(\pi^\lambda)=(2n)[\Pi_{\alpha>0}(\delta$

$+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)]$. We would like to show that the sum of the dimensions of the $\pi^{\lambda+e_i}$ $(i=1,\ldots,2n)$ is equal to the dimension of the tensor product $\pi^{\lambda}\otimes\pi_0$; we can infer this from proposition 8.1 if we know that all the $\lambda+e_i$ are dominant integral weights.

Now $\mu=\Sigma_{i=1}^{n}z_i\beta_i^*$ is not a dominant integral weight if and only if $z_i<0$, for some $i\in\{1,\ldots,n\}$. Since $\lambda=\Sigma_{k=1}^{n}c_i\beta_i$ is the highest weight of π^{λ}, the one and only way that $\lambda+e_i$ $i\in\{1,\ldots,n\}$ would not be a dominant integral weight is if $i\neq 1$ and $c_{i-1}=0$. The only way that $\lambda+e_{n+j}, j\in\{1,\ldots,n\}$, would not be a dominant integral weight is if $c_j=0$. So, proposition 8.2 implies that if $\lambda+e_i$ is not a possible highest weight vector, then the dimension formula gives a value of zero. Taken together, propositions 8.1 and 8.2 imply that the irreducible representations that occur in the tensor product $\pi^{\lambda}\otimes\pi_0$ are exactly those $\pi^{\lambda+e_i}$ for which $\lambda+e_i$ is a dominant integral weight. Therefore, we have proven the following.

Theorem 8.3: *The representations of $H=Sp(n)=Sp(n,\mathbb{R})$ that may be assembled with π^{λ} into a representation of $G=Sp(n)\ltimes\mathbb{R}^{2n}$ are those that have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,2n\}$. For all of the possible representations this assemblage is unique.*

IX. EXAMPLE: SO(2*N*)

Let $H=\mathrm{SO}(2n)$; then the simple roots of H are $\beta_1,\ldots,\beta_n$, given by $\beta_i(u_1,\ldots,u_n)=u_i-u_{i+1}$ for $i=1,\ldots,n-1$, and $\beta_n(u_1,\ldots,u_n)=u_{n-1}+u_n$. The fundamental weights are $\beta_i^*,\ldots,\beta_n^*$ given by $\beta_i^*(u_1,\ldots,u_n)=\Sigma_{k=1}^{i}u_k$ for $i\in\{1,\ldots,n-2\}$, $\beta_{n-1}^*(u_1,\ldots,u_n)=\frac{1}{2}(\Sigma_{k=1}^{n-1}u_k-u_n)$, and $\beta_n^*(u_1,\ldots,u_n)=\frac{1}{2}\Sigma_{k=1}^{n}u_k$. It follows that $\delta=\frac{1}{2}\Sigma_{\alpha>0}\alpha=\Sigma_{k=1}^{n}\beta_k^*$. Let $e_1=\beta_1^*$, $e_i=\beta_i^*-\beta_{i-1}^*(2\leqslant i\leqslant n-2)$, $e_{n-1}=\beta_n^*+\beta_{n-1}^*-\beta_{n-2}^*$, $e_n=\beta_n^*-\beta_{n-1}^*$, and $e_{n+j}=-e_j$ for $j=1,\ldots,n$. As in the previous examples, we shall consider the case where π_0 is the "standard" $2n$-dimensional (real) representation of $\mathrm{SO}(2n)$; its highest weight is e_1, and all its weights have multiplicity one.

Proposition 9.1: For any dominant integral weight λ,

$$\sum_{\ell=1}^{2n}\prod_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)=2n\prod_{\alpha>0}(\delta+\lambda,\alpha).\quad(*)$$

Proof: Let $\lambda=\Sigma_{k=1}^{n}c_k\beta_k^*$; then $\lambda+\delta=\Sigma_{k=1}^{n}(c_k+1)\beta_k^*=\Sigma_{k=1}^{n}x_k\beta_k^*$, where $x_k=c_k+1$.

Case A: Fix i and j with $1\leqslant i\leqslant j<n-2$.

Subcase A1: Suppose that $X_{ij}=\Sigma_{k=i}^{j}x_k=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{j}\beta_k=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$ is the same as that given for $\mathrm{SU}(n+1)$. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ can be obtained by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{n+j+1}, and a_k to $-a_k$, for $k=i-1,i,j,j+1$.

Subcase A2: Suppose that $X_{ij}=(\Sigma_{k=i}^{j}x_k)+(\Sigma_{k=j+1}^{n-2}2x_k)+x_{n-1}+x_n=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=(\Sigma_{k=i}^{j}\beta_k)+(\Sigma_{k=j+1}^{n-2}2\beta_k)+\beta_{n-1}+\beta_n=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ is similar to the one given for $\mathrm{SU}(n+1)$; it may be obtained by making the following changes: e_{i-1} to e_i, e_j to e_{n+j+1}, a_{j+1} to $-a_{j+1}$, and a_j to $-a_j$. The proof that $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$ can be obtained from the proof for $\mathrm{SU}(n+1)$ by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{j+1}, a_{i-1} to $-a_{i-1}$, a_i to $-a_i$.

Case B: Fix i and j with $1\leqslant i\leqslant j=n-2$ and suppose that $X_{ij}=\Sigma_{k=i}^{j}x_k=0$. Then all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{n-1}\beta_k=Y_{ij}$ is zero. Now, we shall show that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n-1}+\delta$

$+\lambda,\alpha)$. To do this, still under the assumption that $X_{ij}=0$, we shall consider both products as polynomials in $x_1,\ldots,x_n$, show that they have the same roots, and finally conclude that they differ by a sign.

Let $\gamma=\Sigma_{k=1}^{n}a_k\beta_k$ be a fixed positive root of H. Let $m=m(\gamma)=a_n+a_{n-1}-a_{n-2}-a_i+a_{i-1}$. Now, $(e_{i-1}+\delta+\lambda,\gamma)=(\delta+\lambda,\gamma)+a_i-a_{i-1}=(\delta+\lambda,\gamma)+a_i-a_{i-1}+mX_{ij}=(\delta+\lambda,\gamma)+a_n+a_{n-1}-a_{n-2}-m+mX_{ij}=(\delta+\lambda,\gamma)+(e_{n-1},\gamma)+(e_{n-1}+\delta+\lambda,mY_{ij})=(e_{n-1}+\delta+\lambda,\gamma+mY_{ij})$. Hence, by the same line of reasoning as in the proof for SU$(n+1)$, the products differ by a minus sign. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$ can be obtained by making the following changes: e_i to e_{n+i}, e_{n-1} to e_{2n-1}, and a_k to $-a_k$, for $k=i-1,i,n-2,n-1,n$.

Case C: Fix i and j with $1\leqslant i\leqslant j=n-1$.

Subcase C1: Suppose that $X_{ij}=\Sigma_{k=i}^{n-1}x_k=0,(i<n-1)$. Then all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{n-1}\beta_k=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$ is similar to that given for SU$(n+1)$; it may be obtained by making the following changes: e_{i-1} to e_i, e_j to e_n, a_{j+1} to a_n, and a_j to a_{n-1}. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$ can be obtained from the proof for SU$(n+1)$ by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{2n}, a_{i-1} to $-a_{i-1}$, a_i to $-a_i$, a_j to $-a_{n-1}$, and a_{j+1} to $-a_n$.

Subcase C2: Suppose that $X_{ij}=x_{n-1}=0$. Then all products in $(*)$ are zero except for $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\beta_{n-1}=Y_{ij}$ is zero. Now, we will show that $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$ by considering the two products as polynomials in $x_1,\ldots,x_n$, showing that they have the same roots, and then concluding that they must differ by a factor of -1.

Let γ be as for SU$(n+1)$, and let $m=m(\gamma)=a_{n-2}-2a_{n-1}$. Then, $(e_{n-1}+\delta+\lambda,\gamma)=(\delta+\lambda,\gamma)+a_n+a_{n-1}-a_{n-2}=(\delta+\lambda,\gamma)+a_n+a_{n-1}-a_{n-2}+mX_{ij}=(\delta+\lambda,\gamma)+a_n-a_{n-1}-m+mX_{ij}=(\delta+\lambda,\gamma)+(e_n,\gamma)+(e_n+\delta+\lambda,mY_{ij})=(e_n+\delta+\lambda,\gamma+mY_{ij})$. Hence, by the same line of reasoning as in the proof for SU$(n+1)$, the products differ by a sign. The proof that $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$ is similar; it may be obtained by making the following changes: e_{n-1} to e_{2n-1}, e_n to e_{2n}, a_{n-2} to $-a_{n-2}$, a_{n-1} to $-a_{n-1}$, and a_n to $-a_n$.

Case D: Fix i and j with $1\leqslant i\leqslant j=n$.

Subcase D1: Suppose that $X_{ij}=\Sigma_{k=i}^{n}x_k=0(i<n)$. Then all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{n-1}\beta_k=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$ is similar to that given in case B; it can be obtained by making the following changes: e_n to e_{2n-1}, a_{n-2} to $-a_{n-2}$, and a_{n-1} to $-a_{n-1}$. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$ can be obtained from the one given in case B, if one makes the following changes: e_i to e_{n+i}, and a_k to $-a_k$, $k=i-1,i,n$.

Subcase D2: Suppose that $X_{ij}=\Sigma_{k=i}^{n-2}x_k+x_n=0$ $(i\leqslant n-2)$. Then all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{n-2}\beta_k+\beta_n=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$ is similar to the one given for SU$(n+1)$; it may be obtained by making the following changes: e_{i-1} to e_i, e_j to e_{2n}, a_{j+1} to $-a_n$, and a_j to $-a_{n-1}$. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$ can be obtained from the proof for SU$(n+1)$ by making the following changes: e_{i-1} to e_{n+i}, e_j to e_n, a_j to a_n, a_j to a_{n-1}, a_i to $-a_i$, and a_{i-1} to $-a_{i-1}$.

Subcase D3: Suppose that $X_{ij}=x_n=0$. Then all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\beta_n=Y_{ij}$ is zero. We will now prove that $\Pi_{\alpha>0}(e_{n-1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)$ by considering both products as poly-

nomials in $x_1,\ldots,x_n$, showing that they have the same roots, and finally concluding that they must differ by a sign.

Let γ and $\{a_i\}$ be as for SU$(n+1)$, and let $m=m(\gamma)=a_{n-2}-2a_n$. Then, $(e_{n-1}+\delta+\lambda,\gamma)=(\delta+\lambda,\gamma)+a_n+a_{n-1}-a_{n-2}=(\delta+\lambda,\gamma)+a_n+a_{n-1}-a_{n-2}+mX_{ij}=(\delta+\lambda,\gamma)+a_{n-1}-a_n-m+mX_{ij}=(\delta+\lambda,\gamma)+(e_{2n},\gamma)+(e_{2n}+\delta+\lambda,mY_{ij})=(e_{2n}+\delta+\lambda,\gamma+mY_{ij})$. Hence, by the same line of reasoning as in the proof for SU$(n+1)$, the products must differ by a sign. The proof that $\Pi_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_n+\delta+\lambda,\alpha)$ is similar; it may be obtained by making the following changes: e_{n-1} to e_{2n-1}, e_{2n} to e_n, a_{n-2} to $-a_{n-2}$, a_{n-1} to $-a_{n-1}$, and a_n to $-a_n$.

Since each factor of $\Pi_{\alpha>0}(\delta+\lambda,\alpha)$ is equal to X_{ij} for some i, j, and some case or subcase above, we have shown that the roots of the right-hand side of $(*)$ are contained within the roots of the left-hand side of $(*)$. By comparing degrees and substituting $\lambda=0$, we obtain the result. ●

Proposition 9.2: Fix $j\in\{1,\ldots,n\}$ and consider a dominant integral weight $\lambda=\Sigma_{k=1}^{n}c_k\beta_k^*$ with $c_j=0$; then, if $j\neq n$,

$$\prod_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=0,$$

and

$$\prod_{\alpha>0}(e_{n+j}+\delta+\lambda,\alpha)=0.$$

If $j=n$, then

$$\prod_{\alpha>0}(e_{2n-1}+\delta+\lambda,\alpha)=0,$$

and

$$\prod_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)=0.$$

Proof: If $j\in\{1,\ldots,n-1\}$, then $(e_{j+1}+\delta+\lambda,\beta_j)=-1+1+c_j=0$, and $(e_{n+j}+\delta+\lambda,\beta_j)=-1+1+c_j=0$. If $j=n$, then $(e_{2n-1}+\delta+\lambda,\beta_j)=-1+1+c_j=0$, and $(e_{2n}+\delta+\lambda,\beta_j)=-1+1+c_j=0$. ●

In the tensor product $\pi^\lambda\otimes\pi_0$, any irreducible representation that occurs must have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,2n\}$, and cannot occur more than once. By (1), the sum of the dimensions of the irreducible representations with highest weights $\lambda+e_i$ $(i=1,\ldots,2n)$ is $\Sigma_{\ell=1}^{2n}\Pi_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)$, and $\dim(\pi^\lambda\otimes\pi_0)=\dim(\pi_0)\dim(\pi^\lambda)=(2n)[\Pi_{\alpha>0}(\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)]$. We would like to show that the sum of the dimensions of the $\pi^{\lambda+e_i}$ $(i=1,\ldots,2n)$ is equal to the dimension of the tensor product $\pi^\lambda\otimes\pi_0$; this follows from proposition 9.1 if all the $\lambda+e_i$ are dominant integral weights.

Now $\mu=\Sigma_{i=1}^{n}z_i\beta_i^*$ is not a dominant integral weight if and only if $z_i<0$, for some $i\in\{1,\ldots,n\}$. Since $\lambda=\Sigma_{k=1}^{n}c_i\beta_i$ is the highest weight of π^λ, the one and only way that $\lambda+e_i$ $i\in\{1,\ldots,n\}$ would not be a possible highest weight is if $i\neq 1$ and $c_{i-1}=0$. The only way that $\lambda+e_{n+j}, j\in\{1,\ldots,n\}$, would not be a dominant integral weight is if $c_j=0$, or if $j=n-1$ and $c_n=0$. So, proposition 9.2 implies that if $\lambda+e_i$ is not a possible highest weight, then the dimension formula gives a value of zero. Thus, propositions 9.1 and 9.2 imply that the irreducible representations that occur in the tensor product $\pi^\lambda\otimes\pi_0$ are exactly those $\pi^{\lambda+e_i}$ for which $\lambda+e_i$ is a dominant integral weight. Therefore, we have proven the following:

Theorem 9.3: *The representations of $H=\mathrm{SO}(2n)$ that may be assembled with π^λ into a representation of $G=\mathrm{SO}(2n)\times\mathbb{R}^{2n}$ are those that have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,2n\}$. For each of the possible representations this assemblage is unique.*

X. EXAMPLE: SO($2n+1$)

Let $H=\mathrm{SO}(2n+1)$; then the simple roots of H are $\beta_1,\ldots,\beta_n$, given by $\beta_i(u_1,\ldots,u_n)=u_i-u_{i+1}$ for $i=1,\ldots,n-1$, and $\beta_n(u_1,\ldots,u_n)=u_n$. The fundamental weights are $\beta_1^*,\ldots,\beta_n^*$ given by $\beta_i^*(u_1,\ldots,u_n)=\Sigma_{k=1}^{i}u_k$ for $i=1,\ldots,n-1$ and $\beta_n^*(u_1,\ldots,u_n)=\frac{1}{2}\Sigma_{k=1}^{n}u_k$. It follows that $\delta=\frac{1}{2}\Sigma_{\alpha>0}\alpha=\Sigma_{k=1}^{n}\beta_k^*$. Let $e_1=\beta_1^*$, $e_i=\beta_i^*-\beta_{i-1}^*(2\leqslant i\leqslant n-1)$, $e_n=2\beta_n^*-\beta_{n-1}^*$, $e_{n+j}=-e_j$ for $j=1,\ldots,n$, and $e_0=0$. As in the previous examples, we shall consider the case where π_0 is the "standard" $(2n+1)$-dimensional (real) representation of $\mathrm{SO}(2n+1)$; its highest weight is e_1, and all its weights e_i have multiplicity one.

Proposition 10.1: For any dominant integral weight λ,

$$\sum_{\ell=0}^{2n}\prod_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)=(2n+1)\prod_{\alpha>0}(\delta+\lambda,\alpha).$$

This is equivalent to

$$\sum_{\ell=1}^{2n}\prod_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)=(2n)\prod_{\alpha>0}(\delta+\lambda,\alpha). \quad (*)$$

Proof: Write $\lambda=\Sigma_{k=1}^{n}c_k\beta_k^*$; then $\lambda+\delta=\Sigma_{k=1}^{n}(c_k+1)\beta_k^*=\Sigma_{k=1}^{n}x_k\beta_k^*$, where $x_k=c_k+1$.

Fix i and j with $1\leqslant i\leqslant j\leqslant n$.

Case A: Suppose that $X_{ij}=\Sigma_{k=i}^{j}x_k=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{j}\beta_k=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$ is the same as that given for $\mathrm{SU}(n+1)$. The proof that $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ can be obtained by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{n+j+1}, and a_k to $-a_k$, for $k=i-1,i,j,j+1$.

Case B: Suppose that $X_{ij}=(\Sigma_{k=i}^{j}x_k)+(\Sigma_{k=j+1}^{n-2}2x_k)+x_{n-1}+x_n=0$. It follows that all products in $(*)$ are zero except for: $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)$, $\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$, and $\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$, since, for each of the other products, the factor corresponding to $\alpha=\Sigma_{k=i}^{j}\beta_k+\Sigma_{k=j+1}^{n-2}2\beta_k+\beta_{n-1}+\beta_n=Y_{ij}$ is zero. The proof that $\Pi_{\alpha>0}(e_i+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+j+1}+\delta+\lambda,\alpha)$ is similar to the one given for $\mathrm{SU}(n+1)$; it may be obtained by making the following changes: e_{i-1} to e_i, e_j to e_{n+j+1}, a_{j+1} to $-a_{j+1}$, and a_j to $-a_j$. The proof that $\Pi_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(e_{n+i}+\delta+\lambda,\alpha)$ can be obtained from the proof for $\mathrm{SU}(n+1)$ by making the following changes: e_{i-1} to e_{n+i}, e_j to e_{j+1}, a_{i-1} to $-a_{i-1}$, a_i to $-a_i$.

Since each factor of $\Pi_{\alpha>0}(\delta+\lambda,\alpha)$ is equal to X_{ij} for some i, j, and some case above, we have shown that the roots of the right-hand side of $(*)$ are contained within the roots of the left-hand side of $(*)$. By comparing degrees and substituting $\lambda=0$, we obtain the result. ●

Proposition 10.2: Fix $j\in\{1,\ldots,n-1\}$ *and consider a dominant integral weight* $\lambda=\Sigma_{k=1}^{n}c_k\beta_k^*$ *with* $c_j=0$; *then,*

$$\prod_{\alpha>0}(e_{j+1}+\delta+\lambda,\alpha)=0,$$

and

$$\prod_{\alpha>0}(e_{n+j}+\delta+\lambda,\alpha)=0.$$

Proof: $(e_{j+1}+\delta+\lambda,\beta_j)=-1+1+c_j=0$ and $(e_{n+j}+\delta+\lambda,\beta_j)=-1+1+c_j=0$. ●

Proposition 10.3: If $\lambda=\Sigma_{i=1}^{n-1}c_i\beta_i^*$, *then* $\Pi_{\alpha>0}(e_{2n}+\delta+\lambda,\alpha)=-\Pi_{\alpha>0}(\delta+\lambda,\alpha)$.

Proof: As in proposition 10.1, consider both products as polynomials in $x_1,\ldots,x_n$ and fix $\gamma = \Sigma_{k=1}^{n} a_k\beta_k > 0$. Now, $(e_{2n}+\delta+\lambda,\gamma) = (\delta+\lambda,\gamma) + a_{n-1} - a_n = (\delta+\lambda,\gamma+2(a_{n-1}-a_n)\beta_n)$. Therefore, by the same line of reasoning as in the proof for SU$(n+1)$, the products differ by a sign. ●

Proposition 10.4: If the highest weight of π^λ is $\lambda = \Sigma_{k=i}^{n-1} c_i\beta_i^*$, with $i<n$ and $c_i>0$, then π^λ is not contained in $\pi^\lambda\otimes\pi_0$.

Proof: If $\lambda = \Sigma_{k=i}^{n-1} c_k\beta_k^*$ with $i<n$ and $c_i>0$, then $(\lambda, \Sigma_{k=i}^{n}\beta_k)>0$, so $\lambda - \Sigma_{k=i}^{n}\beta_k = \lambda - e_i$ is a weight of the irreducible representation with highest weight λ; $\lambda - e_n$ is not a weight, since, if it was, the highest weight would be $\lambda + e_n$ and not λ. For the same reason none of the $\lambda - e_{n+i}$ are weights. Since λ has multiplicity one in the weight diagram of π^λ, then it follows that λ has multiplicity n in the weight diagram of the tensor product $\pi^\lambda\otimes\pi_0$, one for each of the irreps with highest weights $e_0,\ldots,e_{n-1}$ and no more. If $j,k\in\{1,\ldots,n\}$, $j\neq k$, then the weight $\lambda+e_k$ is not contained in the irreducible representation with highest weight $\lambda+e_j$, since λ is a weight of the irreducible representation with highest weight $\lambda+e_j$ and $(\lambda,e_k)>0$; so the irreducible representations with highest weights $\lambda+e_j$, $j=1,\ldots,n$ must all occur in the tensor product $\pi^\lambda\otimes\pi_0$. Now, since λ is a weight (of multiplicity one) of the irreducible representations with highest weight $\lambda + e_j$, $j=1,\ldots,n$, and these representations must all occur in $\pi^\lambda\otimes\pi_0$, then it follows that π^λ does not occur in $\pi^\lambda\otimes\pi_0$. ●

In the tensor product $\pi^\lambda\otimes\pi_0$, any irreducible representation that occurs must have highest weight $\lambda+e_i$, for some $i\in\{0,\ldots,2n\}$, and cannot occur more than once. By (1), the sum of the dimensions of the irreducible representations with highest weights $\lambda+e_i$ $(i=0,\ldots,2n)$ is $\Sigma_{\ell=0}^{2n}\Pi_{\alpha>0}(e_\ell+\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)$, and $\dim(\pi^\lambda\otimes\pi_0) = \dim(\pi_0)\dim(\pi^\lambda) = (2n+1)[\Pi_{\alpha>0}(\delta+\lambda,\alpha)/\Pi_{\alpha>0}(\delta,\alpha)]$. We would like to show that the sum of the dimensions of the $\pi^{\lambda+e_i}$ $(i=0,\ldots,2n)$ is equal to the dimension of the tensor product $\pi^\lambda\otimes\pi_0$; this follows from proposition 10.1 if all the $\lambda+e_i$ are dominant integral weights.

Now $\mu = \Sigma_{i=1}^{n} z_i\beta_i^*$ is not a dominant integral weight if and only if $z_i<0$, for some $i\in\{1,\ldots,n\}$. Since $\lambda = \Sigma_{k=1}^{n} c_i\beta_i$ is the highest weight of π^λ, the one and only way that $\lambda+e_i$ $i\in\{1,\ldots,n\}$ would not be a dominant integral weight is if $i\neq 1$ and $c_{i-1}=0$. The only way that $\lambda+e_{n+j}, j\in\{1,\ldots,n\}$, would not be a dominant integral weight is if $c_j=0$. So, proposition 10.2 implies that if $\lambda+e_i$ $(i\neq 2n)$ is not a possible highest weight vector, then the dimension formula gives a value of zero. Together, propositions 10.3 and 10.4 show that if $c_n=0$, then π^λ is not contained in $\pi^\lambda\otimes\pi_0$, and if d_λ and $d_{\lambda+e_{2n}}$ are the values obtained by substituting λ and $\lambda+e_{2n}$ into (1), then $d_\lambda + d_{\lambda+e_{2n}} = 0$. This expresses the fact that neither π^λ nor $\pi^{\lambda+e_{2n}}$ occurs in the tensor product. Taken together, propositions 10.1, 10.2, 10.3, and 10.4 imply that the irreducible representations that occur in the tensor product $\pi^\lambda\otimes\pi_0$ are exactly those $\pi^{\lambda+e_i}$ for which $\lambda+e_i$ is a dominant integral weight, except in the case where $c_n=0$, in which case π^λ does not occur. Therefore, we have proven the following.

Theorem 10.5: *If $\lambda = \Sigma_{k=1}^{n} c_k\beta_k^*$ with $c_i\geqslant 0$ and $c_n>0$, the representations of $H=\mathrm{SO}(2n+1)$ that may be assembled with π^λ into a representation of $G=\mathrm{SO}(2n+1)\ltimes\mathbb{R}^{2n+1}$ are those that have highest weight $\lambda+e_i$, for some $i\in\{0,\ldots,2n\}$. If $c_n=0$, the representations of H that may be assembled with π^λ into a representation of G are those that have highest weight $\lambda+e_i$, for some $i\in\{1,\ldots,2n-1\}$. For all of the possible representations this assemblage is unique.*

XI. EXAMPLE: SO(3)⋉$\mathbb{R}^5$

Let $H=\mathrm{SO}(3)$ and let π_0 be the five-dimensional representation of H; it has weights $e_1 = 2\beta_1$, $e_2=\beta_1$, $e_3=0$, $e_4=-\beta_1$, and $e_5=-2\beta_1$ (all weights have multiplicity one). Now we will consider the case where $G=\mathrm{SO}(3)\ltimes\mathbb{R}^5$. For this group H, we have that $\beta_1^*(u_1) = \frac{1}{2}u_1$. If the highest weight of a representation π^λ of H is $\lambda = c_1\beta_1^*$, then the dimension of π^λ is given by (1); it is c_1+1.

Lemma 11.1: $\Sigma_{k=1}^{5}(c_1+2k-5) = 5(c_1+1)$.

Proof: A direct calculation gives the result. ●

In the tensor product $\pi^\lambda \otimes \pi_0$, any irreducible representation that occurs must have highest weight $\lambda + e_i$, for some $i \in \{1,\ldots,5\}$, and cannot occur more than once. By the dimension formula, the sum of the dimensions of the irreducible representations with highest weights $\lambda + e_i$ $(i = 1,\ldots,5)$ is $\Sigma_{k=1}^{5}(2(c_1+k)-5)$, and $\dim(\pi^\lambda \otimes \pi_0) = \dim(\pi_0)\dim(\pi^\lambda) = 5(2c_1+1)$. We would like to show that the sum of the dimensions of the $\pi^{\lambda+e_i}(i=1,\ldots,5)$ is equal to the dimension of the tensor product $\pi^\lambda \otimes \pi_0$; we can infer this from lemma 11.1 if all the $\lambda + e_i$ are dominant integral weights, that is, if $c_1 \notin \{0,1,2,3\}$; if this is the case, then it follows that the irreducible representations that occur in the tensor product $\pi^\lambda \otimes \pi_0$ are exactly those $\pi^{\lambda+e_i}$ for which $\lambda + e_i$ is a dominant integral weight. By explicit calculation, the same result can be shown when $c_1 \in \{0,1,2,3\}$. Therefore, we have proven the following:

Theorem 11.2: *The representations of* $H = \mathrm{SO}(3)$ *that may be assembled with* π^λ *into a representation of* $G = \mathrm{SO}(3) \ltimes \mathbb{R}^5$ *are those that have highest weight* $\lambda + e_i$, *for some* $i \in \{1,\ldots,5\}$. *For each of the possible representations this assemblage is unique*.

XII. CONCLUSIONS

The possibility of assembling two irreps of H into an indecomposable representation of the semidirect product $G = H \ltimes V$ is shown to be equivalent to the existence of a certain type of tensor operator between the two irreps. This in turn is shown to be equivalent to the occurrence of one irrep in the tensor product of the other with V.

This theory yields a systematic method for evaluating which irreps can be assembled into indecomposable representations. It is applied to various examples, and the results extend those of Cantoni,[1] also giving information about the number of inequivalent indecomposable representations built from any pair of irreps.

Given a specific semidirect product group $G = H \ltimes V$ and a particular irrep π^λ of H, it is straightforward to use the theory developed here to identify all irreps π^μ for which is it possible to assemble π^λ and π^μ into an indecomposable representation of G. In the examples given above, for various groups G of interest in physics, a description is given of all pairs π^λ and π^μ which can be assembled into an indecomposable representation.

Although it is not pursued here, this type of analysis could also be modified for application to infinite-dimensional representations.

ACKNOWLEDGMENTS

The authors wish to acknowledge helpful discussions with Hubert DeGuise and financial support from the Natural Sciences and Engineering Research Council.

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Extra dimensions and nonlinear equations

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(Received 8 November 2002; accepted 20 November 2002)

Solutions of nonlinear multi-component Euler–Monge partial differential equations are constructed in n spatial dimensions by *dimension-doubling*, a method that completely linearizes the problem. Nonlocal structures are an essential feature of the method. The Euler–Monge equations may be interpreted as a boundary theory arising from a linearized bulk system such that all boundary solutions follow from simple limits of those for the bulk. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1543227]

I. INTRODUCTION

For any theory[22] with an infinite number of conservation laws, we may always assemble the conserved currents into a generating function involving a spectral parameter a. If that spectral parameter is independent of any other space–time dimensions in the theory, as is possible in the simplest cases, then effectively the theory possesses an *extra dimension*.[23] Moreover, it is always possible to openly include this extra dimension in some of the dynamical equations, and not just leave it as a *dimension sub rosa*.

For example, suppose a theory is originally expressed in terms of coordinates (x,t) with an infinite number of conserved currents: $\partial_t \rho^{(n)}(x,t)=\partial_x J^{(n)}(x,t)$, $n\in\mathbb{N}$. Then by defining $\rho(x,t,a)\equiv\Sigma_n(n+1)a^n\rho^{(n)}(x,t)$, as opposed to $\Sigma_n a^n\rho^{(n)}(x,t)$, and $J(x,t,a)\equiv\Sigma_n a^{n+1}J^{(n)}(x,t)$, as opposed to $\Sigma_n a^n J^{(n)}(x,t)$, we have rendered all the conservation laws as a single second-order higher-dimensional partial differential equation (PDE): $\partial_t\rho(x,t,a)=\partial_x\partial_a J(x,t,a)$, as opposed to the first-order $\partial_t\rho(x,t,a)=\partial_x J(x,t,a)$. Hence our choice for the current generating functions has fully exposed an extra dimension in the PDEs satisfied by those generating functions. The extra dimension here does not just ride along as a suppressible label for the currents but it appears explicitly, perhaps even unavoidably, in the dynamical equations. Of course this immediately raises issues about whether the theory requires a to appear explicitly for *all* dynamical equations to be cogently expressed in terms of the original plus extra dimensions, and about covariance properties for the theory in the complete set of dimensions.

In this article we address these issues for a simple but very generally applicable class of nonlinear PDE's:[10,17] The first order Euler–Monge (E-M) equations $\partial_t\mathbf{u}=(\mathbf{u}\cdot\nabla)\mathbf{u}$. We find the full dynamics of these *nonlinear* theories are elegantly encoded into a higher dimensional set of *linear* ''heat'' equations obtained through dimension doubling $(\mathbf{x})\to(\mathbf{x},\mathbf{a})$, where for each spatial coordinate x_i there is an *associated coordinate* given by spectral parameter a_i. The original dynamical variables are obtained as spectral parameter boundary limits, $\lim_{\mathbf{a}\to 0}U_i(\mathbf{x},t,\mathbf{a})=u_i(\mathbf{x},t,\mathbf{a})$. The fact that the higher dimensional theory is linearized strongly argues that this is the right approach to take. In the linearized theory, the pairs (x_i,a_i) act like ''light-cone'' variables in the enlarged set of dimensions such that the heat equations for all the dynamical variables are of the form $(\partial/\partial t-\Sigma_{j=1}^{n}\partial^2/\partial a_j\partial x_j)U_i(\mathbf{x},t,\mathbf{a})=0$. Thus the extra dimensions appear explicitly and, indeed, unavoidably in these linearized dynamical equations.

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We also find Nambu brackets[18] of the fields, of all orders up to the full Jacobian, as a remarkable feature of the linearizing maps. We know of only one other field theoretic example[3] where these brackets appear so naturally. Moreover, the linearizing maps are *nonlocal* in all but the simplest, one component case. The nonlocal structures appropriate for E-M equations with two components in two spatial dimensions are evocative of phase factors in Wilson loops (cf. strings), and when the E-M equations describe n component fields in the original n spatial dimensions these structures extend to higher dimensional constructions involving integrals over $n-1$ dimensional submanifolds [cf. $(n-1)$-branes]. In the one dimensional, one component case, the E-M solution is obtained algebraically from the dimensionally-doubled "bulk" solution for all values of the single spectral parameter. In higher dimensional or multi-component cases the dependence of the solutions on the spectral parameters is more involved. Nevertheless, in all cases the solutions of the E-M equations may be obtained from simple limits of those for the bulk.

II. HISTORICAL OVERVIEW AND OBJECTIVES

The Euler–Monge equations first appeared in 18th and 19th century studies of fluid dynamics[10] and analytic geometry.[17] Riemann took up a study of the equations in the context of gas dynamics, discussing the equations as a theory of invariants[20] (for a modern textbook treatment, see Ref. 8). His approach is widely applicable to almost all nonlinear flow problems, although it does not triumph over turbulence. A systematic modern discussion of the E-M equations that synthesizes ideas from both geometry and invariance theory can be found in the review by Dubrovin and Novikov.[9] Most contemporary texts and reviews stress the universal role played by these nonlinear transport equations in accordance with Whitham's theory.[21] Essentially all nonlinear waves, even those in dispersive and dissipative media, involve E-M equations, or simple variants of them, if the nonlinear wavetrains are slowly varying. This makes the equations particularly useful for analyzing the asymptotic behavior of nonlinear solutions. The E-M equations and their conservation laws also serve as a useful starting point in Polyakov's study of turbulence[19] but without yet leading to a general solution of the Navier–Stokes equations.

The first order E-M equation $\partial u/\partial t = u\,\partial u/\partial x$ also gives rise to the Bateman equation[4] upon substituting $u=(\partial\phi/\partial t)/(\partial\phi/\partial x)$. The resulting second order nonlinear PDE is $0=\phi_x^2\phi_{tt}-2\phi_x\phi_t\phi_{tx}+\phi_t^2\phi_{xx}$, and is well known to possess a general implicit solution given by solving $tS_0(\phi)+xS_1(\phi)=\text{const}$, where S_0 and S_1 are arbitrary differentiable functions of $\phi(x,t)$. The structure of this solution incorporates the covariance properties of the PDE: If ϕ is a solution, so is any function of ϕ. In fact, curiously, the generalization of this solution to $n+1$ functions $S_0(\phi), S_i(\phi)$ of $\phi(\mathbf{x},t)$, $\mathbf{x}=(x_1,\ldots,x_n)$, subject to a single constraint $tS_0(\phi)+\Sigma x_i\,S_i(\phi)=0$, is a "universal solution" [14] to *any* equation derived from a Lagrangian which is homogeneous of weight one in the first derivatives of ϕ.

Thus the Euler–Monge equations appear widespread across a very broad landscape of physics and applied mathematics problems, and therefore it is important to understand their solutions at as many levels as possible. To that end we shall map all solutions of the E-M equations in arbitrary dimensions into solutions of second-order linear equations. This type of map is reminiscent of the Cole–Hopf[6,15] transformation (thoroughly reviewed in Ref. 16) used to linearize the Burgers[5,15] nonlinear diffusion equation, but there are important differences here. The Cole–Hopf transformation only works for curl-free $\mathbf{u}$, does not use extra dimensions, and fails for $0=\kappa$ (the diffusivity). The map to follow works for all $\mathbf{u}$, curl-free or otherwise, does use extra dimensions, but works only for $\kappa=0$. (We hope to extend the method to $\kappa\neq 0$ and to include the effects of pressure in subsequent studies.)

III. METHOD AND ELEMENTARY RESULTS

We believe it is best to present our results summarily for the simplest examples of fields with one, two, and three components, and then to extend these results to the general case of n compo-

nents. We leave out most details but we do sketch the salient features of the derivations. In the following, $\mathcal{M}_n$ is the n dimensional nonlinear Euler–Monge operator and $\mathcal{H}_n$ is an associated hyperbolic heat operator (introduced in Ref. 19),

$$\mathcal{M}_n \equiv \frac{\partial}{\partial t} - \sum_{j=1}^{n} u_j \frac{\partial}{\partial x_j}$$
$$\mathcal{H}_n \equiv \frac{\partial}{\partial t} - \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j \partial a_j}. \tag{1}$$

To begin, however, we will generalize these two definitions to allow for an arbitrary function F in the most *elementary* results in one spatial dimension. We find that

$$\frac{\partial}{\partial t} U(x,t,a) = F\left(\frac{\partial}{\partial a}\right) \frac{\partial}{\partial x} U(x,t,a) \tag{2}$$

if and only if

$$\frac{\partial}{\partial t} u(x,t) = F(u(x,t)) \frac{\partial}{\partial x} u(x,t) \tag{3}$$

where

$$U(x,t,a) \equiv \frac{e^{au(x,t)} - 1}{a}$$
$$u(x,t) = \frac{1}{a} \ln(1 + a U(x,t,a)) \tag{4}$$

and F is any function with a formal power series. This simple result follows by direct calculation

$$\left(\frac{\partial}{\partial t} - F\left(\frac{\partial}{\partial a}\right) \frac{\partial}{\partial x}\right) \frac{e^{au(x,t)} - 1}{a} = e^{au(x,t)} \left(\frac{\partial}{\partial t} u(x,t) - F(u(x,t)) \frac{\partial}{\partial x} u(x,t)\right). \tag{5}$$

The formal solution for $U(x,t,a)$ in terms of $U(x,t=0,a)$ is now obviously given by

$$(e^{au(x,t)} - 1)/a = e^{t\, F(\partial/\partial a)\, \partial/\partial x} ((e^{au(x)} - 1)/a) \tag{6}$$

with $u(x,t=0) = u(x)$.

The bulk solution $U(x,t,a)$ may also be viewed as a simple one-parameter deformation of the boundary data $u(x,t)$, with the extra dimension serving as the deformation parameter. In this exceptional one-component case, we may easily extract $u(x,t)$ from $U(x,t,a)$ for any value of the extra dimension a as given by the logarithmic expression above. But, in particular, we may extract $u(x,t)$ as a limit of the bulk solution $u(x,t) = \lim_{a \to 0} U(x,t,a)$. This immediately yields the time series solution[12] to the previous E-M equation as a limit:

$$u(x,t) = \lim_{a \to 0} e^{t\, F(\partial/\partial a)\, \partial/\partial x} \left(\frac{e^{au(x)} - 1}{a}\right) = F^{-1}\left[\sum_{j=0}^{\infty} \frac{t^j}{(1+j)!} \frac{d^j}{dx^j} (F[u(x)])^{1+j}\right], \tag{7}$$

where we assume F (locally) invertible in the last step.[24] While this time series is an immediate consequence of the previous results, we believe it is neither trivial nor obvious. Similar time series solutions are immediate consequences of all our results. For example, one independent field u in spatial dimensions $(x, y_1, \ldots, y_n)$ with dependent "velocity fields" $(u, v_1(u), \ldots, v_n(u))$ leads to

$$\frac{\partial}{\partial t}u(x,\mathbf{y},t)=u(x,\mathbf{y},t)\frac{\partial}{\partial x}u(x,\mathbf{y},t)+\sum_{i=1}^{n}v_i(u(x,\mathbf{y},t))\frac{\partial}{\partial y_i}u(x,\mathbf{y},t) \tag{8}$$

if and only if

$$\int_0^{u(x,\mathbf{y},t)}\mathrm{d}u\,\exp\left(au+\sum_{i=1}^{n}b_iv_i(u)\right)=e^{t(\partial^2/\partial x\partial a+\Sigma_{i=1}^{n}\partial^2/\partial y_i\partial b_i)}\int_0^{u(x,\mathbf{y})}\mathrm{d}u\,\exp\left(au+\sum_{i=1}^{n}b_iv_i(u)\right). \tag{9}$$

Again, this follows by direct calculation, with

$$U(x,\mathbf{y},t,a,\mathbf{b})\equiv\int_0^{u(x,\mathbf{y},t)}\mathrm{d}u\,\exp\left(au+\sum_{i=1}^{n}b_iv_i(u)\right) \tag{10}$$

since

$$\begin{aligned}\left(\frac{\partial}{\partial t}-\frac{\partial^2}{\partial x\partial a}-\sum_{i=1}^{n}\frac{\partial^2}{\partial y_i\partial b_i}\right)&U(x,\mathbf{y},t,a,\mathbf{b})\\&=\left(\frac{\partial}{\partial t}u(x,\mathbf{y},t)-u(x,\mathbf{y},t)\frac{\partial}{\partial x}u(x,\mathbf{y},t)-\sum_{i=1}^{n}v_i(u(x,\mathbf{y},t))\frac{\partial}{\partial y_i}u(x,\mathbf{y},t)\right)\\&\quad\times\exp\left(au(x,\mathbf{y},t)+\sum_{i=1}^{n}b_iv_i(u(x,\mathbf{y},t))\right).\end{aligned} \tag{11}$$

So, as given, the higher dimensional heat equation is satisfied by the integral form $U(x,\mathbf{y},t,a,\mathbf{b})$ if and only if the given one-component generalization of the E-M equations holds. The rhs of Eq. (10) is then just the formal solution of the heat equation.[25]

The last result does not allow for a simple extraction of $u(x,\mathbf{y},t)$ from the integral form of $U(x,\mathbf{y},t,a,\mathbf{b})$ for nonvanishing $a,\mathbf{b}$. However, it does have the simple limit $\lim_{a,\mathbf{b}\to 0}U(x,\mathbf{y},t,a,\mathbf{b})=u(x,\mathbf{y},t)$, so extraction is trivial on the boundary $a,\mathbf{b}\to 0$. This is true of all the other heat equation solutions to follow. Also note, $U(x,\mathbf{y},t,a,\mathbf{b})$ in this one-component case is an integral over the field value. Nevertheless U is still local in all the dimensions, no matter how many.

IV. MULTIPLE COMPONENTS AND NONLOCALITY

Locality in the original spatial dimensions will *not* hold, however, for maps of multi-component fields in higher dimensions. This is first illustrated by the next result,

$$\mathcal{H}_2U=\mathcal{H}_2V=0, \tag{12}$$

if and only if

$$\mathcal{M}_2u=\mathcal{M}_2v=0, \tag{13}$$

where $[\varepsilon(s)\equiv\pm\frac{1}{2}$ for $s\gtrless 0]$

$$U(x,y,t,a,b)\equiv\int_{-\infty}^{\infty}\mathrm{d}r\,\varepsilon(y-r)e^{au(x,r,t)+bv(x,r,t)}\ \frac{\partial u(x,r,t)}{\partial r}$$

$$V(x,y,t,a,b)\equiv\int_{-\infty}^{\infty}\mathrm{d}q\,\varepsilon(x-q)e^{au(q,y,t)+bv(q,y,t)}\ \frac{\partial v(q,y,t)}{\partial q}. \tag{14}$$

Once again this is established by direct calculation, assuming u, v, and their derivatives vanish asymptotically in x,y,

$$\mathcal{H}_2 U(x,y,t,a,b) = e^{au(x,y,t)+bv(x,y,t)}\mathcal{M}_2 u(x,y,t) + b\int_{-\infty}^{\infty} dr\ \varepsilon(y-r) \times e^{au(x,r,t)+bv(x,r,t)}\left(\frac{\partial u(x,r,t)}{\partial r}\mathcal{M}_2 v(x,r,t) - \frac{\partial v(x,r,t)}{\partial r}\mathcal{M}_2 u(x,r,t)\right) \tag{15}$$

$$\mathcal{H}_2 V(x,y,t,a,b) = e^{au(x,y,t)+bv(x,y,t)}\mathcal{M}_2 v(x,y,t) + a\int_{-\infty}^{\infty} dq\ \varepsilon(x-q) \times e^{au(q,y,t)+bv(q,y,t)}\left(\frac{\partial v(q,y,t)}{\partial q}\mathcal{M}_2 u(q,y,t) - \frac{\partial u(q,y,t)}{\partial q}\mathcal{M}_2 v(q,y,t)\right). \tag{16}$$

The converse result then follows by also using the obvious pair of limits $\lim_{a,b\to 0}\mathcal{H}_2 U(x,y,t,a,b) = \mathcal{M}_2 u(x,y,t)$ and $\lim_{a,b\to 0}\mathcal{H}_2 V(x,y,t,a,b) = \mathcal{M}_2 v(x,y,t)$.

As advertised, the two-component map in two spatial dimensions involves a nonlocal transformation between E-M and heat equation solutions: It features line integrals over the original spatial variables. The map is still local in the extra dimensions, however. This nonlocality in the original dimensions persists and is even extended when more components and more spatial dimensions are considered. As a further illustration before giving the generalization to an arbitrary number of dimensions, we have

$$\mathcal{H}_3 U = \mathcal{H}_3 V = \mathcal{H}_3 W = 0, \tag{17}$$

if and only if

$$\mathcal{M}_3 u = \mathcal{M}_3 v = \mathcal{M}_3 w = 0, \tag{18}$$

where

$$\begin{aligned} U(x,y,z,t,a,b,c) &\equiv \int dr\ \varepsilon(y-r)\, e^{au+bv+cw}\ \frac{\partial u(x,r,z,t)}{\partial r} \\ &\quad - c\int\int drds\ \varepsilon(y-r)\ \varepsilon(z-s)\, e^{au+bv+cw}\{u,w\}_{rs}(x,r,s,t), \\ V(x,y,z,t,a,b,c) &\equiv \int ds\ \varepsilon(z-s)\, e^{au+bv+cw}\ \frac{\partial v(x,y,s,t)}{\partial s} \\ &\quad - a\int\int dqds\ \varepsilon(x-q)\ \varepsilon(z-s)\, e^{au+bv+cw}\{v,u\}_{sq}(q,y,s,t), \\ W(x,y,z,t,a,b,c) &\equiv \int \mathrm{d}q\ \varepsilon(x-q)\, e^{au+bv+cw}\ \frac{\partial w(q,y,z,t)}{\partial q} \\ &\quad - b\int\int dqdr\ \varepsilon(x-q)\ \varepsilon(y-r)\, e^{au+bv+cw}\{w,v\}_{qr}(q,r,z,t). \end{aligned} \tag{19}$$

There are a few essential new ingredients needed to complete the argument by direct calculation in this case. Define Poisson brackets as usual by

$$\{u,v\}_{rs}=\frac{\partial u}{\partial r}\frac{\partial v}{\partial s}-\frac{\partial u}{\partial s}\frac{\partial v}{\partial r}, \tag{20}$$

where u and v are any two functions of the independent variables r and s. Then it is straightforward to show

$$\begin{aligned}&\frac{\partial}{\partial t}\{u,v\}_{zy}-\frac{\partial}{\partial x}(u\{u,v\}_{zy})-\frac{\partial}{\partial y}(v\{u,v\}_{zy})-\frac{\partial}{\partial z}(w\{u,v\}_{zy})=\{\mathcal{M}_3u,v\}_{zy}+\{u,\mathcal{M}_3v\}_{zy},\\ &\frac{\partial}{\partial t}\{u,v\}_{xy}-\frac{\partial}{\partial x}(u\{u,v\}_{xy})-\frac{\partial}{\partial y}(v\{u,v\}_{xy})-\frac{\partial}{\partial z}(w\{u,v\}_{xy})\\ &\quad=\{\mathcal{M}_3u,v\}_{xy}+\{u,\mathcal{M}_3v\}_{xy}-\{u,v,w\}_{xyz},\end{aligned} \tag{21}$$

as well as similar relations obtained by permutation of dependent and independent variables. In the last relation we have introduced the totally antisymmetric Nambu triple bracket (i.e., Jacobian, in this three-dimensional case)

$$\{u,v,w\}_{xyz}=\frac{\partial u}{\partial x}\{v,w\}_{yz}+\frac{\partial u}{\partial y}\{v,w\}_{zx}+\frac{\partial u}{\partial z}\{v,w\}_{xy}=\frac{\partial u}{\partial x}\{v,w\}_{yz}+\frac{\partial v}{\partial x}\{w,u\}_{yz}+\frac{\partial w}{\partial x}\{u,v\}_{yz}. \tag{22}$$

Once equipped with such relations, the complete derivation of the heat equation and E-M equivalence is tedious, perhaps, but not subtle. (See the generalization to follow for additional details.)

The nonlocality appearing in our map for three components in three spatial dimensions is two-dimensional: It features surface integrals over pairs of the original spatial dimensions, perhaps evocative of membrane-based phase factors. Nonetheless, the map is still local in the extra dimensions and the E-M solutions are again trivially given by boundary limits of the bulk constructions.

V. GENERAL RESULTS

The nonlocality is extended to $(n-1)$-dimensional integrals when n-component linearizing maps are constructed in n spatial dimensions. This is explicit in the following equations.

$$\mathcal{H}_nU_k(\mathbf{x},t,\mathbf{a})=0 \tag{23}$$

if and only if

$$\mathcal{M}_nu_i(\mathbf{x},t)=0 \tag{24}$$

for $i,k\in\{1,\ldots,n\}$ where

$$\begin{aligned}U_k(\mathbf{x},t,\mathbf{a})\equiv&\int\cdots\int \mathrm{d}q_1\cdots\mathrm{d}q_n\,\delta(q_k-x_k)\left(\frac{e^{a_ku_k}-1}{a_k}\right)\\ &\times\det\begin{pmatrix}\frac{\partial}{\partial q_1}(\varepsilon(q_1-x_1)e^{a_1u_1}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_1-x_1)e^{a_1u_1})\\ \vdots & \ddots & \vdots\\ \frac{\partial}{\partial q_1}(\varepsilon(q_n-x_n)e^{a_nu_n}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_n-x_n)e^{a_nu_n})\end{pmatrix}_{\substack{\text{exclude } k\text{th row}\\ \text{and } k\text{th column}}}.\end{aligned} \tag{25}$$

The equivalence is shown as follows. Consider only the first component (*et sic de similibus*).

$$U_1(\mathbf{x},t,\mathbf{a}) = \int\cdots\int \mathrm{d}q_1\cdots\mathrm{d}q_n\,\delta(q_1-x_1)\left(\frac{e^{a_1u_1}-1}{a_1}\right)$$

$$\times\det\begin{pmatrix} \frac{\partial}{\partial q_2}(\varepsilon(q_2-x_2)e^{a_2u_2}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_2-x_2)e^{a_2u_2}) \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial q_2}(\varepsilon(q_n-x_n)e^{a_nu_n}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_n-x_n)e^{a_nu_n}) \end{pmatrix}$$

$$= \int\cdots\int \mathrm{d}q_2\cdots\mathrm{d}q_n\left(\frac{e^{a_1u_1}-1}{a_1}\right)$$

$$\times\det\begin{pmatrix} \frac{\partial}{\partial q_2}(\varepsilon(q_2-x_2)e^{a_2u_2}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_2-x_2)e^{a_2u_2}) \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial q_2}(\varepsilon(q_n-x_n)e^{a_nu_n}) & \cdots & \frac{\partial}{\partial q_n}(\varepsilon(q_n-x_n)e^{a_nu_n}) \end{pmatrix}(x_1,q_2,\cdots,q_n,t)$$

$$= \int\cdots\int \mathrm{d}q_2\cdots\mathrm{d}q_n\left(\frac{e^{a_1u_1}-1}{a_1}\right)$$

$$\times\varepsilon_{i_2\cdots i_n}\frac{\partial}{\partial q_{i_2}}(\varepsilon(q_2-x_2)e^{a_2u_2})\frac{\partial}{\partial q_{i_3}}(\varepsilon(q_3-x_3)e^{a_3u_3})\cdots\frac{\partial}{\partial q_{i_n}}(\varepsilon(q_n-x_n)e^{a_nu_n}),$$

where in the last expression the i_k dummy indices, $k\in\{2,\ldots,n\}$, are summed from 2 to n, i.e., 1 is excluded. Now we integrate by parts assuming all fields and their derivatives vanish as $x\to\infty$. To do this, there are clearly $n-1$ equivalent choices. We elect to integrate $\partial/\partial q_{i_2}$ by parts to obtain

$$U_1(\mathbf{x},t,\mathbf{a}) = -\varepsilon_{i_2\cdots i_n}\int\cdots\int \mathrm{d}q_2\cdots\mathrm{d}q_n\,\varepsilon(q_2-x_2)e^{a_2u_2}\frac{\partial}{\partial q_{i_2}}\left(\frac{e^{a_1u_1}-1}{a_1}\right)$$

$$\times\frac{\partial}{\partial q_{i_3}}(\varepsilon(q_3-x_3)e^{a_3u_3})\cdots\frac{\partial}{\partial q_{i_n}}(\varepsilon(q_n-x_n)e^{a_nu_n})$$

$$= -\varepsilon_{i_2\cdots i_n}\int\cdots\int \mathrm{d}q_2\cdots\mathrm{d}q_n\,\varepsilon(q_2-x_2)\frac{\partial u_1}{\partial q_{i_2}}$$

$$\times\left(\delta_{i_33}\delta(q_3-x_3)+a_3\varepsilon(q_3-x_3)\frac{\partial u_3}{\partial q_{i_3}}\right)\cdots\left(\delta_{i_nn}\delta(q_n-x_n)+a_n\varepsilon(q_n-x_n)\frac{\partial u_n}{\partial q_{i_n}}\right)e^{\mathbf{a}\cdot\mathbf{u}}.$$

Expanding out the products of the various paired terms in parentheses in the last line gives

$$
\begin{aligned}
U_1(\mathbf{x},t,\mathbf{a}) = &-\varepsilon_{i_2\cdots i_n} a_3\cdots a_n \int\cdots\int \mathrm{d}q_2\mathrm{d}q_3\cdots\mathrm{d}q_n\, \varepsilon(q_2-x_2)\\
&\times\varepsilon(q_3-x_3)\cdots\varepsilon(q_n-x_n)\,\frac{\partial u_1}{\partial q_{i_2}}\,\frac{\partial u_3}{\partial q_{i_3}}\cdots\frac{\partial u_n}{\partial q_{i_n}}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\varepsilon_{i_2\cdots i_n}\sum_{j=3}^{n}\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\,\delta_{ji_j}\\
&\times\left(\prod_{\substack{k=3\\k\neq j}}^{n}\left(a_k\int \mathrm{d}q_k\,\varepsilon(q_k-x_k)\,\frac{\partial u_k}{\partial q_{i_k}}\right)\right)\frac{\partial u_1}{\partial q_{i_2}}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\varepsilon_{i_2\cdots i_n}\sum_{j=3}^{n}\sum_{\substack{k=4\\k>j}}^{n}\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\,\delta_{ji_j}\,\delta_{ki_k}\\
&\times\left(\prod_{\substack{m=3\\m\neq j,k}}^{n}\left(a_m\int \mathrm{d}q_m\,\varepsilon(q_m-x_m)\,\frac{\partial u_m}{\partial q_{i_m}}\right)\right)\frac{\partial u_1}{\partial q_{i_2}}\,e^{\mathbf{a}\cdot\mathbf{u}}-\cdots\\
&-\sum_{j=3}^{n} a_j\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\int \mathrm{d}q_j\,\varepsilon(q_j-x_j)\left(\frac{\partial u_1}{\partial q_2}\,\frac{\partial u_j}{\partial q_j}-\frac{\partial u_1}{\partial q_j}\,\frac{\partial u_j}{\partial q_2}\right)e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\,\frac{\partial u_1}{\partial q_2}\,e^{\mathbf{a}\cdot\mathbf{u}}.
\end{aligned}
$$

That is to say, the result is given in terms of Nambu brackets[18] of all ranks from $n-1$ down to 2 (i.e., Poisson), as well as a final single derivative term. Thus

$$
\begin{aligned}
U_1(\mathbf{x},t,\mathbf{a}) = &-a_3\cdots a_n\int\cdots\int \mathrm{d}q_2\mathrm{d}q_3\cdots\mathrm{d}q_n\,\varepsilon(q_2-x_2)\,\varepsilon(q_3-x_3)\cdots\varepsilon(q_n-x_n)\\
&\times\{u_1,u_3,\ldots,u_n\}_{23\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\sum_{j=3}^{n}\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\left(\prod_{\substack{k=3\\k\neq j}}^{n}\left(a_k\int \mathrm{d}q_k\,\varepsilon(q_k-x_k)\right)\right)\\
&\times\{u_1,u_3,\ldots,u_{j-1},u_{j+1},\ldots,u_n\}_{23\cdots j-1j+1\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\cdots-\sum_{j=3}^{n}\sum_{\substack{k=4\\k>j}}^{n} a_j a_k\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\int \mathrm{d}q_j\,\varepsilon(q_j-x_j)\int \mathrm{d}q_k\,\varepsilon(q_k-x_k)\\
&\times\{u_1,u_j,u_k\}_{2jk}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\sum_{j=3}^{n} a_j\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\int \mathrm{d}q_j\,\varepsilon(q_j-x_j)\,\{u_1,u_j\}_{2j}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\,\frac{\partial u_1}{\partial q_2}\,e^{\mathbf{a}\cdot\mathbf{u}}.
\end{aligned}
$$

In the preceding equation, it is to be understood that the sum $\Sigma_{j=3}^{n}$ in the second term begins at its lower limit with

$$
-a_4\cdots a_n\int\cdots\int \mathrm{d}q_2\mathrm{d}q_4\cdots\mathrm{d}q_n\,\varepsilon(q_2-x_2)\,\varepsilon(q_4-x_4)\cdots\varepsilon(q_n-x_n)\,\{u_1,u_4,\ldots,u_n\}_{24\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}}
$$

and terminates at its upper limit with

$$-a_3\cdots a_{n-1}\int\cdots\int \mathrm{d}q_2\mathrm{d}q_3\cdots\mathrm{d}q_{n-1}\,\varepsilon(q_2-x_2)\,\varepsilon(q_3-x_3)\cdots\varepsilon(q_{n-1}-x_{n-1})$$
$$\times\{u_1,u_3,\cdots,u_{n-1}\}_{23\cdots n-1}\,e^{\mathbf{a}\cdot\mathbf{u}}.$$

Next we act with the heat operator on $U_1(\mathbf{x},t,\mathbf{a})$. The ε's permit the appropriate ''outside'' (i.e., x) partials to be converted, through integration by parts, into ''inside'' (i.e., q) partials. Also, factors of a_i outside the exponentials produce some extra terms from the cross-partials $\partial^2/\partial x_i\partial a_i$ in $\mathcal{H}_n$. We obtain

$$\begin{aligned}
\mathcal{H}_nU_1(\mathbf{x},t,\mathbf{a}) = &-a_3\cdots a_n\int\cdots\int \mathrm{d}q_2\mathrm{d}q_3\cdots\mathrm{d}q_n\,\varepsilon(q_2-x_2)\,\varepsilon(q_3-x_3)\cdots\varepsilon(q_n-x_n)\\
&\times\mathcal{H}_n(\{u_1,u_3,\ldots,u_n\}_{23\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}})\\
&+\sum_{i=3}^{n}\frac{\partial}{\partial a_i}(a_3\cdots a_n)\int\cdots\int \mathrm{d}q_2\mathrm{d}q_3\cdots\mathrm{d}q_n\frac{\partial}{\partial x_i}[\varepsilon(q_2-x_2)\,\varepsilon(q_3-x_3)\cdots\varepsilon(q_n-x_n)]\\
&\times\{u_1,u_3,\ldots,u_n\}_{23\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\sum_{j=3}^{n}\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\left(\prod_{\substack{k=3\\k\neq j}}^{n}\left(a_k\int \mathrm{d}q_k\,\varepsilon(q_k-x_k)\right)\right)\\
&\times\mathcal{H}_n(\{u_1,u_3,\ldots,u_{j-1},u_{j+1},\ldots,u_n\}_{23\cdots j-1j+1\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}})\\
&+\sum_{j=3}^{n}\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\sum_{i=3}^{n}\frac{\partial}{\partial a_i}\frac{\partial}{\partial x_i}\left(\prod_{\substack{k=3\\k\neq j}}^{n}\left(a_k\int \mathrm{d}q_k\,\varepsilon(q_k-x_k)\right)\right)\\
&\times\{u_1,u_3,\ldots,u_{j-1},u_{j+1},\ldots,u_n\}_{23\cdots j-1j+1\cdots n}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-+\cdots-\sum_{j=3}^{n}a_j\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\int \mathrm{d}q_j\,\varepsilon(q_j-x_j)\,\mathcal{H}_n(\{u_1,u_j\}_{2j}\,e^{\mathbf{a}\cdot\mathbf{u}})\\
&+\sum_{i=3}^{n}\frac{\partial}{\partial a_i}\frac{\partial}{\partial x_i}\left(\sum_{j=3}^{n}a_j\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\int \mathrm{d}q_j\,\varepsilon(q_j-x_j)\right)\{u_1,u_j\}_{2j}\,e^{\mathbf{a}\cdot\mathbf{u}}\\
&-\int \mathrm{d}q_2\,\varepsilon(q_2-x_2)\,\mathcal{H}_n\left(\frac{\partial u_1}{\partial q_2}e^{\mathbf{a}\cdot\mathbf{u}}\right).
\end{aligned}$$

The first term (first two lines) on the rhs of $\mathcal{H}_nU_1$ reduces to terms linear in the E-M equations for the u's. The second term (third and fourth lines) and third term (fifth and sixth lines) on the rhs combine to give similar terms linear in the E-M equations. And so it goes with subsequent pairs of terms on the rhs of $\mathcal{H}_nU_1$, until finally the last two terms (last two lines) on the rhs combine to give terms linear in the E-M equations.

To establish these statements, one needs to use several identities involving the action of the heat operator on exponentially weighted derivatives of the component fields, in particular on so-weighted Nambu brackets. For example, these identities range from the simplest for the full Jacobian

$$\begin{aligned}
\mathcal{H}_n(e^{\mathbf{a}\cdot\mathbf{u}}\{u_1,u_2,\ldots,u_n\}_{12\cdots n}) = &\,e^{\mathbf{a}\cdot\mathbf{u}}(\mathbf{a}\cdot\mathcal{M}_n\mathbf{u})\{u_1,u_2,\ldots,u_n\}_{12\cdots n}+e^{\mathbf{a}\cdot\mathbf{u}}(\{\mathcal{M}_nu_1,u_2,\ldots,u_n\}_{12\cdots n}\\
&+\{u_1,\mathcal{M}_nu_2,\ldots,u_n\}_{12\cdots n}+\cdots+\{u_1,u_2,\cdots,\mathcal{M}_nu_n\}_{12\cdots n})
\end{aligned}$$

to those involving lower rank Nambu brackets such as

$$\mathcal{H}_n(e^{\mathbf{a}\cdot\mathbf{u}}\{u_2,u_3,\ldots,u_n\}_{23\cdots n}) = e^{\mathbf{a}\cdot\mathbf{u}}(-\{u_1,u_2,u_3,\ldots,u_n\}_{123\cdots n}+(\mathbf{a}\cdot\mathcal{M}_n\mathbf{u})\{u_2,u_3,\ldots,u_n\}_{23\cdots n}) + e^{\mathbf{a}\cdot\mathbf{u}}(\{\mathcal{M}_n u_2,u_3,\ldots,u_n\}_{23\cdots n}+\{u_2,\mathcal{M}_n u_3,\ldots,u_n\}_{23\cdots n}+\cdots + \{u_2,u_3,\ldots,\mathcal{M}_n u_n\}_{23\cdots n})$$

including that needed to deal with the first rhs line of $\mathcal{H}_n U_1$

$$\mathcal{H}_n(e^{\mathbf{a}\cdot\mathbf{u}}\{u_1,u_3,\ldots,u_n\}_{23\cdots n}) = e^{\mathbf{a}\cdot\mathbf{u}}(\mathbf{a}\cdot\mathcal{M}_n\mathbf{u})\{u_1,u_3,\ldots,u_n\}_{23\cdots n}+e^{\mathbf{a}\cdot\mathbf{u}}(\{\mathcal{M}_n u_1,u_3,\ldots,u_n\}_{23\cdots n} + \{u_1,\mathcal{M}_n u_3,\ldots,u_n\}_{23\cdots n}+\cdots+\{u_1,u_3,\ldots,\mathcal{M}_n u_n\}_{23\cdots n})$$

as well as other relations obtained by permutations of the indices of these, etc., all the way down to the final

$$\mathcal{H}_n(e^{\mathbf{a}\cdot\mathbf{u}}\partial_j u_k(\mathbf{x},t)) = e^{\mathbf{a}\cdot\mathbf{u}}\left(\partial_j(\mathcal{M}_n u_k)+(\mathbf{a}\cdot\mathcal{M}_n\mathbf{u})\partial_j u_k-\sum_i \{u_k,u_i\}_{ji}\right)$$

as needed to deal with the last two rhs lines in $\mathcal{H}_n U_1$. All such identities are straightforward to substantiate by direct calculation.

Thus, given the E-M equations for the u's, the heat equation for U_1 follows. Moreover, the only terms on the rhs of $\mathcal{H}_n U_1$ which survive in the limit of vanishing spectral parameters are the last two lines, which give

$$\lim_{\mathbf{a}\to\mathbf{0}}\mathcal{H}_n U_1(\mathbf{x},t,\mathbf{a}) = \mathcal{M}_n u_1(\mathbf{x},t). \tag{26}$$

Thus, given the heat equation for U_1, the E-M equation for u_1 follows. Similar results obtain for all the other components, so that $\mathcal{H}_n U_k = 0$ iff $\mathcal{M}_n u_j = 0$.

Formally, time evolution in the bulk is once more given by a simple exponentiation

$$\mathbf{U}(\mathbf{x},t,\mathbf{a}) = e^{t\sum_{j=1}^n \partial^2/\partial x_j\partial a_j}\mathbf{U}(\mathbf{x},t=0,\mathbf{a}). \tag{27}$$

This gives a time-series solution on the boundary upon taking the limit $\mathbf{a}\to\mathbf{0}$.

$$\mathbf{u}(\mathbf{x},t) = \lim_{\mathbf{a}\to\mathbf{0}} e^{t\sum_{j=1}^n \partial^2/\partial x_j\partial a_j}\mathbf{U}(\mathbf{x},t=0,\mathbf{a}) \tag{28}$$

with initial boundary data $\mathbf{u}(\mathbf{x}) = \lim_{\mathbf{a}\to\mathbf{0}}\mathbf{U}(\mathbf{x},t=0,\mathbf{a})$. Moreover, the n-fold infinite sequences of conservation laws for the E-M equations in n spatial dimensions are directly encoded into the bulk solutions.

$$\frac{\partial}{\partial t}U_k(\mathbf{x},t,\mathbf{a}) = \nabla\cdot\mathbf{J}_k(\mathbf{x},t,\mathbf{a}), \quad \mathbf{J}_k(\mathbf{x},t,\mathbf{a}) = \nabla_{\mathbf{a}}U_k(\mathbf{x},t,\mathbf{a}), \quad k\in\{1,2,\ldots,n\}. \tag{29}$$

Explicit sequences of charge and current densities on the boundary follow immediately from power series expansions in the a_j. These conservation laws are elementary consequences of the heat equation obeyed by $\mathbf{U}$.

VI. CONCLUSION

This is as far as we have completed the application of the extra dimensional approach to classical nonlinear PDEs. It remains to apply this approach to other types of nonlinear PDEs, in particular to those higher-order extensions of the E-M equations involving dispersion, such as the Korteweg–deVries equation, and to those involving diffusion, such as the Burgers and Navier–Stokes equations. Another immediately obvious challenge is to carry the method over to quantum field theories (QFTs). This will not be done here. However, we suspect that the implementation of

these ideas in QFT will involve the use of quantum Nambu brackets (QNBs), given that the classical versions of these appear above. QNBs have a long-standing notoriety, but recently[7] it has been shown that theirs is an undeserved bad reputation. QNBs can be defined in terms of operators (or in terms of noncommutative geometry) so as to fulfill their expected roles in the quantum evolution of dynamical systems. Perhaps these developments will be useful to meet the challenge of quantizing the E-M equations as well as their higher-order generalizations.

As emphasized previously, the Euler-Monge equations appear widespread throughout physics and the mathematics of nonlinear partial differential equations. Based on the maps we have presented to linearize these equations, we have come to the conclusion that extra dimensions and nonlocal structures are ubiquitous features to be found upon analyzing solutions of such nonlinear partial differential equations, and are quite natural constructs in many physical theories.

ACKNOWLEDGMENTS

Our thanks to Cosmas Zachos for valuable comments, and to Orlando Alvarez for critically reading the manuscript. This research was supported in part by a Leverhulme Emeritus Fellowship and by NSF Award 0073390.

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[22] We dedicate this paper to Peter Freund on the occasion of his becoming Professor Emeritus at the University of Chicago, and thereby begin with general remarks about the origin of extra dimensions, allowing for the possibility that these are similar to but not necessarily on the exact same footing as the original dimensions. For related points of view within the Kaluza–Klein physics framework,[1] see Ref. 2.
[23] More precisely, an extra *bosonic* dimension. A *finite* number of conservation laws evokes extra *fermionic* or *anyonic dimensions*, θ, involving kth order superspace or Grassman variables. This and other noncommutative geometries will not be discussed further here.
[24] Given the close relation of the Monge and Bateman equations, it might be expected that the latter also admits a power series solution of simple form. Indeed this is so. Treating the equation as hyperbolic with initial conditions $\phi(x,0)$

$=f(x)$, $\partial\phi(x,0)/\partial t=g(x)$, the time series solution of the Bateman equation is $\phi(x,t)=f(x)+tg(x)+\Sigma_{j=1}^{\infty}t^{1+j}/(1+j)!d^j/dx^j\ (g(x)^{1+j}/(df(x)/dx)^j)$.

[25] As is true for the Bateman equation and the one-component Monge equation in one spatial dimension, there is a corresponding second order equation for the case of one component in $n+1$ spatial dimensions which our solution satisfies. It is the so-called ''Universal Field Equation'' which may be obtained by elimination of u from the first order equations.[11,12]

Weak transversality and partially invariant solutions

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(Received 31 May 2002; accepted 11 February 2003)

New exact solutions are obtained for several nonlinear physical equations, namely the Navier–Stokes and Euler systems, an isentropic compressible fluid system and a vector nonlinear Schrödinger equation. The solution method makes use of the symmetry group of the system in situations when the standard Lie method of symmetry reduction is not applicable. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1567799]

I. INTRODUCTION

Lie group theory provides very general and efficient methods for obtaining exact analytic solutions of systems of partial differential equations, specially nonlinear ones.[1–9] The different methods have in common that they provide a reduction of the original system. This reduction usually means the reduction of the number of independent variables occurring, possibly a reduction of the number of dependent ones too.

The ''standard,'' or ''classical'' reduction method goes back to the original work of Sophus Lie and is explained in many modern texts.[1–9] Essentially, it amounts to requiring that a solution of the equation should be invariant under some subgroup $G_0 \subseteq G$, where G is the symmetry group of the considered system of equations. The subgroup G_0 must satisfy certain criteria, in order to provide such group invariant solutions (see below).

The purpose of this article is to further develop, compare and apply alternative reduction methods. They have in common the fact that they provide solutions not obtainable by a standard application of Lie's classical method. We shall survey the ''tool kit'' available for obtaining particular solutions of systems of partial differential equations, and further refine some of the tools. In the process we shall obtain new solutions of some physically important equations such as the Navier–Stokes equations, the Euler equations, the equations describing an isentropic compressible fluid model and the vector nonlinear Schrödinger equation.

We shall consider a system of m partial differential equations of order n, involving p independent variables $(x_1, x_2, \ldots, x_p)$ and q dependent variables $(u_1, u_2, \ldots, u_q)$,

$$\Delta_\nu(x, u^{(n)}) = 0, \quad \nu = 1, \ldots, m, \tag{1}$$

where $u^{(n)}$ denotes all partial derivatives of u_α, up to order n.

Lie's classical method of symmetry reduction consists of several steps.

(1) Find the local Lie group G of local point transformations taking solutions into solutions. Realize its Lie algebra $\mathfrak{g}$ in terms of vector fields and identify it as an abstract Lie algebra. The basis vector fields will have the form

$$\mathbf{v}_a = \sum_{i=1}^{p} \xi_a^i(x,u) \frac{\partial}{\partial x^i} + \sum_{\alpha=1}^{q} \varphi_a^\alpha(x,u) \frac{\partial}{\partial u^\alpha}, \quad a = 1,\ldots,r = \dim G. \tag{2}$$

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(2) Classify the subalgebras $\mathfrak{g}_i \subset \mathfrak{g}$ into conjugacy classes under the action of the largest group $\tilde{G}$ leaving the system of equations invariant (we have $G \subseteq \tilde{G}$). Choose a representative of each class.

(3) For each representative subalgebra $\mathfrak{g}_i$ find the invariants $I_\gamma(x_1,\ldots,x_p,u_1,\ldots,u_q)$ of the action of the group $G_i = \langle \exp \mathfrak{g}_i \rangle$ in the space $M \sim X \times U$ of independent and dependent variables. Let us assume that $p+q-s$ functionally independent invariants I_γ exist, at least locally (s is the dimension of the generic orbits of G_i).

(4) Divide (if possible) the invariants I_γ into two sets: $\{F_1,\ldots,F_q\}$ and $\{\xi_1,\ldots,\xi_k\}$, $k = p-s$ in such a manner that the Jacobian relating F_μ and u_α $(\alpha,\mu=1,\ldots,q)$ has maximal rank

$$J = \frac{\partial(F_1,\ldots,F_q)}{\partial(u_1,\ldots,u_q)}, \quad \operatorname{rank} J = q. \tag{3}$$

Then consider F_μ to be functions of the other invariants $\{\xi_i\}$ which serve as the new independent variables and use condition (3) to express the dependent variables u_α in terms of the invariants.

(5) Substitute the obtained expressions for u_α into the original system and obtain the reduced system, involving only invariants. The reduced system will involve only $k = p-s$, $s \geqslant 1$ independent variables.

(6) Solve the reduced system. If the variables ξ^i depend on $x_1,\ldots,x_p$ only, this will yield explicit solutions of system (1). Otherwise, if ξ_i depend also on the original dependent variables u_α, we obtain implicit solutions.

(7) Apply a general symmetry group transformation to these solutions.

This procedure provides a family of particular solutions that can be used to satisfy particular boundary or initial conditions. The classification of subgroups G_i can be viewed as a classification of conditions that can be imposed on the obtained solutions.

We mention that the dimension $r = \dim G$ of the symmetry group may be infinite. However, we shall always consider reductions by finite-dimensional subgroups of G.

Steps 3, 4, and 5 of Lie's method can be reformulated as follows. Take the vector fields $\{\mathbf{v}_a\}$ forming a basis of the considered Lie subalgebra $\mathfrak{g}_i \subset \mathfrak{g}$ and set their characteristics equal to zero

$$Q_a^\alpha = \varphi_a^\alpha(x,u) - \sum_{i=1}^{p} \xi_a^i(x,u)\, u_{x_i}^\alpha = 0, \quad \alpha = 1,\ldots,q, \quad a = 1,\ldots,r_i = \dim \mathfrak{g}_i. \tag{4}$$

Solve the systems (1) and (4) simultaneously.

Several alternative reduction procedures have been proposed, going beyond Lie's classical method and providing further solutions. They all have in common that they add some system of equations to the original system (1) and that the extended system is solved simultaneously. These additional equations replace the characteristic system (4).

In its generality, this was proposed as the method of "differential constraints," [10] and independently as the method of "side conditions." [11,12] Different methods differ by the choice of this system of side conditions.

Basically two different approaches exist in the literature. The first makes further use of the symmetry group G of system (1), the second approach goes beyond this group of point transformations, or even gives up group theory altogether. Let us briefly discuss some of these methods.

(1) "Group invariant solutions without transversality." This method was proposed by Anderson *et al.*[13] quite recently and deals with the situation when the rank condition (3) is not satisfied. It was shown[13] that under certain conditions on the subgroup $G_i \subset G$ one can still obtain G_i invariant solutions. We recall that a group invariant solution, with or without transversality, is transformed into itself by the subgroup $G_i \subset G$.

(2) The method of partially invariant solutions. A solution $u(x)$ is "partially invariant," [3,14,15] under a subgroup $G_i \subset G$ of the invariance group, if G_i, when acting on $u(x)$ sweeps out a manifold of a dimension that is larger than that of the graph of the solution, but less than the dimension of the entire space M. A group G_i may provide both invariant and partially invariant

solutions (see below in Sec. IV). However, if the rank condition (3) for the Jacobian is not satisfied, at least on a set of solutions, then G_i will not provide invariant solutions, but may provide partially invariant ones. If the rank of the Jacobian J is q', with $q'<q$, then we can express $u_1,\ldots,u_{q'}$ in terms of invariants and let $u_{q'+1},\ldots,u_q$ depend on all of the original variables $x_1,\ldots,x_p$. We then substitute the dependent variables back into the original system and obtain a ''partial reduction.'' Solving this system, we obtain the partially invariant solutions. Irreducible partially invariant solutions are partially invariant solutions that are not invariant under the subgroup G_i, nor under any other subgroup G_i' of the symmetry group of the considered equations. Such solutions were constructed for certain nonlinear Klein–Gordon and Schrödinger equations, in Refs. 16 and 17, and for some equations of hydrodynamics in Refs. 18–20.

The theory of partially invariant solutions was further developed by Ondich[21,22] who formulated irreducibility criteria for certain classes of equations. For other applications, see Refs. 23–26.

In terms of Eqs. (4), the method described above boils down to taking only $q'<q$ of Eqs. (4). As we shall show, it is possible to obtain further partially invariant solutions by different methods.

Among methods that go beyond the use of the symmetry group G we mention the following.

(3) The Clarkson–Kruskal direct reduction method[27,28] does not make explicit use of group theory. It is postulated that the dependent variables should be expressed in terms of new dependent variables that depend on fewer independent ones. The corresponding Ansatz is substituted into the original equation, which must then be solved. It has been shown that the direct method is intimately related to the method of conditional symmetries,[29–31] to the ''nonclassical method'' proposed by Bluman and Cole,[32,33] and to potential symmetries.[34] This method can also be interpreted in terms of side conditions.[11,12] The differential constraints added to system (1) in this case have the form of first order quasilinear partial differential equations of the form (4). However the coefficients φ_a^α and ξ_α^i are not related to a Lie point symmetry of Eq. (1).

(4) The group foliation method. The method goes back to Lie, is described by Ovsiannikov[3] and has recently been applied to obtain solutions of self-dual Einstein equations.[35,36] In terms of differential constraints this method amounts to embedding the system (1) into a larger system, consisting of all equations up to some definite order, invariant under the same Lie point symmetry group as (1) (and involving the same variables).

(5) The method of ''partial Lie-point symmetries,'' proposed by Cicogna and Gaeta.[37] This is a modification of the method of conditional symmetries. The method is in some cases easier to use and may provide solutions in cases when the equations of the conditional symmetry method prove to be untractable.

(6) For integrable equations[38] generalized symmetries can be used to generate side conditions. These will be higher order equations, rather than first order ones.

(7) The method of nonlocal symmetries. This consists in extending the space of dependent variables by adding some auxiliary variables, which can be potentials or pseudopotentials associated to the system of equations under analysis.[8,39–41] A nonlocal symmetry will be then a symmetry of the original system augmented with the equations defining the new nonlocal variables.

This article is organized as follows. In Sec. II we introduce the concept of ''weak transversality'' allowing us to formulate the method of ''group invariant solutions without transversality'' [13] in terms of local coordinates (the dependent and independent variables in the equation). We then relate the rank of the matrix of invariants (3) to that of the coefficients of vector fields. This makes the application of the method quite simple, as we shall show in Sec. III. Moreover, the requirement that the transformations be projectable is not needed. The method of weak transversality is applied in Sec. III to obtain new invariant solutions of the Navier–Stokes equations and of the isentropic compressible fluid model. In Sec. IV we establish a relation between partially invariant solutions and the transversality condition. This is then applied to obtain new irreducible partially invariant solutions of the vector nonlinear Schrödinger equation, of the Euler equations, of the Navier–Stokes equations and of the isentropic compressible fluid model in $(3+1)$ dimensions. The concept of the irreducibility of partially invariant solutions is discussed. Some conclusions are presented in the final Sec. V.

II. GROUP INVARIANT SOLUTIONS, STRONG AND WEAK TRANSVERSALITY

Lie's classical method of symmetry reduction was outlined in the Introduction. The first two steps are entirely algorithmic and we shall assume that they have already been performed. Thus, we are given a system of equations (1) and have found its Lie point symmetry group G, the Lie algebra of which is the symmetry algebra $\mathfrak{g}$. The symmetry algebra has dimension r and has a basis realized by vector fields of the form (2). Each vector field has the property that its nth prolongation annihilates the system (1) on its solution set

$$\mathrm{pr}^{(n)}\,\mathbf{v}\,\Delta_\nu\big|_{\Delta_\mu=0}=0,\quad \nu,\,\mu=1,\ldots,m. \tag{5}$$

The functions $\xi_a^i(x,u)$ and $\varphi_a^i(x,u)$ are thus explicitly known.

Let us now consider a subgroup $G_0\subset G$ and its Lie algebra $\mathfrak{g}_0$. A solution $u=f(x)$ of the system (1) is G_0 invariant if its graph $\Gamma_f\sim\{x,f(x)\}$ is a G_0 invariant set

$$g\cdot\Gamma_f=\Gamma_f,\quad g\in G_0. \tag{6}$$

The basis vector fields (2) can be written in evolutionary form[1] as

$$\mathbf{v}_{E,a}=\sum_{\alpha=1}^{q}\left(\varphi_a^\alpha(x,u)-\sum_{i=1}^{p}\xi_a^i(x,u)u_{x_i}^\alpha\right)\partial_{u_\alpha},\quad a=1,\ldots,r. \tag{7}$$

A G_0-invariant solution will satisfy the $q\times r_0$ characteristic equations (4) associated with the basis elements of the Lie algebra $\mathfrak{g}_0$ ($\dim\mathfrak{g}_0=r_0$).

The following matrices play an essential role in symmetry reduction using the symmetry group of the considered system of equations.

(1) The matrices Ξ_1 and Ξ_2 of the coefficients of the vector fields $\mathbf{v}_a$ spanning the algebra $\mathfrak{g}$, or its subalgebra $\mathfrak{g}_0$, and defined as follows:

$$\begin{gathered}\Xi_1=\{\xi_a^i(x,u)\},\quad \Xi_1\in\mathbb{R}^{r\times p},\\ \Xi_2=\{\xi_a^i(x,u),\varphi_a^\alpha(x,u)\},\quad \Xi_2\in\mathbb{R}^{r\times(p+q)},\end{gathered} \tag{8}$$

where $a=1,\ldots,r$ labels the rows, i and α label the columns.

(2) The matrix of characteristics of the vector fields (2) [or (7)] spanning the considered algebra $\mathfrak{g}$ (or its subalgebra $\mathfrak{g}_0$),

$$Q_a^\alpha=\{\mathbf{v}_a^E u_\alpha\},\quad a=1,\ldots,r,\quad \alpha=1,\ldots,q. \tag{9}$$

(3) The Jacobian matrix J of the transformation relating the dependent variables u_α and the invariants of the action of G_0 on the space $M\sim X\times U$ of independent and dependent variables.

Let us now consider a specific subalgebra $\mathfrak{g}_0\subset\mathfrak{g}$ and use it to obtain group invariant solutions via symmetry reduction. If the group G_0 acts regularly and transversally on $M\sim X\times U$ then

$$\mathrm{rank}\{\xi_a^i(x,u)\}=\mathrm{rank}\{\xi_a^i(x,u),\varphi_a^\alpha(x,u)\}. \tag{10}$$

This rank is equal to the dimension of the generic orbits of G_0 on M. If the transversality condition (10) is satisfied, at least locally, for all $\{x,u\}\in M$, then Lie's classical reduction method is directly applicable. Indeed, if (10) is satisfied then the rank of the matrix J of Eq. (3) is maximal, $\mathrm{rank}\,J=q$ (for a proof, see, e.g., Ref. 1, Chap. 3.5). It follows that all dependent variables can be expressed in terms of invariants and a reduction is immediate (to a system with q dependent variables and $p-s$ independent ones, where s is the dimension of the orbit of a generic point under the action of G_0.

If the action of G_0 on M is fiber preserving (i.e., the new independent variables only depend on the old independent ones), Lie's method provides explicit solutions. This happens because the new invariant independent variables z_i can be chosen to depend only on the original independent variables

$$z_i = z_i(x_1, \ldots, x_p), \quad i = 1, \ldots, p-s. \tag{11}$$

More generally, if we have $z_i = z_i(x,u)$, we obtain implicit solutions.

We shall call the rank condition (10) "strong transversality." Quite recently[13] a method was proposed for obtaining group invariant solutions when equation (10) is not satisfied. The method of Ref. 13 can actually be modified and made easier to apply by introducing the concept of "weak transversality."

The local transversality condition will be said to be satisfied in the weak sense if it holds only on a subset $\tilde{M} \subset M$, rather than on the entire space M:

$$\operatorname{rank}\{\xi_a^i(x,u)\}\big|_{\tilde{M}} = \operatorname{rank}\{\xi_a^i(x,u), \varphi_a^\alpha(x,u)\}\big|_{\tilde{M}}. \tag{12}$$

In other words, even if the transversality condition is not in general satisfied, there may exist a class S of functions $u = f(x)$ such that for them the condition (12) holds.

The "weak transversality" method is quite simple, when applicable. It consists of several steps.

(1) Determine the conditions on the functions $u = f(x)$ under which Eq. (12) is satisfied. Solve these conditions to obtain the general form of these functions.

(2) Substitute the obtained expressions into the matrix of characteristics (9) and require that the condition $\operatorname{rank} Q = 0$ be satisfied. This further constrains the functions $f(x)$.

(3) Substitute the obtained expressions into the system (1). By construction, the solutions, if they exist, will be G_0 invariant.

This method can only be applied if the matrix elements in the matrix Ξ_2 depend explicitly on the variables u_α. This poses strong restrictions on the considered algebra $\mathfrak{g}_0$. Step 1 of this method amounts to restricting to a domain where the original Lie method can be applied. Steps 2 and 3 are as in Lie's method. The "weak transversality method" is from this point of view a direct extension of Lie's classical method. Note that this method can be applied both to ordinary and partially differential equations. We shall give some examples of the method in Sec. III.

III. EXAMPLES OF INVARIANT SOLUTIONS OBTAINED BY THE WEAK TRANSVERSALITY METHOD

A. The Navier–Stokes equations

The Navier–Stokes equations in $(3+1)$ dimensions describing the flow of an incompressible viscuous fluid are

$$\vec{u}_t + \vec{u} \cdot \nabla \vec{u} + \nabla p - \nu \nabla^2 \vec{u} = 0, \tag{13}$$

$$\nabla \cdot \vec{u} = 0, \tag{14}$$

where $\vec{u} = (u_1(x,y,z,t), u_2(x,y,z,t), u_3(x,y,z,t))$ is the velocity field, $p = p(x,y,z,t)$ the fluid pressure and ν the viscosity coefficient.

The symmetry properties of these equations have been intensively investigated by many authors from different points of view (see, for instance, Ref. 42 and references therein). It is well known[43] that Eqs. (13) and (14) are invariant under the flow generated by the following vector fields:

$$B_1 = \alpha\, \partial_x + \dot{\alpha} \partial_{u_1} - \ddot{\alpha} x\, \partial_p, \tag{15}$$

$$B_2=\beta\,\partial_y+\dot{\beta}\partial_{u_2}-\ddot{\beta}y\,\partial_p\,, \tag{16}$$

$$B_3=\gamma\,\partial_z+\dot{\gamma}\partial_{u_3}-\ddot{\gamma}z\,\partial_p\,, \tag{17}$$

$$T=\partial_t\,, \tag{18}$$

$$Q=\partial_p\,, \tag{19}$$

$$D=x\partial_x+y\partial_y+z\partial_z+2t\partial_t-u_1\partial_{u_1}-u_2\partial_{u_2}-u_3\partial_{u_3}-2p\partial_p\,, \tag{20}$$

$$L_1=z\partial_y-y\partial_z+u_3\partial_{u_2}-u_2\partial_{u_3,} \tag{21}$$

$$L_2=x\partial_z-z\partial_x+u_1\partial_{u_3}-u_3\partial_{u_1}, \tag{22}$$

$$L_3=y\partial_x-x\partial_y+u_2\partial_{u_1}-u_1\partial_{u_2}, \tag{23}$$

where α,β,γ, and δ are arbitrary functions of time. The operators B_j generate symmetry transformations that can be interpreted as boosts to frames moving with arbitrary velocities $\vec{v(t)}=\lambda(\dot{\alpha},\dot{\beta},\dot{\gamma})$, where λ is a constant. Space translations and Galilei boosts are obtained if α,β, and γ are linear in t. The operators T and Q express the invariance of the Eqs. (13) and (14) under translations of time and pressure, D generates scaling transformations, and L_1,L_2, and L_3 are the generators of the group of the rotations of the Euclidean space.

Example 1: Let us consider the subalgebra generated by L_1, L_2, and L_3. Here we apply the ideas discussed in Sec. II to determine rotationally invariant solutions for the Navier–Stokes equations.

The matrices of the coefficients $\Xi_1=(\xi_a^i(x,u))$ and $\Xi_2=(\xi_a^i(x,u),\phi_a^\alpha(x,u))$ are represented by

$$\Xi_1=\begin{pmatrix} 0 & z & -y \\ -z & 0 & x \\ y & -x & 0 \end{pmatrix}, \quad \Xi_2=\begin{pmatrix} 0 & z & -y & 0 & u_3 & -u_2 \\ -z & 0 & x & -u_3 & 0 & u_1 \\ y & -x & 0 & u_2 & -u_1 & 0 \end{pmatrix}. \tag{24}$$

We observe that the matrix Ξ_1 has rank 2, whereas the matrix Ξ_2 has rank 3. In this situation, the transversality condition is violated in the strong sense. In other words, it is not true that for *every* function $\vec{u}=(u_1,u_2,u_3)$ the ranks of the matrices Ξ_1 and Ξ_2 coincide. In general, the system of characteristics is not compatible, the Jacobian matrix J will not have maximal rank, and it is *not* possible to use the classical symmetry reduction approach. To overcome these difficulties, let us force the matrix Ξ_2 to be of rank 2. This requirement is equivalent to a system of algebraic equations for $\vec{u}$, obtained imposing that the determinants of all 3×3 matrices constructed using the rows and the columns of Ξ_2 be equal to zero. Once this algebraic system is solved, we get the class S of functions $\vec{u}=(u_1,u_2,u_3)$ on which transversality is weakly restored. The class S in this case is characterized by the conditions:

$$u_1=f(x,y,z,t)x, \quad u_2=f(x,y,z,t)y, \quad u_3=f(x,y,z,t)z, \quad p=p(x,y,z,t). \tag{25}$$

The second step consists in solving the characteristic system $Q_k^\alpha(x,u^{(1)})=0$ for the class S of Eqs. (25). This forces the functions f and p to have the form

$$f=f(r,t), \quad p=p(r,t), \tag{26}$$

where $r=\sqrt{x^2+y^2+z^2}$. Relations (26) represent the most general form for the function $\vec{u}$ and p to be rotationally invariant in the Euclidean space. Substituting these expressions for $\vec{u}$ and p into Eqs. (13) and (14), we find the solution

$$\vec{u}=\frac{a(t)}{r^3}\vec{x}, \quad p=\frac{\dot{a}}{r}-\frac{a^2}{2r^4}+b. \tag{27}$$

The same vector fields L_1, L_2, and L_3 provide also a subalgebra of the symmetry algebra of the Euler equations. Anderson *et al.*[13] obtained a class of rotationally invariant solutions of the Euler equations by means of their technique of reduction diagrams. In Ref. 18 partially invariant solutions related to the subalgebra $\{L_1, L_2, L_3\}$ for the equations describing a nonstationary and isentropic flow for an ideal and compressible fluid in $(3+1)$ dimensions have been constructed using the transformation (25). A similar situation is also observed in magnetohydrodynamics.[19] Our solutions of the Navier–Stokes equations coincide with the solutions of the Euler equations found in Ref. 13. Physically that means that the solutions (27) describe a laminar flow for which viscosity plays no role. This phenomenon occurs because the components of the vector $\vec{u}$ in Eq. (27) are all harmonic functions, i.e., they satisfy the Laplace equation, in addition to the Navier–Stokes equations.

Example 2: Now, let us analyze the subalgebra defined by the operators

$$\begin{aligned} D&=x\partial_x+y\partial_y+z\partial_z+2t\partial_t-u_1\partial_{u_1}-u_2\partial_{u_2}-u_3\partial_{u_3}-2p\partial_p,\\ L_3&=y\partial_x-x\partial_y+u_2\partial_{u_1}-u_1\partial_{u_2},\\ X&=t^k\partial_x+k\,t^{k-1}\partial_{u_1}-k\,(k-1)\,t^{k-2}x\,\partial_p,\\ Y&=t^k\partial_y+k\,t^{k-1}\partial_{u_2}-k\,(k-1)\,t^{k-2}y\,\partial_p, \end{aligned} \tag{28}$$

which is a subalgebra of the Galilei–similitude algebra for a given $k\in\mathbb{R}$. It is immediate to check that the local transversality is violated for this subalgebra in the strong sense. The matrix Ξ_2 is now represented by

$$\begin{pmatrix} x & y & z & 2t & -u_1 & -u_2 & -u_3 & -2p \\ y & -x & 0 & 0 & u_2 & -u_1 & 0 & 0 \\ t^k & 0 & 0 & 0 & k\,t^{k-1} & 0 & 0 & -k\,(k-1)\,t^{k-2}x \\ 0 & t^k & 0 & 0 & 0 & k\,t^{k-1} & 0 & -k\,(k-1)\,t^{k-2}y \end{pmatrix}.$$

If we impose that the matrix Ξ_2 should have rank 3 (that is weak transversality), we get

$$u_1=k\frac{x}{t}, \quad u_2=k\frac{y}{t},$$

$$u_3=u_3(x,y,z,t), \quad p=p(x,y,z,t).$$

As a second step, let us solve the characteristic system $Q_a^{\alpha}(x,u^{(1)})=0$, which consists of 16 linear differential equations of first order in the derivatives of the velocity components u_j and the pressure p. The most general function living in the space of the dependent variables and invariant under the flow associated to the generators (28) is

$$u_1=k\frac{x}{t}, \quad u_2=k\frac{y}{t}, \quad u_3=\frac{\alpha\left(\dfrac{t}{z^2}\right)}{z^2}, \tag{29}$$

$$p=-\frac{k(k-1)(x^2+y^2)}{2t^2}+\frac{\beta\left(\frac{t}{z^2}\right)}{z^2}, \tag{30}$$

with α and β arbitrary functions of $t\ z^{-2}$. Substituting into the Navier–Stokes equations (13) and (14), we obtain the following three parameter set of solutions:

$$u_1=k\frac{x}{t},\quad u_2=k\frac{y}{t},\quad u_3=\frac{c_1}{\sqrt{t}}-2\frac{kz}{t}, \tag{31}$$

$$p=\frac{1}{2t^2}\{c_1\sqrt{t}z+k(x^2+y^2+4c_1\sqrt{t}z-2z^2)-k^2(x^2+y^2+4z^2)+2c_2t\}, \tag{32}$$

with $c_1,c_2,k\in\mathbb{R}$. This solution is invariant under the group generated by the algebra (28) and satisfies weak (but not strong) transversality.

B. The isentropic compressible fluid model

The equations describing the nonstationary isentropic flow of a compressible ideal fluid are[44]

$$\vec{u_t}+\vec{u}\cdot\nabla\vec{u}+k\,a\,\nabla a=0, \tag{33}$$

$$a_t+\vec{u}\cdot\nabla a+k^{-1}a\,\nabla\cdot\vec{u}=0, \tag{34}$$

where $\vec{u}=u_1(x,y,z,t)$, $u_2(x,y,z,t)$, $u_3(x,y,z,t)$ is the velocity field, $a=a(x,y,z,t)$ is the velocity of sound, related to the pressure p and the density ρ by the formula $a=(\gamma p/\rho)^{1/2}$, γ is the adiabatic exponent and $k=2/(\gamma-1)$. The symmetry group G of Eqs. (33) and (34) was derived in Ref. 20. For $k\neq 3$, G it is generated by the following vector fields:

$$P_0=\partial_t,\quad P_1=\partial_x,\quad P_2=\partial_y,\quad P_3=\partial_z, \tag{35}$$

$$K_1=t\partial_x+\partial_{u_1},\quad K_2=t\partial_y+\partial_{u_2},\quad K_3=t\partial_z+\partial_{u_3}, \tag{36}$$

$$L_1=z\partial_y-y\partial_z+u_3\partial_{u_2}-u_2\partial_{u_3,}, \tag{37}$$

$$L_2=x\partial_z-z\partial_x+u_1\partial_{u_3}-u_3\partial_{u_1}, \tag{38}$$

$$L_3=y\partial_x-x\partial_y+u_2\partial_{u_1}-u_1\partial_{u_2}, \tag{39}$$

$$F=x\partial_x+y\partial_y+z\partial_z+t\partial_t,\quad G=-t\partial_t+u_1\partial_{u_1}+u_2\partial_{u_2}+u_3\partial_{u_3}+a\,\partial_a. \tag{40}$$

We mention that for $k=3$ the symmetry algebra contains an additional element generating projective transformations. The operators P_i,K_i, and L_i are the infinitesimal generators of space translations, Galilei boosts and rotations, respectively. The operators F and G generate scaling transformations.

Example 3: Let us consider the subalgebra $\{L_3,F+G,K_1,K_2\}$. The matrix Ξ_2 is given by

$$\begin{pmatrix} y & -x & 0 & 0 & u_2 & -u_1 & 0 & 0\\ x & y & z & 0 & u_1 & u_2 & u_3 & a\\ t & 0 & 0 & 0 & 1 & 0 & 0 & 0\\ 0 & t & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \tag{41}$$

and the transversality is again violated in the strong sense, because rank $\Xi_1=3$ and rank $\Xi_2=4$. If we force the matrix Ξ_2 to be of rank 3, then we get the following constraints:

$$u_1=\frac{x}{t}, \quad u_2=\frac{y}{t}, \quad u_3=u_3(x,y,z,t), \quad a=a(x,y,z,t). \tag{42}$$

From the characteristic system $Q_a^{\alpha}(x,u^{(1)})=0$ we deduce

$$u_3=z\,W(t), \quad a=z\,A(t), \tag{43}$$

where W and A are arbitrary functions of time. Now, substituting relations (42) and (43) into the system (33) and (34) we obtain the relation

$$A(t)=\sqrt{-\frac{1}{k}(W^2+W')} \tag{44}$$

and a second order ODE for W

$$W''+2\left(2+\frac{1}{k}\right)WW'+2\left(1+\frac{1}{k}\right)W^3+\frac{4}{k\,t}(W'+W^2)=0. \tag{45}$$

In general, Eq. (45) does not have the Painlevé property. For special values of the parameter k, namely $k=-1$ and $k=-2$, it does. In these cases it can be reduced to a canonical form (see Ref. 45, p.334) via a linear transformation of the type

$$W=\alpha(t)\,U(z(t))+\beta(t). \tag{46}$$

(1) For $k=-1$ we have

$$W''=-2WW'+p(t)\,(W'+W^2), \tag{47}$$

where $p(t)=4/t$. This equation can be integrated and its solution, which is regular, is

$$W=\frac{c_1t^2\left(I_{-5/6}\left(\frac{c_1t^3}{3}\right)+c_2I_{5/6}\left(\frac{c_1t^3}{3}\right)\right)}{I_{1/6}\left(\frac{c_1t^3}{3}\right)+c_2I_{-1/6}\left(\frac{c_1t^3}{3}\right)}, \tag{48}$$

where c_1 and c_2 are constants and $I_n(x)$ is the modified Bessel function of the first kind. Correspondingly we find

$$A=c_1t^2 \tag{49}$$

in Eq. (44).

(2) For $k=-2$ we have

$$W''=-3WW'-W^3+q(t)(W'+W^2), \tag{50}$$

where $q(t)=2/t$. In this case, we can integrate and the general solution is

$$W=\frac{4\,t^3+c_1}{t^4+c_1\,t+c_2}. \tag{51}$$

The solution of Eq. (44) is

$$A=2\sqrt{3}\sqrt{\frac{t^2}{t^4+c_1t+c_2}}, \tag{52}$$

where c_1, and c_2 are constants. The solutions for $k=-1$ and $k=-2$ represent nonscattering waves.

IV. PARTIALLY INVARIANT SOLUTIONS OF SYSTEMS OF DIFFERENTIAL EQUATIONS AND THE TRANSVERSALITY CONDITION

A useful tool applicable to the study of systems of differential equations, and intimately related to the standard Lie approach, is the theory of partially invariant solutions. The relevant notion in this context is the defect δ of a k-dimensional manifold M with respect to a Lie group G. When the group acts on a p-dimensional submanifold $\Gamma\subseteq M$, it sweeps out an orbit $G(\Gamma)$. The manifold Γ will be identified with the graph Γ_f of a function $u=f(x)$, so its dimension will coincide with the number of independent variables (also denoted p). As we already said, the case $G(\Gamma_f)=\Gamma_f$ corresponds to the G-invariance of the manifold. Otherwise, $G(\Gamma_f)$ will be a more generic subset of M. There is no guarantee that this subset will be a submanifold. However, if the intersection between an orbit O of G and Γ_f has a dimension which is constant in a neighborhood N of a point of Γ_f, then there exists a neighborhood $\tilde{G}$ of the identity of G such that the subset $\tilde{G}$ $(N\cap\Gamma_f)$ is a submanifold.[21] In the subsequent considerations, $G(\Gamma_f)$ will be considered as a submanifold.

Let G be a group, acting regularly with s-dimensional orbits. We call the number

$$\delta=\dim G(\Gamma_f)-\dim\Gamma_f \tag{53}$$

the defect δ of the function f with respect to G. The usual G-invariant functions correspond to the case $\delta=0$. A function will be said to be it *generic* if $\delta=m_0=\min\{s,k-p\}$. The more interesting situation is when $0<\delta<m_0$, which is the case we will dealing with. In this case, the function f will be said to be partially invariant.[3]

Let us consider the system (1) of partial differential equations, whose symmetry group G acts on the $p+q$-dimensional space $M=X\times U$. Let $\mathfrak{g}$ be a subalgebra of the symmetry algebra of Δ, and Q the characteristic matrix associated to the set of its generators. Then $u=f(x)$ is a partially invariant solution of Δ with defect δ with respect to $\mathfrak{g}$ if and only if[3,21,46]

$$\operatorname{rank}(Q(x,u^{(1)}))=\delta. \tag{54}$$

The condition (54) provides a system of differential equations involving the dependent variables $u=(u_1,\ldots,u_q)$. In order to determine partially invariant solutions, we can extend the original system Δ by adding the set of differential constraints given by the condition (54). We must then solve the extended system consisting of Eqs. (1) and (54). The equations given by the prescription (54) are less constraining than those required to obtain G-invariance, as in formulas (4). Indeed, condition (4) requires that the rank of Q be zero [compatible with (54) but stronger].

In this section we will study the role of the local transversality condition (and in particular of the notion of weak transversality) in the theory of partially invariant solutions and propose a strategy to find them.

Let us start by noticing that a partially invariant solution of a system of differential equations can be naturally related to the violation of the transversality condition. Indeed, let $\Delta(x,u^{(n)})=0$ be a system of differential equations defined over $M\subset X\times U$ and $u_0=u_0(x_0)$ be a solution of Δ. Let G be an r-dimensional subgroup of the symmetry group of Δ, acting regularly on M, whose generators are given by (2). If the condition

$$\operatorname{rank}(\xi_a^i(x_0,u_0))<\operatorname{rank}(\xi_a^i(x_0,u_0),\phi_a^\alpha(x_0,u_0)) \tag{55}$$

is satisfied, then $u_0=f(x_0)$ is a partially invariant solution of Δ (or possibly a generic one).

Example 4: The vector nonlinear Schrödinger equation

$$i\psi_t+\Delta\psi=(\overline{\psi}\psi)\psi, \tag{56}$$

where $\psi\in\mathbb{C}^N$ and Δ is the Laplace operator in n dimensions, plays an important role in many areas of physics. For instance, in nonlinear optics it describes the interaction of electromagnetic waves propagating with different polarizations in nonlinear media.[47,48] In hydrodynamics, it furnishes a model for the description of the interactions of N water waves in a deep fluid.[49–51] For these and other applications of the vector nonlinear Schrödinger equation, see also Ref. 52.

Let us consider the case of three components ($N=3$) and two spatial dimensions ($n=2$). The symmetry algebra has been computed in Ref. 53. In terms of amplitude and phase, the components of the wave function will be written as $\psi_\mu=\rho_\mu e^{i\omega_\mu}$. The symmetry algebra of Eq. (56) for $N=3$ and $n=2$ has the form

$$\mathfrak{g}=\mathrm{sch}(2)\oplus\mathrm{su}(3). \tag{57}$$

The Schrödinger algebra sch(2) has a basis realized by the vector fields

$$P_1=\partial_x,\quad P_2=\partial_y,\quad K_1=t\partial_x+\frac{1}{2}x\sum_\mu\partial\omega_\mu, \tag{58}$$

$$K_2=t\partial_y+\frac{1}{2}y\sum_\mu\partial\omega_\mu, \tag{59}$$

$$L_{12}=y\partial_x-x\partial_y,\quad M=\sum_\mu\partial\omega_\mu, \tag{60}$$

$$D=2t\partial_t+x\partial_x+y\partial_y-(x^2+y^2)\sum_\mu\partial\omega_\mu, \tag{61}$$

$$C=t^2\partial_t+t\left[x\partial_x+y\partial_y-\sum_\mu\rho_\mu\partial\rho_\mu\right]+\frac{1}{4}(x^2+y^2)\sum_\mu\partial\omega_\mu. \tag{62}$$

We shall not need the algebra su(3) (given in Ref. 53), only its Cartan subalgebra

$$T_1=\partial\omega_1-\partial\omega_2,\quad T_2=\partial\omega_2-\partial\omega_3. \tag{63}$$

Let us consider the subalgebra

$$\{\partial_x,\partial_y,y\,\partial_x-x\,\partial_y+a_1\partial\omega_1+a_2\partial\omega_2+a_3\partial\omega_3\}, \tag{64}$$

generated by the two translations in the plane and a rotation combined with a transformation of the phases. The matrix of the coefficients Ξ_2, given by

$$\begin{pmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\y&-x&a_1&a_2&a_3&0&0&0\end{pmatrix}$$

has rank 3, unless $(a_1,a_2,a_3)=(0,0,0)$. Let us consider the case $a_2=a_3=0$, $a_1\neq0$. We obtain $\rho_i=\rho_i(t)$ $(i=1,2,3)$, $\omega_1=\omega_1(t)$, $\omega_2=\omega_2(t)$, but ω_3 is not an invariant, so we keep $\omega_3=\omega_3(x,y,z,t)$. Substituting into Eq. (56), we obtain

$$\rho_1=\frac{\gamma_1}{\sqrt{t(t-t_0)}},\quad \rho_2=\gamma_2,\quad \rho_3=\gamma_3, \tag{65}$$

$$\omega_1=\frac{x^2}{4(t-t_0)}+\frac{y^2}{4\,t}+\frac{\gamma_1^2}{t_0}\ln\frac{t}{t-t_0}-(\gamma_2^2+\gamma_3^2)\,t, \tag{66}$$

$$\omega_2=\omega_3=\frac{\gamma_1^2}{t_0}\ln\frac{t}{t-t_0}-(\gamma_2^2+\gamma_3^2)\,t. \tag{67}$$

This solution is partially invariant with respect to the subgroup corresponding to the subalgebra (64) with $a_1\neq 0$, $a_2=a_3=0$. Using the expressions (58)–(62) we can check that this solution is in general not invariant under any subgroup of the Schrödinger group Sch(2). The one exception is the limit $t_0\to 0$ when the solution is invariant under rotations generated by L_{12}. Thus this partially invariant solution is in general irreducible and becomes reducible for $t_0\to 0$.

Example 5: Let us consider again the isentropic compressible model [formulas (33) and (34)]. For the subalgebra $\mathfrak{g}=\{K_1,K_2,K_3,P_3\}$ the matrix Ξ_2 is given by

$$\begin{pmatrix} t & 0 & 0 & 0 & 1 & 0 & 0 & 0\\ 0 & t & 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & t & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Here transversality is violated also in the weak sense. The invariants of the corresponding Lie group are $F=u_1t-x, G=u_2\,t-y$, a and t. The matrix J of (3) is not invertible, but we can write

$$u_1=\frac{F(t)+x}{t},\quad u_2=\frac{G(t)+y}{t},\quad a=A(t), \tag{68}$$

but leave u_3 general, i.e., $u_3=u_3(x,y,z,t)$. Substituting Eqs. (68) into (33), (34) we obtain the solution[18]

$$u_1=\frac{x}{t},\quad u_2=\frac{y}{t},\quad u_3=\frac{z+\lambda(\xi_1,\xi_2)}{t+t_0},\quad a=c\left(\frac{1}{t^2(t+t_0)}\right)^{1/k}, \tag{69}$$

where $\xi_1=x/t$, $\xi_2=y/t$, λ is an arbitrary function of ξ_1 and ξ_2, c and t_0 are constants. The rank of the matrix Q_a^α of the characteristics associated to (69) is equal to 1, and therefore this solution is partially invariant with respect to the subalgebra $\mathfrak{g}$, with $\delta=1$. Now let us check if it is reducible under any other subalgebra of the full symmetry algebra (35)–(40). To do this, it is useful to study the kernel K of the characteristic matrix Q for the full symmetry algebra (35)–(40) associated to the solution (69) and to determine its generators $\{\mathbf{k}_1,\ldots,\mathbf{k}_l\}$. It is clear that if at least a subspace of K can be generated by constant vectors, then the solution will be reducible with respect to the subalgebra identified by these vectors.

In the case of the solution (69), the kernel is generated by eight vectors, each having 12 components. It is possible to show that there exists only one constant generator, namely

$$\mathbf{k}=(0,0,0,t_0,0,0,0,0,0,1,0,0).$$

This implies that the solution (69) is reducible with respect to the one-dimensional subalgebra $\{K_3+t_0P_3\}$.

The concept of ''irreducibility'' of a partially invariant solutions needs further clarification. Once a solution $u=f(x)$, partially invariant under G_i is found, it is of course possible to verify whether it is invariant under some other subgroup $G_i'\subset G$. Let this be the case, let G_i' satisfy the

strong transversality condition, and have generic orbits of dimension r_i'. The standard Lie method using the subgroup G_i' would then reduce system (1) to a system with $q-r_i'$ variables. In general, specially for $q-r_i'>1$, we may not be able to solve this system and the methods of partial invariance for the original subgroup G_i may be more tractable. We have already seen an example of this situation, namely, Example 4 above. Solution (65)–(67) is invariant under rotations in the limit $t_0\to 0$. If we look for such an invariant solution directly, we must set $\rho_i=\rho_i(r,t)$, $\omega_i=\omega_i(r,t)$ with $r=\sqrt{x^2+y^2}$. This reduces Eq. (56) to a system of PDE's in two variables. This system is very hard to solve and solution (65)–(67) would be very hard to obtain (without knowing it in advance). If the invariance subgroup G_i' does not satisfy the weak transversality condition, it may not help us at all.

We observe that the violation of the transversality condition is *not* a necessary condition for the existence of partially invariant solutions of a system $\Delta(x,u^{(n)})=0$. In fact, there could be solutions of Δ which are not solutions of the characteristic system, even if it is compatible as an algebraic system.

Example 6: As a matter of fact, a counterexample was provided by Ondich,[21] namely the two variable Laplace equation, expressed in the following form:

$$v=u_x,\quad v_y=w_x,\quad w=u_y,\quad v_x=-w_y. \tag{70}$$

This system is clearly invariant with respect to the translations in the plane, generated by the vector fields $\{\partial_x,\partial_y\}$. The characteristic matrix Q has the form

$$\begin{pmatrix} -u_x & -v_x & -w_x \\ -u_y & -v_y & -w_y \end{pmatrix}. \tag{71}$$

Invariant solutions are obtained if and only if the rank of this matrix is equal to zero. This implies that u, v, and w are constants:

$$u=k,\quad v=\lambda,\quad w=\mu,\quad k,\lambda,\mu\in\mathbb{R}.$$

Let us impose that the rank of Q is equal to 1. This means that the two rows in Eq. (71) are proportional. Then solving the corresponding equations and replacing the result into Eqs. (70), we get the following solution:

$$(u,v,w)=(a\,x+b\,y+c,\,a,\,b),\quad a,\,b\in\mathbb{R}. \tag{72}$$

By construction, this solution is partially invariant with respect to the group of translations in the plane, with defect $\delta=1$. Nevertheless, the transversality condition is satisfied. More generally, the transversality condition is always satisfied if we have $\operatorname{rank}(\xi_a^i(x,u))=\dim\mathfrak{g}$.

We mention that the previous solution (72) can be also obtained starting from the symmetry subalgebra $\{\partial_x,\partial_y,\partial_u\}$ for which both the weak and strong transversality conditions are violated. In this case, the invariants are $I_1=v=a$, $I_2=w=b$, where a and b are arbitrary constants. The function u remains arbitrary. Putting these constraints into Eqs. (70), we recover immediately the solution (72). However, it should be noticed that the analysis of the rank of the characteristic matrix furnishes a complete characterization of the invariant and partially invariant solutions of a system of differential equations, and provides a more general procedure than the use of the invariants. For instance, this second approach does not allow to recognize the solution (72) as a partially invariant one with respect to the subalgebra $\{\partial_x,\partial_y\}$.

Example 7: To show that a symmetry group satisfying the strong transversality can produce both invariant and partially invariant solutions, let us consider the Euler equations for an incompressible nonviscuous fluid in $(3+1)$ dimensions:

$$\vec{u_t}+\vec{u}\cdot\nabla\vec{u}+\nabla p=0, \tag{73}$$

$$\nabla\cdot\vec{u}=0, \tag{74}$$

The symmetry group of the Euler equations is well known.[1,5] It coincides with the symmetry group of the Navier–Stokes equations, except that it contains an additional dilation. Thus, D of Eq. (20) is replaced by

$$D_1=x\partial_x+y\partial_y+z\partial_z+t\partial_t, \tag{75}$$

$$D_2=t\,\partial_t-u_1\partial_{u_1}-u_2\partial_{u_2}-u_3\partial_{u_3}-2p\,\partial_p. \tag{76}$$

We consider here the subgroup of Galilei transformations. Its Lie algebra is given by

$$K_1=t\partial_x+\partial_{u_1},\quad K_2=t\partial_y+\partial_{u_2},\quad K_3=t\partial_z+\partial_{u_3}. \tag{77}$$

Here the transversality holds in the strong sense and indeed an invariant solution will have the form

$$u_1=\frac{x}{t}+F_1(t),\quad u_2=\frac{y}{t}+F_2(t),\quad u_3=\frac{z}{t}+F_3(t),\quad p=P(t). \tag{78}$$

Let us now look for partially invariant solutions of the system (73) and (74) with respect to the same subgroup and impose that the defect be $\delta=2$. Writing down the characteristic system associated to (77) and imposing that rank $Q=2$, we get the following constraints on u_1 and u_2:

$$u_1=\frac{x}{t}-\mu\,\lambda\frac{z}{t}+\mu\,\lambda u_3+h_1(t), \tag{79}$$

$$u_2=\mu\,u_3+\frac{y}{t}-\mu\frac{z}{t}+h_2(t) \tag{80}$$

but $u_3=u_3(x,y,z,t)$ and $p=p(x,y,z,t)$ remain arbitrary.

Substituting the relations (79) and (80) into the Euler equations, and choosing for simplicity $h_1=h_2=0$, we obtain the solution

$$u_1=\frac{1}{t[\mu^2(1+\lambda^2)+1]}\{x[\mu^2(1-2\lambda^2)+1]-3\lambda\mu(\mu y+z)\}+\lambda\,\mu\,t^2F\left(\frac{\lambda y-x}{t},\frac{\lambda\,\mu\,z-x}{t}\right), \tag{81}$$

$$u_2=\frac{1}{t[\mu^2(1+\lambda^2)+1]}\{y[\mu^2(\lambda^2-2)+1]-3\mu(\lambda\mu x+z)\}+\mu\,t^2F\left(\frac{\lambda y-x}{t},\frac{\lambda\,\mu\,z-x}{t}\right), \tag{82}$$

$$u_3=\frac{1}{t[\mu^2(1+\lambda^2)+1]}\{z[\mu^2(1+\lambda^2)-2]-3(\lambda x+y)\}+t^2F\left(\frac{\lambda y-x}{t},\frac{\lambda\,\mu\,z-x}{t}\right), \tag{83}$$

$$p=-\frac{3\mu^2}{t^2(\lambda^2\mu^2+\mu^2+1)}\left(\lambda x+y+\frac{z}{\mu}\right)^2+p(t), \tag{84}$$

where λ, μ are constants, F is an arbitrary function of its arguments and p is an arbitrary function of t. We have checked explicitly that, if F is kept arbitrary, this solution is not invariant under any

subgroup of the symmetry group. Thus, it represents an irreducible partially invariant solution of the Euler equations of defect $\delta=2$, with respect to a subgroup satisfying the strong transversality condition. If

$$F=\left(\frac{\lambda y-x}{t}\right)^{(3a+2b)/a}\Phi\left(\frac{\lambda y-x}{\lambda\,\mu\, z-x}\right),\quad a,b\in\mathbb{R},$$

where Φ is an arbitrary function of its argument, then the solution (81)–(84) is invariant under the subgroup generated by aD_1+bD_2, where D_1 and D_2 are defined in Eqs. (75) and (76).

However, this subgroup provides a reduced system with three independent variables that would be very difficult to solve.

Particularly interesting is the case when partially invariant solutions can be found that satisfy weak but not strong transversality. Indeed, imposing weak transversality basically means that a class of functions $u=f(x)$ is chosen in such a way that the characteristic system is algebraically compatible. This condition is of course not sufficient to guarantee the invariance of these functions under the action of the considered group G. Indeed, if we compute the rank of the matrix Q_a^α on this class of functions, in general it will be not equal to zero. Then, once weak transversality is satisfied, we can choose either to have group invariant solutions, using the method outlined in Sec. III, or to use the class of functions $u=f(x)$ to get partially invariant solutions.

In the next two examples, we will see how this approach can be used to obtain in a simple and straightforward way new classes of solutions of hydrodynamic systems.

Example 8: In Example 2 we studied the algebra (28) which is a subalgebra of the symmetry algebra of both the Euler and the Navier–Stokes equations. We showed that the requirement of weak transversality implies

$$u_1=k\frac{x}{t},\quad u_2=k\frac{y}{t},\tag{85}$$

$$u_3=u_3(x,y,z,t),\quad p=p(x,y,z,t).\tag{86}$$

These formulas define a class of functions which is partially invariant with defect $\delta=2$ with respect to the subalgebra (28). At this stage, we can choose either to have group invariant solutions or partially invariant ones. Indeed, in Example 2 we forced the class of functions (85) and (86) to be a solution of the characteristic system, and then substituting the obtained expressions (29) and (30) into the system (13) and (14) we constructed the group invariant solutions (31) and (32).

Another possibility is to substitute formulas (85) and (86) directly into the Euler equations (73) and (74) or the Navier–Stokes equations (13) and (14) without requiring further invariance properties. For the case of the Euler equations we get the constraints

$$t^2p_x+k\,(k-1)\,x=0,\tag{87}$$

$$t^2p_y+k\,(k-1)\,y=0,\tag{88}$$

$$u_{3z}+\frac{2k}{t}=0,\tag{89}$$

$$u_{3t}+u_3u_{3z}+\frac{k}{t}(x\,u_{3x}+y\,u_{3y})+p_z=0.\tag{90}$$

We solve this system and obtain the following partially invariant solution of the Euler equations:

$$u_1 = k\frac{x}{t}, \quad u_2 = k\frac{y}{t}, \tag{91}$$

$$u_3 = -\frac{2kz}{t} + x^2 F\left(tx^{-1/k}, \frac{y}{x}\right), \tag{92}$$

$$p = -\frac{k(k-1)(x^2+y^2)}{2t^2} - \frac{k(2k+1)z^2}{t^2} + f(t), \tag{93}$$

where $\xi = tx^{-1/k}$, $\eta = y/x$ and $f(t)$ and $F(\xi,\eta)$ are arbitrary functions of their arguments. As always, the question of the irreducibility of this solution arises. To answer it we must invoke the entire symmetry algebra $\mathfrak{g}$ of the Euler equations, namely the algebra (15) and (23) with the dilation D replaced by the two dilations (75) and (76). The result is that solution (91)–(93) is not invariant under any subgroup of the symmetry group, unless the function $F(\xi,\eta)$ satisfies the following linear PDE:

$$\left[\left(c_1\frac{k-1}{k} + c_2\right)\xi - c_3\frac{\xi\eta}{k} - \frac{c_4}{k}\xi^{k+1} + c_5\xi^k\right]F_\xi + [-c_3(\eta^2+1) - c_4\xi^k\eta + c_5\xi^k]F_\eta$$
$$+ (2c_1 + c_2 + 2c_3\eta)F - c_6(4k+1)\xi^{2k} = 0. \tag{94}$$

If this equation is satisfied, the solution is invariant under the subgroup generated by

$$X = c_1D_1 + c_2D_2 + c_3L_3 + c_4B_1 + c_5B_2 + c_3B_3, \tag{95}$$

where $c_1,\ldots,c_6$ are real constants, D_1 and D_2 are the dilations given by Eqs. (75) and (76), L_3 is the generator (23), and the functions appearing in the boosts (15)–(17) are now monomials in t, namely

$$\alpha = t^k, \quad \beta = t^k, \quad \gamma = t^{2k+1}. \tag{96}$$

For any other function $F(\xi,\eta)$ the solution is irreducible. The same procedure can be applied to the Navier–Stokes equations. Repeating the previous steps, we obtain the following solution:

$$u_1 = k\frac{x}{t}, \quad u_2 = k\frac{y}{t}, \tag{97}$$

$$u_3 = -\frac{2kz}{t} + \alpha(x,y,t), \tag{98}$$

$$p = -\frac{k(k-1)(x^2+y^2)}{2t^2} - \frac{k(2k+1)z^2}{t^2} + f(t), \tag{99}$$

where $\alpha(x,y,t)$ satisfies the following equation:

$$\alpha_t + \frac{k}{t}(x\alpha_x + y\alpha_y - 2\alpha) - \nu(\alpha_{xx} + \alpha_{yy}) = 0. \tag{100}$$

We thus obtain a large class of partially invariant solutions of the Navier–Stokes equations parametrized by the solutions of the *linear* partial differential equation (100).

Example 9: Partially invariant solutions with weak transversality can be also found for the case of the compressible fluid model (33) and (34). Let us again consider the subalgebra $\{L_3, F+G, K_1, K_2\}$ and the corresponding weak transversality condition (42). Substituting into Eqs. (33) and (34) we obtain a coupled system of quasilinear first order PDE's, namely,

$$a_x=0, \quad a_y=0,$$

$$u_{3t}+u_3\,u_{3z}+\frac{x}{t}u_{3x}+\frac{y}{t}u_{3y}+k\,a\,a_z=0, \tag{101}$$

$$a_t+u_3\,a_z+\frac{a}{k}\left(\frac{2}{t}+u_{3z}\right)=0.$$

In particular, if we assume $a_z=0$, we reobtain the solution (69). However, the system (101) allows much more general solutions.

V. CONCLUSIONS

A brief comparison of the results of this article and Ref. 13 is in order. In Sec. III we address the same question, as Anderson *et al.* in Ref. 13 do, namely how to obtain ''Group Invariant Solutions Without Transversality'' (their title). The main difference between us is one of outlook. They prove rigorous theorems under well-defined assumptions, in particular that the local group action is projectable. They make efficient use of the geometric theory of differential equations and further develop this theory by introducing the concept of the ''kinematic bundle'' and using kinematic and dynamic reduction diagrams. They use this concept to impose transversality at point of the original fiber bundle.

Our approach is a pragmatic one, aimed at producing new solutions. We use simple and well-known mathematical concepts (though we do not sacrifice mathematical rigour). From the results of Ref. 13 we know that transversality is not always a necessary requirement. We wish to obtain particular solutions when transversality (which we call ''strong transversality'') is not satisfied. From the geometric point of view we restrict to local coordinates (x,u). From the point of view of differential equations these coordinates are the original independent and dependent variables (x,u). The kinematic bundle concepts are then replaced by an equivalent requirement, namely weak transversality. This is formulated in a ''user friendly'' way as the requirement (12) that two matrices should have the same rank. The subtleties of Ref. 13 are then avoided in applications. In particular, we do not require that the group action be projectable (fiber preserving). As an example, consider a system of two first order PDE's with two dependent and two independent variables $\{u_1,u_2,x_1,x_2\}$,

$$x_1u_{1x_1}+x_2u_{1x_2}-u_1=x_2u_{1x_1}F_1(x_2,u_1), \tag{102}$$

$$u_{1x_2}u_{2x_1}-u_{1x_1}u_{2x_2}+u_{1x_1}=u_{2x_1}F_2(x_2,u_1), \tag{103}$$

where F_1 and F_2 are arbitrary. This system is invariant under a group generated by

$$\mathbf{v}_1=u_1\partial_{x_1}, \quad \mathbf{v}_2=x_2\partial_{x_1}+(u_2-x_2)\partial_{u_2}. \tag{104}$$

Clearly the action is neither transversal, nor projectable. Weak transversality is imposed by putting $u_2=x_2$. An invariant solution will have the form $u_2=x_2$, $u_1=\phi(x_2)$. Substituting into (102) and (103) we obtain the group invariant solution

$$u_2=x_2, \quad u_1=cx_2. \tag{105}$$

Notice that the system (102) and (103) is linear if F_1 and F_2 depend on x_2 alone. To see that ''weak transversality without projectability'' is not limited to first order equations, consider the system of two second order PDE's,

$$u_{1x_1}u_{2x_1x_1}-u_{2x_1}u_{1x_1x_1}=(u_{1x_1})^2u_{2x_1x_2}-u_{1x_1}u_{2x_1}u_{1x_1x_2}+u_{2x_1}u_{1x_2}u_{1x_1x_1}-u_{1x_1}u_{1x_2}u_{2x_1x_1}, \tag{106}$$

$$u_{1x_1x_1}=u_{1x_1}u_{1x_1x_2}-u_{1x_2}u_{1x_1x_1}. \tag{107}$$

This system is invariant under the group generated by the algebra (104). The invariant solution with weak transversality is

$$u_2=x_2, \quad u_1=\phi(x_2), \tag{108}$$

where $\phi(x_2)$ is an arbitrary function. The solutions (105) and (108) are not ''irreducible'' and (104) is only a subalgebra of the symmetry algebra of these equations. The point we are making is that the ''weak transversality'' method works for this algebra, even though the corresponding group action (for $\mathbf{v}_1$) is not projectable.

The main conclusion of this article is that one can do considerably more with the symmetry group G of a system of partial differential equations than apply the standard method for finding group invariant solutions.

Indeed, let us assume that the largest group G (of local Lie point transformations) leaving the system (1) invariant has been found and its subgroups classified. For each subgroup G_0, or its Lie algebra $\mathfrak{g}_0$ we should proceed as follows.

(1) Obtain invariant solutions. First check whether the transversality condition (10) is satisfied (in the strong sense). If it is, we apply Lie's classical method. This is always possible since transversality assures that the rank condition (3) is satisfied. If the (strong) transversality condition is not satisfied, we may still be able to obtain solutions invariant under G_0,[13] by imposing ''weak transversality'' on solutions, as described in Sec. II above. This is illustrated in Sec. III by Examples 1, 2, and 3.

(2) Obtain partially invariant solutions. These can be obtained by (at least) three complementary methods. If the transversality condition (10) is not satisfied and weak transversality cannot be imposed, then the characteristic system (4) is not consistent and the rank condition (3) for the invariants is not satisfied. We then choose a subset of $q'<q$ invariants such that we can express q' dependent variables in terms of invariants. The remaining $q-q'$ variables u_α are considered as functions of all the original variables $x_1,\ldots,x_p$. Examples 4 and 5 of Sec. IV are of this type, as are those of Refs. 16 and 17.

If the transversality condition is satisfied for G_0 we may still be able to obtain partially invariant solutions, in addition to the invariant ones. Instead of imposing that the matrix of characteristics (4) have rank zero [i.e., that all Eqs. (4) be satisfied] we require that on solutions we have $\operatorname{rank} Q=\delta$, with $\delta=1,2,\ldots$, as the case may be. This rank condition must be solved explicitly for u_α and the result substituted into Eq. (1) (see Examples 6 and 7). The third possibility is to impose weak transversality (if possible), but still to impose $\operatorname{rank} Q=\delta\geqslant 1$ (see Examples 8 and 9).

(3) Go beyond invariant and partially invariant solutions, either by the method of group foliation,[3,35,36] or by other methods not using the symmetry group G.[27–34]

We emphasize that the weak transversality method is algorithmic and can be implemented as a computer package. It provides both invariant and partially invariant solutions and is widely applicable. Missing at this stage are clear criteria that tell us which approach will be fruitful. Furthermore, the same solution may be obtained by different methods and it is not clear which of these methods will lead to the least amount of calculations. For instance, solutions partially invariant under some subgroup $G_1\subset G$ have been called ''reducible,''[16–22] if they are actually invariant under some other subgroup $G_2\subset G$. However, it may be more difficult to use G_2, than G_1, specially if the dimension of G_2 is small with respect to the number of independent variables.

ACKNOWLEDGMENTS

One of the authors (P.W.) thanks Professors Ian Anderson and Mark Fels for interesting discussions. The research of A.M.G. and of P.W. was partially supported by NSERC of Canada and FCAR du Québec. P.T. benefited from a CRM–ISM fellowship.

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ERRATA

Publisher's Note: "On certain geometric aspects of CP^N harmonic maps" [J. Math. Phys. 44, 813 (2003)]

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[DOI: 10.1063/1.1576171]

Due to an editorial oversight, the authors' originally published work[1] was published a second time in *Journal of Mathematical Physics* on pp. 813–822 of the February 2003 issue (Vol. 44, Issue 2). The Editors and AIP apologize for this publication error. All online versions of the February 2003 article have been corrected to match the original January 2003 article. Proper citation of this work is shown below in Ref. 1.

[1] A. M. Grundland and W. J. Zakrzewski, J. Math. Phys. **44**, 328 (2003).

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Erratum: "Relativistic *N*-boson systems bound by oscillator pair potentials" [J. Math. Phys. 43, 1237 (2002)]

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[DOI: 10.1063/1.1572531]

Eq. (3.7) of the paper defines the function $P(m)$ so that the formulas for $\{s,\overline{h}(s)\}$ yield $e(m)$ exactly, via Eq. (3.5). However, with the scaling parameters $\{\beta,\gamma,\lambda\}$ included, the "running" P which guarantees that Eq. (3.11) of the paper is exact is *not* simply $P(m)$, as claimed, but rather

$$P=P(\mu), \quad \text{where} \quad \mu=m\left(\frac{\beta}{\gamma\lambda}\right)^{1/3}.$$

With this correction, the expression for P is now consistent with the energy scaling formula given in Eq. (3.12) of the paper. In the application to the N-body problem, the expression $P(m)$ in Eq. (1.4) of Theorem 1 must be replaced by

$$P(\mu), \quad \text{where} \quad \mu=m(N/(\gamma(N-1)^2))^{1/3}.$$

The result is then consistent with the explicit N-body lower bound formula given in Eq. (5.7) of the paper. Figures 2 and 3 in the paper should be replaced by the revised Fig. 2 and 3 shown here. The upper and new lower bounds in Fig. 3 converge to the exact N-body energies in the Schrödinger limit $m\to\infty$.

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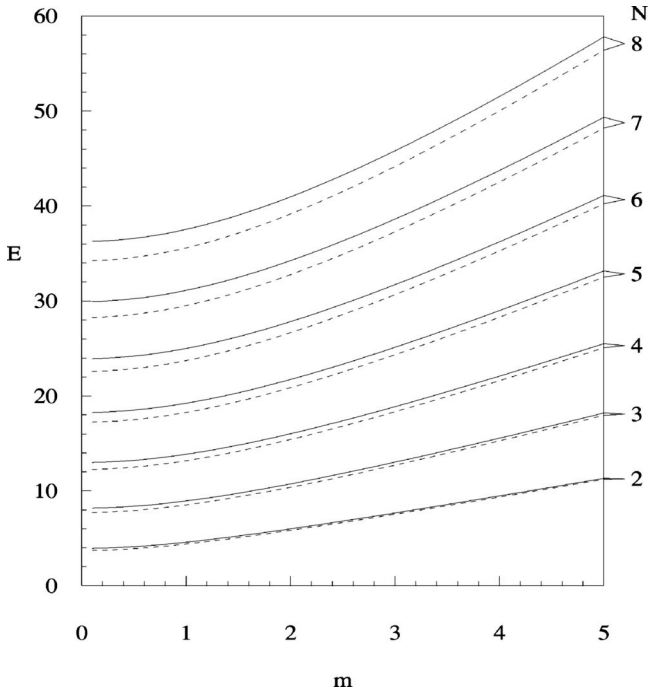

FIG. 2. Upper (full lines) and lower (dashed lines) bounds to the lowest energy $E(m)$ of the N-relativistic harmonic-oscillator problem for $N=2,3,\ldots,8$ obtained by employing the constant values $P=1.376$ and $P=1.5$, respectively, in Eq. (1.4) of Theorem 1.

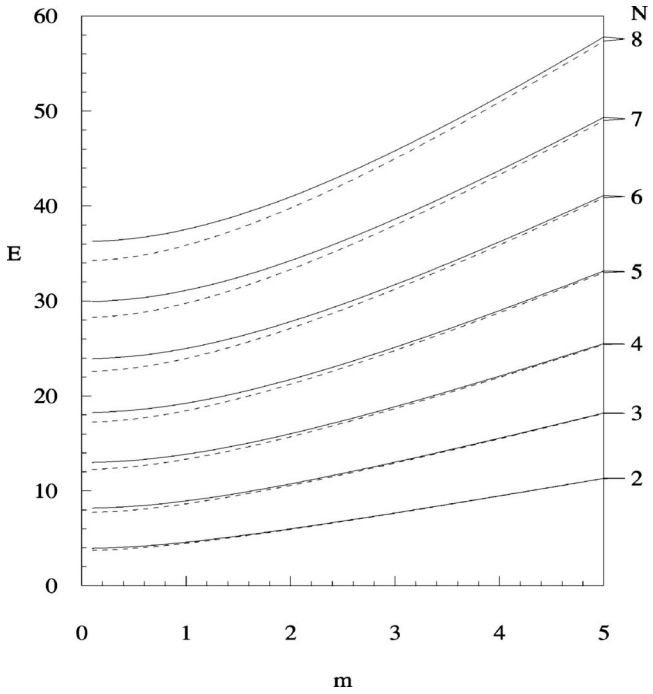

FIG. 3. Upper (full lines) and lower (dashed lines) bounds to the lowest energy $E(m)$ of the N-relativistic harmonic-oscillator problem for $N=2,3,\ldots,8$ obtained by employing the values $P=P(\mu)$, $\mu=m(N/(\gamma(N-1)^2))^{1/3}$, and $P=1.5$, respectively, in Eq. (1.4) of Theorem 1. For $N=2$, the lower bound is exact.

Bell inequalities in four dimensional phase space and the three marginal theorem

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(Received 2 October 2002; accepted 1 April 2003)

We address the classical and quantum marginal problems, namely the question of simultaneous realizability through a common probability density in phase space of a given set of compatible probability distributions. We consider only distributions authorized by quantum mechanics, i.e., those corresponding to complete commuting sets of observables. For four-dimensional phase space with position variables $\vec{q}$ and momentum variables $\vec{p}$, we establish the two following points: (i) given *four* compatible probabilities for (q_1,q_2), (q_1,p_2), (p_1,q_2), and (p_1,p_2), there does not always exist a positive phase space density $\rho(\vec{q},\vec{p})$ reproducing them as marginals; this settles a long standing conjecture; it is achieved by first deriving Bell-type inequalities in phase space which have their own theoretical and experimental interest. (ii) Given instead at most *three* compatible probabilities, there always exist an associated phase space density $\rho(\vec{q},\vec{p})$; the solution is not unique and its general form is worked out. These two points constitute our ''three marginal theorem.'' © *2003 American Institute of Physics.* [DOI: 10.1063/1.1578532]

I. INTRODUCTION

In classical mechanics, position and momentum can be simultaneously specified. Hence phase space density has a well-defined meaning in classical statistical mechanics. In quantum theory the probability density for observing eigenvalues of a complete commuting set (CCS) of observables is specific to the experimental context for measuring that CCS. Joint probabilities for different CCS which contain mutually noncommuting operators are not defined. For example, for a two-dimensional configuration space, with $\vec{q},\vec{p}$ denoting position and momentum, probability densities of anyone of the four CCS (q_1,q_2), (q_1,p_2), (p_1,q_2) or (p_1,p_2) are defined, but not their joint probabilities. The question one may raise is can one define such joint probabilities, e.g., a phase space probability density $\rho(\vec{q},\vec{p})$ such that all its marginals (in agreement with common terminology, by ''marginal'' of a distribution over several variables, we denote integrals of the distribution over a subset of its variables) coincide with the quantum mechanical probabilities for the different individual CCS? This general question was first raised by Martin and Roy.[1]

The Martin–Roy contextuality theorem demonstrates the impossibility of realizing quantum probability densities of all possible choices of the CCS of observables as marginals of one positive definite phase space density. For example, consider a two-dimensional configuration space. Let

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coordinates $q_{1\alpha}$, $q_{2\alpha}$ be obtained from q_1, q_2 by a rotation of arbitrary angle α, and momenta $p_{1\alpha}$, $p_{2\alpha}$ be related similarly to p_1, p_2

$$\begin{pmatrix} q_{1\alpha} \\ q_{2\alpha} \end{pmatrix} = V \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad \begin{pmatrix} p_{1\alpha} \\ p_{2\alpha} \end{pmatrix} = V \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}, \tag{1.1}$$

where

$$V = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}. \tag{1.2}$$

Does there exist for every quantum state (with density operator $\hat{\rho}$) a positive definite phase space density $\rho(\vec{q},\vec{p})$ such that its marginals agree with the corresponding quantum probabilities, i.e.,

$$\int \mathrm{d}p_{1\alpha}\,\mathrm{d}q_{2\alpha}\ \ \rho(\vec{q},\vec{p}) = \langle q_{1\alpha}, p_{2\alpha} |\, \hat{\rho}\, | q_{1\alpha}, p_{2\alpha} \rangle \tag{1.3}$$

for all α ranging from 0 to 2π? They answered this question in the negative by finding a state $\hat{\rho}$ for which Eq. (1.3) for all α are inconsistent with positivity of ρ. Since different α correspond to different experimental contexts, the Martin–Roy theorem is a new Gleason–Kochen–Specker-type contextuality theorem.[2] The positivity of the phase space density $\rho(\vec{q},\vec{p})$ is absolutely crucial for this theorem; otherwise the Wigner distribution function[3] would be a solution of (1.3).

Equations (1.3) constitute conditions on an infinite set of marginals of $\rho(\vec{q},\vec{p})$ (corresponding to the continuously infinite choices for α) to agree with corresponding quantum probability densities. Their inconsistency still leaves open the question of consistency of a finite number of such marginal conditions.

Indeed, the consistency of two marginal conditions where the marginals involve only nonintersecting sets of variables has been known for some time. Cohen and Zaparovanny[4] constructed the most general positive $\rho(\vec{q},\vec{p})$ obeying

$$\int \mathrm{d}\vec{p}\ \rho(\vec{q},\vec{p}) = \langle \vec{q} | \hat{\rho} | \vec{q} \rangle, \quad \int \mathrm{d}\vec{q}\ \rho(\vec{q},\vec{p}) = \langle \vec{p} | \hat{\rho} | \vec{p} \rangle.$$

Their solutions generalize the obvious simple uncorrelated solution for pure states ψ,

$$\rho(\vec{q},\vec{p}) = |\psi(\vec{q})|^2\ |\tilde{\psi}(\vec{p})|^2,$$

where tilde denotes Fourier transform. Based on generalized phase space densities exhibiting position momentum correlations, Roy and Singh[5] constructed a causal quantum mechanics reproducing quantum position and momentum probability densities, thus improving on De Broglie–Bohm mechanics[6] which only reproduced the quantum position probability densities. Later, going much further than the nonintersecting marginals of Cohen *et al.*,[4] Roy and Singh[7] constructed a causal quantum mechanics based on a positive $\rho(\vec{q},\vec{p})$ whose marginals reproduce the quantum probability densities of a chain of $N+1$ different CCS, e.g.,

$$(Q_1, Q_2, \ldots, Q_N),\ (P_1, Q_2, \ldots, Q_N),\ (P_1, P_2, Q_3, \ldots, Q_N), \ldots (P_1, P_2, \ldots, P_N).$$

Here N is the dimension of the configuration space, and each CCS in the chain is obtained from the preceding one by replacing one of the position operators Q_i by the conjugate momentum operator P_i.

Roy and Singh proposed the following definition: a **maximally realistic causal quantum mechanics** is a causal mechanics which simultaneously reproduces the quantum probability densities of the maximum number of different (mutually noncommuting) CCS of observables as marginals of the same positive definite phase space density. They also conjectured that for N-dimensional configuration space this maximum number is $N+1$.

A proof of this long standing conjecture is important for quantum mechanics where it quantifies the extent of simultaneous realizability of noncommuting CCS.

In this paper, we restrict ourselves to the case of $N=2$ degrees of freedom. The general case ($N>2$) will be dealt with in a forthcoming paper. In Sec. II below, we first state the classical and quantum marginal problems and second, show that, given four classical compatible two-variable probability distributions, there does not always exist a positive phase space distribution reproducing them as marginals. In Sec. III, we develop a new tool, "the phase space Bell inequalities," which are the phase space analogues of the standard Bell inequalities[8] for a system of two spin-half particles. We use them in Sec. IV to prove the conjecture for four-dimensional phase space ($N=2$), namely the impossibility of simultaneous realization of quantum probabilities of more than three CCS as marginals. In Sec. V, we explicitly construct the most general phase space distribution which reproduces probabilities of three CCS as marginals. These results, the three marginal theorem, are relevant for the construction of maximally realistic quantum mechanics.

As our results are essentially new theorems for multidimensional Fourier transforms, they are also expected to be useful for classical signal and image processing.[9] The theorems of the present paper and their generalizations to arbitrary N (Ref. 10) considerably advance previous results in the field, which have only dealt with nonintersecting sets of marginals (e.g., time and frequency). A summary of the results of this paper without detailed proofs is being reported separately.[11]

II. FOUR MARGINAL PROBLEM

Let us consider a physical system with two-dimensional configuration space. Let (q_1,p_1) and (q_2,p_2) be a set of canonical variables in the corresponding phase space. We look for a (normalized) probability distribution $\rho(q_1,q_2,p_1,p_2)$ such that

$$\rho(q_1,q_2,p_1,p_2)\geqslant 0\,, \tag{2.1}$$

$$\int \mathrm{d}p_1\,\mathrm{d}p_2\,\rho(q_1,q_2,p_1,p_2)=R(q_1,q_2)\,, \tag{2.2}$$

$$\int \mathrm{d}p_1\,\mathrm{d}q_2\,\rho(q_1,q_2,p_1,p_2)=S(q_1,p_2)\,, \tag{2.3}$$

$$\int \mathrm{d}q_1\,\mathrm{d}p_2\,\rho(q_1,q_2,p_1,p_2)=T(p_1,q_2)\,, \tag{2.4}$$

$$\int \mathrm{d}q_1\,\mathrm{d}q_2\,\rho(q_1,q_2,p_1,p_2)=U(p_1,p_2)\,, \tag{2.5}$$

where the four marginals $R(q_1,q_2)$, $S(q_1,p_2)$, $T(p_1,q_2)$, and $U(p_1,p_2)$, the respective joint probabilities, are given. For consistency we must have

$$R,S,T,U\geqslant 0, \tag{2.6}$$

and

$$\begin{aligned}
\int \mathrm{d}q_2\, R(q_1,q_2) &= \int \mathrm{d}p_2\, S(q_1,p_2)\,,\\
\int \mathrm{d}q_1\, R(q_1,q_2) &= \int \mathrm{d}p_1\, T(p_1,q_2)\,,\\
\int \mathrm{d}q_1\, S(q_1,p_2) &= \int \mathrm{d}p_1\, U(p_1,p_2)\,,\\
\int \mathrm{d}q_2\, T(p_1,q_2) &= \int \mathrm{d}p_2\, U(p_1,p_2)\,.
\end{aligned} \tag{2.7}$$

We shall refer to the following problem as the Classical four marginal problem: *Given four distributions R, S, T, and U, satisfying the consistency conditions, does there always exist a positive $\rho(q_1,q_2,p_1,p_2)$ with these distributions as marginals*?

When the system is quantum mechanical and is described by a state vector $|\Psi\rangle$, each of the four marginals involves a pair of compatible observables and we have

$$\begin{aligned}
R(q_1,q_2) &= |\langle q_1,q_2|\hat{\rho}|q_1,q_2\rangle|^2\,,\\
S(q_1,p_2) &= |\langle q_1,p_2|\hat{\rho}|q_1,p_2\rangle|^2\,,\\
T(p_1,q_2) &= |\langle p_1,q_2|\hat{\rho}|p_1,q_2\rangle|^2\,,\\
U(p_1,p_2) &= |\langle p_1,p_2|\hat{\rho}|p_1,p_2\rangle|^2\,.
\end{aligned} \tag{2.8}$$

In this case, the above consistency conditions are automatically satisfied. We then refer to the problem as the *quantum four marginal problem*. A positive answer to it for all states $\hat{\rho}$ would mean that a realistic interpretation of the quantum results is possible (to the extent that only measurements connected to the four marginals are involved).

We shall see that the answer to both problems is negative.

Let us first show that the classical four marginal problem does not always admit a solution. To this end, consider the following set of marginals:

$$R(q_1,q_2) = \tfrac{1}{2}[\,\delta(q_1-a_1)\,\delta(q_2-a_2)+\delta(q_1-a_1')\,\delta(q_2-a_2')\,]\,, \tag{2.9}$$

$$S(q_1,p_2) = \tfrac{1}{2}[\,\delta(q_1-a_1)\,\delta(p_2-b_2)+\delta(q_1-a_1')\,\delta(p_2-b_2')\,]\,, \tag{2.10}$$

$$T(p_1,q_2) = \tfrac{1}{2}[\,\delta(p_1-b_1)\,\delta(q_2-a_2)+\delta(p_1-b_1')\,\delta(q_2-a_2')\,]\,, \tag{2.11}$$

$$U(p_1,p_2) = \tfrac{1}{2}[\,\delta(p_1-b_1)\,\delta(p_2-b_2')+\delta(p_1-b_1')\,\delta(p_2-b_2)\,]\,, \tag{2.12}$$

which obviously satisfy the consistency conditions (2.6) and (2.7). They possess two essential features. First, their nonfactorized form. Second, in view of the expressions of R, S, and T, the positions of the factors $\delta(p_2-b_2)$ and $\delta(p_2-b_2')$ in the expression of U are not the "natural ones."

Equation (2.9) means that the support of the distribution R in the plane (q_1,q_2) consists in the two points (a_1,a_2) and (a_1',a_2'). As a consequence, any positive ρ satisfying (2.2) should have support from the projection of which on the plane (q_1,q_2) would also consist in those two points. That is

$$\rho = \delta(q_1-a_1)\,\delta(q_2-a_2)\,\alpha(p_1,p_2)+\delta(q_1-a_1')\,\delta(q_2-a_2')\,\alpha'(p_1,p_2)\,, \tag{2.13}$$

where α and α' are some positive distributions. Similarly, from Eqs. (2.3) to (2.5)

$$\rho=\delta(q_1-a_1)\,\delta(p_2-b_2)\beta(p_1,q_2)+\delta(q_1-a_1')\,\delta(p_2-b_2')\beta'(p_1,q_2) \tag{2.14}$$

$$=\delta(p_1-b_1)\,\delta(q_2-a_2)\,\gamma(q_1,p_2)+\delta(p_1-b_1')\,\delta(q_2-a_2')\,\gamma'(q_1,p_2) \tag{2.15}$$

$$=\delta(p_1-b_1)\,\delta(p_2-b_2')\,\eta(q_1,q_2)+\delta(p_1-b_1')\,\delta(p_2-b_2)\,\eta'(q_1,q_2)\,. \tag{2.16}$$

According to Eqs. (2.13)–(2.15)

$$\rho=v\;\delta(q_1-a_1)\,\delta(q_2-a_2)\,\delta(p_1-b_1)\,\delta(p_2-b_2)+v'\,\delta(q_1-a_1')\,\delta(q_2-a_2')\,\delta(p_1-b_1')\,\delta(p_2-b_2')\,, \tag{2.17}$$

with $v\geqslant 0$, $v'\geqslant 0$, $(v+v'=1)$. Clearly, Eqs. (2.16) and (2.17) are incompatible, which establishes the nonexistence of ρ, and settles the classical four marginal problem.

This however does not settle the quantum problem. Actually, the above example obviously cannot be strictly realized through a wave function in accordance with Eqs. (2.8). More than that, this example is so "twisted" that, even after smoothing out the δ measures in Eqs. (2.9)–(2.12), approaching it close enough through a wave function appears as very difficult (if not impossible). Instead, we develop a new mathematical tool.

III. PHASE SPACE BELL INEQUALITIES

Consider any choice of functions $r(q_1,q_2)$, $s(q_1,p_2)$, $t(p_1,q_2)$, and $u(p_1,p_2)$, obeying

$$A\leqslant r(q_1,q_2)+s(q_1,p_2)+t(p_1,q_2)+u(p_1,p_2)\leqslant B\quad(\forall q_1,q_2,p_1,p_2). \tag{3.1}$$

Multiply by $\rho(\vec{q},\vec{p})$, integrate over phase space and use positivity and normalization of $\rho(\vec{q},\vec{p})$. We deduce that the (classical as well as quantum) four marginal problem cannot have a solution unless

$$A\leqslant \int \mathrm{d}q_1\,\mathrm{d}q_2\,r(q_1,q_2)R(q_1,q_2)+\int \mathrm{d}q_1\,\mathrm{d}p_2\,s(q_1,p_2)S(q_1,p_2)$$
$$+\int \mathrm{d}p_1\,\mathrm{d}q_2\,t(p_1,q_2)T(p_1,q_2)+\int \mathrm{d}p_1\,\mathrm{d}p_2\,u(p_1,p_2)U(p_1,p_2)\leqslant B\,. \tag{3.2}$$

Here R, S, T, and U are defined by Eqs. (2.8) in the quantum case. It turns out that a particularly interesting choice is

$$\begin{aligned} r(q_1,q_2)&=\operatorname{sgn}F_1(q_1)\operatorname{sgn}F_2(q_2)\,,\\ s(q_1,p_2)&=\operatorname{sgn}F_1(q_1)\operatorname{sgn}G_2(p_2)\,,\\ t(p_1,q_2)&=\operatorname{sgn}G_1(p_1)\operatorname{sgn}F_2(q_2)\,,\\ u(p_1,p_2)&=-\operatorname{sgn}G_1(p_1)\operatorname{sgn}G_2(p_2)\,, \end{aligned} \tag{3.3}$$

with $A=-2$, $B=+2$ and with F_1, F_2, G_1, and G_2 arbitrary nonvanishing functions. (Note that, with this choice, the sum $r+s+t+u$ assumes only its two extremal values $A=-2$ and $B=+2$, which makes it in a sense optimal.) Then the inequalities (3.2) become a phase space analogue of the Bell inequalities for spin variables.

The necessary conditions (3.2) provide us with an alternative proof that the classical problem does not always admit a solution. Indeed, it is readily seen that they are violated for the marginals (2.9)–(2.12) and functions F's and G's such that

$$F_1(a_1),F_2(a_2),G_1(b_1),G_2(b_2)>0\,,$$

$$F_1(a_1'),F_2(a_2'),G_1(b_1'),G_2(b_2')<0\,.$$

We shall see in the next section that the necessary conditions (3.2) can be violated also in the quantum case. There, the analogy between our correlation inequalities (3.2) [with the choice (3.3)] and Bell inequalities will become more apparent, especially as regards to their implications.

IV. SOLVING THE FOUR MARGINAL QUANTUM PROBLEM

This section is divided into four parts. In the first one, we prove the existence of wave functions which violate the correlation inequalities (3.2). Strictly speaking, this already settles the problem. However, the explicit construction of such wave functions, which we present in Secs. IV B and IV C, is worthwhile in that it exhibits the physical implications of our inequalities. In Sec. IV D, we elaborate on the formal analogy with Bell inequalities.

A. Nonconstructive proof

One first notices that $\chi_1(q_1)\equiv\frac{1}{2}[1+\operatorname{sgn}F_1(q_1)]$ is the characteristic function of some set $S_1\subset\mathbb{R}$, and similarly for F_2, G_1, and G_2, so that Eqs. (3.3) read

$$\begin{aligned} r(q_1,q_2)&=(2\chi_1-1)(2\chi_2-1)\,,\\ s(q_1,p_2)&=(2\chi_1-1)(2\chi_2'-1)\,,\\ t(p_1,q_2)&=(2\chi_1'-1)(2\chi_2-1)\,,\\ u(p_1,p_2)&=-(2\chi_1'-1)(2\chi_2'-1)\,, \end{aligned} \tag{4.1}$$

where χ_i stands for $\chi_i(q_i)$ and χ_i' for $\chi_i'(p_i)$, $(i=1,2)$. Inequalities (3.1) then become

$$0\leqslant\mathcal{P}\leqslant 1\,, \tag{4.2}$$

and in fact $\mathcal{P}(1-\mathcal{P})=0$, where $\mathcal{P}(q_1,q_2,p_1,p_2)$ is given by

$$\mathcal{P}=\chi_1+\chi_2+\chi_1'\chi_2'-\chi_1\chi_2-\chi_1\chi_2'-\chi_1'\chi_2\,. \tag{4.3}$$

Let us define a corresponding quantum operator $\hat{\mathcal{P}}$ by

$$\hat{\mathcal{P}}=\hat\chi_1+\hat\chi_2+\hat\chi_1'\hat\chi_2'-\hat\chi_1\hat\chi_2-\hat\chi_1\hat\chi_2'-\hat\chi_1'\hat\chi_2\,, \tag{4.4}$$

where

$$\begin{aligned} \hat\chi_1&=\int_{S_1}\mathrm{d}q_1\,|q_1\rangle\langle q_1|\otimes\mathbf{1}_2\,,\\ \hat\chi_2&=\mathbf{1}_1\otimes\int_{S_2}\mathrm{d}q_2\,|q_2\rangle\langle q_2|\,,\\ \hat\chi_1'&=\int_{S_1'}\mathrm{d}p_1\,|p_1\rangle\langle p_1|\otimes\mathbf{1}_2\,,\\ \hat\chi_2'&=\mathbf{1}_1\otimes\int_{S_2'}\mathrm{d}p_2\,|p_2\rangle\langle p_2|\,. \end{aligned} \tag{4.5}$$

The $\hat{\chi}$'s are orthogonal projectors ($\hat{\chi}\dagger=\hat{\chi}$, $\hat{\chi}^2=\hat{\chi}$) acting on $\mathcal{H}\equiv L^2(\mathbb{R},\mathrm{d}q_1)\otimes L^2(\mathbb{R},\mathrm{d}q_2)$. [In Eqs. (4.5), S_1, S_2, S_1', S_2' are the supports of $\hat{\chi}_1$, $\hat{\chi}_2$, $\hat{\chi}_1'$, $\hat{\chi}_2'$, respectively. Also, $\int_{S_1} dq_1\,|q_1\rangle\langle q_1|$ is, in standard Dirac notation, the orthogonal projection $\psi(q_1)\to\chi_1(q_1)\psi(q_1)$, whereas $\int_{S_1'}\mathrm{d}p_1\,|p_1\rangle\langle p_1|$ is the orthogonal projection $\tilde{\psi}(p_1)\to\chi_1'(p_1)\tilde{\psi}(p_1)$, $\tilde{\psi}(p_1)$ being the Fourier transform of $\psi(q_1)$, and so on.] The product of two of them involving different indices commutes, so that $\hat{\mathcal{P}}$ is a (bounded) self-adjoint operator.

The inequalities (3.2) to be tested in the quantum context then become, for pure states $\hat{\rho}=|\Psi\rangle\langle\Psi|$,

$$0\leqslant\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle\leqslant 1 \quad \forall\ |\Psi\rangle\in\mathcal{H} \ \text{ with } \ \langle\Psi|\Psi\rangle=1\,, \tag{4.6}$$

or, equivalently,

$$\hat{\mathcal{P}}\geqslant 0 \quad \text{and} \quad \mathbf{1}-\hat{\mathcal{P}}\geqslant 0 \quad \text{in the operator sense.} \tag{4.7}$$

Because $\hat{\chi}_j$ fails to commute with $\hat{\chi}_j'$ ($j=1,2$), $\hat{\mathcal{P}}$ is *not* an orthogonal projector (see below), in contrast to the classical equality $\mathcal{P}^2=\mathcal{P}$. Exploiting this fact leads to the following.

Proposition 1: The operators $\hat{\mathcal{P}}$ and $(\mathbf{1}-\hat{\mathcal{P}})$ cannot be both positive. As a consequence, there is at least one $|\Psi\rangle\neq 0$ such that the inequalities $\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle\geqslant 0$ and $\langle\Psi|(\mathbf{1}-\hat{\mathcal{P}})|\Psi\rangle\geqslant 0$ cannot be simultaneously true. This just means that one of the two inequalities (4.6) is violated for that $|\Psi\rangle$, which settles the question.

Proof of proposition 1: Assume that $\hat{\mathcal{P}}$ and $(\mathbf{1}-\hat{\mathcal{P}})$ are both positive. This would imply

$$\hat{\mathcal{P}}(\mathbf{1}-\hat{\mathcal{P}})\geqslant 0 \tag{4.8}$$

(remember that the product of two positive *commuting* operators is positive).

Now, a straightforward calculation of $\hat{\mathcal{P}}^2$ from Eq. (4.4) yields

$$\hat{\mathcal{P}}^2=\hat{\mathcal{P}}-[\hat{\chi}_1,\hat{\chi}_1'][\hat{\chi}_2,\hat{\chi}_2']\,, \tag{4.9}$$

and Eq. (4.8) would mean that $[\hat{\chi}_1,\hat{\chi}_1'][\hat{\chi}_2,\hat{\chi}_2']$ is a positive operator. That this is wrong is not surprising. Let us show it. Take a factorized $|\Psi\rangle$, namely $|\Psi\rangle=|\Phi_1\rangle\otimes|\Phi_2\rangle$, so that

$$\langle\Psi|\hat{\mathcal{P}}(\mathbf{1}-\hat{\mathcal{P}})|\Psi\rangle=-\langle\Phi_1|i[\hat{\chi}_1,\hat{\chi}_1']|\Phi_1\rangle\langle\Phi_2|i[\hat{\chi}_2,\hat{\chi}_2']|\Phi_2\rangle\,.$$

It is enough to show that, for a given choice of the characteristic functions χ and χ', the real number

$$R[\Phi]\equiv\langle\Phi|i[\hat{\chi},\hat{\chi}']|\Phi\rangle \tag{4.10}$$

can assume both signs when $|\Phi\rangle$ is varied.

Let us define

$$|\Phi^+\rangle=\hat{\chi}\,|\Phi\rangle\,,\quad |\Phi^-\rangle=(\mathbf{1}-\hat{\chi})|\Phi\rangle\,.$$

Using the identity

$$[\hat{\chi},\hat{\chi}']=\hat{\chi}\hat{\chi}'(\mathbf{1}-\hat{\chi})-(\mathbf{1}-\hat{\chi})\hat{\chi}'\hat{\chi}$$

gives $R[\Phi]$ the form

$$R[\Phi]=i\langle\Phi^+|\hat{\chi}'|\Phi^-\rangle-i\langle\Phi^-|\hat{\chi}'|\Phi^+\rangle\,.$$

Obviously, for $|\tilde{\Phi}\rangle=|\Phi^+\rangle-|\Phi^-\rangle$, one has $R[\tilde{\Phi}]=-R[\Phi]$.

This concludes the proof.

Remarks: (1) When the wave function $|\Psi\rangle$ factorizes, i.e., $\Psi(q_1,q_2)=\Phi_1(q_1)\Phi_2(q_2)$, a corresponding probability distribution ρ always exists, namely

$$\rho(q_1,q_2,p_1,p_2)=|\Phi_1(q_1)|^2\,|\Phi_2(q_2)|^2\,|\tilde{\Phi}_1(p_1)|^2\,|\tilde{\Phi}_2(p_2)|^2\,, \tag{4.11}$$

where the $\tilde{\Phi}_i$'s are the Fourier transforms

$$\tilde{\Phi}_i(p_i)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\mathrm{d}q_i\,e^{-ip_iq_i}\,\Phi_i(q_i)\,,\quad (i=1,2). \tag{4.12}$$

Of course, this implies that Eqs. (4.6) are automatically satisfied for such factorized $|\Psi\rangle$'s [which can also be checked from Eq. (4.4)].

(2) The fact (used in the proof) that $\langle\Psi|\hat{\mathcal{P}}(\mathbf{1}-\hat{\mathcal{P}})|\Psi\rangle<0$ for some factorized $|\Psi\rangle$'s is *not* inconsistent with the inequalities $0\leqslant\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle\leqslant 1$ which are satisfied for those $|\Psi\rangle$'s.

B. Construction

We want to find wave functions $|\Psi\rangle$ violating the inequalities (4.6). According to the first of the above remarks, one has to depart from the class of factorized $|\Psi\rangle$'s. The simplest way to do it is to take just a sum of two such products.

Choose first

$$S_1=S_2\equiv S\quad\text{and}\quad S_1'=S_2'\equiv S'\,,$$

so that

$$\hat{\mathcal{P}}=\hat{\chi}\otimes\mathbf{1}_2+\mathbf{1}_1\otimes\hat{\chi}+\hat{\chi}'\otimes\hat{\chi}'-\hat{\chi}\otimes\hat{\chi}-\hat{\chi}\otimes\hat{\chi}'-\hat{\chi}'\otimes\hat{\chi}\,. \tag{4.13}$$

Take next

$$\begin{gathered}|\Psi\rangle=\frac{1}{\sqrt{1+|\lambda|^2}}(|\phi\rangle+\lambda|\varphi\rangle)\quad(\lambda\in\mathbb{C})\,,\\ \text{with}\quad\begin{cases}|\phi\rangle=|\phi_1\rangle\otimes|\phi_2\rangle\,,\quad|\varphi\rangle=|\varphi_1\rangle\otimes|\varphi_2\rangle\,,\\ \langle\phi_1|\phi_1\rangle=\langle\phi_2|\phi_2\rangle=\langle\varphi_1|\varphi_1\rangle=\langle\varphi_2|\varphi_2\rangle=1,\ \langle\phi_1|\varphi_1\rangle=0\,,\end{cases}\end{gathered} \tag{4.14}$$

so that $|\Psi\rangle$ is properly normalized.

For the moment, choose also

$$\phi_1=\phi_2\equiv f\quad\text{and}\quad\varphi_1=\varphi_2\equiv g\,, \tag{4.15}$$

with

$$\langle f|f\rangle=\langle g|g\rangle=1\,,\quad\langle f|g\rangle=0\,. \tag{4.16}$$

Then

$$\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle=\frac{1}{1+|\lambda|^2}[\langle\phi|\hat{\mathcal{P}}|\phi\rangle+(\lambda\langle\phi|\hat{\mathcal{P}}|\varphi\rangle+\text{c.c.})+|\lambda|^2\langle\varphi|\hat{\mathcal{P}}|\varphi\rangle]\,, \tag{4.17}$$

with

$$\langle\phi|\hat{\mathcal{P}}|\phi\rangle = 2\langle f|\hat{\chi}|f\rangle + \langle f|\hat{\chi}'|f\rangle^2 - \langle f|\hat{\chi}|f\rangle^2 - 2\langle f|\hat{\chi}|f\rangle\langle f|\hat{\chi}'|f\rangle\,,$$

$$\langle\varphi|\hat{\mathcal{P}}|\varphi\rangle = 2\langle g|\hat{\chi}|g\rangle + \langle g|\hat{\chi}'|g\rangle^2 - \langle g|\hat{\chi}|g\rangle^2 - 2\langle g|\hat{\chi}|g\rangle\langle g|\hat{\chi}'|g\rangle\,, \tag{4.18}$$

$$\langle\phi|\hat{\mathcal{P}}|\varphi\rangle = \langle f|\hat{\chi}'|g\rangle^2 - \langle f|\hat{\chi}|g\rangle^2 - 2\langle f|\hat{\chi}|g\rangle\langle f|\hat{\chi}'|g\rangle\,.$$

We already know that $0\leqslant\langle\phi|\hat{\mathcal{P}}|\phi\rangle\leqslant 1$ and $0\leqslant\langle\varphi|\hat{\mathcal{P}}|\varphi\rangle\leqslant 1$. Clearly, in view of (4.17), our goal will be reached (namely $\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle<0$ or $\langle\Psi|\hat{\mathcal{P}}|\Psi\rangle>1$) if one can find f and g such that

$$|\langle\phi|\hat{\mathcal{P}}|\varphi\rangle|^2 > \langle\phi|\hat{\mathcal{P}}|\phi\rangle\langle\varphi|\hat{\mathcal{P}}|\varphi\rangle\,. \tag{4.19}$$

We claim that this can be achieved with $S=S'=(0,\infty)$, $f(q)\equiv\langle q|f\rangle$ an even, normalized function in $L^2(-\infty,\infty)$, and

$$g(q)\equiv\langle q|g\rangle = \mathrm{sgn}(q)\, f(q)\,. \tag{4.20}$$

With this choice, Eqs. (4.16) are automatically satisfied and

$$\langle f|\hat{\chi}|f\rangle = \langle g|\hat{\chi}|g\rangle = \langle f|\hat{\chi}|g\rangle = \tfrac{1}{2}\,. \tag{4.21}$$

Also, since the Fourier transforms $\tilde{f}(p)$ and $\tilde{g}(p)$ are, respectively, even and odd functions

$$\langle f|\hat{\chi}'|f\rangle = \langle g|\hat{\chi}'|g\rangle = \tfrac{1}{2}\,. \tag{4.22}$$

As for the nontrivial interference term $\langle f|\hat{\chi}'|g\rangle$, it is given by (see Appendix A)

$$\langle f|\hat{\chi}'|g\rangle = -\frac{i}{\pi}\int_0^\infty \mathrm{d}q \int_0^\infty \mathrm{d}q'\, f^*(q) f(q')\left(\frac{1}{q+q'} - \frac{P}{q-q'}\right). \tag{4.23}$$

At this stage, it is advantageous to take f as a *real* function, so that by symmetry

$$\langle f|\hat{\chi}'|g\rangle = -\frac{i}{\pi}\int_0^\infty \mathrm{d}q \int_0^\infty \mathrm{d}q' \frac{f(q)f(q')}{q+q'}\,.$$

Let us set

$$h(q) = \sqrt{2}\, f(q)\,, \tag{4.24}$$

$$K(q,q') = \frac{1}{\pi}\frac{1}{q+q'}\,. \tag{4.25}$$

Then

$$\langle f|\hat{\chi}'|g\rangle = -\frac{i}{2}\gamma\,, \quad (\gamma\in\mathbb{R}) \tag{4.26}$$

with

$$\gamma = \int_0^\infty \mathrm{d}q \int_0^\infty \mathrm{d}q'\, h(q)\, K(q,q')\, h(q')\,, \tag{4.27}$$

and

$$\|h\|_{L^2(0,\infty)} = 1\,. \tag{4.28}$$

The insertion of Eqs. (4.21), (4.22), and (4.26) in (4.18) gives

$$\langle \phi|\hat{\mathcal{P}}|\phi\rangle = \langle \varphi|\hat{\mathcal{P}}|\varphi\rangle = \tfrac{1}{2},$$

$$\langle \phi|\hat{\mathcal{P}}|\varphi\rangle = -\frac{1}{4}(1+\gamma^2) + \frac{i}{2}\gamma,$$

so that Eq. (4.19) reads

$$(\gamma^2+1)^2 + 4\gamma^2 > 4,$$

which is satisfied provided that

$$|\gamma| > \sqrt{2\sqrt{3}-3} \cong 0.6813. \tag{4.29}$$

Moreover, with $\lambda = \rho e^{i\theta}$, Eq. (4.17) becomes

$$\langle \Psi|\hat{\mathcal{P}}|\Psi\rangle = \frac{1}{2} - \frac{\rho}{2(1+\rho^2)}[(1+\gamma^2)\cos\theta + 2\gamma\sin\theta]. \tag{4.30}$$

We already know that $|\gamma|$ cannot exceed 1, because $|\langle f|\hat{\chi}'|g\rangle|^2 \leqslant \langle f|\hat{\chi}'|f\rangle\langle g|\hat{\chi}'|g\rangle = \frac{1}{4}$. Are there however some h's [subjected to (4.28)] such that γ [given by Eq. (4.27)] fulfils (4.29)? If this occurs we have reached our goal and it only remains to maximize $|\gamma|$ in order to obtain the extremal values of $\langle \Psi|\hat{\mathcal{P}}|\Psi\rangle$ (within the present scheme) through Eq. (4.30). In other words, one has to solve the problem

$$\gamma_0 \equiv \sup_{\substack{\|h\|_{L^2(0,\infty)}=1 \\ h=h^*}} |\langle h|K|h\rangle| = \ ?$$

In Appendix B, it is shown that the (bounded) integral operator K with kernel (4.25) on $L^2(0,\infty)$ is positive and has the purely continuous spectrum $[0,1]$. This immediately entails $\gamma_0 = 1$, and we get

$$\langle \Psi|\hat{\mathcal{P}}|\Psi\rangle|_{\gamma=1} = \frac{1}{2} - \frac{\rho}{1+\rho^2}(\cos\theta + \sin\theta),$$

$$\begin{aligned} \inf_{\lambda} \langle \Psi|\hat{\mathcal{P}}|\Psi\rangle|_{\gamma=1} &= \langle \Psi|\hat{\mathcal{P}}|\Psi\rangle|_{\gamma=\rho=1,\,\theta=\pi/4} = \frac{1-\sqrt{2}}{2} \cong -0.2071, \\ \sup_{\lambda} \langle \Psi|\hat{\mathcal{P}}|\Psi\rangle|_{\gamma=1} &= \langle \Psi|\hat{\mathcal{P}}|\Psi\rangle|_{\gamma=\rho=1,\,\theta=-3\pi/4} = \frac{1+\sqrt{2}}{2} \cong 1.2071. \end{aligned} \tag{4.31}$$

Actually, as discussed in Appendix B, due to the continuous spectrum of K, these extremal values cannot be strictly reached, but only approached arbitrarily close via a family of normalized functions h, e.g.,

$$h_L(q) = \frac{\theta(L-q)}{\sqrt{\ln(L+1)}} \frac{1}{\sqrt{q+1}}, \quad L \to \infty$$

or smoothed forms of this. Of course, other functions h will also do the job (although less perfectly), that is meet the crucial requirement (4.29). Taking, for example, $h(q) = 1/(q+1)$ [which is normalized in $L^2(0,\infty)$], one gets

$$\gamma = \frac{\pi}{4} \cong 0.7854.$$

Finally, collecting the equations (4.14), (4.15), (4.20), and (4.24), together with $\lambda = \pi/4$, $-3\pi/4$, one obtains the wave functions leading to the maximal violations (4.31),

$$\Psi_{\pm}(q_1,q_2) = \frac{1}{2\sqrt{2}}[1 \pm e^{i(\pi/4)}\,\mathrm{sgn}(q_1)\mathrm{sgn}(q_2)]h(|q_1|)h(|q_2|)\,, \tag{4.32}$$

where $h(q)$ stands for some regularized form of $1/\sqrt{q}$, with $\int_0^\infty dq\, h(q)^2 = 1$.

C. Introducing Einstein locality and relative motion

Let us now interpret q_1 and q_2 as the coordinates of two particles (rather than the x and y coordinates of the same particle). Then the wave functions (4.32) describe states of two particles not spatially separated and with zero relative momentum. These two restrictions can be easily disposed of.

First, it can be checked that nothing is essentially changed in the previous derivation if one keeps

$$S_1 = S_1' = (0,\infty)\,, \quad \phi_1(q_1) = f(q_1)\,, \quad \varphi_1(q_1) = \mathrm{sgn}(q_1) f(q_1)\,, \tag{4.33}$$

but replaces

$$S_2 = S_2' = (0,\infty)\,, \quad \phi_2(q_2) = f(q_2)\,, \quad \varphi_2(q_2) = \mathrm{sgn}(q_2) f(q_2)\,, \tag{4.34}$$

by

$$S_2 = (a,\infty)\,, \quad S_2' = (0,\infty)\,, \quad \phi_2(q_2) = f(q_2 - a)\,, \quad \varphi_2(q_2) = \mathrm{sgn}(q_2 - a) f(q_2 - a)\,.$$

Then Eq. (4.32) becomes

$$\Psi_{\pm}(q_1,q_2) = \frac{1}{2\sqrt{2}}[1 \pm e^{i(\pi/4)}\,\mathrm{sgn}(q_1)\mathrm{sgn}(q_2 - a)]h(|q_1|)h(|q_2 - a|)\,,$$

with a arbitrary.

This allows us to let Einstein locality enter the game.

Similarly, nothing is essentially changed if one keeps Eqs. (4.33) but replaces Eqs. (4.34) by

$$S_2 = (0,\infty)\,, \quad S_2' = (P,\infty)\,, \quad \phi_2(q_2) = e^{iPq_2} f(q_2)\,, \quad \varphi_2(q_2) = e^{iPq_2}\,\mathrm{sgn}(q_2) f(q_2)\,.$$

Then Eq. (4.32) becomes

$$\Psi_{\pm}(q_1,q_2) = \frac{1}{2\sqrt{2}}[1 \pm e^{i(\pi/4)}\,\mathrm{sgn}(q_1)\mathrm{sgn}(q_2)]e^{iPq_2}h(|q_1|)h(|q_2|)\,,$$

with P arbitrary.

This allows us to put the two particles in relative motion.

D. Analogy with Bell spin-$\frac{1}{2}$ correlation inequalities

Let us denote by $|+\rangle$ a normalized function f close to the (symmetrized) eigenfunction of the operator K with "eigenvalue" $\lambda_0 = 1$ [i.e., $\gamma \cong 1$ in Eq. (4.26)], and by $|-\rangle$ the orthogonal func-

tion g [as given by Eq. (4.20)]. Consider the subspace $V=\mathrm{span}(|+\rangle,|-\rangle)$ of the full one-particle Hilbert space, together with the orthogonal projector Π onto V. Call Γ (respectively, Γ') the restriction of $\hat{\chi}$ (respectively, $\hat{\chi}'$) to the two-dimensional space V

$$\Gamma=\Pi\,\hat{\chi}\,\Pi\,,\quad \Gamma'=\Pi\,\hat{\chi}'\,\Pi\,.$$

Then Eqs. (4.21), (4.22), and (4.26) tell us that Γ and Γ' are represented in the orthonormal basis $\{|+\rangle,|-\rangle\}$ by the matrices

$$\Gamma=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}=\frac{1}{2}(1+\sigma_x)\,,$$

$$\Gamma'=\begin{pmatrix} \frac{1}{2} & \frac{i}{2}\gamma \\ -\frac{i}{2}\gamma & \frac{1}{2} \end{pmatrix}=\frac{1}{2}(1-\gamma\sigma_y)\,.$$

In the idealized limit $\gamma\to 1$ (and only in this limit), one observes that Γ and Γ' are themselves orthogonal projections $V\to V$

$$\Gamma=\Gamma^\dagger,\quad \Gamma^2=\Gamma\,,$$

$$\Gamma'=\Gamma'^\dagger,\quad \Gamma'^2=\Gamma'\,.$$

This implies that both operators $\hat{\chi}$ and $\hat{\chi}'$ leave the subspace V invariant

$$[\Pi,\hat{\chi}]=[\Pi,\hat{\chi}']=0\,.$$

Indeed, a straightforward calculation shows that

$$[(\mathbf{1}-\Pi)\hat{\chi}\Pi]^\dagger[(\mathbf{1}-\Pi)\hat{\chi}\Pi]=0\,,$$

which entails $(\mathbf{1}-\Pi)\hat{\chi}\Pi=0$ and $\hat{\chi}\Pi=\Pi\hat{\chi}$. The same for $\hat{\chi}'$.

Hence, in the two-particle Hilbert space, the operator (4.13) also leaves invariant $V\otimes V$, and $\overline{\mathcal{P}}:=\hat{\mathcal{P}}\Pi$ assumes the simple form

$$\overline{\mathcal{P}}=\tfrac{1}{2}+\tfrac{1}{4}(\sigma_y^{(1)}\sigma_y^{(2)}-\sigma_x^{(1)}\sigma_x^{(2)}+\sigma_x^{(1)}\sigma_y^{(2)}+\sigma_y^{(1)}\sigma_x^{(2)})\,, \tag{4.35}$$

whereas the maximally violating wave functions (4.32) read

$$|\Psi_\pm\rangle=\frac{1}{\sqrt{2}}(|+\rangle^{(1)}|+\rangle^{(2)}\pm e^{i\pi/4}|-\rangle^{(1)}|-\rangle^{(2)})\,. \tag{4.36}$$

From Eq. (4.35) one can check that

$$\overline{\mathcal{P}}(\mathbf{1}-\overline{\mathcal{P}})=-\tfrac{1}{4}\sigma_z^{(1)}\sigma_z^{(2)}\,, \tag{4.37}$$

which is just the projected form of $\hat{\mathcal{P}}(\mathbf{1}-\hat{\mathcal{P}})=[\hat{\chi}_1,\hat{\chi}_1'][\hat{\chi}_2,\hat{\chi}_2']$, and the expectation value of the operator (4.37) is

$$\langle\Psi_\pm|\overline{\mathcal{P}}(\mathbf{1}-\overline{\mathcal{P}})|\Psi_\pm\rangle=-\tfrac{1}{4}$$

for the wave functions (4.36).

The result (4.31) is also directly recovered from Eqs. (4.35) and (4.36),

$$\langle \Psi_{\pm} | \overline{\mathcal{P}} | \Psi_{\pm} \rangle = \frac{1 \mp \sqrt{2}}{2}.$$

Then one sees that, in the idealized limit $\gamma \to 1$, the original phase space setting up of the problem is formally equivalent to the standard EPR setting up for a two spin-$\frac{1}{2}$ system, together with its classical Bell inequalities.

V. GENERAL SOLUTION OF THE THREE MARGINAL PROBLEM

We have proved here the impossibility of reproducing quantum probabilities of four CCS as marginals. Roy and Singh[7] have given examples to show that reproducing three CCS is possible. In this section, we construct the most general non-negative phase space density which reproduces three different (noncommuting) CCS as marginals. Our results encapsulate the extent to which noncommuting CCS can be simultaneously realized in quantum mechanics.

Among the four marginals R,S,T,U obeying the compatibility conditions (2.7) which are at our disposal, the particular choice of three of them is completely irrelevant. For definiteness, we choose R, T, and U, which we rename $\sigma_0(q_1,q_2)$, $\sigma_1(p_1,q_2)$, and $\sigma_2(p_1,p_2)$.

We assume that these marginals are probability densities in the full mathematical sense, that is they are true (integrable and non-negative) *functions*. This means that we restrict our marginal probability distributions to *absolutely continuous* measures (with respect to Lebesgue measure) in $\mathbb{R}^2$. Notice that such a restriction is automatic in the quantum case, due to Eqs. (2.8).

Likewise, we look for the general solution of the three marginal problem in the class of absolutely continuous measures in the phase space $\mathbb{R}^4$. This means that we want to describe all the solutions ρ of the equations

$$\begin{aligned}
\sigma_0(q_1,q_2) &= \int \mathrm{d}p_1\, \mathrm{d}p_2\, \rho(\vec{q},\vec{p})\,, \\
\sigma_1(p_1,q_2) &= \int \mathrm{d}q_1\, \mathrm{d}p_2\, \rho(\vec{q},\vec{p})\,, \\
\sigma_2(p_1,p_2) &= \int \mathrm{d}q_1\, \mathrm{d}q_2\, \rho(\vec{q},\vec{p})\,,
\end{aligned} \tag{5.1}$$

which belong to $L^1(\mathbb{R}^4, \mathrm{d}^2q\, \mathrm{d}^2p)$.

Notice that this is a restricted problem even in the quantum case, since nothing prevents a probability measure containing a singular part to project on marginals which are L^1 functions. To some extent, the above restrictions can be removed, allowing us to include, e.g., probability measures partly concentrated on submanifolds of the phase space. However, dealing with such extensions at some degree of generality requires painful manipulations, and we shall ignore them here. (Special cases are treated in Refs. 5 and 7). As for the full inclusion of singular measures, it appears as both delicate and of little practical interest.

Let us introduce the one variable marginals

$$\begin{aligned}
\sigma_{01}(q_2) &= \int \mathrm{d}q_1\, \sigma_0(q_1,q_2)\,, \\
\sigma_{12}(p_1) &= \int \mathrm{d}q_2\, \sigma_1(p_1,q_2)\,.
\end{aligned} \tag{5.2}$$

Owing to the compatibility conditions (2.7), these definitions are equivalent to

$$\sigma_{01}(q_2)=\int \mathrm{d}p_1\,\sigma_1(p_1,q_2)\,,$$
$$\sigma_{12}(p_1)=\int \mathrm{d}p_2\,\sigma_2(p_1,p_2)\,. \tag{5.3}$$

As the support properties of the functions σ_j (which are allowed to vanish on some parts of $\mathbb{R}^2$) are not innocent in the forthcoming construction, we need to pay attention to them. Let $\Sigma_j\subset\mathbb{R}^2$ $(j=0,1,2)$ be the essential support of σ_j. The above compatibility conditions, together with the positivity conditions $\sigma_j\geqslant 0$, clearly yield two constraints on the supports Σ_j, namely,

$$\{q_2\in\mathbb{R}\mid \exists\ q_1\in\mathbb{R}\ \text{such that}\ (q_1,q_2)\in\Sigma_0\}=\{q_2\in\mathbb{R}\mid \exists\ p_1\in\mathbb{R}\ \text{such that}\ (p_1,q_2)\in\Sigma_1\}\,,$$
$$\{p_1\in\mathbb{R}\mid \exists\ q_2\in\mathbb{R}\ \text{such that}\ (p_1,q_2)\in\Sigma_1\}=\{p_1\in\mathbb{R}\mid \exists\ p_2\in\mathbb{R}\ \text{such that}\ (p_1,p_2)\in\Sigma_2\}\,. \tag{5.4}$$

To the Σ_j's we associate the subsets E_j's of the phase space defined by

$$E_0=\{\vec{q},\vec{p}\mid (q_1,q_2)\in\Sigma_0,(p_1,p_2)\in\mathbb{R}^2\}\,,$$
$$E_1=\{\vec{q},\vec{p}\mid (p_1,q_2)\in\Sigma_1,(q_1,p_2)\in\mathbb{R}^2\}\,, \tag{5.5}$$
$$E_2=\{\vec{q},\vec{p}\mid (p_1,p_2)\in\Sigma_2,(q_1,q_2)\in\mathbb{R}^2\}\,.$$

Finally, we denote by E the intersection of the E_j's,

$$E=E_0\cap E_1\cap E_2\,. \tag{5.6}$$

Again, due to positivity, any solution ρ of Eqs. (5.1) must have its essential support contained in E.

The three marginal problem in the precise form stated above is then completely solved by the following.

Theorem 1: *(1) The Lebesgue measure of E is not zero and the function ρ_0 defined (a.e.) by*

$$\rho_0(\vec{q},\vec{p})=\begin{cases}\sigma_0(q_1,q_2)\dfrac{1}{\sigma_{01}(q_2)}\sigma_1(p_1,q_2)\dfrac{1}{\sigma_{12}(p_1)}\sigma_2(p_1,p_2) & \text{if } (\vec{q},\vec{p})\in E\,,\\ 0 \quad \text{otherwise,}\end{cases} \tag{5.7}$$

is a non-negative solution of the problem (5.1) in $L^1(\mathbb{R}^4,\mathrm{d}^2q\,\mathrm{d}^2p)$.

(2) The general solution ρ of (5.1) in $L^1(\mathbb{R}^4,\mathrm{d}^2q\,\mathrm{d}^2p)$ is given by

$$\rho(\vec{q},\vec{p})=\rho_0(\vec{q},\vec{p})+\lambda\,\Delta(\vec{q},\vec{p})\,, \tag{5.8}$$

where

$$\lambda\in\left[-\frac{1}{m_+},\frac{1}{m_-}\right] \tag{5.9}$$

and

$$\Delta(\vec{q},\vec{p})=F(\vec{q},\vec{p})-\rho_0(\vec{q},\vec{p})\Bigg[\frac{1}{\sigma_0(q_1,q_2)}\int \mathrm{d}p_1'\,\mathrm{d}p_2'\,F(q_1,q_2,p_1',p_2')$$
$$+\frac{1}{\sigma_1(p_1,q_2)}\int \mathrm{d}q_1'\,\mathrm{d}p_2'\,F(q_1',q_2,p_1,p_2')+\frac{1}{\sigma_2(p_1,p_2)}\int \mathrm{d}q_1'\,\mathrm{d}q_2'\,F(q_1',q_2',p_1,p_2)$$
$$-\frac{1}{\sigma_{01}(q_2)}\int \mathrm{d}q_1'\,\mathrm{d}p_1'\,\mathrm{d}p_2'\,F(q_1',q_2,p_1',p_2')$$
$$-\frac{1}{\sigma_{12}(p_1)}\int \mathrm{d}q_1'\,\mathrm{d}q_2'\,\mathrm{d}p_2'\,F(q_1',q_2',p_1,p_2')\Bigg], \tag{5.10}$$

F being an arbitrary $L^1(\mathbb{R}^4,\mathrm{d}^2q\,\mathrm{d}^2p)$ function with essential support contained in E. The (F-dependent) constants $m_\pm$ in (5.9) are defined as

$$m_+=\operatorname*{ess\,sup}_{(\vec{q},\vec{p})\in E}\frac{\Delta(\vec{q},\vec{p})}{\rho_0(\vec{q},\vec{p})},\quad m_-=-\operatorname*{ess\,inf}_{(\vec{q},\vec{p})\in E}\frac{\Delta(\vec{q},\vec{p})}{\rho_0(\vec{q},\vec{p})}, \tag{5.11}$$

and are both positive if $\Delta\neq 0$ ($m_+=\infty$ or/and $m_-=\infty$ are not excluded).

Proof: (1) To begin with, ρ_0 given by (5.7) is well defined and non-negative. Indeed, due to (5.2) [or (5.3)] and the positivity of the σ_j's, $\sigma_{01}(q_2)$, and $\sigma_{12}(p_1)$ are a.e. nonzero for $(\vec{q},\vec{p})\in E_0$ and E_1 (or E_1 and E_2), so that the denominators in Eq. (5.7) do not vanish on E (except maybe on sets of Lebesgue measure 0).

Next, in order to check that ρ_0 obeys the first equation (5.1), we consider the integral

$$\int \mathrm{d}p_1\int \mathrm{d}p_2\,\rho_0(\vec{q},\vec{p}) \tag{5.12}$$

with this specific order of the p integrations. According to the relations (5.4) and the definition of E, one observes first that the projection of E on the (p_1,p_2) plane is the set Σ_2, so that the integration over p_2 removes the factor σ_2/σ_{12} in ρ_0; and second, that the projections of Σ_1 and Σ_2 on p_1 coincide, so that the integration over p_1 removes the factor σ_1/σ_{01} in ρ_0, and one is left with the expected result $\sigma_0(q_1,q_2)$. We can now write

$$\int \mathrm{d}p_1\,\mathrm{d}p_2\,\rho_0(\vec{q},\vec{p})=\sigma_0(q_1,q_2), \tag{5.13}$$

where thanks to Fubini theorem, the integration order is completely irrelevant. The other two equations (5.1) are derived in a similar way.

This calculation shows at once that the Lebesgue measure of E is not zero and that $\rho_0\in L^1(\mathbb{R}^4,\mathrm{d}^2q\,\mathrm{d}^2p)$.

(2) That any non-negative solution ρ of Eqs. (5.1) admits the representation (5.8)–(5.10) is easy to establish. Indeed, since the essential support of ρ is necessarily contained in E, we are allowed to take $F=\rho$ in Eq. (5.10), which gives [using (5.1)]

$$\Delta(\vec{q},\vec{p})=\rho(\vec{q},\vec{p})-\rho_0(\vec{q},\vec{p})\,. \tag{5.14}$$

Then, from (5.11)

$$m_-=-\operatorname*{ess\,inf}_{(\vec{q},\vec{p})\in E}\left(\frac{\rho}{\rho_0}-1\right)\leqslant 1\,.$$

As $1/m_-\geqslant 1$ in (5.9), we can choose $\lambda=1$, which makes Eq. (5.14) equivalent to the representation (5.8).

It remains to show that any function ρ defined by (5.8)–(5.11) (and thus with essential support E) is a non-negative solution of Eqs. (5.1) in $L^1(\mathbb{R}^4, d^2q\, d^2p)$. In order to prove that ρ satisfies the first equation (5.1), we rearrange pairwise the right-hand side of (5.10) as follows:

$$\Delta = \left[F - \frac{\rho_0}{\sigma_0} \int dp_1' \, dp_2' \, F \right] - \left[\frac{\rho_0}{\sigma_1} \int dq_1' \, dp_2' \, F - \frac{\rho_0}{\sigma_{01}} \int dq_1' \, dp_1' \, dp_2' \, F \right]$$
$$- \left[\frac{\rho_0}{\sigma_2} \int dq_1' \, dq_2' \, F - \frac{\rho_0}{\sigma_{12}} \int dq_1' \, dq_2' \, dp_2' \, F \right]. \tag{5.15}$$

Then, integrating the right-hand side over p_1 and p_2, one finds, by an extensive use of Eqs. (5.2) to (5.4) as in part (1), that the two terms coming from each square bracket cancel each other, leading to

$$\int dp_1 \, dp_2 \, \Delta(\vec{q}, \vec{p}) = 0 \, .$$

This, with (5.8) and (5.13), implies that ρ satisfies the first equation (5.1). That it satisfies the other two equations (5.1) is proved in a similar way.

This calculation also shows that $\rho \in L^1(\mathbb{R}^4, d^2q\, d^2p)$.

Finally

$$\int_E d^2q \, d^2p \, \Delta(\vec{q}, \vec{p}) = 0 \, ,$$

which implies that $m_\pm$ in Eqs. (5.11) are both strictly positive if Δ does not vanish, a.e. on $\mathbb{R}^4$. The positivity of ρ is then a trivial consequence of Eqs. (5.8), (5.9), and (5.11).

The proof is complete.

Remark: Theorem 1, as it is stated above, deals with L^1 functions, and thus excludes the occurrence of Dirac measures. We insist on the fact that this is unnecessarily restrictive. Indeed Dirac measures can be easily accommodated and the theorem suitably rephrased, to the price however of cumbersome mathematical intricacies which we do not want to enter into.

An immediate corollary of Proposition 1 and Theorem 1 is the following.

Theorem 2 (Three marginal theorem): *Let R, S, T, and U be probability distributions for (q_1,q_2), (q_1,p_2), (p_1,q_2), and (p_1,p_2) obeying the consistency conditions (2.7). Given n arbitrary distributions among $\{R,S,T,U\}$, a necessary and sufficient condition for them to be marginals of a probability density in the four-dimensional phase space is $n \leqslant 3$.*

VI. CONCLUSIONS

We have solved the four marginal problem in four-dimensional phase space thus proving a long standing conjecture[7] and vastly improving the first results of Martin and Roy[1] which dealt with infinite number of marginals. To achieve this, we first derived ''phase space Bell inequalities'' which have their own interest. Actually they allow, at least in principle, direct ''experimental'' tests of the orthodox-versus-hidden variable interpretations of quantum mechanics within the position-momentum sector, analogous to those performed within the spin sector.

The technique of phase space Bell inequalities established here has applications to quantum information processing. Generalizing the example (4.11), one can show that for any separable density operator $\hat{\rho}$ one can construct a phase space density obeying the four marginal conditions. Hence, the Bell inequalities (3.2), with R, S, T, and U given by (2.8) must hold for every separable quantum state, irrespective of any physical interpretation of the associated phase space density. Their violation by a quantum state is a signature and even a quantitative measure of entanglement of this state.

We have also constructed the most general positive definite phase space density which has the maximum number of marginals (three) coinciding with corresponding quantum probabilities of three different (noncommuting) CCS. These results should be useful in the construction of maximally realistic quantum theories.

ACKNOWLEDGMENTS

We thank André Martin for collaboration in the initial stages of this work. One of the authors (S.M.R.) thanks A. Fine and A. Garg for some remarks on the three marginal problem many years ago. This work was supported by the Indo-French Centre for the Promotion of Advanced Research, Project No. 1501-02.

APPENDIX A: PROOF OF EQ. (4.23)

Since $S'=(0,\infty)$, one has

$$\hat{\chi}'(p)\tilde{g}(p)=\theta(p)\tilde{g}(p)\,.$$

Assuming first that g belongs to $\mathcal{S}$ (the Schwartz space of infinitely differentiable functions on $\mathbb{R}$ with fast decrease at infinity), one can write

$$(\hat{\chi}'g)(q)=\int_{-\infty}^{\infty}\mathrm{d}q'\,\tilde{\theta}(q-q')g(q')\,,$$

where $\tilde{\theta}$ is the Fourier transform of θ in the distribution-theoretic sense

$$\tilde{\theta}(q)\equiv\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}p\,e^{ipq}\,\theta(p)=\frac{i}{2\pi}\,\frac{P}{q}+\frac{1}{2}\,\delta(q)\,.$$

Then, if f also belongs to $\mathcal{S}$

$$\langle f|\hat{\chi}'|g\rangle=\frac{i}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}q\,f^*(q)\int_{-\infty}^{\infty}\mathrm{d}q'\frac{P}{q-q'}g(q')+\frac{1}{2}\langle f|g\rangle\,.$$

In particular, for even f and odd g, $\langle f|g\rangle$ vanishes, and

$$\langle f|\hat{\chi}'|g\rangle=-\frac{i}{\pi}\int_{0}^{\infty}\mathrm{d}q\,f^*(q)\int_{0}^{\infty}\mathrm{d}q'\left(\frac{1}{q+q'}-\frac{P}{q-q'}\right)g(q')\,,$$

which gives Eq. (4.23) if g coincides with f on $(0,\infty)$. The continuation from $\mathcal{S}$ to $L^2(-\infty,\infty)$ is performed as usual by continuity, using the fact that $\mathcal{S}$ is a dense subspace in $L^2(-\infty,\infty)$.

APPENDIX B: STUDY OF THE OPERATOR *K*

From the very definition of K through the integral kernel (4.25), one has

$$(Kh)(q)=\frac{1}{\pi}\int_{0}^{\infty}\mathrm{d}q'\frac{h(q')}{q+q'}\,.$$

Let us set

$$\overline{h}(u)=e^{u/2}h(e^u)\,.$$

Since $\int_{-\infty}^{\infty}\mathrm{d}u\,|\overline{h}(u)|^2=\int_{0}^{\infty}\mathrm{d}q\,|h(q)|^2$, the correspondence $h\mapsto\overline{h}$ defines a unitary mapping $L^2(0,\infty)\to L^2(-\infty,\infty)$ and

$$\overline{Kh}\,(u)=\int_{-\infty}^{\infty}\mathrm{d}v\;\overline{K}(u-v)\overline{h}(v)\,, \tag{B1}$$

where

$$\overline{K}(u)=\frac{1}{2\pi\cosh\dfrac{u}{2}}\,.$$

Then, another unitary mapping $L^2(-\infty,\infty)\to L^2(-\infty,\infty)$, namely the Fourier transform

$$\tilde{\overline{h}}(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}u\;e^{iku}\,\overline{h}(u)\,,$$

reduces the convolution product in (B1) to an ordinary product

$$\tilde{\overline{Kh}}(k)=\tilde{\overline{K}}(k)\,\tilde{\overline{h}}(k)\,,$$

where

$$\tilde{\overline{K}}(k)\equiv\int_{-\infty}^{\infty}\mathrm{d}u\;e^{iku}\,\overline{K}(u)=\frac{1}{\cosh\pi k}\,. \tag{B2}$$

Therefore, the operator K on $L^2(0,\infty)$ is unitarily equivalent to the multiplicative operator (B2) on $L^2(-\infty,\infty)$. The latter is evidently a positive operator with purely continuous spectrum $[0,\,1]$. Its generalized (non-normalizable) ''eigenfunctions'' are

$$\tilde{\overline{h}}_s(k)=\delta(k-s)\quad(s\in\mathbb{R})\,,$$

with ''eigenvalues'' $\lambda_s=1/\cosh\pi s$, and their preimage in $L^2(0,\infty)$ are

$$h_s(q)=\frac{1}{\sqrt{2\pi q}}\,e^{-is\ln q}\,.$$

Of particular interest for us is the extremal one, with ''eigenvalue'' $\lambda_0=1$,

$$h_0(q)=\frac{1}{\sqrt{2\pi q}}\,.$$

Of course, the corresponding maximal value $\gamma_0=1$ of $\gamma=\langle h|K|h\rangle$ cannot be attained, but only approached arbitrarily close through a family of normalizable functions mimicking $1/\sqrt{q}$. For instance, introducing two cutoffs, ε at small q and L at large q, and setting

$$h_{\varepsilon,L}(q)=\frac{1}{\sqrt{\ln\dfrac{L}{\varepsilon}}}\,\chi_{(\varepsilon,L)}(q)\,\frac{1}{\sqrt{q}}\quad(\|h_{\varepsilon,L}\|=1)\,,$$

one gets

$$\langle h_{\varepsilon,L}|K|h_{\varepsilon,L}\rangle=1-\frac{4}{\pi\ln\dfrac{L}{\varepsilon}}\int_{\sqrt{\varepsilon/L}}^{1}\mathrm{d}x\,\frac{\arctan x}{x}=1-O\left(\frac{1}{\ln\dfrac{L}{\varepsilon}}\right)\,,$$

so that

$$\lim_{\substack{\varepsilon\to 0\\ L\to\infty}} \langle h_{\varepsilon,L}|K|h_{\varepsilon,L}\rangle = 1\ .$$

Notice that one can keep ε fixed (e.g., $\varepsilon=1$) and let L alone go to ∞ without changing anything (this is in fact a consequence of the scale invariance of the operator K), or even choose a family of less singular functions h, like

$$h_L(q) = \frac{1}{\sqrt{\ln(L+1)}}\,\theta(L-q)\,\frac{1}{\sqrt{q+1}}\,.$$

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Higher order trace formulas of the Buslaev–Faddeev-type for the half-line Schrödinger operator with long-range potentials

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(Received 23 January 2003; accepted 4 April 2003)

We deal with trace formulas for half-line Schrödinger operators with long-range potentials. We generalize the Buslaev–Faddeev trace formulas to the case of square integrable potentials. The exact relation between the number of the trace formulas and the number of integrable derivatives of the potential is also given. The main results are optimal. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1579549]

I. INTRODUCTION

The present paper continues to study trace formulas for half-line Schrödinger operators with long-range potentials started previously by one of the authors in Ref. 20. The type of formulas we are concerned with was discovered 50 years ago by Gel'fand–Levitan in their remarkable note,[5] where it was shown that for the eigenvalues $\{\lambda_n\}$ of the regular Sturm–Liouville problem ($0 \leqslant x \leqslant \pi$),

$$\begin{cases} -u''+q(x)u=\lambda u, \\ u(0)=0=u(\pi), \end{cases}$$

the following holds:

$$\sum_{n\geqslant 1}\left\{\lambda_n - n^2 - \frac{1}{2\pi}\int_0^\pi q(x)dx\right\} = -\frac{q(0)+q(\pi)}{4} + \frac{1}{2\pi}\int_0^\pi q(x)dx. \tag{1.1}$$

Relation (1.1), commonly referred to as a trace formula, links a properly regularized trace of the Sturm–Liouville operator with some information on the potential q. Back in 1953 it was a completely new type of formula and its explicit nature originated an intensive search for similar relations eventually in all areas of mathematics dealing with operators. The literature with the key word *trace formula(s)* is enormous and we will not even make an attempt to review it here. We restrict ourselves to just mentioning some of the important stages of its development pertinent to our work.

The original Gel'fand–Levitan trace formula (1.1) belongs to the setting of operators with discrete spectrum (see also Dikii[3] and Podol'skii–Sadovnichii[16] for a recent account). In 1960 Buslaev–Faddeev[2] extended (1.1) to the case of a singular Sturm–Liouville problem,

$$\begin{cases} -u''+q(x)u=\lambda u, x\geqslant 0, \\ u(0)=0, \end{cases} \tag{1.2}$$

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with a short-range real potential q [i.e., integrable on $(0,\infty)$ with the first moment]. In this case, the Schrödinger operator H associated with (1.2) has an absolutely continuous spectrum filling $(0,\infty)$ and only a finite number of eigenvalues $\{\lambda_n\}$ which are all negative. The direct analog of (1.1) reads

$$-\sum_{n\geqslant 1}\lambda_n+\frac{2}{\pi}\int_0^\infty t\left(\theta(t)-\frac{1}{2t}\int_0^\infty q(x)dx\right)dt=-\frac{1}{4}q(0). \tag{1.3}$$

The function θ in (1.3), called the limiting phase, characterizes the absolutely continuous spectrum of H and has a scattering theoretical nature.

In 1971 Faddeev–Zakharov[4] discovered an amazing connection between trace formulas and the conservation laws for the Korteweg–de Vries equation (see also Ref. 8 for a more recent account). The natural Schrödinger operator in this setting is $H=-d^2/dx^2+q(x)$, defined on the whole line with a smooth, fast decaying potential q. The spectral situation here is similar to that of the half-line case and the first Faddeev–Zakharov trace formula reads

$$\sum_{n\geqslant 1}(-\lambda_n)^{1/2}+\frac{1}{2\pi}\int_0^\infty \ln|T(t)|dt=-\frac{1}{4}\int_{-\infty}^\infty q(x)dx, \tag{1.4}$$

where T is the transmission coefficient.

In 1993 Gesztesy–Holden–Simon–Zhao[6] put forward and consistently studied (see, e.g., Ref. 7) local versions of trace formulas which are valid eventually for any real potential. Their first trace relation is

$$E+\lim_{\varepsilon\to 0}\int_E^\infty e^{-\varepsilon t}\{1-2\xi(x,t)\}dt=q(x), \tag{1.5}$$

where E is the low bound of the spectrum of $H=-d^2/dx^2+q(x)$ and $\xi(x,t)$ is the so-called xi-function (see Ref. 7 for details). In the literature, formulas of type (1.5) are related to the trace approach to the inverse scattering problem (see, e.g., Ref. 21, and the literature cited therein).

There is also quite extensive literature on trace formulas in the three-space. We refer to the recent paper[13] by Korotyaev–Pushnitski and further literature cited there.

The list of trace formulas given above is not nearly complete. We mention only one recent development which can be regarded as a breakthrough. In Ref. 10, Killip–Simon introduced a new type of trace formula for Jacobi matrices that yields an exhaustive description of the spectrum of all Hilbert–Schmidt perturbations of the free discrete Schrödinger operator, which answered some open problems on orthogonal polynomials (see, also Ref. 22).

Note that the very term *trace formulas* is due to the fact that they are all related to computing regularized spectral traces of some operators. Moreover, each of (1.1), (1.3)–(1.5) actually represents the first formula in some infinite chain of higher order trace relations representing regularized moments of certain spectral characteristics. The full chain of trace formulas corresponding to (1.3) will be given below [formulas (4.6) and (4.7)].

The present paper deals with trace formulas for long-range potentials [i.e., nonintegrable on $(0,\infty)$]. In the context of the Coulomb potential, such formulas were studied in 1972 by Yafaev[23] and by Kvitsinsky in 1987.[14] For three-dimensional Schrödinger operators, a variant of trace formulas serving long-range potentials was put forward in 1991 by Melin[15] and recently by Bouclet.[1] Our goal is to derive a series of relations which are direct analogs to the Buslaev–Faddeev trace formulas [with the first formula (1.3)]. In 1999 one of the authors[20] proved that

$$-\sum_{n\geqslant 1}\lambda_n^2+2\int_0^\infty\left(\eta(t)+\frac{1}{4\pi\sqrt{t}}\int_0^\infty q^2(x)dx\right)dt=\frac{1}{4}q^2(0), \tag{1.6}$$

where η is the so-called modified spectral shift function that appears in the Koplienko trace formula[11] ($\mathrm{Im}\,\lambda \neq 0$),

$$\mathrm{tr}\{(H-\lambda)^{-1}-(H_0-\lambda)^{-1}-(H_0-\lambda)^{-1}V(H_0-\lambda)^{-1}\} = -\int_{-\infty}^{\infty}\left\{\frac{d^2}{dt^2}(t-\lambda)^{-1}\right\}\eta(t)\,dt, \tag{1.7}$$

where H_0, $H=H_0+V$ are self-adjoint operators such that $V|H_0-i|^{-1/2}$ is Hilbert–Schmidt. In the current paper we use a simpler approach which does not rely on (1.7). We obtain our trace formulas directly from Buslaev–Faddeev's ones using a certain limiting procedure. This way, we also improve on Ref. 20 by imposing in (1.6) weaker conditions on q.

Notation: We will adhere standard notation: $\mathbb{N}=\{1,2,3,\ldots\}$, $\mathbb{R}_+=(0,\infty)$, $\mathbb{C}_+=\{z\in\mathbb{C}:\mathrm{Im}\,z>0\}$, and $\overline{\mathbb{C}_+}=\mathbb{C}_+\cup\mathbb{R}$. All functions are assumed to be measurable and we will use the following Lebesgue classes:

$$L_p := \left\{ f : \|f\|_p^p \equiv \int_{\mathbb{R}_+} |f(x)|^p dx < \infty \right\}, \quad 1 \leqslant p < \infty,$$

$$L_\infty := \left\{ f : \|f\|_\infty \equiv ess \sup_{x\in\mathbb{R}_+} |f(x)| < \infty \right\},$$

and Sobolev classes,

$$W_1^n := \left\{ f : \sum_{m=0}^{n} \int_{\mathbb{R}_+} |f^{(m)}(x)|\,dx < \infty \right\}, \quad f^{(m)}(x) := (d^m/dx^m) f(x).$$

Furthermore, for a linear operator A we denote $\sigma(A)$ the spectrum of A, $\{\lambda_n(A)\}$ are its eigenvalues. By $\mathfrak{S}_p$, $p \geqslant 1$, as usual, we denote the ideal of compact operators A, for which

$$\|A\|_p^p := \sum_n \lambda_n^p(|A|) < \infty, \quad |A| := \sqrt{A^*A}.$$

The most important particular cases: $\mathfrak{S}_1$ is the space of trace class operators, and $\mathfrak{S}_2$ is the Hilbert–Schmidt class.

II. SOME KEY ASYMPTOTICS

In this section we obtain a suitable representation of the solution to the Schrödinger equation satisfying the WKB-type asymptotics at infinity. Such representations are well-known but we need a relation between the number of exact terms and the smoothness of the potential q. The proposition below is a long-range generalization of an analogous statement for L_1-potentials.[19]

Proposition 1: If $q \in L_2, q' \in W_1^{N-1}(\mathbb{R}_+)$ with some $N \in \mathbb{N}$, then the problem

$$\begin{cases} -u'' + q(x)u = k^2 u, \\ \lim\limits_{x\to\infty} u(x,k)\exp\left(-ikx - \dfrac{1}{2ik}\displaystyle\int_0^x q(s)\,ds \right) = 1 \end{cases} \tag{2.1}$$

has a unique bounded solution $u(x,k)$ for all $k \in \mathbb{R}, k \neq 0$. Moreover, for $M(k) := u(0,k)$ the representation

$$M(k)= 1+\sum_{j=2}^{N+1}\frac{m_j}{(-2ik)^j}+\frac{1}{(-2ik)^{N+1}} \times\int_0^\infty \exp\left(2ikx+\frac{1}{ik}\int_0^x q(s)ds\right)q^{(N)}(x)dx+O\left(\frac{1}{k^{N+2}}\right),\quad k\to\infty, \tag{2.2}$$

holds with some coefficients $\{m_j\}$ *depending only on* q.

Proof: It is enough to consider only the case $k\in\mathbb{R}_+$. Set

$$\Theta(x,k):=\exp\left(ikx+\frac{1}{2ik}\int_0^x q(s)ds\right)$$

and observe that $\Theta(x,k)$ satisfies the equation

$$-\Theta''+\{q(x)-q_1(x,k)-k^2\}\Theta=0, \tag{2.3}$$

where

$$q_1(x,k)=\frac{q'(x)}{-2ik}+\frac{q^2(x)}{4k^2}. \tag{2.4}$$

Rewrite (2.1) in the form

$$-u''+\{q(x)-q_1(x,k)-k^2\}u=-q_1(x,k)u \tag{2.5}$$

and note that (2.3) is the homogeneous equation for (2.5). Taking $\Theta(x,k)$ and $\Theta(x,k)\int_0^x\Theta^{-2}(s,k)ds$ as fundamental solutions to (2.3), by variation of parameters, Eq. (2.1) can be represented as

$$u(x,k)=\Theta(x,k)\left\{1+\int_x^\infty q_1(s,k)\Theta(s,k)\left(\int_x^s\Theta^{-2}(t,k)dt\right)u(s,k)ds\right\}. \tag{2.6}$$

Setting $y=\Theta^{-1}u$ and introducing the kernel

$$K(x,s,k)=q_1(s,k)\cdot\Theta^2(s,k)\int_x^s\Theta^{-2}(t,k)dt, \tag{2.7}$$

Eq. (2.6) reads

$$y(x,k)=1+\int_x^\infty K(x,s,k)y(s,k)ds=1+(\mathbb{K}y)(x,k), \tag{2.8}$$

where $\mathbb{K}$ stands for the Volterra integral operator with the kernel $K(x,s)$ (2.7). We show that $\mathbb{K}$ maps L_∞ to L_∞ and then (2.8) can be solved by iteration. Let us estimate

$$\int_x^s\Theta^{-2}(t,k)dt=\int_x^s e^{-2ikt}\cdot\exp\left(-\frac{1}{ik}\int_0^t q(z)dz\right)dt. \tag{2.9}$$

Integrating by parts twice in (2.9) yields

$$\int_x^s\Theta^{-2}(t,k)dt=\left\{\frac{\Theta^{-2}(t,k)}{-2ik}+\frac{q(t)\Theta^{-2}(t,k)}{-4ik^3}\right\}\Bigg|_{t=x}^{t=s}+\frac{1}{4ik^3}\int_x^s\Theta^{-2}(t,k)\left(q'(t)-\frac{q^2(t)}{ik}\right)dt. \tag{2.10}$$

Since $q' \in L_1$ implies $q \in L_\infty$, it follows from (2.10) that

$$\left| \int_x^s \Theta^{-2}(t,k)dt \right| \leqslant \frac{1}{k} + \frac{2\|q\|_\infty + \|q'\|_1}{4k^3} + \frac{\|q\|_2}{4k^4}. \tag{2.11}$$

Due to (2.11) and our conditions on q,

$$\begin{aligned} \int_x^\infty |K(x,s,k)|ds &\leqslant \int_x^\infty |q_1(s,k)| \left| \int_x^s \Theta^{-2}(t,k)dt \right| ds \\ &\leqslant \frac{1}{k^2}\left(1 + \frac{2\|q\|_\infty + \|q'\|_1}{4k^2} + \frac{\|q\|_2}{4k^3}\right)\left(\frac{1}{2}\int_x^\infty |q'(s)|ds + \frac{1}{4k}\int_x^\infty |q(s)|^2 ds\right) \end{aligned} \tag{2.12}$$

and we have

$$\|\mathbb{K}\| = \sup_{\|f\|_\infty = 1} \|\mathbb{K}f\|_\infty \leqslant \left\| \int_x^\infty |K(x,s,k)|ds \right\|_\infty \leqslant \frac{1}{k^2}\left(\frac{\|q'\|_1}{2} + \frac{\|q\|_2}{4k}\right)\left(1 + \frac{2\|q\|_\infty + \|q'\|_1}{4k^2} + \frac{\|q\|_2}{4k^3}\right). \tag{2.13}$$

Estimating (2.13) implies that for some positive constant r_q dependent only on q,

$$\|\mathbb{K}\| \leqslant 1/2 \quad \text{for} \quad k \geqslant r_q, \tag{2.14}$$

Eq. (2.8) can then be solved by iteration,

$$y(x,k) = 1 + \sum_{n=1}^{\infty} \Omega_j(x,k), \quad k \geqslant r_q, \tag{2.15}$$

where $\Omega_j(x,k) = (\mathbb{K}^j 1)(x,k)$, and

$$\|y\|_\infty \leqslant 2 \quad \text{for} \quad k \geqslant r_q. \tag{2.16}$$

This proves the existence.

Now we establish (2.2). To this end, introduce the differential operation

$$D := \frac{d}{dx} + \frac{q(x)}{ik}.$$

It is clear that if $q \in L_2$, $q' \in W_1^{m-1}(\mathbb{R}_+)$ and $f \in W_1^m(\mathbb{R}_+)$, for some $m \geqslant 1$, then

$$D^j f \in L_1, \ \forall \ 1 \leqslant j \leqslant m. \tag{2.17}$$

Denote

$$G(x,s,k) = \Theta^2(s,k)\int_x^s \Theta^{-2}(t,k)dt.$$

Integrating by part, one can easily verify that

$$\int_x^\infty G(x,s,k)f(s)ds = -\frac{1}{2ik}\int_x^\infty f(s)ds - \frac{1}{2ik}\int_x^\infty G(x,s,k)Df(s)ds. \tag{2.18}$$

Equation (2.18) is an integration by parts type formula. Since $q_1 \in W_1^{N-1}$, by (2.17), all $Dq_1, D^2q_1, \ldots, D^{N-1}q_1$ are from L_1, (2.18) can be applied $N-1$ times and the remaining integral will still be absolutely convergent. Setting in (2.15) $x=0$ we have

$$M(k) = 1 + \sum_{j=1}^{\infty} \Omega_j(k), \tag{2.19}$$

where $\Omega_j(k) = \Omega_j(0,k) = (\mathbb{K}^j 1)(0,k)$. Let us now evaluate each term in (2.19). Consider Ω_1 first. Apply (2.18) $N-1$ times to

$$\begin{aligned}
\Omega_1(x,k) &= \int_x^{\infty} G(x,s,k) q_1(s,k) ds \\
&= -\sum_{j=1}^{N-1} \frac{1}{(-2ik)^j} \int_x^{\infty} D^j q_1(s,k) ds + \frac{1}{(-2ik)^{N-1}} \int_x^{\infty} G(x,s,k) D^{N-1} q_1(s,k) ds \\
&= \sum_{j=2}^{N} \frac{\omega_j^{(1)}(x)}{(-2ik)^j} + \frac{1}{(-2ik)^{N-1}} \int_x^{\infty} G(x,s,k) D^{N-1} q_1(s,k) ds + O\left(\frac{1}{k^{N+2}}\right),
\end{aligned} \tag{2.20}$$

where $\omega_j^{(1)}(x)$ are some continuous functions whose expressions are inessential. By (2.10) one has that

$$G(x,s,k) = \frac{1 - \Theta^2(s,k)\Theta^{-2}(x,k)}{-2ik} + O\left(\frac{1}{k^2}\right)$$

and (2.20) reads

$$\begin{aligned}
\Omega_1(x,k) &= \sum_{j=2}^{N+1} \frac{\omega_j^{(1)}(x)}{(-2ik)^j} + \frac{\Theta^{-2}(x,k)}{(-2ik)^{N+1}} \int_x^{\infty} q^{(N)}(s) ds + \frac{\Theta^{-2}(x,k)}{(-2ik)^{N+1}} \int_x^{\infty} \Theta^2(s,k) q^{(N)}(s) ds \\
&\quad + O\left(\frac{1}{k^{N+2}}\right) \\
&= \sum_{j=2}^{N+1} \frac{\omega_j^{(1)}(x)}{(-2ik)^j} - \frac{q^{(N-1)}(x)\Theta^{-2}(x,k)}{(-2ik)^{N+1}} + \frac{\Theta^{-2}(x,k)}{(-2ik)^{N+1}} \int_x^{\infty} \Theta^2(s,k) q^{(N)}(s) ds + O\left(\frac{1}{k^{N+2}}\right).
\end{aligned} \tag{2.21}$$

Setting in (2.21) $x=0$ we finally have

$$\Omega_1(k) = \sum_{j=2}^{N+1} \frac{\omega_j^{(1)}}{(-2ik)^j} + \frac{1}{(-2ik)^{N+1}} \int_0^{\infty} \Theta^2(s,k) q^{(N)}(s) ds + O\left(\frac{1}{k^{N+2}}\right). \tag{2.22}$$

Similarly,

$$\Omega_2(k) = \sum_{j=4}^{N+1} \frac{\omega_j^{(2)}}{(-2ik)^j} + O\left(\frac{1}{k^{N+2}}\right), \quad k \to \infty. \tag{2.23}$$

For the general $1 \leqslant n \leqslant [(N+1)/2]$, where $[x]$ is the greatest integer $n \leqslant x$, we get

$$\Omega_n(k) = \sum_{j=2n}^{N+1} \frac{\omega_j^{(n)}}{(-2ik)^j} + O\left(\frac{1}{k^{N+2}}\right), \quad k \to \infty \tag{2.24}$$

and

$$\Omega_{[(N+1/2)]+1}(k)=O\left(\frac{1}{k^{N+2}}\right),\quad k\to\infty.$$

Since in Ω_j, $j>1$, all terms containing $\int_x^\infty \Theta^2(s,k)q^{(N)}(s)ds$ are included in the error term $o(1/k^{N+1})$, we can get the $N+2$ term if and only if $\int_0^\infty \Theta^2(x,k)q^{(N)}(x)dx=O(1/k)$, $k\to\infty$. From (2.13) and (2.14) is easy to see that

$$\left|\sum_{n\geqslant[(N+1)/2]+1}\Omega_n(k)\right|\leqslant\sum_{n\geqslant[(N+1)/2]+1}\|\mathbb{K}\|^n\leqslant 2\|\mathbb{K}\|^{[(N+1)/2]+1}\leqslant\frac{C_q}{k^{N+2}},$$

where C_q is a constant dependant only on q. Thus,

$$\sum_{n\geqslant[(N+1)/2]+1}\Omega_n(k)=O\left(\frac{1}{k^{N+2}}\right),\quad k\to\infty, \tag{2.25}$$

and combining (2.22)–(2.25) we arrive at

$$\begin{aligned}M(k)&=1+\sum_{n\geqslant 1}\Omega_n(k)\\&=1+\sum_{j=2}^{N+1}\frac{m_j}{(-2ik)^j}+\frac{1}{(-2ik)^{N+1}}\int_0^\infty\Theta^2(s,k)q^{(N)}(s)ds+O\left(\frac{1}{k^{N+2}}\right),\ k\to\infty,\end{aligned}$$

that completes the proof. □

Remark 1: Since, by condition, $q^{(N)}\in L_1$ we conclude that

$$\int_0^\infty\exp\left(2ikx+\frac{1}{ik}\int_0^x q(s)ds\right)q^{(N)}(x)dx=o(1),\quad k\to\infty$$

(*the proof is parallel to that of the Riemann–Lebesgue lemma) and hence the integral term in (2.2) is $o(k^{-N-1})$. The fact that we were able to extract an explicit "intermediate" term between the exact terms $\Sigma_{j=2}^{N+1}(-2ik)^{-j}m_j$ and $O(k^{-N-2})$ will be important in Sec. IV. Proposition 1 actually relates the number of exact terms in (2.2) with the smoothness of q but does not provide a recipe to evaluate coefficients $\{m_j\}$. Explicit formulas for $\{m_j\}$ can be derived, e.g., from Ref. 2.*

III. THE MODIFIED JOST FUNCTION

Introduce the half-line Schrödinger operator $H=-d^2/dx^2+q(x)$ with a Dirichlet boundary condition $u(0)=0$. It is well-known that if $q\in L_1$ then for any $k>0$ the equation $-u''+q(x)u=k^2u$ has the so-called Jost solution $u_0(x,k)$, i.e., a solution subject to the condition that $\lim_{x\to\infty}e^{-ikx}u_0(x,k)=1$. The function $M_0(k):=u_0(0,k)$ is commonly referred to as the Jost function. It is continuous on $\mathbb{R}\setminus\{0\}$ and analytic in $\mathbb{C}_+$ except for isolated poles at $i\sqrt{-\lambda_n}$, where $\{\lambda_n\}$ are (necessarily negative) eigenvalues of H accumulating only at 0. The function $M(k)$, defined in Proposition 1, can then be called *the modified Jost function*. Note that if $q\in L_1$; then

$$M(k)=M_0(k)\exp\left\{\frac{1}{2ik}\int_0^\infty q(x)dx\right\}. \tag{3.1}$$

Given potential q, let $\tilde{q}$ be its smooth cut-off approximation defined by

$$\tilde{q}(x,a)=q(x)\chi_a(x), \tag{3.2}$$

where χ_a is smooth such that $\chi_a(x)=1,0\leqslant x\leqslant a$, and $\chi_a(x)=0,x>a+1$.

It is clear that

$$\tilde{q}(x,a)\to q(x),\quad a\to\infty,$$

which we agree to write just as $\tilde{q}\to q$. In the sequel, we will drop a in $\tilde{q}(x,a)$ and put ~ on top of every object related to $\tilde{q}$.

The following lemma will be a key ingredient in our consideration:

Lemma 1: Let q be real and $q\in L_2$, $q'\in L_1$ and $\tilde{q}$ be defined by (3.2), then

(i) for every $k\in\overline{\mathbb{C}}_+$, $|k|>r_q$, with some $r_q>0$ dependent only on q,

$$\tilde{M}(k)\to M(k),\quad \tilde{q}\to q;$$

(ii) for any $p\geqslant 3/2$;

$$\sum_n |\tilde{\lambda}_n|^p\to\sum_n |\lambda_n|^p,\quad \tilde{q}\to q.$$

Proof: (i) Assume for the time being that $k>0$. In the notation of Proposition 1, by representation (2.15) we have: for any natural number N,

$$\begin{aligned}|M(k)-\tilde{M}(k)|&=|u(0,k)-\tilde{u}(0,k)|\\&=|y(0,k)-\tilde{y}(0,k)|\\&\leqslant\sum_{n=1}^{N}|(\mathbb{K}^n1)(0,k)-(\tilde{\mathbb{K}}^n1)(0,k)|+|(\mathbb{K}^{N+1}y)(0,k)-(\tilde{\mathbb{K}}^{N+1}\tilde{y})(0,k)|\\&\leqslant\sum_{j=1}^{N}\|\mathbb{K}^n-\tilde{\mathbb{K}}^n\|+\|\mathbb{K}^{N+1}-\tilde{\mathbb{K}}^{N+1}\|\|y\|+\|\mathbb{K}^{N+1}(y-\tilde{y})\|.\end{aligned}\tag{3.3}$$

Observing that for any $n\in\mathbb{N}$;

$$\mathbb{K}^n-\tilde{\mathbb{K}}^n=\sum_{m=0}^{n-1}\tilde{\mathbb{K}}^m(\mathbb{K}-\tilde{\mathbb{K}})\mathbb{K}^{n-m-1},$$

and by (2.16), estimate (3.3) for $k\geqslant r_q$ can be continued,

$$\begin{aligned}|M(k)-\tilde{M}(k)|\leqslant\sum_{n=1}^{N}\sum_{m=0}^{n-1}\|\tilde{\mathbb{K}}\|^m\|\mathbb{K}-\tilde{\mathbb{K}}\|\|\mathbb{K}\|^{n-m-1}+\|y\|\sum_{n=0}^{N}\|\tilde{\mathbb{K}}\|^n\|\mathbb{K}-\tilde{\mathbb{K}}\|\|\mathbb{K}\|^{N-n}\\+\|\mathbb{K}\|^{N+1}(\|y\|+\|\tilde{y}\|).\end{aligned}\tag{3.4}$$

But for $k>\max\{r_q,r_{\tilde{q}}\}=r_q$, by (2.14) and (2.16), $\|\tilde{\mathbb{K}}\|,\|\mathbb{K}\|\leqslant 1/2$ and $\|y\|,\|\tilde{y}\|\leqslant 2$ and (3.4) finally yields

$$\begin{aligned}|M(k)-\tilde{M}(k)|&\leqslant\sum_{n=1}^{N-1}n2^{-n}\cdot\|\mathbb{K}-\tilde{\mathbb{K}}\|+N2^{-N+1}\cdot\|\mathbb{K}-\tilde{\mathbb{K}}\|+2^{-N+1}\\&\leqslant 2(1+N2^{-N+1})\|\mathbb{K}-\tilde{\mathbb{K}}\|+2^{-N+1}.\end{aligned}\tag{3.5}$$

Letting in (3.5) $N\to\infty$, we have

$$|M(k)-\tilde{M}(k)|\leqslant 2\|\mathbb{K}-\tilde{\mathbb{K}}\|.\tag{3.6}$$

Show now that $\|\mathbb{K}-\tilde{\mathbb{K}}\|\to 0$ as $a\to\infty$. It follows from (2.4) and (2.7) that

$$\tilde{K}(x,s,k)=K(x,s,k)\quad\text{for}\quad x\leqslant s\leqslant a$$

and hence by (2.12) one obtains

$$\|\mathbb{K}-\widetilde{\mathbb{K}}\|\leqslant\sup_{x\geqslant a}\int_x^\infty|K(x,s,k)-\widetilde{K}(x,s,k)|ds\leqslant\sup_{x\geqslant a}\int_x^\infty\{|K(x,s,k)|+|\widetilde{K}(x,s,k)|\}ds\to 0,\ a\to\infty. \tag{3.7}$$

Combining (3.6) and (3.7) we prove (i) with real k and then using Phragmén–Lindelöf-type arguments we arrive at (i).

(ii) Let $H_0=-d^2/dx^2$ with $u(0)=0$. For the Green's function $G(x,s,\lambda)$ of H_0 one has

$$G(x,y,\lambda)=\frac{1}{i\sqrt{\lambda}}(e^{i\sqrt{\lambda}(x+y)}-e^{i\sqrt{\lambda}|x-y|}),$$

and hence for $\operatorname{Im}\lambda\neq 0$;

$$\|(q-\tilde{q})(H_0-\lambda I)^{-1}\|_2^2=\frac{1}{|\lambda|}\int_0^\infty\int_0^\infty|q(x)-\tilde{q}(x)|^2|e^{i\sqrt{\lambda}(x+y)}-e^{i\sqrt{\lambda}|x-y|}|^2dxdy$$

$$\leqslant\frac{5}{|\lambda|\operatorname{Im}\sqrt{\lambda}}\|q-\tilde{q}\|_2^2\to 0,\ \tilde{q}\to q. \tag{3.8}$$

Due to

$$(H_0-\lambda)^{-1}=(\widetilde{H}-\lambda)^{-1}(I+\tilde{q}(H_0-\lambda)^{-1}),$$

we have

$$\begin{aligned}\|(H-\lambda)^{-1}-(\widetilde{H}-\lambda)^{-1}\|_2&=\|(H-\lambda)^{-1}(\widetilde{H}-H)(\widetilde{H}-\lambda)^{-1}\|_2\\&\leqslant\|(H-\lambda)^{-1}\|\cdot\|(q-\tilde{q})(\widetilde{H}-\lambda)^{-1}\|_2\\&=\|(H-\lambda)^{-1}\|\cdot\|(q-\tilde{q})(H_0-\lambda)^{-1}(I+\tilde{q}(H_0-\lambda)^{-1})^{-1}\|_2\\&\leqslant\|(H-\lambda)^{-1}\|\|(I+\tilde{q}(H_0-\lambda)^{-1})^{-1}\|\cdot\|(q-\tilde{q})(H_0-\lambda)^{-1}\|_2.\end{aligned} \tag{3.9}$$

Since for $\operatorname{Im}\lambda\neq 0$ the first two norms on the right-hand side of (3.9) are finite and, by (3.8), the third one goes to zero and we conclude that

$$\|(H-\lambda)^{-1}-(\widetilde{H}-\lambda)^{-1}\|\leqslant\|(H-\lambda)^{-1}-(\widetilde{H}-\lambda)^{-1}\|_2\to 0,\ \tilde{q}\to q. \tag{3.10}$$

One can now employ some arguments from Ref. 8. Let $\Delta=[a,b]\subset(-\infty,0)$: $a<\inf\{\sigma(H),\sigma(\widetilde{H})\}$, $-1<b\neq\sigma(H),\sigma(\widetilde{H})$, and E_Δ be the spectral projection corresponding to Δ. It follows from (3.10) that[17] in the weak sense,

$$\widetilde{E}_\Delta\to E_\Delta,$$

which implies that

$$\sum_{\tilde{\lambda}_n\in\Delta}|\tilde{\lambda}_n|^p\to\sum_{\lambda_n\in\Delta}|\lambda_n|^p,\ p>0. \tag{3.11}$$

Consider ($p\geqslant 3/2$),

$$\left|\sum_n (|\tilde{\lambda}_n|^p - |\lambda_n|^p)\right| \leqslant \left|\sum_{\tilde{\lambda}_n, \lambda_n < b} (|\tilde{\lambda}_n|^p - |\lambda_n|^p)\right| + \sum_{\tilde{\lambda}_n > b} |\tilde{\lambda}_n|^p + \sum_{\lambda_n > b} |\lambda_n|^p. \tag{3.12}$$

Denote by $q_- = \frac{1}{2}(q - |q|)$ the negative part of q. Since $q_-(x) \leqslant \tilde{q}(x)$ we have $H_- = -d^2/dx^2 + q_-(x) \subseteq \tilde{H}$. Hence, by the standard fact of perturbation theory, $\lambda_n(H_-) \leqslant \tilde{\lambda}_n$ and (all eigenvalues are negative)

$$\sum_n |\tilde{\lambda}_n|^p \leqslant \sum_n |\lambda_n(H_-)|^p. \tag{3.13}$$

From the Lieb–Thirring bounds (see, e.g., Ref. 9),

$$\sum_n |\lambda_n(H_-)|^{3/2}, \ \sum_n |\lambda_n(H)|^{3/2} \leqslant \tfrac{3}{16}\|q_-\|_2^2 \leqslant \tfrac{3}{16}\|q\|_2^2, \tag{3.14}$$

and hence for $p \geqslant 3/2$ by (3.13) and taking into account that $|b| < 1$, we get

$$\sum_{\tilde{\lambda}_n > b} |\tilde{\lambda}_n|^p \leqslant \sum_{\tilde{\lambda}_n > b} |\tilde{\lambda}_n|^{3/2} \leqslant \sum_n |\tilde{\lambda}_n|^{3/2} \leqslant \sum_n |\lambda_n(H_-)|^{3/2} \leqslant \tfrac{3}{16}\|q\|_2^2 < \infty. \tag{3.15}$$

Due to (3.11), (3.14), and (3.15), by the standard $\varepsilon/3$ argument (3.12) yields (ii) and the lemma is proved. □

Remark 2: Since $M(k)$ is analytic in $\mathbb{C}_+$, (i) of Lemma 1 actually holds in $\overline{\mathbb{C}}_+ \backslash \{0\}$.

Remark 3: Lemma 1 improves on one result by Koplienko.[11] *Namely, if (H, H_0): $H_0 = -d^2/dx^2$ with $u(0) = 0$ and $H = H_0 + q$ with $q \in L_2, q' \in L_1$, then the modified spectral shift function $\eta(t)$ for (H, H_0) appearing in (1.7) is differentiable and*

$$\eta'(t) = \pi^{-1} \operatorname{Im} \ln M(\sqrt{t}), \ \ t > 0. \tag{3.16}$$

In Ref. 11, relation (3.16) was proven under stronger conditions involving q''.

IV. TRACE FORMULAS

This section contains the main results of the paper, the Buslaev–Faddeev trace formulas for certain long-range potentials. Relation (3.1), Proposition 1, Lemma 1, and some limiting arguments will let us not only adjust the original Buslaev–Faddeev trace formulas[2] to the long-range setting but also provide sharp conditions on potentials.

Set in (3.1) $M_0 = A_0 e^{i\theta_0}$, where $A_0 = |M_0|$ is the scattering amplitude and θ_0 is the scattering phase. Similarly, $M = Ae^{i\theta}$, where $A = |M|$ can be called *the modified scattering amplitude* and θ_0 *the modified scattering phase*. Relation (3.1) then implies that for $q \in L_1$ and $k > 0$,

$$\theta(k) = \theta_0(k) - \frac{1}{2k}\int_0^\infty q(t)\,dt, \ \ A(k) = A_0(k). \tag{4.1}$$

Following Ref. 2, introduce the sequence $\{Q_n\}_{n \geqslant 1}$:

$$Q_n = \lim_{x \to \infty}\left(V_{n-1}(x) + \sum_{j=1}^{n-2} \frac{j}{n} V_{n-j-1}(x) Q_j \right), \tag{4.2}$$

where

$$V_n(x) = q^{(n-1)}(0) + \sum_{m=1}^{n-1} \binom{l-1}{m} \int_0^x V_m(s) q^{(n-m-1)}(s)\,ds, V_0(x) = 0. \tag{4.3}$$

The following statement is our main result.

Theorem 1: *Suppose that for $q \in L_2(0,\infty)$ and $q' \in W_1^{N-1}(0,\infty), N \in \mathbb{N}$. Then for the modified scattering phase $\theta(k)$ and modified scattering amplitude $A(k)$ the following trace formulas are valid:*

$$(-1)^n \sum_{l=1}^{\infty} (-\lambda_l)^n + \frac{2n}{\pi} \int_0^{\infty} k^{2n-1} \left\{ \theta(k) - \sum_{l=1}^{n-1} \frac{(-1)^{l+1}}{(2k)^{2l+1}} Q_{2l+1} \right\} dk = (-1)^n \frac{n}{2^{2n}} Q_{2n},$$

$$2 \leqslant n \leqslant \frac{N}{2}; \tag{4.4}$$

$$(-1)^n \sum_{l=1}^{\infty} (-\lambda_l)^{n+1/2} - \frac{2n+1}{\pi} \int_0^{\infty} k^{2n} \left\{ \ln A(k) - \sum_{l=1}^{n} \frac{(-1)^{l+1}}{(2k)^{2l}} Q_{2l} \right\} dk$$
$$= (-1)^n \frac{2n+1}{2^{2n+1}} Q_{2n+1}, \quad 1 \leqslant n \leqslant \frac{N-1}{2}; \tag{4.5}$$

where coefficients $\{Q_n\}$ are computed by (4.2) and all integrals are absolutely convergent. In order to extract one additional formula in (4.4)–(4.5) with the absolutely convergent integral it is necessary and sufficient that

$$\frac{1}{k} \int_0^{\infty} \sin\left(2kx - \frac{1}{k} \int_0^x q(s)\,ds \right) q^{(N)}(x)\,dx \in L_1(r,\infty),$$

for some $r > 0$.

Proof: Introduce $\tilde{q}(x)$ by (3.2). Since $\tilde{q} \in L_1((1+x)dx, \mathbb{R}_+)$, then Faddeev–Buslaev trace formulas[2] for $\tilde{\theta}_0(k)$ and $\tilde{A}_0(k)$ apply

$$(-1)^n \sum_{l=1}^{\infty} (-\tilde{\lambda}_l)^n + \frac{2n}{\pi} \int_0^{\infty} k^{2n-1} \left[\tilde{\theta}_0(k) - \sum_{l=0}^{n-1} \frac{(-1)^{l+1}}{(2k)^{2l+1}} \tilde{Q}_{2l+1} \right] dk = (-1)^n \frac{n}{2^{2n}} \tilde{Q}_{2n},$$

$$1 \leqslant n \leqslant \frac{N}{2}; \tag{4.6}$$

$$(-1)^n \sum_{l=1}^{\infty} (-\tilde{\lambda}_l)^{n+1/2} - \frac{2n+1}{\pi} \int_0^{\infty} k^{2n} \left[\ln \tilde{A}_0(k) - \sum_{l=1}^{n} \frac{(-1)^{l+1}}{(2k)^{2l}} \tilde{Q}_{2l} \right] dk$$
$$= (-1)^n \frac{2n+1}{2^{2n+1}} \tilde{Q}_{2n+1}, \quad 1 \leqslant n \leqslant \frac{N-1}{2}. \tag{4.7}$$

In view of (4.1), relations (4.6) and (4.7) transform into

$$(-1)^n \sum_{l=1}^{\infty} (-\tilde{\lambda}_l)^n + \frac{2n}{\pi} \int_0^{\infty} k^{2n-1} \left[\tilde{\theta}(k) - \sum_{l=1}^{n-1} \frac{(-1)^{l+1}}{(2k)^{2l+1}} \tilde{Q}_{2l+1} \right] dk = (-1)^n \frac{n}{2^{2n}} \tilde{Q}_{2n},$$

$$2 \leqslant n \leqslant \frac{N}{2}; \tag{4.8}$$

$$(-1)^n\sum_{l=1}^{\infty}(-\tilde{\lambda}_l)^{n+1/2}-\frac{2n+1}{\pi}\int_0^{\infty}k^{2n}\left[\ln\tilde{A}(k)-\sum_{l=1}^{n}\frac{(-1)^{l+1}}{(2k)^{2l}}\tilde{Q}_{2l}\right]dk$$

$$=(-1)^n\frac{2n+1}{2^{2n+1}}\tilde{Q}_{2n+1},\qquad 1\leqslant n\leqslant\frac{N-1}{2}. \tag{4.9}$$

Since (4.8) and (4.9) are similar we treat only (4.8). Let now in (4.8) $\tilde{q}\to q$. Due to (4.2) and (4.3) one easily has that $\tilde{Q}_j\to Q_j, j\leqslant N$. It follows from Lemma 1 that $\Sigma_l(-\tilde{\lambda}_l)^n\to\Sigma_l(-\lambda_l)^n$ and (4.8) becomes

$$(-1)^n\sum_{l=1}^{\infty}(-\lambda_l)^n+\frac{2n}{\pi}\lim_{\tilde{q}\to q}\int_0^{\infty}k^{2n-1}\left[\tilde{\theta}(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}\tilde{Q}_{2l+1}\right]dk=(-1)^n\frac{n}{2^{2n}}Q_{2n},$$

$$2\leqslant n\leqslant\frac{N}{2}. \tag{4.10}$$

It is only left to pass to the limit under the integral sign in (4.10). To this end, represent this integral as the sum of the integrals over $(0,r)$ and (r,∞) with any $r\geqslant r_q$, where r_q is as in Lemma 1. It can be derived from Ref. 12 that $\int_0^k\tilde{\theta}(t)dt\to\int_0^k\theta(t)dt$ in $L_1(0,r)$ and hence $k\tilde{\theta}(k)\to k\theta(k)$ in $L_1(0,r)$-sense. Thus,

$$\lim_{\tilde{q}\to q}\int_0^r k^{2n-1}\left\{\tilde{\theta}(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}\tilde{Q}_{2l+1}\right\}dk=\int_0^r k^{2n-1}\left\{\theta(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}Q_{2l+1}\right\}dk, \tag{4.11}$$

since $k=0$ is not a singularity of the integrands in (4.11). Consider now the integral over (r,∞). Using the elementary fact

$$f(x)=\sum_{m\geqslant 1}a_m x^m\Rightarrow\ln\{1+f(x)\}=\sum_{m\geqslant 1}b_m x^m,$$

$$b_1=a_1, b_m=a_m-\sum_{j=1}^{m-1}\frac{j}{m}a_{m-j}b_j, m\geqslant 2,$$

it follows form Proposition 1 that for $k\geqslant r_q$ the function

$$\tilde{g}(k):=k^{2n-1}\left\{\tilde{\theta}(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}\tilde{Q}_{2l+1}\right\}-\frac{(-1)^n}{2^{2n}}\cdot\frac{1}{k}\int_0^{\infty}\sin\left(2kx-\frac{1}{k}\int_0^x\tilde{q}(s)ds\right)\tilde{q}^{(N)}(x)dx$$

has a majorant from $L_1(r,\infty)$ and by the dominated convergence theorem

$$g(k)=\lim_{\tilde{q}\to q}\tilde{g}(k)=k^{2n-1}\left\{\theta(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}Q_{2l+1}\right\}$$

$$-\frac{(-1)^n}{2^{2n}}\cdot\frac{1}{k}\int_0^{\infty}\sin\left(2kx-\frac{1}{k}\int_0^x q(s)ds\right)q^{(N)}(x)dx$$

$$\in L_1(r,\infty).$$

The latter means that

$$\lim_{\tilde{q}\to q}\int_r^\infty k^{2n-1}\left\{\tilde{\theta}(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}\tilde{Q}_{2l+1}\right\}dk=\int_r^\infty k^{2n-1}\left\{\theta(k)-\sum_{l=1}^{n-1}\frac{(-1)^{l+1}}{(2k)^{2l+1}}Q_{2l+1}\right\}dk, \tag{4.12}$$

and the integral on the right-hand side of (4.12) converges absolutely if and only if

$$\frac{1}{k}\int_0^\infty \sin\left(2kx-\frac{1}{k}\int_0^x q(s)ds\right)q^{(N)}(x)dx\in L_1(r,\infty)$$

with some positive r. Plug (4.11) and (4.12) into (4.10) and the theorem is proved. □

Corollary 1: If $q\in L_2(0,\infty)$, $q',q''\in L_1(0,\infty)$, *and*

$$\frac{1}{k}\int_0^\infty \sin\left(2kx-\frac{1}{k}\int_0^x q(s)ds\right)q''(x)dx\in L_1(r,\infty),\quad r>0, \tag{4.13}$$

then

$$\sum_{l\geqslant 1}(-\lambda_l)^{3/2}+\frac{3}{\pi}\int_0^\infty\left\{k^2\ln A(k)-\frac{1}{4}q(0)\right\}dk=\frac{3}{8}q'(0)+\frac{3}{8}\int_0^\infty q^2(x)dx. \tag{4.14}$$

If also $q'''\in L_1(0,\infty)$ *and*

$$\frac{1}{k}\int_0^\infty \sin\left(2kx-\frac{1}{k}\int_0^x q(s)ds\right)q'''(x)dx\in L_1(r,\infty),\quad r>0, \tag{4.15}$$

then

$$\sum_{l=1}^{\infty}\lambda_l^2+\frac{4}{\pi}\int_0^\infty\left\{k^3\theta(k)-\frac{1}{8}\left(q'(0)+\int_0^\infty q^2(x)dx\right)\right\}dk=\frac{1}{8}q''(0)-\frac{1}{4}q^2(0). \tag{4.16}$$

Conditions (4.13) and (4.15) are necessary for absolute convergence of the integrals in (4.14) and (4.16), respectively.

Remark 4: It is easy to verify that the function η *defined by*

$$\eta(t)=\frac{1}{\pi}\int_0^t\left(\theta(k)+\frac{1}{2k}\int_0^\infty q(x)\cos 2kx\,dx\right)dk$$

is actually the modified spectral shift function [see (1.6) and Remark 3] and formula (4.16) transforms into (1.6). Relation (1.6) was previously proven in Ref. 20 by different methods under slightly stronger conditions on q. *Note that Corollary 1 gives optimal conditions on* q *for (1.6) to hold with the absolutely convergent integral. In the short-range setting necessary and sufficient conditions for absolute summability of trace relations are recently given in Ref. 18.*

Remark 5: When it comes to long-range potentials there is a certain flexibility in choosing the limiting phase θ. *With a proper choice of* θ *some of the formulas (4.4) may actually simplify.*

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The scattering matrix for the Schrödinger operator with a long-range electromagnetic potential

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(Received 11 November 2002; accepted 17 March 2003)

We consider the Schrödinger operator $H=(i\nabla+A)^2+V$ in the space $L_2(\mathbb{R}^d)$ with long-range electrostatic $V(x)$ and magnetic $A(x)$ potentials. Using the scheme of smooth perturbations, we give an elementary proof of the existence and completeness of modified wave operators for the pair $H_0=-\Delta$, H. Our main goal is to study spectral properties of the corresponding scattering matrix $S(\lambda)$. We obtain its stationary representation and show that its singular part (up to compact terms) is a pseudodifferential operator with an oscillating amplitude which is an explicit function of V and A. Finally, we deduce from this result that, in general, for each $\lambda>0$ the spectrum of $S(\lambda)$ covers the whole unit circle. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1576494]

I. INTRODUCTION

Let the Schrödinger operator H be defined by differential expression

$$H=H(V,A)=(i\nabla+A(x))^2+V(x), \tag{1.1}$$

where the scalar function $V(x)$ and the vector-valued function $A(x)=(A_1(x),\ldots,A_d(x))$ are real valued and called the electrostatic and magnetic potentials, respectively. We assume that the potentials are C^∞-functions satisfying the assumption

$$|\partial_x^\alpha A(x)|+|\partial_x^\alpha V(x)|\leqslant C_\alpha(1+|x|)^{-\rho-|\alpha|},\quad \rho>0, \tag{1.2}$$

for all multi-indices α. Then H is a self-adjoint operator in the space $\mathcal{H}=L_2(\mathbb{R}^d)$ on domain $\mathcal{D}(H)=\mathcal{D}(H_0)$ of the "free" operator $H_0=-\Delta$. Our approach to the scattering theory for the pair H_0, H relies on wave operators with non-trivial identifications $J_\pm$ (depending on the sign of t)

$$W_\pm=W_\pm(H,H_0;J_\pm)=s-\lim_{t\to\pm\infty} e^{iHt}J_\pm e^{-iH_0t}. \tag{1.3}$$

We construct $J_\pm$ as pseudodifferential operators (PDO). Such wave operators were first introduced by Isozaki and Kitada in Ref. 3, where the Enss method was used for the proof of their existence and completeness (the method of Ref. 3 was extended to long-range magnetic potentials in Ref. 13). We show that the long-range scattering fits into the theory of smooth perturbations (in the sense of Kato). This yields, in particular, the stationary (in terms of the resolvent) representation for the corresponding scattering matrix $S(\lambda)$ which allows us to study its structure and spectral properties. Actually, we follow closely Ref. 20, where the case $\rho>1/2$ (and $A=0$) was considered. However consideration of the general case $\rho>0$ is technically much more involved.

The operators $J_\pm$ emerge naturally as PDO with symbols constructed in terms of approximate eigenfunctions $\Psi_\pm(x,\xi)=e^{i\varphi_\pm(x,\xi)}$ of the operator H. Substituting $\Psi=e^{i\varphi}$ in the Schrödinger equation $H\Psi=|\xi|^2\Psi$ and neglecting imaginary terms, we obtain the eikonal equation

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$$|\nabla\varphi|^2-2\langle A,\nabla\varphi\rangle+V(x)+|A(x)|^2-|\xi|^2=0,\quad \nabla=\nabla_x, \tag{1.4}$$

for the phase function $\varphi=\varphi_\pm$. We seek approximate solutions of this equation in the form

$$\varphi_\pm(x,\xi)=\langle\xi,x\rangle+\Phi_\pm(x,\xi) \tag{1.5}$$

where $\Phi_\pm(x,\xi)=o(|x|)$ as $|x|\to\infty$. Such solutions can be constructed by an explicit procedure described in Sec. IV. Then the Schrödinger equation for $\Psi_\pm=e^{i\varphi_\pm}$ is satisfied up to short-range terms (that is, satisfying an estimate of the type (1.2) with $\rho>1$) off any neighborhood of the direction $\hat{x}=\mp\hat{\xi}$. To get rid of the "bad" direction $\hat{x}=\mp\hat{\xi}$, we introduce in the symbol $j_\pm(x,\xi)$ suitable cutoff functions $\zeta_\pm(x,\xi)$, such that $\zeta_\pm$ are asymptotically homogeneous in x of degree 0, $\zeta_\pm(x,\xi)=0$ in a conical neighborhood (in $\mathbb{R}^{2d}$) of the set $\hat{x}=\mp\hat{\xi}$ and $\zeta_\pm(x,\xi)=1$ off somewhat larger neighborhood of this set. At the same time we localize our considerations on a compact energy subinterval of $\mathbb{R}_+=(0,\infty)$. The symbol of the PDO $J_\pm$ can be defined by the equality

$$j_\pm(x,\xi)=e^{i\Phi_\pm(x,\xi)}\zeta_\pm(x,\xi). \tag{1.6}$$

As in Ref. 20, from analytical point of view our approach relies on the limiting absorption principle and the radiation estimates. The first of these results means that the operator $\langle x\rangle^{-p}$, $p>1/2$, is locally H-smooth on any bounded interval disjoint from zero (see Definition 3.1). The second, pertaining to the critical case $p=1/2$, ensures local H-smoothness of the operators $G_j=\langle x\rangle^{-1/2}\nabla_j^\perp$, $j=1,\ldots,d$, where

$$\nabla_j^\perp u=\partial_j u-|x|^{-2}\langle\nabla u,x\rangle x_j,\quad j=1,\ldots,d. \tag{1.7}$$

Let $T_\pm=HJ_\pm-J_\pm H_0$ be the "effective perturbation." It follows from definition (1.6) that both operators $T=T_\pm$ factorize into a sum of products of locally H_0- and H-smooth operators

$$T=\langle x\rangle^{-p}B^{(r)}\langle x\rangle^{-p}+\sum_{j=1}^{d}G_j^*B^{(s)}G_j,\quad p>1/2, \tag{1.8}$$

where the operators $B^{(r)}=B_\pm^{(r)}$, $B^{(s)}=B_\pm^{(s)}$ are bounded. This implies the existence of all wave operators $W_\pm(H,H_0,J_\gamma)$, $W_\pm(H_0,H,J_\gamma^*)$, both for $\gamma=$"$+$" and $\gamma=$"$-$." The operators $W_\pm(H,H_0,J_\pm)$ are isometric since $J_\pm^*J_\pm e^{-iH_0t}f\sim e^{-iH_0t}f$ as $t\to\pm\infty$. For the proof of completeness of $W_\pm(H,H_0,J_\pm)$, we use that, for a suitable choice of the cut-off functions ζ_+ and ζ_-, the operator $J_+J_+^*+J_-J_-^*-I$ is essentially compact. Finally, we check that wave operators (1.3) coincide with wave operators obtained by a time-dependent modification of the free dynamics in the coordinate representation (see Ref. 22). In the special case where $V=0$ and A satisfies assumption (1.2) with $\rho>1/2$ and the additional condition of transversal gauge

$$\langle A(x),x\rangle=0 \tag{1.9}$$

(for $x\in\mathbb{R}^d$ large enough), the identifications $J_\pm$ can be replaced in (1.3) by the identity operator, that is the usual wave operators $W_\pm(H,H_0)$ exist. Thus, we recover the well known result[9] of Loss and Thaller about long-range magnetic scattering.

Since the scattering operator $\mathbf{S}=W_+^*W_-$ commutes with H_0, it reduces in the spectral representation of H_0 to the multiplication by the operator-function $S(\lambda)$, $\lambda>0$, acting in the space $\mathfrak{N}=L_2(\mathbb{S}^{d-1})$ and known as the scattering matrix (SM). Our study of $S(\lambda)$ relies on its stationary representation in terms of the resolvent $R(z)=(H-z)^{-1}$ of the operator H. To describe it, we need to introduce the auxiliary wave operator $W_+(H_0,H_0;J_+^*J_-)$. It commutes with H_0 and hence acts in the spectral representation of H_0 as multiplication by the operator-function $\mathcal{W}(\lambda):\mathfrak{N}\to\mathfrak{N}$. Then (see Refs. 4, 20, 22)

$$S(\lambda)=\mathcal{W}(\lambda)-2\pi i\Gamma_0(\lambda)(J_+^*T_--T_+^*R(\lambda+i0)T_-)\Gamma_0^*(\lambda), \tag{1.10}$$

where

$$(\Gamma_0(\lambda)f)(\omega)=2^{-1/2}k^{(d-2)/2}\hat{f}(k\omega),\quad k=\lambda^{1/2}>0,\ \ \omega\in\mathbb{S}^{d-1},\tag{1.11}$$

is, up to the numerical factor, the restriction of the Fourier transform $\hat{f}=\mathcal{F}f$ to the sphere of radius k. Formula (1.10) is actually of abstract nature and, roughly speaking, is valid always when its right-hand side is well defined.

In our particular case $\mathcal{W}(\lambda)=0$ for all $\lambda>0$. Then, using the resolvent estimates called usually propagation estimates (see Refs. 6, 7, 11), we show that the part of $S(\lambda)$ containing in (1.10) the resolvent of H is a compact operator. Thus, the essential spectrum of $S(\lambda)$ is determined by the explicit operator $-2\pi i\Gamma_0(\lambda)J_+^*T_-\Gamma_0^*(\lambda)$ which we consider as a PDO on the unit sphere. In the general case $\rho>0$ this PDO is determined by its amplitude $a(y,\omega,\omega';\lambda)$ where $\omega,\omega'\in\mathbb{S}^{d-1}$ are close to some point ω_0 and y belongs to the hyperplane orthogonal to ω_0. It turns out that, essentially, $a(y,\omega,\omega';\lambda)=\exp(i\theta(y,\omega,\omega';\lambda))$ where $\theta(y,\omega,\omega;\lambda)\to\infty$ as $|y|\to\infty$. Actually, the asymptotics of $\theta(y,\omega,\omega;\lambda)$ as $|y|\to\infty$ is determined by the asymptotics of $V(x)$ and $A(x)$ as $|x|\to\infty$. For homogeneous potentials of degree $-\rho$, $\rho\in(0,1)$, the function θ is asymptotically homogeneous of degree $1-\rho$ and it has, generically, a logarithmic growth if $\rho=1$. In particular, this implies[21] that the spectrum of the SM covers the whole unit circle $\mathbb{T}$. This situation is completely different from the short-range case where the principal symbol of PDO $S(\lambda)$ equals 1 which corresponds to the Dirac function in its kernel. In this case the spectrum of $S(\lambda)$ consists of eigenvalues accumulating at the point 1 only. Thus, in the long- and short-range cases the singularities and the spectral structure of $S(\lambda)$ are of qualitatively different nature.

A detailed analysis of singularities (as well as asymptotic expansion as $\lambda\to\infty$) of the SM $S(\lambda)$ can be found in Ref. 23 where a method, somewhat different from this paper, was used.

Technically, our paper relies on the PDO calculus. Thus, we treat the operators $J_\pm$ and $T_\pm$ as PDO. For any $\rho\in(0,1)$, they belong to the Hörmander classes $\mathcal{S}^0_{\rho,1-\rho}$ and $\mathcal{S}^{-1}_{\rho,1-\rho}$, respectively. In these classes a convenient PDO calculus can be developed for $\rho>1/2$ only. This creates new difficulties for potentials satisfying (1.2) for $\rho\in(0,1/2]$. Fortunately, the operators $J_\pm$ and $T_\pm$ fit into the framework of PDO with oscillating symbols developed in Ref. 21. Auxiliary results concerning PDO calculus are discussed in Sec. II.

II. PSEUDODIFFERENTIAL OPERATORS

2.1. We need some elementary facts about PDO defined by the equality

$$(Af)(x)=(2\pi)^{-d/2}\int_{\mathbb{R}^d}e^{i\langle\xi,x\rangle}a(x,\xi)\hat{f}(\xi)d\xi,\tag{2.1}$$

where

$$\hat{f}(\xi)=(\mathcal{F}f)(\xi)=(2\pi)^{-d/2}\int_{\mathbb{R}^d}e^{-i\langle\xi,x\rangle}f(x)dx$$

is the Fourier transform of f from the Schwartz class $\mathcal{S}=\mathcal{S}(\mathbb{R}^d)$. We denote by $\mathcal{S}^m_{\rho,\delta}$ the class of symbols $a\in C^\infty(\mathbb{R}^d\times\mathbb{R}^d)$ satisfying, for all multi-indices α and β, the estimates

$$|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)|\leqslant C_{\alpha,\beta}(1+|x|)^{m-\rho|\alpha|+\delta|\beta|}.\tag{2.2}$$

Here and below C,c are different positive constants, whose precise values are of no importance. Moreover, we assume that $a(x,\xi)=0$ for sufficiently large $|\xi|$. We always suppose that $\rho>0$, $\delta<1$ and set $\mathcal{S}^m=\mathcal{S}^m_{1,0}$. The operators A and A^* are well defined as mappings of the Schwartz class $\mathcal{S}$ into itself. The calculus of PDO can be conveniently developed (see, e.g., Ref. 2 or Ref. 17) in the classes $\mathcal{S}^m_{\rho,\delta}$ if $\rho>1/2>\delta$, but it fails in the general case.

To treat the case $\rho\leqslant 1/2$, we need a more special class of PDO with oscillating symbols introduced in Ref. 21. Let us denote by $\mathcal{C}^m(\Phi)$ the class of symbols admitting the representation

$$a(x,\xi)=e^{i\Phi(x,\xi)}b(x,\xi),\quad \Phi\in\mathcal{S}^r,\quad b\in\mathcal{S}^m,\quad r\in[0,1). \tag{2.3}$$

Since $\mathcal{C}^m(\Phi)\subset\mathcal{S}^m_{1-r,r}$, only the case $r\geqslant 1/2$ requires a special study. Occasionally we use the notation $\mathcal{S}^m_{\rho,\delta}$ and $\mathcal{C}^m(\Phi)$ for PDO (2.1) with symbols from these classes. The operator of multiplication by $(1+|x|^2)^{1/2}$ is denoted by $\langle x\rangle$.

Let us collect a necessary information on the calculus of PDO. Note that compared to the standard definition of PDO the roles of the variables x and ξ in (2.1) are interchanged. However, the operator $\mathcal{F}A^*\mathcal{F}^*$ satisfies the usual assumptions. This allows us to recover all results of PDO theory for operators (2.1). We start with an elementary assertion, which can be proven by the standard technique (see, e.g., Ref. 2 or Ref. 17).

Proposition 2.1: Suppose that $a_1\in\mathcal{C}^{m_1}(\Phi)$ *for some* $\Phi\in\mathcal{S}^r$, $r\in[0,1)$, $a_2\in\mathcal{S}^{m_2}$ *and* $a_0(x,\xi)=a_1(x,\xi)a_2(x,\xi)$. *Let* A_j *be the PDO with symbol* a_j, $j=0,1,2$. *Then* A_1A_2 *and* A_2A_1 *are PDO from the class* $\mathcal{C}^m(\Phi)$ *where* $m=m_1+m_2$ *and the PDO* $A_1A_2-A_0$ *and* $A_2A_1-A_0$ *belong to the class* $\mathcal{C}^{m+r-1}(\Phi)$.

The following two assertions are borrowed directly from Ref. 21.

Proposition 2.2: Let $A\in\mathcal{C}^m(\Phi)$. *Then the operator* A *is bounded in the space* $L_2(\mathbb{R}^d)$ *if* $m=0$, *and it is compact if* $m<0$.

Proposition 2.3: Let A_j, $j=1,2$, *be PDO with symbols* $a_j\in\mathcal{C}^0(\Phi)$ *and let* A *be the PDO with symbol* $a_1(x,\xi)a_2(x,\xi)$. *Then both operators* $A-A_1A_2^*$ *and* $A-A_2^*A_1$ *are compact in the space* $L_2(\mathbb{R}^d)$.

To formulate further results on PDO, we need the following technical lemma.

Lemma 2.4: Let $\Omega_0\in C_0^\infty(\mathbb{R}^d)$, $\Omega_0(\xi)=1$ *for* $|\xi|\leqslant R_0-1$ *and* $\Omega_0(\xi)=0$ *for* $|\xi|\geqslant R_0$ *(for some* $R_0>1$*). Let* $\Omega_1\in C^\infty(\mathbb{R}^d)$, $\Omega_1(\xi)=0$ *for* $|\xi|\leqslant R_1$ *and* $\Omega_1(\xi)=1$ *for* $|\xi|\geqslant R_1+1$. *Assume that* $R_1>R_0$. *We denote by* Ω_j, $j=0,1$, *the multiplication operators (in the momentum representation) by the functions* $\Omega_j(\xi)$. *Let* g *be the multiplication operator by a function* $g\in C^\infty(\mathbb{R}^d)$ *such that* $\partial^\alpha g(x)=O(|x|^{n-|\alpha|})$ *as* $|x|\to\infty$ *for some* n *and all* α. *Then the operator* $\Omega_0g\Omega_1=\Omega_0g_0\Omega_1$ *where* $g_0\in\mathcal{S}$.

Proof: In the momentum representation g acts as the convolution with the function $\hat g(\xi)$ where $\hat g\in C^\infty$ except the point zero and decays at infinity, together with all its derivatives, faster that any power of $|\xi|^{-1}$. Therefore $\Omega_0g\Omega_1$ is the integral operator with kernel

$$(2\pi)^{-d/2}\Omega_0(\xi)\hat g(\xi-\xi')\Omega_1(\xi'), \tag{2.4}$$

which equals 0 if $|\xi-\xi'|\leqslant R_1-R_0$. Let $\omega\in C^\infty(\mathbb{R}^d)$, $\omega(\xi)=0$ for $|\xi|\leqslant(R_1-R_0)/2$ and $\omega(\xi)=1$ for $|\xi|\geqslant R_1-R_0$. Then kernel (2.4) is not changed if we replace $\hat g(\xi-\xi')$ by $\hat g_0(\xi-\xi')$ where $\hat g_0(\xi)=\hat g(\xi)\omega(\xi)$ belongs to $\mathcal{S}$. □

Lemma 2.5: Let A *be a PDO with symbol* a *from the class* $\mathcal{S}^m_{\rho,\delta}$ *where* $\rho>0$, $\delta<1$ *and* m *are arbitrary and* $a(x,\xi)=0$ *if* $|\xi|\geqslant R$. *Let* g *and* Ω_1 *be the same as in Lemma 2.4 and* $R_1>R$. *Then for any* p *the operator* $Ag\Omega_1\langle x\rangle^p$ *is bounded in* $L_2(\mathbb{R}^d)$.

Proof: Assuming that p is an even integer and commuting the operators Ω_1 and $\langle x\rangle^p$, we reduce the problem to the case $p=0$. Let Ω_0 be the same as in Lemma 2.4 with $R_0\in(R,R_1)$. Then $Ag\Omega_1=A\Omega_0g\Omega_1$, so that, by Lemma 2.4, we may suppose that $g\in\mathcal{S}$. In the coordinate representation, the operator Ag has kernel

$$(2\pi)^{-d}\int_{\mathbb{R}^d}e^{i\langle\xi,x-x'\rangle}a(x,\xi)d\xi\,g(x'). \tag{2.5}$$

Using the formula $\langle x\rangle^{-k}\langle D_\xi\rangle^k e^{i\langle\xi,x\rangle}=e^{i\langle\xi,x\rangle}$ and integrating by parts, we estimate the kernel (2.5) by $\langle x\rangle^{m-(1-\delta)k}\langle x'\rangle^k|g(x')|$. For sufficiently large k, both functions of x and x' belong to $L_2(\mathbb{R}^d)$, and hence the operator Ag belongs to the Hilbert–Schmidt class. □

Now it easy to check the following two assertions.

Proposition 2.6: Let $A\in\mathcal{C}^m(\Phi)$ for some m. Then the operator $A\langle x\rangle^{-m}$ is bounded in the space $L_2(\mathbb{R}^d)$.

Proof: Assume that $a(x,\xi)=0$ for $|\xi|\geqslant R$. Let Ω_1 be the same operator as in Lemma 2.4 with $R_1>R$ and $\Omega_2=I-\Omega_1$. Clearly, $\langle x\rangle^{-m}\Omega_2$ is a PDO from the class $\mathcal{S}^{-m}$. Therefore, by Proposition 2.1, the PDO $A(\langle x\rangle^{-m}\Omega_2)$ belongs to the class $\mathcal{C}^0(\Phi)$ and hence, by Proposition 2.2, it is bounded. The operator $A\langle x\rangle^{-m}\Omega_1$ is bounded according to Lemma 2.5. □

Proposition 2.7: Suppose that A is a PDO with symbol $a\in\mathcal{C}^m(\Phi)$, for some $\Phi\in\mathcal{S}^r$ with $r\in[0,1)$, and G is a PDO (actually, a differential operator) with symbol $g(x,\xi)=\Sigma_{|s|\leqslant s_0}g_s(x)\xi^s$, where $g_s\in C^\infty(\mathbb{R}^d)$ and $\partial^\alpha g_s(x)=O(|x|^{n-|\alpha|})$ as $|x|\to\infty$ for some n and all α. Let T be the PDO with symbol $t(x,\xi)=|g(x,\xi)|^2a(x,\xi)$. Then the operator $\langle x\rangle^p(G^*AG-T)\times\langle x\rangle^p$ is bounded if $2p=-m-2n+1-r$.

Proof: Let $a_1(x,\xi)$ be the symbol of the PDO $A_1=G^*A$. By direct calculation we show that

$$a_1(x,\xi)-\overline{g(x,\xi)}a(x,\xi)\in C^{m+n+r-1}(\Phi).$$

Assuming that $a(x,\xi)=0$ for $|\xi|\geqslant R$, we introduce the same operators Ω_1,Ω_2 as in Proposition 2.6. Proposition 2.1 implies that, up to terms from the class $C^{m+2n+r-1}(\Phi)$, the operator $A_1G\Omega_2$ has symbol $t(x,\xi)$. Therefore the operator $\langle x\rangle^p(G^*AG\Omega_2-T)\langle x\rangle^p$ is bounded by Proposition 2.6. It remains to take into account that the operator $\langle x\rangle^pA_1G\Omega_1\langle x\rangle^p$ is bounded for any p according to Lemma 2.5. □

For the study of the SM we need to consider PDO defined by their amplitudes. We define such operators in terms of the corresponding sesquilinear forms on $\mathcal{S}\times\mathcal{S}$,

$$(\mathbf{A}f_1,f_2)=(2\pi)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}e^{i\langle\xi'-\xi,x\rangle}\mathbf{a}(x,\xi,\xi')\hat{f}_1(\xi')\overline{\hat{f}_2(\xi)}\,dx\,d\xi d\xi'. \tag{2.6}$$

We suppose that the amplitude $\mathbf{a}(x,\xi,\xi')$ belongs to the class $\mathcal{S}^m_{\rho,\delta,\delta}$ defined quite similarly to $\mathcal{S}^m_{\rho,\delta}$ with ξ replaced by (ξ,ξ') in (2.2) and that $\mathbf{a}(x,\xi,\xi')$ is compactly supported in ξ and ξ'. Again we denote $\mathcal{S}^m=\mathcal{S}^m_{1,0,0}$.

Let us consider [cf. (2.3)] a special class $\mathcal{C}^m(\Theta)$ of amplitudes admitting the representation

$$\mathbf{a}(x,\xi,\xi')=e^{i\Theta(x,\xi,\xi')}\mathbf{b}(x,\xi,\xi'),\quad \Theta\in\mathcal{S}^r,\quad r\in[0,1),\quad \mathbf{b}\in\mathcal{S}^m. \tag{2.7}$$

Such operators reduce to PDO with oscillating symbols.

Proposition 2.8: Let $\mathbf{A}$ be defined by (2.6) with amplitude (2.7). Then $\mathbf{A}=A$ where A is a PDO (2.1) with symbol (2.3) and

$$\Phi(x,\xi)=\Theta(x,\xi,\xi)+\Theta_1(x,\xi),\quad \Theta_1\in\mathcal{S}^{2r-1},$$

$$b(x,\xi)=\mathbf{b}(x,\xi,\xi)+b_1(x,\xi),\quad b_1\in\mathcal{S}^{m+r-1}.$$

In particular, if $\mathbf{b}(x,\xi,\xi)=0$, then A belongs to the class $\mathcal{C}^{m+r-1}(\Phi)$.

This result (its proof can be found in Ref. 21) allows us to extend Propositions 2.2 and 2.6 to operators $\mathbf{A}$ defined by (2.6).

Proposition 2.9: Let $\mathbf{A}\in\mathcal{C}^m(\Theta)$. Then the operator $\mathbf{A}$ is bounded in the space $L_2(\mathbb{R}^d)$ if $m=0$, and it is compact if $m<0$. Moreover, the operator $\mathbf{A}\langle x\rangle^{-m}$ is also bounded.

2.2. The spectral representation of $H_0=-\Delta$ can be constructed in terms of the operator $\Gamma_0(\lambda)$ defined by (1.11). Let $\mathfrak{N}=L_2(\mathbb{S}^{d-1})$ and $(\mathcal{U}f)(\lambda)=\Gamma_0(\lambda)f$, $f\in\mathcal{S}(\mathbb{R}^d)$, $\lambda>0$. Then the operator $\mathcal{U}$ extends by continuity to a unitary operator $\mathcal{U}:L_2(\mathbb{R}^d)\to L_2(\mathbb{R}_+;\mathfrak{N})$, and the operator H_0 is diagonalized by $\mathcal{U}$, that is $(\mathcal{U}H_0f)(\lambda)=\lambda(\mathcal{U}f)(\lambda)$ for $f\in\mathcal{D}(H_0)$.

The operator $\Gamma_0(\lambda)$ is directly related to the spectral family $E_0(\lambda)$ of the operator H_0 and to its resolvent $R_0(z)=(H_0-z)^{-1}$. Set

$$\delta_\varepsilon(H_0-\lambda)=(2\pi i)^{-1}(R_0(\lambda+i\varepsilon)-R_0(\lambda-i\varepsilon)).$$

For any $f_1, f_2 \in \mathcal{S}$ the limit and the derivative below exist and satisfy (see, e.g., Ref. 19)

$$\lim_{\varepsilon \to 0} (\delta_\varepsilon(H_0 - \lambda) f_1, f_2) = \mathrm{d}(E_0(\lambda) f_1, f_2)/\mathrm{d}\lambda = (\Gamma_0(\lambda) f_1, \Gamma_0(\lambda) f_2)_{\mathfrak{N}}.$$

We recall the Sobolev trace theorem.

Proposition 2.10: For $p > 1/2$ the operator-function $\Gamma_0(\lambda)\langle x\rangle^{-p} : \mathcal{H} \to \mathfrak{N}$ is compact and Hölder continuous in norm with respect to the parameter $\lambda > 0$.

For construction of the SM, we have to give a precise definition of the operator $\mathbf{A}^\flat(\lambda) := \Gamma_0(\lambda)\mathbf{A}\Gamma_0^*(\lambda)$ appearing in (1.10) which imposes rather stringent conditions on $\mathbf{A}$. Practically we consider only PDO $\mathbf{A}$ defined by (2.6), although the definition below is of abstract nature. Note that, for a PDO $\mathbf{A}$, the operator $\mathbf{A}^\flat(\lambda)$ is also defined as a PDO on the unit sphere $\mathbb{S}^{\mathrm{d}-1}$. It is convenient to define the operator $\mathbf{A}^\flat(\lambda)$ in terms of its sesquilinear form $(\mathbf{A}^\flat(\lambda) g_1, g_2)$.

Definition 2.11: Let $g_1, g_2 \in C^\infty(\mathbb{S}^{\mathrm{d}-1})$, and let $\psi_1, \psi_2 \in C_0^\infty(\mathbb{R}_+)$ be such that $\psi_1(k) = \psi_2(k) = 1$. Set $\hat{f}_j(\xi) = g_j(\hat{\xi})\psi_j(|\xi|)$, $j = 1,2$. Then

$$(\mathbf{A}^\flat(\lambda) g_1, g_2)_{\mathfrak{N}} := 2k^{2-d} \lim_{\varepsilon \to 0} (\mathbf{A}\delta_\varepsilon(H_0 - \lambda) f_1, \delta_\varepsilon(H_0 - \lambda) f_2), \tag{2.8}$$

provided this limit exists for all $g_1, g_2 \in C^\infty(\mathbb{S}^{d-1})$.

By definition (1.11), if $g \in C^\infty(\mathbb{S}^{d-1})$, $\psi \in C_0^\infty(\mathbb{R}_+)$ and $\hat{f}(\xi) = g(\hat{\xi})\psi(|\xi|)$, then

$$(\Gamma_0(\lambda) f)(\omega) = 2^{-1/2} k^{(d-2)/2} \psi(k) g(\omega), \quad k = \lambda^{1/2}.$$

The operator $\Gamma_0^*(\lambda)$ formally adjoint to $\Gamma_0(\lambda)$ is defined, e.g., for $g \in C^\infty(\mathbb{S}^{d-1})$ by the equality

$$(\Gamma_0^*(\lambda) g)(x) = 2^{-1/2} k^{(\mathrm{d}-2)/2} (2\pi)^{-\mathrm{d}/2} \int_{\mathbb{S}^{\mathrm{d}-1}} e^{ik\langle \omega, x\rangle} g(\omega)\, \mathrm{d}\omega, \quad k = \lambda^{1/2} > 0. \tag{2.9}$$

Therefore Definition 2.11 gives an exact meaning to the formal expression $\Gamma_0(\lambda)\mathbf{A}\Gamma_0^*(\lambda)$.

If $B = \mathcal{F}\mathbf{A}\mathcal{F}^*$ is an integral operator with kernel $B(\xi, \xi')$ which is continuous near the surface $|\xi| = |\xi'| = k$, then, by (1.11) and (2.9), $\mathbf{A}^\flat(\lambda)$ is also an integral operator with kernel

$$b(\omega, \omega'; \lambda) = 2^{-1} k^{\mathrm{d}-2} B(k\omega, k\omega').$$

If $\mathbf{A}$ is a PDO (2.6) with amplitude $\mathbf{a} \in \mathcal{S}^m_{\rho,\delta,\delta}$, then the kernel

$$B(\xi, \xi') = (2\pi)^{-\mathrm{d}} \int_{\mathbb{R}^{\mathrm{d}}} e^{i\langle \xi' - \xi, x\rangle} \mathbf{a}(x, \xi, \xi')\, \mathrm{d}x$$

(understood as an oscillatory integral) of the operator $B = \mathcal{F}\mathbf{A}\mathcal{F}^*$ is well defined and infinitely differentiable off the diagonal $\xi = \xi'$.

Thus, we have the following obvious assertion.

Proposition 2.12: Let $\mathbf{a} \in \mathcal{S}^m_{\rho,\delta,\delta}$ for some $\rho > 0$, $\delta < 1$, and let χ_1 and χ_2 be multiplication operators by $C^\infty(\mathbb{S}^{\mathrm{d}-1})$-functions with disjoint supports. Then $(\chi_1 \mathbf{A} \chi_2)^\flat(\lambda)$ is an integral operator with C^∞-kernel of variables ω, ω' (and $\lambda > 0$).

However due to a possible strong singularity of the function $B(\xi, \xi')$ at $\xi = \xi'$, the operator $\mathbf{A}^\flat(\lambda)$ exists only under special assumptions on $\mathbf{a}(x, \xi, \xi')$. In the case $\mathbf{a} \in \mathcal{C}^m(\Theta)$, $m < -1$, the diagonal singularity of $B(\xi, \xi')$ is weak, so no additional restrictions are required.

Proposition 2.13: Let $\mathbf{A}$ belong to the class $\mathcal{C}^m(\Theta)$ where $m < -1$. Then $\mathbf{A}^\flat(\lambda)$ is well defined for all $\lambda > 0$ and is a compact operator in $\mathfrak{N}$. Moreover, $\mathbf{A}^\flat(\lambda)$ depends norm continuously on λ.

Proof: Indeed,

$$\mathbf{A}^\flat(\lambda) = (\Gamma_0(\lambda)\langle x\rangle^{-p})(\langle x\rangle^p \mathbf{A} \langle x\rangle^p)(\langle x\rangle^{-p} \Gamma_0^*(\lambda)), \quad p = m/2.$$

Since $p>1/2$, Proposition 2.10 applies to the first and third factors. The second factor is bounded in $\mathcal{H}$ by Proposition 2.9. □

Let us now consider the general case $\mathbf{a}\in\mathcal{S}^m_{\rho,\delta,\delta}$ where m is arbitrary. It turns out (see Refs. 8 and 21) that for $m\geqslant -1$ the operator $\mathbf{A}^\flat(\lambda)$ exists if $\mathbf{a}(x,\xi,\xi')=0$ for (x,ξ) belonging to a neighborhood of the conormal bundle of the sphere $|\xi|=k$ and ξ' close to ξ. In view of Proposition 2.12, we may suppose that ξ and ξ' are close to each other or, to put it differently, we can take in Definition 2.11 functions g_1 and g_2 supported in a neighborhood of the same point $\omega_0\in\mathbb{S}^{d-1}$. Let Π_{ω_0} be the hyperplane orthogonal to ω_0, and let $\Omega=\Omega(\omega_0,\gamma)\subset\mathbb{S}^{d-1}$ be determined by the condition $\langle\omega,\omega_0\rangle>\gamma>0$. The number γ can be chosen arbitrary close to 1. We denote by $\zeta=\varkappa(\omega)$ the orthogonal projection of ω on Π_{ω_0}; in particular, we assume that $\varkappa(\omega_0)=0$. We denote by Σ the orthogonal projection of Ω on the hyperplane Π_{ω_0} and identify points $\omega\in\Omega$ and $\zeta=\varkappa(\omega)$. The hyperplane Π_{ω_0} can be identified with $\mathbb{R}^{d-1}$. Let us also consider the unitary mapping $Z=Z_\varkappa: L_2(\Omega)\to L_2(\Sigma)$ defined by

$$(Zu)(\zeta)=(1-|\zeta|^2)^{-1/4}u(\omega),\quad \zeta=\varkappa(\omega). \tag{2.10}$$

The next result (borrowed from Ref. 21) gives conditions of the existence of the operator $\mathbf{A}^\flat(\lambda)$.

Proposition 2.14: Let $\mathbf{a}\in\mathcal{S}^m_{\rho,\delta,\delta}$ *for some* $\rho>0$, $\delta<1$ *with* $\rho+\delta\leqslant 1$. *Suppose that there exists* $\varepsilon>0$ *such that* $\mathbf{a}(x,\xi,\xi')=0$ *if the following two estimates*

$$|\xi-\xi'|<\varepsilon,\quad |\langle\hat{x},\hat{\xi}\rangle|>1-\varepsilon \tag{2.11}$$

are satisfied. Then the operator $\mathbf{A}^\flat(\lambda)$ *is well-defined in the sense of Definition 2.11 for all* $\lambda>0$. *Moreover, the operator* $\mathbf{A}^\flat_\varkappa(\lambda)=Z_\varkappa\mathbf{A}^\flat(\lambda)Z_\varkappa^*$ *is the PDO with sesquilinear form*

$$(\mathbf{A}^\flat_\varkappa(\lambda)u_1,u_2)=(2\pi)^{-d+1}\int_{\mathbb{R}^{d-1}}\int_\Sigma\int_\Sigma e^{i\langle\zeta-\zeta',y\rangle}\mathbf{a}^\flat_\varkappa(y,\zeta,\zeta';\lambda)u_1(\zeta')\overline{u_2(\zeta)}\,d\zeta\,d\zeta'\,dy \tag{2.12}$$

for all $u_1,u_2\in\mathcal{C}_0^\infty(\Sigma)$. *The amplitude* $\mathbf{a}^\flat_\varkappa\in\mathcal{S}^{m+1}_{\rho,\delta,\delta}(\mathbb{R}^{d-1}\times\Sigma\times\Sigma)$ *is given by the formula*

$$\mathbf{a}^\flat_\varkappa(y,\zeta,\zeta';\lambda)=(2\pi k)^{-1}\alpha(\zeta,\zeta')\int_{-\infty}^{\infty}\mathbf{a}((\omega+\omega')z-y/k,k\omega,k\omega')\,dz \tag{2.13}$$

[this integral is taken over a finite interval due to condition (2.11)], where $k=\lambda^{1/2}$, $\zeta=\varkappa(\omega)$, $\zeta'=\varkappa(\omega')$, *and*

$$\alpha(\zeta,\zeta')=2^{-1}\left(\left(\frac{1-|\zeta|^2}{1-|\zeta'|^2}\right)^{1/4}+\left(\frac{1-|\zeta'|^2}{1-|\zeta|^2}\right)^{1/4}\right). \tag{2.14}$$

Consequently, (2.12) is a smooth function of $\lambda>0$ *for all* $u_1,u_2\in\mathcal{C}_0^\infty(\Sigma)$.

Definition 2.15: The function $\mathbf{a}^\flat_\varkappa(y,\zeta,\zeta';\lambda)$ *is called the amplitude of the operator* $\mathbf{A}^\flat(\lambda)$ *in the chart coordinates* $(\omega_0,\varkappa)$.

We emphasize that, from the point of view of PDO theory, in the formula (2.12) ζ plays the role of the space variable and y is the dual one.

A spectral information on PDO with oscillating amplitudes is given in the following assertion (see Ref. 21).

Proposition 2.16: Let $\mathbf{A}: C_0^\infty(\Sigma)\to C^\infty(\Sigma)$, $\Sigma\subset\mathbb{R}^{d-1}$, *be a PDO with amplitude*

$$\mathbf{a}(y,\zeta,\zeta')=e^{i\Theta(y,\zeta,\zeta')}\mathbf{b}(y,\zeta,\zeta'), \tag{2.15}$$

where $\Theta\in\mathcal{S}^r$, $r\in(0,1)$, $\mathbf{b}\in\mathcal{S}^0$. *Suppose that for some points* $y_0\neq 0,\zeta_0\in\Sigma$,

$$|\Theta(\tau y_0,\zeta_0,\zeta_0)|\geqslant c\tau^r, \quad |\nabla_y\Theta(\tau y_0,\zeta_0,\zeta_0)|\geqslant c\tau^{r-1}, \quad c>0, \tag{2.16}$$

for sufficiently large $\tau>0$ *and that*

$$\lim_{\tau\to\infty}\mathbf{b}(\tau y_0,\zeta_0,\zeta_0)=1. \tag{2.17}$$

Then for each $\mu\in\mathbb{T}$ *and arbitrary small neighborhood* Σ_0 *of* ζ_0 *there exists a (Weyl) sequence of functions* $u_n\in C_0^\infty(\Sigma_0)$ *such that*

$$\|u_n\|=1, \quad w-\lim_{n\to\infty}u_n=0, \quad \lim_{n\to\infty}\|\mathbf{A}u_n-\mu u_n\|=0.$$

In particular, the essential spectrum of the operator $\mathbf{A}$ *in the space* $L_2(\Sigma)$ *covers the unit circle* $\mathbb{T}$.

Remark 2.17: A simple version of Proposition 2.16 was proven and used in Ref. 20. Namely, let $\mathbf{a}\in\mathcal{S}^0_{\rho,\delta,\delta}$ with $\rho>1/2>\delta$, and let representation (2.15) hold. Then the conclusion of Proposition 2.16 remains true if, for some $y_0\neq 0,\zeta_0\in\Sigma$, the condition (2.17) is satisfied and

$$\limsup_{\tau\to\infty}\Theta(\tau y_0,\zeta_0,\zeta_0)=\infty \quad \text{or} \quad \liminf_{\tau\to\infty}\Theta(\tau y_0,\zeta_0,\zeta_0)=-\infty. \tag{2.18}$$

III. LIMITING ABSORPTION PRINCIPLE AND RADIATIONS ESTIMATES

3.1. Let us recall some basic notions of the theory of smooth perturbations (see, e.g., Refs. 15 and 19).

Definition 3.1: Let H *be a self-adjoint operator in a Hilbert space* $\mathcal{H}$, $R(z)=(H-z)^{-1}$ *be the resolvent of* H *and* K *be an* H*-bounded operator. The operator* K *is called* H*-smooth (in the sense of Kato) if one of the two equivalent conditions is satisfied*

$$\sup_{f\in\mathcal{D}(\mathcal{H}),\|f\|=1}\int_{-\infty}^{\infty}\|Ke^{-itH}f\|^2\,dt<\infty, \tag{3.1}$$

$$\sup_{\lambda\in\mathbb{R},\varepsilon>0}\|K(R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon))K^*\|<\infty. \tag{3.2}$$

The following definition is essentially more flexible.

Definition 3.2: Let $E(\cdot)$ *be the spectral measure of* H. *Suppose that, for an* H*-bounded operator* K, *and intervals* Λ_n *such that* $\mathbb{R}\setminus\cup_{n=1}^\infty\Lambda_n$ *has the Lebesgue measure zero, the operators* $KE(\Lambda_n)$ *are* H*-smooth. Then we say that* K *is locally* H*-smooth*.

Note that condition (3.2), satisfied for $\lambda\in\Lambda$ only, implies that the operator $KE(\Lambda)$ is H-smooth.

The theory of H-smooth perturbations gives a sufficient condition for the existence of wave operators [which can easily be obtained from (3.1)].

Proposition 3.3: Let H_0, H *be a couple of self-adjoint operators, and let* J *be a bounded operator. Suppose that* $T=HJ-JH_0$ *admits the factorization*

$$T=\sum_{j=1}^{N}K_j^*K_{0,j},$$

where all operators $K_{0,j}$ *are locally* H_0*-smooth and* K_j *are locally* H*-smooth. Denote by* P_0 *and* P *the orthogonal projections on the absolutely continuous subspaces of the operators* H_0 *and* H, *respectively. Then the wave operators*

$$W_\pm(H,H_0;J)=s-\lim_{t\to\pm\infty}e^{itH}J^*e^{-itH_0}P_0$$

and

$$W_{\pm}(H_0,H;J^*)=s-\lim_{t\to\pm\infty} e^{iH_0t}J^*e^{-iHt}P$$

exist.

Note, finally, that for an arbitrary self-adjoint operator H and a compact operator K,

$$s-\lim_{|t|\to\infty} Ke^{-iHt}P=0. \tag{3.3}$$

3.2. Let us return to the Schrödinger operator (1.1). Recall first of all that, although it is really unimportant for our results, under assumption (1.2) the operator H does not have positive eigenvalues (see Refs. 5 and 18 where the proof of Ref. 15 was extended to magnetic potentials). The following well-known result (the limiting absorption principle; see Refs. 1, 10, and 14) can be easily obtained by the Mourre method.

Proposition 3.4: Let assumption (1.2) hold, and let $p>1/2$. *Then the operator function* $\langle x\rangle^{-p}R(z)\langle x\rangle^{-p}$ *is continuous in norm with respect to the parameter* z *in the closed complex plane cut along* $[0,\infty)$ *with exception of the point 0. In particular, the operator* $\langle x\rangle^{-p}E(\Lambda)$ *is* H*-smooth for any compact interval* $\Lambda\subset(0,\infty)$. *The positive spectrum of* H *is absolutely continuous*.

The following resolvent estimates borrowed from Ref. 22 are called radiation estimates.

Proposition 3.5: Let assumption (1.2) hold, and let the operators $\nabla_j^{\perp}$ *be defined by (1.7). Set* $G_j=\langle x\rangle^{-1/2}\nabla_j^{\perp}$. *Then for all* $j=1,\ldots,\mathrm{d}$ *the operators* $G_jE(\Lambda)$ *are* H*-smooth for any compact interval* $\Lambda\subset(0,\infty)$.

Propositions 3.4 and 3.5 are sufficient for the proof of existence and completeness of wave operators. However, our study of the SM requires additional resolvent estimates called usually propagation estimates.

Proposition 3.6: Let assumption (1.2) be fulfilled. Let $Q_{\pm}$ *be the PDO with symbol* $q_{\pm}(x,\xi)\in\mathcal{C}^m(\Phi_{\pm})$ *for some* $\Phi_{\pm}\in\mathcal{S}^r$ *with* $r\in[0,1)$. *Suppose that* $q_{\pm}(x,\xi)=0$ *for* $|\xi|\leqslant\varepsilon$, $|x|\leqslant\varepsilon$ *and that the support of* $q_{\pm}(x,\xi)$ *is contained in the cone*

$$\mp\langle\hat{\xi},\hat{x}\rangle\geqslant\varepsilon,\quad \hat{\xi}=\xi/|\xi|,\quad \hat{x}=x/|x|,$$

for some $\varepsilon\in(0,1)$. *Then the operator-functions*

$$\langle x\rangle^{p-\sigma}Q_+^*R(z)\langle x\rangle^{-p},\quad \langle x\rangle^{-p}R(z)Q_-\langle x\rangle^{p-\sigma},\quad p>1/2,\quad \sigma>m+1,$$

are bounded and continuous in norm with respect to the parameter z *in the region* $\mathrm{Re}\,z\in(\lambda_0,\infty)$, $\lambda_0>0$, $\mathrm{Im}\,z\geqslant0$.

Proposition 3.7: Under the assumptions of Proposition 3.6 the operator function

$$\langle x\rangle^{l}Q_+^*R(z)Q_-\langle x\rangle^{l},\quad \forall l,$$

is bounded and continuous in norm with respect to the parameter z *in the region* $\mathrm{Re}\,z\in(\lambda_0,\infty)$, $\lambda_0>0$, $\mathrm{Im}\,z\geqslant0$.

These two assertions were proven in Refs. 6, 7, and 11 for PDO $Q_{\pm}\in\mathcal{S}^m$. In the case $Q_{\pm}\in\mathcal{C}^m(\Phi_{\pm})$ the proofs are quite similar. In particular, they rely on the Mourre estimate.[10]

IV. THE EIKONAL EQUATION

In this section our goal is to construct approximate eigenfunctions of the Schrödinger operator with long-range electric and magnetic potentials. It is natural to seek these eigenfunctions in the form $\Psi=e^{i\varphi}$ with a real function φ. A simple calculation shows that

$$((i\nabla+A)^2+V-|\xi|^2)\Psi=e^{i\varphi}(|\nabla\varphi|^2-2\langle A,\nabla\varphi\rangle-i\Delta\varphi+V+|A|^2+i\,\mathrm{div}\,A-|\xi|^2), \quad (4.1)$$

where $\nabla=\nabla_x$. Neglecting here the imaginary terms, which turn out to be short-range, we see that the Schrödinger equation reduces to the eikonal equation (1.4) for $\varphi=\varphi_\pm$. Considering this equation, we always remove a conical neighborhood of the direction $\hat{x}=\mp\hat{\xi}$ and require that its right-hand side be short-range (not necessarily zero). We assume that $\varphi_\pm$ has the form (1.5) where $\Phi_\pm=o(|x|)$ as $|x|\to\infty$. Then Eq. (1.4) for $\varphi_\pm$ yields the equation

$$2\langle\xi,\nabla\Phi_\pm(x,\xi)\rangle+|\nabla\Phi_\pm(x,\xi)|^2-2\langle A(x),\xi+\nabla\Phi_\pm(x,\xi)\rangle+V(x)+|A(x)|^2=q_\pm(x,\xi) \quad (4.2)$$

for $\Phi_\pm$ with a short-range term $q_\pm$. Thus, according to (4.1),

$$((i\nabla+A)^2+V-|\xi|^2)(e^{i\varphi_\pm})=e^{i\varphi_\pm}\mathrm{q}_\pm, \quad (4.3)$$

where

$$\mathrm{q}_\pm=q_\pm+i\,\mathrm{div}\,A-i\Delta\Phi_\pm \quad (4.4)$$

is again a short-range term.

Equation (4.2) can be easily solved by iterations. Let us first consider an auxiliary linear equation

$$\langle\xi,\nabla\phi(x,\xi)\rangle+F(x,\xi)=0. \quad (4.5)$$

All estimates below are uniform in ξ if $\lambda_0\leqslant|\xi|\leqslant\lambda_1$ for some $0<\lambda_0<\lambda_1<\infty$.

Lemma 4.1: Suppose that $F=F_\pm$ satisfies for all multi-indices α,β the estimates

$$|\partial_x^\alpha\partial_\xi^\beta F_\pm(x,\xi)|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-\rho-|\alpha|}, \quad \pm\langle\hat{x},\hat{\xi}\rangle\geqslant\kappa,$$

for some $\rho\in(0,1)$ and any $\kappa>-1$. Then the function

$$\phi_\pm(x,\xi)=\pm\int_0^\infty(F_\pm(x\pm t\xi,\xi)-F_\pm(\pm t\xi,\xi))\,\mathrm{d}t \quad (4.6)$$

is a solution of equation (4.5) which satisfies for all α,β and $\kappa>-1$ the estimates

$$|\partial_x^\alpha\partial_\xi^\beta\phi_\pm(x,\xi)|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{1-\rho-|\alpha|}, \quad \pm\langle\hat{x},\hat{\xi}\rangle\geqslant\kappa.$$

The proof can be obtained by a direct differentiation of (4.6), see Ref. 20 for details.

Let us seek $\Phi_\pm=\Phi_\pm^{(N)}$ in the form

$$\Phi_\pm(x,\xi)=\sum_{n=1}^{N}\phi_\pm^{(n)}(x,\xi), \quad (4.7)$$

where the functions $\phi_\pm^{(n)}$ are solutions of equations

$$2\langle\xi,\nabla\phi_\pm^{(1)}\rangle+V-2\langle A,\xi\rangle=0, \quad (4.8)$$

$$2\langle\xi,\nabla\phi_\pm^{(2)}\rangle+|\nabla\phi_\pm^{(1)}|^2-2\langle A,\nabla\phi_\pm^{(1)}\rangle+|A|^2=0, \quad (4.9)$$

$$2\langle\xi,\nabla\phi_\pm^{(n)}\rangle+\sum_{m+p=n}\langle\nabla\phi_\pm^{(m)},\nabla\phi_\pm^{(p)}\rangle-2\langle A,\nabla\phi_\pm^{(n-1)}\rangle=0, \quad n\geqslant3. \quad (4.10)$$

Then the remainder $q_\pm(x,\xi)=q_\pm^{(N)}(x,\xi)$ defined by (4.2) satisfies the equations

$$q_\pm^{(1)}=|\nabla\phi_\pm^{(1)}|^2-2\langle A,\nabla\phi_\pm^{(1)}\rangle+|A|^2,$$
$$q_\pm^{(N)}=\sum_{m+p\geqslant N+1}\langle\nabla\phi_\pm^{(m)},\nabla\phi_\pm^{(p)}\rangle-2\langle A,\nabla\phi_\pm^{(N)}\rangle,\quad N\geqslant 2. \tag{4.11}$$

Using Lemma 4.1, we derive inductively estimates for functions $\phi_\pm^{(n)}$, which gives also estimates for $\Phi_\pm$ and $q_\pm$.

Proposition 4.2: Let assumption (1.2) hold for some $\rho\in(0,1)$ such that ρ^{-1} is not integer and set $N=[\rho^{-1}]$. Then for all multi-indices α,β we have in the region $\pm\langle\hat{x},\hat{\xi}\rangle\geqslant\kappa$ (for any $\kappa>-1$),

$$|\partial_x^\alpha\partial_\xi^\beta\phi_\pm^{(n)}(x,\xi)|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{1-n\rho-|\alpha|}, \tag{4.12}$$

$$|\partial_x^\alpha\partial_\xi^\beta\Phi_\pm(x,\xi)|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{1-\rho-|\alpha|}, \tag{4.13}$$

$$|\partial_x^\alpha\partial_\xi^\beta q_\pm(x,\xi)|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-1-\epsilon-|\alpha|},\quad \epsilon>0. \tag{4.14}$$

Equality (4.4) and estimates (4.13) imply that the function $q_\pm$ on the right-hand side of (4.3) obeys the same bound (4.14) as $q_\pm$.

We note that all assertions of Proposition 4.2 remain true for $\rho=1$, except that in this case the function $\Phi_\pm(x,\xi)=\phi_\pm^{(1)}(x,\xi)$ may have a logarithmic growth as $|x|\to\infty$. Similarly, if ρ^{-1} is integer, then $N=\rho^{-1}$ and the function $\phi_\pm^{(N)}(x,\xi)$ has a logarithmic growth. The assumption that ρ^{-1} is not integer does not of course reduce the generality.

Let us finally give an explicit expression for $\Phi_\pm=\phi_\pm^{(1)}$ in the case $\rho>1/2$,

$$\Phi_\pm(x,\xi)=\pm 2^{-1}\int_0^\infty(V(x\pm t\xi)-V(\pm t\xi)-2\langle A(x\pm t\xi)-A(\pm t\xi),\xi\rangle)\mathrm{d}t. \tag{4.15}$$

V. WAVE OPERATORS

5.1. Here we consider wave operators for the pair of Hamiltonians $H_0=-\Delta$, $H=(i\nabla+A)^2+V$, acting in the space $\mathcal{H}=L_2(\mathbb{R}^d)$. We always assume condition (1.2) on A and V. Below we fix a spectral interval $\Lambda=[\lambda_0,\lambda_1]\subset\mathbb{R}_+=(0,\infty)$. Let $\Phi_\pm$ be the function constructed in Proposition 4.2. We define the identification $J_\pm$ by the formula

$$(J_\pm f)(x)=(2\pi)^{-d/2}\int_{\mathbb{R}^d}e^{i\langle x,\xi\rangle+i\Phi_\pm(x,\xi)}\zeta_\pm(x,\xi)\hat{f}(\xi)\mathrm{d}\xi, \tag{5.1}$$

where the cutoff function

$$\zeta_\pm(x,\xi)=\sigma_\pm(\langle\hat{\xi},\hat{x}\rangle)\,\eta(x)\psi(|\xi|^2),\quad \hat{\xi}=\xi/|\xi|,\quad \hat{x}=x/|x|. \tag{5.2}$$

Here $\sigma_\pm\in C^\infty$ is such that $\sigma_\pm(\tau)=1$ near ± 1 and $\sigma_\pm(\tau)=0$ near ∓ 1, so that it "kills" a conical neighborhood of the bad direction $\hat{x}=\mp\hat{\xi}$ where estimates (4.13) are violated. The function $\eta\in C^\infty(\mathbb{R}^d)$, such that $\eta(x)=0$ near zero and $\eta(x)=1$ for large $|x|$, is introduced only to get rid of the singularity of the function $\hat{x}$ at the point $x=0$. Finally, $\psi\in C_0^\infty(\mathbb{R}_+)$ and $\psi(\lambda)=1$ for $\lambda\in\Lambda$. Thus, our considerations are localized on a bounded disjoint from zero energy interval. Since the function $\Phi_\pm$ satisfies estimates (4.13) on the support of $\zeta_\pm$, the operator $J_\pm$ fits into the framework of PDO with oscillating symbols (see 2.1 in Sec. II). In particular, by Proposition 2.2, $J_\pm$ is a bounded operator on $\mathcal{H}$. Abusing somewhat notation, we write $J_\pm\in\mathcal{C}^0(\Phi_\pm)$.

Our first goal in this section is to show that the pair H_0, H, with identifications J_+ and J_-, fits into the framework of the theory of smooth perturbations, so the wave operators $W_\pm(H,H_0;J_\gamma)$ and $W_\pm(H_0,H;J_\gamma^*)$ exist both for $\gamma=``+"$ and $\gamma=``-"$. The structure of the operators $T_\pm = HJ_\pm - J_\pm H_0$ is described in the following.

Lemma 5.1: The operator $T_\pm$ admits the decomposition $T_\pm = T_\pm^{(s)} + T_\pm^{(r)}$ where $T_\pm^{(s)}, T_\pm^{(r)}$ are, respectively, PDO with symbols

$$t_\pm^{(s)}(x,\xi) = -2i\,\eta(x)e^{i\Phi_\pm(x,\xi)}\langle \xi, \nabla\sigma_\pm(\langle\hat{\xi},\hat{x}\rangle)\rangle\psi(|\xi|^2)$$

$$= -2i\,\eta(x)|x|^{-1}e^{i\Phi_\pm(x,\xi)}(1-\langle\hat{\xi},\hat{x}\rangle^2)\sigma_\pm'(\langle\hat{\xi},\hat{x}\rangle)|\xi|\psi(|\xi|^2) \in \mathcal{C}^{-1}(\Phi_\pm) \qquad (5.3)$$

and $t_\pm^{(r)} \in \mathcal{C}^{-1-\epsilon}(\Phi_\pm)$ for some $\epsilon>0$.

Proof: According to (4.3) and (5.1), we have that

$$(T_\pm f)(x) = (2\pi)^{-d/2}\int_{\mathbb{R}^d} e^{i\langle x,\xi\rangle + i\Phi_\pm(x,\xi)}\tau_\pm(x,\xi)\hat{f}(\xi)d\xi,$$

where

$$\tau_\pm(x,\xi) = q_\pm(x,\xi)\zeta_\pm(x,\xi) - 2i\langle \xi + \nabla\Phi_\pm(x,\xi) - A(x), \nabla\zeta_\pm(x,\xi)\rangle - \Delta\zeta_\pm(x,\xi). \qquad (5.4)$$

We single out here the term

$$\tau_\pm^{(s)}(x,\xi) = -2i\,\eta(x)\langle \xi, \nabla\sigma_\pm(\langle\hat{\xi},\hat{x}\rangle)\rangle\psi(|\xi|^2)$$

decaying as $|x|^{-1}$. According to (1.2), (4.13), and (4.14) all other terms belong to the class $\mathcal{S}^{-1-\epsilon}$. Thus, we define $t_\pm^{(s)}$ and $t_\pm^{(r)}$ by the equalities

$$t_\pm^{(s)}(x,\xi) = e^{i\Phi_\pm(x,\xi)}\tau_\pm^{(s)}(x,\xi), \quad \tau_\pm^{(r)}(x,\xi) = \tau_\pm(x,\xi) - \tau_\pm^{(s)}(x,\xi), \quad t_\pm^{(r)}(x,\xi) = e^{i\Phi_\pm(x,\xi)}\tau_\pm^{(r)}(x,\xi).$$

Then $t_\pm = t_\pm^{(s)} + t_\pm^{(r)}$. □

Our study of the singular part $T_\pm^{(s)}$ relies on

Lemma 5.2: Let T be a PDO with symbol

$$t(x,\xi) = g(x,\xi)w(\langle\hat{x},\hat{\xi}\rangle)\,\eta(x)\psi(|\xi|^2),$$

where $g \in \mathcal{C}^{-1}(\Phi), \Phi \in \mathcal{S}^{1-\rho}$, $\rho>0$, $w \in C^\infty$ and $w(\pm 1)=0$. Let $G_j, j=1,\dots,d$, be the operators defined in Proposition 3.5. Then T admits the representation (1.8), where $p=(1+\rho)/2$ and the operators $B^{(s)}, B^{(r)}$ are bounded.

Proof: Let $B^{(s)}$ and T_j, $j=1,\dots,d$, be the PDO with symbols

$$b^{(s)}(x,\xi) = \langle x\rangle\,|\xi|^{-2}(1-\langle\hat{\xi},\hat{x}\rangle^2)^{-1}t(x,\xi),$$

$$t_j(x,\xi) = \langle x\rangle^{-1}(\xi_j - |x|^{-2}x_j\langle\xi,x\rangle)^2 b^{(s)}(x,\xi).$$

The function $(1-\tau^2)^{-1}w(\tau)$ is C^∞, so that $b^{(s)} \in \mathcal{C}^0(\Phi)$ and hence, by Proposition 2.2, the operator $B^{(s)}$ is bounded. Since G_j is the PDO with symbol

$$g_j(x,\xi) = i\langle x\rangle^{-1/2}(\xi_j - |x|^{-2}x_j\langle\xi,x\rangle)$$

and $t_j = |g_j|^2 b^{(s)}$, we get, by Proposition 2.7 where $m=0$, $n=-1/2$, $r=1-\rho$, that the operator

$$B^{(r)} = \sum_{j=1}^d \langle x\rangle^p (G_j^* B^{(s)} G_j - T_j)\langle x\rangle^p$$

is bounded for $2p=\rho+1$. It remains to remark that $t=\Sigma_{j=1}^{d}t_j$. □

Now it is easy to obtain representation (1.8).

Proposition 5.3: The operators $T_\pm$ admit representation (1.8) for $p>1/2$ and some bounded operators $B_\pm^{(r)}, B_\pm^{(s)}$.

Proof: Let us proceed from Lemma 5.1. Since $t_\pm^{(s)}\in\mathcal{C}^{-1}(\Phi_\pm)$ and $\sigma'_\pm(\tau)=0$ in neighborhoods of the points -1 and 1, Lemma 5.2 can be directly applied to the operators $T_\pm^{(s)}$ for $p_s=(1+\rho)/2$. Since $t_\pm^{(r)}\in\mathcal{C}^{-1-\epsilon}(\Phi_\pm)$, the operator $\langle x\rangle^p T_\pm^{(r)}\langle x\rangle^p$ is bounded for $p_r=(1+\epsilon)/2$ by Proposition 2.6. This leads to (1.8) with $p=\min\{p_s,p_r\}>1/2$. □

It follows from Propositions 3.4 and 3.5 that the triples $\{H_0,H,J_+\}$ and $\{H_0,H,J_-\}$ satisfy the assumptions of Proposition 3.3. This yields

Theorem 5.4: *Suppose that A and V satisfy (1.2). Let $J_\pm=J_\pm(\zeta_\pm)$ be defined by (5.1). Then all wave operators*

$$W_\pm(H,H_0;J_\pm),\quad W_\pm(H_0,H;J_\pm^*) \tag{5.5}$$

and

$$W_\pm(H,H_0;J_\mp),\quad W_\pm(H_0,H;J_\mp^*) \tag{5.6}$$

exist. Operators (5.5) as well as (5.6) are adjoint to each other.

Corollary 5.5: The wave operators satisfy the intertwining property, that is

$$W_\pm(H,H_0;J_\gamma)E_0(X)=E(X)W_\pm(H,H_0;J_\gamma)$$

for all Borel sets $X\subset\mathbb{R}$ and both signs of γ. In particular,

$$\mathrm{Ran}(W_\pm(H,H_0;J_\gamma)E_0(X))\subset E(X)\mathcal{H}. \tag{5.7}$$

5.2. Now we are able to prove the isometricity and completeness of the wave operators $W_\pm(H,H_0;J_\pm)$.

Lemma 5.6: Let A be a PDO with symbol $a\in\mathcal{S}^0$ such that $a(x,\xi)=0$ in some conical neighborhood of the direction $\hat{x}=\pm\hat{\xi}$ at least for sufficiently large $|x|$. Then

$$s-\lim_{t\to\pm\infty}Ae^{-iH_0t}=0.$$

Proof: The stationary point $\xi=x/(2t)$ of the integral

$$(Ae^{-iH_0t}f)(x)=(2\pi)^{-d/2}\int_{\mathbb{R}^d}e^{i\langle\xi,x\rangle-i|\xi|^2t}a(x,\xi)\psi^2(|\xi|^2))\hat{f}(\xi)d\xi \tag{5.8}$$

does not belong to the support of the function $a(x,\xi)$ if $t\to\pm\infty$. Here we have taken into account that according to (3.3) values of $a(x,\xi)$ for bounded x can be neglected. Therefore supposing that $\hat{f}\in C_0^\infty(\mathbb{R}^d)$ and integrating by parts, we estimate integral (5.8) by $C_N(1+|x|+|t|)^{-N}$ for arbitrary N. □

Lemma 5.7: The following relations hold:

$$s-\lim_{t\to\pm\infty}(J_\pm^*J_\pm-\psi^2(H_0))e^{-iH_0t}=0, \tag{5.9}$$

$$s-\lim_{t\to\pm\infty}J_\mp^*J_\mp e^{-iH_0t}=0. \tag{5.10}$$

Proof: By Proposition 2.3, up to compact terms [which are negligible according to (3.3)], $A_1=J_\pm^*J_\pm-\psi^2(H_0)$ and $A_2=J_\mp^*J_\mp$ are PDO with symbols $\zeta_\pm^2(x,\xi)-\psi^2(|\xi|^2)$ and $\zeta_\mp^2(x,\xi)$, respectively. Therefore Lemma 5.6 can be applied to both operators A_1 and A_2. □

Proposition 5.8: Under the assumptions of Theorem 5.4, the operators $W_\pm(H,H_0;J_\pm)$ *are isometric on the subspace* $E_0(\Lambda)\mathcal{H}$ *and*

$$W_\pm(H,H_0;J_\mp)=0, \quad W_\pm(H_0,H;J_\mp^*)=0. \tag{5.11}$$

Proof: The results on the operators $W_\pm(H,H_0;J_\pm)$ and $W_\pm(H,H_0;J_\mp)$ are immediate consequences of (5.9) and (5.10), respectively. The second equality (5.11) is a consequence of the first because $W_\pm(H_0,H;J_\mp^*)=W_\pm^*(H,H_0;J_\mp)$. □

Proposition 5.9: The operators $W_\pm(H,H_0;J_\pm(\zeta_\pm))$ *do not depend on the choice of functions* $\sigma_\pm$ *and* η *in the definition (5.2) provided they satisfy the assumptions formulated at the beginning of this section.*

Proof: Let $\sigma_\pm$, η and $\tilde\sigma_\pm$, $\tilde\eta$ be a couple of such functions, and let $\zeta_\pm$, $\tilde\zeta$ be defined by (5.2). Set $L_\pm=J_\pm(\zeta_\pm)-J_\pm(\tilde\zeta_\pm)$. It suffices to check that $L_\pm e^{-H_0t}\to 0$ strongly as $t\to\pm\infty$ or that

$$s-\lim_{t\to\pm\infty} L_\pm^* L_\pm e^{-iH_0t}=0.$$

By Proposition 2.3, up to a compact term, $A_\pm=L_\pm^*L_\pm$ is the PDO with symbol $(\zeta_\pm(x,\xi)-\tilde\zeta_\pm(x,\xi))^2$, and hence Lemma 5.6 can be applied to both operators $A_\pm$. □

Our main result in this section is the following.

Theorem 5.10: *Under the assumptions of Theorem 5.4, the asymptotic completeness holds,*

$$\mathrm{Ran}(W_\pm(H,H_0;J_\pm)E_0(\Lambda))=E(\Lambda)\mathcal{H}.$$

Proof: By virtue of (5.7) for $X=\Lambda$, it suffices to check that for any $f\in E(\Lambda)\mathcal{H}$ there exists $f_0^{(\pm)}\in E_0(\Lambda)\mathcal{H}$ such that $f=W_\pm(H,H_0;J_\pm)f_0^{(\pm)}$ or, to put it differently, that

$$\lim_{t\to\pm\infty}\|e^{-iHt}f-J_\pm e^{-iH_0t}f_0^{(\pm)}\|=0. \tag{5.12}$$

Let us set $f_0^{(\pm)}=W_\pm(H_0,H;J_\pm^*)f$. Then, by the definition of this wave operator,

$$\lim_{t\to\pm\infty}\|J_\pm^* e^{-iHt}f-e^{-iH_0t}f_0^{(\pm)}\|=0,$$

and hence

$$\lim_{t\to\pm\infty}\|J_\pm J_\pm^* e^{-iHt}f-J_\pm e^{-iH_0t}f_0^{(\pm)}\|=0. \tag{5.13}$$

The second equality (5.11) implies that $\lim_{t\to\pm\infty}\|J_\mp^* e^{-iHt}f\|=0$ and, consequently,

$$\lim_{t\to\pm\infty}\|J_\mp J_\mp^* e^{-iHt}f\|=0. \tag{5.14}$$

By Proposition 2.3, up to a compact term, $J_\pm J_\pm^*+J_\mp J_\mp^*$ is the PDO with symbol $\zeta_\pm^2(x,\xi)+\zeta_\mp^2(x,\xi)$. According to Proposition 5.9, we may assume that the functions $\sigma_\pm$ in (5.2) satisfy the condition $\sigma_+^2(\tau)+\sigma_-^2(\tau)=1$. Then it follows from (5.13) and (5.14) that

$$\lim_{t\to\pm\infty}\|\psi^2(H_0)e^{-iHt}f-J_\pm e^{-iH_0t}f_0^{(\pm)}\|=0.$$

Since the operator $\psi^2(H)-\psi^2(H_0)$ is compact and $\psi^2(H)f=f$, this yields (5.12). □

5.3. Here we find the asymptotics of the function

$$(J_\pm e^{-iH_0t}f)(x)=(2\pi)^{-d/2}\int_{\mathbb{R}^d} e^{i\langle x,\xi\rangle+i\Phi_\pm(x,\xi)-i|\xi|^2t}\zeta_\pm(x,\xi)\hat{f}(\xi)d\xi,\quad f\in\mathcal{S}(\mathbb{R}^d),\quad (5.15)$$

as $t\to\pm\infty$. This will allow us to show that $W_\pm(H,H_0;J_\pm)$ coincide with wave operators defined (see Ref. 22) in terms of a time-dependent modification of the free dynamics e^{-iH_0t}.

Stationary points $\omega(x,t)$ of the phase function in (5.15) are determined by the equation

$$x+(\nabla_\xi\Phi_\pm)(x,\omega(x,t))-2\omega(x,t)t=0,\quad \pm t>0. \quad (5.16)$$

Due to the function $\zeta_\pm(x,\xi)$ we are interested only in points $\omega=\omega(x,t)$ such that $|\omega|^2\in\operatorname{supp}\psi$ and $\pm\langle\hat{\omega},\hat{x}\rangle\geqslant\kappa$ for some $\kappa>-1$. Using estimate (4.13) on $\nabla_\xi\Phi_\pm$, we see that for large $|t|$ equation (5.16) has a unique solution $\omega(x,t)$ and

$$\omega(x,t)=(2t)^{-1}x+O(|t|^{-\rho}) \quad (5.17)$$

uniformly in x such that

$$c_1|t|\leqslant|x|\leqslant c_2|t|,\quad 0<c_1<c_2<\infty. \quad (5.18)$$

Let us set

$$\Xi(x,t)=\langle\omega(x,t),x\rangle+\Phi_\pm(x,\omega(x,t))-|\omega(x,t)|^2t,\quad \pm t>0. \quad (5.19)$$

Applying the stationary phase method to integral (5.15) and taking into account the equality $\sigma_\pm(\langle\hat{\omega}(x,t),\hat{x}\rangle)=1$ for sufficiently large $\pm t$, we find that

$$(J_\pm e^{-iH_0t}f)(x)=e^{\mp\pi id/4}e^{i\Xi(x,t)}(2|t|)^{-d/2}\psi(|\omega(x,t)|^2)\hat{f}(\omega(x,t))+r_\pm(x,t), \quad (5.20)$$

where $r_\pm(x,t)$ tends to zero in $L_2(\mathbb{R}^d)$ as $t\to\pm\infty$. Using Eq. (5.16), we can rewrite expression (5.19) as

$$\Xi(x,t)=|x|^2/(4t)+\Omega(x,t), \quad (5.21)$$

where

$$\Omega(x,t)=\Phi_\pm(x,\omega(x,t))-(4t)^{-1}|(\nabla_\xi\Phi_\pm)(x,\omega(x,t))|^2,\quad \pm t>0. \quad (5.22)$$

It follows from (5.17) that in Eq. (5.20) $\omega(x,t)$ can be replaced by $x/(2t)$. This gives us the following lemma.

Lemma 5.11: Suppose that $|t|$ is sufficiently large. Let $\omega(x,t)$ satisfy equation (5.16), and let $\Xi(x,t)$ be defined by formulas (5.21), (5.22). Define a family of unitary operators by the equality

$$(U_0(t)f)(x)=e^{\mp\pi di/4}e^{i\Xi(x,t)}(2|t|)^{-d/2}\hat{f}((2t)^{-1}x),\quad \pm t>0. \quad (5.23)$$

Then for any function $\zeta_\pm$ defined by (5.2)

$$\lim_{t\to\pm\infty}\|J_\pm(\zeta_\pm)e^{-iH_0t}f-U_0(t)\psi(H_0)f\|.=0,\quad \forall f\in L_2(\mathbb{R}^d).$$

Lemma 5.11 allows us to reformulate the results of Theorems 5.4 and 5.10 as follows.

Proposition 5.12: Suppose that A and V satisfy (1.2). Define $U_0(t)$ by equality (5.23) for sufficiently large $|t|$. Then the wave operators

$$\mathbf{W}_\pm=s-\lim_{t\to\pm\infty}e^{iHt}U_0(t) \quad (5.24)$$

exist, are isometric and $\mathrm{Ran}\,\mathbf{W}_\pm = P\mathcal{H}$. *Furthermore, for any function (5.2) satisfying the assumptions formulated at the beginning of this section*

$$\mathbf{W}_\pm \psi(H_0) = W_\pm(H,H_0;J_\pm(\zeta_\pm)).$$

Proposition 5.12 shows again that the operators $W_\pm(H,H_0;J_\pm(\zeta_\pm))$ do not depend on the choice of functions $\sigma_\pm$ and η in the definition (5.2).

Remark 5.13: If $\Xi(x,t) = |x|^2/(4t)$ in (5.23), then

$$\lim_{t\to\pm\infty} \|e^{-iH_0t}f - U_0(t)f\| = 0, \quad \forall f \in L_2(\mathbb{R}^d),$$

and hence the wave operators (5.24) coincide with

$$W_\pm(H,H_0) = s - \lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t}.$$

If $\rho > 1/2$ then the function (5.22) can be replaced by a simpler expression. Recall first of all that in this case $\Phi_\pm$ is defined by formula (4.15). It follows from (4.13) and (5.17) that in the region (5.18) the functions

$$(4t)^{-1}|\nabla_\xi \Phi_\pm(x,\omega(x,t))|^2 = O(|t|^{1-2\rho}), \quad \Phi_\pm(x,\omega(x,t)) - \Phi_\pm(x,x/(2t)) = O(|t|^{1-2\rho})$$

tend to zero as $|t|\to\infty$. Thus, in place of (5.22) we can set $\Omega(x,t) = \Phi_\pm(x,x/(2t))$ which, according to (4.15), yields the expression

$$\Omega(x,t) = -t\int_0^1 V(sx)\mathrm{d}s + \int_0^1 \langle A(sx),x\rangle \mathrm{d}s.$$

This allows us to simplify considerably the expression for the operators $J_\pm$ in the case $V=0$.

Proposition 5.14: Suppose that $V=0$ *and A satisfies assumption* (1.2) *with* $\rho > 1/2$. *Set*

$$(Jf)(x) = \exp\left(i\int_0^1 \langle A(sx),x\rangle \mathrm{d}s \right) f(x).$$

Then the wave operators $W_\pm(H,H_0;J)$ *exist and coincide [up to the factor* $\psi(H_0)$*] with operators (1.3). If additionally the transversal gauge condition (1.9) is satisfied, then* $J=I$, *so that the same conclusions hold for the usual wave operators* $W_\pm(H,H_0)$.

Remark 5.15: All the results of this section remain true if $V = V_0 + V_1$ and $A = A_0 + A_1$ where V_0 and A_0 satisfy assumption (1.2) and

$$\begin{aligned} |V_1(x)| &\leqslant C(1+|x|)^{-\rho_1}, \\ |A_1(x)| + |\mathrm{div}\, A_1(x)| &\leqslant C(1+|x|)^{-\rho_1} \end{aligned} \tag{5.25}$$

for some $\rho_1 > 1$. In this case the identifications $J_\pm$ can be constructed in terms of the functions V_0 and A_0 only.

Indeed, by multiplication theorem for wave operators, it suffices to check that the usual wave operators for the pair $H(V_0,A_0)$, $H(V,A)$ exist and are complete. Under condition (5.25) this follows from the limiting absorption principle (Proposition 3.4) satisfied by both operators $H(V_0,A_0)$ and $H(V,A)$.

5.4. The direct definition of wave operators (5.24) in Ref. 22 used the function (5.21) with $\Omega(x,t)$ such that

$$\Omega_t(x,t)+t^{-1}\langle x,(\nabla\Omega)(x,t)\rangle+|(\nabla\Omega)(x,t)|^2-\langle A(x),x/t+2\nabla\Omega(x,t)\rangle+V(x)+|A(x)|^2$$
$$=O(|t|^{-1-\varepsilon}),\quad \varepsilon>0, \tag{5.26}$$

and

$$\partial_x^\alpha\Omega(x,t)=O(|t|^{1-\varepsilon-|\alpha|}),\quad |\alpha|=1,2, \tag{5.27}$$

in the region (5.18). These conditions allow to verify with the help of the Cook method the existence of wave operators (5.24). Of course, it is natural to expect that the functions $\Omega(x,t)$ defined in the previous subsection and in Ref. 22 coincide. Let us check it by a direct calculation.

Proposition 5.16: Let $\omega(x,t)$ satisfy equation (5.16) and let $\Omega(x,t)$ be defined by formula (5.22). Then $\Omega(x,t)$ satisfies the conditions (5.26) and (5.27).

Proof: To simplify notation, we omit variables (x,t) and indices "$\pm$." Differentiating (5.22), we find that

$$\Omega_t=(2t)^{-2}|\nabla_\xi\Phi|^2+\sum_j \Phi_{\xi_j}\Big(\partial\omega_j/\partial t-(2t)^{-1}\sum_k \Phi_{\xi_j\xi_k}\partial\omega_k/\partial t\Big), \tag{5.28}$$

$$\Omega_{x_i}=\Phi_{x_i}+\sum_j \Phi_{\xi_j}\Big(\partial\omega_j/\partial x_i-(2t)^{-1}\Big(\Phi_{\xi_jx_i}+\sum_k \Phi_{\xi_j\xi_k}\partial\omega_k/\partial x_i\Big)\Big). \tag{5.29}$$

Differentiating Eq. (5.16), we see that

$$\partial\omega_j/\partial t-(2t)^{-1}\sum_k \Phi_{\xi_j\xi_k}\partial\omega_k/\partial t=-2^{-1}t^{-2}x_j-2^{-1}t^{-2}\Phi_{\xi_j} \tag{5.30}$$

and

$$\partial\omega_j/\partial x_i-(2t)^{-1}\Big(\Phi_{\xi_jx_i}+\sum_k \Phi_{\xi_j\xi_k}\partial\omega_k/\partial x_i\Big)=(2t)^{-1}\delta_{ij}, \tag{5.31}$$

where $\delta_{ii}=1$ and $\delta_{ij}=0$ if $i\neq j$. Comparing (5.28) and (5.30) we obtain that

$$\Omega_t=-2^{-1}t^{-2}\langle x,\nabla_\xi\Phi\rangle-(2t)^{-2}|\nabla_\xi\Phi|^2.$$

Similarly, comparing (5.29) and (5.31), we obtain that

$$\nabla_x\Omega=\nabla_x\Phi+(2t)^{-1}\nabla_\xi\Phi. \tag{5.32}$$

These equalities imply that

$$\Omega_t+t^{-1}\langle x,\nabla_x\Omega\rangle+|\nabla_x\Omega|^2=t^{-1}\langle x+\nabla_\xi\Phi,\nabla_x\Phi\rangle+|\nabla_x\Phi|^2=2\langle\omega,\nabla_x\Phi\rangle+|\nabla_x\Phi|^2,$$

where at the last step we have again used Eq. (5.16). Comparing (5.16) and (5.32), we see also that

$$(2t)^{-1}x+\nabla_x\Omega=\omega+\nabla_x\Phi.$$

Thus, the sum (5.26) can be written as

$$2\langle\omega,\nabla_x\Phi\rangle+|\nabla_x\Phi|^2-2\langle A,\omega+\nabla_x\Phi\rangle+V+|A|^2.$$

It follows from Eq. (4.2) that this expression equals $q(x,\omega(x,t))$ which, by estimate (4.14), is of order $|t|^{-1-\epsilon}$ in the region considered. The condition (5.27) is a consequence of estimates (4.13) and (5.17). □

VI. THE SCATTERING MATRIX

6.1. It follows from Theorems 5.4, 5.10 and Proposition 5.8 that the scattering operator

$$\mathbf{S}=W_+^*(H,H_0;J_+)W_-(H,H_0;J_-)$$

commutes with H_0 and is unitary on the subspace $E_0(\Lambda)\mathcal{H}$. Thus, in the diagonal representation of H_0 (discussed in 2.2 of Sec. II) **S** reduces to the operator of multiplication by the operator function $S(\lambda):\mathfrak{N}\to\mathfrak{N}$ called the SM. It is defined for almost all $\lambda\in(0,\infty)$ and is unitary for almost all $\lambda\in\Lambda$. We suppose that $\lambda\in\Lambda$.

We need a stationary formula for the SM in the case when identifications J_+ and J_- for $t\to+\infty$ and $t\to-\infty$ are different. Below we always assume that the functions $\sigma_\pm$ in definition (5.1) of the operators $J_\pm$ obey the conditions

$$\sigma_+(\tau)=1 \quad \text{for} \quad \tau\in[-\varepsilon,1], \quad \sigma_+(\tau)=0 \quad \text{for} \quad \tau\in[-1,-2\varepsilon] \quad \text{and} \quad \sigma_-(\tau)=\sigma_+(-\tau) \tag{6.1}$$

for some $\varepsilon\in(0,1/2)$. Formally, the SM admits (see, e.g., Ref. 22) the representation (1.10) with $T_\pm=HJ_\pm-J_\pm H_0$. According to Lemma 5.1, $T_\pm=T_\pm^{(s)}+T_\pm^{(r)}$, where $T_\pm^{(s)}$ has symbol $t_\pm^{(s)}$ defined by (5.3) and $T_\pm^{(r)}\in\mathcal{C}^{-1-\epsilon}(\Phi_\pm)$, $\epsilon>0$. It follows from (5.10) that in our case $W_+(H_0,H_0;J_+^*J_-)=0$ and hence $\mathcal{W}(\lambda)=0$. We shall show that other terms in (1.10) satisfy Definition 2.11. Let us set

$$\begin{aligned} S_0(\lambda)&=-2\pi i\Gamma_0(\lambda)J_+^*T_-^{(s)}\Gamma_0^*(\lambda),\\ S_1(\lambda)&=-2\pi i\Gamma_0(\lambda)J_+^*T_-^{(r)}\Gamma_0^*(\lambda),\\ S_2(\lambda)&=2\pi i\Gamma_0(\lambda)T_+^*R(\lambda+i0)T_-\Gamma_0^*(\lambda). \end{aligned} \tag{6.2}$$

Then $S(\lambda)=S_0(\lambda)+S_1(\lambda)+S_2(\lambda)$. We emphasize that these operators depend on the choice of the cutoff functions $\sigma_\pm$ and η in the definition of $J_\pm$, but their sum does not depend on it (see Proposition 5.9).

For the study of the operator $S_2(\lambda)$, we have to consider previously the operator function

$$B(z)=\langle x\rangle^l T_+^*R(z)T_-\langle x\rangle^l, \quad l<(1+\epsilon)/2.$$

Lemma 6.1: The operator function $B(z):\mathcal{H}\to\mathcal{H}$ is bounded and continuous in norm with respect to z in the region $\operatorname{Re}z\in(\lambda_0,\infty),\lambda_0>0$, $\operatorname{Im}z\geqslant 0$.

Proof: Set $p=1+\epsilon-l$. Then $p>l$ and $p>1/2$. Clearly, $B=B_1+B_2+B_3$, where

$$\begin{aligned} B_1(z)&=(\langle x\rangle^p T_+^{(r)}\langle x\rangle^l)^*(\langle x\rangle^{-p}R(z)\langle x\rangle^{-p})(\langle x\rangle^p T_-^{(r)}\langle x\rangle^l),\\ B_2(z)&=(\langle x\rangle^p T_+^{(r)}\langle x\rangle^l)^*(\langle x\rangle^{-p}R(z)T_-^{(s)}\langle x\rangle^l)+(\langle x\rangle^l T_+^{(s)*}R(z)\langle x\rangle^{-p})(\langle x\rangle^p T_-^{(r)}\langle x\rangle^l),\\ B_3(z)&=\langle x\rangle^l T_+^{(s)*}R(z)T_-^{(s)}\langle x\rangle^l. \end{aligned} \tag{6.3}$$

Since $T_\pm^{(r)}\in\mathcal{C}^{-1-\epsilon}(\Phi_\pm)$, it follows from Proposition 2.6 that the operators $\langle x\rangle^p T_\pm^{(r)}\langle x\rangle^l$ are bounded. The second factor in (6.3) satisfies the assumptions of Proposition 3.4. According to (5.3) and (6.1), the operator $T_\pm^{(s)}\in\mathcal{C}^{-1}(\Phi_\pm)$ and its symbol is contained in the cone $\mp\langle\hat{x},\hat{\xi}\rangle\geqslant\varepsilon>0$. Therefore we can apply Proposition 3.6 to the operators

$$\langle x\rangle^{-p}R(z)T_-^{(s)}\langle x\rangle^l, \quad \langle x\rangle^l T_+^{(s)*}R(z)\langle x\rangle^{-p}$$

and Proposition 3.7 to the operator $B_3(z)$. □

Now it is easy to check the following.

Proposition 6.2: The operators $S_1(\lambda)$ *and* $S_2(\lambda)$ *are compact and norm continuous in* $\lambda > 0$.

Proof: Let $l \in (1/2,(1+\epsilon)/2)$. The operator $S_1(\lambda)$ factorizes as

$$S_1(\lambda) = 2\pi i(\Gamma_0(\lambda)\langle x\rangle^{-l})(\langle x\rangle^{-l} J_+ \langle x\rangle^{l})^*(\langle x\rangle^{l} T_-^{(r)} \langle x\rangle^{l})(\Gamma_0(\lambda)\langle x\rangle^{-l})^*,$$

where the operators $\langle x\rangle^{-l} J_+ \langle x\rangle^{l}$ and $\langle x\rangle^{l} T_-^{(r)} \langle x\rangle^{l}$ are bounded according to Proposition 2.6 and the operators $\Gamma_0(\lambda)\langle x\rangle^{-l}$ are compact and norm continuous according to Proposition 2.10. The operator

$$S_2(\lambda) = 2\pi i(\Gamma_0(\lambda)\langle x\rangle^{-l}) B(\lambda + i0)(\Gamma_0(\lambda)\langle x\rangle^{-l})^*$$

is well defined, compact and norm continuous according to Proposition 2.10 and Lemma 6.1. □

6.2. Let us now consider the singular term (6.2). The PDO $\mathbf{A}_0 = -2\pi i J_+^* T_-^{(s)}$ is defined by formula (2.6) with amplitude

$$\mathbf{a}_0(x,\xi,\xi') = -2\pi i \overline{j_+(x,\xi)} t_-^{(s)}(x,\xi').$$

Therefore, by Eqs. (5.1)–(5.3),

$$\mathbf{a}_0(x,\xi,\xi') = -4\pi e^{i\Theta(x,\xi,\xi')} \sigma_+(\langle \hat{x},\hat{\xi}\rangle)\langle \xi', \nabla\sigma_-(\langle \hat{x},\hat{\xi}'\rangle)\rangle \eta^2(x)\psi(|\xi|^2)\psi(|\xi'|^2), \tag{6.4}$$

where

$$\Theta(x,\xi,\xi') = \Phi_-(x,\xi') - \Phi_+(x,\xi) \tag{6.5}$$

and the functions $\Phi_\pm$ are defined in Proposition 4.2. Estimates (4.13) imply the following.

Lemma 6.3: The function $\Theta(x,\xi,\xi')$ *satisfies the estimates*

$$|\partial_x^\alpha \partial_{\xi,\xi'}^\beta \Theta(x,\xi,\xi')| \leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{1-\rho-|\alpha|} \tag{6.6}$$

in the region $\langle \hat{x},\hat{\xi}\rangle \geqslant \kappa$, $-\langle \hat{x},\hat{\xi}'\rangle \geqslant \kappa$ *for any* $\kappa > -1$ *and all* α,β.

Since Θ satisfies the estimates of the class $\mathcal{S}^{1-\rho}$ on the support of $\mathbf{a}_0$, (6.4) has the form (2.7) and hence the operator $\mathbf{A}_0$ fits into the framework of PDO with oscillating amplitudes (see 2.1 in Sec. II). Abusing somewhat notation, we say that $\mathbf{A}_0$ belongs to the class $\mathcal{C}^{-1}(\Theta)$. Moreover, due to the function $\nabla\sigma_-(\langle \hat{x},\hat{\xi}'\rangle)$, the operator $\mathbf{A}_0$ satisfies the assumptions of Proposition 2.14. Below we use the notation and the chart coordinates $(\omega_0,\varkappa)$ introduced in 2.2 in Sec. II. Thus, we have the following.

Proposition 6.4: The operator $S_0(\lambda) = \mathbf{A}_0^\flat(\lambda)$ *is well defined in the sense of Definition 2.11 for all* $\lambda > 0$. *Moreover, in the chart coordinates* $(\omega_0,\varkappa)$, $\mathbf{A}_0^\flat(\lambda)$ *is the PDO with amplitude*

$$\mathbf{a}_0^\flat(y,\zeta,\zeta';\lambda) = (2\pi k)^{-1}\alpha(\zeta,\zeta')\int_{-\infty}^{\infty} \mathbf{a}_0(x,k\omega,k\omega')\,dz,$$

where α *is the function (2.14),* $\zeta = \varkappa(\omega), \zeta' = \varkappa(\omega')$ *and*

$$x = (\omega+\omega')z - y/k, \quad \langle y,\omega_0\rangle = 0. \tag{6.7}$$

It follows from Propositions 2.12 and 2.14 that $(S_0(\lambda)g_1,g_2)$ is a smooth function of λ for $g_j \in C^\infty(\mathbb{S}^{d-1})$. Below we shall see that the operator $S_0(\lambda)$ is bounded in the space $\mathfrak{N}$.

Our next goal is to find a simple expression for a genuinely noncompact part of the operator $S_0(\lambda)$. First, we transform expression (6.4) for $\mathbf{a}_0$ to a more convenient form.

Proposition 6.5: Let $\mathbf{A}_1$ *be the PDO with amplitude*

$$\mathbf{a}_1(x,\xi,\xi')=-2\pi e^{i\Theta(x,\xi,\xi')}\sigma_+(\langle\hat{x},\hat{\xi}\rangle)\langle\xi+\xi',\nabla\sigma_-(\langle\hat{x},\hat{\xi}'\rangle)\rangle\,\eta^2(x)\,\psi(|\xi|^2)\psi(|\xi'|^2), \quad (6.8)$$

where Θ is given by (6.5). Then the operator $\mathbf{A}_1^\flat(\lambda)$ exists and the operator $S_0(\lambda)-\mathbf{A}_1^\flat(\lambda)$ is compact on $\mathfrak{N}$. Moreover, in the chart coordinates $(\omega_0,\varkappa)$, $\mathbf{A}_1^\flat(\lambda)$ is the PDO with amplitude

$$\mathbf{a}_1^\flat(y,\zeta,\zeta';\lambda)=-\alpha(\zeta,\zeta')\int_0^\infty e^{i\Theta(x,k\omega,k\omega')}\langle\omega+\omega',\nabla\sigma_-(\langle\hat{x},\omega'\rangle)\rangle\,\eta^2(x)\mathrm{d}z, \quad (6.9)$$

where x and y,z are related by formula (6.7).

Proof: Comparing (6.4) and (6.8), we see that the difference $\mathbf{B}=\mathbf{A}_0-\mathbf{A}_1$ is a PDO with amplitude

$$\mathbf{b}(x,\xi,\xi')=-2\pi e^{i\Theta(x,\xi,\xi')}\sigma_+(\langle\hat{x},\hat{\xi}\rangle)\langle\xi'-\xi,\nabla\sigma_-(\langle\hat{x},\hat{\xi}'\rangle)\rangle\,\eta^2(x)\,\psi(|\xi|^2)\psi(|\xi'|^2).$$

Since $\mathbf{b}(x,\xi,\xi)=0$, it follows from Proposition 2.8 that the operator $\mathbf{B}$ belongs to the class $\mathcal{C}^{-1-\rho}(\tilde{\Theta})$ for some $\tilde{\Theta}\in\mathcal{S}^{1-\rho}$. Thus, by Proposition 2.13, $\mathbf{B}^\flat(\lambda)$ is a compact operator on $\mathfrak{N}$.

It follows from conditions (6.1) that for ω' sufficiently close to ω the function $\sigma_+(\langle\hat{x},\omega\rangle)=1$ on the support of $\nabla\sigma_-(\langle\hat{x},\omega'\rangle)$. Hence σ_+ may be omitted in (6.8). We also take into account that, due to $\nabla\sigma_-(\langle\hat{x},\omega'\rangle)$, the function $\mathbf{a}_1((\omega+\omega')z-y/k,k\omega,k\omega')$ is supported in the region $z\geqslant 0$ and $\psi(\lambda)=1$ for $\lambda\in\Lambda$. Thus, applying Proposition 2.14 to the PDO $\mathbf{A}_1$, we obtain formula (6.9). □

An obvious drawback of this assertion is that the amplitude $\mathbf{a}_1^\flat$ contains the cutoff function σ_- although the SM does not depend on it.

6.3. Let us show that, up to a compact term, the operator $\mathbf{A}_1^\flat(\lambda)$ does not actually depend on σ_-. Below we always work in fixed chart coordinates $(\omega_0,\varkappa)$ and denote by χ a function from the class $C_0(\Omega)$. Recall, that for fixed $\omega,\omega'\in\Omega(\omega_0,\gamma)$, we always use in $\mathbb{R}^d$ the coordinates $(y,z)\in\mathbb{R}^{d-1}\times\mathbb{R}$ defined by (6.7). Then

$$k\langle\omega'-\omega,x\rangle=\langle\omega-\omega',y\rangle=\langle\zeta-\zeta',y\rangle, \quad (6.10)$$

$$\mathrm{d}x=k^{-d+1}\langle\omega+\omega',\omega_0\rangle\mathrm{d}z\,\mathrm{d}y \quad (6.11)$$

and

$$\langle\omega+\omega',\nabla f(x)\rangle=\partial_z f(x)$$

for any differentiable function f.

Integrating by parts in (6.9) and taking into account that $\sigma_-(\langle\hat{x},\omega'\rangle)$ varies from 1 to 0 as z varies from 0 to ∞, we get that

$$\mathbf{a}_1^\flat(y,\zeta,\zeta';\lambda)=\alpha(\zeta,\zeta')e^{i\Theta(-y/k,k\omega,k\omega')}\eta^2(-y/k)+\mathbf{b}(y,\zeta,\zeta';\lambda), \quad (6.12)$$

where

$$\mathbf{b}(y,\zeta,\zeta';\lambda)=\alpha(\zeta,\zeta')\int_0^\infty e^{i\Theta(x,k\omega,k\omega')}(i\partial_z\Theta(x,k\omega,k\omega')\,\eta^2(x)+\partial_z\eta^2(x))\sigma_-(\langle\hat{x},\omega'\rangle)\mathrm{d}z. \quad (6.13)$$

By Lemma 6.3 and Proposition 2.9, the first term in the right-hand side of (6.12) is the amplitude of a bounded operator in $L_2(\mathbb{S}^{d-1})$. We shall show that $\mathbf{b}$ is the amplitude of a compact operator $\mathbf{B}$. This is obvious for the part of $\mathbf{b}$ which contains $\partial_z\eta^2$ since it is compactly supported in y. To consider the part of $\mathbf{b}$ which contains $\partial_z\Theta$, we use the following.

Lemma 6.6: The function (6.5) satisfies the equality

$$\langle\xi+\xi',\nabla\Theta(x,\xi,\xi')\rangle=\langle\nabla G(x,\xi,\xi'),F(x,\xi,\xi')\rangle+q_0(x,\xi,\xi'), \quad (6.14)$$

where the functions G,F and q_0 are defined by

$$G(x,\xi,\xi')=\langle \xi'-\xi,x\rangle+\Theta(x,\xi,\xi'),$$

$$F(x,\xi,\xi')=2A(x)-\nabla(\Phi_-(x,\xi')+\Phi_+(x,\xi)), \tag{6.15}$$

$$q_0(x,\xi,\xi')=q_-(x,\xi')-q_+(x,\xi)$$

and $q_\pm$ are functions (4.2). The functions F and q_0 satisfy in the region $\langle \hat{x},\hat{\xi}\rangle \geqslant \kappa$, $-\langle \hat{x},\hat{\xi}'\rangle \geqslant \kappa$, for any $\kappa>-1$ and all α,β, the estimates

$$|\partial_x^\alpha \partial_{\xi,\xi'}^\beta F(x,\xi,\xi')|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-\rho-|\alpha|}, \tag{6.16}$$

$$|\partial_x^\alpha \partial_{\xi,\xi'}^\beta q_0(x,\xi,\xi')|\leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-1-\epsilon-|\alpha|}, \quad \epsilon>0. \tag{6.17}$$

Proof: One proceeds from eikonal equation (4.2) for $\Phi_+(x,\xi)$ and $\Phi_-(x,\xi')$ and takes their difference. This yields the equality (6.14). Estimates (6.16) and (6.17) are direct consequences of (4.13) and (4.14), respectively. □

Let us set expression (6.14) into (6.13) and consider the amplitude

$$\mathbf{b}_0(y,\zeta,\zeta';\lambda)=i\alpha(\zeta,\zeta')k^{-1}\int_0^\infty e^{i\Theta(x,k\omega,k\omega')}\langle \nabla G(x,k\omega,k\omega'),F(x,k\omega,k\omega')\rangle\,\eta^2(x)\mathrm{d}z \tag{6.18}$$

corresponding to the first term on the right-hand side of (6.14).

Lemma 6.7: The PDO $\mathbf{B}_0$ with amplitude (6.18) admits the representation $\mathbf{B}_0=\mathbf{B}_1+\mathbf{B}_2$ where $\mathbf{B}_1$, $\mathbf{B}_2$ are PDO with amplitudes

$$\mathbf{b}_1(y,\zeta,\zeta';\lambda)=-k^{-1}\alpha_1(\zeta,\zeta')e^{i\Theta(-y/k,k\omega,k\omega')}\langle \omega_0,F(-y/k,k\omega,k\omega')\rangle\,\eta^2(-y/k), \tag{6.19}$$

$$\mathbf{b}_2(y,\zeta,\zeta';\lambda)=\alpha(\zeta,\zeta')\int_0^\infty e^{i\Theta(x,k\omega,k\omega')}q(x,k\omega,k\omega')\mathrm{d}z. \tag{6.20}$$

Here

$$\alpha_1(\zeta,\zeta')=\langle \omega+\omega',\omega_0\rangle^{-1}\alpha(\zeta,\zeta')$$

and

$$q(x,\xi,\xi')=-k^{-1}\,\mathrm{div}_x(F(x,\xi,\xi')\sigma_-(\langle \hat{x},\hat{\xi}'\rangle)\,\eta^2(x)). \tag{6.21}$$

Proof: According to (6.10), (6.11), the PDO $\mathbf{B}_0$ has integral kernel

$$\begin{aligned}p_0(\zeta,\zeta';\lambda)&=(2\pi)^{-\mathrm{d}+1}\int_{\mathbb{R}^{\mathrm{d}-1}}e^{i\langle \zeta-\zeta',y\rangle}\mathbf{b}_0(y,\zeta,\zeta';\lambda)\mathrm{d}y\\&=i(2\pi)^{-\mathrm{d}+1}k^{\mathrm{d}-2}\alpha_1(\zeta,\zeta')\int_{\langle x,\omega_0\rangle\geqslant 0}\exp(iG(x,k\omega,k\omega'))\\&\quad\times\langle \nabla G(x,k\omega,k\omega'),F(x,k\omega,k\omega')\rangle\sigma_-(\langle \hat{x},\omega'\rangle)\,\eta^2(x)\mathrm{d}x.\end{aligned}$$

Integrating here by parts, we find that $p_0=p_1+p_2$ where

$$p_1(\zeta,\zeta';\lambda)=-\alpha_1(\zeta,\zeta')(2\pi)^{-d+1}k^{-1}\int_{\mathbb{R}^{d-1}}e^{iG(-y/k,k\omega,k\omega')}$$
$$\times\langle\omega_0,F(-y/k,k\omega,k\omega')\rangle\eta^2(-y/k)dy,$$

$$p_2(\zeta,\zeta';\lambda)=\alpha_1(\zeta,\zeta')(2\pi)^{-d+1}k^{d-1}\int_{\langle x,\omega_0\rangle\geqslant 0}e^{iG(x,k\omega,k\omega')}q(x,k\omega,k\omega')dx.$$

The amplitudes of PDO with kernels p_1,p_2 equal $\mathbf{b}_1,\mathbf{b}_2$, respectively. □

Let us consider the operators $\mathbf{B}_1$ and $\mathbf{B}_2$ separately.

Lemma 6.8: The PDO $\mathbf{B}_1$ *with amplitude (6.19) belongs to the class* $\mathcal{C}^{-\rho}(\Theta_0)$, *where*

$$\Theta_0(y,\zeta,\zeta';\lambda)=\Theta_0(-k^{-1}y,k\varkappa(\zeta),k\varkappa(\zeta'))$$

is given by (6.5). In particular, $\chi\mathbf{B}_1\chi$ *is a compact operator in* $L_2(\Sigma)$.

Proof: Since $\langle y,\omega_0\rangle=0$, we have that $|\langle\hat{y},\omega\rangle|\leqslant\varepsilon<1$ and $|\langle\hat{y},\omega'\rangle|\leqslant\varepsilon<1$ for $\omega,\omega'\in\Omega$. According to (6.6), (6.16) this implies that functions Θ and F in (6.19) belong to the classes $\mathcal{S}^{1-\rho}(\mathbb{R}^{d-1})$ and $\mathcal{S}^{-\rho}(\mathbb{R}^{d-1})$, respectively. Thus, $\mathbf{b}_1$ belongs to the class $\mathcal{C}^{-\rho}(\Theta_0)$, and hence $\mathbf{B}_1$ is a compact operator by Proposition 2.9. □

Lemma 6.9: Suppose that a function $q(x,\xi,\xi')$ *equals zero in a conical neighborhood of the set* $\hat{x}=\hat{\xi}'$ *and* $q(x,\xi,\xi')$ *satisfies the estimates (6.17) for* $\langle\hat{x},\hat{\xi}\rangle\geqslant\kappa>-1$ *and all* α,β. *Let* $\mathbf{B}_2$ *be PDO with amplitude (6.20). Then the operator* $\chi\mathbf{B}_2\chi$ *is compact in* $L_2(\Sigma)$.

Proof: Let $\vartheta_0\in C^\infty(\mathbb{R})$ be such that $\vartheta_0(z)=0$ for $z\leqslant 1/2$ and $\vartheta_0(z)=1$ for $z\geqslant 1$ and $\vartheta_1=1-\vartheta_0$. We first consider the operator $\mathbf{B}_{2,0}$ with amplitude

$$\mathbf{b}_{2,0}(y,\zeta,\zeta';\lambda)=\alpha(\zeta,\zeta')\int_{-\infty}^{\infty}e^{i\Theta(x,k\omega,k\omega')}q(x,k\omega,k\omega')\vartheta_0(\langle\omega+\omega',\omega_0\rangle z)dz. \qquad (6.22)$$

Let $f\in C^\infty(\mathbb{R}^d)$, $f(\xi)=1$ for $\xi\in\Omega$ and $f(\xi)=0$ off a small neighborhood of Ω. We introduce an auxiliary PDO $\mathbf{G}$ with amplitude

$$\mathbf{g}(x,\xi,\xi')=f(\xi)f(\xi')\exp(i\Theta(x,\xi,\xi'))q(x,\xi,\xi')\vartheta_0(\langle x,\omega_0\rangle).$$

The function $q\vartheta_0$ equals zero in conical neighborhoods of the sets $\hat{x}=\hat{\xi}'$ and $\hat{x}=-\hat{\xi}$, so that, by Lemma 6.3, Θ satisfies estimates (6.6) on the support of $q\vartheta_0$. Thus, $\mathbf{g}\in C^{-1-\epsilon}(\Theta)$. Comparing (2.13) and (6.22), we see that $\mathbf{B}_{2,0}(\lambda)=2\pi k\mathbf{G}^\flat(\lambda)$. Therefore the operator $\mathbf{B}_{2,0}$ is compact by Proposition 2.13.

Next we consider the PDO $\mathbf{B}_{2,1}$ with amplitude

$$\mathbf{b}_{2,1}(y,\zeta,\zeta';\lambda)=\alpha(\zeta,\zeta')e^{i\Theta(-y/k,k\omega,k\omega')}\int_0^{\infty}e^{i(\Theta(x,k\omega,k\omega')-\Theta(-y/k,k\omega,k\omega'))}q(x,k\omega,k\omega')$$
$$\times\vartheta_1(\langle\omega+\omega',\omega_0\rangle z)dz,$$

where, due to the function ϑ_1, the integral is actually taken over a finite interval. Therefore it follows from Lemma 6.3 that for $\omega,\omega'\in\Omega$ and sufficiently large $|y|$,

$$|\partial_y^\alpha\partial_{\zeta,\zeta'}^\beta e^{i(\Theta(x,k\omega,k\omega')-\Theta(-y/k,k\omega,k\omega'))}|=O(\langle y\rangle^{-\rho-|\alpha|}).$$

Taking also into account that $q\vartheta_1$ satisfies estimates (6.17), we obtain that $\mathbf{b}_{2,1}\in\mathcal{C}^{-1-\rho-\epsilon}(\Theta_0)$. Hence the operator $\chi\mathbf{B}_{2,1}\chi$ is also compact. □

Since the function (6.21) satisfies the assumptions of this lemma, it applies directly to the operator with amplitude (6.20). Moreover, the same conclusion is true if the role of $q(x,\xi,\xi')$ is played by the function $q_0(x,\xi,\xi')\sigma_-(\langle\hat{x},\omega'\rangle)$, where q_0 is defined by (6.15). This yields

Proposition 6.10: The PDO **B** *with amplitude (6.13) is compact in* $L_2(\Sigma)$.

Thus, we have verified that all terms in the right-hand side of (1.10) are well defined as bounded operators in the space $\mathfrak{N}$. As shown in Ref. 22, this justifies the representation (1.10) for the SM $S(\lambda)$. Since $(S(\lambda)g_1,g_2)$ is a smooth function of λ for $g_j\in C^\infty(\mathbb{S}^{d-1})$, it follows from unitarity of $S(\lambda)$ that actually $S(\lambda)$ is a strongly continuous operator-function of $\lambda>0$. Moreover, comparing Propositions 6.5 and 6.10, we see that, modulo compact operators, the SM $S(\lambda)$ can be considered as a PDO with amplitude given by the first term on the right-hand side of (6.12). Finally, neglecting again compact operators, we can omit in this term $\alpha(\zeta,\zeta')$ because $\alpha(\zeta,\zeta)=1$ and $\eta^2(-y/k)$ because it is 1 for sufficiently large $|y|$.

Let us summarize the results obtained in the following theorem.

Theorem 6.11: *Let condition (1.2) hold and let* $J_\pm$ *be defined by (5.1) where the function (5.2) satisfies the assumption (6.1). Then the SM* $S(\lambda)$ *for the pair* H_0, H *with identifications* $J_\pm$ *admits representation (1.10) where* $\mathcal{W}(\lambda)=0$. *The function* $S(\lambda):\mathfrak{N}\to\mathfrak{N}$ *is strongly continuous in* $\lambda>0$. *If* χ_1 *and* χ_2 *are multiplications by* $C^\infty(\mathbb{S}^{d-1})$ *functions with disjoint supports, then the operator* $\chi_1 S(\lambda)\chi_2$ *is compact. Finally, up to a compact term,* $S(\lambda)$ *is the PDO on* $\mathbb{S}^{d-1}$ *with amplitude given in arbitrary chart coordinates* $(\omega_0,\varkappa)$ *by the formula*

$$\mathbf{s}(y,\zeta,\zeta';\lambda)=\exp(i\Theta(-\lambda^{-1/2}y,\lambda^{1/2}\omega,\lambda^{1/2}\omega')). \tag{6.23}$$

6.4. Using Theorem 6.11, we can now describe the spectrum of the SM. Recall that the function $\Theta(x,\xi,\xi')$ is defined by formula (6.5) where $\Phi_\pm$ are constructed in Proposition 4.2. Let us consider the first approximation $\mathbf{V}(x,\xi)=\phi_-^{(1)}(x,\xi)-\phi_+^{(1)}(x,\xi)$ to the function $\Theta(x,\xi,\xi)$. According to (4.15)

$$\mathbf{V}(x,\xi)=2^{-1}\int_{-\infty}^{\infty}(V(t\xi)-V(x+t\xi)+2\langle A(x+t\xi)-A(t\xi),\xi\rangle)\mathrm{d}t. \tag{6.24}$$

Note that the function $\mathbf{V}$ does not depend on the projection of x on the direction of ξ. Typically, for asymptotically homogeneous functions $V(x)$ and $A(x)$ of order $-\rho$, the function $\mathbf{V}(x,\xi)$ is asymptotically homogeneous function of x as $|x|\to\infty$ of order $1-\rho$ if $\rho\in(0,1)$ and it has a logarithmic growth if $\rho=1$.

Theorem 6.12: *Let condition (1.2) hold and suppose that for some* $x_0\neq 0$, $\omega_0\in\mathbb{S}^{d-1}$, $\langle x_0,\omega_0\rangle=0$, *and* $k>0$ *the function (6.24) satisfies the conditions*

$$\limsup_{\tau\to\infty}\mathbf{V}(\tau x_0,k\omega_0)=\infty \quad\text{or}\quad \liminf_{\tau\to\infty}\mathbf{V}(\tau x_0,k\omega_0)=-\infty \tag{6.25}$$

if $\rho>1/2$ *or*

$$|\mathbf{V}(\tau x_0,k\omega_0))|\geqslant c\tau^{1-\rho},\quad |\nabla\mathbf{V}(\tau x_0,k\omega_0))|\geqslant c\tau^{-\rho},\quad c>0, \tag{6.26}$$

for sufficiently large $\tau>0$ *if* $\rho\in(0,1/2]$. *Then the spectrum of the SM* $S(\lambda)$ *coincides for* $\lambda=k^2$ *with the unit circle* $\mathbb{T}$.

Proof: It follows from definition (4.7) and estimates (4.12) for $n\geqslant 2$ that

$$|\partial_x^\alpha(\Theta(x,\xi,\xi)-\mathbf{V}(x,\xi))|\leqslant C_\alpha(1+|x|)^{1-2\rho-|\alpha|},\quad \langle x,\xi\rangle=0,\quad |\alpha|=0,1.$$

Thus, the function $\Theta(\tau x_0,k\omega_0,k\omega_0)$ where $\langle x_0,\omega_0\rangle=0$ also satisfies conditions (6.25) or (6.26). Let us consider the chart diffeomormism $(\omega_0,\varkappa)$ and the PDO $S_0^\varkappa(\lambda)$ with amplitude (6.23). We apply Proposition 2.16 to the operator $\chi_0^\varkappa S_0^\varkappa(\lambda)\chi_0^\varkappa$ where $\chi_0^\varkappa\in C_0^\infty(\Sigma)$ and $\chi_0^\varkappa(\zeta)=1$ in a neighborhood of the point $\zeta_0=0$. Conditions (2.16) [or (2.18)] for $\zeta_0=0$ and $y_0=-x_0$ are satisfied according to (6.26) [or (6.25)]. Therefore for each $\mu\in\mathbb{T}$ there exists a Weyl sequence u_n such that $\|u_n\|=1$, $u_n\to 0$ weakly and

$$\chi_0^\varkappa S_0^\varkappa(\lambda)\chi_0^\varkappa u_n-\mu u_n\to 0$$

~strongly as $n\to\infty$. Moreover, we may assume that supports of u_n are contained in an arbitrary neighborhood of the point $0\in\Pi_{\omega_0}$. Let the operator Z be defined by formula (2.10) and $\chi_0(\omega)=\chi_0^{\varkappa}(\zeta)$. It follows from Theorem 6.11 that $f_n=Z^*u_n$ is a Weyl sequence for the operator $\chi_0 S(\lambda)\chi_0$. Let $\chi_1\in C^\infty(\mathbb{S}^{d-1})$ be supported on the set where $\chi_0(\omega)=1$. Then supp $(1-\chi_0)\cap\operatorname{supp}\chi_1=\varnothing$ and hence, by Theorem 6.11, the operator $(1-\chi_0)S(\lambda)\chi_1$ is compact. Without losing generality, we assume that $\chi_0 f_n=\chi_1 f_n=f_n$. Since both terms on the right-hand side of the estimate

$$\|S(\lambda)f_n-\mu f_n\|\leqslant\|\chi_0 S(\lambda)\chi_0 f_n-\mu f_n\|+\|(1-\chi_0)S(\lambda)\chi_1 f_n\|$$

tend to zero as $n\to\infty$, the spectrum of the SM $S(\lambda)$ covers the unit circle. Finally, we take into account that $S(\lambda)$ is unitary, so that its spectrum actually coincides with $\mathbb{T}$. □

We emphasize that, at least in the cases $V=0$ or $A=0$, the conditions (6.25) and (6.26) are fulfilled for all points k at the same time.

According to Proposition 5.14 and Theorem 6.12, the following result is true for the SM defined in terms of the usual wave operators.

Proposition 6.13: Let $V=0$ and let A satisfy estimates (1.2) for $\rho\in(1/2,1)$ and the transversal condition (1.9) (at least for large $|x|$). Suppose that the corresponding function

$$\mathbf{V}(x,\xi)=\int_{-\infty}^{\infty}\langle A(x+t\xi),\xi\rangle\,dt$$

satisfies condition (6.25) for some point (x_0,ω_0), $\omega_0\in\mathbb{S}^{d-1}$, $\langle x_0,\omega_0\rangle=0$. Then the spectrum of the SM $S(\lambda)$ covers the unit circle $\mathbb{T}$ for all $\lambda>0$.

As an example of a potential satisfying the assumptions of Proposition 6.13 we note (for $d=2$) the potential $A(x)=\gamma|x|^{-1-\rho}(-x_2,x_1)$, $|x|\geqslant R$, $\rho\in(1/2,1)$, $\gamma\neq 0$. In this case for any $(x,\xi)\in\mathbb{R}^{2d}$, $\langle x,\xi\rangle=0$, $|x|\geqslant R$,

$$\mathbf{V}(x,\xi)=\pm\gamma v_0|x|^{1-\rho},\quad v_0=\int_{-\infty}^{\infty}\langle u\rangle^{-1-\rho}du>0,$$

if $\hat{\xi}$ is obtained from $\hat{x}$ by rotation at the angle $\pm\pi/2$. Thus, condition (6.25) is satisfied.

Of course, Proposition 6.13 remains true for all $\rho>0$, but, if $\rho\leqslant 1/2$, then the SM is defined in terms of modified wave operators and condition (6.25) should be replaced by (6.26). On the contrary, if $\rho=1$, then under transversal condition (1.9) $\mathbf{V}(x,\xi)$ has typically the finite limits as $|x|\to\infty$, so that the essential spectrum of $S(\lambda)$ might be a subset of $\mathbb{T}$. This is the case for the Aharonov–Bohm potential $A(x)=\gamma|x|^{-2}(-x_2,x_1)$; for more general potentials of this type, see Ref. 16.

Proposition 6.13 contradicts a preceding result of Nicoleau. It is claimed in Ref. 12 that under the assumptions of Proposition 6.13 the operator $S(\lambda)-I$ is compact. This is incompatible with the assertion that the essential spectrum of $S(\lambda)$ covers the unit circle.

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General realization of $N=4$ supersymmetric quantum mechanics and its applications

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(Received 24 February 2002; accepted 23 March 2003)

Based upon the general supercharges which involve not only generators C_j of the Clifford algebra C(4,0) with positive metric, but also operators of third order, $C_jC_kC_l$, the general form of $N=4$ supersymmetric quantum mechanics (SSQM), which brings out the richer structures, is realized. Then from them, a one-dimensional physical realization and a new multidimensional physical realization of $N=4$ SSQM are respectively obtained by solving the constraint conditions. As applications, $N=4$ dynamical superconformal symmetries, which possess both the $N=4$ supersymmetries and the usual dynamical conformal symmetries, are studied in detail by considering two simple superpotentials k/x and ωx, and their corresponding superalgebraic structures, which are spanned by eight fermionic generators and six bosonic generators, are established as well. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1578531]

I. INTRODUCTION

Since the idea of supersymmetry was applied to quantum mechanical systems[1,2] to discover dynamical supersymmetry in ordinary quantum mechanics in order to explain the degeneracies of energy spectra extensively studies have been undertaken over the last twenty years in many aspects such as atomic physics,[3–5] nuclear physics,[6] many-body systems,[7,8] and so on. According to Witten,[2] a supersymmetric quantum mechanical system is characterized by the existence of N Hermitian supercharges Q^α which, together with the supersymmetric Hamiltonian H of this system, satisfy the following superalgebraic structure:

$$\begin{aligned} &\{Q^\alpha,\ Q^\beta\}=2\,\delta_{\alpha\beta}H, \quad \alpha,\beta=1,2,\ldots,N,\\ &(Q^\alpha)^\dagger=Q^\alpha, \quad [H,\ Q^\alpha]=0, \end{aligned} \tag{1}$$

where $\{,\}$ and $[,]$ denote an anticommutator and a commutator, respectively. We call Eq. (1) a supersymmetric quantum mechanical algebra, denoted by SS(N). When $N=2$, the simplest nontrivial realization of SS(2) was first given by Witten,[2]

$$\begin{aligned} Q^1&=\tfrac{1}{2}\{p\sigma_1+U(x)\sigma_2\},\\ Q^2&=\tfrac{1}{2}\{p\sigma_2-U(x)\sigma_1\}, \end{aligned} \tag{2}$$

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$$H^W=\tfrac{1}{2}\{p^2+[U(x)]^2+U'(x)\sigma_3\},$$

where $p=-i\,(\mathrm{d}/\mathrm{d}x)$, $U'(x)\equiv(\mathrm{d}/\mathrm{d}x)\,U(x)$, $U(x)$ is generally called a superpotential, and σ_i $(i=1,\ 2,\ 3)$ are the usual Pauli matrices.[9] This supersymmetric Hamiltonian H^W describes a quantum mechanical system of a spin-$\frac{1}{2}$ particle moving on a line (x axis).

While $N=2$ supersymmetric quantum mechanics (SSQM) has drawn much attention[10,11] due to its simpler mathematical structure, however, there were only a few attempts at studying $N=4$ SSQM,[12–20] which possesses the higher degeneracies than the $N=2$ SSQM. For example, in one dimension, fourfold degeneracies of energy spectrum may typically occur in the $N=4$ SSQM, whereas double degeneracies in the $N=2$ SSQM. All the supercharges considered in many papers have the following form:

$$Q^\alpha=\frac{1}{\sqrt{2}}\sum_{j=1}^{r}A_j^\alpha C_j,\quad \alpha=1,2,\ldots,N=4, \tag{3}$$

where A_j^α are first-order differential operators with respect to, bosonic degrees of freedoms, the Cartesian coordinates $\{x_n|n=1,\ 2,\ldots,\ d\}$ and the corresponding momentum operators $\{p_n=-i\,(\partial/\partial x_n)\equiv -i\,\partial_n|n=1,\ 2,\ldots,\ d\}$ in d-dimensional space, and C_j, fermionic degrees of freedoms, are generators of the Clifford algebra C(r,0) with positive metric in r-dimensional flat carrier space.[21,22] They satisfy

$$[x_n,\ p_m]=i\,\delta_{nm},\quad n,m=1,2,\ldots,d,$$

$$\{C_j,\ C_l\}=2\,\delta_{jl},\quad C_j^\dagger=C_j,\quad j,l=1,2,\ldots,r, \tag{4}$$

$$[x_n,\ C_j]=[p_n,\ C_j]=0.$$

Obviously, for arbitrary N, the supercharges (3), being linear combinations of the fermionic operators C_j multiplied by the bosonic operators A_j^α, are natural generalizations of the supercharges in Witten's realization (2) of $N=2$ SSQM.

In fact, when $r\geqslant 4$, the Clifford algebra C(r,0), after a graded structure introduced, may yield a superalgebra.[23,24] The generators C_j of C(r,0), together with operators of odd orders in C_j, span the odd space of this superalgebra, in which anticommuting operations among all these odd elements are allowed. For example, the odd space of the superalgebra associated with C(4,0) is spanned by the odd elements C_j $(j=1,\ 2,\ 3,\ 4)$ and $C_jC_kC_l$ $(1\leqslant j<k<l\leqslant 4)$. The purpose of this paper is to realize the general form of $N=4$ SSQM in arbitrary dimension starting from the general supercharges in which the fermionic degrees of freedoms include all the odd elements of the superalgebra associated with C(4,0). As we shall see below, this realization brings out the richer structures.

This paper is arranged as follows. In Sec. II, the general form of $N=4$ SSQM is studied in detail by means of the Clifford algebras C(4,0) and C(0,3). In Sec. III, a one-dimensional physical realization and a new multidimensional physical realization for the $N=4$ SSQM are, respectively, obtained by solving the constraint conditions. In Sec. IV, as applications, $N=4$ superconformal quantum mechanics in one dimension, which is expanded from the one-dimensional realization of $N=4$ SSQM obtained in Sec. III, is discussed in detail by considering two simple superpotentials k/x and ωx, and their corresponding superalgebraic structures are established. A simple summary is given in the final section.

Throughout this paper we shall adopt units wherein $\hbar=m=1$, the symbol $[x]$ means taking an integer part of the real number x, and T in the expression A^T is referred to as transpose of the matrix A.

II. GENERAL FORM OF $N=4$ SSQM

For $N=4$, the four supercharges take the following general form:

$$Q^{\alpha}=\frac{1}{\sqrt{2}}\left(\sum_{j} A_j^{\alpha}C_j+\frac{i}{3!}\sum_{jklm}\epsilon_{jklm}D_j^{\alpha}C_kC_lC_m\right), \qquad \alpha, j, k, l, m=1,2,3,4, \tag{5}$$

where ϵ_{jklm} is a four-dimensional Levi-Civita symbol, C_j are the generators of the Clifford algebra C(4,0), A_j^{α} and D_j^{α} are the Hermitian first-order differential operators of the d-dimensional coordinates $\{x_n\}$ and momentum operators $\{p_n\}$. Clearly, the supercharges (3) are the special cases of those given by Eq. (5) with setting $D_j^{\alpha}=0$.

Substituting Eq. (5) into the first equation of Eq. (1), we may obtain the corresponding supersymmetric Hamiltonian

$$H=\frac{1}{2}(U+VC_1C_2C_3C_4)+\frac{1}{2}\sum_{l}^{q}\sum_{j\,k}\wp_{jk}^{l}B_l\Gamma_{jk}, \tag{6}$$

where

$$(1)\quad U=\sum_{j}[(A_j^{\alpha})^2+(D_j^{\alpha})^2], \quad \text{for any } \alpha;$$

$$(2)\quad V=i\sum_{j}[A_j^{\alpha}, D_j^{\alpha}], \quad \text{for any } \alpha;$$

$$(3)\quad i[A_j^{\alpha}, A_k^{\alpha}]+i[D_j^{\alpha}, D_k^{\alpha}]+\frac{1}{2}\sum_{mn}\epsilon_{jkmn}(\{A_m^{\alpha}, D_n^{\alpha}\}-\{A_n^{\alpha}, D_m^{\alpha}\})$$

$$=-\sum_{l=1}^{q}\wp_{jk}^{l}B_l, \quad \text{for any } \alpha;$$

$$(4)\quad \sum_{j}(\{A_j^{\alpha}, A_j^{\beta}\}+\{D_j^{\alpha}, D_j^{\beta}\})=0, \quad \alpha\neq\beta; \tag{7}$$

$$(5)\quad [A_j^{\alpha}, A_k^{\beta}]-[A_k^{\alpha}, A_j^{\beta}]+[D_j^{\alpha}, D_k^{\beta}]-[D_k^{\alpha}, D_j^{\beta}]=-i\sum_{mn}\epsilon_{jkmn}(\{A_n^{\alpha}, D_m^{\beta}\}+\{A_n^{\beta}, D_m^{\alpha}\}),$$

$$\alpha\neq\beta;$$

$$(6)\quad \sum_{j}([A_j^{\alpha}, D_j^{\beta}]+[A_j^{\beta}, D_j^{\alpha}])=0, \ \alpha\neq\beta;$$

$$(7)\quad \Gamma_{jk}\equiv\frac{i}{4}[C_j, C_k].$$

In Eq. (6), q antisymmetric matrices $\wp^{l}$ ($\wp_{jk}^{l}=-\wp_{kj}^{l}$) and Hermitian operators B_l have to be determined by the third equation in Eq. (7).

Now introduce the following linear transformations:

$$A_i^{\bar{\alpha}}=\Xi_{ij}^{\bar{\alpha}}A_j^4, \quad A_j^4\equiv A_j, \quad \bar{\alpha}=1,2,3,$$

$$D_i^{\bar{\alpha}}=\Xi_{ij}^{\bar{\alpha}}D_j^4, \quad D_j^4\equiv D_j. \tag{8}$$

In order to satisfy the first, second, fourth, and sixth equations in Eq. (7), $\Xi^{\bar{\alpha}}$ should be real antisymmetric,

$$(\Xi^{\bar{\alpha}})^T=(\Xi^{\bar{\alpha}})^{-1}=-\Xi^{\bar{\alpha}}, \tag{9}$$

and satisfy

$$\{\Xi^{\bar{\alpha}}, \ \Xi^{\bar{\beta}}\}=-2\delta_{\bar{\alpha}\bar{\beta}}, \tag{10}$$

that is, $\Xi^{\bar{\alpha}}$ constitute the Clifford algebra C(0,3) with negative metric. The third and fifth equations in Eq. (7) require further that $\Xi^{\bar{\alpha}}$ and $\wp^l$ satisfy

$$\Xi_{jk}^{\bar{\alpha}}\epsilon_{jkmn}=-2\Xi_{mn}^{\bar{\alpha}}, \tag{11}$$

$$[\Xi^{\bar{\alpha}}, \ \wp^l]=0. \tag{12}$$

Equation (12) shows that the number of antisymmetric matrices $\wp^l$ is three, i.e., $l=1, 2, 3$. It follows that matrix representations of $\Xi^{\bar{\alpha}}$ and $\wp^l$ that satisfy Eqs. (9), (10), and (12) may be taken as[12,22]

$$\Xi^1=\begin{pmatrix} i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}, \quad \Xi^2=\begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix}, \quad \Xi^3=\begin{pmatrix} 0 & \sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}, \tag{13}$$

$$\wp^1=\begin{pmatrix} 0 & i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix}, \quad \wp^2=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad \wp^3=\begin{pmatrix} -i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}. \tag{14}$$

With the help of Eqs. (8) and (13), the four supercharges (5), in which the differential operators A_j and D_j now are independent of the index α, read

$$\begin{aligned}
Q^1&=\frac{1}{\sqrt{2}}[A_2C_1-A_1C_2+A_4C_3-A_3C_4 \\
&\quad +i(D_2C_2C_3C_4+D_1C_3C_4C_1+D_4C_1C_2C_4+D_3C_1C_2C_3)], \\
Q^2&=\frac{1}{\sqrt{2}}[A_3C_1-A_4C_2-A_1C_3+A_2C_4 \\
&\quad +i(D_3C_2C_3C_4+D_4C_3C_4C_1-D_1C_1C_2C_4-D_2C_1C_2C_3)], \\
Q^3&=\frac{1}{\sqrt{2}}[A_4C_1+A_3C_2-A_2C_3-A_1C_4 \\
&\quad +i(D_4C_2C_3C_4-D_3C_3C_4C_1-D_2C_1C_2C_4+D_1C_1C_2C_3)], \\
Q^4&=\frac{1}{\sqrt{2}}[A_1C_1+A_2C_2+A_3C_3+A_4C_4 \\
&\quad +i(D_1C_2C_3C_4-D_2C_3C_4C_1+D_3C_1C_2C_4-D_4C_1C_2C_3)].
\end{aligned} \tag{15}$$

By making use of Eqs. (8), (13), and (14), we can obtain from the third equation in Eq. (7) constraint conditions that A_j and D_j need satisfying

$$\begin{aligned}
B_1 &= -i[A_1, A_4] - i[D_1, D_4] - \{A_2, D_3\} + \{A_3, D_2\} \\
&= +i[A_2, A_3] + i[D_2, D_3] + \{A_1, D_4\} - \{A_4, D_1\}, \\
B_2 &= -i[A_2, A_4] - i[D_2, D_4] + \{A_1, D_3\} - \{A_3, D_1\} \\
&= -i[A_1, A_3] - i[D_1, D_3] + \{A_2, D_4\} - \{A_4, D_2\}, \\
B_3 &= -i[A_3, A_4] - i[D_3, D_4] - \{A_1, D_2\} + \{A_2, D_1\} \\
&= +i[A_1, A_2] + i[D_1, D_2] + \{A_3, D_4\} - \{A_4, D_3\}.
\end{aligned} \tag{16}$$

Correspondingly, the supersymmetric Hamiltonian (6) becomes

$$\begin{aligned}
H = \frac{1}{2}\sum_{j=1}^{4} [A_j^2 + D_j^2] + [B_1(\Gamma_{14} + \Gamma_{32}) + B_2(\Gamma_{24} + \Gamma_{13}) + B_3(\Gamma_{34} + \Gamma_{21})] \\
+ \frac{i}{2}\sum_{j=1}^{4} [A_j, D_j] C_1 C_2 C_3 C_4.
\end{aligned} \tag{17}$$

Similar to $N=2$ SSQM,[10] we may further rewrite the four supercharges (15) in the raising/lowering form, which are closely related to the factorization method,[25]

$$Q_1^{\pm} = \frac{1}{\sqrt{2}}(Q_4 \mp iQ_1), \quad Q_2^{\pm} = \frac{1}{\sqrt{2}}(Q_2 \mp iQ_3), \tag{18}$$

and satisfy $Q_\mu^{\mp} = (Q_\mu^{\pm})^{\dagger}$ $(\mu = 1, 2)$, after redefining the four generators C_j $(j = 1, 2, 3, 4)$ of C(4,0) as

$$C_1^{\pm} = \tfrac{1}{2}(C_1 \pm iC_2), \quad C_2^{\pm} = \tfrac{1}{2}(C_3 \pm iC_4). \tag{19}$$

Thus, the four supercharges (15) and the supersymmetric Hamiltonian (17) can be written, respectively, in the forms

$$\begin{aligned}
Q_1^+ &= (A_1 - iA_2)C_1^+ + (A_3 - iA_4)C_2^+ - i(D_1 - iD_2)[C_2^+, C_2^-]C_1^+ + i(D_3 - iD_4)[C_1^+, C_1^-]C_2^+, \\
Q_1^- &= (A_1 + iA_2)C_1^- + (A_3 + iA_4)C_2^- + i(D_1 + iD_2)[C_2^+, C_2^-]C_1^- - i(D_3 + iD_4)[C_1^+, C_1^-]C_2^-, \\
Q_2^+ &= (A_3 - iA_4)C_1^- - (A_1 - iA_2)C_2^- - i(D_3 - iD_4)[C_2^+, C_2^-]C_1^- + i(D_1 - iD_2)[C_1^+, C_1^-]C_2^-, \\
Q_2^- &= (A_3 + iA_4)C_1^+ - (A_1 + iA_2)C_2^+ + i(D_3 + iD_4)[C_2^+, C_2^-]C_1^+ - i(D_1 + iD_2)[C_1^+, C_1^-]C_2^+,
\end{aligned} \tag{20}$$

and

$$\begin{aligned}
H = \frac{1}{2}\sum_{j=1}^{4} [A_j^2 + D_j^2] + \Big\{ -B_1(C_1^+C_2^- - C_1^-C_2^+) + iB_2(C_1^+C_2^- + C_1^-C_2^+) + \frac{1}{2}B_3([C_1^+, C_1^-] \\
- [C_2^+, C_2^-]) \Big\} - \frac{i}{2}\sum_{j=1}^{4} [A_j, D_j][C_1^+, C_1^-][C_2^+, C_2^-].
\end{aligned} \tag{21}$$

It is easy to check that Eqs. (20) and (21) satisfy SS(4) [see Eq. (1)], which now becomes

$$\{Q_\mu^+, Q_\nu^-\}=2\delta_{\mu\nu}H, \quad \mu,\nu=1,2,$$

$$\{Q_\mu^\pm, Q_\nu^\pm\}=0, \quad [H, Q_\mu^\pm]=0. \tag{22}$$

III. PHYSICAL REALIZATIONS OF $N=4$ SSQM

By virtue of the results obtained in Sec. II, we shall discuss in this section two physical realizations of $N=4$ SSQM through choosing the concrete forms for A_j and D_j in Eqs. (20) and (21) to ensure the kinetic energy and potential energy terms appear in the corresponding $N=4$ supersymmetric Hamiltonian.

A. One-dimensional realization

Take

$$A_4=p=-i\frac{d}{dx}, \quad D_{\bar{n}}=0, \quad \bar{n}=1,2,3, \tag{23}$$

and the other components $A_{\bar{n}}$ and D_4 are real functions of x. Substituting them into the constraint conditions (16) gives rise to

$$D_4=\frac{A_1'}{2A_1}=\frac{A_2'}{2A_2}=\frac{A_3'}{2A_3}, \tag{24}$$

where the prime means derivation with respect to x. In order to satisfy Eq. (24), we may choose for simplicity

$$A_{\bar{n}}=k_{\bar{n}}W, \tag{25}$$

where $k_{\bar{n}}$ are constants, and W, here referred to as a superpotential, is an arbitrary real function of x. Accordingly, we have

$$D_4=\frac{W'}{2W}. \tag{26}$$

It follows by inserting Eqs. (25) and (26) into Eqs. (20) and (21) that the four supercharges and $N=4$ supersymmetric Hamiltonian in one dimension have, respectively, the following forms:

$$\begin{aligned}
Q_1^+&=(-ip+k_3W)C_2^+ +k^-WC_1^+ +\frac{W'}{2W}[C_1^+, C_1^-]C_2^+,\\
Q_1^-&=(+ip+k_3W)C_2^- +k^+WC_1^- +\frac{W'}{2W}[C_1^+, C_1^-]C_2^-,\\
Q_2^+&=(-ip+k_3W)C_1^- -k^-WC_2^- -\frac{W'}{2W}[C_2^+, C_2^-]C_1^-,\\
Q_2^-&=(+ip+k_3W)C_1^+ -k^+WC_2^+ -\frac{W'}{2W}[C_2^+, C_2^-]C_1^+,
\end{aligned} \tag{27}$$

where $k^\pm\equiv k_1\pm ik_2$, and

$$H=\frac{1}{2}p^2+\frac{1}{2}k^2W^2+\frac{1}{2}\left(\frac{W'}{2W}\right)^2+\left\{-k_1W'(C_1^+C_2^--C_1^-C_2^+)+ik_2W'(C_1^+C_2^-+C_1^-C_2^+)\right.$$
$$\left.+\frac{1}{2}k_3W'([C_1^+,C_1^-]-[C_2^+,C_2^-])\right\}-\frac{1}{2}[C_1^+,C_1^-][C_2^+,C_2^-]\left(\frac{W'}{2W}\right)'\equiv\frac{1}{2}p^2+V(x;C_j), \tag{28}$$

with $k^2=k_1^2+k_2^2+k_3^2$. Obviously, the Hamiltonian (28) possesses a usual kinetic energy term $\frac{1}{2}p^2$ and a potential function $V(x;C_j)$, so this resulting realization, Eqs. (27) and (28), may be applied to the real quantum mechanical systems provided that W and C_j are appropriately taken.

For the sake of convenient applications, let us further discuss the explicit matrix form for the one-dimensional $N=4$ SSQM given by Eqs. (27) and (28). In fact the Clifford algebra C(4,0) is isomorphic to the well-known Dirac algebra in the relativistic quantum mechanics,[26] here we may take the following matrix representation for C_j:

$$C_{\bar{m}}=\begin{pmatrix}0 & i\sigma_{\bar{m}}\\ -i\sigma_{\bar{m}} & 0\end{pmatrix},\quad \bar{m}=1,2,3,\quad C_4=\begin{pmatrix}0 & I_{2\times2}\\ I_{2\times2} & 0\end{pmatrix}, \tag{29}$$

where $I_{2\times2}$ is a 2×2 unit matrix, then the four supercharges (27) and the supersymmetric Hamiltonian (28) read, respectively,

$$Q_1^+=\begin{pmatrix}0 & 0 & \eta^+ & \varepsilon^-\\ 0 & 0 & 0 & 0\\ 0 & -\varepsilon^- & 0 & 0\\ 0 & \zeta^+ & 0 & 0\end{pmatrix},\quad Q_2^+=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & \eta^+ & \varepsilon^-\\ \varepsilon^- & 0 & 0 & 0\\ -\zeta^+ & 0 & 0 & 0\end{pmatrix}, \tag{30}$$

where $\eta^{\pm}\equiv p\pm i[k_3W+(W'/2W)]$, $\zeta^{\pm}\equiv p\pm i[k_3W-(W'/2W)]$, $\varepsilon^{\pm}\equiv\mp ik^{\pm}W$, and

$$H=\frac{1}{2}p^2+\frac{1}{2}k^2W^2+\frac{1}{2}\left(\frac{W'}{2W}\right)^2$$
$$+\frac{1}{2}\begin{pmatrix}-\left(\frac{W'}{2W}\right)' & & & \\ & -\left(\frac{W'}{2W}\right)' & & \\ & & \left(\frac{W'}{2W}\right)'+2k_3W' & 2k^-W'\\ & & 2k^+W' & \left(\frac{W'}{2W}\right)'-2k_3W'\end{pmatrix}. \tag{31}$$

A comparison between Eq. (31) and the third equation in Eq. (2) shows that in one dimension the matrix form of $N=4$ supersymmetric Hamiltonian is quasidiagonal, whereas the one of $N=2$ supersymmetric Hamiltonian is completely diagonal. (The quasidiagonal form of $N=2$ supersymmetric Hamiltonian appear in multidimension only, for example, see Ref. 27.)

Especially, when $k^{\pm}=0$, it follows from Eq. (31) that we may obtain a completely diagonal $N=4$ supersymmetric Hamiltonian

$$\ddot{H}=\frac{1}{2}p^2+\frac{1}{2}k_3^2W^2+\frac{1}{2}\left(\frac{W'}{2W}\right)^2+\frac{1}{2}\begin{pmatrix}-\left(\frac{W'}{2W}\right)' & & & \\ & -\left(\frac{W'}{2W}\right)' & & \\ & & \left(\frac{W'}{2W}\right)'+2k_3W' & \\ & & & \left(\frac{W'}{2W}\right)'-2k_3W'\end{pmatrix}$$
$$\equiv \mathrm{diag}[\ddot{H}_1,\ \ddot{H}_2,\ \ddot{H}_3,\ \ddot{H}_4]. \tag{32}$$

Note that in Eq. (32) the first and second diagonal component Hamiltonians $\ddot{H}_1$ and $\ddot{H}_2$ are identical, but neither of them can be abandoned because of requirement of SS(4). The corresponding supercharges $\ddot{Q}_\mu^\pm$ $(\mu=1,2)$ may be directly obtained by setting $k^\pm=0$ in Eq. (30). Since $\ddot{H}$ commutes with $\ddot{Q}_\mu^\pm$, the energy spectra of $\ddot{H}_i$ $(i=1,2,3,4)$ are identical except for the ground state, which is also an elementary property of SSQM. Consequently, $\ddot{H}_i$ are called superpartner Hamiltonians.

Let four-component spinor eigenfunction of $\ddot{H}$ be $\ddot{\psi}=[\ddot{\psi}_1,\ \ddot{\psi}_2,\ \ddot{\psi}_3,\ \ddot{\psi}_4]^T$, in which $\ddot{\psi}_i$ $(i=1,2,3,4)$ are, respectively, eigenfunctions of $\ddot{H}_i$ belonging to energy eigenvalues $\ddot{E}_i$. In terms of the third equation in Eq. (22), the four eigenfunctions $\ddot{\psi}_1,\ \ddot{\psi}_2,\ \ddot{\psi}_3,\ \ddot{\psi}_4$ may be related by the four supercharges $\ddot{Q}_\mu^\pm$, or, more concretely, by the four first-order differential operators $\eta^\pm$ and $\zeta^\pm$ given in Eq. (30)

$$\ddot{\psi}_3 \overset{\eta^+}{\rightarrow} \ddot{\psi}_1=\ddot{\psi}_2 \overset{\zeta^+}{\rightarrow} \ddot{\psi}_4 \quad \text{and} \quad \ddot{\psi}_3 \overset{\eta^-}{\leftarrow} \ddot{\psi}_1=\ddot{\psi}_2 \overset{\zeta^-}{\leftarrow} \ddot{\psi}_4. \tag{33}$$

Similar to $N=2$ case,[10] the $N=4$ supersymmtery of some $N=4$ supersymmetric quantum mechanical system is broken if this system has no zero-energy ground state, and is unbroken if this system has a zero-energy ground state. A typical structure of the fourfold degenerate energy spectrum of $\ddot{H}$ is illustratively depicted in Fig. 1, which $N=4$ supersymmetry is broken.

Furthermore, introduce

$$X_3=\frac{1}{2}\sum_\mu\ [C_\mu^+,\ C_\mu^-], \quad X^\pm=\mp C_1^\pm C_2^\pm, \tag{34}$$

which satisfy

$$[X_3,\ X^\pm]=\pm 2X^\pm, \quad [X^+,\ X^-]=X_3, \tag{35}$$

that is, X_3 and $X^\pm$ span an internal SO(3) algebra. Due to the fact $[\ddot{H},\ X_3]=0$, we may use the values of X_3 to label the energy spectra of $\ddot{H}_i$ $(i=1,2,3,4)$. With the help of Eq. (29), the matrix representation of X_3 is

$$X_3=\begin{pmatrix}1 & & & \\ & -1 & & \\ & & 0 & \\ & & & 0\end{pmatrix}. \tag{36}$$

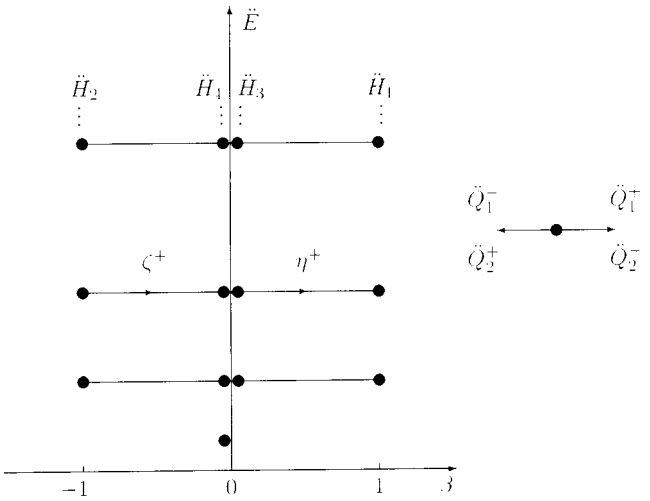

FIG. 1. Typical structure of the fourfold degenerate energy spectrum of $\ddot{H}$ given by Eq. (32). The energy spectra of H_1, H_2, H_3, H_4 correspond to the $\beta=1, -1, 0, 0$ sectors, respectively. The eigenstate belonging to some energy level (dot) may be connected with its left or right eigenstate by the supercharges $\ddot{Q}_\mu^\pm$ $(\mu=1,2)$, or, concretely, by the first-order differential operators $\eta^\pm$ and $\zeta^\pm$ along the horizontal line.

Denoting the values of X_3 by $\beta=1, -1, 0$ and 0, then the energy spectrum of $\ddot{H}_1$ belongs to the $\beta=1$ sector, that of $\ddot{H}_2$ to the $\beta=-1$ sector and so on. Hence, though the first and second superpartner Hamiltonians $\ddot{H}_1$ and $\ddot{H}_2$ are identical, their energy spectra belong to the different sectors, respectively; though the third and fourth superpartner Hamiltonians $\ddot{H}_3$ and $\ddot{H}_4$ are different, their energy spectra belong to the same $\beta=0$ sector.

B. New multidimensional realization

The $N=4$ SSQM obtained in Sec. II itself is valid for the arbitrary dimensions. In this section we shall put forward a new multidimensional physical realization of $N=4$ SSQM by taking the following matrix forms for the Hermitian operators A_4 and D_4 in Eq. (20):

$$A_4=\sum_{j=1}^{d}(p_j+L_j)\tau_j, \quad D_4=\sum_{j=1}^{d}F_j\tau_j, \tag{37}$$

and the other components, $D_{\bar{n}}=0$ $(\bar{n}=1,2,3)$, $A_{\bar{n}}$, together with L_j and F_j in Eq. (37), are the real functions of the coordinates $\{x_n\}$ in d-dimensional space. Here, τ_j are a set of Hermitian matrices which we assume to commute with p_j, L_j, F_j, and C_j. The fact that τ_j commute with C_j implies that they should be, respectively, considered as

$$\tau_j\sim I_{4\times4}\otimes\tau_j, \quad C_j\sim C_j\otimes I_{t\times t}, \tag{38}$$

where the subscript 4 is the dimension of the matrix representation of C(4,0), and the subscript t stands for the order of the matrices τ_j. Note that in the present realization the number of matrices τ_j is equal to the dimensions of space. In order to produce the usual kinetic energy term, we may, after substituting Eq. (37) into Eq. (21), take τ_j $(j=1,2,\ldots,d)$ so that

$$\{\tau_j, \ \tau_l\}=2\delta_{jl}, \tag{39}$$

that is, τ_j constitute the Clifford algebra C(d,0) as well.

The constraint conditions (16) require that

$$2A_{\bar{n}}F_j=\partial_j A_{\bar{n}},\quad \bar{n}=1,2,3,\quad j=1,2,\ldots,d. \tag{40}$$

Similar to the one-dimensional case [see Eq. (25)], a simple choice for Eq. (40) is

$$A_{\bar{n}}=k_{\bar{n}}W, \tag{41}$$

where $k_{\bar{n}}$ are constants, the superpotential W is a real function of $\{x_n\}$. In consequence, we have

$$F_j=\frac{\partial_j W}{2W}. \tag{42}$$

It follows by substituting Eqs. (37), (41), and (42) into Eq. (21) that we have the $N=4$ supersymmetric Hamiltonian in d-dimensional space,

$$\begin{aligned}H=&\frac{1}{2}\sum_j^d(-i\partial_j+L_j)^2+\frac{1}{2}k^2W^2+\frac{1}{2}\sum_j^d\left(\frac{\partial_j W}{2W}\right)^2-\frac{1}{2}\sum_{k<l}^d\mathcal{F}_{kl}\tau_{kl}+\sum_j^d\tau_j(\partial_j W)\\&\times\left\{-k_1(C_1^+C_2^--C_1^-C_2^+)+ik_2(C_1^+C_2^-+C_1^-C_2^+)+\frac{1}{2}k_3([C_1^+,C_1^-]-[C_2^+,C_2^-])\right\}\\&-\frac{1}{2}[C_1^+,C_1^-][C_2^+,C_2^-]\left\{\sum_j^d\left(\partial_j\frac{\partial_j W}{2W}\right)+\sum_{k<l}^d\left(\left\{-i\partial_k,\frac{\partial_l W}{2W}\right\}+2L_k\frac{\partial_l W}{2W}\right)\tau_{kl}\right\},\end{aligned} \tag{43}$$

where $\tau_{kl}\equiv(i/2)[\tau_k,\tau_l]$, and $\mathcal{F}_{kl}\equiv\partial_k L_l-\partial_l L_k$. The vector potential L_i naturally generates a gauge field interaction structure in d-dimensional space so that $\mathcal{F}_{kl}$ may be seen as the strength of vector field. The terms $\mathcal{F}_{kl}\tau_{kl}$ and $\{-i\partial_k,\partial_l W/2W\}\tau_{kl}$ generalize the Pauli coupling and the orbit-spin coupling interactions, respectively. For the simple three-dimensional case, these interpretations are more distinct. We take conveniently τ_j as the Pauli matrices

$$\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \tau_2=\begin{pmatrix}0&i\\-i&0\end{pmatrix},\quad \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{44}$$

then the supersymmetric Hamiltonian (43) becomes

$$\begin{aligned}H=&\frac{1}{2}(\vec{p}+\vec{L})^2+\frac{1}{2}k^2W^2+\frac{1}{2}\left(\frac{\nabla W}{2W}\right)^2+\frac{1}{2}\nabla\cdot\left(\frac{\nabla W}{2W}\right)\begin{pmatrix}-I_{4\times4}&0\\0&I_{4\times4}\end{pmatrix}\\&+\frac{1}{2}\vec{B}\cdot\vec{\tau}-\frac{1}{2}\left(\frac{\nabla W}{2W}\right)\times(-i\nabla+\vec{L})\cdot\vec{\tau},\end{aligned} \tag{45}$$

where ∇ is a three-dimensional gradient operator, $\vec{B}\cdot\vec{\tau}\equiv\nabla\times\vec{L}\cdot\vec{\tau}$ and $(\nabla W/2W)\times(-i\nabla)\cdot\vec{\tau}$ are the usual Pauli coupling term and the orbit-spin coupling interaction, respectively.[9] It can be seen that in three dimension the new realized $N=4$ supersymmetric Hamiltonian (45) is an 8×8 matrix, whereas the original one (17) or (21), in which A_j and D_j are taken as some appropriate first-order differential operator functions of the three-dimensional coordinates and momentum operators, is a 4×4 matrix.

Of course, in Eq. (37), we may also take $A_4=\Sigma_j(ip_j+\tilde{L}_j)\tilde{\tau}_j$, $D_4=\Sigma_j\tilde{F}_j\tilde{\tau}_j$, and $A_{\bar{n}}$, $\tilde{L}_j$ and $\tilde{F}_j$ are the functions of $\{x_n\}$ as well. Thus, the Hermiticities of the supercharges $Q_\alpha^\pm$ require that $\tilde{L}_j$ and $\tilde{F}_j$ should be pure imaginary, and $\tilde{\tau}_i$ should be anti-Hermitian. The convenient choices $\tilde{L}_i=iL_j$, $\tilde{F}_j=iF_j$, and $\tilde{\tau}_j=i\tau_j$ [i.e., $\tilde{\tau}_j$ constitute the Clifford algebra C(0,d) with negative metric] will lead to the same results as Eq. (43).

IV. APPLICATIONS

In this section, using the diagonal matrix realization (32) of $N=4$ SSQM in one dimension, we shall study in detail $N=4$ SCQM, which, discussed first by Fubini *et al.*,[28] is a generalization of $N=4$ SSQM, by considering two simple superpotentials k/x and ωx. Here the main task is to find a set of special exactly solvable potentials which can be brought into the framework of $N=4$ SCQM and the corresponding superalgebraic structures.

(1) The first example is a one-dimensional superpotential

$$W(x)=\frac{k}{x}, \tag{46}$$

where k is a real constant, and $x\in(-\infty,\ \infty)$. Substituting Eq. (46) into Eq. (30) combined with $k^{\pm}=0$ and $k_3=1$ and Eq. (32), we may obtain, respectively, the supercharges

$$\overline{Q}_1^{+}=\begin{pmatrix}0&0&\overline{\eta}^{+}&0\\0&0&0&0\\0&0&0&0\\0&\overline{\zeta}^{+}&0&0\end{pmatrix},\quad \overline{Q}_2^{+}=\begin{pmatrix}0&0&0&0\\0&0&\overline{\eta}^{+}&0\\0&0&0&0\\-\overline{\zeta}^{+}&0&0&0\end{pmatrix}, \tag{47}$$

where $\overline{\eta}^{\pm}=p\pm i(k-\frac{1}{2})(1/x)$, $\overline{\zeta}^{\pm}=p\pm i(k+\frac{1}{2})(1/x)$, and the supersymmetric Hamiltonian

$$H^{\mathrm{sc}}=\frac{1}{2}p^2+\frac{1}{2x^2}\begin{pmatrix}k^2-\frac{1}{4}&&&\\&k^2-\frac{1}{4}&&\\&&k^2-2k+\frac{3}{4}&\\&&&k^2+2k+\frac{3}{4}\end{pmatrix}\equiv\mathrm{diag}[H_1^{\mathrm{c}},\ H_2^{\mathrm{c}},\ H_3^{\mathrm{c}},\ H_4^{\mathrm{c}}]. \tag{48}$$

It may be further verified that H^{sc}, together with the dilatation generator D and the conformal generator K, which are given explicitly by

$$D=-\tfrac{1}{4}\{p,x\},\quad K=\tfrac{1}{2}x^2 \tag{49}$$

fulfills the same commutation relations of the conformal algebra SO(2,1)[29–31]

$$[D,H^{\mathrm{sc}}]=-iH^{\mathrm{sc}},\quad [D,K]=iK,\quad [H^{\mathrm{sc}},K]=2iD, \tag{50}$$

as its four superpartner Hamiltonians H_i^{c} ($i=1,2,3,4$). Hence, H^{sc} given by Eq. (48) is the so-called superconformal Hamiltonian,[28] which possesses not only the $N=4$ supersymmetry but also the dynamical conformal symmetry. Different from the results of Fubini *et al.*,[28] here we realize successfully a $N=4$ superconformal quantum mechanics (SCQM) in one dimension.[33–35] However, the realization of $N=4$ SCQM obtained in Ref. 28, holding uniquely in two dimension, can not be reduced to the one-dimensional or extended to more than two-dimensional cases. Furthermore, in the quartet structure of H^{sc}, three superpartner Hamiltonians $H_1^{\mathrm{c}}(=H_2^{\mathrm{c}})$, H_3^{c}, H_4^{c} are different, whereas in the quartet structure in Ref. 28 only two different superpartner Hamiltonians, $H_1^{\mathrm{c}}(=H_2^{\mathrm{c}})$ and $H_3^{\mathrm{c}}(=H_4^{\mathrm{c}})$, appear.

Let the four-component spinor eigenfunction of H^{sc} be $\psi^{\mathrm{sc}}=[\psi_1^{\mathrm{c}},\ \psi_2^{\mathrm{c}},\ \psi_3^{\mathrm{c}},\ \psi_4^{\mathrm{c}}]^T$, where ψ_i^{c} ($i=1,2,3,4$) are, respectively, the eigenfunctions of H_i^{c} belonging to the energy eigenvalues E_i^{c}. According to the transformation property (33), ψ_i^{c} are related by $\overline{\eta}^{\pm}$ and $\overline{\zeta}^{\pm}$ given in Eq. (47). In order to look for the eigenfunctions and energy eigenvalues of H^{sc}, we check first whether or not a zero-energy ground state exists by solving the following four first-order differential equations

$$\overline{Q}_{\mu}^{\pm}\,\psi_0^{\mathrm{sc}}=0,\quad \mu=1,2, \tag{51}$$

where $\psi_0^{\mathrm{sc}}\equiv[\psi_{0,1}^{\mathrm{c}},\ \psi_{0,2}^{\mathrm{c}},\ \psi_{0,3}^{\mathrm{c}},\ \psi_{0,4}^{\mathrm{c}}]^T$ stands for a zero-energy eigenfunction. It is clear that neither of the four solutions to Eq. (51),

$$\begin{aligned}
&\psi_{0,1}^{\mathrm{c}}\sim x^{-(2k-1)/2},\\
&\psi_{0,2}^{\mathrm{c}}\sim x^{+(2k+1)/2},\\
&\psi_{0,3}^{\mathrm{c}}\sim x^{+(2k-1)/2},\\
&\psi_{0,4}^{\mathrm{c}}\sim x^{-(2k+1)/2}
\end{aligned} \tag{52}$$

is normalizable on $(-\infty,\infty)$ so that neither of H_i^{c} has zero-energy level. Hence, the supersymmetry of the $N=4$ superconformal quantum mechanical system described by H^{sc} is broken. From the SSQM point of view, we know that either of H_i^{c} $(i=1,2,3,4)$ has the same energy spectrum as the other three superpartner Hamiltonians, with E_i^{c} being larger than zero. Consider the special case of $k=1/2$, it follows immediately from Eq. (48) that the conformal Hamiltonian $\breve{H}_4^{\mathrm{c}}=\frac{1}{2}p^2+(1/x^2)$ is the superpartner of the Hamiltonian $\breve{H}_1=\frac{1}{2}p^2$ $(=\breve{H}_2=\breve{H}_3)$ of a free particle. Therefore, the normalizable eigenfunctions of H_i^{c} in Eq. (48) corresponding to some positive definite energy $E_i^{\mathrm{c}}>0$ are the normalizable wave plane eigenfunctions,[37] i.e., the Bessel functions, $\psi_i^{\mathrm{c}}=\sqrt{x}J_{\lambda_i}(x\sqrt{2E_i})$ $(i=1,2,3,4)$, with $\lambda_i=k+(-)^i[i/3]$.

Now let us establish a superalgebra that governs the above $N=4$ superconformal quantum mechanical system described by H^{sc}, in which both SS(4) and SO(2,1) should be contained. Direct calculations show that the five generators of SS(4) and three generators of SO(2,1) are not closed under the anticommutation and commutation relations, for example, commuting the generators $\overline{Q}_{\mu}^{\pm}$ of SS(4) and the generator K of SO(2,1) yields new operators

$$S_{\mu}^{\pm}=xC_{\mu}^{\pm},\quad \mu=1,2. \tag{53}$$

Thus, we obtain the following closed (anti)commutation relations:

$$\begin{aligned}
&(1)\ \{\overline{Q}_{\mu}^{+},\ \overline{Q}_{\nu}^{-}\}=2\delta_{\mu\nu}H^{\mathrm{sc}},\quad \{\overline{Q}_{\mu}^{\pm},\ \overline{Q}_{\nu}^{\pm}\}=0,\quad \mu,\ \nu=1,2;\\
&(2)\ \{S_{\mu}^{+},\ S_{\nu}^{-}\}=2\delta_{\mu\nu}K,\quad \{S_{\mu}^{\pm},\ S_{\nu}^{\pm}\}=0;\\
&(3)\ \{\overline{Q}_{\mu}^{\pm},\ S_{\nu}^{\mp}\}=\delta_{\mu\nu}(k+(-)^{\mu}X_3\pm 2iD)+2(\delta_{\mu\nu}-1)(\delta_{\mu 1}X^{\pm}+\delta_{\mu 2}X^{\mp}),\\
&\qquad \{\overline{Q}_{\mu}^{\pm},\ S_{\nu}^{\pm}\}=0;\\
&(4)\ [D,\ H^{\mathrm{sc}}]=-iH^{\mathrm{sc}},\quad [D,\ K]=iK,\quad [H^{\mathrm{sc}},\ K]=2iD;\\
&(5)\ [X_3,\ X^{\pm}]=\pm 2X^{\pm},\quad [X^{+},\ X^{-}]=X_3;\\
&(6)\ [H^{\mathrm{sc}},\ \overline{Q}_{\mu}^{\pm}]=0,\quad [D,\ \overline{Q}_{\mu}^{\pm}]=-\tfrac{1}{2}i\overline{Q}_{\mu}^{\pm},\quad [K,\ \overline{Q}_{\mu}^{\pm}]=\pm 2S_{\mu}^{\pm};\\
&\qquad [H^{\mathrm{sc}},\ S_{\mu}^{\pm}]=\pm 2\overline{Q}_{\mu}^{\pm},\quad [D,\ S_{\mu}^{\pm}]=\tfrac{1}{2}iS_{\mu}^{\pm},\quad [K,\ S_{\mu}^{\pm}]=0;\\
&(7)\ [H^{\mathrm{sc}},\ X_3]=0,\quad [D,\ X_3]=0,\quad [K,\ X_3]=0;\\
&\qquad [H^{\mathrm{sc}},\ X^{\pm}]=0,\quad [D,\ X^{\pm}]=0,\quad [K,\ X^{\pm}]=0;
\end{aligned} \tag{54}$$

$$(8)\quad [X_3,\ \overline{Q}_\mu^{\pm}]=\pm(-)^{\mu+1}\overline{Q}_\mu^{\pm},\quad [X^{\pm},\ \overline{Q}_\mu^{\pm}]=\pm(1-\delta_{\mu 1})\overline{Q}_1^{\pm},$$

$$[X^{\pm},\ \overline{Q}_\mu^{\mp}]=\mp(1-\delta_{\mu 2})\overline{Q}_2^{\mp},\quad [X_3,\ S_\mu^{\pm}]=\pm(-)^{\mu+1}S_\mu^{\pm},$$

$$[X^{\pm},\ S_\mu^{\pm}]=\pm(1-\delta_{\mu 1})\overline{S}_1^{\pm},\quad [X^{\pm},\ S_\mu^{\mp}]=\mp(1-\delta_{\mu 2})\overline{S}_2^{\mp}.$$

In practice the eight fermionic generators $S_\mu^{\pm}$, $\overline{Q}_\mu^{\pm}$ ($\mu=1, 2$) and six bosonic generators $H^{\rm sc}$, D, K, X_3, and $X^{\pm}$ span a superalgebra SU(1,1|2).[34,35] The first equation in the second set of equations in Eq. (54) indicates that the fermionic generators $S_\mu^{\pm}$ may be seen as square roots of the conformal generator K, which is similar as the supercharges are the square roots of the supersymmetric Hamiltonian. Similar to SO(2,1), the superconformal symmetry described by SU(1,1|2) is dynamical since $H^{\rm sc}$ does not commute with $S_\mu^{\pm}$, D and K. It is obvious that besides SS(4), SO(2,1), and SO(3) [see the fifth set of equations in Eq. (54)], SU(1,1|2) contains a Lie superalgebra OSp(2,1) as its subalgebra,[23] which, spanned by either $\{S_1^{\pm}, \overline{Q}_1^{\pm}, H^{\rm sc}, D, K, X_3\}$ or $\{S_2^{\pm}, \overline{Q}_2^{\pm}, H^{\rm sc}, D, K, X_3\}$, has been used to study $N=2$ SCQM.[28,32] Since the generators of SO(2,1) commute with those of SO(3) [see the seventh set of equations in Eq. (54)], SU(1,1|2) contains a maximum Lie subalgebra $\mathrm{SO}(3)\times\mathrm{SO}(2,1)$. Consequently, we have the following two group chains:

$$\mathrm{SU}(1,1|2)\supset\left\{\begin{matrix}\mathrm{OSp}(2,1)\supset\mathrm{SO}(2)\times\mathrm{SO}(2,1)\\ \mathrm{SO}(3)\times\mathrm{SO}(2,1)\end{matrix}\right\}\supset\underset{X_3}{\mathrm{SO}(2)}\times\underset{H^{\rm sc}}{\mathrm{SO}(2)}. \tag{55}$$

(2) The second example is a linear superpotential on the half-line,

$$W(x)=\omega x, \tag{56}$$

where ω is a real constant, and $x\in(0,\ \infty)$. Substitution into Eq. (30) combined with $k^{\pm}=0$ and $k_3=1$ and Eq. (32) gives, respectively, the supercharges

$$\tilde{Q}_1^{+}=\begin{pmatrix}0&0&\tilde{\eta}^{+}&0\\0&0&0&0\\0&0&0&0\\0&\tilde{\zeta}^{+}&0&0\end{pmatrix},\quad \tilde{Q}_2^{+}=\begin{pmatrix}0&0&0&0\\0&0&\tilde{\eta}^{+}&0\\0&0&0&0\\-\tilde{\zeta}^{+}&0&0&0\end{pmatrix}, \tag{57}$$

where $\tilde{\eta}^{\pm}\equiv p\pm i[\omega x+(1/2x)]$, $\tilde{\zeta}^{\pm}\equiv p\pm i[\omega x-(1/2x)]$, and the corresponding supersymmetric Hamiltonian

$$\tilde{H}=\frac{1}{2}p^2+\frac{1}{2}\omega^2x^2+\begin{pmatrix}\frac{3}{8x^2}&&&\\&\frac{3}{8x^2}&&\\&&-\frac{1}{8x^2}+\omega&\\&&&-\frac{1}{8x^2}-\omega\end{pmatrix}\equiv\mathrm{diag}[\tilde{H}_1,\ \tilde{H}_2,\ \tilde{H}_3,\ \tilde{H}_4]. \tag{58}$$

Note that the set of potential functions $\tilde{V}_i$ ($i=1, 2, 3, 4$) corresponding to the four superpartner Hamiltonians $\tilde{H}_i$ is different from the well-known radial harmonic oscillator potential $V_{\rm ho}(l)=\frac{1}{2}\omega^2x^2+[l(l+1)/2x^2]$,[9] in which the angular momentum quantum number l must be positive integer, though, from the point of view of mathematics, $\tilde{V}_i$ in Eq. (58) are the special cases of

$V_{\rm ho}(l)$ for l taking some special values: $\tilde{V}_1=\tilde{V}_2=V_{\rm ho}(l=\frac{1}{2})$, $\tilde{V}_3=V_{\rm ho}(l=-\frac{1}{2})+\omega$, and $\tilde{V}_4=V_{\rm ho}(l=-\frac{1}{2})-\omega$. It may be easily inferred by using Theorem X.7 in Ref. 36 that all $\tilde{H}_i$ are Hermitian on the half-line $(0,\infty)$ since either of $\tilde{V}_i$ is in the limit point case in both zero and infinity. Let the four-component spinor eigenfunction of $\tilde{H}$ be $\tilde{\psi}=[\tilde{\psi}_1,\tilde{\psi}_2,\tilde{\psi}_3,\tilde{\psi}_4]^T$, where $\tilde{\psi}_i$ $(i=1,2,3,4)$ are, respectively, the eigenfunctions of $\tilde{H}_i$ belonging to the energy eigenvalues $\tilde{E}_i$, and are related by the four first-order differential operators $\tilde{\eta}^{\pm}$ and $\tilde{\zeta}^{\pm}$ given in Eq. (57),

$$\tilde{\psi}_3 \overset{\tilde{\eta}^+}{\rightarrow} \tilde{\psi}_1=\tilde{\psi}_2 \overset{\tilde{\zeta}^+}{\rightarrow} \tilde{\psi}_4 \quad \text{and} \quad \tilde{\psi}_3 \overset{\tilde{\eta}^-}{\leftarrow} \tilde{\psi}_1=\tilde{\psi}_2 \overset{\tilde{\zeta}^-}{\leftarrow} \tilde{\psi}_4. \tag{59}$$

We notice that the quantum mechanical system described by $\tilde{H}$ has no additional symmetry that can be, together with the $N=4$ supersymmetry, embedded in a larger supersymmetry (for example, the superconformal symmetry). If we rewrite $\tilde{H}$ as

$$\tilde{H}=\dot{H}_0^{\rm sc}+\omega^2 K+\omega Y_3, \tag{60}$$

where $\dot{H}_0^{\rm sc}$ is the supersymmetric Hamiltonian given by Eq. (31) combined with $k_3=k^{\pm}=0$ and $W(x)=\omega x$, and Y_3 is a constant matrix,

$$\dot{H}_0^{\rm sc}=\frac{1}{2}p^2+\begin{pmatrix} \frac{3}{8x^2} & & & \\ & \frac{3}{8x^2} & & \\ & & -\frac{1}{8x^2} & \\ & & & -\frac{1}{8x^2} \end{pmatrix}, \quad Y_3=\begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}, \tag{61}$$

then using the same analysis employed in the last example, it is easy to find that $\dot{H}_0^{\rm sc}$ is a superconformal Hamiltonian since it satisfies not only SO(2,1), with the dilatation generator $D=-\frac{1}{4}\{p,x\}$ and the conformal generator $K=\frac{1}{2}x^2$, but also SS(4), with the four supercharges $\dot{Q}_{\mu}^{\pm}$ $(\mu=1,2)$

$$\dot{Q}_1^+=\begin{pmatrix} 0 & 0 & p+\frac{i}{2x} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & p-\frac{i}{2x} & 0 & 0 \end{pmatrix}, \quad \dot{Q}_2^+=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & p+\frac{i}{2x} & 0 \\ 0 & 0 & 0 & 0 \\ -p+\frac{i}{2x} & 0 & 0 & 0 \end{pmatrix}. \tag{62}$$

Introducing extra three operators

$$Y_3=\frac{1}{2}\sum_{\mu}(-1)^{\mu+1}[C_{\mu}^+, C_{\mu}^-], \quad Y^{\pm}=\pm C_2^{\mp}C_1^{\pm}, \tag{63}$$

which constitute SO(3) as well [see the fifth set of equations in Eq. (64)], it follows that $\dot{Q}_{\mu}^{\pm}$, $S_{\mu}^{\pm}$, $\dot{H}_0^{\rm sc}$, D, K, Y_3, and $Y^{\pm}$ satisfy the following closed superalgebraic structure:

$$
\begin{aligned}
&(1)\ \{\dot{Q}_\mu^+,\dot{Q}_\nu^-\}=2\delta_{\mu\nu}\dot{H}_0^{\mathrm{sc}},\quad \{\dot{Q}_\mu^\pm,\dot{Q}_\nu^\pm\}=0,\quad \mu,\nu=1,2;\\
&(2)\ \{S_\mu^+,S_\nu^-\}=2\delta_{\mu\nu}K,\quad \{S_\mu^\pm,S_\nu^\pm\}=0;\\
&(3)\ \{\dot{Q}_\mu^\pm,S_\nu^\mp\}=\delta_{\mu\nu}(\pm 2iD+Y_3),\quad \{\dot{Q}_\mu^\pm,S_\nu^\pm\}=(-)^\mu(1-\delta_{\mu\nu})2Y^\mp;\\
&(4)\ [D,\dot{H}_0^{\mathrm{sc}}]=-i\dot{H}_0^{\mathrm{sc}},\quad [D,K]=iK,\quad [\dot{H}_0^{\mathrm{sc}},K]=2iD;\\
&(5)\ [Y_3,Y^\pm]=\pm 2Y^\pm,\quad [Y^+,Y^-]=Y_3;\\
&(6)\ [\dot{H}_0^{\mathrm{sc}},\dot{Q}_\mu^\pm]=0,\quad [D,\dot{Q}_\mu^\pm]=-\tfrac{1}{2}i\dot{Q}_\mu^\pm,\quad [K,\dot{Q}_\mu^\pm]=\pm S_\mu^\pm;\\
&\qquad [\dot{H}_0^{\mathrm{sc}},S_\mu^\pm]=\pm\dot{Q}_\mu^\pm,\quad [D,S_\mu^\pm]=\tfrac{1}{2}iS_\mu^\pm,\quad [K,S_\mu^\pm]=0;\\
&(7)\ [\dot{H}_0^{\mathrm{sc}},Y_3]=0,\quad [D,Y_3]=0,\quad [K,Y_3]=0;\\
&\qquad [\dot{H}_0^{\mathrm{sc}},Y^\pm]=0,\quad [D,Y^\pm]=0,\quad [K,Y^\pm]=0;\\
&(8)\ [Y_3,\dot{Q}_\mu^\pm]=\mp\dot{Q}_\mu^\pm,\quad [Y^\pm,\dot{Q}_\mu^\pm]=\pm(-)^{\mu+1}\dot{Q}_\nu^\mp,\quad [Y^\pm,\dot{Q}_\mu^\mp]=0;\\
&\qquad [Y_3,S_\mu^\pm]=\mp S_\mu^\pm,\quad [Y^\pm,S_\mu^\pm]=\pm(-)^\mu S_\nu^\mp,\quad [Y^\pm,S_\mu^\mp]=0;
\end{aligned}
\tag{64}
$$

where $S_\mu^\pm$ has been given by Eq. (53). We denote the above superalgebra by SC(4), which, different from SU(1,1|2) defined by Eq. (54), has the same subgroup structure as SU(1,1|2), i.e.,

$$
\mathrm{SC}(4)\supset\begin{Bmatrix}\mathrm{OSp}(2,1)\supset\mathrm{SO}(2)\times\mathrm{SO}(2,1)\\ \mathrm{SO}(3)\times\mathrm{SO}(2,1)\end{Bmatrix}\supset\underset{Y_3}{\mathrm{SO}(2)}\times\underset{\dot{H}_0^{\mathrm{sc}}}{\mathrm{SO}(2)}.
\tag{65}
$$

To determine the eigenfunctions and energy eigenvalues of $\tilde{H}$ by algebraic method, it is convenient to regroup the previous operators $\dot{H}_0^{\mathrm{sc}}$, D, K, $\dot{Q}_\mu^\pm$, and $S_\mu^\pm$ as

$$
\begin{aligned}
&T_3=\frac{1}{2\omega}\dot{H}_0^{\mathrm{sc}}+\frac{\omega}{2}K,\quad T^\pm=\frac{1}{2\omega}\dot{H}_0^{\mathrm{sc}}-\frac{\omega}{2}K\mp iD,\\
&L_\mu^\pm=\frac{1}{2\sqrt{\omega}}\dot{Q}_\mu^\pm-\frac{\sqrt{\omega}}{2}S_\mu^\pm,\quad R_\mu^\pm=\frac{1}{2\sqrt{\omega}}\dot{Q}_\mu^\pm+\frac{\sqrt{\omega}}{2}S_\mu^\pm.
\end{aligned}
\tag{66}
$$

Note that $R_\mu^\pm$ ($\mu=1,2$) are up to normalization constants the supercharges $\tilde{Q}_\mu^\pm$ associated with $\tilde{H}$, i.e., $R_\mu^\pm=(1/2\sqrt{\omega})\tilde{Q}_\mu^\pm$. Owing to the fact $\tilde{H}=2\omega(T_3+\frac{1}{2}Y_3)$, there exists a simple relation between the energy eigenvalues $\tilde{E}_i$ ($i=1,2,3,4$) of $\tilde{H}_i$ and the energy eigenvalues e_i ($i=1,2,3,4$) of $T_{i,3}$, the ith diagonal component of T_3,

$$
\tilde{E}_i=e_i+\Delta_i,\quad \Delta_i=(-)^{i+1}\frac{1}{2}\left[\frac{i}{3}\right],
\tag{67}
$$

and their corresponding eigenfunctions are identical. Therefore, the eigenfunctions and energy eigenvalues of $\tilde{H}$ may be directly obtained provided that those of T_3 are known. With the help of Eq. (64), the closed anticommutation and commutation relations satisfied by the six bosonic operators T_3, $T^\pm$, Y_3, $Y^\pm$ and eight fermionic operators $L_\mu^\pm$, $R_\mu^\pm$, read

$$
\begin{aligned}
&(1)\ [T_3,\ T^{\pm}]=\pm T^{\pm},\quad [T^{+},\ T^{-}]=-2T_3;\\
&(2)\ [Y_3,\ Y^{\pm}]=\pm 2Y^{\pm},\quad [Y^{+},\ Y^{-}]=Y_3;\\
&(3)\ \{L_{\mu}^{+},\ L_{\mu}^{-}\}=T_3-\tfrac{1}{2}Y_3,\quad \{L_{\mu}^{\pm},\ L_{\nu}^{\pm}\}=\{L_{\mu}^{\pm},\ L_{\nu}^{\mp}\}=0;\\
&(4)\ \{R_{\mu}^{+},\ R_{\mu}^{-}\}=T_3+\tfrac{1}{2}Y_3,\quad \{R_{\mu}^{\pm},\ R_{\nu}^{\pm}\}=\{R_{\mu}^{\pm},\ R_{\nu}^{\mp}\}=0;\\
&(5)\ \{L_{\mu}^{\pm},\ R_{\nu}^{\mp}\}=\delta_{\mu\nu}T^{\mp},\quad \{L_{\mu}^{\pm},\ R_{\nu}^{\pm}\}=(-1)^{\nu}(1-\delta_{\mu\nu})Y^{\mp};\\
&(6)\ [T_3,\ Y^{\pm}]=0,\quad [T_3,\ Y_3]=0,\quad [T^{\pm},\ Y^{\pm}]=0,\\
&\qquad [T^{\pm},\ Y_3]=0,\quad [T^{\pm},\ Y^{\mp}]=0;\\
&(7)\ [T_3,\ L_{\mu}^{\pm}]=\pm\tfrac{1}{2}L_{\mu}^{\pm},\quad [T^{\pm},\ L_{\mu}^{\mp}]=0,\quad [T^{\pm},\ L_{\mu}^{\pm}]=\pm L_{\mu}^{\mp};\\
&\qquad [T_3,\ R_{\mu}^{\pm}]=\pm\tfrac{1}{2}R_{\mu}^{\pm},\quad [T^{\pm},\ R_{\mu}^{\pm}]=0,\quad [T^{\pm},\ R_{\mu}^{\mp}]=\mp L_{\mu}^{\mp};\\
&(8)\ [Y_3,\ L_{\mu}^{\pm}]=\mp L_{\mu}^{\pm},\quad [Y^{\pm},\ L_{\mu}^{\mp}]=0,\quad [Y^{\pm},\ L_{\mu}^{\pm}]=\pm(-1)^{\mu+1}L_{\nu}^{\mp};\\
&\qquad [Y_3,\ R_{\mu}^{\pm}]=\mp R_{\mu}^{\pm},\quad [Y^{\pm},\ R_{\mu}^{\mp}]=0,\quad [Y^{\pm},\ R_{\mu}^{\pm}]=\pm(-1)^{\mu+1}L_{\nu}^{\mp},
\end{aligned}
\tag{68}
$$

where $\mu,\ \nu=1,\ 2$. We observe from Eq. (68) that (1) the first set of equations indicates that T_3, $T^{\pm}$ constitute SO(2,1) also, where T_3 is a compact operator with a discrete spectrum, and T^{+} (T^{-}) raises (lowers) the energy eigenvalues of T_3 by 1 unit. (2) Similar to SU(1,1|2), the superalgebra determined by Eq. (68) contains $\mathrm{SO}(2,1)\times\mathrm{SO}(3)$ as its maximum Lie subalgebra as well, moreover, the values of Y_3 [see Eq. (61)] may be used to label the energy eigenvalues e of T_3 or $\tilde{E}$ of $\tilde{H}$. (3) T_3 and $R_{\mu}^{\pm}$ (or T_3 and $L_{\mu}^{\pm}$, $\mu=1,\ 2$) do not form SS(4), therefore, the energy spectrum of T_3 is not fourfold degenerate. (4) The first column of equations in the seventh and eighth sets of equations show that R_{μ}^{+} and L_{μ}^{+} raise the energy eigenvalues of T_3 by $\frac{1}{2}$ unit meanwhile lower the values of Y_3 by 1 unit, whereas R_{μ}^{-} and L_{μ}^{-} lower the energy eigenvalues of T_3 by $\frac{1}{2}$ unit meanwhile raise the values of Y_3 by 1 unit.

Now turn to the eigenfunctions and energy eigenvalues of $\tilde{H}$ by means of the similar approach as used in the last example. Solving the following four equations:

$$
\tilde{Q}_{\mu}^{\pm}\,\tilde{\psi}_0=0,\quad \mu=1,2,
\tag{69}
$$

where $\tilde{\psi}_0\equiv[\tilde{\psi}_{0,1},\ \tilde{\psi}_{0,2},\ \tilde{\psi}_{0,3},\ \tilde{\psi}_{0,4}]^{T}$ stands for the zero-energy eigenfunction, gives rise to

$$
\begin{aligned}
&\tilde{\psi}_{0,1}\sim\frac{1}{\sqrt{x}}\exp(-\omega x^2/2),\\
&\tilde{\psi}_{0,2}\sim\frac{1}{\sqrt{x}}\exp(+\omega x^2/2),\\
&\tilde{\psi}_{0,3}\sim\sqrt{x}\exp(+\omega x^2/2),\\
&\tilde{\psi}_{0,4}\sim\sqrt{x}\exp(-\omega x^2/2).
\end{aligned}
\tag{70}
$$

It is not difficult to find by simple calculations that of the four eigenfunctions $\tilde{\psi}_{0,i}$ ($i=1,\ 2,\ 3,\ 4$), only $\tilde{\psi}_{0,4}$ is square-integrable on the interval $(0,\ \infty)$, whose normalized form is

$$\tilde{\psi}_{0,4}=\sqrt{\omega x}\exp(-\omega x^2/2), \tag{71}$$

that is, only $\tilde{H}_4$ has a normalizable zero-energy ground state, whereas the other three superpartner Hamiltonians $\tilde{H}_1$, $\tilde{H}_2$, $\tilde{H}_3$ do not have. Of course, $\tilde{\psi}_{0,4}$ is also the normalizable ground state eigenfunction of the fourth diagonal component $T_{4,3}$ of T_3, with its corresponding energy being larger than zero. With the help of the superalgebraic relations (68), the eigenfunctions $\tilde{\psi}_{n',i}$ ($n'=1, 2, \ldots$; $i=1, 2, 3, 4$) for arbitrary excited states may be obtained from $\tilde{\psi}_{0,4}$ through two steps: first applying n times the raising operator T^+ to $\tilde{\psi}_{0,4}$ produces all the excited states $\tilde{\psi}_{n',4}$ ($n'=1, 2, \ldots$) of $T_{4,3}$, and then acting, respectively, once and twice on $\tilde{\psi}_{n',4}$ with $\tilde{Q}^-_\mu$ or R^-_μ or L^-_μ gives the other excited states $\tilde{\psi}_{n,i'}$ ($n=0, 1, \ldots$; $i'=1, 2, 3$), i.e., all the eigenfunctions of $\tilde{H}_{i'}$ or $T_{i',3}$. With the help of Rodrigus' formula for the generalized Laguerre polynomial $L^a_n(x)$ of positive integer n and real parameter a in argument x, we can finally obtain by induction

$$\begin{aligned}
\tilde{\psi}_{n,1}&=\sqrt{2\omega x}\exp(-\omega x^2/2)L^0_n(\omega x^2),\\
\tilde{\psi}_{n,2}&=\sqrt{2\omega x}\exp(-\omega x^2/2)L^0_n(\omega x^2),\\
\tilde{\psi}_{n,3}&=\sqrt{\frac{2x}{n+1}}(\omega x)\exp(-\omega x^2/2)L^1_n(\omega x^2),\\
\tilde{\psi}_{n,4}&=\sqrt{\frac{2x}{n+1}}(\omega x)\exp(-\omega x^2/2)L^1_n(\omega x^2),\\
n&=0,\ 1,\ 2,\ldots .
\end{aligned} \tag{72}$$

Thus, the energy eigenvalues, $\tilde{E}_i$ and e_i ($i=1, 2, 3, 4$) related by Eq. (67), that correspond to the same normalized eigenfunctions (72), of $\tilde{H}_i$ and $T_{i,3}$ are, respectively,

$$\begin{aligned}
\tilde{E}_1&=2\omega(e_1+\Delta_1)=2\omega(n+1), \quad e_1=n+1,\\
\tilde{E}_2&=2\omega(e_2+\Delta_2)=2\omega(n+1), \quad e_2=n+1,\\
\tilde{E}_3&=2\omega(e_3+\Delta_3)=2\omega(n+1), \quad e_3=n+1/2,\\
\tilde{E}_4&=2\omega(e_4+\Delta_4)=2\omega n, \quad e_4=n+1/2,\\
n&=0,\ 1,\ 2,\ldots .
\end{aligned} \tag{73}$$

Equation (73) shows clearly that the $N=4$ supersymmetry of the quantum mechanical system described by $\tilde{H}$ is unbroken since its ground state energy is zero, and the fourfold degeneracies may be observed above the second level. However, the quartet energy spectrum structure of T_3, which is not fourfold degenerate, involves two sets of double degenerate spectra, moreover, the corresponding supersymmetry is broken since its ground state energy is $\frac{1}{2}$. The energy spectrum structures of $\tilde{H}$ and T_3 are depicted in Fig. 2 and Fig. 3, respectively. The solutions to the Schrödinger equations with the potentials $ax^2+(b/x^2)$ for different a's and b's may be obtained by different approaches, see Refs. 28, 29, 37–39.

V. SUMMARY

In this paper, we obtained the general form of $N=4$ SSQM in arbitrary dimension, starting from the general form of four supercharges, in which the fermionic degrees of freedoms include

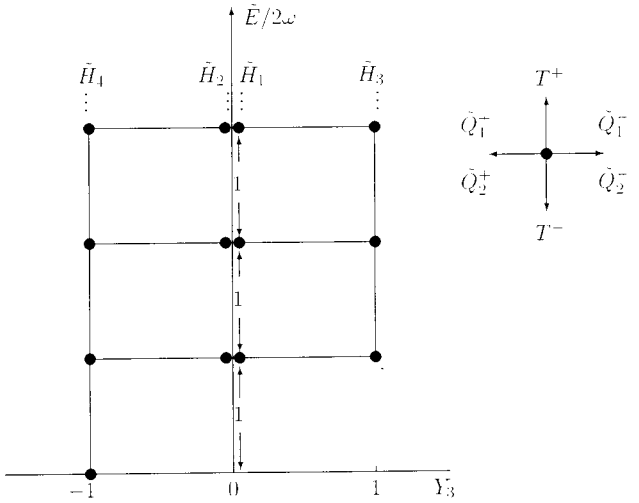

FIG. 2. Fourfold degenerate energy spectrum of $\tilde{H}$ given by Eq. (73), which $N=4$ supersymmetry is unbroken since its ground state energy is zero. Each eigenstate (dot) is connected with its surrounding eigenstates (dots) by the supercharges $\tilde{Q}_\mu^\pm$ $(\mu=1,2)$ along the horizontal line, and by the raising/lowering operators $T^\pm$ along the vertical line.

all the odd elements, C_j and $C_jC_kC_l$, of the superalgebra associated with the Clifford algebra C(4,0). Then, from them, we gave the one-dimensional physical realization and the new multidimensional physical realization for the $N=4$ SSQM by solving their respective constraint conditions. As applications, we studied in detail, on the base of the one-dimensional realization, two superconformal quantum mechanical systems with their superpotentials being k/x and ωx, which possess both the $N=4$ supersymmetries and the dynamical conformal symmetries, and established their corresponding superalgebraic structures, which are spanned by the eight fermionic generators and six bosonic generators. Our next work is to apply the general realizations of $N=4$ SSQM obtained in this paper to the other possible (quasi-) exactly solvable potentials, for example, listed in Refs. 10 and 40, and to discussing the nonlinear $N=4$ SSQM based on the deformations of Eq.

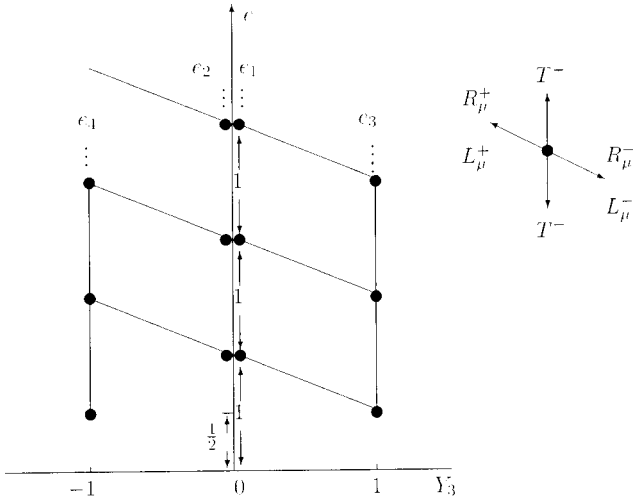

FIG. 3. Quartet structure of the energy spectrum of T_3 related tightly to $\tilde{H}$ [see Eq. (73)]. Different from that of $\tilde{H}$ exhibited in Fig. 2, T_3 possesses two sets of double degenerate spectra with the corresponding supersymmetry being broken. Each eigenstate (dot) is connected with its surrounding eigenstates (dots) by the fermionic operators $R_\mu^\pm$, $L_\mu^\pm$ $(\mu=1,2)$ along the slanting line, and by the raising/lowering operators $T^\pm$ along the vertical line.

(22),[41] which is similar to the deformations of angular momentum algebra.[42,43] From the point of view of mathematics, it is also of interest to investigate the representations of SU(1,1|2) and SC(4) and their relations to the classical Lie superalgebras.[23,44,45]

ACKNOWLEDGMENTS

This work was supported by Chinese National Natural Science Foundation (10275038), Major State Basic Research Development Programs (G2000077400 and G2000077604) and Tsinghua Natural Science Foundation.

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Exponentially accurate error estimates of quasiclassical eigenvalues. II. Several dimensions

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(Received 16 February 2002; accepted 24 March 2003)

We study the behavior of truncated Rayleigh–Schrödinger series for low-lying eigenvalues of the time-independent Schrödinger equation, in the semiclassical limit $\hbar \searrow 0$. In particular we prove that if the potential energy satisfies certain conditions, there is an optimal truncation of the series for the eigenvalues, in the sense that this truncation is exponentially close to the exact eigenvalue. These results were already discussed for the one-dimensional case in a previous article. This time we consider the multi-dimensional problem, where degeneracy plays a central role. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1581353]

I. INTRODUCTION

Perhaps one of the most elementary facts in quantum physics is that, for a sufficiently deep potential well, the eigenvalue problem defined by the time-independent Schrödinger equation admits normalizable solutions. Equivalently, if one considers Planck's constant as a parameter, the equation

$$H(\hbar)\tilde{\Psi}(\hbar;x) := \left[-\frac{\hbar^2}{2}\Delta_x + V(x) \right] \tilde{\Psi}(x) = E(\hbar)\tilde{\Psi}(\hbar;x) \tag{1}$$

is expected to have eigenvalues near the bottom of the potential well, in the semiclassical limit $\hbar \searrow 0$.

Along with the problem of existence of low-lying eigenvalues, one is also interested in the behavior of the corresponding perturbation series in powers of $\hbar$, the so-called Rayleigh–Schrödinger (R-S) series. It is well known that, in general, the R-S series are not convergent but only asymptotic to the solutions of Eq. (1). However, one often wants to consider truncations of these series as good approximations to the actual eigenvalues/eigenvectors. This raises the natural question of whether or not one can find an optimal truncation that minimizes the difference between the exact eigenvalues/eigenvectors and the corresponding truncated R-S series.

In this article we aim to find exponentially accurate asymptotics to the solutions of (1). We shall assume that the potential energy $V(x)$ satisfies the following conditions:

H1 $V(x)$ is a C^∞ real function on $\mathbb{R}^d$ such that $\liminf_{|x|\to\infty} V(x) =: V_\infty > 0$.

H2 $V(x)$ has a unique global minimum $V(0) = 0$ at $x = 0$.

H3 The global minimum of $V(x)$ is nondegenerate in the sense that

$$\mathrm{Hess}_V(0) = \mathrm{diag}[\omega_1^2, \ldots, \omega_d^2]$$

has only strictly positive eigenfrequencies $\omega_1, \ldots, \omega_d$.

H4 $V(x)$ has an analytic extension to a neighborhood of the region $S_\delta = \{z : |\mathrm{Im}\, z_i| \leqslant \delta + \epsilon\}$ for some

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$\delta>0$ and $\epsilon>0$ arbitrarily small. Without loss we may assume that $\delta\leqslant 1$.

H5 $V(z)$ satisfies $|V(z)|\leqslant M\exp(\tau|z|^2)$ uniformly in S_δ, for some positive constants $M>0$ and $\omega_0/4\geqslant\tau>0$ where ω_0 denotes the lowest eigenfrequency of $\mathrm{Hess}_V(0)$.

We shall prove that one can truncate the R-S series so that the difference between the truncated series and the actual eigenvalue/eigenvector can be made smaller than $\Lambda\exp(-\Gamma/\hbar)$ where the positive constants Λ and Γ are explicitly calculated. Our construction is based entirely on a straighforward application of the formal R-S perturbation theory. These results extend those in Ref. 19, where we discussed optimal truncation for the one-dimensional problem. We follow the method explained in that article, which indeed is related with one developed by Hagedorn and Joye to study approximate solutions to the time-dependent Schrödinger equation.[4] Roughly speaking, we calculate upper bounds for each term in the R-S series for both eigenvalues and eigenfuctions. Then we combine these to obtain a recursion relation that yields an estimate for the growth of these terms. From that we compute an estimate of the difference of the two sides of (1) after truncation at order N; this estimate behaves like $ab^N\hbar^{N/2}(N!)^{1/2}$. For each $\hbar$ we choose N to minimize this quantity. This and some standard results of functional analysis yield our results. The main change with respect to Ref. 19 comes from the fact that, in several dimensions, we need to consider degenerate perturbation theory. There are also several technical nuissances which require special treatment.

The study of this problem is not new, of course. The first proof of existence of low-lying eigenvalues and asymptotic R-S series was presented by Combes *et al.* in 1983. Their proof, which involves Dirichlet–Newmann bracketing techniques, only considers the one-dimensional problem. Shortly after, Simon gave another proof, based on geometric arguments, that is valid in several dimensions.[16] This problem was also studied by Helffer and Sjöstrand in the broader framework of microlocal analysis of self-adjoint pseudodifferential operators.[6] From these works, it is known that eigenvalues/eigenfunctions near the bottom of the potential well admit asymptotic expansions in half-powers of $\hbar$, where the leading orders are given by the corresponding eigenvalues/eigenfunctions of the harmonic oscillator aproximation. These results require only to assume that the potential energy satisfies H1–H3, although further information has been obtained in Ref. 6 for potentials with analytic continuation in a neighborhood of the minimum. In particular, it is proved in Theorem 4.6 of Ref. 6 that the low-lying eigenvalues/eigenfunctions can be exponentially approximated by truncated series.

The last result mentioned above is based on the rather involved theory of analytic pseudodifferential operators.[18] On the other hand, the work by Hagedorn and Joye[4] suggests that a much simpler method, involving only formal R-S series, may be used to contruct exponentially accurate aproximations to the eigenvalues/eigenfunctions of (1). Indeed, the constructive method developed in this work relies upon only some elementary notions on complex and functional analysis. Moreover, we obtain explicit upper bounds to the growth of the R-S coefficients. Our construction might be used for numerical computation, although the many constants that we define along the way have not been optimized for that purpose. However, there is a tradeoff in our approach which consists on the need of somewhat stronger assumptions about the potential energy, namely, hypothesis H5. We finally would like to point out that our technique could be used to study the time-independent Born–Oppenheimer approximation.

Results analogous to those discussed in this work have also been obtained for a class of C^∞ potentials. Bambusi *et al.*[1] have studied exponentially accurate quasimodes up to an error of order $\exp(-\mathrm{const}/\hbar^{1/\rho})$ with $\rho>1$, when the potential energy is Gevrey of order $\mu>1$. Furthermore, their estimate on the error is uniform in $\hbar$ for all eigenvalues in $[0,\hbar^\delta]$ with $0<\delta<1$. The construction of those quasimodes is based upon quantization of the Birkhorff normal forms for the classical Hamiltonian associated to (1). Since their proof relies on the KAM theorem,[3] the authors assume that the eigenfrequencies $\omega_1,\ldots,\omega_d$ satisfy the nonresonant condition $|\Sigma_i\omega_i k_i|^{-1}\leqslant C(\Sigma_i|k_i|)^\alpha$, for $C>0$, $\alpha>0$, and for every nontrivial set of integers $(k_1,\ldots,k_d)$. Under similar assumptions, Popov[12,13] has proved more general results by quantization of the KAM theory.

This article is organized as follows. In Sec. II we make a transformation of Eq. (1), and some technical results are proven. In Sec. III we construct some operators through recursion relations,

which allow us to calculate the several correction terms involved in the formal series for eigenvalues and eigenvectors. In particular, this construction allows us to consider the cases where degeneracy occurs. Because of the tranformation done in Sec. II, we obtain a manageable recursion relation for the nth term of the R-S series. Then we state and prove an estimate of the growth of these terms. In Sec. IV we define a residual error function for Eq. (1) and prove an estimate for it. The main results are stated precisely in Sec. V. The Appendix is devoted to a computation needed in Sec. IV.

II. PRELIMINARIES

In this work we shall use the standard multi-index notation: for $\alpha=(\alpha_1,\ldots,\alpha_d)\in\mathbb{Z}_+^d$ and $x=(x_1,\ldots,x_d)\in\mathbb{R}^d$, we denote $|\alpha|:=\alpha_1+\cdots+\alpha_d$, $\alpha!:=\alpha_1!\cdot\cdots\cdot\alpha_d!$, $x^\alpha:=x_1^{\alpha_1}\cdot\cdots\cdot x_d^{\alpha_d}$, $D^\alpha:=\partial_{x_1}^{\alpha_1}\cdot\cdots\cdot\partial_{x_d}^{\alpha_d}$, and $x^2:=x_1^2+\cdots+x_d^2$. For $z=(z_1,\ldots,z_d)\in\mathbb{C}^d$, we denote $|z|^2:=z_1z_1^*+\cdots+z_dz_d^*$.

We first transform (1) by scaling $x\to\hbar^{1/2}x$ and then dividing the whole equation by $\hbar$. This unitary transformation scales the eigenvalues and eigenfunctions as $E\to\hbar^{-1}E$ and $\tilde{\Psi}(x)\to\tilde{\Psi}(\sqrt{\hbar}x)$, respectively. The transformed equation may be written as

$$[-\tfrac{1}{2}\Delta_x+V(\hbar;x)]\tilde{\Psi}(\hbar;x)=E(\hbar)\tilde{\Psi}(\hbar;x). \tag{2}$$

Because of hypothesis H3, $V(x)$ admits a Taylor expansion up to any order n. Thus we can write

$$V(\hbar;x)=\frac{1}{2}\sum_{i,j=1}^{d}A_{ij}x_ix_j+W(\hbar;x),$$

where the function $W(\hbar;x)$ can be asymptotically approximated by

$$W(\hbar;x)=\sum_{l=3}^{n}\hbar^{(l-2)/2}\sum_{|\alpha|=l}\frac{D^\alpha V(0)}{\alpha!}x^\alpha+O(\hbar^{(n-1)/2}x^{|\alpha|=n+1}). \tag{3}$$

Hypothesis H4 implies furthermore that the Taylor series (3) is convergent inside the open polydisc $\{z\in\mathbb{C}^d:|z_i|\leqslant\delta\}$. Upper bounds on the derivatives of $V(x)$ can be easily obtained by using the Cauchy integral formula. They are stated and proved below in Lemma 2.

Now we can rewrite (2) as

$$[H_0+W(\hbar;x)]\tilde{\Psi}(\hbar;x)=E(\hbar)\tilde{\Psi}(\hbar;x), \tag{4}$$

where, in suitable Cartesian coordinates,

$$H_0=-\frac{1}{2}\Delta_x+\frac{1}{2}\sum_{i=1}^{d}\omega_i^2x_i^2$$

is a harmonic oscillator Hamiltonian with eigenfrequencies $\omega_1,\ldots,\omega_d$. The eigenfunctions of H_0 are therefore

$$\Phi_\alpha(x)=\left(\pi^{-d}\prod_{i=1}^{d}\omega_i\right)^{1/4}(2^{|\alpha|}\alpha!)^{-1/2}\exp\left(-\frac{1}{2}\sum_{i=1}^{d}\omega_ix_i^2\right)\prod_{i=1}^{d}h_{\alpha_i}(\sqrt{\omega_i}x_i), \tag{5}$$

where $h_j(y)$ denotes the Hermite polynomial of degree j. The corresponding eigenvalues are $e_\alpha=\Sigma_{i=1}^{d}\omega_i\alpha_i+d/2$.

In the semiclassical limit we want to consider $W(\hbar,x)$ as a perturbation of H_0. Then we can propose formal Rayleigh–Schrödinger series for both $E(\hbar)$ and $\tilde{\Psi}(\hbar;x)$:

$$\tilde{\Psi}(x)\sim\tilde{\psi}_0(x)+\hbar^{1/2}\tilde{\psi}_1(x)+\hbar^{2/2}\tilde{\psi}_2(x)+\hbar^{3/2}\tilde{\psi}_3(x)+\hbar^{4/2}\tilde{\psi}_4(x)+\cdots, \tag{6}$$

$$E(\hbar)\sim\mathcal{E}_0+\hbar^{1/2}\mathcal{E}_1+\hbar^{2/2}\mathcal{E}_2+\hbar^{3/2}\mathcal{E}_3+\hbar^{4/2}\mathcal{E}_4+\cdots. \tag{7}$$

In this work we essentially follow the standard, formal method to compute the R-S coefficients (see, e.g., Ref. 11, Chap. XVI), although alternatively we could use the technique developed by Kato (Ref. 10 Chaps. VII and VIII). However, this last approach seems rather difficult to implement here, in particular when degeneracy occurs. Concerning asymptotics in degenerate perturbation theory, we must mention the approach developed by Hunziker–Pillet.[8,9]

We now insert (6) and (7) into (2) and equate powers of $\hbar^{1/2}$. The zeroth-order equation yields $H_0\psi_0=\mathcal{E}_0\psi_0$. Then $\mathcal{E}_0=e$ and $\psi_0\in G$, where e is some eigenvalue of H_0 with multiplicity g and associated eigenspace G. For $n=1,2,\ldots$, we have

$$(H_0-e)\tilde{\psi}_n+\sum_{l=1}^{n}\tilde{T}^{(l+2)}\tilde{\psi}_{n-l}=\sum_{l=1}^{n}\mathcal{E}_l\tilde{\psi}_{n-l}, \tag{8}$$

where we define

$$\tilde{T}^{(l)}:=\sum_{|\alpha|=l}\frac{1}{\alpha!}D^{\alpha}V(0)x^{\alpha}.$$

Existence of solutions to the set of equations (8) can be shown by explicit construction, as the one we shall develop in Sec. III. Also, the correction terms $\tilde{\psi}_n$ satisfies the following property:

Lemma 1: Let $P_{|\alpha|\leqslant l}$ be the projection onto the subspace spanned by $\{\Phi_\alpha:|\alpha|\leqslant l\}$ and $a=a_e$ be the smallest non-negative integer such that $G\subseteq\mathrm{Ran}(P_{|\alpha|\leqslant a})$. Then, for each $n\geqslant 1$, $\tilde{\psi}_n\in\mathrm{Ran}(P_{|\alpha|\leqslant a+3n})$

Proof: First, decompose $\tilde{\psi}_n=P_{|\alpha|\leqslant a}\tilde{\psi}_n+(1-P_{|\alpha|\leqslant a})\tilde{\psi}_n=:\tilde{\psi}_n^{(1)}+\tilde{\psi}_n^{(2)}$. We have to prove the assertion only for $\tilde{\psi}_n^{(2)}$. Equation (8) yields

$$\tilde{\psi}_n^{(2)}=(H_0-e)_r^{-1}(1-P_{|\alpha|\leqslant a})\left[\sum_{l=1}^{n}\mathcal{E}_l\tilde{\psi}_{n-l}-\sum_{l=1}^{n}\tilde{T}^{(l+2)}\tilde{\psi}_{n-l}\right],$$

where $(H_0-e)_r^{-1}$ is the inverse of the restriction of H_0-e onto $\mathrm{Ran}(1-P_{|\alpha|\leqslant a})$. Since

$$\mathrm{Ran}((H_0-e)_r^{-1}(1-P_{|\alpha|\leqslant a})P_{|\alpha|\leqslant a+3n})\subset\mathrm{Ran}(P_{|\alpha|\leqslant a+3n}),$$

it is sufficient to show that

$$\left(\sum_{l=1}^{n}\mathcal{E}_l\tilde{\psi}_{n-l}-\sum_{l=1}^{n}\tilde{T}^{(l+2)}\tilde{\psi}_{n-l}\right)\in P_{|\alpha|\leqslant a+3n}. \tag{9}$$

Now use mathematical induction. For $n=1$, the assertion $\tilde{T}^{(3)}\tilde{\psi}_0\in P_{|\alpha|\leqslant a+3}$ follows from the fact that $\tilde{T}^{(3)}$ contains terms that are at most proportional to the third power of creation operators, and that $\tilde{\psi}_0\in G\subset P_{|\alpha|\leqslant a}$. Assuming that statement is true for $s=1,\ldots,n-1$, then it is trivially true for the first term in (9). Also, a simple calculation with ladder operators shows that $x^{\alpha}\varphi\in\mathrm{Ran}(P_{|\beta|\leqslant a+3(n-l)+|\alpha|})$ whenever $\varphi\in\mathrm{Ran}(P_{|\beta|\leqslant a+3(n-l)})$. Finally, we have $3(n-l)+2+l=3n+2(1-l)\leqslant 3n$ for $l=1,\ldots,n$. □

The set of recursive equations (8) is not suitable for the purpose of finding the sharp upper bounds for the R-S coefficients that we shall need later. It turns out to be convenient to transform the problem in the following way: Let $\{\Phi_\alpha(x)\}$ be a basis of eigenvectors of H_0. For a given eigenvalue e of H_0, let us define a new operator A_e by

$$A_e\Phi_\alpha(x) = \begin{cases} \Phi_\alpha(x), & \text{if } \Phi_\alpha(x)\in G, \\ |e-e_\alpha|^{-1/2}\Phi_\alpha(x), & \text{otherwise,} \end{cases}$$

where e_α is the eigenvalue associated to $\Phi_\alpha(x)$. Then extend A_e to the whole Hilbert space $\mathcal{H}$ by linearity. So defined, A_e is a bounded operator with unit norm but unbounded inverse. However, $\mathrm{Ran}(P_{|\alpha|\leqslant a+3n})$ is clearly in the domain of A_e^{-1} for each $n\in\mathbb{N}$. This fact allows us to consider the equivalent set of equations

$$H_e\psi_n+\sum_{l=1}^{n} T^{(l+2)}\psi_{n-l}=\sum_{l=1}^{n}\mathcal{E}_l A_e^2\psi_{n-l}, \tag{10}$$

where $H_e:=A_e(H_0-e)A_e$, $T^{(m)}:=A_e\tilde{T}^{(m)}A_e$, and $\psi_m=A_e^{-1}\tilde{\psi}_m$. The operator H_e satisfies

$$H_e\Phi_\alpha(x) = \begin{cases} 0, & \text{if } \Phi_\alpha(x)\in G, \\ \dfrac{e-e_\alpha}{|e-e_\alpha|}\Phi_\alpha(x), & \text{otherwise.} \end{cases}$$

Therefore the norm of H_e is equal to 1. In Sec. III we shall prove that both $|\mathcal{E}_n|$ and $\|\psi_n\|$ essentially grow as $b^n\sqrt{n!}$ for large n.

We conclude this section with an assortment of technical lemmas. Lemma 2 states certain estimates on the derivatives of the potential energy. In Lemma 3 we show a key upper bound to the norm of the operators $T^{(l)}P_{|\alpha|\leqslant n}$. Finally, in Lemma 4 we state results about certain expressions involving factorials that we shall use extensively in the sequel.

Lemma 2: Assume $V(x)$ satisfies H4. Then there are constants C_1 and C_2 such that, for $l\geqslant 1$,

$$\sum_{|\alpha|=l}\frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|}\leqslant C_1C_2^l.$$

If $V(x)$ also satisfies H5, then there exists a constant C_0 such that

$$\frac{\delta^{|\alpha|}}{\alpha!}|D^\alpha V(x)|\leqslant C_0\exp(2\tau x^2). \tag{11}$$

Proof: Let Γ_i be a circle of radius δ in the complex plane, centered at x_i. Then the Cauchy integral formula applied to $V(x)$, which makes sense because of hypothesis H4, states that for each multi-index $\alpha=(\alpha_1,\ldots,\alpha_d)$

$$D^\alpha V(x)=\frac{\alpha!}{(2\pi i)^d}\int_{\Gamma_1}dz_1\cdots\int_{\Gamma_d}dz_d\frac{V(z)}{\Pi_{i=1}^d(z_i-x_i)^{\alpha_i+1}},$$

which implies

$$|D^\alpha V(x)|\leqslant\frac{\alpha!}{\delta^{|\alpha|}}\max_{z_i\in\Gamma_i}|V(z)|. \tag{12}$$

Let us prove (11) first. Because of H5,

$$\max_{z_i\in\Gamma_i}|V(z)|\leqslant M\prod_{i=1}^{d}\max_{z_i\in\Gamma_i}\exp(\tau|z_i|^2)\leqslant M\prod_{i=1}^{d}\exp(\tau|x_i+\delta|^2)\leqslant M\exp(2d\tau\delta^2)\exp(2\tau x^2),$$

so (12) implies (11), after defining $C_0=M\exp(2d\tau\delta^2)$. If now the Γ_i's are circles centered at zero, we have (without assuming H5)

$$\frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|}\leqslant\max_{z_i\in\Gamma_i}|V(z)|=:c<\infty.$$

Then

$$\sum_{|\alpha|=l}\frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|}\leqslant c\sum_{|\alpha|=l}1$$

for all l. The last summation is the number of different ways to sum d non-negative integers such as the result is equal to l. That is,

$$\sum_{|\alpha|=l}1=\frac{(l+d-1)!}{l!(d-1)!}\leqslant\frac{1}{(d-1)!}(l+d-1)^{d-1}.$$

Therefore, we have

$$\sum_{|\alpha|=l}\frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|}\leqslant\frac{c}{(d-1)!}(l+d-1)^{d-1}\leqslant C_1C_2^l$$

with obvious definition of C_1, and C_2 being either equal to $(d-1)\max_{l\geqslant1}\log(l+d-1)/l$ (when $d>1$) or equal to 1 (when $d=1$). □

Lemma 3: For $|\alpha|\geqslant2$, $n\geqslant0$ *and some constant* $\gamma>0$,

$$\|A_e x^\alpha A_e P_{|\beta|\leqslant n}\|\leqslant\gamma^2\left(\frac{2}{\omega_0}\right)^{(|\alpha|-2)/2}\left[\frac{(n+|\alpha|-1)!}{(n+1)!}\right]^{1/2}.$$

As a consequence,

$$\|T^{(l)}P_{|\beta|\leqslant n}\|\leqslant C_3\kappa^{(l-2)/2}\left[\frac{(n+l-1)!}{(n+1)!}\right]^{1/2}$$

for some $C_3>0$ *and* $\kappa\geqslant2$.

Proof: For a single coordinate x_i, we have

$$x_i=\frac{1}{\sqrt{2\omega_i}}(a_i+a_i^*)\tag{13}$$

where a_i and a_i^* are the associated ladder operators. Consider any $\varphi=\Sigma_\beta d_\beta\Phi_\beta\in\mathcal{H}$. Define $J_G:=\{\text{multi-indices }\beta:\Phi_\beta\in G\}$. Then

$$\begin{aligned}a_i^*A_e\varphi&=\sum_{\beta\in J_G}d_\beta a_i^*\Phi_\beta+\sum_{\beta\notin J_G}d_\beta|e-e_\beta|^{-1/2}a_i^*\Phi_\beta\\&=\sum_{\beta\in J_G}d_\beta\sqrt{\beta_i+1}\,\Phi_{\beta+1_i}+\sum_{\beta\notin J_G}d_\beta|e-e_\beta|^{-1/2}\sqrt{\beta_i+1}\,\Phi_{\beta+1_i}\end{aligned}$$

where $\beta+1_i:=(\beta_1,\ldots,\beta_i+1,\ldots,\beta_d)$. Thus,

$$\|a_i^* A_e \varphi\|^2 = \sum_{\beta \in J_G} |d_\beta|^2 (\beta_i + 1) + \sum_{\beta \notin J_G} |d_\beta|^2 |e - e_\beta|^{-1} (\beta_i + 1)$$

$$\leqslant (1+a) \sum_{\beta \in J_G} |d_\beta|^2 + \sum_{\beta \notin J_G} |d_\beta|^2 |e - e_\beta|^{-1} (\beta_i + 1)$$

because $\beta \in J_G$ implies $\beta_i \leqslant |\beta| \leqslant a$. Moreover,

$$\frac{\beta_i + 1}{|e - e_\beta|} = \frac{1}{\omega_i} \frac{\omega_i (\beta_i + \frac{1}{2})}{|e - e_\beta|} + \frac{\frac{1}{2}}{|e - e_\beta|} \leqslant \frac{1}{\omega_i} \frac{e_\beta}{|e - e_\beta|} + \frac{\frac{1}{2}}{|e - e_\beta|}.$$

Since $\sigma(H_0)$ has no accumulation points and $e_\beta \neq e$ for all $\beta \notin J_G$, $\inf_{\beta \notin J_G} |e - e_\beta| > 0$. Furthermore, since $\lim_{|\beta| \to \infty} e_\beta |e - e_\beta|^{-1} = 1$, $\sup_{\beta \notin J_G} e_\beta |e - e_\beta|^{-1} < \infty$. Thus,

$$|e - e_\beta|^{-1} (\beta_i + 1) \leqslant \frac{1}{\omega_i} \sup_{\beta \notin J_G} e_\beta |e - e_\beta|^{-1} + \frac{1}{2} \sup_{\beta \notin J_G} |e - e_\beta|^{-1} =: K_1 < \infty,$$

which implies

$$\|a_i^* A_e\|^2 \leqslant \max\{(1+a), K_1\} \leqslant \max_{\{\omega_i\}} \max\{(1+a), K_1\}. \tag{14}$$

A similar calculation yields

$$\|a_i A_e\|^2 \leqslant \max\{|1-a|, K_2\} \leqslant \max_{\{\omega_i\}} \max\{|1-a|, K_2\} \tag{15}$$

for some $K_2 < \infty$. Therefore,

$$\|x_i A_e\| \leqslant \frac{1}{\sqrt{2\omega_i}} \|a_i A_e\| + \frac{1}{\sqrt{2\omega_i}} \|a_i^* A_e\| \leqslant \frac{1}{\sqrt{2\omega_0}} (\|a_i A_e\| + \|a_i^* A_e\|) \leqslant \gamma,$$

where ω_0 is the lowest eigenfrequency of H_0, and we use the sum of the right-hand sides of (14) and (15) to define γ. Taking the adjoint yields

$$\|A_e x_i\| \leqslant \gamma.$$

Since $|\alpha| \geqslant 2$, we can write $x^\alpha = x_i x^{\alpha'} x_j$ for some x_i, x_j, with $|\alpha'| = |\alpha| - 2$. Then

$$\begin{aligned} \|A_e x^\alpha A_e P_{|\beta| \leqslant n}\| &\leqslant \|A_e x_i x^{\alpha'} P_{|\beta| \leqslant n+1} x_j A_e P_{|\beta| \leqslant n}\| \\ &\leqslant \|A_e x_i\| \|x_j A_e\| \|x^{\alpha'} P_{|\beta| \leqslant n+1}\| \\ &\leqslant \gamma^2 \left(\frac{2}{\omega_0}\right)^{|\alpha'|/2} \left[\frac{(n + |\alpha'| + 1)!}{(n+1)!}\right]^{1/2} \\ &= \gamma^2 \left(\frac{2}{\omega_0}\right)^{(|\alpha| - 2)/2} \left[\frac{(n + |\alpha| - 1)!}{(n+1)!}\right]^{1/2}, \end{aligned} \tag{16}$$

where we use Lemma 5.1 of Ref. 4 to bound $\|x^{\alpha'} P_{|\beta| \leqslant n+1}\|$. The last statement follows from the definition of $T^{(l)}$ and the first part of Lemma 2, along with the definitions $C_3 = C_1 \gamma^2 \delta^{-2} C_2^2$ and $\kappa = \max\{2, 2\omega_0^{-1} \delta^{-2} C_2^2\}$. □

Lemma 4: Let $\kappa \geqslant 2$ be the number defined in Lemma 3. Then we have the following.

(1) For each integer $a \geqslant 0$ there is a constant $C_4 = C_4(a)$ so that, for all $m \geqslant 0$,

$$\sum_{l=0}^{m}\left[\frac{(1+a+m-l)!(1+a+l)!}{(1+a+m)!}\right]^{1/2}\leqslant C_4.$$

(2) For all $a\geqslant -1$ *there is a constant* C_5 *so that, for all* $m\geqslant 0$,

$$\sum_{l=0}^{m}\kappa^{-5l/2}\left[\frac{(1+a+3m-2l)!(1+a+m-l)!}{(1+a+3m-3l)!(1+a+m)!}\right]^{1/2}\leqslant C_5.$$

(3) For each $a\geqslant 0$ *there is a constant* $C_6=C_6(a)$ *so that, for all* $m\geqslant 0$,

$$\sum_{l=1}^{m}\kappa^{-5l/2}\left[\frac{(1+a+m-l)!(1+a+l)!}{(1+a)!(a+m)!}\right]^{1/2}\leqslant C_6.$$

Proof: Statements (1) and (2) are shown in Lemma 2 of Ref. 19. To prove (3), notice that for $1\leqslant l\leqslant m-1$ we have

$$\frac{(1+a+l)!(1+a+m-l)!}{(a+m)!(1+a)!}=(1+a+l)\frac{\prod_{s=1}^{m-l}(1+a+s)}{\prod_{s=l}^{m-1}(1+a+s)}=(1+a+l)\prod_{s=1}^{m-l}\frac{1+a+s}{l+a+s}\leqslant 1+a+l.$$

Therefore

$$\sum_{l=1}^{m}\kappa^{-5l/2}\left[\frac{(1+a+l)!(1+a+m-l)!}{(a+m)!(1+a)!}\right]^{1/2}\leqslant\sum_{l=1}^{m}\kappa^{-5l/2}(1+a+l)^{1/2},$$

where the right-hand side converges to some constant $C_6(a)<\infty$. □

III. COMPUTATION OF THE R-S COEFFICIENTS

Let us assume that the zeroth-order eigenvalue e is g-fold degenerate, with associated eigenspace G. We allow g to be equal to 1. Let P be the projector onto G and $Q:=1-P$. Up to zeroth-order, ψ_0 can be any vector in G, which we may require to be normalized, $\|\psi_0\|=1$. Two cases may arise from solving (10) at higher order. Either the zeroth-order degeneracy is preserved at all orders, or it is removed to some extent at higher order. Let us start by discussing the former case, which trivially includes the nondegenerate one.

A. Degeneracy is preserved

Fix $\psi_0\in G$, with $\|\psi_0\|=1$. The first-order equation is

$$H_e\psi_1+T^{(3)}\psi_0=\mathcal{E}_1A_e^2\psi_0. \tag{17}$$

Let us multiply by P. Noting that $PH_e=0$ and $PA_e^2\psi_0=\psi_0$, we obtain

$$PT^{(3)}P\psi_0=\mathcal{E}_1\psi_0.$$

This is the secular equation for the finite-dimensional, self-adjoint operator $\Lambda^{(1)}:=PT^{(3)}P$. Since we assume that the zeroth-order degeneracy is not broken at any order, $\Lambda^{(1)}$ must have only one eigenvalue. Let us call it λ_1. Then $\mathcal{E}_1=\lambda_1$. Now multiply (17) by Q. We obtain

$$H_eQ\psi_1=-QT^{(3)}\psi_0.$$

Let us introduce more notation. For any vector $\psi\in\mathcal{H}$, define $\psi^{\parallel}:=P\psi$ and $\psi^{\perp}:=Q\psi$. Also, let $(H_e)_{\perp}$ be the restriction of H_e to $\mathrm{Ran}(Q)$. So defined, $(H_e)_{\perp}$ is invertible. Then we have

$$\psi_1^{\perp}=\Xi^{(1,\perp)}\psi_0,$$

where $\Xi^{(1,\perp)}:=(H_e)_\perp^{-1}(-QT^{(3)})$. So far $\psi_1^\parallel$ remains undefined.

The second-order equation is

$$H_e\psi_2+T^{(3)}\psi_1+T^{(4)}\psi_0=\mathcal{E}_2A_e^2\psi_0+\lambda_1A_e^2\psi_1. \tag{18}$$

Multiply (18) by P. After some algebra involving the definitions of $\Lambda^{(1)}$ and $\Xi^{(1,\perp)}$, we obtain

$$(PT^{(3)}\Xi^{(1,\perp)}P+PT^{(4)}P)\psi_0=\mathcal{E}_2\psi_0.$$

Then $\mathcal{E}_2$ has to be equal to the unique eigenvalue of

$$\Lambda^{(2)}:=P(T^{(3)}\Xi^{(1,\perp)}+T^{(4)})P.$$

That is, $\mathcal{E}_2=\lambda_2$. Now multiply (18) by Q to obtain

$$H_e\psi_2^\perp+QT^{(3)}(\psi_1^\parallel+\psi_1^\perp)+QT^{(4)}\psi_0=\lambda_1A_e^2\psi_1^\perp,$$

which yields

$$\psi_2^\perp=\Xi^{(2,\perp)}\psi_0+\Xi^{(1,\perp)}\psi_1^\parallel,$$

where we define

$$\Xi^{(2,\perp)}:=(H_e)_\perp^{-1}[(\lambda_1A_e^2-QT^{(3)})\Xi^{(1,\perp)}+QT^{(4)}]$$

and no requirement is imposed on either $\psi_2^\parallel$ or $\psi_1^\parallel$.

The third-order equation is

$$H_e\psi_3+T^{(3)}\psi_2+T^{(4)}\psi_1+T^{(5)}\psi_0=\mathcal{E}_3A_e^2\psi_0+\lambda_2A_e^2\psi_1+\lambda_1A_e^2\psi_2.$$

Following the procedure already described, we obtain

$$\Lambda^{(3)}\psi_0=\mathcal{E}_3\psi_0,$$

where

$$\Lambda^{(3)}:=P(T^{(3)}\Xi^{(2\perp)}+T^{(4)}\Xi^{(1,\perp)}+T^{(5)})P$$

has only one eigenvalue λ_3. Thus $\mathcal{E}_3=\lambda_3$. Also

$$\psi_3^\perp=\Xi^{(3,\perp)}\psi_0+\Xi^{(2,\perp)}\psi_1^\parallel+\Xi^{(1,\perp)}\psi_2^\parallel,$$

where

$$\Xi^{(3,\perp)}:=(H_e)_\perp^{-1}[(\lambda_1A_e^2-QT^{(3)})\Xi^{(2,\perp)}+(\lambda_2A_e^2-QT^{(4)})\Xi^{(1,\perp)}-QT^{(5)}]$$

and nothing is said about $\psi_3^\parallel$, $\psi_2^\parallel$ or $\psi_1^\parallel$.

As one can see, $\mathcal{E}_n$ and $\psi_n^\perp$ can be calculated through recursive definition of certain operators. The form of these operators is now easy to guess:

Proposition 1: For $n=1,2,\ldots$, *recursively define*

$$\Xi^{(1,\perp)}:=-(H_e)_\perp^{-1}QT^{(3)},$$

$$\Xi^{(n,\perp)}:=(H_e)_\perp^{-1}\left[-QT^{(n+2)}+\sum_{p=1}^{n-1}(\lambda_{n-p}A_e^2-QT^{(n+2-p)})\Xi^{(p,\perp)}\right],$$

where λ_l *is, by assumption, the unique eigenvalue of*

$$\Lambda^{(l)} := PT^{(l+2)}P + \sum_{p=1}^{n-1} PT^{(l+2-p)}\Xi^{(p,\perp)}P.$$

Then, given $\psi_0 \in G$, $\mathcal{E}_n = \lambda_n$ *and*

$$\psi_n = \Xi^{(n,\perp)}\psi_0 + \sum_{p=1}^{n-1} \Xi^{(n-p,\perp)}\psi_p^{\parallel} + \psi_n^{\parallel},$$

where $\psi_1^{\parallel}, \ldots, \psi_n^{\parallel}$ *are vectors arbitrarily chosen from* G.

This construction will be generalized in Proposition 2, from which the proof of Proposition 1 can be easily read out. To rule out arbitrariness, we set $\psi_n^{\parallel} = 0$ for all $n \geqslant 1$, which is equivalent to absorbing those vectors into ψ_0 and renormalizing.

The recursive expressions for the operators $\Lambda^{(n)}$ and $\Xi^{(n,\perp)}$ can be translated into recursive expressions for $\mathcal{E}_n$ and ψ_n. The result is

$$\mathcal{E}_n = \sum_{p=0}^{n-1} \langle T^{(n+2-p)} P_{|\alpha| \leqslant a} \psi_0, \psi_p \rangle,$$

$$\psi_n = (H_e)_{\perp}^{-1} \left[-QT^{(n+2)}\psi_0 + \sum_{p=1}^{n-1} (\mathcal{E}_{n-p}A_e^2 - QT^{(n+2-p)})\psi_p \right].$$

Furthermore, we can easily obtain the following inequalities:

$$|\mathcal{E}_n| \leqslant \sum_{l=1}^{n} \|T^{(l+2)} P_{|j| \leqslant a}\| \|\psi_{n-l}\|,$$

$$\|\psi_n\| \leqslant \sum_{l=1}^{n-1} |\mathcal{E}_l| \|\psi_{n-l}\| + \sum_{l=1}^{n} \|T^{(l+2)} P_{|j| \leqslant a+3(n-l)}\| \|\psi_{n-l}\|.$$

By resorting to Lemma 3, we finally obtain

$$|\mathcal{E}_n| \leqslant C_3 \sum_{l=1}^{n} \kappa^{l/2} \left[\frac{(1+a+l)!}{(1+a)!} \right]^{1/2} \|\psi_{n-l}\|,$$

$$\|\psi_n\| \leqslant \sum_{l=1}^{n-1} |\mathcal{E}_l| \|\psi_{n-l}\| + C_3 \sum_{l=1}^{n} \kappa^{l/2} \left[\frac{(1+a+3n-2l)!}{(1+a+3n-3l)!} \right]^{1/2} \|\psi_{n-l}\|.$$

As an immediate consequence, we have the following.

Theorem 1: *For each* $a \geqslant 0$, *there is* $b > 0$ *so that*

$$|\mathcal{E}_n| \leqslant \kappa^{3n} b^n [(1+a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n} b^n [(1+a+n)!]^{1/2},$$

for all $n \geqslant 1$.

A proof of this theorem is in Ref. 19, where the somewhat simpler one-dimensional problem is discussed. Alternatively, one can modify the proof of Theorem 3.2 below to get somewhat tighter bounds.

B. Degeneracy is removed

Let us examine the case where the zeroth-order degeneracy is partially removed only at first order.

First-order: Now the operator $\Lambda^{(1)}=PT^{(3)}P$ has $k\geqslant 2$ distinct eigenvalues $\lambda_{1,1},\ldots,\lambda_{1,k}$. Let $G_1,\ldots,G_k$ be the corresponding eigenspaces, and let $P^{(1)},\ldots,P^{(k)}$ be their orthogonal projections. Set $\mathcal{E}_1=\lambda_{1,i}$. Then ψ_0 must lie in G_i. As before, $\psi_1^{\perp}=\Xi^{(1,\perp)}\psi_0$ with $\Xi(1,\perp) \coloneqq(He)\perp-1(-QT(3))$.

Second-order: Because of the choice for $\mathcal{E}_1$ we have

$$H_e\psi_2+T^{(3)}\psi_1+T^{(4)}\psi_0=\mathcal{E}_2A_e^2\psi_0+\lambda_{1,i}A_e^2\psi_1. \tag{19}$$

Multiply (19) by $P^{(j)}$

$$P^{(j)}T^{(3)}\psi_1+P^{(j)}T^{(4)}\psi_0=\mathcal{E}_2P^{(j)}\psi_0+\lambda_{1,i}P^{(j)}\psi_1. \tag{20}$$

Note that $P=\Sigma_{j=1}^{k}P^{(j)}$. Then, for any vector ψ, we have $\psi^{\|}=\Sigma_{j=1}^{k}\psi^{(j)}$. On the other hand,

$$P^{(j)}T^{(3)}\psi^{\|}=\sum_{l=1}^{k}P^{(j)}PT^{(3)}PP^{(l)}\psi^{\|}=\sum_{l=1}^{k}P^{(j)}\Lambda^{(1)}P^{(l)}\psi^{\|}=\sum_{l=1}^{k}\lambda_{1,l}P^{(j)}P^{(l)}\psi^{\|}=\lambda_{1,j}\psi^{(j)}. \tag{21}$$

Therefore, $\Sigma_{l\neq i}P^{(i)}T^{(3)}\psi_n^{(l)}=0$. The identity (21) yields

$$P^{(j)}T^{(3)}\psi_1=P^{(j)}T^{(3)}\psi_1^{\|}+P^{(j)}T^{(3)}\psi_1^{\perp}=\lambda_{1,j}\psi_1^{(j)}+P^{(j)}T^{(3)}\psi_1^{\perp}. \tag{22}$$

Now insert (22) into (20). For $j=i$ we have

$$P^{(i)}T^{(4)}\psi_0+P^{(i)}T^{(3)}\psi_1^{\perp}=\mathcal{E}_2\psi_0.$$

Define

$$\Lambda^{(2,i)}\coloneqq P^{(i)}(T^{(4)}+T^{(3)}\Xi^{(1,\perp)})P^{(i)}.$$

Then we obtain $\Lambda^{(2,i)}\psi_0=\mathcal{E}_2\psi_0$. By assumption $\Lambda^{(2,i)}$ has only one eigenvalue $\lambda_{2,i}$. Therefore $\mathcal{E}_2=\lambda_{2,i}$.

For $j\neq i$ we have

$$P^{(j)}T^{(4)}\psi_0+P^{(j)}T^{(3)}\psi_1^{\perp}+\lambda_{1,j}\psi_1^{(j)}=\lambda_{1,i}P^{(j)}\psi_1$$

because $P^{(j)}\psi_0=0$ whenever $j\neq i$. Rearranging terms we finally obtain $\psi_1^{(j)}=\Xi^{(1,j)}\psi_0$, where we define

$$\Xi^{(1,j)}\coloneqq(\lambda_{1,i}-\lambda_{1,j})^{-1}P^{(j)}(T^{(4)}+T^{(3)}\Xi^{(1,\perp)})P^{(i)}. \tag{23}$$

So far no requirement is imposed to $\psi_1^{(i)}$.

Now multiply (19) by Q,

$$H_e\psi_2^{\perp}+QT^{(4)}\psi_0+QT^{(3)}\psi_1=\lambda_{1,i}A_e^2\psi_1^{\perp}. \tag{24}$$

Since

$$QT^{(3)}\psi_1=QT^{(3)}\psi_1^{\perp}+\sum_{l\neq i}QT^{(3)}\psi_1^{(l)}+QT^{(3)}\psi_1^{(i)}$$

$$=QT^{(3)}\Xi^{(1,\perp)}\psi_0+\sum_{l\neq i}QT^{(3)}\Xi^{(1,l)}\psi_0+QT^{(3)}\psi_1^{(i)},$$

(24) yields

$$H_e\psi_2^{\perp} = -QT^{(4)}\psi_0 + \lambda_{1,i}A_e^2\Xi^{(1,\perp)}\psi_0 - QT^{(3)}\Xi^{(1,\perp)}\psi_0 - \sum_{l\neq i} QT^{(3)}\Xi^{(1,l)}\psi_0 - QT^{(3)}\psi_1^{(i)}.$$

From there we obtain

$$\psi_2^{\perp} = \Xi^{(2,\perp)}\psi_0 + \Xi^{(1,\perp)}\psi_1^{(i)},$$

where

$$\Xi^{(2,\perp)} := (H_e)_{\perp}^{-1}\left[\lambda_{1,i}\Xi^{(1,\perp)}A_e^2 - QT^{(3)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) - QT^{(4)}\right].$$

Third-order:

$$H_e\psi_3 + T^{(3)}\psi_2 + T^{(4)}\psi_1 + T^{(5)}\psi_0 = \mathcal{E}_3A_e^2\psi_0 + \lambda_{2,i}A_e^2\psi_1 + \lambda_{1,i}A_e^2\psi_2. \tag{25}$$

Multiply by $P^{(j)}$, rearrange terms, and use (21) to obtain

$$\begin{aligned}
\mathcal{E}_3P^{(j)}\psi_0 &= P^{(j)}T^{(3)}\psi_2 + P^{(j)}T^{(4)}\psi_1 + P^{(j)}T^{(5)}\psi_0 - \lambda_{2,i}\psi_1^{(j)} - \lambda_{1,i}\psi_2^{(j)} \\
&= P^{(j)}T^{(3)}(\psi_2^{\perp} + \psi_2^{\parallel}) + P^{(j)}T^{(4)}\left(\psi_1^{\perp} + \sum_{l\neq i}\psi_1^{(l)} + \psi_1^{(i)}\right) \\
&\quad + P^{(j)}T^{(5)}\psi_0 - \lambda_{2,i}\psi_1^{(j)} - \lambda_{1,i}\psi_2^{(j)} \\
&= P^{(j)}T^{(3)}\psi_2^{\perp} + P^{(j)}T^{(4)}\left(\psi_1^{\perp} + \sum_{l\neq i}\psi_1^{(i)} + \psi_1^{(i)}\right) \\
&\quad + P^{(j)}T^{(5)}\psi_0 - (\lambda_{1,i} - \lambda_{1,j})\psi_2^{(j)} - \lambda_{2,i}\psi_1^{(j)}.
\end{aligned} \tag{26}$$

For $j = i$ we have

$$\begin{aligned}
\mathcal{E}_3\psi_0 &= P^{(i)}T^{(3)}\Xi^{(2,\perp)}\psi_0 + P^{(i)}T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right)\psi_0 \\
&\quad + P^{(i)}T^{(5)}\psi_0 + P^{(i)}T^{(3)}\Xi^{(1,\perp)}\psi_1^{(i)} + P^{(i)}T^{(4)}\psi_1^{(i)} - \lambda_{2,i}\psi_1^{(i)}.
\end{aligned}$$

Let us note that

$$P^{(i)}T^{(4)}\psi^{(i)} + P^{(i)}T^{(3)}\Xi^{(1,\perp)}\psi^{(i)} = \Lambda^{(2,i)}\psi^{(i)} = \lambda_{2,i}\psi^{(i)}.$$

Thus we obtain $\mathcal{E}_3\psi_0 = \Lambda^{(3,i)}\psi_0$, where

$$\Lambda^{(3,i)} := P^{(i)}\left[T^{(5)} + T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) + T^{(3)}\Xi^{(2,\perp)}\right]P^{(i)}.$$

By assumption $\Lambda^{(3,i)}$ has only one eigenvalue $\lambda_{3,i}$ so $\mathcal{E}_3 = \lambda_{3,i}$.

Now for $j \neq i$ we can rewrite (26) as

$$\begin{aligned}
(\lambda_{1,i} - \lambda_{1,j})\psi_2^{(j)} &= P^{(j)}T^{(5)}\psi_0 + P^{(j)}T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right)\psi_0 + P^{(j)}T^{(3)}\Xi^{(2,\perp)}\psi_0 - \lambda_{2,i}\Xi^{(1,j)}\psi_0 \\
&\quad + P^{(j)}T^{(3)}\Xi^{(1,\perp)}\psi_1^{(i)} + P^{(j)}T^{(4)}\psi_1^{(i)}.
\end{aligned}$$

Now use (23) and define

$$\Xi^{(2,j)}:=(\lambda_{1,i}-\lambda_{1,j})^{-1}P^{(j)}\left[T^{(5)}+T^{(4)}\left(\Xi^{(1,\perp)}+\sum_{l\neq i}\Xi^{(1,l)}\right)+T^{(3)}\Xi^{(2,\perp)}-\lambda_{2,i}\Xi^{(1,j)}\right]P^{(i)}$$

to obtain

$$\psi_2^{(j)}=\Xi^{(2,j)}\psi_0+\Xi^{(1,j)}\psi_1^{(i)}.$$

The last step is to multiply (25) by Q,

$$H_e\psi_3^{\perp}=Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2+Q(\lambda_{2,i}A_e^2-T^{(4)})\psi_1-QT^{(5)}\psi_0. \tag{27}$$

We have

$$\begin{aligned}Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2&=Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2^{\perp}+\lambda_{1,i}A_e^2Q\psi_2^{\parallel}-QT^{(3)}\sum_{l\neq i}\psi_2^{(l)}-QT^{(3)}\psi_2^{(i)}\\&=Q(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(2,\perp)}\psi_0+Q(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(1,i)}\psi_1^{(i)}\\&\quad-QT^{(3)}\sum_{l\neq i}\Xi^{(2,l)}\psi_0-QT^{(3)}\sum_{l\neq i}\Xi^{(1,l)}\psi_1^{(i)}-QT^{(3)}\psi_2^{(i)}\\&=-QT^{(3)}\psi_2^{(i)}+Q\left[(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(1,\perp)}-\sum_{l\neq i}T^{(3)}\Xi^{(1,l)}\right]\psi_1^{(1)}\\&\quad+Q\left[(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(2,\perp)}-\sum_{l\neq i}T^{(3)}\Xi^{(2,l)}\right]\psi_0,\end{aligned} \tag{28}$$

and similarly

$$Q(\lambda_{2,i}A_e^2-T^{(4)})\psi_1=Q\left[(\lambda_{2,i}A_e^2-T^{(4)})\Xi^{(1,\perp)}-\sum_{l\neq i}T^{(4)}\Xi^{(1,l)}\right]\psi_0-QT^{(4)}\psi_1^{(i)}. \tag{29}$$

Insert (28) and (29) in (27) and multiply the whole equation by $(H_e)_{\perp}^{-1}$ to obtain

$$\psi_3^{\perp}=\Xi^{(3,\perp)}\psi_0+\Xi^{(2,\perp)}\psi_1^{(i)}+\Xi^{(1,\perp)}\psi_2^{(i)}$$

with

$$\begin{aligned}\Xi^{(3,\perp)}:=(H_e)_{\perp}^{-1}\Bigg[&(\lambda_{1,i}\Xi^{(2,\perp)}+\lambda_{2,i}\Xi^{(1,\perp)})A_e^2-QT^{(5)}-QT^{(4)}\left(\Xi^{(1,\perp)}+\sum_{l\neq i}\Xi^{(1,l)}\right)\\&-QT^{(5)}\left(\Xi^{(2,\perp)}+\sum_{l\neq i}\Xi^{(2,l)}\right)\Bigg].\end{aligned}$$

As before, one can guess the solution for arbitrary n. Let us summarize hypotheses and results:

Proposition 2: Define

$$\Lambda^{(1)}:=PT^{(3)}P,$$

$$\Xi^{(1,\perp)}:=-(H_e)_{\perp}^{-1}QT^{(3)}.$$

Suppose that $\Lambda^{(1)}$ *has* k *distinct eigenvalues* $\lambda_{1,1},\ldots,\lambda_{1,k}$ *with eigenspaces* $G_1,\ldots,G_k$. *Let* $P^{(1)},\ldots,P^{(k)}$ *be the associated projection operators. Given* $1\leqslant i\leqslant k$ *and* $j\neq i$, *set*

$$\Lambda^{(2,i)}:=P^{(i)}(T^{(4)}+T^{(3)}\Xi^{(1,\perp)})P^{(i)},$$

$$\Xi^{(1,j)}:=(\lambda_{1,i}-\lambda_{1,j})^{-1}P^{(j)}(T^{(4)}+T^{(3)}\Xi^{(1,\perp)})P^{(i)},$$

$$\Xi^{(2,\perp)}:=(H_e)_{\perp}^{-1}\left[\lambda_{1,i}\Xi^{(1,\perp)}A_e^2-QT^{(4)}-QT^{(3)}\left(\Xi^{(1,\perp)}+\sum_{l\neq i}\Xi^{(1,l)}\right)\right].$$

And then recursively define

$$\Lambda^{(n,i)}:=P^{(i)}\left(T^{(n+2)}+\sum_{s=1}^{n-1}T^{(n+2-s)}\Xi^{(s,\perp)}+\sum_{s=1}^{n-2}\sum_{l\neq i}T^{(n+2-s)}\Xi^{(s,l)}\right)P^{(i)},$$

$$\Xi^{(n-1,j)}:=(\lambda_{1,i}-\lambda_{1,j})^{-1}P^{(j)}\left(T^{(n+2)}+\sum_{s=1}^{n-1}T^{(n+2-s)}\Xi^{(s,\perp)}+\sum_{s=1}^{n-2}\sum_{l\neq i}T^{(n+2-s)}\Xi^{(s,l)}-\sum_{s=2}^{n-1}\lambda_{s,i}\Xi^{(n-s,j)}\right)P^{(i)},$$

$$\Xi^{(n,\perp)}:=(H_e)_{\perp}^{-1}\left[\sum_{s=1}^{n-1}\lambda_{s,i}\Xi^{(n-s,\perp)}A_e^2-QT^{(n+2)}-\sum_{s=1}^{n-1}QT^{(s+2)}\left(\Xi^{(n-s,\perp)}+\sum_{l\neq i}\Xi^{(n-s,l)}\right)\right],$$

where $\lambda_{s,i}$ *is, by assumption, the unique eigenvalue of* $\Lambda^{(s,i)}$ *when* $s\geqslant 2$.

Let $\mathcal{E}_n,\psi_n$ *be the R-S coefficients. Then* $\mathcal{E}_1$ *has to be equal to one of the eigenvalues of* $\Lambda^{(1)}$, *let us say* $\mathcal{E}_1=\lambda_{1,i}$. *Consequently,* $\psi_0\in G_i$ *and*

$$\mathcal{E}_n=\lambda_{n,i}, \tag{30}$$

$$\psi_{n-1}^{(j)}=\Xi^{(n-1,j)}\psi_0+\sum_{s=1}^{n-1}\Xi^{(n-s-1,j)}\psi_s^{(i)}, \tag{31}$$

$$\psi_n^{\perp}=\Xi^{(n,\perp)}\psi_0+\sum_{s=1}^{n-1}\Xi^{(n-s,\perp)}\psi_s^{(i)}, \tag{32}$$

$$\psi_n=\psi_n^{\perp}+\sum_{j\neq i}\psi_n^{(j)}+\psi_n^{(i)}.$$

The vectors $\psi_1^{(i)},\ldots,\psi_n^{(i)}$ *are arbitrarily chosen from* G_i.

Proof: Use mathematical induction. Because of the discussion above, we only have to prove the inductive step. Thus, let us assume that $\mathcal{E}_m$, $\psi_{m-1}^{(j)}$ and $\psi_m^{\perp}$ are given by (30)–(32), for $m=2,\ldots,n$. Let us compute $\mathcal{E}_{n+1}$, $\psi_n^{(j)}$ and $\psi_{n+1}^{\perp}$. The $(n+1)$-st-order equation is

$$H_e\psi_{n+1}+\sum_{p=0}^{n}T^{(n+3-p)}\psi_p=\sum_{s=0}^{n}\mathcal{E}_{n+1-s}A_e^2\psi_s. \tag{33}$$

We have

$$\sum_{p=0}^{n} T^{(n+3-p)}\psi_p = T^{(n+3)}\psi_0 + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{\perp} + \sum_{p=1}^{n} T^{(n+3-p)}\sum_{l\neq i}\psi_p^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}$$

$$= T^{(n+3)}\psi_0 + T^{(n+2)}\Xi^{(1,\perp)}\psi_0 + \sum_{p=2}^{n} T^{(n+3-p)}\left(\Xi^{(p,\perp)}\psi_0 + \sum_{s=1}^{p-1}\Xi^{(p-s,\perp)}\psi_s^{(i)}\right)$$

$$+ d\sum_{l\neq i} T^{(n+2)}\Xi^{(1,l)}\psi_0 + \sum_{p=2}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\left(\Xi^{(p,l)}\psi_0 + \sum_{s=1}^{p-1}\Xi^{(p-s,l)}\psi_s^{(i)}\right)$$

$$+ \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}$$

$$= \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-1}\sum_{p=s+1}^{n} T^{(n+3-p)}\Xi^{(p-s,\perp)}\psi_s^{(i)}$$

$$+ \sum_{s=1}^{n-2}\sum_{p=s+1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p-s,l)}\psi_s^{(i)} + \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)}\psi_s^{(i)}$$

$$= \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-1}\sum_{m=1}^{n-s} T^{(n+3-s-m)}\Xi^{(m,\perp)}\psi_s^{(i)} + \sum_{s=1}^{n-2}\sum_{m=1}^{n-1-s}\sum_{l\neq i} T^{(n+3-s-m)}\Xi^{(m,l)}\psi_s^{(i)}$$

$$+ \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)}\psi_s^{(i)}$$

where we use that $\Sigma_{p=1}^{r}\Sigma_{s=1}^{p-1}F_{sp} = \Sigma_{s=1}^{r-1}\Sigma_{p=s+1}^{r}F_{sp}$ and then we change index $p\to m = p-s$. Let us multiply (33) by $P^{(i)}$. Since $P^{(i)}H_e = 0$ and $P^{(i)}A_e^2 = A_e^2P^{(i)} = P^{(i)}$, we obtain

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p = \mathcal{E}_{n+1}\psi_0 + \sum_{s=1}^{n}\lambda_{n+1-s,i}\psi_s^{(i)}. \tag{34}$$

The left-hand side can be written as

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p = P^{(i)}\left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-2} P^{(i)}\left(T^{(n+3-s)} + \sum_{m=1}^{n-s} T^{(n+3-s-m)}\Xi^{(m,\perp)}\right.$$

$$\left. + \sum_{m=1}^{n-1-s}\sum_{l\neq i} T^{(n+3-s-m)}\Xi^{(m,l)}\right)\psi_s^{(i)} + P^{(i)}\left(T^{(3)}\Xi^{(1,\perp)} + T^{(4)}\right)\psi_{n-1}^{(i)}$$

$$+ \sum_{l\neq i} P^{(i)}T^{(3)}\psi_n^{(l)} + P^{(i)}T^{(3)}\psi_n^{(i)}.$$

By the argument that leads to (21), we know that $\Sigma_{l\neq i}P^{(i)}T^{(3)}\psi_n^{(l)} = 0$. Also $\psi_s^{(i)} = P^{(i)}\psi_s^{(i)}$. Then

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p=\Lambda^{(n+1,i)}\psi_0+\sum_{s=1}^{n}\Lambda^{(n+1-s,i)}\psi_s^{(i)}. \tag{35}$$

Inserting (35) into (34) we conclude

$$\Lambda^{(n+1,i)}\psi_0=\mathcal{E}_{n+1}\psi_0.$$

Now let us multiply (33) by $P^{(j)}$ for $j\neq i$. Since $P^{(j)}\psi_0=0$, we have

$$\lambda_{1,i}\psi_n^{(j)}=\sum_{p=0}^{n} P^{(j)}T^{(n+3-p)}\psi_p-\sum_{s=1}^{n-1}\lambda_{n+1-s,i}\psi_s^{(j)}. \tag{36}$$

The right-hand side can be manipulated in the same way as before. The result is

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p-\sum_{s=1}^{n-1}\lambda_{n+1-s,i}\psi_s^{(j)}=(\lambda_{1,i}-\lambda_{1,j})\Xi^{(n,j)}\psi_0+\sum_{s=1}^{n-1}(\lambda_{1,i}-\lambda_{1,j})\Xi^{(n-s,j)}\psi_s^{(i)}$$
$$+\sum_{l=1}^{k} P^{(j)}T^{(3)}\psi_n^{(l)}.$$

As proven in (21), the last term above is equal to $\lambda_{1,j}\psi_n^{(j)}$. Thus (36) leads to

$$\psi_n^{(j)}=\Xi^{(n,j)}\psi_0+\sum_{s=1}^{n-1}\Xi^{(n-s,j)}\psi_s^{(i)}.$$

Finally, multiply (33) by Q,

$$H_e\psi_{n+1}^{\perp}=\sum_{p=1}^{n}\lambda_{n+1-p,i}A_e^2\psi_p^{\perp}-\sum_{p=0}^{n}QT^{(n+3-p)}\psi_p. \tag{37}$$

For the first term we have

$$\sum_{p=1}^{n}\lambda_{n+1-p,i}A_e^2\psi_p^{\perp}=\sum_{s=1}^{n}\lambda_{n+1-s,i}A_e^2\Xi^{(s,\perp)}\psi_0+\sum_{p=2}^{n}\sum_{s=1}^{p-1}\lambda_{n+1-p,i}A_e^2\Xi^{(p-s,\perp)}\psi_s^{(i)}$$
$$=\sum_{s=1}^{n}\lambda_{n+1-s,i}A_e^2\Xi^{(s,\perp)}\psi_0+\sum_{s=1}^{n-1}\sum_{m=1}^{n-s}\lambda_{n+1-s-m,i}A_e^2\Xi^{(m,\perp)}\psi_s^{(i)},$$

and for the second one

$$\sum_{p=0}^{n}QT^{(n+3-p)}\psi_p=Q\left(T^{(n+3)}+\sum_{p=1}^{n}T^{(n+3-p)}\Xi^{(p,\perp)}+\sum_{p=1}^{n-1}\sum_{l\neq i}T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$
$$+\sum_{s=1}^{n-2}Q\left(T^{(n+3-s)}+\sum_{m=1}^{n-s}T^{(n+3-s-m)}\Xi^{(m,\perp)}\right.$$
$$\left.+\sum_{m=1}^{n-1-s}\sum_{l\neq i}T^{(n+3-s-m)}\Xi^{(m,l)}\right)\psi_s^{(i)}+\quad Q(T^{(3)}\Xi^{(1,\perp)}+T^{(4)})\psi_{n-1}^{(i)}$$
$$+\sum_{l\neq i}QT^{(3)}\psi_n^{(l)}+QT^{(3)}\psi_n^{(i)}.$$

Then insert these expressions into (37). After multiplying the whole equation by $(H_e)_\perp^{-1}$ we obtain the desired result. □

As before, we set $\psi_n^{(i)}=0$ for all $n=1,2,\ldots$. Consequently, ψ_n will be orthogonal to ψ_0 and

$$\psi_n=\left(\Xi^{(n,\perp)}+\sum_{l\neq i}\Xi^{(n,l)}\right)\psi_0.$$

The following expressions will be useful later:

$$\Lambda^{(n,i)}\psi_0=P^{(i)}T^{(n+2)}\psi_0+\sum_{s=1}^{n-2}P^{(i)}T^{(n+2-s)}\psi_s+P^{(i)}T^{(3)}\psi_{n-1}^{\perp}, \tag{38}$$

$$\psi_n^{\perp}=(H_e)_\perp^{-1}\left[\sum_{s=1}^{n-1}\mathcal{E}_sA_e^2\psi_{n-s}^{\perp}-QT^{(n+2)}\psi_0-\sum_{s=1}^{n-1}QT^{(s+2)}\psi_{n-s}\right], \tag{39}$$

$$\psi_{n-1}^{(j)}=(\lambda_{1,i}-\lambda_{1,j})^{-1}\left(P^{(j)}T^{(n+2)}\psi_0+\sum_{s=1}^{n-2}P^{(j)}T^{(n+2-s)}\psi_s+P^{(j)}T^{(3)}P_{|j|\leqslant a+3(n-1)}\psi_{n-1}^{\perp}-\sum_{s=2}^{n-1}\mathcal{E}_s\psi_{n-s}^{(j)}\right). \tag{40}$$

Next, let us estimate the growth of these coefficients. Since $\mathcal{E}_n\psi_0=\Lambda^{(n,i)}\psi_0$,

$$\begin{aligned}|\mathcal{E}_n|&=|\langle\psi_0,\Lambda^{(n,i)}\psi_0\rangle|\\&\leqslant|\langle\psi_0,P^{(i)}T^{(n+2)}\psi_0\rangle|+\sum_{s=1}^{n-2}|\langle\psi_0,P^{(i)}T^{(n+2-s)}\psi_s\rangle|+|\langle\psi_0,P^{(i)}T^{(3)}\psi_{n-1}^{\perp}\rangle|\\&\leqslant\|T^{(n+2)}P_{|\alpha|\leqslant a}\|+\sum_{s=1}^{n-2}|\langle T^{(n+2-s)}\psi_0,\psi_s\rangle|+|\langle T^{(3)}\psi_0,\psi_{n-1}^{\perp}\rangle|\\&\leqslant\|T^{(n+2)}P_{|\alpha|\leqslant a}\|+\sum_{s=1}^{n-2}\|T^{(n+2-s)}P_{|\alpha|\leqslant a}\|\|\psi_s\|+\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|\\&=\sum_{s=2}^{n}\|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\|+\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|.\end{aligned} \tag{41}$$

This calculation follows from (38), the self-adjointness of $T^{(l)}$, and Lemma 1.

From the definition of H_e, it is straightforward to see that $\|(H_e)_\perp^{-1}\|=1$. Also, $\|A_e\|=1$. Thus, from (39) we have

$$\begin{aligned}\|\psi_n^{\perp}\|&\leqslant\sum_{s=1}^{n-1}|\mathcal{E}_s|\|\psi_{n-s}^{\perp}\|+\|T^{(n+2)}P_{|\alpha|\leqslant a}\|\|\psi_0\|+\sum_{s=1}^{n-1}\|T^{(s+2)}P_{|\alpha|\leqslant a+3(n-s)}\|\|\psi_{n-s}\|\\&=\sum_{s=1}^{n-1}|\mathcal{E}_s|\|\psi_{n-s}^{\perp}\|+\sum_{s=1}^{n}\|T^{(s+2)}P_{|\alpha|\leqslant a+3(n-s)}\|\|\psi_{n-s}\|.\end{aligned} \tag{42}$$

Finally let us consider (40):

$$\|\psi_{n-1}^{(j)}\| \leqslant |\lambda_{1,i}-\lambda_{1,j}|^{-1}\left(\|T^{(n+2)}P_{|\alpha|\leqslant a}\|\|\psi_0\| + \sum_{s=1}^{n-2} \|P^{(j)}T^{(n+2-s)}\|\|\psi_s\| + \|P^{(j)}T^{(3)}\|\|\psi_{n-1}^{\perp}\| + \sum_{s=2}^{n-1} |\mathcal{E}_s|\|\psi_{n-s}^{(j)}\| \right).$$

Set $C_7 := \min_{j\neq i}|\lambda_{1,i}-\lambda_{1,j}|^{-1}$. Also, let us notice that $\|P^{(j)}T^{(n+2-s)}\| = \|T^{(n+2-s)}P^{(j)}\| = \|T^{(n+2-s)}P_{|\alpha|\leqslant a}P^{(j)}\| \leqslant \|T^{(n+2-s)}P_{|\alpha|\leqslant a}\|$. Thus,

$$\|\psi_{n-1}^{(j)}\| \leqslant C_7 \sum_{s=2}^{n-1} |\mathcal{E}_s|\|\psi_{n-s}^{(j)}\| + C_7 \sum_{s=2}^{n} \|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\| + C_7\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|. \quad (43)$$

These inequalities will allow us to obtain upper bounds for the growth of R-S coefficients. In the following theorem we make use of Lemmas 3 and 4.

Theorem 2: *Let k be the number of subspaces as defined in Proposition 3.2. Define $b_1 := C_3[kC_6+(2+a)^{1/2}]$, $b_2 := 8C_7[b_1C_4+C_3(2+a)^{1/2}+kC_3C_6]$ and $b_3 := b_1C_4+C_3C_5[1+b_2(k-1)]$. Then for any $b \geqslant \max\{b_1,b_2,b_3,1\}$ and for $n=1,2,\ldots$,*

$$|\mathcal{E}_n| \leqslant b_1\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}, \quad (44)$$

$$\|\psi_{n-1}^{(l)}\| \leqslant b_2\kappa^{3(n-1)}b^{n-2}[(a+n)!]^{1/2}, \quad (45)$$

$$\|\psi_n^{\perp}\| \leqslant b_3\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}. \quad (46)$$

Proof: Assume the estimates are true for $s=1,\ldots,n-1$. This implies that

$$\|\psi_s\| \leqslant [b_3+b_2(k-1)]\kappa^{3s}b^{s-1}[(1+a+s)!]^{1/2} \leqslant \kappa^{3s}kb^s[(1+a+s)!]^{1/2} \quad (47)$$

for $s \leqslant n-2$. We shall use the second inequality in (47) to prove (44) and (45), and the first one to prove (46).

Let us start showing (44). Applying Lemmas 3 and 4, statement 2, we obtain

$$\begin{aligned}\sum_{s=2}^{n} \|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\| &\leqslant C_3k\sum_{s=2}^{n} \kappa^{s/2}\left[\frac{(1+a+s)!}{(1+a)!}\right]^{1/2}\kappa^{3(n-s)}b^{n-s}[(1+a+n-s)!]^{1/2} \\ &\leqslant C_3k\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}\sum_{s=2}^{n} \kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{1/2} \\ &\leqslant kC_3C_6\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}.\end{aligned}$$

Thus, (41) yields

$$\begin{aligned}|\mathcal{E}_n| &\leqslant kC_3C_6\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}+C_3\kappa^{3(n-1)}b_3b^{n-3}\kappa^{1/2}(2+a)^{1/2}[(a+n)!]^{1/2} \\ &\leqslant kC_3C_6\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}+C_3(2+a)^{1/2}\kappa^{3n}b^{n-2}[(a+n)!]^{1/2} \\ &\leqslant b_1\kappa^{3n}b^{n-2}[(a+n)!]^{1/2},\end{aligned}$$

which completes the proof of (44).

To prove (45) we start from (43) and proceed in the same fashion:

$$\|\psi_{n-1}^{(j)}\| \leqslant C_7\kappa^{3n}b_1b_2b^{n-3}\sum_{s=2}^{n-1}[(a+s)!(1+a+n-s)!]^{1/2}+C_3C_7\kappa^{3n}b_3b^{n-3}(2+a)^{1/2}$$

$$\times[(a+n)!]^{1/2}+C_3C_7k\kappa^{3n}b^{n-2}\sum_{s=2}^{n}\kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!}\right]^{1/2}$$

$$\leqslant C_7b_1\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}\sum_{m=1}^{n-2}\left[\frac{(1+a+m)!(a+n-m)!}{(a+n)!}\right]^{1/2}$$

$$+C_3C_7(2+a)^{1/2}\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}$$

$$+C_3C_7k\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}\sum_{s=2}^{n}\kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{1/2},$$

where we have changed index $s\to m=s-1$ in the first term. From this and statements 1 and 3 of Lemma 4, we obtain

$$\|\psi_{n-1}^{(j)}\| \leqslant 8C_7[b_1C_4+C_3(2+a)^{1/2}+kC_3C_6]\kappa^{3(n-1)}b^{n-2}[(a+n)!]^{1/2}$$

$$=b_2\kappa^{3(n-1)}b^{n-2}[(a+n)!]^{1/2},$$

so (45) is done. Consequently, (47) must be valid for $s=n-1$.

Finally, let us show (46). Note that the first term of (42) is bounded like the first term of (43). Applying statement 2 of Lemma 4, it follows that

$$\|\psi_n^{\perp}\| \leqslant b_1b_3\kappa^{3n}b^{n-3}C_6[(a+n)!]^{1/2}+C_3[1+b_2(k-1)]\kappa^{3n}b^{n-2}[(1+a$$

$$+n)!]^{1/2}\sum_{s=1}^{n}\kappa^{-5s/2}\left[\frac{(1+a+3n-2s)!(1+a+n-s)!}{(1+a+3n-3s)!(1+a+n)!}\right]^{1/2}$$

$$\leqslant b_1C_6\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}+C_3[1+b_2(k-1)]C_5\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}$$

$$=b_3\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2} \quad .$$

□

Corollary 1:

$$|\mathcal{E}_n| \leqslant \kappa^{3n}b^{n-1}[(a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n}kb^n[(1+a+n)!]^{1/2}.$$

For the case where degeneracy is partly broken only up to second order, one needs to define certain operators $\Lambda^{(n,i_1,i_2)}$, $\Xi^{(n-2,i_1,i_2)}$, $\Xi^{(n,\perp)}$ for $n\geqslant 3$, in addition to those already defined in the last subsection. Now ψ_0 would be required to lie in a certain subspace $G_{i_1,1_2}\subset G_{i_1}\subset G$, and one would be able to determine ψ_n module an arbitrary component in $G_{i_1,1_2}$. This scheme may be extended to the general case. But the complexity of the set of equations that recursively defines those operators rapidly becomes wild. For that reason, we do not go further. We assume instead that, in general,

$$|\mathcal{E}_n| \leqslant \kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2},$$

for some positive integer w, which may depend on where degeneracy splits.

IV. THE TWO-SIDE ERROR FUNCTION

The upper bounds for $|\mathcal{E}_n|$ and $\|\psi_n\|$ will allow us to estimate the error made in the Schrödinger equation when truncated series are inserted on it. Here we basically follow the technique developed by Hagedorn and Joye in Ref. 4. Concretely, for $N\geqslant 1$ define

$$E_N := e+\sum_{n=1}^{N-1}\hbar^{n/2}\mathcal{E}_n, \quad \Psi_N(x) := \psi_0(x)+\sum_{n=1}^{N-1}\hbar^{n/2}\psi_n(x).$$

These are the truncations at order N of the R-S series. We define

$$\xi_N(x) := A_e[H_0+W(\hbar;x)-E_N]A_e\Psi_N(x)=\left[H_e+A_eW(\hbar;x)A_e-\sum_{j=1}^{N-1}\hbar^{j/2}\mathcal{E}_jA_e^2\right]\sum_{m=0}^{N-1}\hbar^{m/2}\psi_m(x). \tag{48}$$

We call $\xi_N(x)$ the two-side error function since it is the difference between both sides of the Schrödinger equation when exact eigenvalues and eigenfunctions are replaced by truncated series. It can be portrayed in a more suitable way through a number of cancellations. The calculation is outlined in the Appendix. The result is

$$\xi_N(x)=\sum_{n=0}^{N-1}\hbar^{n/2}A_eW^{[N-n+1]}(\hbar;x)A_e\psi_n(x)-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{m-j}(x).$$

Here $W^{[j]}(\hbar;x)$ is the tail of the Taylor series of $V(\hbar;x)$:

$$W^{[j]}(\hbar;x)=V(\hbar;x)-\sum_{l=2}^{j}\hbar^{(l-2)/2}\sum_{|\alpha|=l}\frac{D^\alpha V(0)}{\alpha!}x^\alpha=\hbar^{(j-1)/2}\sum_{|\alpha|=j+1}\frac{D^\alpha V(\zeta_j)}{\alpha!}x^\alpha,$$

where $\zeta_j=\zeta_j(x)=\Theta_j x$ with $\Theta_j\in(0,1)$, as the Taylor theorem states. So we have

$$\xi_N(x)=\hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\frac{D^\alpha V(\zeta_n)}{\alpha!}A_ex^\alpha A_e\psi_n(x)-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{l=n-N+1}^{N-1}\mathcal{E}_lA_e^2\psi_{n-l}(x). \tag{49}$$

Our main result in the next section relies on an upper bound of the L^2-norm of $(H-E_N)A_e\psi_N=A_e^{-1}\xi_N$. Note that, for each $N\geqslant 2$, ξ_N is in the domain of the unbounded operator A_e^{-1}. This estimate on the two-side error function is stated as follows:

Theorem 3: *There are positive constants A, B and N_0 so that*

$$\|A_e^{-1}\xi_N(x)\|\leqslant\sum_{n=N}^{2N}AB^N\hbar^{N/2}[(2+a+n)!]^{1/2}$$

whenever $N_0\leqslant N$ and $\hbar\leqslant 1$.

To estimate the norm of $A_e^{-1}\xi_N$, we first set a suitable closed region around the bottom of the potential well. Then we compute that norm inside and outside of that region. Most of the work is involved in the outside estimate, which requires control on the growth of derivatives of $V(x)$ far away from the minimum of $V(x)$. For that reason we shall summarize it as a separate lemma. Here the hypothesis H5 becomes crucial.

For $R>0$, let us define

$$\chi_R(x)=\begin{cases}1 & \text{if } \sum_i^d \omega_i x_i^2\leqslant R^2,\\ 0 & \text{otherwise.}\end{cases}$$

Lemma 5: Set $R=\sqrt{6N+2a+d-4}$. *Given a multi-index* α, *with* $|\alpha|\geqslant 2$, *and* $n=0,\ldots,N-1$, *there exists certain constants* C_8 *and* C_9 *such that*

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta_n)x^{\alpha'}(1-\chi_R)P_{|\beta|\leqslant a+3n+1}\right\| \leqslant C_8 C_9^{(3n+2+a)/2}\frac{(3n+a+d)^{(d-1)/2}}{\left(1-\frac{\tau}{\omega_0}\right)^{|\alpha|/2}}\left[\frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}\right]^{1/2},$$

where $|\alpha'|=|\alpha|-1$, $\omega_0=\min\{\omega_1,\ldots,\omega_d\}$, *and* $[\![J]\!]$ *stands for the largest integer less than or equal to* J.

Proof: Since $|\zeta_n|\leqslant|x|$, the first part of Lemma 3 implies

$$\frac{\delta^{|\alpha|}}{\alpha!}|D^{\alpha}V(\zeta_n)|\leqslant C_0\exp(2\tau x^2). \tag{50}$$

Let us consider an eigenfunction $\Phi_\beta(x)$ of H_0. We have

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2=\int_{\mathbb{R}^d}\left|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)\right|^2 x^{2\alpha'}|\Phi_\beta(x)|^2[1-\chi_R(x)]d^dx$$
$$\leqslant C_0^2\int_{\mathbb{R}^d}e^{4\tau x^2}x^{2\alpha'}|\Phi_\beta(x)|^2[1-\chi_R(x)]d^dx,$$

where we have dropped the index n in ζ_n. Now change variables $x_i\to y_i=\sqrt{\omega_i}x_i$ to get

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2$$
$$\leqslant C_0^2\left(\prod_{i=1}^{d}\omega_i^{-\alpha_i'-1/2}\right)\int_{\mathbb{R}^d}e^{\Sigma_i 4(\tau/\omega_i)y_i^2}y^{2\alpha'}|\Phi_\beta(y)|^2[1-\chi_R(y)]d^dy$$
$$\leqslant C_0^2\left(\prod_{i=1}^{d}\omega_i^{-\alpha_i'-1/2}\right)\int_{\mathbb{R}^d}e^{4(\tau/\omega_0)y^2}y^{2\alpha'}|\Phi_\beta(y)|^2[1-\chi_R(y)]d^dy$$
$$=D_1^2\left\|e^{2(\tau/\omega_0)y^2}y^{\alpha'}(1-\chi_R)\Phi_\beta(y)\right\|^2, \tag{51}$$

where D_1 is defined in the obvious way. In the new variables

$$\chi_R(y)=\begin{cases}1 & \text{if } y^2\leqslant R^2,\\ 0 & \text{otherwise.}\end{cases}$$

Using the new variables in (5), we see that $\Phi_\beta(y)$ is an eigenfunction of the normalized harmonic oscillator operator

$$H_0'=-\tfrac{1}{2}\Delta_y+\tfrac{1}{2}y^2$$

with energy $e_\beta=|\beta|+d/2$. For $d\geqslant 2$ this operator is equal to

$$H_0'=\frac{1}{2}\left(-\frac{\partial^2}{\partial r^2}-\frac{d-1}{r}\frac{\partial}{\partial r}+\frac{\mathcal{L}^2}{r^2}+r^2\right)$$

in spherical coordinates, where $\mathcal{L}^2$ is the angular momentum operator defined on S^{d-1}. The eigenvalues now read $e=2n+q+d/2$ and the eigenfunctions are

$$\Psi_{k,q,\nu}(r,\omega)=\left[\frac{2k!}{\Gamma(k+q+d/2)}\right]^{1/2} r^q L_k^{q+d/2-1}(r^2)\exp\left(-\frac{r^2}{2}\right)Y_{q,\nu}(\omega).$$

Here $Y_{q,\nu}(\omega)$ are the normalized eigenfunctions of $\mathcal{L}^2$, with quantum numbers q,ν. For each $q=0,1,\ldots$ there are ν_q values of ν. Although the explicit formula for ν_q is rather clumsy, there is a simple bound for it, namely $\nu_q \leqslant C_d e^{\mu_d q}$. This bound suffices for the purpose of our proof. $L_k^j(x)$ denotes the Laguerre polynomial. By Lemma 6.2 of Ref. 4, this polynomial satisfies $|L_k^{q+d/2-1}(x)|\leqslant x^k/k!$ for all $x>4k+2q+d$. Finally, by equating the expressions for the energy, we obtain $|\beta|=2k+q$.

Now $\Phi_\beta(y)$ is certain linear combination of $\Psi_{k,q,\nu}(r,\omega)$,

$$\Phi_\beta(y)=\sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}} c_{k,q,\nu}\Psi_{k,q,\nu}(r,\omega)$$

with $\Sigma|c_{k,q,\nu}|^2=1$. From (51), it follows that

$$\begin{aligned}\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2 &\leqslant D_1^2\sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}}\left\|e^{2(\tau/\omega_0)y^2}y^{\alpha'}(1-\chi_R)\Psi_{k,q,\nu}(y)\right\|^2\\ &\leqslant D_1^2\sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}}\frac{2k!A_{d-1}}{\Gamma(k+q+d/2)}\int_R^\infty e^{-(1-4\tau/\omega_0)r^2}r^{2(|\alpha|-1+q)}\\ &\quad\times|L_k^{q+d/2-1}(r^2)|^2 r^{d-1}dr,\end{aligned}$$

where A_{d-1} is the area of the $(d-1)$ dimensional unit sphere. We also have used that $y^{2|\alpha'|}\leqslant r^{2|\alpha'|}=r^{2(|\alpha|-1)}$. Since $R\geqslant\sqrt{2|\alpha|+d}$, Lemma 6.2 of Ref. 4 applies so

$$\begin{aligned}&\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2\\ &\leqslant D_1^2\sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}}\frac{2A_{d-1}}{k!\Gamma(k+q+d/2)}\int_R^\infty e^{-(1-4\tau/\omega_0)r^2}r^{2|\alpha|+2q+4k+d-3}dr\\ &= D_1^2\sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}}\frac{2A_{d-1}}{k!\Gamma(k+q+d/2)}\frac{\Gamma(|\alpha|+q+2k+d/2-1)}{2(1-4\tau/\omega_0)^{|\alpha|+q+2k+d/2-1}}\\ &= D_1^2A_{d-1}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}}\sum_{\substack{k,q:\\ 2k+q=|\beta|}}\frac{\nu_q}{k!\Gamma(k+q+d/2)}\\ &= D_1^2A_{d-1}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}}\sum_{k=0}^{[\![|\beta|/2]\!]}\frac{\nu_{|\beta|-2k}}{k!\Gamma(|\beta|-k+d/2)}\\ &\leqslant D_1^2A_{d-1}C_d e^{\mu_d|\beta|}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}}\sum_{k=0}^{[\![|\beta|/2]\!]}\frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k+d/2)}.\end{aligned}\tag{52}$$

For $|\beta|\geqslant 1$, $|\beta|-k+d/2\geqslant 1+d/2\geqslant 2$ for all $0\leqslant k\leqslant[\![|\beta|/2]\!]$. Since $\Gamma(x)$ is an increasing function for $x\geqslant 2$, we have

$$\sum_{k=0}^{[\![|\beta|/2]\!]} \frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k-d/2)} \leqslant \sum_{k=0}^{[\![|\beta|/2]\!]} \frac{1}{k!(|\beta|-k)!} \leqslant \frac{1}{|\beta|!} \sum_{k=0}^{|\beta|} \binom{|\beta|}{k} = \frac{1}{|\beta|!} 2^{|\beta|}.$$

For $|\beta|=0$, the sum above is smaller than $2/\sqrt{\pi}$. Therefore

$$\sum_{k=0}^{[\![|\beta|/2]\!]} \frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k-d/2)} \leqslant \frac{2}{\sqrt{\pi}|\beta|!} 2^{|\beta|}$$

for all $|\beta| \geqslant 0$. Thus (52) becomes

$$\left\| \frac{\delta^{|\alpha|}}{\alpha!} D^\alpha V(\zeta) x^{\alpha'} (1-\chi_R) \Phi_\beta(x) \right\|^2 \leqslant D_2^2 2^{|\beta|} e^{\mu_d |\beta|} \frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{|\beta|!(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}}$$

with $D_2^2 := 2D_1^2 A_{d-1} C_d \pi^{-1/2}$.

Now consider any $\varphi \in \mathrm{Ran}(P_{|\beta| \leqslant 3n+a+1})$ so $\varphi = \Sigma_{|\beta| \leqslant 3n+a+1} c_\beta \Phi_\beta(x)$. Then the Hölder inequality implies that

$$\left\| \frac{\delta^{|\alpha|}}{\alpha!} D^\alpha V(\zeta) x^{\alpha'} (1-\chi_R) P_{|\beta| \leqslant a+3n+1} \varphi \right\|^2 \leqslant \|\varphi\|^2 \sum_{|\beta| \leqslant 3n+a+1} \left\| \frac{\delta^{|\alpha|}}{\alpha!} D^\alpha V(\zeta) x^{\alpha'} (1-\chi_R) \Phi_\beta(x) \right\|^2.$$

Therefore

$$\begin{aligned}
&\left\| \frac{\delta^{|\alpha|}}{\alpha!} D^\alpha V(\zeta) x^{\alpha'} (1-\chi_R) P_{|\beta| \leqslant a+3n+1} \right\|^2 \\
&\quad \leqslant D_2^2 \frac{2^{3n+a+1} e^{\mu_d (3n+a+1)}}{\left(1-\dfrac{4\tau}{\omega_0}\right)^{3n+|\alpha|+a+d/2}} \sum_{|\beta| \leqslant 3n+a+1} \frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{|\beta|!} \\
&\quad \leqslant D_2^2 \frac{2^{3n+a+1} e^{\mu_d (3n+a+1)}}{(1-4\tau/\omega_0)^{3n+|\alpha|+a+d/2}} \sum_{|\beta| \leqslant 3n+a+1} \frac{(|\alpha|+|\beta|+[\![d/2]\!]-1)!}{|\beta|!}
\end{aligned}$$

where we use that $0<(1-4\tau/\omega_0)<1$. The terms under the summation sign are increasing in $|\beta|$. Also,

$$\begin{aligned}
\sum_{|\beta| \leqslant 3n+a+1} 1 &= \sum_{s=0}^{3n+a+1} \#\{\beta : |\beta| = s\} \\
&= \sum_{s=0}^{3n+a+1} \frac{(s+d-1)!}{s!(d-1)!} \\
&\leqslant \sum_{s=0}^{3n+a+1} \frac{(s+d-1)^{d-1}}{(d-1)!} \\
&\leqslant \frac{(3n+a+d)^{d-1}}{(d-1)!} (3n+a+2),
\end{aligned}$$

and, moreover, $(3n+2+a)/(3n+1+a) \leqslant 2$. Thus,

$$\begin{aligned}
&\left\| \frac{\delta^{|\alpha|}}{\alpha!} D^\alpha V(\zeta) x^{\alpha'} (1-\chi_R) P_{|\beta| \leqslant a+3n+1} \right\|^2 \\
&\quad \leqslant D_2^2 \frac{2^{3n+a+2} e^{\mu_d (3n+a+1)}}{(1-4\tau/\omega_0)^{3n+|\alpha|+a+d/2}} (3n+a+d)^{d-1} \frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}.
\end{aligned}$$

Now define $C_8 := D_2 e^{-\mu_d/2} (1-4\tau/\omega_0)^{1-d/4}$ and $C_9 := [2e^{\mu_d}/(1-4\tau/\omega_0)]^{1/2}$. □

Proof of Theorem 3: Recall that we assume that $\delta \leqslant 1$. We already know, from Theorem 2, that $b \geqslant 1$. From the proof of Lemma 3, we also know that $\|x_i A_e\| \leqslant \gamma$. Now, from (49), it follows that

$$\begin{aligned}
\|A_e^{-1}\xi_N(x)\| \leqslant & \hbar^{N/2} \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \left\| \frac{D^\alpha V(\zeta_n)}{\alpha!}(1-\chi_R(x))x^\alpha A_e \psi_n(x) \right\| \\
& + \hbar^{N/2} \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \left\| \frac{D^\alpha V(\zeta_n)}{\alpha!}\chi_R(x)x^\alpha A_e \psi_n(x) \right\| \\
& + \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{l=n-N+1}^{N-1} \|\mathcal{E}_l A_e \psi_{n-l}(x)\| \\
\leqslant & \hbar^{N/2} \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \left\| \frac{D^\alpha V(\zeta_n)}{\alpha!}(1-\chi_R(x))x^{\alpha'} P_{|\beta|\leqslant 3n+a+1} \right\| \|x_i A_e\| \|\psi_n(x)\| \\
& + \hbar^{N/2} \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \left\| \frac{D^\alpha V(\zeta_n)}{\alpha!}\chi_R(x)x^{\alpha'} P_{|\beta|\leqslant 3n+a+1} \right\| \|x_i A_e\| \|\psi_n(x)\| \\
& + \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{l=n-N+1}^{N-1} |\mathcal{E}_l| \|\psi_{n-l}(x)\|, \qquad (53)
\end{aligned}$$

where we split x^α into $x^{\alpha'}x_i$, which is possible for some coordinate x_i because $|\alpha| \geqslant 2$. Then $|\alpha'| = |\alpha| - 1$. Let us estimate each term on the right hand side of (53) individually. Applying Lemma 5 and the estimates for $\|x_\alpha A_e\|$ and $\|\psi_n\|$, we obtain

$$\begin{aligned}
\text{first term} \leqslant & \hbar^{N/2} \sum_{n=0}^{N-1} \sum_{|\alpha|=N+2-n} \delta^{|\alpha|} C_8 C_9^{(3n+a+2)/2} \left(1-\frac{4\tau}{\omega_0}\right)^{-|\alpha|/2} (3n+a+d)^{(d-1)/2} \\
& \times \left[\frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}\right]^{1/2} \gamma \kappa^{3n} b^{n+w} [(1+a+n)!]^{1/2} \\
\leqslant & C_8 \gamma \hbar^{N/2} b^{N+w} \delta^{-(N+2)} C_9^{(3N+a+d+1)/2} \left(1-\frac{4\tau}{\omega_0}\right)^{-(N+2)/2} (3N+a+d-3)^{(d-1)/2} \\
& \times \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2n+N+[\![d/2]\!]+a+2)!(n+a+1)!}{(3n+a)!}\right]^{1/2} \sum_{|\alpha|=N+2-n} 1.
\end{aligned}$$

From the proof of Lemma 2, we know that $\Sigma_{|\alpha|=N+2-n} 1 \leqslant [(d-1)!]^{-1}(N+d+1)^{d-1}$. Let us define $A_1 := \gamma \delta^{-2} b^w C_8 C_9^{(a+d+1)/2} [(d-1)!(1-4\tau/\omega_0)]^{-1}$ and $B_1 := \delta^{-1} C_9^{3/2} b (1-4\tau/\omega_0)^{-1}$. Then

$$\begin{aligned}
\text{first term} \leqslant & A_1 B_1^N \hbar^{N/2} (N+d+1)^{d-1} (3N+a+d-3)^{(d-1)/2} \\
& \times \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2n+N+[\![d/2]\!]+a+2)!(n+a+1)!}{(3n+a)!}\right]^{1/2}.
\end{aligned}$$

Note that $(2n+N+[\![d/2]\!]+a+2)! \leqslant (2n+N+a+2)!(2n+N+[\![d/2]\!]+a+2)^{[\![d/2]\!]}$. Then

$$\begin{aligned}\text{first term} &\leqslant A_1 B_1^N \hbar^{N/2}(3N+a+d-3)^{(d-1)/2}(N+d+1)^{d-1}(3N+a+[\![d/2]\!])^{[\![d/2]\!]/2}\\ &\times[(2+a+N)!]^{1/2}\sum_{n=0}^{N-1}\kappa^{3n}\left[\frac{(2+a+N+2n)!(1+a+n)!}{(a+3n)!(2+a+N)!}\right]^{1/2}\\ &\leqslant A_1 B_1^N \kappa^{3N}\hbar^{N/2}(3N+a+d-3)^{(d-1)/2}(N+d+1)^{d-1}(3N+a+[\![d/2]\!])^{[\![d/2]\!]/2}\\ &\times[(2+a+N)!]^{1/2}\max_{1\leqslant l\leqslant N}\left[\frac{(3N-3l+a+1)(3N-3l+a+2)}{(N-l+a+2)}\right]^{1/2}\\ &\times\sum_{l=1}^{N}\kappa^{-5l/2}\left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!}\right]^{1/2}.\end{aligned}$$

The change of index $n\to l=N-n$ was performed in the last sumation above. Now we need to apply Lemma 4, statement 2, to obtain

$$\begin{aligned}\text{first term} &\leqslant C_5 A_1 B_1^N \kappa^{3N}\hbar^{N/2}(3N+a+d-3)^{(d-1)/2}(N+d+1)^{d-1}(3N+a+[\![d/2]\!])^{[\![d/2]\!]/2}\\ &\times[3(3N+a+2)]^{1/2}[(2+a+N)!]^{1/2}.\end{aligned}$$

Finally, define N_1 as the smallest integer such that the inequality

$$(3N+a+[\![d/2]\!])^{[\![d/2]\!]/2}(3N+a+d-3)^{(d-1)/2}(N+d+1)^{d-1}[3(3N+a+2)]^{1/2}\leqslant\kappa^N$$

holds for all $N\geqslant N_1$. Then, whenever $N\geqslant N_1$,

$$\text{first term}\leqslant C_5 A_1 B_1^N \kappa^{4N}\hbar^{N/2}[(2+a+N)!]^{1/2}.$$

Statement 2 of Lemma 2 yields

$$\frac{\delta^{|\alpha|}}{\alpha!}|D^\alpha V(\zeta(x))|\leqslant C_0\exp\left(\frac{2\tau d}{\omega_0^2}R^2\right)=C_0\exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right]\exp\left(\frac{12\tau d}{\omega_0^2}N\right)$$

on the support of $\chi_R(x)$. Thus, the second term of (53) satisfies

$$\begin{aligned}\text{second term} &\leqslant \hbar^{N/2}\gamma\delta^{-(N+2)}C_0\exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right]\exp\left(\frac{12\tau d}{\omega_0^2}N\right)\\ &\times\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\|x^{\alpha'}P_{|\beta|\leqslant 3n+a+1}\|\|\psi_n(x)\|\\ &\leqslant \hbar^{N/2}\gamma\delta^{-(N+2)}C_0\exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right]\exp\left(\frac{12\tau d}{\omega_0^2}N\right)\\ &\times\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\kappa^{(|\alpha|-1)/2}\left[\frac{(a+|\alpha|+3n)!}{(1+a+3n)!}\right]^{1/2}\kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2}\\ &\leqslant \hbar^{N/2}\gamma\delta^{-(N+2)}C_0\exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right]\exp\left(\frac{12\tau d}{\omega_0^2}N\right)b^{N+w}\kappa^{(N+1)/2}\\ &\times\sum_{n=0}^{N-1}\kappa^{5n/2}\left[\frac{(2+a+N+2n)!(1+a+n)!}{(1+a+3n)!}\right]^{1/2}\sum_{|\alpha|=N-n+2}1.\end{aligned}$$

Define $A_2:=\gamma\delta^{-2}\kappa^{1/2}C_0 b^w\exp[2\pi d(2a+d-4)][(d-1)!]^{-1}$ and $B_2:=\delta^{-1}\kappa^{1/2}b\exp(12\tau d/\omega_0^2)$. Then, following the argument we have used to estimate the first term, we obtain

$$\text{second term} \leqslant A_2 B_2^N \hbar^{N/2} (N+d+1)^{d-1} \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(1+a+3n)!} \right]^{1/2}$$

$$\leqslant A_2 B_2^N \kappa^{3N} \hbar^{N/2} (N+d+1)^{d-1} [(2+a+N)!]^{1/2}$$

$$\times \max_{1 \leqslant l \leqslant N} \left[\frac{2+a+3N-3l}{2+a+N-l} \right]^{1/2} \sum_{l=1}^{N} \kappa^{-5l/2} \left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!} \right]^{1/2}$$

$$\leqslant 3^{1/2} C_5 A_2 B_2^N \kappa^{3N} \hbar^{N/2} (N+d+1)^{d-1} [(2+a+N)!]^{1/2}.$$

Now define N_2 such that $(N+d+1)^{d-1} \leqslant \kappa^N$ for every $N \geqslant N_2$. Then

$$\text{second term} \leqslant 3^{1/2} C_5 A_2 B_2^N \kappa^{4N} \hbar^{N/2} [(2+a+N)!]^{1/2}.$$

For the third term of (53), we only need to use the first statement of Lemma 4. The result is

$$\text{third term} \leqslant \sum_{n=N}^{2N} C_4 \kappa^{3n} b^{n+2w} \hbar^{N/2} [(1+a+n)!]^{1/2}.$$

To complete the proof define $N_0 = \max\{N_1, N_2\}$, $A = \max\{C_5 A_1, 3^{1/2} C_5 A_2, C_4 b^{2w}\}$ and $B = \max\{\kappa^4 B_1, \kappa^3 B_2, \kappa^3 b\}$. □

V. OPTIMAL TRUNCATION

In this section we shall prove that exact eigenvalues and eigenfunctions of $H(\hbar) := -\frac{1}{2}\Delta_x + V(\hbar, x)$ can be approximated by truncated R-S series, up to an exponentially small error. To that end, we shall use our estimate of the norm $A_e^{-1} \xi_N(x)$. We shall also need a couple of results. The first is a lower bound for the distance between perturbed eigenvalues that degenerate at $\hbar = 0$. The second is a ''reverse'' definition of asymptoticness.

Let us consider two distinct eigenvalues of $H(\hbar)$, $E(\hbar)$ and $E'(\hbar)$, which converge to the same eigenvalue of H_0 as $\hbar$ goes to 0. Also, let us assume that their asymptotic series have only a finite number of common R-S coefficients. That is,

$$E(\hbar) \sim e + \mathcal{E}_1 \hbar^{1/2} + \ldots + \mathcal{E}_{M-1} \hbar^{(M-1)/2} + \mathcal{E}_M \hbar^{M/2} + \mathcal{E}_{M+1} \hbar^{(M+1)/2} + \ldots,$$

$$E'(\hbar) \sim e + \mathcal{E}_1 \hbar^{1/2} + \ldots + \mathcal{E}_{M-1} \hbar^{(M-1)/2} + \mathcal{E}'_M \hbar^{M/2} + \mathcal{E}'_{M+1} \hbar^{(M+1)/2} + \ldots,$$

with $\mathcal{E}_M \neq \mathcal{E}'_M$. Then,

$$E(\hbar) - E'(\hbar) \sim (\mathcal{E}_M - \mathcal{E}'_M) \hbar^{M/2} + (\mathcal{E}_{M+1} - \mathcal{E}'_{M+1}) \hbar^{(M+1)/2} + \ldots,$$

so we expect that the difference between these exact eigenvalues be bounded below by $O(\hbar^{M/2})$. Since the series above is asymptotic, there are $C_M > 0$ and $\hbar_a(M) > 0$ so that

$$|E(\hbar) - E'(\hbar) - (\mathcal{E}_M - \mathcal{E}'_M) \hbar^{M/2}| \leqslant C_M \hbar^{(M+1)/2},$$

whenever $\hbar \leqslant \hbar_a(M)$. Then

$$|E(\hbar) - E'(\hbar)| \geqslant |\mathcal{E}_M - \mathcal{E}'_M| \hbar^{M/2} - C_M \hbar^{(M+1)/2}.$$

Set $\hbar_b(M) = |\mathcal{E}_M - \mathcal{E}'_M| / 2C_M$. Then for $\hbar \leqslant \hbar_b(M)$,

$$C_M \hbar^{(M+1)/2} \leqslant \tfrac{1}{2} |\mathcal{E}_M - \mathcal{E}'_M| \hbar^{M/2}.$$

Thus for $\hbar \leqslant \hbar_1 := \min\{\hbar_a(M), \hbar_b(M)\}$ we have

$$|E(\hbar)-E'(\hbar)|\geqslant \tfrac{1}{2}|\mathcal{E}_M-\mathcal{E}'_M|\hbar^{M/2}.$$

Let us denote $\mathcal{E}_M-\mathcal{E}'_M$ as $\Delta\mathcal{E}_M$. Therefore, so far we know the following.

Lemma 6: Let $E(\hbar)$ and $E'(\hbar)$ be distinct eigenvalues of $H(\hbar)$, which degenerate at $\hbar=0$. Then either

(1) $|E(\hbar)-E'(\hbar)|\leqslant O(\hbar^{N/2})$ for all non-negative integers N, or

(2) there exists M and $\hbar_1=\hbar_1(M)$ such that

$$|E(\hbar)-E'(\hbar)|\geqslant \tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2}$$

whenever $\hbar\leqslant\hbar_1$.

Remark: It is clear that Lemma 6 is also valid when several eigenvalues of $H(\hbar)$ converge to the same eigenvalue of H_0. As a shorthand, we will say that $E(\hbar)$ is *quasi-degenerate* if the condition 1 in the lemma above occurs.

Lemma 7: Suppose $\Sigma_{n=0}f_n\beta^n$ is asymptotic to $f(\beta)$ in the sense that given $N\geqslant N_0\geqslant M$, there exists C_N and $\beta(N)$ such that for all $\beta\leqslant\beta(N)$

$$\left| f(\beta)-\sum_{n=0}^{N-1} f_n\beta^n \right| < C_N\beta^N.$$

Then given $\epsilon>0$, there exists $\beta(\epsilon)>0$, such that for each $\beta\leqslant\beta(\epsilon)$ there is an $N(\beta)\geqslant N_0$ (maybe equal to ∞), so that

$$\left| f(\beta)-\sum_{n=0}^{N-1} f_n\beta^n \right| \leqslant \epsilon\beta^M \tag{54}$$

whenever $N_0\leqslant N<N(\beta)$.

Proof: Fix $\epsilon>0$. Define $\beta_1(N_0)=(\epsilon C_{N_0}^{-1})^{1/(N_0-M)}$. Then for $N>N_0$, recursively choose positive numbers $\beta_1(N)$ that satisfy

$$\beta_1(N)<\min\{(\epsilon C_N^{-1})^{1/(N-M)},\beta_1(N-1)\}.$$

Then

$$\left| f(\beta)-\sum_{n=0}^{N-1} f_n\beta^n \right| \leqslant (C_N\beta^{N-M})\beta^M \leqslant (C_N\beta_1(N)^{N-M})\beta^M \leqslant \epsilon\beta^M$$

whenever $\beta<\beta_1(N)$.

Define $\beta(\epsilon)=\beta_1(N_0)$, and define

$$N(\beta)=\begin{cases} N+1 & \text{if} \quad \beta_1(N+1)<\beta\leqslant\beta_1(N), \\ \infty & \text{if} \quad \beta<\beta_1(N) \quad \text{for all } N. \end{cases}$$

Then (54) holds whenever $N_0\leqslant N\leqslant N(\beta)$. □

Let $\{e_I\}_{I=0}^{\infty}$ be an arrangement in increasing order of the eigenvalues of H_0, counting multiplicities. Theorem 1.1 of Ref. 16 states that given a non-negative integer J, we can choose $\hbar_0$ so that for each $\hbar\leqslant\hbar_0$ there are at least $J+K$ eigenvalues of $H(\hbar)$, counting multiplicities. Furthermore, each one of them converges to one of the first $J+K$ eigenvalues of H_0. In the following proposition, we study the behavior of truncations of the R-S series of $E^J(\hbar)$, the Jth eigenvalue of $H(\hbar)$. We set K so that $e_{J+K}>e_J$.

Proposition 3: Let $E(\hbar)=E^J(\hbar)$ be a non-quasi-degenerate eigenvalue of $H(\hbar)$, which converges to $e=e_J$. Let $E_N(\hbar)$ be the associated R-S series, truncated at order N. Let N_0 be as defined in Theorem 3. Then there exists $\hbar_e>0$ and, for each $\hbar\leqslant\hbar_e$ there is an $N_e(\hbar)\geqslant N_0$ such that

$$|E_N(\hbar)-E(\hbar)|\leqslant\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}$$

for all $N_0\leqslant N\leqslant N_e(\hbar)$.

Proof: We shall consider the case where there exists another eigenvalue of $H(\hbar)$ that converges to e. The proof can be easily simplified to accomodate the opposite situation, which is studied in Proposition 3 of Ref. 19. So said, let $E'(\hbar)$ be another eigenvalue of $H(\hbar)$ converging to e as $\hbar\searrow 0$. By Lemma 6, there are M and $\hbar_1$ so that $|E(\hbar)-E'(\hbar)|\geqslant\frac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2}$ for $\hbar\leqslant\hbar_1$. Without loss we may assume that $N_0\geqslant M$. To simplify the proof, we furthermore assume that no other eigenvalue of $H(\hbar)$ converges to e. Let G_e be the eigenspace associated to e.

Now set $N_1(\hbar)$ as the largest $N\geqslant N_0$ such that

$$\sum_{n=N_1(\hbar)}^{2N_1(\hbar)} AB^n\hbar^{(n-M)/2}[(2+a+n)!]^{1/2}\leqslant\frac{1}{4}|\Delta\mathcal{E}_M|.$$

Then, from Theorem 3 it follows that

$$\|[H(\hbar)-E_N(\hbar)]A_e\Psi_N(\hbar;x)\|\leqslant\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\leqslant\frac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2}$$

whenever $\hbar\leqslant\hbar_0:=\min\{1,|\Delta\mathcal{E}_M|^{-2/M}\}$ and $N_0\leqslant N\leqslant N_1(\hbar)$. On the other hand, note that $\Psi_N=\psi_0+\varphi_N$, where φ_N is orthogonal to $\psi_0\in G_e$ because of the normalization we chose for the correction terms ψ_n. Since $A_e\psi_0=\psi_0$, we conclude that $\|A_k\Psi_N(\hbar;x)\|\geqslant 1$. So Theorem 3 implies that

$$\|[H(\hbar)-E_N(\hbar)]A_e\Psi_N(\hbar;x)\|\leqslant\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\|A_e\Psi_N(\hbar;x)\|. \tag{55}$$

We may assume that $E_N(\hbar)\notin\sigma(H(\hbar))$, so $[H(\hbar)-E_N(\hbar)]$ is invertible. It follows that

$$\left\{\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\right\}^{-1}\leqslant\|[H(\hbar)-E_N(\hbar)]^{-1}\|.$$

Because H is self-adjoint, $\|(H-E)^{-1}\|=\mathrm{dist}\{E,\sigma(H)\}^{-1}$ by the spectral theorem. Thus,

$$\mathrm{dist}\{E_N(\hbar),\sigma(H)\}\leqslant\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\leqslant\frac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{56}$$

for $\hbar\leqslant\hbar_0$ and $N_0\leqslant N\leqslant N_1(\hbar)$. Let Δ be the minimum nonzero distance between the first $J+K$ eigenvalues of H_0. Since $E_I(\hbar)\to e_I$, we can set $\hbar_\Delta>0$ so that for $0\leqslant I\leqslant J+K$, $|E_I(\hbar)-e_I|\leqslant\frac{1}{4}\Delta$ if $\hbar\leqslant\hbar_\Delta$. That implies that, for $\hbar\leqslant\hbar_\Delta$ and $E''(\hbar)\in\sigma(H(\hbar))\backslash\{E(\hbar),E'(\hbar)\}$,

$$|E^{\#}(\hbar)-E''(\hbar)|\geqslant\tfrac{1}{2}\Delta$$

where $E^{\#}$ denotes either E or E'. Now set $\hbar_2=(\Delta/|\Delta\mathcal{E}_M|)^{2/M}$. Then for $\hbar\leqslant\hbar_2$ we have $\frac{1}{2}\Delta\geqslant\frac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2}$. As a consequence,

$$|E(\hbar)-E''(\hbar)|\geqslant\tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2},$$

$$|E(\hbar)-E'(\hbar)|\geqslant \tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2},$$

which ultimately implies that

$$\operatorname{dist}\{E(\hbar),\sigma(H)\backslash E(\hbar)\}\geqslant \tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{57}$$

whenever $\hbar\leqslant\min\{\hbar_0,\hbar_1,\hbar_\Delta,\hbar_2\}$. Since $E_N(\hbar)$ is asymptotic to $E(\hbar)$, we may apply Lemma 7. Then there is $\hbar_3>0$ such that for each $\hbar\leqslant\hbar_3$ we can fix $N_2(\hbar)\geqslant N_0$ so that

$$|E(\hbar)-E_N(\hbar)|\leqslant \tfrac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{58}$$

for $N_0\leqslant N\leqslant N_2(\hbar)$.

Now (57), (58) and the second inequality of (56) imply that

$$\operatorname{dist}\{E_N(\hbar),\sigma(H)\}=|E(\hbar)-E_N(\hbar)|$$

whenever $\hbar\leqslant\min\{\hbar_0,\hbar_1,\hbar_2,\hbar_3,\hbar_\Delta\}=:\hbar_e$ and $N_0\leqslant N\leqslant\min\{N_1(\hbar),N_2(\hbar)\}=:N_e(\hbar)$. □

Remark: The number $N_e(\hbar)$ defined in the proof must indeed be equal to $N_1(\hbar)$. Assume that $N_e(\hbar)<N_1(\hbar)$, and consider $N_e(\hbar)\leqslant N\leqslant N_1(\hbar)$. Then $E_N(\hbar)$ has to be near some eigenvalue $E''(\hbar)$ different to $E(\hbar)$. By reducing $\hbar$, $E_N(\hbar)$ approaches to $E(\hbar)$ while keeping itself close to $E''(\hbar)$, which leads to a contradiction.

Remark: $N_e(\hbar)$ grows like $g/\hbar$, as one can see from the proof of Theorem 4 below.

The requirement of $E(\hbar)$ to be non-quasi-degenerate can be relaxed, and we formulate the following weaker version of Proposition 3. The proof is a straighforward variation of it.

Proposition 4: Let $E(\hbar)=E^J(\hbar)$ be an eigenvalue of $H(\hbar)$, which converges to $e=e_J$. Let $E_N(\hbar)$ be the associated R-S series, truncated at order N. Also let $E^{\#}(\hbar)$ be any eigenvalue of $H(\hbar)$ that satisfies the condition 1 of Lemma 6 [including $E(\hbar)$ itself.] Then there exists $\hbar_e>0$ so that for each $\hbar\leqslant\hbar_e$ there is an $N_e(\hbar)\geqslant N_0$ such that

$$|E_N(\hbar)-E^{\#}(\hbar)|\leqslant\sum_{n=N}^{2N}AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}$$

for all $\hbar\leqslant\hbar_e$, $N_0\leqslant N\leqslant N_e(\hbar)$, and $E^{\#}(\hbar)$.

In the following theorem we assume the hypotheses of Proposition 3. An analogous result follows from the hypotheses of Proposition 4.

Theorem 4: *Assume the hypotheses of Proposition 3. Then for each $0<g<B^{-2}$, there is $\hbar_g>0$ such that for each $\hbar\leqslant\hbar_g$ there exists $N(\hbar)$ such that*

$$|E_{N(\hbar)}(\hbar)-E(\hbar)|\leqslant\Lambda\exp\left(-\frac{\Gamma}{\hbar}\right)$$

for some $\Lambda>0$ and $\Gamma>0$ independent of $\hbar$.

Proof: Fix $0<g<B^{-2}$. Then $0<B^2g<1$; consequently there is $\Omega>0$ such that $B^2g=\exp(-\Omega)$. Consider the function

$$f(\hbar):=Ag\exp\left(-\frac{\Omega(1+a)}{4}\right)\hbar^{-(4+a+M)/2}\exp\left(-\frac{\Omega g}{4\hbar}\right).$$

It is clear that $f(\hbar)>0$ on $(0,\infty)$ has a single maximum, and $f(\hbar)\to0$ as $\hbar\to0$ or $\hbar\to\infty$. Now set

$$\hbar_4=\sup\{\hbar:f(\hbar)\ \text{ is increasing and }\ f(\hbar)\leqslant\tfrac{1}{4}|\Delta\mathcal{E}_M|\}.$$

Then set

$$\hat{\hbar}_g = \sup\left\{\hbar : \hbar \leqslant \min\{\hbar_e, \hbar_4\} \text{ and } \left[\!\left[\frac{g}{\hbar}\right]\!\right] \geqslant 2 + a + 2N_0\right\}.$$

Now for $\hbar \leqslant \hat{\hbar}_g$ define $N(\hbar)$ by $2 + a + 2N(\hbar) = [\![g/\hbar]\!]$. So defined, $N(\hbar) \geqslant N_0$. On the other hand, since we can assume $B \geqslant 1$ and $2 + a + n \leqslant g/\hbar$ for $N(\hbar) \leqslant n \leqslant 2N(\hbar)$ we have

$$\begin{aligned}\sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}[(2+a+n)!]^{1/2} &\leqslant \sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}(2+a+n)^{(2+a+n)/2} \\ &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} [B^2\hbar(2+a+n)]^{(2+a+n)/2} \\ &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} (B^2 g)^{(2+a+n)/2}.\end{aligned}$$

Now use that $B^2 g = \exp(-\Omega) < 1$ and the fact that $x^n \geqslant x^{n+1}$ if $x \leqslant 1$ to obtain

$$\begin{aligned}\sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}[(2+a+n)!]^{1/2} &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} \exp\left\{-\frac{\Omega}{2}[2+a+N(\hbar)]\right\} \\ &= A\hbar^{-(2+a)/2} e^{-(\Omega/4)(2+a)}[1+N(\hbar)]\exp\left\{-\frac{\Omega}{4}[2+a+2N(\hbar)]\right\} \\ &\leqslant A\hbar^{-(2+a)/2} e^{-(\Omega/4)(2+a)}[2+a+2N(\hbar)]\exp\left[-\frac{\Omega}{4}\left(\frac{g}{\hbar}-1\right)\right] \\ &\leqslant Age^{-(\Omega/4)(1+a)}\hbar^{-(4+a+M)/2}\exp\left(-\frac{\Omega g}{4\hbar}\right)\hbar^{M/2} \\ &\leqslant f(\hbar_4)\hbar^{M/2} \qquad (59) \\ &\leqslant \tfrac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2}. \qquad (60)\end{aligned}$$

Thus, $N(\hbar) \leqslant N_e(\hbar)$. Therefore, Proposition 3 holds for $\hbar < \hat{\hbar}_g$, which along with (59) implies

$$|E_{N(\hbar)}(\hbar) - E(\hbar)| \leqslant Age^{-(\Omega/4)(1+a)}\hbar^{-(4+a)/2}\exp\left(-\frac{\Omega g}{4\hbar}\right),$$

for all $\hbar \leqslant \hat{\hbar}_g$. Finally, define

$$\hbar_g = \max\left\{\hbar \leqslant \hat{\hbar}_g : \hbar^{-(4+a)/2}\exp\left(-\frac{\omega g}{8\hbar}\right) \leqslant 1\right\}.$$

Then the assertion is true for all $\hbar \leqslant \hbar_g$ with $\Gamma := \Omega g/8$ and $\Lambda := Ag\exp(-\Omega(1+a)/4)$. □

*Proposition 5: Let $E(\hbar)$ be a non-quasi-degenerate eigenvalue of $H(\hbar)$, with eigenspace G_E. Let P_E be the (orthogonal) projector onto G_E. Let $\tilde{\Psi}_N(\hbar;x)$ be the N*th *truncation of the R-S series (6). Let $\hbar_e$ and $N_e(\hbar)$ be defined as in Proposition 3. Then for each $\hbar \leqslant \hbar_e$ and $N_0 \leqslant N \leqslant N_e(\hbar)$,*

$$\left\| \frac{\tilde{\Psi}_N(\hbar;x)}{\|\tilde{\Psi}_N(\hbar;x)\|} - \frac{P_E\tilde{\Psi}_N(\hbar;x)}{\|P_E\tilde{\Psi}_N(\hbar;x)\|} \right\| \leqslant 16|\Delta\mathcal{E}_M|^{-1}\sum_{n=N}^{2N} AB^n\hbar^{(n-M)/2}[(2+a+n)!]^{1/2}$$

for some $M \leqslant N_0$.

Proof: Notice that (55) means that

$$\|[H(\hbar)-E_N(\hbar)]\|\tilde{\Psi}_N(\hbar;x)\|^{-1}\tilde{\Psi}_N(\hbar;x)\| \leqslant \sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}.$$

On the other hand, we can write

$$\|\tilde{\Psi}_N(\hbar;x)\|^{-1}\tilde{\Psi}_N(\hbar;x) = w_N\|P_E\tilde{\Psi}_N(\hbar;x)\|^{-1}P_E\tilde{\Psi}_N(\hbar;x)+\Omega_N(\hbar;x),$$

where $\Omega_N(\hbar;x)$ is orthogonal to G_E, and $|w_N|^2+\|\Omega_N(\hbar;x)\|^2=1$. Since these functions are defined up to a global phase, we can assume that indeed $0<w_n\leqslant 1$. Then the normalization condition implies

$$\|\Omega_N(\hbar;x)\| \geqslant \|\Omega_N(\hbar;x)\|^2 = 1-|w_N|^2 = (1+w_N)(1-w_N) \geqslant 1-w_N.$$

So we have

$$\|\|\tilde{\Psi}_N(\hbar;x)\|^{-1}\tilde{\Psi}_N(\hbar;x)-\|P_E\tilde{\Psi}_N(\hbar;x)\|^{-1}P_E\tilde{\Psi}_N(\hbar;x)\| \leqslant 2\|\Omega_N(\hbar;x)\|. \tag{61}$$

Since

$$[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x) = [H(\hbar)-E_N(\hbar)]\frac{\tilde{\Psi}_N(\hbar;x)}{\|\tilde{\Psi}_N(\hbar;x)\|} - w_N[E(\hbar)-E_N(\hbar)]\frac{P_E\tilde{\Psi}_N(\hbar;x)}{\|P_E\tilde{\Psi}_N(\hbar;x)\|},$$

it follows from Proposition 3 that

$$\|[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)\| \leqslant 2\sum_{n=N}^{2N} AB^n\hbar^{n/2}[(2+a+n)!]^{1/2} \tag{62}$$

for $\hbar\leqslant\hbar_e$ and $N_0\leqslant N\leqslant N_e(\hbar)$.

Recall that $E_N(\hbar)\notin\sigma(H(\hbar))$. From the fact that $[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)$ is orthogonal to G_E, it follows that

$$\|\Omega_N(\hbar;x)\| \leqslant \|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\|\|[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)\|, \tag{63}$$

where $[H(\hbar)-E_N(\hbar)]_\perp$ is the restriction of $[H(\hbar)-E_N(\hbar)]$ to the subspace orthogonal to G_E. For simplicity, let us assume that there is only one distinct eigenvalue $E'(\hbar)$ that converges to the same eigenvalue of H_0 as $E(\hbar)$. Since

$$\mathrm{dist}\{E_N(\hbar),\sigma(H)\backslash E(\hbar)\} \geqslant \tfrac{1}{2}\mathrm{dist}\{E(\hbar),\sigma(H)\backslash E(\hbar)\},$$

the spectral theorem along with (57) implies that

$$\|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\| \leqslant 4|\Delta\mathcal{E}_M|^{-1}\hbar^{-M/2}. \tag{64}$$

The assertion now follows from (61)–(64). □

Remark: The assumption of non-quasi-degeneracy of $E(\hbar)$ is critical, as one can see in the argument that leads to (64).

The last result of this section concerns the optimal truncation for the eigenfunctions of $H(\hbar)$. It follows from Proposition 5 in the same way as Theorem 4 does from Proposition 3:

Theorem 5: *Fix* $0\leqslant g\leqslant B^{-2}$. *Let* Λ *and* Γ *be defined as in Theorem 4. Then there exists* $\hbar'_g>0$ *such that for each* $\hbar\leqslant\hbar'_g$ *there is* $N(\hbar)$ *so that*

$$\left\| \frac{\tilde{\Psi}_{N(\hbar)}(\hbar;x)}{\|\tilde{\Psi}_{N(\hbar)}(\hbar;x)\|} - \frac{P_E\tilde{\Psi}_{N(\hbar)}(\hbar;x)}{\|P_E\tilde{\Psi}_{N(\hbar)}(\hbar;x)\|} \right\| \leqslant 16|\Delta\mathcal{E}_M|\Lambda \exp\left(-\frac{\Gamma}{\hbar}\right).$$

Proof: Define

$$f'(\hbar) := Ag \exp\left(-\frac{\Omega(1+a)}{4}\right)\hbar^{-(4+a+2M)/2}\exp\left(-\frac{\Omega g}{4\hbar}\right),$$

$$\hbar_4' := \sup\{\hbar : f'(\hbar) \text{ is increasing and } f(\hbar) \leqslant \tfrac{1}{4}|\Delta\mathcal{E}_M|\},$$

$$\hat{\hbar}_g' := \sup\left\{\hbar : \hbar \leqslant \min\{\hbar_e, \hbar_4'\} \text{ and } \left[\!\left[\frac{g}{\hbar}\right]\!\right] \geqslant 2+a+2N_0\right\}.$$

$$\hbar_g' := \max\left\{\hbar \leqslant \hat{\hbar}_g' : \hbar^{-(4+a+M)/2}\exp\left(-\frac{\omega g}{8\hbar}\right) \leqslant 1\right\}.$$

Now proceed as in the proof of Theorem 4. □

ACKNOWLEDGMENTS

We thank George Hagedorn for his unconditional support and help. We also thank the referee for suggestions and valuable comments. This work was partially supported by National Science Foundation Grant No. DMS-0071692.

APPENDIX: COMPUTATION OF ξ_N

Here we simplify the formula (48) by using the identity (10). This calculation is formally identical the one done in Ref. 19, with some notational change. We reproduce it here for a sake of convenience:

$$\begin{aligned}\xi_N &= \left[H_e + A_eWA_e - \sum_{j=1}^{N-1}\hbar^{j/2}\mathcal{E}_jA_e^2\right]\sum_{m=0}^{N-1}\hbar^{m/2}\psi_m \\ &= \sum_{m=0}^{N-1}\hbar^{m/2}H_e\psi_m + \sum_{m=0}^{N-1}\hbar^{m/2}A_eWA_e\psi_m - \sum_{j=1}^{N-1}\sum_{m=0}^{N-1}\hbar^{(j+m)/2}\mathcal{E}_jA_e^2\psi_m.\end{aligned}$$

We use $A_eWA_e = \Sigma_{j=3}^{N+2}\hbar^{(j-2)/2}T^{(j)} + A_eW^{[N+2]}A_e$ and change the index by $j \to j-2$. Using $H_e\psi_0 = 0$, we then obtain

$$\begin{aligned}\xi_N &= \sum_{m=1}^{N-1}\hbar^{m/2}H_e\psi_m + \sum_{m=0}^{N-1}\sum_{j=1}^{N}\hbar^{(m+j)/2}T^{(j+2)}\psi_m + \sum_{m=0}^{N-1}\hbar^{m/2}A_eW^{[N+2]}A_e\psi_m \\ &\quad - \sum_{m=0}^{N-1}\sum_{j=1}^{N-1}\hbar^{(j+m)/2}\mathcal{E}_jA_e^2\psi_m = \sum_{n=1}^{N-1}\hbar^{n/2}H_e\psi_n + \sum_{n=1}^{N-1}\hbar^{n/2}\sum_{j=1}^{n}T^{(j+2)}\psi_{n-j} \\ &\quad + \sum_{n=N}^{2N-1}\hbar^{n/2}\sum_{j=n-N+1}^{N}T^{(j+2)}\psi_{n-j} + \sum_{m=0}^{N-1}\hbar^{m/2}A_eW^{[N+2]}A_e\psi_m - \sum_{n=1}^{N-1}\hbar^{n/2}\sum_{j=1}^{n}\mathcal{E}_jA_e^2\psi_{n-j} \\ &\quad - \sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{n-j}.\end{aligned}$$

The first, second and fifth terms of last equation cancel because of (10). In the third term define $m = n-j$ and then $p = n-N$. This yields

$$
\begin{aligned}
\xi_N &= \sum_{n=N}^{2N-1} \hbar^{n/2} \sum_{m=n-N}^{N-1} T^{(n-m+2)}\psi_m + \sum_{m=0}^{N-1} \hbar^{m/2} A_e W^{[N+2]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j} \\
&= \sum_{p=0}^{N-1} \sum_{m=p}^{N-1} \hbar^{(p+N)/2} T^{(p+N-m+2)}\psi_m + \sum_{m=0}^{N-1} \hbar^{m/2} A_e W^{[N+2]} A_e \psi_m \\
&\quad - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j} \\
&= \sum_{m=0}^{N-1} \hbar^{m/2} \sum_{p=0}^{m} \hbar^{(p+N-m)/2} T^{(p+N-m+2)}\psi_m \\
&\quad + \sum_{m=0}^{N-1} \hbar^{m/2} A_e W^{[N+2]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j} \\
&= \sum_{m=0}^{N-1} \hbar^{m/2} \left[\sum_{i=2}^{m+2} \hbar^{(i+N-m-2)/2} T^{(i+N-m)} + A_e W^{[N+2]} A_e \right] \psi_m - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j}.
\end{aligned}
$$

Finally, note that $\hbar^{(j-2/2)} T^{(j)} + A_e W^{[j+1]} A_e = A_e W^{[j]} A_e$. Therefore, it follows that

$$
\xi_N = \sum_{m=0}^{N-1} \hbar^{m/2} A_e W^{[N-m+1]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{m-j}.
$$

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Dynamical symmetry breaking and the Nambu–Goldstone theorem in the Gaussian wave functional approximation

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(Received 27 January 2003; accepted 17 March 2003)

We analyze the group-theoretical ramifications of the Nambu–Goldstone (NG) theorem in the self-consistent relativistic variational Gaussian wave functional approximation to spinless field theories. In an illustrative example we show how the Nambu–Goldstone theorem would work in the O(N) symmetric ϕ^4 scalar field theory, if the residual symmetry of the vacuum were lesser than O($N-1$), e.g., if the vacuum were O($N-2$), or O($N-3$), . . . symmetric. (This does not imply that any of the ''lesser'' vacua is actually the absolute energy minimum: stability analysis has not been done.) The requisite number of NG bosons would be ($2N-3$), or ($3N-6$), . . . , respectively, which may exceed N, the number of elementary fields in the Lagrangian. We show how the requisite new NG bosons would appear even in channels that do not carry the same quantum numbers as one of N ''elementary particles'' [scalar field quanta, or Castillejo–Dalitz–Dyson (CDD) poles] in the Lagrangian, i.e., in those ''flavor'' channels that have no CDD poles. The corresponding Nambu–Goldstone bosons are composites (bound states) of pairs of massive elementary (CDD) scalar fields excitations. As a nontrivial example of this method we apply it to the physically more interesting 't Hooft σ model (an extended $N_f=2$ bosonic linear σ model with four scalar and four pseudoscalar fields), with spontaneously and explicitly broken chiral $O(4)\times O(2)\simeq SU_R(2)\times SU_L(2)\times U_A(1)$ symmetry. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1576907]

I. INTRODUCTION

The proof of the Nambu–Goldstone (NG) theorem[1–5] in the Gaussian wave functional approximation[6–13] used to be an open problem for over 30 years, see Refs. 14–17. The first proof was given in the O(2) symmetric ϕ^4 theory,[17] and then straightforwardly extended to O(4) in Ref. 18; the crucial assumption was that the ground state be O($N-1$) symmetric, i.e., that only one (scalar) field develops a vacuum expectation value (VEV). [That assumption is justified when the remaining $N-1$ fields are pseudoscalars, as in the Gell-Mann–Levy model, otherwise CP symmetry is (spontaneously) broken.] By the standard NG boson counting methods,[3,4] for every spontaneously broken symmetry Lie group generator there is one NG boson. As the Lie algebra O(N) has $N(N-1)/2$ generators, for a ground state (vacuum) with an O($N-1$) residual symmetry the number of NG bosons ought to be $N(N-1)/2-(N-1)(N-2)/2=N-1$. That is exactly the number of available fields in the Lagrangian. What happens when the residual symmetry in the ground state is ''smaller'' than O($N-1$) and there should be more than $N-1$ NG bosons?

In this paper we shall extend our proof of the NG theorem in the Gaussian approximation[17,18] to the O(N) symmetric ϕ^4 theory when the symmetry of the ground state is dynamically broken to some (proper) subgroup of O($N-1$), in this specific case to one of the following symmetries: $O(N-2)\times O(2)$, $O(N-3)\times O(3)$, . . . , $O(N/2)\times O(N/2)$ for N even, or $O((N-1)/2)\times O((N$

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$+1)/2$) for N odd. As we shall show, the residual symmetry pattern is dictated by the absolute minimum of the O(N) ϕ^4 model's ground state energy, which in turn depends on the dynamics (gap equation) in the Gaussian approximation, as well as the free parameters. Absolute minimization of the vacuum energy will not been done in this paper, only a search for the extremal and/or saddle points. In a different model or approximation, or for different values of the free parameters the residual symmetry might be different. In any case, with such an asymmetric ground state the number of NG bosons must exceed $N-1$, the largest number of ''elementary'' scalar fields available in the Lagrangian (at least one field must develop the vacuum expectation value and thus cannot create or destroy single NG bosons). Nevertheless the canonical number of massless spinless excitations appears in the spectrum.[4] Our proof should leave no doubt as to the composite nature of the NG bosons in the Gaussian approximation.

This paper falls into five sections and two Appendixes. First, in Sec. II we define the O(N) ϕ^4 model and the Gaussian approximation. In Sec. III we show exactly how the requisite number of massless NG (bosonic bound) states appear and that all the ''broken symmetry'' Nöther currents remain conserved, as the symmetry of the vacuum is reduced. NG bosons invariably appear in the Gaussian approximation to the O(N) ϕ^4 model in those channels that also contain CDD poles, so in Sec. IV we extend our proof to the 't Hooft ϕ^4 model which does not have this property. There we show how various bound NG states appear, or disappear as the symmetries of the ground state and/or the Lagrangian change. Finally, in Sec. V we draw our conclusions and set them in a wider context. In the Appendixes we present some technical details omitted in the main part of the paper.

II. PRELIMINARIES

A. The O(N) symmetric scalar ϕ^4 model

At first we confine ourselves to the O(N) symmetric scalar ϕ^4 theory for the sake of simplicity. All scalar field theories with other spontaneously broken internal symmetries can be reduced to some subgroup of O(N). Of course, in such cases there will be interaction terms other than the simple ϕ^4 one shown below. The Lagrangian density of this theory is

$$\mathcal{L}=\tfrac{1}{2}(\partial_\mu \boldsymbol{\phi})^2 - V(\boldsymbol{\phi}^2), \tag{1}$$

where

$$\boldsymbol{\phi}=(\phi_0,\phi_1,\phi_2,\ldots,\phi_{N-1})=(\sigma,\boldsymbol{\pi}),$$

is a column vector and

$$V(\boldsymbol{\phi}^2)=-\frac{1}{2}\mu_0^2\boldsymbol{\phi}^2+\frac{\lambda_0}{4}(\boldsymbol{\phi}^2)^2.$$

We assume here that λ_0 and μ_0^2 are not only positive, but such that spontaneous symmetry breakdown (SSB) occurs in the Gaussian approximation (GA) introduced below.

B. The Gaussian variational method

1. The Gaussian ground state ("vacuum")

The Rayleigh–Ritz variational approximation to quantum field theories is based on the (''elliptical'') Gaussian ground state (vacuum) functional Ansatz, Refs. 9–11, 13,

$$\Psi_0[\vec{\phi}]=\mathcal{N}\exp\left(-\frac{1}{4\hbar}\int d\mathbf{x}\int d\mathbf{y}[\phi_i(\mathbf{x})-\langle\phi_i(\mathbf{x})\rangle]G_{ij}^{-1}(\mathbf{x},\mathbf{y})[\phi_j(\mathbf{y})-\langle\phi_j(\mathbf{y})\rangle]\right), \tag{2}$$

where $\mathcal{N}$ is the normalization constant, and one sums all repeated (roman lettered) indices from 0 to $N-1$. $\langle\phi_i(\mathbf{x})\rangle$ is the vacuum expectation value (VEV) of the ith spinless field which henceforth we will assume to be translationally invariant $\langle\phi_i(\mathbf{x})\rangle=\langle\phi_i(0)\rangle\equiv\langle\phi_i\rangle$ and

$$G_{ij}(\mathbf{x},\mathbf{y})=\frac{1}{2}\delta_{ij}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{\sqrt{\mathbf{k}^2+m_i^2}}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}.$$

We have explicitly kept $\hbar$ (while setting the velocity of light $c=1$) to keep track of quantum corrections and count the number of ''loops'' in our calculation. Then the ''vacuum'' (ground state) energy density becomes

$$\begin{aligned}\mathcal{E}(m_i,\langle\phi_i\rangle)=&-\frac{1}{2}\mu_0^2\langle\boldsymbol{\phi}\rangle^2+\frac{\lambda_0}{4}[\langle\boldsymbol{\phi}\rangle^2]^2+\hbar\sum_{i=0}^{N-1}\left[I_1(m_i)-\frac{1}{2}(\mu_0^2+m_i^2)I_0(m_i)\right]\\&+\frac{\lambda_0}{4}\left\{6\hbar\sum_{i=0}^{N-1}\langle\phi_i\rangle^2I_0(m_i)+2\hbar\sum_{i\neq j=0}^{N-1}\langle\phi_i\rangle^2I_0(m_j)+\hbar^2\sum_{i=0}^{N-1}I_0^2(m_i)\right.\\&\left.+\hbar^2\sum_{i\neq j=0}^{N-1}I_0(m_i)I_0(m_j)\right\},\end{aligned}\tag{3}$$

where

$$I_0(m_i)=\frac{1}{2}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{\sqrt{\mathbf{k}^2+m_i^2}}=i\int\frac{d^4k}{(2\pi)^4}\frac{1}{k^2-m_i^2+i\epsilon}=G_{ii}(\mathbf{x},\mathbf{x}),\tag{4}$$

$$I_1(m_i)=\frac{1}{2}\int\frac{d\mathbf{k}}{(2\pi)^3}\sqrt{\mathbf{k}^2+m_i^2}=-\frac{i}{2}\int\frac{d^4k}{(2\pi)^4}\log(k^2-m_i^2+i\epsilon)+\text{const.}\tag{5}$$

We may identify $\hbar I_1(m_i)$ with the familiar ''zero-point'' energy density of a free scalar field of mass m_i.

The divergent integrals $I_{0,1}(m_i)$ are understood to be regularized via an UV momentum cutoff Λ. Thus we have introduced a new free parameter into the calculation. This was bound to happen in one form or another, since even in the renormalized perturbation theory one must introduce a new dimensional quantity (the ''renormalization scale/point'') at the one loop level. We treat this model as an effective theory and thus keep the cutoff without renormalization. (There are several renormalization schemes for the Gaussian approximation, but they show signs of instability and ultimately seem to lead to ''triviality.'' [12])

2. The vacuum energy minimization equations

We vary the energy density with respect to the field vacuum expectation values $\langle\phi_i\rangle$ and the ''dressed'' masses m_i. The extremization condition with respect to the field vacuum expectation values reads

$$\left(\frac{\partial\mathcal{E}(m_i,\langle\phi_i\rangle)}{\partial\langle\phi_j\rangle}\right)_{\min}=0,\quad j\in 0,1,\ldots,N-1;\tag{6}$$

or explicitly

$$\langle\phi_j\rangle\left[-\mu_0^2+\lambda_0\left(\langle\boldsymbol{\phi}\rangle^2+3\hbar I_0(m_j)+\hbar\sum_{j\neq i=0}^{N-1}I_0(m_i)\right)\right]_{\min}=0.\tag{7}$$

The second set of energy extremization equations reads

$$\left(\frac{\partial\mathcal{E}(m_i,\langle\phi_i\rangle)}{\partial m_j}\right)_{\min}=0,\quad j\in 0,1,\ldots,N-1,\tag{8}$$

or

$$m_j^2+\mu_0^2=\lambda_0\left(3\langle\phi_j^2\rangle+\hbar\sum_{j\neq k=0}^{N-1}\langle\phi_k^2\rangle+3\hbar I_0(m_j)+\hbar\sum_{j\neq k=0}^{N-1}\hbar I_0(m_k)\right)_{\min}. \tag{9}$$

Equations (7) and (9) can be identified with the (truncated) Schwinger–Dyson (SD) equation[13,19] for the one- and two-point Green functions, see Refs. 17 and 18. The solutions to these equations plus the additional minimization requirements (positive-definite second derivatives matrix, i.e., the positive definiteness of its principal minors, which will not be discussed here) determine the symmetry of the ground state (vacuum).

3. The vacuum symmetry

Now one ordinarily assumes that only one of the scalar fields ϕ_i (by convention the $i=0$ one) develops a nonzero VEV, i.e., $\langle\phi_0\rangle\neq 0$ and then one proceeds with the proof of the NG theorem. [The validity of this assumption, of course, depends on the values of the bare parameters in the Lagrangian and the cutoff Λ, or the values of the renormalized parameters, if one insists on renormalization. One may also have an unbroken symmetry: with all the fields having a zero VEV, $\langle\phi_i\rangle=0,\ i\in 0,1,\ldots,N-1$, the gap equations (7) and (9) lead to all the masses m_i being equal. In other words the N fields form an O(N) multiplet, so we may say that the symmetry of the vacuum is O(N), i.e., not broken.]

In the conventional case the scalar field masses are $m_0=M; m_1=m_2=m_3=\cdots=\mu$, i.e., the $(N-1)$ fields $\phi_i;\ i\in 1,2,\ldots,N-1$, of mass $m_i=\mu$, form an $(N-1)$-plet and the residual symmetry of the vacuum is O$(N-1)$. That, however, is not the only logical possibility: one may assume that more than one field develops VEV. This, of course, means that the (residual) symmetry of the vacuum is ''lesser'' than the one in the (''canonical'') case with only one VEV. [In the Born approximation such a vacuum might be reducible to the ''one VEV'' vacuum by means of an O(N) transformation (if it lies in the same ''orbit'' of the symmetry group[20]), but in the Gaussian approximation dynamical symmetry breaking may lead to an irreducibly different ground state.]

The decision which of these possibilities actually takes place can be made on the basis of comparing their respective ground state energies. In the case with an O$(N-1)$ symmetric ground state, the vacuum energy, or effective potential is

$$\begin{aligned}&\mathcal{E}(M,\mu,\langle\phi_0\rangle)_{\min}\\&\quad=-\frac{1}{2}\mu_0^2\langle\phi_0\rangle^2+\frac{\lambda_0}{4}\langle\phi_0\rangle^4+\hbar\left[I_1(M)-\frac{1}{2}(\mu_0^2+M^2)I_0(M)\right]\\&\qquad+(N-1)\hbar\left[I_1(\mu)-\frac{1}{2}(\mu_0^2+\mu^2)I_0(\mu)\right]+\frac{\lambda_0}{4}\{2\hbar\langle\phi_0\rangle^2[3I_0(M)+(N-1)I_0(\mu)]\\&\qquad+3\hbar^2I_0^2(M)+(N-1)\hbar^2I_0(\mu)[2I_0(M)+(N+1)I_0(\mu)]\}.\end{aligned} \tag{10}$$

Similar expressions for ground states with lesser symmetries than O$(N-1)$ can be derived by applying the corresponding gap equations (7) and (9) to Eq. (3). The question of the *absolute* energy minimum will not be pursued in this paper, however. For the purpose of argument we shall assume that alternative ground states exist and are stable, i.e., energetically favorable to the standard one.

If two (or more) scalar fields' VEV are simultaneously nonzero, e.g., if $\langle\phi_0\rangle=v_1\neq 0$ and $\langle\phi_j\rangle=v_2\neq 0;\ j\in 1,2,\ldots,N-1\ \langle\phi_i\rangle=0;\ i\in 1,2,\ldots,j-1,j-2,\ldots,N-1$, we may change the scalar field labels such that the fields with nonzero VEVs are labeled successively $0,1,\ldots,k$ without loss of generality. In such a case the masses m_i may also take on different values.

For simplicity's sake we assume that only two fields have nonvanishing vacuum expectation values (extension to three, or more VEVs follows by straightforward analogy), $\phi_0,\phi_1\neq 0$ (we label their masses $m_0=M,\ m_1=\mu_1$). The remaining $(N-2)$ fields $\phi_i;\ i\in 2,\ldots,(N-1)$, with

mass $m_i=\mu_2$, form an $(N-2)$-plet. In that case, it is clear that the residual symmetry of the ground state is (at least) $O(N-2)$, i.e., that the $O(N)$ symmetry has been dynamically (spontaneously) broken to (at least) $O(N-2)$. We say "at least" because, when the masses $m_0=M=m_1=\mu_1$ are equal there is additional O(2) symmetry of the vacuum. Similar comments are valid in the case when more than two fields develop VEVs. Of course, the residual symmetry of the vacuum determines the number of the NG bosons. Next we turn to the case of two fields with VEV as worked out in Appendix A. We have shown in Appendix A that there are only two distinct mass solutions $M=\mu_1, \neq \mu_2$ to Eqs. (A12)–(A15). Thus the residual symmetry of the vacuum is $O(N-2)\times O(2)$, and the corresponding number of NG bosons must be $(2N-4)$. In the following we shall see how all these NG bosons come about.

III. THE NAMBU–GOLDSTONE THEOREM

A. The two-body equation

In Refs. 17 and 18 it was shown that in the Gaussian approximation to the O(2) and O(4) ϕ^4 model, the Nambu–Goldstone particles appear in the *two-particle spectra*, i.e., that they are massless bound states of two different massive elementary excitations with an admixture of the (massive elementary) one-body state with the same quantum numbers (the CDD pole). This admixture of the one-body state is crucial for the masslessness of the NG state (it also proved to be a source of confusion). As there are at most $(N-1)$ such elementary particles/CDD poles (one field adopts a VEV so it cannot create or destroy single NG bosons), it appears that there can be at most $(N-1)$ NG bosons in this theory. There are $N(N-1)/2$ (distinct) pairs of elementary particles in this model, however, and an equal number of distinct (potentially bound) two-body states. Thus there can be at most $N(N-1)/2$ NG bosons, precisely the maximum number allowed by the $O(N)$ Lie group generator counting. Next we must show that the number of "broken symmetry generators" corresponds precisely to the number of massless bound states and that the corresponding Nöther currents are conserved.

The two-body equation of motion in the Gaussian approximation is equivalent to the four-point Schwinger–Dyson (or Bethe–Salpeter) equation (for proof of this equivalence, see Refs. 9 and 21). All the NG channels obey a generic four-point SD equation that reads

$$D_{ij,ij}(s)=V_{ij,ij}(s)+V_{ij,kl}(s)\Pi_{kl,mn}(s)D_{mn,ij}(s), \tag{11}$$

where $D(s)$ is the four-point Green function $(N\times N)$ matrix (scattering amplitude), $\Pi(s)$ is the polarization function matrix and $V(s)$ is the potential matrix; ij denote the $O(N)$ indices of the two constituents, with the generic solution

$$\mathbf{D}(s)=\mathbf{V}(s)[1-\mathbf{V}(s)\mathbf{\Pi}(s)]^{-1}, \tag{12}$$

where $s=(p_1+p_2)^2\equiv P^2$ is the center-of-mass (CM) energy. These matrices may reduce to a direct sum of submatrices depending on the residual symmetry of the system. Such effective two-body propagators can also be written in the following form (see Ref. 22):

$$D_\alpha(s)\simeq\frac{g_\alpha^2}{s-m_\alpha^2}, \tag{13}$$

where m_α is the effective mass in channel α. The difference between various $O(N)$ "flavor" sectors appears in the polarization functions $\Pi(s)$ and potentials $V(s)$: more specifically in $(N-2)$ channels $[(i=0,\ j\subset 2,\ldots N-1)\equiv M\mu_2]$ the said matrices are diagonal and have the form

$$\Pi_{M\mu_2}(s)=I_{M\mu_2}(s)=i\hbar\int\frac{d^4k}{(2\pi)^4}\frac{1}{[k^2-M^2+i\epsilon][(k-P)^2-\mu_2^2+i\epsilon]}, \tag{14}$$

$$V_{M\mu_2}(s)=2\lambda_0\left[1+\left(\frac{2\lambda_0\langle\phi_0\rangle^2}{s-\mu_2^2}\right)\right]=2\lambda_0\left[1+\frac{M^2}{s-\mu_2^2}\right], \tag{15}$$

and another $(N-2)$ channels $[(i=1,\ j\subset 2,\ldots,N-1)\equiv\mu_1\mu_2$ have the form

$$\Pi_{\mu_1\mu_2}(s)=I_{\mu_1\mu_2}(s)=i\hbar\int\frac{d^4k}{(2\pi)^4}\frac{1}{[k^2-\mu_2^2+i\epsilon][(k-P)^2-\mu_1^2+i\epsilon]}, \tag{16}$$

$$V_{\mu_1\mu_2}(s)=2\lambda_0\left[1+\left(\frac{2\lambda_0\langle\phi_1\rangle^2}{s-\mu_2^2}\right)\right]=2\lambda_0\left[1+\frac{\mu_1^2}{s-\mu_2^2}\right]. \tag{17}$$

The poles $1/(s-\mu_{1,2}^2)$ in Eqs. (15) and (17) are called the Castillejo–Dalitz-Dyson (CDD) poles and correspond to one-particle states in the theory. Now due to Eqs. (A12)–(A15) these two channels happen to be equivalent in this case, but that degeneracy is accidental (for a different example see Sec. IV).

B. Massless (Nambu–Goldstone) two-body states

With an $O(N-2)\times O(2)$ residual symmetry there should be $(2N-4)=(N-2)+(N-2)$ NG bosons. This number of NG bosons quickly exceeds the number of available fields in the Lagrangian: $2(N-2)>(N-1)$ for $N>3$. Thus, there are not enough scalar fields to provide for all the NG bosons in case of nonstandard symmetry breaking. Does this mean that the NG theorem breaks down in such a case?

As in Ref. 17, we shall prove that at zero CM energy $P=0$, the matrix $[1-V_{M\mu_2}(0)\Pi_{M\mu_2}(0)]$ vanishes. We use Eq. (A6) to write

$$\begin{aligned}V_{M\mu_2}(0)&=2\lambda_0\left[1-\frac{M^2}{\mu_2^2}\right],\\ \Pi_{M\mu_2}(0)&=\hbar\left(\frac{I_0(M)-I_0(\mu_2)}{M^2-\mu_2^2}\right)\end{aligned} \tag{18}$$

then use Eq. (33) to obtain the final result

$$V_{M\mu_2}(0)\Pi_{M\mu_2}(0)=1. \tag{19}$$

Thus the inverse propagator Eq. (12) evaluated at zero momentum vanishes,

$$D^{-1}_{M\mu_2}(0)=[1-V_{M\mu_2}(0)\Pi_{M\mu_2}(0)]V_{M\mu_2}(0)^{-1}=0, \tag{20}$$

which is equivalent to the result $m^2_{M\mu_2}=0$. Similarly for the remaining $(N-2)$ $\mu_1\mu_2$ channels. Q.E.D.

Note that the proof in no way depended on the fact that $\mu_1=M$. In other words, if the gap Eqs. (A12)–(A15) allowed a solution such that $\mu_1\neq M$ and $\langle\phi_1\rangle=0$, the NG theorem would still hold. But, then the CDD poles would decouple in the latter $(N-2)$ channels, i.e., there would be no CDD poles in these channels. This shows that, at least in principle, $(N-2)$ NG bosons could be pure bound states with no single particle admixtures. In Sec. IV we shall give an example of a model with a gap equation that allows such solutions.

C. Conservation of Nöther currents

There are $N-2[a\subset 2,\ldots,N-1]$ dynamically broken $O(N)$ symmetry Nöther current matrix elements corresponding to

$$J^a_{\mu 5}(p',p)=\langle\phi^a(p')|J_\mu(0)|\phi_0(p)\rangle=(p'+p)_\mu+q_\mu\left(\frac{M^2}{q^2-\mu_2^2}\right)-\Gamma^{M\mu_2}_{\mu 5}(q)D_{M\mu_2}(q), \quad (21)$$

where $\Gamma^{M\mu_2}_{\mu 5}(q)$ is

$$\Gamma^{M\mu_2}_{\mu 5}(q)=i\int\frac{d^4k}{(2\pi)^4}\left[(2k+q)_\mu+q_\mu\left(\frac{M^2}{q^2-\mu_2^2}\right)\right]\frac{1}{[k^2-M^2][(k+q)^2-\mu_2^2]}$$
$$=\frac{q_\mu}{q^2}\left[\frac{\mu_2^2}{2\lambda_0}(V_{M\mu_2}(0)\Pi_{M\mu_2}(0)-V_{M\mu_2}(q^2)\Pi_{M\mu_2}(q^2))\right]. \quad (22)$$

Inserting the vertex $\Gamma^{M\mu_2}_{\mu 5}(q)$, Eq. (22) together with the two-body propagator $D_{M\mu_2}(q^2)$, Eq. (12) into Eq. (21) one finds

$$J^a_{\mu 5}(p',p)=(p'+p)_\mu+q_\mu\left(\frac{M^2}{q^2-\mu_2^2}\right)-\frac{q_\mu}{q^2}\left[\frac{\mu_2^2}{2\lambda_0}\right]V_{M\mu_2}(q^2)=(p'+p)_\mu+q_\mu\left(\frac{M^2-\mu_2^2}{q^2}\right), \quad (23)$$

where $q^\nu=(p'-p)^\nu$. This current is manifestly devoid of a pole at $q^2=\mu_2^2$. The composite state plays precisely the role of the Nambu–Goldstone boson in the conservation of the dynamically broken O(N) symmetry Nöther currents,[1] i.e., in the basic O(N) symmetry Ward–Takahashi identity, cf. Refs. 23 and 24,

$$q^\nu J^a_{\nu 5}(p',p)=(p'^2-\mu_2^2)-(p^2-M^2), \quad (24)$$

that follows directly from Eq. (23). Similarly for the remaining $N-2$ $[a\subset 2,\ldots,N-1]$ dynamically broken O(N) symmetry Nöther current matrix elements corresponding to

$$J^a_{\mu 5}(p',p)=\langle\phi^a(p')|J_\mu(0)|\phi_1(p)\rangle=(p'+p)_\mu+q_\mu\left(\frac{\mu_1^2}{q^2-\mu_2^2}\right)-\Gamma^{\mu_1\mu_2}_{\mu 5}(q)D_{\mu_1\mu_2}(q). \quad (25)$$

The identity of the two ''gap,'' or CDD masses $\mu_1=M$ and the concomitant ''excess'' O(2) vacuum symmetry are consequences of the simplicity of the vacuum equation (7) that only depends on one O(N) algebraic invariant.[4,20] That, in turn, is a consequence of the fact that we are dealing with fields in the fundamental irrep. of O(N) and the requirement that the Lagrangian (1) be renormalizable, i.e., at most of the fourth power in the fields. The assumption of a second VEV $\langle\phi_3\rangle=\langle\pi^0\rangle\neq 0$ is particularly unrealistic in the Gell-Mann–Levy model [O($N=4$) ϕ^4 model],[25] because of the negative parity of the π fields: their nonzero VEV would imply spontaneous breaking of P and CP ''parities.'' In Sec. IV we give an example of a ϕ^4 model with an internal symmetry that leads to a gap equation with distinct mass solutions and potentially exotic NG bound states.

IV. THE 't HOOFT MODEL

A. Definition of the model

't Hooft's[26] extension of the linear sigma model Lagrangian reads

$$\mathcal{L}_{\rm tH}=\mathrm{tr}[(\partial_\mu M\partial^\mu M^\dagger)+\mu^2 MM^\dagger]-\tfrac{1}{2}(\lambda_1-\lambda_2)[\mathrm{tr}(MM^\dagger)]^2$$
$$-\lambda_2\,\mathrm{tr}[(MM^\dagger)^2]+2\kappa[e^{i\theta}\det M+\text{c.c.}], \quad (26)$$

where

$$M=\frac{1}{\sqrt{2}}(\Sigma+i\Pi),$$

$$\Sigma=\frac{1}{\sqrt{2}}(\sigma+\boldsymbol{\alpha}\cdot\boldsymbol{\tau}), \tag{27}$$

$$\Pi=\frac{1}{\sqrt{2}}(\eta+\boldsymbol{\pi}\cdot\boldsymbol{\tau}).$$

Equation (26) is equivalent to the following:

$$\begin{aligned}\mathcal{L}_{\mathrm{tH}}=&\frac{1}{2}[(\partial_\mu\sigma)^2+(\partial_\mu\boldsymbol{\pi})^2+(\partial_\mu\eta)^2+(\partial_\mu\boldsymbol{\alpha})^2]+\frac{\mu^2}{2}[\sigma^2+\boldsymbol{\pi}^2+\eta^2+\boldsymbol{\alpha}^2]\\&+2\kappa\cos\theta[\sigma^2+\boldsymbol{\pi}^2-\eta^2-\boldsymbol{\alpha}^2]-4\kappa\sin\theta[\sigma\eta-\boldsymbol{\pi}\cdot\boldsymbol{\alpha}]-\frac{\lambda_1}{8}[\sigma^2+\boldsymbol{\pi}^2+\eta^2+\boldsymbol{\alpha}^2]^2\\&-\frac{\lambda_2}{2}[(\sigma\boldsymbol{\alpha}+\eta\boldsymbol{\pi})^2+(\boldsymbol{\pi}\times\boldsymbol{\alpha})^2]\end{aligned} \tag{28}$$

which describes the dynamics of the two chiral meson quartets, $(\sigma,\boldsymbol{\pi})$ and $(\boldsymbol{\alpha},\eta)$, in this model, and λ_1, λ_2, κ, θ are the bare coupling constants. Nonvanishing angle θ leads to the explicit (not spontaneous) CP violation in this model, so we set it equal to zero. Thus we see that the 't Hooft model consists of two coupled Gell-Mann–Lévy (GML) linear sigma models,[25] one with a light and the other with a heavy quartet of mesons.

Note that the symmetries of various parts of the interaction Lagrangian also vary, see Appendix B: (i)

$$\lambda_1\neq 0,\quad \lambda_2=\kappa=\theta=0 \tag{29}$$

implies O(8) symmetry. (ii)

$$\lambda_1\neq 0\neq\lambda_2,\quad \kappa=\theta=0 \tag{30}$$

implies $O(4)\times O(2)$ symmetry. (iii)

$$\lambda_1\neq 0\neq\lambda_2,\quad \kappa\neq 0=\theta \tag{31}$$

implies O(4) symmetry. And the number of NG bosons must change accordingly.

B. The gap equations

The first set of energy minimization equations (7) reads

$$0=-v(\mu_0^2+4\kappa)+\frac{\lambda_1}{2}v[v^2+3I_0(m_\sigma)+3I_0(m_\alpha)+3I_0(m_\pi)+I_0(m_\eta)]+3\lambda_2 vI_0(m_\alpha), \tag{32}$$

$$m_\sigma^2=-\mu_0^2-4\kappa+\frac{\lambda_1}{2}v[v^2+3I_0(m_\sigma)+3I_0(m_\alpha)+3I_0(m_\pi)+I_0(m_\eta)]+3\lambda_2 I_0(m_\alpha), \tag{33}$$

$$m_\alpha^2 = -\mu_0^2 - 4\kappa + \left(\frac{\lambda_1}{2} + \lambda_2\right)v^2 + \frac{\lambda_1}{2}[I_0(m_\sigma) + 5I_0(m_\alpha) + 3I_0(m_\pi) + I_0(m_\eta)] + \lambda_2[I_0(m_\sigma) + 2I_0(m_\pi)], \tag{34}$$

$$m_\pi^2 = -\mu_0^2 - 4\kappa + \frac{\lambda_1}{2}v^2 + \frac{\lambda_1}{2}[v^2 + I_0(m_\sigma) + 3I_0(m_\alpha) + 5I_0(m_\pi) + I_0(m_\eta)] + \lambda_2[I_0(m_\eta) + 2I_0(m_\alpha)], \tag{35}$$

$$m_\eta^2 = -\mu_0^2 - 4\kappa + \frac{\lambda_1}{2}v^2 + \frac{\lambda_1}{2}[v^2 + 3I_0(m_\sigma) + 3I_0(m_\alpha) + 3I_0(m_\pi) + I_0(m_\eta)] + 3\lambda_2 I_0(m_\pi), \tag{36}$$

where the divergent integral $I_0(m_i)$ is given by Eq. (4). For simplicity in the following we use the following short-hand notation $\alpha = m_\alpha^2; \eta = m_\eta^2; \sigma = m_\sigma^2; \pi = m_\pi^2$. Equations (32)–(36) can be solved for

$$\begin{aligned}
\Pi_{\alpha\eta}(0) &= \frac{I_0(\alpha) - I_0(\eta)}{\alpha - \eta} = \frac{1}{(\lambda_1^2 - \lambda_2^2)}\left(\lambda_1 + \lambda_2\left(\frac{\pi - \sigma}{\alpha - \eta}\right)\right), \\
\Pi_{\pi\sigma}(0) &= \frac{I_0(\alpha) - I_0(\eta)}{\alpha - \eta} = \frac{-1}{(\lambda_1^2 - \lambda_2^2)}\left(\lambda_1\frac{\pi}{\sigma - \pi} + \lambda_2\frac{\left(\alpha - \eta - \frac{\lambda_2}{\lambda_1}\sigma\right)}{\sigma - \pi}\right), \\
\Pi_{\pi\alpha}(0) &= \frac{I_0(\alpha) - I_0(\pi)}{\alpha - \pi} = \frac{1}{(\lambda_1^2 - 2\lambda_1\lambda_2 - 3\lambda_2^2)}\left(\lambda_1\left(1 - \frac{8\kappa}{\alpha - \pi}\right) + \lambda_2\frac{\eta - 8\kappa}{\alpha - \pi}\right), \\
\Pi_{\sigma\eta}(0) &= \frac{I_0(\sigma) - I_0(\eta)}{\sigma - \eta} \\
&= \frac{1}{(\lambda_1^2 - 2\lambda_1\lambda_2 - 3\lambda_2^2)}\left((\lambda_1 - 2\lambda_2)\left(\frac{8\kappa - \eta}{\sigma - \eta}\right) - 3\lambda_2\frac{\alpha - \pi - 8\kappa - \frac{\lambda_2}{\lambda_1}\sigma}{\sigma - \eta}\right),
\end{aligned} \tag{37}$$

whence follows

$$\Pi_{\pi\eta}(0) = \frac{I_0(\pi) - I_0(\eta)}{\pi - \eta} = \frac{1}{\lambda_1(\pi - \eta)}(8\kappa + \pi - \eta + \lambda_2(\alpha - \eta)\Pi_{\eta\alpha}(0) - 3\lambda_2(\alpha - \pi)\Pi_{\pi\alpha}(0)), \tag{38}$$

$$\begin{aligned}
\Pi_{\alpha\sigma}(0) &= \frac{I_0(\sigma) - I_0(\alpha)}{\sigma - \alpha} \\
&= \frac{1}{\lambda_1(\sigma - \alpha)}\left(8\kappa + \frac{\lambda_2}{\lambda_1}\sigma - \alpha + \lambda_2(\sigma - \pi)\Pi_{\pi\sigma}(0) - 3\lambda_2(\alpha - \pi)\Pi_{\pi\alpha}(0)\right).
\end{aligned}$$

C. The Nambu–Goldstone theorem in the isotensor pseudoscalar sector

Note that there are $8 \times 8 = 64$ possible initial or final two-body states here. Thus there are $64 \times 64 = 4096$ possible channels, but only $4 \times 7 = 28$ distinct pairs of particles, or equivalently at most 28 possible NG bosons. The last statement holds under the proviso of exact O(8) symmetry being broken to a discrete (non-Lie) symmetry, however. Otherwise there are fewer than 28 NG bosons, and when O(8) is explicitly broken down to $O(4) \times O(2)$, or O(4) by one of the terms in

the Lagrangian equation (26), there are even fewer than that. This fact tells us that many channels must be coupled and that the residual symmetry plays a crucial role in this coupling. We shall not look at every possible channel in this paper, but rather concentrate only on the exotic ones, in this case the isotensor, so as to show the existence of pure bound state NG bosons without CDD admixtures.

We may use the residual vacuum symmetry, e.g., the O(3) isospin invariance to split this 64×64 matrix equation into six invariant subspaces: three flavor channels [(a) isoscalar; (b) isovector; and (c) isotensor] of either parity. In the two-body, or Bethe–Salpeter (BS) equation for the four-point Green functions $D_{ij}(s)$, the indices i,j denote the isospin of the two-body initial and final states, respectively.

The negative parity (pseudoscalar) isotensor two-body equation is a single-channel one and straightforward to solve, see Eq. (12). We look at the zero CM energy $P=0$ function $V_{\pi\alpha}(0)\Pi_{\pi\alpha}(0)$; we use

$$V_{\pi\alpha}^{(I=2)}=\lambda_1+\lambda_2 \tag{39}$$

and Eq. (37) to obtain the final result

$$V_{\pi\alpha}^{(I=2)}(0)\Pi_{\pi\alpha}(0)=-\left(\frac{\lambda_1+\lambda_2}{\lambda_1^2-2\lambda_1\lambda_2-3\lambda_2^2}\right)\left(\lambda_1\left(1-\frac{8\kappa}{\alpha-\pi}\right)+\lambda_2\frac{\eta-8\kappa}{\alpha-\pi}\right) \quad . \tag{40}$$

Now set $\lambda_2=\kappa\to 0$ and find

$$\lim_{\lambda_2=\kappa\to 0} V_{\pi\alpha}^{(I=2)}(0)\Pi_{\pi\alpha}(0)=1. \tag{41}$$

The propagator Eq. (12) evaluated at zero momentum can be written as

$$D_{\pi\alpha}^{(I=2)}(0)=\frac{g_{\pi\alpha}^2}{-m_{\pi\alpha}^2}=\frac{V_{\pi\alpha}(0)}{1-V_{\pi\alpha}(0)\Pi_{\pi\alpha}(0)}, \tag{42}$$

whence it follows that

$$\begin{aligned} m_{\pi\alpha}^2&=\left[\frac{1}{\lambda_1+\lambda_2}-\left(\frac{1}{\lambda_1^2-2\lambda_1\lambda_2-3\lambda_2^2}\right)\left(\lambda_1\left(1-\frac{8\kappa}{\alpha-\pi}\right)+\lambda_2\frac{\eta-8\kappa}{\alpha-\pi}\right)\right]\left(\frac{\alpha-\pi}{v}\right)^2 \\ &=\mathcal{O}(\lambda_2)+\mathcal{O}(\kappa). \end{aligned} \tag{43}$$

Thus we see that the effective (pseudo) NG boson mass in this channel is proportional to λ_2, and/or κ, the two O(8) symmetry breaking parameters.

Q.E.D.

V. SUMMARY AND CONCLUSIONS

In summary, we have (1) proven the NG theorem in the variational Gaussian wave functional approximation to the O(N) symmetric ϕ^4 model when the symmetry of the ground state is a proper subgroup of O($N-1$); (2) proven conservation of Nöther currents corresponding to the dynamically broken symmetries; (3) proven the same NG theorem in the exotic isotensor channel of the 't Hooft model in the limit $\lambda_2=\kappa\to 0$. The NG bosons are massless bound states of two massive constituents. We emphasize that our proofs do not depend on the specific values of the bare parameters, or of the cutoff in the theory, so long as the system is in the spontaneously broken phase with appropriate symmetry.

We should like to put these results into their proper logical and chronological setting. The variational method in quantum field theory (QFT) is based on the Schrödinger representation and goes by the name of Gaussian approximation to the ground state wave functional. This method, in

its various guises, was pioneered by Schiff, Rosen, and Kuti[6–8] in the 1960s and 1970s, and later revived and elaborated in the 1980s by Barnes and Ghandour,[9,13] and by Symanzik[10] and by Consoli, Stevenson and collaborators.[11,12,16] Related formalisms based on effective potentials and other functional methods were discussed in Refs. 8, 16, 12 and references cited therein. Most of these studies addressed the ϕ^4 scalar field theory that is also the prime example of the Nambu–Goldstone (NG) theorem,[1–5] an exact result in the O(N) symmetric ϕ^4 scalar theory with spontaneous internal symmetry breaking.

The NG theorem was first shown *not* to be satisfied by the solutions to the mass, or ''gap'' equations in the Gaussian approximation by Kamefuchi and Umezawa in 1964,[14] practically simultaneously with the general proofs of the NG theorem.[3–5] This fact was subsequently rediscovered several times[15,16] and this unsatisfactory situation persisted until 1994.[17] Various conjectures as to the reasons for this failure and as to potential remedies were advanced during this period of time. It was first shown in Ref. 17 that this apparent breakdown of the NG theorem is not an intrinsic shortcoming of the Gaussian wave functional approximation, but rather a consequence of incomplete previous analyses. In other words, the NG theorem is satisfied, but the NG bosons are not excitations of the elementary scalar fields, as initially expected. Rather, they are massless bound states of two massive elementary scalar excitations, in close analogy with Nambu's[1] proof of the NG theorem in a self-interacting fermion theory. NG bosons are solutions to the two-body [or Bethe–Salpeter (BS)] equation in the Gaussian approximation. That equation was only rarely considered in the literature,[7,9] and never before Ref. 17 in the context of spontaneous symmetry breaking of purely bosonic models.

In this light the result is simple enough to understand, yet it drew strong, albeit unpublished criticism and affirmation.[27] Perhaps the underlying reason for the misunderstanding by some was the implication of the proof that the ϕ^4 scalar field theory could have bound states, which, as ''everybody knew,'' (Georgi in Ref. 27) disagrees with various ''rigorous no-go'' and ''triviality'' theorems in the same theory.[28] (For more recent results comparing constructive QFT to the Gaussian approximation in $1+1$ dimensional field theories, see Ref. 29.) The said theorems hold only in the limit of an infinite cutoff, however, in which the Gaussian approximation also becomes trivial.[11] For finite cutoffs, on the other hand, this is a nontrivial theory that may contain bound states.

Soon after the first proof in Ref. 17 it was also shown along the lines of Ref. 3 that the NG theorem also follows from the Gaussian effective potential, Ref. 30, but that proof did not shed much light on the mechanisms that made the NG bosons come about. Only later, in Refs. 31 and 32, it was explicitly shown how this formal proof relates to the Gaussian two-body equations of motion. Another source of confusion was the apparent doubling of degrees of freedom, at least in some ''flavor'' (internal symmetry) channels, *viz.* the existence of massive ''elementary'' and massless bound states in the same channel. This problem was resolved in Ref. 31, wherein the Källen–Lehmann spectral function was calculated in appropriate channels of the model. This spectral function clearly shows the presence of massless NG states and the absence of the massive single-particle excitations. That also constitutes a proof of the NG theorem along Gilbert's lines, Ref. 5, within the Gaussian wave functional approximation. Thus we have confirmed all the well-known proofs of the NG theorem in the Gaussian approximation.

The NG theorem is the simplest example of a Ward–Takahashi identity, which follows from the underlying internal symmetry of the ϕ^4 model. Ward–Takahashi identities typically relate $(n-1)$-point Green functions to n-point functions and/or matrix elements of Nöther currents. These identities were developed by Lee in the linear sigma model at the perturbative one loop level,[23] and by Symanzik for arbitrary orders of perturbation theory,[24] so we shall call them the Lee–Symanzik (LS) identities.

The *exact*, i.e., nonperturbative Green functions satisfy an infinite set of coupled integro-differential equations called the Schwinger–Dyson equations.[19] The iterative/perturbative solutions to the SD equations form (infinite/finite) sets of Feynman diagrams. If one decouples the SD equations for higher order Green functions from the lower order ones (in popular jargon, if one truncates the SD equations), one may obtain tractable equations and find their solutions that sum

infinite, albeit incomplete sets of Feynman diagrams. It has been known at least since 1980, Ref. 9, that the Gaussian approximation to the unbroken symmetry ϕ^4 theory corresponds to one such truncation of the SD equations. But, truncated SD equations need not obey the conservation laws of the original SD equations of motion, i.e., LS identities may be violated by the truncation. To our knowledge, no proof of LS identities had been given for truncated SD equations, i.e., for infinite classes of diagrams in the bosonic linear sigma model prior to Ref. 17, although a similar proof had been given by Nambu and Jona-Lasinio in their fermionic model some 30 years before.[1] Thus we have shown that the Gaussian functional approximation constitutes a closed, self-consistent symmetry-preserving approximation to the Schwinger–Dyson equations.

ACKNOWLEDGMENTS

One of the authors (V.D.) would like to acknowledge a center-of-excellence (COE) Professorship for the year 2000/2001 and the hospitality of RCNP. The same author also thanks Professor Paul Stevenson for valuable conversations and correspondence relating to the Gaussian functional approximation.

APPENDIX A: THE GAP EQUATIONS WITH TWO VEVs

The first set of energy minimization equations (7) read

$$\mu_0^2=\lambda_0[v^2+3\hbar I_0(M)+\hbar I_0(\mu_1)+(N-2)\hbar I_0(\mu_2)], \tag{A1}$$

$$\mu_0^2=\lambda_0[v^2+\hbar I_0(M)+3\hbar I_0(\mu_1)+(N-2)\hbar I_0(\mu_2)], \tag{A2}$$

$$v^2=\langle\phi_0\rangle^2+\langle\phi_1\rangle^2=\langle\boldsymbol{\phi}\rangle^2, \tag{A3}$$

$$\langle\phi_i\rangle=0 \qquad i=2,\ldots,N-1, \tag{A4}$$

where the divergent integral $I_0(m_i)$, Eq. (4) is understood to be regularized via an UV momentum cutoff Λ, either three-, or four dimensional. The second set of gap equations (7) read

$$M^2=-\mu_0^2+\lambda_0[2\langle\phi_0\rangle^2+\langle\boldsymbol{\phi}\rangle^2+3\hbar I_0(M)+\hbar I_0(\mu_1)+(N-2)\hbar I_0(\mu_2)], \tag{A5}$$

$$\mu_1^2=-\mu_0^2+\lambda_0[2\langle\phi_1\rangle^2+\langle\boldsymbol{\phi}\rangle^2+\hbar I_0(M)+3\hbar I_0(\mu_1)+(N-2)\hbar I_0(\mu_2)], \tag{A6}$$

$$\mu_2^2=-\mu_0^2+\lambda_0[\langle\boldsymbol{\phi}\rangle^2+\hbar I_0(M)+\hbar I_0(\mu_1)+N\hbar I_0(\mu_2)]. \tag{A7}$$

Upon inserting Eq. (A1) into Eq. (A5), the following coupled ''gap'' equations emerge:

$$M^2=2\lambda_0\langle\phi_0\rangle^2+2\lambda_0\hbar[I_0(M)-I_0(\mu_1)]=2\lambda_0\langle\phi_0\rangle^2, \tag{A8}$$

$$\mu_1^2=2\lambda_0\langle\phi_1\rangle^2-2\lambda_0\hbar[I_0(M)-I_0(\mu_1)]=2\lambda_0\langle\phi_1\rangle^2, \tag{A9}$$

$$M^2-\mu_1^2=2\lambda_0(\langle\phi_0\rangle^2-\langle\phi_1\rangle^2+2\lambda_0+\hbar[I_0(M)-I_0(\mu_1)]), \tag{A10}$$

$$\mu_2^2=2\lambda_0\hbar[I_0(\mu_2)-I_0(M)]=2\lambda_0\hbar[I_0(\mu_2)-I_0(\mu_1)]. \tag{A11}$$

Note that these equations lead to

$$I_0(M)-I_0(\mu_1)=0, \tag{A12}$$

$$M^2-\mu_1^2=2\lambda_0(\langle\phi_0\rangle^2-\langle\phi_1\rangle^2)=0, \tag{A13}$$

which, in turn have at least one solution, $\mu_1=M$ and $\langle\phi_0\rangle^2=\langle\phi_1\rangle^2$, that are solutions to a single nontrivial gap equation

$$M^2 = 2\lambda_0 \langle \phi_1 \rangle^2, \tag{A14}$$

$$\mu_2^2 = 2\lambda_0 \hbar [I_0(\mu_2) - I_0(M)], \tag{A15}$$

with two unknowns one of which is kept fixed, cf. Ref. 18. This gap equation has been solved numerically in Ref. 18: it admits only massive solutions $M > \mu > 0$, however, for real, positive values of λ_0, μ_0^2 and real ultraviolet cutoff Λ in the momentum integrals $I_0(m_i)$. In other words, the "would be NG boson fields" ($\phi_{1,2,\ldots,N-1}$) excitations are all massive ($\mu > 0$) in the MFA. This looks like a breakdown of the NG theorem in this approximation, but, as discussed in Refs. 17 and 18, there is a solution by way of the two-body (Bethe–Salpeter) equation.

APPENDIX B: SYMMETRIES OF THE 't HOOFT MODEL

The two field quartets, $(\sigma, \boldsymbol{\pi})$ and $(\boldsymbol{\alpha}, \eta)$, have different "chiral" $O(4) = O(3) \times O(3) \simeq SU_L(2) \times SU_R(2)$,

$$\delta_5 \sigma = \boldsymbol{\beta} \cdot \boldsymbol{\pi}, \tag{B1}$$

$$\delta_5 \eta = -\boldsymbol{\beta} \cdot \boldsymbol{\alpha}, \tag{B2}$$

$$\delta_5 \boldsymbol{\alpha} = \boldsymbol{\beta} \eta, \tag{B3}$$

$$\delta_5 \boldsymbol{\pi} = -\boldsymbol{\beta} \sigma, \tag{B4}$$

isospin

$$\delta \sigma = 0, \tag{B5}$$

$$\delta \eta = 0, \tag{B6}$$

$$\delta \boldsymbol{\alpha} = -\varepsilon \times \boldsymbol{\alpha}, \tag{B7}$$

$$\delta \boldsymbol{\pi} = -\varepsilon \times \boldsymbol{\pi}, \tag{B8}$$

and $U_A(1) \simeq O(2)$ transformation properties

$$\delta_5^0 \sigma = \beta \eta, \tag{B9}$$

$$\delta_5^0 \eta = -\beta \sigma, \tag{B10}$$

$$\delta_5^0 \boldsymbol{\alpha} = \beta \boldsymbol{\pi}, \tag{B11}$$

$$\delta_5^0 \boldsymbol{\pi} = -\beta \boldsymbol{\alpha}. \tag{B12}$$

The Lie algebra O(4) has two Casimir operators, but there is only one invariant in the $(\frac{1}{2}, \frac{1}{2})$ representation with one meson quartet, *viz.* (i) $[\sigma^2 + \boldsymbol{\pi}^2]$, whereas with two quartets one has three invariants: (i) above, (ii) $[\eta^2 + \boldsymbol{\alpha}^2]$, and (iii) $[\eta\sigma - \boldsymbol{\alpha} \cdot \boldsymbol{\pi}]$. Any odd power of the third invariant (iii) violates CP. Even without the third invariant the algebraic structure of the Lagrangian is rich enough to allow for multiple vacua [solutions to the energy minimization equations (6)] even in the (first) Born approximation. For example, Eq. (6) applied directly to the 't Hooft interaction (26) in the Born approximation allow two nonzero VEVs $[\langle \sigma \rangle_{0B} = v_{0B} \neq 0$ and $\langle \alpha_3 \rangle_{0B} = v_{1B} \neq 0]$,

$$-\mu_0^2 - 4\kappa + \frac{\lambda_1}{2}[v_{0B}^2 + v_{1B}^2] + \lambda_2 v_{1B}^2 = 0, \tag{B13}$$

$$-\mu_0^2+4\kappa+\frac{\lambda_1}{2}[v_{0\mathrm{B}}^2+v_{1\mathrm{B}}^2]+\lambda_2 v_{1\mathrm{B}}^2=0. \tag{B14}$$

Their solutions are

$$\langle\sigma\rangle_{0\mathrm{B}}=v_{0\mathrm{B}}=\frac{\mu_0^2}{\lambda_1+\lambda_2}-4\frac{\kappa}{\lambda_2}, \tag{B15}$$

$$\langle\alpha_3\rangle_{0\mathrm{B}}=v_{1\mathrm{B}}=\frac{\mu_0^2}{\lambda_1+\lambda_2}+4\frac{\kappa}{\lambda_2}, \tag{B16}$$

leading to a nontrivially broken ground state. Note, however, that (i) $\lambda_2\to 0$ is a singular limit point, i.e., these vacua are not continuously connected with the more conventional vacua at $\lambda_2=0$, and (ii) the two kinds of vacua/energy minima coincide whenever $\kappa=0$ and $\lambda_2\neq 0$. Hence it is possible for the system to be in an unconventional vacuum even with infinitesimally small λ_2 and κ when they vanish with a fixed nonzero ratio. This makes it plausible that unusual vacua may also appear in this model when the symmetry is broken dynamically, i.e., by ''loop'' effects. This doubling of vacua is a consequence of multiple (two) independent algebraic invariants in the Lagrangian (26) which in turn led to multiple (two) VEVs, in agreement with the general theory.[4,20]

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 7 JULY 2003

A "periodic table" for supersymmetric *M*-theory compactifications

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(Received 24 September 2002; accepted 31 March 2003)

We develop a systematic method for classifying supersymmetric orbifold compactifications of *M*-theory. By restricting our attention to Abelian orbifolds with low order, in the special cases where elements do not include coordinate shifts, we construct a "periodic table" of such compactifications, organized according to the orbifolding group (order $\leqslant 12$) and dimension (up to 7). An intriguing connection between supersymmetric orbifolds and G_2 structures is explored. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1581972]

I. INTRODUCTION

Manifolds with SU(N) holonomy have been a source of significant interest for mathematicians and physicists alike. Indeed, the importance of $K3$ manifolds and Calabi–Yau threefolds in the arena of consistent superstring background geometries could hardly be overstated. Aside from their undisputed beauty, compactification on these spaces allows for important control of supersymmetry which, in turn, permits ready access to potentially testable phenomenological consequences of string theory itself. It is for such reasons that understanding the geometry of these objects, including the classification of associated gauge bundles,[1–3] has been such a relevant and fruitful endeavor. It is nowadays accepted, however, that there exists a more fundamental 11-dimensional underpinning, code-named *M*-theory, which appropriately describes nonperturbative aspects of fundamental physics. In contrast to the situation in perturbative string theory, within the context of *M*-theory the most important geometric compactification spaces have special holonomy.[4–6]

The connection between *M*-theory and four-dimensional $N=1$ supersymmetric models of particle physics is provided by 11-dimensional supergravity on compact seven manifolds with G_2 holonomy. Considerably less is known about these objects as compared to the case of Calabi–Yau manifolds. In light of the above discussion, however, it is important to develop a useful classification of the relevant supersymmetric *M*-theory models. The rudiments of a mathematical classification scheme for G_2 holonomy seven manifolds, each a resolution of an orbifold of a seven torus, has been provided by Joyce.[7] The purpose of this paper is to describe a complementary scheme, based on physics, of a class of seven-dimensional orbifold constructions which meet the criterion of $N=1$ supersymmetry preservation.

In previous papers[8–11] we described various technical aspects of the extraction of effective physics from *M*-theory. Generally, our techniques apply to global orbifold compactifications, and rely on significant constraints which follow from the requirement of chiral anomaly cancellation pointwise in 11 dimensions, most notably on distinguished even-dimensional submanifolds. Recently,[12] we have described how to obtain a pair of particular four-dimensional $N=1$ super Yang–Mills theories with chiral matter content from an *M*-theoretic intersecting brane-world scenario. In that paper we included a scan of multiplicities of supersymmetric *M*-theory orbifold

models of a particular class. In this paper we derive this scan, explaining in more detail the physical and mathematical criteria involved in finding such models.

Presupposing an ultimate connection between M-theory and standard model four-dimensional physics, a seven-dimensional compactification space must be Ricci-flat and admit singularities.[13] For these reasons, the class of toroidal orbifolds T^7/Γ, for a finite group Γ, holds special interest. The necessary geometrical singularities are of finite quotient type, and hence readily permit mathematical analysis. Each is modelled on $(M^1)^{7-n}\times\mathbb{R}^n/G$ for some subgroup $G\subset\Gamma$, where $M^1=S^1$ or the unit interval $I^1=S^1/\mathbb{Z}_2$. Moreover, as we shall see in this paper, under the right conditions one can explicitly describe a well-defined lift of the action of Γ to the 11-dimensional spinorial supercharge. This allows us to determine how much supersymmetry is preserved on the various fixed-point loci ("fixed-planes") of spacetime $T^7/\Gamma\times\mathbb{R}^{3,1}$.

The mathematical problem of identifying candidate compactification spaces with supersymmetric fixed-planes is quite elegant, and divides neatly into four parts. First of all, we must decide on a class of tori to orbifold. A torus T^7 is determined by a choice of a rank seven lattice $\Lambda\subset\mathbb{R}^7$. Throughout this paper we will assume that the lattice has the form $\Lambda:=A_1\oplus A_2^3$, i.e., the direct sum of three copies of the usual hexagonal lattice in the complex plane with one copy of $\mathbb{Z}$. More generally, our analysis applies to compactification on tori T^n modelled on lattices $A_1^a\oplus A_2^b$ with $a+2\,b=n$, $1\leqslant n\leqslant 7$. These are by no means the only lattices from which we could construct our tori. In fact, a particularly interesting case, especially as regards the discussion in Sec. V of this paper, is that of the irreducible lattice $A_7\subset\mathbb{R}^7$, whose automorphism group is one of the maximal finite subgroups of the group G_2. We choose to restrict attention to our particular class of decomposable lattices simply because it is both sufficiently general to subsume the orbifolds studied previously, and easy in this setting to describe the action on the 11-dimensional supercharge in the Clifford algebra.

The second step in identifying the desired supersymmetric orbifolds is to choose a particular class of groups Γ acting on T^7. An action on the torus is an action on $\mathbb{R}^7$ that preserves the lattice Λ. We will consider only group actions which respect the decomposition of Λ into direct summands. Thus, an element $g\in\Gamma$ acts as $\exp(2\pi i\vec{f})$, where $\vec{f}=(f_1,f_2,f_3,f_4)$, with $f_{1,2,3}\in\mathbb{Z}/6$ and $f_4\in\mathbb{Z}/2$. In this way we define a class of representations in which each element acts by rotations in two-dimensional subplanes plus the possibility of a parity reversal on one real coordinate. We call such actions "pseudoplanar representations," and groups which admit such representations "pseudoplanar groups." This eliminates, for the time being, orbifolds constructed from non-Abelian orbifolding groups, an omission we hope to rectify in future work.

Having restricted ourselves to pseudoplanar groups, next we need to enumerate all possible actions. For organizational purposes we wish to index the candidate orbifolds of T^n by their orbifolding groups Γ. For reasons of bounding complexity, in this paper we restrict attention to finite Abelian groups Γ of order $\leqslant 12$. The method we use, explained in detail in Sec. II, consists of classifying the Λ-compatible representations of Γ on $\mathbb{R}^7$, using the decomposition into irreducible characters to determine equivalence classes of group actions. Properly taking into account the automorphisms of the group Γ allows us to distinguish inequivalent group actions, and a matrix formalism makes quick work of computing the dimensions of the fixed-planes corresponding to each element of Γ, and provides for a concise accounting of various geometric data associated with each orbifold.

Finally, given this data, we must have a criterion for determining the exact amount of supersymmetry preserved on each fixed-plane. This fourth and final ingredient is provided by a systematic analysis of lifts of Γ to actions on 11-dimensional spinors. The necessary properties of Clifford algebra are reviewed in Sec. III A, and the criterion, our supersymmetric restriction theorem, is summarized in Table VI. We apply this criterion to the full class of groups Γ acting compatibly on our lattice Λ. In this way, we identify and classify the relatively small number of orbifolds T^n/Γ which maintain some supersymmetry at all points, constructions we refer to as *supersymmetric orbifolds*.

In the language of Ref. 12, the orbifolds considered here are all *hard* orbifolds, i.e., there are no fixed-point-free coordinate "shifts" in the Γ action, since we act directly through a represen-

TABLE I. The "periodic table" listing all supersymmetric, hard, pseudoplanar Abelian orbifolds T^n/Γ of M-theory, for cases $|\Gamma| \leqslant 12$. The labeling system is explained in Sec. II.

Γ	1	2	3	4	5	6	7
$\mathbb{Z}_2$	(1)*			(4)	(5)		
$\mathbb{Z}_3$				(4)			
$\mathbb{Z}_4$				(04)	(14)	(24)	(34)
$\mathbb{Z}_2\times\mathbb{Z}_2$					(014)*	(222)	(223)
$\mathbb{Z}_2\times\mathbb{Z}_3$				(004)	(140)*	(222)	(322)
					(104)		
$\mathbb{Z}_2\times\mathbb{Z}_4$					(00104)*	(10104)*	(20104)*
						(00222)	(00322)
						(01122)	(01222)
							(10222)
							(11122)
$(\mathbb{Z}_2)^3$							(2220001)*
							(1111111)
$(\mathbb{Z}_3)^2$							
$(\mathbb{Z}_2)^2\times\mathbb{Z}_3$					(1000004)*	(0020220)	(0122022)*
							(0122020)
							(0030220)
$\mathbb{Z}_3\times\mathbb{Z}_4$							

tation on the space $\mathbb{R}^7$ over $T^7=\mathbb{R}^7/\Lambda$. By contrast, Joyce's examples of orbifolds of T^7 admitting a resolution as a G_2 manifold[7] are all *soft* orbifolds. In Sec. V we use the first class of G_2 resolvable examples studied by Joyce[14,15] as a launching point for a discussion of the relationship between supersymmetric orbifolds of T^7 and the notion of a G_2-structure (a weaker, necessary condition for the orbifold to admit a G_2 holonomy resolution).

We have collected the results of our search, accounting for all pseudoplanar orbifold groups with low order, into a so-called periodic table of orbifolds, which we include in this introduction as Table I. In Table I we exhibit each supersymmetric orbifold T^n/Γ, with rows corresponding to distinct pseudoplanar groups Γ, listed by increasing group order, and columns corresponding to the representation dimensions $1\leqslant n\leqslant 7$. In each block of this table are listed the complete set of hard supersymmetric orbifolds corresponding to associated n-dimensional representations of Γ compatible with our lattices. Each orbifold is indicated by a particular *label*, which codifies the group action of Γ on T^n in a manner explained in detail in Sec. II. For a subset of the supersymmetric orbifolds, the corresponding orbifold label has an asterix appended. These models are those which split off a separate $S^1/\mathbb{Z}_2$ factor. Such models are the only ones which have 10-dimensional fixed-planes. Owing to this distinction, there is a more direct connection between this class of supersymmetric orbifolds and perturbative heterotic string models than is the case for the orbifolds listed without stars.

There are two natural extensions of our work in this paper which we plan to investigate in the near future. First, we would like to remove the pseudoplanar and abelian restrictions on the Γ action, allowing instead any $\Gamma\subset\mathrm{Aut}(\Lambda)$. In particular this will allow many non-Abelian group actions, which in turn will require a generalization of the supersymmetric restriction proof of Sec. III C. An important step towards such a formulation is described in Sec. IV. It would also be quite valuable to reformulate both the analysis herein and the anomaly cancellation compatibility checks in Refs. 11 and 12 using the theory of principal bundles on orbifolds. In this setting both the supersymmetric restriction criterion and anomaly cancellation mechanism should find expression in the language of characteristic classes of such bundles.

II. HARD ORBIFOLDS, SUPERSYMMETRY, AND CHARACTERS

Each distinct representation R, with real dimension $n\leqslant 7$, of any finite group $\Gamma\subset\mathrm{Aut}(T^n)$, can be used to define an orbifold T^n/Γ, and a corresponding compactification scheme in M-theory.

In this section we describe some useful tools for efficiently accounting for large numbers of such constructions, and explain how these feed naturally into an algorithm for selecting those which satisfy a particular criterion: that the 11-dimensional supercharge Q have nonvanishing components at all points in M^{11}. This is done in two steps. First we review some standard results pertaining to representations of finite groups. Then we explain some original technology which adapts these results to the special purpose of sifting through all possible representations and finding those which satisfy our criterion.

A. Representations of finite Abelian groups

Let Γ be an Abelian (commutative) group, and $\rho:\Gamma\to GL_n(\mathbb{C})$ an n-dimensional complex matrix representation of Γ, i.e., ρ is a homomophism of groups. Since Γ is Abelian, $g_1 g_2 = g_2 g_1$ for all $g_i \in \Gamma$, and each element $g \in \Gamma$ equals its own conjugacy class. A basic result in the theory of representations of finite groups states that for a group of order q, with s conjugacy classes, there are, up to equivalence, s distinct irreducible representations $R_1,\ldots,R_s$ over $\mathbb{C}$. Moreover, if R_i has dimension n_i, then

$$q := \sum_{i=1}^{s} (n_i)^2 \tag{2.1}$$

(Ref. 16, Theorem 2.3). When applied to an Abelian group Γ, this shows that each $n_i = 1$, i.e., that each of the irreducible representations of Γ is itself a *character* (one-dimensional representation) of the group.

In fact, it is a simple matter to describe all the characters of a finite Abelian group. Any finite Abelian group Γ can be written as a direct product of m cyclic groups of orders $q_1,\ldots,q_m$, respectively, so that

$$q = |\Gamma| = q_1 q_2 \cdots q_m . \tag{2.2}$$

A typical element of Γ can be represented by the m-tuple $\vec{a} := (a_1,a_2,\ldots,a_m)$, where $0 \leqslant a_i < q_i$, with composition of elements given by componentwise addition followed by reduction of the ith component to its least non-negative remainder modulo r_i, $i=1,\ldots,m$. Then corresponding to each m-tuple $\vec{c} := [c_1,c_2,\ldots,c_m]$, where $0 \leqslant c_i < r_i$, there exists a character

$$\Gamma_{\vec{c}}(\vec{a}) := \exp\left(2\pi\imath \sum_{i=1}^{m} \left(\frac{a_i c_i}{r_i} \right) \right) \tag{2.3}$$

of Γ, and all q characters arise in this way (Ref. 16, Theorem 2.4). The identity element of Γ corresponds to the trivial character.

The obvious correspondence between the characters $\vec{c}$ and elements $\vec{a}$ of Γ is not canonical. Even though they are each composed of m-tuples of integers modulo q_i, $i=1,\ldots,m$, the isomorphism between these is only well-defined up to an automorphism of the group Γ.

Any n dimensional representation of an Abelian group Γ can be written as a direct sum of n of its characters $\Gamma_{\vec{c}}$, i.e., by the data of an n-tuple $\{\vec{c}^1,\ldots,\vec{c}^n\}$ of m-tuples $\vec{c}^j := [c^j_1,\ldots,c^j_m]$, for $j=1,\ldots,n$. Two such representations are considered *equivalent* if these n-tuples agree as unordered lists.

B. Character tables and *C*-matrices

The set of hard orbifolds T^n/Γ is equivalent to the set of distinct n-dimensional representations of Γ consistent with the lattice that defines T^n. If Γ is a finite Abelian group, then these, in turn, are equivalent to the possible ways to order sets with elements chosen freely from among the characters of Γ, allowing for repetition. It is, therefore, a straightforward exercise, in principle, to construct comprehensive lists of hard orbifolds T^n/Γ. This is so because it is also straightforward

TABLE II. The "elemental" character tables for the groups $\mathbb{Z}_2$, $\mathbb{Z}_3$, and $\mathbb{Z}_4$.

$\mathbb{Z}_2$	Ω	Γ	$\mathbb{Z}_3$	Ω	Σ	$\overline{\Sigma}$	$\mathbb{Z}_4$	Ω	Ψ	Σ	$\overline{\Psi}$
1	+	+	**1**	+	+	+	**1**	+	+	+	+
α	+	−	β	+	1/3	−1/3	γ	+	1/4	1/2	−1/4
			β^2	+	−1/3	1/3	γ^2	+	1/2	+	1/2
							γ^3	+	−1/4	1/2	1/4

to determine the characters for any finite Abelian group, using the following simple algorithm. (As described above, we shall limit our discussion to the case of pseudoplanar groups.)

Each pseudoplanar group is given by the direct product of some number each of $\mathbb{Z}_2$, $\mathbb{Z}_3$, and $\mathbb{Z}_4$ factors. For each of these three "elemental" groups, the list of characters are contained in the character tables exhibited in Table II. In these tables, the elements of the group are enumerated rowwise, while each column corresponds to a distinct character. (Our convention differs from that used in the mathematical literature, wherein character tables typically list group elements as columns and characters as rows. Our choice of convention is more suited to the particular application to physics described in this paper.) For the case of $\mathbb{Z}_2$ the characters are real, i.e., each describes a group action on one real coordinate; in our case this corresponds to an action on an A_1 lattice; a plus sign in the table indicates a trivial action, while a minus sign indicates a sign change $x \to -x$ on the associated coordinate. For the groups $\mathbb{Z}_3$ and $\mathbb{Z}_4$ the nontrivial characters are complex; i.e., each describes a group action on a pair of real coordinates; in our case this corresponds to an action on an A_2 lattice; a plus sign indicates a trivial action, other rational numbers indicate the fraction of a complete counterclockwise rotation in the plane spanned by the relevant A_2 lattice. Such entries are defined modulo 1.

It is useful to assemble the entries of a given character table for a group Γ into a "character matrix" $\sigma(\Gamma)$. The data in Table II can be written as

$$\sigma(\mathbb{Z}_2)=\begin{pmatrix} 0 & 0 \\ 0 & 1/2 \end{pmatrix}, \quad \sigma(\mathbb{Z}_3)=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1/3 & -1/3 \\ 0 & -1/3 & 1/3 \end{pmatrix}, \quad \sigma(\mathbb{Z}_4)=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/4 & 1/2 & -1/4 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & -1/4 & 1/2 & 1/4 \end{pmatrix}.$$

We adopt the convention that trivial actions (plus signs in the character tables) are represented in the character matrix with zeros, and parity reversals (minus signs in the character tables) are represented with the fraction 1/2. The character matrix for a generic pseudoplanar group with m elemental factors $\Gamma = G_1 \times \cdots \times G_m$, is obtained by combining the character matrices $\sigma(G_i)$ as an outer sum. For instance, the character matrix $\sigma(\mathbb{Z}_2 \times \mathbb{Z}_3)$ can be written as a a two-by-two array of three-by-three block matrices, wherein the upper left block is computed by adding the upper left entry in $\sigma(\mathbb{Z}_2)$ to the entire matrix $\sigma(\mathbb{Z}_3)$, the second block in the first row of blocks in $\sigma(\mathbb{Z}_2 \times \mathbb{Z}_3)$ is given by adding the entry $\sigma(\mathbb{Z}_2)_{12}$ to the entire matrix $\sigma(\mathbb{Z}_3)$, and so forth. The matrix $\sigma(\mathbb{Z}_2 \times \mathbb{Z}_3)$ formed in this way can be usefully re-expressed in terms of a character table, with the result shown in Table III. In Table III, all rational entries are defined modulo 1. Furthermore, a trivial action, denoted by a zero in the corresponding character matrix, is represented in the character table by a plus sign. Finally, on complex characters an entry 1/2, describing a 180 degree rotation, is represented in the table by a minus sign. Upon reconstituting the character matrix $\sigma(\mathbb{Z}_2 \times \mathbb{Z}_3)$ into Table III we have inserted a useful naming convention for the group elements and characters; we have named the order-two generating element α and the order-three generating element β. Similarly, we have named the trivial character Ω, the order two character Λ, the order-three characters Σ and $\overline{\Sigma}$ and the order-six characters Ψ and $\overline{\Psi}$.

By repeating the operation of combining character matrices as outer sums, in the manner described above, the character matrix and, equivalently, the character table for any pseudoplanar

TABLE III. The character table for the group $\mathbb{Z}_2\times\mathbb{Z}_3$.

$\mathbb{Z}_2\times\mathbb{Z}_3$	Ω	Σ	$\overline{\Sigma}$	Λ	Ψ	$\overline{\Psi}$
1	+	+	+	+	+	+
β	+	1/3	−1/3	+	1/3	−1/3
β^2	+	−1/3	1/3	+	−1/3	1/3
α	+	+	+	−	−	−
$\alpha\beta$	+	1/3	−1/3	−	−1/6	1/6
$\alpha\beta^2$	+	−1/3	1/3	−	1/6	−1/6

group can be generated readily from the three elemental character matrices $\sigma(\mathbb{Z}_2)$, $\sigma(\mathbb{Z}_3)$, and $\sigma(\mathbb{Z}_4)$. For an illustration in the case $\Gamma=(\mathbb{Z}_2)^3$, see Table VII. Here $\Omega:=\Gamma_{[0,0,0]}$ is the trivial character, and the group elements down the left-hand side are indexed in the usual binary ordering:

$$1:=(0,0,0)\,,\quad \gamma:=(0,0,1)\,,\quad \beta:=(0,1,0)\,,\ldots,\alpha\beta\gamma:=(1,1,1).$$

In general, however, there is quite a lot of physically irrelevant redundancy in the full character table for a given orbifolding group Γ. For instance, in the case of $\Gamma=\mathbb{Z}_2\times\mathbb{Z}_3$, the characters which we have named Σ and Ψ describe group actions on a complex coordinate z. However, if we describe these same characters in terms of their actions on the complex conjugate $\overline{z}$, these same characters would appear to act precisely as do $\overline{\Sigma}$ and $\overline{\Psi}$ on the original coordinate z. Thus, complex characters are physically indistinguishable from their conjugates. Since conjugate pairs of characters can be can be mapped into each other by a merely semantical renaming of the coordinates, we can more efficiently describe the relevant representation theory of this group by considering a restricted set of essential nontrivial characters. For the case of $\Gamma=\mathbb{Z}_2\times\mathbb{Z}_3$, these would be Λ, Σ and Ψ. At the same time, elements with order greater than two have nontrivial inverses. These inverse elements have precisely the same locus of fixed-points in the physical space T^n/Γ as do the original elements. So we can characterize the geometry of a given orbifold in terms of a representative set of essential nontrivial elements, thereby removing this second, physical, redundancy.

The number of nontrivial representative elements of any finite Abelian group is equivalent to the number of essential nontrivial characters. This number provides a "physical rank" r of the group. By including only the essential nontrivial elements and characters, we can replace the full character table with an "abbreviated character table." For the case of $\Gamma=\mathbb{Z}_2\times\mathbb{Z}_3$, we would thereby replace Table III with the abbreviated character table shown in Table IV. Notice that we may choose at will the ordering of the elements (rows) and, independently, the ordering of the characters (columns) when we construct a character table; there is no *a priori* canonical ordering. Notice, as well, that no information is sacrificed by replacing a full character table with an abbreviated character table.

By multiplying the abbreviated character table by the order of the group we define an integer-valued, square $r\times r$ matrix, which we denote $C(\Gamma)$. For the case of $\Gamma=\mathbb{Z}_2\times\mathbb{Z}_3$, this is easily obtained from Table IV by multiplying the entries by 6, which is the order of $\mathbb{Z}_2\times\mathbb{Z}_3$. In this way we determine

TABLE IV. The abbreviated character table for the group $\mathbb{Z}_2\times\mathbb{Z}_3$.

$\mathbb{Z}_2\times\mathbb{Z}_3$	Γ	Σ	Ψ
α	1/2	0	1/2
β	0	1/3	1/3
$\alpha\beta$	1/2	1/3	−1/6

TABLE V. The representation $R=(322)$ of the group $\mathbb{Z}_2\times\mathbb{Z}_3$.

$\mathbb{Z}_2\times\mathbb{Z}_3$	x_1	x_2	x_3	z_1	z_2
α	$-$	$-$	$-$	$+$	$-$
β	$+$	$+$	$+$	1/3	1/3
$\alpha\beta$	$-$	$-$	$-$	1/3	$-1/6$

$$C(\mathbb{Z}_2\times\mathbb{Z}_3)=\begin{pmatrix} 3 & 0 & 3 \\ 0 & 2 & 2 \\ 3 & 2 & -1 \end{pmatrix}. \tag{2.4}$$

Of course, owing to the freedom to independently rearrange the rows and the columns of the abbreviated character matrix, the corresponding matrix $C(\Gamma)$ is defined only up to similar reorderings. However, such flexibility can always be used to render the C-matrix symmetrical. We deem this canonical. It is also possible, while keeping $C(\Gamma)$ symmetrical, to arrange the rows and columns so that the corresponding elements and characters have monotonically increasing order. This too, we deem canonical.

All the information described by Table III is also contained in the matrix $C(\mathbb{Z}_2\times\mathbb{Z}_3)$ shown in (2.4). It is interesting that quite a lot of information pertaining to properties of any finite Abelian group, including the complete representation theory can be codified in a symmetric matrix $C\in \mathrm{GL}(r,\mathbb{Z})$. As it turns out, the matrices $C(\Gamma)$ are valuable tools in the search for supersymmetric orbifolds. The matrices $C(\Gamma)$ for each of the pseudoplanar groups with group order $\leqslant 12$ are listed in the Appendix.

C. The enumeration of distinct orbifolds

A representation of Γ is designated by choosing a set of real and complex characters, including the possibility of degeneracy, from the list of essential nontrivial characters. Generally, order-two characters are real, while characters with higher order are complex. Therefore, if we select a order-two characters and b higher-order characters, the corresponding representation will act on $n=a+2b$ real dimensions, $2b$ of which are complexified. Since the set of essential nontrivial characters correlates with the columns of the matrix $C(\Gamma)$, we can unambiguously designate a representation by an ordered list of r multiplicities, each indicating the number of real coordinates transforming according to a corresponding character. The ordering of the multiplicities corresponds to the ordering of the characters described by the rows of the C matrix. Of course, the multiplicities corresponding to complex characters are necessarily even, while those corresponding to order-two characters may be even or odd.

As an example, in the case of the group $\Gamma=\mathbb{Z}_2\times\mathbb{Z}_3$, the physical rank is 3, and the corresponding C-matrix is given by (2.4). In this case, each representation is given by a 3-tuple, $R=(a_1,a_2,a_3)$, where a_1, a_2 and a_3 are the number of real coordinates transforming according to the characters Λ, Σ, and Ψ, respectively. In this case, $a_1\in\mathbb{N}$ since the character Γ is real, and $a_{2,3}\in 2\,\mathbb{N}$ since the characters Σ and Ψ are complex. To be quite specific, the representation of $\mathbb{Z}_2\times\mathbb{Z}_3$ described by the three-tuple $R=(3\,2\,2)$ is a representation which acts on $3+2+2=7$ real coordinates. In this case, however, four of the real coordinates are complexified as two complex coordinates. The first multiplicity (3) in the label (322) indicates that three real coordinates, say $x_{1,2,3}$ transform according to the character Λ, the second multiplicity (2) indicates that two real coordinates, combined into one complex coordinate, say z_1, transform according to the character Σ, and the third multiplicity (2) indicates that one more complex coordinate, say z_2, transforms according to the character Ψ. The corresponding group actions are shown in Table V.

The particular orbifold T^n/Γ which corresponds to a given representation R generically includes a locus of special points which remain invariant under elements of Γ. These generically constitute hyperplanes of various dimensionalities which intersect, forming an intricate network.

One of our primary concerns is to decide what sorts of physics, in the form of localized states, are described by these planes and their intersections. In the next section we will describe in detail how one studies the issue of how many supercharges are retained on these. A primary consideration in this regard is, of course, to describe the number of dimensions which are spanned by the fixed-planes associated with each group element.

There is a simple formula which allows one to compute the set of dimensions corresponding to the r representative nontrivial elements. This formula is most easily described in terms of another useful matrix, which we call $M(\Gamma)$, obtained from $C(\Gamma)$ by replacing all zero entries with ones, and all nonzero entries by zeros. By way of illustration, we focus again on the example $\Gamma = \mathbb{Z}_2 \times \mathbb{Z}_3$. In this case, this prescription, applied to $C(\mathbb{Z}_2 \times \mathbb{Z}_3)$, as given in (2.4), yields

$$M(\mathbb{Z}_2 \times \mathbb{Z}_3) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} . \tag{2.5}$$

For a given orbifold, described by the representation R of a group Γ, the dimensionality of the fixed-planes of each representative element is described by another r-tuple, $d(R)$, given by

$$d(R) = (\,11 - n\,)\,\mathbf{1} + R\,M\,, \tag{2.6}$$

where $\mathbf{1}$ is the row vector with ones in each entry and $n = R \cdot \mathbf{1} = \Sigma_i a_i$. As an example, for the particular orbifold described by $R = (322)$, we compute $n = 7$ and

$$d(122) = (11-7)\,(1 \quad 1 \quad 1) + (3 \quad 2 \quad 2) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = (6 \quad 7 \quad 4)\,. \tag{2.7}$$

Thus, the respective fixed-planes associated with the elements α, β, and $\alpha\beta$ have dimensionality 6, 7, and 4. This result can be verified from the precise group actions in Table V.

Now we have all the information we need to form comprehensive lists of all pseudoplanar orbifolds, including all the data pertaining to the group actions. First we choose a group Γ. Then, we form lists of orbifolds T^n/Γ, for each value of $1 \leqslant n \leqslant 7$ by sequencing through the ordered partitions of n into r non-negative integers, in the manner described above. For the case of $T^7/(\mathbb{Z}_2 \times \mathbb{Z}_3)$ orbifolds, for example, we create the sequence of 3-tuples (a_1, a_2, a_3) which describe ordered partitions of $n = 7$ into sums of $r = 3$ nonnegative integers, subject to the constraints that $a_1 \in \mathbb{N}$ and $a_{2,3} \in 2\,\mathbb{N}$. The complete list of such 3-tuples is given in the usual ascending order in mod 7 arithmetic, as (106), (124), (142), (160), (304), (322), (340), (502), (520), (700). We describe these ordered sets of multiplicities as orbifold *labels*. In each case the corresponding group actions can be determined by dividing the C-matrix by the group order and then selecting rows from this divided C-matrix with the appropriate multiplicity indicated by the corresponding label. The group actions for the orbifold $T^7/(\mathbb{Z}_2 \times \mathbb{Z}_3)_{(322)}$, described above, were obtained in precisely this way, and stand as an example of this methodology.

D. The periodic table

We use the algorithm described in the previous paragraph to systematically cycle through each orbifold label of each pseudoplanar group, obtaining all of the relevant group actions in each case. In each instance, each element of Γ can be represented, by arranging the coordinates judiciously, by a set of three fractional rotations (f_1, f_2, f_3) describing counterclockwise rotations in respective planes spanned by three A_2 lattices, plus possibility of a parity reversal in one real coordinate, which we codify as the binary choice $P \in \{0,1\}$, describing the respective absence or presence of a parity reversal.

As it turns out, the values of $(f_1, f_2, f_3 \mid P)$ for each element of Γ corresponding to a given orbifold label provide all the data necessary to resolve the amount of supersymmetry on the corresponding orbifold plane. The precise corrrespondence is derived in the next section, where it is presented as a supersymmetric restriction theorem. This result says that an orbifold plane is supersymmetric if and only if there is at least one way to add or subtract the three corresponding fractions f_i to obtain, in the case $P=0$, an even integer, or, in the case $P=1$, any integer (even or odd).

For our restricted class of lattices, a given element is compatible only if the three f_i are each elements of the set $\{0, 1/2, \pm 1/3, \pm 1/4, \pm 1/6\}$ mod 1. (There are, therefore $7^3 \times 2 = 686$ possibilities for each element.) It is possible to have compatible elements which do not have compatible products. For example, in the case $\Gamma = \mathbb{Z}_3 \times \mathbb{Z}_4$, there are several models which pass the criteria of the supersymmetric restriction theorem, except that the representations in question involve order-twelve rotations in at least one plane. These would be acceptable as supersymmetric orbifolds of $\mathbb{R}^n$, but not of T^n, because there is no lattice in $\mathbb{C}$ compatible with such a rotation. The number of global orbifolds T^n/Γ is therefore much smaller than the number of orbifold singularities which can be modelled locally as $\mathbb{R}^n/\Gamma$.

The search for supersymmetric orbifolds consists of four steps. First, for a given choice of Γ and n, we generate the complete list of compatible orbifold labels. Second, for each orbifold label, we use the matrix $C(\Gamma)$ to determine the data $(f_1, f_2, f_3 \mid P)$ for each of the r representative elements. Third, we apply the supersymmetric restriction theorem to remove each orbifold which has any element whose data does not meet the restriction criterion. Fourth, we examine the list of orbifolds which satisfy these restrictions, and we remove cases which are redundant. We have created a number of Mathematica functions which fully automate this process, and have used this to generate Table I which appears in the introduction. In this way, we can easily generalize our periodic table to arbitrary group order.

Our periodic table includes all of the hard global *M*-theory orbifolds described previously by other authors as well as by ourselves. For instance the $S^1/\mathbb{Z}_2$ model corresponds to the original *M*-theory model described in Refs. 17 and 18. The four T^4/Γ models correspond to the four global orbifold limits of $K3$. The $T^5/\mathbb{Z}_2$ model was discussed in Refs. 19 and 20. (It was the study of that simple model which first implicated wandering five-branes as a means of unifying ostensibly unique vacua into classes linked by phase transitions.) The four starred models T^5/Γ correspond to the four global orbifold limits of $K3 \times S^1/\mathbb{Z}_2$ and were studied in Refs. 8–10 and 21. The $T^7/(\mathbb{Z}_2)^3$ model with label (2220001) was described in Ref. 11 and the $T^7/(\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_3)$ with label (0122022) was described in Ref. 12. Finally, resolutions of the softenings of the $T^7/(\mathbb{Z}_2)^3$ model with label (1111111) were presented by Joyce in Refs. 14, 15, and 7 as prototype G_2 manifolds, and studied by Acharya as candidate *M*-theory compactification spaces[22,23] (see also Sec. V).

III. A SUPERSYMMETRIC RESTRICTION THEOREM

In the bulk of M^{11} (i.e., at all points not within the locus of orbifold fixed-planes) the 11-dimensional supercharge is completely preserved. It is within the locus of fixed-planes, therefore, that the issue of supercharge preservation becomes important. Since the supercharge transforms nontrivially under elements of Γ, only those components of Q which remain invariant are not projected to zero on those spacetime points inert under those same elements. The invariant components of Q typically resolve as a d-dimensional spinor, where d is the total dimension of the invariant locus associated with that element near a given point. Precisely how many irreducible $\mathrm{SO}(d-1,1)$-spinors are included in this set determines the amount of local sypersymmetry preserved on that fixed plane. For the sorts of pseudoplanar orbifolds defined above, it is possible to delineate a concise criterion for selecting those which, in this way, retain supersymmetry. In this section, which is relatively technical, we derive this supersymmetric restriction theorem. We start by establishing notational conventions and stating the result, and then prove it by analyzing the question of how the spinorial supercharge is influenced by lifts of various elements of finite subgroups of SO(10,1).

A. Notations

We use space–time coordinates $x^I \equiv \{x^0, x^i\}$, where $i = 1, \ldots, 3, 5, \ldots 11$, and gamma matrices Γ_I, which satisfy the Clifford algebra $\{\Gamma_I, \Gamma_J\} = 2\,\eta_{IJ}$, where $\eta_{IJ} = \mathrm{diag}(-+\cdots+)$ is the flat metric. The gamma matrices are chosen such that Γ_0 is anti-Hermitian, $\Gamma_0^\dagger = -\Gamma_0$, and Γ_i are Hermitian, $\Gamma_i^\dagger = \Gamma_i$. It is sometimes useful to define $\Gamma_4 = i\,\Gamma_0$. Another useful identity is $\Gamma_{11} = i\,\Gamma_1 \cdots \Gamma_{10}$. The matrices $\Gamma_{IJ} = \frac{1}{2}[\,\Gamma_I, \Gamma_J\,]$ are the generators of spin (11). We define a complex structure by writing the six real coordinates $x_{5,\ldots,10}$ in terms of three complex coordinates, according to $z_{1,2,3} \equiv x_{5,7,9} + i\,x_{6,8,10}$.

Consider an element which acts as simultaneous rotations in three complex planes, with coordinates z_1, z_2, and z_3, and possibly a parity flip on one real coordinate x^{11},

$$\alpha : (\,z_1, z_2, z_3; x^{11}) \to (\,e^{i\,\theta_1} z_1, e^{i\,\theta_2} z_2, e^{i\,\theta_3} z_3; (-)^P x^{11}\,), \tag{3.1}$$

with $\theta_i = 2\,\pi\,f_i$. The three rational numbers f_i describe the fraction of a complete rotation imparted, respectively, on the three complex planes. The parameter $P \in \{0,1\}$ indicates whether or not the element includes a parity flip. The order of α is given by the least common positive integer multiple of the denominators of the reduced form of the three f_i's and also $(1/2)^P$.

For a given choice of $(\,f_1, f_2, f_3 \,|\, P\,)$, Eq. (3.1) describes a particular global SO(10,1) transformation plus the possibility of a parity transformation. On spinors this induces $\psi \to \Omega\,\psi$, where

$$\Omega = \exp(\,\tfrac{1}{4}\,\theta^{IJ}\,\Gamma_{IJ}\,)\,(\,\Gamma_{11}\,)^P \tag{3.2}$$

and where θ^{IJ} are the parameters of the SO(10,1) transformation. From (3.1) we read off the nonvanishing parameters as $\theta^{5,6} = -\theta^{6,5} \equiv \theta_1$, $\theta^{7,8} = -\theta^{8,7} \equiv \theta_2$, and $\theta^{9,10} = -\theta^{10,9} \equiv \theta_3$. Thus we can rewrite (3.2) as

$$\Omega = \exp(\,\tfrac{1}{2}\,\theta_1\,\Gamma_{5,6}\,)\,\exp(\,\tfrac{1}{2}\,\theta_2\,\Gamma_{7,8}\,)\,\exp(\,\tfrac{1}{2}\,\theta_3\,\Gamma_{9,10}\,)(\,\Gamma_{11}\,)^P\,. \tag{3.3}$$

The supercharge Q is an 11-dimensional Majorana spinor, which transforms precisely as $Q \to \Omega\,Q$. It is useful to append subscripts to spinors, and to spinorial operators, to indicate dimensionality. We thus write the 11-dimensional supercharge Q as $Q_{(11)}$ to indicate that this field takes its values in spin (11). Similarly, we write the operator Ω, defined in (3.3), as $\Omega_{(11)}$ to indicate that this object operates on 11-dimensional spinors.

If the fixed-point locus associated with an element (3.1) has dimensionality d, then, in the neighborhood of this locus, the structure group is broken from SO(10,1) down to $\mathrm{SO}(d-1,1) \times \mathrm{SO}(11-d)$. Accordingly, we write the supercharge as a tensor product of an $\mathrm{SO}(d-1,1)$ fixed-plane spinor and an $\mathrm{SO}(11-d)$ "normal" spinor, as $Q_{(11)} = Q_{(d)} \otimes Q_{(11-d)}$. Similarly, the operator Ω decomposes as $\Omega_{(11)} = \Omega_{(d)} \otimes \Omega_{(11-d)}$. In order to resolve the amount of unbroken fixed-plane supersymmetry, we solve the equation $Q_{(11)} = \Omega_{(11)}\,Q_{(11)}$, and then count the degrees of freedom which describe the most general solution.

The analysis described below is completely general, modulo irrelevant reordering of coordinates. Thus, in this section we consider the element $(\,0, 0, f \,|\, 0\,)$ equivalent to $(\,0, f, 0 \,|\, 0\,)$, for instance.

B. Statement of the theorem

The conclusions which we draw in each of the seven cases discussed in Sec. III C can be easily summarized as follows. The condition for supersymmetry on a fixed-plane associated with any element $\alpha \in \Gamma$, of the special sort characterized by (3.1), is

$$f_1 \pm f_2 \pm f_3 \in \begin{cases} 2\,\mathbb{Z}, & P = 0 \\ \mathbb{Z}, & P = 1 \end{cases} \tag{3.4}$$

TABLE VI. The seven sorts of elements, listed along with the associated fixed-plane dimensionality and the generic amount of supersymmetry retained when the conditions listed in (3.4) are satisfied. The $d=6$ and the $d=4$ cases have exceptions. In the $d=6$ case, if $f=1/2$ then the supersymmetry is merely halved, not quartered. In the $d=4$ case if $|f_1|$, $|f_2|$, and $|f_3|$ are drawn, one each, from either set (1/2, 1/3, 1/6) or (1/2, 1/4, 1/4) then supersymmetry is merely quartered, not eighthed.

$(f_1, f_2, f_3 \mid (-)^P)$	d_{fixed}	SUSY
$(0,0,0 \mid -)$	10	1/2
$(0,0,f \mid +)$	9	NONE
$(0,0,f \mid -)$	8	NONE
$(0,f,\pm f \mid +)$	7	1/2
$(0,f,\pm f \mid -)$	6	1/4*
$(f_1,f_2,f_3 \mid +)$	5	1/4
$(f_1,f_2,f_3 \mid -)$	4	1/8*

for any one of the four possible choices of unspecified signs. If condition (3.4) is satisfied, then supersymmetry is generically reduced to the minimal amount possible in the dimensionality of the fixed plane. Exceptions occur in cases where $P=1$, when one of the sums in (3.4) gives an even integer and another gives an odd integer. In such cases, the fixed-plane supersymmetry is twice the minimal amount. These results are reflected in Table VI.

Note that this result applies to orbifolds $\mathbb{R}^7/\Gamma$ as well as to orbifolds T^7/Γ. In the former case, there is no restriction on the choices of the f_i's other than that they should be rational. In the latter case, there are additional constraints which follow from the requirement that $\Gamma \subset \mathrm{Aut}(T^7)$. For the cases described in Sec. III C, this requirement amounts to the restriction that $f_{1,2,3}$ must be chosen from the set $\{0, 1/2, \pm 1/3, \pm 1/4, \pm 1/6\}$ mod 1.

C. Proof of the theorem

The result is established by explicitly analyzing how the spinorial supercharge is influenced by lifts of various elements of finite subgroups of SO(10,1).

Ten-dimensional fixed-planes: The only transformation (3.1) which has 10-dimensional fixed-planes is an order-two element acting as $(f_1,f_2,f_3 \mid P)=(0,0,0 \mid 1)$. In this case, the supercharge transforms as $Q_{(11)} \to \Gamma_{11} Q_{(11)}$. We decompose $Q_{(11)}$ according to $Q_{(11)}=Q_{(10)R} \oplus Q_{(10)L}$, where $Q_{(10)R,L}=\pm \Gamma_{11} Q_{(10)R,L}$ are 10-dimensional Majorana–Weyl projections of $Q_{(11)}$. The fixed-plane condition, $Q_{(11)}=\Omega_{(11)} Q_{(11)}$ can now be written

$$Q_{(10)\,R,L}=\pm Q_{(10)\,R,L}\,. \tag{3.5}$$

This equation is easy to solve. On the fixed-plane we have $Q_{(11)} \to Q_{(10)R}$. Thus, the bulk supersymmetry is *halved* on the fixed-planes.

Nine-dimensional fixed-planes: Nine-dimensional fixed-planes correspond to elements $(f_1,f_2,f_3 \mid P)=(0,0,f \mid 0)$, where $f \neq 0$ mod 1. In this case, the supercharge transforms as $Q_{(11)} \to \Omega_{(11)} Q_{(11)}$, where

$$\Omega_{(11)}=\exp(\pi f \Gamma_9 \Gamma_{10})\,. \tag{3.6}$$

We write $Q_{(11)}$ as a tensor product of a nine-dimensional fixed-plane spinor with an SO(2) "normal" spinor, according to $Q_{(11)}=Q_{(9)} \otimes Q_{(2)}$. Similarly, we use the following representation for the gamma matrices,

$$\Gamma_\mu = \hat{\Gamma}_\mu \otimes \mathbf{1}, \quad \mu = 1, \ldots, 8,$$
$$\Gamma_{8+i} = \hat{\Gamma}_9 \otimes \sigma_i, \quad i = 1,2, \tag{3.7}$$
$$\Gamma_{11} = \hat{\Gamma}_9 \otimes \sigma_3,$$

where $\{\hat{\Gamma}_\mu, \hat{\Gamma}_9\}$ are nine-dimensional gamma matrices and σ_i are the Pauli matrices. In addition, we decompose the normal spinors according to $Q_{(2)} = Q_{(2)R} + Q_{(2)L}$ where $Q_{(2)R,L} = \pm \sigma_3 Q_{(2)R,L}$. Using these conventions, and also the identity $\sigma_1 \sigma_2 = i \sigma_3$, we can write

$$Q_{(11)} = Q_{(9)} \otimes (Q_{(2)R} + Q_{(2)L}),$$
$$\Omega_{(11)} = \exp(i \pi f \mathbf{1} \otimes \sigma_3). \tag{3.8}$$

The fixed-plane condition $Q_{(11)} = \Omega_{(11)} Q_{(11)}$ can now be written as

$$Q_{(9)} \otimes Q_{(2)R,L} = e^{\pm i \pi f} Q_{(9)} \otimes Q_{(2)R,L}. \tag{3.9}$$

Because there are no nontrivial solutions to either of these equations, subject to the restriction that $f \neq 0 \bmod 1$, we conclude that, as we approach a fixed-nine-plane, $Q_{(11)} \to 0$. Thus supersymmetry is broken completely on any nine-dimensional fixed-plane associated with an element (3.1).

Eight-dimensional fixed-planes: Eight-dimensional fixed-planes correspond to elements $(f_1, f_2, f_3 \mid P) = (0, 0, f \mid 1)$, where $f \neq 0 \bmod 1$. In this case, the supercharge transforms as $Q_{(11)} \to \Omega_{(11)} Q_{(11)}$, where

$$\Omega_{(11)} = \exp(\pi f \Gamma_9 \Gamma_{10}) \Gamma_{11}. \tag{3.10}$$

We write $Q_{(11)}$ as a tensor product of an eight-dimensional fixed-plane spinor with an SO(3) "normal" spinor, according to $Q_{(11)} = Q_{(8)} \otimes Q_{(3)}$, and we represent the gamma matrices precisely as in (3.7). In addition we decompose the SO(7,1) spinors via $Q_{(8)} = Q_{(8)R} + Q_{(8)L}$ where $Q_{(8)R,L} = \pm \hat{\Gamma}_9 Q_{(8)R,L}$, and write the normal spinors as $Q_{(3)} = Q_{(2)R} + Q_{(2)L}$, where $Q_{(2)R,L} = \pm \sigma_3 Q_{(2)R,L}$. We introduce a useful shorthand notation whereby $L \equiv Q_{(2)L}$ and $R \equiv Q_{(2)R}$. Using these conventions, and also the identity $\sigma_1 \sigma_2 = i \sigma_3$, we can write

$$Q_{(11)} = (Q_{(8)R} + Q_{(8)L}) \otimes (R + L),$$
$$\Omega_{(11)} = \exp(i \pi f \mathbf{1} \otimes \sigma_3) \hat{\Gamma}_9 \otimes \sigma_3. \tag{3.11}$$

The fixed-plane condition $Q_{(11)} = \Omega_{(11)} Q_{(11)}$ can now be written

$$Q_{(8)R,L} \otimes R = \pm e^{i \pi f} Q_{(8)R,L} \otimes R,$$
$$Q_{(8)R,L} \otimes L = \mp e^{-i \pi f} Q_{(8)R,L} \otimes L. \tag{3.12}$$

Because there are no nontrivial solutions to any of these four equations, subject to the restriction that $f \neq 0 \bmod 1$, we conclude that, as we approach an eight-dimensional fixed-plane, $Q_{(11)} \to 0$. Thus, supersymmetry is broken completely on any eight-dimensional fixed-plane associated with an element (3.1).

Seven-dimensional fixed-planes: Seven-dimensional fixed-planes correspond to elements $(f_1, f_2, f_3 \mid P) = (0, f, f' \mid 0)$, where $f \neq 0 \bmod 1$ and $f' \neq 0 \bmod 1$. In this case, the supercharge transforms as $Q_{(11)} \to \Omega_{(11)} Q_{(11)}$, where

$$\Omega_{(11)} = \exp(\pi f \Gamma_7 \Gamma_8) \exp(\pi f' \Gamma_9 \Gamma_{10}). \tag{3.13}$$

We write $Q_{(11)}$ as a tensor product of a seven-dimensional fixed-plane spinor with an SO(4) ''normal'' spinor according to $Q_{(11)}=Q_{(7)}\otimes Q_{(4)}$. Similarly, we use the following representation for the gamma matrices,

$$\begin{aligned}\Gamma_{\mu}&=\hat{\Gamma}_{\mu}\otimes\mathbf{1}, \quad \mu=1,\ldots,6,\\ \Gamma_{6+i}&=\hat{\Gamma}_{7}\otimes\gamma_{i}, \quad i=1,\ldots,4,\\ \Gamma_{11}&=\hat{\Gamma}_{7}\otimes\gamma_{5},\end{aligned} \tag{3.14}$$

where $\{\hat{\Gamma}_{\mu},\hat{\Gamma}_{7}\}$ are the seven-dimensional Gamma matrices and γ_i are four-dimensional gamma matrices. In addition, we decompose the normal SO(4) SO(4)$\rightarrow$SO(2)$\times$SO(2), where SO(2)$\times$SO(2) is a convenient maximal subgroup of SO(4). Thus, we write the ''normal'' spinor as $Q_{(4)}=Q_{(2)}\otimes Q_{(2)}$, and the four-dimensional gamma matrices as $\gamma_{1,2}=\sigma_{1,2}\otimes\mathbf{1}$ and $\gamma_{3,4}=\sigma_3\otimes\sigma_{1,2}$, where σ_i are Pauli matrices. Also, using the identities $\gamma_5=\gamma_1\gamma_2\gamma_3\gamma_4$ and $\sigma_1\sigma_2=i\,\sigma_3$, we derive $\gamma_5=-\sigma_3\otimes\sigma_3$. This allows us to rewrite (3.14) as

$$\begin{aligned}\Gamma_{1,\ldots,6}&=\hat{\Gamma}_{1,\ldots,6}\otimes\mathbf{1}\otimes\mathbf{1},\\ \Gamma_{7,8}&=\hat{\Gamma}_{7}\otimes\sigma_{1,2}\otimes\mathbf{1},\\ \Gamma_{9,10}&=\hat{\Gamma}_{7}\otimes\sigma_{3}\otimes\sigma_{1,2},\\ \Gamma_{11}&=-\hat{\Gamma}_{7}\otimes\sigma_{3}\otimes\sigma_{3}.\end{aligned} \tag{3.15}$$

Note that the normal spinor can be decomposed as $Q_{(4)}=Q_{(4)\,R}+Q_{(4)\,L}$ where $Q_{(4)\,R,L}=\pm\gamma_5\,Q_{(4)\,R,L}$. In terms of SO(2)$\times$SO(2)$\subset$SO(4), however, these same objects can be written as

$$\begin{aligned}Q_{(4)R}&=Q_{(2)R}\otimes Q_{(2)L}+Q_{(2)L}\otimes Q_{(2)R},\\ Q_{(4)L}&=Q_{(2)R}\otimes Q_{(2)R}+Q_{(2)L}\otimes Q_{(2)L},\end{aligned} \tag{3.16}$$

where $Q_{(2)\,R,L}=\pm\sigma_3\,Q_{(2)\,R,L}$. Using these results we can decompose the 11-dimensional supercharge in two steps. First, we write $Q_{(11)}=Q_{(7)}\otimes(\,Q_{(4)\,R}+Q_{(4)\,L}\,)$ and then we rewrite the terms $Q_{(4)\,R,L}$ using (3.16). We now define $LL\equiv Q_{(2)L}\otimes Q_{(2)L}$, and similar expressions for LR, RL, and RR. Using these definitions, and also the conventions introduced above, we can write

$$\begin{aligned}Q_{(11)}&=Q_{(7)}\otimes(\,LL+LR+RL+RR\,),\\ \Omega_{(11)}&=\exp(\,i\,\pi\,f\,\mathbf{1}\otimes\sigma_3\otimes\mathbf{1}+i\,\pi\,f'\,\mathbf{1}\otimes\mathbf{1}\otimes\sigma_3\,).\end{aligned} \tag{3.17}$$

The fixed-plane condition $Q_{(11)}=\Omega_{(11)}\,Q_{(11)}$ can now be written as

$$\begin{aligned}Q_{(7)}\otimes LL&=e^{-i\,\pi\,(f+f')}\,Q_{(7)}\otimes LL,\\ Q_{(7)}\otimes LR&=e^{-i\,\pi\,(f-f')}\,Q_{(7)}\otimes LR,\\ Q_{(7)}\otimes RL&=e^{+i\,\pi\,(f-f')}\,Q_{(7)}\otimes RL,\\ Q_{(7)}\otimes RR&=e^{+i\,\pi\,(f+f')}\,Q_{(7)}\otimes RR.\end{aligned} \tag{3.18}$$

Therefore, as we approach a fixed-seven-plane, the bulk supercharge is projected according to

$$Q_{(11)}\rightarrow\begin{cases} Q_{(7)}\otimes(\,LL+RR\,), & f+f'\in 2\,\mathbb{Z},\\ Q_{(7)}\otimes(\,LR+RL\,), & f-f'\in 2\,\mathbb{Z},\end{cases} \tag{3.19}$$

and is projected to zero if neither of these conditions are met. Thus we retain some supersymmetry on a fixed-seven-plane if and only if one of the two sums $f\pm f'$ is an even integer. This is the case only if $f=\pm f'$ mod 1. In such cases, the bulk supersymmetry is *halved* on the fixed-plane in question.

Six-dimensional fixed-planes: Six-dimensional fixed-planes correspond to elements $(f_1,f_2,f_3\,|\,P)=(0,f,f'\,|\,1)$, where $f\neq 0$ mod 1 and $f'\neq 0$ mod 1. In this case the supercharge transforms as $Q_{(11)}\rightarrow\Omega_{(11)}\,Q_{(11)}$, where

$$\Omega_{(11)}=\exp(\,\pi f\,\Gamma_7\,\Gamma_8\,)\exp(\,\pi f'\,\Gamma_9\,\Gamma_{10}\,)\,\Gamma_{11}\,. \tag{3.20}$$

We write $Q_{(11)}$ as a tensor product of a six-dimensional fixed-plane spinor with an SO(5) ''normal'' spinor according to $Q_{(11)}=Q_{(6)}\otimes Q_{(5)}$, and we represent the Gamma matrices precisely as in (3.15). In addition, we decompose the SO(5,1) spinors via $Q_{(6)}=Q_{(6)\,R}+Q_{(6)\,L}$, where $=Q_{(6)\,R,L}=\pm\hat{\Gamma}_7\,Q_{(6)\,R,L}$, and write the normal SO(5) spinors as $Q_{(5)}=Q_{(4)\,R}\oplus Q_{(4)\,L}$, where $Q_{(4)\,R,L}$ are given by (3.16). Now, using the notation introduced above, we can write

$$\begin{aligned} Q_{(11)}&=(\,Q_{(6)R}+Q_{(6)L}\,)\otimes(\,LL+LR+RL+RR\,),\\ \Omega_{(11)}&=-\exp(\,i\,\pi f\,\mathbf{1}\otimes\sigma_3\otimes\mathbf{1}+i\,\pi f'\,\mathbf{1}\otimes\mathbf{1}\otimes\sigma_3\,)\,\hat{\Gamma}_7\otimes\sigma_3\otimes\sigma_3\,. \end{aligned} \tag{3.21}$$

The fixed-plane condition $Q_{(11)}=\Omega_{(11)}\,Q_{(11)}$ can now be written as

$$\begin{aligned} rQ_{(6)\,R,L}\otimes LL&=\mp e^{-i\,\pi(f+f')}\,Q_{(7)}\otimes LL,\\ Q_{(6)\,R,L}\otimes LR&=\pm e^{-i\,\pi(f-f')}\,Q_{(7)}\otimes LR,\\ Q_{(6)\,R,L}\otimes RL&=\pm e^{+i\,\pi(f-f')}\,Q_{(7)}\otimes RL,\\ Q_{(6)\,R,L}\otimes RR&=\mp e^{+i\,\pi(f+f')}\,Q_{(7)}\otimes RR\,. \end{aligned} \tag{3.22}$$

Therefore, as we approach a fixed-six-plane, the bulk supercharge is projected according to

$$Q_{(11)}\rightarrow\begin{cases} Q_{(6)L}\otimes(\,LL+RR\,), & f+f'\in 2\,\mathbb{Z},\\ Q_{(6)R}\otimes(\,LR+RL\,), & f-f'\in 2\,\mathbb{Z},\\ Q_{(6)R}\otimes(\,LL+RR\,), & f+f'\in 2\,\mathbb{Z}+1,\\ Q_{(6)L}\otimes(\,LR+RL\,), & f-f'\in 2\,\mathbb{Z}+1\,. \end{cases} \tag{3.23}$$

and is projected to zero if none of these conditions is met. Thus, we retain some supersymmetry on a fixed-six-plane if and only if one of the two sums $f\pm f'$ is integer (even or odd). In generic cases of this sort, the bulk supersymmetry is *quartered* on the fixed-plane in question. [A special case is when $(\,f\,,f'\,)=(\,1/2\,,1/2\,)$, in which case supersymmetry is merely *halved*. In that special case the difference $f-f'=0$ is an even integer, while the sum $f+f'=1$ is an odd integer; therefore, on the fixed-plane, $Q_{(11)}$ retains nonvanishing components of both the first and also the third case in (3.23).] Note that in the cases where the supersymmetry is quartered the element α necessarily has even order N. In those cases there is necessarily an order-two element in Γ, namely $\alpha^{N/2}$, for which $(f_1,f_2,f_3\,|\,P)=(0,0,0\,|\,1)$. The fixed-plane associated with $\alpha^{N/2}$ is 10-dimensional, while the six-plane associated with α is a submanifold of this ten-plane.

Five-dimensional fixed-planes: Five-dimensional fixed-planes correspond to elements $(f_1,f_2,f_3\,|\,P)=(f_1,f_2,f_3\,|\,0\,)$, where $f_{1,2,3}\neq 0$ mod 1. In this case, the supercharge transforms as $Q_{(11)}\rightarrow\Omega_{(11)}\,Q_{(11)}$, where

$$\Omega_{(11)}=\exp(\pi f_1\Gamma_5\Gamma_6)\exp(\pi f_2\Gamma_7\Gamma_8)\exp(\pi f_3\Gamma_9\Gamma_{10}). \tag{3.24}$$

We write $Q_{(11)}$ as a tensor product of a five-dimensional fixed-plane spinor with a normal spinor according to $Q_{(11)}=Q_{(5)}\otimes Q_{(6)}$. Similarly, we use the following representation for the gamma matrices,

$$\begin{aligned}\Gamma_\mu&=\gamma_\mu\otimes\mathbf{1},\quad \mu=1,\ldots,4,\\ \Gamma_{4+i}&=\gamma_5\otimes\hat{\Gamma}_i,\quad i=1,\ldots,6,\\ \Gamma_{11}&=\gamma_5\otimes\hat{\Gamma}_7.\end{aligned} \tag{3.25}$$

where $\{\gamma_\mu,\gamma_5\}$ are five-dimensional gamma matrices and $\hat{\Gamma}_i$ are six-dimensional gamma matrices. In addition, we decompose the normal SO(6) spinors using the decomposition $\mathrm{SO}(6)\rightarrow\mathrm{SO}(2)\times\mathrm{SO}(2)\times\mathrm{SO}(2)$, where $\mathrm{SO}(2)\times\mathrm{SO}(2)\times\mathrm{SO}(2)$ is a convenient maximal subgroup of SO(6). Thus, we write the normal spinor as $Q_{(6)}=Q_{(2)}\otimes Q_{(2)}\otimes Q_{(2)}$, and the six-dimensional gamma matrices as $\hat{\Gamma}_{1,2}=\sigma_{1,2}\otimes\mathbf{1}\otimes\mathbf{1}$ and $\hat{\Gamma}_{3,4}=\sigma_3\otimes\sigma_{1,2}\otimes\mathbf{1}$, and $\hat{\Gamma}_{5,6}=\sigma_3\otimes\sigma_3\otimes\sigma_{1,2}$, where $\sigma_{1,2,3}$ are Pauli matrices. Now, using the relation $\hat{\Gamma}_7=i\hat{\Gamma}_1\cdots\hat{\Gamma}_6$ we then derive $\hat{\Gamma}_7=\sigma_3\otimes\sigma_3\otimes\sigma_3$. Using these expressions, it is possible to rewrite (3.25) as

$$\begin{aligned}\Gamma_{1,\ldots,4}&=\gamma_{1,\ldots,4}\otimes\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1},\\ \Gamma_{5,6}&=\gamma_5\otimes\sigma_{1,2}\otimes\mathbf{1}\otimes\mathbf{1},\\ \Gamma_{7,8}&=\gamma_5\otimes\sigma_3\otimes\sigma_{1,2}\otimes\mathbf{1},\\ \Gamma_{9,10}&=\gamma_5\otimes\sigma_3\otimes\sigma_3\otimes\sigma_{1,2},\\ \Gamma_{11}&=\gamma_5\otimes\sigma_3\otimes\sigma_3\otimes\sigma_3.\end{aligned} \tag{3.26}$$

We now define $LLL\equiv Q_{(2)\,L}\otimes Q_{(2)\,L}\otimes Q_{(2)\,L}$, and similar expressions for LLR, LRL, LRR, RRR, RRL, RLR, and RLL, where $Q_{(2)\,R,L}=\pm\sigma_3\,Q_{(2)\,R,L}$. In terms of these definitions and conventions, we can write

$$\begin{aligned}Q_{(11)}&=Q_{(5)}\otimes(RRR+RLL+LRL+LLR+LLL+LRR+RLR+RRL),\\ \Omega_{(11)}&=\exp(i\pi f_1\,\mathbf{1}\otimes\sigma_3\otimes\mathbf{1}\otimes\mathbf{1}+i\pi f_2\,\mathbf{1}\otimes\mathbf{1}\otimes\sigma_3\otimes\mathbf{1}+i\pi f_3\,\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1}\otimes\sigma_3).\end{aligned} \tag{3.27}$$

The fixed-plane condition $Q_{(11)}=\Omega_{(11)}Q_{(11)}$ can now be written as

$$\begin{aligned}Q_{(5)}\otimes LLL&=e^{-i\pi(f_1+f_2+f_3)}LLL,\quad Q_{(5)}\otimes RRR=e^{+i\pi(f_1+f_2+f_3)}RRR\\ Q_{(5)}\otimes LLR&=e^{-i\pi(f_1+f_2-f_3)}LLR,\quad Q_{(5)}\otimes RRL=e^{+i\pi(f_1+f_2-f_3)}RRL\\ Q_{(5)}\otimes LRL&=e^{-i\pi(f_1-f_2+f_3)}LRL,\quad Q_{(5)}\otimes RLR=e^{+i\pi(f_1-f_2+f_3)}RLR\\ Q_{(5)}\otimes LRR&=e^{-i\pi(f_1-f_2-f_3)}RLL,\quad Q_{(5)}\otimes RLL=e^{+i\pi(f_1-f_2-f_3)}LRR.\end{aligned}$$

Therefore, as we approach a fixed-five-plane, the bulk supercharge is projected according to

$$Q_{(11)}\rightarrow\begin{cases}Q_{(5)}\otimes(RRR+LLL), & f_1+f_2+f_3\in 2\,\mathbb{Z},\\ Q_{(5)}\otimes(RLL+LRR), & f_1-f_2-f_3\in 2\,\mathbb{Z},\\ Q_{(5)}\otimes(LRL+RLR), & f_1-f_2+f_3\in 2\,\mathbb{Z},\\ Q_{(5)}\otimes(LLR+RRL), & f_1+f_2-f_3\in 2\,\mathbb{Z},\end{cases} \tag{3.28}$$

and is projected to zero if none of these conditions are met. Thus, we retain some supersymmetry on a fixed-five-plane if and only if at least one of the four sums $f_1 \pm f_2 \pm f_3$ is an even integer. In generic cases of this sort, the bulk supersymmetry is *quartered* on the fixed-plane in question.

Four-dimensional fixed-planes: Four-dimensional fixed-planes correspond to elements $(f_1, f_2, f_3 \,|\, P) = (f_1, f_2, f_3 \,|\, 1)$, where $f_{1,2,3} \neq 0 \bmod 1$. In this case the supercharge transforms as $Q_{(11)} \to \Omega_{(11)} Q_{(11)}$, where

$$\Omega_{(11)} = \exp(\pi f_1 \Gamma_5 \Gamma_6) \exp(\pi f_2 \Gamma_7 \Gamma_8) \exp(\pi f_3 \Gamma_9 \Gamma_{10}) \Gamma_{11}. \tag{3.29}$$

We write $Q_{(11)}$ as a tensor product of a four-dimensional fixed-plane spinor with a normal spinor according to $Q_{(11)} = Q_{(4)} \otimes Q_{(7)}$, and we represent the gamma matrices precisely as in (3.25). Furthermore, we decompose the four-dimensional spinors as $Q_{(4)} = Q_{(4)\,R} + Q_{(4)\,L}$ where $Q_{(4)\,R,L} = \pm \gamma_5 Q_{(4)\,R,L}$. We also write the SO(7) normal spinor as $Q_{(7)} = Q_{(6)R} \oplus Q_{(6)L}$. Finally, we can decompose the chiral six-dimensional spinors $Q_{(6)R,L}$ into two-dimensional chiral spinors as descried above. Using these conventions, we can write

$$\begin{aligned} Q_{(11)} &= (Q_{(4)\,R} + Q_{(4)\,L}) \otimes (RRR + RLL + LRL + LLR + LLL + LRR + RLR + RRL), \\ \Omega_{(11)} &= \exp(i\pi f_1 \, \mathbf{1} \otimes \sigma_3 \otimes \mathbf{1} \otimes \mathbf{1} + i\pi f_2 \, \mathbf{1} \otimes \mathbf{1} \otimes \sigma_3 \otimes \mathbf{1} + i\pi f_3 \, \mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} \otimes \sigma_3) \, \gamma_5 \\ &\quad \otimes \sigma_3 \otimes \sigma_3 \otimes \sigma_3. \end{aligned} \tag{3.30}$$

The fixed-plane condition $Q_{(11)} = \Omega_{(11)} Q_{(11)}$ can now be written as

$$\begin{aligned} &Q_{(4)\,R,L} \otimes LLL = \mp e^{-i\pi(f_1+f_2+f_3)} LLL, \quad Q_{(4)\,R,L} \otimes RRR = \pm e^{+i\pi(f_1+f_2+f_3)} RRR, \\ &Q_{(4)\,R,L} \otimes LLR = \pm e^{-i\pi(f_1+f_2-f_3)} LLR, \quad Q_{(4)\,R,L} \otimes RRL = \mp e^{+i\pi(f_1+f_2-f_3)} RRL, \\ &Q_{(4)\,R,L} \otimes LRL = \pm e^{-i\pi(f_1-f_2+f_3)} LRL, \quad Q_{(4)\,R,L} \otimes RLR = \mp e^{+i\pi(f_1-f_2+f_3)} RLR, \\ &Q_{(4)\,R,L} \otimes LRR = \mp e^{-i\pi(f_1-f_2-f_3)} RLL, \quad Q_{(4)\,R,L} \otimes RLL = \pm e^{+i\pi(f_1-f_2-f_3)} LRR. \end{aligned}$$

Therefore, as we approach a fixed-four-plane, the bulk supercharge is projected according to

$$Q_{(11)} \to \begin{cases} Q_{(4)L} \otimes LLL + Q_{(4)R} \otimes RRR, & f_1+f_2+f_3 \in 2\,\mathbb{Z}, \\ Q_{(4)R} \otimes LRL + Q_{(4)L} \otimes RLR, & f_1-f_2+f_3 \in 2\,\mathbb{Z}, \\ Q_{(4)R} \otimes RRL + Q_{(4)L} \otimes LLR, & f_1+f_2-f_3 \in 2\,\mathbb{Z}, \\ Q_{(4)L} \otimes RLL + Q_{(4)R} \otimes LRR, & f_1-f_2-f_3 \in 2\,\mathbb{Z}, \\ Q_{(4)R} \otimes LLL + Q_{(4)L} \otimes RRR, & f_1+f_2+f_3 \in 2\,\mathbb{Z}+1, \\ Q_{(4)L} \otimes LRL + Q_{(4)R} \otimes RLR, & f_1-f_2+f_3 \in 2\,\mathbb{Z}+1, \\ Q_{(4)L} \otimes RRL + Q_{(4)R} \otimes LLR, & f_1+f_2-f_3 \in 2\,\mathbb{Z}+1, \\ Q_{(4)R} \otimes RLL + Q_{(4)L} \otimes LRR, & f_1-f_2-f_3 \in 2\,\mathbb{Z}+1, \end{cases} \tag{3.31}$$

and is projected to zero if none of these conditions are met. Thus, we retain some supersymmetry on a fixed-four-plane if and only if any one of the four sums $f_1 \pm f_2 \pm f_3$ is an integer (even or odd). In generic cases of this sort, supersymmetry is *eighthed* on the fixed-plane in question.

There are special cases, however. For instance, for each of the two cases where (f_1, f_2, f_3) are given by $(1/2, 1/3, 1/6)$ and by $(1/2, 1/4, 1/4)$, one sum $f_1 - f_2 - f_3 = 0$ is an even integer, while another sum $f_1 + f_2 + f_3 = 1$ is an odd integer. Therefore, on the fixed-plane, $Q_{(11)}$ retains nonvanishing components of both the fourth and the also the fifth case in (3.31). Thus, supersymmetry is merely quartered to $D=4, N=2$, rather than eighthed to $D=4, N=1$, in these cases. (If the

fixed-four-plane in question is a submanifold of the fixed-plane of another element of Γ, one needs to account for the action of this other element as well before drawing conclusions as to the amount of fixed-plane supersymmetry.)

Note that the pairs of summands indicated in (3.31) have correlations owing to the Majorana constraint on $Q_{(11)}$. As a result, the two apparent summands in each of these expressions actually describe the same degrees of freedom. In terms of the choices we have made, this gives rise to a Majorana spinor supercharge in four dimensions. The pairs which appear in (3.31) represent left- and right-handed chiral projections of this four-dimensional Majorana supercharge. As is well known, in four dimensions spinor fields which are Majorana may be equally well represented in terms of either chiral projection.

IV. GENERALIZATION TO NON-ABELIAN ORBIFOLD GROUPS

One obvious extension of our criterion, still for orbifolds of tori of our class, is to consider *all* the automorphisms of the underlying lattices. In addition to the rotations and flips we have already considered, the only new type of ''generating'' automorphism to deal with is the permutations of the coordinates x^i. In fact, one can easily lift these permutation actions to spinors. Here are the details.

The lattices of our class are all of the form

$$\Lambda = (A_1)^a \oplus (A_2)^b \ , \tag{4.1}$$

with $a+2b=n$, the dimension of the orbifold. Such a lattice has an automorphism group of order $2^a \cdot a! \cdot b! \cdot 12^b$, a product of four factors. Let's check where these two pairs of factors come from.

The first pair, $2^a \cdot a!$, keeps track of the sign flips on each of a possible x^i (the 2^a), and permutations of the same a x^i's (the $a!$). We have already described a way to lift the flips to spinors, via Γ_i, so we only need to lift the permutations. The second pair, $b! \cdot 12^b$, keeps track of the permutations of the b different copies of A_2, i.e., of corresponding ordered pairs (x^i, x^{i+1}) (giving the $b!$), and automorphisms internal to each of the b A_2's (giving the 12^b, as the automorphism group of the A_2 lattice is the dihedral group D_6 of order 12). Consider a single A_2 lattice in the ''(x,y)-plane.'' The dihedral automorphism group D_6 consists entirely of the identity, rotations by $r^k := 2\pi k/6$, $k=1,2,3,4,5$, and flips $(s, sr, sr^2, sr^3, sr^4, sr^5)$ across lines through opposite vertices or opposite edge centers of the period hexagon (we can assume that s is the flip across the x-axis sending $y \mapsto -y$). In particular, D_6 is generated by a rotation r and a flip s, for each of which we have already described a lift to spinors. What remains is again to describe the effect of the permutation automorphisms on spinors.

Since every permutation of the x^i can be expressed as a product of simple transpositions $x^i \leftrightarrow x^j$, $i \neq j$, it suffices to write out the lift of such a transposition. Imagine the (x^i, x^j)-plane. Rotation counterclockwise by $\pi/2$ radians sends $x^i \mapsto x^j$ and $x^j \mapsto -x^i$. This is represented in the Clifford algebra by

$$\exp\left(\frac{\pi}{4} \Gamma_{ij} \right) = \cos(\pi/4) + \sin(\pi/4)\, \Gamma_i \Gamma_j = \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} \Gamma_i \Gamma_j \right) . \tag{4.2}$$

Now compose this with the flip sending $x^i \mapsto -x^i$ given by Γ_i, yielding

$$\Gamma_i \cdot \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} \Gamma_i \Gamma_j \right) = \frac{\sqrt{2}}{2} (\Gamma_i + \Gamma_j) . \tag{4.3}$$

We can build any permutation we like out of a product of these, and in particular all of the remaining automorphisms come from mixing these with the rotations and flips as above. By adding such permutations, we can obtain a complete supersymmetric restriction criterion for all orbifolds modelled on lattices of type (4.1). In particular, this allows one to check the supersym-

TABLE VII. Character table for the group $(\mathbb{Z}_2)^3$.

$(\mathbb{Z}_2)^3$	Ω	$\Gamma_{[0,0,1]}$	$\Gamma_{[0,1,0]}$	$\Gamma_{[0,1,1]}$	$\Gamma_{[1,0,0]}$	$\Gamma_{[1,0,1]}$	$\Gamma_{[1,1,0]}$	$\Gamma_{[1,1,1]}$
1	+	+	+	+	+	+	+	+
γ	+	−	+	−	+	−	+	−
β	+	+	−	−	+	+	−	−
$\beta\gamma$	+	−	−	+	+	−	−	+
α	+	+	+	+	−	−	−	−
$\alpha\gamma$	+	−	+	−	−	+	−	+
$\alpha\beta$	+	+	−	−	−	−	+	+
$\alpha\beta\gamma$	+	−	−	+	−	+	+	−

metry constraints for a large class of *non-Abelian* orbifold groups. The generalized supersymmetric restriction theorem, including the extension to non-Abelian orbifold groups, will be discussed in a forthcoming paper.

V. SOFT ORBIFOLDS AND G_2-STRUCTURES

Consider the supersymmetric orbifold of $\Gamma=(\mathbb{Z}_2)^3$ labeled (1111111) in Table I. The corresponding representation of Γ on $\mathbb{R}^7$ is given by the direct sum of the seven nontrivial characters $\Gamma_{[i,j,k]}$, each with multiplicity one. The character table for $\Gamma=\langle\alpha,\beta,\gamma\rangle$ is given in Table VII, and, by following the prescription given in Sec. II C, we see that the action of these generators on the coordinate 7-tuple $(x_1,\ldots,x_7)$ is given by

$$\alpha: \quad (x_1,x_2,x_3,-x_4,-x_5,-x_6,-x_7), \tag{5.1}$$

$$\beta: \quad (x_1,-x_2,-x_3,x_4,x_5,-x_6,-x_7), \tag{5.2}$$

$$\gamma: \quad (-x_1,x_2,-x_3,x_4,-x_5,x_6,-x_7). \tag{5.3}$$

Note that this Γ-action preserves the G_2-invariant differential 3-form φ_0 on $\mathbb{R}^7$,

$$\varphi_0 := dx_{123}+dx_{145}+dx_{167}+dx_{246}-dx_{257}-dx_{347}-dx_{356},$$

where $dx_{ijk}:=dx_i\wedge dx_j\wedge dx_k$. Such an action defines a G_2-*structure* on the orbifold T^7/Γ.

Our supersymmetric hard orbifold (1111111) is one of a family of orbifolds considered by Joyce. [In fact, in the notation of Ref. 15 Eqs. (23)–(25), ours corresponds to $b_1=b_2=c_1=c_3=c_5=0$. We will refer to notation and examples from Ref. 7 instead.] It was his goal to construct compact manifolds with holonomy group G_2. To this end he developed in Refs. 14, 15, and 7 a machinery which, starting with a sufficiently simple orbifold admitting a G_2-structure, establishes the existence of such a metric on a ''resolution'' of the orbifold. Joyce's method depends on the existence of certain *R-data* (''*R*'' for resolution) which, for a given orbifold with G_2-structure, may yield a large number of topologically distinct G_2 holonomy manifolds as resolutions.

In Ref. 7 Secs. 12.2, 3, and 5 three paricular softenings are considered. The actions of the generators of Γ take the form

$$\alpha: \quad (x_1,x_2,x_3,-x_4,-x_5,-x_6,-x_7), \tag{5.4}$$

$$\beta: \quad (x_1,-x_2,-x_3,x_4,x_5,b-x_6,-x_7), \tag{5.5}$$

$$\gamma: \quad (-x_1,x_2,-x_3,x_4,c-x_5,x_6,\tfrac{1}{2}-x_7)\ , \tag{5.6}$$

with $b,c\in\{0,\frac{1}{2}\}$. In fact, Joyce considers the three cases

$$(b,c)=(0,\tfrac{1}{2})\,,\quad (\tfrac{1}{2},0)\,,\quad \text{and } (\tfrac{1}{2},\tfrac{1}{2})\,,$$

and shows that each of these admits a set of R-data defining a G_2 holonomy resolution. In each case the generators α, β, and γ act with fixed-points as before, but some other elements, like

$$\beta\gamma:\quad (-x_1,-x_2,x_3,x_4,c-x_5,b+x_6,\tfrac{1}{2}+x_7)\ , \tag{5.7}$$

act freely. Thus softening an orbifold has the effect of simplifying the singularities. The singularities of the orbifold (1111111) are too complicated to visibly admit a compatible set of R-data, hence his interest in various softenings with simpler singularities. Furthermore, at least for these simplest examples, the set of fixed-plane dimensions associated to a hard orbifold contains as subsets those of all of its softenings. For this reason, one expects that much of the supersymmetric restriction analysis of Sec. III can be usefully adapted to the case of soft orbifolds.

It is clear that having a G_2-structure on a hard orbifold implies such a structure on all of its softenings. This raises the intriguing question of the relationship between our supersymmetry condition and such G_2-structures: Do all supersymmetric hard orbifolds (and hence all of their softenings) carry a G_2-structure? What about the converse: Do all orbifolds with a G_2-structure arise via softening from supersymmetric hard orbifolds? What about the more subtle issue of resolvability as a G_2-manifold (i.e., existence of compatible R-data)? These are all questions to be addressed in future work.

VI. CONCLUSIONS

We have described a systematic method for classifying supersymmetric orbifold compactifications of M-theory, specifically hard orbifolds defined by pseudo-planar representations of Abelian groups of order $\leqslant 12$. Although we stopped our ''periodic table'' (Table I) at order 12, the methods developed here apply to groups of arbitrary order, and the algorithmics are such that such an extension (using Mathematica) is computationally feasible.

It is physically relevant that we demand orbifold actions be compatible with particular lattices. By doing this we are able to keep control over two separate problems. On the one hand we are studying aspects of supersymmetric singularities. On the other hand, however, we are at the same time learning something about which sets of such singularities, and their neighborhoods, can be assembled together to create a global supersymmetric compactification space. Elucidating the relationship between our own supersymmetric configurations of singularities and those of intersecting branes as studied by other groups[24–35] seems an important direction for further investigation.

Furthermore, we touch upon the interesting mathematical problem of classifying G_2 manifolds. The vast majority of known compact G_2 holonomy manifolds arise by Joyce's resolution of singularities from orbifolds of T^7. Physically one expects that seven-dimensional supersymmetric compactification spaces of the sort we are studying should admit such G_2 resolutions. In order to compare in general Joyce's ''resolution data'' to the constraints arising from our global supersymmetric restriction, it seems necessary to formulate the restriction for the soft orbifolds of the introduction, as all of Joyce's examples are of this sort.

ACKNOWLEDGMENTS

One of the authors (C.F.D.) would like to thank P. Candelas, N. Hitchin, and X. de la Ossa of the Mathematics Institute, Oxford for interesting and encouraging discussions. The second author (M.F.) is grateful to Mária and Emil Martinka, for hospitality, encouragement and halušky at the Slovak Institute for Basic Research, Podvazie Slovakia, where some of this paper was prepared.

APPENDIX: THE *C*-MATRICES FOR SELECTED GROUPS

By applying the simple algorithm described in Sec. II B, we are able to derive the C-matrix for any pseudoplanar group $\Gamma = G_1 \times \cdots \times G_n$, where $G_i \in \{\mathbb{Z}_2, \mathbb{Z}_3, \mathbb{Z}_4\}$ for $1 \leqslant i \leqslant n$. In Tables VIII and IX we exhibit these for all cases for which $|\Gamma| \leqslant 12$.

TABLE VIII. The C-matrices for pseudoplanar Abelian groups of order $\leqslant 8$.

$$C(\mathbb{Z}_2) = 1$$

$$C(\mathbb{Z}_3) = 1$$

$$C(\mathbb{Z}_4) = \left(\begin{array}{c|c} 0 & 2 \\ \hline 2 & 1 \end{array}\right)$$

$$C(\mathbb{Z}_2\times\mathbb{Z}_2) = \begin{pmatrix} 0 & 2 & 2 \\ 2 & 0 & 2 \\ 2 & 2 & 0 \end{pmatrix}$$

$$C(\mathbb{Z}_2\times\mathbb{Z}_3) = \left(\begin{array}{c|c|c} 3 & 0 & 3 \\ \hline 0 & 2 & 2 \\ \hline 3 & 2 & -1 \end{array}\right)$$

$$C(\mathbb{Z}_2\times\mathbb{Z}_4) = \left(\begin{array}{ccc|cc} 0 & 0 & 0 & 4 & 4 \\ 0 & 4 & 4 & 0 & 4 \\ 0 & 4 & 4 & 4 & 0 \\ \hline 4 & 0 & 4 & 2 & 2 \\ 4 & 4 & 0 & 2 & -2 \end{array}\right)$$

$$C(\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2) = \begin{pmatrix} 4 & 0 & 4 & 0 & 4 & 0 & 4 \\ 0 & 4 & 4 & 0 & 0 & 4 & 4 \\ 4 & 4 & 0 & 0 & 4 & 4 & 0 \\ 0 & 0 & 0 & 4 & 4 & 4 & 4 \\ 4 & 0 & 4 & 4 & 0 & 4 & 0 \\ 0 & 4 & 4 & 4 & 4 & 0 & 0 \\ 4 & 4 & 0 & 4 & 0 & 0 & 4 \end{pmatrix}$$

TABLE IX. The C-matrices for pseudoplanar Abelian groups of orders 9 and 12.

$$C(\mathbb{Z}_3\times\mathbb{Z}_3) = \begin{pmatrix} 0 & 3 & 3 & -3 \\ 3 & 0 & 3 & 3 \\ 3 & 3 & -3 & 0 \\ -3 & 3 & 0 & 3 \end{pmatrix}$$

$$C(\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_3) = \left(\begin{array}{ccc|c|ccc} 0 & 6 & 6 & 0 & 0 & 6 & 6 \\ 6 & 0 & 6 & 0 & 6 & 0 & 6 \\ 6 & 6 & 0 & 0 & 6 & 6 & 0 \\ \hline 0 & 0 & 0 & 4 & 4 & 4 & 4 \\ \hline 0 & 6 & 6 & 4 & 4 & -2 & -2 \\ 6 & 0 & 6 & 4 & -2 & 4 & -2 \\ 6 & 6 & 0 & 4 & -2 & -2 & 4 \end{array}\right)$$

$$C(\mathbb{Z}_3\times\mathbb{Z}_4) = \left(\begin{array}{c|c|c|c|cc} 0 & 0 & 6 & 0 & 6 & 6 \\ \hline 0 & 4 & 0 & 4 & 4 & 4 \\ \hline 6 & 0 & 3 & 6 & 3 & -3 \\ \hline 0 & 4 & 6 & 4 & -2 & -2 \\ \hline 6 & 4 & 3 & -2 & -5 & 1 \\ 6 & 4 & -3 & -2 & 1 & -5 \end{array}\right)$$

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Group-invariant solutions of relativistic and nonrelativistic models in field theory

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(Received 4 March 2003; accepted 12 March 2003)

In this paper we present a method of constructing explicit classes of solutions of the Chaplygin and Born–Infeld systems of equations in $1+1$ dimensions. The approach adopted here is based on the symmetry reduction method for PDE's. A systematic use of the subgroup structure of the invariance group is made to generate symmetry variables. We concentrate only on the case when the symmetry variables are invariants of the subgroups having dimension one. The set of symmetry variables enables us to reduce, after some transformation, the original equations to many possible ODE's. We describe in detail how a composition of Lie subalgebras and singularity analysis applied to these systems provides us with classes of analytic solutions. Several new types of algebraic, rational and solitonlike solutions (among them kinks, bumps and multiple wave solutions) have been obtained in explicit form. We discuss also the existence of several classes of separable solutions admitted by the Chaplygin and Born–Infeld equations. Some physical interpretation of these results in the areas of fluid dynamics and field theory are given. [DOI: 10.1063/1.1576496]

I. INTRODUCTION

The motion of a d-brane in $(d+1)$ spatial dimensions moving in $(d+1,1)$-dimensional space–time is described by the Nambu–Goto (NG) action as given by Jackiw.[1] If $X^\mu=(X^0,X^1,\ldots,X^d,X^{d+1})$ describes the target space–time (in which the d-brane moves), and $\phi^\alpha=(\phi^0,\phi^1,\ldots,\phi^d)$ are world-volume variables which parametrize the d-dimensional extended object evolving in ϕ^0, then the Nambu–Goto action reads

$$I_{\mathrm{NG}}=\int d\phi^0\, d\phi^1\cdots d\phi^d\, \sqrt{(-1)^d \det\left(\frac{\partial X^\mu}{\partial\phi^\alpha}\frac{\partial X_\mu}{\partial\phi^\beta}\right)}. \tag{1}$$

This action is parametrization invariant, and in particular two different choices of the parametrization lead, respectively, to a nonrelativistic fluid dynamical model (the Chaplygin gas) and a relativistic fluid (the Born–Infeld model). In both cases, we choose $(X^1,X^2,\ldots,X^d)$ to coincide with $(\phi^1,\phi^2,\ldots,\phi^d)$ and rename them as the spatial vector $\mathbf{r}$ in d dimensions. The remaining variables X^0, X^{d+1}, and ϕ^0 are treated separately.

A. The Chaplygin gas

We now discuss the two distinct parametrizations, beginning with the nonrelativistic fluid. We define

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$$X^+ = \frac{1}{\sqrt{2}}(X^0 + X^{d+1}) = t, \quad X^- = \frac{1}{\sqrt{2}}(X^0 - X^{d+1}) = \theta(\mathbf{r},t) \tag{2}$$

and then identify t with $\sqrt{2\lambda}\,\phi^0$, where $\lambda \geqslant 0$ is a constant. This is called the light-cone parametrization. The Nambu–Goto action (1) then reduces to the Chaplygin action[1]

$$I_\lambda = -2\sqrt{\lambda}\int dt\, d\mathbf{r}\, \sqrt{\theta_t + \tfrac{1}{2}(\nabla\theta)^2}. \tag{3}$$

This action leads to the Euler–Lagrange equations of the form

$$\frac{\partial}{\partial t}\left(\frac{1}{\sqrt{\theta_t + \frac{1}{2}(\nabla\theta)^2}}\right) + \nabla\cdot\left(\frac{\nabla\theta}{\sqrt{\theta_t + \frac{1}{2}(\nabla\theta)^2}}\right) = 0, \tag{4}$$

which is known as the Chaplygin equation.[2] It should be noted that this equation is equivalent to the following system of differential equations for the density $\rho(\mathbf{r},t)$ and velocity potential $\theta(\mathbf{r},t)$ of a fluid in the interactive case ($\lambda \neq 0$)

$$\rho_t + (\nabla\rho)\cdot(\nabla\theta) + \rho\,(\nabla^2\theta) = 0, \tag{5}$$

$$\theta_t + \frac{1}{2}(\nabla\theta)^2 = \frac{\lambda}{\rho^2}. \tag{6}$$

These equations (5) and (6) correspond, respectively, to the equation of continuity and Euler's force equation for an ideal nonrelativistic fluid of zero vorticity, in which the pressure P is related to the density ρ by the equation[1]

$$P = \frac{-2\lambda}{\rho}. \tag{7}$$

The velocity $\mathbf{v}$ of the fluid is simply the gradient of the potential $\mathbf{v} = \nabla\theta$. It is possible to eliminate the variable ρ by using Eq. (6) to express it in terms of θ. In this way the system (5) and (6) reduces to Eq. (4).

In the free case ($\lambda = 0$) the variable ρ becomes completely independent, and the equations (5) and (6) are decoupled. Equation (6) can be solved for θ, and then equation (5) solved for ρ. A detailed discussion of the symmetry group in one spatial dimension can be found in Ref. 3. This case is not derived from the Nambu–Goto d-brane.

B. The Born–Infeld model

For the relativistic model, the variable X^0 is renamed ct, where c is the speed of light, and is also identified with $c\phi^0$. The remaining target space variable X^{d+1} is renamed $\theta(\mathbf{r},t)/c$, a function of $\mathbf{r}$ and t. This is called the Cartesian parametrization. The Nambu–Goto action (1) then reduces to the Born–Infeld action[1]

$$I_a = -a\int dt\, d\mathbf{r}\, \sqrt{c^2 - (\partial_\mu\theta)^2}. \tag{8}$$

The corresponding Euler–Lagrange equation is found to be

$$\partial^\nu\left(\frac{1}{\sqrt{c^2 - (\partial_\mu\theta)^2}}\,\partial_\nu\theta\right) = 0, \tag{9}$$

which in turn corresponds to the Born–Infeld equations

$$\rho_t + \nabla \cdot \left(\nabla\theta \sqrt{\frac{\rho^2 c^2 + a^2}{c^2 + (\nabla\theta)^2}} \right) = 0, \tag{10}$$

$$\theta_t + \rho c^2 \sqrt{\frac{c^2 + (\nabla\theta)^2}{\rho^2 c^2 + a^2}} = 0. \tag{11}$$

It should be noted that at the limit where $c \to \infty$ the relativistic Born–Infeld model reduces to the nonrelativistic Chaplygin model discussed previously, where λ is identified with $a^2/2$.[1] A solution $\theta_{NR}(\mathbf{r},t)$ of the Chaplygin equation (4) is thus related to its relativistic counterpart $\theta_R(\mathbf{r},t)$ for the Born–Infeld equations (9). This will be discussed in further detail in Sec. III C.

C. Objective and organization

The objective of this paper is to use the method of symmetry reduction (MSR) to determine group-invariant solutions of the Chaplygin and Born–Infeld equations. For simplicity, we shall restrict ourselves to the interactive one-dimensional case (that is in one spatial dimension x and time t). In future work, it will be our objective to extend this analysis to two-dimensional and supersymmetric generalizations[1,4,5] of this theory.

In Sec. II we begin by describing the structure of the six-dimensional Lie algebra which generates the symmetries of the system of Eqs. (5) and (6) of the Chaplygin gas. We also classify the associated one-parameter subalgebras in terms of conjugacy classes. Indeed, since the partial differential equations involved have only two independent variables, a one-dimensional subalgebra (which generates a one-dimensional orbit) will be sufficient to reduce the system to ordinary differential equations of the second order. In Sec. III we proceed to use MSR to determine solutions which are invariant under the various subalgebras, and compare the resulting solutions to those determined by Jackiw with the Legendre method of Riemann coordinates.[1] We use the link between the Chaplygin and Born–Infeld models to generate solutions of the Born–Infeld model. In Sec. IV we discuss the separation of variables admitted by the Chaplygin and Born–Infeld equations, which enables us to construct the families of solitonlike solutions. Finally, Sec. V summarizes the results and contains a future outlook concerning the possible extension of the classical Lie approach to partially invariant solutions (of defect $\delta=1$) for the Chaplygin and Born–Infeld equations.

II. THE SYMMETRY GROUP AND CLASSIFICATION OF SUBALGEBRAS

Let us now investigate the group of symmetries of the interactive Chaplygin gas in one spatial dimension. This fluid is now governed by the system of equations

$$\theta_t + \frac{1}{2}(\theta_x)^2 = \frac{\lambda}{\rho^2}, \quad \rho_t + \rho_x\theta_x + \rho\,\theta_{xx} = 0, \tag{12}$$

obtained from Eqs. (5) and (6) by taking $\mathbf{r}=x$. Following the standard method for determining the symmetry algebra of a system of differential equations,[6] we find that the symmetry algebra $\mathcal{G}$ of the system (12) is spanned by the six independent vector fields

$$\begin{gathered} P_1=\partial_x, \quad P_0=\partial_t, \quad B=t\partial_x+x\partial_\theta, \quad Z=\partial_\theta, \\ D_1=x\partial_x+2t\partial_t+\rho\partial_\rho, \quad D_2=x\partial_x+2\theta\partial_\theta-\rho\partial_\rho. \end{gathered} \tag{13}$$

The commutation relations of the Lie algebra $\mathcal{G}$ are given in Table I.

The vector fields P_1 and P_0 generate translations in space and time, respectively, while Z generates a translation in the dependent variable $\theta(\mathbf{r},t)$. The element B corresponds to a Galilean

TABLE I. Commutation table for the Lie algebra $\mathcal{G}$.

$X\backslash Y$	D_1	D_2	B	Z	P_1	P_0
D_1	0	0	B	0	$-P_1$	$-2P_0$
D_2	0	0	$-B$	$-2Z$	$-P_1$	0
B	$-B$	B	0	0	$-Z$	$-P_1$
Z	0	$2Z$	0	0	0	0
P_1	P_1	P_1	Z	0	0	0
P_0	$2P_0$	0	P_1	0	0	0

boost so that $\{P_0,P_1,B\}$ generate the Galilean algebra in one spatial dimension. The fields D_1 and D_2 correspond to two different types of dilatation. The group G of symmetries is obtained by integrating the vector fields in $\mathcal{G}$ and it acts on the independent and dependent variables as

$$\begin{aligned}\tilde{x} &= e^{d_1+d_2}((x-x_0)+b(t-t_0)),\\ \tilde{t} &= e^{2d_1}(t-t_0),\\ \tilde{\theta} &= e^{2d_2}(\theta+b(x-x_0)+\tfrac{1}{2}b^2(t-t_0)+z),\\ \tilde{\rho} &= e^{d_1-d_2}\rho,\end{aligned} \tag{14}$$

where $g=(d_1,d_2,b,x_0,t_0,z)$ is an arbitrary element of G, all the parameters being real numbers.

The Levi decomposition of the algebra $\mathcal{G}$ is given by

$$\mathcal{G}=\{D_1,D_2,B\}\ \textcircled{+}\ \{P_1,P_0,Z\}=\mathcal{L}\ \textcircled{+}\ \mathcal{N}, \tag{15}$$

where $\mathcal{L}=\{D_1,D_2,B\}$ and $\mathcal{N}=\{P_1,P_0,Z\}$ is an Abelian ideal, so that we can directly apply the method of subalgebra classification[7] to give the nonequivalent one-dimensional splitting and nonsplitting subalgebras of $\mathcal{G}$. The splitting subalgebras are given by

$$\mathcal{L}_1=\{D_1\},\quad \mathcal{L}_2=\{D_2\},\quad \mathcal{L}_3=\{B\},\quad \mathcal{L}_{4,a}=\{D_1+aD_2,\ a\in\Re/\{0\}\},$$

$$\mathcal{L}_{5,\varepsilon}=\{D_1+D_2+\varepsilon B,\ \ \varepsilon=\pm1\},$$

as subalgebras of $\mathcal{L}$, and by

$$\mathcal{N}_1=\{P_0\},\quad \mathcal{N}_2=\{P_1\},\quad \mathcal{N}_3=\{Z\},\quad \mathcal{N}_{4,\varepsilon}=\{Z+\varepsilon P_0,\varepsilon=\pm1\}, \tag{16}$$

as subalgebras of $\mathcal{N}$. The nonsplitting subalgebras in $\mathcal{G}$ are given by

$$\begin{aligned}&\mathcal{K}_{1,\varepsilon}=\{D_1+\varepsilon Z,\ \ \varepsilon=\pm1\},\quad \mathcal{K}_{2,\varepsilon}=\{D_1-D_2+\varepsilon P_1,\ \ \varepsilon=\pm1\},\\ &\mathcal{K}_{3,\varepsilon}=\{D_2+\varepsilon P_0,\ \ \varepsilon=\pm1\},\quad \mathcal{K}_{4,\varepsilon}=\{B+\varepsilon P_0,\ \ \varepsilon=\pm1\}.\end{aligned} \tag{17}$$

All of these subalgebras, except $\mathcal{N}_3$ which does not contain any derivative with respect to the independent variables x and t, will give rise to a reduction process and to invariant solutions.

III. SYMMETRY REDUCTION AND GROUP-INVARIANT SOLUTIONS

In this section, we use the method of characteristics to determine the invariants and reduced differential equations corresponding to each subalgebra listed in Sec. II. In particular for ODE's of second order it is possible to determine whether they are of Painlevé type (i.e., whether all their

TABLE II. Invariants of the subalgebras of the Lie algebra $\mathcal{G}$.

Subalgebra	Symmetry variable	Function θ	Function ρ
$\mathcal{L}_1=\{D_1\}$	$\xi=\frac{\sqrt{t}}{x}$	$\theta=F(\xi)$	$\rho=\sqrt{t}G(\xi)$
$\mathcal{L}_2=\{D_2\}$	$\xi=t$	$\theta=x^2F(\xi)$	$\rho=\frac{1}{x}G(\xi)$
$\mathcal{L}_3=\{B\}$	$\xi=t$	$\theta=F(\xi)+\frac{1}{2\xi}x^2$	$\rho=G(\xi)$
$\mathcal{L}_{4,-1}=\{D_1-D_2\}$	$\xi=x$	$\theta=\frac{1}{t}F(\xi)$	$\rho=tG(\xi)$
$\mathcal{L}_{4,1}=\{D_1+D_2\}$	$\xi=\sqrt{\frac{t}{x}}$	$\theta=tF(\xi)$	$\rho=G(\xi)$
$\mathcal{L}_{4,a}=\{D_1+aD_2,\ a\neq\pm1,0\}$	$\xi=t^{1/2}x^{-[1/(1+a)]}$	$\theta=t^aF(\xi)$	$\rho=t^{[(1-a)/2]}G(\xi)$
$\mathcal{L}_{5,\varepsilon}=\{D_1+D_2+\varepsilon B,\ \varepsilon=\pm1\}$	$\xi=\frac{2x}{t}-\varepsilon\ln t$	$\theta=\frac{1}{2}tF(\xi)+\frac{\varepsilon}{4}\xi t\ln t+\frac{1}{8}t(\ln t)^2$	$\rho=G(\xi)$
$\mathcal{N}_1=\{P_0\}$	$\xi=x$	$\theta=F(\xi)$	$\rho=G(\xi)$
$\mathcal{N}_2=\{P_1\}$	$\xi=t$	$\theta=F(\xi)$	$\rho=G(\xi)$
$\mathcal{N}_{4,\varepsilon}=\{Z+\varepsilon P_0,\ \varepsilon=\pm1\}$	$\xi=x$	$\theta=F(\xi)+\varepsilon t$	$\rho=G(\xi)$
$\mathcal{K}_{1,\varepsilon}=\{D_1+\varepsilon Z,\ \varepsilon=\pm1\}$	$\xi=\frac{\sqrt{t}}{x}$	$\theta=F(\xi)+\varepsilon\ln x$	$\rho=xG(\xi)$
$\mathcal{K}_{2,\varepsilon}=\{D_1-D_2+\varepsilon P_1,\ \varepsilon=\pm1\}$	$\xi=x-\frac{1}{2}\varepsilon\ln t$	$\theta=\frac{1}{t}F(\xi)$	$\rho=tG(\xi)$
$\mathcal{K}_{3,\varepsilon}=\{D_2+\varepsilon P_0,\ \varepsilon=\pm1\}$	$\xi=xe^{-\varepsilon t}$	$\theta=x^2F(\xi)$	$\rho=\frac{1}{x}G(\xi)$
$\mathcal{K}_{4,\varepsilon}=\{B+\varepsilon P_0,\ \varepsilon=\pm1\}$	$\xi=\varepsilon x-\frac{1}{2}t^2$	$\theta=F(\xi)+\xi t+\frac{1}{6}t^3$	$\rho=G(\xi)$

critical points are independent of the initial data). When it is possible, we determine explicit solutions of the Chaplygin and Born–Infeld equations, and compare the former to the ones determined by Jackiw.[1]

A. Reduction of the system

Passing systematically through all subgroups of G with orbits of codimension one, we obtain all symmetry variables. Substituting each of these into the equations (12) we reduce them to a system of ODE's. The result of this analysis can be summarized as follows, where ξ is the symmetry variable, $F(\xi)$ and $G(\xi)$ are invariant functions related to θ and ρ, respectively, and have to be determined using the reduced differential equations. The different classes of symmetry reductions are summarized in Tables II and III. They lead us to 14 different types of solutions.

B. Group-invariant solutions of the Chaplygin model

Let us now discuss certain classes of solutions to the Chaplygin equations obtained from the solutions to the reduced equations determined in Sec. III A. We perform a singularity analysis to determine which of these reduced ODE's can be transformed to the standard Painlevé form.

For the case $\mathcal{L}_1$, we get

$$\theta(x,t)=\frac{1}{4\sqrt{a_0}}\ln\left(\frac{\sqrt{a_0}x^2+t}{\sqrt{a_0}x^2-t}\right)+c_0,\quad \rho(x,t)=\sqrt{\frac{2\lambda}{a_0}}\left(\frac{t^2-a_0x^4}{x^3}\right),\tag{18}$$

where a_0 and c_0 are real constants, and $a_0\neq0$. The velocity is given by

TABLE III. Reduced equations of the subalgebras of the Lie algebra $\mathcal{G}$.

Subalgebra	Equation in G	Equation in F
$\mathcal{L}_1$	$G=\sqrt{\lambda}(\frac{1}{2}\xi F_\xi+\frac{1}{2}\xi^4(F_\xi)^2)^{-1/2}$	$\xi^2F_{\xi\xi}=\xi F_\xi+4\xi^4(F_\xi)^2$
$\mathcal{L}_2$	$G=\sqrt{\lambda}(F_\xi+2F^2)^{-1/2}$	$F_{\xi\xi}+4FF_\xi=0$
$\mathcal{L}_3$	$G=\sqrt{\lambda}(F_\xi)^{-1/2}$	$\xi F_{\xi\xi}-2F_\xi=0$
$\mathcal{L}_{4,-1}$	$G=\sqrt{\lambda}(\frac{1}{2}(F_\xi)^2-F)^{-1/2}$	$FF_{\xi\xi}-(F_\xi)^2+F=0$
$\mathcal{L}_{4,1}$	$G=\sqrt{\lambda}(F+\frac{1}{2}\xi F_\xi+\frac{1}{8}\xi^6(F_\xi)^2)^{-1/2}$	$-\frac{3}{8}\xi F_\xi+\frac{3}{4}\xi^5FF_\xi-\frac{1}{8}\xi^2F_{\xi\xi}+\frac{1}{4}\xi^6FF_{\xi\xi}=0$
$\mathcal{L}_{4,a}$	$G=\sqrt{\lambda}\left(aF+\frac{1}{2}\xi F_\xi+\frac{1}{2(a+1)^2}\xi^{2a+4}(F_\xi)^2\right)^{-1/2}$	$\frac{1}{2}a(1-a)F+(\frac{1}{8}-\frac{1}{2}a)\xi F_\xi+\frac{(1-a)}{2(1+a)^2}\xi^{2a+4}(F_\xi)^2+\frac{a(a+2)}{(a+1)^2}\xi^{2a+3}FF_\xi-\frac{1}{8}\xi^2F_{\xi\xi}+\frac{a}{(a+1)^2}\xi^{2a+4}FF_{\xi\xi}=0$
$\mathcal{L}_{5,\varepsilon}$	$G=\sqrt{\lambda}(\frac{1}{2}F-\frac{1}{2}\varepsilon F_\xi+\frac{1}{2}(F_\xi)^2-\frac{1}{2}\xi F_\xi+\frac{1}{4}\varepsilon\xi)^{-1/2}$	$2\varepsilon F_\xi+2\xi^2F_{\xi\xi}-\varepsilon\xi+2F_{\xi\xi}-1-8FF_{\xi\xi}=0$
$\mathcal{N}_1$	$G=\sqrt{\lambda}(\frac{1}{2}(F_\xi)^2)^{-1/2}$	$0=0$
$\mathcal{N}_2$	$G=\sqrt{\lambda}(F_\xi)^{-1/2}$	$F_{\xi\xi}=0$
$\mathcal{N}_{4,\varepsilon}$	$G=\sqrt{\lambda}(\varepsilon+\frac{1}{2}(F_\xi)^2)^{-1/2}$	$F_{\xi\xi}=0$
$\mathcal{K}_{1,\varepsilon}$	$G=\sqrt{\lambda}\left(\frac{1}{2\xi}F_\xi+\frac{1}{2}\xi^2(F_\xi)^2-\varepsilon\xi F_\xi+\frac{1}{2}\right)^{-1/2}$	$F_\xi-\xi F_{\xi\xi}+4\varepsilon\xi^3F_{\xi\xi}+4\xi^3(F_\xi)^2=0$
$\mathcal{K}_{2,\varepsilon}$	$G=\sqrt{\lambda}(-F-\frac{1}{2}\varepsilon F_\xi+\frac{1}{2}(F_\xi)^2)^{-1/2}$	$F+\frac{3}{4}\varepsilon F_\xi+FF_{\xi\xi}+\frac{1}{8}F_{\xi\xi}-(F_\xi)^2=0$
$\mathcal{K}_{3,\varepsilon}$	$G=\sqrt{\lambda}(-\varepsilon\xi F_\xi+2F^2+2\xi FF_\xi+\frac{1}{2}\xi^2(F_\xi)^2)^{-1/2}$	$F_\xi+\xi F_{\xi\xi}-8\varepsilon FF_\xi+2\xi\varepsilon(F_\xi)^2-4\varepsilon\xi FF_{\xi\xi}=0$
$\mathcal{K}_{4,\varepsilon}$	$G=\sqrt{\lambda}(\xi+\frac{1}{2}(F_\xi)^2)^{-1/2}$	$\xi F_{\xi\xi}-\frac{1}{2}F_\xi=0$

$$v(x,t)=\frac{xt}{t^2-a_0x^4}. \tag{19}$$

This solution is defined for $\sqrt{a_0}x^2>|t|$. It is noticeable that at $t=0$ this solution reduces to $\theta=c_0$, $\rho=\sqrt{2\lambda a_0}x$. Thus, we have a zero velocity and linear density of the fluid.

In an analysis performed on the Chaplygin gas in one spatial dimension, Jackiw[1] considered the following method in order to determine solutions of the Chaplygin gas equations. A Legendre transform is used to exchange the independent variables (x,t) with the dependent ones (θ,ρ). In fact, the new independent variables used are

$$s=\sqrt{2\lambda}/\rho,\quad p=\frac{\partial\theta}{\partial x}=\theta_x, \tag{20}$$

where p is exactly the velocity $v(x,t)$. The following function of s and p is then defined:

$$\Psi(p,s)=\theta(x,t)-t\theta_t-x\theta_x. \tag{21}$$

From the equations (12) it is easily shown that

$$\Psi(p,s)=\theta(x,t)+\tfrac{1}{2}t(p^2-s^2)-xp \tag{22}$$

and so

$$\frac{\partial\Psi}{\partial p}=tp-x,\quad \frac{\partial\Psi}{\partial s}=-ts. \tag{23}$$

The equations (12) can then be rewritten as the linear equation

$$\frac{\partial^2\Psi}{\partial p^2}-\frac{\partial^2\Psi}{\partial s^2}+\frac{2}{s}\frac{\partial\Psi}{\partial s}=0. \tag{24}$$

The general solution of (24) is given in terms of two arbitrary functions $f=f(p+s)$ and $g=g(p-s)$ (where $p\pm s$ are called Riemann coordinates),

$$\Psi(p,s)=f(p+s)-sf'(p+s)+g(p-s)+sg'(p-s). \tag{25}$$

It is easy to show that the solution (18) corresponds to Jackiw's solution where

$$\Psi(p,s)=\frac{1}{4\sqrt{a_0}}\ln\left(\frac{s+p}{s-p}\right)+c_0+\frac{1}{2\sqrt{a_0}}\frac{sp}{(s-p)(s+p)}, \tag{26}$$

and

$$f(z)=\frac{1}{4\sqrt{a_0}}\ln z+\frac{1}{2}c_0,\quad g(-z)=-\frac{1}{4\sqrt{a_0}}\ln z+\frac{1}{2}c_0.$$

where, for each of the functions f and g, the variable z represents the corresponding argument as described in Eq. (25).

For $\mathcal{L}_2$, we have

$$\theta(x,t)=-a_0x^2\left(\frac{1+e^{4a_0(t-t_0)}}{1-e^{4a_0(t-t_0)}}\right),\quad \rho(x,t)=\sqrt{\frac{\lambda}{2a_0^2}}\,\frac{1}{x}, \tag{27}$$

$$v(x,t)=-2a_0x\left(\frac{1+e^{4a_0(t-t_0)}}{1-e^{4a_0(t-t_0)}}\right), \tag{28}$$

where a_0 and t_0 are real constants, and $a_0\neq 0$. This solution has a singularity at line $t=t_0$ which seems to indicate that it does not correspond to a physical theory at time t_0. As $t\to+\infty$, θ approaches the function $f_+(x)=ax^2$, and as $t\to-\infty$ it approaches $f_-(x)=-ax^2$. The density ρ has a pole at $x=0$ and is constant in time. This solution corresponds to the function (25) given explicitly by

$$\Psi(p,s)=-\frac{sp}{4a_0}+\frac{1}{8a_0}(p^2-s^2)\ln\left(\frac{p+s}{p-s}\right)+\frac{1}{2}t_0(p^2-s^2),$$

where

$$f(z)=\frac{t_0}{4}z^2+\frac{1}{8a_0}z^2\ln z,\quad g(z)=\frac{t_0}{4}z^2-\frac{1}{8a_0}z^2\ln z. \tag{29}$$

For $\mathcal{L}_3$, we have

$$\theta(x,t)=\frac{x^2}{2t}+\frac{\lambda t^3}{3a_0^2}+c_0,\quad \rho(x,t)=\frac{a_0}{t}, \tag{30}$$

so that the velocity is now

$$v(x,t)=\frac{x}{t}, \tag{31}$$

where a_0 and c_0 are real constants, and $a_0 \neq 0$. There is a pole singularity at $t=0$. As $t \to \infty$, the velocity potential θ becomes unbounded and the density ρ approaches zero. The velocity (31) is linear in x, but also approaches zero as $t \to \infty$. This solution corresponds to the case

$$\Psi(p,s) = c_0 - \frac{a_0 s^3}{3\sqrt{2\lambda}}, \tag{32}$$

where f and g in (25) are given by

$$f(z) = \frac{1}{2}\left(c_0 + \frac{1}{6\sqrt{2\lambda}} a_0 z^3 \right), \quad g(z) = \frac{1}{2}\left(c_0 - \frac{1}{6\sqrt{2\lambda}} a_0 z^3 \right).$$

It is interesting to note that the solution (32) of the equation (24) is invariant under translation by the variable p. This means that invariance under Galilean boost of the original set (12) implies a p-invariant solution for (24).

For $\mathcal{L}_{4,-1}$, we have

$$\theta(x,t) = \frac{2}{kt}\sinh^2\left(\frac{1}{2}\sqrt{k}(x+c_0) \right), \quad \rho(x,t) = \sqrt{\frac{k\lambda}{2}} \frac{t}{\sinh^2(\frac{1}{2}\sqrt{k}(x+c_0))}, \tag{33}$$

where k and c_0 are real constants. It is possible to rewrite this solution in a more familiar form. If we take $c_0 = i\pi/\sqrt{k}$ and define $a_0 = \frac{1}{2}\sqrt{k}$, we obtain the solution

$$\theta(x,t) = -\frac{1}{2a_0^2 t}\cosh^2(a_0 x), \quad \rho(x,t) = \sqrt{2\lambda}\frac{a_0 t}{\cosh^2(a_0 x)}, \tag{34}$$

$$v(x,t) = -\frac{1}{a_0 t}\cosh(a_0 x) \ \ \sinh(a_0 x), \tag{35}$$

which is exactly the soliton solution given by Jackiw.[1] This solution is not singular in x. The density ρ is zero at time $t=0$ and becomes unbounded as $t \to \infty$. This solution corresponds to the case

$$\Psi(p,s) = \frac{p}{2a_0}\ln\left(\frac{s+p}{s-p} \right) - \frac{s}{a_0}, \tag{36}$$

where $\Psi(p,s) =$ (25) with

$$f(z) = g(-z) = \frac{z}{2a_0}\ln z.$$

For $\mathcal{L}_{4,1}$, we get

$$\theta(x,t) = a_0 t - \frac{a_1}{2}x, \quad \rho(x,t) = \sqrt{\frac{\lambda}{\frac{1}{8}a_1^2 + a_0}}. \tag{37}$$

Here ρ and v are constant. In this case, the variables p and s defined in Eq. (20) are both constant, and so the change of variable $(x,t) \to (s,p)$ is noninvertible. This singular solution therefore cannot be found from the general solution proposed by Jackiw in the sense that we cannot find corresponding functions $\Psi(p,s)$, $f(z)$, and $g(z)$.

For the case $\mathcal{L}_{4,a}$ with $a \neq \pm 1,0$, we have to solve the equation for F listed in Table III. The analysis of this equation gives rise to a family of ODE's which do not enter the classification of Painlevé–Gambier[8,9] since they do not possess the Painlevé property.[10]

For $\mathcal{L}_{5,\varepsilon}$, the method of symmetry reduction on ODE's can be used to reduce the order of the equation for F listed in Table III. Using the infinitesimal symmetry generator $2\partial_x + x\partial_F$, we make the following change of variable:[6]

$$y = 4F - x^2, \quad w = \tfrac{1}{2}x, \tag{38}$$

which allows us to rewrite the equation as

$$2(y-1)w_{yy} + 16(1-y)(w_y)^3 + 4\varepsilon(w_y)^2 = 0. \tag{39}$$

Setting $z(y) = w_y$, we obtain the first-order ODE

$$2(y-1)z_y + 16(1-y)z^3 + 4\varepsilon z^2 = 0, \tag{40}$$

which is Abel's equation of the first kind, and therefore does not possess explicit analytical solutions.[11] In the literature[12] one can find existence theorems for solutions of (40) with property $z_y(0) = 0$ and $\lim_{u\to\infty} z(u) = 0$. For some solutions their Taylor expansions were found and others are given in the tables.[12]

For $\mathcal{N}_1$, $\theta = \theta(x)$ is an arbitrary function of x and we have

$$\rho = \frac{\sqrt{2\lambda}}{\theta_x}, \tag{41}$$

$$v(x,t) = \theta_x \neq 0. \tag{42}$$

Thus, any static velocity potential will satisfy the system of equations (12) provided that the density is also static and is related to θ through equation (41). Such a solution cannot be obtained from the general solution (25) since the change of variables $(x,t) \to (s,p)$ is again singular. Indeed, we have $s = p = \theta_x$.

For $\mathcal{N}_2$, we have

$$\theta(x,t) = \frac{\lambda}{a_0^2}t + c_0, \quad \rho(x,t) = a_0. \tag{43}$$

Here we obtain uniform (in x) solutions where the potential θ evolves in time in a linear manner. Thus, the velocity is zero and the density constant in both time and space.

For $\mathcal{N}_{4,\varepsilon}$, we have

$$\theta(x,t) = a_0 x + \varepsilon t + a_1, \quad \rho(x,t) = \sqrt{\frac{\lambda}{\frac{1}{2}a_0^2 + \varepsilon}}, \tag{44}$$

and

$$v(x,t) = a_0, \tag{45}$$

where a_0 and a_1 are constants. Again, we have a trivial constant solution.

For $\mathcal{K}_{1,\varepsilon}$, we get

$$\theta(x,t) = \tfrac{1}{2}\varepsilon \ln(x^2 - 2\varepsilon t) + c_0, \quad \rho(x,t) = \frac{\sqrt{2\lambda}(x^2 - 2\varepsilon t)}{\sqrt{4\varepsilon t - x^2}}, \tag{46}$$

$$v(x,t) = \frac{\varepsilon x}{x^2 - 2\varepsilon t}. \tag{47}$$

The two cases $\varepsilon = 1$ and $\varepsilon = -1$ are qualitatively different. When $\varepsilon = 1$ we require $2t < x^2 < 4t$ for the solution to be defined. When $\varepsilon = -1$ the condition becomes $-2t < x^2 < -4t$, which implies that the density ρ is real-valued only for negative values of t. Thus, it does not correspond to a physical density. The solution (46) corresponds to the case

$$\Psi(p,s) = \frac{1}{2}\varepsilon \frac{(s^2 - 3p^2)}{(p^2 - s^2)} - \frac{1}{2}\varepsilon \ln(p^2 - s^2) + \frac{1}{2}\varepsilon \ln 2 + c_0, \tag{48}$$

where $\Psi(p,s) =$ (25) with

$$f(z) = g(z) = \frac{1}{2}\varepsilon \ln\left(\frac{\sqrt{2}}{z}\right) - \frac{3}{4}\varepsilon + \frac{1}{2}c_0.$$

For $\mathcal{K}_{2,\varepsilon}$, we get

$$\theta(x,t) = te^{4\varepsilon(x_0 - x)}, \quad \rho(x,t) = \frac{\sqrt{\lambda}}{e^{2\varepsilon(x_0 - x)}\sqrt{1 + 8t^2 e^{4\varepsilon(x_0 - x)}}}, \tag{49}$$

$$v(x,t) = -4\varepsilon t e^{4\varepsilon(x_0 - x)}. \tag{50}$$

Thus ρ is always a finite, nonzero and positive function, while θ becomes infinite as $x \to -\infty$ or $|t| \to \infty$. This solution corresponds to the case

$$\Psi(p,s) = \tfrac{1}{4}\varepsilon p \ln(\tfrac{1}{2}(s^2 - p^2)) - x_0 p, \tag{51}$$

where $\Psi(p,s) =$ (25) with

$$f(z) = -g(-z) = \tfrac{1}{4}\varepsilon z \ln z - (\tfrac{1}{2}x_0 + \tfrac{1}{8}\varepsilon \ln 2)z.$$

For $\mathcal{K}_{3,\varepsilon}$, we have

$$\theta(x,t) = \tfrac{1}{2}(e^{a_0 + 2\varepsilon t} + \varepsilon x^2), \quad \rho(x,t) = \frac{\sqrt{\lambda}}{\sqrt{\varepsilon e^{a_0 + 2\varepsilon t} + \frac{1}{2}x^2}}, \tag{52}$$

$$v(x,t) = \varepsilon x. \tag{53}$$

Here θ and ρ are always nonzero, finite and positive. As $t \to \infty$ or $|x| \to \infty$, θ becomes unbounded and ρ approaches zero. This solution corresponds to the case

$$\Psi(p,s) = \tfrac{1}{4}\varepsilon(s^2 + p^2) - \tfrac{1}{4}\varepsilon(s^2 - p^2)\ln(\tfrac{1}{2}\varepsilon(s^2 - p^2)) + \tfrac{1}{4}\varepsilon(s^2 - p^2)a_0 - \varepsilon p^2, \tag{54}$$

where $\Psi(p,s) =$ (25) with

$$f(z) = g(-z) = -\tfrac{3}{8}\varepsilon z^2 - \tfrac{1}{8}\varepsilon a_0 z^2 + \tfrac{1}{8}\varepsilon z^2 \ln(z^2/2).$$

For $\mathcal{K}_{4,\varepsilon}$, we have

$$\theta(x,t) = \varepsilon x t - \frac{1}{3}t^3 + \frac{2}{3}a_0\varepsilon \frac{(\varepsilon x - \frac{1}{2}t^2)^{3/2}}{\sqrt{\lambda - a_0^2/2}} + c_0, \quad \rho(x,t) = \sqrt{\frac{\lambda - a_0^2/2}{\varepsilon x - \frac{1}{2}t^2}}, \tag{55}$$

$$v(x,t) = \varepsilon t + \frac{a_0}{\sqrt{\lambda - a_0^2/2}} \left(\varepsilon x - \frac{1}{2} t^2 \right)^{1/2}, \tag{56}$$

where $x > \frac{1}{2}t^2$ (in the case where $\varepsilon = 1$) or $x < -\frac{1}{2}t^2$ (in the case where $\varepsilon = -1$). This solution corresponds to the case

$$\Psi(p,s) = \frac{1}{6}\varepsilon p^3 + \frac{1}{3}\varepsilon \frac{a_0^3}{(2\lambda)^{3/2}} s^3 - \frac{1}{2}\varepsilon p s^2 + \frac{2}{3}\varepsilon \frac{a_0}{(2\lambda)^{3/2}} \sqrt{\lambda - a_0^2/2}\, s^3, \tag{57}$$

where $\Psi(p,s) =$ (25) with

$$f(z) = \frac{1}{12}\varepsilon z^3 - \frac{1}{12}\varepsilon \frac{a_0^3}{(2\lambda)^{3/2}} z^3 - \frac{1}{6}\varepsilon \frac{a_0}{(2\lambda)^{3/2}} \sqrt{\lambda - a_0^2/2}\, z^3,$$

$$g(z) = \frac{1}{12}\varepsilon z^3 + \frac{1}{12}\varepsilon \frac{a_0^3}{(2\lambda)^{3/2}} z^3 + \frac{1}{6}\varepsilon \frac{a_0}{(2\lambda)^{3/2}} \sqrt{\lambda - a_0^2/2}\, z^3.$$

It has therefore been demonstrated that for the subalgebras of types $\{\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3, \mathcal{L}_{4,-1}\}$ and $\{\mathcal{K}_{1,\varepsilon}, \mathcal{K}_{2,\varepsilon}, \mathcal{K}_{3,\varepsilon}, \mathcal{K}_{4,\varepsilon}\}$, the invariant solutions fall into the general solution (25) given by Jackiw. However, for the subalgebras $\{\mathcal{L}_{4,1}, \mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_{4,\varepsilon}\}$, the transformations $(x,t) \to (s,p)$ are noninvertible and so the invariant solutions are not included in the general solution (25).

C. Solutions of the Born–Infeld model

Each solution of the Chaplygin equations (12) can be used to obtain an equivalent solution of the relativistic Born–Infeld equations (10) and (11) in one spatial dimension. Since the Chaplygin and Born–Infeld models involve two distinct parametrizations of the Nambu–Goto target space variables X^0 and X^{d+1}, we equate these variables to both their relativistic and nonrelativistic representations:

$$X^0 = c t_R = \frac{1}{\sqrt{2}} (t_{NR} + \theta_{NR}(t_{NR}, \mathbf{r})), \tag{58}$$

$$X^{d+1} = \frac{1}{c}\theta(t_R, \mathbf{r}) = \frac{1}{\sqrt{2}} (t_{NR} - \theta_{NR}(t_{NR}, \mathbf{r})). \tag{59}$$

Renaming the time variables $T = (1/c)\, t_{NR}$ and $t = t_R$, we obtain the following method of solution transformation described by Jackiw.[1] If $\theta_{NR}(\mathbf{r},t)$ is a solution of the Chaplygin equation (4), then a solution $\theta_R(\mathbf{r},t)$ of the Born–Infeld equation can be determined as follows. First, determine the function $T(\mathbf{r},t)$ from the equation

$$T + \frac{1}{c^2}\theta_{NR}(\mathbf{r},T) = \sqrt{2}t, \tag{60}$$

then

$$\theta_R(\mathbf{r},T) = \frac{1}{\sqrt{2}} c^2 T - \frac{1}{\sqrt{2}}\theta_{NR}(\mathbf{r},T) = c^2(\sqrt{2}T - t) \tag{61}$$

is an associated Born–Infeld solution. Since the equation (60) cannot always be solved explicitly for $T(\mathbf{r},t)$ it follows that explicit Born–Infeld solutions cannot always be found in this manner. For instance, in the case of $\mathcal{L}_1$, the Born–Infeld solution is

$$\theta_R(x,t) = \frac{1}{\sqrt{2}}c^2T - \frac{1}{4\sqrt{2a_0}}\ln\left(\frac{\sqrt{a_0}x^2+T}{\sqrt{a_0}x^2-T}\right) - \frac{c^2}{\sqrt{2}}a_1, \tag{62}$$

where $T(x,t)$ satisfies the equation

$$T + \frac{1}{c^2}\left(\frac{1}{4\sqrt{a_0}}\ln\left(\frac{\sqrt{a_0}x^2+T}{\sqrt{a_0}x^2-T}\right)\right) + a_1 = \sqrt{2}t \tag{63}$$

and the density (for any general solution θ_R) is

$$\rho_R(x,t) = \frac{a(\theta_R)_t}{c^2\sqrt{c^2-\partial_\mu(\theta_R)\partial^\mu(\theta_R)}}. \tag{64}$$

However, for the subalgebras $\mathcal{L}_{4,1}$, $\mathcal{N}_1$, $\mathcal{N}_2$, $\mathcal{N}_{4,\varepsilon}$, and $\mathcal{K}_{2,\varepsilon}$, we do obtain explicit Born–Infeld solutions equivalent to the corresponding Chaplygin solutions.

For $\mathcal{L}_{4,1}$, we have

$$\begin{aligned}\theta_R(x,t) &= \frac{\frac{1}{\sqrt{2}}a_0x + \left(1-\frac{a_1}{c^2}\right)c^2t}{1+\frac{a_1}{c^2}}\ ,\\ \rho_R(x,t) &= \frac{a\left(1-\frac{a_1}{c^2}\right)}{\left(1+\frac{a_1}{c^2}\right)\sqrt{c^2+\frac{a_0^2}{2(1+a_1/c^2)^2}}}.\end{aligned} \tag{65}$$

This represents a travelling wave solution.

For $\mathcal{N}_1$, we have

$$\theta_R(x,t) = c^2t - \sqrt{2}f(x), \quad \rho_R(x,t) = -\frac{a}{\sqrt{2}\left(\frac{df}{dx}\right)}, \tag{66}$$

where $f=f(x)$ is an arbitrary function, and is in fact the nonrelativistic solution $\theta_{NR}=f(x)$. This is a generalized travelling wave (i.e., Riemann wave). The gradient catastrophe occurs where $df/dx=0$, which allows a shock wave.

For $\mathcal{N}_2$, we have

$$\theta_R(x,t) = a_0t + c_0, \quad \rho_R(x,t) = \frac{-aa_0}{c\sqrt{c^4-a_0^2}}, \tag{67}$$

where $|a_0|<c^2$. This is a trivial solution since using the invariance with respect to t leads us to a constant solution.

For $\mathcal{N}_{4,\varepsilon}$, we have

$$\theta_R(x,t) = \frac{1}{1+\frac{\varepsilon}{c^2}}((c^2-\varepsilon)t+a_0x+a_1), \quad \rho_R(x,t) = \frac{-a(c^2-\varepsilon)}{c^2\sqrt{4\varepsilon+a_0^2}}, \tag{68}$$

where if $\varepsilon=-1$ then $|a_0|>2$. This represents a travelling wave.

For $\mathcal{K}_{2,\varepsilon}$, we have

$$\theta_R(x,t)=\frac{c^2t(c^2-e^{4\varepsilon(x_0-x)})}{(c^2+e^{4\varepsilon(x_0-x)})},$$
$$\rho_R(x,t)=\frac{-a(c^4-e^{8\varepsilon(x_0-x)})}{\sqrt{4c^4e^{4\varepsilon(x_0-x)}(c^2+e^{4\varepsilon(x_0-x)})^2+64c^8t^2e^{4\varepsilon(x_0-x)}}}. \tag{69}$$

This is a kink-type solution.

IV. THE METHOD OF DIFFERENTIAL CONSTRAINTS

We determined in Sec. III that the group-invariant solutions of the Chaplygin system (12) were either singular or derivable from the general solution of the second-order partial differential equation (24). A further generalization of the classical symmetry reduction is the introduction of the general ''side conditions'' method.[13] This method includes all known methods for determining special classes of solutions of PDE's (among others group-invariant solutions, nonclassical and weak symmetries, partially invariant solutions, separation of variables, and many others). Differential constraints possess a group interpretation as ''conditional symmetries.''[14–16] It consists basically in modifying the original system by adding to it certain compatible differential constraints. The overdetermined system of equations obtained in this way admits, in some cases, a larger class of Lie point symmetry groups, and consequently can provide new classes of solutions of the original system. In this section our choice of differential constraints is motivated by our main aim which is the construction of multiplicative separation of dependent variables

$$u_i(x,t)=f_i(x)g_i(t),\quad i=1,2, \tag{70}$$

for some functions f_i and g_i of one variable. Here, u_1 and u_2 stand for ρ and θ, respectively. Ansatz (70) corresponds to the following second-order differential constraints:

$$\partial_x\partial_t \ln u_i=0,\quad i=1,2. \tag{71}$$

Note that the differential constraints (71) are no longer restricted to be first-order PDE's provided by the characteristics of symmetries generated by (13). Hence, according to Ref. 6 solutions of the overdetermined system composed of the Chaplygin equations (12) [or Born–Infeld equations (10), (11)] subjected to (71) are no longer group-invariant solutions.

We now show that these forms of constraints are compatible with the Chaplygin system (12) and enable us to construct several families of solitonlike solutions. Indeed, substituting (70) into (12) we obtain a system of differential equations

$$g_{2,t}f_2+\frac{1}{2}g_2^2(f_{2,x})^2=\frac{\lambda}{f_1^2g_1^2},$$
$$g_{1,t}f_1+g_1g_2f_{1,x}f_{2,x}+g_1g_2f_1f_{2,xx}=0. \tag{72}$$

Eliminating function f_1g_1 from (72) we obtain

$$-\tfrac{1}{2}g_{2,tt}f_2-g_2g_{2,t}(f_{2,x})^2+g_2g_{2,t}f_2f_{2,xx}=0. \tag{73}$$

Integrating with respect to t and relabeling the functions f_2 and g_2 as f and g, respectively, we obtain

$$-\tfrac{1}{2}g_tf-\tfrac{1}{2}g^2(f_x)^2+\tfrac{1}{2}g^2ff_{xx}=\gamma(x). \tag{74}$$

Let us consider separately three cases, namely (a) the case in which $\gamma(x)$ vanishes everywhere, (b) the case where $\gamma(x)=f$ and $ff_{xx}-(f_x)^2=f$, and (c) the case where $\gamma(x)=f$ and $ff_{xx}-(f_x)^2=-f$. It is easy to show that in case (a), when $\gamma(x)=0$ identically, the solution of the system (74) takes the form

$$\theta(x,t)=\frac{2K_2}{K_3(K_2t+K_1)}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right),$$
$$\rho(x,t)=\sqrt{\frac{K_3\lambda}{2}}\frac{K_2t+K_1}{K_2\sinh^2(\frac{1}{2}\sqrt{K_3}(x+x_0))}. \tag{75}$$

For $K_3\neq 0$ and $t\neq -K_1/K_2$, the expressions (75) represent a bump-type solution. Making use of the transformations (60) and (61), we get a solution of the Born–Infeld equation (9),

$$\theta_R(x,t)=-\frac{c^2K_1}{\sqrt{2}K_2}\pm\frac{c^2}{\sqrt{2}K_2}\sqrt{2K_2^2t^2+2\sqrt{2}K_1K_2t+K_1^2-\frac{8K_2^2}{c^2K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)}. \tag{76}$$

This is a bump-type solution, called in literature a Gaussian solution.[17]

In the cases (b) and (c), the equation (74) can be integrated to give the solutions

$$\theta(x,t)=-\frac{2\sqrt{2}}{K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\left(\frac{1+e^{2\sqrt{2}(t+K_1)}}{1-e^{2\sqrt{2}(t+K_1)}}\right),$$
$$\rho(x,t)=\sqrt{\lambda}\left\{\frac{4}{K_3}\frac{\sinh^2(\frac{1}{2}\sqrt{K_3}(x+x_0))}{(1-e^{2\sqrt{2}(t+K_1)})^2}\left(-4e^{2\sqrt{2}(t+K_1)}+\cosh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\right.\right.$$
$$\left.\left.\times(1+e^{2\sqrt{2}(t+K_1)})^2\right)\right\}^{-1/2} \tag{77}$$

and

$$\theta(x,t)=\frac{2\sqrt{2}}{K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\tan(\sqrt{2}(t_0-t)),$$
$$\rho(x,t)=\sqrt{\lambda}\left\{\frac{4}{K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\right.$$
$$\left.\times\left(\cosh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\tan^2(\sqrt{2}(t_0-t))-\sec^2(\sqrt{2}(t_0-t))\right)\right\}^{-1/2}, \tag{78}$$

respectively. For $K_3\neq 0$ and $t\neq(\sqrt{2}/4)\ln 1-K_1$, the solution (77) represents a bump-type solution. With a specific choice of the constants K_1, K_3, and x_0 such that the density ρ is nonsingular at $x=0$, we get for the solution (77) the functions

$$\theta(x,t)=\frac{1}{\sqrt{2}}\cosh^2 x\left(\frac{1+e^{2\sqrt{2}t}}{1-e^{2\sqrt{2}t}}\right),$$
$$\rho(x,t)=\frac{\sqrt{\lambda}}{\cosh x}\left(\frac{(1-e^{2\sqrt{2}t})^2}{4e^{2\sqrt{2}t}+(1+e^{2\sqrt{2}t})^2\sinh^2 x}\right)^{1/2}. \tag{79}$$

These functions are represented in Figs. 1 and 2. For the solution (78), the same choice for the constants K_1, K_3, and x_0, along with $t_0=0$, lead to

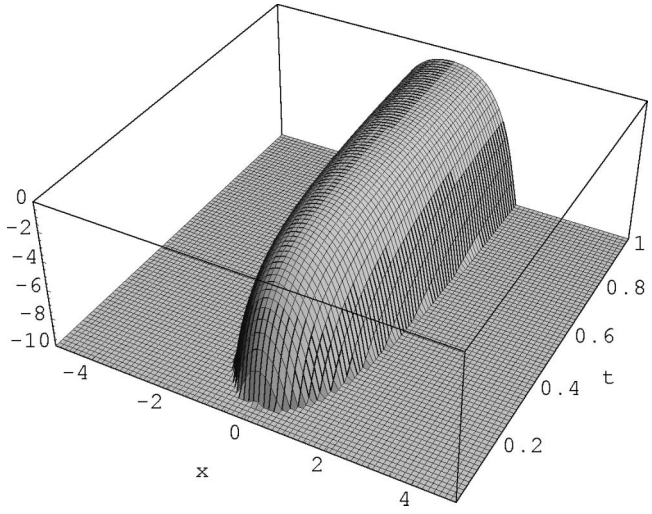

FIG. 1. The function $\theta(x,t)$ in Eq. (79).

$$\theta(x,t) = \frac{1}{\sqrt{2}}\cosh^2 x \tan(\sqrt{2}t),$$
$$\rho(x,t) = \frac{\sqrt{\lambda}}{\cosh x}\left(\frac{1}{\sec^2(\sqrt{2}t)+\sinh^2 x \tan^2(\sqrt{2}t)}\right)^{1/2}. \tag{80}$$

These functions are represented in Figs. 3 and 4. For this solution (78), the function $\theta(x,t)$ includes discontinuities at $t=t_0+n(\sqrt{2}\pi/4)$, where n is an integer. The density $\rho(x,t)$ is defined and continuous everywhere and is a multibump solution.

Once again, we obtain the Born–Infeld solutions,

$$\theta_R(x,t) = c^2(\sqrt{2}T-t), \tag{81}$$

where $T(x,t)$ satisfies the equations

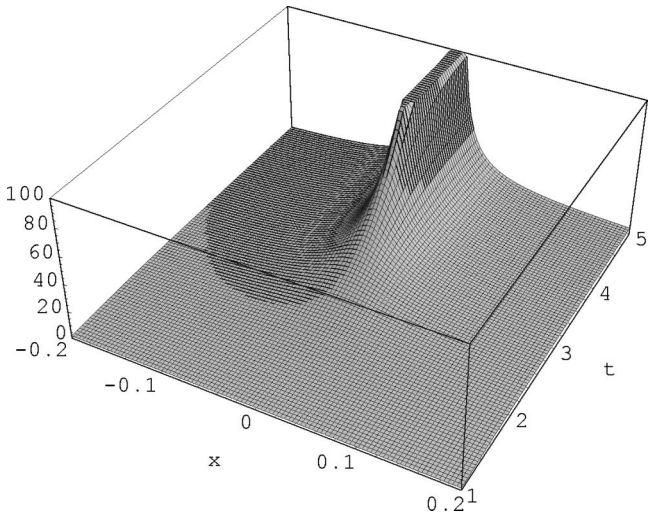

FIG. 2. The function $\rho(x,t)$ in Eq. (79).

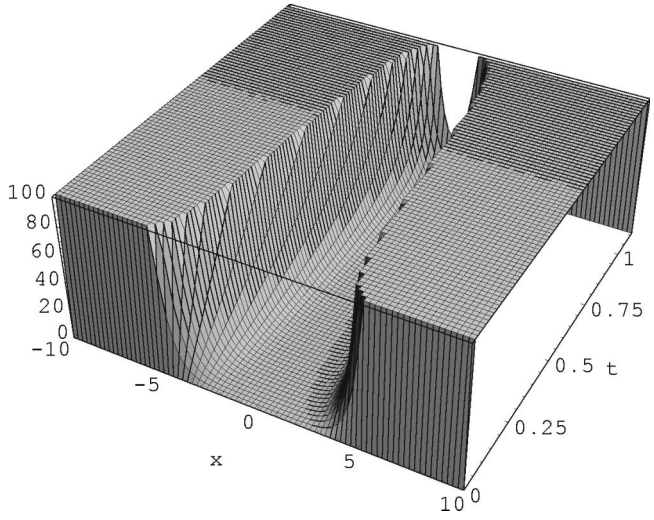

FIG. 3. The function $\theta(x,t)$ in Eq. (80).

$$T+\frac{1}{c^2}\left(-\frac{2\sqrt{2}}{K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\left(\frac{1+e^{2\sqrt{2}(T+K_1)}}{1-e^{2\sqrt{2}(T+K_1)}}\right)\right)=\sqrt{2}t \tag{82}$$

and

$$T+\frac{1}{c^2}\left(\frac{2\sqrt{2}}{K_3}\sinh^2\left(\frac{1}{2}\sqrt{K_3}(x+x_0)\right)\tan(\sqrt{2}(t_0-T))\right)=\sqrt{2}t, \tag{83}$$

respectively.

It is manifest that the solution (75), corresponding to case (a) is simply a generalization of the solution (33), found in Sec. III for the case $\mathcal{L}_{4,-1}$. In fact, solution (33) is the special case where $K_2=1$, $K_1=0$. By the simple change of variable $t\rightarrow(1/K_2)(t-K_1)$, (33) can be transformed to its generalized counterpart (75). For each of the solutions (77) and (78), corresponding to cases (b) and (c), respectively, the Jacobian of the transformation

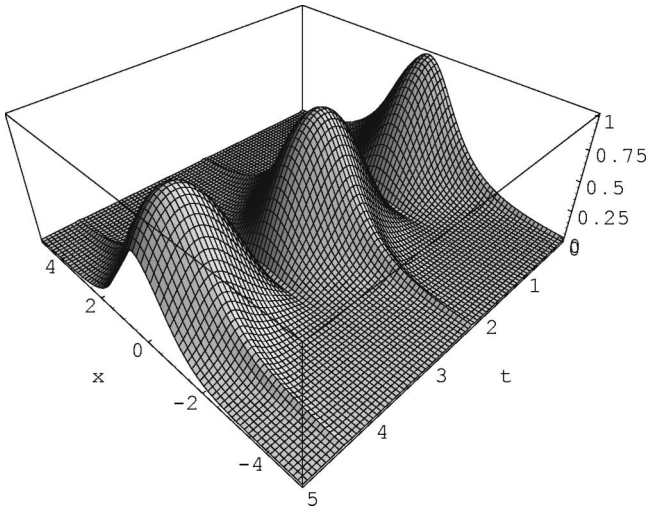

FIG. 4. The function $\rho(x,t)$ in Eq. (80).

$$J = \frac{\partial(p,s)}{\partial(x,t)} \tag{84}$$

is nonzero. This would indicate that the change of variables is invertible. However, attempts to invert the transformation lead to transcendental trigonometric equations for the variables x and t in both cases, so it is not possible to determine equivalent functions $\Psi(p,s)$. Therefore, we cannot determine whether or not the solutions (77) and (78) correspond to the general solution of Jackiw.[1]

V. CONCLUDING REMARKS

Group-invariant solutions of the Chaplygin gas equations have been determined for the one-dimensional subalgebras of the general Chaplygin Lie algebra. In addition, based on these solutions, a number of explicit solutions of the Born–Infeld relativistic model have been determined. The nonsingular solutions [where the transformation $(x,t)\rightarrow(s,p)$ is invertible] were found to be linked to special cases of the general solution described by Jackiw's approach.[1] Certain classes of solutions were found in which the density ρ of the fluid is constant in both time and space. These solutions were found not to be included in the classification presented in Ref. 1. In some cases, the reduced equations for the subalgebras $\mathcal{L}_2$, $\mathcal{N}_2$, and $\mathcal{N}_{4,\varepsilon}$ satisfy the first and fifth Painlevé equations.[10] In summary, we can state that the symmetry reduction method in the version presented here proved to be a useful tool in the sense that in the cases of Chaplygin and Born–Infeld it led to many new interesting solutions, among them kinks, bumps, and multiwave solutions.

A question arises as to whether our approach can be extended to obtain partially invariant solutions[18] with defect structure $\delta=1$. Further, can it provide new classes of solutions which will describe more diverse types of solutions than those found in group-invariant cases. This will be discussed in more detail in a future work.

ACKNOWLEDGMENTS

The authors' research was partially supported by research grants from NSERC of Canada and FCAR du Québec.

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Exact duality transformations for sigma models and gauge theories

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(Received 6 September 2002; accepted 26 March 2003)

We present an exact duality transformation in the framework of statistical mechanics for various lattice models with non-Abelian global or local symmetries. The transformation applies to sigma models with variables in a compact Lie group G with global $G\times G$-symmetry (the chiral model) and with variables in coset spaces G/H and a global G-symmetry [for example, the nonlinear O(N) or $\mathbb{RP}^N$ models] in any dimension $d\geqslant 1$. It is also available for lattice gauge theories with local gauge symmetry in dimensions $d\geqslant 2$ and for the models obtained from minimally coupling a sigma model of the type mentioned above to a gauge theory. The duality transformation maps the strong coupling regime of the original model to the weak coupling regime of the dual model. Transformations are available for the partition function, for expectation values of fundamental variables (correlators and generalized Wilson loops) and for expectation values in the dual model which correspond in the original formulation to certain ratios of partition functions (free energies of dislocations, vortices or monopoles). Whereas the original models are formulated in terms of compact Lie groups G and H, coset spaces G/H and integrals over them, the configurations of the dual model are given in terms of representations and intertwiners of G and H. They are spin networks and spin foams. The partition function of the dual model describes the group theoretic aspects of the strong coupling expansion in a closed form.
[DOI: 10.1063/1.1580071]

I. INTRODUCTION

The most prominent example of an exact duality transformation in statistical mechanics is the transformation for the two-dimensional Ising model.[1] It is an exact transformation which changes the variables of the full partition function of the model and maps the high temperature regime of the original model to the low temperature regime of the dual model and conversely (for the Ising model, the original and the dual model coincide).

In the following, we make use of the correspondence of quantum field theory in the Euclidean (imaginary time) formulation in d space dimensions plus time with equilibrium statistical mechanics in $d+1$ dimensions and often use the words *path integral*, *action*, and *coupling* for *partition function*, *energy*, and *temperature*, respectively.

The duality transformation of the Ising model was subsequently generalized to more general lattice systems with $\mathbb{Z}_2$ symmetries,[2] namely systems in d-dimensions whose variables are $\mathbb{Z}_2$-valued k-forms, $0\leqslant k\leqslant d$, i.e., spin models with global $\mathbb{Z}_2$ symmetry, pure lattice gauge theories with local $\mathbb{Z}_2$ gauge symmetry, theories for $\mathbb{Z}_2$-valued antisymmetric tensor fields, and so on, and to their counterparts with U(1)-symmetries,[3] in particular to the XY-model and pure U(1) gauge theory on the lattice.[3,4] For lattice models with Abelian symmetries, there exists an essentially complete picture,[5] and the systems to which the duality transformation applies include even

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some Higgs models,[6] namely U(1)-lattice gauge theory minimally coupled to a U(1)-valued scalar field, i.e., a Higgs field with frozen radial component.

All these examples of the Abelian duality transformation have some features in common. They map the strong coupling regime of the original model to the weak coupling regime of the dual model. This is a consequence of the change of variables employed in the transformation which essentially involves the Fourier decomposition of the interaction terms e^{-S} for some action S. For example, this replaces U(1)-variables by integers $\mathbb{Z}$ and maps Boltzmann weights with narrow peaks to weights with wide peaks and conversely. The structure of the dual model can be sketched as follows. If, say in a sigma model, the variables are originally associated with the points of the lattice and the interaction terms with the bonds, then the variables of the dual model which are introduced by the Fourier expansion are located at the bonds. In a second step one removes the old variables by performing the relevant sums or integrals which yields additional Boltzmann weights, often constraints, for each point.

As a consequence of the strong–weak nature of the duality transformation, the dual partition function contains essential information on the strong coupling expansion of the original model. In fact, if one understands how the Fourier coefficients of the Boltzmann weight depend on the coupling, the summands of the dual partition function are precisely the terms of the strong coupling expansion and can be sorted by the magnitude of their contribution at strong coupling.

A systematic generalization of these transformations to systems with non-Abelian symmetries proved to be difficult. The calculation of strong coupling expansions of pure non-Abelian lattice gauge theory (see, for example Ref. 7) already exhibits some features of the dual model which one wishes to construct. Fourier expansion is generalized to character decomposition, and the dual variables are irreducible representations of the symmetry group, generalizing the wave numbers of the Fourier series. The main technical difficulties are first to solve the integrals over the variables of the original model in a systematic way, and second to disentangle the lattice combinatorics in order to make the structure of the dual model transparent. Both problems can be overcome if one deals with the non-Abelian group variables at a sufficiently abstract level and if one uses an efficient diagrammatic notation.

The first examples of non-Abelian generalizations were an explicit calculation for pure SU(2) lattice gauge theory in $d=3$ dimensions[8] and, much less obviously, the equivalence of lattice BF-theory (similar to pure lattice Yang–Mills theory, but with δ-functions as the Boltzmann weights) to certain topological state sum models.[9] This correspondence was developed in a nonperturbative approach to quantum gravity. For review articles, see, for example, Refs. 10 and 11. The approach to quantum gravity by quantizing a discrete version of the gauge theory formulation of general relativity has lead to the definition of spin foams.[12–14] A spin foam is an abstract two-complex, consisting of vertices, edges, and faces whose faces are labeled with irreducible representations of some symmetry group while the edges are labeled with compatible intertwiners. Spin foams can be understood as a higher dimensional analog of spin networks. A spin network is a graph whose edges are labeled with representations and whose vertices are labeled with compatible intertwiners (precise definitions of spin networks and spin foams are given below in Sec. III B).

Spin foams provide the appropriate language for a generalization of the exact duality transformation to pure non-Abelian lattice gauge theory in arbitrary dimension $d \geqslant 2$ whose gauge group is a generic compact Lie group G. See Refs. 15 and 16 for lattice gauge theory on hypercubic lattices and Refs. 17 and 18 for the generalization to more general lattices and quantum groups rather than Lie groups.

In this article, we extend the non-Abelian duality transformation to a large class of sigma models whose variables take values in G or G/H, G a compact Lie group and H a Lie subgroup, and which have certain global or local symmetries. (The author is grateful to Alan Sokal who suggested to study this generalization.) This includes, for example, the chiral, the O(N) and $\mathbb{RP}^N$ models, and the models that are obtained from minimally coupling such a sigma model to a non-Abelian lattice gauge theory, for example, some generalized Higgs models with frozen radial degree of freedom.

The duality transformation retains its key properties, namely that it provides a strong–weak relation, that it yields a closed form of the strong coupling expansion of the original model, and that it maps expectation values of the dual model to ratios of partition functions (free energies of dislocations, vortices, or monopoles) in the original formulation and conversely. It therefore relates the fundamental variables of one formulation with some topological defects (collective properties) in the other.

The transformation maps the original model which is formulated in terms of compact Lie groups G and H, functions on G and integrals over G or G/H, to the dual model which is given in terms of the irreducible representations and intertwiners of G and H. The transformation can be understood as a particular application of a Tannaka-Kreĭn-type duality relating groups to their representation categories. That these categories will appear in the dual formulation had already been proposed in Ref. 19. The dual model can be formulated using merely the language of category theory. In the simplest case, it uses the category of finite-dimensional representations of the symmetry group G. This can be extended to more general categories that do not arise as the representation categories of compact Lie groups. The generalization of lattice gauge theory to quantum groups[17,18] is one example. For more details on the relation of groups and quantum groups with certain tensor categories, see, for example, Ref. 20. In this article, we do not explicitly use the language of category theory, but rather present diagrams in addition to the explicit formulas so that one can easily infer the categorial formulation from these diagrams.

While the configurations of the model dual to lattice gauge theory are spin foams,[15] one obtains spin networks as the configurations of the model dual to a sigma model. We thus call the dual models *spin foam models* and *spin network models*, respectively. As the notions of spin networks and spin foams have been developed in an approach to quantum gravity, but might not be familiar to the reader working on statistical mechanics, we try to make this article self-contained and therefore review all relevant definitions and also some background material on the representation theory of compact Lie groups.

The present article is organized as follows. In Sec. II, we summarize some background material on the representation theory of compact Lie groups and introduce a convenient diagrammatical notation. In Sec. III, we present our notation for the lattices we use, namely graphs and abstract two-complexes, and we recall the definitions of spin networks and spin foams. In Sec. IV, we present the duality transformation for the lattice chiral model with symmetry group G. This is generalized in Sec. V to the nonlinear sigma model with variables in coset spaces G/H and in Sec. VI to the nonlinear sigma model for G/H coupled to a lattice gauge theory with gauge group G. We conclude in Sec. VII where we discuss applications, directions for future research, and open questions.

II. MATHEMATICAL BACKGROUND

In this section, we review some basic concepts and results from the representation theory of compact Lie groups. The material presented here is largely textbook knowledge, (see, for example, Refs. 21 and 22 where most of the proofs can be found). The purely algebraic evaluation of the group integrals was first given in Ref. 15; our diagrammatic language follows Refs. 17 and 18.

A. Representation functions

Let G be a compact Lie group. This notion includes in particular any finite group (with the discrete topology). We denote finite-dimensional complex vector spaces on which G is represented by V_ρ and by $\rho: G \to \mathrm{Aut}\, V_\rho$ the corresponding group homomorphisms. Since each finite-dimensional complex representation of G is equivalent to a unitary representation, we select a set $\tilde{\mathcal{R}}_G$ containing one unitary representation of G for each equivalence class of finite-dimensional representations. The tensor product, the direct sum, and taking the dual are supposed to be closed operations on this set. This amounts to a particular choice of representation isomorphisms $\rho_1 \otimes \rho_2 \leftrightarrow \rho_3$ etc., $\rho_j \in \tilde{\mathcal{R}}_G$, which is implicit in our formulas. We furthermore denote by $\mathcal{R}_G \subseteq \tilde{\mathcal{R}}_G$ the subset of irreducible representations.

For a representation $\rho \in \widetilde{\mathcal{R}}_G$, the dual representation is denoted by ρ^*, and the dual vector space of V_ρ by V_ρ^*. The dual representation is given by $\rho^*: G \mapsto \mathrm{Aut}\, V_\rho^*$, where

$$\rho^*(g): V_\rho^* \to V_\rho^*, \quad \eta \mapsto \eta \circ \rho(g^{-1}), \tag{2.1}$$

i.e., $(\rho^*(g)\,\eta)(v) = \eta(\rho(g^{-1})v)$ for all $v \in V_\rho$. There exists a one-dimensional "trivial" representation of G which is isomorphic to $\mathbb{C}$.

For the unitary representations V_ρ, $\rho \in \widetilde{\mathcal{R}}_G$, we have standard (sesquilinear) scalar products $\langle \cdot;\cdot \rangle$ and orthonormal bases $\{e_j\}_j$. Therefore, we can define a bijective antilinear map $*: V_\rho \to V_\rho^*$ induced by the scalar product,

$$*(v) := (w \mapsto \langle v; w \rangle), \quad v \in V_\rho, \tag{2.2}$$

and construct the dual bases $\{\eta^j\}_j$ by $\eta^j := *(e_j)$. Identifying $(V_\rho^*)^* = V_\rho$, this yields $\langle e_j; e_k \rangle = \eta^j(e_k) = \delta_{jk}$ and furthermore induces a scalar product on V_ρ^*, namely $\langle \eta^j; \eta^k \rangle = \eta^k(e_j)$, $1 \leqslant j,\ k \leqslant \dim V_\rho$.

The matrix elements of the representation matrices $\rho(g)$ define complex-valued functions,

$$t_{jk}^{(\rho)}: G \to \mathbb{C}, \quad g \mapsto t_{jk}^{(\rho)}(g) := \eta^j(\rho(g)e_k) = (\rho(g))_{jk}, \tag{2.3}$$

where $\rho \in \widetilde{\mathcal{R}}_G$, $1 \leqslant j,\ k \leqslant \dim V_\rho$. They are called *representation functions* of G and form a commutative and associative unital algebra over $\mathbb{C}$,

$$C_{\mathrm{alg}}(G) := \{t_{jk}^{(\rho)} :\ \rho \in \widetilde{\mathcal{R}}_G, 1 \leqslant j,k \leqslant \dim V_\rho\}, \tag{2.4}$$

whose product is given by the matrix elements of the tensor product of representations,

$$(t_{jk}^{(\rho)} \cdot t_{\ell m}^{(\sigma)})(g) := t_{j\ell,km}^{(\rho\otimes\sigma)}(g), \tag{2.5}$$

where $\rho, \sigma \in \widetilde{\mathcal{R}}_G$, $1 \leqslant j,\ k \leqslant \dim V_\rho$ and $1 \leqslant \ell,\ m \leqslant \dim V_\sigma$.

We find the following expressions involving the group unit $e \in G$,

$$t_{jk}^{(\rho)}(e) = \delta_{jk}, \tag{2.6}$$

products of group elements,

$$t_{jk}^{(\rho)}(g \cdot h) = \sum_{\ell=1}^{\dim V_\rho} t_{j\ell}^{(\rho)}(g) \cdot t_{\ell k}^{(\rho)}(h), \tag{2.7}$$

and inverse group elements,

$$t_{jk}^{(\rho)}(g^{-1}) = (\rho(g)^{-1})_{jk} = \overline{(\rho(g))_{kj}} = \overline{t_{kj}^{(\rho)}(g)}, \tag{2.8}$$

as well as

$$t_{jk}^{(\rho)}(g^{-1}) = \eta^j(\rho(g)^{-1}e_k) = (\rho^*(g)\,\eta^j)(e_k) = \langle \eta^k; \rho^*(g)\,\eta^j \rangle = t_{kj}^{(\rho^*)}(g), \tag{2.9}$$

so that for unitary representations, the dual representation is just the conjugate one. The bar denotes complex conjugation.

B. Peter–Weyl decomposition and theorem

The structure of the algebra $C_{\mathrm{alg}}(G)$ can be understood if $C_{\mathrm{alg}}(G)$ is considered as a representation of $G \times G$ by combined left and right translation of the function argument,

$$(G\times G)\times C_{\mathrm{alg}}(G)\to C_{\mathrm{alg}}(G),\quad ((g_1,g_2),f)\mapsto(h\mapsto f(g_1^{-1}hg_2)). \tag{2.10}$$

It can then be decomposed into its irreducible components as a representation of $G\times G$.

Theorem 2.1 (Peter–Weyl decomposition): Let G be a compact Lie group.

(1) There is an isomorphism

$$C_{\mathrm{alg}}(G)\cong\bigoplus_{\rho\in\mathcal{R}_G}(V_\rho\otimes V_\rho^*) \tag{2.11}$$

of representations of $G\times G$. Here the direct sum runs over the equivalence classes of finite-dimensional irreducible representations of G. The direct summands $V_\rho\otimes V_\rho^*$ are irreducible as representations of $G\times G$.

(2) The direct sum in (2.11) is orthogonal with respect to the L^2-scalar product on $C_{\mathrm{alg}}(G)$ which is formed using the Haar measure of G on the left-hand side, and using the standard scalar products on the right-hand side,

$$\langle t_{jk}^{(\rho)};t_{\ell m}^{(\sigma)}\rangle_{L^2}:=\int_G\overline{t_{jk}^{(\rho)}(g)}\cdot t_{\ell m}^{(\sigma)}(g)dg=\frac{1}{\dim V_\rho}\delta_{\rho\sigma}\delta_{j\ell}\delta_{km}, \tag{2.12}$$

where $\rho,\ \sigma\in\mathcal{R}_G$ are irreducible. The Haar measure is denoted by $\int_G$ and normalized so that $\int_G dg=1$.

If G is finite, the Haar measure coincides with the normalized summation over all group elements. The decomposition (2.11) directly corresponds to our notation of the representation functions $t_{jk}^{(\rho)}$ for irreducible $\rho\in\mathcal{R}_G$.

Corollary 2.2: Each representation function $f\in C_{\mathrm{alg}}(G)$ can be decomposed according to (2.11),

$$f(g)=\sum_{\rho\in\mathcal{R}_G}\sum_{j,k=1}^{\dim V_\rho}\hat{f}_{jk}^{(\rho)}t_{jk}^{(\rho)}(g),\quad\text{where}\ \ \hat{f}_{jk}^{(\rho)}=\dim V_\rho\int_G\overline{t_{jk}^{(\rho)}(g)}f(g)dg. \tag{2.13}$$

For any algebraic $f\in C_{\mathrm{alg}}(G)$, all except finitely many coefficients $f_{jk}^{(\rho)}$ are zero. The analytical aspects of $C_{\mathrm{alg}}(G)$ are given by the Peter–Weyl theorem.

Theorem 2.3 (Peter–Weyl theorem): Let G be a compact Lie group. Then $C_{\mathrm{alg}}(G)$ is dense in $L^2(G)$ with respect to the L^2-norm.

We use the Peter–Weyl theorem in order to complete $C_{\mathrm{alg}}(G)$ with respect to the L^2-norm to $L^2(G)$. Functions $f\in L^2(G)$ then correspond to square summable series in (2.13). These series are invariant under a reordering of summands, and their limits commute with group integrations. We make use of these invariances in the duality transformation. If G is a finite group, $C_{\mathrm{alg}}(G)$ is a finite-dimensional vector space so that the corresponding results hold trivially.

We can summarize these ideas and state that the algebraic structure of $C_{\mathrm{alg}}(G)$ is sufficient to determine the structure of the larger function space $L^2(G)$.

C. Character decomposition

The *characters* of G are the algebraic class functions, i.e., those functions $f\in C_{\mathrm{alg}}(G)$ that satisfy $f(hgh^{-1})=f(g)$ for all $g,\ h\in G$.

Proposition 2.4: For class functions $f\in C_{\mathrm{alg}}(G)$, the Peter–Weyl decomposition (2.13) specializes to the *character decomposition*

$$f(g)=\sum_{\rho\in\mathcal{R}_G}\hat{f}_\rho\chi^{(\rho)}(g),\quad\text{where}\ \ \hat{f}_\rho=\int_G\overline{\chi^{(\rho)}(g)}f(g)dg. \tag{2.14}$$

Here

$$\chi^{(\rho)} := \sum_{j=1}^{\dim V_\rho} t_{jj}^{(\rho)} \tag{2.15}$$

denotes the character of the representation $\rho \in \widetilde{\mathcal{R}}_G$. For irreducible ρ, $\sigma \in \mathcal{R}_G$, the orthogonality relation (2.12) implies

$$\langle \chi^{(\rho)}; \chi^{(\sigma)} \rangle_{L^2} = \int_G \overline{\chi^{(\rho)}(g)} \chi^{(\sigma)}(g) dg = \delta_{p\sigma}. \tag{2.16}$$

D. Algebraic evaluation of group integrals

For the duality transformation, it is important to understand the Haar measure of G in the picture of the Peter–Weyl decomposition (2.11). First we decompose a generic representation function into representation functions of irreducible representations.

Proposition 2.5: Let G be a compact Lie group and $\rho \in \widetilde{\mathcal{R}}_G$ be a finite-dimensional unitary representation of G with the complete decomposition

$$V_\rho \cong \bigoplus_{j=1}^{k} V_{\tau_j}, \quad \tau_j \in \mathcal{R}_G, k \in \mathbb{N}, \tag{2.17}$$

into irreducible components τ_j. Let $P^{(j)}: V_\rho \to V_{\tau_j} \subseteq V_\rho$ be the G-invariant orthogonal projectors associated with the above decomposition. Then

$$t_{mn}^{(\rho)}(g) = \sum_{j=1}^{k} \sum_{p,q=1}^{\dim V_{\tau_j}} \overline{P_{pm}^{(j)}} t_{pq}^{(\tau_j)}(g) P_{qn}^{(j)}, \tag{2.18}$$

where $P_{qn}^{(j)} = \langle w_q^{(j)}; v_n \rangle$. Here $\{v_i\}_i$ denotes an orthonormal basis of V_p and $\{w_i^{(j)}\}_i$ an orthonormal basis of $V_{\tau_j} \subseteq V_\rho$.

Proof: The representation function is Peter–Weyl decomposed by inserting $\mathbb{1} = \Sigma_{j=1}^{k} P^{(j)}$ twice into the right-hand side of $t_{mn}^{(\rho)}(g) = \langle v_m; \rho(g) v_n \rangle$. We use G-invariance $[P^{(j)}, \rho(g)] = 0$ and transversality $P^{(i)} P^{(j)} = \delta_{ij} P^{(j)}$ in order to obtain

$$t_{mn}^{(\rho)}(g) = \sum_{j=1}^{k} \langle v_m; P^{(j)} \rho(g) P^{(j)} v_n \rangle. \tag{2.19}$$

Here $\rho(g) P^{(j)} = \tau_j(g) P^{(j)}$ and

$$P^{(j)} = \sum_{p=1}^{\dim V_{\tau_j}} w_p^{(j)} \cdot \vartheta^{(j)p}, \tag{2.20}$$

where $\{\vartheta^{(j)i}\}_i$ denotes a basis dual to $\{w_i^{(j)}\}_i$. Inserting (2.20) into (2.19), we obtain (2.18). □

For representation functions of an irreducible representation $\rho \in \mathcal{R}_G$, the Haar measure is

$$\int_G t_{jk}^{(\rho)}(g) dg = \begin{cases} 1, & \text{if } \rho \text{ is trivial,} \\ 0, & \text{otherwise,} \end{cases} \tag{2.21}$$

as a consequence of its left–right translation invariance. This can be applied to (2.18) in order to derive an entirely algebraic expression for the Haar measure.

Corollary 2.6: Let G be a compact Lie group and $\rho \in \widetilde{\mathcal{R}}_G$ be a finite-dimensional unitary representation of G with the decomposition (2.17). Assume that precisely the first ℓ components $\tau_1,\ldots,\tau_\ell$, $0 \leqslant \ell \leqslant k$, are equivalent to the trivial representation. Then the Haar measure of a representation function $t^{(\rho)}_{mn}$, $1 \leqslant m,\ n \leqslant \dim V_\rho$, is given by

$$\int_G t^{(\rho)}_{mn}(g)dg = \sum_{j=1}^{\ell} \overline{P^{(j)}_m} P^{(j)}_n . \tag{2.22}$$

Here we have omitted the vector indices corresponding to the one-dimensional representations.

In our calculations, we will refer to Corollary 2.6 in a context in which the integrand is a product of representation functions of irreducible representations. This motivates the following definition.

Definition 2.7: Let G be a compact Lie group and $\rho_1,\ldots,\rho_r \in \mathcal{R}_G$, $r \in \mathbb{N}$, be finite-dimensional irreducible representations of G. The *Haar intertwiner*,

$$T: \bigotimes_{\ell=1}^{r} V_{\rho_\ell} \to \bigotimes_{\ell=1}^{r} V_{\rho_\ell}, \tag{2.23a}$$

is the linear map defined by its matrix elements

$$T_{m_1 m_2 \ldots m_r ; n_1 n_2 \ldots n_r} := \int_G t^{(\rho_1)}_{m_1 n_1}(g) t^{(\rho_2)}_{m_2 n_2}(g) \cdots t^{(\rho_r)}_{m_r n_r}(g) dg. \tag{2.23b}$$

Proposition 2.8: The Haar intertwiner T of (2.23) satisfies

$$T_{m_1 m_2 \ldots m_r ; n_1 n_2 \ldots n_r} = \sum_j \overline{P^{(j)}_{m_1 m_2 \ldots m_r}} P^{(j)}_{n_1 n_2 \ldots n_r}, \tag{2.24}$$

for the projectors

$$P^{(j)}_{n_1 n_2 \ldots n_r} := \langle w^{(j)}; e^{(\rho_1)}_{n_1} \otimes e^{(\rho_2)}_{n_2} \otimes \cdots \otimes e^{(\rho_r)}_{n_r} \rangle, \tag{2.25}$$

with the definitions of Proposition 2.5, as well as for all $h \in G$,

$$T = (\rho_1(h) \otimes \cdots \otimes \rho_r(h)) \circ T = T \circ (\rho_1(h) \otimes \cdots \otimes \rho_r(h)), \tag{2.26}$$

$$T \circ T = T. \tag{2.27}$$

The first equation (2.24) is a consequence of Corollary 2.6 while (2.26) and (2.27) follow from the translation invariance of the Haar measure. In particular, T forms a morphism of representations (*intertwiner*) of G. The map T has been studied in a more general context in Ref. 18.

In the subsequent sections, we will apply Corollary 2.6 in rather complicated calculations. It is therefore convenient to introduce diagrams which visualize the structure of the indices in these formulas (Fig. 1).

The diagrams are read from top to bottom. We draw directed lines which are labeled with representations $\rho \in \widetilde{\mathcal{R}}_G$ of G. If the arrow points down, the line denotes the identity map of V_p [Fig. 1(a)]. If the arrow points up, it refers to the identity map of the dual representation V^*_ρ. A representation function $t^{(\rho)}_{mn}$ is denoted by a box with an incoming and an outgoing line (b), and a product of representation functions by boxes placed next to each other (c). The Haar intertwiner is visualized by the box labeled T in (d), and the calculation of T given by (2.23b) is shown in diagram (e) where the full dots represent the projectors, and the dotted line indicates the simultaneous summation over them.

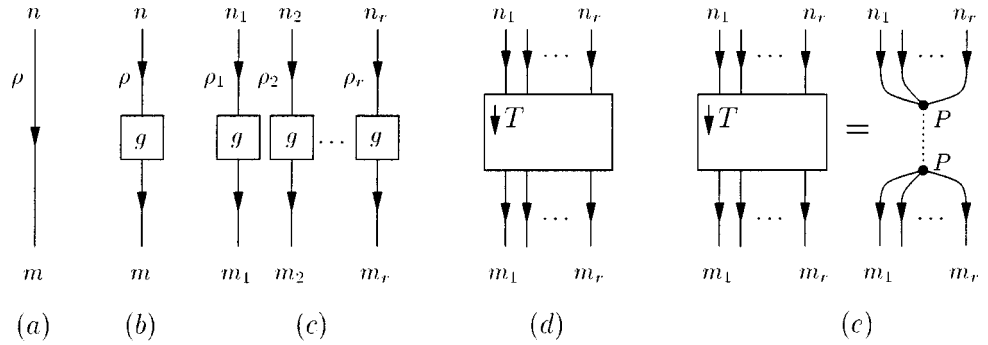

FIG. 1. Diagrams to visualize the index structure in the calculation of group integrals. (a) The identity map of V_ρ; (b) a representation function $t^{(\rho)}_{mn}$; (c) a product of representation functions $t^{(\rho_1)}_{m_1n_1}\cdots t^{(\rho_r)}_{m_rn_r}$; (d) the Haar intertwiner; and (e) the calculation of the Haar intertwiner (2.23b).

E. Coset spaces and spherical functions

In the study of coset spaces G/H, we allow H to be any Lie subgroup of G. First we recall some basic definitions.

Definition 2.9: Let G be a compact Lie group and $H\leqslant G$ be a Lie subgroup.

(1) A finite-dimensional irreducible representation V_ρ of G is said to be of *class-1 with respect to H* if V_ρ contains an H-invariant vector $0\neq v_0\in V_\rho$, i.e., $\rho(h)v_0=v_0$ for all $h\in H$. The subset $\mathcal{R}_H^G\subseteq\mathcal{R}_G$ denotes the set of class-1 representations of G with respect to H.

(2) H is called a *massive* subgroup of G if for each class-1 representation $\rho\in\mathcal{R}_H^G$, the subspace of H-invariant vectors,

$$\mathrm{Inv}_H^{(\rho)}=\{v\in V_\rho:\ \rho(h)v=v\quad\text{for all}\ \ h\in H\},\tag{2.28}$$

is one-dimensional.

Proposition 2.10: Let G be a compact Lie group, $H\leqslant G$ a Lie subgroup, and $\rho\in\mathcal{R}_G$ a finite-dimensional irreducible representation of G. The subspace of H-invariant vectors in V_ρ is spanned by the (not necessarily linearly independent) vectors

$$v^{(k)}:=\sum_{j=1}^{\dim V_\rho} v_j^{(k)}e_j:\quad\text{where}\ \ v_j^{(k)}:=\int_H t^{(\rho)}_{jk}(h)\,dh.\tag{2.29}$$

Here $\{e_j\}_j$ denotes the standard orthonormal basis of V_ρ, and $1\leqslant k\leqslant\dim V_\rho$.

The motivation for studying H-invariant vectors is given by the following result which allows us to construct functions on the space G/H of left cosets, i.e., functions on G that are constant on the cosets gH.

Proposition 2.11: Let $0\neq v^{(k)}\in V_\rho$ be an H-invariant vector. Then the *generalized spherical functions*

$$H^{(\rho)}_{jk}(g):=\sum_{\ell=1}^{\dim V_\rho} t^{(\rho)}_{j\ell}(g)v^{(k)}_\ell,\tag{2.30}$$

$1\leqslant j\leqslant\dim V_\rho$, are constant on the cosets $gH\in G/H$ and therefore induce functions $H^{(\rho)}_{jk}:G/H\to\mathbb{C}$, $x\mapsto H^{(\rho)}_{jk}(x):=H^{(\rho)}_{jk}(g_x)$, where $g_x\in G$ is a representative of the coset $x=g_xH\in G/H$.

Combining the Peter–Weyl decomposition (2.13) of $C_{\mathrm{alg}}(G)$ with the above ideas, we can construct the algebraic functions $C_{\mathrm{alg}}(G/H)$ on the coset space.

Corollary 2.12: Let G be a compact Lie group and $H\leqslant G$ be a Lie subgroup. Denote the dimensions of the H-invariant subspaces by $\kappa_\rho:=\dim\mathrm{Inv}_H^{(\rho)}$ and choose the orthonormal basis $\{e_j\}_j$ of each V_ρ so that precisely $e_1,\ldots,e_{\kappa_\rho}$ are H-invariant. Then the functions

$$H^{(\rho)}_{jk}: G/H \to \mathbb{C}, \quad x \mapsto H^{(\rho)}_{jk}(x) := t^{(\rho)}_{jk}(g_x), \tag{2.31}$$

$\rho \in \mathcal{R}^G_H$, $1 \leqslant j \leqslant \dim V_\rho$, $1 \leqslant k \leqslant \kappa_\rho$, form a basis of $C_{\text{alg}}(G/H)$. These functions satisfy the orthogonality relation,

$$\langle H^{(\rho)}_{jk}; H^{(\sigma)}_{\ell m} \rangle_{L^2} = \int_{G/H} \overline{H^{(\rho)}_{jk}(x)} H^{(\sigma)}_{\ell m}(x) dx = \frac{1}{\dim V_\rho} \delta_{\rho\sigma} \delta_{j\ell} \delta_{km}. \tag{2.32}$$

Remark 2.13: (1) Spherical functions exist only for class-1 representations as $\kappa_\rho \neq 0$ only there.

(2) In the case of a massive subgroup H, there is $\kappa_\rho = 1$ for all class-1 representations $\rho \in \mathcal{R}^G_H$. The second index of the spherical functions can thus be omitted, i.e.,

$$H^{(\rho)}_{j}: G/H \to \mathbb{C}, \quad x \mapsto H^{(\rho)}_{j}(x) := t^{(\rho)}_{j1}(g_x), \tag{2.33}$$

where $1 \leqslant j \leqslant \dim V_\rho$.

(3) If $H \trianglelefteq G$ is a normal subgroup, there is $\kappa_\rho = \dim V_\rho$ for all class-1 representations. In other words, for a given irreducible representation $\rho \in \mathcal{R}_G$ of G, either all representation functions $t^{(\rho)}_{jk}$, $1 \leqslant j, k \leqslant \dim V_\rho$, are spherical functions, or none of them is.

Example 2.14: (1) The spheres $S^N \cong \mathrm{SO}(N+1)/\mathrm{SO}(N)$ or $S^N \cong \mathrm{O}(N+1)/\mathrm{O}(N)$ are formed using massive subgroups.

(2) Odd spheres can alternatively be obtained from $S^{2N+1} \cong \mathrm{SU}(N+1)/\mathrm{SU}(N)$ or $S^{2N+1} \cong \mathrm{U}(N+1)/\mathrm{U}(N)$, in particular $S^3 \cong \mathrm{SU}(2)$. The spherical functions of S^3 can thus be constructed either as functions on SO(4)/SO(3) using the construction sketched above or from the identification $S^3 \cong \mathrm{SU}(2)$. For the latter approach, see the introductory part of Ref. 23.

(3) Other coset spaces which are of interest in the context of sigma models are $\mathbb{RP}^{N-1} \cong \mathrm{O}(N)/(\mathrm{O}(N-1) \times \mathrm{O}(1))$ as a special case of the Grassmanian $G^{\mathbb{R}}_{kN} \cong \mathrm{O}(N)/(\mathrm{O}(N-k) \times \mathrm{O}(k))$ and their complex counterparts $\mathbb{CP}^{N-1} \cong \mathrm{U}(N)/(\mathrm{U}(N-1) \times \mathrm{U}(1))$ and $G^{\mathbb{C}}_{kN} \cong \mathrm{U}(N)/(\mathrm{U}(N-k) \times \mathrm{U}(k))$.

Remark 2.15: Any function $f: G/H \to \mathbb{C}$ naturally extends to a function $\widetilde{f}: G \to \mathbb{C}$ which is constant on the cosets, i.e., $\widetilde{f}(gh) = \widetilde{f}(g)$ for all $g \in G$, $h \in H$. Obviously $f(x) = \widetilde{f}(g_x)$ for all $x \in G/H$ and an arbitrary representative $g_x \in G$ of x. Integrals over G/H can thus be evaluated using integrals over G,

$$\int_{G/H} f(x) dx = \int_G \widetilde{f}(g) dg. \tag{2.34}$$

As the context is usually clear, we omit the tilde ($\widetilde{\ }$) from now on.

The analog of the Haar intertwiner (2.23) for coset spaces can be defined as follows.

Definition 2.16: Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup, and $\rho_1, \ldots, \rho_r \in \mathcal{R}^G_H$, $r \in \mathbb{N}$, be of class-1 with respect to H. The *coset space Haar map*,

$$I: \bigotimes_{\ell=1}^{r} V_{\rho_\ell} \to \bigotimes_{\ell=1}^{r} V_{\rho_\ell}, \tag{2.35a}$$

is the linear map defined by its matrix elements

$$I_{m_1 m_2 \ldots m_r ; n_1 n_2 \ldots n_r} := \int_{G/H} H^{(\rho_1)}_{m_1 n_1}(x) H^{(\rho_2)}_{m_2 n_2}(x) \cdots H^{(\rho_r)}_{m_r n_r}(x) dx, \tag{2.35b}$$

where $1 \leqslant m_\ell \leqslant \dim V_{\rho_\ell}$ and $1 \leqslant n_\ell \leqslant \kappa_{\rho_\ell}$.

Proposition 2.17: The coset space Haar map (2.35) satisfies

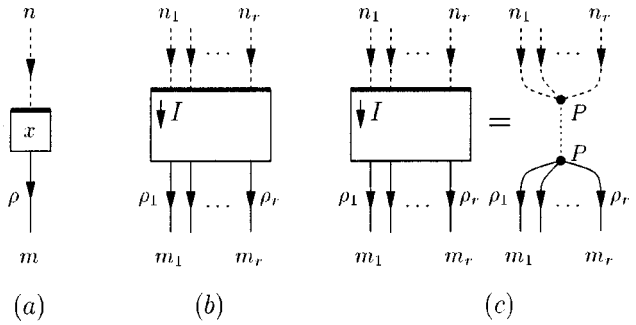

FIG. 2. (a) A spherical function $H^{(\rho)}_{mn}(x)$; (b) the coset space Haar map; and (c) its calculation in terms of G-invariant projectors (2.36), see Proposition 2.17.

$$I_{m_1 m_2 \ldots m_r ; n_1 n_2 \ldots n_r} = \sum_j \overline{P^{(j)}_{m_1 m_2 \ldots m_r}} P^{(j)}_{n_1 n_2 \ldots n_r}, \tag{2.36}$$

with the notation of Proposition 2.8, as well as for all $h \in G$,

$$I = (\rho_1(h) \otimes \cdots \otimes \rho_r(h)) \circ I, \tag{2.37}$$

which makes use of the left action of G on G/H. If in addition $H \trianglelefteq G$ is a normal subgroup, then I satisfies for all $y \in G/H$,

$$I = I \circ (\rho_1(y) \otimes \cdots \otimes \rho_r(y)), \tag{2.38}$$

using the notation $\rho_\ell(y) := \rho_\ell(g_y)$ for any representative g_y of y.

Proof: Equations (2.36) and (2.37) follow from Proposition 2.8 and Remark 2.15. The same is true for (2.38) if we write it for a representative of the coset $y \in G/H$. □

Observe that the coset space Haar map is in general not an intertwiner of G. However, for any fixed choice of indices $n_\ell \in \{1,\ldots,\kappa_{\rho_\ell}\}$, it defines a G-invariant vector $\tilde{I}_{n_1 n_2 \ldots n_r} \in \otimes_{\ell=1}^r V_{\rho_\ell}$.

We visualize spherical functions $H^{(\rho)}_{mn}(x)$ and the coset space Haar map as in Fig. 2. The contraction of indices whose range is restricted to $\{1,\ldots,\kappa_\rho\}$ is represented by dashed lines. They do not correspond to representations of G and are therefore not labeled with any symbol such as ρ. A thick line in the box for $H^{(\rho)}_{mn}$ and in the coset space Haar map I indicates that the indices on this side are special. Figure 2(c) shows the calculation (2.36).

If $H \trianglelefteq G$ is a normal subgroup, $\kappa_\rho = \dim V_\rho$ for all class-1 representations so that the dashed lines become solid again as they do correspond to representations of G. In particular Definition 2.16 and Proposition 2.17 restrict to Definition 2.7 and Proposition 2.8, respectively, if $H = \{e\}$ is the trivial group. The special case when H is a massive subgroup is also of interest.

Corollary 2.18: If $H \leqslant G$ is a massive subgroup, then $\kappa_\rho = 1$ for the class-1 representations. Therefore all indices n_ℓ can be omitted from the expressions so that the Haar map reduces to a map

$$I : \mathbb{C} \to \bigotimes_{\ell=1}^r V_{\rho_\ell}, \tag{2.39}$$

defined by its matrix elements

$$I_{m_1 m_2 \ldots m_r} := \int_{G/H} H^{(\rho_1)}_{m_1}(x) H^{(\rho_2)}_{m_2}(x) \cdots H^{(\rho_r)}_{m_r}(x) dx. \tag{2.40}$$

Equation (2.36) specializes to

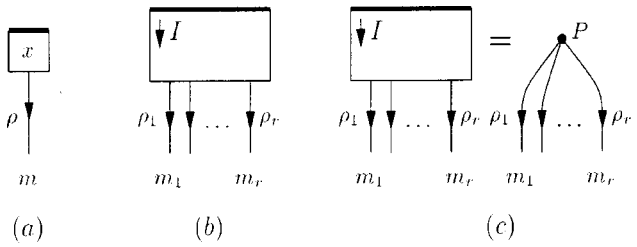

FIG. 3. The specialization of Fig. 2 to the case of a massive subgroup $H \leqslant G$, see Corollary 2.18.

$$I_{m_1 m_2 \ldots m_r} = \sum_j \overline{P^{(j)}_{m_1 m_2 \ldots m_r}}, \tag{2.41}$$

and (2.37) indicates that I defines a G-invariant vector $I \in \otimes_{\ell=1}^{r} V_{\rho_\ell}$.

The situation for massive subgroups is illustrated in Fig. 3. Further properties of the diagrams used in Fig. 3 can be deduced as in the introductory section of Ref. 23.

F. The center of the group

If representation functions are restricted to the center $Z(G)$, we obtain representation functions of the Abelian group $Z(G)$.

Lemma 2.19: Let G be a compact Lie group and $X \in Z(G)$. Then for any irreducible unitary representation ρ of G and $1 \leqslant i,\ j \leqslant \dim V_\rho$,

$$t^{(\rho)}_{ij}(X) = \delta_{ij} \cdot \tilde{t}^{(\rho)}(X), \tag{2.42}$$

where $\tilde{t}^{(\rho)}: Z(G) \to \mathbb{C}$ is a representation of the center $Z(G)$ which is induced by ρ.

Proof: By Schur's lemma, the center is mapped to multiples of the unit matrix. □

G. Special properties of some groups

For $G = U(1)$, all finite-dimensional irreducible representations are one-dimensional. They are denoted by $V_k \cong \mathbb{C}$ and characterized by integers $k \in \mathbb{Z}$ (wave numbers of the Fourier series). In the unitary case, their representation functions are given by $t^{(k)}(g) = g^k$, $g \in \mathrm{U}(1)$, and their duals by $t^{(k^*)}(g) = g^{-k}$. All representation functions are characters, $\chi^{(k)}(g) = t^{(k)}(g) = e^{ik\varphi}$, where we write $g = e^{i\varphi} \in \mathrm{U}(1)$.

From the representation functions and the definition (2.5), we can calculate the tensor product which is again one-dimensional,

$$V_{k_1} \otimes \cdots \otimes V_{k_n} \cong V_{\Sigma_{\ell=1}^n k_\ell}. \tag{2.43}$$

It is isomorphic to the trivial representation if and only if

$$\sum_{\ell=1}^{n} k_\ell = 0. \tag{2.44}$$

Since all irreducible representations are one-dimensional, the Haar intertwiner (2.23),

$$T: \bigotimes_{\ell=1}^{r} V_{k_\ell} \to \bigotimes_{\ell=1}^{r} V_{k_\ell}, \tag{2.45}$$

is just multiplication by a number. We have $T = 1$ if (2.44) holds and $T = 0$ otherwise. The sum over projectors (2.24) is either empty or contains a single unique term.

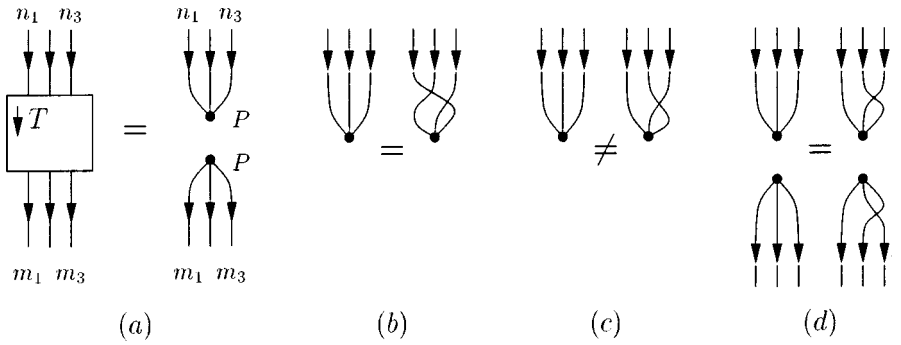

FIG. 4. (a) Simplification of (2.24) for $G=\mathrm{SU}(2)$ in the case of three tensor factors; (b)–(d) Even if we do not write the dotted line anymore, this does not mean that any conceivable symmetry holds.

We write the elements of the cyclic groups $G=\mathbb{Z}_N$ as roots of unity, $e^{2\pi i\ell/N}$, $\ell\in\{0,\ldots,N-1\}$, and parametrize their finite-dimensional irreducible unitary representations $V_k\cong\mathbb{C}$ by $k\in\{0,\ldots,N-1\}$. Representation functions and characters are $t^{(k)}(g)=g^k$, $t^{(k^*)}(g)=g^{-k}$, $\chi^{(k)}=t^{(k)}$, and (2.43) and (2.44) still hold if the sums are taken modulo N.

For $G=\mathrm{SU}(2)$, we characterize the finite-dimensional irreducible representations V_j, $\dim V_j=2j+1$, by non-negative half-integers $j\in 1/2\mathbb{N}_0$. Parametrizing elements of SU(2) by

$$g(\vartheta,\underline{n})=\mathbb{1}\cos\frac{\vartheta}{2}+i\underline{\sigma}\cdot\underline{n}\sin\frac{\vartheta}{2}, \tag{2.46}$$

where $\vartheta\in[0,4\pi)$, $\underline{n}\in S^2\subseteq\mathbb{R}^3$ and $\underline{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are the Pauli matrices, the characters are given by

$$\chi^{(j)}(g)=\frac{\sin((2j+1)\vartheta/2)}{\sin\vartheta/2}, \tag{2.47}$$

in particular for the fundamental representation $\chi^{(1/2)}(g)=\cos\vartheta/2$.

Since for SU(2) there are no higher multiplicities in the decomposition of $V_{j_1}\otimes V_{j_2}$, the space of invariant projectors $V_{j_1}\otimes V_{j_2}\otimes V_{j_3}\to\mathbb{C}$ has a dimension of at most one. For three irreducible representations, we can therefore omit the summation over projectors from (2.24) as is illustrated in Fig. 4(a) and impose the conditions $|j_1-j_2|\leqslant j_3\leqslant j_1+j_2$, etc. instead. This provides a substantial simplification. However, the three-valent vertex that appears there has in general only a cyclic but not a full symmetry [Figs. 4(b)–4(d)] so that one still has to take the ordering of the tensor factors into account. Neglecting this subtlety is a common mistake.

H. Some character decompositions

For the duality transformation, we will apply the character decomposition to the Boltzmann weight $f(g)=\exp(-s(g))$ whose local action $s:G\to\mathbb{R}$ is an L^2-integrable class function that is bounded below. The most common example is the *Wilson action*,

$$s(g)=-\frac{\beta}{2\dim V_\rho}(\chi^{(\rho)}(g)+\overline{\chi^{(\rho)}(g)}), \tag{2.48}$$

where ρ denotes the fundamental representation of G and β is the inverse temperature or inverse coupling constant.

For $G=\mathrm{U}(1)$, the Wilson action reads $s(g)=-\beta\cos\varphi$, $g=e^{i\varphi}$. The character decomposition coincides with the Fourier series,

$$f(g)=\sum_{k=-\infty}^{\infty}\hat{f}_k e^{ik\varphi},\quad \hat{f}_k=\frac{1}{2\pi}\int_{\theta}^{2\pi}e^{-ik\varphi}\exp(-s(e^{i\varphi}))d\varphi=I_k(\beta),\tag{2.49}$$

where $I_k(\beta)$ denote modified Bessel functions.

For $G=\mathbb{Z}_N$, $g=e^{2\pi i\ell/N}$, we write this decomposition as

$$f(g)=\sum_{k=1}^{N-1}\hat{f}_k e^{2\pi ik\ell/N},\quad \hat{f}_k=\frac{1}{N}\sum_{\ell=0}^{N-1}e^{-2\pi ik\ell/N}\exp(-s(e^{2\pi i\ell/N})).\tag{2.50}$$

For $G=\mathrm{SU}(2)$, we have the Wilson action $s(g)=-\beta\cos\vartheta/2$, and the character expansion of $f(g)=\exp(-s(g))$ is given by

$$f(g)=\sum_{j\in(1/\nu)\mathbb{N}_0}\hat{f}_j\frac{\sin((2j+1)\vartheta/2)}{\sin\vartheta/2},\quad \hat{f}_j=\frac{2j+1}{\beta}I_{2j+1}(\beta).\tag{2.51}$$

Another common action is the *heat kernel* or *generalized Villain action* which is given for any compact Lie group in terms of the character decomposition of the corresponding Boltzmann weight,

$$f(g)=\sum_{\rho\in\mathcal{R}_G}\hat{f}_\rho\chi^{(\rho)}(g),\quad \hat{f}_\rho=\dim V_\rho\cdot\exp\left(-\frac{C_\rho}{2\beta}\right),\tag{2.52}$$

where C_ρ denotes the eigenvalue of a quadratic Casimir operator in the representation ρ. For example, we have for $G=\mathrm{U}(1)$,

$$\hat{f}_k=\exp\left(-\frac{k^2}{2\beta}\right),\tag{2.53}$$

and for $G=\mathrm{SU}(2)$,

$$\hat{f}_j=(2j+1)\exp\left(-\frac{j(j+1)}{2\beta}\right).\tag{2.54}$$

In all these cases, the Boltzmann weight $f(g)=\exp(-s(g))$ has a sharp peak at the group unit if β is large (weak coupling, low temperature) which facilitates a perturbative treatment whereas the peak is very wide for small β (strong coupling, high temperature). For small β, however, the dominant contribution to the character expansions listed above originates from the ''small'' representations of G. An expansion in terms of irreducible representations of G therefore provides us with a strong coupling expansion. This is most obvious for the heat kernel action where at small β the representations with small Casimir eigenvalue dominate.

More details on strong coupling expansion techniques can be found in Ref. 7. For spherical functions, see Ref. 22 and in particular for S^N also Ref. 24.

III. NOTATION AND DEFINITIONS

A. Graphs and abstract two-complexes

In order to formulate sigma models and gauge theories on very general lattices, it is sufficient to focus on the combinatorial structure of the lattices rather than on the details of their embedding into some space or space–time manifold. Therefore we employ the notions of graphs and abstract two-complexes. Sigma models are defined on graphs so that we obtain the same expressions for their partition function in any dimension $d\geqslant 1$. Similarly, gauge theories are defined on abstract two-complexes, and we obtain a uniform description of gauge theories valid in any dimension $d\geqslant 2$.

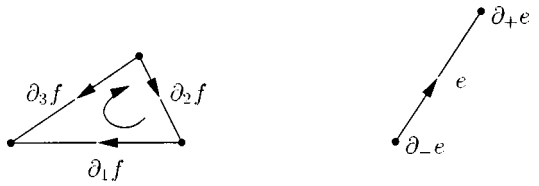

FIG. 5. The maps $\partial_\pm$, ∂_j and ϵ_j and the conditions (3.3). Here $N(f)=3$, $\epsilon_1 f=+1$, $\epsilon_2 f=+1$ and $\epsilon_3 f=(-1)$.

The following definitions differ slightly from what is standard, but will prove most convenient for the purpose of the duality transformation.

Definition 3.1: An *oriented* (or *directed*) *graph* (V,E) consists of finite sets V (vertices) and E (edges) together with maps

$$\partial_+ : E \to V \quad \text{(end point of an edge)}, \tag{3.1a}$$

$$\partial_- : E \to V \quad \text{(starting point of an edge)}. \tag{3.1b}$$

The notion of an abstract two-complex extends this definition and also includes faces whose boundary consists of a sequence of edges.

Definition 3.2: An *oriented two-complex* (V,E,F) is an oriented graph (V,E) together with a finite set F (*faces*) and maps

$$N : F \to \mathbb{N} \quad \text{(number of edges in the boundary of a face)}, \tag{3.2a}$$

$$\partial_j : F \to E \quad \text{(the } j\text{th edge in the boundary of a face)}, \tag{3.2b}$$

$$\epsilon_j : F \to \{-1,+1\} \quad \text{(its orientation)}, \tag{3.2c}$$

such that

$$\partial_{-\epsilon_j f} \partial_j f = \partial_{\epsilon_{j+1} f} \partial_{j+1} f, \quad 1 \leqslant j \leqslant N(f)-1, \tag{3.3a}$$

$$\partial_{-\epsilon_{N(f)} f} \partial_{N(f)} f = \partial_{\epsilon_1 f} \partial_1 f, \tag{3.3b}$$

for all $f \in F$.

The conditions (3.3) state that the edges in the boundary of a face $f \in F$ are in cyclic ordering from $\partial_{N(f)} f$ to $\partial_1 f$ where one encounters the edges with the orientation given by $\epsilon_j f$ (see Fig. 5). Observe that (3.3) contains combinatorial information similar to the condition $\partial \circ \partial = 0$ on the boundary operator ∂ in Abelian simplicial homology.

In the subsequent calculations, it is convenient to use the following abbreviations.

Definition 3.3: Let (V,E,F) denote an oriented two-complex. For a given edge $e \in E$, the sets

$$e_+ := \{f \in F:\ e = \partial_j f,\ \epsilon_j f = (+1) \quad \text{for some } j,\ 1 \leqslant j \leqslant N(f)\}, \tag{3.4a}$$

$$e_- := \{f \in F:\ e = \partial_j f,\ \epsilon_j f = (-1) \quad \text{for some } j,\ 1 \leqslant j \leqslant N(f)\}, \tag{3.4b}$$

contain all faces that have the edge e in their boundary with positive $(+)$ or negative $(-)$ orientation, and we write $\delta e := e_+ \cup e_-$ for the coboundary of an edge $e \in E$. For a given face $f \in F$, the set

$$f_0 := \{v \in V:\ v = \partial_- \partial_j f \quad \text{for some } j,\ 1 \leqslant j \leqslant N(f)\} \tag{3.5}$$

denotes all vertices that belong to the boundary of the face f. Finally, the sets

$$f_+ := \{e \in E:\ e = \partial_j f,\ \epsilon_j f = (+1) \quad \text{for some } j,\ 1 \leqslant j \leqslant N(f)\}, \tag{3.6a}$$

$$f_- := \{e \in E:\ e = \partial_j f,\ \epsilon_j f = (-1) \quad \text{for some } j,\ 1 \leqslant j \leqslant N(f)\}, \tag{3.6b}$$

contain all edges in the boundary of the face f that occur with positive $(+)$ or negative $(-)$ orientation, and $\partial f := f_+ \cup f_-$ denotes the full boundary of $f \in F$.

We have formulated our definitions of graphs and two-complexes so that they have only a finite number of vertices, edges, and faces. This condition ensures that our partition functions are well defined. The collections of points, links, and plaquettes of standard hyper-cubic lattices form a special case of oriented two-complexes in the obvious manner.

B. Spin networks and spin foams

Spin networks were introduced by Penrose[25] in the context of a quantization of space–time geometry. A spin network with symmetry group G is a graph together with a coloring of its edges with irreducible representations of G and a coloring of its vertices with compatible intertwiners (representation morphisms). For the subsequent calculations it is most convenient to separate the notions of graph and coloring and to speak of a *spin network* that *lives on a graph*.

Definition 3.4: Let G be a compact Lie group and (V,E) be an oriented graph. A *spin network* (τ,Q) with symmetry group G on (V,E) is a coloring of the edges with irreducible representations of G,

$$\tau: E \to \mathcal{R}_G, \quad e \mapsto \tau_e, \tag{3.7a}$$

together with a coloring of the vertices $v \in V$ with compatible intertwiners,

$$Q^{(v)} \in \mathrm{Hom}_G\left(\bigotimes_{\substack{e \in E:\\ v = \partial_+ e}} V_{\tau_e},\ \bigotimes_{\substack{e \in E:\\ v = \partial_- e}} V_{\tau_e} \right). \tag{3.7b}$$

The tensor product in the domain is over the ''incoming'' edges and that in the image over the ''outgoing'' edges.

Spin networks appeared first in the context of quantum gravity. There they define, for example, the physical states in the loop formulation of gauge theories and the kinematical states of loop quantum gravity.[26] The observables of non-Abelian lattice gange theory can also be constructed from spin networks.[15,16] They are given by the *spin network functions* (Definition 6.3 below).

The concept of a spin network can be generalized by introducing additional representations at the vertices, called *charges*, and by modifying the compatibility condition (3.7b) accordingly.

Definition 3.5: Let G be a compact Lie group, (V,E) an oriented graph, and $\rho: V \to \mathcal{R}_G$, $v \mapsto \rho_v$ assign an irreducible representation of G to each vertex. A *spin network* (τ,Q,ρ) *with charges* ρ is a coloring of the edges with irreducible representations,

$$\tau: E \to \mathcal{R}_G, \quad e \mapsto \tau_e, \tag{3.8a}$$

together with a coloring of the vertices $v \in V$ with compatible intertwiners,

$$Q^{(v)} \in \mathrm{Hom}_G\left(\left(\bigotimes_{\substack{e \in E:\\ v = \partial_+ e}} V_{\tau_e} \right) \otimes V_{\rho_v},\ \bigotimes_{\substack{e \in E:\\ v = \partial_- e}} V_{\tau_e} \right). \tag{3.8b}$$

We show in this article that spin networks with charges appear as the configurations in the dual expression for correlators in sigma models, and that they characterize the observables of generalized Higgs models.

A higher dimensional analog of spin networks is the concept of spin foams. Spin foams also appeared first in the context of quantum gravity.[12–14]

Definition 3.6: Let G be a compact Lie group and (V,E,F) be an oriented two-complex. A *spin foam* (ρ,P) with symmetry group G on (V,E,F) is a coloring of the faces with finite-dimensional irreducible representations of G,

$$\rho:F\to\mathcal{R}_G,\quad f\mapsto\rho_f, \tag{3.9a}$$

together with a coloring of the edges $e\in E$ with compatible intertwiners,

$$P^{(e)}\in\mathrm{Hom}_G\Big(\bigotimes_{f\in e_+}\rho_f,\ \bigotimes_{f\in e_-}\rho_f\Big). \tag{3.9b}$$

The tensor product in the domain is over the representations at the ''incoming'' faces, that in the image over the ''outgoing'' ones. Incoming and outgoing are here defined by the relative orientations of the edges and faces.

These spin foams are often called *closed spin foams* as opposed to *open spin foams* which are bounded by a spin network. Open spin foams can be understood as the higher dimensional analog of spin networks with charges and are defined as follows.

Definition 3.7: Let G be a compact Lie group, (V,E,F) define an oriented two-complex, and (τ,Q) be a spin network on (V,E). A *spin foam* (ρ,P,τ,Q) *bounded by* the spin network (τ,Q) is a coloring of the faces with finite-dimensional irreducible representations,

$$\rho:F\to\mathcal{R}_G,\quad f\mapsto\rho_f, \tag{3.10a}$$

together with a coloring of the edges $e\in E$ with compatible intertwiners,

$$P^{(e)}\in\mathrm{Hom}_G\Big(\Big(\bigotimes_{f\in e_+}V_{\rho_f}\Big)\otimes V_{\tau_e},\ \bigotimes_{f\in e_-}V_{\rho_f}\Big). \tag{3.10b}$$

IV. THE CHIRAL MODEL

In this section, we develop the duality transformation for the chiral model with a symmetry group G that is a compact Lie group. This model forms the basis for the generalizations to the nonlinear sigma model with variables in a coset space G/H and to the generalized Higgs models in which the chiral model or the nonlinear sigma model is coupled to a lattice gauge theory.

A. Partition function

Definition 4.1: Let G be a compact Lie group and (V,E) be an oriented graph. Let $s:G\to\mathbb{R}$ be an L^2-integrable and bounded class function that satisfies $s(g^{-1})=s(g)$. The *lattice chiral model* with action s is defined by the partition function

$$Z=\Big(\prod_{v\in V}\int_G dg_v\Big)\prod_{e\in E}w(g_{\partial_+e}\cdot g_{\partial_-e}^{-1}), \tag{4.1}$$

whose *Boltzmann weight* is given by $w(g)=\exp(-s(g))$.

Remark 4.2: (1) The set of configurations is the product $G^V:=G\times\cdots\times G$ of one copy of G per vertex $v\in V$. The partition sum is just the Haar measure of G^V. There is an interaction term for each edge $e\in E$ relating the variables at the two end points, g_{∂_+e} and g_{∂_-e}.

(2) It is possible to choose different actions $s_e:G\to\mathbb{R}$ for each edge $e\in E$ so that one obtains Boltzmann weights $w_e(g)=\exp(-s_e(g))$. This is useful, for example, if one wishes to study inhomogeneous or anisotropic systems or nonregular lattices for which one would introduce geometric factors in order to compensate for the different lengths of the various edges. All calculations presented below generalize to this case, too, but we try to keep the notation simple and do not write down the additional index e in the following sections.

Lemma 4.3: Orientation reversal of any edge $e \in E$ is a symmetry of the lattice chiral model. The model therefore depends only on the unoriented graph. Orientation reversal of an edge $e \in E$ maps $g_{\partial_- e} \mapsto g_{\partial_+ e}$ and conversely, which leaves the action invariant since $s(g^{-1}) = s(g)$.

Our subsequent calculations are most transparent for the generic case in which the partition function can depend on the orientations even though this generality is not required for the common examples.

Proposition 4.4: The lattice chiral model (4.1) has got a global left–right $G \times G$-symmetry. Let $h, \tilde{h} \in G$. Then the transformation

$$g_v \mapsto h \cdot g_v \cdot \tilde{h}^{-1}, \tag{4.2}$$

for all $v \in V$, is a symmetry of the action $s(g_{\partial_+ e} \cdot g_{\partial_- e}^{-1})$ for each edge $e \in E$ because s is a class function.

B. Expectation values

The observables of the lattice chiral model are all possible expectation values of functions $G^V \to \mathbb{C}$ that are compatible with the symmetries. With the help of the Peter–Weyl decomposition, it is possible to calculate the generic form of these observables. For the chiral model, one obtains the well-known n-point functions. We present the full calculation here because it illustrates the method and this method generalizes to the more complicated models for which we derive new results in the subsequent sections.

Theorem 4.5: Each algebraic function $f: G^V \to \mathbb{C}$ that is compatible with the global $G \times G$-symmetry (4.2) is a linear combination of functions (*observables*) of the following type,

$$f_{\rho,P,Q}(\{g_v\}_{v \in V}) = \left(\prod_{v \in V} \sum_{\ell_v, m_v = 1}^{\dim V_{\rho_v}} \right) P_{\underbrace{\ell_v \ldots}_{v \in V}} Q_{\underbrace{m_v \ldots}_{v \in V}} \prod_{v \in V} t^{(\rho_v)}_{\ell_v m_v}(g_v). \tag{4.3}$$

Here

$$\rho: V \to \mathcal{R}_G, \quad v \mapsto \rho_v \tag{4.4}$$

associates an irreducible representation of G with each vertex, and

$$P: \bigotimes_{v \in V} V_{\rho_v} \to \mathbb{C}, \quad Q: \bigotimes_{v \in V} V^*_{\rho_v} \to \mathbb{C}, \tag{4.5}$$

are intertwiners of G.

Remark 4.6: (1) By the notation

$$\prod_{v \in V} \sum_{\ell_v, m_v = 1}^{\dim V_{\rho_v}} = \underbrace{\sum_{\ell_v, m_v = 1}^{\dim V_{\rho_v}} \cdots \sum_{\ell_v, m_v = 1}^{\dim V_{\rho_v}}}_{v \in V} \tag{4.6}$$

we mean that there is one sum over ℓ_v and m_v for each vertex $v \in V$. Similarly,

$$P_{\underbrace{\ell_v \cdots}_{v \in V}} \tag{4.7}$$

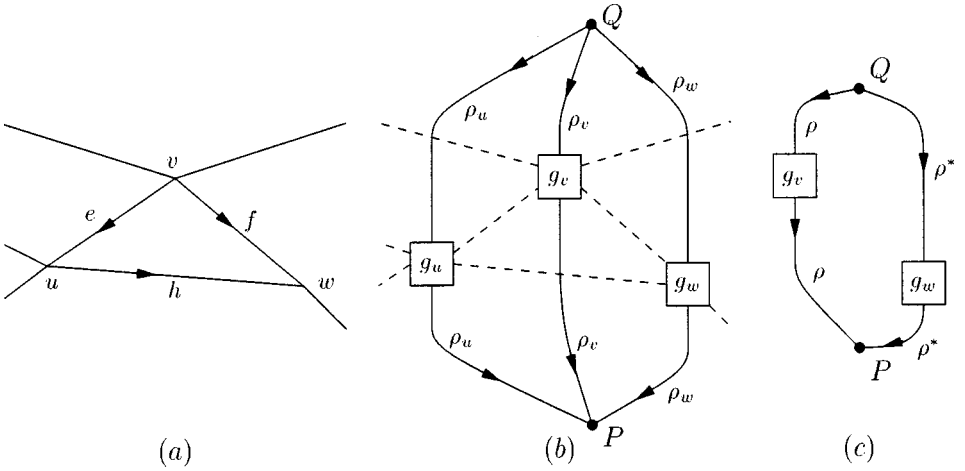

FIG. 6. (a) An oriented graph with vertices u, v, w and edges e, f, h. (b) The structure of the observable (4.3) of the lattice chiral model on that graph. (c) The two-point function (4.8).

indicates that the symbol P has got one index ℓ_v for each $v \in V$. It is also understood that the ordering of tensor factors in (4.5) corresponds to the ordering of indices of P and Q in (4.3). We use this notation frequently in the subsequent calculations.

(2) The structure of the observable (4.3) is illustrated in Fig. 6(b).

(3) The irreducible representations ρ_v describe the charges that are located at the vertices $v \in V$. If there are precisely k vertices whose ρ_v is nontrivial, the normalized expectation value of the observable is a k-point function. For each $v \in V$, there is a representation function $t^{(\rho_v)}_{\ell_v m_v}$ that describes the G-dependence of the observable, and the intertwiners P and Q involve its indices ℓ_v and m_v and are used in order to obtain a globally $G\times G$-invariant expression. The well-known two-point function for two vertices v, $w \in V$ is the normalized expectation value of

$$\chi^{(\rho)}(g_v \cdot g_w^{-1}) = \sum_{\ell_v, m_v = 1}^{\dim V_\rho} t^{(\rho)}_{\ell_v m_v}(g_v) \cdot t^{(\rho^*)}_{\ell_w m_w}(g_w) \cdot \delta_{\ell_v \ell_w} \delta_{m_v m_w} \tag{4.8}$$

[Fig. 6(c)]. It forms a special case of (4.3) in which the only nontrivial representations are a charge ρ at v and an anti-charge ρ^* at w, and the intertwiners are trivial, $P_{\ell_v \ell_w} = \delta_{\ell_v \ell_w}$, etc.

(4) As a consequence of the Peter–Weyl theorem, the L^2-integrable functions that are compatible with the global $G\times G$-symmetry are in the closure of the set of all algebraic $f_{\rho,P,Q}$, i.e., they can be obtained as limits of square summable series of functions $f_{\rho,P,Q}$.

Proof of Theorem 4.5: Algebraic functions $f: G^V \to \mathbb{C}$ are elements $f \in \otimes_{v \in V} C_{\mathrm{alg}}(G)$ and therefore have the Peter–Weyl decomposition

$$f(\{g_v\}_{v \in V}) = \left(\prod_{v \in V} \sum_{\rho_v \in \mathcal{R}_G} \right) \left(\prod_{v \in V} \sum_{j_v, k_v = 1}^{\dim V_{\rho_v}} \right) \hat{f}^{(\rho_v, \ldots)}_{j_v \ldots, k_v \ldots} \prod_{v \in V} t^{(\rho_v)}_{j_v k_v}(g_v). \tag{4.9}$$

If f satisfies the global $G\times G$-symmetry, we can apply (4.2) for each vertex, and as this holds for arbitrary h, $\tilde{h} \in G$, we can integrate the result over h and $\tilde{h}$,

$$\begin{aligned} f(\{g_v\}_{v \in V}) = \int_{G\times G} dh d\tilde{h} \left(\prod_{v \in V} \sum_{\rho_v \in \mathcal{R}_G} \right) \left(\prod_{v \in V} \sum_{j_v, k_v = 1}^{\dim V_{\rho_v}} \right) \hat{f}^{(\rho_v, \ldots)}_{j_v \ldots, k_v \ldots} \\ \times \prod_{v \in V} \sum_{\ell_v, m_v = 1}^{\dim V_{\rho_v}} t^{(\rho_v)}_{j_v \ell_v}(h) t^{(\rho_v)}_{\ell_v m_v}(g_v) t^{(\rho_v)}_{m_v k_v}(\tilde{h}^{-1}). \end{aligned} \tag{4.10}$$

We apply (2.9), writing $t^{(\rho_v)}_{m_v k_v}(\tilde{h}^{-1}) = t^{(\rho_v^*)}_{k_v m_v}(\tilde{h})$, and move all summations to the front of the expression. Then we sort the products by the arguments g_v, h, and $\tilde{h}$,

$$f(\{g_v\}_{v\in V}) = \left(\prod_{v\in V}\sum_{\rho_v\in\mathcal{R}_G}\right)\left(\prod_{v\in V}\sum_{j_v,k_v,\ell_v,m_v=1}^{\dim V_{\rho_v}}\right)\hat{f}^{(\rho_v,\ldots)}_{j_v\ldots,k_v\ldots}\left(\prod_{v\in V} t^{(\rho_v)}_{\ell_v m_v}(g_v)\right)$$
$$\times\left(\int_G\prod_{v\in V} t^{(\rho_v)}_{j_v\ell_v}(h)\,dh\right)\left(\int_G\prod_{v\in V} t^{(\rho_v^*)}_{k_v m_v}(\tilde{h})\,d\tilde{h}\right). \tag{4.11}$$

The integrals over G can be evaluated using (2.24) so that

$$f(\{g_v\}_{v\in V}) = \left(\prod_{v\in V}\sum_{\rho_v\in\mathcal{R}_G}\right)\sum_{P\in\mathcal{P}}\sum_{Q\in\mathcal{Q}}\left(\prod_{v\in V}\sum_{\ell_v,m_v=1}^{\dim V_{\rho_v}}\right)\tilde{f}^{(\rho_v,\ldots)}P_{\underbrace{\ell_v\ldots}_{v\in V}}Q_{\underbrace{m_v\ldots}_{v\in V}}\left(\prod_{v\in V} t^{(\rho_v)}_{\ell_v m_v}(g_v)\right), \tag{4.12}$$

where

$$\tilde{f}^{(\rho_v,\ldots)} = \left(\prod_{v\in V}\sum_{j_v,k_v=1}^{\dim V_{\rho_v}}\right)\hat{f}^{(\rho_v,\ldots)}_{j_v\ldots,k_v\ldots}\overline{P_{\underbrace{j_v\ldots}_{v\in V}}Q_{\underbrace{k_v\ldots}_{v\in V}}}. \tag{4.13}$$

Here $\mathcal{P}$ denotes a basis of the space of G-invariant projectors

$$\bigotimes_{v\in V} V_{\rho_v}\to\mathbb{C}, \tag{4.14}$$

whose elements $P\in\mathcal{P}$ are normalized so that $P^2=P$ where the trivial representation is embedded as $\mathbb{C}\subseteq\otimes_{v\in V}V_{\rho_v}$. Similarly, $\mathcal{Q}$ denotes a basis of G-invariant projectors

$$\bigotimes_{v\in V} V^*_{\rho_v}\to\mathbb{C}, \tag{4.15}$$

with the analogous normalization. The expression (4.12) is a linear combination of observables of the form (4.3). □

Remark 4.7: The global $G\times G$-symmetry can be realized as the translation symmetry of the multiple Haar measure because for each $v\in V$, h, $\tilde{h}\in G$ and any function $u\in C_{\text{alg}}(G)$,

$$\int_G u(g_v)\,dg_v = \int_G u(h\cdot g_v\cdot\tilde{h}^{-1})\,dg_v\,. \tag{4.16}$$

As the Boltzmann weight is invariant, the expectation value of any non-invariant function $f':G^V\to\mathbb{C}$ under the partition function vanishes. Note that this holds for any finite graph (V,E).

Similarly, the expectation value vanishes for any function that is not invariant under simultaneous orientation reversal of all edges which corresponds to taking the dual of all representations and which is realized by the inversion symmetry of the Haar measure,

$$\int_G u(g_v)\,dg_v = \int_G u(g_v^{-1})\,dg_v\,. \tag{4.17}$$

Therefore all interesting observables are functions $G^V\to\mathbb{R}$.

C. Duality transformation

The duality transformation consists of two steps. First, we character expand the Boltzmann weight of the original partition function (4.1) of the lattice chiral model. This introduces sums over all irreducible representations of G for each edge as the new dual variables. Furthermore, this step is responsible for the strong–weak or high temperature–low temperature relation of the duality transformation as we have explained in Sec. II H.

The second step is to employ the methods outlined in Sec. II D in order to solve all integrals over G and therefore to remove the old variables from the partition function.

We start with the partition function (4.1) and insert the character expansion (2.14) of the Boltzmann weight for each edge $e \in E$,

$$Z = \left(\prod_{v \in V} \int_G dg_v \right) \prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_G} \hat{w}_{\tau_e} \chi^{(\tau_e)}(g_{\partial_+ e} \cdot g_{\partial_- e}^{-1}). \tag{4.18}$$

The character can be simplified using (2.7) and (2.9),

$$\chi^{(\tau_e)}(g_{\partial_+ e} \cdot g_{\partial_- e}^{-1}) = \sum_{p_e, q_e = 1}^{\dim V_{\tau_e}} t^{(\tau_e)}_{p_e q_e}(g_{\partial_+ e}) t^{(\tau_e^*)}_{p_e q_e}(g_{\partial_- e}). \tag{4.19}$$

The sums are moved to the front of the expression, and we sort the product of representation functions by the vertex $v \in V$ of their arguments g_v:

$$Z = \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_G} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right) \left(\prod_{e \in E} \sum_{p_e, q_e = 1}^{\dim V_{\tau_e}} \right) \prod_{v \in V} \int_G dg_v \left(\prod_{\substack{e \in E: \\ v = \partial_+ e}} t^{(\tau_e)}_{p_e q_e}(g_v) \right) \left(\prod_{\substack{e \in E: \\ v = \partial_- e}} t^{(\tau_e^*)}_{p_e q_e}(g_v) \right). \tag{4.20}$$

Here the last two products are over all edges $e \in E$ that have $v = \partial_\pm e$. The integrals over G can be evaluated using (2.24),

$$Z = \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_G} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right) \left(\prod_{e \in E} \sum_{p_e, q_e = 1}^{\dim V_{\tau_e}} \right) \prod_{v \in V} \sum_{S^{(v)} \in \mathcal{S}^{(v)}} \overline{S^{(v)}_{\underbrace{p_e \cdots}_{\substack{e \in E: \\ v = \partial_+ e}} \underbrace{p_e \cdots}_{\substack{e \in E: \\ v = \partial_- e}}}} S^{(v)}_{\underbrace{q_e \cdots}_{\substack{e \in E: \\ v = \partial_+ e}} \underbrace{q_e \cdots}_{\substack{e \in E: \\ v = \partial_- e}}}, \tag{4.21}$$

where $\mathcal{S}^{(v)}$, $v \in V$, denotes a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e \in E: \\ v = \partial_- e}} V^*_{\tau_e} \right) \to \mathbb{C}, \tag{4.22}$$

which are normalized so that $S^{(v)2} = S^{(v)}$ if the trivial representation $\mathbb{C}$ is embedded in the big tensor product. We obtain the following result.

Theorem 4.8 (Dual partition function): Let G be a compact Lie group and (V,E) denote an oriented graph. The partition function of the lattice chiral model (4.1) is equal to

$$Z = \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_G} \right) \left(\prod_{v \in V} \sum_{S^{(v)} \in \mathcal{S}^{(v)}} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right) \left(\prod_{e \in E} \sum_{p_e, q_e = 1}^{\dim V_{\tau_e}} \right) \prod_{v \in V} \overline{S^{(v)}_{\underbrace{p_e \cdots}_{\substack{e \in E: \\ v = \partial_+ e}} \underbrace{p_e \cdots}_{\substack{e \in E: \\ v = \partial_- e}}}} S^{(v)}_{\underbrace{q_e \cdots}_{\substack{e \in E: \\ v = \partial_+ e}} \underbrace{q_e \cdots}_{\substack{e \in E: \\ v = \partial_- e}}}, \tag{4.23}$$

where $\mathcal{S}^{(v)}$ is a basis of G-invariant projectors (4.22).

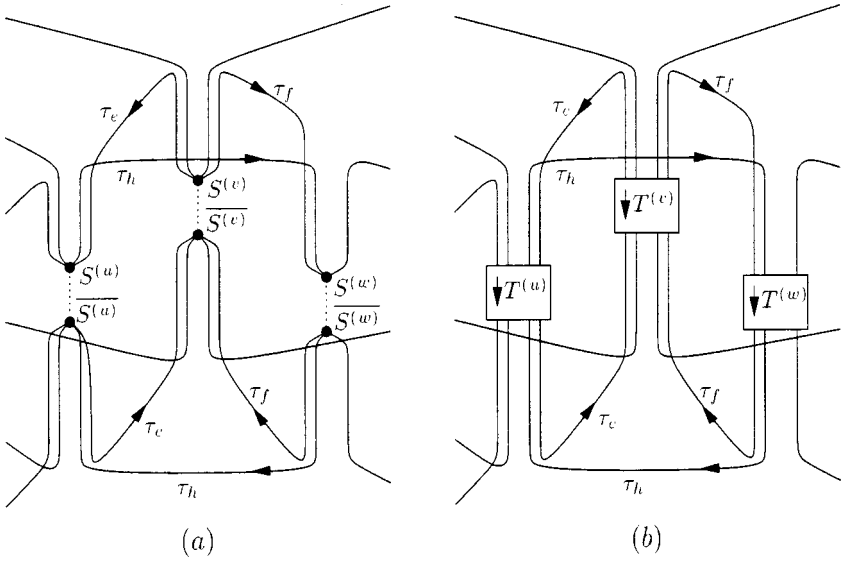

FIG. 7. (a) The spin network that appears in the dual partition function (4.23) of the lattice chiral model on the graph of Fig. 6(a). (b) The alternative expression (4.25) for the same graph.

Remark 4.9: (1) This dual partition function can be described in words as follows. The partition sum consists of a sum over all colorings of the edges $e \in E$ with irreducible representations τ_e of G and over all colorings of the vertices $v \in V$ with compatible intertwiners $S^{(v)}$. Compatible here means that each $S^{(v)}$ corresponds to a map from the tensor product of the representations at the incoming edges $e \in E: v = \partial_+ e$ to the tensor product of the outgoing edges $e \in E: v = \partial_- e$,

$$S^{(v)}: \left(\bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} V_{\tau_e} \right) \to \left(\bigotimes_{\substack{e \in E: \\ v = \partial_- e}} V_{\tau_e} \right). \tag{4.24}$$

Indeed, such an $S^{(v)}$ is related to the one appearing in (4.22) by the canonical isomorphisms $\mathrm{Hom}_G(V \otimes W^*, \mathbb{C}) \cong \mathrm{Hom}_G(V, W)$. The Boltzmann weight of the dual partition function consists of the character expansion coefficients $\hat{w}_{\tau_e}$ for each edge $e \in E$ and of a spin network given by the $S^{(v)}$ whose indices are contracted by the summations over p_e and q_e. This is illustrated in Fig. 7(a).

(2) The dual partition function of the lattice chiral model is therefore given by a sum over spin networks. We call such a model *a spin network model* in analogy to the spin foam models which arise as the dual formulation of lattice gauge theory. The two layers of Fig. 7(a) reflect the chiral structure given by the twofold global G-symmetry. The fact that the spin networks extend over the entire graph is a consequence of the global nature of the symmetry.

(3) We comment on the Abelian special case below in Sec. IV D.

(4) There is an alternative form of the dual partition function which uses a diagrammatical formulation similar to that developed in Ref. 18 for lattice gauge theory. This result is given in the following corollary and illustrated in Fig. 7(b).

Corollary 4.10: From the intermediate step (4.20) of the proof, we obtain the following slightly different expression which involves the Haar intertwiner (2.23) instead of the sum over projectors $S^{(v)}$:

$$Z=\left(\prod_{e\in E}\sum_{\tau_e\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\hat{w}_{\tau_e}\right)\left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\tau_e}}\right)\prod_{v\in V}T^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_-e}},\underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_-e}}},\tag{4.25}$$

where for each $v\in V$, the Haar intertwiner $T^{(v)}$ is a map

$$T^{(v)}:\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\tau_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\tau_e}\right)\to\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\tau_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\tau_e}\right).\tag{4.26}$$

The next step is the generalization of Theorem 4.8 to the expectation value of the observable (4.3),

$$\langle f_{\rho,P,Q}\rangle=\frac{1}{Z}\left(\prod_{v\in V}\int_G dg_v\right)\left(\prod_{e\in E}w(g_{\partial_+e}\cdot g_{\partial_-e}^{-1})\right)\left(\prod_{v\in V}\sum_{\ell_v,m_v=1}^{\dim V_{\rho_v}}\right)P_{\underbrace{\ell_v\ldots}_{v\in V}}Q_{\underbrace{m_v\ldots}_{v\in V}}\prod_{v\in V}t^{(\rho_v)}_{\ell_v m_v}(g_v).\tag{4.27}$$

Again, we character expand the Boltzmann weight, simplify the characters that occur in the expression and reorganize everything. The step that generalizes (4.20) then reads

$$\begin{aligned}\langle f_{\rho,P,Q}\rangle=&\frac{1}{Z}\left(\prod_{e\in E}\sum_{\tau_e\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\hat{w}_{\tau_e}\right)\left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\tau_e}}\right)\left(\prod_{v\in V}\sum_{\ell_v,m_v=1}^{\dim V_{\rho_v}}\right)P_{\underbrace{\ell_v\ldots}_{v\in V}}Q_{\underbrace{m_v\ldots}_{v\in V}}\\&\times\prod_{v\in V}\int_G dg_v\left(\prod_{\substack{e\in E:\\ v=\partial_+e}}t^{(\tau_e)}_{p_eq_e}(g_v)\right)\left(\prod_{\substack{e\in E:\\ v=\partial_-e}}t^{(\tau_e^*)}_{p_eq_e}(g_v)\right)t^{(\rho_v)}_{\ell_v m_v}(g_v).\end{aligned}\tag{4.28}$$

Compared with (4.20), there is an additional factor $t^{(\rho_v)}_{\ell_v m_v}$ for each $v\in V$ under the integral. Solving the integrals, we obtain the following result.

Theorem 4.11 (Dual observable): Let G be a compact Lie group, (V,E) be an oriented graph, and $f_{\rho,P,Q}$ denote an observable of the form (4.3). Then the expectation value (4.27) of $f_{\rho,P,Q}$ in the lattice chiral model is equal to

$$\begin{aligned}\langle f_{\rho,P,Q}\rangle=&\frac{1}{Z}\left(\prod_{v\in V}\sum_{\ell_v,m_v=1}^{\dim V_{\rho_v}}\right)P_{\underbrace{\ell_v\ldots}_{v\in V}}Q_{\underbrace{m_v\ldots}_{v\in V}}\left(\prod_{e\in E}\sum_{\tau_e\in\mathcal{R}_G}\right)\left(\prod_{v\in V}\sum_{S^{(v)}\in\tilde{\mathcal{S}}^{(v)}}\right)\left(\prod_{e\in E}\hat{w}_{\tau_e}\right)\\&\times\left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\tau_e}}\right)\prod_{v\in V}\overline{S^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_-e}}\ell_v}}S^{(v)}_{\underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_-e}}m_v}.\end{aligned}\tag{4.29}$$

For each vertex $v\in V$, $\tilde{\mathcal{S}}^{(v)}$ denotes a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\tau_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\tau_e}\right)\otimes V_{\rho_v}\to\mathbb{C}\tag{4.30}$$

with the usual normalization.

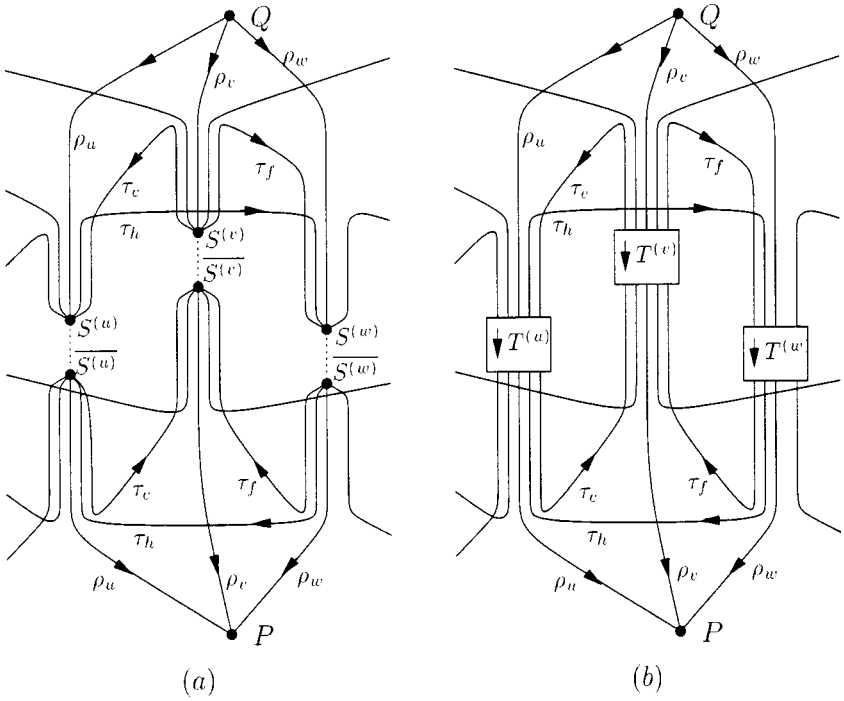

FIG. 8. (a) The dual expression (4.29) for the expectation value of the observable shown in Fig. 6(b), cf. the dual partition function in Fig. 7(a). (b) The alternative formulation (4.31).

Remark 4.12: (1) Compared with the dual partition function (4.23), the new features are the sums over the ℓ_v and m_v and the matrix elements of P and Q from the definition of the observable (4.3). The remainder of the expression has the same structure as the dual partition function except for the fact that the intertwiners $S^{(v)}$ have changed. They now include the charges ρ_v, $v \in V$, of the observable in the compatibility condition (4.30), and the spin networks of the dual partition function are coupled to these charges—the ℓ_v and m_v appear as additional indices of the $S^{(v)}$. The numerator of the dual expression is therefore given by a sum over spin networks with charges (Definition 3.5). This is illustrated in Fig. 8(a).

(2) Equation (4.29) shows that an expectation value of an observable is mapped to a ratio of partition functions in the dual picture, say $\langle f_{\rho,P,Q}\rangle = Z(\rho)/Z$. The numerator $Z(\rho)$ is similar to the partition function, but the spin networks appearing there are now coupled to the charges of the observable, i.e., the numerator corresponds to the partition function in the presence of ''background charges.''

(3) Again there exists an alternative formulation based on the intermediate step (4.28) and involving the Haar intertwiner. This is stated in the following corollary and shown in Fig. 8(b).

Corollary 4.13: From the intermediate step (4.28) of the proof, we obtain,

$$\langle f_{\rho,P,Q}\rangle = \frac{1}{Z}\left(\prod_{v\in V}\sum_{\ell_v,m_v=1}^{\dim V_{\rho_v}}\right) P_{\underbrace{\ell_v\ldots}_{v\in V}}{}^{\underbrace{m_v\ldots}_{v\in V}} \left(\prod_{e\in E}\sum_{\tau_e\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\hat{w}_{\tau_e}\right)\left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\tau_e}}\right) \times \prod_{v\in V} T^{(v)}{}^{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ \ell_v\,,\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ m_v}, \tag{4.31}$$

where the Haar intertwiner $T^{(v)}$ for any given $v \in V$ is a map

$$T^{(v)}:\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\tau_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V^*_{\tau_e}\right)\otimes V_{\rho_v}\to\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\tau_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V^*_{\tau_e}\right)\otimes V_{\rho_v}. \tag{4.32}$$

D. The Abelian special case

In this section, we illustrate the specialization to the Abelian case in detail.

For $G=\mathrm{U}(1)$, the partition function reads

$$Z=\left(\prod_{v\in V}\frac{1}{2\pi}\int_0^{2\pi}d\varphi_v\right)\prod_{e\in E}\exp(-s(e^{i(\varphi_{\partial_+ e}-\varphi_{\partial_- e})})) \tag{4.33}$$

for some action $s:U(1)\to\mathbb{R}$. For $G=\mathbb{Z}_N$ we have

$$Z=\left(\prod_{v\in V}\frac{1}{N}\sum_{\ell_v=0}^{N-1}\right)\prod_{e\in E}\exp(-s(e^{2\pi i(\ell_{\partial_+ e}-\ell_{v_- e})/N})), \tag{4.34}$$

i.e., the chiral model restricts to the XY-model if $G=\mathrm{U}(1)$, to the $\mathbb{Z}_N$-vector Potts model if $G=\mathbb{Z}_N$, and in particular to the Ising model if $G=\mathbb{Z}_2$. The dual partition function (4.23) contains a sum over irreducible representations for each edge which becomes in the Abelian case a sum over $\mathbb{Z}$ or $\mathbb{Z}_N$ (Sec. II G).

As all irreducible representations are one-dimensional, the indices of $S^{(v)}$ in (4.23) are absent, and the sum over projectors restricts to the constraint (2.44), therefore for $G=\mathrm{U}(1)$,

$$Z=\left(\prod_{e\in E}\sum_{k_e=-\infty}^{\infty}\right)\left(\prod_{v\in V}\delta\left(\sum_{\substack{e\in E:\\ v=\partial_+ e}}k_e-\sum_{\substack{e\in E:\\ v=\partial_- e}}k_e\right)\right)\left(\prod_{e\in E}\hat{w}_{k_e}\right), \tag{4.35}$$

where we write $\delta(x)$ for the constraint that $x=0$. For $G=\mathbb{Z}_N$, the sum over the k_e is over $\{0,\ldots,N-1\}$ and all arithmetic involving the k_e is modulo N. The coefficients $\hat{w}_k$ are the character expansion coefficients of the Boltzmann weight [see (2.49) and (2.50)].

Equation (4.35) is the well-known dual expression of the partition function at a stage before the constraints are solved (see, for example, Refs. 3 and 5). The solution of these constraints then depends on the dimension and on the topology of the lattice. For $G=\mathrm{U}(1)$ one obtains the solid-on-solid model in $d=2$ and $\mathbb{Z}$-lattice gauge theory in $d=3$ (Ref. 3) whereas for $G=\mathbb{Z}_N$, one finds again the $\mathbb{Z}_N$-vector Potts model in $d=2$ with the self-duality of the Ising model[1] as a special case for $N=2$, and a $\mathbb{Z}_N$-lattice gauge theory in $d=3$ whose $N=2$ case was studied in Ref. 2.

In the Abelian situation, the dual partition function (4.35) contains only a coloring at one level, namely the sum over all colorings of edges with irreducible representations (wave numbers). The generalization to non-Abelian symmetry groups introduces as a second level the sum over all colorings of the vertices with compatible intertwiners. This second coloring restricts to the familiar constraint of the form (2.44) if G is Abelian.

The symmetry compatible functions (4.3) read in the Abelian case $G=\mathrm{U}(1)$ [or $G=\mathbb{Z}_N$]

$$\underbrace{f_{\ell_v\ldots}}_{v\in V}(\{g_v\}_{v\in V})=\prod_{v\in V}g_v^{\ell_v}, \tag{4.36}$$

where the $\ell_v\in\mathbb{Z}$ [or $\ell_v\in\{0,\ldots,N-1\}$] specify the charges located at the vertices. The dual of the expectation value (4.29) is then given by

$$\langle \underbrace{f_{\ell_v \ldots}}_{v \in V} \rangle = \frac{1}{Z} \left(\prod_{e \in E} \sum_{k_e = -\infty}^{\infty} \right) \left(\prod_{v \in V} \delta \left(\sum_{\substack{e \in E: \\ v = \partial_+ e}} k_e - \sum_{\substack{e \in E: \\ v = \partial_- e}} k_e + \ell_v \right) \right) \left(\prod_{e \in E} \hat{w}_{k_e} \right) \tag{4.37}$$

for $G = \mathrm{U}(1)$ and the obvious aualog for $G = \mathbb{Z}_N$.

Already in the Abelian case, the duality transformation maps the expectation value to a ratio of partition functions whose numerator is a modification of the partition function in which the presence of background charges has modified the constraints or compatibility conditions.

E. Expectation values of the dual model

As Theorem 4.11 shows, the dual expression for the expectation value of an observable is given by a ratio of partition functions. In particular, this dual expression does not coincide with any expectation value under the dual partition function.

It is therefore an interesting problem to study the natural observables of the dual partition function and to transform these expressions back to the original formulation. From the Abelian special case it is familiar that the transformation maps expectation values to ratios of partition functions and therefore correlators constructed from fundamental variables to free energies of collective excitations and conversely (see, for example, Refs. 5 and 27).

For lattice gauge theory with gauge group $G = \mathrm{U}(1)$ in $d = 4$ dimensions, for example, there exist particular expectation values of the dual partition function which describe the correlators of world-lines of magnetic monopoles.[27] If one transforms these expressions back to the original picture, one obtains ratios of partition functions $Z(X)/Z$. The numerator can be understood as the partition function of the model in the presence of a background magnetic field probing monopoles, and the ratio $Z(X)/Z = e^{-F}$ is related to the free energy F of this monopole configuration. A first natural generalization to the non-Abelian case was given by the correlation functions of center monopoles in Ref. 16, expressions which have been studied in lattice gauge theory for some time, but which have not been seen in the context of the duality transformation.

In the Abelian sigma models, the analog of the magnetic monopoles is given by dislocations, vortices, or world lines of vortices, depending on the dimension and on the precise model. In the following, we present the analogous definition for the lattice chiral model with non-Abelian symmetry group G which we call *center dislocation* as it uses the center $Z(G)$ of the symmetry group G similarly to the center monopoles in order to parametrize the observables and because it specializes to the *dislocations* studied in Ref. 2 in the case $G = \mathbb{Z}_2$.

Definition 4.14: Let G be a compact Lie group, (V,E) be an oriented graph, and $X: E \to Z(G), e \mapsto X_e$ assign an element of the center $Z(G)$ to each edge $e \in E$. The *center dislocation* is the following function $\mathcal{O}_X: (\mathcal{R}_G)^V \to \mathbb{C}$ of the configurations of the dual partition function (4.23),

$$\mathcal{O}_X(\{\tau_e\}_{e \in E}) := \prod_{e \in E} \tilde{t}^{(\tau_e)}(X_e), \tag{4.38}$$

where $\tilde{t}^{(\tau_e)}$ denotes the representation functions of $Z(G)$ induced from the representation $\tau_e \in \mathcal{R}_G$ (Lemma 2.19).

We can now employ the techniques of Sec. IV C in order to transform the expectation value of the center dislocation back to the original picture.

Theorem 4.15: The normalized expectation value of the center dislocation (4.38) under the dual partition function (4.23) is equal to

$$\langle \mathcal{O}_X \rangle_{\mathrm{dual}} = \frac{1}{Z} \left(\prod_{v \in V} \int_G dg_v \right) \prod_{e \in E} w(g_{\partial_+ e} \cdot g_{\partial_- e}^{-1} \cdot X_e). \tag{4.39}$$

Proof: Start from (4.39), insert the expansion of $w(g)$ and apply Lemma 2.19. The proof is entirely analogous to that of Theorem 4.8 with one additional factor $\tilde{t}^{(\tau_e)}(X_e)$ for each edge $e \in E$ in the integrand. □

Remark 4.16: The expectation value of the dual observable takes the form of a ratio of partition functions in the original formulation. This is essentially the converse of Theorem 4.11. The numerator can again be viewed as the partition function in the presence of a background field X.

In the Abelian case, we have $Z(G)=G$. The possible choices for fields X depend on the particular group and on the dimension and topology of the lattice. They have been carefully studied for several models.

(1) If $G=\mathrm{U}(1)$ and (V,E) is a two-dimensional cubic lattice, then the disorder parameter of the XY-model, which is related to the free energy of a vortex–antivortex pair, is of the form (4.39). In higher dimensions, this generalizes to vortex strings, vortex sheets, etc.
(2) For $G=\mathbb{Z}_2$ we obtain the dislocations of Ref. 2 as the simplest dual observables. Their expectation value is again related to their free energies.

There are more general functions $(\mathcal{R}_G)^V \to \mathbb{C}$ whose expectation value under the dual partition function can be calculated. Let $e_0 \in E$ be an edge and $\sigma \in \mathcal{R}_G$ be an irreducible representation of G. Then we can study the indicator function,

$$\mathcal{O}_{e_0,\sigma}(\{\tau_e\}_{e\in E}) = \delta_{\tau_{e_0}\sigma}, \tag{4.40}$$

which probes whether the representation σ is assigned to the edge e_0. The center dislocations can be expressed as linear combinations of these indicator functions,

$$\mathcal{O}_X(\{\tau_e\}_{e\in E}) = \left(\prod_{e\in E}\sum_{\sigma_e\in\mathcal{R}_G}\right)\prod_{e\in E}\mathcal{O}_{e,\sigma_e}\tilde{t}^{(\sigma_e)}(X_e). \tag{4.41}$$

The expectation value of an indicator function (4.40) under the dual partition function (4.23) is then equal to

$$\langle \mathcal{O}_{e_0,\sigma}\rangle_{\mathrm{dual}} = \frac{1}{Z}\left(\prod_{v\in V}\int_G dg_v\right)\prod_{e\in E}\tilde{w}_e^{(e_0,\sigma)}(g_{\partial_+ e}\cdot g_{\partial_- e}^{-1}), \tag{4.42}$$

where the Boltzmann weight $w(g)$ is modified at the edge e_0,

$$\tilde{w}_e^{(e_0,\sigma)}(g) = \begin{cases} w(g), & \text{if } e\neq e_0, \\ \displaystyle\sum_{\rho\in\mathcal{R}_G}\delta_{\rho,\sigma}\hat{w}_\rho\chi^{(\rho)}(g), & \text{if } e=e_0, \end{cases} \tag{4.43}$$

In general, a function involving the indicator functions in the dual formulation leads to a convolution of the Boltzmann weight in the original picture.

Remark 4.17: (1) The definition of dual expectation values presented here is restricted to functions of the irreducible representations at the edges. It is also conceivable to make use of functions of the intertwiners at the vertices.

(2) Indicator functions similar to (4.40) have been used to construct geometrical observables in the spin foam model of three-dimensional quantum gravity.[28]

F. The strong–weak relation

The dual partition function (4.23) of the lattice chiral model is strong–weak dual to the original formulation (4.1). This follows from the properties of the character expansion of the Boltzmann weight and is most transparent for the heat kernel action (2.52). The only β-dependent term of the dual partition function is the product

$$\prod_{e\in E}\hat{w}_{\tau_e}=\exp\left(-\frac{1}{2\beta}\sum_{e\in E}C^{(2)}_{\tau_e}\right), \tag{4.44}$$

where the inverse temperature β appears in the denominator! The result for the Wilson action of $G=\mathrm{U}(1)$ or $G=\mathrm{SU}(2)$ looks more complicated and involves modified Bessel functions, but it is qualitatively quite similar. In all these cases, the term corresponding to (4.44) has a sharp peak as a function of the $C^{(2)}_{\tau}$ if β is small.

The β-dependence (4.44) of the dual partition function also encodes essential information on the strong coupling expansion of the lattice chiral model. For small β, the dominant contribution to (4.44) comes from spin networks (assignments of representations to the edges of the graph) whose sum of the quadratic Casimir eigenvalues over all edges is very small. It is now possible to sort them by the value of this sum so that the configurations of the dual partition function are precisely the terms of the strong coupling expansion!

V. THE NONLINEAR SIGMA MODEL

We construct the lattice nonlinear sigma model with variables in some coset space G/H, where $H\leqslant G$ is a Lie subgroup of G, starting from the chiral model. One half of the $G\times G$-symmetry of the chiral model is used to couple elements $h\in H$ to the action term. Integration over h then makes sure that the action is constant on the cosets gH and therefore defines a model with variables in G/H.

A. Partition function

Lemma 5.1: Let G be a compact Lie group and $H\leqslant G$ be a Lie subgroup. Let $f\in L^2(G)$ be a class function of G with character expansion

$$f(g)=\sum_{\rho\in\mathcal{R}_G}\hat{f}_\rho\chi^{(\rho)}(g). \tag{5.1}$$

(1) For any $g_1,\ g_2\in G$,

$$\int_H f(g_1\cdot h\cdot g_2^{-1})dh=\sum_{\rho\in\mathcal{R}_H^G}\hat{f}_\rho\sum_{j=1}^{\dim V_\rho}\sum_{k=1}^{\kappa_\rho}H^{(\rho)}_{jk}(g_1)H^{(\rho^*)}_{jk}(g_2), \tag{5.2}$$

using the conventions of Sec. II E.

(2) The function f defines a map $\tilde{f}:G/H\times G/H\to\mathbb{C}$,

$$\tilde{f}(x,y):=\int_H f(g_x\cdot h\cdot g_y^{-1})dh, \tag{5.3}$$

where $g_x,\ g_y\in G$ denote representatives of the cosets $x,\ y\in G/H$.

(3) The function $\tilde{f}(x,y)$ has a global left G-symmetry, i.e., for any $g\in G,\ x,\ y\in G/H$,

$$\tilde{f}(g\cdot x,g\cdot y)=\tilde{f}(x,y). \tag{5.4}$$

(4) If in addition $f(g^{-1})=f(g)$, then $\tilde{f}(x,y)=\tilde{f}(y,x)$.

Remark 5.2: If H is a massive subgroup of G, then $\kappa_\rho = 1$ for the class-1 representations. In this case, any L^2-function $G/H \times G/H \to \mathbb{C}$ with the symmetry (5.4) is of the form (5.2). This statement does, however, not extend to the case of generic Lie subgroups $H \leqslant G$. We define the lattice nonlinear sigma model for Boltzmann weights of the special form (5.2).

Definition 5.3: Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup, and (V,E) denote an oriented graph. Let $s: G \to \mathbb{R}$ be an L^2-integrable and bounded class function that satisfies $s(g^{-1}) = s(g)$. Construct $\tilde{w}: G/H \times G/H \to \mathbb{R}$ from $w(g) = \exp(-s(g))$ as in Lemma 5.1. The *lattice nonlinear sigma model* is defined by the partition function

$$Z = \left(\prod_{v \in V} \int_{G/H} dx_v \right) \prod_{e \in E} \tilde{w}(x_{\partial_+ e}, x_{\partial_- e}). \tag{5.5}$$

Proposition 5.4: The lattice nonlinear sigma model has got a global left-G symmetry. For any fixed $g \in G$, the transformation

$$x_v \mapsto g \cdot x_v, \tag{5.6}$$

for all $v \in V$, is a symmetry of the weight $\tilde{w}(x_{\partial_+ e}, x_{\partial_- e})$. In the special case in which $H \trianglelefteq G$ is a normal subgroup, there is also a global right-G/H symmetry. Let $y \in G/H$. Then the transformation

$$x_v \mapsto x_v \cdot y^{-1}, \tag{5.7}$$

for all $v \in V$, is also a symmetry of the weight.

Example 5.5: The Boltzmann weights $\tilde{w}(x,y) := \exp(-\tilde{s}(x,y))$ of the lattice N-vector model [the O(N) nonlinear sigma model] and of the $\mathbb{RP}^{N-1}$-model are of the type of Lemma 5.1. For the N-vector model, $G = \mathrm{O}(N)$, $H = \mathrm{O}(N-1)$, and

$$\tilde{s}(\underline{x},\underline{y}) = -\beta \underline{x} \cdot \underline{y}, \tag{5.8}$$

where $\underline{x}$, $\underline{y} \in S^{N-1} \subseteq \mathbb{R}^N$, and the dot denotes the standard scalar product. For the $\mathbb{RP}^{N-1}$-model, $G = \mathrm{O}(N)$, $H = \mathrm{O}(N-1) \times \mathbb{Z}_2$, and

$$\tilde{s}(\underline{x},\underline{y}) = -\frac{\beta}{2} (\underline{x} \cdot \underline{y})^2, \tag{5.9}$$

for representatives $\underline{x}$, $\underline{y}$ of classes in $\mathbb{RP}^{N-1} \cong S^{N-1}/\mathbb{Z}_2$. On cubic lattices, there exists in both cases a suitable naïve continuum (or weak field) limit in which the lattice constant tends to zero and the lattice action towards the action of the corresponding continuum model.

Remark 5.6: (1) The partition function again depends only on the unoriented graph.

(2) If $H = \{e\}$ is the trivial group, then any representation function is a generalized spherical function. The nonlinear sigma model for G/H coincides in this case with the chiral model for G, and the global $G \times G$-symmetry is restored.

B. Expectation values

The observables of the lattice nonlinear sigma model can be found by the same methods as for the chiral model (Sec. IV B). The calculation is very similar so that we just state the results.

Theorem 5.7: Each algebraic function $(G/H)^V \to \mathbb{C}$ that is compatible with the global left-G symmetry (5.6) is a linear combination of observables of the following type,

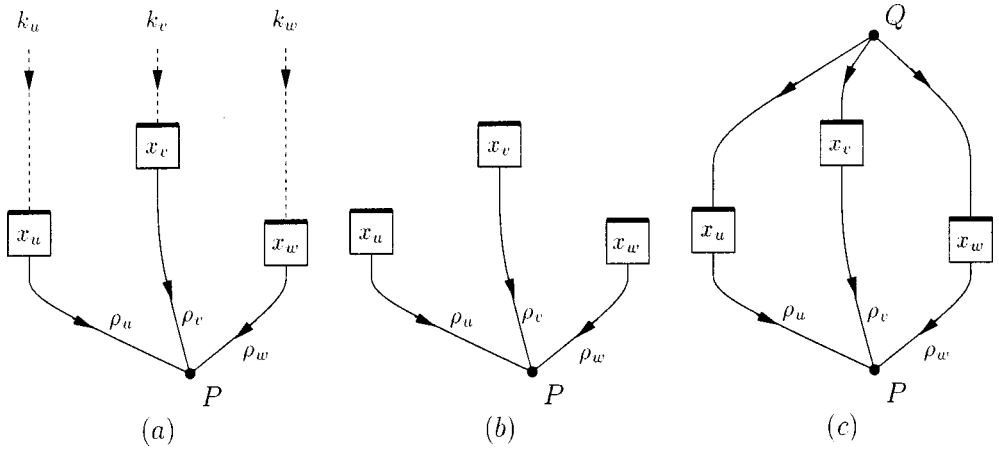

FIG. 9. (a) The observable (5.10) of the lattice nonlinear sigma model on the graph of Fig. 6. (b) The same function for the case of a massive subgroup $H \leqslant G$. (c) The observable (5.14) if $H \trianglelefteq G$ is a normal subgroup.

$$f_{\rho,P,k_v\ldots}(\{x_v\}_{v\in V}) = \left(\prod_{v\in V}\sum_{\ell_v=1}^{\dim V_{\rho_v}}\right) P_{\underbrace{\ell_v\ldots}_{v\in V}} \prod_{v\in V} H^{(\rho_v)}_{\ell_v,k_v}(x_v), \tag{5.10}$$

where

$$\rho: V \to \mathcal{R}_H^G, \quad v \mapsto \rho_v, \tag{5.11}$$

assigns a class-1 representation of G with respect to H to each vertex; $k_v \in \{1,\ldots,\kappa_{\rho_v}\}$ for all $v \in V$, and

$$P: \bigotimes_{v\in V} V_{\rho_v} \to \mathbb{C} \tag{5.12}$$

is an intertwiner of G.

Remark 5.8: (1) The structure of the function (5.10) is illustrated in Fig. 9(a).

(2) The well-known two-point function for a charge-anticharge pair ρ, ρ^* at $v, w \in V$ is a special case,

$$f_{k_v,k_v}(x_v,x_w) = \sum_{j_v=1}^{\dim V_\rho} H^{(\rho)}_{j_v k_v}(x_v) H^{(\rho^*)}_{j_w k_w}(x_w)\, \delta_{j_v j_w}, \tag{5.13}$$

for fixed k_v, $k_w \in \{1,\ldots,\kappa_\rho\}$.

(3) If H is a massive subgroup of G, we have $\kappa_\rho = 1$ for the class-1 representations so that the indices k_v can be omitted from all expressions [Fig. 9(b)].

Theorem 5.9: If in addition $H \trianglelefteq G$ is a normal subgroup, then the algebraic functions $(G/H)^V \to \mathbb{C}$ that are compatible with both the global left-G and the global right-G/H symmetry are linear combinations of observables of the following form,

$$f_{\rho,P,Q}(\{x_v\}_{v\in V}) = \left(\prod_{v\in V}\sum_{\ell_v=1}^{\dim V_{\rho_v}}\sum_{\ell_v=1}^{\kappa_{\rho_v}}\right) P_{\underbrace{\ell_v\ldots}_{v\in V}} Q_{\underbrace{k_v\ldots}_{v\in V}} \prod_{v\in V} H^{(\rho_v)}_{\ell_v k_v}(x_v). \tag{5.14}$$

Here

$$\rho: V \to \mathcal{R}_H^G, \quad v \mapsto \rho_v, \tag{5.15}$$

assigns a class-1 representation of G with respect to H to each vertex and

$$P: \bigotimes_{v \in V} V_{\rho_v} \to \mathbb{C}, \quad Q: \bigotimes_{v \in V} V_{\rho_v}^* \to \mathbb{C}, \tag{5.16}$$

are intertwiners of G.

Remark 5.10: (1) Figure 9(c) illustrates the structure of the observables (5.14) if $H \trianglelefteq G$ is a normal subgroup. Here the indices k_v of (5.10) are no longer independent, but rather exhibit a G/H-symmetry under which invariance is required. Therefore we need the second intertwiner Q. Furthermore, $\kappa_\rho = \dim V_\rho$ for all class-1 representations so that the dashed lines have become solid.

(2) In particular for $H = \{e\}$, we recover the observable (4.3) of the chiral model.

(3) In order to have nonvanishing expectation values, the observable not only has to be invariant under the symmetries (5.6) and (5.7) (if applicable), but also under orientation reversal (Remark 4.7).

C. Duality transformation

The duality transformation for the nonlinear sigma model is very similar to that of the chiral model. We summarize the main steps which differ from the calculation for the chiral model and focus directly on the most general case, the dual of an expectation value, from which the transformation of the partition function can be easily inferred.

We start with an observable $f_{\rho,P,Q}$ of the form (5.14). If $H \trianglelefteq G$ is a normal subgroup, then Q is an intertwiner of G. Otherwise, Q is arbitrary so that we obtain the function (5.10) for geueric $k_v \in \{1,\ldots,\kappa_{\rho_v}\}$, $v \in V$.

We start with the expectation value of the observable (5.14) under the partition function (5.5),

$$\begin{aligned}\langle f_{\rho,P,Q} \rangle = \frac{1}{Z} \left(\prod_{v \in V} \int_{G/H} dx_v \right) \left(\prod_{e \in E} \tilde{w}(x_{\partial_+ e}, x_{\partial_- e}) \right) \\ \times \left(\prod_{v \in V} \sum_{\ell_v=1}^{\dim V_{\rho_v}} \sum_{k_v=1}^{\kappa_{\rho_v}} \right) P_{\underbrace{\ell_v \ldots}_{v \in V}} \overline{Q_{\underbrace{k_v \ldots}_{v \in V}}} \prod_{v \in V} H^{(\rho_v)}_{\ell_v k_v}(x_v),\end{aligned} \tag{5.17}$$

and insert for each $e \in E$ the expansion of Lemma 5.1,

$$\tilde{w}(x_{\partial_+ e}, x_{\partial_- e}) = \sum_{\tau_e \in \mathcal{R}_H^G} \hat{w}_{\tau_e} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} H^{(\tau_e)}_{j_e m_e}(x_{\partial_+ e}) H^{(\tau_e^*)}_{j_e m_e}(x_{\partial_- e}), \tag{5.18}$$

where the $\hat{w}_\tau$ are the character expansion coefficients of the function $w(g) = \exp(-s(g))$ of Definition 5.3. The reorganized expression then reads

$$\begin{aligned}\langle f_{\rho,P,Q} \rangle = \frac{1}{Z} \left(\prod_{v \in V} \sum_{\ell_v=1}^{\dim V_{\rho_v}} \sum_{k_v=1}^{\kappa_{\rho_v}} \right) P_{\underbrace{\ell_v \ldots}_{v \in V}} \overline{Q_{\underbrace{k_v \ldots}_{v \in V}}} \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_H^G} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right) \left(\prod_{e \in E} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} \right) \\ \times \prod_{v \in V} \int_{G/H} dx_v \left(\prod_{\substack{e \in E: \\ v = \partial_+ e}} H^{(\tau_e)}_{j_e m_e}(x_v) \right) \left(\prod_{\substack{e \in E: \\ v = \partial_- e}} H^{(\tau_e^*)}_{j_e m_e}(x_v) \right) H^{(\rho_v)}_{\ell_v k_v}(x_v),\end{aligned} \tag{5.19}$$

so that we can evaluate the integrals over G/H using (2.36),

$$\int_{G/H} dx_v(\cdots) = \sum_{S^{(v)} \in \tilde{\mathcal{S}}^{(v)}} \overline{S^{(v)}_{\underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} \ell_v}} S^{(v)}_{\underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} k_v}. \tag{5.20}$$

Here $\tilde{\mathcal{S}}^{(v)}$, $v \in V$, denotes a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V^*_{\tau_e} \right) \otimes V_{\rho_v} \to \mathbb{C} \tag{5.21}$$

with the usual normalization. We obtain the following result.

Theorem 5.11 (Dual observable): Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup, and (V,E) denote an oriented graph. The expectation value (5.17) of the observable of the lattice nonlinear sigma model is equal to the expressions

$$\begin{aligned}
\langle f_{\rho,P,Q} \rangle = & \frac{1}{Z} \left(\prod_{v\in V} \sum_{\ell_v=1}^{\dim V_{\rho_v}} \sum_{\kappa_v=1}^{\kappa_{\rho_v}} \right) P_{\underbrace{\ell_v \cdots}_{v\in V}} \overline{Q_{\underbrace{k_v \cdots}_{v\in V}}} \left(\prod_{e\in E} \sum_{\tau_e \in \mathcal{R}_H^G} \right) \left(\prod_{e\in E} \hat{w}_{\tau_e} \right) \\
& \times \left(\prod_{e\in E} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} \right) \prod_{v\in V} I^{(v)}_{\underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} \ell_v ; \underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} k_v}
\end{aligned} \tag{5.22}$$

$$\begin{aligned}
= & \frac{1}{Z} \left(\prod_{v\in V} \sum_{\ell_v=1}^{\dim V_{\rho_v}} \sum_{k_v=1}^{\kappa_{\rho_v}} \right) P_{\underbrace{\ell_v \cdots}_{v\in V}} \overline{Q_{\underbrace{k_v \cdots}_{v\in V}}} \times \left(\prod_{e\in E} \sum_{\tau_e \in \mathcal{R}_H^G} \right) \left(\prod_{v\in V} \sum_{S^{(v)} \in \tilde{\mathcal{S}}^{(v)}} \right) \left(\prod_{e\in E} \hat{w}_{\tau_e} \right) \\
& \times \left(\prod_{e\in E} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} \right) \prod_{v\in V} \overline{S^{(v)}_{\underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{j_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} \ell_v}} S^{(v)}_{\underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_+ e}} \underbrace{m_e \cdots}_{\substack{e\in E:\\ v=\partial_- e}} k_v}.
\end{aligned} \tag{5.23}$$

Here $\tilde{\mathcal{S}}^{(v)}$, $v \in V$, denotes a basis of G-invariant projectors (5.21), and the $\hat{w}_\tau$ are the character expansion coefficients of the function $w(g) = \exp(-s(g))$ where $s(g)$ is the class function of Definition 5.3. The coset space Haar map $I^{(v)}$, $v \in V$, in (5.22) is a map

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V_{\tau_e} \right) \otimes V_{\rho_v} \to \left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V_{\tau_e} \right) \otimes V_{\rho_v}. \tag{5.24}$$

Remark 5.12: (1) The dual expression (5.22) for the observable of the nonlinear sigma model is very similar to the dual observable of the chiral model in Theorem 4.11. The differences are the ranges of the indices which follow from the choice of the subgroup $H \leqslant G$. The structure of the dual observable is illustrated in Fig. 10(a) if $H \leqslant G$ is a generic, non-normal subgroup, in Fig. 10(b) if H is a massive subgroup, and in Fig. 10(c) for the case of a normal subgroup $H \trianglelefteq G$. Figures 10(a)–10(c) correspond to (5.22). The diagrams for the other formulation (5.23) are obtained by the replacements shown in Figs. 2(c) or 3(c).

(2) Again, the dual expression for the observable of the chiral model can be obtained from (5.23) for a trivial subgroup $H = \{e\}$.

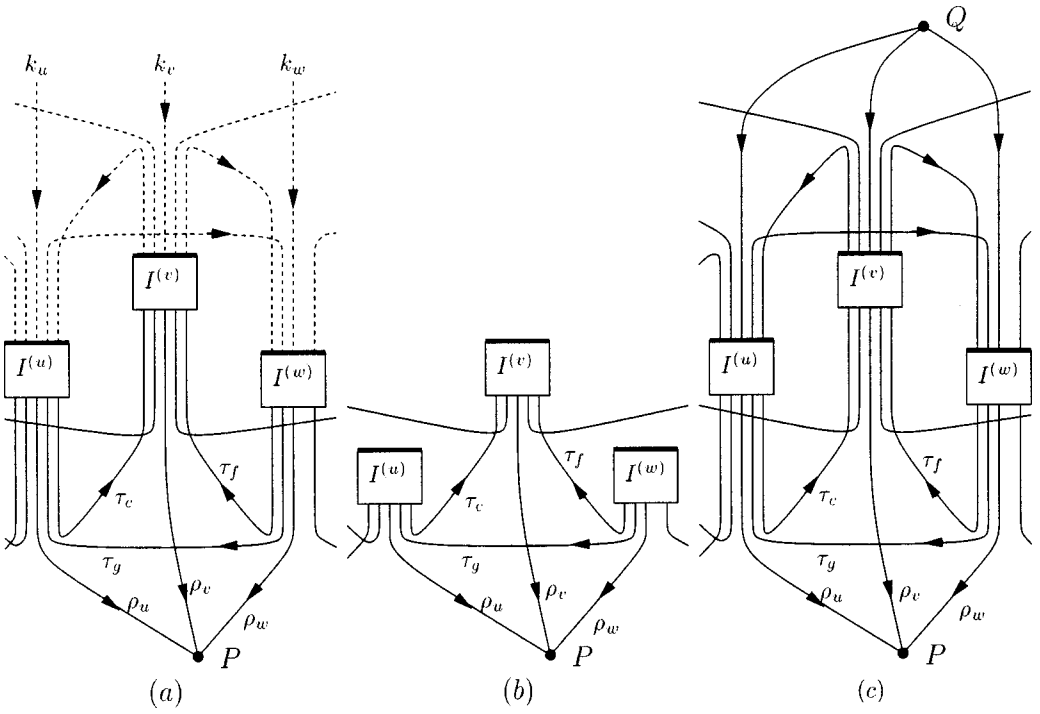

FIG. 10. (a) The structure of the dual form (5.22) for the expectation value of an observable of the lattice nonlinear sigma model on the graph of Fig. 6(a). (b) The special case of a massive subgroup $H \leqslant G$. (c) The situation for a normal subgroup $H \trianglelefteq G$.

(3) If one seeks a purely categorial picture of the dual nonlinear sigma model, one should generally view all representations as representations of H. Otherwise the integrals over H, which are still implicitly present in the spherical functions, would not be honest intertwiners. The dashed lines with open ends labeled k_v then enumerate different trivial representations of H. The special cases of massive and normal subgroups, however, are easier and can be handled already in the context of the representations of G.

The dual expression for the partition function can be calculated by specializing the numerator of (5.22) to the trivial observable. This result is given in the following corollary and visualized in Fig. 11.

Corollary 5.13 (Dual partition function): Let G be a compact Lie group with a Lie subgroup $H \leqslant G$ and (V,E) be an oriented graph. The partition function (5.5) of the lattice nonlinear sigma model is equal to

$$Z = \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_H^G} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right) \left(\prod_{e \in E} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} \right) \prod_{v \in V} I^{(v)}_{\underbrace{j_e \ldots}_{\substack{e \in E: \\ v=\partial_+ e}} \underbrace{j_e \ldots}_{\substack{e \in E: \\ v=\partial_- e}} ; \underbrace{m_e \ldots}_{\substack{e \in E: \\ v=\partial_+ e}} \underbrace{m_e \ldots}_{\substack{e \in E: \\ v=\partial_- e}}} \tag{5.25}$$

$$= \left(\prod_{e \in E} \sum_{\tau_e \in \mathcal{R}_H^G} \right) \left(\prod_{v \in V} \sum_{S^{(v)} \in \mathcal{S}^{(v)}} \right) \left(\prod_{e \in E} \hat{w}_{\tau_e} \right)$$
$$\times \left(\prod_{e \in E} \sum_{j_e=1}^{\dim V_{\tau_e}} \sum_{m_e=1}^{\kappa_{\tau_e}} \right) \prod_{v \in V} \overline{S^{(v)}_{\underbrace{j_e \ldots}_{\substack{e \in E: \\ v=\partial_+ e}} \underbrace{j_e \ldots}_{\substack{e \in E: \\ v=\partial_- e}}}} S^{(v)}_{\underbrace{m_e \ldots}_{\substack{e \in E: \\ v=\partial_+ e}} \underbrace{m_e \ldots}_{\substack{e \in E: \\ v=\partial_- e}}} . \tag{5.26}$$

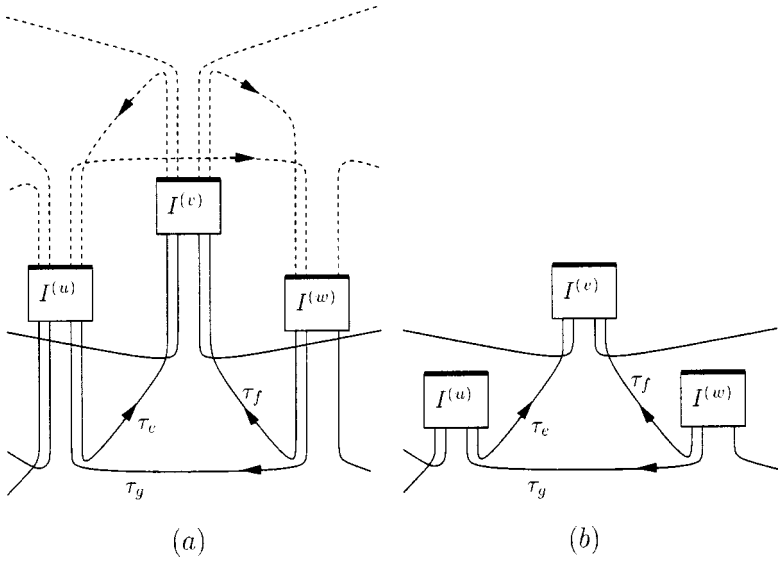

FIG. 11. (a) The structure of the dual partition function (5.25) of the lattice nonlinear sigma model on the graph of Fig. 6. (b) The special case of a massive subgroup $H \leqslant G$.

Here $\mathcal{S}^{(v)}$, $v \in V$, denotes a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e \in E: \\ v = \partial_- e}} V^*_{\tau_e} \right) \to \mathbb{C} \tag{5.27}$$

with the usual normalization, and the coset space Haar map $I^{(v)}$ is a linear map

$$\left(\bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e \in E: \\ v = \partial_- e}} V_{\tau_e} \right) \to \left(\bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} V_{\tau_e} \right) \otimes \left(\bigotimes_{\substack{e \in E: \\ v = \partial_- e}} V_{\tau_e} \right). \tag{5.28}$$

D. Expectation values of the dual model

If the natural observables of the dual partition function are again constructed from the labelling of the edges with representations, the result is the same as for the lattice chiral model in Sec. IV E, restricted to the class-1 representations. The analog of (4.39) is then

$$\langle \mathcal{O}_X \rangle_{\text{dual}} = \frac{1}{Z} \left(\prod_{v \in V} \int_{G/H} dx_v \right) \prod_{e \in E} \tilde{w}(X_e \cdot x_{\partial_+ e}; x_{\partial_- e}). \tag{5.29}$$

VI. THE GENERALIZED HIGGS MODELS

In this section, we couple the chiral model and the nonlinear sigma model to lattice gauge theory. In some particular cases, this yields certain Higgs models with frozen radial component which motivates the title of this section. Before we study the coupled models, it is useful to summarize the results of the duality transformation for lattice gauge theory[15–17] in the language of the present article.

A. Lattice gauge theory

Definition 6.1: Let G be a compact Lie group, (V,E,F) be an oriented two-complex, and $s: G \to \mathbb{R}$ be an L^2-integrable class function of G that is bounded below and satisfies $s(g^{-1}) = s(g)$ for all $g \in G$. The partition function of *lattice gauge theory* with gauge group G is defined by

$$Z=\left(\prod_{e\in E}\int_G dg_e\right)\prod_{f\in F}u(g_f),\quad g_f:=g_{\partial_1 f}^{\epsilon_1 f}\cdots g_{\partial_{N(f)}f}^{\epsilon_{N(f)}f},\tag{6.1}$$

where $u(g)=\exp(-s(g))$.

The set of configurations of lattice gauge theory is the product G^E of one copy of G for each edge $e\in E$. The ordered product of group elements attached to the edges in the boundary of the face $f\in F$ is denoted by g_f. The Boltzmann weight exhibits a local gauge symmetry.

Proposition 6.2: Let $h:V\to G$, $v\mapsto h_v$, associate a group element with each vertex. The Boltzmann weight $u(g_f)=\exp(-s(g_f))$ in (6.1) is invariant under the local gauge transformations

$$g_e\mapsto h_{\partial_+ e}\cdot g_e\cdot h_{\partial_- e}^{-1},\tag{6.2}$$

for all $e\in E$.

This definition of lattice gauge theory is motivated by the fact that on regular hypercubic lattices, the Wilson action tends towards the continuum Yang–Mills action in the weak field limit of vanishing lattice constant. The group elements g_e attached to the edges of the lattice correspond to the parallel transports of the gauge connection along these edges. For more details on lattice gauge theory, see, for example, Refs. 29 and 30.

The most general observable of lattice gauge theory whose expectation value under the partition function (6.1) can be calculated is constructed from spin networks. Each algebraic function $G^E\to\mathbb{C}$ that is invariant under the transformation (6.2) is a linear combination of *spin network functions*. They generalize the notion of Wilson loops and are defined as follows.

Definition 6.3: Let G be a compact Lie group, (V,E,F) be an oriented two-complex, and (σ,Q) be a spin network (Definition 3.4). The *spin network function* of (σ,Q) associates with each configuration a complex number,

$$W_{\sigma,Q}(\{g_e\}_{e\in E}):=\left(\prod_{e\in E}\sum_{k_e,\ell_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{e\in E}t_{k_e\ell_e}^{(\sigma_e)}(g_e)\right)\left(\prod_{v\in V}Q^{(v)}_{\underbrace{\ell_e\cdots}_{\substack{e\in E:\\ v=\partial_- e}}\ \underbrace{k_e\cdots}_{\substack{e\in E:\\ v=\partial_+ e}}}\right).\tag{6.3}$$

Remark 6.4: (1) The above definition uses the spin network (σ,Q) to label edges with representations and vertices with intertwiners, and then employs a representation function for each edge in order to obtain a function $G^E\to\mathbb{C}$.

(2) All edges $e\in E$ for which $V_{\sigma_e}\cong\mathbb{C}$ is the trivial representation contribute only a factor 1 to the expression (6.3). For an ordinary Wilson loop, for example, all edges are labeled with the trivial representation except for those edges that are part of the loop. These are labeled with the fundamental representation of G. The intertwiners $Q^{(v)}$ (if nonvanishing) are in this case uniquely determined up to normalization.

(3) The spin network function (6.3) can be *evaluated* by putting $g_e=e$ (group unit) for all edges $e\in E$. The result is an invariant of G which is often called the *value* of the spin network (σ,Q).

(4) If G is Abelian, then the set $\mathcal{R}_G$ of irreducible representations forms an additive group, and all irreducible representations are one-dimensional. Thus $W_{\sigma,Q}$ can be decomposed into a sum of products of ordinary Wilson loops.

We have the following dual expressions for the partition function and the expectation value of a spin network function.[15,17]

Theorem 6.5 (Dual partition function): Let G be a compact Lie group. The partition function (6.1) of lattice gauge theory is equal to the expression

$$Z=\left(\prod_{f\in F}\sum_{\tau_f\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\sum_{U^{(e)}\in\mathcal{U}(e)}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{v\in V}C(v)\right).\tag{6.4}$$

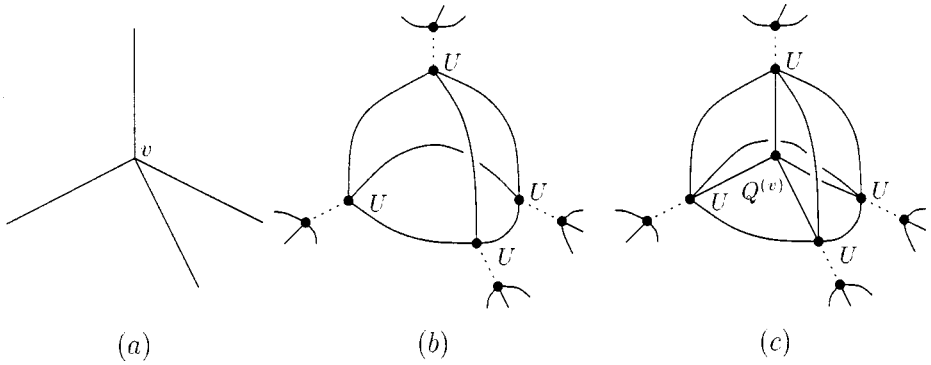

FIG. 12. (a) A two-complex with a vertex v attached to four edges. There are six faces, one between each pair of edges. (b) The spin network $C(v)$ of (6.6) that appears in the dual partition function of lattice gauge theory and (c) the spin network (6.14) from the dual of an expectation value.

Here $\mathcal{U}^{(e)}$, $e \in E$, denotes a basis of G-invariant projectors

$$\left(\bigotimes_{f \in e_+} V_{\tau_f} \right) \otimes \left(\bigotimes_{f \in e_-} V_{\tau_f}^* \right) \to \mathbb{C}. \tag{6.5}$$

The $\hat{u}_\tau$ are the coefficients of the character expansion of the Boltzmann weight $u(g)$. The weights per vertex $C(v)$ are given by a trace involving representations and projectors in the neighborhood of the vertex $v \in V$,

$$C(v) = \left(\prod_{\substack{f \in F: \\ v \in f_0}} \sum_{n_f=1}^{\dim V_{\tau_f}} \right) \left(\prod_{\substack{e \in E: \\ v = \partial + e}} \overline{U^{(e)}_{\underbrace{n_f n_f \ldots}_{f \in e_+} \underbrace{n_f n_f \ldots}_{f \in e_-}}} \right) \left(\prod_{\substack{e \in E: \\ v = \partial - e}} U^{(e)}_{\underbrace{n_f n_f \ldots}_{f \in e_+} \underbrace{n_f n_f \ldots}_{f \in e_-}} \right). \tag{6.6}$$

Here the range $f \in F: v \in f_0$ of the first product refers to all faces $f \in F$ that contain the vertex v in their boundary. The second product is over the range $e \in E: v = \partial_+ e$ of all edges that have v as their endpoint, etc. (see Sec. III A).

Remark 6.6: (1) For each edge $e \in E$, the projectors (6.5) are related by natural isomorphisms to intertwiners

$$\bigotimes_{f \in e_+} V_{\tau_f} \to \bigotimes_{f \in e_-} V_{\tau_f}, \tag{6.7}$$

from the tensor product of the representations at the ''incoming'' faces to the tensor product at the ''outgoing'' ones.

(2) The dual partition function (6.4) labels the faces with irreducible representations of G and the edges with compatible intertwiners in the sense of (6.7). The configurations of the dual partition function are therefore spin foams (Definition 3.6) so that the dual model is a spin foam model. Compared with the situation for the sigma models, all the labels appear one level ''higher,'' i.e., at the faces rather than at the edges, and at the edges rather than the vertices.

(3) The expression $C(v)$ for given projectors $U^{(e)}$ is itself a spin network. Figure 12(b) visualizes it for a vertex with four edges attached. In particular, for $G = \mathrm{SU}(2)$, the $C(v)$ are the $6j$-symbols of SU(2). The collection of all $C(v)$ in a two-complex is illustrated in Fig. 13(a).

(4) The spin networks of the dual partition function for lattice gauge theory decompose into one independent $C(v)$ for each vertex. This is a consequence of the local G-symmetry and is in contrast to the chiral model whose dual partition function involves two spin networks that extend over the entire graph, reflecting the two-fold global G-symmetry. For the nonlinear sigma model

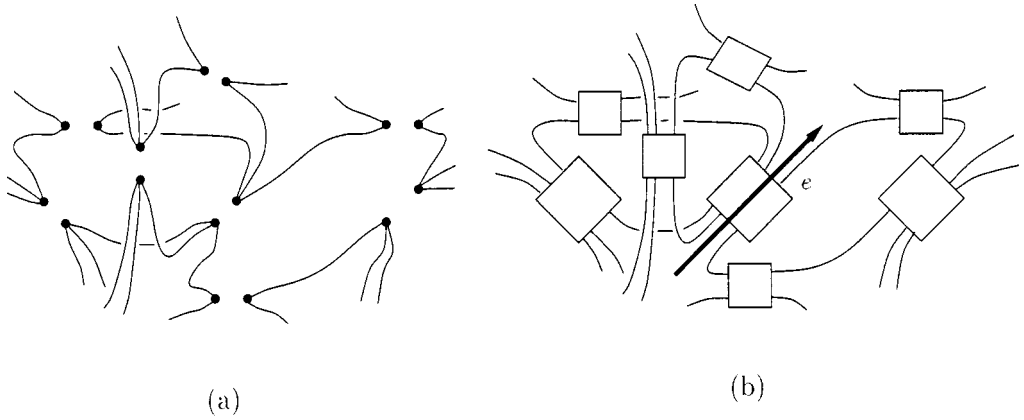

FIG. 13. An edge $e \in E$ in the boundary of three faces, two triangles and one quadrilateral. (a) The structure of the spin networks $C(v)$ in the dual partition function of lattice gauge theory (6.4). (b) The alternative formulation (6.8) using the Haar intertwiner. We have omitted labels and arrows in both diagrams.

with a massive subgroup $H \leqslant G$, the dual partition function still contains one spin network that extends over the entire graph which corresponds to a single global G-symmetry.

(5) Again there exists an alternative formulation using the Haar intertwiner rather than the sum over projectors which is stated in the following corollary. This result agrees with the purely diagrammatical picture of Ref. 18 and is illustrated in Fig. 13(b). Upon use of (2.24), we recover (6.4) and Fig. 13(a).

Corollary 6.7: Let G be a compact Lie group and (V,E,F) denote an oriented two-complex. The partition function of lattice gauge theory (6.4) is equal to

$$Z = \left(\prod_{f \in F} \sum_{\tau_f \in \mathcal{R}_G} \right) \left(\prod_{f \in F} \hat{u}_{\tau_f} \right) \left(\prod_{f \in F} \prod_{v \in f_0} \sum_{n(f,v)=1}^{\dim V_{\tau_f}} \right) \prod_{e \in E} T^{(e)}_{\underbrace{n(f,\partial_+ e)\ldots}_{f \in e_+} \underbrace{n(f,\partial_+ e)\ldots}_{f \in e_-} ; \underbrace{n(f,\partial_- e)\ldots}_{f \in e_+} \underbrace{n(f,\partial_- e)\ldots}_{f \in e_-}}, \tag{6.8}$$

where $T^{(e)}$, $e \in E$, denotes the Haar intertwiner (2.23) for the following representations:

$$T^{(e)} : \left(\bigotimes_{f \in e_+} V_{\tau_f} \right) \otimes \left(\bigotimes_{f \in e_-} V^*_{\tau_f} \right) \to \left(\bigotimes_{f \in e_+} V_{\tau_f} \right) \otimes \left(\bigotimes_{f \in e_-} V^*_{\tau_f} \right). \tag{6.9}$$

Finally, the analogous statements are available for expectation values of spin network functions.

Theorem 6.8 (Dual observable): Let G be a compact Lie group, (V,E,F) be an oriented two-complex, and Z denote the partition function (6.1) of lattice gauge theory. The expectation value of the spin network function (6.3),

$$\begin{aligned} \langle W_{\sigma,Q} \rangle = \frac{1}{Z} \left(\prod_{e \in E} \int_G dg_e \right) \prod_{f \in F} u(g_{\partial_1 f}^{\epsilon_1 f} \cdots g_{\partial_{N(f)} f}^{\epsilon_{N(f)} f}) \left(\prod_{e \in E} \sum_{k_e, \ell_e = 1}^{\dim V_{\sigma_e}} \right) \\ \times \left(\prod_{e \in E} t^{(\sigma_e)}_{k_e \ell_e}(g_e) \right) \left(\prod_{v \in V} Q^{(v)}_{\underbrace{\ell_e \ldots}_{\substack{e \in E: \\ v = \partial_- e}} \; \underbrace{k_e \ldots}_{\substack{e \in E: \\ v = \partial_+ e}}} \right), \end{aligned} \tag{6.10}$$

is equal to the following expressions:

$$\langle W_{\sigma,Q}\rangle = \frac{1}{Z}\left(\prod_{f\in F}\sum_{\tau_f\in\mathcal{R}_G}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{f\in F}\prod_{v\in f_0}\sum_{n(f,v)=1}^{\dim V_{\tau_f}}\right)\left(\prod_{e\in E}\sum_{k_e,\ell_e=1}^{\dim V_{\sigma_e}}\right)$$
$$\times\left(\prod_{v\in V} Q^{(v)}_{\underbrace{\ell_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ \underbrace{k_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}}\right)\prod_{e\in E} T^{(e)}_{\underbrace{n(f,\partial_+e)\ldots n(f,\partial_+e)\ldots k_e}_{f\in e_+}\ \underbrace{n(f,\partial_+e)\ldots}_{f\in e_-}\ ;\underbrace{n(f,\partial_-e)\ldots}_{f\in e_+}\ \underbrace{n(f,\partial_-e)\ldots \ell_e}_{f\in e_-}} \tag{6.11}$$

$$= \frac{1}{Z}\left(\prod_{f\in F}\sum_{\tau_f\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\sum_{U^{(e)}\in\tilde{\mathcal{U}}^{(e)}}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{v\in V}\tilde{C}(v)\right). \tag{6.12}$$

Here $\tilde{\mathcal{U}}^{(e)}$, $e\in E$, denotes a basis of G-invariant projectors

$$\left(\bigotimes_{f\in e_+} V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-} V^*_{\tau_f}\right)\otimes V_{\sigma_e}\to\mathbb{C}. \tag{6.13}$$

The weights per vertex $\tilde{C}(v)$ are given by a trace involving representations and projectors in the neighborhood of the vertex $v\in V$,

$$\tilde{C}(v) = \left(\prod_{\substack{e\in E:\\ v=\partial_+ e}}\sum_{k_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_- e}}\sum_{\ell_e=1}^{\dim V_{\sigma_e}}\right) Q^{(v)}_{\underbrace{\ell_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ \underbrace{k_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}}\left(\prod_{\substack{f\in F:\\ v\in f_0}}\sum_{n_f=1}^{\dim V_{\tau_f}}\right)$$
$$\times\left(\prod_{\substack{e\in E:\\ v=\partial_+ e}}\overline{U^{(e)}_{\underbrace{n_f n_f\ldots}_{f\in e_+}\ \underbrace{n_f\ldots k_e}_{f\in e_-}}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_- e}} U^{(e)}_{\underbrace{n_f n_f\ldots}_{f\in e_+}\ \underbrace{n_f\ldots \ell_e}_{f\in e_-}}\right). \tag{6.14}$$

The Haar intertwiner $T^{(e)}$, $e\in E$, in (6.11) is a map

$$T^{(e)}:\left(\bigotimes_{f\in e_+} V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-} V^*_{\tau_f}\right)\otimes V_{\sigma_e}\to\left(\bigotimes_{f\in e_+} V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-} V^*_{\tau_f}\right)\otimes V_{\sigma_e}. \tag{6.15}$$

Remark 6.9: (1) The general pattern is already familiar: The dual of the expectation value is given by a ratio of partition functions whose numerator is a modification of the partition function, here given by the background spin network (σ,Q) to which the spin foams couple. The structure remains unchanged, just the compatibility condition is modified so that the numerator of the dual expectation value is given by a sum over all spin foams bounded by the spin network (σ,Q) (Definition 3.7).

(2) The spin networks $\tilde{C}(v)$ of (6.14) are shown in Fig. 12(c). Compared with (b), there is in addition a piece of the spin network (σ,Q) in the middle of the diagram.

Similarly to the sigma models, we can again ask what are the natural functions whose expectation value under the dual partition function we can study. A construction using the center $Z(G)$, which is essentially analogous to Sec. IV E, was given in Ref. 16. In the language of the present article, it reads as follows.

Definition 6.10: Let G be a compact Lie group, (V,E,F) be an oriented two-complex, and $X:F\to Z(G)$, $f\mapsto X_f$ assign an element of the center to each face $f\in F$. The *center monopole correlator* is the following function $\mathcal{O}_X:(\mathcal{R}_G)^E\to\mathbb{C}$ of the configurations of the dual partition function (6.4),

$$\mathcal{O}_X(\{\tau_f\}_{f\in F}) := \prod_{f\in F}\tilde{t}^{(\tau_f)}(X_f), \tag{6.16}$$

where $\tilde{t}^{(\tau_f)}$ denotes the representation functions of $Z(G)$ of Lemma 2.19.

Theorem 6.11: The expectation value of the center monopole correlator under the dual partition function (6.4) reads in the original formulation

$$\langle \mathcal{O}_X \rangle_{\text{dual}} = \frac{1}{Z} \left(\prod_{e \in E} \int_G dg_e \right) \prod_{f \in F} u(gf \cdot X_f). \tag{6.17}$$

For a deliberate choice of X, this expression restricts to the monopole correlator[27] of U(1)-lattice gauge theory in $d=4$ and coincides with the $\mathbb{Z}_N$ center monopoles and vortices which are being studied in SU(N)-lattice gauge theory.

A construction using indicator functions in the dual formulation, which probe whether a particular face $f \in F$ is assigned a given representation $\tau_f \in \mathcal{R}_G$, results in a convolution of the Boltzmann weight in the original formulation. This construction proceeds in complete analogy to Sec. IV E.

B. The generalized Higgs model

In this section, we study the models that can be obtained by coupling a nonlinear sigma model with variables in G/H to a lattice gauge theory with gauge group G. When we study these models, we keep a particular Abelian special case in mind, namely the U(1)-Higgs model with frozen radial component for which Einhorn and Savit[6] have developed a duality transformation. In all the following steps, the lattice chiral model will be contained as a special case of the nonlinear sigma model for the choice $H=\{e\}$.

If we wish to couple a lattice gauge theory to the nonlinear sigma model, we have to make use of the left-action of G on G/H. A similar coupling has already been performed when we passed from the chiral model to the nonlinear sigma model. In Lemma 5.1, we have used the action of H by right-multiplication on G in order to couple one variable $h \in H$ for each edge to the variables of the chiral model. The collection of all the integrals over H for each edge just describes a lattice gauge theory with gauge group H and zero action for the gauge fields. Therefore we have coupled the chiral model with symmetry group G to a lattice gauge theory with gauge group H. The result of this ''nondynamical'' gauge field is merely to average over the cosets and therefore to give rise to a model with variables in G/H.

In this section, we couple a ''second'' gauge field with gauge group G to the chiral model which is dynamical and which realizes a lattice gauge theory as described in the previous section.

Definition 6.12: Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup, and (V,E,F) denote an oriented two-complex. Let $s_s, s_g : G \to \mathbb{R}$ be L^2-integrable class functions that are bounded below and satisfy $s_s(g^{-1}) = s_s(g)$, $s_g(g^{-1}) = s_g(g)$. The function s_g is called the *gauge action* and s_s is the *sigma model action.* Define furthermore the Boltzmann weight $u(g) = \exp(-s_g(g))$ and, using Lemma 5.1, a function $\tilde{w} : G/H \times G/H \to \mathbb{R}$ from $w(g) = \exp(-s_s(g))$. Then the generalized lattice Higgs model is given by the partition function

$$Z = \left(\prod_{e \in E} \int_G dg_e \right) \left(\prod_{v \in V} \int_{G/H} dx_v \right) \left(\prod_{f \in F} u(g_{\partial_1 f}^{\epsilon_1 f} \cdots g_{\partial_{N(f)} f}^{\epsilon_{N(f)} f}) \right) \left(\prod_{e \in E} \tilde{w}(g_e^{-1} \cdot x_{\partial_+ e}, x_{\partial_- e}) \right). \tag{6.18}$$

Remark 6.13: (1) This definition combines the partition sum of gauge theory, integration over G for each edge, with that of the nonlinear sigma model, integration over G/H for each vertex. The configurations of the partition function are elements of $G^E \times (G/H)^V$. The Boltzmann weight $u(g_f)$ of lattice gauge theory is unchanged whereas the Boltzmann weight of the nonlinear sigma model $\tilde{w}(x,y)$ is modified to $\tilde{w}(g^{-1} \cdot x, y)$ in order to implement the minimal coupling. We use g^{-1} rather than g here so that the subsequent results are consistent with the left-cosets which we have chosen for the nonlinear sigma model and with the notation established in the previous section for gauge theory.

(2) The expression does again not depend on the orientations as $\tilde{w}(g^{-1}\cdot x,y)=\tilde{w}(x,g\cdot y)$. Also we could choose different Boltzmann weights $u_f(g)$ for each face $f\in F$ and $\tilde{w}_e(x,y)$ for each edge $e\in E$.

(3) Many Higgs models with frozen radial modes appear as special cases of Definition 6.12 (see, for example, Ref. 7).

Proposition 6.14: The total Boltzmann weight of the generalized lattice Higgs model (6.18) has got a local left-G symmetry. For each function $h:V\to G$, $v\mapsto h_v$, which assigns a group element to each vertex, the Boltzmann weight is invariant under the transformations

$$\begin{aligned} x_v &\mapsto h_v\cdot x_v\,,\\ g_e &\mapsto h_{\partial_+ e}\cdot g_e\cdot h_{\partial_- e}^{-1}, \end{aligned} \tag{6.19}$$

for all $v\in V$ and $e\in E$. If in addition $H\trianglelefteq G$ is a normal subgroup, there is also a global right-G/H symmetry. Then the Boltzmann weight is invariant for each $y\in G/H$ under the transformation

$$x_v\mapsto x_v\cdot y^{-1}, \tag{6.20}$$

for all $v\in V$.

C. Expectation values

Using similar methods as in the previous sections, one can calculate all functions $G^E\times(G/H)^V\to\mathbb{C}$ that are compatible with these symmetries and therefore determine all observables whose expectation values under the partition function can be calculated.

Theorem 6.15: Any algebraic function $G^E\times(G/H)^V\to\mathbb{C}$ that is invariant under the transformations (6.19) is a linear combination of functions of the form

$$\begin{aligned} f_{\sigma,\rho,P,k_v\ldots}(\{g_e\}_{e\in E},\{x_v\}_{v\in V}) &= \left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{v\in V}\sum_{j_v=1}^{\dim V_{\rho_v}}\right)\left(\prod_{v\in V} P^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ j_v}\right)\\ &\quad\times\left(\prod_{e\in E} t^{(\sigma_e)}_{p_e q_e}(g_e)\right)\left(\prod_{v\in V} H^{(\rho_v)}_{j_v k_v}(x_v)\right). \end{aligned} \tag{6.21}$$

Here $\sigma:E\to\mathcal{R}_G$, $e\mapsto\sigma_e$ assigns an irreducible representation of G to each edge $e\in E$, and $\rho:V\to\mathcal{R}_H^G$, $v\mapsto\rho_v$ assigns a class-1 representation to each vertex $v\in V$. There are intertwiners of G,

$$P^{(v)}\in\mathrm{Hom}_G\left(\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}} V_{\sigma_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}} V^*_{\sigma_e}\right)\otimes V_{\rho_v},\mathbb{C}\right), \tag{6.22}$$

for each vertex, and the indices k_v are arbitrary, $k_v\in\{1,\ldots,\kappa_{\rho_v}\}$. If in addition $H\trianglelefteq G$ is a normal subgroup, then the invariant functions are of the form

$$\begin{aligned} f_{\sigma,\rho,P,Q}(\{g_e\}_{e\in E},\{x_v\}_{v\in V}) &= \left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{v\in V}\sum_{j_v=1}^{\dim V_{\rho_v}}\sum_{k_v=1}^{\kappa_{\rho_v}}\right) Q_{\underbrace{k_v\ldots}_{v\in V}}\left(\prod_{v\in V} P^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ j_v}\right)\\ &\quad\times\left(\prod_{e\in E} t^{(\sigma_e)}_{p_e q_e}(g_e)\right)\left(\prod_{v\in V} H^{(\rho_v)}_{j_v k_v}(x_v)\right), \end{aligned} \tag{6.23}$$

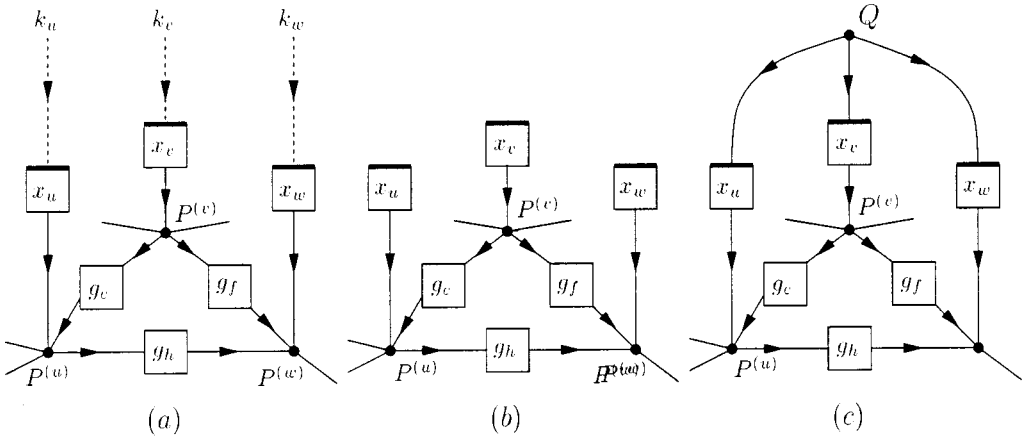

FIG. 14. The structure of the observables of the generalized Higgs model on the graph of Fig. 6(a). (a) The case (6.21) of a generic subgroup $H \leqslant G$. (b) The special case of a massive subgroup $H \leqslant G$ and (c) the situation (6.23) for a normal subgroup $H \trianglelefteq G$.

where σ, ρ, and P are as above, and Q is an intertwiner of G,

$$\bigotimes_{v \in V} V^*_{\rho_v} \to \mathbb{C}. \tag{6.24}$$

Remark 6.16: (1) These functions combine a spin network function of the type (6.3) given by the spin network (σ,P) with an observable of the type (5.10) specified by ρ and by the k_v or by ρ and Q, respectively. They are characterized by a spin network with charges (σ,P,ρ) (Definition 3.5). The fact that the local gauge transformation (6.19) also affects the variables x_v of the sigma model does not only fix the structure of the minimal coupling term, but also enforces the compatibility condition (6.22) between the spin network function and the sigma model observables. The structure of the functions (6.21) and (6.23) is illustrated in Figs. 14(a)–14(c) for the generic case, for a massive and for a normal subgroup.

(2) The chiral model coupled to a lattice gauge theory is contained as the special case for $H=\{e\}$. In this case, all dashed lines in Fig. 14(b) become solid.

D. Duality transformation

The duality transformation for the partition function (6.18) and for the expectation values of the functions (6.21) and (6.23) are straightforward using the methods established in the preceding sections. Since the expressions become very long, we only quote the results. As the very number of sum and product signs is probably deterring at first sight, we carefully comment on the meaning of the various terms and refer to the figures for illustration.

Theorem 6.17 (Dual partition function): Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup, and (V,E,F) denote an oriented two-complex. The partition function of the generalized lattice Higgs model (6.18) is equal to the following expressions,

$$Z=\left(\prod_{e\in E}\sum_{\eta_e\in\mathscr{R}_H^G}\right)\left(\prod_{f\in F}\sum_{\tau_f\in\mathscr{R}_G}\right)\left(\prod_{e\in E}\hat{w}_{\eta_e}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{f\in F}\prod_{v\in f_0}\sum_{n(f,v)=1}^{\dim V_{\tau_f}}\right)\left(\prod_{e\in E}\sum_{i_e,\ell_e=1}^{\dim V_{\eta_e}}\sum_{m_e=1}^{\kappa_{\eta_e}}\right)$$
$$\times\left(\prod_{v\in V}I^{(v)}_{\underbrace{i_e\cdots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{\ell_e\cdots}_{\substack{e\in E:\\ v=\partial_-e}};\ \underbrace{m_e\cdots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{m_e\cdots}_{\substack{e\in E:\\ v=\partial_-e}}}\right)\left(\prod_{e\in E}T^{(e)}_{\underbrace{n(f,\partial_+e)\cdots}_{f\in e_+}\underbrace{n(f,\partial_+e)\cdots}_{f\in e_-}i_e;\underbrace{n(f,\partial_-e)\cdots}_{f\in e_+}\underbrace{n(f,\partial_-e)\cdots}_{f\in e_-}\ell_e}\right) \tag{6.25}$$

$$=\left(\prod_{e\in E}\sum_{\eta_e\in\mathscr{R}_H^G}\right)\left(\prod_{v\in V}\sum_{S^{(v)}\in\mathscr{S}^{(v)}}\right)\left(\prod_{f\in F}\sum_{\tau_f\in\mathscr{R}_G}\right)\left(\prod_{e\in E}\sum_{U^{(e)}\in\mathscr{U}^{(e)}}\right)\left(\prod_{e\in E}\hat{w}_{\eta_e}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)$$
$$\times\left(\prod_{e\in E}\sum_{m_e=1}^{\kappa_{\eta_e}}\right)\left(\prod_{v\in V}S^{(v)}_{\underbrace{m_e\cdots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{m_e\cdots}_{\substack{e\in E:\\ v=\partial_-e}}}\right)\prod_{v\in V}D(v), \tag{6.26}$$

where for each $v\in V$,

$$D(v)=\left(\prod_{\substack{f\in F:\\ v\in f_0}}\sum_{n_f=1}^{\dim V_{\tau_f}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_-e}}\sum_{\ell_e=1}^{\dim V_{\eta_e}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_+e}}\sum_{i_e=1}^{\dim V_{\eta_e}}\right)\overline{S^{(v)}_{\underbrace{i_e\cdots}_{\substack{e\in E:\\ v=\partial_+e}}\ \underbrace{\ell_e\cdots}_{\substack{e\in E:\\ v=\partial_-e}}}}$$
$$\times\left(\prod_{\substack{e\in E\\ v=\partial_+e}}\overline{U^{(e)}_{\underbrace{n_f\cdots n_f\cdots i_e}_{f\in e_+f\in e_-}}}\right)\left(\prod_{\substack{e\in E\\ v=\partial_-e}}\overline{U^{(e)}_{\underbrace{n_f\cdots n_f\cdots\ell_e}_{f\in e_+f\in e_-}}}\right). \tag{6.27}$$

Here $\hat{u}_\tau$ and $\hat{w}_\eta$ denote the character expansion coefficients of the functions $u(g)$ and $w(g)$ of Definition 6.12. For each edge $e\in E$, $\mathcal{U}^{(e)}$ is a basis of G-invariant projectors

$$\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}\to\mathbb{C}, \tag{6.28}$$

and for each vertex $v\in V$, $\mathcal{S}^{(v)}$ denotes a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\eta_e}\right)\to\mathbb{C}. \tag{6.29}$$

The coset space Haar map $I^{(v)}$, $v\in V$, in (6.25) is a map

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\eta_e}\right)\to\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_-e}}V^*_{\eta_e}\right), \tag{6.30}$$

while the Haar intertwiner $T^{(e)}$, $e\in E$, maps

$$\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}\to\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}. \tag{6.31}$$

Remark 6.18: (1) We first comment on the dual partition function in the form (6.26). The dual partition sum comprises the partition sums of both the nonlinear sigma model and of lattice gauge

theory. For the nonlinear sigma model, we have a sum over all colorings of the edges with class-1 representations η_e and a sum over all colorings of the vertices with compatible intertwiners $S^{(v)}$ where the compatibility condition (6.29) is the same as for the nonlinear sigma model. For lattice gauge theory, there are additional sums over all colorings of the faces with irreducible representations τ_f and of the edges with compatible intertwiners $U^{(e)}$. This compatibility condition (6.28) is, however, not the same as in lattice gauge theory. The minimal coupling term has modified this condition so that each spin foam appearing in the dual of the gauge theory sector is bounded by the spin network that occurs in the dual of the nonlinear sigma model. In other words, the spin network diagrams of the high temperature expansion of the nonlinear sigma model appear as spin network functions whose expectation value is calculated under the partition function of gauge theory. The minimal coupling term of the generalized Higgs model could have been found from this entirely dual point of view.

(2) In addition to the character expansion coefficients, we find under the dual partition sum several spin networks. There is one would-be spin network from the nonlinear sigma model, given by the representations V_{η_c} and by the intertwiners $S^{(v)}$ which extends over the entire graph. It does not form a proper spin network because the summation over the indices m_e extends only over $1,...,\kappa_{\rho_e}$, i.e., over the H-invariant subspaces of the representations. This is the same type of network that is usually denoted by dashed lines and has already appeared in the dual partition function of the nonlinear sigma model [see the top layer of Fig. 11(a)].

(3) Under the partition sum, there are furthermore the spin networks denoted by $D(v)$ for each vertex. They are similar to the spin networks $C(v)$ from the dual partition function of lattice gauge theory (6.6), but include in addition a part of the spin network given by the representations V_{η_e} and the intertwiners $\overline{S^{(v)}}$. The difference between the $C(v)$ of lattice gauge theory and the $D(v)$ appearing here is essentially the same as that of the $C(v)$ and the $\widetilde{C}(v)$, cf. Figs. 12(b) and 12(c). The neighborhood of a vertex with the spin network $D(v)$ and the dashed lines of the would-be spin network is shown in Fig. 15(a).

(4) The structure of the dual partition function (6.26) of the generalized Higgs model can be explained in other words starting from the corresponding expression of the chiral model [Fig. 7(a)]. First, we are concerned with the nonlinear sigma model rather than with the chiral model. This was implemented by coupling elements $h \in H$ to one chiral half of the model which corresponds to the top layer in Fig. 7(a), and then by averaging over the subgroup in Lemma 5.1. This averaging is the reason why the top layer of Fig. 11(a) consists of dashed lines (''would-be spin network''). Then we have minimally coupled lattice gauge theory to the other chiral half which corresponds to the spin network in the bottom layer of Fig. 7(a). The effect of the minimal coupling term is that lattice gauge theory just considers this spin network as an observable to which it couples its spin foams. The bottom layer of Fig. 7(a) is therefore treated as the spin network function in the expectation value of lattice gauge theory, and becomes disconnected, leading to Fig. 12(c) for lattice gauge theory and to Fig. 15(a) for the generalized Higgs model.

(5) As usual, there is an alternative formulation of the dual partition function which uses the Haar intertwiners and Haar maps rather than sums over projectors. This version is given in the first equation (6.25).

(6) As G acts transitively on G/H, one can easily fix a ''unitary'' gauge by choosing $h_v := g_{x_v}^{-1}$ in (6.19) where g_{x_v} is a representative of x_v. This step is often convenient because it removes the scalar degrees of freedom from the model. For the duality transformation it is, however, pointless because the corresponding symmetry is already manifest in the dual picture.

Finally, the duality transformation is also available for the expectation value of the observable (6.23). The result is stated in the following theorem which contains the most complicated formulas we are going to present. We formulate the result for the correlator in the form (6.23). If $H \leqslant G$ is a non-normal subgroup, then the requirement that Q is G-invariant can be dropped so that one recovers the expression (6.21) for generic $k_v \in \{1,...,\kappa_{\rho_v}\}$.

Theorem 6.19 (Dual observable): Let G be a compact Lie group, $H \leqslant G$ be a Lie subgroup,

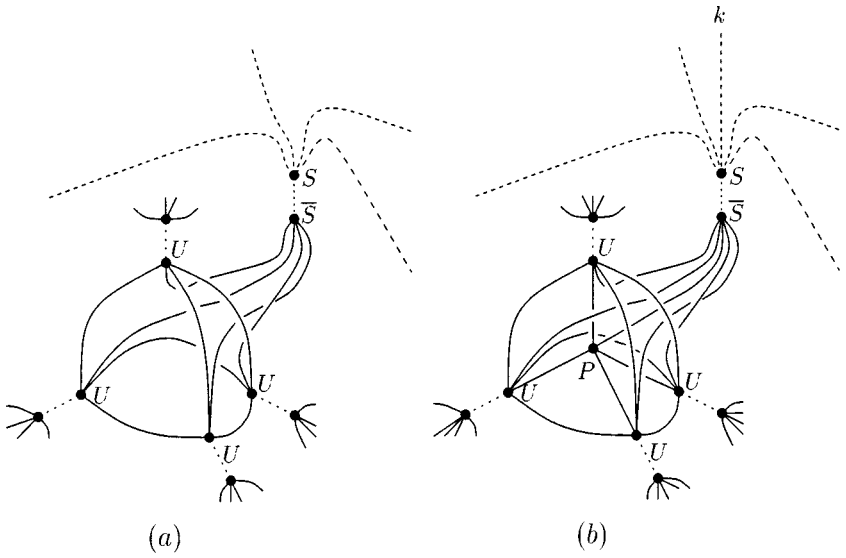

FIG. 15. (a) The dual partition function (6.26) of the generalized Higgs model in the neighborhood of a vertex with a spin network $D(v)$ of (6.27). (b) The analogous diagram for the dual expression (6.33) of the expectation value of an observable (6.21).

and (V,E,F) denote an oriented two-complex. The expectation value of the function (6.23) under the partition function of the generalized Higgs model is equal to

$$\begin{aligned}
\langle f_{\sigma,\rho,P,Q}\rangle = \frac{1}{Z}&\left(\prod_{e\in E}\sum_{p_e,q_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{v\in V}\sum_{j_v=1}^{\dim V_{\rho_v}}\sum_{k_v=1}^{\kappa_{\rho_v}}\right)Q_{\underbrace{k_v\ldots}_{v\in V}}\left(\prod_{v\in V}P^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ j_v}\right)\left(\prod_{e\in E}\sum_{\eta_e\in\mathcal{R}_H^G}\right)\\
&\times\left(\prod_{f\in F}\sum_{\tau_f\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\hat{w}_{\eta_e}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{f\in F}\prod_{v\in f_0}\sum_{n(f,v)=1}^{\dim V_{\tau_f}}\right)\left(\prod_{e\in E}\sum_{i_e,\ell_e=1}^{\dim V_{\eta_e}}\sum_{m_e=1}^{\kappa_{\eta_e}}\right)\\
&\times\left(\prod_{v\in V}I^{(v)}_{\underbrace{i_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{\ell_e\ldots}_{\substack{e\in E:\\ v-\partial_- e}}\ j_v\,;\,\underbrace{m_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{m_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ k_v}\right)\\
&\times\left(\prod_{e\in E}T^{(e)}_{\underbrace{n(f,\partial_+e)\ldots n(f,\partial_+e)\ldots i_e}_{f\in e_+}\ \underbrace{p_e}_{f\in e_-}\,;\,\underbrace{n(f,\partial_-e)\ldots n(f,\partial_-e)\ldots \ell_e}_{f\in e_+}\ \underbrace{q_e}_{f\in e_-}}\right)\qquad(6.32)\\
=\frac{1}{Z}&\left(\prod_{v\in V}\sum_{k_v=1}^{\kappa_{\rho_v}}\right)Q_{\underbrace{k_v\ldots}_{v\in V}}\left(\prod_{e\in E}\sum_{\eta_e\in\mathcal{R}_H^G}\right)\left(\prod_{v\in V}\sum_{S^{(v)}\in\tilde{\mathcal{S}}^{(v)}}\right)\left(\prod_{f\in F}\sum_{\tau_f\in\mathcal{R}_G}\right)\left(\prod_{e\in E}\sum_{U^{(e)}\in\tilde{\mathcal{U}}^{(e)}}\right)\\
&\times\left(\prod_{e\in E}\hat{w}_{\eta_e}\right)\left(\prod_{f\in F}\hat{u}_{\tau_f}\right)\left(\prod_{e\in E}\sum_{m_e=1}^{\kappa_{\eta_e}}\right)\left(\prod_{v\in V}S^{(v)}_{\underbrace{m_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{m_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}\ k_v}\right)\prod_{v\in V}\tilde{D}(v),
\end{aligned}$$

(6.33)

where

$$\tilde{D}(v)=\left(\prod_{\substack{f\in F:\\ v\in f_0}}\sum_{n_f=1}^{\dim V_{\tau_f}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_- e}}\sum_{\ell_e=1}^{\dim V_{\eta_e}}\sum_{q_e=1}^{\dim V_{\sigma_e}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_+ e}}\sum_{i_e=1}^{\dim V_{\eta_e}}\sum_{p_e=1}^{\dim V_{\sigma_e}}\right)$$
$$\times\sum_{j=1}^{\dim V_{\rho_v}}\times P^{(v)}_{\underbrace{p_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{q_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}}\ \overline{j S^{(v)}_{\underbrace{i_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{\ell_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}}\ j}\left(\prod_{\substack{e\in E\\ v=\partial_+ e}}\overline{U^{(e)}_{\underbrace{n_f\ldots}_{f\in e_+}\underbrace{n_f\ldots}_{f\in e_-}\ i_e p_e}}\right)$$
$$\times\left(\prod_{\substack{e\in E\\ v=\partial_- e}}U^{(e)}_{\underbrace{n_f\ldots n_f\ldots}_{f\in e_+ f\in e_-}\ \ell_e q_e}\right). \tag{6.34}$$

For each edge $e\in E$, $\tilde{\mathcal{U}}^{(e)}$ denotes a basis of G-invariant projectors

$$\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}\otimes V_{\sigma_e}\to\mathbb{C}, \tag{6.35}$$

and for each vertex $v\in V$, $\tilde{\mathcal{S}}^{(v)}$ is a basis of G-invariant projectors

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}}V^*_{\eta_e}\right)\otimes V_{\rho_v}\to\mathbb{C}. \tag{6.36}$$

The coset space Haar map $I^{(v)}$, $v\in V$, in (6.32) is a map

$$\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}}V^*_{\eta_e}\right)\otimes V_{\rho_v}\to\left(\bigotimes_{\substack{e\in E:\\ v=\partial_+ e}}V_{\eta_e}\right)\otimes\left(\bigotimes_{\substack{e\in E:\\ v=\partial_- e}}V^*_{\eta_e}\right)\otimes V_{\rho_v}, \tag{6.37}$$

while the Haar intertwiner $T^{(e)}$, $e\in E$, maps

$$\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}\otimes V_{\sigma_c}\to\left(\bigotimes_{f\in e_+}V_{\tau_f}\right)\otimes\left(\bigotimes_{f\in e_-}V^*_{\tau_f}\right)\otimes V^*_{\eta_e}\otimes V_{\sigma e}. \tag{6.38}$$

Remark 6.20: (1) The features that are new in the dual expectation value (6.32) compared with the dual partition function (6.25) are first the sums and intertwiners from the definition (6.23). The presence of the spherical functions $H^{(\rho_v)}_{j_v k_v}$ for each vertex $v\in V$ has lead to an additional representation V_{ρ_v} in the coset space Haar map (6.37) and thus to a modification of the compatibility condition (6.36). The presence of the representation function $t^{(\sigma_e)}_{p_e q_c}$ has resulted in an additional representation V_{σ_e} of the Haar intertwiner (6.38) and thus in a modification of the compatibility condition (6.35). The correlator (6.23), which is given by a spin network with charges, has modified the numerator of (6.23) so that the configurations of the dual picture, spin foams bounded by spin networks, are now themselves bounded by the given spin network with charges. The structure of (6.33) is illustrated in Fig. 15(b) which shows the spin network $\tilde{D}(v)$ in the neighborhood of a vertex.

(2) For the special cases in which H is normal or massive, the situation is completely analogous to the nonlinear sigma model. The only changes in these cases apply to the open ends of the dashed lines labeled k_v.

E. Expectation values of the dual model

It is possible to construct natural observables for the dual partition function of the generalized Higgs model in the same way as for the nonlinear sigma model and for lattice gauge theory. If these observables only probe the representations η_e assigned to the edges and τ_f assigned to the faces, the result is the product of a dual observable of the nonlinear sigma model and one of lattice gauge theory, both independent of each other.

F. The Abelian special case

In analogy to Sec. IV D, we show the Abelian special case of the generalized Higgs model for $G=U(1)$, $H=\{e\}$, in greater detail.

We write $e^{i\varphi_e}\in U(1)$, $e\in E$, for the variables of lattice gauge theory and $e^{i\vartheta_v}$, $v\in V$, for the sigma model. The partition function (6.18) then reads

$$Z=\left(\prod_{v\in V}\frac{1}{2\pi}\int_0^{2\pi}d\vartheta_v\right)\left(\prod_{e\in E}\frac{1}{2\pi}\int_0^{2\pi}d\varphi_e\right)\left(\prod_{f\in F}\exp(-s_g(e^{i\Sigma_{j=1}^{N(f)}(\epsilon_j f)\cdot\varphi_{\partial_j f}}))\right)$$
$$\times\left(\prod_{e\in E}\exp(-s_s(e^{i(\vartheta_{\partial_+ e}-\vartheta_{\partial_- e}+\varphi_e)}))\right). \tag{6.39}$$

This is the U(1)-Higgs model studied by Einhorn and Savit.[6] The dual expression for the partition function, Eq. (6.26), specializes to

$$Z=\left(\prod_{e\in E}\sum_{\ell_e=-\infty}^{\infty}\right)\left(\prod_{f\in F}\sum_{k_f=-\infty}^{\infty}\right)\left(\prod_{e\in E}\hat{w}_{\ell_e}\right)\left(\prod_{f\in F}\hat{u}_{k_f}\right)$$
$$\times\left(\prod_{v\in V}\delta\left(\sum_{\substack{e\in E:\\ v=\partial_+ e}}\ell_e-\sum_{\substack{e\in E:\\ v=\partial_- e}}\ell_e\right)\right)\left(\prod_{e\in E}\delta\left(\sum_{f\in e_+}k_f-\sum_{f\in e_-}k_f+\ell_e\right)\right), \tag{6.40}$$

where $\hat{w}_\ell$ and $\hat{u}_k$ are the Fourier coefficients of $w(g)=\exp(-s_s(g))$ and $u(g)=\exp(-s_g(g))$, $g\in\mathrm{U}(1)$, respectively. This expression combines the dual partition function (4.35) of the XY-model with that of U(1)-lattice gauge theory and implements the minimal coupling by the compatibility condition encoded in the constraint. It agrees with the result of Ref. 6 before the constraint is integrated.

Since the labellings of the edges with integers ℓ_e and of the faces with integers k_f are Abelian, we can visualize (6.40) as a sum over all closed lines living on the edges together with a sum over all closed surfaces living on the faces where each surface is either closed or bounded by one of the lines.

If we use the Villain action for both the sigma model and gauge theory, i.e., $\hat{w}_\ell=e^{-\ell^2/2\beta_1}$ and $\hat{u}_k=e^{-k^2/2\beta_2}$, then the total exponent of the dual Boltzmann weight is the length of the lines weighted with $1/\beta_1$ plus the area of the surfaces weighted with $1/\beta_2$. This is the effective (open) string model for the strong coupling regime of the U(1)-Higgs model.

The observables (6.23) reduce to functions

$$f_{p_v\ldots,q_e\ldots}(\{\vartheta_v\}_{v\in V};\{\varphi_e\}_{e\in E}):=\left(\prod_{v\in V}e^{ip_v\vartheta_v}\right)\left(\prod_{e\in E}e^{iq_e\varphi_e}\right), \tag{6.41}$$

which describe charges $p_v\in\mathbb{Z}$ at the vertices $v\in V$ and Wilson loops $q_e\in\mathbb{Z}$ at the edges $e\in E$ provided that for each $v\in V$, the following compatibility condition holds:

$$\sum_{\substack{e\in E:\\ v=\partial_+ e}}q_e-\sum_{\substack{e\in E:\\ v=\partial_- e}}q_e+p_v=0. \tag{6.42}$$

The dual of the expectation value then reads

$$\langle f_{p_v \ldots, q_e \ldots} \rangle = \frac{1}{Z} \left(\prod_{e \in E} \sum_{\ell_e = -\infty}^{\infty} \right) \left(\prod_{f \in F} \sum_{k_f = -\infty}^{\infty} \right) \left(\prod_{e \in E} \hat{w}_{\ell_e} \right) \left(\prod_{f \in F} \hat{u}_{k_f} \right) \times \left(\prod_{v \in V} \delta \left(\sum_{\substack{e \in E: \\ v = \partial_+ e}} \ell_e - \sum_{\substack{e \in E: \\ v = \partial_- e}} \ell_e + p_v \right) \right) \left(\prod_{e \in E} \delta \left(\sum_{f \in e_+} k_f - \sum_{f \in e_-} k_f + \ell_e + q_e \right) \right), \tag{6.43}$$

i.e., the closed lines of (6.40) now couple to the charges p_v, $v \in V$, and can thus end at one of these charges while the surfaces are either closed or bounded by the lines or by the background Wilson loop q_e, $e \in E$.

This is the picture which is generalized to sums over spin networks and spin foams in the non-Abelian case.

VII. DISCUSSION

We have presented an exact duality transformation for the partition functions and expectation values of observables of the lattice chiral model, of the lattice nonlinear sigma model, and of a class of generalized Higgs models. We conclude with various miscellaneous comments on applications, limitations, and open questions.

Throughout the present article, we have chosen *ultra-local* actions, i.e., the action is a sum over all edges (or faces) and can be calculated independently for each edge (or face). A generalization to more complicated, less local, actions is straightforward. Observe that the character expansion of the Boltzmann weight is always a series of charges (or spin network functions) and that we can perform the duality transformation for generic expectation values of these charges (or spin network functions).

The dual form of the partition function can be used for numerical studies. From the Abelian special case it is familiar (see, for example, Ref. 31) that for some observables the original model is much easier to simulate whereas for others the simulations are much more efficient in the dual model. At present, algorithms are being developed for pure SU(2)-lattice gauge theory in three dimensions[32] and for a technically closely related model[33] in the context of quantum gravity.

If one wishes to implement Monte Carlo algorithms for the dual model, one has to make sure that the importance sampling is applied to a positive measure. While the character expansion coefficients of the common Boltzmann weights are positive, the situation is less clear for the spin networks [such as the $C(v)$ of (6.6)] which appear under the dual partition sum. At least for the O(4)-symmetric nonlinear sigma model and for the SU(2)-symmetric chiral model, these spin networks have non-negative real values.[34] Should there be alternating signs in other models, one has to associate the sign with the observable which is measured while the modulus can be dealt with by the importance sampling. This is familiar, for example, from the sign problems in the simulation of fermionic systems.

It might finally be more than a mere coincidence that the dual partition function resembles a cluster decomposition. The lack of efficient cluster algorithms for gauge theories may have a natural explanation in the dual picture where the weights $C(v)$ of lattice gauge theory are localized at the vertices as opposed to the spin network which appears in the dual sigma model and which extends over the entire lattice.

We emphasize that there are intermediate steps in the duality transformation, for example (4.20) and (5.19), in which both the old and the new variables are present and which resemble an extended ''phase space'' path integral whose weight, however, does not have any obvious positivity properties. Upon solving all sums, one recovers the original partition function with positive Boltzmann weights, while performing the integrals, one obtains the dual expression, again with positive weights (at least in some cases which we have listed above).

In the Abelian case, there are higher level generalizations of sigma models and gauge theories in which the fundamental variables are located not at vertices or edges, but rather at higher level, e.g., at cubes, hypercubes etc., and described by discretized k-forms.[2,3] This construction does not have any obvious generalization to the non-Abelian case. Any such model would make use of a suitable definition of non-Abelian cohomology.

We also stress that the non-Abelian generalization of the duality transformation parallels the Abelian special case only up to the point where one solves the constraints. In the non-Abelian situation, there are no longer just constraints, but rather sums over compatible intertwiners so that there exists no obvious step which generalizes the integration of the constraints. This restricts us to the original lattice as opposed to the Abelian case in which one usually passes to a suitable "dual" lattice. This can, however, also be seen as an advantage because our generalization is therefore independent of the topology of the lattice. The case of nontrivial topology in Abelian systems was studied in Ref. 35.

An interesting generalization of lattice gauge theory is available in $d \leqslant 4$ dimensions in the dual formulation where one can replace the gauge group by a quantum group.[17,18] This includes in particular supergroups as the gauge groups. Similar constructions in which the category of representations of a compact Lie group in the dual formulation is replaced by more general categories have already been known from the definition of topological invariants and from topological quantum field theory, (see, for example, Refs. 36 and 37). From the formulas stated in the present article, one obtains at least a formal topological invariant from the partition functions if the Boltzmann weights, say, $w(g)$, are replaced by δ-functions $w(g)=\delta(g)$ and similarly $\hat{w}_\rho = \dim V_\rho$ in the dual picture. Noncompact Lie groups have recently attracted attention in the context of quantum gravity, (see, for example, Ref. 38).

What has been missing so far is, first, a generalization which includes fermions (this is mainly due to the still rather limited understanding of fermions in a non perturbative formulation) and, second, an analog of the vortex–spin wave decomposition of Refs. 39 and 40.

The present article is entirely written in the Lagrangian language of path integrals and expectation values. All results are in one-to-one correspondence to the analogous statements in the Hamiltonian formulation which involves the quantum statistical operator e^{-H}. Matrix elements of this operator can be calculated in the dual picture from sums over spin networks and spin foams. (A detailed study is in preparation.)

As far as the strong–weak relation of the duality transformation is concerned, we stress that the dual partition function provides a closed form for the strong coupling expansion which makes it possible to separate the group combinatorics from the lattice combinatorics. This has been advocated in the context of high-order strong coupling expansions (see, for example, Refs. 7 and 41). The key to the duality transformation was to abstract from a particular group and to focus on the structures that are common to all compact Lie groups. It remains a considerable challenge to evaluate the dual expressions for particular groups, Boltzmann weights, and shapes of the lattice.

As far as the construction of strong coupling expansions in gauge theories is concerned, it is interesting to note that there exists an effective string model which describes the strong coupling regime of Abelian lattice gauge theories. In the non-Abelian case, however, mere strings are insufficient, and the world-sheets of the strings should rather be allowed to branch according to the combinatorics of the representation theory. A familiar example is the strong coupling calculation of the static three-quark potential in QCD. The lack of branchings of the world-sheets causes the string picture to break down when spin foams appear as the fundamental nonperturbative structure.

ACKNOWLEDGMENTS

The author is grateful to Emmanuel College, Cambridge, for a Research Fellowship. I thank Alan Sokal who suggested to extend the techniques of the duality transformation to sigma models. I am also grateful to John Barrett, Alan Macfarlane, Shahn Majid, Robert Oeckl, Daniele Oriti, Arttu Rajantie, Nuno Romão, Tony Sudbury, and Toby Wiseman for valuable discussions and for comments on the relevant literature.

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Entropic repulsion for a Gaussian lattice field with certain finite range interaction

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(Received 15 January 2003; accepted 10 April 2003)

Consider the centered Gaussian field on $\mathbb{Z}^d$, $d \geqslant 2l+1$, with covariance matrix given by $(\Sigma_{j=l}^{K} q_j(-\Delta)^j)^{-1}$ where Δ is the discrete Laplacian on $\mathbb{Z}^d$, $1 \leqslant l \leqslant K$ and $q_j \in \mathbb{R}, l \leqslant j \leqslant K$ are constants satisfying $\Sigma_{j=l}^{K} q_j r^j > 0$ for $r \in (0,2]$ and a certain additional condition. We show the probability that all spins are positive in a box of volume N^d decays exponentially at a rate of order $N^{d-2l} \log N$ and under this hard-wall condition, the local sample mean of the field is repelled to a height of order $\sqrt{\log N}$. This extends the previously known result for the case that the covariance is given by the Green function of simple random walk on $\mathbb{Z}^d$ (i.e., $K=l=1, q_1=1$). © *2003 American Institute of Physics.* [DOI: 10.1063/1.1581354]

I. INTRODUCTION

We consider the continuous spin lattice models with massless interaction which can be thought of as an effective modelization of the random interface. The configuration $\phi = \{\phi_x\}_{x \in \mathbb{Z}^d} \in \mathbb{R}^{\mathbb{Z}^d}$ is interpreted as a (discretized) interface embedded in the $d+1$-dimensional space and the spin ϕ_x at the site $x \in \mathbb{Z}^d$ denotes the height of the interface. Formally speaking, for the Hamiltonian $H(\phi)$, the corresponding Gibbs measure is defined by

$$P(d\phi) = \frac{1}{Z} \exp\{-H(\phi)\} \prod_{x \in \mathbb{Z}^d} d\phi_x,$$

where $d\phi_x$ is Lebesgue measure on $\mathbb{R}$ and Z is a normalization factor. When the (formal) Hamiltonian is given by $H_0(\phi) = \Sigma_{\langle x,y \rangle} V(\phi_x - \phi_y)$ for appropriate potential V where the summation is taken over all nearest neighbor sites x and y, this model is called the massless fields model and recently the study of this model has been rapidly developing from both dynamical and statical aspects (cf. Ref. 14).

One of the problems related to the interfaces is the study of the effect of a hard wall. In this article we consider the problem of the entropic repulsion, that is, to examine the asymptotic behavior of the lattice massless fields under the condition that the height variables are all positive in a large finite box (cf. Ref. 20). To consider such asymptotics plays an important role in the construction of droplets on a hard wall (cf. Refs. 1 and 3) and also it is closely related to the problem of the wetting transition (cf. Refs. 6 and 8). For Gaussian case (harmonic crystal) it has been studied in Refs. 4, 5, 9, and 10 with several boundary conditions and a non-Gaussian case (anharmonic crystal) was studied in Ref. 11. But these results treated the Hamiltonian $H_0(\phi)$, the so-called $\nabla\phi$ models.

The purpose of this article is to investigate the entropic repulsion for a much more wide class of interactions determined by certain quadratic potentials. Namely, we consider the following (formal) Hamiltonian $H_1(\phi)$ instead of $H_0(\phi)$:

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$$H_1(\phi)=\sum_{j=1}^{K} q_j \sum_{x\in\mathbb{Z}^d} V((-\Delta)^{j/2}\phi_x) \qquad \text{with } V(r)=r^2, \tag{1}$$

where $K\in\mathbb{N}$, $q=\{q_j\}_{1\leqslant j\leqslant K}\in\mathbb{R}^K$ and Δ is the discrete Laplacian on $\mathbb{Z}^d$. If j is odd, we consider $\Sigma_{x\in\mathbb{Z}^d}((-\Delta)^{j/2}\phi_x)^2$ as $\Sigma_{i=1}^{d}\Sigma_{x\in\mathbb{Z}^d}((-\Delta)^{[j/2]}\nabla_i\phi_x)^2$ where $[j/2]$ is an integral part of $j/2$ and ∇_i is the discrete gradient on $\mathbb{Z}^d$ for ith direction. Similarly to the $\nabla\phi$ case, this Hamiltonian has a continuum symmetry, i.e., changing the value of heights by adding a constant at each site does not change the Hamiltonian. When $d\geqslant 2l+1$ for $l=\min\{j;q_j\neq 0\}$, a corresponding infinite volume Gibbs measure actually exists and is characterized by DLR equations. It determines a Gaussian field on $\mathbb{Z}^d$; see Sec. II for more details.

The Hamiltonian $H_1(\phi)$ is related to several physical and mathematical models. For example, in the model of the membrane such as a lipid bilayer, the energy of the interface separating the water phase and the lipid phase is given by

$$H(\phi)=\sum_{x\in\mathbb{Z}^d}(\kappa_1(\nabla\phi_x)^2+\kappa_2(\Delta\phi_x)^2),$$

where κ_1 and κ_2 are called lateral tension and bending rigidity, respectively (cf. Refs. 23 and 26). And also when $d=1$, $K=2$ and $q_1=0, q_2>0$, this model corresponds to the integration of random walks which was studied in Ref. 25 (see Ref. 16 for the continuum version).

In Sec. II, we give a precise formulation of our model and state the results. The proof will be given in Secs. III and IV. Finally, in Sec. V we show the asymptotics of the Green function and the convergence of the capacity which are used in the proof. The strategy of the proof is similar to those for $\nabla\phi$ models. However, in our case, since we do not have the random walk representation of conditional expectation and covariance as $\nabla\phi$ models (cf. Refs. 2 and 5), we need to consider another conditioning argument which depends on the Markov property of the ϕ field and the range of the interaction.

II. MODEL AND RESULTS

Let $q(r)=\Sigma_{j=1}^{K}q_j r^j$, $q=\{q_j\}_{1\leqslant j\leqslant K}\in\mathbb{R}^K$, be a polynomial of degree $K\in\mathbb{N}$. Define $J_\varepsilon(x,y)=q(\varepsilon I-\Delta)(x,y)$ for $\varepsilon\geqslant 0$ and $x,y\in\mathbb{Z}^d$, where I is an identity matrix and Δ is the discrete Laplacian on $\mathbb{Z}^d$ determined by

$$(-\Delta)(x,y)=\begin{cases} -\dfrac{1}{2d} & \text{if } |x-y|=1,\\ 1 & \text{if } |x-y|=0,\\ 0 & \text{otherwise,}\end{cases}$$

and for $j\geqslant 2$

$$(-\Delta)^j(x,y)=\sum_{z_i\in\mathbb{Z}^d;\ i=1,2,\ldots,j-1}(-\Delta)(x,z_1)(-\Delta)(z_1,z_2)\cdots(-\Delta)(z_{j-1},y).$$

We will denote $J_0(x,y)$ by $J(x,y)$. At first we assume the following:

Assumption 1:

(i) $d\geqslant 2l+1$ where $l=\min\{j;q_j\neq 0\}$,
(ii) $\Sigma_{j=l}^{K}q_j r^j>0$ for every $0<r\leqslant 2$.

For any absolutely summable function $f:\mathbb{Z}^d\to\mathbb{R}$, we will denote its Fourier transform by $\hat{f}(\theta)=\Sigma_{x\in\mathbb{Z}^d}e^{i\theta\cdot x}f(x)$, $\theta\in[-\pi,\pi]^d$. It is easy to see that J_ε is translation invariant and $\hat{J}_\varepsilon(\theta)=\Sigma_{x\in\mathbb{Z}^d}e^{i\theta\cdot x}J_\varepsilon(0,x)=\Sigma_{j=l}^{K}q_j(\varepsilon+\mu(\theta))^j$ where $\mu(\theta)=(1/d)\Sigma_{i=1}^{d}(1-\cos\theta_i)$ is the Fourier

transform of $-\Delta$. From Assumption 1 and the fact that $\mu(\theta)=(1/2d)|\theta|^2+o(|\theta|^2)$ as $|\theta|\to 0$, $\hat{J}_\varepsilon(\theta)\geqslant 0$ and $\hat{J}_\varepsilon(\theta)^{-1}$ is integrable over $[-\pi,\pi]^d$ for any $\varepsilon\geqslant 0$ small enough. Hence, in this case, J_ε is positive definite, i.e., $\Sigma_{x,y\in\mathbb{Z}^d}J_\varepsilon(x,y)\xi_x\xi_y\geqslant 0$ for every $\xi=\{\xi_x\}_{x\in\mathbb{Z}^d}$ of finite range and the equality holds only when $\xi\equiv 0$. Therefore, J_ε^{-1} exists and it is also positive definite (cf. Chap. 13 of Ref. 13). Thus the centered Gaussian field on $\mathbb{Z}^d$ with covariance matrix $G=J^{-1}$ exists. We will denote its law on $\Omega\equiv\mathbb{R}^{\mathbb{Z}^d}$ by P. The infinite volume measure P is characterized by the following DLR equation as an infinite Gibbs distribution (cf. Ref. 13):

$$P(\cdot\,|\mathcal{F}_{\{x\}^c})=\mathcal{N}\left(-J(0,0)^{-1}\sum_{y\neq x}J(x,y)\phi_y,\,J(0,0)^{-1}\right)\qquad P\text{-a.s. }\phi,$$

where $\mathcal{F}_{\{x\}^c}=\sigma(\phi_y;y\neq x)$ is the σ-field generated by $\{\phi_y;y\neq x\}$ and $\mathcal{N}(m,\sigma^2)$ denotes the normal distribution with mean m and variance σ^2. Positivity of the variance $J(0,0)^{-1}$ follows from the positive definiteness of J.

Remark 2.1: Formally speaking, by summation by parts the measure P is represented as

$$P(d\phi)=\frac{1}{Z}\exp\left\{-\sum_{j=1}^{K}\left(\frac{1}{2d}\right)^{a_j}q_j\sum_{x\in\mathbb{Z}^d}((-\Delta)^{j/2}\phi_x)^2\right\}\prod_{x\in\mathbb{Z}^d}d\phi_x,$$

where $a_j=1$ if j is odd and $a_j=0$ if j is even. Hence P corresponds to the Gibbs measure with Hamiltonian $H_1(\phi)$ defined by (1).

Remark 2.2: By Lemma 5.1 below, we have

$$\mathrm{Cov}(\phi_x,\phi_y)\sim\frac{C}{|x-y|^{d-2l}}\quad\text{as }|x-y|\to\infty,$$

for some constant C when $d\geqslant 2l+1$. This implies that the field has a long range correlation similar to the $\nabla\phi$ interface model.

The following second assumption implies $G(x,y)=J^{-1}(x,y)\geqslant 0$ for all $x,y\in\mathbb{Z}^d$ which ensures that we can use a FKG inequality for the measure P (cf. Ref. 24).

Assumption 2: There exists a sequence of positive small numbers $\{\varepsilon_k\}_{k\geqslant 1}$ such that $\varepsilon_k\downarrow 0$ as $k\to\infty$ and $J_{\varepsilon_k}^{-1}(x,y)\geqslant 0$ for all $x,y\in\mathbb{Z}^d$ and $k\geqslant 1$.

We have the following example which satisfies our two assumptions.

Example: $q(r)=\alpha_0 r^l\Pi_{j=1}^{K-l}(\alpha_j r+\beta_j)$, where $\alpha_j,\beta_j>0$ for every $0\leqslant j\leqslant K-l$ and $1\leqslant l\leqslant K$.

Proof: Assumption 1 is obvious. We will check Assumption 2. For this $q(r)$, J_ε^{-1} is given by

$$\frac{1}{\alpha_0}((\varepsilon I-\Delta)^{-1})^l\prod_{j=1}^{K-l}(\alpha_j(\varepsilon I-\Delta)+\beta_j I)^{-1}.$$

However, $(-\Delta)^{-1}$ is the Green function of the d-dimensional simple random walk on $\mathbb{Z}^d$ and $(\alpha(\varepsilon I-\Delta)+\beta I)^{-1}$ is the Green function of the random walk with killing rate $(\varepsilon\alpha+\beta)/[\alpha(\varepsilon+1)+\beta]$ and killing starting at time 0 if $\alpha,\beta>0$ for any $\varepsilon\geqslant 0$. Thus all components of $(\varepsilon I-\Delta)^{-1},(\alpha_j(\varepsilon I-\Delta)+\beta_j I)^{-1}$ are positive and accordingly $J_\varepsilon^{-1}(x,y)>0$ for all $x,y\in\mathbb{Z}^d$ and $\varepsilon\geqslant 0$. □

Our attention will be focused on the following entropic repulsion event,

$$\Omega_N^+=\{\phi\in\Omega;\phi_x\geqslant 0\ \text{ for all }\ x\in V_N\},$$

where $V_N=NV\cap\mathbb{Z}^d, N\in\mathbb{N}$ and $V=[-1,1]^d$.

The first result is on the asymptotics of the probability of the event Ω_N^+. We always assume Assumptions 1 and 2.

Theorem 2.1: *There exist $C_1,C_2>0$ such that*

$$-C_1 \leqslant \liminf_{N\to\infty} \frac{1}{N^{d-2l}\log N} \log P(\Omega_N^+) \leqslant \limsup_{N\to\infty} \frac{1}{N^{d-2l}\log N} \log P(\Omega_N^+) \leqslant -C_2.$$

Remark 2.3: This theorem implies that in our model, the order of the decay of $P(\Omega_N^+)$ depends on the minimum degree l of the polynomial $q(r)$ and not on the maximum degree K of $q(r)$, namely the maximum range of the interaction of the (formal) Hamiltonian $H_1(\phi)$ defined by (1). This is because the asymptotics of the correlation of the field depends on l and not on K, and also formally speaking, if $\Sigma_{x\in\mathbb{Z}^d}((-\Delta)^{l/2}\phi_x)^2$ is small, then $\Sigma_{x\in\mathbb{Z}^d}((-\Delta)^{j/2}\phi_x)^2$ becomes small for every $l+1 \leqslant j \leqslant K$ and so the energy $H_1(\phi)$ becomes small.

By using these bounds, we obtain the asymptotics of the local sample mean of the height variables under the conditional probability $P(\cdot|\Omega_N^+)$ as $N\to\infty$. This implies that the field is repelled to the height of order $\sqrt{\log N}$ by a hard-wall at least under average.

Theorem 2.2: *Let $1-2l/d<\gamma\leqslant 1$ be fixed. Then for every $a<2G(0,0)\{(-1+\gamma)d+2l\}$, we have*

$$\lim_{N\to\infty} \sup_{\substack{z\in V_N, r>0 \\ V_{rN^\gamma}(z)\subset V_N}} P(\overline{\phi}_{z,rN^\gamma} \leqslant \sqrt{a\log N} | \Omega_N^+) = 0, \tag{2}$$

and there exists some $b>0$ such that

$$\lim_{N\to\infty} \sup_{\substack{z\in V_N, r>0 \\ V_{rN}(z)\subset V_N}} P(\overline{\phi}_{z,rN} \geqslant \sqrt{b\log N} | \Omega_N^+) = 0, \tag{3}$$

where $V_R(z)=z+V_R$ is a box with side-length $2R$ and centered at z and $\overline{\phi}_{z,R}=(1/|V_R(z)|)\Sigma_{x\in V_R(z)}\phi_x$ denotes the local sample mean of the height variables on $V_R(z)$.

Remark 2.4: The case that $K=l=1$ and $q_l=1$ was studied in Ref. 5. In this case, it is proved that the constants C_1 and C_2 in Theorem 2.1 coincide with each other. In our case, by the proof of Theorem 2.1 below, we can see that the constant C_1 of the lower bound is given by $C_1=2lq_lC_lG(0,0)$ where $C_l=Cap_l(V)\equiv\inf\{(1/2d)^l(\psi,(-\Delta_c)^l\psi)_{L^2(\mathbb{R}^d)}; \psi\in H_0^l(\mathbb{R}^d), \psi\geqslant 1_V\}$, Δ_c is the continuous Laplacian on $\mathbb{R}^d$, $(\cdot,\cdot)_{L^2(\mathbb{R}^d)}$ denotes $L^2(\mathbb{R}^d)$-scalar product and H_0^l denotes the usual Sobolev space with norm $(\psi,(-\Delta_c)^l\psi)_{L^2(\mathbb{R}^d)}^{1/2}$. If $K=l=1$ and $q_l=1$, this constant coincides with that in Ref. 5. To obtain the same constant (or good upper bound), the technique of subgrid conditioning argument was used in Ref 5. When considering such kind of conditioning argument, conditional expectation of height variable can be represented as the linear sum of the height variables of conditioned sites. In the $\nabla\phi$ case, each coefficient is given by the hitting probability of the simple random walk on $\mathbb{Z}^d$ and this is non-negative. But in our case, both positive coefficient and negative coefficient appear and we cannot obtain the estimate of the conditional expectations from below or above under the event Ω_N^+ at all. By this reason, we have not been able to prove the upper and lower bounds with the same constant.

Also in Ref. 5, Theorem 2.2 is proved for each height variable ϕ_x instead of the local sample mean of the height $\overline{\phi}_{z,rN^\gamma}$. In our model, since the well-known FKG criterion (cf. Corollary 1.7 of Ref. 15) does not hold, we cannot use FKG inequality for the conditioned measure $P(\cdot|\Omega_N^+)$. This causes the great difficulty to estimate the several expectations with respect to the measure $P(\cdot|\Omega_N^+)$. That is why we can prove Theorem 2.2 only for the local sample mean of the height variables.

Remark 2.5: We have restricted our discussion to the infinite volume Gaussian field P with $d\geqslant 2l+1$. It might be natural and interesting to consider the finite volume measure P_N with zero boundary condition outside V_N and investigate the behavior of $P_N(\Omega_{\delta N}^+)$ and $P_N(\cdot|\Omega_{\delta N}^+)$ for $0<\delta\leqslant 1$ in arbitrary dimensions. When $0<\delta<1$ and $d\geqslant 2l+1$, we can modify our proof and obtain similar results to Theorems 2.1 and 2.2. But when $0<\delta<1$ and $d\leqslant 2l$, since we do not have the estimate of the covariance given as in Proposition 1.6.7 of Ref. 19 for the $\nabla\phi$ case, we

have not obtained the corresponding results. Also, because of the same reason as Remark 2.4, it seems much more difficult to consider the boundary effect (i.e., the case where $\delta=1$*) even if* $d \geqslant 2l+1$.

III. PROOF OF THEOREM 2.1

A. Proof of the lower bound

We will use two-scale decomposition originally introduced in the proof of Proposition 4.1 of Ref. 10.

Step 1: Let $\phi^0=\{\phi_x^0\}_{x\in\mathbb{Z}^d}$ and $\phi^1=\{\phi_x^1\}_{x\in\mathbb{Z}^d}$ be two independent centered Gaussian fields with covariances

$$E[\phi_x^0\phi_y^0]=J^{-1}(x,y)-J_\varepsilon^{-1}(x,y)\equiv G_\varepsilon^{(0)}(x,y),$$

$$E[\phi_x^1\phi_y^1]=J_\varepsilon^{-1}(x,y)\equiv G_\varepsilon^{(1)}(x,y),$$

respectively. We will choose a parameter $\varepsilon>0$ along the sequence $\{\varepsilon_k\}_{k\geqslant 1}$ of Assumption 2 and for convenience omit the subscript k. Note that $\widehat{G_\varepsilon^{(0)}}(\theta)=(\Sigma_{j=l}^K q_j(\mu(\theta))^j)^{-1}-(\Sigma_{j=l}^K q_j(\varepsilon+\mu(\theta))^j)^{-1}$, $\widehat{G_\varepsilon^{(1)}}(\theta)=(\Sigma_{j=l}^K q_j(\varepsilon+\mu(\theta))^j)^{-1}$ and by Assumptions 1 and 2, the fields ϕ^0,ϕ^1 exist for any $\varepsilon>0$ small enough. The original field $\phi=\{\phi_x\}_{x\in\mathbb{Z}^d}$ is represented as the sum of these two fields: $\phi=\phi^0+\phi^1$. We will keep the notation P for the joint law of ϕ^0 and ϕ^1. By using the inversion formula and Lebesgue's dominated convergence theorem, it is easy to see that $\lim_{\varepsilon\to 0} G_\varepsilon^{(0)}(x,y)=0$ for every $x,y\in\mathbb{Z}^d$. We denote by $P_{\alpha,N}(\alpha>0)$ the law of the random field $\{\phi_x^0+\sqrt{\alpha\log N},\phi_x^1\}_{x\in\mathbb{Z}^d}$, which is still a Gaussian field with the same covariance as $\{\phi^0,\phi^1\}$ under P, but the mean of the ϕ^0-field is shifted.

For $\mathcal{F}^0=\sigma(\phi_x^0;x\in\mathbb{Z}^d)$, we have

$$P(\Omega_N^+)\geqslant E[P(\phi_x^0+\phi_x^1\geqslant 0 \text{ for all } x\in V_N|\mathcal{F}^0)I(\phi_x^0\geqslant\sqrt{\alpha\log N} \text{ for all } x\in V_N)].$$

Since ϕ^0 and ϕ^1 are independent, on $\{\phi_x^0\geqslant\sqrt{\alpha\log N}$ for all $x\in V_N\}$ we have

$$P(\phi_x^0+\phi_x^1\geqslant 0 \text{ for all } x\in V_N|\mathcal{F}^0)\geqslant P(\phi_x^1\geqslant-\sqrt{\alpha\log N} \text{ for all } x\in V_N).$$

Thus, we obtain $\log P(\Omega_N^+)\geqslant T_0+T_1$ where

$$T_0=\log P(\phi_x^0\geqslant\sqrt{\alpha\log N} \text{ for all } x\in V_N),$$

$$T_1=\log P(\phi_x^1\geqslant-\sqrt{\alpha\log N} \text{ for all } x\in V_N).$$

We will estimate T_0 in Steps 2 and 3 and T_1 in Step 4.

Step 2: Since $\lim_{\varepsilon\to 0} G_\varepsilon^{(0)}(0,0)=0$, in a completely analogous manner to the proof of (4.13) of Ref. 10 we can prove that for every $\alpha'>\alpha$ there exists $\varepsilon'>0$ such that for all $\varepsilon\leqslant\varepsilon'$

$$\lim_{N\to\infty} P_{\alpha',N}(\phi_x^0\geqslant\sqrt{\alpha\log N} \text{ for all } x\in V_N)=1. \tag{4}$$

Moreover, we have

$$\lim_{N\to\infty}\frac{1}{N^{d-2l}\log N}H_N(P_{\alpha',N}|P)=\frac{1}{2}\alpha' q_l\mathcal{C}_l, \tag{5}$$

where $H_N(P_{\alpha',N}|P)=E^{P_{\alpha',N}}[\log dP_{\alpha',N}/dP|_{\mathcal{F}_{V_N}}]$, $\mathcal{F}_{V_N}=\sigma(\phi_x;x\in V_N)$. We will prove this equality later. Combining (4) and (5) with entropy inequality (cf. Lemma 5.4.21 of Ref. 12), we obtain

$$\liminf_{N\to\infty}\frac{1}{N^{d-2l}\log N}T_0\geqslant-\frac{1}{2}\alpha q_l\mathcal{C}_l, \tag{6}$$

for every $\alpha>0$ and $\varepsilon>0$ small enough.

Step 3: It is easy to see that $H_N(P_{\alpha',N}|P)=\frac{1}{2}\alpha'\log N\langle 1_{V_N},(G^{(0)}_{\varepsilon,(N)})^{-1}1_{V_N}\rangle_{V_N}$ where $G^{(0)}_{\varepsilon,(N)}$ is a restriction of $G^{(0)}_\varepsilon$ to $V_N\times V_N$ and $\langle\cdot,\cdot\rangle_{V_N}$ denotes the $l^2(V_N)$-scalar product. So all we need to prove (5) is

$$\lim_{N\to\infty}\frac{1}{N^{d-2l}}\langle 1_{V_N},(G^{(0)}_{\varepsilon,(N)})^{-1}1_{V_N}\rangle_{V_N}=q_l\mathcal{C}_l, \tag{7}$$

for fixed $\varepsilon>0$ small enough. By the variational formula, we have for any $\psi\in L^2(V)$,

$$\langle\psi_N,(G^{(0)}_{\varepsilon,(N)})^{-1}\psi_N\rangle_{V_N}=\sup_{f\in L^2(V_N)}\{2\langle\psi_N,f\rangle_{V_N}-\langle f,G^{(0)}_{\varepsilon,(N)}f\rangle_{V_N}\}, \tag{8}$$

where $\psi_N(x)=\psi(x/N)$. By Assumption 2 and the definition of ϕ^0-field, we have $G^{(0)}_\varepsilon(x,y)\leqslant G(x,y)$ for every $x,y\in\mathbb{Z}^d$. The lower bound of (7) is an easy consequence of this fact, (8) and Lemma 5.2.

Next, we will prove the upper bound. By (8) we have

$$\langle 1_{V_N},(G^{(0)}_{\varepsilon,(N)})^{-1}1_{V_N}\rangle_{V_N}\leqslant\sup_{f\in L^2(\mathbb{Z}^d)}\{2\langle h_N,f\rangle_{V_N}-\langle f,G^{(0)}_\varepsilon f\rangle_{V_N}\}=\langle h_N,(G^{(0)}_\varepsilon)^{-1}h_N\rangle_{\mathbb{Z}^d},$$

where $h\in C_0^\infty(\mathbb{R}^d)$ with $h=1$ on V and $h_N(x)=h(x/N)$. It is easy to see that $\widehat{(G^{(0)}_\varepsilon)^{-1}}(\theta)-\widehat{G^{-1}}(\theta)\leqslant C(\Sigma_{j=l}^K q_j(\mu(\theta))^j)^2$ for some $C=C(\varepsilon)>0$ and every $\theta\in[-\pi,\pi]^d$. Hence by Parseval identity we know that

$$\langle h_N,((G^{(0)}_\varepsilon)^{-1}-G^{-1})h_N\rangle_{\mathbb{Z}^d}\leqslant\frac{C}{(2\pi)^d}\int_{[-\pi,\pi]^d}|\widehat{h_N}(\theta)|^2\left(\sum_{j=l}^K q_j(\mu(\theta))^j\right)^2 d\theta=C\langle h_N,J^2h_N\rangle_{\mathbb{Z}^d}.$$

Thus

$$\begin{aligned}\frac{1}{N^{d-2l}}\langle 1_{V_N},(G^{(0)}_{\varepsilon,(N)})^{-1}1_{V_N}\rangle_{V_N}&\leqslant\frac{1}{N^{d-2l}}(\langle h_N,Jh_N\rangle_{\mathbb{Z}^d}+C\langle h_N,J^2h_N\rangle_{\mathbb{Z}^d})\\&=\left(\frac{1}{2d}\right)^l q_l(h,(-\Delta_c)^lh)_{L^2(\mathbb{R}^d)}(1+o(1)),\end{aligned}$$

as $N\to\infty$, where the last equality follows from the fact that

$$\frac{1}{N^{d-2j}}\langle\psi_N,(-\Delta)^j\psi_N\rangle_{\mathbb{Z}^d}=\left(\frac{1}{2d}\right)^j(\psi,(-\Delta_c)^j\psi)_{L^2(\mathbb{R}^d)}(1+o(1)), \tag{9}$$

as $N\to\infty$, for every $\psi\in C_0^\infty(\mathbb{R}^d)$ and $j\geqslant 1$. Finally, taking $\liminf_{N\to\infty}$ and infimum over h we obtain the upper bound.

Step 4: By Assumption 2, we can use FKG inequality for ϕ^1-field (cf. Ref. 24). Therefore, elementary Gaussian estimate yields

$$\liminf_{N\to\infty}\frac{1}{N^{d-2l}\log N}T_1=0\quad\text{if}\quad\alpha\geqslant 4lG(0,0). \tag{10}$$

By (10) and (6), we can complete the proof. □

B. Proof of the upper bound

We consider the conditioning argument which corresponds to the even-odd procedure for $\nabla\phi$ case (cf. Ref. 11).

Step 1: Let $A_N=V_N\cap(K+1)\mathbb{Z}^d$, $\tilde{A}_N=\{x\in A_N;\mathrm{dist}(x,A_N^c)>K\}$ and $B_N=V_N-\tilde{A}_N$. Define $\mathcal{F}_{B_N}=\sigma(\phi_x;x\in B_N)$. Then by the Gibbsian description of P, $\{\phi_x\}_{x\in\tilde{A}_N}$ are independent Gaussian random variables with mean $m_x=-J(0,0)^{-1}\Sigma_{y\neq x}J(x,y)\phi_y$ and variance $\sigma^2=J(0,0)^{-1}$ under $P(\cdot\,|\mathcal{F}_{B_N})$. Define $C_N=\{x\in\tilde{A}_N;m_x\leqslant a_N\}$ for $a_N=\sqrt{\alpha\log N},\alpha>0$. Note that C_N is an $\mathcal{F}_{B_N}$-measurable random set and different from the $\nabla\phi$ case; m_x contains the sum for y with $J(x,y)<0$. For $0<\varepsilon<1$, we have

$$\begin{aligned}P(\Omega_N^+)&=E\left[\prod_{x\in\tilde{A}_N}P(\phi_x\geqslant 0|\mathcal{F}_{B_N})I(\Omega^+(B_N))\right]\\&\leqslant E\left[\prod_{x\in\tilde{A}_N}P(\phi_x\geqslant 0|\mathcal{F}_{B_N})I(|C_N|\geqslant\varepsilon|\tilde{A}_N|)\right]+P(\Omega^+(B_N)\cap\{|C_N|\leqslant\varepsilon|\tilde{A}_N|\})\\&\equiv T_0+T_1,\end{aligned}$$

where $\Omega^+(D)=\{\phi\in\Omega;\phi(x)\geqslant 0\text{ for all }x\in D\}$ for every $D\subset\mathbb{Z}^d$.

Step 2: Since $\{\phi_x-m_x\}_{x\in\tilde{A}_N}$ are centered Gaussian random variables under $P(\cdot\,|\mathcal{F}_{B_N})$, by following the argument of the proof of (2.16) of Ref. 11, we obtain

$$\limsup_{N\to\infty}\frac{1}{N^{d-2l}\log N}\log T_0=-\infty\quad\text{if}\quad\alpha<4l\sigma^2.$$

Step 3: Let $h(x,y)=-J(0,0)^{-1}J(x,y)$. Then m_x can be represented as

$$m_x=\sum_{\substack{y\neq x\\ h(x,y)>0}}h(x,y)\phi_y+\sum_{\substack{y\neq x\\ h(x,y)<0}}h(x,y)\phi_y\equiv m_x^+ + m_x^-.$$

Now on $\Omega^+(B_N)$, $m_x^+\geqslant 0$ and $m_x^-\leqslant 0$. Especially on $(C_N)^c$, $m_x^+\geqslant a_N$ since $m_x=m_x^++m_x^-\geqslant a_N$. Thus on $\Omega^+(B_N)\cap\{|C_N|\leqslant\varepsilon|\tilde{A}_N|\}$, we have

$$S_N^+\equiv\frac{1}{|\tilde{A}_N|}\sum_{x\in\tilde{A}_N}m_x^+\geqslant(1-\varepsilon)a_N.$$

Since S_N^+ is a linear sum of $\{\phi_x\}_{x\in B_N}$ this is a centered Gaussian, hence

$$T_1\leqslant P(S_N^+\geqslant(1-\varepsilon)a_N)\leqslant\exp\left\{-\frac{(1-\varepsilon)^2a_N^2}{2\mathrm{Var}(S_N^+)}\right\}.$$

By using the fact that $h(x,y)$ is independent of N and $G(x,y)\geqslant 0$ for all $x,y\in\mathbb{Z}^d$,

$$\begin{aligned}\mathrm{Var}(S_N^+)&=E\left[\left(\frac{1}{|\tilde{A}_N|}\sum_{x\in\tilde{A}_N}\sum_{\substack{y\neq x\\ h(x,y)>0}}h(x,y)\phi_y\right)^2\right]\\&\leqslant\frac{C}{|V_N|^2}E\left[\left(\sum_{x\in V_N}\phi_x\right)^2\right]\\&\leqslant\frac{C}{N^{2d}}\langle 1_{V_N},G_{(N)}1_{V_N}\rangle_{V_N}\\&=O(N^{-d+2l}),\end{aligned}$$

as $N\to\infty$, where $C>0$ is a constant independent of N and $G_{(N)}$ is a restriction of G to $V_N \times V_N$. The last equality follows from Lemma 5.2.

Finally, we obtain

$$\limsup_{N\to\infty} \frac{1}{N^{d-2l}\log N} \log T_1 \leqslant -C_2,$$

for some constant $C_2>0$ and complete the proof. □

IV. PROOF OF THEOREM 2.2

A. Proof of (2)

We will use the modified version of the conditioning argument which was used in Refs. 5 and 11. To obtain the independent field under conditioning, we consider thicker walls.

For fixed $L\in 2\mathbb{N}$ large enough, define $M_L=(L\mathbb{Z}\times\mathbb{Z}\times\cdots\times\mathbb{Z})\cup(\mathbb{Z}\times L\mathbb{Z}\times\mathbb{Z}\times\cdots\times\mathbb{Z})\cup\cdots\cup(\mathbb{Z}\times\cdots\times\mathbb{Z}\times L\mathbb{Z})$, $A_L=(\cup_{j=-[K/2]}^{[K/2]}(M_L+j\mathbf{1}))+(L/2)\,\mathbf{1}$, $A_L^c=\mathbb{Z}^d\backslash A_L$, $V_{rN\gamma}(z)=z+V_{rN\gamma}$, $\Lambda_N=V_N\cap L\mathbb{Z}^d$ and $\Lambda_{rN\gamma}(z)=V_{rN\gamma}(z)\cap L\mathbb{Z}^d$, where $z\in\mathbb{Z}^d$, $r>0$, $0<\gamma\leqslant 1$, $[a]$ denotes the integral part of a and $\mathbf{1}=(1,1,\ldots,1)$. A_L^c consists of separated d-dimensional cells with centered at $L\mathbb{Z}^d$ and side-length $L-2[K/2]-2$. We will denote a cell with centered at the origin and side-length $L-2[K/2]-2$ by B_L and the matrix inverse of $(J(x,y))_{x,y\in B_L}$ by $(G^L(x,y))_{x,y\in B_L}$. Next let $\mathcal{F}_{A_L}=\sigma(\phi_x;x\in A_L)$ and $\tilde{\phi}_x=E[\phi_x|\mathcal{F}_{A_L}]$. Under $P(\cdot|\mathcal{F}_{A_L})$, $\{\phi_x\}_{x\in\Lambda_N}$ are independent Gaussian random variables with mean $\{\tilde{\phi}_x\}_{x\in\Lambda_N}$ and by the Gibbsian description of P we have $\mathrm{Cov}(\phi_x,\phi_y|\mathcal{F}_{A_L})=\mathrm{Cov}(\phi_x,\phi_y|\mathcal{F}_{B_L^c})$ for $x,y\in B_L$, where $\mathcal{F}_{B_L^c}=\sigma(\phi_x;x\notin B_L)$. The following lemma follows from this fact and Theorems (1.5) and (1.6) of Ref. 18 (see also Sec. 4 of Ref. 17).

Lemma 4.1: (i) $\mathrm{Cov}(\phi_x,\phi_y|\mathcal{F}_{A_L})=G^L(x,y)$ *for every* $x,y\in B_L$.

(ii) For each fixed $x,y\in B_L$, $G^L(x,y)\to G(x,y)$ *as* $L\to\infty$.

By the translation invariance and the Gibbsian description of P, $\mathrm{Cov}(\phi_x,\phi_y|\mathcal{F}_{A_L})=G^L(x,y)$ if $x,y\notin A_L$ belong to the same cell of A_L^c and $\mathrm{Cov}(\phi_x,\phi_y|\mathcal{F}_{A_L})=0$ if $x,y\notin A_L$ belong to the different cells of A_L^c. Also, we have $G^L(0,0)>0$ for any $L\in 2\mathbb{N}$ large enough. The crucial step in the proof of (2) is the following:

Lemma 4.2: Let $1-2l/d<\gamma\leqslant 1$ *be fixed and take* $a<2G^L(0,0)\{(-1+\gamma)d+2l\}$. *Then for every* $\delta>0$

$$\lim_{N\to\infty} \sup_{\substack{z\in V_N, r>0\\ \Lambda_{rN^\gamma}(z)\subset V_N}} P(R_{\Lambda_{rN^\gamma}(z)}[0,\sqrt{a\log N}]\geqslant\delta|\Omega_N^+)=0,$$

where $R_D=(1/|D|)\,\Sigma_{x\in D}\delta_{\phi_x}$ *for each* $D\subset\mathbb{Z}^d$.

We will prove this lemma at the end. Once we have shown Lemma 4.2, in the similar way to the proof of (4.2) of Ref. 5 we can prove the following.

Lemma 4.3: Let $1-2l/d<\gamma\leqslant 1$ *be fixed and take* $a<2G(0,0)\{(-1+\gamma)d+2l\}$. *Then for every* $\delta>0$

$$\lim_{N\to\infty} \sup_{\substack{z\in V_N, r>0\\ V_{rN^\gamma}(z)\subset V_N}} P(R_{V_{rN^\gamma}(z)}[0,\sqrt{a\log N}]\geqslant\delta|\Omega_N^+)=0.$$

By using Lemma 4.3, we first prove (2).

Proof of (2): Let $a<2G(0,0)\{(-1+\gamma)d+2l\}$ be fixed. For every $a<a'<2G(0,0)\{(-1+\gamma)d+2l\}$, $\delta>0$ and $z\in V_N$, $r>0$ with $V_{rN^\gamma}(z)\subset V_N$, we have

$$P(\overline{\phi}_{z,rN^\gamma} \leqslant \sqrt{a \log N} | \Omega_N^+) = P(\{\overline{\phi}_{z,rN^\gamma} \leqslant \sqrt{a \log N}\} \cap \{R_{V_{rN^\gamma(z)}}[0, \sqrt{a' \log N}] \geqslant \delta\} | \Omega_N^+)$$
$$+ P(\{\overline{\phi}_{z,rN^\gamma} \leqslant \sqrt{a \log N}\} \cap \{R_{V_{rN^\gamma(z)}}[\sqrt{a' \log N}, \infty) \geqslant 1-\delta\} | \Omega_N^+).$$

By Lemma 4.3, the first term goes to 0 as $N \to \infty$. Next, on $\{R_{V_{rN^\gamma(z)}}[\sqrt{a' \log N}, \infty) \geqslant 1-\delta\} \cap \Omega_N^+$, we have $\overline{\phi}_{z,rN^\gamma} \geqslant (1-\delta)\sqrt{a' \log N}$. Hence the second term is less than $P((1-\delta)\sqrt{a' \log N} \leqslant \overline{\phi}_{z,rN^\gamma} \leqslant \sqrt{a \log N} | \Omega_N^+)$ which equals 0 for $\delta > 0$ small enough. □

Proof of Lemma 4.2:

Step 1: We will denote $\Lambda_{N^\gamma}(0)$ by Λ_N^γ. Set

$$I_N(a) = \{x \in \Lambda_N^\gamma ; \phi_x \leqslant \sqrt{a \log N}\},$$

$$\tilde{I}_N(a) = \{x \in \Lambda_N^\gamma ; \tilde{\phi}_x \leqslant \sqrt{a \log N}\}, \quad \tilde{I}_N(a)^c = \{x \in \Lambda_N^\gamma ; \tilde{\phi}_x > \sqrt{a \log N}\}.$$

As the proof of Lemma 4.4 of Ref. 5, on Ω_N^+ we have

$$\{R_{\Lambda_N^\gamma}[0, \sqrt{a \log N}] \geqslant \delta\} \subseteq \{|\tilde{I}_N(a')| \geqslant \delta' |\Lambda_N^\gamma|\} \cup \{|I_N(a) \cap \tilde{I}_N(a')^c| \geqslant (\delta - \delta')|\Lambda_N^\gamma|\} \equiv J_0 \cup J_1,$$

for each $0 < \delta' < \delta$ and $a' > a$.

Step 2: Since $\{\phi_x\}_{x \in \Lambda_N^\gamma}$ are independent Gaussian random variables under $P(\cdot | \mathcal{F}_{A_L})$, we have

$$P(J_0 \cap \Omega_N^+) \leqslant E_N\left[\prod_{x \in \Lambda_N^\gamma} P(\phi_x \geqslant 0 | \mathcal{F}_{A_L}) I(|\tilde{I}_N(a')| \geqslant \delta' |\Lambda_N^\gamma|)\right].$$

Note that $|\Lambda_N^\gamma| = CN^{\gamma d}$ for some $C > 0$ independent of N. Then in the same way as in Step 2 of the proof of Theorem 2.1 upper bound, we can obtain

$$P(J_0 \cap \Omega_N^+) \leqslant \exp\left\{-C \frac{\sqrt{G^L}}{\sqrt{\log N}} N^{\gamma d - a'/2G^L}\right\},$$

for some constant $C > 0$, where $G^L = G^L(0,0)$. Hence for every $a < a' < 2G^L\{(-1+\gamma)d + 2l\}$, we know that

$$P(J_0 \cap \Omega_N^+) \leqslant \exp\{-CN^{d-2l+\varepsilon}\}, \tag{11}$$

for some $C, \varepsilon > 0$. By this inequality and Theorem 2.1 lower bound, we obtain that $\lim_{N \to \infty} P(J_0 | \Omega_N^+) = 0$.

Step 3: Define

$$C_N = \{|\{x \in \Lambda_N^\gamma ; \phi_x - \tilde{\phi}_x \leqslant -(\sqrt{a'} - \sqrt{a})\sqrt{\log N}\}| \geqslant (\delta - \delta')|\Lambda_N^\gamma|\},$$

$$D_x = \{\phi_x - \tilde{\phi}_x \leqslant -(\sqrt{a'} - \sqrt{a})\sqrt{\log N}\}.$$

If $x \in I_N(a) \cap \tilde{I}_N(a')^c$, then the event D_x occurs, so we have $P(J_1 \cap \Omega_N^+) \leqslant P(C_N)$. For $x \in \Lambda_N^\gamma$,

$$P(D_x | \mathcal{F}_{A_L}) \leqslant \exp\left\{-\frac{(\sqrt{a'} - \sqrt{a})^2 \log N}{2G^L}\right\}. \tag{12}$$

Next, for every $\beta \in \mathbb{R}$,

$$
\begin{aligned}
T_1 &\equiv E\left[\exp\left\{N^\beta \frac{1}{|\Lambda_N^\gamma|}\sum_{x\in\Lambda_N^\gamma} I(\phi_x-\tilde{\phi}_x \leqslant -(\sqrt{a'}-\sqrt{a})\sqrt{\log N})\right\}\right] \\
&\geqslant E\left[\exp\left\{N^\beta \frac{1}{|\Lambda_N^\gamma|}\sum_{x\in\Lambda_N^\gamma} I(\phi_x-\tilde{\phi}_x \leqslant -(\sqrt{a'}-\sqrt{a})\sqrt{\log N})\right\} I(C_N)\right] \\
&\geqslant \exp\{(\delta-\delta')N^\beta\} P(C_N).
\end{aligned}
$$

Using the independence of $\{\phi_x-\tilde{\phi}_x\}_{x\in\Lambda_N^\gamma}$ under $P(\cdot|\mathcal{F}_{A_L})$ and (12),

$$
\begin{aligned}
T_1 &= E\left[\prod_{x\in\Lambda_N^\gamma} E\left[\exp\left\{N^\beta \frac{1}{|\Lambda_N^\gamma|} I(\phi_x-\tilde{\phi}_x \leqslant -(\sqrt{a'}-\sqrt{a})\sqrt{\log N})\right\}\middle| \mathcal{F}_{A_L}\right]\right] \\
&= E\left[\prod_{x\in\Lambda_N^\gamma}\left\{\left(\exp\left\{N^\beta\frac{1}{|\Lambda_N^\gamma|}\right\}-1\right)P(D_x|\mathcal{F}_{A_L})+1\right\}\right] \\
&\leqslant \left\{\left(\exp\left\{N^\beta\frac{1}{|\Lambda_N^\gamma|}\right\}-1\right)\exp\left\{-\frac{(\sqrt{a'}-\sqrt{a})^2\log N}{2G^L}\right\}+1\right\}^{|\Lambda_N^\gamma|} \\
&\leqslant \exp\left\{\left|\Lambda_N^\gamma\right|\left(\exp\left\{N^\beta\frac{1}{|\Lambda_N^\gamma|}\right\}-1\right)\exp\left\{-\frac{(\sqrt{a'}-\sqrt{a})^2\log N}{2G^L}\right\}\right\}.
\end{aligned}
$$

Hence we obtain

$$
P(J_1\cap\Omega_N^+) \leqslant \exp\{-(\delta-\delta')N^\beta\}\exp\{CN^{\gamma d-(\sqrt{a'}-\sqrt{a})^2/2G^L}(\exp\{CN^{\beta-\gamma d}\}-1)\},
$$

for some $C>0$. Now taking $\beta=\gamma d-(\sqrt{a'}-\sqrt{a})^2/2G^L$, we know that

$$
\limsup_{N\to\infty}\frac{1}{N^\beta}\log P(J_1\cap\Omega_N^+) \leqslant -(\delta-\delta'). \tag{13}
$$

Since $\beta>d-2l$ for $a<a'<2G^L\{(-1+\gamma)d+2l\}$, by (13) and Theorem 2.1 lower bound we obtain $\lim_{N\to\infty} P(J_1|\Omega_N^+)=0$.

Completely the same way, we can obtain the estimates (11) and (13) independent of $z\in V_N$, $r>0$ with $\Lambda_{rN^\gamma}(z)\subset V_N$ for $\Lambda_{rN^\gamma}(z)$ instead of Λ_N^γ and complete the proof. □

B. Proof of (3)

Take $z\in V_N$, $r>0$ so that $V_{rN}(z)\subset V_N$. By Chebyshev inequality and the Brascamp–Lieb inequality (cf. Ref. 7), which can be applied to the conditioned measure $P(\cdot|\Omega_N^+)$ (cf. Appendix of Ref. 11), we have

$$
P(\overline{\phi}_{z,rN}\geqslant\sqrt{b\log N}|\Omega_N^+) \leqslant \exp\left\{-\frac{|V_{rN}(z)|^2}{2\langle 1_{V_{rN}(z)}, G1_{V_{rN}(z)}\rangle_{V_N}}((\sqrt{b\log N}-E[\overline{\phi}_{z,rN}|\Omega_N^+])\vee 0)^2\right\}.
$$

Hence, by Lemma 5.2, we have only to prove that

$$
\limsup_{N\to\infty}\frac{1}{\sqrt{\log N}}E[\overline{\phi}_{z,rN}|\Omega_N^+] \leqslant C,
$$

for some constant $C>0$ and this estimate follows from the same argument as in the proof of Lemma 4.7 of Ref. 5. □

V. SOME TECHNICAL LEMMAS

In this section we show the asymptotics of the Green function and the convergence of the capacity which are used in Secs. III and IV.

Lemma 5.1: Let $d \geqslant 2l+1$. Then, it holds that

$$\lim_{|x|\to\infty} \frac{G(0,x)}{|x|^{-d+2l}} = \frac{1}{q_l}\gamma.$$

γ is given by

$$\gamma = \frac{1}{(2\pi)^d} \int_0^\infty \int_{\mathbb{R}^d} \exp\left\{ i\zeta\cdot\omega - \left(\frac{1}{2d}\right)^l |\omega|^{2l} t \right\} d\omega dt,$$

where $\zeta \in \mathbb{S}^{d-1}$ and the right hand side is independent of the choice of $\zeta \in \mathbb{S}^{d-1}$.

Proof: We follow the argument of Sec. 3 of Ref. 21 (see also Sec. 5 of Ref. 22). By the inversion formula we know that

$$G(0,x) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \hat{G}(\theta) e^{ix\cdot\theta} d\theta.$$

Since we can write $q_l \hat{G}(\theta) = \int_0^\infty \exp\{-[1/q_l \hat{G}(\theta)]\, u\} du$, we have

$$\begin{aligned}(2\pi)^d q_l G(0,x) &= \int_0^\infty \int_{[-\pi,\pi]^d} \exp\left\{ ix\cdot\theta - \frac{1}{q_l}\hat{G}(\theta)^{-1} u \right\} d\theta du \\ &= |x|^{-d+2l} \int_0^\infty \int_{[-\pi|x|,\pi|x|]^d} \exp\left\{ i\frac{x}{|x|}\cdot\omega - \frac{1}{q_l}\hat{G}\left(\frac{\omega}{|x|}\right)^{-1} |x|^{2l} t \right\} d\omega dt,\end{aligned}$$

where the last equality follows from the change of variables $u = |x|^{2l} t$, $\theta = \omega/|x|$. Define

$$\Gamma(t,x) = \int_{[-\pi|x|,\pi|x|]^d} \exp\left\{ i\frac{x}{|x|}\cdot\omega - \frac{1}{q_l}\hat{G}\left(\frac{\omega}{|x|}\right)^{-1} |x|^{2l} t \right\} d\omega.$$

Since $\hat{G}(\theta)^{-1} = \hat{J}(\theta) = \Sigma_{j=l}^K q_j (\mu(\theta))^j$, $\mu(\theta) = (1/2d)\,|\theta|^2 (1+o(1))$ and $(\partial/\partial\theta_i)\,\mu(\theta) = (1/d)\,\theta_i (1+o(1))$ as $|\theta| \to 0$, in the similar way to the proof of Lemma 3.1 of Ref. 21, we can prove that $|\Gamma(t,x)| \leqslant C(t^{-1/2l} \wedge t^{-d/2l})$ for some $C>0$ independent of $x \in \mathbb{Z}^d \setminus \{0\}$ and the rhs is integrable with respect to $\int_0^\infty \cdot\, dt$ when $d \geqslant 2l+1$. Hence by Lebesgue's dominated convergence theorem, we have

$$\lim_{|x|\to\infty} \frac{(2\pi)^d q_l G(0,x)}{|x|^{-d+2l}} = \int_0^\infty \lim_{|x|\to\infty} \Gamma(t,x)\, dt.$$

Now by using the asymptotics of $\hat{G}(\theta)^{-1}$ as $|\theta| \to 0$ and Assumption 1, the absolute value of the integrand of $\Gamma(t,x)$ is bounded by $\exp\{-C|\omega|^{2l} t\}$ for some $C>0$ which is integrable with respect to $\int_{\mathbb{R}^d} \cdot\, d\omega$ and $1/q_l\, \hat{G}(\omega/|x|)^{-1} |x|^{2l} t$ converges to $(1/2d)^l |\omega|^{2l} t$ as $|x| \to \infty$. Hence by Lebesgue's dominated convergence theorem again, we obtain

$$\lim_{|x|\to\infty}\Gamma(t,x)=\int_{\mathbb{R}^d}\lim_{|x|\to\infty}\exp\left\{i\frac{x}{|x|}\cdot\omega-\frac{1}{q_l}\hat{G}\left(\frac{\omega}{|x|}\right)^{-1}|x|^{2l}t\right\}d\omega$$

$$=\int_{\mathbb{R}^d}\exp\left\{i\zeta\cdot\omega-\left(\frac{1}{2d}\right)^{l}|\omega|^{2l}t\right\}d\omega,$$

where $\zeta\in\mathbb{S}^{d-1}$ and the right hand side is independent of $\zeta\in\mathbb{S}^{d-1}$. □

Let $g_l(x)=\gamma|x|^{-d+2l}$ and define the integral operator K_V^l on $L^2(V)$ by

$$K_V^l f(x)=\int_V g_l(x-y)f(y)dy,\quad x\in V.$$

Using Lemma 5.1 and (9), in a way similar to Sec. 2 of Ref. 2 and the Appendix of Ref. 5, we can obtain the following lemma.

Lemma 5.2: Let $d\geqslant 2l+1$, $f\in C(V;\mathbb{R})$ *and* $(G_{(N)})^{-1}$ *be a matrix inverse of* $G_{(N)}$. *Set* $f_N(x)=f(x/N)$. *Then*

$$\lim_{N\to\infty}N^{-d-2l}\langle f_N,G_{(N)}f_N\rangle_{V_N}=\frac{1}{q_l}\langle f,K_V^l f\rangle_V,$$

$$\lim_{N\to\infty}N^{-d+2l}\langle 1_{V_N},(G_{(N)})^{-1}1_{V_N}\rangle_{V_N}=q_l Cap_l(V).$$

ACKNOWLEDGMENTS

I would like to express my sincere thanks to Professor T. Funaki for many helpful discussions and his encouragement. The problem was suggested by Professor H. Spohn.

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Foldy–Wouthuysen transformation for relativistic particles in external fields

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(Received 16 November 2001; accepted 11 April 2003)

A method of Foldy–Wouthuysen transformation for relativistic spin-1/2 particles in external fields is proposed. It permits the determination of the Hamilton operator in the Foldy–Wouthuysen representation with any accuracy. Interactions between a particle having an anomalous magnetic moment and nonstationary electromagnetic and electroweak fields are investigated. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1579991]

I. INTRODUCTION

The Foldy–Wouthuysen (FW) representation[1] occupies a special place in the quantum theory. This is mainly due to the fact that the Hamiltonian and all operators in this representation are block-diagonal (diagonal in two spinors). For relativistic particles in external fields, operators have the same form as in the nonrelativistic quantum theory. Therefore, the FW representation in the relativistic quantum theory is similar to the nonrelativistic quantum theory. The basic advantages of the FW representation are described in Refs. 1 and 2 (see also below).

The transformation to the FW representation (FW transformation) holds only in the one-particle approximation where the radiative corrections are not calculated in a consistent way but are phenomenologically taken into account by including extra terms in the Dirac equation (see Ref. 3). The one-particle description is feasible even for ultrarelativistic particles if the external field is so weak that the probability of pair production or bremsstrahlung losses can be neglected for a given interaction energy of a particle. The range of applicability of this description is fairly wide and includes, in particular, the relativistic particle scattering and the interaction of relativistic particles with matter and external fields.

In the nonrelativistic case, there exist a lot of good methods of FW transformation with taking into account relativistic corrections.[1,4–6] However, they are not useful for relativistic particles. The known methods of solving this problem[9–12] either lead to cumbersome calculations or the field of their use is limited by the first approximation in field parameters. None of these methods permits an exact FW transformation for the particular cases described in Refs. 5, 7, and 8. Therefore, the FW representation does not take the right stand in the relativistic quantum theory. The Dirac and Melosh[13] representations are mostly used.

FW transformation can also be performed for particles with spin $s>1/2$.[7,14]

In the present work, a method of FW transformation for relativistic particles in external fields is proposed. This method permits obtaining a Hamiltonian of any accuracy by successive approximations, as a power series in the external field potentials and their derivatives. In some cases, this method permits performing an exact FW transformation.

The relativistic system of units $\hbar=c=1$ is used.

II. GENERAL PROPERTIES OF THE FOLDY–WOUTHUYSEN REPRESENTATION

The basic advantages of the FW representation are due to its specific properties.

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The relations between the operators in the FW representation are similar to those between the respective classical quantities. In this representation, the operators have the same form as in the nonrelativistic quantum theory. Only the FW representation possesses these properties considerably simplifying the transition to the semiclassical description. The FW representation provides the best possibility of obtaining a meaningful classical limit of the relativistic quantum theory.

For example, the Hamiltonian for a free particle fully agrees with that of classical physics:

$$\mathcal{H}_{\mathrm{FW}}=\beta\sqrt{m^2+\mathbf{p}^2},\qquad \mathbf{p}=-i\boldsymbol{\nabla}, \tag{1}$$

in contrast with the Hamiltonian in the Dirac representation.[1,15] The position operator in the Dirac representation is the radius-vector, $\mathbf{r}$.[15] It corresponds to the mean position operator for the free particle in the FW representation,[1]

$$\mathbf{r}_{\mathrm{D}}=\mathbf{r}+\frac{i\beta\boldsymbol{\alpha}}{2\epsilon}-\frac{i\beta(\boldsymbol{\alpha}\cdot\mathbf{p})\mathbf{p}+[\boldsymbol{\Sigma}\times\mathbf{p}]p}{2\epsilon(\epsilon+m)p},\qquad p\equiv|\mathbf{p}|,\qquad \epsilon=\sqrt{m^2+p^2}.$$

Here and below the following designations for the matrices are used:

$$\boldsymbol{\gamma}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ -\boldsymbol{\sigma} & 0\end{pmatrix},\qquad \beta\equiv\gamma^0=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\qquad \boldsymbol{\alpha}=\beta\boldsymbol{\gamma}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{pmatrix},$$

$$\boldsymbol{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix},\qquad \boldsymbol{\Pi}=\beta\boldsymbol{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & -\boldsymbol{\sigma}\end{pmatrix},$$

where $0,1,-1$ mean the corresponding 2×2 matrices and $\boldsymbol{\sigma}$ is the Pauli matrix.

In the FW representation, the problem of "*zitterbewegung*" motion never arises.[2,15] The operators $\mathbf{l}=\mathbf{r}\times\mathbf{p}$ and $\boldsymbol{\Sigma}/2$ define the angular momentum and the spin for the free particle, respectively. In this representation, unlike the Dirac one, each of them is a constant of motion (see Ref. 1). The corresponding operators conserving in the Dirac representation are

$$\mathbf{l}_{\mathrm{D}}=\mathbf{r}_{\mathrm{D}}\times\mathbf{p},$$

$$\frac{\boldsymbol{\Sigma}_{\mathrm{D}}}{2}=\frac{\boldsymbol{\Sigma}}{2}-\frac{i\beta[\boldsymbol{\alpha}\times\mathbf{p}]}{2\epsilon}-\frac{[\mathbf{p}\times[\boldsymbol{\Sigma}\times\mathbf{p}]]}{2\epsilon(\epsilon+m)}.$$

The total angular momentum operator, $\mathbf{j}$, is a constant of motion in both representations, because

$$\mathbf{j}_{\mathrm{D}}=\mathbf{l}_{\mathrm{D}}+\frac{\boldsymbol{\Sigma}_{\mathrm{D}}}{2}=\mathbf{l}+\frac{\boldsymbol{\Sigma}}{2}=\mathbf{j}.$$

The FW representation is very convenient for describing the particle polarization. In this representation, polarization operators have simple forms. For example, the three-dimensional polarization operator equals the matrix $\boldsymbol{\Pi}$.[16,17] In the Dirac representation, this operator depends on the particle momentum:[16,17]

$$\mathbf{O}\equiv\boldsymbol{\Pi}_{\mathbf{D}}=\boldsymbol{\Pi}-\gamma^5\frac{\mathbf{p}}{\epsilon}-\frac{\mathbf{p}(\boldsymbol{\Pi}\cdot\mathbf{p})}{\epsilon(\epsilon+m)}.$$

For particles interacting with external fields, it also depends on the external field parameters.[17]

Thus, in the Dirac representation all operators corresponding to the basic classical quantities are defined by cumbersome expressions. These operators should also depend on the external field parameters for particles interacting with external fields.

The FW representation helps one to prove that the particle position can be measured up to its Compton wavelength.[1,15] However, this property is valid only for a particle not strongly interacting with external fields if the one-particle approximation is attainable. Otherwise, the effect of pair production prevents the use of both the Dirac equation (even with some corrections) and the ''traditional'' Hamilton approach. Obviously, in this case the FW transformation cannot be used either.

The FW transformation possesses another important property. The relativistic wave equations and all operators are block-diagonal (diagonal in two spinors). This property permits separating positive and negative energy states.[1] Of course, extraction of even parts of operators becomes unnecessary.

The detailed analysis performed in Ref. 18 shows that the wave functions in both the Dirac and FW representations are equal to each other only approximately, and they do not coincide. In these papers, the nonrelativistic case was considered and relativistic corrections were taken into account.

An analogous conclusion follows from the results obtained in Ref. 11. In this work, a more general situation has been investigated for the relativistic particle not strongly interacting with an electromagnetic field. It has been found that the upper spinors in the Dirac and FW representations are approximately proportional to each other, but this property is not exact.

Thus, the preferable employment of the FW representation is evident, although the relativistic wave equations are more complicated in this representation.

III. METHODS OF THE FOLDY–WOUTHUYSEN TRANSFORMATION

In the classical work by Foldy and Wouthuysen,[1] two different transformations, for free relativistic particles and for nonrelativistic particles in electromagnetic fields have been carried out. In the general case, transformation to a new representation described by the wave function Ψ' is performed with the unitary operator U:

$$\Psi' = U\Psi = e^{iS}\Psi,$$

where $\Psi = \binom{\phi}{\chi}$ is the wave function (bispinor) in the Dirac representation. As

$$\Psi = U^{-1}\Psi', \qquad i\frac{\partial}{\partial t}\Psi = \mathcal{H}\Psi, \qquad i\frac{\partial}{\partial t}\Psi' = \mathcal{H}'\Psi',$$

the following transformation can be carried out:

$$i\frac{\partial}{\partial t}\Psi = \mathcal{H}U^{-1}\Psi',$$

$$i\frac{\partial}{\partial t}\Psi = i\frac{\partial}{\partial t}(U^{-1}\Psi') = i\frac{\partial U^{-1}}{\partial t}\Psi' + iU^{-1}\frac{\partial \Psi'}{\partial t} = \left(i\frac{\partial U^{-1}}{\partial t} + U^{-1}\mathcal{H}'\right)\Psi',$$

$$U\mathcal{H}U^{-1}\Psi' = \left(iU\frac{\partial U^{-1}}{\partial t} + \mathcal{H}'\right)\Psi'.$$

Hence, the Hamilton operator in the new representation takes the form[1,19]

$$\mathcal{H}' = U\mathcal{H}U^{-1} - iU\frac{\partial U^{-1}}{\partial t}, \tag{2}$$

or

$$\mathcal{H}' = U\left(\mathcal{H} - i\frac{\partial}{\partial t}\right)U^{-1} + i\frac{\partial}{\partial t}.$$

There is an error in this transformation in Ref. 20.

The Hamiltonian can be split into operators commuting and noncommuting with the operator β:

$$\mathcal{H}=\beta m+\mathcal{E}+\mathcal{O}, \quad \beta\mathcal{E}=\mathcal{E}\beta, \quad \beta\mathcal{O}=-\mathcal{O}\beta. \tag{3}$$

The Hamiltonian $\mathcal{H}$ is Hermitian. We assume that both operators $\mathcal{E}$ and $\mathcal{O}$ are also Hermitian. For free Dirac particles $\mathcal{E}=0$, $\mathcal{O}=\boldsymbol{\alpha}\cdot\mathbf{p}$, and the operator S has the form

$$S=-i\beta\boldsymbol{\alpha}\cdot\mathbf{p}\theta(\mathbf{p}), \tag{4}$$

where θ is a function of the momentum operator. If we choose

$$\theta(\mathbf{p})=\frac{1}{2p}\arctan\left(\frac{p}{m}\right),$$

the transformed Hamiltonian $\mathcal{H}'$ contains no odd operators[1,20] and we obtain Eq. (1),

$$\mathcal{H}'=\beta\sqrt{m^2+\mathbf{p}^2}.$$

For nonrelativistic particles in an electromagnetic field, the FW transformation can be performed with the operator[1,20]

$$S=-\frac{i}{2m}\beta\mathcal{O}. \tag{5}$$

The transformed Hamiltonian can be written in the form

$$\mathcal{H}'=\mathcal{H}+i[S,\mathcal{H}]+\frac{i^2}{2!}[S,[S,\mathcal{H}]]+\frac{i^3}{3!}[S,[S,[S,\mathcal{H}]]]+\cdots-\dot{S}-\frac{i}{2!}[S,\dot{S}]-\frac{i^2}{3!}[S,[S,\dot{S}]]-\cdots, \tag{6}$$

where $[\cdots,\cdots]$ means a commutator. As a result of this transformation, we find

$$\mathcal{H}'=\beta\epsilon+\mathcal{E}'+\mathcal{O}', \qquad \beta\mathcal{E}'=\mathcal{E}'\beta, \qquad \beta\mathcal{O}'=-\mathcal{O}'\beta, \tag{7}$$

where the odd operator $\mathcal{O}'$ is now $O(1/m)$. This procedure can be repeated to obtain the required accuracy. Another form of the nonrelativistic FW transformation was given by Ericksen[5] (see also Ref. 21).

There are also other methods for obtaining the block-diagonal form of the Hamiltonian or the Lagrangian. The so-called elimination method of Pauli[22] permits us excluding the lower spinor from relativistic wave equations. As a result, the wave function of the final Pauli equation is the upper Dirac spinor, ϕ. This means that the upper Dirac spinor is also an eigenfunction of the transformed Hamiltonian. However, this property is not exact. The Pauli method was analyzed in detail in Refs. 18 and 21. It was shown that this method gives the right first approximation. Nevertheless, relativistic corrections of higher orders are incorrect. It is quite natural because a direct Pauli's reduction leads to a neglect of the contribution of the lower spinor.[18] The relation between the exact wave function in the FW representation and the upper Dirac spinor has been found in Ref. 11 in the relativistic case.

A more exact variant of the elimination method had been proposed earlier by Berestetskii and Landau[23] (see also Refs. 4 and 24). They showed that it was possible to find a nonunitary operator V for which

$$\psi=V\phi \tag{8}$$

is a two-component wave function with a correct norm. An appropriate form of the operator V can be obtained from the condition

$$\int \psi^\dagger \psi \, dV = \int (\phi^\dagger \phi + \chi^\dagger \chi) dV = 1.$$

The relation between the Dirac spinors can be expressed in the general form $\chi = Q\phi$. Therefore,

$$V^\dagger V = 1 + Q^\dagger Q.$$

If we additionally assume that the operator V is Hermitian, then both this operator and the Hamiltonian can be found by successive approximations.[4,23–25]

Of course, the elimination method is much simpler. However, it is mostly intuitive. Its validity is proved only by the coincidence of the results obtained by the FW and Akhiezer–Berestetskii–Landau methods.[21]

Another method of diagonalization of relativistic wave equations was proposed by Korner and Thompson.[6] In this work, the Lagrangian approach was used. The Korner–Thompson method is similar to the FW method. It also includes a successive decrease in the maximum order of odd terms. The results obtained by the FW and Korner–Thompson methods agree (see Ref. 12).

Thus, several nonrelativistic transformation methods give the same results. However, the FW transformation method has been justified in the best way.

In several cases, FW transformation can be performed exactly.[5,7,8] An exact FW transformation has also been performed for a wide class of external fields in Ref. 26. In this work, involutive symmetries of relativistic wave equations have been used. However, the transformed Hamiltonians contain ''nontraditional'' space reflection operators. The reduction of Hamiltonians to the ''traditional'' form is a difficult problem. It has not been investigated in Ref. 26. However, this reduction is necessary to do for solving many problems (e.g., finding particle and spin motion equations).

Generally, FW transformation for relativistic particles in external fields is complicated. The transformation methods explained in Refs. 9 and 10 require cumbersome calculations. A variant of the elimination method useful for relativistic particles has been developed in Ref. 11. On eliminating the lower spinor from the relativistic wave equations, the final equation for the upper spinor takes the form[11]

$$i\frac{\partial \phi}{\partial t} = F\left(\mathbf{r}, \mathbf{p}, i\frac{\partial}{\partial t}\right)\phi, \tag{9}$$

where F is the operator function. Further calculations are analogous to those in the Akhiezer–Berestetskii–Landau method. A new wave function with a correct norm, ψ, expressed by Eq. (8) is introduced. Substituting it for ϕ into Eq. (9), one can find the Hamilton operator for the relativistic particle.

The relativistic wave equation for an upper spinor similar to Eq. (9) is found by the Lagrangian approach.[12]

However, it is difficult to find a second approximation by using the relativistic variant of the elimination method proposed in Ref. 11. It is easier to determine relativistic corrections of higher orders.[12]

The right two-component wave function in the FW representation, ψ, does not coincide with the upper Dirac spinor, ϕ.[11] This conclusion is in agreement with the results obtained in Ref. 18.

There are other difficult problems. The diagonalization of relativistic wave equations needs carefulness, especially in the time-dependent case. As mentioned in Refs. 19 and 27, in the latter case $\mathcal{H}'$ is not equivalent to $\mathcal{H}$ since these operators have different matrix elements. Rather, $U\mathcal{H}U^{-1}$ is. There is a danger that one can arrive at a block-diagonal representation differing from the FW one even in the time-independent case. For example, the transformation performed in Ref. 8 (this is the Melosh transformation indeed[28]) leads to a block-diagonal Hamiltonian that differs from the Hamiltonian in the FW representation.[29] Therefore, the application of noncanonical

transformation methods is restricted by the necessity of verifying the results by comparing them with the corresponding results obtained by the canonical transformation method in some particular cases. Of course, other transformation methods may be simpler or less cumbersome. Nevertheless, the FW method is safer and substantiated very well.

In the present work, a relativistic extension to the FW method is proposed.

IV. EXACT FOLDY–WOUTHUYSEN TRANSFORMATION

Consider some cases of the exact FW transformation.

In Eq. (3), the operators β and $\mathcal{O}^2$ commute ($\beta\mathcal{O}^2=-\mathcal{O}\beta\mathcal{O}=\mathcal{O}^2\beta$). Therefore, the operator $\mathcal{O}^2$ is even.

The operator S can be defined by an expression similar to Eq. (4):

$$S=-i\frac{\beta\mathcal{O}}{C}\theta, \tag{10}$$

where C and θ are the functions of $\mathcal{O}^2$ and the operator C satisfies the following conditions:

$$C^2=\mathcal{O}^2, \qquad [\beta,C]=0. \tag{11}$$

It follows from conditions (11) that the operator C is also even.

It is possible to use the following formal definition of this operator:

$$C=\sqrt{\mathcal{O}^2}. \tag{12}$$

Relations (11) and (12) define the square root of matrix operators. To unambiguously define the square root, these relations should be complemented by the condition that the square root of the unit matrix $\mathcal{I}$ is equal to the unit matrix. This definition of the square root coincides with those of Refs. 1, 20, and 26. For example, for free particles,

$$\mathcal{O}=\boldsymbol{\alpha}\cdot\mathbf{p}, \qquad \mathcal{O}^2=\mathcal{I}\mathbf{p}^2, \qquad C=\mathcal{I}\sqrt{\mathbf{p}^2}\equiv\mathcal{I}|\mathbf{p}|.$$

Further, the symbol of the unit matrix $\mathcal{I}$ will be omitted.

Since

$$\mathcal{O}^2=-\beta\mathcal{O}\beta\mathcal{O}, \qquad C=\sqrt{-\beta\mathcal{O}\beta\mathcal{O}}, \qquad f(\mathcal{O}^2)=f(C^2),$$

the operators $\beta\mathcal{O},C,\mathcal{O}^2$, and θ commute with each other. The operator θ is the angle of rotation of the basic vector set in the spinor space.

The unitary transformation operator, U, can be written in the form

$$U=\cos\theta+\frac{\beta\mathcal{O}}{C}\sin\theta. \tag{13}$$

A FW transformation is exact if the external field is stationary and the operators $\mathcal{E}$ and $\mathcal{O}$ commute:

$$[\mathcal{E},\mathcal{O}]=0. \tag{14}$$

In this particular case,

$$[\mathcal{E},\beta\mathcal{O}]=\beta[\mathcal{E},\mathcal{O}]=0.$$

Condition (14) is a sufficient but not necessary condition of the exact transformation.

The Hamilton operator in the new representation takes the form

$$\mathcal{H}'=\left(\cos\theta+\frac{\beta\mathcal{O}}{C}\sin\theta\right)\mathcal{H}\left(\cos\theta-\frac{\beta\mathcal{O}}{C}\sin\theta\right)$$
$$=(\beta m+\mathcal{O})\left(\cos\theta-\frac{\beta\mathcal{O}}{C}\sin\theta\right)^2+\mathcal{E}$$
$$=(\beta m+\mathcal{O})\left(\cos 2\theta-\frac{\beta\mathcal{O}}{C}\sin 2\theta\right)+\mathcal{E}$$
$$=\beta(m\cos 2\theta+C\sin 2\theta)+\mathcal{O}\left(\cos 2\theta-\frac{m}{C}\sin 2\theta\right)+\mathcal{E}.$$

The Hamiltonian $\mathcal{H}'$ is even if the odd term (proportional to $\mathcal{O}$) vanishes. This takes place if

$$\tan 2\theta=\frac{C}{m}. \tag{15}$$

This equation has two solutions, θ_1 and θ_2, differing in $\pi/2$. Since

$$\tan 2\theta=\frac{2\tan\theta}{1-\tan^2\theta},\quad \tan\theta=\frac{\tan 2\theta}{1\pm\sqrt{1+\tan^2 2\theta}},$$

they are defined by the relations

$$\tan\theta_1=\frac{C}{\epsilon+m},\qquad \tan\theta_2=-\frac{C}{\epsilon-m},\qquad \epsilon=\sqrt{m^2+C^2}=\sqrt{m^2+\mathcal{O}^2}. \tag{16}$$

Thus, there are two unitary transformations of the operator $\mathcal{H}$ to an even form. They are characterized by the angles θ_1 and θ_2, where the angle θ_1 corresponds to the FW transformation.

As a result of both transformations, one of the spinors (lower for θ_1 and upper for θ_2) becomes zero as for free particles.

Note that the transformation under consideration is also similar to the Melosh transformation.[13]

If condition (14) is satisfied, then the Hamilton operator in the FW representation is defined exactly:

$$\mathcal{H}'=\beta\epsilon+\mathcal{E}. \tag{17}$$

Unlike Refs. 9, 10, and 11, Eq. (17) contains exact expressions for the Hamiltonian derived in Refs. 5, 7, and 8 as particular cases.

The transformation operator U can be written in nonexponential form. After the calculation of $\sin\theta_1$ and $\cos\theta_1$ with formulas (16),

$$\sin\theta_1=\frac{C}{\sqrt{2\epsilon(\epsilon+m)}},\qquad \cos\theta_1=\sqrt{\frac{\epsilon+m}{2\epsilon}},$$

we obtain the following expression:

$$U^{\pm}=\frac{\epsilon+m\pm\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}, \tag{18}$$

where $U^+\equiv U$, $U^-\equiv U^{-1}$. This expression agrees with the well-known formula for free particles.[1] Since $(\beta\mathcal{O})^\dagger=\mathcal{O}\beta=-\beta\mathcal{O}$, the operator U is unitary. A simultaneous change of signs

of $\sin\theta_1$ and $\cos\theta_1$ does not affect the final result because the wave functions Ψ,Ψ' are determined up to a sign. The direct calculation of the Hamilton operator in the FW representation also leads to Eq. (17) in accordance with formulas (2), (3), (14), and (18).

Another class of Hamiltonians permitting exact FW transformation has been investigated in Ref. 26.

V. EXACT TRANSFORMATION FOR PARTICLES IN ELECTROWEAK FIELDS

Let us consider the interaction of a relativistic spin-1/2 particle, possessing an anomalous magnetic moment (AMM), with stationary electromagnetic and electroweak fields. The Hamiltonian of the electromagnetic interaction is defined by the Dirac–Pauli equation:[30]

$$\mathcal{H}_{\mathrm{DP}}=\boldsymbol{\alpha}\cdot\boldsymbol{\pi}+\beta m+e\Phi+\mu'(-\mathbf{\Pi}\cdot\mathbf{H}+i\boldsymbol{\gamma}\cdot\mathbf{E}),\qquad \boldsymbol{\pi}=\mathbf{p}-e\mathbf{A}, \tag{19}$$

where μ' is AMM, Φ, $\mathbf{A}$ and $\mathbf{E}$, $\mathbf{H}$ are the potentials and the strengths of an electromagnetic field. This equation is derived in the one-particle approximation and is useful when an electromagnetic field is not extremely strong (see Ref. 11).

The weak interaction Hamiltonian should be added to the Hamiltonian of Eq. (19). The weak interaction does not conserve the spatial parity. For the interaction transferred by neutral currents, the standard model gives the following expression for the parity-nonconserving weak interaction Hamiltonian in the approximation of a small transferred momentum:[31]

$$\mathcal{H}_{\mathrm{PNC}}=-\frac{G}{\sqrt{2}}(C_1\gamma^5+C_2\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}')n(\mathbf{r}),\qquad \gamma^5=\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}, \tag{20}$$

where G is the Fermi constant, $\boldsymbol{\sigma}'$ is the Pauli matrix for matter particles, and $n(\mathbf{r})$ is the density of matter particles. For the interactions with nuclei, $n(\mathbf{r})$ characterizes the density of nucleons of a certain kind, and $\boldsymbol{\sigma}'$ should be replaced by the nucleus spin. Formulas (19) and (20) do not change if the external fields are nonstationary. The matter particles are considered to be at rest.

The coefficients C_1,C_2 are different for different pairs of interacting particles. The Hamiltonians corresponding to the interactions with different matter particles should be summed-up. The signs in formula (20) depend on the definition of the coefficients C_1,C_2 and matrix γ^5. The total Hamiltonian equals

$$\mathcal{H}=\mathcal{H}_{\mathrm{DP}}+\mathcal{H}_{\mathrm{PNC}}. \tag{21}$$

In this case, in formulas (3), (16)–(18) we have

$$\begin{aligned}\mathcal{E}&=e\Phi-\mu'\mathbf{\Pi}\cdot\mathbf{H},\\ \mathcal{O}&=\boldsymbol{\alpha}\cdot\boldsymbol{\pi}+i\mu'\boldsymbol{\gamma}\cdot\mathbf{E}-\frac{G}{\sqrt{2}}(C_1\gamma^5+C_2\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}')n(\mathbf{r})\\ &=\beta\left[\boldsymbol{\gamma}\cdot\boldsymbol{\pi}+i\mu'\boldsymbol{\alpha}\cdot\mathbf{E}-\frac{G}{\sqrt{2}}(C_1\beta\gamma^5+C_2\boldsymbol{\gamma}\cdot\boldsymbol{\sigma}')n(\mathbf{r})\right].\end{aligned} \tag{22}$$

Let us consider some particular cases where Hamiltonian (21) satisfies condition (14). For these cases the FW transformation is exact. The general case will be analyzed in the next section.

The exact Hamiltonian in the FW representation is given by Eq. (17), where $\mathcal{E}$ is defined by Eq. (22), and

$$\epsilon=\left\{ m^2-\left[\boldsymbol{\gamma}\cdot\boldsymbol{\pi}+i\mu'\boldsymbol{\alpha}\cdot\mathbf{E}-\frac{G}{\sqrt{2}}(C_1\beta\gamma^5+C_2\boldsymbol{\gamma}\cdot\boldsymbol{\sigma}')n(\mathbf{r})\right]\right\}^{1/2}$$

$$=\Bigg\{ m^2+\boldsymbol{\pi}^2+\beta\mu'(\boldsymbol{\Sigma}\cdot[\boldsymbol{\pi}\times\mathbf{E}]-\boldsymbol{\Sigma}\cdot[\mathbf{E}\times\boldsymbol{\pi}]-\boldsymbol{\nabla}\cdot\mathbf{E})+\mu'^2\mathbf{E}^2-e\boldsymbol{\Sigma}\cdot\mathbf{H}$$

$$+\frac{G}{\sqrt{2}}(C_1\{\boldsymbol{\Sigma}\cdot\boldsymbol{\pi},n(\mathbf{r})\}_+-C_2\{\boldsymbol{\sigma}'\cdot\boldsymbol{\pi},n(\mathbf{r})\}_+ +C_2[\boldsymbol{\Sigma}\times\boldsymbol{\sigma}']\cdot\boldsymbol{\nabla}n(\mathbf{r})-2\beta\mu'C_2[\boldsymbol{\Sigma}\times\boldsymbol{\sigma}']\cdot\mathbf{E}n(\mathbf{r}))$$

$$+\frac{G^2}{2}n^2(\mathbf{r})[C_1^2+3C_2^2-2C_2(C_1+C_2)\boldsymbol{\Sigma}\cdot\boldsymbol{\sigma}']\Bigg\}^{1/2}. \tag{23}$$

Hence, the operator $U^{\pm}$ is expressed by formulas (18), (22), and (23). Although Eq. (23) is formally exact, the small terms proportional to C_1^2, C_1C_2, C_2^2 are wittingly negligible in the approximation of a small transferred momentum.

Formulas (17), (22), and (23) describe the exact Hamilton operator in the FW representation in the following particular cases:

(a) in the presence of only weak interaction ($\Phi=0,\mathbf{A}=0,\mathbf{E}=0,\mathbf{H}=0$);
(b) for Dirac particles ($\mu'=0$) in magnetic and weak fields ($\Phi=0,\mathbf{E}=0$);
(c) for uncharged particles with AMM in electric and weak fields ($e=0,\mathbf{A}=0,\mathbf{H}=0$);
(d) for particles with AMM moving in the plane orthogonal to a static uniform magnetic field ($\Phi=0,\mathbf{E}=0,P_z=0,C_1=C_2=0$);
(e) for uncharged particles with AMM moving in the plane orthogonal to a static uniform magnetic field. A static electric field (possibly nonuniform) is also orthogonal to the magnetic field ($e=0,\mathbf{E}\perp\mathbf{H},P_z=0,C_1=C_2=0$).

In two cases [(d) and (e)], $\mathbf{H}=H\mathbf{e}_z$, and in the case (e), the electric field strength does not depend on z. Otherwise, $\mathrm{rot}\,\mathbf{E}\neq 0$ and the magnetic field is not constant ($\partial\mathbf{H}/\partial t\neq 0$). Therefore, in these cases the operator $p_z=-i(\partial/\partial z)$ commutes with the Hamilton operator and has eigenvalues $P_z=\mathrm{const}$. Consequently, the consideration of the particular case $P_z=0$ is quite reasonable. All these cases satisfy condition (14).

Formulas (17), (22), and (23) agree with all exact expressions of the operator $\mathcal{H}'$ derived for uncharged particles with AMM in an electrostatic field, Dirac particles in a static magnetic field, and particles with AMM moving in the plane orthogonal to a static uniform magnetic field in Refs. 5, 7, 8. The weak interaction is not considered in these works.

VI. GENERAL CASE

In the general case, relativistic particles interact with external fields. We suggest performing the FW transformation in two stages. First, a transformation similar to the FW transformation for free particles is performed for particles in external fields. Second, a transformation similar to the FW transformation for nonrelativistic particles is carried out.

We assume that the external fields are not extremely strong and the transformed Hamiltonian can be expressed as a power series in the field potentials and their derivatives. The external fields can be nonstationary.

In the general case, formula (17) is not exact because $\mathcal{E}$ depends on the coordinates and contains Dirac matrices. We should calculate the commutator of the operators U and $\mathcal{E}-i(\partial/\partial t)$:

$$U\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)U^{-1}=\mathcal{E}-i\frac{\partial}{\partial t}+\left[U,\mathcal{E}-i\frac{\partial}{\partial t}\right]U^{-1}.$$

In this case, it is necessary to compute some commutators containing inverse operators and square roots of the operators. These commutators can be calculated using the following exact formulas which are valid for arbitrary operators A and B:[32]

$$[A^{-1},B]=A^{-1}[B,A]A^{-1}, \tag{24}$$

$$[A,B]=\tfrac{1}{4}\{A^{-1},[A^2,B]\}_+-\tfrac{1}{4}[[A,[A,B]],A^{-1}], \tag{25}$$

where $A^{-1}\equiv 1/A$ and $\{\ldots,\ldots\}_+$ stands for the anticommutator. If A is the square root of the operators and the commutator of the operators is small compared to their product, i.e.,

$$|[A,B]|\ll|AB|,$$

formulas (24) and (25) allow us to obtain the quantity $[A,B]$ with any accuracy by the method of successive approximations (see Ref. 32). As a rule, this condition is satisfied since it is equivalent to the inequality

$$\frac{\hbar c}{E}\ll l_c, \tag{26}$$

where E is the total energy including the rest energy and l_c is the characteristic size of the nonuniformity region of the external field. For the nonrelativistic particle, the quantity $\hbar c/E$ is equal to the Compton wavelength.

First, it is necessary to perform a unitary transformation with operator (18). After this operation, the Hamiltonian $\mathcal{H}'$ still contains odd terms proportional to the derivatives of the potentials. Let us write the operator $\mathcal{H}'$ as

$$\mathcal{H}'=\beta\epsilon+\mathcal{E}'+\mathcal{O}', \qquad \beta\mathcal{E}'=\mathcal{E}'\beta, \qquad \beta\mathcal{O}'=-\mathcal{O}'\beta, \tag{27}$$

where

$$\epsilon=\sqrt{m^2+\mathcal{O}^2},$$

$$\mathcal{E}'=i\frac{\partial}{\partial t}+\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}-\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}, \tag{28}$$

$$\mathcal{O}'=\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}-\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}.$$

Since

$$ABA=\tfrac{1}{2}(\{A^2,B\}_+-[A,[A,B]]),$$

relation (28) for the operator $\mathcal{E}'$ takes the form

$$\mathcal{E}'=\mathcal{E}-\frac{1}{4}\left[\frac{\epsilon+m}{\sqrt{\epsilon(\epsilon+m)}},\left[\frac{\epsilon+m}{\sqrt{\epsilon(\epsilon+m)}},\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\right]\right]+\frac{1}{4}\left[\frac{\beta\mathcal{O}}{\sqrt{\epsilon(\epsilon+m)}},\left[\frac{\beta\mathcal{O}}{\sqrt{\epsilon(\epsilon+m)}},\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\right]\right]. \tag{29}$$

The odd terms are small compared to both ϵ and the initial Hamiltonian $\mathcal{H}$. This circumstance allows us to apply the usual scheme of the nonrelativistic FW transformation.[1,20]

Second, the transformation should be performed with the following operator:

$$U'=\exp(iS'),\quad S'=-\frac{i}{4}\beta\left\{\mathcal{O}',\frac{1}{\epsilon}\right\}_+=-\frac{i}{4}\left[\frac{\beta}{\epsilon},\mathcal{O}'\right]. \tag{30}$$

The further calculations are similar to those given in Ref. 20. The particle mass should be replaced by the operator ϵ noncommuting with the operators $\mathcal{E}',\mathcal{O}'$. If only major corrections are taken into account, then the transformed Hamiltonian equals

$$\mathcal{H}''=\beta\epsilon+\mathcal{E}'+\frac{1}{4}\beta\left\{\mathcal{O}'^2,\frac{1}{\epsilon}\right\}_+. \tag{31}$$

This is the Hamiltonian in the FW representation.

To obtain the desired accuracy, the calculation procedure with the transformation operator (30) (S' is replaced by S'',S''', etc.) should be repeated multiply.

Let us calculate the Hamiltonian in the FW representation for the relativistic particle with AMM interacting with a nonstationary electroweak field. The Hamiltonian in the Dirac representation is defined by formulas (19)–(21). The transformed Hamiltonian is defined by Eq. (30), where the operator $\mathcal{O}'$ contains the field strengths and does not contain the field potentials. Let us deduce the Hamiltonian to within first-order terms in the field strengths and their first derivatives and second-order terms in the field potentials. The terms of the second order and higher in the field strengths and their derivatives and the first-order terms containing derivatives of the second order and higher of the field strengths will be omitted.

Since we neglect the second-order quantities in $\mathcal{O}'$, the operator $\mathcal{O}'$ does not make any contribution to the Hamiltonian $\mathcal{H}''$ at the second stage of transformation defined by formula (31). As a result, we obtain the following equation for the Hamiltonian in the FW representation:

$$\mathcal{H}''=\beta\epsilon+\mathcal{E}',$$

$$\begin{aligned}\mathcal{E}'=e\Phi&+\frac{e}{8}\left\{\frac{1}{\epsilon(\epsilon+m)},(\boldsymbol{\Sigma}\cdot[\boldsymbol{\pi}\times\mathbf{E}]-\boldsymbol{\Sigma}\cdot[\mathbf{E}\times\boldsymbol{\pi}]-\boldsymbol{\nabla}\cdot\mathbf{E})\right\}_+\\&+\frac{e}{32}\left\{\frac{2\epsilon^2+2\epsilon m+m^2}{\epsilon^4(\epsilon+m)^2},\boldsymbol{\pi}\cdot\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{E}+\mathbf{E}\cdot\boldsymbol{\pi})\right\}_+\\&-\mu'\boldsymbol{\Pi}\cdot\mathbf{H}+\beta\frac{\mu'}{4}\left\{\frac{1}{\epsilon(\epsilon+m)},[(\mathbf{H}\cdot\boldsymbol{\pi})(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi})+(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{H})+2\pi(\boldsymbol{\pi}\cdot\mathbf{j}+\mathbf{j}\cdot\boldsymbol{\pi})]\right\}_+,\end{aligned} \tag{32}$$

where $\mathbf{j}=\boldsymbol{\nabla}\times\mathbf{H}-(1/4\pi)(\partial\mathbf{E}/\partial t)$ is the external current density, and ϵ is determined by formulas (23) and (27). It is important that the operators $\epsilon,\mathcal{E}'$ are found at the first stage, i.e., at the transformation with operator (18).

In the weak field approximation,

$$\epsilon=\epsilon'+\beta\frac{\mu'}{4}\left\{\frac{1}{\epsilon'},(\boldsymbol{\Sigma}\cdot[\boldsymbol{\pi}\times\mathbf{E}]-\boldsymbol{\Sigma}\cdot[\mathbf{E}\times\boldsymbol{\pi}]-\boldsymbol{\nabla}\cdot\mathbf{E})\right\}_+-\frac{e}{4}\left\{\frac{1}{\epsilon'},\boldsymbol{\Sigma}\cdot\mathbf{H}\right\}_++\frac{G}{4\sqrt{2}}\left\{\frac{1}{\epsilon'},W\right\}_+$$

and

$$\mathcal{H}''=\beta\epsilon'+e\Phi+\frac{1}{4}\left\{\left(\frac{\mu_0 m}{\epsilon'+m}+\mu'\right)\frac{1}{\epsilon'},(\mathbf{\Sigma}\cdot[\boldsymbol{\pi}\times\mathbf{E}]-\mathbf{\Sigma}\cdot[\mathbf{E}\times\boldsymbol{\pi}]-\boldsymbol{\nabla}\cdot\mathbf{E})\right\}_+$$
$$+\frac{\mu_0 m}{16}\left\{\frac{2\epsilon'^2+2\epsilon' m+m^2}{\epsilon'^4(\epsilon'+m)^2},\boldsymbol{\pi}\cdot\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{E}+\mathbf{E}\cdot\boldsymbol{\pi})\right\}_+-\frac{1}{2}\left\{\left(\frac{\mu_0 m}{\epsilon'}+\mu'\right),\mathbf{\Pi}\cdot\mathbf{H}\right\}_+$$
$$+\frac{\mu'}{4}\left\{\frac{1}{\epsilon'(\epsilon'+m)},[(\mathbf{H}\cdot\boldsymbol{\pi})(\mathbf{\Pi}\cdot\boldsymbol{\pi})+(\mathbf{\Pi}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{H})+2\pi(\boldsymbol{\pi}\cdot\mathbf{j}+\mathbf{j}\cdot\boldsymbol{\pi})]\right\}_+ +\frac{G}{4\sqrt{2}}\left\{\frac{1}{\epsilon'},W\right\}_+, \tag{33}$$

where

$$\epsilon'=\sqrt{m^2+\boldsymbol{\pi}^2},\qquad W=C_1\{\mathbf{\Sigma}\cdot\boldsymbol{\pi},n(\mathbf{r})\}_+-C_2\{\boldsymbol{\sigma}'\cdot\boldsymbol{\pi},n(\mathbf{r})\}_++C_2[\mathbf{\Sigma}\times\boldsymbol{\sigma}']\cdot\boldsymbol{\nabla}n(\mathbf{r}), \tag{34}$$

and $\mu_0=e/(2m)$ is the Dirac magnetic moment.

Unlike works,[9–11] formula (33) includes, as particular cases, the exact expressions for the Hamiltonian in the FW representation obtained in Refs. 5, 7, and 8. Formulas (32)–(34) also agree with the results obtained in Refs. 9, 10, 11, 33, and 34. A detailed analysis shows that the method of FW transformation used in Ref. 11 does not allow one to take into consideration the terms proportional to the double commutators of ϵ with $e\Phi$ and $\mu'\mathbf{\Pi}\cdot\mathbf{H}$ ($e[\epsilon,[\epsilon,\Phi]]$ and $\mu'[\epsilon,[\epsilon,\mathbf{\Pi}\cdot\mathbf{H}]]$). The terms proportional to $\mathbf{E}$ and $\mathbf{H}$ in the Hamiltonian obtained in Ref. 11 coincide with those in Refs. 9 and 10 and Eq. (33). However, only the Dirac particles were considered in Ref. 9, the derivatives of the field strengths were neglected in Ref. 10, and the nonrelativistic Hamiltonian with relativistic corrections was found in Ref. 33.

VII. PARTICLE AND SPIN MOTION EQUATIONS

Thus, the FW representation is very convenient for describing the particle and spin motion owing to the simple forms of operators. In order to derive corresponding quantum equations, it is necessary to compute the commutators of the Hamiltonian with the same operators as in the nonrelativistic theory. The kinetic momentum operator of particles in an electromagnetic field equals $\boldsymbol{\pi}=\mathbf{p}-e\mathbf{A}$.[35] The equation of particle motion in the electromagnetic field is defined in terms of the commutator of the Hamiltonian with this operator:

$$\frac{d\boldsymbol{\pi}}{dt}=i[\mathcal{H}'',\boldsymbol{\pi}]-e\frac{\partial\mathbf{A}}{dt}.$$

To determine the quantum equation of particle motion, we take into account Eq. (33) for the Hamiltonian,

$$\frac{d\boldsymbol{\pi}}{dt}=e\mathbf{E}+\beta\frac{e}{4}\left\{\frac{1}{\epsilon'},([\boldsymbol{\pi}\times\mathbf{H}]-[\mathbf{H}\times\boldsymbol{\pi}])\right\}_+$$
$$+\frac{1}{4}\left\{\left(\frac{\mu_0 m}{\epsilon'+m}+\mu'\right)\frac{1}{\epsilon'},[\boldsymbol{\nabla}(\mathbf{\Sigma}\cdot[\mathbf{E}\times\boldsymbol{\pi}])-\boldsymbol{\nabla}(\mathbf{\Sigma}\cdot[\boldsymbol{\pi}\times\mathbf{E}])+\Delta\mathbf{E}]\right\}_+$$
$$-\frac{\mu_0 m}{16}\left\{\frac{2\epsilon'^2+2\epsilon' m+m^2}{\epsilon'^4(\epsilon'+m)^2},(\boldsymbol{\pi}\cdot\boldsymbol{\nabla})\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{E}+\mathbf{E}\cdot\boldsymbol{\pi})\right\}_+ +\frac{1}{2}\left\{\left(\frac{\mu_0 m}{\epsilon'}+\mu'\right),\boldsymbol{\nabla}(\mathbf{\Pi}\cdot\mathbf{H})\right\}_+$$
$$-\frac{\mu'}{4}\left\{\frac{1}{\epsilon'(\epsilon'+m)},[(\mathbf{\Pi}\cdot\boldsymbol{\pi})\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{H})+(\boldsymbol{\nabla}(\mathbf{H}\cdot\boldsymbol{\pi}))(\mathbf{\Pi}\cdot\boldsymbol{\pi})+2\pi\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{j}+\mathbf{j}\cdot\boldsymbol{\pi})]\right\}_+. \tag{35}$$

The equation of spin motion is defined by the formula

$$\frac{d\mathbf{\Pi}}{dt}=i[\mathcal{H}'',\mathbf{\Pi}].$$

For particles in a nonstationary electroweak field, it takes the form

$$\begin{aligned}\frac{d\mathbf{\Pi}}{dt}=&\left\{\left(\frac{\mu_0 m}{\epsilon'+m}+\mu'\right)\frac{1}{\epsilon'},[\mathbf{\Pi}\times[\mathbf{E}\times\boldsymbol{\pi}]]\right\}_+ +\left\{\left(\frac{\mu_0 m}{\epsilon'}+\mu'\right),[\mathbf{\Sigma}\times\mathbf{H}]\right\}_+\\ &-\frac{\mu'}{2}\left\{\frac{1}{\epsilon'(\epsilon'+m)},([\mathbf{\Sigma}\times\boldsymbol{\pi}](\boldsymbol{\pi}\cdot\mathbf{H})+(\mathbf{H}\cdot\boldsymbol{\pi})[\mathbf{\Sigma}\times\boldsymbol{\pi}])\right\}_+\\ &-\frac{G}{2\sqrt{2}}\left\{\frac{1}{\epsilon'},(C_1\{[\mathbf{\Sigma}\times\boldsymbol{\pi}],n(\mathbf{r})\}_+ +C_2[\mathbf{\Sigma}\times[\boldsymbol{\sigma}'\times\boldsymbol{\nabla}n(\mathbf{r})]])\right\}_+ .\end{aligned}\tag{36}$$

The corresponding equation for stationary electroweak fields was derived in Ref. 34.

The transition to the semiclassical description is also simple. For free particles, the lower spinor is equal to zero in the FW representation. For particles in external fields, the maximum ratio of the lower and upper spinors is of the first order of W_{int}/E, where W_{int} is the energy of the particle interaction with external fields. Thus, we obtain $(\chi^\dagger\chi)/(\phi^\dagger\phi)\sim(W_{\mathrm{int}}/E)^2$. Therefore, the contribution of the lower spinor is negligible and the transition to the semiclassical equations is performed by averaging the operators in the equations for the upper spinor. It is usually possible to neglect the commutators between the coordinate and kinetic momentum operators and between different components of the kinetic momentum operator (see Ref. 36). As a result, the operators $\boldsymbol{\sigma},\boldsymbol{\sigma}'$, and $\boldsymbol{\pi}$ should be substituted by the corresponding classical quantities: the average spin, $\boldsymbol{\xi}$ ($\boldsymbol{\xi}'$ for matter particles), and the kinetic momentum. For the latter quantity we retain the designation $\boldsymbol{\pi}$. The semiclassical equations of particle and spin motion are

$$\begin{aligned}\frac{d\boldsymbol{\pi}}{dt}=&e\mathbf{E}+\frac{e}{\epsilon'}[\boldsymbol{\pi}\times\mathbf{H}]-\frac{1}{2}\left(\frac{\mu_0 m}{\epsilon'+m}+\mu'\right)\frac{1}{\epsilon'}[2\boldsymbol{\nabla}(\boldsymbol{\xi}\cdot[\boldsymbol{\pi}\times\mathbf{E}])-\Delta\mathbf{E}]\\ &-\frac{\mu_0 m}{4}\cdot\frac{2\epsilon'^2+2\epsilon' m+m^2}{\epsilon'^4(\epsilon'+m)^2}(\boldsymbol{\pi}\cdot\boldsymbol{\nabla})\boldsymbol{\nabla}(\boldsymbol{\pi}\cdot\mathbf{E})+\left(\frac{\mu_0 m}{\epsilon'}+\mu'\right)\boldsymbol{\nabla}(\boldsymbol{\xi}\cdot\mathbf{H})\\ &-\frac{\mu'}{\epsilon'(\epsilon'+m)}[(\boldsymbol{\xi}\cdot\boldsymbol{\pi})\boldsymbol{\nabla}(\mathbf{H}\cdot\boldsymbol{\pi})+2\pi\boldsymbol{\nabla}(\mathbf{j}\cdot\boldsymbol{\pi})],\end{aligned}\tag{37}$$

$$\begin{aligned}\frac{d\boldsymbol{\xi}}{dt}=&2\left(\frac{\mu_0 m}{\epsilon'+m}+\mu'\right)\frac{1}{\epsilon'}[\boldsymbol{\xi}\times[\mathbf{E}\times\boldsymbol{\pi}]]+2\left(\frac{\mu_0 m}{\epsilon'}+\mu'\right)[\boldsymbol{\xi}\times\mathbf{H}]\\ &-\frac{2\mu'}{\epsilon'(\epsilon'+m)}(\mathbf{H}\cdot\boldsymbol{\pi})[\boldsymbol{\xi}\times\boldsymbol{\pi}]-\frac{G}{\sqrt{2}\epsilon'}(2C_1[\boldsymbol{\xi}\times\boldsymbol{\pi}]n(\mathbf{r})+C_2[\boldsymbol{\xi}\times[\boldsymbol{\xi}'\times\boldsymbol{\nabla}n(\mathbf{r})]]).\end{aligned}\tag{38}$$

Equation (37) shows that the particle motion depends on the spin orientation. The corresponding term determines the Stern–Gerlach force.

It is not as convenient to use the Dirac representation to derive quantum equations of particle and spin motion in a similar manner. In this case, it is necessary to extract the polarization operator, **O**, from the obtained equations. This problem is rather difficult because the operator **O** in the Dirac representation is defined by the cumbersome expression given in Ref. 17.

For particles in external fields, the FW transformation also changes the form of the kinetic momentum operator. In particular, the equation of spin motion in the Dirac representation depends on the operator $\boldsymbol{\pi}_{\mathrm{D}}=U^{-1}\boldsymbol{\pi}U$ just as the corresponding equation in the FW representation depends

on the operator $\boldsymbol{\pi}$. However, these two equations differ in their functional dependence on $\boldsymbol{\pi}$. The use of the FW representation protects from both an error in derived equations of particle and spin motion and an incorrect interpretation of these equations.

Another method of transition to the semiclassical description is based on the trajectory-coherent solution of the Dirac equation.[37]

VIII. DISCUSSION

As mentioned above, the proposed method permits obtaining a transformed Hamiltonian to within first-order terms in the field parameters after the first transformation. In this case, all the other canonical methods need several transformations.[1,5,6,10,12,20,21] Therefore, the method described above can be successfully used even for solving nonrelativistic problems. For this purpose, the transformation operator, U, can be expanded in a series of $1/m$. Of course, such an expansion is helpful only in the case of transformation of the operator $\mathcal{E}-i(\partial/\partial t)$. The transformation of other operators leads to the appearance of the term $\beta\epsilon$ in Eq. (31).

Consider the classical example of the FW transformation for a nonrelativistic Dirac particle in an electromagnetic field. We calculate the Hamiltonian to within terms of orders of $(p/m)^4$ and p^2W/m^3, where W means $e\Phi$, $e\mathbf{A}$ (see Refs. 1 and 20). In this approximation, the first double commutator in Eq. (29) is negligible and the second one is equal to

$$\frac{1}{4}\left[\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}},\left[\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}},\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\right]\right]=\frac{1}{2m^2}\left[\boldsymbol{\gamma}\cdot\boldsymbol{\pi},\left[\boldsymbol{\gamma}\cdot\boldsymbol{\pi},\left(\mathcal{E}-i\frac{\partial}{\partial t}\right)\right]\right]$$

$$=\frac{e}{2m^2}[\boldsymbol{\Sigma}\cdot(\mathbf{E}\times\boldsymbol{\pi})-\boldsymbol{\Sigma}\cdot(\boldsymbol{\pi}\times\mathbf{E})-\boldsymbol{\nabla}\cdot\mathbf{E}]. \quad (39)$$

As

$$\epsilon=\sqrt{m^2+(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})^2}=\sqrt{m^2+\boldsymbol{\pi}^2-e\boldsymbol{\Sigma}\cdot\mathbf{H}}=m+\frac{\boldsymbol{\pi}^2}{2m}-\frac{\boldsymbol{\pi}^4}{8m^3}-\frac{e}{2m}\boldsymbol{\Sigma}\cdot\mathbf{H},$$

the transformed Hamiltonian is expressed by the well-known formula[1,20]

$$\mathcal{H}''=\beta\left(m+\frac{\boldsymbol{\pi}^2}{2m}-\frac{\boldsymbol{\pi}^4}{8m^3}\right)+e\Phi-\frac{e}{2m}\boldsymbol{\Pi}\cdot\mathbf{H}+\frac{e}{8m^2}[\boldsymbol{\Sigma}\cdot(\mathbf{E}\times\boldsymbol{\pi})-\boldsymbol{\Sigma}\cdot(\boldsymbol{\pi}\times\mathbf{E})-\boldsymbol{\nabla}\cdot\mathbf{E}]. \quad (40)$$

Thus, the proposed method permits obtaining this formula after the computation of only one double commutator. All the other canonical methods require cumbersome calculations.[1,5,12,20,21] For example, the classical method of Foldy and Wouthuysen require three successive transformations and a calculation of numerous commutators. The noncanonical methods (the Pauli's elimination method and others)[4,11,21–25] permit deriving Hamiltonian (40) in an easier way. Nevertheless, the proposed method is very simple even compared to them. Moreover, it gives an opportunity to find a transformed Hamiltonian with any accuracy even for relativistic particles in external fields.

IX. SUMMARY

In this work, a method of FW transformation for relativistic particles in external fields is proposed. This method is simple and reliable. It performs the exact FW transformation as in known particular cases,[5,7,8] as in others. This property distinguishes the proposed method from the other methods developed for relativistic particles.[9–11] The method is based on the well-known elaborations.[1,20] First, a transformation similar to the FW transformation for free particles is performed for particles in external fields. Second, a transformation similar to the FW transformation for nonrelativistic particles is carried out. In the general case, the FW transformation is

approximate. As an example, the Hamilton operator in the FW representation for relativistic particles with AMM interacting with nonstationary electroweak fields is found to within second derivatives of potentials.

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Resolvent convergence in norm for Dirac operator with Aharonov–Bohm field

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(Received 30 January 2003; accepted 10 April 2003)

We consider the Hamiltonian for relativistic particles moving in the Aharonov–Bohm magnetic field in two dimensions. The field has δ-like singularity at the origin, and the Hamiltonian is not necessarily essentially self-adjoint. The self-adjoint realization requires one parameter family of boundary conditions at the origin. We approximate the point-like field by smooth ones and study the problem of norm resolvent convergence to see which boundary condition is physically reasonable among admissible boundary conditions. We also study the effect of perturbations by scalar potentials. Roughly speaking, the obtained result is that the limit self-adjoint realization is different even for small perturbation of scalar potentials according to the values of magnetic fluxes. It changes at half-integer fluxes. The method is based on the resolvent analysis at low energy on magnetic Schrödinger operators with resonance at zero energy and the resonance plays an important role from a mathematical point of view. However it has been neglected in earlier physical works. The emphasis here is placed on this natural aspect. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1580200]

I. INTRODUCTION

The relativistic Hamiltonian of massless particle moving in the Aharonov–Bohm field is formally defined as the operator

$$H^D=\sigma_1\pi_1+\sigma_2\pi_2 \tag{1.1}$$

acting on the space $[L^2]^2=[L^2(\mathbf{R}^2)]^2$, where

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

are the Pauli spin matrices and

$$\pi_j=-i\partial_j-a_{j\alpha},\quad A_{0\alpha}=(a_{1\alpha},a_{2\alpha})=\alpha(-x_2/|x|^2,x_1/|x|^2),\quad \partial_j=\partial/\partial x_j,$$

for $j=1,2$. For notational brevity, we here confine ourselves to the massless Hamiltonian H^D throughout the entire discussion. However, the obtained results easily extend to the Hamiltonian $\sigma_1\pi_1+\sigma_2\pi_2+m\beta$, $\beta=\sigma_3$, with mass $m>0$. Since the vector potential $A_{0\alpha}:\mathbf{R}^2\to\mathbf{R}^2$ is written as

$$A_{0\alpha}=\alpha(-\partial_2\log|x|,\partial_1\log|x|),$$

it has the point-like magnetic field

$$\nabla\times A_{0\alpha}=\partial_1 a_{2\alpha}-\partial_2 a_{1\alpha}=\alpha\Delta\log|x|=2\pi\alpha\delta(x)$$

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with flux α. Let $\theta=\theta(x)$ be the azimuth angle from the positive x_1 axis. Then $A_{0\alpha}$ takes the form $A_{0\alpha}=\alpha\nabla\theta$, and hence

$$H^D=e^{i\alpha\theta}(-i\sigma_1\partial_1-i\sigma_2\partial_2)e^{-i\alpha\theta}$$

in a formal way. When $\alpha\notin\mathbf{Z}$ is not an integer, $e^{i\alpha\theta}$ is a multivalued function, and the magnetic effect comes from the multivaluedness. We always assume that

$$0<\alpha<1. \tag{1.2}$$

If we replace $A_{0\alpha}(x)$ by $-A_{0\alpha}(x)$, it is easily seen that a similar argument applies to the case $-1<\alpha<0$ under a natural modification. However, if $|\alpha|>1$, then the norm resolvent convergence cannot be in general expected. We will later make a brief comment on the matter [Remarks 3.2 and 5.1 (3)]. According to Ref. 12 [see also (Refs. 7–9 and 19)], we know that H^D is not essentially self-adjoint in $[C_0^\infty(\mathbf{R}^2-\{0\})]^2$ and it has the deficiency indices (1,1). If $u\in[L^2]^2$ is in the domain of some self-adjoint extension, then it behaves like

$$u=\begin{pmatrix}(u_{-1}+o(1))r^{-\alpha}\\(u_{-2}+o(1))e^{i\theta}r^{-(1-\alpha)}\end{pmatrix}+o(1),\quad r=|x|\to 0, \tag{1.3}$$

for some pair (u_{-1},u_{-2}) in the polar coordinate system (r,θ) under assumption (1.2). The ratio $\kappa=iu_{-1}/u_{-2}$ can be shown to be a real number independent of u, and the self-adjoint extension H_κ has the domain

$$\mathcal{D}(H_\kappa)=\{u\in[L^2]^2:H^Du\in[L^2]^2,\quad u_{-1}+i\kappa u_{-2}=0\} \tag{1.4}$$

parametrized by κ, $-\infty<\kappa\leqslant\infty$, where

$$u_{-1}=\lim_{|x|\to 0}|x|^\alpha u_1(x),\quad u_{-2}=\lim_{|x|\to 0}|x|^{1-\alpha}e^{-i\theta}u_2(x)$$

for $u={}^t(u_1,u_2)\in[L^2]^2$, and H^Du is understood in the distribution sense. If $\kappa=\infty$, then $u_{-2}=0$ and the lower component has a weak singularity near the origin for $u\in\mathcal{D}(H_\infty)$, while the singularity of upper component is weak in the case $\kappa=0$. It is impossible to impose the boundary condition in which both components of wave functions remain bounded near the origin.

We approximate $2\pi\alpha\delta(x)$ by a smooth field with compact support. Let $b\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$ be given field with flux $\alpha=\int b(x)\,dx/2\pi$ and set

$$b_\varepsilon(x)=\varepsilon^{-2}b(x/\varepsilon)$$

for $\varepsilon>0$ small enough, where the integration without domain is taken over the whole space. Then b_ε preserves the flux $\int b_\varepsilon(x)\,dx=2\pi\alpha$ and it approximates $b_\varepsilon\to 2\pi\alpha\delta(x)$ as $\varepsilon\to 0$ in the distribution sense. We define the potential $A\in C^\infty(\mathbf{R}^2\to\mathbf{R}^2)$ associated with field b by

$$A(x)=(-\partial_2\varphi(x),\partial_1\varphi(x)) \tag{1.5}$$

and set $A_\varepsilon(x)=\varepsilon^{-1}A(x/\varepsilon)$, where

$$\varphi(x)=(2\pi)^{-1}\int \log|x-y|\,b(y)\,dy. \tag{1.6}$$

As is easily seen, A and A_ε satisfy $\nabla\times A=\Delta\varphi=b$ and $\nabla\times A_\varepsilon=b_\varepsilon$. We further define

$$H_\varepsilon^D=\sigma_1\nu_{1\varepsilon}+\sigma_2\nu_{2\varepsilon} \tag{1.7}$$

as the Hamiltonian approximating H^D, where $(\nu_{1\varepsilon},\nu_{2\varepsilon})=-i\nabla-A_\varepsilon$. This Hamiltonian admits a unique self-adjoint realization with domain $\mathcal{D}(H_\varepsilon^D)=[H^1(\mathbf{R}^2)]^2$, $H^s(\mathbf{R}^2)$ being the Sobolev space of order s. As the first main theorem (Theorem 3.1), we obtain that H_ε^D is convergent to H_∞ in the sense (norm resolvent sense) that

$$(H_\varepsilon^D+i)^{-1}\to(H_\infty+i)^{-1},\quad \varepsilon\to 0,$$

in norm. The attempt of approximation to point-like fields has been often done in physical literatures. For example, the approximation by the bounded potential

$$\tilde{A}(x)=\alpha(-x_2/|x|^2,x_1/|x|^2)\quad \text{on } \{|x|>1\},\quad \tilde{A}(x)=0\quad \text{on } \{|x|<1\}$$

has been studied in a series of works (Refs. 15, 16, and 18). A similar problem has been studied for the nonrelativistic particles. We write $L(p,q)=(-i\nabla-p)^2+q$ for the Schrödinger operator with vector and scalar potentials $p:\mathbf{R}^2\to\mathbf{R}^2$ and $q:\mathbf{R}^2\to\mathbf{R}$. Let $A_{0\alpha}$, A, and A_ε be as above. According to Refs. 1 and 11, $L(A_{0\alpha},0)$ is known to have the deficiency indices (2,2) as a symmetric operator over $C_0^\infty(\mathbf{R}^2-\{0\})$, and one of possible self-adjoint extensions has the domain

$$\mathcal{D}=\{u\in L^2: L(A_{0\alpha},0)u\in L^2,\quad \lim_{|x|\to 0}|u(x)|<\infty\}. \tag{1.8}$$

If $u\in\mathcal{D}$, then the wave function u remains bounded around the origin. This is not the case for the relativistic particles, as stated above. The self-adjoint operator with domain $\mathcal{D}$ is often called the Aharonov–Bohm Hamiltonian (Ref. 3) and we denote it by L_{AB}. We have proved in Ref. 22 that $L(A_\varepsilon,0)$ converges to L_{AB} in the norm resolvent sense. The difference between the nonrelativistic and relativistic cases can be explained as follows. Since the spin matrices satisfy the anticommutator relation $\sigma_j\sigma_k+\sigma_k\sigma_j=2\delta_{jk}$ and since $\sigma_1\sigma_2=i\sigma_3$ and

$$[\nu_{1\varepsilon},\nu_{2\varepsilon}]=\nu_{1\varepsilon}\nu_{2\varepsilon}-\nu_{2\varepsilon}\nu_{1\varepsilon}=ib_\varepsilon,$$

we take the square to obtain the Pauli operator

$$(H_\varepsilon^D)^2=\begin{pmatrix}\nu_{1\varepsilon}^2+\nu_{2\varepsilon}^2-b_\varepsilon & 0\\ 0 & \nu_{1\varepsilon}^2+\nu_{2\varepsilon}^2+b_\varepsilon\end{pmatrix}=\begin{pmatrix}L(A_\varepsilon,-b_\varepsilon) & 0\\ 0 & L(A_\varepsilon,b_\varepsilon)\end{pmatrix}.$$

Then $L(A_\varepsilon,\mp b_\varepsilon)$ have additional δ-like potentials $\mp b_\varepsilon\sim\mp 2\pi\alpha\delta(x)$ for $\varepsilon>0$ small enough. The repulsive potential b_ε makes the lower component vanish near the origin, but the attractive one $-b_\varepsilon$ makes the upper component singular.

We define the unitary operator $J_\varepsilon:L^2\to L^2$ or $[L^2]^2\to[L^2]^2$ by

$$(J_\varepsilon f)(x)=\varepsilon^{-1}f(x/\varepsilon). \tag{1.9}$$

Then we have $L(A_\varepsilon,\mp b_\varepsilon)=\varepsilon^{-2}J_\varepsilon L(A,\mp b)J_\varepsilon^*$ and

$$(L(A_\varepsilon,\mp b_\varepsilon)+1)^{-1}=\varepsilon^2 J_\varepsilon(L(A,\mp b)+\varepsilon^2)^{-1}J_\varepsilon^*.$$

Thus the proof of Theorem 3.1 is reduced to the analysis on the behavior of resolvent $(L(A,\mp b)+\varepsilon^2)^{-1}$ as $\varepsilon\to 0$. In particular, it is significant that $L(A,-b)$ has a resonance state at zero energy. We can represent $L(A,\pm b)$ as

$$L(A,\pm b)=\nu_\pm\nu_\mp=\nu_\mp^*\nu_\mp, \tag{1.10}$$

so that the operators are both non-negative, where $\nu_\pm=\nu_1\pm i\nu_2$ with $(\nu_1,\nu_2)=-i\nabla-A$. A simple calculation yields the relation

$$\nu_+=-ie^{-\varphi}(\partial_1+i\partial_2)e^{\varphi} \tag{1.11}$$

for φ defined by (1.6). Hence the equation $L(A,-b)u=0$ has a bounded solution behaving like

$$\tilde{\rho}=e^{-\varphi(x)}=|x|^{-\alpha}(1+O(|x|^{-1})), \quad |x|\to\infty.$$

Such a solution is called a resonance state. On the other hand, $L(A,b)$ can be shown to have no resonance state at zero energy. Thus the two operators $L(A,\pm b)$ have the different spectral property at zero energy. It seems that this essential aspect has not been recognized in earlier physical literatures.

We discuss the effect of perturbations by scalar potentials in the latter sections. The obtained result (Theorem 5.1) strongly depends on flux α, and the limit self-adjoint extension H_κ changes at $\alpha=1/2$. What is interesting is that it occurs even for small perturbation of scalar potentials. We set

$$V_\varepsilon(x)=\varepsilon^{-1}V(x/\varepsilon)$$

for $V\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$, and we define $H_\varepsilon(V_\varepsilon)$ by

$$H_\varepsilon(V_\varepsilon)=H_\varepsilon^D+V_\varepsilon=\sigma_1\nu_{1\varepsilon}+\sigma_2\nu_{2\varepsilon}+V_\varepsilon. \tag{1.12}$$

Roughly speaking, the operator $H+V=\sigma_1\nu_1+\sigma_2\nu_2+V$ is said to have a resonance state at zero energy, if the equation $(H+V)u=0$ admits a bounded but not square integrable solution. The precise definition is formulated in Sec. V (Definition 5.1). If $H+V$ do not have a resonance state at zero energy, then $H_\varepsilon(V_\varepsilon)$ is proved to converge to H_∞ for $0<\alpha<1/2$ and to H_0 for $1/2<\alpha<1$ in the norm resolvent sense. If $\alpha=1/2$, then $H_\varepsilon(V_\varepsilon)$ is convergent to H_κ for some κ determined from the above resonance state $\tilde{\rho}$ of $L(A,-b)$. If, on the other hand, $H+V$ has a resonance state at zero energy, then the situation is completely reversed. We obtain that $H_\varepsilon(V_\varepsilon)$ is convergent to H_0 for $0<\alpha\leqslant 1/2$ and to H_∞ for $1/2<\alpha<1$.

Our motivation of the study on the convergence to point-like fields comes from an application to the scattering of Dirac particles by magnetic fields (Refs. 2, 7, and 14). For example, the asymptotic behavior of the amplitude in the scattering by the small disk has been calculated under a certain impenetrable boundary condition in the book [Ref. 2 (Sec.7.10)]. The behavior changes discontinuously at half-integer fluxes. Another motivation is to study the scattering of Dirac particles by electromagnetic fields with small support in the interaction of cosmic string with matter (Ref. 7). The amplitude there has been also explicitly calculated for the electric potential of characteristic function of the small disk, and its asymptotic behavior has been shown to take a different form at half-integer fluxes as the support of electromagntic field shrinks. This phenomenon also seems to be closely related to the resonance at zero energy of magnetic Schrödinger operators. However, such a discontinuity at half-integer fluxes in the asymptotic form is completely hidden behind this explicit calculation using the Bessel functions. The argument developed here seems to account for this phenomenon partly. The present work is the first step toward analyzing this problem from a mathematical point of view.

The spectral problems for Dirac Hamiltonians with Aharonov–Bohm fields in two dimensions has been recently discussed from various aspects by several authors. For example, Sitenko (Ref. 21) has studied the vacuum polarization effects in the background of singular magnetic vortex for all self-adjoint extensions, and Falomir and Pisani (Ref. 13) have determined the spectrum in the presence of a uniform magnetic field.

II. KREIN THEORY ON SELF-ADJOINT EXTENSION

In this section we discuss the self-adjointness of the symmetric operator H^D defined by (1.1). This is defined as an operator acting on $[C_0^\infty(\mathbf{R}^2-\{0\})]^2$. We write

$$H^D=\begin{pmatrix} 0 & \pi_- \\ \pi_+ & 0 \end{pmatrix}, \quad \pi_\pm=\pi_1\pm i\,\pi_2,$$

and denote by $\overline{H^D}$ and $(H^D)^*$ the closure and adjoint of H^D in $[L^2]^2$. Let

$$\Sigma_\pm = \mathrm{Ker}\,((H^D)^* \mp i) = \{u \in [L^2]^2 : ((H^D)^* \mp i)u = 0\}.$$

The pair (n_+, n_-), $n_\pm = \dim \Sigma_\pm$, is called the deficiency indices of H^D. As is well known, H^D has self-adjoint extensions if and only if $n_+ = n_-$.

We shall show that $n_+ = n_- = 1$. Suppose that

$$((H^D)^* - i)u = 0, \quad u = {}^t(u_1, u_2) \in [L^2]^2. \tag{2.1}$$

Then u_2 satisfies

$$(\pi_+ \pi_- + 1)u_2 = (\pi_1^2 + \pi_2^2 + 1)u_2 = 0$$

in $\mathbf{R}^2 \setminus \{0\}$, and u_1 is given by $u_1 = -i\pi_- u_2$. The operator $\pi_\pm$ has the representation

$$\pi_+ = e^{i\theta}(-i\partial_r + r^{-1}(\partial_\theta - i\alpha)), \quad \pi_- = e^{-i\theta}(-i\partial_r - r^{-1}(\partial_\theta - i\alpha))$$

in terms of the polar coordinates (r, θ), and

$$\pi_1^2 + \pi_2^2 = (-i\nabla - A_{0\alpha})^2 = -\partial_r^2 - r^{-1}\partial_r + r^{-2}(-i\partial_\theta - \alpha)^2.$$

We write $H_\nu(z) = H_\nu^{(1)}(z)$ for the Hankel function of first kind. All Hankel functions are throughout understood to be of the first kind. Since

$$(z^\nu H_\nu(az))' = az^\nu H_{\nu-1}(az) \tag{2.2}$$

by formula, it follows that

$$(H_{1-\alpha}(ir)e^{i\theta}) = H'_{1-\alpha}(ir) - i(1-\alpha)r^{-1}H_{1-\alpha}(ir) = H_{-\alpha}(ir).$$

If we make use of this relation, then the solution $u \in [L^2]^2$ to (2.1) takes the form

$$u_2 = cH_{1-\alpha}(ir)e^{i\theta}, \quad u_1 = -icH_{-\alpha}(ir) = -ice^{i\alpha\pi}H_\alpha(ir)$$

with constant c. This is the solution corresponding to angular momentum $l = 0$. The solutions with momentum $l \geqslant 1$ are obtained by

$$u_2 = cH_{l+1-\alpha}(ir)e^{i(l+1)\theta}, \quad u_1 = -icH_{l-\alpha}(ir)e^{il\theta},$$

but these are not in $[L^2]^2$ because of the strong singularity near the origin. The same reasoning applies to solutions with momentum $l < 0$. Thus we see that $\Sigma_+ = \{u \in [L^2]^2 : u = c\psi_+\}$ is the one-dimensional space spanned by

$$\psi_+ = N_\alpha \begin{pmatrix} -i^{1+2\alpha}H_\alpha(ir) \\ H_{1-\alpha}(ir)e^{i\theta} \end{pmatrix}, \quad \|\psi_+\|_{L^2} = 1, \tag{2.3}$$

where

$$N_\alpha = (\sin \alpha\pi)^{1/2}/2. \tag{2.4}$$

The normalization constant N_α is calculated by use of the formula

$$2\pi \int_0^\infty r|H_\alpha(ir)|^2 \, \mathrm{d}r = 4\alpha/(\sin \alpha\pi).$$

Similarly $\Sigma_- = \{u \in [L^2]^2 : u = c\psi_-\}$ is spanned by

$$\psi_- = N_\alpha \begin{pmatrix} i^{1+2\alpha} H_\alpha(ir) \\ H_{1-\alpha}(ir) e^{i\theta} \end{pmatrix}, \quad \|\psi_-\|_{L^2} = 1, \tag{2.5}$$

with the same constant N_α.

The Krein theory determines a family of all possible self-adjoint extensions. According to Theorem X.2 and its Corollary of Ref. 20 there is a one-to-one correspondence between the unitary mapping $U:\Sigma_+ \to \Sigma_-$ and the self-adjoint extension H_U, which acts as

$$H_U u = \overline{H}^D v + i v_+ - i U v_+$$

on the domain $\mathcal{D}(H_U) = \{u \in [L^2]^2 : u = v + v_+ + U v_+, \ v \in \mathcal{D}(\overline{H}^D), \ v_+ \in \Sigma_+\}$.

Lemma 2.1: Let J be the isometry operator defined by

$$J = -(\overline{H}^D - i)(\overline{H}^D + i)^{-1} : \Sigma_+^\perp \to \Sigma_-^\perp$$

where $\Sigma_\pm^\perp = \mathrm{Ran}\,(\overline{H}^D \pm i)$ is the orthogonal complement of $\Sigma_\pm$. Then the resolvent $(H_U + i)^{-1}$ is represented as

$$(H_U + i)^{-1} = (1/2i)(1 + (U \oplus J)) : [L^2]^2 = \Sigma_+ \oplus \Sigma_+^\perp \to [L^2]^2 = \Sigma_- \oplus \Sigma_-^\perp .$$

Proof: Let $f \in [L^2]^2$ and set $u = (1/2i)(1 + (U \oplus J))f$. We decompose f into $f = h + g$, where $h \in \Sigma_+$ and $g \in \Sigma_+^\perp$. Then

$$u = (1/2i)((1 + J)g + (1 + U)h).$$

Since $g \in \Sigma_+^\perp = \mathrm{Ran}(\overline{H}^D + i)$, we can write $g = (\overline{H}^D + i)\tilde{g}$ for some $\tilde{g} \in \mathcal{D}(\overline{H}^D)$. Thus $(1 + J)g = 2i\tilde{g} \in \mathcal{D}(\overline{H}^D)$, and hence $u \in \mathcal{D}(H_U)$. We calculate

$$(H_U + i)u = (1/2i)((\overline{H}^D + i)(1 + J)g + (H_U + i)(1 + U)h).$$

Then we obtain $(H_U + i)u = g + h = f$, so that $u = (H_U + i)^{-1} f$. This proves the lemma. □

We examine what boundary condition H_U satisfies at the origin. When $\nu > 0$ is not an integer, $H_\nu(z)$ is represented as

$$H_\nu(z) = J_\nu(z) + i N_\nu(z) = (i/\sin \nu\pi)(e^{-i\nu\pi} J_\nu(z) - J_{-\nu}(z))$$

in terms of Bessel functions, and it obeys

$$H_\nu(z) = -(i/\sin \nu\pi)(1/\Gamma(1 - \nu))(z/2)^{-\nu}(1 + O(|z|^{2\nu}) + O(|z|^2)), \quad |z| \to 0.$$

We now use the abstract lemma in Ref. 20 (p.138). According to the notation there, we have

$$\mathcal{D}((H^D)^*) = \mathcal{D}(\overline{H}^D) \oplus_{\overline{H}^D} \Sigma_+ \oplus_{\overline{H}^D} \Sigma_- .$$

This implies that $v = {}^t(v_1, v_2) \in \mathcal{D}(\overline{H}^D)$ obeys

$$\int_0^{2\pi} v_1(r,\theta)\, \mathrm{d}\theta = o(r^{-\alpha}), \quad \int_0^{2\pi} v_2(r,\theta) e^{-i\theta}\, \mathrm{d}\theta = o(r^{-(1-\alpha)})$$

as $r = |x| \to 0$. The other Fourier coefficients vanish at the origin. Hence $u = {}^t(u_1, u_2) \in \mathcal{D}(H_U)$ satisfies

$$\int_0^{2\pi} u_1(r,\theta)\, \mathrm{d}\theta = 2\pi(u_{-1} + o(1)) r^{-\alpha}, \quad \int_0^{2\pi} u_2(r,\theta) e^{-i\theta}\, \mathrm{d}\theta = 2\pi(u_{-2} + o(1)) r^{-(1-\alpha)}$$

for some pair (u_{-1},u_{-2}) as in (1.3). The unitary mapping U acts as the multiplication $e^{i\zeta}\times$ for some ζ, $-\pi<\zeta\leqslant\pi$, between the one-dimensional spaces $\Sigma_{\pm}$. If we take account of the above behavior of Hankel functions, then the ratio $\kappa=iu_{-1}/u_{-2}$ is calculated as the real number

$$\kappa=(2^{2\alpha-1}\Gamma(\alpha)/\Gamma(1-\alpha))\tan(\zeta/2) \tag{2.6}$$

independent of $u\in\mathcal{D}(H_U)$. Thus we can obtain the family $\{H_\kappa\}$ of self-adjoint extensions with domain $\mathcal{D}(H_\kappa)$ parametrized as in (1.4). If $\zeta=\pi$ and hence $\kappa=\infty$, then

$$\mathcal{D}(H_\infty)=\{u={}^t(u_1,u_2)\in[L^2]^2:H^Du\in[L^2]^2,\quad \lim_{|x|\to 0}|x|^{1-\alpha}e^{-i\theta}u_2(x)=0\},$$

and if $\zeta=0$ and hence $\kappa=0$, then

$$\mathcal{D}(H_0)=\{u={}^t(u_1,u_2)\in[L^2]^2:H^Du\in[L^2]^2,\quad \lim_{|x|\to 0}|x|^{\alpha}u_1(x)=0\}.$$

Roughly speaking, only one component of Dirac wave functions has a weak singularity near the origin in the two special cases $\kappa=\infty$ and $\kappa=0$, while both the components have in general strong singularities in the other cases. Thus it is not allowed as a boundary condition that both the components remain bounded near the origin.

We denote by $(\ ,\ )_{L^2}$ the scalar product in L^2 or $[L^2]^2$. We write

$$f\otimes g=(\ \cdot\ ,g)_{L^2}f:L^2\to L^2$$

for the integral operator with kernel $f(x)\,\overline{g(y)}$, and use a similar notation for the operator $u\otimes v:[L^2]^2\to[L^2]^2$ defined by $(u\otimes v)w=(w,v)_{L^2}u$. This operator is represented in the matrix form

$$u\otimes v=(u_j\otimes v_k)_{1\leqslant j,k\leqslant 2},\quad u_j\otimes v_k:L^2\to L^2,$$

for $u={}^t(u_1,u_2)$ and $v={}^t(v_1,v_2)$ in $[L^2]^2$.

We end the section by deriving the relation between the two resolvents $(H_\kappa+i)^{-1}$ and $(H_\infty+i)^{-1}$. Since $U:\Sigma_+\to\Sigma_-$ takes the form $U=e^{i\zeta}(\psi_-\otimes\psi_+)$, it follows from Lemma 2.1 that

$$(H_\kappa+i)^{-1}-(H_{\kappa'}+i)^{-1}=(1/2i)(e^{i\zeta}-e^{i\zeta'})(\psi_-\otimes\psi_+),$$

where κ and κ' are related to ζ and ζ' through (2.6), respectively. If, in particular, $\zeta'=\pi$, then we obtain

$$(H_\kappa+i)^{-1}=(H_\infty+i)^{-1}+(1/2i)(e^{i\zeta}+1)(\psi_-\otimes\psi_+). \tag{2.7}$$

This relation plays a basic role in the future argument. This is a special case of the Krein formula between resolvents. We refer to Ref. 5 (Chap. VII) for the general Krein theory for self-adjoint extensions.

III. NORM RESOLVENT CONVERGENCE

We consider the problem as to which self-adjoint extension is realized as a norm resolvent limit of Hamiltonians with smooth magnetic fields having small support when the support is shrinking. Let H_ε^D be defined by (1.7). The aim here is to prove the following theorem.

Theorem 3.1: *Assume (1.2). Then H_ε^D is convergent to H_∞ in the norm resolvent sense as $\varepsilon\to 0$.*

Remark 3.1: The potential associated with given field $b\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$ is not uniquely determined. Let $\tilde{A}\in C^\infty(\mathbf{R}^2\to\mathbf{R}^2)$ be another potential having b as a field. Then it takes the form $\tilde{A}$

$=A+\nabla g$ with some $g\in C^\infty(\mathbf{R}^2\to\mathbf{R})$. If $g(x)\to 0$ at infinity, we can prove the norm resolvent convergence for $\tilde{A}_\varepsilon=\varepsilon^{-1}\tilde{A}(x/\varepsilon)$ also. This can be shown in the course of the proof of the theorem.

Before going into the proof, we fix the notation and introduce several auxiliary operators. We assume for brevity that the field $b\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$ has support in the unit disk. According to Ref. 22 (Lemma 2.1) [see (2.2) there], we can construct a potential $a\in C^\infty(\mathbf{R}^2\to\mathbf{R}^2)$ associated with field b such that

$$a(x)=(a_1(x),a_2(x))=A_{0\alpha}(x)=\alpha(-x_2/|x|^2,x_1/|x|^2) \tag{3.1}$$

for $|x|>2$. Then we define

$$p_j=-i\partial_j-a_j,\quad p_{j\varepsilon}=-i\partial_j-a_{j\varepsilon}$$

for $j=1,2$, and

$$K=\sigma_1 p_1+\sigma_2 p_2,\quad K_\varepsilon=\sigma_1 p_{1\varepsilon}+\sigma_2 p_{2\varepsilon},$$

where $a_\varepsilon(x)=\varepsilon^{-1}a(x/\varepsilon)=(a_{1\varepsilon}(x),a_{2\varepsilon}(x))$. Both K and K_ε are self-adjoint operators with domain $[H^1(\mathbf{R}^2)]^2$.

We again denote by $L(p,q)=(-i\nabla-p)^2+q$ the Schrödinger operator with vector potential p and scalar one q. According to this notation, we further define

$$L=L(a,0)=p_1^2+p_2^2,\quad L_\varepsilon=L(a_\varepsilon,0)=p_{1\varepsilon}^2+p_{2\varepsilon}^2 \tag{3.2}$$

and

$$L_\pm=L(a,\pm b)=p_1^2+p_2^2\pm b,\quad L_{\pm\varepsilon}=L(a_\varepsilon,\pm b_\varepsilon).$$

These are self-adjoint operators with domain $H^2(\mathbf{R}^2)$. If we set

$$p_\pm=p_1\pm ip_2,\quad p_{\pm\varepsilon}=p_{1\varepsilon}\pm ip_{2\varepsilon},$$

then $L_\pm=p_\pm p_\mp=p_\mp^* p_\mp$ and $L_{\pm\varepsilon}=p_{\pm\varepsilon}p_{\mp\varepsilon}$ as in (1.10). We can easily show

$$p_{+\varepsilon}(L_{-\varepsilon}+1)^{-1}=(L_{+\varepsilon}+1)^{-1}p_{+\varepsilon},\quad p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}=(L_{-\varepsilon}+1)^{-1}p_{-\varepsilon} \tag{3.3}$$

and the resolvent $(K_\varepsilon+i)^{-1}$ is calculated as

$$(K_\varepsilon+i)^{-1}=\begin{pmatrix} -i(L_{-\varepsilon}+1)^{-1} & p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1} \\ (L_{+\varepsilon}+1)^{-1}p_{+\varepsilon} & -i(L_{+\varepsilon}+1)^{-1}\end{pmatrix}. \tag{3.4}$$

We now assert that

$$(K_\varepsilon+i)^{-1}\to(H_\infty+i)^{-1},\quad \varepsilon\to 0, \tag{3.5}$$

in norm. To prove the assertion, we analyze the behavior as $\varepsilon\to 0$ of $(L_{\pm\varepsilon}+1)^{-1}$. By (3.1), $a_\varepsilon(x)\to A_{0\alpha}(x)$ as $\varepsilon\to 0$ for $x\neq 0$, and hence we have

$$L_{\pm\varepsilon}\to L(A_{0\alpha},0)=(-i\nabla-A_{0\alpha})^2$$

on $C_0^\infty(\mathbf{R}^2-\{0\})$. As stated in Sec. I, the limit operator $L(A_{0\alpha},0)$ has the deficiency indices (2,2). The Krein theory yields a family $\{L_U\}$ of all possible self-adjoint extensions which is parametrized by 2×2 unitary mapping U from one deficiency subspace to the other one. The operator L_U is realized as a differential operator with some boundary conditions at the origin. If w belongs to $\mathcal{D}(L_U)$, then w behaves like

$$w=(w_{-0}r^{-\alpha}+w_{+0}r^{\alpha}+o(r^{\alpha}))+(w_{-1}r^{-(1-\alpha)}+w_{+1}r^{1-\alpha}+o(r^{1-\alpha}))e^{i\theta}+o(r)$$

near the origin for some coefficients $w_{\pm l}$, $l=0,1$, and there exist 2×2 matrices $B_{\pm}$ for which the boundary condition is described as the relation

$$B_{-}\begin{pmatrix} w_{-0} \\ w_{-1} \end{pmatrix}+B_{+}\begin{pmatrix} w_{+0} \\ w_{+1} \end{pmatrix}=0$$

between these four coefficients. For later references, we distinguish the two special operators among the family of self-adjoint extensions. One is the Aharonov–Bohm Hamiltonian L_{AB} with domain

$$\mathcal{D}(L_{AB})=\{w\in L^2: L(A_{0\alpha},0)w\in L^2, \quad w_{-0}=w_{-1}=0\}$$

and the other is L_Z with domain

$$\mathcal{D}(L_Z)=\{w\in L^2: L(A_{0\alpha},0)w\in L^2, \quad w_{+0}=w_{-1}=0\}.$$

Let $J_{\varepsilon}: L^2\to L^2$ be the unitary operator defined by (1.9). Then we have

$$(L_{\pm\varepsilon}+1)^{-1}=\varepsilon^2 J_{\varepsilon}(L_{\pm}+\varepsilon^2)^{-1}J_{\varepsilon}^{*},$$

so that the behavior as $\varepsilon\to 0$ of resolvents $(L_{\pm\varepsilon}+1)^{-1}$ strongly depends on the spectral structure of $L_{\pm}$ at low energy. We explain the resonance state at zero energy in some details. We have assumed in (1.2) that $0<\alpha<1$. Hence it follows from the Aharonov–Casher theorem (Ref. 4) that $L_{\pm}=p_{\mp}^{*}p_{\mp}$ has no bound states at zero energy. It should be noted that L_{-} has bound states in the case that $\alpha>1$, even if $L_{-}\geqslant 0$ is non-negative. The resonance space $E_{\pm}$ at zero energy of $L_{\pm}$ is defined by

$$E_{\pm}=\{u\in C^{\infty}(\mathbf{R}^2): L_{\pm}u=0, \quad u \text{ is bounded}\}.$$

We look at the structure of the resonance spaces. We consider E_{-} only. A similar reasoning applies to E_{+} also. We recall the facts obtained in Ref. 22 (Sec. V): (1) $\dim E_{-}\leqslant 2$. (2) If $\dim E_{-}=2$, then E_{-} is spanned by the linearly independent pair

$$e_l(x)=r^{-\nu}e^{il\theta}+g_l, \quad \nu=|l-\alpha|, \quad l=0,1,$$

where the remainder term $g_l\in L^2\cap C^{\infty}$ falls off like $\partial^{\beta}g_l=O(|x|^{-\nu-1-|\beta|})$. (3) If $\dim E_{-}=1$, then E_{-} is spanned by the linear combination

$$e(x)=c_l r^{-\alpha}+c_2 r^{-1+\alpha}e^{i\theta}+g, \quad |c_1|+|c_2|\neq 0,$$

where $g\in L^2\cap C^{\infty}$ obeys the bound as above at infinity. If $u\in E_{-}$, then

$$L_{-}u=p_{+}^{*}p_{+}u=p_1^2u+p_2^2u-bu=0, \quad b\in C_0^{\infty}(\mathbf{R}^2),$$

by definition, and we have by Lemma 4.3 in Ref. 22 (or by the argument used for its proof) that p_1u and p_2u are in L^2. This implies that $p_{\pm}u$ are also in L^2 and hence it follows by use of partial integration that $p_{+}u=0$ for $u\in E_{-}$. Let φ be defined by (1.6). The function φ behaves like $\varphi(x)=\alpha\log|x|+O(|x|^{-1})$ at infinity, so that $e^{\varphi(x)}=|x|^{\alpha}(1+O(|x|^{-1}))$. Recall that $a\in C^{\infty}(\mathbf{R}^2\to\mathbf{R}^2)$ has the property (3.1). The potential a takes the form

$$a=(-\partial_2\varphi(x),\partial_1\varphi(x))+\nabla h=A+\nabla h \tag{3.6}$$

for some $h\in C^{\infty}(\mathbf{R}^2\to\mathbf{R})$, where h obeys $h=O(|x|^{-1})$ at infinity. We can write

$$p_{+}=-ie^{ih}e^{-\varphi}(\partial_1+i\partial_2)e^{\varphi}e^{-ih} \tag{3.7}$$

as in (1.11) and similarly for $p_- = p_+^*$. Thus we see that $e^{\varphi} e^{-ih} u$ is an entire function for $u \in E_-$. This implies that $E_- = \{c\rho\}$ is the one-dimensional space spanned by $\rho = e^{ih} e^{-\varphi}$, and the resonance state ρ behaves like

$$\rho(x) = |x|^{-\alpha}(1 + O(|x|^{-1})), \quad |x| \to \infty. \tag{3.8}$$

On the other hand, we can show in a similar way that $\dim E_+ = 0$. If we take account of these facts, then Theorem 6.1 in Ref. 22 implies the following lemma.

Lemma 3.1: As $\varepsilon \to 0$, one has

$$(L_{+\varepsilon} + i)^{-1} \to (L_{AB} + i)^{-1}, \quad (L_{-\varepsilon} + i)^{-1} \to (L_Z + i)^{-1},$$

in norm.

Remark 3.2: If $\alpha > 1$, then it follows from the Aharonov–Casher theorem in Ref. 4 that L_- has the zero eigenvalue with multiplicity $[\alpha]$, $[\alpha]$ being the greatest integer not exceeding α. Hence $L_{-\varepsilon} = \varepsilon^{-2} J_\varepsilon L_- J_\varepsilon^*$ has also eigenstates at zero energy. But L_Z never has an eigenstate at zero energy. Thus $L_{-\varepsilon}$ is not convergent to L_Z in norm resolvent sense. It seems that $(L_{-\varepsilon} + i)^{-1}$ is strongly convergent to $(L_Z + i)^{-1}$, so that Theorem 3.1 remains true in the strong sense even for $\alpha > 1$. We do not go into the details here.

We calculate the resolvent $(H_\infty + i)^{-1}$. Consider the equation $(H_\infty + i)u = f$ for $f = {}^t(f_1, f_2) \in [C_0^\infty(\mathbf{R}^2 - \{0\})]^2$. Then $u = {}^t(u_1, u_2)$ satisfies

$$(L(A_{0\alpha}, 0) + 1)u_2 = \pi_+ f_1 - i f_2, \quad u_1 = i\pi_- u_2 - i f_1$$

for the Aharonov–Bohm potential $A_{0\alpha}(x)$. We see that $u \in \mathcal{D}(H_\infty)$ implies $u_2 \in \mathcal{D}(L_{AB})$. Thus $u_2 = (L_{AB} + 1)^{-1}(\pi_+ f_1 - i f_2)$ and

$$u_1 = -i(1 - \pi_-(L_{AB} + 1)^{-1}\pi_+) f_1 + \pi_-(L_{AB} + 1)^{-1} f_2,$$

so that we have

$$(H_\infty + i)^{-1} = \begin{pmatrix} i\pi_-(L_{AB} + 1)^{-1}\pi_+ - i & \pi_-(L_{AB} + 1)^{-1} \\ (L_{AB} + 1)^{-1}\pi_+ & -i(L_{AB} + 1)^{-1} \end{pmatrix}. \tag{3.9}$$

Lemma 3.2: One has the relation

$$1 - \pi_-(L_{AB} + 1)^{-1}\pi_+ = (L_Z + 1)^{-1}.$$

Proof: We note that the operator on the left-hand side of the relation is bounded. Let $f, g \in C_0^\infty(\mathbf{R}^2 - \{0\})$. By (3.1), there exists $\delta > 0$ such that $\pi_\pm f = p_{\pm\varepsilon} f$ and $\pi_\pm g = p_{\pm\varepsilon} g$ for $0 < \varepsilon < \delta$. Since

$$(\pi_-(L_{AB} + 1)^{-1}\pi_+ f, g)_{L^2} = \lim_{\varepsilon \to 0} ((L_{+\varepsilon} + 1)^{-1} p_{+\varepsilon} f, p_{+\varepsilon} g)_{L^2}$$

by Lemma 3.1, it follows from (3.3) that

$$((1 - \pi_-(L_{AB} + 1)^{-1}\pi_+) f, g)_{L^2} = \lim_{\varepsilon \to 0} ((L_{-\varepsilon} + 1)^{-1} f, g)_{L^2}.$$

This, together with Lemma 3.1 again, proves the lemma. □

We denote by $Op(\varepsilon^\nu)$ and $op(\varepsilon^\nu)$ the classes of bounded operators B_ε acting on L^2 or $[L^2]^2$ such that the operator norm of B_ε obeys the bound $\|B_\varepsilon\| = O(\varepsilon^\nu)$ and $\|B_\varepsilon\| = o(\varepsilon^\nu)$, respectively, as $\varepsilon \to 0$. We now prove Theorem 3.1, accepting the three lemmas below as proved. The proof of the lemmas is done in the next section.

Lemma 3.3: $\chi(L_+ + \varepsilon^2)^{-1}\chi = Op(\varepsilon^0)$ for $\chi \in C_0^\infty(\mathbf{R}^2 \to \mathbf{R})$.

Lemma 3.4: $p_{\pm\varepsilon}(L_{+\varepsilon}+1)^{-1}\to\pi_{\pm}(L_{AB}+1)^{-1}$ *in norm as* $\varepsilon\to 0$.

Lemma 3.5: $\chi(L_{-}+\varepsilon^2)^{-1}\chi=Op(\varepsilon^{-2\alpha})$ *for* $\chi\in C_0^{\infty}(\mathbf{R}^2\to\mathbf{R})$.

Proof of Theorem 3.1: We first prove (3.5). The two resolvents $(K_\varepsilon+i)^{-1}$ and $(H_\infty+i)^{-1}$ are represented by (3.4) and (3.9), respectively. If we use Lemma 3.2, then

$$(H_\infty+i)^{-1}=\begin{pmatrix} -i(L_Z+1)^{-1} & \pi_-(L_{AB}+1)^{-1} \\ (L_{AB}+1)^{-1}\pi_+ & -i(L_{AB}+1)^{-1}\end{pmatrix}.$$

By Lemma 3.4, we have $p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}\to\pi_-(L_{AB}+1)^{-1}$ and

$$(L_{+\varepsilon}+1)^{-1}p_{+\varepsilon}=(p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1})^*\to(\pi_-(L_{AB}+1)^{-1})^*=(L_{AB}+1)^{-1}\pi_+ .$$

Hence Lemma 3.1 implies (3.5). Next we prove the norm resolvent convergence for the operator H_ε^D in question. Let $A\in C^\infty(\mathbf{R}^2\to\mathbf{R}^2)$ be defined by (1.5). Then $A=a-\nabla h$ by (3.6), and

$$(H_\varepsilon^D+i)^{-1}=\exp(-ih_\varepsilon)(K_\varepsilon+i)^{-1}\exp(ih_\varepsilon),$$

where $h_\varepsilon(x)=h(x/\varepsilon)$. By definition, $K=\varepsilon J_\varepsilon^* K_\varepsilon J_\varepsilon$ is independent of ε. We have

$$(K+i\varepsilon)^{-1}=\begin{pmatrix} -i\varepsilon(L_-+\varepsilon^2)^{-1} & p_-(L_++\varepsilon^2)^{-1} \\ (L_{+\varepsilon}+\varepsilon^2)^{-1}p_+ & -i\varepsilon(L_++\varepsilon^2)^{-1}\end{pmatrix} \tag{3.10}$$

and $(K_\varepsilon+i)^{-1}=\varepsilon J_\varepsilon(K+i\varepsilon)^{-1}J_\varepsilon^*$. For any $\delta>0$ small enough, we can take $M>0$ so large that $|h_\varepsilon(x)|<\delta$ for $|x|\geqslant\varepsilon M$, and hence $|\exp(\pm ih_\varepsilon)-1|<2\delta$ for x as above. On the other hand, we can prove that

$$\varepsilon\|\chi_M(K+i\varepsilon)^{-1}\chi_M\|=O(\varepsilon)+O(\varepsilon^{2(1-\alpha)})$$

for the characteristic function χ_M of $\{|x|<M\}$. In fact, Lemma 3.3 yields

$$\|\chi_M(L_++i\varepsilon^2)^{-1}p_+\chi_M\|+\|\chi_M p_-(L_++i\varepsilon^2)^{-1}\chi_M\|=O(1),\quad \varepsilon\to 0,$$

by elliptic estimate. Note that $\chi_{\varepsilon M}=J_\varepsilon\chi_M J_\varepsilon^*$ for $\chi_{\varepsilon M}(x)=\chi_M(x/\varepsilon)$. Hence

$$\begin{aligned}\|(K_\varepsilon+i)^{-1}\chi_{\varepsilon M}\|^2&=\|(K_\varepsilon+i)^{-1}J_\varepsilon\chi_M\|^2\\ &=\|\chi_M J_\varepsilon^*(K_\varepsilon-i)^{-1}(K_\varepsilon+i)^{-1}J_\varepsilon\chi_M\|\\ &=O(\varepsilon)\,\|\chi_M((K+i\varepsilon)^{-1}-(K-i\varepsilon)^{-1})\chi_M\|\to 0\end{aligned}$$

by Lemmas 3.3 and 3.5, and also $\|(H_\varepsilon^D+i)^{-1}\chi_{\varepsilon M}\|\to 0$ by gauge transformation. Thus we obtain

$$\|(H_\varepsilon^D+i)^{-1}-(K_\varepsilon+i)^{-1}\|\to 0.$$

This, together with (3.5), completes the proof. □

IV. RESOLVENT ANALYSIS AT LOW ENERGY ON SCHRÖDINGER OPERATORS I

We shall prove Lemmas 3.3, 3.4, and 3.5 which remain unproved. Throughout the section, we denote by $\chi\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$ a real function such that $\operatorname{supp}\chi\subset B_M$ and $\chi=1$ on $B_{M/2}$, where $B_M=\{|x|<M\}$ for $M\gg 1$ fixed arbitrarily. We further denote by $k\in\mathbf{C}$ a small complex number with $\operatorname{Im}k>0$.

Let $L=L(a,0)$ be as in (3.2). We first make a brief review on the spectral property of L from Ref. 22. Let $L_c^2=\{u\in L^2:\operatorname{supp}u\subset B_M\}$ be the space of L^2 functions with support in B_M. Then we know that there exists a limit

$$G_0 = \lim_{k\to 0} (L-k^2)^{-1}$$

and the limit operator $G_0: L^2_c \to L^2_{-1}$ is bounded into the weighted L^2 space $L^2_{-1} = L^2(\mathbf{R}^2; \langle x\rangle^{-2}\,dx)$, where $\langle x\rangle = (1+|x|^2)^{1/2}$. By (3.1), L coincides with

$$L = L(A_{0\alpha}, 0) = -\partial_r^2 - r^{-1}\partial_r + r^{-2}(-i\partial_\theta - \alpha)^2$$

on $\{|x|>2\}$, and hence $u_l(x) = r^\nu e^{il\theta}$, $\nu = |l-\alpha|$, satisfies $Lu_l = 0$ there. If we define ω_l by

$$\omega_l = c_l(1-\chi)u_l + c_l G_0[L,\chi]u_l, \quad c_l = (l+\nu)^{1/2}/2\nu, \tag{4.1}$$

for $l = 0,1$, then ω_l behaves like

$$\omega_l = c_l r^\nu e^{il\theta} + O(1) \tag{4.2}$$

as $r = |x| \to \infty$, and it solves $L\omega_l = 0$. Such a solution is shown to be unique [see Ref. 22 (Lemma 4.3)]. The argument here is based on the proposition below, which has been proved as Proposition 4.2 in Ref. 22.

Proposition 4.1: Let the notation be as above and let $\nu = |l-\alpha|$ again. Then

$$\chi(L-k^2)^{-1}\chi = \chi G_0 \chi + \sum_{l=0,1} \gamma_l(k) i^{-2\nu} k^{2\nu} (\chi\omega_l \otimes \chi\omega_l) + Op(|k|^2), \quad |k| \to 0,$$

for some coefficients $\gamma_l(k)$, and $\gamma_l(k)$ behaves like

$$\gamma_l(k) = \gamma_l + o(1) \tag{4.3}$$

as $|k| \to 0$, where

$$\gamma_l = -(2^{1-2\nu}\Gamma(1-\nu))/((l+\nu)\Gamma(\nu)). \tag{4.4}$$

The precise value of γ_l is not required to prove the lemmas, but it is important in studying the effect of perturbation by scalar potentials in the latter sections.

Next we consider the operator $L_+ = L(a,b) = L + b$. We shall show that $(L_+ - k^2)^{-1}$ admits an expansion similar to that in Proposition 4.1. We have the relation

$$(L_+ - k^2)^{-1} = (L-k^2)^{-1}(1 + b(L-k^2)^{-1})^{-1} \tag{4.5}$$

by the resolvent identity. Since L_+ has neither bound states nor resonance states at zero energy, $1 + bG_0: L^2_c \to L^2_c$ has the bounded inverse

$$T = (1 + bG_0)^{-1}: L^2_c \to L^2_c.$$

We see that there exists a limit

$$G_+ = \lim_{k\to 0} (L_+ - k^2)^{-1}$$

and the limit operator $G_+ = G_0 T: L^2_c \to L^2_{-1}$ is bounded. The inverse T is represented as

$$T = LG_+ = 1 - bG_+ : L^2_c \to L^2_c \tag{4.6}$$

and it follows that the adjoint operator $T^* = 1 - G_+ b: L^2_{\mathrm{loc}} \to L^2_{\mathrm{loc}}$ is well defined as an operator from the space L^2_{loc} of locally square integrable functions into itself. If we define

$$\omega_{+l} = T^*\omega_l = \omega_l - G_+ b\omega_l \tag{4.7}$$

for $l=0,1$, then ω_{+l} solves $L_+\omega_{+l}=0$ and obeys (4.2) at infinity.

Proposition 4.2: Let the notation be as above. Then

$$\chi(L_+-k^2)^{-1}\chi=\chi G_+\chi+\sum_{l=0,1}\gamma_{+l}(k)i^{-2\nu}k^{2\nu}(\chi\omega_{+l}\otimes\chi\omega_{+l})+Op(|k|^2)$$

for some coefficients $\gamma_{+l}(k)$ *obeying* $\gamma_{+l}(k)=\gamma_l+o(1)$ *as in Proposition 4.1.*

Proof: We start with the relation

$$\chi(L_+-k^2)^{-1}\chi=\chi(L-k^2)^{-1}(1+b(L-k^2)^{-1})^{-1}\chi$$

obtained from (4.5). Set

$$E(k)=\sum_{l=0,1}\gamma_l(k)i^{-2\nu}k^{2\nu}(\omega_l\otimes\omega_l):L^2_c\to L^2_{\mathrm{loc}}.$$

Then we have

$$(1+b(L-k^2)^{-1})^{-1}=(1+TbE(k))^{-1}T+Op(|k|^2)$$

by Proposition 4.1, and hence $(L_+-k^2)^{-1}$ is expanded as

$$\chi(L_+-k^2)^{-1}\chi=G_1+G_2(k)+Op(|k|^2),$$

where $G_1=\chi G_0T\chi=\chi G_+\chi$ and

$$G_2(k)=\chi E(k)(1+TbE(k))^{-1}T\chi+\chi G_0((1+TbE(k))^{-1}-1)T\chi.$$

We can calculate $G_2(k)$ as

$$G_2(k)=\chi(1-G_0Tb)E(k)(1+TbE(k))^{-1}T\chi=\chi T^*E(k)\left(\sum_{j=0}^{\infty}(-1)^j(TbE(k))^j\right)T\chi.$$

Hence it follows from (4.7) that

$$G_2(k)=\sum_{0\leqslant l,m\leqslant 1}\gamma_{lm}(k)(\chi\omega_{+l}\otimes\chi\omega_{+m})$$

for some 2×2 matrix $(\gamma_{lm}(k))_{0\leqslant l,m\leqslant 1}$. The components obey $\gamma_{lm}(k)=O(|k|^2)$ for $l\neq m$, and $\gamma_{ll}(k)=\gamma_l i^{-2\nu}k^{2\nu}(1+o(1))$. This completes the proof. □

Proof of Lemma 3.3: The lemma follows from Proposition 4.2. □

Proof of Lemma 3.4: We have

$$\chi((L_++i\varepsilon^2)^{-1}-(L_+-i\varepsilon^2)^{-1})\chi=Op(\varepsilon^{2\alpha})+Op(\varepsilon^{2(1-\alpha)})$$

by Proposition 4.2. Since $J_\varepsilon^*(L_{+\varepsilon}+i)^{-1}J_\varepsilon=\varepsilon^2(L_++i\varepsilon^2)^{-1}$, it follows that

$$\|\chi_\varepsilon(L_{+\varepsilon}+i)^{-1}\|^2=\|\chi J_\varepsilon^*(L_{+\varepsilon}+i)^{-1}(L_{+\varepsilon}-i)^{-1}J_\varepsilon\chi\|=O(\varepsilon^{2+2\alpha})+O(\varepsilon^{2+2(1-\alpha)}),$$

where $\chi_\varepsilon(x)=\chi(x/\varepsilon)$. Hence

$$\|\chi_\varepsilon(L_{+\varepsilon}+1)^{-1}\|=O(\varepsilon^{1+\alpha})+O(\varepsilon^{1+(1-\alpha)}).$$

If we set $u_\varepsilon=(L_{+\varepsilon}+1)^{-1}f$ for $f\in L^2$, then u_ε satisfies the equation

$$(L_{+\varepsilon}+1)u_\varepsilon=(p_{1\varepsilon}^2+p_{2\varepsilon}^2)u_\varepsilon+b_\varepsilon u_\varepsilon+u_\varepsilon=f$$

and obeys the bound

$$\|\chi_\varepsilon u_\varepsilon\|_{L^2}=(O(\varepsilon^{1+\alpha})+O(\varepsilon^{1+(1-\alpha)}))\|f\|_{L^2}. \tag{4.8}$$

Thus we have

$$\|\chi_\varepsilon p_{j\varepsilon} u_\varepsilon\|_{L^2}=(O(\varepsilon^{\alpha})+O(\varepsilon^{1-\alpha}))\|f\|_{L^2} \tag{4.9}$$

by elliptic estimate. A similar argument applies to $v=(L_{AB}+1)^{-1}f$. Note that

$$J_\varepsilon^*(L_{AB}+1)^{-1}J_\varepsilon=\varepsilon^2(L_{AB}+\varepsilon^2)^{-1}.$$

The Green kernel of $(L_{AB}-k^2)^{-1}$ is explicitly represented in terms of the Bessel functions after separation into the polar coordinates, and it admits an expansion similar to $(L_+-k^2)^{-1}$. Thus we obtain

$$\|\chi_\varepsilon v\|_{L^2}=(O(\varepsilon^{1+\alpha})+O(\varepsilon^{1+(1-\alpha)}))\|f\|_{L^2} \tag{4.10}$$

and

$$\|\chi_\varepsilon \pi_j v\|_{L^2}=(O(\varepsilon^{\alpha})+O(\varepsilon^{1-\alpha}))\|f\|_{L^2}. \tag{4.11}$$

By (3.1), $p_j=\pi_j$ on $\{|x|>2\}$, so that $(1-\chi_\varepsilon)(\pi_j-p_{j\varepsilon})=0$. Since $\chi_\varepsilon=1$ on $\operatorname{supp} b_\varepsilon$, $w_\varepsilon=u_\varepsilon-v$ satisfies

$$(1-\chi_\varepsilon)(p_{1\varepsilon}^2+p_{2\varepsilon}^2+1)w_\varepsilon=0$$

and it follows from (4.8) and (4.10) that

$$\|(1-\chi_\varepsilon)p_{j\varepsilon}w_\varepsilon\|_{L^2}=(O(\varepsilon^{\alpha})+O(\varepsilon^{1-\alpha}))\|f\|_{L^2}.$$

This, together with (4.9) and (4.11), yields

$$\|p_{j\varepsilon}(L_{+\varepsilon}+1)^{-1}-\pi_j(L_{AB}+1)^{-1}\|=O(\varepsilon^{\alpha})+O(\varepsilon^{1-\alpha})$$

and the proof is complete. □

We move to the proof of Lemma 3.5. We analyze the behavior as $|k|\to 0$ of $(L_--k^2)^{-1}$. Decompose b into the product $b=b^{1/2}|b|^{1/2}$, where $b^{1/2}=|b|^{1/2}\operatorname{sgn} b$ with $\operatorname{sgn} b=b/|b|$. Then we have

$$(L_--k^2)^{-1}=(L-k^2)^{-1}+(L-k^2)^{-1}|b|^{1/2}Z(k)^{-1}b^{1/2}(L-k^2)^{-1} \tag{4.12}$$

by repeated use of the resolvent identity, where

$$Z(k)=1-b^{1/2}(L-k^2)^{-1}|b|^{1/2}.$$

Since L_- has a resonance state at zero energy, $1-b^{1/2}G_0|b|^{1/2}:L^2\to L^2$ is not invertible. Let

$$X=\{v\in L^2: v=b^{1/2}G_0|b|^{1/2}v\}.$$

According to Ref. 22, $\dim X=1$, and $v\in X$, $v\neq 0$, satisfies $(v,|b|^{1/2}\omega_0)_{L^2}\neq 0$ and $(v,|b|^{1/2}\omega_1)_{L^2}=0$ for ω_l defined by (4.1). We normalize $\eta_0\in X$ as

$$(\eta_0,|b|^{1/2}\omega_0)_{L^2}=1,\quad (\eta_0,|b|^{1/2}\omega_1)_{L^2}=0 \tag{4.13}$$

and define

$$\rho_0=G_0|b|^{1/2}\eta_0. \tag{4.14}$$

Then ρ_0 solves $L_-\rho_0=0$ and behaves like

$$\rho_0(x)=(2\pi\alpha)^{-1/2}r^{-\alpha}+g, \quad r\to\infty, \tag{4.15}$$

with some $g\in L^2$ [see (5.8) and (5.9) in Ref. 22]. Thus ρ_0 spans the resonance space E_- of L_- at zero energy, because $\dim E_-=1$ as shown already in Sec. III.

Proposition 4.3: Let $\rho_0\in E_-$ be the resonance state defined above. Then

$$\chi(L_--k^2)^{-1}\chi=\gamma_-(k)i^{2\alpha}k^{-2\alpha}(\chi\rho_0\otimes\chi\rho_0)+Op(|k|^0), \quad |k|\to 0,$$

for some coefficient $\gamma_-(k)$ obeying $\gamma_-(k)=-1/\gamma_0+o(1)$, γ_0 being as in (4.4).

Proof: For brevity, we prove the lemma when $b(x)\geqslant 0$. If $b(x)$ is not non-negative, $b^{1/2}G_0|b|^{1/2}$ is not necessarily self-adjoint. The argument below undergoes a slight change, but it is not serious. We skip the detail. Let Q_0 and Q be the orthogonal projections defined by $Q_0=\eta_1\otimes\eta_1$ and $Q=1-Q_0$, where $\eta_1=\eta_0/\|\eta_0\|_{L^2}$. Since $1-b^{1/2}G_0b^{1/2}$:Ran $Q\to$Ran Q is invertible and since

$$Q_0((b^{1/2}\omega_1)\otimes(b^{1/2}\omega_1))=((b^{1/2}\omega_1)\otimes(b^{1/2}\omega_1))Q_0=0$$

by (4.13), it follows from Proposition 4.1 that the inverse $Z(k)^{-1}$ takes the form

$$Z(k)^{-1}=\gamma(k)i^{2\alpha}k^{-2\alpha}(\eta_0\otimes\eta_0)+Op(|k|^0)$$

for some coefficient $\gamma(k)$ having the property in the proposition. This yields the relation. □

Proof of Lemma 3.5: The lemma follows from Proposition 4.3. □

Remark 4.1: Proposition 4.1 remains true for $\chi\nabla(L-k^2)^{-1}\chi$. For example, we have

$$\chi\nabla(L-k^2)^{-1}\chi=\chi\nabla G_0\chi+\sum_{l=0,1}\gamma_l(k)i^{-2\nu}k^{2\nu}(\chi\nabla\omega_l\otimes\chi\omega_l)+Op(|k|^2).$$

This follows by elliptic estimate. A similar relation is true for $(L_+-k^2)^{-1}$ in Proposition 4.2.

We end the section by making a brief comment on the limit as $\varepsilon\to 0$ of the resolvent $(K\pm i\varepsilon)^{-1}$ calculated in (3.10). We formally write $(K\pm i0)^{-1}$ for the limit $\lim_{\varepsilon\to 0}(K\pm i\varepsilon)^{-1}$. If we combine (3.10) with Propositions 4.2, 4.3 and Remark 4.1, then we see that these limits have the different properties according as $0<\alpha<1/2$, $\alpha=1/2$ or $1/2<\alpha<1$:

$$\text{if} \quad 0<\alpha<1/2, \quad (K\pm i0)^{-1} \quad \text{exists and} \quad (K+i0)^{-1}=(K-i0)^{-1},$$

$$\text{if} \quad \alpha=1/2, \quad (K\pm i0)^{-1} \quad \text{exists but} \quad (K+i0)^{-1}\neq(K-i0)^{-1},$$

$$\text{if} \quad 1/2<\alpha<1, \quad (K\pm i0)^{-1} \quad \text{does not exist.}$$

It is obvious by gauge transformation that $H=\sigma_1\nu_1+\sigma_2\nu_2$ preserves the same property as above. This means that H has a property similar to the three dimensional Laplacian for the case $0<\alpha<1/2$ and to the one- or two-dimensional Laplacian for the case $1/2<\alpha<1$.

V. EFFECT OF SCALAR POTENTIALS AND RESONANCE STATE

The remaining three sections are devoted to the study on the effect of perturbation by scalar potentials. We assume that $V\in C_0^\infty(\mathbf{R}^2\to\mathbf{R})$ satisfies

$$\lambda_0=(V\rho_0,\rho_0)_{L^2}\neq 0 \tag{5.1}$$

for ρ_0 spanning the resonance space of L_- at zero energy. We set $V_\varepsilon(x)=\varepsilon^{-1}V(x/\varepsilon)$ and define $K_\varepsilon(V_\varepsilon)$ by

$$K_\varepsilon(V_\varepsilon)=K_\varepsilon+V_\varepsilon=\sigma_1 p_{1\varepsilon}+\sigma_2 p_{2\varepsilon}+V_\varepsilon,$$

which is self-adjoint with domain $\mathcal{D}(K_\varepsilon(V_\varepsilon))=[H^1(\mathbf{R}^2)]^2$. We study the norm resolvent convergence for this Hamiltonian. The obtained result is invariant under gauge transformations. In particular, it remains true for the Hamiltonian $H_\varepsilon^D+V_\varepsilon$.

We define the resonance state at zero energy of the operator

$$K+V=\sigma_1 p_1+\sigma_2 p_2+V=\sum_{j=1}^{2}\sigma_j(-i\partial_j-a_j)+V$$

before formulating the result. The definition is different according as $0<\alpha\leqslant 1/2$ or $1/2<\alpha<1$. By (3.7), we have $p_+=-2i\,e^{ih}e^{-\varphi}\overline{\partial}e^{\varphi}e^{-ih}$, where $\overline{\partial}=(1/2)(\partial_1+i\partial_2)$. The Cauchy–Riemann operator $\overline{\partial}$ has the fundamental solution $(1/\pi)(x_1+ix_2)^{-1}$. We denote by $\overline{\partial}^{-1}$ the convolution operator

$$\overline{\partial}^{-1}=(1/\pi)\,(x_1+ix_2)^{-1}*.$$

According to this notation, we define

$$p_+^{-1}=-(2i)^{-1}e^{ih}e^{-\varphi}\overline{\partial}^{-1}e^{\varphi}e^{-ih}$$

and $p_-^{-1}=(p_+^{-1})^*$. By definition, we have $p_\pm p_\pm^{-1}=1$.

Lemma 5.1: One has the relations

$$p_-G_+=p_+^{-1},\quad G_+p_+=p_-^{-1}$$

on bounded functions with compact support.

Proof: We prove only the first relation. The second one follows by taking the adjoint. We set $w_1=p_+^{-1}f$ for a function f as in the lemma. Then $w_1\in L^2$ and it solves $p_+w_1=f$. If, on the other hand, we set $w_2=p_-G_+f\in L^2_{-1}$, then w_2 satisfies

$$p_+w_2=p_+p_-G_+f=L_+G_+f=f$$

and $w_2\in L^2$. In fact, we have $\|p_-G_+f\|_{L^2}<\infty$ by a simple use of partial integration. Set $w=e^{\varphi}e^{-ih}(w_1-w_2)$. Then w is an entire function. Note that $e^{\varphi}=O(|x|^{\alpha})$ at infinity for $0<\alpha<1$. Since $w_1-w_2\in L^2$, we can easily show that $w=0$, and hence $w_1=w_2$. Thus the lemma is obtained. □

We now recall that $G_+:L^2_c\to L^2_{-1}$ is bounded. Hence

$$|V|^{1/2}p_+^{-1}|V|^{1/2}=|V|^{1/2}p_-G_+|V|^{1/2}:L^2\to L^2$$

is bounded by elliptic estimate, and also it follows by adjoint that

$$|V|^{1/2}p_-^{-1}|V|^{1/2}=|V|^{1/2}G_+p_+|V|^{1/2}:L^2\to L^2$$

is bounded.

We first consider the case $0<\alpha\leqslant 1/2$. We write $V^{1/2}=|V|^{1/2}/V$ and define $\Phi=\{u\in[L^2]^2:Z_0u=-u\}$, where

$$Z_0=V^{1/2}F_0|V|^{1/2},\quad F_0=\begin{pmatrix}0 & p_-G_+\\ G_+p_+ & 0\end{pmatrix}. \tag{5.2}$$

Since $Z_0:[L^2]^2\to[L^2]^2$ is a compact operator, it follows that $\dim\Phi<\infty$. As is easily seen from Lemma 5.1, $v=F_0|V|^{1/2}u$ with $u\in\Phi$ belongs to $L^2\times L^\infty$ and it solves $(K+V)v=0$. We further define $\Phi_0=\{u\in\Phi:(u,|V|^{1/2}\tilde{\rho}_0)_{L^2}=0\}$ with $\tilde{\rho}_0=(\rho_0,0)$. By definition, we have $\dim\Phi/\Phi_0\leqslant 1$.

Lemma 5.2: If $u\in\Phi_0$, then $v=F_0|V|^{1/2}u$ is in $[L^2]^2$ and hence v becomes a bound state associated with zero eigenvalue. If, conversely, v is a bound state, then $u=-V^{1/2}v$ belongs to Φ_0.

Proof: Let $u={}^t(u_1,u_2)\in\Phi_0$ and $v={}^t(v_1,v_2)=F_0|V|^{1/2}u$. Then $(u_1,|V|^{1/2}\rho_0)=0$ by assumption, and it is easy to see that $v_1\in L^2$. Since $\rho_0=ce^{-\varphi}e^{ih}$ for some $c\neq 0$, $v_2=p_-^{-1}|V|^{1/2}u_1$ behaves like

$$v_2(x)=c\,(u_1,|V|^{1/2}\rho_0)_{L^2}e^{\varphi}e^{-ih}(x_1-ix_2)^{-1}+O(|x|^{-2+\alpha}),\quad |x|\to\infty, \tag{5.3}$$

for another $c\neq 0$. Hence it follows that

$$(u_1,|V|^{1/2}\rho_0)_{L^2}=0\Leftrightarrow v\in[L^2]^2. \tag{5.4}$$

This proves the first statement. The second one is also easy to prove. If $v\in[L^2]^2$ satisfies $(K+V)v=0$, then $v=-F_0Vv$. Hence we have

$$u=-V^{1/2}v=V^{1/2}F_0Vv=Z_0V^{1/2}v=-Z_0u,$$

which, together with (5.4), implies that $u\in\Phi_0$. □

If $\dim\Phi/\Phi_0=1$, then the above lemma implies that $(K+V)v=0$ has a solution $v={}^t(v_1,v_2)\in L^2\times L^\infty$ with $(v,V\tilde{\rho}_0)_{L^2}\neq 0$, and hence it follows from (5.3) that v_2 behaves like

$$v_2(x)=cr^{-1+\alpha}e^{i\theta}(1+o(1)),\quad r=|x|\to\infty,$$

for $c\neq 0$. The converse is also true.

We move to the case $1/2<\alpha<1$. Recall that $\lambda_0\neq 0$ by assumption (5.1). This enables us to define the projection

$$P=\lambda_0^{-1}(V^{1/2}\tilde{\rho}_0\otimes|V|^{1/2}\tilde{\rho}_0):[L^2]^2\to[L^2]^2. \tag{5.5}$$

Let $Q=1-P$. We further define

$$\Psi=\{u\in[L^2]^2:QZ_0Qu=-u\},\quad \Psi_0=\{u\in\Psi:(u,Z_0^*|V|^{1/2}\tilde{\rho}_0)_{L^2}=0\}.$$

We again have $\dim\Psi/\Psi_0\leqslant 1$.

Lemma 5.3: If $u\in\Psi_0$, then $v=F_0|V|^{1/2}u$ becomes a bound state associated with zero eigenvalue. If, conversely, v is a bound state, then $u=-V^{1/2}v$ belongs to Ψ_0.

Proof: If $u\in\Psi_0$, then $PZ_0u=0$ and it follows that

$$u=-QZ_0Qu=-Z_0u=-V^{1/2}F_0|V|^{1/2}u=-V^{1/2}v.$$

This shows that $|V|^{1/2}u=-Vv$ and hence $(K+V)v=0$. If we write $v=F_0|V|^{1/2}u=-F_0|V|^{1/2}Z_0u$, then the first statement follows from (5.4). To prove the second one, we repeat the same computation as in the proof of Lemma 5.2 to obtain the relation $u=-Z_0u$. Since $v=-F_0Vv\in[L^2]^2$, it again follows from (5.4) that

$$(u,|V|^{1/2}\tilde{\rho}_0)_{L^2}=-(v,V\tilde{\rho}_0)_{L^2}=0.$$

This implies that $Pu=0$ and we obtain $u\in\Psi_0$. □

Lemma 5.4: If $\dim\Psi/\Psi_0=1$, then $(K+V)v=0$ has a solution such that $v={}^t(v_1,v_2)\in L^\infty\times L^2$ and

$$v_1(x)=cr^{-\alpha}(1+o(1)),\quad |x|\to\infty,$$

for $c\neq 0$. The converse is also true.

Proof: Let $u\in\Psi$ be a representative of Ψ/Ψ_0. We set $v=F_0|V|^{1/2}u-\mathrm{d}\tilde{\rho}_0$, where

$$\mathrm{d}=\lambda_0^{-1}(u,Z_0^*|V|^{1/2}\tilde{\rho}_0)_{L^2}\neq 0.$$

Then $(Vv,\tilde{\rho}_0)_{L^2}=0$, and $v_1(x)=-\mathrm{d}\rho_0(x)(1+o(1))$ at infinity. We show that $(K+V)v=0$. To see this, we calculate

$$V^{1/2}v=Z_0u-PZ_0u=QZ_0u=-u.$$

Since $K\tilde{\rho}_0=0$, we obtain $Kv=|V|^{1/2}u=-Vv$. We claim that $v_2\in L^2$. This follows from (5.4), because $(u,|V|^{1/2}\tilde{\rho}_0)_{L^2}=-(Vv,\tilde{\rho}_0)_{L^2}=0$. Thus the first statement is established. We shall prove the converse. Let $v\in L^\infty\times L^2$ be a solution to $(K+V)v=0$ with the properties in the lemma. We assert that v takes the form $v=-F_0Vv+c_0\tilde{\rho}_0$ for some $c_0\neq 0$. To see this, we set $w=v+F_0Vv$. Then $Kw=0$ and the first component w_1 behaves like $w_1=cr^{-\alpha}(1+o(1))$ for $c\neq 0$ in the lemma, because $v_1\notin L^2$ behaves in a similar way by assumption. Thus $w=c_0\tilde{\rho}_0$. The constant $c_0\neq 0$ is determined as

$$c_0=\lambda_0^{-1}(F_0Vv,V\tilde{\rho}_0)_{L^2}=\lambda_0^{-1}(V^{1/2}v,Z_0^*|V|^{1/2}\tilde{\rho}_0)_{L^2}$$

by use of (5.4). In fact, we have

$$(-F_0Vv+c_0\tilde{\rho}_0,V\tilde{\rho}_0)_{L^2}=(Vv,\tilde{\rho}_0)_{L^2}=(Vv_1,\rho_0)_{L^2}=0$$

because $v_2\in L^2$. If we set $u=-V^{1/2}v$, then $u\in[L^2]^2$ satisfies the relation $u=-Z_0u+PZ_0u=-QZ_0u$. Hence we have $u\in\Psi$, and also it follows that

$$(u,Z_0^*|V|^{1/2}\tilde{\rho}_0)_{L^2}=-(V^{1/2}v,Z_0^*|V|^{1/2}\tilde{\rho}_0)_{L^2}=-\lambda_0c_0\neq 0.$$

This implies the second statement, and the proof is complete. □

We combine Lemmas 5.2, 5.3, and 5.4 to formulate the precise definition of resonance state at zero energy.

Definition 5.1: The operator $K+V$ is said to admit a resonance state at zero energy, if the following condition is fulfilled.

(1) Assume that $0<\alpha\leqslant 1/2$. The equation $(K+V)v=0$ has a solution such that $v={}^t(v_1,v_2)\in L^2\times L^\infty$ and

$$v_2(x)=r^{-1+\alpha}e^{i\theta}(1+o(1)),\quad |x|\to\infty.$$

(2) Assume that $1/2<\alpha<1$ and that (5.1) is fulfilled. $(K+V)v=0$ has a solution such that $v={}^t(v_1,v_2)\in L^\infty\times L^2$ and

$$v_1(x)=r^{-\alpha}(1+o(1)),\quad |x|\to\infty.$$

We note that the definition is invariant under gauge transformations. We are now in a position to state the second main theorem.

Theorem 5.1: *Assume that the flux α satisfies (1.2) and that $K+V$ has no bound states at zero energy. Then one has the following three statements.*

(1) Let $0<\alpha<1/2$. If $K+V$ does not have a resonance state at zero energy, then $K_\varepsilon(V_\varepsilon)$ converges to H_∞ in the norm resolvent sense, and if $K+V$ has a resonance state, then $K_\varepsilon(V_\varepsilon)$ converges to H_0.

(2) Let $\alpha=1/2$. Assume that $K+V$ does not have a resonance state at zero energy, so that $(1+Z_0)^{-1}:[L^2]^2\to[L^2]^2$ exists as a bounded operator. Define the real number λ_2 by

$$\lambda_2=((1+Z_0)^{-1}V^{1/2}\tilde{\rho}_0,|V|^{1/2}\tilde{\rho}_0)_{L^2}$$

with $\tilde{\rho}_0 = {}^t(\rho_0, 0) \in [L^2]^2$. *Then* $K_\varepsilon(V_\varepsilon)$ *converges to* H_κ *with* $\kappa = \tan(\zeta/2)$ *determined through (2.6) with*

$$\zeta = \arg((i\lambda_2 - \gamma_0)/(i\lambda_2 + \gamma_0)),$$

where $\gamma_0 = -2$ *is as in Proposition 4.1. If* $K+V$ *has a resonance state, then* $K_\varepsilon(V_\varepsilon)$ *converges to* H_0.

(3) Let $1/2 < \alpha < 1$. *Assume that (5.1) is fulfilled. If* $K+V$ *does not have a resonance state at zero energy, then* $K_\varepsilon(V_\varepsilon)$ *converges to* H_0, *and if* $K+V$ *has a resonance state, then* $K_\varepsilon(V_\varepsilon)$ *converges to* H_∞.

The theorem is proved in the next section. We follow the argument used in the proof of Theorem 1.2.5 in Ref. 6 and of Theorem 3.3 in Ref. 10. The major part of the argument is again occupied by the resolvent analysis at low energy of magnetic Schrödinger operator with resonance state at zero energy. We end the section by making some brief comments on the theorem.

Remark 5.1: (1) If $V(x) \geqslant 0$ or $V(x) \leqslant 0$ and if it is sufficiently small but not identically zero, then $K+V$ has neither bound state nor resonance state at zero energy. The theorem asserts that the limit Hamiltonian changes at $\alpha = 1/2$ even for small perturbations of scalar potentials, and also it is interesting that the situation is completely reversed when $K+V$ has a resonance state. (2) The same reason as in Remark 3.2 applies to $K_\varepsilon(V_\varepsilon) = \varepsilon^{-1} J_\varepsilon (K+V) J_\varepsilon^*$. The norm convergence is not true without assuming that $K+V$ has no bound states at zero energy. (3) The restriction (1.2) is technical. The same results as in the theorem seem to remain true even for $\alpha > 1$ in the strong convergence sense, so that the limit Hamiltonian changes at half-integer fluxes. (4) The assumption (5.1) also seems to be technical. This is used for proving the third statement only, and a similar assumption has been used in Ref. 10 for the analysis on resolvents at low energy of Schrödinger operators in two dimensions. However the idea in the recent work (Ref. 17) may make it possible to remove the assumption.

VI. PROOF OF THEOREM 5.1

We prove Theorem 5.1 in this section. The proof requires several new lemmas on the behavior at low energy of resolvents of magnetic Schrödinger operators besides the propositions in Sec. IV. In formulating these lemmas, we use $\chi \in C_0^\infty(\mathbf{R}^2 \to \mathbf{R})$ with the same meaning as ascribed in Sec. IV and denote by $o_2(\varepsilon^\sigma)$ remainder terms with L^2 norm obeying the bound $o(\varepsilon^\sigma)$. We further define $\xi_l(x)$ by

$$\xi_l(x) = H_\nu(ir) e^{il\theta}, \quad \nu = |l - \alpha|, \tag{6.1}$$

for $l = 0,1$. According to this notation, we have

$$\psi_+ = N_\alpha \begin{pmatrix} -i^{1+2\alpha}\xi_0 \\ \xi_1 \end{pmatrix}, \quad \psi_- = N_\alpha \begin{pmatrix} i^{1+2\alpha}\xi_0 \\ \xi_1 \end{pmatrix}$$

by (2.3) and (2.5).

Lemma 6.1: Let ω_{+l} *be defined by (4.7). Then*

$$(L_{+\varepsilon} + 1)^{-1} J_\varepsilon \chi = \sum_{l=0,1} \beta_{+l}(\varepsilon) i^\nu \varepsilon^{1+\nu} (\xi_l \otimes \chi \omega_{+l}) + Op(\varepsilon^2)$$

for some coefficient $\beta_{+l}(\varepsilon)$, *and* $\beta_{+l}(\varepsilon)$ *behaves like* $\beta_{+l}(\varepsilon) = \beta_l + o(1)$ *as* $\varepsilon \to 0$, *where*

$$\beta_l = i(2\pi)^{-1/2} (2^{-\nu} \Gamma(1-\nu)/(l+\nu)^{1/2}) \sin \nu\pi. \tag{6.2}$$

Lemma 6.2: Let β_0 *be as above and let* γ_0 *be as in Proposition 4.1. Let* ρ_0 *be the resonance state defined by (4.14). Then*

$$(L_{-\varepsilon}+1)^{-1}J_\varepsilon\chi=-i^\alpha(\beta_0/\gamma_0)\varepsilon^{1-\alpha}((\xi_0+o_2(1))\otimes\chi\rho_0)+Op(\varepsilon).$$

Lemma 6.3: One has

$$p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}J_\varepsilon\chi=Op(\varepsilon).$$

Lemma 6.4: One has

$$p_{+\varepsilon}(L_{-\varepsilon}+1)^{-1}J_\varepsilon\chi=i^{-\alpha}(\beta_0/\gamma_0)\varepsilon^{1-\alpha}((\xi_1+o_2(1))\otimes\chi\rho_0)+Op(\varepsilon).$$

We proceed to proving Theorem 5.1, accepting the above lemmas as proved. The proof of these lemmas is done in Sec. VII.

Proof of Theorem 5.1: For brevity, we assume throughout the proof that $V(x)\geqslant 0$, so that the operator Z_0 defined by (5.2) becomes self-adjoint. We write $R_\varepsilon=(K_\varepsilon(V_\varepsilon)+i)^{-1}$. Then we obtain

$$R_\varepsilon=(K_\varepsilon+i)^{-1}-(K_\varepsilon+i)^{-1}V_\varepsilon^{1/2}X_\varepsilon^{-1}V_\varepsilon^{1/2}(K_\varepsilon+i)^{-1}$$

from the resolvent identity, where $X_\varepsilon=1+V_\varepsilon^{1/2}(K_\varepsilon+i)^{-1}V_\varepsilon^{1/2}$. We define Y_ε by

$$Y_\varepsilon=J_\varepsilon^*X_\varepsilon J_\varepsilon=1+V^{1/2}(K+i\varepsilon)^{-1}V^{1/2}.$$

Then R_ε is rewritten as

$$R_\varepsilon=(K_\varepsilon+i)^{-1}-\varepsilon^{-1}((K_\varepsilon+i)^{-1}J_\varepsilon V^{1/2})Y_\varepsilon^{-1}((K_\varepsilon-i)^{-1}J_\varepsilon V^{1/2})^*.$$

We analyze the behavior as $\varepsilon\to 0$ of operators on the right-hand side. By Theorem 3.1, $(K_\varepsilon+i)^{-1}\to(H_\infty+i)^{-1}$. If we make use of relation (3.3), then we can obtain

$$(K_\varepsilon\pm i)^{-1}=\begin{pmatrix}\mp i(L_{-\varepsilon}+1)^{-1} & p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}\\ p_{+\varepsilon}(L_{-\varepsilon}+1)^{-1} & \mp i(L_{+\varepsilon}+1)^{-1}\end{pmatrix}$$

from (3.4). By Lemmas 6.1–6.4, we have

$$(K_\varepsilon+i)^{-1}J_\varepsilon V^{1/2}=(\beta_0/\gamma_0)N_\alpha^{-1}i^{-\alpha}\varepsilon^{1-\alpha}((\psi_-+o_2(1))\otimes q_0)+Op(\varepsilon),\tag{6.3}$$

where $q_0={}^t(V^{1/2}\rho_0,0)$. Similarly $((K_\varepsilon-i)^{-1}J_\varepsilon V^{1/2})^*$ takes the form

$$((K_\varepsilon-i)^{-1}J_\varepsilon V^{1/2})^*=(\overline{\beta_0}/\gamma_0)N_\alpha^{-1}i^{\alpha}\varepsilon^{1-\alpha}(q_0\otimes(\psi_++o_2(1)))+Op(\varepsilon).\tag{6.4}$$

The operator $(K+i\varepsilon)^{-1}$ also has been calculated as

$$(K+i\varepsilon)^{-1}=\begin{pmatrix}-i\varepsilon(L_-+\varepsilon^2)^{-1} & p_-(L_++\varepsilon^2)^{-1}\\ (L_++\varepsilon^2)^{-1}p_+ & -i\varepsilon(L_++\varepsilon^2)^{-1}\end{pmatrix}$$

in (3.10). By (4.2) and (4.7), ω_{+0} obeys $\omega_{+0}=(1/2)\alpha^{-1/2}r^\alpha+g$ for some $g\in L^2_{-1}$, and it solves $L_+\omega_{+0}=0$ uniquely (see Lemma 4.3 of Ref. 22). Since $L_+=p_+p_-$ with

$$p_-=p_+^*=ie^{ih}e^{\varphi}(-\partial_1+i\partial_2)e^{-\varphi}e^{-ih},$$

we see that $p_-\omega_{+0}=0$. In fact, ω_{+0} is given by $\omega_{+0}=ce^{ih}e^{\varphi}$ for some constant $c\neq 0$. Thus we have

$$V^{1/2}p_-(L_++\varepsilon^2)^{-1}V^{1/2}=V^{1/2}(p_-G_++\varepsilon^{2(1-\alpha)}\gamma_{+1}(i\varepsilon)(p_-\omega_{+1}\otimes\omega_{+1}))V^{1/2}+Op(\varepsilon^2)$$

by Proposition 4.2 (see Remark 4.1) and similarly for $V^{1/2}(L_++\varepsilon^2)^{-1}p_+V^{1/2}$. Hence it follows from Proposition 4.3 that

$$Y_\varepsilon = 1 + Z_0 - i\gamma_-(i\varepsilon)\varepsilon^{1-2\alpha}(q_0 \otimes q_0) + \varepsilon^{2(1-\alpha)}Z_1(\varepsilon) + Op(\varepsilon),$$

where $\gamma_-(i\varepsilon) = -1/\gamma_0 + o(1)$ as $\varepsilon \to 0$ and

$$Z_1(\varepsilon) = \gamma_{+1}(i\varepsilon)V^{1/2}\begin{pmatrix} 0 & p_-\omega_{+1}\otimes\omega_{+1} \\ \omega_{+1}\otimes p_-\omega_{+1} & 0 \end{pmatrix}V^{1/2}. \tag{6.5}$$

Note that $p_- = \pi_-$ on $\{|x|>2\}$, and recall the form of operator π_- (see Sec. II). Then it follows from (4.7) that $p_-\omega_{+1} = cr^{-\alpha} + g$ for some $c \neq 0$. We see by Lemma 5.1 (or by the argument in the proof) that the remainder term g is in L^2. Since $p_-\omega_{+1}$ satisfies $p_+p_-\omega_{+1} = L_+\omega_{+1} = 0$, we have $p_-\omega_{+1} = c\rho_0$ for another $c \neq 0$, and hence

$$Z_1(\varepsilon) = c\gamma_{+1}(i\varepsilon)(q_0 \otimes q + q \otimes q_0) \tag{6.6}$$

with $q = {}^t(0, V^{1/2}\omega_{+1})$. The argument is different from now on according as $0<\alpha<1/2$, $\alpha = 1/2$ or $1/2<\alpha<1$.

(1) Assume that $0<\alpha<1/2$. If $K+V$ has neither bound nor resonance state at zero energy, then the bounded inverse $(1+Z_0)^{-1}:[L^2]^2 \to [L^2]^2$ exists, and hence Y_ε has an inverse bounded uniformly in ε. Thus it follows that $R_\varepsilon \to (H_\infty + i)^{-1}$ in norm. Next we consider the case when $K+V$ has a resonance state. Since $K+V$ has no bound states by assumption, $\dim \Phi = 1$ and $\dim \Phi_0 = 0$. Let Φ be spanned by $q_1 \in [L^2]^2$ with $\|q_1\|_{L^2} = 1$. Then $\lambda_1 = (q_1, q_0)_{L^2} \neq 0$ by definition. We denote by $\Pi_1 = q_1 \otimes q_1$ the projection on Φ and write $\Pi = 1 - \Pi_1$ for the projection on the orthogonal complement $\Phi^\perp$. Then $\Pi(1+Z_0)\Pi:\Phi^\perp \to \Phi^\perp$ has an bounded inverse and $\Pi_1(q_0 \otimes q_0)\Pi_1 = |\lambda_1|^2\Pi_1$. Thus Y_ε^{-1} takes the form

$$Y_\varepsilon^{-1} = -i(\gamma_0/|\lambda_1|^2)\varepsilon^{2\alpha-1}(q_1 \otimes q_1) + op(\varepsilon^{2\alpha-1}). \tag{6.7}$$

Since $\Gamma(1-\alpha)\Gamma(\alpha) = \pi/(\sin \alpha\pi)$ by formula, a direct calculation yields

$$|\beta_0|^2/\gamma_0 = -\sin \alpha\pi/4 = -N_\alpha^2 \tag{6.8}$$

by (2.4). We combine (6.3), (6.4), (6.7), and (6.8) to obtain that

$$R_\varepsilon = (H_\infty + i)^{-1} - i(\psi_- \otimes \psi_+) + op(\varepsilon^0).$$

This determines $\zeta = 0$ by (2.7) and hence $\kappa = 0$ by (2.6). Thus we obtain that $R_\varepsilon \to (H_0 + i)^{-1}$.

(2) If $\alpha = 1/2$, then Y_ε takes the form

$$Y_\varepsilon = 1 + Z_0 + (i/\gamma_0)(q_0 \otimes q_0) + op(\varepsilon^0)$$

and $\gamma_0 = -2$. Assume that zero is not a resonance energy. If we set $q_2 = (1+Z_0)^{-1}q_0$, then the real number λ_2 in the theorem is represented as $\lambda_2 = (q_2, q_0)_{L^2}$, and Y_ε^{-1} is calculated as

$$\begin{aligned} Y_\varepsilon^{-1} &= (1 + (i/\gamma_0)(q_2 \otimes q_0))^{-1}(1+Z_0)^{-1} + op(\varepsilon^0) \\ &= (1 - (i/(\gamma_0 + i\lambda_2))(q_2 \otimes q_0))(1+Z_0)^{-1} + op(\varepsilon^0). \end{aligned}$$

Thus we obtain

$$R_\varepsilon = (H_\infty + i)^{-1} + c_2(\psi_- \otimes \psi_+) + op(\varepsilon^0)$$

with $c_2 = \lambda_2/(\gamma_0 + i\lambda_2)$, and

$$e^{i\zeta} = 2ic_2 - 1 = (i\lambda_2 - \gamma_0)/(i\lambda_2 + \gamma_0).$$

This determines $\kappa = \tan(\zeta/2)$ through (2.6). If $K+V$ has a resonance state, the lemma below yields the desired relation

$$R_\varepsilon=(H_\infty+i)^{-1}-i(\psi_-\otimes\psi_+)+op(\varepsilon^0)=(H_0+i)^{-1}+op(\varepsilon^0).$$

Lemma 6.5: Under the above situation, one has

$$(q_0,Y_\varepsilon^{-1}q_0)_{L^2}=i\gamma_0+o(1),\quad \varepsilon\to 0.$$

Proof: If we again denote by Π_1 and $\Pi=1-\Pi_1$ the projections on Φ and $\Phi^\perp$, respectively, then

$$Y_{11}=\Pi_1(1+Z_0)\Pi_1=0,\quad Y_{01}=\Pi(1+Z_0)\Pi_1=0,\quad Y_{10}=\Pi_1(1+Z_0)\Pi=0,$$

and $Y_{00}=\Pi(1+Z_0)\Pi:\Phi^\perp\to\Phi^\perp$ is invertible. We write

$$q_0=\Pi q_0+\Pi_1 q_0=r_0+r_1.$$

We set $D=(i/\gamma_0)(q_0\otimes q_0)$ and decompose it into the sum

$$D=\sum_{0\leqslant j,k\leqslant 1}D_{jk},\quad D_{jk}=(i/\gamma_0)(r_j\otimes r_k).$$

We represent $Y_\varepsilon=1+Z_0+D+op(\varepsilon^0)$ in the matrix form

$$Y_\varepsilon=\begin{pmatrix}Y_{00}+D_{00} & D_{01}\\ D_{10} & D_{11}\end{pmatrix}+op(\varepsilon^0):\begin{pmatrix}\Phi^\perp\\ \Phi\end{pmatrix}\to\begin{pmatrix}\Phi^\perp\\ \Phi\end{pmatrix}.$$

By (5.4), $r_1\neq 0$, and hence $D_{11}:\Phi\to\Phi$ is invertible. We have

$$D_{11}^{-1}=-i\gamma_0\|r_1\|_{L^2}^{-4}(r_1\otimes r_1)$$

and $D_{00}-D_{01}D_{11}^{-1}D_{10}=0$. If we make use of this relation, then

$$Y_\varepsilon^{-1}=\begin{pmatrix}Y_{00}^{-1} & -Y_{00}^{-1}D_{01}D_{11}^{-1}\\ -D_{11}^{-1}D_{10}Y_{00}^{-1} & D_{11}^{-1}(1+D_{10}Y_{00}^{-1}D_{01}D_{11}^{-1})\end{pmatrix}+op(\varepsilon^0).$$

We compute

$$(r_0,Y_{00}^{-1}D_{01}D_{11}^{-1}r_1)_{L^2}=(r_0,Y_{00}^{-1}r_0)_{L^2},\quad (r_1,D_{11}^{-1}D_{10}Y_{00}^{-1}r_0)_{L^2}=(Y_{00}^{-1}r_0,r_0)_{L^2}$$

and

$$(r_1,D_{11}^{-1}(1+D_{10}Y_{00}^{-1}D_{01}D_{11}^{-1})r_1)_{L^2}=i\gamma_0+(Y_{00}^{-1}r_0,r_0)_{L^2}.$$

This completes the proof of the lemma. □

(3) The final case is $1/2<\alpha<1$. The projection $P=\lambda_0^{-1}(q_0\otimes q_0):[L^2]^2\to[L^2]^2$ is defined by (5.5). Set $Q=1-P$ again. Then

$$Y_\varepsilon=\tau(\varepsilon)P+Q+Z_0+\varepsilon^{2(1-\alpha)}Z_1(\varepsilon)+Op(\varepsilon),$$

where

$$\tau(\varepsilon)=1-i\lambda_0\gamma_-(i\varepsilon)\varepsilon^{1-2\alpha}=\varepsilon^{1-2\alpha}(i\lambda_0/\gamma_0+o(1)).$$

We can easily prove that

$$(\tau(\varepsilon)P+Q)^{-1}=\delta(\varepsilon)P+Q,\quad (1+QZ_0P)^{-1}=1-QZ_0P,$$

where $\delta(\varepsilon)=1/\tau(\varepsilon)=\varepsilon^{2\alpha-1}(-i\gamma_0/\lambda_0+o(1))$. The two relations yield

$$Y_\varepsilon=(\tau(\varepsilon)P+Q)(1+QZ_0P)T_\varepsilon$$

and hence we have

$$Y_\varepsilon^{-1}=T_\varepsilon^{-1}(\delta(\varepsilon)(P-QZ_0P)+Q), \tag{6.9}$$

where

$$T_\varepsilon=1+QZ_0Q+\delta(\varepsilon)(1-QZ_0)PZ_0+\varepsilon^{2(1-\alpha)}QZ_1(\varepsilon)+Op(\varepsilon).$$

By (6.6), we see that $QZ_1(\varepsilon)Q=0$. Let $\Sigma_0=\mathrm{Ran}\,P$ and $\Sigma=\mathrm{Ran}\,Q$. The second factor on the right-hand side of (6.9) has the matrix representation

$$\delta(\varepsilon)(P-QZ_0P)+Q=\begin{pmatrix}\delta(\varepsilon)P & 0\\ -\delta(\varepsilon)QZ_0P & Q\end{pmatrix}:\begin{pmatrix}\Sigma_0\\ \Sigma\end{pmatrix}\to\begin{pmatrix}\Sigma_0\\ \Sigma\end{pmatrix}, \tag{6.10}$$

while T_ε takes the form $T_\varepsilon=(T_{jk}(\varepsilon))_{0\leqslant j,k\leqslant 1}$, where

$$T_{00}=P(1+Op(\varepsilon^{2\alpha-1}))P,\quad T_{01}=P(\delta(\varepsilon)Z_0+Op(\varepsilon))Q,$$

$$T_{10}=Q(Op(\varepsilon^{2\alpha-1})+Op(\varepsilon^{2(1-\alpha)}))P,\quad T_{11}=Q(1+Z_0-\delta(\varepsilon)Z_0PZ_0+Op(\varepsilon))Q.$$

The inverse T_ε^{-1} can be calculated as $T_\varepsilon^{-1}=(S_{jk}(\varepsilon))_{0\leqslant j,k\leqslant 1}$, where

$$S_{00}=(T_{00}-T_{01}T_{11}^{-1}T_{10})^{-1},\quad S_{01}=-T_{00}^{-1}T_{01}(T_{11}-T_{10}T_{00}^{-1}T_{01})^{-1},$$

$$S_{10}=-T_{11}^{-1}T_{10}(T_{00}-T_{01}T_{11}^{-1}T_{10})^{-1},\quad S_{11}=(T_{11}-T_{10}T_{00}^{-1}T_{01})^{-1}.$$

We now analyze the behavior as $\varepsilon\to 0$ of inverse Y_ε^{-1}. We first deal with the resonance case. We claim that Y_ε^{-1} takes the form

$$Y_\varepsilon^{-1}=\begin{pmatrix}Pop(\varepsilon^{2\alpha-1})P & POp(\varepsilon^0)Q\\ QOp(\varepsilon^0)P & QOp(\varepsilon^{1-2\alpha})Q\end{pmatrix}. \tag{6.11}$$

Note that

$$(f\otimes q_0)Q=0,\quad Q(q_0\otimes f)=0$$

for $f\in[L^2]^2$. Hence we combine (6.11) with (6.3) and (6.4) to obtain that $R_\varepsilon\to(H_\infty+i)^{-1}$. When $K+V$ has a resonance state at zero energy,

$$\dim\Psi=\dim\mathrm{Ker}(Q+QZ_0Q)=1$$

and $\dim\Psi_0=0$. Let Ψ be spanned by $q_3\in[L^2]^2$ with $\|q_3\|_{L^2}=1$. We denote by $Q_3=q_3\otimes q_3$ the projection on Ψ and decompose $Q=Q_3+Q(1-Q_3)=Q_3+Q_4$. Since $\dim\Psi_0=0$, $\lambda_3=(Z_0q_3,q_0)_{L^2}\neq 0$. The operator T_{11} is represented in the form

$$T_{11}=Q_4(1+Z_0+Op(\varepsilon^{2\alpha-1}))Q_4-(\delta(\varepsilon)|\lambda_3|^2/\lambda_0)Q_3+Q_4Op(\varepsilon^{2\alpha-1})Q_3+Q_3Op(\varepsilon^{2\alpha-1})Q_4.$$

Hence

$$T_{11}^{-1}=-(\tau(\varepsilon)\lambda_0/|\lambda_3|^2)Q_3+QOp(\varepsilon^0)Q.$$

As is easily seen, $T_{00}^{-1}=P(1+op(\varepsilon^0))P$. Similarly we have

$$(T_{11}-T_{10}T_{00}^{-1}T_{01})^{-1}=-(\tau(\varepsilon)\lambda_0/|\lambda_3|^2)Q_3+QOp(\varepsilon^0)Q$$

and $(T_{00}-T_{01}T_{11}^{-1}T_{10})^{-1}=P(1+op(\varepsilon^0))P$. Thus we obtain

$$T_\varepsilon^{-1}=\begin{pmatrix} P(1+op(\varepsilon^0))P & (\lambda_0/|\lambda_3|^2)PZ_0Q_3+Pop(\varepsilon^0)Q \\ Q(Op(\varepsilon^0)+Op(\varepsilon^{3-4\alpha}))P & QOp(\varepsilon^{1-2\alpha})Q \end{pmatrix}.$$

This, together with (6.9) and (6.10), implies that

$$Y_\varepsilon^{-1}=\begin{pmatrix} \delta(\varepsilon)P(1-(\lambda_0/|\lambda_3|^2)Z_0Q_3Z_0+op(\varepsilon^0))P & POp(\varepsilon^0)Q \\ QOp(\varepsilon^0)P & QOp(\varepsilon^{1-2\alpha})Q \end{pmatrix}.$$

Since $PZ_0Q_3Z_0P=(|\lambda_3|^2/\lambda_0)P$, (6.11) follows at once. If $K+V$ does not have a resonance state, then $\dim\Psi=0$, and $T_{11}(\varepsilon):\Sigma\to\Sigma$ admits an inverse bounded uniformly in ε. We repeat the same argument as above to obtain that

$$Y_\varepsilon^{-1}=\begin{pmatrix} \delta(\varepsilon)P(1+op(\varepsilon^0))P & POp(\varepsilon^0)Q \\ QOp(\varepsilon^0)P & QOp(\varepsilon^{1-2\alpha})Q \end{pmatrix},$$

so that $Y_\varepsilon^{-1}\sim -i(\gamma_0/\lambda_0^2)\varepsilon^{2\alpha-1}(q_0\otimes q_0)$. Hence we have

$$R_\varepsilon=(H_\infty+i)^{-1}-i(\psi_-\otimes\psi_+)+op(\varepsilon^0)=(H_0+i)^{-1}+op(\varepsilon^0)$$

in the same way as in case (1). Thus the proof of the theorem is now complete. □

VII. RESOLVENT ANALYSIS AT LOW ENERGY ON SCHRÖDINGER OPERATORS II

The last section is devoted to proving Lemmas 6.1–6.4 which remain unproved. The argument here is based on the following proposition obtained as Proposition 7.1 in Ref. 22. The proposition has been proved for $(L_\varepsilon-i)^{-1}$, but the argument there applies to $(L_\varepsilon-\sigma^2)^{-1}$, $\mathrm{Im}\,\sigma>0$, without any serious modification.

Proposition 7.1: Let L_ε be defined by (3.2) and let $\sigma\in\mathbf{C}$ be as above. Then

$$(L_\varepsilon-\sigma^2)^{-1}J_\varepsilon\chi=\sum_{l=0,1}\beta_l(\varepsilon)\sigma^\nu\varepsilon^{1+\nu}(\mu_l\otimes\chi\omega_l)+Op(\varepsilon^2)$$

for some coefficients $\beta_l(\varepsilon)$, where $\mu_l(x)=H_\nu(\sigma r)e^{il\theta}$ and $\beta_l(\varepsilon)$ behaves in the same manner as in Lemma 6.1.

Proof of Lemma 6.1: We use the relations $J_\varepsilon^*(L_{+\varepsilon}+1)^{-1}J_\varepsilon=\varepsilon^2(L_++\varepsilon^2)^{-1}$ and $b_\varepsilon J_\varepsilon=\varepsilon^{-2}J_\varepsilon b$. Then we have

$$(L_{+\varepsilon}+1)^{-1}J_\varepsilon\chi=(L_\varepsilon+1)^{-1}J_\varepsilon\chi-(L_\varepsilon+1)^{-1}J_\varepsilon b(L_++\varepsilon^2)^{-1}\chi$$

by the resolvent identity. We apply Proposition 7.1 with $\sigma=i$ to $(L_\varepsilon+1)^{-1}J_\varepsilon b$ and Proposition 4.2 with $k=i\varepsilon$ to $\chi(L_++\varepsilon^2)^{-1}\chi$. Since $\omega_{+l}=\omega_l-G_+b\omega_l$ by (4.7) and since $\mu_l=\xi_l$ for $\sigma=i$, the desired relation is obtained. □

Proof of Lemma 6.2: We have

$$(L_{-\varepsilon}+1)^{-1}J_\varepsilon\chi=(L_\varepsilon+1)^{-1}J_\varepsilon\chi+(L_\varepsilon+1)^{-1}J_\varepsilon b(L_-+\varepsilon^2)^{-1}\chi$$

by the resolvent identity. The first operator on the right-hand side is of class $Op(\varepsilon)$ by Proposition 7.1. We apply Proposition 4.3 to $\chi(L_-+\varepsilon^2)^{-1}\chi$ in the second operator. Since

$$(b\rho_0,\omega_0)_{L^2}=(b^{1/2}G_0|b|^{1/2}\eta_0,|b|^{1/2}\omega_0)_{L^2}=(\eta_0,|b|^{1/2}\omega_0)_{L^2}=1$$

and since $(b\rho_0,\omega_1)_{L^2}=(\eta_0,|b|^{1/2}\omega_1)_{L^2}=0$ by (4.13), the desired relation again follows from Proposition 7.1 with $\sigma=i$. □

Proof of Lemma 6.3: Since $p_{-\varepsilon}^* p_{-\varepsilon}=p_{+\varepsilon}p_{-\varepsilon}=L_{+\varepsilon}$, we have

$$(p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1})^* p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}=(L_{+\varepsilon}+1)^{-1}-(L_{+\varepsilon}+1)^{-2}$$

and hence

$$\|p_{-\varepsilon}(L_{+\varepsilon}+1)^{-1}J_\varepsilon\chi\|^2=\|\chi(\varepsilon^2(L_++\varepsilon^2)^{-1}-\varepsilon^4(L_++\varepsilon^2)^{-2})\chi\|.$$

By Proposition 4.2, $\|\chi(L_++\varepsilon^2)^{-1}\chi\|=O(1)$ as $\varepsilon\to 0$. This implies that

$$\|\chi(L_++\varepsilon^2)^{-1/2}\|=O(1).$$

Thus the bound in the lemma is obtained. □

Proof of Lemma 6.4: We prove the lemma only in the simple case that $b(x)\geqslant 0$. We assert that

$$p_{+\varepsilon}(L_{-\varepsilon}-i)^{-1}J_\varepsilon\chi=-i^{(3-\alpha)/2}(\beta_0/\gamma_0)\varepsilon^{1-\alpha}((\tau_1+o_2(1))\otimes\chi\rho_0)+Op(\varepsilon), \tag{7.1}$$

where $\tau_1(x)=H_{1-\alpha}(i^{1/2}r)e^{i\theta}$. This implies the lemma. In fact, we use (3.3) to obtain

$$p_{+\varepsilon}(L_{-\varepsilon}+1)^{-1}=(1-(1+i)(L_{+\varepsilon}+1)^{-1})p_{+\varepsilon}(L_{-\varepsilon}-i)^{-1}$$

and it follows from Lemma 3.1 that

$$(1-(1+i)(L_{+\varepsilon}+1)^{-1})\tau_1\to f_1=(1-(1+i)(L_{AB}+1)^{-1})\tau_1$$

strongly in L^2. The function $f_1\in L^2$ satisfies $(\pi_1^2+\pi_2^2+1)f_1=0$. Hence it takes the form $f_1(x)=g(r)e^{i\theta}$, where g solves

$$-g''-r^{-1}g'+((1-\alpha)^2r^{-2}+1)g=0.$$

Thus $f_1=cH_{1-\alpha}(ir)e^{i\theta}=c\xi_1$ for some coefficient c. Since $u\in\mathcal{D}(L_{AB})$ vanishes at the origin, $f_1-\tau_1$ also vanishes, so that c is determined as $c=i^{(1-\alpha)/2}$. Hence we see that (7.1) implies the relation of the lemma.

We shall show (7.1). We make use of the relation

$$(L_{-\varepsilon}-i)^{-1}J_\varepsilon\chi=(L_\varepsilon-i)^{-1}J_\varepsilon\chi+(L_\varepsilon-i)^{-1}J_\varepsilon b(L_--i\varepsilon^2)^{-1}\chi$$

to decompose

$$p_{+\varepsilon}(L_{-\varepsilon}-i)^{-1}J_\varepsilon\chi=I_1(\varepsilon)+I_2(\varepsilon),$$

where $I_1(\varepsilon)=p_{+\varepsilon}(L_\varepsilon-i)^{-1}J_\varepsilon\chi$ and

$$I_2(\varepsilon)=p_{+\varepsilon}(L_\varepsilon-i)^{-1}J_\varepsilon b(L_--i\varepsilon^2)^{-1}\chi.$$

Since $p_{-\varepsilon}p_{+\varepsilon}=L_{-\varepsilon}=L_\varepsilon-b_\varepsilon$, it follows from Proposition 4.1 that

$$\|I_1(\varepsilon)\|^2=\|\chi J_\varepsilon^*(L_\varepsilon+i)^{-1}(L_\varepsilon-b_\varepsilon)(L_\varepsilon-i)^{-1}J_\varepsilon\chi\|=O(\varepsilon^2).$$

To evaluate $I_2(\varepsilon)$, we use Proposition 4.3 with $k=i^{1/2}\varepsilon$ for $b(L_--i\varepsilon^2)^{-1}\chi$. Then

$$I_2(\varepsilon)=p_{+\varepsilon}(L_\varepsilon-i)^{-1}J_\varepsilon\chi(\gamma_-(k)i^\alpha\varepsilon^{-2\alpha}(b\rho_0\otimes\chi\rho_0)+Op(\varepsilon^0)),$$

where $\gamma_-(k)$ obeys $\gamma_-(k)=-1/\gamma_0+o(1)$. Since $p_{+\varepsilon}(L_\varepsilon-i)^{-1}J_\varepsilon\chi=Op(\varepsilon)$ as is seen from the proof of Lemma 6.3, (7.1) follows from the lemma below at once. □

Lemma 7.1: One has the relation

$$p_{+\varepsilon}(L_\varepsilon - i)^{-1} J_\varepsilon b\rho_0 = i^{3(1-\alpha)/2}\beta_0 \varepsilon^{1+\alpha}\tau_1 + o_2(\varepsilon^{1+\alpha}).$$

Proof: Since $b^{1/2}G_0 b^{1/2}\eta_0 = \eta_0$, it follows from (4.14) that $b\rho_0 = b^{1/2}\eta_0$. We write

$$g_\varepsilon = \varepsilon^{-(1+\alpha)} p_{+\varepsilon}(L_\varepsilon - i)^{-1} J_\varepsilon b\rho_0 = \varepsilon^{-(1+\alpha)}\Lambda(\varepsilon)\eta_0,$$

where $\Lambda(\varepsilon) = p_{+\varepsilon}(L_\varepsilon - i)^{-1} J_\varepsilon b^{1/2}$. To prove the lemma, it suffices to show that

$$g_\varepsilon \to g_0 = i^{3(1-\alpha)/2}\beta_0\tau_1$$

strongly in L^2. We first show that $\|g_\varepsilon\|_{L^2} \to \|g_0\|_{L^2}$. If we make use of the relation $p_{+\varepsilon}^* p_{+\varepsilon} = L_{-\varepsilon} = L_\varepsilon - b_\varepsilon$, then a simple calculation yields

$$\Lambda(\varepsilon)^*\Lambda(\varepsilon) = (\varepsilon^2/2)(\Pi(\varepsilon) + \Pi(\varepsilon)^*) - \varepsilon^2\Pi(\varepsilon)^*\Pi(\varepsilon),$$

where $\Pi(\varepsilon) = b^{1/2}(L - i\varepsilon^2)^{-1}b^{1/2}$. We apply Proposition 4.1 with $k = i^{1/2}\varepsilon$ to $\Pi(\varepsilon)$. Then

$$\Pi(\varepsilon) = b^{1/2}G_0 b^{1/2} + \sum_{l=0,1} \gamma_l(k) i^{-\nu}\varepsilon^{2\nu}(b^{1/2}\omega_l \otimes b^{1/2}\omega_l) + Op(\varepsilon^2).$$

Since $(\eta_0, b^{1/2}\omega_0)_{L^2} = 1$ and $(\eta_0, b^{1/2}\omega_1)_{L^2} = 0$ by (4.13), we have

$$\Pi(\varepsilon)\eta_0 = \eta_0 + \gamma_0(k) i^{-\alpha}\varepsilon^{2\alpha} b^{1/2}\omega_0 + o_2(\varepsilon^{1+\alpha})$$

and similarly for $\Pi(\varepsilon)^*\eta_0$ with coefficient $\gamma_0(k)i^{-\alpha}$ replaced by $\overline{\gamma_0(k)} i^{\alpha}$. Thus

$$\|g_\varepsilon\|_{L^2}^2 = \varepsilon^{-2(1+\alpha)}\|\Lambda(\varepsilon)\eta_0\|_{L^2}^2 = -\gamma_0 \cos(\alpha\pi/2) + o(1).$$

On the other hand, we use the formula

$$\|\tau_1\|_{L^2}^2 = 2\pi \int_0^\infty r|H_{1-\alpha}(i^{1/2}r)|^2 \, dr = 2/\sin(\alpha\pi/2)$$

to obtain that

$$\|g_0\|_{L^2}^2 = |\beta_0|^2\|\tau_1\|_{L^2}^2 = 2|\beta_0|^2/\sin(\alpha\pi/2).$$

Since $2|\beta_0|^2/\sin(\alpha\pi/2) = -\gamma_0\cos(\alpha\pi/2)$ by (6.8), it follows that $\|g_\varepsilon\|_{L^2} \to \|g_0\|_{L^2}$. Next we shall show that $g_\varepsilon \to g_0$ is weak. Let $f \in C_0^\infty(\mathbf{R}^2 - \{0\})$. Then $p_{-\varepsilon} f = \pi_- f$ for $\varepsilon > 0$ small enough, and

$$(g_\varepsilon, f)_{L^2} = \varepsilon^{-(1+\alpha)}((L_\varepsilon - i)^{-1} J_\varepsilon b^{1/2}\eta_0, \pi_- f)_{L^2}.$$

We have

$$(L_\varepsilon - i)^{-1} J_\varepsilon b^{1/2}\eta_0 = i^{\alpha/2}\beta_0 \varepsilon^{1+\alpha}\tau_0 + o_2(\varepsilon^{1+\alpha})$$

by Proposition 7.1 with $\sigma = i^{1/2}$, where $\tau_0 = H_\alpha(i^{1/2}r)$. Hence it follows that

$$(g_\varepsilon, f)_{L^2} \to i^{\alpha/2}\beta_0(\pi_+\tau_0, f)_{L^2}.$$

By (2.2), we can calculate

$$\pi_+\tau_0 = -i^{3/2}H_{\alpha-1}(i^{1/2}r)e^{i\theta} = -i^{3/2}e^{i(1-\alpha)\pi}\tau_1 = i^{3/2-2\alpha}\tau_1.$$

This shows that $g_\varepsilon \to g_0$ is weak, and the proof is complete. □

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Regularity for Lorentz metrics under curvature bounds

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(Received 27 January 2003; accepted 11 April 2003)

Let (**M**, **g**) be an $(n+1)$-dimensional space–time, with bounded curvature, with respect to a bounded framing. If (**M**, **g**) is vacuum, or satisfies a weak condition on the stress-energy tensor, then it is shown that (**M**, **g**) locally admits coordinate systems in which the Lorentz metric **g** is well-controlled in the (space–time) Sobolev space $L^{2,p}$, for any $p<\infty$. This result is essentially optimal. The result allows one to control the regularity of limits of sequences of space–times, with uniformly bounded curvature, and has applications to the structure of boundaries and extensions of space–times. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1580199]

I. INTRODUCTION

A well-known issue in the geometry of space–times is to understand the regularity of metrics with given bounds on the curvature tensor. This issue is closely connected to the diffeomorphism invariance of general relativity and the problem of choosing a good gauge, i.e., local coordinate system, in which the metric has optimal regularity. It is not at all clear if the most commonly used local coordinates, namely harmonic or wave coordinates, have such optimal regularity; in any case, this has not been addressed in the literature. The regularity issue also arises frequently in the analysis and discussions of the behavior at the boundary and definitions of singularities for space–times. For instance, if the curvature remains bounded on approach to a possible boundary or singularity of space–time, it is important to understand how smooth the metric remains. If the metric remains sufficiently smooth (in some local coordinates), it may then be possible to extend the space–time through the boundary or the singularity to a larger space–time, essentially then removing the purported boundary or singularity; see Refs. 1–4 for further discussion.

More specifically, it has been an open problem for some time, cf. Refs. 2 and 5–7 for instance, whether a space–time (**M**, **g**) which has curvature bounded in L^{∞} in a suitable sense has coordinate charts in which the metric components $\mathbf{g}_{\alpha\beta}$ are in $C^{1,\gamma}\cap L^{2,p}$, for any $\gamma<1$, $p<\infty$. Here $C^{k,\gamma}$ is the Hölder space of functions whose kth derivatives are Hölder continuous of order γ, while $L^{k,p}$ is the Sobolev space of functions with k weak derivatives in L^{p}. Previous work (see the references above) only gives bounds on the metric components in $C^{0,\gamma}$, so that one has a loss of one derivative.

The first purpose of this article is to provide an affirmative solution to this problem, at least for vacuum space–times or space–times satisfying a weak condition on the stress-energy tensor. Second, this result is applied to examine the regularity of limits of sequences of space–times, or that of space–times with curvature defined only distributionally in L^{∞}. Also included is a preliminary discussion of behavior at the boundary, and the related extension problem, for space–times in any dimension.

The solution of the corresponding regularity problem in Riemannian geometry has been known for some time, and it is useful to state the exact result in this context before considering the Lorentzian analog. Thus, let (M,g) be a Riemannian n-manifold, with say C^{∞} smooth metric g. Suppose there exists a point $p\in M$ such that

$$\mathrm{dist}_g(p,\partial M)\geqslant 1. \tag{1.1}$$

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Let $R=R_{ijkl}$ denote the Riemann curvature tensor of (M,g), and let $B_p(r)$ denote the geodesic ball of radius r about p in (M,g). Suppose one has bounds

$$|R|_{L^\infty(B_p(1))}\leqslant C,\ \ \mathrm{vol}_g B_p(\tfrac{1}{2})\geqslant v_o\,, \tag{1.2}$$

for arbitrary constants $C<\infty$, $v_o>0$. Then there exists a constant $r_o>0$, depending only on C, v_o and n, such that the ball $B_p(r_o)$ admits a coordinate chart $U=\{u_k\}$, in which the metric g is $C^{1,\gamma}\cap L^{2,p}$, for any $\gamma<1$, $p<\infty$. Further, there exists a constant R_o, depending only on C, v_o, n and p, such that

$$\|g_{ij}\|_{L^{2,p}}\leqslant R_o\,, \tag{1.3}$$

where the norm is taken over the ball $B_p(r_o)$. A proof of this result may be found in Ref. 8, for instance. By Sobolev embedding $C^{1,\gamma}\subset L^{2,p}$, for $\gamma=1-n/p$, so that (1.3) also gives a bound on g_{ij} in $C^{1,\gamma}$.

This degree of regularity under the bound (1.2) is almost optimal. There are examples of metrics satifying (1.2) which are not $C^{1,1}$ in any coordinate system. Using somewhat more sophisticated analytic techniques, one can show that g_{ij} is in the Zygmund space C^2_*, cf. Ref. 9 (Prop. III.10.2).

The point here is that the estimate (1.3) applies to *all* metrics satisfying the bound (1.2). Thus, while (1.3) may be obvious for a given, possibly explicit, smooth metric, (1.3) applies to the space of all sufficiently smooth metrics, as well as their limits, provided (1.2) holds. In addition, one has an *a priori* bound on the size of the region where (1.3) holds.

A direct analog of this result for Lorentzian metrics is false, due to the existence of large families of nonflat space–times for which the curvature norm $|\mathbf{R}|^2=\mathbf{R}_{ijkl}\mathbf{R}^{ijkl}$ vanishes identically. Thus, consider, for instance, the class of vacuum plane-fronted gravitational waves on $\mathbb{R}^4$, with metric of the form

$$\mathbf{g}=-dudv-h(x,y,u)du^2+(dx^2+dy^2), \tag{1.4}$$

$$\Delta_{(x,y)}h=0. \tag{1.5}$$

For such metrics, the two possible scalar invariants in the curvature tensor, namely

$$|\mathbf{R}|^2=\langle\mathbf{R},\mathbf{R}\rangle=\mathbf{R}_{ijkl}\mathbf{R}^{ijkl}\quad\text{and}\quad\langle\mathbf{R},{*}\mathbf{R}\rangle=\mathbf{R}_{ijkl}({*}\mathbf{R})^{ijkl},$$

vanish identically. The vacuum Einstein equations impose only the condition (1.5), i.e., that h is harmonic as a function of (x,y). Thus, the function h may be an arbitrary function of u, and so is not controlled in any Hölder or Sobolev space. It is thus clear that there is no coordinate system in which a general metric $\mathbf{g}$ of the form (1.4) is controlled in $L^{2,p}$, or even C^0.

To deal with this situation, one imposes bounds on the components of $\mathbf{R}$ in a fixed coordinate system or framing. An efficient way to do this is to choose a future-directed unit timelike vector $T=e_0$ and extend it to an orthonormal frame e_α, $0\leqslant\alpha\leqslant n$, where the space–time dimension is $n+1$. Since the space $T^\perp$ orthogonal to T is spacelike and $O(n)$ is compact, the particular choice of framing for $T^\perp$ is unimportant. The norm of $\mathbf{R}$ w.r.t. T is then defined as

$$|\mathbf{R}|^2_T=\sum\ (R_{ijkl})^2, \tag{1.6}$$

where the components are w.r.t. the framing e_α.

Observe that if, at a point $p\in\mathbf{M}$, the vector $T=T_p$ is contained in a compact subset W of the future interior null cone $T^+_p\mathbf{M}$, then the norms (1.6) are all equivalent, with constant depending only on W. Hence, if K is a compact subset of the space–time $(\mathbf{M},\mathbf{g})$ and T is a continuous vector

field on K, then T (or more precisely, Im T, where T is viewed as a section of the tangent bundle), lies within a compact subset of $T^+\mathbf{M}$, where $T^+\mathbf{M}$ is the bundle of future interior null cones in the tangent bundle $T\mathbf{M}$.

To state the main result, we need the following definition, which is essentially just a normalization on the size of the region to be considered in ($\mathbf{M}$, $\mathbf{g}$), as is (1.1).

Definition 1: Let Ω be a domain in a smooth Lorentz manifold ($\mathbf{M}$, $\mathbf{g}$). Then Ω satisfies the size conditions if the following holds: The domain Ω admits a smooth time function t, with $c_o^{-1} \leqslant \|\nabla t\| \leqslant c_o$, for an arbitrary but fixed constant $c_o < \infty$. Further, one has

$$C_1 = B_p(1) \times [-1,1] \subset\subset \Omega, \tag{1.7}$$

i.e., the one-cylinder C_1 has compact closure strictly contained in Ω. Here $B_p(r)$ is the geodesic r-ball about a point p in S, where $S = S_0 = t^{-1}(0)$ and the metric g on S is that induced from $\mathbf{g}$. The product $B_p(1) \times [-1,1]$ is identified with a subset of Ω by the flow of ∇t, i.e., $(q,s) \to \gamma_q(s)$, where $\gamma_q(s)$ is the flow line of ∇t, starting at q and terminating on the s-level set $S_s = t^{-1}(s)$.

Let $T = \nabla t / \|\nabla t\|$ be the corresponding future-directed unit timelike vector field, and set

$$D = \text{Im}\, T|_{C_1} \subset\subset T^+\Omega. \tag{1.8}$$

The size conditions represent a Lorentzian analog of the condition (1.1). They can always be realized by choosing Ω to be a sufficiently small open set in ($\mathbf{M}$, $\mathbf{g}$) and rescaling the metric up sufficiently. Essentially, they just serve to normalize the data.

The main result of the article is then the following:

Theorem 2: *Let Ω be a domain in a vacuum $(n+1)$-dimensional space–time ($\mathbf{M}$, $\mathbf{g}$), $n \geqslant 2$, satisfying the size conditions. Suppose that there are constants $C < \infty$ and $v_o > 0$ such that*

$$|\mathbf{R}|_T \leqslant C, \quad \text{vol}_g B_p(\tfrac{1}{2}) \geqslant v_o. \tag{1.9}$$

Then there exists a constant $r_o > 0$, depending only on C, v_o, c_o, D, (and n), and a coordinate system (τ, x_i), $1 \leqslant i \leqslant n$, on the r_o-cylinder

$$C_{r_o} = D_p(r_o) \times [-r_o, r_o] \subset C_1, \tag{1.10}$$

such that the components of the metric $\mathbf{g}_{\alpha\beta}$ are in $C^{1,\gamma} \cap L^{2,p}$, for any $\gamma < 1$, $p < \infty$. Here $D_p(r)$ is the geodesic r-ball about p in the level set $\tau = 0$ and the product structure is that induced by the flow of $\nabla\tau$.

Further, there exists a constant $R_o < \infty$, depending only on C, v_o, c_o, D and the exponent p, such that, on C_{r_o},

$$\|\mathbf{g}_{\alpha\beta}\|_{L^{2,p}} \leqslant R_o. \tag{1.11}$$

More precisely, for any $k \leqslant 2$, and $0 \leqslant \alpha, \beta \leqslant n$,

$$\|\partial_\mu^k \mathbf{g}_{\alpha\beta}\|_{L_x^{2-k,p}} \leqslant R_o, \tag{1.12}$$

where ∂_μ^k denotes any k-fold space–time partial derivative and the spatial $L_x^{2-k,p}$ norm is taken over any spatial slice $\{\tau = \text{const}\}$ in C_{r_o}. The constant R_o is independent of τ in $[-r_o, r_o]$.

The coordinates in Theorem 2 are geometrically natural; the time coordinate τ is a Gaussian (equidistant) coordinate, while the spatial coordinates are chosen to be harmonic on the spatial slices $\{\tau = \text{const}\}$. It is not clear if there exist space–time harmonic (or wave) coordinates, in which $\mathbf{g}$ has this degree of regularity.

The condition that ($\mathbf{M}$, $\mathbf{g}$) is vacuum, i.e., $\mathbf{Ric}_\mathbf{g} = 0$, is used in only in minor way. It is used, via the Bianchi identity, only to obtain L^p bounds on the second time derivatives $\partial_\tau \partial_\tau \mathbf{g}_{0\alpha}$ of the

components $\mathbf{g}_{0\alpha}$. This is equivalent to bounds on the second time derivatives on the components of the shift vector of the coordinates, i.e., a bound on the acceleration of the shift. Such acceleration components do not appear in any component of the curvature tensor $\mathbf{R}$. All other estimates on $\partial_\gamma^k \mathbf{g}_{\alpha\beta}$ are independent of the Einstein equations.

The vacuum condition can be weakened to an assumption on the stress-energy tensor $\mathcal{T}$ in the Einstein equations, of the form

$$\|\nabla_T \mathcal{T}\|_{L_x^{-1,p}} \leqslant C. \tag{1.13}$$

Here $L_x^{-1,p}$ is the dual space of $L_o^{1,q}$, the space of $L_x^{1,q}$ functions of compact support on spatial slices $\{\tau = \text{const}\}$ within C_{r_o}, $p^{-1}+q^{-1}=1$.

The condition (1.13) will be satisfied automatically for many physically natural matter fields, cf. Remark 4.

Theorem 2 is formulated in such a way that it is easy to pass to limits. Thus, suppose $(\mathbf{M}_i, \mathbf{g}_i)$ is a sequence of smooth space–times satisfying the hypotheses of the theorem. There exist then domains $\Omega_i \subset (\mathbf{M}_i, \mathbf{g}_i)$, points $p_i \in \Omega_i$ such that the size conditions (1.7) and (1.8) hold, with D_i uniformly compact in $T^+\Omega_i$, (i.e., T does not become arbitrarily close to null cones). If (1.9) and (1.13) hold uniformly on Ω_i, then there is a subsequence which converges to a limit $C^{1,\gamma} \cap L^{2,p}$ space–time $(\mathbf{M}, \mathbf{g})$, defined at least on an r_o-cylinder C_{r_o}. Further, the convergence to the limit is $C^{1,\gamma}$ and weak $L^{2,p}$, and the bound (1.12) holds on the limit.

Define a Lorentz manifold $(\mathbf{M}, \mathbf{g})$ to be weakly regular if $\mathbf{g}$ is a continuous Lorentz metric, with $\mathbf{g} \in L^{1,2}_{loc}(\mathbf{M})$. It is well-known, cf. Refs. 1 and 10, for example, that such metrics have a well-defined curvature tensor $\mathbf{R}$ in the sense of distributions. This leads to the following corollary.

Corollary 3: Let $(\mathbf{M}, \mathbf{g})$ *be a weakly regular Lorentz manifold, and let* $\Omega \subset\subset \mathbf{M}$ *be a domain with compact closure in* $\mathbf{M}$. *Suppose the size conditions hold locally on* Ω, *in that the constant* $\frac{1}{2}$ *is replaced by a small constant* δ_o *so that* $B_p(\delta_o) \subset\subset \mathbf{M}$, *for any* $p \in \Omega$. *Suppose also the bounds (1.9) hold locally and uniformly on* δ_o *cylinders as in (1.7), centered at any* $p \in \Omega$.

Then Ω *may be covered by a finite atlas of charts in which the metric* $\mathbf{g} = \mathbf{g}_{\alpha\beta}$ *satisfies all the bounds in (1.12), except for the* L_x^p *bound on* $\partial_\tau \partial_\tau \mathbf{g}_{0\alpha}$. *The bounds in (1.12) depend, near* $\partial\Omega$, *on the distance of* $\partial\Omega$ *to* $\partial\mathbf{M}$.

If in addition the bound (1.13) holds distributionally on $\mathbf{M}$ *[e.g.,* $(\mathbf{M}, \mathbf{g})$ *is a weak solution of the vacuum equations], then all bounds in (1.12) hold locally on* $(\Omega, \mathbf{g})$.

We refer to the proof of Corollary 3 below for the precise meaning that (1.13) holds distributionally.

The proof of Theorem 2 and Corollary 3 follow in Sec. II, while Sec. III concludes the article with several remarks and extensions of these results, together with some open problems.

II. PROOFS OF THE RESULTS

In this section, we prove Theorem 2 and Corollary 3. For clarity, the proof of Theorem 2 is divided into several steps, each treating basically separate issues. In the following, as already above, space–time quantities are generally denoted in boldface while spatial quantities are not in boldface.

A. Step I (Initial choice of domain)

Let $B_p(r)$ be the intrinsic geodesic ball about p in S. Since S is achronal in the cylinder C_1 from (1.7), the extrinsic radius of $B_p(r)$ is bounded below for r small. Thus, if γ is any spacelike curve in $(\mathbf{M}, \mathbf{g})$ from p to $x \in \partial B_p(r_1) \subset S$, for r_1 small, then the length $L(\gamma)$ satisfies $L(\gamma) \geqslant l_o r_1$; the constants l_o and r_1 depend only on c_o and D in Definition 1.

Let $\mathcal{D}_{r_1}$ be the domain of dependence of $B_p(r_1)$ in the manifold $(\mathbf{M}, \mathbf{g})$. Thus, by choosing r_1 sufficiently small, again depending only on c_o, D, one has

$$\mathcal{D}_{r_1} \subset\subset \Omega, \tag{2.1}$$

i.e., $\mathcal{D}_{r_1}$ has compact closure in Ω.

The region $\mathcal{D}_{r_1}$ is globally hyperbolic and hence any pair of time-related points in $\mathcal{D}_{r_1}$ may be joined by a timelike maximizing geodesic in $\mathcal{D}_{r_1}$. Recall from Definition 1 that the curves γ_x are the flow lines of ∇t through x. For $r_2 > 0$ small (to be determined below), let

$$q = \gamma_p(-r_2), \tag{2.2}$$

so $q \ll p$, i.e., q is to the past of p. For x to the future of p, $x \gg p$, let

$$\tau(x) = \mathrm{dist}_{\mathbf{g}}(x,q) - \mathrm{dist}_{\mathbf{g}}(p,q), \tag{2.3}$$

so that $\tau(p) = 0$ and $\tau(x) > 0$, for $x \gg p$. The distance $\tau(x)$ is realized by a maximizing timelike geodesic $\sigma_v(\tau) = \exp_q(\tau + \tau_o)v$ from q to x; here $v \in T_q^+\mathbf{M}$, with $\mathbf{g}(v,v) = -1$, and $\tau_o = \mathrm{dist}_{\mathbf{g}}(p,q)$. This normalization gives $p = \sigma_{v_o}(0)$, for some $v_o \in T_q^+\mathbf{M}$. Let

$$N = \nabla \tau$$

be the corresponding unit timelike vector field, so that N is the tangent vector to geodesics σ issuing from q. Although N is well-defined and smooth along the individual geodesics $\sigma_v(\tau)$ [for any τ until one reaches the boundary of $(\mathbf{M}, \mathbf{g})$], at points where the exponential map $\exp_q$ has cut or conjugate points, N is not uniquely defined. Of course, past such cut or conjugate points, the geodesics $\sigma_v(\tau)$ are no longer maximal. Thus, in general, τ is merely Lipschitz and N, as a vector field, is defined only almost everywhere to the future of q. At the end of step I (via the work in step V), it will be seen that in fact τ and N are smooth, in suitable domains of a definite size. In the following, unless stated otherwise, all geodesics are assumed to be maximal, i.e., they are not continued past the conjugate or cut points of q.

Next, let $\Sigma = \Sigma_0 = \tau^{-1}(0)$ and similarly let Σ_τ be the τ-level set of τ in $\mathcal{D}_{r_1}$. Since the geodesics are maximal, $\sigma_v(\tau) \in \Sigma_\tau$, and $p \in \Sigma = \Sigma_0$. Again, in general, Σ_τ is only Lipschitz. For $r_2 \leqslant r_1$, consider the intrinsic geodesic ball $B_p(r_2) \subset S$ and let

$$\mathcal{C} = \{x \in \mathcal{D}_{r_1} : x = \sigma(\tau),\ \ \tau \leqslant r_2, \quad \text{and} \ \ \sigma(\tau) \cap B_p(r_2) \neq \varnothing\} \subset \mathcal{D}_{r_1}. \tag{2.4}$$

This is the "cone" of maximal geodesics σ starting at q, hitting S within $B_p(r_2)$, and terminating at time $\tau = r_2$.

Observe that the vector field N restricted to $\mathcal{C}$ stays within a compact subset of $T^+\mathbf{M}$. In fact, since N is parallel along its geodesic flow lines, this needs to be verified only at the base point q, where it holds by construction. It then follows from the curvature bound (1.9) and the remarks following (1.6) that

$$|\mathbf{R}|_N \leqslant C_1 = C_1(C,D). \tag{2.5}$$

Now the curvature bound (2.5) and the Rauch comparison theorem (cf. Ref. 11, for instance) imply that if r_2 is sufficiently small, depending (explicitly) only on C_1, then the exponential map $\exp_q$ restricted to the interior future null cone in T_q^+, has no conjugate points in $\mathcal{C}$. Thus, $\exp_q$ is of maximal rank, and so a local diffeomorphism on $\mathcal{C}$. In fact, for r_1 is sufficiently small, again depending only on C and c_o, no timelike or null geodesic within $\mathcal{D}_{r_1}$ has conjugate points, and so $\exp_x$ is of maximal rank on timelike geodesics in $\mathcal{D}_{r_1}$, $\forall x \in \mathcal{D}_{r_1}$.

Since $\mathcal{D}_{r_1}$ is globally hyperbolic and without timelike conjugate points, it follows then from Ref. 11 (Thm. 11.16, for instance) that any pair of points $x, y \in \mathcal{D}_{r_1}$ with $y \gg x$, may be joined by a *unique* maximizing timelike geodesic in $\mathcal{D}_{r_1}$, provided $\mathcal{D}_{r_1}$ is future one-connected (i.e., any pair of timelike curves joining x and y are homotopic through timelike curves).

In general, $\mathcal{D}_{r_1}$ need not be future one-connected. Consider, for example, the past null cone of two-dimensional Minkowski space in hyperbolic coordinates $t \in (-\infty, 0)$, $\phi \in (-\infty, \infty)$,

$$-dt^2+t^2d\phi^2.$$

If ϕ is identified periodically, with any period, then the resulting space–time is globally hyperbolic but not future one-connected. The future exponential map based at any point q has cut points; if the period of ϕ is sufficiently small, or if q is sufficiently close to $\{0\}$, then cut points occur arbitrarily close to q.

However, $\mathcal{D}_{r_1}$ is future one-connected if it has a simply connected Cauchy surface S, i.e., $S \equiv S_{r_1}=S\cap\mathcal{D}_{r_1}$, for S as in (1.7) ff. To see this, let γ_1, γ_2 be two timelike curves with common endpoints in $\mathcal{D}_{r_1}$. The flow of the timelike vector field ∇t gives a strong deformation retraction of $\gamma_1\cup\gamma_2$ onto a closed loop $\lambda_1\cup\lambda_2$ in S. If S is simply connected, then λ_1 may be deformed into λ_2 within S. These two homotopies, timelike along ∇t and spacelike along the Cauchy surfaces S_t, may be performed simultaneously, but with the latter at a larger speed than the former, to produce a timelike homotopy from γ_1 to γ_2.

We will prove later that S (or more precisely, a domain in S of a definite size) is simply connected. However, in order not to overburden the arguments that follow with such further issues, we assume in the following, through step IV, that the Cauchy surface $S\subset\mathcal{D}_{r_1}$ is simply connected. This hypothesis will be removed in step V, using the results obtained in the previous steps.

It follows then that the exponential map $\exp_q$ is a diffeomorphism onto $\mathcal{C}$, when restricted to a suitable domain in $T_q^+\mathbf{M}$. The time function τ is smooth in $\mathcal{C}\setminus\{q\}$, as are the level sets $\Sigma_\tau\cap\mathcal{C}$, and there is a unique maximizing geodesic from q to any point in $\mathcal{C}$.

From now on, we consider $\Sigma_\tau\subset\mathcal{C}$, and so let Σ_τ denote the prior Σ_τ intersected with $\mathcal{C}$. The level sets Σ_τ form a foliation of $\mathcal{C}$ by equidistant spacelike hypersurfaces, with unit normal N.

B. Step II (Initial curvature and volume estimates)

The geodesic congruence σ on $(\mathcal{C},\mathbf{g})$ satisfies the Riccati or transport equation

$$K'+K^2+\mathbf{R}_N=0. \tag{2.6}$$

Here $K=D^2\tau$ is the second fundamental form or extrinsic curvature of the leaves Σ_τ, $\mathbf{R}_N$ is the symmetric bilinear form given by $\mathbf{R}_N(X)=\langle\mathbf{R}(N,X)X,N\rangle$ and $'$ is the covariant derivative in the direction N. Hence, the bound (2.5) gives

$$|K'+K^2|\leq C_1.$$

This estimate holds on Σ_τ, for all $\tau\in[-r_2,r_2]$. It then follows by standard comparison theory for the Riccati ODE (2.6) that if r_2 is sufficiently small, depending only on c_o, D, and C_1, then

$$|K|_{L^\infty}\leq C_2, -|K'|_{L^\infty}\leq C_2, \tag{2.7}$$

on all Σ_τ, $\tau\in[-r_2/2,r_2]$. The constant C_2 depends only on r_2 and C_1. The Gauss equation relating the curvature $\mathbf{R}$ of the ambient manifold $(\mathbf{M},\mathbf{g})$ with that of the spatial slices Σ_τ reads

$$\mathbf{R}_{ijkl}=R_{ijkl}+K_{ik}K_{jl}-K_{il}K_{jk}, \tag{2.8}$$

for spatial components $(ijkl)$. This, together with the bounds (2.5) and (2.7), thus gives the bound

$$|R_g|_{L^\infty}\leq C_3, \tag{2.9}$$

on Σ_τ, $\tau\in[-r_2/2,r_2]$. Let dK be the exterior derivative (w.r.t. the connection induced by g) of K, when K is viewed as a one-form with values in $T\Sigma_\tau$, i.e., $dK(X,Y,Z)=(\nabla_XK)(Y,Z)-(\nabla_YK)(X,Z)$. The Gauss–Codazzi equations are

$$dK=\mathbf{R}^N,$$

where $\mathbf{R}^N(X,Y,Z)=\langle \mathbf{R}(N,X),Y,Z\rangle$. Hence, (2.5) also implies

$$|dK|_{L^\infty}\leqslant C_3. \tag{2.10}$$

We record also the well-known constraint equations:

$$\begin{aligned} \delta K &= -dH-\mathbf{Ric}(N),\\ R-|K|^2+H^2 &= 2\mathbf{Ric}(N,N)+\mathbf{R}, \end{aligned} \tag{2.11}$$

where $H=$ tr K is the mean curvature and the operators δ and d are taken on Σ_τ.

Next, we use the bounds above to obtain a lower volume bound on the spatial slices Σ_τ, $\tau\in[-r_2/2,r_2]$, from that on the slice $S=S_0$ in (1.9). To do this, let $\hat{S}=S\cap\mathcal{C}$. The domain $\hat{S}$ may be written as a graph over $\Sigma=\Sigma_0\subset\mathcal{C}$ via the time coordinate τ in the usual way. Thus, each geodesic $\sigma=\sigma_v$ intersects Σ and $\hat{S}$ in exactly two points $\sigma(\tau_1)$, $\sigma(\tau_2)$, with $|\tau_i|\leqslant r_2$. For $x=\sigma_v(\tau_1)\in\Sigma$, let $u(x)=\tau_2-\tau_1$, so that $\sigma_v(\tau_2)\in\hat{S}$. This gives a diffeomorphism $\phi:\Sigma\to\hat{S}$, and hence

$$\text{vol } \hat{S}=\int_{\hat{S}}dV_{\hat{S}}=\int_\Sigma \phi^*(dV_{\hat{S}})=\int_\Sigma J dV_\Sigma,$$

where $J=\det D\phi$ is the Jacobian of ϕ. Since both $\hat{S}$ and Σ are spacelike, the function u is a Lipschitz function (cf. Ref. 1) whose (weak) derivative is uniformly bounded, since both normal vectors N and T lie in compact subsets of interior null cones. In addition, the (uniform) time τ exponential map, mapping Σ to Σ_τ, has Jacobian uniformly bounded above and below on $[-r_2/2,r_2]$, by the bound (2.7). (Recall that $H=$tr K measures the infinitesimal volume expansion or contraction.) It follows that the Jacobian J is uniformly bounded below (depending only on C, D). Hence,

$$\text{vol } \Sigma\geqslant v_1\cdot\text{vol } \hat{S}. \tag{2.12}$$

Now the lower bound on vol $B_p(\frac{1}{2})\subset S$ in (1.9) does not immediately imply a lower bound on vol $\hat{S}$ (it could *a priori* happen that most all of the volume of $B_p(\frac{1}{2})$ occurs outside $\hat{S}$). However, in this case one can repeat all the estimates (2.6)–(2.9) when the construction of $\mathcal{C}$ is based at other center points q' in place of q. Thus, for $p'\in B_p(\frac{1}{2})\subset S$, define q' as in (2.2) and let $\mathcal{C}'$ be then as in (2.4). The same estimates as above then hold in $\mathcal{C}'$. The corresponding domains $\hat{S}'=S\cap\mathcal{C}'$ give a covering of $B_p(\frac{1}{2})\subset S$. Hence the volume bound in (1.9) and the estimates above now do give the existence of points $p_o\in B_p(\frac{1}{2})\subset S$ such that

$$\text{vol } \Sigma_{p_o}\geqslant v_2>0, \tag{2.13}$$

where Σ_{p_o} is the level set of τ (i.e., τ_o) containing p_o and $v_2=v_2(v_o,D,C_1)$. [The local estimate (2.12) does not in fact depend on the absence of future cut points of $\exp_q$, cf. the discussion concerning (2.59) below.]

Recall the standard volume comparison theorem in Riemannian geometry: if (N,g) is a Riemannian n-manifold, with $\text{Ric}_g\geqslant-(n-1)k$, then the ratio

$$\frac{\text{vol } D(r)}{\text{vol } D_k(r)},$$

is monotone nonincreasing in r. Here $D(r)$ denotes the volume of a geodesic r-ball at any fixed point, while $D_k(r)$ is the geodesic r-ball in the n-dimensional space form of constant curvature k. It then follows from the curvature bound (2.9), together with (2.13), that the geodesic balls $D_{p_o}(r)\subset(\Sigma_{p_o},g)$ satisfy

$$\text{vol } D_{p_o}(r)\geqslant v_3 r^n,$$

for all $r\leqslant r_2$, where v_3 depends only on v_2 and C_3.

Observe that a similar estimate also holds for geodesic balls on other spatial slices Σ_τ, with $\Sigma_0=\Sigma_{p_o}$, for $\tau\in[-r_2/2,r_2]$. Namely, the L^∞ bound on K in (2.7) bounds the infinitesimal distortion in the spatial metrics, and hence distances and volumes, under the flow of N. It follows that within the cylinder $\mathcal{C}_o$ centered at p_o, the volume estimate above holds for balls $D_{p_\tau}(r)\subset\Sigma_\tau$; thus, for $p_\tau=\sigma_{v_o}(\tau)$, where $p_o=\sigma_{v_o}(0)$, and for $r\leqslant r_2$, one has

$$\text{vol } D_{p_\tau}(r)\geqslant v_4 r^n, \tag{2.14}$$

$v_4=v_4(v_o,C,D)$. An upper bound on the volume of vol $D_{p_\tau}(r)$ of the form (2.14) follows immediately from the curvature bound (2.9).

In the construction above, we have shifted the original base point p to a new base point p_o. However, one may now use these estimates to obtain equivalent volume bounds for the slices Σ_τ within the original cylinder $\mathcal{C}$ centered at p. This may be done by constructing a suitable chain, of bounded cardinality, of overlapping cylinders $\mathcal{C}_i$ from $\mathcal{C}_o$ to $\mathcal{C}$. One then uses the arguments above on each $\mathcal{C}_i$, together with the fact that upper and lower volume bounds of spatial slices are equivalent to upper and lower volume bounds of each cylinder $\mathcal{C}_i$.

Thus, in the following, we work on the original cylinder $\mathcal{C}$ from (2.4) centered at p; the bound (2.14) holds with p in place of p_o.

C. Step III (Local coordinates)

In this step, we define the cylinder C_{r_o} and the local coordinate system on it, and obtain in addition some initial estimates on $\mathbf{g}_{\alpha\beta}$. The local coordinates are Gaussian in time and harmonic in space (Gaussian-harmonic coordinate system).

Thus, the function τ from (2.3) is chosen as the time coordinate on $\mathcal{C}$. To construct spatial harmonic coordinates, start with the slice $\Sigma=\Sigma_0$ within $\mathcal{C}$. By (2.9) and (2.14), one has the bounds

$$|R_g|\leqslant C_3, \text{vol}_g D_p(r_2)\geqslant v_4. \tag{2.15}$$

It then follows, for instance from the discussion in Sec. I, that there exists $r_o>0$, depending only on C_3 and v_4, such that the geodesic ball $D_p(r_o)\subset\Sigma$ admits a harmonic coordinate system $\{x_i\}$, $1\leqslant i\leqslant n$, in which the spatial metric $g=\mathbf{g}|_\Sigma$ is controlled in $L^{2,p}$, i.e.,

$$\|g_{ij}\|_{L^{2,p}}\leqslant R_o, \tag{2.16}$$

where the $L^{2,p}$ norm is taken on $D_p(r_o)$, and $R_o=R_o(C_3,v_4,p)$. The harmonic functions x_i are solutions to the Dirichlet problem

$$\Delta_g x_i=0,\ x_i|_{\partial D}=\phi_i, \tag{2.17}$$

where $D=D_p(r_o)$ and ϕ_i are suitably chosen boundary values (approximating linear-type functions, cf. Ref. 8).

Let $\phi_{i,\tau}=\phi_i\circ\psi_\tau$, where ψ_τ is the time τ flow from Σ_τ to Σ_0 along the integral curves of N. Thus, ψ_τ maps a domain $D_\tau\subset\Sigma_\tau$ diffeomorphically onto D and $\phi_{i,\tau}$ are functions defined on ∂D_τ. It follows that

$$N(\phi_{i,\tau})=1 \quad \text{at} \quad \partial D_\tau. \tag{2.18}$$

Define the functions x_i on D_τ to be solutions to the Dirichlet problem

$$\Delta_{g_\tau} x_i=0, \quad x_i|_{\partial D_\tau}=\phi_{i,\tau}. \tag{2.19}$$

By (2.9) and (2.14), the estimate (2.15) holds uniformly on D_τ, for $\tau\in[-r_2/2,r_2]$. Hence, as with Σ_0, $r_o>0$ may be chosen, depending only on C_3 and v_4, such that the functions $\{x_i\}$ form a harmonic coordinate system on $D_\tau\subset\Sigma_\tau$, on which one has the bounds

$$\|g_{ij}\|_{L^{2,p}}\leq R_o, \tag{2.20}$$

where the $L^{2,p}$ norm is taken on D_τ and $g=g_\tau$. The estimate (2.20) holds for all $|\tau|\leq r_o$.

This construction gives the local coordinate system (τ,x_i), $1\leq i\leq n$, on the r_o-cylinder

$$C_{r_o}=D_p(r_o)\times[-r_o,r_o] \tag{2.21}$$

about p, where the product structure is defined by the flow of $\nabla\tau$. For the remainder of the proof, Σ_τ is now redefined to be its intersection with C_{r_o}, i.e., $\Sigma_\tau\equiv D_\tau$.

The metric $\mathbf{g}$ in these coordinates has the form

$$\mathbf{g}=(-1+|\xi|^2)(d\tau)^2+g_{ij}(dx_i+\xi_i d\tau)(dx_j+\xi_j d\tau), \tag{2.22}$$

where $\xi=\{\xi_i\}$ is the shift vector. Thus,

$$\partial/\partial\tau=N+\xi,$$

with $N=\nabla\tau$. The lapse function α of this foliation satisfies $\alpha\equiv 1$.

On each slice $\Sigma_\tau\subset C_{r_o}$, one has good spatial control, namely for $g_{ij}=\mathbf{g}_{ij}=\mathbf{g}|_{\Sigma\tau}$, (2.20) holds. As usual, Latin indices i,j, denote spatial variables, i.e., $1\leq i,j\leq n$, while Greek indices α, β denote space–time variables, $0\leq\alpha,\beta\leq n$.

In the following, all Sobolev norms $L^{k,p}$ are understood to be spatial norms, i.e., the derivatives and norms are taken on spatial leaves Σ_τ. Thus, for emphasis or clarity, we sometimes write $L^{k,p}_x$ in place of $L^{k,p}$. All estimates will be independent of τ, for $\tau\leq r_o$.

D. Step IV ($L^{2,p}$ estimates of $g_{\alpha\beta}$)

In this next step, we extend the estimate (2.20) to include the remaining terms $\mathbf{g}_{0\alpha}$, $0\leq\alpha\leq n$, and also obtain estimates on the time derivatives of $\mathbf{g}_{\alpha\beta}$.

Before beginning, we first improve the estimate (2.7) on the second fundamental form. Recall the Simons (or Bochner-Weitzenbock) formula (cf. Ref. 12, Chap. 1I):

$$D^*DK=\delta dK+d\delta K-\mathcal{R}(K)$$

on (Σ_τ,g_τ), where the term $\mathcal{R}(K)$ is linear in the curvature and K; the exact form of $\mathcal{R}(K)$ plays no role in the argument, but for completeness is given by $\mathcal{R}(K)=Ric\circ K+K\circ Ric-2R\circ K$, where $R\circ K$ is the action of the curvature tensor R on symmetric bilinear forms. The elliptic operator $D^*D=-trD^2$ is the so-called rough Laplacian.

In the following, we frequently write $f\in L^{k,p}$ or $f\in L^{k,p}_x$ as shorthand for f is uniformly bounded in $L^{k,p}$ along the spatial slices Σ_τ, $|\tau|\leq r_o$.

By (2.10), $dK\in L^\infty$, and hence $\delta dK\in L^{-1,p}_x$, for all $p<\infty$; recall that these spaces are defined as following (1.13). Similarly, by (2.11), since $dd=0$,

$$d\delta K=d(\mathbf{Ric}N)\in L^{-1,p}_x; \tag{2.23}$$

here we recall that the operators δ and d are spatial. The term $\mathcal{R}(K)$ is also bounded in L^∞. Hence, one has

$$D^*DK = Q_1, \tag{2.24}$$

where Q_1 is uniformly bounded in $L_x^{-1,p}$, for any $p<\infty$, while K is uniformly bounded in L^∞. By (2.20), the coefficients of D^*D in the local coordinates $\{x_i\}$ are controlled in $L^{2,p}\subset C^{1,\gamma}$. It then follows from standard elliptic regularity theory, cf. Ref. 13, that

$$|K|_{L_x^{1,p}} \leqslant C_2, \tag{2.25}$$

where $C_2 = C_2(C, v_o, c_o, D, p)$, on all spatial slices Σ_τ, $|\tau| \leqslant r_o$.

E. Spatial estimates

Here, we prove that the components $\mathbf{g}_{0\alpha}$ also satisfy the $L^{2,p} = L_x^{2,p}$ estimate (2.20) uniformly on Σ_τ. One has $N = \mathbf{g}^{0\alpha}\partial_\alpha$, $\nabla x_i = \mathbf{g}^{i\alpha}\partial_\alpha$. Hence, $N(x_i) = \langle N, \nabla x_i\rangle = \mathbf{g}^{0\alpha}\mathbf{g}^{i\beta}\mathbf{g}_{\alpha\beta} = \mathbf{g}^{0i}$.

To obtain estimates on $N(x_i)$, differentiate the harmonic coordinate condition (2.17), in the normal (i.e., N) direction. Let $x_i' = N(x_i)$. Since $\Delta x_i = 0$, a standard computation [cf. Ref. 12, (1.184) for example] gives

$$\Delta x_i' = -\Delta' x_i = \langle D^2 x_i, K\rangle - \langle dx_i, \delta K + \tfrac{1}{2} dH\rangle. \tag{2.26}$$

Here, as above and in the following, all metric quantities in (2.26) are on spatial slices Σ_τ.

By (2.25), K is uniformly bounded in $L^{1,p}$. The term $D^2 x_i$ is also uniformly bounded in $L^{1,p}$, since by (2.20) the spatial metric is uniformly bounded in $L^{2,p}$ and hence the coordinate functions are uniformly bounded in $L^{3,p}$. Further, both δK and dH are uniformly bounded in L^p. Thus,

$$\Delta x_i' = Q_2,$$

where Q_2 is uniformly bounded in L^p, $|\tau| \leqslant r_o$. As before, the coefficients of Δ are controlled in $L^{2,p}$. Further, by construction, cf. (2.18), $x_i' = 1$ on $\partial\Sigma_\tau$. Hence, standard elliptic regularity again gives

$$\|x_i'\|_{L^{2,p}} = \|\mathbf{g}^{0i}\|_{L^{2,p}} \leqslant C_4, \tag{2.27}$$

where $C_4 = C_4(C, v_o, c_o, D, p)$. Observe also that

$$\mathbf{g}^{00} = -1 \tag{2.28}$$

(since the lapse function $\alpha \equiv 1$). Hence $\mathbf{g}^{0\alpha} \in L^{2,p}$, i.e., the $L^{2,p}$ norm of $\mathbf{g}^{0\alpha}$ is uniformly bounded, $0 \leqslant \alpha \leqslant n$.

From this and (2.20), it is then an elementary exercise in linear algebra to see that

$$\|\mathbf{g}_{\alpha\beta}\|_{L^{2,p}} \leqslant C_5. \tag{2.29}$$

Briefly, $\mathbf{g}^{0\gamma} = (\det \mathbf{g}_{\alpha\beta})^{-1} A_{0\gamma}$, where $A_{0\gamma}$ is the $(0,\gamma)$ cofactor in the matrix $\mathbf{g}_{\alpha\beta}$. The cofactor A_{00} involves only g_{ij}, and hence by (2.20), $A_{00} \in L^{2,p}$. Thus $\det \mathbf{g}_{\alpha\beta} \in L^{2,p}$. The same reasoning on $\mathbf{g}^{0\alpha}$ then gives $A_{0\alpha} \in L^{2,p}$, for all α. Each determinant A_{0k} may be expanded along the first column to obtain a linear form in the variables $\mathbf{g}_{0i}$, with coefficients $(n-1)\times(n-1)$ determinants. Thus, one has a linear system of n equations in n unknowns $\mathbf{g}_{0i}$. The matrix of this system is the $(n-1)$-compound G_{n-1} of the matrix $[g_{ij}]$, i.e., $(G_{n-1})_{kl} = \det A_{kl}$, where A_{kl} is the (k,l) cofactor of $[g_{ij}]$. Since $[g_{ij}]$ is nonsingular, and since $[g_{ij}]$ nonsingular implies that G_{n-1} is nonsingular (cf. Ref. 14, §1.4 for instance), it follows that this linear system is invertible.

The components $\mathbf{g}_{0i}$ are rational expressions in $\{g_{ij}\}$ and $\{A_{0k}\}$, each of which is now bounded in $L^{2,p}$. Hence $\mathbf{g}_{0i}$ is bounded in $L^{2,p}$. Finally, since $1=\mathbf{g}^{0\alpha}\mathbf{g}_{\alpha 0}=\mathbf{g}^{00}\mathbf{g}_{00}+\mathbf{g}^{0i}\mathbf{g}_{i0}$, it follows from (2.28) that $\mathbf{g}_{00}$ is also bounded in $L^{2,p}$. This establishes the bound (2.29).

Recall that $\partial_\tau = N+\xi$, while $\langle N,\partial_i\rangle = 0$, $i>0$, by construction. Since $\langle \partial_i,\partial_\tau\rangle = \mathbf{g}_{i0}$ is bounded in $L^{2,p}$, it follows that $\langle \xi,\partial_i\rangle$ is bounded in $L^{2,p}$. Hence the shift vector $\xi=\{\xi_i\}$ is bounded in $L^{2,p}$,

$$\|\xi\|_{L^{2,p}} \leqslant C_6. \tag{2.30}$$

This completes the $L^{2,p}$ estimates of $\mathbf{g}_{\alpha\beta}$ in spatial directions.

F. First time derivatives

Next we turn to estimates on the time derivatives of $\mathbf{g}_{\alpha\beta}$, i.e., $L^{1,p}$ estimates for $\partial_\tau \mathbf{g}_{\alpha\beta}$. To begin, using the Leibniz rule, and the fact that $[\partial_\alpha,\partial_\tau]=0$, it suffices to estimate

$$\langle \nabla_{\partial_\alpha}\partial_\tau,\partial_\beta\rangle = \langle \nabla_{\partial_\alpha}N,\partial_\beta\rangle + \langle \nabla_{\partial_\alpha}\xi,\partial_\beta\rangle. \tag{2.31}$$

Suppose first $\alpha>0$, $\beta>0$, so $(\alpha,\beta)=(i,j)$. The first term in (2.31) is then K_{ij}, which is bounded in $L^{1,p}$ by (2.25), while the second term is also bounded in $L^{1,p}$ by (2.30) [and the $L^{2,p}$ spatial bounds on $\mathbf{g}_{\alpha\beta}$ in (2.29)]. This gives uniform $L^{1,p}$ bounds on $\partial_\tau g_{ij}$, i.e.,

$$\|\partial_\tau g_{ij}\|_{L^{1,p}_x} \leqslant C_7. \tag{2.32}$$

It follows of course that also

$$\|\partial_{x_k}\partial_\tau g_{ij}\|_{L^p_x} \leqslant C_7.$$

The bounds on $\partial_\tau \mathbf{g}_{0\alpha}$ require more work. Writing $\partial_\tau = N+\xi$ as above, the $L^{2,p}$ spatial estimates above imply that $\xi(\mathbf{g}_{0\alpha})$ is bounded in $L^{1,p}$, so one needs to obtain $L^{1,p}$ bounds on $N(\mathbf{g}_{0\alpha})$.

Recall that $x_i' = N(x_i) = \mathbf{g}^{0i}$. Hence $N(\mathbf{g}^{0i}) = NN(x_i) = x_i''$. To obtain estimates on x_i'', differentiate the equation (2.17) in the N direction twice. This gives

$$\Delta x_i'' = -(2\Delta' x_i' + \Delta'' x_i). \tag{2.33}$$

Here, as before, all metric quantities are on the spatial slices Σ_τ. It has already been proved that $x_i' \in L^{2,p}$. From the form of Δ' in (2.26), one then easily sees that

$$\Delta' x_i' \in L^p.$$

Next, one has

$$\Delta'' x_i = N\langle D^2 x_i, K\rangle - N\langle dx_i, \delta K + \tfrac{1}{2} dH\rangle. \tag{2.34}$$

To estimate these terms, let e_α be a local orthonormal basis on Σ_τ, with $\nabla_{e_\alpha} e_\beta = 0$ at any fixed point in Σ_τ. Then the first term in (2.34) may be written

$$N\langle D^2 x_i, K\rangle = N(D^2 x_i(e_a,e_b))\cdot K(e_a,e_b) + D^2 x_i(e_a,e_b)\cdot N(K(e_a,e_b)).$$

By (2.25) and (2.7), $K_{ab} \in L^{1,p}$ and $NK_{ab} \in L^p$, while by (2.20), $D^2 x_i \in L^{1,p}$. Thus

$$D^2 x_i(e_a,e_b)\cdot N(K(e_a,e_b)) \in L^p. \tag{2.35}$$

Further $N(D^2 x_i(e_a,e_b)) = N\langle \nabla_{e_a} dx_i, e_b\rangle = \langle \nabla_N \nabla_{e_a} dx_i, e_b\rangle$, so that

$$N(D^2 x_i(e_a,e_b)) = \langle \nabla_{e_a}\nabla_N dx_i, e_b\rangle + \langle R(N,e_a)dx_i, e_b\rangle - \langle \nabla_{e_b} dx_i, \nabla_{e_a} N\rangle. \tag{2.36}$$

The curvature term in (2.36) is bounded in L^∞, while the last term equals $\langle D^2 x_i(e_b), K(e_a)\rangle$, which is bounded in L^∞. For the first term, one has

$$\langle \nabla_{e_a}\nabla_N dx_i, e_b\rangle = e_a\langle \nabla_N dx_i, e_b\rangle = e_a\langle \nabla_{e_b} dx_i, N\rangle = -e_a(K(dx_i, e_b)). \tag{2.37}$$

Since $K \in L^{1,p}$, this term is bounded in L^p. Combining these estimates, it follows that the first term in (2.34) is bounded in L^p.

For the next term in (2.34), $N\langle dx_i, dH\rangle = \langle \nabla_N dx_i, dH\rangle + \langle dx_i, \nabla_N dH\rangle = \langle \nabla_{dH} dx_i, N\rangle + \langle N, \nabla_{dx_i} dH\rangle$, so that

$$N\langle dx_i, dH\rangle = -2K(dH, dx_i), \tag{2.38}$$

which is bounded in L^p.

Finally, $-N\langle dx_i, \delta K\rangle = Ne_a K(dx_i, e_a) - NK(\nabla_{e_a} e_a, dx_i) - NK(e_a, \nabla_{e_a} dx_i)$. By (2.7), the latter two terms are in L^∞. For the first term, $Ne_a K(dx_i, e_a) = e_a NK(dx_i, e_a) - (\nabla_{e_a} N)(K(dx_i, e_b))$. The latter term here is $-[K(e_a)](K(dx_i, e_b))$, which is bounded in L^p by (2.25). For the first term, since $NK(dx_i, e_a)$ is bounded in L^∞, $e_a NK(dx_i, e_a) = \mathrm{div}(N(K(dx_i)))$ is bounded in $L^{-1,p}$, since the derivatives e_a are spatial. This shows that

$$N\langle dx_i, \delta K\rangle \in L^{-1,p}. \tag{2.39}$$

Thus, combining these estimates on (2.33) gives a uniform bound on $\Delta x_i''$ in $L^{-1,p}$. On the boundary $\partial\Sigma_\tau$, one has $x_i'' = 0$. It then follows from elliptic regularity as before [as in (2.24)] that

$$N(\mathbf{g}^{0i}) = x_i'' \in L^{1,p}.$$

Of course, by (2.28), $N(\mathbf{g}^{00}) = 0$. As above, $\mathbf{g}_{0i}$ is a rational expression in $\{g_{ij}\}$ and $\{A_{0k}\}$. The bound (2.32) implies that each of these has N-derivative in $L^{1,p}$ and hence, by the same arguments as before, $N(\mathbf{g}_{0\alpha}) \in L^{1,p}$. This gives uniform bounds

$$\|\partial_\tau \mathbf{g}_{\alpha\beta}\|_{L^{1,p}_x} \leqslant C_8. \tag{2.40}$$

This completes the estimates for the first time derivatives on spatial slices. In particular, all Christoffel symbols are bounded in $L^{1,p}_x$.

G. Second time derivatives

Finally, we obtain L^p estimates on the second time derivatives $\partial_\tau\partial_\tau \mathbf{g}_{\alpha\beta}$. To do this, take ∂_τ of the term $\langle \nabla_{\partial_\alpha}\partial_\tau, \partial_\beta\rangle$ in (2.31). One then obtains

$$\langle \nabla_{\partial_\alpha}\nabla_{\partial_\tau}\partial_\tau, \partial_\beta\rangle + \langle \mathbf{R}(\partial_\tau, \partial_\alpha)\partial_\tau, \partial_\beta\rangle.$$

The curvature term is bounded in L^p, in fact L^∞. (This uses the fact that ξ is controlled, so the framing is controlled.)

Write $\nabla_{\partial_\tau}\partial_\tau = \Gamma^\gamma_{00}\partial_\gamma$. Hence

$$\langle \nabla_{\partial_\alpha}\nabla_{\partial_\tau}\partial_\tau, \partial_\beta\rangle = \Gamma^\gamma_{00}\langle \nabla_{\partial_\alpha}\partial_\gamma, \partial_\beta\rangle + \partial_\alpha(\Gamma^\gamma_{00})\langle \partial_\gamma, \partial_\beta\rangle.$$

By the first derivative estimates above, the Christoffel symbols are bounded in $L^{1,p}_x$. The first term is a product of Christoffel symbols, and hence is bounded in $L^{1,p/2}_x \subset L^{np/(2n-p)}$, by Sobolev embedding. For $p > n$ (recall that p is arbitrarily large), $L^{np/(2n-p)} \subset L^p$. Thus the first term is bounded in L^p.

For the second term, if $\alpha > 0$, then $\partial_\alpha(\Gamma^\gamma_{00})$ is bounded in L^p by (2.40). Hence, this gives

$$\|\partial_\tau\partial_\tau g_{ij}\|_{L^p} \leqslant C_9, \tag{2.41}$$

uniformly in τ. It remains to estimate the second time derivatives of $\mathbf{g}_{0\alpha}$. These correspond to the second order time behavior of the shift vector ξ.

These estimates are the most involved, and are the only estimates dependent on the Einstein equations. To obtain these estimates, one needs to differentiate (2.17) three times in the normal N direction. Thus, from (2.17) again,

$$\Delta x_i''' = -3\Delta' x_i'' - 3\Delta'' x_i' - \Delta''' x_i . \tag{2.42}$$

Recall $x_i' = \mathbf{g}^{0i}$ is bounded in $L^{2,p}$, while $x_i'' = N(\mathbf{g}^{0i})$ is bounded in $L^{1,p}$. From previous work, it is then straightforward to bound the first two terms on the left in (2.42).

To see this, one has

$$\Delta' x_i'' = \langle D^2 x_i'', K\rangle - \langle dx_i'', \delta K + \tfrac{1}{2} dH\rangle,$$

which is bounded in $L_x^{-1,p}$, since $x_i'' \in L_x^{1,p}$. To estimate the term $\Delta'' x_i'$, one just replaces x_i in the estimates (2.34)–(2.39) by $N(x_i)$. Using the fact that $N(x_i) \in L^{2,p}$, one sees by checking term by term that this is bounded in $L^{-1,p}$.

It remains to analyze

$$\Delta''' x_i = NN\langle D^2 x_i, K\rangle - NN\langle dx_i, \delta K + \tfrac{1}{2} dH\rangle. \tag{2.43}$$

To begin,

$$NN\langle D^2 x_i, K\rangle = \langle \nabla_N \nabla_N D^2 x_i, K\rangle + 2\langle \nabla_N D^2 x_i, \nabla_N K\rangle + \langle D^2 x_i, \nabla_N \nabla_N K\rangle. \tag{2.44}$$

By the Riccati equation (2.6), $\nabla_N K$ is bounded in L^∞, while by the estimate on (2.36), $\nabla_N D^2 x_i$ is bounded in L^p. Hence, the middle term in (2.44) is bounded in L^p. For the last term, taking the N-derivative of the Riccati equation (2.6) gives

$$\langle D^2 x_i, \nabla_N \nabla_N K\rangle = -2\langle D^2 x_i, (\nabla_N K)K\rangle - \langle D^2 x_i, \nabla_N \mathbf{R}_N\rangle. \tag{2.45}$$

The first term in (2.45) is bounded in L^∞. The second (curvature) term in (2.45) will be analyzed below.

For the first term in (2.44), one needs to take N-derivatives of all terms following (2.35) to (2.37). The only one which is not bounded in $L^{-1,p}$ by previous estimates is the term

$$N\langle \mathbf{R}(N, e_a) dx_i, e_b\rangle = (\nabla_N \mathbf{R})(N, e_a, dx_i, e_b) + \text{lower order}. \tag{2.46}$$

We return again to this curvature term below, and proceed with the second term in (2.43).

Again, to estimate this, one takes N-derivatives of the estimates in (2.38) to (2.39). This gives first

$$NK(dH, dx_i) \in L^p,$$

since NK is bounded. For the δK term, modulo lower order terms, this is of the form

$$\begin{aligned} N\langle \nabla_N \nabla_{e_a} K(dx_i), e_a\rangle &= N\langle \nabla_{e_a} \nabla_N K(dx_i), e_a\rangle + N\langle \mathbf{R}(N, e_a) K(dx_i), e_a\rangle \\ &= \langle \nabla_N \nabla_{e_a} \nabla_N K(dx_i), e_a\rangle + (\nabla_N \mathbf{R})(N, e_a, K(dx_i), e_a) \\ &= \langle \nabla_{e_a} \nabla_N \nabla_N K(dx_i), e_a\rangle + (\nabla_N \mathbf{R})(N, e_a, K(dx_i), e_a) \\ &\quad + \langle \mathbf{R}(N, e_a) \nabla_N K(dx_i), e_a\rangle; \end{aligned}$$

the equalities here are understood to be modulo lower order terms. Modulo terms bounded in L^p, this may be rewritten as

$$\nabla_{e_a}(\nabla_N \mathbf{R})(N,K(dx_i),N,e_a)+(\nabla_N \mathbf{R})(N,e_a,K(dx_i),e_a). \tag{2.47}$$

Combining these estimates gives then uniform $L_x^{-1,p}$ bounds on all terms in (2.43), except for the four curvature terms of the form $(\nabla_N \mathbf{R})N$.

We obtain bounds on the curvature terms via the contracted second Bianchi identity on $(\mathbf{M}, \mathbf{g})$:

$$\boldsymbol{\delta}\mathbf{R} = -\mathbf{dRic},$$

or more precisely, cf. Ref. 12, (16.3),

$$\boldsymbol{\delta}\mathbf{R}(X,Y,Z) = -\mathbf{dRic}(Y,Z,X). \tag{2.48}$$

Write, on $\mathbf{M}$,

$$(\nabla_N \mathbf{R})N = -\boldsymbol{\delta}\mathbf{R}+\delta\mathbf{R} = \mathbf{dRic}+\delta\mathbf{R}, \tag{2.49}$$

where the divergences $\boldsymbol{\delta}$, δ are the space–time and spacelike divergences on Σ_τ, respectively.

Now the space–time curvature $\mathbf{R}$ is bounded in L^∞ (in bounded framings). Hence the spatial divergence $\delta\mathbf{R}$ is bounded in $L_x^{-1,p}$, for any $p<\infty$. Thus, the curvature term (2.46) may be rewritten, modulo $L_x^{-1,p}$, as

$$(\nabla_N \mathbf{R})(N,e_a,dx_i,e_b) = \mathbf{dRic}(dx_i,e_b,e_a) \in L_x^{-1,p},$$

where the last estimate follows since all derivatives of **Ric** are taken in spatial directions. Similarly, for the second curvature term in (2.47), one has, for the same reasons, modulo $L_x^{-1,p}$,

$$(\nabla_N \mathbf{R})(N,e_a,K(dx_i),e_a) = \mathbf{dRic}(K(dx_i),e_b,e_a) \in L_x^{-1,p}.$$

This leaves left the two curvature terms:

$$\langle D^2 x_i, \nabla_N \mathbf{R}_N\rangle \quad \text{and} \quad \nabla_{e_a}(\nabla_N \mathbf{R})(N,K(dx_i),N,e_a). \tag{2.50}$$

The second term is of form $\delta\mathbf{dRic}(N,K(dx_i))$ (to leading order), which cannot be controlled without the Einstein equation, since it involves differentiation in the N direction. Similarly,

$$\nabla_N \mathbf{R}_N = \mathbf{dRic}(N,\cdot,\cdot), \quad \text{modulo } L_x^{-1,p}, \tag{2.51}$$

is not controlled without the Einstein equations.

Dropping the usual constants, the Einstein equations on $(\mathbf{M}, \mathbf{g})$ are

$$\mathbf{Ric} - \frac{\mathbf{R}}{2} g = \mathcal{T}, \tag{2.52}$$

where $\mathcal{T}$ is the stress-energy tensor. Suppose $(\mathbf{M}, \mathbf{g})$ is vacuum, or more generally, suppose the stress-energy tensor $\mathcal{T}$ satisfies

$$d\mathcal{T}(N,e_a,e_b) \in L_x^{-1,p}, \tag{2.53}$$

where e_a, e_b are spatial. Since the Einstein equations and the bound (2.5) imply that $\nabla_{e_a}\mathcal{T}(N) \in L_x^{-1,p}$, (2.53) is equivalent to

$$\nabla_N \mathcal{T} \in L_x^{-1,p}, \text{ or } \mathcal{L}_N \mathcal{T} \in L_x^{-1,p}, \tag{2.54}$$

where $\mathcal{L}_N$ denotes the Lie derivative in the direction N.

Combining the bound (2.53) with the estimates obtained above on the terms in (2.42) then gives

$$\Delta x_i''' = \Delta NN(\mathbf{g}^{0i}) \in L_x^{-2,p}, \tag{2.55}$$

since $\delta\mathbf{dRic}(N,K(dx_i)) \in L_x^{-2,p}$, not $L_x^{-1,p}$. As before, since the coefficients of the Laplacian are well-controlled (i.e., bounded in $L^{2,p}$), and the functions x_i''' have 0 boundary values, elliptic regularity gives

$$NN(\mathbf{g}^{0i}) \in L^p.$$

(One sees this from duality in the standard way, using the fact that $\Delta: L_o^{2,p} \to L^p$ is an isomorphism, cf. also Ref. 15.)

Applying the linear algebra argument as before then gives the bound

$$\partial_\tau \partial_\tau \mathbf{g}_{0\alpha} \in L^p. \tag{2.56}$$

This completes all of the estimates on $\mathbf{g}_{\alpha\beta}$. We refer to Remark 4 below for further discussion on use of the Einstein equations. Finally, the assumptions (2.53) or (2.54) are equivalent to (1.13). To see this, both T and N lie within a compact subset of $T^+\Omega$. Since the covariant derivative w.r.t. T or N involves only the pointwise behavior of these vector fields, one may replace T by N in (1.13), which then corresponds to (2.54).

H. Step V (Issue of cut points)

In this final step, we show that by passing to a smaller cylinder if necessary, of definite size within C_{r_o}, the exponential map $\exp_{q'}$ at a suitable base point q' has no future cut points. By the work above, this will complete the proof.

To begin, return to the "cone" $\mathcal{C}$ in (2.4). Let V be the collection of timelike unit vectors in $T_q^+\mathcal{D}_{r_1}$ for which there is a maximal geodesic σ_v issuing from q and terminating in $\mathcal{C}$. Let

$$\tilde{\mathcal{C}} = \{sv : v \in V, s \leq r_1\} \subset T_q^+\mathcal{D}_{r_1}, \tag{2.57}$$

so that in particular $\exp_q \tilde{\mathcal{C}}$ contains $\mathcal{C}$. Here, as in step I, r_1 is chosen so that no geodesic $\sigma_v(s)$, for $v \in V$, has conjugate points with $s \leq r_1$. Of course the geodesics $\sigma_v(s)$ now are no longer necessarily maximal. Since $\exp_q$ is of maximal rank on $\tilde{\mathcal{C}}$, we work on the pullback $(\tilde{\mathcal{C}}, \tilde{\mathbf{g}})$, where

$$\tilde{\mathbf{g}} = (\exp_q)^* \mathbf{g}. \tag{2.58}$$

The domain $\tilde{\mathcal{C}}$ is a compact connected cone in $T_q\mathbf{M}$, w.r.t. the vector space structure. By the Gauss lemma, the straightline generators of this cone are geodesics in the $\tilde{\mathbf{g}}$ metric. Let $\tilde{\tau}$ denote the distance to the origin $\{0\}$ w.r.t. $\tilde{\mathbf{g}}$, within $\tilde{\mathcal{C}}$. This is now a smooth function on $\tilde{\mathcal{C}} \setminus \{0\}$, and serves as the parameter for the geodesics from $\{0\}$. Inside the cutlocus of $\exp_q$ on $\tilde{\mathcal{C}}$ (i.e., where $\exp_q$ is a diffeomorphism), $\tilde{\tau}$ is just the lift of the function τ from (2.3), up to an additive constant.

The level sets $\tilde{\Sigma}_{\tilde{\tau}} \subset \tilde{\mathcal{C}}$ of τ are smooth, and hence the images $\exp_q \tilde{\Sigma}_{\tilde{\tau}}$ are smoothly immersed submanifolds in $\mathcal{C}$. The original Lipschitz level surface Σ_τ is just the part of $\exp_q \tilde{\Sigma}_{\tilde{\tau}}$ contained in the domain $U^\tau = \{x : \tau(x) \geq \tau\} \cap \mathcal{C}$. Observe that the timelike exponential map $\exp_0$ of $(\tilde{\mathcal{C}}, \tilde{\mathbf{g}})$ based at 0 is a diffeomorphism onto $\tilde{\mathcal{C}}$; this map has no conjugate or cut points within $\tilde{\mathcal{C}}$.

Thus, we are now in exactly the same situation as at the end of step I, with $(\tilde{\mathcal{C}}, \tilde{\mathbf{g}})$ in place of $(\mathcal{C}, \mathbf{g})$. Set $\tilde{S} = (\exp_q)^{-1}(\mathcal{C}) \subset \tilde{\mathcal{C}}$, so that $\tilde{S}$ is an embedded hypersurface in $\tilde{\mathcal{C}}$. Since $\exp_q$ is a local isometry of $\tilde{S}$ onto $\hat{S}$, one has

$$\mathrm{vol}_{\tilde{g}} \tilde{S} \geq \mathrm{vol}_g \hat{S}. \tag{2.59}$$

Hence, by the same reasoning as in step II, the volume estimate (2.14) holds on the smooth hypersurfaces $\tilde{\Sigma}_{\tilde{\tau}}$.

We may thus apply the work in steps II–IV to conclude that there is an $r_o>0$, depending only on C, D, c_o, v_o, and an r_o-cylinder $\tilde{C}_{r_o}\subset\tilde{\mathcal{C}}$, centered on $\tilde{p}$, on which there are coordinates $(\tilde{\tau},\tilde{x}_i)$ in which the metric $\tilde{\mathbf{g}}$ is controlled in $L^{2,p}$ in the sense that (1.12) holds.

It remains to prove the existence of a suitable cylinder C' "downstairs," i.e., within $(\Omega,\mathbf{g})$, with these properties. Thus, let $\tilde{\Sigma}_{\tilde{\tau}}$ now denote the part of $\tilde{\Sigma}_{\tilde{\tau}}$ contained in $\tilde{C}_{r_o}$. Each $\tilde{\Sigma}_{\tilde{\tau}}$ is an n-ball, topologically. Recall, as in step II, that $\tilde{S}\cap\tilde{C}_{r_o}$ is a graph over $\tilde{\Sigma}_{\tilde{\tau}_o}$, for some $\tilde{\tau}_o$. Hence, $\tilde{S}\cap\tilde{C}_{r_o}$ is also an n-ball topologically. By construction, both $\tilde{\Sigma}_{\tilde{\tau}_o}$ and $\tilde{S}\cap\tilde{C}_{r_o}$ have a uniform lower bound on their volume and size, i.e., $\mathrm{dist}_{\tilde{g}}(\tilde{p},\partial(\tilde{S}\cap\tilde{C}_{r_o}))\geqslant r_3>0$ (and similarly for $\tilde{\Sigma}_{\tilde{\tau}_o}$). These bounds depend only on the initial bounds on C, v_o and D, c_o.

Let U be the interior of the cutlocus of $\exp_q|_{\tilde{\mathcal{C}}}$. The domain U is starshaped w.r.t. the origin $\{0\}$ in $T_q^+\mathcal{D}_{r_1}$. Further, again by construction, $\tilde{S}\cap\tilde{C}_{r_o}$ is contained in the closure $\overline{U}$ of U. If $(\tilde{S}\cap\tilde{C}_{r_o})\cap\partial U\neq\varnothing$, one may perturb it slightly, along the geodesic straight lines to $\{0\}$, to obtain an n-ball $\tilde{S}'\subset\tilde{C}_{r_o}$ with $\tilde{S}'\subset U$. As before, the ball $\tilde{S}'$ has a definite lower bound on its volume and its size.

The exponential map $\exp_q$ now gives a diffeomorphism, in fact an isometry, from $(\tilde{S}',\tilde{g})$ to (S',g), $S'=\exp_q\tilde{S}'$. Let $\mathcal{D}'$ be the domain of dependence of S' in $(\mathbf{M},\mathbf{g})$. This gives a globally hyperbolic region $\mathcal{D}'\subset(\mathbf{M},\mathbf{g})$, with a simply connected Cauchy surface of definite size and volume. The work of steps I–IV may now be applied to this situation within $(\mathbf{M},\mathbf{g})$ to produce a new cylinder C', centered at p, satisfying the bounds (1.12).

This completes the proof of Theorem 2. ■

It is an open question whether Theorem 2 holds without an assumption of the form (1.13), i.e., whether there exist coordinate systems in which (1.12) holds under only the bounds (1.9).

Remark 4: From the physical point of view, most stress-energy tensors $\mathcal{T}$ derive from matter fields satisfying a hyperbolic system of PDE, of first or second order. In such a situation, these equations can frequently be used to interchange a time derivative $\nabla_N\mathcal{T}$ on spatial slices, with a spatial derivative $\nabla_X\mathcal{T}$, modulo lower order terms, e.g., $(\nabla_N\mathcal{T})(X)\sim(\nabla_X\mathcal{T})(N)$, modulo lower order terms. This is exactly the process used via the second Bianchi identity above. For instance, this is easily seen to be the case for electromagnetic fields, via use of the Maxwell equation $\mathbf{dF}=0$.

When the matter equations allow for such time–space replacement, modulo lower order terms, the condition (1.13) is of course not necessary in Theorem 2.

Next we turn to the proof of Corollary 3.

Let $(\mathbf{M},\mathbf{g})$ be a weakly regular space–time, satisfying the size conditions, and satisfying the bound (1.9) distributionally. Thus, the components of $\mathbf{R}$, well-defined as distributions, are in fact bounded in L^∞.

Any such space–time $(\mathbf{M},\mathbf{g})$ is a limit of a sequence of (C^∞) smooth space–times $(\mathbf{M},\mathbf{g}_k)$, cf. Ref. 10 (Theorem 4), for instance. The metrics $\mathbf{g}_k$ are obtained in the usual way by taking the convolution of $\mathbf{g}$ with a sequence of smooth mollifiers. The local size conditions and local volume bound in (1.9), with δ_o in place of $\frac{1}{2}$, depend only on the C^0 behavior of the metric. Since the convergence to the limit is C^0, it follows that local size conditions and local volume bounds hold uniformly on the sequence $(\mathbf{M},\mathbf{g}_k)$. Similarly, the fact that $|\mathbf{R}|_T$ is bounded on $(\mathbf{M},\mathbf{g}_k)$ implies that the curvature $|\mathbf{R}_{\mathbf{g}_k}|_{T_k}$ of $(\mathbf{M},\mathbf{g}_k)$ is uniformly bounded, for unit timelike vector fields $T_k\to T$, as $k\to\infty$.

It then follows from Theorem 2 that for any $p\in\Omega$, there are r_o-cylinders $((C_{r_o})_k,p_k)\subset\subset(\mathbf{M},\mathbf{g}_k)$, with $p_k\to p$, and coordinates on $(C_{r_o})_k$ in which the metric $\mathbf{g}_k$ is controlled: this in the sense that the bounds (1.12) hold, with the exception of the bound on $\partial_0\partial_0\mathbf{g}_{0\alpha}$. Since the bounds on C, v_o and D, c_o, hold uniformly on $(\mathbf{M},\mathbf{g}_k)$, and p_k remains a bounded

distance away from $\partial\mathbf{M}$, it follows that there is a limit cylinder $(C_{r_o},p)\subset(\mathbf{M},\mathbf{g})$ on which (1.12) holds, again except for the bound on $\partial_0\partial_0\mathbf{g}_{0\alpha}$.

This proves the first part of Corollary 1.3. For the second part, one needs to make sense of the condition (1.13) on $(\mathbf{M}, \mathbf{g})$. It suffices to do this locally, i.e., on cylinders $C_{r_o}\subset(\mathbf{M},\mathbf{g})$. Of course $\nabla_N\mathbf{Ric}$, or equivalently $\nabla_N\mathcal{T}$, is well-defined in $L^{-1,p}(\Omega)$, (since $\mathbf{Ric}\in L^\infty$), but one needs to define it in $L^{-1,p}(\Sigma_\tau)$.

To do this, from the above, we know that $g_\tau=\mathbf{g}|_{\Sigma_\tau}$ is in $L^{2,p}_x(\Sigma_\tau)$, for any $\Sigma_\tau\subset C_{r_o}$. Let h be a symmetric bilinear form in $L^{1,q}(\Sigma_\tau)$, of compact support, for a given τ. Extend h into C_{r_o} by the flow of N, so that $\mathcal{L}_N h=0$. Hence, h is defined on all $\Sigma_\tau\subset C_{r_o}$. Formally, or alternately on the smooth approximations $(\mathbf{M},\mathbf{g}_k)$ of $(\mathbf{M}, \mathbf{g})$, one has

$$\int_{\Sigma_\tau}\langle h,\nabla_N\mathbf{Ric}\rangle dV=\int_{\Sigma_\tau}N\langle h,\mathbf{Ric}\rangle dV-\int_{\Sigma_\tau}\langle\nabla_N h,\mathbf{Ric}\rangle dV. \tag{2.60}$$

Observe that $\nabla_N h=\mathcal{L}_N h+h(\nabla_{\partial_a}N,\partial_b)+h(\partial_a,\nabla_{\partial_b}N)=h(K(\partial_a),\partial_b)+h(K(\partial_b),\partial_a)$. Since $K\in L^{1,p}(\Sigma_\tau)$ and p is large, it follows $\nabla_N h$ is well-defined in $L^q(\Sigma_\tau)$, for any τ. Hence, the second term in (2.60) is well-defined (since $\mathbf{Ric}$ is bounded in L^∞).

For the first term on the right in (2.60), one has

$$\int_{\Sigma_\tau}N\langle h,\mathbf{Ric}\rangle dV=\frac{d}{d\tau}\int_{\Sigma_\tau}\langle h,\mathbf{Ric}\rangle dV-\int_{\Sigma_\tau}\langle h,\mathbf{Ric}\rangle H dV. \tag{2.61}$$

The second term in (2.61) is well-defined, since again $H\in L^{1,p}\subset C^\alpha$. Thus, to define (1.13) on C_{r_o}, we require that the derivative

$$\frac{d}{d\tau}\int_{\Sigma_\tau}\langle h,\mathbf{Ric}\rangle dV, \text{ or equivalently, } \frac{d}{d\tau}\int_{\Sigma_\tau}\langle h,\mathcal{T}\rangle dV \tag{2.62}$$

exist for all $\tau\in[-r_o,r_o]$, for any h as above. Under this condition, the bound (1.13) on C_{r_o} is then equivalent to a uniform bound on (2.62), for all $\tau\in[-r_o,r_o]$.

Given this definition of the condition (1.13) on the limit C_{r_o}, it follows from the same proof as in Theorem 2 that $\partial_0\partial_0\mathbf{g}_{0\alpha}$ is uniformly bounded in $L^p(\Sigma_\tau)$, $|\tau|\leqslant r_o$. This completes the proof of Corollary 3. ■

III. DISCUSSION AND CONCLUDING REMARKS

We conclude the paper with several remarks extending the validity of Theorem 2, together with some open problems.

Theorem 2 gives the existence of cylinders C of a definite size in the interior of $\mathbf{M}$, and a definite distance away from any boundary $\partial\mathbf{M}$, on which there exist coordinates in which the metric is controlled in $L^{2,p}$. Of course, by rescaling up suitably to realize the size conditions, applying Theorem 2, and then rescaling back down, the cylinders C may be chosen to be arbitrarily close to $\partial\mathbf{M}$. (This is already implicit in Corollary 3.) However, the coordinates may change in the (smaller and smaller) cylinders as one approaches $\partial\mathbf{M}$.

The main reason it is necessary to stay a definite distance away from $\partial\mathbf{M}$ in the proof is that one needs to work in globally hyperbolic regions, as in (2.1), which are future one-connected. If $\mathbf{M}$ is globally hyperbolic and future one-connected to begin with, then it is no longer necessary to stay a given distance away from $\partial\mathbf{M}$. We describe an alternate version of Theorem 2 in this context.

Thus, suppose $(\mathbf{M}, \mathbf{g})$ is globally hyperbolic and future one-connected; [for instance, $(\mathbf{M}, \mathbf{g})$ has a simply connected Cauchy surface]. Choose any point $q\in\mathbf{M}$ and timelike unit vector $N_o\in T^+_q\mathbf{M}$. Let $V\subset T^+_q\mathbf{M}$ be the compact cone of unit vectors forming a fixed angle θ with N_o, and

let $\mathcal{C}=\exp_q \pi v$, $v \in V$, be the corresponding "cone" in $(\mathbf{M}, \mathbf{g})$. Also, let N be the corresponding vector field tangent to the geodesics $\sigma_v(\tau)=\exp_q(\pi v)$, and let Σ_τ be the level sets of τ in $\mathcal{C}$. We make the following assumptions: there exist constants $C<\infty$ and $v_o>0$ such that

$$|\mathbf{R}|_N \leqslant C, \quad \text{within } \mathcal{C}, \tag{3.1}$$

$$\text{vol } \Sigma_\tau \geqslant v_o \cdot (\text{diam } \Sigma_\tau)^n. \tag{3.2}$$

Although (3.2) is understood to hold for all $\tau \leqslant r_1$, for a fixed r_1, the methods used in step II show that it suffices to assume (3.2) holds for a fixed $\tau_o>0$, where the size τ_o depends only on C in (3.1). The bound (3.2) is of course scale-invariant.

We then have the following result, valid at least up to a point in $\partial\mathbf{M}$.

Corollary 5: Let $(\mathbf{M}, \mathbf{g})$ *be a globally hyperbolic, future one-connected space–time satisfying the assumptions (3.1) and (3.2). Suppose also* $(\mathbf{M}, \mathbf{g})$ *is vacuum, or more generally, satisfies (1.13). Then there exist small constants* $d_o>0$, *and* $r_o>0$, *depending only on* C, v_o, N_o *and* θ, *such that if*

$$\sigma_{N_o}(\tau) \in \mathbf{M}, \ \forall \tau < d_o,$$

then there exist coordinates (τ, x_i) *on the cylinder*

$$C_{r_o}(d_1)=D_p(r_o d_o)\times[d_1/2, d_1] \subset \mathbf{M}, \tag{3.3}$$

in which the metric satisfies the bounds (1.12). Here d_1 *is the largest value such that* $d_1 \leqslant d_o$ *and* $C_{r_o}(d_1)$ *is contained in* $\mathbf{M}$.

The proof of this result is exactly the same as that of Theorem 2. In fact, it is simpler, since the issues of global hyperbolicity and future one-connected are assumed, and one works with N in place of the vector field T from Definition 1. Thus, for d_o small as above, and for $C(V)$ the cone on V in $T_q\mathbf{M}$, the exponential map $\exp_q$ restricted to $(C(V)\backslash\{q\})\cap B_0(d_1)$ is a diffeomorphism onto $(\mathcal{C}\cap B_q(d_1))$, where $B_q(d_1)=\exp_q(B_0(d_1))$. The domain $\mathcal{C}\cap B_q(d_1)$ plays exactly the same role as $\mathcal{C}$ in step I. All the estimates of steps II–IV then proceed just as before and are uniform for $\tau \in [d_1/2, d_1]$. ■

Remark 6: One may also derive a version of Theorem 2, (or Corollary 3), without the lower volume bound in (1.9). Thus, one has a uniform spatial curvature bound (2.9), either on the slices $\Sigma_\tau \subset \mathcal{C}$ downstairs, or on the slices $\widetilde{\Sigma}_{\tilde{\tau}} \subset \widetilde{\mathcal{C}}$ upstairs in $T_q\mathbf{M}$. [The bound (2.9) does not require any *a priori* volume bound.] If the volume Σ_τ or $\widetilde{\Sigma}_{\tilde{\tau}}$ is very small, then the injectivity radius of g_τ is very small, i.e., the spatial metric g_τ is highly collapsed in the sense of Cheeger-Gromov. However (as before), the Rauch comparison theorem implies that the intrinsic exponential map on Σ_τ or $\widetilde{\Sigma}_{\tilde{\tau}}$ is still of maximal rank on geodesic balls of a definite size (depending only on the curvature bound). Suppose first one works in the situation of $\Sigma_\tau \subset \mathcal{C}$. Then just as before in timelike directions, one can lift the metric g_τ up to the tangent space by pulling back by its exponential map, i.e., consider the metric $\tilde{g}_\tau=(\exp_{p_\tau})^* g_\tau$ defined on balls in $T_{p_\tau}\Sigma_\tau$. The metric $\tilde{g}_\tau$ has a uniform lower bound on the volumes of small balls. All the arguments in steps II–IV can then be carried out as before on this "unwrapped" space–time and the corresponding unwrapped cylinder $\widetilde{C}_{r_o}$. This gives coordinates $(\tilde{\tau}, \tilde{x}_i)$ for $\widetilde{C}_{r_o}$ on which the metric $\tilde{\mathbf{g}}$ satisfies the bounds (1.12). The same procedure holds when working with $\widetilde{\Sigma}_{\tilde{\tau}}$. These coordinates upstairs within $T_q\mathbf{M}$ give then "multi-valued" coordinates downstairs in $(\mathbf{M}, \mathbf{g})$.

To conclude, we mention two open problems. First, for certain purposes, the L^∞ bound on the curvature in (1.11) may be viewed as too strong. It would be of interest to know if a version of Theorem 2 holds with suitable L^p bounds on $|\mathbf{R}|_T$, $p>n/2$, in place of L^∞ bounds.

Second, it would be very interesting if the Einstein equations could be used to remove the dependence of these results on bounds on the full curvature, i.e., if bounds on the full curvature could be replaced by bounds on the Ricci curvature, possibly introducing other hypotheses not related to curvature. This seems to be a challenging problem; cf. Ref. 16 for some further discussion.

ACKNOWLEDGMENT

This work was partially supported by NSF Grant No. DMS 0072591.

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Exterior differential systems, Janet–Riquier theory and the Riemann–Lanczos problems in two, three, and four dimensions

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(Received 22 August 2002; accepted 23 December 2002)

We discuss the Riemann–Lanczos problems in two, three, and four dimensions using the theory of exterior differential systems and Janet–Riquier theory. We show that the Riemann–Lanczos problem in two dimensions is always a system in involution. For each of the two possible signatures we give the general solution in both instances and show that the occurrence of characteristic coordinates need not affect the result. In three dimensions, the Riemann–Lanczos problem is not in involution as an identity occurs. This does not prevent the existence of singular solutions and we give an example for the *reduced* Gödel space–time. A prolongation of this problem, whereby an integrability condition is added, leads to a prolonged system in involution. The Riemann–Lanczos problem in four dimensions is not in involution and needs to be prolongated as Bampi and Caviglia suggested. But *singular* solutions of it can be found and we give examples for the Gödel, Kasner, and Debever–Hubaut space–times. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1566095]

I. INTRODUCTION

The problem of generating the space–time Weyl conformal curvature tensor C_{abcd} from a tensor potential is called the **Weyl–Lanczos problem** and the analogous problem for the Riemann curvature tensor the Riemann–Lanczos problem.

The Lanczos tensor potential admits the following index symmetries,

$$L_{[ab]c}=L_{abc}, \tag{1}$$

where $a,b,c,s=0,1,2,3$ for four dimensions and

$$L_{[abc]}=0. \tag{2}$$

Apart from these, we may impose two gauge conditions: the differential gauge condition

$$L_{ab}{}^{s}{}_{;s}=0, \tag{3}$$

where ";" indicates covariant differentiation and we often write $f_{ab}=L_{ab}{}^{s}{}_{;s}$, and the algebraic gauge or trace free condition

$$L_{a}{}^{s}{}_{s}=0. \tag{4}$$

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Lanczos discovered the Weyl–Lanczos equations,[1] where he introduced a Lagrangian based on the double dual of the Riemann tensor R_{abcd}. The Lanczos tensor L_{abc} arose as a Lagrange multiplier for this Lagrangian. Lanczos found an expression for the Weyl tensor in terms of certain Lagrange multipliers L_{abc}, namely,

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}+g_{bc}L_{(ad)}+g_{ad}L_{(bc)}-g_{bd}L_{(ac)}-g_{ac}L_{(bd)} + \tfrac{2}{3}L^{ms}{}_{m;s}(g_{ac}g_{bd}-g_{ad}g_{bc}), \tag{5}$$

where $L_{ad}=L_a{}^s{}_{d;s}-L_a{}^s{}_{s;d}$. These are *the Weyl–Lanczos equations*. Further, if we impose (3) and (4) above, we can simplify (5) considerably to

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}-g_{bc}L^s{}_{ad;s}-g_{ad}L^s{}_{bc;s}+g_{bd}L^s{}_{ac;s}+g_{ac}L^s{}_{bd;s}. \tag{6}$$

Many solutions to (6) are known and solutions for vacuum space–times can be found in Ref. 2.

We can also attempt to express the Riemann curvature tensor in terms of a comparable tensor potential $\hat{L}_{abc}$ which leads to the **Riemann–Lanczos problem**. Udeschini Brinis[3] had wanted to describe the space–time Riemann tensor in terms of a Lanczos tensor $\hat{L}_{abc}$ and proposed the Riemann–Lanczos relations

$$R_{abcd}=\hat{L}_{abc;d}-\hat{L}_{abd;c}+\hat{L}_{cda;b}-\hat{L}_{cdb;a}. \tag{7}$$

But the difficulties with the relations (7) were pointed out in two papers by Bampi and Caviglia[4,5] where they proved existence of theorems for solutions of (5) and (7). Whereas the Weyl–Lanczos problem is always in involution, the Riemann–Lanczos problem is *not* and only singular solutions of it can occur if the problem is **not** modified. Bampi and Caviglia showed the following.

(i) The Weyl–Lanczos problem (5) or (6) has nonsingular solutions for $n=4, 5$, where n is the dimension of the space–time manifold M.
(ii) For $n=4$ the Riemann–Lanczos problem (7) has no nonsingular solutions but it does have "singular" solutions which means that the Cartan characters do not adopt their maximal values.
(iii) The differential gauge condition (3) has no effect on the existence or nonexistence of solutions of either (5) or (7).

Bampi and Caviglia[5] also suggested a prolongation of the Riemann–Lanczos equations to make them a system in involution.

In the Riemann–Lanczos problem, we meet Eq. (2) and possibly (3) but **not** (4), which leaves us with 20 independent components for the $\hat{L}_{abc}$ in four dimensions. *We always assume that the cyclic conditions* (2) *hold* but **not** *the trace-free conditions* (4). If Eqs. (4) were to hold, we would have

$$R=4\hat{L}^{nk}{}_{k;n}=-4\hat{L}^{nk}{}_{n;k}=0,$$

which would lead to inconsistencies. Because we are only going to talk about the Riemann–Lanczos problem in this article, we will change notation from $\hat{L}_{abc}$ to L_{abc} from now on. We will also write the Riemann–Lanczos equations in solved form as

$$f^{(R)}_{abcd}:=R_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}. \tag{8}$$

The paper by Massa and Pagani[6] concerning a modification of the Riemann–Lanczos problem used a different approach to the above work of Bampi and Caviglia. Accordingly, we do not consider Ref. 6 here. As Ref. 7 is based on Ref. 6 it is also not applicable here.

II. EXTERIOR DIFFERENTIAL SYSTEMS

First we introduce some theory of exterior differential systems (EDSs) which we are going to apply to the Riemann–Lanczos problems in two, three, and four dimensions. Good and detailed accounts of the theory of exterior differential systems can be found in Refs. 8–10.

A. Exterior differential systems and Pfaffian systems

We denote a formal N-dimensional manifold by $\mathcal{M}$ of which the space–time manifold M is an n-dimensional submanifold. Then, for a collection of differential forms we define an **exterior differential system** (EDS) as a collection of one-forms $\alpha^{(1)}_{i_1}$, two-forms $\alpha^{(2)}_{i_2}$ and so on up to p-forms $\alpha^{(p)}_{i_p}$ and possibly zero-forms on our formal N-dimensional manifold $\mathcal{M}$. A **Pfaffian system** $\mathcal{P}$ is a special EDS containing only one-forms θ^α and 0-forms.[11–13] We denote the **rank** of $\mathcal{P}$ by s which is given by the number s of independent one-forms in $\mathcal{P}$. Consider now the collection of all vector fields on $\mathcal{M}$ denoted by $\mathcal{X}(\mathcal{M})$. There is a subset of $\mathcal{X}(\mathcal{M})$ given by all those vector fields which annihilate the Pfaffians in $\mathcal{P}$,

$$\mathcal{D} := \{X \in \mathcal{X}(\mathcal{M}) \,|\, \theta^\alpha(X) = 0, \quad \alpha = 1,...,s\},$$

so that the number of independent vector fields in $\mathcal{D}$ is $N-s$. We call $\mathcal{D}$ the **dual system** to $\mathcal{P}$. For any Pfaffian system $\mathcal{P}$, we can also look at its **derived system** $\mathcal{P}'$ for which we can write[14]

$$\mathcal{P}' := \{\theta^\alpha \in \mathcal{P} | d\theta^\alpha(X,Y) = 0, \quad \forall X, Y \in \mathcal{D}, \quad \alpha = 1,...,s\},$$

where $\mathcal{P}' \subset \mathcal{P}$ always holds. Further, we denote by $\overline{\mathcal{D}}$

$$\overline{\mathcal{D}} := \{Y \in \mathcal{X}(\mathcal{M}) | d\theta^\alpha(X,Y) = 0, \quad \forall X \in \mathcal{D}, \quad \forall \alpha = 1,...,s\}.$$

Pfaffian systems are classified according to the ease with which they can be integrated. The most familiar Pfaffian systems are also the simplest, namely, **complete Pfaffian systems** to which the celebrated **Frobenius theorem** applies. We say that a Pfaffian system $\mathcal{P}$ is *complete* if and only if $\mathcal{P} = \mathcal{P}'$ holds, or, in other words $\mathcal{D} = \overline{\mathcal{D}}$. *In general, Pfaffian systems are not complete* but each Pfaffian system can be enlarged by adding further one-forms until it becomes complete or becomes inconsistent. The minimal enlarged Pfaffian system which is complete is known as the **associated system** $\mathcal{A}(\mathcal{P})$ of $\mathcal{P}$ and its dimension is called the **class** c of $\mathcal{P}$. Sometimes, $\mathcal{A}(\mathcal{P})$ is also called the **Cartan system** $C(\mathcal{P})$.[15] Further, the dual space of $C(\mathcal{P})$ usually denoted by $C(\mathcal{D}) = C(\mathcal{P})^\perp$ is the space containing all Cauchy characteristic vector fields.

A good account of Pfaffian systems characterized by Vessiot vector fields can be found in Refs. 14 and 16 and many examples are given in Ref. 17. A Vessiot vector field system $\mathcal{D} = \mathcal{P}^\perp$ is complete means then that $[\mathcal{D},\mathcal{D}] \subseteq \mathcal{D}$ for all $Y \in \mathcal{D}$ which is equivalent to $\overline{\mathcal{D}} = \mathcal{D}$.

When a vector field system $\mathcal{D}$ or Pfaffian system $\mathcal{P}$ fails to be complete, a slightly weaker condition may hold on some subsystem of $\mathcal{D}$. Such a possibility is that a vector field system is in **involution**, which is defined as follows:

Definition 1: Involutory subsystem of a vector field system. An involutory subsystem $\mathcal{T}$ of a vector field system $\mathcal{D}$ is a subsystem $\mathcal{T}$ of $\mathcal{D}$ such that $[\mathcal{T},\mathcal{T}] \subseteq \mathcal{D}$, which means that $\mathcal{T}$ is closed relative to $\mathcal{D}$ but not relative to $\mathcal{T}$ itself.

B. Integral elements and Cartan characters

All definitions in this section are based on Ref. 18 which relies on Cartan's original work whereas the work in Ref. 19 varies slightly from Ref. 9 in some definitions. When an EDS Σ or a Pfaffian system $\mathcal{P}$ is given, we try to find manifolds on which all the differential forms of Σ or $\mathcal{P}$ are annihilated. We will construct tangent spaces to such manifolds, where the dimension of each of them can be deduced from a sequence of non-negative integers called the Cartan characters. Such tangent spaces are called *integral elements* and are defined as follows.

Definition 2: Integral element. A p-dimensional subspace $(E^p)_x$ at a point x of the tangent space $T_x(\mathcal{M})$ of a N-dimensional manifold $\mathcal{M}$ is called an integral element of an EDS Σ if $\alpha^i_j(E^p)_x=0$ at x for all forms α^i_j in Σ, which means that all differential forms of Σ are annihilated on $(E^p)_x$ at $x\in\mathcal{M}$.

Once we have found such a p-dimensional integral element $(E^p)_x\subset T_x\mathcal{M}$ spanned by $V^1,\ldots,V^p$, we look for vectors $V_x^{p+1}\in T_x\mathcal{M}$ in such a way that the space generated by $(E^p)_x$ and V_x^{p+1} forms a $(p+1)$-dimensional integral element. The conditions on such a tangent vector V_x^{p+1} at the point $x\in\mathcal{M}$ are

$$\begin{aligned}
&\alpha^1_{i_1}(V_x^{p+1})=0, \quad 1\leqslant i_1\leqslant k_1,\\
&\alpha^2_{i_2}(V^{j_1},V_x^{p+1})=0, \quad 1\leqslant i_2\leqslant k_2, \quad 1\leqslant j_1\leqslant p,\\
&\vdots\\
&\alpha^{p+1}_{i_{p+1}}(V^1,V^2,\ldots,V^p,V_x^{p+1})=0, \quad 1\leqslant i_{p+1}\leqslant k_{p+1}.
\end{aligned} \tag{9}$$

The vectors V_x^{p+1} that satisfy the above system of linear equations generate the **polar space** $H((E^p)_x)^\perp$ of $(E^p)_x$, where $H((E^p)_x)$ is the polar system (9). Depending on the ranks of the polar systems generated, we can divide integral elements into three classes which are called **regular, ordinary**, and **singular**. We look at the subsystem $\alpha^1_1(V^1_x)=\cdots=\alpha^1_{k_1}(V^1_x)=0$ of (9), where $s_0(x)=r(H(E^0)_x)$ is its rank. From this, we obtain the integer

$$s_0:=\max_{\{x\in\mathcal{M}\}}(r(H((E^0)_x)))$$

called the **zeroth Cartan character**. We define a **regular point** $x\in\mathcal{M}$ to be a point where $s_0(x)=s_0$. Then, a one-dimensional integral element $(E^1)_x$ is an **ordinary** integral element if x is a regular point. Let the polar space of $(E^1)_x$ in $T_x\mathcal{M}$ have rank $r(H((E^1)_x))=s_1(x)+s_0(x)$. From this, we define

$$s_1:=\max_{\{x\in\mathcal{M},V^2\in T_x\mathcal{M}\}}r(H((E^1)_x))-s_0,$$

which is called the **first Cartan character**. If, for $x\in\mathcal{M}$, $s_1(x)=s_1$ holds, then the integral element $(E^1)_x$ is called **regular**. A two-dimensional integral element $(E^2)_x$ then is called **ordinary** if it contains at least one regular one-dimensional integral element. We define inductively as follows.

Definition 3: Cartan characters. The pth Cartan character is inductively defined as

$$s_p=\max_{\{x\in\mathcal{M},V^{p+1}\in T_x\mathcal{M}\}}r(H((E^p)_x))-\sum_{i=0}^{p-1}s_i.$$

Based on this we can state that a p-dimensional integral element $(E^p)_x$ is called **ordinary** if it contains at least one $(p-1)$-dimensional regular integral element. A p-dimensional integral element is called **regular** if its polar space $H((E^p)_x)$ has maximal rank $r(H((E)^p)_x)=s_p$. All other integral elements are called **singular**.

Note that a sequence of integral elements $(E^0)_x\subset(E^1)_x\subset\cdots\subset(E^p)_x$ at a point $x\in\mathcal{M}$ is called a **regular chain** of integral elements if all its $(E^k)_x$, $1\leqslant k\leqslant p-1$, are regular and $(E^p)_x$ is at least ordinary. The maximal dimension an ordinary integral element can adopt is called the **genus** g of Σ or $\mathcal{P}$. Integral elements are the tangent planes to manifolds which are solution manifolds for a given EDS Σ and Pfaffian systems $\mathcal{P}$ and defined as follows.

Definition 4: Integral manifolds. An integral manifold $\mathcal{N}$ of an EDS Σ on $\mathcal{M}$ is a p-dimensional submanifold $\mathcal{N}$ of $\mathcal{M}$ such that each k-dimensional vector subspace $(E^k)_x\subset T_x\mathcal{N}$ for $1\leqslant k\leqslant p$ annihilates all the k-forms in the EDS Σ.

C. Reduced characters and involution

If we wish to look for specific integral manifolds transversal to some given submanifold, we must introduce an **independence condition** $\Omega=\omega^1\wedge\cdots\wedge\omega^n\neq 0$, which is sometimes also called the *volume element*, where the ω^i are one-forms characterizing such a submanifold. If we select $x^1,\ldots,x^n$ as local independent coordinates, where we will use brackets to indicate powers of x^i such as in $(x^i)^n$, then Ω is given by $\Omega=dx^1\wedge\cdots\wedge dx^n$. All integral elements on which Ω *does not vanish* are called **admissible integral elements** according to Ref. 10 and we can define the following.

Definition 5: Involutive systems. An EDS with independence condition (Σ,Ω) *is in involution with respect to* Ω *at a point* $x\in\mathcal{M}$ *means that there exists an* **admissible ordinary** *integral element of dimension n of* (Σ,Ω) *at x.*

In order to determine the reduced characters, we need to introduce the **reduced polar systems** $H^{\mathrm{red}}((E^p)_x)$ which are defined as polar systems, where one suppresses all components involving $\omega^1,\ldots,\omega^n$ in each one-form of a given (9). We then define the reduced rank $s_0'(x)$ $:=r(H^{\mathrm{red}}((E^0)_x))$ and $s_0':=\max(_{\{x\in\mathcal{M}\}}s_0'(x))$ so that we can define the reduced characters inductively as follows.

Definition 6: Reduced Cartan characters. The reduced Cartan characters s_p' *are inductively defined as*

$$s_p':=\max(_{\{x\in\mathcal{M},V_x^{p+1}\in T_x\mathcal{M}\}}r(H^{\mathrm{red}}((E^p)_x)))-\sum_{i=0}^{p-1}s_i'\,.$$

For a Pfaffian system $(\mathcal{P},\Omega)$ the reduced Cartan characters can also be computed in the following way. Given a Pfaffian system $\mathcal{P}$ consisting of s one-forms θ^α with independence condition Ω $=\omega^1\wedge\cdots\wedge\omega^n\neq 0$, we denote by π^λ all the extra $N-s-n$ one-forms such that $(\theta^\alpha,\omega^i,\pi^\lambda)$, $1\leqslant\alpha\leqslant s$, form a coframe on our formal N-dimensional manifold $\mathcal{M}$. Once we have chosen such one-forms π^λ, we can write each $d\theta^\alpha$ as

$$d\theta^\alpha=A^\alpha_{\lambda i}\pi^\lambda\wedge\omega^i+\tfrac{1}{2}B^\alpha_{ij}\omega^i\wedge\omega^j+\tfrac{1}{2}C^\alpha_{\lambda\kappa}\pi^\lambda\wedge\pi^\kappa(\mathrm{mod}\mathcal{I}(\mathcal{P})),\tag{10}$$

where $\mathcal{I}(\mathcal{P})$ is the differential ideal generated by $\mathcal{P}$. In Eqs. (10), the terms $A^\alpha_{\lambda i}$ form the **tableau matrix** and we call the terms B^α_{ij} the **torsion terms**, where the notion of torsion here has nothing to do with affine connections. The Pfaffian system is called **quasi-linear** if all the $C^\alpha_{\lambda\kappa}=0$. We say that the torsion can be absorbed if a suitable transformation Φ

$$\Phi:\pi^\lambda\to\pi^\lambda+p_i^\lambda\omega^i$$

with

$$\tilde{B}^\alpha_{ij}=B^\alpha_{ij}+A^\alpha_{\lambda j}p_i^\lambda-A^\alpha_{\lambda i}p_j^\lambda\,,\tag{11}$$

can be found such that $\tilde{B}^\alpha_{ij}=0$. When $B^\alpha_{ij}\neq 0$ in every coframe $(\theta^\alpha,\omega^e,\pi^\lambda)$, the system possesses integrability conditions which will prevent it from being in involution. From the tableau matrix $A^\alpha_{\lambda i}$, we can determine the reduced Cartan characters directly[8,10] because $r(A^\alpha_{\lambda 1})=s_1'$ and the rank of

$$\begin{pmatrix}A^\alpha_{\lambda 1}\\A^\alpha_{\lambda 2}\end{pmatrix}$$

is equal to $s_1'+s_2'$ and so on. There are many versions of **Cartan's test for involution**,[9] some of which one can find in Refs. 8 and 10, and we state it as follows.

Theorem 1: *Cartan's test for involution. A Pfaffian system* $(\mathcal{P}, \Omega)$ *is in involution means that* $s_0 = s_0'$, $s_1 = s_1', \ldots, s_p = s_p'$ *and a coframe transformation can be found such that* **all** *its torsion terms* B_{ij}^{α} *vanish identically.*

An important question is whether and when ordinary integral manifolds exist and whether, given some initial data, they are unique. The **Cartan–Kähler theorems**[8,10] give some answers to these questions for real-analytic systems. They reduce to the **Cauchy–Kovalevskaya theorem** when the number of equations equals the number of unknowns given by m so that $n = m$.[20] The first Cartan–Kähler theorem specifies under which conditions a unique integral manifold of dimension p can be constructed from a $(p-1)$-dimensional one. The second theorem states that under certain conditions a chain of regular integral manifolds of increasing dimension exists.[8–10] If there is no general solution for a given EDS (Σ, Ω), then there could be identities or integrability conditions so that we must **prolong** the system by adding in these conditions and by enlarging the space of our formal jet coordinates to higher order, where in Refs. 8 and 10 a detailed account of this procedure can be found. The key result for prolongations in the real analytic case is given by the **Cartan–Kuranishi theorem** which states that an EDS (Σ, Ω) which is not in involution and not inconsistent becomes either involutive or inconsistent after a **finite** number of prolongations.[21]

Comment: We should point out that in Refs. 22–24 there is a quantity similar to the Cartan characters also introduced by Cartan[9] called the **degré d'arbitraire**. Einstein had introduced the **strength** of a system of equations in his last unified field theory of electromagnetism and gravity in order to measure how strongly such a system restricts the solution. A discussion between him and Cartan on this subject is presented in Ref. 25. Sué finally compared Cartan's degree of arbitrariness and Einstein's strength in Refs. 23 and 24 for linear systems of equations. Seiler derived a relation between this degree of arbitrariness and the Cartan characters for nonlinear, overdetermined higher-order systems of PDEs.[22]

Before we introduce Janet–Riquier theory, we illustrate the above theory with the example of a coordinate transformation to Euclidean coordinates in two dimensions. For the line element we therefore have

$$ds^2 = y^2 dx^2 + dy^2 = du^2 + dU^2,$$

where u, U are the Euclidean coordinates. For this to hold we must have

$$y^2 = p^2 + P^2, \quad 0 = pq + PQ, \quad 1 = q^2 + Q^2,$$

where we introduced the Monge notation

$$p := \frac{\partial u}{\partial x}, \quad q := \frac{\partial u}{\partial y}, \quad r := \frac{\partial^2 u}{\partial x^2}, \quad s := \frac{\partial^2 u}{\partial x \partial y}, \quad t := \frac{\partial^2 u}{\partial y^2},$$

$$P := \frac{\partial U}{\partial x}, \quad Q := \frac{\partial U}{\partial y}, \quad R := \frac{\partial^2 U}{\partial x^2}, \quad S := \frac{\partial^2 U}{\partial x \partial y}, \quad T := \frac{\partial^2 U}{\partial y^2}.$$

These are local coordinates on a jet bundle $\mathcal{J}^2(\mathbb{R}^2, \mathbb{R}^2)$ with $N = 2 + 2 + 4 + 6 = 14$ formal dimensions, where we have $n = 2$ independent and $m = 2$ dependent variables. After differentiating the above equations, we obtain a Pfaffian system $\mathcal{P}$ with $s = 12$ independent one-forms which can locally be expressed as

$$\theta^1 = du - p\,dx - q\,dy,$$

$$\theta^2 = dU - P\,dx - Q\,dy,$$

$$\theta^3 = dp - r\,dx - s\,dy,$$

$$\theta^4 = dP - R\,dx - S\,dy,$$

$$\begin{aligned}
\theta^5 &= dq - s\,dx - t\,dy,\\
\theta^6 &= dQ - S\,dx - T\,dy,\\
\theta^7 &= p\,dr + r\,dp + P\,dR + R\,dP,\\
\theta^8 &= q\,dr + r\,dq + Q\,dR + R\,dQ + dy,\\
\theta^9 &= p\,ds + s\,dp + P\,dS + S\,dP - dy,\\
\theta^{10} &= q\,ds + s\,dq + Q\,dS + S\,dQ,\\
\theta^{11} &= p\,dt + t\,dp + P\,dT + T\,dP,\\
\theta^{12} &= q\,dt + t\,dq + Q\,dT + T\,dQ.
\end{aligned} \tag{12}$$

As the rank of $\mathcal{D}$ is $N-s=14-12=2$, where $s=12$, the system (12) can dually be characterized by two Vessiot vector fields V^1, V^2 generating $\mathcal{D}$, where

$$\begin{aligned}
V^i = {} & V^i_x\frac{\partial}{\partial x} + V^i_y\frac{\partial}{\partial y} + (pV^i_x + qV^i_y)\frac{\partial}{\partial u} + (PV^i_x + QV^i_y)\frac{\partial}{\partial U} + (rV^i_x + sV^i_y)\frac{\partial}{\partial p} + (RV^i_x + SV^i_y)\frac{\partial}{\partial P}\\
& + (sV^i_x + tV^i_y)\frac{\partial}{\partial q} + (SV^i_x + TV^i_y)\frac{\partial}{\partial Q} + V^i_r\frac{\partial}{\partial r} + V^i_R\frac{\partial}{\partial R} + V^i_s\frac{\partial}{\partial s} + V^i_S\frac{\partial}{\partial S} + V^i_t\frac{\partial}{\partial t} + V^i_T\frac{\partial}{\partial T},
\end{aligned}$$

$$i=1,2, \tag{13}$$

and the coefficients V^i_r, V^i_R, V^i_s, V^i_S, V^i_t, V^i_T are determined through the condition that the six one-forms $\theta^7,\ldots,\theta^{12}$ are annihilated by V^1, V^2. Because here we have $d\theta^\alpha(V^1,V^2)\equiv 0$, we find that the system (12) is *complete*. It means that $C(\mathcal{P})=\mathcal{D}$ so that $c=2$ and, therefore, both V^1 and V^2 are Cauchy characteristics. They form an involution of maximal dimension $g=2$ and because $s=12$ and $s=s_0=s_0'$, then $s_0=s_0'=12$. We see that $t=\partial^2 u/\partial y^2=0$ and $T=\partial^2 U/\partial y^2=0$ so that the solution must be linear in y. The general solution is then given by

$$\begin{aligned}
u &= y\cos(x+\epsilon)+a, & U &= y\sin(x+\epsilon)+b,\\
p &= -y\sin(x+\epsilon), & P &= y\cos(x+\epsilon),\\
q &= \cos(x+\epsilon), & Q &= \sin(x+\epsilon),\\
r &= -y\cos(x+\epsilon), & R &= -y\sin(x+\epsilon),\\
s &= -\sin(x+\epsilon), & S &= \cos(x+\epsilon),\\
t &= 0, & T &= 0,
\end{aligned}$$

where $\{a,b,\epsilon\}$ are arbitrary constants corresponding to the translational and rotational degrees of freedom. This also gives a local parametrization of the two-dimensional integral manifold which corresponds to this solution.

III. JANET–RIQUIER THEORY

In the original Janet–Riquier theory of systems of partial differential equations (PDEs), there was an algorithm created to explain how a given system of PDEs could be brought into passive orthonomic form. Passivity is the *absence* of integrability conditions and orthonomicity is a form of *ordering* of the partial derivatives of a system. The passive orthonomic system of a system of PDEs was the predecessor of what is now called a formally integrable system or involutory system of PDEs. A theory created by Riquier[26] and developed by Janet[27,28] and later by Thomas [29] now called Janet–Riquier theory helps to decide such questions. A good account of this theory as in the

form as created in Refs. 26, 27 and 29 is given in Russian by S. P. Finikov.[30] In order to obtain intrinsic results Spencer[31] and then Goldschmidt[32] introduced a new coordinate independent approach based on homological algebra. An account of this theory can be found in Ref. 33.

There are many algorithms which have been implemented by algebraic computing. Some of them are concerned with the choice of particular rankings such as the REDUCE package DINV by Gerdt.[34] Reid[35] developed a computer package based on MAPLE which brings a system into *solved form*, which is a modification of an orthonomic system.[36] Seiler[22,37] uses the theory of the involutive symbol, which is a modernized version of the original Janet–Riquier theory, to determine whether systems are in involution. Janet–Riquier theory is well illustrated by the Janet example[28,33,37] and applications to general relativity have previously been made such as in Refs. 38–40.

For a system of partial differential equations (=system of PDEs) of order q, which we will denote by $\mathcal{R}_q$ from now on, we use $x^1,\ldots,x^n$ for the independent variables, where we will use brackets to indicate powers of any x^i such as in $(x^i)^n$, and u^α for the m dependent variables. Their derivatives on the jet bundle of order q, denoted by $\mathcal{J}^q(\mathbb{R}^n,\mathbb{R}^m)$, are denoted by $u^\alpha_{,J}$, where J is a multi-index. We associate a **monomial** $x^J=(x^1)^{j_1}\cdot\cdots\cdot(x^n)^{j_n}$ with each partial derivative $u^\alpha_{,J}$, where $J=(j_1,\ldots,j_n)$ is a **multi-index** and $\|J\|=j_1+\ldots+j_n$ is the order of the derivative. This means that to each set of partial derivatives of each dependent variable u^α corresponds a unique set of monomials.

Then, we **order the partial derivatives** of a system of PDEs in a systematic way. Very often we will use an inverse lexicographic ordering based on $x^n>\ldots>x^2>x^1$ on their partial derivatives so that $u_{,n}>\ldots>u_{,2}>u_{,1}$ and so on. A **ranking** amongst *all* partial derivatives is defined as follows.

Definition 7: Ranking of derivatives. A ranking of derivatives is a total ordering $\mathcal{R}_>$ of all the partial derivatives $u^\alpha_{,J}$ (for m, n fixed) satisfying the two following conditions (where J and K are multi-indices).

(i) *If $\|J\|>\|K\|$, then $u^\alpha_{,J}>u^\alpha_{,K}$.*
(ii) *If $u^\alpha_{,J^1}>u^\alpha_{,J^2}$, then $(u^\alpha_{,J^1})_{,K}>(u^\alpha_{,J^2})_{,K}$ for any multi-index K.*

A special subclass of these rankings are called **orderly rankings** which are rankings such that (*i*) holds for different indices α referring to different unknowns u^α (see Ref. 41 for more details). Then, the system can be brought into a more organized form called **orthonomic form**. This is achieved by determining the partial derivative highest in the ranking in each equation of $\mathcal{R}_q$ and calling it the **leading** derivative of the equation. Once this equation is solved for its leading derivative which then becomes the only term on its LHS, we call it a **principal** derivative. All other partial derivatives of that order which are not in the set of principal derivatives are called **parametric derivatives**. Based on this we can define an orthonomic system.

Definition 8: Orthonomic system. A system of partial differential equations $\mathcal{R}_q$ of order q is orthonomic with respect to a given ranking $\mathcal{R}_>$ if

(i) *all the PDEs are solved with respect to their leading derivatives*;
(ii) *no two leading derivatives are the same; and*
(iii) *no parametric derivative in any equation of $\mathcal{R}_q$ can be a principal derivative in another equation of $\mathcal{R}_q$ or even a partial derivative of any order of a principal derivative.*

Those independent variables by means of which we can differentiate the principal derivative of an equation without reintroducing a derivative already produced by means of differentiating another principal derivative are called **multiplicative variables** for the equation. This induces multiplicative variables for the monomials corresponding to the partial derivatives.[33] To avoid nonintrinsic results, one introduces special coordinates called **δ-regular coordinates** and uses the theory of the **involutive symbol** of a system $\mathcal{R}_q$ which we will introduce next.

A. Involutive symbol and formal integrability

In order to determine the **symbol** of a system of PDEs only the highest-order partial derivatives of each equation in $\mathcal{R}_q$ matter. We denote the quantities corresponding to each partial derivative $u^{\alpha}_{,J}$ by V^{α}_{J} and define the symbol $\mathcal{M}_q$ as follows.

Definition 9: Symbol of $\mathcal{R}_q$. A system of partial differential equations $\mathcal{R}_q$ of order q, locally described by p equations in solved form as $\Phi^{\tau}(x^i,u^{\alpha},u^{\alpha}_{,J})=0$ for $\tau=1,...,p$, has a solution space $\mathcal{M}_q$ for the unknowns V^{α}_{J} with $\alpha=1,...,m$, $\|J\|=q$:

$$\mathcal{M}_q:\sum_{\alpha,\|J\|=q}\left(\frac{\partial\Phi^{\tau}}{\partial u^{\alpha}_{,J}}\right)V^{\alpha}_{J}=0, \tag{14}$$

where we formally differentiate with respect to the $u^{\alpha}_{,J}$. $\mathcal{M}_q$ is called the **symbol of** $\mathcal{R}_q$.

For simplicity the matrix rather than the map is usually regarded as the symbol of $\mathcal{R}_q$. We associate with each symbol equation its multiplicative variables which are the same as the multiplicative variables which its corresponding equation in $\mathcal{R}_q$ adopts. Then, we determine the **class of an equation** in $\mathcal{M}_q$ by counting the number of multiplicative variables it adopts—a number denoted by k such that $0\leqslant k\leqslant n$—and define

$$\beta^{(k)}_{q}:=\text{number of equations of class } k \text{ in } \mathcal{M}_q(\text{or}\mathcal{R}_q).$$

The definition of the **Cartan characters** $\alpha^{(k)}_{q}$ is based on the $\beta^{(k)}_{q}$ and is given by

$$\alpha^{(k)}_{q}:=m\cdot\binom{n+q-k-1}{q-1}-\beta^{(k)}_{q}, \tag{15}$$

where $m\cdot\Sigma_{k=1}^{n}\binom{n+q-k-1}{q-1}$ is the total number of partial derivatives of order q that a system $\mathcal{R}_q$ will have. Earlier in this article, we denoted the $n+1$ Cartan characters of an EDS by s_k, $k=0,1,2,\ldots,n$ but here we write s_k, $k,=1,2,\ldots,n$ as $\alpha^{(k)}_{q}$ as Janet–Riquier theory does not give s_0. In δ-regular coordinates $\alpha^{(k)}_{q}$ equals the number of parametric derivatives of class k and order q. When no identities are present, the symbol is said to be involutive, which can be equivalently expressed as[33] follows.

Theorem 2: *Involutive symbol. In a δ-regular coordinate system the following conditions are equivalent*:

(i) *The symbol $\mathcal{M}_q$ is involutive.*
(ii) $\dim(\mathcal{M}_{q+1})=\Sigma^{n}_{k=1}k\cdot\alpha^{(k)}_{q}$.
(iii) *The rank r of $\mathcal{M}_{q+1}$ is* $r(\mathcal{M}_{q+1})=\Sigma^{n}_{k=1}k\cdot\beta^{(k)}_{q}$.
(iv) *Prolongation with respect to* **nonmultiplicative variables** *does not lead to any new equations.*

But a system of equations $\mathcal{R}_q$ which has an involutive symbol $\mathcal{M}_q$ can still admit integrability conditions. They can be revealed by means of projecting our prolonged system $\mathcal{R}_{q+1}$, which is obtained by differentiating $\mathcal{R}_q$ with respect to all its n independent variables, back onto $\mathcal{R}_q$. In general, we will denote first projections onto lower-order systems by $\mathcal{R}^{(1)}_{q+r}=\pi^{(q+r+1)}_{q+r}(\mathcal{R}_{q+r+1})$. If $\mathcal{R}^{(1)}_{q}$ is not identical to $\mathcal{R}_q$, then integrability conditions occur. If they are identical we can characterize a *formally integrable system* $\mathcal{R}_q$ as[33,37] a system of partial differential equations $\mathcal{R}_q$ for which $\mathcal{R}^{(1)}_{q+r}=\mathcal{R}_{q+r}$ for all $r\geqslant 0$. A special situation occurs when $\mathcal{M}_q$ is involutive *and* $\mathcal{R}_q$ is formally integrable.[37] Then, we obtain ideal systems of equations which are called involutive systems of equations.

Definition 10: Involutive systems of equations. A system of equations $\mathcal{R}_q$ is involutive if and only if its symbol $\mathcal{M}_q$ is involutive and $\mathcal{R}_q$ is formally integrable.

There exists an important criterion for involution that tells us that we only need to prolong once for an involutive system to prove this:

Theorem 3: *Criterion for involution. $\mathcal{R}_q$ is a system in involution means that its symbol $\mathcal{M}_q$ is involutive and $\mathcal{R}^{(1)}_{q}=\mathcal{R}_q$.*

We will now apply the above theory to the Riemann–Lanczos problem.

IV. THE RIEMANN–LANCZOS PROBLEM

In the Bampi–Caviglia papers[4,5] the Riemann–Lanczos problem in four dimensions was written as an EDS. Here we are going to introduce a Pfaffian system based on (8) which differs slightly from that in Ref. 4 because we incorporate the cyclic conditions (2) as well. Independently of the space–time dimension n, we can use the exterior differentials of Eqs. (8) in solved form together with the *contact conditions* K_{abc} to obtain the system

$$\begin{aligned} df^{(R)}_{abcd} &= (R_{abcd,e}+\alpha_{abcde})dx^e - dP_{abcd}+dP_{abdc}-dP_{cdab}+dP_{cdba}+\Gamma^n_{ad}(dL_{nbc}+dL_{ncb}) \\ &\quad -\Gamma^n_{ac}(dL_{nbd}+dL_{ndb})+\Gamma^n_{bc}(dL_{nad}+dL_{nda})-\Gamma^n_{bd}(dL_{nac}+dL_{nca}), \\ K_{abc} &= dL_{abc}-P_{abce}dx^e, \\ dK_{abc} &= dx^e\wedge dP_{abce}, \end{aligned} \tag{16}$$

where α_{abcde} is given by

$$\alpha_{abcde}=\Gamma^n_{ad,e}(L_{nbc}+L_{ncb})-\Gamma^n_{ac,e}(L_{nbd}+L_{ndb})+\Gamma^n_{bc,e}(L_{nad}+L_{nda})-\Gamma^n_{bd,e}(L_{nac}+L_{nca}). \tag{17}$$

The (x^a, L_{abc}, P_{abcd}) are local jet coordinates on $\mathcal{J}^1(\mathbb{R}^n,\mathbb{R}^m)$ with $P_{abcd}=\partial L_{abc}/\partial x^d$ when projected onto our space–time manifold and m is the number of independent Lanczos components L_{abc}. A Vessiot vector field $V\in\mathcal{D}$ is then locally given as

$$V=V^e\frac{\partial}{\partial x^e}+V^eP_{abce}\frac{\partial}{\partial L_{abc}}+V_{abcd}\frac{\partial}{\partial P_{abcd}}, \tag{18}$$

where m of the $n\cdot m$ components V_{abcd} are defined through the requirement that $df^{(R)}_{abcd}(V)=0$. This leads to the m independent equations

$$\begin{aligned} V_{\{abcd\}} &= V^e[R_{abcd,e}+\alpha_{abcde}+\Gamma^n_{ad}(P_{nbce}+P_{ncbe})-\Gamma^n_{ac}(P_{nbde}+P_{ndbe})+\Gamma^e_{bc}(P_{nade}+P_{ndae}) \\ &\quad -\Gamma^n_{bd}(P_{nace}+P_{ncae})], \end{aligned} \tag{19}$$

where $\{abcd\}$ denotes the Riemann-type symmetrization performed over the indices $abcd$. Before we comment on the Riemann–Lanczos problem in four dimensions, we look at the two- and three-dimensional cases.

A. The Riemann–Lanczos problem in two dimensions

First, we consider the Riemann–Lanczos problem in a two-dimensional space–time. In two space–time dimensions there is only one independent Riemann–Lanczos equation $f^{(R)}_{1212}$. We have two given independent variables x^1, x^2, two dependent variables L_{121}, L_{122} and four Monge derivatives P_{1211}, P_{1212}, P_{1221}, P_{1222} so that $(x^1,x^2,L_{121},L_{122},P_{1211},P_{1212},P_{1221},P_{1222})$ are local coordinates on the jet bundle $\mathcal{J}^1(\mathbb{R}^2,\mathbb{R}^2)$ with $N=2+2+4=8$. We leave the metric tensor components completely arbitrary so that $f^{(R)}_{1212}$ is given as

$$f^{(R)}_{1212}=R_{1212}-2P_{1212}+2P_{1221}+2L_{121}(\Gamma^1_{12}-\Gamma^2_{22})-2L_{122}(\Gamma^1_{11}+\Gamma^2_{12})=0. \tag{20}$$

We define α_{1212e} in the two-dimensional case to be

$$\alpha_{1212e}=R_{1212,e}-2L_{121}(\Gamma^1_{12,e}-\Gamma^2_{22,e})-2L_{122}(\Gamma^1_{11,e}+\Gamma^2_{12,e}), \tag{21}$$

where $e=1,2$. The Pfaffian system derived from (20) is locally given by

$$\theta^1=\alpha_{12121}dx^1+\alpha_{12122}dx^2-2dP_{1212}+2dP_{1221}+2(\Gamma^1_{12}-\Gamma^2_{22})dL_{121}-2(\Gamma^1_{11}+\Gamma^2_{12})dL_{122},$$

$$\theta^2=dL_{121}-P_{1211}dx^1-P_{1212}dx^2, \tag{22}$$

$$\theta^3=dL_{122}-P_{1221}dx^1-P_{1222}dx^2,$$

where θ^1 is the exterior derivative of $f^{(R)}_{abcd}$ and θ^2, θ^3 are the two contact conditions and $d\theta^2$, $d\theta^3$ their exterior derivatives. The zeroth character is $s_0=3$, since we only have to count the number of one-forms in (22). Omitting all the terms involving dx^1, dx^2 in the one-forms in (22), the same number is obtained so that $s_0'=3$, leading to our first result $s_0=s_0'=3$. Further characters were obtained to be $s_1=s_1'=2$ and $s_2=s_2'=1$. A detailed discussion of the polar systems and their Cartan characters for this case can be found in Ref. 42.

We can also compute the characters using the tableau, and by determining the torsion we then find out whether the system possesses integrability conditions. In order to form a complete coframe for our example (22), we have to add three one-forms π^Λ, where Λ now is a *collective index* with $\Lambda\in\{1211,1221,1222\}$, to the five one-forms θ^1, θ^2, θ^3, ω^1, ω^2 and so we choose

$$\pi_{1211}:=dP_{1211},\quad \pi_{1221}:=dP_{1221},\quad \pi_{1222}:=dP_{1222}.$$

The dP_{1212} can be expressed through θ^1 as

$$dP_{1212}=\pi_{1221}+((\tfrac{1}{2}\alpha_{12121}+(\Gamma^1_{12}-\Gamma^2_{22})(P_{1211}-(\Gamma^1_{11}+\Gamma^2_{12})P_{1221}))\omega^1$$
$$+((\tfrac{1}{2}\alpha_{12122}+(\Gamma^1_{12}-\Gamma^2_{22})(P_{1212}-(\Gamma^1_{11}+\Gamma^2_{12})P_{1222}))\omega^2(\mathrm{mod}\ \{\theta^\alpha\}). \tag{23}$$

Having accomplished this, we can then expand the exterior derivatives of the contact conditions as

$$d\theta^1\equiv 0,$$

$$d\theta^2\equiv-\pi_{1211}\wedge\omega^1-\pi_{1221}\wedge\omega^2+((\tfrac{1}{2}\alpha_{12121}+(\Gamma^1_{12}-\Gamma^2_{22})P_{1211}-(\Gamma^1_{11}+\Gamma^2_{12})P_{1221}))\omega^1\wedge\omega^2, \tag{24}$$

$$d\theta^3\equiv-\pi_{1221}\wedge\omega^1-\pi_{1222}\wedge\omega^2\quad(\mathrm{mod}\ \mathcal{I}(\mathcal{P})).$$

Therefore, we obtain for the tableau matrices

$$A^\alpha_{\Lambda 1}=\begin{pmatrix}0&0&0\\-1&0&0\\0&-1&0\end{pmatrix},\quad A^\alpha_{\Lambda 2}=\begin{pmatrix}0&0&0\\0&-1&0\\0&0&-1\end{pmatrix},$$

where $\alpha=1,2,3$ and Λ is one of the collective indices $\Lambda\in\{1211,1221,1222\}$. This leads to $s_1'=2$, $s_2'=1$, and the only nonvanishing torsion term is given by

$$B^2_{12}=-[\tfrac{1}{2}\alpha_{12121}-(\Gamma^1_{12}-\Gamma^2_{22})P_{1211}+(\Gamma^1_{11}+\Gamma^2_{12})P_{1221}]. \tag{25}$$

If we wish to absorb the torsion coefficients, we must find a transformation Φ with $\pi^\lambda\to\pi^\lambda+p^\lambda_i\omega^i$ and quantities p^λ_i such that

$$0=\tilde{B}^\alpha_{ij}=B^\alpha_{ij}+A^\alpha_{\lambda j}p^\lambda_i-A^\alpha_{\lambda i}p^\lambda_j.$$

In our case this leads to the system

$$0=A^1_{\Lambda 2}p^\Lambda_1-A^1_{\Lambda 1}p^\Lambda_2,$$

$$0 = B^2_{12} + A^2_{\Lambda 2} p^\Lambda_1 - A^2_{\Lambda 1} p^\Lambda_2 , \tag{26}$$

$$0 = A^3_{\Lambda 2} p^\Lambda_1 - A^3_{\Lambda 1} p^\Lambda_2 .$$

One solution *ansatz* to fulfill (26) is to choose $p^2_1 := B^2_{12}$ while all other p^Λ_i vanish: thus the torsion is absorbed and the system is therefore in involution.[9,10] Adding the exterior derivative of the differential gauge condition $L_{12}{}^s{}_{;s} = 0$ does not change the involutivity. Obviously then $s_0 = s'_0 = 4$ so that the set of Cartan characters (s_0, s_1, s_2) in this case is given by (4, 2, 0). Detailed calculations and a REDUCE code are given in Ref. 42.

Next, we use Janet–Riquier theory to reproduce these results. We have a system of equations $\mathcal{R}_1$ with $n = m = 2$, $q = 1$ and the symbol $\mathcal{M}_1$ consists only of a single equation

$$-2V_{1212} + 2V_{1221} = 0, \tag{27}$$

which is of class 2 whatever the choice of the orderly ranking. (Note that here and in subsequent sections, where Janet–Riquier theory is applied, the *symbol variables* V_{abcd}, V_{abcde} have no connection with Vessiot vector fields V.) This yields

$$\alpha^{(1)}_1 = 2, \quad \alpha^{(2)}_1 = 1.$$

Trivially, all variables are multiplicative variables and the symbol of one equation is always involutive. We have $\dim(\mathcal{R}_1) = 5$ and $\dim(\mathcal{M}_1) = 3$ and our prolonged system of equations $\mathcal{R}_2$ consists of $f^{(R)}_{1212}$, $f^{(R)}_{1212,1}$, $f^{(R)}_{1212,2}$. No integrability conditions can be created because

$$\dim(\mathcal{R}^{(1)}_1) = \dim(\mathcal{R}_2) - \dim(\mathcal{M}_2) = 9 - 4 = 5 = \dim(\mathcal{R}_1),$$

and the system is linear so that formal integrability is demonstrated and the system $\mathcal{R}_1$ is involutive.

If we incorporate the differential gauge condition $L_{ab}{}^s{}_{;s} = 0$, then $\mathcal{M}_1$ is formed by

$$\begin{aligned} -2V_{1212} + 2V_{1221} &= 0, \\ g^{11}V_{1211} + g^{12}V_{1221} + g^{12}V_{1212} + g^{22}V_{1222} &= 0, \end{aligned} \tag{28}$$

which again has all its equations of class 2 whatever the choice of the orderly ranking be and so we obtain $\alpha^{(1)}_1 = 2$, $\alpha^{(2)}_1 = 0$. The result is that $\mathcal{R}_1$ is formally integrable and involutive.[42] We conclude that *the Riemann–Lanczos problem in two dimensions is always in involution and the differential gauge condition does not affect the result*. The Cartan characters (s_0, s_1, s_2) are (3, 2, 1) when no differential gauge condition is imposed but (4, 2, 0) when it is imposed.

We can give the general solution for the two-dimensional Riemann–Lanczos problem explicitly. First, we look at the general two-dimensional space–time with Lorentzian signature and line element in characteristic coordinates x^1, x^2 written as

$$ds^2 = -e^{2\rho} dx^1 dx^2,$$

where ρ is an arbitrary function of x^1, x^2. We find that the general solution is of the form

$$\begin{aligned} L_{121} &= e^{2\rho} f_1(x^1) - \tfrac{1}{4} e^{2\rho} \rho_{,x^1}, \\ L_{122} &= e^{2\rho} f_2(x^2) + \tfrac{1}{4} e^{2\rho} \rho_{,x^2}, \end{aligned} \tag{29}$$

where $f_1(x^1)$, $f_2(x^2)$ are two arbitrary functions depending on one local coordinate each. This is in agreement with the result for the Cartan characters claiming that the general solution depends on two arbitrary functions of one variable each. The symbol derived from $f^{(R)}_{1212}$, $L_{12}{}^s{}_{;s}$ is

$$0 = -2V_{1212} + 2V_{1221},$$
$$0 = -V_{1212} - V_{1221}, \tag{30}$$

from which we obtain $\beta_1^{(1)} = \beta_1^{(2)} = 1$ based on the ranking stemming from $x^2 \succ x^1$. This leads to $\alpha_1^{(1)} = \alpha_1^{(2)} = 1$, which **cannot be** the intrinsic result as we already solved the two-dimensional problem in the previous section. We conclude that the above coordinate frame is not δ-regular and we need to perform a coordinate transformation of the form

$$d\tilde{x}^1 = a_{11}dx^1 + a_{12}dx^2, \quad d\tilde{x}^2 = a_{21}dx^1 + a_{22}dx^2$$

in order to obtain the correct values for $\alpha_1^{(1)}$, $\alpha_1^{(2)}$. After such a transformation, the new symbol in orthonomic form is

$$V_{1222} = -\frac{a_{21}}{a_{22}} V_{1221},$$
$$V_{1212} = -\frac{a_{11}}{a_{12}} V_{1211}. \tag{31}$$

Now, both equations are of class 2 so that $\beta_1^{(1)} = 0$, $\beta_1^{(2)} = 2$, which produces $\alpha_1^{(1)} = 2$, $\alpha_1^{(2)} = 0$ which is the known intrinsic result for the Cartan characters.

For spaces with Euclidean signature we can write their line element as

$$ds^2 = e^{2\rho}((dx^1)^2 + (dx^2)^2),$$

where ρ is again an arbitrary function of x^1, x^2. We obtain the solution

$$L_{121} = e^{2\rho}(f_1(x^1 + x^2) - \tfrac{1}{2}\rho_{,x^2}),$$
$$L_{122} = e^{2\rho}(f_2(x^1 - x^2) + \tfrac{1}{2}\rho_{,x^1}), \tag{32}$$

and the intrinsic values for the characters are $\alpha_1^{(1)} = 2$, $\alpha_1^{(2)} = 0$.

B. The Riemann–Lanczos problem in three dimensions

In three space–time dimensions with local coordinates x^1, x^2, x^3, we obtain eight independent components of the Lanczos tensor, namely, L_{121}, L_{122}, L_{131}, L_{133}, L_{232}, L_{233}, L_{123}, L_{132} when imposing the cyclic conditions (2). Each of them has three first-order partial derivatives so that we use the jet bundle $\mathcal{J}^1(\mathbb{R}^3, \mathbb{R}^8)$ with formal dimension $N = 3 + 8 + 8 \cdot 3 = 35$ to express the EDS. We obtain the six independent Riemann–Lanczos equations whose exterior derivatives are $df_{1212}^{(R)}$, $df_{1313}^{(R)}$, $df_{2323}^{(R)}$, $df_{1213}^{(R)}$, $df_{1223}^{(R)}$, $df_{1323}^{(R)}$. We find that the Riemann–Lanczos problem in three dimensions is not in involution and its reduced characters (s_0', s_1', s_2', s_3') are (14, 8, 7, 3), where detailed calculations can be found in Ref. 42. We can test this result with the REDUCE code given in Ref. 42 and immediately obtain (8, 7, 3) for the reduced characters (s_1', s_2', s_3') and that the system is not in involution. It is sufficient to use an *arbitrary diagonalized line element* which describes three-dimensional space–times completely as is shown in Ref. 43.

We can also use the tableau matrix to calculate this result. First, we must complete our set of 14 one-forms together with the three ω^e to a complete coframe consisting of $N = 35$ elements by introducing the 18 π^Λ such that $(df_{abcd}^{(R)}, K_{abc}, \omega^e, \pi^\Lambda)$ forms a cobasis on $\mathcal{M}$. We introduce the 18 π^Λ using collective indices Λ with $\Lambda = 1,...,18$ with the following correspondence between $\pi^\Lambda \leftrightarrow dP_{abcd}$:

$$\pi^1 \leftrightarrow dP_{1211}, \quad \pi^2 \leftrightarrow dP_{1221}, \quad \pi^3 \leftrightarrow dP_{1311},$$

$$\pi^4 \leftrightarrow dP_{1331}, \quad \pi^5 \leftrightarrow dP_{2321}, \quad \pi^6 \leftrightarrow dP_{2331},$$

$$\pi^7 \leftrightarrow dP_{1231}, \quad \pi^8 \leftrightarrow dP_{1321}, \quad \pi^9 \leftrightarrow dP_{1222},$$

$$\pi^{10} \leftrightarrow dP_{1312}, \quad \pi^{11} \leftrightarrow dP_{1332}, \quad \pi^{12} \leftrightarrow dP_{2322},$$

$$\pi^{13} \leftrightarrow dP_{2332}, \quad \pi^{14} \leftrightarrow dP_{1232}, \quad \pi^{15} \leftrightarrow dP_{1322},$$

$$\pi^{16} \leftrightarrow dP_{1333}, \quad \pi^{17} \leftrightarrow dP_{2333}, \quad \pi^{18} \leftrightarrow dP_{1233}.$$

When using the correspondence $\theta^\alpha \leftrightarrow K_{abc}$ the eight dK_{abc} can be recast as

$$\begin{aligned}
d\theta^1 &\equiv -\pi^1\wedge\omega^1 - \pi^2\wedge\omega^2 - \pi^7\wedge\omega^3 + \pi^{10}\wedge\omega^3 - \pi^8\wedge\omega^3 + \tfrac{1}{2}B^1_{i2}\omega^i\wedge\omega^2 + \tfrac{1}{2}B^1_{i3}\omega^i\wedge\omega^3,\\
d\theta^2 &\equiv -\pi^2\wedge\omega^1 - \pi^9\wedge\omega^2 - 2\pi^{14}\wedge\omega^3 - \pi^5\wedge\omega^3 + \tfrac{1}{2}B^2_{i3}\omega^i\wedge\omega^3,\\
d\theta^3 &\equiv -\pi^3\wedge\omega^1 - \pi^{10}\wedge\omega^2 - \pi^4\wedge\omega^3 + \tfrac{1}{2}B^3_{i3}\omega^i\wedge\omega^3,\\
d\theta^4 &\equiv -\pi^4\wedge\omega^1 - \pi^{11}\wedge\omega^2 - \pi^{16}\wedge\omega^3,\\
d\theta^5 &\equiv -\pi^5\wedge\omega^1 - \pi^{12}\wedge\omega^2 - \pi^{13}\wedge\omega^3 + \tfrac{1}{2}B^5_{i3}\omega^i\wedge\omega^3,\\
d\theta^6 &\equiv -\pi^6\wedge\omega^1 - \pi^{13}\wedge\omega^2 - \pi^{17}\wedge\omega^3,\\
d\theta^7 &\equiv -\pi^7\wedge\omega^1 - \pi^{14}\wedge\omega^2 - \pi^{18}\wedge\omega^3,\\
d\theta^8 &\equiv -\pi^8\wedge\omega^1 - \pi^{15}\wedge\omega^2 - \tfrac{1}{2}\pi^{11}\wedge\omega^3 - \tfrac{1}{2}\pi^8\wedge\omega^3 - \tfrac{1}{2}\pi^6\wedge\omega^3 + \tfrac{1}{2}B^8_{i3}\omega^i\wedge\omega^3 \pmod{\mathcal{I}(\mathcal{P})}.
\end{aligned} \tag{33}$$

Using the tableau matrices derived from (33) we obtain $s_1' = 8$, $s_2' = 7$ and $s_3' = 3$. We also find that all remaining torsion coefficients B^α_{ij} in (33) can be absorbed so that no integrability conditions occur at this stage. However, because we have the rank deficiency in the reduced polar matrix leading to $s_2 = s_2' + 1$, the system admits an identity and is **not in involution**. This makes prolongation necessary, but the process of prolongation often becomes simpler when Janet–Riquier theory is used in the way that we now show.

The symbol $\mathcal{M}_1$ for the unprolonged Riemann–Lanczos problem in three dimensions consists of the six linear equations derived from $f^{(R)}_{1212}$, $f^{(R)}_{1313}$, $f^{(R)}_{2323}$, $f^{(R)}_{1213}$, $f^{(R)}_{1223}$, $f^{(R)}_{1323}$ and is given in orthonomic form as (where nonmultiplicative variables are indicated by a $\cdot$)

$$\begin{aligned}
&V_{1212} = V_{1221} && x^1x^2\cdot\\
&V_{1313} = V_{1331} && x^1x^2x^3\\
&V_{2323} = V_{2332} && x^1x^2x^3\\
&V_{1213} = V_{1231} - V_{1312} + V_{1321} && x^1x^2x^3\\
&V_{1223} = 2V_{1232} - V_{1322} + V_{2321} && x^1x^2x^3\\
&V_{1323} = \frac{1}{2}(V_{1332} + V_{1233} + V_{2331}) && x^1x^2x^3.
\end{aligned}$$

We imposed the ranking $x^3 \succ x^2 \succ x^1$ which then induced the ranking $P_{abc3} \succ P_{abc2} \succ P_{abc1}$ and amongst each set P_{abce} the ranking $P_{233e} \succ P_{232e} \succ P_{132e} \succ P_{123e} \succ P_{133e} \succ P_{131e} \succ P_{122e} \succ P_{121e}$. From this we now obtain $\beta^{(1)}_1 = 0$, $\beta^{(2)}_1 = 1$, $\beta^{(3)}_1 = 5$ and $\alpha^{(1)}_1 = 8$, $\alpha^{(2)}_1 = 7$, $\alpha^{(3)}_1 = 3$. The above results are intrinsic because we used δ-regular coordinates.[42]

In order to see whether the symbol is involutive, we differentiate each equation with respect to x^1, x^2, x^3 from which we can produce $\mathcal{M}_2$, where its sparse coefficient matrix is given and explained in detail in Ref. 42. We obtain $r(\mathcal{M}_2)=18$ which does not coincide with the total number of multiplicative variables

$$\sum_{k=1}^{3} k\cdot\beta_1^{(k)}=17\neq r(\mathcal{M}_2)=18,$$

so that $\mathcal{M}_1$ is it not involutive. Therefore, we prolong $\mathcal{R}_1$ to $\mathcal{R}_2$ which consists of 24 equations, 18 of which are the partial derivatives S_{abcde} of the six $f^{(R)}_{abcd}$. We order the S_{abcde} such that $S_{abc33}\succ S_{abc23}\succ S_{abc22}\succ S_{abc13}\succ S_{abc12}\succ S_{abc11}$ and then amongst each set $S_{233ij}\succ S_{232ij}\succ S_{132ij}\succ S_{123ij}\succ S_{133ij}\succ S_{131ij}\succ S_{122ij}\succ S_{121ij}$. We find that the prolonged symbol $\mathcal{M}_2$ in orthonomic form is given by

$$\begin{array}{lll}
\boxed{1} & V_{12112}=V_{12211} & x^1\ \cdot\ \cdot\\
\boxed{2} & V_{12122}=V_{12212} & x^1\ x^2\ \cdot\\
\boxed{3} & V_{12123}=2V_{12312}-V_{13212}+V_{23211} & x^1\ x^2\ \cdot\\
\boxed{4} & V_{13113}=V_{13311} & x^1\ \cdot\ \cdot\\
\boxed{5} & V_{13123}=V_{13312} & x^1\ x^2\ \cdot\\
\boxed{6} & V_{13133}=V_{13313} & x^1\ x^2\ x^3\\
\boxed{7} & V_{23213}=V_{23312} & x^1\ \cdot\ \cdot\\
\boxed{8} & V_{23223}=V_{23322} & x^1\ x^2\ \cdot\\
\boxed{9} & V_{23233}=V_{23323} & x^1\ x^2\ x^3\\
\boxed{10} & V_{12113}=V_{12311}-V_{13112}+V_{13211} & x^1\ \cdot\ \cdot\\
\boxed{11} & V_{13122}=2V_{13212}-V_{12312}-V_{23211} & x^1\ x^2\ \cdot\\
\boxed{12} & V_{12133}=\frac{3}{2}V_{12313}-\frac{1}{2}V_{13312}+\frac{1}{2}V_{23311} & x^1\ x^2\ x^3\\
\boxed{13} & V_{12213}=2V_{12312}-V_{13212}+V_{23211} & x^1\ \cdot\ \cdot\\
\boxed{14} & V_{12223}=2V_{12322}-V_{13222}+V_{23212} & x^1\ x^2\ \cdot\\
\boxed{15} & V_{12233}=\frac{3}{2}V_{12323}+\frac{1}{2}V_{23312}-\frac{1}{2}V_{13322} & x^1\ x^2\ x^3\\
\boxed{16} & V_{13213}=\frac{1}{2}(V_{13312}+V_{12313}+V_{23311}) & x^1\ \cdot\ \cdot\\
\boxed{17} & V_{13223}=\frac{1}{2}(V_{13322}+V_{12323}+V_{23312}) & x^1\ x^2\ \cdot\\
\boxed{18} & V_{13233}=\frac{1}{2}(V_{13323}+V_{12333}+V_{23313}) & x^1\ x^2\ x^3,
\end{array}$$

where the groups of three equations each correspond to $f^{(R)}_{1212,i}$, $f^{(R)}_{1313,i}$, $f^{(R)}_{2323,i}$, $f^{(R)}_{1213,i}$, $f^{(R)}_{1223,i}$, $f^{(R)}_{1323,i}$ so that $\boxed{1}\leftrightarrow f^{(R)}_{1212,1}$ and so on. This system produces six equations of class 1, 7 of class 2 and 5 of class 3 leading to $\beta_2^{(1)}=6$, $\beta_2^{(2)}=7$, $\beta_2^{(3)}=5$. The total number of multiplicative variables equals 35 and, if $\mathcal{M}_2$ were involutive, we would have to obtain $r(\mathcal{M}_3)=35$. From differentiating $\mathcal{R}_2$ with respect to all three space–time coordinates, we obtain the symbol $\mathcal{M}_3$ and find that $r(\mathcal{M}_3)=35$, which means that $\mathcal{M}_2$ is involutive.[42] But we can show that the symbol equation ∂_3 [Eq. (3)], where $3\leftrightarrow\boxed{3}$ above, can also be created as a linear combination

$$\partial_3[\text{Eq. (3)}]=2\partial_2[\text{Eq. (16)}]+2\partial_3[\text{Eq. (11)}]-2\partial_3[\text{Eq. (13)}]-\partial_2[\text{Eq. (5)}]-\partial_1[\text{Eq. (7)}] \tag{34}$$

using formal differentiation so that $r(\mathcal{M}_3)=\Sigma_{k=1}^{3}\, k\cdot\beta_2^{(k)}=35$. However, it turns out that when (34) is rewritten in terms of the full equations from $\mathcal{R}_3$ as

$$I=f^{(R)}_{1212,33}+f^{(R)}_{1313,22}+f^{(R)}_{2323,11}-2\,f^{(R)}_{1323,12}-2\,f^{(R)}_{1213,23}+2\,f^{(R)}_{1223,13}, \tag{35}$$

it is not a trivial identity any longer and cannot be obtained by means of any linear combination of the $f^{(R)}_{abcd}$ and their derivatives $f^{(R)}_{abcd,e}$ so that $r(\mathcal{R}_3)=6+18+36=60$. We have

$$\dim(\mathcal{R}_1)=18,\quad \dim(\mathcal{M}_1)=18,$$

$$\dim(\mathcal{R}_2)=56,\quad \dim(\mathcal{M}_2)=30,$$

$$\dim(\mathcal{R}_3)=100,\quad \dim(\mathcal{M}_3)=45,$$

which leads us to the important consequence that

$$\dim(\mathcal{R}_2^{(1)})=\dim(\mathcal{R}_3)-\dim(\mathcal{M}_3)=100-45=55=\dim(\mathcal{R}_2)-1.$$

This means that **one integrability condition of the form (35) occurs**. Our new system of equations has to be given by

$$0=f^{(R)}_{abcd},$$

$$0=f^{(R)}_{abcd,e}, \tag{36}$$

$$0=I.$$

We find that the symbol of (36) is simply given by the previous $\mathcal{M}_2$ together with

$$V_{12323}=\frac{1}{(\Gamma^3_{12}-\Gamma^3_{13})}[V_{23312}(\Gamma^3_{13}-\Gamma^3_{12})+2\Gamma^3_{33}V_{12312}-V_{13322}(2\Gamma^1_{11}+\Gamma^3_{12}+\Gamma^3_{13})], \tag{37}$$

which adopts three multiplicative variables. Therefore, we obtain for (36)

$$\beta^{(1)}_{2,(1)}=6,\beta^{(2)}_{2,(1)}=7,\beta^{(3)}_{2,(1)}=6\ \text{ so that }\ \alpha^{(1)}_{2,(1)}=18,\alpha^{(2)}_{2,(1)}=9,\alpha^{(3)}_{2,(1)}=2.$$

We see that $r(\mathcal{M}_3^{(1)})=r(\mathcal{M}_3)+3=38$ because the three derivatives resulting from (37) are linearly independent and because $r(\mathcal{R}_3^{(1)})=r(\mathcal{R}_1)+r(\mathcal{R}_2^{(1)})+35+3=63$ which leads to

$$\dim(\mathcal{R}_2^{(2)})=\dim(\mathcal{R}_3^{(1)})-\dim(\mathcal{M}_3^{(1)})=97-42=55=\dim(\mathcal{R}_2^{(1)}).$$

Because $r(\mathcal{M}_3^{(1)})=\Sigma_{k=1}^{3}\, k\cdot\beta^{(k)}_{2,(1)}=6+14+18=38$, $\mathcal{M}_2^{(1)}$ is involutive and, because $\dim(\mathcal{R}_2^{(2)})=\dim(\mathcal{R}_2^{(1)})=55$, there are no integrability conditions that can occur and so the system $\mathcal{R}_2^{(1)}$ is in involution.

Even though the above prolongation of the Riemann–Lanczos problem mathematically leads to a prolonged system in involution, this prolonged system (36) does not respect general covariance. This is not satisfactory from a general relativity point of view and we are going to suggest a covariant version of the above prolongation. Instead of adding the partial derivatives to our equations, we look at the following new system of equations:

$$0=f^{(R)}_{abcd}, \tag{38}$$

$$0 = f^{(R)}_{abcd;e}\,.$$

The symbol of this modified system obviously coincides with that of the system formed by $f^{(R)}_{abcd}$, $f^{(R)}_{abcd,e}$ and, again, we obtain for the rank of $\mathcal{M}_3$ that $r(\mathcal{M}_3)=\Sigma^3_{k=1}\,k\cdot\beta^k_2=35$ so that $\mathcal{M}_2$ is involutive. We now have to see whether the linear combination (34) also holds for the full covariant system here. Calculations show that this is not the case and we obtain a covariant version of the above integrability condition in solved form given by

$$I_{\mathrm{Cov}}=f^{(R)}_{1212;33}+f^{(R)}_{1313;22}+f^{(R)}_{2323;11}-f^{(R)}_{1323;12}-f^{(R)}_{1323;21}-f^{(R)}_{1213;23}-f^{(R)}_{1213;32}+f^{(R)}_{1223;13}+f^{(R)}_{1223;31}\,. \tag{39}$$

This condition can be rewritten again in solved form as

$$I_{\mathrm{Cov}}=B_{12123;3}+B_{13132;2}+B_{23231;1}\,. \tag{40}$$

where $B_{abcde}:=f^{(R)}_{ab[cd;e]}$ which amounts to the covariant derivatives of the Bianchi identities for the R_{abcd} involved in (40). We can rewrite I_{Cov} (Ref. 44) in a more concise form using **bivectors**, where we introduce the bivector-indices $\underline{A}:=12$, $\underline{B}:=31$, $\underline{C}:=23$. The integrability condition I_{Cov} can then be expressed as

$$I_{\mathrm{Cov}}=f^{(R)}_{\underline{AA};(33)}+f^{(R)}_{\underline{BB};(22)}+f^{(R)}_{\underline{CC};(11)}+2(f^{(R)}_{\underline{AC};(13)}+f^{(R)}_{\underline{BC};(12)}+f^{(R)}_{\underline{AB};(23)})=\sum_{x,y=1}^{3}\sum_{X,Y=1}^{3}f^{(R)}_{XY;(xy)}\,. \tag{41}$$

Our new covariantly prolonged system is then given by

$$\begin{aligned} 0&=f^{(R)}_{abcd}\,,\\ 0&=f^{(R)}_{abcd;e}\,,\\ 0&=I_{\mathrm{Cov}}\,. \end{aligned} \tag{42}$$

It is $r(\mathcal{R}^{(1)}_2)=6+19=25$, $r(\mathcal{R}^{(1)}_3)=6+19+38=63$ as well as $r(\mathcal{M}^{(1)}_2)=19$, $r(\mathcal{M}^{(1)}_3)=38$ so that $\mathcal{M}^{(1)}_3$ coincides with the previous symbol for the prolongation involving partial derivatives. Once again it is $\dim(\mathcal{R}^{(2)}_2)=\dim(\mathcal{R}^{(1)}_2)=55$. We find that the system (42) also consists of a system in involution which respects general covariance. Therefore, we prefer (42) as a prolongation to a second-order system in involution for the Riemann–Lanczos problem in three dimensions and we conclude the following.

Theorem 4: *Proposition. The Riemann–Lanczos problem in three dimensions is not in involution. Its reduced characters* (s'_0,s'_1,s'_2,s'_3) *are (14, 8, 7, 3). They modify to (17, 8, 7, 0) when the differential gauge conditions are imposed. The Riemann–Lanczos problem becomes involutive after one prolongation which is obtained by adding either of the integrability conditions (35) or (40) and now its Cartan characters* $(\alpha^{(1)}_2,\alpha^{(2)}_2,\alpha^{(3)}_2)$ *for* $\mathcal{R}^{(1)}_2$ *are (18, 9, 2).*

C. The problem in four dimensions and singular solutions

In the Bampi–Caviglia papers[4,5] the Riemann–Lanczos problem was written as an EDS and found not to be in involution in four dimensions. In their second paper[5] they introduced a prolongation to create an involutive system. Our Pfaffian system for four dimensions is given by (16), where $n=4$ and the number of independent Lanczos components L_{abc} is $m=20$. We obtain (x^a,L_{abc},P_{abcd}) local jet coordinates on $\mathcal{J}^1(\mathbb{R}^4,\mathbb{R}^{20})$ with $N=4+20+80=104$ formal dimensions. For a Vessiot vector field V, 20 of the 80 components V_{abcd} are defined through the requirement that $df^{(R)}_{abcd}(V)=0$ given by (19). The 60 remaining components $V_{abcd}-V_{\{abcd\}}$ can be chosen arbitrarily for the first Vessiot vector field. As shown in Ref. 4 a rank deficiency between the s_i and the s'_i occurs due to six identities and the system (16) fails to be involutive.

The reduced Cartan characters can be computed using the REDUCE computer code in Ref. 42 based on the EDS package by Hartley.[45] For a number of space–times such as the conformally flat, Kasner, Gödel, some Debever types, and plane wave space–times we verified that the reduced Cartan characters $(s_0',s_1',s_2',s_3',s_4')$ were (40, 20, 19, 15, 6) when the differential gauge condition (3) was not included and (40, 20, 19, 15, 0) when it was included but *neither* differential system is *in involution*.[42]

Nevertheless, singular solutions exist and occur when some of the integral elements are *singular* so that the characters are not maximal. In the remaining sections of this article, we will give a examples of singular solutions for the Riemann–Lanczos problem mostly in four dimensions.

D. Debever-type space–times: Example

We expect singular solutions to occur for most of the Debever type space–times for which a line element is given by

$$ds^2=dt^2-f^2(t,y,z)dx^2-dy^2-dz^2 \tag{43}$$

with $f(t,y,z)$ being one of the functions given in Refs. 46 and 47. Specifically, for a Debever space–time with $f=y^2$ of Petrov type *D* we are interested in singular solutions such that

$$\pounds_\xi L_{abc}=0 \tag{44}$$

is possible using $\pounds_\xi R_{abcd}=0$ and the fact that $\nabla\pounds_\xi=\pounds_\xi\nabla$ for ξ any Killing vector field (=KV). There are three KVs corresponding to the ignorable coordinates *t, x*, and *z* and the components of the fourth KV are $\xi^4=(z,0,0,t)$.[48] The only nonvanishing independent Riemann–Lanczos equations are $f^{(R)}_{txty},f^{(R)}_{xyxy},f^{(R)}_{xzyz}$. A singular solution with vanishing Lie derivatives along Killing directions is then given by

$$L_{txt}=C_1y^4,\quad L_{tyz}=C_2y^{-2},\quad L_{xyx}=C_3y^2+y^3,$$

where C_1,C_2,C_3 are arbitrary constants. On a submanifold of (16) with $f^{(R)}_{abcd}=0$ for the above line element this solution corresponds to a singular integral manifold for which the (reduced) characters are $s_0=s_0'=3$ while all higher characters vanish. The Vessiot vector fields which span the tangent spaces of this singular solution manifold are locally given as

$$\begin{aligned}
V^1&=\frac{\partial}{\partial t},\\
V^2&=\frac{\partial}{\partial x},\\
V^3&=\frac{\partial}{\partial y}+4C_1y^3\frac{\partial}{\partial L_{txt}}-2C_2y^{-3}\frac{\partial}{\partial L_{tyz}}-4C_2y^{-3}\frac{\partial}{\partial L_{tzy}}+(2C_3y+3y^2)\frac{\partial}{\partial L_{xyx}}+4C_1y^3\frac{\partial}{\partial L_{xzz}}\\
&\quad+12y^2\frac{\partial}{\partial P_{txty}}+6C_2y^{-4}\frac{\partial}{\partial P_{tyzy}}+12C_2y^{-4}\frac{\partial}{\partial P_{tzyy}}+2(C_3+3y)\frac{\partial}{\partial P_{xyxy}}+12y^2\frac{\partial}{\partial P_{xzzy}},\\
V^4&=\frac{\partial}{\partial z},
\end{aligned} \tag{45}$$

where we substituted

$$V^3_{txty}=12y^2,\quad V^3_{tyzy}=6C_2y^{-4},\quad V^3_{xyxy}=2(C_3+3y),$$

and where $V^3_{txty}=V^3_{xzzy}$ and $V^3_{tzyy}=2V^3_{tyzy}$.

E. Singular solution for Gödel space–time

Gödel space–time is a perfect fluid space–time admitting closed timelike curves with line element

$$ds^2=a^2(dt^2-dx^2-dz^2+\tfrac{1}{2}e^{2x}dy^2+2e^x dtdy). \tag{46}$$

It is well known[49] that this space–time admits a G_5 as an isometry group of which three Killing vectors ξ^1,ξ^2,ξ^3 are based on the ignorable coordinates *t, y, z*. The other two are given by

$$\xi^4=\frac{\partial}{\partial x}-y\frac{\partial}{\partial y},\quad \xi^5=-2e^{-x}\frac{\partial}{\partial t}+y\frac{\partial}{\partial x}+\left(e^{-2x}-\frac{1}{2}y^2\right)\frac{\partial}{\partial y}.$$

But here, the Riemann–Lanczos problem does not admit singular solutions which inherit all the space–time symmetries. However, it is possible to find singular solutions with $\pounds_\xi L_{abc}=0$ imposed for the three Killing vectors based on ignorable coordinates and we find the solution[42]

$$L_{txy}=-\frac{a^2}{8}e^x,\quad L_{tyx}=\frac{a^2}{8}e^x,\quad L_{txt}=-\frac{a^2}{8},\quad L_{xyy}=\frac{3a^2}{16}e^{2x}.$$

This solution does not satisfy all the differential gauge conditions (3) however.[42] The tangent spaces of this singular integral manifold are spanned by four Vessiot vector fields which are locally given as

$$\begin{aligned}
V^1&=\frac{\partial}{\partial t},\\
V^2&=\frac{\partial}{\partial x}+\frac{a^2}{8}e^x\frac{\partial}{\partial L_{txy}}+\frac{a^2}{8}e^x\frac{\partial}{\partial L_{tyx}}+\frac{3a^2}{8}e^{2x}\frac{\partial}{\partial L_{xyy}}+\frac{1}{3}e^x\left(\frac{5a}{16}-\frac{1}{2}-e^{2x}\frac{3a}{16}\right)\frac{\partial}{\partial P_{txyx}}\\
&\quad-\frac{1}{3}e^x\left(\frac{5a}{16}-\frac{1}{2}-e^{2x}\frac{3a}{16}\right)\frac{\partial}{\partial P_{tyxx}}+\frac{3}{4a}e^{2x}\frac{\partial}{\partial P_{xyyx}},\\
V^3&=\frac{\partial}{\partial y},\\
V^4&=\frac{\partial}{\partial z},
\end{aligned} \tag{47}$$

where $V^2_{tyxx}=V^2_{txyx}$.

Note that the solution above is *also a singular solution* to the **reduced** Gödel space–time when we choose the line element

$$ds^2=a^2(dt^2-dx^2+\tfrac{1}{2}e^{2x}dy^2+2e^x dtdy) \tag{48}$$

to describe the reduced Gödel space–time.

F. Kasner space–time

For Kasner space–time we choose the line element

$$ds^2=dt^2-t^{2p_1}dx^2-t^{2p_2}dy^2-t^{2p_3}dz^2. \tag{49}$$

Kasner space–time admits a G_3 based on the three ignorable coordinates x, y, z. If we impose $\pounds_\xi L_{abc}=0$, the six nonvanishing components of the Riemann–Lanczos equations are $f^{(R)}_{txtx}, f^{(R)}_{tyty}, f^{(R)}_{tztz}, f^{(R)}_{xyxy}, f^{(R)}_{xzxz}, f^{(R)}_{yzyz}$. The last three equations can be solved for $L_{txx}, L_{tyy}, L_{tzz}$. But, inserting this solution into the first three equations leads to the inconsistent solution

$$L_{txx}=-\tfrac{1}{4}p_1t^{2p_1-1}, \quad P_{txxt}=(\tfrac{1}{2}-\tfrac{3}{4}p_1)p_1t^{2p_1-2},$$

$$L_{tyy}=-\tfrac{1}{4}p_2t^{2p_2-1}, \quad P_{tyyt}=(\tfrac{1}{2}-\tfrac{3}{4}p_2)p_2t^{2p_2-2},$$

$$L_{tzz}=-\tfrac{1}{4}p_3t^{2p_3-1}, \quad P_{tzzt}=(\tfrac{1}{2}-\tfrac{3}{4}p_3)p_3t^{2p_3-2},$$

because $P_{abcd}\neq\partial L_{abc}/\partial x^d$. However, there are singular solutions for which some of the components L_{abc} are linear in either x, y or z with no Lie symmetries along Killing directions. We find that

$$L_{txt}=C_1t^{2p_1-2}x, \quad L_{txx}=C_4t^{2p_1-1},$$

$$L_{tyt}=C_2t^{2p_2-2}y, \quad L_{tyy}=C_5t^{2p_2-1},$$

$$L_{tzt}=C_3t^{2p_3-2}z, \quad L_{tzz}=C_6t^{2p_3-1},$$

$$L_{xyx}=C_7t^{-2p_3}y, \quad L_{xyy}=C_{10}t^{-2p_3}x,$$

$$L_{xzx}=C_8t^{-2p_2}z, \quad L_{xzz}=C_{11}t^{-2p_2}x,$$

$$L_{yzy}=C_9t^{-2p_1}z, \quad L_{yzz}=C_{12}t^{-2p_1}y$$

is a singular solution for Kasner space–time for the following constants:

$$C_4=\frac{C_1}{(p_1-1)}-\frac{p_1}{2}, \quad C_5=\frac{C_2}{(p_2-1)}-\frac{p_2}{2},$$

$$C_6=\frac{C_3}{(p_3-1)}-\frac{p_3}{2}, \quad C_7=\frac{p_1C_2}{2-p_1},$$

$$C_8=\frac{p_1C_3}{2-p_1}, \quad C_9=\frac{p_2C_3}{2-p_2},$$

$$C_{10}=\frac{-p_2C_1}{2-p_2}, \quad C_{11}=\frac{-p_3C_1}{2-p_3},$$

$$C_{12}=\frac{-p_3C_2}{2-p_3}.$$

A computer code, which determines the rather longish expressions for C_1, C_2, C_3 in terms of p_1, p_2, p_3, can be found in Ref. 42.

V. CONCLUSION

In two dimensions, the Riemann–Lanczos problem is very simple and we showed that it is always in involution. The general solution was given for both possible choices of signature, Lorentzian and Euclidean.

In three dimensions, a prolongation becomes necessary to make it a system in involution. An integrability condition based on the derivatives of the Bianchi identities occurs when we use

Janet–Riquier theory and introduce the second-order partial derivatives S_{abcde} as new jet coordinates. A singular solution for the unprolonged problem for the reduced Gödel space–time is given.

The Riemann–Lanczos problem in four dimensions is not in involution as already shown in Ref. 4. But singular solutions for the Riemann–Lanczos problem do exist and we found some for Kasner, Gödel, and a Debever-type spacetime.

ACKNOWLEDGMENTS

Both authors thank D. Hartley and W. M. Seiler for valuable discussions as well as Professor L. S. Xanthis. We are grateful to Professor C. Hoenselaers for pointing out Refs. 38–40,50 to us. A.G. would like to thank the Swiss National Science Foundation (SNSF) and the Dr Robert Thyll-Dürr Foundation.

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The Weyl–Lanczos equations and the Lanczos wave equation in four dimensions as systems in involution

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(Received 22 August 2002; accepted 23 December 2002)

The Weyl–Lanczos equations in four dimensions form a system in involution. We compute its Cartan characters explicitly and use Janet–Riquier theory to confirm the results in the case of all space–times with a diagonal metric tensor and for the plane wave limit of space–times. We write the Lanczos wave equation as an exterior differential system and, with assistance from Janet–Riquier theory, we compute its Cartan characters and find that it forms a system in involution. We compare these Cartan characters with those of the Weyl-Lanczos equations. All results hold for the real analytic case. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1566096]

I. INTRODUCTION

A. The Weyl–Lanczos equations and the Lanczos tensor wave equation in four dimensions

Lanczos[1] generated the space–time Weyl conformal tensor C_{abcd} from a tensor potential L_{abc} by covariant differentiation such that C_{abcd} is given by

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}+g_{bc}L_{(ad)}+g_{ad}L_{(bc)}-g_{bd}L_{(ac)}-g_{ac}L_{(bd)} + \tfrac{2}{3}L^{ms}{}_{m;s}(g_{ac}g_{bd}-g_{ad}g_{bc}), \tag{1}$$

where $L_{ad}=L_a{}^s{}_{d;s}-L_a{}^s{}_{s;d}$ and ";" denotes covariant differentiation. We call (1) the Weyl–Lanczos equations. The index symmetries of the Lanczos tensor L_{abc} have to match the symmetries of (1) and so it is usual to impose

$$L_{abc}=L_{[ab]c} \tag{2}$$

and

$$L_{[abc]}=0. \tag{3}$$

and the trace-free (gauge) condition

$$L_a{}^s{}_s=0. \tag{4}$$

The algebraic Eqs. (2)–(4) leave us with only 16 independent components for the L_{abc}. If we then introduce the differential gauge conditions

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$$L_{ab}{}^{s}{}_{;s}=0, \tag{5}$$

which we often denote by $f_{ab}:=L_{ab}{}^{s}{}_{;s}$, we can simplify (1) considerably to get

$$C_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}-g_{bc}L^{s}{}_{ad;s}-g_{ad}L^{s}{}_{bc;s}+g_{bd}L^{s}{}_{ac;s}+g_{ac}L^{s}{}_{bd;s}. \tag{6}$$

We will denote the Weyl–Lanczos equations in solved form as

$$f_{abcd}=C_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}+g_{bc}L^{s}{}_{ad;s}+g_{ad}L^{s}{}_{bc;s}-g_{bd}L^{s}{}_{ac;s}-g_{ac}L^{s}{}_{bd;s}. \tag{7}$$

We note that Eqs. (5) and (6) constitute a system of 16 linear first-order partial differential equations in four dimensions. It was already shown in Ref. 2 for the real analytic case that the above four-dimensional Weyl–Lanczos equations consist of an exterior differential system (EDS) in involution with respect to the space–time variables.

From the Weyl–Lanczos problem it is possible to generate a Lanczos tensor wave equation and from this the Penrose wave equation for the Weyl tensor C_{abcd} can be derived.[3] It is given by

$$\Box L_{abc}+2R^{s}_{c}L_{abs}-R^{s}_{a}L_{bcs}-R^{s}_{b}L_{cas}-g_{ac}R^{ls}L_{lbs}+g_{bc}R^{ls}L_{las}-\tfrac{1}{2}RL_{abc}=J_{abc}, \tag{8}$$

where

$$J_{abc}=\tfrac{1}{2}R_{c[a;b]}-\tfrac{1}{6}g_{c[a}R_{;b]}, \quad \Box L_{abc}=g^{sm}L_{abc;s;m}.$$

Penrose's nonlinear wave equation for the space–time Weyl tensor[4]

$$\Box C_{abcd}-C_{ab}{}^{sm}C_{smcd}+4C_{asm[c}C^{m}{}_{d]}{}^{s}{}_{b}+\frac{R}{4}C_{abcd}=J_{[ab][c;d]}+J_{[cd][a;b]}-{}^{*}J^{*}_{[ab][c;d]}-{}^{*}J^{*}_{[cd][a;b]} \tag{9}$$

was derived in Ref. 3 from (8) and can be found for all dimensions $n\geqslant 4$. It was not derived from the wave equations for the Lanczos tensor candidate, which was given for $n=5$ by Edgar and Höglund.[5] We postpone to a later paper the discussion of the five-dimensional Weyl–Lanczos problem and the related tensor wave equation for the Lanczos potential. It is not clear from the published tensor wave equation of Edgar and Höglund[5] in five dimensions that there is still an *independent* derivation of the Penrose wave equation from it as in four dimensions.

In this article, we are going to compute the Cartan characters for the Weyl–Lanczos equations in four dimensions explicitly using both EDS theory and Janet–Riquier theory[6,7] and we will derive corresponding results for the four-dimensional wave equation.

II. WEYL–LANCZOS EQUATIONS IN FOUR DIMENSIONS

The theory of exterior differential systems (EDSs) can be found in many places such as in Refs. 8–11. In Ref. 2 it was shown that the Weyl–Lanczos relations in four dimensions are a system in involution with respect to the space–time variables. They constitute a system in involution as compared to the Riemann–Lanczos equations, which do not, even in vacuum space–times when $C_{abcd}=R_{abcd}$, because each problem is based on different partial differential equations. (Of course, this is carrying formality about vacuum space–times to excessive lengths. Why choose a system of PDEs which is not in involution in preference to one which is in involution?)

A. The Weyl–Lanczos equations as an EDS

We introduce the local coordinates (x^{e},L_{abc},P_{abcd}) on the jet bundle $\mathcal{J}^{1}(\mathbb{R}^{4},\mathbb{R}^{16})$ which form our formal manifold $\mathcal{M}$ of formal dimension $N=4+16+64=84$. The exterior derivatives of the f_{abcd} and of $f_{ab}=L_{ab}{}^{s}{}_{;s}$ constitute our first 16 one-forms. We also have to add 16 **contact condi-**

tions K_{abc} in order to make sure that the P_{abcd} can be considered as partial derivatives of the L_{abc} when projected onto the space–time manifold. We obtain the Pfaffian system $\mathcal{P}$ as given in Ref. 2,

$$\begin{aligned} df_{abcd}=&[C_{abcd,e}+\alpha_{abcde}+\gamma_{abcde}]dx^e-dP_{abcd}+dP_{abdc}-dP_{cdab}+dP_{cdba}+g_{bc}g^{ns}dP_{nads}\\ &+g_{ad}g^{ns}dP_{nbcs}-g_{bd}g^{ns}dP_{nacs}-g_{ac}g^{ns}dP_{nbds}+\Gamma^n_{ad}(dL_{nbc}+dL_{ncb})-\Gamma^n_{ac}(dL_{nbd}\\ &+dL_{ndb})+\Gamma^n_{bc}(dL_{nad}+dL_{nda})-\Gamma^n_{bd}(dL_{nac}+dL_{nca})-g_{bc}g^{ns}(\Gamma^m_{ns}dL_{mad}+\Gamma^m_{as}dL_{nmd}\\ &+\Gamma^m_{ds}dL_{nam})-g_{ad}g^{ns}(\Gamma^m_{ns}dL_{mbc}+\Gamma^m_{bs}dL_{nmc}+\Gamma^m_{cs}dL_{nbm})+g_{bd}g^{ns}(\Gamma^m_{ns}dL_{mac}\\ &+\Gamma^m_{as}dL_{nmc}+\Gamma^m_{cs}dL_{nam})+g_{ac}g^{ns}(\Gamma^m_{ns}dL_{mbd}+\Gamma^m_{bs}dL_{nmd}+\Gamma^m_{ds}dL_{nbm}),\end{aligned}$$

$$\begin{aligned} df_{ab}=&(P_{abns}g^{ns}_{,e}-L_{mbn}\Gamma^m_{as,e}-L_{amn}\Gamma^m_{bs,e}-L_{abm}\Gamma^m_{ns,e})dx^e+g^{ns}(dP_{abns}-\Gamma^m_{as}dL_{mbn}-\Gamma^m_{bs}dL_{amn}\\ &-\Gamma^m_{ns}dL_{abm}),\end{aligned}$$

$$K_{abc}=dL_{abc}-P_{abce}dx^e, \tag{10}$$

where α_{abcde} and γ_{abcde} are given in Appendix A. The system (10) consists of a system in involution in the real analytic case and does not possess any Cauchy characteristics. The Cartan characters (s_0,s_1,s_2,s_3,s_4) were computed to be (32,16,16,16,0) or (16,16,16,16,0) due to df_{abcd} and df_{ab} vanishing identically when pulled back onto the submanifold with $f_{abcd}=0$, $f_{ab}=0$ for a number of space–times in a computation based on REDUCE computer codes.[12]

We can also compute the reduced Cartan characters for (10) using the tableau matrix. First, we must complete $(df_{abcd},df_{ab},\omega^e)$ so that it turns into a complete coframe on $\mathcal{M}$, say $(df_{abcd},df_{ab},K_{abc},\omega^e,\pi^\Lambda)$ by adding $N-s-n=48$ new one-forms π^Λ. Accordingly, we add the 48 new cobasis elements chosen as

$$\pi^\Lambda\leftrightarrow dP_{abc1},\quad \Lambda=1,...,16,$$

$$\pi^\Lambda\leftrightarrow dP_{abc2},\quad \Lambda=17,...,32,$$

$$\pi^\Lambda\leftrightarrow dP_{abc3},\quad \Lambda=33,...,48,$$

where the ordering of the P_{abcd} based on the indices *abc* is given in Appendix A and where Λ is a collective index subject to Einstein's summation convention and corresponding to the set of indices *abc*. Here, the independence condition Ω is given by $\Omega=\omega^1\wedge\omega^2\wedge\omega^3\wedge\omega^4$,where $\omega^1=dx^1$, $\omega^2=dx^2$, $\omega^3=dx^3$, $\omega^4=dx^4$. We can now express the 16 dK_{abc}, where the α below are arranged in the same way as the L_{abc} in Appendix A, as

$$d\theta^\alpha=A^\alpha_{\Lambda1}\pi^\Lambda\wedge\omega^1+A^\alpha_{\Lambda2}\pi^\Lambda\wedge\omega^2+A^\alpha_{\Lambda3}\pi^\Lambda\wedge\omega^3-dP_{abc4}\wedge\omega^4. \tag{11}$$

Further calculations are based on the assumption that we can express each of the 16 dP_{abc4} in (11) as a distinct linear combination of the df_{abcd}, K_{abc}, $dL_{ab}{}^{s}{}_{;s}$ and the ω^e.[12] We obtain the only nonvanishing components of the tableau matrices $A^\alpha_{\Lambda1}$, $A^\alpha_{\Lambda2}$ and $A^\alpha_{\Lambda3}$ to be $A^\alpha_{\Lambda1}=A^\alpha_{\Lambda2}=A^\alpha_{\Lambda3}=-1$ if α and Λ refer to the same group of indices *abc*. This leads to

$$\begin{pmatrix} A^\alpha_{\Lambda1}\\ A^\alpha_{\Lambda2}\\ A^\alpha_{\Lambda3}\\ A^\alpha_{\Lambda4}\end{pmatrix}=\begin{pmatrix} A & 0 & 0\\ 0 & A & 0\\ 0 & 0 & A\\ X_1 & X_2 & X_3\end{pmatrix},$$

which is a 64×48 matrix, and where X_1, X_2, X_3 stand for $A^\alpha_{\Lambda4}$ and each A is given by the 16×16 matrix $A:=-\mathbb{I}_{16}$. From this we can immediately deduce that the reduced characters are

$s_1'=s_2'=s_3'=16$ and $s_4'=0$. However, this method does not supply s_0' but here clearly $s_0=s_0'=s=32$ which is simply the number of independent one-forms in (10) so that $(s_0',s_1',s_2',s_3',s_4')$ is given by (32, 16, 16, 16, 0). When (10) is pulled back onto the submanifold, where $f_{abcd}=0$ and $f_{ab}=0$, we get (16, 16, 16, 16, 0). One can show that the torsion terms B_{ij}^{α} can be made to vanish through applying a corresponding coframe transformation. This rather cumbersome calculation can be carried out using a REDUCE code in Ref. 12 based on the package EDS.[13]

B. The Weyl–Lanczos equations as a system of PDEs

The theory in this section and for the Lanczos wave equation below is based on a modernized version of Janet–Riquier theory[14–16] which can be found in Refs. 17 and 7. A review together with some results on the Riemann–Lanczos problems in two and three dimensions is given in Ref. 12.

Here, we use (6) and (5) as our first-order system of PDEs denoted by $\mathcal{R}_1$. Using a computer code in Ref. 12, we derived the symbol $\mathcal{M}_1$ for any space–time with diagonal metric

$$ds^2=a_1(dx^1)^2-a_2(dx^2)^2-a_3(dx^3)^2-a_4(dx^4)^2, \tag{12}$$

where a_1, a_2, a_3, a_4 depend on all space–time variables. We replace the four components L_{121}, L_{131}, L_{141}, L_{122} and their partial derivatives by solving (4) for them and we choose an ordering $\succ$ for the P_{abce} in such a way that $P_{abc4}\succ P_{abc3}\succ P_{abc2}\succ P_{abc1}$ and then the sets of P_{abce} ordered according to $\mathcal{R}_{\succ}^{(W,4)}$ for each $e=1, 2, 3, 4$, where $\mathcal{R}_{\succ}^{(W,4)}$ is given in Appendix A. This produces an orderly ranking and induces such a ranking amongst the *symbol variables* V_{abcd}.[7,17] Then, $\mathcal{M}_1$ is given in orthonomic form by

$$\begin{aligned}
&(f_{1212})\quad V_{3434}=\frac{a_4}{a_1}V_{1331}+\frac{a_3}{a_1}V_{1441}-\frac{a_4}{a_2}V_{2332}-\frac{a_3}{a_2}V_{2442}+V_{3443},\\
&(f_{1213})\quad V_{2434}=\frac{a_4}{a_1}V_{1321}-\frac{a_4}{a_2}V_{2322}+V_{2443}+V_{3442},\\
&(f_{1313})\quad V_{2424}=\frac{a_4}{a_3}V_{2323}+V_{2442}-\frac{a_2a_4}{a_1a_3}V_{1331}-\frac{a_2}{a_3}V_{3443},\\
&(f_{1214})\quad V_{2334}=V_{2343}+\frac{a_3}{a_2}V_{2422}+V_{3432}-\frac{a_3}{a_1}V_{1421},\\
&(f_{1314})\quad V_{2324}=\frac{a_2}{a_1}V_{1431}+V_{2342}-V_{2423}-\frac{a_2}{a_3}V_{3433},\\
&(f_{1323})\quad V_{1424}=\frac{a_4}{a_3}V_{1323}-\frac{a_4}{a_3}V_{1233}+V_{1442}-\frac{a_4}{a_3}V_{2331},\\
&(f_{1223})\quad V_{1434}=\frac{a_4}{a_2}V_{1232}-\frac{a_4}{a_2}V_{1322}+V_{1443}+\frac{a_4}{a_2}V_{2321},\\
&(f_{1224})\quad V_{1334}=V_{1343}+\frac{a_3}{a_2}V_{1422}-\frac{a_3}{a_2}V_{2421}-\frac{a_3}{a_2}V_{1242},\\
&(f_{1234})\quad V_{1234}=V_{1243}+V_{1342}-V_{1432}-V_{2341}+V_{2431},\\
&(f_{1324})\quad V_{1324}=V_{1243}+V_{1342}-V_{1423}+V_{2431},
\end{aligned} \tag{13}$$

$$(L_{12}{}^{s}{}_{;s}) \quad V_{1244}=-\frac{a_4}{a_3}V_{2331}-V_{2441}+\frac{a_4}{a_3}V_{1332}+V_{1442}-\frac{a_4}{a_3}V_{1233},$$

$$(L_{13}{}^{s}{}_{;s}) \quad V_{1344}=-\frac{a_4}{a_2}V_{1322}-\frac{a_4}{a_3}V_{1333}+\frac{a_4}{a_2}V_{2321}-V_{3441},$$

$$(L_{14}{}^{s}{}_{;s}) \quad V_{1444}=-\frac{a_4}{a_2}V_{1422}-\frac{a_4}{a_3}V_{1433}+\frac{a_4}{a_2}V_{2421}+\frac{a_4}{a_3}V_{3431},$$

$$(L_{23}{}^{s}{}_{;s}) \quad V_{2344}=-\frac{a_4}{a_1}V_{1231}+\frac{a_4}{a_1}V_{1321}-\frac{a_4}{a_2}V_{2322}-\frac{a_4}{a_3}V_{2333},$$

$$(L_{24}{}^{s}{}_{;s}) \quad V_{2444}=-\frac{a_4}{a_1}V_{1241}+\frac{a_4}{a_1}V_{1421}-\frac{a_4}{a_2}V_{2422}-\frac{a_4}{a_3}V_{2433},$$

$$(L_{34}{}^{s}{}_{;s}) \quad V_{3444}=-\frac{a_4}{a_1}V_{1341}+\frac{a_4}{a_1}V_{1431}+\frac{a_4}{a_2}V_{2342}-\frac{a_4}{a_2}V_{2432}-\frac{a_4}{a_3}V_{2432}.$$

All 16 equations in (13) are of class 4 because all variables x^1, x^2, x^3, x^4 are multiplicative variables for each equation so that we obtain $\beta_1^{(1)}=0$, $\beta_1^{(2)}=0$, $\beta_1^{(3)}=0$, $\beta_1^{(4)}=16$. For the sum $\Sigma_{k=1}^{4}\beta_1^{(k)}=16$, and because we only have 16 equations, this means that we are already using coordinates which are δ-regular.[12] Then, the Cartan characters are $\alpha_1^{(1)}=16$, $\alpha_1^{(2)}=16$, $\alpha_1^{(3)}=16$, $\alpha_1^{(4)}=0$ according to the formula[7,12,17]

$$\alpha_q^{(k)}=m\binom{n+q-k-1}{q-1}-\beta_q^{(k)}. \tag{14}$$

Now, we must verify that our symbol is involutive and we prolong f_{abcd}, f_{ab} by differentiating each equation in $\mathcal{R}_1$ with respect to x^1, x^2, x^3, x^4 to obtain $\mathcal{R}_2$. We find that we can rewrite the prolonged symbol $\mathcal{M}_2$ of $\mathcal{R}_2$ in such a way that each equation contains a distinct component V_{abcde} so that $r(\mathcal{M}_2)=64$.[12] But we also have $\Sigma_{k=1}^{4}k\cdot\beta_1^{(k)}=64$ which means that $\mathcal{M}_1$ is involutive. In order to show that the system is formally integrable, we have to verify that the canonical projection of $\mathcal{R}_2$ from second to first order $\pi_1^2(\mathcal{R}_2)$ coincides with $\mathcal{R}_1$ itself. Our system is a linear system of PDEs and therefore involution follows.[12]

For a general space–time, the calculations are more cumbersome and in Ref. 12 we looked at the plane-wave limit which all space–times possess. A good account of the plane-wave limit of space–times is given in Ref. 18. All space–times can locally be expressed using a line element

$$ds^2=2dx^1dx^2+a(dx^3)^2+2b_3dx^2dx^3+2b_4dx^2dx^4-c_{33}(dx^3)^2-2c_{34}dx^3dx^4-c_{44}(dx^4)^2, \tag{15}$$

where a, b_3, b_4, c_{33}, c_{34}, c_{44} are functions of all four coordinates. When a plane-wave limit is taken, the metric (15) becomes[18]

$$ds^2=2dx^1dx^2-C_{33}(dx^3)^2-2C_{34}dx^3dx^4-C_{44}(dx^4)^2, \tag{16}$$

where C_{33}, C_{34}, and C_{44} are arbitrary functions of x^1 only. We can determine the symbol for the metric (16) but we see that for whatever ranking we choose, the coordinates are not δ-regular.[12] We perform a linear coordinate transformation[17] which we choose to be

$$\begin{aligned} d\tilde{x}^1&=a_{11}dx^1+a_{12}dx^2,\\ d\tilde{x}^2&=a_{21}dx^1+a_{22}dx^2, \end{aligned} \tag{17}$$

$$d\tilde{x}^3 = dx^3,$$

$$d\tilde{x}^4 = dx^4,$$

where $a_{11}=a_{12}=a_{21}=1/\sqrt{2}$, $a_{22}=-1/\sqrt{2}$. This produces a new, only slightly different metric line element for (16) which is

$$ds^2=(d\tilde{x}^1)^2-(d\tilde{x}^2)^2-C_{33}(d\tilde{x}^3)^2-2C_{34}d\tilde{x}^3d\tilde{x}^4-C_{44}(d\tilde{x}^4)^2. \tag{18}$$

Even though this seems a minor transformation, the change from **characteristic** to **noncharacteristic coordinates**, which are now δ-regular, is necessary in order to obtain the Cartan characters. Then, we evaluate $f_{abcd}=0$, $f_{ab}=0$ for the new line element (16) and order the P_{abcd} such that $P_{abc1}>P_{abc2}>P_{abc3}>P_{abc4}$ instead, whereas we leave the ordering in each set P_{abce} unchanged as in $\mathcal{R}_{>}^{(W,4)}$ which leads to an orderly ranking. In this way we obtain an orthonomic system, where each symbol equation is of the form[12]

$$V_{abc1}=f(g_{a'b'},V_{c'd'e'f'}). \tag{19}$$

This system is composed of 16 equations all of class 4 which leads to $\beta_1^{(1)}=\beta_1^{(2)}=\beta_1^{(3)}=0$, $\beta_1^{(4)}=16$ and therefore to the Cartan characters $\alpha_1^{(1)}=\alpha_1^{(2)}=\alpha_1^{(3)}=16$ and $\alpha_1^{(4)}=0$. We obtained the further result that $r(\mathcal{M}_2)=\Sigma_{k=1}^4 k\cdot\beta_1^{(k)}=64$ and that no integrability conditions occur[12] so that the Weyl–Lanczos equations consist of a system in involution for all plane-wave limits of space–times with Cartan characters (16, 16, 16, 0).

III. LANCZOS WAVE EQUATION IN FOUR DIMENSIONS

In this section, we look at the Lanczos wave equation at first as an EDS and then as a system of PDEs. We again determine the Cartan characters and show that it consists of a system in involution in the real analytic case using each theory, a result which can be derived from the scalar wave equation directly.

A. The Lanczos wave equation as an EDS

We describe the Lanczos tensor wave equation in terms of an EDS on a jet bundle $\mathcal{J}^2(\mathbb{R}^4,\mathbb{R}^{16})$ with formal dimension $N=4+16+64+160=244$ and the local coordinates $(x^e,L_{abc},P_{abcd},S_{abcde})$ composed by 4 space–time coordinates x^e, 16 L_{abc}, 64 P_{abcd}, and 160 S_{abcde}. The S_{abcde} are the variables corresponding to the second-order partial derivatives of the L_{abc} when projected onto our space–time manifold. We denote the components of the wave equation in solved form by $\mathcal{W}_{abc}$.

In addition to the exterior derivations of $\mathcal{W}_{abc}$, we need to add two sets of contact conditions, K_{abc} and K_{abcd}, when we write the Lanczos wave equation as an EDS. Altogether, we obtain the Pfaffian system

$$d\mathcal{W}_{abc}=d\mathcal{W}_{abc},$$

$$K_{abc}=dL_{abc}-P_{abce}dx^e, \tag{20}$$

$$K_{abcd}=dP_{abcd}-S_{abcde}dx^e.$$

There $d\mathcal{W}_{abc}$ are the exterior derivatives of the components of the wave equation in solved form which are locally given by

$$\begin{aligned}d\mathcal{W}_{abc}=&[\Box L_{abc}+2R^s_cL_{abs}-R^s_aL_{bcs}-R^s_bL_{cas}-g_{ac}R^{ls}L_{lbs}+g_{bc}R^{ls}L_{las}-\tfrac{1}{2}RL_{abc}-J_{abc}]_{,e}dx^e\\&+g^{sm}[dS_{abcms}-\Gamma^n_{am,s}dL_{nbc}-\Gamma^n_{ms,s}dL_{anc}-\Gamma^n_{cm,s}dL_{abn}-\Gamma^n_{as}dP_{nbcm}+\Gamma^n_{as}\Gamma^k_{nm}dL_{kbc}\\&+\Gamma^n_{as}\Gamma^k_{bm}dL_{nkc}+\Gamma^n_{as}\Gamma^k_{cm}dL_{nbk}-\Gamma^n_{bs}dP_{ancm}+\Gamma^n_{bs}\Gamma^k_{am}dL_{knc}+\Gamma^n_{bs}\Gamma^k_{nm}dL_{akc}\end{aligned}$$

$$+\Gamma^n_{bs}\Gamma^k_{cm}dL_{ank}-\Gamma^n_{cs}dP_{abnm}+\Gamma^n_{cs}\Gamma^k_{am}dL_{kbn}+\Gamma^n_{cs}\Gamma^k_{bm}dL_{akn}+\Gamma^n_{cs}\Gamma^k_{nm}dL_{abk}$$
$$-\Gamma^n_{ms}dP_{abcn}+\Gamma^n_{ms}\Gamma^k_{an}dL_{kbc}+\Gamma^n_{ms}\Gamma^k_{bn}dL_{akc}+\Gamma^n_{ms}\Gamma^k_{cn}dL_{abk}]+2R^s_c dL_{abs}-R^s_a dL_{bcs}$$
$$-R^s_b dL_{cas}-g_{ac}R^{ls}dL_{lbs}+g_{bc}R^{ls}dL_{las}-\tfrac{1}{2}RdL_{abc}. \tag{21}$$

For a number of space–times, we could show that the Cartan characters (s_0,s_1,s_2,s_3,s_4) are given by (96, 64, 48, 32, 0) and that the system is in involution.[12]

Again, we can determine the reduced Cartan characters using the tableau matrices $A^\alpha_{\Lambda i}$. First, we complete $(dW_{abc},K_{abc},K_{abcd},\omega^e)$ to a coframe on our formally 244-dimensional jet-bundle. In (20) we have 96 one-forms to which we add the 4 one-forms $\omega^1=dx^1$, $\omega^2=dx^2$, $\omega^3=dx^3$, $\omega^4=dx^4$ so that we need to add a further 144 forms π^Λ in order to obtain a complete coframe of $N=244$ one-forms. Again, Λ is a collective index subject to Einstein's summation convention, this time replacing complete sets of indices *abcd* in dS_{abcde}. In order to obtain intrinsic values, we choose to replace all components dS_{abcde}, where either *d* or *e* are $=4$, first, and so on based on x^4 being our first coordinate, then x^3, then x^2, and x^1 last. The correspondence of $\pi^\Lambda\leftrightarrow dS_{abcde}$ is given in detail in Appendix B. We solve each $d\mathcal{W}_{abc}$ for a distinct dS_{abc11}. Because $dK_{abc}=0$ (mod $(\mathcal{P})$), we only need to consider dK_{abcd} when computing the tableau matrices and the reduced Cartan characters. We can now write the 64 dK_{abcd} as

$$d\theta^\alpha\equiv A^\alpha_{\Lambda 2}\pi^\Lambda\wedge\omega^2+A^\alpha_{\Lambda 3}\pi^\Lambda\wedge\omega^3+A^\alpha_{\Lambda 4}\pi^\Lambda\wedge\omega^4-dS_{abc11}\wedge\omega^1+B^\alpha_{ij}\omega^i\wedge\omega^j. \tag{22}$$

From this we find that the only nonvanishing tableau matrix components $A^\alpha_{\Lambda i}$ for $i\neq 1$ are given by $A^\alpha_{\Lambda i}=-1$ when the indices α and Λ correspond to the same set of indices *abcd* as given in Appendix B and $A^\alpha_{\Lambda i}=0$ otherwise. This leads to

$$\begin{pmatrix} A^\alpha_{\Lambda 4}\\ A^\alpha_{\Lambda 3}\\ A^\alpha_{\Lambda 2}\\ A^\alpha_{\Lambda 1}\end{pmatrix}=\begin{pmatrix} 0 & 0 & A\\ 0 & B & 0\\ C & 0 & 0\\ X_1 & X_2 & X_3\end{pmatrix},$$

which is a 160×144 matrix and where X_1, X_2, X_3 stand for $A^\alpha_{\Lambda 1}$ and A is a 64×64 matrix with $A=-\mathbb{I}_{64}$, B is a 48×48 matrix with $B=-\mathbb{I}_{48}$ and C is a 32×32 matrix with $C=-\mathbb{I}_{32}$ so that the total rank $r=144$ is obtained. We obtain $s'_1=64$, $s'_2=48$, $s'_3=32$, and $s'_4=0$, meaning that the set of reduced Cartan characters $(s'_0,s'_1,s'_2,s'_3,s'_4)$ is (96, 64, 48, 32, 0). Computer codes show that we can find a coframe transformation such that the torsion terms B^α_{ij} can be absorbed and the system is in involution with Cartan characters (96, 64, 48, 32, 0) for a number of space–times.[12]

B. The Lanczos wave equation as a system of PDEs

We denote the system (8) formed by the 16 components of the wave equation by $\mathcal{R}_{2,\text{wave}}$, where the index "2" refers to the order of the system. Due to the definition of the symbol $\mathcal{M}_q$ of a system of PDEs $\mathcal{R}$, only the highest-order derivatives lead to terms in the symbol so that the only terms contributing to the symbol $\mathcal{M}_{2,\text{wave}}$ are parts of the $\Box L_{abc}$-terms. The 16 equations for the symbol for an arbitrary space–time each look like

$$V_{abc44}=\frac{1}{g^{44}}(g^{11}V_{abc11}+g^{22}V_{abc22}+g^{33}V_{abc33}+2g^{12}V_{abc12}+2g^{13}V_{abc13}+2g^{14}V_{abc14}$$
$$+2g^{23}V_{abc23}+2g^{24}V_{abc24}+2g^{34}V_{abc34}). \tag{23}$$

We can easily see that by ordering the S_{abcde} in such a way that $S_{abc44}>S_{abc34}>S_{abc33}>S_{abc24}>S_{abc23}>S_{abc22}>S_{abc14}>S_{abc13}>S_{abc12}>S_{abc11}$ based on $x^4>x^3>x^2>x^1$ and by choosing for each set of S_{abcij} the ordering $\mathcal{R}^{(\text{wave},4)}_>$ given in Appendix B, an orderly ranking is achieved.

Because all equations of form (23) are of class 4, it means that $\beta_2^{(4)}=16$ is the maximal value for $\beta_2^{(4)}$ and $\beta_2^{(1)}=\beta_2^{(2)}=\beta_2^{(3)}=0$ so that the Cartan characters are $\alpha_2^{(1)}=64$, $\alpha_2^{(2)}=48$, $\alpha_2^{(3)}=32$, $\alpha_2^{(4)}=0$. Further calculations show that $\mathcal{M}_{2,\text{wave}}$ is involutive and *no integrability conditions occur* because the system is linear so that the Lanczos wave equation in four dimensions consists of a system in involution with Cartan characters (64, 48, 32, 0).[12]

We can also derive this result directly from the *scalar wave equation*

$$\Box\Psi=0, \tag{24}$$

where Ψ is our scalar component depending on x^1, x^2, x^3, x^4. We use a formal manifold $\mathcal{M}$ with $N=19$ formal dimensions of which a local basis is given by the four x^e, one dependent variable Ψ, four P_e and ten S_{ef} on our jet bundle $\mathcal{J}^2(\mathbb{R}^4,\mathbb{R})$. We obtain $\beta_2^{(1)}=\beta_2^{(2)}=\beta_2^{(3)}=0$ and $\beta_2^{(4)}=1$ and the characters are $\alpha_2^{(1)}=4$, $\alpha_2^{(2)}=3$, $\alpha_2^{(3)}=2$, $\alpha_2^{(4)}=0$. The symbol of a single equation is always involutive and we further find that $r(\mathcal{M}_3)=4$ and therefore $\dim(\mathcal{M}_3)=16$ whereas $r(\mathcal{R}_3)=5$ and $\dim(\mathcal{R}_3)=30$. We also find that $\dim(\mathcal{R}_2)=14$ and

$$\dim(\mathcal{R}_2^{(1)})=\dim(\mathcal{R}_3)-\dim(\mathcal{M}_3)=30-16=14,$$

so that we conclude that $\dim(\mathcal{R}_2)=\dim(\mathcal{R}_2^{(1)})=14$. Because the system is linear, no integrability conditions can occur and the scalar wave equation (24) consists of a system in involution with characters (4, 3, 2, 0). Note that in the case of the Lanczos wave equation, we are dealing with 16 equations because we have 16 independent components L_{abc} and find the correspondence between the two sets of characters is here given by

$$16\cdot(4,3,2,0)=(64,48,32,0).$$

If we compare the characters of the Weyl–Lanczos equations with those of the Lanczos wave equation, we need to prolongate the Weyl–Lanczos equations once to second order. But for an involutive system the characters of the symbol $\mathcal{M}_{q+r}$ of the prolonged system together with the $\beta_{q+r}^{(k)}$ are directly determined by[7,17]

$$\alpha_{q+r}^k=\sum_{i=k}^{n}\binom{r+i-k-1}{r-1}\alpha_q^{(i)},\quad \beta_{q+r}^k=\sum_{i=k}^{n}\binom{r+i-k-1}{r-1}\beta_q^{(i)},$$

where in our case $n=4$, $m=16$, $q=1$, and $r=1$, which leads to the result (48, 32, 16, 0) for $(\alpha_2^{(1)},\alpha_2^{(2)},\alpha_2^{(3)},\alpha_2^{(4)})$ for the prolonged Weyl–Lanczos equations. This shows that, based on the $\alpha_2^{(k)}$ for both systems, the Weyl–Lanczos equations are more restrictive than the Lanczos wave equation with characters (64,48,32,0). The general solution of the Weyl–Lanczos equations only depends on 16 arbitrary functions of three variables whereas the general solution for the Lanczos wave equations contains 32 arbitrary functions of three variables.

IV. CONCLUSION

We obtained the Cartan characters (s_0,s_1,s_2,s_3,s_4) for the Weyl–Lanczos equations given as a Pfaffian system in involution which are (32, 16, 16, 16, 0) and (16, 16, 16, 16, 0) when pulled back onto the submanifold where the Weyl–Lanczos equations themselves vanish identically. These results were obtained assisted by REDUCE codes based on the EDS package. Using Janet–Riquier theory the Cartan characters were obtained to be (16, 16, 16, 0) for a diagonalized space–time and for the plane wave limit taken of any space–time and these systems were in involution.

We showed that the Lanczos wave equation also consists of a Pfaffian system in involution and that its Cartan characters are given by (96, 64, 48, 32, 0). We also found that the Lanczos wave equation was less restrictive than the Weyl–Lanczos equations allowing for 32 arbitrary

functions of three variables as opposed to only 16 which can also be derived from the scalar wave equation. In practice many of the arbitrary functions involved may amount to gauge contributions though. All results hold for the real analytic case.

ACKNOWLEDGMENTS

Both authors wish to thank D. Hartley and W. M. Seiler for valuable discussions as well as Professor L. S. Xanthis. A.G. would like to thank the Swiss National Science Foundation (SNSF) and the Dr Robert Thyll-Dürr Foundation.

APPENDIX A: THE WEYL–LANCZOS EQUATIONS

Here, we give the expressions for the α_{abcde} and the γ_{abcde} occurring in the EDS for the Weyl–Lanczos equations given by (10):

$$\alpha_{abcde}=\Gamma^n_{ad,e}(L_{nbc}+L_{ncb})+\Gamma^n_{bc,e}(L_{nad}+L_{nda})-\Gamma^n_{ac,e}(L_{nbd}+L_{ndb})-\Gamma^n_{bd,e}(L_{nac}+L_{nca}). \tag{A1}$$

The quantity γ_{abcde} is given by

$$\begin{aligned}\gamma_{abcde}=&g_{bc}[P_{nads}g^{ns}_{,e}-L_{mad}(\Gamma^m_{ns}g^{ns})_{,e}-L_{nmd}(\Gamma^m_{as}g^{ns})_{,e}-L_{nam}(\Gamma^m_{ds}g^{ns})_{,e}]+g_{ad}[P_{nbcs}g^{ns}_{,e}\\&-L_{mbc}(\Gamma^m_{ns}g^{ns})_{,e}-L_{nmc}(\Gamma^m_{bs}g^{ns})_{,e}-L_{nbm}(\Gamma^m_{cs}g^{ns})_{,e}]-g_{bd}[P_{nacs}g^{ns}_{,e}-L_{mac}(\Gamma^m_{ns}g^{ns})_{,e}\\&-L_{nmc}(\Gamma^m_{as}g^{ns})_{,e}-L_{nam}(\Gamma^m_{cs}g^{ns})_{,e}]-g_{ac}[P_{nbds}g^{ns}_{,e}-L_{mbd}(\Gamma^m_{ns}g^{ns})_{,e}-L_{nmd}(\Gamma^m_{bs}g^{ns})_{,e}\\&-L_{nbm}(\Gamma^m_{ds}g^{ns})_{,e}]+g_{bc,e}[P_{nads}g^{ns}-L_{mad}(\Gamma^m_{ns}g^{ns})-L_{nmd}(\Gamma^m_{as}g^{ns})-L_{nam}(\Gamma^m_{ds}g^{ns})]\\&+g_{ad,e}[P_{nbcs}g^{ns}-L_{mbc}(\Gamma^m_{ns}g^{ns})-L_{nmc}(\Gamma^m_{bs}g^{ns})-L_{nbm}(\Gamma^m_{cs}g^{ns})]-g_{bd,e}[P_{nacs}g^{ns}\\&-L_{mac}(\Gamma^m_{ns}g^{ns})-L_{nmc}(\Gamma^m_{as}g^{ns})-L_{nam}(\Gamma^m_{cs}g^{ns})]-g_{ac,e}[P_{nbds}g^{ns}-L_{mbd}(\Gamma^m_{ns}g^{ns})\\&-L_{nmd}(\Gamma^m_{bs}g^{ns})-L_{nbm}(\Gamma^m_{ds}g^{ns})].\end{aligned} \tag{A2}$$

When introducing the collective index Λ for the additional coframe elements π^Λ, we ordered the L_{abc} according to

$$\begin{aligned}&L_{133}<L_{144}<L_{123}<L_{132}<L_{124}<L_{142}<L_{134}<L_{143}<L_{232}<L_{233}<L_{242}<L_{244}\\&\quad<L_{234}<L_{243}<L_{343}<L_{344}\end{aligned}$$

from which we deduce the ordering for the $\pi^\Lambda \leftrightarrow dP_{abce}$ in such a way that the dP_{abce} are arranged like the L_{abc} above. The π^Λ are then labeled:

$$\pi^1 \leftrightarrow dP_{1331},\ldots,\quad \pi^{16}\leftrightarrow dP_{3441},$$

$$\pi^{17} \leftrightarrow dP_{1332},\ldots,\quad \pi^{32}\leftrightarrow dP_{3442},$$

$$\pi^{33} \leftrightarrow dP_{1333},\ldots,\quad \pi^{48}\leftrightarrow dP_{3443}.$$

When expressing the Weyl–Lanczos equations as a system of PDEs, we used the standard orderly ranking (if not stated otherwise explicitly) which is based on the ordering $P_{abc4}>P_{abc3}>P_{abc2}>P_{abc1}$. Then, amongst each set of the P_{abci} we order them according to

$$\begin{aligned}&P_{344i}>P_{343i}>P_{243i}>P_{234i}>P_{244i}>P_{242i}>P_{233i}>P_{232i}>P_{143i}>P_{134i}>P_{142i}>P_{124i}>P_{132i}\\&\quad>P_{123i}>P_{144i}>P_{133i}.\end{aligned}$$

This leads to an orderly ranking for the P_{abcd} for the Weyl–Lanczos equations denoted by $\mathcal{R}^{(W,4)}_>$.

APPENDIX B: THE LANCZOS WAVE EQUATION

Here, we specify the correspondence between the π^{Λ} and the dS_{abcde} for the Lanczos wave equation. For both i,j fixed we assume that the dS_{abcij} are ordered according to the ordering of the L_{abc} in Appendix A. For the first 64 π^{Λ}, where we have used the fact that $x^4>x^3>x^2>x^1$ for our independent variables in order to obtain intrinsic results, we obtain the labeling (for the pairs of indices $ij=44$, 34, 24, 14)

$$\pi^{1}\leftrightarrow dS_{13344},\ldots,\quad \pi^{16}\leftrightarrow dS_{34444},$$

$$\pi^{7}\leftrightarrow dS_{13334},\ldots,\quad \pi^{32}\leftrightarrow dS_{34434},$$

$$\pi^{33}\leftrightarrow dS_{13324},\ldots,\quad \pi^{48}\leftrightarrow dS_{34424},$$

$$\pi^{49}\leftrightarrow dS_{13314},\ldots,\quad \pi^{64}\leftrightarrow dS_{34414}.$$

Then, the next 48 π^{Λ} are given by (for $ij=33$, 23, 13)

$$\pi^{65}\leftrightarrow dS_{13333},\ldots,\quad \pi^{80}\leftrightarrow dS_{34433},$$

$$\pi^{81}\leftrightarrow dS_{13323},\ldots,\quad \pi^{96}\leftrightarrow dS_{34423},$$

$$\pi^{97}\leftrightarrow dS_{13313},\ldots,\quad \pi^{112}\leftrightarrow dS_{34413}.$$

The last 32 π^{Λ} are denoted as follows (for $ij=22$, 12)

$$\pi^{113}\leftrightarrow dS_{13322},\ldots,\quad \pi^{128}\leftrightarrow dS_{34422},$$

$$\pi^{129}\leftrightarrow dS_{13312},\ldots,\quad \pi^{144}\leftrightarrow dS_{34412}.$$

We assumed that all the dS_{abc11} can be solved for by the 16 exterior derivatives of the wave equation $d\mathcal{W}_{abc}$ and expressed the dS_{abc11} in this way.

Using Janet–Riquier theory, an orderly ranking $\mathcal{R}_{>}^{(\text{wave},4)}$ for the 160 second-order partial derivatives S_{abcde} for the Lanczos wave equation is based on

$$S_{abc44}>S_{abc34}>S_{abc33}>S_{abc24}>S_{abc23}>S_{abc22}>S_{abc14}>S_{abc13}>S_{abc12}>S_{abc11}$$

and then amongst each set S_{abcij} for i,j fixed in the same way as for the P_{abci} in Appendix A, namely,

$$S_{344ij}>S_{343ij}>S_{243ij}>S_{234ij}>S_{244ij}>S_{242ij}>S_{233ij}>S_{232ij}>S_{143ij}>S_{134ij}>S_{142ij}>S_{124ij}>S_{132ij}$$
$$>S_{123ij}>S_{144ij}>S_{133ij}.$$

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A space–time in toroidal coordinates

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(Received 18 July 2002; accepted 26 March 2003)

We present an exact solution of Einstein's field equations in toroidal coordinates. The solution has three regions: an interior with a string equation of state; an Israel boundary layer; and an exterior with constant isotropic pressure and constant density, locally isometric to anti–de Sitter space–time. The exterior can be a cosmological vacuum with negative cosmological constant. The size and mass of the toroidal loop depend on the size of Λ. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1580999]

I. INTRODUCTION

There has been increasing interest in space–times with nonspherical topology and negative cosmological constant. Much of the discussion has focused on structures with horizons in anti–de Sitter (AdS) space–times.[1–5] Vanzo[6] pointed out that, in AdS space, there are black hole solutions with genus g horizons. Aminneborg *et al.* (ABHP)[1] discussed space–times locally isometric to AdS with horizons of arbitrary genus. While many current models of the universe seem to indicate that Λ is positive, there are some models with $\Lambda<0$.[7] Aside from their physical relevance to the actual structure of the Universe, solutions in AdS are very interesting as a comparison case to asymptotically flat solutions. For example, Hawking and Page[8] have discussed the relevance of a negative Λ to black hole thermal stability. The $2+1$ Bañados–Teitelboim–Zanelli[9] black hole solution and its $3+1$ black string[10] lift have generated a large literature.[11]

In this work we discuss a toroidal fluid solution embedded in a locally AdS exterior. There is an overall metric scale factor which depends on the size of Λ. The solution has three regions:

(i) an interior solution with an equation of state, $\rho+p_{\varphi}=0$;
(ii) an Israel[12] boundary layer with surface stress energy S_{ij} and stringlike content $S_{00}+S_{\varphi\varphi}=0$; and
(iii) an exterior with constant isotropic pressure, constant density, and a negative cosmological constant. Just as in the ABHP study, the exterior metric is locally isometric to AdS. The solution models an extended loop with interior structure. The size of the loop and its mass depend on the cosmological constant. The solution can be used to model both micro loops or very large loop structures, depending on the size of Λ.

There have been other discussions of circular string structures. Frolov, Israel and Unruh[13] started with an axially symmetric space–time and discussed the relation between internal string structure and angular deficit, then transformed the metric to toroidal coordinates to discuss the mass structure of circular cosmic strings. Using toroidal coordinates, Hughes *et al.*[14] studied weak field loops. Sen and Banerjee[15] have discussed a solution for a circular cosmic string loop in cylindrical coordinates. Because often a particular choice of surfaces can simplify the solution of the field equations, we begin with toroidal coordinates.

Cartesian toroids are discussed in the next section. In Sec. III we write the field equations for the space–time and develop the interior and exterior solutions. Matching conditions are presented in the fourth section. The Israel boundary layer is described in the fifth section. In Sec. VI we

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discuss the mass, and the final section concludes with a general discussion.

II. CARTESIAN TOROIDS

The relation between Cartesian coordinates (x,y,z) and toroidal coordinates (η,ϑ,φ) on $\mathcal{R}^3$ is[16]

$$x=a\frac{\sinh(\eta)\cos(\varphi)}{\cosh(\eta)-\cos(\vartheta)}, \tag{1a}$$

$$y=a\frac{\sinh(\eta)\sin(\varphi)}{\cosh(\eta)-\cos(\vartheta)}, \tag{1b}$$

$$z=a\frac{\sin(\vartheta)}{\cosh(\eta)-\cos(\vartheta)}, \tag{1c}$$

with $0\leqslant\eta<\infty$, $0\leqslant\vartheta\leqslant 2\pi$, $0\leqslant\varphi\leqslant 2\pi$. Here "$a$" is a constant scale factor.

In toroidal coordinates, the Euclidean metric $dx^2+dy^2+dz^2$ becomes

$$dL^2=\frac{a^2}{[\cosh(\eta)-\cos(\vartheta)]^2}[d\eta^2+d\vartheta^2+\sinh^2(\eta)d\varphi^2]. \tag{2}$$

The torus $\eta=\eta_0$ described by dL^2 has a circular cross section with circumference $2\pi a\,\mathrm{csch}(\eta_0)$, and the center of the toroid circular cross section is a distance $a\coth(\eta_0)$ from the origin. The equation of the $\varphi=0$, $y=0$ circles, Eq. (1b), is[17]

$$[x-a\coth(\eta_0)]^2+z^2=a^2\,\mathrm{csch}^2(\eta_0).$$

As η_0 increases, the radius of the loop decreases and the torus approaches the flat torus, a distance "a" from the origin. Looking down the z-axis (about which φ has range $0\leqslant\varphi\leqslant 2\pi$) at the torus, one sees two concentric circles. The $\vartheta=$constant surfaces, $0\leqslant\vartheta\leqslant 2\pi$, are spheres centered on the z-axis. From Eq. (1) these spheres have equation

$$(x^2+y^2+z^2-a^2)/2az=\cot(\vartheta),$$

which defines the relation of ϑ to the torus.

III. SPACE–TIME

For the curved space torus, one must construct two different metrics, an exterior for $0\leqslant\eta\leqslant\eta_0$ and an interior for $\eta_0\leqslant\eta\leqslant\infty$. The metric that we use to describe the space–time is a simple generalization of the flat space metric:

$$ds^2=\frac{a^2}{[\cosh(\eta)-\cos(\vartheta)]^2}[-h^2(\eta)dt^2+e^{2\mu(\eta)}d\eta^2+d\vartheta^2+h^2(\eta)d\varphi^2]. \tag{3}$$

Note that metric (3) cannot reduce to the Minkowski metric.

A. Field equations

We write Einstein's field equations using the conventions of Misner, Thorne, and Wheeler[18] and Wald.[19] The field equations are ($G=c=1$)

$$G_{\alpha\beta}=8\pi T_{\alpha\beta}. \tag{4}$$

Using flow vector $\hat{u}^\alpha\hat{u}_\alpha=-1$, the energy-momentum tensor for a fluid is given in terms of principal pressures as

$$T_{\alpha\beta}=\rho\hat{u}_\alpha\hat{u}_\beta+p_1\hat{x}_\alpha\hat{x}_\beta+p_2\hat{y}_\alpha\hat{y}_\beta+p_3\hat{z}_\alpha\hat{z}_\beta. \tag{5}$$

In the following development, we write the field equations allowing for fluid anisotropy. We do not include Λ explicitly in the stress-energy tensor but will interpret the stress-energy associated with a metric solution in terms of Λ if appropriate. Using metric (3) above with $\Psi=\cosh(\eta)-\cos(\vartheta)$ and $u^\alpha\partial_\alpha=(\Psi/ah)\partial_t$, the field equations are

$$\begin{aligned}8\pi\rho a^2e^{2\mu}&=-8\pi p_\varphi a^2e^{2\mu}\\&=-\cosh^2(\eta)-2\cosh(\eta)\cos(\vartheta)+3+2\sinh(\eta)\Psi(h'/h)-\Psi^2(h''/h)+\Psi^2\mu'(h'/h)\\&\quad-2\Psi\mu'\sinh(\eta)+e^{2\mu}[-3+\cos^2(\vartheta)+2\cosh(\eta)\cos(\vartheta)],\end{aligned} \tag{6a}$$

$$\begin{aligned}8\pi p_\eta a^2e^{2\mu}&=3\cosh^2(\eta)-3-4\Psi\sinh(\eta)(h'/h)+\Psi^2(h'/h)^2\\&\quad+e^{2\mu}[3-2\cosh(\eta)\cos(\vartheta)-\cos^2(\vartheta)],\end{aligned} \tag{6b}$$

$$\begin{aligned}8\pi p_\vartheta a^2e^{2\mu}&=\cosh^2(\eta)-3+2\cosh(\eta)\cos(\vartheta)-2\Psi\sinh(\eta)[2(h'/h)-\mu']\\&\quad+\Psi^2[2(h''/h)-2\mu'(h'/h)+(h'/h)^2]+3e^{2\mu}\sin^2(\vartheta),\end{aligned} \tag{6c}$$

where $\partial h/\partial\eta$ and $\partial\mu/\partial\eta$ are abbreviated by h' and μ'.

B. Interior solution

Let $h^2=[d_0\sinh(\eta)-b_0]^2$, $e^{2\mu}=1$. The interior metric is

$$g^{\text{in}}_{\alpha\beta}dx^\alpha dx^\beta=(a/\Psi)^2[-h^2dt^2+d\eta^2+d\vartheta^2+h^2d\varphi^2]. \tag{7}$$

The energy-momentum components for g^{in} are

$$8\pi a^2\rho=-8\pi a^2p_\varphi=(b_0/h)[\cosh^2(\eta)-\cos^2(\vartheta)], \tag{8a}$$

$$8\pi a^2p_\eta=(\Psi/h^2)\{(d_0^2+b_0^2)\Psi-2b_0h[\cosh(\eta)+\cos(\vartheta)]\}, \tag{8b}$$

$$8\pi a^2p_\vartheta=(\Psi/h^2)[(d_0^2+b_0^2)\Psi-4b_0h\cos(\vartheta)]. \tag{8c}$$

The equation of state is

$$\rho+p_\varphi=0. \tag{9}$$

The interior metric has quadratic Weyl invariant

$$C_{\alpha\beta\mu\nu}C^{\alpha\beta\mu\nu}=\frac{4}{3}d_0^2\frac{\Psi^4}{a^4h^4}[b_0\sinh(\eta)+d_0]^2, \tag{10}$$

and Ricci scalar

$$R_{\alpha\beta}g^{\alpha\beta}_{\text{in}}=-\frac{2\Psi}{a^2h^2}\{(d_0^2+b_0^2)\Psi-2b_0h[\cosh(\eta)+2\cos(\vartheta)]\}. \tag{11}$$

C. Exterior solution

The solution to be used in the toroid exterior is

$$g^{\text{ex}}_{\alpha\beta}dx^\alpha dx^\beta=\frac{a^2}{[\cosh(\eta)-\cos(\vartheta)]^2}[-h^2(\eta)dt^2+e^{2\mu(\eta)}d\eta^2+d\vartheta^2+h^2(\eta)d\varphi^2]. \tag{12}$$

In order to describe a cosmological vacuum, p_η will have to be constant. The cosine terms should vanish. From the general field equations we write p_η, grouping the terms:

$$\begin{aligned}8\pi p_\eta a^2 e^{2\mu} &= 3\cosh^2(\eta) - 3 - 4\sinh(\eta)\cosh(\eta)(h'/h) + 3e^{2\mu} + \cosh^2(\eta)(h'/h)^2 \\ &+ \cos(\vartheta)[-2\cosh(\eta)e^{2\mu} + 4\sinh(\eta)(h'/h) - 2\cosh(\eta)(h'/h)^2] \\ &+ \cos^2(\vartheta)[-e^{2\mu} + (h'/h)^2].\end{aligned}$$

To eliminate the $\cos^2$ term, take $(h'/h)^2 = e^{2\mu}$. The cosine term then becomes

$$4\cos(\vartheta)e^{\mu}[-\cosh(\eta)e^{\mu} + \sinh(\eta)].$$

Requiring this term to vanish provides one nontrivial solution

$$e^{\mu} = \sinh(\eta)/\cosh(\eta), \quad h = \cosh(\eta). \tag{13}$$

Substituting (13), the energy-momentum components of g^{ex} are

$$8\pi\rho = -3/a^2, \tag{14a}$$

$$8\pi p_\eta = 8\pi p_\vartheta = 8\pi p_\varphi = 3/a^2. \tag{14b}$$

This can be a space–time with negative cosmological constant $\Lambda = -3/a^2$. The metric is conformally flat and has constant negative Ricci scalar $R = -12/a^2$. $g^{\alpha\beta}_{\text{ex}}$ is locally isometric to the AdS metric.

IV. MATCHING INTERIOR TO EXTERIOR

The two metrics to be joined are

$$\begin{aligned}g^{\text{in}}_{\alpha\beta}dx^\alpha dx^\beta &= \frac{a^2}{\Psi^2}\{-[d_0\sinh(\eta) - b_0]^2 dt^2 + d\eta^2 + d\vartheta^2 + [d_0\sinh(\eta) - b_0]^2 d\varphi^2\}, \\ g^{\text{ex}}_{\alpha\beta}dx^\alpha dx^\beta &= \frac{a^2}{\Psi^2}\left[-\cosh^2(\eta)dt^2 + \frac{\sinh^2(\eta)}{\cosh^2(\eta)}d\eta^2 + d\vartheta^2 + \cosh^2(\eta)d\varphi^2\right].\end{aligned} \tag{15}$$

Matching the metrics one obtains

$$\cosh(\eta_0) = d_0\sinh(\eta_0) - b_0.$$

Matching the extrinsic curvature yields

$$d_0\cosh(\eta_0) = \sinh(\eta_0).$$

The bounding surface is thus defined by

$$\cosh(\eta_0) = \frac{b_0}{d_0^2 - 1}, \tag{16a}$$

$$\sinh(\eta_0) = \frac{d_0 b_0}{d_0^2 - 1}, \tag{16b}$$

with

$$b_0^2+d_0^2=1. \tag{17}$$

This implies that both b_0 and d_0 are less than 1. On the boundary the stresses are

$$8\pi a^2\rho=-8\pi a^2 p_\varphi=[b_0^2\cos^2(\vartheta)-1], \tag{18a}$$

$$8\pi a^2 p_\eta=\Psi b_0[-3+b_0\cos(\vartheta)], \tag{18b}$$

$$8\pi a^2 p_\vartheta=\Psi b_0[-1+3b_0\cos(\vartheta)]. \tag{18c}$$

A problem with the matching is that p_η does not smoothly join to the exterior stress. This mismatch would lead to a dynamic boundary. Therefore, an Israel boundary layer will be developed.

V. THE BOUNDARY LAYER

A. Position of the layer

If the interior and exterior solutions do not match derivatives but join over an Israel surface layer,[12] then the position of the boundary will be set by matching only h at $\eta=\eta_0$. For the exterior we have

$$h=\cosh(\eta), \quad e^\mu=\sinh(\eta)/\cosh(\eta).$$

For the interior

$$h=d_0\sinh(\eta)-b_0, \quad e^{2\mu}=1.$$

Matching the interior and exterior at $\eta=\eta_0$ provides

$$\cosh(\eta_0)=d_0\sinh(\eta_0)-b_0.$$

Note that the $e^{2\mu}$ term need not match, since it is the coefficient of $d\eta^2$ and the match is for η constant surfaces. Rearranging, we have the bounding surface

$$\cosh(\eta_0)=\frac{b_0+\mathbb{k}d_0(b_0^2+d_0^2-1)^{1/2}}{d_0^2-1}, \quad \mathbb{k}=(\pm 1), \tag{19a}$$

$$\sinh(\eta_0)=\frac{d_0b_0+\mathbb{k}(b_0^2+d_0^2-1)^{1/2}}{d_0^2-1}. \tag{19b}$$

B. Parameter constraints

Constraints can be set on d_0 and b_0 by requiring

$$\sinh(\eta_0)>0, \quad \cosh(\eta_0)>0, \quad \rho_{\text{interior}}>0.$$

Both of the hyperbolic functions in Eq. (19) have a sign choice which is the same for both functions. There are eight possible parameter $(\mathbb{k},d_0,b_0)$ combinations for both $d_0^2>1$ and $d_0^2<1$ for a total of 16 cases. The hyperbolic conditions eliminate eight and the density constraint five more. The three remaining allowed parameter combinations with their constraints are

$$(1)\ \ d_0^2>1:[\mathbb{k}=+1,\ d_0>0,\ b_0>0],\ \text{no constraints},$$

$$(2)\ \ d_0^2>1:[\mathbb{k}=-1,\ d_0>0,\ b_0>0],\ \ \sqrt{b_0^2+d_0^2-1}<\left|\frac{b_0}{d_0}\right|,\ \ \sqrt{b_0^2+d_0^2-1}<|d_0 b_0|, \tag{20}$$

$$(3)\ \ d_0^2<1:[\mathbb{k}=-1,\ d_0>0,\ b_0>0],\ \ \sqrt{b_0^2+d_0^2-1}>\left|\frac{b_0}{d_0}\right|,\ \ \sqrt{b_0^2+d_0^2-1}>|d_0 b_0|.$$

The algebraic details are in the Appendix.

C. Extrinsic curvature

We are interested in a space–time that could describe a loop of matter with an energy density equal to the loop tension over a bounding Israel surface layer at $\eta=\eta_0$. The stress-energy content of the surface layer S_{ij} (Ref. 12) is given by

$$8\pi S_{ij}=\gamma_{ij}-\gamma h_{ij}^{(b)} \tag{21}$$

with $h_{ij}^{(b)}$ the metric of the bounding torus. γ_{ij} is the difference between the extrinsic curvatures of the exterior and interior metrics on the boundary

$$\gamma_{ij}=K_{ij}^{\mathrm{ex}}-K_{ij}^{\mathrm{in}}=\langle K_{ij}\rangle.$$

Calculating the general extrinsic curvature on the bounding torus $\eta=\eta_0$ with unit normal n_α we have

$$K_{ij}=-n_{\alpha;\beta}h_i^\alpha h_j^\beta,$$

$$K_{ij}=n_\alpha\Gamma_{ij}^\alpha=-(n_\alpha/2)g^{\alpha\beta}g_{ij,\beta}.$$

With $\Psi=\cosh(\eta)-\cos(\vartheta)$ and $\eta^\alpha\partial_\alpha=\partial/\partial\eta$, we have for the extrinsic curvatures on the boundary

$$K_{00}=(n_\alpha\eta^\alpha)\frac{\Psi^2}{2e^{2\mu}}\frac{\partial}{\partial\eta}(h^2/\Psi^2), \tag{22a}$$

$$K_{\varphi\varphi}=-K_{00}, \tag{22b}$$

$$K_{\vartheta\vartheta}=(n_\alpha\eta^\alpha)\frac{\Psi^2}{2e^{2\mu}}\frac{\partial}{\partial\eta}(1/\Psi^2). \tag{22c}$$

$K_{\vartheta\vartheta}$ will match across the boundary with the metrics we have found. Using Eq. (22a) and forming K_{00} we have

$$K_{00}=\frac{h}{\Psi}[\Psi h'-h\sinh(\eta)]. \tag{23}$$

Establishing the difference between inner and outer spaces and matching h on the boundary, the discontinuity in the extrinsic curvature is

$$\langle K_{00}\rangle=h[\sinh(\eta_0)-d_0\cosh(\eta_0)].$$

Therefore the boundary layer has a stress energy content

$$8\pi S_{00}=\cosh(\eta_0)[d_0\cosh(\eta_0)-\sinh(\eta_0)]=-8\pi S_{\varphi\varphi}. \tag{24}$$

Requiring $S_{00}>0$ and substituting for $\cosh(\eta_0)$ and $\sinh(\eta_0)$ from Eq. (19) implies $\mathbb{k}=1$. Thus one parameter set remains:

$$d_0^2 > 1 : [\mathbb{k} = +1,\ d_0 > 0,\ b_0 > 0]. \tag{25}$$

The stress energy content of the boundary layer represents a toroidal loop with a stringlike equation of state.

VI. MASS

When the generator of time translations is Killing vector ξ^ν, then the Einstein four-momentum $p^\mu = \sqrt{-g} T^\mu_\nu \xi^\nu$ is conserved and a mass can be associated with three-volume dV_μ,

$$M = \int_{3vol} \sqrt{-g} T^\mu{}_\nu \xi^\nu dV_\mu,$$

where $dV_\mu = t,_\mu d\eta d\vartheta d\varphi$. Substituting we have the mass inside the torus:

$$M = \frac{2\pi b_0 a^2}{8\pi} \int_{\eta_0}^{\infty} \int_0^{2\pi} \frac{h}{\Psi^3} [\cosh(\eta) + \cos(\vartheta)] d\vartheta d\eta$$

$$= \frac{\pi b_0 a^2}{8 \sinh^4(\eta_0)} \{4 d_0 \sinh(\eta_0) \cosh^2(\eta_0) - b_0 [2 \sinh^2(\eta_0) + 3]\}. \tag{26}$$

A similar calculation can be repeated for the mass associated with the surface layer. In the Israel formalism the surface stress energy is defined in geodesic coordinates as the thickness ε of the layer approaches zero:

$$S_{\mu\nu} = \lim_{\varepsilon \to 0} \int_0^\varepsilon T_{\mu\nu} dx. \tag{27}$$

Start with the definition of the mass in a three-volume and take the limit as the distance between tori goes to zero:

$$M' = \int_{3vol} \sqrt{-g} T^\mu{}_\nu \xi^\nu dV_\mu = \int_{3vol} \sqrt{-g} T^0{}_\nu \xi^\nu d\eta d\vartheta d\varphi.$$

In the limit of zero layer thickness

$$M' = \lim_{\varepsilon \to 0} \int \int \int_{\eta_0 - \varepsilon}^{\eta_0} \sqrt{-g_{tt} g_{\vartheta\vartheta} g_{\varphi\varphi} g_{\eta\eta}}\ T^0{}_\nu \xi^\nu d\eta d\vartheta d\varphi. \tag{28}$$

Assume that the limit can be taken inside the integral and that over the range of the $\eta-$ integral that $\sqrt{-g_{tt} g_{\vartheta\vartheta} g_{\varphi\varphi}}$ is approximately constant and takes its value on η_0:

$$M' = \int \int \sqrt{-g_{tt}(\eta_0, \vartheta) g_{\vartheta\vartheta}(\eta_0, \vartheta) g_{\varphi\varphi}(\eta_0, \vartheta)}\ d\vartheta d\varphi \lim_{\varepsilon \to 0} \int_{\eta_0 - \varepsilon}^{\eta_0} (T^0{}_\nu \xi^\nu \sqrt{g_{\eta\eta}} d\eta),$$

$$M' = \int \int \sqrt{-g_{tt} g_{\vartheta\vartheta} g_{\varphi\varphi}}\ S^0{}_\nu \xi^\nu d\vartheta d\varphi.$$

Integration results in

$$M' = \frac{a h^2}{4} [d_0 - \tanh(\eta_0)] \frac{2\pi}{\sinh(\eta_0)}. \tag{29}$$

VII. DISCUSSION

In summary, we have obtained a fluid solution to the field equations that describes a positive density torus with a boundary layer, embedded in a locally AdS exterior. The solution has two parameters, d_0 and b_0 with a restricted range. The fluid and boundary layers both have a stringlike equation of state. The solution can describe a variety of structures, depending on the parameter value chosen. First consider the size of the loop, $R_\vartheta = a\,\mathrm{csch}(\eta_0)$. For the allowed parameter set we have, in the limit $b_0^2 \gg |d_0^2 - 1|$,

$$\frac{R_\vartheta[\mathbb{k}=+1,\, d_0^2>1]}{a} \sim \frac{d_0-1}{b_0}.$$

R_ϑ/a can become very small and the torus will approach the flat torus a distance "a" from the center of the torus loop. The size of the loop depends on the scale parameter, "a." The size of the scale factor is determined by the cosmological constant. From the field equations we have

$$\frac{8\pi G}{c^2}\rho_{\text{exterior}} = -\frac{3}{a^2}, \quad |\Lambda| = \frac{3}{a^2}. \tag{30}$$

For example, if this density is roughly the same order as the critical density, we would have $|\rho| \sim 10^{-27}$ kg/m^3 and one finds that $a \sim 10^{28}$ m. If the solution is used to describe a primordial universe with a large negative Λ, the scale factor could be much smaller and micro loops could be possible.

The mass description is also dependent on the size of the scale factor. We have from Eq. (26) for the fluid interior

$$M = \frac{\pi b_0 a^2}{8}\left[\frac{4d_0}{\sinh(\eta_0)} + \frac{4d_0}{\sinh^3(\eta_0)} - \frac{2b_0}{\sinh^2(\eta_0)} - \frac{3b_0}{\sinh^4(\eta_0)}\right].$$

For the surface layer we have Eq. (29),

$$M' = \frac{\pi}{2} a h^2 [d_0 - \tanh(\eta_0)] \frac{1}{\sinh(\eta_0)}.$$

One thing that is immediately obvious is the different dependence on the scale parameter. In the large b_0 limit taken above we have

$$M' \sim \frac{\pi}{2} a b_0,$$

$$M \sim \frac{\pi}{4} a^2 (d_0^2 - 1).$$

The fluid inside the torus does not depend on b_0 in this limit. In the current universe, if $a \gg 1$ and if $b_0 \ll a$, the fluid inside the torus can dominate the mass because of the scale factor. If $b_0 \sim a$ and $d_0 \to 1$, the mass in the surface layer could dominate the loop structure. While the size of the thin-loop torus depends on "a," the "fat" torus can extend much closer in to the origin. As above, if, in the primordial universe, the cosmological constant was negative and much larger, the scale factor, "a," could be quite small. The solution could then describe micro loops with the surface layer the dominant mass contribution.

Several extensions of this solution might be possible. Adding time dependence to generate an oscillating loop for a Casimir calculation would be quite interesting. Time dependence could also

be used to check the evolution and stability over time of a primordial loop. This solution could also be regarded as a step toward generating multi segment Brevik–Nielson[20] loops with metric dependent tensions.

APPENDIX: MATCHING CONSTRAINTS

The hyperbolic functions are, with $S(b_0,d_0):=(b_0^2+d_0^2-1)^{1/2}$,

$$\cosh(\eta_0)=\frac{b_0+\mathbb{k}d_0S}{d_0^2-1},\quad \mathbb{k}=(\pm 1), \tag{A1a}$$

$$\sinh(\eta_0)=\frac{d_0b_0+\mathbb{k}S}{d_0^2-1}. \tag{A1b}$$

The conditions to be satisfied are

$$\sinh(\eta_0)>0,$$

$$\cosh(\eta_0)>0.$$

The cosh function is always positive and $\sinh(\eta_0)$ is positive because the range for the interior metric is $\eta_0<\eta<\infty$. The parameters must always satisfy the condition

$$b_0^2+d_0^2>1.$$

The equal sign with $S=0$ is not a possibility since that would imply an exact match of interior and exterior.

1. $\sinh(\eta_0)>0$

$$\frac{d_0b_0+\mathbb{k}S}{d_0^2-1}>0$$

A: $d_0^2>1$, $\mathbb{k}=+1$, $0<d_0b_0+S$
- (1) ($d_0>0$, $b_0>0$) condition satisfied
- (2) ($d_0<0$, $b_0<0$) condition satisfied
- (3) ($d_0>0$, $b_0<0$) condition satisfied if $|d_0b_0|<S$
- (4) ($d_0<0$, $b_0>0$) condition satisfied if $|d_0b_0|<S$

B: $d_0^2>1$, $\mathbb{k}=-1$, $0<d_0b_0-S$
- (5) ($d_0>0$, $b_0>0$) condition satisfied if $S<|d_0b_0|$
- (6) ($d_0<0$, $b_0<0$) condition satisfied if $S<|d_0b_0|$
- (7) ($d_0>0$, $b_0<0$) condition excluded
- (8) ($d_0<0$, $b_0>0$) condition excluded

C: $d_0^2<1$, $\mathbb{k}=+1$, $0<-d_0b_0-S$
- (9) ($d_0>0$, $b_0>0$) condition excluded
- (10) ($d_0<0$, $b_0<0$) condition excluded
- (11) ($d_0>0$, $b_0<0$) condition satisfied if $S<|d_0b_0|$
- (12) ($d_0<0$, $b_0>0$) condition satisfied if $S<|d_0b_0|$

D: $d_0^2<1$, $\mathbb{k}=-1$, $0<-d_0b_0+S$
- (13) ($d_0>0$, $b_0>0$) condition satisfied if $|d_0b_0|<S$
- (14) ($d_0<0$, $b_0<0$) condition satisfied if $|d_0b_0|<S$
- (15) ($d_0>0$, $b_0<0$) condition satisfied
- (16) ($d_0<0$, $b_0>0$) condition satisfied

Summary of Condition 1

$d_0^2>1$, $\mathbb{k}=-1$, $(d_0>0, b_0<0)$ and $(d_0<0, b_0>0)$ are excluded
$d_0^2<1$, $\mathbb{k}=+1$, $(d_0>0, b_0>0)$ and $(d_0<0, b_0<0)$ are excluded

2. $\cosh(\eta_0)>0$

$$\frac{b_0+d_0\mathbb{k}S}{d_0^2-1}>0$$

A: $d_0^2>1$, $\mathbb{k}=+1$, $0<b_0+d_0S$
(1) $(d_0>0, b_0>0)$ condition satisfied
(2) $(d_0<0, b_0<0)$ condition excluded
(3) $(d_0>0, b_0<0)$ condition satisfied if $|b_0|<d_0S$
(4) $(d_0<0, b_0>0)$ condition satisfied if $|b_0|>|d_0|S$
B: $d_0^2>1$, $\mathbb{k}=-1$, $0<b_0-d_0S$
(5) $(d_0>0, b_0>0)$ condition satisfied if $d_0S<b_0$
(6) $(d_0<0, b_0<0)$ condition satisfied if $|d_0|S>|b_0|$
(7) $(d_0<0, b_0>0)$ condition satisfied
(8) $(d_0>0, b_0<0)$ condition excluded
C: $d_0^2<1$, $\mathbb{k}=+1$, $0<-b_0-d_0S$
(9) $(d_0>0, b_0>0)$ condition excluded
(10) $(d_0<0, b_0<0)$ condition satisfied
(11) $(d_0>0, b_0<0)$ condition satisfied if $|b_0|>d_0S$
(12) $(d_0<0, b_0>0)$ condition satisfied if $b_0<|d_0|S$
D: $d_0^2<1$, $\mathbb{k}=-1$, $0<-b_0+d_0S$
(13) $(d_0>0, b_0>0)$ condition satisfied if $|b_0|<d_0S$
(14) $(d_0<0, b_0<0)$ condition satisfied if $|b_0|>|d_0|S$
(15) $(d_0<0, b_0>0)$ condition excluded
(16) $(d_0>0, b_0<0)$ condition satisfied
Summary of Condition 2
$d_0^2>1$, $\mathbb{k}=+1$, $(d_0<0, b_0<0)$ is excluded
$d_0^2>1$, $\mathbb{k}=-1$, $(d_0>0, b_0<0)$ is excluded
$d_0^2<1$, $\mathbb{k}=+1$, $(d_0>0, b_0>0)$ is excluded
$d_0^2<1$, $\mathbb{k}=-1$, $(d_0<0, b_0>0)$ is excluded
When the constraints for the two conditions are put together, the cases
$k=+1$, $d_0<0$, $b_0>0$, are eliminated for both $d_0^2>1$ and $d_0^2<1$.
Summary of existing cases after hyperbolic conditions are imposed

$$d_0^2>1:\mathbb{k}=+1 \tag{A2}$$

$$(d_0>0,\ b_0>0)$$

$$(d_0>0,\ b_0<0):\ |d_0b_0|<S,\ \left|\frac{b_0}{d_0}\right|<S$$

$$d_0^2>1:\mathbb{k}=-1 \tag{A3}$$

$$(d_0>0,\ b_0>0):S<|d_0b_0|,\ S<\left|\frac{b_0}{d_0}\right|$$

$$(d_0<0,\ b_0<0):\ S<|d_0b_0|,\ S>\left|\frac{b_0}{d_0}\right|$$

$$d_0^2<1:\mathbb{k}=+1 \tag{A4}$$

$$(d_0>0,\ b_0<0): S<|d_0 b_0|,\ S<\left|\frac{b_0}{d_0}\right|$$

$$d_0^2<1: \mathbb{k}=-1 \tag{A5}$$

$$(d_0>0,\ b_0>0):\ S>|d_0 b_0|,\ S>\left|\frac{b_0}{d_0}\right|$$

$$(d_0<0,\ b_0<0):\ S>|d_0 b_0|,\ S<\left|\frac{b_0}{d_0}\right|$$

$$(d_0>0,\ b_0<0).$$

Now we require the fluid density inside the torus to be positive:

$$8\pi a^2\rho=(b_0/h)[\cosh^2(\eta_0)-\cos^2(\vartheta)]>0.$$

$\cosh(\eta_0)$ will always be greater than 1 since it equals 1 at $\eta=0$, which is outside of the torus interior. In the interior $\eta_0\leqslant\eta\leqslant\infty$. We have

$$\frac{b_0}{d_0\sinh(\eta_0)-b_0}>0,$$

$$\frac{1}{\frac{d_0}{b_0}\sinh(\eta_0)-1}>0,$$

$$\frac{d_0}{b_0}\,\frac{b_0 d_0+\mathbb{k}S}{d_0^2-1}>1.$$

3. $d_0^2>1$

$$d_0^2+\mathbb{k}\frac{d_0}{b_0}S>d_0^2-1$$

$$-\mathbb{k}\frac{d_0}{b_0}S<1$$

$\mathbb{k}=+1$, $(b_0>0,\ d_0>0)$ and $(b_0<0,\ d_0<0)$. No constraints

$\mathbb{k}=-1$, $(b_0>0,\ d_0>0)$ and $(b_0<0,\ d_0<0)$ with constraint $\left|\frac{d_0}{b_0}\right|S<1$

4. $d_0^2<1$

$$-d_0^2-\mathbb{k}\frac{d_0}{b_0}S>1-d_0^2$$

$$-\mathbb{k}\frac{d_0}{b_0}S>1$$

$$\mathbb{k}=+1,\ (b_0<0,\ d_0>0)\ \text{with constraint}\ S>\left|\frac{b_0}{d_0}\right| \tag{A6}$$

$$\mathbb{k}=-1,\ (b_0>0,\ d_0>0)\ \text{and}\ (b_0<0,\ d_0<0)\ \text{with constraint}\ S>\left|\frac{b_0}{d_0}\right|$$

Summarizing all constraints provides

$$d_0^2>1:\mathbb{k}=+1 \tag{A7}$$

$$(d_0>0,\ b_0>0)$$

$$(d_0>0,\ b_0<0):\ |d_0b_0|<S,\ \left|\frac{b_0}{d_0}\right|<S,\ S<\left|\frac{b_0}{d_0}\right|\ \text{is excluded}$$

$$d_0^2>1:\mathbb{k}=-1 \tag{A8}$$

$$(d_0>0,\ b_0>0):S<|d_0b_0|,\ S<\left|\frac{b_0}{d_0}\right|$$

$$(d_0<0,\ b_0<0):\ S<|d_0b_0|,\ S>\left|\frac{b_0}{d_0}\right|,\ S<\left|\frac{b_0}{d_0}\right|\ \text{is excluded}$$

$$d_0^2<1:\mathbb{k}=+1 \tag{A9}$$

$$(d_0>0,\ b_0<0):S<|d_0b_0|,\ S<\left|\frac{b_0}{d_0}\right|,\ S>\left|\frac{b_0}{d_0}\right|\ \text{is excluded}$$

$$d_0^2<1:\mathbb{k}=-1 \tag{A10}$$

$$(d_0>0,\ b_0>0):\ S>|d_0b_0|,\ S>\left|\frac{b_0}{d_0}\right|$$

$$(d_0<0,\ b_0<0):\ S>|d_0b_0|,\ S<\left|\frac{b_0}{d_0}\right|,\ S>\left|\frac{b_0}{d_0}\right|\ \text{is excluded}$$

$$(d_0>0,b_0<0)\ \text{is excluded}$$

The three allowed parameter combinations are

$$d_0^2>1:\mathbb{k}=+1\ \ (d_0>0,\ b_0>0)$$

$$d_0^2>1:\mathbb{k}=-1\ \ (d_0>0,\ b_0>0):S<|d_0b_0|,\ S<\left|\frac{b_0}{d_0}\right|$$

$$d_0^2<1:\mathbb{k}=-1\ \ (d_0>0,\ b_0>0):\ S>|d_0b_0|,\ S>\left|\frac{b_0}{d_0}\right|$$

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Prolongation methods and Cartan characters for the three-dimensional Riemann–Lanczos problem

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(Received 21 February 2003; accepted 26 March 2003)

The Riemann–Lanczos problem in two dimensions is in involution and its general solution is known. The three-dimensional Riemann–Lanczos problem is not in involution and needs to be prolongated. We write the three-dimensional Riemann–Lanczos problem as an exterior differential system and prolong it to second order. Using algebraic computing we find that we have to add an integrability condition to make it a system in involution. We also suggest a prolongation of the three-dimensional Riemann–Lanczos problem in the same way as Bampi and Caviglia did for four dimensions. After supplementing this three-dimensional system with an integrability condition, it becomes involutive with Cartan characters (17,8,2) or (20,10,3) if no cyclic conditions are imposed. We present the relevant sections of REDUCE computer codes by means of which these results were obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1578181]

I. INTRODUCTION

Apart from the Weyl conformal tensor, which can be expressed by means of a third-order tensor potential, an expression which was first found by Lanczos,[1] we can also express the Riemann tensor using a third-order tensor potential. This third-order tensor potential is usually called the **Lanczos tensor** and its components are denoted by L_{abc}. For the Weyl–Lanczos problem as well as for the Riemann–Lanczos problem the Lanczos tensor components L_{abc} are subject to the following symmetry condition,

$$L_{abc}=L_{[ab]c}, \tag{1}$$

and, sometimes, we also impose the cyclic conditions

$$L_{[abc]}=0. \tag{2}$$

In this paper we confine ourselves to the discussion of the **Riemann-Lanczos equations** which were first published in Ref. 2 as

$$R_{abcd}=L_{abc;d}-L_{abd;c}+L_{cda;b}-L_{cdb;a}. \tag{3}$$

For practical reasons we will often write Eqs. (3) in solved form as

$$f^{(R)}_{abcd}=R_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a} \tag{4}$$

denoted by $f^{(R)}_{abcd}$. If we impose (1) together with (2), we obtain two independent components L_{abc} in two dimensions, eight independent components in three dimensions and 20 independent components L_{abc} in four dimensions. We also have one independent Riemann–Lanczos equation in

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two dimensions, six independent in three dimensions and 20 independent Riemann–Lanczos equations in four dimensions. Unless stated otherwise we will not impose the differential gauge conditions

$$L_{ab}{}^{s}{}_{;s}=0\,. \tag{5}$$

We *never* assume the trace-free gauge conditions

$$L_{a}{}^{s}{}_{s}=0 \tag{6}$$

to hold for the Riemann–Lanczos problem because then we would automatically obtain $R=0$ for the Ricci scalar which leads to inconsistencies.

As explained in Refs. 3 and 4, Eqs. (3) do not form a system in involution in four dimensions and a prolongation is presented there. The work in this article is based on Refs. 3–6 for the Riemann–Lanczos problem as an exterior differential system. First, we are going to present a few results already known for the Riemann–Lanczos problems in two and three dimensions. Then we are going to use the theory of **exterior differential systems (EDS)** and algebraic computing to present two different prolongations for the three-dimensional Riemann–Lanczos problem to make it involutive, and, we compute its **Cartan characters**. Algebraic computing supports the calculations as some can be very cumbersome such as the computation of the Cartan characters. There are programs developed by Wahlquist and Estabrook based on MATEMATICA which compute Cartan characters, and, applications of these programs can be found in Ref. 7. Here, we are going to use the REDUCE package EDS by Hartley[8] and present the relevant sections of computer codes we used in Appendices A, B and C.

II. THE RIEMANN–LANCZOS PROBLEM AS AN EDS

Exterior differential systems (EDS) in general and Cartan characters in particular are discussed in Refs. 9–13. We can express the Riemann–Lanczos problem as an exterior differential system (EDS) as it was done in Ref. 3. We use a first-order jet bundle $\mathcal{J}^1(\mathbb{R}^n,\mathbb{R}^m)$, where n denotes the number of local space–time coordinates and m is the number of independent Lanczos components L_{abc}. Local coordinates are then given by (x^e,L_{abc},P_{abcd}) characterizing a formal manifold $\mathcal{M}$ of dimension $N=n+m+n\cdot m$. The EDS itself is formed by

$$\begin{aligned} df^{(R)}_{abcd}&=d(R_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}),\\ K_{abc}&=dL_{abc}-P_{abce}dx^e\ , \end{aligned} \tag{7}$$

where sometimes $f^{(R)}_{abcd}=0$ is also assumed, which in subsequent cases does not change any of the results obtained except that it reduces the values of the zeroth Cartan characters s_0 and their reduced counterparts s_0'. The K_{abc} are the **first-order contact conditions** and the P_{abcd} coincide with $P_{abcd}=\partial L_{abc}/\partial x^d$ when projected onto the space–time manifold. Next, we briefly recast the results already known for the Riemann–Lanczos problems in two and in three dimensions. Some of these results were obtained using Janet–Riquier theory[14–16] of which modernized versions can be found in Refs. 17–19.

A. The Riemann–Lanczos problem in two dimensions

The Riemann–Lanczos problem in two dimensions was discussed in Refs. 5 and 6. We choose $(x^1,x^2,L_{121},L_{122},P_{1211},P_{1212},P_{1221},P_{1222})$ as local coordinates on $\mathcal{J}^1(\mathbb{R}^2,\mathbb{R}^2)$ so that the corresponding formal manifold $\mathcal{M}$ is eight-dimensional. We leave the metric tensor components completely arbitrary and obtain the only independent Riemann–Lanczos equation in solved form,

$$f^{(R)}_{1212}=R_{1212}-2P_{1212}+2P_{1221}+2L_{121}(\Gamma^1_{12}-\Gamma^2_{22})-2L_{122}(\Gamma^1_{11}+\Gamma^2_{12})\ , \tag{8}$$

where Γ^a_{bc} are the Christoffel symbols. We can write the Pfaffian system derived from (8) as

$$\theta^1=\alpha_{12121}dx^1+\alpha_{12122}dx^2-2dP_{1212}+2dP_{1221}+2(\Gamma^1_{12}-\Gamma^2_{22})dL_{121}-2(\Gamma^1_{11}+\Gamma^2_{12})dL_{122},$$

$$\theta^2=dL_{121}-P_{1211}dx^1-P_{1212}dx^2\ , \tag{9}$$

$$\theta^3=dL_{122}-P_{1221}dx^1-P_{1222}dx^2\ ,$$

where θ^1 is the exterior derivative of $f^{(R)}_{abcd}$ and the one-forms θ^2,θ^3 are the two contact conditions. The quantity α_{1212e} is given by

$$\alpha_{1212e}=R_{1212,e}-2L_{121}(\Gamma^1_{12,e}-\Gamma^2_{22,e})-2L_{122}(\Gamma^1_{11,e}+\Gamma^2_{12,e}) \tag{10}$$

for $e=1,2$. We obtained the result that the Riemann–Lanczos problem in two dimensions is in involution with Cartan characters $(s_0,s_1,s_2)=(3,2,1)$.[5,6] If the exterior derivative of (5) given by $dL_{12}{}^s_{;s}=0$ is included in (9), the problem remains in involution with Cartan characters $(s_0,s_1,s_2)=(4,2,0)$. These results are confirmed using Janet–Riquier theory.[6]

The general solution to the Riemann–Lanczos problem in two dimensions is known.[5] For a space–time with Lorentzian signature given by

$$ds^2=-e^{2\rho}dx^1dx^2\ ,$$

where ρ is an arbitrary function of x^1 and x^2, the general solution is

$$L_{121}=e^{2\rho}(f_1(x^1)-\tfrac{1}{4}\rho_{,1})\ ,\quad L_{122}=e^{2\rho}(f_2(x^2)+\tfrac{1}{4}\rho_{,2})\ ,$$

where $f_1(x^1),f_2(x^2)$ are two arbitrary functions depending on one local coordinate each. For spaces with Euclidean signature given by

$$ds^2=e^{2\rho}((dx^1)^2+(dx^2)^2)\ ,$$

where ρ is again an arbitrary function of x^1 and x^2, the general solution is

$$L_{121}=e^{2\rho}(f_1(x^1+x^2)-\tfrac{1}{2}\rho_{,2})\ ,\quad L_{122}=e^{2\rho}(f_2(x^1-x^2)+\tfrac{1}{2}\rho_{,1})\ .$$

Both solutions depend on two arbitrary functions of one variable each, a fact which reflects the intrinsic meaning of the highest nonvanishing Cartan character which is in the two above cases $s_1=2$. (Here we also imposed the differential gauge condition $L_{12}{}^s_{;s}=0$. For more details see Ref. 5.)

B. The Riemann–Lanczos problem in three dimensions

In three space–time dimensions with local coordinates x^1, x^2, x^3, we obtain eight independent components of the Lanczos tensor, namely, L_{121}, L_{122}, L_{131}, L_{133}, L_{232}, L_{233}, L_{123}, L_{132} when imposing the cyclic conditions (2). Each of the components has three first-order partial derivatives so that we use the jet bundle $\mathcal{J}^1(\mathbb{R}^3,\mathbb{R}^8)$ with formal dimension $N=3+8+24=35$ to express the EDS. There are six independent Riemann–Lanczos equations whose exterior derivatives are $df^{(R)}_{1212}$, $df^{(R)}_{1313}$, $df^{(R)}_{2323}$, $df^{(R)}_{1213}$, $df^{(R)}_{1223}$, $df^{(R)}_{1323}$ and eight contact conditions K_{abc}. In this way, we obtain for the zeroth Cartan character and its reduced counterpart $s_0=s_0'=6+8=14$. Using the above local coordinates the EDS is then again of the form (7). It is sufficient to consider line elements with diagonalized metric tensor because of Ref. 20.

As discussed in detail in Ref. 6 an identity occurs so that for the second Cartan character $s_2=s_2'+1$ leading to $s_2'=7$ and to $s_2=8$. This means that the necessary condition for a system to be in involution requiring that each Cartan character coincides with its reduced counterpart[9,10,13] is not fulfilled and the three-dimensional Riemann–Lanczos problem is not in involution and its reduced characters (s_0',s_1',s_2',s_3') are (14,8,7,3). This result was confirmed with the REDUCE code given in Appendix A.

We also used Janet–Riquier theory to examine the three-dimensional Riemann–Lanczos problem further. After a prolongation to second order we found that the *integrability condition I*, given in solved form as

$$I = f^{(R)}_{1212,33} + f^{(R)}_{1313,22} + f^{(R)}_{2323,11} - 2\, f^{(R)}_{1323,12} - 2\, f^{(R)}_{1213,23} + 2\, f^{(R)}_{1223,13}, \tag{11}$$

had to be added so that the new prolonged system is given by

$$0 = f^{(R)}_{abcd}, \quad 0 = f^{(R)}_{abcd,e}, \quad 0 = I\ . \tag{12}$$

In Ref. 5 it is shown in detail that the system (12) consists of a system in involution with Cartan characters (18,9,2) when (2) is also imposed. There, the integrability condition (11) is also expressed in a better form respecting general covariance, namely, as I_{Cov}:

$$\begin{aligned} I_{Cov} &= 2(f^{(R)}_{1212;(33)} + f^{(R)}_{1313;(22)} + f^{(R)}_{2323;(11)} - f^{(R)}_{1323;(12)} - f^{(R)}_{1213;(23)} + f^{(R)}_{1223;(13)}) \\ &= B_{12123;3} + B_{13132;2} + B_{23231;1} = 0\ , \end{aligned} \tag{13}$$

where the B_{abcde} are $B_{abcde} = f^{(R)}_{ab[cd;e]}$, which reduce to the Bianchi identities for the R_{abcd} involved. The covariantly prolonged system, where we add the covariant derivatives instead of the partial derivatives, is then given by

$$0 = f^{(R)}_{abcd}, \quad 0 = f^{(R)}_{abcd;e}, \quad 0 = I_{Cov}\ . \tag{14}$$

This also forms a system in involution again with Cartan characters (18,9,2),[5] and we prefer it to (12) because it is based on covariant differentiation rather than partial differentiation. Next, we are going to present two different prolongation methods based on the theory of exterior differential systems (EDS) which will lead to the same result.

III. A PROLONGATION USING EDS AND JET BUNDLES

In this section we show that we can use computer algebra to express the systems (12) and (14) as EDS and obtain results in agreement with those for the three-dimensional Riemann–Lanczos problem based on Janet–Riquier theory. We introduce S_{abcde} as second-order jet coordinates so that our local coordinates are now given by $(x^e, L_{abc}, P_{abcd}, S_{abcde})$ on a jet bundle $\mathcal{J}^2(\mathbb{R}^3, \mathbb{R}^8)$ with formal dimension $N = 3 + 8 + 24 + 48 = 83$. Again, we obtain $P_{abcd} = \partial L_{abc}/\partial x^d$ and $S_{abcde} = \partial^2 L_{abc}/\partial x^d \partial x^e$ if P_{abcd} and S_{abcde} are projected onto the space–time manifold. The prolonged system is then given by

$$\begin{aligned} f^{(R)}_{abcd} &= R_{abcd} - L_{abc;d} + L_{abd;c} - L_{cda;b} + L_{cdb;a}\ , \\ K_{abc} &= dL_{abc} - P_{abce} dx^e, \quad K_{abcd} = dP_{abcd} - S_{abcde} dx^e\ , \end{aligned} \tag{15}$$

where K_{abcd} are the **second-order contact conditions**. When applying a computer code of which extracts are given in Appendix B, combined with the one in Appendix A to this system, we find that (15) is clearly *not in involution* with reduced Cartan characters (s'_1, s'_2, s'_3) given by (18,9,3) with (2) imposed and given by (21,11,4) otherwise. However, if we add either of the conditions I_{Cov} or I, respectively, and augment (15) to the system

$$\begin{aligned} I_{Cov} &= B_{12123;3} + B_{13132;2} + B_{23231;1} \qquad (\text{or } I), \\ f^{(R)}_{abcd} &= R_{abcd} - L_{abc;d} + L_{abd;c} - L_{cda;b} + L_{cdb;a}\ , \\ f^{(R)}_{abcd;e} &= R_{abcd;e} - L_{abc;de} + L_{abd;ce} - L_{cda;be} + L_{cdb;ae} \quad (\text{or } f^{(R)}_{abcd,e}), \\ K_{abc} &= dL_{abc} - P_{abce} dx^e, \end{aligned} \tag{16}$$

$$K_{abcd}=dP_{abcd}-S_{abcde}dx^e\ ,$$

the system (16) turns out to be in involution with its set of Cartan characters (s_1,s_2,s_3) being (17,8,2) if (2) is imposed or (20,10,3) if no cyclic conditions are imposed. These results were obtained using computer codes of which details are given in the Appendixes A and B. We could derive the results for all metrics of the form

$$ds^2=(dx^1)^2-b\cdot(dx^2)^2-c\cdot(dx^3)^2\ , \tag{17}$$

where the functions b and c depend on one local coordinate each, or where either or both were precisely given in terms of local coordinates. Further, the results were also obtained for some space–times typically given with nondiagonal line element such as the reduced Gödel space–time. The restrictions of the results are due to limited memory available for computing. We believe that when the use of memory is economized further, we will be able to generalize these results to all three-dimensional spacetimes.

There is a reason why we do not obtain the Cartan characters (18,9,2), as we did when using Janet–Riquier theory, when we apply the theory of exterior differential systems. If we look at the system (15), we obtain its reduced characters to be (18,9,3) and that the system is not in involution. Using the integrability condition I_{Cov} (or I), we can express one of the S_{abcde} in terms of the other such second-order jet variables plus lower-order terms. We then build our integral elements for the system (16) which are our tangent spaces of an integral manifold representing a solution to our system of equations (for details see Refs. 9–13). When we construct the first **integral element** $(E^1)_x$ at a point $x\in\mathcal{M}$, we express one of the dS_{abcde} through the others which causes the value of the first reduced Cartan character s_1' to drop by one from 18 to $s_1'=17$. The same procedure applies at the second stage for a two-dimensional integral element $(E^2)_x$ so that $s_2'=8$, and, at the third stage for a three-dimensional integral element $(E^3)_x$ we have $s_3'=2$. Because the system (16) is involutive, which we could show for all spacetimes of type (17) using algebraic computing, these are equally the values for the Cartan characters themselves. Therefore, we obtain for the Cartan characters (17,8,2) with (2) imposed or (20,10,3) otherwise when we use the theory of EDS. This does not contradict the values obtained in Ref. 5 based on Janet–Riquier theory. The above results for the Cartan characters and for involutivity were computed using computer codes based on extracts of a code given in Appendix B added to a modified version of that in Appendix A for metric line elements as explained above based on (17). Next, we will examine whether the same kind of prolongation as suggested in Ref. 4 for four dimensions does lead to an involutive system in three dimensions.

IV. A PROLONGATION BASED ON TENSOR DECOMPOSITIONS

It is instructive to look at a prolongation for the Riemann–Lanczos problem in three dimensions constructed in the same way as Bampi and Caviglia did in Ref. 4 for four dimensions and to see whether this leads to an involutive system in three dimensions. We are going to use the local coordinates (x^a,L_{abc},P_{abcd}) again but not the S_{abcde} in this approach. In order to obtain a complete coframe with $N=3+8+24=35$ elements [or $N=3+9+27=39$ if we do not impose the cyclic conditions (2)] and from that to obtain further coordinates, we introduce the 18 new one-forms [or 21 if (2) is not imposed]

$$\omega_{abcd}=dP_{abcd}-dP_{\{abcd\}}=(\overline{\omega}_{abcde}+\hat{\omega}_{abcde})dx^e\ , \tag{18}$$

where the brackets $\{abcd\}$ indicate a Riemann-type symmetry imposed on the indices $abcd$.[3] The quantities $\overline{\omega}_{abcde}$ and $\hat{\omega}_{abcde}$ have the same symmetry conditions as in Ref. 4 only here for three dimensions, namely,

$$\begin{aligned}\overline{\omega}_{abcde}&=\overline{\omega}_{[ab][cd]e}=-\overline{\omega}_{cdabe}\,,\\ \hat{\omega}_{abcde}&=\hat{\omega}_{[ab](cd)e}\,.\end{aligned} \tag{19}$$

Even though we are not going to use the S_{abcde}, which correspond to the second-order partial derivatives $S_{abcde}=\partial^2 L_{abc}/\partial x^d \partial x^e$ when projected onto the spacetime manifold, it has to hold

$$S_{abc[de]}=\overline{\omega}_{abc[de]}+\hat{\omega}_{abc[de]}+A_{abc[de]}=0\,,$$

where the quantity $A_{abcde}=A_{\{abcd\}e}$ is given by

$$A_{abcde}=\frac{1}{4}\left(\frac{\partial f^{(R)}_{abcd}}{\partial x^e}-S_{abcde}+S_{abdce}-S_{cdabe}+S_{cdbae}\right)\,, \tag{20}$$

and does no longer contain any terms involving S_{abcde}. Now, we add the $\overline{\omega}_{abcde}$ and $\hat{\omega}_{abcde}$ as new coordinates of a formal manifold $\mathcal{M}$ with local coordinates $(x^e, L_{abc}, P_{abcd}, \overline{\omega}_{abcde}, \hat{\omega}_{abcde})$ of formal dimension $N=3+9+27+63=102$ without the cyclic conditions and $N=3+8+24+54=89$ when taking the cyclic conditions (2) into account. Our prolonged EDS in three dimensions using this prolongation method is then given by

$$\begin{aligned}
f^{(R)}_{abcd}&=R_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}\,,\\
\mathcal{W}_{abcde}&=\overline{\omega}_{abc[de]}+\hat{\omega}_{abc[de]}+A_{abc[de]}\,,\\
K_{abc}&=dL_{abc}-P_{abce}dx^e,\\
K_{abcd}&=dP_{abcd}-(\overline{\omega}_{abcde}+\hat{\omega}_{abcde}+A_{abcde})dx^e,\\
d\mathcal{W}_{abcde}&=d\overline{\omega}_{abc[de]}+d\hat{\omega}_{abc[de]}+B_{abc[de]f}dx^f\,,
\end{aligned} \tag{21}$$

where $dA_{abcde}=B_{abc[de]f}dx^f$ and $B_{abcdef}=B_{abcd(ef)}=B_{\{abcd\}ef}$ for the same reasons as discussed in Ref. 4, and K_{abcd} are the one-forms corresponding to the second-order contact conditions expressed in terms of the variables $\overline{\omega}_{abcde}$ and $\hat{\omega}_{abcde}$. Using a computer code producing the system (21) of which details are given in Appendix C below, we see that the system (21) is clearly *not in involution* with reduced characters (18,9,3) if (2) is imposed or (21,11,4) if (2) is not imposed. Using the commands *torsion* and *prolong* from the EDS package,[8] which suggests prolongations wherever possible, we see that an integrability condition has to be added to (21) in order to make it an involutive system. After some calculations and further algebraic computations, we find that we have to add *precisely* I_{Cov} given in (13) [or I given in (11) also possible] again, which is *the same integrability condition* as for the EDS before and also the one obtained by Janet–Riquier theory. The new augmented system is now given by

$$\begin{aligned}
I_{Cov}&=B_{12123;3}+B_{13132;2}+B_{23231;1}\qquad(\text{or } I),\\
f^{(R)}_{abcd}&=R_{abcd}-L_{abc;d}+L_{abd;c}-L_{cda;b}+L_{cdb;a}\,,\\
\mathcal{W}_{abcde}&=\overline{\omega}_{abc[de]}+\hat{\omega}_{abc[de]}+A_{abc[de]}\,,\\
K_{abc}&=dL_{abc}-P_{abce}dx^e,\\
K_{abcd}&=dP_{abcd}-(\overline{\omega}_{abcde}+\hat{\omega}_{abcde}+A_{abcde})dx^e,\\
d\mathcal{W}_{abcde}&=d\overline{\omega}_{abc[de]}+d\hat{\omega}_{abc[de]}+B_{abc[de]f}dx^f\,.
\end{aligned} \tag{22}$$

We find that the system (22) is involutive with Cartan characters (17,8,2) if we impose the cyclic conditions (2) and with Cartan characters (20,10,3) otherwise. Again, these results were obtained for metrics of the form (17) and the results were computed using computer codes based on those

given in Appendixes A and C. We conclude that in three dimensions it is not sufficient to simply prolong the Riemann–Lanczos problem to a second-order system but we must also add the integrability condition $ICov$ (or I) to make it a system in involution.

V. CONCLUSION

As opposed to two dimensions, in three dimensions the Riemann–Lanczos problem is not in involution and we showed that when we prolongate it to second order using the theory of exterior differential systems and add the integrability condition $ICov$ (or I), it turns into an involutive system with Cartan characters (17,8,2) with cyclic conditions imposed or with characters (20,10,3) when no cyclic conditions are imposed. This confirms a result given in Ref. 5, where Janet–Riquier theory was used.

When we use the prolongation method by Bampi and Caviglia[4] applied to three dimensions, we find that this prolonged system is clearly not in involution in three dimensions. However, after supplementing it with the *same integrability condition* $ICov$ (or I), it becomes involutive and its Cartan characters are again (17,8,2) with (2) imposed or (20,10,3) otherwise. The above results were obtained for space–times which admit metric line elements of type (17) using algebraic computing based on the REDUCE package EDS. It is of interest to improve the efficiency of the computer codes further so that we can obtain the above results for all three-dimensional space–times using algebraic computing.

ACKNOWLEDGMENTS

The author would like to thank D. Hartley, T. Wolf and W. M. Seiler for valuable discussions. The author would also like to thank the Dr. Robert Thyll-Dürr Foundation for further support and the Région Centre for a grant at the University of Tours.

APPENDIX A: EDS AND COMPUTER ALGEBRA

The REDUCE package EDS by D. Hartley[8] is a very reliable algebraic computing package when one wants to calculate properties of EDS. In Ref. 8 important commands such as **eds**, **contact**, **pde2eds**, **pullback**, **lift**, **restrict**, **characters**, **involution**, **torsion**, and **prolong** are explained in detail. They and further available commands perform all important calculations for exterior differential systems efficiently.

The computer code, which creates the unprolonged Riemann–Lanczos equations in three dimensions, is given next, where a version for four dimensions can be found in Ref. 6. We use the package EXCALC here first to create the differential forms for the exterior differential system used later on because some of the jet variables below do contain nontensorial indices. The package EDS uses the contravariant components of quantities in all expressions whereas EXCALC uses covariant components (see Ref. 21 for details on REDUCE packages). After that we use the package EDS to calculate properties of our exterior differential system so created. First, we introduce the notation used in the computer codes below, where all indices run over the three space–time dimensions denoted by t, x, y here.

chr(a,−b,−c)	Christoffel symbols,
Rie(−a,−b,−c,−d)	Components of the Riemann tensor,
Ric(−a,−b), R	Ricci tensor and Ricci scalar,
f(−a,−b,−c,−d), w1(−a,−b,−c,−d)	Riemann-Lanczos equations, ext. derivatives,
gau(−a,−b), w2(−a,−b)	Differential gauge conditions, ext. der.s,
L(−a,−b,−c)	Components of the Lanczos potential,
P(−a,−b,−c,−d)	First-order jet variables of L(−a,−b,−c),
S(−a,−b,−c,−d,−e)	Second-order jet variables of L(−a,−b,−c),
V(−a,−b,−c,−d,−e,−f)	Third-order jet variables of L(−a,−b,−c),
w3(−a,−b,−c)	First-order contact conditions.

```
load excalc;
on div; on nero;
pform {b,c}=0; fdomain b=b(t,x,y); fdomain c=c(t,x,y);
coframe o(t)=d t,
        o(x)=d x,
        o(y)=d y with metric
           g=o(t)*o(t)-b*o(x)*o(x)-c*o(y)*o(y);
frame e;
riemannconx om;
pform curv(a,b)=2; pform chr(a,-b,-c)=0;
curv(a,-b):=d om(a,-b)+om(a,-c) ^ om(c,-b);
chr(a,-b,-c):=e(-c)_|om(a,-b);

%Computation of the curvature tensors:
pform {Rie(a,b,c,d),Ric(a,b),Wey(a,b,c,d)}=0;
index_symmetries curv(a,b)     : antisymmetric in {a,b};
index_symmetries Rie(a,b,c,d)  : antisymmetric in {a,b}, {c,d}
                                 symmetric in {{a,b},{c,d}};
index_symmetries Ric(a,b)      : symmetric in {a,b};
index_symmetries Wey(a,b,c,d) : antisymmetric in {a,b}, {c,d}
                                 symmetric in {{a,b},{c,d}};
Rie(a,b,c,d):==e(d)_|(e(c)_|curv(a,b));
Rie(-a,-b,-c,-d):=Rie(-a,-b,-c,-d);
Ric(-a,-b):=g(n,s)*Rie(-n,-a,-s,-b);
R:=g(a,b)*Ric(-a,-b);
Wey(-a,-b,-c,-d):=Rie(-a,-b,-c,-d)+(1/2)*R*(g(-a,-c)*g(-b,-d)
                        -g(-a,-d)*g(-b,-c))
                        -(g(-a,-c)*Ric(-b,-d)-g(-b,-c)*Ric(-a,-d)
                          +g(-b,-d)*Ric(-a,-c)-g(-a,-d)*Ric(-b,-c));

pform {L(-a,-b,-c),P(-a,-b,-c,-d)}=0;
index_symmetries L(-a,-b,-c)     : antisymmetric in {-a,-b};
index_symmetries P(-a,-b,-c,-d) : antisymmetric in {-a,-b};
%First part of the cyclic conditions if imposed:
L(-x,-y,-t):=L(-t,-y,-x)-L(-t,-x,-y);
P(-x,-y,-t,-t):=P(-t,-y,-x,-t)-P(-t,-x,-y,-t);
P(-x,-y,-t,-x):=P(-t,-y,-x,-x)-p(-t,-x,-y,-x);
P(-x,-y,-t,-y):=P(-t,-y,-x,-y)-P(-t,-x,-y,-y);

%Creation of Covariant Derivatives KD(-a,-b,-c,-d) of L(-a,-b,-c):
pform K(-a,-b,-c)=1; pform KD(-a,-b,-c,-d)=0;
index_symmetries K(-a,-b,-c)      : antisymmetric in {-a,-b};
index_symmetries KD(-a,-b,-c,-d) : antisymmetric in {-a,-b};
K(-a,-b,-c):=P(-a,-b,-c,-n)*o(n)-L(-n,-b,-c)*om(n,-a)
                -L(-a,-n,-c)*om(n,-b)-L(-a,-b,-n)*om(n,-c);

KD(-a,-b,-c,-d):=e(-d)_|K(-a,-b,-c);
%Riemann-Lanczos equations:
pform {f(-a,-b,-c,-d),gau(-a,-b)}=0;
pform {w1(-a,-b,-c,-d),w2(-a,-b),w3(-a,-b,-c)}=1;
```

```
index_symmetries f(-a,-b,-c,-d)  : antisymmetric in {-a,-b}, {-c,-d}
                                   symmetric in {{-a,-b},{-c,-d}};
index_symmetries w1(-a,-b,-c,-d) : antisymmetric in {-a,-b}, {-c,-d}
                                   symmetric in {{-a,-b},{-c,-d}};
index_symmetries gau(-a,-b)      : antisymmetric in {-a,-b};
index_symmetries w2(-a,-b)       : antisymmetric in {-a,-b};
index_symmetries w3(-a,-b,-c)    : antisymmetric in {-a,-b};
f(-a,-b,-c,-d):=Rie(-a,-b,-c,-d)-KD(-a,-b,-c,-d)+KD(-a,-b,-d,-c)
                -KD(-c,-d,-a,-b)+KD(-c,-d,-b,-a);
gau(-a,-b)     :=KD(-a,-b,s,-s);
%PART(*): Creation of EDS
w1(-a,-b,-c,-d):=d f(-a,-b,-c,-d);
w2(-a,-b):=d gau(-a,-b);
w3(-a,-b,-c):=d L(-a,-b,-c)-P(-a,-b,-c,-n)*o(n);
load eds;
coframing({o(a),d L(-a,-b,-c),d P(-a,-b,-c,-d)});
myedsrr:=EDS({w3(-a,-b,-c),f(-a,-b,-c,-d)},{o(a)});
myedsr:=lift myedsrr;

%If necessary, store ''myedsr'' in an output file.
% PART (**): Computation of Cartan characters
%Computation of the Cartan characters, torsion, checks for
%involution, linearity and further properties.
%Reload ''myedsr'' first if output file was created and load eds:
on ranpos;      %''on genpos'' if more memory available
characters myedsr;
involutive myedsr;
quasilinear myedsr; semilinear myedsr;
torsion myedsr; tableau myedsr;
prolong myedsr;
end;
```

This produces the result that the Riemann–Lanczos problem in three dimensions is not in involution with reduced characters (18,9,3) if the cyclic conditions are imposed or (21,11,4) if they are not imposed.

APPENDIX B: THE PROLONGED RIEMANN–LANCZOS PROBLEM USING JET BUNDLES

Here, we give the important sections of a computer code producing the prolonged EDS including the integrability condition $ICov$ (or I) as discussed in Sec. III. This part has to be combined with the code given in Appendix A omitting part (*) and part (**). Here, we use the further notation:

f4(-a,-b,-c,-d,-e), f7(-a,-b,-c,-d,-e,-f)	1st and 2nd-order partial derivatives of Riemann-Lanczos equations,
m1(-a,-b,-c,-d,-e), m2(-a,-b,-c,-d,-e,-f)	1st and 2nd-order covariant derivatives of Riemann-Lanczos equations,
w5(-a,-b,-c,-d),w6(-a,-b,-c,-d,-e)	2nd and 3rd-order contact conditions.

```
%Impose cyclic conditions for S(-x,-y,-t,-a,-b) and
%V(-x,-y,-t,-a,-b,-c) if they were imposed before.
```

```
%In dLtoP, dPtoS, dStoV below, replacements are made for all
%components L, P, S listed separately, which is abbreviated here:
dLtoP:={d L(-t,-x,-t)=P(-t,-x,-t,-n)*o(n), ...};
dPtoS:={d P(-t,-x,-t,-t)=S(-t,-x,-t,-t,-n)*o(n), ...};
dStoV:={d S(-t,-x,-t,-t,-t)=V(-t,-x,-t,-t,-t,-n)*o(n), ...};

%Creation of Integrability Condition Int (denoted by I in text):
pform{f4(-a,-b,-c,-d,-e),f7(-a,-b,-c,-d,-e,-f)}=0;
pform{w5(-a,-b,-c,-d),w6(-a,-b,-c,-d,-e)}=1;
let dLtoP; let dPtoS;
f4(-a,-b,-c,-d,-e):=e(-e)_|w1(-a,-b,-c,-d);
clearrules dLtoP; clearrules dPtoS;
w4(-a,-b,-c,-d,-e):=d f4(-a,-b,-c,-d,-e);
let dLtoP; let dPtoS; let dStoV;
f7(-a,-b,-c,-d,-e,-f):=e(-f)_|w4(-a,-b,-c,-d,-e);
clearrules dLtoP, dPtoS, dStoV;
Int:=f7(-t,-x,-t,-x,-y,-y)+f7(-t,-y,-t,-y,-x,-x)
   +f7(-x,-y,-x,-y,-t,-t)-2*f7(-t,-x,-t,-y,-x,-y)
   -2*f7(-t,-y,-x,-y,-t,-x)+2*f7(-t,-x,-x,-y,-t,-y);
w5(-a,-b,-c,-d):=d P(-a,-b,-c,-d)-S(-a,-b,-c,-d,-n)*o(n);
w6(-a,-b,-c,-d,-e):=d S(-a,-b,-c,-d,-e)-V(-a,-b,-c,-d,-e,-n)*o(n);

%Creation of Covariant Integrability Condition ICov:
pform{wc1(a,b,c,d),wc2(a,b,c,d,e),wc4(a,b,c,d,e)}=1;
pform{m1(a,b,c,d,e),m2(a,b,c,d,e,f),m4(a,b,c,d,e,f)}=0;
wc1(-a,-b,-c,-d):=f4(-a,-b,-c,-d,-n)*o(n)-f(-n,-b,-c,-d)*om(n,-a)
                  -f(-a,-n,-c,-d)*om(n,-b)-f(-a,-b,-n,-d)*om(n,-c)
                  -f(-a,-b,-c,-n)*om(n,-d);
m1(-a,-b,-c,-d,-e):=e(-e)_|wc1(-a,-b,-c,-d);
wc2(-a,-b,-c,-d,-e):=d m1(-a,-b,-c,-d,-e);
let dLtoP; let dPtoS; let dStoV;
m2(-a,-b,-c,-d,-e,-f):=e(-f)_|wc2(-a,-b,-c,-d,-e);
clearrules dLtoP; clearrules dPtoS; clearrules dStoV;
wc4(-a,-b,-c,-d,-e):=
m2(-a,-b,-c,-d,-e,-n)*o(n)-m1(-n,-b,-c,-d,-e)*om(n,-a)
   -m1(-a,-n,-c,-d,-e)*om(n,-b)-m1(-a,-b,-n,-d,-e)*om(n,-c)
   -m1(-a,-b,-c,-n,-e)*om(n,-d)-m1(-a,-b,-c,-d,-n)*om(n,-e);
m4(-a,-b,-c,-d,-e,-f):=e(-f)_|wc4(-a,-b,-c,-d,-e);
ICov:=
m4(-t,-x,-t,-x,-y,-y)+m4(-t,-y,-t,-y,-x,-x)+m4(-x,-y,-x,-y,-t,-t)
   -m4(-t,-x,-t,-y,-x,-y)-m4(-t,-x,-t,-y,-y,-x)-m4(-t,-y,-x,-y,-t,-x)
   -m4(-t,-y,-x,-y,-x,-t)+m4(-t,-x,-x,-y,-t,-y)+m4(-t,-x,-x,-y,-y,-t);


%Creating an EDS including ICov (or including Int and partial
%derivatives f4 instead of covariant derivatives m1 below):
load eds;
coframing({o(a),d L(a,b,c),d P(a,b,c,d),d S(a,b,c,d,e)});
myedsrr:=EDS({w3(-a,-b,-c),w5(-a,-b,-c,-d),f(-a,-b,-c,-d),
```

```
m1(−a,−b,−c,−d,−e),ICov},{o(a)});
myedsr:=lift myedsrr;
```

%Apply part (**) of Appendix A next for the ''myedsr'' created here.

We applied part (**) of the code in Appendix A above to our output file ''myedsr'' created here. Results show that this prolonged system including $ICov$ (or I) is then in involution with Cartan characters (17,8,2) when the cyclic conditions are imposed and with characters (20,10,3) otherwise.

APPENDIX C: THE PROLONGED RIEMANN-LANCZOS PROBLEM AS GIVEN IN SEC. IV

Here, we give the relevant parts of a computer code producing the EDS for the prolongation given in Sec. IV. We will use the further notation:

f1(−a,−b,−c,−d),w10(−a,−b,−c,−d)	Riemann-Lanczos equations without P(−a,−b,−c,−d), exterior derivatives of f1,
A1(−a,−b,−c,−d,−e)	quantities A_{abcde} introduced in (20),
B2(−a,−b,−c,−d,−e,−f)	quantities B_{abcdef} introduced in (21),
R1(−a,−b,−c,−d,−e),R2(−a,−b,−c,−d,−e)	quantities $\overline{\omega}_{abcde}, \hat{\omega}_{abcde}$ in (19),
w7(−a,−b,−c,−d)	contact conditions involving R1, R2.

```
%3-dimensional Riemann-Lanczos Problem:Bampi-Caviglia Prolongation:
%combine this code with the first part of the code in Appendix A
%omitting part (*) and part (**); introduce rule dLtoP again, then:
pform{f1(a,b,c,d),f2(a,b,c,d,e),A1(a,b,c,d,e),A2(a,b,c,d,e), B2(a,b,c,d,e,f)}=0;
pform{w7(a,b,c,d),w8(a,b,c,d,e),w9(a,b,c,d,e),w10(a,b,c,d)}=1;
f1(−a,−b,−c,−d):=f(−a,−b,−c,−d)+P(−a,−b,−c,−d)−P(−a,−b,−d,−c)
                                  +P(−c,−d,−a,−b)−P(−c,−d,−b,−a);
w10(−a,−b,−c,−d):=d f1(−a,−b,−c,−d); let dLtoP;
A1(−a,−b,−c,−d,−n):=(1/4)*(e(−n)_|w10(−a,−b,−c,−d));
clearrules dLtoP;
dPtoR1:={d P(−t,−x,−t,−t)=(R1(−t,−x,−t,−t,−n)+R2(−t,−x,−t,−t,−n)
                          +A1(−t,−x,−t,−t,−n))*o(n),...};
%Impose cyclic conditions on R1 and R2 if necessary, then:
f2(−a,−b,−c,−d,−e):=
  R1(−a,−b,−c,−d,−e)−R1(−a,−b,−c,−e,−d)+R2(−a,−b,−c,−d,−e)
−R2(−a,−b,−c,−e,−d)+A1(−a,−b,−c,−d,−e)−A1(−a,−b,−c,−e,−d);
A2(−a,−b,−c,−d,−e):=d A1(−a,−b,−c,−d,−e); let dLtoP; let dPtoR1;
B2(−a,−b,−c,−d,−e,−f):=e(−f)_|A2(−a,−b,−c,−d,−e);
clearrules dLtoP; clearrules dPtoR1;

w7(−a,−b,−c,−d):=d P(−a,−b,−c,−d)−(R1(−a,−b,−c,−d,−n)
                  +R2(−a,−b,−c,−d,−n)+A1(−a,−b,−c,−d,−n))*o(n);
w8(−a,−b,−c,−d,−e):=d R1(−a,−b,−c,−d,−e)−d R1(−a,−b,−c,−e,−d)
                    +d R2(−a,−b,−c,−d,−e)−d R2(−a,−b,−c,−e,−d)
    +(B2(−a,−b,−c,−d,−e,−n)−B2(−a,−b,−c,−e,−d,−n))*o(n);
w9(−a,−b,−c,−d,−e):=d R1(−a,−b,−c,−d,−e)−d R1(−a,−b,−c,−e,−d)
                    +d R2(−a,−b,−c,−d,−e)−d R2(−a,−b,−c,−e,−d)
                    +d A1(−a,−b,−c,−d,−e)−d A1(−a,−b,−c,−e,−d);
load eds;
coframing({o(a),d L(−a,−b,−c),d P(−a,−b,−c,−d),
          d R1(−a,−b,−c,−d,−e),d R2(−a,−b,−c,−d,−e)});
```

```
%Prior to adding Int or ICov to the EDS here, it is necessary
%to create Int and ICov expressed in the variables R1,R2, then:
myedsrr:=EDS({w3(-a,-b,-c),w7(-a,-b,-c,-d),w8(-a,-b,-c,-d,-e),
        f(-a,-b,-c,-d),f2(-a,-b,-c,-d,-e),ICov},{o(a)});
myedsr:=lift myedsrr;
```

After using part (**) of the code given in Appendix A applied to the file ''myedsr'' created here we obtained that the system is in involution with Cartan characters (17,8,2) if the cyclic conditions are imposed and (20,10,3) otherwise.

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The algebraic entropy of classical mechanics[a)]

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(Received 14 October 2002; accepted 3 March 2003)

We describe the ''Lie algebra of classical mechanics,'' modelled on the Lie algebra generated by kinetic and potential energy of a simple mechanical system with respect to the canonical Poisson bracket. It is a polynomially graded Lie algebra, a class we introduce. We describe these Lie algebras, give an algorithm to calculate the dimensions c_n of the homogeneous subspaces of the Lie algebra of classical mechanics, and determine the value of its entropy $\lim_{n\to\infty} c_n^{1/n}$. It is $1.825\,423\,774\,201\,08\ldots$, a fundamental constant associated with classical mechanics. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1576904]

I. INTRODUCTION. CLASSES OF LIE ALGEBRAS

The class of 'simple mechanical systems' is defined by pairs (Q,V), where the configuration space Q is a real Riemannian manifold and the potential energy V is a smooth real function on Q. The phase space T^*Q has a canonical Poisson bracket and a kinetic energy $T:T^*Q\to\mathbb{R}$ associated with the metric on Q. In general, the smooth functions on a Poisson manifold form a Lie algebra under the Poisson bracket. In the case of a simple mechanical system, we are given two distinguished functions, namely the kinetic and potential energies, and one can ask what Lie algebra they generate under the Poisson bracket.

In this paper we study, not the Lie algebra generated by a *particular* V and T, but the Lie algebra defined by the whole *class* of simple mechanical systems. That is, one should think of the dimension of Q as being arbitrarily large, and the metric and potential energies also being arbitrary.

This question arose out of very practical considerations of the calculations required to derive high-order symplectic integrators by splitting and composition, used in applications including molecular, celestial, and accelerator dynamics.[17,10] The vector field X which is to be integrated is split as $X=A+B$, where A and B have the same properties (e.g., Hamiltonian) as X, but can be integrated exactly. We write $\exp(tX)$ for the time-t flow of X. The most common such integrator is the leap-frog method

$$\varphi(\tau):=\exp(\tfrac{1}{2}\tau A)\exp(\tau B)\exp(\tfrac{1}{2}\tau A),$$

where the small parameter τ is the time step.

From the Baker–Campbell–Hausdorff formula,[7] the map $\varphi(\tau)$ can be represented (up to any power in τ) as a flow $\exp(\tau\tilde{X})$, where

$$\tilde{X}=A+B+\tau^2(\tfrac{1}{12}[B,[B,A]]-\tfrac{1}{24}[A,[A,B]])+\mathcal{O}(\tau^4). \tag{1}$$

Because it is the flow of a vector field $\mathcal{O}(\tau^2)$-close to the original one, the integrator is second order. The function $\tilde{X}$ is called the *modified vector field* in the numerical integration literature.[10]

For simple mechanical systems, we split the Hamiltonian as $H=T+V$. The flow of (the Hamiltonian vector field of) V can of course always be calculated easily, but calculating the flow

[a)]Dedicated to Gerhard Wanner on the occasion of his 60th birthday. Of trees and the counting of trees, may there be no end!

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of the kinetic energy T requires that Q have integrable (and even fairly simple) geodesics. Because the Lie algebras of Hamiltonian vector fields and of Hamiltonian functions are isomorphic under $[X_T, X_V] = X_{\{V,T\}}$, there is a series formally identical to Eq. (1) involving the Hamiltonians T and V with respect to the Poisson bracket.

In the series of Eq. (1) we see the Lie algebra generated by A and B entering. Such series, for example in the proof of the BCH formula, are usually considered in the context of the free Lie algebra $L(A,B)$ with two generators A and B. One can in fact consider the more general composition

$$\prod_{i=1}^{s} \exp(a_i \tau A) \exp(b_i \tau B) = \exp(Z), \tag{2}$$

where $Z \in L(A,B)$. Requiring $Z = \tau(A+B) + O(\tau^{p+1})$ for some integer $p > 1$ gives a system of equations in the a_i and b_i which must be satisfied for the method to have order p.[17,24] In the case of general A and B, then, at each order $n = 1, \ldots, p$ there are $\dim L_n(A,B)$ such *order conditions*. Here $L_n(A,B)$ is the subspace of $L(A,B)$ consisting of homogeneous elements of order n. Witt's formula[7] states that

$$\dim L_n(A,B) = \frac{1}{n} \sum_{d|n} \mu(d) 2^{n/d}, \tag{3}$$

where $\mu(d)$ is the Möbius function defined by $\mu(1) = 1$, $\mu(d) = (-1)^k$ if d is the product of k distinct primes, and $\mu(d) = 0$ otherwise. Notice that in this case

$$\dim L_n(A,B) \sim \frac{2^n}{n};$$

the dimensions grow exponentially with n. The base (2 in this case) of the exponent is called the *entropy* of $L(A,B)$. In general, the entropy of a graded vector space $\bigoplus L_n$ is

$$\limsup_{n \to \infty} (\dim L_n)^{1/n},$$

if this limit exists.[21] [We shall use generalizations of Witt's formula[12,19] to calculate the dimensions and entropies of other free Lie algebras, see Eqs. (15), (17) below.]

In this approach it is assumed that there are no Lie identities satisfied by the vector fields A and B. This is reasonable if one wants the method to work for all A and B. However, in the case of simple mechanical systems, the Lie algebra is *never* free, regardless of T, V, or the dimension of the system. There are always identities satisfied by kinetic and potential energy. The simplest of these is

$$\{V, \{V, \{V, T\}\}\} \equiv 0. \tag{4}$$

For, working in local coordinates (q,p) with $T = \frac{1}{2} p^T M(q) p$, and recalling the canonical Poisson bracket

$$\{A,B\} := \sum_i \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i},$$

we have that

$$\{V,T\} = \sum_{i,j} \frac{\partial V}{\partial q_i} M_{ij}(q) p_j$$

is of degree 1 in p, and that

$$\{V,\{V,T\}\}=\sum_{i,j}\frac{\partial V}{\partial q_i}M_{ij}\frac{\partial V}{\partial q_j} \tag{5}$$

is a function of q only. So V and $\{V,\{V,T\}\}$ commute.

Thus, it was realized early on[16] that in deriving high-order integrators as in Eq. (2) for simple mechanical systems, the order conditions corresponding to $\{V,\{V,\{V,T\}\}\}$ and to all its higher Lie brackets can be dropped. This means that more efficient integrators can be designed for this class of systems. Much work has been done on this special case, both because of its intrinsic theoretical and practical importance, and because it allows such big improvements over the general case. For example, one can design special (corrector or processor) methods of the form $\varphi\psi\varphi^{-1}$,[3] special methods for nearly integrable systems such as the solar system,[4,23] special methods involving exact evaluation of the forces associated with the modified potential [Eq. (5)],[5] and so on—see Ref. 17 for a survey. All of these studies rely on the structure of the Lie algebra generated by kinetic and potential energy. Bases for this Lie algebra have been constructed, more or less by hand, for small orders.[5,6,20] In particular, Murua[20] associates a unique tree of a certain type to each independent order condition of symplectic Runge–Kutta–Nyström methods (very closely related to the problem considered here), and enumerates these up to order 6. (Iserles *et al.*[11] extend this approach to some other classes of polynomial vector fields.) However, a systematic description of the entire Lie algebra is clearly preferred.[18]

Not many classes of Lie algebras have been completely described. Here are two examples from the literature. First, Duchamp and Krob[9] completely describe all partially-commutative Lie algebras

$$L(A_1,\ldots,A_n;[A_i,A_j]=0,(i,j)\in C),$$

where C specifies the pairs of commuting variables. Second, Kirillov, Kontsevich, and Molev[13] studied the Lie algebra L generated by two vector fields on $\mathbb{R}$ in general position, conjectured that

$$\sum_{\sigma\in S_4}(-1)^{\mathrm{sgn}(\sigma)}[x_{\sigma(1)},x_{\sigma(2)},x_{\sigma(3)},x_{\sigma(4)},y]=0 \quad \forall x_1,x_2,x_3,x_4,y\in L \tag{6}$$

generates all identities, and calculated the dimensions of its homogeneous subspaces and the asymptotic growth of their dimension. If their conjecture is true, L is a *PI-algebra*,[2,8] one which the identities which hold in the Lie algebra [such as Eq. (6)] are satisfied by *all* elements of the Lie algebra.

Returning to the case of simple mechanical systems, it is clear that every Lie bracket of T and V is a homogeneous polynomial in p. Furthermore, the degrees of these polynomials combine in a natural way. We therefore introduce the following class $\mathfrak{P}$ of Lie algebras.

We use the notation $[XY]:=[X,Y]$, $[XYZ]:=[X,[Y,Z]]$, and for sets $\mathfrak{X}$, $\mathcal{Y}$, $[\mathfrak{X}\mathcal{Y}]:=[\mathfrak{X},\mathcal{Y}]$ $:=\{[X,Y]:X\in\mathfrak{X},Y\in\mathcal{Y}\}$.

Definition 1: A Lie algebra L is of class $\mathfrak{P}$ (polynomially graded) if it is graded, i.e., $L=\bigoplus_{n\geqslant 0}L_n$, and its homogeneous subspaces L_n satisfy

$$[L_n,L_m]\subseteq L_{n+m-1} \text{ if } n>0 \text{ or } m>0,$$
$$[L_0,L_0]=0. \tag{7}$$

Note that this implies $[(L_0)^{n+1}L_n]=0$ for all n. We call the grading of L its grading by degree.

For example, the Lie algebra generated by kinetic and potential energy is of class $\mathfrak{P}$, where the grading is by total degree in p. The Lie algebra of all polynomial vector fields on a linear space is of class $\mathfrak{P}$, where the grading is by total degree. We will give more examples later.

Such a grading is quite different from the natural grading of a free Lie algebra. Two important differences are that (i) It is not Abelian. For, $[L_2,[L_0,L_0]]=0$ while $[L_0,[L_0,L_2]]\subseteq L_0$. (ii) It is not finite, in the sense that elements of L_n are Lie brackets of unboundedly many other elements of L. For example, the bracket of any number of elements of degree 1 is still of degree 1.

We also need the concept of a Lie algebra which is free in a certain class.

Definition 2 (Ref. 8): Let F be a Lie algebra of class $\mathfrak{P}$ generated by a set $\mathfrak{X}$. Then F is called a free Lie algebra in the class $\mathfrak{P}$, freely generated by the set $\mathfrak{X}$, if for any Lie algebra R of class $\mathfrak{P}$, every mapping $\mathfrak{X}\to R$ can be extended to a unique homomorphism $F\to R$. We write $F=L_{\mathfrak{P}}(\mathfrak{X})$.

In addition to the grading by degree, $L_{\mathfrak{P}}(\mathfrak{X})$ also carries the standard grading which we call the grading by *order*, generated by $\mathrm{order}(X)=1$ for all generators $X\in\mathfrak{X}$ and $\mathrm{order}([Y,Z])=\mathrm{order}(Y)+\mathrm{order}(Z)$. [The term *order* is chosen here because it corresponds to order in the sense of numerical integrators, as in Eq. (1).]

Because of the importance of the grading by degree for Lie algebras generated by kinetic and potential energy, we make the following definition.

Definition 3: The Lie algebra $L_{\mathfrak{P}}(A,B)$, free in the class $\mathfrak{P}$, where A has degree 2 and B has degree 0, is called the Lie algebra of classical mechanics.

Two Lie algebras of class $\mathfrak{P}$ are easy to describe. First, the Lie algebra with k generators of degree $\geqslant 1$ which is free in the class $\mathfrak{P}$ is just the standard free Lie algebra on k generators—the degrees can never decrease if the Lie algebra has no elements of degree 0. Second, the Lie algebra with generators $\mathfrak{X}=\{X_1,\ldots,X_k\}$ of degree 0 and generators $\mathcal{Y}=\{Y_1,\ldots,Y_l\}$ of degree 1, free in the class $\mathfrak{P}$, is $\mathcal{Y}\oplus\bigoplus_{n\geqslant 0}[\mathcal{Y}^n\mathfrak{X}]$, and only contains elements of degree 0 and 1. (In both of these cases, the grading by degree is in fact Abelian.)

However, we want to describe the Lie algebra of classical mechanics, $L_{\mathfrak{P}}(A,B)$. This is the simplest nontrivial case as it includes the essential feature of $\mathfrak{P}$ that degrees can both increase and decrease under Lie brackets.

The paper is organized as follows. In Sec. II, we give a construction which describes $L_{\mathfrak{P}}(A,B)$ as the direct sum of an Abelian and a free Lie algebra, both with an infinite number of generators. In Sec. III, we enumerate the dimensions of the homogeneous (by order) components of $L_{\mathfrak{P}}(A,B)$ and hence in Sec. IV numerically compute its entropy. Section V considers special cases (e.g., of mechanical systems with Euclidean metric; these turn out not to be free in the class $\mathfrak{P}$) and other examples of polynomially graded Lie algebras.

II. STRUCTURE OF THE LIE ALGEBRA OF CLASSICAL MECHANICS

Let $\psi: L(A,B)\to L_{\mathfrak{P}}(A,B)$ be the unique homomorphism from the free Lie algebra to the free Lie algebra of class $\mathfrak{P}$. The kernel $\ker\psi$ can be thought of as the set of identities of $L_{\mathfrak{P}}(A,B)$. For example, we showed above [Eq. (4)] that $[BBBA]\in\ker\psi$. This implies that $[CBBBA]\in\ker\psi$ for all $C\in L(A,B)$. However, we will see below that $[BBBA]$ is not the only generator of the ideal $\ker\psi$.

Our description of $L_{\mathfrak{P}}(A,B)$ is based on the following two observations. First, suppose one wants to describe the Lie algebra with three generators A,B,C which is free in the class of Lie algebras with $C=0$. Since C generates all identities in this class, this Lie algebra is just $L(A,B)$: one merely has to drop the generator C. To generalize this idea, suppose the free Lie algebra $L(A,B)$ can be factored as $\bigoplus_i L(\mathfrak{X}_i)$ for certain generating sets $\mathfrak{X}_i$ with elements in $L(A,B)$, such that some subset $\mathcal{Y}$ of $\cup_i\mathfrak{X}_i$ generates all the identities in $\mathfrak{P}$. Then, we have

$$L_{\mathfrak{P}}(A,B)\cong\bigoplus_i L(\mathfrak{X}_i\backslash(\mathcal{Y}\cap\mathfrak{X}_i)), \tag{8}$$

again we merely drop these generators.

If $\mathcal{Y}$ only generates *some* of the identities of $\mathfrak{P}$, then dropping these generators gives a sum of free Lie algebras which is surjectively homomorphic to $L_{\mathfrak{P}}(A,B)$. This can be used to get upper bounds for the dimensions of the homogeneous subspaces of $L_{\mathfrak{P}}(A,B)$.

Second, given a description of $L_{\mathfrak{P}}(A,B)$ as such a sum [Eq. (8)] of free Lie algebras, we can apply standard techniques to describe it in detail, for example, to construct bases, to compute its dimensions with respect to degree and/or order, and to compute the asymptotic growth of these dimensions.

We begin by stating the crucial tool we shall use, the Lazard factorization of free Lie algebras.

Theorem 1: (Refs. 14, 7, 15) *Let $\mathfrak{X}$ and $\mathcal{Y}$ be sets of generators. Then*

$$L(\mathfrak{X}\cup\mathcal{Y})\cong L(\mathcal{Y})\oplus L(\cup_{n\geqslant 0}[\mathcal{Y}^n\mathfrak{X}]).$$

Applying the Lazard factorization to $L(A,B)$ with $\mathfrak{X}=\{A\}$, $\mathcal{Y}=\{B\}$, gives

$$L(A,B)\cong B\oplus L(A,[BA],[BBA],[BBBA],\dots)$$

where the elements $[B^nA]$ for $n\geqslant 3$ are all identities in $\mathfrak{P}$. Thus, $L_{\mathfrak{P}}(A,B)$ is surjectively homomorphic to $B\oplus L(A,[BA],[BBA])$. The three generators have degrees 2 (A), 1 ($[BA]$), and 0 ($[BBA]$). The idea now is to eliminate this new element of degree 0. (Formally, the generators $[B^nA]$, $n\geqslant 3$, do remain in the generating set; but they and all succeeding Lie brackets of them will be dropped at the final stage when we pass to $L_{\mathfrak{P}}(A,B)$, so we do not need to keep track of them and just indicate them by $*$.) This gives

$$\begin{aligned}L(A,B)&\cong B\oplus L(A,[BA],[BBA],*)\\&\cong B\oplus[BBA]\oplus L(A,[BA],[BBA,A],[BBA,BA],[BBA,BBA,A]),*),\end{aligned}$$

where the generators now have degrees 2, 1, 1, 0, and 0, respectively. Continuing in this way we get the following.

Theorem 2: *Let the degree of A be 2 and the degree of B be 0 with respect to the polynomial grading [Eq. (7)]. Then for all $k\geqslant 0$ we have the following isomorphism*:

$$L(A,B)\cong\mathcal{Z}_k\oplus L(A,\mathfrak{X}_k,\mathcal{Y}_k,*),$$

where

$$\begin{gathered}\mathfrak{X}_0=\varnothing,\quad \mathfrak{X}_{k+1}=\mathfrak{X}_k\cup[\mathcal{Y}_k,A],\\ \mathcal{Y}_0=\{B\},\quad \mathcal{Y}_{k+1}=[\mathcal{Y}_k,\mathfrak{X}_k]\cup[\mathcal{Y}_k,\mathcal{Y}_k,A]=[\mathcal{Y}_k,\mathfrak{X}_{k+1}],\\ \mathcal{Z}_0=\varnothing,\quad \mathcal{Z}_{k+1}=\mathcal{Z}_k\cup\mathcal{Y}_k,\end{gathered}\tag{9}$$

and $*$ represents generators which are zero in $\mathfrak{P}$, i.e., elements of the kernel of the homomorphism $L(A,B)\to L_{\mathfrak{P}}(A,B)$. The generating sets have the following properties.

(1) All elements of $\mathcal{Y}_k$ and $\mathcal{Z}_k$ have degree 0, and all elements of $\mathfrak{X}_k$ have degree 1.
(2) The Lie algebra spanned by $\mathcal{Z}_k$ is Abelian.
(3) $\mathfrak{X}_k=[\mathcal{Z}_k,A]$.
(4) All elements of $\mathcal{Y}_k$ and $\mathcal{Z}_k$ have odd order, and all elements of $\mathfrak{X}_k$ have even order.
(5) The element of smallest order in $\mathcal{Y}_k$ is $(-1)^k[[BA]^kB]$, with order $2k+1$.
(6) The element of largest order in $\mathcal{Y}_k$ is B_k, defined recursively by $B_0=B$, $B_{k+1}=[B_k,[B_k,A]]$. It has order $2^{k+1}-1$.
(7) The finite sets $\mathfrak{X}_k$ and $\mathcal{Z}_k$ converge to infinite sets $\mathcal{Z}$ and $\mathfrak{X}=[\mathcal{Z},A]$ in the sense that the sets

$$\{X{:}X\in\mathfrak{X}_k,\text{order}(X)\leqslant n\}$$

are all equal for $k\geqslant n/2$. We have

$$L(A,B)\cong\mathcal{Z}\oplus L(A,\mathfrak{X},*)$$

and

$$L_{\mathfrak{P}}(A,B)\cong\mathcal{Z}\oplus L(A,\mathfrak{X}).\tag{10}$$

TABLE I. Elements of degree 0 and order $\leqslant 11$ (i.e., functions of q only or modified potentials of simple mechanical systems) appearing at iteration k of Eq. (9). The new elements are numbered consecutively $Z_1, Z_2, \ldots$ The degree 1 elements $X_n := [Z_n, A]$ also appear.

k	$\mathcal{Y}_k$	Order
1	$Z_1 = B$	1
2	$Z_2 = [Z_1, X_1]$ $(= [BBA])$	3
3	$Z_3 = [Z_2, X_1]$ $(= [BBA, BA])$	5
	$Z_4 = [Z_2, X_2]$ $(= [BBA, [BBA, A]])$	7
4	$Z_5 = [Z_3, X_1]$ $(= [[BBA, BA], BA])$	7
	$Z_6 = [Z_3, X_2]$ $(= [[BBA, BA], [BBA, A]])$	9
	$Z_7 = [Z_3, X_3]$	11
	$Z_8 = [Z_4, X_1]$	9
	$Z_9 = [Z_4, X_2]$	11
5	$Z_{10} = [Z_5, X_1]$	9
	$Z_{11} = [Z_5, X_2]$	11
	$Z_{12} = [Z_6, X_1]$	11
	$Z_{13} = [Z_8, X_1]$	11
6	$Z_{14} = [Z_{10}, X_1]$	11

(8) The sizes of the sets $\mathfrak{X}_k$ and $\mathcal{Y}_k$ obey the iteration

$$\begin{aligned} |\mathfrak{X}_{k+1}| &= |\mathfrak{X}_k| + |\mathcal{Y}_k|, \\ |\mathcal{Y}_{k+1}| &= |\mathcal{Y}_k|\,|\mathfrak{X}_{k+1}| \end{aligned} \tag{11}$$

with initial conditions $|\mathfrak{X}_0| = 0$, $|\mathcal{Y}_0| = 1$. This iteration generates the sequence of $|\mathfrak{X}_k|$ values

$$0,1,2,4,12,108,10\,476,108\,625\,644,\ldots; \tag{12}$$

there is a constant $\gamma \approx 1.1555$ such that for sufficiently large k, $|\mathfrak{X}_k| = [\gamma^{2^k}]$.

Proof: The iteration results from successive elimination of elements of degree 0, each iteration introducing only a finite number of new elements nonzero in $\mathfrak{P}$, which have degrees 0 and 1. The other points then follow easily. The final description of $L_{\mathfrak{P}}(A,B)$, Eq. (10), follows because the generators of $L(A,\mathfrak{X},*)$ have degree 2 (A), 1 $(\mathfrak{X})$, or are identically zero $(*)$. Therefore $L(A,\mathfrak{X},*)$ contains no elements of degree 0, so $L_{\mathfrak{P}}(A,\mathfrak{X}) = L(A,\mathfrak{X})$. The sequence of Eq. (12) is Sloane's sequence A001696,[22] which comes from the same iteration [Eq. (11)]; the reference there to Ref. 1 shows how to establish its doubly-exponential growth. ●

The rapid growth of the sets $\mathfrak{X}_k$ and $\mathcal{Y}_k$ means that it is impossible to carry out the iteration exactly very far. In practice the generating set $\mathcal{Z}$ can be found up to any order n by dropping any terms of order $>n$ as soon they appear in $\mathcal{Y}_k$ (i.e., by quotienting all Lie algebras by the ideal consisting of all elements of order $>n$). We then have $\mathcal{Y}_{[(n+1)/2]} = 0$ and the iteration terminates.

The results of the six iterations required when $n = 12$ are shown in Table I. We name the elements of $\mathcal{Z}$ $Z_1, Z_2, \ldots$ as they are successively generated by the algorithm. This gives a short description of the elements of $(L_{\mathfrak{P}})_n(A,B)$ of order $\leqslant 12$ in terms of 14 elements of degree 0, 14 elements of degree 1, and 1 element of degree 2, which generate a total of 283 elements of order $\leqslant 12$ (see Tables II and III).

III. DIMENSIONS OF THE HOMOGENEOUS COMPONENTS

We now turn to the enumeration of $\mathfrak{X}_k$ and $\mathcal{Y}_k$ by order. We introduce the generating functions

$$x_k(t) = \sum_{n=1}^{\infty} |\{X \in \mathfrak{X}_k : \mathrm{order}(X) = n\}|\, t^n,$$

TABLE II. Dimensions of Lie algebras graded by order. Column 2: Of the free Lie algebra with two generators. Column 3: Of the Lie algebra of classical mechanics, $L_{\mathfrak{P}}(A,B)$ where A (kinetic energy) has degree 2 in p and B (potential energy) has degree 0 in p, i.e., is a function of q only. Column 4: Number of modified potentials of order n in $L_{\mathfrak{P}}(A,B)$. Column 5: Upper bound for maximum number of linearly independent Poisson brackets of order n when $M=\mathbb{R}^n$ with the Euclidean metric, i.e., $A=p^{\mathrm{T}}p$. Column 6: As column 5, but $V(q)$ is a cubic polynomial.

n	$\dim L_n(A,B)$	$\dim(L_{\mathfrak{P}})_n(A,B)$	$[t^{n+1}]x(t)$	Euclidean	Cubic
1	2	2	1	2	2
2	1	1		1	1
3	2	2	1	2	2
4	3	2		2	2
5	6	4	1	4	3
6	9	5		5	3
7	18	10	2	10	6
8	30	14		14	6
9	56	25	3	25	10
10	99	39		39	12
11	186	69	6	69	19
12	335	110		110	22
13	630	194	12	193	
14	1161	321		320	
15	2182	557	24	555	
16	4080	941		938	
17	7710	1638	50	1631	
18	14 532	2798		2787	
19	27 594	4878	107	4857	
20	52 377	8412		8376	
21	99 858	14 692	232	14 624	
22	190 557	25 519		25 399	
23	364 722	44 683	508	44 460	
24	698 870	77 993		77 594	
25	1 342 176	136 928	1124	136 191	
26	2 580 795	240 013		238 684	
27	4 971 008	422 360	2513	419 916	
28	9 586 395	742 801		738 375	
29	18 512 790	1 310 121	5665	130 199	
30	35 790 267	2 310 451		2 295 702	
31	69 273 666	4 083 436	12 858	4 056 416	
32	134 215 680	7 218 252		7 169 109	
33	260 300 986	12 781 038	29 356	12 691 109	
34	505 286 415	22 638 741		22 474 996	
35	981 706 806	40 152 860	67 371	39 853 452	
36	1 908 866 960	71 247 291		70 701 714	
37	3 714 566 310	126 559 227	155 345	125 562 178	
38	7 233 615 333	224 917 313		223 099 566	
39	14 096 302 710	400 080 000	359 733	396 759 314	
40	27 487 764 474	711 997 958		705 941 791	

$$\tilde{y}_k(t)=\sum_{n=1}^{\infty}\left|\{Y\in\mathcal{Y}_k:\mathrm{order}(Y)=n\}\right|t^n,\quad \tilde{z}_k(t)=\sum_{n=1}^{\infty}\left|\{Z\in\mathcal{Z}_k:\mathrm{order}(Z)=n\}\right|t^n$$

which from Eq. (9) obey

$$x_0=0,\quad \tilde{y}_0=0,\quad \tilde{z}_0=t,$$

$$x_{k+1}=x_k+t\tilde{y}_k,\quad \tilde{y}_{k+1}=\tilde{y}_k x_{k+1},\quad \tilde{z}_{k+1}=\tilde{z}_k+\tilde{y}_k.$$

We can eliminate the t-dependence of this map by introducing $y_k=t\tilde{y}_k$ and $z_k=t\tilde{z}_k$. Then $z_k\equiv x_k$ for all k and the rest of the system is

TABLE III. Dimensions of $L_{\mathfrak{P}}(A,B)$, graded by degree m and by order n.

n	m total	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2	1	0	1													
2	1	0	1														
3	2	1	0	1													
4	2	0	1	0	1												
5	4	1	0	2	0	1											
6	5	0	2	0	2	0	1										
7	10	2	0	4	0	3	0	1									
8	14	0	4	0	6	0	3	0	1								
9	25	3	0	9	0	8	0	4	0	1							
10	39	0	9	0	14	0	11	0	4	0	1						
11	69	6	0	20	0	23	0	14	0	5	0	1					
12	110	0	18	0	37	0	32	0	17	0	5	0	1				
13	194	12	0	46	0	62	0	46	0	21	0	6	0	1			
14	321	0	42	0	90	0	97	0	60	0	25	0	6	0	1		
15	557	24	0	107	0	165	0	144	0	80	0	29	0	7	0	1	
16	941	0	90	0	229	0	274	0	206	0	100	0	34	0	7	0	1

$$x_0=0, \quad y_0=t^2,$$
$$x_{k+1}=x_k+y_k, \quad y_{k+1}=y_k x_{k+1}. \tag{13}$$

The polynomials $x_k(t)$ converge to a formal power series $x(t)$. The polynomials $y_k(t)$ converge, again in the sense of formal power series, to 0. The power series $x(t)$ completely determines the dimensions of the homogeneous components of $(L_{\mathfrak{P}})_n(A,B)$ [including its abelian part $\mathcal{Z}$, because $z_k(t)=x_k(t)/t$]. We find

$$x(t)=t^2+t^4+t^6+2t^8+3t^{10}+6t^{12}+12t^{14}+24t^{16}+50t^{18}+107t^{20}+232t^{22}+508t^{24}+1124t^{26}$$
$$+2513t^{28}+5665t^{30}+12858t^{32}+29356t^{34}+67371t^{36}+\cdots. \tag{14}$$

(For example, the $1+1+1+2+3+6=14$ generators of weight $\leqslant 12$ are given in Table I.) Amazingly, this power series has appeared before (apparently as a curiosity) from the same iteration [Eq. (13), and it appears as Sloane's sequence A045761[22]].

The classical formula of Witt [Eq. (3)] can be extended to free Lie algebras with more general generating sets.[12,19] For any set $\mathcal{A}$ with generating function $a(t)=\Sigma_{n>0}|\{A\in\mathcal{A}:\text{order}(A)=n\}|t^n$, the dimensions $c_n=\dim L_n(\mathcal{A})$ of the homogeneous components of the graded Lie algebra $L(\mathcal{A})=\bigoplus_{n>0}L_n(\mathcal{A})$ are given by

$$c_n=\sum_{d|n}\frac{1}{d}\mu(d)b_{n/d}, \tag{15}$$

where

$$-\log(1-a(t))=\sum_{n>0}b_n t^n.$$

In Maple, one can compute the dimensions easily by `c=EULERi(INVERT(a))` (these functions are available in Ref. 22), where a and c are the sequences of coefficients of $a(t)$ and $c(t)$, respectively.

We apply Eq. (15) to $L_{\mathfrak{P}}(A,B)\cong\mathcal{Z}\oplus L(A,\mathfrak{X})$. The generating function for the grading by order of $\{A\}\cup\mathfrak{X}$ is $t+x(t)$. This gives the dimensions listed in Table II for $1\leqslant n\leqslant 40$. A dramatic reduction in the dimensions compared to those of the free Lie algebra of rank 2 is evident.

More generally still, Kang and Kim[12] consider the grading of a free Lie algebra by an abelian semigroup S which satisfies the finiteness condition that any $s \in S$ is a sum of other elements of S in only finitely many ways. Then we have

$$\dim L_s(\mathcal{A}) = \sum_{d|s} \frac{1}{d} \mu(d) b_{s/d} \tag{16}$$

where

$$-\log(1-a(t)) = \sum_{s \in S} b_s t^s$$

and $d|s$ means that there exists $\tau \in S$ such that $d\tau = s$, in which case we write $s/d = \tau$.

We can use this to calculate the dimensions of $L_{\mathfrak{P}}(A,B)$ with respect to the bigrading by order and degree. We first simplify the grading by degree [Eq. (7)] by introducing $\text{degree}'(x) := \text{degree}(x) - 1$. Then (as long as no elements of degree 0 enter, which now holds), the semigroup of the grading by degree′ is isomorphic to the non-negative integers under addition. Including the grading by order gives $S = \mathbb{Z}^{>0} \times \mathbb{Z}^{\geqslant 0}$. Note that the finiteness condition holds for S since it holds for $\mathbb{Z}^{>0}$. Since $\text{order}(A) = 2$, $\text{degree}'(A) = 1$, and $\text{degree}'(X) = 0$ for all $X \in \mathcal{X}$, the generating function of $\{A\} \cup \mathcal{X}$ is $ut + x(t)$ and we apply Eq. (16) with

$$b_{t,u} = -[t^n u^m] \log(1 - ut - x(t)).$$

This gives the dimensions for $n, m \leqslant 16$ as shown in Table III.

IV. ASYMPTOTICS OF THE DIMENSIONS AND CALCULATION OF THE ENTROPY

From Eq. (15), the asymptotic growth of the dimensions c_n is determined by the analytic structure—the location and type of the singularities—of $-\log(1-a(t))$. These correspond to zeros and singularities of $1-a(t)$. In particular, if $1-a(t)$ has a simple zero at $t = \alpha$ and no other zero with $|t| \leqslant \alpha$, then

$$c_n \sim \frac{1}{n} \left(\frac{1}{\alpha} \right)^n \tag{17}$$

and the Lie algebra has entropy $1/\alpha$.

The generating function of $\{A\} \cup \mathcal{X}$ is $t + x(t)$. We therefore need to study the analytic structure of the function $1 - (t + x(t))$. We therefore study the map of Eq. (13) considered as a map

$$\varphi : \mathbb{C}^2 \to \mathbb{C}^2, \quad (x,y) \mapsto (x+y, y(x+y))$$

with initial conditions $x = 0$, $y = t^2$. If the iterates of the map converge to $(x^*,0)$ say, then $x(t) = x^*$. Curiously, the map preserves the area $(1/y)\, dx \wedge dy$, although this plays no role in the analysis.

The map φ has a line of degenerate fixed points $(x,0)$ with eigenvalues x and 1. The fixed points with $|x| > 1$ are unstable and one can show that the fixed points with $|x| < 1$ are stable. The map remembers its initial condition, and the function $x(t)$ is the x-coordinate of the fixed point reached from initial condition $(0,t^2)$.

We can see immediately that (i) for t real and positive, $x(t)$ is strictly increasing; and (ii) if the map converges then $|x(t)| \leqslant 1$. For t real and positive, the sequence $\{y_k\}$ is increasing, and if there is a k such that $y_k > 1$, then $x_k \to \infty$. Therefore we define

$$\beta = \inf\{t \in \mathbb{R}^+ : x_k(t) \to \infty\}.$$

Because

$$|x_{k+1}|\leqslant|x_k|+|z_k|,\quad |z_{k+1}|=|z_k||x_{k+1}|,$$

the map converges in the disk $\{t:|t|<\beta\}$.

We can get a crude bound on β immediately, but more detailed knowledge requires a numerical study of the map φ. Let t be real, let $I(x,y)=y+x-1+\sqrt{2y}$, and suppose $x>0$, $y>0$, and $I(x,y)<0$. Then

$$\begin{aligned} I\circ\varphi-I&=y(x+y)+x+y-1+\sqrt{2y(x+y)}-(y+x-1+\sqrt{2y})\\ &=y(x+y)+\sqrt{2y}(\sqrt{x+y}-1)\leqslant y(1-\sqrt{2y})+\sqrt{2y}\sqrt{1-\sqrt{2y}}-1)\\ &\leqslant y(1-\sqrt{2y})+\sqrt{2y}(1-\tfrac{1}{2}\sqrt{2y})-1)=-\sqrt{2}y^{3/2}<0. \end{aligned}$$

Therefore, the orbit must stay in the bounded region $x>0$, $y>0$, $I(x,y)<0$, with x_k increasing and y_k decreasing. Therefore the orbit converges to some fixed point $(x,0)$. [Here the curve $x=1-\sqrt{2y}-y$ was chosen because it is a good approximation of the stable manifold of (1,0).] Since $I(0,t^2)<0$ for $0<t^2<2-\sqrt{3}$, we have $\beta>\sqrt{2-\sqrt{3}}>0.51$. Better approximations of β can be obtained as the roots of $I\circ\varphi^k(0,\beta^2)=0$ (i.e., by requiring the kth iterate to land in the trapping region), but these must be calculated numerically. On the other hand, $x_2=t^2+t^4>1$ if $t>0.79$, so we have the bounds $0.51<\beta<0.79$.

We have that $dx(t)/dt>0$ on $[0,\beta)$, with $x(0)=0$ and $x(\beta)=1$; and $1-t$ is decreasing. Therefore $1-t-x(t)$ has exactly one zero in $[0,\beta)$, and it is simple. The zero is α, the reciprocal of the required entropy of $L_{\mathfrak{P}}(A,B)$. The numerical value of α can be determined by solving $1-t-x(t)=0$ numerically. [In MATLAB, by `function x=f(t); x=0; y=t^2; while y>1e-16, x=x+y; y=y*x; end; x=1-t-x;` and `alpha=fsolve('f',0.5).`] This gives the value of the entropy of $L_{\mathfrak{P}}(A,B)$ as

$$1/\alpha=1.825\,423\,774\,201\,08\cdots. \tag{18}$$

Are there any other solutions to $1-t-x(t)=0$? Because the coefficients of $x(t)$ are all non-negative, there can be none in the disk $|t|\leqslant\alpha$. To say more we have to proceed numerically. First, if $|x_k|$ and $|y_k|$ get too large then the orbit blows up. Let

$$D=\{(x,y)\in\mathbb{C}^2:|y|>2|x|>2\}.$$

Suppose $(x_k,y_k)\in D$. Then

$$|x_{k+1}|\geqslant||y_k|-|x_k||>|x_k|>1$$

and

$$|y_{k+1}|=|x_{k+1}||y_k|>2|x_{k+1}|,$$

i.e., we have $(x_{k+1},y_{k+1})\in D$. The orbit then stays in D and cannot converge—in fact, it must blow up doubly exponentially. The first iterate $(x_1,y_1)=(t^2,t^4)$ is in D if $|t|>\sqrt{2}$, and the second iterate $(x_2,y_2)=(t^2+t^4,t^4(t^2+t^4))$ is in D if $|t|>1.272\,02$. In practice, if an iterate enters this region one can immediately stop the calculation and report that the map diverges.

Using this criterion we computed the function $x(t)$ numerically. See Figs. 1 and 2.

We have made the following numerical observations.

(1) The singularity of $x(t)$ closest to the origin is at
$$t=\beta=1/1.582\,079\,127\,34\cdots. \tag{19}$$
(2) There are no zeros of $1-t-x(t)$ in the disk $|t|<\beta$.
(3) The map converges only in a connected, simply connected region with a fractal boundary.

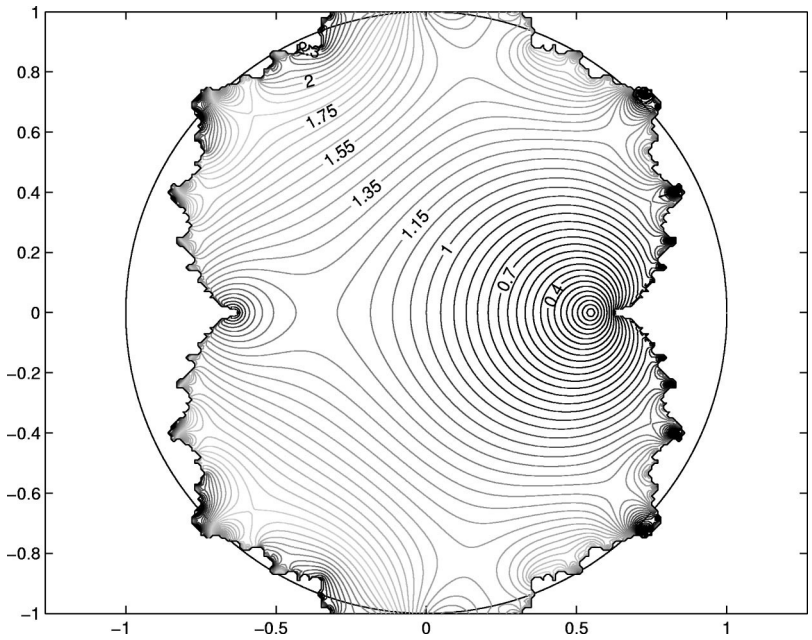


FIG. 1. Contour plot of $|1-t-x(t)|$, showing its main zero at $t=\alpha=1/1.8254\cdots$ and other zeros (two sequences approaching $t=\beta$). The unit circle is also shown.

(4) The function $x(t)$ is analytic everywhere inside this region but has a square root singularity everywhere on its boundary.
(5) For each point z on the boundary, $x(t)\sim 1-a(t-z)^{1/2}$ for some constant a depending on z, as $t\to z$.

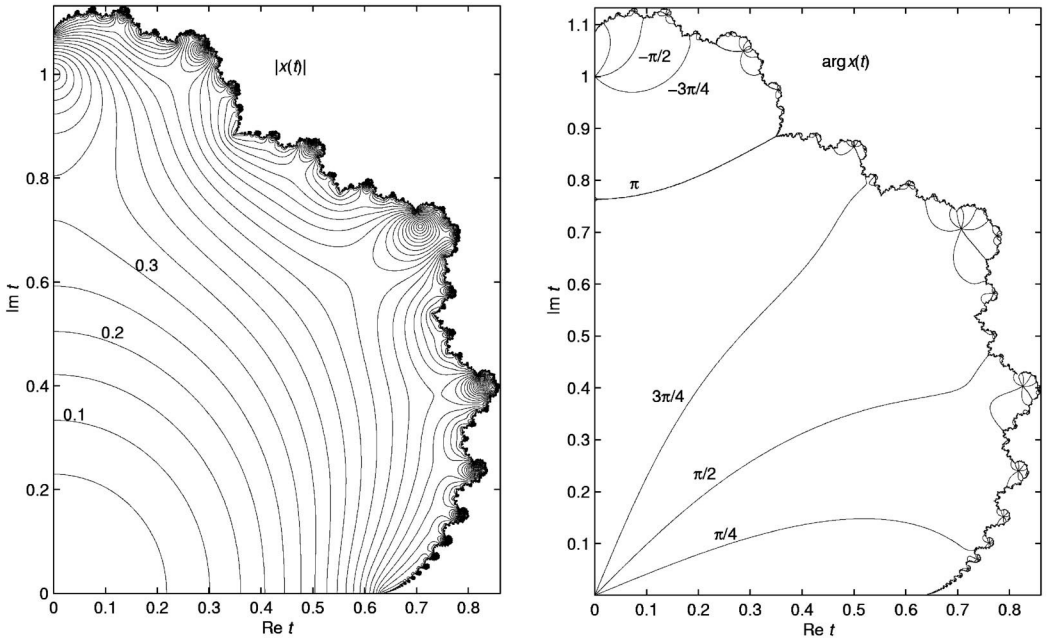


FIG. 2. Contour plots of $|x(t)|$ (left, contour interval 0.05) and arg $x(t)$ (right).

(6) There is only one zero of $1-t-x(t)$ in $|t|\leqslant\beta$.
(7) The other zeros of $1-t-x(t)$ form two infinite sequences α_n, $\overline{\alpha_n}$, with $\mathrm{Re}(\alpha_n)>\beta$ for all n and $\lim_{n\to\infty}\alpha_n=\beta$.

Because of the fractal nature of the boundary, we are unlikely to be able to solve the map φ or find α in closed form. Observation (4) would imply that this boundary forms a natural boundary for the function $x(t)$. Observation (5) would imply that the number of modified potentials of order n, $[t^{n+1}]x(t)$, is $\mathcal{O}(n^{-3/2}\beta^{-n})$. Observation (6) would imply that the next term in the asymptotic growth of $c_n=\dim(L_{\mathfrak{P}})_n(A,B)$ comes from the square root singularity at $t=\beta$. Indeed, by computing c_n numerically for $n<80$ we find that

$$c_n\sim n^{-1}\alpha^{-n}-\begin{cases}1.51n^{-1/2}\beta^{-n} & n \text{ odd}\\ 1.61n^{-3/2}\beta^{-n} & n \text{ even}\end{cases}$$

and

$$[t^{n+1}]x(t)\sim 0.9628n^{-3/2}\beta^{-n}$$

for n even. These are all consistent with the observed singularity structure of $1-t-x(t)$.

V. DISCUSSION

A. Physical interpretation of the generators

There is a particularly nice interpretation of $L_{\mathfrak{P}}(A,B)\cong\mathcal{Z}\oplus L(A,\mathfrak{X})$ in the specific case of simple mechanical systems. In local coordinates, let $A=T(p)=\frac{1}{2}p^TM(q)p$ be the kinetic energy, where $M(q)$ is the inverse of the metric (or mass matrix), and let $B=V(q)$ be the potential energy. The set $\mathcal{Z}$ consists of functions of q only, and we think of them as modified potentials. Elements of the span of $\mathcal{Z}$,

$$\sum_{Z\in\mathcal{Z}}a_Z\tau^{\mathrm{degree}(Z)}Z=a_1\tau V+a_2\tau^3M(V',V')+\cdots,$$

and their flows, can be evaluated explicitly and used to construct high-order integrators of the full system $T+V$ [see Eq. (23) for more terms]. Now consider the generator $X=[Z,A]\in\mathfrak{X}$. It is the cotangent lift of the gradient flow of the modified potential Z; we have $X=M(q)(Z(q),p)$ and Hamilton's equations are

$$\dot q=M(q)Z'(q)=\mathrm{div}_{M^{-1}(q)}Z=:f(q),\quad \dot p=-f'(q)^{\mathrm{T}}p.$$

So in a sense the modified potentials and the kinetic energy together contain a complete description of the Lie algebra.

B. Euclidean mechanical systems

Recall that on each manifold M, each simple mechanical system (say with kinetic energy T and potential energy V) generates a Lie algebra of class $\mathfrak{P}$. Therefore there is a homomorphism $\psi(M,T,V)$ from $L_{\mathfrak{P}}(A,B)$ onto this Lie algebra. One can ask whether the system (M,T,V) is in general position, i.e., if the two Lie algebras are actually isomorphic and $\ker\psi(M,T,V)=0$. This is unlikely, because of the existence of identities such as Eq. (6) in Lie algebras of vector fields. One can therefore consider larger *classes* of systems and ask whether they are in general position. That is, does the class satisfy any identities other than those corresponding to the grading by degree [Eq. (7)]? We conjecture that for the class of all simple mechanical systems, it does not.

Conjecture 1: The only identities satisfied by all simple mechanical systems are those due to the grading by degree. That is,

$$\bigcap_{M,T,V} \ker \psi(M,T,V) = 0.$$

This is best discussed by introducing a smaller class which we shall see is *not* in general position. Namely, let $M=\mathbb{R}^n$ with the Euclidean metric. Then in coordinates the kinetic energy is $T(p)=\frac{1}{2}\Sigma_{i=1}^{n} p_i^2$. The first few modified potentials are then

$$Z_1 = V,$$

$$Z_2 = [BBA] = V'(V'),$$

$$Z_3 = [BBA,BA] = 2V''(V',V'),$$

$$Z_4 = [BBA,[BBA,A]] = 4V''(V''(V'),V'),$$

$$Z_5 = [[BBA,BA],BA] = 2V'''(V',V',V') + 4V''(V''(V'),V'),$$

where we regard the kth derivative of V as a real-valued symmetric linear function on k vectors. Each modified potential of order $2n-1$ is a linear combination of the scalar elementary differentials of order n of V. Each such differential can be associated to a free tree with n nodes. (See, for example, Ref. 10 for a discussion of elementary differentials and trees.) The number of such trees for $n \geqslant 1$ is (Sloane's A000055[22]) 1, 1, 1, 2, 3, 6, 11, 23, 47, 106, 235, ... This should be compared with the number of modified potentials in Eq. (14), namely 1, 1, 1, 2, 3, 6, 12, 24, 50, 107, 232, ... There are three interesting consequences.

(i) For $n \leqslant 6$, the sequences are the same. In fact, one can check that in the modified potentials of orders $2n-1 \leqslant 11$, all trees appear, in invertible linear combinations, so these modified potentials are in general independent.

(ii) For $n=7,8,9$, there are more modified potentials than free trees. In particular, only 11 of the 12 modified potentials of order 13 can be linearly independent. This proves that the class of *Euclidean* mechanical systems is not in general position.

(iii) For $n \geqslant 10$, there are fewer modified potentials than free trees. In fact, the former have entropy $1/\beta = 1.582\cdots$ while the latter (since the free trees have entropy given by Otter's constant, $2.955\cdots$) have entropy $\sqrt{2.955\cdots} = 1.719\cdots$. Thus, for large n, only certain combinations of the trees appear in $\mathcal{Z}$.

So far we have only considered the modified potentials $\mathcal{Z}$ themselves. If these are independent, then $\mathcal{X}=[\mathcal{Z},A]$ is independent too. However, there is still a possibility for extra identities to hold in the Lie algebra generated by A and $\mathcal{X}$. A term of order n and degree m is a sum of elementary differentials of V and p, corresponding to trees with $(n+m+1)/2$ nodes, of which m leaves are labeled p and the remaining nodes are labeled V. In this case we find that for $(n+m+1)/2 \leqslant 7$ there are always sufficient labeled free trees to prevent forced dependencies among the Lie brackets. For example, of the 11 free trees with 7 nodes, there are 12, 20, 24, 18, 9, 3, and 1 trees in which $m=0$, 1, 2, 3, 4, 5, and 6 leaves are colored p, respectively. The dimensions of the corresponding homogeneous subspaces of $L_{\mathfrak{P}}(A,B)$ with $(n+m+1)/2=7$ are (from Table III) 12, 18, 20, 14, 8, 3, and 1, respectively. Thus, only in the case $m=0$, corresponding to the modified potentials themselves, is a dependency forced in this way.

The algorithm for $L_{\mathfrak{P}}(A,B)$ [Eqs. (9) and (13)] can be modified to take into account the dependencies amongst the Lie brackets in the Euclidean case. To get an upper bound on the dimensions and entropy of the Lie algebra in this case, we assume that the dependency appears only when forced. Let c_n be the number of free trees with n nodes. At iteration k, we already have $z_{k,2n} := [t^{2n}]\tilde{z}_k$ elements of order $2n-1$ in $\mathcal{Z}_k$, and $y_{k,2n} := [t^{2n}]\tilde{y}_k$ elements of order $2n-1$ have just been created in $\mathcal{Y}_k$. If $z_{k,2n}+y_{k,2n} > c_n$, we replace $\mathcal{Y}_k$ by a smaller set, of $c_n - z_{k,2n} - y_{k,2n}$ elements, which together with the order $2n-1$ elements of $\mathcal{Z}_k$, forms a basis of the c_n elementary differentials. In terms of the generating functions, we add the final step to the iteration of Eq. (13):

$$y_{k+1} \leftarrow \sum_{n \geqslant 1} \min(y_{k+1,2n}, c_n - z_{k+1,2n}) t^{2n}. \tag{20}$$

Let the resulting limiting formal series be $x_E(t)$, $y_E(t)$, and $z_E(t)$. The generating function for $x_E(t)$ is then computed to be

$$x_E(t) = t^2 + t^4 + t^6 + 2t^8 + 3t^{10} + 6t^{12} + 11t^{14} + 23t^{16} + 47t^{18} + 102t^{20} + 221t^{22} + 484t^{24} + 1069t^{26} + 2386t^{28} + 5364t^{30} + 12143^{32} + 27645t^{34} + 63259t^{36} + \cdots \tag{21}$$

which should be compared with Eq. (14). At order 14, 16, and 18 the dimensions are limited by the number of elementary differentials, but for $n>9$, $[t^{2n}]x_E(t) < [t^{2n}]x(t) < c_n$. Because the new map on generating functions, Eq. (20), is not analytic, it is harder to determine the location of its smallest singularity. We found the smallest root of successive polynomial truncations of $1 - t - x_E(t)$ and extrapolated these results to obtain

$$1/\alpha_E = 1.825\,0339\cdots, \quad 1/\beta_E = 1.574\cdots. \tag{22}$$

These are upper bounds for the entropy of the class of Euclidean mechanical systems and their modified potentials, respectively.

(Murua[20] has also considered this case, in the context of order conditions for Hamiltonians of the form $\frac{1}{2}\Sigma p_i^2 + V(q)$. He finds a unique independent tree of a certain type for each order condition, and enumerates these up to order 6. It would be interesting to compare the two approaches at higher order.)

The situation is quite different for non-Euclidean, i.e., general, mechanical systems. Repeating the above calculation for a general kinetic energy $T(p) = \frac{1}{2} p^T M(q) p$, we get the following modified potentials. The associated trees will be explained below.

$$Z_1 = V = \bullet$$

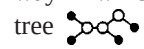
$$Z_2 = [BBA] = M(V',V') =$$

$$Z_3 = [BBA,BA] = 2M(V',V''(M(V'))) + M'(V',V',M(V')) = 2$$

$$Z_4 = [BBA,[BBA,A]]$$
$$= 4V'(M(V''(M(V''(M(V')))))) + 3V'(M(V''(M(M'(V',V'))))) + M(M'(V',V'),M'(V',V')) \tag{23}$$
$$= 4 \quad + 3$$

$$Z_5 = [[BBA,BA],BA] = 4V'(M(V''(M(V''(M(V')))))) + 2V'''(M(V'),M(V'),M(V')) + 6M'(V',M(V'),V''(M(V'))) + M'(V',V',M(V''(M(V')))) + M'(V',M(V'),M'(V',V')) + M''(M(V'),M(V'),V',V')$$
$$= 4 \quad + 2 \quad + 6 \quad + \quad + \quad + \quad .$$

In this case each modified potential of order $2n-1$ is a scalar elementary differential of *V and M*. These correspond to bicolored free trees with $2n-1$ nodes, of which n nodes are labeled V (shown as solid circles above) and $n-1$ nodes are labeled M (shown as open circles above); the

latter must have at least two branches since a derivative of M has at least two indices. Of the 1, 1, 3, 11, 47, and 235 free trees of order 1, 3, 5, 7, 9, and 11 respectively, exactly 1, 1, 2, 8, 34, and 175 of them can be colored (labeled) in this way. The calculation above shows that of these colorable trees, precisely one coloring of 1, 1, 2, and 7 of these colorable trees occur in the modified potentials of orders $\leqslant 7$. (The other colorings of these trees do not occur, because of the way in which the trees at each order are built from the trees of lower order. The colorable 7-node tree  also does not occur.) It is clear that there is enormously much more freedom in this case than in the (Euclidean, $T(p)=\frac{1}{2}\Sigma p_i^2$) case considered previously. Therefore, we believe that all the modified potentials are independent in this case. This supports Conjecture 1.

C. Other polynomially graded Lie algebras

We close with a list of some other Lie algebras of class $\mathfrak{P}$. In each case one can consider the case of two generators A and B of degrees 2 and 0 and the induced homomorphism from $L_{\mathfrak{P}}(A,B)$.

(1) The case of classical mechanics. The objects are real functions on a cotangent bundle, homogeneous polynomial in p. This can be specialized to the following cases.
   (a) Q any Riemannian manifold, any potential energy, degree(X) is the total degree of X in p. Entropy is $\leqslant 1.8254\cdots$ [Eq. (18)] with Conjecture 1 implying equality.
   (b) $Q=\mathbb{R}^n$ with the Euclidean metric. Entropy is $\leqslant 1.8250\cdots$ [Eq. (22)]. It is remarkable that these two Lie algebras, not previously distinguished from each other in the literature, differ starting at order 13, and have slightly different entropy.
   (c) $Q=\mathbb{R}^n$, functions polynomial in p *and* q. We can then introduce a bigrading by degree in p and by degree in q. To get a new Lie algebra, one of the generators has to be degree 0 in each grading, which forces Q Euclidean, $A=\frac{1}{2}\Sigma p_i^2$, $B=V(q)$ polynomial. For example, we have computed the dimensions of the Lie algebra generated by cubic potentials for small n in Table II—they are remarkably small. See Ref. 11 for an analysis of this case in terms of special types of trees.

(2) Homogeneous polynomial vector fields on $\mathbb{R}^m$ graded by total degree in $x_1,\ldots,x_k$ for some $1\leqslant k\leqslant m$. In the case $k=m$, the vector fields in $\mathfrak{X}$ associated with $L(A,B)$ [degree(A)$=2$, degree(B)$=0$] are associated with free trees in which each node has degree at most 2 (since only the first two derivatives of A are nonzero). Their numbers are 1, 1, 1, 2, 3, 6, 11, 23 (so far the same as for the free trees), then 46, 98, 207, 451, ... (Sloane's A001190[22]), which gives an upper bound for the number of independent elements of $\mathcal{Z}$ of each odd order. These grow more slowly than the free trees, and even more slowly than $\mathcal{Z}$, with entropy 1.5758, compared to 1.5821 [Eq. (19)] for $\mathcal{Z}$. Perhaps in this case the trees $\mathfrak{T}$ generate the Lie algebra as $\mathfrak{T}\oplus L(A,[\mathfrak{T},A])$?

(3) As the previous item, but multigrading by total degree in different subsets of the variables.

(4) Homogeneous polynomial vector fields with the variables partitioned (x,y) with $x\in\mathbb{R}^k$, $y\in\mathbb{R}^m$, and the vector fields of the form $p(\partial/\partial x)+q(\partial/\partial y)$ with either $\text{degree}_y(q)\leqslant\text{degree}_y(p)+1$, or $p\equiv 0$ and $\text{degree}_y(q)=0$. Simple mechanical systems form examples of this class. So do high-order ODEs of the form $y^{(n)}=f(y,\ldots,y^{(n-2)})$ when rewritten as first-order systems

$$\dot{x}_i=x_{i+1},\quad i=0,\ldots,n-2,$$
$$\dot{x}_{n-1}=f(x_1,\ldots,x_{n-2}),$$

with $x_i=y^{(i)}$, $k=n-1$, and $m=1$.

(5) Consider the Schrödinger equation

$$i\dot{\psi} = \nabla^2 \psi + V(x)\psi,$$

where ∇^2 is the Euclidean Laplacian. The two operators ∇^2 and $V(x)$ generate a Lie algebra of class $\mathfrak{P}$, where the grading is by degree of the differential operators. For example,

$$[\nabla^2, V]\psi = \nabla \cdot (V\psi) + V\nabla \cdot \psi$$

is of degree 1,

$$[V, V, \nabla^2]\psi = (\nabla \cdot (V^2))\psi$$

is of degree 0, and

$$[V, V, V, \nabla^2]\psi \equiv 0.$$

ACKNOWLEDGMENTS

We would like to thank Mark Sofroniou and Reinout Quispel for pointing out the connection to free trees. R.M. would like to thank Ernst Hairer and Gerhard Wanner for their hospitality at the University of Geneva where this paper was written.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 7 JULY 2003

Towards the complete classification of homogeneous two-component integrable equations

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(Received 4 December 2001; accepted 7 February 2003)

In this article we suggest an improved method for classifying general two-component integrable evolution equations, homogeneous in a given weighting scheme. This method relies on linear changes of variables and on an appropriate splitting of the solution space. To illustrate the method, we implement the classification of coupled KdV-type equations. We show that there are five nontriangular systems possessing higher order generalized symmetries. One of these systems is previously unknown. This seems to be the first classification of coupled integrable equations homogeneous in a given weighting scheme, without any restrictions on the form of the main matrix. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1580998]

I. INTRODUCTION

Among many different approaches to the problem of classification of integrable evolution equations, the most successful ones are based on the existence of infinitely many conservation laws or generalized symmetries. These two methods were extensively used by many authors (cf. Mikhailov, Shabat, and Sokolov[25] or Mikhailov, Shabat, and Yamilov[26]) and they led to the discovery of many new systems, both *S*-integrable and *C*-integrable in Calogero's terminology.[4]

In the present article we consider two-component systems of evolution equations homogeneous in a given weighting scheme. More precisely, we are interested in the general case, i.e., in the systems whose main matrices are not of any special form.

We suggest a method for completely classifying such equations possessing higher order generalized symmetries. It is based on techniques widely used in the field of classification of integrable equations. We think that our method offers an improvement with respect to other versions, since it consists of a simultaneous reduction of the equation and the symmetry to a canonical form, while in general one only searches for the canonical forms of the equation.

To illustrate the method, we present the case of coupled KdV-type equations and apply the techniques similar to the ones used in our previous articles[9–11] about the systematic classification of integrable symmetrically-coupled KdV-type,[9] Burgers-type[10] and mKdV/pKdV-type equations.[11]

Coupled integrable systems come up in many physical applications. From the mathematical point of view, the interest in them has recently been rekindled as a consequence of the key result of Sanders and Wang[31] who showed that the list of known integrable homogeneous, autonomous polynomial scalar evolution equations with linear leading terms is exhaustive, whereas more general classes of equations, such as scalar complex evolution equations involving the complex conjugate, were not yet treated in complete generality. (We recall that scalar complex equations can be equivalently written as two-component systems of real equations for the real and imaginary parts.)

Two-component integrable systems have often been considered in the literature. Unfortunately, to implement classifications of such systems is usually an intractable problem. The only attempt to investigate very general two-component systems was done by Mikhailov, Shabat, and

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Sokolov[25] and Svinolupov,[33] who worked with Burgers- and Schrödinger-type vector equations.

It thus became necessary to consider narrower classes of equations in order to do a complete classification. It was noticed that many important integrable equations are homogeneous as differential polynomials in a certain weighting scheme. Several classes of homogeneous equations were thus dealt with by many authors. We will mention here the works of Gerdt and Zharkov,[14] Sanders and Wang,[31] Olver and Sokolov,[29,30] Meshkov[20,24] and Foursov.[8–11]

Coupled KdV-type equations were first considered by Hirota and Satsuma,[17,32] who showed that the system

$$\begin{cases} u_t = u_{xxx} + uu_x + vv_x, \\ v_t = -2v_{xxx} - uv_x \end{cases} \tag{1}$$

possesses multi-soliton solutions and infinitely many conservation laws. Another similar integrable equation was found by Ito,[18]

$$\begin{cases} u_t = u_{xxx} + 3uu_x + 3vv_x, \\ v_t = vu_x + uv_x, \end{cases} \tag{2}$$

who showed that it possesses a recursion operator and an infinite number of nontrivial conservation laws. Yet another integrable equation of this type was found by Drinfeld and Sokolov[6] in the study of the Kac–Moody algebras

$$\begin{cases} u_t = 3vv_x, \\ v_t = 2v_{xxx} + vu_x + 2uv_x. \end{cases} \tag{3}$$

Its recursion operator was recently found by Wang.[35]

Other two-component KdV-type equations were considered by Fuchssteiner,[13] Nutku and Oğus,[27] Gerdt and Zharkov,[14] Zharkov,[39] and Foursov.[8,9] Several new integrable equations were found, all reducible to a triangular form.

More generally, one can consider multi-component KdV-type equations. This is the path taken by Antonowicz and Fordy,[1] Ma,[21] and Ma and Pavlov,[22] among others. They have considered multi-dimensional coupled KdV-type systems and were able to find several generalizations of the scalar Hamiltonian operators that provide us with a bi-Hamiltonian structure for these systems. Along the same vein, Gürses and Atalay Karasu[15,16] attempted to classify multi-dimensional KdV equations of the type

$$u_t^i = b_j^i u_{xxx}^j + s_{jk}^i u^j u_x^k \tag{4}$$

that possess a recursion operator of degree 4. They found the conditions on b's and s's that insure integrability in the recursion operator sense, but they were unable to find the general solution. Another drawback of this approach is that *a priori* one does not know the degree of the recursion operator. For example, the Drinfeld–Sokolov equation is of type (4), but its recursion operator is of degree 6.

Yet another path to the classification problem was followed by Ayşe Karasu[19] who has investigated the two-component KdV-type equations that pass the Painlevé PDE test.[37] She presented 15 classes of such equations. Her classification has a big disadvantage: the equations were considered in the most general form and many of the systems are far too complicated to be worked with. Using scaling in all variables and linear changes of dependent variables, these 15 classes could have been reduced to a much simpler form.

II. STATEMENT OF THE PROBLEM

Definition 1: Let us consider a system of two equations

$$\begin{cases} u_t = F[u,v], \\ v_t = G[u,v]. \end{cases} \tag{5}$$

Here $F[u,v]=F(u,v,u_x,v_x,u_{xx},\dots)$ denotes a differential polynomial function of u and v, i.e., a function of u, v and their x-derivatives. This equation can be interpreted as a scalar complex equation in the variable $z=u+iv$ involving its complex conjugate $\overline{z}=u-iv$.

Definition 2: A system (5) is called *decoupled* or *triangular* if it involves either an equation depending only on u or an equation depending only on v.

For a decoupled system, we can first solve the equation depending on only one variable and then, using it, reduce the other equation to an x,t-dependent one-component equation. As a consequence, one function has no effect on the other and thus these equations are less interesting for applications. In our classifications we will only consider equations that cannot be decoupled by a change of variables.

Remark: There are in fact two more reasons not to consider decouplable equations. First, Fokas' conjecture is certainly false for them. Second, the number of decouplable equations is extremely large even in the simplest cases, rendering any thorough investigation of them impossible.

Definition 3: A second system of t-independent evolution equations,

$$\begin{cases} u_t = Q_1[u,v], \\ v_t = Q_2[u,v], \end{cases} \tag{6}$$

is said to be a *generalized symmetry* of (5) if their flows formally commute:

$$\mathbf{D_K}(\mathbf{Q}) - \mathbf{D_Q}(\mathbf{K}) = \mathbf{0}. \tag{7}$$

Here $\mathbf{Q}=(Q_1,Q_2)$, $\mathbf{K}[u,v]=(F[u,v],G[u,v])$ and $\mathbf{D_K}$ denotes the Fréchet derivative of $\mathbf{K}$ defined by $\mathbf{D_K}(\mathbf{Q})=(d/d\varepsilon)\,\mathbf{K}[\mathbf{u}+\varepsilon\mathbf{Q}[\mathbf{u}]]|_{\varepsilon=0}$. For a more detailed explanation of generalized symmetries, see Ref. 28.

Definition 4: Let us call the system (5) *integrable* if it possesses infinitely many generalized symmetries.

We remark that in all the known cases it is sufficient to produce only a certain fixed number of generalized symmetries to guarantee integrability. The property of possessing a fixed number of generalized symmetries has the advantage of being easy to verify. But for every class of equations we have to choose carefully the necessary number of symmetries. One symmetry would be the most convenient case, but it is well-known that one symmetry is not enough to insure the existence of an infinite number thereof. The first counter-example is due to Bakirov[2] (see Ref. 3 for a proof).

Fokas[7] has thus conjectured that for an n-component system it suffices to produce n higher symmetries. Quite recently, van der Kamp and Sanders[34] have found an example of a two-component system possessing exactly two higher-order symmetries. We note, however, that there is no pattern for the orders of the two symmetries in this ''anomalous'' example, the system being of order 7 and the two symmetries of orders 11 and 29. Moreover, the Bakirov and van der Kamp–Sanders systems are trivially decoupled, while in this work we consider only ''truly'' coupled equations. And for all the known cases of integrable non-decouplable equations Fokas' conjecture is still valid (as a matter of fact, only one higher symmetry seems to be enough in all these cases). Since all the known symmetry ''pathologies'' occur only for decoupled systems, it is reasonable to continue to rely on Fokas' conjecture for integrability of nondecoupled systems.

The classification problem: to find all nontriangularizable equations of a given class that possess a higher order generalized symmetry of a certain specified class. Implementing this clas-

sification for several different classes of symmetries will provide us the equations possessing several higher-order symmetries. Using Fokas' conjecture, we can thus conclude that these equations are integrable.

III. CLASSIFICATION OF HOMOGENEOUS EQUATIONS

For a given PDE, it is relatively easy to check the existence of higher-order generalized symmetries. However, if one is interested in finding all equations from a certain class possessing this property, the problem becomes significantly harder. At first, several attempts were made to classify general classes of scalar and coupled integrable equations. It was soon realized that is in an intractable problem in practically all cases of interest. The only classification that was successfully (and satisfactorily) completed is the case of general second-order evolution equations $u_t = F(t,x,u,u_x,u_{xx})$ (see Ref. 25).

As a consequence, it became necessary to consider narrower classes in order to be able to investigate them completely. It was noticed that many integrable evolution equations are homogeneous as differential polynomials in a certain weighting scheme (i.e., they possess a scaling Lie symmetry). Moreover, the right-hand sides of symmetries of such equations can be split into homogeneous components, each of which is a symmetry itself. Therefore, without loss of generality, we can restrict our attention to homogeneous symmetries.

Definition 5: Let us introduce the following *weighting scheme* on the space of differential functions. It will assign weight n to the dependent variables u,v and weight 1 to the x-differentiation. The weight of a monomial is the sum of the weights of its factors and the weight of a PDE $u_t = P[u]$ is $\deg P - n$.

When $n=2$, we will call this weighting the *KdV weighting*. The Hirota–Satsuma, Ito, and Drinfeld–Sokolov equations, as well as the trivially coupled KdV equation, are homogeneous in this weighting.

In the case when both the equation and the symmetry are homogeneous in a certain weighting scheme, the classification problem reduces to solving (large) systems of polynomial equations, called the *obstruction equations*. For scalar equations, this system can be easily resolved by Gröbner basis techniques. However, for general classes of coupled homogeneous equations the resulting system is highly nonlinear and it seems to be impossible to solve it in any case of interest. The method we suggest in the next section uses linear transformations of variables to reduce this general problem to 17 subcases, thereby reducing the dimension of the solution space by two or three. In each of the 17 cases, we can then successfully solve the corresponding system of polynomial equations, at least for coupled KdV-type equations.

To compute the symmetries, we use a MAPLE package written by the author. This package uses the same algorithm as the MATHEMATICA package created by Olver.[29] The latter package was successfully used to implement several classifications of integrable equations (e.g., Olver and Sokolov[29,30] and Foursov[8–11]).

Even though it is quite simple to directly compute the symmetry condition (7), the obtained system of polynomial equations is often too big to be dealt with as a whole. To overcome this difficulty, Olver[29] suggested splitting the commutator (7) into homogeneous parts as algebraic polynomials. This way, one first computes the coefficients of linear monomials, then of quadratic ones, of cubic ones, etc. On every step we can either completely resolve the corresponding system or reduce it to the Gröbner basis form (and then consider each branch separately, if necessary). This method allows one to significantly simplify the problem in the majority of cases. A more detailed explanation and examples of the algorithm can be found in Ref. 29 or 8.

IV. ALGORITHM

Definition 6: Consider a nondegenerate system of two evolution equations

$$\begin{cases} u_t = \alpha u_k + \beta v_k + \text{lower order terms}, \\ v_t = \gamma u_k + \delta v_k + \text{lower order terms}, \end{cases} \tag{8}$$

where u_k and v_k are kth order derivatives with respect to x. By a *nondegenerate* system I mean a system that does involve the kth order derivatives (i.e., not all of α, β, γ, δ vanish). We call the matrix $A=\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & \delta\end{smallmatrix}\right)$ the *main matrix* of the system (8). In vector notation we will write the system as

$$\mathbf{u}_t = A\mathbf{u}_k + \text{lower order terms}, \tag{9}$$

where $\mathbf{u}=(u,v)$.

Proposition 7: If the system of the form $\mathbf{u}_t=B\mathbf{u}_k+\cdots$ is a generalized symmetry of $\mathbf{u}_t=A\mathbf{u}_k+\cdots$, then the two main matrices commute, i.e., $[A,B]=0$.

Proposition 8: Under a general linear invertible change of dependent variables

$$\mathbf{w}=K\mathbf{u} \tag{10}$$

(where K is an invertible matrix) the system (9) is mapped to the system $\mathbf{w}_t=A'\mathbf{w}_k+\cdots$ with the main matrix $A'=KAK^{-1}$.

Corollary 9: By a linear invertible change of dependent variables (10) a system of type (9) can be reduced to a system with the main matrix in Jordan canonical form.

Definition 10: We say that the equation $\mathbf{u}_t=A\mathbf{u}_k+\cdots$ is in *canonical form* if the main matrix A is of one of the following forms:

$$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad \begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix},\quad \begin{pmatrix}1 & 0\\ 0 & a\end{pmatrix},\quad \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \tag{11}$$

where a is a constant satisfying $|a|\geqslant 1$, $a\neq 1$.

Remark: The subcases $a=1$ and $a=0$ are written separately for three reasons. First, in the known cases, the solution set for either of these two values is different from the solution set for a generic value of a. Thus this branching seems to be always necessary. Moreover, in case $a=1$, the main matrix commutes with all the other matrices and thus any linear transformation (10) preserves this canonical form. Last, but not least, the conditions $a\neq 1$ and $a\neq 0$ are crucial for successful solving of the obstruction equations.

Corollary 11: Any nondegenerate system (9) can be reduced to canonical form by a linear transformation of type (10). Moreover, the canonical form of the main matrix is unique and well-defined.

The proof is a straightforward application of the fact that a nonzero coefficient of the main matrix can be rescaled to 1 by an appropriate scaling in t. We remark that in general there seems to be no canonical form for the lower order terms. In all the five cases, we can still rescale u and v. And in the case of unit main matrix, any transformation of type (10) is allowed. As a consequence, if one wants to know whether the given system is integrable, he has to reduce it first to canonical form and then compare it to the known integrable equations of this type modulo transformations of type (10) preserving this particular canonical form.

To simplify the symmetry in a way similar to the way we treated the equation, we use the following proposition from linear algebra.

Proposition 12: Two commuting 2×2 matrices can be simultaneously reduced to (a multiple of) their Jordan canonical forms by a transformation $A\rightarrow KAK^{-1}$ for some nondegenerate matrix K.

Remark: This proposition is false for matrices of higher dimension. Thus our method will have to be slightly modified for these cases.

Proposition 13: If the system of the form $\mathbf{u}_t=B\mathbf{u}_k+\cdots$ is a generalized symmetry of $\mathbf{u}_t=A\mathbf{u}_k+\cdots$ with A in canonical form (11), then B can be reduced to Jordan canonical form by a transformation of type (10).

The proof relies on the trivial fact that if $\mathbf{u}_t=\mathbf{Q}$ is a symmetry, so is $\mathbf{u}_t=k\mathbf{Q}$ for any constant k.

Definition 14: We say that the symmetry $\mathbf{u}_t = B\mathbf{u}_m + \cdots$ is in *canonical form* if its main matrix B is of one of the following forms:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & a \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{12}$$

where $a \neq 1$ and $b \neq 0$ are constants.

This list is somewhat different from (11), since we can only apply the changes of variables (10) that preserve all canonical forms of the equation (9).

We have thus put together all the building blocks to prove the following key result.

Theorem 15: By a linear change of variables of type (10), every nondegenerate equation of the type (9) can be reduced to canonical form, simultaneously with its nondegenerate symmetries of type $\mathbf{u}_t = B\mathbf{u}_m + \cdots$.

This simple trick is crucial for implementing successful classifications of integrable equations. Indeed, as a rule, the greater is the number of arbitrary parameters in the main matrices, the harder are the required computations. Writing the equations and the symmetries in canonical form allows one to reduce the number of parameters to at most 1 for each canonical matrix, thereby paving the road for complete classification of many classes of integrable equations.

We remark that not all the canonical main matrices for the equation and for the symmetry are pairwise commuting. There are eight noncommuting pairs. As a consequence, in order to completely classify the equations of a certain type possessing generalized symmetries of a certain (different) type, both of type (9), it is sufficient to consider equations and symmetries with the pairs of main matrices belonging to the list of 17 commuting pairs of canonical matrices.

V. CLASSIFICATION OF COUPLED KdV-TYPE INTEGRABLE EQUATIONS

To illustrate our method, we will show how it helps to resolve the problem of classification of coupled KdV-like equations. We choose this class because we think it is the simplest class of coupled homogeneous equations to deal with, and at the same time a very interesting one. Moreover, it is the class most often considered in the literature. We would like to note that in spite of all the efforts, only particular subclasses were completely investigated. The algorithm we suggest allowed us to finally solve this problem and to find one new integrable equation.

Let us thus consider evolution equations of weight 3 in the KdV weighting, i.e., the equations of the form

$$\begin{cases} u_t = \alpha u_{xxx} + \beta v_{xxx} + \lambda_1 u u_x + \lambda_2 v u_x + \lambda_3 u v_x + \lambda_4 v v_x, \\ v_t = \gamma u_{xxx} + \delta v_{xxx} + \mu_1 u u_x + \mu_2 v u_x + \mu_3 u v_x + \mu_4 v v_x. \end{cases} \tag{13}$$

As shown in Sec. III, we can reduce any equation of this type to an equation having its main matrix in canonical form. We implemented six classifications of equations of this type. To be precise, we searched for equations possessing symmetries of orders 4, 5, 6, 7, 8 and 9. The polynomial equations that appear during the classification can be solved using Gröbner basis techniques in the majority of subcases. When the main matrix of the equation is $\mathrm{diag}(1,a)$, the MAPLE's ''grobner'' package is not efficient for solving the corresponding systems. However, we can do some additional splitting of the solution space and successfully treat each branch separately. In this way, we were able to prove the following three theorems.

Theorem 16: A two-component system of evolution equations (13) that possesses a symmetry of weight 4, 6 or 8 in the KdV weighting is reducible to triangular form by some linear change of dependent variables (10).

Theorem 17: A two-component system of evolution equations (13) possesses a symmetry of weight 5 in the KdV weighting, if and only if it is reducible [by a linear change of dependent variables (10) and/or a rescaling] either to triangular form or to one of the following four equations:

$$\begin{cases} u_t = u_{xxx} + uu_x + vv_x, \\ v_t = -2v_{xxx} - uv_x, \end{cases} \tag{14}$$

$$\begin{cases} u_t = u_{xxx} + 3uu_x + 3vv_x, \\ v_t = vu_x + uv_x, \end{cases} \tag{15}$$

$$\begin{cases} u_t = u_{xxx} + v_{xxx} + 2vu_x + 2uv_x, \\ v_t = v_{xxx} - 9uu_x + 6vu_x + 3uv_x + 2vv_x, \end{cases} \tag{16}$$

$$\begin{cases} u_t = u_{xxx} + 2vu_x + uv_x, \\ v_t = uu_x. \end{cases} \tag{17}$$

We remark that (14) is the Hirota–Satsuma system, (15) is the Ito system, while (17) is the rescaled Drinfeld–Sokolov equation in our canonical form. The system (16) seems to be new. Our computations show that it possesses generalized symmetries of orders 5, 7, 9, 11, 13, 15 and 17, as well as conserved densities of weights 2, 4, 6, 8, 10, 12 and 14. We have thus a very good reason to conjecture that it is integrable, i.e., that it possesses infinitely many generalized symmetries.

Theorem 18: A two-component system of evolution equations (13) possesses a symmetry of weights 7 or 9 in the KdV weighting, if and only if it is reducible [by a linear change of dependent variables (10) and/or a rescaling] either to triangular form, to one of (14)–(17), or else to the following system:

$$\begin{cases} u_t = 4u_{xxx} + 3v_{xxx} + 4uu_x + vu_x + 2uv_x, \\ v_t = 3u_{xxx} + v_{xxx} - 4vu_x - 2uv_x - 2vv_x. \end{cases} \tag{18}$$

Remark: The system (18) is not presented here in canonical form. We prefer this form, since all its coefficients are integer-valued. In canonical form, the main matrix is $\mathrm{diag}(1, -(7+3\sqrt{5})/2)$ and the coefficients depend on $\sqrt{5}$.

The system (18) possesses generalized symmetries of orders 7, 9, 11, 13 and 17, as well as conserved densities of weights 2, 4, 8, 10, 12 and 14. Therefore it is also very likely to be integrable. We remark that its symmetry pattern is rather unusual. It is also characteristic of the Ramani equation,[5] as well as of several equations found by Drinfeld and Sokolov[6] in the study of Kac–Moody algebras.

The explicit form of the system (18) seems to be new. (It was also found by Meshkov,[23] independently of us.) We did an extensive search in the literature, but were unable to find any explicit equation equivalent to (18). It appears, however, albeit implicitly, in a paper of Wilson[38] in the study of equations related to the Kac–Moody algebra $C_2^{(1)}$.

To end up, we would like to remark that *a priori* we do not know the order of the first higher-order symmetry. In this article we have limited our attention to the symmetries of order at most 9. Similar computations can of course be made in order to search for symmetries of yet higher order. These computations become rapidly very time-consuming as the order increases. We do not implement them here, since we think that it is highly unlikely any new integrable equations can be found in this way.

VI. CONCLUSIONS

In this article we have presented an improved method allowing one to implement complete classifications of two-component homogeneous integrable evolution equations. Applying these techniques to KdV-type equations, we were able to find a new integrable equation. (Another application, to Sawada–Kotera and Kaup–Kupershmidt-type equations, can be found in Ref. 12.)

An interesting open problem is to produce recursion operators for this new system (16), as well as for the system (18), whose recursion operator seems to be unknown. Jing Ping Wang[36] demonstrated that the system (18) does not possess symmetries of orders $10n+5$. We thus conjecture that if this recursion operator exists, its degree should be 10.

Another interesting direction is to generalize this method to consider more general classes of systems. For example, coupled equations homogeneous in *some* weighting scheme is a particularly interesting class. This would require finding equivalence classes under *general transformations of variables* preserving the evolutionary form of the equation. This problem is resolved by Cartan's equivalence method. Unfortunately, this seems to be impossible at the current stage of development of computer algebra tools, as there is no package allowing one to tackle the problem of classification of equivalence classes for systems of PDEs. However, such packages are currently under development. Their successful realization would allow one to find the complete list of integrable coupled homogeneous evolution equations.

ACKNOWLEDGMENTS

I would like to thank Gérard Jacob, Peter Olver, Michel Petitot, and Luis Valero Elizondo for helpful discussions, Jing Ping Wang for investigating the new integrable equations, Marc Moreno Maza for checking my solutions and the Computer Science department at the INSA of Rennes for its hospitality.

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Isospectrality of spherical MHD dynamo operators: Pseudo-hermiticity and a no-go theorem

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(Received 8 August 2002; accepted 13 March 2003)

The isospectrality problem is studied for the operator of the spherical hydromagnetic α^2-dynamo. It is shown that this operator is formally pseudo-Hermitian (J-symmetric) and lives in a Krein space. Based on the J-symmetry, an operator intertwining Ansatz with first-order differential intertwining operators is tested for its compatibility with the structure of the α^2-dynamo operator matrix. An intrinsic structural inconsistency is obtained in the set of associated matrix Riccati equations. This inconsistency is interpreted as a no-go theorem which forbids the construction of isospectral α^2-dynamo operator classes with the help of first-order differential intertwining operators. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1573741]

I. INTRODUCTION

The magnetic fields of stars and planets are generated by the homogeneous dynamo effect in moving electrically conducting fluids.[1] This effect is explained within the framework of magnetohydrodynamics (MHD), but its experimental demonstration was missing until recently. In 1999, the first successful dynamo experiments in Riga and Karlsruhe[2] opened up a new way for the laboratory investigation of homogeneous dynamos. In connection with the data analysis for the existing experiments and the design of new dynamo experiments there is a growing interest in the spectral properties of dynamos. Of particular interest is the question of whether isospectral dynamos can exist. The first numerical results on this topic were published in Refs. 3, 4, but rigorous results are still missing.

As a step towards clarification of this issue, we study in the present paper the question of whether operator intertwining techniques from quantum mechanics (QM) can be adopted to MHD dynamo models. In case of an affirmative answer we would obtain an efficient tool for constructing isospectral classes of MHD dynamo operators. Otherwise we would get a no-go theorem which would forbid a straight analogy with quantum mechanical models.

Let us start by recalling some essentials of operator intertwining transformations in QM.[5] Two operators H_0 and H_1 are said to be intertwined if there exist operators A_+ and A_- so that

$$H_1 A_+ = A_+ H_0, \quad A_- H_1 = H_0 A_- . \tag{1}$$

For the corresponding eigenfunctions ϕ_0 and ϕ_1 holds, up to normalization,

$$\phi_1 = A_+ \phi_0, \quad A_- \phi_1 = \phi_0,$$

and the operators H_0 and H_1 are isospectral, except for those states that are annihilated by A_+ or A_-. In the case of one-dimensional Schrödinger operators $H_0 = p^2 + V_0(x)$ and $H_1 = p^2 + V_1(x)$ with the momentum operator given as $p = -i\partial_x$, the intertwining operators can be chosen as first-order differential operators,

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$$A_+ = A := ip + f, \quad A_- = A^\dagger = -ip + f. \tag{2}$$

Structural compatibility of H_0 and H_1 with the intertwining relations (1) requires that the function $f(x)$ and the potentials $V_0(x)$, $V_1(x)$ are connected by the consistency conditions

$$V_1 = V_0 + 2f',$$

$$-f' + f^2 = V_0 - E, \tag{3}$$

$$f' + f^2 = V_1 - E, \tag{4}$$

where the prime denotes differentiation with respect to x; and E is a constant of integration. Linearization of the Riccati differential equations (3), (4) shows that this constant can be interpreted as eigenvalue of the Schrödinger operators H_0 and H_1,

$$H_0\chi_0 = E\chi_0, \quad \text{for} \quad f = -\frac{\chi_0'}{\chi_0}, \tag{5}$$

$$H_1\chi_1 = E\chi_1, \quad \text{for} \quad f = \frac{\chi_1'}{\chi_1}, \tag{6}$$

where χ_0 and χ_1 are formal, and not necessarily normalized eigenfunctions of H_0 and H_1, respectively. They are connected by the product relation

$$\chi_0\chi_1 = c, \tag{7}$$

with c a nonvanishing constant. It is straightforward to verify that the shifted Schrödinger operators are factorizable in terms of the intertwining operators,

$$H_0 - E = A^\dagger A, \quad H_1 - E = AA^\dagger.$$

First-order differential intertwining transformations of type (2) are known as Darboux transformations[6] and are widely used to generate isospectral operator classes from given operators with known spectra.[5,7,8] In particular, intertwining constructions are a basic ingredient of supersymmetric quantum mechanical models[5,9] and their generalizations to pseudo-supersymmetric systems.[10,11] As it was demonstrated in Ref. 12, a double-intertwining (double commutation) method can provide a tool for inserting additional eigenvalues in spectral gaps of given background Schrödinger and Jacobi operators.

Motivated by the large number of exact results on isospectral classes obtained by operator intertwining constructions, it is natural to investigate whether MHD dynamo operators are also suitable for this technique. For this purpose we study in the present paper the simplest mean-field MHD dynamo configuration—the spherical α^2-dynamo.[1] In terms of the radial momentum operator $p = -i(\partial_r + 1/r)$ the 2×2 operator matrix of the α^2-dynamo is given as

$$\hat{H}_l[\alpha] \equiv \begin{pmatrix} -p^2 - \dfrac{l(l+1)}{r^2} & \alpha(r) \\ p\alpha(r)p + \alpha(r)\dfrac{l(l+1)}{r^2} & -p^2 - \dfrac{l(l+1)}{r^2} \end{pmatrix}, \tag{8}$$

and lives on the domain

$$\mathcal{D}(\hat{H}_l[\alpha]) := \left\{ \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} : \ \psi \in \tilde{\mathcal{H}} \equiv \mathcal{H} \oplus \mathcal{H}, \ \mathcal{H} = L_2(\Omega, r^2 dr), \right.$$

$$\Omega=[0,1],\ \ \psi(1)=0,\ \ r\psi(r)|_{r\to 0}\to 0\},$$

in the Hilbert space $\tilde{\mathcal{H}}$. (A brief outline of the derivation of the α^2-dynamo operator matrix from the MHD mean-field induction equation can be found in the Appendix.) It describes the coupled l-modes of the poloidal and toroidal magnetic field components in a mean-field dynamo model with helical turbulence function $\alpha(r)$. The function $\alpha(r)$ does not depend on l and we assume that it is real-valued, positive definite, bounded, and sufficiently smooth on Ω: $\mathrm{Im}\,\alpha=0$, $0<\alpha\leqslant c_1<\infty$, $\alpha\in C^4(\Omega)$. The idealized boundary condition $\psi(r=1)=0$ corresponds to a superconducting spherical boundary shell and is chosen here to ensure simplicity of the subsequent considerations.[13] For more realistic models with a close relation to stellar dynamos, the spherical fluid configurations confined to $r<1$ can be assumed as embedded in empty space. The boundary condition should then be replaced by $\hat{B}_l\psi|_{r=1}=0$ with $\hat{B}_l=\mathrm{diag}[\partial_r+(l+1)/r,1]$ (see, e.g., Ref. 1) what will require a more general approach than that presented in the present paper.

Exploring the fundamental symmetry of the α^2-dynamo operator matrix we find in Sec. II that $\hat{H}_l[\alpha]$ acts as a symmetric operator on the Hilbert space $\tilde{\mathcal{H}}$ when this is endowed with an indefinite metric J. That means the α^2-dynamo operator matrix is a J-symmetric (formally J-self-adjoint) operator,

$$\hat{H}_l[\alpha]=\hat{H}_l^\sharp[\alpha]:=J\hat{H}_l^\dagger[\alpha]J,$$

living in a Krein space $\tilde{\mathcal{K}}=\tilde{\mathcal{H}}_J$.[14] J-self-adjointness is a natural property of operators from different fields of physics. Examples are, e.g., the super-symmetric Dirac operator,[15] PT-symmetric non-Hermitian Hamiltonians in QM[10,16] as well as the Wheeler–DeWitt operator for a cosmological Friedman–Robertson–Walker model coupled to a real massive scalar field.[10] Since the recent paper series[10,11,17] of Mostafazadeh on non-Hermitian operators with real spectra, J-self-adjoint operators are also known as pseudo-Hermitian operators.

In analogy with the simple quantum mechanical model described above, we base our isospectrality analysis on an intertwining Ansatz for two α^2-dynamo operators with helical turbulence functions $\alpha_0(r)$, $\alpha_1(r)$,

$$\hat{H}_{l_0}[\alpha_0]-EI=-\hat{A}\hat{A}^\sharp,\quad \hat{H}_{l_1}[\alpha_1]-EI=-\hat{A}^\sharp\hat{A},$$

and intertwining operator matrices $\hat{A}$, $\hat{A}^\sharp$ that are first-order differential operators,

$$\hat{A}:=iR(r)p+Q(r),\quad \hat{A}^\sharp:=-ipR^\sharp(r)+Q^\sharp(r).$$

This Ansatz leads to a set of six consistency conditions on the matrices $R(r)$ and $Q(r)$ which are studied in Sec. III. It is shown that one pair of conditions fixes the structure of $R(r)$ in terms of the helical turbulence functions $\alpha_0(r)$ and $\alpha_1(r)$. A second pair is equivalent to the symmetry relations $B=B^\sharp$, $U=U^\sharp$ on the matrix functions

$$B:=R^\sharp Q,$$

$$U:=R[Q^\sharp-(R^\sharp)']=RBR^{-1}-R(R^\sharp)',$$

and can be regarded as an implicit consequence of the J-pseudo-Hermiticity of the operator matrices $\hat{H}_{l_0}[\alpha_0]$ and $\hat{H}_{l_1}[\alpha_1]$. (The prime denotes the derivative with respect to r.) The remaining two conditions can be transformed into a pair of coupled matrix Riccati differential equations (MREs) on B and U.

The consistency of the six conditions is analyzed in Sec. IV with the help of a step-by-step reduction of their complexity. First, we conclude from the limiting behavior of the MREs for $r\to 0$ that the angular mode numbers l_0 and l_1 in the two dynamo operator matrices should be connected by the incremental relation $l_1=l_0+1$. Then we use the J-symmetry of B to derive from

the coupled MREs a system of coupled nonlinear ordinary differential equations (ODEs) involving the helical turbulence functions $\alpha_0(r)$ and $\alpha_1(r)$. Analyzing these ODEs, we are able to show the existence of an inherent contradiction between them. As an implication, we arrive at a no-go theorem which states that the six consistency conditions cannot be fulfilled simultaneously and that, hence, the structure of the α^2-dynamo operator matrices is not suitable for an operator intertwining technique based on an Ansatz with first-order differential intertwining operators.

In the concluding section (V) we briefly discuss some other methods which could be useful for studying isospectrality issues of the dynamo operator matrix and which possibly could provide a technique to construct classes of isospectral spherical α^2-dynamo operators.

II. *J*-SYMMETRY OF THE DYNAMO OPERATOR MATRIX

In this section, we study the fundamental symmetry J of the α^2-dynamo operator matrix (8) which allows us to choose an appropriate Ansatz for the intertwining operators A_+ and A_-.

We start our consideration by introducing the auxiliary operator

$$Q[\alpha] := p\alpha p + \alpha \frac{l(l+1)}{r^2},$$

defined on the domain

$$\mathcal{D}(Q) = \{\phi:\ \ \phi \in \mathcal{H} = L_2(\Omega, r^2 dr), \phi(1) = 0,\ \ r\phi(r)|_{r\to 0} \to 0\},$$

in the Hilbert space $\mathcal{H}$. The operator $Q[\alpha]$ is a formally self-adjoint singular differential operator $Q = Q^\dagger$ which acts as symmetric operator on $\mathcal{H}$. [In the subsequent compatibility analysis of the operator intertwining construction we restrict our attention to symmetric (formally self-adjoint) operators. For simplicity, we leave questions of self-adjoint extensions and corresponding generalized boundary conditions[18,19] for the bi-component functions ψ aside.] In terms of $Q[\alpha]$ the dynamo operator matrix and its formal adjoint read as

$$\hat{H}_l[\alpha] = \begin{pmatrix} -Q[1] & \alpha \\ Q[\alpha] & -Q[1] \end{pmatrix}, \quad \hat{H}_l^\dagger[\alpha] = \begin{pmatrix} -Q[1] & Q[\alpha] \\ \alpha & -Q[1] \end{pmatrix},$$

so that the fundamental (canonical) symmetry can be obtained as

$$\hat{H}_l[\alpha] = \hat{H}_l^\sharp[\alpha] := J\hat{H}_l^\dagger[\alpha]J, \quad J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{9}$$

Diagonalizing the matrix J,

$$J \to \eta = S^T J S, \quad S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad \eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

we see that $\hat{H}_l[\alpha]$ is equivalent to the operator matrix,

$$\breve{H}_l[\alpha] = S^T \hat{H}_l[\alpha] S = \frac{1}{2} \begin{pmatrix} Q[\alpha-2] + \alpha & -Q[\alpha] + \alpha \\ Q[\alpha] - \alpha & Q[-\alpha-2] - \alpha \end{pmatrix},$$

with the property $\breve{H}_l[\alpha] = \eta \breve{H}_l[\alpha]^\dagger \eta$. The fundamental η-symmetry of the operator matrix $\breve{H}_l[\alpha]$ implies that $\mathcal{D}(\breve{H}_l)$ could be endowed with the indefinite metric η so that $\breve{H}_l[\alpha]$ becomes a symmetric operator on $\mathcal{D}(\breve{H}_l)$. Due to the invariance of the signature under the transformation S the domain $\mathcal{D}(\hat{H}_l)$ can also be endowed with a natural indefinite inner product $[\cdot,\cdot]_J$ defined by the metric J,

$$[x,y]_J := (x,Jy), \quad x,y \in \tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H},$$

where $(\cdot,\cdot)$ denotes the usual inner (scalar) product in the Hilbert space $\tilde{\mathcal{H}}$. This means that $\hat{H}_l[\alpha]$ is a J-symmetric operator which acts as symmetric operator in a Krein space $\tilde{\mathcal{K}} = \tilde{\mathcal{H}}_J$,

$$[\hat{H}_l x,y]_J = [x,\hat{H}_l^\sharp y]_J .$$

[For surveys on operators in Krein spaces (Hilbert spaces with additional indefinite inner product structures) we refer to the mathematical literature.[14,20]] From its operator-matrix representation (9) we see that J is self-adjoint, involutory and unitary,

$$J^\dagger = J, \quad J^2 = I, \quad J^{-1} = J^\dagger,$$

so that $\hat{H}_l[\alpha]$ is a J-pseudo-Hermitian operator in the sense of Refs. 10, 11, 17.

The eigenvalues of J-pseudo-Hermitian operators are known[10,14,20] to be either real or to come in complex-conjugate pairs. Here we illustrate this property by passing from the eigenvalue problem for the linear operator pencil,

$$\hat{L}_l[\alpha,\lambda]\psi := (\hat{H}_l[\alpha] - \lambda)\psi = 0,$$

to the eigenvalue problem $L_l[\alpha,\lambda]\psi_1 = 0$ for the associated quadratic operator pencil $L_l[\alpha,\lambda]$. This pencil can be derived explicitly from the Ansatz

$$\psi = \begin{pmatrix} \psi_1 \\ \dfrac{1}{\alpha}[Q[1]+\lambda]\psi_1 \end{pmatrix},$$

with $\alpha(r) \neq 0$. As result we obtain

$$L_l[\alpha,\lambda]\psi_1 \equiv \left\{ [Q[1]+\lambda]\frac{1}{\alpha}[Q[1]+\lambda] - Q[\alpha] \right\} \psi_1 = 0$$

$$= (A_2\lambda^2 + A_1\lambda + A_0)\psi_1 = 0.$$

The operators

$$A_0 := Q[1]\frac{1}{\alpha}Q[1] - Q[\alpha], \quad A_1 := Q[1]\frac{1}{\alpha} + \frac{1}{\alpha}Q[1], \quad A_2 := \frac{1}{\alpha},$$

are formally self-adjoint on $\mathcal{D}(Q)$ so that the functionals $a_j := (A_j\psi_1,\psi_1)$, $j = 1,2,3$ are real-valued: $\mathrm{Im}\, a_j = 0$.

From the quadratic equation

$$(L_l[\alpha,\lambda]\psi_1,\psi_1) = a_2\lambda^2 + a_1\lambda + a_0 = 0,$$

we conclude that the eigenvalues of the J-pseudo-Hermitian dynamo operator matrix $\hat{H}_l$ and its associated pencil L_l occur as eigenvalue pairs,[21]

$$\lambda_\pm = \frac{1}{2a_2}(-a_1 \pm \sqrt{a_1^2 - 4a_0a_2}).$$

Obviously, the sign of the discriminant $\Delta := a_1^2 - 4a_0a_2$ defines whether $\lambda_\pm$ are both real or pairwise complex conjugate. The transition from real eigenvalues $\lambda_\pm$ to complex ones occurs at $\Delta = 0$ where the eigenvalue becomes two-fold degenerate $\lambda_+ = \lambda_- = \lambda_0 = -a_1/2a_2$. This general

behavior of $\lambda_\pm$ confirms the results of numerical simulations,[4] which showed that a scaling of the helical turbulence function α leads to a pairwise intersection of real eigenvalue branches of $\hat{H}_l$ and a transition at the intersection points to a pair of complex conjugate eigenvalues.

We note that at the two-fold degenerate points λ_0 of the spectrum with $\Delta=0$ a Jordan–Keldysh chain[22] exists for the linear operator pencil,

$$\hat{L}_l(\lambda_0)\psi=0, \quad \hat{L}_l(\lambda_0)\chi=\psi,$$

as well as for the quadratic operator pencil,

$$L_l(\lambda_0)\psi_1=0, \quad L_l(\lambda_0)\chi_1+\partial_\lambda L_l(\lambda_0)\psi_1=0.$$

Both are built up from eigenvectors ψ, ψ_1 and associated vectors χ, χ_1, respectively.

III. CONSISTENCY CONDITIONS AND MATRIX RICCATI EQUATIONS

The fundamental J-symmetry (J-pseudo-Hermiticity) of the α^2-dynamo operator matrix provides a natural Ansatz for an intertwining construction which respects this symmetry:

$$\hat{H}_{l_0}[\alpha_0]-EI=-\hat{A}\hat{A}^\sharp, \quad \hat{H}_{l_1}[\alpha_1]-EI=-\hat{A}^\sharp\hat{A}. \tag{10}$$

In general, the operator matrix $\hat{A}$ could be an nth-order differential operator of the form

$$\hat{A}=\sum_{k=1}^{n} R_k(r)(ip)^k+Q(r),$$

with 2×2 matrices $R_k(r)$ and $Q(r)$ as coefficients. For simplicity, we restrict our attention in the present paper to the first-order differential operator,

$$\hat{A}=iR(r)p+Q(r), \tag{11}$$

with J-adjoint $\hat{A}^\sharp=-ipR^\sharp(r)+Q^\sharp(r)$. Here we define the $\sharp$-operation for a given 2×2 matrix C as

$$C^\sharp=JC^\dagger J=JC^{*T}J.$$

An asterisk and superscript ''^{T}'' denote complex conjugation and transposition, respectively.

Let us introduce the abbreviations

$$K_{0,1}:=I-\alpha_{0,1}\sigma_-,$$

$$M_{0,1}:=K_{0,1}\frac{l_{0,1}(l_{0,1}+1)}{r^2}+EI-\alpha_{0,1}\sigma_+,$$

with the nilpotent matrices $\sigma_\pm$ defined as

$$\sigma_+:=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \quad \sigma_-:=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}.$$

The shifted α^2-dynamo operator matrices in (10) take then the short form

$$\hat{H}_{l_{0,1}}[\alpha_{0,1}]-EI=-pK_{0,1}p-M_{0,1}. \tag{12}$$

Substituting (11) and (12) into the intertwining Ansatz (10), making use of commutation relations like $[p,R(r)]=-iR'(r)$ and equating the coefficient matrices of the p^2, p, I terms we obtain the following six consistency conditions:

$$\hat{H}_{l_0}: \quad p^2: \ RR^\sharp = K_0, \tag{13}$$

$$p: \ RQ^\sharp - QR^\sharp - R(R^\sharp)' + R'R^\sharp = 0, \tag{14}$$

$$I: \ QQ^\sharp - R(R^\sharp)'' + R(Q^\sharp)' - Q(R^\sharp)' = M_0; \tag{15}$$

$$\hat{H}_{l_1}: \quad p^2: \ R^\sharp R = K_1, \tag{16}$$

$$p: \ -R^\sharp Q + Q^\sharp R = 0, \tag{17}$$

$$I: \quad Q^\sharp Q - (R^\sharp Q)' = M_1. \tag{18}$$

For a successful intertwining construction these matrix equations should be fulfilled simultaneously. So, the main task consists in finding explicit solution sets for (13)–(18). Alternatively, we should obtain intrinsic contradictions within this equation system which could be interpreted as a no-go theorem forbidding this construction for α^2-dynamo operator matrices.

We start our analysis with Eqs. (13) and (16). From the tautologies $RR^\sharp R = RR^\sharp R$ and $R^\sharp RR^\sharp = R^\sharp RR^\sharp$ follows:

$$RK_1 = K_0 R, \quad K_1 R^\sharp = R^\sharp K_0,$$

what with

$$R = \begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix}, \quad R^\sharp = \begin{pmatrix} r_{22}^* & r_{12}^* \\ r_{21}^* & r_{11}^* \end{pmatrix}$$

yields

$$r_{12} = 0, \quad \frac{\alpha_1}{\alpha_0} = \frac{r_{11}}{r_{22}} = \frac{r_{11}^*}{r_{22}^*}. \tag{19}$$

Hence, we can set

$$r_{11} = |r_{11}| e^{i\gamma}, \quad r_{22} = |r_{22}| e^{i\gamma}, \quad r_{21} = |r_{21}| e^{i(\gamma+\varepsilon)}.$$

Using this and (19) in

$$RR^\sharp = K_0 = \begin{pmatrix} 1 & 0 \\ -\alpha_0 & 1 \end{pmatrix}, \quad R^\sharp R = K_1 = \begin{pmatrix} 1 & 0 \\ -\alpha_1 & 1 \end{pmatrix},$$

we find

$$R = e^{i\gamma} \begin{pmatrix} \sqrt{\dfrac{\alpha_1}{\alpha_0}} & 0 \\ -\dfrac{1}{2}\sqrt{\alpha_0 \alpha_1}(1 + i \tan \varepsilon) & \sqrt{\dfrac{\alpha_0}{\alpha_1}} \end{pmatrix}, \tag{20}$$

where the phases γ and ε are still undefined.

As a next step we analyze Eqs. (14) and (17). It is easily seen that defining the matrices

$$U:=R[Q^\sharp-(R^\sharp)'],\quad B:=R^\sharp Q, \tag{21}$$

these equations are equivalent to the J-symmetry relations

$$U=U^\sharp,\quad B=B^\sharp.$$

Due to the different symmetry content of B and Q it is natural to consider B as the primary structural element of the intertwining construction, and Q as a secondary one. So, we perform our subsequent investigation in terms of B and R. Explicitly, the J-symmetry is realized by the matrix structure

$$B=\begin{pmatrix} b_1+ib_4 & b_2 \\ b_3 & b_1-ib_4 \end{pmatrix},\quad \operatorname{Im} b_k=0,\quad k=1,\ldots,4. \tag{22}$$

Furthermore, we exclude Q from (21) to obtain

$$U=RBR^{-1}-R(R^\sharp)'. \tag{23}$$

Introducing the notation $N:=R^{-1}R'$ and substituting (23) into the symmetry relation $U=U^\sharp$ yields the additional constraint

$$[B,K_1^{-1}]=N^\sharp-N. \tag{24}$$

From Eq. (20) we find

$$N=i\gamma' I+\begin{pmatrix} -q & 0 \\ f & q \end{pmatrix},$$

$$q=\frac{1}{2}\left(\frac{\alpha_0'}{\alpha_0}-\frac{\alpha_1'}{\alpha_1}\right), \tag{25}$$

$$f=-\frac{\alpha_1}{2}\left[\frac{\alpha_0'}{\alpha_0}(1+i\tan\varepsilon)+i\frac{\varepsilon'}{\cos^2\varepsilon}\right], \tag{26}$$

so that (24) transforms to

$$\alpha_1\begin{pmatrix} b_2 & 0 \\ -2ib_4 & -b_2 \end{pmatrix}=-2i\gamma' I+\begin{pmatrix} 2q & 0 \\ f^*-f & -2q \end{pmatrix}.$$

Finally, we arrive at the following restrictions on the phase γ and the components b_2 and b_4 of the matrix B:

$$\gamma'=0,\quad b_2=\frac{2q}{\alpha_1},\quad b_4=\frac{\operatorname{Im} f}{\alpha_1}=-\frac{1}{2}\left(\frac{\alpha_0'}{\alpha_0}\tan\varepsilon+\frac{\varepsilon'}{\cos^2\varepsilon}\right). \tag{27}$$

Summarizing the implications of the first four consistency conditions, we see that they are free of intrinsic contradictions. From the initially eight arbitrary complex-valued functions contained in the matrices R and Q, only the three real-valued functions (b_1,b_3,ε) are still undefined. Together with the helical turbulence functions (α_0,α_1) and the constants $(\gamma,E,l_0,l_1)\in\mathbb{R}^2\times\mathbb{Z}_+^2$, we expect them to be highly fine-tuned by the remaining two consistency conditions (15) and (18).

Let us study these conditions now. Making use of the definitions of U and B in (21), their implications

$$Q^\sharp-(R^\sharp)'=R^{-1}U, \tag{28}$$

$$(Q^\sharp)'-(R^\sharp)''=-R^{-1}R'R^{-1}U+R^{-1}U',$$

$$Q=(R^\sharp)^{-1}B, \tag{29}$$

and setting at the end $RR^\sharp=K_0$, $R^\sharp R=K_1$ according to Eqs. (13), (16), we find that (15) and (18) transform to the matrix Riccati equations (MREs)

$$U'=M_0-UK_0^{-1}U, \tag{30}$$

$$B'=-M_1+BK_1^{-1}B. \tag{31}$$

Similar to the linearization of the scalar Riccati equations mentioned in (3)–(6) of the Introduction, the MREs (30), (31) can be linearized by an Ansatz,[23,24]

$$U=VW^{-1},\quad V,W\in\mathbb{C}^{2\times 2},\quad \det(W)\neq 0, \tag{32}$$

$$B=XY^{-1},\quad X,Y\in\mathbb{C}^{2\times 2},\quad \det(Y)\neq 0. \tag{33}$$

As result we arrive at the equation systems

$$\begin{pmatrix}V'\\W'\end{pmatrix}=\begin{pmatrix}0 & M_0\\ K_0^{-1} & 0\end{pmatrix}\begin{pmatrix}V\\W\end{pmatrix},\quad \begin{pmatrix}X'\\Y'\end{pmatrix}=-\begin{pmatrix}0 & M_1\\ K_1^{-1} & 0\end{pmatrix}\begin{pmatrix}X\\Y\end{pmatrix}. \tag{34}$$

The 4×2 matrices

$$\begin{pmatrix}V\\W\end{pmatrix},\begin{pmatrix}X\\Y\end{pmatrix}\in\mathbb{C}^{4\times 2}$$

are defined up to $GL(2,\mathbb{C})\times GL(2,\mathbb{C})$-transformations

$$\begin{pmatrix}\tilde V\\ \tilde W\end{pmatrix}=\begin{pmatrix}VG_0\\ WG_0\end{pmatrix},\quad \begin{pmatrix}\tilde X\\ \tilde Y\end{pmatrix}=\begin{pmatrix}XG_1\\ YG_1\end{pmatrix},\quad G_0,G_1\in GL(2,\mathbb{C}),$$

and can be interpreted as homogeneous coordinates of two points on a complex Grassmann manifold $G_2(\mathbb{C}^4)$ which consists of 2-dimensional complex subspaces in $\mathbb{C}^4$ (see, e.g., Refs. 23, 24). The matrices $U=VW^{-1}$ and $B=XY^{-1}$ are the corresponding affine coordinates of these points.

Differentiating (34) and substituting $V=K_0W'$, $X=-K_1Y'$, it is easily seen that the equation systems (34) are equivalent to the second-order matrix differential equations,

$$\begin{aligned}(\partial_r K_0\partial_r-M_0)W&=0,\\ (\partial_r K_1\partial_r-M_1)Y&=0.\end{aligned} \tag{35}$$

This implies that the matrices $\tilde W=r^{-1}W$, $\tilde Y=r^{-1}Y$ should be formal (non-normalized) solutions of the eigenvalue equations for the dynamo operator matrices $\hat H_{l_0}[\alpha_0]$, $\hat H_{l_1}[\alpha_1]$, respectively,

$$\hat H_{l_0}[\alpha_0]\tilde W=E\tilde W,\quad \hat H_{l_1}[\alpha_1]\tilde Y=E\tilde Y.$$

A comparison with the simple QM model from the Introduction shows that the intertwining operator matrix $\hat A$ should be expressible in terms of W or Y, and that W and Y should be connected by a product invariant like (7). With the help of (28), (29) and (34) we find

$$\hat A=R(ip-Y'Y^{-1})=(ip+K_0W'W^{-1}K_0^{-1})R.$$

In order to obtain the product invariant which connects W and Y, we use a slightly modified version of (23),

$$U=RB^{\sharp}R^{-1}-R(R^{\sharp})',$$

and substitute from (32)–(34),

$$U=RR^{\sharp}W'W^{-1}, \quad B^{\sharp}=-(Y^{\sharp})^{-1}(Y^{\sharp})'R^{\sharp}R,$$

so that

$$W'W^{-1}=-(R^{\sharp})^{-1}(Y^{\sharp})^{-1}(Y^{\sharp})'R^{\sharp}-(R^{\sharp})^{-1}(R^{\sharp})'. \tag{36}$$

This equation is of the type $g=g_1n$, $(\partial_r g)g^{-1}=(\partial_r g_1)g_1^{-1}+g_1(\partial_r n)n^{-1}g_1^{-1}$. Hence, integration of (36) yields the product invariant,

$$Y^{\sharp}R^{\sharp}W=C, \quad \det(C)\neq 0,$$

with C a constant nonsingular matrix.

So far, we have obtained a 1:1 generalization of the intertwining technique from the simple QM example described in the Introduction to our J-symmetric dynamo operator model. It remains to test whether the MREs of this model are consistent. This will be the subject of the next section.

IV. NO-GO THEOREM

In order to test the pair of MREs (30), (31) for consistency, we make use of (23), (24) as well as the relation

$$N+K_1^{-1}N^{\sharp}K_1=K_1^{-1}K_1'=K_1',$$

and transform the MRE for U [Eq. (30)] into an equivalent MRE for B. As result, we arrive at the following pair of MREs:

$$B'=R^{-1}M_0R-K_1^{-1}BB+BK_1'+[NN^{\sharp}+(N^{\sharp})']K_1, \tag{37}$$

$$B'=-M_1+BK_1^{-1}B, \tag{38}$$

which should be satisfied simultaneously. The corresponding consistency test will be performed in two steps:

(1) From the limiting behavior at $r\to 0$ we will derive a relation between l_0 and l_1.

(2) We will extract from Eqs. (37), (38) a system of nonlinear ODEs for the helical turbulence functions α_0,α_1 and for the components $b_1,\ldots,b_4$ of the matrix B. By mutual substitutions of these ODEs we will find an inconsistency which can be interpreted as a no-go theorem.

A. Limiting behavior at $r\to 0$

From the assumed nonsingular behavior of the helical turbulence functions at $r\to 0$ follows that they can be approximated as

$$\alpha_{0,1}(r\to 0)\approx c_{0,1}+a_{0,1}r+\mathcal{O}(r^2) \quad , \quad c_{0,1}\neq 0.$$

Substituting this approximation in a slightly rewritten version of the defining equation (35) for the matrix Y,

$$\left[I\partial_r^2-\alpha_1'\sigma_-\partial_r-\frac{l_1(l_1+1)}{r^2}I-\begin{pmatrix} E & -\alpha_1 \\ \alpha_1 & E-\alpha_1^2 \end{pmatrix}\right]Y=0, \tag{39}$$

we obtain the estimate

$$Y(r\to 0)\approx r^{-l_1}\left(I+\frac{a_1}{2}\sigma_- r+\mathcal{O}(r^2)\right)(r^{2l_1+1}C_+ + C_-),$$

where C_+, C_- are arbitrary nonsingular constant matrices $\det(C_\pm)\neq 0$. Correspondingly, it holds

$$Z:=Y'Y^{-1}\approx -l_1 r^{-1}I+\frac{a_1}{2}\sigma_- +\mathcal{O}(r), \tag{40}$$

$$B=-K_1 Y'Y^{-1}\approx l_1 r^{-1}I-[c_1 l_1 r^{-1}+(l_1+1/2)a_1]\sigma_- +\mathcal{O}(r). \tag{41}$$

A comparison of (41) with (22) shows that the components b_2 and b_4 of the matrix B vanish at least as

$$b_2, b_4\approx\mathcal{O}(r), \quad \text{for } r\to 0.$$

Furthermore, we find with the help of Eqs. (25), (26) and (27) that $q\approx\mathcal{O}(r)$ and, hence, $a_0/c_0 = a_1/c_1$, as well as $q', f, f'\approx\mathcal{O}(1)$ which implies $N, N^\sharp, (N^\sharp)'\approx\mathcal{O}(1)$.

We are now well prepared to perform a partial consistency test of (37) and (38) by comparing the singular terms of these equations in the vicinity of the origin $r=0$. From the MREs (37) and (38) we find

$$-K_1^{-1}K_1' Z - Z' = \frac{l_0(l_0+1)}{r^2}I - K_1^{-1}ZK_1 Z - ZK_1' +\mathcal{O}(1), \tag{42}$$

$$-K_1^{-1}K_1' Z - Z' = -\frac{l_1(l_1+1)}{r^2}I + ZZ +\mathcal{O}(1), \tag{43}$$

respectively. Substituting Z from (40) and equating the coefficients of the r^{-2}, r^{-1}-terms we obtain from Eq. (42),

$$l_1 = l_0+1, \quad a_1 = 0,$$

and, hence, also $a_0=0$. Equation (43) is automatically satisfied, because Y is defined by the corresponding linearized equation (39). The incremental relation $l_1=l_0+1$ is well known from ladder operator constructions for spherically symmetric Hamiltonians in QM.[5] This is not surprising, because this ladder operator construction can be recovered from the intertwining construction (10) for the α^2-dynamo operator matrices by the two-step transition: 1. $\alpha_0=\alpha_1=\alpha$, 2. $\alpha\to 0$.

B. Systems of coupled nonlinear ODEs and their inconsistency

The system of eight coupled nonlinear ODEs for the components $b_1,\ldots,b_4$ of the matrix B is easily obtained from the MREs (37), (38), e.g., with the help of the matrix multiplication package of MATHEMATICA©. For our analysis it is sufficient to consider only the simplest four equations of this system, i.e., the σ_+ and I projections of (37) and (38):

$$b_2' = 2b_1 b_2 + \alpha_1(1+b_2^2), \tag{44}$$

$$= -2b_1 b_2 - \frac{\alpha_0^2}{\alpha_1}, \tag{45}$$

$$b_1' = b_1^2 + b_2 b_3 - b_4^2 - E - \frac{l_1(l_1+1)}{r^2} + \alpha_1 b_1 b_2, \tag{46}$$

$$= -b_1^2 - b_2 b_3 + b_4^2 + E + \frac{l_0(l_0+1)}{r^2} - \alpha_1' b_2 + \frac{\alpha_0^2}{2} + q' - q^2. \tag{47}$$

Equating the right-hand-sides of (44), (45) and using $b_2 = 2q/\alpha_1$ from (27) we are able to express b_1 as

$$b_1 = -\frac{4q^2 + \alpha_0^2 + \alpha_1^2}{8q}. \tag{48}$$

Taking into account that $q = \partial_r \ln(\alpha_0/\alpha_1)/2$ according to (25) and that the helical turbulence functions α_0 and α_1 do not depend on l_0 or l_1 we conclude from Eq. (48) that b_1 should not depend on l_0 or l_1 too. On the other hand, the addition of (46) and (47) together with the relation $l_0 = l_1 - 1$ gives

$$2b_1' = -\frac{2l_1}{r^2} + 2q\left(b_1 - \frac{\alpha_1'}{\alpha_1}\right) + \frac{\alpha_0^2}{2} + q' - q^2,$$

which by integration leads to a function b_1 which depends on l_1. That means, the term depending on l_1 cannot be compensated by a combination of l_1-independent terms. This is an obvious contradiction to (48) and we have to conclude that the consistency conditions (13)–(18) cannot be fulfilled simultaneously. This means that we are lead to the

No-go theorem: The structure of the MHD α^2-dynamo operator matrix is incompatible with an operator intertwining technique which is based on first-order differential intertwining operators.

A similar situation occurs also for three-dimensional spherically symmetric models in QM.[5] There the l-dependent centrifugal term sets so strong restrictions on the form of the allowed potential that an intertwining construction built on first-order differential intertwining operators is only possible for the following three cases: the constant potential $V(r) = \text{const}$, the Coulomb potential $V(r) \propto 1/r$, and the potential of the three-dimensional isotropic harmonic oscillator with $V(r) \propto r^2$. Richer classes of allowed potentials are only found for models in their s states, when $l = 0$. Such states are *a priori* excluded for the α^2-dynamo operator matrix due to its construction [see Eq. (A5)].

V. CONCLUDING REMARKS

In the present paper, we have tested the MHD α^2-dynamo operator matrix for its compatibility with the simplest variant of an intertwining construction based on *first-order* differential intertwining operators. The operators have been chosen in accordance with the fundamental J-symmetry (pseudo-Hermiticity) of the operator matrix and lead to a set of six matrix equations as consistency conditions. With the help of a step-by-step reduction of the complexity we have extracted their basic structural elements and have shown that they contain an intrinsic inconsistency. So, we have to conclude that the structure of the α^2-dynamo operator matrix is not compatible with the considered first-order differential intertwining Ansatz. This fact is the subject of the formulated no-go theorem.

It remains to test whether intertwining constructions can be built from second-order or higher-order differential intertwining operators. Energy shift operators based on second-order differential expressions are known for harmonic oscillators with time-dependent frequencies and additional $1/r^2$-term[25] as well as for the spherically symmetric oscillator and the Coulomb potential.[5] A generalization of the technique to the MHD α^2-dynamo operator matrix seems realistic.

Another approach for a clarification of the considered isospectrality problem could consist in a generalization of the Gelfand–Levitan technique for vector-valued Sturm–Liouville problems.[26]

Concerning its general structure, the α^2-dynamo operator matrix $\hat{H}_l[\alpha]$ is a singular non-self-adjoint matrix Sturm–Liouville operator which by a unitary transformation can be recast into the standard form

$$-\partial_r P_2(r)\partial_r + P_0(r).$$

In 1998, Jodeit and Levitan[26] analyzed the isospectrality problem for matrix Sturm–Liouville operators with $P_2(r)=I$ and $P_0(r)$ a symmetric matrix. They showed that if two vector-valued Sturm–Liouville problems are isospectral then the eigenfunctions of one problem can be constructed from the eigenfunctions of the other problem with the help of a matrix Gelfand–Levitan transformation. So, a generalization of this technique to Sturm-Liouville problems with nonsymmetric $P_0(r)$ and $P_2(r)\neq I_2$ would naturally cover the isospectrality problem for the MHD α^2-dynamo operator matrix.

ACKNOWLEDGMENTS

We would like to thank G. Gerbeth for numerous discussions and C. Tretter for useful comments. This project was supported by the German Research Foundation, DFG, under Grant No. GE-682/12-1.

APPENDIX A: DERIVATION OF THE α^2-DYNAMO OPERATOR MATRIX FROM THE MEAN-FIELD INDUCTION EQUATION

For completeness we sketch here the main steps of the derivation of the 2×2 operator matrix $\hat{H}_l[\alpha]$ for a model with helical turbulence function $\alpha(r)$. The outline follows the technique for models with $\alpha=\text{const}$ as presented in Ref. 1.

The spherical MHD mean-field α^2-dynamo in its kinematic regime is described by the induction equation for the magnetic field,

$$\partial_t \mathbf{B} = \boldsymbol{\nabla}\times(\alpha\mathbf{B}) + \nu_m \Delta \mathbf{B}, \tag{A1}$$

supplemented by the condition $\boldsymbol{\nabla}\cdot\mathbf{B}=0$. The magnetic diffusivity ν_m is assumed to be constant and the helical turbulence function α to depend only on the distance from the origin $\alpha=\alpha(r)$. Decomposition into toroidal and poloidal components $\mathbf{B}=\mathbf{B_t}+\mathbf{B_p}$ and setting $\mathbf{B_p}=\boldsymbol{\nabla}\times\mathbf{A_t}$ allows for a decomposition of the induction equation (A1):

$$\partial_t \mathbf{B_t} = \boldsymbol{\nabla}\times(\alpha\boldsymbol{\nabla}\times\mathbf{A_t}) - \nu_m \boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{B_t}, \tag{A2}$$

$$\partial_t \mathbf{A_t} = \alpha\mathbf{B_t} - \nu_m \boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{A_t}. \tag{A3}$$

Furthermore, the fields $\mathbf{B_t}$ and $\mathbf{A_t}$ can be represented as

$$\mathbf{A_t} = -\mathbf{r}\times\boldsymbol{\nabla}F_1, \quad \mathbf{B_t} = -\mathbf{r}\times\boldsymbol{\nabla}F_2,$$

where F_1 and F_2 are single-valued scalar functions which are normalized on the unit sphere S^2 by the condition

$$\int_{S^2} F_{1,2}\ d\omega = 0. \tag{A4}$$

With the help of the relations

$$\Delta(\mathbf{r}\times\boldsymbol{\nabla}F_1) = \mathbf{r}\times\boldsymbol{\nabla}\Delta F_1,$$

$$\boldsymbol{\nabla}\times[\alpha\boldsymbol{\nabla}\times(-\mathbf{r}\times\boldsymbol{\nabla}F_1)] = \mathbf{r}\times\boldsymbol{\nabla}\left[\frac{1}{r}(\partial_r\alpha)(\partial_r r F_1) + \alpha\Delta F_1\right],$$

$$\alpha \mathbf{r}\times\nabla F_2 = \mathbf{r}\times\nabla(\alpha F_2),$$

Eqs. (A2) and (A3) can be rewritten as

$$\mathbf{r}\times\nabla[\,\nu_m \Delta F_1 + \alpha F_2 - \partial_t F_1] = 0,$$

$$\mathbf{r}\times\nabla\left[\,\nu_m \Delta F_2 - \frac{1}{r}(\partial_r \alpha)(\partial_r r F_1) - \alpha \Delta F_1 - \partial_t F_2\right] = 0.$$

It follows that the expressions in the square brackets are functions of r and t alone which must vanish due to the normalization condition (A4) and its implication $\int_{S^2} \Delta F_{1,2}\, d\omega = 0$. By re-scaling of r and t one sets the magnetic diffusivity to unity $\nu_m = 1$ and the boundary conditions at $r = 1$.

With the help of a series expansion in spherical harmonics,

$$F_{1,2} = \sum_{l,m,n} e^{\lambda_{l,n} t} F_{1,2}^{(l,m,n)}(r) Y_l^m(\theta,\phi) \in L^2(\Omega, r^2 dr) \otimes L^2(S^2, d\omega), \quad \Omega = [0,1],$$

one obtains the eigenvalue problem

$$\Delta_l F_1^{(l,m,n)} + \alpha F_2^{(l,m,n)} = \lambda_{l,n} F_1^{(l,m,n)},$$

$$\Delta_l F_2^{(l,m,n)} - \frac{1}{r}(\partial_r \alpha)(\partial_r r F_1^{(l,m,n)}) - \alpha \Delta_l F_1^{(l,m,n)} = \lambda_{l,n} F_2^{(l,m,n)}.$$

Here we used the notation $\Delta_l = (1/r^2)\,\partial_r r^2 \partial_r - l(l+1)/r^2$ and the fact that due to the symmetry of the dynamo configuration[1] the eigenvalues $\lambda_{l,n}$ depend only on l and n. We note that the normalization condition (A4) implies

$$F_{1,2}^{(l=0,m,n)} = 0. \tag{A5}$$

Finally, the substitutions $p = -i(\partial_r + 1/r)$, $\psi_{1,2} = F_{1,2}^{(l,m,n)} \in L^2(\Omega, r^2 dr)$ lead to the eigenvalue problem for the α^2-dynamo operator matrix $\hat{H}_l[\alpha]$ as it is given in Eq. (8) of the Introduction.

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Special solution of the inhomogeneous Bloch equation

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(Received 20 June 2002; accepted 3 April 2003)

A solution of the inhomogeneous Bloch equation is given for a class of three-dimensional time-varying magnetic fields by finding the fundamental system in terms of a set of the three independent solutions of the homogeneous Bloch equation. This class is distinguished by requiring a nonlinear relation between one of the magnetic field components and the other two components and their derivatives. A brief discussion of the magnetic field class characteristics and an illustrative example are given. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1579992]

I. INTRODUCTION

Since the Bloch equation[1] was proposed in 1946, various workers have tried to solve it analytically. As yet few exact solutions are known.[2] Very recently, an interesting solution was found to the homogeneous Bloch equation.[3] This was done by solving the Riccati equation to which the homogeneous Bloch equation reduces.[4] The reason why we persist in solving the homogeneous Bloch equation analytically is due to the fact that the inhomogeneous Bloch equation is uniquely solved by finding a fundamental system in terms of a set of three independent solutions of the homogeneous Bloch equation. By linearizing the Riccati equation, a set of three solutions of the homogeneous Bloch equation are found.[5] The fundamental matrix in terms of these solutions becomes singular. This means two of them serve as independent solutions. We have clarified the utility and limitation of this approach to solve the homogeneous Bloch equation.

The purpose of this paper is to find a fundamental system of solutions using the standard method of solving the Riccati equation.[6] We thus discover a solution of the inhomogeneous Bloch equation for a class of time-varying magnetic fields.

In Sec. II we solve the Riccati equation and find a set of three independent solutions of the homogeneous Bloch equation. Then in Sec. III we give a solution of the inhomogeneous Bloch equation using the fundamental system of solutions. A brief discussion of the magnetic field class characteristics and an illustrative example are given in Sec. IV. The final section is devoted to our conclusions.

II. THE RICCATI EQUATION

The Bloch equation for magnetization with infinite relaxation times is a homogeneous system of three first-order linear differential equations, and given by

$$\dot{\mathbf{M}} = -\gamma(\mathbf{B}\times\mathbf{M}), \tag{1}$$

where an overdot means differentiation with respect to time. Here **M** and **B** are the magnetization vector and the applied magnetic field, respectively, and γ is the gyromagnetic ratio.

It immediately follows from Eq. (1) that the magnitude of the magnetization vector is preserved. Thus we can define **m** by

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$$\mathbf{m}=\frac{\mathbf{M}}{|\mathbf{M}|}, \tag{2}$$

which obeys the Bloch equation, i.e.,

$$\dot{\mathbf{m}}=-\gamma(\mathbf{B}\times\mathbf{m}), \tag{3}$$

with

$$\mathbf{m}\cdot\mathbf{m}=1. \tag{4}$$

Let us introduce the two variables, ξ and η, defined by

$$m_1+i\,m_2=\xi(1-m_3), \tag{5}$$

and

$$m_1-i\,m_2=\frac{1}{\eta}(m_3-1); \tag{6}$$

then we find

$$\xi=\frac{m_1+i\,m_2}{1-m_3}=\frac{1+m_3}{m_1-i\,m_2}, \tag{7}$$

and

$$\eta=-\frac{1-m_3}{m_1-i\,m_2}=-\frac{m_1+i\,m_2}{1+m_3}, \tag{8}$$

and the relationships between ξ and η such that

$$\xi\eta^*=\xi^*\eta=-1, \tag{9}$$

$$\xi\xi^*=\frac{1+m_3}{1-m_3}, \tag{10}$$

and

$$\eta=-\frac{1-m_3}{1+m_3}\xi. \tag{11}$$

Differentiating Eq. (7) with respect to time and substituting Eq. (3) into it, we find the Riccati equation,

$$\dot{\xi}=\tfrac{1}{2}\gamma(B_2+i\,B_1)\,\xi^2-i\,\gamma B_3\,\xi+\tfrac{1}{2}\gamma(B_2-i\,B_1). \tag{12}$$

Similarly, we also find the same Riccati equation for η. Here use has been made of the relationship

$$B_1\,m_2-B_2\,m_1=-\tfrac{1}{2}(B_2+i\,B_1)(m_1+i\,m_2)-\tfrac{1}{2}(B_2-i\,B_1)(m_1-i\,m_2). \tag{13}$$

Let z be defined by

$$z=\left(\frac{B_2-i\,B_1}{B_2+i\,B_1}\right)^{1/2}; \tag{14}$$

then we find

$$z = \pm i\, e^{i\psi}, \tag{15}$$

where

$$B_2 \pm i\, B_1 = \pm i\, B_0\, e^{\mp i\psi}, \tag{16}$$

with

$$B_0 = \sqrt{B_1^2 + B_2^2}, \tag{17}$$

and

$$\psi = \cos^{-1}\left(\frac{B_1}{B_0}\right) = \sin^{-1}\left(\frac{B_2}{B_0}\right) = \tan^{-1}\left(\frac{B_2}{B_1}\right). \tag{18}$$

Having assigned the two phases of z to ξ and η, we define

$$\xi = -i\, e^{i\psi} u, \tag{19}$$

and

$$\eta = i\, e^{i\psi} v. \tag{20}$$

Thus we find the relationships from Eqs. (9), (10), and (11):

$$u v^* = u^* v = 1, \tag{21}$$

$$u u^* = \frac{1+m_3}{1-m_3}, \tag{22}$$

and

$$v = \frac{1-m_3}{1+m_3} u. \tag{23}$$

Since u is defined by Eq. (19),

$$\xi = z u, \tag{24}$$

with

$$z = -i\, e^{i\psi}, \tag{25}$$

then the Riccati equation (12) turns out to be

$$z \dot{u} = \tfrac{1}{2}\gamma(B_2 - i B_1)(u^2+1) - (\dot{z} + i\,\gamma B_3 z)\, u. \tag{26}$$

Notice that the Riccati equation (26) can be solved by requiring the coefficient of u to be proportional to the coefficient of u^2+1;

$$\dot{z} + i\,\gamma B_3 z = i\, C\, \tfrac{1}{2}\gamma(B_2 - i B_1), \tag{27}$$

where C is an arbitrary real constant. This produces a separation of the variables, u and z, and leads to an expression for z consistent with the previous definition after solving the resulting first-order linear differential equation.[6]

Using Eqs. (16) and (25), we rewrite Eq. (27) in the form

$$\dot{z} = i(-\gamma B_3 + \tfrac{1}{2} C\, \gamma B_0) z\,. \tag{28}$$

The solution of Eq. (28) is easily found and given by

$$z = -i\, e^{i\psi}, \tag{29}$$

where

$$\psi = \int_{t_0}^{t} \left[-\gamma B_3(\tau) + \frac{1}{2} C\, \gamma B_0(\tau) \right] d\tau\,. \tag{30}$$

Substituting Eq. (27) into Eq. (26), we find

$$\dot{u} = \tfrac{1}{2} \gamma B_0 (u^2 - i\, C\, u + 1)\,, \tag{31}$$

where we have used Eqs. (16) and (25).

Solving Eq. (31), we find two solutions:

$$u_1 = i\, \alpha + \beta \tan(\beta \chi)\,, \tag{32}$$

and

$$u_2 = i\, \alpha - \beta \cot(\beta \chi)\,, \tag{33}$$

where α and β are given by

$$\alpha = \tfrac{1}{2} C\,, \tag{34}$$

and

$$\beta = \sqrt{1 + \alpha^2}\,, \tag{35}$$

and

$$\chi = \frac{1}{2} \gamma \int_{t_0}^{t} B_0(\tau)\, d\tau\,. \tag{36}$$

Similarly we find the solutions for η as

$$\eta = i\, e^{i\psi} v\,, \tag{37}$$

with

$$v = \frac{1}{(u\, u^*)} u\,, \tag{38}$$

where v is the solution of the differential equation;

$$\dot{v} = -\tfrac{1}{2} \gamma B_0 (v^2 + i\, C\, v + 1)\,. \tag{39}$$

We thus find the solutions of Eq. (39),

$$v_1 = -[i\,\alpha + \beta \tan(\beta\,\chi)]\,, \tag{40}$$

and

$$v_2 = -[i\,\alpha - \beta \cot(\beta\,\chi)]\,. \tag{41}$$

The solutions of the Riccati equation for ξ and η have the same forms.

We have found two solutions of the Riccati equation (12):

$$\xi_1 = -i\,e^{i\psi} u_1 = e^{i\psi}[\alpha - i\,\beta \tan(\beta\,\chi)]\,, \tag{42}$$

and

$$\xi_2 = -i\,e^{i\psi} u_2 = e^{i\psi}[\alpha + i\,\beta \cot(\beta\,\chi)]\,. \tag{43}$$

The Riccati equation (12) can be cast in the more convenient form

$$\dot{\xi} = i\,\dot{\chi}\,e^{-i\psi}\,\xi^2 - i\,\dot{\chi}_3\,\xi - i\,\dot{\chi}\,e^{i\psi}\,, \tag{44}$$

where

$$\chi_3 = \gamma \int_{t_0}^{t} B_3(\tau)\,d\tau\,. \tag{45}$$

Here we have used Eqs. (16), (17), and (36).

By using the solutions (42) and (43), we can find a third solution of the Riccati equation (44). Since $\xi_i\,,(i=1,2)$ are the solutions of Eq. (44), we have

$$\dot{\xi} - \dot{\xi}_i = i\,\dot{\chi}\,e^{-i\psi}(\xi^2 - \xi_i^2) - i\,\dot{\chi}_3(\xi - \xi_i) \quad (i=1,2)\,, \tag{46}$$

namely,

$$\frac{\dot{\xi} - \dot{\xi}_i}{\xi - \xi_i} = i\,\dot{\chi}\,e^{-i\psi}(\xi + \xi_i) - i\,\dot{\chi}_3 \quad (i=1,2)\,. \tag{47}$$

Thus we find

$$\frac{\dot{\xi} - \dot{\xi}_1}{\xi - \xi_1} - \frac{\dot{\xi} - \dot{\xi}_2}{\xi - \xi_2} = i\,\dot{\chi}\,e^{-i\psi}(\xi_1 - \xi_2)\,. \tag{48}$$

The solution of the differential equation (48) is

$$\frac{\xi - \xi_1}{\xi - \xi_2} = C_1 \exp\left\{ i \int_{t_0}^{t} \dot{\chi}(\tau) e^{-i\psi(\tau)}[\xi_1(\tau) - \xi_2(\tau)]\,d\tau \right\}, \tag{49}$$

where C_1 is a constant of integration. The third solution is obtained by substituting Eqs. (42) and (43) into Eq. (49). The result turns out to be

$$\frac{\xi_3 - \xi_1}{\xi_3 - \xi_2} = \tan(\beta\,\chi)\,, \tag{50}$$

where we have chosen C_1 as

$$C_1 = \tan[\beta\,\chi(t_0)]\,. \tag{51}$$

Thus we find

$$\xi_3 = e^{i\psi}\left[\alpha - i\,\beta\frac{1+\tan(\beta\chi)}{1-\tan(\beta\chi)}\right] = e^{i\psi}\left[\alpha + i\,\beta\frac{1+\cot(\beta\chi)}{1-\cot(\beta\chi)}\right]. \tag{52}$$

III. THE FUNDAMENTAL SYSTEM

A set of three solutions of the homogeneous Bloch equation is obtained from the Riccati equation (12) corresponding to equations Eqs. (42), (43), and (52).

Let $\mathbf{m}^{(i)}$ $(i=1,2,3)$, be

$$m_1^{(i)} = \frac{\xi_i + \xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{53}$$

$$m_2^{(i)} = -\,i\,\frac{\xi_i - \xi_i^*}{1+\xi_i\,\xi_i^*}, \tag{54}$$

and

$$m_3^{(i)} = -\,\frac{1-\xi_i\,\xi_i^*}{1+\xi_i\,\xi_i^*}; \tag{55}$$

then the fundamental matrix K is defined by

$$(K)_{ij} = K_{ij} = m_i^{(j)} \quad (i,j=1,2,3)\,. \tag{56}$$

Here use has been made of the definitions of ξ and η, Eqs. (5) and (6), respectively, together with Eq. (9).

Substituting Eqs. (42), (43), and (52) into Eqs. (53), (54), and (55), we write out the elements of the fundamental matrix here:

$$K_{11} = m_1^{(1)} = \frac{1}{\beta^2}\{\alpha[1+\cos(2\beta\chi)]\cos\psi + \beta\sin(2\beta\chi)\sin\psi\}, \tag{57}$$

$$K_{21} = m_2^{(1)} = \frac{1}{\beta^2}\{\alpha[1+\cos(2\beta\chi)]\sin\psi - \beta\sin(2\beta\chi)\cos\psi\}, \tag{58}$$

$$K_{31} = m_3^{(1)} = -\left(\frac{1-\alpha^2}{\beta^2}\right)\frac{1}{2}[1+\cos(2\beta\chi)] + \frac{1}{2}[1-\cos(2\beta\chi)], \tag{59}$$

$$K_{12} = m_1^{(2)} = \frac{1}{\beta^2}\{\alpha[1-\cos(2\beta\chi)]\cos\psi - \beta\sin(2\beta\chi)\sin\psi\}, \tag{60}$$

$$K_{22} = m_2^{(2)} = \frac{1}{\beta^2}\{\alpha[1-\cos(2\beta\chi)]\sin\psi + \beta\sin(2\beta\chi)\cos\psi\}, \tag{61}$$

$$K_{32} = m_3^{(2)} = -\left(\frac{1-\alpha^2}{\beta^2}\right)\frac{1}{2}[1-\cos(2\beta\chi)] + \frac{1}{2}[1+\cos(2\beta\chi)], \tag{62}$$

$$K_{13} = m_1^{(3)} = \frac{1}{\beta^2}\{\alpha[1-\sin(2\beta\chi)]\cos\psi + \beta\cos(2\beta\chi)\sin\psi\}, \tag{63}$$

$$K_{23}=m_2^{(3)}=\frac{1}{\beta^2}\{\alpha[1-\sin(2\beta\chi)]\sin\psi-\beta\cos(2\beta\chi)\cos\psi\}, \tag{64}$$

and

$$K_{33}=m_3^{(3)}=-\left(\frac{1-\alpha^2}{\beta^2}\right)\frac{1}{2}[1-\sin(2\beta\chi)]+\frac{1}{2}[1+\sin(2\beta\chi)]. \tag{65}$$

First of all we have to calculate the determinant of the fundamental matrix. The result turns out to be

$$\det K=\frac{2\alpha}{\beta^3}=C\left(\frac{2}{\sqrt{4+C^2}}\right)^3. \tag{66}$$

This means that the fundamental matrix is nonsingular and the three solutions of the homogeneous Bloch equation are linearly independent.

The homogeneous Bloch equation (3) is written in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{m}=A\,\mathbf{m}, \tag{67}$$

where the normalized magnetization vector $\mathbf{m}$ is a column vector and A is 3×3 matrix and given by

$$A=\begin{pmatrix} 0 & \gamma B_3 & -\gamma B_2 \\ -\gamma B_3 & 0 & \gamma B_1 \\ \gamma B_2 & -\gamma B_1 & 0 \end{pmatrix}. \tag{68}$$

The homogeneous Bloch equation turns out to be

$$\dot{K}_{ij}=\dot{m}_i^{(j)}=A_{ik}\,m_k^{(j)}=A_{ik}\,K_{kj}\quad(i,j=1,2,3), \tag{69}$$

where we assume summation over repeated indices and

$$(A)_{ij}=A_{ij}. \tag{70}$$

Thus we find

$$\dot{K}=A\,K. \tag{71}$$

Similarly, we find

$$\det\dot{K}=\dot{K}_{ij}\,K_{ij}^C=A_{ik}\,K_{kj}\,K_{ij}^C=A_{ik}\,\delta_{ki}\det K=\mathrm{tr}\,A\det K, \tag{72}$$

where K_{ij}^C is the cofactor of K_{ij} and

$$K_{ik}\,K_{jk}^C=\delta_{ij}\det K. \tag{73}$$

The solution of the differential equation (72) is

$$\det K=\det K(t_0)\exp\left[\int_{t_0}^{t}\mathrm{tr}\,A(\tau)\,d\tau\right], \tag{74}$$

with

$$\operatorname{tr} A = 0 . \tag{75}$$

Thus we find that Eq. (66) is exactly the solution we want.

The inhomogeneous Bloch equation has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{m} = A\,\mathbf{m} + \mathbf{b} , \tag{76}$$

where the column vector **b** is given by

$$b_i = -\frac{m_i}{T_i} \quad (i = 1, 2, 3) . \tag{77}$$

Here $T_i \quad (i = 1, 2, 3)$ are relaxation times.

The fundamental system of solutions of the homogeneous system is a set of three linearly independent magnetization vector, $\mathbf{m}^{(i)} \quad (i = 1, 2, 3)$. Using the fundamental matrix K defined by Eq. (56), the unique solution to the inhomogeneous system (76) is

$$\mathbf{m} = K K^{-1}(t_0)\,\mathbf{m}(t_0) + K \int_{t_0}^{t} K^{-1}(\tau)\,\mathbf{b}(\tau)\,d\tau , \tag{78}$$

where the inverse matrix of K is defined by

$$K^{-1} = \frac{\operatorname{adj} K}{\det K} , \tag{79}$$

with

$$(\operatorname{adj} K)_{ij} = K^{C}_{ji} . \tag{80}$$

The cofactors of $K_{ij} \quad (i, j = 1, 2, 3)$, are listed in the Appendix.

IV. CHARACTERISTICS OF THE MAGNETIC FIELD CLASS AND ILLUSTRATIVE EXAMPLE

In this section we give a brief discussion of the import of the restriction imposed on the magnetic field through the relation (81) below and an illustrative example of precession.

Differentiating Eq. (30) with respect to time, we find

$$\gamma B_3 = \frac{\dot{B}_1 B_2 - B_1 \dot{B}_2}{B_1^2 + B_2^2} + \frac{1}{2} C\,\gamma \sqrt{B_1^2 + B_2^2} , \tag{81}$$

where we have used Eq. (18). The third component of the magnetic field is expressed by the other two independent time-varying magnetic field components. The effect of the assumption (27) is to restrict the acceptable domain of the magnetic field variation to the region of $(\mathbf{B}, \dot{\mathbf{B}})$-space where the relationship (81) holds.

To discuss the characteristics of the magnetic field class we give some insight to the meaning of the restriction (81) which must be satisfied by the applied magnetic field in order to obtain the solution which is developed in the article.

The simplest practical discussion would center on the behavior of the third component when the first two components are harmonically varying;

$$\mathbf{B}(t) = (B_0(t)\cos(\omega t), B_0(t)\sin(\omega t), B_3(t)) , \tag{82}$$

with ω being a constant angular velocity (harmonic frequency). The restriction (81) leads to the relation

$$B_3(t) = -\frac{\omega}{\gamma} + \frac{1}{2} C B_0(t) . \tag{83}$$

This immediately suggests the effect of the variation of the constant C as a controlling influence on the third component of the applied magnetic field; the effects of variation of harmonic frequency, gyromagnetic ratio and the magnitude of the harmonic field thus being easily interpreted.

If the magnitude of the harmonic field, B_0, is time-independent, we then find the well-known solution of classical precession.

V. CONCLUSIONS

We have found a solution of the inhomogeneous Bloch equation for a class of time-varying magnetic fields. This has been done by finding the fundamental system in terms of a set of the three independent solutions of the homogeneous Bloch equation.

Notice that we can find a solution of the homogeneous Bloch equation in another form:

$$\mathbf{m}^{(1)} + \mathbf{m}^{(2)} = \frac{2\alpha}{\beta} \mathbf{m}^{(4)} , \tag{84}$$

where

$$\mathbf{m}^{(4)} = \left(\frac{1}{\beta} \cos\psi, \frac{1}{\beta} \sin\psi, \frac{\alpha}{\beta} \right)^{\mathrm{T}} . \tag{85}$$

Here we have used Eqs. (57) to (62). This is a generalized solution of the classical precession which can be decomposed into the two independent solutions, $\mathbf{m}^{(1)}$ and $\mathbf{m}^{(2)}$.

In general, the Riccati equation (44) can be rewritten in the form

$$\dot{u} = \dot{\chi} u^2 - i(\dot{\psi} + \dot{\chi}_3) u + \dot{\chi} , \tag{86}$$

where

$$\xi = -iue^{i\psi} . \tag{87}$$

It seems to be difficult to find a general solution of Eq. (86), because $\dot{\chi}_3$ is contained in the coefficient of u. The simplest soluble case is to be imposed the restriction as

$$\dot{\psi} + \dot{\chi}_3 = C\dot{\chi} . \tag{88}$$

This is exactly the same as Eq. (81).

Also note that the solutions obtained by using the linearized Riccati equation[5] were restricted to the case of

$$C = \pm 2 \quad \text{or} \quad \alpha = \pm 1 , \tag{89}$$

in which some simplifications of the solutions (57)–(65) occur.

ACKNOWLEDGMENTS

I am indebted to Y. Takahashi for the discussions at earlier stages of this work. I thank M. Kawasaki for continual discussions about solutions of the Bloch equation.

APPENDIX: THE COFACTORS OF K_{ij} $(i, j=1, 2, 3)$

We list here the cofactors of the element of the fundamental matrix K:

$$K_{11}^{C}=\frac{1}{2}\left(\frac{1-\alpha^2}{\beta^3}\right)[1-\cos(2\beta\chi)-\sin(2\beta\chi)]\cos\psi - \frac{1}{\beta^2}\left\{\alpha[\cos(2\beta\chi)-\sin(2\beta\chi)]\sin\psi-\frac{1}{2}\beta[1+\cos(2\beta\chi)+\sin(2\beta\chi)]\cos\psi\right\}, \tag{A1}$$

$$K_{21}^{C}=\frac{1}{2}\left(\frac{1-\alpha^2}{\beta^3}\right)[1-\cos(2\beta\chi)-\sin(2\beta\chi)]\sin\psi + \frac{1}{\beta^2}\left\{\alpha[\cos(2\beta\chi)-\sin(2\beta\chi)]\cos\psi+\frac{1}{2}\beta[1+\cos(2\beta\chi)+\sin(2\beta\chi)]\sin\psi\right\}, \tag{A2}$$

$$K_{31}^{C}=\frac{\alpha}{\beta^3}[1-\cos(2\beta\chi)-\sin(2\beta\chi)], \tag{A3}$$

$$K_{12}^{C}=\frac{1}{2}\left(\frac{1-\alpha^2}{\beta^3}\right)[1+\cos(2\beta\chi)-\sin(2\beta\chi)]\cos\psi - \frac{1}{\beta^2}\left\{\alpha[\cos(2\beta\chi)+\sin(2\beta\chi)]\sin\psi-\frac{1}{2}\beta[1-\cos(2\beta\chi)+\sin(2\beta\chi)]\cos\psi\right\}, \tag{A4}$$

$$K_{22}^{C}=\frac{1}{2}\left(\frac{1-\alpha^2}{\beta^3}\right)[1+\cos(2\beta\chi)-\sin(2\beta\chi)]\sin\psi + \frac{1}{\beta^2}\left\{\alpha[\cos(2\beta\chi)+\sin(2\beta\chi)]\cos\psi+\frac{1}{2}\beta[1-\cos(2\beta\chi)+\sin(2\beta\chi)]\sin\psi\right\}, \tag{A5}$$

$$K_{32}^{C}=\frac{\alpha}{\beta^3}[1+\cos(2\beta\chi)-\sin(2\beta\chi)], \tag{A6}$$

$$K_{13}^{C}=-\frac{1}{\beta}\left(1-\frac{1-\alpha^2}{\beta^2}\right)\sin(2\beta\chi)\cos\psi+\frac{2\alpha}{\beta^2}\cos(2\beta\chi)\sin\psi, \tag{A7}$$

$$K_{23}^{C}=-\frac{1}{\beta}\left(1-\frac{1-\alpha^2}{\beta^2}\right)\sin(2\beta\chi)\sin\psi-\frac{2\alpha}{\beta^2}\cos(2\beta\chi)\cos\psi, \tag{A8}$$

and

$$K_{33}^{C}=\frac{2\alpha}{\beta^3}\sin(2\beta\chi). \tag{A9}$$

The determinant of the fundamental matrix is found by using Eqs. (A1) to (A9):

$$\det K = K_{i1} K^C_{i1} = K_{i2} K^C_{i2} = K_{i3} K^C_{i3} = \frac{2\alpha}{\beta^3}. \tag{A10}$$

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Quaternionic roots of SO(8), SO(9), F_4 and the related Weyl groups

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(Received 1 January 2003; accepted 31 March 2003)

The root systems of SO(8), SO(9) and F_4 are constructed by quaternions. Triality manifests itself as permutations of pure quaternion units e_1, e_2 and e_3. It is shown that the automorphism groups of the associated root systems are the finite subgroups of O(4) generated by left-right actions of unit quaternions on the root systems. The relevant finite groups of quaternions, the binary tetrahedral and binary octahedral groups, play essential roles in the construction of the Weyl groups and their conjugacy classes. The relations between the Dynkin indices, standard orthogonal vector and the quaternionic weights are obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1578177]

I. INTRODUCTION

The Lie groups SO(8), SO(9), F_4 and their Lie algebras have generated more interest[1] regarding their use in building massless supersymmetry and supergravity multiplets of the superstring theories and M-theory,[2] respectively. The SO(8) is the light-cone little group of the superstring theories in $9+1$ dimensions, which are certain limits of a bigger theory, called M-theory existing in $10+1$ dimensions. The massless degrees of freedom of M-theory require certain irreducible representations of SO(9). If algebraic structures play any role in ultimate unification of the fundamental forces, the F_4 seems to be a natural symmetry in which SO(9) can be embedded with a triply symmetric way.

In what follows we construct the root systems of SO(8), SO(9) and F_4 in terms of quaternions[3] and their Weyl group elements as pairs of unit quaternions acting on the quaternion weights from left and right. We show that the quaternion elements of the binary tetrahedral group and the binary octahedral group are relevant structures both for the root systems as well as the Weyl group elements of SO(8) and F_4, respectively. The SO(9) plays a transition stage between SO(8) and F_4.

For the root systems of these Lie algebras and their weights form lattices in four-dimensional Euclidean space, it is expected that their automorphism groups are the finite subgroups of O(4). The defining representation of O(4) can be constructed by the actions of a pair of unit quaternions (p,r) on an arbitrary quaternion q as $q\rightarrow pqr$ and $q\rightarrow p\bar{q}r$ with $\bar{q}$ being quaternion conjugate of q. The finite subgroups of O(4) can be classified with the use of finite subgroups of quaternions.[4]

We have organized the article as follows: The O(4) group of quaternions are introduced in Sec. II along with the binary tetrahedral group and the binary octahedral group of quaternions with their relevant subgroups, coset structures and the conjugacy classes. In Sec. III, we introduce the quaternionic simple roots of SO(8), construct its root system and its Weyl group with quaternions. The conjugacy classes of the Weyl group with its subgroup structures and extension of the Weyl group by the Dynkin diagram symmetry of SO(8) have been explicitly constructed.

The SO(9) root system and its Weyl group have been studied in Sec. IV. A similar analysis for

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TABLE I. The conjugacy classes of $2A_4$.

Conjugacy classes and orders of elements	Elements in the conjugacy classes denoted also by their total numbers
1	1
2	-1
4	$6 : 3_+ \oplus 3_- : \pm e_i,\ i=1,2,3$
6	$4_+ : \{\frac{1}{2}(1+e_1+e_2+e_3), \frac{1}{2}(1+e_1-e_2-e_3), \frac{1}{2}(1-e_1-e_2+e_3), \frac{1}{2}(1-e_1+e_2-e_3)\}$
6	$\overline{4}_+$: conjugates of 4_+
3	$4_- = -4_+$: negatives of 4_+
3	$\overline{4}_- = -\overline{4}_+$: negatives of $\overline{4}_+$

the F_4 algebra has been done in Sec. V. Embeddings of SO(9) in F_4, extension of $W(F_4)$ by the Dynkin diagram symmetry, relations between the Dynkin indices and the quaternionic weights and a number of interesting aspects of the Weyl groups have been worked out in relevant sections. Finally, in Sec. VI we discuss our results along with their possible use in four-dimensional crystallography as well as the superstring theories and M-theory.

II. THE O(4) SYMMETRY OF QUATERNIONS

A quaternion $q=\Sigma_{a=0}^{3} q_a e_a$ with q_a real numbers and $e_a(e_0=1,e_1,e_2,e_3)$ quaternion units is a vector in four-dimensional Euclidean space where pure quaternions satisfy the relations

$$e_i e_j = -\delta_{ij} + \epsilon_{ijk} e_k, \quad i,j,k=1,2,3. \tag{1}$$

Here δ_{ij} and ϵ_{ijk} are the usual Kronecker and Levi-Civita symbols, respectively. The quaternions of unit norm $q\overline{q}=\overline{q}q=1$ with quaternion conjugate $\overline{q}=q_0-\Sigma_{i=1}^{3} q_i e_i$ form a group isomorphic to SU(2). The finite subgroups of quaternions relevant to our discussions are the quaternion group $Q=\langle 2,2,2\rangle$ of order 8, the binary octahedral group $T=\langle 3,3,2\rangle=2A_4$ of order 24 and the binary octahedral group $O=\langle 4,3,2\rangle=2S_4$ of order 48. [There are a number of notations in the literature for the finite subgroups of quaternions. (The notation for the finite subgroups of quaternions $\langle p,q,r\rangle$ which is introduced by Coxeter and Moser[5] means the group generators A,B,C satisfy the relations $A^p=B^q=C^r=Z, Z^2=1$.) We will interchangeably use all; however, we will mainly follow the notations of the Atlas of Finite Groups.[6] The group $G=AB$ denotes any group having a normal subgroup structure A, for which the corresponding quotient group has structure B. The finite groups of quaternions are of this type, e.g., $2A_4$, $2S_4$ and $2A_5$ are the double covers of the tetrahedral, octahedral and icosahedral groups where 2 stands for the center of the group. The group $G=A\times B$ (or $G=A:B$ in the notation of Ref. 6) is the semi-direct product of two groups A and B where A is the invariant subgroup and B is the quotient group. An important difference from the previous case is that a copy of B lies within the group G. The direct product of two groups is denoted by $G=A\times B$.] The conjugacy classes of $2A_4$ and $2S_4$ will be used when we construct the Weyl groups $W(D_4)$, $W(B_4)$ and $W(F_4)$ of the Lie algebras SO(8), SO(9) and F_4, respectively, and they are given in Tables I and II. The positive and negative subscripts are self-explanatory and are chosen such that these discrete quaternions will also stand for positive and negative roots of the Lie algebras of interest.

For completeness, here we introduce the important properties of the O(4) symmetry of quaternions. A pair of unit quaternions (p,r), with $p\overline{p}=r\overline{r}=1$, multiplying an arbitrary quaternion q from left and right,

$$(p,r): q \to pqr = e^{\alpha P} q e^{\beta R}, \tag{2}$$

leaves the quaternion norm $q\overline{q}=\overline{q}q$ invariant. Here $P=-\overline{P}$ and $R=-\overline{R}$ are pure quaternions. It can be shown that the determinant of the 4×4 matrix corresponding to the transformation (2) is

TABLE II. The conjugacy classes of $2S_4$.

Conjugacy classes and orders of elements	Elements in the conjugacy classes denoted also by their total numbers
1	1
2	-1
4	$6=3_+\oplus 3_-:\pm e_i,\ i=1,2,3$
6	$8_+=4_+\oplus\overline{4}_+:\frac{1}{2}(1\pm e_1\pm e_2\pm e_3)$
3	$8_-=-8_+:\frac{1}{2}(-1\pm e_1\pm e_2\pm e_3)$
4	$6_+\oplus 6_-;6_+=\left\{\frac{1}{\sqrt{2}}(e_1\pm e_2),\frac{1}{\sqrt{2}}(e_2\pm e_3),\frac{1}{\sqrt{2}}(e_3\pm e_1)\right\}, 6_-=-6_+$
8	$6'_+:\left\{\frac{1}{\sqrt{2}}(1\pm e_1),\frac{1}{\sqrt{2}}(1\pm e_2),\frac{1}{\sqrt{2}}(1\pm e_3)\right\}$
8	$6'_-=-6'_+:\left\{\frac{1}{\sqrt{2}}(-1\pm e_1),\frac{1}{\sqrt{2}}(-1\pm e_2),\frac{1}{\sqrt{2}}(-1\pm e_3)\right\}$

$+1$, thereby indicating that it is an element of the SO(4) subgroup. The left and right rotations in (2) are actually representing a double rotation through the angles $\alpha+\beta$, $\alpha-\beta$ about planes generated by vectors $(O,P-R,1+RP)$ and $(O,P+R,1-RP)$, respectively.[7] The two planes are orthogonal to each other. In addition to the transformation in (2) one can define a transformation

$$(p,r)^*:q\rightarrow p\overline{q}r, \tag{3}$$

which also leaves $q\overline{q}=\overline{q}q$ invariant. Since (3) leaves $p+r$ invariant and changes sign of $p-r$ for general unit quaternions p and r, it follows that $(p,r)^*$ is a rotary reflection having determinant -1. Therefore (p,r) and $(p,r)^*$ generate the group O(4). Below we give some properties of the group elements:

$$\begin{gathered}(a,b)(c,d)=(ac,db),\quad (a,b)^{-1}=(a^{-1},b^{-1})=(\overline{a},\overline{b}),\\ (a,b)^*(c,d)^*=(a\overline{d},\overline{c}b),\quad (a,b)^{*-1}=(b,a)^*,\\ (a,b)(c,d)^*=(ac,db)^*,\\ (a,b)^*(c,d)=(a\overline{d},\overline{c}b)^*.\end{gathered} \tag{4}$$

The element $(1,1)^*$ acts as a conjugation $(1,1)^*:q\rightarrow\overline{q}$, which leaves the SO(4) invariant:

$$(1,1)^*(a,b)(1,1)^{*-1}=(\overline{b},\overline{a})^*(1,1)^{\times}=(\overline{b},\overline{a})\in \mathrm{SO}(4). \tag{5}$$

This shows that SO(4) is an invariant subgroup of O(4) dividing O(4) into two cosets generated by the elements (a,b) and $(a,b)(1,1)^*=(a,b)^*\neq(1,1)^*(a,b)=(\overline{b},\overline{a})^*$ for a general element (a,b). The quotient group $\mathrm{O}(4)/\mathrm{SO}(4)=2=Z_2$ is represented by $(1,1)^*$ and $(1,1)$, a copy of which is within the group O(4). Therefore we have the semi-direct product structure $\mathrm{O}(4)=\mathrm{SO}(4)\rtimes 2$. The SO(3) subgroup of SO(4) is generated by the elements $(a,\overline{a})$, which can be extended to O(3) by $(1,1)^*$. But we note that $(1,1)^*$ and the SO(3) elements are commutative as we have

$$(a,\overline{a})(1,1)^*=(1,1)^*(a,\overline{a})=(a,\overline{a})^*. \tag{6}$$

This relation proves that O(3) has a direct product structure $\mathrm{O}(3)=2\times\mathrm{SO}(3)$.

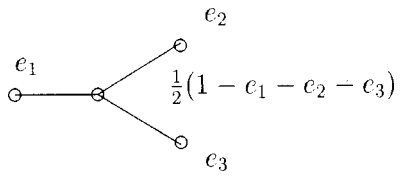

FIG. 1. Dynkin diagram of SO(8) with unit quaternions.

Quaternions can be represented by 2×2 unitary matrices where the quaternion units have the correspondence $1\rightarrow I, e_i\rightarrow -i\sigma_i$ where I is the 2×2 unit matrix while σ_i are the Pauli matrices. The transformations (2) and (3) can be written in terms of 2×2 unitary matrices in the forms

$$e^{-i\alpha\vec{n}\cdot\vec{\sigma}}\begin{pmatrix} q_0+iq_3 & iq_1+q_2 \\ iq_1-q_2 & q_0-iq_3 \end{pmatrix} e^{-i\beta\vec{m}\cdot\vec{\sigma}}$$

and

$$e^{-i\alpha\vec{n}\cdot\vec{\sigma}}\begin{pmatrix} q_0-iq_3 & -iq_1-q_2 \\ -iq_1+q_2 & q_0+iq_3 \end{pmatrix} e^{-i\beta\vec{m}\cdot\vec{\sigma}},$$

respectively. Determinants of the matrices q and $q^\dagger$ are left invariant corresponding to the norms of the vectors q and $\overline{q}$, respectively.

The finite subgroups of O(4) can be obtained from the finite subgroups of quaternions by the rules given in (4). We will analyze some of them when we deal with the Weyl groups $W(D_4)$, $W(B_4)$ and $W(F_4)$ as well as the full automorphism groups of the root systems. In an earlier publication[8] we have introduced a general method to construct the conjugacy classes of the Coxeter group H_4. A similar method also applies here in the construction of conjugacy classes of the Weyl groups of interest.

III. THE ROOT SYSTEM OF SO(8) AND ITS WEYL GROUP $W(D_4)$

In this section we will construct the root system of SO(8) and its automorphism group with quaternions. In one publication[3] one of us (MK) has given the root systems of SO(8), SO(9) and F_4 in terms of quaternions. However, no one has since then constructed the automorphism groups of their root systems as finite subgroups of O(4) using quaternions.

The scalar product of two quaternions q_1 and q_2 can be defined by $(q_1,q_2)=\frac{1}{2}(q_1\overline{q_2}+q_2\overline{q_1})$. In the four-dimensional Euclidean space the quaternion units $e_a(a=0,1,2,3)$ with this scalar product form an orthonormal basis. The familiar orthogonal vector system l_i $(i=1,2,\ldots,r)$ used for the construction of root systems of Lie algebras[9] is given for $r=4$ in terms of the quaternion units as

$$l_1=\frac{1}{\sqrt{2}}(1+e_1),\quad l_2=\frac{1}{\sqrt{2}}(1-e_1),\quad l_3=\frac{1}{\sqrt{2}}(e_2+e_3),\quad l_4=\frac{1}{\sqrt{2}}(e_2-e_3). \tag{7}$$

The Dynkin diagram of SO(8) with quaternion simple roots scaled by $\sqrt{2}$ is depicted in Fig. 1. [Root systems of SO(8), SO(9) and F_4 will be represented by quaternions scaled by $\sqrt{2}$.]

The positive roots of SO(8) with the simple roots in Fig. 1 are

$$r_+=\{1,e_1,e_2,e_3,\tfrac{1}{2}(1\pm e_1\pm e_2\pm e_3)\}=\{1,3_+,4_+,\overline{4}_+\}. \tag{8}$$

The nonzero roots including their negatives form the set $T=V_0\oplus V_1\oplus V_2$, where

$$V_0=\{\pm e_a\quad (a=0,1,2,3)\}=\{\pm 1,3_+,3_-\}, \tag{9a}$$

TABLE III. The conjugacy classes of $W(D_4)$ with quaternions.

Class	Order	Type	No. of elements
1	1	(1,1)	1
2	2	$(-1,1)$	1
3	4	$(3_+,\pm 1)\oplus(\pm 1,3_+)$	12
4	3	$(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)$	32
5	6	$-[(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)]$	32←Coxeter element
6	2	$\pm(e_1,e_1),\pm(e_2,e_3),\pm(e_3,e_2)$	6
7	2	$\pm(e_2,e_2),\pm(e_3,e_1),\pm(e_1,e_3)$	6
8	2	$\pm(e_3,e_3),\pm(e_2,e_1),\pm(e_1,e_2)$	6
9	2	$(p,p)^*=(r_+,r_+)^*$[a]	12
10	2	$-(r_+,r_+)^*$	12
11	4	$\pm(e_1r_+,r_+)^*$	24
12	4	$\pm(e_2r_+,r_+)^*$	24
13	4	$\pm(e_3r_+,r_+)^*$	24

[a]r_+ represent the positive quaternionic roots in (8).

$$V_1=\{4_+\oplus 4_-\}, \tag{9b}$$

$$V_2=\{\overline{4}_+\oplus\overline{4}_-\}=\overline{V}_1 \tag{9c}$$

form the binary tetrahedral group $2A_4$ of order 24. The set V_0 is the quaternion group Q of order 8 and represents the vertices of a hyperoctahedron in four dimensions.[4] Similarly the sets of quaternions V_1 and V_2 each represent a hyperoctahedron, however any two sets, say V_1 and V_2, form a hypercube in four dimensions. The symmetry of the root system of SO(8) is the symmetry of three congruent hyperoctahedrons. The quaternion group V_0 is an invariant subgroup of $2A_4$ where V_1 and $\overline{V}_1$ are the cosets obtained by multiplying V_0 on the left by

$$t=\tfrac{1}{2}(1+e_1+e_2+e_3),\quad t^2=-\overline{t},\ \text{i.e.,}\quad V_1=t\ V_0\ \text{ and }\ \overline{V}_1=\overline{t}V_0=V_2. \tag{10}$$

In fact $(t,\overline{t})$ is an SO(3) group element permuting the pure quaternion units e_i $i=1,2,3$ in the cyclic order

$$t\ e_i\overline{t}=e_{i+1}\ \text{ mod }\ 3,\quad i=1,2,3. \tag{11}$$

The binary tetrahedral group can be written as $T=V_0{:}3$ where 3 is the cyclic group of order 3.

The Weyl group of $W(D_4)$ of SO(8) is generated by reflections with respect to the hyperplanes orthogonal to the simple roots. An arbitrary quaternion q is reflected by the quaternionic root $\alpha'=\sqrt{2}\alpha$ where α is unit quaternion

$$q\to q-\frac{2(q,\alpha')}{(\alpha',\alpha')}\alpha'=-\alpha\overline{q}\alpha=-(\alpha,\alpha)^*. \tag{12}$$

The generators of $W(D_4)$ in terms of the unit quaternion simple roots can be written as

$$-(e_1,e_1)^*,\ -(e_2,e_2)^*,\ -(e_3,e_3)^*,\ -(\overline{t,t})^*. \tag{13}$$

A computer calculation leading to the 192 elements of $W(D_4)$ with 13 conjugacy classes is given in Table III.

There is, however, a simpler way to obtain the group elements of $W(D_4)$ by hand. We start with the quaternion group V_0, elements of which are the roots of $SU(2)^4$ subalgebra of SO(8). The automorphism group of the set V_0 is just the set of elements

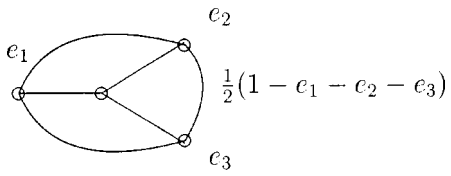

FIG. 2. The cyclic Dynkin diagram symmetry.

$$(V_0,V_0) \text{ and } (V_0,V_0)^* \tag{14}$$

forming a group of order $32\times 2=64$. Before proceeding further we note the following products of sets $V_a(a=0,1,2)$ satisfying the relations

$$V_a\ V_b=V_{a+b} \text{ mod } 3; \quad a,b=0,1,2. \tag{15}$$

The group elements of $W(D_4)$ can be generated by multiplying (14) by the element $a=(t,t)$ with $a^3=(1,1)$ on the left or on the right. Since $a=(t,t)$ is one of the elements of the set (V_1,V_1) we have a great number of choices for the coset representatives. Instead of choosing a particular element we use the whole set of elements (V_1,V_1) to generate the rest of elements $W(D_4)$. Multiplying (14) by (V_1,V_1) and $(V_1,V_1)^2=(V_2,V_2)$ and using (15) we obtain the sets of elements

$$W(D_4): \begin{matrix}(V_0,V_0),\ (V_1,V_1),\ (V_2,V_2)\\ (V_0,V_0)^*,\ (V_1,V_1)^*,\ (V_2,V_2)^*\end{matrix}. \tag{16}$$

Using (4) and (15) we can show that the elements in (16) form a group of order $32\times 6=192$, the conjugacy classes of which are the elements given in Table III. Obviously, the elements of $W(D_4)$ in (16) leave the root system Φ_{D_4} of SO(8),

$$\Phi_{D_4}=V_0\oplus V_1\oplus V_2, \tag{17}$$

invariant. However, the full automorphism group of Φ_{D_4} is not the Weyl group $W(D_4)$. The Dynkin diagram symmetry resulting in the simple roots $t\ e_i\overline{t}=e_{i+1}$ with $(e_4=e_1)$ shown in (11) can be represented by an element of SO(4), $b=(t,\overline{t})$ with $b^3=(1,1)$. The cyclic symmetry of the simple roots is shown in Fig. 2. All Dynkin diagram symmetries leave the associated Weyl groups invariant. In the present example that means

$$bW(D_4)\ b^{-1}=W(D_4). \tag{18}$$

Adjoining the generator b to $W(D_4)$ one generates a larger group which we denote by $\text{Aut}'\ \Phi_{D_4}=W(D_4)\rtimes Z_3$. The $\text{Aut}'\ \Phi_{D_4}$ is not the full automorphism of Φ_{D_4}. One can, by exchanging any pair of e_i and leaving the third term intact, extend the $\text{Aut}'\ \Phi_{D_4}$ to $\text{Aut}\ \Phi_{D_4}$ which we will discuss later. With the action of $b=(t,\overline{t})\in(V_1,V_2)$ on the elements of $W(D_4)$ in (16) on the left or right one generates the elements of the $\text{Aut}'\ \Phi_{D_4}$:

$$\text{Aut}'\ \Phi_{D_4}=\{(V_a,V_b)\oplus(V_a,V_b)^*\} \text{ with } a,b=0,1,2. \tag{19}$$

Here we have altogether 18 sets of 32 sets of quaternions which form a group of order 576. Interestingly enough, it exploits the whole set of elements of the binary tetrahedral group $T=\Phi_{D_4}$ with all possible combinations. Therefore we can concisely write (19) as

$$\text{Aut}'\ \Phi_{D_4}=\{(T,T)\oplus(T,T)^*\}. \tag{20}$$

TABLE IV. The conjugacy classes of Aut′ Φ_{D_4} of order 576.

Class	Order	Type	No. of elements
1	1	(1,1)	1
2	2	$(-1,1)$	1
3	6	$(4_+,1)\oplus(1,\overline{4}_+)$	8
4	6	$(\overline{4}_+,1)\oplus(1,4_+)$	8
5	3	$-[(4_+,1)\oplus(1,\overline{4}_+)]$	8
6	3	$-[(\overline{4}_+,1)\oplus(1,4_+)]$	8
7	4	$(3_+,\pm 1)\oplus(\pm 1,3_+)$	12
8	3	$(4_+,\overline{4}_+)$	16
9	3	$(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)$	32
10	6	$-[(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)]$	32
11	6	$-(4_+,\overline{4}_+)$	16
12	3	$(\overline{4}_+,4_+)$	16
13	6	$-(\overline{4}_+,4_+)$	16
14	12	$(4_+,6)\oplus(6,\overline{4}_+)$	48
15	12	$(\overline{4}_+,6)\oplus(6,4_+)$	48
16	2	$(3_+,3_+)\oplus(-3_+,3_+)$	18
17	2	$(12_+,12_+)^*$	12
18	2	$-(12_+,12_+)^*$	12
19	4	$(3_+r_+,r_+)^*\oplus(-3_+r_+,r_+)^*$	72
20	6	$(4_+r_+,r_+)^*$	48
21	6	$(\overline{4}_+r_+,r_+)^*$	48
22	6	$-(4_+r_+,r_+)^*$	48
23	6	$-(\overline{4}_+r_+,r_+)^*$	48

The elements (T,T) form a finite subgroup of SO(4) of order 288. The conjugacy classes of Aut′ Φ_{D_4} are given in Table IV.

The full automorphism group of Φ_4 is obtained by extending the Aut′ Φ_4 by a generator $c=-((1/\sqrt{2})(e_2-e_3),(1/\sqrt{2})(e_2-e_3))^*$ which leads to the transformations $1\to 1$, $e_1\to e_1$, $e_2\leftrightarrow e_3$. The Dynkin diagram symmetry of this transformation is shown in Fig. 3.

The Aut′ Φ_4 is invariant under conjugation by the generator c

$$c\ \ \mathrm{Aut}'\ \ \Phi_4\ \ c^{-1}=\mathrm{Aut}'\ \ \Phi_4, \tag{21}$$

so that the full automorphism group Aut $\Phi_4=$ Aut′ $\Phi_4:Z_2$. It is also true that

$$c\ W(D_4)\ c^{-1}=W(D_4). \tag{22}$$

Therefore the generators b and c generate a group $D_3\approx S_3$ satisfying the generation relations

$$c\ \ b\ \ c^{-1}=b^{-1}. \tag{23}$$

Therefore now the Aut Φ_4 can be written as

$$\mathrm{Aut}\ \ \Phi_4=W(D_4)\rtimes S_3. \tag{24}$$

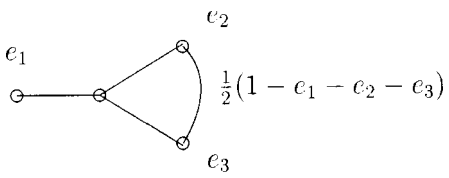

FIG. 3. The Dynkin diagram symmetry of SO(8) exchanging two simple roots leaving the other root intact.

This is the group of order 1152 which is also isomorphic to the Weyl group of F_4. Had we extended $W(D_4)$ by c we would have obtained the Weyl group of SO(9),

$$W(B_4)=W(D_4)\rtimes Z_2 \tag{25}$$

of order 384. The details of these works will be dealt with in the following sections.

We now turn back to further aspects of the root system of SO(8) and its Weyl group $W(D_4)$. The weight vector of any irreducible representation of SO(8) is represented by a quaternion $q=q_0+q_1e_1+q_2e_2+q_3e_3$. The relations between the quaternion components of a weight vector and the Dynkin indices $\wedge=(a_1,a_2,a_3,a_4)$ and the Weyl vector δ are given by

$$q_0=\frac{1}{\sqrt{2}}(a_1+2a_2+a_3+a_4),\quad q_1=\frac{1}{\sqrt{2}}a_1,\quad q_2=\frac{1}{\sqrt{2}}a_4,\quad q_3=\frac{1}{\sqrt{2}}a_3, \tag{26a}$$

$$\delta=\frac{1}{\sqrt{2}}(5+e_1+e_2+e_3). \tag{26b}$$

The Dynkin diagram symmetry on the indices (a_1,a_4,a_3) is now transformed to an S_3 symmetry on the pure quaternion units e_1, e_2 and e_3. This symmetry is even more apparent in the dimension formula which we do not want to illustrate for it is lengthy. However, similar triality symmetries can be shown on the Weyl group $W(D_4)$. The highest weights of some low dimensional irreducible representations of SO(8) are given in the quaternion weights versus Dynkin indices in Table V. When we examine the character table of $W(D_4)$ we note that the elements $\pm(e_1,e_1)$, $\pm(e_2,e_3)$ and $\pm(e_3,e_2)$ are in the same conjugacy classes which together with the elements $(-1,1)$ and $(1,1)$ form an elementary Abelian subgroup of $W(D_4)$ denoted by $2^3=Z_2^3$. Obviously this is an invariant subgroup where the quotient group $S_4=W(D_4)/Z_2^3$ is generated by the set of elements

$$(e_3,e_3)^*,\quad (t,t)^*. \tag{27}$$

The generators $(e_3,e_3)=(e_3,e_3)^*(1,1)^*$ and $(t,t)=(t,t)^*(1,1)^*$ generate the tetrahedral subgroup A_4 of S_4 of order 12. The A_4 involves the generators (e_3,e_3), (e_2,e_1), (e_1,e_2) and $(1,1)$ which form the elementary Abelian group 2^2 (Klein's fier-gruppe); under the cyclic group generator $a=(t,t)$ of order 3, the Klein's four-group is left invariant. This analysis reveals the whole skeleton of the Weyl group $W(D_4)$,

$$W(D_4)=2^3\rtimes S_4=2^3\rtimes A_4\rtimes 2=2^3\rtimes 2^2\rtimes 3\rtimes 2. \tag{28}$$

We could have chosen the generators of S_4 as

$$(e_2,e_2)^*\ \text{ and }\ (t,t)^*, \tag{29}$$

which leave the same elementary Abelian group 2^3 invariant. A closer inspection of Table III (class numbers 6, 7, 8) shows that we have three alternative choices for the elementary Abelian group 2^3 and two choices for S_4 generators for each elementary abelian group of order 8. This is another explicit indication that the $W(D_4)$ is invariant under an outer automorphism of S_3.

IV. THE ROOT SYSTEM OF SO(9) AND ITS WEYL GROUP $W(B_4)$

The standard simple roots of SO(9) with the orthogonal vectors l_i $(i=1,2,3,4)$[7] and its positive roots are

$$l_1-l_2,\quad l_2-l_3,\quad l_3-l_4,\quad l_4, \tag{30a}$$

TABLE V. The highest weights of some low dimensional irreducible representations of SO(8) with quaternions versus Dynkin indices.

Dimension	Dynkin indices	Quaternion weight
8_v	(1000)	$\frac{1}{\sqrt{2}}(1+e_1)$
8_s	(0001)	$\frac{1}{\sqrt{2}}(1+e_2)$
8_c	(0010)	$\frac{1}{\sqrt{2}}(1+e_3)$
28	(0100)	$\sqrt{2}$
35_v	(2000)	$\sqrt{2}(1+e_1)$
35_s	(0002)	$\sqrt{2}(1+e_2)$
35_c	(0020)	$\sqrt{2}(1+e_3)$
56_v	(0011)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_2+e_3)$
56_s	(1010)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_3+e_1)$
56_c	(1001)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_1+e_2)$
112_v	(3000)	$\frac{3}{\sqrt{2}}(1+e_1)$
112_s	(0003)	$\frac{3}{\sqrt{2}}(1+e_2)$
112_c	(0030)	$\frac{3}{\sqrt{2}}(1+e_3)$

$$l_i \pm l_j, \quad 1 \leqslant i \leqslant j \leqslant 4, \qquad l_i, \quad 1 \leqslant i \leqslant 4. \tag{30b}$$

Its Dynkin diagram with quaternion simple roots scaled by $\sqrt{2}$ is shown in Fig. 4.

The scaled quaternion roots of SO(9) will be given by the sets of quaternions

$$\Phi_{B_4}: V_0, \quad V_1, \quad V_2 \quad \text{and} \quad V_x' = \left\{ \begin{array}{l} \frac{1}{2}(\pm 1 \pm e_1) \\ \frac{1}{2}(\pm e_2 \pm e_3) \end{array} \right\}. \tag{31}$$

The set in V_x' is the scaled short roots. The actual short roots of unit norm are denoted by the set $V_x = \sqrt{2} V_x'$. The first three simple roots in Fig. 4 are the simple roots of SO(8). The reflection by the simple root $\alpha_4 = \sqrt{2}\alpha_4' = (1/\sqrt{2})(e_2 - e_3)$ can be computed by

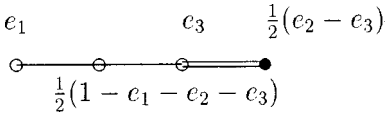

FIG. 4. Dynkin diagram of SO(9) with scaled quaternion simple roots.

TABLE VI. The conjugacy classes of $W(B_4)$ with quaternions.

Class	Order	Type of elements	No. of elements
1	1	(1,1)	1
2	2	$(-1,1)$	1
3	4	$(\pm e_i,\pm 1), i=1,2,3$	12
4	2	$\{\pm(e_d,e_d),\pm(e_d,e_1),\pm(e_1,e_d), d=2,3\}$	12
5	2	$\pm\{(e_1,e_1),(e_2,e_3),(e_3,e_2)\}$	6
6	2	$\pm\{(a_{12},a_{31}),(a_{31},a_{12}),(a_{23},a_{23})\}$[a]	24
7	8	$\pm\{(a_{01},a_{23}),(a_{23},a_{01}),(a_{02},a_{12}),\ (a_{12},a_{02}),(a_{03},a_{31}),(a_{31},a_{03})\}$	48
8	3	$\{(4_+,4_+),(\overline{4}_+,\overline{4}_+)\}$	32
9	6	$-\{(4_+,4_+),(\overline{4}_+,\overline{4}_+)\}$	32
10	4	$\{(a_{01},a_{01}),(a_{02},a_{03}),(a_{03},a_{02})\}$	12
11	4	negatives of elements of class (10)	12
12	2	$\{(e_a.e_a)^*,(4_+,4_+)^*,(\overline{4}_+,\overline{4}_+)^*, a=0,1,2,3\}$	12
13	2	negatives of elements in class (12)	12
14	4	$\pm\{(e_de_a,e_a)^*,(e_d4_+,4_+)^*,(e_d\overline{4}_+,\overline{4}_+)^*, d=1,2\ \&\ a=0,1,2,3\}$	48
15	4	$\pm\{(e_1e_a,e_a)^*,(e_2\overline{4}_+,\overline{4}_+),(e_34_+,4_+), a=0,1,2,3\}$	24
16	6	$\{(\overline{4}_+a_{02},a_{02})^*,(\overline{4}_+a_{12},a_{12})^*,(\overline{4}_+a_{03},a_{03})^*,(\overline{4}_+a_{31},a_{31})^*\}$	32
17	6	negatives of elements in class (16)	32
18	4	$\pm\{(e_ia_{23},a_{23})^*,(e_ia_{01},a_{01})^*, i=1,2,3\}$	24
19	2	$\{(a_{01},a_{01})^*,(a_{23},a_{23})^*\}$	4
20	2	negatives of elements in class (19)	4

[a] $a_{ab}=(1/\sqrt{2})(e_a\pm e_b)$.

$$q\to q'=q-\frac{2(q,\alpha_4)}{(\alpha_4,\alpha_4)}\alpha_4 \quad \text{with} \quad (\alpha_4,\alpha_4)=1,$$
$$q'=-\alpha_4\overline{q}\alpha_4. \tag{32}$$

The group elements of $W(B_4)$ then can be generated by the reflection generators

$$-(e_1,e_1)^*,\ -(\overline{t,t})^*,\ -(e_3,e_3)^*,c=-\left(\frac{1}{\sqrt{2}}(e_2-e_3),\frac{1}{\sqrt{2}}(e_2-e_3)\right)^*. \tag{33}$$

The elements of the Weyl group $W(B_4)$ are given in Table VI with their conjugacy classes. The elements of $W(B_4)$ not only involve the set (V_x,V_x) but also (V_y,V_z), (V_z,V_y) and their star elements. Here the sets of V_y and V_z are obtained from V_x by cyclic permutation of e_1, e_2, and e_3,

$$V_y=\left\{\begin{array}{l}\frac{1}{\sqrt{2}}(\pm 1\pm e_2)\\ \\ \frac{1}{\sqrt{2}}(\pm e_3\pm e_1)\end{array}\right\},\quad V_z=\left\{\begin{array}{l}\frac{1}{\sqrt{2}}(\pm 1\pm e_3)\\ \\ \frac{1}{\sqrt{2}}(\pm e_1\pm e_2)\end{array}\right\}. \tag{34}$$

Since $W(D_4)$ is invariant under the action of the element c as shown in (22) the elements of $W(B_4)$ can also be obtained from the elements of $W(D_4)$ in (16) by multiplication of c with those in (16) on the left. This can be achieved in a simpler way by using the multiplication table of the sets V_0, V_1, V_2, V_x, V_y and V_z given in Table VII.

By multiplying the elements of $W(D_4)$ in (16) by (V_x,V_x) on the left we obtain the elements of $W(B_4)$ in pairs of sets

TABLE VII. The multiplication table of the sets $V_0, V_1, V_2, V_x, V_y, V_z$. (It is the same multiplication table of the group S_3.)

	V_0	V_1	V_2	V_x	V_y	V_z
V_0	V_0	V_1	V_2	V_x	V_y	V_z
V_1	V_1	V_2	V_0	V_z	V_x	V_y
V_2	V_2	V_0	V_1	V_y	V_z	V_x
V_x	V_x	V_y	V_z	V_0	V_1	V_2
V_y	V_y	V_z	V_x	V_2	V_0	V_1
V_z	V_z	V_x	V_y	V_1	V_2	V_0

$$\begin{gathered}(V_0,V_0),(V_1,V_1),(V_2,V_2),\\ (V_0,V_0)^*,(V_1,V_1)^*,(V_2,V_2)^*,\\ (V_x,V_x),(V_y,V_z),(V_z,V_y),\\ (V_x,V_x)^*,(V_y,V_z)^*,(V_z,V_y)^*.\end{gathered} \tag{35}$$

This is a group of order $12\times 32=384$ elements generated by the generators of $W(B_4)$ in (33) leaving the root system of SO(9) in (31) invariant. The invariance of the elements of $W(D_4)$ can also be shown concisely in the following relations

$$\begin{gathered}(V_x,V_x)^*(V_a,V_a)(V_x,V_x)^{*-1}=(V_b,V_b),\\ a,b=0,1,2\\ (V_x,V_x)^*(V_a,V_a)^*(V_x,V_x)^{*-1}=(V_b,V_b)^*,\end{gathered} \tag{36}$$

which implies that $W(B_4)=W(D_4):Z_2$. We also note that the generator $c=-((1/\sqrt{2})(e_2-e_3),(1/\sqrt{2})(e_2-e_3))^*$ together with the elements of the elementary Abelian group of order 8, $\pm(e_1,e_1),\pm(e_2,e_3),\pm(e_3,e_2),\pm(1,1)$ given before, form an elementary Abelian group 2^4 of order 16. The same elements of S_4 generated by the generators in (27) leave the group 2^4 invariant, which implies that the Weyl group has the form $W(B_4)=2^4\rtimes S_4=2^4\rtimes 2^2\rtimes 3\rtimes 2$.

A few other facts about SO(9) are in order. The positive roots in terms of the scaled quaternions read as follows:

$$1,e_1,e_2,e_3,\quad \tfrac{1}{2}(1\pm e_1\pm e_2\pm e_3),\quad \tfrac{1}{2}(1\pm e_1),\quad \tfrac{1}{2}(e_2\pm e_3). \tag{37}$$

The transformation between the weight vector in the Dynkin basis and the quaternion basis as well as the Weyl vector in terms of quaternions are given as follows:

$$q_0=\frac{1}{\sqrt{2}}(a_1+2(a_2+a_3)+a_4),\ \ q_1=\frac{1}{\sqrt{2}}a_1,\ \ q_2=\frac{1}{\sqrt{2}}(a_3+a_4),\ \ q_3=\frac{1}{\sqrt{2}}a_3, \tag{38a}$$

$$\delta=\frac{1}{\sqrt{2}}(6+e_1+2e_2+e_3). \tag{38b}$$

The highest weights of some of the low dimensional irreducible representations of SO(9) are given in Table VIII. Embedding of SO(9) in F_4 will be discussed in the next section. The Coxeter elements are all in the same conjugacy classes. One can choose the products of the generators in an arbitrary order. Without loss of generality we can construct the Coxeter element as the products

TABLE VIII. Some of the low dimensional irreducible representations of SO(9) in quaternion basis versus Dynkin indices.

Dimension	Dynkin indices	Quaternion weights
9	(1000)	$\frac{1}{\sqrt{2}}(1+e_1)$
16	(0001)	$\frac{1}{\sqrt{2}}(1+e_2)$
36	(0100)	$\sqrt{2}$
44	(2000)	$\sqrt{2}(1+e_1)$
84	(0010)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_2+e_3)$
126	(0002)	$\sqrt{2}(1+e_2)$
128	(1001)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_1+e_2)$

$$M=\left(\frac{1}{\sqrt{2}}(e_2-e_3),\frac{1}{\sqrt{2}}(e_2-e_3)\right)^*(e_3,e_3)^*\left(\frac{1}{2}(1-e_1-e_2-e_3),\frac{1}{2}(1-e_1-e_2-e_3)\right)^*(e_1,e_1)^*. \tag{39}$$

A simple calculation leads to the element

$$M=\left(\frac{1}{\sqrt{2}}(1+e_3),\frac{1}{\sqrt{2}}(e_1-e_3)\right) \tag{40}$$

with the right property $M^8=(1,1)$. When we convert M to the 4×4 matrix in the quaternion basis and calculate the eigenvalues we obtain the complex exponents with the correct Coxeter exponents of SO(9).

V. THE AUTOMORPHISM GROUP OF F_4 ROOT SYSTEM

The simple roots of F_4 in the standard orthogonal basis are given in the respective order:

$$l_2-l_3,\quad l_3-l_4,\quad l_4,\quad \tfrac{1}{2}(l_1-l_2-l_3-l_4). \tag{41}$$

The Dynkin diagram and the scaled quaternionic simple roots of F_4 are shown in Fig. 5. The positive scaled roots and the Weyl vector in terms of quaternions are

$$1,e_1,e_2,e_3,\quad \tfrac{1}{2}(1\pm e_1\pm e_2\pm e_3),$$

$$\tfrac{1}{2}(1\pm e_1),\quad \tfrac{1}{2}(1\pm e_2),\quad \tfrac{1}{2}(1\pm e_3), \tag{42a}$$

$$\tfrac{1}{2}(e_2\pm e_3),\quad \tfrac{1}{2}(e_1\pm e_3),\quad \tfrac{1}{2}(e_1\pm e_2),$$

$$\delta=\frac{1}{\sqrt{2}}(8+3e_1+2e_2+e_3). \tag{42b}$$

The relations between the quaternion weights and the Dynkin indices are determined as

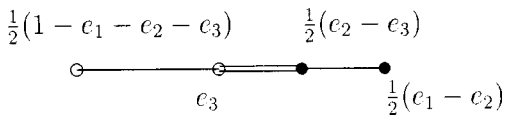

FIG. 5. The Dynkin diagram of F_4 with the scaled roots of quaternions.

$$q_0=\frac{1}{\sqrt{2}}(2a_1+3a_2+2a_3+a_4),\quad q_1=\frac{1}{\sqrt{2}}(a_2+a_3+a_4),$$
$$q_2=\frac{1}{\sqrt{2}}(a_2+a_3),\quad q_3=\frac{1}{\sqrt{2}}a_2. \tag{43}$$

Some low dimensional representations using quaternions are given in Table IX. The complete root system of F_4 consists of the sets of elements

$$V_0,\ V_1,\ V_2,\ V_x',\ V_y',\ \text{and}\ V_z', \tag{44}$$

where

$$V_y'=\left\{\begin{array}{c}\frac{1}{2}(\pm 1\pm e_2)\\ \frac{1}{2}(\pm e_3\pm e_1)\end{array}\right\},\quad V_z'=\left\{\begin{array}{c}\frac{1}{2}(\pm 1\pm e_3)\\ \frac{1}{2}(\pm e_1\pm e_2)\end{array}\right\}. \tag{45}$$

The roots of F_4 in (45) represent the weights of the spinor representation $\underline{16}$ of SO(9). A cyclic symmetry on e_1,e_2 and e_3 leaves (44) invariant, however it replaces $(\overline{45})$ by the pairs V_z',V_x' and V_x',V_y', which indicate that the spinor representation $\underline{16}$ and thereby the roots of SO(9) can be embedded in F_4 three symmetric ways. The three alternative ways of SO(9) roots in F_4 are

$$V_0,\quad V_1,\quad V_2,\quad V_i\quad (i=x,y,z), \tag{46}$$

TABLE IX. Some of the low dimensional irreducible representations of F_4 with the quaternion highest weights.

Dimension	Dynkin indices	Quaternion weights
26	(0001)	$\frac{1}{\sqrt{2}}(1+e_1)$
52	(1000)	$\sqrt{2}$
273	(0010)	$\sqrt{2}+\frac{1}{\sqrt{2}}(e_1+e_2)$
324	(0002)	$\sqrt{2}(1+e_1)$
1053	(1001)	$\sqrt{2}+\frac{1}{\sqrt{2}}(1+e_1)$
1053′	(2000)	$2\sqrt{2}$
1274	(0100)	$\sqrt{2}+\frac{1}{\sqrt{2}}(1+e_1+e_2+e_3)$
2652	(0003)	$\frac{3}{\sqrt{2}}(1+e_1)$

one i at a time. The Weyl group $W(F_4)$ can be generated from the reflection generators of simple roots in Fig. 5. We have already obtained it from $W(D_4)$ as an extension by the Dynkin diagram symmetry of SO(8). Now we can determine the elements more explicitly as sets of elements of the binary octahedral group.

The Weyl group $W(B_4)$ is not an invariant subgroup of $W(F_4)$. But by the transformation

$$b\ W(B_4)\ b^{-1}=W'(B_4) \tag{47}$$

with $b=(t,\overline{t})$ and $b^3=(1,1)$, we generate new sets of elements representing $W(B_4)$ in $W(F_4)$. Indeed a left and right application of b,b^2 and b^3 on the set of elements $W(B_4)$ in (35) generate the whole set of elements of $W(F_4)$:

$$(V_a,V_b),(V_a,V_b)^*,\quad a=0,1,2, \tag{48a}$$

$$(V_i,V_j),(V_i,V_j)^*,\quad i,j=x,y,z. \tag{48b}$$

We have $9\times 4=36$ pair of sets each involving 32 elements which yield the order $36\times 32=1152$ of $W(F_4)$. The elements in (48a) constitute the group of order 576, an extension of $W(D_4)$ by b. The set of elements

$$(V_a,V_b),(V_i,V_j),\quad a=0,1,2,\quad i,j=x,y,z, \tag{49}$$

also form a different group of order 576, a finite subgroup of SO(4). Several other interesting subgroups can be determined. The embedding of the Weyl group $W(B_4)$ in $W(F_4)$ in three different ways and selection of those elements from (48a) is straightforward.

We have noted in (24) that the Aut $\Phi_{D_4}=W(D_4):S_3$. Indeed Aut $\Phi_{D_4}\approx W(F_4)$ and, using the cosets of $W(D_4)$, we can prove that

$$W(F_4)=W(D_4):S_3. \tag{50}$$

We recall from (16) that the elements of $W(D_4)$ are of the form

$$(V_a,V_a),\ (V_a,V_a)^*,\quad a=0,1,2. \tag{51}$$

We can readily show that the elements of $W(F_4)$ in (48a) can be generated by applying the generators $A=(V_1,V_2)$ and $B=(V_x,V_x)$ with $A^3=B^2=(V_0,V_0)$ on the left of the elements of $W(D_4)$ in (51) since the $W(D_4)$ is an invariant subgroup of $W(F_4)$:

$$\begin{aligned} A\ W(D_4)\ A^{-1}&=W(D_4),\\ B\ \ W(D_4)\ \ B^{-1}&=W(D_4). \end{aligned} \tag{52}$$

Now we can show that the coset representatives A and B generate the group $D_3=S_3$. We recall that the generation relations of a dihedral group D_n is given by[5] $b\ a\ b^{-1}=a^{n-1}$, $a^n=b^2=1$. Here A and B satisfy the relation

$$B\ A\ B^{-1}=A^2=A^{-1}. \tag{53}$$

Therefore $W(F_4)$ is the semi-direct product of $W(D_4)$ with S_3:

$$W(F_4)=W(D_4)\rtimes S_3. \tag{54}$$

The conjugacy classes of $W(F_4)$ are given in Table X.

The automorphism group Aut Φ_{F_4} of the root system of F_4 can be obtained by adding another generator determined from the Dynkin diagram symmetry of F_4 diagram to the Weyl group

TABLE X. The conjugacy classes of $W(F_4)$ with quaternions.

Class	Order	Type of elements	No. of elements
1	1	$(1,1)$	1
2	2	$(-1,1)$	1
3	4	$(6,1)\oplus(1,6)$	12
4	2	$(3_+,3_+)\oplus(3_+,3_-)$	18
5	3	$(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)$	32
6	6	$-[(4_+,4_+)\oplus(\overline{4}_+,\overline{4}_+)]$	32
7	3	$(4_+,\overline{4}_+)\oplus(\overline{4}_+,4_+)$	32
8	6	$-[(4_+,\overline{4}_+)\oplus(\overline{4}_+,4_+)]$	32
9	6	$(8_+,1)\oplus(1,8_+)$	16
10	3	$-[(8_+,1)\oplus(1,8_+)]$	16
11	12	$(3_+,8_+)\oplus(3_+,8_-)\oplus(8_+,3_+)\oplus(8_-,3_+)$	96←Coxeter element
12	2	$(6_+,6_+)\oplus(6_+,6_-)$	72
13	8	$(6_+,6'_+)\oplus(6_+,6'_-)\oplus(6'_+,6_+)\oplus(6'_-,6_+)$	144
14	4	$(6'_+,6'_+)$	36
15	4	$-(6'_+,6'_+)$	36
16	2	$(1,1)^*\oplus(3_+,3_+)^*\oplus(4_+,4_+)^*\oplus(\overline{4}_+,\overline{4}_+)^*$	12
17	2	$-[(1,1)^*\oplus(3_+,3_+)^*\oplus(4_+,4_+)^*\oplus(\overline{4}_+,\overline{4}_+)^*]$	12
18	4	$(3_+r'_+,r'_+)^*\oplus(3_-r'_+,r'_+)^*,(r'_+=e_a,4_+,\overline{4}_+,a=0,1,2,3)$	72
19	2	$(6_+,6_+)^*\oplus(6'_+,6'_+)^*$	12
20	2	$-[(6_+,6_+)^*\oplus(6'_+,6'_+)^*]$	12
21	4	$(3_+r''_+,r''_+)^*\oplus(3_-r''_+,r''_+)^*,(r''_+=6_+,6'_+)$	72
23	6	$-(8_+r'_+,r'_+)^*$	96
24	6	$(8_+r''_+,r''_+)^*$	96
25	6	$-(8_+r''_+,r''_+)^*$	96

generators of F_4. The Dynkin diagram symmetry of F_4 is obtained by exchanging the short and long roots which is shown in Fig. 6. In an explicit form, exchanges of long and short roots

$$\frac{1}{2}(1-e_1-e_2-e_3)\leftrightarrow\frac{1}{\sqrt{2}}(e_1-e_2),\quad e_3\leftrightarrow\frac{1}{\sqrt{2}}(e_2-e_3), \tag{55}$$

will result in the transformation

$$1\rightarrow\frac{1}{\sqrt{2}}(1+e_1),\ e_1\rightarrow\frac{1}{\sqrt{2}}(1-e_1),\quad e_2\rightarrow\frac{1}{\sqrt{2}}(e_2+e_3),\ e_3\rightarrow\frac{1}{\sqrt{2}}(e_2-e_3). \tag{56}$$

This transformation is a rotation in four-dimensional space which exchanges the following sets of roots of F_4,

$$V_0\leftrightarrow V_x,\quad V_1\leftrightarrow V_y,\quad V_2\leftrightarrow V_z, \tag{57}$$

and can be represented by the generator

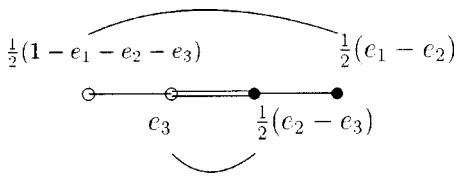

FIG. 6. The Dynkin diagram symmetry of F_4.

$$d=\left(\frac{1}{\sqrt{2}}(e_2+e_3),-e_2\right)\in(V_x,V_0). \tag{58}$$

When it is put in the form of Eq. (2) it turns out that it is a rotation by π in the plane determined by the quaternions $q_1=0$, $q_2=(1/\sqrt{2})(e_2+e_3)-e_2$ and $q_3=1-(1/\sqrt{2})(1+e_1)$. It is clear from (56) that while $q_1=0$ remains fixed q_2 and q_3 are transformed to their negatives $q_2\rightarrow -q_2$ and $q_3\rightarrow -q_3$.

Since the Dynkin diagram symmetry exchanges the simple roots leading to the interchange of the generators of $W(F_4)$ pairwise, the Weyl group of F_4 is left invariant:

$$d\ \ W(F_4)\ \ d^{-1}=W(F_4). \tag{59}$$

It can be extended to the Aut Φ_{F_4} by a left multiplication of d on the elements of $W(F_4)$ in (46). This can also be achieved by the left multiplication of (V_x,V_0) on $W(F_4)$ leading to the result

$$(V_a,V_b),\quad (V_i,V_j),\quad (V_a,V_i),\quad (V_i,V_a),\quad a,b=0,1,2, \tag{60a}$$

$$(V_a,V_b)^*,\quad (V_i,V_j)^*,\quad (V_a,V_i)^*,\quad (V_i,V_a)^*,\quad i,j=x,y,z. \tag{60b}$$

The Aut Φ_{F_4} is a group of order 2304 whose SO(4) subgroup is of order 1152. Interestingly enough the Aut Φ_{F_4} is the group fully generated by the elements of the binary octahedral group O. That means the elements in (60) can be written as

$$(O,O)\oplus(O,O)^*. \tag{61}$$

In summary, we have the following isomorphisms:

$$\begin{aligned}&\text{Aut}\ \ \Phi_{F_4}=\{(O,O)\oplus(O,O)^*\},\\ &\text{Aut}\ \ \Phi_{D_4}=W(F_4),\\ &\text{Aut}\ \ \Phi'_{D_4}=\{T,T)\oplus(T,T)^*\},\end{aligned} \tag{62}$$

with the subgroup sequence

$$\text{Aut}\ \ \Phi'_{D_4}\subset\text{Aut}\ \ \Phi_{D_4}\subset\text{Aut}\ \ \Phi_{F_4}. \tag{63}$$

The conjugacy classes of Aut Φ_{F_4} are given in Table XI.

One of the interesting subgroups of $W(F_4)$ is of order 384 isomorphic to $W(B_4)$, however it does not leave the root system of SO(9) in any form given by (46) invariant. The group elements are given as follows:

$$\begin{aligned}&(V_0,V_0),\quad (V_1,V_2),\quad (V_2,V_1),\\ &(V_0,V_0)^*,\quad (V_1,V_2)^*,\quad (V_2,V_1)^*,\end{aligned} \tag{64a}$$

$$\begin{aligned}&(V_x,V_x),\quad (V_y,V_y),\quad (V_z,V_z),\\ &(V_x,V_x)^*,\quad (V_y,V_y)^*,\quad (V_z,V_z)^*.\end{aligned} \tag{64b}$$

The set of elements in (64a) form a group of order 192 with 16 conjugacy classes and leaves the roots system of SO(8) invariant, however this group is not the Weyl group generated by the reflections on simple roots.

TABLE XI. Conjugacy classes of the group Aut Φ_{F_4} of order 2304.

Class	Order	Type	No. of elements
1	1	(1,1)	1
2	2	$(-1,1)$	1
3	4	$(3_+,\pm 1)\oplus(\pm 1,3_+)$	12
4	4	$(6_+,\pm 1)\oplus(\pm 1,6_+)$	24
5	6	$(8_+,1)\oplus(1,8_+)$	16
6	3	$-[(8_+,1)\oplus(1,8_+)]$	16
7	8	$(6'_+,1)\oplus(1,6'_+)$	12
8	8	$-[(6'_+,1)\oplus(1,6'_+)]$	12
9	2	$(3_+,\pm 3_+)$	18
10	2	$(6_+,\pm 3_+)\oplus(\pm 3_+,6_+)$	72
11	12	$(8_+,\pm 3_+)\oplus(\pm 3_+,8_+)$	96
12	8	$(6'_+,\pm 3_+)\oplus(\pm 3_+,6'_+)$	72
13	2	$(6_+,\pm 6_+)$	72
14	12	$(8_+,\pm 6_+)\oplus(\pm 6_+,8_+)$	192
15	8	$(6_+,\pm 6'_+)\oplus(\pm 6'_+,6_+)$	144
16	3	$(8_+,8_+)$	64
17	6	$-(8_+,8_+)$	64
18	24	$(8_+,6'_+)\oplus(6'_+,8_+)$	96
19	24	$-[(8_+,6'_+)\oplus(6'_+,8_+)]$	96
20	4	$(6'_+,6'_+)$	36
21	4	$-(6'_+,6'_+)$	36
22	2	$(r_+,r_+)^*(r_+=1,3_+,4_+,\overline{4}_+,6_+,6'_+)$	24
23	2	$-(r_+,r_+)^*$	24
24	4	$(\pm 6_+ r_+,r_+)^*$	288
25	4	$(\pm 3_+ r_+,r_+)^*$	144
26	6	$(8_+ r_+,r_+)^*$	192
27	6	$-(\pm 8_+ r_+,r_+)^*$	192
28	8	$(6'_+ r_+,r_+)^*$	144
29	8	$-(6'_+ r_+,r_+)^*$	144

VI. CONCLUSIONS

We are motivated by the work of P. Ramond and his collaborators[1] to construct the elements of the Weyl groups $W(D_4)$, $W(B_4)$ and $W(F_4)$ with pairs of quaternions. We have observed that the group Aut Φ_{F_4} is isomorphic to the finite subgroup of O(4) of order 2304 represented by the quaternion elements of the binary octahedral group O in the form $(O,O)\oplus(O,O)^*$. Several subgroups of this group have potential interest, in particular, those corresponding to the Weyl groups $W(D_4)$, $W(B_4)$ and $W(F_4)$. The group $(T,T)\oplus(T,T)^*$, where T stands for the quaternion elements of the binary tetrahedral group, is the extension of the Weyl group $W(D_4)$ by the cyclic symmetry of the Dynkin diagram of SO(8).

The triality of SO(8) and the embedding of $W(B_4)$ in the $W(F_4)$ by a cyclic symmetry involves the permutation symmetry of pure quaternion units e_1, e_2, e_3. The weights of irreducible representations of any of these Lie algebras have been constructed with quaternions and the relations between the Dynkin indices and the standard orthogonal vectors in four dimensions have been established. The symmetry between the vector, spinor and conjugate spinor representations of SO(8) is a manifestation of the S_3 symmetry imposed on the quaternion units e_i. The conjugacy classes of the Weyl groups and the automorphism groups have been constructed. It has been also noted that without a need of computer calculation one can construct the conjugacy classes by hand using the conjugacy classes of the binary tetrahedral and binary octahedral groups.

The groups we have dealt with have the potential importance in four-dimensional crystallography. They involve a great number of crystallographic point groups in three dimensions as subgroups which we have pointed out the general structure without referring to any particular example.

The most important aspect of our work perhaps is that the root systems of the Lie algebras of SO(8) and F_4 have a multiplication structure which led to a straightforward method for the construction of their automorphism groups. We are optimistic that the quaternionic representations of the root systems and the automorphism groups of SO(8), SO(9) and F_4 may pave a new road for further insights toward the symmetries of supersrings in ten dimensions and M-theory in 11 dimensions.

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A geometric description of Routh's procedure. Addendum: "Legendre transformation and analytical mechanics: A geometric approach" [J. Math. Phys. 44, 1709 (2003)]

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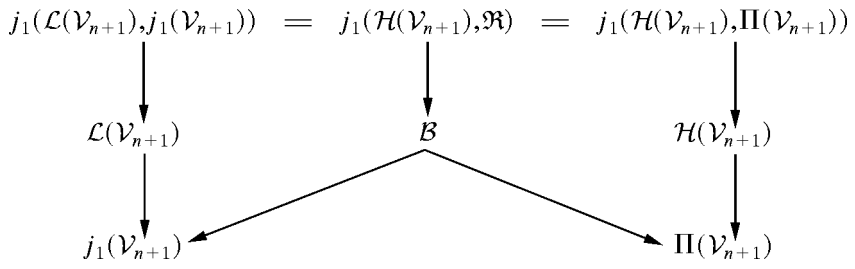
(Received 28 January 2003; accepted 19 March 2003)

The geometrical framework developed in J. Math. Phys. **44**, 1709 (2003) is applied in order to obtain a geometric description of Routh's procedure. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1576495]

I. INTRODUCTION

In a recent paper,[1] a new geometrical framework for a unified formulation of Lagrangian and Hamiltonian dynamics has been proposed. The analysis provides a gauge-invariant extension to nonautonomous systems of classical results due to Tulczyjew.

The core of the procedure developed in Ref. 1 may be summarized into the following diagram:



(1.1)

in which:

$\mathcal{V}_{n+1}$, $j_1(\mathcal{V}_{n+1})$ and $\Pi(\mathcal{V}_{n+1})$ denote, respectively, the configuration space–time, the velocity space–time and the phase space of a holonomic system with n degrees of freedom. All spaces are fibered over the real line $\mathfrak{R}$ through the absolute time function t.

$\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})$ and $\mathcal{H}(\mathcal{V}_{n+1})\to\Pi(\mathcal{V}_{n+1})$ denote principal fiber bundles with structural group $(\mathfrak{R},+)$, called, respectively, the *Lagrangian* and the *Hamiltonian bundles*. The latter have been introduced in Ref. 2 (see also Ref. 1 and references therein) to give a geometric arrangement to the gauge structure of classical mechanics.

$j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$, $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\Pi(\mathcal{V}_{n+1}))$ and $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ are the first-jet bundles, respectively, associated with the fibrations $\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})$, $\mathcal{H}(\mathcal{V}_{n+1})\to\Pi(\mathcal{V}_{n+1})$ and $\mathcal{H}(\mathcal{V}_{n+1})\to\mathfrak{R}$. All bundles are mutually diffeomorphic, and represent the generalization of the so-called *Tulczyjew triple* $T^*(T(M))\leftrightarrow T(T^*(M))\leftrightarrow T^*(T^*(M))$ (see, for example, Refs. 3 and 4). Moreover, all spaces are principal fiber bundles over a base manifold $\mathcal{B}$, endowed with a canonical symplectic structure.

In the resulting geometrical setting, a central role is played by the space $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$. In fact, the assignment of Lagrangian or Hamiltonian dynamics—expressed geometrically through sections $l:j_1(\mathcal{V}_{n+1})\to\mathcal{L}(\mathcal{V}_{n+1})$ or $h:\Pi(\mathcal{V}_{n+1})\to\mathcal{H}(\mathcal{V}_{n+1})$—gives rise in a natural way to corresponding surfaces in $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$. By the very definition of $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, these latter have

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the nature of first-order differential equations yielding the evolution of the system. Switching from the Lagrangian to the Hamiltonian description of dynamics is then merely switching between two different representations of the same surface in $j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$, related to each other by what is usually referred to as the Legendre transformation.

II. THE ROUTH'S PROCEDURE

Given a mechanical system as above, assume that the configuration space–time $\mathcal{V}_{n+1}$ is fibered over a $r+1$-dimensional manifold $\mathcal{V}_{r+1}$, in turn fibered over $\mathfrak{R}$ through absolute time t.

Typically, this is the situation occurring in the study of systems with geometrical symmetries, summarized into a Lie group G acting freely and properly on $\mathcal{V}_{n+1}$, the base space $\mathcal{V}_{r+1}$ being then identified with the quotient space $\mathcal{V}_{r+1}:=\mathcal{V}_{n+1}/G$.

In what follows, we shall refer the manifolds $\mathcal{V}_{r+1}$ and $\mathcal{V}_{n+1}$ to local fibered coordinates t,q^α and t,q^α,q^a, respectively ($\alpha=1,\ldots,r$, $a=r+1,\ldots,n$), subject to the transformation laws

$$\overline{t}=t+c, \quad \overline{q}^\beta=\overline{q}^\beta(t,q^\alpha), \quad \overline{q}^b=\overline{q}^b(t,q^\alpha,q^a).$$

Now, let $j_1(\mathcal{V}_{r+1})$ denote the first-jet bundle of $t:\mathcal{V}_{r+1}\to\mathfrak{R}$ and $\mathcal{N}:=j_1(\mathcal{V}_{r+1})\times_{\mathcal{V}_{r+1}}\mathcal{V}_{n+1}$ be the fiber product over $\mathcal{V}_{r+1}$ between $j_1(\mathcal{V}_{r+1})$ and $\mathcal{V}_{n+1}$.

We shall put on $j_1(\mathcal{V}_{r+1})$, $j_1(\mathcal{V}_{n+1})$ and $\mathcal{L}(\mathcal{V}_{n+1})$, respectively, jet and fibered coordinates expressed by (the significant part of) $t,q^\alpha,q^a,\dot{q}^\alpha,\dot{q}^a,\dot{u}$. The latter undergo the transformation laws[1,2]

$$\overline{\dot{q}}^\beta=\frac{\partial\overline{q}^\beta}{\partial q^\alpha}\dot{q}^\alpha+\frac{\partial\overline{q}^\beta}{\partial t}, \quad \overline{\dot{q}}^b=\frac{\partial\overline{q}^b}{\partial q^a}\dot{q}^a+\frac{\partial\overline{q}^b}{\partial q^\alpha}\dot{q}^\alpha+\frac{\partial\overline{q}^b}{\partial t}, \quad \overline{\dot{u}}=\dot{u}+\frac{\partial f}{\partial q^a}\dot{q}^a+\frac{\partial f}{\partial q^\alpha}\dot{q}^\alpha+\frac{\partial f}{\partial t}$$

with $f(t,q^\alpha,q^a)\in\mathcal{F}(\mathcal{V}_{n+1})$.

In view of these, it is a straightforward matter to verify the affine nature of the fibration $j_1(\mathcal{V}_{n+1})\to\mathcal{N}$.

Therefore, all the arguments stated in Ref. 1 apply equally well to the *affine principal fibration* $\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})\to\mathcal{N}$. In particular, referring systematically the reader to Ref. 1 for proofs, comments, and notations, one has the following.

Given any point $z\in\mathcal{N}$, let us denote by $\mathcal{L}(\mathcal{V}_{n+1})^*_z$ the space of affine sections $\sigma_z:j_1(\mathcal{V}_{n+1})_z\to\mathcal{L}(\mathcal{V}_{n+1})_z$, $j_1(\mathcal{V}_{n+1})_z$ and $\mathcal{L}(\mathcal{V}_{n+1})_z$ being the fibers over z of $j_1(\mathcal{V}_{n+1})$ and $\mathcal{L}(\mathcal{V}_{n+1})$, respectively. In coordinates, every $\sigma_z\in\mathcal{L}(\mathcal{V}_{n+1})^*_z$ admits a representation of the form

$$\dot{u}=\xi_0+\xi_a\dot{q}^a.$$

There exists a one-parameter group of translations acting on $\mathcal{L}(\mathcal{V}_{n+1})^*_z$; the quotient of $\mathcal{L}(\mathcal{V}_{n+1})^*_z$ under this action will be denoted by $j_1(\mathcal{V}_{n+1})^*_z$.

Introducing the spaces $\mathcal{L}(\mathcal{V}_{n+1})^*:=\cup_{z\in\mathcal{N}}\mathcal{L}(\mathcal{V}_{n+1})^*_z$ and $j_1(\mathcal{V}_{n+1})^*:=\cup_{z\in\mathcal{N}}j_1(\mathcal{V}_{n+1})^*_z$, we obtain an affine principal fibration $\mathcal{L}(\mathcal{V}_{n+1})^*\to j_1(\mathcal{V}_{n+1})^*\to\mathcal{N}$, *dual* of $\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})\to\mathcal{N}$ in the sense described in Ref. 1. We refer $\mathcal{L}(\mathcal{V}_{n+1})^*$ to local coordinates $t,q^\alpha,q^a,\dot{q}^\alpha,\xi_a,\xi_0$, subject to transformation laws

$$\overline{\xi}_b=\left(\xi_a+\frac{\partial f}{\partial q^a}\right)\frac{\partial q^a}{\partial\overline{q}^b}, \quad \overline{\xi}_0=\xi_0+\xi_a\left(\frac{\partial\overline{q}^a}{\partial q^\alpha}\dot{q}^\alpha+\frac{\partial q^a}{\partial\overline{t}}\right)+\frac{\partial f}{\partial\overline{q}^\alpha}\overline{\dot{q}}^\alpha+\frac{\partial f}{\partial\overline{t}}$$

with $f(t,q)\in\mathcal{F}(\mathcal{V}_{n+1})$. In particular, $j_1(\mathcal{V}_{n+1})^*$ coincides with the quotient space $\mathcal{L}(\mathcal{V}_{n+1})^*/(\partial/\partial\xi_0)$ generated by the action induced by the fundamental vector field $\partial/\partial\xi_0$.

Denoting by $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ and $j_1(\mathcal{L}(\mathcal{V}_{n+1})^*,j_1(\mathcal{V}_{n+1})^*)$ the first-jet bundles, respectively, associated with the principal bundles $\mathcal{L}(\mathcal{V}_{n+1})\to j_1(\mathcal{V}_{n+1})$ and $\mathcal{L}(\mathcal{V}_{n+1})^*\to j_1(\mathcal{V}_{n+1})^*$, there exists a canonical diffeomorphism $\psi:j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))\to j_1(\mathcal{L}(\mathcal{V}_{n+1})^*,j_1(\mathcal{V}_{n+1})^*)$. Referring $j_1(\mathcal{L}(\mathcal{V}_{n+1}),j_1(\mathcal{V}_{n+1}))$ ($\simeq j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$) to local co-

ordinates t, q^α, q^a, p_0, p_α, p_a, q^α, $\dot{q}^a$, $\dot{p}_0$, $\dot{p}_\alpha$, $\dot{p}_a$ and $j_1(\mathcal{L}(\mathcal{V}_{n+1})^*, j_1(\mathcal{V}_{n+1})^*)$ to local jet-coordinates t, q^α, q^a, $\dot{q}^\alpha$, ξ_a, ξ_0, ξ_{0_t}, $\xi_{0_{q^\alpha}}$, $\xi_{0_{q^a}}$, $\xi_{0_{\dot{q}^\alpha}}$, $\xi_{0_{\xi_a}}$, the diffeomorphism ψ is described by the relations

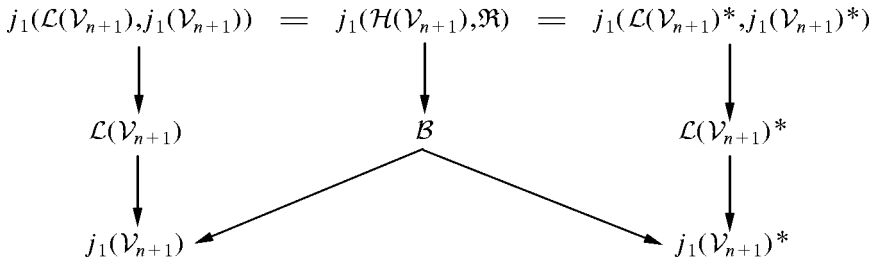
$$t=t, \quad q^\alpha=q^\alpha, \quad q^a=q^a, \quad \dot{q}^\alpha=\dot{q}^\alpha, \quad \xi_a=p_a, \quad \xi_0=p_0+p_\alpha\dot{q}^\alpha,$$

$$\xi_{0_t}=\dot{p}_0, \quad \xi_{0_{q^\alpha}}=\dot{p}_\alpha, \quad \xi_{0_{q^a}}=\dot{p}_a, \quad \xi_{0_{\dot{q}^\alpha}}=p_\alpha, \quad \xi_{0_{\xi_a}}=-\dot{q}^a.$$

Following Ref. 1, we shall identify systematically both $j_1(\mathcal{L}(\mathcal{V}_{n+1}), j_1(\mathcal{V}_{n+1}))$ and $j_1(\mathcal{L}(\mathcal{V}_{n+1})^*, j_1(\mathcal{V}_{n+1})^*)$ with $j_1(\mathcal{H}(\mathcal{V}_{n+1}), \mathfrak{R})$, referred to local coordinates t, q^α, q^a, p_0, p_α, p_a, $\dot{q}^\alpha$, $\dot{q}^a$, $\dot{p}_0$, $\dot{p}_\alpha$, $\dot{p}_a$, and we shall regard the relation

$$\xi_0=p_0+p_\alpha\dot{q}^\alpha=\dot{u}-p_a\dot{q}^a \tag{2.1}$$

as a coordinate transformation on $j_1(\mathcal{H}(\mathcal{V}_{n+1}), \mathfrak{R})$. Equation (2.1) represents changes of trivialization of the principal bundle $j_1(\mathcal{H}(\mathcal{V}_{n+1}), \mathfrak{R}) \to \mathcal{B}$. Once again, the previous discussion may be summarized into the commutative diagram



(2.2)

analogous of (1.1).

Now, let $l: j_1(\mathcal{V}_{n+1}) \to \mathcal{L}(\mathcal{V}_{n+1})$ be a Lagrangian section, locally expressed as (see Refs. 1 and 2)

$$\dot{u}=L(t,q,\dot{q}). \tag{2.3}$$

As pointed out in Ref. 1, the surface $\mathcal{E} := j_1(l)(j_1(\mathcal{V}_{n+1}))$, image of $j_1(\mathcal{V}_{n+1})$ under the first-jet extension $j_1(l)$ of l, carries complete information on dynamics. Indeed, the surface $\mathcal{E}$ is described by the equations

$$p_0=-\frac{\partial L}{\partial \dot{q}^\alpha}\dot{q}^\alpha-\frac{\partial L}{\partial \dot{q}^a}\dot{q}^a+L, \quad \dot{p}_0=\frac{\partial L}{\partial t}, \quad p_\alpha=\frac{\partial L}{\partial \dot{q}^\alpha}, \tag{2.4a}$$

$$\dot{p}_\alpha=\frac{\partial L}{\partial q^\alpha}, \quad p_a=\frac{\partial L}{\partial \dot{q}^a}, \quad \dot{p}_a=\frac{\partial L}{\partial q^a} \tag{2.4b}$$

providing, as pointed out in the Introduction, a set of ordinary differential equations for the determination of the evolution of the system.

Making use of the right vertical arrows of the diagram (2.2), we may project $\mathcal{E}$ into $\mathcal{L}(\mathcal{V}_{n+1})^*$ and $j_1(\mathcal{V}_{n+1})^*$, so generating two maps $\Lambda_l: j_1(\mathcal{V}_{n+1}) \to \mathcal{L}(\mathcal{V}_{n+1})^*$ and $\lambda_l: j_1(\mathcal{V}_{n+1}) \to j_1(\mathcal{V}_{n+1})^*$ locally expressed as

$$\Lambda_l, \quad p_a=\frac{\partial L}{\partial \dot{q}^a}, \quad \xi_0=L-\frac{\partial L}{\partial \dot{q}^a}\dot{q}^a; \tag{2.5a}$$

$$\lambda_l, \quad p_a = \frac{\partial L}{\partial \dot{q}^a}. \tag{2.5b}$$

Under the regularity assumption $\| \partial^2 L / \partial \dot{q}^a \partial \dot{q}^b \| \neq 0$, the map λ_l may be (locally) inverted so that the composite map $\Lambda_l \circ \lambda_l^{-1}$ defines a section $r: j_1(\mathcal{V}_{n+1})^* \to \mathcal{L}(\mathcal{V}_{n+1})^*$. The explicit representation of r may be achieved by solving Eqs. (2.5b) with respect to the variables $\dot{q}^a$ and substituting the result into the second equation (2.5a). In this way we get the final expression

$$\xi_0 = -R(t,q^\alpha,q^a,\dot{q}^\alpha,p_a) := L(t,q^\alpha,q^a,\dot{q}^\alpha,p_a) - p_a \dot{q}^a(t,q^\alpha,q^a,\dot{q}^\alpha,p_a). \tag{2.6}$$

The function R involved in Eq. (2.6) is commonly known as the *Routhian function*.[5] Accordingly, the maps (2.5) and the section (2.6) are, respectively, the *Routh Maps* and the *Routhian section* associated with l.

At this point, it is a straightforward matter to verify that the image space $j_1(r)(j_1(\mathcal{V}_{n+1})^*) \subset j_1(\mathcal{H}(\mathcal{V}_{n+1}),\mathfrak{R})$ [$j_1(r)$ denoting the first-jet extension of r] coincides with the surface $\mathcal{E}$ generated by the given Lagrangian section l. In other words, through the Routhian section r, we obtain a representation of the surface $\mathcal{E}$ in terms of the variables t, q^α, $\dot{q}^\alpha$, p_a, ξ_0, given by the equations

$$\xi_0 = -R(t,q^\alpha,q^a,\dot{q}^\alpha,p_a), \quad \dot{p}_0 = -\frac{\partial R}{\partial t}, \quad \dot{q}^a = \frac{\partial R}{\partial p_a}, \tag{2.7a}$$

$$\dot{p}_a = -\frac{\partial R}{\partial q^a}, \quad \dot{p}_\alpha = -\frac{\partial R}{\partial q^\alpha}, \quad p_\alpha = -\frac{\partial R}{\partial \dot{q}^\alpha}. \tag{2.7b}$$

Once again, Eqs. (2.7) fix the evolution of the system. In particular, writing the equations of motion in the form (2.7) is especially worthwhile whenever the variables q^a $(a = r+1,\ldots,n)$ are cyclic[6] in the Lagrangian function $L(t,q,\dot{q}) \in \mathcal{F}(j_1(\mathcal{V}_{n+1}))$ involved in Eq. (2.3). Indeed, under the stated circumstance, the Routhian function $R(t,q^\alpha,\dot{q}^\alpha,p_a)$ is independent of the variables q^a too. Therefore, the first set of Eqs. (2.7b) imply the evolution equations $p_a = c_a$ const. Due to this fact, by Eqs. (2.7) themselves we derive the decoupled differential equations

$$\frac{d}{dt}\left(\frac{\partial R}{\partial \dot{q}^\alpha}\right) - \frac{\partial R}{\partial q^\alpha} = 0, \quad \dot{q}^a = \frac{\partial R}{\partial p_a} \tag{2.8}$$

with $R(t,q^\alpha,\dot{q}^\alpha,c_a)$, and with the constants c_a fixed by the initial data. Equations (2.8) are the well-known Routh's equations[5] yielding a reduction of the problem of motion.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Integrable systems and reductions of the self-dual Yang–Mills equations

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(Received 5 April 2003; accepted 9 April 2003)

Many integrable equations are known to be reductions of the self-dual Yang–Mills equations. This article discusses some of the well known reductions including the standard soliton equations, the classical Painlevé equations and integrable generalizations of the Darboux–Halphen system and Chazy equations. The Chazy equation, first derived in 1909, is shown to correspond to the equations studied independently by Ramanujan in 1916. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1586967]

I. INTRODUCTION

The self-dual Yang–Mills (SDYM) equations (a system of equations for Lie algebra-valued functions of $\mathbb{C}^4$) play a central role in the field of integrable systems and also play a fundamental role in several other areas of mathematics and physics.

From the perspective of integrable systems, the study of the SDYM equations became particularly intriguing when, in 1985, R. S. Ward[59] conjectured that

> *... many (and perhaps all?) of the ordinary and partial differential equations that are regarded as being integrable or solvable may be obtained from the self-dual gauge field equations (or its generalizations) by reduction.*

That the SDYM equations are a rich source of integrable systems is suggested by the fact that they are the compatibility condition of an associated linear problem which admits enormous freedom if one allows the associated Lie algebra (the so-called gauge algebra) to be arbitrary. In light of this and other results, the SDYM equations are often referred to as the master integrable system. The SDYM equations provide us with a means of generating and classifying many integrable systems and they also give a unified geometrical framework in which to analyze them. Moreover, in the context of the inverse scattering transform, an integrable equation admits well-behaved solutions obtained via the related linear problems.

The SDYM equations are of great importance in their own right and have found a remarkable number of applications in both physics and mathematics. These equations arise in the context of gauge theory,[49] in classical general relativity,[63,39] and can be used as a powerful tool in the analysis of four-manifolds.[29]

For finite-dimensional gauge groups the integrability of the SDYM equations can be understood from both the inverse scattering transform and geometric points of view.[58,13,26] An excellent reference related to the geometric aspects is Mason and Woodhouse.[41] Our point of view deals

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with the algebraic and analytic aspects and novel reductions via infinite-dimensional gauge algebras.

The use of certain infinite-dimensional gauge algebras in the self-dual Yang–Mills equations is an important development in the theory. Using these Lie algebras, reductions of the SDYM equations to many important equations including the Kadomtsev–Petviashvili, Davey–Stewartson, $2+1$-dimensional n-wave, and Chazy equations have been found. Recently a generalized Darboux–Halphen system has been obtained as a reduction of the SDYM equations with an infinite-dimensional gauge algebra.[7] These equations are solvable via an associated linear problem, yet their solutions do not possess the Painlevé property—the characteristic singularity structure often thought to be the hallmark of integrability. A special case of the Darboux–Halphen system is equivalent to the generalized Chazy equation. Much work remains to be done in order to identify the class of infinite-dimensional gauge algebras for which the SDYM equations are integrable. These investigations force us to take a much closer look at the idea of integrability itself.

Throughout we will present geometrical interpretations and reasoning whenever we believe that they provide a deeper insight into the reduction process and the properties of the resulting equations. However, this article has been written with the nongeometer in mind. We hope that our survey will be accessible to a wide variety of researchers from many different branches of mathematics and physics.

In Sec. II we introduce the self-dual Yang–Mills equations and their underlying linear problem. In Sec. III we discuss reductions of the SDYM equations to integrable PDEs. Many of the reductions in this section can be found in Ablowitz and Clarkson.[1] In this section we also consider reductions to PDEs when the underlying Lie algebra is infinite dimensional. Such reductions include the Kadomtsev–Petviashvili and Davey–Stewartson equations. In Sec. IV we describe reductions of the SDYM equations with finite-dimensional Lie algebras to ODEs. In particular, the integrable cases of the equations of motion of a spinning top are recovered, together with some generalizations. We also describe the reductions of SDYM to the Painlevé equations due to Mason and Woodhouse.[41] Finally, Sec. V considers the reduction of the SDYM with an infinite-dimensional Lie algebra to a generalized Darboux–Halphen system whose general solution is densely branched about movable singularities and can contain movable natural barriers. This equation in turn has reductions to the Chazy equation and integrable generalizations of the Chazy equation.

II. THE SDYM EQUATIONS

In this section we motivate the SDYM equations from the points of view of both integrable systems and gauge theory.

A. Linear problems and integrable systems

Recall that many $1+1$-dimensional integrable systems are solved via related linear problems of the form

$$\mathbf{\Psi}_x = X\mathbf{\Psi}, \tag{1}$$

$$\mathbf{\Psi}_t = T\mathbf{\Psi}, \tag{2}$$

where X and T are square matrices of the same dimension which are functions of x, t, and the spectral parameter ζ. The compatibility of these equations (i.e., $\mathbf{\Psi}_{xt}=\mathbf{\Psi}_{tx}$) is equivalent to

$$X_t - T_x + [X,T] = 0. \tag{3}$$

In 1973, Ablowitz *et al.*[10,11] solved the inverse scattering problem in the case

$$X = \begin{pmatrix} -i\zeta & q(x,t) \\ r(x,t) & i\zeta \end{pmatrix}, \quad T = \begin{pmatrix} A & B \\ C & -A \end{pmatrix}, \tag{4}$$

where A,B,C are (Laurent) polynomials in ζ.

Below we list several choices of T that yield a number of integrable equations which will be discussed in later sections.

(i) The Korteweg–de Vries equation:

$$q_t+6qq_x+q_{xxx}=0,$$

$$T=\begin{pmatrix} -4i\zeta^3+2iq\zeta-q_x & 4q\zeta^2+2iq_x\zeta-(2q^2+q_{xx}) \\ -4\zeta^2+2q & 4i\zeta^3-2iq\zeta+q_x \end{pmatrix}$$

$$(r=-1).$$

(ii) The nonlinear Schrödinger equation:

$$iq_t=q_{xx}\pm 2q^2q^*,$$

$$T=\begin{pmatrix} 2i\zeta^2+iqr & -2q\zeta-iq_x \\ 2r\zeta+ir_x & -2i\zeta^2-iqr \end{pmatrix}$$

$$(r=\mp q^*).$$

(iii) The sine-Gordon equation:

$$u_{xt}=\sin u$$

$$T=\zeta^{-1}\begin{pmatrix} \frac{1}{4}i\cos u & \frac{1}{4}i\sin u \\ \frac{1}{4}i\sin u & -\frac{1}{4}i\cos u \end{pmatrix} \tag{5}$$

$$(q=-r=-\tfrac{1}{2}u_x).$$

It should be noted that the dependence on the spectral parameter and the restriction to 2×2 systems given by (4) is not the only choice for which the inverse scattering problem can be solved for Eq. (3) (see, for example, Refs. 3 and 57).

A simple, natural, and highly symmetric generalization of the linear problem (1) and (2) to four variables; x_1, x_2, t_1, t_2 is given by

$$\left(\frac{\partial}{\partial x_1}+\zeta\frac{\partial}{\partial x_2}\right)\Psi=(X_1+\zeta X_2)\Psi, \tag{6}$$

$$\left(\frac{\partial}{\partial t_1}+\zeta\frac{\partial}{\partial t_2}\right)\Psi=(T_1+\zeta T_2)\Psi, \tag{7}$$

where X_1, X_2; T_1, T_2 are functions from $\mathbb{C}^4$ to $\mathfrak{sl}(n;\mathbb{C})$—the Lie algebra of $n\times n$ trace-free matrices with complex-valued entries. The compatibility of this system is equivalent to the self-dual Yang–Mills equations with gauge algebra $\mathfrak{sl}(n;\mathbb{C})$ (see Sec. II C below). From the general form of this linear problem it is clear that many integrable equations are reductions of the self-dual Yang–Mills equations because their associated linear problems arise as reductions of the linear problem for the SDYM equations. Notice, however, that the right sides of Eqs. (6) and (7) are linear in ζ whereas in the AKNS scheme, the right side of Eq. (2) can be a Laurent polynomial in ζ. However, it turns out that reductions of (6) and (7) can have much more general dependence on the spectral parameter.

B. The Yang–Mills equations

Non-Abelian gauge theories first appeared in the seminal work of Yang and Mills[65] as a non-Abelian generalization of Maxwell's equations. Let G be a Lie group (referred to as the gauge group) with Lie algebra LG and let $\{x^\mu\}_{\mu=0,\ldots,3}$ be coordinates on a four-dimensional manifold M which can be $\mathbb{R}^4$, $\mathbb{R}^{1,3}$ or $\mathbb{R}^{2,2}$. Given $A_\mu(\mathbf{x}) \in \mathrm{LG}$, we introduce the covariant derivatives

$$D_\mu = \partial_\mu - A_\mu, \tag{8}$$

and their commutators

$$F_{\mu\nu} = -[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu - [A_\mu, A_\nu]. \tag{9}$$

The fact that the Yang–Mills equations have a natural geometric interpretation was recognized early on in the history of gauge theory. The covariant derivatives (8) can be used to obtain a local representation of a connection on a principal fiber bundle over M. The one-form $A := A_\mu dx^\mu$ is called the *connection one-form* and $F := \frac{1}{2} F_{\mu\nu} dx^\mu dx^\nu$ the *curvature two-form* of the connection. F can also be expressed as the exterior covariant derivative of A given by

$$F = DA := dA - A \wedge A.$$

Recall that the Hodge dual operator on the four-dimensional manifold M takes any two-form $T = \frac{1}{2} T_{\mu\nu} dx^\mu \wedge dx^\nu$ to the dual two-form $*T = \frac{1}{2} \varepsilon_{\mu\nu}{}^{\gamma\delta} T_{\gamma\delta} dx^\mu \wedge dx^\nu$ where $\varepsilon_{\mu\nu\gamma\delta}$ is totally antisymmetric with $\varepsilon_{0123} = 1$ and the standard metric on M is used to raise and lower indices. The Yang–Mills equations then have the simple form

$$D*F = 0$$

together with the Bianchi identity

$$DF = 0,$$

which follows from the definitions of exterior covariant derivative D and F. Note that under the gauge transformation

$$A_\mu \mapsto g^{-1} A_\mu g + g^{-1} \partial_\mu g, \quad g \in \mathrm{G}, \tag{10}$$

the components of the curvature two-form transform as

$$F_{\mu\nu} \mapsto g^{-1} F_{\mu\nu} g, \tag{11}$$

which corresponds to the transformation of the fibers by the right action of the structure group G on the principal bundle.

C. The self-dual Yang–Mills equations

The Yang–Mills equations are a set of coupled, second-order PDEs in four dimensions for the LG-valued gauge potential functions A_μ's, and are extremely difficult to solve in general. It is, however, possible to obtain a special class of first-order reductions of the full Yang–Mills equations by noting that any F that satisfies

$$*F = \lambda F \tag{12}$$

for some constant λ, also satisfies the Yang–Mills equations by virtue of the Bianchi identity: $DF = 0$. From (12) we must have

$$**F = \lambda * F = \lambda^2 F. \tag{13}$$

However, $**F = gF$ where $g = \det[g_{\mu\nu}]$ is the determinant of the metric on M. Hence

$$\lambda = \begin{cases} \pm 1 & \text{on } \mathbb{R}^4,\ \mathbb{R}^{2,2}; \\ \pm i & \text{on } \mathbb{R}^{3,1}. \end{cases}$$

All real solutions of the equations $*F = \pm iF$ are trivial. On $\mathbb{R}^4$ and $\mathbb{R}^{2,2}$, the equations $*F = (-)F$ are called the (anti-)self-dual Yang–Mills equations. We will work in $\mathbb{R}^4$ with the standard metric

$$ds^2 = (dx^0)^2 + (dx^1)^2 + (dx^2)^2 + (dx^3)^2.$$

The SDYM equations now take the form

$$F_{01} = F_{23}, \quad F_{02} = F_{31}, \quad F_{03} = F_{12}. \tag{14}$$

We introduce the null coordinates

$$\sigma = \frac{1}{\sqrt{2}}(x^1 + ix^2), \quad \tau = \frac{1}{\sqrt{2}}(x^0 - ix^3),$$

$$\tilde{\sigma} = \frac{1}{\sqrt{2}}(x^1 - ix^2), \quad \tilde{\tau} = \frac{1}{\sqrt{2}}(x^0 + ix^3).$$

It then follows from $A = A_\mu dx^\mu = A_\sigma d\sigma + A_{\tilde{\sigma}} d\tilde{\sigma} + A_\tau d\tau + A_{\tilde{\tau}} d\tilde{\tau}$ that

$$A_0 = \frac{1}{\sqrt{2}}(A_\tau + A_{\tilde{\tau}}), \quad A_1 = \frac{1}{\sqrt{2}}(A_\sigma + A_{\tilde{\sigma}}),$$

$$A_2 = \frac{i}{\sqrt{2}}(A_\sigma - A_{\tilde{\sigma}}), \quad A_3 = -\frac{i}{\sqrt{2}}(A_\tau - A_{\tilde{\tau}}),$$

and the SDYM equations become

$$F_{\sigma\tau} = 0, \quad F_{\tilde{\sigma}\tilde{\tau}} = 0, \quad F_{\sigma\tilde{\sigma}} + F_{\tau\tilde{\tau}} = 0. \tag{15}$$

Equations (15) are the compatibility condition of the isospectral linear problem

$$(\partial_\sigma + \zeta\partial_{\tilde{\tau}})\boldsymbol{\Psi} = (A_\sigma + \zeta A_{\tilde{\tau}})\boldsymbol{\Psi}, \tag{16}$$

$$(\partial_\tau - \zeta\partial_{\tilde{\sigma}})\boldsymbol{\Psi} = (A_\tau - \zeta A_{\tilde{\sigma}})\boldsymbol{\Psi}, \tag{17}$$

where ζ is the spectral parameter and $\boldsymbol{\Psi}$ is a local section of the Yang–Mills fiber bundle. The compatibility condition is simply $(\partial_\tau - \zeta\partial_{\tilde{\sigma}})(\partial_\sigma + \zeta\partial_{\tilde{\tau}})\boldsymbol{\Psi} = (\partial_\sigma + \zeta\partial_{\tilde{\tau}})(\partial_\tau - \zeta\partial_{\tilde{\sigma}})\boldsymbol{\Psi}$. On using Eqs. (16) and (17), this gives

$$[F_{\sigma\tau} - \zeta(F_{\sigma\tilde{\sigma}} + F_{\tau\tilde{\tau}}) + \zeta^2 F_{\tilde{\sigma}\tilde{\tau}}]\boldsymbol{\Psi} = 0.$$

The gauge transformation (10) can be understood by setting $\boldsymbol{\Psi} = g\tilde{\boldsymbol{\Psi}}$ in (16) and (17) and demanding that the A_μ's transform so as to preserve the form of these equations.

A very compact way of writing the SDYM equations was introduced by Pohlmeyer.[48] Following Yang,[64] and working with the Lie algebra su(2), Pohlmeyer noted that the vanishing of $F_{\sigma\tau}$ and $F_{\tilde{\sigma}\tilde{\tau}}$ allows us to write (locally)

$$A_\sigma=(\partial_\sigma C)C^{-1},\quad A_\tau=(\partial_\tau C)C^{-1},$$

$$A_{\tilde{\sigma}}=(\partial_{\tilde{\sigma}}D)D^{-1},\quad A_{\tilde{\tau}}=(\partial_{\tilde{\tau}}D)D^{-1},$$

for some C and D in the Lie group G. Letting $J=C^{-1}D\in\mathrm{G}$ we see that the last equation in (15) becomes

$$\partial_{\tilde{\sigma}}(J^{-1}\partial_\sigma J)+\partial_{\tilde{\tau}}(J^{-1}\partial_\tau J)=0. \tag{18}$$

III. EXAMPLES OF REDUCTIONS

Perhaps the simplest reductions of the SDYM equations are those in which the A_μ's are taken to be independent of certain coordinates. With the exception of the reduction to the Ernst equation, all reductions in this section will be with respect to translational symmetries. That is, the A_μ's will be taken to depend only on two linear combinations of the variables x^0, x^1, x^2, and x^3 (or equivalently σ, $\tilde{\sigma}$, τ, and $\tilde{\tau}$).

A. The nonlinear Schrödinger equation

Following Mason and Sparling,[40] let us consider the case in which the Lie algebra is $\mathfrak{sl}(2;\mathbb{C})$ (trace-free 2×2 matrices over the field of complex numbers) and the A_μ's are functions of $x=\sigma+\tilde{\sigma}$ and $t=\tilde{\tau}$ only. We use the gauge freedom and take $A_\sigma=0$. (Note that this involves solving a linear equation for g.)

In terms of the matrix-valued functions $P:=A_\tau$, $Q:=A_{\tilde{\sigma}}$ and $R:=A_{\tilde{\tau}}$, the self-dual Yang–Mills equations (15) are

$$P_x=0, \tag{19}$$

$$Q_x-P_t-[P,R]=0, \tag{20}$$

$$R_x-Q_t-[Q,R]=0. \tag{21}$$

Note that Eqs. (19)–(21) are invariant if P, Q, and R all undergo the same constant similarity transformation. Hence if P is independent of t it can be put into canonical form. In particular, if it is diagonalizable we can, without loss of generality, assume it has the form

$$P=\begin{pmatrix}k & 0\\ 0 & -k\end{pmatrix},$$

for some constant k. From Eq. (20) we see that Q_x must have zero diagonal part. Hence we can take

$$Q=\begin{pmatrix}0 & q\\ -r & 0\end{pmatrix}.$$

Equation (20) gives the parametrization of the off-diagonal elements of R in terms of q and r. So up to a constant (which can be gauged away), Eq. (21) gives

$$R=\frac{1}{2k}\begin{pmatrix}qr & q_x\\ r_x & -qr\end{pmatrix},$$

together with the equations

$$2kq_t=q_{xx}+2q^2r,$$

$$2kr_t=-r_{xx}-2qr^2.$$

Choosing $k=i/2$, $r=\pm q^*$, gives the nonlinear Schrödinger equation

$$iq_t=q_{xx}\pm 2|q|^2q.$$

B. The Korteweg–de Vries equation

Mason and Sparling[40] also considered the above reduction for the case in which P is not diagonalizable. Let P take the canonical form

$$P=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}.$$

We then find that

$$Q=\begin{pmatrix}v & 1\\ w & -v\end{pmatrix},$$

where $w=v_x-v^2$ (up to an arbitrary function of t),

$$R=\frac{1}{8}\begin{pmatrix}4(v_x-v^2)_x & -8v_x\\ v_{xxx}-4vv_{xx}-2v_x^2+4v^2v_x & -4(v_x-v^2)_x\end{pmatrix}$$

and $u=-v_x$ satisfies the Korteweg–de Vries equation

$$u_t=\tfrac{1}{4}u_{xxx}+3uu_x.$$

C. The sine-Gordon equation

Suppose that the A_μ's depend on $x=\sigma$ and $t=\tilde{\sigma}$ only. If we use a gauge in which $A_{\tilde{\sigma}}=0$, then the linear problem (16) and (17) for the SDYM equations becomes

$$\partial_x\Psi=(A_\sigma+\zeta A_{\tilde{\tau}})\Psi,\quad \partial_t\Psi=-\frac{1}{\zeta}A_\tau\Psi.$$

Here we choose the Lie algebra to be $\mathfrak{su}(2)$ so that the A_μ's are skew-Hermitian. We introduce the parametrization

$$A_\sigma=-\frac{i}{2}\begin{pmatrix}c & 0\\ 0 & -c\end{pmatrix},\quad A_\tau=-\frac{i}{2}\begin{pmatrix}0 & a-ib\\ a+ib & 0\end{pmatrix},\quad A_{\tilde{\tau}}=-\frac{i}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

(Ref. 14), where a,b,c are real functions of x and t. The SDYM equations are equivalent to

$$\frac{\partial a}{\partial x}=-bc,\quad \frac{\partial b}{\partial x}=ac,\quad \frac{\partial c}{\partial t}=-b. \tag{22}$$

It follows from the first two equations of (22) that a^2+b^2 is independent of x. We choose $a^2+b^2=1$ and introduce the parametrization $a=\cos u$, $b=\sin u$. This gives $c=\partial u/\partial x$. The third equation in (22) then becomes the sine-Gordon equation

$$u_{xt}=-\sin u.$$

D. The *N*-wave equations

Following Chakravarty and Ablowitz,[14] we consider the case in which the A_μ's are functions of σ and τ only and the Lie algebra is $\mathfrak{su}(n;\mathbb{R})$. In this case, from the self-duality equation $F_{\tilde{\sigma}\tilde{\tau}}=0$, it follows that $[A_{\tilde{\sigma}},A_{\tilde{\tau}}]=0$. We take

$$A_{\tilde{\sigma}}=\mathrm{diag}(a_1,a_2,\ldots,a_n), \quad A_{\tilde{\tau}}=\mathrm{diag}(b_1,b_2,\ldots,b_n),$$

where the a_j's and b_j's are constants (we can use a gauge transformation to make them constant). Using the parametrization $A_\sigma=[A_{ij}]$ and $A_\tau=[B_{ij}]$, the vanishing of $F_{\sigma\tilde{\sigma}}+F_{\tau\tilde{\tau}}$ implies that $[A_\sigma,A_{\tilde{\sigma}}]+[A_\tau,A_{\tilde{\tau}}]=0$, which gives

$$A_{ij}=\lambda_{ij}B_{ij},$$

where

$$\lambda_{ij}=-\frac{b_i-b_j}{a_i-a_j}, \quad i\neq j,$$

and we have assumed that the a_j's are distinct. Finally, the vanishing of $F_{\sigma\tau}$ gives the N-wave interaction equations,

$$\frac{\partial B_{ij}}{\partial\sigma}-\lambda_{ij}\frac{\partial B_{ij}}{\partial\tau}=\sum_{k=1}^{n}(\lambda_{ik}-\lambda_{kj})B_{ik}B_{kj}. \tag{23}$$

In the case $N=3$ and in which B is skew-Hermitian, Eq. (23) becomes the three-wave interaction equation.[66] The equation (23) for arbitrary N was studied by Ablowitz and Haberman.[3]

E. The chiral field equations

A number of important reductions of the SDYM equations come directly from Eq. (18). If J depends only on $x=\sigma+\tilde{\sigma}$ and $t=\tau+\tilde{\tau}$, then Eq. (18) becomes the chiral field equation

$$(J^{-1}J_x)_x+(J^{-1}J_t)_t=0. \tag{24}$$

Using $\sigma=(1/\sqrt{2})(x^1+ix^2)$, $\tilde{\sigma}=(1/\sqrt{2})(x^1-ix^2)$, Ward[61,60] obtained a $2+1$-dimensional generalization of Eq. (24) by considering a reduction of Eq. (18) in which J depends on $t=\tau+\tilde{\tau}$ and σ and $\tilde{\sigma}$. This gives

$$(J^{-1}J_t)_t+(J^{-1}J_\sigma)_{\tilde{\sigma}}=0, \tag{25}$$

which has been studied by Manakov and Zakharov[38] and Villarroel.[56] More generally, Ward obtains the equation

$$\begin{aligned}-(J^{-1}J_t)_t+(J^{-1}J_x)_x+(J^{-1}J_y)_y+a[(J^{-1}J_y)_x-(J^{-1}J_x)_y]+b[(J^{-1}J_t)_y-(J^{-1}J_y)_t]\\ +c[(J^{-1}J_x)_t-(J^{-1}J_t)_x]=0,\end{aligned} \tag{26}$$

where (a,b,c) is spacelike $(-a^2+b^2+c^2=1)$ or timelike $(-a^2+b^2+c^2=-1)$. If (a,b,c) is timelike, then Eq. (26) can be transformed to (25).

F. The Ernst equation

Following L. Witten,[62] we let J in Eq. (18) be a function of $\rho=\sqrt{(x^1)^2+(x^2)^2}$ and $z=x^3$ only. That is, $\rho^2=2\sigma\tilde{\sigma}$ and $z=(i/\sqrt{2})(\tau-\tilde{\tau})$. Equation (18) becomes

$$\rho^{-1}(\rho J^{-1}J_\rho)_\rho+(J^{-1}J_z)_z=0. \tag{27}$$

When J is a real symmetric matrix in $\mathrm{SL}(2;\mathbb{R})$, we can parametrize J as

$$J=\frac{1}{f}\begin{pmatrix}1 & g\\ g & f^2+g^2\end{pmatrix}.$$

In terms of this parametrization, Eq. (27) becomes

$$f\Delta f=\nabla f\cdot\nabla f-\nabla g\cdot\nabla g,$$

$$f\Delta g=2(\nabla f)\cdot(\nabla g),$$

where $\nabla:=(\partial_\rho,\partial_z)$ and $\Delta:=\partial_\rho^2+\rho^{-1}\partial_\rho+\partial_z^2$ are the axisymmetric forms of the gradient and Laplacian on $\mathbb{R}^3$, respectively, in cylindrical-polar coordinates. Introducing the variable $\mathcal{E}:=f+ig$, this system can be written compactly as

$$\Re(\mathcal{E})\Delta\mathcal{E}=\nabla\mathcal{E}\cdot\nabla\mathcal{E}. \tag{28}$$

Equation (28) is called the Ernst equation and describes stationary axisymmetric space–times in general relativity.[30] The function $\mathcal{E}$ is known as the Ernst potential.

G. Toda molecule

In this reduction we choose the Lie algebra to be simple and of rank N [e.g., $\mathfrak{sl}(N+1;\mathbb{C})$]. We use the basis $\{H_j,E_j^+,E_j^-\}_{j=1}^N$, which satisfies

$$\begin{gathered}[H_i,H_j]=0,\quad [E_i^+,E_j^-]=\delta_{ij}H_j,\\ [H_i,E_j^+]=K_N^{ji}E_j^+,\quad [H_i,E_j^-]=-K_N^{ji}E_j^-,\end{gathered} \tag{29}$$

where $K_N=[K_N^{ij}]$ is a Cartan matrix. Recall that an $N\times N$-matrix K is called a Cartan matrix if it satisfies the following properties:

(1) $K^{ii}=2$.
(2) K^{ij} is a nonpositive integer if $i\neq j$.
(3) $K^{ij}=0$ if and only if $K^{ji}=0$.
(4) K is positive definite with rank N.

We choose the A_μ's to be functions of σ and $\tilde{\sigma}$ only and of the form

$$A_\sigma=\sum_{k=1}^N u_k(\sigma,\tilde{\sigma})H_k,\quad A_{\tilde{\sigma}}=\sum_{k=1}^N v_k(\sigma,\tilde{\sigma})H_k,$$

$$A_\tau=\sum_{k=1}^N w_k(\sigma,\tilde{\sigma})E_k^+,\quad A_{\tilde{\tau}}=\sum_{k=1}^N w_k(\sigma,\tilde{\sigma})E_k^-.$$

Substituting the above A_μ's into the self-duality equations and using the commutation relations (29), a straightforward calculation shows that the functions u_k and v_k, $k=1,2,\ldots,N$ can be eliminated from the resulting equations, which then yield

$$\Delta\phi_i=-\sum_{j=1}^N K_N^{ij}\exp(\phi_j),\quad i=1,2,\ldots,N, \tag{30}$$

where $w_i=\exp(\phi_i/2)$ and $\Delta\phi=\phi_{\sigma\tilde{\sigma}}$. Equations (30) are known as the Toda molecule equations.[46] The case $N=1$ corresponds to the Liouville equation $\Delta\phi_1=-2\exp(\phi_1)$.

The above analysis can be repeated for the case in which a basis $\{H_j, E_j^+, E_j^-\}_{j=0}^N$ satisfies the relations (29) in which $\tilde{K}_N$ is now taken to be an extended Cartan matrix. An $(N+1)\times(N+1)$ matrix is said to be an extended Cartan matrix if and only if it is of rank N and satisfies properties 1–3 above. Note that, in particular, an extended Cartan matrix possesses a zero eigenvalue because it is not of maximal rank. This gives the Toda lattice equation

$$\Delta\phi_i = -\sum_{j=1}^{N} \tilde{K}_N^{ij} \exp(\phi_j), \quad i=0,1,\ldots,N. \tag{31}$$

In particular, if we take

$$\tilde{K}_N = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots & \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & & & -1 & 2 & -1 \\ -1 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix},$$

then Eq. (31) becomes the two-dimensional Darboux–Toda equation

$$\Delta\phi_i = \exp(\phi_{i-1}) - 2\exp(\phi_i) + \exp(\phi_{i+1}), \tag{32}$$

where $\phi_i = \phi_{i+N+1}$. The system (32) was known to Darboux[28] in the nineteenth century.

H. Infinite-dimensional algebras and 2+1 equations

In Ref. 9, Ablowitz, Chakravarty, and Takhtajan considered reductions of the SDYM equations in which the Lie algebra is the infinite-dimensional Lie algebra of formal matrix differential operators in an auxiliary variable y. They then considered reductions in which the A_μ's depend only on two space–time variables. The resulting equations then depends on three variables.

1. The 2+1-dimensional N-wave equation

First consider a reduction in which the A_μ's are functions of $x=\sigma$ and $t=\tau$ only. Then the resulting SDYM linear system is given by

$$\partial_x\Psi = (A_\sigma + \zeta A_{\tilde{\tau}})\Psi,$$

$$\partial_t\Psi = (A_\tau - \zeta A_{\tilde{\sigma}})\Psi,$$

where Ψ is a function of x,t,y and ζ. Choose a gauge in which $A_{\tilde{\tau}}=B$ and $A_{\tilde{\sigma}}=C$, where B and C are constant, commuting $n\times n$ matrices. We take the remaining gauge potentials of the form $A_\sigma = U + B\partial_y$ and $A_\tau = V + C\partial_y$, where $U(x,y,t), V(x,y,t) \in \mathfrak{sl}(n,\mathbb{C})$. By taking $\Psi = Ge^{-\zeta y}$, we obtain a simpler, reduced linear system from above,

$$\partial_x G = (U + B\partial_y)G, \tag{33}$$

$$\partial_t G = (V + C\partial_y)G, \tag{34}$$

in terms of the function $G(x,y,t)$. The system (33) and (34) is the standard linear system related to the $2+1$-dimensional N-wave equations. The compatibility of (33) and (34) is

$$\partial_t U - \partial_x V + [U,V] - C\partial_y U + B\partial_y V = 0, \quad [B,V] = [C,U],$$

which gives

$$[B,\partial_t Q]-[C,\partial_x Q]-C[B,\partial_y Q]+B[C,\partial_y Q]+[[B,Q],[C,Q]]=0,$$

where $U=[B,Q]$ and $V=[C,Q]$. In the case when B and C are diagonal and Q is off-diagonal, these equations can be transformed to the $2+1$ N-wave equations

$$\frac{\partial Q_{ij}}{\partial t}=a_{ij}\frac{\partial Q_{ij}}{\partial x}+b_{ij}\frac{\partial Q_{ij}}{\partial y}+\sum_{k=1}^{n}(a_{ik}-a_{kj})Q_{ik}Q_{kj},$$

where a_{ij}, b_{ij} are suitable constants depending on the matrix elements of B and C.

2. KP, mKP, and DS equations

Chakravarty, Kent, and Newman[21] also obtained the Kadomtsev–Petviashvili, modified Kadomtsev–Petviashvili, and Davey–Stewartson equations directly as reductions of the SDYM equations with an infinite-dimensional Lie algebra of formal matrix differential operators. If the A_μ's are assumed to depend on $x=\sigma+\tilde{\sigma}$ and $t=\tau$ only, then the linear problem (16) and (17) becomes

$$\partial_x\mathbf{\Psi}=(A_\sigma+\zeta A_{\tilde{\tau}})\mathbf{\Psi}, \tag{35}$$

$$\partial_t\mathbf{\Psi}=(A_\tau+\zeta[A_\sigma+A_{\tilde{\sigma}}]+\zeta^2 A_{\tilde{\tau}})\mathbf{\Psi}. \tag{36}$$

The connection components are taken to be of the form

$$A_\sigma=U_0+U_1\partial_y,\quad A_{\tilde{\sigma}}=-(B_0+B_1\partial_y),\quad A_\tau=V_0+V_1\partial_y+V_2\partial_y^2,\quad A_{\tilde{\tau}}=A,$$

where the coefficients are 2×2 matrix-valued functions of x and t. In order to simplify the integrability conditions of (35) and (36), we demand (as in the $2+1$ N-wave case) that the spectral parameter ζ be eliminated from this system after a change of variable of the form $\mathbf{\Psi}=G\mathrm{e}^{-\zeta y}$. It can be shown that this requirement implies that $U_1=V_2=B_1+A$ and $V_1=U_0+B_0$. Subsequently, the system (35) and (36) becomes

$$\partial_x G=(U_0+A\partial_y)G, \tag{37}$$

$$\partial_t G=(V_0+[U_0+B_0]\partial_y+A\partial_y^2)G. \tag{38}$$

Appropriate choices of the matrices A, B, U, and V give the linear problem for the KP, mKP, and DS equations (see Ref. 21).

Another notable reduction with an infinite-dimensional gauge algebra was considered in Ref. 39 by Mason and Newman. They showed that the SDYM equations with the Lie algebra of the Lie group of volume preserving diffeomorphisms on a four-manifold, in which the A_μ's are independent of the space-time coordinates σ, $\tilde{\sigma}$, τ, and $\tilde{\tau}$, are equivalent to the self-dual Einstein equations. In particular, the reduction to the Plebanski heavenly equation is given in Ref. 22. This equation in turn has a reduction to the Monge–Ampere equation.

I. The SDYM hierarchy

In Ref. 9, the authors studied an infinite hierarchy of equations whose first member was the SDYM system. Each member of the hierarchy has the same underlying spectral problem, and the higher flows are derived from an infinite sequence of nonlocal conservation laws associated with the SDYM equations. Furthermore, many well known integrable hierarchies in $1+1$- and $2+1$-dimensions are derived from the symmetry reductions of the self-dual hierarchy.

In an appropriate gauge, the kth member of the SDYM hierarchy is given by

$$\partial_{\tau_k}A_\sigma-\partial_\sigma\Phi_{k-1}+[A_\sigma,\Phi_{k-1}]=0, \tag{39}$$

where Φ_n is given recursively by

$$(\partial_{\tilde{\tau}} - \mathrm{ad}\, A_{\tilde{\tau}})\Phi_{n+1} = -(\partial_\sigma - \mathrm{ad}\, A_\sigma)\Phi_n - \partial_{\tilde{\sigma}} A_\sigma \delta_{n0}, \quad n = 0,1,\ldots,$$

and $\Phi_0 = -A_{\tilde{\sigma}}$. Equation (39) is the compatibility condition for the system

$$D_1\Psi = \mathcal{A}_1\Psi, \quad D_2\Psi = \mathcal{A}_2\Psi, \tag{40}$$

where, for $k = 2,3,\ldots$,

$$D_1 = \partial_\sigma + \zeta\partial_{\tilde{\tau}}, \quad \mathcal{A}_1 = A_\sigma + \zeta A_{\tilde{\tau}},$$

$$D_k = \partial_{\tau_k} - \zeta^{k-1}\partial_{\tilde{\sigma}}, \quad \mathcal{A}_k = (\zeta^{k-1}\Phi)_+, \quad \Phi = \sum_{n=0}^{\infty} \Phi_n \zeta^{-n},$$

and $(F)_+$ denotes the power series part of the Laurent expansion of F about $\zeta = 0$. Note that if $k = 2$, then $D_2 = \partial_\tau - \zeta\partial_{\tilde{\sigma}}$ and $\mathcal{A}_2 = A_\tau - \zeta A_{\tilde{\sigma}}$, where $\tau = \tau_2$ and we have identified A_τ with Φ_1. In this case the linear problem (40) becomes the standard linear problem for the SDYM equations.

As mentioned above, the reduction of the SDYM equations to the $1+1$- and $2+1$-dimensional integrable equations can be extended to a reduction of the SDYM hierarchy to the corresponding hierarchies. In this way, we can obtain, for example, both the $1+1$- and $2+1$-dimensional N-wave hierarchies. In particular, the Davey–Stewartson equation (DS) can be obtained as the second member of the $2+1$-dimensional N-wave hierarchy. See Ref. 9 for details.

IV. ODE REDUCTIONS

A. Integrable tops

The equations of motion for a spinning top have played a fundamental role in the early development of the theory of integrable systems.

1. The Euler–Arnold–Manakov top

In this reduction, following Chakravarty, Ablowitz, and Clarkson,[18,19] we take the Lie algebra to be $\mathfrak{sl}(n;\mathbb{C})$ and we assume that the A_μ's are functions of $t = \sigma$ only. The vanishing of $F_{\tilde{\sigma}\tilde{\tau}}$ demands that $A_{\tilde{\sigma}}$ and $A_{\tilde{\tau}}$ commute. We take these matrices to be diagonal and of the form

$$A_{\tilde{\sigma}} = \mathrm{diag}(a_1, a_2, \ldots, a_n), \quad A_{\tilde{\tau}} = \mathrm{diag}(b_1, b_2, \ldots, b_n),$$

where the a_j's and b_j's are constants. The equation $F_{\sigma\tilde{\sigma}} + F_{\tau\tilde{\tau}} = 0$ is now the algebraic equation $[A_\sigma, A_{\tilde{\sigma}}] + [A_\tau, A_{\tilde{\tau}}] = 0$, which gives the elements of $A_\sigma = [A_{ij}]$ in terms of the elements of $A_\tau = [B_{ij}]$ as

$$A_{ij} = -\frac{b_j - b_i}{a_j - a_i} B_{ij}, \quad i \neq j,$$

provided $a_i \neq a_j$, $b_i \neq b_j$ for $i \neq j$.

Choosing $a_i = b_i^2$, $i = 1,\ldots,n$, and A_σ and A_τ to be skew-symmetric, we have $A_{ij} = -(b_i + b_j)^{-1} B_{ij}$ and the vanishing of $F_{\sigma\tau}$ gives

$$\frac{dB_{ij}}{dt} = \sum_{k=1}^{n} \left(\frac{1}{b_j + b_k} - \frac{1}{b_k + b_i} \right) B_{ik} B_{kj}. \tag{41}$$

Equations (41) were first considered by Manakov[37] and Arnold[12] and are the equations of motion for a free n-dimensional rigid body about a fixed point. In the case $n = 3$, we obtain Euler's equations for a free spinning body about a fixed point,

$$\frac{dL_1}{dt}=\gamma_1 L_2 L_3, \quad \frac{dL_2}{dt}=\gamma_2 L_3 L_1, \quad \frac{dL_3}{dt}=\gamma_3 L_1 L_2, \tag{42}$$

where

$$L_1=B_{23}, \quad L_2=B_{31}, \quad L_3=B_{12}, \quad I_1=-(b_2+b_3), \quad I_2=-(b_3+b_1), \quad I_3=-(b_1+b_2),$$

and

$$\gamma_1=\frac{I_2-I_3}{I_2 I_3}, \quad \gamma_2=\frac{I_3-I_1}{I_3 I_1}, \quad \gamma_3=\frac{I_1-I_2}{I_1 I_2}.$$

In Eq. (42), (L_1,L_2,L_3) is the angular momentum in the body frame and the I_k's are the principal moments of inertia. Reductions to other integrable tops, including the Kowalevsaya top, are described in Refs. 18 and 19.

B. The Painlevé equations

With the exception of the reduction to the Ernst equation, all of the above reductions have been with respect to translational symmetries. In other words, the reductions have all resulted from considering A_μ's that depend only on one or more linear combination of the variables σ, $\tilde{\sigma}$, τ, and $\tilde{\tau}$. In this section we follow Mason and Woodhouse[41,42] and obtain reductions to the Painlevé equations by considering reductions by conformal symmetries.

The Painlevé equations are the following six classically known ODEs:

$$P_I \quad u''=6u^2+t,$$

$$P_{II} \quad u''=2u^3+tu+\alpha,$$

$$P_{III} \quad u''=\frac{1}{u}u'^2-\frac{1}{t}u'+\frac{1}{t}(\alpha u^2+\beta)+\gamma u^3+\frac{\delta}{u},$$

$$P_{IV} \quad u''=\frac{1}{2u}u'^2+\frac{3}{2}u^3+4tu^2+2(t^2-\alpha)u+\frac{\beta}{u},$$

$$P_V \quad u''=\left\{\frac{1}{2u}+\frac{1}{u-1}\right\}u'^2-\frac{1}{t}u'+\frac{(u-1)^2}{t^2}\left(\alpha+\frac{\beta}{u}\right)+\frac{\gamma u}{t}+\frac{\delta u(u+1)}{u-1},$$

$$P_{VI} \quad u''=\frac{1}{2}\left\{\frac{1}{u}+\frac{1}{u-1}+\frac{1}{u-t}\right\}u'^2-\left\{\frac{1}{t}+\frac{1}{u-1}+\frac{1}{u-t}\right\}u'$$
$$+\frac{u(u-1)(u-t)}{t^2(t-1)^2}\left\{\alpha+\frac{\beta t}{u^2}+\frac{\gamma(t-1)}{(u-1)^2}+\frac{\delta t(t-1)}{(u-t)^2}\right\}.$$

These equations have played a very important role in integrable systems. Indeed they arise from similarity reductions of classical soliton equations and as monodromy preserving deformation equations associated with linear systems of ODEs with rational coefficients.

The SDYM equations are invariant under the group of conformal transformations (transformations that preserve the metric up to an over all factor). The metric on $\mathbf{R}^4$ in null coordinates, $d\sigma\, d\tilde{\sigma}+d\tau\, d\tilde{\tau}$, is proportional to $\varepsilon_{\alpha\beta\gamma\delta}dx^{\alpha\beta}dx^{\gamma\delta}$, where $[x^{\alpha\beta}]$ is the skew-symmetric singular matrix

$$[x^{\alpha\beta}]=\begin{pmatrix} 0 & \lambda & \sigma & \tilde{\tau} \\ -\lambda & 0 & -\tau & \tilde{\sigma} \\ -\sigma & \tau & 0 & 1 \\ -\tilde{\tau} & -\tilde{\sigma} & -1 & 0 \end{pmatrix}, \tag{43}$$

where $\lambda=\sigma\tilde{\sigma}+\tau\tilde{\tau}$.

Consider a mapping of the form $x\mapsto y=gxg^T$, where $g\in \mathrm{GL}(4;\mathbb{C})$. Then the mapping $x\mapsto y/y^{23}$ generates a conformal transformation of $\mathbb{C}^4$ as it maps the space of matrices of the form (43) into itself. In fact, every proper conformal transformation arises in this way. The generators of the conformal transformations are called conformal Killing vectors. In order to calculate the associated conformal Killing vectors we consider a one-parameter family of transformations given by $g=\exp(\epsilon K)=I+\epsilon K+O(\epsilon^2)$, where $K\in \mathfrak{gl}(4;\mathbb{C})$. Hence $y=x+\epsilon(Kx+xK^T)+O(\epsilon^2)$. Consider the case in which the matrix K has a 1 in the $\mu\nu$ component and zeros elsewhere. In components we have

$$y^{\alpha\beta}=x^{\alpha\beta}+\epsilon(x^{\alpha\nu}\delta^{\beta\mu}-x^{\beta\nu}\delta^{\alpha\mu})+O(\epsilon^2).$$

So

$$x^{\alpha\beta}\mapsto\tilde{x}^{\alpha\beta}=y^{\alpha\beta}/y^{23}=x^{\alpha\beta}+\epsilon(x^{\alpha\nu}\delta^{\beta\mu}-x^{\beta\nu}\delta^{\alpha\mu}+x^{\alpha\beta}q^{\mu\nu})+O(\epsilon^2),$$

where $q^{\mu\nu}=x^{3\nu}\delta^{2\mu}-x^{2\nu}\delta^{3\mu}$. By considering the appropriate components of $[x^{\alpha\beta}]$ we find

$$\sigma\mapsto\sigma+\epsilon(x^{0\nu}\delta^{2\mu}-x^{2\nu}\delta^{0\mu}+\sigma q^{\mu\nu})+O(\epsilon^2),$$

$$\tilde{\sigma}\mapsto\tilde{\sigma}+\epsilon(x^{1\nu}\delta^{3\mu}-x^{3\nu}\delta^{1\mu}+\tilde{\sigma}q^{\mu\nu})+O(\epsilon^2),$$

$$\tau\mapsto\tau+\epsilon(x^{2\nu}\delta^{1\mu}-x^{1\nu}\delta^{2\mu}+\tau q^{\mu\nu})+O(\epsilon^2),$$

$$\tilde{\tau}\mapsto\tilde{\tau}+\epsilon(x^{0\nu}\delta^{3\mu}-x^{3\nu}\delta^{0\mu}+\tilde{\tau}q^{\mu\nu})+O(\epsilon^2).$$

It follows that the conformal Killing vector $X_{\mu\nu}$ associated with the matrix K which is one in the $\mu\nu$-entry and zero elsewhere, is

$$X_{00}=\sigma\partial_\sigma+\tilde{\tau}\partial_{\tilde{\tau}},\quad X_{20}=-\sigma\tilde{\tau}\partial_\sigma-\tilde{\sigma}\tilde{\tau}\partial_{\tilde{\sigma}}+\sigma\tilde{\sigma}\partial_\tau-\tilde{\tau}^2\partial_{\tilde{\tau}},$$

$$X_{01}=\tilde{\sigma}\partial_{\tilde{\tau}}-\tau\partial_\sigma,\quad X_{21}=\tau\tilde{\tau}\partial_\sigma-\tilde{\sigma}^2\partial_{\tilde{\sigma}}-\tau\tilde{\sigma}\partial_\tau-\tilde{\sigma}\tilde{\tau}\partial_{\tilde{\tau}},$$

$$X_{10}=\tilde{\tau}\partial_{\tilde{\sigma}}-\sigma\partial_\tau,\quad X_{30}=\sigma^2\partial_\sigma-\tau\tilde{\tau}\partial_{\tilde{\sigma}}+\sigma\tau\partial_\tau+\sigma\tilde{\tau}\partial_{\tilde{\tau}},$$

$$X_{11}=\tilde{\sigma}\partial_{\tilde{\sigma}}+\tau\partial_\tau,\quad X_{31}=-\sigma\tau\partial_\sigma-\tilde{\sigma}\tau\partial_{\tilde{\sigma}}-\tau^2\partial_\tau+\sigma\tilde{\sigma}\partial_{\tilde{\tau}},$$

$$X_{02}=\partial_{\tilde{\tau}},\quad X_{22}=-\tilde{\sigma}\partial_{\tilde{\sigma}}-\tilde{\tau}\partial_{\tilde{\tau}},$$

$$X_{03}=-\partial_\sigma,\quad X_{23}=\tilde{\tau}\partial_\sigma-\tilde{\sigma}\partial_\tau,$$

$$X_{12}=\partial_{\tilde{\sigma}},\quad X_{32}=-\tau\partial_{\tilde{\sigma}}+\sigma\partial_{\tilde{\tau}},$$

$$X_{13}=\partial_\tau,\quad X_{33}=-\sigma\partial_\sigma-\tau\partial_\tau.$$

Note that there are 15 independent conformal Killing vectors since $X_{00}+X_{11}+X_{22}+X_{33}=0$. This corresponds to the fact that we could have taken $g\in \mathrm{SL}(4;\mathbb{C})$, which would mean that the trace of K is zero.

The Painlevé equations correspond to reductions of the SDYM equations when the Lie algebra is $\mathfrak{sl}(2;\mathbb{C})$. The conformal Killing vectors of these reductions correspond to the following four-parameter subgroups of GL(4;$\mathbb{C}$). Mason and Woodhouse[42] call these the Painlevé groups:

$$P_I,\ P_{II}\ \begin{pmatrix} a_4 & a_3 & a_2 & a_1 \\ 0 & a_4 & a_3 & a_2 \\ 0 & 0 & a_4 & a_3 \\ 0 & 0 & 0 & a_4 \end{pmatrix},$$

$$P_{III}\ \begin{pmatrix} a_4 & a_2 & 0 & 0 \\ 0 & a_4 & 0 & 0 \\ 0 & 0 & a_3 & a_1 \\ 0 & 0 & 0 & a_3 \end{pmatrix},$$

$$P_{IV}\ \begin{pmatrix} a_3 & a_2 & a_1 & 0 \\ 0 & a_3 & a_2 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix},$$

$$P_V\ \begin{pmatrix} a_2 & a_1 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix},$$

$$P_{VI}\ \begin{pmatrix} a_4 & 0 & 0 & 0 \\ 0 & a_3 & 0 & 0 \\ 0 & 0 & a_2 & 0 \\ 0 & 0 & 0 & a_1 \end{pmatrix}.$$

The conformal Killing vectors associated with the Painlevé equations are discussed below.

P_I, P_{II}: The conformal Killing vectors associated with the Painlevé subgroup given above are of the form

$$a_1X_{03}+a_2(X_{02}+X_{13})+a_3(X_{01}+X_{12}+X_{23})+a_4(X_{00}+X_{11}+X_{22}+X_{33}).$$

In this case the vector multiplying a_4 is zero. More generally for the reductions described for other Painlevé equations below, the conformal Killing vector associated with a_4 is a linear combination of the conformal Killing vectors associated with a_1, a_2, and a_3.

The vectors multiplying a_1, a_2, and a_3 are, respectively,

$$\tilde{X}_1=-\partial_\sigma,$$

$$\tilde{X}_2=\partial_\tau+\partial_{\tilde{\tau}},$$

$$\tilde{X}_3=(\tilde{\tau}-\tau)\partial_\sigma+\partial_{\tilde{\sigma}}-\tilde{\sigma}\partial_\tau+\tilde{\sigma}\partial_{\tilde{\tau}}.$$

We now choose new variables w^1, w^2, w^3, and t, such that

$$\tilde{X}_i(w^j)=\delta_i^j,\quad \tilde{X}_i(t)=0,\quad i,j=1,2,3. \tag{44}$$

A particular choice is

$$w^1=-\sigma+\tilde{\sigma}(\tilde{\tau}-\tau)-\tfrac{2}{3}\tilde{\sigma}^3,\quad w^2=\tilde{\tau}-\tfrac{1}{2}\tilde{\sigma}^2,\quad w^3=\tilde{\sigma},\quad t=\tilde{\tau}-\tau-\tilde{\sigma}^2.$$

Using the gauge freedom, we let the one-form A have the form

$$A=W_j dw^j,$$

where the W_j's are functions of t only. That is, the gauge freedom has been used to choose the coefficient of dt to be zero. Hence,

$$A=-W_1 d\sigma+([\tilde{\tau}-\tau-2\tilde{\sigma}^2]W_1-\tilde{\sigma}W_2+W_3)d\tilde{\sigma}-\tilde{\sigma}W_1 d\tau+(\tilde{\sigma}W_1+W_2)d\tilde{\tau},$$

from which we can read the values of A_σ, $A_{\tilde{\sigma}}$, A_τ, and $A_{\tilde{\tau}}$. The SDYM equations are

$$W_1'=0,\quad W_2'=[W_1,W_3],\quad W_3'=[W_2,tW_1+W_3].$$

From these equations it follows that three conserved quantities are $l=\mathrm{Tr}(W_1W_2)$, $m=\mathrm{Tr}(W_3W_1+\frac{1}{2}W_2^2)$, and $n=\mathrm{Tr}(W_2W_3)$.

Using the residual gauge freedom, W_1 can be put into one of the canonical forms,

$$\begin{pmatrix} k & 0 \\ 0 & -k \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

where k is a constant. The first case leads to P_{II} while the second leads to P_I. If we choose y to be one of the roots of the gauge-invariant equation

$$\det([W_1,yW_2-W_3])=0\,,$$

we find that (up to simple rescalings) y solves the appropriate Painlevé equation.

For the other Painlevé equations, we list the conformal Killing vectors, the choices for the w^j's and t, and the reduced SDYM equations.

P_{III}

$$\tilde{X}_1=\tilde{\tau}\partial_\sigma-\tilde{\sigma}\partial_\tau,$$

$$\tilde{X}_2=-\tau\partial_\sigma+\tilde{\sigma}\partial_{\tilde{\tau}},$$

$$\tilde{X}_3=-\sigma\partial_\sigma-\tilde{\sigma}\partial_{\tilde{\sigma}}-\tau\partial_\tau-\tilde{\tau}\partial_{\tilde{\tau}}.$$

$$w^1=-\tau/\tilde{\sigma},\quad w^2=\tilde{\tau}/\tilde{\sigma},\quad w^3=-\log\tilde{\sigma},\quad t=\tilde{\sigma}^{-1}\sqrt{\sigma\tilde{\sigma}+\tau\tilde{\tau}}.$$

$$W_1'=0,\quad tW_2'=2[W_3,W_2],\quad W_3'=2t[W_1,W_2].$$

P_{IV}

$$\tilde{X}_1=\partial_{\tilde{\tau}},$$

$$\tilde{X}_2=-\tau\partial_\sigma+\partial_{\tilde{\sigma}}+\tilde{\sigma}\partial_{\tilde{\tau}},$$

$$\tilde{X}_3=\sigma\partial_\sigma+\tau\partial_\tau.$$

$$w^1=\tilde{\tau}-\tfrac{1}{2}\tilde{\sigma}^2,\quad w^2=-\sigma/\tau,\quad w^3=\log\tau,\quad t=\tilde{\sigma}+\sigma/\tau.$$

$$W_1'=0,\quad W_2'=[tW_2+W_3,W_1],\quad W_3'=[W_3,W_2]. \tag{45}$$

P_V

$$\tilde{X}_1=-\tau\partial_\sigma+\tilde{\sigma}\partial_{\tilde{\tau}},$$

$$\tilde{X}_2=\sigma\partial_\sigma+\tilde{\sigma}\partial_{\tilde{\sigma}}+\tau\partial_\tau+\tilde{\tau}\partial_{\tilde{\tau}},$$

$$\tilde{X}_3=-\tilde{\sigma}\partial_{\tilde{\sigma}}-\tilde{\tau}\partial_{\tilde{\tau}}.$$

$$w^1=\tilde{\tau}/\tilde{\sigma},\quad w^2=\log([\sigma\tilde{\sigma}+\tau\tilde{\tau}]/\tilde{\sigma}),\quad w^3=\log(\tau/\tilde{\sigma}),\quad t=\sigma/\tau+\tilde{\tau}/\tilde{\sigma}.$$

$$W_1'=0,\quad W_2'=[W_3,W_1],\quad tW_3'=[tW_1+W_2,W_3].$$

P_{VI}

$$\tilde{X}_1=-\sigma\partial_\sigma-\tau\partial_\tau,$$

$$\tilde{X}_2=-\tilde{\sigma}\partial_{\tilde{\sigma}}-\tilde{\tau}\partial_{\tilde{\tau}}$$

$$\tilde{X}_3=\tilde{\sigma}\partial_{\tilde{\sigma}}+\tau\partial_\tau.$$

$$w^1=-\log\sigma,\quad w^2=-\log\tilde{\tau},\quad w^3=\log(\tilde{\sigma}/\tilde{\tau}),\quad t=-(\tau\tilde{\tau})/(\sigma\tilde{\sigma}).$$

$$W_1'=0,\quad tW_2'=[W_2,W_3],\quad t(1-t)W_3'=[W_3,tW_1+W_2].$$

1. Reduction of the linear problem

Note that each of the symmetry reductions of the SDYM equations to one of the Painlevé equations extends to a reduction of the linear problem (16) and (17). However, in finding a reduction of the linear problem, the spectral parameter ζ must also be transformed. The symmetries of the field equations are lifted to symmetries of the linear problem. For P_{VI} we extend the reduction above to the linear problem (16) and (17) by restricting $\mathbf{\Psi}$ to have the form $\mathbf{\Psi}(\sigma,\tau,\tilde{\sigma},\tilde{\tau};\zeta)=\psi(t;\lambda)$, where $\lambda=\tilde{\tau}/(\sigma\zeta)$. Note that then

$$\tau\partial_\tau\mathbf{\Psi}=-\tilde{\sigma}\partial_{\tilde{\sigma}}\mathbf{\Psi}=t\partial_t\psi,\quad \text{and}\quad \tilde{\tau}\partial_{\tilde{\tau}}\mathbf{\Psi}=-\sigma\partial_\sigma\mathbf{\Psi}=t\partial_t\psi+\lambda\partial_\lambda\psi.$$

The linear problem (16) and (17) then becomes

$$\partial_\lambda\psi=-\left[\frac{W_2}{\lambda-1}-\frac{W_1+W_2+W_3}{\lambda-1}+\frac{W_3}{\lambda-t}\right]\psi,\quad \partial_t\psi=\frac{W_3}{\lambda-t}\psi. \tag{46}$$

The system of equations (46) is the isomonodromy problem for P_{VI}. The compatibility of (46) gives Eqs. (45), which are equivalent to P_{VI}. Isomonodromy problems for the above reductions

to P_I–P_V can be obtained in the same way. Indeed, it is often easier to identify a reduction to one of the Painlevé equations from the form of the isomonodromy problem. By comparing the isomonodromy problem to those in the literature, we can identify the component that will satisfy the appropriate Painlevé equation.

V. THE DARBOUX–HALPHEN SYSTEM

In this section we consider a reduction of the SDYM equations to an integrable generalization of the classical Darboux–Halphen system. Its general solution is densely branched and contains a movable natural barrier.

Consider the reduction of the SDYM equations in which the A_μ's are functions of $t:=-x^0$ only. This gives the well known Nahm equations[43]

$$\dot{A}_1=[A_2,A_3], \quad \dot{A}_2=[A_3,A_1], \quad \dot{A}_3=[A_1,A_2], \tag{47}$$

where we have chosen a gauge in which $A_0\equiv 0$.

Using $\mathfrak{diff}(S^3)$, the infinite-dimensional Lie algebra of vector fields on S^3, we choose the components of the connection to be of the form

$$A_i(t)=\sum_{j,k=1}^{3} O_{ij}M_{jk}(t)X_k\,. \tag{48}$$

The X_k's are divergence-free vector fields on S^3 and satisfy the $\mathfrak{su}(2)$ commutation relations

$$[X_i,X_j]=\sum_{k=1}^{3} \varepsilon_{ijk}X_k\,, \tag{49}$$

where ε_{ijk} is totally antisymmetric and $\varepsilon_{123}=1$. The SO(3) matrix $[O_{ij}]$ is used to represent the points of S^3 (see, e.g., Ref. 55) and the action of the vector fields X_i on O_{jk} is given by[6]

$$X_iO_{jk}=\sum_{l=1}^{3} \varepsilon_{ikl}O_{jl}\,. \tag{50}$$

Substituting Eq. (48) into Eq. (47) and using (49) and (50) together with the identities

$$\sum_{i,j,k=1}^{3} \varepsilon_{ijk}O_{ip}O_{jq}O_{kr}=\varepsilon_{pqr}\,, \quad \sum_{i=1}^{3} \varepsilon_{ijk}\varepsilon_{imn}=\delta_{jm}\delta_{kn}-\delta_{jn}\delta_{km},$$

yields

$$\dot{M}=(\mathrm{Adj}\,M)^T+M^TM-(\mathrm{Tr}\,M)M, \tag{51}$$

where $(\mathrm{Adj}\,M):=(\det M)M^{-1}$ is the adjoint of M and the dot denotes differentiation with respect to t. Equation (51) was first derived in Ref. 20. Equation (51) was also derived in Ref. 34 where it was shown to represent an SU(2) invariant hypercomplex four-manifold. Since the Weyl curvature of a hypercomplex four-manifold is self-dual, Eq. (51) describes a class of self-dual Weyl Bianchi IX space–times with Euclidean signature.[15]

In order to solve Eq. (51) we first introduce a simple factorization. If the eigenvalues of the symmetric part, M_s, of M are distinct, then M_s can be diagonalized using a (complex) orthogonal matrix P. In this case we may write

$$M=M_s+M_a=P(d+a)P^{-1},$$

where $d:=\mathrm{diag}\,(\omega_1,\omega_2,\omega_3)$, $\omega_i\neq\omega_j$, $i\neq j$, and the nonzero elements of the skew-symmetric matrix a are denoted as $a_{12}=-a_{21}=\tau_3$, $a_{23}=-a_{32}=\tau_1$ and $a_{31}=-a_{13}=\tau_2$. Using the above factorization of M, Eq. (51) can be transformed into

$$\begin{aligned}\dot\omega_1&=\omega_2\omega_3-\omega_1(\omega_2+\omega_3)+\tau^2,\\ \dot\omega_2&=\omega_3\omega_1-\omega_2(\omega_3+\omega_1)+\tau^2,\\ \dot\omega_3&=\omega_1\omega_2-\omega_3(\omega_1+\omega_2)+\tau^2,\end{aligned}\tag{52}$$

where $\tau^2:=\tau_1^2+\tau_2^2+\tau_3^2$ and

$$\dot\tau_1=-\tau_1(\omega_2+\omega_3),\quad \dot\tau_2=-\tau_2(\omega_3+\omega_1),\quad \dot\tau_3=-\tau_3(\omega_1+\omega_2),\tag{53}$$

together with the linear equation

$$\dot P+Pa=0,\tag{54}$$

for the matrix P. The system (52) with $\tau^2=0$ is the classical Darboux–Halphen system which appeared in Darboux's analysis of triply orthogonal surfaces[27] and was later solved by Halphen.[32] Halphen also studied and solved Eqs. (52)–(56),[31] which are linearizable in terms of Fuchsian differential equations with three regular singular points.

Taking the differences between the various equations in (52) results in

$$\omega_1=-\frac{1}{2}\frac{d}{dt}\ln(\omega_2-\omega_3),\quad \omega_2=-\frac{1}{2}\frac{d}{dt}\ln(\omega_3-\omega_1),\quad \omega_3=-\frac{1}{2}\frac{d}{dt}\ln(\omega_1-\omega_2).$$

Together with Eqs. (53), these equations show that

$$\begin{aligned}\alpha^2&:=\frac{\tau_1^2}{(\omega_1-\omega_2)(\omega_3-\omega_1)},\\ \beta^2&:=\frac{\tau_2^2}{(\omega_2-\omega_3)(\omega_1-\omega_2)},\\ \gamma^2&:=\frac{\tau_3^2}{(\omega_3-\omega_1)(\omega_2-\omega_3)}\end{aligned}\tag{55}$$

are constants. Without loss of generality we choose α, β, and γ to have nonnegative real parts. Hence, provided the symmetric part of M has distinct eigenvalues, Eq. (51) reduces to the third-order system (52), where

$$\tau^2=\alpha^2(\omega_1-\omega_2)(\omega_3-\omega_1)+\beta^2(\omega_2-\omega_3)(\omega_1-\omega_2)+\gamma^2(\omega_3-\omega_1)(\omega_2-\omega_3),\tag{56}$$

together with the linear equation (54) for P. In Refs. 47 and 33, solutions of equations (52)–(56) for special choices of α, β, and γ were determined in terms of automorphic forms.

Note that the system (52) with τ^2 as in (56) is invariant under the transformation

$$t\mapsto\mu(t):=\frac{at+b}{ct+d},\quad \omega_j(t)\mapsto\frac{\omega_j(\mu(t))}{(ct+d)^2}+\frac{c}{ct+d},\quad ad-bc=1.$$

We introduce the μ-invariant function

$$s := \frac{\omega_1 - \omega_3}{\omega_2 - \omega_3}. \tag{57}$$

Differentiating Eq. (57) and using the system (52) yields $\dot{s} = 2s(\omega_1 - \omega_2)$. Repeating this process gives $\ddot{s} = 2(\dot{s} - 2\omega_3 s)(\omega_1 - \omega_2)$. Solving these two equations together with (57) for the ω's gives

$$\begin{aligned} \omega_1 &= -\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s(s-1)}, \\ \omega_2 &= -\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s-1}, \\ \omega_3 &= -\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}}{s}. \end{aligned} \tag{58}$$

Substituting the parametrization (58) into any of the equations in (52) shows that $s(t)$ must satisfy

$$\{s,t\} + \frac{\dot{s}^2}{2}V(s) = 0, \tag{59}$$

where

$$\{s,t\} := \frac{d}{dt}\left(\frac{\ddot{s}}{\dot{s}}\right) - \frac{1}{2}\left(\frac{\ddot{s}}{\dot{s}}\right)^2$$

is the Schwarzian derivative and V is given by

$$V(s) = \frac{1-\beta^2}{s^2} + \frac{1-\gamma^2}{(s-1)^2} + \frac{\beta^2+\gamma^2-\alpha^2-1}{s(s-1)}. \tag{60}$$

The general solution of Eq. (59) is given implicitly by

$$t(s) = \frac{u_1(s)}{u_2(s)}, \tag{61}$$

where $u_1(s)$ and $u_2(s)$ are two independent solutions of the Fuchsian differential equation

$$\frac{d^2u}{ds^2} + \frac{1}{4}V(s)u = 0 \tag{62}$$

with regular singular points at 0, 1, and ∞. The transformation

$$u(s) = s^{c/2}(1-s)^{(a+b-c+1)/2}\chi(s) \tag{63}$$

maps Eq. (62) to the Gauss hypergeometric equation

$$s(1-s)\frac{d^2\chi}{ds^2} + [c-(a+b+1)s]\frac{d\chi}{ds} - ab\chi = 0, \tag{64}$$

where $a = (1+\alpha-\beta-\gamma)/2$, $b = (1-\alpha-\beta-\gamma)/2$, and $c = 1-\beta$ (see, e.g., Refs. 45 and 2). Note that from the general solution $s(t)$ of Eq. (59) we can reconstruct the ω_j's from Eqs. (58) and the τ_j's then follow from (55).

From Eq. (61), if α, β, and γ are non-negative real numbers such that $\alpha+\beta+\gamma<1$, then the upper- (or lower-) half s-plane is mapped to a triangular region in the t-plane whose sides are the

arcs of circles and whose vertices subtend angles of $\alpha\pi$, $\beta\pi$, and $\gamma\pi$. Moreover, if α, β, and γ are either 0 or reciprocals of integers, then s is an analytic function of t on the interior of a circle on the complex sphere $\mathbb{C}\cup\infty$ but cannot be analytically extended across any point of the circle. That is, the circle is a natural barrier for the function $s(t)$.

The solution procedure just outlined allows us to obtain explicit expressions for the conserved quantities for the generalized Darboux–Halphen system (52) and (56). In Ref. 36, it was shown that the classical Darboux–Halphen system admits no meromorphic first integrals. In Ref. 17, the first integrals for the full system (52) and (56) were found and shown to be branched and transcendental involving hypergeometric functions. The existence of these integrals is consistent with Ref. 36 because even in the classical case they are branched despite the fact that the general solution is single-valued.

Fix two linearly independent solutions u_1 and u_2 of Eq. (62) with Wronskian

$$W(u_1,u_2)=u_1u_2'-u_2u_1'=1, \tag{65}$$

where prime denotes differentiation with respect to s. Then the general solution of Eq. (59) is given implicitly by

$$t(s)=\frac{J_2u_1(s)-J_1u_2(s)}{I_2u_1(s)-I_1u_2(s)}, \tag{66}$$

where I_α and J_α, $\alpha=1,2$, are constants satisfying $I_1J_2-I_2J_1=1$. Differentiating Eq. (66) twice and using (65) gives

$$I_2u_1-I_1u_2=\dot{s}^{1/2}, \quad I_2u_1'-I_1u_2'=\tfrac{1}{2}\dot{s}^{-3/2}\ddot{s}. \tag{67}$$

Solving the linear equations (67) for I_1 and I_2 gives

$$I_\alpha=\frac{d\phi_\alpha}{dt}, \quad \phi_\alpha=\dot{s}^{-1/2}u_\alpha(s), \quad \alpha=1,2. \tag{68}$$

The constants J_1 and J_2 are then obtained from Eqs. (66) and (68) together with the normalization $I_1J_2-I_2J_1=1$. They are given by

$$J_\alpha=tI_\alpha-\phi_\alpha, \quad \alpha=1,2\,.$$

So, the I_α and J_α, taken to be functions of $t,s,\dot{s}$ and $\ddot{s}$ are first integrals for the Schwarzian equation. In terms of the Darboux–Halphen variables, these quantities are

$$\phi_\alpha=\sqrt{2r(\omega_i)}\,u_\alpha(s(\omega_i))\,, \quad I_\alpha=\sqrt{\frac{2}{r(\omega_i)}}\,u_\alpha'(s(\omega_i))-(\omega_1-\omega_2-\omega_3)\sqrt{\frac{r(\omega_i)}{2}}\,u_\alpha(s(\omega_i))\,,$$

where $r(\omega_i)=\sqrt{(\omega_2-\omega_3)/(\omega_1-\omega_2)(\omega_1-\omega_3)}$ and $s(\omega_i)$ is given by Eq. (57).

In terms of these variables, the Darboux–Halphen system (52) and (56) can be written as the Hamiltonian system

$$\dot{\phi}_\alpha=\frac{\partial H}{\partial I_\alpha}=I_\alpha\,, \quad \dot{I}_\alpha=-\frac{\partial H}{\partial\phi_\alpha}=0\,, \quad H=\frac{I_1^2+I_2^2}{2}, \quad \alpha=1,2, \tag{69}$$

subject to the algebraic constraint

$$\phi_1I_2-\phi_2I_1=W(u_1,u_2)=1. \tag{70}$$

The canonical coordinates $\{I_\alpha,\phi_\alpha\}$ are analogs of the action-angle variables for the Darboux–Halphen system. The phase space dynamics of the system is restricted to the constraint subspace

given by Eq. (70). This represents a three-dimensional complex quadric. Poisson–Nambu structures for the generalized Darboux–Halphen system (52) and (56) are presented in Ref. 17 which are similar to those for rigid body dynamics in three dimensions.[44,54] The system is also written as a gradient flow in Ref. 16.

A. The Chazy equation

Let ω_1, ω_2, ω_3 be a solution of (52) with $\tau=0$ and define $y:=-2(\omega_1+\omega_2+\omega_3)$. Then y is a solution of the equation[17,18]

$$\frac{d^3y}{dt^3}=2y\frac{d^2y}{dt^2}-3\left(\frac{dy}{dt}\right)^2, \tag{71}$$

which was studied by Chazy.[23–25] Furthermore, given a solution y of the Chazy equation (71), let ω_1, ω_2, and ω_3 be the three roots of the cubic equation

$$\omega^3+\frac{1}{2}y\omega^2+\frac{1}{2}\frac{dy}{dz}\omega+\frac{1}{12}\frac{d^2y}{dt^2}=0.$$

If the ω_j's are distinct, then they solve the classical Darboux–Halphen system [i.e., the system (52) with $\tau=0$].

The general solution of the Chazy equation is given by

$$y(t(s))=6\frac{d}{dt}\ln\chi_1(s),\quad t(s)=\chi_2(s)/\chi_1(s), \tag{72}$$

where χ_1 and χ_2 are two independent solutions of the special hypergeometric equation

$$s(1-s)\frac{d^2\chi}{ds^2}+\left(\frac{1}{2}-\frac{7}{6}s\right)\frac{d\chi}{ds}-\frac{1}{144}\chi=0.$$

On replacing χ_1 and χ_2 with the independent linear combinations $a\chi_1+b\chi_2$ and $c\chi_1+d\chi_2$, $ad-bc=1$, it can be seen from Eq. (72) that the Chazy equation admits the symmetry

$$y(t)\mapsto\tilde{y}(t)=(ct+d)^{-2}y\left(\frac{at+b}{ct+d}\right)-\frac{6c}{ct+d},\quad ad-bc=1. \tag{73}$$

As well as having a general solution in terms of special hypergeometric functions as described above, the Chazy equation (71) is related to the theory of modular functions.[8,53] Indeed, a particular solution of (71) is given by

$$y(t):=i\pi E_2(t), \tag{74}$$

where

$$E_2(t):=1+\frac{6}{\pi^2}\sum_{m=1}^{\infty}\sum_{n=-\infty}^{\infty}\frac{1}{(mt+n)^2} \tag{75}$$

is the second Eisenstein series. [Note that the series (75) is not absolutely convergent, so the order of the sum is important.] The second Eisenstein series can also be written as the Fourier series

$$E_2(t)=1-24\sum_{n=1}^{\infty}\sigma_1(n)q^n,\quad q=\mathrm{e}^{2\pi it},$$

where $\sigma_1(n)$ is the sum of the divisors of n.

Furthermore, the solution (74) can be written in terms of a special logarithmic potential,

$$y(t)=\frac{1}{2}\frac{d}{dt}\ln\Delta(t), \tag{76}$$

where Δ is the discriminant cusp form of weight 12, which satisfies

$$\Delta(\mu(t))=(ct+d)^{12}\Delta(t), \quad \mu\in \mathrm{PSL}(2;\mathbf{Z}). \tag{77}$$

This shows that there is a deep connection between the Chazy equation and the theory of modular forms.

The discriminant modular form has the well known representation

$$(2\pi)^{-12}\Delta(t)=q\prod_{n=1}^{\infty}(1-q^n)^{24}=\sum_{n=1}^{\infty}\tau(n)q^n,$$

where $q=\mathrm{e}^{2\pi it}$ and the coefficient function $\tau(n)$ is called the Ramanujan τ-function (see, e.g., Ref. 52). From Eqs. (76) and (74) it can be shown that Δ satisfies the homogeneous ODE of degree 4;

$$\Delta^3\frac{d^4\Delta}{dt^4}-5\Delta^2\frac{d\Delta}{dt}\frac{d^3\Delta}{dt^3}-\frac{3}{2}\Delta^2\left(\frac{d^2\Delta}{dt^2}\right)^2+12\Delta\left(\frac{d\Delta}{dt}\right)^2\frac{d^2\Delta}{dt^2}-\frac{13}{2}\left(\frac{d\Delta}{dt}\right)^4=0.$$

Rankin[51] first showed that the discriminant cusp form satisfies this equation. Since Δ has no zeros or poles and satisfies a homogeneous equation it is the natural analog of the τ function that appears in Hirota's method (see, e.g., Sec. 3.3 of Ref. 4).

Note that the characterization of the Ramanujan coefficients $\tau(n)$ is a major problem in number theory. These famous numbers arise naturally as the Fourier coefficients of $\Delta(t)$ when we write the Chazy equation in the above homogeneous form.

Furthermore, there is another important correspondence between the Chazy equation and Ramanujan's work. In 1916 Ramanujan[50] proved that the functions

$$P(q)=1-24\sum_{n=1}^{\infty}\sigma_1(n)q^n,$$

$$Q(q)=1+240\sum_{n=1}^{\infty}\sigma_3(n)q^n,$$

$$R(q)=1-504\sum_{n=1}^{\infty}\sigma_5(n)q^n,$$

where $\sigma_k(n)=\Sigma_{d|n}d^k$, $k=1,3,5$ (sum of the divisors of n to the kth power), satisfy

$$q\frac{dP}{dq}=\frac{1}{12}(P^2-Q),$$

$$q\frac{dQ}{dq}=\frac{1}{3}(PQ-R), \tag{78}$$

$$q\frac{dR}{dq}=\frac{1}{2}(PR-Q^2).$$

Using $q=e^{2\pi it}$, $\tau=\pi t$, the equations (78) take the form

$$\frac{dP}{d\tau}=\frac{i}{6}(P^2-Q),$$

$$\frac{dQ}{d\tau}=\frac{2i}{3}(PQ-R), \tag{79}$$

$$\frac{dR}{d\tau}=i(PR-Q^2).$$

Using the first of the above equations to find Q: $Q=P^2+6i\,dP/d\tau$, the second equation implies $R=-9(d^2P/d\tau^2)+9iP\,(dP/d\tau)+P^3$. Then the last of the above equations yields

$$\frac{d^3\tilde{y}}{d\tau^3}=2y\frac{d^2\tilde{y}}{d\tau^2}-3\left(\frac{d\tilde{y}}{d\tau}\right)^2,$$

where $P(q)=-i\tilde{y}(\tau)$. Finally, in terms of $\tilde{y}(\tau)=\pi^{-1}y(t)$, y satisfies the Chazy equation (71). Thus the special solution (74) yields $y(t)=i\pi E_2(t)=i\pi P(q)$. Knowing $P(q)$, from (78) we can obtain the other functions $Q(q)$ and $R(q)$ directly. Moreover, since we know the general solution of the Chazy equation, we know the general solution of the equations of Ramanujan. Note that Q and R are also called the normalized Eisenstein series E_4 and E_6 (see, e.g., Ref. 35).

As an historical postscript we note that Chazy and Ramanujan both worked on the same equation at nearly the same time, but apparently they did not know this!

B. The generalized Chazy equation

Let $(\omega_1,\omega_2,\omega_3)$ be a solution of (52)–(56). Ablowitz, Chakravarty, and Halburd[5,7] showed that

$$y:=-2(\omega_1+\omega_2+\omega_3)=-2\operatorname{Tr}M \tag{80}$$

solves

$$\frac{d^3y}{dt^3}-2y\frac{d^2y}{dt^2}+3\left(\frac{dy}{dt}\right)^2=\frac{4}{36-n^2}\left(6\frac{dy}{dt}-y^2\right)^2, \tag{81}$$

if and only if either $\alpha=\beta=\gamma=:2/n$ or exactly one of the parameters α, β, γ is $2/n$ and the other two are $\frac{1}{3}$. Equation (81) was also studied by Chazy[23–25] and is usually referred to as the *generalized Chazy equation* [to contrast it with the classical Chazy equation (71), which is the special case $n=\infty$].

It follows from Eqs. (58) and (80) that the general solution of (81) is given by

$$y(t)=\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{s}^6}{s^4(s-1)^4}. \tag{82}$$

In Chazy's analysis of Eq. (81) he showed that its solution is given by

$$y(t)=\frac{1}{2}\frac{d}{dt}\ln\frac{\dot{J}^6}{J^4(J-1)^3}, \tag{83}$$

where the Schwarz function J solves Eq. (59) with (60) and $\alpha=1/n$, $\beta=\frac{1}{3}$, $\gamma=\frac{1}{2}$. The function J, and hence y, is single-valued if n is an integer greater than 1. The choice $n=\infty$ again corresponds to the classical Chazy equation (71).

Equations (82) and (83) suggest that there is a relationship between J and the special Schwarzian triangle functions s described above. In the case when s corresponds to the choice $\alpha=\beta=\gamma=2/n$, it can be shown that

$$J=\frac{4}{27}\frac{(s^2-s+1)^3}{s^2(s-1)^2},$$

and, similarly, when $\alpha=2/n$, $\beta=\gamma=\frac{1}{3}$, we have

$$J=-4s(s-1)$$

(see Ref. 5).

VI. SUMMARY AND DISCUSSION

The SDYM equations are a rich source of integrable systems. The classical soliton equations in $1+1$ dimensions and the well known Painlevé quations P_I-P_{VI} are reductions of the SDYM equations with finite-dimensional Lie algebras. Reductions of the SDYM equations using infinite-dimensional algebras are of particular interest. They yield the classical $2+1$-dimensional soliton equations, the Chazy equations and a ninth-order generalization of the Darboux–Halphen system.

ACKNOWLEDGMENTS

This work was supported by NSF Grant No. DMS-007092 and Royal Society Grant No. 22204.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Topological phenomena in the real periodic sine-Gordon theory

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(Received 26 March 2003; accepted 9 April 2003)

The set of real finite-gap sine-Gordon solutions corresponding to a fixed spectral curve consists of several connected components. A simple explicit description of these components obtained by the authors recently is used to study the consequences of this property. In particular this description allows to calculate the topological charge of solutions (the averaging of the x-derivative of the potential) and to show that the averaging of other standard conservation laws is the same for all components. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1588742]

I. INTRODUCTION. ALGEBRO-GEOMETRICAL SOLUTIONS AND THE REALITY REDUCTIONS. THE TOPOLOGICAL CHARGE

The algebro-geometrical (or finite-gap) solutions play a very important role in the modern theory of soliton equations with periodic and quasiperiodic boundary conditions. The main property characterizing these solutions is the following: the wave function of the auxiliary linear operator is meromorphic in the spectral parameter on the finite part of an algebraic Riemann surface. This allows one to apply the powerful tools of classical algebraic geometry, and to write explicit representations for solutions and wave functions in terms of Riemann Θ-functions of several variables. Usually the algebro-geometrical solutions are dense in the space of the periodic ones, and if the nonlinearity tends to zero, they degenerate to finite Fourier sums. Therefore their role in the soliton theory is rather similar to the role of finite Fourier series for the linear PDEs.

The algebro-geometrical solutions of solition equations were first introduced in Ref. 1 in 1974 dedicated to the integration of the Korteveg–de Vries (KdV) equation with periodic boundary conditions. Real nonsingular periodic algebro-geometrical KdV solutions can be characterized by the following property: the number of gaps (forbidden bands or zones) in the spectrum of the auxiliary Schrödinger operator acting in the Hilbert space $L_2(R)$ is finite. This characterization is not valid for other systems [for example, the spectrum of non-self-adjoint auxiliary operator for the self-focusing nonlinear Schrödinger equation (NLS) has no gaps for any regular potential], but nevertheless the algebro-geometrical solutions are called finite-gap.

The complete theory of algebro-geometrical KdV solutions involving the spectral theory of periodic (quasiperiodic) finite-gap Schrödinger operators on the line and its unification with algebraic geometry and analysis on the Riemann surfaces, time dynamics and algebro-geometric hamiltonian aspects was constructed in Refs. 2–7 (see in the survey article, Ref. 8) and in Refs. 9 and 10. Complex finite-gap solutions of the NLS and sine-Gordon (SG) equations were constructed in Refs. 11 and 12. Finite-gap solutions of the $2+1$ Kadomtsev–Petviashvili (KP) eqation were constructed in Ref. 13 on a basis of a purely algebraic formulation of the finite-gap approach developed in this article. The algebro-geometric spectral theory of the stationary periodic 2D

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Schrödinger operator was developed in Refs. 14 and 15. In these papers it was shown that the proper analog of the finite-gap constraint in the two-dimensional case is the following: the restriction of the Bloch variety to one energy level is algebraic, and the spectral data is ''collected'' at this energy level only. Such potentials can be treated as ''integrable'' at one energy. It means that the wave functions for this energy and arbitrary complex quaismomenta can be written explicitly in terms of Riemann Θ-functions, but the information about the spectral properties at other energies is very restricted.

The algebro-geometrical approach allows us to obtain explicit compact formulas for solutions. But the Θ-functions of several variables are very complicated from the analytic point of view; therefore the existence of such formulas does not lead sometimes to the simple solution of the problem of selecting physically or geometrically meaningful solutions among generic complex ones. For example, it is very easy to describe reality conditions for the KdV, defocusing NLS or sinh-Gordon equation

$$\frac{\partial^2 u}{\partial \xi \partial \eta} = 4 \sinh u(\xi, \eta)$$

(in all these cases the auxiliary linear operators are self-adjoint). However, the reality reductions for the self-focusing NLS or the sine-Gordon equation found in Ref. 16 are rather nontrivial. It was shown in Ref. 15 that analogous reductions are responsible for the absence of magnetic field in the theory of the 2D Schrödinger operator. A good review of reality reductions can be found in Ref. 17.

The sine-Gordon equation

$$u_{tt} - u_{xx} + \sin u(x,t) = 0 \tag{1}$$

derived in the 19th century geometry in the light-cone representation

$$u_{\xi\eta} = 4 \sin u, \quad u = u(\xi, \eta), \tag{2}$$

where

$$x = 2(\xi + \eta), \quad t = 2(\xi - \eta), \quad \partial_\xi = 2\partial_x + 2\partial_t, \quad \partial_\eta = 2\partial_x - 2\partial_t \tag{3}$$

is one of the most important systems of the soliton theory. One of its distinguished properties is the folowing. Usually if we fix the spectral curve (or equivalently all local conservation laws), then the level set is a connected Jacobi torus. It is true for KdV, defocusing and self-focusing NLS and for both real reductions of the KP equation. But in the sine-Gordon case the level set is a union of 2^m real Jacobi tori, where m denotes the number of pairs of negative branch points. As a corollary, the result of averaging a generic functional depends not only on the spectral curve, but also on the component. This property is also essential if we calculate the action-angle variables (this problem was studied in Refs. 18 and 19).

The averaged densities of conservation laws arose naturally as Hamiltonians of the Whitham equations. These equations describe the evolution of parameters of the asymptotic solutions in the form of a slowly varying N-phase wavetrains. The Whitham equations for the sine-Gordon were derived in Ref. 20, but the connectivity components of the level sets were not discussed. Let us point out that the Whitham equations are hyperbolic only in the ''stable'' case, when all branch point are negative and the number of components is always greater than 1.

It is possible to extract from the calculations of Ref. 20 that for all classical local conservation laws except the topological charge the result of averaging is the same for all components, but this property was never pointed out explicitly. In Sec. IV we give a simple explanation of it.

Remark: The number of real tori was calculated in Ref. 16, and their characterization in terms of the complex Jacobi torus was obtained in Ref. 21, see also Ref. 22. An elementary description of these tori was obtained by the authors in Refs. 23 and 24 (see Sec. II below).

Another interesting property of the sine-Gordon equation is the following. In the theory of constant negative curvature surfaces $u(\xi,\eta)$ denotes the angle between asymptotic lines. In the theory of Josephson junctions u has the meaning of a phase. In both situations it is defined up to an additive constant $c=2\pi n$. Therefore, it is natural to call a solution $u(x,t)$ space-periodic with the period T if $\exp\{iu(x+T)\}=\exp\{iu(x)\}$. The integer n such that $u(x+T)=u(x)+2\pi n$ is called **topological charge**: the real number $\overline{n}=n/T$ denotes the **density of topological charge**. These quantities are the ''most stable'' conservation laws surviving all real periodic nonintegrable perturbations. The density of topological charge can be naturally extended to all nonsingular quasi-periodic solutions using the formula

$$\overline{n}=\lim_{T\to\infty}[u(x+T)-u(x)]/2\pi T.$$

One of the most natural problems is the following: *how to calculate the topological charge of real periodic SG solutions in terms of the spectral data: the Riemann surface and the divisor*. It turned out that nobody succeeded to extract the answer from the explicit description of the real components described in terms of the Jacobi torus and Θ-functional formulas, found in Refs. 21 and 22. An attempt was made almost 20 years ago in Ref. 18 to solve this problem. For this purpose the so-called ''Algebro-Topological'' approach was developed in Ref. 18, and an interesting formula was proposed. However, as it was pointed out in Ref. 19, the idea of the proof presented in Ref. 18 works only if the spectral curve is sufficiently close to a degenerate one. A complete solution using a new development of the main idea of Ref. 18 was obtained only recently by the authors in Refs. 23 (for the so-called stable curves) and 24 for generic ones. Our proof is based on a new effective description of the real components in terms of divisors. We present a summary of these results in Sec. III.

Remark: Formally we can define topological charge for any nonsingular complex solution. But if the solution has poles, this quantity became ill-defined, and no natural nonsingularity condition in terms of the spectral data for complex potentials is known. It explains why only real solutions are discussed.

II. FINITE-GAP SINE-GORDON SOLUTIONS

The ''soliton-type'' solutions of sine-Gordon were found already in the 19th century using substitution discovered by Bianchi and S. Lie. Now this method is called ''Backlund transformation.''

In the early 1970s G. Lamb found out (see Ref. 25) that the sine-Gordon equation is analogous to KdV in the following sense: the so-called ''inverse scattering method'' can be applied to it. The modern approach was started in Ref. 26. The critical point of this approach is the following zero-curvature representation for SG,

$$\Psi_x=\tfrac{1}{4}(U+V)\Psi,\quad \Psi_t=\tfrac{1}{4}(U-V)\Psi, \tag{4}$$

where

$$U=U(\lambda,x,t)=\begin{bmatrix} i(u_x+u_t) & 1 \\ -\lambda & -i(u_x+u_t)\end{bmatrix}, \tag{5}$$

$$V=V(\lambda,x,t)=\begin{bmatrix} 0 & -\dfrac{1}{\lambda}e^{iu} \\ e^{-iu} & 0.\end{bmatrix}. \tag{6}$$

To construct generic complex finite-gap SG solutions, assume that we have the following spectral data:

(1) A nonsingular hyperelliptic Riemann surface Γ $[\mu^2=R(\lambda)]$, where $R(\lambda)=\Pi_{k=0}^{2g}(\lambda-E_k)$, such that $E_0=0$ and $E_i\neq E_j, i,j=0,1,\ldots,2g$. It has exactly $2g+2$ branch points $E_0=0$, $E_1,\ldots,E_{2g},\infty$; the genus of Γ is equal to g. A point $\gamma\in\Gamma$ is by definition a pair of complex numbers $\gamma=(\lambda,\mu)$ such that $\mu^2=R(\lambda)$.
(2) A divisor D of degree g, i.e., set (or formal sum) of g points $D=\gamma_1+\cdots+\gamma_g$.

For generic data Γ,D there exists an unique two-component "Baker–Akhiezer" vector-function $\Psi(\gamma,x,t)$ such that the following hold.

(1) For fixed (x,t) the function $\Psi(\gamma,x,t)$ is meromorphic in the variable $\gamma\in\Gamma$ outside the points $0,\infty$ and has at most first order poles at the divisor points γ_k, $k=1,\ldots,g$.
(2) $\Psi(\gamma,x,t)$ has essential singularities at the points $0,\infty$ with the following asymptotics:

$$\Psi(\gamma,x,t)=\begin{pmatrix}1+o(1)\\ i\sqrt{\lambda}+O(1)\end{pmatrix}e^{i\sqrt{\lambda}(x+t)/4}\quad\text{as}\quad\lambda\to\infty, \tag{7}$$

$$\Psi(\gamma,x,t)=\begin{pmatrix}\phi_1(x,t)+o(1)\\ i\sqrt{\lambda}\phi_2(x,t)+O(\lambda)\end{pmatrix}e^{-(i/\sqrt{\lambda})[(x-t)/4]}\quad\text{as}\quad\lambda\to 0, \tag{8}$$

where $\phi_1(x,t)$, $\phi_2(x,t)$ are some functions of the variables x,t.

Denote the divisor of zeros of the first component ψ_1 by $D(x,t)=\Sigma_j\gamma_j(x,t)$. The vector-function $\Psi(\gamma,x,t)$ satisfies to the zero-curvature equations (4) with potential given by the formula

$$u(x,t)=i\ln\frac{\phi_2(x,t)}{\phi_1(x,t)}, \tag{9}$$

and the function $u(x,t)$ solves the SG equation (2). In terms of the divisor of zeros $D(x,t)$ the potenital $u(x,t)$ can be easily written explicitly:

$$e^{iu(x,t)}=\frac{\Pi_{j=1}^{g}(-\lambda_j(x,t))}{\sqrt{\Pi_{j=1}^{2g}E_j}}. \tag{10}$$

The x and t dynamics of the divisor $D(x,t)$ can be described in terms of Dubrovin equations (see Ref. 24). From (10) it follows that the potential $u(x,t)$ is singular at the point (x_0,t_0) if and only if one of the points $\gamma_k(x_0,t_0)$ coincides with 0 or ∞. Collisions of two or more divisor points result in singularities in the solutions of Dubrovin equations, but all symmetric combinations of the divisor points including the potential $u(x,t)$ remain nonsingular.

Remark: The first component ψ_1 of the Baker–Akhiezer vector-function Ψ is a partial case of the general scalar two-point Baker–Akhiezer functions satisfying to the second order linear Schrödinger equation $L_1\psi_1=0$ invented in Ref. 14. Here we have

$$L_1=\frac{\partial^2}{\partial\xi\partial\eta}+A(\xi,\eta)\frac{\partial}{\partial\eta}+W(\xi,\eta),$$

$-A=\partial_\xi\log\phi_1$. In this special case our surface Γ is hyperelliptic, the selected points coincide with $0,\infty$ and corresponding local parameters are chosen as $\sqrt{\lambda},1/\sqrt{\lambda}$. The second function ψ_2 satisfies to similar equation $L_2\psi_2=0$ where the operator L_2 is obtained from L_1 by the so-called Laplace transformations and vice versa. It is known that cyclic Laplace chains of length 2 lead to the SG equation in the general complex case (see Ref. 27).

Lemma 1: Assume that the spectral data (Γ,D), $D=\gamma_1+\cdots,\gamma_g$ *satisfy the following reality constraints*:

(1) The set of branch points of the Riemann surface Γ *contains real points or complex conjugate pairs of points only, and all real branch points are nonpositive. Without loss of generality we*

may assume that the first $2m+1$ *of them,* $E_0=0$, E_1, E_2, $\ldots$, E_{2m}, *are real and* $0>E_1>E_2>\cdots>E_{2m}$, *and for* $k>m$ *we have* $E_{2k}=\overline{E}_{2k-1}$, $\operatorname{Im} E_{2k}\neq 0$. *Then the spectral curve* Γ *is real and admits a* $\mathbb{Z}_2\times\mathbb{Z}_2$*-group of involutions generated by the standard holomorphic involution*

$$\sigma:\Gamma\to\Gamma: \quad \sigma(\lambda,\mu)=(\lambda,-\mu), \tag{11}$$

transposing the sheets, and by the antiholomorphic involution

$$\tau:\Gamma\to\Gamma: \quad \tau(\lambda,\mu)=(\overline{\lambda},\overline{\mu}) \tag{12}$$

(*complex conjugation*).

(2) *There exists a meromophic differential* Ω *with two simple poles at the points* $0,\infty$ *such that the zeros of* Ω *are located at the points* $D+\tau D$. *We shall call such divisors* **admissible**. *Without loss of generality we can normalize* Ω *to be real*: $\tau\Omega=\overline{\Omega}$.

Then the potential $u(x,t)$ *is real and nonsingular*.

Remark: The constraints on the spectral curve were found in Ref. 12. The characterization of admissible divisors and the proof of nonsingularity were obtained in Ref. 16.

It is easy to check (see, for example, Ref. 24)

Lemma 2: If D *is an admissible divisor, then the divisor of zeros* $D(x,t)=\gamma_1(x,t)+\cdots+\gamma_g(x,t)$ *is admissible for all* x,t

Assume that we have a real meromorphic differential Ω with exactly two simple poles at the points $0,\infty$. We can associate an admissible divisor D to it if and only if $2g$ zeros of Ω can be presented as a union of two subsets D and D_1 such that $D_1=\tau D$. It is possible if and only if all real roots of Ω have even multiplicity.

Definition 1: Assume that the spectral curve Γ *satisfies the reality conditions formulated above. A real meromorphic differential* Ω *on* Γ *with exactly two simple poles at the points* $0,\infty$ *is called* **admissible** *if the multiplicity of all real roots is even.*

Without loss of generality we may assume that the residues of Ω at the points 0 and ∞ are equal to $+1$ and -1, respectively. Then we have

$$\Omega=\left(1-\frac{\lambda P_{g-1}(\lambda)}{R(\lambda)^{1/2}}\right)\frac{d\lambda}{2\lambda}, \tag{13}$$

where $P_{g-1}(\lambda)$ is a polynomial of degree at most $g-1$ with real coefficients. Let us call the polynomial $P_{g-1}(\lambda)$ **admissible** if Ω is an admissible differential.

Denote the map associating an admissible polynomial with an admissible divisor by $\Pi:D\to P_{g-l}(\lambda)$. The inverse map Π^{-1} is multivalued. If $P_{g-1}(\lambda)$ is an admissible polynomial, then the equation

$$\begin{aligned}\mu&=\lambda P_{g-1}(\lambda),\\ R(\lambda)&=\mu^2\end{aligned} \tag{14}$$

has $2g+1$ roots. One of them is the point (0,0), the other $2g$ roots form g pairs. To define an admissible divisor we have to choose one point from each pair: therefore we have at most 2^g possibilities depending on the number of real points. In the generic case we have no real roots, so the number is equal to 2^g in this case.

The description of connected components suggested by the authors in Refs. 23 and 24 is based on the following simple observation:

Consider a pair of functions of the real variable λ:

$$f_{\pm}(\lambda)=\pm\frac{\sqrt{R(\lambda)}}{\lambda}. \tag{15}$$

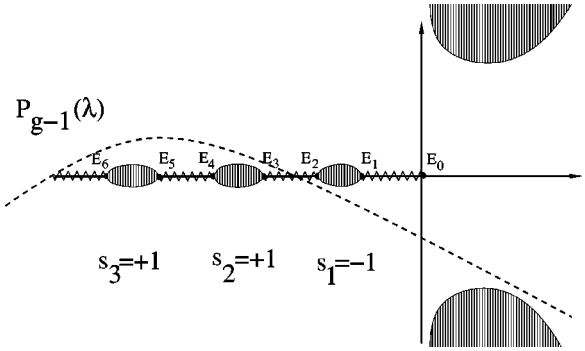

FIG. 1. The graph of $P_{g-1}(\lambda)$ and the forbidden domains.

We assume that the functions $f_{\pm}(\lambda)$ are defined only for such $\lambda \neq 0$ that $R(\lambda) \geqslant 0$, i.e., these functions are real-valued. Let us draw the graphs of these functions $y=f_{+}(\lambda)$, $y=f_{-}(\lambda)$, and fill in the following domains (see Fig. 1):

$$\lambda<0, y^2<\frac{R(\lambda)}{\lambda^2}, \qquad \lambda>0, y^2>\frac{R(\lambda)}{\lambda^2}. \tag{16}$$

Lemma 3: The polynomial $P_{g-1}(\lambda)$ is admissible if and only if the graph of $P_{g-1}(\lambda)$ does not cross the black open domains (but it can touch their boundaries).

Now we can associate with each admissible polynomial a **topological type**, i.e., a collection of m numbers $s_k=\pm 1$, $k=1,\ldots,m$, defined by the following rule:

$$s_k=1 \text{ if } P_{g-1}(\lambda) \geqslant f_{+}(\lambda) \text{ as } E_{2k} \leqslant \lambda \leqslant E_{2k-1},$$

$$s_k=-1 \text{ if } P_{g-1}(\lambda) \leqslant f_{-}(\lambda) \text{ as } E_{2k} \leqslant \lambda \leqslant E_{2k-1}.$$

Using simple algebraic estimates (see Ref. 24) it is easy to check:

Lemma 4: Each topological type is presented by the convex subset in the space of polynomials P_{g-1}. Each of these 2^m connected components is nonempty and depends continuously on the branch points $E_1,\ldots,E_{2g}$.

The x and t dynamics of admissible divisors may be rather nontrivial (a number of numeric experiments are discussed in Ref. 22). In contrast with the self-adjoint case (KdV, defocusing NLS, sinh-Gordon) the admissible position of a given divisor point depends on the position of other ones (the admissibility constraints are nonlocal). The trajectory of a single divisor point may be not well-defined because divisor points may collide and a small variation of parameters near the collision point results in a bifurcation of trajectories. If the potential $u(x,t)$ is periodic with the period T, the corresponding divisor is generically periodic only modulo permutations. But the following properties can be easily proved using the characterization formulated above.

Lemma 5: Projections of the points of admissible divisors to the λ-plane could not lie in the segments $[E_1,E_0]$, $[E_3,E_2]$, $\ldots,(-\infty,E_{2m}]$. Moreover, it is possible to choose an open neighborhood of these segments such that the projections of these points could not lie in it.

Lemma 6: Assume that the projection of a point $\gamma_s=(\lambda_s,\mu_s)$ of an admissible divisor to the λ-plane lie in the segments $[E_{2k},E_{2k-1}]$; then $\mu_s<0$ if $s_k=1$ and $\mu_s>0$ if $s_k=-1$.

III. THE TOPOLOGICAL CHARGE OF REAL SOLUTIONS

It is well-known (see, for example, Refs. 21 and 22) that after the Abel transform the x-dynamics of sine-Gordon corresponds to the motion along the straight line

$$\vec{X}=\vec{X}_0+\vec{U}x, \tag{17}$$

in the Jacobi torus, where $\vec{U}$ denotes the noramalized vector of b-periods of the quasimomentum differential dp:

$$U^k=-\frac{1}{2\pi}\oint_{b_k} dp. \tag{18}$$

Let us recall that by definition dp is a meromorphic differential with zero a-periods and two second order poles at 0, ∞ such that

$$dp=\begin{cases}\left(\dfrac{1}{8\sqrt{\lambda}}+o\left(\dfrac{1}{\lambda}\right)\right)d\lambda \quad \text{as} \quad \lambda\to\infty,\\ \left(\dfrac{1}{8\lambda\sqrt{\lambda}}+o\left(\dfrac{1}{\lambda}\right)\right)d\lambda \quad \text{as} \quad \lambda\to 0.\end{cases} \tag{19}$$

The real part of the Jacobi torus is isomorphic to the factor $\mathbb{R}^n/\mathbb{Z}^n$, therefore we can apply the following simple analytic lemma:

Lemma 7: Let $u(\vec{X}), X\in\mathbb{R}^n$ *be a smooth function in* $\mathbb{R}^n$ *such that* $\exp(iu(\vec{X}))$ *is single-valued on the torus* $\mathbb{R}^n/\mathbb{Z}^n$, *i.e.*, $\exp(iu(\vec{X}+\vec{N}))=\exp(iu(\vec{X}))$ *for any integer vector* $\vec{N}$. *Denote by* $u(x)$ *restriction of* $u(\vec{X})$ *to the straight line* $\vec{X}=\vec{X}_0+x\cdot\vec{U}$. *Then the density of topological charge* $\overline{n}=\lim_{T\to\infty}[u(x+T)-u(x)]/2\pi T$ *is well-defined; it does not depend on the point* $\vec{X}_0$ *and can be expressed by the following formula:*

$$\overline{n}=\sum_{k=1}^{n} n_k U^k, \tag{20}$$

where $\vec{U}=(U^1,U^2,\ldots,U^n)$, *and* n_k *are topological charges along the basic cycles* $\mathcal{A}_k, k=1,\ldots,n$:

$$u(X^1,X^2,\ldots,X^k+1,\ldots,X^n)-u(X^1,X^2,\ldots,X^k,\ldots,X^n)=2\pi n_k. \tag{21}$$

The main step is the calculation of the charges along the basic cycles $\mathcal{A}_k$. To obtain a convenient answer the choice of canonical basis is very important. For **stable** surfaces (surfaces without complex branch points) the proper system of a-cycles was constructed in Ref. 18.

We work with the following system of cuts $[E_1,E_0],[E_3,E_2],\ldots,(-\infty,E_{2g}]$. Let us denote the sheet containing the line $\lambda\in\mathbb{R},\lambda>0$ $\mu>0$ by G_+ and the second sheet by G_- (see Fig. 2).

For the generic real curves with $2m$ negative branch points $E_1,\ldots,E_{2m}$ and $g-m$ complex adjoint pairs $E_{2j-1},E_{2j}=\overline{E}_{2j-1}$, $j=m+1,\ldots,g$, we choose first m a-cycles exactly as in the stable case. The last $g-m$ a-cycles should be chosen as coverings on Γ over the path on the λ-plane connecting the points E_{2j-1} and E_{2j} for $j>m$. All these paths should not meet each other. All of them should cross positive part of the line $\lambda>0$ in one point κ_j (i.e., in two points of Riemann surface) such that $\kappa_{m+1}<\kappa_{m+2}<\cdots<\kappa_g$. This basis depends on the order of the complex conjugate pairs only (see Fig. 3).

We assume also that the cycles $b_1,b_2,\ldots,b_m$ are the ovals lying over the segments $[E_2,E_1]$, $[E_4,E_3]$, $[E_{2m},E_{2m-1}]$, respectively.

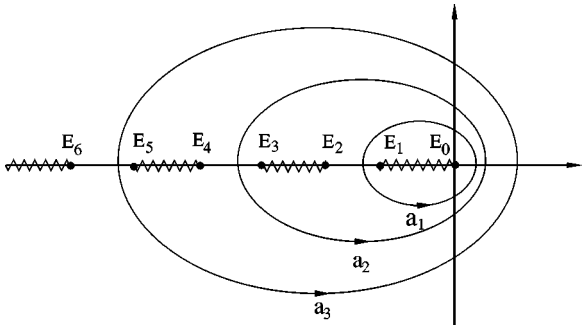

FIG. 2. The basic *a*-cycles: the stable case.

For the complex conjugate pairs of branch points $E_{2j},E_{2j-1},j>m$, we make the cuts connecting each of these points with $i\infty$ or $-i\infty$ such that the cuts do not intersect the real line. As before we denote the sheet containing the line $\lambda\in\mathbb{R},\lambda>0$ $\mu>0$ by G_+ and the second sheet by G_-. The orientation of the cycles $b_l,l=1,\ldots,m$, coincides with the standard orientation of the negative semi-line $\mathbb{R}_-$ at the sheet G_+; they are opposite at the sheet G_-.

Consider a basic cycle $\mathcal{A}_k$ on the real component of Jacobi torus, represented by the closed curve B_k on this torus. The image of this cycle in the surface Γ (i.e., image of it under the inverse Abel map) is a closed oriented curve C_k (may be consisting from several connected components) homological to the cycle $a_k\in H_1(\Gamma,\mathbb{Z})$. From Lemma 5 it follows that this curve does not touch the closed segments on the real line $[-\infty,E_{2m}],\ldots,[E_3,E_2],[E_1,0]$, and if it crosses the negative semi-line at the inteval $[E_{2l},E_{2l-1}]$, then it happens in the sheet G_+ if $(-1)^{l-1}s_l>0$ and in the sheet G_- if $(-1)^{l-1}s_l<0$. From formula (10) it follows that the topological charge along the cycle $\mathcal{A}_k$ is given by

$$n_k=\tilde{C}_k\circ\mathbb{R}_-, \tag{22}$$

where $\tilde{C}_k$ is the projection of C_k to the λ-plane, and $\circ$ denotes the intersection index of curves on the λ-plane. Taking into account that any intersection with the negative semi-line is the intersection with one of the *b*-cycles we obtain the following.

Lemma 8: The topological charge along the cycle $\mathcal{A}_k$ on the real torus in the Jacobian variety is equal to the intersection index of the corresponding curve C_k with the **counting cycle of the real component** *on the Riemann surface* Γ,

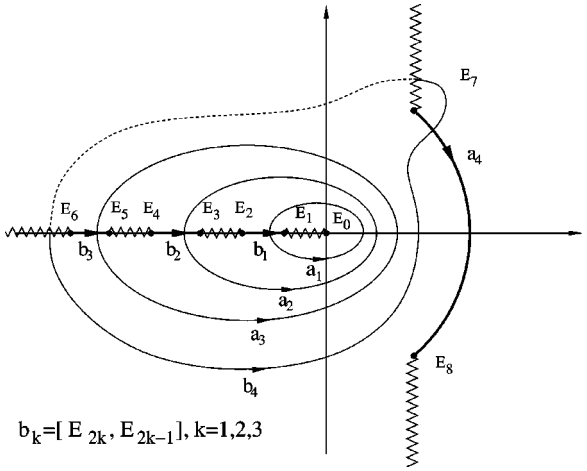

FIG. 3. The basic cycles: the generic case.

$$n_k = C_k \circ \left(\sum_{l=1}^{m} (-1)^{l-1} s_l b_l \right). \tag{23}$$

Let us mention that the cycle C_k is homotopic to a_k on Γ. Therefore $C_k \circ b_l = \delta_{kl}$ and

$$\begin{gathered} n_k = (-1)^{k-1} s_k \quad \text{for } k \leqslant m, \\ n_k = 0 \quad \text{for } k > m. \end{gathered} \tag{24}$$

Combining (20) with (24), we obtain our main result:

Theorem 1: *For any real solution the density of topological charge along the variable x is given by the formula*

$$\overline{n} = \frac{1}{2} \sum_{k=1}^{m} (-1)^{k-1} s_k U^k, \tag{25}$$

where the components U^k of the vector $\vec{U}$ are defined by (18).

IV. AVERAGING OF THE LOCAL CONSERVATION LAWS AND TOPOLOGICAL TYPES

For a generic functional

$$F[u] = \int f(e^{iu}, e^{-iu}, u_x, u_{xx}, \ldots, u_t, u_{tx}, u_{txx}, \ldots) dx \tag{26}$$

the result of averaging over a real componet of the Jacobi torus depends on the topolgical type. For example, by averaging of u_x we get the topological charge. But if we average the sine-Gordon Hamiltonian

$$H[u] = \int \left[\frac{u_t^2}{2} + \frac{u_x^2}{2} + (1 - \cos(u)) \right] dx, \tag{27}$$

the result is the same for all components. Therefore it is natural to formulate the following:

Problem: How to characterize the functionals such that the averaging does not depend on the topological type.

A complete classification seems to be a complicated problem. But it is rather easy to formulate a natural sufficient condition.

If $f(e^{iu}, e^{-iu}, u_x, u_{xx}, \ldots, u_t, u_{tx}, u_{txx}, \ldots)$ is a polynomial of its arguments, then it can be written as a symmetric rational function of the divisor coordinates $f = \tilde{f}(\lambda_1(x,t), \ldots, \lambda_g(x,t), \mu_1(x,t), \ldots, \mu_g(x,t))$.

Lemma 9: Consider the following form on the $\underbrace{\Gamma \times \Gamma \times \cdots \times \Gamma}_{g \text{ times}}$

$$W_f = \tilde{f}(\lambda_1, \ldots \lambda_g, \mu_1, \ldots, \mu_g) \prod_{k<l} (\lambda_k - \lambda_l) \prod_{k=1}^{g} \frac{d\lambda_k}{\mu_k}. \tag{28}$$

If we fix all divisor points except γ_1, we obtain a meromorphic differential on Γ with poles only at 0 and ∞. Assume that the residues of this differential are equal to 0 identically in $\gamma_2, \ldots, \gamma_g$. Then for a given spectral curve the averaging does not depend on the topological type.

Proof: Following Ref. 20 we can calculate the averaging of $F[u]$ using the formula

$$\overline{F[u]} = C \oint_{a_1} \cdots \oint_{a_g} W_f, \tag{29}$$

where C is the normalization constant, and **all cycles a_k have the proper topological type**. The last condition was not discussed in Ref. 20. The deformations of the integration cycles do not affect the integral if we do not cross 0. If the condition of Lemma 9 is fulfilled, then we can move the integration path through 0 and ''reach'' any topological type without changing the integral.

As a corollary we immediately get the following statement:

Theorem 2: *Assume that the functional $F[u]$ is invariant with respect to the following symmetries*: $\sigma_k:(\lambda_k,\mu_k)\to(\lambda_k,-\mu_k)$, $\sigma_k:(\lambda_l,\mu_l)\to(\lambda_l,\mu_l)$ *for* $l\neq k$. *Then the result of averaging does not depend on the topological type.*

Important example: Consider the densities of ''higher SG Hamiltonians'' defined as odd expansion coefficients of the function

$$\frac{\Psi_x(\lambda,x,t)}{\Psi(\lambda,x,t)} \tag{30}$$

at the points 0 and ∞. Direct calculation shows that

$$\frac{\Psi_x}{\Psi} = \frac{1}{4}\left[\frac{\Psi_\xi}{\Psi} + \frac{\Psi_\eta}{\Psi}\right], \tag{31}$$

where

$$\frac{\Psi_\xi}{\Psi} = i\frac{\mu + Q^\xi(\lambda)}{(\lambda-\lambda_1(x,t))\cdots(\lambda-\lambda_g(x,t))}, \tag{32}$$

$$\frac{\Psi_\eta}{\Psi} = i\frac{[\mu+\lambda Q^\eta(\lambda)][-\lambda_1(x,t),\ldots,(-\lambda_g(x,t))]}{\lambda(\lambda-\lambda_1(x,t))\cdots(\lambda-\lambda_g(x,t))\sqrt{E_1\cdots E_{2g}}}, \tag{33}$$

and $Q^\xi(\lambda)$, $Q^\eta(\lambda)$ are polynomials of degree $g-1$ determined by the following conditions:

$$Q^\xi(\lambda_k(x,t)) = \mu_k(x,t), \quad Q^\eta(\lambda_k(x,t)) = \frac{\mu_k(x,t)}{\lambda_k(x,t)}. \tag{34}$$

We see that the odd part of $\Psi_x\Psi^1$ depends on $\lambda_k(x,t)$ but not $\mu_k(x,t)$. Therefore the averaging of the ''higher SG Hamiltonians'' does not depend on the topological type.

P.G.G. was partially supported by the RFBR Grant No. 01-01-00874-A. Numerical simulations were partially performed on a computer, donated to PGG by the Humboldt Foundation. S.P.N. was partially supported by NSF Grant No. DMS 0072700.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Generation of asymptotic solitons of the nonlinear Schrödinger equation by boundary data

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(Received 15 December 2002; accepted 9 April 2003)

This article is about the focusing nonlinear Schrödinger equation on the half-line. The initial function vanishes at infinity while boundary data are local perturbations of periodic or quasi-periodic (finite-gap) functions. We study the corresponding scattering problem for the Zakharov–Shabat compatible differential equations, the representation of the solution of the nonlinear Schrödinger equation in the quarter of the (x,t)-plane through functions, which satisfy Marchenko integral equations. We use this formalism to investigate the asymptotic behavior of the solution for large time. We prove that under certain conditions a periodic (quasi-periodic) behavior at infinity of boundary data generates an unbounded train of asymptotic solitons running away from the boundary. The asymptotics of the solution shows that boundary data with periodic behavior as time tends to infinity generates a train of such asymptotic solitons even in the case when the initial function is identically zero. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1588465]

I. INTRODUCTION

The nonlinear Schrödinger equation is one of the most important completely integrable nonlinear equations. It has various applications in nonlinear optics, hydrodynamics, quantum field theory, etc. After the Korteweg–de Vries equation, the nonlinear Schrödinger equation was the second for which an inverse scattering transform was discovered by V. E. Zakharov and A. B. Shabat.[41,42] During the next three decades the nonlinear Schrödinger equation was studied by a large number of researchers of different orientation ranging from pure mathematics to applied physics. We mention only some results related to the Cauchy problem for the nonlinear Schrödinger equation on the whole line with initial functions vanishing at infinity.[16] The solvability of the Cauchy problem was proved and a representation for the solution was obtained via the Gelfand–Levitan–Marchenko equation or, alternatively, via the solution of a Riemann–Hilbert problem for an analytic matrix-valued function. It was also proved that the nonlinear Schrödinger equation with vanishing initial data is a completely integrable infinite-dimensional Hamiltonian system.

In the last decade there has been an increase activity in the investigation of initial boundary value problems on the half line. Among publications,[2–14,17–25,29–40] devoted to this problem, the more interesting and significant results were obtained by A. S. Fokas[18] and A. S. Fokas and A. R. Its.[22] Below we will use a modification of this approach. In the framework of the Fokas–Its approach we recently found characteristic properties of the scattering data for the compatible Zakharov–Shabat eigenvalue problem associated with focusing and defocusing nonlinear Schrödinger equations on the half-axis with initial and boundary functions of Schwartz type.[9]

In this article we consider a more complicated problem where boundary data have a periodic or quasi-periodic behavior as t tends to infinity. Our main goal is to study the asymptotic behavior

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of a solution. To the best of our knowledge such a problem was not considered elsewhere. So, we consider the Dirichlet and/or the Neumann initial-boundary value problem for the focusing nonlinear Schrödinger equation:

$$iq_t+q_{xx}+2|q|^2q=0, \quad \text{with} \quad x,t\in\mathbb{R}_+, \tag{1.1}$$

$$q(x,0)=u(x), \quad \text{with} \quad x\in\mathbb{R}_+, \tag{1.2}$$

$$q(0,t)=v(t) \quad \text{or} \quad q_x(0,t)=v_1(t) \quad \text{with} \quad t\in\mathbb{R}_+, \tag{1.3}$$

$$u(0)=v(0) \qquad \text{or} \quad u_x(0)=v_1(0), \tag{1.4}$$

where $u(x)$ vanishes as $x\to\infty$, and the boundary values are perturbations

$$v(t)=\alpha(t)+\hat{v}(t), \quad \hat{v}(t)\to 0, \quad t\to+\infty, \tag{1.5}$$

$$v_1(t)=\beta(t)+\hat{v}_1(t), \quad \hat{v}_1(t)\to 0, \quad t\to+\infty \tag{1.6}$$

of "finite-gap" functions $\alpha(t)$ and $\beta(t)$, which are periodic or quasi-periodic. The functions $\hat{v}(t)$ and $\hat{v}_1(t)$ vanish at $+\infty$. The definition of "finite-gap" functions $\alpha(t)$ and $\beta(t)$ will be given later.

We assume that the solution $q(x,t)$ of the NLS equation for $x,t\in\mathbb{R}_+$ is infinitely differentiable, continuous with all its derivatives up to the boundary $\{x=0\}\cup\{t=0\}$ of the quarter xt-plane and $q(x,t)\in\mathcal{S}(\mathbb{R}_+)$ in x for any fixed $t\in\mathbb{R}_+$, where $\mathcal{S}(\mathbb{R}_+)$ is the space of infinitely differentiable functions on $\mathbb{R}_+$ such that derivatives of any order $n\geqslant 0$ vanish at infinity faster than any negative power of x:

$$\mathcal{S}(\mathbb{R}_+)=\{u(x)\in C^\infty(\mathbb{R}_+)\,|\,x^m u^{(n)}(x)\in L^\infty(\mathbb{R}_+) \quad \text{for any} \quad m,n\geqslant 0\}.$$

They will be referred as "Schwartz functions." So the initial function $u(x)$ and $\hat{v}(t)$, $\hat{v}_1(t)$ are of Schwartz type. Standard notations will be used throughout the article:

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix}, \quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix}, \quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Our study of the solution $q(x,t)$ is based on simultaneous spectral analysis of two eigenvalue problems, one for the linear x-equation

$$\begin{gathered} w_x+ik\sigma_3 w=Q(x,t)w,\\ Q(x,t)=\begin{pmatrix}0&q(x,t)\\-\overline{q}(x,t)&0\end{pmatrix}, \end{gathered} \tag{1.7}$$

the other for the linear t-equation

$$\begin{gathered} w_t+2ik^2\sigma_3 w=\hat{Q}(x,t,k)w,\\ \hat{Q}(x,t,k)=2kQ(x,t)-i(Q^2(x,t)+Q_x(x,t))\sigma_3. \end{gathered} \tag{1.8}$$

Equations (1.7) and (1.8) are the well-known Zakharov–Shabat,[41] or Ablowitz–Kaup–Newel–Segur,[1] system of linear equations associated to q. Both equations are compatible if and only if $q(x,t)$ satisfies the nonlinear Schrödinger equation (1.1).

The main goal of this article is to study the scattering problem for compatible differential equations (1.7) and (1.8), the representation of the solution $q(x,t)$ through functions satisfying Marchenko integral equations, and the asymptotic behavior of $q(x,t)$ as $t\to+\infty$. We prove that

the principal (nonvanishing) part of the asymptotics is a series of asymptotic solitons. The asymptotics of the solution shows that boundary functions $v(t)$ or $v_1(t)$ with periodic behavior at infinity generate a train of such solitons even in the case when the initial data $u(x)$ vanish identically.

Now let us introduce the so-called *finite-gap functions* $\alpha(t)$ and $\beta(t)$. We refer to the Appendix for more details.

Let $\mathcal{X}$ be the hyperelliptic Riemann surface of genus g given by the equation

$$z^2=\prod_{j=0}^{g}(k-E_j)(k-\overline{E_j}),$$

with $E_j\in\mathbb{C}$, $\operatorname{Im}E_j>0$, $E_i\neq E_j$ for $i\neq j$, and $\operatorname{Re}E_0\leqslant\operatorname{Re}E_1\leqslant\cdots\leqslant\operatorname{Re}E_g$. $\mathcal{X}$ is a double covering of the complex k-plane $\overline{\mathbb{C}}=\mathbb{C}\cup\{\infty\}$ obtained by gluing two copies of $\overline{\mathbb{C}}$ along cuts γ_j whose endpoints are the $2g+2$ branch points E_j, $\overline{E_j}$. Let

$$\pi:\mathcal{X}\to\overline{\mathbb{C}}$$

be the canonical projection on the k-plane. Each point in the k-plane has two preimages on $\mathcal{X}$, except for the $2g+2$ branch points. Denote the preimage of $k=\infty$ on the upper (lower) sheet of $\mathcal{X}$ by $\mathcal{P}=\infty^+$ (respectively $\mathcal{P}=\infty^-$). We fix the branch of the square root by relation

$$\sqrt{\prod_{j=0}^{g}(k-E_j)(k-\overline{E_j})}=\pm k^{g+1}[1+\mathrm{O}(k^{-1})],\quad k\to\infty^{\pm}\in\mathcal{X}_{\pm}. \tag{1.9}$$

Let $D=\mathcal{P}_1+\cdots+\mathcal{P}_g$ be a nonspecial integral divisor on $\mathcal{X}\setminus\{\infty^+,\infty^-\}$ and let $\phi(t,\mathcal{P})$ be the Baker–Akhiezer vector function on $\mathcal{X}$ whose divisor of poles is D. That means

(i) $\phi(t,\mathcal{P})$ is meromorphic on $\mathcal{X}\setminus\{\infty^+,\infty^-\}$ with divisor of poles D; and
(ii) the product $\phi(t,\mathcal{P})\exp\{2\,\mathrm{i}k^2(\mathcal{P})t\}$ is analytic in the neighborhoods of $\infty^{\pm}$.

The Baker–Akhiezer vector-function satisfies the following equation:[28]

$$\phi_t+2\mathrm{i}k^2\sigma_3\phi=\hat{Q}_g(t,k)\phi, \tag{1.10}$$

where $k=\pi(\mathcal{P})$ is the canonical projection of $\mathcal{P}\in\mathcal{X}$ on the complex k-plane and

$$\hat{Q}_g(t,k)=2kQ_g(t)-\mathrm{i}(Q_g^2(t)+Q_{1g}(t))\sigma_3,$$

$$Q_g(t)=\begin{pmatrix}0 & \alpha(t)\\ -\overline{\alpha}(t) & 0\end{pmatrix},\quad Q_{1g}(t)=\begin{pmatrix}0 & \beta(t)\\ -\overline{\beta}(t) & 0\end{pmatrix}.$$

Definition: $\alpha(t)$ and $\beta(t)$ are called *finite-gap* if (1.10) has a solution which is a Baker–Akhiezer vector-function on some hyperelliptic Riemann surface $\mathcal{X}$ of finite genus.

The explicit representation of $\phi(t,\mathcal{P})$ given in the Appendix yields corresponding representations for $\alpha(t)$ and $\beta(t)$ through theta functions which leads to their periodicity or quasiperiodicity in $t\in\mathbb{R}$.

A. First case: Re $E_0<0$

So, $E_0=\mathrm{i}a-b$ with $a>0$ and $b>0$. Assume the solution $q(x,t)$ of the Dirichlet or Neumann problem (1.1)–(1.6) exists and satisfies the smoothness assumptions mentioned above. Then we prove that

$$q(x,t)=2\overline{K}_2(x,x,t), \tag{1.11}$$

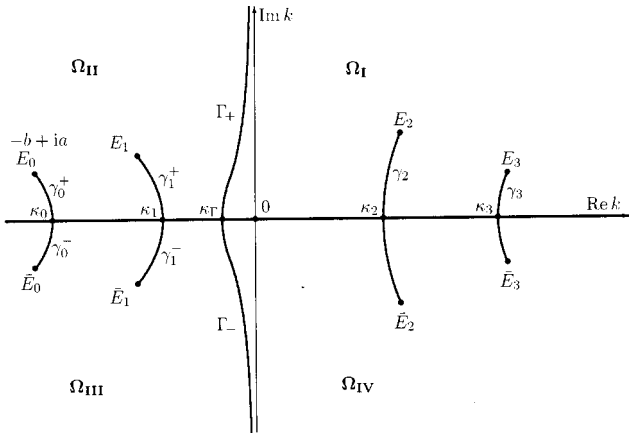

FIG. 1. Spectrum Σ of (1.10).

where $\overline{K}_2(x,y,t)$ together with some $K_1(x,y,t)$ satisfy the linear integral Marchenko equations:

$$K_1(x,y,t)-\int_x^\infty \overline{K}_2(x,z,t)H(z+y,t)\mathrm{d}z=0 \quad \text{for} \quad 0\leqslant x<y<\infty, \tag{1.12}$$

$$\overline{K}_2(x,y,t)+\overline{H}(x+y,t)+\int_x^\infty K_1(x,z,t)\overline{H}(z+y,t)\mathrm{d}z=0 \tag{1.13}$$

with kernel

$$H(x,t)=\sum_{k_j\in\Omega_I} m_j^1 \mathrm{e}^{\mathrm{i}k_j x+4\mathrm{i}k_j^2 t}+\sum_{z_j\in\Omega_{II}} m_j^2 \mathrm{e}^{\mathrm{i}z_j x+4\mathrm{i}z_j^2 t}+\frac{1}{2\pi}\int_{\partial\Omega_{II}} c(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2 t}\mathrm{d}k$$
$$+\frac{1}{2\pi}\int_{-\infty}^{\infty} r(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2 t}\mathrm{d}k. \tag{1.14}$$

(i) Ω_I, $\Omega_{II}\subset\mathbb{C}$ are some domains defined by the spectrum of the t-equation (1.10) with finite-gap coefficients $\alpha(t)$ and $\beta(t)$. See Fig. 1 above.

(ii) The function $r(k)$, eigenvalues $k_j\in\Omega_I$ and numbers m_j^1 $(j=1,\ldots,l)$ are uniquely defined only by initial data $u(x)$.

(iii) The remaining scattering data $c(k)$, eigenvalues $z_j\in\Omega_{II}$ and numbers m_j^2 $(j=1,\ldots,m)$ depend on both initial and boundary data.

Note that $H(x,t)$ is only defined for $x\geqslant 0$ because for $x<0$ the integral over the infinite contour $\partial\Omega_{II}$ does not converge.

Theorem 1: *Let $q(x,t)$ be the solution of the nonlinear problem (1.1)–(1.6) given by (1.11)–(1.14). Let $E_0=-b+\mathrm{i}a$. We assume $b<0$ and $\min_{1\leqslant j\leqslant m}\mathrm{Re}\, z_j>-b$. Let $N\in\mathbb{N}$ and*

$$G_N(t)=\left\{x\in\mathbb{R}_+ \;\middle|\; x>4bt-\frac{1}{2b}\log t^{N+1}\right\}.$$

Then, $q(x,t)$ has in $G_N(t)$ the following asymptotics, for $t\to\infty$:

$$|q(x,t)|^2=\sum_{j=1}^{[(N+1)/2]}\frac{4a^2}{\cosh^2[2a(x-4bt-x_j)+\log t^{2j-1/2}]}+o(1),$$

where

$$x_j = x_j^{(0)} + \frac{1}{2\pi}\int_{-\infty}^{-b} \frac{\log[1+|\rho(\lambda)|^2]}{(\lambda+b)^2+a^2}\,d\lambda,$$

$$\rho(\lambda) = r(\lambda) + c(\lambda),$$

and the numbers $x_j^{(0)}$ *depend on* γ_0^+ *and* $c(k)$.

Remark: If there exist eigenvalues z_j with $\mathrm{Re}\, z_j < -b$, then the asymptotics of the function $|q(x,t)|^2$ will contain additionally a finite number of ordinary solitons

$$\sum_{\mathrm{Re}\, z_j < -b} \frac{4\,\mathrm{Im}^2 z_j}{\cosh^2[2\,\mathrm{Im}\, z_j(x+4\,\mathrm{Re}\, z_j t - y_j)]}$$

which move faster than asymptotic solitons away from the boundary in the domain $x > 4bt$ and correspond to those eigenvalues $z_j \in \Omega_{\mathrm{II}}$ for which $\mathrm{Re}\, z_j < -b$.

It is easy to see that asymptotic solitons given by Theorem 1 are similar to ordinary solitons but their velocities depend on t. In contrast with ordinary solitons they are not exact solutions of the nonlinear equation, however they satisfy it with increasing accuracy when $t \to \infty$. For this reason such objects are called asymptotic solitons. The number of these asymptotic solitons increases to infinity when $t \to \infty$ if the observation domain in the neighborhood of the solution front is extended correspondingly.

B. Second case: Re $E_0 > 0$

Now let us consider the case when the finite-gap function $\alpha(t)$ or $\beta(t)$ are such that all branch points E_j have a positive real part. In contrast with the first case, such boundary functions do not generate asymptotic solitons.

Theorem 2: *Let the boundary functions be such that* $\mathrm{Re}\, E_0 > 0$. *Then, the solution* $q(x,t)$ *has in the domain*

$$x > z_0 t,$$

$$z_0 = \min_{1 \le j \le m} |\mathrm{Re}\, z_j| - \varepsilon, \quad \varepsilon > 0,$$

the following asymptotics, for $t \to \infty$*:*

$$|q(x,t)|^2 = \sum_{j=1}^{m} \frac{4\,\mathrm{Im}^2 z_j}{\cosh^2[2\,\mathrm{Im} z_j(x+4\,\mathrm{Re}\, z_j t - y_j)]} + o(1).$$

If in addition $\{z_j \in \Omega_{\mathrm{II}}\} = \varnothing$, *then, in the same domain for* $t \to \infty$,

$$|q(x,t)|^2 = \frac{1}{4\pi t}\log\left[1 + \left|\rho\left(-\frac{x}{4t}\right)\right|^2\right] + o(t^{-1}),$$

with

$$\rho(k) = r(k) + c(k), \quad z_0 > 0 \ \textit{arbitrary}.$$

Qualitatively these results do not depend on whether the initial function $u(x)$ is identically zero or not. In the case $u(x) \equiv 0$ the scattering function $r(k)$ is also identically zero, and $\rho(k)$ depends on the boundary data only. Thus we have the following

Summary: (1) Boundary data $v(t)$ *or* $v_1(t)$ *with periodic or quasi-periodic behavior such that* $\mathrm{Re}\, E_0 < 0$ *generate an unbounded train of asymptotic solitons which run away from the boundary.*

(2) For boundary data $v(t)$ or $v_1(t)$ with periodic or quasi-periodic behavior such that $\mathrm{Re}\, E_0>0$, *only a finite number of ordinary solitons may exist.*

(2′) If in addition the set of eigenvalues $\{z_j \in \Omega_{\mathrm{II}}\}$ is empty, then the solution $q(x,t)$ does not contain any soliton.

Generated by eigenvalues $k_j \in \Omega_{\mathrm{I}}$ [in this case $u(x) \not\equiv 0$] ordinary solitons run to the boundary $x=0$ and they are absorbed by the boundary in finite time.

II. BASIC SOLUTIONS

Let us write the x- and t-equations in the form

$$W_x = U(x,t,k)W, \tag{2.1}$$

$$W_t = V(x,t,k)W, \tag{2.2}$$

where $U(x,t,k)$ and $V(x,t,k)$ are 2×2 matrices given by

$$U(x,t,k) = Q(x,t) - \mathrm{i}k\sigma_3,$$

$$V(x,t,k) = 2kQ(x,t) - \mathrm{i}(Q^2(x,t) + Q_x'(x,t))\sigma_3 - 2\mathrm{i}k^2\sigma_3.$$

Lemma 1: Let the system (2.1) and (2.2) be compatible for all k. Let $W(x,t,k)$ satisfy the x-equation (2.1) for all t, and let $W(x_0,t,k)$ satisfy the t-equation (2.2) for some $x=x_0$ (including the case $x_0=\infty$).

Then $W(x,t,k)$ satisfies the t-equation for all x.

Proof: See, e.g., Ref. 9. □

Notations: The over-bar denotes the complex conjugation; $\mathbb{C}_{\pm}$ denotes the upper (lower) complex half plane; I, II, III, IV are the first, second, third and fourth quadrants of the complex plane. If A is a 2×2 matrix, we denote A^- the first column of A, and A^+ the second column of A:

$$A = (A^- \quad A^+) = \begin{pmatrix} a_1^- & a_1^+ \\ a_2^- & a_2^+ \end{pmatrix}.$$

We denote $[A,B]=AB-BA$ the commutator of two matrices A and B.

In this section we shall introduce three solutions of both x- and t-equations. They are called ''basic'' solutions.

C. First basic solution

First of all, since $q(x,t)\to 0$ as $x\to\infty$, then we can choose the 2×2 matrix-valued *Jost solution* of the x-equation (1.7) as the first basic solution. It has the integral representation (see, e.g., Ref. 16)

$$\Psi(x,t,k) = \left(\mathrm{e}^{-\mathrm{i}kx\sigma_3} + \int_x^{\infty} K(x,y,t)\mathrm{e}^{-\mathrm{i}ky\sigma_3}\mathrm{d}y \right) \mathrm{e}^{-2\mathrm{i}k^2t\sigma_3}, \tag{2.3}$$

where

$$K(x,y,t) = \begin{pmatrix} K_1(x,y,t) & -\overline{K_2}(x,y,t) \\ K_2(x,y,t) & \overline{K_1}(x,y,t) \end{pmatrix}$$

with $K_1, K_2 \in C^{\infty}(\mathbb{R}_+\times\mathbb{R}_+\times\mathbb{R}_+)$ and of Schwartz type in $x+y$ for any $t\in\mathbb{R}_+$. Moreover, $K(x,x,t)$ and $Q(x,t)$ are connected by

$$[\sigma_3, K(x,x,t)] = Q(x,t)\sigma_3. \tag{2.4}$$

This last equality leads to the important formula

$$q(x,t)=2\overline{K_2}(x,x,t) \tag{1.11}$$

for the solution $q(x,t)$ of the nonlinear Schrödinger equation (1.10). $\Psi(x,t,k)$ satisfies the x-equation (1.7). It also satisfies the t-equation (1.8) with $x=\infty$, because $e^{-ik(x+2kt)\sigma_3}$ satisfies both Eqs. (1.7) and (1.8) for $Q(x,t)\equiv 0$. Then, Lemma 1 implies that $\Psi(x,t,k)$ satisfies the t-equation for any $x\in\mathbb{R}_+$, both equations being assumed compatible.

The integral representation (2.3) and Lemma 1 imply the following properties of the matrix-valued Jost solution $\Psi(x,t,k)$ (cf. Ref. 16).

Proposition: The first basic solution $\Psi(x,t,k)$ has the following properties:

(1) $\Psi(x,t,k)$ satisfies both x-and t-equations (1.7) and (1.8).
(2) $\Psi(x,t,k)=\sigma_2\overline{\Psi}(x,t,k)\sigma_2$ for $k\in\mathbb{R}$.
(3) $\det\Psi(x,t,k)\equiv 1$ for $k\in\mathbb{R}$.
(4) $\Psi(x,t,k)$ is C^∞ in $(x,t,k)\in\mathbb{R}_+\times\mathbb{R}_+\times\mathbb{R}$.
(5) $\Psi^+(x,t,k)$ is analytic in $k\in\mathbb{C}_+$, and $\Psi^-(x,t,k)$ is analytic in $k\in\mathbb{C}_-$.
(6) $\sigma_2\overline{\Psi}^-(x,t,k)=i\Psi^+(x,t,\overline{k})$ for any $k\in\mathbb{C}_-$.
(7) For $k\to\infty$,

$$e^{ikx+2ik^2t}\Psi^-(x,t,k)=\begin{pmatrix}1\\0\end{pmatrix}+O(k^{-1}) \quad \text{if} \quad \operatorname{Im}k\leqslant 0,$$

$$e^{-ikx-2ik^2t}\Psi^+(x,t,k)=\begin{pmatrix}0\\1\end{pmatrix}+O(k^{-1}) \quad \text{if} \quad \operatorname{Im}k\geqslant 0.$$

D. Second basic solution

Now let us introduce the second basic solution $\Phi(x,t,k)$ of the x- and t-equations which satisfies the initial condition

$$\Phi(0,0,k)=\sigma_0. \tag{2.5}$$

It can be represented as a product of two 2×2 matrices:

$$\Phi(x,t,k)=\varphi(x,t,k)\hat{\varphi}(t,k), \tag{2.6}$$

where $\varphi(x,t,k)$ satisfies the x-equation under the condition $\varphi(0,t,k)=\sigma_0$, and $\hat{\varphi}(t,k)$ satisfies the t-equation with $x=0$ under the initial condition $\hat{\varphi}(0,k)=\sigma_0$. Lemma 1 implies that $\Phi(x,t,k)$ satisfies both equations (1.7) and (1.8). The existence of the solution $\varphi(x,t,k)$ and its integral representation

$$\varphi(x,t,k)=e^{-ikx\sigma_3}+\int_{-x}^{x}A(x,y,t)e^{-iky\sigma_3}dy \tag{2.7}$$

with some integral kernel $A(x,y,t)$ is proved in Ref. 9. $\hat{\varphi}(t,k)$ can be found as solution of the Volterra integral equation:

$$\hat{\varphi}(t,k)=e^{-2ik^2t\sigma_3}+\int_0^t e^{2ik^2(\tau-t)}\hat{Q}(0,\tau,k)\hat{\varphi}(\tau,k)d\tau, \tag{2.8}$$

where

$$\hat{Q}(0,t,k)=2k\begin{pmatrix}0 & v(t)\\ -\overline{v}(t) & 0\end{pmatrix}+i|v(t)|^2\sigma_3+i\begin{pmatrix}0 & v_1(t)\\ \overline{v_1}(t) & 0\end{pmatrix}.$$

For $\hat{\varphi}(t,k)$ the following integral representation,

$$\hat{\varphi}(t,k)=\mathrm{e}^{-2\mathrm{i}k^2t\sigma_3}+\int_{-t}^{t}B(t,s)\mathrm{e}^{-2\mathrm{i}k^2s\sigma_3}\mathrm{d}s+k\int_{-t}^{t}C(t,s)\mathrm{e}^{-2\mathrm{i}k^2s\sigma_3}\mathrm{d}s, \tag{2.9}$$

can be found in Ref. 9. In the present case $A(x,y,t)$, $B(t,s)$ and $C(t,s)$ are C^∞ and bounded.

The integral representations (2.6)–(2.9) yield the following properties of $\Phi(x,t,k)$.

Proposition: The second basic solution $\Phi(x,t,k)$ has the following properties:

(1) $\Phi(x,t,k)$ *satisfies both x- and t-equations.*
(2) $\overline{\Phi(x,t,\overline{k})}=\sigma_2\Phi(x,t,k)\sigma_2$ *for any* $k\in\mathbb{C}$.
(3) $\det\Phi(x,t,k)\equiv 1$ *for* $k\in\mathbb{C}$.
(4) $\Phi(x,t,k)\in C^\infty(\mathbb{R}_+\times\mathbb{R}_+\times\mathbb{C})$.
(5) $\Phi(x,t,k)$ *is an entire function in* $k\in\mathbb{C}$.
(6) For $k\in\mathbb{C}$, $k\to\infty$,

$$\Phi(x,t,k)=\left[I+\mathrm{O}(k^{-1})+\mathrm{O}\left(\frac{\mathrm{e}^{2\mathrm{i}kx\sigma_3}}{k}\right)+\mathrm{O}\left(\frac{\mathrm{e}^{4\mathrm{i}k^2t\sigma_3}}{k}\right)\right]\mathrm{e}^{-\mathrm{i}k(x+2kt)\sigma_3}.$$

(7) For $k\in\Omega_1$, $k\to\infty$,

$$\mathrm{e}^{\mathrm{i}kx+2\mathrm{i}k^2t}\Phi^-(x,t,k)=\begin{pmatrix}1\\0\end{pmatrix}+\mathrm{O}(k^{-1}).$$

The last asymptotic relation can be easily proved using large k asymptotics for $\varphi^{\mp}(x,t,k)$ and $\hat{\varphi}^-(t,k)$.

E. Third basic solution

The third basic solution involves a *Floquet–Bloch solution* of the equation (1.10). We have supposed that the functions $\alpha(t)$ and $\beta(t)$ are finite-gap. This means that there exists a hyperelliptic Riemann surface $\mathcal{X}$ and a Baker–Akhiezer vector-function $\phi(t,\mathcal{P})$, $\mathcal{P}\in\mathcal{X}$, which satisfies (in t) the equation (1.10). Using theta function theory (Appendix or Ref. 15) one can write

$$\phi(t,\mathcal{P})=\chi(t,\mathcal{P})\exp\left(-\mathrm{i}t\int_{\underline{E}_g}^{\mathcal{P}}\Omega(\mathcal{Q})\right).$$

Let $D=\mathcal{P}_1+\cdots+\mathcal{P}_g$ be the divisor of poles of $\phi(t,\mathcal{P})$. For all $t\in\mathbb{R}$ the function $\chi(t,\mathcal{P})$ is defined on $\mathcal{X}\backslash\{\mathcal{P}_1,\ldots,\mathcal{P}_g\}$. Moreover, $\Omega(\mathcal{P})$ is an Abelian differential on $\mathcal{X}$ characterized by the following properties:

(1) It is holomorphic on $\mathcal{X}\backslash\{\infty^{\pm}\}$.
(2) It has the following behavior for $\mathcal{P}\to\infty^{\pm}$:

$$\Omega(\mathcal{P})=\pm\mathrm{d}(2k^2)+\mathrm{O}\left(\frac{\mathrm{d}k}{k^2}\right),$$

where $k=k(\mathcal{P})$.
(3) It satisfies the normalization conditions:

$$\int_{a_j}\Omega(\mathcal{P})=0,\quad j=1,\ldots,g,$$

where $a_1,\ldots,a_g$ are suitable one-cycles on $\mathcal{X}$.

More details about $\phi(t,\mathcal{P})$ are given in the Appendix.

Let $e(t,k)$ be the projection of $\phi(t,\mathcal{P})$ on the upper sheet $\mathcal{X}_+$, namely $e(t,k)=\phi(t,\mathcal{P})$, where $\mathcal{P}\in\mathcal{X}_+$ and $\pi(\mathcal{P})=k$. This function $e(t,k)$ satisfies (1.10) in $t\in\mathbb{R}$, and it is meromorphic away from $\Sigma\cup\{\infty\}$ where

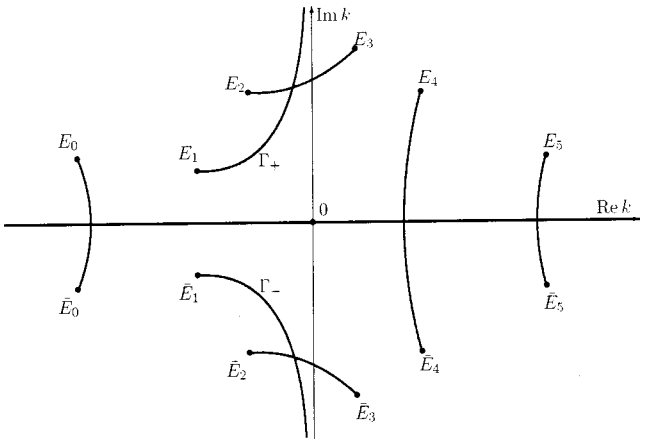

FIG. 2. The second type of Σ.

$$\Sigma := \left\{ k \in \mathbb{C} \,\middle|\, \operatorname{Im} \mu(k) = \operatorname{Im} \int_{\overline{E}_g}^{\mathcal{P}} \Omega(\mathcal{P}') = 0 \right\}.$$

It is known[15] that the function $\mu(k)$ can be written in the form

$$\mu(k) = \int_{\overline{E}_g}^{k} \frac{s^{g+2} + \mu_1 s^{g+1} + \cdots + \mu_{g+2}}{X(s)} \mathrm{d}s,$$
$$X(s) = \sqrt{\prod_{j=0}^{g} (s - E_j)(s - \overline{E_j})}. \tag{2.10}$$

This integral representation shows that

$$\Sigma = \mathbb{R} \cup \Gamma \cup \gamma_0 \cup \cdots \cup \gamma_g,$$

where $\mathbb{R}$ is the real axis in the complex k-plane, Γ is an infinite contour on $\mathbb{C}$, asymptotic to the imaginary axis $\mathrm{i}\mathbb{R}$ and invariant by complex conjugation, and the γ_j's are finite arcs whose endpoints are the branch points E_j and $\overline{E_j}$. We denote

$$\Sigma_E = \{E_0, \overline{E_0}, \ldots, E_g, \overline{E_g}\},$$
$$\Sigma_\kappa = \{\kappa_j \,|\, \kappa_j \quad \text{self-intersection of} \quad \Sigma\}. \tag{2.11}$$

There exist two types of Σ:

(1) For the first type the complex plane $\mathbb{C}$ is divided into two nonintersecting left and right "half-planes" by Γ (Fig. 1).
(2) The second type of Σ is that when Γ does not divide the plane $\mathbb{C}$. It consists of two connected parts $\Gamma_\pm \subset \mathbb{C}_\pm$ with endpoints $E_+ = E_{j_0}$ and $E_- = \overline{E}_{j_0}$ for some $0 \leqslant j_0 \leqslant g$ (Fig. 2).

Away from endpoints, γ_j and Γ are analytic curves. In what follows we will consider only cases where Σ is of the first type. Let us denote

$$\Omega_{\mathrm{I}} = \{k \in \mathbb{C} \,|\, \operatorname{Im} k > 0, \operatorname{Im} \mu(k) > 0\},$$
$$\Omega_{\mathrm{II}} = \{k \in \mathbb{C} \,|\, \operatorname{Im} k > 0, \operatorname{Im} \mu(k) < 0\},$$

$$\Omega_{\mathrm{III}}=\{k\in\mathbb{C}|\operatorname{Im}k<0,\operatorname{Im}\mu(k)>0\},$$

$$\Omega_{\mathrm{IV}}=\{k\in\mathbb{C}|\operatorname{Im}k<0,\operatorname{Im}\mu(k)<0\}. \tag{2.12}$$

So, we obtain a partition of the complex k-plane:

$$\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{III}}\cup\Omega_{\mathrm{IV}}\cup\Sigma=\mathbb{C},$$

where

$$\Sigma=\{k\in\mathbb{C}|\operatorname{Im}\mu(k)=0\}=\mathbb{R}\cup\Gamma\cup\gamma_0\cup\cdots\cup\gamma_g,$$

$$\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}=\{k\in\mathbb{C}|\operatorname{Im}\mu(k)>0\},$$

$$\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}=\{k\in\mathbb{C}|\operatorname{Im}\mu(k)<0\}.$$

Now we input the matrix-valued Floquet–Bloch solution

$$\mathcal{E}(t,k)=\begin{pmatrix} e_1(t,k) & -\overline{e_2}(t,\overline{k}) \\ e_2(t,k) & \overline{e_1}(t,\overline{k}) \end{pmatrix}$$

of (1.10), which is bounded in $t\in\mathbb{R}$ for $k\in\Sigma$. We remind that $e(t,k)$ is C^∞ in $t\in\mathbb{R}$ and $k\in\Sigma\setminus(\Sigma_\kappa\cup\Sigma_E)$. It is meromorphic away from $\Sigma\cup\{\infty\}$.

For $k\in\mathbb{C}\setminus\Sigma$ the matrix-valued function $\mathcal{E}(t,k)$ is unbounded in $t\in\mathbb{R}$. However, its first column $\mathcal{E}^-(t,k)$ has exponential decay in the domain $\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$ as $t\to\infty$ and the second column $\mathcal{E}^+(t,k)$ has exponential decay in the domain $\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}$:

$$\mathcal{E}^{\mp}(t,k)=\mathrm{O}(\mathrm{e}^{\pm 2\operatorname{Im}\mu(k)t}),\quad t\to\infty.$$

But, they grow exponentially when $k\in\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}$ and $k\in\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$, respectively. The determinant

$$\det\mathcal{E}(t,k)=\Delta(k)=1+e_2(0,k)\overline{e_2}(0,\overline{k}) \tag{2.13}$$

does not vanish at any $k\neq E_j,\overline{E_j}$.

Examples: The simplest examples of finite-gap boundary data are as follows. If $g=0$, there exist only two branch points E_0 and $\overline{E_0}$. Let us put $E_0=\mathrm{i}a-b$, $a>0$, $b>0$.

Then the function $\mu(k)$ has the form

$$\mu(k)=2(k-b)\sqrt{(k+b)^2+a^2},$$

$$X(k)=\sqrt{(k+b)^2+a^2},$$

and the function $e(t,k)$ can be written as

$$e(t,k)=\begin{pmatrix} 1 \\ \dfrac{\mathrm{i}\mathrm{e}^{-\mathrm{i}\omega t}}{a}(k+b-X(k)) \end{pmatrix}\mathrm{e}^{-\mathrm{i}\mu(k)t}.$$

Using Eq. (1.10) one finds

$$\alpha(t)=a\mathrm{e}^{2\mathrm{i}\omega t},$$

$$\beta(t)=2\mathrm{i}ab\mathrm{e}^{2\mathrm{i}\omega t},$$

where $\omega=a^2-2b^2$. This case of simplest periodic behavior of boundary data was studied in Ref. 10. The genus $g=1$ produces elliptic functions $\alpha(t)$ and $\beta(t)$ which are periodic in $t\in\mathbb{R}$. For $g\geqslant 2$ the functions $\alpha(t)$ and $\beta(t)$ can also be periodic. In general, these functions are quasi-periodic in $t\in\mathbb{R}$ with finite number of frequencies.

We introduce the third basic solution as follows. Let $\hat{\Psi}(t,k)$ be a solution of the Volterra integral equation

$$\hat{\Psi}(t,k)=\mathcal{E}(t,k)-\int_t^\infty \mathcal{E}(t,k)\mathcal{E}^{-1}(\tau,k)[\hat{Q}(0,\tau,k)-\hat{Q}_0(\tau,k)]\hat{\Psi}(\tau,k)\mathrm{d}\tau, \tag{2.14}$$

where $\hat{Q}(0,t,k)$ is as in (2.8), and

$$\hat{Q}_0(t,k)=\begin{pmatrix} \mathrm{i}|\alpha(t)|^2 & 2k\alpha(t)+\mathrm{i}\beta(t) \\ -2k\overline{\alpha}(t)+\mathrm{i}\beta(t) & -\mathrm{i}|\alpha(t)|^2 \end{pmatrix},$$

which means the matrix $\hat{\Psi}(t,k)$ satisfies the t-equation with $x=0$ under the asymptotic condition $\hat{\Psi}(t,k)=\mathcal{E}(t,k)+o(1)$ as $t\to\infty$. We input the matrix

$$Y(x,t,k)=\varphi(x,t,k)\hat{\Psi}(t,k), \quad k\in\Sigma, \tag{2.15}$$

where $\varphi(x,t,k)$ is as in (2.7). Lemma 1 implies that $Y(x,t,k)$ is a solution of the x- and t-equations with

$$\det Y(x,t,k)=\det\mathcal{E}(t,k)=\Delta(k), \quad k\in\Sigma.$$

For k outside of Σ the function $\hat{\Psi}(t,k)$, hence also $Y(x,t,k)$, is unbounded in $t\in\mathbb{R}_+$. The matrix-valued function $Y(x,t,k)$ has the same analytic properties in $k\in\mathbb{C}$ as $\mathcal{E}(t,k)$, since the Green matrix $\mathcal{E}(t,k)\mathcal{E}^{-1}(\tau,k)$ is an entire function in $k\in\mathbb{C}$, and the integral equation (2.14) is of Volterra type with $\tau\in(t,\infty)$. Therefore, $Y^-(x,t,k)$ is meromorphic in the domain $\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$, and $Y^+(x,t,k)$ is meromorphic in $\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}$.

The properties of the solution $Y(x,t,k)$ follow from the integral representation (2.7) and from the integral Volterra equation (2.14):

Proposition: The third basic solution $Y(x,t,k)$ has the following properties:

(1) $Y(x,t,k)$ *is a solution of both x- and t-equations.*
(2) $Y(x,t,k)=\sigma_2\overline{Y}(x,t,\overline{k})\sigma_2$ *for* $k\in\Sigma$.
(3) $\det Y(x,t,k)=\Delta(k)$ *for* $k\in\Sigma$.
(4) $Y(x,t,k)\in C^\infty(\mathbb{R}_+\times\mathbb{R}_+\times\Sigma')$ *where* $\Sigma'=\Sigma\backslash(\Sigma_\kappa\cup\Sigma_E)$.
(5) $Y^+(x,t,k)$ *is meromorphic in* $k\in\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}$.
(6) $Y^-(x,t,k)$ *is meromorphic in* $k\in\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$.
(7) $\sigma_2\overline{Y^-}(x,t,k)=\mathrm{i}Y^+(x,t,\overline{k})$ *for* $k\in\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$.
(6) For $k\in\Omega_{\mathrm{II}}$, $k\to\infty$,

$$\mathrm{e}^{\mathrm{i}kx+2\mathrm{i}k^2t}Y^-(x,t,k)=\begin{pmatrix}1\\0\end{pmatrix}+\mathrm{O}(k^{-1}).$$

III. "SCATTERING" (TRANSITION) MATRICES

Definition (scattering matrices): The basic solutions we have introduced are clearly linearly dependent:

$$\Phi(x,t,k)=\Psi(x,t,k)S(k),$$

$$Y(x,t,k)=\Phi(x,t,k)P(k), \tag{3.1}$$

$$Y(x,t,k)=\Psi(x,t,k)R(k).$$

The matrices $S(k)$, $P(k)$ and $R(k)$ depend neither on x nor on t because by virtue of the x-equation they do not depend on x, and by virtue of the t-equation they do not depend on t. Hence for $k\in\mathbb{R}$ and for $k\in\Sigma$ we have

$$S(k)=\Psi^{-1}(0,0,k), \quad k\in\mathbb{R};$$

$$P(k)=Y(0,0,k), \quad k\in\Sigma; \tag{3.2}$$

$$R(k)=S(k)P(k), \quad k\in\mathbb{R}.$$

Let us study the properties of these "scattering" (transition) matrices. Properties of $S(k)$ follow from the scattering problem for the x-equation with $t=0$. Indeed, consider the problem on the whole x-axis by putting

$$q(x,0)=\hat{u}(x)=\begin{cases}0 & \text{for} \quad x\in(-\infty,0],\\ u(x) & \text{for} \quad x\in[0,\infty).\end{cases}$$

For simplicity, and to make considerations more transparent, we also suppose that

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}u(x)\bigg|_{x=0}=\frac{\mathrm{d}^n}{\mathrm{d}t^n}v(t)\bigg|_{t=0}=\frac{\mathrm{d}^n}{\mathrm{d}t^n}v_1(t)\bigg|_{t=0}=0 \tag{3.3}$$

for any $n\geqslant 0$. Let $\tilde{\Psi}(x,k)$ be the Jost solution[16] normalized by

$$\tilde{\Psi}(x,k)=\mathrm{e}^{-\mathrm{i}kx\sigma_3} \quad \text{for} \quad x<0,$$

and let $\tilde{T}(k)$ be the transition matrix for that case, i.e.,

$$\tilde{\Psi}(x,k)=\Psi(x,0,k)\tilde{T}(k).$$

Putting $x=0$ we find $S(k)\equiv\tilde{T}(k)$. Hence the "scattering" matrix $S(k)$ has all properties of the transition matrix $\tilde{T}(k)$.[16]

Properties of $S(k)$: The scattering matrix $S(k)$ satisfies

(i) $S(k)=\sigma_2\overline{S(k)}\sigma_2$ *for* $k\in\mathbb{R}$;
(ii) $\det S(k)\equiv 1$ *for* $k\in\mathbb{R}$;
(iii) $S(k)\in C^\infty(\mathbb{R})$.

For the half-axis case there are additional properties:

(iv) $S(k)=\begin{pmatrix} s_2^+(k) & -s_1^+(k)\\ -s_2^-(k) & s_1^-(k)\end{pmatrix}$ *where* $s_j^+(k)=\Psi_j^+(0,0,k)$.
(v) *The first line* $(s_2^+(k) \quad -s_1^+(k))$ *is analytic in* $k\in\mathbb{C}_+$.
(vi) *The second line* $(-s_2^-(k) \quad s_1^-(k))$ *is analytic in* $k\in\mathbb{C}_-$. [For an arbitrary function $\hat{u}(x)$, $x\in\mathbb{R}$, these analytic properties do not hold; $s_2^+(k)$ and $s_1^-(k)$ are only analytic functions in $k\in\mathbb{C}_+$ and $k\in\mathbb{C}_-$, respectively. In our case $\hat{u}(x)\equiv 0$ for $x<0$, therefore $s_1^+(k)$ and $s_2^-(k)$ are also analytic functions in $k\in\mathbb{C}_\pm$.]

(vii) *If* $k\in\mathbb{C}_+$ *and* $k\to\infty$,

$$s_2^+(k)=1+\mathrm{O}(k^{-1}),$$
$$s_1^+(k)=\mathrm{O}(k^{-1}).$$

(viii) *Under condition* (3.3) $s_1^+(k)\in\mathcal{S}(\mathbb{R})$ *and* $s_2^+(k)-1$ *is the Fourier transform of a complex-valued function* $f(y)\in\mathcal{S}(\mathbb{R}_+)$.

Proof: To prove the last item we use limit formulas

$$s_1^+(k)=\lim_{x\to-\infty}\mathrm{e}^{-\mathrm{i}kx}\Psi_1^+(x,0,k),$$

$$s_2^+(k)=\lim_{x\to-\infty}\mathrm{e}^{-\mathrm{i}kx}\Psi_2^+(x,0,k),$$

which follow from the definition of the matrix $S(k)$. If one puts

$$\chi_j(x,k)=\mathrm{e}^{-\mathrm{i}kx}\Psi_j^+(x,0,k),$$

the x-equation yields

$$\chi_1'+2\mathrm{i}k\chi_1=\hat{u}(x)\chi_2,\quad \chi_1(x,k)\to0\quad\text{as}\quad x\to+\infty,$$

$$\chi_2'=-\overline{\hat{u}(x)}\chi_1,\quad \chi_2(x,k)\to1\quad\text{as}\quad x\to+\infty.$$

Integrating these equations we find

$$\chi_1(x,k)=-\int_x^\infty \mathrm{e}^{2\mathrm{i}k(y-x)}\hat{u}(y)\chi_2(y,k)\mathrm{d}y,$$

$$\chi_2(x,k)=1+\int_x^\infty\overline{\hat{u}(y)}\chi_1(y,k)\mathrm{d}y,$$

and therefore

$$s_1^+(k)=-\int_{-\infty}^\infty\hat{u}(x)\mathrm{e}^{2\mathrm{i}kx}\chi_2(x,k)\mathrm{d}x=-\int_{-\infty}^\infty\hat{u}(x)\mathrm{e}^{2\mathrm{i}kx}\mathrm{d}x-\int_{-\infty}^\infty\hat{u}(x)\mathrm{e}^{2\mathrm{i}kx}\mathrm{d}x\int_0^\infty\overline{K}_1(x,x+y)\mathrm{e}^{\mathrm{i}ky}\mathrm{d}y,$$

$$s_2^+(k)=1+\int_{-\infty}^\infty\overline{\hat{u}(x)}\chi_1(x,k)\mathrm{d}x=1-\int_0^\infty\mathrm{e}^{\mathrm{i}kx}\mathrm{d}x\int_{-\infty}^\infty\overline{\hat{u}(y)}\overline{K}_2(y,y+x)\mathrm{d}y,$$

where $\overline{K}_1(x,y)$ and $\overline{K}_2(x,y)$ are entries of the kernel of triangular integral transformation (2.3). Taking into account that both functions $\overline{K}_1(x,y)$ and $\overline{K}_2(x,y)$ are of Schwartz type and that $\hat{u}(x)$ is of Schwartz type on the whole axis, which follows from (3.3), we arrive to the statement of the last item. □

The matrix $S(k)=\Psi^{-1}(0,0,k)$ is determined by the function $u(x)\in\mathcal{S}(\mathbb{R}_+)$. The entries of this matrix are not independent and can be recovered from one known function. Let $s(k)\equiv s_1^+(k)/s_2^+(k)$ be given and let

$$\Sigma_{\mathrm{d}}^{\mathrm{ic}}=\{k_1,\ldots,k_n\}=\{k_j\in\mathbb{C}_+|s_2^+(k_j)=0\}$$

be the set of zeros of the analytic function $s_2^+(k)$. Since $\det S(k)\equiv1$, then $|s_2^+(k)|^2+|s_1^+(k)|^2\equiv1$ for any $k\in\mathbb{R}$. This identity yields the well-known formula:

$$s_2^+(k)=\prod_{k_j\in\mathbb{C}_+}\frac{k-k_j}{k-\overline{k_j}}\exp\left\{\frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\frac{\log[1+|s(\lambda)|^2]\mathrm{d}\lambda}{\lambda-k}\right\}. \tag{3.4}$$

The remaining entries of $S(k)$ are also recovered:

$$s_1^+(k)=s(k)s_2^+(k),\quad s_2^-(k)=-\overline{s_1^+}(\overline{k}),\quad s_1^-(k)=\overline{s_2^+}(\overline{k}).$$

So, the function $s_2^+(k)$ may vanish at some points $k_j\in\mathbb{C}_+$ and the set $\Sigma_{\mathrm{d}}^{\mathrm{ic}}$ is not empty. Moreover, these zeros can be multiple and there can exist limit points on the real axis $\mathbb{R}$.[16] To avoid these difficulties we shall consider a subset $\mathcal{S}_0(\mathbb{R}_+)$ of functions $u(x)\in\mathcal{S}(\mathbb{R}_+)$ for which $s_2^+(k)$ has a finite number of simple zeros in $\mathbb{C}_+$ and $s_2^+(k)\neq 0$ for $k\in\mathbb{R}$.

Let us briefly discuss the discrete spectrum of the x-problem. The main relation of the x-scattering problem is

$$\frac{1}{s_2^+(k)}\Phi^-(x,t,k)=\Psi^-(x,t,k)+r(k)\Psi^+(x,t,k)\quad\text{for}\quad k\in\mathbb{R}, \tag{3.5}$$

where

$$r(k)=-\frac{s_2^-(k)}{s_2^+(k)}. \tag{3.6}$$

The function $F(x,t,k)=\Phi^-(x,t,k)/s_2^+(k)$ is analytic in $k\in\mathbb{C}_+$ with the exception of a discrete set

$$\Sigma_{\mathrm{d}}^{\mathrm{ic}}=\{k_j\in\mathbb{C}_+|s_2^+(k_j)=0,\quad j=1,2,\ldots,n\},$$

where it has poles. If

$$s_2^+(k_j)=\det(\Phi^-(x,t,k_j)\quad\Psi^+(x,t,k_j))=0,$$

then $\Phi^-(x,t,k_j)=\gamma_j^1\Psi^+(x,t,k_j)$. Hence,

$$\mathrm{res}_{k_j}F(x,t,k)=c_j^1\Psi^+(x,t,k_j)$$

with

$$c_j^1=\frac{\gamma_j^1}{\dot{s}_2^+(k_j)},\quad j=1,2,\ldots,n,$$

$$\gamma_j^1=\frac{1}{s_1^+(k_j)}.$$

The dot denotes differentiation w.r.t. k. Note that $s_1^+(k_j)\neq 0$ because otherwise we come to a contradiction: $\Psi_+(x,t,k_j)\equiv 0$ since $\Psi_1^+(0,0,k_j)=s_1^+(k_j)=0$ and $\Psi_2^+(0,0,k_j)=s_2^+(k_j)=0$. The set of zeros $\Sigma_{\mathrm{d}}^{\mathrm{ic}}$ is finite because $s_2^+(k)\to 1$ as $k\to\infty$ and we have supposed that $s_2^+(k)\neq 0$ for any $k\in\mathbb{R}$. We also assume that zeros are simple, i.e., $\dot{s}_2^+(k_j)\neq 0$.

Using asymptotics of the function $\Phi^-(x,t,k)$ at $k=\infty$, for $\mathrm{Im}\,k\geqslant 0$, we find

$$F(x,t,k)=\left[\begin{pmatrix}1\\0\end{pmatrix}+\mathrm{O}(|k|^{-1})\right]\mathrm{e}^{-\mathrm{i}kx-2\mathrm{i}k^2t}\quad\text{for}\quad|k|\to\infty,\ k\in\Omega_1, \tag{3.7}$$

which will be used below. So, we come to the following:

Properties of $r(k)$: The reflection coefficient $r(k)$ satisfies the following.

(i) $r(k)\in\mathcal{S}(\mathbb{R})$. [For arbitrary functions $u(x)$ which do not satisfy (3.3) the reflection coefficient $r(k)$ does not belong to the Schwartz space $\mathcal{S}(\mathbb{R})$ since, for example, $\lim_{k\to\infty}2ikr(k)=u(0)\neq 0$.]

(ii) $r(k)$ *is the ratio of two functions* $-s_2^-(k)$ *and* $s_2^+(k)$ *which are analytic in* $k\in\mathbb{C}_-$ and $k\in\mathbb{C}_+$, respectively.

Properties of $t(k)$*: The transmission coefficient is given by* $t(k)=[s_2^+(k)]^{-1}$ *with*

$$s_2^+(k)=\prod_{k_j\in\mathbb{C}_+}\frac{k-k_j}{k-\overline{k_j}}\exp\left\{\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{\log[1+|s(\lambda)|^2]d\lambda}{\lambda-k}\right\}, \tag{3.4}$$

$\mathrm{Im}\,k_j>0$, $j=1,\ldots,n$, *and* $k_i\neq k_j$ *for* $i\neq j$. *Moreover,* $|s(k)|=|r(k)|$.

These properties follow from the x-scattering problem on the whole axis and can be found in Ref. 16. We also take into account that for the half-axis case $s_2^-(k)=-\overline{s_1^+}(\overline{k})$ is analytic in $k\in\mathbb{C}_-$ and the constants γ_j^1 are not independent parameters (that takes place for whole axis), and they are given in terms of the value of $s_1^+(k)$ at k_j:

$$\gamma_j^1=\frac{1}{s_1^+(k_j)}.$$

Analytic properties of the "scattering" matrix $P(k)$ are derived from the defining relation, i.e., from (3.2), (2.15), and (2.14):

$$P(k)=\mathcal{E}(0,k)+\int_0^{\infty}\mathcal{E}(0,k)\mathcal{E}^{-1}(t,k)[\hat{Q}(0,t,k)-\hat{Q}_0(t,k)]\hat{\Psi}(t,k)dt.$$

We stress only the main properties of $P(k)=\begin{pmatrix}p_1^-(k) & p_1^+(k)\\ p_2^-(k) & p_2^+(k)\end{pmatrix}$.

Properties of $P(k)$*: The scattering matrix* $P(k)$ *satisfies the following.*

(i) $P(k)=\sigma_2\overline{P(\overline{k})}\sigma_2$ *for* $k\in\Sigma$.
(ii) $\det P(k)\equiv\Delta(k)$ *for* $k\in\Sigma$.
(iii) $P(k)$ *is* C^{∞} *for* $k\in\Sigma'$.
(iv $P^+(k)$ *is meromorphic in* $k\in\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{III}}$.
(v) $P^-(k)$ *is meromorphic in* $k\in\Omega_{\mathrm{II}}\cup\Omega_{\mathrm{IV}}$.
(vi) $P(k)=\sigma_0+O(k^{-1})$, $k\in\Sigma$, $k\to\infty$.

Below we need to study properties of the "scattering" matrix $R(k)$ introduced by Eqs. (3.1) and (3.2). If we denote

$$R(k)=\begin{pmatrix}R_{\mathrm{II}}(k) & R_{\mathrm{I}}(k)\\ R_{\mathrm{IV}}(k) & R_{\mathrm{III}}(k)\end{pmatrix},$$

then

$$R_{\mathrm{I}}(k)=-\overline{R}_{\mathrm{IV}}(\overline{k}),\quad R_{\mathrm{III}}(k)=\overline{R}_{\mathrm{II}}(\overline{k})\quad\text{for } k\in\Sigma.$$

Moreover,

$$R_{\mathrm{II}}(k)=p_1^-(k)s_2^+(k)-p_2^-(k)s_1^+(k) \tag{3.8}$$

is meromorphic in $k\in\Omega_{\mathrm{II}}$ [hence $R_{\mathrm{III}}(k)$ is meromorphic in $k\in\Omega_{\mathrm{III}}$] and

$$R_{\mathrm{IV}}(k)=p_2^-(k)s_1^-(k)-p_1^-(k)s_2^-(k) \tag{3.9}$$

is meromorphic in $k \in \Omega_{IV}$ [hence $R_I(k)$ is meromorphic in $k \in \Omega_I$]. We remind that the branch of the square root (1.9) is fixed throughout the article and we deal with a single-valued analytic branch of the function $\mu(k)$ defined in (2.10).

From (3.1) we derive

$$Y^+(x,t,k) = R_I(k)\Psi^-(x,t,k) + R_{III}(k)\Psi^+(x,t,k).$$

Hence,

$$R_I(k) = \det(Y^+(x,t,k) \quad \Psi^+(x,t,k)),$$

$$R_{III}(k) = \det(\Psi^-(x,t,k) \quad Y^+(x,t,k)).$$

Let us put $x=0$, and $k = k_1 + ik_2 \in \Omega_I$. Using (2.3), (2.15), and (2.14) for large enough t we obtain

$$|R_I(k)| \leqslant C_1(k)\exp[8(k_1^0 k_2^0 - k_1 k_2)t],$$

where $C_1(k)$ is independent of t, and

$$k_1^0 k_2^0 = \max_{1 \leqslant j \leqslant n} [\mathrm{Re}\, k_j \mathrm{Im}\, k_j],$$

where $k_j \in \Omega_I$ is an eigenvalue of the x-scattering problem. Taking into account the analyticity of $R_I(k)$ in $k \in \Omega_I \backslash D$, choosing k large enough and putting $t \to \infty$ we find $R_I(k) \equiv 0$ for any $k \in \Omega_I$, hence also $R_{IV}(k) \equiv 0$ for any $k \in \Omega_{IV}$. So, we come to the main property of the compatible scattering problem for x- and t-equations.

Properties of $R(k)$: Let $\Gamma \cap \mathbb{R} = \{\kappa_\Gamma\}$. Then, for $k \in [\kappa_\Gamma, \infty)$, the "scattering" matrix $R(k)$ is diagonal:

$$R(k) = \begin{pmatrix} \rho_-(k) & 0 \\ 0 & \rho_+(k) \end{pmatrix}$$

with

$$\rho_+(k) = \frac{p_2^+(k)}{s_2^+(k)} = \frac{p_1^+(k)}{s_1^+(k)},$$

$$\rho_-(k) = \frac{p_1^-(k)}{s_1^-(k)} = \frac{p_2^-(k)}{s_2^-(k)}, \tag{3.10}$$

and the important relation

$$\frac{p_1^+(k)}{p_2^+(k)} \equiv \frac{s_1^+(k)}{s_2^+(k)}. \tag{3.11}$$

This relation means that $s(k) = s_1^+(k)/s_2^+(k)$, which is meromorphic on $\mathbb{C}_+$, is a meromorphic continuation of $p(k) = p_1^+(k)/p_2^+(k)$, which is meromorphic on Ω_I.

The asymptotic behavior of $S(k)$ and $P(k)$ yields the following asymptotic expansions, for $k \to \pm\infty$:

$$R_{\mathrm{II}}(k)=1+\frac{\rho_1}{k}+\cdots,$$

$$R_{\mathrm{IV}}(k)=\frac{\omega_1}{k}+\frac{\omega_2}{k^2}+\cdots.$$

Since $R_{\mathrm{IV}}(k)\equiv 0$ for $k\in[\kappa_\Gamma,\infty)$, then its asymptotic behavior is

$$R_{\mathrm{IV}}(k)=\mathrm{O}(k^{-\infty}) \quad \text{for} \quad k\to-\infty.$$

Hence,

$$R_{\mathrm{IV}}(k),\ \ R_{\mathrm{I}}(k)\in C^\infty(\mathbb{R}\backslash(\Sigma\kappa\cap\mathbb{R})),$$

$$R_{\mathrm{IV}}(k)\equiv 0 \quad \text{for} \quad k\in[\kappa_\Gamma,\infty), \tag{3.12}$$

$$R_{\mathrm{I}}(k)\equiv 0 \quad \text{for} \quad k\in[\kappa_\Gamma,\infty).$$

Therefore $R_{\mathrm{IV}}(k)$, $R_{\mathrm{I}}(k)$ and all their derivatives vanish at $k=\kappa_\Gamma$.

Since $\det R(k)\equiv\Delta(k)$, then

$$\rho_-(k)\rho_+(k)=|\rho_+(k)|^2\equiv\Delta(k).$$

Hence, $\rho_\pm(k)$ can be written

$$\rho_\pm(k)=\sqrt{\Delta(k)}\,\mathrm{e}^{\pm\mathrm{i}\nu(k)}, \quad k\in[\kappa_\Gamma,\infty) \tag{3.13}$$

for some real function $\nu(k)$ defined for $k\in[\kappa_\Gamma,\infty)$. This function has an analytic continuation also denoted $\nu(k)$ on $\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{IV}}$. This continuation satisfies $\nu(k)=\overline{\nu(\overline{k})}$ and tends to zero when $k\to\infty$ in view of the asymptotics of $s_2^+(k)$ and $p_2^+(k)$. It has logarithmic singularities at the points of the divisor D and different boundary values on cuts γ_j.

Indeed, in view of (3.10),

$$p_j^+(k)=\rho_+(k)\,s_j^+(k) \quad \text{for} \quad j=1,2. \tag{3.14}$$

$\rho_+(k)$ must have poles at the points of the divisor D and at the points where $s_1^+(k)$ and $s_2^+(k)$ vanish. On the other hand, $s_1^+(k)$ and $s_2^+(k)$ must simultaneously vanish at poles in view of the analyticity of the functions $p_j^+(k)$ in the domain $\Omega_{\mathrm{I}}\backslash D$. Hence $\Psi^+(x,t,k)$ is identically zero when k is a pole, which is impossible. So $\rho_+(k)$ is analytic in $k\in\Omega_{\mathrm{I}}$ with the exception of the points of the divisor D where it has simple poles. Hence the functions $p_j^+(k)$ and $s_j^+(k)$ have a common set of zeros, possibly empty, in Ω_{I}.

Other statements about $\nu(k)$ are very easy. So, for $R_{\mathrm{II}}(k)$ which is meromorphic in $k\in\Omega_{\mathrm{II}}$ we obtain

$$R_{\mathrm{II}}(k)=\frac{s_2^+(k)}{p_2^+(k)}\Delta(k)=\sqrt{\Delta(k)}\,\mathrm{e}^{-\mathrm{i}\nu(k)} \quad \text{for} \quad k\in\Gamma_+. \tag{3.15}$$

The last formula follows from relations

$$R_{\mathrm{II}}(k)=p_1^-(k)s_2^+(k)-p_2^-(k)s_1^+(k),$$

$$p_1^+(k)s_2^+(k)-p_2^+(k)s_1^+(k)=0.$$

Hence, $R_{\mathrm{II}}(k)$ has a meromorphic continuation to Ω_{I}, where it coincides with the function $\Delta(k)/\rho_+(k)$. Therefore $R_{\mathrm{II}}(k)$ does not vanish for $k\in[\kappa_\Gamma,\infty)\cup\Gamma_+$, and its only zeros are among the $z_j\in\Omega_{\mathrm{II}}$. Let $\Sigma_{\mathrm{d}}^{\mathrm{bc}}$ be the set of zeros of $R_{\mathrm{II}}(k)$:

$$\Sigma_{\mathrm{d}}^{\mathrm{bc}}=\{z_1,\ldots,z_m\}=\{z_j\in\Omega_{\mathrm{II}}|R_{\mathrm{II}}(z_j)=0\}.$$

Let

$$\rho(k):=\frac{R_{\mathrm{IV}}(k)}{R_{\mathrm{II}}(k)}.$$

As above we also assume the number of zeros of $R_{\mathrm{II}}(k)$ is finite and they are simple, i.e., $\dot{R}_{\mathrm{II}}(z_j)\neq 0$.

Properties of $\rho(k)$ and $R_{\mathrm{II}}(k)$: $\rho(k)$ and $R_{\mathrm{II}}(k)$ have the following properties:

(1) They satisfy the determinant relation

$$1+|\rho(k)|^2=\frac{\Delta(k)}{|R_{\mathrm{II}}(k)|^2},\quad k\in\mathbb{R}. \tag{3.16}$$

(2) $\rho(k),R_{\mathrm{II}}(k)\in C^\infty(\mathbb{R}\backslash(\Sigma_\kappa\cap\mathbb{R}))$ *and* $\rho(k)\equiv 0$ *for* $k\in[\kappa_\Gamma,\infty)$.

(3) $R_{\mathrm{II}}(k)=\sqrt{\Delta(k)}\,\mathrm{e}^{-\mathrm{i}\nu(k)}$ *for* $k\in[\kappa_\Gamma,\infty)$, *where* $\nu(k)$ *is real-valued and has an analytic continuation to* $\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{IV}}$.

(4) $\rho(k)$ *and all its derivatives have jumps at the real points* $\kappa_j<\kappa_\Gamma$*:*

$$\rho^{(l)}(\kappa_j-0)-\rho^{(l)}(\kappa_j+0)=f^{(l)}(\kappa_j),\quad l=0,1,\ldots, \tag{3.17}$$

where $f(k)$ *is defined for* $k\in\gamma_j^+=\gamma_j\cap\overline{\Omega}_{\mathrm{II}}$ by

$$f(k)=2\mathrm{i}\,\frac{\sqrt{\Pi_{i=0}^{g}(k-E_i)(k-\overline{E_i})}}{R_{\mathrm{II}}(k-0)R_{\mathrm{II}}(k+0)}\prod_{l=1}^{g}\frac{1}{k-\lambda_l},$$
$$\lambda_l=\pi(\mathcal{P}_l),\quad D=\mathcal{P}_1+\cdots+\mathcal{P}_g. \tag{3.18}$$

(5) The function

$$\rho(k)-r(k)=\frac{p_2^-(k)}{R_{\mathrm{II}}(k)s_2^+(k)}$$

has a meromorphic continuation to Ω_{II}.

Proof: The fourth item will be proved in the next section. The last item follows from Eqs. (3.8) and (3.9) which yield

$$p_1^-(k)=R_{\mathrm{IV}}(k)s_1^+(k)+R_{\mathrm{II}}(k)s_1^-(k)=R_{\mathrm{II}}(k)[1/s_2^+(k)+s_1^+(k)(\rho(k)-r(k))],$$

$$p_2^-(k)=R_{\mathrm{IV}}(k)s_2^+(k)+R_{\mathrm{II}}(k)s_2^-(k)=R_{\mathrm{II}}(k)s_2^+(k)[\rho(k)-r(k)]\quad\text{for}\quad k\in\mathbb{R}_-,$$

and the difference $\rho(k)-r(k)$ has a meromorphic continuation to the domain Ω_{II} because the l.h.s. is meromorphic in $k\in\Omega_{\mathrm{II}}$. Hence, the r.h.s. must have a meromorphic continuation to the domain Ω_{II}.

Besides we remind that $p_1^+(k)/p_2^+(k)=s_1^+(k)/s_2^+(k)$ has a meromorphic continuation to the domain $\mathbb{C}_+$, i.e., this ratio has no jump over the arcs γ_j^+.

The second main relation of the compatible scattering problem is

$$G(x,t,k)=\frac{1}{R_{\mathrm{II}}(k)}Y^-(x,t,k)=\Psi^-(x,t,k)+\rho(k)\Psi^+(x,t,k)\quad\text{for}\quad k\in\mathbb{R}. \tag{3.19}$$

The function $G(x,t,k)$ is analytic in $k\in\Omega_{\mathrm{II}}$, $k\neq z_j$ with poles at z_j's. Singularities at the points $\lambda_j=\pi(\mathcal{P}_j)$, $\mathcal{P}_j\in D$, are reduced since the divisor D does not depend on x and t, and $Y^-(x,t,k)$ and $R_{\mathrm{II}}(k)$ have simple poles at λ_j simultaneously. If $R_{\mathrm{II}}(z_j)=0$, $j=1,\ldots,m$, then $Y^-(x,t,z_j)$ and $\Psi^+(x,t,z_j)$ are linearly dependent:

$$Y^-(x,t,z_j)=\gamma_j^2\Psi^+(x,t,z_j),$$

hence

$$\mathrm{res}_{z_j}G(x,t,k)=c_j^2\Psi^+(x,t,z_j),$$

$$c_j^2=\frac{\gamma_j^2}{\dot{R}_{\mathrm{II}}(z_j)}$$

(the dot denotes differentiation with respect to k) with

$$\gamma_j^2=\frac{p_1^-(z_j)}{s_1^+(z_j)}=\frac{p_2^-(z_j)}{s_2^+(z_j)}.$$

Using asymptotics of the function $Y^-(x,t,k)$ at $k=\infty$ with $k\in\Omega_{\mathrm{II}}$, we find

$$G(x,t,k)=\left[\begin{pmatrix}1\\0\end{pmatrix}+\mathrm{O}(|k|^{-1})\right]\mathrm{e}^{-\mathrm{i}kx-2\mathrm{i}k^2t} \tag{3.20}$$

for $|k|\to\infty$, $k\in\Omega_{\mathrm{II}}$.

This asymptotic formula will be used in the next section. □

IV. THE MAIN INTEGRAL EQUATIONS

The main relations of the compatible scattering problem follow from (3.1), (3.2) and (3.5), (3.19):

$$F(x,t,k)=\Psi^-(x,t,k)+r(k)\Psi^+(x,t,k) \quad \text{for} \quad k\in\mathbb{R}, \tag{4.1}$$

$$G(x,t,k)=\Psi^-(x,t,k)+\rho(k)\Psi^+(x,t,k) \quad \text{for} \quad k\in\mathbb{R}. \tag{4.2}$$

These relations give

$$G(x,t,k)-F(x,t,k)=c(k)\Psi^+(x,t,k), \tag{4.3}$$

where $c(k)$ can be written as follows

$$c(k)=\rho(k)-r(k)=\begin{cases}-r(k) & \text{for} \quad k\in[\kappa_\Gamma,\infty),\\ \dfrac{p_2^-(k)}{s_2^+(k)\,R_{\mathrm{II}}(k)} & \text{for} \quad k\in(-\infty,\kappa_\Gamma].\end{cases} \tag{4.4}$$

Hence, $c(k)$ has a meromorphic continuation from the interval $(-\infty,\kappa_\Gamma]$ to the domain Ω_{II}, because $p_2^-(k)$, $s_2^+(k)$ and $R_{\mathrm{II}}(k)$ are meromorphic in $k\in\Omega_{\mathrm{II}}$. Hence, (4.3) is also true for $k\in\overline{\Omega}_{\mathrm{II}}$. The function $c(k)$ has poles at the z_j's, where $s_2^+(z_j)=R_{\mathrm{II}}(z_j)=0$. Since the number of zeros of $s_2^+(k)$ and $R_{\mathrm{II}}(k)$ is finite and they are simple, all poles of $c(k)$ are simple and their number is finite. Indeed, we only have to check the case $s_2^+(z_0)=R_{\mathrm{II}}(z_0)=0$. Due to (3.8) we also find $p_2^-(z_0)=0$. Poles which are related to the divisor D are reduced.

In view of the continuation of $c(k)$ to Ω_{II} we have the following relation on Γ_+:

$$\frac{Y^-(x,t,k-0)}{R_{\rm II}(k-0)}-\frac{\Phi^-(x,t,k+0)}{s_2^+(k+0)}=c(k)\Psi^+(x,t,k)\quad\text{for}\quad k\in\Gamma_+. \tag{4.5}$$

To deduce the integral equations of the inverse scattering problem let us put

$$h^-(x,t,k)=G(x,t,k)-\begin{pmatrix}1\\0\end{pmatrix}e^{-ikx-2ik^2t}\quad\text{for}\quad k\in(-\infty,\kappa_\Gamma],$$

$$h^+(x,t,k)=F(x,t,k)-\begin{pmatrix}1\\0\end{pmatrix}e^{-ikx-2ik^2t}\quad\text{for}\quad k\in[k_\Gamma,\infty\rangle.$$

$h^-(x,t,k)$ has different left and right boundary values at each $k\in\gamma_j^+=\gamma_j\cap\overline{\Omega}_{\rm II}$:

$$\begin{aligned}h^-(x,t,k-0)-h^-(x,t,k+0)&=G(x,t,k-0)-G(x,t,k+0)\\&=\frac{Y^-(x,t,k-0)R_{\rm II}(k+0)-Y^-(x,t,k+0)R_{\rm II}(k-0)}{R_{\rm II}(k+0)R_{\rm II}(k-0)}.\end{aligned}$$

Since $R_{\rm II}(k)=\det(Y^-(x,t,k)\ \ \Psi^+(x,t,k))$ one can find

$$\begin{aligned}&Y^-(x,t,k-0)R_{\rm II}(k+0)-Y^-(x,t,k+0)R_{\rm II}(k-0)\\&\quad=Y^-(x,t,k-0)\det(Y^-(x,t,k+0)\quad\Psi^+(x,t,k))\\&\qquad-Y^-(x,t,k+0)\det(Y^-(x,t,k-0)\quad\Psi^+(x,t,k))\\&\quad=\det(Y^-(x,t,k+0)\quad Y^-(x,t,k-0))\Psi^+(x,t,k)\\&\quad=\det(e(0,k+0)\quad e(0,k-0))\Psi^+(x,t,k).\end{aligned}$$

Comparing analytic properties of

$$\det(e(0,k+0)\quad e(0,k-0))\ \text{ and }\ \frac{2i\sqrt{X(k)}}{(k-\lambda_1)\cdots(k-\lambda_g)},\quad \lambda_l=\pi(\mathcal{P}_l),\quad D=\sum_{l=1}^g\mathcal{P}_l$$

as functions on the Riemann surface $\mathcal{X}$ we infer that they coincide. Therefore

$$h^-(x,t,k-0)-h^-(x,t,k+0)=f(k)\Psi^+(x,t,k),\quad k\in\gamma_j^+=\gamma_j\cap\overline{\Omega}_{\rm II}, \tag{4.6}$$

where

$$f(k)=2i\frac{\sqrt{\Pi_{j=0}^g(k-E_j)(k-\overline{E_j})}}{R_{\rm II}(k-0)R_{\rm II}(k+0)}\prod_{l=1}^g\frac{1}{k-\lambda_l}.$$

Taking into account analytic continuation of the relation (4.3) to $\Omega_{\rm II}$ we find that for $k\in\gamma_j^+$

$$[c(k-0)-c(k+0)]\Psi^+(x,t,k)=G(x,t,k-0)-G(x,t,k+0),$$

and as above

$$c(k-0)-c(k+0)=f(k),\quad k\in\gamma_j^+, \tag{4.7}$$

where $c(k\mp0)$ are the left and right boundary values of $c(k)$ on γ_j^+.

Let us consider the integral

$$J(x,y,t)=\frac{1}{2\pi}\int_{-\infty}^{\kappa_\Gamma}h^-(x,t,k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\mathrm{d}k+\frac{1}{2\pi}\int_{\kappa_\Gamma}^{\infty}h^+(x,t,k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\mathrm{d}k.$$

Using Eqs. (4.1)–(4.3) and (2.3) we find

$$J(x,y,t)=\begin{pmatrix}K_1\\K_2\end{pmatrix}(x,y,t)+\begin{pmatrix}0\\1\end{pmatrix}F_s(x+y,t)+\int_x^\infty\begin{pmatrix}-\overline{K}_2\\\overline{K}_1\end{pmatrix}(x,z,t)F_s(z+y,t)\mathrm{d}z,$$

where

$$\begin{aligned}F_s(x,t)&=\frac{1}{2\pi}\int_{-\infty}^{\kappa_\Gamma}\rho(k)\mathrm{e}^{\mathrm{i}k(x+y)+4\mathrm{i}k^2t}\mathrm{d}k+\frac{1}{2\pi}\int_{\kappa_\Gamma}^{\infty}r(k)\mathrm{e}^{\mathrm{i}k(x+y)+4\mathrm{i}k^2t}\mathrm{d}k\\&=\frac{1}{2\pi}\int_{-\infty}^{\kappa_\Gamma}c(k)\mathrm{e}^{\mathrm{i}k(x+y)+4\mathrm{i}k^2t}\mathrm{d}k+\frac{1}{2\pi}\int_{-\infty}^{\infty}r(k)\mathrm{e}^{\mathrm{i}k(x+y)+4\mathrm{i}k^2t}\mathrm{d}k.\end{aligned}$$

On the other hand, using estimates (3.7) and (3.20) of $F(x,t,z)$ and $G(x,t,z)$ for large k, taking into account (4.3), (4.5) and (4.6), and applying the Jordan lemma, we find

$$\begin{aligned}J(x,y,t)=&\mathrm{i}\sum_{\substack{k_j\in\Omega_\mathrm{I}\\ s_2^+(k_j)=0}}\mathrm{res}_{k_j}[h^+(x,t,k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}]+\mathrm{i}\sum_{\substack{z_j\in\Omega_\mathrm{II}\\ R_\mathrm{II}(z_j)=0}}\mathrm{res}_{z_j}[h^-(x,t,k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}]\\&-\frac{1}{2\pi}\int_{\Gamma_+}[h^-(x,t,k)-h^+(x,t,k)]\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\mathrm{d}k-\frac{1}{2\pi}\sum_{\gamma_j^+\in\overline{\Omega}_\mathrm{II}}\int_{\gamma_j^+}[h^-(x,t,k-0)\\&-h^-(x,t,k+0)]\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\mathrm{d}k\\=&-\sum_{k_j\in\Omega_\mathrm{I}}m_j^1\mathrm{e}^{\mathrm{i}k_jy+2\mathrm{i}k_j^2t}\Psi^+(x,t,k_j)-\sum_{z_j\in\Omega_\mathrm{II}}m_j^2\mathrm{e}^{\mathrm{i}z_jy+2\mathrm{i}z_j^2t}\Psi^+(x,t,z_j)\\&-\frac{1}{2\pi}\int_{\Gamma_+}c(k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\Psi^+(x,t,k)\mathrm{d}k-\frac{1}{2\pi}\sum_{\gamma_j^+\in\overline{\Omega}_\mathrm{II}}\int_{\gamma_j^+}f(k)\mathrm{e}^{\mathrm{i}ky+2\mathrm{i}k^2t}\Psi^+(x,t,k)\mathrm{d}k.\end{aligned}$$

Finally, we have the following integral equations of the inverse scattering:

$$K_1(x,y,t)-\int_x^\infty\overline{K}_2(x,z,t)H(z+y,t)\mathrm{d}z=0\quad\text{for}\quad 0\leqslant x<y<\infty,\tag{4.8}$$

$$\overline{K}_2(x,y,t)+\overline{H}(x+y,t)+\int_x^\infty K_1(x,z,t)\overline{H}(z+y,t)\mathrm{d}z=0,\tag{4.9}$$

with the kernel

$$\begin{aligned}H(x,t)=&\sum_{k_j\in\Omega_\mathrm{I}}m_j^1\mathrm{e}^{\mathrm{i}k_jx+4\mathrm{i}k_j^2t}+\sum_{z_j\in\Omega_\mathrm{II}}m_j^2\mathrm{e}^{\mathrm{i}z_jx+4\mathrm{i}z_j^2t}+\frac{1}{2\pi}\sum_{\gamma_j^+\in\overline{\Omega}_\mathrm{II}}\int_{\gamma_j^+}f(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k\\&+\frac{1}{2\pi}\left(\int_{-\infty}^{\kappa_\Gamma}+\int_{\Gamma_+}\right)c(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k+\frac{1}{2\pi}\int_{-\infty}^{\infty}r(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k.\end{aligned}\tag{4.10}$$

The coefficients m_j^1 and m_j^2 are given by

$$m_j^1=[\mathrm{i}s_1^+(k_j)\dot{s}_2^+(k_j)]^{-1},$$
$$m_j^2=p_1^-(z_j)[\mathrm{i}s_1^+(z_j)\dot{R}_{\mathrm{II}}(z_j)]^{-1}=p_2^-(z_j)[\mathrm{i}s_2^+(z_j)\dot{R}_{\mathrm{II}}(z_j)]^{-1}=-\mathrm{i}\ \mathrm{res}_{z_j}c(k). \tag{4.11}$$

Taking into account the jump relations (4.7) for $c(k)$ on γ_j^+ the kernel $H(x,t)$ can be written in the form (1.14). For further analysis of the kernel properties we rewrite this kernel (4.10) as follows:

$$H(x,t)=\sum_{k_j\in\Omega_{\mathrm{I}}} m_j^1\mathrm{e}^{\mathrm{i}k_jx+4\mathrm{i}k_j^2t}+\sum_{z_j\in\Omega_{\mathrm{II}}} m_j^2\mathrm{e}^{\mathrm{i}z_jx+4\mathrm{i}z_j^2t}+\frac{1}{2\pi}\sum_{\gamma_j^+\in\Omega_{\mathrm{II}}^-}\int_{\gamma_j^+} f(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k$$
$$+\frac{1}{2\pi}\int_{-\infty}^{\kappa_\Gamma}\rho(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k+\int_{\Gamma_+} c(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k+\frac{1}{2\pi}\int_{\kappa_\Gamma}^{\infty} r(k)\mathrm{e}^{\mathrm{i}kx+4\mathrm{i}k^2t}\mathrm{d}k, \tag{4.12}$$

using the relation

$$c(k)+r(k)=\rho(k). \tag{4.13}$$

For any fixed $t\in\mathbb{R}_+$ the function $H(x,t)$ will be rapidly decreasing for $x\to\infty$, if (3.17) and (4.13) are fulfilled. Indeed, using the method of steepest descent and integration by parts we see that $H(x,t)=\mathrm{O}(x^{-\infty})$ because $c(k)$, $r(k)$, $\rho(k)$ are C^∞ away from self-intersection points κ_j and, according to their asymptotic behavior, they vanish at infinity as well as their derivatives of any order. The integrated terms vanish at the points $k=\kappa_j\mp 0$ because of relations (3.17) on jumps of $\rho(k)$ and their derivatives and

$$\frac{\mathrm{d}^m}{\mathrm{d}k^m}(\rho(k)-c(k)-r(k))\bigg|_{k=\kappa_\Gamma}=0,\quad m=0,1,2,\ldots, \tag{4.14}$$

which follows from (4.13). The contribution of the stationary point $[k_{\mathrm{st}}=-(x+y)/(8t)\in\mathbb{R}_-]$ is given by the Schwartz type function $\rho(k)$. Hence $H(x,t)$ is rapidly decreasing for $x\to\infty$ for any fixed t.

On the other hand, using (4.9) for $y=x$ one can prove that $H(x,t)\in C^\infty(\mathbb{R}_+\times\mathbb{R}_+)$ and is of Schwartz type, $H(x,t)=\mathrm{O}(x^{-\infty})$, as $x\to\infty$, since $K_1(x,y,t)$ and $K_2(x,y,t)$ belong to $C^\infty(\mathbb{R}_+\times\mathbb{R}_+\times\mathbb{R}_+)$ and are of Schwartz type also as $x+y\to\infty$, and Eq. (4.9) is a Volterra integral equation with respect to the kernel $H(x,t)$. Using the method of steepest descent and integrating by parts as above, taking into account the discontinuity of $\rho(k)$ at the points $\kappa_j<\kappa_\Gamma$ and its vanishing with all derivatives at the point κ_Γ we find that relations (3.17) must be fulfilled because $H(x,t)=\mathrm{O}(x^{-\infty})$.

Remark: For $t=0$ the kernel $H(x,t)|_{t=0}$ coincides with the kernel

$$H_0(x)=\sum_{k_j\in\mathbb{C}_+} m_j^1\mathrm{e}^{\mathrm{i}k_jx}+\frac{1}{2\pi}\int_{-\infty}^{\infty} r(k)\,\mathrm{e}^{\mathrm{i}kx}\mathrm{d}k,$$

because in this case ($t=0$) the integrals over the boundary of Ω_{II} can be evaluated by using jump relations (4.7) and the residues of the function $c(k)$. After integration we find that $H(x,0)=H_0(x)$. Then Marchenko integral equations with kernel $H_0(x)$ yield that $q(x,0)=u(x)$.

Definition (scattering data): Now it is natural to introduce the set

$$\mathcal{R}=\{k_1,\ldots,k_n\in\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{II}};\ z_1,\ldots,z_m\in\Omega_{\mathrm{II}};\ \ r(k),\rho(k),R_{\mathrm{II}}(k)\} \tag{4.15}$$

and to call $\mathcal{R}$ the *scattering data* for the compatible system of differential equations (1.7) and (1.8) with $q(x,t)$ satisfying (1.1)–(1.6).

The kernel $H(x,t)$ of the Marchenko equations is completely defined by the scattering data $\mathcal{R}$ because the missing coefficients m_j^1, m_j^2 of (4.11) and the functions $f(k)$, $c(k)$ can be determined from scattering data values.

We remind that both finite-gap functions $\alpha(t)$, $\beta(t)$ and the corresponding Riemann surface $\mathcal{X}$ are given. Therefore, the function

$$\Delta(k)=\det \mathcal{E}(t,k)$$

is also known. It immediately follows from properties proved above that scattering data $\mathcal{R}$ satisfy the following conditions.

Condition A:

(1) $r(k)\in\mathcal{S}(\mathbb{R})$.
(2) $r(k)=b(k)/a(k)$, where $b(k):=-s_2^-(k)$ is analytic in $k\in\mathbb{C}_-$, and $a(k):=s_2^+(k)$ is analytic for $k\in\mathbb{C}_+$ and has the form

$$a(k)=\prod_{j=1}^{n}\frac{k-k_j}{k-\overline{k_j}}\exp\left[\frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\frac{\log(1+|r(s)|^2)\mathrm{d}s}{s-k}\right],\quad k\in\mathbb{C}_+.$$

Condition B:

(1) $\rho(k),R_{\mathrm{II}}(k)\in C^\infty(\mathbb{R}\backslash(\Sigma_\kappa\cap\mathbb{R}))$ and $\rho(k)\equiv 0$ for $k\in[\kappa_\Gamma,\infty)$.
(2) $R_{\mathrm{II}}(k)$ is analytic in $k\in\Omega_{\mathrm{II}}$, where it has a finite number of zeros $z_1,\ldots,z_m$, each of multiplicity 1.
(3) $\rho(k)$ and $R_{\mathrm{II}}(k)$ are connected by

$$1+|\rho(k)|^2=\frac{\Delta(k)}{|R_{\mathrm{II}}(k)|^2},\quad k\in\mathbb{R}.$$

(4) $R_{\mathrm{II}}(k)=\sqrt{\Delta(k)}\,\mathrm{e}^{-\mathrm{i}\nu(k)}$ for $k\in[\kappa_\Gamma,\infty)$, where $\nu(k)$ is a real-valued function with analytic continuation to $\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{IV}}$.
(5) $\rho(k)$ and all its derivatives have jumps at the real points $\kappa_j<\kappa_\Gamma$:

$$\rho^{(l)}(\kappa_j-0)-\rho^{(l)}(\kappa_j+0)=f^{(l)}(\kappa_j),\quad l=0,1,\ldots,$$

where $f(k)$ is defined for $k\in\gamma_j^+=\gamma_j\cap\overline{\Omega}_{\mathrm{II}}$ by

$$f(k)=2\mathrm{i}\frac{\sqrt{\Pi_{j=0}^{g}(k-E_j)(k-\overline{E_j})}}{R_{\mathrm{II}}(k-0)R_{\mathrm{II}}(k+0)}\prod_{l=1}^{g}\frac{1}{k-\lambda_l},\quad \lambda_l=\pi(\mathcal{P}_l).$$

Condition C:

(1) The function $c(k)=\rho(k)-r(k)$ extends analytically to Ω_{II}, where it has a finite number of poles $z_1,\ldots,z_m$, all simple, and satisfies the jump relations:

$$c(k-0)-c(k+0)=f(k),\quad k\in\gamma_j^+.$$

One can think that properties A–C are characteristic, i.e., that they are also sufficient for numbers $k_1,\ldots,k_n$, $z_1,\ldots,z_m$ and functions $r(k)$, $\rho(k)$, $R_{\mathrm{II}}(k)$ to be the scattering data of a compatible system of x- and t-equations (1.7) and (1.8) with $q(x,t)$ satisfying (1.1)–(1.6).

Anyway, formula (1.11) and Marchenko integral equations (4.8) and (4.9) represent a solution of the focusing nonlinear Schrödinger equation if the kernel (4.10) is sufficiently smooth and rapidly decreasing as $x\to\infty$. It follows from statements of the next section.

V. GENERATION OF ASYMPTOTIC SOLITONS BY BOUNDARY DATA

Let $\mathcal{R}=\{k_1,\ldots,k_n\in\Omega_{\mathrm{I}}\cup\Omega_{\mathrm{II}};\ z_1,\ldots,z_m\in\Omega_{\mathrm{II}};r(k),\rho(k),R_{\mathrm{II}}(k)\}$ be data satisfying conditions A–C. Then the following statements are true.

Statements: (1) The xt-integral equation

$$K(x,y,t)+\mathcal{H}(x+y,t)+\int_x^\infty K(x,z,t)\mathcal{H}(z+y,t)\mathrm{d}z=0,$$
$$0\leqslant x<y<\infty,\quad 0\leqslant t<\infty, \tag{5.1}$$

with the 2×2 matrix kernel

$$\mathcal{H}(x,t)=\begin{pmatrix} 0 & H(x,t)\\ -\overline{H}(x,t) & 0\end{pmatrix},$$

where $H(x,t)$ is given by (4.10), is uniquely solvable in the space $L^1(x,\infty)$ for any $x\geqslant 0$ and $t\geqslant 0$.

(2) The solution $K(x,y,t)$ belongs to $C^\infty(\mathbb{R}_+\times\mathbb{R}_+\times\mathbb{R}_+)$, it and all its derivatives decrease faster than any negative power of $x+y$, for $x+y\to\infty$, and t fixed.

(3) The matrix

$$\Psi(x,t,k)=\left[\mathrm{e}^{-\mathrm{i}kx\sigma_3}+\int_x^\infty K(x,y,t)\mathrm{e}^{-\mathrm{i}ky\sigma_3}\mathrm{d}y\right]\mathrm{e}^{-2\mathrm{i}k^2t\sigma_3}$$

satisfies the symmetry condition

$$\Psi(x,t,k)=\sigma_2\overline{\Psi}(x,t,k)\sigma_2\quad\text{for}\quad k\in\mathbb{R}$$

and is a solution of the x-equation (1.7) with $Q(x,t)$ given by

$$Q(x,t)=\sigma_3K(x,x,t)\sigma_3-K(x,x,t). \tag{5.2}$$

(4) $\Psi(x,t,k)$ is a solution of the x- and t-equations constructed from the matrix $Q(x,t)$ and its derivative $Q_x(x,t)$, using Eqs. (5.2), (1.7), (1.8) and (2.4).

Statement 1 follows from the following lemma about the solvability of the xt-integral equation.

Lemma 2: Let $\mathcal{R}$ be data satisfying conditions A–C. *Then, the xt-integral equation (5.1) is uniquely solvable in the space $L^1(x,\infty)$.*

Proof: Under conditions A–C the integral operator of the xt-integral equation is compact in the space $L^1(x,\infty)$. Then, by Fredholm theory the xt-integral equation has a unique solution if the homogeneous equation has no nonzero solution. If a nonzero solution does exist in $L^1(x,\infty)$, in view of the homogeneity of the integral equation, it is bounded, hence it belongs to $L^2(x,\infty)$. The integral operator is clearly skew-Hermitian in $L^2(x,\infty)$, so we obtain a contradiction, because the only solution in this case is zero. □

We omit proofs of the remaining statements because they are almost the same as in Ref. 16. Now let us sketch the proof of the main result.

Sketch of proof of Theorem 1: For study of the asymptotic behavior of the solution $q(x,t)$ we use the integral equation (5.1), which is uniquely solvable in the space $L^1(x,\infty)$ and, due to the statements above, represents a C^∞ and fast decreasing function $q(x,t)$. We carry out the asymptotic analysis of the integral equation by reducing the problem to degenerated integral equations, obtaining a determinant formula for the solution and its asymptotics as $t\to\infty$.

Taking into account properties A–C and using the method of steepest descent and integration by parts we come to the following decomposition of the scalar kernel $H(x,t)$ as $t\to\infty$:

$$H(x,t)=H_N(x,t)+H_1(x,t)+R_0(x,t)+R_1(x,t), \tag{5.3}$$

where $H_N(x,t)$ is a degenerate one:

$$H_N(x+y,t)=\mathrm{e}^{-(a+\mathrm{i}b)(\xi+\eta)}\sum_{m=0}^{N-1}\frac{d_m(t)}{m!t^{m+3/2}}(\xi+\eta)^m,$$

$$\xi=x-4bt,\quad \eta=y-4bt.$$

$R_0(x+y,t)$ is given in terms of $\rho(k)$ by

$$R_0(x+y,t)=\frac{1}{\sqrt{16\pi t}}\rho\left(-\frac{x+y}{8t}\right)\exp\left[\frac{\mathrm{i}\pi}{4}-4\mathrm{i}t\left(\frac{x+y}{8t}\right)^2\right].$$

$H_1(x+y,t)$ and $R_1(x+y,t)$ admit the estimates

$$|H_1(x+y,t)|\leqslant C_1|\xi+\eta|^N\ t^{-N-3/2}\mathrm{e}^{-a(\xi+\eta)},$$

$$|R_1(x+y,t)|\leqslant C_2t^{-3/2}\left|\rho''\left(-\frac{x+y}{8t}\right)\right|.$$

Let $\hat{H}$ be the integral operator which acts in $L^2(x,\infty)$ by

$$(\hat{H}f)(y)=\int_x^\infty\begin{pmatrix}0 & H(y+z,t)\\ -\overline{H}(y+z,t) & 0\end{pmatrix}\begin{pmatrix}f_1(y)\\ f_2(y)\end{pmatrix}\mathrm{d}z.$$

Then the Marchenko integral equations take the form

$$\begin{gathered}(I+\hat{H})K=G,\\ K=(K_1\ \ K_2),\quad G=(0\ \ \overline{H}).\end{gathered}\tag{5.4}$$

Under conditions A–C, (5.4) has a unique solution $\hat{H}$ in $L^2(x,\infty)$ and

$$\|(I+\hat{H})^{-1}\|\leqslant 1.$$

Let $\hat{H}_N$, $\hat{R}_0$, $\hat{H}_1$, $\hat{R}_1$ be the corresponding integral operators in $L^2(x,\infty)$ given by the kernels H_N, R_0, H_1, R_1. We look for a solution of (5.4) in the form

$$K=\tilde{K}+\psi,$$

where $\tilde{K}$ satisfies

$$\begin{gathered}(I+\hat{H}_N+\hat{R}_0)\tilde{K}=G_N+G_0,\\ G_N=(0\ \ \overline{H}_N),\quad G_0=(0\ \ \overline{R}_0).\end{gathered}\tag{5.5}$$

Then, $\psi=K-\tilde{K}$ satisfies

$$(I+\hat{H})\psi=G_1-\hat{H}_1\tilde{K}-\hat{R}_1\tilde{K},$$

$$G_1=(0\ \ \overline{H}_1+\overline{R}_1).$$

The last equation yields the estimate

$$\|\psi\|=\|K-\tilde{K}\|\leqslant C(N)t^{-1/2+\epsilon}$$

in the domain $\Omega_N(t)$ with $0<\epsilon<\frac{1}{2}$. This estimate allows us to consider below the integral equation (5.5) instead of (5.4).

The next step is as follows. Let $L=(L_1(x,y,t)\quad L_2(x,y,t))$ be a solution of

$$(I+\hat{R}_0)L=G_R,$$
$$G_R=(0\quad \overline{R}_0). \tag{5.6}$$

Then, the solution $\tilde{K}$ of (5.5) can be written in the form

$$\tilde{K}=L+(I+\hat{Q})M, \tag{5.7}$$

where $I+\hat{Q}=(I+\hat{R}_0)^{-1}$, and $\hat{Q}$ is an integral operator. The kernel $Q(y,z)$ of this operator has an explicit representation via the vector-function $L(y,z)$. The substitution of (5.7) into (5.5) yields a degenerate integral equation

$$M+\hat{H}_N(I+\hat{Q})M=G_N-\hat{H}_N L. \tag{5.8}$$

The next decisive step is that (5.6) can be explicitly solved in the limit $t\to\infty$. Namely, it is possible to show[26] that for $t\to\infty$

$$\|L_1(x,y,t)-L_1^{(\infty)}(x,y,t)\|_{C([X,\infty))}=o(1),$$
$$\|L_2(x,y,t)-L_2^{(\infty)}(x,y,t)\|_{L^2(X,\infty)}=o(1),\quad t\to\infty,$$

where

$$L_1^{(\infty)}(x,y,t)=-\frac{2}{\sqrt{\pi}}e^{\pi i/4}\int_X^\infty N(X,Z)\rho(-Z-Y)\exp(4it[X^2-Y^2+2(X-Y)Z])dZ,$$

$$L_2^{(\infty)}(x,y,t)=\frac{1}{\sqrt{t}}N(X,Y)\exp[4it(X+Y)^2],\quad X=\frac{x}{t},\quad Y=\frac{y}{t},$$

with

$$N(X,Y)=\frac{1}{4\sqrt{\pi}}e^{\pi i/4}\rho(-X-Y)\exp\left(\frac{i}{2\pi}\int_X^\infty\frac{\ln[1+|\rho(-X-S)|^2]}{S-Y-i0}dS\right).$$

This explicit formula and the degenerate integral equation (5.8) allow us to complete the proof of Theorem 1 in the same way as in Ref. 26. □

Sketch of proof of Theorem 2: In the case of Theorem 2, when $\min_{0\leqslant j\leqslant g}\mathrm{Re}\,E_j>0$, the kernel $H(x,t)$ has the form

$$H(x,t)=\sum_{k_j\in\Omega_{\mathrm{I}}}m_j^1e^{ik_jx+4ik_j^2t}+\sum_{z_j\in\Omega_{\mathrm{II}}}m_j^2e^{iz_jx+4iz_j^2t}+\frac{1}{2\pi}\left(\int_{-\infty}^{\kappa_\Gamma}+\int_{\Gamma_+}\right)c(k)e^{ikx+4ik^2t}dk$$
$$+\frac{1}{2\pi}\int_{-\infty}^{\infty}r(k)e^{ikx+4ik^2t}dk.$$

Therefore the corresponding decomposition as $t\to\infty$ will be similar to (5.3), but now the degenerate kernel has an ordinary solitonic form:

$$H_N(x,t)=\sum_{k_j\in\Omega_{\mathrm{I}}} m_j^1 \mathrm{e}^{\mathrm{i}k_j x+4\mathrm{i}k_j^2 t}+\sum_{z_j\in\Omega_{\mathrm{II}}} m_j^2 \mathrm{e}^{\mathrm{i}z_j x+4\mathrm{i}z_j^2 t}.$$

It is easy to see that such a kernel generates

(i) solitons which move to the right, i.e., away from the boundary (they correspond to the eigenvalues $k_j\in\Omega_{\mathrm{I}}$ and $z_j\in\Omega_{\mathrm{II}}$ with negative real part),
(ii) and other solitons which move to the left (they correspond to the eigenvalues $k_j\in\Omega_{\mathrm{I}}$ with positive real part) and which are absorbed by the boundary $x=0$ in finite time.

The proof of Theorem 2 we carry out by the same approach as above, using Ref. 27. □

APPENDIX: FINITE-GAP FUNCTIONS

Let $\mathcal{X}$ be the hyperelliptic Riemann surface of genus g given by the equation

$$z^2=\prod_{j=0}^{g}(k-E_j)(k-\overline{E}_j),$$

where $\mathrm{Im}\,E_j>0$, $E_i\neq E_j$ for $i\neq j$. This Riemann surface is a double covering of the complex k-plane $\overline{\mathbb{C}}=\mathbb{C}\cup\{\infty\}$ obtained by gluing two copies of $\overline{\mathbb{C}}$ along cuts γ_j whose endpoints are the $2g+2$ branch points E_j, $\overline{E}_j$. Let

$$\pi:\mathcal{X}\to\overline{\mathbb{C}}$$

be the canonical projection on the k-plane, and let $k=k(\mathcal{P})=\pi(\mathcal{P})$ be the image of a point $\mathcal{P}\in\mathcal{X}$. Each point $k\in\overline{\mathbb{C}}$ has two preimages on $\mathcal{X}$, except for the $2g+2$ branch points. Denote the preimage of $k=\infty$ on the upper (lower) sheet $\mathcal{X}^+$ ($\mathcal{X}^-$) of $\mathcal{X}$ by $\mathcal{P}=\infty^+$ ($\mathcal{P}=\infty^-$). We fix the branch of the square root by the asymptotic behavior

$$\sqrt{\prod_{j=0}^{g}(k-E_j)(k-\overline{E}_j)}=\pm k^{g+1}[1+\mathrm{O}(k^{-1})],\qquad k\to\infty^{\pm}\in\mathcal{X}_{\pm}. \tag{A1}$$

Let $D=\mathcal{P}_1+\cdots+\mathcal{P}_g$ be a nonspecial integral divisor on $\mathcal{X}\backslash\{\infty^+,\infty^-\}$ and let $\phi(t,\mathcal{P})$ be the Baker–Akhiezer vector function on $\mathcal{X}$ whose divisor of poles is D:

(i) $\phi(t,\mathcal{P})$ is meromorphic on $\mathcal{X}\backslash\{\infty^+,\infty^-\}$ with divisor of poles D;
(ii) the product $\phi(t,\mathcal{P})\exp\{2\,\mathrm{i}k^2(\mathcal{P})t\}$ is analytic at $\infty^{\pm}$.

The Baker–Akhiezer function satisfies the following equation:[28]

$$\phi_t+2\mathrm{i}k^2\sigma_3\phi=\hat{Q}_g(t,k)\phi, \tag{A2}$$

where $k=k(\mathcal{P})$, $\mathcal{P}\in\mathcal{X}$, and

$$\hat{Q}_g(t,k)=2kQ_g(t)-\mathrm{i}(Q_g^2(t)+Q_{1g}(t))\sigma_3$$

$$Q_g(t)=\begin{pmatrix}0 & \alpha(t)\\ -\overline{\alpha}(t) & 0\end{pmatrix},\quad Q_{1g}(t)=\begin{pmatrix}0 & \beta(t)\\ -\overline{\beta}(t) & 0\end{pmatrix}.$$

Definition: The functions $\alpha(t)$ and $\beta(t)$ are called *finite-gap* if there exists a Baker–Akhiezer vector-function on a hyperelliptic Riemann surface $\mathcal{X}$ of finite genus which is a solution of (A2).

The function $\phi(t,\mathcal{P})$ can be written[28] through Riemann theta functions. To establish this representation we need to define several notions.

The first is a homology basis on the hyperelliptic Riemann surface $\mathcal{X}$. It is a system of equivalent classes of closed, noncontractible, oriented contours on $\mathcal{X}$. Two contours are considered equivalent if their difference (the union with the orientation of one contour reversed) forms the oriented boundary of a surface in $\mathcal{X}$. The equivalence classes will be referred to by representatives. Two contour representatives of the same class are called homologous cycles. The integral of any meromorphic differential without residues gives the same value over any two homologous cycles. The system of homology classes is a linear space with integer coefficients $H_1(\mathcal{X},\mathbb{Z})$. The zero element is the equivalence class of contractible oriented loops on $\mathcal{X}$. It is a topological result that this space has dimension $2g$. Let c_1 and c_2 be two oriented closed contours on $\mathcal{X}$. The intersection number $c_1\cdot c_2$ is defined as the number of times c_2 crosses c_1 from the right of c_1, minus the number of times c_2 crosses c_1 from the left. The intersection number is a skew-symmetric bilinear form on $H_1(\mathcal{X},\mathbb{Z})$. A *canonical homology basis* is a symplectic basis, i.e., a basis $\{a_1,\ldots,a_g;b_1,\ldots,b_g\}$ of $H_1(\mathcal{X},\mathbb{Z})$ such that

$$a_j\cdot a_k=b_j\cdot b_k=0,\quad a_j\cdot b_l=\delta_{jl}.$$

This does not make the basis unique, even up to homology equivalence of class representatives. Any linear transformation with integer coefficients of the basis elements will preserve the intersection number but modify the particular basis. One can select a particular homology basis in order to simplify the formulas that we will write down, but the results themselves, by uniqueness, are independent of this choice. Once the homology cycles a_j are fixed, the dual cycles b_j are determined by the intersection relation up to transformation of the form:

$$b_j\to b_j+\sum_{l=1}^{g} s_{jl}a_l,$$

where the s_{jl}'s are integers and $s_{lj}=s_{jl}$.

The next ingredient we need are the *normalized holomorphic differentials, Riemann theta functions, Abel map and Jacobian variety*. The space of *holomorphic differentials* on $\mathcal{X}$ has dimension g, with basis $\{\omega_1(\mathcal{P}),\ldots,\omega_g(\mathcal{P})\}$ that can be written

$$\omega_j(\mathcal{P})=\frac{\Sigma_{i=0}^{g}c_{ji}k^i(\mathcal{P})}{X_{\mathcal{X}}(\mathcal{P})}\,\mathrm{d}k(\mathcal{P}),$$

where $X_{\mathcal{X}}(\mathcal{P})$ is a lifting of the function $X(k)$ from the cut plane to the Riemann surface $\mathcal{X}$: if $\mathcal{P}$ is on the first sheet of $\mathcal{X}$, then $X_{\mathcal{X}}(\mathcal{P})=X(k(\mathcal{P}))$, and if $\mathcal{P}$ is on the second sheet of $\mathcal{X}$, then $X_{\mathcal{X}}(\mathcal{P})=-X(k(\mathcal{P}))$. The coefficients c_{jl} are uniquely determined by the normalization relations:

$$\int_{a_l}\omega_j(\mathcal{P})=\delta_{jl}.$$

These *normalized holomorphic differentials* define the b-period matrix B by

$$B_{jl}=\int_{b_l}\omega_j(\mathcal{P}).$$

This matrix is symmetric with imaginary part positive definite.

Associated with B there is a *Riemann theta function* Θ defined by the Fourier series

$$\Theta(u_1,\ldots,u_g)=\sum_{\mathbf{n}\in\mathbb{Z}^g}\exp\{\pi\mathrm{i}(B\mathbf{n},\mathbf{n})+2\pi\mathrm{i}(\mathbf{n},\mathbf{u})\}.$$

where $\mathbf{u}\in\mathbb{C}^g$ and $(\mathbf{n},\mathbf{u})=n_1u_1+\cdots+n_gu_g$.

Let $\{\mathbf{e}_j|j=1,\ldots,g\}$ be the standard basis of $\mathbb{C}^g$ and let $B\mathbf{e}_j$ be the jth column of the matrix B. Let $\Lambda\subset\mathbb{C}^g$ be the lattice generated by the vectors $\mathbf{e}_j$ and $B\mathbf{e}_j$ for $j=1,\ldots,g$. Then, by definition, the *Jacobian variety* of $\mathcal{X}$ is the complex torus $\mathrm{Jac}\mathcal{X}=\mathbb{C}^g/\Lambda$. The *Abel map* $\mathbf{A}:\mathcal{X}\to\mathrm{Jac}\mathcal{X}$ is defined by

$$A_j(\mathcal{P},\mathcal{P}_0)=\int_{\mathcal{P}_0}^{\mathcal{P}}\omega_j(\mathcal{Q}),\quad j=1,\ldots,g,$$

where $\mathcal{P}_0\in\mathcal{X}$ is arbitrarily fixed, and $\mathcal{Q}$ is the integration variable. The *Abel map* is extended by linearity to integral divisors. If D is a divisor of degree 0, then $\mathbf{A}(D,\mathcal{P}_0)$ do not depend on the choice of $\mathcal{P}_0$. Abel's theorem states that if $D=D^+-D^-$ is the divisor of a meromorphic function on $\mathcal{X}$ with D^+, D^- the divisors of zeros and poles, then $\mathbf{A}(D,\mathcal{P}_0)=0$ in $\mathrm{Jac}\mathcal{X}$. Besides, for any nonspecial integral divisor $D=\mathcal{P}_1+\cdots+\mathcal{P}_g$ of degree g there exists a vector $\mathbf{w}(D)$ such that the Riemann theta function $\Theta[\mathbf{A}(\mathcal{P},\mathcal{P}_0)+\mathbf{w}(D)]$ defined on $\mathcal{X}$ cut along of the cycles a_j and b_j has precisely g zeros which are the points $\mathcal{P}_j$. The vector $\mathbf{w}(D)$ is defined by

$$\mathbf{w}(D)=-\mathbf{A}(D,\mathcal{P}_0)-\mathbf{K},$$

where the Riemann constant $\mathbf{K}=(K_1,\ldots,K_g)\in\mathbb{C}^g/\Lambda$ is defined by

$$K_j=\frac{1}{2}-\frac{B_{jj}}{2}+\sum_{\substack{l=1\\ l\neq j}}^{g}\int_{a_l}\left(\int_{\mathcal{P}_0}^{\mathcal{Q}}\omega_j\right)\omega_l.$$

Next, we consider on $\mathcal{X}$ a meromorphic Abel differential Ω which is holomorphic except at ∞^+ and ∞^-, where it has the behavior

$$\Omega(\mathcal{P})=\pm\mathrm{d}(2k^2(\mathcal{P}))+\mathrm{O}\left(\frac{\mathrm{d}k(\mathcal{P})}{k^2(\mathcal{P})}\right),\quad \mathcal{P}\to\infty^{\pm},$$

and which is normalized by the conditions

$$\int_{a_j}\Omega(\mathcal{Q})=0,\quad j=1,2,\ldots,g.$$

Note that $\Omega(\mathcal{P})$ has no residues. Let $\mathbf{V}=(V_1,\ldots,V_g)\in\mathbb{C}^g$ defined by

$$V_j=\frac{1}{2\pi\mathrm{i}}\int_{b_j}\Omega.$$

Finally we consider the *Abel integral* $L(\mathcal{P})$ *of logarithmic kind*, which is characterized by the following asymptotics:

$$\mathrm{d}L(\mathcal{P})=\pm\mathrm{d}\log k(\mathcal{P})+\mathrm{O}\left(\frac{\mathrm{d}k(\mathcal{P})}{k^2(\mathcal{P})}\right),\quad \mathcal{P}\to\infty^{\pm},$$

and by the normalization conditions:

$$\int_{a_j}\mathrm{d}L(\mathcal{Q})=0,\quad j=1,\ldots,g.$$

Then, the *Baker–Akhiezer vector function* $\phi(t,\mathcal{P})$ has the form

$$\phi(t,\mathcal{P})=\chi(t,\mathcal{P})\exp\left(-\mathrm{i}t\int_{E_g}^{\mathcal{P}}\Omega(\mathcal{Q})\right),$$

where $\chi(t,\mathcal{P})=(\chi_1(t,\mathcal{P})\ \ \chi_2(t,\mathcal{P}))$ with

$$\chi_1(t,\mathcal{P})=\frac{\Theta[\mathbf{A}(\mathcal{P},\mathcal{P}_0)+\mathbf{w}(D)+t\mathbf{V}]}{\Theta[\mathbf{A}(\infty^+,\mathcal{P}_0)+\mathbf{w}(D)+t\mathbf{V}]}\times\frac{\Theta[\mathbf{A}(\infty^+,\mathcal{P}_0)+\mathbf{w}(D)]}{\Theta[\mathbf{A}(\mathcal{P},\mathcal{P}_0)+\mathbf{w}(D)]}\mathrm{e}^{\mathrm{i}\Omega_0 t},$$

$$\chi_2(t,\mathcal{P})=2\mathrm{i}\frac{\Theta[\mathbf{A}(\mathcal{P},\mathcal{P}_0)+\mathbf{w}(D)+t\mathbf{V}-2\mathbf{A}(\infty^-,\mathcal{P}_0)]}{\Theta[\mathbf{w}(D)+t\mathbf{V}-\mathbf{A}(\infty^-,\mathcal{P}_0)]}\times\frac{\Theta[\mathbf{A}(\infty^-,\mathcal{P}_0)+\mathbf{w}(D)]}{\Theta[\mathbf{A}(\mathcal{P},\mathcal{P}_0)+\mathbf{w}(D)]}\mathrm{e}^{L(\mathcal{P})}\mathrm{e}^{-\mathrm{i}\Omega_0 t}.$$

The constant Ω_0 is defined by the relations

$$\int_{\mathcal{P}_0}^{\mathcal{P}}\Omega(\mathcal{Q})\mp\Omega_0=\pm 2k^2(\mathcal{P})+\mathrm{O}\left(\frac{1}{k(\mathcal{P})}\right),\quad \mathcal{P}\to\infty^{\pm}.$$

For any $t\in\mathbb{R}$ the vector function $\chi(t,\mathcal{P})$ is bounded on $\mathcal{X}$ except at the points of the divisor $D=\mathcal{P}_1+\cdots+\mathcal{P}_g$. Therefore, $\phi(t,\mathcal{P})$ is the Floquet–Bloch solution of the equation (A2). This representation for Baker–Akhiezer vector-function was first derived by A. R. Its in 1975. The asymptotic expansions of the Baker–Akhiezer function at $\infty^{\pm}$ and Eq. (A2) give representations for the finite-gap functions $\alpha(t)$ and $\beta(t)$ through theta functions from which their periodicity in $t\in\mathbb{R}$, or, in general, their quasi-periodicity if $g\geqslant 2$ is derived.

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Lax equations scattering and KdV

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(Received 5 April 2003; accepted 9 April 2003)

The study of the Korteveg–de Vries (KdV) equation is considered as a special chapter of potential scattering where the dynamic scattering equation is a set of coupled ''Lax'' equations. With this approach, all points of view and all tools of potential scattering have their counterpart in the standard inverse scattering transform, which appears as a straightforward consequence. If the approach is transposed to the quarterplane problem, it shows a generalization to KdV of the solutions obtained by Fokas in the linearized KdV problem, but unfortunately the last step is iterative and complicated. The method can also be used to study NLS. [DOI: 10.1063/1.1589179]

I. SCATTERING BY LAX EQUATIONS

We consider a special chapter of potential scattering where the ''dynamic equation'' is a set of coupled (Lax) equations. We already wrote down basic properties, transformation properties, consistency relations, and explicit expansions of solutions.[1–4] Here we recall the approach and we show how it can be applied to boundary value problems.

The nonlinear KdV equation

$$\frac{\partial V}{\partial t}+\frac{1}{4}V'''-\frac{3}{2}VV'=0, \tag{1.1}$$

where ''prime'' denotes x-derivative, is the condition for the existence of continuous second derivatives of two-vector solutions F of two linear (Lax) equations

$$\frac{\partial F}{\partial x}=\mathbf{M}F, \quad \frac{\partial F}{\partial t}=\mathbf{N}F, \tag{1.2}$$

where the matrices $\mathbf{M}$ and $\mathbf{N}$ depend on k, x, t, as follows:

$$\mathbf{M}=\mathbf{M}_0+\mathbf{V}(x,t)=:\begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix}+\begin{pmatrix} 0 & 0 \\ V(x,t) & 0 \end{pmatrix}, \tag{1.3}$$

$$\mathbf{N}=k^2\mathbf{M}_0+\begin{pmatrix} V_1 & V_0 \\ k^2V_0+V_2 & -V_1 \end{pmatrix}=:k^2\mathbf{M}_0+\mathbf{W}, \tag{1.4}$$

$$V_0=\tfrac{1}{2}V(x,t), \quad V_1=-\tfrac{1}{4}V', \quad V_2=\tfrac{1}{2}V^2-\tfrac{1}{4}V''. \tag{1.5}$$

It is clear from (1.2) that if F exists, it has the form

$$F=\begin{pmatrix} f \\ f' \end{pmatrix}. \tag{1.6}$$

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We note that since **M** and **N** have zero-trace, the matrix determinant $\det(F,G)$ of two solutions of (1.2) does not depend on x or t. For a given function $V(x,t)$, which is solution of (1.1), the space $\mathcal{F}$ of solutions F of (1.2) is two-dimensional. Assuming now on demand that $V(x,t)$ goes to zero "rapidly enough" as $x\to\pm\infty$ with fixed t or $t\to\pm\infty$ with fixed x, we can define "scattering problems" if we can construct "Jost solutions" F with given asymptotic properties, which are written here in terms of the function

$$E(k,x,t)=\begin{pmatrix}1\\ ik\end{pmatrix}\exp[i(kx+k^3t)]=\begin{pmatrix}e\\ e'\end{pmatrix}:$$

$$\overleftarrow{F}(k,x,t)-E(k,x,t)=o(|x|^{-1}) \quad \text{fixed } t,\ x\to\infty, \tag{1.7}$$

$$\hat{F}(k,x,t)-E(-k,x,t)=o(|x|^{-1}) \quad \text{fixed } t,\ x\to-\infty, \tag{1.8}$$

$$\vec{F}(k,x,t)-E(k,x,t)=o(|t|^{-1}) \quad \text{fixed } x,\ t\to\infty, \tag{1.9}$$

$$\check{F}(k,x,t)-E(-k,x,t)=o(|t|^{-1}) \quad \text{fixed } x,\ t\to-\infty. \tag{1.10}$$

For $k\neq 0$, $F(k,)$ and $F(-k,)$ are a basis in the space $\mathcal{F}$, so that

$$\hat{F}(k,)=\hat{\eta}(k)\overleftarrow{F}(-k,)+\hat{\eta}(k)\overleftarrow{F}(k,), \tag{1.11}$$

$$\overleftarrow{F}(k,)=\eta(k)\vec{F}(k,)+\xi(k)\vec{F}(-k,), \tag{1.12}$$

$$\check{F}(k,)=\check{\eta}(k)\vec{F}(-k,)+\check{\xi}(k)\vec{F}(k,). \tag{1.13}$$

Each of these relations is associated to an inverse one, for example, (1.12) to

$$\vec{F}(k,)=\eta(-k)\overleftarrow{F}(k,)-\xi(k)\overleftarrow{F}(-k,). \tag{1.14}$$

Inserting the reverse relation in the direct relation yields the unitarity relation, here

$$\eta(k)\,\eta(-k)-\xi(k)\,\xi(-k)=1. \tag{1.15}$$

Similar relations exist for the other coefficients.

For real V, which is the case here, the Jost solutions take conjugate values as $k\to-k$ in $\mathbb{R}$ and the coefficients written above behave accordingly. It is clear that these "global scattering" coefficients depend only on k, hence they are invariants in the x, t, plane.

Beside the global scattering problem defined above, we can now define scattering problems by $V(x,t)$, fixed x or fixed t. Scattering coefficients can be related to the global ones by retracing from the functions F the usual Jost solutions of this scattering problem. As an example, on a fixed t axis, assuming $|V(x,t)|\in L^1_1(\mathbb{R})$, the Schrödinger scattering problem on the axis has coefficients $R_+(k,t)$, $T(k,t)$. From their asymptotic behavior, we see that the Jost solutions $\binom{f^+}{f'^+}$ and $\binom{f^-}{f'^-}$ are equal to $\overleftarrow{F}$, respectively, $\hat{F}$, times trivial phase factors so that

$$\hat{\eta}(k)=[T(k)]^{-1}, \tag{1.16}$$

$$\hat{\xi}(k)=[T(k)]^{-1}R^+(k,t)\exp[2ik^3t]. \tag{1.17}$$

One recognizes in Eq. (1.16) the usual KdV invariant. As for Eq. (1.7), it gives trivially the "standard IST" (inverse scattering transform) where $V(x,t)$ is constructed from $T(k)$ (bound states) and $R^+(k,t)$, so that the boundary value problem with data $V(x,t_0)$ in L^1_1 is solved for any finite t. A similar analysis can be done on a fixed x axis.[3,4] If a spectral measure is identified in global scattering from the scattering by $V(x,t)$ on a full x-axis, the corresponding Jost solutions or

transformation kernels are solutions[3,4] of integral equations whose kernel involves this measure multiplied by $(k+k')^{-1}$, and going to a t-axis is formally done if we replace this factor by $(k^3+k'^3)^{-1}(k^2-kk'+k'^2)$. This symmetry is particularly obvious in the multisolitonic case, but does exist in all others. The IST on axes are nothing but a trivial consequence of translation invariance in the global scattering problem.

The situations become quite different if two half-axes are involved, as an elbow: if we try solving an inverse problem from informations on each axis, we define "*de facto*" a scanning of $V(x,t)$, which must be possible and consistent! What still makes our global scattering approach interesting is that all the conditions for solving the problem can be reproduced on a linear companion problem in such a way that if a solution of the linear problem does exist, we can transpose it. Fokas[5] gave a general approach to linear problems of this kind, by using Fourier representations of solutions. Now let us recall two properties of the Fourier representations.

(a) If a function f is known only on $\mathbb{R}^+$, it has an infinity of Fourier representations, corresponding to different continuations on $\mathbb{R}^-$.
(b) In many cases, a given Fourier integral may be written in terms of various measures, with different supports in the complex plane.

Fokas[6] was able to extend his ideas to nonlinear cases, but we do not follow the same lines. As a tool for transposing to the nonlinear case, we notice that if a function $V(x)$ is derived from a transformation kernel $K(x,y)$ represented[7] by an expansion over products of solutions, allowances seen for Fourier transforms are transposed: (a) the transformation kernels corresponding to different continuations of V outside the interval where it is considered on an axis give the same functions on the interval and (b) the support of a measure giving the transformation kernel can be displaced in the complex plane. In what follows we use these remarks, together with the global scattering approach.

II. CONSISTENCY CONDITIONS

The condition that $V(x,t)$ solves KdV can also be expressed in terms of global Jost solutions: it follows from the zero trace property and the differentiability that

$$\frac{\partial}{\partial t}\det[\mathbf{V}E,F]=\frac{\partial}{\partial x}\det[\mathbf{W}E,F], \tag{2.1}$$

where E can be evaluated for $\pm k$, F can be any solution of (1.2), and they can be chosen independently, so that for a given sort of F there exists two independent relations (2.1), one with $E(k,)$ and $F(k,)$, the other one with $E(-k,)$ and $F(k,)$.

In the following we are interested in functions $V(x,t)$ that go to zero, together with their two first derivatives, as $x\to+\infty$, fixed $t\geqslant 0$. Two independent consistency conditions can be written. Satisfying both conditions is necessary and sufficient for V to satisfy KdV, and it appears that their most convenient formulation is

$$\frac{\partial}{\partial t}\int_0^\infty dy\,\det[F(-k,y,t),\mathbf{V}(y,t)E(\pm k,y,t)]=-\det[F(-k,0,t),\mathbf{W}(k^2,0,t)E(\pm k,0,t)], \tag{2.2}$$

and, explicitly,

$$\begin{aligned}\dot{I}_1&=\frac{\partial}{\partial t}\int_0^\infty dy f(-k,y,t)e(-k,y,t)V(y,t)\\&=f'(-k,0,t)e(-k,0,t)[V_1(0,t)-ikV_0(0,t)]\\&\quad-f(-k,0,t)e(-k,0,t)[V_2(0,t)+ikV_1(0,t)+k^2V_0(0,t)],\end{aligned} \tag{2.3}$$

$$\dot{I}_2=\frac{\partial}{\partial t}\int_0^\infty dy f(-k,y,t)e(k,y,t)V(y,t)$$
$$=f'(-k,0,t)e(k,0,t)[V_1(0,t)+ikV_0(0,t)]$$
$$-f(-k,0,t)e(k,0,t)[V_2(0,t)-ikV_1(0,t)+k^2V_0(0,t)], \tag{2.4}$$

where we used the value $\exp[i(kx+k^3t)]$ of the first component e of E.

III. COMPANION LINEAR PROBLEM

We study solutions F_L of the pair of equations

$$\frac{\partial F_L}{\partial x}=\mathbf{M}_0F_L+\mathbf{V}E, \quad \frac{\partial F_L}{\partial t}=\mathbf{N}_0F_L+\mathbf{W}_LE, \tag{3.1}$$

where $\mathbf{W}_L$ is defined as $\mathbf{W}$ but with $V_2=-1/4V''$. It is readily shown that F_L is twice continuously diffrentiable if and only if V satisfies LKdV:

$$\frac{\partial V}{\partial t}+\frac{1}{4}V'''=0. \tag{3.2}$$

The consistency conditions are derived as in Sec. II and the one corresponding to (2.3) will be written concisely as

$$\frac{\partial}{\partial t}\int_0^\infty dy\ \det[E^\pm,VE^-]_y=-\det[E^\pm,W_LE^-]_{x=0}, \tag{3.3}$$

and, explicitly,

$$\frac{\partial}{\partial t}\int_0^\infty dy V(y,t)=-V_2(0,t), \tag{3.4}$$

$$\frac{\partial}{\partial t}\int_0^\infty e^{-2i(ky+k^3t)}V(y,t)dy=-e^{-2ik^3t}[2k^2V_0(0,t)+2ikV_1(0,t)+V_2(0,t)]. \tag{3.5}$$

IV. THE LINEAR QUARTERPLANE PROBLEM

We wish to construct $V(x,t)$ which is a solution of Eq. (3.2) and has prescribed values $V(x,0)$, $x\geqslant 0$, $V(0,t)$, $0\leqslant t$ (satisfying convenient general constraints). This can be done by identifying completely a representation of $V(x,t)$. Now, it is obvious that $V(x,t)$ has plenty of possible representations (e.g., Laplace in time) in terms of separable solutions of Eq. (3.2). But **it is not before the tricky idea of Fokas**[5] that a special one enables us to manage the $V(0,t)$ condition. I recall the representations of Fokas with my view and my notations ($k\to -k$ compared to Fokas). We set

$$V(x,t)=-2\frac{\partial}{\partial x}\int_{\mathbb{R}}\exp[2i(k'x+k'^3t)]\xi(k')dk'-2\frac{\partial}{\partial x}\int_\Lambda\exp[2i(k'x+k'^3t)]\tau(k')dk', \tag{4.1}$$

where Λ consists of the ray $k=|k|e^{i\pi/3}$, oriented from ∞ to 0, and the ray $k=|k|e^{2i\pi/3}$, oriented from 0 to ∞. This choice of contour is a **joker** because for $t=0$, the integral over Λ vanishes for any $x>0$ if the function $\tau(k)$ is holomorphic in $\bar{\Lambda}$, which we take as a working assumption. Hence the Fourier transform determines $\xi(k)$ from the data $V(x,0)$. To determine $\tau(k)$, we recall that Eqs. (3.4) and (3.5) are necessary and sufficient for V to satisfy Eq. (3.2), but (3.4) can be

forgotten since it is a special value of (3.5), the value $k=0$, provided that $V\in L_1^1(\mathbb{R}^+)$ and $V(x,t)$ is continuous at (0,0), which we assume. Thus it remains to enforce Eq. (3.5), which we do after substituting into it Eq. (4.1) and subtracting the calculated part due to $\xi(k)$: on the right hand side, the V_i's are replaced by, say, δV_i, and we get

$$2\frac{\partial}{\partial t}\int_\Lambda dk'\frac{k'\tau(k')}{k'-k}e^{2i(k'^3-k^3)t}=-e^{-2ik^3t}[2k^2\delta V_0(0,t)+2ik\delta V_1(0,t)+\delta V_2(0,t)]. \quad (4.2)$$

Identifying the powers of k, we see that τ is bijectively related by Fourier transforms to any of the δV_1's. We can derive it from δV_0 and then calculate δV_1 and δV_2:

$$2i\int_\Lambda dk'k'\tau(k')e^{2ik'^3t}=-\delta V_0(0,t), \quad (4.3)$$

$$\tau(k')=-\frac{3k'}{2\pi i}\int_0^\infty e^{-2ik'^3t}\delta V_0(0,t), \quad (4.4)$$

and we see that τ indeed satisfies the working assumption.

V. THE NONLINEAR QUARTERPLANE PROBLEM

We gave transformation operators adapted to studies on x-axes and others adapted to studies on t-axes. Both give representations of $V(x,t)$ but we did not emphasize the fact that like in the linear case and like in ordinary potential scattering, there are many more or less equivalent representations and we wish to use this freedom as trickily as Fokas did it in the linear case. As a matter of fact, assume $V(x,0)\in L_1^1(0,\infty)$ and look for $V(x,t)$, fixed $t\geqslant 0$, in $L_1^1(0,\infty)$. We know that there exists a kernel $\kappa(x,y,t)$ such that

$$\overleftarrow{f}(k,x,t)=e^{i(kx+k^3t)}+\int_x^\infty \kappa(x,y,t)e^{i(ky+k^3t)}dy, \quad (5.1)$$

$$V(x,t)=-2\frac{\partial}{\partial x}\kappa(x,x,t). \quad (5.2)$$

We know that κ can be expanded into products $(ef)(k,x,t)$ and that this can be done in several equivalent ways, for instance by "continuing" $V(x,t)$, fixed t, for $x<0$, keeping V in $L_1^1(\mathbb{R})$. Discrete spectrum values and continuous ones may be selected, but they are not independent, and we can also move in the complex plane the part corresponding to the spectrums. Hence, we decide to seek $\kappa(x,y,t)$ as

$$\kappa(x,y,t)=\kappa^s(x,y,t)+\kappa^\tau(x,y,t), \quad (5.3)$$

$$\kappa^\tau(x,y,t)=\int_\Lambda e^{i(k'y+k'^3t)}f(k',x,t)\tau(k')dk'. \quad (5.4)$$

For $t=0$, with our assumption on $V(x,0)$, f is holomorphic in $\mathrm{Im}\,k'\geqslant 0$, and it follows that κ^τ vanishes at any $x\geqslant 0$, $t=0$, if $\tau(k')$ is holomorphic in Λ. We take it as a working assumption on τ. Then $\kappa^s(x,y,0)=\kappa(x,y,0)$ can be constructed as a transformation operator on the $t=0$ line. It is defined directly from $\overleftarrow{f}(k,x,0)$ after $\overleftarrow{f}$ has been constructed from $V(x,0)$ by solving the Volterra integral equation:

$$\overleftarrow{F}(k,x,0)=\begin{pmatrix}1\\ ik\end{pmatrix}e^{ikx}-\int_x^\infty dy\begin{pmatrix}\cos k(y-x) & -\dfrac{\sin k(y-x)}{k}\\ k\sin k(y-x) & \cos k(y-x)\end{pmatrix}\mathbf{V}(y,0)\overleftarrow{F}(k,y,0), \tag{5.5}$$

$$\kappa^s(x,y,0)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-iky}[\overleftarrow{f}(k,x,0)-e^{ikx}]dk. \tag{5.6}$$

It can also be derived by the Faddeev–Marchenko methods as an expansion over products $e(k,x,t)\ f(k,x,t)$, since it is the kernel associated to scattering coefficients readily written at $x=0$ in terms of $f(\pm k,0,0)$. They correspond to a "potential" $V(x,0)$ continued by 0 for negative x. The expansion involves an integral over $k\in\mathbb{R}$ and a finite sum over the eigenvalues $i\kappa_\ell$, $\ell=1,2,...,N$. Introducing the auxiliary notations

$$g(k,x,t)=e(k,x,t)f(k,x,t), \tag{5.7}$$

$$\tilde{g}(k,x,t)=e(-k,x,t)f(k,x,t), \tag{5.8}$$

it is clear that the expansions of $\kappa(x,y,t)$ yield

$$V(x,t)=\int d\omega(k')g'(k',x,t), \tag{5.9}$$

where g' is the x derivative of g, and the measure $d\omega(k')$ consists of three parts, with separate supports: $\mathbb{R}$ (continuous spectrum), $i\kappa_\ell$ (discrete spectrum), and Λ (ternary support, as we shall call it). Let us insert now Eq. (5.9) in Eqs. (2.2) and (2.3). We are able to calculate explicitly all the integrals over y thanks to a number of formulas that follow from Eqs. (1.2)–(1.5), and are reproduced below, with dots indicating time derivatives and notations condensed for convenience:

$$g''=2ikg'+Vg, \tag{5.10}$$

$$\dot{g}=(k^2+\tfrac{1}{2}V)g'-\tfrac{1}{4}(V'+2ikV)g, \tag{5.11}$$

$$\dot{g}'=(2ik^3+\tfrac{1}{2}ikV+\tfrac{1}{4}V')g+(k^2V-\tfrac{1}{2}ikV'+\tfrac{1}{2}V^2-\tfrac{1}{4}V'')g, \tag{5.12}$$

$$g(-k)g'(k')-g(k')g'(-k)=-\frac{k'+k}{k'-k}\frac{\partial}{\partial x}[g(-k)g(k')]-\frac{i}{k'-k}\frac{\partial}{\partial x}[g(-k)g'(k')-g(k')g'(-k)], \tag{5.13}$$

$$\tilde{g}''=-2ik\tilde{g}'+V\tilde{g}, \tag{5.14}$$

$$\tilde{g}=(k^2+\tfrac{1}{2}V)\tilde{g}'-\tfrac{1}{4}(V'-2ikV)\tilde{g}, \tag{5.15}$$

$$\tilde{g}'=(-2ik^3-\tfrac{1}{2}ikV+\tfrac{1}{4}V')\tilde{g}'+\left(k^2V+\tfrac{1}{2}ikV'+\frac{V^2}{2}-\tfrac{1}{4}V''\right)\tilde{g}, \tag{5.16}$$

$$\tilde{g}(-k)g'(k')-g(k')\tilde{g}'(-k)=-\frac{k'-k}{k'+k}\frac{\partial}{\partial x}[\tilde{g}(-k)g(k')]-\frac{i}{k'+k}\frac{\partial}{\partial x}[\tilde{g}(-k)g'(k')-g(k')\tilde{g}'(-k)]. \tag{5.17}$$

All calculations are elementary but lengthy. The results are

$$\dot{I}_1 = -e^{-ik^3t}\{f'(-k,0,t)[\alpha(t)+ikC(t)]-f(-k,0,t)[ik\alpha(t)+\beta(t)-\gamma(t)-k^2C(t)]\}$$
$$= e^{-ik^3t}\{f'(-k,0,t)[V_1(0,t)-ikV_0(0,t)]-f(-k,0,t)[V_2(0,t)+ikV_1(0,t)+k^2V_0(0,t)]\}, \tag{5.18}$$

$$\dot{I}_2 = -e^{ik^3t}\{f'(-k,0,t)[\alpha(t)-ikC(t)]-f(-k,0,t)[-ik\alpha(t)+\beta(t)-\gamma(t)-k^2C(t)]\}$$
$$= e^{ik^3t}\{f'(-k,0,t)[V_1(0,t)+ikV_0(0,t)]-f(-k,0,t)[V_2(0,t)-ikV_1(0,t)+k^2V_0(0,t)]\}, \tag{5.19}$$

where

$$\alpha = \frac{1}{2}\int d\omega(k')\left\{\frac{1}{2}V(0,t)g(k',0,t)+ik'g'(k',0,t)\right\}, \tag{5.20}$$

$$\beta = \frac{1}{2}\int d\omega(k')\left\{\frac{1}{2}V'(0,t)g(k',0,t)+iV(0,t)k'g(k',0,t)\right\}, \tag{5.21}$$

$$\gamma = \frac{1}{2}\int d\omega(k')\left\{\frac{1}{2}V(0,t)g'(k',0,t)+2k'^2g'(k',0,t)\right\}, \tag{5.22}$$

$$C = \frac{1}{2}\int d\omega(k')g'(k',0,t). \tag{5.23}$$

Equating the two values that appear on the right hand side of $\dot{I}_1$ (respectively, $\dot{I}_2$), we obtain a linear system for f and f'. The cancelling of coefficients ensures the consistency and the equality of k powers; more precisely, setting

$$P = \alpha + V_1 + ik(V_0 - C) \tag{5.24}$$

we get

$$f'(-k,0,t)P(k,t)-f(-k,0,t)[-ikP(k,t)+V_2(0,t)-\gamma(t)+\beta(t)]=0,$$
$$f'(-k,0,t)P(-k,t)-f(-k,0,t)[ikP(-k,t)+V_2(0,t)-\gamma(t)+\beta(t)]=0. \tag{5.25}$$

Hence

$$V_0(0,t) = C(t), \tag{5.26}$$

$$V_1(0,t) = -\alpha(t), \tag{5.27}$$

$$V_2(0,t) = \beta(t) - \gamma(t). \tag{5.28}$$

The transformation kernel that produces Eq. (5.9) is

$$\kappa(x,y,t) = -\frac{1}{2}\int d\omega(k')f(k',x,t)e^{i(k'x+k'^3t)}. \tag{5.29}$$

As it is inserted into (5.1), it produces for $g(k,x,t)$ and $g'(k,x,t)$ linear integral equations that enable us to construct functions from $d\omega$ (they are the Cauchy form of the Gelfand–Levitan–Marchenko equations):

$$g(k,x,t) = e^2(k,x,t)\left[1-\frac{i}{2}\int \frac{d\omega(k')}{k+k'+i\epsilon}g(k',x,t)\right], \tag{5.30}$$

$$g'(k,x,t)=e^2(k,x,t)\left\{2ik-\frac{i}{2}\int\frac{d\omega(k')}{k+k'+i\epsilon}[g'(k',x,t)+2ikg(k',x,t)]\right\}. \tag{5.31}$$

The $\epsilon(\to 0^+)$ which appears comes from a regularizing of the infinite integral on y which is necessary only when $\mathbb{R}$ is the support of the concerned part of $d\omega$. From (5.31) we see that the right hand side of (5.23) contains only one independent piece of information, which is $d\omega(k')$. If we succeed to get it from $V_0(0,t)$ by solving Eq. (5.26), not only do we obtain $d\omega(k)$ and $g(k,0,t)$, but (readily) $V_1(0,t)$ and $V_2(0,t)$ from (5.27) and (5.28) and [by solving (5.30) and (5.31) for $x\neq 0$], $V(x,t)$ and all this in a consistent way with KdV requirements. The problem is therefore solved as in the linear case, provided this set of three equations has a solution $d\omega(k')$ with the desired supports:

$$g(k,t)=e^{2ik^3t}\left[1-\frac{i}{2}\int\frac{d\omega(k')}{k+k'+i\epsilon}g(k',t)\right], \tag{5.32}$$

$$g'(k,t)=e^{2ik^3t}\left\{2ik-\frac{i}{2}\int\frac{d\omega(k')}{k+k'+i\epsilon}[g'(k',t)+2ikg(k',t)]\right\}, \tag{5.33}$$

$$V(0,t)=\int d\omega(k')g'(k',t), \tag{5.34}$$

where we used the condensed notation $g(k',t)$ for $g(k',0,t)$. As for the support conditions, we know the value of $d\omega(k)$ on $\mathbb{R}$ [continuous spectrum of $V(x,0)$] and on the imaginary half axis [discrete spectrum of $V(x,0)$] and we must make sure that the value $d\tau(k)$ on Λ enables the Fokas joker. So as to make the iterations easy to follow, we leave $d\omega$ everywhere it is possible. First we display Eq. (5.34) in favor of $\tau(k)dk$, the measure completing it to $d\omega$ being collectively called $d\sigma$:

$$\int_\Lambda dk'\,\tau(k')2ik'e^{2ik'^3t}=V(0,t)-\int d\sigma(k')2ik'e^{2ik'^3t}+\frac{i}{2}\int d\omega(k)e^{2ik^3t}\int\frac{d\omega(k')}{k'+k+i\epsilon}[g'(k',t)+2ikg(k',t)]. \tag{5.35}$$

Both sides are limited to $t>0$ and inverting yields $\tau(k)$:

$$\tau(k'')=\tau_0(k'')+\frac{3k''}{2\pi}\int_0^\infty e^{-2ik''^3t}dt\left\{\int d\omega(k)e^{2ik^3t}\int\frac{d\omega(k')}{k'+k+i\epsilon}[g'(k',t)+2ikg(k',t)]\right\}, \tag{5.36}$$

$$\tau(k)=\tau_0(k)+N(g,g',\tau). \tag{5.37}$$

This equation should be combined with (5.32) and (5.33) which read in concise notations as

$$g=g_0+L(g,\tau), \tag{5.38}$$

$$g'=g_0'+M(g,g',\tau). \tag{5.39}$$

The set of equations is studied more easily in the case without discrete spectrum, where $d\sigma=\rho(k)dk$ [known from $V(x,0)$]. In any case we have to prove the convergence of the algorithm

$$\tau_{n+1}(k)=\tau_0(k)+N(g_n,g_n',\tau_n), \tag{5.40}$$

$$g_{n+1}=g_0+L(g_n,\tau_n), \tag{5.41}$$

$$g'_{n+1}=g'_0+M(g_n,g'_n,\tau_n). \tag{5.42}$$

It is possible to do it if conveniently defined norms $\|\rho\|$ **and** $\|\tau_0\|$ are small enough and the result can be extended if there is a discrete spectrum. This, of course, is a poor result compared to the standard IST! We sketch the proof only in the oversimplified case where $V(x,0)$ is set equal to zero $(x>0)$. Thus we meet only k integrals over Λ, where $e^{\pm 2ik^3t}$ is a number of modulus one and where we can use the bound, for any function f:

$$\left|\int_\Lambda f(k)dk\right| \leqslant \int_0^\infty \{|f(|k|e^{i\pi/3})|+|f(|k|e^{2i\pi/3})|\}d|k|. \tag{5.43}$$

In the following, this integral will be denoted for convenience as $\int_{|\Lambda|}|f(k)|dk$.

Now, from the formula

$$\tau_0(k)=\frac{3k}{2\pi}\int_0^\infty e^{-2ik^3t}V(0,t)dt \tag{5.44}$$

we can show that if $V\in L^2(0,\infty)\cap L^1(0,\infty)$, which is a cheap assumption, for $k\in\Lambda$, there exists T and $\overline{\tau}$ with

$$|\tau_0(k)|\leqslant\frac{|k|}{1+|k|}T_0(|k|)\leqslant\overline{\tau_0}, \tag{5.45}$$

where $T_0(|k|)$ is in $L^2(\mathbb{R})$, and its norm is smaller than the number, say, $\overline{\tau_0}$. Suppose now the inequality (5.44) holds for $\tau(k)$, with $\overline{T}$, $\overline{\tau}$. Then one easily shows from (5.38) and (5.39) that $|g|$ and $|k|^{-1}|g'|$ are bounded. Using now the sup norm for $|g|$ and $|k|^{-1}|g|$, the L^2 norm of $(1+|k|)|k|^{-1}|\tau(k)|$ for τ, we show that the operator (L,M,N) acting on (g,g',τ) is contracting if $\|\tau_0\|$ is small enough and that the working assumptions are satisfied.

VI. ALTERNATIVE KERNEL, FINAL REMARKS AND POSSIBLE EXTENSIONS

(a) What makes the method work is that $\kappa(x,y,t)$ [or $\kappa(x,x,t)$] and therefore $V(x,t)$, is "separated" into two parts, a part I that reduces at $t=0$ to the kernel of the global scattering problem defined at $t=0$ from $V(x,0)$ $(x>0)$ and zero $(x<0)$, and a part II that does not contribute to $V(x,0)$ at $x\geqslant 0$. One can try to obtain this separation property in another way, by combining a similar part I to a part II that reduces at $t=0$ to the kernel of the global scattering problem defined at $t=0$ from an unknown $V(x,0)$ $(x<0)$, and zero $(x\geqslant 0)$. The kernel constructed from I and II has therefore the separation property. It has an expansion over products of solutions but involving both $\check{f}$ and $\hat{f}$. This last fact, however, does not alter very much the developments of Sec. V and one gets to three equations similar to (5.32)–(5.34). Working on this alternative method is now our current interest because the separation on the axis $t=0$ is natural: as a matter of fact, all the developments can be written "exactly" in the purely multisolitonic case.

(b) In previous papers[3] we showed that transformation kernels related to t-axes are easily constructed: it is often sufficient to replace $(k+k')^{-1}$ inside equations like (5.38) by $(k^3+k'^3)^{-1}(k^2-kk'+k'^2)$ and rewrite it by means of integrals over t. Hence there are approaches on t-axes similar to those on x-axes. It is not impossible that combining an x-approach and a t-approach eventually brings a linearization of the quarterplane problem.

(c) We have shown a global scattering by a set of two linear equations whose C^2 consistency is expressed by KdV and is such that another set of equations, whose C^2 consistency is expressed by LKdV, shows the linear limit of solutions. A quite similar situation exists for at least another set of two linear equations:

$$\frac{\partial H}{\partial x}=\mathbf{m}H, \quad \frac{\partial H}{\partial t}=\mathbf{n}H, \tag{6.1}$$

where

$$\mathbf{m}=\begin{pmatrix} -ik & v \\ u & ik \end{pmatrix}, \tag{6.2}$$

$$\mathbf{n}=\begin{pmatrix} 2ik^2+iuv & -i\dfrac{\partial v}{\partial x}-2kv \\ i\dfrac{\partial u}{\partial x}-2ku & -2ik^2-iuv \end{pmatrix}. \tag{6.3}$$

They are C^2-consistent if the fields u and v satisfy the nonlinear system,

$$\begin{aligned} &\frac{\partial v}{\partial t}+i\frac{\partial^2 v}{\partial x^2}-2iuv^2=0, \\ &\frac{\partial u}{\partial t}-i\frac{\partial^2 u}{\partial x^2}+2iu^2v=0, \end{aligned} \tag{6.4}$$

which for $v=-cu^*$, real c, reduces to NLS:

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial x^2}+2c|u|^2u=0. \tag{6.5}$$

Potential scattering, both on x- and t-axes, can be managed as in the KdV case.

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The Davey–Stewartson I equation on the quarter plane with homogeneous Dirichlet boundary conditions

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(Received 5 May 2003; accepted 5 May 2003)

Dromions are exponentially localized coherent structures supported by nonlinear integrable evolution equations in two spatial dimensions. In the study of *initial-value* problems on the plane, such solutions occur only if one imposes nontrivial boundary conditions at infinity, a situation of dubious physical significance. However, it is established here that dromions appear naturally in the study of *boundary-value* problems. In particular, it is shown that the long time asymptotics of the solution of the Davey–Stewartson I equation in the quarter plane with arbitrary initial conditions and with zero Dirichlet boundary conditions is dominated by dromions. The case of nonzero Dirichlet boundary conditions is also discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1588744]

I. INTRODUCTION

We consider the Davey–Stewartson (DS) I equation:[1]

$$iq_t+\tfrac{1}{2}(q_{xx}+q_{yy})-(\varphi_x+|q|^2)q=0, \tag{1.1a}$$

$$\varphi_{xx}-\varphi_{yy}+2|q|^2x=0. \tag{1.1b}$$

In the context of water waves this equation is the shallow water limit of the Benney–Roskes[2] equation in the case of dominant surface tension. In this case $q(x,y,t)$ is the amplitude of a surface wave packet and φ is the velocity potential of the associated mean flow. In general the DSI equation provides a two-dimensional generalization of the nonlinear Schrödinger equation and can be derived from general asymptotic considerations.[3]

We introduce characteristic coordinates and we also replace the second order equation (1.1b) by two first order equations: Let ξ,η, $U_1(\xi,\eta,t)$, $U_2(\xi,\eta,t)$, be defined by

$$\xi=x+y, \quad \eta=x-y, \quad U_1=-\varphi_\eta-\tfrac{1}{2}|q|^2, \quad U_2=-\varphi_\xi-\tfrac{1}{2}|q|^2. \tag{1.2}$$

Then the DSI equation becomes

$$iq_t+q_{\xi\xi}+q_{\eta\eta}+(U_1+U_2)q=0, \tag{1.3a}$$

$$U_{1_\xi}=\tfrac{1}{2}|q|^2_\eta, \tag{1.3b}$$

$$U_{2_\eta}=\tfrac{1}{2}|q|^2_\xi. \tag{1.3c}$$

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Indeed, writing Eq. (1.1a) in characteristic coordinates and using the definitions of U_1, U_2, we find Eq. (1.3a). Also the definition of U_1 implies $U_{1_\xi} = -\varphi_{\eta\xi} - |q|^2_\xi/2$; writing Eq. (1.1b) in characteristic coordinates and using this equation to replace $\varphi_{\eta\xi}$, we find Eq. (1.3b), and similarly for Eq. (1.3c).

A. Formulation of the problem

Let the complex-valued function $q(\xi,\eta,t)$ and the real-valued functions $U_1(\xi,\eta,t)$, $U_2(\xi,\eta,t)$, satisfy Eqs. (1.3) in the domain

$$0<\xi<\infty, \quad 0<\eta<\infty, \quad t>0, \tag{1.4}$$

with the following initial and boundary conditions:

$$\begin{gathered} q(\xi,\eta,0)=q_0(\xi,\eta), \quad 0<\xi<\infty, \quad 0<\eta<\infty, \\ q(0,\eta,t)=0, \quad U_1(0,\eta,t)=u_1(\eta,t), \quad 0<\eta<\infty, \quad t>0, \\ q(\xi,0,t)=0, \quad U_2(\xi,0,t)=u_2(\xi,t), \quad 0<\xi<\infty, \quad t>0, \end{gathered} \tag{1.5}$$

where the functions $q_0(\xi,\eta)$, $u_1(\eta,t)$, $u_2(\xi,t)$ have sufficient smoothness and they also decay as $\xi\to\infty$ and $\eta\to\infty$.

Notations:

(i) Bar denotes complex conjugation.
(ii) $M_{11}, M_{12}, M_{21}, M_{22}$ denote the (11), (12), (21), (22) entries of the 2×2 matrix M.
(iii) M_D, M_0 denote the diagonal and the off-diagonal parts of the 2×2 matrix M.

Theorem 1.1: Given $q_0(\xi,\eta)$, define the vector $(M_1(\xi,\eta,k), M_2(\xi,\eta,k))^T$ by

$$\begin{gathered} M_{1_\xi} - ikM_1 = -\tfrac{1}{2}q_0 M_2, \quad M_{2_\eta} = \tfrac{1}{2}\overline{q_0}M_1, \quad 0<\xi<\infty, \quad 0<\eta<\infty, \quad \operatorname{Im} k\leqslant 0, \\ \lim_{\xi\to\infty} M_1 = 0, \quad M_2(\xi,0,k)=1. \end{gathered} \tag{1.6}$$

Given q_0 and M_2, define $S_0(k,l)$ by

$$S_0(k,l)=\frac{1}{4\pi}\int_0^\infty\int_0^\infty d\xi\, d\eta\, q_0(\xi,\eta)M_2(\xi,\eta,k)e^{-ik\xi-il\eta}, \quad \operatorname{Im} k\leqslant 0, \quad \operatorname{Im} l\leqslant 0. \tag{1.7}$$

Given S_0, u_1, u_2, define $\hat{S}(\xi,\eta,t)$ by

$$i\hat{S}_t+\hat{S}_{\xi\xi}+\hat{S}_{\eta\eta}+(u_1(\eta,t)+u_2(\xi,t))\hat{S}=0, \quad 0<\xi<\infty, \quad 0<\eta<\infty, \quad t>0, \tag{1.8a}$$

$$\hat{S}(\xi,\eta,0)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk\,dl\, e^{ik\xi+il\eta}S_0(k,l), \quad 0<\xi<\infty, \quad 0<\eta<\infty, \tag{1.8b}$$

$$\hat{S}(\xi,0,t)=0, \quad 0<\xi<\infty, \quad t>0, \tag{1.8c}$$

$$\hat{S}(0,\eta,t)=0, \quad 0<\eta<\infty, \quad t>0. \tag{1.8d}$$

Given $\hat{S}$, define the 2×2 matrices $M^+(\xi,\eta,t,k)$ and $M^-(\xi,\eta,t,k)$ as the solution of the following nonlocal Riemann-Hilbert problem:

(i) M^+ and M^- are analytic for $\operatorname{Im} k>0$ and $\operatorname{Im} k<0$, respectively.

(ii) $M^{\pm}=I+O(1/k),\ k\to\infty,\ \mathrm{Im}\,k\neq 0.$

(iii) For real k, M^{+} and M^{-} satisfy the following jump condition,

$$\begin{aligned}\begin{pmatrix}M_{11}^{+}\\ M_{21}^{+}\end{pmatrix}(\xi,\eta,t,k)-\begin{pmatrix}M_{11}^{-}\\ M_{21}^{-}\end{pmatrix}(\xi,\eta,t,k)&=-\int_{-\infty}^{\infty}dl\overline{S(l,k,t)}e^{-il\xi-ik\eta}\begin{pmatrix}M_{12}^{+}\\ M_{22}^{+}\end{pmatrix}(\xi,\eta,t,l),\\ \begin{pmatrix}M_{12}^{+}\\ M_{22}^{+}\end{pmatrix}(\xi,\eta,t,k)-\begin{pmatrix}M_{12}^{-}\\ M_{22}^{-}\end{pmatrix}(\xi,\eta,t,k)&=-\int_{-\infty}^{\infty}dlS(k,l,t)e^{il\eta+ik\xi}\begin{pmatrix}M_{11}^{-}\\ M_{21}^{-}\end{pmatrix}(\xi,\eta,t,l),\end{aligned}\tag{1.9}$$

where

$$S(k,l,t)=\frac{1}{4\pi^2}\int_0^{\infty}\int_0^{\infty}d\xi d\eta\hat{S}(\xi,\eta,t)e^{-ik\xi-il\eta}.\tag{1.10}$$

This Riemann–Hilbert problem has a unique global solution.

Define $q(\xi,\eta,t)$ by

$$q=2i\lim_{k\to\infty}(kM_{12}).\tag{1.11}$$

Then q satisfies (1.3) and (1.5).

Remark 1.1: Although the evolution of the scattering data $S(k,l,t)$ is in principle determined by Eqs. (1.8), the relevant time dependence is complicated. In turn, this makes it difficult to determine the long time behavior of the solution M of the RH problem (1.9). This difficulty can be bypassed by formulating an *inverse problem* for $S(k,l,t)$. Since Eq. (1.8a) is precisely the one studied in Ref. 4, the relevant analysis is identical with the one presented in Ref. 4: (a) If u_1 and u_2 are time-independent, then the analysis of (1.8) is intimately related with the analysis of the time-independent Schrödinger equation

$$\psi_{xx}+(u(x)+k^2)\psi=0,$$

where u is either u_1 or u_2. After a long time the solution of (1.8) is dominated by the *discrete* spectrum of u_1 and of u_2. If u_1 and u_2 have N_1 and N_2 discrete eigenvalues, respectively, then the long time asymptotics of q is given by an (N_1,N_2)-*breather* solution. (b) If u_1 and u_2 are time-dependent, then the analysis of (1.8) is related with the analysis of the time-dependent Schrödinger equation. Assuming a certain completeness relation for the eigenfunctions of the time-dependent Schrödinger equation, the long time asymptotics of the solution q is dominated again by the associated discrete spectrum; in this case the solution is dominated by an (N_1,N_2)-*dromion* solution.

Remark 1.2: The explicit form of the (N_1,N_2)-dromion solution can be found in Ref. 4, see also Refs. 5 and 6. Dromion solutions are exponentially decaying in both ξ and η. However, in contrast to the one-dimensional solitons, these solutions do *not* preserve their form upon interaction and therefore can exchange energy. These coherent strucures can be driven everywhere in the quarter-plane $\xi\geqslant 0,\eta\geqslant 0$, by choosing a suitable motion for $u_1(\eta,t),u_2(\xi,t)$.

Remark 1.3: A characteristic feature of boundary-value problems for integrable evolution partial differential equations (PDEs) in one spatial dimension is that the (spectral) functions defining the associated Riemann–Hilbert problems *cannot* in general be expressed explicitly in terms of the given boundary conditions.[7] Explicit formulas can be obtained only for a particular class of boundary conditions which are referred to in Ref. 7 as *linearizable*. The situation is similar for boundary-value problems in two spatial dimensions. We emphasize that Eqs. (1.8) are explicitly defined in terms of the given initial conditions, thus the homogeneous Dirichlet problem (1.3)–(1.5) belongs to the class of linearizable conditions. It is shown below that for nonhomogeneous Dirichlet boundary conditions, the equations defining $\hat{S}$, in addition to the *given* Dirichlet boundary conditions, also involve the *unknown* Neumann boundary values.

Proposition 1.1: Let the complex-valued function $q(\xi,\eta,t)$ satisfy a nonhomogeneous Dirichlet boundary-value problem in the quarter plane, namely, Eqs. (1.3)–(1.5), where $q(0,\eta,t)=0$ and $q(\xi,0,t)=0$ are replaced by

$$q(0,\eta,t)=g_0(\eta,t), \quad q(\xi,0,t)=f_0(\xi,t), \tag{1.12}$$

and the functions g_0, f_0 have sufficient smoothness and they also decay as $\eta\to\infty, \xi\to\infty$. *Assume* that there exists a global solution.

This solution can be expressed by Eq. (1.11) through the solution of the Riemann–Hilbert problem defined in Theorem 1.1. This problem is uniquely defined in terms of the function $\hat{S}(\xi,\eta,t)$ which satisfy the following:

(i) $\hat{S}$ solves the linear evolution PDE

$$i\hat{S}_t+\hat{S}_{\xi\xi}+\hat{S}_{\eta\eta}+(u_1+u_2)\hat{S}+\int_0^{\xi} d\tilde{\xi}F_1(\xi,\tilde{\xi},t)\hat{S}(\tilde{\xi},\eta,t)+\int_0^{\eta} d\tilde{\eta}F_2(\eta,\tilde{\eta},t)\hat{S}(\xi,\tilde{\eta},t)=0, \tag{1.13}$$

where

$$F_1(\xi,\tilde{\xi},t)=\frac{1}{4}[\overline{f_1}(\tilde{\xi},t)f_0(\xi,t)-\overline{f_0}(\tilde{\xi},t)f_1(\xi,t)]-\frac{1}{16}f(\xi,t)\overline{f}(\tilde{\xi},t)\int_{\tilde{\xi}}^{\xi} d\xi'|f(\xi',t)|^2,$$

$$F_2(\eta,\tilde{\eta},t)=\frac{1}{4}[\overline{g_1}(\tilde{\eta},t)g_0(\eta,t)-\overline{g_0}(\tilde{\eta},t)g_1(\eta,t)]-\frac{1}{16}g(\eta,t)\overline{g}(\tilde{\eta},t)\int_{\tilde{\eta}}^{\eta} d\eta'|g(\eta',t)|^2,$$

and $g_1(\eta,t), f_1(\xi,t)$ denote the Neumann boundary values $q_\xi(0,\eta,t), q_\eta(\xi,0,t)$.

(ii) $\hat{S}$ satisfies the initial and boundary conditions

$$\hat{S}(\xi,\eta,0)=\hat{S}_0(\xi,\eta), \quad \hat{S}(\xi,0,t)=\pi f_0(\xi,t), \quad \hat{S}(0,\eta,t)=\pi g_0(\eta,t), \tag{1.14}$$

where $\hat{S}_0(\xi,\eta)$ is defined in terms of $q_0(\xi,\eta)$ by the rhs of Eq. (1.7).

Remark 1.4: In the case of boundary-value problems for evolution PDEs in one spatial dimension, the unknown boundary values can be characterized in terms of the given boundary conditions through the analysis of certain *global relations*.[7,8] Such global relations exist in two spatial dimensions and can also be used for the characterization of the unknown boundary values. This analysis, which is rather complicated, will be presented elsewhere.

B. Organization of the article

The DSI equation admits a Lax pair formulation. The t-independent part of the Lax pair [see Eqs. (4.2)] is analyzed in Sec. II. The specific form of the t-part of the Lax pair [see Eqs. (3.4)] depends on the specific form of the boundary conditions. The t-part of the Lax pair for the homogeneous and nonhomogeneous Dirichlet cases is discussed in Secs. III and V, respectively. The proof of Theorem 1.1 is presented in Sec. IV. Section VI contains further discussion.

II. THE t-INDEPENDENT PART OF THE LAX PAIR

Throughout this section we *suppress the t-dependence*. The t-independent part of the Lax pair is given by Eq. (4.2). Analyzing this equation in characteristic coordinates we find the following:

Proposition 2.1: Let the vectors

$$\begin{pmatrix} M_{11}^+ \\ M_{21}^+ \end{pmatrix}, \begin{pmatrix} M_{12}^+ \\ M_{22}^+ \end{pmatrix}, \begin{pmatrix} M_{11}^- \\ M_{21}^- \end{pmatrix}, \begin{pmatrix} M_{12}^- \\ M_{22}^- \end{pmatrix}, \tag{2.1}$$

which are functions of ξ,η,k, be defined by

$$M_{11}^{+}=1-\frac{1}{2}\int_0^{\xi}d\xi' qM_{21}^{+},\quad M_{12}^{+}=-\frac{1}{2}\int_0^{\xi}d\xi' e^{ik(\xi-\xi')}qM_{22}^{+},$$

$$M_{21}^{+}=-\frac{1}{2}\int_{\eta}^{\infty}d\eta' e^{ik(\eta'-\eta)}\overline{q}M_{11}^{+},\quad M_{22}^{+}=1+\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}M_{12}^{+},$$

$$M_{11}^{-}=1-\frac{1}{2}\int_0^{\xi}d\xi' qM_{21}^{-},\quad M_{12}^{-}=\frac{1}{2}\int_{\xi}^{\infty}d\xi' e^{ik(\xi-\xi')}qM_{22}^{-},\tag{2.2}$$

$$M_{21}^{-}=\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}e^{ik(\eta'-\eta)}M_{11}^{-},\quad M_{22}^{-}=1+\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}M_{12}^{-},$$

where $q(\xi,\eta)$ has sufficient smoothness and decay. Then we have the following.

(1) The first two vectors in (2.1) are analytic in k for $\operatorname{Im}k>0$, while the last two vectors in (2.1) are analytic for $\operatorname{Im}k<0$.

(2) For real k, the vectors (2.1) satisfy the relationships

$$\begin{pmatrix}M_{11}^{+}\\M_{21}^{+}\end{pmatrix}(\xi,\eta,k)-\begin{pmatrix}M_{11}^{-}\\M_{21}^{-}\end{pmatrix}(\xi,\eta,k)=-\int_{-\infty}^{\infty}dl\overline{S(l,k)}e^{-il\xi-ik\eta}\begin{pmatrix}M_{12}^{+}\\M_{22}^{+}\end{pmatrix}(\xi,\eta,l),\tag{2.3a}$$

$$\begin{pmatrix}M_{12}^{+}\\M_{22}^{+}\end{pmatrix}(\xi,\eta,k)-\begin{pmatrix}M_{12}^{-}\\M_{22}^{-}\end{pmatrix}(\xi,\eta,k)=-\int_{-\infty}^{\infty}dlS(k,l)e^{il\eta+ik\xi}\begin{pmatrix}M_{11}^{-}\\M_{21}^{-}\end{pmatrix}(\xi,\eta,l),\tag{2.3b}$$

where $S(k,l)$ is defined by

$$S(k,l)=\frac{1}{4\pi}\int_0^{\infty}\int_0^{\infty}d\xi d\eta q(\xi,\eta)M_{22}^{-}(\xi,\eta,k)e^{-ik\xi-il\eta},\quad \operatorname{Im}k\leqslant 0,\quad \operatorname{Im}l\leqslant 0.\tag{2.4}$$

(3) The vectors (2.1) have the following behavior for large k:

$$M_{11}^{\pm}=1+O\left(\frac{1}{k}\right),\quad M_{22}^{\pm}=1+O\left(\frac{1}{k}\right),\quad M_{12}^{\pm}=O\left(\frac{1}{k}\right),\quad M_{21}^{\pm}=O\left(\frac{1}{k}\right),\quad k\to\infty,\quad \operatorname{Im}k\neq 0.\tag{2.5}$$

Proof:

(1) The vector $(M_{11}^{+},M_{21}^{+})^{T}$ satisfies a system of linear Volterra integral equations with kernel analytic in k for $\operatorname{Im}k>0$ (since $\eta'\geqslant\eta$). Thus this vector is analytic for $\operatorname{Im}k>0$ and similarly for the other vectors.

(2) Let the matrices $\Psi^{+}(\xi,\eta,k)$ and $\Psi^{-}(\xi,\eta,k)$ be defined by

$$\Psi^{\pm}=\begin{pmatrix}M_{11}^{\pm}e^{ik\eta} & M_{12}^{\pm}e^{-ik\xi}\\ M_{21}^{\pm}e^{ik\eta} & M_{22}^{\pm}e^{-ik\xi}\end{pmatrix}.\tag{2.6}$$

Then

$$\Psi_{11}^{+}=e^{ik\eta}-\frac{1}{2}\int_0^{\xi}d\xi' q\Psi_{21}^{+},\quad \Psi_{12}^{+}=-\frac{1}{2}\int_0^{\xi}d\xi' q\Psi_{22}^{+},$$

$$\Psi_{21}^{+}=\frac{1}{2}\int_{\eta}^{\infty}d\eta'\overline{q}\Psi_{11}^{+},\quad \Psi_{22}^{+}=e^{-ik\xi}+\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}\Psi_{12}^{+},$$

$$\Psi_{11}^{-}=e^{ik\eta}-\frac{1}{2}\int_0^{\xi}d\xi' q\Psi_{21}^{-},\quad \Psi_{12}^{-}=\frac{1}{2}\int_{\xi}^{\infty}d\xi' q\Psi_{22}^{-},\tag{2.7}$$

$$\Psi_{21}^{-}=\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}\Psi_{11}^{-},\quad \Psi_{22}^{-}=e^{-ik\xi}+\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}\Psi_{12}^{-}.$$

Subtracting the equations defining the vectors $(\Psi_{12}^{+},\Psi_{22}^{+})^T$ and $(\Psi_{12}^{-},\Psi_{22}^{-})^T$ we find

$$\Psi_{12}^{+}-\Psi_{12}^{-}=-\frac{1}{2}\int_0^{\infty}d\xi' q\Psi_{22}^{-}-\frac{1}{2}\int_0^{\xi}d\xi' q(\Psi_{22}^{+}-\Psi_{22}^{-}),\tag{2.8a}$$

$$\Psi_{22}^{+}-\Psi_{22}^{-}=\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}(\Psi_{12}^{+}-\Psi_{12}^{-}).\tag{2.8b}$$

Using the definition of $S(k,l)$, it follows that the first term of the rhs of Eq. (2.8a) equals

$$-\int_{-\infty}^{\infty}dlS(k,l)e^{il\eta}.$$

Comparing Eqs. (2.8) with the equation satisfied by $(\Psi_{11}^{-},\Psi_{21}^{-})^T$ we find Eq. (2.3b) written in terms of the functions $\Psi^{\pm}$ instead of the functions $M^{\pm}$.

Similarly subtracting the equations defining the vectors $(\Psi_{11}^{+},\Psi_{21}^{+})^T$ and $(\Psi_{11}^{-},\Psi_{21}^{-})^T$ we find Eq. (2.3a), where instead of $-\overline{S(l,k)}$ we have the function

$$T(k,l)=-\frac{1}{4\pi}\int_0^{\infty}\int_0^{\infty}d\xi d\eta\overline{q}(\xi,\eta)M_{11}^{+}(\xi,\eta,k)e^{ik\eta+il\xi}.\tag{2.9}$$

We will now show that

$$T(k,l)=-\overline{S(l,k)}.\tag{2.10}$$

Indeed, the vectors $(\Psi_{11}^{+},\Psi_{21}^{+})^T$ and $(\Psi_{12}^{-},\Psi_{22}^{-})^T$ satisfy the equations

$$\Psi_{11_{\xi}}^{+}=-\tfrac{1}{2}q\Psi_{21}^{+},\quad \overline{\Psi_{12_{\xi}}^{-}}=-\tfrac{1}{2}\overline{q}\,\overline{\Psi_{22}^{-}},$$

$$\Psi_{21_{\xi}}^{+}=\tfrac{1}{2}\overline{q}\Psi_{11}^{+},\quad \overline{\Psi_{22_{\eta}}^{-}}=\tfrac{1}{2}q\,\overline{\Psi_{12}^{-}}.$$

Hence

$$(\Psi_{11}^{+}(k)\overline{\Psi_{12}^{-}(l)})_{\xi}=-(\Psi_{21}^{+}(k)\overline{\Psi_{22}^{-}(l)})_{\eta},$$

where for convenience of notation we have suppressed the (ξ,η) dependence. Integrating this equation we find

$$\int_0^\infty d\eta[\Psi_{11}^+(k)\overline{\Psi_{12}^-(l)}|_{\xi=\infty}-\Psi_{11}^+(k)\overline{\Psi_{12}^-(l)}|_{\xi=0}]=-\int_0^\infty d\xi[\Psi_{21}^+(k)\overline{\Psi_{22}^-(l)}|_{\eta=0}$$
$$-\Psi_{21}^+(k)\overline{\Psi_{22}^-(l)}|_{\eta=0}].$$

Using Eq. (2.7) to compute the boundary values appearing above, for example,

$$\Psi_{12}^-|_{\xi=\infty}=\Psi_{21}^+|_{\eta=\infty}=0,\quad \Psi_{11}^+(k)|_{\xi=0}=e^{ik\eta},\quad \Psi_{22}^-(l)|_{\eta=0}=e^{-il\xi},$$

we find

$$\int_0^\infty d\eta e^{ik\eta}\int_0^\infty d\xi'\,\overline{q}\overline{\Psi_{22}^-(l)}=\int_0^\infty d\xi e^{il\xi}\int_0^\infty d\eta'\,\overline{q}\Psi_{11}^+(k).$$

The lhs of this equation is the complex conjugate of $S(l,k)$, while the rhs equals $-T(k,l)$.

(3) Equations (2.2) and integration by parts imply Eqs. (2.5). Q.E.D.

III. THE *t*-PART OF THE LAX PAIR FOR THE HOMOGENOUS DIRICHLET CASE

In what follows we first derive the t-part of the Lax pair for the vector $(\Psi_{12}^-,\Psi_{22}^-)^T$.

Proposition 3.1: Assume that there exists a function $q(\xi,\eta,t)$ with sufficient smoothness and decay which satisfies Eqs. (1.3)–(1.5). Let the vector $\Psi=(\Psi_1,\Psi_2)^T$ satisfy

$$\Psi_1(\xi,\eta,t,k)=\frac{1}{2}\int_\xi^\infty d\xi' q(\xi',\eta,t)\Psi_2(\xi',\eta,t,k), \tag{3.1a}$$

$$\Psi_2(\xi,\eta,t,k)=e^{-ik\xi}+\frac{1}{2}\int_0^\eta d\eta'\,\overline{q}(\xi,\eta',t)\Psi_1(\xi,\eta',t,k),\quad \mathrm{Im}\,k\leqslant 0. \tag{3.1b}$$

Then the function $\psi_1(\eta,t,k)$ defined by

$$\psi_1(\eta,t,k)=\Psi_1(0,\eta,t,k)$$

solves

$$i\psi_{1_t}+\psi_{1_{\eta\eta}}+u_1(\eta,t)\psi_1-\left(k^2\psi_1+\frac{1}{2}q_\xi(0,\eta,t)\right)-i\int_{-\infty}^\infty dl\,\gamma(k-l,t)\psi_1(\eta,t,l)=0, \tag{3.2}$$

where

$$\gamma(k,t)=\frac{i}{2\pi}\int_0^\infty d\xi u_2(\xi,t)e^{-ik\xi}. \tag{3.3}$$

Proof: We will first show that if $(\Psi_1,\Psi_2)^T$ satisfies Eqs. (3.1) and $q(\xi,\eta,t)$ satisfies Eqs. (1.3)–(1.5), then

$$\Psi_{1_t}=i(\partial_\xi-\partial_\eta)^2\Psi_1+iq(\partial_\xi-\partial_\eta)\Psi_2+iU_1\Psi_1-iq_\eta\Psi_2+v_1, \tag{3.4a}$$

$$\Psi_{2_t}=-i(\partial_\xi-\partial_\eta)^2\Psi_2-i\overline{q}(\partial_\xi-\partial_\eta)\Psi_1-iU_2\Psi_2-i\overline{q}_\xi\Psi_1+v_2, \tag{3.4b}$$

where the vector $v=(v_1,v_2)^T$ is given by

$$v(\xi,\eta,t,k)=-ik^2\Psi(\xi,\eta,t,k)+\int_{-\infty}^{\infty}dl\,\gamma(k-l,t)\Psi(\xi,\eta,t,l). \tag{3.5}$$

Indeed, the vector $\Psi=(\Psi_1,\Psi_2)^T$ satisfies

$$\Psi_{1_\xi}=-\tfrac{1}{2}q\Psi_2,\quad \Psi_{2_\eta}=\tfrac{1}{2}\overline{q}\Psi_1. \tag{3.6}$$

Suppose that Ψ satisfies equations similar with (3.4) but with $v=0$. It is straightforward to verify that the compatibility condition of Eq. (3.4) with $v=0$, and of Eqs. (3.6) yields Eqs. (1.3). Actually, if Eqs. (1.3) are valid, then Eqs. (3.4) and (3.6) are compatible for any vector v given by

$$v(\xi,\eta,t,k)=\int_{-\infty}^{\infty}dl\Gamma(k,l,t)\Psi(\xi,\eta,t,l).$$

The precise form of Γ depends on the boundary conditions that Ψ and q satisfy. Indeed, Ψ_1 can be written in the form

$$\Psi_1=-\int_{\xi}^{\infty}d\xi'\Psi_{1_{\xi'}}\quad\text{or}\quad \Psi_{1_t}=-\int_{\xi}^{\infty}d\xi'(\Psi_{1_t})_{\xi'}.$$

By replacing in the above equation Ψ_{1_t} by $A+v_1$, where A is defined in the rhs of Eq. (3.4a), we find

$$v_1=-\lim_{\xi\to\infty}[i(\partial_\xi-\partial_\eta)^2\Psi_1+iq(\partial_\xi-\partial\eta)\Psi_2+iU_1\Psi_1-iq_\eta\Psi_2]-\int_{\xi}^{\infty}d\xi'v_{1_{\xi'}}.$$

Using

$$\lim_{\xi\to\infty}q=\lim_{\xi\to\infty}\Psi_1=0,$$

the term in the bracket vanishes. Also

$$v_{1_\xi}=\int_{-\infty}^{\infty}dl\Gamma\Psi_{1_\xi}=\int_{-\infty}^{\infty}dl\Gamma\left(-\frac{q_1}{2}\Psi_2\right)=-\frac{q_1}{2}v_1.$$

Hence

$$v_1=\frac{1}{2}\int_{\xi}^{\infty}d\xi'q_1v_2. \tag{3.7a}$$

Similarly starting with

$$\Psi_2=\int_0^{\eta}d\eta'\Psi_{2_{\eta'}}+e^{-ik\xi}\quad\text{or}\quad \Psi_{2_t}=\int_0^{\eta}d\eta'(\Psi_{2_t})_{\eta'},$$

we find

$$v_2=[i(\partial_\xi-\partial_\eta)^2\Psi_2+i\overline{q}(\partial_\xi-\partial_\eta)\Psi_1+iU_2\Psi_2+i\overline{q}_\xi\Psi_1]_{\eta=0}+\frac{1}{2}\int_0^{\eta}d\eta'\overline{q}v_1.$$

Using

$$\Psi_1|_{\eta=0}=q|_{\eta=0}=0,\quad(\partial_\xi-\partial_\eta)^2\Psi_2|_{\eta=0}=-k^2e^{-ik\xi},$$

it follows that

$$v_2 = -ik^2 e^{-ik\xi} + iu_2(\xi,t)e^{-ik\xi} + \frac{1}{2}\int_0^\eta d\eta' \overline{q} v_1. \tag{3.7b}$$

Equations (3.7) imply that the term $-ik^2 \exp[-ik\xi]$ gives rise to $-ik^2\Psi$, while the term

$$iu_2(\xi,t)e^{-ik\xi} = \int_{-\infty}^{\infty} dl\, \gamma(k-l,t)e^{-il\xi} \tag{3.8}$$

gives rise to the term $\int_{-\infty}^{\infty} dl\, \gamma(k-l,t)\Psi(l)$. Also Eq. (3.8) implies that $\gamma(k,t)$ is given by Eq. (3.3).

Equation (3.2) follows from the evaluation of Eq. (3.4a) at $\xi=0$. In this respect we note

$$\Psi_{1_{\xi\eta}}|_{\xi=0} = -\tfrac{1}{2}[q_\eta \Psi_2 + q\Psi_{2\eta}]_{\xi=0} = 0,$$

since $q(0,\eta,t) = q_\eta(0,\eta,t) = 0$. Also

$$\Psi_{1_{\xi\xi}}|_{\xi=0} = -\tfrac{1}{2}[q_\xi \Psi_2 + q\Psi_{2\xi}]_{\xi=0} = -\tfrac{1}{2} q_\xi(0,\eta,t),$$

since $\Psi_2(0,\eta,t,k) = 1$. Q.E.D.

Using Eq. (3.2), it is now straightforward to obtain the time evolution of $S(k,l,t)$:

Proposition 3.2: Let $S(k,l,t)$ be defined by Eq. (2.4), where $M_{22}^-(\xi,\eta,t,k) = \Psi_2 \exp[-ik\xi]$, Ψ_2 is defined in terms of $q(\xi,\eta,t)$ in Eqs. (3.1), and q evolves in time according to Eqs. (1.3)–(1.5). Let

$$\hat{S}(\xi,\eta,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk dl e^{ik\xi + il\eta} S(k,l,t). \tag{3.9}$$

Then $\hat{S}$ satisfies Eqs. (1.8).

Proof: Using $(M_{12}^-, M_{22}^-)^T = e^{-ik\xi}(\Psi_1,\Psi_2)^T$, it follows that the vector $\Psi = (\Psi_1,\Psi_2)^T$ satisfies Eqs. (3.1). Also

$$S(k,l,t) = \frac{1}{4\pi}\int_0^\infty\int_0^\infty d\xi d\eta q(\xi,\eta)e^{-il\eta}\Psi_2(\xi,\eta,k) = \frac{1}{2\pi}\int_0^\infty d\eta e^{-il\eta}\Psi_1(0,\eta,t,k), \tag{3.10}$$

where the first equality uses the definition of S [see Eq. (2.4)] and the second equality uses Eq. (3.1a). Hence using $\Psi_1(0,\eta,t,k) = \psi_1(\eta,t,k)$ and replacing in Eq. (3.9) S by the rhs of Eq. (3.10) we find

$$\hat{S}(\xi,\eta,t) = \int_{-\infty}^{\infty} dk e^{ik\xi}\psi_1(\eta,t,k). \tag{3.11}$$

In order to find the time evolution of $\hat{S}$ we need to take the k-Fourier transform of Eq. (3.2). In this respect we note that if $q(0,\eta,t) = 0$, Eqs. (3.1) imply

$$\psi_1 = -\frac{1}{2}\frac{q_\xi(0,\eta,t)}{k^2} + O\left(\frac{1}{k^3}\right), \quad k\to\infty. \tag{3.12}$$

Using this estimate, Eq. (3.2) implies Eq. (1.8a). In this respect we note that the k-Fourier transform of $k^2\psi_1 + \frac{1}{2}q_\xi(0,\eta,t)$ equals $\hat{S}_{\xi\xi}$. Indeed, if $s(x)$ denotes the Fourier transform of ψ,

$$s(x)=\int_{-\infty}^{\infty}e^{ikx}\psi(k)dk,\quad x>0, \tag{3.13}$$

and if $\psi(k)$ for large k is given by

$$\psi(k)=\frac{\alpha}{k^2}+O\left(\frac{1}{k^3}\right),\quad k\to\infty, \tag{3.14}$$

then

$$\frac{d^2s}{dx^2}=\int_{-\infty}^{\infty}e^{ikx}[\alpha-k^2\psi(k)]dk. \tag{3.15}$$

In order to derive this result we note that the definition of $s(x)$ can be rewritten as

$$s(x)=\int_{-\infty}^{\infty}e^{ikx}\left[\psi(k)+\frac{\alpha}{1+k^2}\right]dk+\alpha\int_{-\infty}^{\infty}\frac{e^{ikx}}{1+k^2}dk;$$

the second integral above can be computed explicitly and equals πe^{-x}. Thus

$$\frac{d^2s}{dx^2}=\int_{-\infty}^{\infty}e^{-ikx}\left[\frac{\alpha k^2}{1+k^2}-\psi(k)\right]dk+\alpha\pi e^{-x};$$

simplifying the rhs of this equation we find (3.15).

Since $\psi_1(0,t,k)=\Psi_1(0,0,t,k)=0$, Eq. (3.11) implies $\hat{S}(\xi,0,t)=0$. Also

$$\hat{S}(0,\eta,t)=\int_{-\infty}^{\infty}dk\,\psi_1(\eta,t,k)=0,$$

since ψ_1 is analytic for $\mathrm{Im}\,k<0$ and is of $O(1/k^2)$ as $k\to\infty$ [see Eq. (3.12)]. Q.E.D.

IV. PROOF OF THEOREM 1.1

In both Secs. II and III it was *assumed* that $q(\xi,\eta,t)$ exists, it is smooth, and it has sufficient decay. Then, under this assumption, it was shown in Sec. II that q can be obtained through the solution of a RH problem uniquely defined in terms of $S(k,l,t)$. Furthermore, it was shown in Sec. III that S satisfies Eqs. (1.8). We will now prove that $q(\xi,\eta,t)$ can be constructed through the solution of the RH problem (1.9) *without* the *a priori* assumption of existence. Furthermore, this result is valid *without* the need for the norms of $q_0(\xi,t),u_1(\eta,t),u_2(\xi,t)$ to be small.

The function $S_0(k,l)$ is defined through the solution $(M_1(\xi,\eta),M_2(\xi,\eta))^T$ of the linear integral equations (1.6). These equations are of Volterra type, and thus, if $q_0\in L_1$, are always solvable.

The Fourier transform $\hat{S}(\xi,\eta,t)$ of the function $S(k,l,t)$ satisfies the linear PDE (1.8a) with the initial condition $\hat{S}_0(\xi,\eta)$ and with homogeneous Dirichlet boundary conditions. Thus if $u_1(\eta,t),u_2(\xi,t)$ have sufficient smoothness and decay, $S(k,l,t)$ is well defined.

If the functions $S,S_k,S_l\in L_2$ for fixed t, the RH problem (1.9) has a global solution provided that its homogeneous version has only the *trivial* solution. This is indeed the case:[4] Let μ satisfy Eqs. (1.9) but with $\mu=O(1/k)$ as $k\to\infty$. The jump conditions imply

$$\mu_{11}^{+}(k)-\mu_{11}^{-}(k)=-\int_{-\infty}^{\infty}dl\overline{S(l,k)}e^{-il\xi-ik\eta}\mu_{12}^{+}(l), \tag{4.1a}$$

$$\mu_{12}^{+}(k)-\mu_{12}^{-}(k)=-\int_{-\infty}^{\infty}dlS(k,l)e^{il\eta+ik\xi}\mu_{11}^{-}(l), \tag{4.1b}$$

where for convenience of notation we have suppressed the ξ,η,t dependence of μ,S. Multiplying Eq. (4.1a) by $\overline{\mu_{11}^{-}(\overline{k})}$, Eq. (4.1b) by $\overline{\mu_{22}^{+}(\overline{k})}$, integrating over k, and adding the resulting equations we find an equation whose lhs equals

$$\int_{-\infty}^{\infty}dk(|\mu_{11}^{-}(k)|^2+|\mu_{12}^{+}(k)|^2),$$

while the rhs is imaginary [in this derivation we have used that the integrals of $\overline{\mu_{11}^{-}(\overline{k})}\mu_{11}^{+}(k)$ and of $\overline{\mu_{22}^{+}(\overline{k})}\mu_{12}^{-}(k)$ vanish since these products are analytic for $\mathrm{Im}\,k>0$ and $\mathrm{Im}\,k<0$, respectively, and are of $O(1/k^2)$ as $k\to\infty$]. Hence, $\mu_{11}^{-}=\mu_{12}^{+}=0$.

For the proof of the fact that $q(\xi,\eta,0)=q_0(\xi,\eta)$ we note that $q(\xi,\eta,0)$ is defined through the RH problem (1.9) but with $S_0(k,l)$ instead of $S(k,l,0)$. By repeating the analysis of Sec. II where $q(\xi,\eta,t)$ is now replaced by the given function $q_0(\xi,\eta)$, it follows that $q_0(\xi,\eta)$ is characterized by precisely the same RH problem as the problem characterizing $q(\xi,\eta,0)$. [We note that $(M_1,M_2)^T=(M_{12}^{-},M_{22}^{-})^T$.] Hence the unique solution of this RH problem implies $q(\xi,\eta,0)=q_0(\xi,\eta)$.

We now show that if $q(\xi,\eta,t)$ is defined through the solution of the RH problem (1.9), then q satisfies the DSI equation. This proof is based on the extended version of the dressing method presented in Ref. 9. The dressing method can be used to show that if M solves an appropriate RH problem, then M also solves both parts of the associated Lax pair. Hence, using the compatibility condition of this pair, q solves the relevant nonlinear PDE.

We first show that M solves the t-independent part of the Lax pair

$$M_x+\sigma_3M_y-ik[\sigma_3,M]+QM=0, \tag{4.2}$$

where

$$\xi=x+y,\quad \eta=x-y,\quad \sigma_3=\mathrm{diag}(1,-1),\quad Q=\begin{pmatrix}0 & q\\ -\overline{q} & 0\end{pmatrix}, \tag{4.3}$$

and $[,]$ denotes the usual matrix commutator. Indeed, the jump condition of the RH problem can be written in the form

$$M^{+}(x,y,t,k)-M^{-}(x,y,t,k)=\int_{-\infty}^{\infty}dl\tilde{M}(x,y,t,l)F(x,y,t,k,l), \tag{4.4}$$

where $\tilde{M}$ denotes the matrix with first and second column vectors $(M_{11}^{-},M_{21}^{-})^T$ and $(M_{12}^{+},M_{22}^{+})^T$, respectively, and F denotes the off-diagonal matrix with

$$F_{12}(x,y,t,k,l)=-S(k,l,t)e^{ik(x+y)+il(x-y)}, \tag{4.5a}$$

$$F_{21}(x,y,t,k,l)=\overline{F_{12}(x,y,t,l,k)}. \tag{4.5b}$$

Using

$$F_{12x}=i(k+l)F_{12},\quad F_{21x}=-i(k+l)F_{21},$$

$$F_{12y}=i(k-l)F_{12},\quad F_{21y}=i(k-l)F_{21},$$

and writing these equations in a matrix form, we find

$$F_x = il\sigma_3 F - ikF\sigma_3, \quad F_y = i(k-l)F. \tag{4.6}$$

Let the operators D_x, D_y be defined by

$$D_x M = M_x + ikM\sigma_3, \quad D_y M = M_y - ikM. \tag{4.7}$$

These definitions and Eqs. (4.6) imply that

$$D_x \int_{-\infty}^{\infty} dl \tilde{M}(l) F(k,l) = \int_{-\infty}^{\infty} dl (D_x \tilde{M}(l)) F(k,l),$$

$$D_y \int_{-\infty}^{\infty} dl \tilde{M}(l) F(k,l) = \int_{-\infty}^{\infty} dl (D_y \tilde{M}(l)) F(k,l),$$

where for simplicity of notation we have suppressed the x,y,t dependence. Hence, both $D_x M$ and $D_y M$ satisfy the same jump condition as M. Using the fact that QM also satisfies the same jump condition, it follows that the expression

$$D_x M + \sigma_3 D_y M + QM \tag{4.8}$$

satisfies the same jump condition as M. Using

$$M = I + \frac{M^{(1)}(x,y,t)}{k} + \frac{M^{(2)}(x,y,t)}{k^2} + O\left(\frac{1}{k^3}\right), \tag{4.9}$$

it follows that the large k behavior of the expression (4.8) is given by

$$(Q - i[\sigma_3, M^{(1)}]) + O\left(\frac{1}{k}\right).$$

Hence if we define Q by

$$Q(x,y,t) = i[\sigma_3, M^{(1)}], \tag{4.10}$$

the expression (4.8) satisfies the homogeneous version of the RH problem, therefore it vanishes and M satisfies equation (4.2). We note that Q is off diagonal; furthermore Eq. (4.5b) implies certain symmetry relations for M, which in turn implies that $(Q)_{21} = -\overline{(Q)}_{12}$. In summary, if M satisfies the RH problem (1.9) and if q is defined through M by Eq. (1.11), then M satisfies the t-independent part of the Lax pair.

We now show that M also satisfies the t-part of the Lax pair. For this purpose, rather than assuming that S satisfies Eq. (1.8a) we first assume that $S(k,l,t)$ satisfies the equation

$$iS_t - (k^2 + l^2)S + \int_{-\infty}^{\infty} d\nu (-i)\gamma_1(\nu - l, t) S(k, \nu, t) + i\gamma_2(\nu, t) S(k - \nu, l, t), \tag{4.11}$$

where the functions γ_1, γ_2 are defined by

$$\gamma_1(\nu,t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\eta u_1(\eta, t) e^{i\nu\eta}, \quad \gamma_2(\nu,t) = -\frac{i}{2\pi} \int_{-\infty}^{\infty} d\xi u_2(\xi, t) e^{-i\nu\xi}. \tag{4.12}$$

These equations imply that F satisfies the evolution equation

$$F_t = ik^2 F\sigma_3 - il^2 \sigma_3 F + \int_{-\infty}^{\infty} d\nu (\Gamma(x,y,t,\nu - l) F(x,y,t,k,\nu) - F(x,y,t,k-\nu,l)\Gamma(x,y,t,\nu)), \tag{4.13}$$

where Γ is defined by

$$\Gamma(x,y,t,\nu)=e^{i\nu y}\,\mathrm{diag}(e^{-i\nu x}\gamma_1(\nu),e^{i\nu x}\gamma_2(\nu)). \tag{4.14}$$

Indeed, using

$$F_{12}(x,y,t,k,l)=-S(k,l,t)e^{ik\xi+il\eta},\quad \Gamma_{11}(x,y,t,\nu)=e^{-i\nu\eta}\gamma_1(\nu,t),$$
$$\Gamma_{22}(x,y,t,\nu)=e^{i\nu\xi}\gamma_2(\nu,t),$$

the (12) component of Eq. (4.13) yields Eq. (4.11).

The time dependence of F suggests the introduction of the operator D_t defined by

$$D_tM=M_t-ik^2M\sigma_3+\int_{-\infty}^{\infty}d\nu M(x,y,t,k-\nu)\Gamma(x,y,t,\nu). \tag{4.15}$$

Indeed it can be shown that

$$D_t\int_{-\infty}^{\infty}dl\tilde{M}(l)F(k,l)=\int_{-\infty}^{\infty}dl(D_t\tilde{M}(l))F(k,l).$$

This equation is a direct consequence of the definition of D_t and of Eq. (4.13) provided that

$$\int_{-\infty}^{\infty}dl\int_{-\infty}^{\infty}d\nu\tilde{M}(l)\Gamma(\nu-l)F(k,\nu)=\int_{-\infty}^{\infty}dl\int_{-\infty}^{\infty}d\nu\tilde{M}(l-\nu)\Gamma(\nu)F(k,l);$$

this equality is established by replacing on the rhs $l-\nu$ by ν and then exchanging l and ν in the resulting equation.

Since D_tM satisfies the same jump condition as M, following the same logic as in the derivation of Eq. (4.2) it follows that

$$-D_tM+i\sigma_3D_y^2M+BD_yM+AM=0, \tag{4.16}$$

where the matrices $A(x,y,t)$ and $B(x,y,t)$ will be chosen by the requirement that the lhs of Eq. (4.16) is of $O(1/k)$ as $k\to\infty$. In this respect we first introduce the following notations for the $O(1/k)$ term of M [see Eq. (4.9)]:

$$M^{(1)}(x,y,t)=\begin{pmatrix}a & b\\ c & d\end{pmatrix}. \tag{4.17}$$

Equation (4.10) yields

$$b=\frac{q}{2i},\quad c=\frac{\overline{q}}{2i}. \tag{4.18}$$

The $O(1/k)$ term of Eq. (4.2) implies

$$M_x^{(1)}+\sigma_3M_y^{(1)}-i[\sigma_3,M^{(2)}]+QM^{(1)}=0. \tag{4.19}$$

The diagonal and off-diagonal parts of this equation yield

$$\partial_xM_D^{(1)}+\sigma_3\partial_yM_D^{(1)}+QM_O^{(1)}=0, \tag{4.20}$$

$$\partial_xM_O^{(1)}+\sigma_3\partial_yM_O^{(1)}-i[\sigma_3,M_O^{(2)}]+QM_D^{(1)}=0. \tag{4.21}$$

Equation (4.20) implies

$$a_\xi = -\frac{|q|^2}{4i}, \quad d_\eta = \frac{|q|^2}{4i}. \tag{4.22}$$

Using the definitions of D_t and D_y, Eq. (4.16) becomes

$$M_t = -ik^2[\sigma_3, M] - ikBM + 2k\sigma_3 M_y + AM + BM_y + i\sigma_3 M_{yy} - \int_{-\infty}^{\infty} d\nu M(x,y,t,k-\nu)\Gamma(x,y,t,\nu). \tag{4.23}$$

The $O(k)$ term of this equation yields

$$B = -[\sigma_3, M^{(1)}],$$

thus [comparing with Eq. (4.10)]

$$B = iQ. \tag{4.24}$$

The $O(1)$ term of Eq. (4.23) yields

$$-i[\sigma_3, M^{(2)}] - iBM^{(1)} + 2\sigma_3 M_y^{(1)} + A - \int_{-\infty}^{\infty} d\nu \Gamma(x,y,t,\nu) = 0. \tag{4.25}$$

Using Eq. (4.19) to replace the first two terms of this equation we find

$$-M_x^{(1)} + \sigma_3 M_y^{(1)} + A - \int_{-\infty}^{\infty} d\nu \Gamma(x,y,t,\nu) = 0.$$

Solving this equation for A and using the definition of Γ [Eqs. (4.14) and (4.12)] we find

$$A_{11} = 2a_\eta + iu_1, \quad A_{12} = 2b_\eta, \quad A_{21} = 2c_\xi, \quad A_{22} = 2d_\xi - iu_2. \tag{4.26}$$

In summary, if the time evolution of $S(k,l,t)$ is given by Eq. (4.11), where γ_1 and γ_2 are defined by Eq. (4.12), then the time evolution of M is given by (4.23) where $B = iQ$ and the components of the matrix A are given by Eqs. (4.26).

Letting

$$M = \Psi \operatorname{diag}(e^{-ik\eta}, e^{ik\xi}), \tag{4.27}$$

and using that the y-derivative of the above diagonal matrix equals ik times this matrix, it follows that the time evolution of Ψ is given by

$$\Psi_t = i\sigma_3\partial_y^2\Psi + iQ\partial_y\Psi + A\Psi + ik^2\Psi\sigma_3 - \int_{-\infty}^{\infty} d\nu \Psi(x,y,t,k-\nu)\operatorname{diag}(\gamma_1(\nu,t), \gamma_2(\nu,t)). \tag{4.28}$$

With a particular choice of the constants of integration, Eqs. (4.22) yield

$$a = \frac{i}{4}\int_0^\xi d\xi' |q|^2, \quad d = -\frac{i}{4}\int_0^\eta d\eta' |q|^2. \tag{4.29}$$

Then the first and the fourth of equations (4.26) become

$$A_{11} = i\left(\frac{1}{2}\int_0^\xi d\xi' |q|_\eta^2 + u_1(\eta,t)\right), \quad A_{22} = -i\left(\frac{1}{2}\int_0^\eta d\eta' |q|_\xi^2 + u_2(\xi,t)\right).$$

Using these expressions as well as Eqs. (4.18), Eqs. (4.26) become

$$A_{11}=iU_1, \quad A_{12}=-iq_\eta, \quad A_{21}=-i\overline{q}_\xi, \quad A_{22}=-iU_2. \tag{4.30}$$

Denoting by $(\Psi_1,\Psi_2)^T$ the second column vector of Ψ, replacing A in Eq. (4.28) by Eqs. (4.30), and noting that $\gamma_2=-\gamma$, where γ is defined by Eq. (3.3), Eq. (4.28) implies that Ψ_1,Ψ_2 satisfy precisely Eqs. (3.4) where the vector v is defined by Eq. (3.5).

The vector $(\Psi_1,\Psi_2)^T$ also satisfies

$$\Psi_{1\xi}=-\tfrac{1}{2}q\Psi_2, \quad \Psi_{2\eta}=\tfrac{1}{2}\overline{q}\Psi_1. \tag{4.31}$$

It can be verified that the compatibility of Eqs. (3.4) and (4.31) yields Eqs. (1.3).

It remains to (a) show that the Fourier transform of Eq. (4.11) yields Eq. (1.8a); (b) justify the choice of the constants of integration of Eqs. (4.22); and (c) establish that $q(0,\eta,t)=q(\xi,0,t)=0$. These interelated facts can be proved by ''reversing'' the relevant arguments used in Sec. III.

Q.E.D.

V. THE *t*-PART OF THE LAX PAIR FOR THE NONHOMOGENEOUS CASE

For simplicity of notation throughout this section we suppress the t-dependence.

Proposition 5.1: Let the vector Ψ satisfy Eqs. (3.1) where q satisfies Eqs. (1.3) on the quarter plane. Then the function $\psi_1(\eta,k)=\Psi_1(0,\eta,k)$ satisfies the following equation:

$$i\psi_{1_t}+\psi_{1_{\eta\eta}}-\left[k^2\psi_1+\frac{ikq}{2}+\frac{q_\xi}{2}+\frac{q}{8}\int_0^\eta d\eta'|q|^2\right]+u_1\psi_1-i\int_{-\infty}^{\infty}dl[\gamma(k-l)+\delta(k-l,k)+\varepsilon(k-l,k)]\psi_1(\eta,l)-\frac{q_\xi}{4}\int_0^\eta d\eta'\overline{q}\psi_1+\frac{q}{4}\int_0^\eta d\eta'\overline{q}_\xi\psi_1-\frac{1}{16}\int_0^\eta d\eta'|q|^2\int_0^{\eta'}d\hat{\eta}\overline{q}\psi_1=0, \tag{5.1}$$

where q,q_ξ in the first bracket are evaluated at $(0,\eta)$; $|q|,\overline{q}\psi_1,\overline{q}_\xi\psi_1$ in the integrals with respect to $d\eta'$ are evaluated at $(0,\eta')$; $\overline{q}\psi_1$ in the integral with respect to $d\hat{\eta}$ is evaluated at $(0,\hat{\eta})$; γ is defined by Eq. (3.3); and δ,ε are defined by

$$\delta(l,k)=\frac{i}{8\pi}\int_0^\infty\int_0^\infty d\xi d\hat{\xi}[\overline{q}_\eta(\xi,0)q(\hat{\xi}+\xi,0)-\overline{q}(\xi,0)q_\eta(\hat{\xi}+\xi,0)]e^{-ik\hat{\xi}-il\xi}, \tag{5.2}$$

$$\varepsilon(l,k)=-\frac{i}{32\pi}\int_0^\infty\int_0^\infty\int_0^\infty d\xi d\hat{\xi}d\xi'\overline{q}(\xi,0)|q(\hat{\xi}+\xi,0|^2q(\xi+\hat{\xi}+\xi',0)e^{-ik\hat{\xi}-ik\xi'-il\xi}. \tag{5.3}$$

Proof: We first show that Ψ satisfies Eqs. (3.4) where v is defined by Eq. (3.5) with the additional term

$$\int_{-\infty}^{\infty}dl(\delta(k-l,k)+\varepsilon(k-l,k))\Psi(\xi,\eta,l).$$

Indeed, proceeding as in the proof of Proposition 3.1 we find that the forcing of the equation satisfied by v_2 involves the following additional terms:

$$\frac{i}{4}\left[\overline{q}_\eta(\xi,0)\int_\xi^\infty d\xi' q(\xi',0)e^{-ik\xi'}-\overline{q}(\xi,0)\int_\xi^\infty d\xi' q_\eta(\xi',0)e^{-ik\xi'}\right]$$
$$-\frac{i}{16}\overline{q}(\xi,0)\int_\xi^\infty d\xi'|q(\xi',0)|^2\int_{\xi'}^\infty d\xi'' q(\xi'',0)e^{-ik\xi''}. \tag{5.4}$$

For the computation of these additional terms we have used the following expressions, where for convenience of notation we have suppressed the k-dependence:

$$\psi_1(\xi,0)=\frac{1}{2}\int_\xi^\infty d\xi' q(\xi',0)e^{-ik\xi'}, \quad \psi_2(\xi,0)=e^{-ik\xi},$$

$$\psi_{1_\xi}(\xi,0)=-\tfrac{1}{2}q(\xi,0)e^{-ik\xi},$$

$$\psi_{1_\eta}(\xi,0)=\frac{1}{2}\int_\xi^\infty d\xi' q_\eta(\xi',0)e^{-ik\xi'}+\frac{1}{4}\int_\xi^\infty d\xi'|q(\xi',0)|^2\psi_1(\xi',0), \tag{5.5}$$

$$\psi_{2_{\xi\xi}}(\xi,0)=-k^2e^{-ik\xi},$$

$$\psi_{2_{\eta\xi}}(\xi,0)=\tfrac{1}{2}\overline{q}_\xi(0,\eta)\psi_1(\xi,0)-\tfrac{1}{4}|q|^2(\xi,0)e^{-ik\xi},$$

$$\psi_{2_{\eta\eta}}(\xi,0)=\tfrac{1}{2}\overline{q}_\eta(\xi,0)\psi_1(\xi,0)+\tfrac{1}{2}\overline{q}(\xi,0)\psi_{1_\eta}(\xi,0).$$

Denoting the first bracket in (5.4) by

$$\int_\xi^\infty d\xi' A(\xi,\xi')e^{-ik\xi'}=\int_{-\infty}^\infty dl\,\delta(k-l,k)e^{-il\xi},$$

replacing $k-l$ by l and $\xi'-\xi$ by $\hat{\xi}$, we find

$$\int_0^\infty d\hat{\xi}A(\xi,\hat{\xi}+\xi)e^{-ik\hat{\xi}}=\int_{-\infty}^\infty dl\,\delta(l,k)e^{il\xi},$$

which yields (5.2). Similarly denoting the second term in (5.4) by

$$\int_\xi^\infty d\xi' A(\xi,\xi')\int_{\xi'}^\infty d\xi'' B(\xi'')e^{-ik\xi''}=\int_{-\infty}^\infty dl\,\varepsilon(k-l,k)e^{-il\xi},$$

replacing $k-l$ by l, $\xi''-\xi'$ by $\hat{\hat{\xi}}$, and $\xi'-\xi$ by $\hat{\xi}$, we find

$$\int_0^\infty d\hat{\xi}A(\xi,\hat{\xi}+\xi)\int_0^\infty d\hat{\hat{\xi}}B(\hat{\hat{\xi}}+\hat{\xi}+\xi)e^{-ik(\hat{\xi}+\hat{\hat{\xi}})}=\int_{-\infty}^\infty dl\,\varepsilon(l,k)e^{il\xi},$$

which yields (5.3).

Equation (5.1) follows by evaluating Eq. (3.4a) at $\xi=0$. For this computation we use the following equations, where again for convenience of notation we have suppressed the k-dependence:

$$\psi_2(0,\eta)=1+\frac{1}{2}\int_0^\eta d\eta'\,\overline{q}(0,\eta')\psi_1(0,\eta'),\quad \psi_{2_\eta}(0,\eta)=\tfrac{1}{2}\overline{q}(0,\eta)\psi_1(0,\eta),$$

$$\psi_{2_\xi}(0,\eta)=-ik+\frac{1}{2}\int_0^\eta d\eta'\,\overline{q}_\xi(0,\eta')\psi_1(0,\eta')-\frac{1}{4}\int_0^\eta d\eta'\,|\overline{q}(0,\eta')|^2\psi_2(0,\eta'),$$

$$\psi_{1_{\xi\xi}}(0,\eta)=-\tfrac{1}{2}q_\xi(0,\eta)\psi_2(0,\eta)-\tfrac{1}{2}q(0,\eta)\psi_{2_\xi}(0,\eta),\tag{5.6}$$

$$\psi_{1_{\xi\eta}}(0,\eta)=-\tfrac{1}{2}q_\eta(0,\eta)\psi_2(0,\eta)-\tfrac{1}{4}|q(0,\eta)|^2\psi_1(0,\eta).$$

Q.E.D.

Proposition 5.2: Let $S(k,l,t)$ be defined by Eq. (2.4), where $M_{22}^-=\Psi_2\exp[-ik\xi]$, Ψ is defined in terms of q in Eqs. (3.1) and q evolves in time according to Eq. (1.3). Let $\hat{S}$ be defined in terms of S by Eq. (3.9). Then $\hat{S}$ satisfies the equation

$$i\hat{S}_t+\hat{S}_{\xi\xi}+\hat{S}_{\eta\eta}+(u_1+u_2)\hat{S}+\int_0^\xi d\tilde{\xi}F_1(\xi,\tilde{\xi},t)\hat{S}(\tilde{\xi},\eta,t)+\int_0^\eta d\tilde{\eta}F_2(\eta,\tilde{\eta},t)\hat{S}(\xi,\tilde{\eta},t)=0,\tag{5.7}$$

where

$$F_1(\xi,\tilde{\xi},t)=\frac{1}{4}[\overline{q}_\eta(\tilde{\xi},0)q(\xi,0)-\overline{q}(\tilde{\xi},0)q_\eta(\xi,0)]-\frac{1}{16}q(\xi,0)\overline{q}(\tilde{\xi},0)\int_{\tilde{\xi}}^\xi d\xi'\,|q(\xi',0)|^2,$$

$$F_2(\eta,\tilde{\eta},t)=\frac{1}{4}[\overline{q}_\xi(0,\tilde{\eta})q(0,\eta)-\overline{q}(0,\tilde{\eta})q_\xi(0,\eta)]-\frac{1}{16}q(0,\eta)\overline{q}(0,\tilde{\eta})\int_{\tilde{\eta}}^\eta d\eta'\,|q(0,\eta')|^2.\tag{5.8}$$

Furthermore, $\hat{S}$ satisfies the boundary conditions

$$\hat{S}(\xi,0,t)=\pi q(\xi,0),\quad \hat{S}(0,\eta,t)=\pi q(0,\eta).\tag{5.9}$$

Proof: The analog of Eq. (3.12) is now

$$\psi_1=\frac{-iq(0,\eta)/2}{k}-\frac{q_\xi/2+(q/8)\int_0^\eta d\eta'|q(0,\eta')|^2}{k^2}+O\left(\frac{1}{k^3}\right),\quad k\to\infty.\tag{5.10}$$

Equation (3.11) yields

$$\hat{S}(\xi,0,t)=\int_{-\infty}^\infty dke^{ik\xi}\Psi_1(0,0,t,k)=\frac{1}{2}\int_{-\infty}^\infty dke^{ik\xi}\int_0^\infty d\xi'\,q(\xi',0)e^{-ik\xi'}=\pi q(\xi,0).$$

Furthermore,

$$\hat{S}(0,\eta,t)=\int_{-\infty}^\infty dk\Psi_1(0,\eta,t,k)=\int_{-\infty}^\infty dk\left[\Psi_1(0,\eta,t,k)+\frac{i}{2}\frac{q(0,\eta)}{k}\right]-\frac{i}{2}\int_{-\infty}^\infty\frac{dk}{k}q(0,\eta),$$

$$=\pi q(0,\eta),$$

since $\Psi_1(0,\eta,t,k)$ is analytic for $\mathrm{Im}\,k<0$.

Taking the Fourier transform of Eq. (5.1) and using the estimate (5.10) we find Eq. (5.7). In this respect we note that if we denote the bracket on the rhs of Eq. (5.2) by $A(\xi,\hat{\xi})$, then the contribution of the term involving γ is given by

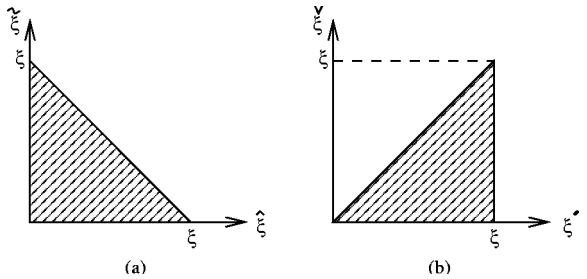

FIG. 1. The change of variables from $(\tilde{\xi},\ \hat{\xi})$ to $(\check{\xi},\ \xi')$.

$$
\begin{aligned}
&-i\int_{-\infty}^{\infty}dl\int_{-\infty}^{\infty}dk\,\gamma(k-l,t)\psi_1(l)e^{ik\xi}\\
&\quad=\frac{1}{8\pi}\int_{-\infty}^{\infty}dl\int_{-\infty}^{\infty}dk\int_0^{\infty}d\xi'\int_0^{\infty}d\hat{\xi}A(\xi',\hat{\xi})e^{-ik\hat{\xi}-i(k-l)\xi'+ik\xi}\psi_1(l)\\
&\quad=\frac{1}{4}\int_0^{\infty}d\xi'\int_0^{\infty}d\hat{\xi}A(\xi',\hat{\xi})\,\delta(\hat{\xi}-(\xi-\xi'))\hat{S}(\xi',\eta,t)\\
&\quad=\frac{1}{4}\int_0^{\infty}d\xi'\,\theta(\xi-\xi')A(\xi',\xi-\xi')\hat{S}(\xi',\eta,t),
\end{aligned}
$$

where $\psi_1(l)=\psi_1(\eta,l)$. Similarly the contribution of the term involving δ is given by

$$
\begin{aligned}
&-\frac{1}{32}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dkdl\int_0^{\infty}\int_0^{\infty}\int_0^{\infty}d\tilde{\xi}d\hat{\xi}d\xi'\overline{q}(\tilde{\xi},0)|q(\hat{\xi}+\tilde{\xi},0|^2q(\tilde{\xi}+\hat{\xi}\\
&\quad+\xi',0)e^{-ik\hat{\xi}-ik\xi'-i(k-l)\tilde{\xi}+ik\xi}\psi_1(l)\\
&\quad=-\frac{q(\xi,0)}{16}\int_0^{\infty}d\tilde{\xi}\int_0^{\infty}d\hat{\xi}\,\theta(\xi-\tilde{\xi}-\hat{\xi})\overline{q}(\tilde{\xi},0)|q(\hat{\xi}+\tilde{\xi},0)|^2\hat{S}(\tilde{\xi},\eta)\\
&\quad=-\frac{q(\xi,0)}{16}\int_0^{\xi}d\tilde{\xi}\int_0^{\xi-\tilde{\xi}}d\hat{\xi}\overline{q}(\tilde{\xi},0)|q(\hat{\xi}+\tilde{\xi},0)|^2\hat{S}(\tilde{\xi},\eta).
\end{aligned}
$$

The area of integration is depicted in Fig. 1(a). Making the change of variables $\xi'=\hat{\xi}+\tilde{\xi}$, $\check{\xi}=\tilde{\xi}$, the area of integration is mapped to the area depicted in Fig. 1(b). Thus the relevant integral becomes

$$
\frac{-q(\xi,0)}{16}\int_0^{\xi}d\check{\xi}\left(\int_{\check{\xi}}^{\xi}d\xi'|q(\xi',0)|^2\right)\overline{q}(\check{\xi},0)\hat{S}(\check{\xi},\eta).
$$

Also regarding the last term of Eq. (5.1) we note that taking its Fourier transform we find

$$
\frac{-q(0,\eta)}{16}\int_0^{\eta}d\eta'|q(0,\eta')|^2\int_0^{\eta'}d\hat{\eta}\overline{q}(0,\hat{\eta})\hat{S}(\xi,\hat{\eta},t).
$$

Changing the order of the integration we find that the relevant contribution involves the last term of F_2, see Eq. (5.8). Q.E.D.

VI. DISCUSSION

In the last decade considerable progress has been made in the understanding of boundary-value problems for integrable nonlinear evolution PDEs in *one* spatial dimension. For example, two of the articles in this special issue are concerned with this development.[10,11] Here, to our knowledge for the first time, a boundary-value problem is solved in *two* spatial dimensions.

It has been emphasized by the author that an important difference between initial- and boundary-value problems is the following: For initial-value problems one needs to perform the spectral analysis of the t-independent part of the Lax pair only, while for boundary-value problems the spectral analysis of *both* parts of the Lax pair is needed. In this respect we recall the following developments:

(i) It is interesting that the spectral analysis of the t-part of the Lax pair (in addition to that of the t-independent part) was first considered not for an equation in one spatial dimension but for an equation in two spatial dimensions, namely the DSI equation: In Ref. 4 Eqs. (1.3) were solved on the plane, but with nontrivial boundary conditions at infinity,

$$U_1(\xi,\eta,t)\to u_1(\eta,t), \quad \xi\to\infty; \quad U_2(\xi,\eta,t)\to u_2(\xi,t), \quad \eta\to\infty.$$

The authors of Ref. 4, rather than performing the explicit spectral analysis of the relevant t-dependent eigenvalue equation, made use of a certain completeness relation (of course the derivation of this relation is based on the spectral analysis of the Schrödinger eigenvalue equation).

(ii) In Ref. 12 the *independent* spectral analysis of the two parts of the Lax pair of the nonlinear Schrödinger equation led to the formulation of the solution in terms of *two* Riemann–Hilbert (RH) problems, which had to be solved in sequence.

(iii) In Ref. 13 the above two RH problems were combined and the solution q was expressed in terms of a *single* RH problem. This RH problem has the distinctive and very useful feature of involving jump matrices with *explicit* exponential (x,t) dependence.

(iv) It was shown in Ref. 14 that the above RH problem can be derived in a straightforward manner by performing the *simultaneous* spectral analysis of the Lax pair. The rigorous proof that the solution of this RH problem yields the unique solution of the given initial-boundary value problem was presented in Refs. 7 and 8.

In the present article we have implemented for Eqs. (1.3)–(1.5) the construction of (i) above. The main reason for using (i) instead of (iv) is the fact that for the case of homogeneous Dirichlet boundary conditions the analysis of the t-part of the Lax pair is very similar to the analysis presented in Ref. 4.

The implementation of (iv) for the initial-boundary value problem formulated in Proposition 1.1 remains open. Furthermore, the analysis of the associated global relation, which characterizes g_1 and f_1 in terms of g_0, f_0 and q_0, also remains open.

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The *n*-component KP hierarchy and representation theory

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(Received 26 March 2003; accepted 9 April 2003)

It is the aim of the present article to give all formulations of the *n*-component KP hierarchy and clarify connections between them. The generalization to the *n*-component KP hierarchy is important because it contains many of the most popular systems of soliton equations, like the Davey–Stewartson system (for $n=2$), the two-dimensional Toda lattice (for $n=2$), the *n*-wave system (for $n\geqslant 3$) and the Darboux–Egoroff system. It also allows us to construct natural generalizations to the Davey–Stewartson and Toda lattice systems. Of course, the inclusion of all these systems in the *n*-component KP hierarchy allows us to construct their solutions by making use of vertex operators. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1590055]

I. INTRODUCTION

The remarkable link between the soliton theory and the group GL_∞ was discovered in the early 1980s by Sato[40] and developed, making use of the spinor formalism, by Date, Jimbo, Kashiwara, and Miwa.[7–9,24] The basic object that they considered is the KP hierarchy of partial differential equations, which they studied through a sequence of equivalent formulations that we describe below. The first formulation is a deformation (or Lax) equation of a formal pseudo-differential operator $L=\partial+u_1\partial^{-1}+u_2\partial^{-2}+\cdots$, introduced in Refs. 40 and 52:

$$\frac{\partial L}{\partial x_n}=[B_n,L], \quad n=1,2,\ldots. \tag{1}$$

Here u_i are unknown functions in the indeterminates x_1, $x_2,\ldots$, and $B_n=(L^n)_+$ stands for the differential part of L^n. The second formulation is given by the following zero curvature (or Zakharov–Shabat) equations:

$$\frac{\partial B_m}{\partial x_n}-\frac{\partial B_n}{\partial x_m}=[B_n,B_m], \quad m,n=1,2,\ldots. \tag{2}$$

These equations are compatibility conditions for the following linear system

$$Lw(x,z)=zw(x,z), \quad \frac{\partial}{\partial x_n}w(x,z)=B_nw(x,z), \quad n=1,2,..., \tag{3}$$

on the wave function

$$w(x,z)=(1+w_1(x)z^{-1}+w_2(x)z^{-2}+\cdots)e^{x_1z+x_2z^2+\cdots}. \tag{4}$$

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Provided that (2) holds, the system (3) has a unique solution of the form (4) up to multiplication by an element from $1+z^{-1}\mathbb{C}[\![z^{-1}]\!]$. Introduce the wave operator

$$P=1+w_1(x)\partial^{-1}+w_2(x)\partial^{-2}+\cdots, \tag{5}$$

so that $w(x,z)=Pe^{x_1z+x_2z^2+\cdots}$. Then the existence of a solution of (3) is equivalent to the existence of a solution of the form (5) of the following Sato equation, which is the third formulation of the KP hierarchy:[41,52]

$$\frac{\partial P}{\partial x_k}=-(P\circ\partial\circ P^{-1})_-\circ P, \quad k=1,2,..., \tag{6}$$

where the formal pseudo-differential operators P and L are related by

$$L=P\circ\partial\circ P^{-1}. \tag{7}$$

Let $P^*=1+(-\partial)^{-1}\circ w_1+(-\partial)^{-2}\circ w_2+\cdots$ be the formal adjoint of P and let

$$w^*(x,z)=(P^*)^{-1}e^{-x_1z-x_2z^2-\cdots}$$

be the adjoint wave function. Then the fourth formulation of the KP hierarchy is the following bilinear identity:

$$\mathrm{Res}_{z=0}w(x,z)w^*(x',z)dz=0 \quad \text{for any } x \text{ and } x'. \tag{8}$$

Next, this bilinear identity can be rewritten in terms of Hirota bilinear operators defined for an arbitrary polynomial Q as follows:

$$Q(D)f(x)\cdot g(x)\overset{\text{def}}{=}Q\left(\frac{\partial}{\partial y}\right)(f(x+y)g(x-y))\big|_{y=0}. \tag{9}$$

Towards this end, introduce the famous τ-function $\tau(x)$ by the formulas

$$w(x,z)=\Gamma^+(z)\tau/\tau, \quad w^*(x,z)=\Gamma^-(z)\tau/\tau. \tag{10}$$

Here $\Gamma^{\pm}(z)$ are the vertex operators defined by

$$\Gamma^{\pm}(z)=e^{\pm(x_1z+x_2z^2+\cdots)}e^{\mp(z^{-1}\tilde{\partial}/\partial x_1+z^{-2}\tilde{\partial}/\partial x_2+\cdots)}, \tag{11}$$

where $\tilde{\partial}/\partial x_j$ stands for $(1/j)(\partial/\partial x_j)$. The τ-function exists and is uniquely determined by the wave function up to a constant factor. Substituting the τ-function in the bilinear identity (8) we obtain the fifth formulation of the KP hierarchy as the following system of Hirota bilinear equations:

$$\sum_{j=0}^{\infty}S_j(-2y)S_{j+1}(\tilde{D})e^{\sum_{r=1}^{\infty}y_rD_r}\tau\cdot\tau=0. \tag{12}$$

Here $y=(y_1,y_2,\ldots)$ are arbitrary parameters and the elementary Schur polynomials S_j are defined by the generating series

$$\sum_{j\in\mathbb{Z}}S_j(x)z^j=\exp\sum_{k=1}^{\infty}x_kz^k. \tag{13}$$

The τ-function formulation of the KP hierarchy allows one to construct easily its N-soliton solutions. For that introduce the vertex operator:[8,9]

$$\Gamma(z_1,z_2)=:\Gamma^+(z_1)\Gamma^-(z_2):\tag{14}$$

(where the sign of normal ordering $::$ means that partial derivatives are always moved to the right), and show using the bilinear identity (8) that if τ is a solution of (12), then $(1+a\Gamma(z_1,z_2))\tau$, where $a, z_1, z_2\in\mathbb{C}^\times$, is a solution as well. Since $\tau=1$ is a solution, the function

$$f_N\equiv(1+a_1\Gamma(z_1^{(1)},z_2^{(1)}))\cdots(1+a_N\Gamma(z_1^{(N)},z_2^{(N)}))\cdot 1\tag{15}$$

is a solution of (12), too. This is the τ-function of the N-soliton solution.

The first application of the KP hierarchy, as well as its name, comes from the fact that the simplest nontrivial Zakharov–Shabat equation, namely (2) with $m=2$ and $n=3$, is equivalent to the Kadomtsev–Petviashvili equation if we let $x_1=x$, $x_2=y$, $x_3=t$, $u=2u_1$:

$$\frac{3}{4}\frac{\partial^2 u}{\partial y^2}=\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}-\frac{3}{2}u\frac{\partial u}{\partial x}-\frac{1}{4}\frac{\partial^3 u}{\partial x^3}\right).\tag{16}$$

Recall also that the celebrated KdV and Boussinesq equations are simple reductions of (16). Since the functions u and τ are related by

$$u=2\frac{\partial^2}{\partial x^2}\log\tau,\tag{17}$$

the functions $2(\partial^2/\partial x^2)\log f_N$ are solutions of (16), called the N-soliton solutions.

The connection of the KP hierarchy to the representation theory of the group GL_∞ is achieved via the spinor formalism. Consider the Clifford algebra $C\ell$ on generators ψ_j^+ and ψ_j^- ($j\in 1/2+\mathbb{Z}$) and the following defining relations (i.e., $\psi_i^\pm$ are free charged fermions):

$$\psi_i^+\psi_j^-+\psi_j^-\psi_i^+=\delta_{i,-j},\quad \psi_i^\pm\psi_j^\pm+\psi_j^\pm\psi_i^\pm=0.\tag{18}$$

The algebra $C\ell$ has a unique irreducible representation in a vector space F (resp. F^*) which is a left (resp. right) module admitting a nonzero vector $|0\rangle$ (resp. $\langle 0|$) satisfying

$$\psi_j^\pm|0\rangle=0\ \ (\text{resp. } \langle 0|\psi_{-j}^\pm=0)\quad \text{for } j>0.\tag{19}$$

These representations are dual to each other with respect to the pairing

$$\langle\langle 0|a,b|0\rangle\rangle=\langle 0|ab|0\rangle$$

normalized by the condition $\langle 0|1|0\rangle=1$.

The Lie algebra gl_∞ embeds in $C\ell$ by letting

$$r(E_{ij})=\psi_{-i}^+\psi_j^-.\tag{20}$$

Exponentiating gives a representation R of the group GL_∞ on F and F^*. Let, for $n\in\mathbb{Z}$,

$$\alpha_n=\sum_{j\in 1/2+\mathbb{Z}}\psi_{-j}^+\psi_{j+n}^-\quad\text{for } n\neq 0,\quad \alpha_0=\sum_{j>0}\psi_{-j}^+\psi_j^--\sum_{j<0}\psi_j^-\psi_{-j}^+.\tag{21}$$

and consider the following operator on F:

$$H(x)=\sum_{n=1}^{\infty}x_n\alpha_n.\tag{22}$$

For a positive integer m let

$$\langle \pm m| = \langle 0|\psi^{\pm}_{1/2}\cdots\psi^{\pm}_{m-1/2} \in F^* \quad \text{and} \quad |\pm m\rangle = \psi^{\pm}_{-m+1/2}\cdots\psi^{\pm}_{-1/2}|0\rangle \in F.$$

Then the Fock space is realized on the vector space of polynomials $B=\mathbb{C}[x_1,x_2,\ldots;Q,Q^{-1}]$ via the isomorphism $\sigma: F \tilde{\to} B$ defined by

$$\sigma(a|0\rangle) = \sum_{m\in\mathbb{Z}} \langle m|e^{H(x)}a|0\rangle Q^m. \tag{23}$$

This remarkable isomorphism is called the boson-fermion correspondence and goes back to the work of Skyrme[44] and many other physicists; this beautiful form of it is an important part of the work of Date, Jimbo, Kashiwara, and Miwa.[8,9,24]

Using that

$$[\alpha_m,\alpha_n] = m\delta_{m,-n} \tag{24}$$

(i.e., that the α_n are free bosons), it is not difficult to show that the isomorphism σ is characterized by the following two properties:[27]

$$\sigma(|m\rangle) = Q^m, \quad \sigma\alpha_n\sigma^{-1} = \frac{\partial}{\partial x_n} \quad \text{and} \quad \sigma\alpha_{-n}\sigma^{-1} = nx_n \quad \text{if } n>0. \tag{25}$$

Using (25), it is easy to recover the following well-known properties of the boson-fermion correspondence.[8,9,27] Introduce the fermionic fields

$$\psi^{\pm}(z) = \sum_{j\in 1/2+\mathbb{Z}} \psi^{\pm}_j z^{-j-1/2}.$$

Then one has

$$\sigma\psi^{\pm}(z)\sigma^{-1} = Q^{\pm 1}z^{\pm\alpha_0}\Gamma^{\pm}(z), \tag{26}$$

$$\sigma\left(\sum_{i,j\in 1/2+\mathbb{Z}} r(E_{ij})z_1^{i-1/2}z_2^{-j-1/2}\right)\sigma^{-1} = \frac{1}{z_1-z_2}\Gamma(z_1,z_2). \tag{27}$$

Hence $\Gamma(z_1,z_2)$ lies in a "completion" of the Lie algebra gl_∞ acting on B via the boson-fermion correspondence. Therefore, the group GL_∞ and its "completion" act on B and Date, Jimbo, Kashiwara, and Miwa show that all elements of the orbit $\mathcal{O}=\mathrm{GL}_\infty\cdot 1$ and its completions satisfy the bilinear identity (12). Since $\Gamma(z_1,z_2)^2=0$ and $\Gamma(z_1,z_2)$ lies in a completion of gl_∞, we see that $\exp a\Gamma(z_1,z_2)=1+a\Gamma(z_1,z_2)$ leaves a completion of the orbit $\mathcal{O}$ invariant, which explains why (15) are solutions of the KP hierarchy.

Since the orbit $\mathrm{GL}_\infty|0\rangle$ (which is the image of $\mathcal{O}$ in the fermionic picture) can be naturally identified with the cone over a Grassmannian, we arrive at the remarkable discovery of Sato that solutions of the KP hierarchy are parametrized by an infinite-dimensional Grassmannian.[41]

It was subsequently pointed out in Refs. 27 and 30 that the bilinear Eq. (8) (in the bosonic picture) corresponds to the following remarkably simple equation on the τ-function in the fermionic picture:

$$\sum_{k\in 1/2+\mathbb{Z}} \psi^+_k\tau\otimes\psi^-_{-k}\tau = 0. \tag{28}$$

This is the fermionic formulation of the KP hierarchy. Since (1) is equivalent to

$$\mathrm{Res}_{z=0}\psi^+(z)\tau\otimes\psi^-(z)\tau = 0, \tag{29}$$

it is clear from (10) and (11) that Eqs. (8) and (29) are equivalent. Since $\tau=|0\rangle$ obviously satisfies (1) and $R\otimes R(\mathrm{GL}_\infty)$ commutes with the operator $\Sigma_k \psi_k^+\otimes\psi_{-k}^-$, we see why any element of $R(\mathrm{GL}_\infty)|0\rangle$ satisfies (28). Thus, the most natural approach to the KP hierarchy is to start with the fermonic formulation (28), go over to the bilinear identity (8) and then to all other formulations (see Refs. 27, 30, and 25). This approach was generalized in Ref. 33.

Our basic idea is to start once again with the fermonic formulation of KP, but then use the *n*-component boson-fermion correspondence, also considered by Date, Jimbo, Kashiwara, and Miwa.[7,24] This leads to a bilinear equation on a matrix wave function, which in turn leads to a deformation equation for a matrix formal pseudo-differential operator, to matrix Sato equations and to matrix Zakharov–Shabat-type equations.

The corresponding linear problem has been already formulated in Sato's paper[41] and Date, Jimbo, Kashiwara, and Miwa[7] have written the corresponding bilinear equation for the wave function, but the connection between these formulations remained somewhat obscure.

It is the aim of the present article to give all formulations of the *n*-component KP hierarchy and clarify connections between them. The generalization to the *n*-component KP is important because it contains many of the most popular systems of soliton equations, like the Davey–Stewartson system (for $n=2$), the two-dimensional Toda lattice (for $n=2$), and the *n*-wave system (for $n\geqslant 3$). It also allows us to construct natural generalizations of the Davey–Stewartson and Toda lattice systems. Of course, the inclusion of all these systems in the *n*-component KP hierarchy allows us to construct their solutions by making use of vertex operators.

Hirota's direct method[23] requires some guesswork to introduce a new function (the τ-function) for which the equations in question take a bilinear form. The inclusion of the equations in the *n*-component KP hierarchy provides a systematic way of construction of the τ-functions, the corresponding bilinear equations and a large family of their solutions.

The difficulty of the τ-function approach lies in the fact that the hierarchy contains too many Hirota bilinear equations. To deal with this difficulty we introduce the notion of an energy of a Hirota bilinear equation. We observe that the most interesting equations are those of lowest energy. For example, in the $n=1$ case the lowest energy $(=4)$ nontrivial equation is the classical KP equation in the Hirota bilinear form, in the $n=2$ case the lowest energy $(=2)$ equations form the two-dimensional Toda chain and the energy 2 and 3 equations form the Davey–Stewartson system in the bilinear form, and in the $n\geqslant 3$ case the lowest energy $(=2)$ bilinear equations form the *n*-wave system in the bilinear form.

The Hirota bilinear equations of the *n*-component KP hierarchy also play a role in the theory of theta functions of Riemann surfaces. To be more specific, Maffei[35] shows that the theta function of a Riemann surfaces gives a τ function for the *n*-component KP hierarchy. He then uses the results of Sec. III D, formula (80), to show that such a theta function satisfies the Fay trisecant formula. He also shows that more complicated relations in the hierarchy give some theta relations obtained by Gunning in Ref. 20.

There is a new phenomenon in the *n*-component case, which does not occur in the one-component case: the τ-function and the wave function are a collection of functions $\{\tau_\alpha\}$ and $\{W_\alpha\}$ parametrized by the elements of the root lattice M of type A_{n-1}. The set $\mathrm{supp}\ \tau=\{\alpha\in M|\tau_\alpha\neq 0\}$ is called the support of the τ-function τ. We show that $\mathrm{supp}\ \tau$ is a convex polyhedron whose edges are parallel to roots; in particular, $\mathrm{supp}\ \tau$ is connected, which allows us to relate the behavior of the *n*-component KP hierarchy at different points of the lattice M. It is interesting to note that the ''matching conditions'' which relate the functions W_α and W_β, $\alpha,\beta\in M$, involve elements from the subgroup of translations of the Weyl group (Ref. 25, Chap. 6) of the loop group $\mathrm{GL}(\mathbb{C}[z,z^{-1}])$ and are intimately related to the Bruhat decomposition of this loop group (see Ref. 40). We are planning to study this in a future publication.

The behavior of solutions obtained via vertex operators in the *n*-component case is much more complicated than for the ordinary KP hierarchy. In particular, they are not necessarily multisoliton solutions (i.e., a collection of waves that preserve their form after interaction). For that reason we call them the multisolitary solutions. Some of the multisolitary solutions turn out to be the so called dromion solutions, which have become very popular recently.[6,19,22,21] These solutions decay

exponentially in all directions (and they are not soliton solutions; in particular, they exist only for $n>1$). It is a very interesting problem for which values of parameters the multisolitary solutions are soliton or dromion solutions.

Note also that the Krichever method for construction of the quasiperiodic solutions of the KP hierarchy as developed in Refs. 42 and 43 applies to the n-component KP (see, e.g., Ref. 35).

As shown in Refs. 41 and 8, the mth reduction of the KP hierarchy, i.e., the requirement that L^m is a differential operator, leads to the classical formulation of the celebrated KdV hierarchy for $m=2$, Boussinesq for $m=3$ and all the Gelfand–Dickey hierarchies for $m>3$. The totality of τ-functions for the mth reduced KP hierarchy turns out to be the orbit of the vacuum under the loop group of SL_m.

We define in a similar way the $[m_1,m_2,\dots,m_n]$-reduction of the n-component KP and show that the totality of τ-functions is the orbit of the vacuum vector under the loop group of $\mathrm{SL}_{m_1+\cdots+m_n}$ (see also Ref. 5). Even the case that all $m_j=1$ turns out to be extremely interesting (it is trivial if $n=1$), as it gives the $1+1$ n-wave system for $n\geqslant 3$, the Darboux-Egoroff system from topological field theory (see also Ref. 50) and the decoupled nonlinear Schrödinger (or AKNS) system for $n=2$. We note that the $[1,1,\dots,1]$-reduced n-component KP, which we call the n-component NLS hierarchy, admits a natural generalization to the case of an arbitrary simple Lie group G (the n-component NLS corresponding to GL_n). These hierarchies, which might be called the GNLS hierarchies, contain the systems studied by many authors (Refs. 10, 52, 53, and 33, among others).

The article is set out as follows. In Sec. II we explain the construction of the semi-infinite wedge representation F of the group GL_∞ and write down the equation of the GL_∞-orbit $\mathcal{O}$ of the vacuum $|0\rangle$ (Proposition 2.1). This equation is called the KP hierarchy in the fermionic picture. As usual, the Plücker map makes $\mathcal{O}$ a $\mathbb{C}^\times$-bundle over an infinite-dimensional Grassmannian. We describe the ''support'' of $\tau\in\mathcal{O}$ (Proposition 2.2).

In Sec. III we introduce the n-component bosonization and write down the fermionic fields in terms of bosonic ones via vertex operators (Theorem 3.1). This allows us to transport the KP hierarchy from the fermionic picture to the bosonic one (66) and write down the n-component KP hierarchy as a system of Hirota bilinear Eqs. (70). We describe the support of a τ-function in the bosonic picture (Proposition 3.1). At the end of the section we list all Hirota bilinear equations of lowest energy (73)–(79).

We start Sec. IV with an exposition of the theory of matrix formal pseudo-differential operators, and prove the crucial Lemma 4.1. This allows us to reformulate the n-component KP hierarchy (66) in terms of formal pseudo-differential operators [see (95) and (103)]. Using the crucial lemma we show that the bilinear Eq. (66) is equivalent to the Sato Eq. (113) and matching conditions (107) on the wave operators $P^+(\alpha)$. We show that Sato equation is the compatibility condition of Sato's linear problem (121) on the wave function (Proposition 4.3), and that compatibility of Sato equation implies the equivalent Lax and Zakharov–Shabat equations (Lemma 4.3). We prove that compatibility conditions completely determine the wave operators $P^+(\alpha)$ once one of them is given (Proposition 4.1). At the end of the section we write down explicitly the first Sato and Lax equations and relations between them.

In Sec. V we show that many well-known $2+1$ soliton equations are the simplest equations of the n-component KP hierarchy, and deduce from Sec. IV expressions for their τ-functions and the corresponding Hirota bilinear equations.

Using vertex operators we write down in Sec. VI the N-solitary solutions (219) of the n-component KP and hence of all its relatives. We discuss briefly the relation of this general solution to the known solutions to the relatives.

In Sec. VII we discuss the $[m_1,m_2,\dots,m_n]$-reductions of the n-component KP hierarchy. They reduce the $2+1$ soliton equations to $1+1$ soliton equations. We show that at the group theoretic level it corresponds to a reduction from GL_∞ (or rather a completion of it) to the subgroup $\mathrm{SL}_{m_1+\cdots+m_n}(\mathbb{C}[t,t^{-1}])$ (Proposition 7.1). We discuss in more detail the $[1,1,\dots,1]$-reduced n-component KP, which is a generalization of the NLS system and which admits further generalization to any simple Lie group.

In Sec. VIII we introduce the Lie algebra $W_{1+\infty}(\mathrm{gl}_n)$ and describe the Orlov–Schulman–Adler–Shiota–van Moerbeke formula for the n-component KP hierarchy. This formula gives a connection between the action of $W_{1+\infty}(\mathrm{gl}_n)$ on a tau function and the Orlov-Schulman symmetries of the wave function.

II. THE SEMI-INFINITE WEDGE REPRESENTATION OF THE GROUP GL_∞ AND THE KP HIERARCHY IN THE FERMIONIC PICTURE

Consider the infinite complex matrix group

$$\mathrm{GL}_\infty=\{A=(a_{ij})_{i,j\in\mathbb{Z}+1/2}|A \text{ is invertible and all but a finite number of } a_{ij}-\delta_{ij} \text{ are } 0\}$$

and its Lie algebra

$$\mathrm{gl}_\infty=\{a=(a_{ij})_{i,j\in\mathbb{Z}+1/2}| \text{ all but a finite number of } a_{ij} \text{ are } 0\}$$

with bracket $[a,b]=ab-ba$. The Lie algebra gl_∞ has a basis consisting of matrices E_{ij}, $i,j\in\mathbb{Z}+1/2$, where E_{ij} is the matrix with a 1 on the (i,j)th entry and zeros elsewhere.

Let $\mathbb{C}^\infty=\oplus_{j\in\mathbb{Z}+1/2}\mathbb{C}v_j$ be an infinite-dimensional complex vector space with fixed basis $\{v_j\}_{j\in\mathbb{Z}+1/2}$. Both the group GL_∞ and its Lie algebra gl_∞ act linearly on $\mathbb{C}^\infty$ via the usual formula:

$$E_{ij}(v_k)=\delta_{jk}v_i.$$

The well-known semi-infinite wedge representation is constructed as follows.[27] The semi-infinite wedge space $F=\Lambda^{1/2\infty}\mathbb{C}^\infty$ is the vector space with a basis consisting of all semi-infinite monomials of the form $v_{i_1}\wedge v_{i_2}\wedge v_{i_3}\wedge\cdots$, where $i_1>i_2>i_3>\cdots$ and $i_{\ell+1}=i_\ell-1$ for $\ell\gg 0$. We can now define representations R of GL_∞ and r of gl_∞ on F by

$$R(A)(v_{i_1}\wedge v_{i_2}\wedge v_{i_3}\wedge\cdots)=Av_{i_1}\wedge Av_{i_2}\wedge Av_{i_3}\wedge\cdots, \tag{30}$$

$$r(a)(v_{i_1}\wedge v_{i_2}\wedge v_{i_3}\wedge\cdots)=\sum_k v_{i_1}\wedge v_{i_2}\wedge\cdots\wedge v_{i_{k-1}}\wedge av_{i_k}\wedge v_{i_{k+1}}\wedge\cdots. \tag{31}$$

These equations are related by the usual formula:

$$\exp(r(a))=R(\exp a) \quad \text{for } a\in\mathrm{gl}_\infty.$$

The representation r of gl_∞ can be described in terms of a Clifford algebra. Define the wedging and contracting operators ψ_j^+ and ψ_j^- $(j\in\mathbb{Z}+1/2)$ on F by

$$\psi_j^+(v_{i_1}\wedge v_{i_2}\wedge\cdots)=\begin{cases}0 & \text{if } j=i_s \text{ for some } s,\\ (-1)^s v_{i_1}\wedge v_{i_2}\cdots\wedge v_{i_s}\wedge v_{-j}\wedge v_{i_{s+1}}\wedge\cdots & \text{if } i_s>-j>i_{s+1};\end{cases}$$

$$\psi_j^-(v_{i_1}\wedge v_{i_2}\wedge\cdots)=\begin{cases}0 & \text{if } j\neq i_s \text{ for all } s,\\ (-1)^{s+1} v_{i_1}\wedge v_{i_2}\wedge\cdots\wedge v_{i_{s-1}}\wedge v_{i_{s+1}}\wedge\cdots & \text{if } j=i_s.\end{cases}$$

These operators satisfy the following relations $(i,j\in\mathbb{Z}+1/2,\lambda,\mu=+,-)$:

$$\psi_i^\lambda\psi_j^\mu+\psi_j^\mu\psi_i^\lambda=\delta_{\lambda,-\mu}\delta_{i,-j}, \tag{32}$$

hence they generate a Clifford algebra, which we denote by $\mathcal{C}\ell$.

Introduce the following elements of F $(m\in\mathbb{Z})$:

$$|m\rangle=v_{m-1/2}\wedge v_{m-3/2}\wedge v_{m-5/2}\wedge\cdots.$$

It is clear that F is an irreducible $\mathcal{C}\ell$-module such that

$$\psi_j^{\pm}|0\rangle = 0 \quad \text{for } j > 0. \tag{33}$$

It is straightforward that the representation r is given by the following formula:

$$r(E_{ij}) = \psi_{-i}^{+}\psi_j^{-}. \tag{34}$$

Define the *charge decomposition*

$$F = \bigoplus_{m \in \mathbb{Z}} F^{(m)} \tag{35}$$

by letting

$$\text{charge}(v_{i_1} \wedge v_{i_2} \wedge \cdots) = m \quad \text{if } i_k + k = \frac{1}{2} + m \quad \text{for } k \gg 0. \tag{36}$$

Note that

$$\text{charge}(|m\rangle) = m \quad \text{and} \quad \text{charge}(\psi_j^{\pm}) = \pm 1. \tag{37}$$

It is clear that the charge decomposition is invariant with respect to $r(\mathrm{gl}_\infty)$ [and hence with respect to $R(\mathrm{GL}_\infty)$]. Moreover, it is easy to see that each $F^{(m)}$ is irreducible with respect to gl_∞ (and GL_∞). Note that $|m\rangle$ is its highest weight vector, i.e.,

$$r(E_{ij})|m\rangle = 0 \quad \text{for } i < j,$$

$$r(E_{ii})|m\rangle = 0 \ \ (\text{resp.} = |m\rangle) \quad \text{if } i > m \ \ (\text{resp. if } i < m).$$

The main object of our study is the GL_∞-orbit

$$\mathcal{O} = R(\mathrm{GL}_\infty)|0\rangle \subset F^{(0)}$$

of the vacuum vector $|0\rangle$.

Proposition 2.1:[27] *A nonzero element τ of $F^{(0)}$ lies in $\mathcal{O}$ if and only if the following equation holds in $F \otimes F$:*

$$\sum_{k \in \mathbb{Z}+1/2} \psi_k^{+} r \otimes \psi_{-k}^{-} \tau = 0. \tag{38}$$

Proof: It is clear that $\Sigma_k \psi_k^{+}|0\rangle \otimes \psi_{-k}^{-}|0\rangle = 0$ and it is easy to see that the operator $\Sigma_k \psi_k^{+} \otimes \psi_{-k}^{-} \in \mathrm{End}(F \otimes F)$ commutes with $R(g) \otimes R(g)$ for any $g \in \mathrm{GL}_\infty$. It follows that $R(g)|0\rangle$ satisfies (38). For the proof of the converse statement (which is not important for our purposes) see Ref. 27 or 30. □

Equation (38) is called the *KP hierarchy in the fermionic picture*.

Note that any nonzero element τ from the orbit $\mathcal{O}$ is of the form

$$\tau = u_{-1/2} \wedge u_{-3/2} \wedge u_{-5/2} \wedge \cdots, \quad \text{where } u_j \in \mathbb{C}^\infty \quad \text{and } u_{-k} = v_{-k} \quad \text{for } k \gg 0. \tag{39}$$

This allows us to construct a canonical map φ: $\mathcal{O} \to \mathrm{Gr}$ by $\varphi(\tau) = \Sigma_i \mathbb{C} u_{-i} \subset \mathbb{C}^\infty$, where Gr consists of the subspaces of $\mathbb{C}^\infty$ containing $\Sigma_{j=k}^{\infty} \mathbb{C} v_{-j-1/2}$ for $k \gg 0$ as a subspace of codimension k. It is clear that the map φ is surjective with fibers $\mathbb{C}^\times$.

A more general approach using the spin group of the above Clifford algebra is given in Ref. 32. As in the KP case there is a connection to Matrix models, see, e.g., Refs. 4 and 51.

Consider the free $\mathbb{Z}$-module $\widetilde{L}$ with the basis $\{\delta_j\}_{j \in 1/2+\mathbb{Z}}$, let $\widetilde{\Delta}\,(\text{resp. } \widetilde{\Delta}_0) = \{\delta_i - \delta_j | i, j \in 1/2 + \mathbb{Z}\,(\text{resp. } i, -j \in 1/2 + \mathbb{Z}_+), i \neq j\}$, and let $\widetilde{M} \subset \widetilde{L}$ (resp. $\widetilde{M}_0 \subset \widetilde{L}$) be the $\mathbb{Z}$-span of $\widetilde{\Delta}\,(\text{resp. } \widetilde{\Delta}_0)$. We define the weight of a semi-infinite monomial by

$$\text{weight}(\psi_{i_1}^{+}\cdots\psi_{i_s}^{+}\psi_{j_1}^{-}\cdots\psi_{j_t}^{-}|0\rangle)=\delta_{-i_1}+\cdots+\delta_{-i_s}-\delta_{j_1}-\cdots-\delta_{j_t}. \tag{40}$$

Note that weights of semi-infinite monomials from $F^{(0)}$ lie in $\widetilde{M}_0$. Given $\tau\in F$ we denote by $f\,\text{supp}\,\tau$, and call it the *fermionic support of* τ, the set of weights of semi-infinite monomials that occur in τ with a nonzero coefficient.

Proposition 2.2: If $\tau\in\mathcal{O}$, *then f supp* τ *is the intersection of* $\widetilde{M}_0$ *with a convex polyhedron with vertices in* $\widetilde{M}_0$ *and edges in* $\widetilde{\Delta}_0$.

Proof: According to the general result (Ref. 40, Lemma 4), the edges of the convex hull of $f\,\text{supp}\,\tau$ must be parallel to the elements of $\widetilde{\Delta}_0$. But if the difference of weights of two semi-infinite monomials is a multiple of $\delta_i-\delta_j$, then it is clearly equal to $\pm(\delta_i-\delta_j)$. Hence edges of the convex hull of $f\,\text{supp}\,\tau$ are elements of $\widetilde{\Delta}_0$, and the proposition follows. □

III. THE *n*-COMPONENT BOSONIZATION AND THE KP HIERARCHY IN THE BOSONIC PICTURE

Using a bosonization one can rewrite (38) as a system of partial differential equations. There are, however, many different bosonizations. In this article we focus on the *n*-component bosonizations, where $n=1,2,\ldots$.

For that purpose we relabel the basis vectors v_i and with them the corresponding fermionic operators (the wedging and contracting operators). This relabeling can be done in many different ways, see, e.g., Ref. 46. The simplest one is the following.

Fix $n\in\mathbb{N}$ and define for $j\in\mathbb{Z}$, $1\leqslant j\leqslant n$, $k\in\mathbb{Z}+1/2$:

$$v_k^{(j)}=v_{nk-(1/2)(n-2j+1)},$$

and correspondingly:

$$\psi_k^{\pm(j)}=\psi_{nk\pm(1/2)(n-2j+1)}^{\pm}.$$

Notice that with this relabeling we have

$$\psi_k^{\pm(j)}|0\rangle=0 \quad \text{for } k>0.$$

The charge decomposition (36) can be further decomposed into a sum of *partial charges* which are denoted by charge_j, $j=1,\ldots,n$, defined for a semi-infinite monomial $v\equiv v_{i_1}\wedge v_{i_2}\wedge\cdots$ of weight $\Sigma_i a_i\delta_i$ by

$$\text{charge}_j(v)=\sum_{k\in\mathbb{Z}}a_{kn+j-1/2}, \tag{41}$$

which is equivalent to

$$\text{charge}_j\ \ \psi_k^{\pm(i)}=\pm\delta_{ij}, \quad \text{charge}_j|0\rangle=0.$$

Another important decomposition is the *energy decomposition* defined by

$$\text{energy}|0\rangle=0, \quad \text{energy}\ \ \psi_k^{\pm(j)}=-k. \tag{42}$$

Note that energy is a non-negative number which can be calculated by

$$\text{energy}(v)=\sum_{k\in 1/2+\mathbb{Z}}a_k\left(\left[\frac{k}{n}\right]+\frac{1}{2}\right). \tag{43}$$

Introduce the fermionic fields ($z\in\mathbb{C}^{\times}$):

$$\psi^{\pm(j)}(z)\overset{\text{def}}{=}\sum_{k\in\mathbb{Z}+1/2}\psi_k^{\pm(j)}z^{-k-1/2}. \tag{44}$$

Next we introduce bosonic fields ($1\leqslant i,j\leqslant n$):

$$\alpha^{(ij)}(z)\equiv\sum_{k\in\mathbb{Z}}\alpha_k^{(ij)}z^{-k-1}\overset{\text{def}}{=}:\psi^{+(i)}(z)\psi^{-(j)}(z):, \tag{45}$$

where $::$ stands for the *normal ordered product* defined in the usual way (λ, $\mu=+$ or $-$):

$$:\psi_k^{\lambda(i)}\psi_\ell^{\mu(j)}:=\begin{cases}\psi_k^{\lambda(i)}\psi_\ell^{\mu(j)} & \text{if } \ell>0,\\ -\psi_\ell^{\mu(j)}\psi_k^{\lambda(i)} & \text{if } \ell<0.\end{cases} \tag{46}$$

One checks (using, e.g., the Wick formula) that the operators $\alpha_k^{(ij)}$ satisfy the commutation relations of the affine algebra $\mathrm{gl}_n(\mathbb{C})\hat{}$ with central charge 1, i.e.,

$$[\alpha_p^{(ij)},\alpha_q^{(k\ell)}]=\delta_{jk}\alpha_{p+q}^{(i\ell)}-\delta_{i\ell}\alpha_{p+q}^{(kj)}+p\,\delta_{i\ell}\delta_{jk}\delta_{p,-q}, \tag{47}$$

and that

$$\alpha_k^{(ij)}|m\rangle=0 \quad \text{if } k>0 \quad \text{or } k=0 \quad \text{and } i<j. \tag{48}$$

The operators $\alpha_k^{(i)}\equiv\alpha_k^{(ii)}$ satisfy the canonical commutation relation of the associative oscillator algebra, which we denote by $\mathfrak{a}$:

$$[\alpha_k^{(i)},\alpha_\ell^{(j)}]=k\,\delta_{ij}\delta_{k,-\ell}, \tag{49}$$

and one has

$$\alpha_k^{(i)}|m\rangle=0 \quad \text{for } k>0. \tag{50}$$

It is easy to see that restricted to $\mathrm{gl}_n(\mathbb{C})\hat{}$, $F^{(0)}$ is its basic highest weight representation (see Ref. 25, Chap. 12). The $\mathrm{gl}_n(\mathbb{C})\hat{}$-weight of a semi-infinite monomial v is as follows:

$$\Lambda_0+\sum_{j=1}^{n}\text{charge}_j(v)\,\delta_j-\text{energy}(v)\,\tilde{\delta}. \tag{37}$$

Here Λ_0 is the highest weight of the basic representation, $\{\delta_j\}$ is the standard basis of the weight lattice of $\mathrm{gl}_n(\mathbb{C})$ and $\tilde{\delta}$ is the primitive imaginary root (Ref. 25, Chap. 7).

In order to express the fermionic fields $\psi^{\pm(i)}(z)$ in terms of the bosonic fields $\alpha^{(ii)}(z)$, we need some additional operators Q_i, $i=1,\ldots,n$, on F. These operators are uniquely defined by the following conditions:

$$Q_i|0\rangle=\psi_{-1/2}^{+(i)}|0\rangle, \quad Q_i\psi_k^{\pm(j)}=(-1)^{\delta_{ij}+1}\psi_{k\mp\delta_{ij}}^{\pm(j)}Q_i. \tag{52}$$

They satisfy the following commutation relations:

$$Q_iQ_j=-Q_jQ_i \quad \text{if } i\neq j, \quad [\alpha_k^{(i)},Q_j]=\delta_{ij}\delta_{k0}Q_j. \tag{53}$$

Theorem 3.1:[7,24]

$$\psi^{\pm(i)}(z)=Q_i^{\pm1}z^{\pm\alpha_0^{(i)}}\exp\left(\mp\sum_{k<0}\frac{1}{k}\alpha_k^{(i)}z^{-k}\right)\exp\left(\mp\sum_{k>0}\frac{1}{k}\alpha_k^{(i)}z^{-k}\right). \tag{54}$$

Proof: See Ref. 46.

The operators on the right-hand side of (54) are called vertex operators. They made their first appearance in string theory (cf. Ref. 16).

We shall use below the following notation:

$$|k_1,\ldots,k_n\rangle = Q_1^{k_1}\cdots Q_n^{k_n}|0\rangle. \tag{55}$$

Remark 3.1: One easily checks the following relations:

$$[\alpha_k^{(i)},\psi_m^{\pm(j)}] = \pm\delta_{ij}\psi_{k+m}^{\pm(j)}.$$

They imply formula (54) for $\psi^{\pm(i)}(z)$ except for the first two factors, which require some additional analysis.

We can describe now the n-component boson-fermion correspondence. Let $\mathbb{C}[x]$ be the space of polynomials in indeterminates $x=\{x_k^{(i)}\}$, $k=1,2,\ldots$, $i=1,2,\ldots,n$. Let L be a lattice with a basis $\delta_1,\ldots,\delta_n$ over $\mathbb{Z}$ and the symmetric bilinear form $(\delta_i|\delta_j)=\delta_{ij}$, where δ_{ij} is the Kronecker symbol. Let

$$\epsilon_{ij} = \begin{cases} -1 & \text{if } i>j, \\ 1 & \text{if } i\leqslant j. \end{cases} \tag{56}$$

Define a bimultiplicative function $\epsilon: L\times L\to\{\pm 1\}$ by letting

$$\epsilon(\delta_i,\delta_j) = \epsilon_{ij}. \tag{57}$$

Let $\delta=\delta_1+\cdots+\delta_n$, $M=\{\gamma\in L|(\delta|\gamma)=0\}$, $\Delta=\{\alpha_{ij}:=\delta_i-\delta_j|i,j=1,\ldots,n,i\neq j\}$. Of course M is the root lattice of $\mathrm{sl}_n(\mathbb{C})$, the set Δ being the root system.

Consider the vector space $\mathbb{C}[L]$ with basis e^γ, $\gamma\in L$, and the following twisted group algebra product:

$$e^\alpha e^\beta = \epsilon(\alpha,\beta)e^{\alpha+\beta}. \tag{58}$$

Let $B=\mathbb{C}[x]\otimes_{\mathbb{C}}\mathbb{C}[L]$ be the tensor product of algebras. Then the n-component boson-fermion correspondence is the vector space isomorphism

$$\sigma: F\xrightarrow{\sim} B, \tag{59}$$

given by

$$\sigma(\alpha_{-m_1}^{(i_1)}\cdots\alpha_{-m_s}^{(i_s)}|k_1,\ldots,k_n\rangle) = m_1\cdots m_s x_{m_1}^{(i_1)}\cdots x_{m_s}^{(i_s)}\otimes e^{k_1\delta_1+\cdots+k_n\delta_n}. \tag{60}$$

The transported charge and energy then will be as follows:

$$\mathrm{charge}(p(x)\otimes e^\gamma) = (\delta|\gamma), \quad \mathrm{charge}_j(p(x)\otimes e^\gamma) = (\delta_j|\gamma), \tag{61}$$

$$\mathrm{energy}(x_{m_1}^{(i_1)}\cdots x_{m_s}^{(i_s)}\otimes e^\gamma) = m_1+\cdots+m_s+\tfrac{1}{2}(\gamma|\gamma). \tag{62}$$

We denote the transported charge decomposition by

$$B = \bigoplus_{m\in\mathbb{Z}} B^{(m)}.$$

The transported action of the operators $\alpha_m^{(i)}$ and Q_j looks as follows:

$$\sigma\alpha_{-m}^{(j)}\sigma^{-1}(p(x)\otimes e^\gamma) = mx_m^{(j)}p(x)\otimes e^\gamma, \quad \text{if } m>0,$$

$$\sigma\alpha_m^{(j)}\sigma^{-1}(p(x)\otimes e^{\gamma})=\frac{\partial p(x)}{\partial x_m}\otimes e^{\gamma},\quad \text{if } m>0,$$
$$\sigma\alpha_0^{(j)}\sigma^{-1}(p(x)\otimes e^{\gamma})=(\delta_j|\gamma)p(x)\otimes e^{\gamma}, \tag{63}$$
$$\sigma Q_j\sigma^{-1}(p(x)\otimes e^{\gamma})=\epsilon(\delta_j,\gamma)p(x)\otimes e^{\gamma+\delta_j}.$$

Using the isomorphism σ we can reformulate the KP hierarchy (38) in the bosonic picture as a hierarchy of Hirota bilinear equations.

We start by observing that (38) can be rewritten as follows:

$$\mathrm{Res}_{z=0}dz\left(\sum_{j=1}^{n}\psi^{+(j)}(z)\tau\otimes\psi^{-(j)}(z)\tau\right)=0,\quad \tau\in F^{(0)}. \tag{64}$$

Here and further $\mathrm{Res}_{z=0}dz\Sigma_j f_j z^j$ (where f_j are independent of z) stands for f_{-1}. Notice that for $\tau\in F^{(0)}$, $\sigma(\tau)=\Sigma_{\gamma\in M}\tau_\gamma(x)e^{\gamma}$. Here and further we write $\tau_\gamma(x)e^{\gamma}$ for $\tau_\gamma\otimes e^{\gamma}$. Using Theorem 3.1, Eq. (64) turns under $\sigma\otimes\sigma: F\otimes F\xrightarrow{\sim}\mathbb{C}[x',x'']\otimes(\mathbb{C}[L']\otimes\mathbb{C}[L''])$ into the following equation:

$$\mathrm{Res}_{z=0}dz\left(\sum_{j=1}^{n}\sum_{\alpha,\beta\in M}\epsilon(\delta_j,\alpha-\beta)z^{(\delta_j|\alpha-\beta)}\exp\left(\sum_{k=1}^{\infty}(x_k^{(j)'}-x_k^{(j)''})z^k\right)\right.$$
$$\left.\times\exp\left(-\sum_{k=1}^{\infty}\left(\frac{\partial}{\partial x_k^{(j)'}}-\frac{\partial}{\partial x_k^{(j)''}}\right)\frac{z^{-k}}{k}\right)\tau_\alpha(x')(e^{\alpha+\delta_j})'\tau_\beta(x'')(e^{\beta-\delta_j})''\right)=0. \tag{65}$$

Hence for all $\alpha,\beta\in L$ such that $(\alpha|\delta)=-(\beta|\delta)=1$ we have

$$\mathrm{Res}_{z=0}\left(dz\sum_{j=1}^{n}\epsilon(\delta_j,\alpha-\beta)z^{(\delta_j|\alpha-\beta-2\delta_j)}\exp\left(\sum_{k=1}^{\infty}(x_k^{(j)'}-x_k^{(j)''})z^k\right)\right.$$
$$\left.\times\exp\left(-\sum_{k=1}^{\infty}\left(\frac{\partial}{\partial x_k^{(j)'}}-\frac{\partial}{\partial x_k^{(j)''}}\right)\frac{z^{-k}}{k}\right)\tau_{\alpha-\delta_j}(x')\tau_{\beta+\delta_j}(x'')\right)=0. \tag{66}$$

Now making the change of variables

$$x_k^{(j)}=\tfrac{1}{2}(x_k^{(j)'}+x_k^{(j)''}),\quad y_k^{(j)}=\tfrac{1}{2}(x_k^{(j)'}-x_n^{(j)''}),$$

(66) becomes

$$\mathrm{Res}_{z=0}\left(dz\sum_{j=1}^{n}\epsilon(\delta_j,\alpha-\beta)z^{(\delta_j|\alpha-\beta-2\delta_j)}\exp\left(\sum_{k=1}^{\infty}2y_k^{(j)}z^k\right)\exp\left(-\sum_{k=1}^{\infty}\frac{\partial'}{\partial y_k^{(j)}}\frac{z^{-k}}{k}\right)\right.$$
$$\left.\times\tau_{\alpha-\delta_j}(x+y)\tau_{\beta+\delta_j}(x-y)\right)=0. \tag{67}$$

We can rewrite (67) using the elementary Schur polynomials defined by (13):

$$\sum_{j=1}^{n}\epsilon(\delta_j,\alpha-\beta)\sum_{k=0}^{\infty}S_k(2y^{(j)})S_{k-1+(\delta_j|\alpha-\beta)}\left(-\frac{\tilde{\partial}}{\partial y^{(j)}}\right)\tau_{\alpha-\delta_j}(x+y)\tau_{\beta+\delta_j}(x-y)=0. \tag{68}$$

Here and further we use the notation

$$\frac{\tilde{\partial}}{\partial y}=\left(\frac{\partial}{\partial y_1},\frac{1}{2}\frac{\partial}{\partial y_2},\frac{1}{3}\frac{\partial}{\partial y_3},\ldots\right).$$

Using Taylor's formula we can rewrite (68) once more:

$$\sum_{j=1}^{n}\epsilon(\delta_j,\alpha-\beta)\sum_{k=0}^{\infty}S_k(2y^{(j)})S_{k-1+(\delta_j|\alpha-\beta)}\left(-\frac{\tilde{\partial}}{\partial u^{(j)}}\right)$$
$$\times e^{\Sigma_{j=1}^{n}\Sigma_{r=1}^{\infty}y_r^{(j)}\partial/\partial u_r^{(j)}}\tau_{\alpha-\delta_j}(x+u)\tau_{\beta+\delta_j}(x-u)|_{u=0}=0. \tag{69}$$

This last equation can be written as the following generating series of Hirota bilinear equations:

$$\sum_{j=1}^{n}\epsilon(\delta_j,\alpha-\beta)\sum_{k=0}^{\infty}S_k(2y^{(j)})S_{k-1+(\delta_j|\alpha-\beta)}(-\widetilde{D^{(j)}})e^{\Sigma_{j=1}^{n}\Sigma_{r=1}^{\infty}y_r^{(j)}D_r^{(j)}}\tau_{\alpha-\delta_j}\cdot\tau_{\beta+\delta_j}=0 \tag{70}$$

for all $\alpha,\beta\in L$ such that $(\alpha|\delta)=-(\beta|\delta)=1$. Hirota's dot notation used here and further is explained in the Introduction [see (9)].

Equation (70) is known (see Refs. 7, 8, and 24) as the *n*-component KP hierarchy of Hirota bilinear equations. This equation still describes the group orbit: $\sigma(\mathcal{O})=\sigma R\sigma^{-1}(\mathrm{GL}_\infty)\cdot 1$.

Remark 3.2: Equation (70) is invariant under the transformations $\alpha\mapsto\alpha+\gamma$, $\beta\mapsto\beta+\gamma$, where $\gamma\in M$. Transformations of this type are called Schlesinger transformations.

Let $\tau=\Sigma_{\gamma\in L}\tau_\gamma(x)e^\gamma\in B$; the set $\mathrm{supp}\ \tau=_{\mathrm{def}}\{\gamma\in L|\tau_\gamma\neq 0\}$ is called the *support* of τ.

Proposition 3.1: Let $\tau\in\mathbb{C}[[x]]\otimes\mathbb{C}[M]$ be a solution to the KP hierarchy (67). Then supp τ is the intersection of M with a convex polyhedron with vertices in M and edges parallel to elements of Δ.

Proof: Consider the linear map $\overline{\sigma}:\tilde{L}\to L$ defined by $\overline{\sigma}(\delta_j)=\delta_{(j+1/2)\bmod n}$, where $a\bmod n$ stands for the element of the set $\{1,\ldots,n\}$ congruent to $a\bmod n$. Then it is easy to see that for $\tau\in F$ we have

$$\mathrm{supp}\ \ \sigma(\tau)=\overline{\sigma}(f\ \ \mathrm{supp}\ \ \tau).$$

Now Proposition 3.1 follows from Proposition 2.2. □

The indeterminates $y_k^{(j)}$ in (70) are free parameters, hence the coefficient of a monomial $y_{k_1}^{(j_1)}\cdots y_{k_s}^{(j_s)}$ $(k_i\in\mathbb{N},k_1\leqslant k_2\leqslant\cdots,j_i\in\{1,\ldots,n\})$ in Eq. (70) gives us a Hirota bilinear equation of the form

$$\sum_{i=1}^{n}\sum_{\alpha,\beta}Q_{k;\alpha,\beta}^{(j)}(D)\tau_{\alpha-\delta_i}\cdot\tau_{\beta+\delta_i}=0, \tag{71}$$

where $Q_{k,\alpha,\beta}^{(j)}$ are polynomials in the $D_r^{(i)}$, $k=(k_1,\ldots,k_s)$, $j=(j_1,\ldots,j_s)$ and $\alpha,\beta\in L$ are such that $(\alpha|\delta)=-(\beta|\delta)=1$. Each of these equations is a partial differential equation (PDE) in the indeterminates $x_k^{(j)}$ on functions τ_γ, $\gamma\in M$.

Recall that an expression $Q(D)\tau_\alpha\cdot\tau_\beta$ is identically zero if and only if $\alpha=\beta$ and $Q(D)=-Q(-D)$. The corresponding Hirota bilinear equation is then called *trivial* and can be disregarded.

Let us point out now that the energy decomposition (62) induces the following energy decomposition on the space of Hirota bilinear equations:

$$\mathrm{energy}(Q_{k;\alpha,\beta}^{(j)}(D)\tau_{\alpha-\delta_i}\cdot\tau_{\beta+\delta_i})=k_1+\cdots+k_s+\tfrac{1}{2}((\alpha|\alpha)+(\beta|\beta)). \tag{72}$$

It is clear that the energy of a nontrivial Hirota bilinear equation is at least 2.

Below we list the Hirota bilinear equations of lowest energy for each *n*.

$n=1$. In this case we may drop the superscript in $D_k^{(1)}$ and the subscript in τ_α (which is 0). Each monomial $y_{k_1}\cdots y_{k_s}$ gives a Hirota bilinear equation of the form

$$Q_k(D)\tau\cdot\tau=0$$

of energy $k_1+\cdots+k_s+1$. An easy calculation shows that the lowest energy of a nontrivial equation is 4, and that there is a unique nontrivial equation of energy 4, the classical KP equation in the Hirota bilinear form:

$$(D_1^4-4D_1D_3+3D_2^2)\tau\cdot\tau=0. \tag{73}$$

$n\geqslant 2$. There is an equation of energy 2 for each unordered pair of distinct indices i and k (recall that $\alpha_{ik}=\delta_i-\delta_k$ are roots):

$$D_1^{(i)}D_1^{(k)}\tau_0\cdot\tau_0=2\tau_{\alpha_{ik}}\tau_{\alpha_{ki}}. \tag{74}$$

Furthermore, for each ordered pair of distinct indices i and j there are three equations of energy 3:

$$(D_2^{(i)}+D_1^{(i)2})\tau_0\cdot\tau_{\alpha_{ij}}=0, \tag{75}$$

$$(D_2^{(j)}+D_1^{(j)2})\tau_{\alpha_{ij}}\cdot\tau_0=0, \tag{76}$$

$$D_1^{(i)}D_2^{(j)}\tau_0\cdot\tau_0+2D_1^{(j)}\tau_{\alpha_{ij}}\cdot\tau_{\alpha_{ji}}=0. \tag{77}$$

$n\geqslant 3$. There is an equation of energy 2 and an equation of energy 3 for each ordered triple of distinct indices i, j, k:

$$D_1^{(k)}\tau_0\cdot\tau_{\alpha_{ij}}=\epsilon_{ik}\epsilon_{kj}\epsilon_{ij}\tau_{\alpha_{ik}}\tau_{\alpha_{kj}}, \tag{78}$$

$$D_2^{(k)}\tau_0\cdot\tau_{\alpha_{ij}}=\epsilon_{ij}\epsilon_{kj}\epsilon_{ik}D_1^{(k)}\tau_{\alpha_{ik}}\cdot\tau_{\alpha_{kj}}. \tag{79}$$

[Note that (76) is a special case of (79) where $k=j$.]

$n\geqslant 4$. There is an algebraic equation of energy 2 for each ordered quadruple of distinct indices i, j, k, ℓ:

$$\epsilon_{ij}\epsilon_{k\ell}\tau_0\tau_{\alpha_{ik}+\alpha_{j\ell}}+\epsilon_{i\ell}\epsilon_{jk}\tau_{\alpha_{ik}}\tau_{\alpha_{j\ell}}+\epsilon_{ik}\epsilon_{j\ell}\tau_{\alpha_{i\ell}}\tau_{\alpha_{jk}}=0. \tag{80}$$

Equations (74)–(80), together with an algebraic equation of energy 3 for each ordered sextuple of distinct indices similar to (80), form a complete list of nontrivial Hirota bilinear equations of energy $\leqslant 3$ of the n-component KP hierarchy.

IV. THE ALGEBRA OF FORMAL PSEUDO-DIFFERENTIAL OPERATORS AND THE n-COMPONENT KP HIERARCHY AS A DYNAMICAL SYSTEM

The KP hierarchy and its n-component generalizations admit several formulations. The one given in the previous section obtained by the field theoretical approach is the τ-function formulation given by Date, Jimbo, Kashiwara, and Miwa.[7] Another well-known formulation, introduced by Sato,[41] is given in the language of formal pseudo-differential operators. We will show that this formulation follows from the τ-function formulation given by Eq. (66).

We shall work over the algebra $\mathcal{A}$ of formal power series over $\mathbb{C}$ in indeterminates ξ and $x=(x_k^{(j)})$, where $k=1,2,...$ and $j=1,...,n$. The indeterminate ξ will be viewed as a variable and the $x_k^{(j)}$ as parameters. Let

$$\partial = \frac{\partial}{\partial \xi}.$$

A *formal $n\times n$ matrix pseudo-differential operator* is an expression of the form

$$P(\xi,x,\partial) = \sum_{j\leqslant N} P_j(\xi,x)\partial^j, \tag{81}$$

where P_j are $n\times n$ matrices over $\mathcal{A}$. The largest N such that $P_N \neq 0$ is called the *order* of $P(\xi,x,\partial)$ [write $\operatorname{ord} P(\xi,x,\partial) = N$]. The coefficient P_{-1} is called the *residue* of P (write $\operatorname{Res}_\partial P = P_{-1}$). Let Ψ denote the vector space over $\mathbb{C}$ of all expressions (81). We have a linear isomorphism $s:\Psi \to \operatorname{Mat}_n(\mathcal{A}((z)))$ given by $s(P(\xi,x,\partial)) = P(\xi,x,z)$. The matrix series $P(\xi,x,z)$ in indeterminates ξ, x and z is called the *symbol* of $P(\xi,x,\partial)$.

Now we may define a product $\circ$ on Ψ making it an associative algebra:

$$s(P\circ Q) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n s(P)}{\partial z^n} \partial^n s(Q).$$

We shall often drop the multiplication sign $\circ$ when no ambiguity may arise. Letting $\Psi(m) = \{P \in \Psi \,|\, \operatorname{ord}\Psi \leqslant m\}$, we get a $\mathbb{Z}$-filtration of the algebra Ψ:

$$\cdots \Psi(m+1) \supset \Psi(m) \supset \Psi(m-1) \supset \cdots. \tag{82}$$

One defines the differential part of $P(\xi,x,\partial)$ by $P_+(\xi,x,\partial) = \Sigma_{j=0}^N P_j(\xi,x)\partial^j$, and let $P_- = P - P_+$. We have the corresponding vector space decomposition:

$$\Psi = \Psi_- \oplus \Psi_+. \tag{83}$$

One defines a linear map $*:\Psi\to\Psi$ by the following formula:

$$\left(\sum_j P_j \partial^j\right)^* = \sum_j (-\partial)^j \circ {}^t P_j. \tag{84}$$

Here and further ${}^tP$ stands for the transpose of the matrix P. Note that $*$ is an anti-involution of the algebra Ψ. In terms of symbols the anti-involution $*$ can be written in the following closed form:

$$P^*(\xi,x,z) = \left(\exp \partial \frac{\partial}{\partial z}\right) {}^t P(\xi,x,-z). \tag{85}$$

It is clear that the anti-involution $*$ preserves the filtration (82) and the decomposition (83).

Introduce the following notation:

$$z\cdot x^{(j)} = z\xi + \sum_{k=1}^{\infty} z^k x_k^{(j)}, \quad e^{z\cdot x} = \operatorname{diag}(e^{z\cdot x^{(1)}},\ldots,e^{z\cdot x^{(n)}}).$$

The algebra Ψ acts on the space U_+ (resp. U_-) of formal oscillating matrix functions of the form

$$\sum_{j\leqslant N} P_j z^j e^{z\cdot x}\left(\text{resp. } \sum_{j\leqslant N} P_j z^j e^{-z\cdot x}\right), \quad \text{where } P_j \in \operatorname{Mat}_n(\mathcal{A}),$$

in the obvious way:

$$P(\xi,x)\partial^j e^{\pm z\cdot x} = P(\xi,x)(\pm z)^j e^{\pm z\cdot x}.$$

We can now prove the following fundamental lemma.

Lemma 4.1: For $P,Q\in\Psi$ one has

$$\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})({}^tQ(\xi-\eta,x',-z)e^{z(\eta-\xi)})dz=\mathrm{Res}_{\partial}P(\xi,x,\partial)\circ Q^*(\xi,x',\partial)\circ e^{\eta\partial}. \quad (86)$$

Proof: We first prove Eq. (86) for $\eta=0$, i.e.,

$$\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})({}^tQ(\xi,x',-z)e^{-z\xi})dz=\mathrm{Res}_{\partial}P(\xi,x,\partial)\circ Q^*(\xi,x',\partial). \quad (87)$$

For this purpose we let $P(\xi,x,\partial)=\Sigma_i P_i\partial^i$ and ${}^tQ(\xi,x',\partial)=\Sigma_j Q_j(-\partial)^j$. Then the left-hand side of (87) is

$$\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})({}^tQ(\xi,x',-z)e^{-z\xi})dz=\sum_{i+j=-1}P_i\ {}^tQ_j. \quad (88)$$

The right-hand side of (87) is equal to $\mathrm{Res}_{\partial}\Sigma_{i,j}P_i\partial^{i+j}\,{}^tQ_j$. Since $\binom{k-1}{k}=0$ for $k>0$ we deduce that this is equal to

$$\begin{aligned}\mathrm{Res}_{\partial}\sum_{i,j}P_i\partial^{i+j}\ {}^tQ_j&=\mathrm{Res}_{\partial}\sum_{i,j}\sum_{k=0}^{\infty}\binom{i+j}{k}\frac{\partial^k\ {}^tQ}{\partial\xi^k}\partial^{i+j-k}\\&=\sum_{i+j+1=k\geqslant 0}\binom{i+j}{k}\frac{\partial^k\ {}^tQ}{\partial\xi^k}\partial^{i+j-k}\\&=\sum_{i+j=-1}P_i\ {}^tQ_j,\end{aligned}$$

which is equal to (88). This proves (87). Next, we use Taylor's formula and rewrite the left-hand side of (86):

$$\begin{aligned}&\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})({}^tQ(\xi-\eta,x',-z)e^{z(\eta-\xi)})dz\\&=\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})\sum_{k=0}^{\infty}\frac{(-\eta)^k}{k!}\frac{\partial^k}{\partial\xi^k}({}^tQ(\xi,x',-z)e^{-z\xi})dz\\&=\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})\sum_{k=0}^{\infty}\frac{(-\eta)^k}{k!}\sum_{\ell=0}^{k}\binom{k}{\ell}\frac{\partial^{\ell}\ {}^tQ(\xi,x',-z)}{\partial\xi^{\ell}}(-z)^{k-\ell}e^{-z\xi}dz\\&=\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})\sum_{k=0}^{\infty}\frac{(\eta)^k}{k!}{}^t((-\partial)^kQ(\xi,x',\partial))e^{-z\xi}dz. \quad (89)\end{aligned}$$

Using (87) we find that the last line of (89) is equal to

$$\mathrm{Res}_{\partial}\sum_{k=0}^{\infty}\frac{(\eta)^k}{k!}P(\xi,x,\partial)\circ Q^*(\xi,x',\partial)\circ\partial^k,$$

which is equal to the right-hand side of (86). □

As a consequence of this lemma one finds the following corollary.

Corollary 4.1: The equality

$$\mathrm{Res}_{z=0}(P(\xi,x,z)e^{z\xi})({}^tQ(\xi',x',-z)e^{-z\xi'})dz=0 \quad (90)$$

is equivalent to

$$(P(\xi,x,\partial)\circ Q^*(\xi,x',\partial))_- = 0. \tag{91}$$

Proof: Substitute $\xi' = \xi - \eta$ in (90). Now use Lemma 4.1 and one obtains that

$$\mathrm{Res}_\partial P(\xi,x,\partial)\circ Q^*(\xi,x',\partial)\circ e^{\eta\partial} = 0.$$

Next write $e^{\eta\partial} = \Sigma_{j=0}^{\infty}(\partial^j/j!)\,\eta^j$ and (91) follows immediately. The converse is proved in a similar way. □

In this article we will sometimes use infinite order pseudo-differential operators. Following Mulase[37] we define a valuation

$$\mathrm{val}_x : \mathcal{A}\backslash\{0\} \to \{0,1,2,3,\ldots\}$$

by

$$\mathrm{val}_x x_k^{(j)} = \mathrm{energy}(x_k^{(j)}) = k$$

and take a completion of Ψ defined as follows:

$$\hat{\Psi} = \left\{ P = \sum_{j\in\mathbb{Z}} P_j\partial^j \,\middle|\, P_j \in \mathcal{A} \quad \text{and there is a positive real number } C_P \right.$$
$$\left. \text{and positive integers } M_P \text{ and } N_P \text{ such that } \mathrm{val}_x P_j > C_P j - N_P \quad \text{for all } j > M_P \right\}.$$

The completion $\hat{\Psi}$ has a natural associative algebra structure. We refer for more information to Refs. 36 and 37. It is straightforward to check the following:

Remark 4.1: Lemma 4.1 and Corollary 4.1 also hold for $P,Q \in \hat{\Psi}$.

We proceed now to rewrite the formulation (66) of the *n*-component KP hierarchy in terms of formal pseudo-differential operators.

Let $1 \leqslant a,\ b \leqslant n$ and recall formula (66) where α is replaced by $\alpha + \delta_a$, β by $\beta - \delta_b$ and all $x_1^{(j)}$ for $1 \leqslant j \leqslant n$ by $x_1^{(j)} + \xi$:

$$\mathrm{Res}_{z=0}\left(dz \sum_{j=1}^{n} \epsilon(\delta_j, \alpha + \delta_a - \beta + \delta_b) z^{(\delta_j|\alpha+\delta_a-\beta+\delta_b-2\delta_j)} \exp\left(\sum_{k=1}^{\infty} (x_k^{(j)\prime} - x_k^{(j)\prime\prime}) z^k \right) \right.$$
$$\left. \times \exp\left(-\sum_{k=1}^{\infty} \left(\frac{\partial}{\partial x_k^{(j)\prime}} - \frac{\partial}{\partial x_k^{(j)\prime\prime}} \right) \frac{z^{-k}}{k} \right) \tau_{\alpha+\alpha_{a_j}}(\xi',x')\,\tau_{\beta-\alpha_{b_j}}(\xi'',x'') \right) e^{z(\xi'-\xi'')} = 0$$
$$(\alpha,\beta \in M). \tag{92}$$

For each $\alpha \in \mathrm{supp}\ \tau$ we define the (matrix valued) functions

$$V^{\pm}(\alpha,\xi,x,z) = (V_{ij}^{\pm}(\alpha,\xi,x,z))_{i,j=1}^{n} \tag{93}$$

as follows:

$$V_{ij}^{\pm}(\alpha,\xi,x,z) \overset{\text{def}}{=} \epsilon(\delta_j, \alpha + \delta_i) z^{(\delta_j|\pm\alpha+\alpha_{ij})} \exp\left(\pm \sum_{k=1}^{\infty} x_k^{(j)} z^k \right)$$
$$\times \exp\left(\mp \sum_{k=1}^{\infty} \frac{\partial}{\partial x_k^{(j)}} \frac{z^{-k}}{k} \right) \tau_{\alpha\pm\alpha_{ij}}(\xi,x)/\tau_\alpha(\xi,x) e^{\pm z\xi}. \tag{94}$$

It is easy to see that Eq. (92) is equivalent to the following bilinear identity:

$$\mathrm{Res}_{z=0} V^+(\alpha,\xi,x,z)\ {}^tV^-(\beta,\xi',x',z)dz=0 \quad \text{for all} \quad \alpha,\beta\in M. \tag{95}$$

Define $n\times n$ matrices $W^{\pm(m)}(\alpha,\xi,x)$ by the following generating series [cf. (94)]:

$$\sum_{m=0}^{\infty} W_{ij}^{\pm(m)}(\alpha,\xi,x)(\pm z)^{-m}=\epsilon_{ji}z^{\delta_{ij}-1}\left(\exp\mp\sum_{k=1}^{\infty}\frac{\partial}{\partial x_k^{(j)}}\frac{z^{-k}}{k}\right)\tau_{\alpha\pm\alpha_{ij}}(\xi,x))/\tau_\alpha(\xi,x). \tag{96}$$

Note that

$$W^{\pm(0)}(\alpha,\xi,x)=I_n, \tag{97}$$

$$W_{ij}^{\pm(1)}(\alpha,\xi,x)=\begin{cases}\pm\epsilon_{ji}\tau_{\alpha\pm\alpha_{ij}}/\tau_\alpha & \text{if } i\neq j,\\ -\tau_\alpha^{-1}\dfrac{\partial\tau_\alpha}{\partial x_1^{(i)}} & \text{if } i=j,\end{cases} \tag{98}$$

$$W_{ij}^{\pm(2)}(\alpha,\xi,x)=\begin{cases}\mp\epsilon_{ji}\dfrac{\partial\tau_{\alpha\pm\alpha_{ij}}}{\partial x_1^{(j)}}\Big/\tau_\alpha & \text{if } i\neq j,\\ \left(\mp\dfrac{1}{2}\dfrac{\partial\tau_\alpha}{\partial x_2^{(i)}}+\dfrac{1}{2}\dfrac{\partial^2\tau_\alpha}{\partial x_1^{(i)2}}\right)\Big/\tau_\alpha & \text{if } i=j.\end{cases} \tag{99}$$

We see from (94) that $V^\pm(\alpha,\xi,x,z)$ can be written in the following form:

$$\begin{aligned}V^\pm(\alpha,\xi,x,z)&=\left(\sum_{m=0}^{\infty}W^{\pm(m)}(\alpha,\xi,x)R^\pm(\alpha,\pm z)(\pm z)^{-m}\right)e^{\pm z\cdot x}\\&=\sum_{m=0}^{\infty}W^{\pm(m)}(\alpha,\xi,x)(\pm z)^{-m}R^\pm(\alpha,\pm z)S^\pm(x,\pm z)e^{z\xi},\end{aligned} \tag{100}$$

where

$$\begin{aligned}R^\pm(\alpha,z)&=\sum_{i=1}^{n}\epsilon(\delta_i,\alpha)E_{ii}(\pm z)^{\pm(\delta_i|\alpha)},\\ S^\pm(x,z)&=\sum_{i=1}^{n}e^{\pm\sum_{j=1}^{\infty}x_j^{(i)}(\pm z)^j}E_{ii}.\end{aligned} \tag{101}$$

Here and further E_{ij} stands for the $n\times n$ matrix whose (i,j) entry is 1 and all other entries are zero. Now it is clear that $V^\pm(\alpha,\xi,x,z)$ can be written in terms of formal pseudo-differential operators

$$\begin{aligned}P^\pm(\alpha)\equiv P^\pm(\alpha,\xi,x,\partial)&=I_n+\sum_{m=1}^{\infty}W^{\pm(m)}(\alpha,\xi,x)\partial^{-m}.\\ R^\pm(\alpha)=R^\pm(\alpha,\xi,\partial)\quad&\text{and}\quad S^\pm=S^\pm(x,\partial)\end{aligned} \tag{102}$$

as follows:

$$V^\pm(\alpha,\xi,x,z)=P^\pm(\alpha)R^\pm(\alpha)e^{\pm z\cdot x}=P^\pm(\alpha)R^\pm(\alpha)S^\pm e^{\pm zx}. \tag{103}$$

Since obviously

$$R^-(\alpha,\partial)^{-1}=R^+(\alpha,\partial)^* \quad \text{and} \quad S^-(x,\partial)^{-1}=S^+(x,\partial)^*, \tag{104}$$

using Corollary 4.1 and Remark 4.1 we deduce from the bilinear identity (95)

$$(P^+(\alpha,\xi,x,\partial)R^+(\alpha-\beta,\partial)S^+(x-x',\partial)P^-(\beta,\xi,x'\partial)^*)_-=0 \tag{105}$$

for any $\alpha,\ \beta\in\text{supp}\ \tau$.

Furthermore, put $x=x'$. Then one deduces from (105) with $\alpha=\beta$ that

$$P^-(\alpha)=(P^+(\alpha)^*)^{-1}, \tag{106}$$

since $R^\pm(0)=I_n$ and $P^\pm(\alpha)\in I_n+\Psi_-$. Equations (105) and (106) imply

$$(P^+(\alpha)R^+(\alpha-\beta)P^+(\beta)^{-1})_-=0 \quad \text{for all} \quad \alpha,\beta\in\text{supp}\ \tau. \tag{107}$$

In the rest of this article we sometimes write $P(\alpha)$, $W(\alpha)^{(k)}$ instead of $P^+(\alpha)$ and $W(\alpha)^{+(k)}$.

Proposition 4.1: Given $\beta\in supp\ \tau$, all the pseudo-differential operators $P(\alpha)$, $\alpha\in supp\ \tau$, are completely determined by $P(\beta)$ from Eqs. (107). Moreover, if $\alpha=\beta+\alpha_{ij}$, then

$$P(\alpha)=\left(\left(\epsilon_{ij}\partial+\frac{\partial\log W_{ij}^{(1)}(\beta)}{\partial x_1^{(i)}}\right)E_{ii}-\frac{\epsilon_{ij}}{W_{ij}^{(1)}(\beta)}E_{ji}+\sum_{\substack{k=1\\k\neq i,j}}^{n}\epsilon_{ik}\epsilon_{jk}\left(E_{kk}-\frac{W_{kj}^{(1)}(\beta)}{W_{ij}^{(1)}(\beta)}E_{ik}\right)\right)P(\beta). \tag{108}$$

Proof: For $P=I_n+\Sigma_{j=1}^{\infty}W^{(j)}\partial^{-j}$ we have

$$P^{-1}=I_n-W^{(1)}\partial^{-1}+(W^{(1)2}-W^{(2)})\partial^{-2}+\cdots. \tag{109}$$

We have for $i\neq j$:$R(\alpha_{ij})=A\partial+B+C\partial^{-1}$, where

$$A=\epsilon_{ij}E_{ii}, \quad B=\sum_{\substack{k=1\\k\neq i,j}}^{n}\epsilon_{ik}\epsilon_{jk}E_{kk}, \quad C=\epsilon_{ji}E_{jj}. \tag{110}$$

Let $\alpha,\beta\in M$ be such that $\alpha-\beta=\alpha_{ij}$. It follows from (109) and (107) that $P(\alpha)R(\alpha-\beta)P(\beta)^{-1}=(P(\alpha)R(\alpha-\beta)P(\beta)^{-1})_+=A\partial+B+W^{(1)}(\alpha)A-AW^{(1)}(\beta)$, or equivalently

$$P(\alpha)(A\partial+B+C\partial^{-1})=(A\partial+B+W^{(1)}(\alpha)A-AW^{(1)}(\beta))P(\beta).$$

Using (110),

$$\begin{aligned}W_{ii}^{(1)}(\alpha)-W_{ii}^{(1)}(\beta)&=W_{ii}^{(1)}(\beta+\alpha_{ij})-W_{ii}^{(1)}(\beta)\\&=-\tau_{\beta+\alpha_{ij}}^{-1}\frac{\partial\tau_{\beta+\alpha_{ij}}}{\partial x_i^{(1)}}+\tau_\beta^{-1}\frac{\partial\tau_\beta}{\partial x_i^{(1)}}\\&=\epsilon_{ij}\frac{\partial\log(\epsilon_{ji}\tau_{\beta+\alpha_{ij}}/\tau_\beta)}{\partial x_i^{(1)}}=\epsilon_{ij}\frac{\partial\log W_{ij}^{(1)}(\beta)}{\partial x_i^{(1)}},\end{aligned}$$

and for $k\neq i$

$$W_{ki}^{(1)}(\alpha)=W_{ki}^{(1)}(\beta+\alpha_{ij})=\epsilon_{ik}\frac{\tau_{\beta+\alpha_{ij}+\alpha_{ki}}}{\tau_{\beta+\alpha_{ij}}}=\epsilon_{ik}\frac{\tau_{\beta+\alpha_{kj}}}{\tau_\beta}\frac{\tau_\beta}{\tau_{\beta+\alpha_{ij}}}=\epsilon_{ji}\epsilon_{ik}\epsilon_{jk}\frac{W_{kj}^{(1)}(\beta)}{W_{ij}^{(1)}(\beta)},$$

we obtain (108).

Due to Proposition 3.2 for any $\alpha,\beta \in \operatorname{supp} \tau$ there exist a sequence $\gamma_1,\dots,\gamma_k$ such that $\alpha=\gamma_1$, $\beta=\gamma_k$ and $\gamma_i-\gamma_{i+1}\in\Delta$ for all $i=1,...,k-1$. The proposition now follows. □

We call operators of the form (108) which produce new wave functions Schlesinger–Bäcklund differential operators (see Ref. 49).

Remark 4.2: The functions $P^+(\alpha,\xi,x,z)$ $(\alpha\in M)$ determine the τ-function $\Sigma_\alpha \tau_\alpha(\xi,x)e^\alpha$ up to a constant factor. Namely, we may recover $\tau_\alpha(\xi,x)$ from functions $P^+_{jj}(\alpha,x,z)$ as follows. We have from (96)

$$\log P^+_{jj}(\alpha,\xi,x,z)=\log \tau_\alpha\left(x^{(p)}_\ell+\delta_{\ell,1}\xi-\frac{\delta_{jp}}{\ell z^\ell}\right)-\log \tau_\alpha(x^{(p)}_\ell+\delta_{\ell,1}\xi).$$

Putting $\xi=0$ and applying to both sides the operator $\partial/\partial z-\Sigma_{k\geqslant 1}z^{-k-1}\partial/\partial x^{(j)}_k$ (that kills the first summand on the right), we obtain

$$\left(\frac{\partial}{\partial z}-\sum_{k\geqslant 1} z^{-k-1}\frac{\partial}{\partial x^{(j)}_k}\right)\log P^+_{jj}(\alpha,x,z)=\sum_{k\geqslant 1} z^{-k-1}\frac{\partial}{\partial x^{(j)}_k}\log \tau_\alpha(x).$$

Hence

$$\frac{\partial}{\partial x^{(j)}_m}\log \tau_\alpha(x)=\operatorname{Res}_{z=0}dz\ \ z^m\left(\frac{\partial}{\partial z}-\sum_{k\geqslant 1} z^{-k-1}\frac{\partial}{\partial x^{(j)}_k}\right)\log P^+_{jj}(\alpha,x,z). \tag{111}$$

This determines $\tau_\alpha(x)$ and hence $\tau_\alpha(\xi,x)$ up to a constant factor. It follows from (98) and Proposition 3.2 that these constant factors are the same for all α.

Introduce the following formal pseudo-differential operators $L(\alpha)$, $C^{(j)}(\alpha)$, $L^{(j)}(\alpha)$ and differential operators $B_m(\alpha)$ and $B^{(j)}_m(\alpha)$:

$$\begin{aligned}
&L(\alpha)\equiv L(\alpha,\xi,x,\partial)=P^+(\alpha)\circ\partial\circ P^+(\alpha)^{-1},\\
&C^{(j)}(\alpha)\equiv C^{(j)}(\alpha,\xi,x,\partial)=P^+(\alpha)E_{jj}P^+(\alpha)^{-1},\\
&L^{(j)}(\alpha)\equiv C^{(j)}(\alpha)L(\alpha)=P^+(\alpha)E_{jj}\circ\partial\circ P^+(\alpha)^{-1},\\
&B_m(\alpha)\equiv(L(\alpha)^m)_+=(P^+(\alpha)\circ\partial^m\circ P^+(\alpha)^{-1})_+,\\
&B^{(j)}_m(\alpha)\equiv(L^{(j)}(\alpha)^m)_+=(P^+(\alpha)E_{jj}\circ\partial^m\circ P^+(\alpha)^{-1})_+.
\end{aligned} \tag{112}$$

Using Corollary 4.1 we can now derive the Sato equations from Eq. (95):

Lemma 4.2: Each formal pseudo-differential operator $P=P^+(\alpha)$ satisfies the Sato equations:

$$\frac{\partial P}{\partial x^{(j)}_k}=-(PE_{jj}\circ\partial^k\circ P^{-1})_-\circ P=B^{(j)}_k P-PE_{jj}\circ\partial^k. \tag{113}$$

Proof: Notice first that

$$\begin{aligned}
&\left(\frac{\partial}{\partial x_k^{(j)}}-B_k^{(j)}(\alpha)\right)V^+(\alpha,x,z)\\
&\quad=\left(\frac{\partial}{\partial x_k^{(j)}}-B_k^{(j)}(\alpha)\right)P^+(\alpha)R^+(\alpha)e^{z\cdot x}\\
&\quad=\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}R^+(\alpha)+P^+(\alpha)R^+(\alpha)E_{jj}\partial^k-B_k^{(j)}(\alpha)P^+(\alpha)R^+(\alpha)\right)e^{z\cdot x}\\
&\quad=\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}+P^+(\alpha)E_{jj}\partial^k-B_k^{(j)}(\alpha)P^+(\alpha)\right)R^+(\alpha)e^{z\cdot x}\\
&\quad=\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}+L^{(j)}(\alpha)^kP^+(\alpha)-B_k^{(j)}(\alpha)P^+(\alpha)\right)R^+(\alpha)e^{z\cdot x}\\
&\quad=\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}+(L^{(j)}(\alpha)^k)_-P^+(\alpha)\right)R^+(\alpha)e^{z\cdot x}.
\end{aligned}$$

Next apply $\partial/\partial x_k^{(j)}-B_k^{(j)}(\alpha)$ to the Eq. (95) for $\alpha=\beta$ to obtain

$$\mathrm{Res}_{z=0}dz\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}+(L^{(j)}(\alpha)^k)_-\right)(P^+(\alpha)R^+(\alpha)e^{z\cdot x})^t(P^-(\alpha)R^-(\alpha)e^{-z\cdot x'})=0.$$

Now apply Corollary 4.1 and (106) to obtain

$$\left(\left(\frac{\partial P^+(\alpha)}{\partial x_k^{(j)}}+(L^{(j)}(\alpha)^k)_-P^+(\alpha)\right)P^+(\alpha)^{-1}\right)_-=0,$$

which proves the lemma. □

Proposition 4.2: Consider the formal oscillating functions $V^+(\alpha,xi,x,z)$ *and* $V^-(\alpha,\xi,x,z)$, $\alpha\in M$, *of the form (103), where* $R^\pm(\alpha,z)$ *are given by (101) and* $P^\pm(\alpha,xi,x,\partial)\in I_n+\Psi_-$. *Then the bilinear identity (95) for all* $\alpha,\beta\in supp\ \tau$ *is equivalent to the Sato Eq. (113) for each* $P=P^+(\alpha)$ *and the matching condition (105) for all* $\alpha,\beta\in supp\ \tau$.

Proof: We have proved already that the bilinear identity (95) implies (113) and (105). To prove the converse, denote by $A(\alpha,\beta,\xi,xi',x,x')$ the left-hand side of (95). The same argument as in the proof of Lemma 4.2 shows that

$$\left(\frac{\partial}{\partial x_k^{(j)}}-B_k^{(j)}(\alpha)\right)A(\alpha,\beta,\xi,\xi',x,x')=0, \tag{114}$$

$$A(\alpha,\beta,\xi,\xi',x,x')=0,\quad \text{if } x_k^{(i)}=x_k'^{(i)}\quad \text{for } k\geqslant 1, \tag{115}$$

where $B_k^{(j)}(\alpha)$ is defined by (112).

Denote by $A_1(\alpha,\beta)$ the expression for $A(\alpha,\beta,\xi,\xi',x,x')$ in which we set $x_k^{(j)}=x_k'^{(j)}=0$ for all k. Expanding $A(\alpha,\beta,\xi,\xi',x,x')$ in a power series in $x_k^{(i)}-x_k'^{(i)}$ for $k\geqslant 1$, we see from (114) and (115) that it remains to prove

$$A_1(\alpha,\beta)=0. \tag{116}$$

But the same argument as in the proof of Lemma 4.1 shows that

$$A_1(\alpha,\beta)=\mathrm{Res}_\partial W^+(\alpha,\xi,\partial)R^+(\alpha-\beta,\partial)W^-(\beta,\xi,\partial)*e^{y\partial}dz,$$

where $y=\xi-\xi'$. Hence, (116) follows from (105). □

Fix $\alpha\in M$; we have introduced above a collection of formal pseudo-differential operators $L\equiv L(\alpha)$, $C^{(i)}\equiv C^{(i)}(\alpha)$ of the form

$$\begin{gathered} L=I_n\partial+\sum_{j=1}^{\infty}U^{(j)}(\xi,x)\partial^{-j}, \\ C^{(i)}=E_{ii}+\sum_{j=1}^{\infty}C^{(i,j)}(\xi,x)\partial^{-j},\quad i=1,2,...,n, \end{gathered} \tag{117}$$

subject to the conditions

$$\sum_{i=1}^{n}C^{(i)}=I_n,\quad C^{(i)}L=LC^{(i)},\quad C^{(i)}C^{(j)}=\delta_{ij}C^{(i)}. \tag{118}$$

They satisfy the following set of equations for some $P\in I_n+\Psi_-$:

$$\begin{gathered} LP=P\partial, \\ C^{(i)}P=PE_{ii}, \\ \frac{\partial P}{\partial x_k^{(i)}}=-(L^{(i)k})_-P,\quad \text{where } L^{(i)}=C^{(i)}L. \end{gathered} \tag{119}$$

Notice that the first and last equations of (119) imply that

$$\frac{\partial P}{\partial\xi}=\sum_{i=1}^{n}\frac{\partial P}{\partial x_1^{(i)}},$$

since $L=I_n\partial+\Sigma_i(L^{(i)})_-$.

Proposition 4.3: The system of Eqs. (119) has a solution $P\in I_n+\Psi_-$ if and only if we can find a formal oscillating function of the form

$$W(\xi,x,z)=\left(I_n+\sum_{j=1}^{\infty}W^{(j)}(\xi,x)z^{-j}\right)e^{z\cdot x} \tag{120}$$

that satisfies the linear equations

$$LW=zW,\quad C^{(i)}W=WE_{ii},\quad \frac{\partial W}{\partial x_k^{(i)}}=B_k^{(i)}W. \tag{121}$$

Proof (119)⇒(121): Put $W=Pe^{z\cdot x}$. Then we have

$$LW = LPe^{z\cdot x} = P\partial e^{z\cdot x} = zPe^{z\cdot x} = zW;$$

$$C^{(i)}W = C^{(i)}Pe^{z\cdot x} = PE_{ii}e^{z\cdot x} = Pe^{z\cdot x}E_{ii} = WE_{ii};$$

$$\frac{\partial W}{\partial x_k^{(i)}} = \frac{\partial P}{\partial x_k^{(i)}} + P\frac{\partial e^{z\cdot x}}{\partial x_k^{(i)}} = -(L^{(i)k})_- Pe^{z\cdot x} + z^k PE_{ii}e^{z\cdot x} = -(L^{(i)k})_- W + PE_{ii}\partial^k e^{z\cdot x}$$

$$= -(L^{(i)k})_- W + C^{(i)}P\partial^k e^{z\cdot x} = -(L^{(i)k})_- W + C^{(i)}L^k Pe^{z\cdot x} = -(L^{(i)k})_- W + L^{(i)k}W = B_k^{(i)}W.$$

(121)⇒(119): Define $P\in\Psi$ by $W=Pe^{z\cdot x}$. If $LW=zW$, then $LPe^{z\cdot x}=zPe^{z\cdot x}=P\partial e^{z\cdot x}$, hence $LP=P\partial$.

If $C^{(i)}W=WE_{ii}$, then $C^{(i)}Pe^{z\cdot x}=Pe^{z\cdot x}E_{ii}=PE_{ii}e^{z\cdot x}$, hence $C^{(i)}P=PE_{ii}$.

Finally, the last equation of (121) gives $(\partial/\partial x_k^{(i)})(Pe^{z\cdot x}) = -(L^{(i)k})_- Pe^{z\cdot x} + L^{(i)k}Pe^{z\cdot x}$. Since we have already proved the first two equations of (119), we derive (as above) $L^{(i)k}Pe^{z\cdot x} = z^k Pe^{z\cdot x} = P\partial e^{z\cdot x}/\partial x_k^{(i)}$. Hence $(\partial P/\partial x_k^{(i)})e^{x\cdot z} = -(L^{(i)k})_- Pe^{x\cdot z}$, which proves that P satisfies the Sato equations. □

Remarks 4.3: (a) It is easy to see that the collection of formal pseudo-differential operators $\{L, C^{(1)},\ldots,C^{(n)}\}$ of the form (117) and satisfying (118) can be simultaneously conjugated to the trivial collection $\{\partial, E_{11},\ldots,E_{nn}\}$ by some $P\in I_n+\Psi_-$. It follows that the solution of the form (120) to the linear problem (121) is unique up to multiplication on the right by a diagonal matrix of the form

$$D(z) = \exp -\sum_{j=1}^{\infty} a_j z^{-j}/j, \tag{122}$$

where the a_j are diagonal matrices over $\mathbb{C}$ (indeed, this is the case for the trivial collection). The space of all solutions of (121) in formal oscillating functions is obtained from one of the form (120) by multiplying on the right by a diagonal matrix over $\mathbb{C}((z))$. For that reason the (matrix valued) functions

$$W^+(\alpha,\xi,x,z) = P^+(\alpha)e^{x\cdot z}, \quad \alpha\in \text{supp}\ \tau, \tag{123}$$

are called the *wave functions* for τ. The formal pseudo-differential operator $P^+(\alpha)$ is called the wave operator. The functions $W^-(\alpha,\xi,x,z)=P^-(\alpha)e^{-x\cdot z}$ are called the adjoint wave functions and the operators $P^-(\alpha)$ [which are expressed via $P^+(\alpha)$ by (106)] are called the adjoint wave operators. Note that $V^+(\alpha,\xi,x,z)$ are solutions of (121) as well since they are obtained by multiplying $W^+(\alpha,xi,x,z)$ on the right by $R^+(\alpha,z)$.

(b) Multiplying the wave function $W^+(\alpha,\xi,x,z)$ on the right by $D(z)$ given by (122) corresponds to multiplying the corresponding τ-function by $\exp tr\Sigma_{k=1}^{\infty}a_k x_k$, where $x_k = \text{diag}(x_k^{(1)},\ldots,x_k^{(n)})$.

(c) The collection $\{L, C^{(1)},\ldots,C^{(n)}\}$ determines uniquely $P\in I_n+\Psi_-$ up to the multiplication of P on the right by a formal pseudo-differential operator with constant coefficients from $I_n+\Psi_-$.

We shall now rewrite the compatibility conditions of the system (119) [or equivalent compatibility conditions of the system (121)] in the form of Lax equations and Zakharov–Shabat equations.

Lemma 4.3: If for every $\alpha\in M$ the formal pseudo-differential operators $L\equiv L(\alpha)$ and $C^{(j)}\equiv C^{(j)}(\alpha)$ of the form (117) satisfy conditions (118) and if the Eqs. (119) have a solution $P\equiv P(\alpha)\in I_n+\Psi_-$, then the differential operators $B_k^{(j)}\equiv B_k^{(j)}(\alpha)=(L^{(j)}(\alpha)^k)_+$ satisfy one of the following equivalent conditions:

$$\frac{\partial L}{\partial x_k^{(j)}} = [B_k^{(j)}, L],$$

$$\frac{\partial C^{(i)}}{\partial x_k^{(j)}} = [B_k^{(j)}, C^{(i)}], \tag{124}$$

$$\frac{\partial L^{(i)}}{\partial x_k^{(j)}} = [B_k^{(j)}, L^{(i)}], \tag{125}$$

$$\frac{\partial B_\ell^{(i)}}{\partial x_k^{(j)}} - \frac{\partial B_k^{(j)}}{\partial x_\ell^{(i)}} = [B_k^{(j)}, B_\ell^{(i)}]. \tag{126}$$

Proof (cf. Ref. 43): To derive the first equation of (124) we differentiate the equation $LP = P\partial$ by $x_k^{(j)}$:

$$\frac{\partial L}{\partial x_k^{(j)}} P + L \frac{\partial P}{\partial x_k^{(j)}} = \frac{\partial P}{\partial x_k^{(j)}} \partial,$$

and substitute Sato's equation [see (119)]. Then one obtains

$$\frac{\partial L}{\partial x_k^{(j)}} P = (B_k^{(j)} L - L B_k^{(j)}) P,$$

from which we derive the desired result. The second equation of (124) is proven analogously: differentiate $C^{(i)}P = PE_{ii}$, substitute Sato's equation and use the fact that $[L^{(j)k}, C^{(i)}] = 0$.

Next we prove the equivalence of (124), (125), and (126). The implication (124)⇒(125) is trivial. To prove the implication (125)⇒(124) note that $L = \Sigma_{j=1}^n L^{(j)}$ implies that the first equation of (124) follows immediately. As for the second one, we have

$$\frac{\partial C^{(i)}}{\partial x_k^{(j)}} = \left(\frac{\partial L^{(i)}}{\partial x_k^{(j)}} - C^{(i)} \frac{\partial L}{\partial x_k^{(j)}} \right) L^{-1} = ([B_k^{(j)}, L^{(i)}] - C^{(i)}[B_k^{(j)}, L]) L^{-1}$$

$$= ([B_k^{(j)}, C^{(i)}] L) L^{-1} = [B_k^{(j)}, C^{(i)}].$$

Next, we prove the implication (125)⇒(126). Since both $\partial/\partial x_k^{(j)}$ and $ad\, B_k^{(j)}$ are derivations, (125) implies

$$\frac{\partial L^{(i)\ell}}{\partial x_k^{(j)}} = [B_k^{(j)}, L^{(i)\ell}].$$

Hence:

$$\left(\frac{\partial B_\ell^{(i)}}{\partial x_k^{(j)}} - \frac{\partial B_k^{(j)}}{\partial x_\ell^{(i)}} - [B_k^{(j)}, B_\ell^{(i)}] \right) + \left(\frac{\partial (L^{(i)\ell})_-}{\partial x_k^{(j)}} - \frac{\partial (L^{(j)k})_-}{\partial x_\ell^{(i)}} + [(L^{(j)k})_-, (L^{(i)\ell})_-] \right)$$

$$= [B_k^{(j)}, L^{(i)\ell}] - [B_\ell^{(i)}, L^{(j)k}] - [B_k^{(j)}, B_\ell^{(i)}] + [(L^{(j)k})_-, (L^{(i)\ell})_-] = [L^{(j)k}, L^{(i)\ell}] = 0.$$

Since $\Psi_- \cap \Psi_+ = \{0\}$, both terms on the left-hand side are zero, proving (126).

Finally, we prove the implication (126)⇒(125). We rewrite (126):

$$\frac{\partial L^{(i)\ell}}{\partial x_k^{(j)}}-[B_k^j,L^{(i)\ell}]=\frac{\partial (L^{(i)\ell})_-}{\partial x_k^{(j)}}+\frac{\partial B_k^{(j)}}{\partial x_\ell^{(i)}}-[B_k^{(j)},(L^{(i)\ell})_-].$$

This right-hand side has order $k-1$, hence

$$\frac{\partial L^{(i)\ell}}{\partial x_k^{(j)}}-[B_k^{(j)},L^{(i)\ell}]\in\Psi(k-1)\quad\text{for every}\quad \ell>0. \tag{127}$$

Now suppose that $\partial L^{(i)}/\partial x_k^{(j)}-[B_k^{(j)},L^{(i)}]\neq 0$. Then

$$\lim_{\ell\to\infty}\operatorname{ord}\left(\frac{\partial L^{(i)\ell}}{\partial x_k^{(i)}}-[B_k^{(j)},L^{(i)\ell}]\right)=\infty,$$

which contradicts (127). □

Equations (124) and (125) are called *Lax type* equations. Equations (126) are called the *Zakharov–Shabat-type* equations. The latter are the compatibility conditions for the linear problem (121). Indeed, since $(\partial/\partial x_k^{(j)})(\partial/\partial x_\ell^{(i)})W=(\partial/\partial x_\ell^{(i)})(\partial/\partial x_k^{(j)})W$, one finds

$$0=\frac{\partial}{\partial x_k^{(j)}}(B_\ell^{(i)}W)-\frac{\partial}{\partial x_\ell^{(i)}}(B_k^{(j)}W)=\left(\frac{\partial B_\ell^{(i)}}{\partial x_k^{(j)}}-\frac{\partial B_k^{(j)}}{\partial x_\ell^{(i)}}-[B_k^{(j)},B_\ell^{(i)}]\right)W.$$

Notice that as a by-product of the proof of Proposition 4.4, we obtain complementary Zakharov–Shabat equations:

$$\frac{\partial (L^{(i)\ell})_-}{\partial x_k^{(j)}}-\frac{\partial (L^{(j)k})_-}{\partial x_\ell^{(i)}}=[(L^{(i)\ell})_-,(L^{(j)k})_-]. \tag{128}$$

Proposition 4.4: Sato Eq. (113) on $P\in I_n+\Psi_-$ *imply Eqs. (126) on differential operators* $B_k^{(i)}=(L^{(i)k})_+$.

Proof is the same as that of the corresponding part of Lemma 4.3. □

Remark 4.4: The above results may be summarized as follows. The *n*-component KP hierarchy (70) of Hirota bilinear equations on the τ-function is equivalent to the bilinear Eq. (95) on the wave function, which is related to the τ-function by formula (94) and Remark 4.2. The bilinear Eq. (95) for each $\alpha=\beta$ implies the Sato Eq. (113) on the formal pseudo-differential operator $P\equiv P(\alpha)$. Moreover, Eq. (113) on $P(\alpha)$ for each α together with the matching conditions (105) are equivalent to the bilinear identity (95). Also, the Sato equation [or rather (119)] is a compatibility condition for the linear problem (121) for the wave function. The Sato equation in turn implies the system of Lax-type Eq. (125) [or equivalent systems (124) or (126), which is the most familiar form of the compatibility condition] on formal pseudo-differential operators $L^{(i)}$ [resp. L and $C^{(i)}$ satisfying constraints (118)]. The latter formal pseudo-differential operators are expressed via the wave function by formulas (112) and (100)–(103).

We next write down explicitly some of the Sato Eq. (113) on the matrix elements $W_{ij}^{(s)}$ of the coefficients $W^{(s)}(\xi,x)$ of the pseudo-differential operator

$$P=I_n+\sum_{m=1}^{\infty}W^{(m)}(\xi,x)\partial^{-m}.$$

We shall write W_{ij} for $W_{ij}^{(1)}$ to simplify notation. We have for $i\neq k$

$$\frac{\partial W_{ij}}{\partial x_1^{(k)}}=W_{ik}W_{kj}-\delta_{jk}W_{ij}^{(2)}, \tag{129}$$

$$\frac{\partial W_{ij}^{(2)}}{\partial x_1^{(k)}} = W_{ik}W_{kj}^{(2)} - \delta_{jk}W_{ij}^{(3)}. \tag{130}$$

Next, calculating $\partial W_{ij}/\partial x_2^{(k)}$ from (113) and substituting (129) and (130) in these equations, we obtain

$$\frac{\partial W_{ij}}{\partial x_2^{(k)}} = W_{ik}\frac{\partial W_{kj}}{\partial x_1^{(k)}} - \frac{\partial W_{ik}}{\partial x_1^{(k)}}W_{kj} \quad \text{if } k \neq i \quad \text{and } k \neq j, \tag{131}$$

$$\frac{\partial W_{ij}}{\partial x_2^{(j)}} = 2\frac{\partial W_{jj}}{\partial x_1^{(j)}}W_{ij} - \frac{\partial^2 W_{ij}}{\partial x_1^{(j)2}} \quad \text{if } i \neq j, \tag{132}$$

$$\frac{\partial W_{ij}}{\partial x_2^{(i)}} = -2\frac{\partial W_{ii}}{\partial x_1^{(i)}}W_{ij} + \frac{\partial^2 W_{ij}}{\partial x_1^{(i)2}} \quad \text{if } i \neq j, \tag{133}$$

$$\frac{\partial W_{ii}}{\partial x_2^{(i)}} = \frac{\partial^2 W_{ii}}{\partial x_1^{(i)2}} + 2\sum_{p\neq i} W_{ip}\frac{\partial W_{pi}}{\partial x_1^{(i)}} - 2W_{ii}\partial W_{ii} + 2\partial W_{ii}^{(2)}. \tag{134}$$

Remark 4.5: Substituting expressions for the $W_{ij} = W_{ij}^{(1)}(\alpha = 0, x)$ given by (98), the above equations turn into the Hirota bilinear equations found in Sec. III D as follows:

(129) for $i = j \Rightarrow$(74)
(129) for $i \neq j \Rightarrow$(78)
(133)$\Rightarrow$(75)
(132)$\Rightarrow$(76)
(131) for $i = j \Rightarrow$(77) (with j replaced by k),
(131) for $i \neq j \Rightarrow$(79).

We now write down explicitly some of the Lax Eqs. (124) of the n-component KP hierarchy and auxiliary conditions (118) for the formal pseudo-differential operators

$$L = I_n\partial + \sum_{j=1}^{\infty} U^{(j)}(\xi, x)\partial^{-j} \quad \text{and} \quad C^{(i)} = E_{ii} + \sum_{j=1}^{\infty} C^{(i,j)}(\xi, x)\partial^{-j} \ (i = 1, \ldots, n). \tag{135}$$

For the convenience of the reader, recall that x stands for all indeterminates $x_i^{(k)}$, where $i = 1,2,\ldots$ and $k = 1,\ldots,n$, that the auxiliary conditions are

$$\sum_{i=1}^{n} C^{(i)} = I_n, \quad C^{(i)}C^{(j)} = \delta_{ij}C^{(i)}, \quad C^{(i)}L = LC^{(i)}, \tag{136}$$

and that the Lax equations of the n-component KP hierarchy are

$$\frac{\partial L}{\partial x_i^{(k)}} = [B_i^{(k)}, L], \tag{137a}$$

$$\frac{\partial C^{(\ell)}}{\partial x_i^{(k)}} = [B_i^{(k)}, C^{(\ell)}], \tag{137b}$$

where $B_i^{(k)} = (C^{(k)}L^i)_+$. For example, we have

$$B_1^{(k)} = E_{kk}\partial + C^{(k,1)}, \quad B_2^{(k)} = E_{kk}\partial^2 + C^{(k,1)}\partial + 2E_{kk}U^{(1)} + C^{(k,2)}. \tag{138}$$

Denote by $C_{ij}^{(k,\ell)}$ and $U_{ij}^{(k)}$ the (i,j)th entries of the $n\times n$ matrices $C^{(k,\ell)}$ and $U^{(k)}$, respectively. Then the ∂^{-1} term of the second Eq. (136) gives

$$C_{ij}^{(k,1)}=0 \quad \text{if } i\neq k \quad \text{and } j\neq k, \quad \text{or } i=j=k, \tag{139}$$

$$C_{kj}^{(k,1)}=-C_{kj}^{(j,1)}. \tag{140}$$

Hence the matrices $C^{(j,1)}$ are expressed in terms of the functions

$$A_{ij}:=C_{ij}^{(j,1)} \quad (\text{note that } A_{ii}=0).$$

The ∂^{-2} term of the second Eq. (136) allows one to express most of the $C_{ij}^{(k,2)}$ in terms of the A_{ij}:

$$C_{ij}^{(k,2)}=-A_{ik}A_{kj} \quad \text{if } i\neq k \quad \text{and } j\neq k, \tag{141}$$

$$C_{k,k}^{(k,2)}=\sum_{p=1}^{n} A_{kp}A_{pk}. \tag{142}$$

Furthermore, the ∂^{-1} term of the Lax Eq. $(137b)_1$ gives

$$\frac{\partial A_{ij}}{\partial x_1^{(k)}}=A_{ik}A_{kj} \quad \text{for distinct } i,j,k, \tag{143}$$

$$C_{ij}^{(j,2)}=-\frac{\partial A_{ij}}{\partial x_1^{(j)}} \quad \text{for } i\neq j, \tag{144}$$

$$C_{ij}^{(i,2)}=\sum_{\substack{p=1\\ p\neq i}}^{n}\frac{\partial A_{ij}}{\partial x_1^{(p)}} \quad \text{for } i\neq j. \tag{145}$$

The ∂^{-2} term of that equation gives for $i\neq j$ (recall that $\partial=\partial/\partial x_1^{(1)}+\cdots+\partial/\partial x_1^{(n)}$):

$$C_{ij}^{(i,3)}=-\frac{\partial C_{ij}^{(i,2)}}{\partial x_1^{(j)}}+A_{ij}C_{jj}^{(i,2)}-\sum_{p=1}^{n}(A_{ip}\partial A_{pj}+C_{ip}^{(i,2)}A_{pj}), \tag{146}$$

$$C_{ij}^{(j,3)}=-\sum_{\substack{p=1\\ p\neq i}}^{n}\frac{\partial C_{ij}^{(j,2)}}{\partial x_1^{(p)}}-A_{ij}C_{ii}^{(j,2)}+\sum_{p=1}^{n}A_{ip}C_{pj}^{(j,2)}. \tag{147}$$

Substituting (141), (142), and (145) [resp. (141), (142), and (144)] in (146) [resp. in (147)] we obtain for $i\neq j$

$$C_{ij}^{(i,3)}=-\left(\partial-\frac{\partial}{\partial x_1^{(i)}}\right)^2 A_{ij}-2\sum_{\substack{p=1\\ p\neq i}}^{n}A_{ip}A_{pi}A_{ij}, \tag{148}$$

$$C_{ij}^{(j,3)}=\frac{\partial^2 A_{ij}}{\partial x_1^{(j)2}}+2\sum_{\substack{p=1\\ p\neq j}}^{n}A_{ij}A_{jp}A_{pj}. \tag{149}$$

Furthermore, the ∂^0 and ∂^{-1} terms of the Lax Eq. $(137a)_1$ give respectively for $i\neq j$

$$U_{ij}^{(1)}=-\partial A_{ij}, \tag{150}$$

$$\frac{\partial U_{ii}^{(1)}}{\partial x_1^{(j)}} = -\partial(A_{ij}A_{ji}). \tag{151}$$

Finally, the ∂^{-1} term of the Lax Eq. $(137b)_2$ gives

$$\frac{\partial A_{ij}}{\partial x_2^{(j)}} = -2A_{ij}U_{jj}^{(1)} - C_{ij}^{(j,3)} \quad \text{for } i \neq j, \tag{152}$$

$$\frac{\partial A_{ij}}{\partial x_2^{(i)}} = \partial^2 A_{ij} - 2\partial C_{ij}^{(i,2)} - C_{ij}^{(i,3)} + 2U_{ii}^{(1)}A_{ij} \quad \text{for } i \neq j, \tag{153}$$

$$\frac{\partial A_{ij}}{\partial x_2^{(k)}} = A_{ik}\frac{\partial A_{kj}}{\partial x_1^{(k)}} - A_{kj}\frac{\partial A_{ik}}{\partial x_1^{(k)}} \quad \text{for } i \neq k \quad \text{and } j \neq k. \tag{154}$$

Finally, we write down explicitly expressions for $U^{(1)}$ and $C^{(i,1)}$ in terms of τ-functions. Recall that

$$P = I_n + \sum_{j=1}^{\infty} W^{(j)}\partial^{-j},$$

$$L = P\partial P^{-1} = I_n\partial + \sum_{j=1}^{\infty} U^{(j)}\partial^{-j},$$

$$C^{(i)} = PE_{ii}P^{-1} = E_{ii} + \sum_{j=1}^{\infty} C^{(i,j)}\partial^{-j}.$$

Using (152) we have

$$U^{(1)} = -\partial W^{(1)}, \tag{155}$$

$$U^{(2)} = W^{(1)}\partial W^{(1)} - \partial W^{(2)}, \tag{156}$$

$$C^{(i,1)} = [W^{(1)}, E_{ii}], \tag{157}$$

$$C^{(i,2)} = [W^{(2)}, E_{ii}] + [E_{ii}, W^{(1)}]W^{(1)}. \tag{158}$$

Using (98) we obtain from (155) and (157), respectively

$$U_{ij}^{(1)} = \begin{cases} -\epsilon_{ji}\partial(\tau_{\alpha+\alpha_{ij}}/\tau_\alpha) & \text{if } i \neq j, \\ \partial\left(\dfrac{\partial\tau_\alpha}{\partial x_1^{(i)}} \Big/ \tau_\alpha\right) & \text{if } i = j, \end{cases} \tag{159}$$

$$A_{ij} \equiv C_{ij}^{(j,1)} = \epsilon_{ji}\tau_{\alpha+\alpha_{ij}}/\tau_\alpha. \tag{160}$$

[Recall that by (139) and (140) all the matrices $C^{(k,1)}$ can be expressed via the functions A_{ij}.] Using (98) and (99) and (156) and (158) one also may write down the matrices $U^{(2)}$ and $C^{(i,2)}$ in terms of τ-functions, but they are somewhat more complicated and we will not need them anyway.

V. THE DARBOUX-EGOROFF SYSTEM, THE *n*-WAVE INTERACTION EQUATIONS, THE GENERALIZED TODA CHAIN AND THE GENERALIZED DAVEY–STEWARTSON EQUATIONS AS SUBSYSTEMS OF THE *n*-COMPONENT KP

In this section we show that some well-known soliton equations, as well as their natural generalizations, are the simplest equations of the various formulations of the *n*-component KP hierarchy. To simplify notation, let

$$t_i = x_2^{(i)}, \quad x_i = x_1^{(i)}. \tag{161}$$

Let $n \geqslant 3$. Then the *n*-component KP in the form of Sato equation contains the system (129) of $n(n-1)(n-2)$ equations on n^2-n functions $W_{ij}\,(i \neq j)$ in the indeterminates x_i (all other indeterminates being parameters):

$$\frac{\partial W_{ij}}{\partial x_k} = W_{ik} W_{kj} \quad \text{for distinct } i,j,k. \tag{162}$$

This is sometimes called the *n*-wave equation. The τ-function is given by the formula (98) for a fixed $\alpha \in M$:

$$W_{ij} = \epsilon_{ji} \tau_{\alpha+\alpha_{ij}} / \tau_\alpha. \tag{163}$$

Substituting this in (162) gives the Hirota bilinear Eq. (78):

$$D_1^{(k)} \tau_\alpha \cdot \tau_{\alpha+\alpha_{ij}} = \epsilon_{ik}\epsilon_{kj}\epsilon_{ij} \tau_{\alpha+\alpha_{ik}} \tau_{\alpha+\alpha_{kj}}. \tag{164}$$

Note that due to (157), $W_{ij} = A_{ij}$ if $i \neq j$, hence (162) is satisfied by the A_{ij} as well.

One usually adds to (162) the following equations, whose group theoretical meaning we shall explain in Sec. VII:

$$\partial W_{ij} = 0, \quad i \neq j. \tag{165}$$

Using (119), this is equaivalent to

$$\sum_{k=1}^{n} \frac{\partial W_{ij}}{\partial x_k} = 0.$$

If one adds the symmetry $W_{ij} = W_{ji}$ one obtains the Darboux–Egoroff system:

$$\frac{\partial W_{ij}}{\partial x_k} = W_{ik} W_{kj} \quad \text{for distinct } i,j,k,$$

$$\sum_{k=1}^{n} \frac{\partial W_{ij}}{\partial x_k} = 0, \tag{166}$$

$$W_{ij} = W_{ji}.$$

These equations describe certain flat diagonal metrics and classifiy (locally) massive topological field theories see Refs. 12–15. For a group theoretical interpretation of this system as a subsystem of the *n*-component KP we refer to Ref. 50.

Let now $a = \mathrm{diag}(a_1,...,a_n)$, $b = \mathrm{diag}(b_1,...,b_n)$ be arbitrary diagonal matrices over $\mathbb{C}$. We reduce the system (162) to the plane:[11]

$$x_k = a_k x + b_k t.$$

A direct calculation shows that (162) reduces then to the following equation on the matrix $W=(W_{ij})$ (note that its diagonal entries do not occur):

$$\left[a,\frac{\partial W}{\partial t}\right]-\left[b,\frac{\partial W}{\partial x}\right]=[\![a,W],[b,W]\!]+b\partial Wa-a\partial Wb. \tag{167}$$

Hence, imposing the constraint (165), we obtain the famous $1+1$ n-wave system (cf. Refs. 11 and 38):

$$\left[a,\frac{\partial W}{\partial t}\right]-\left[b,\frac{\partial W}{\partial x}\right]=[\![a,W],[b,W]\!]. \tag{168}$$

Let now

$$x_k=a_kx+b_kt-y. \tag{169}$$

Then Eq. (167) gives

$$\left[a,\frac{\partial W}{\partial t}\right]-\left[b,\frac{\partial W}{\partial x}\right]-a\frac{\partial W}{\partial y}b+b\frac{\partial W}{\partial y}a=[\![a,W],[b,W]\!]. \tag{170}$$

If we let

$$Q_{ij}=-(a_i-a_j)W_{ij},$$

Eq. (170) turns into the following system, which is called in Ref. 1, (5.4.30a,c), the $2+1$ n-wave interaction equations ($i\neq j$):

$$\frac{\partial Q_{ij}}{\partial t}=a_{ij}\frac{\partial Q_{ij}}{\partial x}+b_{ij}\frac{\partial Q_{ij}}{\partial y}+\sum_k\ (a_{ik}-a_{kj})Q_{ik}Q_{kj}, \tag{171}$$

where

$$a_{ij}=(b_i-b_j)/(a_i-a_j),\quad b_{ij}=b_i-a_ia_{ij}. \tag{172}$$

On the other hand, letting (we assume that $a_1>\cdots>a_n$)

$$w_{ij}=W_{ij}/(a_i-a_j)^{1/2}, \tag{173}$$

the Eq. (177) gives for $i\neq j$

$$\frac{\partial w_{ij}}{\partial t}-a_{ij}\frac{\partial w_{ij}}{\partial x}-b_{ij}\frac{\partial w_{ij}}{\partial y}=\sum_k\ \epsilon_{ijk}w_{ik}w_{kj}, \tag{174}$$

where

$$\epsilon_{ijk}=\frac{a_ib_k+a_kb_j+a_jb_i-a_kb_i-a_jb_k-a_ib_j}{((a_i-a_k)(a_k-a_j)(a_i-a_j))^{1/2}}. \tag{175}$$

Imposing the constraint $\overline{w_{ij}}=-w_{ji}$, we obtain from (174) the following Hamiltonian system (considered in Ref. 38, pp. 175, 242, for $n=3$ and called there the $2+1$ three-wave system) ($i<j$):

$$\frac{\partial w_{ij}}{\partial t}-a_{ij}\frac{\partial w_{ij}}{\partial x}-b_{ij}\frac{\partial w_{ij}}{\partial y}=\frac{\partial H}{\partial\overline{w_{ij}}}, \tag{176}$$

where

$$H=\sum_{\substack{i,k,j\\ i<k<j}} \epsilon_{ijk}(w_{ik}w_{kj}\overline{w}_{ij}+\overline{w}_{ik}\overline{w}_{kj}w_{ij}). \tag{177}$$

Finally, let $n=3$ and let $u_1=iw_{13}$, $u_2=i\overline{w}_{13}$, $u_3=iw_{12}$, $a_1=-a_{23}$, $b_1=-b_{23}$, $a_2=-\overline{a}_{13}$, $b_2=-\overline{b}_{13}$, $a_3=-a_{12}$, $b_3=-b_{13}$. Then, after imposing the constraint $\epsilon_{132}=1$, Eqs. (176) turn into the well-known 2+1 three-wave interaction equations [see Ref. 1, (5.4.27)]:

$$\frac{\partial u_j}{\partial t}+a_j\frac{\partial u_j}{\partial x}+b_j\frac{\partial u_j}{\partial y}=i\overline{u}_k\overline{u}_\ell, \tag{178}$$

where (j,k,ℓ) is an arbitrary cyclic permutation of 1, 2, 3.

Let $n\geqslant 2$. Then the n-component KP in the form of Sato equations contains the following subsystem of the system of Eq. (129) for arbitrary $\alpha\in M$ on the functions $W_{ij}(\alpha)$ in the indeterminates x_i (all other indeterminates being parameters):

$$\frac{\partial W_{ii}(\alpha)}{\partial x_j}=W_{ij}(\alpha)W_{ji}(\alpha)\quad \text{if } i\neq j. \tag{179}$$

The τ-function is given by (98) ($\alpha\in M$)

$$W_{ij}(\alpha)=\begin{cases}\epsilon_{ji}\tau_{\alpha+\alpha_{ij}}/\tau_\alpha & \text{if } i\neq j,\\ -\dfrac{\partial}{\partial x_i}\log\tau_\alpha & \text{if } i=j.\end{cases} \tag{180}$$

Substituting this in (179) gives the Hirota bilinear Eq. (74):

$$D_iD_j\tau_\alpha\cdot\tau_\alpha=2\tau_{\alpha+\alpha_{ij}}\tau_{\alpha-\alpha_{ij}}. \tag{181}$$

In order to rewrite (179) in a more familiar form, let for $i\neq j$

$$U_{ij}(\alpha)=\log\epsilon_{ji}W_{ij}(\alpha)=\log(\tau_{\alpha+\alpha_{ij}}/\tau_\alpha). \tag{182}$$

Note that $\log(\tau_{\alpha+\alpha_{ij}}/\tau_\alpha)=-\log(\tau_{(\alpha+\alpha_{ij})-\alpha_{ij}}/\tau_{\alpha+\alpha_{ij}}$. Hence from (180) we obtain

$$U_{ij}(\alpha)=-U_{ji}(\alpha+\alpha_{ij})\quad \text{if } i\neq j. \tag{183}$$

Furthermore, we have

$$\begin{aligned}\frac{\partial^2}{\partial x_i\partial x_j}U_{ij}(\alpha)&=\frac{\partial^2}{\partial x_i\partial x_j}\log\tau_{\alpha+\alpha_{ij}}-\frac{\partial^2}{\partial x_i\partial x_j}\log\tau_\alpha\\ &=\frac{\partial W_{ii}(\alpha)}{\partial x_j}-\frac{\partial W_{ii}(\alpha+\alpha_{ij})}{\partial x_j}\\ &=W_{ij}(\alpha)W_{ji}(\alpha)-W_{ij}(\alpha+\alpha_{ij})W_{ji}(\alpha+\alpha_{ij})\\ &=-\frac{\tau_{\alpha+\alpha_{ij}}}{\tau_\alpha}\frac{\tau_{\alpha-\alpha_{ij}}}{\tau_\alpha}+\frac{\tau_{\alpha+2\alpha_{ij}}}{\tau_{\alpha+\alpha_{ij}}}\frac{\tau_\alpha}{\tau_{\alpha+\alpha_{ij}}}\\ &=e^{U_{ij}(\alpha+\alpha_{ij})-U_{ij}(\alpha)}-e^{U_{ij}(\alpha)-U_{ij}(\alpha-\alpha_{ij})}.\end{aligned}$$

Thus the functions $U_{ij}(\alpha)\,(i\neq j)$ satisfy the following generalized Toda chain [with constraint (183)]:

$$\frac{\partial^2 U_{ij}(\alpha)}{\partial x_i \partial x_j} = e^{U_{ij}(\alpha+\alpha_{ij})-U_{ij}(\alpha)} - e^{U_{ij}(\alpha)-U_{ij}(\alpha-\alpha_{ij})}. \tag{184}$$

Note also that (162) for distinct i, j and k becomes

$$\frac{\partial U_{ij}(\alpha)}{\partial x_k} = \epsilon_{ik}\epsilon_{kj}\epsilon_{ji} e^{U_{ij}(\alpha)+U_{ik}(\alpha)+U_{kj}(\alpha)}. \tag{185}$$

One should be careful about the boundary conditions. Let $S=\operatorname{supp}\tau$; recall that by Proposition 2.4, S is a convex polyhedron with vertices in M and edges parallel to roots. It follows that (184) should be understood as follows:

(i) If $\alpha\notin S$, then $U_{ij}(\alpha)=0$ and (184) is trivial.
(ii) If $\alpha\in S$, but $\alpha+\alpha_{ij}\notin S$, then (184) is trivial.
(iii) If $\alpha\in S$, but $\alpha-\alpha_{ij}\notin S$, then the second term on the right-hand side of (184) is removed.
(iv) If $\alpha\in S$, $\alpha+\alpha_{ij}\in S$, but $\alpha+2\alpha_{ij}\notin S$, then the first term on the right-hand side of (184) is removed.

Let now $n=2$, and let $u_n=U_{12}(n\alpha_{12})$. Then we get the usual Toda chain:

$$\frac{\partial^2 u_n}{\partial x_1 \partial x_2} = e^{u_{n+1}-u_n} - e^{u_n-u_{n-1}}, \quad n\in\mathbb{Z}. \tag{186}$$

It is a part of the Toda lattice hierarchy discussed in Ref. 47.

Let $n\geqslant 2$. Then the n-component KP in the form of Sato equations contains the system of Eqs. (132), (133), (131) and (129) for $j\neq k$ on n^2 functions W_{ij} in the indeterminates x_k and $t_k\,(k=1,\ldots,n)$ (all other indeterminates being parameters):

$$\frac{\partial W_{ij}}{\partial t_j} = -\frac{\partial^2 W_{ij}}{\partial x_j^2} + 2\frac{\partial W_{jj}}{\partial x_j} W_{ij} \quad \text{if } i\neq j, \tag{187}$$

$$\frac{\partial W_{ij}}{\partial t_i} = \frac{\partial^2 W_{ij}}{\partial x_i^2} - 2\frac{\partial W_{ii}}{\partial x_i} W_{ij} \quad \text{if } i\neq j, \tag{188}$$

$$\frac{\partial W_{ij}}{\partial t_k} = W_{ik}\frac{\partial W_{kj}}{\partial x_k} - \frac{\partial W_{ik}}{\partial x_k} W_{kj} \quad \text{if } i\neq k \quad \text{and } j\neq k, \tag{189}$$

$$\frac{\partial W_{ij}}{\partial x_k} = W_{ik}W_{kj} \quad \text{if } i\neq k \quad \text{and } j\neq k. \tag{190}$$

This is a system of n^3-n evolution Eqs. (187)–(189) and $n(n-1)^2$ constraints (190) which we call the generalized Davey–Stewartson system.

Note that the τ-functions of this system are given by (98), where we may take $\alpha=0$. The corresponding to (187)–(190) Hirota bilinear equations are (76), (75), (77) if $i=j$ and (79) if $i\neq j$; (74) if $i=j$ and (78) if $i\neq j$, respectively.

Now, note that letting

$$\varphi_{ij} = \frac{1}{2}\left(\frac{\partial W_{ii}}{\partial x_i} + \frac{\partial W_{jj}}{\partial x_j} + \frac{\partial W_{ii}}{\partial x_j} + \frac{\partial W_{jj}}{\partial x_i}\right) (=\varphi_{ji})$$

and subtracting (188) from (187) we obtain using (190)

$$\frac{\partial W_{ij}}{\partial t_j}-\frac{\partial W_{ij}}{\partial t_i}=-\left(\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial x_j^2}\right)W_{ij}+2W_{ij}(\varphi_{ij}-W_{ij}W_{ji}). \tag{191}$$

Also, from (190) we obtain

$$\frac{\partial^2\varphi_{ij}}{\partial x_i\partial x_j}=\frac{1}{2}\left(\frac{\partial}{\partial x_i}+\frac{\partial}{\partial x_j}\right)^2(W_{ij}W_{ji}). \tag{192}$$

Let now $n=2$; to simplify notation, let

$$q=W_{12},\quad r=W_{21},\quad \varphi=\varphi_{12}=\varphi_{21}.$$

Then, making the change of indeterminates

$$s=-2i(t_1+t_2),\quad t=-2i(t_1-t_2),\quad x=x_1+x_2,\quad y=x_1-x_2, \tag{193}$$

Eqs. (191) and (192) turn into the decoupled Davey–Stewartson system:

$$\begin{aligned} i\frac{\partial q}{\partial t}&=-\frac{1}{2}\left(\frac{\partial^2 q}{\partial x^2}+\frac{\partial^2 q}{\partial y^2}\right)+q(\varphi-qr),\\ i\frac{\partial r}{\partial t}&=\frac{1}{2}\left(\frac{\partial^2 r}{\partial x^2}+\frac{\partial^2 r}{\partial y^2}\right)-r(\varphi-qr),\\ \frac{\partial^2\varphi}{\partial x^2}-\frac{\partial^2\varphi}{\partial y^2}&=2\frac{\partial^2(qr)}{\partial x^2}. \end{aligned} \tag{194}$$

Due to (98), the corresponding τ-functions are given by the following formulas, where we let $\tau_n=\tau_{n\alpha_{12}}$:

$$q=-\tau_1/\tau_0,\quad r=\tau_{-1}/\tau_0,\quad \varphi=-\frac{\partial^2}{\partial x^2}\log\tau_0, \tag{195}$$

the Hirota bilinear equations being (cf. Ref. 22)

$$\begin{aligned} (iD_t+\tfrac{1}{2}D_x^2+\tfrac{1}{2}D_y^2)\tau_1\cdot\tau_0&=0,\\ (-iD_t+\tfrac{1}{2}D_x^2+\tfrac{1}{2}D_y^2)\tau_{-1}\cdot\tau_0&=0,\\ (D_x^2-D_y^2)\tau_0\cdot\tau_0&=2\tau_1\tau_{-1}. \end{aligned} \tag{196}$$

Finally, imposing the constraint

$$r=\kappa\overline{q},\quad \text{where}\ \ \kappa=\pm 1, \tag{197}$$

we obtain the classical Davey–Stewartson system

$$\begin{aligned} i\frac{\partial q}{\partial t}+\frac{1}{2}\left(\frac{\partial^2 q}{\partial x^2}+\frac{\partial^2 q}{\partial y^2}\right)&=(\varphi-\kappa|q|^2)q,\\ \frac{\partial^2\varphi}{\partial x^2}-\frac{\partial^2\varphi}{\partial y^2}&=2\kappa\frac{\partial^2|q|^2}{\partial x^2}. \end{aligned} \tag{198}$$

Remark 5.1: It is interesting to compare the above results with that obtained via the Lax equations. To simplify notation, let $U_i=U_{ii}^{(1)}$. Substituting (149) [resp. (148)] in (152) [resp. (153)], we obtain for $i\neq j$

$$\frac{\partial A_{ij}}{\partial t_j}=-\frac{\partial^2 A_{ij}}{\partial x_j^2}-2A_{ij}U_j-2\sum_{k\neq j}A_{ij}A_{jk}A_{kj}, \tag{199}$$

$$\frac{\partial A_{ij}}{\partial t_i}=\frac{\partial^2 A_{ij}}{\partial x_i^2}+2A_{ij}U_i+2\sum_{k\neq i}A_{ij}A_{ik}A_{ki}. \tag{200}$$

These equation together with (143), (151), and (154) give a slightly different version of the generalized DS system (recall that $A_{ij}=W_{ij}$ if $i\neq j$ and $U_i=-\partial W_{ii}$). For $n=2$ we get again the classical DS system after the change of indeterminates (193) if we let $\varphi=-\frac{1}{2}(U_1+U_2)$.

Finally, we explain what happens in the well-known case $n=1$. In this case $C^{(1)}=1$ and auxiliary conditions (136) are trivial. Lax Eq. (137b) is trivial as well, and Lax Eq. (137a) becomes

$$\frac{\partial L}{\partial x_i}=[B_i,L],\quad i=1,2,..., \tag{201}$$

where $L=\partial+\Sigma_{j=1}^{\infty}u_j(x)\partial^{-j}$, $\partial=\partial/\partial x_1$ and $B_i=(L^i)_+$. Thus, the KP hierarchy is a system of partial differential Eqs. (201) on unknown functions u_1, u_2,... in indeterminates x_1, x_2,.... By Lemma 3.6, (201) is equivalent to the following system of Zakharov–Shabat equations:

$$\frac{\partial B_\ell}{\partial x_k}-\frac{\partial B_k}{\partial x_\ell}=[B_k,B_\ell]. \tag{202}$$

By (138) we have

$$B_1=\partial,\quad B_2=\partial^2+2u_1. \tag{203}$$

Furthermore, we have

$$B_3=\partial^3+3u_1\partial+3u_2+3\frac{\partial u_1}{\partial x_1}. \tag{204}$$

Thus we see that Eqs. $(202)_{k,1}$ are all trivial, the first nontrivial equation of (202) being

$$\frac{\partial B_2}{\partial x_3}-\frac{\partial B_3}{\partial x_2}=[B_3,B_2].$$

Substituting in it (203) and (204), the coefficients of ∂^0 and ∂^1 give, respectively,

$$2\frac{\partial u_1}{\partial x_3}-2\frac{\partial^2 u_1}{\partial x_1\partial x_2}-6u_1\frac{\partial u_1}{\partial x_1}=3\frac{\partial u_2}{\partial x_2}-3\frac{\partial^2 u_2}{\partial x_1^2}, \tag{205}$$

$$6\frac{\partial u_2}{\partial x_1}=3\frac{\partial u_1}{\partial x_2}-\frac{\partial^2 u_1}{\partial x_1^2}. \tag{206}$$

Differentiating (205) by x_1 and substituting $\partial u_2/\partial x_1$ from (206) gives a PDE on $u=2u_1$, where we let $x_1=x$, $x_2=y$, $x_3=t$:

$$\frac{3}{4}\frac{\partial^2 u}{\partial y^2}=\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}-\frac{3}{2}u\frac{\partial u}{\partial x}-\frac{1}{4}\frac{\partial^3 u}{\partial x^3}\right). \tag{207}$$

This is the classical KP equation. Due to (159), the connection between u and the τ-function is given by the famous formula

$$u=2\frac{\partial^2}{\partial x^2}\log\tau. \tag{208}$$

Substituting u in (207) gives the Hirota bilinear Eq. (73).

VI. SOLITON AND DROMION SOLUTIONS

We turn now to the construction of solutions of the n-component KP hierarchy. As in Ref. 9 we make use of the vertex operators (54). When transported via the n-component boson-fermion correspondence σ from F to $B=\mathbb{C}[x]\otimes\mathbb{C}[L]$, they take the following form:

$$\psi^{\pm(i)}(z)=Q_i^{\pm 1}z^{\pm\alpha_0^{(i)}}\left(\exp\pm\sum_{k=1}^{\infty}z^k x_k^{(i)}\right)\left(\exp\mp\sum_{k=1}^{\infty}\frac{z^{-k}}{k}\frac{\partial}{\partial x_k^{(i)}}\right). \tag{209}$$

Note that for $z,w\in\mathbb{C}^\times$ such that $|w|<|z|$ we have (λ, $\mu=+$ or $-$)

$$\psi^{\lambda(i)}(z)\psi^{\mu(j)}(w)=(z-w)^{\delta_{ij}\lambda\mu}Q_i^{\lambda 1}Q_j^{\mu 1}z^{\lambda\alpha_0^{(i)}}w^{\mu\alpha_0^{(j)}}\exp\sum_{k=1}^{\infty}(\lambda z^k x_k^{(i)}+\mu w^k x_k^{(j)})$$
$$\times\exp-\sum_{k=1}^{\infty}\left(\lambda\frac{z^{-k}}{k}\frac{\partial}{\partial x_k^{(i)}}+\mu\frac{w^{-k}}{k}\frac{\partial}{\partial x_k^{(j)}}\right). \tag{210}$$

We let for $0<|w|<|z|$

$$\Gamma_{ij}(z,w)\overset{\text{def}}{=}\psi^{+(i)}(z)\psi^{-(j)}(w)=(z-w)^{-\delta_{ij}}Q_iQ_j^{-1}z^{\alpha_0^{(i)}}w^{-\alpha_0^{(j)}}\exp\sum_{k=1}^{\infty}(z^k x_k^{(i)}-w^k x_k^{(j)})$$
$$\times\exp-\sum_{k=1}^{\infty}\left(\frac{z^{-k}}{k}\frac{\partial}{\partial x_k^{(i)}}-\frac{w^{-k}}{k}\frac{\partial}{\partial x_k^{(j)}}\right). \tag{211}$$

Using (210), we obtain for $|z_1|>|z_2|>\cdots>|z_{2N-1}|>|z_{2N}|>0$

$$\Gamma_{i_1i_2}(z_1,z_2)\cdots\Gamma_{i_{2N-1}i_{2N}}(z_{2N-1},z_{2N})$$
$$=\prod_{1\le k\le\ell\le 2N}(z_k-z_\ell)^{(-1)^{k+\ell}\delta_{i_ki_\ell}}Q_{i_1}Q_{i_2}^{-1}\cdots Q_{i_{2N-1}}Q_{i_{2N}}^{-1}\prod_{m=1}^{2N}z_m^{(-1)^{m-1}\alpha_0^{(i_m)}}$$
$$\times\exp\left(-\sum_{m=1}^{2N}\sum_{k=1}^{\infty}(-1)^m z_m^k x_k^{(m)}\right)\exp\left(\sum_{m=1}^{2N}\sum_{k=1}^{\infty}(-1)^m\frac{z_m^{-k}}{k}\frac{\partial}{\partial x_k^{(m)}}\right). \tag{212}$$

We may analytically extend the right-hand side of (212) to the domain $\{z_i \neq 0,\ z_i \neq z_j \text{ if } i \neq j,\ i,j = 1,...,2N\}$. Then we deduce from (212) for $N=2$ that in this domain we have

$$\Gamma_{i,i_2}(z_1,z_2)\Gamma_{i_3,i_4}(z_3,z_4) = \Gamma_{i_3,i_4}(z_3,z_4)\Gamma_{i,i_2}(z_1,z_2), \tag{213}$$

$$\Gamma_{ij}(z_1,z_2)^2 \equiv \lim_{\substack{z_3 \to z_1 \\ z_4 \to z_2}} \Gamma_{ij}(z_1,z_2)\Gamma_{ij}(z_3,z_4) = 0. \tag{214}$$

Remark 6.1: Let $A=(a_{ij})$ be a $n \times n$ matrix over $\mathbb{C}$ and let $z_i,\ w_i\ (i=1,...,n)$ be nonzero complex numbers such that $z_i \neq w_j$. Due to (34) the sum

$$\Gamma_A(z,w) = \sum_{i,j=1}^{n} a_{ij}\Gamma_{ij}(z_i,w_j) \tag{215}$$

lies in a completion of $r(\mathrm{gl}_\infty)$.

By (213) and (214) we obtain

$$\exp \Gamma_A(z,w) = \prod_{i,j=1}^{n} (1 + a_{ij}\Gamma_{ij}(z_i,w_j)). \tag{216}$$

Lemma 6.1: (a) If τ is a solution of the n-component KP hierarchy (70) of Hirota bilinear equations, then $(\exp \Gamma_A(z,w))\tau$ is a solution as well for any complex $n \times n$ matrix A and any $z = (z_1,...z_n),\ w=(w_1,...,w_n) \in \mathbb{C}^{\times n}$ such that $z_i \neq w_j$.

(b) For any collection of complex $n \times n$-matrices $A_1,...,A_N$ and any collection $z^{(1)},...,z^{(N)}$, $w^{(1)},...,w^{(N)} \in \mathbb{C}^{\times n}$ with all coordinates distinct, the function

$$\exp \Gamma_{A_1}(z^{(1)},w^{(1)}) \cdots \exp \Gamma_{A_N}(z^{(N)},w^{(N)}) \cdot 1 \tag{217}$$

is a solution of the n-component KP hierarchy (70).

Proof: (a) follows from Proposition 2.1 and Remark 6.1. (b) follows from (a) since the function $1 = \sigma|0\rangle$ satisfies (38). □

We call (217) the *N-solitary τ-function* (of the *n*-component KP hierarchy).

In order to write down (217) in a more explicit form, introduce the lexicographic ordering on the set S of all triples $s=(p,i,j)$, where $p \in \{1,...,N\},\ i,j \in \{1,...,n\}$ (i.e., $s_1 < s_2$ if $p_1 < p_2$, or $p_1 = p_2$ and $i_1 < i_2$ or $p_1 = p_2$, $i_1 = i_2$ and $j_1 < j_2$). Given N $n \times n$ complex matrices $A_p = (a_{ij}^{(p)})$, we let $a_s = a_{ij}^{(p)}$ for $s=(p,i,j) \in S$; given in addition two sets of nonzero complex numbers z_s and w_s, all distinct, parametrized by $s \in S$, introduce the following constants:

$$c(s_1,...,s_r) = \prod_{k=1}^{r} a_{s_k} \prod_{\ell=k+1}^{r} \epsilon_{i_k i_\ell}\epsilon_{i_k j_\ell}\epsilon_{j_k i_\ell}\epsilon_{j_k j_\ell} \prod_{1 \leq k < \ell \leq r} \frac{(z_{s_k} - z_{s_\ell})^{\delta_{i_k i_\ell}}(w_{s_k} - w_{s_\ell})^{\delta_{j_k j_\ell}}}{(z_{s_k} - w_{s_\ell})^{\delta_{i_k j_\ell}}(w_{s_k} - z_{s_\ell})^{\delta_{j_k i_\ell}}}. \tag{218}$$

Then the *N*-solitary solution (217) can be written as follows:

$$1 + \sum_{r=1}^{Nn^2} \sum_{(1,1,1) \leq s_1 < \cdots < s_r \leq (N,n,n)} c(s_1,...,s_r) \left(\exp \sum_{k=1}^{r} \sum_{m=1}^{\infty} (z_{s_k}^m x_m^{(i_k)} - w_{s_k}^m x_m^{(j_k)}) \right) e^{\sum_{k=1}^{r} \alpha_{i_k j_k}}. \tag{219}$$

Let $n=1$. Then the index set S is naturally identified with the set $\{1,...,N\}$, the two sets of complex numbers we denote by z_{2j-1} and z_{2j}, $j=1,...,N$, and we let $A_p = (z_{2p-1} - z_{2p})^{-1} a_p$, where a_p are some constants. Then (219) becomes the well-known formula (see Ref. 9) for the τ-function of the *N*-soliton solution:

$$\tau^{(N)}=1+\sum_{r=1}^{N}\sum_{1\leqslant j_1<\cdots<j_r\leqslant N}\prod_{k=1}^{r}a_{j_k}\prod_{1\leqslant k<\ell\leqslant 2r}(z_{j_k}-z_{j_\ell})^{(-1)^{k+\ell}}\exp\sum_{k=1}^{r}\sum_{m=1}^{\infty}(z_{j_{2k-1}}^m-z_{j_{2k}}^m)x_m. \tag{220}$$

Letting $x_1=x$, $x_2=y$, $x_3=t$ and all other indeterminates constants $x_4=c_4,\ldots$, we obtain, due to (208), the soliton solution of the classical KP Eq. (207):

$$u(t,x,y)=2\frac{\partial^2}{\partial x^2}\log\tau^{(N)}(x,y,t,c_4,c_5,\ldots). \tag{221}$$

In particular, the τ-function of the one-soliton solution is

$$\tau^{(1)}(x,y,t)=1+\frac{a}{z_1-z_2}\exp((z_1-z_2)x+(z_1^2-z_2^2)y+(z_1^3-z_2^3)t+\text{const}), \tag{222}$$

and we get the corresponding one-soliton solution of the classical KP Eq. (207):

$$u(x,y,t)=\frac{(z_1-z_2)^2}{2}\cosh^{-2}\left(\frac{1}{2}((z_1-z_2)x+(z_1^2-z_2^2)y+(z_1^3-z_2^3)t)+\text{const}\right). \tag{223}$$

Let $n=2$. Then any $\tau\in\mathbb{C}[x]\otimes\mathbb{C}[M]$ can be written in the form

$$\tau=\sum_{\ell\in\mathbb{Z}}\tau_\ell e^{\ell\alpha_{12}},\quad \text{where}\quad \tau_\ell\equiv\tau_{\ell\alpha_{12}}.$$

For a N-solitary solution $\tau^{(N)}$ given by (219) we then have

$$\tau_\ell^{(N)}=\delta_{\ell.0}+\sum_{r=1}^{4N}\sum_{(s_1,\ldots,s_r)}c(s_1,\ldots,s_r)\exp\sum_{k=1}^{r}\sum_{m=1}^{\infty}(z_{s_k}^m x_m^{(i_k)}-w_{s_k}^m x_m^{(j_k)}), \tag{224}$$

where $(s_1,\ldots,s_r)$ run over the subset $(225)_2$ of S^r, where

$$\begin{cases}(1,1,1)\leqslant s_1<s_2\cdots<s_r\leqslant(N,n,n)\\ \#\{(i_k,j_k)|i_k>j_k\}-\#\{(i_k,j_k)|i_k<j_k\}=\ell.\end{cases} \tag{225}$$

Letting [cf. (195)]

$$q=-\frac{\tau_1(x,y,t,c,c_3^{(1)},\ldots)}{\tau_0(x,y,t,c,c_3^{(1)},\ldots)},\quad r=\frac{\tau_{-1}(x,y,t,c,c_3^{(1)},\ldots)}{\tau_0(x,y,t,c,c_3^{(1)},\ldots)},$$
$$\varphi=-\frac{\partial^2}{\partial x^2}(\log\tau_0(x,y,t,c,c_3^{(1)},\ldots)), \tag{226}$$

where $x=x_1^{(1)}+x_2^{(1)}$, $y=x_1^{(1)}-x_2^{(1)}$, $t=-2i(x_2^{(1)}-x_2^{(2)})$, $c=-2i(x_2^{(1)}+x_2^{(2)})$ and all other indeterminates $x_k^{(j)}$ are arbitrary constants $c_k^{(j)}$, we obtain an N-solitary solution of the decoupled Davey–Stewartson system (194).

We turn now to the classical Davey–Stewartson system (198) for $\kappa=-1$. The constraint (197) gives

$$\tau_1/\tau_0=\overline{\tau_{-1}/\tau_0}.$$

One way of satisfying this constraint is to let

$$a_{ij}^{(p)}=(-1)^{i+j}\overline{a}_{ji}^{(p)},\quad z_{(p,i,j)}=-\overline{w}_{(p,j,i)},$$
$$c_2=0,\quad c_k^{(j)}\in i^{k+1}\mathbb{R}. \tag{227}$$

We shall concentrate now on the case $N=1$. It will be convenient to use the following notation:

$$x_1=x_1^{(1)},\quad x_2=x_1^{(2)},$$

$$z_{ij}=z_{(1,i,j)},\quad a_i=a_{(1,i,i)}\in\mathbb{R}_+(1\leqslant i,j\leqslant 2),\quad a_3=a_{(1,1,2)}\in\mathbb{C},$$

$$C(z,w)=\frac{z-w}{z+\overline{w}},\quad D(z,w)=\frac{|a_3|^2}{(z+\overline{z})(w+\overline{w})},$$

$$A_j(z)=(z+\overline{z})\left(x_j-(-1)^j it\frac{z-\overline{z}}{4}\right)+\sum_{k=3}^{\infty}(z^k-(-\overline{z})^k)c_k^{(j)}\quad (j=1,2),$$

$$A_3(z,w)=zx_1+\overline{w}z_2+it\left(\frac{z^2}{4}+\frac{\overline{w}^2}{4}\right)+\sum_{k=3}^{\infty}(z^kc_k^{(1)}-(-\overline{w})^kc_k^{(2)}).$$

Then $q=-\tau_1/\tau_0$ and $\varphi=-\frac{1}{2}(\partial/\partial x_1+\partial/\partial x_2)^2\log\tau_0$ is a solution of (198), where

$$\tau_1=a_3e^{A_3(z_{12},z_{21})}(1+a_1C(z_{12},z_{11})e^{A_1(z_{11})})(1+a_2C(\overline{z}_{21},\overline{z}_{22})e^{A_2(z_{22})}), \tag{228a}$$

$$\tau_0=(1+a_1e^{A_1(z_{11})})(1+a_2e^{A_2(z_{22})})+D(z_{12},z_{21})e^{A_3(z_{12},z_{21})+\overline{A_3(z_{12},z_{21})}}(1+a_1|C(z_{12},z_{21})|^2e^{A_1(z_{11})})$$
$$\times(1+a_2|C(z_{21},z_{22})|^2e^{A_2(z_{22})}). \tag{228b}$$

Consider now two special cases of (228a) and (228b):

$$(D)\quad z_1\equiv z_{11}=z_{12}\quad\text{and}\quad z_2\equiv z_{22}=z_{21},$$

$$(S)\quad a_i=0\quad (i=1,2),$$

and let $T=D$ or S. Then (228a) and (228b) reduce to

$$\tau_1=a_3e^{A_3(z_1,z_2)}\ \text{ in both cases,} \tag{229a}$$

$$\tau_0^{(T)}=(1+\delta_{TD}a_1e^{A_1(z_1)})(1+\delta_{TD}a_2e^{A_2(z_2)})+D(z_1,z_2)e^{A_1(z_1)+A_2(z_2)}, \tag{229b}$$

so that $q^{(T)}=-\tau_1/\tau_0^{(T)}$, $\varphi^{(T)}=-\frac{1}{2}(\partial/\partial x_1+\partial/\partial x_2)^2\log\tau_0^{(T)}$ is a solution of (198).

In order to rewrite $q^{(T)}$ in a more familiar form, let ($j=1$, 2 and $a_j(z_j+\overline{z_j})>0$)

$$p_j^{(T)}=(a_j(z_j+\overline{z_j}))^{-1/2}\quad\text{if } T=D\quad\text{and }=1\quad\text{if } T=S,$$

$$\mu_1=\mu_{1R}+i\mu_{1I}=\tfrac{1}{2}\overline{z}_1,\quad \mu_2=\mu_{2R}+i\mu_{2I}=\tfrac{1}{2}z_2,$$

$$m_j^{(T)}=2\sqrt{2}\mu_{jR}p_j^{(T)}e^{-\sum_{k=3}^{\infty}(-1)^j((-1)^j2\mu_j)^kc_k^{(j)}},$$

$$\xi_j=2x_j+2\mu_{jI}t,\quad \tilde{\xi}_j=\frac{1}{\mu_{jR}}\log\frac{|m_j^{(T)}|}{\sqrt{2\mu_{jR}}},$$

$$\rho^{(T)}=-a_3p_1^{(T)}p_2^{(T)}.$$

Then we obtain the following expression for $q^{(T)}$:

$$\frac{4\rho^{(T)}(\mu_{1R}\mu_{2R})^{1/2}\exp\{-(\mu_{1R}(\xi_1-\tilde{\xi}_1)+\mu_{2R}(\xi_2-\tilde{\xi}_2))+i(-(\mu_{1I}\xi_1+\mu_{2I}\xi_2)+(|\mu_1|^2+|\mu_2|^2)t+\arg m_1 m_2)\}}{((\delta_{TD}+\exp(-2\mu_{1R}(\xi_1-\tilde{\xi}_1))(\delta_{TD}+\exp(-2\mu_{2R}(\xi_2-\tilde{\xi}_2))+|\rho^{(T)}|^2)}.$$

The function $q^{(D)}$ is precisely the (1,1)-dromion solution of the Davey–Stewartson Eqs. (198) with $\kappa=-1$ found in Ref. 19 (provided that $\mu_{jR}\in\mathbb{R}_+$). On the other hand, if we let $\mu_{1I}=\mu_{2I}=0$, then $q^{(T)}$ reduces to the two-dimensional breather solution found in Ref. 6. Finally, $q^{(S)}$ is a one-solution solution.

Recall that the dromion solutions of the DS equation were originally discovered in Refs. 6, 18, and 19 (see also Ref. 22). The dromion solutions of the DS equation were first studied from the point of view of the spinor formalism in Ref. 21.

Similarly, we obtain the following solutions of the two-dimensional Toda chain (186):

$$u_\ell=\begin{cases}\log(\tau_{\ell+1}^{(N)}/\tau_\ell^{(N)}) & \text{if } -N\leqslant\ell\leqslant N-1,\\ 0 \quad \text{otherwise,}\end{cases} \tag{230}$$

where the τ-functions $\tau_\ell^{(N)}$ are obtained from (224) by letting all indeterminates $x_m^{(j)}$ with $m>1$ be arbitrary constants:

$$\tau_\ell^{(N)}=\delta_{\ell,0}+\sum_{r=1}^{4N}\sum_{(s_1,\dots,s_r)}c(s_1,\dots,s_r)c_{s_1}\cdots c_{s_r}\exp\sum_{k=1}^{r}(x_{i_k}z_{s_k}-x_{j_k}w_{s_k}), \tag{231}$$

where $(s_1,\dots,s_r)$ runs over $(225)_2$ and $c_s\,(s\in S)$ are arbitrary constants.

Let now $n\geqslant 3$. Then we obtain solutions of the $2+1$ n-wave system (170) as follows. For $1\leqslant i,\ j\leqslant n$ let

$$\tau_{ij}^{(N)}=\delta_{ij}+\sum_{r=1}^{Nn^2}\sum_{(s_1,\dots,s_r)}c_{s_1}\cdots c_{s_r}\exp\sum_{k=1}^{r}(a_{i_k}x+b_{i_k}t-y)z_{s_k}-(a_{j_k}x+b_{j_k}t-y)w_{s_k}, \tag{232}$$

where $(s_1,\dots,s_r)$ runs over $(225)_n$ and $c_s\,(s\in S)$ are arbitrary constants. Then $W_{ij}=\epsilon_{ji}\tau_{ij}/\tau_0\,(i\neq j)$ is a solution of (170), and $Q_{ij}=\epsilon_{ij}(a_i-a_j)\tau_{ij}/\tau_0\,(i\neq j)$ is a solution of (171).

VII. $[m_1,m_2,\dots,m_n]$-REDUCTIONS OF THE n-COMPONENT KP HIERARCHY

Fix a positive integer $m\geqslant n$ and let $m_1+m_2+\cdots+m_n$ be a partition of m into n parts. Let $\omega_j=\exp 2\pi i/m_j$ for $j=1,2,\dots,n$. Introduce the following m^2 fields ($1\leqslant i,j\leqslant n,\ 1\leqslant k\leqslant m_i,\ 1\leqslant\ell\leqslant m_j$):[46]

$$\alpha^{(ijk\ell)}(z)\equiv\sum_{p\in\mathbb{Z}}\alpha_p^{(ijk\ell)}z^{-p-1}=:\psi^{+(i)}(\omega_i^k z)\psi^{-(j)}(\omega_j^\ell z):, \tag{233}$$

where the normal ordering is defined by (46). Note that

$$\alpha^{(ijm_im_j)}(z)=\alpha^{(ij)}(z), \tag{234}$$

where $\alpha^{(ij)}(z)$ are the bosonic fields, defined by (45), which generate the affine algebra $\mathrm{gl}_n(\mathbb{C})\hat{}$ with central charge 1 [see (47)]. It is easy to check that for arbitrary m, the fields $\alpha^{(ijk\ell)}(z)$ generate the affine algebra $\mathrm{gl}_m(\mathbb{C})\hat{}$ with central charge 1. In other words, all the operators $\alpha_p^{(ijk\ell)}$ ($1\leqslant i,j\leqslant n,\ 1\leqslant k\leqslant m_i,\ 1\leqslant\ell\leqslant m_j,\ p\in\mathbb{Z}$) together with 1 span $\mathrm{gl}_m(\mathbb{C})\hat{}$ in its representation in F with central charge 1, the charge decomposition being the decomposition into irreducibles. Hence, using (54), (60) and (63), we obtain the vertex operator realization of this representation of $\mathrm{gl}_m(\mathbb{C})\hat{}$ in the vector space B (see Ref. 46 for details).

Now, restricted to the subalgebra $\mathrm{sl}_m(\mathbb{C})\hat{}$, the representation in $F^{(0)}$ is not irreducible any more, since $\mathrm{sl}_m(\mathbb{C})\hat{}$ commutes with all the operators

$$\beta^{(s)}_{km_n}=\sqrt{\frac{m_n}{m}}\sum_{i=1}^{n}\alpha^{(i)}_{km_i},\quad k\in\mathbb{Z}. \tag{235}$$

In order to describe the irreducible part of the representation of $\mathrm{sl}_m(\mathbb{C})\hat{}$ in $B^{(0)}$ containing the vacuum 1, we choose the complementary generators of the oscillator algebra $\mathfrak{a}$ contained in $\mathrm{sl}_m(\mathbb{C})\hat{}$ $(k\in\mathbb{Z})$:

$$\beta^{(j)}_k=\begin{cases}\alpha^{(j)}_k & \text{if } k\notin m_j\mathbb{Z},\\ \dfrac{M_{j+1}\alpha^{(j+1)}_{\ell m_{j+1}}-m_{j+1}(\alpha^{(1)}_{\ell m_1}+\alpha^{(2)}_{\ell m_2}+\cdots+\alpha^{(j)}_{\ell m_j})}{\sqrt{M_{j+1}(M_{j+1}-m_{j+1})}} & \text{if } k=\ell m_j \text{ and } 1\leqslant j<n,\end{cases} \tag{236}$$

where $M_j=m_1+m_2+\cdots+m_{j-1}$ and $M_1=0$. So the operators (235) and (236) also satisfy relations (49). Hence, introducing the new indeterminates

$$y^{(j)}_k=\begin{cases}x^{(j)}_k & \text{if } k\notin m_j\mathbb{N},\\ \dfrac{M_{j+1}x^{(j+1)}_{\ell m_{j+1}}-(m_1x^{(1)}_{\ell m_1}+m_2x^{(2)}_{\ell m_2}+\cdots+m_jx^{(j)}_{\ell m_j})}{\sqrt{M_{j+1}(M_{j+1}-m_{j+1})}} & \text{if } k=\ell m_j \text{ and } 1\leqslant j<n,\\ \dfrac{m_1x^{(1)}_{\ell m_1}+m_2x^{(2)}_{\ell m_2}+\cdots+m_nx^{(n)}_{\ell m_n}}{\sqrt{mm_n}} & \text{if } k=\ell m_n \text{ and } j=n,\end{cases} \tag{237}$$

we have $\mathbb{C}[x]=\mathbb{C}[y]$ and

$$\sigma(\beta^{(j)}_k)=\frac{\partial}{\partial y^{(j)}_k}\quad\text{and}\quad\sigma(\beta^{(j)}_{-k})=ky^{(j)}_k\quad\text{if } k>0. \tag{238}$$

Now it is clear that the irreducible with respect to $\mathrm{sl}_m(\mathbb{C})\hat{}$ subspace of $B^{(0)}$ containing the vacuum 1 is the vector space

$$B^{(0)}_{[m_1,m_2,\ldots,m_n]}=\mathbb{C}[y^{(j)}_k|1\leqslant j<n,\quad k\in\mathbb{N},\quad\text{or } j=n,\quad k\in\mathbb{N}\backslash m_n\mathbb{Z}]\otimes\mathbb{C}[Q]. \tag{239}$$

The vertex operator realization of $\mathrm{sl}_m(\mathbb{C})\hat{}$ in the vector space $B^{(0)}_{[m_1,m_2,\ldots m_n]}$ is then obtained by expressing the fields (233) in terms of vertex operators (54), which are expressed via the operators (236), the operators $Q_iQ_j^{-1}$ and $\alpha^{(i)}_0-\alpha^{(j)}_0$ $(1\leqslant i<j\leqslant n)$ (see Ref. 46 for details).

The n-component KP hierarchy of Hirota bilinear equations on $\tau\in B^{(0)}=\mathbb{C}[y]\otimes\mathbb{C}[M]$ when restricted to $\tau\in B^{(0)}_{[m_1,m_2,\ldots,m_n]}$ is called the $[m_1,m_2,\ldots,m_n]$-th *reduced* KP *hierarchy*. It is obtained from the n-component KP hierarchy by making the change of variables (237) and putting zero all terms containing partial derivates by $y^{(n)}_{m_n}$, $y^{(n)}_{2m_n}$, $y^{(n)}_{3m_n},\ldots$.

It is clear from the definitions and results of Sec. IV that the condition on the n-component KP hierarchy to be $[m_1,m_2,\ldots,m_n]$th reduced, i.e.,

$$\sum_{j=1}^{n}\frac{\partial\tau}{\partial x^{(j)}_{km_j}}=0,\quad\text{for all } k\in\mathbb{N},$$

implies the following equivalent conditions (cf. Ref. 9):

$$\left(\sum_{j=1}^{n} L(\alpha)^{km_j} C^{(j)}\right)_- = 0, \tag{240}$$

$$\sum_{j=1}^{n} \frac{\partial W(\alpha)}{\partial x_{km_j}^{(j)}} = W(\alpha) \sum_{j=1}^{n} z^{km_j} E_{jj}, \tag{241}$$

$$\sum_{j=1}^{n} \frac{\partial \tau}{\partial x_{m_j}^{(j)}} = \lambda \tau, \quad \text{for some } \lambda \in \mathbb{C}. \tag{242}$$

It follows from (240) that these conditions automatically imply that all of them hold if all m_j are replaced by any, but the same, multiple of m_j.

The totality of solutions of the $[m_1,m_2,\ldots,m_n]$th reduced KP hierarchy is given by the following.

Proposition 7.1: Let $\mathcal{O}_{[m_1,m_2,\ldots,m_n]}$ *be the orbit of 1 under the (projective) representation of the loop group* $\mathrm{SL}_m(\mathbb{C}[t,t^{-1}])$ *corresponding to the representation of* $\hat{\mathrm{sl}}_m$ *in* $B^{(0)}_{[m_1,m_2,\ldots,m_n]}$. *Then*

$$\mathcal{O}_{[m_1,m_2,\ldots,m_n]} = \sigma(\mathcal{O}) \cap B^{(0)}_{[m_1,m_2,\ldots,m_n]}.$$

In other words, the τ-functions of the $[m_1,m_2,\ldots,m_n]$*th reduced KP hierarchy are precisely the τ-functions of the KP hierarchy in the variables* $y_k^{(j)}$, *which are independent of the variables* $y_{\ell m_n}^{(n)}$, $\ell \in \mathbb{N}$.

Proof is the same as of a similar statement in Ref. 27. □

Remark 7.1: The above representation of $\mathrm{sl}_m(\mathbb{C})\hat{}$ in $B^{(0)}_{[m_1,m_2,\ldots,m_n]}$ is a vertex operator construction of the basic representation corresponding to the element of the Weyl group S_m of $\mathrm{sl}_m(\mathbb{C})$ consisting of n cycles of length m_1, $m_2,\ldots,m_n$ (see Refs. 26 and 46). In particular, for $n=1$ this is the principal realization,[34] and for $m=1$ this is the homogeneous realization. $[m]$th reduced one-component KP was studied in a great detail in Ref. 8 (see also Ref. 27).

Let $n=1$. Then the $[2]$-reduced KP hierarchy becomes the celebrated KdV hierarchy on the differential operator $S \equiv (L^2)_+ = \partial^2 + u$, where $u = 2u_1$:

$$\frac{\partial}{\partial x_{2n+1}} S^{1/2} = [(S^{n+1/2})_+, S^{1/2}], \quad n = 1,2,..., \tag{243}$$

the first equation of the hierarchy being the classical Korteweg–deVries equation

$$4\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3} + 6u\frac{\partial u}{\partial x}. \tag{244}$$

Of course, the $[3]$-reduced KP is the Boussinesq hierarchy, and the general $[m]$-reduced KPs are the Gelfand–Dickey hierarchies.

Let $n=2$. The equations of the $[1,1]$-reduced two-component KP are independent of x, hence Eq. (194) becomes independent of x and φ becomes 0 [see (195)]. Thus, Eq. (94) turns into the decoupled nonlinear Schrödinger system (called also the AKNS system):

$$\begin{aligned} i\frac{\partial q}{\partial t} &= -\frac{1}{2}\frac{\partial^2 q}{\partial y^2} - q^2 r, \\ i\frac{\partial r}{\partial t} &= \frac{1}{2}\frac{\partial^2 r}{\partial y^2} + q r^2. \end{aligned} \tag{245}$$

Thus (245) is a part of the [1,1]-reduced two-component KP. For that reason the one-reduced two-component KP is sometimes called the nonlinear Schrödinger hierarchy. Of course, under the constraint (197), we get the nonlinear Schrödinger equation

$$i\frac{\partial q}{\partial t}=-\frac{1}{2}\frac{\partial^2 q}{\partial y^2}-\kappa|q|^2 q. \tag{246}$$

Similarly, under the same reduction the two-dimensional Toda chain (186) turns into the one-dimensional Toda chain

$$\frac{\partial^2 u_n}{\partial x^2}=e^{u_n-u_{n-1}}-e^{u_{n+1}-u_n}(\text{here } x=2y_1^{(1)}). \tag{247}$$

Thus, the one-dimensional Toda chain is a part of the nonlinear Schrödinger hierarchy. It was studied from the representation theoretical point of view in Ref. 45.

Let $n\geqslant 3$. Since the constraint (165) is contained among the constraints of the [1,1,...,1]-reduced n-component KP hierarchy, we see that the $1+1$ n-wave system (168) is a part of the [1,1,...,1]-reduced n-component KP hierarchy. Note also that the [1,1,...,1]-reduction of the n-component KP reduces the $2+1$ n-wave interaction system (171) into the $1+1$ system (168).

Since the nonlinear Schrödinger system (245) is a part of the [1,1]-reduced two-component KP hierarchy, the [1,1,...,1]-reduced n-component KP hierarchy will be called the n-component NLS. Let us give here its formulation since it is especially simple.

Given a $n\times n$ matrix $C(z)=\Sigma_j C_j z^j$, we let

$$C(z)_-=\sum_{j<0} C_j z^j, \quad C(z)_+=\sum_{j\geqslant 0} C_j z^j.$$

Also, given a diagonal complex matrix $a=\mathrm{diag}(a_1,...,a_n)$ we let

$$x_k^a=\sum_{j=1}^n a_k x_k^{(j)}, \quad \frac{\partial}{\partial x_k^a}=\sum_{j=1}^n a_k\frac{\partial}{\partial x_k^{(j)}}.$$

Let $\mathfrak{h}$ denote the set of all traceless diagonal matrices over $\mathbb{C}$.

The n-component NLS hierarchy is the following system on matrix valued functions,

$$P(\alpha)\equiv P(\alpha,x,z)=1+\sum_{j>0} W^{(j)}(\alpha,x)z^{-j}, \quad \alpha\in M,$$

where $x=\{x_k^{(a)}|a\in\mathfrak{h},k=1,2,...\}$:

$$\frac{\partial P(\alpha)}{\partial x_k^{(\alpha)}}=-(P(\alpha)\alpha P(\alpha)^{-1}z^k)_- P(\alpha) \tag{248}$$

with additional matching conditions

$$(P(\alpha)R(\alpha-\beta,z)P(\beta)^{-1})_-=0, \quad \alpha,\beta\in M, \tag{249}$$

where $R(\gamma,z)\equiv R^+(\gamma,z)$ is defined by (101).

This formulation implies the Lax form formulation if we consider $C^{(a)}(x,z)=P(\alpha)aP(\alpha)^{-1}$ for each $a\in\mathfrak{h}$ and fixed α. Consider a family of commuting matrix valued functions of the form

$$C^{(a)} \equiv C^{(a)}(x,z) = a + \sum_{j>0} C_j^{(a)}(x) z^{-j},$$

depending linearly on $a \in \mathfrak{h}$, and let $B_k^{(a)} = (C^{(a)} z^k)_+$. Then the Lax form of the n-component NLS is

$$\frac{\partial C^{(a)}}{\partial x_k^{(b)}} = [B_k^{(b)}, C^{(a)}], \quad a,b \in \mathfrak{h}, \quad k = 1,2,\ldots. \tag{250}$$

The equivalent zero curvature form of the n-component NLS is

$$\frac{\partial B_\ell^{(a)}}{\partial x_k^{(b)}} - \frac{\partial B_k^{(b)}}{\partial x_\ell^{(a)}} = [B_k^{(b)}, B_\ell^{(a)}], \quad a,b \in \mathfrak{h}, \quad k,\ell = 1,2,\ldots. \tag{251}$$

Since for the $[1,1,\ldots,1]$-reduced n-component KP one has $L = \partial$, i.e., all $U^{(j)} = 0$, we see from Remark 5.1 that the n-component NLS in the form (250) contains the following system of equations on functions $A_{ij} \equiv (C_1^{E_{jj}})_{ij}$ $(i \neq j)$:

$$\frac{\partial A_{ij}}{\partial t_j} = -\frac{\partial^2 A_{ij}}{\partial x_j^2} - 2\sum_{k \neq j} A_{ij} A_{jk} A_{kj},$$

$$\frac{\partial A_{ij}}{\partial t_i} = \frac{\partial^2 A_{ij}}{\partial x_i^2} + 2\sum_{k \neq i} A_{ij} A_{ik} A_{ki},$$

$$\frac{\partial A_{ij}}{\partial t_k} = A_{ik}\frac{\partial A_{kj}}{\partial x_k} - A_{kj}\frac{\partial A_{ik}}{\partial x_k}, \quad \text{if } i \neq k, \quad j \neq k, \tag{252}$$

$$\frac{\partial A_{ij}}{\partial x_k} = A_{ik} A_{kj}, \quad \text{if } i \neq k, \quad j \neq k,$$

$$\sum_k \frac{\partial A_{ij}}{\partial x_k} = \sum_k \frac{\partial A_{ij}}{\partial t_k} = 0.$$

This reduces to (215) if $n = 2$.

Remark 7.2: Equations (248), (250), and (251) still make sense if we consider an arbitrary algebraic group G and a reductive commutative subalgebra $\mathfrak{h}$ of its Lie algebra $\mathfrak{g}$. The functions $P(\alpha)$ take values in $G(\mathcal{A}((z)))$ and the functions $C^{(a)}$ take values in $\mathfrak{g}(\mathcal{A}((z)))$. If G is a simply laced simple Lie group, the element $R(\gamma,z) \in G(\mathbb{C}[z,z^{-1}])$ in matching conditions (249) can be generalized as follows. Let $\mathfrak{h}$ be a Cartan subalgebra of $\mathfrak{g}$, normalize the Killing form on $\mathfrak{g}$ by the condition that $(\alpha|\alpha) = 2$ for any root α, and identify $\mathfrak{h}$ with $\mathfrak{h}^*$ using this form. Let $M(\text{resp. } L) \subset \mathfrak{h}^* = \mathfrak{h}$ be the root (resp. weight) lattice and let $\epsilon(\alpha,\beta)$: $M \times M \to \{\pm 1\}$ be a bimultiplicative function such that $\epsilon(\alpha,\alpha) = (-1)^{(1/2)(\alpha|\alpha)}$, $\alpha \in M$. Define $R(\alpha,z) \in H(\mathbb{C}[z,z^{-1}])$ for each α as follows:

$$R(\alpha,z) = c_\alpha z^\alpha, \tag{253}$$

where in any finite-dimensional representation V of G, $c_\alpha \in H$ and $z^\alpha \in H$ for $z \in \mathbb{C}^\times$ are defined by

$$c_\alpha(v) = \epsilon(\beta,\alpha) v, \quad z^\alpha(v) = z^{(\alpha|\beta)} v \quad \text{if } v \in V_\beta. \tag{254}$$

Note that this GNLS hierarchy is closely related to the Bruhat decomposition in the loop group $G(\mathbb{C}((z)))$.

It is clear that we get the τ-function of the $[\ell,\ell,...,\ell]$th reduced n-component KP hierarchy if we let in (217)

$$w_s = \omega_s z_s, \quad s \in S, \tag{255}$$

where ω_s are arbitrary ℓth roots of 1. The totality of τ-functions is (a completion of) the orbit of $1 \in B^{(0)}$ under the group $\mathrm{SL}_m(\mathbb{C}[t,t^{-1}])$.

VIII. $W_{1+\infty}(\mathrm{gl}_n)$ AND THE ORLOV–SCHULMAN–ADLER–SHIOTA–VAN MOERBEKE FORMULA

In recent years Adler, Shiota, and van Moerbeke[2,3] proved a formula, conjectured by Orlov and Schulman,[39] which connects the action of $W_{1+\infty}$ on the tau-function of the one-component KP hierarchy to the so-called ''additional symmetries'' of the wave function. These Orlov–Schulman symmetries were also independently found by Fokas and Santini in Ref. 18. In this section we shall give a generalization of this formula, obtained by one of the authors in Ref. 48, for the n-component KP case.

In the spirit of Refs. 28, 29, and 41, we introduce the bosonic fields

$$J^{(ab,\ell)}(z) = \sum_{k\in\mathbb{Z}} J_k^{(ab,\ell)} z^{-k-\ell-1} = :\frac{\partial^\ell \psi^{+(a)}(z)}{\partial z^\ell} \psi^{-(b)}(z):, \tag{256}$$

and their generating series

$$J^{(ab)}(y,w) =: :\psi^{+(a)}(y)\psi^{-(b)}(w): = \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} J^{(ab,\ell)}(w) = \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \sum_{k\in\mathbb{Z}} J_k^{(ab,\ell)} w^{-k-\ell-1}. \tag{257}$$

It is straightforward, but tedious, to check that these operators satisfy the following commutation relations:

$$[J_k^{(ab,\ell)}, J_p^{(cd,q)}] = \delta_{bc} \sum_{m=0}^{q} \binom{q}{m} [k+l]_m J_{k+\ell+p+q-m}^{(ad,\ell+q-m)} - \delta_{ad} \sum_{m=0}^{\ell} \binom{\ell}{m} [p+q]_m J_{k+\ell+p+q-m}^{(cb,\ell+q-m)}$$
$$+ \delta_{ad}\delta_{bc}\delta_{k,-p}(-)^\ell \ell! q! \binom{k+\ell}{\ell+q+1},$$

where $[x]_m = x(x-1)(x-2)\cdots(x-m+1)$. Hence these operators $J_k^{(ab,\ell)}$ together with 1 satisfy the commutation relations of the Lie algebra $W_{1+\infty}(\mathrm{gl}_n)$, the central extension of the Lie algebra of differential operators on $(\mathbb{C}[t,t^{-1}])^n$, where the central element acts as 1. If one substitutes (54) into (257) and using (63), one obtains the following vertex operator expression for the generating series of the fields $J^{(ab,\ell)}(w)$:

$$J^{(ab)}(y,w) = \frac{1}{(y-w)^{\delta_{ab}}}(X^{(ab)}(y,w) - \delta_{ab}), \quad \text{where}$$

$$X^{(ab)}(y,w) = \epsilon(\delta_a,\delta_b) e^{\delta_a - \delta_b} y^{\delta_a} w^{-\delta_b} \widetilde{X}^{(ab)}(y,w), \quad \text{and} \tag{258}$$

$$\widetilde{X}^{(ab)}(y,w) = \exp\left(\sum_{k=1}^{\infty} (x_k^{(a)} y^k - x_k^{(b)} w^k)\right) \exp\left(-\sum_{k=1}^{\infty} \left(\frac{\partial}{\partial x_k^{(a)}} \frac{y^{-k}}{k} - \frac{\partial}{\partial x_k^{(b)}} \frac{w^{-k}}{k}\right)\right).$$

In order to give the Orlov–Schulman–Adler–Shiota–van Moerbeke (OSASM) formula, we have to introduce some infinite order pseudo-differential operators for $\alpha \in \operatorname{supp} \tau$:

$$\Gamma = \xi I_n + \sum_{a=1}^{n} \sum_{k=1}^{\infty} k x_k^{(a)} \partial^{k-1} E_{aa},$$

$$M(\alpha) = P^+(\alpha) R^+(\alpha) S^+(\alpha) \xi S^+(\alpha)^{-1} R^+(\alpha)^{-1} P^+(\alpha)^{-1} = P^+(\alpha) R^+(\alpha) \Gamma R^+(\alpha)^{-1} P^+(\alpha)^{-1}, \tag{259}$$

$$C^{(ij)}(\alpha) = P^+(\alpha) R^+(\alpha) S^+(\alpha) E_{ab} S^+(\alpha)^{-1} R^+(\alpha)^{-1} P^+(\alpha)^{-1}.$$

Notice that Γ, $M(\alpha)$, $C^{(ij)}(\alpha) \in \hat{\Psi}$. One has the following linear problem for the wave function $V^+(\alpha, \xi, x, z)$:

$$\begin{aligned} L(\alpha) V^+(\alpha, \xi, x, z) &= z V^+(\alpha, \xi, x, z), \\ M(\alpha) V^+(\alpha, \xi, x, z) &= \frac{\partial V^+(\alpha, \xi, x, z)}{\partial z}, \\ C^{(ij)}(\alpha) V^+(\alpha, \xi, x, z) &= V^+(\alpha, \xi, x, z) E_{ij} \\ B_k^{(j)}(\alpha) V^+(\alpha, \xi, x, z) &= \frac{\partial V^+(\alpha, \xi, x, z)}{\partial x_k^{(j)}}. \end{aligned} \tag{260}$$

In the spirit of Sec. VIII. We introduce

$$Y_k^{(ab,\ell)}(\alpha) = M(\alpha)^\ell L(\alpha)^{k+\ell} C^{(ab)}(\alpha), \tag{261}$$

and define

$$\begin{aligned} Y^{(ab)}(\alpha, y, w) &= \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \sum_{k \in \mathbb{Z}} w^{-k-\ell-1} Y_k^{(ab,\ell)}(\alpha) \\ &= \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \sum_{k \in \mathbb{Z}} w^{-k-\ell-1} M(\alpha)^\ell L(\alpha)^{k+\ell} C^{(ab)}(\alpha). \end{aligned} \tag{262}$$

Let $\delta(w-z) = \Sigma_{n \in \mathbb{Z}} w^{-n} z^{n-1}$. Using (259) we calculate

$$\begin{aligned} Y^{(ab)}(\alpha, y, w) V^+(\alpha, \xi, x, z) &= \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \sum_{k \in \mathbb{Z}} w^{-k-\ell-1} M(\alpha)^\ell L(\alpha)^{k+\ell} C^{(ab)}(\alpha) V^+(\alpha, \xi, x, z) \\ &= \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \sum_{k \in \mathbb{Z}} w^{-k-\ell-1} z^{k+\ell} \frac{\partial^\ell V^+(\alpha, \xi, x, z)}{\partial z^\ell} E_{ab} \\ &= \delta(w-z) \sum_{\ell=0}^{\infty} \frac{(y-w)^\ell}{\ell!} \frac{\partial^\ell V^+(\alpha, \xi, x, z)}{\partial z^\ell} E_{ab} \\ &= \delta(w-z) V^+(\alpha, \xi, x, y) E_{ab}. \end{aligned} \tag{263}$$

The deduction of the OSASM formula is based on two things; (1) the bilinear identity (64) in a slightly modified form (with all $x_1^{(i)}$'s replaced by $x_1^{(i)} + \xi$), viz.,

$$\mathrm{Res}_{z=0}dz\sum_{j=1}^{n}\psi^{+(j)}(z)e^{z\xi}\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)e^{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}\otimes\psi^{-(j)'}(z)$$
$$\times e^{-z\xi'}\tau_{\beta+\delta_j-\delta_k}(\xi'x')(e^{\beta+\delta_j-\delta_k})'=0, \tag{264}$$

and (2) the commutation relations (32), which we rewrite as follows:

$$\psi^{\lambda(i)}(w)\psi^{\mu(j)}(z)+\psi^{\mu(j)}(z)\psi^{\lambda(i)}(w)=\delta_{\lambda_j-\mu}\delta_{ij}\delta(w-z). \tag{265}$$

Now, let $\psi^{+(a)}(y)e^{y\xi}\psi^{-(b)}(w)e^{w\xi}\otimes 1$ act on the bilinear identity (264). We obtain, using (265),

$$\mathrm{Res}_{z=0}dz\sum_{j=1}^{n}\{\psi^{+(j)}(z)\psi^{+(a)}(y)\psi^{-(b)}(w)e^{(z+y-w)\xi}-\delta_{jb}\psi^{+(a)}(y)e^{y\xi}\delta(w-z)\}$$
$$\times\tau_{\alpha+\delta_i+\delta_b-\delta j-\delta_a}(\xi,x)e^{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}\otimes\psi^{-(j)'}(z)e^{-z\xi'}\tau_{\beta+\delta_j-\delta_k}(\xi'x')(e^{\beta+\delta_j-\delta_k})'=0. \tag{266}$$

Since $\psi^{+(a)}(y)\psi^{-(b)}(w)=J^{(ab)}(y,w)-\delta_{ab}/(y-w)$ and since we can subtract a multiple of (264), we can replace $\psi^{+(a)}(y)\psi^{-(b)}(w)$ by $J^{(ab)}(y,w)$. Now remove the tensor product and the factors $e^{\alpha+\delta_i}$ and $(e^{\beta+\delta_k})'$ and divide by $\tau_\alpha(\xi,x)\tau_\beta(\xi',x')$. Notice that by doing this, the action of $J^{(ab)}(y,w)$ is no longer well-defined. For that reason we introduce $\mathbb{J}^{(ab)}(y,w)$ as follows:

$$(y-w)^{\delta_{ab}}\mathbb{J}^{(ab)}(y,w)\tau_\gamma(\xi,x)=\{\epsilon(\delta_a,\delta_b)\epsilon(\delta_a-\delta_b,\gamma)y^{(\delta_a|\gamma)}w^{-(\delta_b|\gamma)}e^{y\cdot x^{(a)}-w\cdot x^{(b)}}$$
$$\times e^{-\eta^{(a)}(x,y)+\eta^{(b)}(x,w)}-\delta_{ab}\}e^{(y-w)\xi}\tau_\gamma(x,t),$$

where $\eta^{(a)}(x,z)=\Sigma_{k=1}^{\infty}(\partial/\partial x_k^{(a)})(z^{-k}/k)$. So (266) turns into

$$\mathrm{Res}_{z=0}dz\left\{\delta(w,z)V_{ia}^{+}(\alpha,\xi,x,y)V_{kb}^{-}(\beta,\xi',x',z)+\sum_{j=1}^{n}e^{-\eta^{(j)}(x,z)}\right.$$
$$\left.\times\left(\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)}\right)V_{ij}^{+}(\alpha,\xi,x,z)V_{kj}^{-}(\beta,\xi',x'z)\right\}=0.$$

Using (263) one obtains

$$\mathrm{Res}_{z=0}dz\left\{E_{ii}\left(Y^{(ab)}(\alpha,y,w)V^{+}(\alpha,\xi,x,z)+\sum_{j=1}^{n}e^{-\eta^{(j)}(x,z)}\right.\right.$$
$$\left.\left.\times\left(\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)}\right)\right)V^{+}(\alpha,\xi,x,z)E_{jj}\right\}^{t}V^{-}(\beta,\xi',x',z)=0.$$

Now notice that

$$e^{-\eta^{(j)}(x,z)}\left(\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)}\right)V^{+}(\alpha,\xi,x,z)E_{jj}$$
$$=\sum_{k=0}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)V^{+}(\alpha,\xi,x,z)$$
$$=\left\{\left(\sum_{k=1}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)\right)_{-}+\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)}E_{jj}\right\}V^{+}(\alpha,\xi,x,z),$$

hence

$$\mathrm{Res}_{z=0} dz E_{ii} \left(Y^{(ab)}(\alpha,y,w) + \sum_{j=1}^{n} \sum_{k=0}^{\infty} c_{jk} L(\alpha)^{-k} C^{(j)}(\alpha) \right) V^{+}(\alpha,\xi,x,z) \ {}^{t}V^{-}(\beta,\xi',x',z) = 0.$$

Now take $\beta=\alpha$ and use Corollary 4.1 and Remark 4.1; one obtains

$$E_{ii} \left(Y^{(ab)}(\alpha,y,w)_{-} + \sum_{j=1}^{n} \left(\sum_{k=0}^{\infty} c_{jk} L(\alpha)^{-k} C^{(j)}(\alpha) \right)_{-} \right) = 0.$$

Hence

$$\begin{aligned} &-E_{ii} Y^{(ab)}(\alpha,y,w)_{-} V^{+}(\alpha,\xi,x,z) \\ &\quad = E_{ii} \sum_{j=1}^{n} e^{-\eta^{(j)}(x,z)} \left(\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)} \right) V^{+}(\alpha,\xi,x,z) E_{jj} \\ &\qquad - \frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_b-\delta_a}(\xi,x)}{\tau_{\alpha}(\xi,x)} E_{ii} V^{+}(\alpha,\xi,x,z). \end{aligned}$$

So we obtain the following generalization of the Orlov–Schulman–Adler–Shiota–van Moerbeke formula.

Theorem 8.1:

$$\begin{aligned} &-(Y^{(ab)}(\alpha,y,w)_{-} V^{+}(\alpha,\xi,x,z))_{ij} \\ &\quad = \left\{ e^{-\eta^{(j)}(x,z)} \left(\frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)} \right) - \frac{\mathbb{J}^{(ab)}(y,w)\tau_{\alpha+\delta_b-\delta_a}(\xi,x)}{\tau_{\alpha}(\xi,x)} \right\} V^{+}_{ij}(\alpha,\xi,x,z). \end{aligned} \tag{267}$$

Introducing the modes of

$$\mathbb{J}^{(ab)}(y,w) = \sum_{\ell=0}^{\infty} \frac{(y-w)^{\ell}}{\ell!} \sum_{k\in\mathbb{Z}} \mathbb{J}^{(ab,\ell)}_{k} w^{-k-\ell-1}, \tag{268}$$

one has the following.

Corollary 8.1:

$$\begin{aligned} &-((M(\alpha)^{\ell} L(\alpha)^{k+\ell} C^{(ab)}(\alpha))_{-} V^{+}(\alpha,\xi,x,z))_{ij} \\ &\quad = \left\{ e^{-\eta^{(j)}(x,z)} \left(\frac{\mathbb{J}^{(ab,\ell)}_{k}\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(\xi,x)}{\tau_{\alpha+\delta_i-\delta_j}(\xi,x)} \right) - \frac{\mathbb{J}^{(ab,\ell)}_{k}\tau_{\alpha+\delta_b-\delta_a}(\xi,x)}{\tau_{\alpha}(\xi,x)} \right\} V^{+}_{ij}(\alpha,\xi,x,z). \end{aligned}$$

Proof: Compare in (267) the expansions for the vertex operators $Y^{(ab)}(\alpha,y,w)$ as in (262) and $\mathbb{J}^{(ab)}(y,w)$ as in (268). □

ACKNOWLEDGMENTS

We would like to thank A. S. Fokas for asking one of us to write a paper for this volume. We are grateful to E. Medina for calling our attention to Ref. 21. The second named author would like to thank MIT for the kind hospitality. V.K. was supported in part by NSF Grant No. DMS-9970007.

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Additional symmetries and solutions of the dispersionless KP hierarchy

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(Received 15 January 2003; accepted 9 April 2003)

The dispersionless KP hierarchy is considered from the point of view of the twistor formalism. A set of explicit additional symmetries is characterized and its action on the solutions of the twistor equations is studied. A method for dealing with the twistor equations by taking advantage of hodograph type equations is proposed. This method is applied for determining the orbits of solutions satisfying reduction constraints of Gelfand–Dikii type under the action of additional symmetries. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1587873]

I. INTRODUCTION

The so-called dispersionless hierarchies[1–9] provide an interesting type of nonlinear integrable model which cannot be studied by the standard schemes of the KP theory and require an entirely new approach. From the point of view of the Lax formalism, dispersionless hierarchies arise as the quasiclassical limits of Lax pair equations performed by replacing operators by phase space functions and commutators by Poisson brackets. In this way, when dealing with dispersionless hierarchies, instead of the associated auxiliary linear system of the standard formalism of integrable systems the underlying equations to be solved are of Hamilton–Jacobi type.

Several methods of solution of dispersionless hierarchies have been formulated. In Refs. 3 and 4 (see also Refs. 11 and 12) Kodama and Gibbons gave a direct method based on the use of reductions in which the dependent variables depend on a finite number of unknown functions. The corresponding reduced hierarchy becomes an infinite set of compatible hydrodynamic systems solvable by hodographic techniques. A $\overline{\partial}$ scheme has been proposed by Konopelchenko *et al.* in Refs. 13–15, which introduces an associated $\overline{\partial}$ equation of Hamilton–Jacobi type. In this article we deal with the twistorial method of Takasaki and Takebe,[9,10] Two important advantages of this method are the following.

(1) It provides a convenient scheme for describing the symmetries.
(2) All local solutions can be determined by means of the twistor method.

The main aim of this article is to present a technique for deriving explicit examples of both additional symmetries and solutions of dispersionless hierarchies within the framework of the twistor formalism. It requires a new formulation of the twistor equations which involves a certain type of generating function for canonical transformations of twistor data as well as the use of hodograph equations. To show our strategy, we concentrate on the dispersionless KP (dKP) hierarchy, which is the prototype of this kind of integrable hierarchy. Its Lax pair formulation involves a phase space with a canonical pair of coordinates (p,x) and an associated Poisson bracket

$$\{F,G\}=\frac{\partial F}{\partial p}\frac{\partial G}{\partial x}-\frac{\partial F}{\partial x}\frac{\partial G}{\partial p}.$$

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It is useful to introduce an enlarged Lax formalism with a pair of canonically conjugate variables $\mathcal{L}=\mathcal{L}(p,\mathbf{t})$ and $\mathcal{M}=\mathcal{M}(p,\mathbf{t})$ (i.e. $\{\mathcal{L},\mathcal{M}\}=1$) depending on p and an infinite set of time parameters

$$\mathbf{t}:=(t_1=x,t_2,\ldots,t_n,\ldots),$$

which are assumed to admit expansions of the form

$$\mathcal{L}=p+\sum_{n\geqslant 1}\frac{u_n(\mathbf{t})}{p^n},\quad \mathcal{M}=\sum_{n\geqslant 2}nt_n\mathcal{L}^{n-1}+x+\sum_{n\geqslant 1}\frac{v_n(\mathbf{t})}{\mathcal{L}^{n+1}},\tag{1}$$

as $p\to\infty$ and $\mathcal{L}\to\infty$, respectively. The Lax equations of the dKP hierarchy are

$$\frac{\partial\mathcal{L}}{\partial t_n}=\{\mathcal{B}_n,\mathcal{L}\},\quad \frac{\partial\mathcal{M}}{\partial t_n}=\{\mathcal{B}_n,\mathcal{M}\},\quad n\geqslant 2,\tag{2}$$

where

$$\mathcal{B}_n:=(\mathcal{L}^n)_{\geqslant 0}.$$

Here $(\mathcal{F})_{\geqslant 0}$ denotes the projection of a Laurent series $\mathcal{F}$ in the variable p on the subspace generated by the non-negative powers of p [we will also use the notation $(\mathcal{F})_{\leqslant -1}:=\mathcal{F}-(\mathcal{F})_{\geqslant 0}$]. The system of compatibility equations

$$\frac{\partial\mathcal{B}_m}{\partial t_n}-\frac{\partial\mathcal{B}_n}{\partial t_m}+\{\mathcal{B}_m,\mathcal{B}_n\}=0,\quad m\neq n,\tag{3}$$

yields an infinite set of nonlinear equations for the coefficients u_n of the expansion (1) of $\mathcal{L}$. In particular for $(n,m)=(2,3)$ one gets the dKP equation (Zabolotskaya–Khokhlov equation)

$$(u_t-3uu_x)_x=\tfrac{3}{4}u_{yy},\quad u:=u_1,t:=t_3,y:=t_2.\tag{4}$$

This is an interesting nonlinear model with applications, in the study of quasi-plane sound beams,[17] quasi-transonic flows past thin wings[18] or Einstein-Weyl spaces.[19]

In the next section we first describe in brief the twistor approach to the solutions and symmetries of the dKP hierarchy. Then we present a class of additional symmetries depending on arbitrary functions of one variable, the action of which can be explicitly determined. As a particular case they include the symmetries of the dKP equation found by Dunajski, Mason and Tod in Ref. 19. The first part of Sec. III is devoted to a new formulation of twistor equations which is appropriate for dealing with the transformation laws of solutions under the action of symmetries. In the second part of Sec. III we show how solutions of the dKP hierarchy satisfying reduction constraints of Gelfand–Dikii type transform under the class of additional symmetries introduced in Sec. II. Finally, some explicit examples are worked out.

II. SYMMETRIES IN THE TWISTOR FORMALISM

A. Twistorial structure of the dKP hierarchy

The twistor formalism of the dKP hierarchy is based on the degenerate symplectic form[9]

$$\omega:=\mathrm{d}p\wedge\mathrm{d}x+\sum_{n\geqslant 2}\mathrm{d}\mathcal{B}_n\wedge\mathrm{d}t_n,\tag{5}$$

which plays the role of the Gindikin bundle[16] of curved twistor theory. The form ω encodes both the Lax equations and their compatibility conditions into the simple system

$$\omega = \mathrm{d}\mathcal{L} \wedge \mathrm{d}\mathcal{M}, \qquad \omega \wedge \omega = 0. \tag{6}$$

From the first equation we have that

$$\mathrm{d}\left(\mathcal{M}\mathrm{d}\mathcal{L} + p\,\mathrm{d}x + \sum_{n\geqslant 2} \mathcal{B}_n \mathrm{d}t_n \right) = 0,$$

so that there exists a generating function $S = S(\mathcal{L}, \mathbf{t})$ for the canonical transformation $(p,x) \mapsto (\mathcal{L}, \mathcal{M})$ satisfying

$$\mathrm{d}S = \mathcal{M}\mathrm{d}\mathcal{L} + p\,\mathrm{d}x + \sum_{n\geqslant 2} \mathcal{B}_n \mathrm{d}t_n,$$

or equivalently

$$\mathcal{M} = \frac{\partial S}{\partial \mathcal{L}}, \quad p = \frac{\partial S}{\partial x}, \quad \mathcal{B}_n = \frac{\partial S}{\partial t_n}, \quad n \geqslant 2. \tag{7}$$

Notice that from (1) and the first equation of (7) it follows that S can be defined as

$$S(\mathcal{L}, \mathbf{t}) = \sum_{n\geqslant 1} t_n \mathcal{L}^n - \sum_{n\geqslant 1} \frac{v_n(\mathbf{t})}{n} \mathcal{L}^{-n}.$$

The twistor scheme for solving the dKP hierarchy is based on the following result.[9]

Theorem 1: *Let (P(p,x),X(p,x)) be a pair of canonically conjugate variables (i.e. $\{P,X\}=1$). Then we have the following:*

(1) Given two functions $(\mathcal{L}(p,\mathbf{t}), \mathcal{M}(p,\mathbf{t}))$ of the form (1) such that the composite functions $(P(\mathcal{L},\mathcal{B}), X(\mathcal{L},\mathcal{B}))$ have Laurent series expansions in p satisfying the twistor equations

$$(P(\mathcal{L},\mathcal{M}))_{\leqslant -1} = 0, \quad (X(\mathcal{L},\mathcal{M}))_{\leqslant -1} = 0, \tag{8}$$

then $(\mathcal{L},\mathcal{M})$ gives a solution of the dKP hierarchy (2). The pair

$$(P(p,x), X(p,x))$$

is called the twistor data *of the solution $(\mathcal{L},\mathcal{M})$.*

(2) Each solution of the dKP hierarchy admits a set $(P(p,x), X(p,x))$ of twistor data.

In general, we cannot assume the existence of appropriate solutions $(\mathcal{L},\mathcal{M})$ of (8). For example, the canonical variables

$$P := p^2 x, \quad X := \frac{1}{p}, \tag{9}$$

determine the twistor equations

$$(\mathcal{L}^2 \mathcal{M})_{\leqslant -1} = 0, \quad \left(\frac{1}{\mathcal{L}} \right)_{\leqslant -1} = 0,$$

which obviously have no solutions satisfying (1).

B. Symmetry transformations

One of the main features of the twistor equations is that the symmetry properties of the dKP hierarchy can be formulated in a convenient way.[9] Indeed, the natural group acting on the set of twistor data $(P(p,x),X(p,x))$ is the group of canonical transformations generated by one-parameter groups of the form

$$\begin{aligned} &\exp(s\{F,\cdot\}):(P,X)\mapsto(P(s),X(s)), \quad F=F(p,x),\\ &P(s):=P(\exp(s\{F,\cdot\})p,\exp(s\{F,\cdot\})x),\\ &X(s):=X(\exp(s\{F,\cdot\})p,\exp(s\{F,\cdot\})x), \end{aligned} \tag{10}$$

where

$$\exp(s\{F,\cdot\})G:=G+s\{F,G\}+\frac{s^2}{2}\{F,\{F,G\}\}+\cdots.$$

The following theorem can be proved.[9]

Theorem 2: *A one-parameter group of canonical transformations (10) induces an action* $(\mathcal{L},\mathcal{M})\mapsto(\mathcal{L}(s),\mathcal{M}(s))$ *on the set of solutions of the dKP hierarchy determined by the flow*

$$\frac{\partial\mathcal{L}}{\partial s}=\{\mathcal{L},F(\mathcal{L},\mathcal{M})_{\leqslant -1}\}, \quad \frac{\partial\mathcal{M}}{\partial s}=\{\mathcal{M},F(\mathcal{L},\mathcal{M})_{\leqslant -1}\}. \tag{11}$$

Let us consider symmetries of the dKP hierarchy generated by double series of the form

$$F(\mathcal{L},\mathcal{M})=\sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}c_{ij}\mathcal{L}^i\mathcal{M}^j. \tag{12}$$

We will concentrate on the $(r+1)$th *truncated dKP hierarchies* defined as the sets of the first $r+1$ flows of the dKP hierarchy $(r\geqslant 2)$. Thus in order to analyze their symmetries we may set $t_n=0,\forall n\geqslant r+1$, and so we may write

$$\mathcal{M}=(r+1)t_{r+1}\mathcal{L}^r+rt_r\mathcal{L}^{r-1}+\cdots+x+\mathcal{O}\left(\frac{1}{\mathcal{L}^2}\right). \tag{13}$$

By substituting this expansion in (12), a series expansion of F in powers of $\mathcal{L}$ is obtained. Let us now investigate those symmetries of the $(r+1)$th truncated dKP hierarchy which do not involve the action of higher dKP flows. To this end, we have to avoid terms of the form $\{(\mathcal{L}^n)_{\geqslant 0},\mathcal{L}\}$ with $n>(r+1)$ on the right-hand side of the first equation in (11). Hence we impose $c_{ij}=0$ for $(i+jr)>(r+1)$, so that F can be expressed in the form

$$F(\mathcal{L},\mathcal{M})=\sum_{n\leqslant r+1}\alpha_n\left(\frac{\mathcal{M}}{(r+1)\mathcal{L}^r}\right)\mathcal{L}^n, \tag{14}$$

with $\alpha_n(t)$ being arbitrary smooth functions. Furthermore, Eq. (11) for $\mathcal{L}$ can be written as

$$\frac{\partial\mathcal{L}}{\partial s}=\frac{\partial F}{\partial\mathcal{M}}+\{F(\mathcal{L},\mathcal{M})_{\geqslant 0},\mathcal{L}\}, \tag{15}$$

and it is easy to see that only those terms in (14) with $n\geqslant 1$ contribute to $\partial u/\partial s$.

Therefore, we conclude that the symmetries of the $(r+1)$th truncated dKP hierarchy which do not involve higher dKP flows and define a nontrivial action on the coefficient u are of the form

$$F(\mathcal{L},\mathcal{M})=\sum_{n=1}^{r+1}\alpha_n\left(\frac{\mathcal{M}}{(r+1)\mathcal{L}^r}\right)\mathcal{L}^n. \tag{16}$$

This means that, under these conditions, there are essentially $r+1$ types of symmetry generators of the $(r+1)$th truncated dKP hierarchy given by

$$F_i(\mathcal{L},\mathcal{M}):=\alpha\left(\frac{\mathcal{M}}{(r+1)\mathcal{L}^r}\right)\mathcal{L}^i,\quad i=1,\ldots,r+1, \tag{17}$$

with $\alpha=\alpha(t)$ being an arbitrary function.

The action of the one-parameter groups generated by F_i on the coefficient u can be explicitly found. Indeed, by identifying the coefficients of $1/p$ in both members of (15) one gets a first-order *linear* partial differential equation for

$$u(s,\mathbf{t}):=\exp(s\{F_i,\cdot\})u(\mathbf{t}),$$

the integration of which provides the symmetry transformation

$$u=u(\mathbf{t})\mapsto\tilde{u}=u(s,\mathbf{t}).$$

Let us illustrate these facts by considering the case $r=2$. We observe that (13) implies that near points t in the region of analyticity of α

$$\alpha\left(\frac{\mathcal{M}}{3\mathcal{L}^2}\right)=\alpha(t)+\frac{2}{3}y\alpha'(t)\frac{1}{\mathcal{L}}+\left(\frac{1}{3}x\alpha'(t)+\frac{2}{9}y^2\alpha''(t)\right)\frac{1}{\mathcal{L}^2}+\mathcal{O}\left(\frac{1}{\mathcal{L}^3}\right). \tag{18}$$

One finds the following results for the corresponding three generators (17):

(1) F_1

From (15) we have

$$\frac{\partial\mathcal{L}}{\partial s}=\alpha'\left(\frac{\mathcal{M}}{3\mathcal{L}^2}\right)\frac{1}{3\mathcal{L}}+\alpha(t)\frac{\partial\mathcal{L}}{\partial x},$$

so that

$$\frac{\partial u}{\partial s}=\alpha(t)\frac{\partial u}{\partial x}+\frac{1}{3}\alpha'(t). \tag{19}$$

The solution of this equation is

$$u=U(x+s\alpha(t),y,t)+\tfrac{1}{3}s\alpha'(t),$$

where U is an arbitrary function. It leads to the symmetry

$$\tilde{u}=u(x+s\alpha(t),y,t)+\tfrac{1}{3}s\alpha'(t). \tag{20}$$

(2) F_2

In this case (15) becomes

$$\frac{\partial\mathcal{L}}{\partial s}=\frac{1}{3}\alpha'\left(\frac{\mathcal{M}}{3\mathcal{L}^2}\right)+\frac{2}{3}y\alpha'(t)\frac{\partial\mathcal{L}}{\partial x}+\alpha(t)\frac{\partial\mathcal{L}}{\partial y},$$

and the equation for u is

$$\frac{\partial u}{\partial s}=\frac{2}{3}y\alpha'(t)\frac{\partial u}{\partial x}+\alpha(t)\frac{\partial u}{\partial y}+\frac{2}{9}y\alpha''(t), \tag{21}$$

which has the solution

$$u=U(x+\tfrac{2}{3}sy\alpha'(t)+\tfrac{1}{3}s^2\alpha(t)\alpha'(t),y+s\alpha(t),t)+\tfrac{2}{9}sy\alpha''(t)+\tfrac{1}{9}s^2\alpha(t)\alpha''(t),$$

where U is an arbitrary function. The corresponding symmetry transformation of the dKP equation is

$$\tilde{u}=u(x+\tfrac{2}{3}sy\alpha'(t)+\tfrac{1}{3}s^2\alpha(t)\alpha'(t),y+s\alpha(t),t)+\tfrac{2}{9}sy\alpha''(t)+\tfrac{1}{9}s^2\alpha(t)\alpha''(t). \tag{22}$$

(3) F_3

Now Eq. (15) takes the form

$$\frac{\partial\mathcal{L}}{\partial s}=\frac{1}{3}\alpha'\left(\frac{\mathcal{M}}{3\mathcal{L}^2}\right)\mathcal{L}+\left(\frac{1}{3}x\alpha'(t)+\frac{2}{9}y^2\alpha''(t)\right)\frac{\partial\mathcal{L}}{\partial x}+\frac{2}{3}y\alpha'(t)\frac{\partial\mathcal{L}}{\partial y}+\alpha(t)\frac{\partial\mathcal{L}}{\partial t},$$

which implies

$$\frac{\partial u}{\partial s}=\left(\frac{1}{3}x\alpha'(t)+\frac{2}{9}y^2\alpha''(t)\right)\frac{\partial u}{\partial x}+\frac{2}{3}y\alpha'(t)\frac{\partial u}{\partial y}+\alpha(t)\frac{\partial u}{\partial t}+\frac{1}{3}\alpha'(t)u+\frac{1}{9}x\alpha''(t)+\frac{2}{27}y^2\alpha'''(t). \tag{23}$$

The solution of this equation is

$$u=(c'(t))^{2/3}U\left(x(c'(t))^{1/3}+\frac{2}{9}y^2\frac{c''(t)}{(c'(t))^{2/3}},y(c'(t))^{2/3},s+c(t)\right)$$
$$+\frac{1}{9}x\frac{c''(t)}{c'(t)}+\frac{2}{27}y^2\left(\frac{c'''(t)}{c'(t)}-\frac{4}{3}\left(\frac{c''(t)}{c'(t)}\right)^2\right),$$

where U is an arbitrary function and $c(t)$ is such that $c'(t)=1/\alpha(t)$. Hence, by defining $T:=T(s,t)$ through the implicit relation

$$c(T)=s+c(t),$$

and by taking into account that

$$T':=\frac{\partial T}{\partial t}=\frac{c'(t)}{c'(T)},$$

one finds that the symmetry transformation determined by (23) is

$$\tilde{u}=(T')^{2/3}u\left(x(T')^{1/3}+\frac{2}{9}y^2\frac{T''}{(T')^{2/3}},y(T')^{2/3},T\right)+\frac{1}{9}x\frac{T''}{T'}+\frac{2}{27}y^2\left(\frac{T'''}{T'}-\frac{4}{3}\left(\frac{T''}{T'}\right)^2\right). \tag{24}$$

The three symmetries (20), (22), and (24) coincide with the symmetries of the dKP equation found by Dunajski, Mason, and Tod.[19] by analyzing equivalence transformations of Einstein–Weyl spaces.

1. Transformation law of twistor data

According to (10) the dKP symmetry generated by (17) corresponds to a canonical transformation law of the twistor data determined by the Hamiltonian system

$$\frac{\mathrm{d}p}{\mathrm{d}s}=\{\alpha(\rho)p^i,p\},\quad \frac{\mathrm{d}x}{\mathrm{d}s}=\{\alpha(\rho)p^i,x\},\tag{25}$$

where we are denoting

$$\rho:=\frac{x}{(r+1)p^r}.$$

In terms of (p,ρ) this system becomes

$$\frac{\mathrm{d}p}{\mathrm{d}s}=-\frac{\alpha'(\rho)}{r+1}p^{i-r},\quad \frac{\mathrm{d}\rho}{\mathrm{d}s}=i\frac{\alpha(\rho)}{r+1}p^{i-r-1},\tag{26}$$

and by taking into account that the Hamiltonian function

$$h:=\alpha(\rho)p^i$$

is a constant of the motion it follows that the solution of (25) can be written as

$$p(s)=\frac{p}{(j_\rho)^{1/(r+1)}},\quad x(s)=(r+1)j\,p(s)^r.\tag{27}$$

Here $j=j(s,\rho,h)$ is the evolution law of the variable ρ. That is to say, it is the solution of the initial value problem

$$\frac{\partial j}{\partial s}=\beta(\rho,h),\quad j(0,\rho,h)=\rho,\tag{28}$$

where

$$\beta(\rho,h):=\frac{i}{r+1}\left(\frac{\alpha(\rho)}{h}\right)^{(r+1)/i}h.$$

The expressions (27) define the action of the additional symmetries (17) on the twistor data. It is important to observe that the solution of (28) satisfies

$$s=\int_\rho^{j(s,\rho,h)}\frac{\mathrm{d}\rho}{\beta(\rho,h)},$$

and, as a consequence, one deduces that the first-order derivatives of j with respect to ρ and h are

$$\begin{aligned} j_\rho&=\left(\frac{\alpha(j)}{\alpha(\rho)}\right)^{(r+1)/i},\\ j_h&=s\left(\frac{i}{r+1}-1\right)\left(\frac{\alpha(j)}{h}\right)^{(r+1)/i}=\left(\frac{i}{r+1}-1\right)\frac{s}{p(s)^{r+1}}. \end{aligned}\tag{29}$$

As we will see below, these relations will be useful for determining the action of the additional symmetries on the solutions of the twistor equations.

III. SOLUTIONS OF THE dKP HIERARCHY

A. Generating functions and hodograph equations

We are going to present a scheme for solving twistor equations which is particularly suitable to investigate the action of the additional symmetries introduced in the above section. An ingre-

dient of our analysis is the use of a type of generating functions for canonical transformations of twistor data,[20] which allows us to introduce hodograph type equations to formulate part of the constraints imposed by the twistor equations.

Let $(P(p,x),X(p,x))$ be a pair of canonically conjugate variables. Then for each positive integer r we have

$$\mathrm{d}P\wedge\mathrm{d}X=\mathrm{d}p\wedge\mathrm{d}x=\mathrm{d}(p^{r+1})\wedge\mathrm{d}\rho,\quad \rho:=\frac{x}{(r+1)p^r}.$$

Hence there exists an associated generating function $J_r:=J_r(P,\rho)$ of the canonical transformation $(p,x)\mapsto(P,X)$ such that

$$\mathrm{d}J_r=p^{r+1}\mathrm{d}\rho+X\mathrm{d}P,$$

or equivalently

$$p^{r+1}=\frac{\partial J_r(P,\rho)}{\partial\rho},\quad X=\frac{\partial J_r(P,\rho)}{\partial P}. \tag{30}$$

In this way by denoting

$$\mathcal{M}_r:=\frac{\mathcal{M}}{(r+1)\mathcal{L}^r},$$

we deduce

$$\frac{\partial}{\partial p}J_r(P(\mathcal{L},\mathcal{M}),\mathcal{M}_r)=\frac{\partial J_r}{\partial P}(P(\mathcal{L},\mathcal{M}),\mathcal{M}_r)\frac{\partial P(\mathcal{L},\mathcal{M})}{\partial p}+\frac{\partial J_r}{\partial\rho}(P(\mathcal{L},\mathcal{M}),\mathcal{M}_r)\frac{\partial\mathcal{M}_r}{\partial p}$$

$$=X(\mathcal{L},\mathcal{M})\frac{\partial P(\mathcal{L},\mathcal{M})}{\partial p}+\mathcal{L}^{r+1}\frac{\partial\mathcal{M}_r}{\partial p},$$

and by taking into account that

$$\mathcal{L}^{r+1}\frac{\partial\mathcal{M}_r}{\partial p}=\frac{1}{r+1}\frac{\partial(\mathcal{L}\mathcal{M})}{\partial p}-\frac{\partial S}{\partial p},$$

where S is the function introduced in (7), we deduce that

$$X(\mathcal{L},\mathcal{M})=\frac{(\partial/\partial p)\,(S+J_r(P(\mathcal{L},\mathcal{M}),\mathcal{M}_r)-[1/(r+1)]\mathcal{L}\mathcal{M})}{(\partial/\partial p)\,P(\mathcal{L},\mathcal{M})}. \tag{31}$$

This formula enables us to state the following:

Theorem 3: *In terms of the function*

$$\mathcal{S}_r:=S+J_r(P(\mathcal{L},\mathcal{M}),\mathcal{M}_r)-\frac{1}{r+1}\mathcal{L}\mathcal{M}, \tag{32}$$

the second twistor equation $(X(\mathcal{L},\mathcal{M}))_{\leqslant -1}=0$ *is equivalent to the following two conditions*

(1) The expansion of $\mathcal{S}_r$ *in powers of* p *satisfies*

$$(\mathcal{S}_r)_{\leqslant -1}=0. \tag{33}$$

(2) At each zero p_i *of* $\partial P(\mathcal{L},\mathcal{M})/\partial p$ *it is verified that*

$$\frac{\partial \mathcal{S}_r}{\partial p}(p_i,\mathbf{t})=0. \tag{34}$$

Henceforth we will refer to (34) as the *hodograph equations*.

A natural problem is to determine generating functions $J_r(P,\rho)$ leading to solvable twistor equations. In this sense, an important class arises when $P=P(p,x)$ is independent of x and has a finite-order expansion as $p\to\infty$:

$$P(p)=\sum_{n=-\infty}^{N} a_n p^n.$$

The corresponding generating function J_0 is of the form

$$J_0(P,x)=f(P)+g(P)x,$$

where $g(P)$ is the inverse function of $P=P(p)$. As a consequence

$$J_0(P(\mathcal{L},\mathcal{M}),\mathcal{M})=f(P(\mathcal{L}))+\mathcal{L}\mathcal{M},$$

$$\mathcal{S}_0=S+f(P(\mathcal{L})).$$

It can be shown that, provided $f(P(p))$ admits a Laurent expansion as $p\to\infty$, the twistor equations determined by J_0 have a solution. Moreover, it turns out that solving the hodograph equations for $\mathcal{S}_0$ is enough for computing $\mathcal{L}$. Let us illustrate these facts with the following important example

Gelfand–Dikii reductions: If we set

$$J_0(P,x)=f(P^{1/m})+P^{1/m}x, \quad f(P^{1/m}):=\sum_{n=-\infty}^{\infty} c_n P^{n/m}, \tag{35}$$

for a given integer $m>1$, the associated twistor data are

$$P=p^m, \quad X=\frac{1}{mp^{m-1}}(f'(p)+x). \tag{36}$$

Then, the first twistor equation is

$$\mathcal{L}^m=(\mathcal{L})_{\geqslant 0},$$

so that

$$\mathcal{L}^m=p^m+q_{m-2}(\mathbf{u})p^{m-2}+\cdots+q_1(\mathbf{u})p+q_0(\mathbf{u}), \tag{37}$$

where the functions $q_i(\mathbf{u})$ depend on the $(m-1)$ first coefficients $\mathbf{u}:=(u_1,\ldots,u_{m-1})$ of the expansion (1) of $\mathcal{L}$. This constraint defines the mth Gelfand–Dikii reduction of the dKP hierarchy.

For example the first few reductions are

$$m=2, \quad \mathcal{L}^2=p^2+2u_1,$$

$$m=3, \quad \mathcal{L}^3=p^3+3u_1p+3u_2,$$

$$m=4, \quad \mathcal{L}^4=p^4+4u_1p^2+4u_2p+6u_1^2+4u_3.$$

To determine $\mathcal{L}$ we must find the $(m-1)$ unknowns u_i as functions of $\mathbf{t}$ through the second twistor equation. Thus, according to Theorem 2, we impose

$$\mathcal{S}_0 = S + f(\mathcal{L}) = (S + f(\mathcal{L}))_{\geqslant 0} = \sum_{n\geqslant 1} (t_n + c_n)(\mathcal{L}^n)_{n\geqslant 0} + c_0 .$$

Hence, by using (37) we can express $\mathcal{S}_0$ as a function of $(p,\mathbf{t},\mathbf{u})$. If we now impose the hodograph equations (34), we get $(m-1)$ implicit equations

$$\left(\sum_{n\geqslant 1} (t_n + c_n) \frac{\partial}{\partial p} (\mathcal{L}^n)_{n\geqslant 0} \right) \Bigg|_{p=p_i(\mathbf{u})} = 0, \quad i = 1,\ldots,m-1, \tag{38}$$

which determine the functions $u_i(\mathbf{t})$ and, consequently, $\mathcal{L}$. Furthermore, by eliminating p in (37) we can express p as a function $p = p(\mathcal{L},\mathbf{t})$, which under substitution into

$$S = \sum_{n\geqslant 1} t_n \mathcal{L}^n - \left(\sum_{n\geqslant 1} t_n \mathcal{L}^n - f(\mathcal{L}) \right)_{\leqslant -1},$$

leads to $\mathcal{M} = \partial S/\partial \mathcal{L}$. Thus, it is easy to see that the functions $\mathcal{L}$ and $\mathcal{M}$ are solutions of the twistor equations which satisfy (1) and, therefore, they solve the dKP hierarchy Henceforth these solutions will be called *Gelfand–Dikii solutions* of the dKP hierarchy.

For instance, if $m = 2$ (dKdV reduction),

$$\mathcal{L}^2 = p^2 + 2u, \quad u := u_1,$$

and we set $t_n = 0$, $\forall n > 3$, one gets the hodograph relation

$$3ut + x = F(u), \tag{39}$$

which solves the dKdV equation $u_t = 3uu_x$. Here

$$F(u) := - = \frac{\partial}{\partial p} \sum_{n\geqslant 1} c_n \cdot (\mathcal{L}^n)_{n\geqslant 0}\big|_{p=0}$$

can be assumed to be an arbitrary smooth function of u. Some elementary solutions provided by (39) are

$$F(u) = cu, \quad u = -\frac{x}{3t-c},$$

$$F(u) = cu^2, \ \ u = \frac{1}{2c}(3t + \sqrt{9t^2 + 4cx}), \tag{40}$$

$$F(u) = cu^3, \ \ u = \frac{f}{2c} + \frac{2t}{f}, \ \ f := \left(4x + 4c^2 \sqrt{x^2 - \frac{4t^3}{c}} \right)^{1/3}.$$

B. The action of additional symmetries on Gelfand–Dikii solutions

Our aim now is to characterize solutions of the dKP hierarchy by applying the symmetry transformations (17) to Gelfand–Dikii solutions. Obviously we may start from solutions of the hodograph equations (38) and then perform the corresponding symmetry transformation. However, in order to do it we need to know how the coefficients u_i of the expansion (1) of $\mathcal{L}$ transform under the symmetries (17), which requires us to solve a system of first-order linear partial differential equations. We are trying instead an alternative way consisting in determining the generating

functions $J_r(P,\rho)$ for the transformed twistor data and then solving the corresponding twistor equations according to the scheme of Theorem 3. In this alternative procedure the problem reduces to solving a system of implicit algebraic equations.

The dKP symmetry generated by (17) acts on twistor data according to the canonical transformation (27). In particular, the twistor data (36) for the Gelfand–Dikii reductions transform as

$$P(s)=\left(\frac{p}{(j_\rho)^{1/(r+1)}}\right)^m,$$
$$X(s)=\frac{P^{(m-1)/m}}{m}(f'(P^{1/m})+(r+1)j\,P^{r/m}). \tag{41}$$

Hence, by taking into account that j is a function of (s,ρ,h), it follows that

$$p^{r+1}=j_\rho P^{(r+1)/m}=\frac{\partial}{\partial\rho}(jP^{(r+1)/m})-\hat{h}_\rho j_h P^{(r+1)/m},$$

$$X=\frac{\partial}{\partial P}(f(P)^{1/m}+jP^{(r+1)/m})-\hat{h}_P j_h P^{(r+1)/m},$$

where

$$\hat{h}=\hat{h}(P,\rho):=h(p(P,\rho),\rho)=\alpha(\rho)p(P,\rho)^i.$$

By using now (29) we deduce

$$p^{r+1}=\frac{\partial J_r^{(i)}(P,\rho)}{\partial\rho},\quad X=\frac{\partial J_r^{(i)}(P,\rho)}{\partial P}, \tag{42}$$

where

$$J_r^{(i)}(s,P,\rho):=f(P^{1/m})+j(s,\rho,\hat{h})P^{(r+1)/m}+s\left(1-\frac{i}{r+1}\right)\hat{h}(P,\rho). \tag{43}$$

Wide families of solutions of the $(r+1)$th truncated dKP can be found by solving the twistor equations associated with the generating functions (43). The calculations are simple but long and require computer aid. To illustrate the strategy for computing these solutions let us consider the family of generating functions $J_r^{(i)}$ with

$$i=r+1\geqslant m. \tag{44}$$

The choice $i=r+1$ means that we are dealing with the orbits of Gelfand–Dikii solutions under the action of the symmetry generator

$$F_{r+1}(\mathcal{L},\mathcal{M}):=\alpha\left(\frac{\mathcal{M}}{(r+1)\mathcal{L}^r}\right)\mathcal{L}^{r+1}. \tag{45}$$

Thus, according to (29) the function j in (43) is determined from α through the solution of the initial value problem

$$\frac{\partial j}{\partial s}=\alpha(\rho),\quad j(0,\rho)=\rho. \tag{46}$$

Hence j is independent of h and by setting s to be a constant, we may take j as a function of ρ only. Therefore, the generating functions $J_r^{(i)}$ that we are considering are

$$J_r(P,\rho)=f\left(P^{1/m}\right)+j(\rho)\,P^{(r+1)/m}. \tag{47}$$

Notice that

$$P=\frac{p^m}{(j_\rho)^{m/(r+1)}}, \tag{48}$$

so that the first twistor equation reads

$$\mathbb{L}^m=(\mathbb{L}^m)_{\geqslant 0}, \tag{49}$$

where

$$\mathbb{L}:=\frac{\mathcal{L}}{j_\rho(\mathcal{M}_r)}, \quad \mathcal{M}_r:=\frac{\mathcal{M}}{(r+1)\mathcal{L}^r}. \tag{50}$$

From (1) one deduces at once that the integer powers of $\mathcal{L}$ have expansions of the form

$$\begin{aligned}\mathcal{L}^N&=p^N+\cdots+a_n(u_1,\ldots,u_{N-n-1})p^n+\cdots+b_n(u_1,\ldots,u_{N+n-1})\frac{1}{p^n}+\cdots,\\ \frac{1}{\mathcal{L}^N}&=\frac{1}{p^N}+\cdots+c_n(u_1,\ldots,u_{n-N-1})\frac{1}{p^n}+\cdots.\end{aligned} \tag{51}$$

Furthermore, (1) implies that for any smooth function $g=g(t)$ the composite function $g(\mathcal{M}_r)$ can be expanded in the form

$$\begin{aligned}g(\mathcal{M}_r)&=g\left(t_{r+1}+\frac{rt_r}{r+1}\frac{1}{\mathcal{L}}+\cdots+\frac{v_n(\mathbf{t})}{r+1}\frac{1}{\mathcal{L}^n}+\cdots\right)\\ &=g(t_{r+1})+\frac{rt_r}{r+1}g'(t_{r+1})\frac{1}{p}+\cdots+d_n(\mathbf{t},u_1,\ldots,u_{n-2},v_1,\ldots,v_{n-r-1})\frac{1}{p^n}+\cdots.\end{aligned} \tag{52}$$

Thus, from (51) and (52) and by taking into account (44), we deduce that $\mathbb{L}$ is of the form

$$\mathbb{L}=(q_m(\mathbf{t},\mathbf{u})p^m+\cdots+q_1(\mathbf{t},\mathbf{u})p+q_0(\mathbf{t},\mathbf{u}))^{1/m}, \tag{53}$$

where $\mathbf{u}:=(u_1,\ldots,u_{m-1})$.

Two different cases arise.

(1) $\mathbf{r}=\mathbf{m}-1,\mathbf{m}$. This is the simplest situation since from (51)–(53) it follows at once that

$$\mathcal{S}_r=\left(\sum_{s=1}^{r}\frac{r-s+1}{r+1}t_s\mathcal{L}^s+\gamma\mathbb{L}^{m+n}+j(\mathcal{M}_r)\mathbb{L}^{r+1}\right)_{\geqslant 0}$$

is a function depending of $(p,\mathbf{t})$ and $\mathbf{u}=(u_1,\ldots,u_{m-1})$. Therefore, the $(m-1)$ hodograph equations

$$\frac{\partial\mathcal{S}_r}{\partial p}(p_i,\mathbf{t})=0, \tag{54}$$

where $p_i=p_i(\mathbf{t},\mathbf{u})$ are the zeros of $\partial\mathbb{L}^m/\partial p$, are enough for determining $\mathbf{u}$.

(2) $\mathbf{r}\geqslant\mathbf{m}+\mathbf{1}$. The function $\mathcal{S}_r=(\mathcal{S}_r)_{\geqslant 0}$ depends on $(p,\mathbf{t})$ and $\tilde{\mathbf{u}}=(u_1,\ldots,u_{r-1})$, so that in addition to the $(m-1)$ hodograph equations (54) a set of $(r-m)$ new equations involving $\mathbf{t}$ and $\tilde{\mathbf{u}}$ are required. These additional equations are supplied by vanishing the coefficients of the negative powers $1/p^n$ $(n=1,\ldots,r-m)$ in

$$(\mathbb{L}^m)_{\leqslant -1}=0.$$

C. Examples

In the following examples we exhibit solutions u of the dKP equation (4) depending on an arbitrary function $j=j(\rho)$. They are orbits of Gelfand–Dikii solutions u_0 under the action of the symmetry generated by (45). Notice that according to (45)–(46) we can obtain u_0 by setting $j=\rho$ in the expression of u.

(1) For

$$r=m=2, \quad f(P^{1/2}):=\gamma P^{7/2},$$

the generating function (47) becomes

$$J_2(P,\rho)=\gamma P^{7/2}+j(\rho)P^{3/2}, \quad \rho:=\frac{x}{3p^2}, \tag{55}$$

and $\mathbb{L}^2$ takes the form

$$\begin{aligned}\mathbb{L}^2&=(\mathbb{L}^2)_{\geqslant 0}\\ &=\frac{p^2}{(j'(t))^{2/3}}-\frac{4}{9}\frac{yj''(t)}{(j'(t))^{5/3}}p+\frac{2u_1}{(j'(t))^{2/3}}-\frac{2}{9}\frac{xj''(t)}{(j'(t))^{5/3}}-\frac{4}{27}\frac{y^2j'''(t)}{(j'(t))^{5/3}}+\frac{20}{81}\frac{y^2(j''(t))^2}{(j'(t))^{8/3}}.\end{aligned} \tag{56}$$

Hence $\partial\mathbb{L}^2/\partial p$ has a unique zero given by

$$p_1=\frac{2}{9}y\frac{j''(t)}{j'(t)}.$$

Moreover, the expression of

$$\mathcal{S}_2=(\tfrac{1}{3}y\mathcal{L}^2+\tfrac{2}{3}x\mathcal{L}+\gamma\mathbb{L}^7+j(\mathcal{M}_2)\mathbb{L}^3)_{\geqslant 0}$$

as a function of p can be computed by using (57) and the expansion

$$\begin{aligned}j(\mathcal{M}_2)=j(t)+\frac{2}{3}yj'(t)\frac{1}{p}+\left(\frac{x}{3}j'(t)+\frac{2}{9}y^2j''(t)\right)\frac{1}{p^2}\\ +\left(-\frac{2}{3}yj'(t)u_1+\frac{4}{81}y^3j'''(t)+\frac{2}{9}xyj''(t)\right)\frac{1}{p^3}+\mathcal{O}\left(\frac{1}{p^4}\right).\end{aligned}$$

In this way the hodograph equation $(\partial\mathcal{S}_2/\partial p)|_{p=p_1}=0$ turns out to be an equation for $u=u_1$, which yields the following solution of the dKP equation

$$u=\frac{F}{105\gamma}-\frac{6j(t)j'(t)^{4/3}}{F}+\frac{9j'(t)j''(t)x+6j'(t)j'''(t)y^2-8j''(t)^2y^2}{81(j'(t))^2}, \tag{57}$$

where

$$F:=\gamma^{2/3}(-7350j'(t)^{4/3}j''(t)y^2-33075j'(t)^{7/3}x+105\sqrt{35\,G})^{1/3},$$

$$G:=\frac{1}{\gamma}(648j(t)^3j'(t)^4+140\gamma j'(t)^{8/3}j''(t)^2y^4+1260\gamma j'(t)^{11/3}j''(t)xy^2+2835\gamma j'(t)^{14/3}x^2).$$

(2) By setting

$$r=m=3,\quad f(P^{1/3}):=\gamma P^{7/3},$$

in (47) one finds that the first two coefficients of the expansion (1) of $\mathcal{L}$ are given by

$$u=u_1=-\frac{1}{1024\,j_1^2}(90\,j_2^2t^2-72\,j_1j_3t^2-128\,j_1j_2y+Z^2), \tag{58}$$

$$u_2=\frac{-21\,\gamma j_1^8j_2t\,Z^4+F\,Z^2+8388608\,j_1^{59/4}y+2359296\,j_1^{55/4}j_2t^2}{114688\,\gamma j_1^{11}Z}, \tag{59}$$

where

$$j_i:=\frac{\partial^i j}{\partial\rho^i}(t_4),\quad i\geqslant 0,$$

$$F:=-16384\,j_0j_1^{47/4}+7168\,\gamma j_1^{10}j_2x-13440\,\gamma j_1^9j_2^2ty+5670\,\gamma j_1^8j_2^3t^3$$
$$+2016\,\gamma j_1^{10}j_4t^3-7560\,\gamma j_1^9j_2j_3t^3+10752\,\gamma j_1^{10}j_3ty,$$

and $Z=Z(x,y,t,t_4)$ is a root of the equation

$$49\,j_1^{30}\gamma^2Z^{10}+(5\,637\,144\,576\,\gamma j_1^{151/4}x+2\,113\,929\,216\,\gamma j_1^{147/4}j_2\,ty-1\,610\,612\,736\,j_0^2j_1^{75/2}$$
$$+396\,361\,728\,\gamma j_1^{147/4}j_3t^3-297\,271\,296\,\gamma\,j_1^{143/4}j_2^2t^3)Z^4+422\,212\,465\,065\,984\,j_1^{87/2}y^2$$
$$+33\,397\,665\,693\,696\,j_1^{83/2}j_2^2t^4+237\,494\,511\,599\,616\,j_1^{85/2}j_2t^2y=0.$$

ACKNOWLEDGMENTS

The authors are grateful to Professor F. Guil for showing them the relevance of generating functions for canonical transformations of twistor data to get solutions of the dKP hierarchy. This work was partially supported by CICYT Project No. BFM2002-01607.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Extended resolvent and inverse scattering with an application to KPI

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(Received 10 January 2003; accepted 9 April 2003)

We present in detail an extended resolvent approach for investigating linear problems associated to $2+1$ dimensional integrable equations. Our presentation is based as an example on the nonstationary Schrödinger equation with potential being a perturbation of the one-soliton potential by means of a decaying two-dimensional function. Modification of the inverse scattering theory as well as properties of the Jost solutions and spectral data as follows from the resolvent approach are given. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1587874]

I. INTRODUCTION

The extended resolvent approach to the study of the spectral theory of differential operators was developed in Refs. 1–8 as a method that from one side unifies all known approaches of the inverse scattering theory, such as dressing transformation, nonlocal Riemann–Hilbert problem, d-bar method and, from the other side, enables considering operators of more generic type, say, with nontrivial asymptotic behavior at space infinity. Our presentation is based on the study of the well known differential operator

$$\mathcal{L}(x,\partial_x)=i\partial_{x_2}+\partial_{x_1}^2-u(x),\quad x=(x_1,x_2), \tag{1.1}$$

i.e., the nonstationary Schrödinger equation $\mathcal{L}(x,\partial_x)\Phi(x,k)=0$ which is the linear problem associated to the Kadomtsev–Petviashvili I equation (KPI):[9]

$$(u_t-6uu_{x_1}+u_{x_1x_1x_1})_{x_1}=3u_{x_2x_2}. \tag{1.2}$$

This equation has been known to be integrable for about three decades.[10,11] The Cauchy problem for this equation with rapidly decaying initial data was studied by using the inverse scattering method in Refs. 12–15. At the same time, it is well known that (1.2) is a $(2+1)$-dimensional generalization of the famous Korteweg–de Vries (KdV) equation. Indeed, if $u_1(t,x_1)$ obeys KdV, then

$$u(t,x_1,x_2)=u_1(t,x_1+\mu x_2+3\mu^2 t) \tag{1.3}$$

solves (1.2) for an arbitrary constant $\mu\in\mathbb{R}$. Thus, it is natural to consider solutions of (1.2) that are not decaying in all directions at space infinity but have one-dimensional rays with behavior of

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the type (1.3). The scattering theory for the simplest example of such potentials in (1.1) was developed in Ref. 16. There, the Cauchy problem for the KPI equation was considered with initial data

$$u(x)=u_1(x_1)+u_2(x), \tag{1.4}$$

where $u_1(x_1)$ is the zero time value of the one-soliton solution of the KdV equation and $u_2(x)$ is a smooth real function that decays rapidly enough on the (x_1,x_2)-plane. We consider here a simplified case of (1.3) in which $\mu=0$. The generic case is reconstructed by means of the Galileo invariance of (1.2), that is, if $u(t,x)$ is a solution of KPI, then

$$\tilde{u}(t,x_1,x_2)=u(t,x_1+\mu x_2+3\mu^2 t,x_2+6\mu t) \tag{1.5}$$

also obeys this equation.

In Ref. 1 it was mentioned that the standard approach to the spectral theory of the operator (1.1) based on the integral equation for the Jost solution fails for potentials of the above type. In Ref. 16 the direct problem was studied by using a modified integral equation for the Jost solution, i.e., an equation that involves as background solution the Jost solution of the one-soliton potential and corresponding Green's function. An appropriate Jost solution was introduced and it was shown that, in addition to a standard jump across the real k-axis, where k is the spectral parameter, it also has a jump across a segment of the imaginary axis of the complex k-plane. In the modified formulation of the direct and inverse problems given in Ref. 16 some essential properties of the Jost solutions and relations between spectral data were stated without proof. The reason for this was that a technique based on the Jost solutions themselves is not enough for the study of these properties and especially for investigating relations among spectral data. This gap can be filled effectively in the framework of the extended resolvent approach that we present in detail in this article. The outline of the article is as follows. In Sec. II we give the basic notions of the resolvent approach. In particular, we demonstrate that in this framework the known results for a decaying potential in (1.1) follow readily. In Sec. III we consider the theory of the two-dimensional operator (1.1) with the pure one-dimensional $[u_2(x)\equiv 0$ in (1.4)] one-soliton potential $u_1(x_1)$. In Sec. IV we apply the resolvent approach to the operator (1.1) with a potential $u(x)$ that is a perturbation of this one-dimensional potential. We introduce and study the properties of the corresponding resolvent and Green's functions, Jost and auxiliary Jost solutions and advanced/retarded solutions. In Sec. IV E we investigate the properties of the spectral data and derive their characterization equations. In Sec. V we summarize the main aspects of the spectral theory developed in the framework of the extended resolvent approach.

II. BASIC OBJECTS OF THE RESOLVENT APPROACH

A. Extension of differential operators and resolvent

Let $\mathcal{A}=\mathcal{A}(x,\partial_x)$ denote a differential operator with kernel

$$A(x,x')=\mathcal{A}(x,\partial_x)\delta(x-x'), \quad x=(x_1,x_2), \tag{2.1}$$

$\delta(x)=\delta(x_1)\delta(x_2)$ being the two-dimensional δ-function. Here we consider the two-dimensional situation, but the whole procedure can be applied in any dimension. In what follows we consider differential operators whose kernels $A(x,x')$ belong to the space $\mathcal{S}'$ of tempered distributions of the four real variables x and x'. Differential operators are polynomials with respect to the derivatives. In order to exploit this property we introduce the **extension** of differential operators, i.e., to any differential operator $\mathcal{A}$ we associate the differential operator $A(s)$ with kernel

$$A(x,x';s)\equiv e^{-s(x-x')}A(x,x')=\mathcal{A}(x,\partial_x+s)\delta(x-x'), \tag{2.2}$$

where all variables x, x', $s\in\mathbb{R}^2$. Under the above condition kernels of the extended operators form a subclass in the space $\mathcal{S}'$ of tempered distributions $A(x,x';s)$ of six real variables. We

consider generic elements $A(x,x';s)$, $B(x,x';s)$, etc., of this space $\mathcal{S}'$ as operators (not necessarily differentiable) $A(s)$, $B(s)$, etc., with the standard composition rule

$$(AB)(x,x';s)=\int dx''\,A(x,x'';s)\,B(x'',x';s). \tag{2.3}$$

Since the kernels are distributions this composition is neither necessarily defined for all pairs of operators nor necessarily associative. On the space of these distributions we define the operation of Hermitian conjugation $A^\dagger$ as

$$A^\dagger(x,x';s)=\overline{A(x',x;-s)}, \tag{2.4}$$

where bar denotes complex conjugation and in the case of matrix operators the matrix on the r.h.s. must be transposed.

The kernels of the extended differential operators depend polynomially on the variables $s=(s_1,s_2)$ so that the analytic continuation of the kernels with respect to these variables is admissible. In what follows we denote such kernels as $A(x,x';\mathbf{s})$ using boldface font for the complex variable $\mathbf{s}$ which has s as real part. So, for the variable $\mathbf{s}$ we write

$$\mathbf{s}=\mathbf{s}_\Re+i\mathbf{s}_\Im=(\mathbf{s}_1,\mathbf{s}_2)\in\mathbb{C}^2,\quad \mathbf{s}_\Re\equiv s\in\mathbb{R}^2. \tag{2.5}$$

In the following we will use the same notation $\mathbf{k}=\mathbf{k}_\Re+i\mathbf{k}_\Im\equiv k+i\mathbf{k}_\Im$ for the other complex spectral parameter $\mathbf{k}\in\mathbb{C}$ we introduce.

Thanks to (2.2) continuation (2.5) (analytic for the differential operators) is given by

$$A(x,x';\mathbf{s})=e^{-i\mathbf{s}_\Im(x-x')}A(x,x';\mathbf{s}_\Re). \tag{2.6}$$

Since this formula is well defined in the space $\mathcal{S}'$ for any operator $A(s)$, it can be used as the definition of the continuation (in general not analytic) of a generic $A(s)$ in the complex domain, $\mathbf{s}\in\mathbb{C}^2$.

An operator A can have an inverse in the sense of the composition law (2.3), say $AA^{-1}=I$ or $A^{-1}A=I$ (in general left and right inverse can be different), where I is the unity operator in $\mathcal{S}'$,

$$I(x,x';s)=\delta(x-x'). \tag{2.7}$$

Thanks to (2.6) continuation to the complex domain of the operator inverse to (extended) differential operator $A(s)$ equals to the inverse of continued differential operator $A(\mathbf{s})$. Therefore, we can impose to the inverse the additional condition that the product

$$A(\mathbf{s}+\mathbf{s}')^{-1}A(\mathbf{s})^{-1},\quad \mathbf{s},\mathbf{s}'\in\mathbb{C}, \tag{2.8}$$

is a bounded function of $\mathbf{s}'$ in a neighborhood of $\mathbf{s}'=0$. Then, if the inversion $A^{-1}(s)$ exists, it is unique and, therefore, in the following in order to guarantee the uniqueness of the inverse we will always require that this condition is fulfilled.

In order to clarify the meaning of the introduced extension of differential operators it is convenient to consider the ''shifted'' Fourier transform

$$A(p;\mathbf{s})=\frac{1}{(2\pi)^2}\int dx\int dx'\,e^{i(p-\mathbf{s}_\Im)x+i\mathbf{s}_\Im x'}A(x,x';\mathbf{s}_\Re), \tag{2.9}$$

where $p\in\mathbb{R}^2$, $px=p_1x_1+p_2x_2$, and $\mathbf{s}\in\mathbb{C}^2$ and to consider it as the kernel of the operator $A(s)$ in the transformed p space. In this space the extension of a differential operator $\mathcal{A}$ with constant coefficients is particularly simple. Indeed, we have $A(p;\mathbf{s})=a(\mathbf{s})\delta(p)$, where $a(\mathbf{s})$ is a polynomial in $\mathbf{s}$. For the kernel of the inverse operator we get trivially $A^{-1}(p;\mathbf{s})=\delta(p)/a(\mathbf{s})$ and condition (2.8) means that possible terms proportional to $\delta(a(\mathbf{s}))$ must be omitted.

Let D_j denote the extension of the differential operator ∂_{x_j} $(j=1,2)$, i.e., according to (2.2) let

$$D_j(x,x';s)=(\partial_{x_j}+s_j)\,\delta(x-x'),\quad j=1,2. \tag{2.10}$$

In terms of the Fourier transform (2.9) $D_j(p;\mathbf{s})=\mathbf{s}_j\delta(p)$ and then $D_j^{-1}(p;\mathbf{s})=\mathbf{s}_j^{-1}\delta(p)$, so that inverting (2.9) we get

$$D_j^{-1}(x,x';s)=e^{-s(x-x')}[\,\theta(x_j-x_j')-\theta(-s_j)\,]\,\delta(x_{j+1}-x_{j+1}'), \tag{2.11}$$

where $j+1\equiv(j+1)\mathrm{mod}2$. These operators are just the standard resolvents of the operators ∂_{x_j}. This observation motivates the name extended resolvent for the mathematical object we introduced. In fact, we added a complex (spectral) parameter not to the operator itself but to the operators ∂_{x_j}. Below we discuss the relevance of this modification and compare our approach to the standard spectral theory of differential operators.

By (2.10) we have that $D_j(x,x';\mathbf{s})=(\partial_{x_j}+\mathbf{s}_j)\,\delta(x-x')$ that is, of course, an analytic (polynomial) function of $\mathbf{s}$. But for the continuation of the inverse operator we get by (2.11) and (2.6)

$$D_j^{-1}(x,x';\mathbf{s})=e^{-\mathbf{s}(x-x')}[\,\theta(x_j-x_j')-\theta(-\mathbf{s}_{j\Re})\,]\,\delta(x_{j+1}-x_{j+1}'), \tag{2.12}$$

that is not analytic with respect to $\mathbf{s}_j$. Moreover, let us perform the operation inverse to imbedding (2.2), i.e., to any operator $A(s)$ with kernel $A(x,x';s)$ we associate its "hat-kernel"

$$\hat{A}(x,x';s)=e^{s(x-x')}A(x,x';s). \tag{2.13}$$

It is clear that these objects (in the generic case) do not belong to the space $\mathcal{S}'(\mathbb{R}^6)$ of distributions, while we still can use their composition relation

$$\widehat{(AB)}(x,x';s)=\int dx''\,\hat{A}(x,x'';s)\,\hat{B}(x'',x';s) \tag{2.14}$$

derived from (2.3). Let now $A(s)$ be the extension of a differential operator $\mathcal{A}$. Then of course $\hat{A}(x,x';s)=A(x,x')$, i.e., the kernel of the original differential operator. In particular this means that $\hat{A}(x,x';s)$ is independent of the variables s. At the same time, as demonstrated by example (2.11), for an operator inverse to a differential operator, the dependence on s of the kernel $\widehat{A^{-1}}(x,x';s)$ is in general nontrivial, for instance,

$$\widehat{D_j^{-1}}(x,x';s)=[\,\theta(x_j-x_j')-\theta(-s_j)\,]\,\delta(x_{j+1}-x_{j+1}'). \tag{2.15}$$

Using the "hat-operation," for any differential operator $\mathcal{A}(x,\partial_x)$, equalities $AA^{-1}=A^{-1}A=I$ take the form

$$\mathcal{A}(x,\partial_x)\widehat{A^{-1}}(x,x';s)=\mathcal{A}^{\mathrm{d}}(x',\partial_{x'})\widehat{A^{-1}}(x,x';s)=\delta(x-x'), \tag{2.16}$$

where $\mathcal{A}^{\mathrm{d}}$ is the operator dual to $\mathcal{A}$. Thus the hat-kernel (2.13) of the operator inverse to an extended differential operator gives a two-parametric ($s\in\mathbb{R}^2$) family of Green's functions of the operator $\mathcal{A}$. In what follows for equalities of the type (2.16) we use the following special notation,

$$\vec{\mathcal{A}}\,\widehat{A^{-1}}(s)=\widehat{A^{-1}}(s)\tilde{\mathcal{A}}=I, \tag{2.17}$$

where $\vec{\mathcal{A}}$ denotes the operator $\mathcal{A}$ applied to the x-variable of the function $\widehat{A^{-1}}(x,x';s)$ and $\tilde{\mathcal{A}}$ denotes the operator dual to $\mathcal{A}$ applied to the x'-variable of the same kernel. We also see that any discontinuity of the kernel $\widehat{A^{-1}}(x,x';s)$ with respect to the s-variables belongs to the null space of

the operator $\mathcal{A}$ and its dual. The same is valid for the derivatives of such kernels with respect to the s-variables. Let us mention that for kernels continued by means of (2.6) we have by (2.13) the relation

$$A(x,x';\mathbf{s})=e^{-\mathbf{s}(x-x')}\hat{A}(x,x';\mathbf{s}_{\mathfrak{R}}), \tag{2.18}$$

and for the inversion $A^{-1}(\mathbf{s})$ of a differential operator $A(\mathbf{s})$

$$A(\mathbf{s})\frac{\partial A^{-1}(\mathbf{s})}{\partial\overline{\mathbf{s}}_j}=\frac{\partial A^{-1}(\mathbf{s})}{\partial\overline{\mathbf{s}}_j}A(\mathbf{s})=0. \tag{2.19}$$

Thus the d-bar derivatives of the inverse operator also annulate the differential operator and its dual, while by (2.13)

$$\left(\frac{\partial A^{-1}(\mathbf{s})}{\partial\overline{\mathbf{s}}_j}\right)\widehat{\ }\Big|_{\mathbf{s}_{\mathfrak{I}}=0}=\frac{1}{2}\frac{\partial\widehat{A^{-1}}(s)}{\partial s_j},\quad s=\mathbf{s}_{\mathfrak{R}}, \tag{2.20}$$

where both derivatives are considered in the sense of distributions.

B. Resolvent approach in the case of rapidly decaying potential

1. Definition of the resolvent

The extension of operator $\mathcal{L}(x,\partial_x)$ in (1.1) is given by

$$L(s)=L_0(s)-U, \tag{2.21}$$

where

$$L_0=iD_2+D_1^2 \tag{2.22}$$

has kernel

$$L_0(x,x';s)=[i(\partial_{x_2}+s_2)+(\partial_{x_1}+s_1)^2]\delta(x-x'), \tag{2.23}$$

and U, which is called the potential operator, has kernel

$$U(x,x';s)=u(x)\,\delta(x-x'), \tag{2.24}$$

which is independent of s. Below we always suppose that $u(x)$ is real, which by (2.4) is equivalent to

$$L^{\dagger}=L. \tag{2.25}$$

The main object of our approach is the (extended) resolvent $M(s)$ of the operator $L(s)$, which is defined as the inverse of the operator L, that is, M satisfies

$$LM=ML=I, \tag{2.26}$$

and obeys condition (2.8). The main advantage of using the extended resolvent is that its derivatives with respect to s are given in terms of its reduced values that are just the Jost solutions (and their generalizations) of the linear problem under consideration. In their turn discontinuities and derivatives of these solutions lead us to the spectral data, again given as ''further'' reductions of the resolvent. Let us consider first the resolvent M_0 of the bare operator L_0. In terms of the Fourier transformation (2.9) and thanks to condition (2.8) we get for the kernel of this operator $M_0(p;\mathbf{s})=\delta(p)(i\mathbf{s}_2+\mathbf{s}_1^2)^{-1}$. Inverting transformation (2.9) we get for the hat-kernel

$$\hat{M}_0(x,x';s)=\frac{1}{2\pi i}\int_{\mathbf{k}_\Im=s_1} d\mathbf{k}_\Re[\theta(x_2-x_2')-\theta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)]\,\Phi_0(x,\mathbf{k})\Psi_0(x',\mathbf{k}), \tag{2.27}$$

where we introduced the functions

$$\Phi_0(x,\mathbf{k})=e^{-i\mathbf{k}x_1-i\mathbf{k}^2x_2},\quad \Psi_0(x,\mathbf{k})=e^{i\mathbf{k}x_1+i\mathbf{k}^2x_2}, \tag{2.28}$$

where $\mathbf{k}=\mathbf{k}_\Re+i\mathbf{k}_\Im\in\mathbb{C}$ is a complex (one-dimensional) spectral parameter for which we again use boldface font and also, in order to simplify notation, standard font for its real part, i.e., $\mathbf{k}_\Re\equiv k$. The functions $\Phi_0(x,\mathbf{k})$ and $\Psi_0(x,\mathbf{k})$ which naturally appeared in (2.27) obey the differential equations

$$\mathcal{L}_0(x,\partial_x)\Phi_0(x,\mathbf{k})\equiv(i\partial_{x_2}+\partial_{x_1}^2)\Phi_0(x,\mathbf{k})=0, \tag{2.29}$$

$$\mathcal{L}_0^{\mathrm{d}}(x,\partial_x)\Psi_0(x,\mathbf{k})\equiv(-i\partial_{x_2}+\partial_{x_1}^2)\Psi_0(x,\mathbf{k})=0, \tag{2.30}$$

i.e., solve the nonstationary Schrödinger equation and its dual in the case of zero potential. Thus they can be considered as the Jost solutions for this trivial case. Notice also that they obey the conjugation property

$$\overline{\Phi_0(x,\mathbf{k})}=\Psi_0(x,\overline{\mathbf{k}}). \tag{2.31}$$

By using notation (2.17) we can write

$$\vec{\mathcal{L}}_0\hat{M}_0(s)=\hat{M}_0(s)\tilde{\mathcal{L}}_0=I, \tag{2.32}$$

showing that the hat version of the extended resolvent $\hat{M}_0(s)$ is a two-parametric set of Green's functions of operator (1.1) and its dual. In analogy with these notations we write

$$\vec{\mathcal{L}}_0\Phi_0(\mathbf{k})=0,\quad \Psi_0(\mathbf{k})\tilde{\mathcal{L}}_0=0, \tag{2.33}$$

considering $\Phi_0(\mathbf{k})$ and $\Psi_0(\mathbf{k})$ as "vector" and "covector" with "components" labeled by the variable x.

The resolvent M_0 given in (2.27) obeys the following properties. It is a continuous function of s when $s\neq 0$, it is bounded but discontinuous at $s=0$, it is self-adjoint [cf. (2.25)], that is $M_0^\dagger=M_0$, and from (2.27) we have

$$\frac{\partial\hat{M}_0(s)}{\partial s_1}=\frac{i}{\pi}\int_{\mathbf{k}_\Im=s_1} d\mathbf{k}_\Re\,\overline{\mathbf{k}}\,\delta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)\,\Phi_0(\mathbf{k})\otimes\Psi_0(\mathbf{k}), \tag{2.34}$$

$$\frac{\partial\hat{M}_0(s)}{\partial s_2}=\frac{1}{2\pi i}\int_{\mathbf{k}_\Im=s_1} d\mathbf{k}_\Re\,\delta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)\,\Phi_0(\mathbf{k})\otimes\Psi_0(\mathbf{k}), \tag{2.35}$$

where, in correspondence with the "vector" interpretation of the Jost solutions, the direct product in (2.34), (2.35) is defined in the standard way as an operator with kernel

$$(\Phi_0(\mathbf{k})\otimes\Psi_0(\mathbf{k}))(x,x')=\Phi_0(x,\mathbf{k})\Psi_0(x',\mathbf{k}). \tag{2.36}$$

Derivatives in (2.34) and (2.35) can be considered in the standard sense when $s_1\neq 0$, while in vicinity of $s_1=0$ they must be understood in the distributional sense. It is easy to see that the integral in (2.27) is exponentially divergent when, say, $s_2\to\infty$. Thus, indeed, $\hat{M}_0(x,x';s)\notin\mathcal{S}'(\mathbb{R}^6)$.

2. The resolvent and Hilbert identity

The resolvent of the operator L can also be defined as the solution of the integral equations

$$M=M_0+M_0UM, \quad M=M_0+MUM_0. \tag{2.37}$$

Under a small norm assumption on the potential we expect that the solution M exists and is unique (the same for both integral equations) if the condition (2.8) is required. Taking into account the properties of M_0 given above, we get that thanks to the reality of the potential $u(x)$ the resolvent is self-adjoint,

$$M^\dagger=M, \tag{2.38}$$

$M(s)$ is a continuous function of s when $s\neq 0$ and discontinuous at $s=0$, and by (2.26) has the asymptotic expansion

$$M(s_1,s_2+\mathbf{s}_2')=\frac{I}{i\mathbf{s}_2'}+\frac{L(s)}{\mathbf{s}_2'^2}+\cdots, \quad \mathbf{s}_2'\in\mathbb{C}, \quad \mathbf{s}_2'\to\infty. \tag{2.39}$$

As we mentioned above essential information on the spectrum of the operator $\mathcal{L}$ can be derived from the d-bar derivatives of the resolvent $M(\mathbf{s})$ continued in the complex domain. In order to study these derivatives we use the following analog of the well known Hilbert identity,

$$M'-M=-M'(L'-L)M, \tag{2.40}$$

where L' is another operator of the type (1.1) and M' is its resolvent. Let us choose $U'=U$ and let $L=L(\mathbf{s})$ and $L'=L(\mathbf{s}')$ and the same for their resolvents. Then (2.40) can be written in the form

$$M(\mathbf{s}')-M(\mathbf{s})=-M(\mathbf{s}')(L_0(\mathbf{s}')-L_0(\mathbf{s}))M(\mathbf{s}), \tag{2.41}$$

or by (2.26) as

$$M(\mathbf{s}')-M(\mathbf{s})=M(\mathbf{s}')L_0(\mathbf{s}')(M_0(\mathbf{s}')-M_0(\mathbf{s}))L_0(\mathbf{s})M(\mathbf{s}), \tag{2.42}$$

that gives

$$\frac{\partial M(\mathbf{s})}{\partial\overline{\mathbf{s}}_j}=M(\mathbf{s})L_0(\mathbf{s})\frac{\partial M_0(\mathbf{s})}{\partial\overline{\mathbf{s}}_j}L_0(\mathbf{s})M(\mathbf{s}). \tag{2.43}$$

In terms of hat-kernels as defined in (2.13), thanks to (2.20), we get

$$\frac{\partial\hat{M}(s)}{\partial s_j}=\hat{M}(s)\tilde{\mathcal{L}}_0\frac{\partial\hat{M}_0(s)}{\partial s_j}\vec{\mathcal{L}}_0\hat{M}(s), \quad j=1,2, \tag{2.44}$$

and then by (2.34) and (2.35) for $s_1\neq 0$

$$\frac{\partial\hat{M}(s)}{\partial s_1}=\frac{i}{\pi}\int_{\mathbf{k}_\mathfrak{I}=s_1}d\mathbf{k}_\mathfrak{R}\,\overline{\mathbf{k}}\,\delta(2\mathbf{k}_\mathfrak{R}\mathbf{k}_\mathfrak{I}-s_2)\,\Phi(\mathbf{k})\otimes\Psi(\mathbf{k}), \tag{2.45}$$

$$\frac{\partial\hat{M}(s)}{\partial s_2}=\frac{1}{2\pi i}\int_{\mathbf{k}_\mathfrak{I}=s_1}d\mathbf{k}_\mathfrak{R}\,\delta(2\mathbf{k}_\mathfrak{R}\mathbf{k}_\mathfrak{I}-s_2)\,\Phi(\mathbf{k})\otimes\Psi(\mathbf{k}), \tag{2.46}$$

where we introduced the functions

$$\Phi(x,\mathbf{k})=\int dx'\,(\mathcal{L}_0^{\mathrm{d}}(x',\partial_{x'})G(x,x',\mathbf{k}))\Phi_0(x',\mathbf{k}), \tag{2.47}$$

$$\Psi(x',\mathbf{k})=\int dx\,\Psi_0(x,\mathbf{k})\,\mathcal{L}_0(x,\partial_x)\,G(x,x',\mathbf{k}), \tag{2.48}$$

with $G(x,x',\mathbf{k})$ defined as a specific value of the resolvent itself

$$G(x,x',\mathbf{k})=\hat{M}(x,x';\mathbf{k}_{\mathfrak{I}},2\mathbf{k}_{\mathfrak{R}}\mathbf{k}_{\mathfrak{I}}). \tag{2.49}$$

In what follows we consider the function $G(x,x',\mathbf{k})$ as the kernel of the operator $G(\mathbf{k})$ and the functions $\Phi(x,\mathbf{k})$ and $\Psi(x',\mathbf{k})$ as vector $\Phi(\mathbf{k})$ and covector $\Psi(\mathbf{k})$. For shortness we write equations of the type (2.47)–(2.49) as

$$\Phi(\mathbf{k})=G(\mathbf{k})\vec{\mathcal{L}}_0\Phi_0(\mathbf{k}),\quad \Psi(\mathbf{k})=\Psi_0(\mathbf{k})\vec{\mathcal{L}}_0G(\mathbf{k}), \tag{2.50}$$

$$G(\mathbf{k})=\hat{M}(s)|_{s=(\mathbf{k}_{\mathfrak{I}},2\mathbf{k}_{\mathfrak{R}}\mathbf{k}_{\mathfrak{I}})}. \tag{2.51}$$

Relation (2.49) shows that the function $G(x,x',\mathbf{k})$ is in one-to-one correspondence with the resolvent $\hat{M}(x,x';s)$ iff $\mathbf{k}_{\mathfrak{I}}\neq 0$, that is, iff the points along the above mentioned discontinuity of the resolvent at $s=0$ are excluded. In order to study this discontinuity we introduce the following notation for the specific limits of the resolvent at this point of discontinuity,

$$G_{\pm}(x,x')=\lim_{s_2\to\pm 0}\lim_{s_1\to 0}\hat{M}(x,x';s), \tag{2.52}$$

where the limit $s_1\to 0$ is independent of the sign. Now we choose in (2.42) both s and s' real, $s_1'=s_1=0$ and consider the limits $s_2'\to\pm 0$, $s_2\to\mp 0$. We get

$$G_+-G_-=G_{\pm}\vec{\mathcal{L}}_0(G_{0,+}-G_{0,-})\vec{\mathcal{L}}_0G_{\mp}, \tag{2.53}$$

where $G_{0,\pm}$ is defined in terms of the bare resolvent $\hat{M}_0$ like in (2.52), so that by (2.27) we have

$$G_{0,\pm}(x,x')=\frac{\pm\theta(\pm(x_2-x_2'))}{2\pi i}\int dk\,\Phi_0(x,k)\Psi_0(x',k), \tag{2.54}$$

and

$$G_{0,+}-G_{0,-}=\frac{1}{2\pi i}\int dk\,\Phi_0(k)\otimes\Psi_0(k). \tag{2.55}$$

Inserting this relation in the r.h.s. of (2.53) we derive the equality

$$G_+-G_-=\frac{1}{2\pi i}\int dk\,\Phi_{\pm}(k)\otimes\Psi_{\mp}(k), \tag{2.56}$$

where we introduced the functions $\Phi_{\pm}(x,k)$ and $\Psi_{\pm}(x,k)$, which, in analogy with (2.50) and using the same notation, are defined by

$$\Phi_{\pm}(k)=G_{\pm}\vec{\mathcal{L}}_0\Phi_0(k),\quad \Psi_{\pm}(k)=\Psi_0(k)\vec{\mathcal{L}}_0G_{\pm}. \tag{2.57}$$

Next we consider in detail the properties of all the objects introduced so far, $G(\mathbf{k})$, $\Phi(\mathbf{k})$, $\Psi(\mathbf{k})$, $G_{\pm}(\mathbf{k})$, $\Phi_{\pm}(k)$, and $\Psi_{\pm}(k)$.

3. Properties of the Green's function

Thanks to (2.17) it is clear that $G(\mathbf{k})$ defined in (2.49) is a Green's function of the operator $\mathcal{L}$ depending on the complex parameter $\mathbf{k}$,

$$\vec{\mathcal{L}}G(\mathbf{k})=G(\mathbf{k})\vec{\mathcal{L}}=I. \tag{2.58}$$

Properties of this Green's function follow from the properties of $M(s)$. In particular, thanks to the definition (2.4) and to (2.38) (i.e., reality of the potential u) we get

$$\overline{G(x,x',\mathbf{k})}=G(x',x,\overline{\mathbf{k}}). \tag{2.59}$$

Applying the reduction (2.49) to equalities (2.37) we get that this function obeys the integral equations

$$G(\mathbf{k})=G_0(\mathbf{k})+G_0(\mathbf{k})UG(\mathbf{k}),\quad G(\mathbf{k})=G_0(\mathbf{k})+G(\mathbf{k})UG_0(\mathbf{k}), \tag{2.60}$$

where the Green's function $G_0(\mathbf{k})$ of the operator $\mathcal{L}_0$ is defined by the general formula (2.51) in terms of M_0 and thanks to (2.27) it equals

$$G_0(x,x',\mathbf{k})=\frac{1}{2\pi i}\int dk'\,[\,\theta(x_2-x_2')-\theta(\mathbf{k}_\Im k')\,]\,\Phi_0(x,\mathbf{k}'+k)\Psi_0(x',\mathbf{k}+k'). \tag{2.61}$$

By (2.60) it is easy to check that the function

$$g(x,x',\mathbf{k})=e^{i\mathbf{k}(x_1-x_1')+i\mathbf{k}^2(x_2-x_2')}G(x,x',\mathbf{k}) \tag{2.62}$$

is a bounded function of its arguments and that

$$\lim_{\mathbf{k}\to\infty} g(x,x',\mathbf{k})=0 \tag{2.63}$$

if the potential $u(x)$ decays rapidly enough. The function $G(x,x',\mathbf{k})$ is a continuously differentiable function of $\mathbf{k}$ in the whole complex plane $\mathbb{C}$ with exception of the real axis $\mathbf{k}_\Im=0$, as follows from (2.49). By (2.45) and (2.46) for $\mathbf{k}_\Im\neq 0$ we have

$$\frac{\partial G(\mathbf{k})}{\partial \mathbf{k}_\Re}=\frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi i}\Phi(\mathbf{k})\otimes\Psi(\mathbf{k}),\quad \frac{\partial G(\mathbf{k})}{\partial \mathbf{k}_\Im}=\frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi}\Phi(\mathbf{k})\otimes\Psi(\mathbf{k}), \tag{2.64}$$

so that in the complex domain this Green's function is analytic,

$$\frac{\partial G(\mathbf{k})}{\partial \overline{\mathbf{k}}}=0,\quad \mathbf{k}_\Im\neq 0, \tag{2.65}$$

and discontinuous at the real axis.

The Hilbert identity (2.41) allows us also to find relations among the Green's function at different values of the parameter $\mathbf{k}$. For this sake we choose $\mathbf{s}_1'=\mathbf{s}_1=s_1\in\mathbb{R}$ and let $\mathbf{s}_2',\mathbf{s}_2\in\mathbb{C}$. By (2.23) $\mathcal{L}(s_1,\mathbf{s}_2')-\mathcal{L}(s_1,\mathbf{s}_2)=i(\mathbf{s}_2'-\mathbf{s}_2)I$. Inserting this equality in (2.41) we can divide both parts by $\mathbf{s}_2'-\mathbf{s}_2$ and thanks to condition (2.8) we get

$$M(s_1,\mathbf{s}_2')M(s_1,\mathbf{s}_2)=i\frac{M(s_1,\mathbf{s}_2')-M(s_1,\mathbf{s}_2)}{\mathbf{s}_2'-\mathbf{s}_2}. \tag{2.66}$$

In terms of the hat-kernel of the resolvent by (2.18) we then have

$$\int dx'\, e^{(\mathbf{s}_2'-\mathbf{s}_2)x_2'}\hat{M}(x,x';s_1,\mathbf{s}_{2\mathfrak{R}}')\hat{M}(x',x'';s_1,\mathbf{s}_{2\mathfrak{R}})$$

$$= i\frac{e^{(\mathbf{s}_2'-\mathbf{s}_2)x_2''}\hat{M}(x,x'';s_1,\mathbf{s}_{2\mathfrak{R}}')-e^{(\mathbf{s}_2'-\mathbf{s}_2)x_2}\hat{M}(x,x'';s_1,\mathbf{s}_{2\mathfrak{R}})}{\mathbf{s}_2'-\mathbf{s}_2}.$$

Next we perform the Fourier transform with respect to the difference $\mathbf{s}_{2\mathfrak{I}}'-\mathbf{s}_{2\mathfrak{I}}$ and denote $\mathbf{s}_{2\mathfrak{R}}'=s_2'$, $\mathbf{s}_{2\mathfrak{R}}=s_2$. We get for $s_1'=s_1$

$$\int dx_1'\,\hat{M}(x,x';s')\hat{M}(x',x'';s)=i\hat{M}(x,x'';s')[\theta(x_2''-x_2')-\theta(s_2-s_2')]$$

$$-i\hat{M}(x,x'';s)[\theta(x_2-x_2')-\theta(s_2-s_2')].$$

Finally, we introduce $\mathbf{k}_{\mathfrak{I}}=s_1'=s_1$, $\mathbf{k}_{\mathfrak{R}}=s_2/(2s_1)$, $k'=(s_2'-s_2)/(2s_1)$. Then $s'=(\mathbf{k}_{\mathfrak{I}},2(\mathbf{k}_{\mathfrak{R}}+k')\mathbf{k}_{\mathfrak{I}})$ and $s=(\mathbf{k}_{\mathfrak{I}},2\mathbf{k}_{\mathfrak{R}}\mathbf{k}_{\mathfrak{I}})$ and using definition (2.49) we can rewrite the above equality in terms of the Green's function as

$$\int dx_1'\,G(x,x',\mathbf{k}+k')G(x',x'',\mathbf{k})$$

$$= iG(x,x'',\mathbf{k}+k')[\theta(x_2''-x_2')-\theta(-\mathbf{k}_{\mathfrak{I}}k')]-iG(x,x'',\mathbf{k})[\theta(x_2-x_2')-\theta(-\mathbf{k}_{\mathfrak{I}}k')],$$

$$\mathbf{k}\in\mathbb{C},\quad k'\in\mathbb{R}. \tag{2.67}$$

Properties of the functions $G_{\pm}(x,x')$ as well follow from the properties of the resolvent. Both of them are also Green's functions of the operator (1.1) and its dual,

$$\vec{\mathcal{L}}G_{\pm}=G_{\pm}\tilde{\mathcal{L}}=I, \tag{2.68}$$

obey the conjugation property

$$\overline{G_{\pm}(x,x')}=G_{\mp}(x',x), \tag{2.69}$$

and the integral equations

$$G_{\pm}=G_{0,\pm}+G_{0,\pm}UG_{\pm},\quad G_{\pm}=G_{0,\pm}+G_{\pm}UG_{0,\pm}, \tag{2.70}$$

where $G_{0,\pm}$ is given in (2.54).

The limiting values of the Green's function $G(\mathbf{k})$ on the real axis in a sense must be close to the Green's functions $G_{\pm}$. Indeed, introducing notations

$$G^{\pm}(x,x',k)=G(x,x',k\pm i0),\quad k\in\mathbb{R}, \tag{2.71}$$

we see by (2.49) that they are given by the following limits of the resolvent

$$G^{\pm}(x,x',k)=\lim_{\varepsilon\to+0}\hat{M}(x,x';\pm\varepsilon,\pm 2k\varepsilon), \tag{2.72}$$

so like in (2.52) they correspond to $\hat{M}(s)$ at $s=0$. But the resolvent is discontinuous at this point, so in the generic situation these limits are different. In order to find relations between them we again start from (2.42) choosing both s' and s to be real. Performing for s' the limiting procedure (2.72) and for s the one in (2.52) we get

$$G^{\sigma}(k)-G_{\pm}=(G_{\pm}\tilde{\mathcal{L}}_0)(G_0^{\sigma}(k)-G_{0,\pm})(\vec{\mathcal{L}}_0G^{\sigma}(k)), \tag{2.73}$$

where $k\in\mathbb{R}$ and $\sigma=+,-$. Then, thanks to (2.54) and definitions (2.57) we get from (2.73)

$$G^{\sigma}(k)-G_{\pm}=\frac{\mp 1}{2\pi i}\int dk'\ \theta(\mp\sigma(k-k'))\Phi_{\pm}(k')\otimes(\Psi_0(k')\vec{\mathcal{L}}_0G^{\sigma}(k)), \tag{2.74}$$

where for the "covector" $\Psi_0(k')\vec{\mathcal{L}}_0G^{\sigma}(k)$ we used a shorthand notation analogous to that in (2.50). Finally, let us mention that the relation between G_+ and G_- was given in (2.56).

4. Jost and advanced/retarded solutions. Bilinear representation for the resolvent

We have shown that the derivatives of the resolvent and its discontinuities are given in terms of the functions $\Phi(\mathbf{k})$, $\Psi(\mathbf{k})$, $\Phi_{\pm}(k)$, and $\Psi_{\pm}(k)$ which in their turn are obtained as special reductions of the resolvent. Here we describe the properties of these functions. Thanks to (2.33) and (2.58) it follows directly from definitions (2.50) that the functions $\Phi(x,\mathbf{k})$ and $\Psi(x,\mathbf{k})$ obey the nonstationary Schrödinger equation with potential $u(x)$ and its dual, that is,

$$\vec{\mathcal{L}}\Phi(\mathbf{k})=0,\quad \Psi(\mathbf{k})\tilde{\mathcal{L}}=0, \tag{2.75}$$

where we use the same notation as in (2.33). Thanks to (2.59) we get the conjugation property

$$\overline{\Phi(x,\mathbf{k})}=\Psi(x,\overline{\mathbf{k}}) \tag{2.76}$$

and the integral equations for these functions,

$$\Phi(\mathbf{k})=\Phi_0(\mathbf{k})+G_0(\mathbf{k})U\Phi(\mathbf{k}),\quad \Psi(\mathbf{k})=\Psi_0(\mathbf{k})+\Psi(\mathbf{k})UG_0(\mathbf{k}), \tag{2.77}$$

follow if we apply $\tilde{\mathcal{L}}_0\Phi_0$ from the right to the first equation in (2.60) and $\Psi_0\vec{\mathcal{L}}_0$ from the left to the second one. Thanks to (2.61) they are just the standard[12] equations for the Jost solution of the nonstationary Schrödinger equation and its dual. Thus, in what follows we refer to $\Phi(x,\mathbf{k})$ and $\Psi(x,\mathbf{k})$ as Jost solutions and to $G(x,x',\mathbf{k})$ as to the Green's function of the Jost solutions. By (2.65) these solutions are analytic functions of the spectral parameter $\mathbf{k}$ for $\mathbf{k}_\jmath\neq 0$ and are discontinuous at the real axis. Inserting (2.51) into (2.50) we get by (2.18) and (2.28) the standard representation

$$\Phi(x,\mathbf{k})=e^{-i\mathbf{k}x_1-i\mathbf{k}^2x_2}\chi(x,\mathbf{k}),\quad \Psi(x,\mathbf{k})=e^{i\mathbf{k}x_1+i\mathbf{k}^2x_2}\xi(x,\mathbf{k}), \tag{2.78}$$

where

$$\chi(x,\mathbf{k})=\int dx'\ (ML_0)(x,x';\mathbf{s}),\quad \xi(x',\mathbf{k})=\int dx\ (L_0M)(x,x';\mathbf{s}), \tag{2.79}$$

for $\mathbf{s}=(-i\mathbf{k},-i\mathbf{k}^2)$. From (2.77) we get that χ and ξ are normalized at infinity,

$$\lim_{\mathbf{k}\to\infty}\chi(x,\mathbf{k})=\lim_{\mathbf{k}\to\infty}\xi(x,\mathbf{k})=1, \tag{2.80}$$

while the potential $u(x)$ is reconstructed by their means as

$$u(x)=-2i\lim_{\mathbf{k}\to\infty}\mathbf{k}\partial_{x_1}\chi(x,\mathbf{k})=2i\lim_{\mathbf{k}\to\infty}\mathbf{k}\partial_{x_1}\xi(x,\mathbf{k}). \tag{2.81}$$

Solutions $\Phi(x,\mathbf{k})$ and $\Psi(x,\mathbf{k})$ obey orthonormality relation, i.e., their "scalar product" equals

$$\frac{1}{2\pi}\int dx_1\ \Psi(x,\mathbf{k}+k')\Phi(x,\mathbf{k})=\delta(k'),\quad \mathbf{k}\in\mathbb{C},\quad k'\in\mathbb{R}. \tag{2.82}$$

In order to prove it we apply $\tilde{\mathcal{L}}_0\Phi_0(\mathbf{k})$ to (2.67) from the right. Thanks to (2.28) and (2.62) the integrand in the first term on the r.h.s. of (2.67) is rapidly decaying when $x_2''\to\infty$ and we can integrate by parts, that gives zero due to (2.33). Thus by recalling (2.50) we obtain

$$\int dx_1' G(x,x',\mathbf{k}+k')\Phi(x',\mathbf{k}) = -i[\theta(x_2-x_2') - \theta(-\mathbf{k}_\Im k')]\Phi(x,\mathbf{k}) \tag{2.83}$$

and by taking the complex conjugate and using the conjugation properties (2.59) and (2.76)

$$\int dx_1'\Psi(x',\mathbf{k}+k')G(x',x,\mathbf{k}) = i[\theta(x_2-x_2') - \theta(-\mathbf{k}_\Im k')]\Psi(x,\mathbf{k}+k'). \tag{2.84}$$

Next we apply $\Psi_0(\mathbf{k}+k')\vec{\mathcal{L}}_0$ to (2.83) from the left and recalling (2.50) and (2.28) we have

$$\int dx_1' \Psi(x',\mathbf{k}+k')\Phi(x',\mathbf{k}) = \int dx\, \Psi_0(x,\mathbf{k}+k')\,\delta(x_2-x_2')\Phi(x,\mathbf{k}) - i\int dx\, \Psi_0(x,\mathbf{k}+k') \times[\theta(x_2-x_2') - \theta(-\mathbf{k}_\Im k')]u(x)\Phi(x,\mathbf{k}). \tag{2.85}$$

Now (2.82) follows if we consider (2.84) for G_0 and Ψ_0, insert it in the second term on the r.h.s. of (2.85) and use the first equation in (2.77).

The properties of the functions $\Phi_\pm(x,k)$ and $\Psi_\pm(x,k)$ are derived analogously from their definition (2.57). By (2.68) they obey

$$\vec{\mathcal{L}}\Phi_\pm(k) = 0, \quad \Psi_\pm(k)\tilde{\mathcal{L}} = 0. \tag{2.86}$$

Their conjugation property

$$\overline{\Phi_\pm(x,k)} = \Psi_\mp(x,k) \tag{2.87}$$

and the integral equations

$$\Phi_\pm(k) = \Phi_0(k) + G_{0,\pm}U\Phi_\pm(k), \quad \Psi_\pm(k) = \Psi_0(k) + \Psi_\pm(k)UG_{0,\pm}, \tag{2.88}$$

follow from their definition and Eqs. (2.70), where the Green's function $G_{0,\pm}$ is defined in (2.54). Thus $\Phi_\pm(x,k)$ and $\Psi_\pm(x,k)$ are just the standard[12] advanced/retarded solutions of the nonstationary Schrödinger equation and its dual. Correspondingly, in what follows we refer to $G_\pm(x,x')$ as to the Green's function of the advanced/retarded solutions. In analogy with derivation of (2.82) we can get the orthonormality relation

$$\frac{1}{2\pi}\int dx_1\, \Psi_\pm(x,k+k')\Phi_\mp(x,k) = \delta(k'), \quad k,k'\in\mathbb{R}. \tag{2.89}$$

The properties of the Jost solutions enable us to reconstruct $M(s)$ from (2.45) in the form

$$\hat{M}(x,x';s) = \frac{1}{2\pi i}\int_{\mathbf{k}_\Im=s_1} d\mathbf{k}_\Re\,[\theta(x_2-x_2') - \theta(2\mathbf{k}_\Re\mathbf{k}_\Im - s_2)]\,\Phi(x,\mathbf{k})\Psi(x',\mathbf{k}) \tag{2.90}$$

that generalizes (2.27) to the case of nonzero potentials. Indeed, thanks to (2.78) and to the boundedness of χ and ξ the integral, on the interval fixed by the θ-functions, is convergent, the kernel $M(x,x';s) = e^{-s(x-x')}\hat{M}(x,x';s)$ has zero limit for $s_2\to\infty$ in accordance with (2.39), and expression (2.45) for the derivative of $M(s)$ with respect to s_1 follows from (2.90) at $s_1\neq 0$ thanks to the analyticity of the Jost solutions at $\mathbf{k}_\Im\neq 0$. At the same time we know that the resolvent must be continuous at $s_1=0$ when $s_2\neq 0$. In order to formulate this property, we introduce in analogy with (2.71) a specific notation for the limiting values of the Jost solutions at the real axis, i.e.,

$$\Phi^{\pm}(x,k)=\Phi(x,k\pm i0), \quad \Psi^{\pm}(x,k)=\Psi(x,k\pm i0). \tag{2.91}$$

Then the above mentioned condition of continuity reads as

$$\int dk\,\Phi^{+}(k)\otimes\Psi^{+}(k)=\int dk\,\Phi^{-}(k)\otimes\Psi^{-}(k). \tag{2.92}$$

Representation (2.90) plays a crucial role in the resolvent approach since it enables us to express all objects of the spectral theory in terms of the Jost solutions. In particular, thanks to (2.51), for the Green's function of the Jost solutions we get

$$G(x,x',\mathbf{k})=\frac{1}{2\pi i}\int dk'\,[\,\theta(x_2-x_2')-\theta(\mathbf{k}_\Im k')\,]\,\Phi(x,\mathbf{k}+k')\Psi(x',\mathbf{k}+k'), \tag{2.93}$$

that in its turn generalizes (2.61). Moreover, from (2.90) one can get an expression of the advanced/retarded Green's functions in terms of the limiting values of the Jost solutions. Applying the limiting procedure (2.52) to (2.90) we get

$$G_{\pm}(x,x')=\frac{\pm\,\theta(\pm(x_2-x_2'))}{2\pi i}\int dk\,\Phi^{\sigma}(x,k)\Psi^{\sigma}(x',k), \tag{2.94}$$

where $\sigma=+,-$ and we used notation (2.91) for the limiting values of the Jost solutions at the real axis. Condition (2.92) guarantees that the $G_{\pm}$'s are independent of the sign σ as it must be.

From the behavior at large s_2 of the bilinear representation (2.90), comparing with (2.39) we obtain also the following important property of the Jost solutions:

$$\frac{1}{2\pi}\int_{x_2'=x_2} d\mathbf{k}_{\Re}\,\Psi(x',\mathbf{k})\Phi(x,\mathbf{k})=\delta(x_1-x_1'), \tag{2.95}$$

which can be considered a completeness relation.

5. Relations among Jost and advanced/retarded solutions. Spectral data

In the previous section, in the framework of the extended resolvent approach, we obtained in (2.93) a bilinear representation in terms of the Jost solutions of the Green's function for the Jost solutions and in (2.94) of the Green's function for the advanced/retarded solutions. We derived also Eq. (2.74) relating these Green's functions. We can now exploit these results for deriving relations among the advanced/retarded and Jost solutions on the real axis and use them to introduce the spectral data. In fact, applying $\tilde{\mathcal{L}}_0\Phi_0(k)$ to (2.74) from the right, recalling definitions (2.50) and (2.57), we get (notice that $k\in\mathbb{R}$)

$$\Phi^{\sigma}(k)=\int dk'\,\Phi_{\pm}(k')r_{\pm}^{\sigma}(k',k), \quad \sigma=+,-, \tag{2.96}$$

while the relations among $\Psi^{\sigma}(k)$ and $\Psi_{\pm}(k)$ can be derived analogously or follow by conjugation properties (2.76) and (2.87). Here we introduced the spectral data

$$r_{\pm}^{\sigma}(k',k)=\delta(k'-k)\mp\theta(\pm\sigma(k'-k))r^{\sigma}(k',k), \quad k',k\in\mathbb{R}, \tag{2.97}$$

$$r^{\sigma}(k',k)=\frac{\Psi_0(k')\vec{\mathcal{L}}_0G^{\sigma}(k)\tilde{\mathcal{L}}_0\Phi_0(k)}{2\pi i}\equiv\frac{\Psi_0(k')\vec{\mathcal{L}}_0\Phi^{\sigma}(k)}{2\pi i}. \tag{2.98}$$

Recalling ''vector'' and ''covector'' notations [cf. (2.47), (2.48), and (2.50)], the ''expectation values'' at the numerator have the following explicit expressions:

$$\Psi_0(k')\vec{\mathcal{L}}_0 G^\sigma(k)\tilde{\mathcal{L}}_0\Phi_0(k)=\int dx\int dx'\,\Psi_0(x,k')(\mathcal{L}_0(x,\partial_x)\mathcal{L}_0^{\mathrm{d}}(x',\partial_{x'})G^\sigma(x,x',k))\Phi_0(x',k), \tag{2.99}$$

$$\Psi_0(k')\vec{\mathcal{L}}_0\Phi^\sigma(k)=\int dx\,\Psi_0(x,k')\mathcal{L}_0(x,\partial_x)\Phi^\sigma(x,k), \tag{2.100}$$

showing that they are functions of k' and k only.

In order to get the advanced/retarded solutions in terms of the boundary values of the Jost ones we use (2.94) and the limiting values (2.71) of (2.93) on the real axis. Then

$$G^\sigma(k)-G_\pm=\frac{\mp 1}{2\pi i}\int dk'\;\theta(\pm\sigma(k'-k))\Phi^\sigma(k')\otimes\Psi^\sigma(k'),\quad \sigma=+,-, \tag{2.101}$$

and in the same way as above we readily derive

$$\Phi_\pm(k)=\int dk'\,\Phi^\sigma(k')\overline{r_\pm^{-\sigma}(k,k')}. \tag{2.102}$$

Now inserting these expressions into (2.96) and taking into account the orthonormality properties (2.82) and (2.89) of the Jost and advanced/retarded solutions we derive that the spectral data obey characterization equations,[17] which we discuss below in Sec. IV E 2 in a more general situation.

The alternative spectral data defined as

$$F^\sigma(k,k')=\int dk''\,\overline{r_\pm^{-\sigma}(k'',k)}r_\pm^{-\sigma}(k'',k'), \tag{2.103}$$

where the r.h.s. is independent of the choice of $\pm$ thanks to the above mentioned characterization equations, allow expressing the discontinuity of the Jost solutions across the real axis as

$$\Phi^\sigma(k)=\int dk'\,\Phi^{-\sigma}(k')F^{-\sigma}(k',k). \tag{2.104}$$

The inverse problem can be formulated in the standard way by using the fact that the Jost solution $\Phi(x,\mathbf{k})$ is an analytic function of $\mathbf{k}$ for $\mathbf{k}_\mathfrak{I}\neq 0$, has the discontinuity (2.104) at the real axis and obeys the normalization condition given by (2.78) and (2.80). In Ref. 5 we also demonstrated that the inverse problem can be formulated in terms of the resolvent itself. Here we skip this for brevity, as well as many other results that follow from the extended resolvent approach, like the introduction and properties of the dressing operators,[5] derivation of the time evolution of the spectral data corresponding to the KPI equation and algorithmic construction of time evolutions compatible with the given linear problem.[4]

III. CASE OF ONE-DIMENSIONAL POTENTIAL

A. Main definitions

In this section we consider the spectral theory of the differential operator (1.1) when the perturbation $u_2(x)$ in (1.4) is identically zero, i.e., we consider the extended differential operator

$$L_1(s)=L_0(s)-U_1,\quad U_1(x,x';s)=u_1(x_1)\delta(x-x'), \tag{3.1}$$

where $L_0(s)$ is defined in (2.22). Here and in the following we use the subscript 1 for all objects related to the case of a one-dimensional potential. In addition we choose u_1 to be the one-soliton solution of the KdV equation at the initial time $t=0$, that is,

$$u_1(x_1)=\frac{-2\kappa^2}{\cosh^2\kappa(x_1-x_0)}, \tag{3.2}$$

where x_0 and $\kappa>0$ are arbitrary constants. This choice is sufficient for showing the main peculiar aspects of the imbedding of a one-dimensional potential into two dimensions and is particularly convenient, since all objects relevant to the extended resolvent approach to inverse scattering can be explicitly given.

The Jost and dual Jost solutions [cf. (2.78)] are given by

$$\Phi_1(x,\mathbf{k})=e^{-i\mathbf{k}x_1-i\mathbf{k}^2x_2}\chi_1(x,\mathbf{k}),\quad \Psi_1(x,\mathbf{k})=e^{i\mathbf{k}x_1+i\mathbf{k}^2x_2}\xi_1(x,\mathbf{k}), \tag{3.3}$$

where as always we use boldface font for the complex spectral parameter $\mathbf{k}$, and

$$\chi_1(x_1,\mathbf{k})=\frac{\mathbf{k}-i\kappa\tanh\kappa(x_1-x_0)}{\mathbf{k}-i\kappa},\quad \xi_1(x_1,\mathbf{k})=\frac{\mathbf{k}+i\kappa\tanh\kappa(x_1-x_0)}{\mathbf{k}+i\kappa}. \tag{3.4}$$

They satisfy the differential equations

$$\vec{\mathcal{L}}_1\Phi_1(\mathbf{k})=0,\quad \Psi_1(\mathbf{k})\tilde{\mathcal{L}}_1=0, \tag{3.5}$$

and are analytic in the complex $\mathbf{k}$-plane with the exception of a pole at $\mathbf{k}=i\kappa$ and at $\mathbf{k}=-i\kappa$, correspondingly. Strictly speaking, in order to deal with Jost solutions defined in the standard way one would have to consider, for instance, $\Phi_1(x,\mathbf{k})$ multiplied by $(\mathbf{k}-i\kappa)/(\mathbf{k}+i\kappa\,\mathrm{sgn}\,\mathbf{k}_\Im)$, but this would introduce unnecessary complications. So, these Jost solutions have no discontinuity at the real axis and when we are considering their value at the real axis we can omit the superscript $\pm$. They obey, however, the conjugation property (2.76).

It is convenient to introduce the residua of functions $\Phi_1(x,\mathbf{k})$ and $\Psi_1(x,\mathbf{k})$ at the poles and their values at the conjugate points. We write

$$\operatorname*{res}_{\mathbf{k}=i\kappa}\Phi_1(x,\mathbf{k})=i\sqrt{\frac{\kappa}{\pi}}e^{\kappa x_0}\varphi_1(x),\quad \Phi_1(x,-i\kappa)=\frac{e^{-\kappa x_0}}{2\sqrt{\kappa\pi}}\varphi_1(x), \tag{3.6}$$

$$\operatorname*{res}_{\mathbf{k}=-i\kappa}\Psi_1(x,\mathbf{k})=-i\sqrt{\frac{\kappa}{\pi}}e^{\kappa x_0}\psi_1(x),\quad \Psi_1(x,i\kappa)=\frac{e^{-\kappa x_0}}{2\sqrt{\kappa\pi}}\psi_1(x), \tag{3.7}$$

where

$$\varphi_1(x)=\frac{\sqrt{\kappa\pi}\,e^{i\kappa^2x_2}}{\cosh\kappa(x_1-x_0)},\quad \psi_1(x)=\overline{\varphi_1(x)}. \tag{3.8}$$

Functions φ_1 and ψ_1 satisfy the differential equations

$$\vec{\mathcal{L}}_1\varphi_1=0,\quad \psi_1\tilde{\mathcal{L}}_1=0. \tag{3.9}$$

The equation

$$\operatorname*{res}_{\mathbf{k}=i\kappa}\Phi_1(x,\mathbf{k})=2i\kappa e^{2\kappa x_0}\Phi_1(x,-i\kappa), \tag{3.10}$$

or an analogous equation for Ψ_1, closes the formulation of the inverse problem for this Jost solution.

The orthonormality relation for the Jost solutions is not modified with respect to (2.82),

$$\frac{1}{2\pi}\int dx_1\,\Psi_1(x,\mathbf{k}+k')\Phi_1(x,\mathbf{k})=\delta(k'),\quad k'\in\mathbb{R},\quad \mathbf{k}\in\mathbb{C}, \tag{3.11}$$

but now it is accompanied by the scalar products

$$\int dx_1\,\psi_1(x)\Phi_1(x,\mathbf{k})=\int dx_1\,\Psi_1(x,\mathbf{k})\varphi_1(x)=0,\quad |\mathbf{k}_\Im|<\kappa, \tag{3.12}$$

$$\frac{1}{2\pi}\int dx_1\psi_1(x)\varphi_1(x)\equiv\frac{1}{2\pi}\int dx_1|\psi_1(x)|^2\equiv\frac{1}{2\pi}\int dx_1|\varphi_1(x)|^2=1, \tag{3.13}$$

where condition $|\mathbf{k}_\Im|<\kappa$ in (3.12) is necessary for the convergence of the integral. On the other side, the completeness relation is essentially modified with respect to the case of decaying potential (2.95) considered above, since we have

$$\int_{x_2'=x_2} d\mathbf{k}_\Re\,\Phi_1(x,\mathbf{k})\Psi_1(x',\mathbf{k})+\theta(\kappa-|\mathbf{k}_\Im|)\varphi_1(x)\psi_1(x')\Big|_{x_2'=x_2}=2\pi\delta(x_1-x_1'). \tag{3.14}$$

B. Resolvent

The resolvent $M_1(s)$ according to our general definition is the inverse, in the sense of (2.26), of the extended operator (3.1) and its hat-kernel obeys the equations

$$\vec{\mathcal{L}}_1\hat{M}_1(s)=\hat{M}_1(s)\tilde{\mathcal{L}}_1=I. \tag{3.15}$$

Taking into account that the completeness relation (3.14) is modified with respect to (2.95) and that this relation is the first order term of the asymptotic expansion of the resolvent as $s_2\to\infty$, it is natural to expect that the bilinear representation (2.90) is also modified by an additional term proportional to the product $\varphi_1(x)\psi_1(x')$. In fact we get

$$\hat{M}_1(x,x';s)=\frac{1}{2\pi i}\Bigg(\int_{\mathbf{k}_\Im=s_1} d\mathbf{k}_\Re[\,\theta(x_2-x_2')-\theta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)\,]\,\Phi_1(x,\mathbf{k})\Psi_1(x',\mathbf{k})$$
$$+\theta(\kappa-|s_1|)\,[\,\theta(x_2-x_2')-\theta(-s_2)\,]\varphi_1(x)\psi_1(x')\Bigg). \tag{3.16}$$

Performing the transformation (2.13) and taking into account the properties of the Jost solutions and of the functions $\varphi_1(x)$ and $\psi_1(x')$ one can check that $M_1(x,x';s)\in\mathcal{S}'$ and obeys integral equations of the kind (2.37) with $U=U_1$. The second term in (3.16) is different from zero in the interval $|s_1|<\kappa$, it compensates the discontinuities of the first term at $s_1=\pm\kappa$, which are consequence of the pole singularities of $\Phi_1(x,\mathbf{k})$ and $\Psi_1(x,\mathbf{k})$. On the other side, this term introduces a discontinuity in $M_1(s)$ at $s_2=0$ for all $|s_1|<\kappa$ and not only at $s_1=0$ as it was for the resolvent of the decaying case. By direct calculations one can prove the regularity with respect to s-variables of

$$\hat{M}_{1,\mathrm{reg}}(s)=\hat{M}_1(s)-\Gamma(s)\,\varphi_1(x)\psi_1(x'), \tag{3.17}$$

where

$$\Gamma(s)=\frac{\operatorname{sgn}s_1}{(2\pi)^2}\log\frac{s_2+2is_1(s_1-\kappa)}{s_2+2is_1(s_1+\kappa)}, \tag{3.18}$$

the logarithm being the principal part with the cut along the negative real axis. Thus, we see that the extended resolvent in the case of one-dimensional potentials gets logarithmic singularities at the points $s=(\pm\kappa,0)$. The singular part of the resolvent has the structure of a direct product.

C. Properties of the resolvent and Green's functions

For the discontinuity of the resolvent at $s_2=0$ we get from (3.16)

$$\lim_{s_2\to+0}\hat{M}_1(s)-\lim_{s_2\to-0}\hat{M}_1(s)=\frac{\theta(\kappa-|s_1|)}{2\pi i}\varphi_1\otimes\psi_1, \tag{3.19}$$

which also follows from (3.17). For all other values of s the resolvent (3.16) has derivatives with respect to s of the form of (2.34), (2.35):

$$\frac{\partial\hat{M}_1(s)}{\partial s_1}=\frac{i}{\pi}\int_{\mathbf{k}_\Im=s_1}d\mathbf{k}_\Re\,\overline{\mathbf{k}}\,\delta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)\,\Phi_1(\mathbf{k})\otimes\Psi_1(\mathbf{k}), \tag{3.20}$$

$$\frac{\partial\hat{M}_1(s)}{\partial s_2}=\frac{1}{2\pi i}\int_{\mathbf{k}_\Im=s_1}d\mathbf{k}_\Re\,\delta(2\mathbf{k}_\Re\mathbf{k}_\Im-s_2)\,\Phi_1(\mathbf{k})\otimes\Psi_1(\mathbf{k}), \tag{3.21}$$

which at the vicinity of the point $s_1=0$ have to be considered in the distributional sense. Thus, we can introduce the Green's function $G_1(x,x',\mathbf{k})$ of the Jost solutions by using the same definition as in (2.51). Then, from (3.16) we get the bilinear representation

$$\begin{aligned}G_1(x,x',\mathbf{k})=&\frac{1}{2\pi i}\int dk'\,[\,\theta(x_2-x_2')-\theta(\mathbf{k}_\Im k')\,]\,\Phi_1(x,k'+\mathbf{k})\Psi_1(x',k'+\mathbf{k})\\&+\frac{\theta(\kappa-|\mathbf{k}_\Im|)}{2\pi i}[\,\theta(x_2-x_2')-\theta(-\mathbf{k}_\Re\mathbf{k}_\Im)\,]\varphi_1(x)\psi_1(x'),\end{aligned} \tag{3.22}$$

which was already derived in Ref. 16, but starting from another point of view. It is easy to check that this Green's function obeys the conjugation property (2.59) and that the function $g_1(x,x',\mathbf{k})$ defined like in (2.62) has property (2.63). Taking into account that the resolvent obeys (2.37) with $U=U_1$ we get that the Green's function obeys integral equations of the type (2.60),

$$G_1(\mathbf{k})=G_0(\mathbf{k})+G_0(\mathbf{k})U_1G_1(\mathbf{k}),\quad G_1(\mathbf{k})=G_0(\mathbf{k})+G_1(\mathbf{k})U_1G_0(\mathbf{k}), \tag{3.23}$$

it is analytic when $\mathbf{k}_\Re\mathbf{k}_\Im\neq0$, continuous up to the borders of these quadrants, and in this region in analogy with (2.64) we obtain

$$\frac{\partial G_1(\mathbf{k})}{\partial\mathbf{k}_\Im}=\frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi}\Phi_1(\mathbf{k})\otimes\Psi_1(\mathbf{k}). \tag{3.24}$$

In addition to the standard discontinuity at the real axis, the Green's function has also a discontinuity

$$G_1(+0+i\mathbf{k}_\Im)-G_1(-0+i\mathbf{k}_\Im)=\frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi i}\,\theta(\kappa-|\mathbf{k}_\Im|)\,\varphi_1\otimes\psi_1 \tag{3.25}$$

at the imaginary axis when $|\mathbf{k}_\Im|<\kappa$. Using (3.17) one can prove that the function $G_1(\mathbf{k})-\gamma(\mathbf{k})\,\varphi_1\otimes\psi_1$, where

$$\gamma(\mathbf{k})=\Gamma(s)|_{s=(\mathbf{k}_\Im,2\mathbf{k}_\Re\mathbf{k}_\Im)}\equiv\frac{\operatorname{sgn}\mathbf{k}_\Im}{(2\pi)^2}\log\frac{\mathbf{k}-i\kappa}{\mathbf{k}+i\kappa}, \tag{3.26}$$

is a bounded continuous function of $\mathbf{k}$ in vicinity of the cut $\mathbf{k}_{\Re}=0$, $|\mathbf{k}_{\Im}|<\kappa$ with exception of the point $\mathbf{k}=0$. As a consequence the regularized function

$$G_{1,\mathrm{reg}}(\mathbf{k})=G_1(\mathbf{k})+2\pi i\,\gamma(\mathbf{k})(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_{\Im}-i\kappa)\Phi_1(\mathbf{k})\otimes\Psi_1(\mathbf{k}) \tag{3.27}$$

has finite limits at the points $\mathbf{k}=\pm i\kappa$, while it is discontinuous at $\mathbf{k}_{\Re}=0$ and $\mathbf{k}_{\Im}=0$. In (3.27) the multiplier $(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_{\Im}-i\kappa)$ compensates the poles of $\Phi_1(\mathbf{k})$ and $\Psi_1(\mathbf{k})$. Note that the regularized function $g_{1,\mathrm{reg}}(\mathbf{k})$ constructed from $G_{1,\mathrm{reg}}(x,x',\mathbf{k})$ like in (2.62) is bounded with respect to x and has finite limits when $x\to\infty$.

Let us mention that in the case of the Jost solutions Φ_1 and Ψ_1 the integrals in definitions (2.47) and (2.48) are divergent and they must be conveniently regularized in the following way:

$$\Phi_1(x,\mathbf{k})=\lim_{\varepsilon\to+0}\int dx'\,(G_1(\mathbf{k})\tilde{\mathcal{L}}_0)(x,x')\Phi_0(x',\mathbf{k})e^{i\varepsilon\mathbf{k}_{\Im}x'_2}, \tag{3.28}$$

$$\Psi_1(x,\mathbf{k})=\lim_{\varepsilon\to+0}\int dx'\,e^{-i\varepsilon\mathbf{k}_{\Im}x'_2}\Psi_0(x',\mathbf{k})(\vec{\mathcal{L}}_0G_1(\mathbf{k}))(x',x), \tag{3.29}$$

where $\mathbf{k}_{\Im}\neq0$. As the result of this regularization we get (see Refs. 2 and 4) a modification of the integral equations for the Jost solutions with respect to the standard ones[10,12–15] that are not applicable in the case of one-dimensional potentials. In particular, in spite of the cut that $G_1(x,x',\mathbf{k})$ has on the imaginary axis, we have

$$\Phi_1(+0+i\mathbf{k}_{\Im})-\Phi_1(-0+i\mathbf{k}_{\Im})=2i\sqrt{\kappa\pi}e^{\kappa x_0}\delta(\mathbf{k}_{\Im}-\kappa)\varphi_1 \tag{3.30}$$

in agreement with (3.6).

When $s_1=0$ the kernel $\hat{M}_1(s)$ is discontinuous at $s_2=0$. This means that we have to introduce the advanced/retarded Green's functions like in (2.52). By (3.16) we get the following bilinear representation for these Green's functions in terms of the Jost solutions on the real axis:

$$G_{1,\pm}(x,x')=\frac{\pm\theta(\pm(x_2-x'_2))}{2\pi i}\left(\int dk\,\Phi_1(x,k)\Psi_1(x',k)+\varphi_1(x)\psi_1(x')\right). \tag{3.31}$$

The singular part of these Green's functions is equal to zero, as follows from (3.18). These Green's functions obey the conjugation property (2.69).

Now turning back to the discontinuity of the resolvent with respect to s_2 when $s_1\neq0$ we get from (2.51) for these limits

$$\lim_{s_2\to\pm0\mathbf{k}_{\Im}}(\hat{M}_1(s)|_{s_1=\mathbf{k}_{\Im}})=G_1(\pm0+i\mathbf{k}_{\Im}). \tag{3.32}$$

Relations among Green's functions follow from the bilinear representation (3.16) for the resolvent. For the boundary values of the Green's function of the Jost solutions at the real axis we use notations (2.72). Then by (3.22) they are finite for all finite k but discontinuous at $k=0$ and by (3.31)

$$G_1^{\sigma}(k)-G_{1,\pm}=\frac{\mp1}{2\pi i}\int dk'\,\theta(\mp\sigma(k-k'))\Phi_1(k')\otimes\Psi_1(k')\mp\frac{\theta(\mp\sigma k)}{2\pi i}\varphi_1\otimes\psi_1,\quad \sigma=+,-. \tag{3.33}$$

Other relations of such kind, say, among advanced and retarded Green's functions, can be derived analogously.

IV. INVERSE SCATTERING TRANSFORM ON NONTRIVIAL BACKGROUND: TWO-DIMENSIONAL PERTURBATION OF THE SOLITON SOLUTION

A. Resolvent

We investigate, now, the operator $\mathcal{L}$ in (1.1) with a potential of the form (1.4), where $u_1(x_1)$ is the one-soliton solution (3.2) and $u_2(x)$ is a generic real, smooth and rapidly decaying function on the plane (x_1,x_2), "small" in some sense, so that it can be considered a two-dimensional perturbation of the one-soliton solution. According to our general approach we introduce the extension $L(s)$ of $\mathcal{L}$ and the inverse of this extension, i.e., its extended resolvent $M(s)$. In the previous sections we considered the special case $u_2(x)\equiv 0$ and studied in detail the properties of the corresponding resolvent $M_1(s)$. Therefore, it is convenient to exploit these results and to use for constructing the resolvent $M(s)$, instead of the integral equations (2.37), the following ones,

$$M(s)=M_1(s)+M_1(s)U_2M(s), \quad M(s)=M_1(s)+M(s)U_2M_1(s), \tag{4.1}$$

where $U_2(x,x';s)=u_2(x)\delta(x-x')$. We assume that, thanks to the "smallness" requirement on $u_2(x)$, both equations admit a unique solution $M(x,x';s)$ in $\mathcal{S}'(\mathbb{R}^6)$. This requirement, in addition, guarantees that the solution $M(x,x';s)$ inherits the properties of $M_1(x,x';s)$, in particular that $M(x,x';s)$ is a distribution with respect to $x-x'$, a smooth function with respect to $x+x'$ and a continuous function of s, when $s_1\neq 0$ and $s_2\neq 0$. Therefore, the Hilbert identities (2.40) and (2.42) are valid also in our case, since the composition of operators appearing in them exist and are associative. The Hilbert identity (2.40) can be used for proving that equations (4.1) have the same solution. In fact, if we choose M to be a solution of the first equation in (4.1) [and then solution of the second equation in (2.26)] and M' to obey the second equation in (4.1) [the first in (2.26), correspondingly], then we obtain $M'=M$. Notice that, in addition, this proves that $M(s)$ is Hermitian, i.e., it obeys (2.38) like in the decaying and one-dimensional cases. Instead, the Hilbert identity (2.42) can be used for studying the properties of the resolvent in the s variable. However, as we did for the integral equations (4.1) defining $M(s)$, it is more convenient to rewrite it in terms of the one-dimensional operator $L_1(s)$ and resolvent $M_1(s)$ as follows:

$$M(\mathbf{s}')-M(\mathbf{s})=M(\mathbf{s}')L_1(\mathbf{s}')(M_1(\mathbf{s}')-M_1(\mathbf{s}))L_1(\mathbf{s})M(\mathbf{s}). \tag{4.2}$$

Then, in analogy with (2.44) we get for the derivatives of the hat-kernel of the resolvent

$$\frac{\partial\hat{M}(s)}{\partial s_j}=\hat{M}(s)\overleftarrow{\mathcal{L}}_1\frac{\partial\hat{M}_1(s)}{\partial s_j}\vec{\mathcal{L}}_1\hat{M}(s), \quad j=1,2, \quad s_2\neq 0.$$

Inserting here (3.20) and (3.21) we get for the derivatives of $\hat{M}(s)$ the same equations (2.45) and (2.46) of the decaying case, where the Jost solutions are defined now as [cf. (2.50)]

$$\Phi(\mathbf{k})=G(\mathbf{k})\overleftarrow{\mathcal{L}}_1\Phi_1(\mathbf{k}), \quad \Psi(\mathbf{k})=\Psi_1(\mathbf{k})\vec{\mathcal{L}}_1G(\mathbf{k}), \tag{4.3}$$

with the Green's function $G(x,x',\mathbf{k})$ defined by (2.51) as in the decaying case. We excluded here the value $s_2=0$, where $M_1(s)$ is discontinuous.

For the study of the discontinuity at $s_2=0$ of $M(s)$ inherited from $M_1(s)$, following the results of Sec. III, we have to consider separately the cases $s_1=0$ and $s_1\neq 0$. The boundary values of the resolvent in the first case, $\lim_{s_2\to\pm 0}\hat{M}(s)|_{s_1=0}$, define the advanced/retarded Green's functions like in (2.52). In the case $s_1\neq 0$ for the boundary values of the resolvent thanks to (2.51) we have in analogy with (3.32) that

$$\lim_{s_2\to\pm 0\mathbf{k}_\mathfrak{I}}(\hat{M}(s)|_{s_1=\mathbf{k}_\mathfrak{I}})=G(\pm 0+i\mathbf{k}_\mathfrak{I}). \tag{4.4}$$

Now we consider the properties of these Green's functions in detail.

B. The Green's function of the Jost solutions

1. Properties of $G(\mathbf{k})$

We proved above that the definition (2.51) of the Green's function $G(\mathbf{k})$ of the Jost solutions is applicable in the case we are considering now. Then directly by (4.1) we get that $G(\mathbf{k})$ satisfies the integral equations

$$G(\mathbf{k})=G_1(\mathbf{k})+G_1(\mathbf{k})U_2G(\mathbf{k}),\quad G(\mathbf{k})=G_1(\mathbf{k})+G(\mathbf{k})U_2G_1(\mathbf{k}). \tag{4.5}$$

Taking into account that $\mathcal{L}=\mathcal{L}_1-U_2$ it is easy to check that $G(\mathbf{k})$ obeys the differential equations (2.58) and the conjugation property (2.59). According to the remark we already made above for the resolvent $M(s)$, $G(\mathbf{k})$ has the same domains of analyticity as $G_1(\mathbf{k})$. Precisely, it is analytic in the region $\mathbf{k}_\Re\mathbf{k}_\Im\neq 0$, where it obeys (2.64) and (2.65), and continuous up to the borders, it has a cut at $\mathbf{k}_\Im=0$ as in the decaying case and an additional cut at $\mathbf{k}_\Re=0$ when $|\mathbf{k}_\Im|<\kappa$. Using notation (2.71) for the boundary values of the Green's function at the real axis, we get

$$\lim_{\sigma\mathbf{k}_\Im\to+0} G(\pm 0+i\mathbf{k}_\Im)=\lim_{\pm k\to+0} G^\sigma(k)\equiv G^\sigma(\pm 0),\quad \sigma=+,-. \tag{4.6}$$

Notice that by inserting (4.5) into the definitions (4.3) of the Jost solutions we get the integral equations

$$\Phi(\mathbf{k})=\Phi_1(\mathbf{k})+G_1(\mathbf{k})U_2\Phi(\mathbf{k}),\quad \Psi(\mathbf{k})=\Psi_1(\mathbf{k})+\Psi(\mathbf{k})U_2G_1(\mathbf{k}), \tag{4.7}$$

which can be also considered to define the Jost solutions.

2. Discontinuity of $G(\mathbf{k})$ across the imaginary axis

As always in order to study the properties of the resolvent at a discontinuity we use the Hilbert identity. Choosing in (4.2) both $\mathbf{s}$ and $\mathbf{s}'$ to be real and $s_1=s_1'$, we have

$$\lim_{s_2\to+0}\hat{M}(s)-\lim_{s_2\to-0}\hat{M}(s)=(\lim_{s_2\to\pm 0}\hat{M}(s)\tilde{\mathcal{L}}_1)(\lim_{s_2\to+0}\hat{M}_1(s)-\lim_{s_2\to-0}\hat{M}_1(s))(\vec{\mathcal{L}}_1\lim_{s_2\to\mp 0}\hat{M}(s)),$$

which, by (4.4), is the discontinuity of the Green's function across the imaginary axis. By using (3.22) for the discontinuity of $G_1(\mathbf{k})$ we obtain

$$G(+0+i\mathbf{k}_\Im)-G(-0+i\mathbf{k}_\Im)=\frac{\theta(\kappa-|\mathbf{k}_\Im|)}{2\pi i\ \mathrm{sgn}\,\mathbf{k}_\Im}(G(\pm 0+i\mathbf{k}_\Im)\tilde{\mathcal{L}}_1\varphi_1)\otimes(\psi_1\vec{\mathcal{L}}_1G(\mp 0+i\mathbf{k}_\Im)), \tag{4.8}$$

where in brackets ''vector'' and ''covector'' notation like in (2.50) is used and the direct product is defined as in (2.36). Applying operations $\psi_1\vec{\mathcal{L}}_1$ and $\tilde{\mathcal{L}}_1\varphi_1$ to this equality from the left and from the right, correspondingly, we get in the region $\kappa>|\mathbf{k}_\Im|>0$

$$\left[1-\frac{\psi_1\vec{\mathcal{L}}_1G(-0+i\mathbf{k}_\Im)\tilde{\mathcal{L}}_1\varphi_1}{2\pi i\ \mathrm{sgn}\,\mathbf{k}_\Im}\right]\left[1+\frac{\psi_1\vec{\mathcal{L}}_1G(+0+i\mathbf{k}_\Im)\tilde{\mathcal{L}}_1\varphi_1}{2\pi i\ \mathrm{sgn}\,\mathbf{k}_\Im}\right]=1, \tag{4.9}$$

where the ''expectation values'' in the numerator have explicit expressions analogous to those in (2.99). Under our assumptions on the potential both multipliers on the l.h.s. are regular in this region so they have no zeroes. Denoting the right multiplier as $A(\mathbf{k}_\Im)$ we get

$$A(\mathbf{k}_\Im)=\left(1\pm\frac{\psi_1\vec{\mathcal{L}}_1G(\pm 0+i\mathbf{k}_\Im)\tilde{\mathcal{L}}_1\varphi_1}{2\pi i\mathrm{sgn}\,\mathbf{k}_\Im}\right)^{\pm 1}, \tag{4.10}$$

which has no zeroes for any $|\mathbf{k}_\Im|<\kappa$,

$$A(\mathbf{k}_\jmath)\neq 0, \tag{4.11}$$

and by (2.59) and the second equality in (3.8) obeys the conjugation property

$$\overline{A(\mathbf{k}_\jmath)}=A(-\mathbf{k}_\jmath). \tag{4.12}$$

The function $A(\mathbf{k}_\jmath)$ is defined inside the interval $|\mathbf{k}_\jmath|<\kappa$, it is continuous for all $\mathbf{k}_\jmath\neq 0$ and using for the limiting values at $\mathbf{k}_\jmath=\pm 0$ notation of the type (2.71), $A^\pm=\lim_{\mathbf{k}_\jmath\to\pm 0}A(\mathbf{k}_\jmath)$, we get by (4.6) and (4.10)

$$A^\pm=1\pm\frac{\psi_1\vec{\mathcal{L}}_1G^\pm(+0)\tilde{\mathcal{L}}_1\varphi_1}{2\pi i}. \tag{4.13}$$

Thanks to (4.11) both these constants $A^\pm$ are different from zero and by (4.12) they are mutually conjugate,

$$\overline{A^-}=A^+. \tag{4.14}$$

If we introduce the functions

$$\varphi(\mathbf{k}_\jmath)=G(+0+i\mathbf{k}_\jmath)\tilde{\mathcal{L}}_1\varphi_1,\quad \psi(\mathbf{k}_\jmath)=A(\mathbf{k}_\jmath)(\psi_1\vec{\mathcal{L}}_1G(-0+i\mathbf{k}_\jmath)), \tag{4.15}$$

where the multiplier $A(\mathbf{k}_\jmath)$ in the last equality is introduced for convenience, the discontinuity of the Green's function at the imaginary axis (4.8) can be written in their terms as

$$G(+0+i\mathbf{k}_\jmath)-G(-0+i\mathbf{k}_\jmath)=\theta(\kappa-|\mathbf{k}_\jmath|)\frac{\varphi(\mathbf{k}_\jmath)\otimes\psi(\mathbf{k}_\jmath)}{2\pi iA(\mathbf{k}_\jmath)\operatorname{sgn}\mathbf{k}_\jmath}. \tag{4.16}$$

Thanks to (4.10) this equality gives the following relations symmetric to (4.15),

$$\varphi(\mathbf{k}_\jmath)=A(\mathbf{k}_\jmath)(G(-0+i\mathbf{k}_\jmath)\tilde{\mathcal{L}}_1\varphi_1),\quad \psi(\mathbf{k}_\jmath)=\psi_1\vec{\mathcal{L}}_1G(+0+i\mathbf{k}_\jmath). \tag{4.17}$$

Notice that using the first equality in (4.15) and the second equality in (4.17) we get by (4.5) the integral equations for these functions

$$\varphi(\mathbf{k}_\jmath)=\varphi_1+G_1(+0+i\mathbf{k}_\jmath)U_2\varphi(\mathbf{k}_\jmath),\quad \psi(\mathbf{k}_\jmath)=\psi_1+\psi(\mathbf{k}_\jmath)U_2G_1(+0+i\mathbf{k}_\jmath), \tag{4.18}$$

$|\mathbf{k}_\jmath|<\kappa$, which can also be considered to define them.

The values of the Green's function on the two sides of the cut along the imaginary axis can be obtained by using the derivatives of the Green's function (2.64), whose validity can be extended to the case we are now considering if the Jost solutions are defined as in (4.3). Performing the limits $\mathbf{k}_\mathfrak{R}\to\pm 0$ we get in the strip $|\mathbf{k}_\jmath|<\kappa$

$$G(\pm 0+i\mathbf{k}_\jmath)=G^\sigma(\pm 0)+\frac{\sigma}{2\pi}\int_0^{\mathbf{k}_\jmath}d\alpha\,\Phi(\pm 0+i\alpha)\otimes\Psi(\pm 0+i\alpha),\quad \sigma=\operatorname{sgn}\mathbf{k}_\jmath, \tag{4.19}$$

where we used the second equality in (4.6).

3. Behavior of $G(\mathbf{k})$ at the end points of the cut

In order to study the behavior of the Green's function in the vicinities of the points $\mathbf{k}=\pm i\kappa$ [where $G_1(\mathbf{k})$ is singular] we use (3.27) and introduce the regularized Green's function $G_{\text{reg}}(\mathbf{k})$ as solution of the integral equation

$$G_{\text{reg}}(\mathbf{k})=G_{1,\text{reg}}(\mathbf{k})+G_{1,\text{reg}}(\mathbf{k})U_2G_{\text{reg}}(\mathbf{k}), \tag{4.20}$$

which thanks to properties of $G_{1,\mathrm{reg}}$ has finite limits at points $\mathbf{k}=\pm i\kappa$. Subtracting (4.20) from (4.5) and using (3.27) we get

$$G(\mathbf{k})-G_{\mathrm{reg}}(\mathbf{k})=-2\pi i\gamma(\mathbf{k})(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_\mathfrak{I}-i\kappa)\Phi_1(\mathbf{k})\otimes\Psi_1(\mathbf{k})[I+U_2G(\mathbf{k})]$$
$$+G_{1,\mathrm{reg}}(\mathbf{k})U_2[G(\mathbf{k})-G_{\mathrm{reg}}(\mathbf{k})].$$

Under the assumption of unique solvability of (4.20) and thanks to the identity $I+U_2G(\mathbf{k})=\vec{\mathcal{L}}_1G(\mathbf{k})$ we derive from this equality for the Green's function in vicinity of these points the following representation:

$$G(\mathbf{k})=G_{\mathrm{reg}}(\mathbf{k})-\frac{2\pi i\gamma(\mathbf{k})(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_\mathfrak{I}-i\kappa)(G_{\mathrm{reg}}(\mathbf{k})\tilde{\mathcal{L}}_1\Phi_1(\mathbf{k}))\otimes(\Psi_1(\mathbf{k})\vec{\mathcal{L}}_1G_{\mathrm{reg}}(\mathbf{k}))}{1+2\pi i\gamma(\mathbf{k})(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_\mathfrak{I}-i\kappa)(\Psi_1(\mathbf{k})\vec{\mathcal{L}}_1G_{\mathrm{reg}}(\mathbf{k})\tilde{\mathcal{L}}_1\Phi_1(\mathbf{k}))}. \quad (4.21)$$

In analogy with (4.15), (4.17) we introduce the regular parts of the functions $\varphi(x,\mathbf{k}_\mathfrak{I})$, $\psi(x,\mathbf{k}_\mathfrak{I})$ at $\mathbf{k}_\mathfrak{I}=\pm\kappa$:

$$\varphi_{\mathrm{reg},\pm}=G_{\mathrm{reg}}(\pm i\kappa)\tilde{\mathcal{L}}_1\varphi_1,\quad \psi_{\mathrm{reg},\pm}=\psi_1\vec{\mathcal{L}}_1G_{\mathrm{reg}}(\pm i\kappa) \quad (4.22)$$

and the ''expectation values''

$$B_\pm=\psi_1\vec{\mathcal{L}}_1G_{\mathrm{reg}}(\pm i\kappa)\tilde{\mathcal{L}}_1\varphi_1. \quad (4.23)$$

Then by (3.6), (3.7) we have that

$$2\pi\lim_{\mathbf{k}\to\pm i\kappa}(\mathbf{k}\,\mathrm{sgn}\,\mathbf{k}_\mathfrak{I}-i\kappa)(\Psi_1(\mathbf{k})\vec{\mathcal{L}}_1G_{\mathrm{reg}}(\mathbf{k})\tilde{\mathcal{L}}_1\Phi_1(\mathbf{k}))=iB_\pm,$$

and thus using the above notations we get the asymptotic relation

$$G(\mathbf{k})=G_{\mathrm{reg}}(\pm i\kappa)+\frac{\gamma(\mathbf{k})\varphi_{\mathrm{reg}}(\pm\kappa)\otimes\psi_{\mathrm{reg}}(\pm\kappa)}{1-\gamma(\mathbf{k})B_\pm}+o(1),\quad \mathbf{k}\to\pm i\kappa. \quad (4.24)$$

Summarizing, the Green's function $G(\mathbf{k})$, like $G_1(\mathbf{k})$, has a discontinuity on the segment $|\mathbf{k}_\mathfrak{I}|<\kappa$ of the imaginary axis, but in general it is not necessarily singular at the end points of this segment. Indeed, if $B_+=0$, then at $\mathbf{k}\to i\kappa$ the logarithmic behavior of $\gamma(\mathbf{k})$ in the numerator of (4.24) is not compensated, so the Green's function $G(\mathbf{k})$ has a logarithmic singularity at the point $\mathbf{k}=i\kappa$, like in the special case considered in Sec. II. However, if

$$B_+\neq 0, \quad (4.25)$$

then the logarithmic behaviors of numerator and denominator in (4.24) compensate and we get a finite result. Taking into account the conjugation property $B_-=\overline{B_+}$, this is also valid for the point $\mathbf{k}=-i\kappa$, so in this case at the end points of the cut we have

$$G(\pm i\kappa)=G_{\mathrm{reg}}(\pm i\kappa)-\frac{\varphi_{\mathrm{reg},\pm}\otimes\psi_{\mathrm{reg},\pm}}{B_\pm}. \quad (4.26)$$

Applying to (4.24) the operations $\psi_1\vec{\mathcal{L}}_1$ from the left and $\tilde{\mathcal{L}}_1\varphi_1$ from the right we get for $A(\mathbf{k}_\mathfrak{I})$ by (4.10) that

$$A(\pm\kappa)=1 \quad (4.27)$$

independently of the value of B_+.

C. Jost solutions

1. Properties of Jost solutions

From the properties of the Green's function $G(\mathbf{k})$ studied in Sec. II it follows that the Jost solutions $\Phi(\mathbf{k})$ and $\Psi(\mathbf{k})$ introduced in (4.3) are analytic in the region $\mathbf{k}_{\mathfrak{R}}\mathbf{k}_{\mathfrak{I}}\neq 0$, and continuous up to the borders, have a discontinuity at $\mathbf{k}_{\mathfrak{I}}=0$ as in the decaying case and an additional discontinuity at $\mathbf{k}_{\mathfrak{R}}=0$ when $|\mathbf{k}_{\mathfrak{I}}|<\kappa$. By (2.59) the Jost solutions obey the conjugation property (2.76). Moreover, the functions $\chi(x,\mathbf{k})$ and $\xi(x,\mathbf{k})$ defined as in (2.78) are bounded both in the x-variables and obey condition (2.80).

The discontinuity of the Jost solution $\Phi(\mathbf{k})$ at $\mathbf{k}_{\mathfrak{R}}\to\pm 0$ follows from (4.16) by means of (4.3), i.e., by applying $\check{\mathcal{L}}_1\Phi_1(\pm 0+i\mathbf{k}_{\mathfrak{I}})$ to (4.16) from the right. By (3.30) the discontinuity of $\Phi_1(\mathbf{k})$ at the imaginary axis is proportional to φ_1. Under condition (4.25) we have representation (4.26) thanks to which $G(i\kappa)\check{\mathcal{L}}_1\varphi_1=0$ by (4.22), (4.23). So the discontinuity of $\Phi_1(\mathbf{k})$ in the first equality in (4.3) does not contribute to the discontinuity of $\Phi(\mathbf{k})$ and we get by (4.16)

$$\Phi(x,+0+i\mathbf{k}_{\mathfrak{I}})-\Phi(x,-0+i\mathbf{k}_{\mathfrak{I}})=\theta(\kappa-|\mathbf{k}_{\mathfrak{I}}|)\varphi(x,\mathbf{k}_{\mathfrak{I}})w(\mathbf{k}_{\mathfrak{I}}), \tag{4.28}$$

where

$$w(\mathbf{k}_{\mathfrak{I}})=\frac{\psi(\mathbf{k}_{\mathfrak{I}})\check{\mathcal{L}}_1\Phi_1(i\mathbf{k}_{\mathfrak{I}})}{2\pi iA(\mathbf{k}_{\mathfrak{I}})\operatorname{sgn}\mathbf{k}_{\mathfrak{I}}},\quad |\mathbf{k}_{\mathfrak{I}}|<\kappa, \tag{4.29}$$

and again thanks to (4.25) we can omit specification of the limiting procedure for $\Phi_1(\pm 0+i\mathbf{k}_{\mathfrak{I}})$ in the r.h.s. Below in (4.38) and (4.42) we give the behavior of $\varphi(\mathbf{k}_{\mathfrak{I}})$ and $w(\mathbf{k}_{\mathfrak{I}})$ that enables to prove that in the limit $B(\kappa)\to 0$ one gets $\delta(\mathbf{k}_{\mathfrak{I}}-\kappa)$ in the r.h.s. of (4.28).

If we use for the numerator of (4.29) the explicit expression

$$\psi(\mathbf{k}_{\mathfrak{I}})\check{\mathcal{L}}_1\Phi_1(i\mathbf{k}_{\mathfrak{I}})=\int dx(\mathcal{L}_1^{\mathrm{d}}(x,\partial_x)\psi(x,\mathbf{k}_{\mathfrak{I}}))\Phi_1(x,i\mathbf{k}_{\mathfrak{I}}),$$

we recover the spectral data $w(\mathbf{k}_{\mathfrak{I}})$ describing the discontinuity of the Jost solutions introduced in Ref. 16. Using (4.3) and (4.15)–(4.17) $w(\mathbf{k}_{\mathfrak{I}})$ can be rewritten as

$$w(\mathbf{k}_{\mathfrak{I}})=\frac{\psi_1\vec{\mathcal{L}}_1G(-0+i\mathbf{k}_{\mathfrak{I}})\check{\mathcal{L}}_1\Phi_1(i\mathbf{k}_{\mathfrak{I}})}{2\pi i\ \operatorname{sgn}\mathbf{k}_{\mathfrak{I}}}\equiv\frac{\psi_1\vec{\mathcal{L}}_1\Phi(-0+i\mathbf{k}_{\mathfrak{I}})}{2\pi i\ \operatorname{sgn}\mathbf{k}_{\mathfrak{I}}}, \tag{4.30}$$

or

$$w(\mathbf{k}_{\mathfrak{I}})=\frac{\psi_1\vec{\mathcal{L}}_1G(+0+i\mathbf{k}_{\mathfrak{I}})\check{\mathcal{L}}_1\Phi_1(i\mathbf{k}_{\mathfrak{I}})}{2\pi iA(\mathbf{k}_{\mathfrak{I}})\operatorname{sgn}\mathbf{k}_{\mathfrak{I}}}\equiv\frac{\psi_1\vec{\mathcal{L}}_1\Phi(+0+i\mathbf{k}_{\mathfrak{I}})}{2\pi iA(\mathbf{k}_{\mathfrak{I}})\operatorname{sgn}\mathbf{k}_{\mathfrak{I}}}. \tag{4.31}$$

From the first equality here and the conjugation properties of all the objects involved we have

$$\overline{w(-\mathbf{k}_{\mathfrak{I}})}=\frac{\Psi_1(i\mathbf{k}_{\mathfrak{I}})\vec{\mathcal{L}}_1\varphi(\mathbf{k}_{\mathfrak{I}})}{2\pi iA(\mathbf{k}_{\mathfrak{I}})\operatorname{sgn}\mathbf{k}_{\mathfrak{I}}},\quad |\mathbf{k}_{\mathfrak{I}}|<\kappa. \tag{4.32}$$

Notice that by (2.59), (4.15), and (4.17) we get the conjugation property

$$\overline{\varphi(x,\mathbf{k}_{\mathfrak{I}})}=\psi(x,-\mathbf{k}_{\mathfrak{I}}), \tag{4.33}$$

which motivates the introduction of the multiplier $A(\mathbf{k}_{\mathfrak{I}})$ in (4.15). Then, by conjugation of (4.28) we get for the dual Jost solution

$$\Psi(x,+0+i\mathbf{k}_{\mathfrak{I}})-\Psi(x,-0+i\mathbf{k}_{\mathfrak{I}})=\theta(\kappa-|\mathbf{k}_{\mathfrak{I}}|)\psi(x,\mathbf{k}_{\mathfrak{I}})\overline{w(-\mathbf{k}_{\mathfrak{I}})}. \tag{4.34}$$

Thus we see that the discontinuity of the Jost solutions across the imaginary axis is given not in their terms, but in terms of the functions $\varphi(x,\mathbf{k}_\jmath)$, $\psi(x,\mathbf{k}_\jmath)$ introduced in (4.15) [or (4.17)]. From their definition it follows that they obey equations (2.75): $\tilde{\mathcal{L}}\varphi(\mathbf{k}_\jmath)=0$ and $\psi(\mathbf{k}_\jmath)\tilde{\mathcal{L}}=0$, and can be considered a generalization of the functions $\varphi_1(x)$, $\psi_1(x)$ to the case u_2 different from zero. However, they acquire a nontrivial dependence on $\mathbf{k}_\jmath$ and cannot be obtained as specific values of the Jost solutions. Due to the properties of the Green's function these solutions are discontinuous at $\mathbf{k}_\jmath=0$. In the following we refer to $\varphi(x,\mathbf{k}_\jmath)$ and $\psi(x,\mathbf{k}_\jmath)$ as auxiliary Jost solutions.

2. Behavior of Jost solutions and spectral data at the end points of the cut

The asymptotic behavior of the Jost solutions easily results from the asymptotic property of the Green's function given in (4.24). Applying $\tilde{\mathcal{L}}_1\varphi_1$ from the right and using definitions (4.22) and (4.23) we get

$$G(\mathbf{k})\tilde{\mathcal{L}}_1\varphi_1=\frac{\varphi_{\mathrm{reg},\pm}}{1-\gamma(\mathbf{k})B_\pm}+o(1),\quad \mathbf{k}\to\pm i\kappa. \tag{4.35}$$

Then, from the definitions (4.3) of the Jost solution and properties (3.6), (3.7) of the Jost solutions of the one-soliton case, we derive the asymptotic behavior

$$\Phi(\mathbf{k})=\sqrt{\frac{\kappa}{\pi}}\frac{ie^{\kappa x_0}\varphi_{\mathrm{reg},+}}{(\mathbf{k}-i\kappa)(1-\gamma(\mathbf{k})B_+)}+O(1),\quad \mathbf{k}\to+i\kappa, \tag{4.36}$$

$$\Phi(\mathbf{k})=\frac{e^{-\kappa x_0}\varphi_{\mathrm{reg},-}}{2\sqrt{\kappa\pi}(1-\gamma(\mathbf{k})B_-)}+o(1),\quad \mathbf{k}\to-i\kappa, \tag{4.37}$$

while the behavior of $\Psi(\mathbf{k})$ follows from conjugation property (2.76) and relations $\overline{\varphi_{\mathrm{reg},\pm}}=\psi_{\mathrm{reg},\mp}$ that follow from (4.22). As regards the auxiliary Jost solution $\varphi(\mathbf{k}_\jmath)$, by its definition (4.15) and (4.35) we get in the same way

$$\varphi(\mathbf{k}_\jmath)=\frac{\varphi_{\mathrm{reg},\pm}}{1-\gamma(+0+i\mathbf{k}_\jmath)B_\pm}+o(1),\quad \mathbf{k}_\jmath\to\pm\kappa, \tag{4.38}$$

and asymptotics for $\psi(\mathbf{k}_\jmath)$ follow again by the conjugation property (4.33). We see that the behavior of the Jost and auxiliary Jost solutions at the points $\mathbf{k}_\jmath=\pm\kappa$ is determined by the value of B_+. If $B_+=0$ the behavior of the Jost solutions is like in the case $u_2\equiv 0$ [cf. (3.6) and (3.7)] and the auxiliary Jost solutions are finite and nonzero at these points. If $B_+\neq 0$, the behavior of both types of Jost solutions is modified at these points by the multiplier $(\log||\mathbf{k}_\jmath|-\kappa|)^{-1}$ as follows from (3.26). In particular, in this case we have

$$\varphi(\pm\kappa)=\psi(\pm\kappa)=0. \tag{4.39}$$

Now we apply $\tilde{\mathcal{L}}_1\varphi_1$ from the right to (4.19) with the upper sign and cancel $G^\sigma(\pm 0)\tilde{\mathcal{L}}_1\varphi_1$ thanks to (4.39). Then by (4.31) and the conjugation properties (2.76) and (4.12) we get the following expression of $\varphi(x,\mathbf{k}_\jmath)$ in terms of the Jost solution,

$$\varphi(x,\mathbf{k}_\jmath)=i\int_{\kappa\,\mathrm{sgn}\,\mathbf{k}_\jmath}^{\mathbf{k}_\jmath}d\alpha\,A(\alpha)\overline{w(-\alpha)}\Phi(x,+0+i\alpha), \tag{4.40}$$

which, as we will see below, is necessary for closing the inverse problem.

For the spectral data $A(\mathbf{k}_\jmath)$ in (4.10) we can use the first equality in (4.17) and in the case $B_+\neq 0$ also (4.40), and, then, by (4.27) and (4.31) we obtain the relation

$$A(\mathbf{k}_\jmath)=1+i\int_{\kappa\ \mathrm{sgn}\ \mathbf{k}_\jmath}^{\mathbf{k}_\jmath} d\alpha\, w(\alpha)\overline{w(-\alpha)}A^2(\alpha),$$

giving the explicit expression of $A(\mathbf{k}_\jmath)$ in terms of the spectral data $w(\mathbf{k}_\jmath)$,

$$A(\mathbf{k}_\jmath)=\left(1-i\int_{\kappa\ \mathrm{sgn}\ \mathbf{k}_\jmath}^{\mathbf{k}_\jmath} d\alpha\, w(\alpha)\overline{w(-\alpha)}\right)^{-1}, \tag{4.41}$$

which also is necessary for closing the inverse problem.

For the spectral data $w(\mathbf{k}_\jmath)$ we can use the second equality in (4.31) and taking into account that by (4.22) and (4.23) $\psi_1\vec{\mathcal{L}}_1\varphi_{\mathrm{reg},\pm}=B_\pm$ we get by (4.36) and (4.37) the asymptotic behaviors

$$w(\mathbf{k}_\jmath)=\frac{i\sqrt{\kappa}e^{\kappa x_0}B_+}{2\pi^{3/2}(\kappa-\mathbf{k}_\jmath)(1-\gamma(+0+i\mathbf{k}_\jmath)B_+)}+O(1),\quad \mathbf{k}_\jmath\to\kappa-0, \tag{4.42}$$

$$w(\mathbf{k}_\jmath)=\frac{ie^{-\kappa x_0}B_-}{4\sqrt{\kappa}\pi^{3/2}(1-\gamma(+0+i\mathbf{k}_\jmath)B_-)}+o(1),\quad \mathbf{k}_\jmath\to-\kappa+0. \tag{4.43}$$

Notice that for $B_+=0$ both these asymptotics are equal to zero, while as we mentioned above, in the product on the r.h.s. of (4.28) one gets δ-function in this case.

Concluding this study of the properties of the Jost solutions and spectral data at the points $\mathbf{k}_\jmath=\pm\kappa$, let us emphasize that, in order to get relations among different spectral data, which are crucial for solving the inverse problem, as for instance (4.32) used in getting (4.40), it is necessary to use different representations for the spectral data, like (4.30) and (4.31), in terms of different solutions of the nonstationary Schrödinger equation and its dual. These representations can be obtained in the framework of the resolvent approach, while they cannot be derived if one deals only with equations for the Jost solutions (cf. Ref. 16).

3. Bilinear representation for the resolvent and Green's functions

Now, we can derive a bilinear representation of the resolvent in terms of the Jost solutions. We proved that for $s_2\neq0$ its derivative with respect to s_2 obeys (2.46), so using notations (4.4) for the limiting values at $s_2=0$ we get

$$\hat{M}(x,x';s)=\frac{1}{2\pi i}\int dk\,[\theta(x_2-x_2')-\theta(2ks_1-s_2)]\,\Phi(x,k+is_1)\Psi(x',k+is_1)$$
$$+\mathrm{sgn}\,s_1[\theta(x_2-x_2')-\theta(-s_2)][G(x,x';+0+is_1)-G(x,x';-0+is_1)].$$

Then, thanks to (4.16), we get the following generalization of the bilinear representation (3.16) for the resolvent of the perturbed potential:

$$\hat{M}(x,x';s)=\frac{1}{2\pi i}\int dk\,[\theta(x_2-x_2')-\theta(2ks_1-s_2)]\,\Phi(x,k+is_1)\Psi(x',k+is_1)$$
$$+\frac{\theta(\kappa-|s_1|)}{2\pi iA(s_1)}[\theta(x_2-x_2')-\theta(-s_2)]\varphi(x,s_1)\psi(x',s_1). \tag{4.44}$$

If we consider the kernel $M(x,x';s)$ defined by (2.13), then both terms on the r.h.s. give distributions belonging to $\mathcal{S}'$. For the first term this follows from the mentioned properties of the functions χ and ξ, defined as in the decaying case by (2.78), and for the second term from the fact that $e^{-s_1x_1}\varphi(x,s_1)$ and $e^{s_1x_1}\psi(x,s_1)$ are bounded at space infinity when $|s_1|<\kappa$. Equation (2.45)

at $s_1 \neq 0$ follows from the analyticity of the Jost solutions and from the derivatives of (4.40) and of the analogous equation for $\psi(s_1)$. The absence of a discontinuity at $s_1=0$ in the case $s_2 \neq 0$ like in the derivation of (2.92) is equivalent to the condition

$$\int dk\, \Phi^+(k) \otimes \Psi^+(k) + \frac{\varphi^+ \otimes \psi^+}{A^+} = \int dk\, \Phi^-(k) \otimes \Psi^-(k) + \frac{\varphi^- \otimes \psi^-}{A^-}, \tag{4.45}$$

where we used notation (2.91) also for the limiting values of the auxiliary Jost solutions on the real axis

$$\varphi^{\pm}(x) = \lim_{\pm \mathbf{k}_\Im \to +0} \varphi(x, \mathbf{k}_\Im), \quad \psi^{\pm}(x) = \lim_{\pm \mathbf{k}_\Im \to +0} \psi(x, \mathbf{k}_\Im). \tag{4.46}$$

Thanks to (2.76) and (4.33) these limiting values obey the conjugation properties

$$\overline{\Phi^{\pm}(x,k)} = \Psi^{\mp}(x,k), \quad \overline{\varphi^{\pm}(x)} = \psi^{\mp}(x), \quad k \in \mathbb{R}. \tag{4.47}$$

By (2.49) the bilinear representation (4.44) for the resolvent leads to the following bilinear representation for the Green's function of the Jost solutions:

$$\begin{aligned} G(x,x',\mathbf{k}) = {} & \frac{1}{2\pi i} \int dk' \, [\, \theta(x_2 - x_2') - \theta(\mathbf{k}_\Im k')\,] \, \Phi(x, k' + \mathbf{k}) \Psi(x', k' + \mathbf{k}) \\ & + \frac{\theta(\kappa - |\mathbf{k}_\Im|)}{2\pi i A(\mathbf{k}_\Im)} [\, \theta(x_2 - x_2') - \theta(-\mathbf{k}_\Re \mathbf{k}_\Im)\,] \varphi(x, \mathbf{k}_\Im) \psi(x', \mathbf{k}_\Im), \end{aligned} \tag{4.48}$$

which generalizes (3.22). Below we use this bilinear representation for deriving relations between the Jost and advanced/retarded solutions.

D. Discontinuity of the resolvent at $s=0$

1. The advanced/retarded Green's functions and solutions

Above we investigated the behavior of the resolvent when at least one of the variables s_1 or s_2 is different from zero. As we have seen in the case of decaying potentials, it is just the study of the discontinuity of the resolvent at $s=0$ that leads to relations between Jost and advanced/retarded solutions which can be used for defining the spectral data. In the present case of a perturbed one-soliton potential the method is pretty close and, therefore, we omit details and we mainly present the peculiarities of this case. First, we introduce the advanced/retarded Green's functions as specific limits of the resolvent in the same way as in (2.52). It is straightforward to prove that they obey equations (2.68) and (2.69) and integral equations (2.70). In order to find the difference between the advanced and the retarded Green's function we use the Hilbert identity in the form (4.2), which, according to our previous discussion, in the case of a perturbed one-soliton potential is more convenient than (2.42). So we choose in (4.2) both s and s' real, $s_1' = s_1 = 0$ and consider the limits $s_2' \to \pm 0$, $s_2 \to \mp 0$. We get

$$G_+ - G_- = G_\pm \tilde{\mathcal{L}}_1 (G_{1,+} - G_{1,-}) \vec{\mathcal{L}}_1 G_\mp,$$

which by (3.31) gives for the discontinuity the representation

$$G_+ - G_- = \frac{1}{2\pi i} \left(\int dk\, \Phi_\pm(k) \otimes \Psi_\mp(k) + \varphi_\pm \otimes \psi_\mp \right), \tag{4.49}$$

where we introduced not only, in analogy with (2.57), the advanced/retarded solutions $\Phi_\pm(k)$, $\Psi_\pm(k)$ but also the auxiliary advanced/retarded solutions $\varphi_\pm$, $\psi_\pm$ defined by

$$\Phi_{\pm}(k)=G_{\pm}\tilde{\mathcal{L}}_1\Phi_1(k),\quad \varphi_{\pm}=G_{\pm}\tilde{\mathcal{L}}_1\varphi_1, \tag{4.50}$$

$$\Psi_{\pm}(k)=\Psi_1(k)\vec{\mathcal{L}}_1G_{\pm},\quad \psi_{\pm}=\psi_1\vec{\mathcal{L}}_1G_{\pm}. \tag{4.51}$$

It is easy to check that these functions $\Phi_{\pm}(x,k)$, $\Psi_{\pm}(x,k)$ and $\varphi_{\pm}(x)$, $\psi_{\pm}(x)$ are solutions of the differential equations (2.86) and obey a conjugation property, i.e., (2.87) for $\Phi_{\pm}(x,k)$, $\Psi_{\pm}(x,k)$, and

$$\overline{\varphi_{\pm}}=\psi_{\mp} \tag{4.52}$$

for the auxiliary solutions.

The bilinear representation (4.44) for the resolvent, thanks to (2.52), gives the following representation for the advanced/retarded Green's functions in terms of the Jost and auxiliary Jost solutions on the real axis,

$$G_{\pm}(x,x')=\frac{\pm\theta(\pm(x_2-x_2'))}{2\pi i}\left(\int dk\,\Phi^{\sigma}(x,k)\Psi^{\sigma}(x',k)+\frac{\varphi^{\sigma}(x)\psi^{\sigma}(x')}{A^{\sigma}}\right), \tag{4.53}$$

where we used notations (2.91) for the limiting values of the Jost solutions at the real axis and where the l.h.s. is independent on the sign $\sigma=+,-$ due to condition (4.45).

2. Relations among Green's functions $G^{\pm}(k)$ and $G_{\pm}$

The difference among the limiting values of the Green's function $G(\mathbf{k})$ on the two sides of the real axis and the advanced/retarded Green's functions, like in the case of the decaying potential, can be presented in two forms. The first one follows from (4.48) in the limits $\mathbf{k}\to k\pm i0$ and (4.53):

$$G^{\sigma}(k)-G_{\pm}=\frac{\mp 1}{2\pi i}\left(\int dk'\;\theta(\pm\sigma(k'-k))\,\Phi^{\sigma}(k')\otimes\Psi^{\sigma}(k')+\theta(\mp\sigma k)\,\frac{\varphi^{\sigma}\otimes\psi^{\sigma}}{A^{\sigma}}\right). \tag{4.54}$$

A second type of relation, analogous to (2.74), can be derived from the Hilbert identity (4.2). Taking into account definitions (2.72) and (2.52) we get

$$G^{\sigma}(k)-G_{\pm}=G_{\pm}\tilde{\mathcal{L}}_1(G_1^{\sigma}(k)-G_{1,\pm})\vec{\mathcal{L}}_1G^{\sigma}(k),\quad k\in\mathbb{R},$$

so that we can use (3.33) and definitions (4.50) and (4.51) to derive

$$\begin{aligned}G^{\sigma}(k)-G_{\pm}=&\frac{\mp 1}{2\pi i}\int dk'\;\theta(\mp\sigma(k-k'))\Phi_{\pm}(k')\otimes(\Psi_1(k')\vec{\mathcal{L}}_1G^{\sigma}(k))\\&\mp\frac{\theta(\mp\sigma k)}{2\pi i}\,\varphi_{\pm}\otimes(\psi_1\vec{\mathcal{L}}_1G^{\sigma}(k)),\quad \sigma=+,-.\end{aligned} \tag{4.55}$$

Now we can use relations (4.54) and (4.55) in order to get relations among Jost and advanced/retarded solutions, introduce spectral data and get characterization equations such that, in particular, condition (4.45) is accomplished.

E. Spectral data

1. Relations among Jost and advanced/retarded solutions

In order to derive these relations we again use definitions (4.3) and (4.15) for $\mathbf{k}=k\in\mathbb{R}$ and apply $\tilde{\mathcal{L}}_1\Phi_1(k)$ and $\tilde{\mathcal{L}}_1\varphi_1$ to (4.55) from the right (the latter one to the limit of (4.55) at $k\to+0$). Then by (2.91), (4.13), (4.46), and (4.50) we get

$$\Phi^{\sigma}(k)=\int dk'\;\Phi_{\pm}(k')r_{\pm}^{\sigma}(k',k)+\varphi_{\pm}r_{\pm}^{\sigma}(k),\quad \sigma=+,-, \tag{4.56}$$

$$\varphi^{\sigma}=\int dk'\,\Phi_{\pm}(k')\tau_{\pm}^{\sigma}(k')+\varphi_{\pm}(A^{\sigma})^{\theta(\mp\sigma)}, \tag{4.57}$$

generalizing (2.96), where we introduced spectral data [cf. (2.97) and (2.98)] by means of relations

$$r_{\pm}^{\sigma}(k,k')=\delta(k-k')\mp\theta(\pm\sigma(k-k'))r^{\sigma}(k,k'), \tag{4.58}$$

$$r^{\sigma}(k,k')=\frac{\Psi_1(k)\vec{\mathcal{L}}_1G^{\sigma}(k')\tilde{\mathcal{L}}_1\Phi_1(k')}{2\pi i}\equiv\frac{\Psi_1(k)\vec{\mathcal{L}}_1\Phi^{\sigma}(k')}{2\pi i}, \tag{4.59}$$

$$r_{\pm}^{\sigma}(k)=\mp\theta(\mp\sigma k)r^{\sigma}(k), \tag{4.60}$$

$$r^{\sigma}(k)=\frac{\psi_1\vec{\mathcal{L}}_1G^{\sigma}(k)\tilde{\mathcal{L}}_1\Phi_1(k)}{2\pi i}\equiv\frac{\psi_1\vec{\mathcal{L}}_1\Phi^{\sigma}(k)}{2\pi i}, \tag{4.61}$$

$$\tau_{\pm}^{\sigma}(k)=\mp\theta(\pm\sigma k)\tau^{\sigma}(k), \tag{4.62}$$

$$\tau^{\sigma}(k)=\frac{\Psi_1(k)\vec{\mathcal{L}}_1G^{\sigma}(+0)\tilde{\mathcal{L}}_1\varphi_1}{2\pi i}\equiv\frac{\Psi_1(k)\vec{\mathcal{L}}_1\varphi^{\sigma}}{2\pi i}. \tag{4.63}$$

We write equations (4.56) and (4.57) in a more compact form as

$$(\Phi^{\sigma},\,\varphi^{\sigma})=(\Phi_{\pm},\,\varphi_{\pm})*\mathcal{R}_{\pm}^{\sigma}, \tag{4.64}$$

and omit equations for Ψ and ψ that can be obtained analogously, or by conjugation. Here we introduced the matrix operator

$$\mathcal{R}_{\pm}^{\sigma}(k,k')=\begin{pmatrix} r_{\pm}^{\sigma}(k,k') & \tau_{\pm}^{\sigma}(k) \\ r_{\pm}^{\sigma}(k') & (A^{\sigma})^{\theta(\mp\sigma)} \end{pmatrix}. \tag{4.65}$$

$\mathcal{R}^{\dagger}$ denotes the Hermitian conjugate operator. Solutions $\Phi(x,k)$ and $\varphi(x)$ [$\Psi(x,k)$ and $\psi(x)$] have been combined in a row (correspondingly, column), where only the first element depends on k. For two operators $\mathcal{R}$ and $\mathcal{R}'$ with elements $\mathcal{R}_{ij}$, $\mathcal{R}'_{ij}$ with dependence on the arguments k, k' like in (4.65) we introduce a composition $*$ that gives a matrix of the same form with elements

$$\begin{aligned}
(\mathcal{R}*\mathcal{R}')_{11}(k,k')&=\int dk''\,\mathcal{R}_{11}(k,k'')\mathcal{R}'_{11}(k'',k')+\mathcal{R}_{12}(k)\mathcal{R}'_{21}(k'),\\
(\mathcal{R}*\mathcal{R}')_{12}(k,k')&=\int dk''\,\mathcal{R}_{11}(k,k'')\mathcal{R}'_{12}(k'')+\mathcal{R}_{12}(k)\mathcal{R}'_{22},\\
(\mathcal{R}*\mathcal{R}')_{21}(k,k')&=\int dk''\,\mathcal{R}_{21}(k'')\mathcal{R}'_{11}(k'',k')+\mathcal{R}_{22}\mathcal{R}'_{21}(k'),\\
(\mathcal{R}*\mathcal{R}')_{22}(k,k')&=\int dk''\,\mathcal{R}_{21}(k'')\mathcal{R}'_{12}(k'')+\mathcal{R}_{22}\mathcal{R}'_{22}.
\end{aligned} \tag{4.66}$$

The unity matrix in the set of such operators is given by

$$\mathcal{I}(k,k')=\begin{pmatrix} \delta(k-k') & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.67}$$

In the same way we define the product of the matrix by the row (from the left) and by column (from the right) of the type used in (4.64). This composition is also denoted by an asterisk to emphasize that the integration is performed in the first (upper) element only.

Equation (4.64) gives the boundary values of the Jost solutions in terms of the advanced/retarded ones. In order to get the inverse relations we apply the same procedures as above to Eq. (4.54) and in analogy with (2.102) in terms of the introduced notations we get

$$(\Phi_{\pm}, \varphi_{\pm}) = (\Phi^{\sigma}, \varphi^{\sigma}) * (W^{\sigma})^{-1} (\mathcal{R}_{\pm}^{-\sigma})^{\dagger}, \tag{4.68}$$

where we introduced the constant matrix

$$W^{\sigma} = \begin{pmatrix} 1 & 0 \\ 0 & A^{\sigma} \end{pmatrix}. \tag{4.69}$$

Alternative spectral data that relate values of the Jost solutions computed on the two sides of the real axis appear if we insert $(\Phi_{\pm}, \varphi_{\pm})$ from (4.68) into (4.64) for opposite sign of σ. Thus we get

$$(\Phi^{\sigma}, \varphi^{\sigma}) = (\Phi^{-\sigma}, \varphi^{-\sigma}) * (W^{-\sigma})^{-1} \mathcal{F}^{-\sigma}, \tag{4.70}$$

where we denoted

$$\mathcal{F}^{\sigma} = (\mathcal{R}_{\pm}^{-\sigma})^{\dagger} * \mathcal{R}_{\pm}^{-\sigma}. \tag{4.71}$$

Finally let us note that Eqs. (4.58)–(4.63) together with Eqs. (4.31), (4.40), and (4.41) solve completely the so-called direct problem, furnishing all spectral data and the auxiliary function $\varphi(x, \mathbf{k}_3)$ in terms of the Jost solution $\Phi(x, \mathbf{k})$ and the functions $\Phi_1(x, \mathbf{k})$ and $\varphi_1(x)$ relative to the one-soliton potential.

Below we discuss the properties of these spectral data and relations between them.

2. Characterization equations for spectral data

Inserting (4.68) in (4.64) we get relation $(\Phi^{\sigma}, \varphi^{\sigma}) = (\Phi^{\sigma}, \varphi^{\sigma})(W^{\sigma})^{-1} (\mathcal{R}_{\pm}^{-\sigma})^{\dagger} * \mathcal{R}_{\pm}^{\sigma}$, $\sigma = +, -$, so taking into account the asymptotic behavior of the Jost solutions with respect to the x-variables we derive the characterization equation

$$(\mathcal{R}_{\pm}^{-\sigma})^{\dagger} * \mathcal{R}_{\pm}^{\sigma} (W^{\sigma})^{-1} = \mathcal{I} \tag{4.72}$$

for the spectral data $\mathcal{R}_{\pm}^{\sigma}$. Another characterization equation follows by inserting (4.64) into (4.68):

$$\mathcal{R}_{\pm}^{\sigma} (W^{\sigma})^{-1} * (\mathcal{R}_{\pm}^{-\sigma})^{\dagger} = \mathcal{I}, \tag{4.73}$$

and the third one is the condition that the r.h.s. of (4.71) is independent of the choice of the sign $\pm$:

$$(\mathcal{R}_{+}^{\sigma})^{\dagger} * \mathcal{R}_{+}^{\sigma} = (\mathcal{R}_{-}^{\sigma})^{\dagger} * \mathcal{R}_{-}^{\sigma}. \tag{4.74}$$

These equations generalize the characterization equations of the case of decaying potential.[17] We see that (4.72) and (4.73) are just the condition that the "triangular operators" $\mathcal{R}_{\pm}^{\sigma}$ are invertible and that $(\mathcal{R}_{\pm}^{-\sigma})^{\dagger}$ is the inverse of $\mathcal{R}_{\pm}^{\sigma} (W^{\sigma})^{-1}$. They define, say, $\mathcal{R}_{\pm}^{-}$ if $\mathcal{R}_{\pm}^{+}$ is given. Thus essential restrictions on the spectral data are imposed by (4.74), that is a consequence of the reality condition on the potential $u(x)$. Thanks to (4.64) this equation proves (4.45). By (4.65) we write (4.74) as a system of three equations (for some sign σ):

$$\left(\int_{k'}^{+\infty}-\int_{-\infty}^{k}\right)dk''\,\overline{r^{\sigma}(k'',k)}r^{\sigma}(k'',k')=\operatorname{sgn}k\;\theta(kk')\,\overline{r^{\sigma}(k)}r^{\sigma}(k')+\sigma r^{\sigma}(k,k')+\sigma\overline{r^{\sigma}(k',k)},\tag{4.75}$$

$$[\,\theta(k)A^{\sigma}+\theta(-k)]\overline{r^{\sigma}(k)}=\sigma\left(\int_{0}^{+\infty}-\int_{-\infty}^{k}\right)dk'\,\overline{r^{\sigma}(k',k)}\,\tau^{\sigma}(k')-\tau^{\sigma}(k),\tag{4.76}$$

$$|A^{\sigma}|^{2}=\int dk\,\operatorname{sgn}k\,|\tau^{\sigma}(k)|^{2}+1.\tag{4.77}$$

Characterization equations for the spectral data (4.71) look simpler,

$$(\mathcal{F}^{\sigma})^{\dagger}=\mathcal{F}^{\sigma},\quad (\mathcal{F}^{\sigma})^{-1}=(W^{-\sigma})^{-1}\mathcal{F}^{-\sigma}(W^{\sigma})^{-1},\tag{4.78}$$

to which we have to add the requirement that $\mathcal{F}^{\sigma}$ can be decomposed in the product (4.71) of two sets of triangular operators (4.65).

3. Discontinuities of spectral data

The cuts of the Jost solutions intersect on the complex plane at $k=0$. Thanks to property (4.6) for the Green's function we get by (4.3) that the Jost solution obeys property

$$\lim_{\sigma\mathbf{k}_{\mathfrak{J}}\to+0}\Phi(\pm 0+i\mathbf{k}_{\mathfrak{J}})=\Phi^{\sigma}(\pm 0),\quad \sigma=+,-,\tag{4.79}$$

which means that it is necessary to pay special attention to the properties of the spectral data at this point $k=0$. Thus taking the limits $\mathbf{k}_{\mathfrak{J}}\to\sigma 0$ in (4.28) we get for the boundary values of the Jost and auxiliary Jost solutions the relation

$$\Phi^{\sigma}(+0)-\Phi^{\sigma}(-0)=\varphi^{\sigma}w^{\sigma}.\tag{4.80}$$

The spectral data $r^{\sigma}(k,k')$ are defined in (4.59) in terms of the Jost solution $\Psi_1(k)$, which is a continuous function of k, and of $\Phi^{\sigma}(k')$ which is discontinuous at $k'=0$. Therefore $r^{\sigma}(k,k')$ is continuous with respect to k and k' with a possible discontinuity at $k'=0$. Precisely, by (4.59), (4.63), and (4.80) we get

$$r^{\sigma}(k,+0)-r^{\sigma}(k,-0)=\tau^{\sigma}(k)w^{\sigma}.\tag{4.81}$$

The spectral data $\tau^{\sigma}(k)$ are continuous at $k=0$ and from their definition (4.63) and the definitions (4.10) and (4.29) of A and w we derive

$$\tau^{\sigma}(0)=\sigma A^{\sigma}\overline{w^{-\sigma}}.\tag{4.82}$$

The spectral data $r^{\sigma}(k)$ are discontinuous at $k=0$ as follows from their definition (4.61). Taking into account (4.30) and (4.31), we get the relations

$$r^{\sigma}(+0)=\sigma A^{\sigma}w^{\sigma},\tag{4.83}$$

$$r^{\sigma}(-0)=\sigma w^{\sigma}.\tag{4.84}$$

These behaviors at $k=0$ are compatible with the characterization equations. In fact, choosing $k'=\pm 0$ in (4.75) we get (4.76) and analogously (4.76) at $k=\pm 0$ gives (4.77).

F. Inverse problem and time evolution

Let now be given the spectral data, i.e., function $w(\mathbf{k}_{\mathfrak{J}})$ and, say, $\mathcal{R}^{+}_{\pm}$. Function $w(\mathbf{k}_{\mathfrak{J}})$ is continuously differentiable on the interval $|\mathbf{k}_{\mathfrak{J}}|<\kappa$ except for the point $\mathbf{k}_{\mathfrak{J}}=0$, where it has

bounded limits $w^{\pm}$. Moreover, $w(\mathbf{k}_\mathfrak{I})$ has the asymptotic behaviors (4.42), (4.43) and $A(\mathbf{k}_\mathfrak{I})$ defined by (4.41) is bounded on this interval and has finite limits $A^{\pm}$ at zero. The spectral data $\mathcal{R}_{\pm}^{+}$ obey the characterization equation (4.74), or, more explicitly the characterization equations (4.75)–(4.77) for its elements in (4.65) and relations (4.81)–(4.84). The matrix operator $\mathcal{R}_{\pm}^{+}$ also admits inverse, so that the spectral data $\mathcal{R}_{\pm}^{-}$ can be introduced by (4.72) or (4.73) with the triangularity property given in (4.65), which means that the spectral data $\mathcal{F}^{-}$ can be defined by (4.71). Taking into account that the Jost solution $\Phi(x,\mathbf{k})$ is analytic in the complex $\mathbf{k}$-plane with a discontinuity across the real axis, given by the first equation in (4.70) for $\sigma=+$, and with a discontinuity across the interval $|\mathbf{k}_\mathfrak{I}|<\kappa$ of the imaginary axis, given by (4.28), and has an asymptotic normalization at $\mathbf{k}\to\infty$ given by (2.78) and (2.80), the Cauchy–Green formula yields

$$\Phi(x,\mathbf{k})=e^{-i\mathbf{k}x_1-i\mathbf{k}^2x_2}+\frac{1}{2\pi i}\int dk'\frac{e^{i(k'-\mathbf{k})x_1+i(k'^2-\mathbf{k}^2)x_2}}{k'-\mathbf{k}}\Bigg(\int dk''\Phi^{-}(x,k'')[\mathcal{F}_{11}^{-}(k'',k')-\delta(k''-k')]+\frac{\varphi^{-}(x)}{A^{-}}\mathcal{F}_{21}^{-}(k')\Bigg)-\frac{1}{2\pi i}\int_{-\kappa}^{\kappa}\frac{d\alpha\, w(\alpha)}{\alpha+i\mathbf{k}}e^{-(\alpha+i\mathbf{k})x_1-i(\alpha^2+\mathbf{k}^2)x_2}\varphi(x,\alpha). \tag{4.85}$$

Notice that the singular behavior (4.42) of $w(\alpha)$ at $\alpha=\kappa$ is smoothed by (4.38) and, consequently, the integral on the r.h.s. is well defined. It is necessary to emphasize that equalities (4.40) and (4.85) were derived under condition (4.25) that excludes the case $u_2(x)\equiv 0$. Indeed, in this case $G_{\mathrm{reg}}(i\kappa)=G_{1,\mathrm{reg}}(i\kappa)$ so that by (4.23) $B(\kappa)=0$.

The integral equation (4.85) together with (4.40) solves the inverse problem. In fact, considering (4.40) and the limits of (4.85) as $\mathbf{k}\to k-i0$, $k\in\mathbb{R}$, and as $\mathbf{k}\to+0+i\mathbf{k}_\mathfrak{I}$, we obtain a system of three linear integral equations for $\{\Phi^{-}(x,k),\Phi(x,+0+i\mathbf{k}_\mathfrak{I}),\varphi(x,\mathbf{k}_\mathfrak{I})\}$, whose solution is uniquely determined in terms of the spectral data. When these boundary values are determined, the Jost solution for generic $\mathbf{k}\in\mathbb{C}$ is given by (4.85) and then the potential is reconstructed in the standard way by (2.78), (2.81) as

$$u(x)=\frac{1}{\pi}\frac{\partial}{\partial x_1}\Bigg[\int dk\, e^{ikx_1+ik^2x_2}\Bigg(\int dk'\Phi^{-}(x,k')[\mathcal{F}_{11}^{-}(k',k)-\delta(k'-k)]+\frac{\varphi^{-}(x)}{A^{-}}\mathcal{F}_{21}^{-}(k)\Bigg)-i\int_{-\kappa}^{\kappa}d\alpha\, w(\alpha)\, e^{-\alpha x_1-i\alpha^2x_2}\varphi^{-}(x,\alpha)\Bigg]. \tag{4.86}$$

Since, in the resolvent approach, all spectral data can be given as special reductions of the extended resolvent, one can derive directly (see Ref. 4 for details) the time evolution of the spectral data related to a solution of (1.2). We omit here these calculations and give only the final result on the time evolution of the spectral data:[16]

$$\mathcal{F}^{-}(k,k',t)=\begin{pmatrix} e^{-4ik^3t} & 0\\ 0 & 1\end{pmatrix}\mathcal{F}^{-}(k,k')\begin{pmatrix} e^{4ik'^3t} & 0\\ 0 & 1\end{pmatrix},\quad k,k'\in\mathbb{R}, \tag{4.87}$$

$$w(\mathbf{k}_\mathfrak{I},t)=e^{4\mathbf{k}_\mathfrak{I}^3t}w(\mathbf{k}_\mathfrak{I}), \tag{4.88}$$

$$A(\mathbf{k}_\mathfrak{I},t)=A(\mathbf{k}_\mathfrak{I}). \tag{4.89}$$

Taking the time evolution (4.88) into account we get that (4.42) and (4.43) are preserved under the dynamics and like in the pure one-soliton case

$$\kappa(t)=\kappa,\quad x_0(t)=x_0+4\kappa^2t, \tag{4.90}$$

where $x_0(t)$ is the parameter of the one-soliton solution (3.2).

V. CONCLUSION

We presented the main aspects of what we call the extended resolvent approach to the spectral theory of differential operators and we tested it in the two-dimensional case of the nonstationary Schrödinger equation with decaying and nondecaying potentials at large distances in the plane. We showed that a specific advantage of this approach is that the extended resolvent $M(s)$ of the differential operator (1.1), which depends on a parameter $s \in \mathbb{R}^2$, can be used as a general tool for finding all mathematical objects, such as Green's functions, Jost and auxiliary Jost solutions, advanced/retarded solutions and spectral data, which result to be necessary for developing the spectral theory. In fact, the introduction of all these quantities follow naturally from the study of departure from analyticity of the extended resolvent and of its discontinuities, together with its reductions. In particular, the different Green's functions involved in the theory are values (in general limiting values) of the resolvent $M(s)$ at different specific points s, which are suggested by the behavior in s of $M(s)$ itself. Moreover, the study of the properties of all these objects is reduced to the study of the resolvent $M(s)$, which can be accomplished by using Hilbert-type identities and the bilinear representation (2.90). This representation gives the extended resolvent in terms of the Jost solutions and supplies a simple and straightforward way of deriving relations between different kinds of solutions of the linear problem, constructing spectral data and deriving relations between them, as well as characterization equations.

ACKNOWLEDGMENTS

This work was supported in part by the Russian Foundation for Basic Research (Grant No. 02-01-00484) and by PRIN 2002 ''Sintesi.''

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Novel integrable reductions in nonlinear continuum mechanics via geometric constraints

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(Received 15 December 2002; accepted 9 April 2003)

The nonlinear equations that describe solitonic behavior in physical systems have, to-date, typically been derived by approximation or expansion methods. Here, by contrast, hidden integrable structure is revealed in diverse areas of nonlinear continuum mechanics through natural geometric constraints. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1589155]

I. INTRODUCTION

The basic equations of hydrodynamics, magnetohydrodynamics, and finite deformation elasticity are intrinsically nonlinear. The extent to which these and other governing equations of nonlinear continuum mechanics naturally admit integrable structure and are accordingly amenable to the powerful techniques of modern soliton theory remains an important open question. Hitherto, whereas solitonic phenomena have been observed in widely diverse areas in nature, the nonlinear equations that describe solitons have typically been derived by approximation or expansion methods. It is well-established that solitonic equations arise naturally out of the geometry of those privileged classes of surfaces that admit invariance under Bäcklund transformations.[1] Soliton systems that occur, without resort to approximation, in nonlinear physics or continuum mechanics have been relatively unknown. The prime exception is the Ernst equation which constitutes a reduction of Einstein's equations in general relativity.[2] However, the Ernst equation may be formulated as an elliptic counterpart of a classical Bianchi system descriptive of a class of hyperbolic surfaces constrained to admit a Bäcklund transformation.[1] Indeed, the celebrated Harrison transformation for the Ernst equation as set down in Ref. 3 is the counterpart of a classical Bäcklund transformation for the Bianchi system. This important paradigm motivates an investigation into how appropriate geometric constraints imposed on nonlinear physical models might reveal hidden integrable structure. Here, we bring together in a single account recent work by the authors on the application of geometric constraints to reveal hidden integrable structure over a range of nonlinear physical models in

(i) hydrodynamics,
(ii) magnetohydrodynamics,
(iii) the kinematics of ideal fiber-reinforced materials, and
(iv) elastostatics of shell membranes.

Integrable connections in the theory of liquid crystals have recently been uncovered in Ref. 4.

II. HYDRODYNAMICS BACKGROUND. GENESIS OF THE NLS EQUATION

The celebrated nonlinear Schrödinger (NLS) equation

$$\mathrm{i}\frac{\partial q}{\partial t}+\frac{\partial^2 q}{\partial x^2}+\nu|q|^2 q=0 \tag{2.1}$$

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models a wide range of physical phenomena. It was originally derived in explicit form in the context of the self-focusing of optical beams in nonlinear media.[5,6] However, the origins of the NLS equation or, equivalently, if $\nu>0$, of the Heisenberg spin equation[7]

$$\frac{\partial \mathbf{S}}{\partial t}=\mathbf{S}\times\frac{\partial^2 \mathbf{S}}{\partial x^2}, \quad \mathbf{S}^2=1, \tag{2.2}$$

go back to work in hydrodynamics at the beginning of the 20th century. Thus, Da Rios,[8] in 1906, in a study of the motion of an isolated inextensible vortex filament in an unbounded fluid, derived, via what is essentially the localized induction approximation (LIA), a pair of nonlinear coupled equations for the temporal evolution of the curvature and torsion of the filament. These equations may be conjugated to produce the NLS equation.[9] The original and subsequent results by Da Rios were collected in a survey by Levi-Civita.[10] An interesting account of the rediscovery of the work of Da Rios has been given by Ricca.[11]

The origins of the NLS equation then seem to reside in hydrodynamics, albeit via approximation. That it arises in hydrodynamics in the guise of the Heisenberg spin equation but rather via a geometric constraint was established only recently by Rogers.[12] The origins of that study go back to a long outstanding problem in hydrodynamics posed by Gilbarg[13] which seeks to delimit the circumstances under which a motion is uniquely determined by its geometry.

It was Prim[14] who established that any steady motion governed by the classical hydrodynamic system

$$\operatorname{div}\mathbf{q}=0, \tag{2.3a}$$

$$\rho(\mathbf{q}\cdot\nabla)\mathbf{q}+\nabla p=\mathbf{0} \tag{2.3b}$$

is uniquely determined by its streamline pattern unless it has constant velocity magnitude $q=|\mathbf{q}|$ along individual streamlines or, equivalently, in the absence of stagnation points, unless

$$\operatorname{div}\mathbf{t}=0, \tag{2.4}$$

where $\mathbf{t}$ is the unit tangent to the streamline. In the above, $\mathbf{q}=q\mathbf{t}$ is the fluid velocity and p,ρ are the pressure and constant density, respectively. If the geometric condition (2.4) holds, then there exists a multiplicity of flows which exhibit the same streamline pattern since the system (2.3) and (2.4) is seen to be invariant under $(p,\mathbf{q})\rightarrow(f(p),\sqrt{f'(p)}\,\mathbf{q})$.

The Gilbarg problem has been investigated by, *inter alia*, not only Prim[14] but also Howard,[15] Wasserman,[16] and Marris.[17] In Ref. 18, it has been established that, remarkably, this classical problem may be decomposed into a study of the solitonic Heisenberg spin equation (2.2) with $\mathbf{S}=\mathbf{t}$ subject to the condition (2.4). The results carry over, *mutatis mutandis*, to the steady motion of an inviscid and thermally nonconducting gas with arbitrary equation of state as well as to magnetohydrostatics.[12,18,19]

In the sequel, an account of the derivation of the Heisenberg spin equation in hydrodynamics and magnetohydrostatics is presented. The classical Gilbarg problem is reformulated as the problem of solving the Heisenberg spin equation subject to the geometric constraint (2.4).

III. GEOMETRIC PRELIMINARIES

The nature of the geometric constraint (2.4) prompts the adoption of a characterization of a three-dimensional vector field $\mathbf{f}$ inherent in a study of anholonomic coordinate systems by Vranceanu.[20] Thus, the orthonormal basis $\{\mathbf{t},\mathbf{n},\mathbf{b}\}$ is introduced along the tangential, principal normal and binormal directions to the vector lines of nonvanishing $\mathbf{f}$. This formulation has been previously used to derive kinematic properties in hydrodynamics by Marris and Passman.[21] In that context, as here, $\mathbf{f}$ is identified with the velocity field $\mathbf{q}$.

Let

$$\frac{\delta}{\delta s}=\mathbf{t}\cdot\nabla,\quad \frac{\delta}{\delta n}=\mathbf{n}\cdot\nabla,\quad \frac{\delta}{\delta b}=\mathbf{b}\cdot\nabla \tag{3.1}$$

denote the directional derivatives in the tangential, principal normal and binormal directions, respectively. It proves convenient to introduce the notation[22]

$$\theta_{ns}=\mathbf{n}\cdot\frac{\delta\mathbf{t}}{\delta n},\quad \theta_{bs}=\mathbf{b}\cdot\frac{\delta\mathbf{t}}{\delta b}, \tag{3.2}$$

in terms of which

$$\operatorname{div}\mathbf{t}=\left(\mathbf{t}\frac{\delta}{\delta s}+\mathbf{n}\frac{\delta}{\delta n}+\mathbf{b}\frac{\delta}{\delta b}\right)\cdot\mathbf{t}=\theta_{ns}+\theta_{bs}. \tag{3.3}$$

In a similar manner,

$$\operatorname{div}\mathbf{n}=-\kappa+\mathbf{b}\cdot\frac{\delta\mathbf{n}}{\delta b},\quad \operatorname{div}\mathbf{b}=\mathbf{n}\cdot\frac{\delta\mathbf{b}}{\delta n}, \tag{3.4}$$

where κ denotes the curvature of the **t**-field. Moreover,

$$\operatorname{curl}\mathbf{t}=\left(\mathbf{t}\times\frac{\delta}{\delta s}+\mathbf{n}\times\frac{\delta}{\delta n}+\mathbf{b}\times\frac{\delta}{\delta b}\right)\mathbf{t}=\Omega_s\mathbf{t}+\kappa\mathbf{b}, \tag{3.5}$$

where

$$\Omega_s=\mathbf{t}\cdot\operatorname{curl}\mathbf{t}=\mathbf{b}\cdot\frac{\delta\mathbf{t}}{\delta n}-\mathbf{n}\cdot\frac{\delta\mathbf{t}}{\delta b}. \tag{3.6}$$

Further,

$$\begin{aligned}\operatorname{curl}\mathbf{n}&=-(\operatorname{div}\mathbf{b})\mathbf{t}+\Omega_n\mathbf{n}+\theta_{ns}\mathbf{b},\\ \operatorname{curl}\mathbf{b}&=(\kappa+\operatorname{div}\mathbf{n})\mathbf{t}-\theta_{bs}\mathbf{n}+\Omega_b\mathbf{b},\end{aligned} \tag{3.7}$$

where

$$\begin{aligned}\Omega_n&=\mathbf{n}\cdot\operatorname{curl}\mathbf{n}=\mathbf{t}\cdot\frac{\delta\mathbf{n}}{\delta b}-\tau,\\ \Omega_b&=\mathbf{b}\cdot\operatorname{curl}\mathbf{b}=-\tau-\mathbf{t}\cdot\frac{\delta\mathbf{b}}{\delta n},\end{aligned} \tag{3.8}$$

with τ the torsion of the **t**-field. The quantities Ω_s, Ω_n, and Ω_b are termed abnormalities of the **t**, **n**, and **b**-fields, in turn. Combination of (3.6) and (3.8) produces the important relation

$$\Omega_s+\Omega_n+\Omega_b=2(\Omega_s-\tau). \tag{3.9}$$

This connection between the abnormalities appears in another guise in the treatise of Weatherburn.[23] Therein, Ω_s, Ω_n, and Ω_b are called the total moments of the **t**, **n**, and **b**-fields, respectively.

The identity curl grad $\phi=\mathbf{0}$, on use of the intrinsic decompositions (3.5) and (3.7), produces the commutator relations

$$\frac{\delta^2}{\delta n\,\delta b}-\frac{\delta^2}{\delta b\,\delta n}=-\Omega_s\frac{\delta}{\delta s}+\operatorname{div}\mathbf{b}\,\frac{\delta}{\delta n}-(\kappa+\operatorname{div}\mathbf{n})\frac{\delta}{\delta b}, \tag{3.10a}$$

$$\frac{\delta^2}{\delta b\,\delta s}-\frac{\delta^2}{\delta s\,\delta b}=-\Omega_n\frac{\delta}{\delta n}+\theta_{bs}\frac{\delta}{\delta b}, \tag{3.10b}$$

$$\frac{\delta^2}{\delta s\,\delta n}-\frac{\delta^2}{\delta n\,\delta s}=-\kappa\frac{\delta}{\delta s}-\theta_{ns}\frac{\delta}{\delta n}-\Omega_b\frac{\delta}{\delta b}. \tag{3.10c}$$

The system governing the directional derivatives of the orthonormal triad $\{\mathbf{t},\mathbf{n},\mathbf{b}\}$ reads

$$\frac{\delta}{\delta s}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}=\begin{pmatrix}0 & \kappa & 0\\ -\kappa & 0 & \tau\\ 0 & -\tau & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix},$$

$$\frac{\delta}{\delta n}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}=\begin{pmatrix}0 & \theta_{ns} & \Omega_b+\tau\\ -\theta_{ns} & 0 & -\operatorname{div}\mathbf{b}\\ -(\Omega_b+\tau) & \operatorname{div}\mathbf{b} & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}, \tag{3.11}$$

$$\frac{\delta}{\delta b}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}=\begin{pmatrix}0 & -(\Omega_n+\tau) & \theta_{bs}\\ \Omega_n+\tau & 0 & \kappa+\operatorname{div}\mathbf{n}\\ -\theta_{bs} & -(\kappa+\operatorname{div}\mathbf{n}) & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}.$$

The compatibility of this linear system, on application of the commutator relations (3.10), gives rise to nine conditions on the eight geometric parameters $\kappa,\tau,\Omega_s,\Omega_n,\operatorname{div}\mathbf{n},\operatorname{div}\mathbf{b},\theta_{ns}$, and θ_{bs}, viz.,

$$\frac{\delta\theta_{ns}}{\delta b}+\frac{\delta}{\delta n}(\tau+\Omega_n)=(\kappa+\operatorname{div}\mathbf{n})(\Omega_s-2\Omega_n-2\tau)+\operatorname{div}\mathbf{b}\,(\theta_{bs}-\theta_{ns})+\Omega_s\kappa, \tag{3.12a}$$

$$\frac{\delta}{\delta b}(\tau+\Omega_n-\Omega_s)+\frac{\delta\theta_{bs}}{\delta n}=(\kappa+\operatorname{div}\mathbf{n})(\theta_{ns}-\theta_{bs})+\operatorname{div}\mathbf{b}\,(\Omega_s-2\Omega_n-2\tau), \tag{3.12b}$$

$$\frac{\delta}{\delta b}\operatorname{div}\mathbf{b}+\frac{\delta}{\delta n}(\kappa+\operatorname{div}\mathbf{n})=(\tau+\Omega_n)(\tau+\Omega_n-\Omega_s)-\theta_{ns}\theta_{bs}-\tau\Omega_s-(\operatorname{div}\mathbf{b})^2-(\kappa+\operatorname{div}\mathbf{n})^2, \tag{3.12c}$$

$$\frac{\delta}{\delta s}(\tau+\Omega_n)+\frac{\delta\kappa}{\delta b}=-\Omega_n\theta_{ns}-(2\tau+\Omega_n)\theta_{bs}, \tag{3.12d}$$

$$\frac{\delta\theta_{bs}}{\delta s}=-\theta_{bs}^2+\kappa(\kappa+\operatorname{div}\mathbf{n})-\Omega_n(\tau+\Omega_n-\Omega_s)+\tau(\tau+\Omega_n), \tag{3.12e}$$

$$\frac{\delta}{\delta s}(\kappa+\operatorname{div}\mathbf{n})-\frac{\delta\tau}{\delta b}=-\Omega_n\operatorname{div}\mathbf{b}-\theta_{bs}(2\kappa+\operatorname{div}\mathbf{n}), \tag{3.12f}$$

$$\frac{\delta\kappa}{\delta n}-\frac{\delta\theta_{ns}}{\delta s}=\kappa^2+\theta_{ns}^2+(\tau+\Omega_n)(3\tau+\Omega_n)-\Omega_s(2\tau+\Omega_n), \tag{3.12g}$$

$$\frac{\delta}{\delta s}(\tau+\Omega_n-\Omega_s)=-\theta_{ns}(\Omega_n-\Omega_s)+\kappa\,\mathrm{div}\,\mathbf{b}+\theta_{bs}(-2\tau-\Omega_n+\Omega_s), \tag{3.12h}$$

$$\frac{\delta\tau}{\delta n}+\frac{\delta}{\delta s}\mathrm{div}\,\mathbf{b}=-\kappa(\Omega_n-\Omega_s)-\theta_{ns}\mathrm{div}\,\mathbf{b}+(\kappa+\mathrm{div}\,\mathbf{n})(-2\tau-\Omega_n+\Omega_s). \tag{3.12i}$$

Solitonic equations inherent in subsystems of these compatibility conditions have been isolated via the application of certain geometric constraints in Ref. 24. Here, it is shown how the classical hydrodynamic system (2.3) subject to the geometric constraint (2.4) when adjoined to an appropriate subset of the system (3.12), namely, (3.12d)–(3.12f), produces an integrable Heisenberg spin equation that prevails on the constant pressure surfaces. The residual conditions in (3.12) constrain the foliation of these soliton surfaces.

In what follows, it will emerge that the geometric constraint (2.4) imposed on the hydrodynamic system (2.3) implies the vanishing abnormality condition

$$\Omega_n=0. \tag{3.13}$$

Magnetohydrodynamic motions in which this condition arises in conjunction with (2.4) have been previously investigated by Rogers and Kingston.[25] The geometric constraint (3.13) implies the existence of functions Φ and Ψ such that

$$\mathbf{n}=\Psi\nabla\Phi. \tag{3.14}$$

Since $\mathbf{n}$ is parallel to the normal to the surfaces $\Sigma_n:\Phi=\mathrm{const}$, the vector lines of $\mathbf{t}$ (commonly termed the s-lines) constitute geodesics thereon. The vector lines of $\mathbf{b}$ (the b-lines) are necessarily parallels.[23]

On introduction of a parametrization of the surfaces Σ_n wherein

$$\frac{\delta}{\delta s}=\frac{\partial}{\partial s},\quad \frac{\delta}{\delta b}=\frac{1}{\gamma}\frac{\partial}{\partial b}, \tag{3.15}$$

the commutator relation (3.10b) shows that

$$\theta_{bs}=\frac{\partial}{\partial s}\ln\gamma. \tag{3.16}$$

Thus, with the s-lines and b-lines taken as parametric curves on the surfaces Σ_n, the surface metric of an individual such surface adopts the form

$$\mathrm{I}_n=ds^2+\gamma^2(s,b)db^2, \tag{3.17}$$

where γ is constrained by the relation (3.16).

The Gauss–Weingarten equations for an individual surface Σ_n become

$$\begin{aligned}\frac{\partial}{\partial s}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}&=\begin{pmatrix}0 & \kappa & 0\\ -\kappa & 0 & \tau\\ 0 & -\tau & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix},\\ \frac{1}{\gamma}\frac{\partial}{\partial b}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}&=\begin{pmatrix}0 & -\tau & \theta_{bs}\\ \tau & 0 & \kappa+\mathrm{div}\,\mathbf{n}\\ -\theta_{bs} & -(\kappa+\mathrm{div}\,\mathbf{n}) & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\\ \mathbf{b}\end{pmatrix}.\end{aligned} \tag{3.18}$$

Moreover, if $\mathbf{r}$ denotes the generic position vector to a surface Σ_n, then

$$\frac{\partial \mathbf{r}}{\partial s}=\mathbf{t}, \quad \frac{\partial \mathbf{r}}{\partial b}=\gamma \mathbf{b}, \tag{3.19}$$

and compatibility requires that the **t**-field be such that

$$\frac{\partial \mathbf{t}}{\partial b}=\frac{\partial}{\partial s}\left(h\mathbf{t}\times\frac{\partial \mathbf{t}}{\partial s}\right), \tag{3.20}$$

where

$$h=\gamma\kappa^{-1}. \tag{3.21}$$

IV. THE HEISENBERG SPIN EQUATION IN HYDRODYNAMICS AND MAGNETOHYDROSTATICS

If we now set $\mathbf{q}=q\mathbf{t}$, then decomposition of the hydrodynamic system (2.3) yields

$$\frac{\delta q}{\delta s}+q\,\mathrm{div}\,\mathbf{t}=0, \tag{4.1}$$

together with

$$\frac{\delta p}{\delta s}=\rho q^2\,\mathrm{div}\,\mathbf{t}, \quad \frac{\delta p}{\delta n}=-\rho q^2\kappa, \quad \frac{\delta p}{\delta b}=0. \tag{4.2}$$

On use of the commutator relations (3.10), it is seen that the compatibility conditions for the pressure field require that

$$2\left(\frac{\delta \ln q}{\delta n}\right)\mathrm{div}\,\mathbf{t}=-\frac{\delta \kappa}{\delta s}+\theta_{bs}\kappa-\frac{\delta}{\delta n}\mathrm{div}\,\mathbf{t}+2\kappa\,\mathrm{div}\,\mathbf{t},$$

$$2\left(\frac{\delta \ln q}{\delta b}\right)\mathrm{div}\,\mathbf{t}=\kappa\Omega_n-\frac{\delta}{\delta b}\mathrm{div}\,\mathbf{t}, \tag{4.3}$$

$$2\kappa\left(\frac{\delta \ln q}{\delta b}\right)=-\mathrm{div}\,(\kappa\mathbf{b})-\Omega_s\,\mathrm{div}\,\mathbf{t}.$$

These relations confirm Prim's result[14] that the hydrodynamic motions described by the classical system (2.3) are completely determined by their geometry except when $\mathrm{div}\,\mathbf{t}=0$. On the other hand, if $\mathrm{div}\,\mathbf{t}=0$, then (4.3) shows that if $\kappa\neq 0$, then

$$\theta_{bs}=\frac{\delta}{\delta s}\ln\kappa=\frac{\partial}{\partial s}\ln\kappa, \tag{4.4a}$$

$$\Omega_n=0. \tag{4.4b}$$

Combination of the relation (3.16) with (4.4a) yields

$$\gamma=\nu\kappa, \tag{4.5}$$

where $\partial\nu/\partial s=0$. Here, we may set $\nu=1$ without loss of generality since ν may be absorbed into the b-coordinate. It is readily shown that the residual condition

$$\frac{\delta}{\delta b}\ln q=-\frac{1}{2\kappa}\mathrm{div}\,\kappa\mathbf{b} \tag{4.6}$$

is compatible with the relation

$$\frac{\delta q}{\delta s}=0 \tag{4.7}$$

on use of the geometric compatibility conditions (3.12). It is noted that (4.7) is equivalent, by virtue of the continuity equation (2.3a), to the geometric condition $\operatorname{div}\mathbf{t}=0$ if stagnation points are excluded. It was with hydrodynamic motions subject to the condition (4.7) that the doctoral thesis of Howard in 1953 was concerned.[15]

The relation (4.5), in view of (3.20) and (3.21), shows that, remarkably, for such hydrodynamic motions, the **t**-field satisfies the integrable Heisenberg spin equation. The result is encapsulated in the following:

Theorem 1: *In steady hydrodynamic motions with*

$$\operatorname{div}\mathbf{t}=0 \tag{4.8}$$

and $\kappa\neq 0$, *the unit tangent to the streamlines on individual constant pressure surfaces is governed by the solitonic Heisenberg spin equation*

$$\frac{\partial \mathbf{t}}{\partial b}=\frac{\partial}{\partial s}\left(\mathbf{t}\times\frac{\partial \mathbf{t}}{\partial s}\right), \tag{4.9}$$

where s denotes arc length of the streamlines and b parametrizes the binormal lines. Conversely, any solution of the Heisenberg spin equation subject to the constraint (4.8) gives rise to steady hydrodynamic motions via integration of the compatible linear system (4.2), (4.6), and (4.7) for p and q^2.

In light of the above result, the classical Gilbarg problem reduces to that of the foliation of NLS soliton surfaces according to the geometric constraint (4.8). The integrable Heisenberg spin equation reduction subject to (4.8) likewise obtains for the steady spatial motion of a Prim gas[12] and indeed for that of a gas with general equation of state

$$\rho=\rho(p,\eta),\quad \left.\frac{\partial \rho}{\partial \eta}\right|_{p}>0. \tag{4.10}$$

Importantly, it also applies *mutatis mutandis* for the equilibrium equations of an infinitely conducting liquid, namely,[26]

$$\operatorname{div}\mathbf{H}=0,\quad -\mu(\mathbf{H}\cdot\nabla)\mathbf{H}+\nabla\Pi=\mathbf{0}, \tag{4.11}$$

subject to the condition

$$\mathbf{H}\cdot\nabla|\mathbf{H}|=0, \tag{4.12}$$

where **H** denotes the magnetic field, μ is the magnetic permeability assumed constant and $\Pi=p+\frac{1}{2}\mu\mathbf{H}^2$ is the total pressure. In this context, the role of the constant pressure surfaces in hydrodynamics is replaced by the constant total pressure surfaces $\Pi=\text{const}$. The Heisenberg spin connection has been recently exploited by Schief[27] to construct geometric configurations wherein the constant total pressure surfaces comprise nested tori which are foliated in accordance with the condition (4.8). In this case, the constant total pressure surfaces and the isobar surfaces are identical. Remarkably, such equilibrium configurations were earlier obtained in a direct manner by Palumbo,[28,29] who asserted that the constant pressure surfaces coincide with the so-called drift surfaces if and only if the magnetic field lines constitute geodesics on these surfaces. Equilibria of this kind are of importance since they are free of neoclassical transport effects causing increased diffusion and heat conduction.

The above-mentioned nested toroidal configurations represent a particular solution of the complete set of compatibility conditions (3.12) subject to the geometric constraints (4.4) and (4.8). The solution of these constrained compatibility conditions in general remains an open and important problem. In terms of complexity, it represents an extension of a classical problem posed by Hamel[30] (vide Ref. 31).

V. INTEGRABLE STRUCTURE IN IDEAL EQUILIBRIUM MAGNETOHYDRODYNAMICS. THE POHLMEYER–LUND–REGGE MODEL

It is natural to pose an analog of the Gilbarg problem in ideal magnetohydrodynamics. Indeed, work in this direction was initiated by Wasserman in Ref. 32. However, it is only recently that it has been established that any solution of the ideal magnetohydrodynamic equations governing the steady motion of an infinitely conducting incompressible fluid which is such that the Maxwellian and constant total pressure surfaces coincide is embedded in a multiplicity of solutions which share the magnetic field line and streamline geometry.[33] Remarkably, in this case, the magnetohydrodynamic equations reduce to the integrable Pohlmeyer–Lund–Regge model subject to a volume-preserving constraint. Moreover, it may be shown that if the magnetic and velocity fields are aligned or either of them vanishes then the Heisenberg spin connection as discussed in the previous section is retrieved. Here, the Pohlmeyer–Lund–Regge connection to ideal magnetohydrodynamics is described.

A. The magnetohydrodynamic system

The system of magnetohydrodynamic equations adopts the form[26]

$$\operatorname{div}\mathbf{q}=0, \tag{5.1a}$$

$$\rho(\mathbf{q}\cdot\nabla)\mathbf{q}+\nabla p=\frac{1}{\mu}\operatorname{curl}\mathbf{B}\times\mathbf{B}, \tag{5.1b}$$

$$\operatorname{div}\mathbf{B}=0, \tag{5.1c}$$

$$\operatorname{curl}(\mathbf{q}\times\mathbf{B})=\mathbf{0}, \tag{5.1d}$$

or, equivalently,

$$\operatorname{div}\mathbf{q}=0, \tag{5.2a}$$

$$\rho(\mathbf{q}\cdot\nabla)\mathbf{q}-\frac{1}{\mu}(\mathbf{B}\cdot\nabla)\mathbf{B}+\nabla\Pi=\mathbf{0}, \tag{5.2b}$$

$$\operatorname{div}\mathbf{B}=0, \tag{5.2c}$$

$$(\mathbf{q}\cdot\nabla)\mathbf{B}=(\mathbf{B}\cdot\nabla)\mathbf{q}, \tag{5.2d}$$

wherein $\Pi=p+\mathbf{B}^2/2\mu$ is the total pressure and μ designates the magnetic permeability. In the following, we set $\rho=\mu=1$ without loss of generality.

The Faraday equation (5.1d) implies that there exist 'Maxwellian' surfaces Σ which bear the streamlines and magnetic field lines. The commutation property

$$[\mathbf{q}\cdot\nabla,\mathbf{b}\cdot\nabla]=0 \tag{5.3}$$

embodied in (5.2d) implies that there exists a coordinate system (χ, ψ, ω) such that the Maxwellian surfaces are given by $\omega=\text{const}$ and

$$\mathbf{q}\cdot\nabla=\partial_\chi, \quad \mathbf{B}\cdot\nabla=\partial_\psi \tag{5.4}$$

so that if $\mathbf{r}$ denotes the Eulerian coordinate vector then

$$\mathbf{q}=\mathbf{r}_\chi, \quad \mathbf{B}=\mathbf{r}_\psi \tag{5.5}$$

are tangent vectors to the χ and ψ coordinate lines, respectively, on the Maxwellian surfaces. In terms of this coordinate system, the continuity and induction equations (5.2a) and (5.2c) in turn, adopt the form

$$\begin{aligned} \operatorname{div}\mathbf{r}_\chi &= \frac{|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|_\chi}{|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|}=0, \\ \operatorname{div}\mathbf{r}_\psi &= \frac{|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|_\psi}{|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|}=0. \end{aligned} \tag{5.6}$$

Thus, on appropriate reparametrization of the foliation parameter ω, we obtain the volume-preserving condition

$$|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|=1 \tag{5.7}$$

while the equation of motion (5.2b) becomes

$$\mathbf{r}_{\chi\chi}-\mathbf{r}_{\psi\psi}+\Pi_\chi\mathbf{r}_\psi\times\mathbf{r}_\omega+\Pi_\psi\mathbf{r}_\omega\times\mathbf{r}_\chi+\Pi_\omega\mathbf{r}_\chi\times\mathbf{r}_\psi=0. \tag{5.8}$$

It is concluded that the magnetohydrodynamic system (5.2) is equivalent to the system (5.7), (5.8) with the fluid velocity and magnetic field given by (5.5).

B. The Pohlmeyer–Lund–Regge connection

The preceding canonical formulation of the governing equations has as a consequence the following theorem:[33]

Theorem 2: *If the Maxwellian surfaces coincide with the constant total pressure surfaces so that* $\Pi=\Pi(\omega)$ *then the magnetohydrodynamic system (5.1) or, equivalently, (5.2) reduces to the* integrable *Pohlmeyer–Lund–Regge model*

$$\mathbf{r}_{\chi\chi}-\mathbf{r}_{\psi\psi}=\Omega(\omega)\mathbf{r}_\chi\times\mathbf{r}_\psi \tag{5.9}$$

subject to the volume-preserving condition

$$|\mathbf{r}_\chi,\mathbf{r}_\psi,\mathbf{r}_\omega|=1. \tag{5.10}$$

The fluid velocity, magnetic field, and total pressure are given by

$$\mathbf{q}=\mathbf{r}_\chi, \quad \mathbf{B}=\mathbf{r}_\psi, \quad \Pi=-\int \Omega(\omega)\,d\omega, \tag{5.11}$$

respectively.

The Pohlmeyer–Lund–Regge model constitutes an integrable nonlinear σ-model[34,35] which usually consists of the vector equation (5.9) and the admissible constraints

$$\mathbf{r}_\chi^2+\mathbf{r}_\psi^2=1, \quad \mathbf{r}_\chi\cdot\mathbf{r}_\psi=0. \tag{5.12}$$

The latter normalization may always be achieved by means of a suitable coordinate transformation which leaves (5.9) invariant. However, in the present magnetohydrodynamic context, the new coordinate lines on the Maxwellian surfaces do not necessarily coincide with the streamlines and magnetic field lines and the volume-preserving condition (5.10) adopts a less convenient form.

The assumption that the magnetic field is orthogonal to the velocity field constitutes an additional constraint on the magnetohydrodynamic system. This orthogonality condition is not 'geometric' in that it is not preserved by the invariance

$$\begin{pmatrix} \mathbf{q} \\ \mathbf{B} \end{pmatrix} \to \begin{pmatrix} \cosh\lambda & \sinh\lambda \\ \sinh\lambda & \cosh\lambda \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{B} \end{pmatrix}, \quad \lambda = \text{const} \tag{5.13}$$

of the magnetohydrodynamic system.

C. A substitution principle. Bernoulli integrals of motion

The geometric constraint that the Maxwellian surfaces and constant total pressure surfaces coincide is equivalently characterized by

$$\mathbf{q}\cdot\nabla\Pi = 0, \quad \mathbf{B}\cdot\nabla\Pi = 0. \tag{5.14}$$

If $\mathbf{q}$, $\mathbf{B}$ and Π obey these conditions then a function m which is constant on the Maxwellian surfaces so that

$$\mathbf{q}\cdot\nabla m = 0, \quad \mathbf{B}\cdot\nabla m = 0 \tag{5.15}$$

is associated with the multiplicity of solutions $\{\mathbf{q}^*, \mathbf{B}^*, \Pi^*\}$ of the magnetohydrodynamic system (5.2) embodied in the substitution principle

$$\mathbf{q}^* = m\mathbf{q}, \quad \mathbf{B}^* = m\mathbf{B}, \quad \nabla\Pi^* = m^2\nabla\Pi. \tag{5.16}$$

Thus, any solution of the magnetohydrodynamic system wherein the Maxwellian and constant total pressure surfaces coincide is embedded in a multiplicity of solutions which share the streamline and magnetic field line geometry. This property is reflected by the invariance $(\chi, \psi, \omega) \to (\chi^*, \psi^*, \omega^*)$ of the constrained Pohlmeyer–Lund–Regge system (5.9), (5.10), where

$$\chi^* = \frac{\chi}{m(\omega)}, \quad \psi^* = \frac{\psi}{m(\omega)}, \quad \omega^* = \int m^2(\omega)\, d\omega \tag{5.17}$$

and $\Omega^* = \Omega$. It is noted that the admittance of invariance properties of substitution principle type has been previously investigated in magnetohydrodynamics in Refs. 36–38.

In view of the conditions (5.14), it is seen that scalar multiplication of the equation of motion (5.2b) by $\mathbf{q}$ and $\mathbf{B}$, respectively, yields

$$(\mathbf{q} \mp \mathbf{B})\cdot\nabla(\mathbf{q} \pm \mathbf{B})^2 = 0. \tag{5.18}$$

Accordingly, we obtain the two Bernoulli-type integrals of motion

$$(\mathbf{q} \pm \mathbf{B})^2 = 2\mathbb{B}_\pm(\chi \pm \psi, \omega) \tag{5.19}$$

or, equivalently,

$$\mathbf{q}^2 + \mathbf{B}^2 = \mathbb{B}_+ + \mathbb{B}_-, \quad \mathbf{q}\cdot\mathbf{B} = \tfrac{1}{2}(\mathbb{B}_+ - \mathbb{B}_-). \tag{5.20}$$

The latter correspond to the first integrals

$$\mathbf{r}_\chi^2 + \mathbf{r}_\psi^2 = \mathbb{B}_+ + \mathbb{B}_-, \quad \mathbf{r}_\chi\cdot\mathbf{r}_\psi = \tfrac{1}{2}(\mathbb{B}_+ - \mathbb{B}_-) \tag{5.21}$$

of the Pohlmeyer–Lund–Regge model. These may be reduced to the normal form (5.12) by means of a suitable coordinate transformation.

VI. THE KINEMATICS OF IDEAL FIBER-REINFORCED FLUIDS. INTEGRABLE ADMISSIBLE REDUCTIONS

The notion of an ideal fiber-reinforced fluid was introduced in Ref. 39 as a model in the liquid formation process of fiber-resin materials. This model consists of an incompressible fluid which is inextensible along 'fiber' lines that occupy the volume of the fluid by which they are convected. Resin matrix fiber-reinforced materials enjoy abundant engineering applications, particularly in the construction of light laminated shell structures with complicated geometries.

The kinematic conditions that attend the motion of an ideal fiber-reinforced fluid were set down by Spencer.[40] Thus, if a generic fiber direction is characterized by a unit vector $\mathbf{t}$, the kinematic conditions comprise the usual continuity equation

$$\operatorname{div}\mathbf{v}=0 \tag{6.1}$$

together with the condition

$$\frac{\partial \mathbf{t}}{\partial t}+(\mathbf{v}\cdot\nabla)\mathbf{t}=(\mathbf{t}\cdot\nabla)\mathbf{v}. \tag{6.2}$$

The latter constitutes the commutativity condition

$$\frac{d}{dt}\left(\frac{\delta \mathbf{r}}{\delta s}\right)=\frac{\delta}{\delta s}\left(\frac{d\mathbf{r}}{dt}\right), \tag{6.3}$$

where $\mathbf{r}$ is the position vector to a generic fiber and $d/dt=\partial/\partial t+\mathbf{v}\cdot\nabla$. It is interesting to observe that a similar compatibility condition arises in the derivation of soliton equations via privileged motions of inextensible curves. The kinematic conditions combine to show that

$$\frac{d}{dt}\operatorname{div}\mathbf{t}=0 \tag{6.4}$$

and an important subclass of motions is that with[40]

$$\operatorname{div}\mathbf{t}=0. \tag{6.5}$$

The natural reappearance of the geometric constraint (6.5), albeit now with regard to the fiber field, prompts the search for hidden integrable structure within the kinematic conditions (6.1), (6.2). This motivation is enhanced by the presence of the commutativity condition (6.3) as encountered in soliton theory. Here, attention is restricted to steady motion, in which case the kinematic conditions imply that

$$(\mathbf{v}\times\mathbf{t})\cdot\operatorname{curl}(\mathbf{v}\times\mathbf{t})=0, \tag{6.6}$$

whence the $\mathbf{v}\times\mathbf{t}$-field is complex-lamellar so that

$$\mathbf{v}\times\mathbf{t}=\Psi\nabla\Phi \tag{6.7}$$

for some functions Ψ and Φ. Thus, surfaces $\Sigma:\Phi=\text{const}$ exist which bear both the streamlines and fibers.

It is common in the structure of composite materials to have reinforcement by multiple families of fibers. If there exists a second family of fibers with unit tangent $\mathbf{t}^*$ which are convected by the fluid flow $\mathbf{v}$ and which also lie on the surfaces Σ then there exists the additional kinematic constraint

$$(\mathbf{v}\cdot\nabla)\mathbf{t}^*=(\mathbf{t}^*\cdot\nabla)\mathbf{v}, \tag{6.8}$$

where $\mathbf{t}^*$ may be decomposed according to

$$\mathbf{t}^* = \alpha \mathbf{t} + \beta \mathbf{v}. \tag{6.9}$$

Substitution of (6.9) into (6.8) establishes the following result:

Theorem 3: *In steady fiber-reinforced motion, the surfaces* Σ *bearing the stream lines and* $\mathbf{t}$*-fibers contain a second family of fibers*

$$\mathbf{t}^* = \alpha \mathbf{t} + \beta \mathbf{v}, \quad |\mathbf{t}^*| = 1 \tag{6.10}$$

iff

$$\alpha^2 + \beta^2 v^2 + 2\alpha\beta v(\mathbf{T}\cdot\mathbf{t}) = 1, \tag{6.11}$$

where $\mathbf{T}$ *is the unit tangent to the streamlines and*

$$\frac{\delta\alpha}{\delta S} = \frac{\delta\beta}{\delta S} = 0 \tag{6.12}$$

with $\delta/\delta S = \mathbf{T}\cdot\nabla$.

The following result is readily obtained as a consequence of Theorem 3:[41]

Corollary 1: A multiplicity (>2) *of fibers can exist on the surfaces* Σ *iff the geometry of the streamlines and fibers is constrained by*

$$\operatorname{div}\mathbf{T} = 0, \tag{6.13a}$$

$$\frac{\delta}{\delta S}(\mathbf{T}\cdot\mathbf{t}) = 0. \tag{6.13b}$$

Materials with two, three, or more families of embedded fibers have been discussed in the authoritative monograph of Spencer.[42] It is recalled that it is just the geometric condition (6.13a) which in classical hydrodynamics has been seen to lead to the integrable Heisenberg spin equation.

If the fluid velocity $\mathbf{v}$ is decomposed as

$$\mathbf{v} = v_s \mathbf{t} + v_n \mathbf{n} + v_b \mathbf{b} \tag{6.14}$$

in terms of the fiber direction $\mathbf{t}$ and its principal normal $\mathbf{n}$ and binormal $\mathbf{b}$ then insertion into the kinematic conditions (6.1) and (6.2) yields

$$\frac{\delta v_s}{\delta s} = v_n \kappa, \tag{6.15a}$$

$$\frac{\delta v_n}{\delta s} = v_n \theta_{ns} - v_b \Omega_n, \tag{6.15b}$$

$$\frac{\delta v_b}{\delta s} = v_n \Omega_b + v_b \theta_{bs}, \tag{6.15c}$$

$$\frac{\delta v_n}{\delta n} + \frac{\delta v_b}{\delta b} = -v_s \operatorname{div}\mathbf{t} - v_n(\kappa + \operatorname{div}\mathbf{n}) - v_b \operatorname{div}\mathbf{b}. \tag{6.15d}$$

This constitutes an overdetermined system of linear equations for the velocity components v_s, v_n, and v_b with compatibility condition

$$v_s \frac{\delta}{\delta s} \operatorname{div} \mathbf{t} + v_n \frac{\delta}{\delta n} \operatorname{div} \mathbf{t} + v_b \frac{\delta}{\delta b} \operatorname{div} \mathbf{t} = 0. \tag{6.16}$$

In particular, the latter constraint is satisfied if

$$\operatorname{div} \mathbf{t} = 0 \tag{6.17}$$

in which case the commutator relations (3.10) show that (6.15b)–(6.15d) guarantee the existence of a potential Π such that

$$\frac{\delta \Pi}{\delta s} = 0, \tag{6.18a}$$

$$\frac{\delta \Pi}{\delta n} = -v_b, \tag{6.18b}$$

$$\frac{\delta \Pi}{\delta b} = v_n. \tag{6.18c}$$

Moreover, in the case of geometries with

$$\Omega_n = 0, \quad \theta_{bs} = \frac{\delta}{\delta s} \ln \kappa, \tag{6.19}$$

the solution of the residual condition (6.15a) is given explicitly by

$$\Pi = \frac{\delta \chi}{\delta s}, \tag{6.20a}$$

$$\frac{v_s}{\kappa} = \frac{\delta \chi}{\delta b}, \tag{6.20b}$$

where the function χ is, *a priori*, arbitrary. However, insertion of Π as given by (6.20a) into (6.18a) produces a constraint on χ and we obtain:

Theorem 4: *The kinematic equations (6.1), (6.2) of ideal fiber-reinforced spatial flows with geometric constraints*

$$\operatorname{div} \mathbf{t} = 0, \tag{6.21a}$$

$$\Omega_n = 0, \tag{6.21b}$$

$$\theta_{bs} = \frac{\delta}{\delta s} \ln \kappa \tag{6.21c}$$

admit the general solution

$$\mathbf{v} = \kappa \frac{\delta \chi}{\delta b} \mathbf{t} + \frac{\delta^2 \chi}{\delta b \, \delta s} \mathbf{n} - \frac{\delta^2 \chi}{\delta n \, \delta s} \mathbf{b}, \tag{6.22}$$

where

$$\frac{\delta^2 \chi}{\delta s^2} = 0. \tag{6.23}$$

The fibers constitute geodesics on a family of surfaces Σ_n.

It is recalled that the conditions (6.21b) and (6.21c) encapsulate the integrable Heisenberg spin equation while (6.21a) is identical to the constraint encountered in the Gilbarg problem. In the present context, however, the **t**-lines are the fibers. The nested toroidal solutions obtained in Ref. 27 carry over *mutatis mutandis* to provide particular spatial geometries that adhere to the kinematic conditions (6.1) and (6.2).

A. The geometry of planar motion

It is asserted in Ref. 40 that two-dimensional flows of an ideal fiber-reinforced fluid are essentially determined by kinematical considerations. Thus, the pressure p and tension T in the fiber direction can always be determined such that the equations of motion are satisfied. Accordingly, planar motion is especially privileged and the study of its kinematics assumes an added importance. Here, it is established that the kinematic conditions for the planar motion of an ideal fiber-reinforced fluid can be encoded in a single nonlinear third-order equation. Remarkably, the latter is shown to contain a variant of a well-known integrable system in soliton theory.

In the planar kinematic study of ideal fiber-reinforced fluids, the linear system (3.11) reduces to

$$\frac{\delta}{\delta s}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\end{pmatrix}=\begin{pmatrix}0 & \kappa\\ -\kappa & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\end{pmatrix},$$
$$\frac{\delta}{\delta n}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\end{pmatrix}=\begin{pmatrix}0 & \theta\\ -\theta & 0\end{pmatrix}\begin{pmatrix}\mathbf{t}\\ \mathbf{n}\end{pmatrix}, \tag{6.24}$$

where $\theta=\theta_{ns}=\operatorname{div}\mathbf{t}$. The above pair may be interpreted as the Serret–Frenet equations associated with the planar fibers and their orthogonal trajectories, that is the **n**-lines, with $-\theta$ being the curvature of the latter. The nonlinear system of compatibility conditions (3.12) is identically satisfied except for the single condition

$$\frac{\delta\kappa}{\delta n}-\frac{\delta\theta}{\delta s}=\kappa^2+\theta^2. \tag{6.25}$$

Indeed, on use of the commutator relation

$$\frac{\delta^2}{\delta n\,\delta s}-\frac{\delta^2}{\delta s\,\delta n}=\kappa\frac{\delta}{\delta s}+\theta\frac{\delta}{\delta n}, \tag{6.26}$$

it is readily shown that the Serret–Frenet system (6.24) is compatible modulo (6.25). The general solution of the latter geometric condition may be parametrized via

$$\kappa=\frac{\delta\varphi}{\delta s},\quad \theta=\frac{\delta\varphi}{\delta n}, \tag{6.27}$$

where φ is an as yet unspecified function. Moreover, the fluid velocity **v** is now decomposed according to

$$\mathbf{v}=v\,\mathbf{t}+w\,\mathbf{n}, \tag{6.28}$$

whence, on substitution into the kinematic conditions (6.1) and (6.2), one obtains

$$\frac{\delta v}{\delta s}=\kappa w, \tag{6.29a}$$

$$\frac{\delta w}{\delta s} = \theta w, \tag{6.29b}$$

$$\frac{\delta w}{\delta n} = -\theta v, \tag{6.29c}$$

where the relation $\kappa + \operatorname{div}\mathbf{n} = 0$ valid in planar geometry has been employed.

It is natural to take the fiber lines and their orthogonal trajectories as the coordinate lines of an orthogonal system on the plane. Accordingly, if the variables s and n parametrize the **t**- and **n**-lines, respectively, then the metric of the plane adopts the form

$$\mathrm{I} = \phi^2 ds^2 + \psi^2 dn^2, \tag{6.30}$$

where the partial and directional derivatives are related by

$$\frac{\partial}{\partial s} = \phi \frac{\delta}{\delta s}, \quad \frac{\partial}{\partial n} = \psi \frac{\delta}{\delta n}. \tag{6.31}$$

Thus, if **r** is a generic point on the plane then

$$\frac{\delta \mathbf{r}}{\delta s} = \mathbf{t} = \frac{1}{\phi}\frac{\partial \mathbf{r}}{\partial s}, \quad \frac{\delta \mathbf{r}}{\delta n} = \mathbf{n} = \frac{1}{\psi}\frac{\partial \mathbf{r}}{\partial n}. \tag{6.32}$$

In view of (6.27), the geometric quantities κ and θ now admit the parametrization

$$\kappa = \frac{1}{\phi}\frac{\partial \varphi}{\partial s}, \tag{6.33a}$$

$$\theta = \frac{1}{\psi}\frac{\partial \varphi}{\partial n}. \tag{6.33b}$$

Insertion of (6.31) into the commutator relation (6.26) yields

$$\psi_s = \varphi_n \phi, \tag{6.34a}$$

$$\phi_n = -\varphi_s \psi. \tag{6.34b}$$

Here and subsequently, subscripts denote partial derivatives.

It now proves convenient to introduce a quantity ρ according to the relations

$$\frac{\delta \rho}{\delta s} = 1, \tag{6.35a}$$

$$\frac{\delta \rho}{\delta n} = -\frac{v}{w}. \tag{6.35b}$$

Use of the commutator relation (6.26) and the kinematic conditions (6.29a) and (6.29b) shows that the relations (6.35) are indeed compatible. By virtue of (6.35a), the quantity ρ is seen to constitute arc length along the fibers. Moreover, the relations (6.35) combine to yield

$$\mathbf{q} \cdot \nabla \rho = 0 \tag{6.36}$$

while the compatibility of the kinematic conditions (6.29b) and (6.29c) requires, on use of (6.26), that

$$\mathbf{q}\cdot\nabla\theta=0, \tag{6.37}$$

whence we come to the important conclusion that the divergence of the **t**-field constitutes a function of the arc length ρ along the fibers. In fact, in Ref. 41, it has been shown that this geometric property completely characterizes steady planar motions. If we set, for convenience,

$$\theta=\operatorname{div}\mathbf{t}=\frac{\Psi'(\rho)}{\Psi(\rho)} \tag{6.38}$$

then relations (6.33b) and (6.34a) together show that

$$\frac{\psi_s}{\psi}=\frac{\Psi'(\rho)}{\Psi(\rho)}\phi \tag{6.39}$$

while (6.35a) yields

$$\phi=\rho_s, \tag{6.40}$$

whence

$$\psi=\Psi(\rho). \tag{6.41}$$

Herein, an arbitrary function of integration $N(n)$ has been omitted without loss of generality since it may be removed via a suitable reparametrization of the **n**-lines. The relation (6.33b), on use of (6.38) and (6.41), reduces to

$$\varphi_n=\Psi'(\rho) \tag{6.42}$$

while the residual condition (6.34b) shows that

$$\varphi_s=-\frac{\rho_{sn}}{\Psi(\rho)}. \tag{6.43}$$

Elimination of φ between the latter two relations gives rise to the following result:

Theorem 5: *The kinematics of the steady planar motion of an ideal fiber-reinforced fluid is governed by the single third-order nonlinear equation*

$$\left(\frac{\rho_{sn}}{\Psi(\rho)}\right)_n+\Psi''(\rho)\rho_s=0 \tag{6.44}$$

for the arc length ρ along the fibers. Here, Ψ constitutes an arbitrary function of ρ. The one-parameter family of fibers $\mathbf{r}(s,n=\text{const})$ *is obtained by integration of the compatible pair*

$$\mathbf{r}_s=\rho_s\mathbf{t}, \quad \mathbf{r}_n=\Psi(\rho)\mathbf{n} \tag{6.45}$$

while the fluid velocity is given by

$$\mathbf{v}=-\rho_n\mathbf{t}+\Psi(\rho)\mathbf{n}. \tag{6.46}$$

The solution of the Serret–Frenet equations (6.24) reads

$$\mathbf{t}=\begin{pmatrix}\cos\varphi\\ \sin\varphi\end{pmatrix}, \quad \mathbf{n}=\begin{pmatrix}-\sin\varphi\\ \cos\varphi\end{pmatrix}, \tag{6.47}$$

where φ obeys the compatible system

$$\varphi_s = -\frac{\rho_{sn}}{\Psi(\rho)}, \quad \varphi_n = \Psi'(\rho). \tag{6.48}$$

B. An integrable reduction. Generation of fiber distributions

To proceed, it proves convenient to reformulate the third-order equation (6.44) as a coupled system of equations, namely,

$$\rho_{sn} = \mu\Psi(\rho), \quad \mu_n = -\Psi''(\rho)\rho_s. \tag{6.49}$$

The latter admits the first integral

$$\mu^2 - \alpha\rho_s^2 = I(s) \tag{6.50}$$

if Ψ is constrained by

$$\Psi''(\rho) + \alpha\Psi(\rho) = 0, \tag{6.51}$$

where α constitutes an arbitrary constant. On use of an appropriate reparametrization of the fiber lines, the function I may be scaled to $0, \pm 1$. In particular, if $\alpha = I = 1$ and

$$\Psi(\rho) = \sin\rho, \tag{6.52}$$

the parametrization

$$\mu = \epsilon\cosh\omega, \quad \rho_s = \epsilon\sinh\omega, \quad \epsilon^2 = 1 \tag{6.53}$$

of the relation (6.50) results in the following consequence of Theorem 5:

Corollary 2: The specialization $\Psi(\rho) = \sin\rho$ in (6.44) reduces it to the system

$$\rho_s = \epsilon\sinh\omega, \quad \omega_n = \sin\rho \tag{6.54}$$

with associated fluid velocity

$$\mathbf{v} = -\rho_n\mathbf{t} + \sin\rho\,\mathbf{n}, \tag{6.55}$$

where the pair $(\mathbf{t}, \mathbf{n})$ *is given by (6.47) with*

$$\varphi_s = -\epsilon\cosh\omega, \quad \varphi_n = \cos\rho. \tag{6.56}$$

The metric of the plane may be cast into the form

$$\mathrm{I} = \rho_s^2 ds^2 + \omega_n^2 dn^2 \tag{6.57}$$

so that ρ and ω constitute arc length along the **t***-lines and* **n***-lines, respectively.*

If the term $\epsilon\sinh\omega$ in (6.54) is replaced by $\sin\omega$ then the classical Bäcklund equations for surfaces of constant negative Gaussian curvature result.[1] The Gauss equation for such pseudospherical surfaces is the integrable sine-Gordon equation.[43] In the current context, it is readily verified that $\rho + \mathrm{i}\omega$ obey the sine-Gordon equation

$$(\rho + \mathrm{i}\omega)_{sn} = \epsilon\sin(\rho + \mathrm{i}\omega). \tag{6.58}$$

The system (6.54) guarantees that the pair

$$\Phi_s=\frac{\epsilon}{2}\begin{pmatrix}\tan\nu\sinh\omega & -\dfrac{\cosh\omega}{\cos\nu}\\ \dfrac{\cosh\omega}{\cos\nu} & -\tan\nu\sinh\omega\end{pmatrix}\Phi,$$
$$\Phi_n=\frac{1}{2}\begin{pmatrix}0 & \cos(\rho-\nu)\\ -\cos(\rho+\nu) & 0\end{pmatrix}\Phi \tag{6.59}$$

is compatible for any value of the constant parameter ν. In fact, the latter constitutes a 'linear representation' of the nonlinear system (6.54) in the sense of soliton theory and admits an associated Darboux transformation.[1] In this connection, it is noted that, at $\nu=0$, the fundamental solution of (6.59) is given by

$$\Phi|_{\nu=0}=\begin{pmatrix}\cos\varphi/2 & \sin\varphi/2\\ -\sin\varphi/2 & \cos\varphi/2\end{pmatrix}. \tag{6.60}$$

Thus, the 'eigenfunction' Φ encodes the tangent vectors $\mathbf{t}$ and $\mathbf{n}$ via the angle φ. An induced Bäcklund transformation for the fiber distribution on the plane may be obtained in a standard manner by employing the Sym–Tafel formula[1,44] which, in the current context, states that the position vector of the fibers is encapsulated in

$$\Phi^{-1}\frac{\partial\Phi}{\partial\nu}\bigg|_{\nu=0}. \tag{6.61}$$

The above-mentioned results are summarized below:[45]

Theorem 6: *Any solution (ρ,ω) of the integrable system (6.54) together with the associated fiber position vector* $\mathbf{r}$ *and tangent vectors* $\mathbf{t}$, $\mathbf{n}$ *may be mapped to another solution* (ρ',ω') *and fiber distribution* $(\mathbf{r}',\mathbf{t}',\mathbf{n}')$ *by the Bäcklund transformation*

$$\rho'=\rho+2\arctan\left(\cot\nu\frac{1+\xi^2}{1-\xi^2}\right),$$
$$\omega'=-\omega+2\left(\frac{2\xi\sin\nu}{1+\xi^2}\right),$$
$$\varphi'=\varphi+\chi,\quad \chi=-2\arctan\left(\frac{2\xi\cos\nu}{1-\xi^2}\right), \tag{6.62}$$
$$\mathbf{r}'=\mathbf{r}+2\cot\nu\frac{1+\xi^2}{1-\xi^2}\cos\frac{\chi}{2}\left(\cos\frac{\chi}{2}\mathbf{t}+\sin\frac{\chi}{2}\mathbf{n}\right),$$
$$\mathbf{t}'=\cos\chi\,\mathbf{t}+\sin\chi\,\mathbf{n},\quad \mathbf{n}'=-\sin\chi\,\mathbf{t}+\cos\chi\,\mathbf{n},$$

where $\xi=\Phi^1/\Phi^2$ *and* $\epsilon'=-\epsilon$. *Here,* Φ^i *designate the components of a vector-valued solution* Φ *of the linear system (6.59).*

The above Bäcklund transformation may be used to generate explicitly large classes of fiber distributions and associated velocity fields $\mathbf{v}$. This has been discussed in Ref. 45.

In conclusion, it is noted that if we introduce the vector field

$$\mathbf{w}=\sinh\omega\,\mathbf{t}-\epsilon\omega_s\mathbf{n} \tag{6.63}$$

then it is readily shown that

$$(\mathbf{w}\cdot\nabla)\mathbf{n}=(\mathbf{n}\cdot\nabla)\mathbf{w},\quad \operatorname{div}\mathbf{w}=0. \tag{6.64}$$

Consequently, the **n**-lines may also be regarded as inextensible fibers which are convected with the **w**-flow. The inextensibility of the **n**-lines is verified by the relation

$$(\mathbf{w}\cdot\nabla)\omega=0. \tag{6.65}$$

Accordingly, we have established the duality

$$(\mathbf{t},\mathbf{v})\leftrightarrow(\mathbf{n},\mathbf{w}). \tag{6.66}$$

Moreover, it may be shown that such a duality property exists iff the function $\Psi(\rho)$ is constrained by (6.51). Thus, the integrable case is privileged with regard to duality.

C. A Loewner connection. The 2+1-dimensional sine-Gordon system

It has been established that the third-order equation (6.44) embodies the complete set of equations governing steady planar motions. These consist of the geometric system (6.34), that is

$$\psi_s=q\phi,\quad \phi_n=-p\psi, \tag{6.67}$$

where

$$p=\varphi_s,\quad q=\varphi_n, \tag{6.68}$$

along with the kinematic conditions (6.29a) and (6.29c) given by

$$v_s=pw,\quad w_n=-qv \tag{6.69}$$

and the remaining kinematic condition (6.29b) which may be replaced by

$$w=\psi. \tag{6.70}$$

Remarkably, if p and q are arbitrary then the linear system (6.69) may be interpreted as the standard 'scattering problem' associated with the $2+1$-dimensional AKNS hierarchy of soliton equations[46] and (6.67) constitutes its adjoint. The functions v and w may be regarded as eigenfunctions while ψ and ϕ represent adjoint eigenfunctions. Moreover, a 'squared eigenfunction' M may be introduced via the compatible system

$$M_s=\phi w,\quad M_n=-\psi v. \tag{6.71}$$

Squared eigenfunctions play an important role in the construction of binary Darboux transformations in soliton theory.[47]

The reduction (6.68) is admissible and indeed standard in soliton theory. It produces a modified Nizhnik-Veselov-Novikov hierarchy (see, e.g., Ref. 48) which may be regarded as a $2+1$-dimensional version of the potential modified Korteweg–de Vries hierarchy.[46] The latter is compatible with the $2+1$-dimensional sine-Gordon system which constitutes a particular reduction of the so-called LKR system.[48–50] The origins of this master $2+1$-dimensional soliton system reside in gasdynamics in a study by Loewner[51] on the application of infinitesimal Bäcklund transformations to reduce the hodograph equations to appropriate canonical form in subsonic, transsonic and supersonic flow régimes. Indeed, (6.69) is gauge-equivalent to the system as studied by Loewner. It was the discovery of the gasdynamic connection with soliton theory via the LKR system that, in part, motivated the present search for hidden integrability in other classical systems of nonlinear continuum mechanics.

The eigenfunction-adjoint eigenfunction constraint (6.70) appears to be novel. It gives rise to the nonlinearity of the third-order equation (6.44) in that it implicitly relates the function φ to the (adjoint) eigenfunctions.

The above-mentioned $2+1$-dimensional integrable generalization of the classical sine-Gordon equation may be brought into the compact polynomial form

$$\hat{\varphi}_{snt}+\hat{\varphi}_s\eta_{nt}+\hat{\varphi}_n\eta_{st}=0, \tag{6.72a}$$

$$\eta_{sn}=\hat{\varphi}_s\hat{\varphi}_n\,. \tag{6.72b}$$

It arises out of the compatibility conditions associated with the Lax pair[52]

$$\begin{pmatrix} \partial_s & -\hat{\varphi}_s \\ \hat{\varphi}_n & \partial_n \end{pmatrix}\begin{pmatrix} \hat{v} \\ \hat{w} \end{pmatrix}=0, \tag{6.73a}$$

$$\begin{pmatrix} \partial_n\partial_t+\eta_{nt} & -\hat{\varphi}_n\partial_t \\ \hat{\varphi}_s\partial_t & \partial_s\partial_t+\eta_{st} \end{pmatrix}\begin{pmatrix} \hat{v} \\ \hat{w} \end{pmatrix}=0. \tag{6.73b}$$

The 'spatial' part (6.73a) of this Lax pair may be identified with the linear system (6.69) if we set

$$\hat{\varphi}=\varphi, \quad \hat{v}=v, \quad \hat{w}=w. \tag{6.74}$$

It is natural to inquire as to whether the 'temporal' part (6.73b) may also be satisfied in the present context, in which case the angle φ obeys the $2+1$-dimensional sine-Gordon system (6.72) and gives rise to classes of fiber distributions in which t plays the role of a parameter.

Here, we focus on the integrable case as summarized in Corollary 2 with $\epsilon=1$. Thus, insertion of φ_s and φ_n as given by (6.56) into (6.72a) yields

$$(\sinh\omega\sin\rho)_t+\eta_{nt}\cosh\omega-\eta_{st}\cos\rho=0, \tag{6.75}$$

which admits a decomposition into the two equations

$$\eta_{st}=\rho_t\sinh\omega, \quad \eta_{nt}=-\omega_t\sin\rho, \tag{6.76}$$

while the remaining equation (6.72b) reads

$$\eta_{sn}=-\cosh\omega\cos\rho. \tag{6.77}$$

The compatibility conditions $\eta_{stn}=\eta_{nts}=\eta_{snt}$ then produce

$$\rho_{nt}=-\omega_t\cos\rho, \quad \omega_{st}=-\rho_t\cosh\omega. \tag{6.78}$$

These are readily seen to be compatible with the system (6.54). Moreover, if we take into account the relations $v=-\rho_n$ and $w=\psi=\sin\rho$ (cf. (6.55)) then it may be verified that the Lax equation (6.73b) is indeed satisfied. Accordingly, it has been established that the fluid velocity vector $\mathbf{v}$ associated with steady planar motions governed by the integrable system (6.54) and taken with respect to the orthonormal basis ($\mathbf{t}$, $\mathbf{n}$) may be interpreted as an eigenfunction of the $2+1$-dimensional sine-Gordon system (6.72). Even though these integrable motions are not constrained by their parametric dependence on t, the solutions of the sine-Gordon system are special. In fact, the associated specialization of the sine-Gordon system encoded in (6.54), (6.56) and (6.76)–(6.78) may be simplified by the observation that

$$(\rho+\mathrm{i}\omega)_{st}=\mathrm{i}\varphi_s(\rho+\mathrm{i}\omega)_t, \quad (\rho+\mathrm{i}\omega)_{nt}=\mathrm{i}\varphi_n(\rho+\mathrm{i}\omega)_t \tag{6.79}$$

so that

$$\rho_t = \cos\varphi, \quad \omega_t = \sin\varphi \tag{6.80}$$

without loss of generality. Hence, we obtain the compatible systems

$$\begin{gathered}\varphi_s = -\cosh\omega, \quad \varphi_n = \cos\rho,\\ \omega_n = \sin\rho, \quad \rho_s = \sinh\omega,\\ \rho_t = \cos\varphi, \quad \omega_t = \sin\varphi,\end{gathered} \tag{6.81}$$

and

$$\begin{gathered}\eta_{sn} = -\cos\rho\cosh\omega,\\ \eta_{st} = \cos\varphi\sinh\omega,\\ \eta_{nt} = -\sin\varphi\sin\rho,\end{gathered} \tag{6.82}$$

which may directly be shown to constitute a reduction of the sine-Gordon system (6.72). It is interesting that the integrable system (6.81) has been recently discussed by Ferapontov in connection with Laplace transformations and Poisson brackets of hydrodynamic type.[53,54]

VII. INTEGRABILITY IN THE EQUILIBRIUM THEORY OF SHELL MEMBRANES

The study of the equilibrium of shell membranes has a long history going back to work of Lamé and Clapeyron[55] on the symmetric loading of shells of revolution. The classical governing equations of general membrane theory were set down by Lecornu[56] and Beltrami.[57] An extensive account of the membrane theory of shells is presented in the lucid monograph of Novozhilov.[58] Here, a classical system descriptive of the equilibrium of shell membranes under normal loading is investigated. It is established that, remarkably, the nonlinear system comprised of the equilibrium equations augmented by the Gauss–Mainardi–Codazzi equations for the membranes may be located in a large class of integrable systems which has recently been derived in the context of so-called O surfaces.[59]

A. The membrane shell system

In the following, we adopt the standard assumptions of classical shell membrane theory as described in Ref. 58. The geometric properties of the membrane are analyzed in the setting of the classical differential geometry of surfaces Σ embedded in an Euclidean space $\mathbb{R}^3$. If a surface (membrane) $\Sigma:\mathbf{r}=\mathbf{r}(\alpha,\beta)$ with associated normal $\mathbf{N}$ is parametrized in terms of curvature coordinates α, β then the first and second fundamental forms $\mathrm{I}=\mathrm{d}\mathbf{r}\cdot\mathrm{d}\mathbf{r}$, $\mathrm{II}=-\mathrm{d}\mathbf{N}\cdot\mathrm{d}\mathbf{r}$ are given by

$$\begin{gathered}\mathrm{I} = A_1^2 d\alpha^2 + A_2^2 d\beta^2,\\ \mathrm{II} = \kappa_1 A_1^2 d\alpha^2 + \kappa_2 A_2^2 d\beta^2,\end{gathered} \tag{7.1}$$

where $\kappa_1 = 1/R_1$, $\kappa_2 = 1/R_2$ denote the principal curvatures and R_1, R_2 are the corresponding principal radii of curvature. In these coordinates, the Gauss–Mainardi–Codazzi equations adopt the form

$$\left(\frac{A_{2\alpha}}{A_1}\right)_\alpha + \left(\frac{A_{1\beta}}{A_2}\right)_\beta + \kappa_1\kappa_2 A_1 A_2 = 0, \tag{7.2a}$$

$$\kappa_{1\beta} + (\ln A_1)_\beta(\kappa_1 - \kappa_2) = 0, \tag{7.2b}$$

$$\kappa_{2\alpha} + (\ln A_2)_\alpha(\kappa_2 - \kappa_1) = 0, \tag{7.2c}$$

while the classical membrane equilibrium equations reduce to

$$(N_1A_2)_\alpha+\frac{(A_1^2S)_\beta}{A_1}-N_2A_{2\alpha}+A_1A_2p_1=0,$$

$$(N_2A_1)_\beta+\frac{(A_2^2S)_\alpha}{A_2}-N_1A_{1\beta}+A_1A_2p_2=0, \tag{7.3}$$

$$\frac{N_1}{R_1}+\frac{N_2}{R_2}+p_3=0,$$

where N_1,N_2 denote the in-plane normal stress components and $S=N_{12}=N_{21}$ designates the in-plane shear. Here, the functions p_i are the components of the surface loading

$$\mathbf{p}=p_1\mathbf{e}_1+p_2\mathbf{e}_2+p_3\mathbf{e}_3, \tag{7.4}$$

wherein the orthonormal triad $(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)$ is defined by

$$\mathbf{e}_1=\frac{\mathbf{r}_\alpha}{A_1},\quad \mathbf{e}_2=\frac{\mathbf{r}_\beta}{A_2},\quad \mathbf{e}_3=\mathbf{N}=\frac{\mathbf{r}_\alpha\times\mathbf{r}_\beta}{A_1A_2}. \tag{7.5}$$

The system (7.3) results directly from the general theory of thin shells.[58]

For any given membrane geometry and prescribed external surface loading, the membrane equilibrium equations constitute a well-determined linear system for the in-plane stress. However, if conditions are imposed on the in-plane stress then the equilibrium equations constrain the Gauss–Mainardi–Codazzi equations and thereby the geometry of the membrane. Indeed, in the absence of in-plane shear $(S=0)$ with purely normal loading, the equilibrium equations (7.3) reduce to

$$N_{1\alpha}+(\ln A_2)_\alpha(N_1-N_2)=0, \tag{7.6a}$$

$$N_{2\beta}+(\ln A_1)_\beta(N_2-N_1)=0, \tag{7.6b}$$

$$\kappa_1N_1+\kappa_2N_2+p_3=0. \tag{7.6c}$$

The equilibrium equations together with the Gauss–Mainardi–Codazzi equations (7.2) then form a well-determined *coupled nonlinear* system. Thus, under the above-mentioned circumstances, the shape of a membrane in equilibrium is restricted. It is noted that the condition $S=0$ expresses the requirement that the lines of principal stress on the membrane coincide with the lines of curvature.

In the simplest case of a 'homogeneous' stress distribution, that is,

$$N_1=N_2=c=\text{const}, \tag{7.7}$$

the equilibrium equations (7.6) reduce to the classical Young–Laplace equation[60–62]

$$\kappa_1+\kappa_2=-c^{-1}p_3 \tag{7.8}$$

which expresses the fact that the normal loading p_3 is proportional to the mean curvature

$$\mathcal{H}=\kappa_1+\kappa_2 \tag{7.9}$$

of the membrane. In particular, if

$$p_3=\text{const} \tag{7.10}$$

then the membrane is of constant mean curvature while when $p_3=0$ then the membrane is minimal. This connection with classical constant mean curvature and minimal surfaces suggests the detailed study of the case $p_3=\text{const}$. Accordingly, in the following, we focus on the case of vanishing in-plane shear and constant purely normal loading.

B. The O surface connection

It is observed that the equilibrium equations (7.6a) and (7.6b) and the Gauss–Mainardi–Codazzi equations (7.2b) and (7.2c) are identical in form if the correspondence $(N_1,N_2)\leftrightarrow(\kappa_2,\kappa_1)$ is made. In fact, this observation provides the link with integrability. This is readily seen by reformulation of the governing equations. Thus, the change of variables

$$p=\frac{A_{1\beta}}{A_2},\quad q=\frac{A_{2\alpha}}{A_1},$$

$$H_\circ=-\kappa_1 A_1,\quad K_\circ=-\kappa_2 A_2, \tag{7.11}$$

$$H=A_1,\quad K=A_2$$

takes the Gauss–Mainardi–Codazzi equations (7.2) to the equivalent first-order system

$$p_\beta+q_\alpha+H_\circ K_\circ=0, \tag{7.12a}$$

$$H_\beta=pK, \tag{7.12b}$$

$$H_{\circ\beta}=pK_\circ, \tag{7.12c}$$

$$K_\alpha=qH, \tag{7.12d}$$

$$K_{\circ\alpha}=qH_\circ. \tag{7.12e}$$

The unit tangent vectors $\mathbf{e}_1=\mathbf{X}$, $\mathbf{e}_2=\mathbf{Y}$ to the lines of curvature and the normal $\mathbf{e}_3=\mathbf{N}$ are then obtained by solving the Gauss–Weingarten equations

$$\begin{aligned}\begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\\ \mathbf{N}\end{pmatrix}_\alpha&=\begin{pmatrix}0&-p&-H_\circ\\ p&0&0\\ H_\circ&0&0\end{pmatrix}\begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\\ \mathbf{N}\end{pmatrix},\\ \begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\\ \mathbf{N}\end{pmatrix}_\beta&=\begin{pmatrix}0&q&0\\ -q&0&-K_\circ\\ 0&K_\circ&0\end{pmatrix}\begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\\ \mathbf{N}\end{pmatrix},\end{aligned} \tag{7.13}$$

while the position vector $\mathbf{r}$ of the membrane is constructed by integration of the pair

$$\mathbf{r}_\alpha=H\mathbf{X},\quad \mathbf{r}_\beta=K\mathbf{Y}. \tag{7.14}$$

Here, it is important to note that the triplets $(\mathbf{r},H,K)$ and $(\mathbf{r}_\circ,H_\circ,K_\circ)$, where $\mathbf{r}_\circ=\mathbf{N}$, obey the same linear equations, namely, (7.12b), (7.12d), and (7.14) on the one hand and (7.12c), (7.12e), and

$$\mathbf{r}_{\circ\alpha}=H_\circ\mathbf{X},\quad \mathbf{r}_{\circ\beta}=K_\circ\mathbf{Y} \tag{7.15}$$

on the other.

The additional change of variables

$$\tilde{H}=N_2A_1, \quad \tilde{K}=N_1A_2 \tag{7.16}$$

now reduces the equilibrium equations (7.6) to the pair

$$\tilde{H}_\beta=p\tilde{K}, \quad \tilde{K}_\alpha=q\tilde{H} \tag{7.17}$$

subject to the constraint

$$H_\circ\tilde{K}+K_\circ\tilde{H}-p_3HK=0. \tag{7.18}$$

The relations (7.17) represent nothing but another copy of the equations (7.12b) and (7.12d) or (7.12c) and (7.12e). They imply the compatibility of the pair

$$\tilde{\mathbf{r}}_\alpha=\tilde{H}\mathbf{X}, \quad \tilde{\mathbf{r}}_\beta=\tilde{K}\mathbf{Y} \tag{7.19}$$

for some vector-valued function $\tilde{\mathbf{r}}$. Thus, if we interpret $\tilde{\mathbf{r}}$ as the position vector of a surface $\tilde{\Sigma}$ with principal curvatures $\tilde{\kappa}_1=-H_\circ/\tilde{H}$ and $\tilde{\kappa}_2=-K_\circ/\tilde{K}$ then the relations (7.14), (7.15) and (7.19) show that the tangent vectors to the coordinate lines on the membrane Σ, the sphere $\Sigma_\circ$ and the surface $\tilde{\Sigma}$ are parallel. Moreover, since the Gauss–Weingarten equations (7.13) are formulated in terms of the orthonormal triad ($\mathbf{X}$, $\mathbf{Y}$, $\mathbf{N}$) only, we deduce that the surface $\tilde{\Sigma}$ is likewise parametrized in terms of curvature coordinates. Two surfaces parametrized in terms of curvature coordinates which are such that at corresponding points their tangent vectors are parallel are said to be Combescure transforms of each other.[59] It is observed that even though the Combescure transformation has originally been defined for surfaces parametrized in terms of conjugate coordinates, it may readily be shown that it preserves lines of curvature. Accordingly, the surface $\tilde{\Sigma}$ constitutes a Combescure transform of the membrane Σ. The following theorem therefore holds:[63]

Theorem 7: *A shell membrane Σ with vanishing in-plane shear S and constant purely normal loading $\mathbf{p}=p_3\mathbf{N}$ is in equilibrium iff there exists a Combescure transform $\tilde{\Sigma}$ such that the orthogonality condition*

$$\mathsf{H}^{\mathrm{T}}\Lambda\mathsf{K}=0 \tag{7.20}$$

is satisfied, where

$$\mathsf{H}=\begin{pmatrix} H_\circ \\ H \\ \tilde{H} \end{pmatrix}, \quad \mathsf{K}=\begin{pmatrix} K_\circ \\ K \\ \tilde{K} \end{pmatrix}, \quad \Lambda=\begin{pmatrix} 0 & 0 & 1 \\ 0 & -p_3 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{7.21}$$

The in-plane stress components N_1 and N_2 are given by

$$N_1=\frac{\kappa_2}{\tilde{\kappa}_2}=\frac{\tilde{K}}{K}, \quad N_2=\frac{\kappa_1}{\tilde{\kappa}_1}=\frac{\tilde{H}}{H}. \tag{7.22}$$

If one replaces the three-dimensional vectors H, K by their higher-dimensional analogues corresponding to a collection of Combescure transforms and demands that these vectors be orthogonal with respect to a symmetric constant matrix Λ then the general class of integrable O surfaces is obtained.[59] It is important to remark that O surfaces include and generalize classical surfaces such as isothermic, constant mean curvature, minimal, linear Weingarten, Guichard and Petot surfaces and surfaces of constant Gaussian curvature. The membrane O surfaces as identified above are reminiscent of the classical Guichard surfaces which are associated with the matrix

$$\Lambda = \begin{pmatrix} c & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{7.23}$$

In this case, the orthogonality constraint (7.20) reads

$$R_1\tilde{R}_2 + R_2\tilde{R}_1 + c = 0. \tag{7.24}$$

This is precisely the constraint in terms of which Guichard[64] defined his surfaces. In the case of membrane O surfaces, the constraint (7.20) may be written as

$$\tilde{R}_1 + \tilde{R}_2 + p_3 R_1 R_2 = 0, \tag{7.25}$$

which, by construction, is nothing but the normal component equilibrium equation (7.6c).

C. Particular membrane geometries

The above formulation of the governing equations may be exploited to isolate particular classes of membrane O surfaces and investigate their properties.[63] For instance, if the normal loading vanishes, that is $p_3 = 0$, then the orthogonality constraint (7.20) simplifies to

$$\begin{pmatrix} H_\circ \\ \tilde{H} \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} K_\circ \\ \tilde{K} \end{pmatrix} = 0. \tag{7.26}$$

Thus, the latter imposes a restriction on the surface $\tilde{\Sigma}$ while Σ constitutes an arbitrary Combescure transform of $\tilde{\Sigma}$. Since (7.26) may be cast into the form

$$\tilde{\mathcal{H}} = \tilde{\kappa}_1 + \tilde{\kappa}_2 = 0, \tag{7.27}$$

it is evident that any Combescure transform Σ of a minimal surface $\tilde{\Sigma}$ may be considered a membrane which is in equilibrium.

In the case of non-vanishing normal loading, we may impose the admissible conditions

$$\tilde{H} = \mu H - \lambda H_\circ, \quad \tilde{K} = \mu K - \lambda K_\circ, \tag{7.28}$$

where λ and μ constitute arbitrary constants. The orthogonality constraint (7.20) then reduces to

$$\begin{pmatrix} H_\circ \\ H \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 2\lambda & -\mu \\ -\mu & p_3 \end{pmatrix} \begin{pmatrix} K_\circ \\ K \end{pmatrix} = 0 \tag{7.29}$$

or, equivalently,

$$2\lambda\mathcal{K} + \mu\mathcal{H} + p_3 = 0, \tag{7.30}$$

where the Gaussian curvature $\mathcal{K}$ of the membrane is defined by

$$\mathcal{K} = \kappa_1\kappa_2. \tag{7.31}$$

Importantly, the relation (7.30) shows that the membrane adopts the shape of a linear Weingarten surface since the principal curvatures κ_1, κ_2 are functionally dependent and their relation is such that the Gauss and mean curvatures are linearly related.[43] It is well-known that linear Weingarten surfaces are 'solitonic,' that is, their underlying Gauss–Mainardi–Codazzi equations constitute an integrable system. In the case $\lambda = 0$, the above-mentioned constant mean curvature surfaces are retrieved while the condition $\mu = 0$ leads to surfaces of constant Gaussian curvature. Linear

Weingarten surfaces are known to be parallel to surfaces of constant Gaussian curvature provided that $\mu^2-2\lambda p_3\neq 0$. Parallel surfaces are of importance in computer-aided engineering design in which context they are termed ''offset surfaces.'' [65,66] Potential applications of Weingarten surfaces in this context are discussed in Ref. 67. Thus, linear Weingarten surfaces may be regarded as inheriting their integrable nature from surfaces of constant Gaussian curvature (vide Ref. 1).

Canal surfaces[68] may also be identified with membranes in equilibrium. These are the envelopes of one-parameter families of spheres of variable radius. They include surfaces of revolution and classical Dupin cyclides. The latter are defined by the requirement that the lines of curvature consist of circles.[43,68] Dupin surfaces constitute particular members of the integrable class of classical isothermic surfaces (see, e.g., Ref. 69). Details of the significance of canal surfaces in shell membrane theory may be found in Refs. 63 and 70.

D. A linear representation and associated Bäcklund transformation

The integrability of O surfaces is reflected by the existence of Lax pairs and Bäcklund transformations.[59] The existence of Lax pairs for O surfaces implies that the *nonlinear* Gauss–Mainardi–Codazzi and equilibrium equations (7.2), (7.6), and (7.10) may be completely encoded in a pair of *linear* matrix equations via compatibility. Indeed, the following result may be established.[63]

Theorem 8: *The linear system*

$$\begin{pmatrix}\mathcal{X}\\ \mathcal{Y}\\ \mathcal{R}_\circ\\ \mathcal{R}\\ \tilde{\mathcal{R}}\end{pmatrix}_\alpha=\begin{pmatrix}0 & -p & m\tilde{H}-H_\circ & -mp_3H & mH_\circ\\ p & 0 & 0 & 0 & 0\\ H_\circ & 0 & 0 & 0 & 0\\ H & 0 & 0 & 0 & 0\\ \tilde{H} & 0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\mathcal{X}\\ \mathcal{Y}\\ \mathcal{R}_\circ\\ \mathcal{R}\\ \tilde{\mathcal{R}}\end{pmatrix},$$

$$\begin{pmatrix}\mathcal{X}\\ \mathcal{Y}\\ \mathcal{R}_\circ\\ \mathcal{R}\\ \tilde{\mathcal{R}}\end{pmatrix}_\beta=\begin{pmatrix}0 & q & 0 & 0 & 0\\ -q & 0 & m\tilde{K}-K_\circ & -mp_3K & mK_\circ\\ 0 & K_\circ & 0 & 0 & 0\\ 0 & K & 0 & 0 & 0\\ 0 & \tilde{K} & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\mathcal{X}\\ \mathcal{Y}\\ \mathcal{R}_\circ\\ \mathcal{R}\\ \tilde{\mathcal{R}}\end{pmatrix} \tag{7.32}$$

is compatible iff the Gauss–Mainardi–Codazzi equations

$$\begin{gathered}p_\beta+q_\alpha+H_\circ K_\circ=0,\\ H_\beta=pK,\quad H_{\circ\beta}=pK_\circ,\\ K_\alpha=qH,\quad K_{\circ\alpha}=qH_\circ,\end{gathered} \tag{7.33}$$

and the membrane equilibrium equations

$$\begin{gathered}\tilde{H}_\beta=p\tilde{K},\quad \tilde{K}_\alpha=q\tilde{H},\\ H_\circ\tilde{K}+K_\circ\tilde{H}-p_3HK=0\end{gathered} \tag{7.34}$$

are simultaneously satisfied. Here, m is an arbitrary constant parameter.

The Bäcklund transformation for the general class of O surfaces as set down in Ref. 59 is based on the classical fundamental transformation for conjugate nets and its specialization to the classical Ribaucour transformation which preserves lines of curvature.[1] In the case of membrane O surfaces, the associated Bäcklund transformation reads as follows:[63]

Theorem 9: *The Gauss–Mainardi–Codazzi and membrane equilibrium equations (7.33) and (7.34) are invariant under the transformation*

$$\mathsf{H}'=\mathsf{H}-\frac{\overline{H}\mathsf{R}}{M},\quad \mathsf{K}'=\mathsf{K}-\frac{\overline{K}\mathsf{R}}{M},$$
$$p'=p-\frac{\mathcal{Y}\overline{H}}{M},\quad q'=q-\frac{\mathcal{X}\overline{K}}{M},\tag{7.35}$$

where $\mathcal{X},\mathcal{Y},\mathsf{R}=(\mathcal{R}_\circ,\mathcal{R},\tilde{\mathcal{R}})^{\mathrm{T}}$ *constitute a solution of the linear representation (7.32) subject to the admissible quadratic constraint*

$$\mathcal{X}^2+\mathcal{Y}^2+\mathcal{R}_\circ^2=m(2\mathcal{R}_\circ\tilde{\mathcal{R}}-p_3\mathcal{R}^2)\tag{7.36}$$

and

$$\overline{H}=\mathcal{X}_\alpha+p\mathcal{Y}+H_\circ\mathcal{R}_\circ,\quad \overline{K}=\mathcal{Y}_\beta+q\mathcal{X}+K_\circ\mathcal{R}_\circ,$$
$$2M=\mathcal{X}^2+\mathcal{Y}^2+\mathcal{R}_\circ^2.\tag{7.37}$$

The membranes Σ *and* Σ' *are related by*

$$\mathbf{r}'=\mathbf{r}-\frac{\mathcal{R}\mathbf{M}}{M},\quad \mathbf{M}=\mathcal{X}\mathbf{X}+\mathcal{Y}\mathbf{Y}+\mathcal{R}_\circ\mathbf{N}.\tag{7.38}$$

The above Bäcklund transformation may now be used to construct explicitly large classes of membranes in equilibrium with vanishing in-plane shear S and associated in-plane stress components N_1 and N_2 determined by (7.22).

In conclusion, it is noted that if the geometry of the membrane is such that $A_1=A_2$, then the analysis presented here extends to the case $SA_1^2=\text{const}$ since the in-plane shear terms in the equilibrium equations (7.3) vanish. In particular, this applies to membranes of constant mean curvature, membranes of revolution and membranes which adopt the shape of Dupin cyclides. Surfaces constrained by $A_1=A_2$ are ''solitonic'' and termed isothermic surfaces.[43]

ACKNOWLEDGMENTS

The authors acknowledge support for this project under an Australian Research Council grant. One of the authors (C.R.) expresses his gratitude to Professor Carillo of the Dipartimento di Metodi e Modelli Matematici per le Scienzá Applicate, Università di Roma and to Professor Antonio Degasperis of the Dipartimento di Fisica, Università di Roma for support during a visit to Italy during which part of the present text was presented in a lecture series under the title ''Integrability and Continuum Mechanics.''

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

CP^{N-1} harmonic maps and the Weierstrass problem

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(Received 2 December 2002; accepted 9 April 2003)

A Weierstrass-type system of equations corresponding to the CP^{N-1} harmonic maps is presented. The system constitutes a further generalization of our previous construction [J. Math. Phys. **44**, 328 (2003)]. It consists of four first order equations for three complex functions which are shown to be equivalent to the CP^{N-1} harmonic maps. When the harmonic maps are holomorphic (or antiholomorphic) one of the functions vanishes and the system reduces to the previously given generalization of the Weierstrass problem. We also discuss a possible interpretation of our results and show that in our new case the induced metric is proportional to the total energy density of the map and not only to its holomorphic part, as was the case in the previous generalizations. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1586791]

I. INTRODUCTION

A few years ago Konopelchenko, together with his collaborators,[1,2] introduced the subject of Weierstrass representations of surfaces immersed in multidimensional spaces. This has generated quite a lot of interest[3,4] and has led to the connection with the CP^{N-1} harmonic maps. Exploiting this connection, we have recently proposed a generalization of these ideas to the CP^2 (Ref. 5) case and, more recently, managed to generalize it further—to the CP^{N-1} case.[6]

These generalizations lead to the study of immersed surfaces, whose metric is then related to the properties of the corresponding harmonic maps. In the CP^1 case all harmonic maps (from S^2) are holomorphic (or antiholomorphic) and, as the induced metric is characterized by the holomorphic component of the energy, this characterization is complete. This is also the case for the holomorphic CP^{N-1} maps.

In the CP^{N-1} case (for $N>2$) there are harmonic maps which are not holomorphic[7] and for them the above mentioned construction[6] is not complete, as in the general case we would expect the maps to be characterized by the total energy. Hence a further generalization is called for and such a generalization is provided in this article.

In the next section we briefly review the CP^{N-1} harmonic maps (using the formalism as given in Ref. 7) and in the following sections relate these maps to the various versions of the Weierstrass problem.

II. CP^{N-1} HARMONIC MAPS

A. Formulation

The CP^{N-1} models are, in fact, a generalization of the, perhaps the simplest, sigma model, namely, the S^2 model—also called the vector $O(3)$ model. The CP^{N-1} models involve maps from R^2, or S^2 if a nontrivial topology is required, to CP^{N-1}, i.e.,

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$$C \supset \Omega \ni \zeta = \zeta_1 + i\zeta_2 \mapsto z = (z^1, \ldots, z^N) \in C^N, \tag{1}$$

where the homogeneous coordinates $z = (z^1, \ldots, z^N)$ have the following property:

$$z \sim z' = \lambda z \quad \text{for} \quad \lambda \neq 0.$$

Exploiting this projective invariance we can require that

$$z^\dagger \cdot z = 1 \tag{2}$$

holds, where † denotes Hermitian conjugation, and we are still left with the gauge symmetry

$$z \to z' = z e^{i\phi}, \tag{3}$$

where ϕ is a real-valued function.

It is easiest to define the CP^{N-1} models in terms of the Lagrangian density[7]

$$L = \tfrac{1}{4}(D_\mu z)^\dagger \cdot D_\mu z, \quad z^\dagger \cdot z = 1, \tag{4}$$

where the covariant derivatives D_μ act on $z: S^2 \to CP^{N-1}$ according to the formula

$$D_\mu z = \partial_\mu z - (z^\dagger \cdot \partial_\mu z) z. \tag{5}$$

Here the index $\mu = 1,2$ denotes ζ_1 and ζ_2. Note that the covariant derivatives $D_\mu z$ transform under the gauge transformation (3)

$$D_\mu z \to D_\mu z' = (D_\mu z) e^{i\phi}, \tag{6}$$

so that the dependence on the phase ϕ drops out of the Lagrangian density (4) and so the model is really based on CP^{N-1}.

The total Lagrangian is given by

$$\mathcal{L} = \int L \, d\zeta \, d\overline{\zeta} \tag{7}$$

and, if the CP^{N-1} model is defined over S^2, we require that $\mathcal{L}$ is finite.

For the CP^{N-1} sigma model it is convenient to define

$$z = \frac{f}{|f|}, \tag{8}$$

where $|f| = (f^\dagger \cdot f)^{1/2}$. In terms of f the Lagrangian (7) becomes

$$\mathcal{L} = \int \frac{|\overline{\partial} f|^2 + |\partial f|^2}{|f|^4} d\zeta \, d\overline{\zeta}, \tag{9}$$

where $|\partial f|^2 = (\partial f)^\dagger \cdot (\partial f)$ and $|\overline{\partial} f|^2 = (\overline{\partial} f)^\dagger \cdot (\overline{\partial} f)$. The Euler–Lagrange equations for f take the form

$$\left(1 - \frac{f \otimes f^\dagger}{|f|^2}\right)\left[\partial \overline{\partial} f - \partial f \frac{(f^\dagger \cdot \overline{\partial} f)}{|f|^2} - \overline{\partial} f \frac{(f^\dagger \cdot \partial f)}{|f|^2}\right] = 0, \tag{10}$$

where we have introduced the holomorphic and antiholomorphic derivatives

$$\partial = \frac{\partial}{\partial(\zeta_1 + i\zeta_2)} = \frac{\partial}{\partial\zeta}, \quad \overline{\partial} = \frac{\partial}{\partial(\zeta_1 - i\zeta_2)} = \frac{\partial}{\partial\overline{\zeta}}, \tag{11}$$

and bar denotes complex conjugation.

B. Integrability and first conservation laws

As is well known,[8] Eqs. (10) can be written as a compatibility condition for a set of two linear spectral equations for an N-component auxiliary vector Ψ,

$$\begin{aligned} \partial\Psi &= \frac{2}{1+\lambda}[\partial P, P]\,\Psi, \\ \overline{\partial}\Psi &= \frac{2}{1-\lambda}[\overline{\partial} P, P]\,\Psi, \end{aligned} \tag{12}$$

where λ is a spectral parameter and the N by N matrix P is the projector given by

$$P = \frac{1}{|f|^2} f \otimes f^\dagger, \quad P^\dagger = P, \quad P^2 = P. \tag{13}$$

The compatibility conditions for (12) are then

$$[\partial\overline{\partial} P, P] = 0, \tag{14}$$

which, as can be easily checked, are equivalent to Eqs. (10). Note that (14) can be written in the form of a conservation law

$$\partial[\overline{\partial} P, P] + \overline{\partial}[\partial P, P] = 0 \tag{15}$$

or, equivalently, using the tracelessness of the matrix K, as

$$\partial K - \overline{\partial} K^\dagger = 0, \tag{16}$$

where the matrices K and $K^\dagger$ are given by

$$K = [\overline{\partial} P, P] = \frac{\overline{\partial} f \otimes f^\dagger - f \otimes \overline{\partial} f^\dagger}{|f|^2} + \frac{f \otimes f^\dagger}{|f|^4}[(\overline{\partial} f^\dagger \cdot f) - (f^\dagger \cdot \overline{\partial} f)], \qquad \mathrm{Tr}\, K = 0, \tag{17}$$

and consequently

$$K^\dagger = -[\partial P, P] = -\frac{\partial f \otimes f^\dagger - f \otimes \partial f^\dagger}{|f|^2} + \frac{f \otimes f^\dagger}{|f|^4}[(\partial f^\dagger \cdot f) - (f^\dagger \cdot \partial f)].$$

Note that due to the invariance of the Lagrangian (4) under the gauge transformation (3) we can, without any loss of generality, set one of the components of the vector field f, say f_1, to 1. Then, in the CP^1 case, all quantities are expressible through one variable

$$w = \frac{f_2}{f_1} = f_2 \tag{18}$$

and the Euler–Lagrange equations (10) take the form

$$\partial\overline{\partial}w-\frac{2\overline{w}}{(1+|w|^2)}\partial w\overline{\partial}w=0. \tag{19}$$

C. Further conservation laws

Let us note that our matrix K in (17) is given by

$$K=M+L, \tag{20}$$

where

$$M=(1-P)\frac{\overline{\partial}f\otimes f^{\dagger}}{|f|^2} \tag{21}$$

and

$$L=-\frac{f\otimes\overline{\partial}f^{\dagger}}{|f|^2}(1-P). \tag{22}$$

Thus

$$M^{\dagger}=\frac{f\otimes\partial f^{\dagger}}{|f|^2}(1-P),\quad \text{and}\quad L^{\dagger}=-(1-P)\frac{\partial f\otimes f^{\dagger}}{|f|^2}. \tag{23}$$

Next we note that the matrices M and L, separately, satisfy our conservations laws (16). To see this consider

$$\begin{aligned}\partial M-\overline{\partial}M^{\dagger}=&-\partial P\frac{\overline{\partial}f\otimes f^{\dagger}}{|f|^2}+(1-P)\frac{\overline{\partial}\partial f\otimes f^{\dagger}}{|f|^2}+(1-P)\frac{\overline{\partial}f\otimes\partial f^{\dagger}}{|f|^2}-(1-P)\frac{\overline{\partial}f\otimes f^{\dagger}}{|f|^4}\partial|f|^2\\&-\frac{\overline{\partial}f\otimes\partial f^{\dagger}}{|f|^2}(1-P)-\frac{f\otimes\overline{\partial}\partial f^{\dagger}}{|f|^2}(1-P)+\frac{f\otimes\partial f^{\dagger}}{|f|^2}\overline{\partial}P+\frac{f\otimes\partial f^{\dagger}}{|f|^4}(1-P)\overline{\partial}|f|^2.\end{aligned} \tag{24}$$

But

$$\partial P=\frac{\partial f\otimes f^{\dagger}}{|f|^2}+\frac{f\otimes\partial f^{\dagger}}{|f|^2}-\frac{P}{|f|^2}\partial|f|^2 \tag{25}$$

and so we see that all the terms in (24) become

$$\begin{aligned}&(1-P)\left[\partial\overline{\partial}f-\partial f\frac{(f^{\dagger}\cdot\overline{\partial}f)}{|f|^2}-\overline{\partial}f\frac{(f^{\dagger}\cdot\partial f)}{|f|^2}\right]\\&\otimes\frac{f^{\dagger}}{|f|^2}-\frac{f}{|f|^2}\otimes\left[\partial\overline{\partial}f^{\dagger}-\partial f^{\dagger}\frac{(\overline{\partial}f^{\dagger}f)}{|f|^2}-\overline{\partial}f^{\dagger}\frac{(\partial f^{\dagger}\cdot f)}{|f|^2}\right](1-P).\end{aligned} \tag{26}$$

However, due to (10), this is zero. Hence we have two separate conservation laws, namely,

$$\partial M=\overline{\partial}M^{\dagger} \tag{27}$$

and

$$\partial L=\overline{\partial}L^{\dagger}. \tag{28}$$

Next we consider the explicit form of the entries of the matrices M and L. To do this we introduce

$$F_{ij} = f_i \partial f_j - f_j \partial f_i, \tag{29}$$

and

$$G_{ij} = f_i \overline{\partial} f_j - f_j \overline{\partial} f_i. \tag{30}$$

Then, using expressions (29) and (30), we can write the entries of the matrices M and L, equivalently, in the form

$$M_{ij} = \overline{\Phi_i^2} \overline{f_j} \tag{31}$$

and

$$L_{ij} = - f_i \overline{\varphi_j^2}, \tag{32}$$

where we have introduced

$$\varphi_i^2 = \frac{1}{A^2} \overline{f}_k F_{ki}, \quad A = \overline{f_l} f_l \tag{33}$$

and

$$\Phi_i^2 = \frac{1}{A^2} f_k \overline{G_{ki}}, \tag{34}$$

and we have used the convention of implicit summation over repeated indices.

Note that from Eqs. (30), (33), and (34) we have two algebraic constraints, namely,

$$\overline{f_k}\, \varphi_k^2 = 0, \quad f_k \Phi_k^2 = 0, \tag{35}$$

which imply that only $(N-1)$ functions φ_i^2 and $(N-1)$ functions Φ_i^2 are linearly independent. So in our further discussion we take as independent functions $\varphi_2^2, \ldots, \varphi_N^2$ and $\Phi_2^2, \ldots, \Phi_N^2$.

Making use of the symmetry (3) we can set, without any loss of generality, say, $f_1 = 1$, and so we end up with the expressions [for (33), and (34)]

$$\begin{aligned} \varphi_i^2 &= \frac{1}{A^2}[(1 + f_k \overline{f_k})\, \partial f_i - f_i(\overline{f_k}\, \partial f_k)], \\ \overline{\Phi_i^2} &= \frac{1}{A^2}[(1 + f_k \overline{f_k})\, \overline{\partial} f_i - f_i(\overline{f_k}\, \overline{\partial} f_k)], \quad i = 2, \ldots, N, \end{aligned} \tag{36}$$

where

$$A = 1 + |f_2|^2 + \cdots + |f_N|^2.$$

Note that now all the sums over repeated indices run over $k = 2, \ldots, N$.

Next we invert expressions (36) and so express all the derivatives ∂f_i in terms of φ_i^2's and f_i. This way we find that

$$\partial f_i = A\,[\varphi_i^2 + f_i \overline{f}_k \varphi_k^2]. \tag{37}$$

Thus, in particular, for the CP^1 case, Eqs. (37) become

$$\partial f_2 = A^2 \varphi_2^2, \quad A = 1 + |f_2|^2,$$

and f_2 is often denoted by w (see, e.g., Ref. 7), while in the CP^2 case we have

$$\begin{aligned} \partial f_2 &= A[(1+|f_2|^2)\varphi_2^2 + f_2 \overline{f_3}\, \varphi_3^2], \\ \partial f_3 &= A[(1+|f_3|^2)\varphi_3^2 + f_3 \overline{f_2}\, \varphi_2^2], \\ A &= 1 + |f_2|^2 + |f_3|^2. \end{aligned} \tag{38}$$

Note that in Refs. 5 and 6 the functions f_2 and f_3 are denoted by w_1 and w_2, respectively.

Similarly,

$$\overline{\partial} f_i = A\,[\overline{\Phi}_i^2 + f_i\, \overline{f}_k \overline{\Phi}_k^2]. \tag{39}$$

III. THE WEIERSTRASS PROBLEM[1,3]

In the Weierstrass problem we consider two complex functions $\psi = \psi(\zeta, \overline{\zeta})$ and $\phi = \phi(\zeta, \overline{\zeta})$, which satisfy

$$\partial \psi = p\, \phi, \quad \overline{\partial} \phi = -p\, \psi, \quad p = |\phi|^2 + |\psi|^2. \tag{40}$$

Note that we have not specified $\overline{\partial}\psi$, nor $\partial\phi$.

A natural question then arises. Is this problem related to the harmonic maps of the previous sections, presumably corresponding to the case of CP^1?

This is indeed the case as has been discussed in Ref. 4. To see this we put

$$w = \frac{\psi}{\overline{\phi}} \tag{41}$$

and note that

$$\psi = w \frac{(\overline{\partial}\overline{w})^{1/2}}{1+|w|^2}, \quad \phi = \frac{(\partial w)^{1/2}}{1+|w|^2} \tag{42}$$

satisfy (40). In fact, one can show that (19) and (40) are equivalent.

Moreover, we can introduce three real quantities:

$$\begin{aligned} X_1 &= i \int_\gamma [\overline{\psi}^2 + \phi^2] d\zeta - [\psi^2 + \overline{\phi}^2] d\overline{\zeta}, \\ X_2 &= \int_\gamma [\overline{\psi}^2 - \phi^2] d\zeta + [\psi^2 - \overline{\phi}^2] d\overline{\zeta}, \\ X_3 &= -2 \int_\gamma \overline{\psi}\phi d\zeta + \psi \overline{\phi} d\overline{\zeta}, \end{aligned} \tag{43}$$

where γ is any curve from a fixed point to ζ. Then, it is easy to show that if ψ and ϕ satisfy (40), the functions X_i do not depend on the contour of the curve γ but only on its endpoints.

Furthermore, if we treat X_i as components of a vector $\vec{r} = (X_1, X_2, X_3)$ and introduce the metric

$$g_{\zeta\zeta} = (\partial \vec{r}, \partial \vec{r}), \quad g_{\overline{\zeta}\overline{\zeta}} = (\overline{\partial}\vec{r}, \overline{\partial}\vec{r}), \quad g_{\zeta\overline{\zeta}} = (\partial \vec{r}, \overline{\partial}\vec{r}), \tag{44}$$

we find that, for fields which solve (19) on S^2, only $g_{\zeta\bar{\zeta}}$ is nonzero and is given by

$$g_{\zeta\bar{\zeta}} = \frac{|\partial w|^2}{(1+|w|^2)^2} = |Dz|^2, \tag{45}$$

where $D = 1/2(D_1 - iD_2)$, with D_i defined in (5); i.e., is a covariant derivative evaluated with respect to ζ. Note that (45) is a term in the general expression for the energy density of the CP^1 map. However, as all harmonic maps on S^2 satisfy $w = w(\zeta)$,[7] we note that $g_{\zeta\bar{\zeta}}$ is the total energy density of this map. (We are assuming here that we are not dealing with antiholomorphic maps, as in this case we simply interchange the roles of ζ and $\bar{\zeta}$.)

IV. A GENERALIZED WEIERSTRASS REPRESENTATION IN R^M

Having observed that the Weierstrass problem is related to the equations of the CP^1 model, we have in Refs. 5 and 6 presented a CP^{N-1} generalization of the Weierstrass problem. Our generalization was based on the observation that for a generalized Weierstrass system in multi-dimensional spaces we need a set of φ_i and ψ_i which generalize the φ and ψ of the CP^1 case.

Then we noted that the quantities φ_i^2, $i = 2, \ldots, N$, defined in (33), provide such a choice as (37) is a natural CP^{N-1} generalization of (42).

What should we take for the functions ψ_i? In Ref. 6 we argued that (41) suggested that we put

$$\psi_i = f_i \bar{\varphi}_i \tag{46}$$

with no summation over the indices $i = 2, \ldots, N$. Then, to complete the generalization of the Weierstrass system in multi-dimensional spaces, we need relations which would be analogs of (40), i.e., we need to prescribe the first derivatives $\bar{\partial}\varphi_i$ and $\partial\psi_i$ in terms of φ_i and ψ_i.

Note that from (46) we have

$$\partial\psi_i = \partial(f_i \bar{\varphi}_i) = \partial f_i \bar{\varphi}_i + f_i \overline{(\bar{\partial}\varphi_i)}. \tag{47}$$

So, we are left to specify $\bar{\partial}\varphi_i$ in terms of φ_i, f_i and their derivatives. To do this, in Ref. 1, we noted that from (36) we had

$$\bar{\partial}\varphi_i^2 = 2\frac{f_i(\bar{f}_l \partial f_l)}{A^3}(\bar{f}_k \bar{\partial} f_k + f_k \overline{\partial f_k}) + \frac{1}{A^2}[(1+|f|^2)\partial\bar{\partial} f_i - (\bar{f}_k \bar{\partial} f_k)\partial f_i - (f_k \overline{\partial f_k})\partial f_i - \bar{\partial} f_i(\bar{f}_k \partial f_k) - f_i(\overline{\partial f_k}\partial f_k) - f_i(\bar{f}_k\, \partial\bar{\partial} f_k)]. \tag{48}$$

However, Eq. (10) allowed us to eliminate the second derivatives $\partial\bar{\partial} f_i$ from (48) and also we noted that all the terms involving first derivatives $\bar{\partial} f$ and $\partial \bar{f}$ in (48) canceled. Thus we ended up with a simple expression

$$\bar{\partial}\varphi_i = -\frac{\varphi_i}{2A}(f_k \overline{\partial f_k}) - \frac{f_i}{2\varphi_i A^2}(\overline{\partial f_k}\partial f_k) + \frac{f_i}{2\varphi_i A^3}(\overline{\partial f_k} f_k)(\bar{f}_l \partial f_l). \tag{49}$$

Next, taking the complex conjugate of (37),

$$\overline{\partial f_k} = A[\bar{\varphi}_k^2 + \bar{f}_k f_l \bar{\varphi}_l^2], \tag{50}$$

and using (50) we have found

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\} \tag{51}$$

(no summation over i). The second pair of equations for ψ_i then followed from (47), i.e.,

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)] \tag{52}$$

(no summation over i).

Thus, in Ref. 6 we proposed the following form of the generalized Weierstrass system: The **generalized Weierstrass system** in multi-dimensional space is a set of $(2N-2)$ complex functions φ_i and ψ_i, $i=2,\ldots,N$, which obey the following system of equations (no summation over i):

$$\overline{\partial}\varphi_i = -\frac{1}{2}\left\{A\varphi_i(\overline{\varphi}\cdot\psi) + \frac{\psi_i}{\varphi_i\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)]\right\}$$

and

$$\partial\psi_i = A\overline{\varphi}_i\varphi_i^2 + \frac{1}{2}A\psi_i(\overline{\psi}\cdot\varphi) - \frac{1}{2}\frac{|\psi_i|^2}{|\varphi_i|^2\overline{\varphi}_i}[(\overline{\varphi}^2\cdot\varphi^2) + (\overline{\varphi}\cdot\psi)(\overline{\psi}\cdot\varphi)], \tag{53}$$

where

$$A = 1 + \sum_{k=2}^{N}\frac{|\psi_k|^2}{|\varphi_k|^2}.$$

From our construction it is clear that the above system of equations is equivalent to the equations of the CP^{N-1} sigma model (10). Moreover, it is easy to check that the system of equations (53) reduces to Eq. (19) when $N=2$.

V. A MODIFIED GENERALIZED WEIERSTRASS REPRESENTATION

The generalized Weierstrass representation given in the previous section leads to pairs of functions φ_i, ψ_i, $i=2,\ldots,N$, and, as discussed in Ref. 6, to a geometric interpretation in terms of surfaces in R^M for which their metric is given by $|Dz|^2$ [as in the CP^1 case—see (45)]. This is the case for the holomorphic solutions but we know[7] that CP^{N-1} models have harmonic maps which are not holomorphic (even CP^1 has such maps; in this case, antiholomorphic maps, but these can be considered to be complex conjugates of holomorphic ones). But for CP^{N-1}, $N>2$, we have also maps which are neither holomorphic nor antiholomorphic. So can we generalize the Weierstrass problem differently to bring out this property?

In fact, our discussion of the CP^{N-1} models does tell us what to do. We should use both φ_i and Φ_i. Thus we should consider a larger problem and use Φ_i, φ_i, and f_i.

Then taking (36) and repeating the steps as in (48) (and using φ^2 and Φ^2) we get

$$\overline{\partial}\varphi_i^2 = -A\varphi_i^2(\varphi^{\dagger 2}\cdot f) - f_i[(\varphi^{\dagger 2}\cdot\varphi^2) + (f^\dagger\cdot\varphi^2)(\varphi^{2\dagger}\cdot f)], \tag{54}$$

$$\overline{\partial}\Phi_i^2 = -A\Phi_i^2(f^\dagger\cdot\overline{\Phi}^2) - \overline{f}_i[(\Phi^{\dagger 2}\cdot\Phi^2) + (f^\dagger\cdot\overline{\Phi}^2)(\overline{\Phi}^{\dagger 2}\cdot f)]. \tag{55}$$

These equations should then be supplemented with the expressions for ∂f and $\partial\overline{f}$. The latter are given by (37) and (39) and so take the form

$$\partial f_i = A\,[\varphi_i^2 + f_i\,\overline{f}_k\varphi_k^2],$$
$$\overline{\partial} f_i = A\,[\overline{\Phi}_i^2 + f_i\,\overline{f}_k\overline{\Phi}_k^2], \tag{56}$$

where, as usual, $A=1+(f^\dagger\cdot f)$ and all indices, and summations, go over $(2,\ldots,N)$.

These four sets of equations (54)–(56), for three sets of complex functions, f_i, φ_j and Φ_k, constitute our **modified generalized Weierstrass problem**.

Let us make a few comments.

(i) The equations fall into two sets (those involving ∂f_i and φ_j and those involving $\partial\overline{f_i}$ and Φ_j). Both sets are equivalent to the same equations for f_i, namely, (10).

(ii) Instead of taking f_i we could introduce, in analogy with (46), new functions ψ_i and Ψ_i by, say, $\psi_i=f_i\overline{\varphi_i}$ and $\Psi_i=f_i\overline{\Phi}_i$. Then our set of functions would effectively decouple.

(iii) One can consider what happens when f_i are holomorphic; i.e., $\overline{\partial} f_i=0$. Then, as is easy to check, $f^\dagger\cdot\overline{\Phi}^2=0$, which in turn shows that $|\Phi^2|^2=0$, thus demonstrating that $\Phi_i^2=0$, and we are left with (54) and (56) for f_i, φ_j, i.e., with the previous system (53).

VI. GEOMETRICAL ASPECTS

Next we consider some geometrical aspects of our procedure. This requires the introduction of a real vector $X_i\in R^M$ which is a generalization of the vector (43) constructed for CP^1. In Ref. 6 we have introduced such a vector and showed that its properties generalize those of (43).

However, our approach here generalizes the discussion in Ref. 6 and elucidates some of the points made there. Namely, in our new construction we exploit the matrices M and L. We introduce two matrices

$$V=\int_\gamma M\,d\overline{\zeta}+\int_\gamma M^\dagger\,d\zeta \tag{57}$$

and

$$W=\int_\gamma L\,d\overline{\zeta}+\int_\gamma L^\dagger\,d\zeta, \tag{58}$$

and for the components of our vectors we take individual entries of each matrix. As $\mathrm{Tr}\,M=\mathrm{Tr}\,L=0$ we see that V and W have, each, only N^2-1 independent entries so our construction gives us two vectors in R^{N^2-1}.

Notice also that W and V do not depend on the contour of integration γ. This follows from the fact that for an integral

$$Z=\int_\Gamma F(\zeta,\overline{\zeta})\,d\zeta+\overline{F}(\zeta,\overline{\zeta})\,d\overline{\zeta}$$

to be independent of the integration contour Γ the condition is that F and $\overline{F}$ must satisfy

$$\overline{\partial}F=\partial\overline{F},$$

which is the case for V and W due to, respectively, our conservation laws (27) and (28).

Of course we can reexpress our vectors V and W in terms of the Weierstrass functions φ_i, Φ_j and f_k or in terms of φ_i, ψ_j, Φ_k, and Ψ_l.

Note that in the CP^1 case the matrix W is given by

$$W = -\frac{1}{(1+|w|^2)^2}\begin{pmatrix} w\overline{\partial w} & -\overline{\partial w} \\ w^2\overline{\partial w} & -w\overline{\partial w}\end{pmatrix}, \tag{59}$$

and so, given (42), we see that the integrands of the first terms in X_i of (43) have the form

$$x_1 = -i[\overline{L}_{21} - \overline{L}_{12}], \quad x_2 = -[\overline{L}_{21} + \overline{L}_{12}], \quad x_3 = -\overline{L}_{11} = \overline{L}_{22}. \tag{60}$$

So should we consider a new $2(N^2-1)$ vector, the first half of whose components are various entries of the matrix W, and the second half those of V? In the CP^1 case, as shown in Ref. 5, we can restrict ourselves to a vector with only three components. So we add both contributions and consider an N^2-1 component vector given by all the entries (except the top left hand corner one) of the matrix

$$X = \int_\gamma (M+L)\, d\overline{\zeta} + \int_\gamma (M^\dagger + L^\dagger)\, d\zeta. \tag{61}$$

Next we calculate the components of the induced metric

$$g_{\alpha\beta} = \sum_{lk} \frac{\partial X_{kl}}{\partial \alpha}\frac{\partial X_{lk}}{\partial \beta}, \tag{62}$$

where α and β are ζ or $\overline{\zeta}$. But

$$\frac{\partial X}{\partial \overline{\zeta}} = (M + L), \quad \frac{\partial X}{\partial \zeta} = (M^\dagger + L^\dagger), \tag{63}$$

where we are still using the matrix formulation. Hence

$$g_{\overline{\zeta}\overline{\zeta}} = \mathrm{Tr}\,(M+L)^2, \quad g_{\zeta\zeta} = \mathrm{Tr}\,(M^\dagger + L^\dagger)^2, \quad g_{\zeta\overline{\zeta}} = \mathrm{Tr}\,[(M+L)(M^\dagger + L^\dagger)]. \tag{64}$$

However, given the form of M in (21) and L in (22), we see that

$$\mathrm{Tr}\,M^2 = \mathrm{Tr}\,L^2 = \mathrm{Tr}\,(M^\dagger)^2 = \mathrm{Tr}\,(L^\dagger) = \mathrm{Tr}\,L^\dagger M = \mathrm{Tr}\,M^\dagger L = 0, \tag{65}$$

and so we are left with

$$g_{\overline{\zeta}\overline{\zeta}} = 2\,\mathrm{Tr}\,(ML), \quad g_{\zeta\zeta} = 2\,\mathrm{Tr}\,(M^\dagger L^\dagger), \quad g_{\zeta\overline{\zeta}} = \mathrm{Tr}\,[MM^\dagger + LL^\dagger]. \tag{66}$$

Next we observe that

$$\mathrm{Tr}\,MM^\dagger = \mathrm{Tr}\,(1-P)\frac{\overline{\partial f}\otimes f^\dagger}{|f|^2}\frac{f\otimes \partial f^\dagger}{|f|^2} = \frac{\partial f^\dagger \cdot \overline{\partial f}}{|f|^4} - \frac{(\partial f^\dagger \cdot f)(f^\dagger \cdot \overline{\partial f})}{|f|^6} = |Dz|^2, \tag{67}$$

where, as in (45), D denotes the covariant derivative evaluated with respect to ζ. Similarly,

$$\mathrm{Tr}\,LL^\dagger = |\overline{D}z|^2, \tag{68}$$

where $\overline{D}$ is again the covariant derivative but this time evaluated with respect to $\overline{\zeta}$.

Note that, together, the two terms in $g_{\zeta\overline{\zeta}}$ give the total energy density of the map (i.e., $|Dz|^2 + |\overline{D}z|^2$).

What about $g_{\zeta\zeta}$ and $g_{\overline{\zeta}\overline{\zeta}}$? They are given by

$$g_{\bar{\zeta}\bar{\zeta}} = -\operatorname{Tr}(1-P)\frac{\bar{\partial}f\otimes f^{\dagger}\cdot f\otimes\bar{\partial}f^{\dagger}}{|f|^4} = -\operatorname{Tr}(1-P)\frac{\bar{\partial}f\otimes\bar{\partial}f^{\dagger}}{|f|^2}, \tag{69}$$

$$g_{\zeta\zeta} = -\operatorname{Tr}(1-P)\frac{\partial f\otimes f^{\dagger}\cdot f\otimes\partial f^{\dagger}}{|f|^4} = -\operatorname{Tr}(1-P)\frac{\partial f\otimes\partial f^{\dagger}}{|f|^2}, \tag{70}$$

and, at first sight, they appear to be nonvanishing. However, they do, in fact, vanish on the solutions of the CP^{N-1} model, i.e., on the vectors f which satisfy (10), at least those that are defined on S^2. To see this we note that

$$g_{\bar{\zeta}\bar{\zeta}} = \frac{-|f|^2(\bar{\partial}f^{\dagger}\cdot\bar{\partial}f) + (\bar{\partial}f^{\dagger}\cdot f)(f^{\dagger}\cdot\bar{\partial}f)}{|f|^2} \tag{71}$$

and $g_{\zeta\zeta}$ is its complex conjugate.

However, all solutions of (10) defined on S^2 are[7] of the type

$$f = P_+^k g, \tag{72}$$

where g is a holomorphic vector, i.e., $g\neq g(\bar{\zeta})$, and k is some integer taken from the set $\{0,1,\ldots,N-1\}$, and $P_+^l g$ is defined by the successive, i.e., $P_+^l g = P_+(P_+^{l-1}g)$, repetition of the operation

$$P_+ h = \partial h - h\frac{(h^{\dagger}\cdot\partial h)}{|h|^2}. \tag{73}$$

Then, as is known,[7] $P_+^k g$ satisfy

$$(P_+^l g)^{\dagger}\cdot P_+^k g = 0 \quad \text{if} \quad k\neq l, \tag{74}$$

$$\partial P_+^k g = P_+^{k+1}g + P_+^k g\frac{(P_+^k g^{\dagger}\cdot\partial P_+^k g)}{|P_+^k g|^2}, \tag{75}$$

$$\bar{\partial}P_+^k g = -P_+^{k-1}g\frac{|P_+^k g|^2}{|P_+^{k-1}g|^2}. \tag{76}$$

Thus $(\bar{\partial}f^{\dagger}\cdot\bar{\partial}f)=0$ and $(f^{\dagger}\cdot\bar{\partial}f)=0$ and so we see that $g_{\zeta\zeta}=0$ (and so also $g_{\bar{\zeta}\bar{\zeta}}=0$).

VII. THE CP^1 CASE REVISITED

In the CP^1 case it is convenient to calculate its energy momentum tensor

$$T_{\mu\nu} = (D_\mu z)^{\dagger}\cdot D_\nu z + (D_\nu z)^{\dagger}\cdot D_\mu z - \delta_{\mu\nu}|D_\alpha|^2. \tag{77}$$

Then, as is known[7]

$$\bar{\partial}(T_{11} + iT_{12}) = 0 \tag{78}$$

and in the CP^1 case

$$J = T_{11} + iT_{12} = \frac{\partial w\,\bar{\partial}w}{[1+|w|^2]^2}. \tag{79}$$

When the CP^1 model is defined on S^2 we find that $J=0$, which shows that all the harmonic CP^1 maps on S^2 are either holomorphic or antiholomorphic,[7] but for the CP^1 model on R^2, or for CP^{N-1}, $N>2$, J does not have to vanish.

In the CP^1 model case we have (59),

$$W=-\frac{1}{(1+|w|^2)^2}\begin{pmatrix} w\overline{\partial w} & -\overline{\partial w} \\ w^2\overline{\partial w} & -w\overline{\partial w}\end{pmatrix} \tag{80}$$

and

$$V=\frac{\overline{\partial w}}{(1+|w|^2)^2}\begin{pmatrix} -\bar{w} & -\bar{w}^2 \\ 1 & \bar{w}\end{pmatrix}. \tag{81}$$

This allows us to express $\overline{\partial w}$ in terms of $\overline{\partial \bar{w}}$, J and p given by (40). We find

$$\overline{\partial w}=\frac{J(1+|w|^2)^2}{\partial w}=J\,\overline{\partial \bar{w}}\frac{(1+|w|^2)^2}{|\partial w|^2}. \tag{82}$$

However, using (42), we see that

$$p^2=\frac{|\partial w|^2}{(1+|w|^2)^2} \tag{83}$$

and so we have

$$\overline{\partial w}=\overline{\partial \bar{w}}\frac{J}{p^2}. \tag{84}$$

This allows us to combine the two vectors V and W into

$$V+W=\frac{\overline{\partial \bar{w}}}{(1+|w|^2)^2}\begin{pmatrix} -w-R\bar{w} & 1-R\bar{w}^2 \\ R-w^2 & w+R\bar{w}\end{pmatrix}, \tag{85}$$

where $R=J/p^2$.

This explains the origin of the expressions for the components of X_i given in Ref. 4. However, it is clear that this possibility to gather both terms into one expression does not generalize to higher CP^{N-1} models.

VIII. SUMMARY AND CONCLUDING REMARKS

The main aim of this article has been to derive a generalization of the Weierstrass system to the CP^{N-1} case for which the metric of the induced surfaces is determined by the energy density of the corresponding harmonic map.

This has led us to introduce a set of $3N$ complex functions φ_i, Φ_j and f_k which are required to satisfy a system of four classes of first order equations and which are equivalent to the full system of equations of the CP^{N-1} model.

We have also introduced a set of (N^2-1) real quantities X_i, which can be treated as coordinates of a surface immersed in R^{N^2-1} and we have shown that the induced metric of our map is given by

$$ds^2=(|Dz|^2+|\overline{Dz}|^2)\,d\zeta\,d\bar{\zeta}. \tag{86}$$

The study of the generalized Weierstrass representations for surfaces immersed in multidimensional spaces was initiated by Konopelchenko and Landolfi.[3] Our work here, in which we have adopted an alternative approach based on the CP^{N-1} sigma models, provides a generalization of their results.

ACKNOWLEDGMENTS

A.M.G. would like to thank the University of Durham for the award of an Alan Richards fellowship that allowed him to spend two terms in Durham during the academic years 2001 and 2002. Partial support for A.M.G.'s work was provided by a research grant from NSERC of Canada and Fonds FCAR du Gouvernement du Quebec.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Painlevé analysis of the Ricci-flat ordinary differential equations associated with Aloff–Wallach spaces and U(1)-bundles over Fano products

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(Received 10 December 2002; accepted 9 April 2003)

We apply techniques of Painlevé–Kowalewski analysis to certain ODE reductions of the Ricci-flat equations. We particularly focus on two examples when the hypersurface is an Aloff–Wallach space or a circle bundle over a Fano product. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1584207]

I. INTRODUCTION

The difficulty of the Einstein system of partial differential equations has made it natural to consider reductions of this system to ordinary differential equations (ODEs). One way of performing this reduction is to require the Einstein metrics to be of cohomogeneity one, that is, to be invariant under the action of a group with principal orbits of codimension one. In Dancer and Wang (2003b) we studied the cohomogeneity-one Ricci-flat equations in the situation when the isotropy representation of the principal orbit consists of pairwise inequivalent summands. We showed how to choose variables so that the equations became a constrained flow of an ODE system with quadratic nonlinearities.

In Dancer and Wang (2002) we proved some general results about the Painlevé–Kowalewski analysis of this system. This involves looking for solutions of the equations given by *Painlevé expansions*, i.e., meromorphic expansions in (a rational power of) the independent variable. The general philosophy of this method is that the existence of large families of Painlevé expansions should be associated with ''nice'' properties of the equations. In particular, if for each dependent variable in the equations there is a corresponding family of Painlevé expansions which depends on the full number of parameters and in which that dependent variable actually blows up, then this is regarded as a strong indication that the equations are ''integrable.'' A good summary of the modern treatment of Painlevé–Kowalewski analysis may be found in Ablowitz *et al.* (1980) and Adler and van Moerbeke (1982).

This general theory was applied to some examples in Dancer and Wang (2001, 2002, 2003b). Two features were particularly noteworthy.

(i) The existence of Painlevé expansions is often associated with the existence of a solution to a Diophantine problem (in many cases, the existence of an integral point on an elliptic curve). This may single out certain dimensions as special.
(ii) When Painlevé expansions do exist, they sometimes represent metrics of exceptional holonomy.

In this article we shall analyze some further examples, including one which has recently become relevant in string theory (Cvetič *et al.*, 2002a; Gukov and Sparks, 2002; Kanno and Yasui,

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2002). This is the example when the principal orbit is an Aloff–Wallach space SU(3)/U(1). Such spaces depend on two integer parameters, leading to Diophantine questions during the Painlevé analysis. Moreover, the Ricci-flat equations have a subsystem whose solutions represent metrics of Spin(7) holonomy. We find that this Spin(7) subsystem has a family of Painlevé expansions depending on the full number of parameters and representing asymptotically locally conical (ALC) metrics (cf. Theorem 4.5 and Remark 4.6). By contrast, large Painlevé families representing asymptotically conical (AC) metrics are very rare, and their existence imposes strong Diophantine constraints on the Aloff–Wallach space (cf Theorem 4.8).

We also consider the case when the hypersurface belongs to a certain class of circle bundles over a product of two Fano manifolds admitting Kähler–Einstein metrics. These circle bundles are classified by two integers, which, together with the dimensions and first Chern classes of the factors in the base, lead also to Diophantine questions during the Painlevé analysis. As a result, dimension 12 is singled out when considering ALC Ricci-flat metrics. Furthermore, the circle bundles which admit Sasakian–Einstein metrics (up to orientation changes) appear to be singled out in the case of AC Ricci-flat metrics. For this class of bundles, the Ricci-flat equations have a subsystem whose solutions represent Calabi–Yau metrics and can be written down by quadratures.

In order to make this article as self-contained as possible, we include a review of the results of Dancer and Wang (2002, 2003b) on the general cohomogeneity one Ricci-flat system and its Painlevé analysis.

II. THE EQUATIONS

In this section we briefly review the formulation in Dancer and Wang (2003b) of the cohomogeneity one Ricci-flat equations [see also Bérard and Bergery (1982), Dancer and Wang (2000), and Eschenburg and Wang (2000) for background on these equations].

Consider a Riemannian manifold $(\mathcal{M},g)$ with a cohomogeneity one isometric action of a compact Lie group G, whose principal orbit is G/K. We denote by

$$\mathfrak{p}=\mathfrak{p}_1\oplus\cdots\oplus\mathfrak{p}_r$$

the decomposition of the isotropy representation $\mathfrak{p}\approx T_{(K)}(G/K)$ of G/K into irreducible K-representations. We let d_i be the real dimension of $\mathfrak{p}_i$, and let $n=\Sigma_{i=1}^r d_i$ denote the dimension of G/K (so $\dim\mathcal{M}=n+1$). We use d for the vector of dimensions $(d_1,\ldots,d_r)$.

We shall assume that the isotropy representation is *monotypic*, that is, all the $\mathfrak{p}_i$ are distinct as representations of K. In particular if there is a trivial summand it must be one-dimensional. The metric g may now be written as

$$dt^2+g_t, \tag{1}$$

where

$$g_t=e^{q_1(t)}B|_{\mathfrak{p}_1}\perp\cdots\perp e^{q_r(t)}B|_{\mathfrak{p}_r} \tag{2}$$

is a one-parameter family of G-invariant metrics on G/K, B is a fixed background metric on G/K induced from some biinvariant metric on G, and t is a parameter along a geodesic which intersects all principal orbits orthogonally. Note that the factor $\exp(\frac{1}{2}d\cdot q)$ is the ratio of the volume of g_t to that of B.

The scalar curvature of $(G/K,g_t)$ is given by $\mathsf{S}=\Sigma_{w\in\mathcal{W}}A_w e^{w\cdot q}$, where A_w are (nonzero) constants and $\mathcal{W}$ is a finite collection of vectors $w\in\mathbb{Z}^r$ (which depend only on G/K and which we refer to as *weight vectors*).

We shall also assume that the elements of $\mathcal{W}$ span $\mathbb{R}^r$, which is the case when G is semisimple (Dancer and Wang, 2000). We define a non-negative integer ℓ by $r+\ell=|\mathcal{W}|$, and order the weight vectors as $w^{(k)}$ $(1\leqslant k\leqslant r+\ell)$, where $w^{(i+r)}=\Sigma_{j=1}^r \nu_{ij}w^{(j)}(1\leqslant i\leqslant\ell)$, for some constants ν_{ij}.

Note that by the homogeneity properties of the scalar curvature, $w^{(k)}\cdot(1,\ldots,1)=-1$ for all k, so we can deduce that $\Sigma_{j=1}^{r}\nu_{ij}=1$ for all i. We shall refer to the constant $A_{w^{(k)}}$ just as A_k in future.

As explained in Dancer and Wang (2003b), the Ricci-flat equations for g may be viewed as the flow for a Hamiltonian $\bar{H}$ together with the constraint $\bar{H}=0$. The potential term is the scalar curvature S of G/K times the square of the volume distortion factor $\exp(\frac{1}{2}d\cdot q)$. The kinetic energy is given by the signature $(1,r-1)$ quadratic form

$$J(p)=\frac{1}{n-1}\left(\sum_{i=1}^{r}p_i\right)^2-\sum_{i=1}^{r}\frac{p_i^2}{d_i}. \tag{3}$$

In Dancer and Wang (2003b) we showed how to rewrite the Ricci-flat equations as a quadratic system, using ideas from Adler and van Moerbeke (1982). We first define an $(r+\ell)\times r$ matrix $\hat{U}$ by

$$\hat{U}_{ij}=d_j+w_j^{(i)}.$$

Consider the matrix $\Phi:=\hat{U}J\hat{U}^t$, where we have also denoted by J the matrix of the quadratic form given in (3). Now we can choose an $(r+\ell)\times r$ matrix Q satisfying $QDQ^t=\Phi$, where $D=\mathrm{diag}(\epsilon_1,\ldots,\epsilon_r)$ and $\epsilon_1=1$, $\epsilon_i=-1\quad(i>1)$. We may also arrange that Q is of the form

$$\begin{pmatrix} Q_1 \\ \nu Q_1 \end{pmatrix} \tag{4}$$

for some invertible $r\times r$ matrix Q_1.

The Ricci-flat equations for g are now equivalent, after suitable change of dependent and independent variables, to the system

$$z_i'=2z_i\sum_{j=1}^{r}Q_{ij}v_j \qquad (1\leqslant i\leqslant r+\ell), \tag{5}$$

$$v_i'=\epsilon_i\sum_{j=1}^{r+\ell}Q_{ji}z_j \qquad (1\leqslant i\leqslant r), \tag{6}$$

together with the constraints

$$\frac{z_{r+j}}{A_{r+j}}=\prod_{i=1}^{r}\left(\frac{z_i}{A_i}\right)^{\nu_{ji}} \qquad (1\leqslant j\leqslant \ell), \tag{7}$$

and the Hamiltonian constraint

$$\bar{H}\equiv v_1^2-v_2^2-\cdots-v_r^2-\sum_{j=1}^{r+\ell}z_j=0. \tag{8}$$

Remark 2.1: (i) The quantities $z_{r+j}\Pi_{i=1}^{r}z_i^{-\nu_{ji}}$, as well as $\bar{H}$, are conserved by the flow. As discussed in Dancer and Wang (2003b), Eqs. (5) and (6) may be viewed as a Poisson Hamiltonian flow, and the constraints (7) define restriction of this flow to a symplectic leaf. The Ricci-flat equations are then the Hamiltonian flow on this leaf subject to the Hamiltonian constraint (8).

(ii) Note that the choice of Q above is not unique. Indeed, replacing Q by $-Q$ and v_j by $-v_j$ will leave the above system invariant.

(iii) For quadratic systems such as (5) and (6) a general majorization argument shows that formal Painlevé expansions about 0 are convergent in a deleted neighborhood of 0.

III. PAINLEVÉ EXPANSIONS

A. Leading terms

We now review the Painlevé analysis (Dancer and Wang, 2002) of Eqs. (5) and (6). We first look for possible leading terms of the Painlevé expansions of solutions to these equations. Put

$$z_i = \alpha_0^{(i)} s^{m_i} + \cdots, \qquad v_i = \beta_0^{(i)} s^{n_i} + \cdots, \tag{9}$$

where $\alpha_0^{(i)}, \beta_0^{(i)} \neq 0$.

It is straightforward to show that $n_i \geqslant -1$; we shall assume for the moment (see Remark 3.2) that all $m_i \geqslant -2$. Let $S \subset \{1,\ldots,r+\ell\}$ denote the set of indices for which $m_i = -2$ and $T \subset \{1,\ldots,r\}$ denote the set of indices for which $n_i = -1$. It is convenient to introduce an $(r+\ell)\times r$ matrix P defined by

$$P_{ij} = \begin{cases} Q_{ij} & \text{if } i \in S, \\ 0 & \text{if } i \notin S. \end{cases}$$

In Dancer and Wang (2002) we derived the equation

$$m_i = -2\sum_{j\in S} (QDQ^t)_{ij} \quad \alpha_0^{(j)} = -2\sum_{j\in S} (\hat{U}J\hat{U}^t)_{ij} \quad \alpha_0^{(j)} = -2(\Phi^S \hat{\alpha}_0)^{(i)},$$

where Φ^S denotes the $(r+\ell)\times|S|$ matrix obtained by deleting the jth column of $\Phi = \hat{U}J\hat{U}^t$ iff $j \notin S$, and $\hat{\alpha}_0$ denotes the $|S|\times 1$ vector $(\alpha_0^{(i)})_{i\in S}$. Therefore we need

$$(\Phi^S \hat{\alpha}_0)^{(i)} = 1 \quad (i \in S), \tag{10}$$

$$(\Phi^S \hat{\alpha}_0)^{(i)} < 1 \quad (i \notin S). \tag{11}$$

This gives us an algorithm to find the possibilities for S, α_0 and β_0. For each subset S of $\{1,\ldots,r+\ell\}$, we solve (10) for $\hat{\alpha}_0$ and then check if (11) is satisfied. (If $|S| < r+\ell$, then the components $\alpha_0^{(i)}$ with $i \notin S$ will be free.)

Remark 3.1: We showed in Dancer and Wang (2002) that

$$j \in S \quad \text{whenever} \quad w^{(j)} \in \text{Span}\{w^{(i)} \ : \ i \in S\}. \tag{12}$$

This observation drastically reduces the number of sets S to which we have to apply the algorithm.

Remark 3.2: If there are some indices i for which $m_i < -2$, we let $\tilde{S}$ denote the subset of such indices corresponding to the minimal leading power m_i. Remark 3.1 still applies to $\tilde{S}$ and immediately puts some restrictions on $\tilde{S}$.

Now (6) implies that $\Sigma_{j\in\tilde{S}} Q_{ji}\alpha_0^{(j)} = 0$ for $i = 1,\ldots,r$. These r equations are supplemented by the ℓ equations on α_0 coming from the constraints (7). Usually these equations force some or all of the $\alpha_0^{(i)}$ to be zero, giving a contradiction. This is the case in the examples we deal with in this article.

Convergent Painlevé expansions for Eqs. (5)–(8) give local solutions of the cohomogeneity one Ricci-flat equations. In Dancer and Wang (2002) we derived from the leading term behavior (as s tends to 0) of an expansion the behavior of the corresponding Ricci-flat metric.

Theorem 3.3: (Dancer and Wang, 2002) *Let U denote the $r\times r$ matrix consisting of the first r rows of $\hat{U}$. Let ξ be the vector $-dU^{-1}$ and U^{ij} denote the components of U^{-1}. Then $1 - \frac{1}{2}\Sigma_i m_i \xi_i$ is nonzero. Moreover, letting $f_i(t)^2 = e^{q_i(t)}$ in (2), we have the following.*

(I) If $1 - \frac{1}{2}\Sigma_{i=1}^r m_i\xi_i < 0$, then as $s \to 0^+$, we must have $t \to +\infty$ (possibly after changing the sign of t). Asymptotically, we have

$$f_i(t)^2 \sim c_i\, t^{\Sigma_j U^{ij} m_j / (1 - (1/2)\,\Sigma_j m_j \xi_j)}.$$

(II) if $1-\frac{1}{2}\Sigma_{i=1}^{r} m_i\xi_i>0$, *then as* $s\to 0^+$, t *decreases to a finite limit* t^*, *and asymptotically we have*

$$f_i(t)^2 \sim c_i(t-t^*)^{\Sigma_j U^{ij} m_j/(1-(1/2)\,\Sigma_j m_j\xi_j)}.$$

In both (I) and (II), the c_i *are constants which can be explicitly computed in terms of* U^{-1}, m, ξ, α_0 *and the* A_i.

Remark 3.4: Painlevé expansions of type (I) give metrics with a complete end. Two special cases are particularly important in examples.

(a) *AC asymptotics:* If $S=\{1,\ldots,r+\ell\}$ and $T=\{1,\ldots,r\}$, that is, all m_i equal -2 and all n_i equal -1, the leading terms are themselves an exact solution of the equations, corresponding to the Ricci-flat cone over a homogeneous Einstein metric on G/K.
Painlevé expansions with such leading terms will correspond to metrics *asymptotic* to the cone [AC in the terminology of Cvetič *et al.* (2002a)].

(b) *ALC asymptotics:* If we are in case (I) and $\mathfrak{p}_i$ is a *trivial* summand such that $\Sigma_j U^{ij} m_j=0$, then the principal orbits in the Ricci-flat end will be asymptotic to a circle bundle over G/K' with isometric fibers, where K' has Lie algebra $\mathfrak{k}\oplus\mathfrak{p}_i$. An important special case is when the $f_j(t)^2$ for $j\neq i$ grow like t^2. Locally (in t) the metric is now asymptotically that of a circle bundle with isometric fibres over a cone on G/K'. In Cvetič *et al.* (2002a) the terminology *asymptotically locally conical* (or ALC) was introduced to describe such end behavior. The circle is often referred to as the M-theory circle, due to the physical implications discussed, for example, in Brandhuber *et al.* (2001) and Cvetič *et al.* (2002a, b).

B. Resonances

Next one must extend the leading terms of the previous section to full series solutions to Eqs. (5) and (6), in (possibly fractional) powers of s. We write

$$z_i=\sum_{j=0}^{\infty} \alpha_j^{(i)} s^{m_i+(j/N)}, \qquad v_i=\sum_{j=0}^{\infty} \beta_j^{(i)} s^{n_i+(j/N)}, \tag{13}$$

where N is an integer to be determined after all the resonances have been computed.

Equations (5) and (6) will now yield recursion relations involving the α_j,β_j. Schematically, the recursion may be written as

$$\mathcal{T}_j(\alpha_j,\beta_j)=\text{expression} \quad \text{in} \quad \alpha_k,\beta_k \qquad (k<j),$$

where $\mathcal{T}_j$ is a linear operator. The *resonances* of the expansion are the values of j/N for which $\mathcal{T}_j$ is noninvertible; that is, they give the stages in the recursion at which free parameters may enter.

We shall now summarize the calculation of the resonances in Dancer and Wang (2002). The recursion relations are (for $j>0$)

$$\frac{j}{N}\ \alpha_j^{(i)}-2\ \mathrm{diag}(\alpha_0^{(1)},\ldots,\alpha_0^{(r+\ell)})\ Q\widehat{\beta}_j=X_j, \tag{14}$$

$$\left(\frac{j}{N}-1\right)\beta_j^{(p)}-(DP^t\alpha_j)^{(p)}=Y_j^{(p)} \quad (p\in T), \tag{15}$$

$$\left(n_p+\frac{j}{N}\right)\beta_j^{(p)}=\epsilon_p\sum_{i=1}^{r+\ell} Q_{ip}\ \ \alpha_{j-N(m_i-n_p+1)}^{(i)} \quad (p\notin T), \tag{16}$$

where

$$\hat{\beta}_j^{(p)} = \begin{cases} \beta_j^{(p)} & (p \in T), \\ 0 & (p \notin T), \end{cases}$$

$$X_j^{(i)} = \sum_{p \in T} \sum_{k=1}^{j-1} 2Q_{ip}\ \alpha_k^{(i)} \beta_{j-k}^{(p)} + \sum_{p \notin T} \sum_{k=0}^{j-N(n_p+1)} 2Q_{ip}\ \alpha_k^{(i)} \beta_{j-k-N(n_p+1)}^{(p)}, \tag{17}$$

and

$$Y_j^{(p)} = \epsilon_p \sum_{i \notin S} Q_{pi}^t\ \alpha_{j-N(m_i+2)}^{(i)}. \tag{18}$$

Note that $X_j^{(i)}$ and $Y_j^{(p)}$ involve only terms with subscripts $<j$, and the terms $\beta_j^{(p)}$ with $p \notin T$ do not appear on the left-hand side of (14) and (15). Equations (14) and (15) therefore form a subsystem of the full recursion, and in this subsystem we can eliminate α_j by (14).

The following theorem describes the nonzero resonances of the recursion.

Theorem 3.5: (Dancer and Wang, 2002):

(a) The (nonzero) resonances $R = j/N$ of the subsystem (14) and (15) are the roots of the quadratic equation

$$R(R-1) = \lambda, \tag{19}$$

where λ runs over all the eigenvalues of the $|T| \times |T|$ matrix M_T obtained from $M := 2DP^t \operatorname{diag}(\alpha_0^{(1)}, \ldots, \alpha_0^{(r+\ell)})\, Q$ by deleting the pth row and pth column for all p not in T.

(b) If the following conditions,

(i) $m_i \geqslant n_p - 1$ for all $p \notin T$ and $i \notin S$ with $Q_{ip} \neq 0$,

(ii) $Q_{ip} = 0$ for all $p \notin T$ and $i \in S$,

hold, then Eq. (16) reduces to

$$\left(n_p + \frac{j}{N}\right) \beta_j^{(p)} = \epsilon_p \sum_{i \notin S} Q_{ip}\ \alpha_{j-N(m_i-n_p+1)}^{(i)}, \quad p \notin T, \tag{20}$$

where the terms on the right have subscript $\leqslant j$, so the only additional nonzero resonances from (16) are $R = -n_p$ for $p \notin T$.

Remark 3.6: (1) Equations (14)–(16) are valid for $j > 0$. We may also have additional zero resonances, associated to free parameters in α_0, β_0.

(2) In the examples of this article the only case where conditions (i) and (ii) do not hold is $S = \{4,6\}$ in the example of Sec. IV. In this case we can perform a reindexing $j \mapsto j - N(n_p+1)$ for the terms $\beta_j^{(p)}$ where $p \notin T$, and bring the system back into the form considered above. [cf. $S = \{4,5\}$ in Example 5.2 of Dancer and Wang (2002)].

Remark 3.7: As mentioned in Dancer and Wang (2002), $(\beta_0^{(p)})_{p \in T}$ is an eigenvector of M_T with eigenvalue 2, and hence -1, 2 are resonances. The appearance of -1 as a resonance is typical for autonomous systems of differential equations, and is associated to the degree of freedom coming from translating the independent variable. For the Einstein system under consideration, it can be shown that this freedom corresponds to homothetic changes of the metric. We shall see below (Proposition 3.10) that the Hamiltonian constraint fixes one free parameter at $R = 2$.

Existence of nontrivial Painlevé expansions (that is, expansions with free parameters other than translation) therefore requires, at least in the case $|T| = r$, the existence of rational roots of (19) other than -1,2. This can impose constraints on the principal orbit G/K, and in particular can lead to Diophantine conditions involving, for example, the dimension of G/K.

One common situation is that we have a family of principal orbit types indexed by an integer k (often dimension), and that the eigenvalues of M_T are given by rational functions $P_i(k)/Q_i(k)$, where $P_i, Q_i \in \mathbb{Z}[k]$. The condition that the associated resonance should be rational is that

$$Q_i(k)(Q_i(k)+4P_i(k)) \quad \text{is a perfect square.}$$

We are therefore looking for an integral point (k,y) on the hyperelliptic curve

$$y^2=Q_i(k)(Q_i(k)+4P_i(k)). \tag{21}$$

A theorem of Siegel tells us that there are only finitely many solutions [provided that all the roots of $Q_i(Q_i+4P_i)$ are distinct].

In Dancer and Wang (2002, 2003b) we encountered examples of this situation where the orbit G/K is $\mathrm{Sp}(k+1)/\mathrm{Sp}(k)\mathrm{U}(1)$, $\mathrm{Sp}(k+1)\mathrm{Sp}(1)/\mathrm{Sp}(k)\mathrm{Sp}(1)$, and $\mathrm{Sp}(k+1)\mathrm{U}(1)/\mathrm{Sp}(k)\mathrm{U}(1)$. The right-hand side of (21) factorized into polynomials of degree $\leqslant 3$, and we were able to reduce the problem of finding integral points on (21) to that of finding integral points (satisfying certain extra conditions) on an elliptic curve.

C. Compatibility conditions and constraints

By definition, the resonances correspond to the steps in the recursion at which the recursion operator is noninvertible. This means that at each resonance there are compatibility conditions which must be satisfied if the recursion is to proceed.

It often happens that these conditions may only be satisfied by setting to zero free parameters arising from earlier resonances.

However, in all of our examples compatibility holds *automatically* at the top resonance $R=2$. In most cases we can see this from the following proposition.

Proposition 3.8: (Dancer and Wang, 2002) *Suppose that all compatibility conditions hold for* $R=j/N<2$, *and we have*

(i) $m_i \geqslant n_p-1$ *for all* $p\notin T$, $i\notin S$ *with* $Q_{ip}\neq 0$,

(ii) $Q_{ip}=0$ *for all* $p\notin T$ *and* $i\in S$, *and*

(iii) the 2-eigenspace of M_T *is one-dimensional.*

Suppose in addition that **either**

(iv) $m_i+n_p+1>0$ *for all* $p\notin T$ *and* $i\notin S$ *with* $Q_{ip}\neq 0$, **or**

(v) $m_i-n_p+1=0$ *for all* $p\notin T$ *and* $i\notin S$ *with* $Q_{ip}\neq 0$.

Then the compatibility condition holds at $R=2$.

Remark 3.9: Note that condition (iv) holds if $m_i\geqslant 0$ for all $i\notin S$, which is true for all cases in the examples of Secs. IV and V [and the examples of Dancer and Wang (2002)] except the ALC ones.

Condition (v) holds if there exist constants ν_1 and ν_2 such that $\nu_1-\nu_2+1=0$ and $m_i=\nu_1$ for all $i\notin S$, $n_p=\nu_2$ for all $p\notin T$. This situation occurs in the ALC cases of the examples in Secs. IV and V, and in Dancer and Wang (2002).

The Hamiltonian constraint (8) is related to the resonance at $R=2$, as we now explain. After substituting the Painlevé expansion into the Hamiltonian (8), one sees that the constant term in the Hamiltonian is given by a linear combination of $\beta_{2N}^{(p)}$ $(p\in T)$ and $\alpha_{2N}^{(i)}$ $(i\in S)$ plus terms with subscripts less than $2N$. Substituting in an element of the kernel of the recursion operator at $R=2$ (that is, $j=2N$) we have the following:

Proposition 3.10: (Dancer and Wang, 2002) *If all compatibility conditions hold at* $R=2$, *and if*

$$2\sum_{p\in T}\epsilon_p(\beta_0^{(p)})^2+\sum_{i\in S}\alpha_0^{(i)}\neq 0,$$

then the Hamiltonian constraint may always be satisfied by choosing α_{2N},β_{2N} *appropriately. In this situation the Hamiltonian constraint fixes one of the degrees of freedom coming from the resonance* $R=2$.

As $z_{r+j}\Pi_{i=1}^{r} z_i^{-\nu_{ji}}$ $(j=1,\ldots,\ell)$ are constants of the flow, the remaining constraints (7) are equivalent to imposing on α_0 the constraints

$$\frac{\alpha_0^{(r+j)}}{A_{r+j}} = \prod_{i=1}^{r} \left(\frac{\alpha_0^{(i)}}{A_i} \right)^{\nu_{ji}} \quad (1 \leqslant j \leqslant \ell). \tag{22}$$

IV. ALOFF–WALLACH SPACES AS PRINCIPAL ORBITS

We shall now look at a specific example, where the principal orbit G/K is the Aloff–Wallach space $N(k,l)$ (Aloff and Wallach, 1975). Here $N(k,l)$ is defined to be the quotient $\mathrm{SU}(3)/\mathrm{U}(1)_{k,l}$ where $\mathrm{U}(1)_{k,l}$ denotes $\mathrm{U}(1)$ embedded as

$$e^{i\theta} \mapsto \mathrm{diag}(e^{ik\theta}, e^{il\theta}, e^{im\theta})$$

and k,l,m are coprime integers with $k+l+m=0$. Notice that permuting k,l,m does not change the diffeomorphism type of the space. For example $N(1,-1) \approx N(1,0) \approx N(-1,0)$. We exclude the case $\{k,l,m\}=\{1,1,-2\}$ as in this case the isotropy representation does not split as the direct sum of inequivalent irreducible summands.

The second author (Wang, 1982) showed that every $N(k,l)$ admits a homogeneous Einstein metric. It was subsequently shown (Page and Pope, 1984) that there are exactly two such metrics on each $N(k,l)$, except for $N(1,-1)$ and the spaces obtained from it by permutation, when the metric is unique. Explicit formulas are given in Castellani and Romans (1984) [see Cvetič *et al.* (2002b) for a more detailed derivation]. Both Einstein metrics are in fact of weak holonomy G_2, so the cone over them has holonomy contained in Spin(7).

The isotropy representation of $N(k,l)$ is

$$\mathfrak{su}(3)/\mathfrak{u}(1) = \mathfrak{p}_0 \oplus \mathfrak{p}_1 \oplus \mathfrak{p}_2 \oplus \mathfrak{p}_3,$$

where $\mathfrak{p}_0$ is a trivial summand of real dimension one, $\mathfrak{p}_i$ $(i=1,2,3)$ are of real dimension 2, and $\mathrm{U}(1)$ acts on them with weights

$$\pm(k-l), \pm(k-m), \pm(l-m),$$

respectively. We write $\Gamma = k^2+m^2+km = k^2+l^2+kl = l^2+m^2+lm$. We take the background metric B to be the normal metric induced by the trace form $-\mathrm{tr}(XY)$.

The weight vectors in the scalar curvature formula are now as follows:

$$w^{(1)}=(0,-1,0,0), \quad w^{(2)}=(0,0,-1,0), \quad w^{(3)}=(0,0,0,-1),$$

$$w^{(4)}=(1,-2,0,0), \quad w^{(5)}=(1,0,-2,0), \quad w^{(6)}=(1,0,0,-2),$$

$$w^{(7)}=(0,1,-1,-1), \quad w^{(8)}=(0,-1,1,-1), \quad w^{(9)}=(0,-1,-1,1),$$

and the corresponding coefficients are $(A_1,\ldots,A_9)=(6,6,6,-3m^2/4\Gamma,-3l^2/4\Gamma,-3k^2/4\Gamma,-1,-1,-1)$. We give Φ and a choice of Q below:

$$\Phi=\begin{pmatrix}
\frac{1}{2} & 1 & 1 & 0 & 1 & 1 & \frac{3}{2} & \frac{1}{2} & \frac{1}{2}\\
1 & \frac{1}{2} & 1 & 1 & 0 & 1 & \frac{1}{2} & \frac{3}{2} & \frac{1}{2}\\
1 & 1 & \frac{1}{2} & 1 & 1 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{2}\\
0 & 1 & 1 & -2 & 0 & 0 & 2 & 0 & 0\\
1 & 0 & 1 & 0 & -2 & 0 & 0 & 2 & 0\\
1 & 1 & 0 & 0 & 0 & -2 & 0 & 0 & 2\\
\frac{3}{2} & \frac{1}{2} & \frac{1}{2} & 2 & 0 & 0 & -\frac{1}{2} & \frac{3}{2} & \frac{3}{2}\\
\frac{1}{2} & \frac{3}{2} & \frac{1}{2} & 0 & 2 & 0 & \frac{3}{2} & -\frac{1}{2} & \frac{3}{2}\\
\frac{1}{2} & \frac{1}{2} & \frac{3}{2} & 0 & 0 & 2 & \frac{3}{2} & \frac{3}{2} & -\frac{1}{2}
\end{pmatrix},$$

$$Q=\begin{pmatrix}
\frac{1}{\sqrt{2}} & 0 & 0 & 0\\
\sqrt{2} & \frac{\sqrt{6}}{2} & 0 & 0\\
\sqrt{2} & \frac{\sqrt{6}}{3} & \frac{\sqrt{30}}{6} & 0\\
0 & -\frac{\sqrt{6}}{3} & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}}{5}\\
\sqrt{2} & \frac{2\sqrt{6}}{3} & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}}{5}\\
\sqrt{2} & \frac{\sqrt{6}}{3} & \frac{4\sqrt{30}}{15} & \frac{\sqrt{30}}{5}\\
\frac{3}{\sqrt{2}} & \frac{5}{\sqrt{6}} & \frac{\sqrt{30}}{6} & 0\\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & \frac{\sqrt{30}}{6} & 0\\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & -\frac{\sqrt{30}}{6} & 0
\end{pmatrix}.$$

Applying the algorithm of Sec. III we can now find the possible leading terms. It is straightforward to check from Remark 3.2 that no m_i can be less than -2. The subgroup C_3 of permu-

tations of {1,...,9} generated by the order three element (123)(456)(789) acts on the set of possible S, so we list only one possibility from each orbit. The vectors m are similarly permuted. Note that the last three entries in our table are fixed by C_3.

S	m	$\alpha_0^{(i)}$ $(i\in S)$
{4}	$(0,1,1,-2,0,0,2,0,0)$	$-\frac{1}{2}$
{7}	$(6,2,2,8,0,0,-2,6,6)$	-2
{4,5}	$(1,1,2,-2,-2,0,2,2,0)$	$-\frac{1}{2},-\frac{1}{2}$
{4,8}	$(2,7,3,-2,8,0,8,-2,6)$	$-\frac{1}{2},-2$
{4,9}	$(2,3,7,-2,0,8,8,6,-2)$	$-\frac{1}{2},-2$
{4,5,9}	$(3,3,8,-2,-2,8,8,8,-2)$	$-\frac{1}{2},-\frac{1}{2},-2$
{4,5,6}	$(2,2,2,-2,-2,-2,2,2,2)$	$-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}$
{1,...,9}	$(-2,...,-2)$	see below
{1,2,3,7,8,9}	$(-2,-2,-2,-\frac{8}{5},-\frac{8}{5},-\frac{8}{5},-2,-2,-2)$	see below

Remark 4.1: The AC case is when $S=\{1,\ldots,9\}$, and the ALC case is $S=\{1,2,3,7,8,9\}$. For all other choices of S, letting s tend to 0 corresponds to letting arclength t tend to a finite limit, as in (II) of Theorem 3.3.

A. AC case

As mentioned in Remark 3.4(a) the possibilities for α_0 may be computed from the homogeneous Einstein metrics on the principal orbits. Using the formulas of Castellani and Romans (1984) and Cvetič *et al.* (2002b) we find the explicit formula

$$\alpha_0=\left(\frac{2(3+2\cos\phi+\sin\phi)}{3(2+\cos\phi)^2},\frac{2(3+2\cos\phi-\sin\phi)}{3(2+\cos\phi)^2},\frac{(3+2\cos\phi+\sin\phi)(3+2\cos\phi-\sin\phi)}{3(2+\cos\phi)^2},\right.$$
$$-\frac{(\cos\phi-2\sin\phi)^2}{18(2+\cos\phi)^2},-\frac{(\cos\phi+2\sin\phi)^2}{18(2+\cos\phi)^2},-\frac{(2+3\cos\phi)^2}{18(2+\cos\phi)^2},-\frac{(3+2\cos\phi-\sin\phi)^2}{18(2+\cos\phi)^2},$$
$$\left.-\frac{(3+2\cos\phi+\sin\phi)^2}{18(2+\cos\phi)^2},-\frac{2}{9(2+\cos\phi)^2}\right),$$

where

$$\frac{l}{m}=\frac{(3+2\cos\phi+\sin\phi)(\cos\phi+2\sin\phi)}{(3+2\cos\phi-\sin\phi)(\cos\phi-2\sin\phi)}=\frac{4+6\cos\phi+12\sin\phi+5\sin 2\phi}{4+6\cos\phi-12\sin\phi-5\sin 2\phi}. \tag{23}$$

If $\{k,l,m\}\neq\{1,0,-1\}$ there are, for each choice of *ordered* triple (k,l,m), two choices of ϕ in $[0,2\pi)$, corresponding to the two Einstein metrics on $N(k,l)$. Note that the degenerate case $\{k,l,m\}=\{1,1,-2\}$ (that is, $l/m=1,-2$ or $-\frac{1}{2}$) occurs iff $\cos\phi=-1,0,1$ or $-\frac{4}{5}$.

It follows from (23) that $\cos\phi$ is a root of the quartic

$$H(t)=(l+m)^2(5t^2-4)(5t^2+12t+8)-4lm(3t+2)^2. \tag{24}$$

B. ALC case

There are four possibilities for α_0:

(i) $\alpha_0=(\frac{12}{25},\frac{12}{25},\frac{12}{25},m^2\omega,l^2\omega,k^2\omega,-\frac{2}{25},-\frac{2}{25},-\frac{2}{25})$, and

(ii) $\alpha_0=(\frac{3}{5},\frac{3}{5},\frac{3}{10},m^2\omega,l^2\omega,k^2\omega/4,-\frac{1}{20},-\frac{1}{20},-\frac{1}{5})$, and the two other vectors obtained by applying the permutation (123)(789) and shifting the $\frac{1}{4}$ factor cyclically in the middle three indices.

In both cases ω is a free parameter.

The corresponding cohomogeneity one metrics will asymptotically approach a circle bundle of constant radius c_1 over a cone over a homogeneous Einstein metric on $\mathrm{SU}(3)/T^2$. Cases (i)

and (ii) correspond to the four homogeneous Einstein metrics on $SU(3)/T^2$, that is, (i) the normal metric and (ii) the three Kähler–Einstein metrics. As in Theorem 3.3, we may calculate that ω controls the radius c_1 of the M-theory circle.

We can now calculate the resonances, check the compatibility conditions, and find the Painlevé expansions.

S	Rational resonances (multiplicities)	No. of parameters in expansion
{4}	-1,0 (three times), 1 (twice), 2 and $-n_1$	7
{5} or {6}	-1,0 (three times), 1 (three times), 2	7
{7}	-1,0 (three times), 1 (twice), 2 and $-n_4$	7
{4,5}	-1 (twice), 0 (twice), 1 (twice), 2 (twice)	6
{4,8}	-1 (twice), 0 (twice), 1 (twice), 2 (twice)	6
{4,9}	-1 (twice), 0 (twice), 1 (twice), 2 (twice)	6
{4,5,9}	-1 (three times), 0,1,2 (three times)	5
{4,5,6}	-1 (three times), 0,1,2 (three times)	5
{1,...,9}	see below	see below
{1,2,3,7,8,9} (i)	-1,0,$\frac{1}{5}$ (twice), $\frac{4}{5}$ (twice), 2 and $\frac{3}{5}$	5
{1,2,3,7,8,9} (ii)	-1,0,2 and $\frac{3}{5}$	3

Remark 4.2: (i) As before, we have listed one choice of S from each orbit of the permutation group C_3. The exception is when $S=\{4\}$, $\{5\}$ or $\{6\}$, where we have listed each case separately because $S=\{4\}$ is slightly different from the other two (this reflects the fact that the choice of Q to some extent breaks the C_3 symmetry).

(ii) The entry in the final column is the maximum number of parameters among Painlevé families with given set S, after all constraints, including the Hamiltonian constraint, have been imposed. Note that the degree of freedom coming from translation of s is included as a parameter (cf. Remark 3.7).

(iii) The resonances after ''and'' are those arising from Theorem 3.5 (b); that is, they are $-n_a$ $(a \notin T)$ in the cases where $|T|<4$. In the ALC case, $T=\{1,2,3\}$ and the value of n_4 follows from the fourth equation in (6). In the remaining cases we obtain the maximal number of parameters in the expansion by taking n_a $(a \notin T)$ to be zero. If $S=\{7\}$, then n_4 must be 0 or 1.

(iv) Expansions with $N=1$ (i.e., expansions meromorphic in s rather than a fractional power of s) are obtained except when S is $\{1,\ldots,9\}$ or $\{1,2,3,7,8,9\}$.

Let us discuss the AC and ALC cases in more detail.

C. AC case: $S=\{1,\ldots,9\}$

On computing the characteristic polynomial of M_T and applying Theorem 3.5(a), we find that the resonances are the roots of the polynomial

$$f(t)f(1-t),$$

where f is the quartic polynomial

$$f(t)=(t+1)\left(t^3-\frac{4}{3}t^2-\frac{1}{9}t+\frac{4}{27}\left(14\frac{\cos^2\phi(\cos\phi+1)}{(\cos\phi+2)^3}+1\right)\right). \tag{25}$$

The number of nontrivial rational resonances is therefore twice the number of rational roots of the cubic factor in $f(t)$.

We write

$$E_x(t)=t^3-\frac{4}{3}t^2-\frac{1}{9}t+\frac{4}{27}\left(14\frac{x^2(x+1)}{(x+2)^3}+1\right)$$

so that the cubic factor is $E_{\cos\phi}(t)$.

The discriminant of $E_x(t)$ is

$$\left(\frac{2}{27(x+2)^3}\right)^2 F(x),$$

where

$$F(x) = -19\,375x^6 - 28\,660x^5 + 20\,556x^4 + 67\,360x^3 + 66\,544x^2 + 43\,200x + 14\,400. \quad (26)$$

Theorem 4.3: *For all but a finite number of Aloff–Wallach spaces $N(k,l)$, the cubic $E_{\cos\phi}(t)$ has at most one rational root, hence the number of parameters in the AC Painlevé expansion is at most three.*

Proof: Observe that if $E_{\cos\phi}(t)$ has more than one rational root, then all its roots are rational.

We first claim that

$$\{x \in \mathbb{Q} : E_x(t) \text{ has more than one root in } \mathbb{Q}\}$$

is *finite*. This is because the discriminant of $E_x(t)$ must now be the square of a rational, and so we have a rational point on the smooth genus two curve $y^2 = F(x)$, where $F(x)$ is given by (26). Faltings's proof of the Mordell conjecture shows there are only finitely many such points.

Now consider the case of general $\cos\phi$. If $E_{\cos\phi}(t)$ has more than one rational root, then, from above, all its coefficients are rational. Therefore there exists a rational q (depending on ϕ) such that $\cos\phi$ is a root of the cubic

$$c_{q(\phi)}(t) = q(t+2)^3 - t^2(t+1) = (q-1)t^3 + (6q-1)t^2 + 12qt + 8q.$$

Also, we saw earlier that $\cos\phi$ is a root of the quartic $H(t)$ given by (24).

If $c_{q(\phi)}(t)$ is irreducible over $\mathbb{Q}$, then up to a scale factor $H(t)$ must be the product of $c_{q(\phi)}(t)$ and a linear factor. It is straightforward to show, by equating coefficients, that this cannot occur for l/m rational.

It follows that $c_{q(\phi)}(t)$ has a root in $\mathbb{Q}$, which means that the cubic $E_{\cos\phi}(t)$ is $E_x(t)$ for some $x \in \mathbb{Q}$. Hence $\{\cos\phi : E_{\cos\phi}(t)$ has more than one root $\in \mathbb{Q}\}$ is finite, and the claim now follows. □

Remark 4.4: The program Ratpoints of Elkies, Stahlke, and Stoll was used to search for rational points on the curve $y^2 = F(x)$ in the range where the denominator of x is $\leqslant 10^5$. The only points found were $(x,y) = (-1, \pm 15), (0, \pm 120), (1, \pm 405), (-\frac{4}{5}, \pm \frac{648}{25})$. As remarked earlier, these possibilities for $x = \cos\phi$ correspond precisely to the degenerate case $\{k,l,m\} = \{1,1,-2\}$.

D. ALC case: $S = \{1,2,3,7,8,9\}$

The eigenvalues of M_T are given as follows:
case (i): $2, -\frac{4}{25}$ (twice),
case (ii): $2, \frac{1}{5}, -\frac{2}{5}$.

In case (i) we have a full set of rational resonances: $-1, \frac{1}{5}$(twice), $\frac{4}{5}$(twice),2 from the eigenvalues of M_T, 0 as in Remark 3.6 (1) and $\frac{3}{5}$ from 3.5(b), as $n_4 = m_4 + 1 = -\frac{3}{5}$.

In case (ii), $-1,2$ are the only rational resonances from the eigenvalues of M_T. We also have resonances 0 and $\frac{3}{5}$ as in (i).

The compatibility conditions are computed using MAPLE. In (i) we have a free parameter ω_0 at $j=0$, and pick up two more ω_1, ω_2 at $j=1$. (The compatibility condition is vacuous here as $X_1 = Y_1 = 0$.) The compatibility condition at $j=3$ forces ω_0 to equal a certain rational function of ω_1, ω_2, homogeneous of degree two. We pick up a free parameter ω_3 from the kernel of the recursion operator at $j=3$. The compatibility conditions at $j=4$ are now the vanishing of two homogeneous polynomials of degree six in ω_1, ω_2. These polynomials have a common linear factor, so we lose only one free parameter at $j=4$. Now the kernel of the recursion operator at

$j=4$ gives two new free parameters ω_4,ω_5. Now Proposition 3.8 ensures that we can solve the recursion at $j=10$, and the Hamiltonian constraint fixes the parameter here.

The upshot is that $\omega_3,\omega_4,\omega_5$ and one of $\omega_0,\omega_1,\omega_2$ may be regarded as free. We therefore have five free parameters in all (including the position of the singularity).

In (ii) the recursion operator for (14) and (15) is invertible for $j<10$ and we find that $\alpha_1=\hat{\beta}_1=0$ and hence $X_3=Y_3=0$. Therefore $\alpha_3=0$, the compatibility condition holds at $j=3$ and we pick up one free parameter here. The other free parameters are from $j=0$ and the position of the singularity.

Now, the equations for the cohomogeneity one metric to be of Spin(7) holonomy will be a subsystem of the Ricci-flat equations (5) and (6).

Transforming the Spin(7)-equations in Gukov and Sparks (2002) to the variables we use, we find that this subsystem may be written as

$$\zeta_i'=\zeta_i\sum_j C_{ij}\zeta_j \quad (i,j=4,5,6,7,8,9) \tag{27}$$

with the constraints

$$\zeta_4\zeta_7=\zeta_5\zeta_8=\zeta_6\zeta_9. \tag{28}$$

Here ζ_i is the positive square root of x_i and C is the matrix

$$-\begin{pmatrix} m\sqrt{\frac{3}{2\Gamma}} & 0 & 0 & 2\sqrt{2} & 0 & 0 \\ 0 & l\sqrt{\frac{3}{2\Gamma}} & 0 & 0 & 2\sqrt{2} & 0 \\ 0 & 0 & k\sqrt{\frac{3}{2\Gamma}} & 0 & 0 & 2\sqrt{2} \\ -m\sqrt{\frac{3}{2\Gamma}} & 0 & 0 & -1/\sqrt{2} & 3/\sqrt{2} & 3/\sqrt{2} \\ 0 & -l\sqrt{\frac{3}{2\Gamma}} & 0 & 3/\sqrt{2} & -1/\sqrt{2} & 3/\sqrt{2} \\ 0 & 0 & -k\sqrt{\frac{3}{2\Gamma}} & 3/\sqrt{2} & 3/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}.$$

We can now look for Painlevé expansions

$$\zeta_i=\sum_{j=0}^{\infty}\gamma_j^{(i)}s^{\mu_i+j/N} \qquad (i=4,5,6,7,8,9),$$

for (27). If we let S denote the set of indices for which the leading power is -1, we can form matrices $\tilde{C}$ and $\hat{C}$ defined by

$$\text{if } j\in S, \quad \tilde{C}_{ij}=C_{ij}, \quad \hat{C}_{ij}=0;$$

$$\text{if } j\notin S, \quad \tilde{C}_{ij}=0, \quad \hat{C}_{ij}=C_{ij}.$$

It is straightforward to check that

$$\tilde{C}\gamma_0=\mu,$$

and that the recursion relation is

$$\frac{j}{N}\gamma_j^{(i)} - \gamma_0^{(i)}(\tilde{C}\gamma_j)^{(i)} = \sum_{k=1}^{j-1}(\tilde{C}\gamma_{j-k})^{(i)}\gamma_k^{(i)} + \sum_{p\notin S}\sum_{k=0}^{j-N(1+\mu_p)} C_{ip}\gamma_k^{(i)}\gamma_{j-k-N(1+\mu_p)}^{(p)}.$$

In particular the resonances $R=j/N$ are the eigenvalues of $\mathrm{diag}(\gamma_0^{(4)},\ldots,\gamma_0^{(9)})\tilde{C}$ [two of the zero eigenvalues should be removed, as the corresponding free parameters are fixed by the constraints (28)].

We can thus compare the Painlevé expansions of the exceptional holonomy system (27) with those of the full Ricci-flat system having the corresponding leading terms.

Theorem 4.5: *Consider the cohomogeneity one Ricci-flat system for the principal orbit* $N(k,l)=\mathrm{SU}(3)/\mathrm{U}(1)_{k,l}$. *The non-AC Painlevé expansions of the associated quadratic system (5)–(8) which contain metrics of* Spin(7)*-holonomy are given by*

(*I*) *a five-parameter family of ALC metrics containing a four-parameter family of ALC* Spin(7)*-metrics,*

(*II*) *a six-parameter family of metrics with* $S=\{4,5\}$ (*or* $\{5,6\}$ *or* $\{4,6\}$) *containing a three-parameter family of* Spin(7)*-metrics,*

(*III*) *a seven-parameter family of metrics with* $S=\{4\}$ (*or* $\{5\}$ *or* $\{6\}$) *containing a four-parameter family of* Spin(7)*-metrics.*

(See Theorem 4.8 for the AC case.) □

Remark 4.6: The expansion for (27) representing ALC metrics has resonances at $-1,0$ and $\frac{4}{5}$ (twice) (cf. the resonances for the ALC expansion in the full Ricci-flat system). A calculation with MAPLE shows that the compatibility conditions at $\frac{4}{5}$ hold automatically, so we have a four-parameter family of expansions. The metrics are asymptotic to a circle of constant radius c_1 over a cone over the standard normal Einstein metric on $\mathrm{SU}(3)/T^2$.

It is interesting to compare this with the equations studied in Dancer and Wang (2002, 2003a) [see also Cvetič *et al.* (2002b) and Cleyton and Swann (2002)] for cohomogeneity one G_2 metrics with principal orbit $\mathrm{SU}(3)/T^2$. These equations form a three-dimensional system, and there is a Painlevé expansion representing metrics asymptotic to a cone over the standard normal Einstein metric on $\mathrm{SU}(3)/T^2$. The eigenvalues are now $-1,\frac{4}{5}(\text{twice})$, all compatibility conditions hold, and we obtain a three-parameter expansion. In fact, the equations may be explicitly solved in terms of Jacobi functions.

The extra parameter in the Spin(7) system comes from the free parameter at $j=0$, that is, the free leading term $\gamma_0^{(4)}=\gamma_0^{(5)}=\gamma_0^{(6)}$. This parameter determines the radius c_1 of the M-theory circle. The existence of our four-parameter ALC Painlevé expansion suggests that it may be possible to find a more general solution in closed form to the Spin(7) system than the ones discovered in Cvetič *et al.* (2002b) and Kanno and Yasui (2002).

Remark 4.7: In the AC case, we find that the resonances are the roots of the polynomial $f(t)$ that we encountered in (25). [Recall that the AC resonances for the full Ricci-flat system are the roots of $f(t)f(1-t)$.] Theorem 4.3 therefore has the following corollary.

Theorem 4.8: *For all but finitely many Aloff–Wallach spaces, the* Spin(7) *equations have at most one nontrivial rational resonance in the AC case. The corresponding Painlevé expansions have at most two free parameters.* □

V. U(1) BUNDLES OVER PRODUCTS OF EINSTEIN FANO VARIETIES

In this section we examine Painlevé expansions of our Ricci-flat equations (5)–(8) in the case when the ''principal orbits'' are certain circle bundles over a product of two Fano varieties studied in Wang and Ziller (1990). When the Fano varieties are homogeneous, then the principal circle bundles we consider are homogeneous, and so are genuine principal orbits of a cohomogeneity one action on the manifold $\mathcal{M}$. In general, however, there are no symmetries on the Fano varieties or the circle bundles. Nevertheless, it is well known that if we use the Kaluza–Klein construction

for the metrics on the circle bundles, the formalism of cohomogeneity one Einstein metrics leads to the same system of ordinary differential equations as in the homogeneous case.

Let $V_i (i=2,3)$ be respectively smooth Fano varieties admitting Kähler–Einstein metrics h_i. The cohomology group $H^2(V_i,\mathbb{Z})$ is torsion free and so we can write the first Chern class of V_i as $c_i\gamma_i$ where γ_i is an indivisible class and c_i is a positive integer—the first Chern number. The principal circle bundles we will consider are circle bundles over $V_2\times V_3$ whose Euler class is $e_2\gamma_2+e_3\gamma_3\in H^2(V_2,\mathbb{Z})\oplus H^2(V_3,\mathbb{Z})$, where e_i are arbitrary nonzero integers. Note that if e_2 and e_3 have greatest common divisor e_1, then the circle bundle has the bundle whose Euler class is $(e_2/e_1)\,\gamma_2+(e_3/e_1)\,\gamma_3$ as its universal cover. Also, bundles whose Euler classes give rise to the same ordered pair $(|e_2|,|e_3|)$ are related by pull-back via diffeomorphisms of the base. So it is natural and convenient to introduce the quantity

$$\tau:=\left|\frac{e_2}{c_2}\left(\frac{e_3}{c_3}\right)^{-1}\right| \tag{29}$$

and not to distinguish bundles with the same invariant τ.

We will let $d_i=2l_i$ be the real dimension of V_i. Without loss of generality, we may assume that $d_2\leqslant d_3$. We will also normalize the Kähler–Einstein metric h_i so that its Ricci form is $2\pi c_i$ times its Kähler form.

Next we describe the one-parameter families of metrics we will consider on our principal circle bundles. For each such bundle, we choose a connection θ so that its curvature form is harmonic with respect to the product metric $h_2\perp h_3$ on the base. Then we consider one-parameter families of metrics of the form

$$g_t=f_1(t)^2\ (\theta\otimes\theta)\perp\pi^*(f_2(t)^2h_2\perp f_3(t)^2h_3), \tag{30}$$

where π denotes the bundle projection map and f_i are smooth positive functions of the transverse variable t. The scalar curvature of g_t is given by

$$\mathsf{S}(g_t)=\frac{d_2c_2}{f_2(t)^2}+\frac{d_3c_3}{f_3(t)^2}-\frac{1}{4}\left(d_2e_2^2\frac{f_1(t)^2}{f_2(t)^4}+d_3e_3^2\frac{f_1(t)^2}{f_3(t)^4}\right). \tag{31}$$

We shall need some information about Einstein metrics of the form (30) (without the parameter t) on our circle bundles. It was shown by an abstract degree argument in Wang and Ziller (1990) that up to homothety there is a unique Einstein metric in this class of metrics. The special case of these bundles where $V_2=\mathbb{CP}^1$ and $V_3=\mathbb{CP}^2$ was first studied in Witten (1982). These are homogeneous seven-dimensional manifolds with $\mathrm{SU}(3)\cdot\mathrm{SU}(2)\cdot\mathrm{U}(1)$ symmetry. For these manifolds, Castellani, D'Auria, and Fré (1984, p. 627) independently showed the existence of a unique homogeneous Einstein metric (up to homothety). Furthermore, they parametrized the Einstein metrics in terms of the roots of a cubic polynomial whose coefficients depend on a rational expression of c_i and e_i. Finally, they showed that the Einstein manifolds admit a nontrivial Killing spinor only when this rational expression is 1. In our notation, this is the case when $e_i=-c_i$ $(i=2,3)$. Another way to phrase this observation is that the circle bundles with $e_i=-c_i$ $(i=2,3)$ are the only ones where the unique Einstein metric of bundle type is Sasakian–Einstein. This observation holds generally in the situation of Wang and Ziller (1990), and in an even more general context, and is due to Boyer and Galicki (2000). Thus the metric cones over these Einstein circle bundles admit a Calabi–Yau metric.

In the Appendix we will give a similar parametrization (in terms of τ) of the unique Einstein metric on the circle bundles under study. This parametrization will be used in this section.

With the above preliminaries, we are now ready to discuss the Painlevé analysis of (5)–(8) for the present case.

Note first that from (31) we have the weight vectors

$$w^{(1)}=(0,-1,0),\quad w^{(2)}=(0,0,-1),$$

$$w^{(3)}=(1,-2,0),\quad w^{(4)}=(1,0,-2),$$

and corresponding coefficients $(A_1,A_2,A_3,A_4)=(d_2c_2,d_3c_3,-d_2e_2^2/4,-d_3e_3^2/4)$. So $r=3$ and $\ell=1$. It follows that the matrix Φ and a choice of the matrix Q are given by

$$\Phi=\begin{pmatrix} 1-\frac{1}{d_2} & 1 & 1-\frac{2}{d_2} & 1 \\ 1 & 1-\frac{1}{d_3} & 1 & 1-\frac{2}{d_3} \\ 1-\frac{2}{d_2} & 1 & -\frac{4}{d_2} & 0 \\ 1 & 1-\frac{2}{d_3} & 0 & -\frac{4}{d_3} \end{pmatrix},$$

$$Q=\begin{pmatrix} \sqrt{\frac{d_2-1}{d_2}} & 0 & 0 \\ \sqrt{\frac{d_2}{d_2-1}} & \sqrt{\frac{d_2+d_3-1}{d_3(d_2-1)}} & 0 \\ \frac{d_2-2}{\sqrt{d_2(d_2-1)}} & -\sqrt{\frac{d_3}{(d_2-1)(d_2+d_3-1)}} & \sqrt{\frac{d_2+d_3}{d_2+d_3-1}} \\ \sqrt{\frac{d_2}{d_2-1}} & \frac{2d_2+d_3-2}{\sqrt{d_3(d_2-1)(d_2+d_3-1)}} & \sqrt{\frac{d_2+d_3}{d_2+d_3-1}} \end{pmatrix}.$$

The vector ξ in Theorem 3.3 is equal to $[1/(d_2+d_3)](-(d_2+2),-d_3,1)$.

Applying the algorithm in Sec. III, one easily checks that possible leading terms of Painlevé expansions for Eqs. (5) and (6) are as given in the following table.

S	T	m	$\alpha_0^{(i)}$ $(i\in S)$	Remarks
$\{3\}(i)$	$\{2,3\}$	$(0,1,-2,0)$	$-\frac{1}{2}$	$d_2=2$
$\{3\}(ii)$	$\{1,2,3\}$	$\left(\frac{d_2-2}{2},\frac{d_2}{2},-2,0\right)$	$-\frac{d_2}{4}$	$d_2>2$
$\{4\}$	$\{1,2,3\}$	$\left(\frac{d_3}{2},\frac{d_3-2}{2},0,-2\right)$	$-\frac{d_3}{4}$	
$\{3,4\}$	$\{1,2,3\}$	$\left(\frac{d_2+d_3-2}{2},\frac{d_2+d_3-2}{2},-2,-2\right)$	$-\frac{d_2}{4},-\frac{d_3}{4}$	
$\{1,2,3,4\}$	$\{1,2,3\}$	$(-2,-2,-2,-2)$	see below	AC
$\{1,2\}$	$\{1,2\}$	$\left(-2,-2,-2\left(\frac{d_2+d_3-2}{d_2+d_3-1}\right),-2\left(\frac{d_2+d_3-2}{d_2+d_3-1}\right)\right)$	$\frac{d_2}{d_2+d_3-1},\frac{d_3}{d_2+d_3-1}$	ALC

In the above table, we have not yet imposed the constraint (7). When $S=\{1,2,3,4\}$, using (10) and the parametrization of the Einstein metrics on our circle bundles given in the Appendix, we find that

$$\begin{aligned} \alpha_0^{(1)}&=\frac{d_2}{d_2+d_3}\left(\frac{d_3\mu^2+d_2+2}{d_3\mu^2+d_2}\right),\quad \alpha_0^{(2)}=\frac{d_3}{d_2+d_3}\left(\frac{(d_3+2)\mu^2+d_2}{d_3\mu^2+d_2}\right), \\ \alpha_0^{(3)}&=\frac{-d_2}{d_2+d_3}\left(\frac{1}{d_3\mu^2+d_2}\right),\quad \alpha_0^{(4)}=\frac{-d_3}{d_2+d_3}\left(\frac{1}{d_3\mu^2+d_2}\right), \end{aligned} \tag{32}$$

where μ is the parameter introduced in the Appendix and the constraint condition (7) is precisely the requirement that μ is a root of the cubic polynomial φ given by (A1).

When $S=\{1,2\}$, we may let $\alpha_0^{(4)}$ be a free parameter $\omega_0<0$, and the constraint (7) implies that $\alpha_0^{(3)}=(d_2/d_3)\,\tau^2\omega_0$.

Regarding the asymptotics of the metrics corresponding to Painlevé expansions with the above leading term behavior, the AC and ALC cases are as indicated in the table, with $f_1(t)$ approaching a positive constant in the latter case. In the remaining cases, as s approaches 0, the transverse parameter t tends to a finite limit, and the volume of the circle bundles tends to 0. There is always an $f_j(t)$ which blows up, and when $S=\{3\}$ or $\{4\}$ there is always another $f_j(t)$ which tends to a positive constant.

We discuss next the resonances and compatibility conditions for our Painlevé expansions. The results are summarized in the table below.

S	Resonances (multiplicities)	No. of parameters in expansion
$\{3\}$ (i)	-1,0 (twice), 1,2 and $-n_1$	5
$\{3\}$ (ii)	-1,0 (twice), 1 (twice), 2	5
$\{4\}$	-1,0 (twice), 1 (twice), 2	5
$\{3,4\}$	-1 (twice), 0,1,2 (twice)	4
$\{1,2,3,4\}$	$-1,\frac{-2}{n-1},\frac{2}{n-1},\frac{n-3}{n-1},\frac{n+1}{n-1},2$ when $\tau=1$ otherwise see below	4 or 3
$\{1,2\}$	$-1,0,2$, roots of $R(R-1)=\frac{-2}{n-2}$	4 $(n=11)$
	and $-n_3=\frac{n-4}{n-2}$	3 (n$\neq$11)

Remark 5.1: We follow the same conventions as those in Remark 4.2.

(i) Recall that $n=1+d_2+d_3$ *is the dimension of our hypersurfaces and* τ *is given by* (29).

(ii) We may choose $N=1$ in the first four cases, and so we obtain expansions meromorphic in s.

(iii) We have again listed the maximum number of parameters among Painlevé expansions with the same S in the third column. For example, when $S=\{3\}$ and $d_2=2$, we get five parameters when $n_1=0$, four parameters when $n_1=1$ and three parameters when $n_1>1$.

We now give more details regarding the AC and ALC cases.

A. AC cases

When $S=\{1,2,3,4\}$, one finds using MAPLE that the eigenvalues of the matrix M (cf. Theorem 3.5) are 2 and $2(1+\mu^2\pm\sqrt{\delta})/[(d_2+d_3)(d_3\mu^2+d_2)]$ where

$$\delta=(d_3+1)^2\mu^4+2(d_2d_3-d_2-d_3-1)\mu^2+(d_2+1)^2.$$

Hence the rationality conditions for the resonances are that

$$\Delta_{\pm}=1+\left(\frac{8}{d_2+d_3}\right)\left(\frac{1+\mu^2\pm\sqrt{\delta}}{d_3\mu^2+d_2}\right) \tag{33}$$

should be squares in $\mathbb{Q}$.

By the discussion in the Appendix, in the special case when $\tau=1$ (the Sasakian–Einstein case), we have $\mu=1$, and $\delta=(n-1)^2$. Corresponding to Δ_+ we obtain resonances $-2/(n-1)$ and $(n+1)/(n-1)$, and corresponding to Δ_- we obtain resonances $2/(n-1)$ and $(n-3)/(n-1)$ (which are equal when $n=5$).

Lemma 5.2: In the AC case, in order that we have a full set of rational resonances, μ must be rational.

Proof: Note that besides the cubic equation $\varphi(x)=0$, where φ is given by (A1), μ also satisfies the quartic equation

$$F(x)=((d_3+1)^2-r_*^2d_3^2)x^4+2(d_2d_3(1-r_*^2)-d_2-d_3-1)x^2+((d_2+1)^2-r_*^2d_2^2)=0,$$

where r_* is some rational number, because $\sqrt{\delta}/(d_3\mu^2+d_2)$ has to be rational. Let $\eta(x)$ be the minimal polynomial of μ. If η has degree 1, μ is rational, so we may assume that η has degree 2 or 3. In the former case, since it divides φ, we get a contradiction to the fact that φ has a unique real root, as was indicated in the Appendix. In the latter case, up to a constant, φ is the minimal polynomial of μ. If F genuinely has degree 4, since φ must divide F, F has a nonzero rational root in addition to the roots of φ. Since F is even in x, the negative of this root must be μ, which would then be rational. If the coefficient of x^4 in F vanishes, then φ cannot be the minimal polynomial of μ unless the coefficient of x^2 in F vanishes as well. But this leads immediately to a contradiction. □

We do not know if the above lemma remains true under the assumption that there is at least one nontrivial rational resonance.

In any case, let us assume that μ is rational in (33). This imposes a restriction on the circle bundles through (A2). In this situation, if one of $\Delta_\pm$ is a square in $\mathbb{Q}$, then δ must be a square, too. We shall analyze this condition in two steps. First, note that $(\mu^2,\pm\sqrt{\delta})$ are rational points on the curve whose equation is

$$y^2=(d_3+1)^2x^2+2(d_2d_3-d_2-d_3-1)x+(d_2+1)^2.$$

Since $(1,d_2+d_3)$ is also a rational point on this curve it follows that we can parametrize all of its rational points (x_ρ,y_ρ) by lines with rational slope ρ passing through $(1,d_2+d_3)$. Explicitly we have

$$x_\rho=1+\frac{2(d_3(d_2+d_3)+d_3-d_2-(d_2+d_3)\rho)}{\rho^2-(d_3+1)^2}, \tag{34}$$

$$y_\rho=(d_2+d_3)+\rho(x_\rho-1). \tag{35}$$

Second, in order for $x_\rho=\mu^2$ for some positive rational number μ, we must have a rational point (ρ_0,w_0) on the curve

$$\mathcal{C}_\delta: w^2=F_\delta(\rho):=(\rho+d_3+1)(\rho-d_3-1)(\rho-d_3+1)(\rho-2d_2-d_3-1). \tag{36}$$

Note that the underlying circle bundle must then have Euler class satisfying (A2) with $\mu=\sqrt{x_{\rho_0}}$.

Assuming now that δ is a square in $\mathbb{Q}$ as above, it follows by a straightforward computation that requiring Δ_+ or Δ_- to be a square in $\mathbb{Q}$ is equivalent to the existence of a rational point *having first coordinate* ρ_0 on one of the two curves $\mathcal{C}_\pm$ whose respective equations are

$$\mathcal{C}_+: w^2=F_+(\rho):=(d_2+d_3)F_1(\rho)G(\rho), \tag{37}$$

$$\mathcal{C}_-: w^2=F_-(\rho):=(d_2+d_3)F_2(\rho)G(\rho), \tag{38}$$

where

$$F_1(\rho)=(d_2+d_3-4)^2\rho^2-2(d_3(d_2+d_3-4)^2+16(d_2-d_3))\rho+(d_2+d_3-4)^2(d_3^2-1)$$
$$-4(d_2+d_3)(d_2d_3+8)-32d_3^2, \tag{39}$$

$$F_2(\rho)=(d_2+d_3+4)^2\rho^2-2d_3(d_2+d_3+4)^2\rho+(d_2+d_3+4)^2(d_3^2-1)-4d_2d_3(d_2+d_3-8), \tag{40}$$

$$G(\rho)=(d_2+d_3)\rho^2-2d_3(d_2+d_3)\rho+(d_2+d_3)(d_3^2-1)-4d_2d_3. \tag{41}$$

In particular, there is a full set of rational resonances iff there are rational points on all three curves $\mathcal{C}_\delta,\mathcal{C}_\pm$ with the *same* first coordinate ρ.

Note that we do not really need both curves $\mathcal{C}_\pm$ in the above analysis. For a fixed value of x_ρ in (34), there are two corresponding values of ρ, for which the values of y_ρ are negatives of each other. So searching for rational points having the same first coordinate on the two curves is the same as searching for rational points on one of the curves whose first coordinates determine the same x_ρ.

One can check that the right-hand side of (37) has four distinct real roots except when $d_2=d_3=2$, and the right-hand side of (38) always has four distinct real roots. Furthermore, the polynomial $F_\delta(\rho)\cdot F_-(\rho)$ has distinct roots except when $d_2+d_3=8$, in which case there are precisely two roots with multiplicity 2 and the rest have multiplicity 1. The genus of the curve

$$\mathcal{C}:\quad w^2=F_\delta(\rho)\cdot F_-(\rho)$$

is therefore 3 when $d_2+d_3\neq 4$ or 8, and in this situation Faltings' theorem implies that $\mathcal{C}$ has only finitely many rational points. Now consider the situation where (ρ_0,w_1) and (ρ_0,w_2) are rational points on $\mathcal{C}_\delta$ and $\mathcal{C}_-$, respectively. Then (ρ_0,w_1w_2) is a rational point on the curve $\mathcal{C}$. This proves the first assertion in the following theorem.

Theorem 5.3: *Among all the circle bundles under study over a fixed base whose dimension is different from* 4 *or* 8, *there are only finitely many for which the AC Painlevé expansions can have a full set of rational resonances. When the base has dimension* 4 *this happens only for the bundles such that* $\tau=1$, *i.e., the bundles which admit a Sasakian–Einstein metric of bundle type after suitable changes in orientation.*

We now discuss some low-dimensional cases in more detail and along the way prove the second assertion of the above theorem.

Let us first consider the case where $d_2=d_3=2$. In this situation we have circle bundles over $\mathbb{CP}^1\times\mathbb{CP}^1$, and $(c_2,c_3)=(2,2)$. If e_2 and e_3 are coprime, then all the circle bundles are diffeomorphic to $S^2\times S^3$ by a well-known theorem of Smale (1962). Equations (37) and (38) become respectively

$$w^2=-4\cdot 16^2\cdot 5\cdot(\rho^2-4\rho-1),$$

$$w^2=4\cdot 16^2\cdot(\rho-2)^2(\rho^2-4\rho-1).$$

(Note that F_+ reduces to a constant in this case, so the first equation is quadratic in ρ.) Obviously, the same ρ cannot be the first coordinate of two rational points, one on each curve, unless $\rho=2$, which occurs iff $x_\rho=\mu^2=1$. By (A2), we must have $|e_2|=|e_3|$. The total spaces of these bundles are related by pull-back via a diffeomorphism of the base which sends one or both of the first Chern classes of the base factors to their negatives. Thus modulo this pull-back, these are precisely the bundles admitting a Sasakian–Einstein metric of bundle type. This gives the second claim in Theorem 5.3.

If $d_2=2$ and $d_3=4$, the respective curves are given by

$$\mathcal{C}_\delta: w^2=(\rho-5)(\rho+5)(\rho-3)(\rho-9),$$

$$\mathcal{C}_+: w^2=48(\rho-11)(\rho+19)(3\rho^2-24\rho+29),$$

$$\mathcal{C}_-: w^2 = 48(5\rho - 23)(5\rho - 17)(3\rho^2 - 24\rho + 29).$$

Using the program Ratpoints with a bound of 10^5 on $|\rho|$ and on its denominator, we find 14 rational points on $\mathcal{C}_+$, 16 rational points on $\mathcal{C}_-$, and 17 rational points on $\mathcal{C}_\delta$, not counting the point at infinity. Comparing the ρ-coordinates of the rational points found for $\mathcal{C}_\pm$ and $\mathcal{C}_\delta$, we find $\rho = \frac{13}{3}$ as the only common value. By (34), $x_\rho = 1$, and so $\tau = 1$.

The same phenomenon is observed for $(d_2, d_3) = (2,6),(4,4),(2,8),(4,6)$. In other words, for the AC Painlevé expansions under consideration, the requirement of having a full set of rational resonances appears to single out (when $d_2 + d_3 + 1 = n \leqslant 11$) the circle bundles on which the bundle-type Einstein metric is Sasakian–Einstein, modulo orientation change and pull-back. In view of the above numerical evidence and Proposition 5.3, it is tempting to conjecture that this is true in general, perhaps even under the weaker requirement that there is at least one nontrivial rational resonance.

We turn now to the compatibility conditions when $\tau = 1$ (the Sasakian–Einstein case). The positive resonances are at $j/N = 1/(l_2 + l_3)$, $(l_2 + l_3 - 1)/(l_2 + l_3)$, $(l_2 + l_3 + 1)/(l_2 + l_3)$ and 2. We take N to be $l_2 + l_3$, the complex dimension of the base of our bundles. The compatibility condition at $j = 1$ is trivially satisfied since the right-hand side of the recursion relations is zero. We therefore obtain a free parameter ω_1. If compatibility holds up to and including $j = l_2 + l_3 + 1$, then compatibility at the top resonance follows from Proposition 3.8, and one checks that the free parameter entering at that stage can be used to satisfy the Hamiltonian constraint. Hence we get at most a four-parameter Painlevé family.

When $d_2 = d_3 = 2$, we have $N = 2$. The first two nonzero resonances coincide, and the compatibility condition at $j = 3$ is also satisfied. So we obtain a three-parameter family of expansions.

When $d_2 = 2$, $d_3 = 4$, we have $N = 3$. The compatibility condition at $j = 2$ is satisfied, giving rise to a free parameter ω_2. Using MAPLE, one sees that the compatibility condition at $j = 4$ is satisfied iff

$$(10\omega_2 + 97\sqrt{2}\omega_1^2)(-10\omega_2 + 3\sqrt{2}\omega_1^2) = 0.$$

Hence we obtain two three-parameter families of Painlevé expansions by setting one of the two factors in the above equal to 0.

When $d_2 = d_3 = 4$, we have $N = 4$. This time, using MAPLE one sees that the compatibility conditions always hold and we obtain a four-parameter Painlevé family. On the other hand, when $d_2 = 2, d_3 = 6$, the compatibility condition at $j = 3$ holds while that at $j = 5$ is given by

$$\omega_1^2\left(\tfrac{1024}{63}\omega_1^3 + \sqrt{21}\omega_2\right) = 0.$$

So we have two three-parameter Painlevé families.

Exactly the same phenomena occur for the two cases where $d_2 + d_3 = 10$ and we obtain two three-parameter families in each case.

B. ALC cases

When $S = \{1,2\}$, the eigenvalues of the 2×2 matrix M_T are 2 and $-2/(n-2)$. The equation $R(R-1) = -2/(n-2)$ has rational solutions iff $(n-10)/(n-2)$ is a square in $\mathbb{Q}$. By Lemma 4.1 in Dancer and Wang (2001), this happens precisely when $n = 10$ or 11. Since n must be odd in our situation, we have $n = 11$, and the resonances in this case are $-1, 0, \frac{1}{3}, \frac{2}{3}, \frac{7}{9}$ and 2. We therefore take $N = 9$ in the recursion, which we perform using MAPLE.

Recall that we have a free parameter ω_0 in the leading coefficients. At step $j = 3$ the right-hand sides of the recursion relations (14) and (15) vanish and we pick up a free parameter ω_1. At $j = 6$ the compatibility condition requires ω_1 to vanish, and we pick up a free parameter ω_2. It follows then that at $j = 7$ the right-hand sides of (14) and (15) vanish, and we pick up a free parameter ω_3 from (16). The compatibility condition at the top resonance then follows from Proposition 3.8, and as usual the free parameter entering at that point is used to satisfy the

Hamiltonian constraint. Thus, adding in the singularity position, we obtain a four-parameter Painlevé family. If $n \neq 11$, then the only positive rational resonances are $(n-4)/(n-2)$ and 2, and we can let $N=n-2$. The compatibility condition at $(n-4)/(n-2)$ is satisfied because we can show by induction that the right-hand sides of (14) and (15) are zero when j is odd and $\leqslant n-4$. The compatibility condition holds at the top resonance again by Proposition 3.8, and the Hamiltonian constraint is satisfied by fixing the parameter entering at the top resonance. Thus ω_0, the free parameter entering at $j=n-4$, and the singularity position account for a three-parameter Painlevé family.

Finally, we discuss situations in which the metrics represented by the Painlevé expansions we obtained above exhibit special geometry.

Recall from Dancer and Wang (1998, Sec. 2) and Wang and Wang (1998) that when $e_i = -c_i$ for $i=2,3$, the cohomogeneity one Ricci-flat equations have a three-parameter family of explicit (local) Kähler–Einstein solutions, if we include the freedom to add a constant to the independent variable. [Note that $e_i=-c_i, (i=2,3)$ is a *necessary* condition for Ricci-flat Kähler-Einstein metrics.] In the above three-parameter family, there is a one-parameter subfamily of *complete* Calabi–Yau metrics. One can easily check that the ends in this subfamily are asymptotic to the metric cone over the Sasakian–Einstein metric of bundle-type on the circle bundle.

It turns out that when $e_i=-c_i (i=2,3)$, the solution curves of the Ricci-flat system (5)–(8) which lie in the subvariety given by

$$\frac{v_1}{\sqrt{d_2(d_2-1)}}+\frac{\sqrt{d_3}\ v_2}{\sqrt{(d_2-1)(d_2+d_3-1)}}-\frac{v_3}{\sqrt{(d_2+d_3)(d_2+d_3-1)}}=\frac{\sqrt{-z_3}}{\sqrt{d_2}},$$

$$-\frac{\sqrt{d_2-1}}{\sqrt{d_3(d_2+d_3-1)}}v_2-\frac{v_3}{\sqrt{(d_2+d_3)(d_2+d_3-1)}}=\frac{\sqrt{-z_4}}{\sqrt{d_3}},$$

$$\frac{2\sqrt{d_2+d_3-1}}{\sqrt{d_2+d_3}}\ v_3=\frac{1}{\sqrt{d_2}}\frac{z_1}{\sqrt{-z_3}}-\sqrt{d_2}\sqrt{-z_3}-\sqrt{d_3}\sqrt{-z_4}$$

correspond to Calabi–Yau metrics. If we let $\zeta_1=z_1/\sqrt{-z_3}$, $\zeta_2=\sqrt{-z_3}$ and $\zeta_3=\sqrt{-z_4}$, then these variables parametrize the subvariety of Calabi–Yau solutions and (5) and (6) induce on it the system

$$\zeta_i'=\zeta_i\sum_j C_{ij}\zeta_j, \quad i,j=1,2,3,$$

where C is the matrix

$$\begin{pmatrix} 0 & \sqrt{d_2} & \sqrt{d_3} \\ \dfrac{1}{\sqrt{d_2}} & -\dfrac{2}{\sqrt{d_2}} & 0 \\ \dfrac{1}{\sqrt{d_2}} & 0 & -\dfrac{2}{\sqrt{d_3}} \end{pmatrix}.$$

By comparing the Painlevé expansions of this system which have the same leading terms as those of the full Ricci-flat system, we obtain the following.

Theorem 5.4: *Consider the quadratic system (5)–(8) associated to principal circle bundles over a product of two Kähler–Einstein Fano varieties V_2, V_3 with $e_i=-c_i$, $i=2,3$.*

(*I*) *There are two five-parameter families of meromorphic Painlevé expansions representing local Ricci-flat metrics, within each of which is a three-parameter subfamily of Painlevé expansions representing Calabi–Yau metrics.*

(*II*) *There is a four-parameter family of meromorphic Painlevé expansions representing local Ricci-flat metrics, within which lies a two-parameter subfamily representing Calabi–Yau metrics.*

(*III*) *If the base dimension is* $\leqslant 10$*, there is a three-parameter family of Painlevé expansions (four parameters if* V_i *have the same dimension) representing complete Ricci-flat ends with AC asymptotics, within which lies a two-parameter subfamily representing Calabi–Yau metrics.*

The remaining ALC Painlevé families do not contain Calabi-Yau metrics.

□

Remark 5.5: (i) We expect that part (III) of the above theorem should be true without the dimension restriction.

(ii) We can relate our Painlevé expansions to another geometric condition that was first explored by Alfred Gray (1976). This concerns Riemannian metrics which are almost Hermitian with respect to a complex structure J and for which the curvature four-tensor is totally invariant under J. The Kähler condition is a special case of this condition. In Wang and Wang (1998), this condition was used to integrate the Einstein equations of cohomogeneity-one type where the hypersurfaces are circle bundles over a product of Fano manifolds. In particular, it was shown in Lemma 2.14 in Wang and Wang (1998) that local solutions satisfying the above geometric condition depend in general on three-parameters. The Ricci-flat equations we are studying in this section by Painlevé analysis are a special case of the Ricci-flat equations in Wang and Wang (1998). Hence the fact that in dimension 12 we obtained a four-parameter family of ALC Painlevé expansions implies that in that dimension there is a one-parameter family of complete Ricci-flat ends with ALC asymptotics whose curvature four-tensor is not totally invariant under the natural complex structure arising in that situation. On the other hand, MAPLE computations seem to indicate that Gray's condition in our situation is closely related to ALC asymptotics and it is quite probable that our three-parameter families of ALC Painlevé expansions in dimensions $\neq 12$ all satisfy Gray's condition.

ACKNOWLEDGMENTS

The second author was partially supported by NSERC Grant No. OPG0009421. Part of the research for this article uses the symbolic computation program MAPLE 7 and the number theory computation program RATPOINTS 1.4.c of Elkies, Stahlke, and Stoll.

APPENDIX: EXPLICIT PARAMETRIZATION OF EINSTEIN METRICS ON CIRCLE BUNDLES

In this section we indicate how we parametrize the Einstein metrics on the total spaces of the circle bundles we considered in Sec. V. The method is similar to that used in Castellani *et al.* (1984) and in Cvetic (2002b).

We start with the Einstein equations (1.5), (1.6) on p. 222 of Wang and Ziller (1990). In our notation, and in the case when the base consists of two factors, these are

$$x_1\left(\frac{d_2e_2^2}{x_2^2}+\frac{d_3e_3^2}{x_3^2}\right)=4\Lambda,$$

$$\frac{4c_2}{x_2}-2x_1\frac{e_2^2}{x_2^2}=4\Lambda,$$

$$\frac{4c_3}{x_3}-2x_1\frac{e_3^2}{x_3^2}=4\Lambda,$$

where Λ is the Einstein constant and $x_i=f_i^2$ for $i=1,2,3$. Let us multiply all three of the above equations by the factor $x_2x_3/c_2c_3x_1$. For $i=2,3$ let $\sigma_i=e_i/c_i$ (so $\tau=|\sigma_2/\sigma_3|$) and $y_i=x_i/c_ix_1$, and set $W_2^2=\sigma_2^2y_3/y_2$, $W_3^2=\sigma_3^2y_2/y_3$. After subtracting the resulting equations, we obtain

$$d_2W_2^2+(d_3+2)W_3^2=4y_2,$$

$$(d_2+2)W_2^2+d_3W_3^2=4y_3.$$

It follows that

$$(d_2+d_3+2)W_2^2=2(-d_3y_2+(d_3+2)y_3),$$

$$(d_2+d_3+2)W_3^2=2((d_2+2)y_2-d_2y_3).$$

The relation $W_2^2W_3^2=\sigma_2^2\sigma_3^2$ now gives

$$(d_2+d_3+2)^2\sigma_2^2\sigma_3^2=2(F_1^2-F_2^2),$$

where

$$F_1=\frac{1}{\sqrt{2}}(((d_2+2)y_2-d_2y_3)+(-d_3y_2+(d_3+2)y_3))$$

and

$$F_2=\frac{1}{\sqrt{2}}(((d_2+2)y_2-d_2y_3)-(-d_3y_2+(d_3+2)y_3)).$$

We can therefore write

$$F_1=\frac{1}{\sqrt{2}}(d_2+d_3+2)|\sigma_2\sigma_3|\cosh\theta,$$

$$F_2=\frac{1}{\sqrt{2}}(d_2+d_3+2)|\sigma_2\sigma_3|\sinh\theta,$$

for some parameter θ and set $\mu=\exp\theta$. One easily checks now that the Einstein equations become the condition that μ should be a positive root of the cubic polynomial

$$\varphi(x)=\tau d_3x^3-(d_3+2)x^2+\tau(d_2+2)x-d_2. \tag{A1}$$

The x_i in the original Einstein equations are then given by

$$x_2=\frac{x_1}{4}c_2|\sigma_2\sigma_3|((d_3+2)\exp\theta+d_2\exp(-\theta)),$$

$$x_3=\frac{x_1}{4}c_3|\sigma_2\sigma_3|(d_3\exp\theta+(d_2+2)\exp(-\theta)).$$

Since roots of a cubic polynomial are given by Cardano's formula, we may regard the above Einstein metrics as ''explicit.''

Note that for $\mu \leqslant 0$ we have $\varphi(\mu) < 0$, and one easily checks also that φ has a unique positive root. Hence we recover the fact that up to homothety there is a unique solution of the Einstein equations. Our interest here is to parametrize the Einstein metrics in terms of τ. Note that when $\tau = 1$, φ has the unique positive root $\mu = 1$, which represents the unique Sasakian–Einstein metric in the family.

From $\varphi(\mu) = 0$ we obtain the relation

$$\tau = \frac{(d_3+2)\mu^2 + d_2}{\mu(d_3\mu^2 + (d_2+2))}. \tag{A2}$$

One can check that as a function of $\mu > 0$, τ is strictly decreasing, with $\lim_{\mu \to 0} \tau = +\infty$ and $\lim_{\mu \to +\infty} \tau = 0$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Progress in relativistic gravitational theory using the inverse scattering method

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(Received 9 April 2003; accepted 9 April 2003)

The increasing interest in compact astrophysical objects (neutron stars, binaries, galactic black holes) has stimulated the search for rigorous methods, which allow a systematic general relativistic description of such objects. This article is meant to demonstrate the use of the inverse scattering method, which allows, in particular cases, the treatment of rotating body problems. The idea is to replace the investigation of the matter region of a rotating body by the formulation of boundary values along the surface of the body. In this way we construct solutions describing rotating black holes and disks of dust (''galaxies''). Physical properties of the solutions and consequences of the approach are discussed. Among other things, the balance problem for two black holes can be tackled. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1590419]

I. INTRODUCTION

The systematic investigation of neutron stars and binaries consisting of pulsars and other compact objects and the increasing evidence for the existence of (rotating) black holes have stimulated theoretical and numerical studies on rapidly rotating bodies in general relativity. No doubt, realistic stellar models (e.g., neutron star models) require a careful physical analysis of their interior states and processes and, as a consequence, extensive *numerical* calculations. On the other hand, there is widespread interest for explicit solutions of the rotating body problem under simplifying assumptions. Such solutions could provide a deeper insight into physical phenomena connected with spinning matter configurations and, moreover, serve as test beds for the numerical investigations mentioned before. A good example is the Kerr solution, which has enriched our knowledge of rotating black holes in an inestimable way. However, rigorous results for rotating bodies are relatively rare in general relativity. Among other things, this is due to the mathematical difficulties with ''free boundary value problems,'' already known from Newton's gravitational theory, and to the specific complexity of the differential equations of Einstein's theory inside the body. Namely, the shape of the surface of a rotating self-gravitating fluid ball—the best model for astrophysical applications—is a ''compromise'' between gravitational, centrifugal, and pressure forces and not known *a priori*. (The surface is ''free,'' i.e., not fixed from the very beginning.) Though there are powerful (soliton-) techniques to generate (formal) stationary axisymmetric solutions of Einstein's vacuum equations, no algorithm to integrate the interior field equations is available. Hence, at first glance, a boundary value description of rotating bodies seems to be questionable and inadequate. However, there are exceptional cases, in which the surface of the body has a known shape and the surface values provide enough information to construct the complete solution of the vacuum field equations. It is the intention of this article to show that this is true for stationary black holes and disks of dust, which may be considered to be extremely flattened perfect fluid bodies. Moreover, it should become clear that our procedure, which is based

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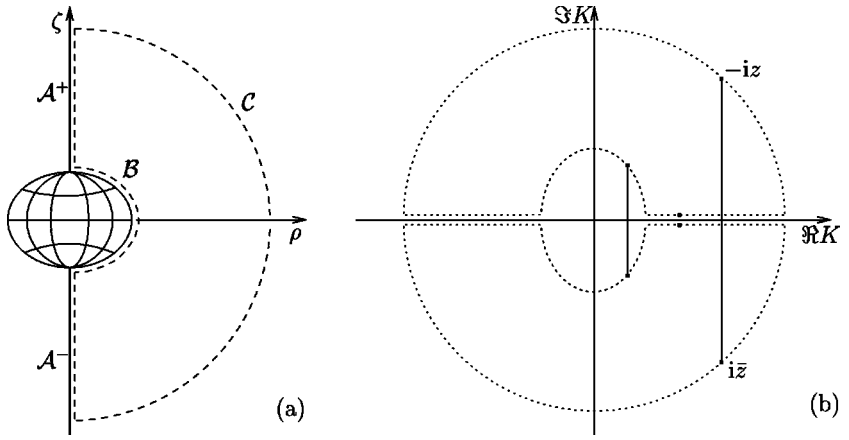

FIG. 1. (a) A slice $\phi=\text{const}$, $t=\text{const}$, (b) two-sheeted Riemann K-surface with branch points (dots) and two cuts (solid lines).[2]

on the inverse scattering method, opens an access to the not yet solved problem of the balance of two black holes and enables, in principle, the construction of black holes surrounded by dust rings (''AGN models'').

Another interesting domain of application for the inverse scattering method is colliding gravitational waves. This theory is out of the scope of our article. We refer to Ref. 1 and references therein.

The present work is mainly based on the Refs. 2 and 3, but it also contains substantial material not published before.

II. THE BOUNDARY VALUE PROBLEM

We consider a simply connected axisymmetric and stationary body and describe its exterior vacuum gravitational field in Weyl–Lewis–Papapetrou coordinates

$$ds^2=e^{-2U}[e^{2k}(d\rho^2+d\zeta^2)+\rho^2 d\phi^2]-e^{2U}(dt+a\,d\phi)^2, \tag{1}$$

where the ''Newtonian'' gravitational potential U, the ''gravitomagnetic'' potential a, and the ''superpotential'' k are functions of ρ and ζ alone. Figure 1(a) shows the boundaries of the vacuum region: $\mathcal{A}^{\pm}$ are the regular parts of the axis of symmetry ($\rho=0$), $\mathcal{B}$ is the surface of the body and $\mathcal{C}$ stands for spatial infinity. Later on, we will integrate along the dashed line and pick up information from the boundary values of the gravitational fields at $\mathcal{A}^{\pm}$, $\mathcal{B}$ and $\mathcal{C}$. The metric (1) allows an Abelian group of motions G_2 with the generators (Killing vectors)

$$\begin{aligned} &\xi^i=\delta^i_t, \quad \xi^i\xi_i<0 \quad \text{(stationarity)},\\ &\eta^i=\delta^i_\phi, \quad \eta^i\eta_i>0 \quad \text{(axisymmetry)}, \end{aligned} \tag{2}$$

where the Kronecker symbols δ^i_t and δ^i_ϕ indicate that ξ^i has only a t-component whereas η^i points in the azimuthal ϕ-direction (its trajectories are closed circles!). Obviously,

$$e^{2U}=-\xi^i\xi_i, \quad a=-e^{-2U}\eta_i\xi^i \tag{3}$$

is a coordinate-free representation of the two relativistic gravitational fields U (generalization of the Newtonian gravitational potential) and a (gravitomagnetic potential). To get a unique definition of U and a, we prescribe their behavior at infinity. Assuming that the space–time has to be flat at large distances from the body and can be described by a Minkowskian line element (1) in cylindrical coordinates, we are led to the boundary conditions

$$\mathcal{C}: \quad U\to 0, \quad a\to 0, \quad k\to 0. \tag{4}$$

Any linear transformation

$$t'=t, \quad \phi'=\phi-\omega t \tag{5}$$

introduces a frame of reference which rotates with a constant angular velocity ω with respect to that asymptotic Minkowski space.

To describe stationarity and axixymmetry in that rotating system one would use the Killing vectors

$$\tilde{\xi}^{i'}=\xi^{i'}+\omega\,\eta^{i'}, \quad \tilde{\eta}^{i'}=\eta^{i'} \tag{6}$$

instead of (2).

Regularity of the metric along $\mathcal{A}^{\pm}$ means

$$\mathcal{A}^{\pm}: \quad a=0, \quad k=0. \tag{7}$$

These conditions express the fact that $\mathcal{A}^{\pm}$ is an axis of symmetry ($a=0$) and ensure elementary flatness along the axis ($k=0$). The behavior of U and a at the surface $\mathcal{B}$ of the body depends on the physical nature of it. Rotating *perfect fluids* are characterized by a *four-velocity field* u^i consisting of a linear combination of the two Killing vectors,

$$u^i=\mathrm{e}^{-V}(\xi^i+\Omega\,\eta^i), \quad u^iu_i=-1, \tag{8}$$

where Ω is the angular velocity of the body, and an *invariant scalar pressure* p, which is, for rigid rotation,

$$\Omega=\Omega_0 \quad (\Omega_0 \text{ a constant}), \tag{9}$$

a function of V alone,

$$p=p(V), \tag{10}$$

as a consequence of the Euler equations. Along the surface of the body (if it exists) the pressure has to vanish, $p(V_0)=0$, i.e., V must be a constant along $\mathcal{B}$,

$$\mathcal{B}: \quad \mathrm{e}^{2V}\equiv-(\xi^i+\Omega_0\,\eta^i)(\xi_i+\Omega_0\,\eta_i)=\mathrm{e}^{2V_0}. \tag{11}$$

That is a further boundary condition. When identifying ω in (5) and Ω_0 we introduce a frame of reference co-rotating with the body and may interprete V as the co-rotating ''Newtonian'' potential, cf. (3) and (11). Interestingly, the event horizon $\mathcal{H}$ of a stationary (axisymmetric) black hole behaves like an ''ordinary'' perfect fluid surface (11). Namely, one can show that a linear combination of the two Killing vectors, $\xi^i+\Omega_{\mathrm{H}}\eta^i$, has a vanishing norm along $\mathcal{H}$,

$$\mathcal{H}: \quad \mathrm{e}^{2V}\equiv(\xi^i+\Omega_{\mathrm{H}}\eta^i)(\xi_i+\Omega_{\mathrm{H}}\eta_i)=0, \tag{12}$$

where Ω_{H} is the angular velocity of the horizon. Hence we may include black holes in our scheme, see Fig. 1(a), for $V_0\to-\infty$ and $\mathcal{H}\equiv\mathcal{B}$. It will turn out that (12) together with the correct positioning of the horizon $\mathcal{H}$ in Weyl–Lewis–Papapetrou coordinates together with the asymptotic behavior (4) of the (invariant) potentials (3) suffices for an explicit construction of the Kerr solution—thus providing a simple constructive uniqueness proof for stationary axisymmetric black holes. On the other hand, the condition (11) is not sufficient to calculate the gravitational field of rotating *perfect fluid balls*. However, in the disk of dust limit of such fluid configurations the

field equations themselves will provide the missing boundary condition along the surface $\mathcal{B}$ of the disk, see Ref. 3. Starting with that completed set of boundary conditions we will be able to construct the global solution for the rigidly rotating disk of dust.

III. THE FIELD EQUATIONS

The vacuum Einstein equations for the metric coefficients k, U, a are equivalent to the Ernst equation

$$(\Re f)\left(f_{,\rho\rho}+f_{,\zeta\zeta}+\frac{1}{\rho}f_{,\rho}\right)=f_{,\rho}^2+f_{,\zeta}^2 \tag{13}$$

for the complex function

$$f(\rho,\zeta)=\mathrm{e}^{2U}+\mathrm{i}b, \tag{14}$$

where b replaces a via

$$a_{,\rho}=\rho\mathrm{e}^{-4U}b_{,\zeta}, \quad a_{,\zeta}=-\rho\mathrm{e}^{-4U}b_{,\rho} \tag{15}$$

and k can be calculated from

$$k_{,\rho}=\rho[U_{,\rho}^2-U_{,\zeta}^2+\tfrac{1}{4}\mathrm{e}^{-4U}(b_{,\rho}^2-b_{,\zeta}^2)], \quad k_{,\zeta}=2\rho[U_{,\rho}U_{,\zeta}+\tfrac{1}{4}\mathrm{e}^{-4U}b_{,\rho}b_{,\zeta}]. \tag{16}$$

As a consequence of the Ernst equation (13), the integrability conditions $a_{,\rho\zeta}=a_{,\zeta\rho}$ and $k_{,\rho\zeta}=k_{,\zeta\rho}$ are automatically satisfied such that the metric functions a and k may be calculated via line integration from the Ernst potential f. Thus, it is sufficient to discuss the Ernst equation alone.

IV. THE LINEAR PROBLEM

The existence of a linear problem (LP) for the Ernst equation[4–9] is the cornerstone of our analysis since it provides a suitable instrument for tackling boundary value problems: the inverse scattering method (ISM). Here we will use a ''local'' version[10] of the linear problem,

$$\begin{aligned}\mathbf{\Phi}_{,z}&=\left\{\begin{pmatrix}B & 0\\ 0 & A\end{pmatrix}+\lambda\begin{pmatrix}0 & B\\ A & 0\end{pmatrix}\right\}\mathbf{\Phi},\\ \mathbf{\Phi}_{,\bar{z}}&=\left\{\begin{pmatrix}\bar{A} & 0\\ 0 & \bar{B}\end{pmatrix}+\frac{1}{\lambda}\begin{pmatrix}0 & \bar{A}\\ \bar{B} & 0\end{pmatrix}\right\}\mathbf{\Phi},\end{aligned} \tag{17}$$

where $\mathbf{\Phi}(z,\bar{z},\lambda)$ is a 2×2 matrix depending on the spectral parameter

$$\lambda=\sqrt{\frac{K-\mathrm{i}\bar{z}}{K+\mathrm{i}z}} \tag{18}$$

as well as on the complex coordinates $z=\rho+\mathrm{i}\zeta$, $\bar{z}=\rho-\mathrm{i}\zeta$, whereas A,B and the complex conjugate quantities $\bar{A}$, $\bar{B}$ are functions of $z,\bar{z}$ (or ρ, ζ) and do not depend on K. From the integrability condition and the formulas

$$\lambda_{,z}=\frac{\lambda}{4\rho}(\lambda^2-1), \quad \lambda_{,\bar{z}}=\frac{1}{4\rho\lambda}(\lambda^2-1) \tag{19}$$

it follows that a matrix polynomial in λ has to vanish. This yields the set of first order differential equations

$$A_{,\bar{z}}=A(\bar{B}-\bar{A})-\frac{1}{4\rho}(A+\bar{B}),\quad B_{,\bar{z}}=B(\bar{A}-\bar{B})-\frac{1}{4\rho}(B+\bar{A}). \tag{20}$$

The system has the ''first integrals''

$$A=\frac{f_{,z}}{f+\bar{f}},\quad B=\frac{\bar{f}_{,z}}{f+\bar{f}}. \tag{21}$$

Resubstituting A and B in the equations (20) one obtains the Ernst equation (13). Thus, the Ernst equation is the integrability condition of the LP (17). Vice versa, if f is a solution to the Ernst equation, the matrix $\mathbf{\Phi}$ calculated from (17) does not depend on the path of integration. The idea of the inverse scattering method (ISM) is to discuss $\mathbf{\Phi}$, for fixed but arbitrary values of $z,\bar{z}$, as a holomorphic function of λ (or K) and to calculate A,B and finally f afterwards. To obtain the desired information about the holomorphic structure in λ, we will integrate the linear system along the dashed line in Fig. 1(b) making use of the conditions (4), (7), (11) or (12). In this way, we will solve the *direct problem* of the ISM and obtain $\mathbf{\Phi}(z,\bar{z},\lambda)$ for $z,\bar{z}\in\mathcal{A}^{\pm},\mathcal{B},\mathcal{C}$. It turns out that the holomorphic structure remains unchanged by an extension of $z,\bar{z}$ off the axis of symmetry into the entire vacuum region such that one can construct functions $\mathbf{\Phi}$ with prescribed properties in λ from which one obtains the desired solution $f(z,\bar{z})$ everywhere in the vacuum region. This second step can be very technical and will, in general, lead to linear integral equations for $\mathbf{\Phi}$. In some circumstances, λ may be replaced by K. For this purpose, it may be helpful to discuss the mapping (18) of the two-sheeted Riemann surface of K onto the λ-plane for different values of ρ, ζ (or equivalently $z,\bar{z}$). Figure 1(b) shows the position of the branch points $K_{\mathrm{B}}=\mathrm{i}\bar{z}$, $\bar{K}_{\mathrm{B}}=-\mathrm{i}z$ for the marked path $\mathcal{A}^{+}\mathcal{C}\mathcal{A}^{-}\mathcal{B}$ of Fig. 1(a). It reflects the slice $\phi=\mathrm{const}$, $t=\mathrm{const}$ [Fig. 1(a)] and indicates, in particular, the position and shape of the body. Note that $\mathbf{\Phi}$ is not defined in the nonvacuum domain inside the circular contour around the origin.

Consider now a Riemann surface with confluent branch points $K_{\mathrm{B}}=\bar{K}_{\mathrm{B}}=\zeta\in\mathcal{A}^{+}$. Here λ degenerates and takes the values $\lambda=-1$ for K's in the lower sheet, say, and $\lambda=+1$ for K's in the upper sheet ($K\neq K_{\mathrm{B}}$).

We will now travel along the dashed line of Fig. 1(a) starting from and returning to any point $\rho=0$, $\zeta\in\mathcal{A}^{+}$. [In Fig. 1(b) this corresponds to the bold faced points on the real axis.] Note that $\lambda=-1$ for all K's ($K\neq\zeta$) in the lower and $\lambda=+1$ for all K's ($K\neq\zeta$) in the upper sheet of the Riemann K-surface belonging to axis values $\rho=0$, $\zeta\in\mathcal{A}^{\pm}$ [the corresponding branch points cling to either side of the real axis in Fig. 1(b)]. For $\rho,\zeta\in\mathcal{C}$, the cut between the branch points [e.g., right solid line in Fig. 1(b)] points over the entire K-surface and puts ''upper'' K values into the lower sheet and ''lower'' K values into the ''upper'' sheet. As a consequence, λ will change from ±1 to ∓1 between $\rho=0$, $\zeta=+\infty$ and $\rho=0$, $\zeta=-\infty$.[11] This ''exchange of sheets'' is important for the solution of the linear problem: The initial value $\mathbf{\Phi}(\rho_0,\zeta_0,\lambda)$ can (and must) be fixed only in *one* sheet of the K-surface. The dependence on K in the other sheet follows by integration of the LP (17) along a suitable path.[11]

We will divide the integration of the LP (17) along the closed dashed line of Fig. 1(a) into two steps:

(i) Integrating along $\mathcal{A}^{+}\mathcal{C}\mathcal{A}^{-}$: This step can be performed without particular knowledge about the body and leads to a ''*general* solution'' for $\mathbf{\Phi}$ on the regular parts $\mathcal{A}^{\pm}$ of the symmetry axis.

(ii) Integrating along $\mathcal{B}$: Here we confine ourselves to black holes and disks of dust.

V. SOLUTION OF THE DIRECT PROBLEM

A. Axis and infinity

Without loss of generality the matrix $\mathbf{\Phi}$ may be assumed to have the structure

$$\mathbf{\Phi}=\begin{pmatrix}\psi(\rho,\zeta,\lambda) & \psi(\rho,\zeta,-\lambda)\\ \chi(\rho,\zeta,\lambda) & -\chi(\rho,\zeta,-\lambda)\end{pmatrix} \tag{22}$$

together with

$$\overline{\psi\left(\rho,\zeta,\frac{1}{\bar{\lambda}}\right)}=\chi(\rho,\zeta,\lambda). \tag{23}$$

Note that both columns of $\mathbf{\Phi}$ are independent solutions of (17). The particular form of (22) is equivalent to

$$\mathbf{\Phi}(-\lambda)=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\mathbf{\Phi}(\lambda)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{24}$$

For $K\to\infty$ and $\lambda=-1$ the functions ψ, χ may be normalized by

$$\psi(\rho,\zeta,-1)=\chi(\rho,\zeta,-1)=1. \tag{25}$$

Finally, the solution to the Ernst equation can be read off at $\lambda=1$ $(K\to\infty)$,

$$f(\rho,\zeta)=\chi(\rho,\zeta,1),\quad (\overline{f(\rho,\zeta)}=\psi(\rho,\zeta,1)). \tag{26}$$

Remarkably enough, the Ernst equation retains its form in the frame of reference co-rotating with the body $(\omega=\Omega_0)$. This is a consequence of (3) and (6) and implies the existence of a linear problem (17) in the co-rotating system. In particular, the $\mathbf{\Phi}$-matrices of both systems of reference are connected by the relation

$$\mathbf{\Phi}'=\left[\begin{pmatrix}1+\Omega_0 a-\Omega_0\rho e^{-2U} & 0\\ 0 & 1+\Omega_0 a+\Omega_0\rho e^{-2U}\end{pmatrix}+i(K+iz)\Omega_0 e^{-2U}\begin{pmatrix}-1 & -\lambda\\ \lambda & 1\end{pmatrix}\right]\mathbf{\Phi}. \tag{27}$$

Henceforth, a prime marks ''co-rotating'' quantities. We can now realize our program and integrate the linear problem (17) along the part $\mathcal{A}^+\mathcal{C}\mathcal{A}^-$ of the dashed line in Fig. 1(a). Using (17) along $\mathcal{A}^\pm$ and (21) one finds for the axis values of $\mathbf{\Phi}$

$$\mathcal{A}^+:\quad \mathbf{\Phi}=\begin{pmatrix}\overline{f(\zeta)} & 1\\ f(\zeta) & -1\end{pmatrix}\begin{pmatrix}F(K) & 0\\ G(K) & 1\end{pmatrix}, \tag{28}$$

$$\mathcal{A}^-:\quad \mathbf{\Phi}=\begin{pmatrix}\overline{f(\zeta)} & 1\\ f(\zeta) & -1\end{pmatrix}\begin{pmatrix}1 & G(K)\\ 0 & F(K)\end{pmatrix}, \tag{29}$$

where $f(\zeta)=f(\rho=0,\zeta)$ is the axis value of the Ernst potential and $F(K),G(K)$ are integration ''constants'' depending on K alone. The particular form of (28) is due to the initial condition $\psi=\chi=1$ for some $\rho_0=0$, $\zeta=\zeta_0\in\mathcal{A}^+$, $\lambda=-1$ (K in the lower sheet), which fixes the second column of $\mathbf{\Phi}$ in (28), cf. (22). The first column corresponds to the upper $(\lambda=1)$ sheet and represents a general integral with the two integration ''constants'' $F(K),G(K)$ which cannot be specified here. Along $\mathcal{C}$, $\mathbf{\Phi}=\mathbf{\Phi}(K)$ does not depend on ρ and ζ, since A and B vanish, cf. (21). The ''exchange of sheets'' along $\mathcal{C}$, see Fig. 1(b), together with (24) leads to the particular form of $\mathbf{\Phi}$

on $\mathcal{A}^-$. The representations (28) and (29) describe the behavior of ψ and χ in both sheets. Nevertheless, one may wish to consider the matrix $\mathbf{\Phi}$ as a whole as a unique function of λ, which is therefore defined on both sheets of the K-surface. From this point of view, the equations (28) and (29) describe $\mathbf{\Phi}$ on one sheet only (say, on the upper sheet). Its values on the other (lower) sheet follow from (24).

Combining (28) and (29) with (27) we obtain the axis values in the co-rotating system,

$$\mathcal{A}^+: \quad \mathbf{\Phi}' = \left[\mathbf{1} + \mathrm{i}(K-\zeta)\Omega_0 \mathrm{e}^{-2U}\begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}\right] \times \left[\begin{pmatrix} \overline{f(\zeta)} & 1 \\ f(\zeta) & -1 \end{pmatrix}\begin{pmatrix} F(K) & 0 \\ G(K) & 1 \end{pmatrix}\right], \tag{30}$$

$$\mathcal{A}^-: \quad \mathbf{\Phi}' = \left[\mathbf{1} + \mathrm{i}(K-\zeta)\Omega_0 \mathrm{e}^{-2U}\begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}\right] \times \left[\begin{pmatrix} \overline{f(\zeta)} & 1 \\ f(\zeta) & -1 \end{pmatrix}\begin{pmatrix} 1 & G(K) \\ 0 & F(K) \end{pmatrix}\right], \tag{31}$$

where $\mathbf{1}$ ist the 2×2 unit matrix. At the branch points $K_\mathrm{B}=\zeta$ of K-surfaces belonging to axis values $\rho=0, \zeta \in \mathcal{A}^\pm$, ψ and χ must be unique, i.e.,

$$\mathcal{A}^+(K_\mathrm{B}=\zeta): \quad \mathbf{\Phi} = \begin{pmatrix} \psi & \psi \\ \chi & -\chi \end{pmatrix} = \begin{pmatrix} \overline{f(\zeta)} & 1 \\ f(\zeta) & -1 \end{pmatrix}\begin{pmatrix} F(\zeta) & 0 \\ G(\zeta) & 1 \end{pmatrix}, \tag{32}$$

$$\mathcal{A}^-(K_\mathrm{B}=\zeta): \quad \mathbf{\Phi} = \begin{pmatrix} \psi & \psi \\ \chi & -\chi \end{pmatrix} = \begin{pmatrix} \overline{f(\zeta)} & 1 \\ f(\zeta) & -1 \end{pmatrix}\begin{pmatrix} 1 & G(\zeta) \\ 0 & F(\zeta) \end{pmatrix}, \tag{33}$$

whence

$$\mathcal{A}^+: \quad F(\zeta) = \frac{2}{f(\zeta)+\overline{f(\zeta)}}, \quad G(\zeta) = \frac{f(\zeta)-\overline{f(\zeta)}}{f(\zeta)+\overline{f(\zeta)}}, \tag{34}$$

$$\mathcal{A}^-: \quad F(\zeta) = \frac{2\, f(\zeta)\overline{f(\zeta)}}{\overline{f(\zeta)}+f(\zeta)}, \quad G(\zeta) = \frac{\overline{f(\zeta)}-f(\zeta)}{f(\zeta)+\overline{f(\zeta)}}. \tag{35}$$

Thus, $F(K)$ and $G(K)$ consist in a unique way of analytic continuations of the real and imaginary parts of the axis values of the Ernst potential $f(\zeta)$. Vice versa, $f(\zeta)$ follows from $F(K), G(K)$ for $K=\zeta$. Interestingly, the determinants of $\mathbf{\Phi}$ and $\mathbf{\Phi}'$ can be expressed in terms of $\Re f$, $\Re f'$ and $F(K)$. From (17) $[\mathrm{Tr}\mathbf{\Phi}_{,z}\mathbf{\Phi}^{-1} = (\ln\det\mathbf{\Phi})_{,z}]$, (21) and (28)–(31), we have

$$\det\mathbf{\Phi} = -2\mathrm{e}^{2U}F(K), \quad \det\mathbf{\Phi}' = -2\mathrm{e}^{2V}F(K), \tag{36}$$

where $\mathrm{e}^{2U}=\Re f$ and $\mathrm{e}^{2V}=\Re f'$ $[U=U(\rho,\zeta), V=V(\rho,\zeta)]$.

We may now interpret the result of (30)–(35) of the integration of the LP along $\mathcal{A}^+\mathcal{C}\mathcal{A}^-$: On the regular parts $\mathcal{A}^\pm$ of the symmetry axis, $\mathbf{\Phi}$ and $\mathbf{\Phi}'$ can explicitly be expressed in terms of the axis values $f(\zeta)$ of the Ernst potential and its analytic continuations $F(K), G(K)$. To calculate $f(\zeta)$ one needs boundary values on $\mathcal{B}$. Accordingly, the integration along $\mathcal{B}$ depends on the physical nature of the rotating body and can be performed in particular cases only. In the next section we will discuss black holes and rigidly rotating disks of dust.

B. Surface

1. One black hole

We identify the surface $\mathcal{B}$ with the horizon $\mathcal{H}$. In Weyl coordinates, the event horizon $\mathcal{H}$ of a single black hole covers the domain,[12]

$$\mathcal{H}: \quad \rho=0, \quad K_1 \geqslant \zeta \geqslant K_2. \tag{37}$$

[In Fig. 1(a), the surface $\mathcal{B}$ degenerates to a "straight line" connecting the regular parts $\mathcal{A}^-, \mathcal{A}^+$ of the axis of symmetry.] Along $\mathcal{H}$, e^{2V} has to vanish [see (12)],

$$\mathcal{H}: \quad e^{2V} \equiv (\xi^i + \Omega_0 \eta^i)(\xi_i + \Omega_0 \eta_i) = 0 \quad (\Omega_0 = \Omega_H). \tag{38}$$

Because of

$$e^{2V} = e^{2U}([1 + \Omega_0 a]^2 - \Omega_0^2 \rho^2 e^{-4U}), \tag{39}$$

cf. (3), this implies

$$\mathcal{H}: \quad 1 + \Omega_0 a = 0. \tag{40}$$

$\mathbf{\Phi}$ and $\mathbf{\Phi}'$ can now be calculated along the horizon $\mathcal{H}$. From (17), (37), (38), (40) and (27) we obtain

$$\mathbf{\Phi} = \begin{pmatrix} \overline{f(\zeta)} & 1 \\ f(\zeta) & -1 \end{pmatrix} \begin{pmatrix} U(K) & V(K) \\ W(K) & X(K) \end{pmatrix},$$

$$\mathcal{H}: \tag{41}$$

$$\mathbf{\Phi}' = 2i\Omega_0 (K - \zeta) \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} U(K) & V(K) \\ W(K) & X(K) \end{pmatrix}.$$

The Ernst equations have to hold at K_1 and K_2 too. Hence, $\mathbf{\Phi}$ and $\mathbf{\Phi}'$ must be continuous in K_1 and K_2. Considering (28)–(31) and (41), we are led to the conditions

$$\begin{aligned} \begin{pmatrix} f_1 & -1 \\ f_1 + 2i\Omega_0(K - K_1) & -1 \end{pmatrix} \begin{pmatrix} F & 0 \\ G & 1 \end{pmatrix} &= \begin{pmatrix} f_1 & -1 \\ 2i\Omega_0(K - K_1) & 0 \end{pmatrix} \begin{pmatrix} U & V \\ W & X \end{pmatrix}, \\ \begin{pmatrix} f_2 & -1 \\ f_2 + 2i\Omega_0(K - K_2) & -1 \end{pmatrix} \begin{pmatrix} 1 & G \\ 0 & F \end{pmatrix} &= \begin{pmatrix} f_2 & -1 \\ 2i\Omega_0(K - K_2) & 0 \end{pmatrix} \begin{pmatrix} U & V \\ W & X \end{pmatrix}, \end{aligned} \tag{42}$$

where $f_1 = f(\zeta = K_1)$ and $f_2 = f(\zeta = K_2)$. Note that f_1 and f_2 are imaginary, see (36).

Eliminating the $UVWX$ matrix, we obtain

$$\mathcal{N} = \left(\mathbf{1} + \frac{\mathbf{F}_1}{2i\Omega_0(K - K_1)} \right) \left(\mathbf{1} + \frac{\mathbf{F}_2}{2i\Omega_0(K - K_2)} \right), \tag{43}$$

where

$$\mathbf{F}_1 = \begin{pmatrix} -f_1 & 1 \\ -f_1^2 & f_1 \end{pmatrix}, \quad \mathbf{F}_2 = \begin{pmatrix} f_2 & -1 \\ f_2^2 & -f_2 \end{pmatrix}, \tag{44}$$

$$\mathcal{N} = \begin{pmatrix} F & -G \\ G & (1 - G^2)/F \end{pmatrix}. \tag{45}$$

Obviously, the elements of $\mathcal{N}$ are regular everywhere in the complex K-plane with the exception of the two simple poles at K_1 and K_2 ($\Im K_1 = 0 = \Im K_2$). The sum of the off-diagonal elements in (45) must be zero. This requirement leads to the constraints

$$f_1 = -f_2, \quad \Omega_0 = \frac{i f_1 (1 + f_1^2)}{(K_1 - K_2)(1 - f_1^2)}. \tag{46}$$

$F(K)$ and $G(K)$ take the form

$$F(K)=\frac{4\Omega_0^2(K^2-K_1^2)+4\mathrm{i}\Omega_0 f_1 K-2f_1^2}{4\Omega_0^2(K^2-K_1^2)},\quad G(K)=\frac{4\mathrm{i}\Omega_0 K_1+2f_1}{4\Omega_0^2(K^2-K_1^2)}. \tag{47}$$

Here we have chosen $K_1=-K_2$, i.e., we have set the horizon in a symmetric position in the ρ, ζ-plane. Making use of (34) and (35) and eliminating Ω_0 by the second constraint equation we obtain the axis potential

$$\mathcal{A}^+:\quad f=\frac{\zeta(1+f_1^2)+(f_1^2-1+2f_1)K_1}{\zeta(1+f_1^2)+(1-f_1^2+2f_1)K_1}. \tag{48}$$

It can be useful to introduce the multipole moments mass M and angular momentum J by an asymptotic expansion of f,

$$M=\frac{1-f_1^2}{1+f_1^2}K_1,\quad \frac{J}{M}=\alpha=\frac{2\mathrm{i}f_1K_1}{1+f_1^2}, \tag{49}$$

and to replace f_1, K_1 in (47), (48) and (46):

$$F(K)=\frac{(K+M)^2+\alpha^2}{K^2+\alpha^2-M^2},\quad G(K)=\frac{2\mathrm{i}M\alpha}{K^2+\alpha^2-M^2}. \tag{50}$$

To represent $f(\zeta)$, a simplifying parametrization is advisible,

$$f_1=\mathrm{i}\tan\varphi/2,\quad \alpha=-M\sin\varphi,\quad K_1=-K_2=\sqrt{M^2-\alpha^2}=M\cos\varphi,\quad \varphi=\overline{\varphi}. \tag{51}$$

This yields

$$\mathcal{A}^+:\quad f=\frac{(\zeta-M)+\mathrm{i}M\sin\varphi}{(\zeta+M)+\mathrm{i}M\sin\varphi}. \tag{52}$$

Finally, the second constraint equation (46) becomes the well-known equation of state of black hole thermodynamics,

$$2M\Omega_0=\frac{M}{\alpha}-\sqrt{\frac{M^2}{\alpha^2}-1}, \tag{53}$$

connecting the angular velocity of the horizon with mass and angular momentum.

2. Two aligned black holes

The same procedure can be used to tackle the balance problem for two black holes. The question is whether the spin-spin repulsion of two aligned stationary black holes can compensate their gravitational attraction.

Here we have two horizons $\mathcal{H}_1$ and $\mathcal{H}_2$,

$$\mathcal{H}_1:\quad \rho=0,\ K_1\geqslant\zeta\geqslant K_2,\quad \mathcal{H}_2:\rho=0,\ K_3\geqslant\zeta\geqslant K_4, \tag{54}$$

separated by a piece of the regular symmetry axis $\mathcal{A}^0$,

$$\mathcal{A}^0:\quad K_2\geqslant\zeta\geqslant K_3. \tag{55}$$

As a characteristic black hole property, the norm of the Killing vectors of the co-rotating frameworks has to vanish along the horizons,

$$\mathcal{H}_1: \quad (\xi_i+\Omega_0^1\eta_i)(\xi^i+\Omega_0^1\eta^i)=0, \quad \mathcal{H}_2: \quad (\xi_i+\Omega_0^2\eta_i)(\xi^i+\Omega_0^2\eta^i)=0, \tag{56}$$

where Ω_0^1,Ω_0^2 are the constant angular velocities of the respective horizons.

Following the arguments for one black hole, we arrive at[13]

$$\mathcal{N}=\prod_{i=1}^{4}\left(\mathbf{1}+\frac{\mathbf{F}_i}{2\mathrm{i}\Omega_i(K-K_i)}\right), \tag{57}$$

where $\Omega_1=\Omega_2=\Omega_0^2$, $\Omega_3=\Omega_4=\Omega_0^2$ and

$$\mathbf{F}_i=(-1)^i\begin{pmatrix} f_i & -1 \\ f_i^2 & -f_i \end{pmatrix}, \tag{58}$$

whence

$$\begin{aligned} F(K)&=\frac{p_4(K)}{(K-K_1)(K-K_2)(K-K_3)(K-K_4)}, \\ G(K)&=\frac{p_2(K)}{(K-K_1)(K-K_2)(K-K_3)(K-K_4)}, \end{aligned} \tag{59}$$

where $p_4(K)$ and $p_2(K)$ are polynomials in K of the indicated orders. From (59) together with (34) and (35) we may read off the axis values of the Ernst potential. For the upper axis we obtain the structure

$$\mathcal{A}^+: \quad f(\zeta)=\frac{q_2(\zeta)}{Q_2(\zeta)}. \tag{60}$$

We need not use the representation of the explicit form of the second order polynomials $q_2(\zeta),Q_2(\zeta)$ and of the constraints resulting from $G=\mathcal{N}_{21}=-\mathcal{N}_{12}$. Namely, from the fact that $f(\zeta)$ is a quotient of polynomials of the same (even) order, it is clear that the desired two black hole solution can be generated by a Bäcklund transformation (in our case by a twofold Bäcklund transformation) from the Minkowski space. (Note that the axis values of the Ernst potential determine solutions of the Ernst equation in a unique way.)

The four constraints $\mathcal{N}_{21}=-\mathcal{N}_{12}$ ensure that the constants K_i, $f_i=-\overline{f_i}$ $(i=1,\ldots,4)$, Ω_0^1,Ω_0^2 may be expressed by two position parameters and the masses and angular momenta of the two black holes.

The Bäcklund generated solution belonging to (60) known as the ''double Kerr solution'' was intensively discussed by several authors.[14,15] It turned out that there are necessarily struts between the ''horizons.'' Since we have shown, by solving the boundary value problem, that Bäcklund generated solutions are the *only* candidates to describe aligned balanced black holes, we may now assert that black holes cannot be balanced at all.

3. Rigidly rotating disks of dust

Disks of dust can be considered to be extremely flattened spheroids [Fig. 2(a)] consisting of perfect fluid matter.[3] One can show that, for rigidly rotating dust, the boundary conditions (4) and (11) have to be complemented by the condition $b'=\mathfrak{I}f'=0$ on the disk ($\mathcal{B}$). This condition follows from the Einstein equations as a transition condition from a divergence-free part of those equations via Gauss's theorem.[3] Thus we have to take into consideration

$$\mathcal{A}^{\pm}: \text{ regularity of } f, \quad \mathcal{B}: \ f'=\mathrm{e}^{2V_0}, \quad \mathcal{C}: \ f\to 1, \tag{61}$$

see Fig. 2(a). On the disk, the linear problem of the co-rotating system of reference takes the form

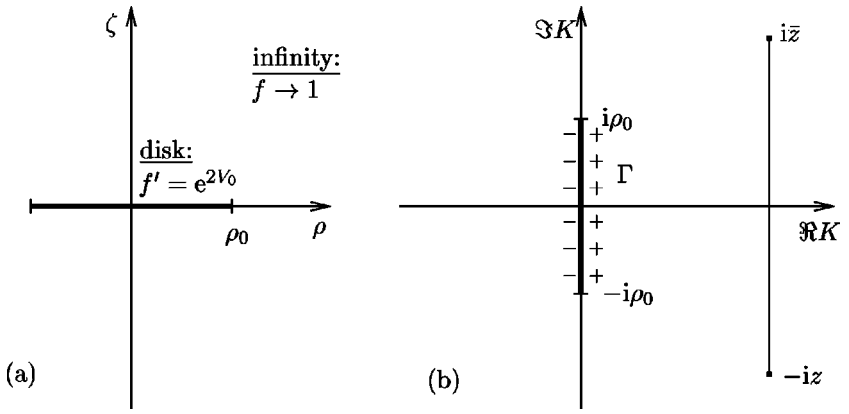

FIG. 2. (a) Boundary value problem for the rotating disk of dust, (b) two-sheeted K-surface of the rotating disk with branch points at $-iz, i\bar{z}$.[2]

$$\mathcal{B}: \quad \mathbf{\Phi}'_{,\rho} = -\frac{\rho}{\sqrt{K^2+\rho^2}(f'+\overline{f'})}\begin{pmatrix} 0 & \overline{f'}_{,\zeta} \\ f'_{,\zeta} & 0 \end{pmatrix}\mathbf{\Phi}', \tag{62}$$

where $\mathbf{\Phi}'$ and f' are the "co-rotating" $\mathbf{\Phi}$-matrix and the "co-rotating" Ernst potential on the disk. This relation must be discussed under the "boundary conditions"

$$\mathbf{\Phi}'(\rho=0,\zeta=0^+,\lambda)|_{\mathcal{B}} = \mathbf{\Phi}'(\rho=0,\zeta=0^+,\lambda)|_{\mathcal{A}^+},$$

cf. (30) and

$$\mathbf{\Phi}'(\rho=0,\zeta=0^-,\lambda)|_{\mathcal{B}} = \mathbf{\Phi}'(\rho=0,\zeta=0^-,\lambda)|_{\mathcal{A}^-},$$

cf. (31).

Again, this discussion allows the construction of $F(K)$ and $G(K)$ and, via (34) and (35), the construction of the axis values $f(\zeta)$ of the Ernst potential. We first take advantage of the symmetry of the problem which implies $\overline{f(\rho,\zeta)} = f(\rho,-\zeta)$ and connects the ζ-derivatives of f' above ($\zeta = 0^+$) and below ($\zeta = 0^-$) the disk

$$\mathcal{B}: \quad \overline{f'}_{,\zeta}|_{\zeta=0^+} = -f'_{,\zeta}|_{\zeta=0^-}. \tag{63}$$

As a consequence, the LP (62) connects the matrix $\overset{\mathrm{A}}{\mathbf{\Phi}}$ above the disk, $\overset{\mathrm{A}}{\mathbf{\Phi}} = \mathbf{\Phi}'(\rho,\zeta=0^+,K)$, with the matrix $\overset{\mathrm{B}}{\mathbf{\Phi}}$ below the disk, $\overset{\mathrm{B}}{\mathbf{\Phi}} = \mathbf{\Phi}'(\rho,\zeta=0^-,K)$,

$$\mathcal{B}: \quad \overset{\mathrm{A}}{\mathbf{\Phi}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\overset{\mathrm{B}}{\mathbf{\Phi}}\mathbf{H}(K), \tag{64}$$

where the matrix $\mathbf{H}(K)$ (the "integration constant") does not depend on $\rho \in \mathcal{B}$. At the rim of the disk we have

$$\overset{\mathrm{A}}{\mathbf{\Phi}}(\rho_0,0,K) = \overset{\mathrm{B}}{\mathbf{\Phi}}(\rho_0,0,K) = \overset{\mathrm{r}}{\mathbf{\Phi}}. \tag{65}$$

Because of (64), the rim matrix $\overset{\mathrm{r}}{\mathbf{\Phi}}{}^{-1}\left(\begin{smallmatrix}0 & -1\\ 1 & 0\end{smallmatrix}\right)\overset{\mathrm{r}}{\mathbf{\Phi}}$ can be expressed in terms of $\overset{\mathrm{A}}{\mathbf{\Phi}}=\mathbf{\Phi}'(\rho,\zeta=0^+,K)$, $\overset{\mathrm{B}}{\mathbf{\Phi}}=\mathbf{\Phi}'(\rho,\zeta=0^-,K)$. Note that $\mathbf{\Phi}$ is considered to be a holomorphic function of λ and therefore a function living on the two-sheeted Riemann K-surface of Fig. 1(b). Hence we have to discuss the rim matrix as a function of K on both sheets.

Any $\mathbf{\Phi}$ multiplied from the right by a matrix function of K is again a solution of the LP. The discussion of the rim matrix simplifies after the following redefinition

$$\mathcal{R}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}\overset{\mathrm{r}}{\mathbf{\Phi}}{}^{-1}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\overset{\mathrm{r}}{\mathbf{\Phi}}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}^{-1}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}^{-1}. \tag{66}$$

Using (30) and (31) we obtain

$$\mathcal{R}=\begin{cases}\mathrm{e}^{2V_0}\mathcal{M}\mathcal{S}^{-1} & \text{on the upper sheet,}\\ -\mathrm{e}^{2V_0}\mathcal{S}^{-1}\mathcal{M} & \text{on the lower sheet,}\end{cases} \tag{67}$$

where

$$\mathcal{M}=\begin{pmatrix}G(K) & (G^2-1)/F\\ -F(K) & -G(K)\end{pmatrix},\quad \mathcal{S}=\begin{pmatrix}f_0\overline{f_0}-4\Omega_0^2K^2 & \mathrm{i}b_0+2\mathrm{i}\Omega_0K\\ \mathrm{i}b_0-2\mathrm{i}\Omega_0K & -1\end{pmatrix} \tag{68}$$

and

$$f_0=\mathrm{e}^{2V_0}+\mathrm{i}b_0=f(\zeta=0^+). \tag{69}$$

Note that $\mathcal{M}=\left(\begin{smallmatrix}0 & -1\\ 1 & 0\end{smallmatrix}\right)\mathcal{N}\left(\begin{smallmatrix}-1 & 0\\ 0 & 1\end{smallmatrix}\right)$.

Obviously, $\operatorname{Tr}\mathcal{R}=\operatorname{Tr}\mathcal{R}^{-1}=0$ and $\mathcal{M}^2=\mathbf{1}$, whence

$$\operatorname{Tr}\mathcal{M}\mathcal{S}^{-1}=\operatorname{Tr}\mathcal{S}\mathcal{M}=0. \tag{70}$$

This relation interlinks $F(K)$ and $G(K)$ and, because of (34) and (35), real and imaginary parts of the axis values $f(\zeta)$ of the Ernst potential.[16,17]

We next wish to determine $F(K)$ and $G(K)$ which in turn determine $f(\zeta)$. To this end we consider $\mathbf{\Phi}(\rho,\zeta,\lambda)$, for fixed coordinates ρ, ζ as a function of λ. We have already used the initial conditions $\psi=\chi=1$ for some $\rho=\rho_0=0$, $\zeta=\zeta_0\in\mathcal{A}^+$ prescribed in one sheet ($\lambda=-1$) of the K-plane. In principle the behavior of $\mathbf{\Phi}$ in both sheets and at all points in the ρ, ζ-plane can be calculated by integrating the LP along a suitable path. However, the coefficients $A(\rho,\zeta)$, $B(\rho,\zeta)$ in the LP (17) are not explicitly known. Nevertheless, their regular behavior outside the disk together with the boundary values on the disk, cf. (61), provides us with defining properties for $\mathbf{\Phi}$. One of them may be taken from Fig. 1(b) together with Fig. 2(b): Since the domain of the disk, $0\leqslant\rho\leqslant\rho_0$, $\zeta=0^{\pm}$, is a nonvacuum domain, where the LP fails, $\mathbf{\Phi}$ at the branch point pairs $K=\mathrm{i}\rho+0^{\pm},-\mathrm{i}\rho+0^{\pm}$, $0\leqslant\rho\leqslant\rho_0$, cannot "pass" through the contour(s) $\Gamma:\Re K=0,-\rho_0\leqslant\Im K\leqslant\rho_0$, i.e., $\mathbf{\Phi}$ has a well-defined jump between opposite points along the contour(s) Γ, see Fig. 2. A careful discussion would show that $\mathbf{\Phi}(\rho,\zeta,\lambda)$, for fixed coordinate values ρ, ζ outside the disk ($\rho,\zeta\notin\mathcal{B}$), is a regular function in λ outside Γ and jumps along Γ, i.e., $\mathbf{\Phi}$ satisfies a (regular) Riemann–Hilbert problem.

Consider now the jump $\mathbf{\Phi}_+^{-1}\mathbf{\Phi}_-$, where the signs indicate the two sides of Γ, cf. Fig. 2(b). The LP tells us that $\mathbf{\Phi}_+^{-1}\mathbf{\Phi}_-$ does not depend on the coordinates and is therefore a function $\mathcal{D}$ of the contour alone,

$$\begin{aligned}\mathbf{\Phi}_+^{-1}\mathbf{\Phi}_-&=\mathcal{D}_{\mathrm{u}}(K),\quad K\in\Gamma_{\mathrm{u}},\\ \mathbf{\Phi}_+^{-1}\mathbf{\Phi}_-&=\mathcal{D}_{\mathrm{l}}(K),\quad K\in\Gamma_{\mathrm{l}},\end{aligned} \tag{71}$$

where u marks the upper and l the lower sheet. Since the jump contours Γ_u, Γ_l and the jump matrices $\mathcal{D}_u$, $\mathcal{D}_l$ are the same for all values of ρ, ζ (i.e., for all Riemann surfaces with different branch points), we may express $\mathcal{D}_u$ and $\mathcal{D}_l$ in terms of the axis values of $\mathbf{\Phi}$,

$$\mathcal{D}_u(K)=\begin{pmatrix} F_+ & 0 \\ G_+ & 1 \end{pmatrix}^{-1}\begin{pmatrix} F_- & 0 \\ G_- & 1 \end{pmatrix}, \quad K\in\Gamma_u. \tag{72}$$

A similar relation for $\mathcal{D}_l$ may be obtained via (24). As a consequence of (71) and (72) the matrix $\mathbf{\Phi}\left(\begin{smallmatrix} F & 0 \\ G & 1 \end{smallmatrix}\right)^{-1}$ does not jump along Γ_u. Because of (27) the same holds for $\mathbf{\Phi}'\left(\begin{smallmatrix} F & 0 \\ G & 1 \end{smallmatrix}\right)^{-1}$ and, finally, for $\mathcal{R}$ as defined in (66). Consider now the Riemann K-surface of the disk rim $\rho=\rho_0$, $\zeta=0$. The cut between the branch points $K_B=\pm i\rho_0$ coincides with the contour Γ_u, Γ_l which are on the two "bridges" connecting crosswise the upper with the lower sheet. Since $\mathcal{R}$ does not jump on Γ_u, we have, according to (67), $(\mathcal{M}\mathcal{S}^{-1})_-=-(\mathcal{S}^{-1}\mathcal{M})_+$. Though $\mathcal{R}$ does not jump, F and G do jump, cf. (72). Note that $F(K)$ and $G(K)$ are unique functions of K. Hence, there is only one contour $\Gamma:\Re K=0,-\rho_0\leqslant\Im K\leqslant\rho_0$, where $\mathcal{M}$ [with the elements $F(K)$, $G(K)$] does jump. Since $\mathbf{\Phi}$ is analytic outside Γ_u,Γ_l, the matrix $\mathcal{M}$ must be analytic outside Γ. Thus we obtain $F(K)$ and $G(K)$ from the Riemann–Hilbert problem,

$$\begin{aligned} &K\in\Gamma: \quad \mathcal{S}\mathcal{M}_-=-\mathcal{M}_+\mathcal{S}, \\ &K\notin\Gamma: \quad \mathcal{M}(K) \text{ analytic in } K, \end{aligned} \tag{73}$$

$\mathcal{S}$ and $\mathcal{M}$ as in (68). (Note that the elements of $\mathcal{S}$, which are polynomials, and the elements of $\mathcal{S}^{-1}$, which are rational functions in K, do not jump along Γ.) There is no jump at the end points of the contour $K=\pm i\rho_0$, $\mathcal{M}(\pm i\rho_0)_-=\mathcal{M}(\pm i\rho_0)_+$. As a consequence, one obtains $\operatorname{Tr}\mathcal{S}(\pm i\rho_0)=0$, i.e., the parameter relation

$$f_0\overline{f_0}+4\Omega_0^2\rho_0^2=1. \tag{74}$$

It turns out that the Riemann–Hilbert problem (73) has a unique solution $\mathcal{M}(K)$ in the parameter region

$$0\leqslant\mu=2\Omega_0^2e^{-2V_0}\rho_0^2<\mu_0=4.629\,661\,84\ldots\,. \tag{75}$$

An important step on the way to this solution is the diagonalization of $\mathcal{S}$. Finally, one obtains $F(K)$, $G(K)$ and the axis values of the Ernst potential $f(\zeta)$ in terms of elliptic theta functions. We need not go this road. As we shall see in the next section, we can use the Riemann–Hilbert problem (73) to formulate a more general Riemann–Hilbert problem which will yield the complete disk of dust solution in terms of hyperelliptic theta functions.

VI. ERNST POTENTIAL EVERYWHERE

A. Kerr solution

In the preceding section, we analyzed the axis values of the Ernst potential. We will now construct the complete solutions $f(\rho,\zeta)$ of our boundary value problems from the information about the behavior along the axis of symmetry gained by the discussion of the direct problem.

There is, of course, no question that the discussion of the black hole case in Sec. V B 1 will lead to the famous Kerr solution [in Weyl coordinates (1)]. The point made here is that this solution describing the stationary rotating black hole can be derived from a boundary value problem.

To achieve our goal it is useful to exploit the gauge freedom of multiplying $\mathbf{\Phi}$ from the right by an arbitrary matrix funktion of K. The transformation

$$\tilde{\mathbf{\Phi}}=\frac{K^2-\alpha^2-M^2}{K[(K+M)^2+\alpha^2]}\mathbf{\Phi}\begin{pmatrix}K+m & \mathrm{i}\alpha\\ \mathrm{i}\alpha & K+m\end{pmatrix} \tag{76}$$

preserves the properties (22)–(25) and enables the calculation of f via (26). Because of (36), (50), (28) and (18), the determinant of $\tilde{\mathbf{\Phi}}$ becomes

$$\det\tilde{\mathbf{\Phi}}=\gamma\frac{(K+\mathrm{i}z)^2}{K^2}(\lambda^2-\lambda_1^2)(\lambda^2-\lambda_2^2),\quad \gamma=\gamma(\rho,\zeta)=-\frac{2\mathrm{e}^{2U(\rho,\zeta)}}{(1-\lambda_1^2)(1-\lambda_2^2)}, \tag{77}$$

where

$$\lambda_i^2=\frac{K_i-\mathrm{i}\overline{z}}{K_i+\mathrm{i}z}\quad (i=1,2). \tag{78}$$

This form of the determinant together with the axis values of $\tilde{\mathbf{\Phi}}$ tells us that $\tilde{\mathbf{\Phi}}$ must be a quadratic matrix polynomial of λ,

$$\tilde{\mathbf{\Phi}}=\frac{K+\mathrm{i}z}{K}(\mathbf{C}+\mathbf{D}\lambda+\mathbf{E}\lambda^2), \tag{79}$$

where the 2×2 matrices $\mathbf{C}$, $\mathbf{D}$, $\mathbf{E}$ are functions of ρ, ζ alone. It can be shown[18] that $\tilde{\mathbf{\Phi}}$ with (77) satisfies the LP. (It is a Bäcklund transformation of the trivial solution $f=1$.)

According to (77), $\tilde{\mathbf{\Phi}}(\rho,\zeta,\lambda_i)$ $(i=1,2)$ must have a null eigenvector b_i in the zeros λ_i,

$$\tilde{\mathbf{\Phi}}(\rho,\zeta,\lambda_i)b_i=0\quad (i=1,2). \tag{80}$$

From the LP it follows that the elements of b_i have to be constants. Hence, the quotient

$$\frac{\tilde{\chi}(\rho,\zeta,\lambda)}{\tilde{\chi}(\rho,\zeta,-\lambda)}=-\frac{C_{21}+D_{21}\lambda+E_{21}\lambda^2}{C_{21}-D_{21}\lambda+E_{21}\lambda^2}, \tag{81}$$

where the coefficients are elements of the matrices $\mathbf{C}$, $\mathbf{D}$, $\mathbf{E}$ must be a constant at $\lambda=\lambda_i$ $(i=1,2)$. The values of the two constants $(i=1,2)$ can be read off from the axis values of $\tilde{\mathbf{\Phi}}$ resulting from (81) together with (28), (29), (50), (51) and (76),

$$\frac{\tilde{\chi}(\lambda_1)}{\tilde{\chi}(-\lambda_1)}=-\mathrm{i}\cot\frac{\varphi}{2},\quad \frac{\tilde{\chi}(\lambda_2)}{\tilde{\chi}(-\lambda_2)}=\mathrm{i}\cot\frac{\varphi}{2}. \tag{82}$$

Note that $\tilde{\chi}(-1)=1$ implies

$$C_{21}-D_{21}+E_{21}=1. \tag{83}$$

These three conditions fix the coefficients C_{21}, D_{21}, E_{21} via a linear algebraic system. Finally, we obtain the Ernst potential everywhere from $f=\tilde{\chi}(1)/\tilde{\chi}(-1)$,

$$f(\rho,\zeta)=\frac{r_1\mathrm{e}^{\mathrm{i}\varphi}+r_2\mathrm{e}^{\mathrm{i}\varphi}-2M\cos\varphi}{r_1\mathrm{e}^{\mathrm{i}\varphi}+r_2\mathrm{e}^{\mathrm{i}\varphi}+2M\cos\varphi}, \tag{84}$$

where

$$r_i^2=(K_i-\zeta)^2+\rho^2\quad (i=1,2)$$

with $K_1=-K_2$ and φ as in (51). This is the Ernst potential f of the Kerr solution in Weyl–Papapetrou coordinates. By virtue of (15) and (16), this potential determines all metric coefficients in the line element (1).

B. Disk of dust solution

In order to construct the $\mathbf{\Phi}$-matrix for arbitrary values of ρ, ζ and λ, let us return to the Riemann–Hilbert problem (73). As we have seen, the matrix $\mathbf{\Phi}\left(\begin{smallmatrix}F & 0\\ G & 1\end{smallmatrix}\right)^{-1}$ does not jump along Γ_u. Analogously, $\mathbf{\Phi}\left(\begin{smallmatrix}1 & G\\ 0 & F\end{smallmatrix}\right)^{-1}$ does not jump along Γ_l. The images Γ_λ of Γ_u and $\Gamma_{-\lambda}$ of Γ_l inherit these properties, which are essential to the following deductions.

To formulate a Riemann-Hilbert problem in the λ-plane, we define two matrices,

$$\begin{aligned}\mathcal{L}:&=\mathbf{\Phi}\begin{pmatrix}1 & G\\ 0 & F\end{pmatrix}^{-1}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\mathcal{M}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & G\\ 0 & F\end{pmatrix}\mathbf{\Phi}^{-1}\\ &=\mathbf{\Phi}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}^{-1}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\mathcal{M}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}\mathbf{\Phi}^{-1}\\ &=\mathbf{\Phi}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\mathbf{\Phi}^{-1},\end{aligned}\tag{85}$$

$$\begin{aligned}\mathcal{Q}:&=\mathrm{e}^{-2V_0}\mathbf{\Phi}\begin{pmatrix}1 & G\\ 0 & F\end{pmatrix}^{-1}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}(\mathcal{S}+w\mathbf{1})\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & G\\ 0 & F\end{pmatrix}\mathbf{\Phi}^{-1}\\ &=\mathrm{e}^{-2V_0}\mathbf{\Phi}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}^{-1}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}(\mathcal{S}+w\mathbf{1})\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}F & 0\\ G & 1\end{pmatrix}\mathbf{\Phi}^{-1},\end{aligned}\tag{86}$$

where

$$w=-\tfrac{1}{2}\mathrm{Tr}\,\mathcal{S}=2\Omega_0^2(K^2+\rho_0^2).$$

Here we have made use of the parameter relation (74). Since $\mathcal{S}$ and w are polynomials in K and therefore rational functions in λ, the matrix $\mathcal{Q}$ has no jump at all. Taking the asymptotics of S and w into account, $\mathcal{Q}$ must take the following polynomial structure in λ:

$$\mathcal{Q}=(K+\mathrm{i}z)^2\begin{pmatrix}q_1 & q_2\\ q_3 & -q_2\end{pmatrix},\quad q_1=k\lambda+l\lambda^3,\quad q_2=m+n\lambda^2+p\lambda^4,\quad q_3=q+r\lambda^2+s\lambda^4,\tag{87}$$

where $k,l,m,n,p;q,r,s$ are functions of ρ, ζ alone. From the definitions (85), (86) and the condition (70), we may derive

$$\mathcal{Q}\mathcal{L}=-\mathcal{L}\mathcal{Q},\tag{88}$$

whereas the particular Riemann-Hilbert problem (73) has the continuation

$$\begin{aligned}&\lambda\in\Gamma_\lambda:\quad(\mathcal{Q}+\mathrm{e}^{-2V_0}w\mathbf{1})\mathcal{L}_-=-\mathcal{L}_+(\mathcal{Q}+\mathrm{e}^{-2V_0}w\mathbf{1}),\\ &\lambda\in\Gamma_{-\lambda}:\quad(\mathcal{Q}-\mathrm{e}^{-2V_0}w\mathbf{1})\mathcal{L}_-=-\mathcal{L}_+(\mathcal{Q}-\mathrm{e}^{-2V_0}w\mathbf{1}),\\ &\lambda\notin\Gamma_\lambda,\Gamma_{-\lambda}:\quad\mathcal{L}\ \text{analytic in}\ \lambda.\end{aligned}\tag{89}$$

The following solution of the regular Riemann–Hilbert problem (89) is based on the diagonalization of $\mathcal{Q}$.

We consider a function Ψ defined by

$$\Psi := \frac{1}{\sqrt{w^2+\mathrm{e}^{4V_0}}} \ln \frac{\hat{\mathcal{L}}_{22}+\sqrt{1+w^2\mathrm{e}^{-4V_0}}\,\hat{\mathcal{L}}_{21}}{\hat{\mathcal{L}}_{22}-\sqrt{1+w^2\mathrm{e}^{-4V_0}}\hat{\mathcal{L}}_{21}}, \tag{90}$$

where

$$\hat{\mathcal{L}} = \mathcal{L}\begin{pmatrix} 1 & \mathcal{Q}_{11} \\ 0 & \mathcal{Q}_{21} \end{pmatrix}. \tag{91}$$

Note that Ψ has no branch points at the zeroes K_1, K_2, $\overline{K_1}=-K_2$ and $\overline{K_2}=-K_1$ of $w^2+\mathrm{e}^{4V_0}$,

$$K_1^2=\rho_0^2\frac{\mathrm{i}-\mu}{\mu},\quad K_2^2=\rho_0^2\frac{\mathrm{i}+\mu}{\mu}\,[\Re K_1<0,\ \Re K_2>0,\quad \mu \text{ as in (75)}] \tag{92}$$

(Ψ is unaffected by a change in the sign of $\sqrt{w^2+\mathrm{e}^{4V_0}}$). It is an odd function of λ (vanishing at $\lambda=0$ and at $\lambda=\infty$). Therefore, the function

$$\hat{\Psi}=\Psi/[\lambda(K+\mathrm{i}z)]=\Psi/\sqrt{(K-\mathrm{i}\overline{z})(K+\mathrm{i}z)} \tag{93}$$

can be discussed as a unique function of K with the following properties:

(i) Along Γ, because of (89), it jumps according to

$$\hat{\Psi}_-=\hat{\Psi}_+ + \frac{2}{\sqrt{(K-\mathrm{i}\overline{z})(K+\mathrm{i}z)}\sqrt{w^2+\mathrm{e}^{4V_0}}} \ln \frac{\sqrt{w^2+\mathrm{e}^{4V_0}}+w}{\sqrt{w^2+\mathrm{e}^{4V_0}}-w}. \tag{94}$$

(ii) Because of

$$\hat{\mathcal{L}}_{21}^2(1+w^2\mathrm{e}^{-4V_0})-\hat{\mathcal{L}}_{22}^2=\mathcal{Q}_{21}^2, \tag{95}$$

$$\mathcal{Q}_{21}=-\frac{2\,f\Omega_0^2\mathrm{e}^{-2V_0}}{f+\overline{f}}(K-K_a)(K-K_b), \tag{96}$$

the behavior for $K\to K_{a/b}$ is given by

$$\hat{\Psi}\to\frac{\pm 2}{\sqrt{(K_{a/b}-\mathrm{i}\overline{z})(K_{a/b}+\mathrm{i}z)(w_{a/b}^2+\mathrm{e}^{4V_0})}}\ln(K-K_{a/b}) \quad \text{as} \quad K\to K_{a/b}. \tag{97}$$

(The ambiguity of sign can be compensated for by the square root.)

(iii) The behavior for $K\to\infty$, because of the definitions of $\mathcal{Q}$ and $\mathcal{L}$, is given by

$$\hat{\Psi}\to\frac{\ln f}{\Omega^2K^3}\text{as}\quad K\to\infty. \tag{98}$$

These properties are realized by the following representation of $\hat{\Psi}$:

$$\hat{\Psi}=\frac{1}{\pi \mathrm{i}}\int_{-\mathrm{i}\rho_0}^{\mathrm{i}\rho_0}\frac{\ln[(\sqrt{w'^2+\mathrm{e}^{4V_0}}+w')/(\sqrt{w'^2+\mathrm{e}^{4V_0}}-w')]}{\sqrt{(K'-\mathrm{i}\bar{z})(K'+\mathrm{i}z)}\sqrt{w'^2+\mathrm{e}^{4V_0}}(K'-K)}\,\mathrm{d}K'$$
$$-2\int_{K_1}^{K_a}\frac{1}{\sqrt{(K'-\mathrm{i}\bar{z})(K'+\mathrm{i}z)(w'^2+\mathrm{e}^{4V_0})}(K'-K)}\,\mathrm{d}K'$$
$$-2\int_{K_2}^{K_b}\frac{1}{\sqrt{(K'-\mathrm{i}\bar{z})(K'+\mathrm{i}z)(w'^2+\mathrm{e}^{4V_0})}(K'-K)}\,\mathrm{d}K', \tag{99}$$

where K_a and K_b have to be determined such that $\hat{\Psi}=\mathcal{O}(K^{-3})$. The lower limits of integration in the last two integrals have been fixed to obtain the correct result in the Newtonian limit $\mu\to 0$ where $K_a/K_1=1+\mathcal{O}(\mu^2)$ and $K_b/K_2=1+\mathcal{O}(\mu^2)$. (A systematic post-Newtonian expansion of the solution is given in Ref. 19.) Note that the last two terms in Eq. (99) may also be interpreted as follows,

$$2\left(\int_{K_1}^{K_a}+\int_{K_2}^{K_b}\right)=2\left(\int_{K_a}^{K_1}\{-\}+\int_{K_2}^{K_b}\right)=\int_{K_a}^{K_b}\{1\}+\int_{K_a}^{K_b}\{2\}, \tag{100}$$

showing that nothing special happens at K_1 and K_2. In this symbolic notation $\{-\}$ indicates that the square root is meant to have the opposite sign with reference to the first term; $\{1\}$ and $\{2\}$ denote different paths in the complex K-plane, which are chosen such that the closed integral

$$\oint=\int_{K_a}^{K_b}\{1\}-\int_{K_a}^{K_b}\{2\}=2\int_{K_1}^{K_2} \tag{101}$$

is performed around a contour enclosing the branch points K_1 and K_2 of $\sqrt{w^2+\mathrm{e}^{4V_0}}$. In the subsequent formulas we normalize K and introduce

$$X=\frac{K}{\rho_0},\quad X_{a/b}=\frac{K_{a/b}}{\rho_0},\quad X_{1/2}=\frac{K_{1/2}}{\rho_0}. \tag{102}$$

An asymptotic expansion of Eq. (99) for $X\to\infty$ $(K\to\infty)$ leads, according to (98), to

$$\ln f=\mu\left[\int_{X_1}^{X_a}\frac{X^2\,\mathrm{d}X}{W}+\int_{X_2}^{X_b}\frac{X^2\,\mathrm{d}X}{W}-\int_{-\mathrm{i}}^{\mathrm{i}}\frac{hX^2\,\mathrm{d}X}{W_1}\right], \tag{103}$$

$$\int_{X_1}^{X_a}\frac{\mathrm{d}X}{W}+\int_{X_2}^{X_b}\frac{\mathrm{d}X}{W}=\int_{-\mathrm{i}}^{\mathrm{i}}\frac{h\mathrm{d}X}{W_1},\qquad \int_{X_1}^{X_a}\frac{X\,\mathrm{d}X}{W}+\int_{X_2}^{X_b}\frac{X\,\mathrm{d}X}{W}=\int_{-\mathrm{i}}^{\mathrm{i}}\frac{hX\mathrm{d}X}{W_1}, \tag{104}$$

where the lower integration limits X_1, X_2 are given by

$$X_1^2=\frac{\mathrm{i}-\mu}{\mu},\quad X_2^2=-\frac{\mathrm{i}+\mu}{\mu}\quad(\Re X_1<0,\quad \Re X_2>0), \tag{105}$$

whereas the upper limits X_a, X_b must be calculated from the integral equations (104). Here we have introduced the abbreviations

$$W=W_1W_2,\quad W_1=\sqrt{(X-\zeta/\rho_0)^2+(\rho/\rho_0)^2},\quad W_2=\sqrt{1+\mu^2(1+X^2)^2}, \tag{106}$$

and

$$h=\frac{\ln(\sqrt{1+\mu^2(1+X^2)^2}+\mu(1+X^2))}{\pi\mathrm{i}\sqrt{1+\mu^2(1+X^2)^2}}. \tag{107}$$

The third integral in (103) as well as the integrals on the right-hand sides in (104) have to be taken along the imaginary axis in the complex X-plane with h and and W_1 fixed according to $\Re W_1<0$ (for ρ, ζ outside the disk) and $\Re h=0$. The task of calculating the upper limits X_a, X_b in (104) from

$$u=\int_{-\mathrm{i}}^{\mathrm{i}}\frac{h\,dX}{W_1},\quad v=\int_{-\mathrm{i}}^{\mathrm{i}}\frac{hXdX}{W_1} \tag{108}$$

is known as Jacobi's inversion problem. Göpel[20] and Rosenhain[21] were able to express the hyperelliptic functions $X_a(u,v)$ and $X_b(u,v)$ in terms of (hyperelliptic) theta functions. Later on it turned out that even the first two integrals in (103) can be expressed by theta functions in u and v! A detailed introduction into the related mathematical theory which was founded by Riemann and Weierstraß may be found in Refs. 22–24. The representation of the Ernst potential (103) in terms of theta functions can be be taken from Stahl's book [see Ref. 22, p. 311, Eq. (5)]. Here is the result: Defining a theta function $\vartheta(x,y;p,q,\alpha)$ by

$$\vartheta(x,y;p,q,\alpha)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}(-1)^{m+n}p^{m^2}q^{n^2}\mathrm{e}^{2mx+2ny+4mn\alpha} \tag{109}$$

one can reformulate the expressions (103) and (104) to give

$$f=\frac{\vartheta(\alpha_0u+\alpha_1v-C_1,\beta_0u+\beta_1v-C_2;p,q,\alpha)}{\vartheta(\alpha_0u+\alpha_1v+C_1,\beta_0u+\beta_1v+C_2;p,q,\alpha)}\,\mathrm{e}^{-(\gamma_0u+\gamma_1v+\mu w)} \tag{110}$$

with u and v as in (108) and

$$w=\int_{-\mathrm{i}}^{\mathrm{i}}\frac{hX^2\mathrm{d}X}{W_1}. \tag{111}$$

The normalization parameters α_0, α_1; β_0, β_1; γ_0, γ_1, the moduli p, q, α of the theta function and the quantities C_1, C_2 are defined on the two sheets of the hyperelliptic Riemann surface related to

$$W=\mu\sqrt{(X-X_1)(X-\overline{X_1})(X-X_2)(X-\overline{X_2})(X-\mathrm{i}\overline{z}/\rho_0)(X+\mathrm{i}z/\rho_0)}, \tag{112}$$

see Fig. 3. There are two normalized Abelian differentials of the first kind,

$$\mathrm{d}\omega_1=\alpha_0\frac{\mathrm{d}X}{W}+\alpha_1\frac{X\mathrm{d}X}{W}, \tag{113}$$

$$\mathrm{d}\omega_2=\beta_0\frac{\mathrm{d}X}{W}+\beta_1\frac{X\mathrm{d}X}{W}, \tag{114}$$

defined by

$$\oint_{a_m}\mathrm{d}\omega_n=\pi\mathrm{i}\,\delta_{mn}\quad(m=1,2;\,n=1,2). \tag{115}$$

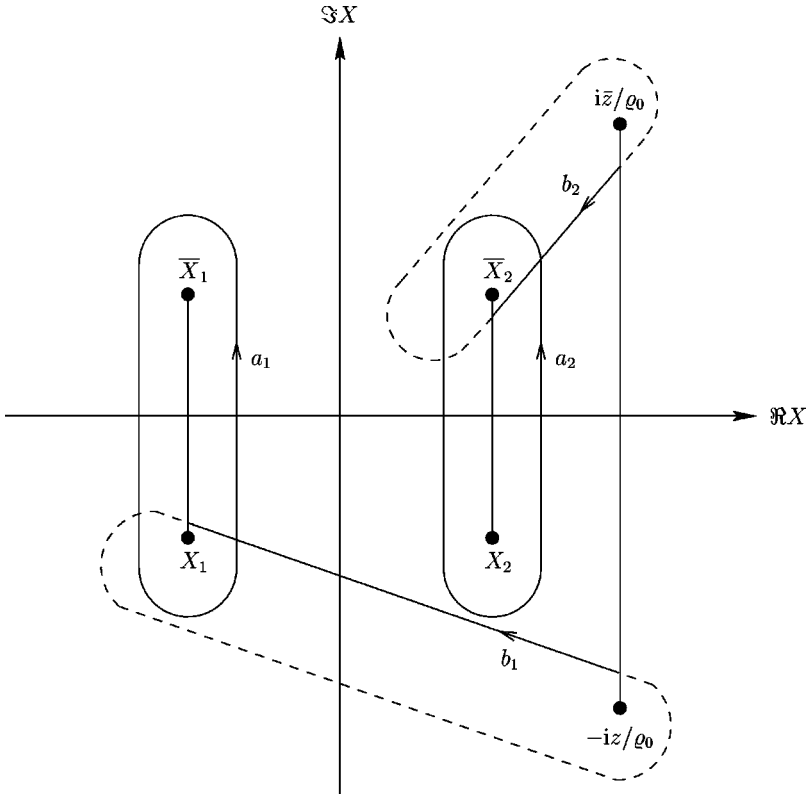

FIG. 3. Riemann surface with cuts between the branch points X_1 and $\overline{X}_1$, X_2 and $\overline{X}_2$, $-\mathrm{i}z/\rho_0$ and $\mathrm{i}\overline{z}/\rho_0$. Also shown are the four periods a_i and b_i $(i=1,2)$. (Continuous/dashed lines belong to the upper/lower sheet defined by $W\to\pm\mu X^3$ as $X\to\infty$.)[3]

Equation (115) consists of four linear algebraic equations and yields the four parameters α_0, α_1, β_0, β_1 in terms of integrals extending over the closed (deformable) curves a_1, a_2. It can be shown that there is one normalized Abelian differential of the third kind,

$$\mathrm{d}\omega=\gamma_0\frac{\mathrm{d}X}{W}+\gamma_1\frac{X\mathrm{d}X}{W}+\mu\frac{X^2\mathrm{d}X}{W}, \tag{116}$$

with vanishing a-periods,

$$\oint_{a_j}\mathrm{d}\omega=0 \qquad (j=1,2). \tag{117}$$

This equation defines γ_0, γ_1 (again via a linear algebraic system). The Riemann matrix

$$(B_{ij})=\begin{pmatrix}\ln p & 2\alpha\\ 2\alpha & \ln q\end{pmatrix} \qquad (i=1,2;\ j=1,2) \tag{118}$$

(with negative definite real part) is given by

$$B_{ij}=\oint_{b_i}d\omega_j \tag{119}$$

and defines the moduli p, q, α of the theta function (109). Finally, the quantities C_1, C_2 can be calculated by

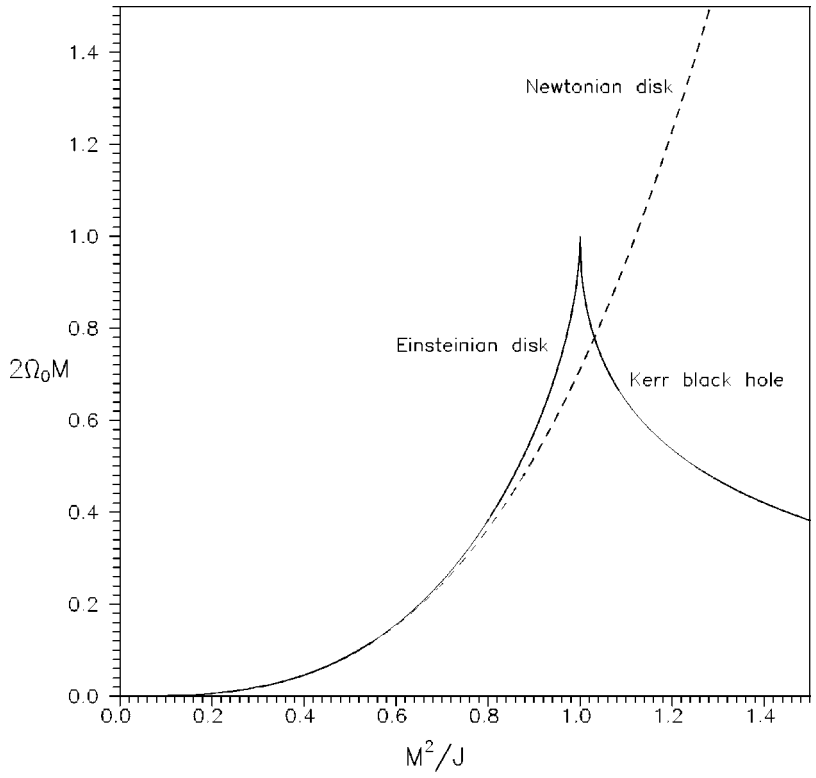

FIG. 4. Relation between $2\Omega_0 M$ and M^2/J for the classical Maclaurin disk (dashed line), the general-relativistic dust disk and the Kerr black-hole.[17]

$$C_i = -\int_{-\mathrm{i}z/\rho_0}^{\infty^+} \mathrm{d}\omega_i \quad (i=1,2), \tag{120}$$

where $+$ denotes the upper sheet. Obviously, all the quantities entering the theta functions and the exponential function in (110) can be expressed in terms of well-defined integrals and depend on the three parameters ρ/ρ_0, ζ/ρ_0, μ. The corresponding "tables" for α_i, β_i, γ_i, C_i, B_{ij}, u, v, w can easily be calculated by numerical integrations. Fortunately, theta series like (109) converge rapidly. For $0<\mu<\mu_0$, the solution (110) is analytic *everywhere* outside the disk—even at the rings $-\mathrm{i}z/\rho_0 = X_1$, X_2. The complete metric, calculated according to (1) and (14)–(16), is given in the Appendix.

In the framework of the completely integrable evolution equations, the solution (110) may be interpreted as a "Bäcklund-like" transformation of well-defined "seed" solutions u,v,w satisfying axisymmetric Laplace equations. The transformation "parameters" $\alpha_0,\beta_0;\alpha_1,\beta_1;\gamma_0,\gamma_1;$ $p,q,\alpha;C_1,C_2$ depend on the six branch points of the two-sheeted Riemann K-surface associated with the function $W=W(X)$, cf. (106), and do not depend on u,v,w. All in all, f is a function of the two parameters ρ_0 and μ and the two cylindrical coordinates ρ and ζ. For $\mu \ll 1$ we obtain the Maclaurin disk as the Newtonian limit.

VII. PHYSICAL DISCUSSION

Since the Kerr black hole is also a two-parameter solution, it might be interesting to compare the behavior of both solutions in dependence on common parameters, say, on mass M and angular momentum J. It must be possible to express the area of the horizon and the disk, the radius ρ_0 of the disk or other physical quantities in terms of M and J. A very illustrative relation is the angular

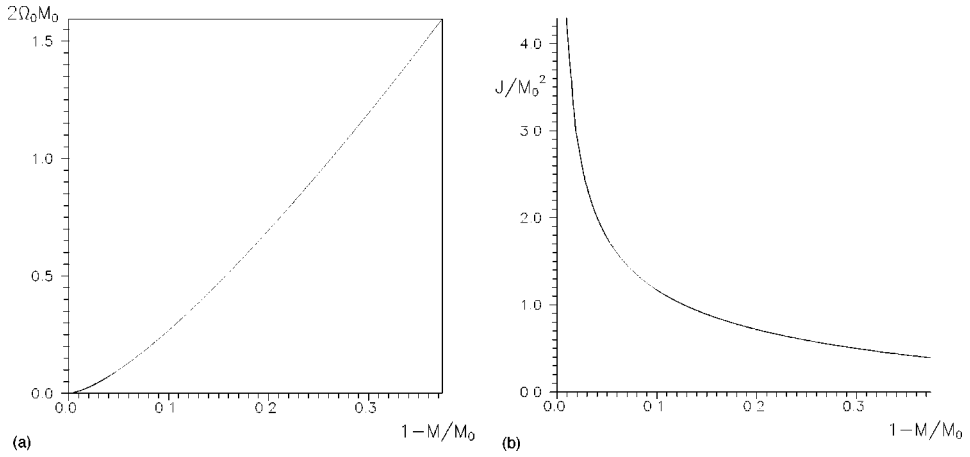

FIG. 5. (a) $\Omega_0 M_0$ and (b) J/M_0^2 as functions of the relative binding energy $(M_0-M)/M_0$ for the disk of dust.[2]

velocity Ω_0 as a function of M and J, since Ω_0 is defined in both cases. For black holes, we have derived the explicit expression (53). Surprisingly, the corresponding disk of dust relation has the same scaling behavior, i.e., $M\Omega_0$ is a function of M^2/J alone. Figure 4 shows this dependence for both solutions.[17] For $M^2/J \to 1$ (corresponding to $\mu \to \mu_0$), where the disk solution becomes identical with the extreme Kerr solution outside the horizon $(\rho^2+\zeta^2>0)$, there is a "phase transition" between the disk and the black hole. Note that for nonvanishing Ω_0, $\rho_0 \to 0$ as $\mu \to \mu_0$. A detailed analysis of the disk solution for $\mu \to \mu_0$, including the discussion of a different, nonasymptotically flat limit of space–time, which is obtained for finite ρ/ρ_0 and ζ/ρ_0 $(\rho^2+\zeta^2 = 0\,!)$, can be found in Ref. 25.

We remark that (110) solves the Bardeen–Wagoner problem[26] explicitly. All metric coefficients in (1) are analytic in ρ, ζ outside the disk and continuous through the disk. From a physical point of view we have an extremely flattened rigidly rotating body and, likewise, a rotating continuous distribution of mass points interacting via gravitational forces alone ("galaxy" model). Figure 5 illustrates the "parametric" collapse of a disk with the total mass-energy M, the baryonic mass M_0, the angular velocity Ω_0 and the angular momentum J towards the black hole limit $(1-M/M_0 = 0.373\,283\,5\ldots)$. Imagine a disk consisting of a fixed number of baryons (fixed M_0): Occupying states with decreasing energy M, it would shrink, thereby shedding angular momentum but increasing its angular velocity. The above mentioned limit of the relative binding energy $1-M/M_0$ corresponds to the extreme black hole limit. Additional physical effects (ergozones, dragging effects, surface mass density,...) as well as further parameter relations have been discussed in Refs. 3 and 27.

The methods outlined in this article could be used to construct self-gravitating disks around a central black hole.

ACKNOWLEDGMENTS

We wish to thank Andreas Kleinwächter for numerous discussions and Jörg Hennig for technical assistance.

APPENDIX: METRIC OF THE RIGIDLY ROTATING DISK OF DUST

The metric functions e^{2U}, a, e^{2k} calcutated from the Ernst potential (110) via (14)–(16) are given as follows:

$$e^{2U}=\frac{\vartheta(\mathbf{c})\vartheta^*(\mathbf{c})\vartheta(\mathbf{a})\vartheta^*(\mathbf{a})}{\vartheta(\mathbf{0})\vartheta^*(\mathbf{0})\vartheta(\mathbf{a}+\mathbf{c})\vartheta^*(\mathbf{a}+\mathbf{c})}e^{-(\gamma_0 u+\gamma_1 v+\mu w)},$$

$$1+\frac{(1+\Omega_0 a)e^{2U}}{\Omega_0\rho}=\frac{\vartheta(\mathbf{0})\vartheta^*(\mathbf{0})\vartheta(\mathbf{a}+2\mathbf{c})\vartheta^*(\mathbf{a})}{\vartheta(\mathbf{c})\vartheta^*(\mathbf{0})\vartheta(\mathbf{a}+\mathbf{c})\vartheta^*(\mathbf{a}+\mathbf{c})},$$

$$e^{2k(\rho,\zeta)}=\frac{\kappa(\rho,\zeta)}{\kappa(0,0)},$$

with

$$\kappa(\rho,\zeta)=\frac{\vartheta(\mathbf{a})\vartheta^*(\mathbf{a})}{\vartheta(\mathbf{0})\vartheta^*(\mathbf{0})}\exp\left(2k_0-\frac{1}{2}\sum_{i,k=1}^{2}a_i a_k\frac{\partial^2\ln\vartheta(\mathbf{x})\vartheta^*(\mathbf{x})}{\partial x_i\partial x_k}\bigg|_{\mathbf{x}=\mathbf{0}}\right),$$

where

$$2k_0=\frac{\mu^2}{4}\int_{-i}^{i}\int_{-i}^{i}dX\,dX'\frac{(\lambda-\lambda')^2}{\lambda\lambda'}\frac{h(X)h(X')(X-X_1)(X-X_2)(X'+X_1)(X'+X_2)}{(X-X')^2},$$

$$\lambda=\sqrt{\frac{X-iz/\rho_0}{X+iz/\rho_0}},\quad \lambda'=\sqrt{\frac{X'-iz/\rho_0}{X'+iz/\rho_0}},$$

$$\vartheta(\mathbf{x})=\vartheta(\mathbf{x};p,q,\alpha)=\vartheta(x_1,x_2;p,q,\alpha),$$

$$\vartheta^*(\mathbf{x})=\vartheta\left(x_1+\frac{i\pi}{2},x_2+\frac{i\pi}{2};p,q,\alpha\right),$$

$$\mathbf{a}=(a_1,a_2)=(\alpha_0 u+\alpha_1 v,\beta_0 u+\beta_1 v),\quad \mathbf{0}=(0,0),\quad \mathbf{c}=(C_1,C_2).$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Twistor theory of hyper-Kähler metrics with hidden symmetries

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(Received 15 January 2003; accepted 9 April 2003)

We review the hierarchy for the hyper-Kähler equations and define a notion of symmetry for solutions of this hierarchy. A four-dimensional hyper-Kähler metric admits a hidden symmetry if it embeds into a hierarchy with a symmetry. It is shown that a hyper-Kähler metric admits a hidden symmetry if it admits a certain Killing spinor. We show that if the hidden symmetry is tri-holomorphic, then this is equivalent to requiring symmetry along a higher time and the hidden symmetry determines a ''twistor group'' action as introduced by Bielawski [*Twistor Quotients of Hyper-Kähler Manifolds* (World Scientific, River Edge, NJ, 2001)]. This leads to a construction for the solution to the hierarchy in terms of linear equations and variants of the generalized Legendre transform for the hyper-Kähler metric itself given by Ivanov and Rocek [Commun. Math. Phys. **182**, 291 (1996)]. We show that the ALE spaces are examples of hyper-Kähler metrics admitting three tri-holomorphic Killing spinors. These metrics are in this sense analogous to the ''finite gap'' solutions in soliton theory. Finally we extend the concept of a hierarchy from that of our earlier work [Commun. Math. Phys. **213**, 641 (2000)] for the four-dimensional hyper-Kähler equations to a generalization of the conformal anti-self-duality equations and briefly discuss hidden symmetries for these equations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1588466]

I. INTRODUCTION

It is well known that finding exact solutions to a nonlinear partial differential equation (PDE) is greatly simplified by the existence of symmetries. In differential geometric language the symmetries of a hyper-Kähler structure or, more generally, anti-self-dual conformal structures in four dimensions, correspond to (conformal) Killing vectors. Equations for hyper-Kähler four-manifolds with conformal Killing vectors have been studied and, in many cases, solved.[11,31,9,10]

Apart from natural Lie-point symmetries, integrable soliton equations possess infinitely many hidden symmetries, which can also be effectively used to construct solutions. It is less well known how to find such solutions in hyper-Kähler geometry (although we will see that such solutions have indeed been found in another guise[3,17,20]). In this article we shall show that hidden symmetries correspond to Killing tensors and spinors (which, classically, occur in Riemannian geometry as additional integrals of the geodesic flow) and propose two methods of finding hyper-Kähler metrics with such symmetries.

We start by briefly reviewing a beautiful construction of Novikov[24] which we shall posit as a motivation and a guiding principle. Consider the Korteveg–de Vries (KdV) equation

$$u_{t_1}=6uu_x-u_{xxx}, \quad \text{where} \quad u=u(x,t_1), \tag{1}$$

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together with the associated hierarchy of equations for $u(x,t_1,t_2,\dots)$

$$\frac{\partial u}{\partial t_i}=\frac{\partial}{\partial x}\frac{\delta H_i}{\delta u}. \tag{2}$$

Here

$$H_0=\int \frac{1}{2}u^2\mathrm{d}x, \quad H_1=\int\left(\frac{1}{2}u_x^2+u^3\right)\mathrm{d}x, \quad H_2=\int\left(\frac{1}{2}u_{xx}^2-\frac{5}{2}u^2u_{xx}+\frac{5}{2}u^4\right)\mathrm{d}x, \ \dots$$

are constants of motions which can be found recursively by solving the Riccati equation. Imposing a constraint

$$\frac{\partial u}{\partial t_k}+c_1\frac{\partial u}{\partial t_{k-1}}+\ \cdots\ +c_k\frac{\partial u}{\partial t_0}=c_0 \tag{3}$$

reduces (1) to an ordinary differential equation (ODE). This ODE is a completely integrable Hamiltonian system with k first integrals in involution. In the simplest nontrivial case the solution is

$$x=\int\frac{\mathrm{d}u}{\sqrt{2u^3+c_1u^2+2c_0u+E}}.$$

In the case of the KdV equation, it is then possible to proceed to obtain explicit formulas for such solutions in terms of theta functions.

For a general integrable system, hidden symmetries are constructed systematically by studying a hierarchy of commuting flows associated to the original equations. A hidden symmetry is then an explicit point symmetry of the hierarchy which, in particular, include the higher flows themselves.

In this article we shall propose an analogous construction of hidden symmetries for the hyper-Kähler equations in four dimensions and its integrable generalizations, which include quaternionic structures in $4k$ dimensions. Recall that a four-dimensional Riemannian manifold $(\mathcal{M},g)$ is hyper-Kähler if it admits three Kähler structures Σ_I, Σ_J, and Σ_K compatible with g and such that the endomorphisms I, J, K given by $g(IX,Y)=\Sigma_I(X,Y)$, etc., satisfy $IJ=K=-JI$. To impose higher symmetries on this system one needs to

(1) reformulate the hyper-Kähler condition on a metric as an integrable PDE (the *heavenly equation*),
(2) construct the associated hierarchy, and
(3) look for solutions invariant under the hidden symmetries, and characterize twistor spaces corresponding to these solutions.

Steps (**1**) and (**2**) were taken in Ref. 27, and Refs. 5, 30, 29, and 8, respectively. We shall review the approach taken in Ref. 8 in Sec. II which focuses on hierarchies associated to four-dimensional hyper-Kähler spaces. This is generalized in Sec. VI to give a hierarchy associated to general conformally ASD spaces both in four dimensions and their higher dimensional generalizations such as quaternion Kähler spaces. The other sections deal with (**3**).

In Secs. III and IV we discuss symmetry and hidden symmetry reduction in the context of the four-dimensional hyper-Kähler equations. In Sec. III we first discuss and classify symmetries of solutions to the hyper-Kähler hierarchy. We use the well known twistor description[31] of the Gibbons–Hawking solution as a guiding example in our analysis of the case of the hierarchy; we show that when the symmetry is triholomorphic, the solutions of the reduced equations are linear and we briefly discuss the corresponding twistor theory. The hyper-Kähler hierarchy is in particular foliated by four-dimensional hyper-Kähler manifolds that admit a hidden symmetry in a variant of the Ivanov and Rocek construction.[17]

In Sec. IV we discuss hyper-Kähler spaces with a hidden symmetry, defined to be a space that embeds into a hierarchy that has a symmetry. In the general case, we show that a hidden symmetry corresponds to the existence of a spinor $K^{B}_{B'_0\dots B'_k}$ satisfying

$$\nabla^{(A}{}_{(A'}K^{B)}_{B'_0\dots B'_k)}=0. \tag{4}$$

When the hidden symmetry is ''triholomorphic'' in an appropriate sense, we find that $K^{B}_{B'_0\dots B'_k}=\nabla^{B}_{(B'_0}L_{B'_1\dots B'_k)}$ for some spinor field $L_{B'_1\dots B'_k}$ satisfying

$$\nabla_{A(A'}L_{B'_1\dots B'_k)}=0. \tag{5}$$

A nonconstant solution $L_{A'_1\dots A'_k}$ to the Killing-spinor equation (5) is said to be a Killing spinor of type $(0,k)$ and is also sometimes known as a solution to the valence-$(0,k)$ twistor equation. If $k=2$, then $K_{AA'}=\nabla^{B'}_{A}L_{A'B'}$ is a triholomorphic Killing vector of the given hyper-Kähler space, and the corresponding metric is of the Gibbons–Hawking form.[12]

If the metric admits a hyper-Kähler hidden symmetry and hence Killing spinor, then the corresponding twistor space admits a globally defined twistor function Q homogeneous of degree k. This is because the existence of a Killing spinor implies that the twistor space of the hyper-Kähler hierarchy admits an action of a Hamiltonian vector field with Hamiltonian Q and factor space $\mathcal{O}(k)$. The hyper-Kähler twistor space therefore arises as an affine bundle over $\mathcal{O}(k)$, described by a cohomology class $f\in H^1(\mathbb{CP}^1,\mathcal{O}(2-k))$. The corresponding space–time can be determined directly and the construction followed through to give explicit formulas for a basis of the self-dual two-forms (and therefore for the metric).

In Sec. V, we demonstrate that the asymptotically locally Euclidean (ALE) spaces constructed by Hitchin[15] and Kronheimer[18,19] admit three triholomorphic hidden symmetries. We show that the corresponding twistor spaces are elliptic fibrations over $\mathcal{O}(k)$ for some k, and the transition functions defining these bundles can be found in terms of elliptic integrals.

Finally in Sec. VI we extend the concept of a hierarchy from that of Ref. 8 for the four-dimensional hyper-Kähler equations to a generalization of the conformal anti-self-duality equations and give a brief discussion of hidden symmetries in this context.

The two-component spinor notation used in the article is summarized in the Appendix.

II. THE HYPER-KÄHLER HIERARCHY

Let $\mathcal{M}$ be a complex four-manifold equipped with a holomorphic metric g and compatible volume form ν; we shall refer to this triple as a *space–time*. For a four-manifold with metric, we have that $T\mathcal{M}=\mathbb{S}\otimes\tilde{\mathbb{S}}$ where $\mathbb{S}$ and $\tilde{\mathbb{S}}$ are the bundles of self-dual and anti-self-dual spinors, respectively, each being rank two complex vector bundles on $\mathcal{M}$. The metric connection necessarily preserves this factorization, and the hyper-Kähler condition is equivalent to the condition that the induced connection on $\tilde{\mathbb{S}}$ be flat. (The I, J, and K act trivially on the $\tilde{\mathbb{S}}$ factor and on the $\mathbb{S}$ factor by Pauli σ matrices.) This implies that, on translation of the one-form indices to indices $A,B,\dots$ denoting membership of $\mathbb{S}$ and $A',B',\dots$ denoting membership of $\tilde{\mathbb{S}}$, the curvature has the form

$$R_{AA'BB'CC'DD'}=\varepsilon_{A'B'}C_{ABCD}\varepsilon_{C'D'}, \quad C_{ABCD}=C_{(ABCD)},$$

where ε_{AB} and $\varepsilon_{A'B'}$ are skew, and $\varepsilon_{AB}\varepsilon_{A'B'}$ induces the metric under $T\mathcal{M}=\mathbb{S}\otimes\tilde{\mathbb{S}}$. In four dimensions this amounts to the ASD vacuum equations

$$\Phi_{ABA'B'}=0, \quad R=0, \quad C_{A'B'C'D'}=0. \tag{6}$$

Here R is the Ricci scalar, $\Phi_{ABA'B'}$ is the trace-free part of the Ricci tensor, and $C_{A'B'C'D'}$ is the SD part of the Weyl tensor (we use the conventions of Penrose and Rindler[26]).

We now show how the geometrical characterization of the hyper-Kähler equations and its hierarchy can be reduced to differential equations. We use a potential formulation, due to Plebański,[27] based on the fact that the equations locally imply the existence of a complex-valued function Θ and coordinate system (w,z,x,y) such that the metric is given by

$$g=2\mathrm{d}w\mathrm{d}x+2\mathrm{d}z\mathrm{d}y-2\Theta_{xx}\mathrm{d}z^2-2\Theta_{yy}\mathrm{d}w^2+4\Theta_{xy}\mathrm{d}w\mathrm{d}z, \tag{7}$$

and Θ satisfies so-called second heavenly equation

$$\Theta_{xw}+\Theta_{yz}+\Theta_{xx}\Theta_{yy}-\Theta_{xy}^2=0. \tag{8}$$

The associated hierarchy is a differential equation with higher times generalizing one of the formulations of the hyper-Kähler equations in terms of potentials. We introduce the coordinates $x^{Ai}, A=0,1, i=0,\ldots n$, on a $(2n+2)$-dimensional manifold $\mathcal{N}$. The dependent variable $\Theta(x^{Ai})$ satisfies the equations

$$\partial_{Ai}\partial_{Bj-1}\Theta-\partial_{Bj}\partial_{Ai-1}\Theta+\{\partial_{Ai-1}\Theta,\partial_{Bj-1}\Theta\}_{yx}=0, \qquad i,j=1,\ldots,n. \tag{9}$$

Here $\{\ldots,\ldots\}_{yx}$ is the Poisson bracket with respect to the Poisson structure $\partial/\partial x^{A0}\wedge\partial/\partial x_{A0}$. [In order to make contact with the above for $n=1$, put $x^{A0}=(y,-x)$ and $x^{A1}=(w,z)$ and note that (8) is (9) with $i=j=1$.]

This hierarchy has a Lax representation

$$L_{Ai}\Phi=\partial_{Ai-1}\Phi+\lambda(\partial_{Ai}\Phi+\{\partial_{Ai-1}\Theta,\Phi\})=0, \tag{10}$$

where $A=0,1$, $i=1,\ldots,n$, λ is an affine coordinate on $\mathbb{CP}^1$ and $\Phi(x^{Ai},\lambda)$ is a function on $\mathcal{N}\times\mathbb{CP}^1$. It is clear that this provides the point of contact with the abstract definition.

It is clear from the form of the equations (10) that the space $\mathcal{N}$ is foliated by four-dimensional hyper-Kähler manifolds parametrized by $x^{Ai}=\text{const}$ for $i\geqslant 2$.

In Ref. 8 the hierarchies were obtained both via a rescursion operator construction and via a twistor construction. We shall summarize these constructions in the remaining part of this section.

Let

$$\Box_\Theta=\partial_x\partial_w+\partial_y\partial_z+\Theta_{yy}\partial_x^2+\Theta_{xx}\partial_y^2-2\Theta_{xy}\partial_x\partial_y$$

denote the wave operator on the ASD background determined by Θ, and let $\mathcal{W}_\Theta=\mathrm{Ker}\ \Box_\Theta$.

Proposition 2.1:[8]

(i) Elements of $\mathcal{W}_\Theta$ can be identified with linearized solutions $\delta\Theta$ [i.e., $(\Theta+\delta\Theta)$ satisfies (8) up to the linear terms in $\delta\Theta$] of the heavenly equation (8).

(ii) Let $(\delta\Theta_1\delta\Theta_2)\in\mathcal{W}_\Theta\times\mathcal{W}_\Theta$. The "recursion operator" $\mathcal{R}$ is defined to be the subspace $\mathcal{R}\subset\mathcal{W}_\Theta\times\mathcal{W}_\Theta$ on which

$$\partial_y(\delta\Theta_2)=(\partial_w-\Theta_{xy}\partial_y+\Theta_{yy}\partial_x)\delta\Theta_1, \qquad -\partial_x(\delta\Theta_2)=(\partial_z+\Theta_{xx}\partial_y-\Theta_{xy}\partial_x)\delta\Theta_1. \tag{11}$$

Note that the recursion operator is only an operator in the usual sense when the subspace $\mathcal{R}$ can be realized as a graph of a genuine operator $R:\mathcal{W}_\Theta\to\mathcal{W}_\Theta$ given by the recursion relations

$$R\,\delta\Theta=\partial_y^{-1}((\partial_w-\Theta_{xy}\partial_y+\Theta_{yy}\partial_x)\delta\Theta), \qquad R\,\delta\Theta=-\partial_x^{-1}((\partial_z+\Theta_{xx}\partial_y-\Theta_{xy}\partial_x)\delta\Theta). \tag{12}$$

This identification with a genuine operator will only be possible when we impose appropriate boundary conditions. However, for the definition of the hierarchy as a local system of equations, we will need only the definition of $\mathcal{R}$ above.

The first few iterations can be explicitly integrated to give

$$w\to y\to -\Theta_x\to\Theta_z\to\cdots,\quad z\to -x\to -\Theta_y\to -\Theta_w\to\cdots.$$

We introduce the new coordinates x^{Ai}, $A=0,\ 1$, $i=0,\ldots,n$. For $i=0,\ 1$, $x^{Ai}=x^{AA'}=(w,z,x,y)$ are coordinates on $\mathcal{M}$, and for $1<i\leqslant n, x^{Ai}$ are the parameters for the new flows (with $2n-2$ dimensional parameter space $\mathbb{X}$). The propagation of Θ along these parameters is determined by the recursion relations $\partial_{Ai+1}\Theta=R\partial_{Ai}\Theta$. However, the consistency conditions imply that in addition Θ satisfies the equations (9) with the Lax system generated by the operators (10).

The twistor theory is summarized in the following:

Theorem 2.2:[8] *There is a 1-1 correspondence between solutions to (9) on $\mathcal{M}\times\mathbb{X}$ and twistor spaces $\mathcal{PT}_n$ defined as follows.*

The twistor space $\mathcal{PT}_n$ is a three-dimensional complex manifold with the following structures:

(1) a projection $\mu:\mathcal{PT}\to\mathbb{CP}^1$,

(2) a section $s:\mathbb{CP}^1\mapsto\mathcal{PT}$ of μ with normal bundle $\mathcal{O}(n)\oplus\mathcal{O}(n)$,

(3) a nondegenerate two-form Σ on the fibers of μ, with values in the pullback from $\mathbb{CP}^1$ of $\mathcal{O}(2n)$.

(4) The choice of coordinate systems and potential Θ in the second Plebanski form for the hierarchy corresponds on the twistor space to a choice of point $[o^{A'}]\in\mathbb{CP}^1$ and canonical homogeneous degree n coordinates ω^A (i.e., $\Sigma=\mathrm{d}\omega^0\wedge\mathrm{d}\omega^1$) on a neighborhood of the fiber of $\mathcal{PT}_n$ over $[o^{A'}]$ defined up to $2n$th order away from this fiber.

Briefly, the space $\mathcal{M}\times\mathbb{X}$ is reconstructed as the moduli space $\mathcal{N}$ of deformations of the section s given in condition (2) above. Then $\mathcal{N}$ is $2n+2$-dimensional and we can introduce coordinates and the function Θ as follows:

We use homogeneous coordinates $\pi_{A'}=(\pi_{0'},\pi_{1'})$ and affine coordinate $\lambda=\pi_{0'}/\pi_{1'}$ on $\mathbb{CP}^1$ so that the point o is represented by $o_{A'}=(0,1)$, or $\lambda=0$. The homogeneous coordinates ω^A [i.e., $(\omega^A,\pi_{A'})\simeq(c^n\omega^A,c\pi_{A'})$ for $c\in\{\mathbb{C}-0\}$] can be pulled back to $\mathcal{N}\times\mathbb{CP}^1$ and the expansion $\omega^A=\pi_{1'}^n\Sigma_{i=0}^n x^{A,i}\lambda^i+O(\lambda^{n+1})$ and this defines coordinates $x^{A,i}$ on $\mathcal{N}$.

Expanding ω^A further, we discover, as shown in Ref. 8, that the twistor coordinates ω^A pulled back to the correspondence space $\mathbb{CP}^1\times\mathcal{N}$ can be expanded further as

$$\omega_n^0=(\pi_{1'})^n\left[x^{0n}+\lambda x^{0n-1}+\cdots+\lambda^n x^{00}+\lambda^{n+1}\frac{\partial\Theta}{\partial x^{10}}+\lambda^{n+2}\frac{\partial\Theta}{\partial x^{11}}+\cdots+\lambda^{2n+1}\frac{\partial\Theta}{\partial x^{1n}}+\cdots\right],$$
$$\omega_n^1=(\pi_{1'})^n\left[x^{1n}+\lambda x^{1n-1}+\cdots+\lambda^n x^{10}+\lambda^{n+1}\frac{\partial\Theta}{\partial x^{00}}+\lambda^{n+2}\frac{\partial\Theta}{\partial x^{01}}+\cdots+\lambda^{2n+1}\frac{\partial\Theta}{\partial x^{0n}}+\cdots\right], \tag{13}$$

and this determines $\Theta(x^{Ai})$ (up to a constant) satisfying (9). The form of the Lax system (10) is determined by the fact that ω^B are solutions to $L_{Ai}\omega^B=0$.

The form of the expansions (13) and Eqs. (9) can be obtained from the fact that the expansion of $\Sigma=\mathrm{d}\omega^0\wedge\mathrm{d}\omega^1$ on $\mathcal{N}\times\mathbb{CP}^1$ in powers of λ must truncate after λ^{2n}.

There is a $2n$-dimensional distribution on the "spin bundle" $D\subset T(\mathcal{N}\times\mathbb{CP}^1)$ that is tangent to the fibers of the projection $\mathcal{N}\times\mathbb{CP}^1\to\mathcal{PT}_n$. The distribution D has an identification with $\mathcal{O}(-1)\otimes\mathbb{C}^{2n}$ and is generated by the Lax system (10).

This correspondence is stable under small perturbations of the complex structure on $\mathcal{PT}_n$ preserving (1)–(3).

One can find the twistor spaces for the four-dimensional hyper-Kähler slices given by $x^{Ai}=\mathrm{const}, i\geqslant 2$, by taking a sequence of $n-1$ blowups of points in the fiber over $o_{A'}\in\mathbb{CP}^1$, the choice of point in the fiber to blow up at the $(n-i+1)$th blowup corresponding precisely to the choice of the values of x^{Ai}. If one wishes to respect Euclidean reality conditions, one can instead blow up complex conjugate points in the fibers over $o_{A'}$ and $\hat{o}_{A'}$.

III. SYMMETRIES OF HYPER-KÄHLER HIERARCHIES

For a hyper-Kähler space, we can characterize conformal symmetries as follows: let $\Sigma^{A'B'}=(\Sigma^{0'0'},\Sigma^{0'1'},\Sigma^{1'1'})$ be a basis of SD two-forms, and let $\Sigma=\Sigma^{A'B'}\pi_{A'}\pi_{B'}$.

Definition 3.1: A solution to the hyper-Kähler equations admits a symmetry if there exists a vector field K on $\mathcal{N}$ together with a lift $\tilde{K}$ to $S^{A'}$ over $\mathcal{N}$ such that $\mathcal{L}_{\tilde{K}}\Sigma=0$.

Here the lift must be $\tilde{K}=K+\phi_{B'}^{A'}\pi_{A'}\partial/\partial\pi_{B'}$ where $\phi_{B'}^{A'}=-\frac{1}{2}\nabla_{BB'}K^{BA'}-\frac{1}{2}\nabla_c K^c\varepsilon_{B'}^{A'}$ according to the standard theory of Lie derivatives of spinors, see Ref. 26.

We will use this also as a definition for symmetries of the hyper-Kähler hierarchy where now Σ will be the pull-back from twistor space to the spin bundle of the corresponding two-form that is homogeneous of degree $2n$ in $\pi_{A'}$.

Definition 3.2: A solution to the hyper-Kähler hierarchy admits a symmetry if there exists a vector field K on $\mathcal{N}$ together with a lift $\tilde{K}$ to $S^{A'}$ over $\mathcal{N}$ such that $\mathcal{L}_{\tilde{K}}\Sigma=0$.

Again, by homogeneity, we must have that the lift must be $\tilde{K}=K+\phi_{B'}^{A'}\pi_{A'}\partial/\partial\pi_{B'}$ where $\phi_{B'}^{A'}$ will be determined by K.

In particular, $\tilde{K}$ is therefore in involution with the Lax distribution D so that it projects down to a global holomorphic vector field $\mathcal{K}$ on the twistor space $\mathcal{PT}$.

We can classify symmetries according to the extent to which they preserve the various structures on $S^{A'}$ or on the twistor space. This is most easily seen by examining the vertical part $\phi=\phi_{A'}^{B'}\pi_{B'}\partial/\partial\pi_{A'}=\tilde{K}-K$ (where here $\tilde{K}$ denotes the horizontal lift of K). The matrix $\phi_{A'}^{B'}$ generically has two constant eigenvalues (the space–time must be of Petrov type N for nonconstant eigenvalues to be admissable).

(1) K will be said to be *triholomorphic* if the eigenvalues of $\phi_{A'}^{B'}$ are equal. The projection of $\tilde{K}$ to the projective spin bundle, $PS^{A'}$, is then horizontal, and the vertical part ϕ of $\tilde{K}$ on $S^{A'}$ is a multiple of the Euler homogeneity operator $\pi^{A'}\partial/\partial\pi^{A'}$, i.e., $\phi_{A'}^{B'}=\mu\,\delta_{A'}^{B'}$. Equivalently, it is triholomorphic if $\mathcal{K}$ is tangent to the fibers of the projection $p:\mathcal{PT}_n\mapsto\mathbb{CP}^1$.

(2) K is said to be Killing if the trace of ϕ vanishes, $\phi_{A'}^{A'}=0$. Then ϕ preserves the form $\pi_{A'}d\pi^{A'}$ on the spin bundle.

(3) K is said to be a homothety if the trace of ϕ, $\phi_{A'}^{A'}$ is constant, i.e., $\mathcal{L}_{\tilde{K}}\varepsilon^{A'B'}\pi_{A'}\mathrm{d}\pi_{B'}=\mu\varepsilon^{A'B'}\pi_{A'}\mathrm{d}\pi_{B'}$ for some constant $\mu\neq0$.

In the case that the symmetry is not triholomorphic, we can further distinguish the case where ϕ, on projection to the projective spin bundle, has one or two zeroes. In the single zero case in particular, $\phi_{A'}^{B'}$ will not be diagonalizable. We will not pursue this distinction here but see Refs. 7 and 10 for a study of such symmetries on $(++--)$ hyper-Kähler space.

A. Examples with triholomorphic Killing symmetry

We first consider well known reductions of the hyper-Kähler equations, and then analogous reductions of the hierarchy.

1. Gibbons–Hawking metrics revisited

The heavenly equation (8) with $R(\Theta_x)=\Theta_z=0$ can be expressed as

$$\mathrm{d}\Theta_x\wedge\mathrm{d}x\wedge\mathrm{d}y+\mathrm{d}w\wedge\mathrm{d}\Theta_x\wedge\mathrm{d}\Theta_y=0. \tag{14}$$

Introduce $p:=\Theta_x$ and perform a Legendre transform

$$F(p,y,w):=px(w,y,p)-\Theta(w,z,y,x(w,y,p)).$$

Then $x=F_p$, $\Theta_y=-F_y$ and (14) yields the wave equation[11]

$$F_{pw}+F_{yy}=0. \tag{15}$$

Implicit differentiation gives

$$\Theta_{yy}=-F_{yy}+\frac{F_{py}}{F_{pp}},\quad \Theta_{xy}=-\frac{F_{py}}{F_{pp}},\quad \Theta_{xx}=\frac{1}{F_{pp}},$$

and so [with the help of (7) and (15)]

$$g=F_{pp}\left(\frac{1}{4}\mathrm{d}y^2+\mathrm{d}w\mathrm{d}p\right)-\frac{1}{F_{pp}}\left(\mathrm{d}z-\frac{F_{pp}}{2}\mathrm{d}y+F_{py}\mathrm{d}w\right)^2=\psi\left(\frac{1}{4}\mathrm{d}y^2+\mathrm{d}w\mathrm{d}p\right)-\psi^{-1}(\mathrm{d}z+\Omega)^2, \tag{16}$$

where $\psi=F_{pp}$ and $\Omega=F_{py}\mathrm{d}w-(F_{pp}/2)\mathrm{d}y$ satisfy the monopole equation $*\mathrm{d}\psi=\mathrm{d}\Omega$ from (15). Thus (16) is of the Gibbons–Hawking form.[12]

The twistor description is as follows: the twistor coordinates pull back to the spin bundle as

$$\omega^0=\pi_{1'}[w+\lambda y-\lambda^2\Theta_x+\lambda^3\Theta_z+\cdots],$$

$$\omega^1=\pi_{1'}[z-\lambda x-\lambda^2\Theta_y-\lambda^3\Theta_w+\cdots]. \tag{17}$$

The vanishing of Θ_z implies that the whole series for ω^0 truncates at second order. Thus the twistor space admits a global section of $\mathcal{O}(2)$, and this is the Hamiltonian with respect to Σ, for the holomorphic vector field corresponding to the Killing field $\partial_z=K^{AA'}\partial_{AA'}$. Conversely, given a triholomorphic symmetry, the triholomorphicity condition means that its lift to the spin bundle $\mathcal{M}$ is horizontal and so, on twistor space, the corresponding holomorphic vector field is tangent to the fibers of μ. It also preserves Σ and so is Hamiltonian with Hamiltonian given by a homogeneity degree-2 global function. We can choose ω^0 to be this preferred section divided by $\pi_{1'}$ so that the series for ω^0 terminates after λ^2.

Substituting the Legendre transform into (17) yields

$$\omega^0=\pi_{1'}[w+\lambda y-\lambda^2 p], \tag{18}$$

$$\omega^1=\pi_{1'}[z-\lambda F_p+\lambda^2 F_y+\lambda^3 F_w+\cdots]\ . \tag{19}$$

With the definition $\Sigma=\mathrm{d}\omega^0\wedge\mathrm{d}\omega^1|_{\lambda=\mathrm{const}}$ the equation (15) can be rewritten as $\Sigma\wedge\Sigma=0$. The basis of SD two-forms can be read off from $\Sigma=\Sigma^{A'B'}\pi_{A'}\pi_{B'}$:

$$\Sigma^{0'0'}=-\mathrm{d}z\wedge\mathrm{d}p+\mathrm{d}y\wedge\mathrm{d}F_p-\mathrm{d}w\wedge\mathrm{d}F_y,\quad \Sigma^{0'1'}=\mathrm{d}z\wedge\mathrm{d}y+\mathrm{d}w\wedge\mathrm{d}F_p,\quad \Sigma^{1'1'}=\mathrm{d}z\wedge\mathrm{d}w,$$

and these determine the metric above.

2. Triholomorphic symmetry reductions of the hierarchy

In this subsection we shall generalize the construction of Gibbons–Hawking metrics described in the last subsection, and generate solutions to the hyper-Kähler hierarchy such that $R^n\Theta_x=\partial_{1n}\Theta=0$. These are the cases of a triholomorphic Killing symmetry.

Proposition 3.3: The hyper-Kähler hierarchy (9) with symmetry $\partial\Theta/\partial x^{1n}=0$ reduces (in appropriate coordinates) to an overdetermined system of $n(2n-1)$ linear equations for $F(t^0,\ldots,t^{2n})$:

$$\frac{\partial^2 F}{\partial t^{i+1}\partial t^j}=\frac{\partial^2 F}{\partial t^i\partial t^{j+1}},\quad i,j=0,\ldots,2n-1. \tag{20}$$

Proof: Let $\mathcal{PT}_n$ be the twistor space from Proposition 2.2, and let $(\omega_n^A, \pi_{A'})$ be homogeneous coordinates on the neighborhood of $\pi_{A'} = o_{A'}$. (In the previous section $\mathcal{PT} := \mathcal{PT}_1$ and $\omega^A := \omega_1^A$ correspond to the standard situation of the nonlinear graviton construction.)

Now impose the symmetry condition, i.e., assume that $R^n\Theta_x = \partial_{1n}\Theta = 0$. Again, the vanishing of $\partial_{1n}\Theta$ implies that the series (13) in λ for ω^0 truncates at degree $2n$. [Thus, $\pi_{1'}^n \omega^0$ is a global holomorphic function of homogeneity degree-$2n$ on $\mathcal{PT}_n$. Conversely, again, this symmetry corresponds to a global holomorphic vector field on $\mathcal{PT}_n$ that is vertical up the fibers of μ and preserves Σ. It therefore is generated by a global Hamiltonian Q homogeneous of degree $2n$, and we can take as before $\omega^0 = Q/\pi_{1'}^n$.]

We can now perform the Legendre transform

$$p^i = \partial_{1i}\Theta, \qquad i = 0, \ldots, n-1, \quad F(p^j, x^{0j}) = \sum_{i=0}^{n-1} p^i x^{1i}(p^j, x^{0j}) - \Theta(x^{0j}, x^{1i}(p^j, x^{0j})), \quad x^{1n} = T. \tag{21}$$

Therefore $\partial_{0i}F = -\partial_{0i}\Theta, \partial_{p_i}F = x^{1i}$. Define 2n+1 functions $(t^0, \ldots, t^{2n})$ by

$$t^{n-i-1} = p^i, \quad i = 0, \ldots, n-1, \quad t^{n+i} = x^{0i}, \quad i = 0, \ldots n.$$

This implies

$$\omega_n^0 = (\pi_{1'})^n [t^{2n} + \lambda t^{2n-1} + \cdots + \lambda^{2n} t^0], \tag{22}$$

$$\omega_n^1 = (\pi_{1'})^n \left[T + \lambda \frac{\partial F}{\partial t^0} + \lambda^2 \frac{\partial F}{\partial t^1} + \cdots + \lambda^{2n+1} \frac{\partial F}{\partial t^{2n}} + \cdots \right] . \tag{23}$$

Equations (20) arise from the vanishing of coefficient λ^{2n+2} in $\mathrm{d}\omega_n^0 \wedge \mathrm{d}\omega_n^1$:

$$\sum_{i=0}^{2n-1} \mathrm{d}t^i \wedge \mathrm{d} \frac{\partial F}{\partial t^{i+1}} = 0.$$

It can also be verified by cross-differentiating that all integrability conditions for the system (20) are satisfied. □

The geometry on twistor space can be understood as follows. The section Q of $\mathcal{O}(2n)$ generates a Hamiltonian flow

$$\mathcal{K} = \varepsilon^{AB} \frac{\partial Q}{\partial \omega^A} \frac{\partial}{\partial \omega^B}, \quad \varepsilon^{AB} = -\varepsilon^{BA}, \quad \varepsilon^{01} = 1,$$

on the extended twistor space $\mathcal{PT}_n$. This flow corresponds to $\mathcal{K}^{AA_1' \ldots A_n'} \partial_{AA_1' \ldots A_n'} = \partial/\partial x^{1n}$ on $\mathcal{N}$. Since Q is constant along $\mathcal{K}$, the quotient space $\mathcal{PT}_n/\mathcal{K}$ is the total space of $\mathcal{O}(2n) \to \mathbb{CP}^1$ where the map to $\mathcal{O}(2n)$ is furnished by $(\omega^A, \pi_{A'}) \to (Q, \pi_{A'})$.

The full twistor space $\mathcal{PT}_n$ is an affine line bundle with trivial underlying translation bundle and so it corresponds to an element $G(Q, \pi_{A'})$ of $H^1(\mathcal{O}(2n), \mathcal{O})$.

Sections of $\mathcal{O}(2n) \to \mathbb{CP}^1$ are parametrized by $\mathbb{C}^{2n+1}$ with coordinates $\mathbf{t} = (t^0, \ldots, t^{2n})$. The $2n+2$-dimensional space of sections of $\mathcal{PT}_n \to \mathbb{CP}^1$ maps onto this with fiber $\mathbb{C}$ parametrized by T. Choosing linear coordinates up the line bundle η and $\tilde{\eta}$ over open sets U and $\tilde{U}$, the problem of lifting a curve $L_{\mathbf{t}}$ in $\mathcal{O}(2n)$ to one in $\mathcal{PT}_n$ is one of finding a trivialization of the line bundle over L_t, i.e., of finding functions $g(\mathbf{t}, \pi_{A'})$ and $\tilde{g}(\mathbf{t}, \pi_{A'})$ such that, on $U \cap \tilde{U}$, $g - \tilde{g} = G$ on restriction to L_t where G is the log of the patching function for the line bundle, and therefore has homogeneity degree zero. We can then take $\eta = T + g$. We can give a formula for g as

$$g(\mathbf{t},\lambda)=\oint_\gamma G(t^{2n}+\zeta t^{2n-1}+\cdots+\zeta^{2n}t^0,\zeta)\mathrm{d}\zeta/(\zeta-\lambda),$$

where the contour γ is taken in $L_t\cap U\cap\tilde{U}$ surrounding ζ in U. With an identical expression for $\tilde{g}$ but with contour $\tilde{\gamma}$ such that $\gamma-\tilde{\gamma}$ surrounds ζ, we see that $g-\tilde{g}=G$ follows from Cauchy's integral formula. Then the expression for the expansion of the coordinate $\eta=T+g$ about $\lambda=0$ is

$$\eta=T+\sum_{i=0}\lambda^i\oint G(Q(t,\zeta),\zeta)\mathrm{d}\zeta/\zeta^{i+1}.$$

It can then be seen that if we define

$$F(\mathbf{t})=\oint_\Gamma\frac{G(t^{2n}+\lambda t^{2n-1}+\cdots+\lambda^{2n}t^0,\lambda)}{\lambda^2}\mathrm{d}\lambda,$$

then F clearly satisfies the equations of (20) and we obtain the expansions (22) for $(\omega^0,\omega^1)=(Q/\pi_1^n,,\pi_1^n,\eta)$. These can then be used to obtain concrete expressions for $\Sigma=\mathrm{d}\omega^0\wedge\mathrm{d}\omega^1$ to determine the geometric structures of the hyper-Kähler hierarchy.

Clearly we have the following.

Lemma 3.4: The full space of the hierarchy is foliated by hyper-Kähler four-manifolds with $x^{Ai}=constant$ *for* $i>1$ *and metric*

$$2\mathrm{d}x^{10}\mathrm{d}x^{01}+2\mathrm{d}x^{11}\mathrm{d}x^{00}-2\frac{\partial^2\Theta}{\partial(x^{10})^2}(\mathrm{d}x^{11})^2-2\frac{\partial^2\Theta}{\partial(x^{00})^2}(\mathrm{d}x^{01})^2-4\frac{\partial^2\Theta}{\partial x^{00}\partial x^{10}}\mathrm{d}x^{01}\mathrm{d}x^{11}. \quad (24)$$

This gives a variant of the Legendre transform of Ivanov and Rocek[17] (see also Ref. 3).

B. Example for $n=2$

We saw above that for $n=1$ the construction is equivalent to the Gibbons–Hawking anzatz. The $n=2$ case goes as follows:

Let $F_i:=\partial_{t^i}F$. Implicit differentiation of $\partial_{0i}F=-\partial_{0i}\Theta,\partial_{p_i}F=x^{1i}$ with respect to p_0,p_1,y yields

$$\Theta_{xx}=-\frac{F_{00}}{M},\quad \Theta_{xy}=\frac{-F_{01}F_{02}+F_{00}F_{12}}{M},\quad \Theta_{yy}=-F_{22}-\frac{F_{00}(F_{12})^2-2F_{01}F_{12}F_{02}+F_{11}(F_{02})^2}{M},$$

where $M:=(F_{01})^2-F_{00}F_{11}$. The metric (7) with $x=x(t^i),z=z(t^i)$ is defined on the surface $F_4=0$. The formula for the metric in terms of F is not very illuminating, but we shall give it for the sake of completeness:

$$\begin{aligned}g=&M^{-1}(F_{10}N\mathrm{d}t^1\mathrm{d}t^2+F_{00}N\mathrm{d}t^0\mathrm{d}t^2+F_{11}(F_{01})^2(\mathrm{d}t^2)^2+F_{11}^3(\mathrm{d}t^3)^2+2F_{01}(F_{11})^2\mathrm{d}t^2\mathrm{d}t^3\\&+2F_{01}(F_{00})^2\mathrm{d}t^0\mathrm{d}t^1+F_{00}^3(\mathrm{d}t^0)^2+F_{00}(F_{01})^2(\mathrm{d}t^1)^2+[F_{11}N+F_{01}F_{00}F_{03}]\mathrm{d}t^1\mathrm{d}t^3\\&+[3F_{01}F_{00}F_{11}-(F_{01})^3+(F_{00})^2F_{03}]\mathrm{d}t^0\mathrm{d}t^3),\end{aligned} \quad (25)$$

where $N:=(F_{01})^2+F_{00}F_{11}$.

IV. HYPER-KÄHLER SPACES WITH HIDDEN SYMMETRIES

If we have a hyper-Kähler space that embeds into a hyper-Kähler hierachy that admits a symmetry we will say that that the original hyper-Kähler space admits a *hidden symmetry*.

The first question we wish to address is of how to recognize when a hyper-Kähler space admits such a hidden symmetry.

Proposition 4.1: If a hyper-Kähler space $\mathcal{M}$ admits a hidden symmetry, then it admits a solution to the equation

$$\nabla^{(A}_{(A'_1}K^{B)}_{A'_2\cdots A'_n)}=0. \tag{26}$$

Proof: This result is most easily seen from the twistor theory. The symmetry vector K gives rise to a global holomorphic vector field $\mathcal{K}$ on the twistor space for $\mathcal{N}$, $\mathcal{PT}_n$. The twistor space $\mathcal{PT}_1$ for $\mathcal{M}$ is a region in the blowup of $\mathcal{PT}_n$ at a number of points. Thus we have a map $p:\mathcal{PT}_1 \to \mathcal{PT}_n$. So rather than consider $\mathcal{K}$ itself, we consider the two-form $\mathcal{K}\lrcorner\nu_n$ weight $2n+2$ where $\nu_n\in\Gamma(\mathcal{PT}_n,\Omega^3(2n+2))$ is given by $\Sigma_n\wedge\pi_{A'}\mathrm{d}\pi^{A'}$.

This two-form can be pulled back to give $p^*\mathcal{K}\lrcorner\nu_n$ a global two-form of weight $2n+2$ on the twistor space $\mathcal{PT}_1$ for $\mathcal{M}$. This two-form can then be pulled back to give a two-form on the spin-bundle $\mathbb{S}^{A'}$ which must take the form

$$\mathcal{K}\lrcorner\nu_n=(K^{AA'_1\cdots A'_{2n-1}}e^{A'_{2n}}_{A}\pi_{A'_1}\cdots\pi_{A'_{2n}}\wedge\pi_{B'}\mathrm{d}\pi^{B'}+\chi_{A'_1\cdots A'_{2n}}\pi^{A'_1}\cdots\pi^{A'_{2n}})\Sigma_1$$

for some $K^{AA'_1\cdots A'_{2n-1}}$ and $\chi_{A'_1\cdots A'_{2n}}$.

The condition that this two-form descends to twistor space is the condition that

$$\pi^{A'}\nabla_{AA'}\lrcorner\mathrm{d}(\mathcal{K}\lrcorner\nu_n)=0.$$

This leads to Eq. (26) and

$$\nabla^{A}_{(A'_1}K_{A'_2\cdots A'_{2n})A}=\chi_{A'_1\cdots A'_{2n}}, \quad \nabla_{A(A'}\chi_{A'_1\cdots A'_{2n})}=0\,.$$

However, it can be checked that these two equations are a consequence of (26), if the first equation is taken to be the definition of $\chi_{A'_1\cdots A'_{2n}}$. □

A. The case of a hidden triholomorphic Killing symmetry

The case of a hidden triholomorphic Killing symmetry reduces to linear equations and can be worked through completely modulo some intergations and solving for implicit functions. This is effectively the case studied by Ivanov and Rocek[17] and generalized by Bielawski.[3]

In the triholomorphic Killing case, we have the following.

Lemma 4.2: Suppose $\mathcal{M}$ admits a hidden triholomorphic Killing symmetry. Then $\chi_{A'_1\cdots A'_{2n}}=0$ and there exists a spinor $\phi_{A'_2\cdots A'_{2n}}$ such that

$$\nabla_{AA'}\phi_{A'_1\cdots A'_{2n}}=K_{A(A'_1\cdots A'_{2n-1}}\varepsilon_{A'_{2n})A'}\,.$$

Proof: The vanishing of $\chi_{A'_1\cdots A'_{2n}}=0$ follows from the fact that $\mathcal{K}$ is tangent to the fibers of twistor space over $\mathbb{CP}^1$. The existence of $\phi_{A'_1\cdots A'_{2n}}$ follows from the fact that $\mathcal{K}$ is Hamiltonian with respect to the symplectic forms Σ_n up the fibers of μ and so is generated by a Hamiltonian $Q\in\Gamma(\mathcal{O}(2n))$. On pullback to the spin bundle $Q=\phi_{A'_1\cdots A'_{2n}}\pi^{A'_1}\cdots\pi^{A'_{2n}}$ and the condition that Q descends to twistor space is $\pi^{A'}\nabla_{AA'}Q=0$ and this gives the equation above. □

The above lemma shows that a Killing spinor on an ASD vacuum determines a function Q homogeneous of degree k on its twistor space $\mathcal{PT}$. This in turn implies the following lemma.

Lemma 4.3: If an ASD vacuum space–time admits a Killing spinor, its twistor space $\mathcal{PT}$ is an affine line bundle over $\mathcal{O}(k)$ with underlying translation bundle $\mathcal{O}(2-k)$.

Proof: The existence of a global twistor function homogeneous of degree k on $\mathcal{PT}$ gives a projection onto $p:\mathcal{PT}\to\mathcal{O}(k)$. Furthermore, the fiber is spanned by the Hamiltonian vector field of Q with respect to Σ, in local coordinates,

$$\mathcal{K}=\varepsilon^{AB}\frac{\partial Q}{\partial \omega^A}\frac{\partial}{\partial \omega^B}.$$

This is a vector field with values in $O(k-2)$. This gives each fiber an affine linear structure which is twisted globally by $\mathcal{O}(2-k)$, since, if a is a local section of $\mathcal{O}(2-k)$ over $\mathbb{CP}^1$, then $a\mathcal{K}$ is a vector whose flows determine an action of $\mathbb{C}$. Thus $\mathcal{PT}\to\mathcal{O}(k)$ is an affine line bundle over $\mathcal{O}(k)$ with underlying translation bundle $\mathcal{O}(2-k)$. □

Such affine line bundles are classified by elements $[f]$ of $H^1(\mathcal{O}(k),\mathcal{O}(2-k))$. In a Cech description, cover $\mathcal{O}(k)$ by open sets, U_i, and represent $[f]$ by its Cech representative $f_{ij}\in\Gamma(\mathcal{O}(2-k),U_i\cap U_j)$. Then $\mathcal{PT}$ is constructed by patching together the total space of $\mathcal{O}(2-k)\to U_i$ to $\mathcal{O}(2-k)\to U_j$ by translating the zero section by f_{ij}. The data $[f]$ therefore determines the twistor space. This proves the first part of the following theorem.

Theorem 4.4: *There is a one-to-one correspondence between ASD vacuum space–times* $(\mathcal{M},g)$ *admitting a valence* $(0,k)$ *Killing spinor and elements* $[f]$ *of* $H^1(\mathcal{O}(k),\mathcal{O}(2-k))$.

In this case, for $k\geqslant 3$, $\mathcal{M}$ *admits a natural map into* $\mathbb{C}^{k+1}=\odot^k\mathbb{S}^{A'}$ *which we coordinate with* $t^{A'_1\cdots A'_k}$. *The hyper-Kähler space* $\mathcal{M}$ *is determined as a subset of* $\mathbb{C}^{k+1}$ *by the* $k-3$ *constraints*

$$f_{A'_1\cdots A'_{k-4}}:=\oint_\Gamma \pi_{A'_1}\cdots\pi_{A'_{k-4}}f(Q,\pi_{A'})\pi\cdot \mathrm{d}\pi=0.$$

The basis of SD two-forms for g *is then given by the restriction of the forms*

$$\Sigma^{A'_1B'_1}=\psi_{B'_2\cdots B'_kA'_2\cdots A'_{k-2}}\mathrm{d}t^{A'_1\cdots A'_k}\wedge \mathrm{d}t^{B'_2\cdots B'_k}{}_{A'_k}, \tag{27}$$

to $\mathcal{M}$, *where*

$$\psi_{A'_1\cdots A'_{2k-4}}=\frac{1}{2\pi i}\oint_\Gamma \pi_{A'_1}\cdots\pi_{A'_{2k-4}}\frac{\partial f}{\partial Q}\pi\cdot\mathrm{d}\pi \tag{28}$$

is a field determined by an arbitrary element of $H^1(\mathcal{O}(k),\mathcal{O}(2-k))$.

Proof: If one wishes to obtain the space–time $(\mathcal{M},g,\nu)$ determined by a given twistor space, the first task is to locate the four-dimensional family of sections of the fibration $\mathcal{PT}\to\mathbb{CP}^1$.

Let $t^{A'_1\cdots A'_k}=t^{(A'_1\cdots A'_k)}$ be coordinates on the $\mathbb{C}^{k+1}=\odot^k\mathbb{S}^{A'}$ parameter space of sections $\sigma_t:\pi_{A'}\to Q=t^{A'_1\cdots A'_k}\pi_{A'_1}\cdots\pi_{A'_k}\in\Gamma(\mathcal{O}(k))$. Sections of $\mathcal{PT}\to\mathbb{CP}^1$ determine sections of $\mathcal{O}(k)$ by projection onto $\mathcal{O}(k)$. However, the affine line bundle $\mathcal{PT}$ only admits a section over some σ_t if the cohomology class $[f]$ vanishes on restriction to σ_t. If $[f]$ vanishes on restriction to σ_t, $\mathcal{PT}$ restricts to become the line bundle $\mathcal{O}(2-k)$ so that there is a $3-k$-dimensional family of sections over σ_t for $3-k>0$ or just the zero-section otherwise.

To obtain explicit formulas, we first note that $[f]$ determines a field

$$f_{A'_1\cdots A'_{k-4}}(t^{B'_1\cdots B'_k})=\oint_{\gamma\subset\sigma_t}\pi_{A'_1}\cdots\pi_{A'_{k-4}}f\pi_{B'}\mathrm{d}\pi^{B'}$$

on $\mathbb{C}^{k+1}$ (here we express the natural pairing as a contour integral over some contour γ_t in σ_t where here χ is a Cech representative). This vanishes at some $t^{A'_1\cdots A'_k}$ iff $[f]$ vanishes on the corresponding σ_t. Thus, for $3-k>0$, $\mathcal{M}$ is fibered over the zero set of $\chi_{A'_1\cdots A'_{k-4}}$ in $\mathbb{C}^{k+1}$ with $3-k$-dimensional fibers, and is simply identified with this zero set for $k\geqslant 3$.

In order to calculate the SD two-forms associated to the space–time, we use the method of Gindikin,[13] and pullback Σ to the spin-bundle. To this end, introduce local homogeneous coordi-

nates $(\pi_{A'},Q,\zeta_i)=(c\pi_{A'},cQ,c^{2-k}\zeta_i)$ on each set U_i of some Stein cover twistor space; here ζ_i is a fiber coordinate up the fibers of the affine line bundle $\mathcal{PT}\to\mathcal{O}(k)$ on U_i with patching relations $\zeta_i=\zeta_j+f_{ij}$ on $U_i\cap U_j$. In these coordinates

$$\Sigma=\mathrm{d}_h Q\wedge\mathrm{d}_h\zeta_i\,,$$

where d_h denotes the exterior derivative in which $\pi_{A'}$ is held constant, i.e., horizontal on the spin bundle over space–time (although slightly confusingly, vertical with respect to the fibration $\mathcal{PT}\to\mathbb{CP}^1$). This form Σ is globally defined on vector fields tangent to the fibers of $\mathcal{PT}\to\mathbb{CP}^1$ as f_{ij} does not depend on ζ_i.

In order to evaluate this, we need to find the values of ζ_i on the sections of $\mathcal{PT}\to\mathbb{CP}^1$. These are obtained by a splitting formula due to Sparling.

On a σ_t for which $f_{A'_1\cdots A'_{k-4}}(t^{B'_1\cdots B'_k})=0$, we can find $\zeta_i(t,\pi_{A'})$ such that

$$\zeta_i(t,\pi_{A'})=\zeta_j(t,\pi_{A'})+f_{ij}(t^{A'_1\cdots A'_k}\pi_{A'_1}\cdots\pi_{A'_k},\pi_{B'})\,. \tag{29}$$

For $k\geqslant 3$ this solution will be unique, but for $k<3$ we will be free to add $x^{A'_1\cdots A'_{k-2}}\pi_{A'_1}\cdots\pi_{A'_{k-2}}$ to the solution.

In the formula for Σ we can rearrange so that we have

$$\Sigma=\mathrm{d}_h Q\wedge\mathrm{d}_h\zeta_i=\mathrm{d}t^{A'_1\cdots A'_k}\wedge\mathrm{d}_h(\pi_{A'_1}\cdots\pi_{A'_k}\zeta_i)\,.$$

Applying d_h to Eq. (29), and multiplying by $k-3$ of the π's, we obtain

$$\mathrm{d}_h(\pi_{A'_1}\cdots\pi_{A'_{k-3}}\zeta_i)=\mathrm{d}_h(\pi_{A'_1}\cdots\pi_{A'_{k-3}}\zeta_j)+\frac{\partial f_{ij}}{\partial Q}\pi_{A'_1}\cdots\pi_{A'_{k-3}}\pi_{B'_1}\cdots\pi_{B'_k}\mathrm{d}t^{B'_1\cdots B'_k}\,.$$

The cocycle $\partial f_{ij}/\partial Q$ defines a class in $H^1(\mathcal{O}(k),\mathcal{O}(2-2k))$ so that the expression above takes values in $\mathcal{O}(-1)$ on $\mathbb{CP}^1$ for each fixed t. Thus the splitting as stated exists and is unique since $H^0(\mathbb{CP}^1,\mathcal{O}(-1))=H^1(\mathbb{CP}^1,\mathcal{O}(-1))=0$. This gives

$$\mathrm{d}_h(\pi_{A'_1}\cdots\pi_{A'_{k-3}}\zeta_i)=k_{i,A'_1\cdots A'_{k-3}B'_1\cdots B'_k}\mathrm{d}t^{B'_1\cdots B'_k}\,,$$

where $k_{i,A'_1\cdots A'_{2k-3}}$ is defined by the splitting relation

$$k_{i,A'_1\cdots A'_{2k-3}}-k_{j,A'_1\cdots A'_{2k-3}}=\pi_{A'_1}\cdots\pi_{A'_{2k-3}}\frac{\partial f_{ij}}{\partial Q}$$

or alternatively the contour integral formula

$$k_{i,A_1,\cdots A'_{2k-3}}=\oint_{\Gamma_i}\rho_{A'_1}\cdots\rho_{A'_{2k-3}}\frac{1}{\pi\cdot\rho}\frac{\partial f_{ij}(Q,\rho_{A'})}{\partial Q}\rho\cdot\mathrm{d}\rho, \tag{30}$$

where for simplicity we assume a two set cover and the contour γ_i is chosen so that $\gamma_i-\gamma_j$ surrounds $\pi=\rho$. It follows that

$$\psi_{A'_1\cdots A'_{2k-4}}=\pi^{A'_{2k-3}}k_{A'_1\cdots A'_{2k-4}A'_{2k-3}}=\oint_{\gamma_i}\rho_{A'_1}\cdots\rho_{A'_{2k-4}}\frac{\partial f_{ij}(Q,\rho_{A'})}{\partial Q}\rho\cdot\mathrm{d}\rho \tag{31}$$

is the field on $\mathbb{C}^{k+1}$ naturally associated to $\partial f/\partial Q$.

We therefore obtain the formula

$$\Sigma = \mathrm{d}t^{A'_1\cdots A'_k} \wedge \pi_{A'_1}\pi_{A'_2}\pi_{A'_3} k_{A'_4\cdots A'_{2k}} \mathrm{d}t^{A'_{k+1}\cdots A'_{2k}}.$$

Define the indexed two-forms $\Sigma^{(B'_1B'_2)|(A'_5\cdots A'_{2k})}$ by

$$\mathrm{d}t^{B'_1\cdots B'_3(A'_4\cdots A'_k} \wedge \mathrm{d}t^{A'_{k+1}\cdots A'_{2k})} = \varepsilon^{(A'_4|(B'_1} \Sigma^{B'_2B'_3)|A'_5\cdots A'_{2k})C'}.$$

(This indexed two-form can be represented as

$$\Sigma^{(B'_1B'_2)|(A'_5\cdots A'_{2k})} = \frac{3k}{2} \mathrm{d}t^{(B'_1B'_2)|(A'_5\cdots A'_{k+1}}_{C'} \wedge \mathrm{d}t^{A'_{k+2}\cdots A'_{2k})C'}$$

$$+ a_k \varepsilon^{(A'_5|(B'_1} \varepsilon^{B'_2)|A'_6} \mathrm{d}t^{A'_7\cdots A'_{k+1}}_{C'D'E'} \wedge \mathrm{d}t^{A'_{k+2}\cdots A'_{2k})C'D'E'},$$

where a_k is a conbinatorial constant depending on k.) With this, we find that a $\pi_{A'}$ is contracted onto $k_{i,A'_1\cdots A'_{2k-3}}$ so that (31) gives

$$\Sigma = \pi_{A'_1}\pi_{A'_2}\psi_{A'_3\cdots A'_{2k-2}} \Sigma^{A'_1\cdots A'_{2k-2}}.$$

Thus, the result follows. □

Remarks:

(i) If $k>3$, then there exists a potential for $\psi_{A'_1\cdots A'_{2k-4}}$,

$$\psi_{A'_1\cdots A'_{2k-4}} = \partial_{A'_{k-3}\cdots A'_{2k-4}} f_{A'_1\cdots A'_{k-4}},$$

where

$$f_{A'_1\cdots A'_{k-4}} = \oint_\Gamma \rho_{A'_1}\cdots\rho_{A'_{k-4}} f \rho\cdot\mathrm{d}\rho.$$

The space–time is a four-dimensional surface $\chi_{A'_1\cdots A'_{k-4}}=0$ in $k+1$-dimensional moduli space of $\mathcal{O}(k)$ sections coordinatized by $x^{A'_1\cdots A'_k}$.

(ii) $k=3$: The field $\psi_{A'_1A'_2}$ does not have a potential, and no conditions have to be imposed on the moduli space of $\mathcal{O}(3)$ to find the space–time. This is because $H^0(\mathbb{CP}^1,\mathcal{O}(3)) = H^0(\mathbb{CP}^1,\mathcal{O}(1)\oplus\mathcal{O}(1))$, and $x^{A'_1A'_2A'_3}$ has as many components as $x^{AA'}$. Ward[32] regards $\psi_{A'_1A'_2}$ as a self-dual Maxwell field on $\mathbb{C}^4$.

(iii) The case $k=2$ implies the existence of a triholomorphic Killing vector and was considered by Tod and Ward in Ref. 31. Now

$$\psi = \oint_\Gamma \frac{\partial f}{\partial Q} \rho\cdot\mathrm{d}\rho$$

is a solution to the three-dimensional wave equation. The relation between our construction and the description of the Gibbons–Hawking metric form in Sec. III A 1 is given by

$$F(x^{A'B'}) = \oint_\Gamma \frac{G(\pi_{A'},Q)}{(\pi\cdot o)^2}\pi\cdot\mathrm{d}\pi, \quad \psi = F_{pp} = \oint_\Gamma (\pi\cdot o)^2 \frac{\partial^2 G}{\partial Q^2}\pi\cdot\mathrm{d}\pi,$$

where

$$x^{A'B'} := \begin{pmatrix} -p & y/2 \\ y/2 & w \end{pmatrix}.$$

B. Relation between the two constructions

In this section we relate the hyper-Kähler slices (4) of the symmetric hierarchy introduced in Sec. III to the method described above.

Proposition 4.5: Let $f \in H^1(\mathcal{O}(2n),\mathcal{O}(2-2n))$ *give rise to the ZRM field* (28) *with* $k=2n$. *Then hyper-Kähler metrics arising from Proposition 3.3 form a subclass of metrics from Proposition 4.4 if*

$$F=\oint_\Gamma (\pi\cdot o)^{-2}G(Q,\pi_{A'})\pi\cdot \mathrm{d}\pi, \quad \textit{where} \quad (\pi\cdot o)^2\frac{\partial G}{\partial Q}=f\in H^1(\mathcal{O}(2n),\mathcal{O}(2-2n)),$$

where $o_{A'}$ *is a constant spinor*.

Proof: Let $(Q,\pi_{A'})$ be homogeneous coordinates on the total space of $\mathcal{O}(2n)$ bundle. Let us choose a constant spinor $o_{A'}$ and parametrize a section of the $\mathcal{O}(2n)\to\mathbb{CP}^1$ by $2n+1$ complex numbers

$$x^{A'_1\cdots A'_{2n}}=\left.\frac{\partial^{2n}Q}{\partial\pi_{A'_1}\cdots\partial\pi_{A'_{2n}}}\right|_{\pi_{A'_i}=o_{A'}}.$$

The coordinates $x^{A'_1\cdots A'_{2n}}$ on $\mathbb{C}^{2n+1}$ correspond to $t^0,\ldots,t^{2n}$ by

$$t^i=\binom{2n}{i}x^{A'_1A'_2\cdots A'_{2n}}o_{A'_1}\cdots o_{A'_i}\iota_{A'_{i+1}}\cdots\iota_{A'_{2n}}(-1)^{n-i}, \quad i=0,\ldots,2n.$$

Define

$$\frac{\partial}{\partial t^i}=\iota^{A'_1}\cdots\iota^{A'_i}o^{A'_{i+1}}\cdots o^{A'_{2n}}\frac{\partial}{\partial x^{A'_1\cdots A'_{2n}}}.$$

Let

$$F=\oint_\Gamma (\pi\cdot o)^{-2}G(Q,\pi_{A'})\pi\cdot \mathrm{d}\pi, \quad \text{where} \quad (\pi\cdot o)^2\frac{\partial G}{\partial Q}=f\in H^1(\mathcal{O}(2n),\mathcal{O}(2-2n)).$$

We have

$$\begin{aligned} f_{A'_1\cdots A'_{2n-4}} &= \oint_\Gamma \pi_{A'_1}\cdots\pi_{A'_{2n-4}}f\pi\cdot\mathrm{d}\pi \\ &= \oint_\Gamma \pi_{A'_1}\cdots\pi_{A'_{2n-4}}(\pi\cdot o)^2\frac{\partial G}{\partial Q}\pi\cdot\mathrm{d}\pi \\ &= o^{A'_{2n-3}}\cdots o^{A'_{2n}}\frac{\partial}{\partial x^{A'_1\cdots A'_{2n}}}\oint_\Gamma(\pi\cdot o)^{-2}G\pi\cdot\mathrm{d}\pi=\frac{\partial F}{\partial x^{A'_1\cdots A'_{2n-4}0'0'0'0'}}. \end{aligned}$$

Therefore fixing $f_{A'_1\cdots A'_{2n-4}}$ is equivalent to fixing $\partial F/\partial t^i$ for $i<2n-3$. Moreover, the global twistor function is given by

$$Q=(\omega_n\cdot\iota)(\pi\cdot\iota)^n=(\pi\cdot\iota)^{2n}\sum_{i=0}^{2n}\lambda^i t^{2n-i}.$$

□

V. ALE SPACES REVISITED; FINITE-GAP SOLUTIONS OF ASD VACUUM EQUATIONS

One way to generalize the Novikov construction of finite gap solutions of the Korteweg–de Vries equation to hyper-Kähler equations would be to study solutions to (8) which are invariant under three commuting hidden symmetries that we shall take to be triholomorphic:

$$\partial_{T_1} := \sum_{i=1}^{k} a_i \frac{\partial}{\partial t_i}, \quad \partial_{T_2} := \sum_{i=1}^{l} b_i \frac{\partial}{\partial t_i}, \quad \partial_{T_3} := \sum_{i=1}^{m} c_i \frac{\partial}{\partial t_i}, \qquad \text{where } a_i, b_i, c_i \text{ are constant,}$$

and the propagation of Θ along the parameters t_i is determined by the recursion relations (9). This would reduce (8) down to an ODE.

Rather than performing the explicit reduction to an ODE, we see from the twistor picture that the twistor space must have three projections onto the total space of the line bundle $\mathcal{O}(n)$ for three values of n. Thus we have a map of the twistor space $\mathcal{PT}$ into $\mathcal{O}(p)\oplus\mathcal{O}(q)\oplus\mathcal{O}(r)$ and so $\mathcal{PT}$ can be realized as a hypersurface in this space (although there may need to be some blowup or resolution of singularities where the map fails to be an embedding). If we realize $\mathcal{PT}$ as the zero set of a function F taking values in a line bundle of degree s, then we must have, for rational curves to have the appropriate normal bundle, that $p+q+r=2+s$.

We will now see that the ALE hyper-Kähler spaces fall precisely into this above class.

It is well known that hyper-Kähler manifolds $(\mathcal{M},g)$, which have the topology of $\mathbb{R}^4$ at infinity, and approach the flat Euclidean metric $\eta=\mathrm{d}x_1^2+\cdots+\mathrm{d}x_4^2$ sufficiently fast, in the sense that

$$g_{ab}=\eta_{ab}+O(r^{-4}), \quad (\partial_a)^p(g_{bc})=O(r^{-4-p}), \quad r^2=x_1^2+\cdots+x_4^2 \tag{32}$$

have to be flat. A weaker asymptotic condition one can impose on g is assymptoticaly locally Euclidean (ALE).

The ALE spaces are noncompact, complete hyper-Kähler manifolds which satisfy (32) only locally for $r\to\infty$. Globally the neighborhood of infinity must look like $S^3/\Gamma\times\mathbb{R}$, where Γ is a finite group of isometries acting freely on S^3 (a Kleinian group). These manifolds belong to the class of *gravitational instantons* because their curvature is localized in a "finite region" of a space–time.

Finite subgroups of $\Gamma\subset\mathrm{SU}(2)$ correspond Platonic solids in $\mathbb{R}^3$. They are the cyclic groups, and the binary dihedral, tetrahedral, octahedral and icosahedral groups (one can think about the last three as Möbius transformations of $S^2=\mathbb{CP}^1$ which leave the points corresponding to vertices of a given Platonic solid fixed). Each of them can be related to a Dynkin diagram of a simple Lie algebra. All Kleinian groups act on $\mathbb{C}^2$, and the "infinity" $S^3\subset\mathbb{C}^2$. Let $(z_1,z_2)\in\mathbb{C}^2$. For each Γ there exist three invariants x,y,z which are polynomials in (z_1,z_2) invariant under Γ. These invariants satisfy some algebraic relations which we list below:

Group	**Dynkin diagram**	**Relation** $F_\Gamma(x,y,z)=0$
cyclic	A_k	$xy-z^k=0$
dihedral	D_{k-1}	$x^2+y^2z+z^k=0$
tetrahedral	E_6	$x^2+y^3+z^4=0$
octahedral	E_7	$x^2+y^3+yz^3=0$
icosahedral	E_8	$x^2+y^3+z^5=0$

In each case

$$\mathbb{C}^2/\Gamma\subset\mathbb{C}^3=\{(x,y,z)\in\mathbb{C}^3, F_\Gamma(x,y,z)=0\}.$$

The manifold $\mathcal{M}$ on which an ALE metric is defined is obtained by minimally resolving the singularity at the origin of $\mathbb{C}^2/\Gamma$. This desingularization is achieved by taking $\mathcal{M}$ to be the zero set of

$$\tilde{F}_\Gamma(x,y,z)=F_\Gamma(x,y,z)+\sum_{i=1}^{r} a_i f_i(x,y,z),$$

where f_i span the ring of polynomials in (x,y,z) which do not vanish when $\partial_x F_\Gamma=\partial_y F_\Gamma=\partial_z F_\Gamma=0$. The dimension r of this ring is equal to the number of nontrivial conjugacy classes of Γ which is $k-1,\ k+1,\ 6,\ 7$ and 8, respectively.[6] Kronheimer[18,19] proved that for each Γ a unique hyper-Kähler metric exists on a minimal resolution $\mathcal{M}$, and that this metric is precisely the ALE metric with $\mathbb{R}^4/\Gamma$ as its infinity. His construction was a combination of the hyper-Kähler quotient[16] with twistor theory.

In each case the twistor space is the three-dimensional hyper-surface $\tilde{F}_\Gamma(x,y,z,\lambda)=0$ in the rank-three bundle $\mathcal{O}(p)\oplus\mathcal{O}(q)\oplus\mathcal{O}(r)\to\mathbb{CP}^1$. Now $x(\lambda)\in\mathcal{O}(p), y(\lambda)\in Q(q), z(\lambda)\in O(r)$ are polynomials in λ, $f_i=f_i(x,y,z)$, and $a_i=a_i(\lambda)$. Therefore

$$\mathcal{PT}\to\mathcal{O}(p),\quad \mathcal{PT}\to\mathcal{O}(q),\quad \mathcal{PT}\to\mathcal{O}(r),$$

and Lemma 4.2 implies that the corresponding hyper-Kähler metrics admit three commuting hidden symmetries, and the heavenly equation (8) reduces to an ODE.

The degrees p,q and r are such that $\tilde{F}_\Gamma(x,y,z,\lambda)$ is a function homogeneous of some degree s. Therefore

$$\tilde{F}_\Gamma:\mathcal{O}(p)\oplus\mathcal{O}(q)\oplus\mathcal{O}(r)\to\mathcal{O}(s).$$

To determine the integers p,q,r,s take the determinants of the above, and notice that the normal bundle to an $\mathcal{O}(1)\oplus\mathcal{O}(1)$ section of $\mathcal{PT}\to\mathbb{CP}^1$ will have the Chern class $p+q+r-s=2$. This gives us the following:

$$\begin{aligned}
A_k\quad & \mathcal{PT}=\{(x,y,z,\lambda)\in\mathcal{O}(k)\oplus\mathcal{O}(k)\oplus\mathcal{O}(2)\to\mathbb{CP}^1,\\
& xy-z^k-a_1z^{k-2}-\cdots-a_{k-1}=0\},\\
D_{k-1}\quad & \mathcal{PT}=\{(x,y,z,\lambda)\in\mathcal{O}(2k)\oplus\mathcal{O}(2k-2)\oplus\mathcal{O}(4)\to\mathbb{CP}^1,\\
& x^2+y^2z+z^k+a_1y^2+a_2y+a_3z^{k-2}+\cdots+a_kz+a_{k+1}=0\},\\
E_6\quad & \mathcal{PT}=\{(x,y,z,\lambda)\in\mathcal{O}(12)\oplus\mathcal{O}(8)\oplus\mathcal{O}(6)\to\mathbb{CP}^1,\\
& x^2+y^3+z^4+y(a_1z^2+a_2z+a_3)+a_4z^2+a_5z+a_6=0\},\\
E_7\quad & \mathcal{PT}=\{(x,y,z,\lambda)\in\mathcal{O}(18)\oplus\mathcal{O}(12)\oplus\mathcal{O}(8)\to\mathbb{CP}^1,\\
& x^2+y^3+yz^3+y^2(a_1z+a_2)+y(a_3z+a_4)+a_5z^2+a_6z+a_7=0\},\\
E_8\quad & \mathcal{PT}=\{(x,y,z,\lambda)\in\mathcal{O}(30)\oplus\mathcal{O}(20)\oplus\mathcal{O}(12)\to\mathbb{CP}^1,\\
& x^2+y^3+z^5+y(a_1z^3+a_2z^2+a_3z+a_4)+a_5z^3+a_6z^2+a_7z+a_8=0\}.
\end{aligned}\tag{33}$$

Note that these spaces are not quite the full nonsingular twistor space as there will be singular points where $\tilde{F}_\Gamma$ vanishes together with its first derivatives. These singularities can, however, be resolved, see Ref. 19.

We observe that these twistor spaces have projections onto $\mathcal{O}(2n)$ for $2n=p,q,r$ and this corresponds to the existence of three independent commuting triholomorphic hidden symmetries. The simplest description along the lines of Sec. IV arises for the lowest value of n, i.e., when we

project onto the z coordinates in the above construction. It is clear from the above formulas that the fibers of this projection are affine conics in the A_k and D_k cases, and affine elliptic curves in the E_k cases.

From now on we shall drop the subscript Γ, because the construction we shall describe applies to all cases. These twistor spaces can all be described as affine line bundles over $\mathcal{O}(r)$ in effect by uniformizing the affine conics or elliptic curves that make up the fibers of $\mathcal{PT}\to\mathcal{O}(r)$. The affine line bundle is determined by a cohomology class in $H^1(\mathcal{O}(r),\mathcal{O}(2-r)$ which can be evaluated as a linear field on $\mathbb{C}^{r+1}$. The ALE space can then be realized as (a branched cover of) the zero set of this linear field in the real slice $\mathbb{R}^{r+1}$ as in Theorem 4.4.

To make the description more concrete, we now find a patching description of the relevant cohomology class in $H^1(\mathcal{O}(r),\mathcal{O}(2-r)$. We exclude the curve(s) on which both $\tilde{F}_x=0$ and $\tilde{F}_y=0$ so that we can cover the twistor space by the two open sets $U,\tilde{U}$ such that $\tilde{F}_x\neq 0$ in U and $\tilde{F}_y\neq 0$ in $\tilde{U}$. We use (y,z,λ) and (x,z,λ) as local coordinates in U and $\tilde{U}$, respectively. The symplectic form Σ on each fiber of $\mathcal{PT}\to\mathbb{CP}^1$ is given by

$$\frac{dy\wedge dz}{\tilde{F}_x} \quad \text{in } U, \quad \text{or} \quad \frac{-dx\wedge dz}{\tilde{F}_y} \quad \text{in } \tilde{U}.$$

These arise from the formula $\Sigma=\oint dx\wedge dy\wedge dz/\tilde{F}$ with the contour being a small circle surrounding $\tilde{F}=0$. The global homogeneous function z gives rise to a homogeneity $r-2$ Hamiltonian vector field X_z tangent to the fibers of $\mathcal{PT}\to\mathcal{O}(r)$. From the formula $X_z\lrcorner\Sigma=dz$ we deduce that

$$X_z=\tilde{F}_x\frac{\partial}{\partial y} \quad \text{in } U, \quad X_z=-\tilde{F}_y\frac{\partial}{\partial x} \quad \text{in } \tilde{U}.$$

We now introduce new coordinates (u,z,λ) and $(\tilde{u},z,\lambda)$ on U and $\tilde{U}$, respectively, where the fiber coordinates in u in $U\to\mathcal{O}(r)$ and $\tilde{u}$ in $\tilde{U}\to\mathcal{O}(r)$ satisfy $X_z(u)=X_z(\tilde{u})=1$. Therefore

$$u(y,z)=\int_\sigma^{\tilde{F}_x=1}\frac{dy}{\tilde{F}_x}, \quad \tilde{u}(x,z)=-\int_\sigma^{\tilde{F}_y=1}\frac{dx}{\tilde{F}_y}$$

for some σ, and the patching function is given on the overlap by

$$f(z,\lambda)=u-\tilde{u}=\int_{\tilde{F}_y=1}^{\tilde{F}_x=1}\frac{dy}{\tilde{F}_x}. \tag{34}$$

In the above formula x should be determined in terms of (y,z,λ) using $\tilde{F}=0$ before the integral is evaluated. The upper and lower limits will then involve $y=y(z,\lambda)$.

In the case of A_k ALE space we can assume that

$$z^k+a_1z^{k-2}+\cdots+a_{k-1}=\prod_{j=1}^{k}(z-p_j(\lambda)), \quad \text{where } p_j\in\Gamma(\mathcal{O}(2)).$$

(See Refs. 15 and 6 for further discussion of this point.) A simple integration yields $f=\ln\Pi_{j=1}^k(z-p_j(\lambda))$, and from Proposition 4.5 we find

$$G=\sum_{j=1}^{k}(z-p_j)(\ln(z-p_j)-1).$$

For D_{k-1} we can redefine z and a_j to get rid of terms linear and quadratic in y, and write

$$\tilde{F}=x^2-y^2z-\prod_{j=1}^{k}(z-q_j(\lambda)) \quad \text{where } q_j\in\Gamma(\mathcal{O}(4)).$$

Now (34) yields

$$f=\frac{1}{\sqrt{z}}\ln\frac{(z-4z\Pi_{j=1}^{k}(z-q_j(\lambda)))^{1/2}+\sqrt{z}}{(1+4z\Pi_{j=1}^{k}(z-q_j(\lambda)))^{1/2}-1}.$$

In the remaining cases E_6, E_7 and E_8 the fibers of $\mathcal{PT}\to\mathcal{O}(r)$ are elliptic curves $x^2=4y^2+g_1y+g_2$ (in case of E_7 one needs to redefine y,z,a_i to obtain this canonical form). The periods g_1,g_2 are polynomials in z of order less or equal to 5 which can be determined from (33). The fibers can therefore be parametrized by the Weierstrass elliptic function. The cohomology class is represented by an elliptic integral

$$f=\frac{1}{2}\int_{y_0}^{y_1}\frac{\mathrm{d}y}{\sqrt{4y^3+g_1y+g_2}},$$

where y_1 and y_0 are roots of $4y^3+g_1y+g_2-\frac{1}{4}=0$ and $12y^2+g_1-1=0$, respectively.

One can now, in principal, take these cohomology classes and integrate them to obtain a linear field with $r-3$ components on $\mathbb{C}^{r+1}$ the vanishing of which will determine the complexified ALE space as a submanifold. This above description is not completely satisfactory for two related reasons. First, the description of the ALE space will not be global; the projection from the true ALE space to $\mathbb{C}^{r+1}$ can be many to one, and can have irregular values. Second, the limits of integration above defining the cohomology classes actually branch and are not completely well defined.

Further work is required to make this a useful description of ALE spaces. It seems likely that these are the only complete hyper-Kähler metrics with three triholomorphic hidden symmetries.

VI. HIERARCHIES FOR THE GENERALIZED CONFORMAL ANTI-SELF-DUALITY EQUATIONS

In this section we extend the concept of a hierarchy from that of Ref. 8 for the four-dimensional hyper-Kähler equations to a generalization of the conformal anti-self-duality equations (and in the process give new and more geometric formulations for the hyper-Kähler hierarchy than in Ref. 8). The guiding motivation for these definitions comes from the twistor theory. However, we first define the various concepts in space–time terms, and then discuss the twistor theory subsequently. We shall, for convenience, work in the holomorphic category. Real versions of the various structures and equations can then be obtained subsequently by demanding the existence of an antiholomorphic involution σ fixing a real slice and with specified action on the various geometric structures.

We will abbreviate the term conformal anti-self-duality to CASD and generalized CASD to GCASD. Unfortunately this terminology is nonstandard but is designed to be consistent with the corresponding discussion for the anti-self-dual Yang–Mills equations given in Ref. 21. The generalization of the CASD case is a mild generalization of quaternionic structures discussed in Ref. 28 and they have been termed paraconformal structures, see Ref. 2, and Grassman structures,[1,4] where many properties, including the twistor theory, of these spaces are studied. Here we shall refer to them as generalized CASD, GCASD, spaces. The hierarchies defined here are a special case of the $\mathcal{P}$-structures of Gindikin (Ref. 14, and references therein).

Definition 6.1: A solution to the GCASD hierarchy consists of the data $(\mathcal{M},\mathbb{S},\tilde{\mathbb{S}},e^{AA'_1\cdots A'_n})$ *defined as follows:* $\mathcal{M}$ *is a manifold of dimension* $r(n+1)$, $\mathbb{S}$ *and* $\tilde{\mathbb{S}}$ *are vector bundles of rank* r *and* 2, *respectively, we use abstract indices* A *and* A' *to denote membership of* $\mathbb{S}$ *and* $\tilde{\mathbb{S}}$, *respec-*

tively; when realized concretely, $A=0,1,\ldots,r-1$ *and* $A'=0',1'$. *The indexed one-form* $e^{AA'_1\cdots A'_n}$, *symmetric over its primed indices, determines an isomorphism* $T\mathcal{M}=\mathbb{S}\otimes\odot^n\tilde{\mathbb{S}}$ *at every point.*

An element $\pi_{A'}$ *of* $\tilde{\mathbb{S}}^*$ *at* $m\in\mathcal{M}$ *determines an* rn*-plane element*

$$z(m)_\pi=\{V\in T_m\mathcal{M}, V\lrcorner e^{AA'_1\cdots A'_n}\pi_{A'_1}\cdots\pi_{A'_n}=0\}.$$

Such an rn*-plane element will be said to be an* α*-plane element at* m. *An* α*-surface is an* rn*-dimensional surface whose tangent space defines an* α*-plane element at each of its points.*

The GCASD hierarchy equations are the requirement that there exists a full family of α*-surfaces, with a unique* α*-surface through each* $z(m)_\pi$.

The notation derives from the identification of these bundles with the spin bundles of a conformal structure in four-dimensions, $r=2$, $n=1$. It will also be convenient to introduce a "clumped" index i for the $n+1$-dimensional vector space $\odot^n\tilde{\mathbb{S}}$. When the indices are realized concretely by a choice of a frame for $\tilde{\mathbb{S}}$ with components labeled by 0 and 1, there is a standard correspondence between the ith component for the clumped index and the component with i 1's and $n-i$ 0's, so that i naturally goes from 0 to n.

We now assume that we have a solution to the CASD hierarchy so that we have a full complement of α-surfaces and that, shrinking $\mathcal{M}$ to a convex neighborhood of a point if necessary, the space of these α-surfaces is a manifold. We can then define the following.

Definition 6.2: The space of such α*-surfaces will be called the twistor space and is denoted* $\mathcal{PT}$.

Twistor space is an $r+1$-dimensional complex manifold.

Theorem 6.3: *The twistor space determines and is determined by the GCASD hierarchy. The correspondence is stable under small deformations of the complex structure of* $\mathcal{PT}$ *or of the GCASD hierarchy.*

Proof: This is a straightforward extension of Penrose's nonlinear graviton construction. The correspondence can be studied by means of the double fibration

$$\begin{array}{ccc} & P\tilde{\mathbb{S}} & \\ p\swarrow & & \searrow q \\ \mathcal{M} & & \mathcal{PT}. \end{array}$$

Points $m\in M$ correspond to rational curves $L_m:=q(p^{-1}(m))\equiv\mathbb{CP}^1$ in $\mathcal{PT}$. The normal bundle of these rational curves is $N=\mathbb{S}\otimes\mathcal{O}(n)$ where $\mathcal{O}(n)$ is the line bundle of Chern class n on $\mathbb{CP}^1$; this follows from the fact that, since the tangent space of $z(m)_\pi$ is the kernel of $e^{AA'_1\cdots A'_n}\pi_{A'_1}\cdots\pi_{A'_n}$, the section of the normal bundle corresponding to a vector V can be identified with $V\lrcorner e^{AA'_1\cdots A'_n}\pi_{A'_1}\cdots\pi_{A'_n}$, a function with values in $\mathbb{S}$ with homogeneity n. However, sections of $\mathcal{O}(n)$ can be identified with functions homogeneous degree n, and so the normal bundle is $\mathbb{S}\otimes\mathcal{O}(n)$ as claimed.

With knowledge of the normal bundle, Kodaira theory can now be applied and shows that, since $H^1(\mathbb{CP}^1,N)=H^1(\mathbb{CP}^1,\mathrm{End}(N))=0$, the moduli space of curves has $\dim(H^0(\mathbb{CP}^1,\mathbb{S}\otimes\mathcal{O}(n))=r(n+1)$ dimensions, contains $\mathcal{M}$ and $T_m\mathcal{M}\equiv\Gamma(\mathbb{S}\otimes\mathcal{O}(n))\equiv\mathbb{S}\otimes\odot^n\tilde{\mathbb{S}}$. Points of $\mathcal{PT}$ clearly then correspond to integrable α-surfaces in $\mathcal{M}$. Kodaira theory also provides the stability of the correspondence under small deformations. See Refs. 22 and 23 for general constructions that apply to these situations. □

Remark: The $\mathcal{P}$-structures of Gindikin are more general but can be understood easily in this context as arising naturally on moduli spaces of rational curves in some complex manifold whose normal bundles are $\mathcal{O}(k_1)\oplus\cdots\oplus\mathcal{O}(k_r)$ with the k_i not being required to be equal. Such prescriptions for the normal bundle are unstable under deformations of the underlying complex manifold

unless no two of the k_i differ by more than one. Under deformations of the complex structure, in the moduli space of such rational curves, the normal bundle will jump so that a dense open set will be the stable case where the normal bundle will be $E\otimes\mathcal{O}(k)\oplus F\otimes\mathcal{O}(k+1)$ with E and F trivial bundles.

This additional generality can be important. For example, if we wish to discuss generalizations of the Ward construction, the twistor space has the structure of a holomorphic vector bundle over a lower dimensional space. In this case, the normal bundle of the rational curves along the fibers is usually taken to have degree 0, whereas the normal bundle of its projection into the bases will usually be required to have a higher degree normal bundle.

These geometric structures fall into the category of involutive G-structures studied by Merkulov.[22,23] In particular, one can exploit his theorems to deduce the existence of connections compatible with the geometric structure. However, for the most part, they must have torsion, although they fall into Merkulov's category of "G-structures with very little torsion."[23]

Lemma 6.4: For $r\geqslant 2$, $n\geqslant 1$, there exists connections on $\mathbb{S}$ and $\widetilde{\mathbb{S}}$ such that the induced connection on TM has torsion with nonvanishing irreducible parts only in $\mathbb{S}\otimes\odot^2\mathbb{S}^*\otimes\odot^{n-2}\widetilde{\mathbb{S}}$ and $\mathbb{S}^*\otimes\odot^{n-4}\widetilde{\mathbb{S}}$ where we take $\odot^n\widetilde{\mathbb{S}}=\mathbb{C}$ for $n=0$ or zero for $n<0$. There exists a unique choice for such a connection when $n>1$ and unique up to a one-form for $n=1$ (which can be taken to be exact with appropriate choices).

Proof: Merkulov reformulates the moduli spaces considered above as Legendrian moduli spaces of holomorphically embedded $\mathbb{CP}^1\times\mathbb{CP}^{r-1}$'s in the projective cotangent bundle $PT^*\mathcal{PT}$ of twistor space. A rational curve, $\mathbb{CP}^1$ in $\mathcal{PT}$ determines its projective conormal bundle in $PT^*\mathcal{PT}$, i.e., the one-forms up to scale that annihilate the tangent space of $\mathbb{CP}^1$. This correspondence is studied by means of the following double fibration

$$\begin{array}{ccc} & P\widetilde{\mathbb{S}}\times P\mathbb{S}\subset P(T^*M) & \\ & \mu\swarrow \qquad \searrow\nu & \\ M & & P(T^*\mathcal{PT})\,. \end{array}$$

Merkulov's method uses the contact line bundle L which is the dual to the tautological line bundle $T^*\mathcal{PT}\to P(T^*\mathcal{PT})$. On restriction to a $\mathbb{CP}^1\times\mathbb{CP}^{r-1}$, it gives $\mathcal{O}(n,1)$ where $\mathcal{O}(p,q)$ is the product of the pullback of $\mathcal{O}(p)$ from $\mathbb{CP}^1$ with the pullback of $\mathcal{O}(q)$ frpm $\mathbb{CP}^{r-1}$.

Merkulov shows that the minimal torsion of an affine connection preserving the G-structure (or obstruction to obtaining a torsion free connection preserving the tensor decomposition of the tangent space) is then measured by a geometrically obtained class in $H^1(\mathbb{CP}^1\times\mathbb{CP}^{r-1},L\otimes\odot^2(J^1L)^*)$ and the freedom in the resulting connection is given by $H^0(\mathbb{CP}^1\times\mathbb{CP}^{r-1},L\otimes\odot^2(J^1L)^*)$.

These groups can be computed as follows. The first jet of a section of $\mathcal{O}(n)$, $n\neq 0$, at a point of $\mathbb{CP}^{r-1}$ can be encoded into the derivative of a homogeneous degree n function with respect to the $r+1$ homogeneous coordinates. The value of the function is then retrieved from this by Euler's homogeneity equations, $\pi_A\partial f/\partial\pi_A=nf$. Thus, the sheaf J^1L on $\mathbb{CP}^1\times\mathbb{CP}^r$ can be understood as the kernel

$$0\to J^1L\to\mathbb{S}^*(n-1,1)\oplus\widetilde{\mathbb{S}}^*(n,0)\xrightarrow{(\pi_A,-\pi_{A'})}\mathcal{O}(n,1)\to 0$$

since, in the third map, we are imposing the requirement that the Euler homogeneity relation for each factor leads to the same value for f.

The cohomology groups $H^i(\mathbb{CP}^1\times\mathbb{CP}^{r-1},L\otimes\odot^2(J^1L)^*)$ can therefore be calculated by consideration of the long exact cohomology sequence arising from the short exact sequence

$$0\to \mathbb{S}^*(-n,0)\oplus\tilde{\mathbb{S}}^*(1-n,-1)\xrightarrow{\odot(\pi_B,\pi_{B'})}\odot^2\mathbb{S}^*(-n,1)\oplus\mathbb{S}\otimes\tilde{\mathbb{S}}(1-n,0)\oplus\odot^2\tilde{\mathbb{S}}(2-n,-1)$$
$$\to L\otimes\odot^2(J^1L^*)\to 0,$$

where π_A and $\pi_{A'}$ are the homogenous coordinates on $\mathbb{CP}^{r-1}$ and $\mathbb{CP}^1$, respectively. □

Note that the Merkulov framework is not quite equivalent to ours in the sense that it only requires knowledge of the total space $P(T^*\mathcal{PT})$ but does not require that it be realized as the projective cotangent bundle of some $\mathcal{PT}$. The results are only inequivalent for $r=1$, $n<3$ and $r=2$, $n=1$. In these cases the results are well known, for example, the full theory of the latter case goes back to Penrose in 1976.[25] The Merkulov framework does not see the curvature conditions that arise from existence of $\mathcal{PT}$, but gives the correct result for the existence of and freedom in choosing compatible torsion-free affine connections.

The cases $r=1$ are also well known, but for $n=1,2$ do not fall satisfactorily into the Merkulov framework. For $n=1$, there is a projective structure, i.e., an equivalence class of torsion-free connections that share the same unparametrized geodesics, with freedom given by a one-form. For $n=2$ there exists a unique torsion-free connection compatible with a conformal structure. For $n=3$ the connection is still torsion-free, but not subsequently for higher n.

The general $n=1$ case was studied in Refs. 28 and 2. It also follows from the calculations of Ref. 2 that the torsion must be nonzero for a nonflat structure in the $n>1$, $r>2$ cases as a consequence of the fact that in these cases the decomposition of the tangent space as a tensor product of $\mathbb{S}$ with $\odot^n\tilde{\mathbb{S}}$ determines a paraconformal structure in which both factors have dimension greater than two, and in that case the torsion-free condition implies flatness.

Lemma 6.5: For $r>1$, the requirement of uniqueness for the α surface through $z(m)_\pi$ is redundant.

Proof: The integrability equations in particular give a propagation equation for π across the α-surface. □

There are a number of specializations of the GCASD equations: hypercomplex, scalar-flat Kähler, Einstein, hyper-Kähler. The hypercomplex and hyper-Kähler cases have straightforward extensions to the hierarchy.

(i) The hyper-complex case for r even, $n=1$, where there exists a flat connection on $\tilde{\mathbb{S}}$ such that the distribution D on $P\tilde{\mathbb{S}}$ is horizontal. This is equivalent to the existence of a fibration $\mathcal{PT}\mapsto\mathbb{CP}^1$. This condition (flatness of the induced connection of 6.4 or a fibration of the associated twistor space over $\mathbb{CP}^1$) can clearly be imposed consistently on any $\mathcal{M}_{r,n}$ to give a hypercomplex hierarchy.

(ii) In case of the hyper-Kähler hierarchy, we require that there exists a connection compatible with 6.4 that induces a flat connection on $\tilde{\mathbb{S}}$ and preserves skew forms ε_{AB} on $\mathbb{S}$ and $\varepsilon_{A'B'}$ on $\tilde{\mathbb{S}}$ such that the forms $\varepsilon_{AB}e^{A(A'_1\cdots A'_n}\wedge e^{B'_1\cdots B'_n)B}$ are closed. This then implies that $\eta=\varepsilon^{A'B'}\pi_{A'}D\pi_{B'}$ and $\eta\wedge\varepsilon_{AB}\pi_{A'_1}\cdots\pi_{A'_n}e^{AA'_1\cdots A'_n}\wedge\pi_{B'_1}\cdots\pi_{B'_n}e^{BB'_1\cdots B'_n}$ descend to $\mathcal{PT}$, in such a way that η is the annihilator of an integrable distribution determining a fibration over $\mathbb{CP}^1$.

A. Reality structures

The imposition of reality conditions is standard; it is imposed by requiring the existence of an anti-holomorphic involution σ on $\mathcal{M}$ that fixes a real slice and preserves the geometric structures (i.e., sends α-surfaces to α-surfaces). In the hyper-Kähler case, we can talk in terms of the signature of the associated metric (although the following conditions can be applied more generally). For Euclidean signature, we require that it induces a quaternionic involution on $\tilde{\mathbb{S}}$ given by $\sigma^2=-1$. In particular there are no nonzero fixed points. It will then also induce a quaternionic involution on $\mathbb{S}$ which will have to be even dimensional and we must also require that the

Hermitian form $\pi^A\hat{\pi}^B\varepsilon_{AB}$ be definite (it is trivially definite for $r=2$). For non-Euclidean signature we can have different signatures for $\pi^A\hat{\pi}^B\varepsilon_{AB}$, or impose a conjugation whose action on $\mathbb{S}$ snf $\widetilde{\mathbb{S}}$ is an ordinary complex conjugation.

The conjugation will also lead to an antiholomorphic involution on the twistor space, without fixed points in the quaternionic case, and with a fixed real slice otherwise. Points of the real slice of $\mathcal{M}$ will then correspond to σ invariant rational curves.

B. Embedding into hierarchies

In the usual definition of a hierarchy, the hierarchy is an overdetermined, but compatible, system of equations which contains the original system. A given solution to the original system may not actually extend to a solution of the hierarchy in general (there can be obstructions, see p. 249 and p. 253, footnote 2, of Ref. 21 for some discussion of this behavior for the Drinfeld Sokolov hierarchies). Furthermore, if such an extension does exist, it will not in general be unique without the imposition of boundary conditions.

Our definition of a hidden symmetry in Sec. IV requires the existence of an extension of a solution to the original equation to the hierarchy that happens to admit a symmetry, but only when thought of as a solution to the hierarchy.

We state the embedding definition in slightly greater generality as for one hierarchy into another:

Definition 6.6: A solution $\mathcal{M}_{r_1,n_1}$ to the GCASD hierarchy embeds into another solution $\mathcal{M}_{r_2,n_2}$, $n_1<n_2$, $r_1\leqslant r_2$, if $\mathcal{M}_{r,n_1}$ embeds into $\mathcal{M}_{r,n_2}$ as a manifold in such a way that the α-surfaces of $\mathcal{M}_{r,n_2}$ intersect $\mathcal{M}_{r,n_1}$ in the α-surfaces of $\mathcal{M}_{r,n_1}$ and all α-surfaces of $\mathcal{M}_{r,n_1}$ arise in this way.

Due to a remarkable theorem of Bernstein and Gindikin,[14] the twistor characterization of such an embedding in the most interesting case, $r_1=r_2$, is remarkably simple:

Theorem 6.7 (Bernstein and Gindikin): *A solution $\mathcal{M}_{r,n_1}$ to the GCASD hierarchy embeds into $\mathcal{M}_{r,n_2}$ iff the twistor space $\mathcal{PT}_{n_1}$ for $\mathcal{M}_{r,n_1}$ is obtained from that $\mathcal{PT}_{n_2}$ for $\mathcal{M}_{r,n_2}$ by choosing submanifolds Γ_1, Γ_2,... of codimension greater than one and S_1, S_2,... of $codimension=1$ and blowing up along each Γ_1, Γ_2,... and taking a branch covers branching with some multiplicity over each S_i.*

In Ref. 8 (see also Sec. III), we embedded $\mathcal{M}_{2,n_1}$ into $\mathcal{M}_{2,n_2}$ by blowing up the twistor space $\mathcal{PT}_{n_2}$ at one point n_2-n_1 times.

Note that it is natural in the quaternionic cases, or in the hyper-CASD cases, to require that the additional structures be compatible. This is straightforward in the hypercomplex case in which one wishes the embedded twistor space to inherit a fibration over $\mathbb{CP}^1$, but when line bundle valued forms need to be pulled back also, there is the problem that the forms that have been pulled back will in general take values in an inappropriate line bundle unless particular care has been taken.

C. Symmetries and hidden symmetries

We can define a symmetry for a GCASD structure to be the requirement that the twistor space admits a global holomorphic vector field $\mathcal{K}$. This will in turn determine global holomorphic vector fields $\widetilde{K}$ on the correspondence space and K on $\mathcal{M}$, such that $\widetilde{K}$ projects to K. The essential requirement on $\widetilde{K}$ will be that it preserves the twistor distribution and this will lead to a generalization of the conformal Killing vector equations on K whose precise form will depend on r and n.

Clearly the concept of hidden symmetry can be applied as before but with greater generality; a solution $\mathcal{M}_{r,n}$ admits a hidden symmetry if it can be embedded as above into an $\mathcal{M}_{r,m}$ that admits an explicit symmetry. This will, as in the proof of Proposition 4.1, lead to a global vector field on $\mathcal{PT}_{r,n}$ with values in a line bundle $\mathcal{L}$ of degree $m-n$ (the restriction of the canonical bundle of $\mathcal{PT}_{r,m}$ tensored with the inverse of that of $\mathcal{PT}_{r,n}$). There will also be a generalization of Theorem 4.4: this global vector field with values in $\mathcal{L}$ will lead to the realization of $\mathcal{PT}_{r,n}$ as the total space of an affine line bundle, with underlying translation bundle $\mathcal{L}^*$, over some reduced

twistor space which will generically be $\mathcal{PT}_{r-1,l}$ where $l=n+m/(r-1)$, if l is an integer, although if l is fractional, or in nongeneric situations, the normal bundle of lines in the reduced twistor space must be $\mathcal{O}(k_1)\oplus\cdots\oplus\mathcal{O}(k_{r-1})$ with $\Sigma k_i=(r-1)n+m$. Thus the original $\mathcal{PT}_{r,n}$ with a hidden symmetry can be determined in terms of a lower dimensional twistor space together with a linear cohomology class on that space.

ACKNOWLEDGMENTS

We are grateful to Nigel Hitchin for helpful comments and for showing us his notes on D_k ALE manifolds. We would also like to thank Toby Bailey, Roger Bielawski, David Calderbank, Simon Gindikin and George Sparling for useful discussions. Both authors are members of EDGE, Research Training Network HPRN-CT-2000-00101. M.D. was partly supported by NATO Grant No. PST.CLG.978984.

APPENDIX: TWO-COMPONENT SPINOR NOTATION

In four complex dimensions orthogonal transformations decompose into products of ASD and SD rotations $\mathrm{SO}(4,\mathbb{C})=(\mathrm{SL}(2,\mathbb{C})\times\widetilde{\mathrm{SL}}(2,\mathbb{C}))/\mathbb{Z}_2$. The spinor calculus in four dimensions is based on this isomorphism. We use the conventions of Penrose and Rindler.[26] The tangent space at each point of $\mathcal{M}$ is isomorphic to a tensor product of the two spin spaces $T^a\mathcal{M}=S^A\otimes S^{A'}$. Spin dyads (o^A,ι^A) and $(o^{A'},\iota^{A'})$ span S^A and $S^{A'}$, respectively. The spin spaces S^A and $S^{A'}$ are equipped with symplectic forms ε_{AB} and $\varepsilon_{A'B'}$ such that $\varepsilon_{01}=\varepsilon_{0'1'}=1$. These antisymmetric objects are used to raise and lower the spinor indices via $\iota_A=\iota^B\varepsilon_{BA}$, $\iota^B=\varepsilon^{AB}\iota_B$. Let Γ_{AB} and $\Gamma_{A'B'}$ be the $\mathrm{SL}(2,\mathbb{C})$ and $\widetilde{\mathrm{SL}}(2,\mathbb{C})$ spin connections. The curvature of the unprimed spin connection $R^A{}_B=\mathrm{d}\Gamma^A{}_B+\Gamma^A{}_C\wedge\Gamma^C{}_B$ decomposes as

$$R^A{}_B=C^A{}_{BCD}\Sigma^{CD}+(1/12)R\Sigma^A{}_B+\Phi^A{}_{BC'D'}\Sigma^{C'D'},$$

and similarly for $R^{A'}{}_{B'}$. Here R is the Ricci scalar, $\Phi_{ABA'B'}$ is the trace-free part of the Ricci tensor R_{ab}, and C_{ABCD} is the ASD part of the Weyl tensor

$$C_{abcd}=\varepsilon_{A'B'}\varepsilon_{C'D'}C_{ABCD}+\varepsilon_{AB}\varepsilon_{CD}C_{A'B'C'D'},$$

and the two-forms $\Sigma^{A'B'}$ span the three-dimensional space of SD two-forms.

Given a complex four-dimensional manifold $\mathcal{M}$ with curved metric g, a twistor in $\mathcal{M}$ is an α-surface, i.e., a null two-dimensional surface whose tangent space at each point is an α plane (a null two-dimensional plane with a SD bi-vector). There are Frobenius integrability conditions for the existence of such α-surfaces through each α-plane element at each point and these are equivalent, after some calculation, to the vanishing of the self-dual part of the Weyl curvature, $C_{A'B'C'D'}$. Thus, given $C_{A'B'C'D'}=0$, we can define a twistor space $\mathcal{PT}$ to be the three complex dimensional manifold of α-surfaces in $\mathcal{M}$. If g is also Ricci flat, then $\mathcal{PT}$ has further structures which are listed in the nonlinear graviton theorem:

Theorem A.1 (Penrose[25]): *There is a 1-1 correspondence between complex ASD vacuum metrics on complex four-manifolds and three-dimensional complex manifolds $\mathcal{PT}$ such that the following hold.*

(i) *There exists a holomorphic projection $\mu:\mathcal{PT}\to\mathbb{CP}^1$.*
(ii) *$\mathcal{PT}$ is equipped with a four complex parameter family of sections of μ each with a normal bundle $\mathcal{O}(1)\oplus\mathcal{O}(1)$ (this will follow from the existence of one such curve by Kodaira theory).*
(iii) *Each fiber of μ has a symplectic structure $\Sigma_\lambda\in\Gamma(\Lambda^2(\mu^{-1}(\lambda))\otimes\mathcal{O}(2))$, where $\lambda\in\mathbb{CP}^1$.*

To obtain real metrics on a real four-manifold, we can require further that the twistor space admit an antiholomorphic involution.

The correspondence space $\mathcal{F}=\mathcal{M}\times\mathbb{CP}^1$ is coordinatized by (x,λ), where x denotes the coordinates on $\mathcal{M}$ and λ is the coordinate on $\mathbb{CP}^1$ that parametrizes the α-surfaces through x in $\mathcal{M}$. We represent $\mathcal{F}$ as the quotient of the primed-spin bundle $S^{A'}$ with fiber coordinates $\pi_{A'}$ by the Euler vector field $\Upsilon=\pi^{A'}\partial/\partial\pi^{A'}$. We relate the fiber coordinates to λ by $\lambda=\pi_{0'}/\pi_{1'}$. A form with values in the line bundle $\mathcal{O}(n)$ on $\mathcal{F}$ can be represented by a homogeneous form α on the nonprojective spin bundle satisfying $\Upsilon\lrcorner\alpha=0$, $\mathcal{L}_\Upsilon\alpha=n\alpha$.

The correspondence space has the alternate definition

$$\mathcal{F}=\mathcal{PT}\times\mathcal{M}\big|_{Z\in l_x}=\mathcal{M}\times\mathbb{CP}^1,$$

where l_x is the line in $\mathcal{PT}$ that corresponds to $x\in\mathcal{M}$ and $Z\in\mathcal{PT}$ lies on l_x. This leads to a double fibration

$$\mathcal{M}\overset{p}{\leftarrow}\mathcal{F}\overset{q}{\rightarrow}\mathcal{PT}. \tag{A1}$$

Points in $\mathcal{M}$ correspond to rational curves in $\mathcal{PT}$ with normal bundle $\mathcal{O}^A(1):=\mathcal{O}(1)\oplus\mathcal{O}(1)$. The normal bundle to l_x consists of vectors tangent to x (horizontally lifted to $T_{(x,\lambda)}\mathcal{F}$) modulo the twistor distribution. We have a sequence of sheaves over $\mathbb{CP}^1$:

$$0\rightarrow D\rightarrow\mathbb{C}^4\rightarrow\mathcal{O}^A(1)\rightarrow 0.$$

The map $\mathbb{C}^4\rightarrow\mathcal{O}^A(1)$ is given by $V^{AA'}\rightarrow V^{AA'}\pi_{A'}$. Its kernel consists of vectors of the form $\pi^{A'}\lambda^A$ with λ^A varying. The twistor distribution is therefore $D=O(-1)\otimes S^A$ and so there is a canonical $L_A\in\Gamma(D\otimes\mathcal{O}(1)\otimes S_A)$ given by $L_A=\pi^{A'}\nabla_{AA'}$. The projective twistor space $\mathcal{PT}$ arises as a quotient of $\mathcal{F}$ by the twistor distribution. Functions on $\mathcal{F}$ which are constant along $L_{A'}$ are called twistor functions.

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Hexagonal circle patterns with constant intersection angles and discrete Painlevé and Riccati equations

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(Received 15 January 2003; accepted 9 April 2003)

Hexagonal circle patterns with constant intersection angles mimicking holomorphic maps z^c and $\log(z)$ are studied. It is shown that the corresponding circle patterns are immersed and described by special separatrix solutions of discrete Painlevé and Riccati equations. The general solution of the Riccati equation is expressed in terms of the hypergeometric function. Global properties of these solutions, as well as of the discrete z^c and $\log(z)$, are established. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1586966]

I. INTRODUCTION. HEXAGONAL CIRCLE PATTERNS AND z^c

The theory of circle patterns is a rich fascinating area having its origin in the classical theory of circle packings. Its fast development in recent years is caused by the mutual influence and interplay of ideas and concepts from discrete geometry, complex analysis and the theory of integrable systems.

The progress in this area was initiated by Thurston's idea[24,17] of approximating the Riemann mapping by circle packings. Classical circle packings consisting of disjoint open disks were later generalized to circle patterns where the disks may overlap (see, for example, Ref. 14). Different underlying combinatorics were considered. Circle patterns with the combinatorics of the square grid were introduced in Ref. 22; hexagonal circle patterns were studied in Refs. 7 and 9.

The striking analogy between circle patterns and the classical analytic function theory is underlined by such facts as the uniformization theorem concerning circle packing realizations of cell complexes with prescribed combinatorics,[4] a discrete maximum principle and Schwarz's lemma,[20] rigidity properties[17,14] and a discrete Dirichlet principle.[22]

The convergence of discrete conformal maps represented by circle packings was proven in Ref. 21. For prescribed regular combinatorics this result was refined. C^∞-convergence for hexagonal packings is shown in Ref. 15. The uniform convergence for circle patterns with the combinatorics of the square grid and orthogonal neighboring circles was established in Ref. 22.

The approximation issue naturally leads to the question about analogs to standard holomorphic functions. Computer experiments give evidence for their existence,[12,16] however not very much is known. For circle packings with hexagonal combinatorics the only explicitly described examples are Doyle spirals,[11,5] which are discrete analogs of exponential maps, and conformally symmetric packings, which are analogs of a quotient of Airy functions.[6] For patterns with overlapping circles more explicit examples are known: discrete versions of $\exp(z)$, $\mathrm{erf}(z)$,[22] z^c, $\log(z)$ (Ref. 3) are constructed for patterns with underlying combinatorics of the square grid; z^c, $\log(z)$ are also described for hexagonal patterns.[7,9]

It turned out that an effective approach to the description of circle patterns is given by the theory of integrable systems (see Refs. 7–9). For example, Schramm's circle patterns are governed by a difference equation which is the stationary Hirota equation (see Ref. 22). This approach proved to be especially useful for the construction of discrete z^c and $\log(z)$ in Refs. 3 and 7–9 with

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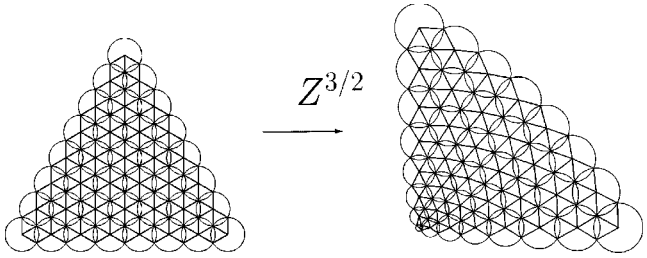

FIG. 1. Hexagonal circle patterns as a discrete conformal map.

the aid of some isomonodromy problem. Another connection with the theory of discrete integrable equations was revealed in Refs. 1–3: embedded circle patterns are described by special solutions of discrete Painlevé II and discrete Riccati equations.

In this article we carry the results of Ref. 3 for square grid combinatorics over to hexagonal circle patterns with constant intersection angles introduced in Ref. 7.

Hexagonal combinatorics are obtained on a sublattice of $\mathbb{Z}^3$ as follows: consider the subset

$$H=\{(k,l,m)\in\mathbb{Z}^3:\ |k+l+m|\leqslant 1\}$$

and join by edges those vertices of H whose (k,l,m)-labels differ by 1 only in one component. The obtained quadrilateral lattice QL has two types of vertices: for $k+l+m=0$ the corresponding vertices have six adjacent edges, while the vertices with $k+l+m=\pm 1$ have only three. Suppose that the vertices with six neighbors correspond to centers of circles in the complex plane $\mathbb{C}$ and the vertices with three neighbors correspond to intersection points of circles with the centers in neighboring vertices. Thus we obtain a circle pattern with hexagonal combinatorics.

Circle patterns where the intersection angles are constant for each of three types of (quadrilateral) faces (see Fig. 1) were introduced in Ref. 7. A special case of such circle patterns mimicking holomorphic map z^c and $\log(z)$ is given by the restriction to an H-sublattice of a special isomonodromic solution of some *integrable system* on the lattice $\mathbb{Z}^3$. Equations for the field variable $z:\mathbb{Z}^3\to\mathbb{C}$ of this system are

$$\begin{aligned}
&q(z_{k,l,m},z_{k,l+1,m},z_{k-1,l+1,m},z_{k-1,l,m})=e^{-2i\alpha_1},\\
&q(z_{k,l,m},z_{k,l,m-1},z_{k,l+1,m-1},z_{k,l+1,m})=e^{-2i\alpha_2},\\
&q(z_{k,l,m},z_{k+1,l,m},z_{k+1,l,m-1},z_{k,l,m-1})=e^{-2i\alpha_3},
\end{aligned}\tag{1}$$

where $\alpha_i>0$ satisfy $\alpha_1+\alpha_2+\alpha_3=\pi$ and

$$q(z_1,z_2,z_3,z_4)=\frac{(z_1-z_2)(z_3-z_4)}{(z_2-z_3)(z_4-z_1)}$$

is the cross-ratio of elementary quadrilaterals of the image of $\mathbb{Z}^3$. Equations (1) mean that the cross-ratios of images of faces of elementary cubes are constant for each type of face, while the restriction $\alpha_1+\alpha_2+\alpha_3=\pi$ ensures their compatibility.

The isomonodromic problem for this system (see Sec. II for the details, where we present the necessary results from Ref. 7) specifies the nonautonomous constraint

$$\begin{aligned}
cz_{k,l,m}=&2k\frac{(z_{k+1,l,m}-z_{k,l,m})(z_{k,l,m}-z_{k-1,l,m})}{z_{k+1,l,m}-z_{k-1,l,m}}+2l\frac{(z_{k,l+1,m}-z_{k,l,m})(z_{k,l,m}-z_{k,l-1,m})}{z_{k,l+1,m}-z_{k,l-1,m}}\\
&+2m\frac{(z_{k,l,m+1}-z_{k,l,m})(z_{k,l,m}-z_{k,l,m-1})}{z_{k,l,m+1}-z_{k,l,m-1}},
\end{aligned}\tag{2}$$

which is compatible with (1) (this constraint in the two-dimensional case with $c=1$ first appeared in Ref. 19). In particular, a solution to (1) and (2) in the subset

$$Q=\{(k,l,m)\in\mathbb{Z}^3 |\ \ k\geqslant 0,\ \ l\geqslant 0,\ \ m\leqslant 0\} \tag{3}$$

is uniquely determined by its values

$$z_{1,0,0},\ \ z_{0,1,0},\ \ z_{0,0,-1}.$$

Indeed, the constraint (2) gives $z_{0,0,0}=0$ and defines z along the coordinate axis $(n,0,0)$, $(0,n,0)$, $(0,0,-n)$. Then all other $z_{k,l,m}$ with $(k,l,m)\in Q$ are calculated through the cross-ratios (1).

Proposition 1:[7] *The solution $z:Q\to\mathbb{C}$ of the system (1) and (2) with the initial data*

$$z_{1,0,0}=1,\ \ z_{0,1,0}=e^{i\phi},\ \ z_{0,0,-1}=e^{i\psi} \tag{4}$$

determines a circle pattern. For all $(k,l,m)\in Q$ with even $k+l+m$ the points $z_{k\pm 1,l,m}$, $z_{k,l\pm 1,m}$, $z_{k,l,m\pm 1}$ lie on a circle with the center $z_{k,l,m}$, i.e., all elementary quadrilaterals of the Q-image are of kite form.

Moreover, Eqs. (1) (see Lemma 1 in Sec. III) ensure that for the points $z_{k,l,m}$ with $k+l+m=\pm 1$, where three circles meet intersection angles are α_i or $\pi-\alpha_i$, $i=1,2,3$ (see Fig. 1 where the isotropic case $\alpha_i=\pi/3$ of regular and $Z^{3/2}$-pattern are shown).

According to Proposition 1, the discrete map $z_{k,l,m}$, restricted on H, defines a circle pattern with circle centers $z_{k,l,m}$ for $k+l+m=0$, each circle intersecting six neighboring circles. At each intersection point three circles meet.

However, for most initial data $\phi,\psi\in\mathbb{R}$, the behavior of the obtained circle pattern is quite irregular: inner parts of different elementary quadrilaterals intersect and circles overlap. Define $Q_H=Q\cap H$.

Definition 1:[7] *The hexagonal circle pattern Z^c, $0<c<2$ with intersection angles $\alpha_1,\alpha_2,\alpha_3$, $\alpha_i>0$, $\alpha_1+\alpha_2+\alpha_3=\pi$ is the solution $z:Q\to\mathbb{C}$ of (1) subject to (2) and with the initial data*

$$z_{1,0,0}=1,\ \ z_{0,1,0}=e^{ic(\alpha_2+\alpha_3)},\ \ z_{0,0,-1}=e^{ic\alpha_3} \tag{5}$$

restricted to Q_H.

Definition 2: A discrete map $z:Q_H\to\mathbf{C}$ is called an immersion if inner parts of adjacent elementary quadrilaterals are disjoint.

The main result of this article is the following theorem.

Theorem 1: *The hexagonal Z^c with constant positive intersection angles and $0<c<2$ is an immersion.*

The proof of this property follows from an analysis of the geometrical properties of the corresponding circle patterns and analytical properties of the corresponding discrete Painlevé and Riccati equations.

The crucial step is to consider equations for the radii of the studied circle patterns in the whole Q-sublattice with even $k+l+m$. In Sec. III, these equations are derived and the geometrical property of immersedness is reformulated as the positivity of the solution to these equations. Using discrete Painlevé and Riccati equations in Sec. IV we present the proof of the existence of a positive solution and thus complete the proof of immersedness. In Sec. VI, we discuss possible generalizations and corollaries of the obtained results. In particular, circle patterns Z^2 and Log with both square grid and hexagonal combinatorics are considered. It is also proved that they are immersions.

II. DISCRETE Z^c VIA A MONODROMY PROBLEM

Equations (1) have the Lax representation:[7]

$$\Phi_{k+1,l,m}(\mu)=L^{(1)}(e,\mu)\Phi_{k,l,m}(\mu),$$

$$\Phi_{k,l+1,m}(\mu)=L^{(2)}(e,\mu)\Phi_{k,l,m}(\mu), \tag{6}$$

$$\Phi_{k,l,m+1}(\mu)=L^{(3)}(e,\mu)\Phi_{k,l,m}(\mu),$$

where μ is the spectral parameter and $\Phi(\mu):\mathbb{Z}^3\to \mathrm{GL}(2,\mathbb{C})$ is the wave function. The matrices $L^{(n)}$ are defined on the edges $e=(p_{out},p_{in})$ of $\mathbb{Z}^3$ connecting two neighboring vertices and oriented in the direction of increasing $k+l+m$:

$$L^{(n)}(e,\mu)=\begin{pmatrix} 1 & z_{in}-z_{out} \\ \mu\dfrac{\Delta_n}{z_{in}-z_{out}} & 1 \end{pmatrix}, \tag{7}$$

with parameters Δ_n fixed for each type of edges. The zero-curvature condition on the faces of elementary cubes of $\mathbb{Z}^3$ is equivalent to Eqs. (1) with $\Delta_n=e^{i\delta_n}$ for properly chosen δ_n. Indeed, each elementary quadrilateral of $\mathbb{Z}^3$ has two consecutive positively oriented pairs of edges e_1,e_2 and e_3,e_4. Then the compatibility condition

$$L^{(n_1)}(e_2)L^{(n_2)}(e_1)=L^{(n_2)}(e_4)L^{(n_1)}(e_3)$$

is exactly one of the equations (1). This Lax representation is a generalization of the one found in Ref. 19 for the square lattice.

A solution $z:\mathbb{Z}^3\to\mathbb{C}$ of Eqs. (1) is called *isomonodromic* if there exists a wave function $\Phi(\mu):\mathbf{Z}^3\to\mathrm{GL}(2,\mathbf{C})$ satisfying (6) and the following linear differential equation in μ:

$$\frac{d}{d\mu}\Phi_{k,l,m}(\mu)=A_{k,l,m}(\mu)\Phi_{k,l,m}(\mu), \tag{8}$$

where $A_{k,l,m}(\mu)$ are some 2×2 matrices meromorphic in μ, with the order and position of their poles being independent of k,l,m. Isomonodromic solutions are important in many applications, in particular, for the first time the isomonodromy method was used to solve a discrete equation appearing in quantum gravity.[13]

The simplest nontrivial isomonodromic solutions satisfy the constraint

$$\begin{aligned} bz_{k,l,m}^2+cz_{k,l,m}+d=&2(k-a_1)\frac{(z_{k+1,l,m}-z_{k,l,m})(z_{k,l,m}-z_{k-1,l,m})}{z_{k+1,l,m}-z_{k-1,l,m}} \\ &+2(l-a_2)\frac{(z_{k,l+1,m}-z_{k,l,m})(z_{k,l,m}-z_{k,l-1,m})}{z_{k,l+1,m}-z_{k,l-1,m}} \\ &+2(m-a_3)\frac{(z_{k,l,m+1}-z_{k,l,m})(z_{k,l,m}-z_{k,l,m-1})}{z_{k,l,m+1}-z_{k,l,m-1}}. \end{aligned} \tag{9}$$

Theorem 2:[7] *Let $z:\mathbf{Z}^3\to\mathbf{C}$ be an isomonodromic solution to (1) with the matrix $A_{k,l,m}$ in (8) of the form*

$$A_{k,l,m}(\mu)=\frac{C_{k,l,m}}{\mu}+\sum_{n=1}^{3}\frac{B^{(n)}_{k,l,m}}{\mu-1/\Delta_n} \tag{10}$$

with μ-independent matrices $C_{k,l,m}$, $B^{(n)}_{k,l,m}$ and normalized by $\mathrm{tr}\,A_{0,0,0}(\mu)=0$. *Then these matrices have the following form:*

$$C_{k,l,m}=\frac{1}{2}\begin{pmatrix} -bz_{k,l,m}-c/2 & bz_{k,l,m}^2+cz_{k,l,m}+d \\ b & bz_{k,l,m}+c/2 \end{pmatrix},$$

$$B^{(1)}_{k,l,m}=\frac{k-a_1}{z_{k+1,l,m}-z_{k-1,l,m}}\begin{pmatrix} z_{k+1,l,m}-z_{k,l,m} & (z_{k+1,l,m}-z_{k,l,m})(z_{k,l,m}-z_{k-1,l,m}) \\ 1 & z_{k,l,m}-z_{k-1,l,m}\end{pmatrix}+\frac{a_1}{2}I,$$

$$B^{(2)}_{k,l,m}=\frac{l-a_2}{z_{k,l+1,m}-z_{k,l-1,m}}\begin{pmatrix} z_{k,l+1,m}-z_{k,l,m} & (z_{k,l+1,m}-z_{k,l,m})(z_{k,l,m}-z_{k,l-1,m}) \\ 1 & z_{k,l,m}-z_{k,l-1,m}\end{pmatrix}+\frac{a_2}{2}I,$$

$$B^{(3)}_{k,l,m}=\frac{m-a_3}{z_{k,l,m+1}-z_{k,l,m-1}}\begin{pmatrix} z_{k,l,m+1}-z_{k,l,m} & (z_{k,l,m+1}-z_{k,l,m})(z_{k,l,m}-z_{k,l,m-1}) \\ 1 & z_{k,l,m}-z_{k,l,m-1}\end{pmatrix}+\frac{a_3}{2}I,$$

and $z_{k,l,m}$ satisfies (9).

Conversely, any solution $z:\mathbb{Z}^3\to\mathbb{C}$ to the system (1) and (9) is isomonodromic with $A_{k,l,m}(\mu)$ given by the formulas above.

The special case $b=a_1=a_2=a_3=0$ with shift $z\to z-d/c$ implies (2).

III. EUCLIDEAN DESCRIPTION OF HEXAGONAL CIRCLE PATTERNS

In this section we describe the circle pattern z^c in terms of the radii of the circles. Such characterization proved to be quite useful for the circle patterns with combinatorics of the square grid.[1,3] In what follows, we say that the triangle (z_1,z_2,z_3) has *positive (negative) orientation* if

$$\frac{z_3-z_1}{z_2-z_1}=\left|\frac{z_3-z_1}{z_2-z_1}\right|e^{i\phi}\quad\text{with}\quad 0\leqslant\phi\leqslant\pi\quad(-\pi<\phi<0).$$

Lemma 1: Let $q(z_1,z_2,z_3,z_4)=e^{-2i\alpha}$, $0<\alpha<\pi$.

(i) *If $|z_1-z_2|=|z_1-z_4|$ and the triangle (z_1,z_2,z_4) has positive orientation, then $|z_3-z_2|=|z_3-z_4|$ and the angle between $[z_1,z_2]$ and $[z_2,z_3]$ is $(\pi-\alpha)$.*

(ii) *If $|z_1-z_2|=|z_1-z_4|$ and the triangle (z_1,z_2,z_4) has negative orientation, then $|z_3-z_2|=|z_3-z_4|$ and the angle between $[z_1,z_2]$ and $[z_2,z_3]$ is α.*

(iii) *If the angle between $[z_1,z_2]$ and $[z_1,z_4]$ is α and the triangle (z_1,z_2,z_4) has positive orientation, then $|z_3-z_2|=|z_1-z_2|$ and $|z_3-z_4|=|z_4-z_1|$.*

(iv) *If the angle between $[z_1,z_2]$ and $[z_1,z_4]$ is $(\pi-\alpha)$ and the triangle (z_1,z_2,z_4) has negative orientation, then $|z_3-z_2|=|z_1-z_2|$ and $|z_3-z_4|=|z_4-z_1|$.*

Lemma 1 and Proposition 1 imply that each elementary quadrilateral of the studied circle pattern has one of the forms enumerated in the lemma.

Proposition 1 allows us to introduce the radius function

$$r(K,L,M)=|z_{k,l,m}-z_{k\pm1,l,m}|=|z_{k,l\pm1,m}-z_{k,l,m}|=|z_{k,l,m}-z_{k,l,m\pm1}|,\tag{11}$$

where (k,l,m) belongs to the sublattice of Q with even $k+l+m$ and (K,L,M) label this sublattice:

$$K=k-\frac{k+l+m}{2},\quad L=l-\frac{k+l+m}{2},\quad M=m-\frac{k+l+m}{2}.\tag{12}$$

The function r is defined on the sublattice

$$\tilde{Q}=\{(K,L,M)\in\mathbf{Z}^3|L+M\leqslant 0,\quad M+K\leqslant 0,\quad K+L\geqslant 0)\}$$

corresponding to Q. Consider this function on

$$\tilde{Q}_H=\{(K,L,M)\in\mathbf{Z}^3|K\geqslant 0,\quad L\geqslant 0,\quad M\leqslant 0,\quad K+L+M=0,+1\}.$$

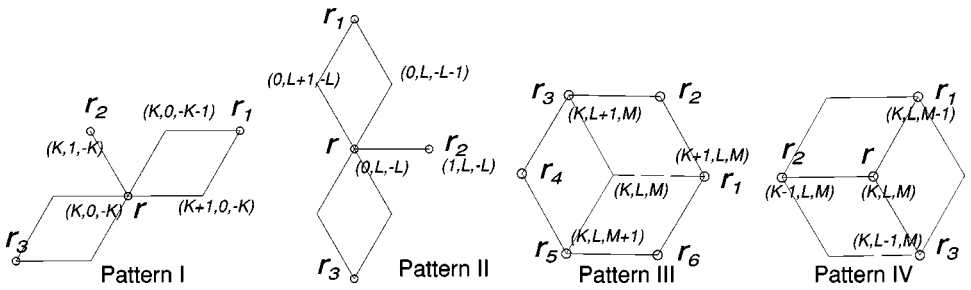

FIG. 2. Equation patterns.

Theorem 3: *Let the solution $z:Q_H\to\mathbb{C}$ of the system (1) and (2) with initial data (4) be an immersion. Then function $r(K,L,M):\tilde{Q}_H\to\mathbb{R}_+$, defined by (11), satisfies the following equations:*

$$(r_1+r_2)(r^2-r_2r_3+r(r_3-r_2)\cos\alpha_i)+(r_3+r_2)(r^2-r_2r_1+r(r_1-r_2)\cos\alpha_i)=0 \tag{13}$$

on the patterns of type I and II as in Fig. 2, with $i=3$ and $i=2$, respectively;

$$(L+M+1)\frac{r_4-r_1}{r_4+r_1}+(M+K+1)\frac{r_6-r_3}{r_6+r_3}+(K+L+1)\frac{r_2-r_5}{r_2+r_5}=c-1 \tag{14}$$

on the patterns of type III, and

$$r(r_1\sin\alpha_3+r_2\sin\alpha_1+r_3\sin\alpha_2)=r_1r_2\sin\alpha_2+r_2r_3\sin\alpha_3+r_3r_1\sin\alpha_1 \tag{15}$$

on the patterns of type IV. Conversely, $r(K,L,M):\tilde{Q}_H\to\mathbb{R}_+$ satisfying Eqs. (13)–(15) is the radius function of an immersed hexagonal circle pattern with constant intersection angles [i.e., corresponding to some immersed solution $z:Q_H\to\mathbb{C}$ of (1) and (2)], which is determined by r uniquely.

Proof: The map $z_{k,l,m}$ is an immersion if and only if all triangles $(z_{k,l,m},z_{k+1,l,m},z_{k,l,m-1})$, $(z_{k,l,m},z_{k,l,m-1},z_{k,l+1,m})$ and $(z_{k,l,m},z_{k+1,l,m},z_{k,l+1,m})$ of elementary quadrilaterals of the map $z_{k,l,m}$ have the same orientation (for brevity we call it the orientation of the quadrilaterals).

Necessity: To get Eq. (14), consider the configuration of two starlike figures with centers at $z_{k,l,m}$ with $k+l+m=1\,(\mathrm{mod}\,2)$ and at $z_{k+1,l,m}$, connected by five edges in the k-direction as shown on the left part of Fig. 3. Let r_i, $i=1,\ldots,6$, be the radii of the circles with the centers at the vertices neighboring $z_{k,l,m}$ as in Fig. 3. As follows from Lemma 1, the vertices $z_{k,l,m}$, $z_{k+1,l,m}$ and $z_{k-1,l,m}$ are collinear. For immersed z^c, the vertex $z_{k,l,m}$ lies between $z_{k+1,l,m}$ and $z_{k-1,l,m}$. Similar facts are true also for the l- and m-directions. Moreover, the orientations of elementary quadrilaterals with the vertex $z_{k,l,m}$ coincides with one of the standard lattice. Lemma 1 defines all angles at $z_{k,l,m}$ of these quadrilaterals. Equation (2) at (k,l,m) gives $z_{k,l,m}$:

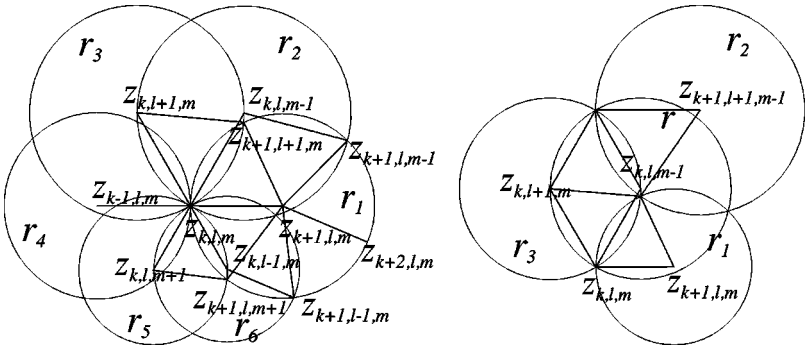

FIG. 3. Circles.

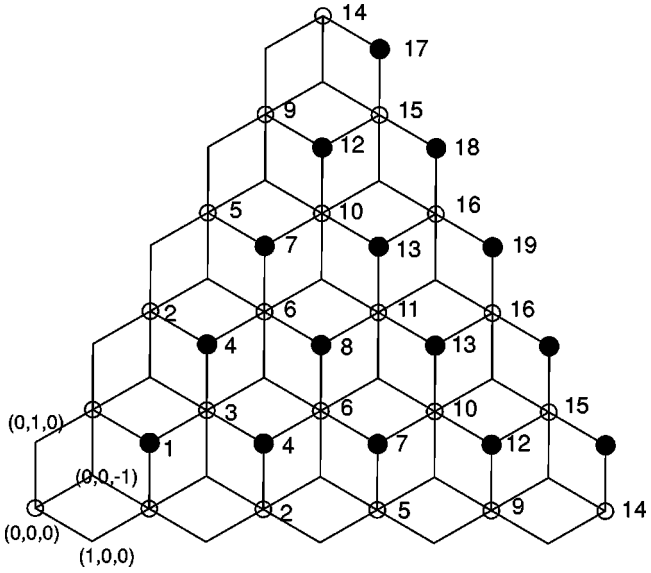

FIG. 4. Computing r in $\tilde{Q}_H$.

$$z_{k,l,m}=\frac{2e^{is}}{c}\left(k\frac{r_1r_4}{r_1+r_4}+l\frac{r_3r_6}{r_3+r_6}e^{i(\alpha_2+\alpha_3)}+m\frac{r_2r_5}{r_2+r_5}e^{i(\alpha_1+\alpha_2+2\alpha_3)}\right),$$

where $e^{is}=(z_{k+1,l,m}-z_{k,l,m})/r_1$. Lemma 1 allows one to compute $z_{k+1,l,m-1}$, $z_{k+1,l+1,m}$, $z_{k+1,l,m+1}$ and $z_{k+1,l-1,m}$ using the form of quadrilaterals (they are shown in Fig. 3). Now Eq. (2) at $(k+1,l,m)$ defines $z_{k+2,l,m}$. Condition $|z_{k+2,l,m}-z_{k+1,l,m}|=r_1$ with the labels (12) yields Eq. (14).

For $l=0$ values $z_{k+1,0,m}$, $z_{k+2,0,m}$, $z_{k+1,0,m-1}$ and the equation for the cross-ratio with α_3 give the radius R with the center at $z_{k+2,0,m-1}$. Note that for $l=0$ the term with r_6 and r_5 drops out of Eq. (14). Using this equation and the permutation $R\to r_1$, $r_1\to r$, $r_2\to r_2$, $r_5\to r_3$, one gets Eq. (13) with $i=3$. The equation for pattern II is derived similarly.

To derive (15), consider the figure on the right part of Fig. 3 where $k+l+m=1\ (\mathrm{mod}\ 2)$ and r_1, r_2, r_3 and r are the radii of the circles with the centers at $z_{k+1,l,m}$, $z_{k+1,l+1,m-1}$, $z_{k,l+1,m}$ and $z_{k,l,m-1}$, respectively. Elementary geometrical considerations and Lemma 1 applied to the forms of the shown quadrilaterals give Eq. (15).

Remark: Equation (15) is derived for $r=r(K,L,M)$, $r_1=r(K,L,M-1)$, $r_2=r(K-1,L,M)$, $r_3=r(K,L-1,M+1)$. However, it holds true also for $r_1=r(K,L,M+1)$, $r_2=r(K+1,L,M)$, $r_3=r(K,L+1,M+1)$ since it gives the radius of the circle through the three intersection points of the circles with radii r_1, r_2, r_3 intersecting at prescribed angles as shown in the right part of Fig. 3. Later, we refer to this equation also for this pattern.

Sufficiency: Now let $r(K,L,M):\tilde{Q}_H\to\mathbf{R}_+$ be some positive solution to (13)–(15). We can rescale it so that $r(0,0,0)=1$. Starting with $r(1,0,-1)$ and $r(0,1,-1)$ one can compute r everywhere in $\tilde{Q}_H$: r in a "black" vertex (see Fig. 4) is computed from (14). [Note that only r at "circled" vertices is used: so to compute $r_{1,1,-1}$ one needs only $r(1,0,-1)$ and $r(0,1,-1)$.] The function r in "white" vertices on the border $\partial\tilde{Q}_H=\{(K,0,-K)|K\in\mathbf{N}\}\cup\{(0,L,-L)|L\in\mathbf{N}\}$ is given by (13). Finally, r in "white" vertices in $Q_H^{int}=Q_H\backslash\partial\tilde{Q}_H$ is computed from (15). In Fig. 4 labels show the order of computing r.

Lemma 2: Any solution $r(K,L,M):\tilde{Q}_H\to\mathbf{R}$ to (13)–(15) with $0\leqslant c\leqslant 2$, which is positive for inner vertices of $\tilde{Q}_H$ defines some $z_{k,l,m}$ satisfying (1) in Q. Moreover, all the triangles $(z_{k,l,m},z_{k+1,l,m},z_{k,l,m-1})$, $(z_{k,l,m},z_{k,l,m-1},z_{k,l+1,m})$ and $(z_{k,l,m},z_{k+1,l,m},z_{k,l+1,m})$ have positive orientation.

Proof of the lemma: One can place the circles with radii $r(K,L,M)$ into the complex plane $\mathbb{C}$ in the way prescribed by the hexagonal combinatorics and the intersection angles. Taking the circle centers and the intersection points of neighboring circles, one recovers $z_{k,l,m}$ for $k+l+m=0,\pm 1$ up to a translation and rotation. Reversing the arguments used in the derivation of (13)–(15), one observes from the forms of the quadrilaterals that Eqs. (1) are satisfied. Now using (1), one recovers z in the whole Q. Equation (15) ensures that the radii r remain positive, which implies the positive orientations of the triangles $(z_{k,l,m},z_{k+1,l,m},z_{k,l,m-1})$, $(z_{k,l,m},z_{k,l,m-1},z_{k,l+1,m})$ and $(z_{k,l,m},z_{k+1,l,m},z_{k,l+1,m})$.

Consider a solution $z:Q\to\mathbb{C}$ of the system (1) and (2) with initial data (4), where ϕ and ψ are chosen so that the triangles $(z_{0,0,0)},z_{1,0,0},z_{0,0,-1})$ and $(z_{0,0,0)},z_{0,0,-1},z_{0,1,0})$ have positive orientations and satisfy conditions $r(1,0,-1)=|z_{1,0,-1}-z_{1,0,0}|$ and $r(0,1,-1)=|z_{0,1,-1}-z_{0,0,-1}|$. The map $z_{k,l,m}$ defines circle pattern due to Proposition 1 and coincides with the map defined by Lemma 2 due to the uniqueness of the solution uniqueness. Q.E.D.

Since the cross-ratio equations and the constraint are compatible, the equations for the radii are also compatible. Starting with $r(0,0,0)$, $r(1,0,-1)$ and $r(0,1,-1)$, one can compute $r(K,L,M)$ everywhere in $\tilde{Q}$.

Lemma 3: Let a solution $r(K,L,M):\tilde{Q}\to\mathbb{R}$ of (13)–(15) be positive in the planes given by equations $K+M=0$ and $L+M=0$. Then it is positive everywhere in $\tilde{Q}$.

Proof: As follows from Eq. (15), r is positive for positive r_i, $i=1,2,3$. As r at $(K,K,-K)$, $(K+1,K,-K-1)$ and $(K,K+1,-K-1)$ is positive, r at $(K,K,K-1)$ is also positive. Now starting from r at $(K,K,-K-1)$ and having $r>0$ at $(N,K+1,-K-1)$ and $(N,K,-K)$, one obtains positive r at $(N,K,-K-1)$ for $0\leqslant N<K$ by the same reason. Similarly, r at $(K,N,-K-1)$ is positive. Thus from positive r at the planes $K+M=0$ and $L+M=0$, we get positive r at the planes $K+M=-1$ and $L+M=-1$. Induction completes the proof.

Lemma 4: Let a solution $r(K,L,M):\tilde{Q}\to\mathbb{R}$ of (13)–(15) be positive in the lines parametrized by n as $(n,0,-n)$ and $(0,n,-n)$. Then it is positive in the border planes of $\tilde{Q}$ specified by $K+M=0$ and $L+M=0$.

Proof: We prove this lemma for $K+M=0$. For the other border plane it is proved similarly. Equation (14) for $(K,L,-K-1)$ gives

$$r_2=r_5\frac{(2L+c)r_1+(2K+c)r_4}{(2K+2-c)r_1+(2L+2-c)r_4}, \tag{16}$$

therefore r_2 is positive provided r_1, r_5 and r_4 are positive. For $K=L$ it reads as

$$r_2=r_5\frac{(2K+c)}{(2K+2-c)}. \tag{17}$$

It allows us to compute recursively r at $(K,K,-K)$ starting with r at $(0,0,0)$. Obviously, $r>0$ for $(K,K,-K)$ if $r>0$ at $(0,0,0)$. This property together with the condition $r>0$ at $(n,0,-n)$ implies the conclusion of the lemma since Eq. (16) gives r everywhere in the border plane of $\tilde{Q}$ specified by $K+M=0$.

Lemmas 3 and 4 imply that the circle pattern z^c is an immersion if $r>0$ at $(N,0,-N)$ and $(0,N,-N)$.

IV. PROOF OF THE MAIN THEOREM. DISCRETE PAINLEVÉ AND RICCATI EQUATIONS

In this section, we prove that all $r(n,0,-n)$, $\forall n\in\mathbb{N}$ are positive only for the initial data $z_{1,0,0}=1$, $z_{0,0,-1}=e^{c\alpha_3}$. For the line $r(0,n,-n)$ the proof is the same. Our strategy is as follows: first, we prove the existence of an initial value $z_{0,0,-1}$ such that $r(n,0,-n)>0$, $\forall n\in\mathbb{N}$. Finally we will show that this value is unique and is $z_{0,0,-1}=e^{c\alpha_3}$.

Proposition 2: Suppose the equation

$$(n+1)(x_n^2-1)\left(\frac{x_{n+1}+x_n/\varepsilon}{\varepsilon+x_nx_{n+1}}\right)-n(1-x_n^2/\varepsilon^2)\left(\frac{x_{n-1}+\varepsilon x_n}{\varepsilon+x_{n-1}x_n}\right)=cx_n\frac{\varepsilon^2-1}{2\varepsilon^2}, \tag{18}$$

where $\varepsilon=e^{i\alpha_3}$, *has a unitary solution* $x_n=e^{i\beta_n}$ *in the sector* $0<\beta_n<\alpha_3$. *Then* $r(n,0,-n)$, $n\geqslant 0$ *is positive.*

Proof: For $z_{1,0,0}=1$ and unitary $z_{1,0,-1}$, the equation for the cross-ratio with α_3 and (2) reduce to (18) with unitary $x_n^2=(z_{n,0,-n-1}-z_{n,0,n})/(z_{n+1,0,-n}-z_{n,0,n})$. Note that for $n=0$ the term with x_{-1} drops out of (18); therefore the solution for $n>0$ is determined by x_0 only. The condition $0<\beta_n<\alpha_3$ means that all triangles $(z_{n,0,-n},z_{n+1,0,n},z_{n,0,-n-1})$ have positive orientation. Hence $r(n,0,-n)$ are all positive. Q.E.D.

Remark: Equation (18) is a special *discrete Painlevé equation*. For a more general reduction of cross-ratio equation see Ref. 18. The case $\varepsilon=i$, corresponding to the orthogonally intersecting circles, was studied in detail in Ref. 3. Here we generalize these results to the case of arbitrary unitary ε. Below we omit the index of α so that $\varepsilon=e^{i\alpha}$.

Theorem 4: *There exists a unitary solution* $x_n=e^{i\beta_n}$ *to (18) in the sector* $0<\beta_n<\alpha$.

Proof: Equation (18) allows us to represent x_{n+1} as a function of n,x_{n-1} and x_n: $x_{n+1}=\Phi(n,x_{n-1},x_n)$. $\Phi(n,u,v)$ maps the torus $T^2=S^1\times S^1=\{(u,v)\in\mathbb{C}:|u|=|v|=1\}$ into S^1 and has the following properties:

(i) For all $n\in\mathbb{N}$ it is a continuous map on $A_I\times\overline{A_I}$ where $A_I=\{e^{i\beta}:\beta\in(0,\alpha)\}$ and $\overline{A_I}$ is the closure of A_I. Values of Φ on the border of $A_I\times\overline{A_I}$ are defined by continuity: $\Phi(n,u,\varepsilon)=-1$, $\Phi(n,u,1)=-\varepsilon$.

(ii) For $(u,v)\in A_I\times A_I$ one has $\Phi(n,u,v)\in A_I\cup A_{II}\cup A_{IV}$, where $A_{II}=\{e^{i\beta}:\beta\in(\alpha,\pi]\}$ and $A_{IV}=\{e^{i\beta}:\beta\in[\alpha-\pi,0)\}$, i.e., x cannot jump in one step from A_I into $A_{III}=\{e^{i\beta}:\beta\in(-\pi,\alpha-\pi)\}$.

Let $x_0=e^{i\beta_0}$. Then $x_n=x_n(\beta_0)$. Define $S_n=\{\beta_0:\ x_k(\beta_0)\in\overline{A_I}\forall\,0\leqslant k\leqslant n\}$. Then S_n is a closed set since Φ is continuous on $A_I\times\overline{A_I}$. As a closed subset of a segment it is a collection of disjoint segments S_n^l.

Lemma 5: There exists sequence $\{S_n^{l(n)}\}$ *such that*

(i) $S_n^{l(n)}$ *is mapped by* $x_n(\beta_0)$ *onto* $\overline{A_I}$ *and*
(ii) $S_{n+1}^{l(n+1)}\subset S_n^{l(n)}$.

The lemma is proved by induction. For $n=0$ it is trivial. Suppose it holds for n. As $S_n^{l(n)}$ is mapped by $x_n(\beta_0)$ onto $\overline{A_I}$, continuity considerations and $\Phi(n,u,\varepsilon)=-1$, $\Phi(n,u,1)=-\varepsilon$ imply $x_{n+1}(\beta_0)$ maps $S_n^{l(n)}$ onto $A_I\cup A_{II}\cup A_{IV}$ and at least one of the segments $S_{n+1}^l\subset S_n^{l(n)}$ is mapped into $\overline{A_I}$. This proves the lemma.

Since the segments of $\{S_n^{l(n)}\}$ constructed in Lemma 5 are nonempty, there exists $\overline{\beta_0}\in S_n$ for all $n\geqslant 0$. For this $\overline{\beta_0}$, the value $x_n(\overline{\beta_0})$ is not on the border of $\overline{A_0}$ since then $x_{n+1}(\beta_0)$ would jump out of $\overline{A_I}$. Q.E.D.

Let r_n and R_n be the radii of the circles of the circle patterns defined by $z_{k,l,m}$ with the centers at $z_{2n,0,0}$ and $z_{2n+1,0,-1}$, respectively. Constraint (2) gives

$$r_{n+1}=\frac{2n+c}{2(n+1)-c}r_n,$$

which is exactly formula (17). From elementary geometric considerations (see Fig. 5) one gets

$$R_{n+1}=\frac{r_{n+1}-R_n\cos\alpha}{R_n-r_{n+1}\cos\alpha}r_{n+1}$$

(recall that $\alpha=\alpha_3$). Define

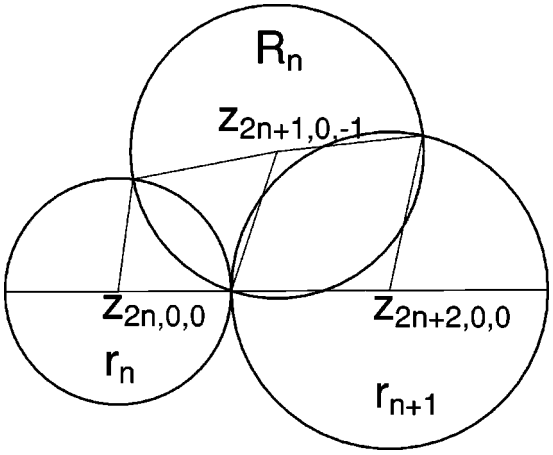

FIG. 5. Circles on the border.

$$p_n=\frac{R_n}{r_n},\quad g_n(c)=\frac{2n+c}{2(n+1)-c}$$

and denote $t=\cos\alpha$. Now, the equation for the radii R, r takes the form

$$p_{n+1}=\frac{g_n(c)-tp_n}{p_n-tg_n(c)}. \tag{19}$$

Remark: Equation (19) can be seen as a discrete version of a *Riccati* equation. This is motivated by the following properties:

(i) The cross-ratio of each four-tuple of its solutions is constant as p_{n+1} is a Möbius transform of p_n.

(ii) The general solution is expressed in terms of solutions of some linear equation: the standard ansatz

$$p_n=\frac{y_{n+1}}{y_n}+tg_n(c) \tag{20}$$

transforms (19) into

$$y_{n+2}+t(g_{n+1}(c)+1)y_{n+1}+(t^2-1)g_n(c)y_n=0. \tag{21}$$

As follows from Theorem 4, Proposition 2, and Lemma 4, Eq. (19) has a positive solution. One may conjecture that there is only one initial value p_0 such that $p_n>0,\ \forall n\in\mathbb{N}$ from the consideration of the asymptotics. Indeed, $g_n(c)\to 1$ as $n\to\infty$, and the general solution of Eq. (21) with limit values of coefficients is $y_n=c_1(-1)^n(1+t)^n+c_2(1-t)^n$. Thus $p_n=y_{n+1}/y_n+tg_n(c)\to -1$ for $c_1\neq 0$. However c_1,c_2 define only the asymptotics of a solution. To relate it to the initial value p_0 is a more difficult problem. Fortunately, it is possible to find the general solution to (21).

Proposition 3: The general solution to (21) is

$$y_n=\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma\left(n+1-\frac{c}{2}\right)}\left(c_1\lambda_1^{n+1-c/2}F\left(\frac{3-c}{2},\frac{c-1}{2},\frac{1}{2}-n,z_1\right)\right.$$
$$\left.+c_2\lambda_2^{n+1-c/2}F\left(\frac{3-c}{2},\frac{c-1}{2},\frac{1}{2}-n,z_2\right)\right), \tag{22}$$

where $\lambda_1=-t-1$, $\lambda_2=1-t$, $z_1=(t-1)/2$, $z_2=-(1+t)/2$ *and* F *is the hypergeometric function.*

Proof: The solution was found by a slightly modified *symbolic method* (see Ref. 10 for the method description and Ref. 2 for the detail). Here, $F(a,b,c,z)$ denotes the standard hypergeometric function which is a solution of the hypergeometric equation

$$z(1-z)F_{zz}+[c-(a+b+1)z]F_z-abF=0 \tag{23}$$

holomorphic at $z=0$. Due to linearity, the general solution of (21) is given by a superposition of any two linearly independent solutions. Direct computation with the series representation of the hypergeometric function

$$\begin{aligned}F&\left(1-\frac{\gamma-1}{2},\frac{\gamma-1}{2},1-\left(x+\frac{\gamma-1}{2}\right),z\right)\\&=1+z\frac{(1-(\gamma-1)/2)(\gamma-1)/2}{(1-(x+(\gamma-1)/2))}+\cdots\\&\quad+z^k\frac{[(1-(\gamma-1)/2)(2-(\gamma-1)/2)\cdots(k-(\gamma-1)/2)][((\gamma-1)/2)(1+(\gamma-1)/2)\cdots(k-1(\gamma-1)/2)]}{(1-(x(\gamma-1)/2))\cdots(k-(x+(\gamma-1)/2))}+\cdots\end{aligned} \tag{24}$$

shows that each summand in (22) satisfies Eq. (21). To finish the proof of Proposition 3, one has to show that the particular solutions with $c_1=0$, $c_2\neq 0$ and $c_1\neq 0$, $c_2=0$ are linearly independent. This fact follows from the following lemma.

Lemma 6: As $n\to\infty$, *function (22) has the asymptotics*

$$y_n\simeq(n+1-\gamma/2)^{(\gamma-1)/2}(c_1\lambda_1^{n+1-\gamma/2}+c_2\lambda_2^{n+1-\gamma/2}). \tag{25}$$

For $n\to\infty$ the series representation (24) implies $F((3-\gamma)/2,(\gamma-1)/2,\frac{1}{2}-n,z_1)\simeq 1$. Stirling's formula

$$\Gamma(x)\simeq\sqrt{2\pi}e^{-x}x^{x-1/2} \tag{26}$$

yields the asymptotics of the factor $\Gamma(n+\frac{1}{2})/\Gamma(n+1-\gamma/2)$. This completes the proof of the lemma and of Proposition (3).

Proposition 4: A solution of the discrete Riccati equation (19) with $\alpha\neq\pi/2$ *is positive for all* $n\geqslant 0$ *if and only if*

$$p_0=\frac{\sin c\alpha/2}{\sin(2-c)\alpha/2}. \tag{27}$$

Proof: For positive p_n, it is necessary that $c_1=0$: this follows from asymptotics (25) substituted into (20). Let us define

$$\begin{aligned}s(z)&=1+z\frac{(1-(\gamma-1)/2)((\gamma-1)/2)}{\frac{1}{2}}+\cdots\\&\quad+z^k\frac{(k-(\gamma-1)/2)\cdots(1-(\gamma-1)/2)((\gamma-1)/2)(k-1+(\gamma-1)/2)}{k!\left(k-\frac{1}{2}\right)\cdots\frac{1}{2}}\cdots.\end{aligned} \tag{28}$$

This is the hypergeometric function $F((3-\gamma)/2,(\gamma-1)/2,\frac{1}{2}-n,z)$ with $n=0$. A straightforward computation with series shows that

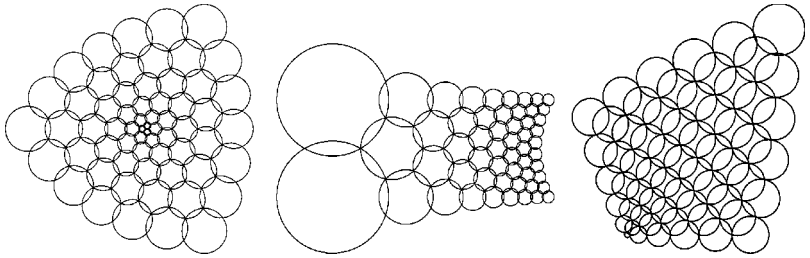

FIG. 6. Hexagonal z^2, Log and square grid $z^{3/2}$.

$$p_0 = 1 + \frac{2(\gamma-1)}{2-\gamma} z + \frac{4z(z-1)}{2-\gamma} \frac{s'(z)}{s(z)}, \tag{29}$$

where $z=(1+t)/2$. Note that p_0 as a function of z satisfies an ordinary differential equation of first order since $s'(z)/s(z)$ satisfies the Riccati equation obtained by a reduction of (23). A computation shows that $[\sin(\gamma\alpha/2)]/[\sin(2-\gamma)\alpha/2]$ satisfies the same ordinary differential eqiation. Since both expression (29) and (27) are equal to 1 for $z=0$, they coincide everywhere.

Q.E.D.

Proof of Theorem 1: Proposition (4) implies that the initial x_0 for which (18) gives positive r is unique and implies the initial values (5) for z^c if $\alpha_i \neq \pi/2$. For the case $\alpha=\pi/2$, any solution for (19) with $p_0>0$ is positive. Nevertheless, as was proved in Ref. 3, x_0 is in this case also unique and is specified by (27). Thus for all $n \in \mathbb{N}$ we have $r(n,0,-n)>0$, $r(0,n,-n)>0$ for the circle pattern z^c. Lemmas 4 and 3 complete the proof.

V. HEXAGONAL CIRCLE PATTERNS z^2 AND Log

For $c=2$, formula (17) gives infinite $r(1,1,-1)$. The way around this difficulty is renormalization $z \to (2-c)z/c$ and a limit procedure $c \to 2-0$, which leads to the renormalization of initial data (see Ref. 7). As follows from (27), this renormalization implies

$$r(0,0,0)=0,\ r(1,0,-1)=\frac{\sin\alpha_3}{\alpha_3}, r(0,1,-1)=\frac{\sin\alpha_2}{\alpha_2},\ r(1,1,-1)=1. \tag{30}$$

Proposition 5: The solution to (13)–(15) with $c=2$ and initial data (30) is positive.

Proof: This follows from Lemmas 3 and 4 since Theorem 4 is true also for the case $c=2$. Indeed, solution x_n is a continuous function of c. Therefore it has a limit value as $c \to 2-0$ and it lies in the sector A_I.

Lemma 2 implies that there exists a hexagonal circle pattern with radius function r.

Definition 3: The hexagonal circle pattern Z^2 has a radius function specified by Proposition 5.

Equations (13)–(15) have the symmetry

$$r \to \frac{1}{r},\ \ c \to 2-c, \tag{31}$$

which is the *duality transformation* (see Ref. 8). The smooth analog $f \to f^*$ for holomorphic functions $f(w), f^*(w)$ is

$$\frac{df(w)}{dw}\frac{df^*(w)}{dw}=1.$$

Note that $\log^*(w)=w^2/2$. The hexagonal circle pattern Log is defined[7] as a circle pattern dual to Z^2. Discrete z^2 and Log are the first two images in Fig. 6.

Theorem 5: *The hexagonal circle patterns Z^2 and* Log *are immersions.*

Proof: For z^2 this follows from Proposition 5. Hence the values of $1/r$, where r is radius function for z^2, are positive except for $r(0,0,0)=\infty$. Lemma 2 completes the proof.

VI. CONCLUDING REMARKS

In this section we discuss corollaries of the obtained results and possible generalizations

A. Square grid circle patterns z^c and Log

Equations (1) extend $z_{k,l,m}$ corresponding to the hexagonal z^2 and Log from Q_H into the three-dimensional lattice Q. The r-function of this extension satisfies Eq. (15). Consider $z_{k,l,m}$ for the hexagonal z^c and Log restricted to one of the coordinate planes, e.g., $l=0$. Then Proposition 1 states that $z_{k,0,m}$ defines some circle pattern with combinatorics of the square grid: each circle has four neighboring circles intersecting it at angles α_3 and $\pi-\alpha_3$. It is natural to call it *square grid* z^c (see the third image in Fig. 6). Such circle patterns are natural generalization of those with orthogonal neighboring and tangent half-neighboring circles introduced and studied in Ref. 22.

Theorem 6: *Square grid* z^c, $0<c\leqslant 2$ *and* Log *are immersions.*

Proof easily follows from Lemma 2.

It is interesting to note that the square grid circle pattern z^c can be obtained from hexagonal one by limit procedure $\alpha_3\to+0$ and by $\alpha_1\to\pi-\alpha_2$. These limit circle patterns still can be defined by (1) and (2) by imposing the self-similarity condition $z_{k,l,m}=f_{l,k-m}$.

B. Square grid circle patterns Erf

For square grid combinatorics and $\alpha=\pi/2$, Schramm[22] constructed circle patterns mimicking holomorphic function $\mathrm{erf}(z)=(2/\pi)\int e^{-z^2}dz$ by giving the radius function explicitly. Namely, let n,m label the circle centers so that the pairs of circles $c(n,m)$, $c(n+1,m)$ and $c(n,m)$, $c(n,m+1)$ are orthogonal and the pairs $c(n,m)$, $c(n+1,m+1)$ and $c(n,m+1)$, $c(n+1,m)$ are tangent. Then

$$r(n,m)=e^{nm} \tag{32}$$

satisfies the equation for a radius function:

$$R^2(r_1+r_2+r_3+r_4)-(r_2r_3r_4+r_1r_3r_4+r_1r_2r_4+r_1r_2r_3)=0, \tag{33}$$

where $R=r(n,m)$, $r_1=r(n+1,m)$, $r_2=r(n,m+1)$, $r_3=r(n-1,m)$, $r_4=r(n,m-1)$. For square grid circle patterns with intersection angles α for $c(n,m)$, $c(n+1,m)$ and $\pi-\alpha$ for $c(n,m)$, $c(n,m+1)$ the governing Eq. (33) becomes

$$R^2(r_1+r_2+r_3+r_4)-(r_2r_3r_4+r_1r_3r_4+r_1r_2r_4+r_1r_2r_3)+2R\cos\alpha(r_1r_3-r_2r_4)=0. \tag{34}$$

It is easy to see that (34) has the same solution (32) and it therefore defines a square grid circle pattern, which is a discrete Erf. A hexagonal analog of Erf is not known.

C. Circle patterns with quasi-regular combinatorics

One can deregularize the prescribed combinatorics by a projection of $\mathbb{Z}^n$ into a plane as follows (see Ref. 23). Consider $\mathbb{Z}^n_+\subset\mathbb{R}^n$. For each coordinate vector $\mathbf{e}_i=(e_i^1,\ldots,e_i^n)$, where $e_i^j=\delta_i^j$ define a unit vector ξ_i in $\mathbb{C}=\mathbb{R}^2$ so that for any pair of indices i,j, vectors ξ_i,ξ_j form a basis in $\mathbb{R}^2$. Let $\Omega\in\mathbb{R}^n$ be some two-dimensional simply connected cell complex with vertices in $\mathbb{Z}^n_+$. Choose some $x_0\in\Omega$. Define the map $P:\Omega\to\mathbb{C}$ by the following conditions:

(i) $P(x_0)=P_0$.
(ii) If x,y are vertices of Ω and $y=x+\mathbf{e}_i$, then $P(y)=P(x)+\xi_i$.

It is easy to see that P is correctly defined and unique.

We call Ω a *projectable* cell complex if its image $\omega = P(\Omega)$ is embedded, i.e., intersections of images of different cells of Ω do not have inner parts. Using projectable cell complexes one can obtain combinatorics of Penrose tilings.

It is natural to define ''discrete conformal map on ω'' as a discrete complex immersion function z on vertices of ω preserving the cross-ratios of the ω-cells. The argument of z can be labeled by the vertices x of Ω. Hence for any cell of Ω, constructed on $\mathbf{e}_k, \mathbf{e}_j$, the function z satisfies the following equation for the cross-ratios:

$$q(z_x, z_{x+\mathbf{e}_k}, z_{x+\mathbf{e}_k+\mathbf{e}_j}, z_{x+\mathbf{e}_j}) = e^{-2i\alpha_{k,j}}, \tag{35}$$

where $\alpha_{k,j}$ is the angle between $\boldsymbol{\xi}_k$ and $\boldsymbol{\xi}_j$, taken positively if (ξ_k, ξ_j) has positive orientation and taken negatively otherwise. Now suppose that z is a solution to (35) defined on the whole $\mathbb{Z}^n_+$. We can define a discrete $z^c: \omega \to \mathbb{C}$ for projectable Ω as a solution to (35) and (36) restricted to Ω. Initial conditions for this solution are of the form (5) so that the restrictions of z to each two-dimensional coordinate lattice is an immersion defining a circle pattern with prescribed intersection angles. This definition naturally generalizes the definition of discrete hexagonal and square grid z^c considered above.

We finish this section with the natural conjecture formulated in Ref. 2.

Conjecture: The discrete $z^c: \omega \to \mathbb{C}$ is an immersion.

The first step in proving this claim is to show that Eq. (35) is compatible with the constraint

$$c f_x = \sum_{s=1}^{n} 2x_s \frac{(f_{x+\mathbf{e}_s} - f_x)(f_x - f_{x-\mathbf{e}_s})}{f_{x+\mathbf{e}_s} - f_{x-\mathbf{e}_s}}. \tag{36}$$

For $n = 3$ this fact is proven in Ref. 7.

ACKNOWLEDGMENTS

S.I.A. was partially supported by the SFB 288 ''Differential Geometry and Quantum Physics'' and EPSRC Grant No. Gr/N30941. A.I.B. was partially supported by the SFB 288 ''Differential Geometry and Quantum Physics'' and the DFG Research Center ''Mathematics for Key Technologies'' (FZT 86) in Berlin.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

The geodesic approximation for lump dynamics and coercivity of the Hessian for harmonic maps

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(Received 19 December 2002; accepted 9 April 2003)

The most fruitful approach to studying low energy soliton dynamics in field theories of Bogomol'nyi type is the geodesic approximation of Manton. In the case of vortices and monopoles, Stuart has obtained rigorous estimates of the errors in this approximation, and hence proved that it is valid in the low speed regime. His method employs energy estimates which rely on a key coercivity property of the Hessian of the energy functional of the theory under consideration. In this article we prove an analogous coercivity property for the Hessian of the energy functional of a general sigma model with compact Kähler domain and target. We go on to prove a continuity property for our result, and show that, for the $\mathbb{C}P^1$ model on S^2, the Hessian fails to be globally coercive in the degree 1 sector. We present numerical evidence which suggests that the Hessian is globally coercive in a certain equivariance class of the degree n sector for $n \geqslant 2$. We also prove that, within the geodesic approximation, a single $\mathbb{C}P^1$ lump moving on S^2 does not generically travel on a great circle. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1586480]

I. INTRODUCTION

Many field theories arising naturally in theoretical high energy physics may be said to be of Bogomol'nyi type. For such theories there is a topological lower bound on the energy of field configurations, and this bound is attained only by solutions of a first order ''self-duality'' equation, the so-called solitons of the theory. The solitons are stable by virtue of their energy-minimizing property, and are generically spatially localized lumps of energy with strongly particlelike characteristics. When static they exert no net force on one another, so the structure of the space of static multisoliton solutions is rather rich. Examples within the context of gauge theory are given by the Yang–Mills–Higgs and Abelian–Higgs models, whose solitons are called monopoles and vortices, respectively. In both these cases, the static models are very well understood and the structure of M_n, the moduli space of static n-soliton solutions, is known in great detail. For monopoles, in particular, the static system is integrable and there are several constructions which generate exact solutions of various degrees of explicitness. Once one introduces time dependence, however, things get much more difficult. No Bogomol'nyi-type field theory (indeed, no Lorentz invariant field theory) in more than $(1+1)$ dimensions is integrable, and the construction of nontrivial exact time-dependent solutions seems impossible.

How then is one to understand the dynamics of moving solitons in these models? The most fruitful approach has turned out to be the geodesic approximation of Manton.[11] Here one argues on physical grounds that the solution of any initial value problem in the n-soliton sector whose initial field is a static solution, and whose initial kinetic energy is small, should be forced to stay close to M_n by energy conservation. Manton suggested that the dynamics should be well approximated by

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a solution of the reduced variational problem where the field configuration is *constrained* to lie on M_n at all times. This reduced dynamics turns out to be geodesic flow on M_n with respect to a natural metric called the L^2 metric, so one has the appealing suggestion that low energy soliton dynamics in Bogomol'nyi-type theories may be understood by studying the Riemannian geometry of their moduli spaces. This is still a highly nontrivial problem, and it was some time before the L^2 metrics on the two-monopole and two-vortex moduli spaces were well understood.[2,17] Since first being proposed, the method of Manton has been extended to deal with dynamical issues other than classical multisoliton scattering. Quantum soliton states[5] are thought to be well approximated by eigenstates of the Laplacian on M_n, for example, and the thermodynamics of soliton gases[12] has been analyzed in terms of the geometry of M_n.

Not all Bogomol'nyi-type field theories are gauge theories. Another class is given by nonlinear sigma models with Kähler target space, for example the $\mathbb{C}P^N$ models. These models are nonlinear in the most fundamental way: the field takes values in a space with no linear structure. However, they have many features in common with the gauge theories mentioned above. There is again a topological lower bound on energy, attained only by solutions of a first order partial differential equation, namely the $\pm$-holomorphic maps—the Cauchy–Riemann conditions play the role of the self-duality equation. The static model is integrable and the structure of M_n is again well understood. The solitons in this case are usually called ''lumps.''

Given the similarities between lumps and their gauge theoretic counterparts, it was natural for Ward to suggest, in the specific context of the $\mathbb{C}P^1$ model on the plane, that the geodesic approximation should be applicable to classical lump dynamics too.[26] A detailed numerical analysis of two-lump scattering within the geodesic approximation followed,[7] as well as generalizations to the $\mathbb{C}P^N$ models.[22] One technical problem encountered in all these studies is that $\mathbb{C}P^N$ lumps have L^2-infinite zero modes on $\mathbb{C}$, so the L^2 metric is only well-defined on the leaves of a foliation of M_n, rather than M_n itself. One interprets this physically as saying that certain parameters in the static n-lump solution are frozen to constant values by infinite inertia. For example, the width of a single $\mathbb{C}P^1$ lump is a free parameter, but is frozen in this fashion. Unfortunately, this freezing appears to be an artifact of the approximation—numerical solutions suggest that a single lump may expand or contract according to the genuine field dynamics. So the geodesic approximation is rather pathological for these models. It is therefore interesting to consider situations where physical space is compact, since the L^2 metric is then guaranteed to be well-defined. In particular, $\mathbb{C}P^1$ lumps on S^2 and T^2 have been studied, and quite a lot is known about the corresponding L^2 geometries.[19–21]

The question remains, of course, whether geodesic flow in M_n really does closely approximate low-energy n-lump dynamics in these theories. For two-vortex and two-monopole dynamics, rigorous results supporting the geodesic approximation have been proved by Stuart.[23,24] He has shown that the solution with initial data $\phi(0) \in \mathsf{M}_2$, $\dot{\phi}(0) \in T_{\phi(0)}\mathsf{M}_2$ of order ϵ (where $\epsilon > 0$ is small), stays pointwise close (order ϵ^2) to its corresponding geodesic in M_2 for a time of order ϵ^{-1}. The key idea in Stuart's analysis is to separate the dynamics into slow and fast time-varying modes by means of the following projection: the true solution $\phi(t)$ is projected onto M_2 to obtain a slow trajectory $\tilde{\phi}$,

$$\phi(t) = \tilde{\phi}(\epsilon t) + \epsilon^2 V(t), \tag{1.1}$$

and a fast varying ''error'' $V(t)$, the projection being chosen so that $V(t)$ is always L^2 orthogonal to $T_{\tilde{\phi}(\epsilon t)}\mathsf{M}_2$. Stuart goes on to prove that an appropriate Sobolev norm of $V(t)$ remains bounded for times of order ϵ^{-1} by bounding this norm in terms of $\mathsf{Hess}_{\tilde{\phi}}$, the quadratic form associated with the second variation of the potential energy functional of the model, which is slowly varying by virtue of energy conservation. It follows that, as expected, the true solution remains close to M_2. That the projected trajectory $\tilde{\phi}$ remains close to geodesic is proved as a separate step.

The whole analysis relies on one's ability to control Sobolev norms of the error in terms of the Hessian. More precisely, the following coercivity property of Hess is crucial:

There exists a constant $\tau>0$ *such that for all* $\tilde{\phi}\in \mathsf{M}_2$ *and all* $V\in H^1$ *with* $V\perp_{L^2} T_{\tilde{\phi}}\mathsf{M}_2$, $\mathsf{Hess}_{\tilde{\phi}}(V,V)\geqslant \tau\|V\|^2_{H^1}$.

This turns out to be slightly easier to prove for vortices than monopoles since the L^2 spectrum of small oscillations about a static vortex has a mass gap due to the Higgs mechanism. No such gap occurs for monopoles.

How much of this framework carries over to sigma models? Since the target space has no linear structure, Eq. (1.1) makes no sense as it stands, and must be replaced. We suggest here that the correct replacement is

$$\phi(t)=\exp_{\tilde{\phi}(\epsilon t)}\epsilon^2 V(t), \tag{1.2}$$

where $\exp{:}TN\to N$ is the exponential map on the target space N. Once again, we should choose $V(t)$ always to be L^2 orthogonal to $T_{\tilde{\phi}(\epsilon t)}\mathsf{M}_n$. In this context, we will prove an analog of Stuart's coercivity lemma for any holomorphic map $\tilde{\phi}$ between compact Kähler manifolds, namely, there exists $\tau(\tilde{\phi})>0$ such that for all $V\in H^1$, $V\perp_{L^2} T_{\tilde{\phi}}\mathsf{M}_n$,

$$\mathsf{Hess}_{\tilde{\phi}}(V,V)\geqslant \tau(\tilde{\phi})\|V\|^2_{H^1}. \tag{1.3}$$

The important difference from Stuart's result is that the constant τ depends on $\tilde{\phi}$, that is, varies with position in M_n. We may define the optimal constant

$$\tau(\tilde{\phi})=\inf\left\{\frac{\mathsf{Hess}_{\tilde{\phi}}(V,V)}{\|V\|^2_{H^1}}: V\neq 0, V\perp_{L^2} T_{\tilde{\phi}}\mathsf{M}_n\right\}>0. \tag{1.4}$$

We prove a result (Theorem 6) which gives sufficient conditions that τ depends continuously on $\tilde{\phi}$, and verify that those conditions hold in the main examples of interest to us. It turns out that M_n for sigma models is generically noncompact, so continuity of $\tau(\tilde{\phi})$ does not guarantee a global bound. In fact, we will show by means of an explicit counterexample that $\tau(\tilde{\phi})>0$ is *not* necessarily bounded away from zero. The counterexample occurs in the simplest nontrivial case, namely the one-lump moduli space of the $\mathbb{C}P^1$ model on S^2, but we believe it is indicative of a generic phenomenon for the $\mathbb{C}P^N$ models on any compact Riemann surface. Roughly speaking, $\tau(\tilde{\phi})\to 0$ as the lump $\tilde{\phi}$ shrinks to zero size. One would expect this to happen quite generically in M_n, wherever a family of holomorphic maps degenerates so that a single isolated lump collapses. This suggests we are never likely to have a global bounding constant τ on M_n as obtained by Stuart for vortices and monopoles. Consequently, the best result one could hope for from an analysis of this type for lumps is that the geodesic approximation is good for a time of order $T\epsilon^{-1}$, where T is some increasing function of $\inf_t \tau(\tilde{\phi}(\epsilon t))$. In this case, the approximation would work well (in the usual sense) so long as the projected geodesic stays away from $\partial_\infty \mathsf{M}_n$, the boundary at infinity of M_n, where $\tau\to 0$. In particular it seems very unlikely that geodesic flow provides a good approximation to the process of single lump collapse itself. Two independent numerical studies of singularity formation in the $\mathbb{C}P^1$ model on the plane support this pessimistic assessment.[3,10]

If we impose extra symmetry on our system, in other words, restrict attention to an admissible equivariance class, then the projected map $\tilde{\phi}$ is confined to a totally geodesic submanifold M_n^{eq} of M_n, and the error V is confined to an infinite dimensional subspace H^1_{eq} of $H^1(\tilde{\phi}^*TN)$. We may define an equivariant version τ^{eq} of τ by taking the infimum only over sections $V\in H^1_{eq}$. Clearly $\tau^{eq}(\tilde{\phi})\geqslant\tau(\tilde{\phi})>0$. For a certain equivariance class for n-lump dynamics in the $\mathbb{C}P^1$ model on S^2, one can prove that τ^{eq} is continuous on M_n^{eq}, which is again noncompact. We will present numerical evidence that $\tau^{eq}(\tilde{\phi})$ *is* globally bounded away from zero for $n\geqslant 2$ in this class. The point is that only *coincident* n-lump collapse can occur within this particular equivariance class, and the problem of vanishing τ does not appear to happen for such collapse. It is possible,

therefore, that the geodesic approximation does give a good model of equivariant multilump collapse, though one should be cautious: there is ample scope for other aspects of Stuart's method to break down as singularities form. There are some grounds for optimism. A recent careful numerical study of lump collapse by Linhart and Sadun found that single lump collapse on the plane differed significantly from that predicted by a truncated geodesic approximation, while coincident two-lump collapse did not.[10]

The rest of this article is structured as follows. In Sec. II we introduce the nonlinear sigma models of interest and briefly review some of their standard properties. We focus in particular on the $\mathbb{C}P^1$ model on S^2, describing what is known about the L^2 geometry on M_n in this case, especially for $n=1$. We present a new result on generic behavior of the geodesic flow in M_1 which implies that (within the geodesic approximation) a single lump generically does *not* travel along great circles on S^2. Precise restrictions on the set of nongeneric initial data are given. In Sec. III we formulate and prove the main result of the article, that the Hessian for these models is coercive on H^1, in the sense described above. In Sec. IV we establish a simple sufficient condition for $\tau(\phi)$ to depend continuously on $\tilde{\phi}\in\mathsf{M}_n$. In Sec. V we show that this condition is met in the case of M_1 for the $\mathbb{C}P^1$ model on S^2. We go on to prove that $\tau\to 0$ as $\tilde{\phi}$ approaches $\partial_\infty \mathsf{M}_1$, so global coercivity fails in this case. Finally, in Sec. VI we consider the case of the n-lump sector of the $\mathbb{C}P^1$ model on S^2 within a given equivariance class, showing that τ^{eq} is continuous. We conjecture that Hess^{eq} is globally coercive for $n\geqslant 2$ and present some numerical results in support of this conjecture.

II. THE $\mathbb{C}P^1$ MODEL ON S^2

For our purposes, a nonlinear sigma model consists of a single field $\phi:\mathbb{R}\times M\to N$, where (M,g) and (N,h) are compact Kähler manifolds, M represents physical space, $\mathbb{R}\times M$ is space–time, equipped with the Lorentzian pseudometric $\eta=dt^2-g$, and N is the target space. Solutions of the model are local extremals of the action,

$$S[\phi]=\frac{1}{2}\int_{\mathbb{R}\times M}\sum_{\alpha}\frac{|d\phi E_\alpha|^2}{|E_\alpha|^2}=\int_{\mathbb{R}}\left(\frac{1}{2}\int_M|\dot{\phi}|^2-E[\phi]\right), \tag{2.1}$$

where $E_0=\partial/\partial t, E_1,\ldots,E_m$ is an orthonormal basis of vector fields on $\mathbb{R}\times M$ and $E[\phi]$ is the harmonic map energy functional for maps $M\to N$. Such solutions are called wave maps in the geometric analysis literature, by analogy with harmonic maps.[18] Indeed, static wave maps are precisely harmonic maps and hence have been the focus of intense study. In particular, Lichnerowicz showed that if a homotopy class $[\phi]$ contains $\pm$-holomorphic representatives, then these minimize energy within that class.[9] So the moduli space of interest within a given class is $\mathsf{M}_{[\phi]}=\mathsf{Hol}_{[\phi]}(M,N)$. For the sake of generality, we will state and prove the coercivity lemma for the Hessian in this general context.

It is important when using the geodesic approximation to know that $\mathsf{M}_{[\phi]}$ is a finite dimensional smooth manifold. This is not always true in the general case of holomorphic maps between Kähler manifolds. We discuss this question in more detail in Sec. III, briefly summarizing some results in the harmonic maps and algebraic geometry literature which allow us to identify classes of sigma model whose moduli spaces are smooth manifolds. For the moment we note that the particular case we have most directly in mind, namely $M=N=S^2$, the $\mathbb{C}P^1$ model on the two-sphere, certainly does have this property.

We now consider the case $M=N=S^2$ in more detail. Each homotopy class $[\phi]\in\pi_2(S^2)$ is labeled by the degree of ϕ, an integer n, which without loss of generality we may assume is nonnegative. The degree n is interpreted physically as the net lump number of the configuration ϕ. The space M_n of degree n holomorphic maps $S^2\to S^2$ is easily constructed explicitly. Choosing stereographic coordinates $z,W\in\mathbb{C}$ on both M and N, such a map is rational of degree n,

$$\phi: z \mapsto W = \frac{a_1 z^n + \cdots + a_{n+1}}{a_{n+2} z^n + \cdots + a_{2n+2}}, \tag{2.2}$$

where a_i are $2n+2$ complex constants, a_1 and a_{n+2} do not both vanish, and the numerator and denominator have no common roots. Since $(a_1,\ldots,a_{2n+2})$ and $(\xi a_1,\ldots,\xi a_{2n+2})$ give the same map for all $\xi \in \mathbb{C}\backslash\{0\}$, we have a natural identification of M_n with a dense open subset of $\mathbb{C}P^{2n+1}$, whence it inherits a natural topology and complex structure.

The metric of interest γ does not descend from the inclusion $\mathsf{M}_n \subset \mathbb{C}P^{2n+1}$, however. To define it, one must think of a tangent vector $X \in T_\phi \mathsf{M}_n$ as a zero mode of the Cauchy–Riemann equations for maps $M \to N$ at the map ϕ. Such a zero mode is a smooth section of $\phi^* TN$, the pullback of the tangent bundle of N by the map ϕ, that is, a rule which assigns to each $p \in M$ a vector $V(p) \in T_{\phi(p)} N$. We may define the L^2 inner product between any pair of sufficiently regular sections X, Y of $\phi^* TN$ by taking their fibrewise inner product in $T_{\phi(p)} N$, then integrating over M,

$$\langle X, Y \rangle_{L^2} = \int_M h(X,Y). \tag{2.3}$$

The L^2 metric on M_n is simply the restriction of $\langle \cdot, \cdot \rangle_{L^2}$ to zero modes. In more concrete terms, one can in principle compute explicit formulas for γ by choosing local coordinates q^i on M_n (for example, the real and imaginary parts of a_i/a_1, on the chart where $a_1 \neq 0$) and expressing the map $\phi(\{q^i\})$ as an explicit function $W(z,\{q^i\})$, so that

$$\gamma = \sum_{ij} \gamma_{ij} dq^i dq^j, \quad \gamma_{ij} = \int_{\mathbb{C}} \frac{dz d\overline{z}}{(1+|z|^2)^2} \frac{1}{(1+|W|^2)^2} \frac{\partial W}{\partial q^i} \frac{\overline{\partial W}}{\partial q^j}. \tag{2.4}$$

In practice, of course, the integrals involved are almost always intractable.

Certainly, the L^2 metric is a natural way of geometrizing M_n. More importantly, it is the Riemannian metric descending from the restriction of the kinetic energy functional $\frac{1}{2}\int_M |\dot{\phi}|^2$ to M_n, and hence the metric whose geodesics are thought to model slow lump dynamics. We shall briefly review what is known about the Riemannian manifold (M_n, γ), and prove a new result about the generic behavior of geodesics in (M_1, γ).

First, (M_n, γ) is manifestly Hermitian, and is in fact Kähler. This was long suspected, owing to a rather general formal argument of Ruback,[15] and has recently been proved rigorously.[21] It is also known that (M_n, γ) is geodesically incomplete.[16] For odd n, (M_n, γ) contains a totally geodesic Lagrangian submanifold naturally identified with the moduli space of static $\mathbb{R}P^2$ n-lumps on $\mathbb{R}P^2$; for $n \geqslant 3$ this submanifold is also incomplete.

There is an isometric action of $G = \mathrm{SO}(3) \times \mathrm{SO}(3)$ on M_n, induced by the natural SO(3) actions on the domain and target spheres, which on M_1 has cohomogeneity 1 (generic G orbits have codimension 1), and in fact, almost completely determines γ. Consequently, an explicit formula for γ is known in this case, and the geometry is particularly well understood. For $n=1$, the no common roots condition on the rational map $W(z) = (a_1 z + a_2)/(a_3 z + a_4)$ is $a_1 a_4 - a_2 a_3 \neq 0$, so we may identify each map with a projective equivalence class $[L]$ of $\mathrm{GL}(2,\mathbb{C})$ matrices. Hence $\mathsf{M}_1 \cong \mathrm{PL}(2,\mathbb{C})$. By identifying S^2 with the unit sphere in $\mathbb{R}^3 \cong \mathfrak{su}(2)$ in the usual way, we may identify the SO(3) action on S^2 with the adjoint SU(2) action, so that γ regarded as a metric on $\mathrm{PL}(2,\mathbb{C})$ is invariant under the left and right PU(2) actions:

$$([U_1],[U_2]): [L] \mapsto [U_1 L U_2]. \tag{2.5}$$

Now every $[L] \in \mathrm{PL}(2,\mathbb{C})$ has a unique polar decomposition

$$[L] = [U(\sqrt{1+\lambda^2}\,\mathbb{I}_2 + \boldsymbol{\lambda}\cdot\boldsymbol{\tau})] \tag{2.6}$$

where $([U],\boldsymbol{\lambda})\in \mathrm{PU}(2)\times\mathbb{R}^3$, $\lambda=|\boldsymbol{\lambda}|$, and τ_1,τ_2,τ_3 are the Pauli spin matrices. Hence $\mathsf{M}_1 \cong \mathrm{PU}(2)\times\mathbb{R}^3\cong \mathrm{SO}(3)\times\mathbb{R}^3$. Physically, the lump corresponding to $([U],\boldsymbol{\lambda})$ has maximum energy density at $-\boldsymbol{\lambda}/\lambda\in S^2$, sharpness proportional to λ and internal orientation $[U]$. The $\lambda=0$ lumps have uniform energy density. The G action in this coordinate system is

$$([U_1],[U_2]):([U],\boldsymbol{\lambda})\mapsto([U_1UU_2],Ad_{U_2}\boldsymbol{\lambda}), \tag{2.7}$$

where again we have used $\mathbb{R}^3\cong\mathfrak{su}(2)$ to identify the fundamental SO(3) action on $\mathbb{R}^3$ with the adjoint SU(2) action on $\mathfrak{su}(2)$. From this we see that the G-orbits are level sets of λ, generically diffeomorphic to $\mathrm{SO}(3)\times S^2$ (when $\lambda>0$), the only exception being $\lambda=0$, which is diffeomorphic to SO(3).

In Ref. 21 it was proved that every G invariant Kähler metric on M_1 may be written

$$\gamma=A_1\,d\boldsymbol{\lambda}\cdot d\boldsymbol{\lambda}+A_2(\boldsymbol{\lambda}\cdot d\boldsymbol{\lambda})^2+A_3\,\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}+A_4(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma})^2+A_1\boldsymbol{\lambda}\cdot(\boldsymbol{\sigma}\times d\boldsymbol{\lambda}), \tag{2.8}$$

where $A_1,\ldots,A_4$ are smooth functions of λ only, all determined from the single function $A_1=A(\lambda)$ by the relations

$$A_2=\frac{A(\lambda)}{1+\lambda^2}+\frac{A'(\lambda)}{\lambda},\quad A_3=\frac{1}{4}(1+2\lambda^2)A(\lambda),\quad A_4=\frac{1}{4\lambda}(1+\lambda^2)A'(\lambda). \tag{2.9}$$

Here $\sigma_1,\sigma_2,\sigma_3$ are the left invariant one-forms on SO(3) dual to the basis $\{i/2\,\tau_a : a=1,2,3\}$ for $\mathfrak{su}(2)\cong\mathfrak{so}(3)$. For the L^2 metric, one finds that

$$A=\frac{4\pi\mu[\mu^4-4\mu^2\log\mu-1]}{(\mu^2-1)^3},\quad \mu=(\sqrt{1+\lambda^2}+\lambda)^2. \tag{2.10}$$

It follows from these formulas that (M_1,γ) has finite volume and diameter, is Ricci positive and has unbounded scalar and holomorphic sectional curvatures. Examining the large λ behavior of γ, one finds that $\partial_\infty\mathsf{M}_1$, the boundary at infinity of M_1, is $S^2\times S^2$. This is natural in two ways: a point in $\partial_\infty\mathsf{M}_1$ should be thought of as a collapsed lump whose width has shrunk to zero. Such a lump is specified by a pair of points p,p' in S^2 because every point except one, p, in the domain gets mapped to the same point p' in the codomain, while p gets mapped to the antipodal point $-p'$. Second, the complex codimension 1 algebraic variety $a_1a_4-a_2a_3=0$ complementary to M_1 in $\mathbb{C}P^3$ is biholomorphic to $\mathbb{C}P^1\times\mathbb{C}P^1$, being the image of the holomorphic embedding

$$([x_1,x_2],[y_1,y_2])\mapsto[x_1y_2,x_1y_1,x_2y_2,x_2y_1]. \tag{2.11}$$

Since $\mathrm{diam}(\mathsf{M}_1,\gamma)<\infty$, $\partial_\infty\mathsf{M}_1$ lies at finite proper distance, so geodesics may reach it in finite time, the origin of the incompleteness already noted. Given that $\partial_\infty\mathsf{M}_1$ has (real) codimension 2, however, one would expect geodesics to miss $\partial_\infty\mathsf{M}_1$ generically. More precisely, one would expect the subset of $T\mathsf{M}_1$ consisting of initial data of geodesics which *do* escape to infinity to have zero measure with respect to the natural measure inherited from γ.

Geodesic flow in (M_1,γ) was studied in detail in Ref. 19. It turns out to be surprisingly complicated given the homogeneity and isotropy of the domain of the sigma model, S^2. Geodesics were found for which the lump spins internally and oscillates between antipodal points. Other geodesics were found where the lump travels along a great circle in S^2, its speed and shape undergoing complicated periodic oscillations. Geodesics do exist for which the lump simply traverses a great circle at constant speed and shape, but the initial data to generate such motion must be chosen very carefully. Nevertheless, all the geodesics found in Ref. 19 confined the lump's position $-\boldsymbol{\lambda}/\lambda$ to some great circle for all time. More precisely, they all confined $\boldsymbol{\lambda}(t)$ to some plane through the origin. The geodesics themselves were obtained by reducing the geodesic problem to low dimensional totally geodesic submanifolds, the fixed point sets of discrete isom-

etries. The question arises, then, whether this "planar property" of the geodesic flow is an artifact of the exceptional symmetries enjoyed by these geodesics, or is a general feature of the dynamics. We shall now prove that the former is the case.

By the G invariance of the metric, it suffices to determine which initial velocities $u \in T_{x(0)}H$ at the point $x(0)=([\mathbb{I}_2],(0,0,\lambda))$ tangent to the hypersurface $H=\{([U],\boldsymbol{\lambda}):\lambda_2=0\}$ generate geodesics which remain in H. We shall call such an initial velocity u a "good" vector. Clearly the set of good initial velocities is conical by time-scaling invariance of geodesic flow. By this we mean that if $u \in T_{x(0)}H$ is good, so is every vector $\xi u \in T_{x(0)}H$, $\xi \in [0,\infty)$, on the ray containing u. The question is then whether the *link* of this cone of good velocity vectors, that is, its intersection with the unit four-sphere in $T_{x(0)}H$, has nonvanishing measure in S^4.

Theorem 1: *Let $u \in T_{x(0)}H$ generate a geodesic through $x(0)$ which remains in H. Then u lies in a codimension 1 cone in $T_{x(0)}H$. For generic $x(0) \in H$, the link of this cone is the suspension of a two-torus. There is at most a nowhere dense subset of H on which the link of the cone is $S^3 \cup S^3$, two three-spheres intersecting in an equatorial two-sphere.*

Proof: Let N be a nonvanishing (but not necessarily unit) normal on H. Then if $x(t)$ remains in H, $\gamma(\dot{x}(t),N(x(t)))=0$ for all t. Differentiating this at $t=0$ and using the fact that $\dot{x}(t)$ is parallel for a geodesic, one finds that $\gamma(\dot{x}(0),\nabla_{\dot{x}(0)}N)=0$, where ∇ is the Levi-Civita connection. Hence, $u=\dot{x}(0)$ must lie in the null space of the symmetric bilinear form

$$B(u,v)=\gamma(u,\nabla_v N), \tag{2.12}$$

that is, $B(u,u)=0$. Clearly this null space is conical. We seek to understand the link of this cone. In this case ($H=\{\lambda_2=0\}$), we may choose

$$N=A_3\frac{\partial}{\partial\lambda_2}+\frac{1}{2}A_1(-\lambda_3\theta_1+\lambda_1\theta_3) \tag{2.13}$$

as our normal field, where θ_a are the left-invariant vector fields on SO(3) dual to σ_a. We may compute $B(u,v)$ by extending u,v to vector fields U,V on M_1, then using the usual formula for ∇ and symmetry of B,[27] to yield

$$B(u,v)=\tfrac{1}{2}N[\gamma(U,V)]|_{x(0)}+\tfrac{1}{2}\gamma([U,N]|_{x(0)},v)+\tfrac{1}{2}\gamma([V,N]|_{x(0)},u). \tag{2.14}$$

A straightforward but lengthy calculation then shows that

$$B=f_1(\lambda)d\lambda_1\sigma_3+f_2(\lambda)d\lambda_3\sigma_1+f_3(\lambda)\sigma_2\sigma_3, \tag{2.15}$$

where

$$f_1=\tfrac{1}{8}(1+\lambda^2)(2A+\lambda A'),\quad f_2=-\tfrac{1}{4}(1+2\lambda^2)A(A+\lambda A'),\quad f_3=\tfrac{1}{16}(1+\lambda^2)AA', \tag{2.16}$$

at the specific point $x(0)=([\mathbb{I}_2],(0,0,\lambda))$. By computing eigenvalues, one sees that, with respect to some orthonormal basis for $T_{x(0)}H$,

$$B(u,u)=f_2(\lambda)(u_2^2-u_3^2)+\sqrt{f_1(\lambda)^2+f_3(\lambda)^2}(u_4^2-u_5^2). \tag{2.17}$$

Note that

$$\frac{8f_1(\lambda)}{1+\lambda^2}=2A+\lambda A'>\frac{2\lambda^1+1}{\lambda^2+1}A+\lambda A'=\gamma\left(\frac{\partial}{\partial\lambda_3},\frac{\partial}{\partial\lambda_3}\right)>0 \tag{2.18}$$

so $f_1(\lambda)$ never vanishes. Consider the set $L=f_2^{-1}(0)\subset[0,\infty)$. If L were dense at λ_0, then by continuity of $A+\lambda A'$, there would be an open interval containing λ_0 such that $A=-\log\lambda+\text{const}$. Given the formula (2.10), A clearly does not coincide with $-\log\lambda+\text{const}$ on any interval, so no such λ_0 exists. Hence the set L is nowhere dense.

Let $\lambda\notin L$. By means of a λ dependent rescaling of the basis, we see that the null space is the locus of the equation

$$\tilde{u}_2^2+\tilde{u}_4^2=\tilde{u}_3^2+\tilde{u}_5^2. \tag{2.19}$$

Clearly $\tilde{u}_1$ may take any value, while $(\tilde{u}_2,\tilde{u}_3,\tilde{u}_4,\tilde{u}_5)$ lies on a cone in $\mathbb{R}^4$ whose link is a two-torus. Alternatively, we may think of the unit sphere in $\mathbb{R}^5$ as the suspension of the unit sphere in $\mathbb{R}^4$ along the $\tilde{u}_1$ direction. Then the intersection of the link of the null space with each three-sphere of constant $\tilde{u}_1\in[-1,1]$ is a scaled two-torus. Assembling the slices together we see that the whole null space has a link which is topologically the suspension of a two-torus.[6] Either way of viewing the null set, it is clearly a codimension 1 cone in $T_{x(0)}H$ as claimed.

It remains to consider the nongeneric case, $\lambda\in L$, for which $f_2(\lambda)=0$. In this case, since $f_1(\lambda)\neq 0$, the cone consists of all vectors for which $u_4=\pm u_5$. The link is the intersection of S^4 with the union of the two orthogonal hyperplanes $(u_4\pm u_5)=0$, which is manifestly a union of two three-spheres intersecting in an equatorial two sphere $(u_4=u_5=0)$. □

We should point out that $u\in\text{null}\,B$ is a necessary but not sufficient condition for the geodesic with initial velocity u to stay in H. It is not certain that the cone of good velocities is all of null B, therefore. Given the explicit formula for A, one would expect to be able to improve the characterization of the nongeneric subset of H (on which null B has link $S^3\cup S^3$) from nowhere dense to discrete or finite. Indeed, one may check graphically that $f_2(\lambda)=0$ has only one solution ($\lambda=0.881$ to three decimal places), so the nongeneric set consists of a single G orbit, $S^1\times\text{SO}(3)$, in H.

Corollary 2: Generically geodesics in (M_1,γ) *do not confine* $\mathbf{\lambda}(t)$ *to a plane through* $\mathbf{0}$. *Consequently, single lumps generically do not stay on great circles while moving on* S^2.

Of course, this corollary refers to the lump dynamics within the geodesic approximation. The question remains: does this give a good model of the full field dynamics?

III. COERCIVITY OF THE HESSIAN

We wish to consider the wave map problem for maps $(\mathbb{R}\times M,dt^2-g)\to(N,h)$, where $(M,g),(N,h)$ are compact Kähler, and the initial data have a certain Sobolev regularity and are close to holomorphic, in a sense to be made precise. The eventual aim is to prove that such wave maps stay close to $\mathsf{Hol}_{[\phi]}(M,N)$ and that their closest trajectory in $\mathsf{Hol}_{[\phi]}(M,N)$ is close to a geodesic. In this section we will prove the main analytic ingredient needed for such a program, along the lines of Stuart's work on vortices.

The first thing to note is that the Cauchy problem for such wave maps with initial data $(\phi_0,\dot{\phi}_0)\in H^k\oplus H^{k-1}$ on the time slice $\{0\}\times M$ is well posed, that is, has a unique solution in the same Sobolev space, with $t\mapsto(\phi(t),\dot{\phi}(t))$ continuous, at least on some open time interval, $t\in(-\epsilon,\epsilon)$, by work of Choquet-Bruhat.[4] Here H^k denotes the space of maps $M\to\mathbb{R}^p$ which are H^k in the usual sense ($\phi,\nabla\phi,\ldots,\nabla^k\phi$ are all L^2) and which take values on $N\subset\mathbb{R}^p$ (isometrically embedded in $\mathbb{R}^p$) almost everywhere. For our purposes, it is convenient to use an alternative intrinsic definition of $H^k(M,N)$, which is only well-defined for $k>\frac{1}{2}\dim M$. With this restriction on k, $H^k(M,N)$ naturally has the structure of a Hilbert manifold. Below we give a brief treatment of both the intrinsic definition and the Hilbert manifold structure of $H^k(M,N)$. For a complete treatment we refer the reader to Ref. 14.

A map $\phi:M\to N$ is said to belong to $H^k(M,N)$ if for any $p\in M$ and any chart (U,Φ) containing p, and any chart (V,Ψ) containing $\phi(p)$, the map $\Psi\circ\phi\circ\Phi^{-1}:\Phi(U)\to\mathbb{R}^n$ belongs to $H^k(\Phi(U),\mathbb{R}^n)$. For this notion to be well-defined we need to ensure that composition by C^∞ diffeomorphisms on the left and on the right takes an H^k map to an H^k map. For composition on the right this is true without any restriction on k. However, for left composition the same result

only holds if we assume $k>\frac{1}{2}\dim M$ (for a discussion of both points see B.1.7 and B.1.9 on p. 182 in Ref. 13). From now on we make a standing assumption that $k>\frac{1}{2}\dim M$, so that the intrinsic definition of $H^k(M,N)$ given above makes sense.

We now exhibit the structure of an infinite dimensional Hilbert manifold on $H^k(M,N)$. Standard facts on embeddings of Sobolev spaces and the density of smooth maps in Sobolev spaces prove the following: There are continuous inclusions $C^\infty(M,N)\hookrightarrow H^k(M,N)\hookrightarrow C^0(M,N)$ and the first inclusion has dense image. From the latter fact it follows that it is sufficient to exhibit charts for $H^k(M,N)$ around only the C^∞ maps.

Given $\phi\in C^\infty(M,N)$ the pullback bundle ϕ^*TN (i.e., the vector bundle over M whose fibre at m is the vector space $T_{\phi(m)}N$) comes equipped with a natural inner product $h\circ(\phi\times\phi)$ and compatible connexion ∇^ϕ, the pullback of the Levi-Civita connection on TN. For any vector bundle E over compact M equipped with an inner product $\langle\ ,\ \rangle$ and compatible connection ∇ there is a natural H^k inner product on smooth sections of E:

$$\langle V,W\rangle_{H^k}=\int_M\langle V,W\rangle+\int_M\langle\nabla V,\nabla W\rangle+\cdots+\int_M\langle\nabla^k V,\nabla^k W\rangle. \tag{3.1}$$

$H^k(E)$ is then defined as the set of finite H^k norm elements of the completion of $C^\infty(E)$ with respect to the norm $\|\cdot\|_{H^k}$. For M compact, this definition of $H^k(E)$ is equivalent to the following alternative definition: given any choice of local coordinates on M and associated bundle trivializations for E, a section belongs to $H^k(E)$ if it is represented by locally H^k functions in these trivializations. The difference is that the connection-dependent definition gives a preferred inner product on $H^k(E)$, i.e., $(H^k(E),\|\cdot\|_{H^k})$ is naturally a Hilbert space.

The point is that $H^k(\phi^*TN)$ is the local model space for the Hilbert manifold $H^k(M,N)$. For each $\phi\in C^\infty(M,N)$, there is a map $\exp_\phi:H^k(\phi^*TN)\to H^k(M,N)$ given by $V(p)\mapsto\exp_{\phi(p)}V(p)$, where $\exp:TN\to N$ is the exponential map on (N,h). It can be shown that $\exp_\phi$ maps a neighborhood of 0 in the Hilbert space $H^k(\phi^*TN)$ bijectively to a neighborhood of ϕ in $H^k(M,N)$. Hence for each $\phi\in C^\infty(M,N)$ there exists some $\epsilon>0$, so that one can define a chart $(U_\phi,\exp_\phi^{-1})$ based at ϕ where

$$U_\phi=\{\exp_\phi(V):V\in H^k(\phi^*TN),\|V\|_{H^k}<\epsilon\}.$$

The local homeomorphism $U_\phi\to B_\epsilon(0)\subset H^k(\phi^*TN)$ is simply given by $\exp_\phi^{-1}$. So we identify H^k maps close to ϕ with H^k sections of ϕ^*TN by deforming ϕ: the deformed map $\exp_\phi(V)$ maps each $p\in M$ to the point in N reached by traveling for unit time along the geodesic with initial data $(\phi(p),V(p))$.

It can be shown that for any two maps $\phi_1,\phi_2\in C^\infty(M,N)$ the change of charts map $\exp_{\phi_2}^{-1}\circ\exp_{\phi_1}:\exp_{\phi_1}^{-1}(U_{\phi_1}\cap U_{\phi_2})\to\exp_{\phi_2}^{-1}(U_{\phi_1}\cap U_{\phi_2})$ is a diffeomorphism between open sets in the Hilbert spaces $H^k(\phi_1^*TN)$ and $H^k(\phi_2^*TN)$. It follows that the collection of charts $\{(U_\phi,\exp_\phi^{-1})|\ \phi\in C^\infty(M,N)\}$ defines a differentiable structure on $H^k(M,N)$ with local model a Hilbert space, i.e., $H^k(M,N)$ is a Hilbert manifold. In fact, the differentiable structure can be shown to be independent of the metric h on N used to define $\exp_\phi$.

Given

(i) a holomorphic map $\tilde{\phi}_0\in\mathsf{Hol}(M,N)$, and
(ii) sections $V_0,X_0,Y_0\in H^k(\tilde{\phi}_0^*TN)$, such that
(iii) V_0,Y_0 are L^2 orthogonal to $T_{\tilde{\phi}_0}\mathsf{Hol}(M,N)$, and
(iv) $X_0\in T_{\tilde{\phi}_0}\mathsf{Hol}(M,N)$,

and $\epsilon>0$ small, the initial value problem with initial data

$$\phi_0=\exp_{\tilde{\phi}_0}\epsilon^2V_0,\quad \dot{\phi}_0=\epsilon X_0+\epsilon^3Y_0 \tag{3.2}$$

has a unique solution in H^k. The idea is to decompose this solution into $\tilde{\phi}(t) \in \mathsf{Hol}(M,N)$ and $V(t) \in H^k(\tilde{\phi}(t)^*TN) \cap T_{\tilde{\phi}(t)}\mathsf{Hol}(M,N)^{\perp_{L^2}}$ by

$$\phi(t) = \exp^{\sim}_{\tilde{\phi}(t)} \epsilon^2 V(t), \tag{3.3}$$

and then show that $\|V\|_{H^k}$ remains bounded for times of order ϵ^{-1}. The starting point is to show that $\|V\|_{H^1}$ is controlled by $\mathsf{Hess}^{\sim}_{\tilde{\phi}}(V,V)$. From now on, all quantities will be considered at a fixed time, and we will denote the holomorphic base map of our local chart in H^k by ϕ rather than $\tilde{\phi}$, to simplify notation.

$\mathsf{Hess}_\phi(X,Y)$ is the second variation of the harmonic map energy E at the holomorphic (hence harmonic) map ϕ. Precisely, given a two-parameter variation $\phi_{s,t}$ of the map ϕ through smooth maps, with $d\phi_{0,0}\partial/\partial s = X, d\phi_{0,0}\partial/\partial t = Y \in \Gamma(\phi^*TN)$,

$$\mathsf{Hess}_\phi(X,Y) = \left.\frac{\partial^2 E[\phi_{s,t}]}{\partial s \partial t}\right|_{s=t=0}. \tag{3.4}$$

There are two useful explicit formulas for Hess.[25] The first uses only compactness of M, not the Kähler property. To write it down we must introduce two new objects. Let $E_i, i = 1,\ldots,m$, be a local frame of smooth orthonormal vector fields on M. Then the rough Laplacian on sections of ϕ^*TN is the second order linear elliptic differential operator

$$\Delta^\phi V = -\operatorname{tr}(\nabla^\phi \nabla^\phi V) = -\sum_{i=1}^m (\nabla^\phi \nabla^\phi V)(E_i, E_i). \tag{3.5}$$

Like the usual Laplacian (on functions or forms) Δ^ϕ is a positive self-adjoint operator. Positivity follows from the identity

$$\int_M h(V, \Delta^\phi V) = \frac{1}{2}\int_M \sum_i h(\nabla^\phi_{E_i} V, \nabla^\phi_{E_i} V). \tag{3.6}$$

We may define a (fiberwise linear) bundle map $\mathfrak{R}^\phi$ on ϕ^*TN by

$$\mathfrak{R}^\phi V = \sum_{i=1}^m R^N(V, d\phi E_i) d\phi E_i, \tag{3.7}$$

where R^N is the curvature tensor on N. Given these, the Hessian is

$$\mathsf{Hess}_\phi(X,Y) = \int_M h(X, \mathfrak{J}^\phi Y) = \langle X, \mathfrak{J}^\phi Y\rangle_{L^2}, \quad \mathfrak{J}^\phi = \Delta^\phi - \mathfrak{R}^\phi. \tag{3.8}$$

The operator $\mathfrak{J}^\phi$, called the Jacobi operator, is itself second order, linear, elliptic and self-adjoint. It follows immediately from this formula that every harmonic map into a manifold of nonpositive sectional curvature is weakly stable [meaning $\mathsf{Hess}_\phi(V,V) \geqslant 0$].

In the case of interest to us, namely M,N compact Kähler, and ϕ holomorphic, one can obtain a more useful and rather simpler formula for Hess. First one defines the Urakawa connection on ϕ^*TN,

$$(\mathfrak{D}^\phi V)(X) := \nabla^\phi_{J^M X} V - J^N \nabla^\phi_X V, \tag{3.9}$$

J^M, J^N being the almost complex structures on M and N.[25] Then

$$\mathsf{Hess}_\phi(V,V) = \tfrac{1}{2}\|\mathfrak{D}^\phi V\|^2_{L^2}. \tag{3.10}$$

Weak stability of holomorphic maps follows immediately from (3.10).

$\mathfrak{D}^\phi V=0$ should be thought of as the linearized Bogomol'nyi equation, so every $V\in\ker\mathfrak{D}^\phi=\ker\mathfrak{J}^\phi$ is a zero mode of the holomorphic map ϕ. For the geodesic approximation to make sense, the space of holomorphic maps close to ϕ must be a smooth manifold whose tangent space at ϕ equals $\ker\mathfrak{J}^\phi$. Sections of ϕ^*TN in the kernel of $\mathfrak{J}^\phi$ are called Jacobi fields along ϕ. A Jacobi field is said to be integrable if it may be generated by a variation of ϕ through harmonic maps, and the map itself is said to be Jacobi integrable if all its Jacobi fields have this property. A fundamental theorem of Adams and Simon[1] states that a harmonic map ϕ between real analytic manifolds is Jacobi integrable if and only if the space of harmonic maps $C^{2,\alpha}$ close to ϕ is a smooth manifold with tangent space $\ker\mathfrak{J}^\phi$ at ϕ. Similar results hold in suitable Sobolev spaces of maps also. In the case where M,N are Kähler (hence real analytic), Lichnerowicz showed that all harmonic deformations of a holomorphic map ϕ are holomorphic,[9] so the space of interest to us, the space of *holomorphic* maps close to ϕ, is a smooth manifold with tangent space $\ker\mathfrak{J}^\phi$ at ϕ, if and only if ϕ is Jacobi integrable. Jacobi integrability of harmonic maps is an active field of research whose current state is summarized in Ref. 8. Particularly relevant to the present article is a theorem of Wood and Lemaire which states that every holomorphic map $S^2\to\mathbb{C}P^N$ is Jacobi integrable. So the moduli space of holomorphic maps for the $\mathbb{C}P^N$ model on S^2 is smooth with tangent space $\ker\mathfrak{J}^\phi$, as we require. A similar result holds for degree n holomorphic maps $\Sigma\to\mathbb{C}P^1$, Σ being a compact Riemann surface of genus g, provided $n>2g-2$, by a standard application of the Riemann–Roch theorem. So the n-lump moduli space of the $\mathbb{C}P^1$ model on Σ also has the required property, with some low degree exceptions.

We may now state and prove our main result.

Theorem 3 [Coercivity of the Hessian]: *Let $\phi:M\to N$ be a holomorphic map between compact Kähler manifolds and Hess_ϕ be the Hessian of the harmonic map energy functional at ϕ. Then there exists a constant $\tau(\phi)>0$ such that for all $V\in H^1(\phi^*TN)$ with $\langle V,\ker\mathfrak{D}^\phi\rangle_{L^2}=0$,*

$$\mathsf{Hess}_\phi(V,V)\geqslant\tau(\phi)\|V\|^2_{H^1}.$$

Proof: Both H^1 and L^2 are Hilbert spaces. We will use $\to$ and $\rightharpoonup$ to denote strong and weak convergence, respectively, the space concerned being explicitly specified. Define the subset $S=\{V\in H^1:\|V\|^2_{H^1}=1,V\perp_{L^2}\ker\mathfrak{D}^\phi\}$ and the quantity

$$\tau(\phi)=\inf_{V\in S}\mathsf{Hess}_\phi(V,V)=\inf_{V\in S}\tfrac{1}{2}\|\mathfrak{D}^\phi V\|^2_{L^2}\geqslant 0. \tag{3.11}$$

We claim that $\tau(\phi)\neq 0$. Assume this is false. Then there exists a sequence $V_i\in S$ such that $\mathfrak{D}^\phi V_i\overset{L^2}{\to}0$. We will repeatedly extract (nested) subsequences from V_i, which we will always denote by the same symbol, V_i. Now V_i is bounded in H^1 so, by the Alaoglu theorem, there exists a subsequence $V_i\overset{H^1}{\rightharpoonup}V$, to some weak limit V. Since $\mathfrak{D}^\phi:H^1\to L^2$ is a bounded linear map, it is continuous with respect to the weak (and strong) topologies on H^1,L^2. It follows that $\mathfrak{D}^\phi V_i\overset{L^2}{\rightharpoonup}\mathfrak{D}^\phi V$. But $\mathfrak{D}^\phi V_i\overset{L^2}{\to}0\Rightarrow\mathfrak{D}^\phi V_i\overset{L^2}{\rightharpoonup}0\Rightarrow\mathfrak{D}^\phi V=0$ by uniqueness of weak limits. Hence $V_i\overset{H^1}{\rightharpoonup}V\in\ker\mathfrak{D}^\phi$.

Now the inclusion $\iota:H^1\hookrightarrow L^2$ is compact by Rellich's lemma, so the bounded set $\{V_i\}\subset H^1$ is compact in L^2. Hence, any sequence in $\{V_i\}$, for example V_i itself, has a subsequence which is strongly convergent in L^2. Once again, denoting this subsequence by V_i, we have $V_i\overset{L^2}{\to}\tilde{V}$. But then $V_i\overset{L^2}{\rightharpoonup}\tilde{V}$ so

$$0=\langle V_i,\ker\mathfrak{D}^\phi\rangle_{L^2}\to\langle\tilde{V},\ker\mathfrak{D}^\phi\rangle_{L^2}. \tag{3.12}$$

Hence $V_i \overset{L^2}{\to} \tilde{V} \in (\ker \mathfrak{D}^\phi)^{\perp_{L^2}}$.

But $\iota: H^1 \hookrightarrow L^2$ is continuous, so $V_i \overset{H^1}{\rightharpoonup} V \Rightarrow \iota V_i \overset{L^2}{\rightharpoonup} \iota V$, and so $\tilde{V} = V$ by uniqueness of weak limits. So $V \in \ker \mathfrak{D}^\phi$ and $V \in (\ker \mathfrak{D}^\phi)^{\perp_{L^2}}$, and hence $V = 0$, so $V_i \overset{L^2}{\to} 0$. Then, by (3.6) and (3.8),

$$
\begin{aligned}
1 &= \|V_i\|_{H^1}^2 = \|V_i\|_{L^2}^2 + \sum_\alpha \|\nabla^\phi_{E_\alpha} V_i\|_{L^2}^2 \\
&= 2\,\mathrm{Hess}_\phi(V_i, V_i) + \|V_i\|_{L^2}^2 + \sum_\alpha 2\langle R^N(d\phi E_\alpha, V_i) d\phi E_\alpha, V_i\rangle_{L^2} \\
&\leqslant 2\,\mathrm{Hess}_\phi(V_i, V_i) + \|V_i\|_{L^2}^2 + C_\phi \|V_i\|_{L^2}^2, \qquad (3.13)
\end{aligned}
$$

where $C_\phi > 0$ is a constant, by compactness of N and the tensorial property of $\mathfrak{R}^N$. Taking limits of both sides of (3.13) and using $\tau(\phi) = 0$ and $V_i \overset{L^2}{\to} 0$, one sees that $1 \leqslant 0$, a contradiction. □

We remark that the L^2 version of this result, that there exists a constant $\tau(\phi) > 0$ such that $\mathrm{Hess}_\phi(V,V) \geqslant \tau(\phi)\|V\|_{L^2}^2$ for all $V \perp_{L^2} \ker \mathfrak{J}^\phi$, is much easier to prove. Since $\mathfrak{J}^\phi$ is elliptic, self-adjoint and positive definite (for weakly stable ϕ), and M is compact, we know immediately that the spectrum of $\mathfrak{J}^\phi$ is discrete and, normal to its kernel, bounded away from 0. The result immediately follows. In fact the optimal constant $\tau_{L^2}(\phi)$ in this case is just the lowest nonvanishing eigenvalue of $\mathfrak{J}^\phi$. Hence the optimal bound is attained in this case, by any eigensection with this eigenvalue. We remark also that the spectrum of $\mathfrak{J}^\phi$ is of independent physical interest since it gives the semiclassical meson spectrum of the sigma model in the topological sector $[\phi]$.

IV. CONTINUITY OF $\tau(\phi)$

Let $\phi_n : M \to N$ be a sequence of smooth holomorphic maps between compact Kähler manifolds, converging in C^1 to a smooth holomorphic map $\phi: M \to N$. From Theorem 3 we have for each n a positive constant $\tau(\phi_n)$ and the positive constant $\tau(\phi)$, which give lower bounds for the ratio $\mathrm{Hess}(V,V)/\langle V, V\rangle_{H_1}$ for any H^1 section of the pullback bundle L^2 orthogonal to all Jacobi fields. In this section we will establish conditions sufficient to guarantee that $\lim_{n\to\infty} \tau(\phi_n) = \tau(\phi)$. In subsequent sections we will show that these conditions are met in the cases of interest to us.

In order to compare various quantities (especially the Hessian and H^1 norm) at different maps, it is convenient to make various identifications so that we can treat all geometric quantities and operators as being defined on the fixed bundle $E = \phi^* TN$. Since $\phi_n \to \phi$, for sufficiently large n each pullback bundle $E_n = \phi_n^* TN$ is topologically equivalent to E. However, since each bundle E_n comes naturally equipped with both an inner product and a compatible connection (both of which occur in the Hessian and the H^1-norm of a section) we would also like to transfer these geometric structures to the bundle E.

Again since $\phi_n \to \phi$, for each $x \in M$ (and for each sufficiently large n) there is a unique minimizing geodesic joining $\phi_n(x)$ to $\phi(x)$. By parallel transporting vectors along this unique geodesic we construct a canonical isometry between the fibers of E and the fibers of E_n at each point $x \in M$, and hence a natural L^2 isometry between E and E_n. Using this isometry we can interpret the natural connection on each E_n as a connection on E, which we shall write ∇_n. Using the connection ∇_n and the (fixed) L^2 metric on E we can now interpret each of the Jacobi operators $\mathfrak{J}^{\phi_n}$ (and hence also the associated symmetric bilinear form Hess_{ϕ_n}) as an operator on sections of the fixed bundle E. Similarly, for each n we get an $H^1_{\phi_n}$ norm on sections of E, by using the connection ∇_n and the fixed L^2 metric. Since the difference of any two connections on E is tensorial, it is clear that for each n (sufficiently large) the $H^1_{\phi_n}$ norm is equivalent to the H^1_ϕ norm on sections of E.

Suppose now that the difference between the connections ∇_n and ∇ tends to zero in the following pointwise sense,

$$|\nabla V - \nabla_n V| \leq a_n |V|, \tag{4.1}$$

where each a_n is a positive number, $a_n \to 0$ as $n \to \infty$, and $|.|$ refers to the natural pointwise norms on the bundles $E \otimes T^*M$ and E, and V is a smooth section of E.

Lemma 4: Suppose that (4.1) holds. Then the following inequalities also hold:

(i) $\quad | \, \|\nabla V\|^2 - \|\nabla_n V\|^2 \, | \leq b_n \|V\|_1^2,$
(ii) $\quad | \, \|V\|_1^2 - \|V\|_{H^1_{\phi_n}}^2 \, | \leq b_n \|V\|_1^2,$
(iii) $\quad | \, \mathrm{Hess}_\phi(V,V) - \mathrm{Hess}_{\phi_n}(V,V) \, | \leq c_n \|V\|_1^2,$

where b_n, c_n are positive numbers which tend to zero as $n \to \infty$, and $\|\cdot\|$ is the L^2 norm on $\Gamma(E)$, $\|\cdot\|_1$ is the H^1 norm on $\Gamma(E)$ defined using the connection ∇ and $\|\cdot\|_{H^1_{\phi_n}}$ is the H^1 norm on $\Gamma(E)$ defined using the connection ∇_n.

Proof: (i) Elementary manipulations involving the triangle inequality, inequality (4.1) and the Cauchy–Schwarz inequality yield the following chain of inequalities:

$$\begin{aligned}
\left| \int_M (|\nabla V|^2 - |\nabla_n V|^2) \right| &\leq \int_M \|\nabla V|^2 - |\nabla_n V|^2| \\
&\leq \int_M | \; |\nabla V| - |\nabla_n V| \; | \cdot | \; |\nabla V| + |\nabla_n V| \; | \\
&\leq \int_M | \; |\nabla V| - |\nabla_n V| \; | \cdot (| \; 2|\nabla V| + |\nabla V - \nabla_n V| \; |) \\
&\leq 2a_n \int_M |V| \; |\nabla V| \; + a_n^2 \int_M |V|^2 \\
&\leq 2a_n \| \; |V| \; \| \cdot \| \; |\nabla V| \; \| + a_n^2 \|V\|^2 \\
&\leq (2a_n + a_n^2) \; \|V\|_1^2.
\end{aligned}$$

Hence the result follows with $b_n = a_n(2 + a_n)$.

(ii) This is immediate from the definition of the H^1 norm and part (i).

(iii) The definition of $\mathfrak{R}^\phi$ [see Eq. (3.7)], together with the compactness of M and the fact that $\phi_n \to \phi$ in C^1 implies that

$$\lim_{n \to \infty} \|\mathfrak{R}^\phi - \mathfrak{R}^{\phi_n}\| = 0. \tag{4.2}$$

Using part (i) and the definition of Hess we have

$$\begin{aligned}
|\mathrm{Hess}_\phi(V,V) - \mathrm{Hess}_{\phi_n}(V,V)| &= |\tfrac{1}{2}\|\nabla V\|^2 - \tfrac{1}{2}\|\nabla_n V\|^2 - \langle \mathfrak{R}^\phi V, V\rangle + \langle \mathfrak{R}^{\phi_n} V, V\rangle| \\
&\leq \tfrac{1}{2} |\|\nabla V\|^2 - \|\nabla_n V\|^2| + |\langle \mathfrak{R}^\phi V, V\rangle - \langle \mathfrak{R}^{\phi_n} V, V\rangle| \\
&\leq b_n \|V\|_1^2 + \|(\mathfrak{R}^\phi - \mathfrak{R}^{\phi_n})V\| \; \|V\| \\
&\leq b_n \|V\|_1^2 + \|\mathfrak{R}^\phi - \mathfrak{R}^{\phi_n}\| \; \|V\|^2.
\end{aligned}$$

The result now follows from (4.2). □

We will also need the following simple proposition on the continuity of L^2 orthogonal projection operators.

Proposition 5: Let $H^k(E)$ denote the H^k sections of E. Let V_n be a sequence of finite dimensional vector subspaces of $H^k(E)$ of constant dimension p which converge to another p-dimensional subspace V of $H^k(E)$ in the following sense: there exists an L^2-orthonormal basis $e_1^n,\ldots,e_p^n$ of V_n and an L^2-orthonormal basis $e_1,\ldots,e_p$ of V so that for each $i=1,\ldots p$, $e_i^n\to e_i$ in H^k as $n\to\infty$. Denote by P_n and P the L^2 orthogonal projections onto $V_n^\perp$ and $V^\perp$, respectively. Then $P_n\to P$ in the operator norm on $B(H^k(E),H^k(E))$, the bounded linear maps between $H^k(E)$ and itself.

Proof: In this proof, norms and inner products without subscripts will refer to L^2 norms and inner products, while H^k norms and inner products will be referred to with the subscript k. Since $P_n v=v-\Sigma_i\langle v,e_i^n\rangle e_i^n$ and $Pv=v-\Sigma_i\langle v,e_i\rangle e_i$ we have

$$\begin{aligned}\|P_n v-Pv\|_k&=\left\|\sum_i\ \langle v,e_i^n\rangle e_i^n-\sum_i\ \langle v,e_i\rangle e_i\right\|_k\\&\leqslant\sum_i\ \|\langle v,e_i^n\rangle e_i^n-\langle v,e_i\rangle e_i\|_k\\&\leqslant\sum_i\ \|\langle v,e_i^n\rangle e_i^n-\langle v,e_i^n\rangle e_i+\langle v,e_i^n\rangle e_i-\langle v,e_i\rangle e_i\|_k\\&\leqslant\sum_i\ |\langle v,e_i^n\rangle|\ \ \|e_i^n-e_i\|_k+\|e_i\|_k|\langle v,e_i^n-e_i\rangle|\\&\leqslant\|v\|\ \left(\sum_i\ \|e_i^n\|\ \ \|e_i^n-e_i\|_k+\|e_i\|_k\|e_i^n-e_i\|\right)\leqslant\|v\|\left(\sum_i\ (1+\|e_i\|_k)\ \ \|e_i^n-e_i\|_k\right).\end{aligned}\tag{4.3}$$

So for all $v\neq 0\in H^k$ we have

$$\frac{\|(P_n-P)v\|_k}{\|v\|_k}\leqslant\frac{\|(P_n-P)v\|_k}{\|v\|}\leqslant\left(\sum_i\ (1+\|e_i\|_k)\ \ \|e_i^n-e_i\|_k\right).\tag{4.4}$$

Since by assumption $e_i^n\to e_i$ strongly in H^k for each i, (4.4) implies that

$$\limsup_{n\to\infty v\neq 0}\frac{\|(P_n-P)v\|_k}{\|v\|_k}=0\tag{4.5}$$

as required. □

We now state the main result of this section, a theorem giving sufficient conditions for $\tau(\phi)$ to depend continuously on the holomorphic map ϕ. The analogous result in Stuart's analysis of slowly moving Abelian Higgs vortices is Lemma 3.2 of Ref. 23 Our proof of Theorem 6 is inspired by Stuart's argument.

Theorem 6: *Let $\phi_n:M\to N$ be a sequence of smooth holomorphic maps between compact Kähler manifolds converging in C^1 to the smooth holomorphic map $\phi:M\to N$. Suppose all the Jacobi fields of ϕ are integrable and that the conclusions of Lemma 4 hold. Then*

$$\lim_{n\to\infty}\tau(\phi_n)=\tau(\phi).$$

Proof: Let $P_n,P:H^1(E)\to H^1(E)$ denote L^2 orthogonal projection onto $\ker\mathfrak{D}^{\phi_n\perp}$ and $\ker\mathfrak{D}^{\phi\perp}$, respectively. Since ϕ is Jacobi integrable, the space of sufficiently C^1-close holomorphic maps is a C^∞ manifold of dimension equal to dim $\ker\mathfrak{D}^\phi$. This also holds for all ϕ_n for all n

sufficiently large. In particular, the subspaces $\ker\mathfrak{D}^{\phi_n}$ satisfy the hypotheses of the previous proposition for any k, and in particular for $k=1$. Hence by the previous proposition we have

$$\|P-P_n\|_1=d_n,$$

for some positive numbers d_n tending to 0 as $n\to\infty$.

We will prove (i) $\tau(\phi)\geqslant\limsup_{n\to\infty}\tau(\phi_n)$ and (ii) $\tau(\phi)\leqslant\liminf_{n\to\infty}\tau(\phi_n)$. From (i) and (ii) it follows that $\lim_{n\to\infty}\tau(\phi_n)$ exists and equals $\tau(\phi)$.

Proof of (i): Consider for any $V\in H^1(E)\cap(\ker\mathfrak{D}^{\phi})^{\perp}$, the section $V_n:=P_nV\in H^1(E)\cap(\ker\mathfrak{D}^{\phi_n})^{\perp}$. Since $\|V-V_n\|_{H^1_\phi}=\|(P-P_n)V\|_{H^1_\phi}\leqslant d_n\|V\|_{H^1_\phi}$ we get

$$|\langle V_n,V_n\rangle_{H^1_\phi}-\langle V,V\rangle_{H^1_\phi}|\leqslant\|V-V_n\|_{H^1_\phi}(\|V\|_{H^1_\phi}+\|V_n\|_{H^1_\phi})\leqslant d_n(d_n+2)\langle V,V\rangle_{H^1_\phi}. \tag{4.6}$$

Using the previous inequality and inequality (ii) of Lemma 4 we have

$$\begin{aligned}|\langle V,V\rangle_{H^1_\phi}-\langle V_n,V_n\rangle_{H^1_{\phi_n}}|&\leqslant|\langle V_n,V_n\rangle_{H^1_{\phi_n}}-\langle V_n,V_n\rangle_{H^1_\phi}|+|\langle V_n,V_n\rangle_{H^1_\phi}-\langle V,V\rangle_{H^1_\phi}|\\&\leqslant b_n\langle V_n,V_n\rangle_{H^1_\phi}+d_n(d_n+2)\langle V,V\rangle_{H^1_\phi}\\&\leqslant f_n\langle V,V\rangle_{H^1_\phi},\end{aligned} \tag{4.7}$$

where $f_n:=(b_n+d_n(d_n+2)(1+b_n))$ is another sequence of positive numbers tending to zero as $n\to\infty$.

Since $V=V_n+K_n$ for some $K_n\in\ker\mathfrak{D}^{\phi_n}$, we have $\mathrm{Hess}_{\phi_n}(V_n,V_n)=\mathrm{Hess}_{\phi_n}(V,V)$. Hence

$$\begin{aligned}&\left|\frac{\mathrm{Hess}_\phi(V,V)}{\langle V,V\rangle_{H^1_\phi}}-\frac{\mathrm{Hess}_{\phi_n}(V_n,V_n)}{\langle V_n,V_n\rangle_{H^1_{\phi_n}}}\right|\\&\quad=\left|\frac{\mathrm{Hess}_\phi(V,V)}{\langle V,V\rangle_{H^1_\phi}}-\frac{\mathrm{Hess}_{\phi_n}(V,V)}{\langle V_n,V_n\rangle_{H^1_{\phi_n}}}\right|\\&\quad\leqslant\frac{\mathrm{Hess}_\phi(V,V)|\langle V,V\rangle_{H^1_\phi}-\langle V_n,V_n\rangle_{H^1_{\phi_n}}|+\langle V,V\rangle_{H^1_\phi}|\mathrm{Hess}_\phi(V,V)-\mathrm{Hess}_{\phi_n}(V,V)|}{\langle V,V\rangle_{H^1_\phi}\langle V_n,V_n\rangle_{H^1_{\phi_n}}}\\&\quad\leqslant\frac{f_n\mathrm{Hess}_\phi(V,V)+c_n\langle V,V\rangle_{H^1_\phi}}{\langle V,V\rangle_{H^1_{\phi_n}}}\leqslant\frac{f_n}{1-f_n}\frac{\mathrm{Hess}_\phi(V,V)}{\langle V,V\rangle_{H^1_\phi}}+\frac{c_n}{1-f_n}.\end{aligned} \tag{4.8}$$

Let $\{V^j\}_{j=1}^{\infty}\in H^1(E)\cap(\ker\mathfrak{D}^{\phi})^{\perp}$ be a minimizing sequence for $\tau(\phi)$ with unit H^1_ϕ norm, that is

$$\lim_{j\to\infty}\frac{\mathrm{Hess}_\phi(V^j,V^j)}{\langle V^j,V^j\rangle_{H^1_\phi}}=\lim_{j\to\infty}\mathrm{Hess}_\phi(V^j,V^j)=\tau(\phi).$$

Hence there exists a positive constant C and numbers ϵ_j tending to zero as $j\to\infty$, such that

$$\mathrm{Hess}_\phi(V^j,V^j)=\tau(\phi)+\epsilon_j$$

and

$$\mathrm{Hess}_{\phi_n}(V^j,V^j)\leqslant C$$

for all j and n. Define $V_n^j = P_n V^j \in H^1(E) \cap (\ker \mathfrak{D}^{\phi_n})^{\perp}$. The two previous facts together with (4.8) imply that

$$\left| \tau(\phi) + \epsilon_j - \frac{\mathrm{Hess}_{\phi_n}(V_n^j, V_n^j)}{\langle V_n^j, V_n^j \rangle_{H^1_{\phi_n}}} \right| \leqslant \frac{C f_n + c_n}{1 - f_n}$$

holds for all j and n. For any fixed n, taking the limit as $j \to \infty$ we see that

$$\tau(\phi_n) \leqslant \tau(\phi) + \frac{C f_n + c_n}{1 - f_n}.$$

Hence for any limit point l of the sequence $\{\tau(\phi_n)\}_{n=1}^{\infty}$ we have $l \leqslant \tau(\phi)$. In particular we have

$$\limsup_{n \to \infty} \tau(\phi_n) \leqslant \tau(\phi)$$

as required.

Proof of (ii): Since the proof of (ii) is very similar in character to the proof of (i) we shall omit some details. Consider the projection PV_n of an element $V_n \in H^1(E) \cap (\ker \mathfrak{D}^{\phi_n})^{\perp}$ into $H^1(E) \cap (\ker \mathfrak{D}^{\phi})^{\perp}$. Several applications of the triangle inequality, together with the inequalities in Lemma 4 and the fact that $P_n \to P$ in H^1, show that there exist two sequences of positive numbers $\{g_n\}$ and $\{h_n\}$ with $\lim_{n \to \infty} g_n = \lim_{n \to \infty} h_n = 0$ so that

$$\left| \langle V_n, V_n \rangle_{H^1_{\phi_n}} - \langle PV_n, PV_n \rangle_{H^1_{\phi}} \right| \leqslant g_n \langle PV_n, PV_n \rangle_{H^1_{\phi}} \tag{4.9}$$

and

$$\left| \langle V_n, V_n \rangle_{H^1_{\phi}} - \langle PV_n, PV_n \rangle_{H^1_{\phi}} \right| \leqslant h_n \langle V_n, V_n \rangle_{H^1_{\phi}} \tag{4.10}$$

hold for any $V_n \in H^1(E) \cap (\ker \mathfrak{D}^{\phi_n})^{\perp}$. These two inequalities, combined with the inequalities of Lemma 4 and the fact that $\mathrm{Hess}_{\phi}(PV_n, PV_n) = \mathrm{Hess}_{\phi}(V_n, V_n)$, prove that

$$\begin{aligned}
&\left| \frac{\mathrm{Hess}_{\phi}(PV_n, PV_n)}{\langle PV_n, PV_n \rangle_{H^1_{\phi}}} - \frac{\mathrm{Hess}_{\phi_n}(V_n, V_n)}{\langle V_n, V_n \rangle_{H^1_{\phi_n}}} \right| \\
&\quad = \left| \frac{\mathrm{Hess}_{\phi}(V_n, V_n)}{\langle PV_n, PV_n \rangle_{H^1_{\phi}}} - \frac{\mathrm{Hess}_{\phi_n}(V_n, V_n)}{\langle V_n, V_n \rangle_{H^1_{\phi_n}}} \right| \\
&\quad \leqslant \frac{\mathrm{Hess}_{\phi_n}(V_n, V_n) \left| \langle V_n, V_n \rangle_{H^1_{\phi_n}} - \langle PV_n, PV_n \rangle_{H^1_{\phi}} \right| + \langle V_n, V_n \rangle_{H^1_{\phi_n}} \left| \mathrm{Hess}_{\phi}(V_n, V_n) - \mathrm{Hess}_{\phi_n}(V_n, V_n) \right|}{\langle V_n, V_n \rangle_{H^1_{\phi_n}} \langle PV_n, PV_n \rangle_{H^1_{\phi}}} \\
&\quad \leqslant \frac{g_n \mathrm{Hess}_{\phi_n}(V_n, V_n) \ \langle PV_n, PV_n \rangle_{H^1_{\phi}} + c_n \langle V_n, V_n \rangle_{H^1_{\phi_n}} \langle V_n, V_n \rangle_{H^1_{\phi}}}{\langle V_n, V_n \rangle_{H^1_{\phi_n}} \langle PV_n, PV_n \rangle_{H^1_{\phi}}} \\
&\quad \leqslant g_n \frac{\mathrm{Hess}_{\phi_n}(V_n, V_n)}{\langle V_n, V_n \rangle_{H^1_{\phi_n}}} + c_n \frac{\langle V_n, V_n \rangle_{H^1_{\phi}}}{\langle PV_n, PV_n \rangle_{H^1_{\phi}}} \leqslant g_n \frac{\mathrm{Hess}_{\phi_n}(V_n, V_n)}{\langle V_n, V_n \rangle_{H^1_{\phi_n}}} + \frac{c_n}{1 - h_n}
\end{aligned} \tag{4.11}$$

holds for any $V_n \in H^1(E) \cap (\ker \mathfrak{D}^{\phi_n})^{\perp}$.

Let $\{V_n^j\}_{j=1}^{\infty} \in H^1(E) \cap (\ker \mathfrak{D}^{\phi_n})^{\perp}$ be a minimizing sequence for $\tau(\phi_n)$ with unit $H^1_{\phi_n}$ norm, that is

$$\lim_{j\to\infty}\frac{\mathsf{Hess}_{\phi_n}(V_n^j,V_n^j)}{\langle V_n^j,V_n^j\rangle_{H^1_{\phi_n}}}=\lim_{j\to\infty}\ \mathsf{Hess}_{\phi_n}(V_n^j,V_n^j)=\tau(\phi_n).$$

Hence there exists a positive constant C and numbers ϵ_n^j tending to zero as $j\to\infty$, such that

$$\mathsf{Hess}_{\phi}(V_n^j,V_n^j)=\tau(\phi_n)+\epsilon_n^j$$

and

$$\mathsf{Hess}_{\phi}(V_n^j,V_n^j)\leqslant C$$

for all j and n. Consider the sequence $\tilde{V}_n^j=PV_n^j\in H^1(E)\cap(\ker\mathfrak{D}^{\phi})^{\perp}$. The two previous facts together with (4.11) imply that

$$\left|\frac{\mathsf{Hess}_{\phi}(\tilde{V}_n^j,\tilde{V}_n^j)}{\langle\tilde{V}_n^j,\tilde{V}_n^j\rangle_{H^1_{\phi}}}-(\tau(\phi)+\epsilon_n^j)\right|\leqslant Cg_n+\frac{c_n}{1-h_n}$$

holds for all j and n. For any fixed n, taking the limit as $j\to\infty$ we see that

$$\tau(\phi)\leqslant\tau(\phi_n)+Cg_n+\frac{c_n}{1-h_n}.$$

Hence for any limit point l of the sequence $\{\tau(\phi_n)\}_{n=1}^{\infty}$ we have $\tau(\phi)\leqslant l$. In particular,

$$\tau(\phi)\leqslant\liminf_{n\to\infty}\tau(\phi_n)$$

as claimed. □

V. THE CASE OF Rat_1

It is interesting to consider the simplest nontrivial case, namely $\mathsf{M}_1=\mathsf{Hol}_1(S^2,S^2)=\mathsf{Rat}_1$, in detail. Although $M=N=S^2$ in this case, it is often helpful to distinguish between domain and codomain by continuing to denote them M,N, respectively. We shall do this when clarity requires. The G action on M_n introduced in Sec. II extends naturally to $C^{\infty}(S^2,S^2)$, and leaves $E[\phi]$ invariant. It follows that $\tau(\phi)$ is constant on G orbits in M_n. Since G acts with cohomogeneity 1 on M_1, it suffices to consider $\tau(\phi)$ for the one-parameter family of maps

$$\phi_{\mu}:z\mapsto\mu z,\quad \mu\in[1,\infty),\tag{5.1}$$

lying on the curve $\Gamma=\{([\mathbb{I}_2],(0,0,\lambda)):\lambda\geqslant 0\}$ in M_1 (so $\mu=(\sqrt{1+\lambda^2}+\lambda)^2$ as in Sec. II). We may think of τ as a positive function $\tau(\mu)$ on $[1,\infty)$. We will first use the results of Sec. IV to prove that $\tau(\mu)$ is continuous. Positivity and continuity of τ ensure that it is bounded away from zero on any compact set. The domain of τ (whether thought of as a function on M_1 or on $[1,\infty)$) is noncompact, however, so we cannot conclude that τ is globally bounded away from zero. The essential question is, then, how does $\tau(\mu)$ behave as $\mu\to\infty$, that is, as the lump collapses to zero width? We will prove that $\tau(\mu)\to 0$.

First we address the issue of continuity. By symmetry, it suffices to consider a sequence of degree 1 holomorphic maps ϕ_n in the curve Γ, labeled by a sequence μ_n in $[1,\infty)$. If $\mu_n\to\hat{\mu}$, then the corresponding maps $\phi_n:z\mapsto\mu_n z$ converge in C^1 to $\hat{\phi}:z\mapsto\hat{\mu}z$. Since every holomorphic map $S^2\to S^2$ is Jacobi integrable, we may apply the results of Sec. IV. We merely need to prove that the pointwise inequality (4.1) on the pullback connexions ∇_n (∇^{ϕ_n} transfered to $\hat{\phi}^*TN$) holds for any such sequence μ_n. Then Lemma 4 applies, and continuity of τ follows from Theorem 6.

We must first construct the canonical isometry between each bundle $\phi_n^* TN$ and the fixed bundle $\hat{\phi}^* TN$ equipped with their L^2 inner products. To this end, it is convenient to define an orthonormal frame $E_1 = \partial/\partial\theta$, $E_2 = \operatorname{cosec}\theta\, \partial/\partial\varphi$ on S^2, where (θ,φ) are the usual polar coordinates, and the corresponding sections $\tilde{E}_i^n = E_i \circ \phi_n \in \Gamma(\phi_n^* TN)$, $\hat{E}_i = E_i \circ \phi \in \Gamma(\phi^* TN)$, $i = 1,2$. Note that varying ϕ within the family Γ sends each fixed $p \in M$ along a geodesic of constant φ in N. Note also that the frame E_1, E_2 is parallel along geodesics of constant φ, so the canonical isometry between $\phi_n^* TN$ and $\hat{\phi}^* TN$ is simply given by the identification

$$\tilde{E}_1^n \equiv \hat{E}_1, \quad \tilde{E}_2^n \equiv \hat{E}_2. \tag{5.2}$$

It is this property which makes polar coordinates particularly natural for our purposes.

In this coordinate system, a holomorphic map $\phi: z \mapsto \mu z$ is

$$(\theta,\varphi) \mapsto (f_\mu(\theta),\varphi), \quad f_\mu(\theta) = 2\cot^{-1}\left(\mu \cot\frac{\theta}{2}\right). \tag{5.3}$$

We will construct the pullback connexion ∇^ϕ by computing its action on $\tilde{E}_i = E_i \circ \phi$, $i = 1,2$. The Levi-Civita connection on S^2 is

$$\nabla E_1 = \cot\theta\, e_2 \otimes E_2, \quad \nabla E_2 = -\cot\theta\, e_2 \otimes E_1, \tag{5.4}$$

or equivalently,

$$\nabla e_1 = \cot\theta\, e_2 \otimes e_2, \quad \nabla e_2 = -\cot\theta\, e_2 \otimes e_1, \tag{5.5}$$

where e_1, e_2 is the coframe dual to E_1, E_2. The following properties of ∇^ϕ are essential for computations:

(a) If $u \in T_p M$, $Y \in \Gamma(\phi^* TN)$ and $f \in C^\infty(M)$, then $\nabla_u^\phi fY = u[f]Y + f\nabla_u^\phi Y$.

(b) If $Y \in \Gamma(\phi^* TN)$ may locally be identified with a vector field $\tilde{Y}$ on N (i.e., $Y = \tilde{Y} \circ \phi$, on a neighborhood of p), then $\nabla_u^\phi Y = \nabla_{d\phi u}^N \tilde{Y}$.

Now $d\phi E_1 = f'_\mu \tilde{E}_1$ and $d\phi E_2 = \operatorname{cosec}\theta \sin f_\mu \tilde{E}_2$, where $'$ denotes differentiation with respect to θ. Hence

$$\nabla_{\tilde{E}_1}^\phi \tilde{E}_1 = \nabla_{\tilde{E}_1}^\phi \tilde{E}_2 = 0,$$

$$\nabla_{\tilde{E}_2}^\phi \tilde{E}_1 = \frac{\sin f_\mu}{\sin\theta} \nabla_{\tilde{E}_2} \tilde{E}_1 = \frac{\sin f_\mu}{\sin\theta} \cot f_\mu \tilde{E}_2 = \frac{\cos f_\mu}{\sin\theta} \tilde{E}_2, \tag{5.6}$$

$$\nabla_{\tilde{E}_2}^\phi \tilde{E}_2 = \frac{\sin f_\mu}{\sin\theta} \nabla_{\tilde{E}_2} \tilde{E}_2 = -\frac{\sin f_\mu}{\sin\theta} \cot f_\mu \tilde{E}_2 = -\frac{\cos f_\mu}{\sin\theta} \tilde{E}_2.$$

Note that when $\mu = 1$, $\phi = \mathrm{Id}$, and $\nabla^{\mathrm{Id}} = \nabla$, so (5.6) should reduce to (5.4), which it does.

Any section of $\phi^* TN$ may be written

$$W = V + J^N U, \quad V = \mathcal{V}(\theta,\varphi)\tilde{E}_1, \quad U = \mathcal{U}(\theta,\varphi)\tilde{E}_1. \tag{5.7}$$

Note that ∇^ϕ commutes with J^N by the Kähler property. By the defining property (a), above, and (5.6), one sees that

$$\nabla^\phi V = \mathcal{V}_\theta\, e_1 \otimes \tilde{E}_1 + \frac{1}{\sin\theta} \mathcal{V}_\varphi\, e_2 \otimes \tilde{E}_2 + \mathcal{V} \frac{\cos f_\mu}{\sin\theta} e_2 \otimes \tilde{E}_2, \tag{5.8}$$

where subscripts θ,φ denote partial derivatives. This gives us explicit formulas for $\nabla^{\hat{\phi}}$ and ∇^{ϕ_n}. Using the identification (5.2) we may transfer a section W of $\hat{\phi}^*TN$ to ϕ_n^*TN, act with ∇^{ϕ_n}, then transfer back using the same identification, calling the result $\nabla_n W$. The difference between $\nabla_n W$ and $\nabla^{\hat{\phi}}W=\hat{\nabla}W$ is, by (5.8),

$$(\hat{\nabla}-\nabla_n)W=\frac{\cos f_{\hat{\mu}}-\cos f_{\mu_n}}{\sin\theta}(\mathcal{V}e_2\otimes\hat{E}_2-\mathcal{U}e_2\otimes\hat{E}_1)=\frac{\cos f_{\hat{\mu}}-\cos f_{\mu_n}}{\sin\theta}J^N W. \tag{5.9}$$

An elementary calculation shows that

$$\frac{\cos f_{\hat{\mu}}-\cos f_{\mu_n}}{\sin\theta}=\frac{(\hat{\mu}^2-\mu_n^2)\sin 2\theta}{2(\hat{\mu}^2\cos^2(\theta/2)+\sin^2(\theta/2))(\mu_n^2\cos^2(\theta/2)+\sin^2(\theta/2))}$$

$$\Rightarrow\left|\frac{\cos f_{\hat{\mu}}-\cos f_{\mu_n}}{\sin\theta}\right|\leqslant\frac{1}{2}\left(1+\frac{1}{\hat{\mu}^2}+\frac{1}{\mu_n^2}+\frac{1}{\hat{\mu}^2\mu_n^2}\right)|\hat{\mu}^2-\mu_n^2|. \tag{5.10}$$

Hence, we have a pointwise bound of the form (4.1),

$$|(\hat{\nabla}-\nabla_n)W|\leqslant a_n|W|, \tag{5.11}$$

where

$$a_n=\frac{1}{2}\left(1+\frac{1}{\hat{\mu}^2}+\frac{1}{\mu_n^2}+\frac{1}{\hat{\mu}^2\mu_n^2}\right)|\hat{\mu}^2-\mu_n^2|\to 0 \tag{5.12}$$

as $n\to\infty$, as required.

Having shown that $\tau(\mu)$ is continuous, we now address its behavior as $\mu\to\infty$. In particular, we will prove that $\lim_{\mu\to\infty}\tau(\mu)=0$. To do this, it suffices to consider only sections of ϕ^*TN of a certain type, which we will call "irrotational," namely those of the form

$$V=\mathcal{V}(\theta)\tilde{E}_1. \tag{5.13}$$

It is straightforward to compute $\mathfrak{D}^\phi V$ for such sections, and hence obtain $\mathsf{Hess}_\phi(V,V)$ as an explicit integral functional of $\mathcal{V}$. It follows from (5.8) that

$$\mathfrak{D}^\phi V=-\left(\mathcal{V}'-\frac{\cos f_\mu}{\sin\theta}\mathcal{V}\right)(e_1\otimes\tilde{E}_2+e_2\otimes\tilde{E}_1). \tag{5.14}$$

The Hessian for irrotational sections is

$$\mathsf{Hess}_\phi(V,V)=\frac{1}{2}\|\mathfrak{D}^\phi V\|_{L^2}^2=2\pi\int_0^\pi d\theta\sin\theta\left(\mathcal{V}'-\frac{\cos f_\mu}{\sin\theta}\mathcal{V}\right)^2. \tag{5.15}$$

We seek to compare this quantity, for irrotational sections L^2 orthogonal to $\ker\mathfrak{D}^\phi$, with $\|V\|_{H^1}^2$. Note that $\ker\mathfrak{D}^\phi$ is six-dimensional, and is spanned by

$$K_\mu^m=-\frac{2\cot^m(\theta/2)}{1+\mu^2\cot^2(\theta/2)}[\cos(1-m)\varphi\,\tilde{E}_1+\sin(1-m)\varphi\,\tilde{E}_2],\quad m=-1,0,1, \tag{5.16}$$

and their images under J^N. This basis is obtained by considering curves in M_1 through ϕ generated by altering the real part of one of the coefficients of the rational map. Every irrotational section V is automatically L^2 orthogonal to $K_\mu^{-1}, K_\mu^0, J^N K_\mu^{-1}, J^N K_\mu^0$ and $J^N K_\mu^1$, so we need only insist that V is L^2 orthogonal to the one and only irrotational section in the basis, K_μ^1, which we will henceforth denote K_μ. Explicitly, we require that

$$\langle V, K_\mu \rangle_{L^2} = -2\pi \int_0^\pi d\theta \sin\theta \frac{\mathcal{V}(\theta)\sin\theta}{\sin^2(\theta/2) + \mu^2 \cos^2(\theta/2)} = 0, \tag{5.17}$$

having rearranged K_μ slightly.

We shall also need an explict formula for $\|V\|_{H_1}$. Equation (5.8) implies that

$$\nabla^\phi V = \mathcal{V}' e_1 \otimes \tilde{E}_1 + \mathcal{V} \frac{\cos f_\mu}{\sin\theta} e_2 \otimes \tilde{E}_2, \tag{5.18}$$

so

$$\begin{aligned} \|V\|_{H^1}^2 = \|\nabla^\phi V\|_{L^2}^2 + \|V\|_{L^2}^2 &= 2\pi \int_0^\pi d\theta \sin\theta \left((\mathcal{V}')^2 + \frac{\cos^2 f_\mu}{\sin^2\theta} \mathcal{V}^2 + \mathcal{V}^2 \right) \\ &= \mathsf{Hess}_\phi(V,V) + \|V\|_{L^2}^2 + 2\pi \int_0^\pi d\theta \, 2\mathcal{V}\mathcal{V}' \cos f_\mu \\ &= \mathsf{Hess}_\phi(V,V) + \|V\|_{L^2}^2 + \langle V, \mathcal{E}_\mu V \rangle_{L^2}, \end{aligned} \tag{5.19}$$

where $\mathcal{E}_\mu \in C^\infty(S^2)$ is the energy density of the map ϕ. To see the last equality, note that ϕ is holomorphic, hence conformal, so

$$f_\mu' = |d\phi E_1| = |d\phi E_2| = \frac{\sin f_\mu}{\sin\theta}. \tag{5.20}$$

Equation (5.19) follows from (5.20) and integration by parts.

It also proves useful to write down the formulas above using cylindrical coordinates instead of spherical polar coordinates on the domain. That is in place of (θ,φ) we use (s,φ) where $s := \log\cot\theta/2$. First notice that with respect to these cylindrical coordinates $f_\mu(s)$ arises by translating one fixed profile by a μ dependent amount. More precisely,

$$f_\mu(s) = f_1(s + \log\mu), \tag{5.21}$$

where

$$f_1(s) = 2\cot^{-1}(\exp s). \tag{5.22}$$

We have an analogous formula for K_μ the irrotational part of the kernel of $\mathfrak{D}^\phi$:

$$K_\mu(s) = \operatorname{sech}(s + \log\mu)\tilde{E}_1. \tag{5.23}$$

It is a routine computation to obtain the following formulas for $\mathsf{Hess}_{\phi_\mu}(V,V)$, $\langle V, \mathcal{E}_\mu V \rangle_{L^2}$ and the L^2, H^1 norms of an irrotational section V from the corresponding formulas using spherical polars already presented

$$\langle V, V \rangle_{L^2} = \int_{-\infty}^\infty ds \operatorname{sech}^2 s \;\; \mathcal{V}^2, \tag{5.24}$$

$$\langle V,\mathcal{E}_\mu V\rangle_{L^2}=\int_{-\infty}^{\infty} ds\,\operatorname{sech}^2(s+\log\mu)\mathcal{V}^2, \tag{5.25}$$

$$\langle V,V\rangle_{H^1}=\int_{-\infty}^{\infty} ds\left(\left(\frac{d\mathcal{V}}{ds}\right)^2+\tanh^2(s+\log\mu)\ \ \mathcal{V}^2+\operatorname{sech}^2 s\ \ \mathcal{V}^2\right), \tag{5.26}$$

$$\mathsf{Hess}_{\phi_\mu}(V,V)=\int_{-\infty}^{\infty} ds\ \ \left(\frac{d\mathcal{V}}{ds}+\tanh(s+\log\mu)\mathcal{V}\right)^2. \tag{5.27}$$

We may now state and prove the main result of this section. We shall denote the map $z\mapsto\mu z$ by ϕ_μ to emphasize its parametric dependence.

Theorem 7 (Global coercivity of the Hessian fails on Rat_1): $\lim_{\mu\to\infty}\tau(\phi_\mu)=0$.

Proof: Define the following sequence of smooth irrotational sections $V_\mu=\mathcal{V}_\mu\tilde{E}_1$ of $\phi_\mu^*TS^2$ where

$$\mathcal{V}_\mu(s)=\operatorname{sech} s-c_\mu K_\mu(s) \tag{5.28}$$

and c_μ is a constant determined by the requirement that $\langle V_\mu,K_\mu\rangle_{L^2}=0$. By our previous remarks, this suffices to ensure that $\mathcal{V}_\mu$ is orthogonal to $\ker\mathfrak{D}^{\phi_\mu}$. Since $V_\mu\in H^1(\phi_\mu^*TS^2)\cap\ker\mathfrak{D}^{\phi_\mu}$ it suffices to prove that

$$\lim_{\mu\to\infty}\frac{\mathsf{Hess}_{\phi_\mu}(V_\mu,V_\mu)}{\langle V_\mu,V_\mu\rangle_{H^1}^2}=0. \tag{5.29}$$

In fact, we will show that

$$\lim_{\mu\to\infty}\frac{\mathsf{Hess}_{\phi_\mu}(V_\mu,V_\mu)}{\langle V_\mu,\mathcal{E}_\mu V_\mu\rangle_{L^2}}=0, \tag{5.30}$$

which implies (5.29) since

$$\|V\|_{H^1}^2=\mathsf{Hess}_{\phi_\mu}(V,V)+\|V\|_{L^2}^2+\langle V,\mathcal{E}_\mu V\rangle_{L^2}>\langle V,\mathcal{E}_\mu V\rangle_{L^2}.$$

To prove (5.30), first notice that since $K_\mu\in\ker\mathfrak{D}^{\phi_\mu}$ we have

$$\mathsf{Hess}_{\phi_\mu}(V_\mu,V_\mu)=\mathsf{Hess}_{\phi_\mu}(\operatorname{sech} s,\operatorname{sech} s).$$

Using the explicit expression for the Hessian in cylindrical coordinates we find

$$\mathsf{Hess}_{\phi_\mu}(\operatorname{sech} s,\operatorname{sech} s)=\int_{-\infty}^{\infty} ds\,\operatorname{sech}^2 s(\tanh s_\mu-\tanh s)^2,$$

where $s_\mu:=s+\log\mu$. Since $|(\tanh s_\mu-\tanh s)^2|<4$ holds for all s,

$$\mathsf{Hess}_{\phi_\mu}(\operatorname{sech} s,\operatorname{sech} s)<4\int_{-\infty}^{\infty} ds\,\operatorname{sech}^2 s=8$$

holds for all μ. Since $\mathsf{Hess}_{\phi_\mu}(V_\mu,V_\mu)$ is bounded for all μ, (5.30) is implied by

$$\lim_{\mu\to\infty}\langle V_\mu,\mathcal{E}_\mu V_\mu\rangle_{L^2}=+\infty. \tag{5.31}$$

To establish (5.31), first introduce for each non-negative pair of integers (m,n) the positive function

$$I_{m,n}(\mu)=\int_{-\infty}^{\infty} ds\,\mathrm{sech}^m s\,\mathrm{sech}^n s_\mu .$$

Clearly, the function $I_{m,n}(\mu)$ is bounded above by the constant $I_{m,0}$. From the definition of c_μ we have

$$c_\mu=\frac{\langle \mathrm{sech}\,,K_\mu\rangle}{\langle K_\mu,K_\mu\rangle}=\frac{I_{3,1}}{I_{2,2}}\ ,$$

and from Eq. (5.25) and the definition of V_μ we have

$$\langle V_\mu,\mathcal{E}_\mu V_\mu\rangle_{L^2}=c_\mu(c_\mu I_{4,0}-2I_{1,3})+I_{2,2}.$$

Since $I_{4,0}$ is a positive constant and $I_{1,3}$, $I_{2,2}$ are positive and bounded above, (5.31) will follow if we can establish that $\lim_{\mu\to\infty}c_\mu=+\infty$. In fact, one can explicitly evaluate the integrals which appear in the definition of c_μ to obtain

$$c_\mu=\frac{I_{3,1}}{I_{2,2}}=\frac{\mu^4-4\mu^2\log\mu-1}{4\mu(\mu^2\log\mu-\mu^2+\log\mu+1)}.$$

Clearly, this implies that $\lim_{\mu\to\infty}c_\mu=+\infty$ as required. □

VI. THE CASE OF Rat_n^{eq}

Staying in the context of the $\mathbb{C}P^1$ model on S^2, but generalizing to any degree sector, $n\geqslant 1$, things become rather more difficult. The reason is that the isometric action of G on $\mathsf{M}_n=\mathsf{Rat}_n$ does not have cohomogeneity 1, except for $n=1$. In general, then, to understand the global behavior of τ one must consider the $4(n-1)$-dimensional orbifold M_n/G, not simply a curve, as in Sec. V. Reduction to a curve *is* possible, however, provided we restrict attention to dynamics within a certain equivariance class. Employing stereographic coordinates z,W on domain and codomain as usual, and defining polar coordinates such that $z=re^{i\varphi}$, one may write the field equation for the $\mathbb{C}P^1$ model on space–time $S^2\times\mathbb{R}$ as

$$\frac{W_{tt}}{(1+r^2)^2}-\left(W_{rr}+\frac{1}{r}W_r+\frac{1}{r^2}W_{\varphi\varphi}\right)-\frac{2\overline{W}}{1+|W|^2}\left(\frac{W_t^2}{(1+r^2)^2}-W_r^2-\frac{1}{r^2}W_\varphi^2\right)=0. \tag{6.1}$$

This supports equivariant solutions within the ansatz

$$W(r,\varphi,t)=r^n q(r,t)e^{in\varphi}. \tag{6.2}$$

Provided $q:[0,\infty)\times(-\epsilon,\epsilon)\to\mathbb{C}$ is nowhere vanishing and has suitable boundary behavior, solutions within this ansatz have degree n. Substituting (6.2) into (6.1) one obtains a $(1+1)$-dimensional hyperbolic partial differential equation for q. The space of static solutions is simply $q(r,t)=c\neq 0$, a complex constant. So the equivariant moduli space is $\mathsf{M}_n^{eq}=\mathsf{Rat}_n^{eq}=\{z\mapsto cz^n: c\neq 0\}\cong\mathbb{C}^\times$, the punctured complex plane. Note that M_n^{eq} is one connected component of the fixed point set in M_n of the isometry group $G^{eq}=\{([\exp -in(\psi/2)\,\tau_3],[\exp i(\psi/2)\,\tau_3]):\psi\in\mathbb{R}\}\cong\mathrm{SO}(2)$, so we are assured that $\mathsf{M}_n^{eq}\subset\mathsf{M}_n$ is totally geodesic. Both the true wave map flow and its geodesic approximant stay within the equivariance class, therefore, and one can again ask to what extent the analytic method of Stuart applies. The equivariant configuration space enjoys a residual U(1) symmetry, namely $W(z)\mapsto e^{i\psi}W(z)$, and the discrete symmetry $W(z)\mapsto 1/W(1/z)$, both of which leave the harmonic map energy unchanged, so we may again restrict attention to a curve in M_n^{eq}, namely $\Gamma=\{z\mapsto\mu z^n:\mu\in[1,\infty)\}$. The situation is actually *simpler* than in the full

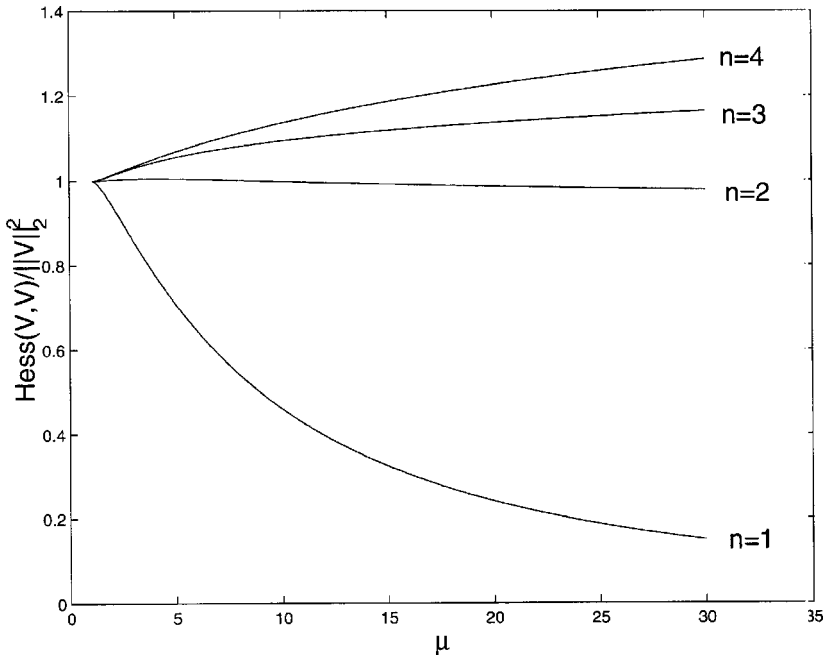

FIG. 1. Plots of the ratio $\mathrm{Hess}_{\phi_\mu}(V_\mu,V_\mu)/\|V_\mu\|^2_{H^1}$ against μ for the first excited state V_μ of the Sturm–Liouville problem (6.8) with $\phi_\mu: z\to\mu z^n$, $n=1,2,3,4$. To facilitate comparison of the curves, in each case the ratio has been normalized by its value at $\mu=1$ (0.30, 0.74, 1.17 and 1.55 respectively, to two decimal places). Note that only for $n=1$ does the ratio tend to 0 as $\mu\to\infty$.

degree 1 case, because now the error, that is, the section of ϕ^*TN along which we exponentiate to get from the holomorphic approximant to the true solution at time t, must also lie within the equivariance class. The only sections of relevance, therefore, are irrotational sections and their J^N images. We may define a new optimal constant $\tau^{eq}(\phi)$, again the infimium of the Hessian for H^1 unit sections L^2 orthogonal to $\ker\mathfrak{D}^\phi$, but now we include only equivariant sections. Since these form a subset of all sections, we have trivially that $\tau^{eq}(\phi)\geqslant\tau(\phi)>0$ by Theorem 3.

Once again, we may think of τ^{eq} as a function of $\mu\in[1,\infty)$. We first show that $\tau^{eq}(\mu)$ is continuous. Since the setup is very similar to Sec. V we use equivalent notation and conventions, and omit several details. In spherical polar coordinates, the map $\phi: z\mapsto\mu z^n$ is

$$(\theta,\varphi)\mapsto(f_\mu(\theta),n\varphi),\quad f_\mu(\theta)=2\cot^{-1}\left(\mu\cot^n\frac{\theta}{2}\right),\tag{6.3}$$

so $d\phi E_1=f'_\mu\tilde{E}_1$ and $d\phi E_2=n\,\mathrm{cosec}\,\theta\cos f_\mu\tilde{E}_2$. It follows that

$$\nabla^\phi\tilde{E}_1=n\frac{\cos f_\mu}{\sin\theta}e_2\otimes\tilde{E}_2,\quad \nabla^\phi\tilde{E}_2=-n\frac{\cos f_\mu}{\sin\theta}e_2\otimes\tilde{E}_1.\tag{6.4}$$

Hence, on an irrotational section $V=\mathcal{V}(\theta)\tilde{E}_1$,

$$\nabla^\phi V=V'e_1\otimes\tilde{E}_1+Vn\frac{\cos f_\mu}{\sin\theta}e_2\otimes\tilde{E}_2.\tag{6.5}$$

Given a general equivariant section $W=V+J^NU$, where V,U are irrotational, we may transfer W to a neighboring bundle $\hat{\phi}^*TN$ (where $\hat{\phi}: z\mapsto\hat{\mu}z$) using the canonical isometry (5.2), act with $\nabla^{\hat{\phi}}$, then transfer back again, to obtain $\hat{\nabla}W$. The difference between this and $\nabla^\phi W$ is

$$(\nabla^{\phi}-\hat{\nabla})W=n\frac{\cos f_{\mu}-\cos f_{\hat{\mu}}}{\sin\theta}J^{N}W. \tag{6.6}$$

Now

$$\begin{aligned}\alpha(\theta)&=\frac{\cos f_{\mu}-\cos f_{\hat{\mu}}}{\sin\theta}\\&=\frac{(\mu^2-\hat{\mu}^2)(\cos(\theta/2)\sin(\theta/2))^{2n-1}}{(\sin^{2n}(\theta/2)+\mu^2\cos^{2n}(\theta/2))(\sin^{2n}(\theta/2)+\hat{\mu}^2\cos^{2n}(\theta/2))}\\&\Rightarrow|\alpha(\theta)|\leqslant\left(1+\frac{1}{\hat{\mu}^2}+\frac{1}{\mu^2}+\frac{1}{\hat{\mu}^2\mu^2}\right)|\hat{\mu}^2-\mu^2|.\end{aligned} \tag{6.7}$$

So the pullback connexion satisfies a pointwise bound of the correct type ($|(\nabla^{\phi}-\hat{\nabla})W|<c(\mu,\hat{\mu})|W|$ where $c\to 0$ as $\mu\to\hat{\mu}$) and we may conclude from the results of Sec. IV that $\tau^{eq}(\mu)$ is continuous.

As for Rat_1, the interesting issue is the large μ behavior of $\tau^{eq}(\mu)$. We are so far unable to prove anything rigorous about $\lim_{\mu\to\infty}\tau^{eq}(\mu)$ (if, indeed, it exists). However, we make the following conjecture:

Conjecture 8: For all $n\geqslant 1$, $\lim_{\mu\to\infty}\tau^{eq}(\mu)$ *exists and is finite. For all* $n>1$, *this limit is not zero.*

If true, the equivariant Hessian is globally coercive for degree n greater than unity. One could at least hope, therefore, to model equivariant lump collapse accurately within the geodesic approximation in the case $n>1$.

To motivate this conjecture, we should describe some numerical work which led directly to the proof of its $n=1$ counterpart, Theorem 7. It is straightforward to write the Jacobi operator on irrotational sections as an explicit ordinary differential operator acting on $\mathcal{V}(\theta)$. The eigenvalue problem for $\mathfrak{J}^{\phi}$ then reduces to a singular Sturm–Liouville problem on $(0,\pi)$, namely

$$-\mathcal{V}''-\cot\theta\mathcal{V}'+n^2\frac{\cos 2f_{\mu}}{\sin^2\theta}\mathcal{V}=\omega^2\mathcal{V}. \tag{6.8}$$

Here $\omega^2\geqslant 0$ is the eigenvalue. The eigenfunctions of this problem form an L^2 orthogonal basis for the space of irrotational sections. In particular, the eigenfunctions outside the kernel, which we shall refer to as "excited states," in analogy with quantum mechanics, form a basis for the irrotational sections orthogonal to $\ker\mathfrak{J}^{\phi}$. If we could prove that $\mathsf{Hess}_{\phi}(V,V)/\|V\|^2_{H^1}=\omega^2\|V\|^2_{L^2}/\|V\|^2_{H^1}$ is bounded uniformly away from zero for all μ and all excited states V, global coercivity of Hess^{eq} would follow. Conversely, if for one of the excited states, $\omega^2\|V\|^2_{L^2}/\|V\|^2_{H^1}\to 0$ as $\mu\to\infty$, global coercivity must fail: the one parameter family of excited states itself provides a counterexample. Unfortunately, the (μ families) of eigensections are rather inaccessible analytically (except in the special case $\mu=n=1$, where they are known exactly). However, they are quite easy to construct numerically, either by employing a specialist Sturm–Liouville solver package, or by using a shooting method. We have tried both strategies, obtaining compatible results from each.

The pertinent results may be summarized as follows. For $n=1,2,3,4$ and for all excited states from second to sixth (ordered by increasing ω^2), the ratio $\mathsf{Hess}_{\phi}(V,V)/\|V\|^2_{H_1}$ appears to remain bounded away from zero as $\mu\to\infty$. More interesting is the first excited state. Here the ratio remains bounded away from zero for $n=2,3,4$, but not for $n=1$. It was by examining the graphs of the $n=1$ first excited eigenstates that the explicit family V_{μ} of the proof of Theorem 7 was devised: the family is designed to have the same qualitative behavior as the numerically generated

eigenstates. In Fig. 1 we present a graph showing the ratio $\mathrm{Hess}_\phi(V,V)/\|V\|^2_{H_1}$ as a function of μ for the first excited states for $n=1,2,3,4$. These data were generated by a shooting method using a fourth order Runge–Kutta scheme with variable θ step. The singularities at $\theta=0,\pi$ were handled by series expansions, so the scheme shot forwards from $\theta=\delta$ and backwards from $\theta=\pi-\delta$, applying a matching condition at $\theta=(\pi/2)$ (δ being a small positive number, typically 0.001). The difference between $n=1$ and the other cases is quite clear. Although it is impossible to be exhaustive numerically, the results suggest that $\mathrm{Hess}_\phi(V,V)/\|V\|^2_{H_1}$ is bounded away from zero for $n>1$, as we have conjectured. Linhart and Sadun in a recent numerical study of lump collapse in the $\mathbb{C}P^1$ model on $\mathbb{C}$ imposed the analogous equivariance condition on their field equation.[10] It is an intriguing coincidence that they found that single lump collapse differs greatly from the predictions of the geodesic approximation (truncated to a finite disk in $\mathbb{C}$), whereas the collapse of two coincident lumps is quite well modeled by the geodesic flow.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

The dynamics of vortices on S^2 near the Bradlow limit

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(Received 1 August 2002; accepted 9 April 2003)

The explicit solutions of the Bogomolny equations for N vortices on a sphere of radius $R^2>N$ are not known. In particular, this has prevented the use of the geodesic approximation to describe the low energy vortex dynamics. In this article we introduce an approximate general solution of the equations, valid for $R^2 \gtrsim N$, which has many properties of the true solutions, including the same moduli space $\mathbb{CP}^N$. Within the framework of the geodesic approximation, the metric on the moduli space is then computed to be proportional to the Fubini–Study metric, which leads to a complete description of the particle dynamics. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1584526]

I. INTRODUCTION

The Abelian Higgs model in the plane is one of the most studied examples of a field theory with topological solitons. The solitons are vortices. At critical coupling there are Bogomolny equations, and it is known that there is a $2N$-dimensional manifold of gauge-inequivalent N-vortex solutions.[6] This is known as the N-vortex moduli space, and denoted $\mathcal{M}_N$. As a manifold, $\mathcal{M}_N \cong \mathbb{C}^N$. There is a natural metric on $\mathcal{M}_N$, arising from the kinetic terms in the Lagrangian of the model, and it has been proved by Stuart[13] that, at least for finite time intervals, geodesic trajectories on the moduli space give a good approximation to the true dynamics of slowly moving vortices.

It is convenient to introduce the standard complex coordinate z on the plane. The locations of the vortices are the N unordered points where the Higgs field vanishes. These points may be regarded as the roots of a monic polynomial in z (monic means that the coefficient of z^N is 1), and the natural coordinates on moduli space are the N complex coefficients of such a polynomial. If a particular geodesic motion is known, then the time dependence of the polynomial is known, and hence the time dependence of the roots can be calculated.

Now, a general formula for the metric on moduli space has been given by Samols,[12] but it is not explicit, so only very special geodesics, with a high degree of symmetry, are understood in detail for $N>2$.[1,9] One vortex just moves at constant speed along a straight line. The geodesic motion for two vortices has been calculated by Samols numerically. The most interesting phenomenon is that, in a head-on collision, two vortices scatter at right angles. Recently, Manton and Speight[11] have found an explicit metric for N well separated vortices, from which the geodesic motion could be computed.

In this article we are interested in the opposite limit. It is possible to consider the Abelian Higgs model with fields defined on any compact surface. We shall only consider the case of a two-sphere with its standard round metric, parametrized by its radius R. There are again Bogomolny equations and a $2N$-dimensional moduli space of N-vortex solutions. As a manifold this is $\mathbb{CP}^N$. However, there is an important geometrical constraint, discovered by Bradlow.[2] This is that the area of the sphere must be greater than $4\pi N$ for nontrivial solutions of the Bogomolny equations to exist. Equivalently, $R^2>N$. The metric on moduli space is known to collapse to zero size as the Bradlow limit $R^2 \searrow N$ is approached. We shall be interested here in the case where R^2

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is slightly greater than N. One should think of this as a situation where the vortices are densely squeezed together. We shall present an approximate general solution of the Bogomolny equations, and, using this, calculate the metric on moduli space directly from its definition. Again the solutions involve a polynomial, and the natural coordinates are the complex coefficients of the polynomial. We shall find that the metric is that of Fubini–Study, with an overall scale factor that depends on R^2-N.

The geodesics on Fubini–Study are quite simple, and hence, in principle, the motion of vortices can be calculated straightforwardly. However, this does involve finding the roots of polynomials with time-varying coefficients, which is not algebraically trivial for three or more vortices. We shall present examples, mainly of two vortex motion. We should also remark that Stuart's proof of the validity of the geodesic approximation for vortex motion does not extend automatically to this regime of being close to the Bradlow limit, so our results on vortex motion remain rather formal at this stage. The particle dynamics we obtain at the end is, nevertheless, quite ''physical.''

The article is structured as follows. In Sec. II we introduce the Bogomolny equations on S^2, which is identified with $\mathbb{CP}^1$. As in Refs. 2 and 4, the equations are defined on complex line bundles over this surface. In Secs. III and IV we explain our approximation for R^2 close to N, and proceed to compute the metric on the moduli space of the approximate solutions. The geodesics of this Fubini–Study metric are then used in Sec. V to give an explicit description of the N-vortex dynamics. Some examples of motions are presented in Sec. VI, and finally in Sec. VII a general result concerning the number of vortex collisions is proved.

II. THE BOGOMOLNY EQUATIONS

According to Bradlow's generalization of the classical vortices over $\mathbb{R}^2$,[2] when the base manifold is the sphere $S^2\cong\mathbb{CP}^1$, the setup for the problem is a complex line bundle $\pi:E\to S^2$ of degree N equipped with a Hermitian metric h. The Higgs field ϕ is now a section of this bundle, and the gauge potentials are the local one-forms of an h-compatible connection D on the bundle. We will take the metric on S^2 to be $g_R:=R^2\times(\text{standard metric on } S^2)$, so that the volume of (S^2,g_R) is $4\pi R^2$.

Letting $\mathcal{A}:=\{h\text{-compatible connections on } E\}$ and $\Gamma(E):=\{\text{global } C^\infty \text{ sections of } E\}$, the Bogomolny equations for $(D,\phi)\in\mathcal{A}\times\Gamma(E)$ are[2,4]

$$D^{0,1}\phi=0, \tag{1}$$

$$F+\tfrac{1}{2}(|\phi|_h^2-1)\,\mathrm{vol}_R=0, \tag{2}$$

where $D^{0,1}$ is the anti-holomorphic part of D, $\mathrm{vol}_R\in\Omega^2(S^2,\mathbb{R})$ is the volume form of the metric g_R, and $-iF$ is the globally defined curvature form of D, so that $F\in\Omega^2(S^2,\mathbb{R})$.

We remark that the problem does not depend essentially on (E,h), because all complex line bundles over S^2 of a given degree N are isomorphic. In fact, for another choice (E',h') there will always be an isomorphism $f:E\to E'$ such that $f^*(h')=h$. It is then not difficult to check that (D,ϕ) is a solution of (1) and (2) on (E',h') if and only if $(f^*D, f^{-1}\circ\phi)$ is a solution on (E,h), where f^*D is the pull-back connection on E. Notice in particular that $\phi\in\Gamma(E')$ and $f^{-1}\circ\phi\in\Gamma(E)$ have the same zeros on S^2, and hence correspond to the same vortex configuration.

We will now define the particular pair (E,h) which is to be used in the remainder of this article. Let $U_1=\mathbb{CP}^1\backslash\{[0,1]\}$, $U_2=\mathbb{CP}^1\backslash\{[1,0]\}$, where we use the standard homogeneous coordinates $[z_0,z_1]$ for points on $\mathbb{CP}^1$, and let $\varphi_i:U_i\to\mathbb{C}$ be the standard complex charts of $\mathbb{CP}^1$ with transition functions $\varphi_1\circ\varphi_2^{-1}=\varphi_2\circ\varphi_1^{-1}:z\mapsto 1/z$. Define $g_{ij}:U_i\cap U_j\to U(1)$ by

$$g_{21}\circ\varphi_2^{-1}(z)=(z/|z|)^N, \qquad g_{12}=1/g_{21}\ , \quad g_{11}=g_{22}=1.$$

Since the g_{ij} satisfy the usual cocycle conditions, it is possible to construct a complex line bundle $\pi: E \to \mathbb{CP}^1$ with trivializations $\psi_i : \pi^{-1}(U_i) \to U_i \times \mathbb{C}$ such that $\psi_i \circ \psi_j^{-1}(p,y) = (p, g_{ij}(p)\, y)$. The Hermitian metric h on E is defined by requiring the unitarity of the trivializations ψ_i, that is, $|\psi_i^{-1}(p,y)|_h^2 = |y|^2$; it is well defined because g_{ij} has values in $U(1)$.

We should now check that $\deg E = N$. Define the real valued one-forms $A_i \in \Omega^1(U_i, \mathbb{R})$ by

$$A_i = \varphi_i^* A \qquad \text{with} \qquad A := \frac{-iN}{2(1+|z|^2)} (\bar{z}\, dz - z\, d\bar{z}) \in \Omega^1(\mathbb{C}, \mathbb{R}). \tag{3}$$

On $U_1 \cap U_2$ one has

$$(\varphi_2^{-1})^*(A_1 - A_2) = \left(\frac{1}{z}\right)^* A - A = i \left(\frac{|z|}{z}\right)^N d\left(\frac{z}{|z|}\right)^N = i\, (\varphi_2^{-1})^*(g_{12}\, dg_{21}),$$

or equivalently

$$(-iA_1) - (-iA_2) = g_{12}\, dg_{21} \ ,$$

which shows that the local forms $-iA_1$ and $-iA_2$ define a connection D_N on E. The curvature $-iF_N$ of D_N is a global two-form on $\mathbb{CP}^1$ determined by $F_N = dA_j$ on U_j. In particular, one can compute that

$$(\varphi_1^{-1})^* F_N = dA = \frac{iN}{(1+|z|^2)^2}\, dz \wedge d\bar{z} = (\varphi_1^{-1})^* \left(\frac{1}{2} \mathrm{vol}_{\sqrt{N}}\right),$$

and hence

$$\deg E := \frac{i}{2\pi} \int_{\mathbb{CP}^1} (-iF_N) = \frac{1}{2\pi} \int_{\mathbb{C}} (\varphi_1^{-1})^* F_N = N.$$

Integrating Eq. (2) over $\mathbb{CP}^1$, and using that $\int_{\mathbb{CP}^1} F = 2\pi \deg E = 2\pi N$, it is clear that for $R^2 < N$ the Bogomolny equations have no solution, and that for $R^2 = N$ any solution (D, ϕ) must satisfy $\phi = 0$ and $F = 1/2\, \mathrm{vol}_{\sqrt{N}} = F_N$. Since we have already constructed a connection D_N on E with curvature $-iF_N$, we have an explicit solution of the Bogomolny equations for the case $R^2 = N$ (which is called the Bradlow limit), and it can be shown that it is unique up to gauge transformations.

For $R^2 > N$ Bradlow has shown,[2] in a more general context, that for any solution (D, ϕ) of (1) and (2), the section ϕ has exactly N zeros (which are called vortices), counting multiplicities. Moreover, the moduli space $\mathcal{M}_N$ of these solutions up to gauge tranformations is parametrized by the positions in $\mathbb{CP}^1$ of these N vortices. Since the vortices are indistinguishable, this moduli space is identified with $(\mathbb{CP}^1)^N / S_N$, where S_N is the group of permutations of N elements.

Now consider the map $\Upsilon : (\mathbb{CP}^1)^N / S_N \to \mathbb{CP}^N$ defined in homogeneous coordinates by

$$[\,[u^1, v^1], \ldots, [u^N, v^N]\,] \mapsto \left[\ \ldots, \sum_{\sigma \in S_N} v^{\sigma(1)} \cdots v^{\sigma(k)} u^{\sigma(k+1)} \cdots u^{\sigma(N)}, \ldots\ \right]_{0 \le k \le N} .$$

With some care, one can verify that Υ is a bijection. In fact, its inverse may be described in the following way. Given $[w_0, \ldots, w_N] \in \mathbb{CP}^N$, consider the nonzero polynomial

$$P(z) = \sum_{k=0}^{N} (-1)^k \frac{N!}{k!(N-k)!} w_k\, z^{N-k} \ ,$$

which has degree $l \leqslant N$. Calling $z_1, \ldots, z_l$ the complex roots of $P(z)$, one has

$$\Upsilon^{-1}([w_0,\ldots,w_N])=[[1,z_1],\ldots,[1,z_l],[0,1],\ldots,[0,1]].$$

Using this bijection, $\mathcal{M}_N$ can also be identified with $\mathbb{CP}^N$.

III. VORTICES NEAR THE BRADLOW LIMIT

Although we have an accurate description of the moduli space $\mathcal{M}_N$, the explicit form of the solutions (D,ϕ) of (1) and (2) is not known. In particular, this has prevented any successful attempt to describe the dynamics of the vortices by means of the well-known geodesic approximation. The purpose of this article is to show that by replacing the exact Bogomolny equations by two other conditions, which should be a good approximation near the Bradlow limit $R^2 \searrow N$, one can obtain the solutions explicitly; they also have $\mathbb{CP}^N$ as their moduli space, and furthermore the dynamics of these ''pseudo-vortices'' is completely computable in the framework of the geodesic approximation.

Since for $R^2=N$ the pair $(D_N,0)\in\mathcal{A}\times\Gamma(E)$ is an exact solution of (1) and (2), we may expect that for R^2 close to N the solutions (D,ϕ) will have $D\approx D_N$ (after a gauge transformation if necessary). We therefore impose $D=D_N$ and look for $\phi\in\Gamma(E)$ such that

$$(D_N,\phi) \text{ is a solution of (1), i.e., } D_N^{0,1}\phi=0; \tag{4}$$

$$(D_N,\phi) \text{ satisfies (2) ''on average,'' i.e., } \int_{\mathbb{CP}^1}\left(F_N+\frac{1}{2}(|\phi|_h^2-1)\,\mathrm{vol}_R\right)=0. \tag{5}$$

[We note in passing that Eq. (4) is analogous to the equation for electron wavefunctions of the first Landau level in the uniform background magnetic field F_N; Eq. (5) is then a wavefunction normalization condition.]

We will now find the explicit solutions of (4) and (5), and then describe their moduli space. Using the local trivialization ψ_1 of E and the chart φ_1 of $\mathbb{CP}^1$ defined before, the equation $D_N^{0,1}\phi=0$ over the domain U_1 is the same as $(\overline{\partial}-iA^{0,1})\phi_1=0$, or, explicitly, using (3),

$$\frac{\partial\phi_1}{\partial\bar{z}}=\frac{-Nz}{2(1+|z|^2)}\phi_1, \tag{6}$$

where $\phi_1\in C^\infty(\mathbb{C})$ is the representative of ϕ with respect to ψ_1.

Equation (6) has the general solution $\phi_1=f(z)(1+|z|^2)^{-N/2}$, with f holomorphic on $\mathbb{C}$. The section ϕ of E determined by ϕ_1, which is only defined over U_1, has a representative ϕ_2 with respect to ψ_2 given by $\phi_2(z)=g_{12}(z)\phi_1(1/z)$, which is smooth on $\mathbb{C}\backslash\{0\}$. But since we are looking for global solutions of (4), ϕ must be extensible to all of $\mathbb{CP}^1$, and this will happen iff $\phi_2(z)$ is smoothly extensible to $\mathbb{C}$. Writing f as a Taylor series, it is then not difficult to check that this requires that the coefficient of z^n vanishes for all $n>N$. Thus any solution ϕ of (4) must have a representative ϕ_1 over U_1 of the form

$$\phi_1(z)=\frac{a_0z^N+\cdots+a_N}{(1+|z|^2)^{N/2}}, \tag{7}$$

and conversely any ϕ_1 of this form determines a global section ϕ of E which is a solution of (4) over U_1, and by continuity over all of $\mathbb{CP}^1$.

If ϕ is represented by ϕ_1 as in (7), then the representative ϕ_2 will be

$$\phi_2(z)=\frac{a_0+\cdots+a_Nz^N}{(1+|z|^2)^{N/2}}$$

and hence, as for (1) and (2), any solution ϕ of (4) has exactly N zeros over $\mathbb{CP}^1$, counting multiplicities.

We now turn to condition (5). Using that $-iF_N$ is the curvature form of a degree N bundle, (5) is equivalent to

$$4\pi(R^2-N)=\int_{\mathbb{CP}^1}|\phi|_h^2\,\mathrm{vol}_R=\int_{\mathbb{C}}|\phi_1|^2\frac{2iR^2}{(1+|z|^2)^2}\,dz\wedge d\bar{z}=4\pi R^2\sum_{k=0}^{N}\frac{k!(N-k)!}{(N+1)!}|a_k|^2\ ,$$

where the last integral is calculated in the Appendix for ϕ_1 of the form (7). We can therefore conclude that ϕ_1 represents a solution ϕ of (4) and (5) iff ϕ_1 is of the form (7) and satisfies the normalization condition

$$\sum_{k=0}^{N}\frac{k!(N-k)!}{(N+1)!}|a_k|^2=1-\frac{N}{R^2}.$$

Calling $\mathcal{D}\subset\mathcal{A}\times\Gamma(E)$ the subspace of solutions of (4) and (5), we thus get a bijection $\alpha:\mathcal{D}\to S^{2N+1}\subset\mathbb{C}^{N+1}$ that maps each $\phi\in\mathcal{D}$, represented by a ϕ_1 like in (7), to the point

$$\left(1-\frac{N}{R^2}\right)^{-1/2}\left(\ldots,\left(\frac{k!(N-k)!}{(N+1)!}\right)^{1/2}a_k,\ldots\right)_{0\leqslant k\leqslant N}. \tag{8}$$

The following step is to determine when two solutions in $\mathcal{D}$ are gauge equivalent. Let therefore (D_N,ϕ) and $(D_N,\tilde{\phi})$ be a pair of solutions, and suppose $g:\mathbb{CP}^1\to U(1)$ is a gauge transformation on E that takes one into the other. Using the usual transformation rule for connection forms under g, and the key fact that the connection is fixed, it is readily shown that g must be constant. So $\tilde{\phi}=e^{i\beta}\phi$ for some $\beta\in\mathbb{R}$. Since the converse is clear, we conclude that (D_N,ϕ) and $(D_N,\tilde{\phi})$ are gauge equivalent iff

$$\tilde{\phi}=e^{i\beta}\phi\ \Leftrightarrow\ \tilde{\phi}_1=e^{i\beta}\phi_1\ \Leftrightarrow\ \tilde{c}=e^{i\beta}c$$

for some $\beta\in\mathbb{R}$, where $c,\tilde{c}\in S^{2N+1}$ are the images of (D_N,ϕ) and $(D_N,\tilde{\phi})$ under the bijection α. Furthermore, notice that this last condition is also equivalent to $\pi(\tilde{c})=\pi(c)$ in $\mathbb{CP}^N$, where $\pi:S^{2N+1}\to\mathbb{CP}^N$ is the usual principal $U(1)$-bundle.

Calling $\mathcal{M}_N$ the moduli space of solutions of (4) and (5) up to gauge transformations, and $p:\mathcal{D}\to\mathcal{M}_N$ the natural projection, we therefore have

$$\begin{array}{ccc}\mathcal{D} & \xrightarrow{\ \alpha\ } & S^{2N+1}\\ \downarrow p & & \downarrow\pi\\ \mathcal{M}_N & \xrightarrow{\ \tilde{\alpha}\ } & \mathbb{CP}^N\end{array} \tag{9}$$

where $\tilde{\alpha}$, defined by the commutativity of the diagram, is, like α, a bijection. The right-hand side of this diagram is a concrete model for the space of solutions $\mathcal{D}$ and its moduli space.

IV. THE METRIC ON THE MODULI SPACE

Using the usual prescriptions of the geodesic approximation (first described in Ref. 10), we will now obtain the metric m on $\mathcal{M}_N$ which, within the framework of this approximation, determines the dynamics of the "pseudo-vortices" (which from now on will be just called vortices).

Suppose one has a curve γ in $\mathcal{D}$:

$$t\overset{\gamma}{\mapsto}(D_N,\phi(t))\in\mathcal{D}\overset{\alpha}{\mapsto}(w_0(t),\ldots,w_N(t))\in S^{2N+1}\ .$$

A natural Hermitian metric on $\mathcal{D}$ is defined by

$$\left\langle \frac{d\gamma}{dt}, \frac{d\gamma}{dt} \right\rangle_{\gamma(t)} := \frac{1}{2} \int_{\mathbb{CP}^1} h(\dot{\phi}(t), \dot{\phi}(t)) \mathrm{vol}_R , \tag{10}$$

where the dot stands for the time derivative. Notice that in this case, as opposed to what happens in Ref. 12, the gauge potentials do not contribute to the metric, since the connection in our space $\mathcal{D}$ is fixed, and thus time independent.

Writing

$$\phi_1(t) = \frac{a_0(t)\, z^N + \cdots + a_N(t)}{(1+|z|^2)^{N/2}}$$

for the usual representative of $\phi(t)$, using the unitarity of ψ_1, and noting that $\dot{\phi}_1 = (1+|z|^2)^{-N/2}(\dot{a}_0 z^N + \cdots + \dot{a}_N)$, one has that

$$\begin{aligned} \left\langle \frac{d\gamma}{dt}, \frac{d\gamma}{dt} \right\rangle_{\gamma(t)} &= \frac{1}{2} \int_{\mathbb{C}} |\dot{\phi}_1|^2 \frac{2iR^2}{(1+|z|^2)^2} dz \wedge d\bar{z} \\ &= 2\pi R^2 \sum_{k=0}^{N} \frac{k!(N-k)!}{(N+1)!} \dot{a}_k \dot{\bar{a}}_k = 2\pi (R^2 - N) \sum_{k=0}^{N} \dot{w}_k \dot{\bar{w}}_k , \end{aligned}$$

again using the integral calculated in the Appendix. We conclude that the Hermitian L^2 metric on $\mathcal{D}$ corresponds via the map α to the restriction to S^{2N+1} of the canonical Hermitian metric on $\mathbb{C}^{N+1}$, up to the constant factor $2\pi(R^2-N)$. This metric will also be called $\langle \cdot, \cdot \rangle$.

According to the usual procedure, the metric m on $\mathcal{M}_N$ is induced from $\langle \cdot, \cdot \rangle$ on $\mathcal{D}$ in the following way. Given $q \in \mathcal{D}$ and a tangent vector $d\gamma/dt \in T_q\mathcal{D}$, let $(d\gamma/dt)_\perp$ be its component perpendicular to the subspace of $T_q\mathcal{D}$ formed by the vectors tangent to curves on $\mathcal{D}$ which are pure gauge transformations, that is, perpendicular to $\ker(p_*)_q$. Then

$$(p^* m)_q \left(\frac{d\gamma}{dt}, \frac{d\gamma}{dt} \right) := \left\langle \left(\frac{d\gamma}{dt} \right)_\perp , \left(\frac{d\gamma}{dt} \right)_\perp \right\rangle_q .$$

We will now compute the metric on $\mathbb{CP}^N$ corresponding to m by the identification $\tilde{\alpha}$. It will also be called m.

Using the diagram (9), the subspace $\ker(p_*)_q \subset T_q\mathcal{D}$ corresponds to the subspace $\ker(\pi_*)_{\alpha(q)} \subset T_{\alpha(q)} S^{2N+1}$. Given $w \in S^{2N+1} \subset \mathbb{C}^{N+1}$, we have that $\ker(\pi_*)_w$ is the one-dimensional real subspace generated by the vector $(d/dt)(e^{it}w)(0) = iw$. Therefore, given a tangent vector $d\gamma/dt = (\dot{\gamma}_0, \ldots, \dot{\gamma}_N) \in T_w S^{2N+1} \subset T_w \mathbb{C}^{N+1}$, we have

$$\left(\frac{d\gamma}{dt} \right)_\perp = \frac{d\gamma}{dt} - \frac{\langle d\gamma/dt, w \rangle}{\langle w, w \rangle} w,$$

so

$$\begin{aligned} \left\langle \left(\frac{d\gamma}{dt} \right)_\perp , \left(\frac{d\gamma}{dt} \right)_\perp \right\rangle_w &= \left\langle \frac{d\gamma}{dt}, \frac{d\gamma}{dt} \right\rangle - \frac{\langle d\gamma/dt, w \rangle \langle w, d\gamma/dt \rangle}{\langle w, w \rangle} \\ &= 2\pi (R^2 - N) \sum_{j,k=0}^{N} (\delta_{jk} - \bar{w}_j w_k)\, \dot{\gamma}_j \dot{\bar{\gamma}}_k , \end{aligned}$$

where the computation in the last step uses that $\langle w, w \rangle = 2\pi(R^2-N)$, since $w \in S^{2N+1}$. Thus $\pi^* m$ is the restriction to S^{2N+1} of the two-tensor in $\mathbb{C}^{N+1}$,

$$2\pi(R^2-N)\sum_{j,k=0}^{N}(\delta_{jk}-\overline{w}_j w_k)\,dw_j\otimes d\overline{w}_k.$$

Now consider the Kähler form μ associated to m. It is defined, as usual, using the imaginary part of m: $\mu=-\operatorname{Im} m\in\Omega^2(\mathbb{CP}^N,\mathbb{R})$. We have

$$\begin{aligned}
\pi^*\mu &= \pi^*(-\operatorname{Im} m)\\
&= -\operatorname{Im}(\pi^* m)\\
&= 2\pi(R^2-N)\frac{i}{2}\sum_{j,k=0}^{N}(\delta_{jk}-\overline{w}_j w_k)\,dw_j\wedge d\overline{w}_k\Big|_{S^{2N+1}}\\
&= 2\pi(R^2-N)\frac{i}{2}\sum_{j,k=0}^{N}\left(\frac{\delta_{jk}}{|w_0|^2+\cdots+|w_N|^2}-\frac{\overline{w}_j w_k}{(|w_0|^2+\cdots+|w_N|^2)^2}\right)dw_j\wedge d\overline{w}_k\Big|_{S^{2N+1}}\\
&= 2\pi(R^2-N)\frac{i}{2}\partial\overline{\partial}\log(|w_0|^2+\cdots+|w_N|^2)\Big|_{S^{2N+1}}\\
&= 2\pi(R^2-N)\,\pi^*\mu_{\mathrm{FS}},
\end{aligned}$$

where μ_{FS} is the Fubini–Study form on $\mathbb{CP}^N$, and the last equality is a well-known result (Ref. 8, p. 160). Since π and $(\pi_*)_w$ are both surjective,

$$\pi^*\mu=\pi^*(2\pi(R^2-N)\mu_{\mathrm{FS}})\qquad\text{implies}\qquad\mu=2\pi(R^2-N)\mu_{\mathrm{FS}}.$$

Therefore $m=2\pi(R^2-N)m_{\mathrm{FS}}$, where m_{FS} is the Fubini–Study metric on $\mathbb{CP}^N$, because a Hermitian metric is uniquely determined by its Kähler form.

V. VORTEX DYNAMICS

Having determined the metric m on the moduli space $\mathcal{M}_N\cong\mathbb{CP}^N$, we will now proceed to explicitly describe its geodesics, which provide an approximate description of the low-energy particle dynamics. Note that $m\propto m_{\mathrm{FS}}$ implies that the geodesics of m are exactly the Fubini–Study geodesics. These are well known (Ref. 8, p. 277) but nevertheless we will rederive them here.

Let $\pi:\mathbb{C}^{N+1}\backslash\{0\}\to\mathbb{CP}^N$ be the natural projection and $\chi_0:U_0\to\mathbb{C}^N$ one of the standard charts of $\mathbb{CP}^N$, where $U_0=\{[w^0,\ldots,w^N]\in\mathbb{CP}^N:w^0\neq 0\}$. Calling $(c^1,\ldots,c^N)$ the coordinate functions of this chart, then by definition of the Fubini–Study metric we have on U_0

$$\mu_{\mathrm{FS}}=\frac{i}{2}\partial\overline{\partial}\log(1+|c^1|^2+\cdots+|c^N|^2)=\frac{i}{2}h_{j\bar{k}}dc^j\wedge d\overline{c}^{\bar{k}}$$

and

$$m_{\mathrm{FS}}=h_{j\bar{k}}dc^j\otimes d\overline{c}^{\bar{k}},$$

with

$$h_{j\bar{k}}=\frac{\delta_{jk}}{1+|c|^2}-\frac{c^k\overline{c}^j}{(1+|c|^2)^2}.\tag{11}$$

For a general Kähler metric the geodesic equations have the simplified form (Ref. 14, p. 4):

$$\ddot{c}^k=-\frac{\partial h_{j\bar{s}}}{\partial c^l}h^{k\bar{s}}\dot{c}^l\dot{c}^j,\qquad\text{where}\qquad h^{k\bar{s}}:=(sk\ \text{entry of}\ [h_{i\bar{j}}]^{-1}).$$

In our case $h^{k\bar{s}}=(1+|c|^2)(\delta^{sk}+c^k\overline{c^s})$, and so the geodesic equations for $(\mathbb{CP}^N,m_{\mathrm{FS}})$ in the chart χ_0 are

$$\ddot{c}=\frac{2\langle\dot{c}\,,c\rangle}{1+\langle c\,,c\rangle}\dot{c}, \tag{12}$$

where $c(t)$ is a curve in $\mathbb{C}^N$ and $\langle\cdot\,,\cdot\rangle$ is the canonical Hermitian product.

Now consider curves in $S^{2N+1}\subset\mathbb{C}^{N+1}$ of the form

$$\gamma(t)=\sin(\omega t)\,y+\cos(\omega t)\,x, \qquad t\in\mathbb{R}, \tag{13}$$

where $x,y\in\mathbb{C}^{N+1}$ are orthonormal with respect to the canonical Hermitian product of $\mathbb{C}^{N+1}$. If $x^0\neq 0$, then $\pi\circ\gamma(t)\notin U_0$ only for a discrete set D of nonzero values of t, and a short computation shows that, in $\mathbb{R}\backslash D$,

$$c(t):=\chi_0\circ\pi\circ\gamma(t)=c(0)+\dot{c}(0)\frac{x^0\sin(\omega t)}{\omega(y^0\sin(\omega t)+x^0\cos(\omega t))}, \tag{14}$$

where

$$c^k(0)=\frac{x^k}{x^0} \quad\text{and}\quad \dot{c}^k(0)=\frac{\omega(y^kx^0-x^ky^0)}{(x^0)^2}, \qquad k=1,\ldots,N. \tag{15}$$

One can verify directly that this $c(t)$ satisfies (12), and therefore $\pi\circ\gamma(t)$ is a geodesic for t in $\mathbb{R}\backslash D$, and by continuity for all t. If $x^0=0$, a similar computation in one of the other standard charts of $\mathbb{CP}^N$ would establish that, also in this case, $\pi\circ\gamma(t)$ is a geodesic.

On the other hand, it is not difficult to verify that every geodesic of $(\mathbb{CP}^N,m_{\mathrm{FS}})$ can be written as $\pi\circ\gamma$, where γ has the form (13). Although one could give a general, chart-independent argument for this, for later convenience we will proceed unnaturally. Namely, using (15), one may simply check that given any $c(0)\in\mathbb{C}^N$ and $\dot{c}(0)\in T_{c(0)}\mathbb{C}^N\cong\mathbb{C}^N$, the geodesic $\pi\circ\gamma(t)$ with

$$\begin{aligned}
x&=(1+|c(0)|^2)^{-1/2}\ (\,1\,,c(0)\,),\\
y&=\omega^{-1}(1+|c(0)|^2)^{-1/2}\left(-\frac{\langle\dot{c}(0),c(0)\rangle}{1+|c(0)|^2},\ \dot{c}(0)-\frac{\langle\dot{c}(0),c(0)\rangle}{1+|c(0)|^2}c(0)\right),\\
\omega&=(1+|c(0)|^2)^{-1/2}\left(|\dot{c}(0)|^2-\frac{|\langle\dot{c}(0),c(0)\rangle|^2}{1+|c(0)|^2}\right)^{1/2},
\end{aligned} \tag{16}$$

has initial position and velocity $\chi_0^{-1}(c(0))$ and $(\chi_0^{-1})_*(\dot{c}(0))$, respectively. This shows that every geodesic starting in U_0 is of the form $\pi\circ\gamma(t)$. Similar calculations in the other standard charts would extend the result to all of $\mathbb{CP}^N$.

We now note two general properties of the geodesics $\pi\circ\gamma(t)$. First, using (11) and (15), one can compute that the velocity of the geodesic, which is a constant of motion, is $|\omega|$. Second, notice that all the geodesics of $(\mathbb{CP}^N,m_{\mathrm{FS}})$ are periodic. It is not difficult to show that for $\omega\neq 0$ the period is $\pi/|\omega|$.

We will now use our knowledge of the geodesics on the moduli space $(\mathbb{CP}^N,m)$ to give an explicit description of the vortex dynamics.

Recall from Sec. III that the solutions $(D_N\,,\phi)\in\mathcal{D}$ with the vortices (zeros of ϕ) in positions $\varphi_1^{-1}(z_1),\ldots,\varphi_1^{-1}(z_N)$ in $\mathbb{CP}^1$ are represented by a function ϕ_1 of the form (7), where we now have

$$a_0z^N+\cdots+a_N\propto(z-z_1)\cdots(z-z_N),$$

and therefore

$$a_k = A\,(-1)^k S_k(z_1,\ldots,z_N), \qquad k=0,\ldots,N,$$

where the S_j are the usual elementary symmetric polynomials, and A is a normalization factor which is nonzero for $R^2>N$. Thus such solutions $(D_N,\phi)\in\mathcal{D}$ correspond by $\pi\circ\alpha$ to [see (8)]

$$\left[\ \ldots,(-1)^k\left(\frac{k!(N-k)!}{(N+1)!}\right)^{1/2} S_k(z_1,\ldots,z_N),\ldots\ \right]_{0\leqslant k\leqslant N}\in\mathbb{CP}^N\cong\mathcal{M}_N$$

and by $\chi_0\circ\pi\circ\alpha$ to $c=(c^1,\ldots,c^N)\in\mathbb{C}^N$, where

$$c^k=(-1)^k\binom{N}{k}^{-1/2} S_k(z_1,\ldots,z_N). \tag{17}$$

Inverting these relations, we can obtain the positions of the N vortices as a function of the coordinates c^k of a given point in the moduli space $\mathbb{CP}^N$. In particular, to the geodesics $c(t)$ of the form (14) corresponds a motion of the vortices determined by

$$w^N+\sum_{k=1}^{N}\binom{N}{k}^{1/2} c^k(t)\,w^{N-k}=(w-z_1(t))\cdots(w-z_N(t)), \tag{18}$$

where the $z_i(t)$ are the coordinates of the vortices in the chart (φ_1,U_1) of $\mathbb{CP}^1$. Thus, since we know all the geodesics of $(\mathbb{CP}^N,m)$, we can determine all the possible N-vortex motions by finding the roots of polynomials of degree N—either analytically for $N\leqslant 4$ or numerically for $N>4$.

Now suppose we are given initial positions $z_i(0)$ and initial velocities $\dot z_i(0)$ for the vortices, where we assume that the $z_i(0)$ are all different. Through (17) and its derivative we can get the corresponding values $c(0),\dot c(0)\in\mathbb{C}^N$, then use (16) to determine which geodesic $c(t)$ corresponds to this initial data, and finally solve (18) to get the motions $z_i(t)$. This general procedure has been used to obtain the various special vortex motions shown below.

We remark that, because (17) is a local diffeomorphism only in the region where the vortices do not coincide, only in this region can we guarantee that the final result $z_i(t)$ has indeed the prescribed initial velocities. This is why we take the $z_i(0)$ all different. If the $z_i(0)$ are not all different, there are some values of $\dot z_i(0)$ that do not correspond to any $z_i(t)$ coming from a geodesic motion.

VI. EXAMPLES OF MOTIONS

Using the method described in the previous section, we now give a few examples of two- and three-vortex motions on the sphere. Figures 1–3 show the initial positions and trajectories in the complex plane via the stereographic projection $\varphi_1:S^2\backslash\{N\}\to\mathbb{C}$. The particular initial positions and velocities used in each case are listed in Table I.

To help with the interpretation of the figures, we recall that the stereographic projection has the property of mapping circles of S^2 (not necessarily great circles) to circles and straight lines in the plane. The inverse φ_1^{-1} has the converse property. Also the circle of unit radius is always shown as a dashed curve; the northern (southern) hemisphere of S^2 projects to the exterior (interior) of that circle.

During the motion shown in Fig. 3, the coordinate $c^1(t)$ of expressions (14) and (18) is always zero. The coordinate $c^2(t)$ is of the form $-a^2+2a(1+a^4)/[2a^3+i\omega\cot(\omega t)]$. Taking one of the roots $z(t)=x(t)+iy(t)$ of (18) and eliminating t from the system $x(t),y(t)$, one obtains that the trajectory on the plane has the simple equation $(x^2+y^2)^2+(1/a^2-a^2)(x^2-y^2)-1=0$. These are special cases of Cassini's ovals and, when projected back to the sphere, look like the joint of a tennis ball.

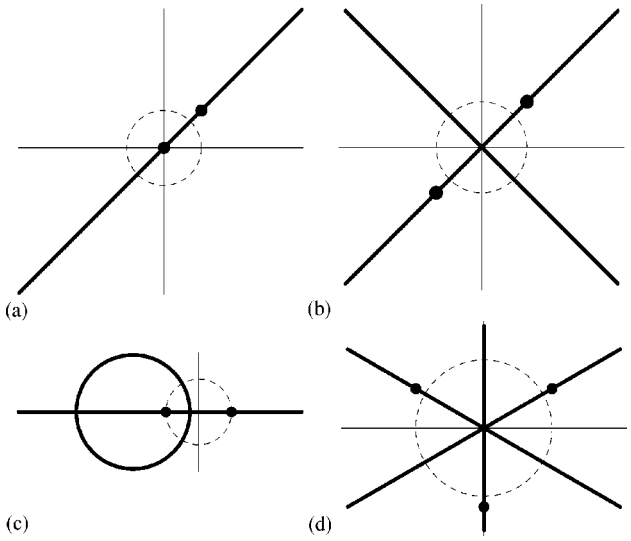

FIG. 1. (a) Two colliding vortices, one of which is at rest. One of the vortices describes a great circle on the sphere that passes through the static position of the other. (b) Head-on collision of two vortices with the same speed. There are two collisions at antipodal points. The total trajectory is the union of two great circles. (c) Head-on collision of two vortices with different initial speeds. Again two collisions occur. The total trajectory is the union of a great circle and another circle. (d) Symmetrical collision of three vortices with equal speeds. The three vortices collide twice at antipodal points. The total trajectory is the union of three great circles.

VII. COINCIDENT PARTICLES AND COLLISIONS

In this section we start by finding an algebraic condition which determines when a point in the moduli space $\mathcal{M}_N \cong \mathbb{CP}^N$ corresponds to a vortex configuration where at least two of the vortices coincide. We then use this condition to show that, for a system of N vortices starting in different positions with arbitrary initial velocities, there are at most $2N-2$ collisions during one period of the motion.

Using diagram (9) and the definition (8) of the bijection α, it is not difficult to recognize that a point $[w_0,\ldots,w_N] \in \mathbb{CP}^N$ corresponds by $\tilde{\alpha}^{-1}$ to the equivalence class in $\mathcal{M}_N$ of a solution ϕ represented by

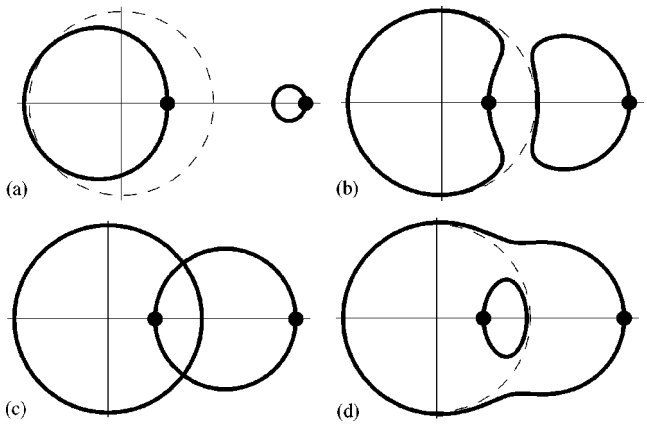

FIG. 2. (a),(b),(d) No collisions occur, and each vortex returns to its initial position after one period. (c) This degenerate case is the same as Fig. 1(c)—one great circle and another circle—in a different orientation.

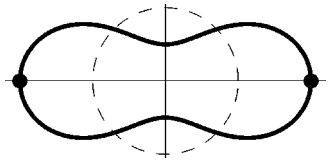

FIG. 3. (*with* $a=2$) No collision takes place and the vortices exchange positions after one period.

$$\phi_1(z) = A\,(1+|z|^2)^{-N/2} \sum_{k=0}^{N} \frac{w_k}{(k!(N-k)!)^{1/2}} z^{N-k},$$

where A is a nonzero normalization factor. Thus, asserting that $[w_0, \ldots, w_N]$ corresponds to a solution with at least two coincident vortices is equivalent to saying that one of the following conditions holds:

(i) $P(z) := \Sigma_{k=0}^{N}[w_k/(k!(N-k)!)^{1/2}]\, z^{N-k}$ has a root of multiplicity at least two;
(ii) $w_0 = w_1 = 0$, which corresponds to a double zero of ϕ at $[0,1] \in \mathbb{CP}^1$.

We now use the following result, whose proof is at the end of this section.

Lemma: For any $n \in \mathbb{N}$, *there is a homogeneous polynomial* S *in* $n+1$ *variables of degree* $2n-2$, *such that* $S(a_0,\ldots,a_n)=0$ *if and only if* $\Sigma_{k=0}^{n} a_k z^{n-k}$ *has a multiple root or* $a_0=a_1=0$.

An explicit formula for S is given in the proof and we note that, up to a sign, S coincides with the discriminant of $\Sigma_k a_k z^{N-k}$ whenever $a_0 \neq 0$.

Using this lemma, it is clear that the points $[w_0,\ldots,w_N] \in \mathbb{CP}^N$, which correspond to at least two coincident vortices, are exactly those of the algebraic hypersurface H of degree $2N-2$ in $\mathbb{CP}^N$ determined by the equation

$$\tilde{S}(\ldots,w_k,\ldots) := S\left(\ldots, \frac{w_k}{(k!(N-k)!)^{1/2}}, \ldots \right) = 0.$$

As we have seen in Sec. V, any motion of N vortices in S^2 corresponds to a Fubini–Study geodesic in $\mathbb{CP}^N$, and these are all of the form $t \mapsto \pi(\sin(\omega t)y + \cos(\omega t)x)$, with $x,y \in \mathbb{C}^{N+1}$ orthonormal and π being the projection from $\mathbb{C}^{N+1}$ to $\mathbb{CP}^N$. By the discussion above, it is also clear that this motion will have a collision of two or more vortices iff the corresponding geodesic intersects H. But since this geodesic lies on the projective line $L = \pi(\mathrm{span}_{\mathbb{C}}\{x,y\}) \subset \mathbb{CP}^N$, and does not intersect itself during one period, we conclude that the number of collisions is not bigger than the cardinality of $L \cap H$.

It is, however, a standard result in algebraic geometry that either $L \subset H$ or $\#(L \cap H) \leqslant \deg H = 2N-2$. In fact, denoting $x=(x_0,\ldots,x_N)$ and $y=(y_0,\ldots,y_N)$ in $\mathbb{C}^{N+1}$, it follows that a point $\pi(ux+vy)$ in L, with $(u,v) \in \mathbb{C}^2 \setminus \{0\}$, belongs to H iff

TABLE I. Initial positions and velocities.

	1(a)	**1(b)**	**1(c)**	**1(d)**	**2(a)**	**2(b)**	**2(c)**	**2(d)**	**3**
$\mathbf{z_1(0)}$	$1+i$	$1+i$	1	$-2i/\sqrt{3}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$a>0$
$\dot{\mathbf{z}}_1\mathbf{(0)}$	$-1-i$	$-1-i$	-3	$2i/\sqrt{3}$	i	i	i	i	i
$\mathbf{z_2(0)}$	0	$-1-i$	-1	$1+i/\sqrt{3}$	2	2	2	2	$-a$
$\dot{\mathbf{z}}_2\mathbf{(0)}$	0	$1+i$	1	$-1-i/\sqrt{3}$	$0.6\,i$	$3.7\,i$	$4\,i$	$4.5\,i$	$-i$
$\mathbf{z_3(0)}$	$\cdots$	$\cdots$	$\cdots$	$-1+i/\sqrt{3}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
$\dot{\mathbf{z}}_3\mathbf{(0)}$	$\cdots$	$\cdots$	$\cdots$	$1-i/\sqrt{3}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$

$$Q(u,v) := \widetilde{S}(ux_0+vy_0,\ldots,ux_N+vy_N)=0.$$

But since $\widetilde{S}$ is homogeneous of degree $2N-2$, so is Q, and therefore there is a factorization (see Ref. 7, p. 31)

$$Q(u,v)=\prod_{i=1}^{2N-2}(\alpha_i u+\beta_i v), \quad \text{for some } (\alpha_i,\beta_i)\in\mathbb{C}^2 .$$

If Q is identically zero we have $L\subset H$. If Q is not identically zero, then the roots of Q are $(\beta_i,-\alpha_i)\neq 0\,\forall i$, and it is apparent that $L\cap H$ consists of the points $\pi(\beta_i x-\alpha_i y)$, which are at most $2N-2$.

We finally conclude that, either the vortices have a motion with at least two of them coincident for all time, which corresponds to $L\subset H$, or there are at most $2N-2$ collisions in one period.

Proof of the lemma: This lemma is a slight generalization of well-known algebraic results, as stated for example in Ref. 5, p. 168, or Ref. 3, p. 178. Consider $P(z)=\Sigma_{k=0}^{n}a_k z^{n-k}$ and its derivative $P'(z)=\Sigma_{k=1}^{n}(n-k+1)a_{k-1}z^{n-k}$, and form the usual resultant

$$\mathcal{R}_{P,P'}(a_0,\ldots,a_n):=\begin{vmatrix} a_0 & & \cdots & a_n & & \\ & \ddots & & & \ddots & \\ & & a_0 & \cdots & & a_n \\ na_0 & & \cdots & a_{n-1} & & \\ & \ddots & & & \ddots & \\ & & na_0 & \cdots & & a_{n-1} \end{vmatrix}$$

where there are $n-1$ rows with the coefficients of P and n rows with the coefficients of P', so that the matrix is $(2n-1)\times(2n-1)$. Applying the usual expansion to the first column of this determinant we get

$$\mathcal{R}_{P,P'}(a_0,\ldots,a_n)=a_0\,S(a_0,\ldots,a_n)$$

with

$$S(a_0,\ldots,a_n) = \begin{vmatrix} a_0 & \cdots & & a_n & & \\ & \ddots & & & \ddots & \\ & & a_0 & \cdots & & a_n \\ (n-1)a_1 & \cdots & a_{n-1} & & & \\ na_0 & \cdots & & a_{n-1} & & \\ & \ddots & & & \ddots & \\ & & na_0 & \cdots & & a_{n-1} \end{vmatrix}$$

$$+(-1)^n n \begin{vmatrix} a_1 & \cdots & a_n & & & \\ a_0 & \cdots & & a_n & & \\ & & \ddots & & \ddots & \\ & & a_0 & \cdots & & a_n \\ na_0 & \cdots & & a_{n-1} & & \\ & \ddots & & & \ddots & \\ & & na_0 & \cdots & & a_{n-1} \end{vmatrix} .$$

Expanding again the first columns of the determinants in $S(0,a_1,\ldots,a_n)$ we get

$$S(0,a_1,\ldots,a_n)=(-1)^n(n-1)\,a_1\,\mathcal{R}_{Q,Q'}+(-1)^n n\,a_1\,\mathcal{R}_{Q,Q'}=(-1)^n(2n-1)\,a_1\,\mathcal{R}_{Q,Q'}$$

where $Q(z)=\Sigma_{k=1}^{n}a_k z^{n-k}$.

Now, if $a_0\neq 0$, by standard results in basic algebra (see Refs. 5 and 3),

$$\mathcal{R}_{P,P'}=(-1)^{n(n-1)/2}a_0\,D(P),$$

where $D(P)$ is the discriminant of P, and therefore

$$S(a_0,\ldots,a_n)=0\Leftrightarrow D(P)=0\Leftrightarrow P \text{ has a multiple root.}$$

If $a_0=0$, then $P(z)=Q(z)$ and

$$S(a_0,\ldots,a_n)=S(0,a_1,\ldots,a_n)=0\Leftrightarrow a_1=0 \text{ or } \mathcal{R}_{Q,Q'}=0.$$

But when $a_1\neq 0$, by the same algebraic results, $\mathcal{R}_{Q,Q'}=0\Leftrightarrow Q=P$ has a multiple root.

We finally conclude that

$$S(a_0,\ldots,a_n)=0\Leftrightarrow P \text{ has a multiple root or } a_0=a_1=0\,.$$

ACKNOWLEDGMENTS

N.S.M. thanks Michael Singer for discussions about the Fubini–Study metric, and also thanks the Pure Mathematics Department, University of Adelaide, for hospitality at the time this work was initiated. J.M.B. is supported by the "*Fundação para a Ciência e Tecnologia*," Portugal, through Research Grant No. SFRH/BD/4828/2001.

APPENDIX

In this appendix we compute integrals of the form

$$\int_{\mathbb{C}}\phi\,\overline{\psi}\frac{2iR^2}{(1+|z|^2)^2}\,dz\wedge d\overline{z}=\int_{\mathbb{R}^2}\phi\,\overline{\psi}\frac{4R^2}{(1+x^2+y^2)^2}\,dx\,dy,$$

where $\phi=(1+|z|^2)^{-N/2}(a_0z^N+\cdots+a_N)$ and $\psi=(1+|z|^2)^{-N/2}(b_0z^N+\cdots+b_N)$.

Write

$$\phi\,\overline{\psi}=\sum_{k,j=0}^{N}a_{N-j}\,\overline{b}_{N-k}\,f_{kj}(z),\quad \text{with}\qquad f_{kj}(z)=\overline{z}^k z^j(1+|z|^2)^{-N}\ .$$

Using polar coordinates and integration by parts,

$$\begin{aligned}I(k,j,N)&:=\int_{\mathbb{R}^2}\frac{f_{kj}(z)}{(1+|z|^2)^2}=\int_0^{2\pi}e^{i(j-k)\theta}\,d\theta\int_0^{\infty}\frac{r^{k+j}}{(1+r^2)^{N+2}}\,r\,dr\\&=2\pi\,\delta_{jk}\int_0^{\infty}\frac{r^{2k+1}}{(1+r^2)^{N+2}}\,dr\\&=\delta_{jk}\frac{-\pi}{N+1}\int_0^{\infty}r^{2k}\frac{d}{dr}\left(\frac{1}{(1+r^2)^{N+1}}\right)dr\\&=\delta_{jk}\frac{2k\pi}{N+1}\int_0^{\infty}\frac{r^{2k-1}}{(1+r^2)^{N+1}}\,dr=\delta_{jk}\frac{k}{N+1}I(k-1,k-1,N-1),\end{aligned}$$

where the vanishing of the boundary terms in the integration by parts is valid for $N\geqslant k\geqslant 1$. Since

$$I(0,0,N-k) = 2\pi \int_0^\infty \frac{r}{(1+r^2)^{N-k+2}}\, dr = \frac{-\pi}{N-k+1}\left[\frac{1}{(1+r^2)^{N-k+1}}\right]_0^\infty = \frac{\pi}{N-k+1},$$

we have

$$I(k,j,N) = \delta_{jk}\frac{k(k-1)\cdots 1}{(N+1)\cdots(N+2-k)}\ I(0,0,N-k) = \frac{k!(N-k)!}{(N+1)!}\,\pi\,\delta_{jk} \quad .$$

The final result is therefore

$$\int_{\mathbb{C}} \phi\,\overline{\psi}\frac{2iR^2}{(1+|z|^2)^2}\, dz\wedge d\overline{z} = 4R^2 \sum_{k=0}^{N} I(k,k,N)\, a_{N-k}\,\overline{b}_{N-k} = 4\pi R^2 \sum_{k=0}^{N} \frac{k!(N-k)!}{(N+1)!}\, a_k\,\overline{b}_k .$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

The moduli space of noncommutative vortices

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(Received 26 September 2002; accepted 9 April 2003)

The Abelian Higgs model on the noncommutative plane admits both BPS vortices and non-BPS fluxons. After reviewing the properties of these solitons, we discuss several new aspects of the former. We solve the Bogomoln'yi equations perturbatively, to all orders in the inverse noncommutivity parameter, and show that the metric on the moduli space of k vortices reduces to the computation of the trace of a $k\times k$-dimensional matrix. In the limit of large noncommutivity, we present an explicit expression for this metric. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1584525]

I. INTRODUCTION AND RESULTS

Vortices are enigmatic objects. Despite the apparent simplicity of the first order equations, no analytic expression for the solution has been found. Moreover, the metric on the moduli space, encoding the interactions of two or more vortices, remains unknown. This is in stark contrast to higher co-dimension solitons, such as monopoles and instantons, where seemingly more complicated equations readily yield results.

Progress may be made in the limit of far separated vortices. By considering the leading order forces experienced by moving vortices, Manton and Speight determined the asymptotic form of the low-energy dynamics.[1] Their expression contains an unknown coefficient that characterizes the exponential return to vacuum of the Higgs field. Although a direct analytic computation of this coefficient appears difficult, a prediction has been given based on T-duality in string theory,[2] and is in agreement with previous numerical results.[3]

Another approach to understanding the dynamics is to deform the background space on which the vortices live. A cunning choice of deformation may ensure that the Bogomoln'yi equations become tractable. For example, it was discovered long ago that the tricky vortex equation is replaced by Liouville's equation when the background is taken to be hyperbolic space.[4] Strachan subsequently showed that this simplification is sufficient to allow an explicit calculation of the moduli space metric.[5] More recently, Baptista and Manton considered the case of k vortices interacting on a sphere of area $A\sim 4\pi k$.[6] An analytic expression for the metric was given in the limit as the area of the sphere shrinks to a critical value, $A\rightarrow 4\pi k$. Curiously, in this limit, the vortex motion exhibits a symmetry enhancement, from the underlying SU(2) symmetry of the sphere to SU$(k+1)$. The physics behind this enhancement remains somewhat puzzling.

Here, we shall again deform the background space so that the dynamics of vortices becomes tractable. This time, we take space to be the flat, noncommutative plane. In two spatial dimensions, noncommutivity is rather natural since it breaks only the discrete parity symmetry, leaving the continuous rotational symmetry intact. Solitons in noncommutative geometry have been extensively studied in recent times (see Ref. 7 for reviews). In particular, aspects of vortices in the noncommutative Abelian Higgs model have been discussed in Refs. 8–10. As we shall review, noncommutivity yields a one-parameter family of metrics on the vortex moduli space, depending on γ, a dimensionless combination of the gauge coupling constant e^2, the Higgs expectation value v and the noncommutivity parameter θ,

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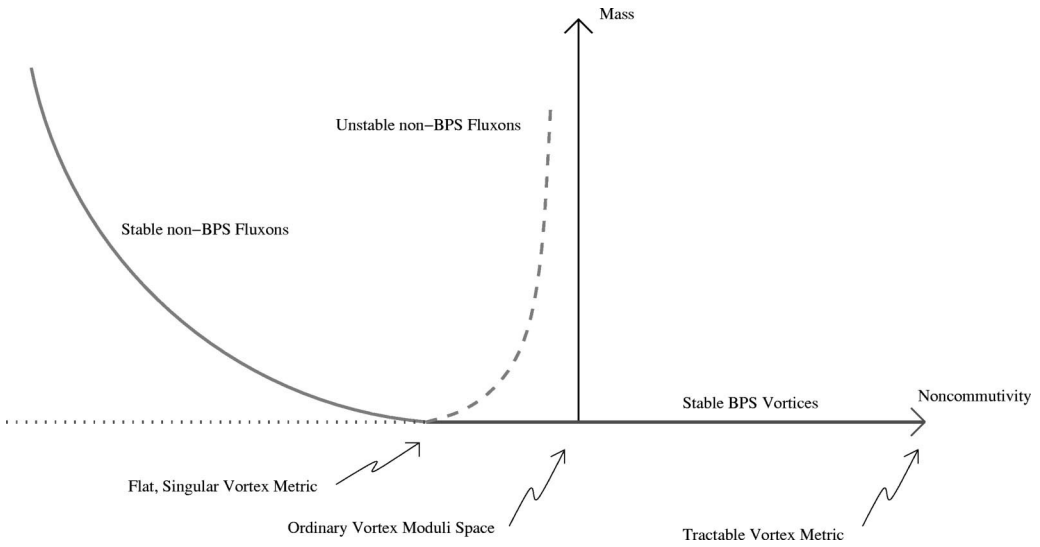

FIG. 1. The vortex phase diagram: BPS vortices exist for $-1\leqslant\gamma\leqslant\infty$, while non-BPS fluxons exist for $\gamma<0$, but are stable only for $\gamma\leqslant-1$.

$$\gamma=\theta e^2 v^2. \tag{1}$$

It was shown by Bak, Lee, and Park[9] that solutions to the Bogomoln'yi equations exist only for $-1\leqslant\gamma\leqslant+\infty$. At the critical point $\gamma=-1$, the vortex solutions coincide with the fluxon solutions discovered in Ref. 11. Here, the moduli space of vortices is endowed with the flat, singular metric on $\mathbf{C}^k/S_k$, and the moduli space approximation breaks down.[9] For $\gamma<-1$, there are no further solutions to the first order vortex equations, but the non-BPS fluxon solutions survive as localized solitons carrying magnetic flux. In contrast, for $-1<\gamma<0$, these non-BPS fluxon solutions are unstable to decay into the BPS vortices which have lower mass. For $\gamma>0$, only the BPS vortex solutions exist. This scenario, which was developed in Ref. 9, is summarized in Fig. 1.

Here we consider only $\gamma>0$, and present three, related, results. First, we derive a $2k$-parameter formal solution to the vortex equations as an all-orders perturbative expansion in γ^{-1}. For arbitrary γ, we then show that the metric on the moduli space of k vortices is given by the trace of a $k\times k$ matrix. This provides the noncommutative extension of Samols' expression in the ordinary commutative case.[12] Finally, in the limit $\gamma\to\infty$, we present an explicit expression for the metric on the moduli space of vortices. For k vortices centered at $z_a\in\mathbb{C}$, $a=1,\ldots,k$, the Kähler potential for the multi-cover of the moduli space is given by

$$\mathcal{K}=\log\det\exp(\overline{z}_a z_b). \tag{2}$$

Modding out by the permutation group S_k, exchanging the z_a, results in the true moduli space metric. This metric has appeared before in the study of noncommutative scalar solitons,[13–16] and we explain the similarities and differences with its appearance in the Abelian Higgs model.

The limit $\gamma\to\infty$ is customarily taken to mean large noncommutivity. However, as is clear from (1), it may also be taken to be the strong coupling limit $e^2\to\infty$, which is commonly used in the context of gauged linear sigma models. Indeed, as we shall see, it is only in this limit that the proper kinetic energy of the noncommutative vortices remains finite. In the ordinary, commutative, Abelian Higgs model, vortices become vanishingly small in this limit but, nevertheless, play an important role as singular worldsheet instantons.[17] We shall see that noncommutivity on the worldsheet resolves these singular vortices, in a manner similar to the resolution of singular U(1) Yang–Mills instantons.

II. THE VORTEX EQUATIONS

The Lagrangian of the Abelian Higgs model at critical coupling is

$$\mathcal{L}=-\frac{1}{4e^2}F_{ij}F^{ij}+\mathcal{D}_i\phi\mathcal{D}^i\phi-\frac{e^2}{2}(\phi\phi^\dagger-v^2)^2.$$

The model admits BPS vortices of mass $2\pi v^2 k$, for any positive integer k, satisfying the first order equations of motion,

$$F_{12}+e^2(\phi\phi^\dagger-v^2)=0,\ \mathcal{D}_{\bar{z}}\phi=0,\ \int F_{12}=2\pi k>0, \tag{3}$$

where we have introduced the complex structure $z=x_1+ix_2$ on the background space. Here we wish to consider the Abelian Higgs model defined on the noncommutative complex plane, such that

$$[z,\bar{z}]=2\theta.$$

It is common practice (see Ref. 7) to take z to be an operator on the Hilbert space $\mathcal{H}$, isomorphic to the Hilbert space of a single harmonic oscillator. We define the usual creation and annihilation operators, satisfying $[a,a^\dagger]=1$, whose action on the orthonormal basis $|n\rangle=0,1,2,\ldots$ is given by

$$a|n\rangle=\sqrt{n}|n-1\rangle,\qquad a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle.$$

For $\theta>0$, the action of all spatial operators may thus be reexpressed as

$$z=\sqrt{2\theta}a,\quad \partial_z\cdot=-\frac{1}{\sqrt{2\theta}}[a^\dagger,\cdot],\quad \int d^2x=2\pi\theta\mathrm{Tr},$$

where Tr is the trace over $\mathcal{H}$. Complex conjugation of the space–time coordinate z is identified with Hermitian conjugation of operators on $\mathcal{H}$. The fields A_z and ϕ are themselves promoted to operators on $\mathcal{H}$. To simplify the equations, we rescale the Higgs field $\phi\to v\phi$, and decompose the gauge potential operator as

$$A_z=\frac{i}{\sqrt{2\theta}}(a^\dagger+C^\dagger).$$

The advantage of this notation is that the magnetic field F_{12} is independent of a and $a^\dagger$, and the vortex equations (3) become the operator equations,

$$1+[C^\dagger,C]=\gamma(\phi\phi^\dagger-1),$$

$$\phi a+C\phi=0, \tag{4}$$

$$\mathrm{Tr}(1+[C^\dagger,C])=-k<0.$$

As promised, the equations depend only on the dimensionless combination $\gamma=\theta e^2v^2$. They are valid only for $\gamma>0$. The rest of this article will be devoted to analyzing these equations. However, for completeness, we first mention the extension to $\theta<0$. Defining $z=\sqrt{-2\theta}a^\dagger$, and $A_z=-i(a+C)/\sqrt{-2\theta}$, we have

$$1+[C^\dagger,C]=\gamma(\phi\phi^\dagger-1),$$

$$\phi a^\dagger+C^\dagger\phi=0, \tag{5}$$

$$\mathrm{Tr}(1+[C^\dagger,C])=+k>0.$$

As depicted in Fig. 1, while the equations (4) are thought to have solutions for all $\gamma>0$,[8] Eqs. (5) have solutions only for $-1\leqslant\gamma\leqslant 0$.[9,10]

Note that under a CP transformation, which is a symmetry of the theory, vortices are mapped to antivortices, while $\theta\to-\theta$. The phase diagram for antivortices is therefore given by reflecting Fig. 1 in the vertical axis. The theory admits both BPS vortex and BPS antivortex solutions only for $|\gamma|\leqslant 1$.

III. THE SOLUTION

We turn now to the solution of the vortex equations (4). Perturbative progress can be made when the dimensionless parameter γ is large. For coincident vortices, the solution to first order in $1/\gamma$ was given in Ref. 8. Here we present an iterative solution, for arbitrary vortex positions, to all orders in $1/\gamma$.

Let us first consider the limit $\gamma\to\infty$. The first equation in (4) now simply becomes $\phi_0\phi_0^\dagger=1$, which can be partially inverted to give

$$\phi_0^\dagger\phi_0=(1-P),$$

where P, a projection operator on $\mathcal{H}$, determines the kernel of ϕ_0: $Ker(\phi_0)=P\mathcal{H}$. In this limit, the gauge potential is given by $C_0=-\phi_0 a\phi_0^\dagger$. After some manipulation, the second and third vortex equations (4) give further constraints on P,

$$(1-P)aP=0,\ \mathrm{Tr}P=k. \tag{6}$$

(In analyzing this final equation, it appears necessary to employ a suitable regularization of the trace over $\mathcal{H}$. We choose $Tr_N\cdot\equiv\Sigma_{n=1}^N\langle n|\cdot|n\rangle$, subsequently taking the limit $N\to\infty$.) Thus the kernel of ϕ_0 is constrained to be a k-dimensional eigenspace of the annihilation operator a. Eigenvectors of a are provided by the coherent states,

$$|z\rangle=\exp(za^\dagger)|0\rangle=\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle,$$

which satisfy $a|z\rangle=z|z\rangle$ for any $z\in\mathbb{C}$. Thus, in general, solutions to the vortex equations in the limit $\gamma\to\infty$ are parametrized by k complex vectors $|z_a\rangle$, $a=1,\ldots,k$, spanning $P\mathcal{H}$, with

$$P=\sum_{a,b=1}^{k}|z_a>(h^{-1})^{ab}\langle z_b|, \tag{7}$$

where the overlap matrix h is defined by

$$h_{ab}=\langle z_a|z_b\rangle=\exp(\overline{z}_a z_b). \tag{8}$$

We therefore find a $2k$ (real) parameter family of solutions. Hearteningly, the number of moduli is in agreement with the ordinary, commutative, vortex equations.[18] In the limit of far-separated vortices, we may think of the z_a as the positions of k unit-flux solitons. Note that this description of $P\mathcal{H}$ becomes singular in the limit as $|z_a\rangle\to|z_b\rangle$ for $a\neq b$. However, as explained nicely in Ref. 15, the underlying eigen-subspace remains smooth in this limit, and is spanned by $|z_a\rangle$ and $a^\dagger|z_a\rangle$.

To extend this analysis away from the $\gamma\to\infty$ limit, we make the expansion

$$\phi=\sum_{m=0}^{\infty}\gamma^{-m}\phi_m, \qquad C=\sum_{m=0}^{\infty}\gamma^{-m}C_m.$$

The resulting iterative equations do not immediately determine the action of ϕ_1 on the eigenspace $P\mathcal{H}$. To resolve this, we make the ansatz that the kernel of ϕ is independent of γ. In other words,

$$\mathrm{Ker}(\phi)=P\mathcal{H}.$$

I have not been able to derive this explicitly from (4), but have been unable to find solutions in which it is not the case. Proceeding with this assumption, we may express the solution to (4) as

$$C_m=-\phi_0 d_m\phi_0^\dagger, \qquad \phi_m=\phi_0\psi_m(1-P),$$

where the operator coefficients ψ_m and d_m are determined by induction, starting from $\psi_0=1$, and with

$$\begin{aligned} d_m&=\psi_m a+\sum_{l=0}^{m-1} d_l(1-P)\psi_{m-l},\\ \psi_m&=\frac{1}{2}(1-P)\sum_{l=0}^{m-1}(d_l^\dagger(1-P)d_{m-l-1}-d_{m-l-1}(1-P)d_l^\dagger)-\frac{1}{2}\sum_{l=1}^{m-1}\psi_l\psi_{m-l}^\dagger. \end{aligned} \tag{9}$$

To summarize, this perturbative solution is uniquely determined by a choice of projector (7) from among the $2k$ parameter family of suitable projectors. An important, open, problem is to determine the radius of convergence of this expansion.

IV. THE LOW-ENERGY DYNAMICS

Let us turn now to the low-energy dynamics of the noncommutative vortices. As usual, we consider the moduli space approximation, in which only the collective coordinates z_a, which determine the projection operator P, are allowed to vary in time. The linearized Bogomoln'yi equations (4) are

$$\begin{aligned} [\dot{C}^\dagger,C]+[C^\dagger,\dot{C}]&=\gamma(\dot{\phi}\phi^\dagger+\phi\dot{\phi}^\dagger),\\ \dot{\phi}a+\dot{C}\phi+C\dot{\phi}&=0, \end{aligned} \tag{10}$$

and are to be augmented with Gauss' law, the equation of motion for A_0. In our operator notation, this reads

$$-[\dot{C}^\dagger,C]+[C^\dagger,\dot{C}]=\gamma(\dot{\phi}\phi^\dagger-\phi\dot{\phi}^\dagger), \tag{11}$$

which can therefore be combined with the first of the Bogomoln'yi equations to give

$$[C^\dagger,\dot{C}]=\gamma\dot{\phi}\phi^\dagger.$$

The low-energy dynamics of the solitons is inherited from the kinetic energy terms of the original field theory in the standard Manton manner,

$$T=2\pi\theta v^2\mathrm{Tr}\left(\frac{1}{\gamma}\dot{C}^\dagger\dot{C}+\dot{\phi}^\dagger\phi\right)\equiv 2\pi\theta v^2 g_{ab}(z)\dot{z}^a\dot{\bar{z}}^b. \tag{12}$$

In the second equality above, we have anticipated the Kählerity of the metric. This property is guaranteed by supersymmetry. To see this, a standard trick is to embed the theory in one with

maximal supersymmetry, living in the maximal space–time dimension. The Abelian Higgs model may be embedded in a $d=5+1$ dimensional theory which is endowed with $\mathcal{N}=1$ supersymmetry (or eight supercharges). The vortex solutions under consideration now become BPS three-branes which preserve half of the supersymmetry. The addition of noncommutivity in two, transverse, spatial directions does not alter this fact, and the low-energy dynamics is thus described by a $d=3+1$, $\mathcal{N}=1$ (four supercharges) nonlinear sigma-model with target space given by the noncommutative vortex moduli space. The metric on the target space is necessarily Kähler.

We start our analysis of the moduli space metric by once again taking the limit $\gamma\to\infty$. As is clear from (12), the low-energy Lagrangian remains finite if we interpret this as $e^2\to\infty$. Since the kinetic terms for the gauge field become negligible in this limit, we have simply

$$\frac{T_0}{2\pi\theta v^2}=\mathrm{Tr}\ \dot{\phi}_0^\dagger\dot{\phi}_0.$$

From (10) and (11) we find that $\dot{\phi}_0=\dot{\phi}_0 P=-\phi_0\dot{P}$, from which we derive the low-energy dynamics purely in terms of the projection operator P,

$$\frac{T_0}{2\pi\theta v^2}=\mathrm{Tr}\ P\ \dot{\phi}_0^\dagger\dot{\phi}_0=\frac{1}{2}\mathrm{Tr}\ \dot{P}\dot{P}. \tag{13}$$

From the definition of the projection operator (7) in terms of the overlap matrix (8) it is simple to derive the explicit form of the metric,

$$\frac{T_0}{2\pi\theta v^2}=\mathrm{tr}\,(\partial_a\overline{\partial_b}\log h)\,\dot{z}^a\dot{\bar{z}}^b, \tag{14}$$

where tr denotes the trace over the $k\times k$ matrix indices of h. The Kähler potential is therefore given by the expression (2) as promised. The expressions (13) and (14) have appeared before in the context of noncommutative solitons.[13–16] Let us pause briefly to review that work and explain the differences with the present case. The seminal work[13] considered pure scalar field theories in noncommutative space–times. It was shown that, in the limit $\theta\to\infty$, *any* projection operator solves the equation of motion. To proceed to finite theta one may work, as we have above, perturbatively in $1/\tilde{\gamma}=1/m^2\theta$ where m is some mass scale of the theory. It was shown that, at first order in $1/\tilde{\gamma}$, only some projection operators survive as solutions to the equations of motion.[15,16] These are precisely those operators satisfying (6) above. At next-to-leading order in $1/\tilde{\gamma}$, these projectors too are lifted, and only isolated solutions remain. This scenario left certain aesthetic puzzles. For example, it was unclear why, *a priori*, the moduli space need be Kähler since the original field theory could not be embedded in a supersymmetric context and the solitons were not BPS. Moreover, the relevant solitons were not the most general solutions to any equations of motion, but rather the surviving approximate solutions at first order in perturbation theory.

In contrast, the appearance of the moduli space in the current context is more natural. It now appears at *zeroth* order in perturbation theory, rather than first, and the solitons are therefore solutions to certain equations of motion (namely those derived in the strict $\gamma\to\infty$ limit). Furthermore, as explained above, the Kähler nature of the target space finds an explanation in terms of supersymmetry.

The explicit metric for noncommutative vortices may be easily extracted from (14). For $k\geqslant 3$, the algebra becomes somewhat entangled, but for $k=2$ it is simple and was given previously in Refs. 14–16. Factoring off an overall center of mass, we have the relative moduli space described in terms of the separation $z=z^1-z^2$ with metric,

$$ds^2=\left(\frac{1}{2}\coth(|z|^2/2)-\frac{|z|^2}{4\sinh^2(|z|^2/2)}\right)dz\,d\bar{z}.$$

Since the two vortices are indistinguishable, we should orbifold this space by the Z_2 action $z \to -z$. It is simple to see that this renders the metric nonsingular at the origin $z=0$.

We would like to extend this discussion beyond the $\gamma \to \infty$ limit. One may consider proceeding by calculating the contributions to the low-energy dynamics perturbatively in $1/\gamma$. Unlike the case of scalar field theories, where these effects induce a potential on the moduli space,[15,16] for the case of vortices they merely correct the metric on the moduli space. The leading order contribution is given by $T = T_0 + T_1/\gamma$ where

$$\frac{T_1}{2\pi\theta v^2} = \mathrm{Tr} P(\dot{P}\dot{P}a(1-P)a^\dagger - a(1-P)\dot{P}\dot{P}a^\dagger).$$

However, this perturbative path appears tedious and illuminates little.

Instead, we finish by deriving the noncommutative extension of Samols' localization theorem.[12] Recall that Samols analyzed the dynamics of k vortices in the ordinary, commutative, Abelian Higgs model. Upon integrating the usual overlap of zero modes over the complex plane, he found that all contributions vanish apart from those arising at the k zeroes of the Higgs field.

Examining our expressions for T_0 and T_1 above, we see that a similar phenomenon has occurred. The trace over the infinite dimensional Hilbert space $\mathcal{H}$ has been reduced to a more manageable trace over a k-dimensional subspace $P\mathcal{H}$. Here we show that this property holds for all values of γ. In order to derive this result, I have found it necessary to introduce the operator ϕ^{-1}. Since $\mathrm{Ker}(\phi) \neq 0$, we must define this operator with care. We require,

$$\phi\phi^{-1} = 1, \quad \phi^{-1}\phi = 1 - P.$$

While the existence of such an operator in not guaranteed for all γ, it is a simple matter to construct it explicitly within the perturbative context of the solution (9),

$$\phi^{-1} = \sum_{m=1}^{\infty} \gamma^{-m} \tilde{\psi}_m \phi_0^\dagger,$$

where the operators $\tilde{\psi}_m$ are defined iteratively as $\tilde{\psi}_0 = 1$ and $\tilde{\psi}_1 = -\psi_1$ with the remainder given by $\tilde{\psi}_m = -\Sigma_{l=1}^m \psi_l \tilde{\psi}_{m-l}$. The result below is therefore only strictly valid for γ within the radius of convergence of the series (9). Wielding this operator allows us to invert the Bogomoln'yi equation to $C = -\phi a \phi^{-1}$, supplying the leverage necessary to pry open the expression for the kinetic energy (12). A little algebra reveals the final result,

$$T = 2\pi\theta v^2 \ \mathrm{Tr}\ P\left(\dot{\phi}^\dagger\dot{\phi} - \frac{1}{\gamma} a \phi^{-1}\dot{C}^\dagger\dot{\phi} \right),$$

which indeed reduces to the trace over the k-dimensional subspace $P\mathcal{H}$ as advertised.

ACKNOWLEDGMENTS

Thanks to Jan Troost and Ashwin Vishwanath for stimulating discussions. I am supported by a Pappalardo fellowship, and thank the Pappalardo family for their generosity. This work was also supported in part by funds provided by the U.S. Department of Energy (D.O.E.) under cooperative research agreement No. DF-FC02-94ER40818.

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A note on monopole moduli spaces

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(Received 10 December 2002; accepted 9 April 2003)

We discuss the structure of the framed moduli space of Bogomolny monopoles for arbitrary symmetry breaking and extend the definition of its stratification to the case of arbitrary compact Lie groups. We show that each stratum is a union of submanifolds for which we conjecture that the natural L^2 metric is hyper-Kähler. The dimensions of the strata and of these submanifolds are calculated, and it is found that for the latter, the dimension is always a multiple of four. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1590056]

I. INTRODUCTION

Recently there has been much interest in monopoles with nonmaximal symmetry breaking at infinity. In particular questions have been raised as to when they are manifolds and when they have hyper-Kähler metrics. This note gathers together some mathematical results concerning the structure of the moduli spaces and their L^2 metrics. These range from theorems which have been proved in full generality through partially proved theorems to outright conjectures.

Recall that we generally expect that moduli spaces of solutions of the self-duality equations and their reductions such as the Bogomolny equations and Nahm's equations should be hyper-Kähler manifolds. One reason for this is that formally such moduli spaces arise as hyper-Kähler quotients. To recall this, fix a compact, connected Lie group G, with Lie algebra $\mathfrak{g}$, and consider the space $\mathcal{A}$ of G-connections (vector potentials) on the trivial G-bundle over flat $\mathbb{R}^4$. By identifying

$$A_0 dx_0 + A_1 dx_1 + A_2 dx_2 + A_3 dx_3$$

with the $\mathfrak{g}\otimes\mathbb{H}$-valued function

$$A_0 + iA_1 + jA_2 + kA_3,$$

where i, j, and k are unit quaternions, $\mathcal{A}$ becomes a quaternionic vector space. Formally, $\mathcal{A}$ can be equipped with the L^2 metric, making it a flat hyper-Kähler manifold. Because $\mathbb{R}^4$ is not compact, the convergence of this metric will depend upon subjecting our connections to suitable asymptotic conditions, and these will be considered in detail below. Setting this aside for the moment, it is a straightforward exercise to check that the hyper-Kähler moment map for the action of the gauge group $\mathcal{G}$ on $\mathcal{A}$ is given by

$$A \mapsto F_A^+ \in \Omega^2(X, \mathfrak{g}) \otimes \mathrm{Im}\,\mathbb{H}.$$

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Hence the hyper-Kähler quotient $\mathcal{A}///\mathcal{G}$ should be the same as the space of anti-self-dual connections divided by the action of the gauge group, and the L^2-metric will descend to define a hyper-Kähler metric on the moduli space.

A monopole on $\mathbb{R}^3$ is a pair $c=(A,\Phi)$, where A is a connection on the trivial G-bundle $E \to \mathbb{R}^3$, and Φ is a section of the adjoint bundle $E\times_G\mathfrak{g}$. The monopole c satisfies the Bogomolny equations

$$\mathrm{d}_A\Phi = *F_A \tag{1.1}$$

if and only if the connection $\Phi dx_0 + A$ is anti-self-dual on $\mathbb{R}\times\mathbb{R}^3$. In particular, from this four-dimensional point of view, Φ cannot vanish at infinity, because it is independent of x_0. Thus the convergence of the L^2 metric and the nondegeneracy of the hyper-Kähler symplectic forms are important issues in this case.

These issues were fully resolved when $G=\mathrm{SU}(2)$ by Atiyah and Hitchin:[2] they showed that the moduli space of (framed) monopoles of charge k is, indeed, a complete hyper-Kähler manifold. Its dimension is $4k$ where the charge of the monopole is k.

For a general compact Lie group of rank r it is expected that the moduli space of monopoles with *maximal symmetry* breaking is a hyper-Kähler manifold although this has not been proved in generality. Except for very simple low charge cases, there are mostly partial results which compute the metric asymptotically near the edge of the moduli space; see, for example, Refs. 4, 5, and 17, and references therein.

The real complications, however, arise when there is *nonmaximal symmetry breaking* which is our primary interest below. The case of SU(3) monopoles with minimal symmetry breaking was treated in detail in Ref. 7, but beyond this little seems to be known.

We shall present here a summary of the results discussed in the article: the reader will have to refer forward for precise definitions.

The full moduli space of (framed) monopoles of mass μ and charge m is denoted by $\mathcal{M}(u,\mu,[\phi]=m)$. Here $0\neq\mu\in\mathfrak{g}$ is arbitrary (*maximal* symmetry breaking is precisely the condition that μ should be regular) and u is a unit vector in $\mathbb{R}^3$. m is a homotopy class, essentially a string of integers. The boundary conditions imposed guarantee that for some $k\in\mathfrak{g}$,

$$\Phi(tu)=\mu-\frac{k}{2t}+o(t^{-1}) \quad \text{for} \quad t\gg 0. \tag{1.2}$$

There is therefore a map $e:\mathcal{M}(u,\mu,[\phi]=m)\to\mathfrak{g}$ which assigns k to (A,Φ). The image $\mathcal{K}$ of e in $\mathfrak{g}$ is not the whole of $\mathfrak{g}$, but rather a disjoint union of $C(\mu)$-orbits

$$\mathcal{K}=C(\mu)k_1\cup C(\mu)k_2\cup\cdots\cup C(\mu)k_n. \tag{1.3}$$

It turns out that the k_j are *integral* elements of $\mathfrak{g}$. The set of all monopoles (A,Φ) with $e(A,\Phi)\in C(\mu)k_j$ is the jth stratum $\mathcal{M}_j$, say, of the moduli space. This was defined in a different way for $G=\mathrm{SU}(r+1)$ in Ref. 19. In general, $\mathcal{M}_j$ does not have dimension divisible by 4, so it cannot be hyper-Kähler. However, if we define, for $k\in\mathcal{K}$,

$$\mathcal{M}(u,\mu,k)=\{(A,\Phi)\in\mathcal{M}(u,\mu,[\phi]=m):e(A,\Phi)=k\} \tag{1.4}$$

[the moduli space of framed monopoles of *type* (μ,k)], then we shall see that $\mathcal{M}(u,\mu,k)$ has dimension divisible by 4 and the natural conjecture is that the L^2 metric makes $\mathcal{M}(u,\mu,k)$ into a hyper-Kähler manifold.

At least one of the strata, $\mathcal{M}_1$, say, must be open, hence of the same dimension as $\mathcal{M}(u,\mu,[\phi]=m)$, but this stratum need not be hyper-Kähler. If, however, $C(\mu)k_1=k_1$, then $\mathcal{M}_1=\mathcal{M}(u,\mu,k_1)$ and then this stratum *is* a candidate to be hyper-Kähler. Notice more generally that if k and k' lie in $C(\mu)k_j$, an element $g\in C(\mu)$ with $\mathrm{ad}(g)k=k'$ can be regarded as a constant gauge transformation which maps $\mathcal{M}(u,\mu,k)$ diffeomorphically to $\mathcal{M}(u,\mu,k')$.

In Sec. IV, magnetic charges $m_1,\ldots,m_s$ and holomorphic charges $h_1,\ldots,h_{r-s}$ are defined for monopoles in $\mathcal{M}(u,\mu,k)$. The information in the magnetic charges is topological and is equivalent to the homotopy class m. In particular, the magnetic charges do not vary from stratum to stratum. By contrast the holomorphic charges determine the stratum $\mathcal{M}_j$. (The number s of magnetic charges is completely determined by the mass μ.)

We shall show that if $\mathcal{M}(u,\mu,k)$ is nonempty, then the charges are all nonnegative, and that

$$\dim \mathcal{M}(u,\mu,k)=4(m_1+\cdots+m_s+h_1+\cdots+h_{r-s}). \tag{1.5}$$

Dimensions of the strata and full moduli space are also determined in Sec. VI.

II. THE MODULI SPACE AS A MANIFOLD

In this section we shall introduce various different monopole moduli spaces and explain carefully which of them are smooth manifolds, and which are likely to admit hyper-Kähler metrics. Throughout we shall be considering *Euclidean* monopoles, that is to say, monopoles on flat $\mathbb{R}^3$. Note that the metric enters the Bogomolny equation (1.1) through the Hodge star operator. Some work has also been done on hyperbolic monopoles, where $\mathbb{R}^3$ is replaced by hyperbolic three-space $\mathcal{H}^3$. It is expected that moduli spaces of hyperbolic monopoles will be diffeomorphic to the corresponding moduli spaces of Euclidean monopoles, but this has not been proved in general. On the other hand, the issue of natural metrics on moduli spaces of hyperbolic monopoles is completely open: all that is known for certain is that the L^2 metric is infinite in this case.

There are two reasons why there are so many different monopole moduli spaces. The first is that the monopoles must be *framed*, and this can be done either at a base-point in $\mathbb{R}^3$ or "at infinity." The second has to do with the specification of the asymptotics of the Higgs field Φ.

A. Notation

In order to discuss monopoles, we shall fix the following:

(i) G is a compact, connected, semi-simple Lie group of rank r. The complexification is denoted G^c and Lie algebra $\mathfrak{g}$.
(ii) If $a\in\mathfrak{g}$, $O_a\subset\mathfrak{g}$ is the orbit of a in $\mathfrak{g}$ under the adjoint action of G. $C(a)\subset G$ is the centralizer of a, with Lie algebra $\mathfrak{c}(a)$.
(iii) As a homogeneous space, $O_a=G/C(a)=G^c/P_a$, where P_a is the appropriate parabolic subgroup. The latter description gives O_a the structure of a compact complex manifold.
(iv) μ and k are commuting elements of $\mathfrak{g}$, $[\mu,k]=0$.
(v) $E\to\mathbb{R}^3$ will denote the trivial principal G-bundle over $\mathbb{R}^3$.

B. Boundary conditions and moduli spaces

The physically natural condition to impose on a solution of the Bogomolny equations is the finite-energy condition

$$\int |F_A|^2=\int |\mathrm{d}_A\Phi|^2<\infty. \tag{2.1}$$

We shall impose apparently rather stronger asymptotic conditions. It follows from the work of Taubes if $G=\mathrm{SU}(2)$, that (2.1) together with (1.1) implies these stronger conditions, but for general groups this must remain a conjecture.

Following Jarvis, we assume the following.

(BC1) Along each straight line, there is a gauge in which

$$\Phi=\mu-\frac{k}{2r}+O\left(\frac{1}{r^{1+\delta}}\right)$$

for all sufficiently large r.

(BC2) In this same gauge,

$$d_A\Phi = \frac{k}{2r^2}\,dr + O\left(\frac{1}{r^{2+\delta}}\right)$$

for all sufficiently large r.

These conditions are closely related to the Bogomolny–Prasad–Sommerfield (BPS) boundary conditions of Ref. 12.

Define

$$\mathcal{C} = \{(A,\Phi): d_A\Phi = *F_A,\ \ (A,\Phi) \text{satisfies BC1 and BC2}\}.$$

Notice that we do not yet fix μ and k: we merely assert that the boundary conditions are satisfied for *some* elements μ and k satisfying

$$\mu \neq 0, \quad [\mu,k] = 0. \tag{2.2}$$

Denote by $\mathcal{G}$ the group of all automorphisms g of E that preserve the boundary conditions (i.e., g and ∇g have limits as r goes to infinity along any straight line, and the limiting values are continuously differentiable when viewed as functions on the sphere at infinity). Then $\mathcal{G}$ acts on $\mathcal{C}$ and we would like to define the monopole moduli space as the quotient $\mathcal{M} = \mathcal{C}/\mathcal{G}$. This will have singularities because $\mathcal{G}$ does not act freely. In addition it will contain components of arbitrarily high dimension. We shall now explain how these two problems are eliminated.

C. The degree of a monopole

The asymptotic value of Φ is a section ϕ, say, of $\mathrm{ad}(E_\infty)$, where E_∞ is the restriction of E to the two-sphere at infinity. Since $\mathrm{ad}(E_\infty)$ is a trivial bundle, we can view ϕ as a continuous map into $\mathfrak{g}$. By BC1, this takes values in the adjoint orbit O_μ. This orbit is preserved by the action of gauge transformations g on E_∞, but $g(\phi) = \mathrm{ad}(g)\phi$, so that this map is not gauge-invariant. However, its homotopy class $m = [\phi]$ *is* gauge invariant, because $\pi_2(G) = 0$, so that any gauge transformation can be deformed to the identity. The homotopy class m is called the *degree* of the monopole. This discussion suggests the definition of spaces

$$\mathcal{C}(O_\mu, [\phi] = m),$$

where the adjoint orbit as well as the homotopy class of ϕ are fixed. This is referred to as the set of monopoles of mass μ and charge m. Note that $O_\mu = G/C(\mu)$.

D. Radial scattering and interior framing

Let $x \in \mathbb{R}^3$ be any point. The moduli space of monopoles framed at x, of mass μ and charge m, is the quotient

$$\mathcal{M}(x, O_\mu, [\phi] = m) = \mathcal{C}(O_\mu, [\phi] = m)/\mathcal{G}(x),$$

where

$$\mathcal{G}(x) = \{g \in \mathcal{G}: g(x) = 1\}.$$

In Ref. 15 Jarvis proved the following:

Theorem 2.1: *There is a natural bijection*

$$r_x : \mathcal{M}(x, O_\mu, [\phi] = m) \to \mathcal{R}(O_\mu, m)$$

where the set on the RHS is the space of all holomorphic maps $v: S^2 \to O_\mu$, *with* $[v] = m$.

In defining $\mathcal{R}(O_\mu, m)$ recall from Sec. II A that O_μ is in a natural way a complex manifold. It is known[6] that $\mathcal{R}(O_\mu, m)$ is a finite-dimensional smooth manifold, often referred to as a space of rational maps. It follows that our framed moduli space can be identified with a smooth manifold. It should be the case that r_x is naturally a diffeomorphism, but to prove that one would have to equip $\mathcal{M}(x, O_\mu, [\phi]=m)$ with a smooth structure. Although this should be possible, we are not aware of a detailed treatment of this issue.

E. Framing at infinity and parallel scattering

To frame monopoles "at infinity" we pick a point $u \in S^2$, viewed as the sphere at infinity in $\mathbb{R}^3$. Returning to BC1, we define

$$\mathcal{C}(u, \mu, [\phi]=m) = \{(A,\Phi) \in \mathcal{C}: \lim_{t\to\infty} \Phi(tu) = \mu, [\phi]=m\}$$

and

$$\mathcal{C}(u, \mu, k) = \{(A,\Phi) \in \mathcal{C}: \Phi(tu) = \mu - k/2t + o(t^{-1})\}$$

and introduce the corresponding gauge group

$$\mathcal{G}(u) = \{g \in \mathcal{G}: \lim_{t\to\infty} g(tu) = 1\}.$$

The corresponding moduli spaces are

$$\mathcal{M}(u, \mu, [\phi]=m) = \mathcal{C}(u, \mu, [\phi]=m)/\mathcal{G}(u) \quad \text{and} \quad \mathcal{M}(\mu, k) = \mathcal{C}(u, \mu, k)/\mathcal{G}(u).$$

The first of these is called the moduli space of (framed) monopoles with mass μ and degree m. The second is called the moduli space of (framed) monopoles of type (μ, k).

These can also be identified with spaces of rational maps:

Theorem 2.2: *(a) There is a natural bijection* $r_u : \mathcal{M}(u, \mu, m) \to \tilde{\mathcal{R}}(O_\mu, m)$. *(b) There is a natural bijection* $\hat{r}_u : \mathcal{M}(u, \mu, k) \to \tilde{\mathcal{R}}(O_{\mu k}, m)$.

Here $\tilde{\mathcal{R}}(O_\mu, m) \subset \mathcal{R}(O_\mu, m)$ is the set of *based* rational maps, that is, those which send $u \in S^2$ to μ. In part (b),

$$O_{\mu k} = G/H_{\mu k} = G^c/P_{\mu k}, \quad \text{where} \quad H_{\mu k} = C(\mu) \cap C(k), \tag{2.3}$$

and $P_{\mu k}$ is the corresponding parabolic subgroup.

Part (a) of this result was proved first by Donaldson[8] for $G = \mathrm{SU}(2)$, then by Hurtubise[11] for classical groups by a generalization of Donaldson's approach. Both parts were proved for general G by Jarvis[13,14] using parallel scattering to associate a rational map to a monopole, and nonlinear analysis to invert this procedure.

We note in passing that Jarvis shows that the restriction of r_u to $\mathcal{M}(u, \mu, k)$ is the composition of $\hat{r}_u$ with the projection $\tilde{\mathcal{R}}(O_{\mu k}, m) \to \tilde{\mathcal{R}}(G^c/P, m)$.

Once again, it is not clear that smooth structures have been defined on these framed moduli spaces. One conjectures that natural smooth structures should exist, such that these bijections are diffeomorphisms.

As we indicated in the Introduction, it is the moduli spaces $\mathcal{M}(u, \mu, k)$ that have dimensions divisible by 4 and which are therefore candidates to be hyper-Kähler spaces. In Proposition 6.2 the dimension of $\tilde{\mathcal{R}}(O_{\mu k}, m)$ will be explicitly computed.

F. Discussion

Let $x(t) = ut$, and consider the bijection $r_{x(t)}$, for t large, of Theorem 2.1. It is tempting to believe that this should approach the map r_u of Theorem 2.2. However, they cannot be compared

directly since they have different targets. But we could divide both sides by the appropriate groups to get bijections

$$\tilde{r}_u : \mathcal{M}(O,[\phi]=m) \to \tilde{\mathcal{R}}(O_\mu, m)/C(\mu) \quad \text{and} \quad \tilde{r}_{x(t)} : \mathcal{M}(O_\mu,[\phi]=m) \to \mathcal{R}(O_\mu, m)/G$$

and then compare them via the natural isomorphism induced by the inclusion of based maps into unbased maps. A straightforward calculation shows that the limit of $\tilde{r}_{tu}(A,\Phi)$ typically does not exist because evaluated in coordinates it blows up. Some kind of renormalization or scaling must be required to find the relationship between the limit of $\tilde{r}_{x(t)}$ and $\tilde{r}_u$.

III. THE L^2 METRIC

Formally, a tangent vector to (A,Φ) in $\mathcal{C}$ is a pair $(\dot{A},\dot{\Phi})$ satisfying the linearization at (A,Φ) of the Bogomolny equations. The L^2 metric gives this vector length-squared equal to

$$\int_{\mathbb{R}^3} (|\dot{A}|^2 + |\dot{\Phi}|^2) \mathrm{d}x; \tag{3.1}$$

due to the noncompactness of $\mathbb{R}^3$, this need not converge. Looking back at BC1 and BC2, it is clear that (3.1) cannot converge if the variation $\dot{\Phi}$ changes μ or k in BC1. It is natural, therefore, to focus on $\mathcal{M}(u,\mu,k)$ as the obvious candidate to carry a hyper-Kähler metric. Our first task is to show that if the Bogomolny equations hold asymptotically, then the pair (μ,k) determines the leading asymptotics of the monopole on the whole of the two-sphere at infinity.

We begin by noting that the boundary conditions imply that the connection A restricts to give a connection a on E_∞ and that BC1 gives

$$\Phi(tz) = \phi(z) - \frac{f(z)}{2t} + o(t^{-1}), \tag{3.2}$$

where ϕ and f are smooth functions of $z \in S^2$ and the framing condition is

$$\phi(u) = \mu, \qquad f(u) = k. \tag{3.3}$$

The Bogomolny equations reduce to

$$\nabla f = 0, \quad \nabla \phi = 0, \quad F_a = \frac{f}{2} \mathrm{dvol}, \tag{3.4}$$

where dvol denotes the standard area-form of the unit two-sphere. A pair (ϕ,f) satisfying (3.3) and (3.4) are called *monopole boundary data*.

We now prove that, up to gauge, the pair (ϕ,f) is completely determined by its value $(\mu,k/2)$ at the base-point u.

Proposition 3.1: Let (ϕ,f) and (ϕ',f') be boundary data for a monopole:

(i) If u and v are in S^2, then there is a $g \in G$ such that $\phi(u) = \mathrm{ad}(g)(\phi(v))$ and $f(u) = \mathrm{ad}(g)(f(v))$.

(ii) If there is an $h \in G$ such that $\phi(u) = \mathrm{ad}(h)(\phi'(u))$ and $f(u) = \mathrm{ad}(h)(f'(u))$, then there is a $g : S^2 \to G$ such that $\phi^g = \phi'$ and $f^g = f'$.

Proof: If $\phi = 0$, this is a trivial case of the results of Ref. 1 classifying equivalence classes or Yang–Mills connections over a Riemann surface. We follow the proof in Ref. 1. Recall that $E_\infty \to S^2$ is a principal G-bundle. Then ϕ and f can be viewed as equivariant maps $E_\infty \to \mathfrak{g}$. Fix a point $p_0 \in E_\infty$ and let $\phi(p_0) = \mu$ and $f(p_0) = k$. Because ϕ and f are covariantly constant they are constant along any horizontal path. If $p \in P$, we can join p_0 to some point pg with a horizontal curve and then $\phi(p) = \mathrm{ad}(g)(\mu)$ and $f(p) = \mathrm{ad}(g)(k)$ as required.

From the discussion in the preceding paragraph it follows that we have a map

$$(\phi,f):E_\infty\to O_{\mu k}=G/H_{\mu k},\quad H_{\mu k}=C(\mu)\cap C(k).$$

Here $O_{\mu k}$ is the orbit of (μ,k). The preimage of the coset $H_{\mu k}$, i.e., the set of all points p in E_∞ at which $\phi(p)=\mu$ and $f(p)=k$, is a reduction of E_∞ to $H_{\mu k}$ which we denote by $E_{\mu k}$. If $p\in E_{\mu k}$, then any horizontal curve is also in $E_{\mu k}$ because ϕ and k are constant along horizontal curves so the connection also reduces to $P_{\mu k}$.

Because S^2 is simply connected, standard results on reduction of bundles to their holonomy subgroups can be used.[16] It follows from the Ambrose–Singer theorem that the holonomy subgroup at p_0 is the subgroup $H\subset H_{\mu k}$ obtained by exponentiating k and that $E_{\mu k}$ reduces to a bundle E_0 with structure group H.

For the final point we need to know that k is an integral element of the Lie algebra. This is done in Ref. 9 and in a different fashion in Ref. 13. We proceed as follows. Because $[\mu,k]=0$ the closure of the subgroup generated by $\exp(t\mu+sk)$ for any t and s will be an Abelian subgroup of G so a torus and hence inside a maximal torus containing H. If λ is any weight of this maximal torus, we can form an associated line bundle which will have integer chern class $\lambda(k)$. It follows that k is an integer element of $\mathfrak{g}$ and that it exponentiates to define a circle subgroup and a homomorphism $\chi:U(1)\to G$.

We have now reduced our original bundle to a subbundle $Q\to S^2$ which is a circle bundle. It has a connection A and a curvature F with $*F=k/2$ a constant so that it is a circle bundle of degree 1. If A' is another connection with curvature $F'=F$, then $A-A'=a$ with $da=0$ so $a=d(\exp(g))$ for $g:S^2\to \mathrm{U}(1)$ and hence the connections A and A' are equal after a gauge transformation.

This gives us a method of constructing the original bundle, connection and Higgs field from the data μ and k. First take the standard U(1) bundle $Q\to S^2$ with its SU(2) invariant connection and fix $q_0\in Q$ in the fiber over the point u. Let $\chi:\mathrm{U}(1)\to G_{\mu k}\subset G$ be the homomorphism defined by exponentiating k. We can then form $Q\times_\chi G$, the associated bundle, using the action $(q,k)z=(qz,\chi(z)^{-1}k)$ for $z\in\mathrm{U}(1)$. This inherits a connection and the Higgs field is defined by $\hat{\phi}([q,k])=\mathrm{ad}(k)(\mu)$. □

Let $\mathcal{C}^\infty$ denote the set of all monopole boundary data (ϕ,f) and let $\mathcal{G}^\infty$ be the space of all gauge transformations at infinity, that is maps $g:S^2\to G$. Define the *moduli space of boundary data* to be the quotient $\mathcal{M}^\infty=\mathcal{C}^\infty/\mathcal{G}^\infty$. We have the boundary map

$$\partial:\mathcal{M}\to\mathcal{M}^\infty, \tag{3.5}$$

which sends (A,Φ) to the value of the Higgs field and curvature at infinity. Our reason for introducing the boundary map is that we believe that the methods of Atiyah and Hitchin[2] can be adapted to show that

Conjecture 3.2: If $\partial(A,\Phi)=\partial(A',\Phi')$, then there is a gauge transformation g such that A^g-A' and $\Phi^g-\Phi'$ are L^2.

The idea here is that if the condition holds, then for some gauge transformation g, Φ^g and Φ' should agree up to order $1/r$, so that $\Phi^g-\Phi'$ will be square integrable. Similar considerations should apply to the difference between the connections.

Let $\mathcal{G}^\infty(u)$ be all gauge transformations which are the identity at u and let $\mathcal{C}^\infty(u,\mu,m)$ be all pairs (ϕ,f) with $\phi(u)=\mu$ and $[\phi]=m$. Denote $\mathcal{M}^\infty(u,\mu,m)=\mathcal{C}^\infty(u,\mu,m)/\mathcal{G}^\infty(u)$. We have the commuting diagram

$$\begin{array}{ccc}\mathcal{M}(u,\mu,m) & \to & \mathcal{M}^\infty(u,\mu,m)\\ \downarrow & & \downarrow\\ \mathcal{M}(O,m) & \to & \mathcal{M}^\infty(O,m)\end{array}$$

where both vertical maps are quotienting by the group $C(\mu)$.

Conjecture 3.2 would imply that the L^2 metric is finite on each of the moduli spaces $\mathcal{M}(u,\mu,k)$ of monopoles of type (μ,k). This suggests the following.

Conjecture 3.3: The spaces $\mathcal{M}(u,\mu,k)$ are hyper-Kähler manifolds.

A natural approach to these conjectures is the analysis of the linearization $\mathcal{D}$ at $(A,\Phi) \in \mathcal{M}(u,\mu,k)$ of (1.1). Combined with the Coulomb gauge-fixing condition, $\mathcal{D}$ becomes a coupled Dirac operator on $\mathbb{R}^3$,

$$\mathcal{D}: C^\infty(\mathbb{R}^3, \mathbb{H}\otimes\mathbb{H}\otimes \mathrm{ad}(E)) \to C^\infty(\mathbb{R}^3, \mathbb{H}\otimes\mathbb{H}\otimes \mathrm{ad}(E)),$$

where $\mathbb{H}$ is regarded as the spin-bundle of $\mathbb{R}^3$. Unfortunately this operator is not "invertible at infinity" and so it is not automatically a Fredholm operator in L^2. Taubes analyzed it in detail when $G=\mathrm{SU}(2)$, but in general, rigorous results about this operator are not available. Nonetheless, it should be possible to find a suitable space of functions such that $\mathcal{D}$ becomes a Fredholm operator, with index calculable in terms of the type data (μ,k). Formally $\mathcal{D}$ is quaternionic, so its L^2 null space will automatically be a quaternionic vector space with compatible inner product. The reader is referred to Ref. 2, Chaps. 3 and 4, for a detailed discussion of the case $G=\mathrm{SU}(2)$.

A. Group actions

Consider $\mathcal{E}$, the group of Euclidean transformations of $\mathbb{R}^3$, which is the semi-direct product of SO(3), the group of rotations and $\mathbb{R}^3$ the group of translations. As the monopole bundle $E\to\mathbb{R}^3$ is trivial the group $\mathcal{E}$ acts on the connection and Higgs field, preserves the Bogomolny equations and commutes with gauge transformations so it acts on the full-unframed moduli space. In general this action disturbs the framings. If $x\in\mathbb{R}^3$, then the subgroup $\mathcal{E}_x$ of transformations preserving x, which is isomorphic to SO(3), acts naturally on the moduli space of monopoles framed at x. If $u\in S^2$, then the subgroup of $\mathcal{E}_u$ of transformations preserving the line through u, which is isomorphic to $\mathrm{SO}(2)\times\mathbb{R}^2$, will act naturally on the moduli space of monopoles framed at u.

As well as these straightforward actions the moduli space $\mathcal{M}(u,\mu,k)$ also carries an action of the full group of Euclidean transformations. For this we need a different description of this moduli space (cf. Ref. 2, pp. 15 and 16). Note that Proposition 3.1 shows that k defines a representation of the circle in G, hence an associated G-bundle over the two-sphere. This carries a natural SO(3)-action and has a unique SO(3)-equivariant connection a and Higgs field ϕ such that $\phi(u)=\mu$ and $f(u)=k$. The moduli space $\mathcal{M}(\mu,k)$ is now defined to consist of configurations (A,Φ,q) where (A,ϕ) is a monopole and q is an isomorphism between $\partial(A,\Phi)$ and (ϕ,f), modulo the group of gauge transformations that approach the identity at infinity. Then $\mathcal{M}(\mu,k)$ has a natural SO(3)-action and can be shown to be diffeomorphic to $\mathcal{M}(u,\mu,k)$. The subtlety is [as in the case $G=\mathrm{SU}(2)$] that the diffeomorphism between $\mathcal{M}(\mu,k)$ and $\mathcal{M}(u,\mu,k)$ is not equivariant with respect to the copy of $\mathrm{SO}(2)\subset\mathrm{SO}(3)$ which fixes the direction u.

B. Discussion

Assuming that the L^2 metric does define a genuine hyper-Kähler metric on $\mathcal{M}(u,\mu,k)$, there are many interesting open questions surrounding it. First of all, there is the issue of whether it is complete for all μ and k. Second, there are questions relating to variation of the parameters μ and k. It is natural to conjecture that the metrics will vary smoothly with μ as long as the corresponding orbit O_μ does not jump. An interesting conjecture of Lee, Weinberg, and Yi[18] suggests that these hyper-Kähler metrics should also behave well with respect to specialization of μ. To state the conjecture, call a path $\mu:[0,\delta]\to\mathfrak{g}$ a *regular* deformation of $\mu_0=\mu(0)$ if $\mu(t)$ is *regular* for all $t>0$. Let $\mathcal{M}_t=\mathcal{M}(u,\mu_t,k)$, and let g_t be the L^2 metric on $\mathcal{M}_t$.

Conjecture 3.4: Given any $0\neq\mu_0\in\mathfrak{g}$, there is a regular deformation μ_t, such that $(\mathcal{M}_t,g_t)$ tends to $(\mathcal{M}_0,g_0)$ as $t\to 0$.

Note that Jarvis[13] describes a "filling-out procedure" which associates to any holomorphic map $v:S^2\to O_{\mu,k}$ a new map $\tilde{v}:S^2\to G/T$ where T is a maximal torus. This would appear to be closely related to the idea of regular deformation of a general element μ, but it says nothing about the behavior of the metrics.

We have now filled in the details of our account in the Introduction up to Eq. (1.4), though we have not yet shown that $\mathcal{K}$ has the structure claimed in (1.3). We turn to that in the next section.

IV. MAGNETIC AND HOLOMORPHIC CHARGES

We will now show how to calculate explicitly the *magnetic charges* of a monopole which determine the homotopy class m and the *holomorphic charges* which determine the strata. We will also make some conjectures about the possible values these can take.

In this section, μ and k are as before. In addition, T is a maximal torus whose Lie algebra $\mathfrak{t}$ contains both μ and k. Recall that a choice of Weyl chamber C in $\mathfrak{t}$ gives rise to a set of simple roots $\alpha_1,\ldots,\alpha_r$ and the corresponding fundamental weights $\lambda_1,\ldots,\lambda_r$ defined by

$$2\frac{\langle\alpha_i,\lambda_j\rangle}{\langle\alpha_i,\alpha_i\rangle}=\delta_{ij}. \tag{4.1}$$

We can always choose a fundamental Weyl chamber C satisfying

$$\alpha_1(\mu)>0,\ldots,\alpha_s(\mu)>0, \text{ and } \alpha_{s+1}(\mu)=0,\ldots,\alpha_r(\mu)=0, \tag{4.2}$$

because this is just the condition that μ is in the closure of C and a particular ordering of the simple roots.

We would like to apply the corresponding fundamental weights to k but this is not possible as we only know that k is in the Lie algebra of the centralizer of μ. We can conjugate k by $C(\mu)$ until it is inside the torus but then we find that $\mathfrak{t}\cap C(\mu)k$ is not a single point but an orbit under $\mathcal{W}_\mu$ the subgroup of the Weyl group stabilising μ. Our first result resolves this problem by showing that we can pick out a unique element $\tilde{k}$ of $\mathfrak{t}\cap C(\mu)k$.

Proposition 4.1: Suppose that the moduli space $\mathcal{M}(u,\mu,k)$ is nonempty and we have fixed a maximal torus containing μ, a fundamental Weyl chamber C with μ in its closure and have ordered the simple roots so they satisfy (4.2). Then there exists a uniquely determined $\tilde{k}\in\mathfrak{t}\cap C(\mu)k$, such that

$$\alpha_{s+1}(\tilde{k})\leqslant 0,\ldots,\alpha_r(\tilde{k})\leqslant 0.$$

Moreover, we have $\lambda_j(\tilde{k})\geqslant 0$ for $j=1,\ldots,r$.

We shall give the proof of this proposition in a moment. For now, we shall use it to define the *charges* of the monopole to be the non-negative integers

$$\lambda_1(\tilde{k}),\ldots,\lambda_r(\tilde{k}).$$

They are naturally divided into *magnetic charges*

$$m_1=\lambda_1(\tilde{k}),\ldots,m_s=\lambda_s(\tilde{k})$$

and the *holomorphic charges*:

$$h_1=\lambda_{s+1}(\tilde{k}),\ldots,h_{r-s}=\lambda_r(\tilde{k}).$$

In some examples the simple roots have a natural ordering and it is convenient not to reorder them. In that case we just choose $\tilde{k}$ to be the unique $\tilde{k}\in\mathfrak{t}\cap C(\mu)k$ such that whenever $\alpha_i(\mu)=0$ we have $\alpha_i(\tilde{k})\leqslant 0$. We then say that $\lambda_i(\tilde{k})$ is a magnetic charge if $\alpha_i(\mu)>0$ and a holomorphic charge if $\alpha_i(\mu)=0$.

The most important point to be made here is that it is easy to show that $\pi_2(O_\mu)=\mathbb{Z}^s$ and the magnetic charges determine the homotopy class of ϕ the Higgs field at infinity (see, for example,

Ref. 3). The magnetic charges therefore cannot change under continuous deformation of a monopole. By contrast, the holomorphic charges can jump under continuous deformation of the monopole.

Note that the strata in the moduli space are all those monopoles with the same $\tilde{k}$.

As well as being non-negative the holomorphic charges satisfy the additional constraint that $\alpha_i(\tilde{k}) \leqslant 0$ for all $i = s+1, \ldots, r$. This is equivalent to

$$\sum_{l=1}^{r-s} \frac{2\langle \alpha_i, \alpha_{l+s} \rangle}{\langle \alpha_{l+s}, \alpha_{l+s} \rangle} h_l + \sum_{j=1}^{s} \frac{2\langle \alpha_i, \alpha_j \rangle}{\langle \alpha_j, \alpha_j \rangle} m_j \leqslant 0, \quad \text{for} \quad i = s+1, \ldots, r. \tag{4.3}$$

We conjecture the following.

Conjecture 4.2: For a given μ there are monopoles with any collection of non-negative magnetic charges $(m_1, \ldots, m_s)$. Given a choice of magnetic charges there are monopoles with any collection of holomorphic charges $(h_1, \ldots, h_{r-s})$ satisfying (4.3).

It should be possible to prove this result using rational maps but it has eluded us. We can prove, however, the following.

Proposition 4.3: For a given μ and choice of magnetic charges there are at most a finite number of possible holomorphic charges satisfying (4.3).

We defer the proof to the next section but note that this gives the following.

Corollary 4.4: There are only a finite number of strata and in particular there must be an open stratum.

Note that this approach gives a nice picture in terms of Dynkin diagrams. For maximal symmetry-breaking, all charges are magnetic (i.e., topological) and the heuristic is that there are m_i fundamental monopoles of type i for each i a node on the Dynkin diagram. For nonmaximal symmetry breaking mark each node i with $\alpha_i(\mu) = 0$. Now each Dynkin node still has associated to it the non-negative integer $\lambda_i(\tilde{k})$. This number is a magnetic charge m_i if i is unmarked, and again the heuristic is that there are m_i fundamental monopoles of type i. If i is a marked node, then $\lambda_i(\tilde{k})$ is a holomorphic charge. This labels the strata and can jump under continuous deformation of the monopole. The possible holomorphic charges are constrained by inequalities which can be deduced from the Dynkin diagram and (4.3).

A. Proof of Proposition 4.1

Let $\mathcal{W}_\mu$ be the subgroup of the Weyl group fixing μ and note that it acts transitively on the set of all fundamental Weyl chambers with μ in their closure.[10]

To prove first that a $\tilde{k}$ exists we follow Jarvis[13] and consider the condition $\alpha(\mu - tk') > 0$ for large enough t and any $k' \in \mathfrak{t} \cap C(\mu)k$. As there are only a finite number of roots we can find an $\epsilon > 0$ such that for all $t \in (0, \epsilon]$ we have that $\alpha(\mu - tk') = 0$ if and only if $\alpha(\mu) = 0$ and $\alpha(k') = 0$ and $\alpha(\mu - tk') > 0$ implies $\alpha(k') = 0$ and $\alpha(k') < 0$. For any such t choose a fundamental Weyl chamber with $\mu - tk'$ in its closure. As $t \to 0$ we see that this has μ in its closure as well. If this is not the fundamental Weyl chamber we first thought of we can move it by $\sigma \in \mathcal{W}_\mu$ until it is and then let $\tilde{k} = \sigma(k')$. Then $\mu - t\tilde{k}$ is in the closure of our fundamental Weyl chamber so that $\alpha_i(\mu) > 0$ for $i = 1, \ldots, s$ and $\alpha_j(\mu) = 0$ and $\alpha_j(\tilde{k}) \leqslant 0$ for $j = s+1, \ldots, r$.

We will see in a moment that $\tilde{k}$ is unique but for now we show that $\lambda_i(\tilde{k}) \geqslant 0$ for all $i = 1, \ldots, r$.

Consideration of the twistor construction for monopoles shows that ϕ and f satisfy the following non-negativity constraint for any direction u. Choose any maximal torus T so that $\phi(u), f(u) \in \mathfrak{t}$. Choose a fundamental Weyl chamber whose closure contains $\phi(u)$ and let $\alpha_1, \ldots, \alpha_r$ be the corresponding simple roots. Define the fundamental weights $\lambda_1, \ldots, \lambda_r$ by (4.1). Then

$$\lambda_i(f(z)) \geqslant 0 \quad \text{for all} \quad i = 1, \ldots, r$$

independent of all the choices made. Note that $\tilde{k}$ is a conjugate of k under an element of $C(\mu)$ and hence corresponds to the k for some different monopole which also satisfies the positivity constraint. Hence we must have $\lambda_i(\tilde{k}) \geqslant 0$ for all $i=1,\ldots,r$.

Consider lastly the uniqueness of $\tilde{k}$. So assume we have $\tilde{k}$ and $\sigma(\tilde{k})$ for $\sigma \in \mathcal{W}_\phi$ and $\alpha_j(\tilde{k}) \leqslant 0$ and $\alpha_j(\sigma(\tilde{k})) \leqslant 0$ for every $i=s+1,\ldots,r$. Let V be the span of the roots $\alpha_{s+1},\ldots,\alpha_r$. This is a root system with Weyl group $\mathcal{W}_\mu$. Let C_{ij} be the inverse of the matrix $D_{ij}=\langle \alpha_i, \alpha_j \rangle$. Then both C and D are symmetric. Define

$$\chi: \mathfrak{t} \to V$$

by

$$\chi(h) = \sum_{j,k=s+1}^{r} \alpha_j(h) C_{jk} \alpha_k .$$

Let σ_l be a simple root reflection for $s+1 \leqslant l \leqslant r$. Then

$$\begin{aligned}
\chi(\sigma_l(h)) &= \sum_{j,k=s+1}^{r} \sigma_l(\alpha_j)(h) C_{jk} \alpha_k \\
&= \chi(h) - \sum_{j,k=s+1}^{r} \frac{2\langle \alpha_j, \alpha_l \rangle}{\langle \alpha_l, \alpha_l \rangle} C_{jk} \alpha_k(h) \\
&= \chi(h) - \frac{2\alpha_l(h)}{\langle \alpha_l, \alpha_l \rangle} \alpha_l .
\end{aligned}$$

Moreover,

$$\begin{aligned}
\sigma_l(\chi(h)) &= \chi(h) - \frac{2\langle \chi(h), \alpha_l \rangle}{\langle \alpha_l, \alpha_l \rangle} \\
&= \chi(h) - \sum_{j,k=s+1}^{r} \alpha_j(h) C_{jk} \frac{2\langle \alpha_k, \alpha_l \rangle}{\langle \alpha_l, \alpha_l \rangle} \\
&= \chi(h) - \frac{2\alpha_l(h)}{\langle \alpha_l, \alpha_l \rangle} \alpha_l \\
&= \chi(\sigma_l(h)).
\end{aligned}$$

It follows that if $\sigma \in \mathcal{W}_\mu$, then $\chi(\sigma(\tilde{k})) = \sigma(\chi(\tilde{k}))$. We also have $\langle \alpha_l, \chi(h) \rangle = \alpha_l(h)$ so that $\chi(\tilde{k})$ and $\chi(\sigma(\tilde{k}))$ are in the closure of the same Weyl chamber in V. Applying Humphreys' 10.3 Lemma B[10] we see that $\chi(\sigma(\tilde{k})) = \sigma(\chi(\tilde{k})) = \chi(\tilde{k})$ and hence $\alpha_i(\tilde{k} - \sigma(\tilde{k})) = 0$ for $i = s+1,\ldots,r$. We have previously seen that $\lambda_i(\tilde{k} - \sigma(\tilde{k})) = 0$ for $i=1,\ldots,s$. Moreover, the span of the $\lambda_1,\ldots,\lambda_s$ is orthogonal to the span of the $\alpha_{s+1},\ldots,\alpha_r$, so together they must span $\mathfrak{t}^*$ and hence $\tilde{k} = \sigma(\tilde{k})$.

B. Proof of Proposition 4.3

Let ϵ be the sum of all the positive roots which are in the span of the simple roots $\alpha_{s+1},\ldots,\alpha_r$. Notice that $\epsilon(\tilde{k}) \leqslant 0$. Recall[10] that a simple root reflection σ_i permutes all the positive roots except α_i which it sends to $-\alpha_i$. So if $s+1 \leqslant i \leqslant r$, we have $\sigma_i(\epsilon) = \epsilon - 2\alpha_i$ so that

$$2\frac{\langle \epsilon, \alpha_i \rangle}{\langle \alpha_i, \alpha_i \rangle} = 2.$$

So we have

$$\epsilon = \sum_{j=1}^{r} 2\frac{\langle \epsilon, \alpha_i \rangle}{\langle \alpha_i, \alpha_i \rangle}\lambda_i = \sum_{j=1}^{s} 2\frac{\langle \epsilon, \alpha_i \rangle}{\langle \alpha_i, \alpha_i \rangle}\lambda_i + \sum_{i=s+1}^{r} 2\lambda_i = \sum_{j=1}^{s} -p_j\lambda_j + \sum_{i=s+1}^{r} 2\lambda_i,$$

where $p_j \geqslant 0$ because if $1 \leqslant j \leqslant s$ we have $\langle \epsilon, \alpha_j \rangle \leqslant 0$. Applying ϵ to $\tilde{k}$ gives

$$0 \leqslant \sum_{i=1}^{r-s} h_i \leqslant \sum_{j=1}^{s} p_j m_j$$

and, as each h_j is non-negative, this means there can only be a finite number of possibilities.

V. EXAMPLES

Let $G = \mathrm{SU}(N)$ and μ be a diagonal matrix with eigenvalues $i\mu_1, i\mu_2, \ldots, i\mu_q$ with multiplicities $n_1, \ldots, n_q$ and assume that $\mu_1 > \mu_2 > \cdots > \mu_q$. Choose the usual fundamental Weyl chamber. That is, if d is any diagonal matrix with entries $id_1, \ldots, id_N$, then it is in the fundamental Weyl chamber if $d_1 > d_2 > \cdots > d_N$. Clearly this has μ in its closure. Define $x_j(d) = d_j$. Then the simple roots are $\alpha_i = x_{i+1} - x_i$ for $i = 1, \ldots, N-1$. The fundamental weights satisfy

$$\lambda_j(d) = d_1 + \cdots + d_j$$

and a weight is magnetic if $j = n_1, n_2, \ldots, n_{q-1}$ and holomorphic otherwise.

Let $\mathbb{C}^N = \mathbb{C}^{n_1} \oplus \cdots \oplus \mathbb{C}^{n_q}$ be the corresponding eigenvalue decomposition of $\mathbb{C}^N$. Assume that on $\mathbb{C}^{n_j}$ the eigenvalues of k are

$$k_{n_1+\cdots+n_{j-1}+1} \leqslant k_{n_1+\cdots+n_{j-1}+2} \leqslant \cdots \leqslant k_{n_1+\cdots+n_j}.$$

Then $\tilde{k}$ is the diagonal matrix with entries $ik_1, \ldots, ik_N$.

Let $\mathcal{M}_j$ be the stratum containing $\mathcal{M}(u, \mu, k)$. It was shown in Ref. 19 that

$$\dim\ \mathcal{M}_j = 4\sum_{i=1}^{N} (k_1 + \cdots + k_i) + \dim\ C(\mu)k,$$

and hence from the definition of the strata in the Introduction,

$$\dim\ (\mathcal{M}(u, \mu, k)) = 4\sum_{i=1}^{N} (k_1 + \cdots + k_i),$$

so the dimension is divisible by four as required for a hyper-Kähler manifold. In Proposition 6.2 we shall show that this result is always true.

Notice that we could find a deformation μ_t of μ by choosing μ_t to be diagonal with entries $i\mu_j(t)$ such that

$$\mu_1(t) > \mu_2(t) > \mu_3(t) > \cdots > \mu_N(t),$$

and, of course, with $\mu(0) = \mu$. It follows from known results on the moduli spaces[12,20] that $\dim \mathcal{M}(u, \mu_t, k) = \dim \mathcal{M}(u, \mu, k)$. In fact, the method used in Ref. 19 to calculate the dimension formula shows that $\mathcal{M}(u, \mu(t), k))$ and $\mathcal{M}(u, \mu, k)$ are diffeomorphic spaces of holomorphic maps. This result was generalized to arbitrary G by Jarvis.[13]

VI. DIMENSIONS

In this section we compute the dimension of the moduli space $\mathcal{M}(u,\mu,m)$ by computing the dimension of $\tilde{\mathcal{R}}(O_\mu,m)$. We shall also compute the dimensions of the strata and the moduli space $\mathcal{M}(u,\mu,k)$ of monopoles of type (μ,k), by computing the dimension of $\tilde{\mathcal{R}}(O_{\mu k},m)$.

Fix a maximal torus T, a fundamental Weyl chamber and a set of simple roots $\alpha_1,\ldots,\alpha_r$. For a root α let $\mathfrak{g}_\alpha$ be the α root space. Denote by B the standard Borel determined by this choice of simple roots. That is the Lie algebra of B contains the root space of every simple root. The parabolic P is determined by the fact that its Lie algebra $\mathfrak{p}$ contains the root spaces for the negative roots $\alpha_{s+1},\ldots,\alpha_r$.

If $f:S^2\to G^c/P$ is a holomorphic map, then we can use it to pull back the tangent bundle to G^c/P and the Riemann–Roch theorem tell us that

$$\dim(H^0(S^2,f^{-1}(TG^c/P)))-\dim(H^1(S^2,f^{-1}(TG^c/P)))=\dim(G^c/P)+c_1(\det(f^{-1}TG^c/P)),$$

where $\det(TG^c/P)$ is the determinant line bundle of $f^{-1}TG^c/P$ and c_1 denotes the first Chern class. Because the group G acts holomorphically on G^c/P every element of $\mathfrak{g}$ defines a holomorphic vector field on G^c/P so we have a surjection of holomorphic vector bundles over S^2

$$\mathfrak{g}\times S^2\to f^{-1}TG^c/P\to 0$$

and it follows from the short exact sequence in cohomology that

$$\dim(H^1(S^2,f^{-1}(TG^c/P)))=0.$$

The tangent space to $\tilde{\mathcal{R}}(G^c/P,m)$ at the function f is just the subset of sections in $H^0(S^2,f^{-1}(TG^c/P))$ which vanish at the base point, say $P\in G^c/P$. This has *real* dimension

$$\dim\mathcal{R}(G^c/P,m)=2(\dim(H^0(S^2,f^{-1}(TG^c/P)))-\dim(G^c/P))=2c_1(\det(f^{-1}TG^c/P)).$$

Each of the fundamental weights $\lambda_1,\ldots,\lambda_s$ extend to one-dimensional representations of P and hence define homogeneous line bundles $L(\lambda_i)$ over G^c/P. The magnetic charges of a holomorphic map f are $m_i=-c_1(f^{-1}(L(\lambda_i)))$. Choose $\tilde{k}$ so that $m_i=\lambda_i(\tilde{k})$. Then $c_1(f^{-1}(L(-\lambda)))=\lambda(\tilde{k})$ for any weight λ.

Let ϵ be the weight defined by the adjoint representation of P on $\mathfrak{p}$. Then the weight defined by the adjoint representation of P on $\mathfrak{g}/\mathfrak{p}$ is $-\epsilon$. The bundle $\det(T(G^c/P)$ is then a homogeneous bundle over G^c/P induced by the character $-\epsilon$ so that

$$c_1(f^{-1}(\det(TG^c/P)))=c_1(f^{-1}(L(-\epsilon)))=\epsilon(\tilde{k}).$$

Hence

$$\dim\tilde{\mathcal{R}}(G^c/P,m)=2\epsilon(\tilde{k}).$$

In the case of maximal symmetry breaking where the parabolic P is a Borel B

$$\epsilon=\sum_{\alpha>0}\alpha=2\sum_{i=1}^{r}\lambda_i,$$

so that

$$\dim\tilde{\mathcal{R}}(G/B,m)=4\sum_{i=1}^{r}m_i.$$

In the nonmaximal symmetry breaking case we can proceed further. Because ϵ is a weight we know that $\epsilon=\Sigma_{i=1}^{r}-n_i\lambda_i$ for some integers n_i. We also know that ϵ is a character of P so invariant under the simple root reflections σ_i for $i=s+1,\ldots,r$. But $\sigma_j(\epsilon)=\epsilon+n_j\alpha_j$ so that we must have

$$\epsilon=\sum_{i=1}^{s}-n_i\lambda_i$$

and hence

$$\dim\tilde{\mathcal{R}}(G^c/P,m)=2\sum_{i=1}^{s}n_im_i.$$

We can obtain some further information about the n_i. First we note that

$$n_i=-2\frac{\langle\epsilon,\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}.$$

Also, if ρ is one-half the sum of the positive roots and $\rho_{\mathfrak{p}}$ is one-half the sum of the positive roots α for which $\mathfrak{g}_{-\alpha}\subset\mathfrak{p}$, then we have that $\epsilon=-2\rho+2\rho_{\mathfrak{p}}$ and hence

$$n_i=2\frac{\langle 2\rho-2\rho_{\mathfrak{p}},\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}=2\left(1-2\frac{\langle\rho_{\mathfrak{p}},\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}\right)\lambda_i$$

using the standard fact that $\rho=\Sigma_{i=1}^{r}\lambda_i$. Hence

$$\dim(\tilde{\mathcal{R}}(G^c/P,m))=4\sum_{i=1}^{s}\left(1-2\frac{\langle\rho_{\mathfrak{p}},\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}\right)m_i,$$

which agrees with the result in Ref. 20. So we have the following proposition.

Proposition 6.1: The dimension of the moduli space $\mathcal{M}(u,\mu,m)$ is

$$4\sum_{i=1}^{s}\left(1-2\frac{\langle\rho_{\mathfrak{p}},\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}\right)m_i.$$

Notice that while the Lie theory guarantees ρ is a weight, the same may not be true of $\rho_{\mathfrak{p}}$ and hence expressions such as

$$2\frac{\langle\rho_{\mathfrak{p}},\alpha_i\rangle}{\langle\alpha_i,\alpha_i\rangle}$$

may not be integers. This is consistent with the fact that for nonmaximal symmetry breaking the moduli space may not be hyper-Kähler for the simple reason that its dimension is not a multiple of four.

Next we calculate $\dim\tilde{\mathcal{R}}(O_{\mu k},m)$ where $P_{\mu k}$ is the parabolic subgroup containing all the positive roots and the negative roots α where $\alpha(\mu)=\alpha(\tilde{k})=0$ and we let $O_{\mu k}=G^c/P_{\mu k}$. This is the parabolic subgroup occurring in (2.3).

Then ϵ is the sum of all these roots so that

$$\epsilon(\tilde{k})=\sum_{\alpha>0}\alpha(\tilde{k})$$

and we have

$$\dim\tilde{\mathcal{R}}(G^c/P_{\mu k},k)=4\left(\sum_{i=1}^{s} m_i+\sum_{j=1}^{r-s} h_j\right).$$

Hence we deduce the following.

Proposition 6.2: The dimension of the moduli space $\mathcal{M}(u,\mu,k)$ is

$$4\left(\sum_{i=1}^{s} m_i+\sum_{j=1}^{r-s} h_j\right).$$

In particular it is divisible by four.

Similarly for the strata, we have the following Corollary.

Corollary 6.3: The dimension of the stratum $\mathcal{M}_j$ containing $\mathcal{M}(u,\mu,k)$ is

$$4\left(\sum_{i=1}^{s} m_i+\sum_{j=1}^{r-s} h_j\right)+\dim C(\mu)-\dim C(\mu)\cap C(k).$$

ACKNOWLEDGMENTS

The first author thanks Michael Eastwood for helpful discussions and the Australian Research Council for support.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Polyhedral scattering of fundamental monopoles

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(Received 12 December 2002; accepted 9 April 2003)

The dynamics of n slowly moving fundamental monopoles in the SU($n+1$) BPS Yang–Mills–Higgs theory can be approximated by geodesic motion on the $4n$-dimensional hyperkähler Lee–Weinberg–Yi manifold. In this article we apply a variational method to construct some scaling geodesics on this manifold. These geodesics describe the scattering of n monopoles which lie on the vertices of a bouncing polyhedron; the polyhedron contracts from infinity to a point, representing the spherically symmetric n-monopole, and then expands back out to infinity. For different monopole masses the solutions generalize to form bouncing nested polyhedra. The relevance of these results to the dynamics of well separated SU(2) monopoles is also discussed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1584208]

I. INTRODUCTION

The dynamics of slowly moving BPS monopoles can be approximated by geodesic motion on the moduli space of static solutions, with the metric determined by the kinetic part of the Lagrangian.[20,23] For two centered SU(2) monopoles the moduli space is the Atiyah–Hitchin manifold and the simplest geodesic corresponds to the 90° scattering of two monopoles in a head-on collision.[3] Unfortunately, for more than two SU(2) monopoles the moduli space metric is not known explicitly, except in the region where all the monopoles are well separated.[12] Despite this fact some geodesics are known.[13,15,16,24] They are obtained by the imposition of appropriate spatial symmetries to yield a one-dimensional manifold of static solutions, which is then automatically a geodesic, since the fixed point set of a group action is always a totally geodesic submanifold.

For BPS monopoles with gauge group SU($n+1$) and maximal symmetry breaking there are n topological charges and correspondingly n types of fundamental monopole, each of which carries a single unit of one of these charges.[25] If there is precisely one fundamental monopole of each type, then the moduli space is $4n$-dimensional and equipped with the hyperkähler Lee–Weinberg–Yi metric,[18] which is known explicitly. The explicit form of the metric allows the possibility of computing some geodesics and hence n-monopole scattering processes for any value

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of n. In this article we apply a variational method to construct some scaling geodesics on this manifold. The approach is to look for central configurations in which the time dependence is only in the form of an overall scaling of the monopole positions. The resulting algebraic equations can then be written as the critical points of a certain energy function,[22] which we minimize using numerical methods. As examples, we find minimal energy configurations, and hence geodesics, for all $n \leqslant 20$. The symmetries of these configurations are analyzed and suggest the existence of icosahedral minima at $n=32$ and $n=72$, which are also constructed. In all cases the associated geodesics describe the scattering of n monopoles which lie on the vertices of a bouncing polyhedron, in the following sense. The polyhedron first contracts from infinity to a point, which in the moduli space represents the spherically symmetric n-monopole. The evolution then reverses with the monopoles located on the vertices of the same polyhedron, but which is now expanding back out to infinity.

For different monopole masses the above solutions generalize to form bouncing nested polyhedra. Our solutions also provide geodesics of the Gibbons–Manton metric,[12] and hence describe the scattering of n SU(2) monopoles, valid in the region where the monopoles are well separated. This reveals a connection with some geodesics obtained earlier using symmetry arguments.

II. POLYHEDRAL SCATTERING

The $4n$-dimensional hyperkähler Lee–Weinberg–Yi manifold is a T^n bundle over a $3n$-dimensional base space. For $i=1,...,n$ let $\theta_i \in S^1$ be the fiber coordinates and $\mathbf{x}_i \in \mathbb{R}^3$ be local coordinates in the base, which may be thought of as the positions in $\mathbb{R}^3$ of each of the n monopoles. The purely kinetic Lagrangian associated with the metric has the form

$$L = g_{ij}\dot{\mathbf{x}}_i \cdot \dot{\mathbf{x}}_j + g_{ij}^{-1}(\dot{\theta}_i + \mathbf{W}_{ik}\cdot\dot{\mathbf{x}}_k)(\dot{\theta}_j + \mathbf{W}_{jl}\cdot\dot{\mathbf{x}}_l)\,, \tag{2.1}$$

where we have used the Einstein summation convention, though this is not to be used in the rest of the article unless explicitly stated. The quantities appearing in the above are given by

$$g_{ii} = m_i + \sum_{j\neq i} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{2.2}$$

$$g_{ij} = \frac{-1}{|\mathbf{x}_i - \mathbf{x}_j|}, \quad i \neq j, \tag{2.3}$$

$$\mathbf{W}_{ii} = \sum_{j\neq i} \mathbf{w}_{ij}\,, \tag{2.4}$$

$$\mathbf{W}_{ij} = -\mathbf{w}_{ij}\,, \quad i \neq j, \tag{2.5}$$

and $\mathbf{w}_{ij}$ is the value at $\mathbf{x}_i$ of the Dirac potential due to the monopole at $\mathbf{x}_j$, that is,

$$\boldsymbol{\nabla}_j \times \mathbf{w}_{ji} = \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}. \tag{2.6}$$

In the above we have scaled out the magnetic charge of a monopole and the positive constants m_i are related to the monopole masses.

The T^n isometry of the metric yields the n conserved charges (here we use the summation convention once more)

$$Q_i = g_{ij}^{-1}(\dot{\theta}_j + \mathbf{W}_{jk}\cdot\dot{\mathbf{x}}_k)\,, \tag{2.7}$$

so that the fiber coordinates are nondynamical degrees of freedom. In this article we shall be concerned with monopoles with no electric charge, so we set $Q_i=0$, for all $i=1,...,n$. In this case the Lagrangian describing the motion in the base space is simply

$$L=\sum_i \left(m_i+\sum_{j\neq i}\frac{1}{x_{ij}}\right)\dot{\mathbf{x}}_i^2-\sum_i\sum_{j\neq i}\frac{1}{x_{ij}}\dot{\mathbf{x}}_i\cdot\dot{\mathbf{x}}_j\,, \tag{2.8}$$

where we have defined $\mathbf{x}_{ij}=\mathbf{x}_i-\mathbf{x}_j$, and $x_{ij}=|\mathbf{x}_{ij}|$. The geodesic equations which follow from (2.8) are

$$m_k\ddot{\mathbf{x}}_k=\sum_{j\neq k}\left(\frac{\ddot{\mathbf{x}}_{jk}}{x_{jk}}+\frac{\mathbf{x}_{jk}|\dot{\mathbf{x}}_{jk}|^2}{2x_{jk}^3}-\frac{\dot{\mathbf{x}}_{jk}\dot{x}_{jk}}{x_{jk}^2}\right). \tag{2.9}$$

As suggested in Ref. 22 we now look for time dependent homothetic solutions of these equations, that is, solutions of the form $\mathbf{x}_k(t)=\alpha(t)\mathbf{y}_k$, with constant $\mathbf{y}_k$. Clearly, such solutions describe monopoles in a fixed configuration, but with the overall scale of the configuration evolving dynamically. Substituting this ansatz into (2.9) yields the equations

$$m_k\mathbf{y}_k+C\sum_{j\neq k}\frac{\mathbf{y}_{jk}}{y_{jk}}=0\,, \tag{2.10}$$

where C is defined to be the quantity

$$C=\frac{\dot{\alpha}^2}{2\ddot{\alpha}\alpha^2}-\frac{1}{\alpha}. \tag{2.11}$$

Obviously, for a nontrivial solution of (2.10) to exist the quantity C must be a constant, and it turns out that only a positive constant produces a physically acceptable solution. By a rescaling of the time variable we may, without loss of generality, set $C=1$. The two constants which appear in the general solution of (2.11) may be absorbed by a linear transformation of t, and the solution we require is given implicitly by

$$t=\sqrt{\alpha+\alpha^2}+\tfrac{1}{2}\log(1+2\alpha+2\sqrt{\alpha+\alpha^2})\,, \tag{2.12}$$

for $t\geqslant 0$. It is clear from (2.12) that the scale $\alpha(t)$ is a monotonically increasing function of t, which for small t has the expansion $\alpha=t^2/4+\cdots$ and for large t has the asymptotic form $\alpha\sim t$.

Note that Eqs. (2.9) are invariant under time reversal $t\mapsto -t$ and also spatial inversion of all the points $\mathbf{x}_k\mapsto-\mathbf{x}_k$. So far we have only addressed the second part of the geodesic motion, when $t\geqslant 0$ and the monopoles are moving away from each other, but the first part with $t<0$ is simply obtained by time reversal in Eq. (2.12), so that the monopoles approach the origin from spatial infinity. Thus the monopoles bounce back off each other, rather than passing through each other, which would have been the result if the time inversion was accompanied by the spatial inversion $\mathbf{x}_k\mapsto-\mathbf{x}_k$. The fact that the first of these scenarios is the correct one can be seen by studying the Lee–Weinberg–Yi manifold in the neighborhood of the origin $\mathbf{x}_k=0$, for all k. Although the metric appears to be singular at the origin, this is merely a coordinate singularity, and if new coordinates are chosen appropriately (these are essentially polar coordinates but with the radial variables related to the monopole positions by $r_k=\sqrt{|\mathbf{x}_k|}$) the metric is seen to be flat in these new coordinates. The fact that the squares of the monopole positions are related to the flat coordinates is the reason that fundamental monopoles of different types bounce back upon collision; had the metric been flat around the origin in the coordinates $\mathbf{x}_k$ then the monopoles would have passed through each other.

The problem of finding scaling geodesics has now been reduced to the algebraic problem of finding sets of n points $\mathbf{y}_k$, which satisfy (2.10) with $C=1$. Our method is to use a variational approach, based on the fact that (2.10) are the equations for critical points of the energy function

$$E=\frac{1}{2}\sum_i m_i|\mathbf{y}_i|^2-\sum_i\sum_{j<i} y_{ij}. \tag{2.13}$$

In this formulation the problem has obvious similarities with the classical problem of finding central configurations[5] (which arise in a similar way when a time dependent homothetic ansatz is used in Newton's equations of motion for gravitating point particles) or equivalently solutions of the one component plasma (OCP) model.[6] The OCP model describes point charges immersed in a uniform background of charge with the opposite sign. Hence there are two competing forces. The first is an attraction towards the origin, represented by exactly the same expression as the first term in (2.13), and repulsion between the points, which in the OCP case is described by the Coulomb energy. The second term in (2.13) plays a similar role in our problem as the Coulomb energy does in the OCP model. The contribution of this nonpositive term produces two-body particle repulsions which can balance the attractive central force, producing stable minimal energy configurations with finite nonzero separations.

In the remainder of this section we shall restrict to the case when all the monopole masses are equal. By rescaling the positions $\mathbf{y}_k$ by the inverse of this common mass we obtain the situation in which all monopole masses are equal to unity, so for the rest of this section we set $m_i=1$ for all $i=1,\ldots,n$.

Although any critical point of the energy (2.13) will provide us with a geodesic on the Lee–Weinberg–Yi manifold we shall concentrate only on local minima, since these are the easiest to find numerically, and ignore any saddle point solutions. Presumably Leech's symmetric configurations,[19] which are sets of particles on a sphere in equilibrium under any force law between pairs of particles, will also yield critical points of (2.13) if the particles are allowed to move off the sphere, but are required to maintain all symmetries of the spherical configuration. Leech's configurations consist of an infinite family of polygons and bipyramids and a finite family with Platonic symmetry.

TABLE I. For $2\leqslant n\leqslant 20$ we list the energy E of the minimizing configuration, its symmetry group G, the distance from the origin of the closest point $r_{\min}$, and the distance from the origin of the furthest point $r_{\max}$.

n	E	G	$r_{\min}$	$r_{\max}$
2	−1.0000	$D_{\infty h}$	1.0000	1.0000
3	−4.5000	D_{3h}	1.7321	1.7321
4	−12.0000	T_d	2.4495	2.4495
5	−24.5916	D_{3h}	3.1018	3.1592
6	−43.9706	O_h	3.8284	3.8284
7	−71.0162	C_1	4.4782	4.5635
8	−107.5011	D_{4d}	5.1841	5.1841
9	−154.5499	D_{3h}	5.8376	5.8718
10	−213.5297	D_{4d}	6.5099	6.5412
11	−285.6593	C_{2v}	7.1648	7.2435
12	−372.7470	Y_h	7.8819	7.8819
13	−475.3419	C_{2v}	8.5186	8.5980
14	−595.4323	D_{6d}	9.2142	9.2749
15	−734.0923	D_3	9.8771	9.9279
16	−892.7338	T	10.5541	10.5925
17	−1072.6591	D_{5h}	11.2308	11.2368
18	−1275.2163	D_{4d}	11.8834	11.9107
19	−1501.5794	C_{2v}	12.5491	12.5987
20	−1753.4547	D_{3h}	13.2348	13.2518

The numerical scheme employed is a multi-start gradient flow algorithm with randomly distributed initial conditions. The energy function (2.13) has the obvious SO(3) invariance associated with a spatial rotation of all n points, and also reflection symmetries which change the sign of any one of the three Cartesian components of all the points. Up to the action of these symmetry groups, all the minimal energy solutions we find are unique.

The case $n=1$ is trivial; the minimal energy solution is a single point at the origin, with $E=0$, and hence the scaling solution is time independent, so no geodesic is obtained. For two points the minimal energy is $E=-1$ which occurs if $\mathbf{y}_1=-\mathbf{y}_2=(0,0,1)$, or any spatial rotation of this configuration. In other words, the two monopoles are at antipodal points on the unit sphere. The associated geodesic describes the head-on collision of two monopoles, in which the spherically symmetric two-monopole is formed, after which the monopoles bounce back off each other. This scattering process was first described by Connell,[9] who discovered that the metric on the centered moduli space of two different fundamental SU(3) monopoles is Taub-NUT with a positive mass parameter.

In Table I we present, for $2\leqslant n\leqslant 20$, the energy E of the minimizing configuration, its symmetry group G, the distance from the origin of the closest point $r_{\min}$, and the distance from the origin of the furthest point $r_{\max}$.

In the examples in Table I where $r_{\min}$ is equal to $r_{\max}$, to the accuracy presented they are in fact precisely equal, indicating that all the points lie on the surface of a sphere of radius $r_{\min}=r_{\max}$. For all the other cases it can be seen that $r_{\min}$ and $r_{\max}$ are very close in value, showing that all n points lie close to, but not exactly on, a sphere. As we shall see later, this feature appears to persist for arbitrarily large values of n, which contrasts sharply with traditional central configurations with a Coulomb interaction, where this property exists only for $n<13$ and beyond this value there are multiple shells.[5] It is interesting to note that a scale invariant geometric energy function exists which also yields minimal energy configurations on a single shell for all numbers

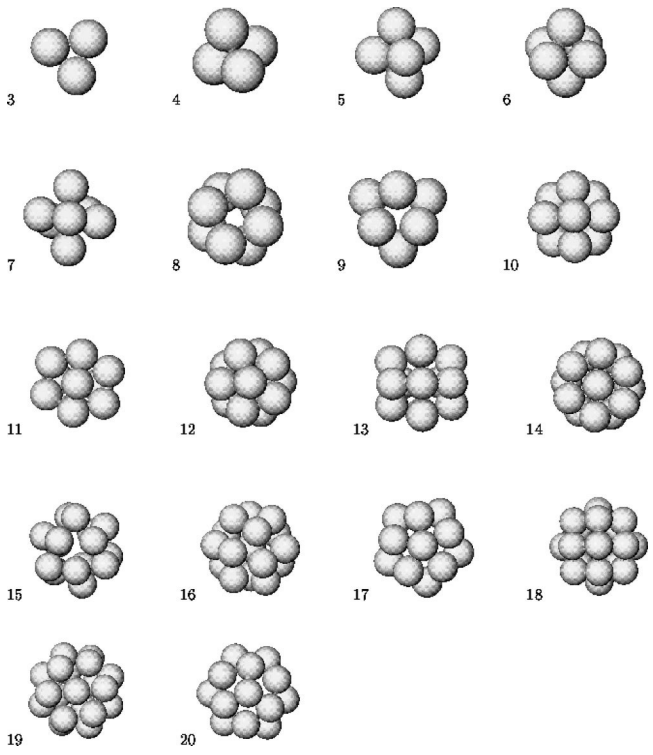

FIG. 1. For $3\leqslant n\leqslant 20$ we display the configurations of n points (not to scale) by plotting spheres around each of the points. In each case the diameter of the spheres is equal to the minimal separation between points, to emphasize the sphere packing behavior.

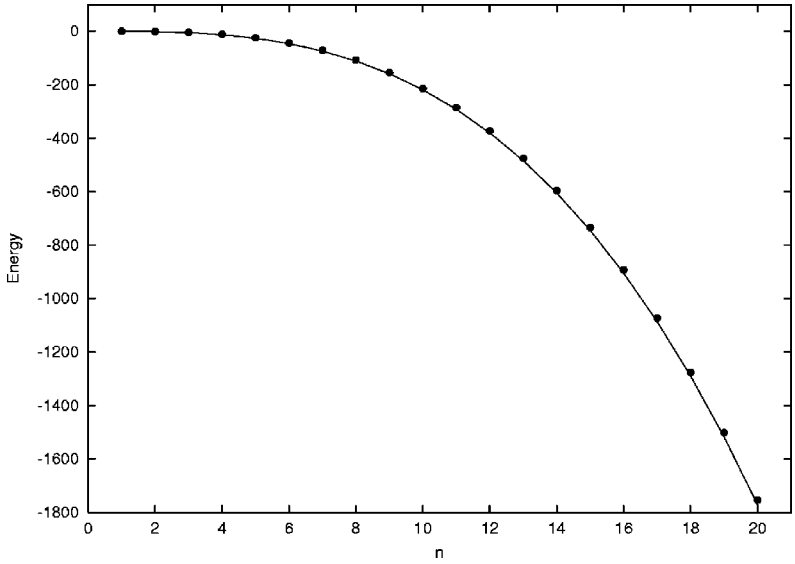

FIG. 2. The energy as a function of n (circles) and the estimate described in the text (curve).

of points.[4] It would be interesting to try and classify the properties of interaction potentials which produce only a single shell.

In Fig. 1 we present, for $3 \leqslant n \leqslant 20$, the minimal energy configurations of n points by plotting spheres around each of the points and in Fig. 2 we plot their energy as a function of n, for $n \leqslant 20$. In each case the diameter of the spheres is equal to the minimal separation between points, to emphasize the sphere packing behavior. As seen from Table I, the size of the configuration (as measured by $r_{\max}$) grows with n, so for clarity we do not display the configurations to scale. Three points lie on the vertices of an equilateral triangle, with edge length equal to 3. For $n > 3$ the points may be considered as forming the vertices of a polyhedron, which generically is a deltahedron, that is, all faces are triangular. For example, four points lie on the vertices of a tetrahedron with edge length equal to 4. For $n = 4,6,8,12$ all points lie exactly on the surface of a sphere, and in fact on the vertices of a tetrahedron, octahedron, square antiprism and icosahedron, respectively.

As can be seen from Table I and Fig. 1 the points are often arranged symmetrically, though the case $n = 7$ is rather anomalous. There is an obvious D_{5h} symmetric candidate for the minimal energy $n = 7$ configuration, in which five points lie on the vertices of a regular pentagon and the two remaining points lie on the fivefold symmetry axis equidistant from the origin. This regular bipyramid is the obvious generalization of the minimal $n = 5$ configuration, which is a bipyramid with a triangular base. However, the minimal energy solution for $n = 7$ is a symmetry breaking perturbation of the bipyramid. There are points at the north and south poles of a sphere of radius 4.5635, and the remaining five points lie in a roughly pentagonal distribution, but all with slightly different heights above or below the equatorial plane and different distances from the origin, which range from 4.4782 to 4.4825. Clearly this prohibits any exact symmetry, even reflection symmetries, so we label the symmetry group as C_1, indicating no point symmetries. As a check it is possible to minimize within the family of D_{5h} symmetric configurations, yielding an energy of $E = -71.0156$, which is indeed slightly higher than the asymmetric minimum with $E = -71.0162$.

To gain insight into minimizing the energy function (2.13) (with $m_k = 1$) it is useful to consider the restricted problem in which all the points are constrained to lie on a sphere of a given radius ρ. The energy of this restricted problem is given by

$$E_\rho = \tfrac{1}{2}\rho^2 n + \rho U, \tag{2.14}$$

where

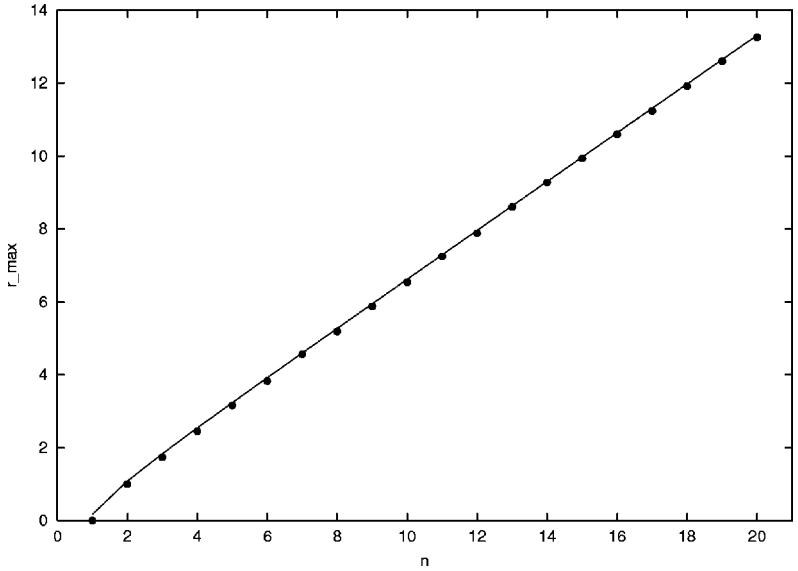

FIG. 3. The size of the configuration $r_{\max}$ as a function of n (circles) and the estimate ρ described in the text (curve).

$$U=-\sum_i \sum_{j<i} |\mathbf{Y_i}-\mathbf{Y_j}|\,, \tag{2.15}$$

for n points $\mathbf{Y_k}=\mathbf{y}_k/\rho$ restricted to lie on the surface of the unit sphere. Minimization of the function U for points on the unit sphere is a problem in discrete geometry which was first posed almost 50 years ago by Fejes Tóth,[11] though it is usually phrased in terms of maximizing the sum of the mutual separations $-U$. There are a number of theorems proved about the extrema of this energy function and in particular there is the lower bound[1]

$$U>\tfrac{1}{2}-\tfrac{2}{3}n^2. \tag{2.16}$$

Using this result in (2.14) we obtain a lower bound for E_ρ which we can then minimize over the radius ρ, finding a minimum value at

$$\rho=\frac{2n}{3}-\frac{1}{2n}, \tag{2.17}$$

to obtain the lower bound

$$E_{\text{sphere}}>-(\tfrac{2}{9}n^3-\tfrac{1}{3}n+\tfrac{1}{8})\,, \tag{2.18}$$

where E_{sphere} denotes the energy (2.13) (with $m_k=1$) under the restriction that all points lie at the same distance from the origin. Clearly when we drop this restriction we have no rigorous lower bound for the unrestricted energy (2.13) which is our main concern, but since our numerical results suggest that in all the minimal energy configurations the points lie very close to the surface of a sphere, then we expect that the quantity in (2.18) will be a good estimate of the minimal energy value, though it will tend to be slightly lower. In Fig. 2 we plot this estimate as the curved line. Clearly the above expectations appear to be realized, in that the estimate is close to the true value, but bounds it from below. In Fig. 3 we compare the estimate (2.17) (curve) for the size of the configuration with the numerical values as measured by $r_{\max}$ (circles). Again it can be seen that the estimate is quite accurate.

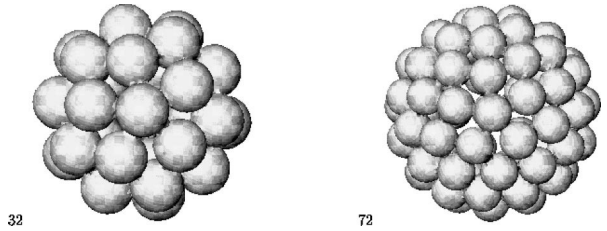

FIG. 4. For $n=32$ and $n=72$ we display the icosahedrally symmetric minimal energy configurations by drawing spheres around the monopoles.

The above discussion suggests that our minimal energy solutions are closely related to those which maximize the sum of the mutual separations for points on a sphere. For $n=2,3,4,8,12$ it is proved that the extremal configurations for this sphere problem are the dipole, triangle, tetrahedron, octahedron and icosahedron, respectively (see Ref. 2 and references therein), which agrees with our results. For $n\leqslant 10$ this problem was investigated numerically by Berman and Hanes[7] and more recently a comprehensive numerical investigation has been performed by Rakhmanov, Saff, and Zhou,[21] who studied all $n\leqslant 200$ and obtained the symmetry groups of the extremal configurations. A comparison of the symmetry groups in Table I with those that appear in Ref. 21 reveals that the groups agree for all cases except $n=7$. (In Ref. 21 the symmetry group for 18 points should read D_{4d} not D_{4h}.) In Ref. 21 the symmetry group for $n=7$ is given as C_2 and in Ref. 7 the configuration is described as two almost antipodal points with the remaining five points sprinkled around an equatorial band. Our configuration for $n=7$ is therefore consistent with a small deformation of the spherical extremal solution, which itself has little symmetry.

For all $1\leqslant n\leqslant 20$ we found only one local minimum of the energy for each value of n, except for $n=16$. For $n=16$ the global minimum with $E=-892.7338$ has tetrahedral symmetry T, but we also found a local minimum with energy $E=-892.7256$ and symmetry D_{4h}. Once again this mirrors the situation in studying extremal problems for points on a sphere.[10]

In order to further investigate the similarites between our solutions and points on the sphere which maximize the sum of the mutual separations we turn our attention to configurations with icosahedral symmetry. For the sphere problem extremal configurations with icosahedral symmetry occur for a sequence of points[21] which begins $n=12,32,72,...$ As we have seen, for $n=12$ our solution has icosahedral symmetry, with the points lying on the vertices of an icosahedron, so it is interesting to compute the minimal energy solutions for $n=32$ and $n=72$, to see if they are icosahedrally symmetric.

In Fig. 4 we display the minimal energy configurations for $n=32$ and $n=72$, using the same method as in Fig. 1. Both configurations contain a single shell and have icosahedral symmetry, as predicted by analogy with the sphere problem. For $n=32$ there are 12 points on the vertices of an icosahedron at a distance of 21.2516 from the origin and a further 20 points at a distance of 21.2680 from the origin. The associated polyhedron is the dual of a truncated icosahedron and the energy is $E=-7233.0539$. For $n=72$ the energy is $E=-82\,780.0335$. There are 12 points at a distance of 47.9338 and 60 points at a distance of 47.9563.

III. DISTINCT MASSES AND SU(2) MONOPOLES

In this section we mention two extensions of the study we have described so far. The first is the obvious generalization to monopoles which are not all of equal mass. As stated earlier, if all monopoles have the same mass, then varying this mass produces the same configuration but scaled by the inverse common mass. Thus, the expectation for sets of distinct masses is that multiple shells will arise, with monopoles grouped into shells according to their mass, so that the heaviest monopoles sit closest to the origin, and with each set of monopoles in a given shell being arranged on the vertices of the polyhedron which arises in the minimization of the relevant number of equal mass monopoles. This nested polyhedron picture is consistent with the numerical results we have

obtained. For example, in the case of two distinct masses and four monopoles of each mass, we set $m_i=1$, for $i=1,..,4$ and $m_i=2$, for $i=5,..,8$; the resulting configuration is that the four heavy monopoles sit on the vertices of a tetrahedron at a distance 1.5940 from the origin and the four light monopoles sit on the vertices of the dual tetrahedron scaled so that they are at a distance 6.3543 from the origin. As another example, with 12 light monopoles (with mass one) and six heavy monopoles (with mass two) the nested polyhedra are an octahedron and an icosahedron with scales 2.6954 and 13.8057, respectively, and oriented so as to preserve their common tetrahedral subgroups. Clearly the relative orientations of sets of nested polyhedra, together with their deformation as very distinct monopole masses are varied towards equality, are interesting problems which are likely to need substantial investigation in each specific case.

The second extension we consider is to relate our results to the dynamics of well separated SU(2) monopoles. Although, for $n>2$, the moduli space metric for n SU(2) monopoles is not known explicitly, the asymptotic metric is known, which is valid in the region where all the monopoles are well separated.[12] This is the Gibbons–Manton metric and it is related to the Lee–Weinberg–Yi metric through some sign changes. Explicitly, the Gibbons–Manton metric is obtained by replacing Eqs. (2.2)–(2.5) by the equations

$$g_{ii}=m_i-\sum_{j\neq i}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}, \tag{3.1}$$

$$g_{ij}=\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}, \quad i\neq j, \tag{3.2}$$

$$\mathbf{W}_{ii}=-\sum_{j\neq i}\mathbf{w}_{ij}, \tag{3.3}$$

$$\mathbf{W}_{ij}=\mathbf{w}_{ij}, \quad i\neq j. \tag{3.4}$$

If the approach of the previous section is now applied to this metric to find time dependent homothetic solutions then, due to the sign changes, the upshot is that Eq. (2.10) is once again obtained, but with the replacement $C\mapsto -C$. In this case the physically acceptable solution is therefore to choose $C=-1$. With this choice both the function $\alpha(t)$ and the positions $\mathbf{y}_k$ that we have found to provide geodesics for the Lee–Weinberg–Yi metric carry over unchanged to produce geodesics of the Gibbons–Manton metric. The difference now is that these geodesics are only valid in the region where all the monopole are well separated, so the solutions break down before they can describe the collision of the monopoles.

For example, for $n=4$, the scaling geodesic describes the scattering of four monopoles on the vertices of a contracting tetrahedron. In fact, by using symmetry arguments, the full geodesic, to which this is a good approximation in the well separated regime, has been found and shows that as the monopoles approach they pass through a monopole solution with cubic symmetry and emerge on the vertices of an expanding tetrahedron which is dual to the incoming one.[15] For this example, even the metric is known exactly in terms of elliptic integrals.[8]

It might be amusing to attempt to identify the outcomes of the various SU(2) monopole scatterings that begin as the contracting polyhedra that we have identified, particularly those with high symmetry. However, a note of caution must be applied in this situation. The Gibbons–Manton metric possesses an n-torus isometry which the true monopole metric does not have for any finite separation. This means that the symmetry of a contracting polyhedron may only be realized in the true SU(2) monopole solution at the limit of infinite separation. As an example of this situation consider the case $n=6$, where the contracting polyhedron is an octahedron. Using the one-to-one correspondence[17] between SU(2) n-monopoles and (an equivalence class of) rational maps between Riemann spheres of degree n we may determine the dimension of the moduli space of octahedrally symmetric SU(2) monopoles of charge six. Degree six polynomials form the carrier space for the 7-dimensional irreducible representation of SU(2) and when this representa-

tion is restricted to the octahedral group it decomposes into irreducible representations of the octahedral group of dimensions one, three and three. Since two polynomials are required to form a rational map this shows that there are no octahedrally symmetric rational maps of degree six, and hence no octahedrally symmetric charge six monopoles. Thus six SU(2) monopoles placed on the vertices of an octahedron break the octahedral symmetry for any finite value of the separation, no matter how large. This contrasts with the above mentioned case of $n=4$ with tetrahedral symmetry. The five-dimensional irreducible representation of SU(2) when restricted to the tetrahedral group decomposes into two one-dimensional representations and a three-dimensional representation. The basis polynomials for the two one-dimensional representations yield a one-parameter family of tetrahedrally symmetric degree three rational maps, which corresponds to the geodesic describing the tetrahedral scattering of four monopoles.[14] Thus, in some cases the symmetry of the scaling geodesics of the Gibbons–Manton metric may be true symmetries of related geodesics in the true moduli space and in others they may not.

IV. CONCLUSION

The scattering of n distinct fundamental monopoles can be approximated by geodesic motion on the Lee–Weinberg–Yi manifold. We have described a variational method to construct some geodesics on this manifold for arbitrary values of n, and applied it to obtain a number of examples. The energy function used in this approach has features similar to that which arises in the classic problem of determining central configurations, but in contrast to central configurations it yields points which lie on a single shell for arbitrary values of n. The geodesics constructed by our method describe the scattering of monopoles on the vertices of a contracting, and then expanding, polyhedron, which generically is a deltahedron. We have found, and exploited, similarities between the deltahedra obtained here and those which arise in the problem of maximizing the sum of the mutual separations for points on a sphere.

ACKNOWLEDGMENTS

We thank Ed Saff and Nikolay Andreev for useful correspondence and acknowledge advanced fellowships from PPARC (RAB) and EPSRC (PMS).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Icosahedral Skyrmions

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(Received 17 October 2002; accepted 9 April 2003)

In this article we aim to determine the baryon numbers at which the minimal energy Skyrmion has icosahedral symmetry. By comparing polyhedra which arise as minimal energy Skyrmions with the dual of polyhedra that minimize the energy of Coulomb charges on a sphere, we are led to conjecture a sequence of magic baryon numbers, $B=7,17,37,67,97,\ldots$, at which the minimal energy Skyrmion has icosahedral symmetry and unusually low energy. We present evidence for this conjecture by applying a simulated annealing algorithm to compute energy minimizing rational maps for all degrees up to 40. Further evidence is provided by the explicit construction of icosahedrally symmetric rational maps of degrees 37, 47, 67 and 97. To calculate these maps we introduce two new methods for computing rational maps with Platonic symmetries. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1584209]

I. INTRODUCTION

Skyrmions are topological solitons in three space dimensions which are candidates for an effective description of nuclei, with an identification between soliton and baryon numbers.[10] Recently, the minimal energy Skyrmions for all baryon numbers $1\leqslant B\leqslant 22$ were computed and their symmetries identified.[3] The baryon density of these Skyrmions is localized around the vertices and edges of polyhedra, which are almost always trivalent, and for $B\geqslant 7$ are composed of 12 pentagons and $2B-14$ hexagons, with only a few exceptions (which can be understood by a symmetry enhancement principle). These Skyrmions have discrete point group symmetries, including occasional Platonic symmetries. For $B=7$ and $B=17$ the minimal energy Skyrmion is particularly symmetric, having icosahedral symmetry Y_h, and the value of the energy is unusually low. However, there are other baryon numbers at which icosahedral Skyrme fields exist, but the minimal energy Skyrmion has less symmetry. This motivates the main question addressed in this article, namely, what are the magic baryon numbers at which the minimal energy Skyrmion has icosahedral symmetry with a resulting unusually low energy?

To gain some insight into this problem we note that, as first observed in Ref. 2, there is a close relationship between the polyhedra which arise as minimal energy Skyrmions and the duals of polyhedra which occur in the problem of minimizing point Coulomb charges on a sphere. This latter problem is often known as the Thomson problem, even though he appears not to have posed it explicitly, and we shall use this nomenclature here. The Thomson problem is well studied for up to 200 points on the sphere[9] and generically the n points sit at the vertices of a combinatoric

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TABLE I. The symmetry group G_B of the minimal energy Skyrmion with baryon number B and the symmetry group H_B of the $2B-2$ points which minimize the Thomson problem.

B	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
G_B	$O(3)$	$D_{\infty h}$	T_d	O_h	D_{2d}	D_{4d}	Y_h	D_{6d}	D_{4d}	D_3	D_{3h}	T_d	O	C_2	T	D_2	Y_h	D_2	D_3	D_{6d}	T_d	D_3
H_B	$O(3)$	$D_{\infty h}$	T_d	O_h	D_{4d}	D_{4d}	Y_h	D_{6d}	T	D_{4d}	D_{3h}	T_d	O	C_2	T	D_2	Y_h	D_2	D_2	D_{6d}	T_d	D_{5h}

deltahedron. Taking the dual of a deltahedron leads to a trivalent polyhedron, which is the class of polyhedra which generically arise for Skyrmions. A Skyrmion polyhedron with baryon number B has $2B-2$ faces, so to identify this with the dual of a Thomson polyhedron requires that we consider $n=2B-2$ Coulomb charges on the sphere. Let us denote by G_B the symmetry of the minimal energy Skyrmion with baryon number B and by H_B the symmetry of the minimal energy Thomson configuration of $2B-2$ points on the sphere. Extracting the information from Refs. 3 and 5 we obtain Table I, in which we compare the symmetries of the minimal energy configurations for each problem.

From Table I it is clear that although a variety of different Platonic, dihedral and cyclic symmetry groups occur, there is a remarkable match for the two problems in 17 out of the 22 cases. Moreover, a closer inspection reveals that in these 17 cases not only do the symmetry groups match, but the combinatorial types of the Skyrmion polyhedron and the dual of the Thomson polyhedron are identical. The five examples that do not coincide, $B=5,9,10,19,22$, show that the topography of the two energy functions is slightly different and suggest that the same factors which determine the polyhedron (or its dual) are important, but perhaps with slightly different weightings. For example, for $B=9$ and $B=10$, which are not particularly low in energy, it is known that Skyrmion configurations exist which have the symmetries required to match to those of the Thomson problem, but that they have very slightly higher energy than the minimal energy Skyrmion. The fact that there is so often an agreement for the two problems leads us to believe that, in the cases where particularly symmetric low energy configurations arise, they will be the minima in both problems. Thus, as a working hypothesis to test, we shall postulate that G_B is the icosahedral group only if H_B is also the icosahedral group. Although the Thomson problem is a difficult one to study numerically, it is certainly much easier than finding minimal energy Skyrmions, so we can take advantage of the known numerical results. Minimal energy configurations are currently available for up to 200 points, that is, $B\leqslant 101$, and of these the values $B=7,17,37,62,67,97$ are selected as magic numbers at which the configuration has icosahedral symmetry and unusually low energy when compared to a numerical fit of all 200 configurations.[9] As we describe later, the case $B=62$ is rather different from the others in the sequence, so we shall leave this example out for the moment. We are thus led to conjecture that there is a sequence $B=7,17,37,67,97,\ldots$ at which the minimal energy Skyrmion has icosahedral symmetry and unusually low energy. In the rest of this article we perform some investigations to test this conjecture, and hence the connection between Skyrmions and the Thomson problem.

II. MINIMIZING RATIONAL MAPS

A static Skyrme field, $\mathrm{U}(\mathbf{x})$, is an SU(2) matrix defined throughout $\mathbb{R}^3$ and satisfying the boundary condition that $U\to 1$ as $|\mathbf{x}|\to\infty$. This boundary condition implies a compactification of space so that the Skyrme field becomes a mapping $U:S^3\mapsto \mathrm{SU}(2)$, and so can be classified by an integer valued winding number

$$B=\frac{1}{24\pi^2}\int \epsilon_{ijk}\,\mathrm{Tr}(\partial_i U\,U^{-1}\partial_j U\,U^{-1}\partial_k U\,U^{-1})\,d^3x, \tag{2.1}$$

which is a topological invariant. This winding number counts the number of solitons in a given field configuration and is identified with baryon number in the application to modeling nuclei.

The energy of a static Skyrme field is given by

$$E=\frac{1}{12\pi^2}\int \mathrm{Tr}\left(-\frac{1}{2}(\partial_i U\,U^{-1})^2-\frac{1}{16}[\partial_i U\,U^{-1},\partial_j U\,U^{-1}]^2\right)d^3x \tag{2.2}$$

and, for each integer B, the problem is to minimize this energy within the class of fields with baryon number B in order to find the minimal energy Skyrmion. This problem has been solved numerically for all $B\leqslant 22$ (Ref. 3) yielding the results presented in Table I for the symmetries of the minimal energy Skyrmions. When we refer to the symmetry of a Skyrmion we do not mean that the Skyrme field itself is invariant under particular spatial rotations, but rather that the effect of a spatial rotation can be undone by the application of the global SO(3) symmetry of the Skyrme model, which acts through the conjugation $U\mapsto \mathcal{O}U\mathcal{O}^{\dagger}$, where $\mathcal{O}\in \mathrm{SU}(2)$ is a constant matrix. In particular this means that the baryon and energy densities [the integrands in (2.1) and (2.2)] are strictly invariant.

It is computationally prohibitive to apply the full numerical scheme to larger values of B at the present time, but fortunately an approximation method has been developed which provides very accurate results. This is the rational map ansatz,[7] where a Skyrme field with baryon number B is constructed from a degree B rational map between Riemann spheres. Although this ansatz does not give exact solutions of the static Skyrme equations, it produces approximations which have energies only a few percent above the numerically computed solutions. Briefly, use spherical coordinates in $\mathbb{R}^3$, so that a point $\mathbf{x}\in\mathbb{R}^3$ is given by a pair (r,z), where $r=|\mathbf{x}|$ is the distance from the origin, and z is a Riemann sphere coordinate giving the point on the unit two-sphere which intersects the half-line through the origin and the point $\mathbf{x}$. Now, let $R(z)$ be a degree B rational map between Riemann spheres, that is, $R=p/q$ where p and q are polynomials in z such that $\max[\deg(p),\deg(q)]=B$, and p and q have no common factors. Given such a rational map the ansatz for the Skyrme field is

$$U(r,z)=\exp\left[\frac{if(r)}{1+|R|^2}\begin{pmatrix}1-|R|^2 & 2\overline{R}\\ 2R & |R|^2-1\end{pmatrix}\right], \tag{2.3}$$

where $f(r)$ is a real profile function satisfying the boundary conditions $f(0)=\pi$ and $f(\infty)=0$, which is determined by minimization of the Skyrme energy of the field (2.3) given a particular rational map R.

Substitution of the rational map ansatz (2.3) into the Skyrme energy functional results in the following expression for the energy

$$E=\frac{1}{3\pi}\int\left(r^2f'^2+2B(f'^2+1)\sin^2 f+\mathcal{I}\frac{\sin^4 f}{r^2}\right)dr\,, \tag{2.4}$$

where $\mathcal{I}$ denotes the integral

$$\mathcal{I}=\frac{1}{4\pi}\int\left(\frac{1+|z|^2}{1+|R|^2}\left|\frac{dR}{dz}\right|\right)^4\frac{2i\;dz\,d\overline{z}}{(1+|z|^2)^2}. \tag{2.5}$$

To minimize the energy (2.4) one first determines the rational map which minimizes $\mathcal{I}$, then given the minimum value of $\mathcal{I}$ it is a simple exercise to find the minimizing profile function. Thus, within the rational map ansatz, the problem of finding the minimal energy Skyrmion reduces to the simpler problem of calculating the rational map which minimizes the function $\mathcal{I}$.

The baryon density of the rational map $R=p/q$ is proportional to the Wronskian

$$w(p,q)=p'q-q'p \tag{2.6}$$

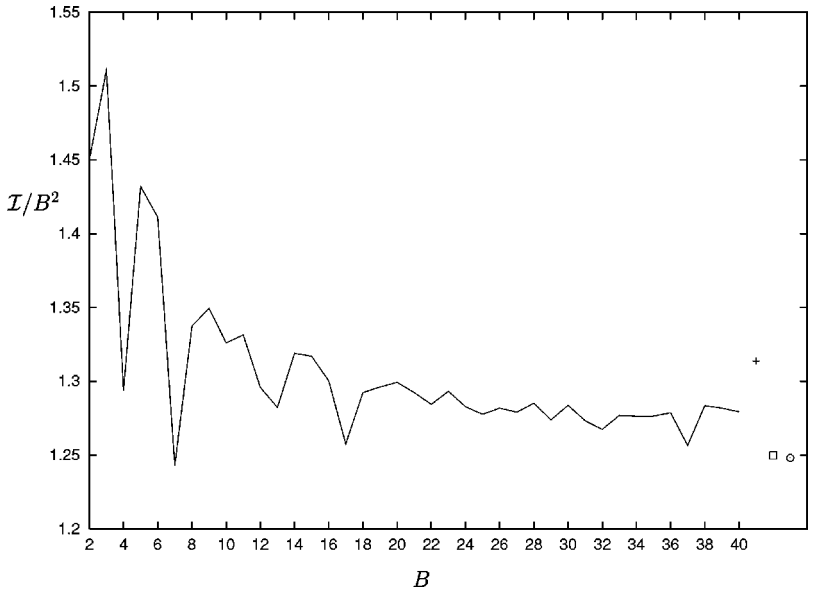

FIG. 1. $\mathcal{I}/B^2$ for $2 \leqslant B \leqslant 40$, as calculated by $\mathcal{I}$ minimizing simulated annealing computations. Also shown are the values of $\mathcal{I}/B^2$ for the icosahedrally symmetric Skyrmions with $B=47$ (cross), $B=67$ (square) and $B=97$ (circle), discussed in the text.

which has $2B-2$ roots, giving the points on the Riemann sphere for which the baryon density vanishes along the corresponding half-lines through the origin. These $2B-2$ points on the sphere give the face-centers of the Skyrmion polyhedron, or equivalently the vertices of the dual polyhedron which is associated with the Thomson problem.

Using a simulated annealing algorithm the $\mathcal{I}$ minimizing rational maps for $1 \leqslant B \leqslant 22$ have been computed[3] and found to be in good agreement with the results of full Skyrme field minimization. Here we extend the simulated annealing computation to $B \leqslant 40$, in an attempt to determine particularly low energy magic numbers. In the Thomson problem the magic numbers are determined by comparing the energy of minimal solutions with the energy of a numerical fit to the data of all known minimal energy solutions—thereby isolating cases where the energy is lower than the expected fit. In the problem of minimizing rational maps it turns out that there is a more natural approach, due to the fact that a useful lower bound exists. Using a simple inequality it is shown in Ref. 7 that $\mathcal{I} \geqslant B^2$. It turns out that examining the excess above this bound, by computing the quantity $\mathcal{I}/B^2$, is a good diagnostic tool for highlighting low energy maps, and in particular is more useful than simply calculating the energy of the associated Skyrme field. We illustrate this in Fig. 1 by plotting $\mathcal{I}/B^2$ for the results of our simulated annealing computations for $2 \leqslant B \leqslant 40$. There are clear dips at the magic numbers $B=7$ and $B=17$, corresponding to the already known low energy icosahedral Skyrmions (see Table I). There are also dips at $B=4$ and $B=13$, where it is known that the Skyrmions also have Platonic symmetry, but this time octahedral (see Table I). However, there is one more major dip at $B=37$, and this is precisely the value predicted as the next magic number in the icosahedral sequence suggested by comparison with the Thomson problem. This result, therefore, provides strong support for our conjectured sequence, providing we can prove that this low energy degree 37 map obtained from simulated annealing does indeed have icosahedral symmetry. This will be discussed in the next section.

Note that the quantity $\mathcal{I}/B^2$ appears to be tending towards an asymptotic value of around 1.28, apart from magic numbers where it drops to around 1.25. It would be interesting to understand this approach to a relatively constant value, as well as its magnitude.

In Fig. 2 we plot the energy per baryon E/B of the Skyrmions constructed from the minimizing maps with $1 \leqslant B \leqslant 40$. The dips at the magic numbers are clearly visible in Fig. 2, reproducing the sequence displayed in Fig. 1. However, in this case the dips are superimposed upon a general

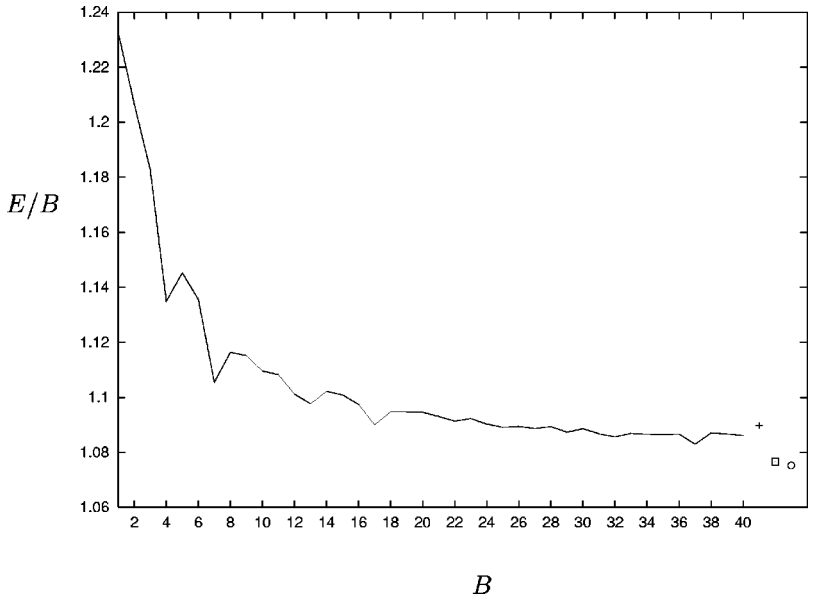

FIG. 2. The energy per baryon E/B of the Skyrmions constructed from the minimizing maps with $1 \leqslant B \leqslant 40$. Also shown are the values of E/B for the icosahedrally symmetric Skyrmions with $B=47$ (cross), $B=67$ (square) and $B=97$ (circle), discussed in the text.

decrease of E/B with increasing B, which is why we regard the quantity $\mathcal{I}/B^2$ as a more useful diagnostic than E/B.

The radius of a Skyrmion produced from the rational map ansatz can be defined as the radial value, r_*, at which the profile function is equal to $\pi/2$. In Fig. 3 we plot r_*^2 as a function of B for $1 \leqslant B \leqslant 40$. This clearly shows that the radius has a $\sqrt{B}$ dependence, and given that all these configurations are reasonably close to the Faddeev–Bogomolny energy bound $E \geqslant |B|$, this means that the energy grows like the square of the radius, as expected for a shell-like structure. Note that

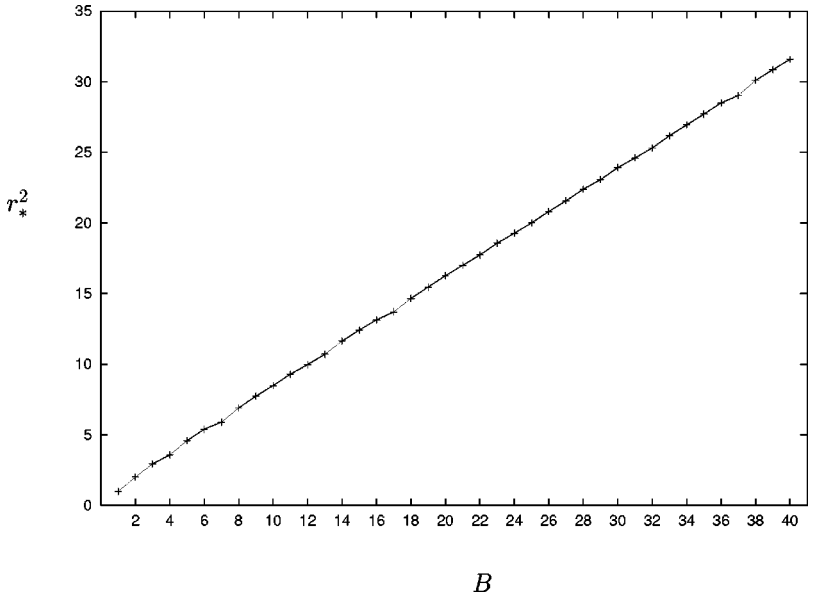

FIG. 3. r_*^2, the squared radius of the Skyrmion, as a function of baryon number B.

at the magic numbers the radius of the Skyrmion is slightly less than expected, presumably due to a more compact arrangement of a particularly symmetric energy density.

III. COMPUTING ICOSAHEDRAL MAPS

Recall that a Skyrmion is symmetric under a group $G \subset \mathrm{SO}(3)$, if a spatial rotation $g \in \mathrm{SO}(3)$ can be compensated by an action of the global SO(3) symmetry. In terms of the rational map approach a spatial rotation acts on the Riemann sphere coordinate z as an SU(2) Möbius transformation. Similarly the global symmetry acts on the Riemann sphere coordinate R of the target two-sphere as an SU(2) Möbius transformation. Hence, a map is G-symmetric if, for each $g \in G$, there exists a target space rotation D_g such that $R(g(z)) = D_g(R(z))$. Since we are dealing with SU(2) transformations the set of target space rotations will form a representation of the double group of G, but we shall continue to call this G.

To determine the existence and compute particular symmetric rational maps is a matter of classical group theory. We are concerned with degree B polynomials which form the carrier space for $B+1$, the $(B+1)$-dimensional irreducible representation of SU(2). Now, as a representation of SU(2) this is irreducible, but if we only consider the restriction to a subgroup G, $\underline{B+1}|_G$, this will, in general, be reducible. What we are interested in is the irreducible decomposition of this representation and tables of these subductions can be found, for example, in Ref. 1.

The simplest case in which a G-symmetric degree B rational map exists is if

$$\underline{B+1}|_G = E + \cdots, \tag{3.1}$$

where E denotes a two-dimensional representation. Here, and in the following, the dots denote other representations which are not relevant. In this case a basis for E consists of two degree B polynomials which can be taken to be the numerator and denominator of the rational map. A subtle point which needs to be addressed is that the two basis polynomials may have a common root, in which case the resulting rational map is degenerate and does not correspond to a genuine degree B map.

More complicated situations can arise, for example, if

$$\underline{B+1}|_G = A_1 + A_2 + \cdots, \tag{3.2}$$

where A_1 and A_2 denote two one-dimensional representations, then a whole one-parameter family of maps can be obtained by taking a constant multiple of the ratio of the two polynomials which are a basis for A_1 and A_2, respectively. An m-parameter family of G-symmetric maps can be constructed if the decomposition contains $(m+1)$ copies of a two-dimensional representation, that is,

$$\underline{B+1}|_G = (m+1)E + \cdots, \tag{3.3}$$

where the m (complex) parameters correspond to the freedom in the choice of one copy of E from $(m+1)E$.

A detailed explanation of how to explicitly calculate any required symmetric map is given in Ref. 7. However, this approach involves computing appropriate projectors which are matrices of size $(B+1)\times(B+1)$, and even with the use of symbolic computational packages this procedure becomes cumbersome for the large values of B that we are interested in here. In this section we therefore describe and apply two new, more convenient, methods for calculating symmetric maps. We shall concentrate on the situation of relevance to this article, where $G = Y$, the icosahedral group, but the methods are applicable for any G.

Before we describe our new approaches we need to recall some facts about representations of the icosahedral group and Klein polynomials of the icosahedron. The icosahedral group Y has the trivial one-dimensional representation A and two two-dimensional representations, which we de-

note by E_1' and E_2', with a prime denoting the fact that these are proper representations of the double group. There are also three-, four-, five- and six-dimensional representations, but we shall not need these here.

Klein polynomials are strictly invariant polynomials for the Platonic groups.[8] Since

$$\underline{13}|_Y = A + \cdots, \tag{3.4}$$

this implies that there is degree 12 invariant polynomial. This is the Klein polynomial given by

$$k_v = z^{11} + 11z^6 - z \tag{3.5}$$

and although it appears to have degree 11, it should be thought of as having degree 12 with one root at infinity. The roots of this polynomial, considered as points on the Riemann sphere, are located at the vertices of a suitably oriented and scaled icosahedron. The same construction, but using the face-centers and mid-points of the edges of the icosahedron, in place of the vertices, produces the Klein polynomials

$$k_f = z^{20} - 228z^{15} + 494z^{10} + 228z^5 + 1, \tag{3.6}$$

$$k_e = z^{30} + 522z^{25} - 10\,005z^{20} - 10\,005z^{10} - 522z^5 + 1, \tag{3.7}$$

which are also Y-invariant, by construction.

A. Polarization

In this subsection we describe our polarization method for computing symmetric maps. It has similar features to the polarization technique used to construct symmetric Nahm data.[6]

Suppose we wish to obtain the symmetric degree B map associated with the decomposition

$$\underline{B+1}|_Y = E + \cdots, \tag{3.8}$$

where E denotes one of the two-dimensional representations. The above fact implies that

$$E \otimes \underline{B+1}|_Y = A + \cdots, \tag{3.9}$$

and, in our polarization method, the invariant polynomial corresponding to this one-dimensional representation is used to construct a basis for the E in (3.8).

It is convenient to work with homogeneous coordinates x,y on the Riemann sphere, that is, $z = x/y$, so that a polynomial in z of degree B corresponds to a homogeneous degree B polynomial in x and y.

Let $(p_L(x,y), q_L(x,y))$ be known degree L polynomials which form a basis for the representation E and let $k(x,y)$ be a degree $B+L$ invariant polynomial which is a basis for the one-dimensional representation in (3.9). Then, since the pair $(\partial_y, -\partial_x)$ transform in the same way as the pair (x,y) under linear SU(2) transformations, this means that the polynomials $p_B(x,y), q_B(x,y)$ defined by

$$p_B(x,y) = p_L(\partial_y, -\partial_x)k(x,y), \quad q_B(x,y) = q_L(\partial_y, -\partial_x)k(x,y) \tag{3.10}$$

have degree B and are the required basis for the two-dimensional representation occuring in (3.8).

As an example of this scheme we now construct the icosahedrally symmetric degree 17 rational map, in an orientation that we shall require later. The relevant decomposition is

$$\underline{18}|_Y = E_2' + \cdots, \tag{3.11}$$

so we first require a known Y-symmetric rational map that is a basis for the representation E_2'. The simplest known example is the degree 7 map[7] (corresponding to the $B=7$ Y_h-symmetric minimal energy Skyrmion)

$$p_7(x,y)=x^7-7x^5y^2-7x^2y^5-y^7, \quad q_7(x,y)=x^7+7x^5y^2-7x^2y^5+y^7. \tag{3.12}$$

Hence we have $B=17$ and $L=7$, so now we require an invariant polynomial $k(x,y)$ of degree $B+L=24$. This is easily found by using an appropriate combination of Klein polynomials, in this case $k(x,y)=k_v^2(x,y)$ is the degree 24 invariant where $k_v(x,y)=x^{11}y+11x^6y^6-xy^{11}$ is the degree 12 Klein polynomial given earlier, when written in terms of homogeneous coordinates. The formula (3.10) then produces

$$\begin{aligned} p_{17}&=z^{17}+17z^{15}+119z^{12}-187z^{10}+187z^7+119z^5+17z^2-1, \\ q_{17}&=z^{17}-17z^{15}+119z^{12}+187z^{10}+187z^7-119z^5+17z^2+1, \end{aligned} \tag{3.13}$$

when written in terms of the inhomogeneous coordinate z. This map is equivalent, after a change of spatial and internal orientation, to the Y_h-symmetric map presented in Ref. 7 that corresponds to the $B=17$ Y_h-symmetric minimal energy Skyrmion. In the following subsection we shall require this map in the orientation presented in (3.13).

Although this method is much easier to implement than the projector algorithm, it turns out that for the icosahedral maps we require in this article there is yet another approach, which is even more effecient.

B. Klein leapfrog

From the previous section we already have two Y-symmetric rational maps, which are $R_7=p_7/q_7$ and $R_{17}=p_{17}/q_{17}$. Here we describe how the other Y-symmetric maps that we require can be obtained from these two by the simple multiplication of invariant Klein polynomials. This way of obtaining higher degree invariant rational maps we refer to as the Klein leapfrog method.

Recall that we wish to determine whether the low energy $\mathcal{I}$ minimizing map of degree 37 that we found earlier is icosahedrally symmetric. The relevant decomposition is

$$\underline{38}|_Y=E_1'+2E_2'+\cdots. \tag{3.14}$$

Both the maps (p_7,q_7) and (p_{17},q_{17}) are a basis for the representation E_2', and the multiplication of these maps by any (integer power of a) Klein polynomial does not change the transformation properties, since Klein polynomials are invariants. Thus, both (k_ep_7,k_eq_7) and (k_fp_{17},k_fq_{17}) are degree 37 Y-symmetric maps. Each map alone is not a valid degree 37 rational map, since the numerator and denominator contain common factors, but taken together they form an acceptable basis for the $2E_2'$ in (3.14). Explicitly,

$$R_{37}=\frac{p_{37}}{q_{37}}=\frac{k_fp_{17}+ck_ep_7}{k_fq_{17}+ck_eq_7}, \tag{3.15}$$

where c is a complex parameter. For $c=0$ or $c=\infty$ the map is clearly degenerate, having degree lower than 37, but for generic values of c the numerator and denominator are coprime.

The Wronskian of this map must be strictly invariant, and indeed it is given by the following combination of Klein polynomials:

$$w(p_{37},q_{37})=k_e^2k_v(80c+28c^2)-k_f^3k_v(68+120c). \tag{3.16}$$

The 72 roots of this polynomial give the face-centers of the Skyrmion polyhedron. Minimizing the integral $\mathcal{I}$ over the one- (complex) parameter family of maps (3.15) results in a minimum at $c=-0.829+0.545i$, where $\mathcal{I}/B^2=1.255$. This is precisely the value found by the minimization

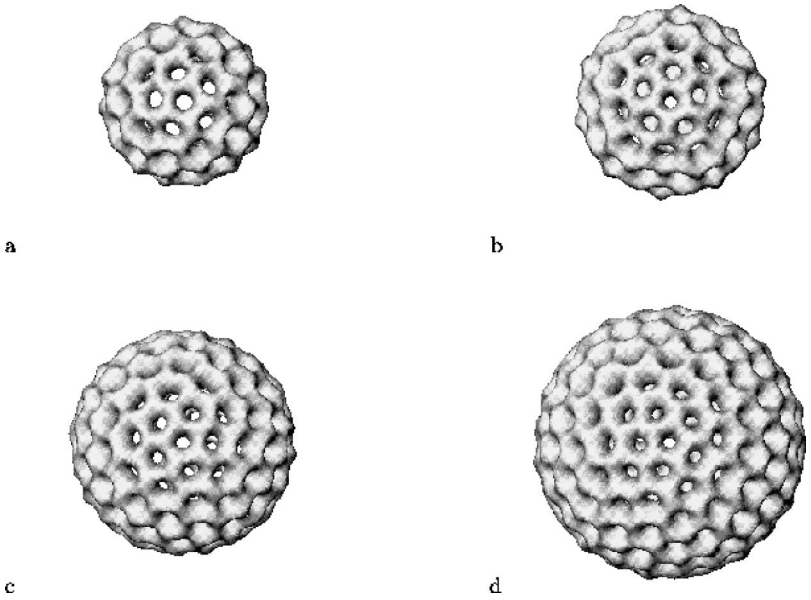

FIG. 4. Baryon density isosurface plots (to scale) for icosahedral Skyrmions with baryon numbers (a) $B=37$, (b) $B=47$, (c) $B=67$, and (d) $B=97$.

over all degree 37 maps, so we confirm that the $\mathcal{I}$ minimizing degree 37 map, and hence the minimal energy $B=37$ Skyrmion, has icosahedral symmetry. Note that the symmetry group is only Y and not Y_h since c is not real. A baryon density isosurface plot for the associated Skyrmion is displayed in Fig. 4(a).

The next magic number in our conjectured icosahedral list is $B=67$. The application of our simulated annealing scheme to extend the results presented in Fig. 1 to such a large value of B would require unreasonable computing resources. We therefore make use of the fact that the quantity $\mathcal{I}/B^2$ appears to approach an asymptotic value of around 1.28, whereas for icosahedral magic numbers the value is closer to 1.25. Therefore we aim to present evidence in support of our conjecture by finding an icosahedral map of degree 67 with $\mathcal{I}/B^2 \approx 1.25$.

The relevant decomposition is

$$\underline{68}|_Y = 2E_1' + 3E_2' + \cdots, \tag{3.17}$$

so we require three degree 67 maps to form a basis for the second component in the above decomposition. These are given by a Klein leapfrog as

$$(k_e k_f p_{17}, k_e k_f q_{17}), \quad (k_e^2 p_7, k_e^2 q_7), \quad (k_f^3 p_7, k_f^3 q_7). \tag{3.18}$$

It might seem strange that $(k_v^5 p_7, k_v^5 q_7)$ is not included, but because $\underline{61}|_Y = 2A + \cdots$, there must be a linear relationship between k_e^2, k_f^3 and k_v^5. In fact, it is given by $1728 k_v^5 = k_e^2 - k_f^3$.[8]

Minimizing over the two- (complex) parameter family of maps

$$R_{67} = \frac{k_e k_f p_{17} + c_1 k_e^2 p_7 + c_2 k_f^3 p_7}{k_e k_f q_{17} + c_1 k_e^2 q_7 + c_2 k_f^3 q_7} \tag{3.19}$$

yields a minimum at $c_1 = -0.292 - 0.816i$, $c_2 = -0.491 + 1.008i$, for which $\mathcal{I}/B^2 = 1.250$. This value is plotted as the square in Fig. 1, and it is clearly consistent with being an icosahedral magic number, as is the energy per baryon of the associated Skyrmion which is plotted as the square in Fig. 2. A baryon density isosurface derived from the minimal Y-symmetric map is displayed in Fig. 4(c).

The next magic number on our list is $B=97$. The required decomposition is

$$\underline{98}|_Y = 3E_1' + 4E_2' + \cdots, \tag{3.20}$$

so there is a three- (complex) parameter family of Y-symmetric maps. Three of the required basis maps are obtained by a Klein leapfrog of the three degree 67 basis maps given above, through the multiplication by k_e. The fourth basis map is a Klein leapfrog of (p_{17}, q_{17}) through the multiplication by k_f^4. The full map is therefore

$$R_{97} = \frac{k_e^2 k_f p_{17} + c_1 k_e^3 p_7 + c_2 k_e k_f^3 p_7 + c_3 k_f^4 p_{17}}{k_e^2 k_f q_{17} + c_1 k_e^3 q_7 + c_2 k_e k_f^3 q_7 + c_3 k_f^4 q_{17}}. \tag{3.21}$$

A minimization over the three complex parameters yields a minimum for $c_1 = 0.705 + 0.699i, c_2 = -0.554 - 1.701i, c_3 = -0.967 + 0.930i$, at which $\mathcal{I}/B^2 = 1.248$. This value is plotted as the circle in Fig. 1, and again it is consistent with being the minimal degree 97 map, producing another icosahedral magic number at $B=97$. A baryon density isosurface of the Skyrmion derived from this minimal Y-symmetric map is displayed in Fig. 4(d). The energy per baryon of this Skyrmion is plotted as the circle in Fig. 2. Given that the rational map ansatz tends to overestimate the energy by around 1% or 2%, then the true energy per baryon of this Skyrmion must be very close to that of the hexagonal lattice,[4] which has $E/B = 1.061$.

Icosahedrally symmetric rational maps, and hence Skyrme fields, exist for many values of B, but rarely are these symmetric configurations those of minimal energy. The simplest example is the degree 11 rational map presented in Ref. 7. For this map $\mathcal{I}/B^2 = 3.84$, which is clearly very large, and indeed the associated $B=11$ Skyrme field has larger energy than 11 well-separated single Skyrmions. This is not very surprising, given that the associated polyhedron is an icosahedron—clearly violating the favorable trivalent property at all vertices. However, in the Thomson problem there are more subtle examples, where there is an icosahedrally symmetric configuration which has reasonably low energy, but not quite as low as a less symmetric minimal energy solution. This situation occurs for the values $B = 22, 47, 82, \ldots$.[9] We shall see if this situation is also mirrored in the Skyrmion problem, by studying Y-symmetric rational maps of degree 47.

The required decomposition is

$$\underline{48}|_Y = E_1' + 2E_2' + \cdots, \tag{3.22}$$

and a basis for the $2E_2'$ is obtained by the Klein leapfrog of R_{17} by k_e and the Klein leapfrog of R_7 by k_f^2. Therefore, the one-parameter family of Y-symmetric maps is

$$R_{47} = \frac{k_e p_{17} + c k_f^2 p_7}{k_e q_{17} + c k_f^2 q_7}. \tag{3.23}$$

Minimizing over c yields a minimum when c is real (so the symmetry extends to Y_h) and takes the value $c = -1.425$, at which $\mathcal{I}/B^2 = 1.314$. This value is plotted as the cross in Fig. 1, and it can be seen that, even though it is reasonably low, it is not consistent with the general trend for minimal energy maps. The associated energy per baryon is plotted as the cross in Fig. 2 and provides further evidence that this is not a minimal energy Skyrmion. This suggests that the same phenomenon of nonminimal icosahedral maps exists in both the Thomson and Skyrme problems, providing yet more evidence for the similarity of these two systems. A baryon density isosurface is displayed in Fig. 4(b) for the Y_h-symmetric Skyrmion obtained from the above map with the minimal value of c. From this figure it can be seen that the Skyrmion polyhedron fits into the required class, as a trivalent polyhedron with 12 pentagonal faces and the remaining faces hex-

agonal. Therefore, the reason for it not to be the minimal energy Skyrmion must be subtle, and probably involves the placement of the pentagons within the polyhedron, when compared to a more favorable but less symmetric distribution.

Finally, we turn to the anomalous case of $B=62$. In the Thomson problem there is an icosahedral magic number at $B=62$, but the relevant decomposition for rational maps is

$$\underline{63}|_Y = A + \text{ irreps of dimension greater than } 2, \tag{3.24}$$

so there is certainly no Y-symmetric degree 62 rational map, and probably no Y-symmetric $B=62$ Skyrmion either. The resolution of this problem is the fact that the polyhedron associated with a Skyrmion is derived from the baryon density, and it is possible that the baryon and energy density of a Skyrmion could have more symmetry than the Skyrme field itself. In terms of the rational map ansatz this corresponds to an enhanced symmetry of the Wronskian, not shared by the rational map.

Recall that the Wronskian is a polynomial of degree $2B-2$, so to see if this is a possible explanation for the case $B=62$ we need to look for Y-invariant polynomials of degree 122. The decomposition

$$\underline{123}|_Y = 2A + \cdots \tag{3.25}$$

reveals that there are two invariants, and in fact they are given by $k_v k_f k_e^3$ and $k_v k_f^4 k_e$. Thus, to address this case we would need to find the family of degree 62 rational maps, (p_{62}, q_{62}), so that the Wronskian takes the form

$$w(p_{62}, q_{62}) = k_v k_f k_e (c_1 k_e^2 + c_2 k_f^3), \tag{3.26}$$

where c_1 and c_2 are arbitrary complex constants. It is difficult to see how to explicitly construct this family, given we do not know the symmetry of the rational map, but it would be interesting if this could be done, to see whether a map with a Y-invariant Wronskian is likely to be the minimal map. However, as far as our definition of icosahedral magic number is concerned, the value $B=62$ does not qualify because the map is not Y-symmetric.

The example of a nonminimal icosahedral $B=22$ Thomson configuration, briefly mentioned above, also appears to fall into the same class.[4] There are no Y-symmetric degree 22 maps, but there is a degree 42 invariant, given by $k_v k_e$, to which the Wronskian of a degree 22 map could be proportional.

IV. CONCLUSION

In this article we have used a comparison between Skyrmion polyhedra and the duals of Thomson polyhedra to predict a sequence of magic baryon numbers at which the Skyrmion has icosahedral symmetry and unusually low energy. We have presented some evidence for our conjecture, through the minimization of the most general rational maps for all degrees up to 40, and by the explicit construction, using two new methods, of some high degree rational maps with icosahedral symmetry.

Our methods could also be used to find other possible minimal energy rational maps and Skyrme fields, with octahedral and tetrahedral symmetries. It is likely that these other Platonic symmetries are more prevalent than icosahedral symmetry, and may account for some of the less pronounced dips in Fig. 1.

Finally, a comparison between the Skyrme crystal and the Skyrme lattice[4] suggests that for large enough baryon numbers the shell-like structure of Skyrmions may give way to a crystal structure. However, even the order of magnitude of B at which this transition might take place is not known, so whether all the icosahedral Skyrmions we have constructed will survive this possible transition remains an open question.

ACKNOWLEDGMENTS

We acknowledge EPSRC (PMS) and PPARC (RAB) for Advanced Fellowships.

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Topological Q-solitons

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(Received 18 November 2002; accepted 9 April 2003)

Static topologically-nontrivial configurations in sigma-models, for spatial dimension $D \geqslant 2$, are unstable. The question addressed here is whether such sigma-model solitons can be stabilized by steady rotation in internal space; that is, rotation in a global SO(2) symmetry. This is the mechanism which stabilizes Q-balls (nontopological solitons). The conclusion is that the Q-mechanism can stabilize topological solitons in $D=2$ spatial dimensions, but not for $D=3$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1584527]

I. INTRODUCTION

Topological solitons (stable, localized, topologically nontrivial solutions in a field theory) have long been of great interest, both for their mathematical properties and for their applications in many areas of physics. In any system admitting such solitons, the nontrivial topology is not sufficient to ensure that the solitons are stable. One obvious reason for this is that topology is, by definition, a nonmetric structure, and so it cannot determine the size of the solitons; for that, one needs to balance the forces acting on the soliton in such a way that it has a preferred size. Recall, for example, the O(n) sigma model in $D+1$ dimensions (with trivial boundary condition at spatial infinity), which is the subject of this article. This system admits topological configurations (textures) whenever the homotopy group $\pi_D(S^{n-1})$ is nontrivial; in particular, for (D,n) equal to (2, 3), (3, 3) or (3, 4). If $D=3$, then solitons tend to shrink—in the pure sigma model, there are no static solutions. In the $D=2$ case, there are static solutions, for example, the Belavin–Polyakov solitons[1] in the O(3) system, but these are unstable.[2,3]

A soliton can always be prevented (or rather discouraged) from spreading out by the addition, if necessary, of a potential (a term involving only the field, and not its gradient). In order to stabilize the soliton size, we also need to introduce something which prevents it from shrinking. There are several possibilities for such an antishrinking mechanism: for example, a Skyrme term involving four (or more) powers of the field gradient, or a gauge field suitably coupled to the sigma-field, or periodic time-dependence (rotation in an internal space). This third possibility also underlies nontopological solitons (Q-balls). In this article, we investigate to what extent the Q-ball mechanism is effective at stabilizing topological sigma-model solitons. We shall see that stationary topological Q-solitons exist in $D=2$ spatial dimensions, but not for $D=3$. This result is analogous to that for the Landau–Lifshitz equation (Heisenberg model of ferromagnetism), as one might have surmised since the static Landau–Lifshitz system is identical to the static sigma model.

II. Q-SOLITONS IN THE O(3) SIGMA MODEL

The O(3) sigma model involves a scalar field taking values on S^2; this field can be represented as a unit three-vector $\vec{\phi}=(\phi_1,\phi_2,\phi_3)$ with $\vec{\phi}\cdot\vec{\phi}=1$. The Lagrangian is

$$\mathcal{L}=\tfrac{1}{2}(\partial_\mu\vec{\phi})\cdot(\partial^\mu\vec{\phi})-V(\phi_3), \tag{1}$$

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where V is some potential function (which, for simplicity, we take to depend only on ϕ_3). The space–time coordinates are $x^\mu=(t,x^j)$, with $j=1,\ldots,D$. The system has a global SO(3) symmetry which is broken, by the potential term, to SO(2). This SO(2) acts only on ϕ_1 and ϕ_2, namely, by changing the phase of $\phi:=\phi_1+\mathrm{i}\phi_2$. The corresponding conserved quantity is

$$Q=\int \mathrm{Im}(\dot{\phi}\overline{\phi})d^Dx. \tag{2}$$

Minimizing the energy of a configuration subject to Q being fixed implies,[4] in particular, that $\vec{\phi}$ has the form

$$\phi(t,x^j)=\psi(x^j)\mathrm{e}^{\mathrm{i}\omega t},\quad \phi_3=\psi_3(x^j), \tag{3}$$

with $|\psi|^2+(\psi_3)^2=1$. Without loss of generality, we shall assume that $\omega\geqslant 0$. Note that $Q=\omega I$, where $I=\int|\psi|^2d^Dx$. The energy of a configuration of the form (3) is $E=E_d+E_k+E_p$, where

$$E_d=\frac{1}{2}\int[|\partial_j\psi|^2+(\partial_j\psi_3)^2]d^Dx,$$

$$E_k=\tfrac{1}{2}I\omega^2=\tfrac{1}{2}Q^2/I,$$

$$E_p=\int V(\psi_3)d^Dx.$$

The boundary condition is $\psi_3\to 1$ as $r\to\infty$, so we need $V(1)=0$.

A stationary Q-lump is a critical point of the energy functional $E[\vec{\psi}]$, subject to Q having some fixed value. Such a Q-lump is (classically) stable if this critical point is a local minimum of E. The usual (Derrick) scaling argument shows that any stationary Q-lump must satisfy

$$(2-D)E_d-DE_p+DE_k=0. \tag{4}$$

Let the positive constant m be defined by $V'(1)=-m^2$; in other words, $V(\psi_3)\approx m^2(1-\psi_3)\approx\frac{1}{2}m^2|\psi|^2$ for $\psi_3\approx 1$. Then, near spatial infinity, the Euler–Lagrange equations corresponding to E imply that

$$\nabla^2\psi-(m^2-\omega^2)\psi=0.$$

So in order to satisfy the boundary condition $\psi\to 0$ as $r\to\infty$, we need $\omega\leqslant m$. The solitons are exponentially localized if $\omega<m$, but less-localized solitons with $\omega=m$ may also exist.

The parameter m is part of the specification of the system, and the parameter Q is set by the initial data. Each of these two parameters has dimensions; the combination Qm^{D-1} is dimensionless, whereas the combination $(Q/m)^{1/D}$ has dimension of length, and determines the size of the soliton. Configurations in this system are classified topologically by their topological charge N (an integer); if $D=2$, then N is the winding number, while if $D=3$, then N is the Hopf number. Let $E(N,Q)$ denote the energy of a configuration (or rather, of data $\vec{\phi},\vec{\phi}_t$) with topological charge N and Noether charge Q.

Let V_0 be the normalized potential function $V_0:=2V/m^2$. Note that $V_0(\psi_3)/|\psi|^2\to 1$ as $\psi_3\to 1$. It is clear from (4) that if $V_0\geqslant|\psi|^2$ everywhere, with $V_0>|\psi|^2$ somewhere, then there can be no solution. So the constant K defined by $K=\min[V_0(\psi_3)/|\psi|^2]$ should satisfy $K\leqslant 1$. It then follows that

$$E_p=m^2\int V_0\geqslant m^2KI=(Km^2/\omega^2)E_k\geqslant(Km^2/\omega^2)E_p, \tag{5}$$

where the final inequality comes from (4). As a consequence, we have

$$Km^2 \leqslant \omega^2 \leqslant m^2. \tag{6}$$

In the $D=3$ case, the first inequality is strict: $Km^2 < \omega^2 \leqslant m^2$.

In two spatial dimensions, it is possible to have $K=1$, which corresponds to the choice $V(\psi_3)=\frac{1}{2}m^2(1-\psi_3^2)$. So here $\omega=m$. This system,[5] and generalizations in which the target space is some other Kähler manifold, arise naturally by dimensional reduction from "pure" sigma models in one dimension higher.[6] The energy satisfies a Bogomolny bound $E(N,Q) \geqslant 4\pi N + mQ$, which (for $N \geqslant 2$) can be saturated: for each value of $N \geqslant 2$ and Q, there is an explicit family $\mathcal{M}$ of stationary multi-soliton solutions such that $E(N,Q)=4\pi N+mQ$. There is no force between the individual solitons: in particular, the total energy has the additive property $E(N_1,Q_1)+E(N_2,Q_2)=E(N_1+N_2,Q_1+Q_2)$. One may use moduli-space methods (as was done in Refs. 7–9 for other sigma-model systems) to investigate the scattering of moving solitons;[5] this involves finite-dimensional mechanics on $\mathcal{M}$. The dynamics turns out to be rather exotic (as is also the case[10–12] for nontopological Q-balls). The solitons are only polynomially localized, and the nonexistence of an $N=1$ soliton is related to this; an $N=1$ configuration tends to shrink in size, and there is no stationary $N=1$ solution.

On the other hand, if $K<1$, then one-solitons can exist. Different choices of V (having $K<1$) seem to lead to similar behavior, but this has yet to be fully investigated; in what follows, we take $V_0=\frac{1}{2}(1-\psi_3^4)$, so $K=\frac{1}{2}$. Let us consider, first, the thin-wall limit,[13] where $Qm^{D-1} \gg 1$. In this limit, the (bulk) contributions E_p and E_k to the energy are very much greater than the (surface) contribution E_d. So, the energy is approximately $E \approx \frac{1}{4}m^2 \int (1-\psi_3^4) + \frac{1}{2}Q^2/\int (1-\psi_3^2)$. Without loss of generality, we may assume that $\psi_3=1$ outside of some compact set. So space is partitioned into three regions: one (with infinite volume) where $\psi_3=1$, the second (with volume A) where $|\psi_3| \neq 1$, and the third (with volume B) where $\psi_3=-1$. Note that E depends on A (and on the value that ψ_3 takes on A), but not on B, and that

$$\frac{\delta E}{\delta \psi_3} = (\omega^2 - m^2\psi_3^2)\psi_3.$$

So for fixed A, the function E has a minimum for $\psi_3=0$ ($\psi_3=\pm\omega/m$ are local maxima). Hence we should set $\psi_3=0$ on A, and the energy becomes

$$E = \tfrac{1}{2}Q^2/A + \tfrac{1}{4}m^2A.$$

Thus for a given value of Q, the energy has the minimum value $E_{\min}=mQ/\sqrt{2}$ when $A=Q\sqrt{2}/m$. Note that $\omega=m/\sqrt{2}$, at the lower end of its allowed range (6).

To make further progress, we need to include the effect of surface tension, in other words include the term E_d. Let us consider, first, the planar case $D=2$. For simplicity, we assume rotational symmetry about a point in the plane: the field is taken to have the form $\psi = \sin(f)\exp(\mathrm{i}N\theta)$ and $\psi_3=\cos(f)$, where $f=f(r)$. The boundary conditions are $f(0)=\pi$ and $f(\infty)=0$, and N is the topological charge. The energy functional $E=E_d+E_k+E_p$ was minimized numerically, for various values of m, Q and N. The term E_k was used in the form $E_k=Q^2/I$, so that one can minimize while keeping Q fixed; the quantity ω does not enter explicitly, but can be derived (via the formula $\omega=Q/I$) once the minimum has been found. In each case that was investigated, a smooth minimum was reached. For $N=1$ and $Qm=3200\pi$ (close to the thin-wall limit), the profile function $f(r)$ is plotted in Fig. 1. We see that there is a region around $r=0$ where $f(r)$ drops rapidly from π to $\pi/2$ (the term E_d prevents this region from shrinking further in size), and then a region (corresponding to A in the argument above) where $f=\pi/2 \Leftrightarrow \psi_3=0$. Outside of this region, the field takes on its asymptotic value $f=0 \Leftrightarrow \psi_3=1$.

Figure 2 displays results for $N=1$, $m=1$ and a range of values of Q. We see that E is very close to being linear in Q (recall that in the Bogomolny case, it is exactly linear): to a very good

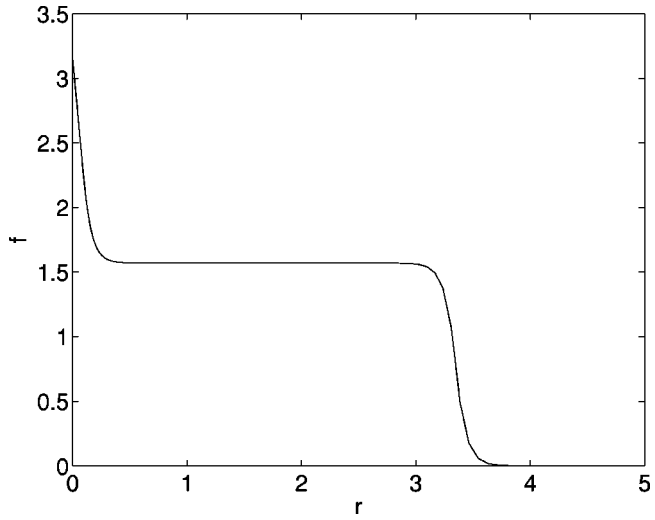

FIG. 1. The profile function $f(r)$ for the one-soliton solution on the plane, with $m=20$ and $Q=160\pi$.

approximation, we have $E=4\pi+3Q/4$. As for ω, we know from (6) that ω has to be in the range $1/\sqrt{2}<\omega<1$, and we see from the figure that this is so; furthermore, $\omega\to 1/\sqrt{2}$ as $Q\to\infty$ (the thin-wall limit[13]), while $\omega\to 1$ as $Q\to 0$ (the thick-wall limit[14]).

In the Bogomolny case[5] mentioned previously, the energy $E(N,Q)$ of a stationary soliton has the feature that, for a given Q, the quantity $E_N:=(4\pi N)^{-1}E(N,NQ)$ is independent of N; in fact, $E_N=1+mQ/4\pi$. This corresponds to the fact that in this Bogomolny-type system, there is no force between stationary solitons. For the potential $V=\frac{1}{4}m^2(1-\psi_3^4)$, however, there are such forces. This can be seen by examining E_N for fixed $Q=4\pi$ and for various values of N. Table I shows the results for $1\leqslant N\leqslant 7$. The energy density of the one-soliton is peaked at the point $r=0$, whereas that for the rotationally-symmetric N-soliton is peaked on a ring. Note that E_N is a decreasing function of N, which suggests that this N-soliton is stable against breakup into solitons of lower topological charge. But this remains to be checked; in particular, one should investigate the vibrational modes about these rotationally-symmetric solutions.

Finally, let us turn to the case of $D=3$ spatial dimensions. Configurations with nonzero Hopf number N look like closed loops, which may be linked or knotted. Static knot-solitons are have been studied in the Faddeev–Skyrme system, where a Skyrme term is added to the Lagrangian: this extra term stabilizes the solitons, which would otherwise shrink.[15–18] The question here is whether there exist stationary Hopf solitons which are stabilized by internal rotation rather than by

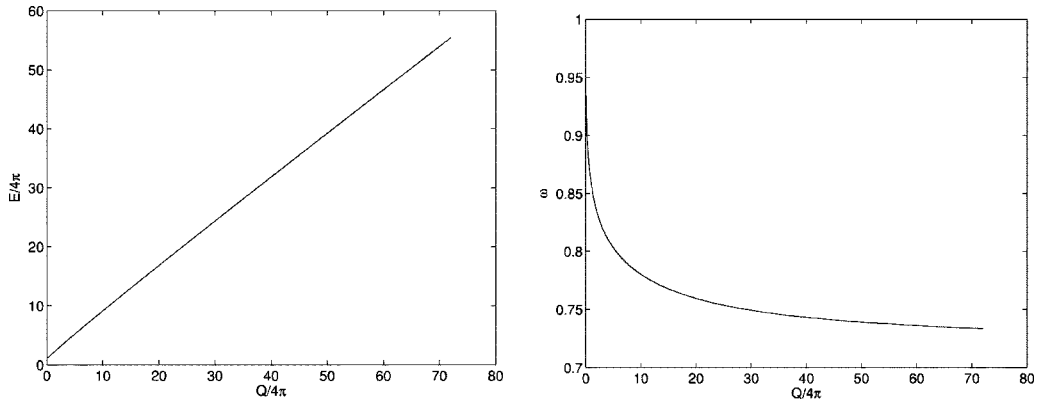

FIG. 2. The energy E and angular frequency ω of the one-soliton, as functions of Q.

TABLE I. Energy $E_N=E(N,NQ)/(4\pi N)$ and frequency ω/m, for $m=1$ and $Q=4\pi$.

N	1	2	3	4	5	6	7
E_N	1.888	1.840	1.826	1.820	1.817	1.816	1.815
ω/m	0.859	0.826	0.817	0.814	0.882	0.811	0.810

a Skyrme term. The answer to this question appears to be negative; what happens is as follows. Consider an $N=1$ configuration. Typically, $\psi_3=1$ at spatial infinity and on a curve which extends to infinity; let us visualize this curve as the z-axis. Second, $\psi_3=-1$ on a closed loop L around the z-axis. Finally, $\psi_3=0$ on a torus around the z-axis, with the loop L in its interior. So the region A in the previous thin-wall analysis is a thickened torus (with the B-region in its interior) resembling a closed string. Numerical experiments indicate that, roughly speaking, the Q-effect supports the thickness of the string, but not its length; the string has a tension which causes its length to shrink. So the configuration collapses, and there is no stationary Hopf soliton in this system. In principle it remains a possibility that for some potential function V, some value of Q, and some nonzero value of the Hopf number N, there might exist a stationary solution, but this seems rather unlikely.

Another way of viewing the situation is as follows. The Q-mechanism provides a lower bound on the quantity I (since ω is bounded above, and $Q=I\omega$ is fixed); this in turn means that the volume of the soliton is bounded below. But surface tension then acts to make the soliton spherical. So we are led to the following conjecture: any stationary Q-ball (whether topological or not) with $\omega<m$, in D spatial dimensions, has O(D) symmetry. (In the Bogomolny case, where $\omega=m$, rotational symmetry is not essential.[5]) For standard Q-balls, this conjecture is known to be true,[13] but it is not immediately clear that the result extends to cases (such as the present one) where the target space is nontrivial. The instability of Hopf Q-solitons is an immediate consequence of the conjecture, since O(3) symmetry implies that the Hopf number is zero.

III. THE O(4) SIGMA MODEL IN 3+1 DIMENSIONS

In this section, we investigate the analogous problem for the O(4) sigma model in three space dimensions. The details of the system are similar to those of the previous section. The field takes values on S^3, and is represented as a unit four-vector $\vec{\phi}=(\phi_0,\phi_1,\phi_2,\phi_3)$. The Lagrangian is (1), as before, but with the potential being allowed to depend on ϕ_0 and ϕ_3: $V=V(\phi_0,\phi_3)$. In general, this breaks the global O(4) symmetry to O(2), the subgroup which rotates ϕ_1 and ϕ_2, leaving ϕ_0 and ϕ_3 fixed. The expressions for E_d, E_k and E_p are the same as before, with $D=3$, except that in E_d there is an extra term involving $(\partial_j\psi_0)^2$.

We take the boundary condition to be $\psi_0\to 1$ as $r\to\infty$ in $\mathbf{R}^3$. The mass m is defined by $V(\psi_0,\psi_3)\approx m^2(1-\psi_0)\approx\frac{1}{2}m^2(|\psi|^2+\psi_3^2)$ for $\psi_0\approx 1$; the function V_0 and the constant K are defined as before. The virial relation from (4) with $D=3$ holds as before, as does the inequality $Km^2<\omega^2\leqslant m^2$.

In Ref. 19, this system was studied, with the potential $V_0=2(1-\psi_0)$. Since in that case we have $K=1$, no soliton solution can exist. The authors of Ref. 19 reach this conclusion for the topologically trivial case $N=0$; they report numerical evidence for a nontrivial solution with $N=1$, but this cannot be correct.

In order to allow the possibility of nontrivial solutions, we need a potential V_0 which has $K<1$; for what follows, we shall take $V_0=\frac{1}{2}(1-\psi_0^4)$ as in the previous section. Then there are solutions, but it appears that they all have trivial topology ($N=0$). One way to see what happens is to consider the thin-wall limit, where $m^2Q\gg 1$. So, the energy is approximately $E\approx\frac{1}{4}m^2\int(1-\psi_0^4)+\frac{1}{2}Q^2/\int|\psi|^2$, and the corresponding variational equations are

$$\xi\psi_0-m^2\psi_0^3=0,\quad \xi\psi-\omega^2\psi=0,\quad \xi\psi_3=0, \tag{7}$$

where $\xi:=m^2\psi_0^4+\omega^2|\psi|^2$ (the ξ-term arises from enforcing the constraint $\vec{\phi}\cdot\vec{\phi}=1$). These equations (7) have a number of solutions, namely,

(i) $\psi_0=0,\ \psi=0,\ \psi_3=\pm 1;$
(ii) $\psi=0,\ \psi_3=0,\ \psi_0=\pm 1;$
(iii) $\psi_0=\psi_3=0,\ |\psi|^2=1;$
(iv) $\psi_3=0,\ \psi_0=\pm\omega/m,\ |\psi|^2=1-\omega^2/m^2.$

So to construct a mimimum-energy configuration, we must partition space $\mathbf{R}^3$ into regions (separated by infinitesimally-thin walls), on each of which one of these relations holds. It is clear that regions on which $\psi_3\neq 0$ contribute only to E_p, and that we can reduce the total energy by instead setting $\psi_3=0,\ \psi_0=1$ on these regions. In other words, ψ_3 ''collapses'' to zero, and is replaced by ψ_0.

This is exactly what one sees in numerical simulations. For example, we may start with the O(3)-symmetric ''hedgehog'' ansatz

$$\psi_0+\mathrm{i}\psi_j\sigma_j=\exp[\mathrm{i}f(r)x^j\sigma_j/r]; \tag{8}$$

here σ_j denotes the Pauli matrices, and the profile function $f(r)$ satisfies the usual boundary conditions $f(0)=\pi,\ f(\infty)=0$. The winding number is $N=1$. Note that $\psi=\psi_1+\mathrm{i}\psi_2$ vanishes on the x^3-axis, and that $\psi_0(0)=-1$. If we now relax the configuration by flowing down the energy gradient, then ψ_3 approaches zero everywhere except at the single point $r=0$; in other words, there is no continuous minimum in this topological class. By contrast, there is a smooth minimum which has $\psi_3\equiv 0$: this is topologically trivial, and is essentially a standard (nontopological) Q-ball.

IV. CONCLUDING REMARKS

We begin with a few remarks on the similarities with stationary topological soliton solutions of the Landau–Lifshitz equation

$$\frac{\partial\vec{\phi}}{\partial t}=-\vec{\phi}\times\frac{\delta E}{\delta\vec{\phi}}. \tag{9}$$

Here $\vec{\phi}$ is a unit three-vector representing the local orientation of magnetization, and the energy E is given by

$$E=\int\left[\frac{1}{2}(\partial_j\vec{\phi})\cdot(\partial_j\vec{\phi})+U(\phi_3)\right]d^Dx. \tag{10}$$

A typical choice for the function U is $U=A(1-\phi_3^2)$, where A is a constant; this corresponds to an easy-axis anisotropy. The boundary condition is $\phi_3\to 1$ as $r\to\infty$. The total magnetization

$$M=\int(1-\phi_3)d^Dx \tag{11}$$

is a conserved quantity. It is clear from scaling that the only static solutions are the Belavin–Polyakov solitons[1] in spatial dimension $D=2$, with $U\equiv 0$. But by allowing time dependence, more solutions are possible. In particular, we may allow periodic time dependence, and look for stationary solutions such that

$$\phi_1+\mathrm{i}\phi_2=\psi(x^j)\mathrm{e}^{\mathrm{i}\nu t},\quad \phi_3=\psi_3(x^j). \tag{12}$$

With this ansatz, the Landau–Lifshitz equation (9) is equivalent to

$$\frac{\delta}{\delta\vec{\phi}}\left(E-\frac{1}{2}\nu M\right)=0. \tag{13}$$

We may think of the solutions as critical points of E, subject to the constraint that M has a given value.[20] The simplest example occurs if $U=\frac{1}{2}\nu(1-\psi_3)$, for then the functional appearing in (13) consists of only the gradient term, and the Belavin–Polyakov solitons are solutions (in $D=2$); these correspond, of course, to the Bogomolny-type Q-lump solitons.[5] The analysis of stationary topological Landau–Lifshitz solitons leads to rather similar results as for Q-solitons (although the dynamics of moving solitons is quite different). In $D=2$, there are topological solutions (called magnetic bubbles—see Ref. 21 for a review); a single soliton is pinned in space, and cannot move.[22] In $D=3$, on the other hand, there are no stationary Hopf solitons;[23] however, such solitons can be stabilized by allowing them to move at constant velocity.[23,24]

Returning to sigma-model dynamics, we have seen that the Q-mechanism stabilizes topological solitons in $D=2$ spatial dimensions, but not in $D=3$. Stabilizing vortex rings (Hopf textures) in $D=3$ is particularly difficult, since there are two length-scales (the length of the loop and its width), each of which has to be fixed. The Q-effect can stabilize the latter, but not the former. One does get stable loops in systems with a Skyrme term,[15,16] and also in systems with a magnetic field sufficiently strongly coupled to the scalar field (minimal coupling is not enough).[25] But in the basic versions of each of these systems, there is only one length-scale; and so the length of the loop is of the same order as (and only slightly greater than) its thickness. It remains an open question as to whether there is a system admitting a stable Hopf soliton in which the two length-scales are significantly different.

A sigma-model soliton in $D=2$ can be thought of as a (straight) sigma-model string in three spatial dimensions. So, for example, the Q-stabilized solitons discussed in this article may find application as cosmic strings. Given an appropriate potential V, long strings with internal rotational energy will be stable, although closed loops will eventually shrink and decay. In this connection, it is worth recalling that, on a cosmological scale, both the width and the length of sigma-model strings are stabilized by cosmological expansion; but stabilizing the length requires a greater rate of expansion than stabilizing the width.[26]

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On the Q-ball profile function

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(Received 1 February 2002; accepted 9 April 2003)

We use analytic and numerical methods to obtain the solution of the Q-ball equation of motion. In particular, we show that the profile function of the three-dimensional Q-ball can be accurately approximated by the symmetrized Woods–Saxon distribution. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1586792]

I. INTRODUCTION

The existence of Q-balls is a general feature of scalar field theories carrying a conserved U(1) charge.[1,2] Q-balls can be understood as bound states of scalar particles and appear as stable classical solutions (nontopological solitons) carrying a rotating time dependent internal phase. They are characterized by a conserved nontopological charge Q (Noether charge) which is responsible for their stability (see, for example, Refs. 3 and 4). These features differentiate the Q-ball interaction properties from those of the topological solitons since here the charge Q can take arbitrary values in a specific range, allowing for the possibility of charge transfer between solitons during the interaction process.

Up till now, comprehensive studies of these objects have been made by using either numerical simulations[3–5] or some analytic considerations.[1,6,7] Recently, in Ref. 8 the explicit relation between the energy and the charge of the Q-balls has been derived using analytic arguments. In particular, a semi-Bogomolny argument in the energy density led to a first order differential equation whose solution, however, did not satisfy the correct boundary conditions and differed considerably from its exact form. In this work, we present a method to obtain an analytic form for the Q-ball profile function which is in good agreement with the numerical results.

We consider the U(1) Goldstone model, given by the Lagrangian

$$\mathcal{L}=\tfrac{1}{2}\partial_\mu\phi\,\partial^\mu\overline{\phi}-\mathrm{U}(|\phi|), \tag{1}$$

where ϕ is a single complex scalar field in three spatial dimensions while the potential $\mathrm{U}(|\phi|)$ is a function of $|\phi|$ only and has a single minimum at $\phi=0$. This is equivalent of stating that there is a sector of scalar particles (mesons) which carry U(1) charge and have mass squared equal to $\frac{1}{2}\mathrm{U}''(0)$. The corresponding energy functional is given by

$$E=\int\left(\frac{1}{2}|\partial_t\phi|^2+\frac{1}{2}|\nabla\phi|^2+\mathrm{U}(|\phi|)\right)d^3x. \tag{2}$$

The model has a global U(1) symmetry and an associated conserved Noether current J_μ exists whose covariant conservation $\partial^\mu J_\mu=0$ leads to the existence of the conserved Noether charge Q given by

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$$Q=\frac{1}{2i}\int(\bar{\phi}\,\partial_t\phi-\phi\,\partial_t\bar{\phi})d^3x. \tag{3}$$

A stationary Q-ball solution has the form

$$\phi=e^{i\omega t}f(r), \tag{4}$$

where $f(r)$ is a real radial profile function which satisfies the ordinary differential equation

$$f''(r)+\frac{2}{r}f'(r)=-\omega^2 f(r)+\mathrm{U}'(f) \tag{5}$$

with the condition $f(\infty)=0$ and $f'(0)=0$. This equation can either be interpreted as describing the motion of a point particle moving in a potential with friction,[1] or in terms of Euclidean bounce solutions.[9] In each case the effective potential being $\mathrm{U}_{\mathrm{eff}}(f)=\omega^2 f^2/2-\mathrm{U}(f)$ leads to constraints on the potential $\mathrm{U}(f)$ and the frequency ω in order for a Q-ball solution to exist. First, the effective mass of f must be negative. If we consider a potential $\mathrm{U}(f)$ which is non-negative and satisfies $\mathrm{U}(0)=\mathrm{U}'(0)=0$, $\mathrm{U}''(0)=\omega_+^2>0$, then one can deduce that $\omega<\omega_+$. Furthermore, the minimum of $\mathrm{U}(f)/f^2$ must be attained at some positive value of f, say $0<f_0<\infty$, and existence of the solution requires that $\omega>\omega_-$ where $\omega_-^2=2\mathrm{U}(f_0)/f_0^2$. Hence, Q-balls exist for all ω in the range $\omega_-<|\omega|<\omega_+$.

Then, the charge and the energy of a stationary Q-ball solution simplify to

$$Q=4\pi\omega\int r^2 f^2(r)\,dr, \tag{6}$$

$$E=4\pi\int\left(\frac{1}{2}\omega^2 f^2(r)+\frac{1}{2}f^{*2}(r)+\mathrm{U}(f)\right)r^2\,dr. \tag{7}$$

It has been observed using numerical and analytic methods that the classical stability of a Q-ball is related with the dependence of its charge on the internal frequency ω. For small internal frequency, close to its minimal value ω_-, the profile function is almost constant, which implies that the charge (6) is large and this corresponds to the so-called thin-wall approximation. On the other hand, for large internal frequency (close to its maximal value ω_+) the profile function (and thus the charge) tends to zero and this corresponds to the thick-wall approximation. In fact, for $\omega\to\omega_+$, the behavior of the charge Q depends on the particular form of the potential and the number of dimensions.[7] In the case studied here we show that $Q\to\infty$ as $\omega\to\omega_+$.

The choice of the potential is not unique; the standard requirement is that the function $\mathrm{U}(f)/f^2$ has a local minimum at some value of f different from zero. For simplicity, we consider the following form,

$$\mathrm{U}(f)=f^2(1+(1-f^2)^2), \tag{8}$$

which implies that in terms of the earlier notation we have that $\omega_+=2$ and $\omega_-=\sqrt{2}$, and therefore stable Q-balls exist for $\sqrt{2}<\omega<2$. In this case, the energy-charge dependence of the Q-balls, obtained in Ref. 8 using a semi-Bogomolny argument, is given by the analytic expression

$$E_{\mathrm{Bog}}=\sqrt{2}\,Q_{\mathrm{Bog}}+\frac{3^{2/3}\pi^{1/3}}{2^{7/6}}Q_{\mathrm{Bog}}^{2/3}+\frac{5\pi^{2/3}}{2^{11/6}3^{2/3}}Q_{\mathrm{Bog}}^{1/3}-\frac{\pi(4+3\pi^2)}{36\sqrt{2}}+\frac{\pi^{4/3}(17-216\pi^2)}{2592\;\;2^{1/6}\;\;3^{1/3}}Q_{\mathrm{Bog}}^{-1/3}$$
$$+\frac{\pi^{5/3}(20-54\pi^2+27\pi^4)}{1944\;\;2^{5/6}\;\;3^{2/3}}Q_{\mathrm{Bog}}^{-2/3}+O(Q_{\mathrm{Bog}}^{-1}). \tag{9}$$

For large Q, the above equation corresponds to the upper energy bound. The same result can be obtained by representing the Q-ball profile function by the Woods–Saxon distribution (i.e., a generalization of the semi-Bogomolny solution) as presented in Ref. 8.

Let us emphasize that neither the semi-Bogomolny nor the Woods–Saxon ansatz describe accurately the Q-ball profile function. In particular, in both cases the derivative of the profile function at the origin is nonzero (that is, different from the required boundary conditions) while the corresponding profile function differs from the exact one obtained by solving numerically the equation of motion. In the next section, we show that the symmetrized Woods–Saxon distribution describes accurately the Q-ball profile function and satisfies the correct boundary conditions.

II. EQUATION OF MOTION

The Q-ball equation of motion (5) for the specific potential (8) is given by

$$f''(r)+\frac{2}{r}f'(r)=(4-\omega^2)f(r)-8f^3(r)+6f^5(r) \tag{10}$$

and satisfies the boundary conditions $f'(0)=0$, $f(\infty)=0$. For large values of the argument r the nonlinear terms in (10) can be neglected and we get the asymptotic behavior $f(r) \sim \exp(-\sqrt{4-\omega^2}\,r)$. The exact solution of (10) should contain only one free parameter ω so that the charge Q, the energy E and the initial value $f(0)$ should in principle be expressed as functions of this parameter. Since Eq. (10) is too complicated to be tackled by analytic methods, we shall seek a suitable ansatz for the profile function and search for relations connecting E, Q and $f(0)$ with ω.

As mentioned earlier, a test profile of the Woods–Saxon type cannot reasonably approximate the Q-ball solution since it fails to satisfy the correct boundary conditions. Nevertheless, it implies an energy-charge relation (9) which holds remarkably well for a wide range of energies, a fact that certainly requires some further investigation. A more general test function that satisfies the correct boundary conditions and has the correct asymptotic behavior is given by the symmetrized Woods–Saxon distribution

$$f(r)=\frac{c}{\sqrt{1+c_1\cosh(\alpha r)}}\,. \tag{11}$$

The values of the arbitrary parameters c, c_1, and α can then be determined by fitting the data of the numerically solved (10). Having done that, we got a very satisfactory agreement in all cases. It is interesting to realize that $f(r)$ satisfies the following differential equation,

$$f''(r)+\frac{2}{r}f'(r)=\frac{\alpha^2}{4}\left(1-\frac{4}{\alpha r}\right)f(r)-\frac{\alpha^2}{c^2}\left(1-\frac{1}{\alpha r}\right)f^3(r)+\frac{3\alpha^2}{4c^4}\left((1-c_1^2)+\frac{2}{3}\frac{c_1^2}{\alpha r}\right)f^5(r)+\mathrm{O}(f^7), \tag{12}$$

which in the limit $\alpha r \gg 4$ looks exactly like (10). It is then quite reasonable to expect that there must be a critical value of $r=r_c$ beyond which the following equations must approximately hold true:

$$\frac{\alpha^2}{4}\left(1-\frac{4}{\alpha r_c}\right)\simeq 4-\omega^2, \tag{13}$$

$$\frac{\alpha^2}{c^2}\left(1-\frac{1}{\alpha r_c}\right)\simeq 8, \tag{14}$$

$$\frac{3\alpha^2}{4c^4}\left((1-c_1^2)+\frac{2}{3}\frac{c_1^2}{\alpha r_c}\right)\simeq 6 \quad . \tag{15}$$

The thin-wall approximation is reached when $c_1\to 0$, so we will assume that $c_1<1$ and we shall neglect the last term on the left hand side of (15). Then the system above gives the approximate solutions

$$c\simeq\sqrt{\frac{2}{3}}\sqrt{1-c_1^2}\sqrt{1+\sqrt{1-\frac{3}{8}\frac{4-\omega^2}{1-c_1^2}}}, \tag{16}$$

$$\alpha\simeq\frac{4\sqrt{2}}{3}\sqrt{1-c_1^2}\left(1+\sqrt{1-\frac{3}{8}\frac{4-\omega^2}{1-c_1^2}}\right), \tag{17}$$

$$\alpha r_c\simeq\frac{1+\sqrt{1-\frac{3}{8}(4-\omega^2)/(1-c_1^2)}}{-\frac{1}{2}+\sqrt{1-\frac{3}{8}(4-\omega^2)/(1-c_1^2)}} \quad . \tag{18}$$

A comparison with values obtained by a direct fit shows that the relations above are quite good. In fact, Eq. (16) is excellent, while Eq. (17) gives the right shape but the actual values for α are on the average 10% higher than expected, implying a faster drop of the profile function. Note that both c and a are slowly varying functions of ω.

The equation of motion (10) can be written as

$$\frac{d}{dr}\left(\frac{1}{2}f^{*2}(r)+\frac{1}{2}\omega^2 f^2(r)-\mathrm{U}(f)\right)=-\frac{2}{r}f'^2(r) \quad . \tag{19}$$

In the absence of the friction term, Eq. (19) would simply imply the conservation of energy for the corresponding mechanical problem. In the presence of friction and upon integrating (19) we get that the initial potential energy equals the work done by friction. This relation can be used to provide a further constraint on the form of (11):

$$\frac{1}{2}\omega^2 f^2(0)-\mathrm{U}(f(0))=-2\int_0^\infty\frac{f'^2(r)}{r}dr \quad . \tag{20}$$

Recall that $f(0)=c/\sqrt{1+c_1}$. Finally, using the symmetrized Woods–Saxon distribution (11), the charge (6) and the energy (7) of the Q-ball can be explicitly evaluated in terms of the parameters c, c_1, and α:

$$Q=4\pi\omega\frac{c^2}{3\alpha^3\sqrt{1-c_1^2}}\cosh^{-1}\left(\frac{1}{c_1}\right)\left(\pi^2+\cosh^{-1}\left(\frac{1}{c_1}\right)^2\right), \tag{21}$$

$$E=4\pi\left[\frac{\alpha^2+4(4+\omega^2)}{8}I_0-\left(2+\frac{\alpha^2}{4c^2}\right)I_1+\left(1+\frac{\alpha^2}{8c^4}(1-c_1^2)\right)I_2\right], \tag{22}$$

where the integrals I_0, I_1, and I_2 are given by

$$I_0=\frac{Q}{4\pi\omega}, \tag{23}$$

TABLE I. Values of the parameters c, c_1, α and $f(0)$ obtained from (11) and numerically $[f(0)_{\text{num}}]$ for different values of ω.

Q	ω	c	c_1	α	$f(0)$	$f(0)_{\text{num}}$
23.68	1.79	1.097	0.12	2.66	1.037	1.024
35	1.72	1.087	0.068	2.60	1.052	1.055
61.6	1.64	1.068	0.0243	2.54	1.056	1.065
149.3	1.57	1.049	0.0031	2.53	1.048	1.056

$$I_1 = c^2 I_0 + c^2 c_1 \frac{d}{dc_1} I_0, \tag{24}$$

$$I_2 = c^4 I_0 + 2c^4 c_1 \frac{d}{dc_1} I_0 + \frac{1}{2} c^4 c_1^2 \frac{d^2}{dc_1^2} I_0 \ . \tag{25}$$

It is readily seen that the actual values for Q and E depend strongly on the value of c_1 especially for small values of c_1. In this region, c_1 can be eliminated in favor of Q to get

$$E = \left(\frac{1}{\omega} + \frac{\omega}{2}\right) Q + \frac{24 + 3\alpha^2}{16\omega} (q\omega)^{1/3} Q^{2/3} + \frac{24 + 3\alpha^2}{8\omega} (q\omega)^{2/3} Q^{1/3} - \frac{(8 + \alpha^2)\,\pi^2}{8\omega} q\omega \ + O(Q^{-1/3}), \tag{26}$$

where

$$q = \frac{4\pi c^2}{3\alpha^3} \ . \tag{27}$$

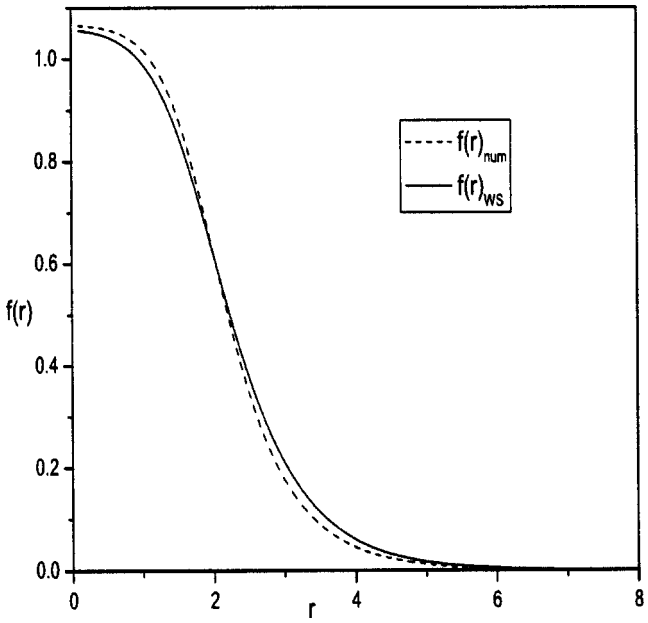

FIG. 1. The profile function $f(r)$ as a function of r for $\omega = 1.64$.

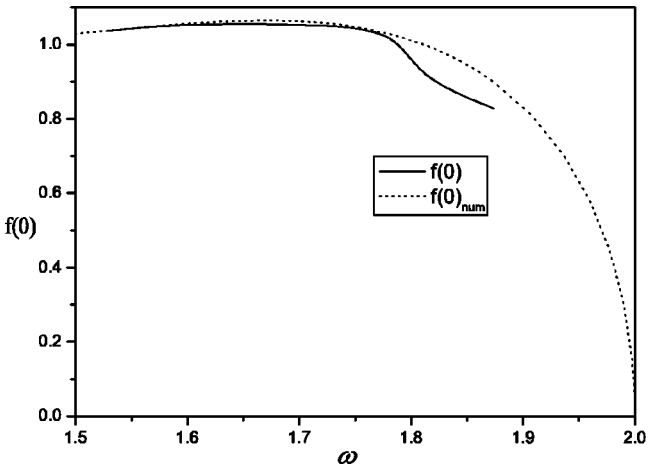

FIG. 2. The frequency dependence of the profile function at the origin $f(0)$.

It is interesting to see that the leading terms of (26) are identical to those of (9) for $\alpha=2\sqrt{2}$, $c=1$, $\omega=\sqrt{2}$. Taking into account the fact that α and c are slowly varying functions of ω helps to explain the wide range of applicability of (9).

As a result, the parameters c, c_1, α, and ω for specific values of the charge Q can be uniquely determined by solving the system of equations: (16), (20), (21), and (22) provided that the energy-charge dependence of the Q-ball is given by (9). We expect the values obtained that way to be quite accurate as long as (9) remains reasonably accurate. In practice, this means that $Q\gtrsim 16$, a value far distant from the values normally associated with the region of the thin-wall approximation. In Table I the values of the arbitrary constants in (11) are presented for different values of Q (or ω). That way, the initial value $f(0)$ can be determined explicitly; a comparison with values obtained numerically show that the symmetrized Woods–Saxon distribution describes accurately the Q-ball profile function.

Finally, Fig. 1 presents the profile function obtained analytically and numerically for $\omega=1.64$. Figure 2 presents the values of the profile function at the origin for different ω obtained numerically and analytically.

III. CONCLUSIONS

In this work, the basic properties of the Q-ball profile function have been extensively studied by means of mainly analytic methods. In particular, it has been shown that the profile function can be accurately approximated by the symmetrized Woods–Saxon distribution, while the corresponding energy and charge can be explicitly evaluated. The approach presented here might prove to be particularly useful in understanding the basic properties of Q-balls such as existence, small vibrations and stability. We believe that a similar line of argument can be applied to study the profile function and the energy-charge dependence in other types of potentials. In fact, we expect that the symmetrized Woods–Saxon distribution will accurately describe all types of Q-balls independently of the exact form of the scalar potential. Work in this direction is currently in progress.

ACKNOWLEDGMENTS

We thank V. Kopeliovich, A. Kouiroukidis, and S. Massen for useful discussions. T.I. thanks the Royal Society and the National Hellenic Research Foundation for a Study Visit Grant.

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Topics in quantum integrable systems

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(Received 15 December 2002; accepted 9 April 2003)

Recent developments in the theory of quantum integrable particle systems in one-dimension with inverse square interactions are reviewed. First the Yangian symmetry is introduced and the energy spectra of the related spin models are discussed. The character of the su$(n)_1$ WZNW theory is shown to be closely related with the Rogers–Szegö polynomial. Second, the infinite dimensional representation for solutions of the Yang–Baxter equation and the reflection equation is given. Based on the representation, the Dunkl operators associated with the classical root systems are constructed. The Macdonald polynomial and its generalization are discussed in connection with the eigenstates for the trigonometric case. Finally, some results on short-range interacting systems are mentioned. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1588743]

I. INTRODUCTION

We define the integrability of quantum systems as an extension of the Liouville theorem for classical systems. The quantum system is integrable when it has M independent mutually commuting conserved operators (M being the number of degrees of freedom). Quantum integrable systems[1] can be classified by the range of interaction. One is short-range interacting systems including the δ-function gas, the Heisenberg XYZ spin chain and the Toda lattice. The other is long-range interacting systems: the most famous systems are due to Calogero,[2] Sutherland,[3] and Moser.[4] See also references in Ref. 5

We consider a system of N identical particles on a line. The Hamiltonians of the Calogero–Sutherland–Moser (CSM) models are written as follows:

$$\mathcal{H}=-\sum_{j=1}^{N}\frac{\partial^2}{\partial z_j{}^2}+2\sum_{1\leqslant j<k\leqslant N}\wp(z_{jk})\cdot(\beta^2-\beta P_{jk}), \tag{1.1}$$

$$\begin{aligned}\mathcal{H}=&-\sum_{j=1}^{N}\frac{\partial^2}{\partial z_j{}^2}+2\sum_{1\leqslant j<k\leqslant N}(\wp(z_{jk})\cdot(\beta^2-\beta P_{jk})+\wp(z_j+z_k)\cdot(\beta^2-\beta Q_jQ_kP_{jk}))\\&+\sum_{j=1}^{N}(\wp(z_j)\cdot(4\alpha^2+4\alpha\overline{\alpha}-2\alpha Q_j)+\wp(2z_j)\cdot(4\overline{\alpha}^2-4\overline{\alpha}Q_j)),\end{aligned} \tag{1.2}$$

where $z_{jk}=z_j-z_k$ and $\wp(z)$ is the Weierstrass $\wp$-function. Note that the original CSM models do not contain internal degrees of freedom expressed by operators P_{jk} and Q_j. The models (1.1) and (1.2) are related to the root system. In this sense, the first one is the A-type, and the second is the BC-type. Another interesting extension is a model confined in an external harmonic potential,

$$\mathcal{H}=-\sum_{j=1}^{N}\frac{\partial^2}{\partial z_j{}^2}+2\sum_{1\leqslant j<k\leqslant N}\frac{\beta^2-\beta P_{jk}}{z_{jk}^2}+\sum_{j=1}^{N}\omega^2 z_j{}^2. \tag{1.3}$$

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Operators P_{jk} and Q_j act on the spin space of the jth and kth particles, and satisfy the relations

$$P_{jk}P_{kl}=P_{kl}P_{jl}=P_{jl}P_{jk}, \quad P_{jk}Q_j=Q_kP_{jk}, \quad Q_jQ_k=Q_kQ_j,$$

$$P_{jk}^2=Q_j{}^2=\mathbb{1}, \quad \text{for } j,k,l \text{ are distinct.}$$

In the case of su(2) spin-$\frac{1}{2}$, these operators may be chosen nontrivially as $P_{jk}=\frac{1}{2}(1+\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k)$, $Q_j=\sigma_j^z$, where $\boldsymbol{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$ are Pauli spin matrices. Hereafter we use su(n) spin generator E_j^{ab} $(a,b=1,2,\ldots,n)$ for the jth spin, $E^{ab}=|a\rangle\langle b|$, satisfying the commutation relations

$$[E_j^{ab},E_k^{cd}]=\delta_{jk}(\delta^{bc}E_j^{ad}-\delta^{da}E_j^{cb}). \tag{1.4}$$

It is noted that the permutation operator P_{jk} is written as

$$P_{jk}=\sum_{a,b=1}^{n}E_j^{ab}E_k^{ba}.$$

Studies of the long-ranged interaction systems have made remarkable developments since the discovery of the integrable variants for spin system.[6,7] A well-known example is the Haldane–Shastry (HS) model,

$$\mathcal{H}_{\mathrm{HS}}=\sum_{1\leqslant j<k\leqslant N}\frac{P_{jk}}{\sin^2(\pi(j-k)/N)}. \tag{1.5}$$

As will be discussed later, the Yangian symmetry is revealed for the HS model with *finite* lattice. This fact gives new insights on interesting subjects such as the fractional statistics, the character formula for the WZNW model, and the affine Hecke algebra.

This article presents some recent results related with the quantum CSM models. In Sec. II the Yangian symmetry is explained. We show that the Haldane–Shastry-type spin chains have the Yangian symmetry, and that the character formula for the level-1 WZNW model is related with the HS chain. Section III deals with the infinite-dimensional representation for solutions of the Yang–Baxter equation (YBE) and the reflection equation (RE). We propose a simple method to give matrix solutions of YBE and RE. In Sec. IV the elliptic Dunkl operator is constructed by use of the infinite-dimensional representation. The Hamiltonians for the elliptic CSM model are expressed in terms of the Dunkl operators. The trigonometric limit is discussed in Sec. V. The trigonometric CSM models are studied from the representation of the affine Hecke algebra. In Sec. VI the Macdonald polynomial associated with the root systems is discussed in relation with the q-deformed trigonometric CSM models. Section VIII is devoted to concluding remarks.

II. YANGIAN SYMMETRY AND CHARACTER FORMULA

A. Yangian symmetry

The Yangian symmetry was first defined by Drinfeld[8] as a Hopf algebra associated with the rational solution of the Yang–Baxter equation. The YBE reads (Fig. 1)

$$R^{12}(\xi_{12})\,R^{13}(\xi_{13})\,R^{23}(\xi_{23})=R^{23}(\xi_{23})\,R^{13}(\xi_{13})\,R^{12}(\xi_{12}), \tag{2.1}$$

where the conventional notation, e.g., $\xi_{ij}=\xi_i-\xi_j$, is used. We call ξ_j spectral parameters.

Operator R^{jk} acts on space $V^{\otimes N}$ as R on the jth and kth space, and as identity on the other spaces. For solutions of the YBE, we can define a monodromy matrix $T(\xi)$, which satisfies the quadratic relation

$$R^{12}(\xi_{12})\overset{1}{T}(\xi_1)\overset{2}{T}(\xi_2)=\overset{2}{T}(\xi_2)\overset{1}{T}(\xi_1)R^{12}(\xi_{12}), \tag{2.2}$$

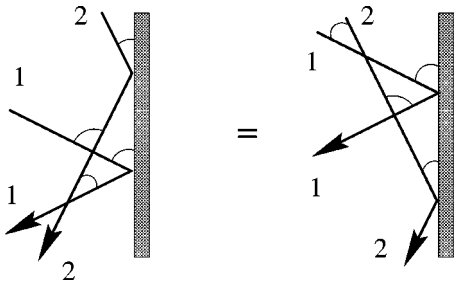

FIG. 1. Yang–Baxter equation (2.1).

where we use the standard notation, $\overset{1}{T}(\xi)=T(\xi)\otimes\mathbb{1}$ and $\overset{2}{T}(\xi)=\mathbb{1}\otimes T(\xi)$. As solutions of the YBE, there are three types of R-matrices: rational, trigonometric, and elliptic ones. When we substitute in the quadratic relation (2.2) a rational su(n) R-matrix $R(u)=u+\hbar P$, we find that matrix elements of the monodromy matrix satisfy commutation relations

$$[T^{ab}(\xi_1),T^{cd}(\xi_2)]=\frac{\hbar}{\xi_{12}}(T^{cb}(\xi_2)\,T^{ad}(\xi_1)-T^{cb}(\xi_1)\,T^{ad}(\xi_2)). \tag{2.3}$$

We refer to $\hbar$ as a ''deformation parameter.'' One defines a set of generators $\{T_l\}$ as a mode expansion of the monodromy matrix $T(\xi)$,

$$T^{ab}(\xi)=\delta^{ab}-\hbar\sum_{k=0}^{\infty}T_k^{ab}\,\xi^{-k-1}. \tag{2.4}$$

The Yangian Y(su(n)) is the algebra constructed from operators T_k^{ab} with commutation relations,

$$[T_l^{ab},T_m^{cd}]=\delta^{bc}\,T_{l+m}^{ad}-\delta^{ad}\,T_{l+m}^{cb}+\hbar\sum_{k=0}^{l-1}(T_{k+m}^{cb}\,T_{l-k-1}^{ad}-T_{l-k-1}^{cb}\,T_{k+m}^{ad}).$$

The above defining relations are simplified when one introduces new generators (Yangian currents) by

$$\begin{aligned}Q_0^{ab}&=T_0^{ab},\\ Q_1^{ab}&=T_1^{ab}+\frac{\hbar}{2}(T_0\,T_0)^{ab},\end{aligned} \tag{2.5}$$

where the notation $(T_0\,T_0)^{ab}=\Sigma_{c=1}^{n}T_0^{ac}\,T_0^{cb}$ is used for brevity. We can show that these currents satisfy the following commutation relations:

$$\begin{aligned}[Q_0^{ab},Q_0^{cd}]&=\delta^{bc}Q_0^{ad}-\delta^{da}Q_0^{cb},\\ [Q_0^{ab},Q_1^{cd}]&=\delta^{bc}Q_1^{ad}-\delta^{da}Q_1^{cb},\\ [Q_0^{ab},[Q_1^{cd},Q_1^{ef}]]&-[Q_1^{ab},[Q_0^{cd},Q_1^{ef}]]\\ &=\frac{\hbar^2}{4}([Q_0^{ab},[(Q_0Q_0)^{cd},(Q_0Q_0)^{ef}]]-[(Q_0Q_0)^{ab},[Q_0^{cd},(Q_0Q_0)^{ef}]]).\end{aligned} \tag{2.6}$$

These are the defining relations for the Yangian Y(su(n)).[8] It is noted that in the limit $\hbar\to 0$ the Yangian algebra Y(su(n)) reduces to the loop algebra for Lie algebra su(n). Due to this, we can

regard the Yangian as the ''deformed Lie algebra.'' The third equation in (2.6) is called the deformed Serre relation. In a precise sense for the Yangian algebra Y(su(n)), we should set the quantum determinant qdet$T(\xi)$ as unity, where the quantum determinant is defined as a center of the Yangian,[9]

$$\mathrm{qdet}T(\xi)=\sum_{\sigma}(-)^{\sigma}T^{1\,\sigma(1)}(\xi)\,T^{2\,\sigma(2)}(\xi+\hbar)\cdots T^{n\,\sigma(n)}(\xi+(n-1)\hbar), \tag{2.7}$$

$$[\mathrm{qdet}T(\xi_1),T^{ab}(\xi_2)]=0,\quad \text{for } a,b=1,2,\ldots,n. \tag{2.8}$$

By definition the Yangian symmetry Y(su(n)) is associated with the quantum integrable colored systems formulated by the rational solution of the YBE, for instance, the XXX–Heisenberg model.[10] The Yangian symmetry in the XXX–Heisenberg spin chain is revealed for the thermodynamical limit. It is a remarkable fact that the Yangian symmetry is realized in the finite-size HS model.[11] As an integrable variant of the HS model, we have the Polychronakos–Frahm (PF) model,[12] which also possesses the Yangian symmetry.[13] The Hamiltonians for these models are respectively written as follows:

$$\mathcal{H}_{\mathrm{HS}}=\sum_{1\leqslant j<k\leqslant N}\frac{z_j z_k}{z_{jk}z_{kj}}P_{jk}, \tag{2.9}$$

$$\mathcal{H}_{\mathrm{PF}}=\sum_{1\leqslant j<k\leqslant N}\frac{1}{z_{jk}^2}P_{jk}. \tag{2.10}$$

We can explicitly construct the Yangian currents $\{Q_0^{ab},Q_1^{ab}\}$ which satisfy the Yangian commutation relations (2.6) and commute with Hamiltonian.

(a) HS model:

$$Q_0^{ab}=\sum_{j=1}^{N}E_j^{ab},$$

$$Q_1^{ab}=\sum_{j,k=1}^{N}{}'\,(E_j E_k)^{ab}\frac{z_j+z_k}{z_{jk}}, \tag{2.11}$$

where Σ' means any two indices do not coincide. For the Yangian currents $\{Q_0^{ab},Q_1^{ab}\}$ to commute with the Hamiltonian $\mathcal{H}_{\mathrm{HS}}$ (2.9), it is required that the coordinates $\{z_j\}$ satisfy

$$\sum_{l=1,\ l\neq j}^{N}\frac{z_j z_l(z_j+z_l)}{z_{jl}^3}=0,\quad \text{for } j=1,2,\ldots,N.$$

This condition is satisfied when

$$z_k=\exp(2\pi\mathrm{i}k/N),\quad \text{for finite } N,$$

$$z_k=\exp(2\gamma k),\quad \text{for } N\to\infty,\ \gamma\in\mathbb{R}.$$

The first case corresponds to the HS model (1.5); all spins are fixed equidistantly on a circle. The second one was studied by Inozemtsev;[14] each spin is on the infinite one-dimensional regular lattice. This model reduces to the XXX–Heisenberg spin chain in a certain limit.

(b) PF model:

$$Q_0^{ab}=\sum_{j=1}^{N}E_j^{ab},$$

$$Q_1^{ab}=-\sum_{j,k=1}^{N}{}' E_j^{ab}\frac{1}{z_{jk}^2}+\sum_{j,k,l=1}^{N}{}' (E_jE_kE_l)^{ab}\frac{1}{z_{jk}z_{kl}}-\sum_{j=1}^{N} E_j^{ab}z_j{}^2. \tag{2.12}$$

In this case the Hamiltonian $\mathcal{H}_{\mathrm{PF}}$ in (2.10) commutes with the Yangian currents $\{Q_0^{ab},Q_1^{ab}\}$ when we set the coordinates as

$$z_j=\sum_{l=1,\ l\neq j}^{N}\frac{2}{z_{jl}^3},\quad \text{for } j=1,2,\ldots,N.$$

This condition means that each spin is fixed on the equilibrium position of the Calogero model (1.3), i.e., $\{z_j\}$ are zeros of the Nth order Hermite polynomial $h_N(x)$:

$$h_N''(x)-2x\,h_N'(x)+2N\,h_N(x)=0.$$

B. Motif

The spectra and their degeneracies of these spin chains can be obtained from Haldane's "motif."[11,15,16] We briefly explain it for the su(2) spin case with N sites. Let us consider a set of pseudo-momenta $m_j\in\{1,2,\ldots,N-1\}$. In terms of pseudo-momenta the energies for HS and PF models are, respectively, given by

$$E_{\mathrm{HS}}=\sum_j m_j(m_j-N), \tag{2.13}$$

$$E_{\mathrm{PF}}=\sum_j (-m_j). \tag{2.14}$$

Remark that the eigenvalues are additive. A set $\{m_j\}$ can be represented by an $(N+1)$-term sequence of 0's and 1's, where a 0 (resp. 1) indicates the absence (presence) of the integer corresponding to the position in the sequence. It is required that consecutive 1's do not occur and that both ends are 0's. These two 0's are sometimes replaced by parenthesis '(' and ')'. This sequence is called "motif." This selection rule shows that motifs are decomposed into a product of "elementary motifs," a series of $(M+1)$ consecutive 0's. Each elementary motif is represented by the Young diagram

$$[M]=\underbrace{\square\square\cdots\square}_{M}$$

and the multiplicities of each motif is calculated as a tensor product of representations of elementary motifs. It is seen that the ground state of the spin chain with $2M$ sites is expressed by motif

$$\underbrace{(101010\ldots0101)}_{2M-1}.$$

For su(n) case, the representation is more involved.[15]

In the following we show that the representation of motif is derived from the Rogers–Szegö polynomial.[17] This polynomial is a special case of the Macdonald polynomial, which will be shown in Sec. VI.

The spectrum of the PF model is simple; energy levels are equally spaced as in (2.14). This fact makes it possible to calculate the partition function $Z_N^{(n)}(q)$ of the N-site su(n) PF spin chain; *modding* the su(n) Calogero model confined in the harmonic potential by the spinless model, the partition function for the PF model is calculated.[18] In the case of su(2), we get

$$Z_N(q)=\sum_{k=0}^{N} q^{(N/2-k)^2}\begin{bmatrix} N \\ k \end{bmatrix}_q, \tag{2.15}$$

where we used the Gaussian q-binomial coefficient (Appendix A),

$$\begin{bmatrix} N \\ k \end{bmatrix}_q=\begin{cases} \dfrac{(q;q)_N}{(q;q)_k\,(q;q)_{N-k}}, & \text{for } 0\leqslant k\leqslant N, \\ 0, & \text{otherwise,} \end{cases}$$

with the q-product $(a;q)_k=(1-a)\,(1-a\,q)\,\cdots(1-a\,q^{k-1})$, $(a;q)_0=1$. The partition function $Z_N(q)$ can be written in a compact form as

$$Z_N(q)=q^{N^2/4}\cdot H_N(x_1=x_2=1;q^{-1}), \tag{2.16}$$

where a function $H_N(x;q)$ is the Rogers–Szegö (RS) polynomial[19] defined by

$$H_N(x;q)=\sum_{k=0}^{N}\begin{bmatrix} N \\ k \end{bmatrix}_q x_1^k\,x_2^{N-k}. \tag{2.17}$$

The RS polynomial is regarded as the q-deformed Hermite polynomial, and we have a generating function,

$$\sum_{N=0}^{\infty}\frac{H_N(x;q)}{(q;q)_N}\,t^N=\frac{1}{(x_1\,t;q)_\infty\,(x_2\,t;q)_\infty}. \tag{2.18}$$

By setting $t\to q\,t$ in the above formula, one obtains the three-term recurrence relation for the RS polynomial,

$$H_N(x;q)=s_{[1]}(x)\,H_{N-1}(x;q)-(1-q^{N-1})\,s_{[1^2]}(x)\,H_{N-2}(x;q), \tag{2.19}$$

where $s_\lambda(x)$ is the Schur function for the Young diagram λ. As the RS polynomial is essentially the partition function of the PF model and the energy of the PF model is additive for the Yangian invariant bases, we obtain the representation for motifs from the recurrence relation (2.19):[17]

$$(\ldots 11)=0,\ (\ldots 10)=\square\otimes(\ldots 1),$$

$$(\ldots 01)=\begin{smallmatrix}\square\\\square\end{smallmatrix}\otimes(\ldots),\quad (\ldots 00)=\square\otimes(\ldots 0)-\begin{smallmatrix}\square\\\square\end{smallmatrix}\otimes(\ldots),$$

with the first three motifs,

$$(\ )=\square,\quad (0)=\square\square,\quad (1)=\begin{smallmatrix}\square\\\square\end{smallmatrix}.$$

One sees that these recurrence relations give the same representation found by Haldane. The first identity means that consecutive 1's are forbidden. This shows that the quasi-particle of the HS and PF models has a fractional exclusion statistics *a là* Haldane.[20] Also one sees that the motif

$$\underbrace{(101010\ldots01)}_{2M-1}$$

gives a trivial representation $[M^2]$. As this motif corresponds to the ground state of the HS and PF models with $2M$ sites, we conclude that the ground state is nondegenerate.

Representation for su(n) motif is related with the generalized RS polynomial $H_N^{(n)}(x;q)$ defined by

$$H_N^{(n)}(x;q)=\sum_{\substack{k_1+\cdots+k_n=N\\ k_j\geqslant 0}}\begin{bmatrix} N \\ k_1,k_2,\ldots,k_n\end{bmatrix}_q x_1^{k_1}x_2^{k_2}\cdots x_n^{k_n}. \tag{2.20}$$

Here we use the q-multinomial coefficients,

$$\begin{bmatrix} N \\ k_1,k_2,\ldots,k_n\end{bmatrix}_q=\begin{cases}\dfrac{(q;q)_N}{(q;q)_{k_1}\cdots(q;q)_{k_n}}, & \text{for } k_1+\cdots+k_n=N,\ k_j\geqslant 0,\\ 0, \quad \text{otherwise.}\end{cases}$$

The partition function $Z_N^{(n)}(q)$ of the PF spin chain is written in terms of the generalized RS polynomial as

$$Z_N^{(n)}(q)=q^{(n-1)/2n\,N^2}\cdot H_N^{(n)} \quad (x_1=\cdots=x_n=1;q^{-1}). \tag{2.21}$$

The generating function of the generalized RS polynomial is given by

$$\sum_{N=0}^{\infty}\frac{H_N^{(n)}(x;q)}{(q;q)_N}t^N=\frac{1}{(x_1t;q)_\infty(x_2t;q)_\infty\cdots(x_nt;q)_\infty}. \tag{2.22}$$

In the same manner for the su(2) case, by setting $t\to q\,t$ in the above equality one gets a recurrence relation for any $(n+1)$-consecutive generalized RS polynomials $H_N^{(n)}(x;q)$,

$$H_N^{(n)}(x;q)=\sum_{k=1}^{n}(-)^{k-1}\frac{(q;q)_{N-1}}{(q;q)_{N-k}}s_{[1^k]}(x)\,H_{N-k}^{(n)}(x;q). \tag{2.23}$$

It is straightforward to translate the above recurrence relation into a language of motifs. We take an example from su(3) case:

$$(\ldots 111)=0, \quad (\ldots 110)=\square\otimes(\ldots 11),$$

$$(\ldots 011)=\begin{array}{|c|}\hline\ \\ \hline\end{array}\otimes(\ldots), \quad (\ldots 001)=\begin{array}{|c|}\hline\ \\ \hline\end{array}\otimes(\ldots 0)-\begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\end{array}\otimes(\ldots),$$

$$(\ldots 101)=\begin{array}{|c|}\hline\ \\ \hline\end{array}\otimes(\ldots 1), \quad (\ldots 010)=\square\otimes(\ldots 01)-\begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\end{array}\otimes(\ldots 0),$$

$$(\ldots 100)=\square\otimes(\ldots 10)-\begin{array}{|c|}\hline\ \\ \hline\end{array}\otimes(\ldots 1),$$

$$(\ldots 000)=\square\otimes(\ldots 00)-\begin{array}{|c|}\hline\ \\ \hline\end{array}\otimes(\ldots 0)+\begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\end{array}\otimes(\ldots).$$

First several motifs are given by

$$(\ )=\square, \quad (0)=\square\square, \quad (1)=\begin{array}{|c|}\hline\ \\ \hline\end{array}, \quad (00)=\square\square\square, \quad (10)=(01)=\begin{array}{|c|}\hline\ \\ \hline\end{array}\square, \quad (11)=\begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\end{array}.$$

In su(3) case the three consecutive 1's are forbidden, and the ground state for a $(3M)$-site spin chain is denoted by motif $(110110110\ldots011)$. In general, one sees that the N-site spin is represented by the Young diagram with N boxes, and that n consecutive 1's cannot occur for the su(n) motif. It should be seen that the ground state for an $(n\times M)$-site spin chain is nondegenerate and given by motif

$$(\underbrace{11\ldots1}_{n-1}0\underbrace{11\ldots1}_{n-1}0\,11\ldots\ldots11\,0\underbrace{11\ldots1}_{n-1}).$$

TABLE I. Representation for motifs, $N=4$.

Motif	$\{m_j\}$	Young diagram	E_{PF}	E_{HS}
(111)	{1,2,3}	$[1^4]$	-6	-10
(011)	{2,3}	$[2^1 1^2]$	-5	-7
(110)	{1,2}	$[2^1 1^2]$	-3	-7
(101)	{1,3}	$[2^1 1^2]\oplus[2^2]$	-4	-6
(010)	{2}	$[2^2]\oplus[3^1 1^1]$	-2	-4
(001)	{3}	$[3^1 1^1]$	-3	-3
(100)	{1}	$[3^1 1^1]$	-1	-3
(000)	{}	$[4^1]$	0	0

One sees also that the motif

$$\underbrace{011\ldots10}_{r}$$

corresponds to the Young diagram $[1^{r+1}]$, but the representation is not given from simple tensor products of each motifs.

Solution of those recurrence relations is explicitly solved as a skew Schur function for the borderstrip which is no 2×2 squares.[21]

In Table I, we list a representation for motifs $N=4$. The representation for the su(n) case ($n<4$) is given by removing the forbidden Young tableaus.

C. Character formula

The Yangian currents $\{Q_0^{ab},Q_1^{ab}\}$ can be constructed from the current operators for level-1 su(n) WZNW theory,[22]

$$[J_l^a,J_m^b]=f^{abc}J_{l+m}^c+\delta^{ab}\,l\,\delta_{l+m,0}. \tag{2.24}$$

In terms of the currents J_m^a, the Yangian currents are expressed as

$$\begin{aligned} Q_0^a&=J_0^a,\\ Q_1^a&=\frac{1}{2}f^{abc}\sum_{m>0}J_{-m}^bJ_m^c-\frac{n}{2(n+2)}W_0^a. \end{aligned} \tag{2.25}$$

We used the zero-mode of the W-current,

$$W^a(z)=\tfrac{1}{2}d^{abc}{:}J^bJ^c{:}(z),$$

where : : denotes the normal ordering. The conserved operators H_m for the Yangian currents are also given in terms of the currents for the su$(n)_1$ WZNW theory. The first two are explicitly written as

$$H_1=L_0\equiv\frac{1}{2(n+1)}\sum_m{:}J_{-m}^aJ_m^a{:}, \tag{2.26a}$$

$$H_2=\sum_{m>0}m\,J_{-m}^aJ_m^a+\frac{n}{(n+1)(n+2)}W_0, \tag{2.26b}$$

where W_0 is the zero-mode of the third order Casimir operator $W(z)$,

$$W(z)=\tfrac{1}{6}d^{abc}{:}J^a{:}J^bJ^c{::}(z).$$

The fact that the energy levels of the PF chain are equally spaced suggests that the Hamiltonian of the PF spin chain can be identified as the Virasoro generator L_0. Through this observation we can show that the partition function $Z_N^{(n)}(q)$ for the large-N limit is realized as the affine character for the level-1 su(n) WZNW theory,

$$\chi_\ell^{(n)}(q)=\lim_{\substack{N\to\infty \\ N\equiv\ell(\mathrm{mod}\ n)}} Z_N^{(n)}(q). \tag{2.27}$$

For the su(2) case we obtain a well-known character formula ($\ell=0,1$),

$$\chi_\ell^{(2)}(q)=\frac{1}{(q;q)_\infty}\sum_{k=-\infty}^{\infty} q^{(k+\ell/2)^2}=\sum_{n^++n^-=\ell(\mathrm{mod}\ 2)}\frac{q^{(n^++n^-)^2/4}}{(q;q)_{n^+}(q;q)_{n^-}}.$$

The second equality is proved in Ref. 23 by using spinon bases.

In the general su(n) case, we can obtain the affine character as the large-N limit of $Z_N^{(n)}(q)$,

$$\chi_{\ell=0}^{(n)}(q)=\frac{1}{(q;q)_\infty^{n-1}}\sum_{k_1=-\infty}^{\infty}\cdots\sum_{k_{n-1}=-\infty}^{\infty} q^{\mathbf{k}^t\cdot\mathbf{A}\cdot\mathbf{k}/2}=1+(n^2-1)\,q+\cdots, \tag{2.28}$$

where $\mathbf{k}^t=(k_1,\ldots,k_{n-1})$ and $\mathbf{A}$ is the Cartan matrix for su(n). A supersymmetric extension of the PF spin chain is also an interesting subject and has been studied in Ref. 24.

III. INFINITE-DIMENSIONAL REPRESENTATION

A. Infinite-dimensional representation

We investigate solutions of the Yang–Baxter equation (2.1). Each solution of the YBE corresponds to an integrable spin chain. Here we shall consider the infinite-dimensional representation for solutions.[25]

We make an ansatz that the R-operator acts on functional space in the following way:

$$(R^{12}(\xi)\,f)(z_1,z_2)=A(z_{12})\,f(z_1,z_2)-B(\xi,z_{12})\,f(z_2,z_1),$$

where functions $A(z)$ and $B(\xi,z)$ are to be determined. By using this ansatz in the YBE (2.1), we get functional equations

$$\begin{aligned}&B(\xi_{12},z_{12})\cdot(A(z_2)\,A(-z_2)-A(z_1)\,A(-z_1))\\&\quad=B(\xi_1,z_1)\,B(\xi_{12},-z_2)\,B(-\xi_2,z_1)-B(-\xi_2,-z_2)\,B(\xi_{12},z_1)\,B(\xi_1,-z_2),\end{aligned} \tag{3.1a}$$

$$B(\xi_1,z_1)\,B(-\xi_2,z_{12})=B(\xi_{12},z_{12})\,B(\xi_1,z_2)+B(-\xi_2,-z_2)\,B(\xi_{12},z_1). \tag{3.1b}$$

One finds that elliptic function solves the above functional equations,

$$A(z)=\sigma_\mu(z),\qquad B(\xi,z)=\sigma_\xi(z),$$

where μ is an arbitrary parameter. See Appendix B for definition and properties of the elliptic function $\sigma_\mu(z)=\sigma_\mu(z;\tau)$. For our convention, we take $R^{jk}(\xi)$ as

$$(R^{12}(\xi)\,f)(z_1,z_2)=\frac{1}{\sigma_\mu(\xi)}(\sigma_\mu(z_{12})\,f(z_1,z_2)-\sigma_\xi(z_{12})\,f(z_2,z_1)), \tag{3.2}$$

which satisfies the unitarity condition, $R^{12}(\xi)\,R^{21}(-\xi)=\mathbb{1}$, and the quasi-classical condition, $R^{12}(\xi)|_{\mu=0}=\mathbb{1}$.

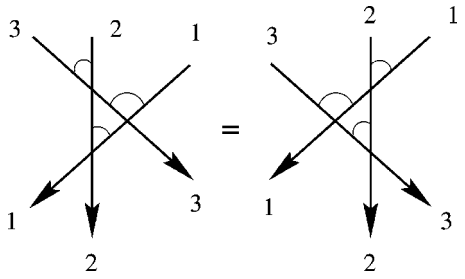

FIG. 2. Reflection equation (3.3).

The YBE is used to formulate integrable systems with the periodic or twisted boundary condition. Recently much attention has been paid on the effects of the boundary condition. In general, the boundary condition should be carefully fixed to keep the integrability; the ''choice'' of the boundary condition is determined by the reflection equation (RE).[26] The RE is written as (see Fig. 2)

$$R^{12}(\xi_{12})\overset{1}{K}(\xi_1)R^{21}(\xi_1+\xi_2)\overset{2}{K}(\xi_2)=\overset{2}{K}(\xi_2)R^{12}(\xi_1+\xi_2)\overset{1}{K}(\xi_1)R^{21}(\xi_{12}), \tag{3.3}$$

where R is a solution of the YBE (2.1). To give the solution of the RE (3.3) associated with the elliptic R-operator (3.2), we make an ansatz that the boundary K-operator acts on functional space as

$$(K(\xi)f)(z)=G(\xi,z)f(z)-H(z)f(-z), \tag{3.4}$$

with functions $G(\xi,z)$ and $H(z)$ to be fixed. Then from the RE (3.3), one obtains functional equations[27]

$$\begin{aligned}
&G(\xi_2,z_2)\sigma_{\xi_1+\xi_2}(z_{12})\sigma_{\xi_{12}}(z_1+z_2)+G(\xi_1,z_1)\sigma_{\mu}(z_1+z_2)\sigma_{\mu}(-z_1-z_2)\\
&\quad+G(\xi_1,-z_2)\sigma_{\xi_1+\xi_2}(z_1+z_2)\sigma_{\xi_{12}}(z_1+z_2)\\
&\quad=G(\xi_1,z_1)\sigma_{\mu}(z_{12})\sigma_{\mu}(z_{21})+G(\xi_1,z_2)\sigma_{\xi_{12}}(z_{12})\sigma_{\xi_1+\xi_2}(z_{12})\\
&\qquad+G(\xi_2,-z_2)\sigma_{\xi_{12}}(z_{12})\sigma_{\xi_1+\xi_2}(z_1+z_2),
\end{aligned} \tag{3.5a}$$

$$\begin{aligned}
&G(\xi_1,z_1)G(\xi_2,z_2)\sigma_{\xi_{12}}(z_{21})+G(\xi_1,z_2)G(\xi_2,z_2)\sigma_{\xi_1+\xi_2}(z_{12})+H(-z_2)H(z_2)\sigma_{\xi_1+\xi_2}(z_1+z_2)\\
&\quad=G(\xi_1,z_1)G(\xi_2,z_1)\sigma_{\xi_1+\xi_2}(z_{21})+G(\xi_1,z_2)G(\xi_2,z_1)\sigma_{\xi_{12}}(z_{12})\\
&\qquad+H(z_1)H(-z_1)\sigma_{\xi_1+\xi_2}(z_1+z_2),
\end{aligned} \tag{3.5b}$$

$$\begin{aligned}
&G(\xi_1,z_1)\sigma_{\xi_1+\xi_2}(z_{21})+G(\xi_1,z_2)\sigma_{\xi_{12}}(z_{12})+G(\xi_2,-z_1)\sigma_{\xi_1+\xi_2}(z_1+z_2)\\
&\quad=G(\xi_2,z_2)\sigma_{\xi_{12}}(z_1+z_2).
\end{aligned} \tag{3.5c}$$

The solution is written as[27]

$$G(\xi,z)=\sum_{r=0}^{3}g_r\sigma_{2\xi}^{r}(z),\qquad H(z)=\sum_{r=0}^{3}g_r\sigma_{2\nu}^{r}(z), \tag{3.6}$$

where parameters g_r and ν are arbitrary. Correspondingly, we have explicit forms for the K-operators,

$$K(\xi)=\sum_{r=0}^{3} g_r\,(\sigma_{2\xi}^r(z)-\sigma_{2\nu}^r(z)\cdot\hat{t}\,). \tag{3.7}$$

As a simple solution we have

$$(K^{\mathrm{I}}(\xi)\,f\,)(z)=\frac{1}{\sigma_{2\nu}(2\xi)}(\sigma_{2\xi}(z)\,f(z)-\sigma_{2\nu}(z)\,f(-z)). \tag{3.8}$$

Here the K-operators are normalized to satisfy the unitarity condition, $K^{\mathrm{I}}(\xi)\,K^{\mathrm{I}}(-\xi)=\mathbb{1}$, and the quasi-classical condition, $K^{\mathrm{I}}(\xi=0)=\mathbb{1}$.

B. Belavin elliptic solutions

In the remainder of this section, we shall show that the Belavin elliptic solutions of the YBE[28] are constructed from the infinite-dimensional R-operator,[29] and that the associated boundary K-matrix is calculated in the same way.[27] The strategy is to restrict the functional space to the finite-dimensional one. We set a positive integer $k\in\mathbb{Z}_+$, and introduce the shift operator $T_k(\xi)$, which acts on the functional space as

$$(T_k(\xi)\,f\,)(z)=f\left(z-\frac{\xi}{k}\right). \tag{3.9}$$

The shift operators satisfy the relations

$$\begin{aligned} &T_k(\xi+\eta)=T_k(\xi)\,T_k(\eta),\\ &[R(\xi),T_k(\eta)\otimes T_k(\eta)]=0. \end{aligned} \tag{3.10}$$

The first one is trivial, and the second follows from the fact that the R-operator (3.2) only depends on the difference z_{12}.

To restrict the functional space to be finite-dimensional, we define the functional space $\mathbf{V}_k(\xi)$ of the theta function; a function $f(z)\in\mathbf{V}_k(\xi)$ is a doubly quasi-periodic function,

$$f(z+1)=f(z),\qquad f(z+\tau)=\alpha_k(z,\xi)\,f(z),$$

where $\alpha_k(z,\xi)\equiv\exp(-2\,\pi\,\mathrm{i}\,k\,z-\pi\,\mathrm{i}\,k\,\tau+2\,\pi\,\mathrm{i}\,\xi)$. It is seen that the elliptic R-operator (3.2), the K-operator (3.7) and the shift operator (3.9) map the functional space in the following way:

$$R(\xi_{12}):\mathbf{V}_k(\xi_1)\otimes\mathbf{V}_k(\xi_2+\mu)\to\mathbf{V}_k(\xi_1+\mu)\otimes\mathbf{V}_k(\xi_2),$$

$$K(\xi):\mathbf{V}_k(\nu-\xi)\to\mathbf{V}_k(\nu+\xi),$$

$$T_k(\xi):\mathbf{V}_k(0)\to\mathbf{V}_k(\xi).$$

Motivated by these properties, we introduce modified elliptic operators $R_k(\xi)$ and $K_k(\xi)$ by

$$R_k(\xi_{12})=T_k(-\xi_1-\mu)\otimes T_k(-\xi_2)\cdot R(\xi)\cdot T_k(\xi_1)\otimes T_k(\xi_2+\mu), \tag{3.11}$$

$$K_k(\xi)=T_k(-\nu-\xi)\cdot K(\xi)\cdot T_k(\nu-\xi), \tag{3.12}$$

both of which preserve the functional space $\mathbf{V}_k(0)$,

$$R_k(\xi):\mathbf{V}_k(0)\otimes\mathbf{V}_k(0)\to\mathbf{V}_k(0)\otimes\mathbf{V}_k(0),$$

$$K_k(\xi):\mathbf{V}_k(0)\to\mathbf{V}_k(0).$$

It is important that a set of the modified operators, $R_k(\xi)$ and $K_k(\xi)$, satisfies both the YBE (2.1) and the RE (3.3). We write explicit forms of the modified operators:

$$(R_k(\xi)\,f)(z_1,z_2)=\sigma_\mu\left(z_{12}+\frac{\mu+\xi}{k};\tau\right)f\left(z_1+\frac{\mu}{k},z_2-\frac{\mu}{k}\right)-\sigma_\xi\left(z_{12}+\frac{\mu+\xi}{k};\tau\right)f\left(z_2-\frac{\xi}{k},z_1+\frac{\xi}{k}\right),$$

$$(K_k(\xi)\,f)(z)=\sum_{r=0}^{3} g_r\left(\sigma^r_{2\xi}\left(z+\frac{\xi+\nu}{k};\tau\right)f\left(z+\frac{2\xi}{k}\right)-\sigma^r_{2\nu}\left(z+\frac{\xi+\nu}{k};\tau\right)f\left(-z-\frac{2\nu}{k}\right)\right).$$

The dimension of the space $\mathbf{V}_k(0)$ is k, and therefore we choose as a basis the θ-function for $a\in\mathbb{Z}_k\equiv\mathbb{Z}/k\mathbb{Z}$:

$$\theta_a(z)=\sum_{n\in\mathbb{Z}}\exp\left(\pi\,\mathrm{i}\,(k\,n+a)^2\frac{\tau}{k}+2\,\pi\,\mathrm{i}\,(k\,n+a)\,z\right)=\vartheta\begin{bmatrix}\alpha/k\\0\end{bmatrix}(kz;k\tau). \tag{3.13}$$

Since the modified R- and K-operators preserve the space $\mathbf{V}_k(0)$, we can define matrix elements of operators by expanding with the θ_a-bases. For the R-operator, we define the $k^2\times k^2$-matrix elements by

$$R_k(\xi)\;\theta_a\otimes\theta_b=\sum_{c,d\in\mathbb{Z}_k}R_k(\xi)_{ac,bd}\,\theta_c\otimes\theta_d\,. \tag{3.14}$$

The boundary K-matrix is also fixed as $k\times k$-matrix,

$$K_k(\xi)\;\theta_a=\sum_{c\in\mathbb{Z}_k}K_k(\xi)_{a,c}\,\theta_c\,. \tag{3.15}$$

Using the property (B5) of the function $\sigma_\mu(z)$, we calculate the matrix elements,

$$R_k(\xi)_{ac,bd}=\delta_{a+b,c+d}\cdot\frac{\vartheta[^{1/2}_{1/2}]'(0;k\,\tau)\;\vartheta[^{(b-a)/k+1/2}_{1/2}](\xi-\mu;k\,\tau)}{\vartheta[^{(b-c)/k+1/2}_{1/2}](\xi;k\,\tau)\;\vartheta[^{(c-a)/k+1/2}_{1/2}](-\mu;k\,\tau)}. \tag{3.16}$$

The same computation results in the elliptic boundary K-matrices[27]

$$K_k(\xi)_{a,c}=\sum_{r=0}^{3}g_r\frac{\vartheta[^{1/2}_{1/2}]'(0;k\,\tau)\;\vartheta[^{-2a/k+1/2}_{1/2}](2\nu-2\xi;k\,\tau)}{\vartheta[^{-(c+a)/k+1/2}_{1/2}](2\nu;k\,\tau)\;\vartheta[^{(c-a)/k+1/2}_{1/2}](-2\xi;k\,\tau)}\times\frac{\vartheta[^{-c/k+\beta_r/2}_{k\alpha_r/2}](\nu+\xi;k\,\tau)}{\vartheta[^{-a/k+\beta_r/2}_{k\alpha_r/2}](\nu-\xi;k\,\tau)}. \tag{3.17}$$

See Appendix B for definitions of α_r and β_r.

To close this section, we note the trigonometric limit of the above results.[30] We set bases e_a for k-dimensional space, $a\in\{-(k-1)/2,-(k-1)/2+1,\ldots,(k-1)/2\}$. The R-matrix is calculated as

$$R(\theta)\,e_a\otimes e_b=\begin{cases}-q^{-1/2}(\theta^{1/2}-\theta^{-1/2})\,e_a\otimes e_b+\theta^{1/2}(q^{1/2}-q^{-1/2})\,e_b\otimes e_a\,, & \text{for } a>b,\\ (\theta^{-1/2}q^{1/2}-\theta^{1/2}q^{-1/2})\,e_a\otimes e_b\,, & \text{for } a=b,\\ -q^{1/2}(\theta^{1/2}-\theta^{-1/2})\,e_a\otimes e_b+\theta^{-1/2}(q^{1/2}-q^{-1/2})\,e_b\otimes e_a\,, & \text{for } a<b.\end{cases} \tag{3.18}$$

This matrix is the Drinfeld's triangular R-matrix. A simple solution of associated boundary K-matrices is computed as

$$K^{\mathrm{I}}(\theta)\, e_a = \begin{cases} -\theta^{-1/2}(p^{1/2}-p^{-1/2})\, e_a + p^{1/2}(\theta^{1/2}-\theta^{-1/2})\, e_{-a}, & \text{for } a>0, \\ (\theta^{1/2}p^{-1/2}-\theta^{-1/2}p^{1/2})\, e_0, & \text{for } a=0, \\ -\theta^{1/2}(p^{1/2}-p^{-1/2})\, e_a + p^{-1/2}(\theta^{1/2}-\theta^{-1/2})\, e_{-a}, & \text{for } a<0. \end{cases} \tag{3.19}$$

We take a simple example from the case of $n=2$. These matrices are written in terms of constant matrices,

$$\begin{aligned} R(\theta) &= \theta^{-1/2}\cdot R - \theta^{1/2}\cdot P\, R^{-1}\, P, \\ K^{\mathrm{I}}(\theta) &= \theta^{1/2}\cdot K^{-1} - \theta^{-1/2}\cdot K, \end{aligned} \tag{3.20}$$

where, with constants p and q, R and K are

$$R = \begin{pmatrix} q^{1/2} & & & \\ & q^{1/2} & q^{1/2}-q^{-1/2} & \\ & & q^{-1/2} & \\ & & & q^{1/2} \end{pmatrix}, \quad K = \begin{pmatrix} 0 & p^{-1/2} \\ p^{1/2} & p^{1/2}-p^{-1/2} \end{pmatrix}.$$

One finds that the following relations are satisfied:

$$\begin{aligned} & R^{12}\, R^{13}\, R^{23} = R^{23}\, R^{13}\, R^{12}, \\ & R - P\, R^{-1}\, P = (q^{1/2}-q^{-1/2})\, P, \\ & K - K^{-1} = p^{1/2}-p^{-1/2}, \\ & (1\otimes K)\, R^{21}\, (K\otimes 1)\, R^{12} = R^{21}\, (K\otimes 1)\, R^{12}\, (1\otimes K). \end{aligned} \tag{3.21}$$

Those are the defining relations for the Hecke algebra of type-B.

IV. ELLIPTIC DUNKL OPERATOR

In this section we consider the integrability of the elliptic CSM models associated with the classical root systems. The integrability is proved, in classical theory, by using the Lax matrix formalism.[31] The Lax matrix formalism has been applied to the quantum theory of the rational and trigonometric models.[7,31] Instead, we shall employ a slightly different approach, namely the Dunkl operator. The Dunkl operator was originally defined as integrable differential-difference operator associated with the root systems[32] and applied to the CSM model.[13,16,33,34] We shall construct the elliptic Dunkl operators based on the infinite-dimensional representation for solutions of the Yang–Baxter equation and the reflection equation discussed in the previous section.

In addition to the YBE (2.1) and the RE (3.3), we introduce the ''conjugate'' reflection equation (RE2, for short),

$$R^{12}(\xi_{21})\, \overset{2}{\overline{K}}(\xi_2)\, R^{21}(\xi_1+\xi_2)\, \overset{1}{\overline{K}}(\xi_1) = \overset{1}{\overline{K}}(\xi_1)\, R^{12}(\xi_1+\xi_2)\, \overset{2}{\overline{K}}(\xi_2)\, R^{21}(\xi_{21}). \tag{4.1}$$

Solutions for the RE2 and for the RE, that is, $\overline{K}(\xi)$ and $K(\xi)$, are related by

$$\overline{K}(\xi) = \hat{t} K(\xi)\, \hat{t}, \tag{4.2}$$

where the operator $\hat{t}$ means the reflection on a single-variable functional space,

$$(\hat{t}_j f)(\ldots, z_j, \ldots) = f(\ldots, -z_j, \ldots). \tag{4.3}$$

Hereafter we shall use the exchange operator $\hat{s}_{j,k}$,

$$(\hat{s}_{j,k} f)(\ldots,z_j,\ldots,z_k,\ldots)=f(\ldots,z_k,\ldots,z_j,\ldots), \tag{4.4}$$

and a parameter $\overline{\nu}$ for solutions of the RE2 [cf. (3.7)].

Based on the method of Refs. 30 and 35, we shall construct the elliptic Dunkl difference operator as variants of the quantum Knizhnik–Zamolodchikov–Bernard equation. For brevity we redefine the shift operator from (3.9) as $\hat{T}=T_{\beta}(\mu)$,

$$(\hat{T} f)(z)=f\left(z-\frac{\mu}{\beta}\right),$$

where β is an arbitrary constant. We recall the commutativity between the R-operator and the shift operator,

$$[R(\xi),\hat{T}\otimes\hat{T}]=0. \tag{4.5}$$

In terms of the infinite-dimensional representations for the R- and K-operators, we can define two sets of the elliptic Dunkl operators by

$$\hat{D}_j(\xi)=R^{j\,j-1}(\xi_{j\,j-1})\cdots R^{j\,1}(\xi_{j\,1})\cdot\hat{T}_j\cdot R^{j\,N}(\xi_{jN})\cdots R^{j\,j+1}(\xi_{j\,j+1}), \tag{4.6}$$

$$\begin{aligned}\hat{Y}_j(\xi)=&R^{j\,j-1}(\xi_{j\,j-1})\cdots R^{j\,1}(\xi_{j\,1})\cdot\hat{T}_j\cdot\overset{j}{K}(\xi_j)\cdot\hat{T}_j^{-1}\times R^{1\,j}(\xi_1+\xi_j)\cdots R^{j-1\,j}(\xi_{j-1}+\xi_j)\\&\cdot R^{j+1\,j}(\xi_{j+1}+\xi_j)\cdots R^{N\,j}(\xi_N+\xi_j)\times\overline{\overset{j}{K}}(\xi_j)\cdot R^{j\,N}(\xi_{j\,N})\cdots R^{j\,j+1}(\xi_{j\,j+1}),\end{aligned} \tag{4.7}$$

where $\overset{j}{K}$ and $\overline{\overset{j}{K}}$ act on the jth space. Using the YBE (2.1) and the RE (3.3) with (4.5), one finds that each set of the quantum Knizhnik–Zamolodchikov (qKZ) type difference operators constitutes a commuting family of operators (an integrable family, hereafter),

$$\begin{aligned}[\hat{D}_j(\xi),\hat{D}_k(\xi)]=0,\\ [\hat{Y}_j(\xi),\hat{Y}_k(\xi)]=0.\end{aligned} \tag{4.8}$$

We assume a parameter μ to be infinitesimal and take a quasi-classical limit in the difference operators. For the A-type operator $\hat{D}_j(\xi)$, we see that

$$\hat{D}_j(\xi)=1-\frac{\mu}{\beta}\left(\frac{\partial}{\partial z_j}-\beta\sum_{k:k\neq j}^{N}(\sigma_{\xi_{jk}}(z_{jk})\,\hat{s}_{j,k}+\rho(\xi_{jk})-\rho(z_{jk}))\right)+O(\mu^2),$$

where the elliptic function $\rho(z)$ is defined by $\rho(z)=(\mathrm{d}/\mathrm{d}z)\log\vartheta_1(z;\tau)$. With a product of functions,

$$\Delta^{\mathrm{A}}(z)=\prod_{1\leqslant j<k\leqslant N}(\vartheta_1(z_{jk};\tau))^{\beta},$$

we gauge-transform the operator $\hat{D}_j(\xi)$ as $\hat{D}_j(\xi)\to\Delta^{\mathrm{A}}(z)\cdot\hat{D}_j(\xi)\cdot\Delta^{\mathrm{A}}(z)^{-1}$. As a result one obtains the A-type elliptic Dunkl operators,

$$\hat{d}_j=\frac{\partial}{\partial z_j}-\beta\sum_{k:k\neq j}^{N}\sigma_{\xi_{jk}}(z_{jk})\,\hat{s}_{j,k},\quad\text{for } j=1,2,\ldots,N, \tag{4.9}$$

which constitute an integrable family,

$$[\hat{d}_j,\hat{d}_k]=0. \tag{4.10}$$

Subtracting terms of order ξ^{-2} (which is a c-number) and setting all rapidities to zero ($\xi\to 0$), we obtain the Hamiltonian of the elliptic CSM model,

$$\mathcal{H}^{\mathrm{A}}=\lim_{\xi\to 0}\sum_{j=1}^{N}\pi(\hat{d}_j^2)=\sum_j\frac{\partial^2}{\partial z_j^2}-\sum_{j,k}\wp(z_{jk})\cdot(-\beta P_{jk}+\beta^2), \tag{4.11}$$

where π means a projection to symmetric functional space, $\hat{s}_{j,k}P_{jk}=\mathbb{1}$. The next-order conserved operator is computed as

$$\lim_{\xi\to 0}\sum_{j=1}^{N}\pi(\hat{d}_j^3)=\sum_j\frac{\partial^3}{\partial z_j^3}+\frac{3}{2}\sum_{j,k}\wp(z_{jk})\cdot\left(\frac{\partial}{\partial z_j}+\frac{\partial}{\partial z_k}\right)\cdot(\beta P_{jk}-\beta^2).$$

For the BC-type, we see that the difference operator is calculated in the quasi-classical limit $\mu\to 0$ as

$$\begin{aligned}\hat{Y}_j(\xi)=1-\frac{\mu}{\beta}\Bigg\{&\frac{\partial}{\partial z_j}-\beta\sum_{k:k\neq j}(\sigma_{\xi_{jk}}(z_{jk})\,\hat{s}_{j,k}+\rho(\xi_{jk})-\rho(z_{jk}))-\beta\sum_{k:k\neq j}(\sigma_{\xi_j+\xi_k}(z_j+z_k)\,\hat{t}_j\hat{t}_k\hat{s}_{j,k}\\&+\rho(\xi_j+\xi_k)-\rho(z_j+z_k))-2\alpha(\sigma_{2\xi_j}(z_j)\,\hat{t}_j+\rho(2\xi_j)-\rho(z_j))-2\overline{\alpha}(\sigma_{\xi_j}(2z_j)\,\hat{t}_j+\rho(\xi_j)\\&-\rho(2z_j))\Bigg\}+O(\mu^2).\end{aligned}$$

Here we have substituted explicit forms of $K(\xi)$ and $\overline{K}(\xi)$. By transforming this operator $\hat{Y}_j^{\mathrm{BC}}\to\Delta^{\mathrm{BC}}(z)\cdot\hat{Y}_j^{\mathrm{BC}}\cdot\Delta^{\mathrm{BC}}(z)^{-1}$ by a product of functions,

$$\Delta^{\mathrm{BC}}(z)=\prod_{1\leqslant j<k\leqslant N}(\vartheta_1(z_{jk};\tau)\,\vartheta_1(z_j+z_k;\tau))^{\beta}\cdot\prod_{j=1}^{N}(\vartheta_1(z_j;\tau))^{2\alpha}(\vartheta_1(2z_j;\tau))^{\overline{\alpha}},$$

we get the BC-type elliptic Dunkl operator,

$$\hat{y}_j=\frac{\partial}{\partial z_j}-\beta\sum_{k:k\neq j}^{N}\{\sigma_{\xi_{jk}}(z_{jk})\,\hat{s}_{j,k}+\sigma_{\xi_j+\xi_k}(z_j+z_k)\,\hat{t}_j\hat{t}_k\hat{s}_{j,k}\}+(-2\alpha\,\sigma_{2\xi_j}(z_j)-2\overline{\alpha}\,\sigma_{\xi_j}(2z_j))\cdot\hat{t}_j. \tag{4.12}$$

It is easily seen that this differential-difference operator is also integrable,

$$[\hat{y}_j,\hat{y}_k]=0. \tag{4.13}$$

The first nontrivial conserved operator, the Hamiltonian of the BC-type, is given by

$$\begin{aligned}\mathcal{H}^{\mathrm{BC}}=\lim_{\xi\to 0}\sum_{j=1}^{N}\pi(\hat{y}_j{}^2)=&\sum_j\frac{\partial^2}{\partial z_j{}^2}-{\sum_{j,k}}'\{\wp(z_{jk})\cdot(-\beta P_{jk}+\beta^2)+\wp(z_j+z_k)\cdot(-\beta Q_jQ_kP_{jk}\\&+\beta^2)\}-\sum_j\{\wp(z_j)\cdot(-2\alpha Q_j+4\alpha^2+4\alpha\overline{\alpha})+\wp(2z_j)\cdot(-4\overline{\alpha}Q_j+4\overline{\alpha}^2)\},\end{aligned} \tag{4.14}$$

where we denote the projection operator π as a restriction to the symmetric space; $\hat{s}_{j,k}P_{jk}=\mathbb{1}$, $\hat{t}_jQ_j=\mathbb{1}$.

V. AFFINE HECKE ALGEBRA

A. Affine Hecke algebra

Mathematical studies for elliptic cases as a well-defined algebra are not completed. On the other hand, the trigonometric case can be formulated in terms of the affine Hecke algebra. We take the trigonometric limit for solutions of the YBE and RE, $\sigma_\mu(z)\to\pi\cot(\pi z)-\pi\cot(\pi\mu)$. In this limit the R- and K-operators are given by

$$R(\theta)=\frac{-1}{q-q^{-1}\theta}(\theta\hat{g}-\hat{g}^{-1})\cdot\hat{s}, \tag{5.1}$$

$$K(\theta)=-\theta^2\hat{r}+\theta(a-a^{-1}-b+b^{-1})+\hat{r}^{-1}, \tag{5.2}$$

where a, b, and q are arbitrary constants. We have introduced the exponential variables for coordinate and rapidity, and defined the so-called Demazure–Lusztig (DL) operators as

$$\hat{g}_{j,k}=\frac{q^{-1}z_j-q\,z_k}{z_j-z_k}\hat{s}_{j,k}+(q-q^{-1})\frac{z_k}{z_j-z_k}, \tag{5.3}$$

$$\hat{r}_j=\frac{-a+a^{-1}-(b-b^{-1})z_j}{1-z_j^{\,2}}+\frac{a+(b-b^{-1})z_j-a^{-1}z_j^{\,2}}{1-z_j^{\,2}}\cdot\hat{t}_j. \tag{5.4}$$

Remark that for the exponential variables, the reflection operator acts as

$$(\hat{t}\,f)(z)=f(z^{-1}).$$

These difference operators satisfy the following relations;

$$\begin{gathered}\hat{g}_{j,j+1}\hat{g}_{j+1,j+2}\hat{g}_{j,j+1}=\hat{g}_{j+1,j+2}\hat{g}_{j,j+1}\hat{g}_{j+1,j+2},\\ \hat{r}_j\hat{g}_{j,j+1}\hat{r}_j\hat{g}_{j,j+1}=\hat{g}_{j,j+1}\hat{r}_j\hat{g}_{j,j+1}\hat{r}_j,\\ (\hat{g}_{j,k}+q)(\hat{g}_{j,k}-q^{-1})=0,\\ (\hat{r}_j+a)(\hat{r}_j-a^{-1})=0.\end{gathered} \tag{5.5}$$

As for the conjugate operator $\overline{K}(\xi)$, we define the operator $\hat{\bar{r}}_j$ which has the same form with the operator $\hat{r}_j$ replacing parameters a and b with c and d, respectively. As we use exponential variables, the action of the shift operator $\hat{T}_j$ is given by

$$(\hat{T}_j f)(\ldots,z_j,\ldots)=f(\ldots,p\,z_j,\ldots), \tag{5.6}$$

where p is an arbitrary parameter.

The difference operators are defined by[36,37]

$$\hat{D}_j=\hat{g}_{j,j-1}\hat{g}_{j-1,j-2}\cdots\hat{g}_{2,1}\cdot\hat{T}_1\cdot\hat{g}_{1,N}^{-1}\hat{g}_{N,N-1}^{-1}\cdots\hat{g}_{j+2,j+1}^{-1}\hat{s}_{1,N}\hat{s}_{1,N-1}\cdots\hat{s}_{1,2}, \tag{5.7}$$

$$\hat{Y}_j=\hat{g}_{j,j-1}\hat{g}_{j-1,j-2}\cdots\hat{g}_{2,1}\cdot\hat{T}_1\hat{\bar{r}}_1\hat{T}_1^{-1}\cdot\hat{g}_{2,1}\hat{g}_{3,2}\cdots\hat{g}_{N,N-1}\times\hat{r}_N^{-1}\cdot\hat{g}_{N,N-1}^{-1}\hat{g}_{N-1,N-2}^{-1}\cdots\hat{g}_{j+1,j}^{-1}. \tag{5.8}$$

Notice that no spectral parameters ξ_j are included. These two operators are given from the qKZ-type difference operators (4.6) and (4.7) by taking limits of the spectral parameters as

$$0\ll\xi_1\ll\xi_2\ll\cdots\ll\xi_N.$$

By construction, trivial is the integrability for these q-difference operators,

$$[\hat{D}_j,\hat{D}_k]=0, \tag{5.9}$$

$$[\hat{Y}_j,\hat{Y}_k]=0. \tag{5.10}$$

We note that the q-difference operators $\hat{D}_j$ and $\hat{Y}_j$ satisfy the relations

$$\hat{g}_{j+1,j}\,\hat{D}_j\,\hat{g}_{j+1,j}=\hat{D}_{j+1}, \tag{5.11}$$

$$\hat{g}_{j+1,j}\,\hat{Y}_j\,\hat{g}_{j+1,j}=\hat{Y}_{j+1},$$

$$\hat{Y}_1^{-1}\cdot(\hat{T}_1\,\hat{r}_1\,\hat{T}_1^{-1})=(\hat{T}_1\,\hat{r}_1\,\hat{T}_1^{-1})^{-1}\cdot\hat{Y}_1-(c-c^{-1}). \tag{5.12}$$

Algebra generated from a set of operators $\{\hat{g}_{j,j+1},\hat{D}_j|j=1,\ldots,N\}$ is called the affine Hecke algebra of type-A while algebra from $\{\hat{g}_{j,j+1},\hat{Y}_j,\hat{T}_1\,\hat{r}_1\hat{T}_1^{-1},\hat{r}_N\}$ is of type-B. We can construct the integrable Hamiltonian systems by

$$\hat{I}_n=\sum_{j=1}^{N}\hat{D}_j{}^n,\quad \hat{J}_n=\sum_{j=1}^{N}\hat{Y}_j{}^n. \tag{5.13}$$

B. A-type

Let us see that the A-type difference operators $\hat{I}_n$ are difference analogue of the trigonometric CSM model. We shall take the quasi-classical limit,

$$p\to 1+\varepsilon+O(\varepsilon^2). \tag{5.14}$$

When we introduce a parameter β by $q=p^{-\beta/2}$, we find that the q-difference operator has a form

$$\hat{D}_j\to 1+\varepsilon\,\hat{d}_j+O(\varepsilon^2),$$

where the differential-difference operator $\hat{d}_j$ is defined by

$$\hat{d}_j=z_j\frac{\partial}{\partial z_j}-\beta\sum_{k<j}\frac{z_k}{z_j-z_k}(\hat{s}_{jk}-1)-\beta\sum_{k>j}\frac{z_j}{z_j-z_k}(\hat{s}_{jk}-1)+\beta\left(j-\frac{N+1}{2}\right). \tag{5.15}$$

The (trigonometric) Dunkl operator satisfies the relations

$$[\hat{d}_j,\hat{d}_k]=0,\quad \hat{s}_{j,j+1}\,\hat{d}_j-\hat{d}_{j+1}\,\hat{s}_{j,j+1}=-\beta, \tag{5.16}$$

which are the quasi-classical limits of (5.9) and (5.11). The Hamiltonians without spin degrees of freedom ($P_{jk}=\mathbb{1}$) are calculated from the operators $\hat{d}_j$ as

$$\mathcal{H}^{\mathrm{A}}=\Delta^{\mathrm{A}}(z)\cdot\sum_{j=1}^{N}\pi(\hat{d}_j{}^2)\cdot\Delta^{\mathrm{A}}(z)^{-1}=\sum_{j=1}^{N}\left(z_j\frac{\partial}{\partial z_j}\right)^2-\beta(\beta-1)\sum_{j,k=1}^{N}\frac{z_j z_k}{(z_j-z_k)^2}, \tag{5.17}$$

where $\Delta^{\mathrm{A}}(z)$ is the ground state wave-function,

$$\Delta^{\mathrm{A}}(z)=\prod_{j=1}^{N}z_j^{-\beta(N-1)}\cdot\prod_{1\leqslant j<k\leqslant N}(z_j-z_k)^{2\beta}.$$

Eigenvalues are computed in the following way.[37,36] We define the ordering for a monomial basis, $z^m = z_1^{m_1} z_2^{m_2} \cdots z_N^{m_N}$. For this basis we define a partition, $|m| = (m_1 \geqslant m_2 \geqslant \cdots \geqslant m_N)$. Ordering is defined as

$$|m| \geqslant |m'| \Leftrightarrow \begin{cases} m_1 \geqslant m_1', \\ m_1 + m_2 \geqslant m_1' + m_2', \\ \cdots \\ m_1 + \cdots + m_N \geqslant m_1' + \cdots + m_N'. \end{cases} \tag{5.18}$$

We recall that the DL operators have forms

$$\hat{g}_{j,k} = q^{-1} \hat{s}_{j,k} - (q - q^{-1}) \frac{z_k}{z_{jk}} (\hat{s}_{j,k} - 1), \quad \hat{g}_{j,k}^{-1} = q \hat{s}_{j,k} - (q - q^{-1}) \frac{z_j}{z_{jk}} (\hat{s}_{j,k} - 1).$$

Thus for the partition $|m|$, the eigenvalue D_j for operator $\hat{D}_j$ is given by

$$D_j = p^{m_j} q^{-N+2j-1}, \tag{5.19}$$

where $\{m_j\}$ is a partition in nonincreasing order, $m_1 \geqslant m_2 \geqslant \cdots \geqslant m_N$. The eigenstates are in fact related with the Macdonald polynomials, which will be discussed later. The eigenvalue E for the A-type CSM model (5.17) is

$$E = \sum_{j=1}^{N} k_j{}^2, \tag{5.20}$$

where the quasi-momenta k_j are given by

$$k_j = m_j + \beta \left(\frac{N+1}{2} - j \right). \tag{5.21}$$

This means that the momenta k_j for the quasi-particles satisfy a condition,

$$k_j - k_{j+1} \geqslant \beta. \tag{5.22}$$

The momenta for bosons and fermions correspond to cases $\beta = 0$ and $\beta = 1$, respectively. One realizes from the Hamiltonian (5.17) that interactions vanish in both cases. In this sense the CSM model with generic β realizes a free particle with "fractional exclusion statistics." A quasi-particle excludes β energy levels, i.e., has a statistical interaction β,[20]

$$\delta G = -\beta \, \delta N, \tag{5.23}$$

where G and N are the number of energy levels and the number of particles, respectively. Remark that the character for the (chiral) A-type CSM model is calculated as[38]

$$Z_\beta(q) = \sum_{n=0}^{\infty} \frac{q^{\beta(n^2-n)/2+n}}{(q;q)_n} x^n. \tag{5.24}$$

This character coincides with the grand partition function for the spinless CSM model confined in the harmonic potential (1.3). It is interesting to see that the cases of $\beta = 0$ and 1 correspond to the free bosons and fermions, respectively,

$$Z_{\beta=0}(q) = \prod_{n=1}^{\infty} \frac{1}{1 - x q^n}, \quad Z_{\beta=1}(q) = \prod_{n=1}^{\infty} (1 + x q^n).$$

The character formula (5.24) suggests that the scattering matrix $S(\xi)$ is related with the statistical interaction by a formula

$$\beta = 1 - \frac{1}{2\pi}\int \mathrm{d}\xi \cdot \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\xi}\log S(\xi)\right). \tag{5.25}$$

This supports the result of the asymptotic Bethe ansatz,[39] by which the S-matrix for the CSM model is computed as

$$S(\xi) = \exp(-\mathrm{i}\pi(\beta-1)\mathrm{sgn}(\xi)). \tag{5.26}$$

C. BC-type

In the following we demonstrate the same calculation for the BC-type. We set $q = p^{-\beta}$, and take a limit $p \to 1+\varepsilon$. The quasi-classical limit (5.14) results in

$$\hat{Y}_j \to 1 + 2\varepsilon\, \hat{y}_j + O(\varepsilon^2),$$

where the BC-type differential-difference operator $\hat{y}_j$ is given by

$$\begin{aligned}\hat{y}_j = {} & z_j\frac{\partial}{\partial z_j} - \beta\sum_{k<j}\frac{z_k}{z_j - z_k}(\hat{s}_{j,k}-1) - \beta\sum_{k>j}\frac{z_j}{z_j-z_k}(\hat{s}_{j,k}-1) - \beta\sum_{k:k\neq j}\frac{1}{z_j z_k - 1}(\hat{t}_j\hat{t}_k\hat{s}_{j,k}-1) \\ & + \beta(j-1) - \left(\frac{\overline{\alpha}}{z_j^{\,2}-1} + \alpha\frac{2}{z_j-1}\right)\hat{t}_j + \left(\frac{\overline{\alpha}}{z_j^{\,2}-1} + \alpha\frac{z_j+1}{z_j-1}\right).\end{aligned} \tag{5.27}$$

The BC-type Dunkl operator $\hat{y}_j$ satisfies the following relations, which may be checked from the properties for $\hat{Y}_j$;

$$[\hat{y}_j, \hat{y}_k] = 0, \quad \hat{s}_{j,j+1}\hat{y}_j - \hat{y}_{j+1}\hat{s}_{j,j+1} = -\beta, \quad \hat{t}_1\hat{y}_1 + \hat{y}_1\hat{t}_1 = 2(\alpha+\overline{\alpha}). \tag{5.28}$$

The Hamiltonian for the trigonometric CSM model is obtained from the Dunkl operator $\hat{y}_j$. A lengthy calculation leads us to

$$\begin{aligned}\mathcal{H}^{\mathrm{BC}} = {} & \Delta^{\mathrm{BC}}(z)\cdot\sum_{j=1}^{N}\pi(\hat{y}_j^{\,2})\cdot\Delta^{\mathrm{BC}}(z)^{-1} \\ = {} & \sum_{j=1}^{N}\left(z_j\frac{\partial}{\partial z_j}\right)^2 - \beta(\beta-1)\sum_{j,k=1}^{N}{}'\left(\frac{z_j z_k}{(z_j-z_k)^2} + \frac{z_j z_k}{(z_j z_k - 1)^2}\right) \\ & - \sum_{j=1}^{N}\left(2\alpha(2\overline{\alpha}+2\alpha-1)\frac{z_j}{(z_j-1)^2} + 4\overline{\alpha}(\overline{\alpha}-1)\frac{z_j^{\,2}}{(z_j^{\,2}-1)^2}\right),\end{aligned} \tag{5.29}$$

where we suppose that there is no internal degree of freedom ($P_{jk} = Q_j = \mathbb{1}$) and define the BC-type ground state wave-function by

$$\Delta^{\mathrm{BC}}(z) = \prod_{j=1}^{N} z_j^{-\beta(N-1)-\overline{\alpha}-\alpha}(z_j-1)^{2\alpha}(z_j^{\,2}-1)^{\overline{\alpha}}\cdot\prod_{1\le j<k\le N}(z_j-z_k)^{\beta}(z_j z_k - 1)^{\beta}.$$

The eigenvalues are calculated in the same method as for the case of the A-type. We recall the DL operators,

$$\hat{r}^{-1} = a + \frac{a + (b-b^{-1})z - a^{-1}z^2}{1-z^2}(\hat{t}-1),$$

$$\hat{T}\,\hat{\bar{r}}\,\hat{T}^{-1}=c^{-1}+\frac{c+(d-d^{-1})\,p\,z-c^{-1}p^2\,z^2}{1-p^2\,z^2}(\hat{T}^2\,\hat{t}-1).$$

One can show that the eigenvalue Y_j for $\hat{Y}_j$ is given by

$$Y_j=q^{2j-2N}\,p^{2m_j}\,c^{-1}\,a. \tag{5.30}$$

Here $\{m_j\}$ is in a nonincreasing order, $m_1\geqslant m_2\geqslant\cdots\geqslant m_N\geqslant 0$. The energy for the BC-type CSM model (5.29) is expressed as

$$E=\sum_{j=1}^{N}(k_j^{\mathrm{BC}})^2, \tag{5.31}$$

where we choose the quasi-momenta k_j^{BC} as

$$k_j^{\mathrm{BC}}=m_j+\beta\,(N-j)+\alpha+\overline{\alpha}. \tag{5.32}$$

One sees that the quasi-particle has a statistical interaction β,

$$k_j^{\mathrm{BC}}-k_{j+1}^{\mathrm{BC}}\geqslant\beta. \tag{5.33}$$

The ''boundary interactions,'' α and $\overline{\alpha}$, only shift the quasi-momenta by a constant, and do not change the statistical interaction. To summarize, the statistical interaction in (5.23) is determined from the bulk property, and is not affected by the boundary effects.

VI. MACDONALD POLYNOMIAL

The difference operators $\hat{D}_j$ and $\hat{Y}_j$ introduced in the previous section are closely related with the Macdonald polynomial.[40] The Macdonald polynomial is defined as the orthogonal polynomial associated with the root system. For the case of the BC-type, it can be generalized to the Koornwinder–Macdonald (KM) polynomial, which contains five arbitrary parameters.[41]

The A_N-type Macdonald polynomial is defined as an eigen-polynomial of the difference operators,

$$\hat{M}_n=\sum_{I\subset\{1,2,\ldots,N\}\atop |I|=n}\prod_{j\in I\atop k\notin I}\frac{q^{-1}\,z_j-q\,z_k}{z_j-z_k}\prod_{j\in I}\hat{T}_j, \tag{6.1}$$

where the operator $\hat{T}_j$ is defined in (5.6). In fact these operators are given from the quantum Dunkl operators $\hat{D}_j$. For example, we have

$$\hat{M}_1=\pi(\hat{I}_1)=\sum_{j=1}^{N}\left(\prod_{k=1\atop k\neq j}^{N}\frac{q^{-1}\,z_j-q\,z_k}{z_j-z_k}\right)\hat{T}_j, \tag{6.2}$$

where $\hat{I}_1=\Sigma_{j=1}^{N}\hat{D}_j$.

On the other hand, the BC-type KM polynomial is introduced as a generalization of the Askey-Wilson polynomial.[42] The KM polynomial is defined as an eigen-polynomial of the operator,

$$\hat{M}_1^{\mathrm{BC}}=\sum_{j=1}^{N}\Psi_j(z)\,(\hat{T}_j-1)+\sum_{j=1}^{N}\Psi_j(z^{-1})\,(\hat{T}_j{}^{-1}-1), \tag{6.3}$$

where functions $\Psi_j(z)$ are defined as

$$\Psi_j(z)=\frac{(1-a_1 z_j)(1-a_2 z_j)(1-a_3 z_j)(1-a_4 z_j)}{(1-z_j{}^2)(1-p z_j{}^2)}\cdot\prod_{\substack{k=1\\k\neq j}}^{N}\frac{(t z_j-z_k)(1-t z_j z_k)}{(z_j-z_k)(1-z_j z_k)}.$$

It should be remarked that we have five arbitrary parameters $\{a_j,t\}$ besides p. It is straightforward to check that the KM operator $\hat{M}_1^{\mathrm{BC}}$ is also given by using the representation of the affine Hecke algebra $\hat{Y}_j$,[43]

$$\hat{W}_1\equiv\pi(\hat{J}_1+\hat{J}_{-1})=\Phi_0+\sum_{j=1}^{N}\Phi_j(z)\cdot(\hat{T}_j{}^2-1)+\sum_{j=1}^{N}\Phi_j(z^{-1})\cdot(\hat{T}_j^{-2}-1). \tag{6.4}$$

In the above equation, functions Φ_0 and $\Phi_j(z)$ are computed as

$$\Phi_j(z)=c\,a^{-1}\frac{(1+c^{-1}d\,p\,z_j)(1-c^{-1}d^{-1}p\,z_j)(1+a\,b^{-1}z_j)(1-a\,b\,z_j)}{(1-z_j{}^2)(1-p^2 z_j{}^2)}$$
$$\times\prod_{\substack{k=1\\k\neq j}}^{N}\frac{q^{-1}z_j-q\,z_k}{z_j-z_k}\cdot\frac{q^{-1}z_j z_k-q}{z_j z_k-1},$$

$$\Phi_0=(c^{-1}a\,q^{1-N}+c\,a^{-1}q^{N-1})\frac{q^{N-1}-q^{-N+1}}{q^2-1}.$$

One thus sees that the KM operator is constructed based on the affine Hecke algebra of type-BC.[44]

Some of eigenfunctions of the Macdonald operator $\hat{M}_1$ are simply calculated from the generating function $F^{(N)}(z;t)$,

$$F^{(N)}(z;t)=\prod_{j=1}^{N}\frac{(q^{-2}z_j t;p)_\infty}{(z_j t;p)_\infty}. \tag{6.5}$$

We can show that the function $F^{(N)}(z;t)$ satisfies a difference equation,

$$(\hat{M}_1 F^{(N)})(z;t)=\left(\sum_{j=1}^{N-1}q^{2j-N+1}\right)F^{(N)}(z;t)+q^{-N+1}F^{(N)}(z;p\,t).$$

Thus when one defines the "generalized Rogers–Askey–Ismail (RAI) polynomial" $C_n^{(N)}(z)$ as

$$F^{(N)}(z;t)=\sum_{n=0}^{\infty}\frac{(q^{-2};p)_n}{(p;p)_n}\cdot C_n^{(N)}(z)\,t^n,$$

one sees that the polynomial is indeed an eigenfunction of $\hat{M}_1$,

$$(\hat{M}_1 C_n^{(N)})(z)=\left(\sum_{j=1}^{N-1}q^{2j-N+1}+q^{-N+1}p^n\right)C_n^{(N)}(z). \tag{6.6}$$

The generalized RAI polynomial $C_n^{(N)}(z)$ coincides with the A-type Macdonald polynomial $P_\lambda(z)$ for Young diagram $\lambda=[n]$.[40] The RS polynomial, which appeared in Sec. II as a generating function for the Yangian invariant spin chain, is a special case of the RAI polynomial,

$$H_n^{(N)}(p)=\lim_{q^{-2}\to 0}C_n^{(N)}(z). \tag{6.7}$$

VII. ELLIPTIC RUIJSENAARS MODEL

The Ruijsenaars model[45] is an elliptic generalization of the Macdonald difference operator (6.1),

$$\hat{\mathcal{D}}_n=\sum_{|I|=n}\prod_{\substack{j\in I\\ k\notin I}}\frac{\vartheta_1(z_{jk}-\mu)}{\vartheta_1(z_{jk})}\prod_{j\in I}\hat{T}_j(\beta), \tag{7.1}$$

where we have used the shift operator, $(\hat{T}_j(\beta)\,f)(\ldots,z_j,\ldots)=f(\ldots,z_j+\beta,\ldots)$.

These integrable operators can be constructed as follows.[46] We rescale the R-operator (3.2) and redefine it by

$$R^{jk}(\xi)=\sigma_\mu(z_{jk})-\sigma_\xi(z_{jk})\,\hat{s}_{jk}. \tag{7.2}$$

We first consider the two-body case. Simple calculation gives

$$R^{21}(\xi)\,\hat{T}_2(\beta)=\frac{\vartheta_1(z_{21}-\mu)\,\vartheta_1'(0)}{\vartheta_1(z_{21})\,\vartheta_1(-\mu)}\hat{T}_2(\beta)+\frac{\vartheta_1(z_{12}+\xi)\,\vartheta_1'(0)}{\vartheta_1(z_{12})\,\vartheta_1(\xi)}\hat{T}_1(\beta)\,\hat{s}_{12},$$

which coincides with the Ruijsenaars operator $\hat{\mathcal{D}}_1$ up to a constant if we set $\xi=-\mu$ and the operator acts on the symmetric space (we replace permutation operators $\hat{s}$ with unity when they are moved to the rightmost). As a generalization of this observation, we have the integrable difference operator defined by

$$\hat{D}(\boldsymbol{\xi})=R^{N,N-1}(\xi_{NN-1})\cdots R^{N,1}(\xi_{N1})\,\hat{T}_N(\beta), \tag{7.3}$$

which reduces to the first order Ruijsenaars operator (up to constant) by suitably setting the spectral parameters,[46]

$$\hat{\mathcal{D}}_1=\lim_{\xi_{jk}\to(k-j)\mu}\hat{D}(\boldsymbol{\xi}). \tag{7.4}$$

This construction can be applied to a generalized elliptic Ruijsenaars model[47] as well. Using a solution of the reflection equation (3.7) and (4.2), the integrable difference operator can be written as

$$\hat{\mathcal{Y}}(\boldsymbol{\xi})=\left(\prod_{k=1}^{\overleftarrow{N-1}}R^{N,k}(\xi_{Nk})\right)^{N}K(\xi_N)\left(\prod_{l=1}^{N-1}R^{l,N}(\xi_l+\xi_N)\right)\hat{T}_N(-\beta)\,\overline{\overset{N}{K}}(\xi_N)\,\hat{T}_N(\beta). \tag{7.5}$$

When we set $\xi_k=-\nu-(k-1)\mu$ in this integrable operator, we obtain an elliptic generalization of the Macdonald–Koornwinder operator,[46]

$$\begin{aligned}\hat{\mathcal{D}}_1^{\mathrm{BC}}=&\sum_{j=1}^{N}\left(\prod_{\substack{k=1\\k\neq j}}^{N}\sigma_\mu(z_{jk})\sigma_\mu(z_j+z_k)\right)\left(\sum_{r=0}^{3}g_r\,\sigma_{2\nu}^r(z_j)\right)\\&\times\left(\sum_{r=0}^{3}\overline{g_r}\,\sigma_{2\nu}^r(z_j+\beta)\,\hat{T}_j^2(\beta)-\sum_{r=0}^{3}\overline{g_r}\,\sigma_{-2(N-1)\mu-2\nu}^r(z_j+\beta)\right)\\&+\sum_{j=1}^{N}\left(\prod_{\substack{k=1\\k\neq j}}^{N}\sigma_\mu(z_{kj})\sigma_\mu(-z_j-z_k)\right)\left(\sum_{r=0}^{3}g_r\,\sigma_{2\nu}^r(-z_j)\right)\end{aligned}$$

$$\times\left(\sum_{r=0}^{3}\overline{g_r}\,\sigma^r_{2\nu}(-z_j+\beta)\,\hat{T}_j^{-2}(\beta)-\sum_{r=0}^{3}\overline{g_r}\,\sigma^r_{-2(N-1)\mu-2\nu}(-z_j+\beta)\right). \tag{7.6}$$

Higher conserved operators for these generalized elliptic Ruijsenaars models are obtained explicitly.[46] Such an approach is further extended to the quantum integrability of elliptic Ruijsenaars models associated with all affine Lie algebras.[48] It was also discussed that for a certain setting of parameters integrable difference operators $\hat{\mathcal{D}}_1$ in (7.4) and $\hat{\mathcal{D}}_1^{\mathrm{BC}}$ in (7.6) preserve a finite dimensional space as in Sec. III B and that we can compute the eigenvalues/eigenfunctions.

VIII. CONCLUDING REMARKS

We have reviewed some salient properties of quantum integrable models with long-range interactions.

In what follows, short-range interaction models are briefly discussed. We remark that the Yangian symmetry is revealed in the Hubbard model[49] and the two-component δ-function interacting fermi gas.[50] In the case of the δ-function interacting fermi gas, one can construct the Dunkl operator as well. We find that the YBE (2.1) is solved by the R-operator,[51]

$$R(\xi)=1-U(\mathrm{sgn}(z)-\coth(\xi))\hat{s}_{j,k}, \tag{8.1}$$

where the function sgn(z) denotes a signature of z,

$$\mathrm{sgn}(z)=\lim_{\gamma\to\infty}\coth(\gamma z)=\begin{cases}+1, & \text{for } z>0,\\ -1, & \text{for } z<0.\end{cases}$$

Almost all the properties studied in Sec. V are preserved for this R-operator; with a shift operator, $(\hat{T}f)(z)=f(z+1)$, one can construct the integrable difference operator,

$$\hat{I}=-\sum_{j=1}^{N}(\hat{T}_j+\hat{T}_j^{-1})+U\sum_{1\leqslant j<k\leqslant N}(\mathrm{sgn}(z_{jk}+1)-\mathrm{sgn}(z_{jk}))(\hat{T}_j+\hat{T}_k^{-1})\,\hat{s}_{j,k}. \tag{8.2}$$

This difference operator corresponds, in the su(2) case, to the strongly correlated electron system[52]

$$\mathcal{H}^{\mathrm{Bariev}}=-\sum_j\{(c^\dagger_{j,\uparrow}c_{j+1,\uparrow}+c^\dagger_{j+1,\uparrow}c_{j,\uparrow})(1-Un_{j,\downarrow})+(c^\dagger_{j,\downarrow}c_{j+1,\downarrow}+c^\dagger_{j+1,\downarrow}c_{j,\downarrow})(1-Un_{j+1,\uparrow})\}, \tag{8.3}$$

where $c_{j,\sigma}$ and $c^\dagger_{j,\sigma}$ are fermion annihilation and creation operators, respectively. It is interesting to see a distinction from the Hubbard model,

$$\mathcal{H}^{\mathrm{Hubbard}}=-\sum_j\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{j,\sigma}c_{j+1,\sigma}+c^\dagger_{j+1,\sigma}c_{j,\sigma})+U\sum_j\left(n_{j,\uparrow}-\frac{1}{2}\right)\left(n_{j,\downarrow}-\frac{1}{2}\right). \tag{8.4}$$

As a continuum limit of (8.3), we obtain the Dunkl operator and the Hamiltonian as follows:

$$\hat{d}_j^{\mathrm{NLS}}=-\mathrm{i}\frac{\partial}{\partial z_j}+\frac{\mathrm{i}\beta}{2}\sum_{k<j}(\mathrm{sgn}(z_{jk})-1)\,\hat{s}_{j,k}+\frac{\mathrm{i}\beta}{2}\sum_{k>j}(\mathrm{sgn}(z_{jk})+1)\,\hat{s}_{j,k}, \tag{8.5}$$

$$\mathcal{H}^{\mathrm{NLS}}=\sum_{j=1}^{N}\pi((\hat{d}_j^{\mathrm{NLS}})^2)=-\sum_{j=1}^{N}\frac{\partial^2}{\partial z_j^{\,2}}+2\beta\sum_{1\leqslant j<k\leqslant N}\delta(z_{jk})\,P_{j,k}. \tag{8.6}$$

We call this system the multi-component nonlinear Schrödinger (NLS) model. This is a generalization of the δ-function gas.

APPENDIX A: GAUSSIAN q-BINOMIAL

The q-binomial satisfies the following relations:

$$\begin{bmatrix} n \\ m \end{bmatrix}_q = \begin{bmatrix} n \\ n-m \end{bmatrix}_q, \quad \begin{bmatrix} n+m \\ m \end{bmatrix}_{q^{-1}} = q^{-mn} \begin{bmatrix} m+n \\ m \end{bmatrix}_q,$$

$$\lim_{q\to 1} \begin{bmatrix} n \\ m \end{bmatrix}_q = \begin{pmatrix} n \\ m \end{pmatrix}, \quad \lim_{n\to\infty} \begin{bmatrix} n \\ m \end{bmatrix}_q = \frac{1}{(q;q)_m}, \tag{A1}$$

$$\begin{bmatrix} n \\ m \end{bmatrix}_q = \begin{bmatrix} n-1 \\ m-1 \end{bmatrix}_q + q^m \begin{bmatrix} n-1 \\ m \end{bmatrix}_q = q^{n-m} \begin{bmatrix} n-1 \\ m-1 \end{bmatrix}_q + \begin{bmatrix} n-1 \\ m \end{bmatrix}_q.$$

We note that the Euler series-product identity is satisfied for infinite q-product series,

$$\sum_{N=0}^{\infty} \frac{t^N}{(q;q)_N} = \frac{1}{(t;q)_\infty}. \tag{A2}$$

APPENDIX B: ELLIPTIC FUNCTION

The elliptic function $\sigma_\mu^r(z) = \sigma_\mu^r(z;\tau)$ is a doubly quasi-periodic function,

$$\sigma_\mu^r(z+1) = \sigma_\mu^r(z), \quad \sigma_\mu^r(z+\tau) = \mathrm{e}^{2\pi \mathrm{i}\mu} \sigma_\mu^r(z), \quad \text{for } \Im\tau > 0. \tag{B1}$$

Here we have defined the function $\sigma_\mu^r(z)$ for $r = 0,1,2,3$ by

$$\sigma_\mu^r(z) = \frac{\vartheta_{r+1}(z-\mu;\tau)\ \vartheta_1'(0;\tau)}{\vartheta_{r+1}(z;\tau)\ \vartheta_1(-\mu;\tau)}, \tag{B2}$$

where

$$\vartheta_1(z) = -\mathrm{i} \sum_{n\in\mathbb{Z}} \exp\left(\mathrm{i}\pi \left(n+\frac{1}{2} \right)^2 \tau + 2\pi \mathrm{i} \left(n+\frac{1}{2} \right) z + \mathrm{i}\pi n \right),$$

$$\vartheta_2(z) = \sum_{n\in\mathbb{Z}} \exp\left(\mathrm{i}\pi \left(n+\frac{1}{2} \right)^2 \tau + 2\pi \mathrm{i} \left(n+\frac{1}{2} \right) z \right),$$

$$\vartheta_3(z) = \sum_{n\in\mathbb{Z}} \exp(\mathrm{i}\pi n^2 \tau + 2\pi \mathrm{i} n z),$$

$$\vartheta_0(z) = \sum_{n\in\mathbb{Z}} \exp(\mathrm{i}\pi n^2 \tau + 2\pi \mathrm{i} n z + \mathrm{i}\pi n),$$

and $\vartheta_4(z) = \vartheta_0(z)$. We mean $\sigma_\mu(z) = \sigma_\mu^0(z)$. Functions $\sigma_\mu^r(z)$ have simple poles at $z = \mathbb{Z} + \tau\mathbb{Z} + \omega_r$ where $\omega_r \equiv (\alpha_r + \beta_r \tau)/2$ are given by $(\omega_0, \omega_1, \omega_2, \omega_3) = (0, 1/2, (1+\tau)/2, \tau/2)$. We summarize some useful formulas for the function $\sigma_\mu(z)$:

$$\begin{gathered} \sigma_\mu(z) = -\sigma_z(\mu), \quad \sigma_\mu(z) = -\sigma_{-\mu}(-z), \\ \sigma_\mu(z)\ \sigma_{-\mu}(z) = \wp(z) - \wp(\mu), \\ \sigma_\lambda(z)\ \sigma_\mu(w) = \sigma_{\lambda+\mu}(w)\ \sigma_\lambda(z-w) + \sigma_\mu(w-z)\ \sigma_{\lambda+\mu}(z), \\ \sigma_\lambda(z)\ \sigma_\mu(z) = \sigma_{\lambda+\mu}(z) \cdot (\zeta(z) - \zeta(\lambda) - \zeta(\mu) - \zeta(z-\lambda-\mu)). \end{gathered} \tag{B3}$$

We also use

$$\vartheta\begin{bmatrix} a \\ b \end{bmatrix}(z;\tau)=\sum_{n\in\mathbb{Z}} \exp(\pi \mathrm{i}(n+a)^2\tau+2\pi\mathrm{i}(n+a)(z+b)). \tag{B4}$$

It is proved by checking the periodicity and the residues that the following equality is satisfied:[29]

$$\sigma_\mu(z;\tau)=\frac{1}{k}\sum_{a=0}^{k-1} \sigma_{\mu+a/k}\left(z;\frac{\tau}{k}\right), \tag{B5}$$

where k is an arbitrary positive integer, $k\in\mathbb{Z}_+$.

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Factorization method and the supersymmetric monopole harmonics

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(Received 9 December 2002; accepted 9 April 2003)

We use the general $\mathcal{N}=1$ supersymmetric formulation of one dimensional sigma models on nontrivial manifolds and its subsequent quantization to formulate the classical and quantum dynamics of the $\mathcal{N}=2$ supersymmetric charged particle moving on a sphere in the field of a monopole. The factorization method is accommodated with the general covariance and it is used to integrate the corresponding system. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1586476]

I. INTRODUCTION

The factorization method was first used by Schrödinger[1] to diagonalize the harmonic oscillator. It may work when the Hamiltonian of the system can be cast as a product of two operators:

$$H=AB. \tag{1.1}$$

A c-number can also be added to the above operator. Most systems treated by this method are one dimensional systems,[2,3] but it has also been considered in other situations.[4]

Recently, Ferapontov and Veselov[5] used factorization to look for integrable Schrödinger operators with magnetic fields on two dimensional surfaces. In the following we will use their approach to the monopole harmonics of Wu and Yang[6] to construct the super-symmetric monopole harmonics. We will show that factorization can be readily used for integrating the $\mathcal{N}=2$ supersymmetric nonrelativistic quantum mechanics[7] of a particle with spin moving on a sphere in the field of a monopole placed at its center. This can be inferred from the fact that the supersymmetric charge of the classical σ-model quantizes as the Dirac operator[8,9] on the manifold. Because the sphere is a two dimensional manifold, in a convenient basis the Dirac operators do not mix the components of the spinors and therefore the Hamiltonian of the system will be

$$H=\frac{1}{2}(Q\overline{Q}+\overline{Q}Q)=\begin{pmatrix} AB & 0 \\ 0 & BA \end{pmatrix},$$

and, because of this, the factorization method will be the natural method to integrate H.

As the factorization method is very simple we will recall some of its features here, in order to make the following computations easier to follow. Therefore, along with (1.1), one considers the reverse order product:

$$\tilde{H}=BA.$$

Then $\tilde{H}$ and H have the same nonzero eigenvalues. Indeed, if λ is an eigenvalue $(\lambda\neq 0)$ of $\tilde{H}$,

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$$\tilde{H}|\tilde{\Psi}_\lambda\rangle=\lambda|\tilde{\Psi}_\lambda\rangle,$$

then

$$|\Psi_\lambda\rangle=A|\tilde{\Psi}_\lambda\rangle$$

obeys

$$H|\Psi_\lambda\rangle=\lambda|\Psi_\lambda\rangle.$$

For the harmonic oscillator,

$$H=a^\dagger a+\tfrac{1}{2}$$

with

$$[a,a^\dagger]=1,$$

introduce

$$\tilde{H}=aa^\dagger+\tfrac{1}{2}=a^\dagger a+\tfrac{3}{2}.$$

The operators H and $\tilde{H}$ are positive operators, and it follows that the vector $|0\rangle$,

$$a|0\rangle=0,$$

is an eigenvector of H, with $\lambda=\frac{1}{2}$, and of $\tilde{H}$, with $\lambda=\frac{3}{2}$, and therefore

$$a^\dagger|0\rangle$$

is an eigenvector of H, corresponding to $\lambda=\frac{3}{2}$. The procedure can be continued:

$$\tilde{\tilde{H}}=H^{(2)}=\tilde{H}+1=H+2.$$

At the nth step

$$H^{(n)}=H+n,$$

with $|0\rangle$ being an eigenvector of $H^{(n)}$ corresponding to

$$\lambda=n+\tfrac{1}{2}.$$

Then H has the same eigenvalue and the corresponding eigenvector is

$$|\Psi_\lambda\rangle=(a^\dagger)^n|0\rangle.$$

We emphasize that the factorization method involves three steps: First, write the Hamiltonian in a factorized way; second, use a trick to cast $\tilde{H}$ in a form similar to that of H (i.e., move the destruction operators to the right in the previous example). The third step is to find the necessary recurrence procedure that yields all the eigenvalues and eigenvectors. This is also the pattern we are going to follow.

In Sec. II we reformulate the method of Ref. 5 for the scalar wave function in the einbein formalism. We show that the recurrence relations are obtained as a consequence of the requirement that the reverse order product BA has the same covariance properties acting on scalar wave vectors as the original product AB. On the sphere this happens because the spin connection

associated with the U(1) gauge group in the tangent space can be chosen to be proportional to the gauge connection corresponding to the monopole at its center,[10] the proportionality factor being exactly the number entering into the Dirac quantization condition.

In Sec. III we formulate the maximal classical supersymmetric action associated with the motion of a charge on a sphere, in the field of a monopole located at its center. The same action can be obtained by considering the supersymmetric one dimensional SU(2)/U(1) nonlinear model and coupling it with the electromagnetic field through a gauge potential equal with the connection, generated by the nonlinear transformation law.[11] The equivalence of these two formulations stems from the aforementioned property: the spin connection and the gauge connection are proportional. Alternatively, the same result follows by restricting the $\mathcal{N}=1$ supersymmetric action corresponding to a charge in the field of a monopole through Lagrange super-multipliers.[12,13] However, we prefer to obtain our model from the existing general superspace σ-model actions,[14,15] by fixing the field content, and choosing the appropriate background. In this way we can follow the natural way of solving models of this sort. We will need only two real anticommuting classical degrees of freedom for the formulation of the classical supersymmetric action. After quantization these real anticommuting degrees of freedom become the gamma matrices. This suggests that the two bosonic degrees of freedom combine with the anticommuting ones in two type-B superfields. Then we fix the appropriate background in the most general renormalizable $\mathcal{N}=1$ type-B superspace σ-model action.[14,15] The quantization of the general superspace σ-models produces the component approach to supersymmetric quantum mechanics, the general formulation of which was pursued in Ref. 16. To quantize our model we use the procedure of Refs. 17 and 18 in which the reparametrization covariance can be obtained with the help of the appropriately defined Noether supercharge.

Section IV is devoted to the diagonalization of this quantum system, while in Sec. V we give some concluding remarks.

II. FACTORIZATION METHOD

The Hamiltonian for the motion of a charge e, on a sphere, in the field of a monopole of strength g, localized at the center of the sphere, is

$$H_N=-\tfrac{1}{4}g^{ab}\nabla_a^{(N)}\nabla_b^{(N)}, \tag{2.1}$$

where g^{ab} is the inverse metric on a sphere

$$ds^2=g_{ab}dx^a dx^b=R^2\sin^2\theta d\phi^2+R^2 d\theta^2, \tag{2.2}$$

and the covariant derivatives are

$$\nabla_b^{(N)}=\partial_b-iA_b^{(N)}, \tag{2.3}$$

and

$$\nabla_a^{(N)}\nabla_b^{(N)}=\partial_a\nabla_b^{(N)}-iA_a^{(N)}\nabla_b^{(N)}-\Gamma_{ab}^c\nabla_c^{(N)}, \tag{2.4}$$

where ∂_a are the derivatives with respect to the coordinates in a patch on the sphere. The gauge connection A_a^N is

$$A_\phi=\frac{eg}{R\sin\theta}(\pm 1-\cos\theta), \tag{2.5}$$

where $\theta<\pi$ for the upper sign and $\theta>0$ for the lower sign. Γ_{ab}^c is the standard Christoffel connection for a sphere, and $N=eg$.

The desired factorization of (2.1) will be obtained by introducing the stereographic projection:

$$\cos\theta = 1 - \frac{2}{1+(x^2+y^2)/4R^2}, \tag{2.6}$$

$$\tan\phi = \frac{y}{x}. \tag{2.7}$$

Defining the complex coordinate

$$z = x + iy, \tag{2.8}$$

the only nonvanishing components of g^{ab} are $g^{z\bar{z}} = g^{\bar{z}z}$ with

$$g^{z\bar{z}} = 2h^{-2} = 2\left(1 + \frac{z\bar{z}}{4R^2}\right)^2. \tag{2.9}$$

Now, in the new coordinates, the Hamiltonian is

$$H_N = -\frac{1}{2} g^{z\bar{z}} \nabla_{\bar{z}}^{(N)} \nabla_z^{(N)} + \frac{N}{4R^2}, \tag{2.10}$$

where

$$\nabla_z^{(N)} = \partial_z - iA_z^{(N)}, \tag{2.11}$$

$$\nabla_{\bar{z}}^{(N)} = \partial_{\bar{z}} - iA_{\bar{z}}^{(N)}, \tag{2.12}$$

and

$$A_z^{(N)} = \tfrac{1}{2}(A_1^{(N)} - iA_2^{(N)}) = -iN\partial_z \ln h, \quad A_{\bar{z}}^{(N)} = A_z^{(N)*}. \tag{2.13}$$

The Christoffel connection does not appear in (2.10) anymore, because its only nonvanishing components are Γ_{zz}^{z} and $\Gamma_{\bar{z}\bar{z}}^{\bar{z}}$. In (2.10) we have used the relation

$$g^{z\bar{z}}[\nabla_z^{(N)}, \nabla_{\bar{z}}^{(N)}] = -\frac{N}{R^2}, \tag{2.14}$$

in order to exhibit the ''destruction operators'' $\nabla_z^{(N)}$ to the right and the ''creation operators'' $\nabla_{\bar{z}}^{(N)}$ to the left. The lowest eigenvalues of H_N are defined by the zero modes of the operators $\nabla_z^{(N)}$. Moreover, as it will be shown, the excited levels of H_N are related to the lowest levels of H_K, with $K > N$. These zero modes are related by the index theorem to topological properties of the manifold, see Ref. 5. Thus we may regard the present method of integrating H_N as a topological one.

In our case the wave vector is a scalar under the reparametrizations of the manifold. In a more general setting we might consider different assignments of spinorial (tensorial) properties to the wave vector. This is the case when one deals with the motion of a charged spin $\frac{1}{2}$ particle on a sphere, when the wave function is a spinor. Then, for a manifestly covariant approach, the appropriate language is the vielbein formalism of general relativity. This is not actually necessary for the case of the scalar wave functions. However, as we will show, even in this case, it allows one to avoid the use of the correct, but rather artificial, similarity transformations[5] in establishing the recurrence relations necessary to apply the factorization method.

Let us now introduce the einbeins for our complex manifold:

$$g_{z\bar{z}} = e_z^{+} e_{\bar{z}}^{-} \eta_{+-}, \tag{2.15}$$

where η_{+-} is the metric in the tangent space in an appropriate basis:

$$\eta_{+-}=\eta_{-+}=\tfrac{1}{2}, \quad \eta^{+-}=\eta^{-+}=2. \tag{2.16}$$

We have

$$e_z^+=e_{\bar{z}}^-=h, \quad e_z^-=e_{\bar{z}}^+=0. \tag{2.17}$$

Using the constant covariance of the einbein

$$\nabla_a e_b^\alpha=\partial_a e_b^\alpha+\omega_a{}^\alpha{}_\beta e_b^\beta-\Gamma_{ab}^c e_c^\alpha=0, \tag{2.18}$$

(2.10) becomes

$$H_N=-\mathcal{D}_-^{(N)}\mathcal{D}_+^{(N)}+\frac{N}{4R^2}, \tag{2.19}$$

where

$$\mathcal{D}_-^{(N)}=e_-^{\bar{z}}(\nabla_{\bar{z}}^{(N)}+\omega_{\bar{z}+}{}^+), \tag{2.20}$$

and

$$\mathcal{D}_+^{(N)}=e_+^z\nabla_z^{(N)}. \tag{2.21}$$

Above, one has

$$e_+^z=e_-^{\bar{z}}=h^{-1}, \tag{2.22}$$

and the nonvanishing components of the spin connection are

$$\omega_z{}^+{}_+=-\omega_{z+}{}^+=\partial_z\ln h, \tag{2.23}$$

$$\omega_{\bar{z}}{}^+{}_+=-\omega_{\bar{z}+}{}^+=-\partial_{\bar{z}}\ln h. \tag{2.24}$$

Consider now the tilde of (2.19):

$$\tilde{H}_N=-[\mathcal{D}_+^{(N)}]_{nc}[\mathcal{D}_-^{(N)}]_{nc}+\frac{N}{4R^2}. \tag{2.25}$$

While (2.19) is manifestly generally covariant (assuming that the wave vector is a world scalar), (2.25) is not manifestly so. By reversing the order of covariant derivatives, the spin connection terms in the covariant derivatives do not match the tensor properties of the terms ahead of them. This is why, in considering the reverse order product above, we appended the nc index to the covariant derivatives, even if their definition (2.20) and (2.21) did not change.

In order to obtain a recurrence relation one would expect (as explained in the Introduction) the operator $\tilde{H}_N$ to be a scalar and act on a scalar wave function. However, then $\tilde{H}_N$ is not manifestly covariant. The manifest covariance of $\tilde{H}_N$ is restored by noting that the gauge connection and the spin connection can be chosen to be proportional:[10]

$$A_a^{(N)}=N\omega_a, \tag{2.26}$$

where $N=eg$ appears in the Dirac quantization condition. Therefore we have the following identity:

$$[\mathcal{D}_+^{(N)}]_{nc}[\mathcal{D}_-^{(N)}]_{nc}=e_+^z\nabla_z^{(N)}e_-^{\bar{z}}(\nabla_{\bar{z}}^{(N)}+\omega_{z+}{}^+)=e_+^z(\nabla_z^{(N+1)}+\omega_{z-}{}^-)e_-^{\bar{z}}\nabla_{\bar{z}}^{(N+1)}=\mathcal{D}_+^{(N+1)}\mathcal{D}_-^{(N+1)}. \tag{2.27}$$

Here the expressions for $\mathcal{D}_+^{(N+1)}$, $\mathcal{D}_-^{(N+1)}$ can be read in the above formula and the expression to the right, above, is fully covariant. Substituting this in $\tilde{H}_N$ and moving the destruction operators to the right with the help of (2.14) we have

$$\tilde{H}_N = H_N{}^{(1)} = H_{N+1} + \frac{2N+1}{4R^2}. \tag{2.28}$$

Therefore the next eigenvalue of H_N is $(3N+2)/4R^2$. The corresponding eigenvector can be obtained from that of $\tilde{H}_N$, given by the condition

$$\nabla_z^{(N+1)} \tilde{\Psi}_1 = 0. \tag{2.29}$$

One has

$$\Psi_1 = \mathcal{D}_-^{(N)} \tilde{\Psi}_1, \tag{2.30}$$

with $\mathcal{D}_-^{(N)}$ defined by (2.20). Even if we deal with two covariant problems, that of H_N and that of $\tilde{H}_N$, the connection between the two sets of eigenvectors is not generally covariant.

The procedure described above can be continued, and at the lth step we get

$$H_N^{(l)} = H_{N+l} + \frac{(2N-1)+l(l+1)}{4R^2}, \tag{2.31}$$

with the eigenvalue

$$\lambda_l = \frac{1}{4R^2}[(2l+1)N + l(l+1)], \tag{2.32}$$

and the corresponding eigenvector of H_N

$$\Psi_l = \mathcal{D}_-^{(N)} \cdots \mathcal{D}_-^{(N+l-1)} \tilde{\Psi}_l, \tag{2.33}$$

where $\mathcal{D}_-^{(P)}$ was defined in (2.20). $\tilde{\Psi}_l$ is the solution of

$$\nabla_z^{(N+l)} \tilde{\Psi}_l = 0. \tag{2.34}$$

The multiplicity of the state Ψ_l is obtained from the condition of finite norm of the states:

$$\int \frac{dz d\bar{z}}{2} h^2 |\tilde{\Psi}_l|^2 < \infty. \tag{2.35}$$

Indeed, the solution of (2.34) is

$$\tilde{\Psi}_l = h^{N+l} f(\bar{z}), \tag{2.36}$$

where $f(\bar{z})$ is an arbitrary polynomial of degree $\leqslant 2(N+l)$, making the degeneracy of the corresponding state $2(N+l)+1$. From the asymptotic behavior of (2.33) in the radial variable, one sees that there are potential problems with normalizability of such states. However, as we checked on examples, due to cancellations of unwanted terms the vector Ψ_l is normalizable. We point out that this result is valid for integer $2N \geqslant 0$. Otherwise ($N<0$) the creation and annihilation operators must be interchanged.

Hence imposing the manifest general covariance of $\tilde{H}_N$ led us to rederive the recurrence relations[5] necessary in order to completely integrate the Hamiltonian H_N. In the next section, using the canonical quantization we will obtain the Hamiltonian for the supersymmetric particle which will be subsequently diagonalized by the factorization method.

III. $\mathcal{N}=2$ SUPERSYMMETRIC QUANTUM MECHANICS ON A SPHERE

We will approach the supersymmetrization of a given bosonic action in the following way. Given the target manifold (whose local coordinates are the bosonic fields which appear in the formulation of the one dimensional σ-model of the system), we look at the dimensionality of the Clifford algebra supported by the tangent space; for the sphere this is two. Therefore, in the present case, the Γ-matrices will be Hermitian matrices and therefore can be obtained from the quantization of the two real anticommuting degrees of freedom. Thus the minimal content of the fields realizing the representation of the supersymmetry algebra will be two real bosonic (the coordinate on the target manifold) and two real anticommuting degrees of freedom. We can fit these degrees of freedom in two type-B superfields. Because the tangent space is two dimensional and the supersymmetry charges must be constructed with the help of the Γ-matrices, one expects the maximal supersymmetry allowable for the system to be $\mathcal{N}=2$. Thus with the help of two type-B superfields we must formulate an $\mathcal{N}=2$ supersymmetric action. This is automatic since our target space manifold admits a complex structure. The above argument is somehow circular because one formulates the problem on the basis of the outcome of the quantization procedure.

Therefore, with the help of the metric $g_{ab}(X^a)$, the gauge connection $A_a{}^{(N)}(X^a)$ and the type-B superfield $X^a(x,\theta)$, we construct the following $\mathcal{N}=1$, one dimensional σ-model:[14,15]

$$S=-i\int dt\,d\theta\left\{\frac{g_{z\bar{z}}}{2}(DX^z\dot{X}^{\bar{z}}+DX^{\bar{z}}\dot{X}^z)+A_zDX^z+A_{\bar{z}}DX^{\bar{z}}\right\}. \tag{3.1}$$

Here

$$D=\frac{\partial}{\partial\theta}+i\theta\frac{d}{dt},\quad D^2=i\frac{d}{dt} \tag{3.2}$$

is the covariant supersymmetric derivative. The superfields, X^z and $X^{\bar{z}}$, are connected through $X^{\bar{z}}=(X^z)^\dagger$ and have the components

$$z=X^z|_{\theta=0},\quad \lambda^z=(DX^z)|_{\theta=0}, \tag{3.3}$$

with

$$\lambda^{z\dagger}=-\lambda^{\bar{z}} \tag{3.4}$$

and

$$\int d\theta\{\cdots\}=D\{\cdots\}|_{\theta=0}. \tag{3.5}$$

The action (3.1) is invariant under the supersymmetry transformations

$$\delta_\epsilon X^{\bar{z}}=\epsilon QX^{\bar{z}}, \tag{3.6}$$

$$\delta_\epsilon X^z=\epsilon QX^z, \tag{3.7}$$

where the supersymmetry shift operator Q is

$$Q=\frac{\partial}{\partial\theta}-i\theta\frac{d}{dt}, \tag{3.8}$$

with

$$Q^2=-i\frac{d}{dt}, \quad \{Q,D\}=0. \tag{3.9}$$

As mentioned before, because of the fact that the target space manifold is complex we will automatically have a second supersymmetry

$$\delta_\eta X^{\bar z}=-i\eta DX^{\bar z}, \tag{3.10}$$

$$\delta_\eta X^{z}=i\eta DX^{z}. \tag{3.11}$$

The two supersymmetry transformations above can be combined in one complex supersymmetry which in component fields $z,\bar z,\lambda^z,\lambda^{\bar z}$ takes the form

$$\delta z=\delta\mu\lambda^z, \quad \delta\lambda^z=i\delta\bar\mu\dot z, \tag{3.12}$$

and

$$\delta\bar z=\delta\bar\mu\lambda^{\bar z}, \quad \delta\lambda^{\bar z}=i\delta\mu\dot{\bar z}, \tag{3.13}$$

where

$$\delta\mu^\dagger=\delta\bar\mu. \tag{3.14}$$

The action (3.1) can also be written in terms of component fields, and the Lagrangian is

$$\mathcal{L}=g_{z\bar z}\dot z\dot{\bar z}+i\frac{g_{z\bar z}}{2}(\lambda^z D\lambda^{\bar z}+\lambda^{\bar z}D\lambda^z)-iF^{(N)}_{z\bar z}\lambda^z\lambda^{\bar z}+A^{(N)}_z\dot z+A^{(N)}_{\bar z}\dot{\bar z}, \tag{3.15}$$

where

$$F_{z\bar z}=\partial_z A_{\bar z}-\partial_{\bar z}A_z, \tag{3.16}$$

and

$$D\lambda^z=\dot\lambda^z+\dot z\Gamma^z_{zz}\lambda^z, \quad D\lambda^{\bar z}=\dot\lambda^{\bar z}+\dot{\bar z}\Gamma^{\bar z}_{\bar z\bar z}\lambda^{\bar z}, \tag{3.17}$$

where Γ^z_{zz} and $\Gamma^{\bar z}_{\bar z\bar z}$ are the only nonvanishing components of the Christoffel connection for the sphere. Equation (3.15) is invariant under (3.12) and (3.13) and by the Noether procedure one can deduce the corresponding supercharges:

$$\bar Q=-\lambda^z g_{z\bar z}\dot{\bar z}, \tag{3.18}$$

$$Q=\lambda^{\bar z}g_{\bar z z}\dot z. \tag{3.19}$$

From (3.15) one infers that one can go to the tangent space indices by making the redefinition

$$\lambda^z=ie^z_+\lambda^+, \tag{3.20}$$

$$\lambda^{\bar z}=ie^{\bar z}_-\lambda^-. \tag{3.21}$$

Then the fermions in (3.15) acquire a standard form:

$$\mathcal{L}=g_{z\bar{z}}\dot{z}\dot{\bar{z}}-\frac{i}{4}(\lambda^{+}\dot{\lambda}^{-}+\lambda^{-}\dot{\lambda}^{+})+\cdots, \tag{3.22}$$

and one concludes that $\lambda^{\pm}$ quantizes as the corresponding $(1/\sqrt{2})\,\Gamma^{\pm}$ matrices:

$$\Gamma^{+}=(\Gamma^{-})^{\dagger}=\begin{pmatrix}0 & 2\\ 0 & 0\end{pmatrix}. \tag{3.23}$$

The canonical conjugate momentum is given by

$$\mathrm{P}_z=g_{z\bar{z}}\dot{\bar{z}}+\frac{i}{2}(\omega_z)_{\alpha\beta}\lambda^{\alpha}\lambda^{\beta}+A_z^{(N)}. \tag{3.24}$$

With the notation

$$\Pi_z=g_{z\bar{z}}\dot{\bar{z}}=\mathrm{P}_z-\frac{i}{2}(\omega_z)_{\alpha\beta}\lambda^{\alpha}\lambda^{\beta}-A_z^{(N)}, \tag{3.25}$$

the corresponding Noether charge can be written

$$Q=\lambda^{z}\Pi_z=ie_{+}^{z}\lambda^{+}\left(\mathrm{P}_z-\frac{i}{2}(\omega_z)_{\alpha\beta}\lambda^{\alpha}\lambda^{\beta}-A_z^{(N)}\right). \tag{3.26}$$

Let us now quantize the supercharge Q.[17,18] As mentioned before $\lambda^{\pm}$ quantizes as the corresponding $(1/\sqrt{2})\,\Gamma^{\pm}$, further P_z goes into $(1/i)(\partial/\partial z)$; therefore in order to maintain the general covariance under quantization we can take the minimal Q:

$$Q=\frac{\Gamma^{+}}{\sqrt{2}}e_{+}^{z}\nabla_z^{(N)}, \tag{3.27}$$

where $\nabla_z^{(N)}$ is the covariant derivative on the spinor wave function:

$$\nabla_z^{(N)}=\partial_z-iA_z^{(N)}-\tfrac{1}{4}\omega_z^{\alpha\beta}\Gamma_{\alpha\beta}, \tag{3.28}$$

and the matrices $\Gamma_{\alpha\beta}$ are

$$\Gamma_{\alpha\beta}=\tfrac{1}{2}[\Gamma_{\alpha},\Gamma_{\beta}], \tag{3.29}$$

where

$$\{\Gamma_{\alpha},\Gamma_{\beta}\}=2\,\eta_{\alpha\beta}. \tag{3.30}$$

Once we have the quantum expression for Q we can define

$$\overline{Q}=Q^{\dagger}, \tag{3.31}$$

with respect to the scalar product corresponding to (2.35), where of course now the scalar wave vector is replaced by the two component wave function. The adjoint of Q is

$$Q^{\dagger}=-\frac{\Gamma^{-}}{\sqrt{2}}e_{-}^{\bar{z}}\nabla_{\bar{z}}^{(N)}, \tag{3.32}$$

with

$$\nabla_{\bar{z}}^{(N)} = \partial_{\bar{z}} - iA_{\bar{z}}^{(N)} - \tfrac{1}{4}\omega_{\bar{z}}^{\alpha\beta}\Gamma_{\alpha\beta}. \tag{3.33}$$

The Q and $\bar{Q}$ so defined obey automatically

$$Q^2 = \bar{Q}^2 = 0, \tag{3.34}$$

because they contain the matrices $\Gamma^{\pm}$ in their definition. Defining the quantum Hamiltonian by

$$H = \tfrac{1}{2}(Q\bar{Q} + \bar{Q}Q), \tag{3.35}$$

H commutes automatically with the supercharges Q and $\bar{Q}$. Thus the quantum ordering in H is completely fixed by supersymmetry and reparametrization covariance. The expression for H is also covariant under the reparametrizations of the manifold and the system has $\mathcal{N}=2$ supersymmetry.

Finally, it might be worth mentioning that by this procedure H is defined from the supersymmetry algebra (3.35) without any recourse to the standard ways of defining it.

IV. SUPERSYMMETRIC MONOPOLE HARMONICS

Diagonalization of the Hamiltonian (3.35) follows now in a rather simple way. Using the constant covariance of the Γ-matrices with respect to vector and spinor indices, (3.35) can be cast in the following form:

$$H = -\tfrac{1}{4}e_+^z e_-^{\bar{z}}[\Gamma^+\Gamma^-\nabla_z^{(N)}\nabla_{\bar{z}}^{(N)} + \Gamma^-\Gamma^+\nabla_{\bar{z}}^{(N)}\nabla_z^{(N)}], \tag{4.1}$$

the products $\Gamma^+\Gamma^-$ and $\Gamma^-\Gamma^+$ being scalars under local rotations in the tangent plane. Moreover, they are projectors:

$$\Gamma^+\Gamma^- = \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma^-\Gamma^+ = \begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix}. \tag{4.2}$$

Therefore, H is a sum of factorized terms. We recognize that the operators multiplying the products $\Gamma^+\Gamma^-$ and $\Gamma^-\Gamma^+$ are connected with the Laplacian appearing in (2.1) with a modified spin connection, due to the nonzero spin of the wave function. In fact, we have

$$H = \left[H_{(N+1/2)} + \frac{(N+\frac{1}{2})}{4R^2}\right]\frac{\Gamma^+\Gamma^-}{4} + \left[H_{(N-1/2)} - \frac{(N-\frac{1}{2})}{4R^2}\right]\frac{\Gamma^-\Gamma^+}{4}. \tag{4.3}$$

This is due to the fact that the spinor components transform with an effective charge $\pm\frac{1}{2}$ under local rotations. As remarked before, one can absorb this ''Lorentz charge'' in the gauge connection leading to a modification of the effective charge of the corresponding components. Using (2.28), it is easy to show that

$$\tilde{H}_{(N-1/2)} - \frac{(N-\frac{1}{2})}{4R^2} = H_{(N+1/2)} + \frac{(N+\frac{1}{2})}{4R^2}. \tag{4.4}$$

However, by the same procedure $\tilde{H}_{(N+1/2)}$ gets connected with $H_{(N+3/2)}$. The connection between $\tilde{H}_{(N+1/2)}$ and $H_{(N-1/2)}$ is the result of a different factorization of H_N in Sec. II. From (2.1) one has

$$H_N = -\mathcal{D}_+^{(N)}\mathcal{D}_-^{(N)} - \frac{N}{4R^2}, \tag{4.5}$$

where

$$\mathcal{D}_{+}^{(N)}=e_{+}^{z}(\nabla_{z}^{(N)}+\omega_{z-}{}^{-}), \tag{4.6}$$

and

$$\mathcal{D}_{-}^{(N)}=e_{-}^{\bar{z}}\nabla_{\bar{z}}^{(N)}. \tag{4.7}$$

Therefore, with respect to this factorization we have

$$\tilde{H}_N=-[\mathcal{D}_{-}^{(N)}]_{nc}[\mathcal{D}_{+}^{(N)}]_{nc}-\frac{N}{4R^2}=-\mathcal{D}_{-}^{(N-1)}\mathcal{D}_{+}^{(N-1)}-\frac{N}{4R^2}=H_{N-1}-\frac{2N-1}{4R^2}, \tag{4.8}$$

and using the identities just derived one has

$$\tilde{H}_{(N+1/2)}+\frac{(N+\frac{1}{2})}{4R^2}=H_{(N-1/2)}-\frac{(N-\frac{1}{2})}{4R^2}. \tag{4.9}$$

We prefer to start with the eigenfunctions of $H_{(N+1/2)}$, because this operator appears in a manifestly positive definite combination in the Hamiltonian.

Therefore, given the eigenvector Ψ of $H_{(N+1/2)}+(N+\frac{1}{2})$, with nonzero eigenvalue, we obtain the corresponding eigenvector of $H_{(N-1/2)}-(N-\frac{1}{2})$ by taking

$$\mathcal{D}_{-}^{(N-1/2)}\Psi, \tag{4.10}$$

with $\mathcal{D}_{-}^{(N-1/2)}$ defined by (2.20). From (4.3) the eigenvalues of H are

$$E_l=\frac{1}{4R^2}(l+1)(l+2N+1), \tag{4.11}$$

with the eigenvector being given by

$$\Psi_l=\begin{pmatrix} \mathcal{D}_{-}^{(N+1/2)}\cdots\mathcal{D}_{-}^{(N+l-1/2)}\tilde{\Psi}_l \\ \mathcal{D}_{-}^{(N-1/2)}\mathcal{D}_{-}^{(N+1/2)}\cdots\mathcal{D}_{-}^{(N+l-1/2)}\tilde{\Psi}_l \end{pmatrix}. \tag{4.12}$$

Therefore we have found the eigenvalues and eigenvectors of the $\mathcal{N}=2$ supersymmetric spinning particle moving on a sphere in the field of a monopole. They are analogous to the eigenfunctions determined in Ref. 19.

V. CONCLUSIONS

Restating the main result, we have supersymmetrized and solved the motion of a charge on a sphere in the field of a monopole at its center.

The factorization method appears to be the natural way to solve this problem. This is because in order to formulate a supersymmetric problem one is basically compelled to use the complex structure of the target space manifold. The quantization scheme for the problem is manifestly taking into account the reparametrizations of the manifold; therefore it is covariant with respect to these reparametrizations. One should remember that one is dealing basically with the algebra of angular momentum and it is quite interesting that following the manifest symmetries of the problem one is led to an alternative integration method. In this context, even if algebraic, this method appears somewhat strange, albeit natural.

One should also stress that the degeneracies of the levels are all finite and it is well known that we deal with a regularization of the Landau electrons. Taking the limit $R^2,N\to\infty$ (with N/R^2 fixed) one obtains the infinitely degenerate states of a planar electron in a constant magnetic field.

In a rather different context, the eigenfunctions obtained in this article may also be studied by methods similar to those used for the harmonic superspace.[20]

ACKNOWLEDGMENTS

We wish to thank Willy Fischler for the question which led to this problem and for subsequent discussions. We have also benefited from discussions with S. Barnes, E. A. Ivanov, A. I. Pashnev, V. Rittenberg and A. B. Zamolodchikov. G.A.M. gratefully ackowledges financial support from a grant by Army Research Laboratory, BAE Systems. L.M. wishes to thank E. Paschos for hospitality at the University of Dortmund, while this work was in progress and is also indebted to A. T. Filippov for making possible his participation in the Symposium of Quantum Gravity and Superstrings, 18–28 June 2001, Dubna, where part of this work was presented. L.M. was supported in part by the National Science Foundation under Grant No. PHY-9870101.

NOTE ADDED

These computations have been posted on the web as a preprint hep-th/0109002. We however did not submit the article as we intended to perform some further checks, which were a little outside the main direction of the paper, to illustrate the usefulness of the factorization method in problems in which general covariance plays an important role. Three months after posting the article on the web a lot of our results have been reobtained by Ref. 21.

While in the process of finalizing our paper, on 21 December 2001, my beloved brother and coauthor on this article suddenly and unexpectedly passed away. For some time afterwards I was unable to touch this article, and this explains the delay by which this article is submitted.

There remains a topic which is not discussed above and it was not covered in Ref. 21 either; it is the action of the rotation group which is a symmetry of the model,[11] and which completely fixes the spin of the excitations in the model. I defer this study to a later publication. (I am indebted to L. Susskind for a discussion of this point.)

It should also be mentioned that the usefulness of the holomorphic approach to closely related problems was recently emphasized in Refs. 22–24.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Fractional charge definitions and conditions

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(Received 10 December 2002; accepted 9 April 2003)

The phenomenon of fractional charge has come to prominence in recent decades through theoretical and experimental discoveries of isolable objects which carry fractions of familiar charge units—electric charge Q, spin S, baryon number B and lepton number L. It is shown here on the basis of a few simple assumptions that all these effects may be described using a generalized version of *charge renormalization* for locally conserved charges, in which many-body correlations can produce familiar adiabatic, continuous renormalization, and in some circumstances nonadiabatic, discrete renormalization. The fractional charges may be carried either by *fundamental particles* or by *fundamental solitons*. This excludes nontopological solitons and also skyrmions: The only known fundamental solitons in three or fewer space dimensions d are the kink ($d=1$), the vortex ($d=2$), and the magnetic monopole ($d=3$). Further, for a charge which is not intrinsically coupled to the topological charge of a soliton, only the kink and the monopole may carry fractional values. The same reasoning enforces fractional local values of $B-L$ for electrically charged elementary particles. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1586793]

I. INTRODUCTION

The ascendancy of elementary particles in thinking about microscopic physics began with atoms and molecules, followed by electrons, photons, and nuclei, then nucleons and neutrinos, quarks, gluons, and W and Z bosons. The pattern of a hierarchy of length scales, with the particles of one scale being compounds of those found at a shorter scale, has replayed itself several times over. Even today there is no observational evidence that this pattern terminates at some scale.

Nevertheless, reasons to question the pattern have emerged. String theory and its developments raise the prospect that at sufficiently short scales the elementary objects are not particles, but rather extended entities. While such studies give exciting directions for discovery at those new scales, they actually support rather than undermine the notion of elementary particles: The additional structure ''inside'' the particles does not change the fact that they still look structureless at sufficiently long scales.

A different reason to worry about the universal validity of the particle description at currently accessible scales has come from theoretical and experimental discoveries of fractional charge. If at the beginning of microscopic physics all kinds of different charges had been observed, with no rational relation among them, progress in understanding would have been impeded seriously indeed. We know that did not happen, but in principle the recent discoveries might herald a new era where precisely such chaos in the pattern of charges could emerge. The purpose of this work is to present some simple definitions and theorems, based on minimal assumptions, from which it follows that fractional charge fits into the familiar framework of charge renormalization, and

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consequently is so tightly constrained that any threat of ''charge chaos'' is precluded.

In the standard model of strong and electroweak interactions there are three isolable, quantized charges observable in vacuum at zero temperature that may be locally conserved, electric charge Q, measured in units of the electron charge e, spin $\vec{S}$, whose projection onto a fixed axis has integer or half-integer values in units of $\hbar$, and the difference between baryon and lepton charge $B-L$, which usually is assumed to have the value 1 for a proton or neutron, and -1 for an electron or neutrino. Despite the existence of an exponentially small effect associated with electroweak instantons, which 't Hooft[1] recognized would produce baryon decay through the Adler–Bell–Jackiw chiral anomaly,[2] and possible additional interactions associated with very high energy scales, B+L also may be treated as conserved in many contexts. If electroweak effects and the difference of light quark masses may be ignored, so that attention is focused exclusively on the strong interactions, then also isospin $\vec{I}$ may be treated as conserved. Even if electromagnetic interactions are included, still I_3, as well as flavor charges of higher generations of quarks—strangeness, charm, bottom, and top—are conserved.

Thus, many isolable, quantized charges observable in the laboratory are exactly or at least quite accurately conserved. It should be noted that besides these charges there are the continuous (i.e., nonquantized), locally conserved charges corresponding to energy and momentum, which precisely because they have a continuum of allowed values need not concern us further here.

At this point it may be worthwhile to discuss a bit more what is meant by the concept ''charge.'' Of course, the prototype example is electric charge, whose conservation follows from the Maxwell equations. Already in classical physics it was understood that the existence of a conserved charge could be deduced from a symmetry of the dynamics. In quantum physics, this is expressed in terms of a unitary (or in the case of time reversal symmetry, antiunitary) operator which commutes with the Hamiltonian. If that symmetry be continuous, then the generators of the symmetry must be self-adjoint operators. In certain cases, such as the generators of the rotation group in three space dimensions, which are identified as the angular momentum or spin of a system under study, the commutation relations among the generators lead directly to the quantization of the allowed values of the charge. However, for electric charge such a deduction has not yet been possible, while for $B-L$ there is not even a framework to discuss the symmetry beyond the statement that phenomenologically established couplings conserve the charge, i.e., all terms in the Lagrangian are invariant under the unitary transformation generated by the operator $B-L$. Thus, in terms of current knowledge, symmetries imply conservation and sometimes even quantization of observable charges, but there is at this point no assurance that all cases of apparently conserved and quantized charges are consequent to symmetries which can be identified in any way other than by recognizing that the charges seem to be conserved.

In relativistic physics, a conserved charge whose local density is defined must be locally conserved. That is, if the charge in some volume changes, the immediately surrounding volume must experience an equal and opposite change in charge, or expressed differently, the rate of change of the charge in a volume is equal and opposite to the net current flowing out of the volume. The reason is easily found by assuming the contradiction to this assertion: If in one inertial frame a conserved charge disappeared in one place and reappeared instantly at a distant place, then in different frames of reference boosted by velocity shifts from the original frame the total charge at certain times either would vanish or would be double the original value, evidently violating charge conservation.

How may charges be measured or observed? Again, the prototype is electric charge, which may be measured through the electromagnetic interaction, either by determining the influence on a particle of a specified electromagnetic field (thus measuring the Lorentz-force charge), or by using test particles with known charges to measure the electric flux coming out of the particle (thus measuring the Gauss-law charge). In the quantum context, these two may be called the Aharonov–Bohm (AB) charge and the local charge, respectively.[3] For other types of charge (i.e., not coupled to gauge fields), one must use more indirect methods, such as counting different spin states of an object, To help understand the conceptual structure, one may introduce hypothetical Abelian gauge fields weakly coupled to any conserved, localizable charge one wishes to measure.

Are there any circumstances in which fractional values of charges may be found, and if so, what are the precise conditions for this to occur? Let us turn to that issue.

II. DEFINITIONS AND THEOREMS

Definition 1 (Elementary particle): In a given medium, and for a given range of length scales, an isolable particle is called *elementary* if its set of conserved charges cannot be constructed from any finite assembly of particles which individually carry fractions and/or subsets of that charge set.

Remarks: In ordinary vacuum at zero temperature, the known elementary particles according to this definition are the proton and neutron, the π^+ and π^0 mesons, the electron, the neutrino, the photon, and the W^+ and Z bosons, plus their antiparticles (the photon, π^0 and Z certainly, and the neutrino possibly, are their own antiparticles). Among this set, all are isolable, but several are unstable against decay to two or more others. These nevertheless are properly considered elementary under the definition, because the summed absolute values of certain charges of the decay products are greater in magnitude than the corresponding charge of the particle, for example, the electrically neutral neutron decays to proton, electron, and antineutrino, of which the first two each carry unit electric charge.

It is significant that protons, and hadrons in general, exhibit strong short-range interactions, so that they really are isolable only at long distance scales. Nevertheless, in nuclear matter it is possible to make an accurate description of the dynamics including quasiparticles with the same charges as neutrons and protons, suitably redefined so that these ''nucleon quasiparticles'' interact weakly. It is a useful perspective to consider these quasiparticles as nucleons whose effective interactions are renormalized by the strong, short-range correlations of the nuclear medium: Each quasinucleon may be viewed as having a nucleon kernel surrounded by a cloud of medium polarization. A very similar approach has been most successful in describing electron quasiparticles in many different condensed-matter systems. Thus, while the definition of an elementary particle may be medium-dependent, there often is a simple correspondence between a set of elementary particles in one medium and a set in a different medium.

Definition 2 (Fundamental particle): A particle is called *fundamental* if it obeys all the criteria for an elementary particle except possibly that of being isolable, and in addition it has no discernible internal structure. This means that at the shortest distance scales such particles correspond to fields appearing in the Lagrangian.

Remarks: This new criterion removes the nucleons and pions from the list above, and introduces instead the quarks and gluons. While these particles are not isolable in vacuum, the fact that quantum chromodynamics (QCD) exhibits asymptotic freedom,[4] meaning weak coupling at short distance scales, implies that at those scales they may be detected and (for quarks) their electric charges measured. As the term ''fundamental'' suggests, the charges of all the known elementary particles in vacuum can be constructed from those of the fundamental particles. In other media, there may be additional fundamental particles in the sense described, and there may be also fundamental solitons, discussed in the theorems below. Again, all elementary particles in these media have charges which may be constructed from those of the fundamental particles and solitons. In this sense, the fundamental objects may be considered the building blocks for everything else.

Definition 3 (Fractional charge): An object which carries only a portion of the charges of finite combinations of elementary particles may be said to carry *fractional charge*. In principle, such a particle might have, for example, the same spin as the electron, but an electric charge which is an irrational fraction of e. There is no known instance like this for particles in vacuum, but in any insulating medium exactly such a phenomenon is found, and in the accepted interpretation this fractional value is treated as a *renormalization* of the electron charge from its value in vacuum. By this definition, the electric charges of quarks are examples of fractional charge, but the fractional values arise because these fundamental particles carry a smaller unit of charge than any (isolable) elementary particle.

Remarks: This definition invites two thought experiments which illuminate it, and also will be useful later. First, imagine a massive particle such as a proton slowly entering an insulating

medium. As it enters, its local charge is reduced and, by the time it has penetrated far inside, the extra charge is found on the surface of the insulator. Thus, total charge is locally conserved throughout the process, but it ends up fractionated between the charge localized on the particle and the charge on the surface. The second experiment, even in vacuum, invokes a slow increase from zero in the value of α, the electromagnetic coupling. As this occurs, the electric field measurable at some distance from a charged particle increases in strength, but not quite proportionally to α, because vacuum polarization increasingly screens the field. Again, charge is locally conserved, because as the coupling increases there is an outward flow of current, with the current density proportional to the electric field at each point.

As mentioned already, the charge which is fractionated is the local charge, while the AB charge remains invariant. This is illustrated by another thought experiment. Imagine a capacitor stuffed with dielectric and set at voltage V. Then an electron of charge $-e$ passing through the capacitor will acquire from the electric field a net energy $-eV$, regardless of the magnitude of the dielectric response. Of course the presence of the dielectric implies an increase in the amount of surface charge on the capacitor plates to achieve the same V as for the plates in vacuum, but once this V is established the effect on the electron is not further modified by the dielectric.

Definition 4 (Breakup): On passing from one medium to another, a particle may undergo *charge breakup*, meaning that on the other side there are several particles instead of one, each with only a portion of the set of charges carried by the one particle in the original medium. This evidently is an intrinsically nonadiabatic process, as the number of mobile degrees of freedom changes discontinuously. Note that charge breakup may occur when, for example, a fast electron enters a conventional insulator, knocking loose a number of electrons each of which penetrates far into the medium. As a result, very little charge may be left on the surface. Nevertheless, there is a big distinction between such a case and one where the surface simply cannot take up charge at all, as occurs when an electron enters from above a two-dimensional layer exhibiting the fractional quantum Hall effect.

Now we are ready for the first theorem.

Theorem 1 (Conservation of particles with fractional charge): An isolable particle that has fractional charge with respect to previously identified elementary particles in its medium must itself be an elementary or a fundamental particle of that medium. (As indicated above, a particle may carry fractional charge with respect to particles in *different* media, as a consequence of medium-dependent charge renormalization.)

Proof: This statement follows directly from the definition of elementary particles, because the charges of this object cannot be produced by any finite assembly of particles carrying integer values of the same charge.

Theorem 2 (Fundamental solitons): The possible soliton carriers of charges which are fractional with respect to those of other elementary particles in a given medium for spatial dimension $d \leqslant 3$ are *fundamental solitons*, of which the known examples are the kink $(d=1)$, the vortex $(d=2)$, and the magnetic monopole $(d=3)$.

Proof: A soliton is an object which in first approximation could be described as a classical field configuration that is classically stable. However, classical stability clearly is not enough because, if addition of energy to the system could enable the disintegration of the soliton, then its conserved charges would have no unconventional carrier, and hence obviously could not be fractional. Furthermore, a soliton in a class all with the same low-energy properties could not carry fractional charge if some other members of the class were capable of disintegration, because all solitons in the class would have the same influence on the medium polarization which determines possible fractional charge.

The kink in $d=1$ may be described by a classical scalar field which has equal potential energy density minima for two or more distinct values of the field. Thus the field can go asymptotically to one value as $x \to +\infty$ and another value as $x \to -\infty$. No finite-action process could destroy this structure, which nevertheless possesses a finite, localized energy in the region between the two asymptotic zones. Consequently the kink has a conserved *topological charge*, and so there would be no contradiction if it carried fractional values of other charges.

In $d=2$, a vortex may be described by a complex scalar field which rotates in phase by $2n\pi$ at large distances from its center as the radial direction rotates by 2π, while the field magnitude approaches a fixed value with increasing radius, again to minimize a potential energy density. In the Abelian Higgs model for such a vortex, gradient energy is kept finite through coupling of the scalar field to a gauge field, which makes the covariant azimuthal gradient negligible at large distances and implies a magnetic flux stored near the center. There is an alternate description of the asymptotic fields, in which the scalar field goes to a fixed constant and the gauge field (pure gauge) corresponds to an Aharonov–Bohm phase factor $e^{2\pi iq/Q}$ relating the phase of a charged particle wave function at, e.g., azimuthal angles $\phi=0$ and $\phi=2\pi$, where Q is the charge of the scalar field and q is the charge of a particle which experiences a nontrivial Aharonov–Bohm effect upon diffraction around the flux. Again, no finite-action process could destroy this structure.

In $d=3$, a configuration again containing a gauge field and perhaps also a scalar field generates a long-range magnetic monopole field, which cannot be destroyed with finite action, regardless of the precise details of the monopole interior. Thus any of these three solitons potentially would be able to carry charges that are pieces or fractions of those carried by elementary particles in the same medium.

Remarks: From the above argument, no other solitons can carry fractional charge, a fact already understood for nontopological solitons.[5] A type of nontopological soliton much discussed recently is the "Q ball,"[6] a configuration of a charged scalar field which carries a very large electric charge, stabilized by the attractive self-interaction of the scalar field. Such a system evidently can be made to disintegrate, and therefore could not carry a fraction of elementary charges.

Perhaps the most famous topological soliton, which according to the above criterion is not fundamental, is the skyrmion, described in the nonlinear sigma model by a four-component scalar field with fixed magnitude. The soliton corresponds to a map from R_3 (with spatial infinity treated as a single point) to S_3. The winding number of the map is an exactly conserved integer, which Skyrme proposed should be identified with baryon number.[7] However, in its coupling to light fermions the skyrmion must have effects equivalent to those of a similar object in the linear sigma model, where a fourth-order polynomial potential density is minimized for a specified magnitude of the Skyrme field. For this structure the topological quantum number could be destroyed with finite action by temporarily creating a zero in the Skyrme field at the center of the skyrmion, and then allowing the topological charge to flow into the zero and disappear.

MacKenzie and Wilczek[8] and D'Hoker and Goldstone[9] each computed flows of baryon current involved in the adiabatic creation of a skyrmion and found integer baryon number, but implicitly left open the possibility that some exotic circumstance might produce a fractional result instead. Their construction works exactly the same way for the original skyrmions or for the almost-stable objects in the linear sigma model, and therefore the argument here shows that one never could obtain fractional charge for this system. There is one apparent way out: Insist that the high-energy behavior indeed is governed by the strict nonlinear sigma model, with fixed magnitude of the Skyrme field. The trouble now is that this theory is well-known to be nonrenormalizable, so that this option is undefined—one only may use the theory with an energy cutoff, which is equivalent to replacing the model with a linear sigma model. Stated differently, using the nonlinear sigma model is making a statement about the behavior at arbitrarily high energies of what should be only an effective field theory. This would be tantamount to introducing new particles associated with those high energy scales.

Theorem 3 (Fractional charge from conventional renormalization): For a fractional charge to be associated with conventional renormalization, the particle must be an electric charge or a magnetic monopole in $d=3$, or a kink in $d=1$. Otherwise (in particular for the vortex in $d=2$), the fractional charge must be intrinsic to the structure of the particle or fundamental soliton.

Proof: For conventional renormalization, as some coupling parameter changes adiabatically there must be a current flow of the relevant charge into or out of the particle in question. Far away from the $d=3$ electric charge, or the magnetic monopole, there is a radial $1/r^2$ field. Thus, a local current density proportional to that field and to the time rate of change of some scalar or pseudo-

scalar parameter would provide a steady net current into the particle. Clearly the long-range field is necessary to give direction as well as the correct radial dependence to the current density. In one space dimension, the different asymptotic behaviors to right and left of the kink field can determine locally the sign and magnitude of a current, again proportional to the time rate of change for some suitable coupling parameter.

Remarks: Thus, in these cases the possibility of creating fractional charge by continuous variation of a suitable parameter is open, while for other isolable objects it is not. In particular, the vortex exhibits no locally observable long-range field, only the globally defined vector potential, so that it cannot guide a continuous current flow from infinity. Note that electrically charged particles in $d=1$ or $d=2$ are not isolable, because the energy for a particle–antiparticle pair diverges with separation. In all cases except the two in $d=3$ and the one in $d=1$ just described, the renormalization cannot be accomplished by a flow from infinity, and therefore must be intrinsic to the structure of the particle. For description of such intrinsic fractional charge as due to discrete renormalization to be meaningful, it must be possible to identify some ''core'' of the particle, with its characteristic conserved charge, to which the medium polarization (leading to net fractional charge) is attached. That turns out to be possible, and therefore at least a useful perspective, for all known cases.

We have seen that among solitons only the fundamental ones (stabilized by long-range physics) can nucleate fractional charge. The obvious corollary is that the only other possible ''kernels'' are those elementary particles which can be taken as given (i.e., determined by short-range physics). Blankenbecler and Boyanovsky[10] have presented another perspective which leads to the same conclusion as the one here for the case of fractional fermion charge induced by topology. They argue that the high-energy coupling of fermions carrying integer values of such a charge is influenced by the asymptotic field of the soliton, and this directly determines the fractional part of the charge localized on the soliton.

III. ILLUSTRATIONS AND COMMENTS

Before going on, it is important to emphasize that the above theorems give necessary conditions for fractional charge—they do not demonstrate that it occurs. Such demonstrations were the important content of works to be cited below.

It has been shown here that the only solitons whose topological charges could have a conventional renormalization to produce fractional values of certain other charges are kinks and monopoles, the two types of object first found by Jackiw and Rebbi (JR)[11] to carry fractional charge—to be precise, fermion number $F=\frac{1}{2}$. Their results were verified elegantly using adiabatic flow methods by Goldstone and Wilczek[12] and by Seiberg and Witten.[13] These methods can be implemented in such a way that the soliton remains intact, while variation of certain couplings ''decorates'' the object with fractional F and perhaps also fractional electric charge.

Fractional local charges are significant only if they are eigenvalues rather than expectation values; they must be ''sharp'' quantum observables. For charges to be sharp, in one space dimension spatial smearing of the corresponding charge density operator is required,[14] while in higher dimensions temporal smoothing is needed as well.[15,3]

Perhaps the most dramatic observation of fractional charge is associated with the fractional quantum Hall effect (FQHE) discovered by Tsui, Störmer, and Gossard.[16] Here Laughlin[17] concluded that the quasiparticles carry a simple fraction of an electron charge, so that an electron entering the medium could break up into several quasiparticles (something dramatically different from the breakup into reduced quasiparticle charge and remnant surface charge when an electron enters a conventional insulator). This result was vindicated in several experiments, by Goldman and Su, de Picciotto *et al.*, Seminadayar *et al.*, and Reznikov *et al.*[18]

Jain's composite-fermion description[19] of odd-denominator FQHE states identifies the composite fermions as electrons whose strong repulsive mutual correlations renormalize their charges to the observed fractional values associated with the quasiparticles, so that it is natural to identify the quasiparticles as electrons dressed by the medium. In that perspective, the AB charge of a quasiparticle should be the same as that of an electron, but it is accepted that the force on the

particle due to a Maxwell electric field $\vec{E}$ parallel to the Hall plane may be obtained by using precisely the fractional local charge already mentioned. In the dressed-electron picture, this is understood as resulting from an induced Chern–Simons field in the Hall plane which partly compensates the effect of the Maxwell field.[20] The large conceptual advantage of this perspective, embodied in composite-fermion theory,[19] is that it not only unifies the description of different FQHE regimes, but also provides a close correspondence with previously familiar condensed-matter systems and their quasielectron excitations.

The original description of a quasihole for simple Hall fractions was given by Laughlin[17] in terms of a fundamental soliton in the form of a special type of vortex—a vortex in the many-body ground-state wave function. This vortex requires neither Higgs nor gauge field, but only is possible under the special conditions for which the Laughlin ansatz gives the ground state wave function. Now one describes the quasihole as a soliton with local charge and AB charge both equal to the same fraction. The ability to describe a quasiparticle either as a fundamental soliton or a dressed electron may be unique to this particular case. Depending on which one chooses, the local charge always is the same fraction, but the AB charge either has fractional or unit value. Of course, all observables are identical in the two descriptions, but as mentioned the electron description has wider and easier application. In these terms, the experiment of Goldman and Su mentioned above was a meaurement of fractional effective AB charge, while the other experiments measuring shot noise were sensitive to fractional local charge.

After JR, besides the independent work of Su, Schrieffer, and Heeger (SSH) on kinks in polyacetylene,[21] there were a number of studies confirming and elaborating on the original finding that solitons can carry fractional charge. Shankar and Witten[22] used bosonization to put fermions and bosons on the same footing in the kink system, taking account of possible back-reaction by fermion on boson degrees of freedom, and confirming the JR result. Su and Schrieffer[23] found examples of kinks in condensed matter models with other rational fractions. Earlier, Witten[24] showed that magnetic monopoles could have fractional electric charge determined by the vacuum angle (or equally well by a crossed electric-magnetic susceptibility like that for a medium with dipolar molecules carrying both electric and magnetic moments). Sikivie[25] put this in the context of conventional insulator behavior, showing that if a monopole passes through a domain wall between different values of the vacuum angle θ, then the change in electric charge of the monopole is exactly compensated by a change in the surface charge spread over the wall.

The work of Witten[24] had two parts. First was a demonstration that the very gauge transformation which has a compact U(1) action on conventional charged particles with quantized electric charge can have a noncompact action on a magnetic monopole, a necessary condition for fractional electric charge on the monopole. (For an extended treatment of this point, see Ref. 26.) The noncompact action of the electric-charge gauge transformation on the dyon is consistent with gauge invariance because in the mutual interaction of two dyons there is besides the normal gauge interaction an extra term, gauge-variant but not contributing to the equations of motion for the pair.[27,28] The conclusion in Theorem 3 above that the monopole satisfies a necessary condition to possess fractional local electric charge is based on a space–time picture of the magnetic field configuration of the monopole (corresponding by a magnetic Gauss law to an absolutely conserved charge), complementary to the topological analysis just mentioned. The second part of Witten's work was a direct construction of the fractional charge from the vacuum angle. Thus he found both necessary and sufficient conditions for the monopole to carry fractional electric local and AB charge. Note that the latter clearly is not conserved when the monopole passes through a domain wall.

As mentioned, Goldstone and Wilczek[12] developed an adiabatic flow analysis showing that F for the JR monopole must change by $\Delta F = \frac{1}{2}$ as the fermion mass is chirally rotated from isoscalar to isovector. Callan[29] considered fermions light even compared to the Coulomb energy required to confine a unit of electric charge within a monopole radius, finding $F = \frac{1}{2}$ appears in a natural way. Over a long period, the notions of electric-magnetic duality, supersymmetry, and JR fermion zero modes were locked together, mutually reinforcing all three.[30,13] In particular, Seiberg and Witten[13] used an adiabatic flow analysis (complementary to that of Goldstone and Wilczek), which allowed

them to follow the change of F and electric charge Q as the isoscalar part of the fermion mass is lowered from infinity, where the fermion is totally decoupled (meaning any fractional part of F must vanish), to a point where the net mass of one member of the fermion isodoublet goes through zero. They were able to establish directly that F becomes fractional, while explicitly treating the electric charge as a discrete quantum variable.

This subject of adiabatic flow brings attention to the beautiful thought experiment of Laughlin,[17] who imagined piercing a fractional quantum Hall layer with an infinitely thin tube of flux, gradually increased from zero to one flux quantum. Through the Faraday effect and the Hall effect this assures the localization of a fractional charge, immediately showing that the quasiparticles of this system must have fractional charge with respect to electrons in a different medium—free ($d=3$) space. The fractional value in itself should not be a surprise, in view of the behavior of normal insulators. However, if we imagine inserting an electron into the layer from above there is no surface in which to leave part of its locally conserved electric charge, so that the charge instead must be deposited on several quasiparticles. This inevitable breakup into many particles was a new and theoretically unanticipated phenomenon.

The concept of fractional soliton charge was at least implicit in the work of Skyrme,[7] who argued that his classical field configuration could be quantized with half-integer isospin and spin (a possibility shown consistent with the usual spin-statistics connection in Ref. 31). Half-integer values would allow the skyrmion to be identified with the nucleon, but by Theorem 2 are impossible without elementary or fundamental isospinor fermions: Modification of the short-distance, high-energy part of the Skyrme action (e.g., replacing the nonlinear constraint in his sigma model with a quartic action in the chiral field) could destabilize the skyrmion, so that its ''topological'' charge would be ''unwound'' in a process with finite action, and therefore in principle is not absolutely conserved. Microscopic analyses agree, indicating that the spin and isospin of the skyrmion will be integer or half-integer as the number of colors of up and down quarks is even or odd,[32] and therefore integer if there are no quarks.

These considerations may be put more dramatically. The fact that the skyrmion is in a class of objects some of which are not conserved immediately implies that there must be some underlying structure to account for spin and isospin charge values that are fractional with respect to the meson charges of the sigma model. Thus at best the skyrmion could be a useful description for reasonably low-energy and long-distance properties of the nucleon. That indeed is the case, but this simple reasoning could have been made at any time after Skyrme's original work. Perhaps an intuitive appreciation of this point contributed to initial resistance to his model. Paradoxically, if the model had been embraced, it might have slowed the approach to quarks and QCD which now gives an intellectual basis for the skyrmion's success in the appropriate domain.

Skyrme's model describes the nucleon entirely in terms of an SU(2) matrix function $\mathrm{U}(\mathbf{r},t)$, while in a ''hybrid'' model the U function is used outside a chosen ''bag'' radius R, and inside are free quarks with angle-dependent boundary condition parametrized by $\mathrm{U}(\mathbf{r})$ at the bag wall.[33] Goldstone and Jaffe[34] showed that the simple boundary condition guessed in Ref. 33 meets the requirement of net integer baryon number B. Thus, for the nucleon it becomes possible to interpolate smoothly between soliton and fundamental-particle (quark) descriptions, and neither can involve intrinsically fractional charges.

An analogous interpolation has been found for FQHE quasiparticles, which for $\nu=1/(2n+1)$ can blow up into arbitrarily spread-out ''baby skyrmions'' when the Zeeman splitting between the two possible electron spin orientations becomes negligible. Thus, adjusting the Zeeman splitting allows interpolation between microscopic quasiparticles and macroscopic solitons. Of course, the charges of the soliton and the quasiparticle are the same. This theoretical result for FQHE follows well-established results for skyrmions of the integer quantum Hall effect with small Zeeman splitting.[35]

The SSH kink analysis[21] shows that in one space dimension ''spinons'' with spin $\frac{1}{2}$ but no charge and ''holons'' with charge $\pm e$ but no spin can travel independently. Kivelson *et al.*[36] proposed that such objects might play a role in the planar dynamics which appears to be critical in high T_C superconductivity. Detailed studies suggested that if so, either these fractional objects are

connected by strings[37] or are able to move only along particular lines in the plane.[38] However, Senthil and Fisher[39] observed that a dynamics which leads to vortices in terms of some effective gauge field could allow the string connecting a spinon and a holon to exhibit zero tension, because the precise path of that string is simply a gauge choice. Hence it becomes imaginable that the two types of particle could move freely in the plane.

The uniqueness of magnetic monopoles among solitons in $d=3$ as possible carriers of fractional particle charge is connected with other special properties, such as the ability to convert the dynamics of the lowest fermion partial wave into a one-dimensional problem on a half-line. This is an example of the fact that the chiral anomaly for electrodynamics with $d=3$ may be written as the product of a magnetic-field contribution which reduces the problem to $d=1$, and an electric-field contribution just like that for QED in $d=1$.[40] The same long-range magnetic field is responsible for the possibility of creating an object with half-integer spin[41] and Fermi–Dirac statistics[42] from spinless bosons in a world with no fundamental fermons, a possibility that we have seen is *not* available to the skyrmion, contrary to casual statements in the literature.

An interesting example of fractional charge is the Higgs–Chern–Simons vortex in Abelian $2+1$ D gauge theory, a soliton which carries a conserved topological charge, the quantized magnetic flux. There is a locally conserved Gauss-law electric charge $Q=\kappa\Phi+q_H$, with κ the Chern–Simons (CS) coupling,[43] Φ the quantized magnetic flux, and q_H the Noether charge of the Higgs field. Evidently Q vanishes by the Gauss law, but of course q_H does not, and is not even conserved if κ varies. Indeed, with the gauge kinetic term F^2 omitted, the resulting ''self-dual'' vortex[44] has vanishing Q density everywhere! This system manifestly violates electric charge conjugation symmetry, and generates fractional values for q_H. The fact that q_H would vary if κ changed implies that κ must be constant if one is to interpret q_H as a conserved fractional charge. With this assumption, one sees that a given value of κ, which is crucial to the dynamics of this soliton, indeed enforces an intrinsic relation between the charge and the soliton structure, maintaining consistency with Theorem 3. For non-Abelian CS theory there must be quantization of κ,[45] but for the Abelian case relevant here there may be some flexibility in the allowed values. The self-dual vortex has been proposed, though without explicit identification as such, to be the charge carrying quasiparticle of the $\nu=5/2$ FQHE state.[46]

Up to now we have not considered fractional spin in this discussion. Of course, in $d=1$ spin is not defined, while in $d=3$ the non-Abelian character of the rotation group assures spin quantization. However, in $d=2$ the logical possibility of fractional spin is open. Paranjape[47] realized that such spin indeed could be induced for solitons carrying both electric charge and magnetic flux; Blankenbecler and Boyanovsky[48] gave a simple exposition of the mechanism. That the familiar connection between spin and statistics holds in $d=2$ for the fractional, charge-conjugation-even part of the spin and the associated part of the statistics was suggested already by Wilczek,[27] and follows from elementary conservation laws:[49,20] To be precise, if one defines $s_e=(s+\overline{s})/2$, the part of the spin symmetric under particle$\leftrightarrow$antiparticle, with $0<|s_e|<\frac{1}{2}$, then there is a contribution to the phase factor on exchange of two indistinguishable particles given by $e^{2\pi i s_e}$.

The one example of fractional charge by conventional renormalization that remains to be discussed is that of the familiar electrically charged elementary particles mentioned at the beginning, the proton and the electron. Suppose we say that the neutron has $B-L=1$, and the neutrino has $B-L=-1$. What is the value of $B-L$ for the charged particles? In first approximation, one may neglect all contributions to QED vacuum polarization except that of electron loops. As a result, the proton is accompanied by a tenuous cloud of electron vacuum polarization, and so has still $B=1$, but $L=\epsilon$. Meanwhile, charge renormalization of the electron implies that it has $L=1-\epsilon$. Thus, $B-L$ for the proton is $1-\epsilon$, and $B-L$ for the electron is $\epsilon-1$. For neutron decay, this gives initial $B-L=1$, and final $B-L=(1-\epsilon)_{\mathrm{p}}+(\epsilon-1)_{\mathrm{e}}-(-1)_{\overline{\nu}}=1$. In principle, it would be consistent with all we know to introduce a new gauge field, weakly coupled to $B-L$. This would allow direct observation of the different local values of $B-L$ for the neutral and the electrically charged particles. However, the main point to make here is that if there is some conserved charge carried by a particle, then it can consistently generate a fractional shift in another

charge carried by that particle. The fact that in some cases this fractional shift is quantized, while in others it can be varied continuously, is important, but the parallelism between the two types of cases may be even more important.

There is a complementary way to view the above discussion, exemplified by consideration of the weak coupling through the new $B-L$ gauge field between a neutron and a proton. What was discussed already shows that the neutron would see a somewhat weaker field due to electron vacuum polarization. Alternately, if one considers the influence of the neutron on the proton, the neutron's $B-L$ field mixes with the electromagnetic field due to the same vacuum polarization, so that it couples to the combination of AB charges $B-\epsilon Q$. The AB charges do not change, but the field acting on them is modified in a nontrivial way. Of course, in line with the principle of reciprocity, either way of calculating the interaction between neutron and proton gives the same answer.

Note that (assuming the neutrino is its own antiparticle) the nonconservation of $B+L$, combined with the conservation of $B-L$, assures that the magnitudes of the electric charges of proton and electron must be equal. This is very close to the assertion that there is a single elementary unit of electric charge (which quarks are able to fractionate because they also possess the additional conserved quantum number triality).

IV. CONCLUSION

This work is designed both as codification and development of an extensive if not entirely coherent literature on fractional charge. The principal results are as follows.

(1) Gauge charge, which in the case of a charge coupled to a local gauge field is the Lorentz-force charge of a particle in classical mechanics or the Aharonov–Bohm charge in quantum mechanics, is a fundamental, quantized attribute of a fundamental particle or an elementary particle built of fundamental particles, never renormalized or fractionated by change in medium, scale, or coupling strength. Gauge charge is not necessarily conserved; for example, there may be processes conserving local charge while allowing excitation of the vacuum to mobilize previously latent particles carrying gauge charge. For a fundamental soliton, there may be gauge charges carrying fractional values compared to those found on elementary particles in the same medium, if so with the fractions equal to the corresponding values for local or Gauss-law charge.
(2) The (locally conserved) local charge of a particle with specified AB charge may have a fractional value in one medium or at one scale with respect to its value in a different medium or at a different scale.
(3) In a given medium an isolable particle may carry a fraction of the local charge of another isolable particle only if the first one is itself elementary, which includes the possibility that it is a fundamental soliton.
(4) Fractional charge may result from conventional, continuous flow if the particle is a $d=1$ kink, or a $d=3$ electric charge or magnetic monopole. Otherwise the fractional value must arise from the intrinsic structure of the particle. In particular, this is the only possible fractional-charge case for a $d=2$ vortex.

The considerations in this work about elementary particles and fundamental solitons show a striking (and typical) duality. The particles and their constituents are established in the dynamics of the smallest distance and highest energy scales, while the stability of the solitons is assured by the dynamics of the largest distance and lowest energy scales.

It is interesting to wonder about possible extensions of this analysis. There may well be novel charges for $d>3$, and in certain circumstances fractional values of these charges. Even within the domain of $d\leqslant 3$ there is a class of issues that remains a matter of art rather than systematic deduction, namely, the determination of the discrete renormalizations which by definition are not directly susceptible to the well-developed techniques used for conventional renormalization. It is

possible that consistency relations of the type developed by Su[50] for the fractional quantum Hall effect would permit this sort of determination.

It may be in order to say something about the role of this article (in a journal issue devoted to exact methods for solitons), which has almost no equations and deals as well with solitons which do and ones which do not exhibit exact integrability, the latter evidently violating the original definition of the term by Zabusky and Kruskal.[51] Mathematical physics uses the notion of exactness in many ways. On one side, emphasized in this issue, one has exactly soluble systems, which can be used to infer generic properties that may be compared with real systems whose dynamics generally will not be exactly soluble. On the other side one finds systems which may not be fully soluble, but the existence of certain local conservation laws still may permit some useful—and exact—statements. This work manifestly is intended as a contribution to the latter category, by determining from mild assumptions some stringent requirements for the occurrence of fractional charge.

ACKNOWLEDGMENTS

A sceptical remark by Jeffrey Goldstone about skyrmions with fractional B was an early stimulus for this study, supported in part by the National Science Foundation under Grant No. PHY-0140192. Michael Dine, Roman Jackiw, Jainendra Jain, Vladimir Korepin, Barry McCoy, and Mikhail Stephanov gave instructive comments and criticisms. The Theoretical Physics Group at the Stanford Linear Accelerator Center (Department of Energy Contract No. DE–AC03–76SF00515) and the Center for Theoretical Physics at the Massachusetts Institute of Technology (Department of Energy Cooperative Agreement No. DF-FC02-94ER40818) provided generous hospitality during a sabbatical leave from Stony Brook.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Sphalerons, spectral flow, and anomalies

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(Received 8 January 2003; accepted 9 April 2003)

The topology of configuration space may be responsible in part for the existence of sphalerons. Here, sphalerons are defined to be static but unstable finite-energy solutions of the classical field equations. Another manifestation of the nontrivial topology of configuration space is the phenomenon of spectral flow for the eigenvalues of the Dirac Hamiltonian. The spectral flow, in turn, is related to the possible existence of anomalies. In this review, the interconnection of these topics is illustrated for three particular sphalerons of SU(2) Yang–Mills–Higgs theory. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1590420]

I. INTRODUCTION

One of the main themes of the present special issue concerns the so-called topological solitons. The field configurations of these classical solutions are characterized by a topologically nontrivial map of the space manifold (or part of it) into some internal space of the model considered. A well-known example is the Skyrme soliton,[1] for which the space manifold S^3 (i.e., the compactified Euclidean space $\mathbb{R}^3$) is mapped into the internal space SU(2). Another example is the magnetic monopole,[2] for which the ''sphere at infinity'' S^2 is mapped into the Higgs vacuum manifold SO(3)/SO(2).

There exist, however, other classical solutions, the so-called sphalerons, which themselves have trivial topology but trace back to nontrivial topology in the configuration space of the fields.[3,4] In this contribution, we intend to give an elementary discussion of sphaleron solutions in Yang–Mills–Higgs theory and the underlying topology. In order to get a clear picture of what goes on, we focus on a single Yang–Mills–Higgs theory and three specific sphalerons.[5–7]

Physically, the topological solitons and the sphalerons play a different role. Solitons are primarily relevant to the equilibrium properties of the theory (e.g., the existence of certain stable asymptotic states), whereas sphalerons are of importance to the dynamics of the theory. The sphaleron[5] of the electroweak standard model,[8] for example, is believed to play a crucial role for baryon-number-violating processes in the early universe (see, e.g., Refs. 9 and 10 for two reviews).

The outline of this article is as follows. In Sec. II, we present the theory considered, to wit, SU(2) Yang–Mills theory with a single complex isodoublet of Higgs fields. This particular Yang–Mills–Higgs theory forms the core of the electroweak standard model of elementary particle physics. In Sec. III, we recall some basic facts about the mapping of spheres into spheres, in particular their homotopy classes. In Sec. IV, we describe three sphaleron solutions and their topological *raison d'être*. In Sec. V, we discuss another manifestation of the nontrivial topology of configuration space, namely the spectral flow of the eigenvalues of the Dirac Hamiltonian. The word ''spectral flow'' is used in a generalized sense, meaning *any* type of rearrangement of the energy levels. Loosely speaking, the spectral flow makes it possible for a sphaleron to acquire a fermion zero-mode. In Sec. VI, we link the spectral flow to the possible occurrence of anomalies (which signal the loss of one or more classical symmetries). In Sec. VII, finally, we present some concluding remarks.

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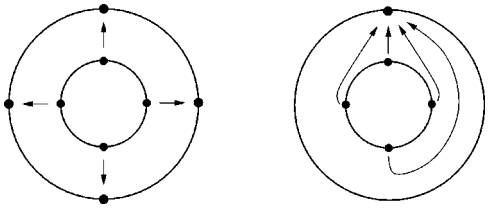

FIG. 1. Two nonhomotopic maps $S^1 \to S^1$, with inner circles mapped into outer circles and matching points indicated. For the figure on the right, the whole inner circle is mapped into a single point of the outer circle.

II. SU(2) YANG–MILLS–HIGGS THEORY

In this article, we consider a simplified version of the electroweak standard model[8] without the hypercharge U(1) gauge field. This means, basically, that we set the weak mixing angle $\theta_w \equiv \arctan(g'/g)$ to zero, where g' and g are the coupling constants of the U(1) and SU(2) gauge groups, respectively. Also, we take only one family of quarks and leptons instead of the three known experimentally.

In general, the fields are considered to propagate in Minkowski space–time with coordinates $x^\mu \in \mathbb{R}$, $\mu = 0,1,2,3$, and metric $g_{\mu\nu}(x) = \text{diag}(+1,-1,-1,-1)$. But occasionally we go over to Euclidean space–time with metric $g_{\mu\nu}(x) = \delta_{\mu\nu}$. Natural units with $\hbar = c = 1$ are used throughout.

The SU(2) Yang–Mills gauge field is denoted by $A_\mu(x) \equiv A^a_\mu(x)\, \tau^a/(2\text{i})$, where the τ^a are the three Pauli matrices acting on weak isospin space and the component fields $A^a_\mu(x)$ are real. (Repeated indices are summed over, unless stated otherwise.) The complex Higgs field transforms as an isodoublet under the SU(2) gauge group and is given by $\Phi(x) = (\Phi_1(x), \Phi_2(x))^t$, where the suffix t stands for transpose [cf. Eq. (5.5) below]. The fermion fields will be discussed in Sec. V.

The classical action of the gauge and Higgs fields reads

$$\Gamma_{\text{YMH}} = \int_{\mathbb{R}^4} \mathrm{d}^4x \, \left\{ \frac{1}{2} \text{tr}\, F_{\mu\nu} F^{\mu\nu} + (D_\mu \Phi)^\dagger (D^\mu \Phi) - \lambda\, (\Phi^\dagger \Phi - \eta^2)^2 \right\}, \tag{2.1}$$

where $F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu + g[A_\mu, A_\nu]$ is the SU(2) Yang–Mills field strength and $D_\mu \Phi \equiv (\partial_\mu + g A_\mu)\Phi$ is the covariant derivative of the Higgs field. The theory has Yang–Mills coupling constant g and quartic Higgs coupling constant λ, but the classical dynamics depends only on the ratio λ/g^2. The parameter η has the dimension of mass and sets the scale of the Higgs expectation value. The three W vector bosons then have equal mass, $M_W = g\,\eta/\sqrt{2}$. The single Higgs scalar boson has a mass $M_H = 2\,\sqrt{\lambda}\,\eta$.

The action (2.1) is invariant under a local gauge transformation

$$\Phi'(x) = \Lambda(x)\, \Phi(x), \quad g A'_\mu(x) = \Lambda(x)\, (\, g A_\mu(x) + \partial_\mu\,)\, \Lambda(x)^{-1}, \tag{2.2}$$

for an arbitrary gauge function $\Lambda(x) \in \text{SU}(2)$. In addition, there are certain global SU(2) and U(1) symmetry transformations which operate solely on the Higgs field.

III. MAPS OF SPHERES INTO SPHERES

Let us consider continuous maps from a connected manifold M to a connected manifold N. Two such maps, f_1 and f_2, are called *homotopic* if the one can be obtained from the other by continuous deformation. More specifically, f_1 and f_2 are homotopic if there exists a continuous map $h:[0,1]\times M \to N$ such that $h(0,m) = f_1(m)$ and $h(1,m) = f_2(m)$ for all $m \in M$. All maps $M \to N$ can be divided into equivalence classes, where two maps are equivalent if they are homotopic (see, e.g., Ref. 11).

We are particularly interested in the case where M and N are the spheres S^m and S^n, respectively. The set of homotopy classes is called the *homotopy group* and is denoted by $\pi_m(S^n)$. Figure 1 shows two maps $S^1 \to S^1$ which are not homotopic. It is clear that in this particular case

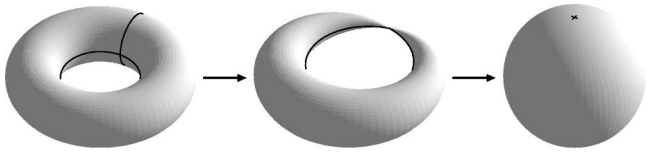

FIG. 2. Left: Cartesian product space $S^1\times S^1$ drawn as a torus, with two circles representing the sets $\{x_0\}\times S^1$ and $S^1\times\{y_0\}$ for some arbitrarily chosen points x_0 and y_0. Middle: surface after shrinking the first of these sets to a point. Right: surface after shrinking the second set to a point, which gives the smash product $S^1\wedge S^1\sim S^2$.

the homotopy classes can be labeled by integer numbers which describe how often the original circle S^1 is wrapped around the target circle S^1. This explains the result $\pi_1(S^1)=\mathbb{Z}$, where $\mathbb{Z}$ denotes the group of integers under addition. The two maps shown in Fig. 1 have winding numbers 1 and 0.

The homotopy classes of $S^n\to S^n$, for $n>1$, can be pictured analogously, since the representation of a sphere S^n in spherical coordinates contains exactly one azimuthal angle $\phi\in[0,2\pi]$. The result is $\pi_n(S^n)=\mathbb{Z}$. Further homotopy groups are $\pi_m(S^n)=\{0\}$ for $m<n$, $\pi_3(S^2)=\mathbb{Z}$, and $\pi_4(S^3)=\mathbb{Z}_2$, where $\mathbb{Z}_2$ denotes the group of integers $\{0,1\}$ under addition modulo 2.

Next, consider families of maps $S^m\to S^n$, where the family parameters themselves form a sphere S^p. In short, consider $S^p\times S^m\to S^n$. Imposing certain constraints, these families of maps can be viewed as maps $S^{p+m}\to S^n$ and classified according to the homotopy groups of spheres.

To this end, we introduce the *smash product*[11] of two spheres S^p and S^m. The smash product $S^p\wedge S^m$ is defined as the Cartesian product $S^p\times S^m$ with the set $(\{x_0\}\times S^m)\cup(S^p\times\{y_0\})$ considered as a single point, for some arbitrarily chosen $x_0\in S^p$ and $y_0\in S^m$. It can be shown that $S^p\wedge S^m$ is homeomorphic to the sphere S^{p+m} (see Fig. 2 for a sketch of the proof).

A simple corollary will be important in the following. Any map $f:S^p\times S^m\to S^n$ can effectively be considered as a map defined on $S^p\wedge S^m$ if $f(x_0,y)$ is independent of y and $f(x,y_0)$ is independent of x, for an appropriate choice of $x_0\in S^p$ and $y_0\in S^m$.

IV. SPHALERONS

The word sphaleron is of Greek origin and means "ready to fall" (see Ref. 5 for the etymology). It is used to denote a static but unstable solution of the classical field equations with finite total energy of the fields.

In this article, only finite-energy configurations of the fields will be considered. By analogy to Morse theory,[12] sphalerons can then be looked for by a minimax procedure[3] if the configuration space of the underlying field theory is multiply connected.

The procedure runs as follows: first, construct a noncontractible p-dimensional sphere S^p in configuration space, then determine its maximal energy configuration, and, finally, "shrink" the sphere to minimize this maximal energy. If the configuration space were compact, this procedure would be guaranteed to give a saddle point. But configuration space is infinite-dimensional and noncompact, so that the minimax procedure produces at best only a candidate solution. It has to be checked explicitly that the appropriate minimax-configuration solves the classical field equations. If this is the case, the minimax-configuration is a genuine sphaleron.

A. Sphaleron S

For the sphaleron S[4,5,13] of the SU(2) Yang–Mills–Higgs theory (2.1), we consider three-space to be compactified by adding the "sphere at infinity." Configuration space is then the space of all static three-dimensional gauge and Higgs field configurations in a particular gauge which have finite energy. The static gauge field can be written as a Lie-algebra-valued one-form,

$$A(x^1,x^2,x^3)\equiv A_m^a(x^1,x^2,x^3)\,\tau^a/(2\mathrm{i})\,\mathrm{d}x^m\,, \tag{4.1}$$

with implicit sums of a and m over $1,2,3$. Furthermore, we use spherical coordinates (r,θ,ϕ) over $\mathbb{R}^3$ and employ the radial gauge condition $A_r=0$, together with $A_0=0$.

Since the energy has to be finite, only those configurations are admissible for which the gauge field tends towards a pure-gauge configuration as $r\to\infty$ and the Higgs field towards its associated vacuum value,

$$g\,A^{\infty}=-\,\mathrm{d}\omega\;\omega^{-1}\,,\quad \Phi^{\infty}=\eta\;\omega\begin{pmatrix}0\\1\end{pmatrix}, \tag{4.2}$$

for a map ω of the "sphere at infinity" S^2 into the gauge group SU(2).

Any loop in configuration space induces a loop in the space of these mappings ω. The corresponding map is denoted by

$$U{:}S^1\times S^2\to \mathrm{SU}(2)\,,\quad (\mu,\theta,\phi)\mapsto U(\mu,\theta,\phi)\,, \tag{4.3}$$

where $\mu\in[0,\pi]$ is the parameter of the loop of configurations and $\theta\in[0,\pi]$ and $\phi\in[0,2\pi]$ are spherical coordinates in three-space.

By imposing certain constraints on this map, we may effectively reduce the set of allowed loops, so that U becomes a map $S^3\to\mathrm{SU}(2)\sim S^3$ which falls into homotopy classes according to $\pi_3(\mathrm{SU}(2))=\pi_3(S^3)=\mathbb{Z}$. To be specific, the map U for $\mu=0$ and $\mu=\pi$ must not depend on θ and ϕ, and the map U for $\theta=0$ has to be independent of μ. Then U is effectively defined on the smash product $S^1\wedge S^2\sim S^3$, as explained in the last paragraph of Sec. III. Now there exist noncontractible loops of field configurations for which the minimax procedure can be performed.

An appropriate expression for the map (4.3) is given by[4]

$$U(\mu,\theta,\phi)=y^1\,(-\mathrm{i}\tau_1)+y^2\,(-\mathrm{i}\tau_2)+y^3\,(-\mathrm{i}\tau_3)+y^4\,\mathbb{1}_2\,, \tag{4.4}$$

with

$$\begin{pmatrix}y^1\\y^2\\y^3\\y^4\end{pmatrix}=\begin{pmatrix}-\sin\mu\,\sin\theta\,\sin\phi\\-\sin\mu\,\sin\theta\,\cos\phi\\\sin\mu\,\cos\mu\,(\cos\theta-1)\\\cos^2\mu+\sin^2\mu\,\cos\theta\end{pmatrix}. \tag{4.5}$$

In order to calculate the winding number of this particular map U, we examine its relation to the standard spherical coordinates on S^3,

$$\begin{pmatrix}z^1\\z^2\\z^3\\z^4\end{pmatrix}=\begin{pmatrix}\cos\theta_2\\\sin\theta_2\,\cos\theta_1\\\sin\theta_2\,\sin\theta_1\,\sin\phi_1\\\sin\theta_2\,\sin\theta_1\,\cos\phi_1\end{pmatrix}, \tag{4.6}$$

with polar angles $\theta_1,\theta_2\in[0,\pi]$ and azimuthal angle $\phi_1\in[0,2\pi]$.

We first observe that the two-vector

$$\vec{w}=\begin{pmatrix}\cos\mu\\\sin\mu\,\cos\theta\end{pmatrix} \tag{4.7}$$

sweeps over the unit disk if μ and θ run from 0 to π. Since rotations map the unit disk onto itself and leave the length of $\vec{w}$ invariant,

$$|\vec{w}|^2=1-\sin^2\mu\,\sin^2\theta\,, \tag{4.8}$$

the relation

$$\begin{pmatrix}\cos\theta_2\\\sin\theta_2\,\cos\theta_1\end{pmatrix}=\begin{pmatrix}\cos\alpha&-\sin\alpha\\\sin\alpha&\cos\alpha\end{pmatrix}\begin{pmatrix}\cos\mu\\\sin\mu\,\cos\theta\end{pmatrix} \tag{4.9}$$

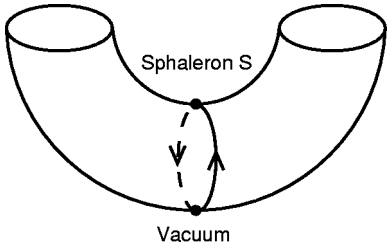

FIG. 3. Sphaleron S on top of a noncontractible loop in configuration space. The field energy is zero for the vacuum and positive for the sphaleron S.

describes an admissible reparametrization of the disc. By choosing $\alpha=-\mu$, we find $y^4=z^1$ and $y^3=z^2$. With $\sin\theta_1\sin\theta_2=\sin\mu\sin\theta$ and $\phi_1=\phi$, we have also $y^1=-z^3$ and $y^2=-z^4$.

The conclusion is that the map U as defined by Eqs. (4.4) and (4.5) covers the target sphere S^3 exactly once. The map U has winding number one (or minus one, depending on the definition of the winding number) and corresponds to a nontrivial element of the homotopy group $\pi_3(S^3)=\mathbb{Z}$.

For the static SU(2) gauge and Higgs fields of the noncontractible loop (NCL), we make the ansatz[4]

$$g\,A(\mu,r,\theta,\phi)=-\,f(r)\;\mathrm{d}U(\mu,\theta,\phi)\;U(\mu,\theta,\phi)^{-1}\,, \tag{4.10a}$$

$$\Phi(\mu,r,\theta,\phi)=\eta\,h(r)\;U(\mu,\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix}+\eta\,(1-h(r))\begin{pmatrix}0\\ \exp(-\mathrm{i}\,\mu)\cos\mu\end{pmatrix}, \tag{4.10b}$$

with the following boundary conditions for the radial functions f and h:

$$\lim_{r\to 0} f(r)/r=0\,,\quad \lim_{r\to\infty} f(r)=1\,, \tag{4.11a}$$

$$\lim_{r\to 0} h(r)=0\,,\quad \lim_{r\to\infty} h(r)=1\,. \tag{4.11b}$$

The energy density of the fields (4.10) turns out to be spherically symmetric. Indeed, the fields of the NCL can also be written in a manifestly spherically symmetric form.[14]

The fields (4.10) of the NCL at $\mu=0$ or π correspond to the Higgs vacuum with $A(x)=0$ and $\Phi(x)=(0,\eta)^t$. This particular configuration is independent of the radial functions f and h and has zero energy according to Eq. (2.1). The NCL configuration at $\mu=\pi/2$ is distinguished by having parity reflection symmetry (the only other configuration of the NCL with this property is the vacuum at $\mu=0$). For given functions f and h, this $\mu=\pi/2$ configuration is also the maximum energy configuration over the NCL. The minimax procedure now consists of adjusting the radial functions f and h while maintaining the boundary conditions (4.11), so that the energy at $\mu=\pi/2$ is minimized. The resulting configuration is the sphaleron S, as sketched in Fig. 3.

Using numerical methods, one finds for the sphaleron energy the value[5]

$$E_{\mathrm{S}}\approx 3.04\times(4\pi/g^2)\,M_W\,, \tag{4.12}$$

which holds for the case of vanishing quartic Higgs coupling constant ($\lambda/g^2=0$). [The sphaleron energy E_{S} has also been calculated for the full SU(2)×U(1) Yang–Mills–Higgs theory of the electroweak standard model. The energy E_{S} is found to be weakly dependent on the mixing angle θ_w, at least near $\theta_w=0$. The emergence of a large magnetic dipole moment $\mu_{\mathrm{S}}\propto(4\pi/g^2)\,g\tan\theta_w/M_W$ is perhaps more interesting. See Refs. 5, 15, and 16 for details.] For large

enough values of λ/g^2, additional solutions appear, the so-called ''deformed sphalerons.'' [17,18] The appearance of these extra sphalerons can be explained[14] by a simple deformation of the energy surface in Fig. 3.

The sphaleron S by itself has trivial topology, with the ''sphere at infinity'' S^2 mapped into the Higgs vacuum manifold $\mathrm{SU}(2)\sim S^3$; cf. Sec. III. [As mentioned in the Introduction, the magnetic monopole[2] in SU(2) Yang–Mills theory with a real isotriplet of Higgs is based on the nontrivial map $S^2\to\mathrm{SO}(3)/\mathrm{SO}(2)\sim S^2$.] Note that the original S ansatz, with the so-called hedgehog structure, was discovered[13] 10 years before the construction of S via the NCL.[4,5]

In the radial gauge, the vacuum configuration of the SU(2) gauge field is uniquely fixed, $gA_m^{\mathrm{vac}}(x^1,x^2,x^3)=0$. If this gauge condition is abandoned, any pure-gauge configuration $gA_m=-\partial_m U\,U^{-1}$, for arbitrary time-independent SU(2)-valued field U, is a possible vacuum configuration. Depending on the topology of three-space, these vacuum configurations may or may not fall into different unconnected classes. This does not happen for our compactification $\mathbb{R}^3\cup S^2_\infty$. But the situation changes if, instead, we choose a one-point compactification $\mathbb{R}^3\cup\{\infty\}$, with all fields approaching a single direction-independent value as $r\to\infty$. Each vacuum configuration then corresponds to a map $S^3\to S^3$ and there are topologically distinct vacuum classes, since $\pi_3(S^3)=\mathbb{Z}$.

In fact, it is possible to perform a gauge transformation on the NCL (4.10) which changes the asymptotic behavior of the gauge fields, so that they can be considered to live on $S^3=\mathbb{R}^3\cup\{\infty\}$. Let $\omega(\mu,r,\theta,\phi)$ be an SU(2)-valued map which approaches $U(\mu,\theta,\phi)$ for $r\to\infty$ and $\mathbb{1}_2$ for $r\to 0$. The radial dependence of $\omega(\mu,r,\theta,\phi)$ implements a path which connects the map $U(\mu,\theta,\phi)=\omega(\mu,\infty,\theta,\phi)$ to the constant map $\mathbb{1}_2=\omega(\mu,0,\theta,\phi)$. [Note that $U(\mu,\theta,\phi)$ for *fixed* μ is a map $S^2\to S^3$ and therefore contractible.]

The crucial point, now, is that the map $\omega(0,r,\theta,\phi)$ is homotopically different from the map $\omega(\pi,r,\theta,\phi)$. [Otherwise, the radial dependence of $\omega(\mu,r,\theta,\phi)$ would yield a contraction of $\omega(\mu,\infty,\theta,\phi)$, considered as a μ-dependent map $S^3\to S^3$, which is impossible.] Both maps $\omega(0,r,\theta,\phi)$ and $\omega(\pi,r,\theta,\phi)$ can also be viewed as maps $S^3\to S^3$, since $\omega(\mu,\infty,\theta,\phi)=U(\mu,\theta,\phi)=\mathbb{1}_2$ for $\mu=0$ and $\mu=\pi$. The conclusion is then that the corresponding vacuum configurations $A_m(x^1,x^2,x^3)$ at $\mu=0$ and $\mu=\pi$ belong to different homotopy classes. This result will be discussed further in Sec. VI A.

B. Sphaleron S*

The three-space of our SU(2) Yang–Mills–Higgs theory (2.1) is again compactified by adding the ''sphere at infinity.'' This time, however, we do not consider one-parameter families (loops) of static finite-energy configurations but two-parameter families (spheres). At spatial infinity, these families are characterized by the map

$$U:S^2\times S^2\to\mathrm{SU}(2)\,,\quad (\mu,\nu,\theta,\phi)\mapsto U(\mu,\nu,\theta,\phi)\,, \tag{4.13}$$

where (μ,ν) are the parameters of the sphere of configurations and (θ,ϕ) are the polar and azimuthal angles of the spherical coordinates in three-space. The parameters μ and ν run from $-\pi/2$ to $+\pi/2$ and the boundary of the (μ,ν)-square at $|\mu|=\pi/2$ or $|\nu|=\pi/2$ is mapped to the same element of SU(2).

Next, restrict the class of mappings U by requiring that $U(\mu,\nu,0,\phi)$ is independent of (μ,ν,ϕ) and $U(-\pi/2,-\pi/2,\theta,\phi)$ independent of (θ,ϕ). Then U is effectively a mapping from S^4 to S^3, which has a nontrivial homotopy structure, $\pi_4(S^3)=\mathbb{Z}_2$. The general idea, now, is to construct a noncontractible sphere, to determine the maximal energy configuration on that sphere and to continuously deform the sphere so that its maximal energy is minimized.[19]

The construction of the required nontrivial map $S^4\to S^3$ is done in two steps. First, a nontrivial map $S^3\to S^2$ is found and, second, an operation is performed to increase the dimension of both spheres.

The relevant map $S^3\to S^2$ is given by the well-known *Hopf fibration*,[11] which can be ex-

plained as follows. Consider the three-sphere S^3 to be a subset of $\mathbb{C}^2$, namely, $\{(z_1,z_2)\,|\,\ |z_1|^2+|z_2|^2=1\}$. Each $\mathbb{C}$-line through the origin in $\mathbb{C}^2$ then intersects with this three-sphere in a great circle S^1. These great circles S^1 form a pairwise disjoint covering of S^3. Two points of S^3 are defined to be equivalent ($\simeq$), if they lie on the same great circle S^1. The corresponding projection,

$$S^3 \to S^3/\simeq , \tag{4.14}$$

is the desired Hopf map, since the topological space $S^3/\simeq$ is homeomorphic to S^2.

The topological equivalence of $S^3/\simeq$ and S^2 can be shown by considering the $\mathbb{C}$-lines which label the great circles S^1 discussed in the previous paragraph. All but one of these $\mathbb{C}$-lines can be parametrized by complex numbers $c \in \mathbb{C}$. Specifically, the coordinates of such a line read

$$(z_1\,,z_2)=(w\,,cw)\,, \quad \text{for} \quad w\in\mathbb{C}\,. \tag{4.15}$$

In addition, there is the single $\mathbb{C}$-line given by

$$(z_1\,,z_2)=(0\,,w)\,, \quad \text{for} \quad w\in\mathbb{C}\,. \tag{4.16}$$

Hence, the total parameter space of $S^3/\simeq$ is given by the one-point-compactified plane, i.e., the Riemann sphere S^2.

The *suspension* of a sphere S^n is essentially the same as the smash product $S^1\wedge S^n$. It can be used to increase the dimension of the spheres appearing in the above discussion. The resulting suspension of the Hopf map corresponds to a nontrivial element of the homotopy group $\pi_4(S^3)=\mathbb{Z}_2$.

In a particular parametrization, the required map (4.13) takes the form[19]

$$\begin{aligned} U(\mu,\nu,\hat{x}) = &(\sin\mu + \mathrm{i}\cos\mu\ \exp[\,+\mathrm{i}(\nu+\pi/2)\,\tau_3\,]\ \hat{x}\cdot\vec{\tau}\ \exp[\,-\mathrm{i}(\nu+\pi/2)\,\tau_3\,])\\ &\times(\sin\mu - \mathrm{i}\cos\mu\ \hat{x}\cdot\vec{\tau})\,, \end{aligned} \tag{4.17}$$

where μ and ν range over $[-\pi/2,\pi/2]$ and describe a two-sphere, as does the unit three-vector $\hat{x}\equiv(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$. The map $U(\mu,\nu,\hat{x})$ is effectively defined on the smash product $S^2\wedge S^2$, since U is independent of $\hat{x}$ for $\mu=\pm\pi/2$ or $\nu=\pm\pi/2$ and independent of μ and ν for $\hat{x}=(0,0,1)$. (Note that the suspended Hopf map also plays a role in the physics of Skyrme solitons.[20])

With the map (4.17) in hand, it is possible to construct a noncontractible sphere (NCS) of static Yang–Mills–Higgs configurations and to obtain the corresponding nontrivial classical solution, the sphaleron S*, just as for the NCL and the sphaleron S of the previous subsection. The construction of S* is, however, rather subtle. Here, we only describe the four basic steps and refer the reader to Ref. 6 for more information.

First, we observe that the map (4.17) singles out the x^3 axis, which suggests the use of the cylindrical coordinates ρ, ϕ, and z, defined by $(x^1,x^2,x^3)=(\rho\cos\phi,\rho\sin\phi,z)$. Then, it is not difficult to construct a NCS of static SU(2) Yang–Mills–Higgs configurations, whose behavior at infinity is governed by the SU(2) matrix (4.17). Specifically, the NCS configurations can be written in terms of six axial functions $f_i(\rho,z)$ and $h_j(\rho,z)$, for $i=0,1,2,3$ and $j=1,2$, with appropriate boundary conditions [for example, $f_0(\rho,z)\to 1$ and $h_1(\rho,z)\to 1$ as $\rho^2+z^2\to\infty$]. The SU(2) gauge and Higgs field configuration of the NCS are by construction axially symmetric.

Second, the configuration at $\mu=\nu=0$ is also invariant under parity reflection and gives the maximum energy of the NCS. Moreover, it can be verified that this $\mu=\nu=0$ configuration, in terms of the six axial functions $f_i(\rho,z)$ and $h_j(\rho,z)$, provides a *self-consistent ansatz* for the SU(2) Yang–Mills–Higgs field equations. Concretely, this means that the ansatz reduces the field equations to precisely six partial differential equations (PDEs) for the six functions $f_i(\rho,z)$ and $h_j(\rho,z)$, with appropriate boundary conditions which trace back in part to the finite-energy condition. (This result agrees with the so-called principle of symmetric criticality,[21] which

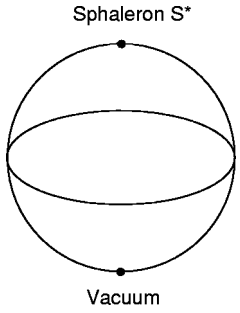

FIG. 4. Sphaleron S* on top of a noncontractible sphere in configuration space.

states that, under certain conditions, it suffices to consider variations that respect the symmetry of the ansatz.) The solution of these PDEs then determines the field configurations of the sphaleron S*. See Fig. 4 for a sketch of configuration space.

Third, the reduced field equations for the sphaleron S* can be solved numerically. For approximately vanishing quartic Higgs coupling constant ($\lambda/g^2 = 1/800$), the numerical solution of the six PDEs with the correct boundary conditions gives the following value for the energy:

$$E_{S^*} \approx 1.91 \times E_S \,, \tag{4.18}$$

where E_S denotes the corresponding energy of the sphaleron S [cf. Eq. (4.12) above]. In fact, the sphaleron S* is found to have the structure of a di-atomic molecule, binding together a sphaleron S and an "anti-sphaleron" $\overline{\text{S}}$. See Ref. 6 for a plot of the energy density and further discussion.

Fourth, the construction of S* via the NCS can be extended to the full $\text{SU}(2)\times\text{U}(1)$ theory of the electroweak standard model by the introduction of one more axial function, $f_4(\rho,z)$, with trivial boundary conditions at infinity. But for nonvanishing weak mixing angle θ_w, there are only preliminary numerical results for the sphaleron S* and it would be worthwhile to obtain accurate results over the full range of values of λ/g^2 and θ_w.

C. *Z*-string

Now consider static field configurations of the SU(2) Yang–Mills–Higgs theory (2.1) which are independent of one spatial coordinate, the z-coordinate, and have vanishing gauge potential in that direction, $A_z = 0$. In order to have finite total energy, the z-direction has to be compact and three-space is taken to be $\mathbb{R}^2 \times S^1$ instead of $\mathbb{R}^3$. Also, choose cylindrical polar coordinates (ρ,ϕ, z) and work in the polar gauge for which $A_\rho = 0$.

Since the energy density in a plane with fixed z has to be finite, the remaining gauge field component A_ϕ reduces to a pure-gauge configuration asymptotically,

$$g\, A_\phi \to -\,(\partial_\phi\, \omega)\;\omega^{-1}\,, \quad \text{as} \quad \rho \to \infty\,, \tag{4.19}$$

for a map $\omega: S^1 \to \text{SU}(2)$. Basically, this means that the plane $\mathbb{R}^2$ is compactified by adding the "circle at infinity."

It is possible to construct a noncontractible sphere of these field configurations by restricting the corresponding maps

$$U: S^2 \times S^1 \to \text{SU}(2)\,, \quad (\mu,\nu,\phi) \mapsto U(\mu,\nu,\phi)\,, \tag{4.20}$$

in such a way that they are effectively defined on the smash product $S^2 \wedge S^1 \sim S^3$. Specifically, the sphere is parametrized by μ and ν which take values in $[-\pi/2, +\pi/2]$. The rim of the (μ,ν)-square is identified and corresponds to a single point on S^2. The map U is restricted to be independent of ϕ if (μ,ν) lies on this rim and independent of (μ,ν) if $\phi = 0$.

An appropriate expression for the map (4.20) is given by[7]

$$U(\mu,\nu,\phi)=V(\mu,\nu,0)^{-1}\,V(\mu,\nu,\phi)\,, \tag{4.21a}$$

$$V(\mu,\nu,\phi)=z^1\,(-\mathrm{i}\tau_1)+z^2\,(-\mathrm{i}\tau_2)+z^3\,(-\mathrm{i}\tau_3)+z^4\,\mathbb{1}_2\,, \tag{4.21b}$$

$$\begin{pmatrix} z^1\\ z^2\\ z^3\\ z^4\end{pmatrix}=\begin{pmatrix} \sin\mu\\ \cos\mu\sin\nu\\ \cos\mu\cos\nu\sin\phi\\ \cos\mu\cos\nu\cos\phi\end{pmatrix}. \tag{4.21c}$$

Note that the factor $V(\mu,\nu,0)^{-1}$ in (4.21a) serves a dual purpose. First, it assures that the rim of the (μ,ν)-square is mapped to a single element, since $V(\mu,\nu,\phi)$ is independent of ϕ on this boundary. Second, it makes U independent of μ and ν if $\phi=0$.

For the two-dimensional SU(2) gauge and Higgs fields of the noncontractible sphere (NCS), we make the ansatz[7]

$$g\,A(\mu,\nu,\rho,\phi)=-f(\rho)\;\mathrm{d}U(\mu,\nu,\phi)\,U(\mu,\nu,\phi)^{-1}\,, \tag{4.22a}$$

$$\Phi(\mu,\nu,\rho,\phi)=\eta\,h(\rho)\,U(\mu,\nu,\phi)\begin{pmatrix}0\\1\end{pmatrix}, \tag{4.22b}$$

with parameters $|\mu|,|\nu|\leqslant\pi/2$. The polar functions f and h have the following boundary conditions:

$$\lim_{\rho\to 0} f(\rho)/\rho=0\,,\quad \lim_{\rho\to\infty} f(\rho)=1, \tag{4.23a}$$

$$\lim_{\rho\to 0} h(\rho)=0\,,\quad \lim_{\rho\to\infty} h(\rho)=1. \tag{4.23b}$$

But no point on this NCS corresponds to a vacuum configuration, since the Higgs field in Eq. (4.22b) vanishes at $\rho=0$ for all values of (μ,ν). Therefore, the point of the NCS at the boundary of the (μ,ν)-square must be connected to the vacuum by an additional line segment. The corresponding ansatz is simply

$$g\,A(\mu,\nu,\rho,\phi)=0\,, \tag{4.24a}$$

$$\Phi(\mu,\nu,\rho,\phi)=\eta\,(1-\sin[\mu\nu]+h(\rho)\sin[\mu\nu]\,)\begin{pmatrix}0\\1\end{pmatrix}, \tag{4.24b}$$

for $[\mu\nu]\equiv\max\{|\mu|,|\nu|\}>\pi/2$ with the parameter range of μ and ν extended to $[-\pi,+\pi]$. The set of configurations (4.21)–(4.24) is like a ''balloon'' which is tied to the ground by a rope.

The energy of the NCS has a global maximum at $\mu=\nu=0$. By minimizing this maximal energy with respect to the functions f and h, one finds the coupled differential equations

$$\rho\,f''-f'=\frac{1}{2}g^2\eta^2\,\rho\,h^2\,(f-1)\,, \tag{4.25a}$$

$$\rho^2\,h''+\rho\,h'=h\,(1-f\,)^2+2\lambda\,\eta^2\,\rho^2 h\,(h^2-1)\,, \tag{4.25b}$$

where the prime indicates a derivative with respect to ρ. The same differential equations, with boundary conditions (4.23), hold for the so-called Z-string,[22–24] which excites the Z boson and Higgs fields of the electroweak standard model.

The Z-string is thus the sphaleron on the NCS given by Eqs. (4.21)–(4.24); see Fig. 5. This particular sphere (balloon) in configuration space will be discussed further in Sec. VI C. Note,

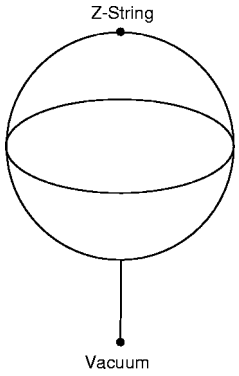

FIG. 5. Z-string on top of a noncontractible sphere (balloon) in configuration space.

finally, that the configurations of the NCS can also be embedded in the full $\mathrm{SU}(2)\times U(1)$ gauge theory of the electroweak standard model; see Ref. 7 for details and numerical results.

V. SPECTRAL FLOW

The classical field configurations of the previous section may serve as background fields for massless Dirac fermions, whose left-handed components form an isodoublet under the SU(2) gauge group and whose right-handed components are gauge singlets. The Dirac equation for the spinor $\Psi(x)$ reads in this case

$$(\mathrm{i}\not{D} - k\,(\Phi_M^\dagger P_L + \Phi_M P_R))\Psi = 0\,, \tag{5.1}$$

with the Yukawa coupling constant k, the Feynman slash notation $\not{D} \equiv \gamma^\mu D_\mu$, and the covariant derivative

$$D_\mu \Psi(x) \equiv [\,\partial_\mu + g A_\mu(x) P_L\,]\Psi(x)\,, \tag{5.2}$$

which shows that only the left-handed fermions interact with the SU(2) gauge field.

The left- and right-handed projectors are, as usual, defined by $P_L \equiv \frac{1}{2}(\mathbb{1} - \gamma_5)$ and $P_R \equiv \frac{1}{2}(\mathbb{1} + \gamma_5)$. With the Minkowski metric of Sec. II, the Dirac matrices obey the following Clifford algebra and Hermiticity conditions:

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\, g^{\mu\nu}\,, \qquad \gamma^{\mu\,\dagger} = \gamma^0 \gamma^\mu \gamma^0\,, \qquad \gamma_5 \equiv \mathrm{i}\,\gamma^0\gamma^1\gamma^2\gamma^3 = \gamma_5^\dagger\,. \tag{5.3}$$

(For the Euclidean metric, all Dirac matrices are chosen Hermitian, $\gamma^{\mu\,\dagger} = \gamma^\mu$.) The space–time manifold considered in this article is flat and there is no need to use the vierbeins (tetrads) explicitly.

The matrix Φ_M in (5.1) contains the two Higgs field components Φ_1 and Φ_2,

$$\Phi_M = \begin{pmatrix} \Phi_2^* & \Phi_1 \\ -\Phi_1^* & \Phi_2 \end{pmatrix}, \tag{5.4}$$

so that

$$\Phi_M \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \Phi\,. \tag{5.5}$$

For the Higgs vacuum with $A_\mu(x) = 0$ and $\Phi_M(x) = \mathrm{diag}(\eta, \eta)$, the effective fermion mass is given by $m = k\,\eta$.

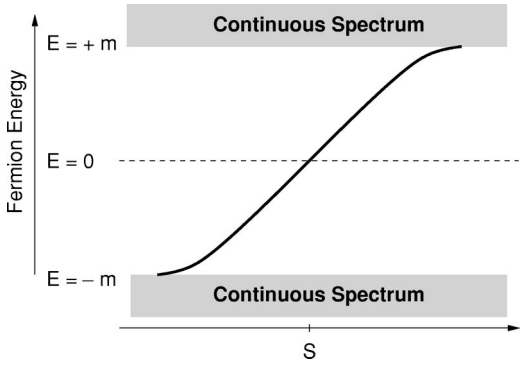

FIG. 6. Spectral flow for a path over the sphaleron barrier (cf. Fig. 3).

The model considered may serve as the starting point for a consistently renormalized quantum field theory with gauge group $SU(2)\times U(1)$ if we include three colors of left-handed quark isodoublets for each left-handed lepton isodoublet, so that the perturbative gauge anomalies[25–28] cancel between the quarks and the leptons.[29,30] (A similar cancellation occurs for the nonperturbative SU(2) anomaly[31] to be discussed in Sec. VI B.) But, for our purpose, it suffices to consider a *single* isodoublet of left-handed fermions, since the fermion isodoublets of the full theory behave identically.

The time-dependent solutions of the Dirac equation (5.1) are, however, not our main interest. Rather, we are interested in the eigenvalues E of the corresponding Dirac Hamiltonian,

$$H=-\mathrm{i}\gamma^0\gamma^m D_m+k\,\gamma^0(\,\Phi_M^\dagger P_L+\Phi_M P_R\,)\,, \tag{5.6}$$

where use has been made of the fact that $A_0=0$ for our gauge field configurations and the covariant derivative D_m, for $m=1,2,3$, has already been given in Eq. (5.2). The eigenvalues E are real, since the Dirac Hamiltonian H is Hermitian.

Now consider periodic one-parameter families (loops) of static background fields. The spectral flow invariant[32] is then defined as the number of eigenvalues that cross zero from below minus the number of eigenvalues that cross zero from above as the loop parameter varies over its range (in a prescribed direction). See, e.g., Ref. 33 for an elementary introduction to the concept of spectral flow.

Even if the spectral flow invariant vanishes, there may still be a nontrivial rearrangement (permutation) of the energy levels. We speak about ''spectral flow'' also in this case. (Mathematicians would perhaps say that there is no spectral flow if the spectral flow invariant is zero.) In addition, we will look for ''spectral flow'' in two-parameter families of background fields (which may be characterized by a different topological invariant).

A. Spectral flow for the sphaleron S

Consider the noncontractible loop (NCL) used in Sec. IV A to construct the sphaleron S, with parameter μ running from 0 to π. At the beginning of the loop ($\mu=0$) and at the end ($\mu=\pi$), the static background field (4.10) is the same vacuum configuration and the spectrum of the Dirac Hamiltonian (5.6) is purely continuous with a mass gap $2m$ according to the Higgs mechanism ($m\propto\eta$). For the sphaleron S at $\mu=\pi/2$, on the other hand, it has been shown[34–38] that the Dirac Hamiltonian H has a single normalizable eigenfunction with eigenvalue zero.

The overall picture, starting from $\mu=0$, is that a negative eigenvalue $E(\mu)$ of the Dirac Hamiltonian H rises above the negative continuous spectrum, crosses zero when the background fields pass the sphaleron barrier ($\mu=\pi/2$), and finally reaches the positive continuous spectrum for $\mu=\pi$. See Fig. 6 for a sketch and Ref. 38 for numerical results.

The nonvanishing spectral flow over the NCL is guaranteed by the Atiyah–Singer index theorem,[39] which relates the analytic index of the four-dimensional Dirac operator (the loop

parameter μ playing the role of an imaginary time) to the topological charge associated with the NCL. Further details will be given in Sec. VI A. Here, we only remark that the NCL gauge field (4.10), defined in Minkowski space, has essentially the same topology as the BPST instanton solution of Euclidean Yang–Mills theory.[40,41]

B. Spectral flow for the sphaleron S*

For the fermion behavior over the noncontractible sphere (NCS) through S*, we need to resort to more abstract reasoning, since no complete numerical or analytic solution has been obtained up till now.

First, consider massless Dirac fermions with *equal* gauge couplings for the right- and left-handed components. It has then been shown that there exist two fermion zero-modes of the four-dimensional Euclidean Dirac operator $i\not{D}_4$, one of each chirality, if the fermions are placed in the background of the constrained instanton I*.[42–44] [Note that a particular time slice through I* corresponds to the three-dimensional configuration of the S* sphaleron. For practical purposes, one may consider I* as a bound state of a BPST instanton I and an anti-instanton $\overline{\text{I}}$, just as the sphaleron S* may be viewed as a composite of a sphaleron S and an anti-sphaleron $\overline{\text{S}}$; see Eq. (4.18) and the lines below.]

Now the instanton I*, which depends on four Euclidean space–time coordinates, can be viewed as a path in configuration space which passes over the S* barrier. (In other words, this path is homotopic to a particular closed loop on the S*-NCS modulo gauge transformations; cf. Fig. 4.) The two zero-modes of $i\not{D}_4$ in the I* background, being time-dependent solutions of the Dirac equation (with imaginary time), can be calculated in the adiabatic approximation, where the state at time t is an eigenstate of the Dirac Hamiltonian with energy $E(t)$. The corresponding "phase factor" is given by

$$\exp\left(-\int_0^t \mathrm{d}t'\, E(t')\right). \tag{5.7}$$

From the normalizability of the zero-mode, it follows that $E(t)$ is positive for $t\to+\infty$ and negative for $t\to-\infty$.

With left- and right-handed chiralities, there are then two energy levels $E^{(1,2)}(t)$ crossing zero from below (these energy levels may, of course, be degenerate). In addition, there are two eigenvalues $E^{(3,4)}(t)$ which cross zero from above, so that the total spectral flow invariant is zero (note that the loop through S* over the NCS is contractible). For these last two eigenvalues, there are no zero-modes of $i\not{D}_4$ because the corresponding four-dimensional wave functions are not normalizable. Thus we have two pairs of levels which cross at zero energy, one left-handed pair and one right-handed pair. Returning to the Dirac Hamiltonian (5.6) with only left-handed fermions interacting with the SU(2) gauge fields, we have the spectral flow of the eigenvalues $E^{(1)}(t)$ and $E^{(3)}(t)$ as shown in Fig. 7.

Recently, numerical results[45] have been obtained for the eigenvalues of the $i\not{D}_4$ operator along a particular path over the I* barrier. It would be interesting to use similar methods to calculate the spectral flow related to S* and also to consider fermion representations other than isodoublet.

C. Spectral flow for the *Z*-string

Finally, we turn to the fermion behavior over the noncontractible sphere (NCS) with the Z-string at the top.[46] First, we choose a path on the NCS (4.21)–(4.24), which starts in the vacuum, passes over the Z-string and ends up in the vacuum.

To be concrete, we put $\nu=0$ in (4.21) and let μ run from $-\pi/2$ to $+\pi/2$. Such a loop is contractible and there is no net spectral flow to be expected (just as for the loop through S* considered in the previous subsection). What happens instead is that one negative eigenvalue $E^{(1)}(\mu,0)$ is raised from the negative continuous spectrum and one positive eigenvalue $E^{(2)}(\mu,0)$ is lowered from the positive continuous spectrum. Both eigenvalues meet at energy zero when the

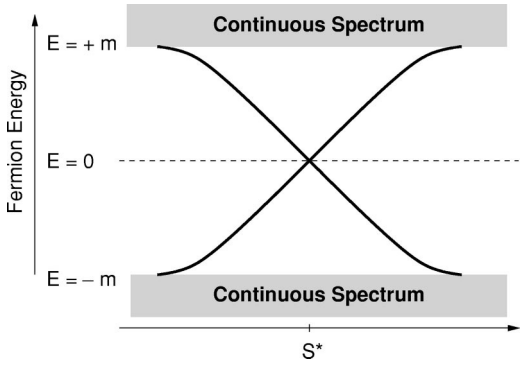

FIG. 7. Spectral flow for a path through the sphaleron S* (cf. Fig. 4).

background fields pass the Z-string configuration ($\mu=\nu=0$), cross and reach the opposite region of continuous eigenvalues (see the picture on the left in Fig. 8). The fermion zero-modes of the Z-string have been studied in Refs. 47 and 48.

We can also consider the behavior of the Dirac eigenvalues over the whole two-parameter family (4.22). Plotted over the (μ,ν)-square, the eigenvalues $E(\mu,\nu)$ form a double cone meeting at $\mu=\nu=0$ (see the picture on the right in Fig. 8).

VI. ANOMALIES

In this section, we review the relation between the sphalerons presented in Sec. IV and so-called anomalies. The connection between sphalerons and anomalies is precisely the spectral flow discussed in Sec. V.

A. Chiral anomaly and fermion number violation

The chiral U(1) anomaly, which turns out to be related to the sphaleron S, eliminates a rigid U(1) symmetry of the classical action, viz., chiral invariance. This anomaly can be found in theories with *massless* fermions, for which there is a classical Ward identity

$$\sum_f \left(\frac{\delta\Gamma_{\rm cl}}{\delta\Psi_f}\ \delta\Psi_f - \delta\bar{\Psi}_f\ \frac{\delta\Gamma_{\rm cl}}{\delta\bar{\Psi}_f} \right) = \partial^\mu j^5_\mu\,, \tag{6.1}$$

where $\Gamma_{\rm cl}$ is the classical action and $\Psi_f(x)$ denotes a Dirac fermion field, with f labeling the different flavors (fermion species). The rigid chiral transformation of the fermion fields is given by

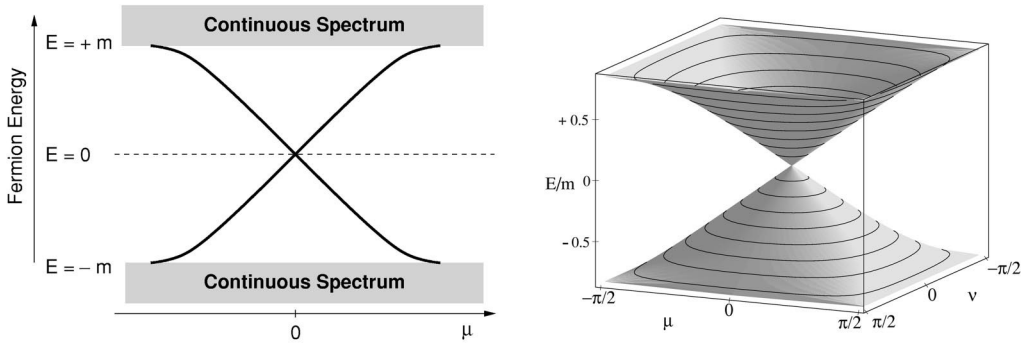

FIG. 8. Spectral flow over the noncontractible sphere (NCS) through the Z-string (cf. Fig. 5). In the picture on the left, the NCS parameter ν is held fixed at the value 0 and μ is varied. In the picture on the right, the Dirac eigenvalues are shown for the NCS patch $|\mu|,|\nu|\leqslant\pi/2$.

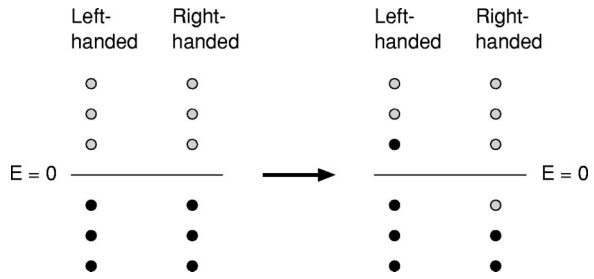

FIG. 9. Opposite spectral flow for left- and right-handed fermions, which leads to the creation of two units of chiral charge. Filled states are drawn black, empty states gray.

$$\delta\Psi_f(x) = \mathrm{i}\gamma_5\,\Psi_f(x)\,, \quad \delta\overline{\Psi}_f(x) = \overline{\Psi}_f(x)\,\mathrm{i}\gamma_5\,. \tag{6.2}$$

Since the left-hand side of (6.1) vanishes for solutions of the classical equations of motion, the current $j^5_\mu(x) \equiv \Sigma_f \overline{\Psi}_f(x)\,\gamma_5\gamma_\mu\Psi_f(x)$ is conserved classically. This implies that the chiral charge $Q_5 \equiv \int \mathrm{d}^3x\, j^5_0(x)$ does not change with time ($t \equiv x^0$),

$$\left.\frac{\mathrm{d}Q_5}{\mathrm{d}t}\right|_{\text{classical}} = 0\,. \tag{6.3}$$

Now suppose that the SU(2) gauge field couples equally to left- and right-handed fermions in the fundamental representation [as is the case for the SU(3) gauge field which is believed to be responsible for quark confinement in the standard model]. Then the spectral flow for a path over the sphaleron S with unit winding number is as shown in Fig. 9: for each isodoublet of fermions a left-handed state crosses zero from below and a right-handed one crosses zero from above. (Essentially the same type of spectral flow has been found[49] in the Schwinger model, i.e., two-dimensional quantum electrodynamics with a massless Dirac fermion.) In the Dirac-sea picture of the second-quantized vacuum, this means that a pair of fermions is created from an initial vacuum state, namely one chiral fermion and one chiral antiparticle corresponding to a hole in the Dirac sea of antichiral negative-energy states. Hence, the total chiral charge Q_5 *changes* by two units per isodoublet, which contradicts the classical conservation equation (6.3).

This result is supported by the Atiyah–Singer index theorem[39] for the four-dimensional chiral Dirac operator (see, e.g., Refs. 50–52). For N isodoublets, the relation between the change of chiral charge and the appropriate characteristic of the background gauge field is simply the integrated version of the perturbative Ward identity for the chiral current containing the Adler–Bell–Jackiw anomaly,[25,26]

$$\sum_{f=1}^{N}\left(\frac{\delta\Gamma}{\delta\Psi_f}\;\delta\Psi_f - \delta\overline{\Psi}_f\;\frac{\delta\Gamma}{\delta\overline{\Psi}_f}\right) = [\,\partial^\mu j^5_\mu\,]\cdot\Gamma + \frac{g^2N}{8\,\pi^2}\,[\,\mathrm{tr}\,\widetilde{F}_{\mu\nu}F^{\mu\nu}]\cdot\Gamma\,, \tag{6.4}$$

where Γ is now the fully quantized vertex functional and the dot denotes an operator insertion.

The anomalous term in Eq. (6.4) includes the Pontryagin density

$$q(x) \equiv -\frac{g^2}{16\,\pi^2}\,\mathrm{tr}\,\widetilde{F}_{\mu\nu}(x)\,F^{\mu\nu}(x)\,, \tag{6.5}$$

with $\widetilde{F}_{\mu\nu} \equiv \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}$. The integral of this density over the space–time manifold M is a *topological invariant* called the Pontryagin index,

$$Q \equiv \int_M \mathrm{d}^4x\;\; q(x)\,. \tag{6.6}$$

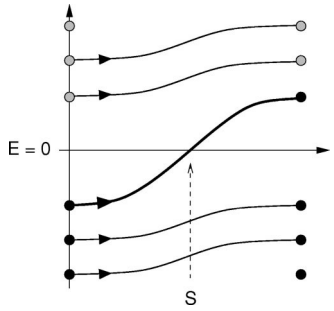

FIG. 10. Spectral flow in the electroweak standard model, where only left-handed fermions interact with the SU(2) gauge fields. S denotes the sphaleron, which has a single fermion zero-mode. The spectral flow leads to a change of fermion number between initial and final states (see text).

For compact space–time manifolds M, the Pontryagin index is an integer number and is also called the winding number or topological ''charge'' (hence, the notation Q).

Next, turn to the simplified version of the electroweak standard model, as described in Secs. II and V. Here, the fermion fields are fundamentally massless, even though they behave as massive particles in the Higgs vacuum. More importantly, the gauge field now couples only to the left-handed parts of the fermion fields; cf. Eqs. (5.1) and (5.2). Hence, the spectral flow for a single fermion flavor is made up of only one state which crosses zero from below. This implies that *fermion number conservation* is violated.[53,54] See Fig. 10 and compare with Fig. 9. (It is, of course, important to define carefully what is meant by ''the fermion number'' of a given state;[55–57] see also the discussion in the last three paragraphs of this subsection.)

The map U given in Sec. IV A essentially provides a map $S^3 \to S^3$, characterized by the topological charge $|Q|=1$. The above considerations can be generalized to other (integer) values of Q and to a model with N_{fam} families of quarks and leptons. The sum of baryon number B and lepton number L is then found to be nonconserved,[53]

$$\Delta(B-L)=0\,, \quad \Delta(B+L)=2\,N_{\text{fam}}\,Q\,, \tag{6.7}$$

where ΔB denotes the change of baryon number between initial and final states and similarly for ΔL.

As explained at the end of Sec. IV A, the NCL can be transformed into a path connecting two topologically distinct vacua in one-point-compactified three-space. The general form of such a vacuum is given by a static pure-gauge configuration,

$$g\,A=-\mathrm{d}\chi\,\chi^{-1}\,, \quad \Phi=\eta\,\chi\begin{pmatrix}0\\1\end{pmatrix}, \tag{6.8}$$

for a map $\chi:\mathbb{R}^3\to \mathrm{SU}(2)$ which approaches $\mathbb{1}_2$ at spatial infinity. The homotopy class to which χ belongs is characterized by the integer *Chern–Simons number*

$$N_{\mathrm{CS}}[\,\chi\,]=-\frac{1}{24\,\pi^2}\int \mathrm{d}^3x\;\epsilon^{klm}\;\mathrm{tr}\{(\partial_k\chi\,\chi^{-1})\,(\partial_l\chi\,\chi^{-1})\,(\partial_m\chi\,\chi^{-1})\}\,. \tag{6.9}$$

The topological charge Q of the map $\omega(\mu,r,\theta,\phi)$, as discussed in the last two paragraphs of Sec. IV A, is then the difference of the Chern–Simons numbers of the vacua at the start and end of the associated path,

$$Q=\Delta N_{\mathrm{CS}}\equiv N_{\mathrm{CS}}[\,\omega(\pi,r,\theta,\phi)\,]-N_{\mathrm{CS}}[\,\omega(0,r,\theta,\phi)\,]\,. \tag{6.10}$$

Of course, it is also possible to map the μ-interval $[0,\pi]$ on the time interval $[-\infty,+\infty]$.

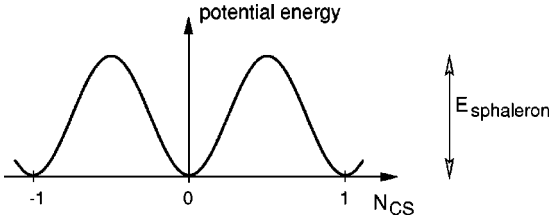

FIG. 11. Potential energy over a slice of configuration space, parametrized by the Chern–Simons number N_{CS}. The height of the energy barrier between topologically different vacua ($N_{\mathrm{CS}}=n\in\mathbb{Z}$) is set by the sphaleron S, which appears in different gauge copies ($N_{\mathrm{CS}}=\frac{1}{2}+n$, for $n\in\mathbb{Z}$). This figure essentially "unwraps" the loop of Fig. 3.

The sphaleron now corresponds to an energy barrier between these vacua, as sketched in Fig. 11. The transition between different vacua can, for example, take place by tunneling *through* the sphaleron barrier[53,54] or by passing *over* the barrier due to a thermal fluctuation of the fields.[5,58] Especially the latter mechanism is expected to contribute significantly to fermion-number-violating processes in the early universe (see, e.g., Refs. 9 and 10).

The rate of fermion-number-violating processes at relatively low energies ($E\ll E_{\mathrm{S}}\approx 10$ TeV) can be calculated from the Euclidean path integral.[54,59] But for a reliable discussion of these processes at high energies ($E\gtrsim E_{\mathrm{S}}$) it is advisable to remain in Minkowski space–time. The problem, then, is that the compactification of four-space which we used as the starting point of our topological considerations is not really physically sensible for Minkowski space–time. The topological charge Q, in particular, need not be an integer quantity in Minkowski space–time. The crucial point here is the role of *energy conservation* for background fields that solve the equations of motion; see, e.g., Ref. 60. The general question of which type of gauge field leads to nontrivial spectral flow remains unanswered for the moment.

There exists, however, a result for *strongly dissipative* SU(2) gauge fields.[55–57] In this case, the spectral flow is given by the difference in winding numbers of the asymptotic vacuum configurations for $t\to\pm\infty$. Roughly speaking, this coincides with the previous result in Euclidean space–time, namely Eq. (6.10) inserted into Eq. (6.7).

For the case of spherically symmetric fields, there is also a result for *generic* (i.e., nondissipative) gauge fields,

$$\Delta(B-L)=0\,,\quad \Delta(B+L)=2\,N_{\mathrm{fam}}\,(\Delta N_{\mathrm{winding}}+\Delta N_{\mathrm{twist}})\,\big|_{\mathrm{spher.\ symm.}}\,. \tag{6.11}$$

The change of $B+L$ is now determined by two integers. The first, $\Delta N_{\mathrm{winding}}$, again corresponds to Eq. (6.10). But the second, $\Delta N_{\mathrm{twist}}$, is an entirely new characteristic of spherically symmetric SU(2) gauge fields, which is related to the asymptotic behavior of the solutions of a (nonlinear) Riccati equation embedded in the (linear) zero-energy Dirac equation.[61] The integer $\Delta N_{\mathrm{twist}}$ is zero for strongly dissipative SU(2) gauge fields. See Ref. 62 for further discussion of the issues involved.

B. Witten's global gauge anomaly

The global SU(2) gauge anomaly, which turns out to be related to the sphaleron S*, differs from the case discussed in the previous subsection in that not just a symmetry of the theory is eliminated but the theory itself.

As mentioned in Sec. V B, the crossing of energy levels for paths over the S* barrier is related to the existence of two normalizable zero-modes of the four-dimensional Euclidean Dirac operator $i\not{D}_4$, one of each chirality. The noncontractible sphere of three-dimensional configurations can also be viewed as a noncontractible loop of four-dimensional configurations. Furthermore, as explained at the end of Sec. IV A, it is possible to pass from a *loop* of gauge field configurations in the radial gauge to a *path* of gauge field configurations without the radial gauge condition. The resulting path has topologically inequivalent vacua at the start and at the end.

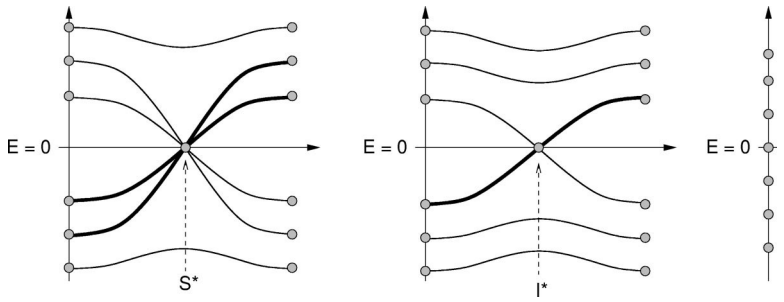

FIG. 12. Left: sketch of the eigenvalues of the Dirac Hamiltonian for a particular path over the S* noncontractible sphere (the theory considered has both left- and right-handed fermions interacting with the SU(2) gauge fields, which is not the case in Fig. 7). Middle: eigenvalues of $i\not{D}_4$ for the corresponding noncontractible loop through the constrained instanton I*. Right: eigenvalues of $i\not{D}_5$ for the corresponding five-dimensional configuration. Each path with an energy level crossing zero from below (thick line) corresponds to a normalizable fermion zero-mode one dimension higher. The sphaleron S* has four fermion zero-modes, the constrained instanton I* two, and the five-dimensional configuration one.

Now consider the change of eigenvalues of $i\not{D}_4$ along such a path. Since for one ''point'' of the path (i.e., the I*-configuration) there are known zero-modes,[44] it is to be expected that some level crossing is occurring also here.

That this is indeed the case has been shown in Ref. 31 by increasing the dimension once more. The one-parameter family of four-dimensional Dirac operators can also be considered as a single five-dimensional one. (In other words, the whole NCS serves as a single background configuration.) It then follows from the so-called mod-2 Atiyah-Singer index theorem[63] that the corresponding five-dimensional Dirac operator has a normalizable zero-mode. For $i\not{D}_4$, this implies that an eigenvalue is crossing zero from negative to positive values as the path is traversed. Simultaneously, there is a second eigenvalue which passes from positive to negative values. This discussion is summarized in Fig. 12, which also gives the corresponding spectral flow in three dimensions. (The mod-2 index theorem guarantees only an odd number of zero-modes for the five-dimensional configuration, but for simplicity we have assumed there is just one. See Ref. 45 for numerical results and further discussion.)

Witten also argued that the spectral flow of $i\not{D}_4$ leads to a global gauge anomaly.[31] In the Euclidean path integral of SU(2) Yang–Mills theory with a single isodoublet of Weyl fermions, there effectively appears a square root of the Dirac determinant,

$$\int \mathcal{D}A_\mu \quad \sqrt{\det i\not{D}_4} \quad \exp\left(\frac{1}{2} \int d^4x \ \mathrm{tr} F_{\mu\nu} F^{\mu\nu} \right), \tag{6.12}$$

if one recalls that two Weyl fermions of opposite chiralities make a single Dirac fermion.

The Dirac determinant in Eq. (6.12) depends on the background gauge fields $A_\mu(x)$ and its square root can be defined as the product of the positive eigenvalues [starting from a given gauge field configuration, say $A_\mu(x)=0$]. The above considerations then show that for a particular *continuous* variation of the gauge fields we end up with gauge fields, which are related to the starting configuration by a large gauge transformation and which have a $\sqrt{\det i\not{D}_4}$ of opposite sign (one positive eigenvalue having become negative; cf. the middle picture of Fig. 12). In the path integral, one has to integrate over all gauge fields (taking out the infinite factor due to gauge invariance afterwards). Hence, for every contribution $\sqrt{\det i\not{D}_4}$ there is also a contribution $-\sqrt{\det i\not{D}_4}$ arising from the gauge-transformed background fields. This implies that the path integral (6.12) vanishes.

More precisely, the path integral over the gauge fields is not well defined, because there is no satisfactory way to restrict the integration over the gauge fields so that a single Weyl isodoublet

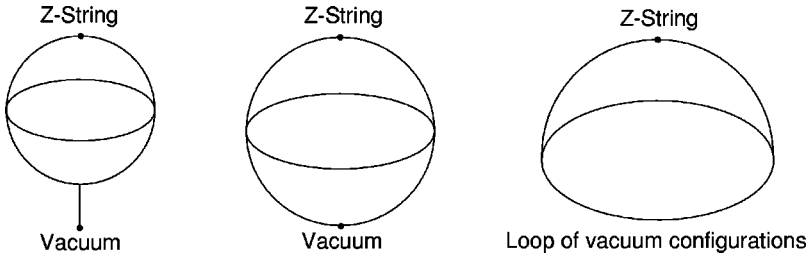

FIG. 13. Z-balloon, Z-sphere and Z-disc.

gives a continuous gauge-invariant contribution. This, then, is the Witten anomaly, which can also be proven without the mod-2 Atiyah–Singer index theorem but with the perturbative Bardeen anomaly instead.[64,65]

C. Z-string global gauge anomaly

Just as for the Witten anomaly and the S* sphaleron of the previous subsection, there exists a global gauge anomaly related to the Z-string sphaleron.[46] In order to explain this anomaly, we need a modified noncontractible sphere (NCS), obtained by continuous deformation of the balloon as given in Sec. IV C. This modification has the advantage of being a real sphere, that is, without degenerate points. The modified NCS still has one point corresponding to the vacuum and one point corresponding to the Z-string (see the picture in the middle of Fig. 13).

For the modified NCS, the z-independent SU(2) gauge field is in the polar gauge $A_\rho = 0$. But like the case of the sphalerons S and S*, it is possible to relax the polar gauge condition and to demand instead that the vacuum reached for $\rho \to \infty$ is the trivial one. Then one ends up with a disc of configurations with a loop of pure-gauge configurations on the boundary (see the picture on the right of Fig. 13). Considering the compactified radial coordinate ρ to be a polar angle θ, the fields are effectively defined on a sphere S^2. The loop of vacuum configurations on this two-sphere, restricted to the smash product $S^1 \wedge S^2$, corresponds to a nontrivial element of the homotopy group $\pi_3(S^3)$.

We keep this in mind for later and turn to the eigenvalues of the four-dimensional Euclidean Dirac operator $i\not{D}_4$, where the time-dependent background fields are taken to be paths over the Z-disc, with the start and end point (not necessarily the same) lying on the rim of vacuum configurations. For any such path passing through the Z-string, we know from Sec. V C that $i\not{D}_4$ has a single normalizable zero-mode corresponding to the eigenvalue of the Dirac Hamiltonian which crosses zero from below.

Now consider a particular family of operators $i\not{D}_4$ corresponding to a family of paths over the Z-disc, which starts from a constant path corresponding to a point on the rim of the disc, passes through a path via the Z-string, and ends up in a pure vacuum path formed by the boundary of the disc (see Fig. 14, where the Z-disc of Fig. 13 has been flattened). This family of four-dimensional Dirac operators sweeps over the whole Z-disc and we expect that there is spectral flow corresponding to the winding number of the underlying map $S^3 \to S^3$. In our case, this means that a single eigenvalue of $i\not{D}_4$ crosses zero. The zero crossing can be expected to occur for the path labeled (3) in Fig. 14.

Like the case of the Witten anomaly in Sec. VI B, this prevents us from defining the square root of the fermion determinant as a continuous gauge-invariant function of the bosonic background fields. Note that our path of four-dimensional configurations begins in a time-independent, topologically trivial vacuum and ends up in a gauge-transformed, time-dependent and topologically nontrivial one.

It is particularly interesting to see how this global gauge anomaly manifests itself in the space of time-independent fermion states. Since the Dirac Hamiltonian is a *real* Hermitian operator, we may choose real energy-eigenstates. Concretely, look at the one-dimensional subspace spanned by

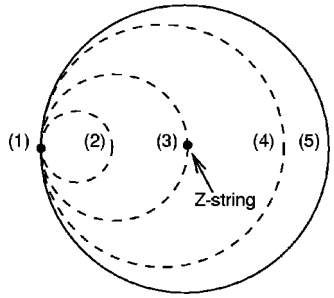

FIG. 14. Five closed loops on the Z-disc (cf. Fig. 13). Loop (1) corresponds to a single point on the boundary, loop (3) passes through the Z-string, and loop (5) consists of the whole boundary of the disc.

the eigenstate which crosses zero from below in the picture on the left in Fig. 8. For the background fields, we use an arbitrary loop on the Z-disc, which circumnavigates the Z-string exactly once and which is parametrized by $\alpha \in [0,2\pi]$. Then the energy eigenstate defines a *real* line bundle over S^1.

It has been shown in Ref. 46 that this bundle is, in fact, the Möbius bundle. A normalized eigenstate $|\Phi(0)\rangle$ transported around the loop ends up as $|\Phi(2\pi)\rangle = -|\Phi(0)\rangle$; see Fig. 15. The phase factor found is determined by the Berry phase for adiabatic transport.[66] The Berry phase π (mod 2π) is of topological origin and does not change under continuous deformation of the loop, as long as the loop of configurations does not touch the fermion degeneracy ''point'' corresponding to the Z-string. This observation also shows that the boundary of the Z-disc (Fig. 13) is a noncontractible loop of vacuum configurations, since the real Berry phase factor -1 on it cannot be continuously changed to $+1$.

The variation of the eigenstate along the rim of the Z-disc defines a projective action of the gauge group on the fermionic matter. There is then a global gauge anomaly, because it is impossible to define a real, continuous, and proper (i.e., nonprojective) representation of the local gauge group on the fermion states. Since the vacuum of quantum field theory is the Dirac sea with all negative-energy eigenstates filled, this also means that the second-quantized vacuum state acquires the Berry phase factor -1. See Sec. 6 of Ref. 46 for further discussion. (We take the opportunity to correct a slip of the pen. In the last sentence of Footnote 6 in Ref. 46, the words ''and vice versa'' must be deleted.)

A similar interpretation of the Witten anomaly in terms of a Berry phase has been given in Ref. 67. There is, however, a crucial difference between the Z-string global gauge anomaly and the Witten anomaly. For the Z-string anomaly, namely, there *does* exist a local counterterm in the action which restores gauge invariance, but at the price of violating Lorentz and CPT invariance.[68] More generally, if gauge invariance is enforced, there appears a new anomaly, the so-called CPT anomaly (see Refs. 69 and 70 for the main result and Ref. 71 for a review).

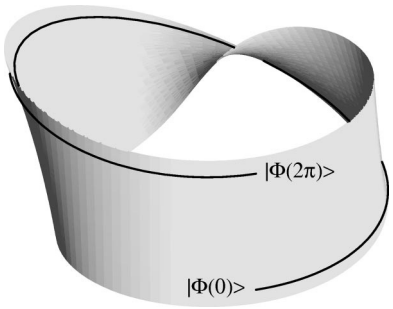

FIG. 15. Möbius bundle structure of the gauge orbit, with loop parameter $\alpha \in [0,2\pi]$. The line represents a normalized real eigenstate $|\Phi(\alpha)\rangle$ of the Dirac Hamiltonian, with $|\Phi(2\pi)\rangle = -|\Phi(0)\rangle$.

VII. CONCLUSION

The space of finite-energy three-dimensional field configurations of SU(2) Yang–Mills–Higgs theory (in short, configuration space) has nontrivial topology,[3,4] which leads to the existence of a new type of classical solutions, the so-called sphalerons. Sphalerons are unstable static finite-energy solutions of the classical field equations, whereas solitons are stable solutions.

In Sec. IV, we have explained the topology behind the S, S*, and Z-string sphalerons[5–7] of the SU(2) Yang–Mills–Higgs theory (2.1). Precisely this theory appears in the electroweak standard model of elementary particle interactions.[8] Knowledge of these classical solutions may, therefore, be of great importance to physics.

Adding chiral fermions to the SU(2) Yang–Mills–Higgs theory, the nontrivial topology of configuration space makes itself felt by the occurence of spectral flow,[32] as discussed in Sec. V. In turn, the general phenomenon of spectral flow is related to the possible existence of anomalies which invalidate certain properties of the classical theory, as discussed in Sec. VI.

The spectral flow over a noncontractible loop through the sphaleron S is related to the chiral U(1) anomaly,[25,26] which corresponds to a breakdown of baryon and lepton number conservation in the electroweak standard model.[53] The spectral flow through the S* and Z-string sphalerons does *not* lead to a global SU(2) gauge anomaly,[31,46] because the electroweak standard model has an *even* number of chiral isodoublets. Still, there is nontrivial spectral flow (more precisely, spectral rearrangement) over configuration space, but its physical implications remain to be clarified (cf. Refs. 44 and 69). Indeed, we need a better understanding of the role of configuration space topology in concrete physical problems, such as the behavior of elementary particle fields at high energies or temperatures.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 8 AUGUST 2003

Monopoles, affine algebras and the gluino condensate

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(Received 28 November 2002; accepted 9 April 2003)

We examine the low-energy dynamics of four-dimensional supersymmetric gauge theories and calculate the values of the gluino condensate for all simple gauge groups. By initially compactifying the theory on a cylinder we are able to perform calculations in a controlled weakly coupled way for a small radius. The dominant contributions to the path integral on the cylinder arise from magnetic monopoles which play the role of instanton constituents. We find that the semi-classically generated superpotential of the theory is the affine Toda potential for an associated twisted affine algebra. We determine the supersymmetric vacua and calculate the values of the gluino condensate. The number of supersymmetric vacua is equal to c_2, the dual Coxeter number, and in each vacuum the monopoles carry a fraction $1/c_2$ of topological charge. As the results are independent of the radius of the circle, they are also valid in the strong coupling regime where the theory becomes decompactified. For gauge groups SU(N), SO(N) and USp($2N$) our results for the gluino condensate are in precise agreement with the ''weak coupling instanton'' expressions (and not with the ''strong coupling instanton'' calculations). For the exceptional gauge groups we calculate the values of the gluino condensate for the first time. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1586477]

I. INTRODUCTION AND SUMMARY OF RESULTS

The goal of this article is to provide new calculations of the values of the gluino condensate $\langle \mathrm{tr}\,\lambda^2 \rangle$ in four-dimensional $\mathcal{N}=1$ supersymmetric Yang-Mills theory for all the simple gauge groups. Our approach is based on the idea[1] that when the space-time is partially compactified on the cylinder $\mathbb{R}^3 \times S^1$, magnetic monopoles play the role of instanton constituents, directly contribute to the path integral and completely determine the values of the gluino condensate. Our results for the gluino condensate are summarized in Table I and a universal formula in terms of Lie algebra data is given in (56). For classical gauge groups our results are in precise agreement with the known expressions derived in the ''weak-coupling instanton'' approach in Refs. 2–5. For the exceptional gauge groups the condensates are calculated for the first time.

It is somewhat of a miracle that some features of gauge theories which have supersymmetry can be understood exactly. Sometimes this success arises from viewing these theories as being embedded in string theory, a classical example being the duality of Maldacena.[6] Generally, however, we can make use of the fact that supersymmetry leads to very restrictive Ward identities, giving rise to powerful holomorphy properties (see the review in Ref. 7). Regarding this later point, the full functional form of certain correlators is fixed up to an overall constant. Sometimes these correlators have a dependence on the couplings which can be identified with specific gauge theory configurations, in particular with instantons, but in other cases this is not so.[8] In the former case, it is tempting to suppose that a semi-classical instanton calculation will yield the value of the correlator. In particular, we have in mind multi-point functions of the gluino operator $\mathrm{tr}\,\lambda^2$ in $\mathcal{N}=1$ supersymmetric gauge theory. It is our thesis that one must be very careful in applying a semi-classical analysis to a strongly-coupled theory and such calculations will only be correct if

TABLE I. The values of the gluino condensate in the Pauli-Villars scheme (2).

Gauge group	$\langle \mathrm{tr}\,\lambda^2\rangle/(\Lambda^3 16\pi^2)$
SU(N)	1
SO(N)	$2^{4/(N-2)-1}$
USp($2N$)	$2^{1-2/(N+1)}$
G_2	$2^{-1/2}3^{1/4}$
F_4	$2^{-1/9}3^{-1/3}$
E_6	$2^{-1/2}3^{-1/4}$
E_7	$2^{-7/9}3^{-1/3}$
E_8	$2^{-13/15}3^{-2/5}5^{-1/6}$

they are performed in a weakly-coupled phase, where semi-classical methods are rigorously justified. It is then possible to infer the value of the correlator in a strongly-coupled phase, if that phase is continuously connected to the weakly-coupled phase by using holomorphicity. It was the misuse of a semi-classical analysis directly in a strongly-coupled phase that led to the gluino condensate puzzle.

This famous puzzle is the inconsistency between two conceptually different approaches followed in the early literature of calculating the gluino condensate in pure $\mathcal{N}=1$ supersymmetric gauge theory. In the first methodology[9–11]—and in the present context the ''suspect'' method, because it involves a semi-classical analysis directly in the strongly-coupled confining phase of the gauge theory—the so-called strong-coupling instanton (SCI) approach, the gluino condensate $\langle \mathrm{tr}\,\lambda^2\rangle$ is determined via an explicit one-instanton calculation of a certain multi-point function of $\mathrm{tr}\,\lambda^2$. Cluster decomposition arguments are then invoked in order to extract the one-point function $\langle \mathrm{tr}\,\lambda^2\rangle$. In the second methodology,[2] the so-called weak-coupling instanton (WCI) approach—and for us the safe method—the calculation is performed with additional matter fields whose presence ensures that the non-Abelian gauge group is broken and the theory is in a weakly-coupled Higgs phase and a ''constrained instanton'' calculation is justified.[12] Holomorphicity is then used to decouple the matter fields and to flow continuously to the confining phase of the original gauge theory. As is well known, these two methods give two different values for the gluino condensate:[2,13,11,5]

$$\left\langle \frac{\mathrm{tr}\,\lambda^2}{16\pi^2}\right\rangle_{\mathrm{SU}(N)} = \begin{cases} \dfrac{2}{[(N-1)!(3N-1)]^{1/N}}\Lambda^3 & \text{SCI,} \\ \Lambda^3 & \text{WCI.} \end{cases} \tag{1}$$

[These results are quoted for an SU(N) gauge theory in the Pauli-Villars scheme with Λ being the corresponding dimensional transmutation scale of the theory defined in Eq. (2) below.] The reason for the discrepancy between the SCI and WCI calculations, as well as the question as to which is correct, has been a long-standing controversy.[2,11,14,15] This controversy was reexamined in Ref. 16 using recently developed multi-instanton methods,[17,18] for a comprehensive review see Ref. 19. By evaluating the k-instanton contribution to gluino correlation functions in the large number of colors limit it was shown that an essential step in the SCI calculation of the gluino condensate, namely the use of cluster decomposition in the instanton sector, is actually invalid. The central idea pursued in Ref. 1 and in the present paper is that there are additional configurations which contribute to the gluino condensate implying that the SCI calculation only gives part of the answer. The existence of other contributions to multi-point correlators of $\mathrm{tr}\,\lambda^2$, which are non-instantonic invalidates the application of cluster decomposition to a purely instantonic contribution.

In Ref. 1 we provided an alternative way to deform the theory in order to connect the confining phase continuously to a weak-coupled phase: in this case a Coulomb rather than a Higgs phase. The idea is to consider the theory partially compactified on the cylinder $\mathbb{R}^3\times S^1$. In this scenario, the gauge field can have a non-trivial Wilson loop around the circle which acts like an

adjoint-valued Higgs field breaking the gauge group to its maximal Abelian subgroup and so the theory is in a Coulomb phase. For small enough radius, the resulting theory is arbitrarily weakly coupled and the gluino condensate can be reliably calculated. It is then argued, based on the usual argument of holomorphy, that the result is actually independent of the radius and is therefore easily extrapolated to the confining phase where the radius goes to infinity and the theory becomes decompactified.

However, there is a significant bonus in this scenario: the additional configurations missing in the instanton calculation can explicitly be identified at small radius with BPS monopoles in the gauge theory with the component of the gauge field around the circle playing the role of a Higgs field. However, we should point out that this in no way means that BPS monopoles quantitatively describe the physics in the decompactification limit. In this scenario, the one-point function $\langle \mathrm{tr}\,\lambda^2\rangle$ directly receives a semi-classical contribution from single monopoles, unlike the SCI situation in $\mathbb{R}^4$, where, as described above, only multi-functions receive contributions. (There are precisely 2 gluino zero modes in the single-monopole background. These are supersymmetric fermion zero modes of the monopole. In distinction with instanton configurations on $\mathbb{R}^4$, there are no, e.g., superconformal gluino zero modes in the monopole background. In fact, classical conformal invariance of the theory is explicitly broken by the compactification on the cylinder.) The monopoles consequently carry fractional topological charge. Hence, the theory on the cylinder uncovers a very pleasing picture of instanton constituents, or instanton partons, that were argued to play an important role in confinement of ordinary QCD.[20–24] The fact that an instanton configuration on the cylinder is actually a composite of fundamental monopoles has been the subject of number of earlier works.[25–30] These generalize the notion of a periodic instanton, or "caloron,"[31–33] to the case when the gauge field has a non-trivial Wilson line around the circle. It is only in this case that the instanton constituents can be pulled apart and identified with monopoles. It turns out that in ordinary QCD the Wilson line of the gauge field around the circle is energetically favored to vanish: in this case the monopoles have no role to play in the physics. On the contrary, as we shall explicitly show, in $\mathcal{N}=1$ supersymmetric gauge theories, a non-trivial superpotential is generated by the monopoles whose supersymmetric vacua have a non-trivial value for the Wilson line and hence monopole effects are important. Other recent references which consider supersymmetric gauge theories on a cylinder and monopole effects are to be found in Refs. 34–36.

In $\mathcal{N}=1$ supersymmetric gauge theories, the first coefficient of the β-function is $b_0=3c_2$, where c_2 is the dual Coxeter number of the gauge group listed in the table in Appendix A. We will use a definition of the dynamical scale Λ in the Pauli–Villars renormalization scheme via the RG-invariant exact relation

$$\Lambda^3=\mu^3\frac{1}{g^2(\mu)}\exp\frac{2\pi i\tau(\mu)}{c_2}. \tag{2}$$

[If one chooses to use instead another exact definition of Λ,[15] more in line with standard QCD conventions, $\tilde{\Lambda}^3=(\mu^3 16\pi^2/3c_2g^2)\exp(-8\pi^2/c_2g^2)$, then the values of the gluino condensate in Table I have to be adjusted accordingly.] Here μ is the Pauli–Villars regulator mass and τ is the usual complexified coupling incorporating both the gauge coupling constant g and the theta angle ϑ:

$$\tau=\frac{\vartheta}{2\pi}+\frac{4\pi i}{g^2}\,. \tag{3}$$

The article is organized in the following way. In Sec. II we consider, in general terms, the effect of compactifying the $\mathcal{N}=1$ gauge theory on $\mathbb{R}^3\times S^1$. In Sec. III we discuss the various semi-classical configurations that can contribute to the functional integral and explain the relation between monopoles and instantons on the cylinder. Regarding this point, our considerations in this article are purely field-theoretical; for an elegant D-brane discussion of the SU(N) dynamics on $\mathbb{R}^3\times S^1$ see Refs. 1 and 25. In Sec. IV we derive the form of the superpotential in the low energy

TABLE II. The associated affine algebra.

Gauge group	Lie algebra	Affine Toda potential
G(Simply-laced)	g	$g^{(1)}$
SO($2r+1$)	b_r	$a^{(2)}_{2r-1}$
USp($2r$)	c_r	$d^{(2)}_{r+1}$
G_2	g_2	$d^{(3)}_4$
F_4	f_4	$e^{(2)}_6$

effective three-dimensional theory generated by monopoles (46). It turns out that this potential is precisely the affine Toda potential for a specific affine algebra. For the simply-laced cases the affine algebra is the untwisted affinization of the Lie algebra of the gauge group while for the non-simply-laced cases it is affine algebra whose Kac–Dynkin diagram is obtained from the untwisted affine diagram with long roots changed to short roots, and vice versa. The affine algebras (in Kac's notation[37]) are listed in Table II. The Toda potential is in complete agreement with M(F)-theory considerations,[38–40] although we will find some additional prefactors that feed into the calculation of the gluino condensate in an essential way. From the superpotential, we find that the number of supersymmetric vacua is equal to dual Coxeter number of the gauge group in complete agreement with the Witten index.[41] The values of the gluino condensate in each vacuum are then found and the results are summarized in Table I. For all classical groups these are in agreement with the WCI results of Refs. 2–5. In Appendix A we summarize our Lie algebra conventions and Appendix B contains a brief discussion of the measure needed for integrating over the collective coordinate space of fundamental monopoles.

II. $\mathcal{N}=1$ GAUGE THEORY ON THE CYLINDER

In this section, we consider the effect of compactifying the pure $\mathcal{N}=1$ gauge theory on a cylinder of radius R. To this end, let us take x_0 to be periodic with period $2\pi R$. We then impose periodic boundary conditions on the gauge field and gluino:

$$v_m(x_\mu,x_0)=v_m(x_\mu,x_0+2\pi R),\quad \lambda(x_\mu,x_0)=\lambda(x_\mu,x_0+2\pi R). \tag{4}$$

(In our notation the four-dimensional indices run over $m,n,\ldots=0,1,2,3$ while our three-dimensional indices run over $\mu,\nu,\ldots=1,2,3$.) Notice that the periodicity of the fermions preserves supersymmetry.

Smooth finite-action gauge fields on the cylinder were classified in Ref. 33. In particular, at finite radius instanton configurations do not exhaust the set of semi-classical contributions. The complete set of semi-classical configurations is characterized by three pieces of data. First, there is a topological or instanton charge (or second Chern class) generalized from $\mathbb{R}^4$ to the cylinder:

$$k=\frac{1}{16\pi^2}\int_{\mathbb{R}^3\times S^1} d^4x\ \ \mathrm{tr}\, v_{mn}{}^*v^{mn}. \tag{5}$$

An important feature of the cylinder is that k is not quantized in integer units. However, when k is an integer there are solutions with action $S=8\pi^2k/g^2-ik\vartheta$ that, for scale size much smaller than R, are identifiable as instantons of the uncompactified theory. The second piece of data involves the Wilson loop of the gauge field around the circle:

$$\oint_{S^1} dx_m\, v_m=\int_0^{2\pi R} dx_0\, v_0\equiv\varphi. \tag{6}$$

We will then define the VEV of φ as the asymptotic value at spatial infinity in $\mathbb{R}^3$:

$$\langle \varphi \rangle = \lim_{|x_\mu| \to \infty} \boldsymbol{\varphi} \cdot \mathbf{H}, \tag{7}$$

where we have fixed a portion of the global gauge symmetry by choosing the Wilson loop (7) to lie within the Cartan subalgebra of the Lie algebra g associated to the gauge group G. (Our Lie algebra conventions are summarized in Appendix A. We will denote $r = \operatorname{rank} G$ vectors in boldface.) This still leaves the freedom to perform global gauge transformations from the Weyl group W_g of G.

A nonzero value for $\langle \varphi \rangle$ acts as an adjoint-valued Higgs field that generically breaks the gauge group to its maximal Abelian subalgebra $\mathrm{U}(1)^r$. The classical moduli space $\mathcal{M}_{\mathrm{cl}}$, parametrized by the vector $\langle \boldsymbol{\varphi} \rangle$, is the quotient

$$\mathcal{M}_{\mathrm{cl}} = \frac{\mathbb{R}^r}{2\pi \cdot \Lambda_W^* \rtimes W_g}, \tag{8}$$

where Λ_W^* is the co-weight lattice. The form of the quotient is explained in the following way: we have already noted that fixing $\langle \varphi \rangle$ to be in the Cartan subalgebra leaves the freedom to perform global gauge transformations in the Weyl group. On top of this, theories with $\langle \boldsymbol{\varphi} \rangle$ differing by 2π times any co-weight vector are equivalent. To see this last point, consider the following topologically nontrivial gauge transformation

$$U(x_0) = \exp\left(\frac{i x_0}{R} \boldsymbol{\omega}^* \cdot \mathbf{H} \right), \tag{9}$$

for any co-weight $\boldsymbol{\omega}^* \in \Lambda_W^*$. This transforms the component of the gauge field around the circle as $v_0 \to v_0 + \boldsymbol{\omega}^* \cdot \mathbf{H}/R$, and hence $\langle \boldsymbol{\varphi} \rangle \to \langle \boldsymbol{\varphi} \rangle + 2\pi \boldsymbol{\omega}^*$. The transformation (9) is periodic in the adjoint representation of the gauge group and consequently in the pure gauge theory where all fields are adjoint-valued $\langle \boldsymbol{\varphi} \rangle$ is identified with $\langle \boldsymbol{\varphi} \rangle + 2\pi \boldsymbol{\omega}^*$. (Because $\boldsymbol{\alpha} \cdot \boldsymbol{\omega}^* \in \mathbb{Z}$ for *any* root $\boldsymbol{\alpha}$ and co-weight $\boldsymbol{\omega}^*$.)

We will find it convenient to choose the VEV $\langle \boldsymbol{\varphi} \rangle$ to lie in a "fundamental cell"

$$0 \leqslant \langle \boldsymbol{\varphi} \rangle \cdot \boldsymbol{\alpha}_i < 2\pi \quad , \quad i = 1, \ldots, r, \tag{10}$$

where $\boldsymbol{\alpha}_i$ are the simple roots of g. [Notice that this region is still an over-parametrization of the quotient (8).] The regions where $\langle \boldsymbol{\varphi} \rangle \cdot \boldsymbol{\alpha}_i = 0$, for some set of i's, correspond to submanifolds of $\mathcal{M}_{\mathrm{cl}}$ where a non-Abelian subgroup of the gauge symmetry is restored.

The final piece of data arises from the fact that finite action configurations can also carry three-dimensional magnetic charge. This is an r-vector-valued quantity $\mathbf{g}$ in the charge space of the unbroken $\mathrm{U}(1)^r$ Abelian symmetry that can be defined via a surface integral over the two-sphere at spatial infinity in $\mathbb{R}^3$ of the magnetic field $B_\mu = \frac{1}{2} \epsilon_{\mu\nu\rho} v_{\nu\rho}$:

$$-\frac{1}{2\pi} \int_{S^2} dS_\mu B_\mu \equiv \mathbf{g} \cdot \mathbf{H}. \tag{11}$$

The magnetic charge is subject to the usual generalization of the Dirac quantization rule[42,43] which requires that

$$\mathbf{g} \in \Lambda_R^*, \tag{12}$$

the co-root lattice of g.

Classically, the Wilson loop $\langle \boldsymbol{\varphi} \rangle$ is not determined and, so, as we have explained, there is a moduli space $\mathcal{M}_{\mathrm{cl}}$ of inequivalent theories. An important question is whether this classical degeneracy persists in the quantum theory. At this point, the behavior depends crucially on whether one has periodic or anti-periodic boundary conditions on the fermions. In the latter—thermal—case,

Ref. 33 argued that nontrivial values of the asymptotic Wilson loop (7) are suppressed in the infinite volume limit. Consequently, the classically flat directions are lifted by thermal quantum corrections and the true vacuum of the theory is $\langle \boldsymbol{\varphi} \rangle = 0$. In this case, the configurations with magnetic charges are not relevant, since they require nonvanishing VEV, and the semi-classical physics is described by instantons only. Remarkably, for the theory on the cylinder, with periodic boundary conditions on the fermions, the argument of Ref. 33 does not apply and, as we shall see in the following sections, the opposite scenario ensues; namely, the following.

(i) The semi-classical physics of the theory on the cylinder is described by configurations of BPS monopoles. There are $r+1$ types of ''fundamental'' monopole which carry only four bosonic and two (adjoint) fermionic zero modes. To those who are sufficiently initiated into monopole calculus in gauge theories with arbitrary gauge group, this will be a surprise: one would expected to have only r such monopoles (each with a magnetic charge equal to one of the r simple roots). The additional monopole, needed to make up the full complement of $r+1$ types, is specific to the compactification on the cylinder since, unlike the other, it is a nontrivial function of ''time'' x_0.[25,26,29,30] The magnetic charge of the new monopole is such that when all $r+1$ types of monopoles are present with a specific degeneracy, the magnetic charges cancel and the resulting configuration carries only a unit of instanton charge. Hence, remarkably, instantons on the cylinder can be understood as composite configurations of monopoles.[25–30]

(ii) The classical moduli space of the gauge theory on the cylinder (6) is lifted in the quantum theory in a nontrivial way. The quantum vacua correspond to a single point in $\mathcal{M}_{\rm cl}$ cell along with an additional c_2-fold degeneracy, which has no counterpart in the classical theory, and corresponds precisely to the expectations based on a refined Witten index[41] and the WCI counting.[44,4]

III. SEMI-CLASSICAL CONFIGURATIONS

In the weak-coupling limit, the path integral is dominated by field configurations which are of minimal action in each topological sector. These configurations satisfy the four-dimensional self-dual, or anti-self-dual, equations $v_{mn} = \pm {}^*v_{mn}$. As we have explained there are two quantum numbers carried by semi-classical configurations: the topological charge and the magnetic charge.

First of all, let us consider solutions which are independent of the coordinate around the circle x_0. These are simply BPS monopoles in the three-dimensional theory[45–48] with the time direction taken to be along x_0. Monopole solutions in a gauge theory with a simple gauge group G can in turn be constructed out of the SU(2) BPS monopole in the following way.[43] The idea is to take a regular embedding $\mathrm{SU}(2) \subset G$, associated to a positive root $\boldsymbol{\alpha}$ of G:

$$\tau^1 = \frac{1}{2}(E_\alpha + E_{-\alpha}), \quad \tau^2 = \frac{1}{2i}(E_\alpha - E_{-\alpha}), \quad \tau^3 = \frac{1}{2}\boldsymbol{\alpha}^* \cdot \mathbf{H}, \tag{13}$$

which obey the SU(2) algebra

$$[\tau^a, \tau^b] = i\epsilon_{abc}\tau^c. \tag{14}$$

(Here, $\boldsymbol{\alpha}^* = 2\boldsymbol{\alpha}/\boldsymbol{\alpha}^2$ is the co-root associated to $\boldsymbol{\alpha}$.) The monopole solution is then

$$v_0(x_\nu) = \Phi^c(v; x_\nu)\tau^c + \frac{1}{2\pi R}\left(\langle \boldsymbol{\varphi} \rangle - \frac{1}{2}(\langle \boldsymbol{\varphi} \rangle \cdot \boldsymbol{\alpha})\boldsymbol{\alpha}^*\right) \cdot \mathbf{H}, \quad v_\mu(x_\nu) = v_\mu^c(v; x_\nu)\tau^c, \tag{15}$$

where $\Phi^c(v; x_\nu)$ is the Higgs field and $v_\mu^c(v; x_\nu)$ are the spatial components of the gauge field (in the gauge $v_0 = 0$) of the SU(2) BPS monopole. The long distance behavior of this solution is

$$\lim_{|x_\mu| \to \infty} \Phi^c(v; x_\nu)\tau^c = \frac{v}{2}\boldsymbol{\alpha}^* \cdot \mathbf{H}, \tag{16}$$

where

$$v = \frac{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}{2\pi R}. \tag{17}$$

For this solution to be well defined, we must have $v>0$, which is automatic if $\boldsymbol{\alpha}$ is a positive root and $\langle\boldsymbol{\varphi}\rangle$ lies in the fundamental cell (10), in which case it has magnetic charge, topological charge and action given by

$$\mathbf{g}=\boldsymbol{\alpha}^*, \quad k=\boldsymbol{\alpha}^*\cdot\frac{\langle\boldsymbol{\varphi}\rangle}{2\pi}, \quad S=\frac{4\pi}{g^2}\,\boldsymbol{\alpha}^*\cdot\langle\boldsymbol{\varphi}\rangle. \tag{18}$$

For completeness, we give the explicit solution for the SU(2) BPS monopole in ''hedgehog'' gauge,

$$v^c_\mu(v;x_\nu)=\epsilon_{\mu\nu c}\frac{x_\nu}{|x|^2}\left(1-\frac{v|x|}{\sinh v|x|}\right), \tag{19a}$$

$$\Phi^c(v;x_\nu)=\frac{x_c}{|x|^2}(v|x|\coth v|x|-1). \tag{19b}$$

The asymptotic value of the magnetic field of the hedgehog solution, as $|x|\to\infty$, is

$$B^c_\mu\to-\frac{x_\mu x^c}{|x|^4}, \tag{20}$$

while in unitary gauge

$$B^c_\mu\to-\frac{x_\mu}{|x|^3}\,\delta^{c3}, \quad B_\mu\equiv B^c_\mu\tau^c\to-\frac{x_\mu}{2|x|^3}\,\boldsymbol{\alpha}^*\cdot H. \tag{21}$$

However, these x_0-independent solutions do not exhaust the set of solutions with a given magnetic charge $\boldsymbol{\alpha}^*$.[25] A whole tower of other solutions which *are* x_0 dependent can be generated in the following way. First of all, we start with the solution (15) with $\langle\boldsymbol{\varphi}\rangle$ lying in the fundamental cell (10). We then write down the same solution with a shifted VEV $\langle\boldsymbol{\varphi}'\rangle=\langle\boldsymbol{\varphi}\rangle+\pi n\boldsymbol{\alpha}^*$, where $n\in\mathbb{Z}$. For this solution to be well defined we must have

$$v'=\frac{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}'\rangle}{2\pi R}=\frac{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}{2\pi R}+\frac{n}{R}>0\,. \tag{22}$$

For $\boldsymbol{\alpha}=\boldsymbol{\alpha}_i$, a simple root, (10) implies that $n\geqslant 0$. Acting on the solution with the (nonperiodic) gauge transformation,

$$V_n(x_0)=\exp\left(\frac{inx_0}{2R}\,\boldsymbol{\alpha}^*\cdot\mathbf{H}\right), \tag{23}$$

has the effect of restoring the VEV $\langle\boldsymbol{\varphi}\rangle$ to its original value. The new solution is then given by

$$\begin{aligned} v_0(x_\nu)&=\Phi^c(v+n/R;x_\nu)\tilde{\tau}^c+\frac{1}{2\pi R}\left(\langle\boldsymbol{\varphi}\rangle-\frac{1}{2}(\langle\boldsymbol{\varphi}\rangle\cdot\boldsymbol{\alpha}+2\pi n)\,\boldsymbol{\alpha}^*\right)\cdot\mathbf{H},\\ v_\mu(x_\nu)&=v^c_\mu(v+n/R;x_\nu)\tilde{\tau}^c, \end{aligned} \tag{24}$$

where v is given as in (17) and the SU(2) generators are conjugated with $V_n(x_0)$:

$$\tilde{\tau}^c = V_n(x_0)\tau^c V_n(x_0)^{-1}. \tag{25}$$

Notice although $V_n(x_0)$ is not a periodic gauge transformation the generators $\tilde{\tau}^c$ *are* periodic functions of x_0. The solution (24) has the same magnetic charge as (15), but the topological charge is $k=\boldsymbol{\alpha}^*\cdot\langle\boldsymbol{\varphi}\rangle/2\pi+n$. This solution can be interpreted as a composite configuration of the original monopole plus an instanton of charge n.

However, there are also towers of solutions of the self-dual equations that have a magnetic charge equal to some *negative* root.[25] We should emphasize that these solutions are *not* anti-monopoles which would satisfy the *anti*-self-dual equations. To construct these solutions we can start with our solution (15) with $\langle\boldsymbol{\varphi}\rangle$ lying in the fundamental cell. We now define a new solution with a VEV $\langle\boldsymbol{\varphi}'\rangle=\kappa_{\boldsymbol{\alpha}}(\langle\boldsymbol{\varphi}\rangle)+\pi n\boldsymbol{\alpha}^*$, where $\kappa_{\boldsymbol{\alpha}}$ is the Weyl reflection in $\boldsymbol{\alpha}$. For the solution to be well defined we must have

$$v'=\frac{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}'\rangle}{2\pi R}=-\frac{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}{2\pi R}+\frac{n}{R}>0. \tag{26}$$

For $\boldsymbol{\alpha}=\boldsymbol{\alpha}_i$, a simple root, this means $n>0$. To reinstall the original VEV, we then perform a Weyl reflection in $\boldsymbol{\alpha}$ and the gauge transformation (23). The resulting solution is

$$\begin{aligned} v_0(x_\nu)&=\Phi^c(n/R-v;x_\nu)\tilde{\tau}^c+\frac{1}{2\pi R}\left(\langle\boldsymbol{\varphi}\rangle-\frac{1}{2}(-\langle\boldsymbol{\varphi}\rangle\cdot\boldsymbol{\alpha}+2\pi n)\boldsymbol{\alpha}^*\right)\cdot\mathbf{H},\\ v_\mu(x_\nu)&=v_\mu^c(n/R-v;x_\nu)\tilde{\tau}^c, \end{aligned} \tag{27}$$

where v is given in (17) and the SU(2) generators are now conjugated with $V_n(x_0)\kappa_{\boldsymbol{\alpha}}$:

$$\tilde{\tau}^c=V_n(x_0)\kappa_{\boldsymbol{\alpha}}\tau^c\kappa_{\boldsymbol{\alpha}}V_n(x_0)^{-1}. \tag{28}$$

It can be easily verified that this solution is again periodic in x_0. The resulting solution has magnetic charge $-\boldsymbol{\alpha}^*$ and topological charge $k=-\boldsymbol{\alpha}^*\cdot\langle\boldsymbol{\varphi}\rangle/2\pi+n$.

It will be important for later to determine the number of adjoint fermion, or gluino, zero modes of these monopole solutions. Each classical solution has at least two adjoint fermion zero modes protected by supersymmetry. These modes can be generated from the purely bosonic solution by acting with the generators of supersymmetry that do not leave the configuration invariant. This gives the universal expression for these supersymmetric modes

$$\lambda_\alpha=\sigma_\alpha^{mn\beta}\xi_\beta v_{mn}, \tag{29}$$

where v_{mn} is the field strength. For future reference we give the long-distance behavior of the supersymmetric fermion zero modes (29) of our fundamental monopole solutions (15) and (27) with $n=1$:

$$\lambda_\alpha=\sigma_\alpha^{mn\beta}\xi_\beta v_{mn}=-2(\sigma^\nu\xi)_\alpha B_\nu\to 4\pi(\mathcal{S}_{\mathrm{F}}\xi)_\alpha\boldsymbol{\alpha}^*\cdot\mathbf{H}, \tag{30}$$

where $\mathcal{S}_{\mathrm{F}}(x)=\sigma_\mu x_\mu/(4\pi|x_\mu|^3)$ is the massless fermion propagator in three dimensions.

Solutions with only the supersymmetric zero modes have four associated bosonic zero modes which correspond to moving the center-of-mass of the monopole in $\mathbb{R}^3$ as well as performing global gauge rotations by $\exp((i/2)\,\Omega\,\boldsymbol{\alpha}^*\cdot\mathbf{H})$. Hence these solutions are special in that they are elementary or ''fundamental'': the other solutions have additional moduli that correspond to pulling the configuration apart into their fundamental constituents.

As might have been expected there are r solutions of the form (15) where $\boldsymbol{\alpha}$ is a simple root $\boldsymbol{\alpha}_i$ lying at the bottom of the more general tower of solutions (24). This gives us $i=1,\ldots,r$ fundamental monopole solutions with two adjoint-valued fermion zero modes, magnetic charge $\boldsymbol{\alpha}_i^*$, and the topological charge $k=\boldsymbol{\alpha}_i^*\cdot\langle\boldsymbol{\varphi}\rangle/2\pi$. Solutions higher in the tower, with $n>0$, have

$2(1+nc_2)$ fermion zero modes,[25,26] as we expect for a configuration of a fundamental monopole and n instantons. In addition to these r fundamental monopoles, there is one other solution that is fundamental.[25,26] This is a solution which has a negative magnetic charge equal to the lowest root $\boldsymbol{\alpha}_0^* \equiv \boldsymbol{\alpha}_0$ (although the solution, as we explained above is *not* an anti-monopole) lying in the second tower (27) with $n=1$ and hence with topological charge $k=-\boldsymbol{\alpha}_0^* \cdot \langle \boldsymbol{\varphi} \rangle / 2\pi + 1$.

Since $\Sigma_{i=0}^{r} k_i^* \boldsymbol{\alpha}_i^* = 0$, the quantum numbers of the solutions suggest that a pure instanton solution, carrying zero magnetic charge and unit topological charge, is a composite configuration with k_i^* fundamental $\boldsymbol{\alpha}_i$ monopoles, for each $i=0,\ldots,r$. (Here k_i^* are the dual "Kac labels," or co-marks, defined in Appendix A.) This turns out to be the case[25,26] and the resulting configuration has exactly $2c_2$ $(4c_2)$ exact fermionic (bosonic) zero modes as expected for a singly-charged instanton with gauge group G.

IV. MONOPOLE CONTRIBUTIONS TO THE SUPERPOTENTIAL

In this section, we will explain how the fundamental monopoles described in the last section lift the classical degeneracy of the theory parametrized by the asymptotic value of the Wilson loop $\langle \boldsymbol{\varphi} \rangle$ (7). The idea is to consider the low energy three-dimensional effective theory corresponding to the massless Abelian components of the fields formed by integrating out all the massive fields.

For this analysis to hold we must first assume there is no root $\boldsymbol{\alpha}$ such that $\langle \boldsymbol{\varphi} \rangle \cdot \boldsymbol{\alpha} = 0$, so that the unbroken gauge group is maximally Abelian $\mathrm{U}(1)^r$. We will also assume that the Wilson line VEV $\langle \boldsymbol{\varphi} \rangle$ lies in the fundamental region (10). After that we can integrate out (1) all non-Abelian fields on $\mathbb{R}^3 \times S^1$, and (2) all the massive Kaluza–Klein modes on S^1, i.e., the modes with nonzero Matsubara frequency $\omega_m = m/R$, to flow to the Abelian theory on $\mathbb{R}^3$. We emphasize that the periodicity in $\langle \boldsymbol{\varphi} \rangle \sim \langle \boldsymbol{\varphi} \rangle + 2\pi \boldsymbol{\omega}^*$, $\boldsymbol{\omega}^* \in \Lambda_W^*$, is a property of the full microscopic theory but not of the low-energy theory on $\mathbb{R}^3$. Indeed, the large gauge transformation (9) is x_0-dependent and has the effect of mixing up the massless and massive Kaluza–Klein modes.

The fields of the low energy theory consist of the Wilson loop $\boldsymbol{\varphi}$, i.e., the component v_0 of the gauge field averaged over the circle, along with r massless photons corresponding to the components of v_μ in the Cartan subalgebra of the gauge group. Along with these bosonic fields there are superpartners corresponding to the Abelian components of the gluino.

It turns out to be convenient to use the fact that massless Abelian gauge fields in three dimensions can be eliminated in favor of scalar fields by a duality transformation. To construct the classical effective action, we start with the action of the pure gauge theory in four dimensions and dimensionally reduce to three dimensions keeping only the Abelian components of the fields. From (6), the component v_0 of the four-dimensional gauge field is replaced by $\boldsymbol{\varphi} \cdot \mathbf{H}/(2\pi R)$ and the resulting three-dimensional effective action is

$$S_{\mathrm{cl}} = \frac{2\pi R}{g^2} \int d^3x \left\{ \frac{1}{4\pi^2 R^2} (\partial_\mu \boldsymbol{\varphi})^2 - \frac{1}{2} (\mathbf{v}_{\mu\nu})^2 + 2i \overline{\boldsymbol{\lambda}} \cdot \overline{\sigma}_\mu \mathcal{D}_\mu \boldsymbol{\lambda} \right\} - \frac{i\vartheta}{8\pi^2} \int d^3x \, \epsilon_{\mu\nu\rho} \partial_\mu \boldsymbol{\varphi} \cdot \mathbf{v}_{\nu\rho} . \tag{31}$$

[It is useful to notice that in our normalization $\mathrm{tr}(\mathbf{a}\cdot\mathbf{H}\ \mathbf{b}\cdot\mathbf{H}) = \mathbf{a}\cdot\mathbf{b}$.] In order to construct the dual description of the three-dimensional gauge field one adds a new term to the action involving a field $\boldsymbol{\sigma}$ which serves as a Lagrange multiplier for the Bianchi identity constraint:

$$S_{\mathrm{cst}} = -\frac{i}{4\pi} \int d^3x \, \epsilon_{\mu\nu\rho} \partial_\mu \boldsymbol{\sigma} \cdot \mathbf{v}_{\nu\rho} = -\frac{i}{2\pi} \int_{S^2} dx_\mu \, \boldsymbol{\sigma} \cdot \mathbf{B}_\mu . \tag{32}$$

The Abelian field strength $\mathbf{v}_{\mu\nu}$ can now be integrated-out of the path integral as a Gaussian field to obtain the classical effective action, whose bosonic part is

$$S_{\mathrm{cl}}^{\mathrm{bos}} = \frac{1}{2\pi R} \int d^3x \left\{ \frac{1}{g^2} (\partial_\mu \boldsymbol{\varphi})^2 + \frac{g^2}{16\pi^2} \left(\partial_\mu \boldsymbol{\sigma} + \frac{\vartheta}{2\pi} \partial_\mu \boldsymbol{\varphi} \right)^2 \right\} . \tag{33}$$

This can be written compactly in terms of the single complex field

$$\mathbf{z}=i(\tau\boldsymbol{\varphi}+\boldsymbol{\sigma}), \tag{34}$$

as

$$S_{\rm cl}^{\rm bos}=\frac{1}{8\pi^2R}\int d^3x\,\frac{1}{\operatorname{Im}\tau}\,\partial^\mu\mathbf{z}^+\cdot\partial_\mu\mathbf{z}. \tag{35}$$

We have eliminated the r massless photons in favor of an r-vector scalar field $\boldsymbol{\sigma}$. Notice that since the magnetic charge $\mathbf{g}$ is quantized in the co-root lattice it follows from (32) that $\boldsymbol{\sigma}$ is physically equivalent to $\boldsymbol{\sigma}+2\pi\boldsymbol{\omega}$ for any weight $\boldsymbol{\omega}\in\Lambda_W$. Once again, we also have the freedom to perform Weyl reflections and so $\boldsymbol{\sigma}$ is valued in the quotient

$$\frac{\mathbb{R}^r}{2\pi\cdot\Lambda_W\rtimes W_g}, \tag{36}$$

to compare with $\boldsymbol{\varphi}$ which is valued in the slightly different quotient (8). Obviously these spaces are the same for the simply-laced groups.

The fact that both (real) scalar fields $\boldsymbol{\varphi}$ and $\boldsymbol{\sigma}$ can be amalgamated into a single complex field $\mathbf{z}$ is no coincidence. Since the original four-dimensional theory was $\mathcal{N}=1$ supersymmetric, the effective theory written in terms of the bosonic fields $\boldsymbol{\varphi}$ and $\boldsymbol{\sigma}$, along with the Abelian components of the gluino $\boldsymbol{\lambda}_\alpha$, must form a representation of four-dimensional $\mathcal{N}=1$ supersymmetry (corresponding to $\mathcal{N}=2$ in three dimensions) which must be a chiral superfield since we have taken the dual of all the vector fields. In particular the bosonic fields must be expressible in terms of a single complex field as we have found in (34).

The $\mathcal{N}=2$ (in 3D) supersymmetric completion of the classical action (35) can be most succinctly expressed in terms of a four-dimensional $\mathcal{N}=1$ chiral superfield $\mathbf{X}$ with scalar component $\mathbf{z}$ and fermionic component $\boldsymbol{\lambda}_\alpha$, the Abelian component of the gluino. The supersymmetric version of (35) written in superspace is then

$$S_{\rm cl}=\frac{1}{8\pi^2R}\int d^3x\,\frac{1}{\operatorname{Im}\tau}\,\mathbf{X}^+\cdot\mathbf{X}\big|_{\theta\theta\overline{\theta\theta}}. \tag{37}$$

Quantum effects can modify the classical expression (37). However, modifications must preserve supersymmetry. As long as we are at a generic point in the classical moduli space, we expect to be able to integrate out all the massive fields to be left with an effective theory in terms of the superfield $\mathbf{X}$. The most general possible low energy effective action, i.e., involving at most two derivatives or four fermions, and preserving $\mathcal{N}=2$ supersymmetry in three dimensions, is

$$S_{\rm eff}=\int d^3x\,\{\mathcal{K}(\mathbf{X},\mathbf{X}^+)\big|_{\theta\theta\overline{\theta\theta}}+\mathcal{W}(\mathbf{X})\big|_{\theta\theta}+\overline{\mathcal{W}}(\mathbf{X}^+)\big|_{\overline{\theta\theta}}\}, \tag{38}$$

which involves an arbitrary D-term $\mathcal{K}(\mathbf{X},\mathbf{X}^+)$ as well as a superpotential $\mathcal{W}(\mathbf{X})$. It is the superpotential that is responsible for lifting the classical degeneracy and which we must determine.

In the classical theory (37) the superpotential vanishes identically. Quantum corrections will modify the theory in a complicated way depending on the couplings. However, the superpotential, by the standard arguments,[49,7,34] must be holomorphic in the fields $\mathbf{X}$ and the complexified coupling τ. In particular, up to the overall factor, the superpotential can only depend on R through the running of τ via the dimensionless quantity $R|\Lambda|$, where Λ is the usual Pauli–Villars scale of strong coupling effects in the pure gauge theory in $\mathbb{R}^4$. [This appears when the fields are not canonically normalized. In our case scalar fields arise from the Wilson line and the dual photon, which are dimensionless. This leads to an overall factor of R/g^2 in Eq. (46) below.] We intend to compute the superpotential at weak-coupling, for which $R\ll|\Lambda|^{-1}$ and the VEV of the effective

Higgs field (17) is large and a semi-classical analysis should be reliable. In this regime the superpotential will receive contributions from the minimal action configurations in each topological sector which have exactly two gluino zero modes; in other words, from the $r+1$ fundamental monopoles described in the last section. As usual holomorphy then forbids any perturbative corrections to the semi-classical contributions and, as a consequence, fixes the R dependence, a fact that ultimately will allow us to take R to be large.

In the presence of the dual photon field $\boldsymbol{\sigma}$, the action of the fundamental monopole associated to the root $\boldsymbol{\alpha}_j$, $j=0,\ldots,r$, is given in terms of the VEV of the scalar field z by

$$S_j = -2\pi i\tau\delta_{j0} - i\tau\boldsymbol{\alpha}_j^*\cdot\langle\boldsymbol{\varphi}\rangle - i\boldsymbol{\alpha}_j^*\cdot\langle\boldsymbol{\sigma}\rangle \equiv -2\pi i\tau\delta_{j0} - \boldsymbol{\alpha}_j^*\cdot\langle\mathbf{z}\rangle. \tag{39}$$

Here τ is the complexified coupling (3).

We determine the form of the superpotential by calculating the monopole contribution to the large distance behavior of the correlator of two components of the massless gluino field

$$\langle\boldsymbol{\lambda}_\alpha(x)\otimes\boldsymbol{\lambda}_\beta(0)\rangle. \tag{40}$$

In the background of the $\boldsymbol{\alpha}_j$ monopole, only the component $\boldsymbol{\lambda}_\alpha \propto \boldsymbol{\alpha}_j$ is nontrivial; in fact from (30) one finds the long-distance behavior to be

$$\boldsymbol{\lambda}_\alpha^{LD}(x) = 4\pi\boldsymbol{\alpha}_j^*\mathcal{S}_{\mathrm{F}}(x-a)_\alpha^\gamma\xi_\gamma, \tag{41}$$

where $\mathcal{S}_{\mathrm{F}}(x)=\sigma_\mu x_\mu/(4\pi|x_\mu|^3)$ is the massless fermion propagator in three dimensions, a_μ is the position of the monopole in $\mathbb{R}^3$ and ξ_α are the Grassmann collective coordinates corresponding to the two supersymmetric zero modes.

In order to evaluate the contribution to the superpotential from the monopole, we need the measure for integrating over the moduli space of the monopole derived in Appendix B. A fundamental monopole has a moduli space that is parametrized by a_μ, the position in $\mathbb{R}^3$ and by the U(1) phase angle $0\leqslant\Omega\leqslant 2\pi$. Along with this, there are two Grassmann collective coordinates ξ_α, corresponding to the two supersymmetric zero modes. From Eq. (79) the measure is

$$\int d\mu_{\mathrm{mon}}^{(\mathrm{j})} = \frac{2}{\boldsymbol{\alpha}_j^2}\frac{\mu^3 R}{g^2}e^{-S_j}\int d^3a\, d\Omega\, d^2\xi. \tag{42}$$

Performing the integrals over the phase angle and the Grassmann collective coordinates, we find that

$$\langle\boldsymbol{\lambda}_\alpha(x)\otimes\boldsymbol{\lambda}_\beta(0)\rangle = \frac{2^6\pi^3\mu^3 R}{g^2\boldsymbol{\alpha}_j^2}\boldsymbol{\alpha}_j^*\otimes\boldsymbol{\alpha}_j^* e^{2\pi i\tau\delta_{j0}+\boldsymbol{\alpha}_j^*\cdot\langle\mathbf{z}\rangle}\int d^3a\,\mathcal{S}_{\mathrm{F}}(x-a)_\alpha^\gamma\mathcal{S}_{\mathrm{F}}(a)_{\beta\gamma}. \tag{43}$$

Amputating this correlator we find the associated vertex in the effective action:

$$\left(\frac{2\pi R}{g^2}\right)^2\frac{2^5\pi^3\mu^3 R}{g^2\boldsymbol{\alpha}_j^2}e^{2\pi i\tau\delta_{j0}+\boldsymbol{\alpha}_j^*\cdot\langle\mathbf{z}\rangle}\ (\boldsymbol{\alpha}_j^*\cdot\boldsymbol{\lambda})^2. \tag{44}$$

In the above, the numerical factor in the bracket reflects our normalization for the kinetic term of $\boldsymbol{\alpha}\cdot\boldsymbol{\lambda}$ which follows from (31). The vertex (44) is generated by a term in the effective potential of the form

$$\frac{4\pi\mu^3 R}{g^2\boldsymbol{\alpha}_j^2}e^{2\pi i\tau\delta_{j0}+\boldsymbol{\alpha}_j^*\cdot\mathbf{X}}. \tag{45}$$

[In order to get the correct numerical factor, notice that the fermionic component of $\mathbf{z}$ and the gluino $\boldsymbol{\lambda}$ are related via $\boldsymbol{\psi}=2^{5/2}\pi^2 g^{-2} R\,\boldsymbol{\lambda}$. This follows from the fact[50] that the superpartner of $\mathbf{v}_0$ is $(\boldsymbol{\lambda}+\overline{\boldsymbol{\lambda}})/\sqrt{2}$.] Hence, summing over the effects of all $r+1$ fundamental monopoles we deduce that the monopole-generated superpotential of the theory is

$$\mathcal{W}_{\text{mono}}(\mathbf{X})=\frac{2\pi\mu^3 R}{g^2}\left(\sum_{j=1}^{r}\frac{2}{\boldsymbol{\alpha}_j^2}e^{\boldsymbol{\alpha}_j^*\cdot\mathbf{X}}+\frac{2}{\boldsymbol{\alpha}_0^2}e^{2\pi i\tau+\boldsymbol{\alpha}_0^*\cdot\mathbf{X}}\right). \tag{46}$$

This is an affine Toda potential for an associated affine algebra. Notice that to give the usual expression for a Toda potential one can remove the pre-factors $2/\boldsymbol{\alpha}_j^2$ by a shift in the field:

$$\mathbf{X}\to\mathbf{X}+\sum_{j=1}^{r}\ln(\boldsymbol{\alpha}_j^2/2)\boldsymbol{\omega}_j+\frac{\boldsymbol{\rho}}{c_2}\left(2\pi i\tau-\sum_{j=0}^{r}\ln(\boldsymbol{\alpha}_j^2/2)\right), \tag{47}$$

where $\boldsymbol{\rho}=\Sigma_{j=1}^{r}\boldsymbol{\omega}_j$ is the Weyl vector. For the simply-laced groups, the associated affine algebra is the untwisted affinization of the original Lie algebra, $g^{(1)}$ in Kac's notation,[37] while for the non-simply-laced groups the corresponding affine algebra is twisted in the way described in Table II. In these cases, the Kac–Dynkin diagram of the affine algebra is obtained from the Kac–Dynkin diagram of the untwisted affinization $g^{(1)}$ by changing long roots into short roots, and vice versa. In Kac's notation[37] this leads to the twisted affinization of a different algebra. The same superpotential has been deduced from entirely different considerations involving M theory compactified on certain eight-dimensional manifolds,[38–40,51,52] although the $2/\boldsymbol{\alpha}_j^2$ prefactors, that we shall find crucial in order to get results for the gluino condensate that agree with other calculations, are absent. It is also interesting that the integrable systems related to the Toda potentials that we have found above are precisely those that appear in the "Seiberg–Witten theory" of the $\mathcal{N}=2$ gauge theory with the same gauge group in four dimensions.[53,54] Naturally this is no accident since the $\mathcal{N}=1$ theory can be obtained from the $\mathcal{N}=2$ theory by soft breaking mass terms.

Importantly, although we have calculated the superpotential in the limit $R\ll|\Lambda^{-1}|$, at weak coupling, there can be no additional dependence on R and the result can be continued to any R, and in particular to the decompactification limit.[34,35]

One may wonder how the superpotential relates to that calculated in Ref. 55 for the three-dimensional $\mathcal{N}=2$ supersymmetric gauge theory. The way that this superpotential arises from the $R\to 0$ limit of our superpotential is explained in a slightly different context in Ref. 34. The point is that to take the three-dimensional limit, one should take it in such a way that the three-dimensional gauge coupling, which is classically given by $g_3^2=g^2/(2\pi R)$, is fixed. In other words, as $R\to 0$, we should simultaneously take the limit $g\to 0$ in the superpotential (46). In this limit, the additional term corresponding to the affine root is removed to give

$$\mathcal{W}_{3\text{-d}}=\frac{\mu^3}{g_3^2}\sum_{j=1}^{r}\frac{2}{\boldsymbol{\alpha}_j^2}e^{\boldsymbol{\alpha}_j^*\cdot\mathbf{X}}. \tag{48}$$

In other words, in this limit, the affine Toda potential becomes the Toda potential for a nonaffine algebra. This is what one expects because the affine term in the superpotential on the cylinder is generated by the additional monopole solution that only exists on the cylinder and not in $\mathbb{R}^3$. The genuinely three-dimensional superpotential (48) is the generalization of that of Ref. 55 from SU(2) to arbitrary gauge group. Just as in the SU(2) case, it does not have a stationary point and therefore the theory does not have a vacuum state.

V. VACUUM STRUCTURE AND THE GLUINO CONDENSATE

The superpotential (46) gives rise to a number of supersymmetric vacua which satisfy

$$\frac{2}{\boldsymbol{\alpha}_j^2} e^{\boldsymbol{\alpha}_j^* \cdot \mathbf{X}} = \frac{2}{\boldsymbol{\alpha}_0^2} k_j^* e^{2\pi i \tau} e^{\boldsymbol{\alpha}_0^* \cdot \mathbf{X}}, \tag{49}$$

for $j=1,\ldots,r$. Writing $\mathbf{X}=\sum_{j=1}^r a_j \boldsymbol{\omega}_j$ we have

$$e^{a_j} = \frac{k_j^* \boldsymbol{\alpha}_j^2 e^{2\pi i \tau}}{2\kappa}, \tag{50}$$

where $\kappa = e^{\sum_{j=1}^r a_j k_j^*}$ is determined self-consistently as the solution of the equation

$$\kappa^{c_2} = e^{2\pi i (c_2-1)\tau} \prod_{j=0}^{r} \left(\frac{k_j^* \boldsymbol{\alpha}_j^2}{2} \right)^{k_j^*}. \tag{51}$$

There are consequently c_2 supersymmetric ground states given by the c_2 roots of (51) which are related by $\mathbf{X} \to \mathbf{X} + 2\pi i \boldsymbol{\rho}/c_2$. (The vector $\boldsymbol{\rho}=\sum_{j=1}^r \boldsymbol{\omega}_j$ is the Weyl vector and recall that $\mathbf{X}$ is identified with $\mathbf{X}+2\pi i \boldsymbol{\rho}$ as a consequence of the fact that $\boldsymbol{\sigma}$ is identified with $\boldsymbol{\sigma}+2\pi\boldsymbol{\rho}$, since $\boldsymbol{\rho} \in \Lambda_W$.) These vacua correspond to a fixed value of $\boldsymbol{\varphi}$:

$$\boldsymbol{\varphi} = \left(\frac{2\pi}{c_2} + \frac{g^2}{4\pi} \ln|\kappa| \right) \boldsymbol{\rho} - \frac{g^2}{4\pi} \sum_{j=1}^{r} \ln(k_j^* \boldsymbol{\alpha}_j^2/2)\, \boldsymbol{\omega}_j, \tag{52}$$

and c_2 values of $\boldsymbol{\sigma}$ given by

$$\boldsymbol{\sigma} = -\frac{\vartheta}{2\pi} \boldsymbol{\varphi} + \frac{\vartheta + 2\pi u}{c_2} \boldsymbol{\rho}, \tag{53}$$

where $u=1,2,\ldots,c_2$. Notice that as expected the c_2 vacua are related by $\vartheta \to \vartheta + 2\pi$.

The value of the superpotential in one of the vacua is

$$\langle \mathcal{W}_{\text{mono}} \rangle = \frac{2\pi\mu^3 R}{g^2} \cdot \frac{e^{2\pi i \tau} c_2}{\kappa} = \frac{2\pi\mu^3 R}{g^2} \cdot \frac{c_2 e^{2\pi i \tau/c_2 + 2\pi i u/c_2}}{\Pi_{j=0}^r (k_j^* \boldsymbol{\alpha}_j^2/2)^{k_j^*/c_2}} = 2\pi R \Lambda^3 \cdot \frac{c_2 e^{2\pi i u/c_2}}{\Pi_{j=0}^r (k_j^* \boldsymbol{\alpha}_j^2/2)^{k_j^*/c_2}}, \tag{54}$$

where in the final expression we have eliminated the Pauli–Villars mass scale μ in favor of the Lambda parameter using the exact relation (2). The value of the gluino condensate in each vacuum can be extracted by using the general relation

$$\left\langle \frac{\operatorname{tr} \lambda^2}{16\pi^2} \right\rangle = b_0^{-1} \Lambda \frac{\partial}{\partial \Lambda} \left\langle \frac{1}{2\pi R} \mathcal{W}_{\text{mono}} \right\rangle, \tag{55}$$

adapted to the three-dimensional superpotential. The first coefficient of the beta-function is $b_0 = 3c_2$ giving

$$\left\langle \frac{\operatorname{tr} \lambda^2}{16\pi^2} \right\rangle = \frac{\Lambda^3 e^{2\pi i u/c_2}}{\Pi_{j=0}^r (k_j^* \boldsymbol{\alpha}_j^2/2)^{k_j^*/c_2}}. \tag{56}$$

The gluino condensate can also be evaluated directly without having to rely on the identity (55). The idea is to consider the fundamental monopole contributions to the one-point function $\langle \operatorname{tr} \lambda^2/16\pi^2 \rangle$ in a given vacuum, say the u^{th}. The contribution of the $\boldsymbol{\alpha}_j$ monopole to the condensate in this vacuum is

$$\left\langle \frac{\mathrm{tr}\,\lambda^2}{16\pi^2} \right\rangle_{j\text{-mono}} = \int d\mu^{(j)}_{\mathrm{mon}} \left. \frac{\mathrm{tr}\,\lambda^2}{16\pi^2} \right|_{j\text{-mono}} . \tag{57}$$

To evaluate (57), we can use the normalization of the adjoint fermion zero modes from Ref. 50,

$$\int d^3a\, d^2\xi \left. \frac{\mathrm{tr}\,\lambda^2}{16\pi^2} \right|_{j\text{-mono}} = \frac{g^2\,\mathrm{Re}\,S_j}{8\boldsymbol{\alpha}_j^2\pi^3 R}. \tag{58}$$

Computing the remaining integral over the phase angle gives

$$\left\langle \frac{\mathrm{tr}\,\lambda^2}{16\pi^2} \right\rangle_{j\text{-mono}} = \frac{\mu^3\,\mathrm{Re}\,S_j}{4\pi^2\boldsymbol{\alpha}_j^2} e^{-S_j}. \tag{59}$$

In the supersymmetric vacua

$$S_j = -2\pi i\tau - \ln\left(\frac{k_j^*\boldsymbol{\alpha}_j^2}{2\kappa} \right) \tag{60}$$

and so inserting the value for κ in (51) we have

$$\left\langle \frac{\mathrm{tr}\,\lambda^2}{16\pi^2} \right\rangle_{j\text{-mono}} = \frac{k_j^*\Lambda^3 e^{2\pi i u/c_2}}{c_2} \cdot \frac{1}{\prod_{j=0}^{r} (\boldsymbol{\alpha}_j^2 k_j^*/2)^{k_j^*/c_2}}. \tag{61}$$

Summing over the contributions from the $r+1$ fundamental monopoles gives (56).

We conclude the section with the observation that in the supersymmetric vacua the $r+1$ fundamental monopoles have equal topological charge

$$\boldsymbol{\alpha}_j \cdot \frac{\langle \boldsymbol{\varphi} \rangle}{2\pi} = 1 - \boldsymbol{\alpha}_0 \cdot \frac{\langle \boldsymbol{\varphi} \rangle}{2\pi} = \frac{1}{c_2} \tag{62}$$

(for $j=1,\ldots,r$) independent of j. In addition, as we have discussed in Sec. III, the configuration which becomes the singly-charged instanton in the uncompactified theory is obtained by considering a multi-monopole solution which consists of k_j^* of the jth fundamental monopole. In this very precise sense they realize the old dream of thinking of the instanton in terms of a set of constituents, or instanton quarks.[20–24] It was anticipated that the instanton quarks would cause, or at least play a major role in, confinement. In the theory on the cylinder this old idea again receives confirmation. Notice that in the quantum vacuum states the dual photon becomes massive which is equivalent to the confinement of the original Abelian electric photons.

APPENDIX A: SOME LIE ALGEBRA CONVENTIONS

In this appendix we give a brief review of particular details of Lie algebras that we will need. For more details on Lie algebras the reader may consult Refs. 56.

Let $\{H^i\}$ be a maximal set of simultaneously diagonalizable, mutually commuting generators, $[H^i,H^j]=0$. The indices i,j run from 1 to r, the *rank* of the Lie algebra. We normalize the Cartan generators to one,

$$\mathrm{tr}(H^iH^j) = \delta^{ij}, \tag{A1}$$

and often think of the r-vector $\mathbf{H}$. The remainder of the generators are the step operators E_α with

$$[\mathbf{H},E_\alpha] = \boldsymbol{\alpha}E_{\boldsymbol{\alpha}}. \tag{A2}$$

The normalization condition (A1) makes the length squared of any long root to be equal to 2.

TABLE III. Lie algebra data.

G	g	c_2	$\{k_i^*\}$	$\{\alpha_i^2\}$
SU($r+1$)	a_r	$r+1$	{1,1,...,1}	{2,...,2}
SO($2r+1$)	b_r	$2r-1$	{1,1,2,...,2,1}	{2,...,2,1}
USp($2r$)	c_r	$r+1$	{1,...,1}	{2,1,...,1,2}
SO($2r$)	d_r	$2r-2$	{1,1,2,...,2,1,1}	{2,...,2}
G_2	g_2	4	{1,2,1}	{2,2,2/3}
F_4	f_4	9	{1,2,3,2,1}	{2,2,2,1,1}
E_6	e_6	12	{1,1,1,2,2,2,3}	{2,...,2}
E_7	e_7	18	{1,1,2,2,2,3,3,4}	{2,...,2}
E_8	e_8	30	{1,2,2,3,3,4,4,5,6}	{2,...,2}

We will denote a set of simple roots as $\boldsymbol{\alpha}_j$, $j=1,\ldots,r$. These span the root lattice Λ_R. The lowest root is then denoted as $\boldsymbol{\alpha}_0$. The co-roots are defined via

$$\boldsymbol{\alpha}^* \equiv \frac{2}{\boldsymbol{\alpha}^2}\boldsymbol{\alpha} \tag{A3}$$

and these span the co-root lattice Λ_R^*. The weight lattice Λ_W is dual to the co-root lattice and is spanned by the fundamental weights $\boldsymbol{\omega}_j$ where

$$\boldsymbol{\omega}_i \cdot \boldsymbol{\alpha}_j^* = \delta_{ij}. \tag{A4}$$

Similarly one can define the co-weight lattice Λ_W^* which is dual to the root lattice and is spanned by the co-weights $\boldsymbol{\omega}_i^*$ where

$$\boldsymbol{\omega}_i^* \equiv \frac{2}{\boldsymbol{\alpha}_i^2}\boldsymbol{\omega}_i. \tag{A5}$$

We will also need to define the dual Kac labels, or co-marks, k_i^*. By definition $k_0^*=1$ and the remaining co-marks are given by the expansion of the lowest co-root in terms of the co-simple-roots:

$$\boldsymbol{\alpha}_0^* = -\sum_{i=1}^{r} k_i^* \boldsymbol{\alpha}_i^*. \tag{A6}$$

Finally

$$c_2 \equiv \sum_{i=0}^{r} k_i^* \tag{A7}$$

is the *dual Coxeter number*. (The Kac labels, or marks, and Coxeter number are similarly defined but will not be needed here.)

In Table III we summarize all the Lie algebra data that we need. As well as listing the dual Kac labels and dual Coxeter number we also list the root lengths $\boldsymbol{\alpha}_j^2$ for $j=0,\ldots,r$. (Note that the set of dual Kac labels and root lengths are ordered in the same way.)

APPENDIX B: THE MONOPOLE COLLECTIVE COORDINATE MEASURE

In this appendix we briefly discuss the measure for integrating over the collective coordinates of a fundamental monopole. A fundamental monopole has a moduli space that is identical to the BPS monopole in SU(2). Therefore, it is parametrized by a_μ, the position in $\mathbb{R}^3$, and by the U(1) phase angle $0\leqslant\Omega\leqslant 2\pi$. Along with this, there are two Grassmann collective coordinates ξ_α,

corresponding to the two supersymmetric zero modes. The measure for integrating over the monopole moduli space is obtained in the standard way by changing variables in the path integral from field fluctuations around the monopole to the monopole's collective coordinates:

$$\int d\mu_{\rm mon} = \mu^3 e^{-S} \int \frac{d^3a}{(2\pi)^{3/2}} J_a \int_0^{2\pi} \frac{d\Omega}{(2\pi)^{1/2}} J_\Omega \int \frac{d^2\xi}{J_F}, \tag{B1}$$

where S is the monopole action (39) and μ is the Pauli–Villars mass scale. The Jacobian factors J_a and J_F were calculated in Ref. 50:

$$J_a = (\mathrm{Re}\, S)^{3/2}, \quad J_F = 2\,\mathrm{Re}\, S, \tag{B2}$$

and S is the monopole action. The remaining Jacobian J_Ω is given by

$$J_\Omega = \frac{2\pi R (\mathrm{Re}\, S)^{1/2}}{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}. \tag{B3}$$

To derive this, we start with the general expression for the bosonic zero mode,

$$Z_m = \frac{\partial v_m^{(\Omega)}}{\partial\Omega} + D_m\Lambda, \tag{B4}$$

where $v_m^{(\Omega)}$ is the Ω-rotated monopole solution in the singular gauge,

$$v_m^{(\Omega)} = e^{i\Omega\tau^3} v_m e^{-i\Omega\tau^3}, \tag{B5}$$

and $D_m\Lambda$ is added to keep the zero mode in the covariant background gauge. Since

$$\frac{\partial v_m^{(\Omega)}}{\partial\Omega} = i\left[\frac{1}{2}\boldsymbol{\alpha}^*\cdot\mathbf{H},\ v_m\right], \tag{B6}$$

the choice of Λ is obvious [recall (16)]:

$$\Lambda = \frac{2\pi R}{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}\ \Phi^c\tau^c - \frac{1}{2}\boldsymbol{\alpha}^*\cdot\mathbf{H}. \tag{B7}$$

This gives

$$Z_m = \frac{2\pi R}{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}\ D_m(\Phi^c\tau^c) = \frac{2\pi R}{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}\ v_{m0}, \tag{B8}$$

and

$$J_\Omega \equiv \sqrt{\langle Z_m | Z_m\rangle} = \frac{2\pi R (\mathrm{Re}\, S)^{1/2}}{\boldsymbol{\alpha}\cdot\langle\boldsymbol{\varphi}\rangle}. \tag{B9}$$

Gathering all factors together, we find that the measure is

$$\frac{\mu^3 R}{g^2}\cdot\frac{2}{\boldsymbol{\alpha}^2}\cdot e^{-S}\int d^3a\ \ d\Omega\ \ d^2\xi. \tag{B10}$$

In contradistinction with the three-dimensional calculation of Ref. 50, our present calculation is locally four-dimensional, i.e., in the path integral we have integrated over the fluctuations around the monopole configuration in $\mathbb{R}^3\times S^1$. Thus, the UV-regularized determinants over nonzero eigenvalues of the quadratic fluctuation operators cancel between fermions and bosons due to supersymmetry as in Ref. 57. The ultra-violet divergences are regularized in the Pauli–Villars scheme, which explains the appearance of the Pauli–Villars mass scale μ.

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Products and ratios of characteristic polynomials of random Hermitian matrices

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(Received 7 April 2003; accepted 9 April 2003)

We present new and streamlined proofs of various formulas for products and ratios of characteristic polynomials of random Hermitian matrices that have appeared recently in the literature. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1587875]

I. INTRODUCTION

In random matrix theory, unitary ensembles of $N\times N$ matrices $\{H\}$ play a central role.[15] Such ensembles are described by a measure $d\alpha$ with finite moments $\int_{\mathrm{R}}|x|^k\,d\alpha(x)<\infty$, $k=0,1,2,...$, and the associated distribution function for the eigenvalues $\{x_i=x_i(H)\}$ of matrices H in the ensembles has the form

$$dP_{\alpha,N}(x)=\frac{1}{Z_N}\Delta(x)^2\,d\alpha(x), \tag{1.1}$$

where $d\alpha(x)=\Pi_{i=1}^{N}d\alpha(x_i)$, $\Delta(x)=\Pi_{N\geqslant i>j\geqslant 1}(x_i-x_j)$ is the Vandermonde determinant for the x_i's, and $Z_N=\int\cdots\int\Delta(x)^2\,d\alpha(x)$ is the normalization constant. The special case $d\alpha(x)=e^{-x^2}dx$ is known as the Gaussian unitary ensemble (GUE). For symmetric functions $f(x)=f(x_1,\ldots,x_N)$ of the x_i's,

$$\langle f\rangle_\alpha\equiv\frac{1}{Z_N}\int\cdots\int f(x)\Delta(x)^2\,d\alpha(x) \tag{1.2}$$

denotes the average of f with respect to $dP_{\alpha,N}$.

Recently there has been considerable interest in the averages of products and ratios of the characteristic polynomials $D_N[\mu,H]=\Pi_{i=1}^{N}(\mu-x_i(H))$ of random matrices with respect to various ensembles. Such averages are used, in particular, in making predictions about the moments of the Riemann-zeta function [see Refs. 12–14 (circular ensembles) and 3 (unitary ensembles)]. Many other uses are described, for example, in Refs. 1, 12, and 17.

By (1.2), for unitary ensembles, such averages have the form

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$$\left\langle \frac{\prod_{j=1}^{K} D_N[\mu_j,H]}{\prod_{j=1}^{M} D_N[\epsilon_j,H]} \right\rangle_\alpha = \frac{1}{Z_N}\int\cdots\int \frac{\prod_{j=1}^{K}\prod_{i=1}^{N}(\mu_j-x_i)}{\prod_{j=1}^{M}\prod_{j=1}^{N}(\epsilon_j-x_i)}\Delta(x)^2\,d\alpha(x). \tag{1.3}$$

In this article we consider certain explicit determinantal formulas for (1.3)—see (2.6), (2.24), (2.36), (3.3), and (3.12) below. Formula (2.6) is due to Brezin and Hikami[3] (see also Ref. 16, and when all the μ_j's are equal, see Ref. 10), whereas (2.24), (2.36), (3.3), and (3.12) are due to Fyodorov and Strahov.[17,11] References 17 and 11 also contain a discussion of the history of these formulas. The formulas (3.3) and (3.12) are particularly useful in proving universality results for the ratios (1.3) in the Dyson limit as $N\to\infty$ (see Ref. 17). For a discussion of other universality results, particularly the work of Brezin–Hikami and Fyodorov in special cases, we again refer the reader to Ref. 17. The asymptotic analysis in Ref. 17 is based on the reformulation of the orthogonal polynomial problem as a Riemann–Hilbert problem by Fokas, Its, and Kitaev.[9] The Riemann–Hilbert problem is then analyzed asymptotically using the noncommutative steepest-descent method introduced by Deift and Zhou,[5] and further developed with Venakides in Ref. 6 to allow for fully nonlinear oscillations, and in Refs. 7 and 8.

Our goal in this article is to give new, streamlined proofs of (2.6)–(3.12), using only the properties of orthogonal polynomials and a minimum of combinatorics. Along the way we will also need an integral version of the classical Binet–Cauchy-formula due to C. Andréief dating back to 1883 (see Lemma 2.1 below).

Let $\pi_j(z)=x^j+\cdots$ denote the jth monic orthogonal polynomial with respect to the measure $d\alpha$,

$$\int_{\mathrm{R}} \pi_j(x)\pi_k(x)d\alpha(x)=c_jc_k\delta_{jk};\quad j,k\geqslant 0, \tag{1.4}$$

where the norming constants c_j's are positive. The key observation in our approach is that for $K=1$ and $M=0$ in (1.3),

$$\langle D_N[\mu,H]\rangle_\alpha=\pi_N(\mu) \tag{1.5}$$

(see Ref. 18). In our words, the orthogonal polynomial $\pi_N(\mu)$ with respect to $d\alpha$ is also precisely the average polynomial $\Pi_{i=1}^{N}(\mu-x_i)$ with respect to $d\mathrm{P}_{\alpha,N}$. Formula (1.5) appears already in the work of Heine in the 1880s (see Ref. 18). Set

$$d\alpha^{[\ell,m]}(t)\equiv \frac{\prod_{j=1}^{\ell}(\mu_j-t)}{\prod_{j=1}^{m}(\epsilon_j-t)}d\alpha(t),\quad \ell,m\geqslant 0, \tag{1.6}$$

$[d\alpha^{[0,0]}(t)\equiv d\alpha(t)]$, and let $\pi_j^{[\ell,m]}(t)$ denote the jth monic orthogonal polynomial with respect to $d\alpha^{[\ell,m]}$. With this notation we see immediately from (1.3) and (1.5) that $\langle \mathrm{Q}_{j=1}^{K}D_N[\mu_j,H]/\mathrm{Q}_{j=1}^{M}D_N[\epsilon_j,H]\rangle_\alpha$ is proportional to $\pi_N^{[K-1,M]}(\mu_K)$. Using a classical determinantal formula of Christoffel (see Ref. 18) for $\pi_N^{[\ell,0]}(\mu)$ and a more recent formula of Uvarov[19] for $\pi_N^{[0,m]}(\mu)$, we are then led (see Sec. II) to (2.6), (2.24), and (2.36) in a rather straightforward way. Formula (3.3) appears to have a different character from (2.6), (2.24), and (2.36), and relies on Lemma 2.1 mentioned above, which computes the integral of the product of two determinants: formula (3.12) follows (see Sec. III) by combining (3.3) with (2.6) and (2.36). In Ref. 17 the authors present a variety of additional formulas for $\langle \mathrm{Q}_{j=1}^{K}D_N[\mu_j,H]/\mathrm{Q}_{j=1}^{M}D_N[\epsilon_j,H]\rangle_\alpha$ for cases of K and M not covered by (2.6)–(3.12): we leave it to the interested reader to verify that the method of this article can also be used to derive these formulas in a straightforward manner.

Remark 1.1: As is well known (see, e.g., Ref. 18), each measure $d\alpha$ gives rise to a tridiagonal operator

$$J=J(d\alpha)=\begin{pmatrix} a_1 & b_1 & 0 & \\ b_1 & a_2 & b_2 & \\ 0 & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \quad b_i>0, \tag{1.7}$$

with generalized eigenfunctions given by the orthonormal polynomials

$$p_j(x)=c_j^{-1}\pi_j(x), \quad j=0,1,..., \tag{1.8}$$

i.e.,

$$b_{j-1}p_{j-1}(x)+a_jp_j(x)+b_jp_{j+1}(x)=xp_j(x), \quad j\geqslant 1, \tag{1.9}$$

where $b_0\equiv 0$. Conversely, modulo certain essential self-adjointness issues, $d\alpha$ is the spectral measure for J in the cyclic subspace generated by J and the vector $e_1(1,0,0,...)^T$ (see, e.g., Ref. 4). It follows that the transformation of measures

$$d\alpha\rightarrow d\alpha^{[\ell,m]} \tag{1.10}$$

leads to the transformation of operators

$$J(d\alpha)\rightarrow J(d\alpha^{[\ell,m]}). \tag{1.11}$$

For appropriate choices of $\mu_1,\ldots,\mu_m$ and $\epsilon_1,\ldots,\epsilon_\ell$, such transformations correspond to removing m points from the spectrum of $J(d\alpha)$ and inserting ℓ points: in the spectral theory literature, such transformations are known as Darboux transformations. The formulas in this article clearly provide formulas for the generalized eigenfunctions $p_j^{[\ell,m]}(x)$ of the Darboux-transformed operator $J(d\alpha^{[\ell,m]})$, as well as the matrix entries, $a_j^{[\ell,m]}$ and $b_j^{[\ell,m]}$, in terms of the corresponding objects for $J(d\alpha)$. Again we leave the details to the reader. Here the elementary formulas

$$b_n^2(d\alpha)=\frac{n+1}{n+2}\frac{Z_n(d\alpha)Z_{n+2}(d\alpha)}{(Z_{n+1}(d\alpha))^2}, \quad a_n(d\alpha)=\frac{d}{dt}\bigg|_{t=0}\log\frac{Z_n(d\alpha_t)}{Z_{n+1}(d\alpha_t)}, \tag{1.12}$$

where $d\alpha_t(x)=e^{tx}d\alpha(x)$, are useful.

Technical Remark 1.2: Formulas (2.6)–(3.12) clearly do not make sense for all values of the parameters. In **all the calculations that follow, we will assume that** $d\alpha$ **has compact support, support** $(d\alpha)=[-Q,Q]$, **say, and that the** μ_i**'s and** ϵ_j**'s are distinct real numbers greater than** Q: under these assumptions, $d\alpha^{[\ell,m]}(t)$ becomes, in particular, a bona fide measure, etc. By analytic continuation one sees that the formulas remain true for complex values of $\{\mu_i\}$ and $\{\epsilon_j\}$, as long as they remain distinct. Furthermore, if the μ_j's and ϵ_j's are distinct, and $\mathrm{Im}(\epsilon_j)\neq 0$ for all j, then we can let $Q\rightarrow\infty$ and so the formulas are true for measures $d\alpha$ with unbounded support. Finally, we can, for example, let $\mu_j\rightarrow\mu_k$ for some $j\neq k$, which leads to formulas involving derivatives of the π_j's, etc.

II. FORMULAS OF CHRISTOFFEL–UVAROV TYPE

We use the notations $d\alpha$, π_j, $d\alpha^{[\ell,m]}$, $\pi_j^{[\ell,m]}$,... of Sec. I. In addition, in all the calculations that follow we assume that $d\alpha$, $\{\mu_j\}$, $\{\epsilon_k\}$ satisfy the conditions described in Technical Remark 1.2 above: the natural analytical continuation of the formulas obtained to complex values of the parameters, and the limit $Q\rightarrow\infty$, is left to the reader.

The following result of Christoffel (see Ref. 18) plays a basic role in what follows.

Lemma 2.1: Consider the measure $d\alpha^{[\ell,0]}(t)=\Pi_{j=1}^{\ell}(\mu_j-t)d\alpha(t)$, *where* $\ell=1,2,...$. *Then the* n*th monic orthogonal polynomial* $\pi_n^{[\ell,0]}(t)$ *associated with the new measure* $d\alpha^{[\ell,0]}(t)$ *can be expressed as follows:*

$$\pi_n^{[\ell,0]}(t)=\frac{1}{(t-\mu_1)\cdots(t-\mu_\ell)}\frac{\begin{vmatrix}\pi_n(\mu_1) & \cdots & \pi_{n+\ell}(\mu_1)\\ \vdots & & \\ \pi_n(\mu_\ell) & \cdots & \pi_{n+\ell}(\mu_\ell)\\ \pi_n(t) & \cdots & \pi_{n+\ell}(t)\end{vmatrix}}{\begin{vmatrix}\pi_n(\mu_1) & \cdots & \pi_{n+\ell-1}(\mu_1)\\ \vdots & & \\ \pi_n(\mu_\ell) & \cdots & \pi_{n+\ell-1}(\mu_\ell)\end{vmatrix}}. \tag{2.1}$$

Proof: Set

$$q_n^{[\ell,0]}(t)=\begin{vmatrix}\pi_n(\mu_1) & \cdots & \pi_{n+\ell}(\mu_1)\\ \vdots & & \\ \pi_n(\mu_\ell) & \cdots & \pi_{n+\ell}(\mu_\ell)\\ \pi_n(t) & \cdots & \pi_{n+\ell}(t)\end{vmatrix}. \tag{2.2}$$

We note that $q_n^{[\ell,0]}(t)$ satisfies the condition $\int t^j q_n^{[\ell,0]}(t)d\alpha(t)=0$ for all $j\in\{0,...,n-1\}$. Also $q_n^{[\ell,0]}(\mu_j)=0$, $j=1,...,\ell$, and so $q_n^{[\ell,0]}(t)/[(\mu_1-t)\cdots(\mu_\ell-t)]$ is a polynomial of degree at most n. Now observe that

$$\int t^j\left[\frac{q_n^{[\ell,0]}(t)}{(\mu_1-t)\cdots(\mu_\ell-t)}\right]d\alpha^{[\ell,0]}(t)=0,\quad 0\leqslant j<n, \tag{2.3}$$

which means that $q_n^{[\ell,0]}(t)$ divided by the product $(\mu_1-t)\cdots(\mu_\ell-t)$ is proportional to the nth monic orthogonal polynomial $\pi_n^{[\ell,0]}(t)$ associated with the new measure $d\alpha^{[\ell,0]}(t)$. Now $q_n^{[\ell,0]}\times(t)$ cannot vanish for any $t=\mu_{\ell+1}>Q$, $\mu_{\ell+1}\notin\{\mu_1,...,\mu_\ell\}$. Indeed, if $q_n^{[\ell,0]}(\mu_{\ell+1})=0$, then there exist $\{\alpha_i\}_{i=0}^{\ell}$, not all zero, such that $p(t)\equiv\Sigma_{i=0}^{\ell}\alpha_i\pi_{n+i}(t)$ vanishes at $\{\mu_i\}_{i=1}^{\ell+1}$. Thus $\tilde{p}(t)\equiv p(t)/\Pi_{i=1}^{\ell+1}(\mu_i-t)$ is a polynomial of order $<n$, and as above, $\tilde{p}(t)$ is orthogonal to t^j, $0\leqslant j<n$, with respect to the measure $d\alpha^{[\ell+1,0]}(t)$. Thus $\tilde{p}(t)\equiv 0$ and hence $\alpha_0=\cdots=\alpha_\ell=0$, which is a contradiction. Replacing ℓ by $\ell-1$, we conclude that

$$\begin{vmatrix}\pi_n(\mu_1) & \cdots & \pi_{n+\ell-1}(\mu_1)\\ \vdots & & \\ \pi_n(\mu_\ell) & \cdots & \pi_{n+\ell-1}(\mu_\ell)\end{vmatrix}\neq 0. \tag{2.4}$$

Taking the limit $t\to\infty$ and noting that the coefficient of the highest degree of $\pi_n^{[\ell,0]}(t)$ should be equal to 1, we find the coefficient of proportionality and establish formula (2.1). □

Representation (2.1) for the monic orthogonal polynomials associated with the measure $d\alpha^{[\ell,0]}(t)$ immediately leads to the following result:

Corollary 2.2: The product of monic orthogonal polynomials $\Pi_{j=0}^{\ell}\pi_n^{[j,0]}(\mu_{j+1})$ *defined with respect to the different measures* $d\alpha^{[j,0]}(t)\equiv(\mu_j-t)\cdots(\mu_1-t)d\alpha(t)$ *is given by the formula*

$$\prod_{j=0}^{\ell}\pi_n^{[j,0]}(\mu_{j+1})=\frac{1}{\Delta(\mu)}\begin{vmatrix}\pi_n(\mu_1) & \cdots & \pi_{n+\ell}(\mu_1)\\ \vdots & & \\ \pi_n(\mu_{\ell+1}) & \cdots & \pi_{n+\ell}(\mu_{\ell+1})\end{vmatrix}, \tag{2.5}$$

where $\Delta(\mu)=\Pi_{\ell+1\geqslant i>j\geqslant 1}(\mu_i-\mu_j)$.

We observe that Corollary 2.2 gives the identity for the average of products of random characteristic polynomials obtained first by Brezin and Hikami.[3]

Theorem 2.3: *Let* $D_N[\mu,H]$ *be the characteristic polynomial of the Hermitian matrix H. The following identity is valid:*

$$\left\langle \prod_{j=1}^{L} D_N[\mu_j,H] \right\rangle_\alpha = \frac{1}{\Delta(\mu)} \begin{vmatrix} \pi_N(\mu_1) & \cdots & \pi_{N+L-1}(\mu_1) \\ \vdots & & \\ \pi_N(\mu_L) & \cdots & \pi_{N+L-1}(\mu_L) \end{vmatrix}, \tag{2.6}$$

where the average is defined by (1.2).

Proof: To prove formula (2.6) we use the representation for the monic orthogonal polynomials in the case $L=1$ given in (1.5),

$$\pi_N(\mu) = \frac{1}{Z_N} \int \cdots \int \prod_{i=1}^{N} (\mu - x_i) \Delta^2(x) d\alpha(x). \tag{2.7}$$

Let $Z_N^{[\ell,0]}$ be defined by

$$Z_N^{[\ell,0]} = \int \cdots \int \Delta^2(x) d\alpha^{[\ell,0]}(x), \quad \ell = 1,2,..., \tag{2.8}$$

where $d\alpha^{[\ell,0]}(x) = \Pi_{i=1}^{N} d\alpha^{[\ell,0]}(x_i)$. With this notation, we have

$$\left\langle \prod_{j=1}^{L} D_N[\mu_j,H] \right\rangle_\alpha = \frac{Z_N^{[L,0]}}{Z_N} = \frac{Z_N^{[L,0]}}{Z_N^{[L-1,0]}} \frac{Z_N^{[L-1,0]}}{Z_N^{[L-2,0]}} \cdots \frac{Z_N^{[1,0]}}{Z_N}. \tag{2.9}$$

Equation (2.7) implies that $\pi_n^{[\ell-1,0]}(\mu_\ell)$ can be represented as the ratio $Z_N^{[\ell,0]}/Z_N^{[\ell-1,0]}$, where $\pi_N^{[0,0]}(\mu) \equiv \pi_N(\mu)$, and $Z_N^{[0,0]} \equiv Z_N$. Thus we obtain

$$\left\langle \prod_{j=1}^{L} D_N[\mu_j,H] \right\rangle_\alpha = \prod_{j=0}^{L-1} \pi_N^{[j,0]}(\mu_{j+1}). \tag{2.10}$$

The above equation together with Corollary 2.2 proves formula (2.6). □

Remark 2.4: Notice [see Eqs. (2.7) and (2.10)] that the average of products of characteristic polynomials can be rewritten as a product of averages. Namely,

$$\left\langle \prod_{j=1}^{L} D_N[\mu_j,H] \right\rangle_\alpha = \prod_{j=1}^{L} \langle D_N[\mu_j,H] \rangle_{\alpha^{[j-1,0]}}, \tag{2.11}$$

where $\langle \cdots \rangle_{\alpha^{[j-1,0]}}$ means the average defined by Eq. (1.2) but with respect to the new measure $d\alpha^{[j-1,0]}(x)$, and $d\alpha(x) \equiv d\alpha^{[0,0]}(x)$.

The formula of Christoffel [Eq. (2.1)] enables us to construct the orthogonal polynomials associated with the measure $d\alpha^{[\ell,0]}(t) = \Pi_{j=1}^{\ell}(\mu_j - t) d\alpha(t)$ in terms of the orthogonal polynomials associated with the measure $d\alpha(t)$. Now we derive a formula due to Uvarov[19] expressing the monic orthogonal polynomials $\pi_n^{[0,m]}(t)$ associated with the measure $d\alpha^{[0,m]}(t) = \Pi_{j=1}^{m}(\epsilon_j - t)^{-1} d\alpha(t)$, again in terms of the monic orthogonal polynomials $\pi_n(t)$ associated with the measure $d\alpha(t)$.

Lemma 2.5: Suppose $0 \leqslant m \leqslant n$. *The monic orthogonal polynomials* $\pi_n^{[0,m]}(t)$ *associated with the measure* $d\alpha^{[0,m]}(t)$ *can be expressed as ratios of determinants.*

$$\pi_n^{[0,m]}(t)=\frac{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_n(\epsilon_1) \\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_n(\epsilon_m) \\ \pi_{n-m}(t) & \cdots & \pi_n(t) \end{vmatrix}}{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_{n-1}(\epsilon_1) \\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_{n-1}(\epsilon_m) \end{vmatrix}}. \tag{2.12}$$

Here the $h_k(\epsilon_j)$'s are the Cauchy transformations of the monic orthogonal polynomials $\pi_k(t)$.

$$h_k(\epsilon_j)=\frac{1}{2\pi i}\int \frac{\pi_k(t)d\alpha(t)}{t-\epsilon_j}. \tag{2.13}$$

Proof: Set

$$q_n^{[0,m]}(t)=\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_n(\epsilon_1) \\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_n(\epsilon_m) \\ \pi_{n-m}(t) & \cdots & \pi_n(t) \end{vmatrix}. \tag{2.14}$$

Now $q_n^{[0,m]}(t)$ is proportional to the nth monic orthogonal polynomial $\pi_n^{[0,m]}(t)$ with respect to the measure $d\alpha^{[0,m]}(t)$. Indeed, first observe that

$$\int \frac{q_n^{[0,m]}(t)}{t-\epsilon_j}d\alpha(t)=0, \quad j=1,...,m. \tag{2.15}$$

Also, for $0\leqslant k<n$,

$$\frac{t^k}{\Pi_{\ell=1}^m(\epsilon_\ell-t)}=\sum_{\ell=1}^m \frac{\beta_\ell}{\epsilon_\ell-t}+p(t) \tag{2.16}$$

for suitable constants $\{\beta_\ell\}$ and for some polynomial $p(t)$ of degree $<n-m$. But for $0\leqslant k<n$,

$$\int t^k q_n^{[0,m]}(t)d\alpha^{[0,m]}(t)=-\sum_{\ell=1}^m \beta_\ell\int \frac{q_n^{[0,m]}(t)}{t-\epsilon_\ell}d\alpha(t)+\int p(t)q_n^{[0,m]}(t)d\alpha(t). \tag{2.17}$$

The terms in the sum are zero by (2.15) and the final integral is zero by the construction (2.14) of $q_n^{[0,m]}(t)$ and the fact that deg $p(t)<n-m$. Thus $q_n^{[0,m]}(t)$ is proportional to $\pi_n^{[0,m]}(t)$. An argument similar to the proof in Lemma 2.1, that

$$\begin{vmatrix} \pi_n(\mu_1) & \cdots & \pi_{n+\ell-1}(\mu_1) \\ \vdots & & \\ \pi_n(\mu_\ell) & \cdots & \pi_{n+\ell-1}(\mu_\ell) \end{vmatrix}\neq 0, \tag{2.18}$$

shows that the denominator in (2.12) does not vanish. Letting $t\to\infty$ in (2.14), and matching leading terms, we prove Lemma 2.5. □

Remark 2.6: In Ref. 19, Uvarov obtains formulas for $\pi_n^{[0,m]}(t)$ of type (2.12) also in the case $m>n$. These formulas can be used to obtain analogs of (2.24) and (2.36) below in the case $M>N$.

Remark 2.7: As noted in Refs. 11 and 17, the Cauchy transformations $h_k(\epsilon)$ of the π_k's occur explicitly, together with the π_k's, in the solution of the Fokas–Its–Kitaev Riemann–Hilbert problem for orthogonal polynomials.[9]

Lemma 2.5 implies the following analog of the Christoffel formula for the Cauchy transforms of monic orthogonal polynomials.

Corollary 2.8: Let $h_k^{[0,m]}(\epsilon)$ be the Cauchy transform of the monic polynomial $\pi_k^{[0,m]}(t)$. with respect to the measure $d\alpha^{[0,m]}(t)$,

$$h_k^{[0,m]}(\epsilon)=\frac{1}{2\pi i}\int \frac{\pi_k^{[0,m]}(t)}{t-\epsilon}d\alpha^{[0,m]}(t). \tag{2.19}$$

Let also $0\leqslant m\leqslant n$. Then $h_n^{[0,m]}(\epsilon)$ has a representation similar to that for the monic orthogonal polynomials $\pi_n^{[\ell,0]}(t)$ [Eq. (2.1)],

$$h_n^{[0,m]}(\epsilon)=\frac{(-1)^m}{(\epsilon-\epsilon_m)\cdots(\epsilon-\epsilon_1)}\frac{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_n(\epsilon_1)\\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_n(\epsilon_m)\\ h_{n-m}(\epsilon) & \cdots & h_n(\epsilon)\end{vmatrix}}{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_{n-1}(\epsilon_1)\\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_{n-1}(\epsilon_m)\end{vmatrix}}. \tag{2.20}$$

Proof: The above representation follows from formula (2.12) and from the fact that

$$\frac{1}{(t-\epsilon_{m+1})\cdots(t-\epsilon_1)}=\sum_{j=1}^{m+1}\frac{1}{t-\epsilon_j}\prod_{k\neq j}\frac{1}{\epsilon_j-\epsilon_k}. \tag{2.21}$$

Indeed we find from formula (2.12) that $h_n^{[0,m]}(\epsilon)$ is the ratio of the determinants. The elements of the last row of the determinant in the numerator are the integrals

$$\frac{1}{2\pi i}\int\frac{\pi_{n-k}(t)d\alpha(t)}{(t-\epsilon)(t-\epsilon_m)\cdots(t-\epsilon_1)},\quad 0\leqslant k\leqslant m.$$

Using identity (2.21) and noting that the only term

$$\frac{1}{t-\epsilon}\frac{1}{(\epsilon-\epsilon_m)\cdots(\epsilon-\epsilon_1)} \tag{2.22}$$

of the sum (2.21) contributes to the determinant, (2.20) follows. □

Equation (2.20) immediately implies the following analogy of (2.5) for the $h_k^{[0,m]}$'s.

Corollary 2.9: Let $0\leqslant m\leqslant n$. Then the product of the Cauchy transforms of monic orthogonal polynomials with respect to the measures $d\alpha^{[0,j]}(t)$, $0\leqslant j\leqslant m$, can be written as a determinant,

$$\prod_{j=0}^{m}h_{n-m+j}^{[0,j]}(\epsilon_{j+1})=\frac{(-1)m(m+1)/2}{\Delta(\epsilon)}\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_n(\epsilon_1)\\ \vdots & & \\ h_{n-m}(\epsilon_{m+1}) & \cdots & h_n(\epsilon_{m+1})\end{vmatrix}. \tag{2.23}$$

Now we derive the identity for the average of the product of inverse random characteristic polynomials.

Theorem 2.10: *Suppose $1\leqslant M\leqslant N$ and let $\gamma_n=-2\pi i/c_n^2$, where c_n is the normality constant defined by Eq. (1.4). Then we have the following formula:*

$$\left\langle \prod_{j=1}^{M} D_N^{-1}[\epsilon_j,H] \right\rangle_\alpha = (-1)^{M(M-1)/2} \frac{\prod_{j=N-M}^{N-1} \gamma_j}{\Delta(\epsilon)} \begin{vmatrix} h_{N-M}(\epsilon_1) & \cdots & h_{N-1}(\epsilon_1) \\ \vdots & & \\ h_{N-M}(\epsilon_M) & \cdots & h_{N-1}(\epsilon_M) \end{vmatrix}. \quad (2.24)$$

Proof: When $M=1$, we use the identity (2.21) together with (2.7) and the relation (see, e.g., Ref. 18)

$$\gamma_{n-1} = -2\pi i n \frac{Z_{n-1}}{Z_n} \quad (2.25)$$

to obtain

$$\langle D_N^{-1}[\epsilon,H] \rangle_\alpha = \gamma_{N-1} h_{N-1}(\epsilon). \quad (2.26)$$

We rewrite the average in Eq. (2.24) as follows:

$$\left\langle \prod_{j=1}^{M} D_N^{-1}[\epsilon_j,H] \right\rangle_\alpha = \frac{Z_N^{[0,M]}}{Z_{N-1}^{[0,M-1]}} \frac{Z_{N-1}^{[0,M-1]}}{Z_{N-2}^{[0,M-2]}} \cdots \frac{Z_{N-M}^{[0,0]}}{Z_N^{[0,0]}}, \quad (2.27)$$

where

$$Z_N^{[0,M]} = \int \cdots \int \Delta^2(x) d\alpha^{[0,M]}(x), \quad (2.28)$$

$Z_N^{[0,0]} \equiv Z_N$ and $d\alpha^{[0,0]}(x) = d\alpha(x)$. The following relation can be observed from Eqs. (2.26) and (2.25):

$$\frac{Z_{N-K}^{[0,m]}}{Z_{N-K-1}^{[0,m-1]}} = -2\pi i (N-K) h_{N-K-1}^{[0,m-1]}(\epsilon_m). \quad (2.29)$$

Inserting this relation in (2.27) we find

$$\left\langle \prod_{j=1}^{M} D_N^{-1}[\epsilon_j,H] \right\rangle_\alpha = \prod_{j=1}^{M} \gamma_{N-j} h_{N-j}^{[0,M-j]}(\epsilon_{M-j+1}). \quad (2.30)$$

Our result (2.24) immediately follows from the above equation and formula (2.23). □

We now repeat the above considerations for the case

$$d\alpha^{[\ell,m]}(t) = \frac{(\mu_1 - t)\cdots(\mu_\ell - t)}{(\epsilon_1 - t)\cdots(\epsilon_m - t)} d\alpha(t). \quad (2.31)$$

The first result is a Christoffel-type formula for the measure (2.31), which is due to Uvarov.[19]

Lemma 2.11: Suppose $0 \leqslant m \leqslant n$. *Then the monic orthogonal polynomials* $\pi_n^{[\ell,m]}(t)$'s *with respect to the measure* $d\alpha^{\ell,m]}(t)$ *have the following representation:*

$$\pi_n^{[\ell,m]}(t)=\frac{1}{(t-\mu_\ell)\cdots(t-\mu_1)}\frac{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_{n+\ell}(\epsilon_1)\\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_{n+\ell}(\epsilon_m)\\ \pi_{n-m}(\mu_1) & \cdots & \pi_{n+\ell}(\mu_1)\\ \vdots & & \\ \pi_{n-m}(\mu_\ell) & \cdots & \pi_{n+\ell}(\mu_\ell)\\ \pi_{n-m}(t) & \cdots & \pi_{n+\ell}(t)\end{vmatrix}}{\begin{vmatrix} h_{n-m}(\epsilon_1) & \cdots & h_{n+\ell}(\epsilon_1)\\ \vdots & & \\ h_{n-m}(\epsilon_m) & \cdots & h_{n+\ell}(\epsilon_m)\\ \pi_{n-m}(\mu_1) & \cdots & \pi_{n+\ell}(\mu_1)\\ \vdots & & \\ \pi_{n-m}(\mu_\ell) & \cdots & \pi_{n+\ell}(\mu_\ell)\end{vmatrix}}. \tag{2.32}$$

Proof: As in the previous cases we define $q_n^{[\ell,m]}(t)$ to be the determinant in the numerator of (2.32). Observe that

$$q_n^{[\ell,m]}(\mu_1)=\cdots=q_n^{[\ell,m]}(\mu_\ell)=0 \tag{2.33}$$

and that

$$\int \frac{q_n^{[\ell,m]}(t)d\alpha(t)}{\epsilon_1-t}=\cdots=\int \frac{q_n^{[\ell,m]}(t)d\alpha(t)}{\epsilon_m-t}=0. \tag{2.34}$$

The next steps are the same as in the proofs of Lemma 2.1 and Lemma 2.5. □

Corollary 2.12:

$$\left\langle \prod_{j=1}^{K} D_N[\mu_j,H] \right\rangle_{\alpha^{[0,M]}}=\frac{1}{\Delta(\mu)}\frac{\begin{vmatrix} h_{N-M}(\epsilon_1) & \cdots & h_{N+K-1}(\epsilon_1)\\ \vdots & & \\ h_{N-M}(\epsilon_M) & \cdots & h_{N+K-1}(\epsilon_M)\\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+K-1}(\mu_1)\\ \vdots & & \\ \pi_{N-M}(\mu_K) & \cdots & \pi_{N+K-1}(\mu_K)\end{vmatrix}}{\begin{vmatrix} h_{N-M}(\epsilon_1) & \cdots & h_N(\epsilon_1)\\ \vdots & & \\ h_{N-M}(\epsilon_M) & \cdots & h_N(\epsilon_M)\end{vmatrix}}. \tag{2.35}$$

Proof: Identity (2.35) follows from Eqs. (2.10) and (2.32) once we note that Eq. (2.32) can be rewritten in a similar manner as Eq. (2.5). □

Finally we generalize Theorems 2.3 and 2.10 and obtain a formula for the average of ratios of characteristic polynomials.

Theorem 2.13: *Suppose* $0\leqslant M\leqslant N$. *Then the average of ratios of characteristic polynomials of* $N\times N$ *Hermitian matrices H is given by the following formula:*

$$\left\langle \frac{\prod_{j=1}^{K} D_N[\mu_j,H]}{\prod_{j=1}^{M} D_N[\epsilon_j,H]} \right\rangle_{\alpha} = \frac{(-1)^{M(M-1)/2} \prod_{j=N-M}^{N-1} \gamma_j}{\Delta(\mu)\Delta(\epsilon)} \begin{vmatrix} h_{N-M}(\epsilon_1) & \cdots & h_{N+K-1}(\epsilon_1) \\ \vdots & & \\ h_{N-M}(\epsilon_M) & \cdots & h_{N+K-1}(\epsilon_M) \\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+K-1}(\mu_1) \\ \vdots & & \\ \pi_{N-M}(\mu_K) & \cdots & \pi_{N+K-1}(\mu_K) \end{vmatrix}. \tag{2.36}$$

Proof: Let $\alpha^{[0,0]} \equiv \alpha$, $Z_n^{[0,0]} \equiv Z_n$. Then we have

$$\left\langle \frac{\prod_{j=1}^{K} D_N[\mu_j,H]}{\prod_{j=1}^{M} D_N[\epsilon_j,H]} \right\rangle_{\alpha} = \frac{Z_N^{[K,M]}}{Z_N^{[0,0]}} = \frac{Z_N^{[K,M]}}{Z_N^{[0,M]}} \frac{Z_N^{[0,M]}}{Z_N^{[0,0]}}, \tag{2.37}$$

i.e.,

$$\left\langle \frac{\prod_{j=1}^{K} D_N[\mu_j,H]}{\prod_{j=1}^{M} D_N[\epsilon_j,H]} \right\rangle_{\alpha} = \left\langle \prod_{j=1}^{K} D_N[\mu_j,H] \right\rangle_{\alpha^{[0,M]}} \left\langle \prod_{j=1}^{M} D_N^{-1}[\epsilon_j,H] \right\rangle_{\alpha}. \tag{2.38}$$

We use Corollary 2.12 and Theorem 2.10 to obtain formula (2.36). □

Remark 2.14: Observe that formulas (2.6) and (2.24) do not follow immediately as special cases of (2.36): some further algebraic manipulation is required. Similarly, the process of adding and removing zeros is clearly reciprocal. More precisely, given $\epsilon_1,\ldots,\epsilon_\ell$, we can construct the polynomials $\pi_n^{[0,\ell]}(t;d\alpha^{[0,\ell]})$ associated with the measure $d\alpha^{[0,\ell]}(t) = (\Pi_{i=1}^{\ell}(\epsilon_i - t)^{-1})dt$ by (2.12): We can then construct $\pi_n^{[\ell,0]}(t;d(\alpha^{[0,\ell]})^{[\ell,0]})$ with $\mu_i = \epsilon_i$, inserting $\pi_n^{[0,\ell]}(t;d\alpha^{[0,\ell]})$ for $\pi_n(t)$ on the right-hand side of (2.1). We should find that $\pi_n^{[\ell,0]}(t;d(\alpha^{[0,\ell]})^{[\ell,0]}) = \pi_n(t;d\alpha)$. However, again, this relation is not immediately clear, and requires further algebraic manipulation.

III. FORMULAS OF TWO-POINT FUNCTION TYPE

The following integral version of the Binet–Cauchy formula is due to Andréief,[2] and plays a basic role in our calculations.

Lemma 3.1: Let $(X,d\mu)$ be a measure space and suppose f_i, $g_j \in L^2(X,d\mu)$ for $1 \leqslant i,j \leqslant k$. Then

$$\int_X \cdots \int_X \det(f_i(x_j))_{1\leqslant i,j\leqslant k} \det(g_i(x_j))_{1\leqslant i,j\leqslant k}\, d\mu(x_1)\cdots d\mu(x_k)$$

$$= k!\, \det\left(\int_X f_i(x) g_j(x) d\mu(x) \right)_{1\leqslant i,j\leqslant k}. \tag{3.1}$$

Proof: Set $c_{ij} = \int_X f_i(x) g_j(x) d\mu(x)$. Then

$$\int_X \cdots \int_X \det(f_i(x_j))_{1\leqslant i,j\leqslant k} \det(g_i(x_j))_{1\leqslant i,j\leqslant k}\, d\mu(x_1)\cdots d\mu(x_k)$$

$$= \sum_{\sigma,\tau\in S_k} \operatorname{sgn}(\sigma)\operatorname{sgn}(\tau) c_{\sigma(1)\tau(1)}\cdots c_{\sigma(k)\tau(k)} = \sum_{\sigma} \operatorname{sgn}(\sigma) \sum_{\tau} \operatorname{sgn}(\tau\circ\sigma) c_{\sigma(1)\tau\circ\sigma(1)}\cdots c_{\sigma(k)\tau\circ\sigma(k)}$$

$$= \sum_{\sigma} (\operatorname{sgn}(\sigma))^2 \sum_{\tau} \operatorname{sgn}(\tau) c_{1\tau(1)}\cdots c_{k\tau(k)} = k!\, \det(c_{ij})_{1\leqslant i,j\leqslant k} \tag{3.2}$$

as desired. In (3.2) we used $\mathrm{sgn}(\tau\circ\sigma)=(\mathrm{sgn}\,\tau)(\mathrm{sgn}\,\sigma)$ and the fact that $c_{\sigma(1)\tau\circ\sigma(1)}\cdots c_{\sigma(k)\tau\circ\sigma(k)}=c_{1\tau(1)}\cdots c_{k\tau(k)}$ for all σ. □

Theorem 3.2: *Let $K\geqslant 1$. Then the following identity is valid:*

$$\left\langle \prod_{j=1}^{K} D_N[\lambda_j,H]D_N[\mu_j,H]\right\rangle_\alpha = \frac{C_{N,K}}{\Delta(\lambda)\Delta(\mu)}\det(W_{I,N+K}(\lambda_i,\mu_j))_{1\leqslant i,j\leqslant K}, \tag{3.3}$$

where

$$W_{I,N+K}(x,y)=\frac{\pi_{N+K}(x)\pi_{N+K-1}(y)-\pi_{N+K}(y)\pi_{N+K-1}(y)}{x-y} \tag{3.4}$$

and

$$C_{N,K}=\frac{\prod_{\ell=N}^{N+K-1} c_\ell^2}{(c_{N+K-1})^{2K}} \tag{3.5}$$

where c_ℓ is again the norming constant for π_ℓ given in (1.4).

Proof: Let $p_j(x)=c_j^{-1}\pi_j(x)$, $j\geqslant 0$, denote the orthonormal polynomials with respect to $d\alpha$. From (1.2) we obtain

$$\left\langle \prod_{j=1}^{K} D_N[\lambda_j,H]D_N[\mu_j,H]\right\rangle_\alpha = \frac{1}{Z_N\Delta(\lambda)\Delta(\mu)}\int\cdots\int \Delta(x,\lambda)\Delta(x,\mu)\,d\alpha(x). \tag{3.6}$$

Adding columns, we see that the Vandermonde determinant $\Delta(x,\lambda)$ has the form

$$\begin{vmatrix} \pi_0(x_1) & \pi_1(x_1) & \cdots & \pi_{N+K-1}(x_1)\\ \vdots & & & \\ \pi_0(x_N) & \pi_1(x_N) & \cdots & \pi_{N+K-1}(x_N)\\ \pi_0(\lambda_1) & \pi_1(\lambda_1) & \cdots & \pi_{N+K-1}(\lambda_1)\\ \vdots & & & \\ \pi_0(\lambda_K) & \pi_1(\lambda_K) & \cdots & \pi_{N+K-1}(\lambda_K)\end{vmatrix} \tag{3.7}$$

and similarly for $\Delta(x,\mu)$. Here $\pi_j(t)=\pi_j^{[0,0]}(t)$. The determinant $\Delta(x,\lambda)$ can be evaluated by a Lagrange expansion of the form

$$\sum_{0\leqslant i_1<i_2<\cdots<i_k\leqslant N+K-1}\sigma_{i_1,\ldots,i_K}\begin{vmatrix}\pi_{i_1}(\lambda_1) & \cdots & \pi_{i_K}(\lambda_1)\\ \vdots & & \\ \pi_{i_1}(\lambda_K) & \cdots & \pi_{i_K}(\lambda_K)\end{vmatrix}\begin{vmatrix}\pi_{j_1}(x_1) & \cdots & \pi_{j_N}(x_1)\\ \vdots & & \\ \pi_{j_1}(x_N) & \cdots & \pi_{j_N}(x_N)\end{vmatrix}, \tag{3.8}$$

where $\sigma_{i_1,\ldots,i_K}=\pm 1$ is an appropriate signature and $\{(j_1,\ldots,j_N):0\leqslant j_1<j_2<\cdots<j_N\leqslant N+K-1\}$ is the complement of $\{i_1,\ldots,i_K\}$ in $\{0,1,\ldots,N+K-1\}$. Multiplying (3.8) by a similar expansion for $\Delta(x,\mu)$, and inserting in (3.6), we obtain a sum of terms of the form

$$\int\cdots\int\begin{vmatrix}\pi_{j_1}(x_1) & \cdots & \pi_{j_K}(x_1)\\ \vdots & & \\ \pi_{j_1}(x_N) & \cdots & \pi_{j_K}(x_N)\end{vmatrix}\begin{vmatrix}\pi_{j_1'}(x_1) & \cdots & \pi_{j_N'}(x_1)\\ \vdots & & \\ \pi_{j_1'}(x_N) & \cdots & \pi_{j_N'}(x_N)\end{vmatrix} d\alpha(x), \tag{3.9}$$

which is equal by Lemma 3.1 to $N!\det(\int \pi_{j_i'}(x)\pi_{j_k}(x)d\alpha(x))_{1\leqslant i,k\leqslant N}=N!\det(\delta_{j_i' j_k}c_{j_k}^2)_{1\leqslant i,k\leqslant N}$. From this we see that

$$\begin{aligned}
&\left\langle \prod_{j=1}^{K} D_N[\lambda_j,H]D_N[\mu_j,H]\right\rangle_\alpha \\
&\quad=\frac{N!}{Z_N\Delta(\lambda)\Delta(\mu)}\sum_{0\leqslant i_1<\cdots<i_k\leqslant N+K-1}\sigma_{i_1,\ldots,i_K}^2\begin{vmatrix}\pi_{i_1}(\lambda_1) & \cdots & \pi_{i_K}(\lambda_1)\\ \vdots & & \\ \pi_{i_1}(\lambda_K) & \cdots & \pi_{i_K}(\lambda_K)\end{vmatrix}\\
&\qquad\times\prod_{k=1}^{N}c_{j_k}^2\begin{vmatrix}\pi_{i_1}(\mu_1) & \cdots & \pi_{i_K}(\mu_1)\\ \vdots & & \\ \pi_{i_1}(\mu_K) & \cdots & \pi_{i_K}(\mu_K)\end{vmatrix}\\
&\quad=\frac{N!\Pi_{q=N}^{N+K-1}c_q^2}{Z_N\Delta(x,\lambda)\Delta(x,\mu)}\sum_{0\leqslant i_1<\cdots<i_k\leqslant N+K-1}\det(p_{i_j}(\lambda_k))_{1\leqslant j,k\leqslant K}\det(p_{i_j}(\mu_k))_{1\leqslant j,k\leqslant K}\\
&\quad=\frac{N!\Pi_{q=N}^{N+K-1}c_q^2}{Z_N\Delta(x,\lambda)\Delta(x,\mu)}\det\left(\sum_{0\leqslant i\leqslant N+K-1}p_i(\lambda_j)p_i(\mu_k)\right)_{1\leqslant j,k\leqslant K},
\end{aligned}\tag{3.10}$$

where the last line follows by applying Lemma 3.1 to the discrete measure $d\mu=\Sigma_{i=0}^{N+K-1}\delta_i$. But, by the Christoffel–Darboux formula,

$$\sum_{0\leqslant i\leqslant N+K-1}p_i(\lambda_j)p_i(\mu_k)=\frac{\pi_{N+K}(\lambda_j)\pi_{N+K-1}(\mu_k)-\pi_{N+K}(\mu_k)\pi_{N+K-1}(\lambda_j)}{\lambda_j-\mu_k},\tag{3.11}$$

which then implies (3.3) as $Z_N=N!\Pi_{\ell=0}^{N-1}c_\ell^2$ (see, e.g., Ref. 18). □

Theorem 3.3: *Suppose* $1\leqslant K\leqslant N$. *Then the following identity is valid:*

$$\left\langle \prod_{j=1}^{K}\frac{D_N[\mu_i,H]}{D_N[\epsilon_j,H]}\right\rangle_\alpha=(-1)^{K(K-1)/2}\gamma_{N-1}^K\frac{\Delta(\epsilon,\mu)}{\Delta^2(\epsilon)\Delta^2(\mu)}\det(W_{H,N}(\epsilon_i,\mu_j))_{1\leqslant i,j\leqslant K},\tag{3.12}$$

where

$$W_{H,N}(x,y)=\frac{h_N(\epsilon)\pi_{N-1}(\mu)-h_{N-1}(\epsilon)\pi_N(\mu)}{\epsilon-\mu}\tag{3.13}$$

and again $h_k(\epsilon)=(1/2\pi i)\int\pi_k(t)d\alpha(t)/(t-\epsilon)$ *is the Cauchy transform of* $\pi_k(t)$ *and* $\gamma_{N-1}=-2\pi i/C_{N-1}^2$. Observe first that by linearity

$$\begin{vmatrix} h_{N-M}(\epsilon_1) & \cdots & h_{N+L-1}(\epsilon_1) \\ \vdots & & \\ h_{N-M}(\epsilon_M) & \cdots & h_{N+L-1}(\epsilon_M) \\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+L-1}(\mu_1) \\ \vdots & & \\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+L-1}(\mu_L) \end{vmatrix} = \int \cdots \int \frac{d\alpha(\lambda)}{(2\pi i)^M \prod_{j=1}^{M} (\lambda_j - \epsilon_j)}$$

$$\times \begin{vmatrix} \pi_{N-M}(\lambda_1) & \cdots & \pi_{N+L-1}(\lambda_1) \\ \vdots & & \\ \pi_{N-M}(\lambda_M) & \cdots & \pi_{N+L-1}(\lambda_M) \\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+L-1}(\mu_1) \\ \vdots & & \\ \pi_{N-M}(\mu_1) & \cdots & \pi_{N+L-1}(\mu_L) \end{vmatrix}. \tag{3.14}$$

Inserting (2.36) on the left-hand side, and using (2.5) to reexpress the integrand on the right-hand side, we obtain the following result, which is of independent interest. The result expresses averages of ratios of characteristic polynomials in terms of averages of products of such polynomials.

Proposition 3.4: Let $1 \leqslant M \leqslant N$. *Then*

$$\left\langle \frac{\prod_{j=1}^{L} D_N[\mu_i, H]}{\prod_{j=1}^{M} D_N[\epsilon_j, H]} \right\rangle_\alpha = \frac{(-1)^{M(M-1)/2} \prod_{j=N-M}^{N-1} \gamma_j}{\Delta(\mu)\Delta(\epsilon)} \int \cdots \int \frac{d\alpha(\lambda)}{(2\pi i)^M \prod_{j=1}^{M} (\lambda_j - \epsilon_j)} \Delta(\lambda, \mu)$$

$$\times \left\langle \prod_{j=1}^{M} D_{N-M}[\lambda_j, H] \prod_{j=1}^{L} D_{N-M}[\mu_j, H] \right\rangle_\alpha. \tag{3.15}$$

Proof of Theorem 3.2: For $M = L = K \leqslant N$, by (3.15) and (3.3),

$$\frac{\Delta(\mu)\Delta(\epsilon)}{(-1)^{K(K-1)/2} \prod_{j=N-K}^{N-1} \gamma_j} \left\langle \frac{\prod_{j=1}^{K} D_N[\mu_i, H]}{\prod_{j=1}^{K} D_N[\epsilon_j, H]} \right\rangle_\alpha$$

$$= \int \cdots \int \frac{d\alpha(\lambda)}{(2\pi i)^M \prod_{j=1}^{M} (\lambda_j - \epsilon_j)} C_{N-K,K} \prod_{i=1}^{K} \prod_{j=1}^{K} (\mu_i - \lambda_j) \det(W_{I,N}(\lambda_i, \mu_j))_{1 \leqslant i,j \leqslant K}. \tag{3.16}$$

But

$$\frac{1}{2\pi i} \int \frac{d\alpha(\lambda_j)}{\lambda_j - \epsilon_j} \prod_{i=1}^{K} (\mu_i - \lambda_j) \frac{\pi_N(\lambda_j)\pi_{N-1}(\mu_k) - \pi_{N-1}(\lambda_j)\pi_N(\mu_k)}{\lambda_j - \mu_k}$$

$$= \frac{1}{2\pi i} \int d\alpha(\lambda_j) \left(1 - \frac{\mu_1 - \epsilon_j}{\lambda_j - \epsilon_j}\right) \left(\prod_{\substack{i=2 \\ i \neq k}}^{K} (\mu_i - \lambda_j) \right) (\pi_N(\lambda_j)\pi_{N-1}(\mu_k) - \pi_{N-1}(\lambda_j)\pi_N(\mu_k))$$

$$= -\frac{1}{2\pi i} \int d\alpha(\lambda_j) \frac{\mu_1 - \epsilon_j}{\lambda_j - \epsilon_j} \left(\prod_{\substack{i=2 \\ i \neq k}}^{K} (\mu_i - \lambda_j) \right) (\pi_N(\lambda_j)\pi_{N-1}(\mu_k) - \pi_{N-1}(\lambda_j)\pi_N(\mu_k)) \tag{3.17}$$

as $\int d\alpha(\lambda_j)\lambda_j^{\ell}\pi_{N-1}(\lambda_j)=\int d\alpha(\lambda_j)\lambda_j^{\ell}\pi_N(\lambda_j)=0$ for $0\leqslant \ell \leqslant K-2<N-1$. Continuing in this way, the integral reduces to $\Pi_{i=1}^{K}(\mu_i-\epsilon_j)W_{H,N}(\epsilon_i,\mu_k)$. Thus we find

$$\frac{\Delta(\mu)\Delta(\epsilon)}{(-1)^{K(K-1)/2}\prod_{j=N-K}^{N-1}\gamma_j}\left\langle \frac{\prod_{j=1}^{K} D_N[\mu_i,H]}{\prod_{j=1}^{K} D_N[\epsilon_j,H]}\right\rangle_{\alpha}=\frac{\Delta(\epsilon,\mu)}{\Delta(\epsilon)\Delta(\mu)}\det(W_{I,N+K}(\lambda_i,\mu_k))_{1\leqslant i,k\leqslant K} \tag{3.18}$$

and (3.12) follows. □

ACKNOWLEDGMENTS

The authors would like to thank Jeff Geronimo for useful conversations and for pointing out the paper of U. B. Uvarov. The authors would also like to thank Nick Witte for many useful remarks. The work of the first author was supported in part by NSF Grant No. DMS-0208577. The work of the second author was supported in part by NSF Grant No. DMS-0296084 and by the Institute for Advanced Study in Princeton. The work of the third author was supported in part by EPSRC Grant No. GR/13838/01 ''Random Matrices close to Unitary or Hermitian'' and by the Brunel University Vice-Chancellor grant.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Monotone Riemannian metrics on density matrices with non-monotone scalar curvature

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(Received 28 November 2002; accepted 20 May 2003)

The theory of monotone Riemannian metrics on the state space of a quantum system was established by Dénes Petz in 1996. In a recent paper he argued that the scalar curvature of a statistically relevant—monotone—metric can be interpreted as an average statistical uncertainty. The present paper contributes to this subject. It is reasonable to expect that states which are more mixed are less distinguishable than those which are less mixed. The manifestation of this behavior could be that for such a metric the scalar curvature has a maximum at the maximally mixed state. We show that not every monotone metric fulfils this expectation, some of them behave in a very different way. A mathematical condition is given for monotone Riemannian metrics to have a local minimum at the maximally mixed state and examples are given for such metrics. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1592874]

I. INTRODUCTION

The quantum mechanical Hilbert space formalism gives a mathematical description of particles with spin of $(n-1)/2$. Concentrating on the spin part of nonrelativistic particles one can build a proper mathematical model in an n dimensional complex Hilbert space. This is the simplest physical realization of an n-level quantum system. The states of an n-level system are identified with the set of positive semidefinite self-adjoint $n\times n$ matrices of trace 1. The states form a closed convex set in the space of matrices and its interior, the set of all strictly positive self-adjoint matrices of trace 1 becomes naturally a differentiable manifold.

The idea in mathematical statistics that a statistical or informational distance between probability measures gives rise to a Riemannian metric is due to Rao[1] and was developed by Amari[2] and Streater[3] among others. Let us see how can one measure the statistical distance between the simplest probability distributions in classical case Ref. 4. Assume, that we have two probability distributions $(p_1,1-p_1)$ and $(p_2,1-p_2)$. Let us now suppose that an experimenter, in making his determination of the value p_1, has only n trials. Because of the unavoidable statistical fluctuations associated with a finite sample, the experimenter cannot know p_1 exactly. After these measurements the experimenter's uncertainty is the size of a typical fluctuation

$$\Delta p_1 = \sqrt{\frac{p_1(1-p_1)}{n}}.$$

We can say that the distributions $(p_1,1-p_1)$ and $(p_2,1-p_2)$ are distinguishable in n trials if the regions of uncertainty do not overlap, that is, if

$$|p_1-p_2| \geqslant \Delta p_1 + \Delta p_2 .$$

Let $k(n,p_1,p_2)$ denote the number of the probability distributions of the form $(p_i,1-p_i)$ between p_1 and p_2 (that is $p_1<p_i<p_2$) each of which is distinguishable in n trials from its neighbors. The statistical distance between the given probability distributions is

$$d(p_1,p_2)=\lim_{n\to\infty}\frac{k(n,p_1,p_2)}{\sqrt{n}}.$$

From the previous equations we find that

$$d(p_1,p_2)=\int_{p_1}^{p_2}\frac{1}{2\sqrt{p(1-p)}}dp=\arccos(\sqrt{p_1p_2}+\sqrt{(1-p_1)(1-p_2)}).$$

This distance function was introduced by Fisher in 1922.

The Fisher informational metric is unique in some sense (i.e., it is the only Markovian monotone distance) in the classical case Ref. 5. A family of Riemannian metrics are called monotone if they are decreasing under stochastic mappings (the exact definition is given below). These metrics play the role of Fisher metric in the quantum case. Monotone Riemannian metrics are important for information-theoretical and statistical considerations on the state space. The study of monotone metrics for parametric statistical manifolds was initiated by Chentsov and Morozova.[6] Petz's classification theorem[7] establishes a correspondence between monotone metrics and operator monotone $f:[0,\infty[\to\mathbb{R}$ functions, such that $f(x)=xf(x^{-1})$ hold for all positive x. In the simplest quantum case, dealing with 2×2 matrices we can use the Stokes parametrization, that is every state D can be uniquely written in the

$$D=\tfrac{1}{2}(I+x_1\sigma_1+x_2\sigma_2+x_2\sigma_2)$$

form, where $(\sigma_i)_{i=1,2,3}$ are the Pauli matrices and $(x_1,x_2,x_3)\in\mathbb{R}^3$ with $x_1^2+x_2^2+x_3^2\leqslant1$. The interior of the set of states can be identified with the open unit ball in $\mathbb{R}^3$ by this parametrization. In this case a monotone Riemannian metric on this manifold can be written in the

$$ds^2=\frac{1}{1-r^2}dr^2+\frac{r^2}{(1+r)f\left(\frac{1-r}{1+r}\right)}d\vartheta^2+\frac{r^2\sin^2\vartheta}{(1+r)f\left(\frac{1-r}{1+r}\right)}d\varphi^2$$

form in polar coordinates.

There is a strong connection between the scalar curvature of these manifolds at a given state and statistical distinguishability and uncertainty of the state. If D_0 is a $n\times n$ density matrix we call geodesic ball the set

$$B_r(D_0)=\{Dn\times n \text{ density matrix: } d(D_0,D)<r\}.$$

The volume of this ball is given by

$$V(B_r(D_0))=\frac{\sqrt{\pi^{n^2-1}}r^{n^2-1}}{\Gamma\left(\frac{n^2+1}{2}\right)}\cdot\left(1-\frac{r(D_0)r^2}{6(n^2+1)}+O(r^4)\right),$$

where $r(D_0)$ is the scalar curvature at the point D_0. According to Ref. 8, the quantity $V(B_r(D_0))$ measures the statistical uncertainty and the scalar curvature measures the average statistical uncertainty. A general explicit formula for the scalar curvature was given by Dittmann[10] (particular cases have been discussed in Refs. 11 and 12). There are many Riemannian metrics on the state space which are statistically relevant in different ways. The state A is more mixed than the state B if for their decreasingly ordered set of eigenvalues $(a_1,\ldots,a_n)$ and $(b_1,\ldots,b_n)$ the inequality

$$\sum_{l=1}^{k}a_l\leqslant\sum_{l=1}^{k}b_l$$

holds for every $1 \leqslant k \leqslant n$.

It is reasonable to expect that the most mixed states are less distinguishable than the less mixed states; for details see Refs. 13 and 14. It means mathematically that in this case the scalar curvature of a Riemann structure should have the following monotonicity property: if D_1 is more mixed than D_2 then $r(D_2)$ should be less then $r(D_1)$, where $r(D)$ denotes the scalar curvature of the manifold at the state D. It has been shown that the Bures metric does not have this monotonicity property for the scalar curvature and moreover it has a global minimum at the most mixed state. Actually in Ref. 9 it was proved that for the Bures metric for every $n \times n$ density matrix D the inequality

$$r(D) \geqslant \frac{(5n^2-4)(n^2-1)}{4}$$

holds. If $n>3$, equality holds iff $D=(1/n)I$. If $n=2$, then $r(D)=24$. This implies that the Bures metric is (trivially) monotone for $n=2$. Indeed all metrics studied thus far in two level quantum systems have monotone scalar curvature. This means that these metrics are compatible with one's statistical view. Do all monotone metrics have this property in the two level quantum system? The answer is no; in this paper we show a family of monotone metrics with non-monotone scalar curvature and we give a condition for monotone metric to have a local minimum at the maximally mixed state.

II. SCALAR CURVATURE ON THE TWO LEVEL QUANTUM SYSTEMS

A. The setup

Let $\mathcal{M}_n^+$ be the space of all complex self-adjoint positive definite $n \times n$ matrices of trace 1 and let $\mathcal{M}_n$ be the real vector space of all self-adjoint traceless $n \times n$ matrices. The space $\mathcal{M}_n^+$ can be endowed with a differentiable structure.[15]

The tangent space T_D at $D \in \mathcal{M}_n^+$ can be identified with $\mathcal{M}_n$. A map

$$K: \mathcal{M}_n^+ \times \mathcal{M}_n \times \mathcal{M}_n \to \mathbb{C}, \quad (D,X,Y) \mapsto K_D(X,Y)$$

will be called a Riemannian metric if the following condition holds: For all $D \in \mathcal{M}_n^+$ the map

$$K_D: \mathcal{M}_n \times \mathcal{M}_n \to \mathbb{C}, \quad (X,Y) \mapsto K_D(X,Y)$$

is a scalar product and for all $X \in \mathcal{M}_n$ the map

$$K_\cdot(X,X): \mathcal{M}_n^+ \to \mathbb{C}, \quad D \mapsto K_D(X,X)$$

is smooth.

We now use differential geometrical notation to define the scalar curvature of the $(\mathcal{M}_n^+, K)$ Riemannian manifold. In this case the Riemannian metric is a

$$K: \mathcal{M}_n^+ \to \mathrm{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R}), \quad D \mapsto ((X,Y) \mapsto K_D(X,Y))$$

map, where $\mathrm{LIN}(U,V)$ denotes the set of linear maps from the vector space U to the vector space V. The derivative of the metric K is a map

$$\mathrm{d}K: \mathcal{M}_n^+ \to \mathrm{LIN}(\mathcal{M}_n, \mathrm{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R})), \quad D \mapsto (X \mapsto ((Y,Z) \mapsto \mathrm{d}K_D(X)(Y,Z))).$$

At a given $D \in \mathcal{M}_n^+$ point for given $X,Y \in \mathcal{M}_n$ tangent vectors the map

$$\tau_{D,X,Y}: \mathcal{M}_n \to \mathbb{R}, \quad Z \mapsto \tfrac{1}{2}(\mathrm{d}K_D(Y)(X,Z) + \mathrm{d}K_D(X)(Z,Y) - \mathrm{d}K_D(Z)(X,Y))$$

is a linear functional. It means that there exists a unique $V_{D,X,Y}\in\mathcal{M}_n$ tangent vector such that for all $Z\in\mathcal{M}_n$ vector

$$K_D(V_{D,X,Y},Z)=\tau_{D,X,Y}(Z)$$

holds. One can define the map

$$\Gamma:\mathcal{M}_n^+\to\mathrm{LIN}(\mathcal{M}_n\times\mathcal{M}_n,\mathcal{M}_n),\quad D\mapsto((X,Y)\mapsto V_{D,X,Y})$$

which is called covariant differentiation. Its derivative is a map

$$\mathrm{d}\Gamma:\mathcal{M}_n^+\to\mathrm{LIN}(\mathcal{M}_n,\mathrm{LIN}(\mathcal{M}_n\times\mathcal{M}_n,\mathcal{M}_n)),\quad D\mapsto(X\mapsto((Y,Z)\mapsto\mathrm{d}\Gamma_D(X)(Y,Z))).$$

The Riemann curvature tensor defined to be

$$R:\mathcal{M}_n^+\to\mathrm{LIN}(\mathcal{M}_n\times\mathcal{M}_n\times\mathcal{M}_n,\mathcal{M}_n),\quad (D,X,Y,Z)\mapsto R_D(X,Y,Z),$$

where

$$R_D(X,Y,Z)=\mathrm{d}\Gamma_D(X)(Y,Z)-\mathrm{d}\Gamma_D(Y)(X,Z)+\Gamma_D(X,\Gamma_D(Y,Z))-\Gamma_D(Y,\Gamma_D(X,Z)).$$

The map

$$\alpha:\mathcal{M}_n^+\times\mathcal{M}_n\times\mathcal{M}_n\to\mathrm{LIN}(\mathcal{M}_n,\mathcal{M}_n),\quad (D,X,Y)\mapsto\alpha_{D,X,Y}=(Z\mapsto R_D(Z,X,Y)),$$

is needed to define the Ricci tensor

$$\mathrm{Ric}:\mathcal{M}_n^+\to\mathrm{LIN}(\mathcal{M}_n\times\mathcal{M}_n,\mathbb{R}),\quad D\mapsto((X,Y)\mapsto\mathrm{Ric}_D(X,Y)),$$

where

$$\mathrm{Ric}_D(X,Y)=\mathrm{Tr}\,\alpha_{D,X,Y}.$$

At a given $D\in\mathcal{M}_n^+$ point for given $X\in\mathcal{M}_n$ tangent vector the map

$$\beta_{D,X}:\mathcal{M}_n\to\mathbb{R},\quad Y\mapsto\mathrm{Ric}_D(X,Y)$$

is a linear functional. It means that there exists a unique $U_{D,X}\in\mathcal{M}_n$ tangent vector such that for all $Y\in\mathcal{M}_n$ vector

$$K_D(U_{D,X},Y)=\beta_{D,X}(Y)$$

holds. From the map

$$\rho:\mathcal{M}_n^+\to\mathrm{LIN}(\mathcal{M}_n,\mathcal{M}_n),\quad D\mapsto\rho_D=((X)\mapsto U_{D,X})$$

we get the scalar curvature of the manifold

$$\mathrm{Scal}:\mathcal{M}_n^+\to\mathbb{R},\quad D\mapsto\mathrm{Tr}\,\rho_D.$$

For further differential geometry details see, for example, Ref. 16.

Let $M_n(\mathbb{C})$ denote the set of complex $n\times n$ matrices and $M_k(M_n)$ denote the set of $k\times k$ matrices with entries $M_n(\mathbb{C})$. If $T:M_n(\mathbb{C})\to M_m(\mathbb{C})$ is a linear map, it induces a linear map $T^{(k)}:M_k(M_n)\to M_k(M_m)$ by

$$T^{(k)}([A_{ij}])=[T(A_{ij})].$$

The map T is called positive if it takes positive operators to positive operators. Say that T is k-positive if $T^{(k)}$ is positive and T is completely positive if it is k-positive for all $k \geqslant 1$.

A linear mapping $T: M_n(\mathbb{C}) \to M_m(\mathbb{C})$ is defined to be stochastic if T is completely positive and trace preserving. For more information on completely positive and stochastic maps see Refs. 13 and 14.

Let $(K^m)_{m \in \mathbb{N}}$ be a family of metrics, such that K^m is a Riemannian metric on $\mathcal{M}_m^+$ for all m. This family of metrics is defined to be monotone if

$$K^m_{T(D)}(T(X),T(X)) \leqslant K^n_D(X,X)$$

for every stochastic mapping $T: M_n(\mathbb{C}) \to M_m(\mathbb{C})$, for every $D \in \mathcal{M}_n^+$ and for all $X \in \mathcal{M}_n$ and for all $m,n \in \mathbb{N}$.

Theorem 2.1: *Petz classification theorem:*[7] *There exists a bijective correspondence between the monotone family of metrics* $(K^n)_{n \in \mathbb{N}}$ *and operator monotone* $f: \mathbb{R}^+ \to \mathbb{R}$ *functions such that* $f(x) = xf(x^{-1})$ *hold for all positive* x. *The metric is given by*

$$K^n_D(X,Y) = \mathrm{Tr}(X(R^{1/2}_{n,D} f(L_{n,D} R^{-1}_{n,D}) R^{1/2}_{n,D})^{-1}(Y)) \tag{1}$$

for all $n \in \mathbb{N}$ *where* $L_{n,D}(X) = DX$, $R_{n,D}(X) = XD$ *for all* $D,X \in M_n(\mathbb{C})$.

A Riemannian metric K is said to be monotone if there is a monotone family of metrics $(K^m)_{m \in \mathbb{N}}$ such that $K = K^n$ for an n. We use the normalization condition for the function f in the previous theorem $f(1) = 1$. Here are some examples of operator monotone functions which generate monotone metrics from Refs. 17 and 18,

$$\frac{1+x}{2}, \quad \frac{2x}{1+x}, \quad \frac{x-1}{\log x}, \quad \frac{2(x-1)^2}{(1+x)(\log x)^2}, \quad \frac{2(x-1)\sqrt{x}}{(1+x)\log x}, \quad \frac{2x^{\alpha+1/2}}{1+x^{2\alpha}}, \quad \frac{\beta(1-\beta)(x-1)^2}{(x^\beta-1)(x^{1-\beta}-1)},$$

where $0 \leqslant \alpha \leqslant 1/2$ and $0 < |\beta| < 1$.

B. Curvature and eigenvalues on $\mathcal{M}_2^+$

There is an explicit formula for scalar curvature in a given $D \in \mathcal{M}_2^+$ state using a monotone metric coming from a suitable f function defined by Eq. (1). To use that result to build up a more explicit formula to our $\mathcal{M}_2^+$ manifold, first introduce the Morozova–Chentsov function related to the monotone function f defined by

$$c(x,y) := \frac{1}{yf(x/y)}. \tag{2}$$

Let us denote by $\partial_1 c(x,y)$ the partial derivative of $c(x,y)$ with respect to its first variable. Define four new functions (as in Ref. 10)

$$h_1(x,y,z) := \frac{c(x,y) - zc(x,z)c(y,z)}{(x-z)(y-z)c(x,z)c(y,z)}, \quad h_3(x,y,z) := \frac{z}{x-y}(\partial_1(\log c)(z,x) - \partial_1(\log c)(z,y)),$$

$$h_2(x,y,z) := \frac{(c(x,z)-c(y,z))^2}{(x-y)^2 c(x,y)c(x,z)c(y,z)}, \quad h_4(x,y,z) := z\partial_1(\log c)(z,x)\partial_1(\log c)(z,y). \tag{3}$$

The terms like $h_i(x,x,z)$ can be computed as a

$$\lim_{y \to x} h_i(x,y,z)$$

limit. We will need a linear combination of these functions

$$h(x,y,z)=h_1(x,y,z)-\tfrac{1}{2}h_2(x,y,z)+2h_3(x,y,z)-h_4(x,y,z). \tag{4}$$

Theorem 2.2: *(see Ref. 10.) Let $\sigma(D)$ be the spectrum of the state $D\in\mathcal{M}_n^+$. Then for the scalar curvature one has the expression*

$$r(D)=\sum_{x,y,z\in\sigma(D)}h(x,y,z)-\sum_{x\in\sigma(D)}h(x,x,x)+\frac{1}{4}(n^2-1)(n^2-2).$$

Corollary 2.1: The scalar curvature at the state $D\in\mathcal{M}_2^+$ with eigenvalues λ_1,λ_2 is given by

$$r(D)=h(\lambda_1,\lambda_1,\lambda_2)+h(\lambda_1,\lambda_2,\lambda_1)+h(\lambda_2,\lambda_1,\lambda_1)+h(\lambda_2,\lambda_2,\lambda_1)+h(\lambda_2,\lambda_1,\lambda_2)$$
$$+h(\lambda_1,\lambda_2,\lambda_2)+\tfrac{3}{2}.$$

Theorem 2.3: *Let $D\in\mathcal{M}_2^+$ and $a=2\lambda_1-1$ where λ_1 is an eigenvalue of D and assume that the monotone metric of $\mathcal{M}_2^+$ comes from a function f. Then the scalar curvature at D is*

$$r(a)=\frac{14(a-1)\left[f'\left(\frac{1-a}{1+a}\right)\right]^2}{(1+a)^3\left[f\left(\frac{1-a}{1+a}\right)\right]^2}+\frac{2(a^2+7a-6)f'\left(\frac{1-a}{1+a}\right)}{(1+a)^2af\left(\frac{1-a}{1+a}\right)}+\frac{8(1-a)f''\left(\frac{1-a}{1+a}\right)}{(1+a)^3f\left(\frac{1-a}{1+a}\right)}$$
$$+\frac{2(1+a)f\left(\frac{1-a}{1+a}\right)}{a^2}+\frac{3a^3+5a^2+8a-4}{2(1+a)a^2}. \tag{5}$$

Proof 1: Through the computation we will use the identities $f'(1)=\frac{1}{2}$ and $2f^{(3)}(1)+3f^{(2)}(1)=0$ which come from the equations $f(x)=xf(1/x)$ and $f(1)=1$. It is easy to recognize that $h_i(y,x,x)=h_i(x,y,x)$ for $i=1,2,3,4$. First let us note the following identities:

$$c(x,x)=\frac{1}{x},\quad c(x,y)=c(y,x),\quad c(x,y)=tc(tx,ty),\quad \forall t\in\mathbb{R}^+,$$
$$\partial_1c(x,x)=-\frac{1}{2x^2},\quad \partial_1^k\partial_2^lc(x,y)=\partial_1^l\partial_2^kc(y,x),\quad c(x,y)=-x\partial_1c(x,y)-y\partial_2c(x,y), \tag{6}$$

which will be used through the computation.

The $h_i(x,x,y)$ and $h_i(x,y,x)$ like limit functions can be computed. For example,

$$h_1(x,x,y)=\lim_{q\to x}h_1(x,q,y)=\lim_{q\to x}\frac{c(x,q)-yc(x,y)c(q,y)}{(x-y)(q-y)c(x,y)c(q,y)}=\frac{c(x,x)-y[c(x,y)]^2}{(x-y)^2[c(x,y)]^2},$$

$$h_4(x,y,x)=\lim_{q\to x}h_4(x,y,q)=\lim_{q\to x}q\frac{\partial_1c(q,x)}{c(q,x)}\frac{\partial_1c(q,y)}{c(q,y)}=x\frac{\partial_1c(x,x)}{c(x,x)}\frac{\partial_1c(x,y)}{c(x,y)}.$$

After taking into account the identities (6) these limit functions can be simplified,

$$h_1(x,x,y)=\frac{1-xy[c(x,y)]^2}{x(x-y)^2[c(x,y)]^2},\quad h_1(x,y,x)=-\frac{1}{2}\frac{c(x,y)+2x\partial_1c(x,y)}{(x-y)c(x,y)}, \tag{7}$$

$$h_2(x,x,y)=x\left(\frac{\partial_1c(x,y)}{c(x,y)}\right)^2,\quad h_2(x,y,x)=\frac{1}{x}\left(\frac{1-xc(x,y)}{(x-y)c(x,y)}\right)^2,$$

$$h_3(x,x,y)=-\frac{y^2c(x,y)[\partial_1c(y,x)]^2+2yc(x,y)\partial_1c(y,x)+xy\partial_1c(x,y)\partial_1c(y,x)}{x[c(x,y)]^2},$$

$$h_3(x,y,x)=-\frac{c(x,y)+2x\partial_1c(x,y)}{2(x-y)c(x-y)},$$

$$h_4(x,x,y)=y\left(\frac{\partial_1c(y,x)}{c(x,y)}\right)^2,\quad h_4(x,y,x)=-\frac{1}{2}\frac{\partial_1c(x,y)}{c(x,y)}.$$

Introducing the suitable sum functions for h_i $(i=1,2,3,4)$,

$$sh_i(x,y):=h_i(x,x,y)+2h_i(x,y,x)+h_i(y,y,x)+2h_i(y,x,y), \tag{8}$$

we get that

$$sh_1(x,y)=\frac{(x+y)(1-xy[c(x,y)]^2)}{xy(x-y)^2[c(x,y)]^2}-\frac{4x\partial_1c(x,y)+2c(x,y)}{(x-y)c(x,y)},$$

$$sh_2(x,y)=\frac{x[\partial_1c(x,y)]^2+y[\partial_1c(y,x)]^2}{[c(x,y)]^2}+2\frac{(x+y)+xy(x+y)[c(x,y)]^2-4xyc(x,y)}{xy(x-y)^2[c(x,y)]^2},$$

$$sh_3(x,y)=\frac{(x+y)(c(x,y)[\partial_{1,2}c(x,y)]^2-\partial_1c(x,y)\partial_1c(y,x))}{[c(x,y)]^2}-\frac{4x\partial_1c(x,y)+2c(x,y)}{(x-y)c(x,y)}, \tag{9}$$

$$sh_4(x,y)=\frac{x[\partial_1c(x,y)]^2+y[\partial_1c(y,x)]^2}{[c(x,y)]^2}-\frac{\partial_1c(x,y)+\partial_1c(y,x)}{c(x,y)}.$$

These sum functions can be expressed by the operator monotone function $f(x)$:

$$sh_1(x,y)=\frac{1}{(x-y)^2}\left(\frac{y(x+y)}{x}[f(x/y)]^2+y-3x+\frac{4x(x-y)}{y}\frac{f'(x/y)}{f(x/y)}\right),$$

$$sh_2(x,y)=\frac{x}{y^2}\left(\frac{f'(x/y)}{f(x/y)}\right)^2+\frac{y^3}{x^4}\left(\frac{f(x/y)f'(y/x)}{[f(y/x)]^2}\right)^2+\frac{2y(x+y)}{x(x-y)^2}[f(x/y)]^2$$
$$-\frac{8y}{(x-y)^2}f(x/y)+\frac{2(x+y)}{(x-y)^2},$$

$$sh_3(x,y)=\frac{-2x(x+y)}{y^3}\left(\frac{f'(x/y)}{f(x/y)}\right)^2-\frac{(x+y)}{x^2}\frac{f'(x/y)f'(y/x)}{[f(x/y)]^2} \tag{10}$$
$$+\frac{2(x^2+2xy-y^2)}{y^2(x-y)}\frac{f'(x/y)}{f(x/y)}+\frac{x(x+y)}{y^3}\frac{f''(x/y)}{f(x/y)}-\frac{2}{x-y},$$

$$sh_4(x,y)=\frac{x}{y^2}\left(\frac{f'(x/y)}{f(x/y)}\right)^2+\frac{y^3}{x^4}\left(\frac{f(x/y)f'(y/x)}{[f(y/x)]^2}\right)^2+\frac{1}{y}\frac{f'(x/y)}{f(x/y)}+\frac{y}{x^2}\frac{f(x/y)f'(y/x)}{[f(y/x)]^2}.$$

The scalar curvature is given by the linear combination of the functions $sh_i(x,y)$:

$$r(D)=sh_1(x,y)-\tfrac{1}{2}sh_2(x,y)+2sh_3(x,y)-sh_4(x,y).$$

The result is the following:

$$r(D)=2\frac{2yf(x/y)-1}{(x-y)^2}+6\frac{2xf'(x/y)-yf(x/y)}{y(x-y)f(x/y)}-\frac{1}{2}\frac{x(8+3y)}{y^3}\left(\frac{f'(x/y)}{f(x/y)}\right)^2-\frac{3}{2}\frac{y}{x^2}\left(\frac{f'(y/x)}{f(y/x)}\right)^2$$
$$+\frac{(3+x)f'(x/y)}{y^2f(x/y)}+2\frac{xf''(x/y)}{y^3f(x/y)}-\frac{f'(y/x)}{xf(y/x)}-\frac{2f'(x/y)f'(y/x)}{x^2[f(y/x)]^2}+\frac{3}{2}. \tag{11}$$

The eigenvalues of D can be expressed by a as

$$\lambda_1=\frac{1+a}{2},\quad \lambda_2=\frac{1-a}{2}.$$

Substituting these into the previous formula and collecting the terms we get Eq. (5). □

Since the scalar curvature formula Eq. (5) is a rather complicated one it is worth mentioning that there is a completely different proof (which is based on Sec. II A) for Theorem 2.3.

Proof 2: There is another parametrization of the state as it was mentioned in the introduction. Let us use the following parametrization for the 2×2 density matrices:

$$\frac{1}{2}\begin{pmatrix}1+r\cos\theta & (r\sin\theta\cos\phi)+i(r\sin\theta\sin\phi)\\ (r\sin\theta\cos\phi)-i(r\sin\theta\sin\phi) & 1-r\cos\theta\end{pmatrix},$$

where (r,θ,ϕ) denote the spherical coordinates, but now $0\leqslant r<1$. In this case the metric is

$$ds^2=\frac{1}{1-r^2}dr^2+\frac{r^2}{(1+r)f\left(\frac{1-r}{1+r}\right)}d\theta^2+\frac{r^2\sin^2\theta}{(1+r)f\left(\frac{1-r}{1+r}\right)}d\phi^2.$$

Let us use the order (r,θ,ϕ) for the coordinates. [For example $\partial_2 t(r,\theta,\phi)$ denotes the partial derivative of $t(r,\theta,\phi)$ with respect to θ.] The g_{ik} metric can be written in the form $g_{ik}=\delta_{ik}\alpha_i(r,\theta,\phi)$. The identities

$$\partial_2\alpha_1=\partial_3\alpha_1=0,\quad \partial_2\alpha_2=\partial_3\alpha_2=0,\quad \partial_3\alpha_3=0$$

will simplify the computation. The Christoffel symbols of the second kind for this Riemannian manifold is

$$\Gamma_{ij}^{\cdot\cdot m}=\sum_{k=1}^{3}\frac{1}{2}g^{km}(\partial_i g_{jk}+\partial_j g_{ik}-\partial_k g_{ij}), \tag{12}$$

where g^{ij} denotes the inverse matrix of g_{ij}. Since $\Gamma_{ij}^{\cdot\cdot m}=\Gamma_{ji}^{\cdot\cdot m}$, there are only seven nonzero independent Christoffel symbols in this case

$$\Gamma_{1,1}^{\cdot\cdot 1}=\frac{r}{1-r^2},\quad \Gamma_{2,2}^{\cdot\cdot 1}=\frac{-r(1-r)}{2(1+r)^2f(c(r))}\left(r^2+3r+2+2r\frac{f'(c(r))}{f(c(r))}\right),\quad \Gamma_{3,3}^{\cdot\cdot 1}=\sin^2\theta\,\Gamma_{2,2}^{\cdot\cdot 1},$$

$$\Gamma_{1,2}^{\cdot\cdot 2}=\frac{-f(c(r))}{r^2(1-r)}\Gamma_{2,2}^{\cdot\cdot 1},\quad \Gamma_{3,3}^{\cdot\cdot 2}=-\sin\theta\cos\theta,\quad \Gamma_{1,3}^{\cdot\cdot 3}=\Gamma_{1,2}^{\cdot\cdot 2},\quad \Gamma_{2,3}^{\cdot\cdot 3}=\frac{\cos\theta}{\sin\theta}, \tag{13}$$

where $c(r)=(1-r)/(1+r)$.

The Riemannian curvature tensor is given by the equation

$$R_{ijkl}=\sum_{n=1}^{3}g_{ln}\left(\partial_i\Gamma_{jk}^{\cdot\cdot n}-\partial_j\Gamma_{ik}^{\cdot\cdot n}+\sum_{m=1}^{3}(\Gamma_{jk}^{\cdot\cdot m}\Gamma_{im}^{\cdot\cdot n}-\Gamma_{ik}^{\cdot\cdot m}\Gamma_{jm}^{\cdot\cdot n})\right). \tag{14}$$

Since $R_{ijkl}=-R_{jikl}$, $R_{ijkl}=-R_{ijlk}$, and $R_{ijkl}=R_{klij}$, there are only three nonzero independent elements of the curvature tensor,

$$R_{1212}=\frac{-r}{(1+r)^4(1-r^2)f(c(r))}\left(2r(1-r)\frac{f''(c(r))}{f(c(r))}-3r(1-r)\left(\frac{f'(c(r))}{f(c(r))}\right)^2+(1+r)(3r-2)\frac{f'(c(r))}{f(c(r))}+\frac{(r^2+r+4)(1+r)^2}{4}\right),$$

$$R_{1313}=\sin^2\theta\ R_{1212}, \tag{15}$$

$$R_{2323}=\frac{r^2(1-r)\sin^2\theta}{(1+r)^4[f(c(r))]^2}\left(r(r+2)\frac{f'(c(r))}{f(c(r))}+\frac{r^2}{1+r}\left(\frac{f'(c(r))}{f(c(r))}\right)^2-\frac{(1+r)^3}{1-r}f(c(r))+\frac{(1+r)(2+r)^2}{4}\right).$$

The Ricci curvature tensor is

$$\mathrm{Ric}_{ij}=\sum_{k,l=1}^{3}g^{kl}R_{lijk}. \tag{16}$$

It is symmetric $\mathrm{Ric}_{ij}=\mathrm{Ric}_{ji}$, and it has three nonzero elements,

$$\mathrm{Ric}_{1,1}=\frac{1}{(1+r)^4}\left(4\frac{f''(c(r))}{f(c(r))}-6\left(\frac{f'(c(r))}{f(c(r))}\right)^2+\frac{2(1+r)(3r-2)}{(1-r)}\frac{f'(c(r))}{f(c(r))}+\frac{(r^2+r+4)(1+r)^2}{2r(1-r)}\right),$$

$$\mathrm{Ric}_{2,2}=\frac{r^2(1-r)}{(1+r)^4f(c(r))}\left(2\frac{f''(c(r))}{f(c(r))}-4\left(\frac{f'(c(r))}{f(c(r))}\right)^2+\frac{(1+r)(r^2+4r-4)}{r(1-r)}\frac{f'(c(r))}{f(c(r))}+\frac{(1+r)^4}{r^2(1-r)}f(c(r))+\frac{(r^3+2r^2+2r-2)(1+r)^2}{2r^2(1-r)}\right), \tag{17}$$

$$\mathrm{Ric}_{3,3}=\sin^2\theta\,\mathrm{Ric}_{2,2}.$$

The scalar curvature at point D is

$$r(D)=\sum_{i,j=1}^{3}g^{ij}\,\mathrm{Ric}_{ji}. \tag{18}$$

Computing $r(D)$ we get Eq. (5). □

The state D is maximally mixed if its eigenvalues are equal, in this case $a=0$. So the scalar curvature has local minimum or maximum at the maximally mixed state if and only if the function $r(a)$ has local minimum or maximum at the origin.

C. Curvature formula at the origin and Radon measures

To find an operator monotone function f such that the scalar curvature has local minimum at the origin we start from the following representation theorem in Ref. 19.

The map $\mu\mapsto f$ defined by

$$f(x)=\int_0^\infty \frac{x(1+t)}{x+t}\,\mathrm{d}\mu(t) \quad \text{for } x>0$$

establishes an affine isomorphism from the class of positive Radon measures $[0,\infty]$ onto the class of operator monotone functions.

We use a modified version of the previous theorem Ref. 20.

Theorem 2.4: *The map $\mu\mapsto f$, defined by*

$$f(x)=\int_0^1 \frac{x}{(1-t)x+t}\,\mathrm{d}\mu(t), \quad \text{for } x>0, \tag{19}$$

establishes a bijection between the class of positive Radon measures on [0,1] and the class of operator monotone functions.

From this representation we get that

$$xf(x^{-1})=\int_0^1 \frac{x}{(1-t)+tx}\,\mathrm{d}\mu(t)=\int_0^1 \frac{x}{(1-t)x+t}\,\mathrm{d}\mu(1-t) \quad .$$

Thus $f(x)=xf(x^{-1})$ holds iff $\mu([0,t])=\mu([1-t,1])$ for all $t\in[0,1]$ and the $f(1)=1$ normalization means that $\mu([0,1])=1$. Let T denote the set of all positive Radon measures on the $[0,1]$ interval such that $\mu(X)=\mu(1-X)$ for every measurable X subset of $[0,1]$ and $\mu([0,1])=1$. Theorem 2.1 and 2.4 imply that there is bijective correspondence between monotone metrics and T.

III. SCALAR CURVATURE

A. Scalar curvatures with local minimum at the origin

For detailed verification of Theorem 3.1 and 3.3 the *Maple* program was used. The Maple worksheet, containing these proofs is available at Ref. 21.

Theorem 3.1: *The series expansion of $r(a)$ at the origin leads to the*

$$r(a)=(6+36f''(1))+a^2\left(\tfrac{100}{3}f^{(4)}(1)-140f''(1)-120f''(1)^2\right)+a^4(352f''(1)^3+616f''(1)^2$$
$$+1092f''(1)-\tfrac{1288}{3}f^{(4)}(1)+\tfrac{392}{45}f^{(6)}(1)-160f''(1)f^{(4)}(1))+O(a^6) \tag{20}$$

approximation.

Proof: From Eq. (5) one may expect that the $1/a$ and $1/a^2$ type divergences occur in this expansion but the behavior derivatives of f not allow this. It is obvious that $r(a)=r(-a)$ from symmetric reasons (not from the formula) this means that the coefficient of $a^{(2n+1)}$ will be zero for all $n\in\mathbb{N}$. We proof this series expansion only up to the order $O(a^4)$ because the coefficient of a^4 can be derived in a similar way, but it needs more complicated formulas. Through the computation we will use the identities

$$f'(1)=\frac{1}{2}, \quad f^{(3)}(1)=-\frac{3}{2}f^{(2)}(1), \quad f^{(5)}(1)=-\frac{15f^{(4)}(1)+60f^{(3)}(1)+60f^{(2)}(1)}{2}$$

which come from the equations $f(x)=xf(1/x)$ and $f(1)=1$. We consider the scalar curvature as a sum of five functions according to the Eq. (5). The series expansion of the summands can be computed in elementary way, but the intermediate formulas are rather complicated. The series expansions of the five summands from Eq. (5) after simplifications are the following:

(1) $-\frac{7}{2}+7(4f''(1)+1)\cdot a-7(8f''(1)^2+4f''(1)+1)\cdot a^2$.
(2) $-6\cdot\frac{1}{a}+(24f''(1)+13)-(28f''(1)+12)\cdot a+(16f^{(4)}(1)-48f''(1)^2-52f''(1)+12)\cdot a^2$.
(3) $8f''(1)+(16f^{(4)}(1)-16f''(1)^2-56f''(1))\cdot a^2$.

(4) $2\cdot\frac{1}{a}^2+4f''(1)+(4/3\,f^{(4)}(1)-4f''(1))\cdot a^2$.
(5) $-2\cdot\frac{1}{a}^2+6\cdot\frac{1}{a}-5+5\cdot a-5\cdot a^2$.

The sum of these expansions leads to Eq. (5) in this theorem. □

Combining Eqs. (19) and (20) we conclude that the scalar curvature has local minimum at the origin if

$$12\left(\int_0^1 t(1-t)\ \mathrm{d}\mu(t)\right)^2-\int_0^1 t(t-1)(20t^2-40t+13)\mathrm{d}\mu(t)<0 \tag{21}$$

holds for a $\mu\in T$. The scalar curvature at the origin is given by

$$6+72\int_0^1 (t^2-t)\ \mathrm{d}\mu(t).$$

It has maximum when $\mu=(1/2)\,\delta_0+(1/2)\,\delta_1$, the corresponding operator monotone function is $f(x)=(1+x)/2$ and then $r(0)=6$. It has minimum when $\mu=\delta_{1/2}$, the corresponding operator monotone function is $f(x)=2x/(1+x)$ and then $r(0)=-12$.

The measure $\mu\in T$ can be transformed into a probability measure μ' on the [0,1] interval such that

$$\int_0^{-1/2} t(1-t)\ \mathrm{d}\mu(t)=\frac{1}{8}\int_0^1 x\ \mathrm{d}\mu'(x)$$

because the $4t(1-t)$ function maps the $2\mu|_{[0,1/2]}$ measure into a probability measure on [0,1]. If λ denotes the Lebesgue measure and

$$\mu(t)|_{[0,1/2]}=\rho(t)\ \mathrm{d}\lambda(t)+\sum a_i\delta_{p_i}$$

then

$$\mu'(x)=\frac{1}{2}\rho\left(\frac{1-\sqrt{1-x}}{x}\right)\frac{1}{\sqrt{1-x}}\mathrm{d}\lambda(x)+\sum 2a_i\delta_{4p_i(1-p_i)}.$$

There is one to one correspondence between probability measures on [0,1] and T. Let m_μ denote the expectation σ_μ^2 the variance and $E_{n,\mu}$ the nth momentum of the μ' measure. Using Eq. (19) and the previous notation one can check the following equalities:

$$f''(1)=-\frac{m_\mu}{2},\quad f^{(4)}(1)=-3m_\mu+\frac{3}{2}E_{2,\mu},\quad f^{(6)}(1)=-90m_\mu-\frac{45}{4}E_{3,\mu}+90E_{2,\mu}.$$

Substituting this into the approximation Eq. (20) one gets the following theorem.

Theorem 3.2: *If for a measure $\mu\in T$ the inequality*

$$m_\mu(3-2m_\mu)<5\sigma_\mu^2$$

holds or if

$$m_\mu(3-2m_\mu)=5\sigma_\mu^2\quad\text{and}\quad -44m_\mu^3+70m_\mu^2+114m_\mu<98E_{3,\mu}$$

then the scalar curvature of the metric induced by the measure μ by the Eq. (19) has local minimum at the origin.

We give examples for monotone metrics which satisfies the previous conditions so the scalar curvature of them has local minimum at the maximally mixed state.

Theorem 3.3: *Let*

$$\frac{7-\sqrt{7}}{14}<p\leqslant\frac{1}{2}$$

and

$$h(p)=\frac{\sqrt{14p^2-14p+4+\sqrt{-640p^4+1280p^3-880p^2+240p+9}}}{2\sqrt{7}} \tag{22}$$

and $0\leqslant q<\frac{1}{2}-h(p)$. *Then the scalar curvature of the* $\mathcal{M}_2^+$ *manifold coming from the operator monotone function*

$$f(x)=\frac{x}{4}\left(\frac{1}{px+1-p}+\frac{1}{(1-p)x+p}+\frac{1}{qx+1-q}+\frac{1}{(1-q)x+q}\right) \tag{23}$$

has local minimum at the origin.

Proof: First one can try to find a $\mu\in T$ measure such that Eq. (21) holds in

$$\mu_p=\tfrac{1}{2}\delta_p+\tfrac{1}{2}\delta_{1-p} \tag{24}$$

form where δ_p is a Dirac measure. Let

$$t_\mu:=12\left(\int_0^1 t(1-t)\ \mathrm{d}\mu(t)\right)^2-\int_0^1 t(t-1)(20t^2-40t+13)\ \mathrm{d}\mu(t) \tag{25}$$

and $t(p)=t_{\mu_p}$. We get that

$$t(p)=p(1-p)(8p^2-8p+3).$$

For all $p\in[0,1/2]$ we have $t(p)>0$. This means that the scalar curvature has local maximum at the origin for all μ_p measures.

Let $p\in[0,1/2]$, $q\in[p,1/2]$, and

$$\mu_{p,q}=\tfrac{1}{4}\delta_p+\tfrac{1}{4}\delta_q+\tfrac{1}{4}\delta_{1-p}+\tfrac{1}{4}\delta_{1-q}. \tag{26}$$

Let $t(p,q)=t_{\mu_{p,q}}$ then

$$t(p,q)=-7(p^4+q^4)+14(p^3+q^3)-6pq(p+q-pq-1)-\tfrac{17}{2}(p^2+q^2)+\tfrac{3}{2}(p+q). \tag{27}$$

After substituting into Eq. (27) the

$$p=\frac{v+\sqrt{v^2-4u}}{2},\quad q=\frac{v-\sqrt{v^2-4u}}{2} \tag{28}$$

formulas one derives that

$$t(u,v)=-8u^2+(28v^2-48v+23)u-(7v^4-14v^3+\tfrac{17}{2}v^2-\tfrac{3}{2}v). \tag{29}$$

The equation $t(u,v)=0$ has two solutions for a given v. Taking into account that $u=pq$ we get the condition $0<u<\frac{1}{4}$. The only solution of the equation $t(u,v)=0$ which fulfills this condition is

$$u(v)=\tfrac{7}{4}v^2-3v+\tfrac{23}{16}-\tfrac{1}{16}\sqrt{560v^4-2240v^3+3320v^2-2160v+529}. \tag{30}$$

If the parameter p is given then q can be computed from the equation $u(p+q)=pq$. There are four solutions for q but only one of them is admissible

$$q(p)=\tfrac{1}{2}-\tfrac{1}{14}\sqrt{84p^2-84p+28+7\sqrt{-640p^4+1280p^3-880p^2+240p+9}} \tag{31}$$

because of the conditions for q. This equation gives positive parameter q if

$$\frac{7-\sqrt{7}}{14}<p\leqslant\frac{1}{2}.$$

One can check that if $0<q<q(p)$ then the function $t(p,q)$ is negative. Then we use Eq. (19) defining a desired $f(z)$ operator monotone function from the $\mu_{p,q}$ measures. □

If we choose $(7-\sqrt{7})/14<p\leqslant\frac{1}{2}$ arbitrary and $q=0$ in the previous theorem then we get that the scalar curvature coming from the operator monotone function

$$f(x)=\frac{x}{4}\left(\frac{1}{(1-p)x+p}+\frac{1}{px+1-p}+\frac{1}{x}+1\right)$$

has local minimum at the origin. In this case series expansion of the scalar curvature at the origin is

$$r(a)=(\tfrac{9}{2}-36p(1-p))-20p(1-p)(14p^2-14p+3)\cdot a^2+O(a^4).$$

One can prove that the minimum at the origin is not only local but global for these functions. The greatest value of the scalar curvature in this case is

$$r(1)=\frac{7}{2}+\frac{1}{p(1-p)}.$$

Here some other examples for operator monotone functions, such that the scalar curvature derived from them has local, but not global minimum at the maximally mixed state,

$$f(x)=\frac{x}{4}\left(\frac{4}{x+1}+\frac{50}{x+49}+\frac{50}{49x+1}\right),\quad f(x)=\frac{250x}{999x+1}+\frac{250x}{x+999}+\frac{x}{x+1}.$$

Numerical computations suggest that the scalar curvature of the Riemannian metric of a three level quantum system induced by the second function has local minimum at the maximally mixed state.

IV. CONCLUSIONS

The Riemannian metrics so far studied on the manifold $\mathcal{M}_n^+$ come from special operator monotone functions according to Theorem 2.1. The metric carries all differential geometrical properties of the manifold, this means that from a suitable function f one can derive all geometrical quantities of the manifold. One of the basic phenomenological problems is to give physical interpretation of differential geometrical quantities.

One can expect that the greatest statistical uncertainty should belong to the most mixed states. This expectation means that the scalar curvature of Riemannian metrics should have a global maximum at the maximally mixed state. We gave several examples for suitable operator monotone functions such that the derived scalar curvatures do not fulfill this expectation and have even a local minimum at the maximally mixed state.

The Kubo–Mori (or Bogoliubov) metric comes from the function $f(x)=(x-1)/\log x$. This is one of the statistically most relevant metrics. It was conjectured in Ref. 17 that the scalar curvature of this metric is monotone in the following sense. If D_1, $D_2 \in \mathcal{M}_n^+$, and D_1 is more mixed than D_2 then $r(D_1) \geqslant r(D_2)$.

ACKNOWLEDGMENTS

The author thanks Dr. Dénes Petz for stimulating discussions and valuable remarks. This work was partially supported by OTKA T32374 and OTKA T43242.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Spontaneous localization of electrons in two-dimensional lattices within the adiabatic approximation

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(Received 30 August 2002; accepted 13 May 2003)

The conditions for spontaneous localization of electrons in an isotropic two-dimensional electron–phonon lattice are investigated within the zero adiabatic approximation. It is shown that the localization occurs when the electron–phonon coupling takes values within certain finite interval of values $g_{c,1}<g<g_{c,2}$. At $g<g_{c,1}$ the energy minimum is attained for the delocalized states and at $g>g_{c,2}$ the strong localization on one lattice site takes place. In this paper we introduce an ansatz which, under a variational principle, allows us to describe all three regimes at the same time. The radius of the electron localization, as a function of electron–phonon coupling constant, is evaluated analytically and shown to fit well the numerical data. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1592873]

I. INTRODUCTION

Low-dimensional systems in general, and electron–phonon systems in particular, attract significant attention both from the experimental and theoretical points of view.[1–8] It is known that in such systems the electron–phonon coupling can be significant and can lead to the formation of localized modes, due to which the electroconducting and/or optical properties of the system can change drastically. In particular, in one-dimensional systems (1DSs) solitonlike states of quasiparticles (electron, hole, exciton) can be formed[9] under certain conditions, namely, when the parameters of the system satisfy the conditions of an adiabatic approximation. The latter is valid when the nonadiabaticity parameter, which is determined as the ratio between the width of the electron band and the characteristic energy of the phonons, is small and when the electron–phonon coupling takes values within a certain finite interval $g_{cr,1}<g<g_{cr,2}$.[10] At weak coupling, when $g<g_{cr,1}$, the quasiparticle is almost free, while at strong coupling, when $g>g_{cr,2}$, a small polaron state is formed which corresponds to the self-trapping of this quasiparticle within one lattice site. Although both solitons and small polarons correspond to the localized quasiparticle states, their transport and stability properties differ significantly: the small polaron motion corresponds to a jumping mechanism and is sensitive to temperature, presence of impurities in the compound, etc., while a soliton, which is localized within several lattice sites, can propagate coherently almost without emitting phonons and is stable due to the mutual compensation between the dispersion and the nonlinearity.

Much less is known about the possibility of spontaneous localization, i.e., the formation of solitonlike states, in 2DSs. First, it is known that in other 2DSs (in plasma, magnetic systems, etc.) 2D solitons might be unstable under the interaction with weak perturbations and, as a result, collapse, i.e., shrink infinitely.[11–13] This shrinking might turn out to be even more important for 'molecular solitons with nonzero velocity, since it is known that the amplitude and the inverse

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radius of localization of 1D solitons increase with the increase of their velocity.[9,14] On the other hand, it is clear that such shrinking of the soliton size is restricted by the discreteness of the system. Some aspects of this problem have been studied for isotropic[15–17] and anisotropic[18,19] 2D crystals. In particular, the possibility of the existence of solitonlike states in 2D lattices has been demonstrated numerically and analytically within various variational schemes. It has turned out that, even within the adiabatic approximation, when the wave vector of the state is chosen to be given by the product of the electron and the renormalized phonon wave functions, the formation of soliton states occurs only within a certain range of the parameters. In the isotropic case this parametric domain can be characterized again by the dimensionless electron–phonon coupling constant: the soliton exists if the condition $g_{c,1}<g<g_{c,2}$ is valid, where the constants $g_{c,1}$ and $g_{c,2}$ are, in general, different from the corresponding constant for the 1DSs. This differs from the 1D case where, once the adiabatic approximation is assumed, the spontaneous localization takes place *formally* for an arbitrary value of the electron–phonon coupling constant.

To understand this better here we present, within the adiabatic approximation, a variational function for a 2D isotropic lattice in such a form that it allows us to describe in a self-consistent way all three electron states: delocalized, spontaneously localized and strongly localized (nearly on one lattice site). We calculate the radius of localization as a function of the electron–phonon coupling constant, and compare these values with the results of the direct numerical calculations of the system of discrete equations. The analytical results show distinctly the existence of the lower critical value $g_{c,1}$ for the formation of solitonlike states, and the transition from soliton states to the small polaron states when $g\to g_{c,2}$.

II. GENERAL DESCRIPTION OF THE MODEL

The quasiparticle states in a 2D lattice where the electron–phonon interaction is taken into account are described by the following Hamiltonian in the site representation

$$\hat{H}=\sum_{\vec{m}}\ \mathcal{E}_0 A^{+}_{\vec{m}}A_{\vec{m}}+\sum_{\vec{m},\vec{n}}\ [-J_{\vec{m},\vec{n}}(A^{+}_{\vec{m}}A_{\vec{n}}+A^{+}_{\vec{n}}A_{\vec{m}})+\chi_{\vec{m},\vec{n}}A^{+}_{\vec{m}}A_{\vec{m}}(\hat{u}_{\vec{m}}-\hat{u}_{\vec{n}})]$$
$$+\sum_{\mu,\vec{n}}\ \frac{\hat{p}^2_{\mu}(\vec{n})}{2M}+\frac{1}{2}\sum_{\mu,\nu,\vec{n},\vec{m}}\ w_{\mu,\nu}(\vec{n},\vec{m})\hat{u}_{\mu}(\vec{n})\hat{u}_{\nu}(\vec{m}). \tag{1}$$

Here $A^{+}_{\vec{m}}$ ($A_{\vec{m}}$) are the creation (annihilation) operators of the quasiparticle on the site $\vec{m}$ with the corresponding radius-vector coordinate $\vec{R}_{\vec{n}}=\vec{e}_x a_x m+\vec{e}_y a_y n,\ m,n=0,\pm 1,\pm 2,\ldots,\ \hat{u}_{\vec{m}}$ and $\hat{p}_{\vec{m}}$ are the molecule displacements operators and the corresponding conjugate momenta, $\mathcal{E}_0$ is the quasiparticle on-site energy, $J_{\vec{m},\vec{n}}$ are the exchange interaction energies, $\chi_{\vec{m},\vec{n}}$ are the electron–phonon coupling constants, $\vec{e}_{\mu}$ is the unit vector along μ axis, $\mu=x,y$. Moreover, a_{μ} is the corresponding lattice spacing, M is the atom mass and $w_{\mu,\nu}(\vec{n},\vec{m})$ are the lattice elasticity coefficients which are assumed to be constant on the grid: $w_{\mu\mu}(\vec{n},\vec{n}\pm\vec{e}_x)=w_{\mu\mu}(\vec{n},\vec{n}\pm\vec{e}_y)=w$.

In the adiabatic approximation the vector state of the system, $|\Psi\rangle$, can be chosen in the multiplicative form[20,18] which, after substitution into the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle=\hat{H}|\Psi\rangle, \tag{2}$$

leads to the following system of discrete equations describing the dynamics of a quasiparticle in a self-consistent deformational potential on a 2D lattice in the nearest neighbor approximation:

$$i\frac{d\varphi_{m,n}}{d\tau}=E_0\varphi_{m,n}-(\varphi_{m+1,n}+\varphi_{m-1,n}+\varphi_{m,n+1}+\varphi_{m,n-1})$$
$$+[U_{m+1,n}-U_{m-1,n}+V_{m,n+1}-V_{m,n-1}]\varphi_{m,n}, \tag{3}$$

$$\frac{d^2U_{m,n}}{d\tau^2} = -K[4U_{m,n} - U_{m+1,n} - U_{m-1,n} - U_{m,n+1} - U_{m,n-1}] + X(|\varphi_{m+1,n}|^2 - |\varphi_{m-1,n}|^2), \quad (4)$$

$$\frac{d^2V_{m,n}}{d\tau^2} = -K[4V_{m,n} - V_{m+1,n} - V_{m-1,n} - V_{m,n+1} - V_{m,n-1}] + X(|\varphi_{m,n+1}|^2 - |\varphi_{m,n-1}|^2). \quad (5)$$

Here we have introduced the dimensionless parameters

$$\tau = \frac{Jt}{\hbar}, \quad U = \frac{u_x\chi}{J}, \quad V = \frac{u_y\chi}{J},$$
$$E_0 = \frac{\mathcal{E}_0 + \mathcal{W}}{J}, \quad K = \frac{\hbar^2 w}{M J^2}, \quad X = \frac{\hbar^2 \chi^2 \hbar^2}{M J^3}, \quad (6)$$

where $u_\mu(\vec{n},t)$ are the average values of the molecule displacements in the μ direction, and $\varphi_{\vec{n}}$ is the probability amplitude of the quasiparticle being located on the $\vec{n}$th site. The total probability is normalized to unity.

The total energy of the system governed by Eqs. (3)–(5) is conserved and can be represented as the following functional:

$$\mathcal{H} = \sum_{\vec{n}} \left\{ \mathcal{E}_0 \varphi_{\vec{n}}^* \varphi_{\vec{n}} - J[\varphi_{\vec{n}}^*(\varphi_{\vec{n}+\vec{e}_x} + \varphi_{\vec{n}-\vec{e}_x}) - \varphi_{\vec{n}}^*(\varphi_{\vec{n}+\vec{e}_y} + \varphi_{\vec{n}-\vec{e}_y})] \right.$$
$$\left. + \varphi_{\vec{n}}^* \varphi_{\vec{n}} \chi \sum_\mu [u_\mu(\vec{n}+\vec{e}_\mu) - u_\mu(\vec{n}-\vec{e}_\mu)] \right\} + \mathcal{W}. \quad (7)$$

Here $\mathcal{W}$, the phonon energy, is the sum of the lattice kinetic and potential energies

$$\mathcal{W} = \frac{1}{2} \sum_{\vec{n},\mu} \left\{ \frac{p_\mu^2(\vec{n})}{M} + w_x[u_\mu(\vec{n}) - u_\mu(\vec{n}-\vec{e}_x)]^2 + w_y[u_\mu(\vec{n}) - u_\mu(\vec{n}-\vec{e}_y)]^2 \right\}. \quad (8)$$

In this paper we consider a square lattice $N_x = N_y = N$ and introduce the quasimomentum representation

$$\vec{k} = k_x\vec{e}_x + k_y\vec{e}_y, \quad k_\mu = \frac{2\pi l_\mu}{N}, \quad l_\mu = 0, \pm 1, \pm 2, \ldots, N/2, \quad (9)$$

using the following transformation:

$$\varphi_{\vec{n}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \Phi(\vec{k}) e^{i\vec{k}\vec{n}}, \quad u_\mu(\vec{n}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} Q_\mu(\vec{k}) e^{i\vec{k}\vec{n}}. \quad (10)$$

The quasiparticle wave function, after excluding the deformational variables in the stationary case, satisfies in this representation the following nonlinear equation:

$$[E(\vec{k}) - E]\Phi(\vec{k}) - \frac{1}{N} \sum_{\vec{k}',\vec{q}} G(\vec{q}) \Phi^*(\vec{k}') \Phi(\vec{k}' + \vec{q}) \Phi(\vec{k} - \vec{q}) = 0, \quad (11)$$

and the corresponding energy functional takes the form

$$E_{\text{tot}} = \sum_{\vec{k}} E(\vec{k}) |\Phi(\vec{k})|^2 - \frac{1}{2N} \sum_{\vec{k}} G(\vec{k}) |\wp(\vec{k})|^2, \quad (12)$$

where

$$E(\vec{k}) = \mathcal{E}_0 - 2J(\cos(k_x) + \cos(k_y)), \tag{13}$$

$$G(\vec{k}) = \frac{\chi^2}{w} \frac{\sin^2(k_x) + \sin^2(k_y)}{\sin^2(k_x/2) + \sin^2(k_y/2)}, \tag{14}$$

$$\wp(\vec{k}) = \sum_{\vec{q}} \Phi^*(\vec{q})\Phi(\vec{q}-\vec{k}) = \sum_{\vec{n}} e^{i\vec{k}\vec{n}} |\varphi_{\vec{n}}|^2. \tag{15}$$

In view of their complexity, Eqs. (3)–(5) can be studied numerically or by using a variational scheme. The numerical studies[18,17] have shown that, depending on the value of electron–phonon coupling, three types of electron ground states occur. To perform an analytical study different forms of the variational functions have been tried, and it has turned out, that the variational functions which had been used, can describe numerical data satisfactorily only in some finite intervals of the coupling constant. Namely, the decreasing exponential function describes the regime of strong localization (strong coupling),[21,17] while hyperbolic[17] and Gaussian[17,16] functions describe the soliton regime (intermediate coupling). But the transition itself from one regime to the other, up to now, has not been described analytically. Here we present a trial function in a form which allows us to describe all three regimes of the coupling constant.

III. VARIATIONAL STUDY

First we note that discrete structures that are periodic in space are characterized by functions which are periodic also in the reciprocal space. Moreover, for $N \gg 1$, the quasimomentum $\vec{k}$ varies as a quasicontinuous function, which allows us to replace the infinite sums by the corresponding integration in the first Brillouin zone. Taking into account these two arguments, we choose the trial function in the form

$$\Phi(\vec{k}) = \Phi(k_x)\Phi(k_y), \quad \Phi(k_\mu) = \frac{2AK(k)}{\pi\sqrt{N}} \mathrm{d}n(u_\mu, k), \tag{16}$$

where $\mathrm{d}n(u_\mu, k)$ is the elliptic Jacobi function of the argument u_μ and of the modulus k, which is assumed to be the variational parameter. The argument of the elliptic function, u, is related to the quasimomentum k_μ by the relation $u_\mu = K(k)ak_\mu/\pi$ where $K(k)$ is the complete elliptic integral of the first kind. Note that we use the standard notations k_μ for the quasimomentum and k for the modulus of the elliptic functions and therefore k_μ and k should be distinguished. The parameter A in (16) can be found from the normalization condition

$$\sum_{\vec{n}} |\varphi_{\vec{n}}|^2 = \sum_{k_\mu} |\Phi(k_\mu)|^2 = 1, \quad A^2 = \frac{\pi^2}{4KE}, \tag{17}$$

where E is the complete elliptic integral of the second kind.

Due to the periodicity of the elliptic function (with period $2K$), the function (16) is also a periodic function (with period 2π) and it describes a spatially localized distribution $\varphi_n = A\cosh^{-1}(\kappa n)$ whose width is controlled by κ. Indeed,

$$\Phi(k_\mu) = \frac{A}{\sqrt{N}} \sum_{n=-(N-1)/2}^{(N-1)/2} \frac{e^{-ik_\mu n}}{\cosh(\kappa n)} = \frac{A}{\sqrt{N}} \left[1 + 4 \sum_{n=1}^{(N-1)/2} \frac{e^{-\kappa n}\cos(k_\mu n)}{1 + e^{-2\kappa n}} \right]. \tag{18}$$

Taking the limit $N \to \infty$ and using the Fourier series of the elliptic function $\mathrm{d}n$, leads to the expression (16) with the Jacobi parameter $q = \exp(i\pi\tau)$, where $\tau = i\kappa/\pi$.

The modulus of the elliptic functions, k, is related to the localization parameter, κ, by

$$\kappa=\pi\frac{K'(k)}{K(k)},\quad K'(k)=K(k'),\quad k'^2=1-k^2. \tag{19}$$

The width of the localized structure, κ, as the variational parameter can be determined by minimizing the energy

$$\frac{dE_{\mathrm{tot}}(\kappa)}{d\kappa}=0. \tag{20}$$

Note that function (16) for large κ is close to a decreasing exponent, and at small κ it reduces to the hyperbolic function. Therefore, such a choice of the trial function generalizes these two limiting cases.

The evaluation of (15) with (16) after integrating over the quasimomentum space gives

$$\wp(k_\mu)=\frac{K}{E}\left[\mathrm{d}n(u)-\frac{cn(u)}{sn(u)}Z(u)\right], \tag{21}$$

where $Z(u)=E(u)-uE/K$ is the Jacobi Z-function and where, according to the normalization condition, $\wp(0)=1$.

To perform further calculations analytically it is convenient to use the representation of the elliptic functions in terms of the ϑ-functions $\vartheta_j(z,q)$, $j=1,2,3,4$ defined by the following standard relations:[22,23]

$$\mathrm{d}n(u)=\frac{\vartheta_4\vartheta_3(z)}{\vartheta_3\vartheta_4(z)},\quad cn(u)=\frac{\vartheta_4\vartheta_2(z)}{\vartheta_2\vartheta_4(z)},\quad sn(u)=\frac{\vartheta_3\vartheta_1(z)}{\vartheta_2\vartheta_4(z)},\quad Z(u)=\frac{\pi}{2K}\frac{\vartheta_4'(z)}{\vartheta_4(z)}. \tag{22}$$

Here $z=\pi u/2K=k_\mu/2$, $\vartheta_j=\vartheta_j(0)$, and $\vartheta_j'(z)=\mathrm{d}\vartheta_j(z)/\mathrm{d}z$.

Next we substitute (22) into (21) and, using the differential relation,[22]

$$\vartheta_4(z)\vartheta_2'(z)-\vartheta_2(z)\vartheta_4'(z)=-\vartheta_3^2\vartheta_1(z)\vartheta_3(z), \tag{23}$$

we obtain the following representation for $\wp(k_\mu)$:

$$\wp(k_\mu)=-\frac{\pi\vartheta_4}{2E\vartheta_3}\frac{\vartheta_2'(z)}{\vartheta_1(z)}. \tag{24}$$

To proceed further with the calculations that involve the complete elliptic integrals it is convenient to use their representation in terms of the ϑ-functions of zero-argument. For the complete elliptic integral of the first kind we have $K=\pi\vartheta_3^2/2$, and for the complete elliptic integral of the second kind several representations are given in textbooks. From (24), using the relation $\vartheta_1'=\vartheta_2\vartheta_3\vartheta_4$, we obtain a new representation,

$$E=-\frac{\pi^2}{4K}\frac{\vartheta_2''}{\vartheta_2}, \tag{25}$$

which is more convenient than others, and, to our knowledge, is absent from most handbooks (see, e.g., Refs. 22–24). This relation will be used below.

The calculation of the first term in the energy expression (12) is straightforward, while the second term requires an approximation. For this we note that the function (14) can be rewritten in several equivalent ways, one of which contains a term that vanishes on the lines $k_x=\pm k_y$ in the $\vec{k}$ plane, while the other vanishes on the lines $k_x=0$ and $k_y=0$. Combining these two representations with different weights α and β, such that $\alpha+\beta=1$, we can set a corresponding weight as a free parameter to be determined by the requirement of producing the best fit to the numerical data.

Taking all this into account, we obtain the following expression for the energy as a function of the variational parameter (12):

$$E_{\rm tot}=\mathcal{E}_0-J\left\{4L+\frac{g}{2}F_1[\alpha F_1+(2-\alpha)F_2]\right\}, \tag{26}$$

where g is the dimensionless electron–phonon coupling constant

$$g=\frac{2\chi^2a^2}{Jw}, \tag{27}$$

and where

$$L=\sum_{k_\mu}|\Phi(k_\mu)|^2\cos(k_\mu)=-\frac{2\vartheta_2}{\vartheta_2''\sinh\kappa}, \tag{28}$$

$$F_1=\frac{1}{N}\sum_{k_\mu}|\wp(k_\mu)|^2=\frac{1}{6}\left(3-4\frac{\vartheta_2}{\vartheta_2''}-\frac{\vartheta_2\vartheta_2'''}{(\vartheta_2'')^2}\right), \tag{29}$$

$$F_2=\frac{1}{N}\sum_{k_\mu}|\wp(k_\mu)|^2\cos(k_\mu)=\frac{L(L\cosh\kappa-1)}{\sinh\kappa}. \tag{30}$$

Substituting (26) into (20), we obtain the following equation for the localization parameter κ as a function of g:

$$g=-\frac{8\,{\rm d}L/{\rm d}\kappa}{2\alpha F_1F_{1,\kappa}+(2-\alpha)(F_{1,\kappa}F_2+F_1F_{2,\kappa})}, \tag{31}$$

where $F_{j,\kappa}={\rm d}F_j/{\rm d}\kappa$.

To analyze Eq. (31), it is necessary to calculate explicitly the derivatives of the functions with respect to the localization parameter. For this one can use equations for ϑ-functions which, when $\tau=i\kappa/\pi$, have the form[22–24]

$$\frac{\partial^2\vartheta_j}{\partial z^2}=4\frac{\partial\vartheta_j}{\partial\kappa},\quad j=\overline{1,4}. \tag{32}$$

In this case the functions in (31) are expressed via the ϑ-functions and their zero argument derivatives. To calculate the functions appearing in (31) at small κ, when the Jacobi parameter $q=\exp(-\kappa)$ is not small, it is convenient to use the ϑ-functions as functions of the small parameter $q'=\exp(-i\pi/\tau)=\exp(-\pi^2/\kappa)$, performing the imaginary Jacobi transformation. Thus, for instance,[22,23]

$$\vartheta_2(z,q)=(-i\tau)^{-1/2}\exp\left(\frac{i\tau'z^2}{\pi}\right)\vartheta_4(z\tau',q'),\quad \tau'=-\frac{1}{\tau}. \tag{33}$$

This allows us to determine the dependence of the localization parameter κ, as a function of g given by Eq. (31), numerically. Our result is presented in Fig. 1, where we see that at $g<g_{c,1}=6$ the localization does not occur, $\kappa=0$, and the ground electron state corresponds to a delocalized state. At $g>g_{c,1}$ there are two different regimes of the localization with the distinct transition from one regime, which corresponds to $\kappa<1$, to the other one with $\kappa>1$. This transition manifests itself as a sharp change of the curve $\kappa(g)$.

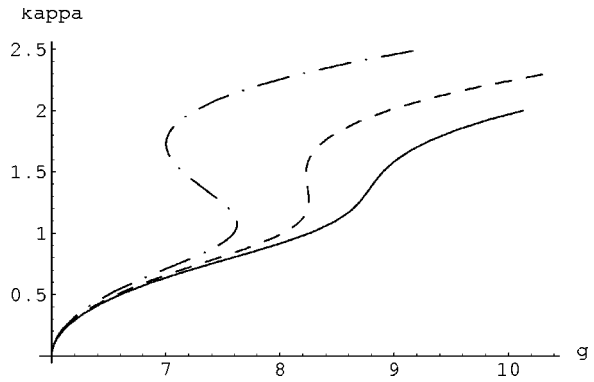

FIG. 1. Dependence of the localization parameter κ on the nonlinearity parameter g as the solution of (20) at $\alpha=0.45$ (solid line), $\alpha=0.5$ (dashed line), and $\alpha=0.6$ (dotted–dashed line).

To compare the results of the variational analysis presented above with the direct numerical calculations of the initial system of discrete equations (3)–(5) it is necessary to calculate the radius of the localization. For the latter the following definition can be used:

$$R^2=\sum_{n,m}(n^2+m^2)|\varphi_{n,m}|^2=-\frac{\mathrm{d}^2}{\mathrm{d}\vec{k}^2}\wp(\vec{k})\bigg|_{\vec{k}=0}. \tag{34}$$

Substituting the explicit expression (24) in (34), we obtain

$$R^2=\frac{2K^2}{3\pi^2}\left[1-\left(\frac{2K}{E}-1\right)k'^2\right]=\frac{1}{6}\left(\frac{\vartheta_1'''}{\vartheta_1'}-\frac{\vartheta_2^{IV}}{\vartheta_2''}\right). \tag{35}$$

The analysis of the last expression shows that at small κ the radius equals $R=\pi/(\sqrt{6}\kappa)$, i.e., it coincides with the radius of the hyperbolic trial function, while at large values of κ it takes the form $R=\sinh^{-1}(\kappa)$ which is equal to the width of localization of the trial function chosen in the form of a decreasing exponential.[17]

In Fig. 2 we present this dependence of the radius of localization as a function of the nonlinearity constant, g, together with the numerical results. The numerical curve shows that $g_{c,1}\approx 5.85$ and $g_{c,2}\approx 7.5$.

While $g_{c,1}$ is well defined as the critical value below which stationary solutions of the model do not exist, $g_{c,2}$ is more difficult to define explicitly: The transition between localized and very strongly localized (small polaron) solutions is not very sharp but one observes that during the transition, the second derivative of the inverse radius of the localization, $d^2(1/R)/dg^2$, is positive near $g_{c,2}$ but negative elsewhere (see Fig. 2 or Ref. 17). If we call $g_{z,1}$ and $g_{z,2}$ the values of g where $d^2(1/R)/dg^2=0$, then we can define $g_{c,2}=(g_{z,1}+g_{z,2})/2$ and from Fig. 2. we see that $R(g_{c,2})\approx 1$ as one would expect intuitively: the solution is essentially localized on one lattice site.

The variational curve, shown in Fig. 2 corresponds to $\alpha=0.45$ and from it one sees that the self-trapped state extends over a few lattice sites when $6<g<8$. In this case the envelope function of the electron distribution changes smoothly from site to site, and the long-wave (continuum) approximation is valid. When $g>9$, the localization is very narrow, virtually, within one lattice site and therefore the lattice discretness is essential and the continuum approximation, obviously, is not valid.

In general, the value of the parameter α introduced in (26) (notice, α is always <1), changes the position of the transition from the soliton regime to the regime of strong localization with respect to g in the interval 8–9 and influences the steepness of the transition. Moreover at $\alpha>0.5$ a bistability takes place, as shown in Fig. 1. Although this bistability can possibly be thought of as an artifact of the variational analysis, its presence indicates that, within the region of the

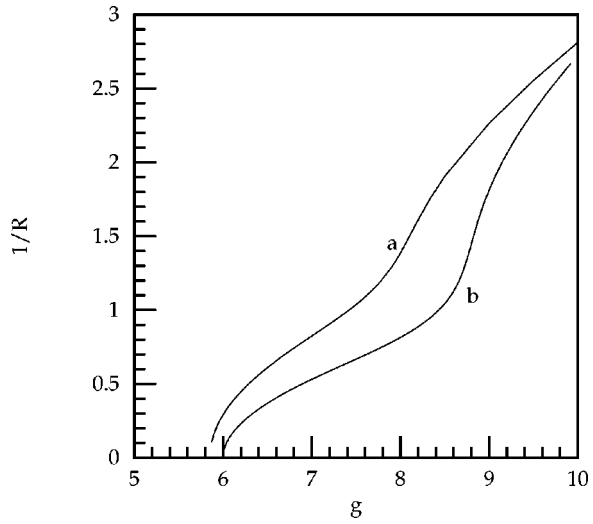

FIG. 2. Inverse radius of localization, $1/R$, as a function of g: (a) Numerical solution of Eqs. (3)–(5), (b) variational curve corresponding to Eq. (35) for $\alpha=0.45$.

transition, $g\approx 8.5$, the self-trapped states are sensitive to the influence of various perturbations, temperature, inclusion of other vibrational modes [i.e., presence of optical mode(s), complex elementary cell of a crystal, account of long-range interactions], etc. Therefore, this bistability can manifest itself in other models. It can possibly be treated as a potential barrier which separates solitonlike states from strongly localized states (the latter ones tend to collapse in the continuum 2D NLSE model).

IV. CONCLUSIONS

We have shown that a 2D lattice with an electron–phonon interaction admits solitonic solutions when the coupling constant g is larger than its lower critical value, $g_{c,1}\approx 5.85$, and lower than its upper critical value, $g_{c,2}\approx 7.5$ ($g_{c,2}\approx 8.5$ for the variational curve). In this interval a solitonic solution is stable with respect to finite and not too large perturbations. The stabilization of such a 2D soliton, which stops it from collapsing or dispersion over the whole lattice, is due to the mutual influence of the nonlinearity, the wave dispersion and the lattice discreteness. As g gets larger than $g_{c,2}$, the self-trapping changes into the regime of strong localization. This transition also manifests itself by the appearance of a bend of the numerical dependence $1/R(g)$, Fig. 2. When the initial function is slightly different from the stationary state its width oscillates around the value that corresponds to the width of the stationary state.[17] A study of the dynamics of such a soliton and its stability with respect to collisions with boundaries is in progress.

Generally speaking, at various values of the electron–phonon coupling different types of electron ground states are realized: small polarons, solitons (large polarons) or almost free electrons.[10] Between the almost free electron states at a weak coupling and the small polaron states at a strong coupling there is a region of the coupling parameter where a soliton state exists and which arises in systems that satisfy the adiabatic approximation. But the properties of the zero adiabatic description of 1D and 2D systems with respect to the self-trapping are qualitatively different. While in 1DS the self-trapping *formally* occurs at an arbitrary value of the coupling constant within the adiabatic approximation, in 2DS, even within the adiabatic approximation, all these three different regimes can be realized depending on the strength of the coupling.

The comparison of the results obtained here with the conditions of the soliton existence in 1D chains[10] shows that solitons in 2D lattices exist at larger values of the electron–phonon coupling constant. Therefore, the properties of systems of similar compounds but possessing a 1D rather than a 2D structure, could differ qualitatively. Indeed, such an example is given by the compara-

tive study of the vibrational modes of double C═O bond of the peptide group, called Amide-I vibrational modes, in biological macromolecules of myoglobin and in photoactive yellow protein, respectively.[25] While myoglobin, which is essentially α-helical, i.e., is a quasi-1D protein and admits the existence of a long-lived photoexcited Amide-I mode with a lifetime >15 ps, photoactive yellow protein, which is predominantly a β-sheet protein, does not, under the same conditions of photoexcitation. Let us add here, that Davydov and Kislukha[26] were the first to predict the self-trapping of Amide-I excitation in a soliton state in α-helical macromolecules due to the electron–phonon coupling with the hydrogen bonds along polypeptide chains, with the lifetime of such a soliton state much higher than that of an isolated Amide-I excitation.[20]

ACKNOWLEDGMENT

This work reported here was supported by a NATO grant.

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On integrable Hamiltonians for higher spin *XXZ* chain

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(Received 9 May 2002; accepted 6 May 2003)

Integrable Hamiltonians for higher spin periodic XXZ chains are constructed in terms of the spin generators; explicit examples for spins up to $\frac{3}{2}$ are given. Relations between Hamiltonians for some $U_q(sl_2)$-symmetric and $U(1)$-symmetric universal r-matrices are studied; their properties are investigated. A certain modification of the higher spin periodic chain Hamiltonian is shown to be an integrable $U_q(sl_2)$-symmetric Hamiltonian for an open chain. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1591054]

I. INTRODUCTION

XXZ spin chains have numerous connections with two-dimensional statistical physics and $(1+1)$-dimensional quantum field theory. They describe interaction of q-deformed spins sitting at the nodes of a one-dimensional lattice. The spin generators S^+, S^-, and S^3 obey the commutation relations of the quantum Lie algebra $U_q(sl_2)$,[1]

$$[S^+,S^-]=\frac{\sin(2\gamma S^3)}{\sin\gamma},\quad [S^3,S^\pm]=\pm S^\pm. \tag{1}$$

We will consider only integrable XXZ spin models. The simplest example in this class is a spin-$\frac{1}{2}$ chain with the Hamiltonian given by

$$H=\sum_n \left(\frac{1}{2}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)+(\cos\gamma)\,S_n^3S_{n+1}^3\right).$$

Higher spin XXZ chains have also been studied[2,3] but the technique of the "R-matrix fusion" used in these works, although sufficient for application of the Bethe ansatz, did not yield explicit expressions for the corresponding Hamiltonians. In fact, only in the spin-1 case such expression was given in the literature.[2] Another method of constructing the higher spin Hamiltonians, based on consideration of the universal (spectral parameter dependent) R-matrix, was proposed in Ref. 4 but lacked at the time important ideas of the Hopf algebra approach to the quantum groups that was developed later. In the present paper we will combine these two ingredients together and construct local integrable Hamiltonians for higher spin XXZ chains explicitly, i.e., in terms of the spin generators. This, in particular, will allow us to give a rigorous derivation of the properties of the Hamiltonians and to prove integrability of a certain open higher spin chain.

The paper is organized as follows. In Sec. II we recall some facts about $U_q(sl_2)$-symmetric universal r-matrix $r(\lambda)$. In Sec. III we construct a $U_q(sl_2)$-symmetric local Hamiltonian $H_{n,n+1}$. Its properties and properties of the corresponding closed chain Hamiltonian $\mathcal{H}$ are discussed in Sec. IV. In particular, we observe that $H_{n,n+1}$ decomposes into a $U(1)$-symmetric bulk Hamiltonian $\hat{H}_{n,n+1}$ plus a universal local boundary term. Section V contains explicit expressions for $H_{n,n+1}$ for spins $\frac{1}{2}$, 1, and $\frac{3}{2}$. In Sec. VI we find a family of universal r-matrices and Hamiltonians

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corresponding to an alternative choice of the co-multiplication. In Sec. VII we construct another family of [$U(1)$-symmetric] universal r-matrices and local Hamiltonians which contains the Hamiltonian $\hat{H}_{n,n+1}$ and the corresponding reflection-symmetric universal r-matrix $r_0(\lambda)$. In Sec. VIII we employ our construction to establish the integrability of certain [$U_q(sl_2)$-symmetric] Hamiltonians for an open chain. Appendix A contains technical details related to $r(\lambda)$ and $r_0(\lambda)$. Appendix B provides some details on computation of the spin-1 and spin-$\frac{3}{2}$ Hamiltonians presented in Sec. V. Appendix C explains a q-trace formula for $H_{n,n+1}$ used in Sec. VIII.

For compactness of notations, we will use in the text both the deformation parameter γ introduced in (1) and $q \equiv e^{i\gamma}$. We assume that q is either real or takes values on the unit circle. In the latter case q is assumed to be generic, i.e., it is not a root of unity.

II. UNIVERSAL *r*-MATRIX

The starting point of the quantum inverse scattering method is the exchange relation

$$R(\lambda)\, L(\lambda+\mu)\otimes L(\mu) = L(\mu)\otimes L(\lambda+\mu)\, R(\lambda)\,, \tag{2}$$

with $\otimes$ understood as the tensor product with respect to an auxiliary space V (below it is the space of 2×2 matrices) and the usual product of operators in the quantum space $\mathfrak{H}$. The R-matrix belongs to $V\otimes V$. Thus (2) is an equation in $V\otimes V\otimes \mathfrak{H}$.

The following L-operator, i.e., an element of $V\otimes\mathfrak{H}$, is consistent with the algebra (1)

$$L(\lambda) = \frac{1}{\sin\gamma}\begin{pmatrix} \sinh[\,\gamma(\lambda+iS^3)\,] & i\sin\gamma\, e^{\gamma\lambda}\, S^- \\ i\sin\gamma\, e^{-\gamma\lambda}\, S^+ & \sinh[\,\gamma(\lambda-iS^3)\,] \end{pmatrix} \tag{3}$$

in the sense that it satisfies Eq. (2) provided that $R(\lambda)=P_V\check{R}(\lambda)$, where

$$\check{R}(\lambda) = i\, e^{\gamma\lambda}\,\sigma^+\otimes\sigma^- + i\, e^{-\gamma\lambda}\,\sigma^-\otimes\sigma^+ + \frac{1}{\sin\gamma}\sinh\left(\gamma\lambda + \frac{i\,\gamma}{2}(1\otimes 1+\sigma^3\otimes\sigma^3)\right). \tag{4}$$

Here σ^a denote the Pauli matrices, $\sigma^\pm=\sigma^1\pm i\sigma^2$, and $P_V=\frac{1}{2}(1\otimes 1+\Sigma_a\sigma^a\otimes\sigma^a)$ is the permutation matrix in $V\otimes V$.

The L-operator (3) decomposes into two λ-independent Borel components,

$$(2\sin\gamma)\, L(\lambda) = e^{\gamma\lambda}L_+ - e^{-\gamma\lambda}L_-\,, \tag{5}$$

which can be utilized to define[5] the co-multiplication (a linear homomorphism $\Delta: U_q(sl_2)\to[U_q(sl_2)]^{\otimes 2}$) in the matrix form,

$$\Delta(L_\pm) = L_\pm \dot{\otimes} L_\pm\,, \tag{6}$$

where Δ acts on the quantum space and $\dot{\otimes}$ denotes the tensor product with respect to $\mathfrak{H}$ and the usual matrix product in V. In explicit form (6) reads

$$\Delta(S^\pm) = S^\pm\otimes q^{-S^3} + q^{S^3}\otimes S^\pm\,,\quad \Delta(S^3) = S^3\otimes 1 + 1\otimes S^3\,. \tag{7}$$

Observe that (4) can be obtained by evaluating the quantum space of $L(\lambda+i/2)$ in the fundamental representation, where $S^\pm=q^{\pm 1/2}\sigma^\pm$ and $S^3=\frac{1}{2}\sigma^3$. In fact, $\check{R}(\lambda)$ and $L(\lambda)$ are, respectively, $V\otimes V$ and $V\otimes\mathfrak{H}$ representations of a more general object, $\check{\mathbf{R}}(\lambda)\in[U_q(sl_2)]^{\otimes 2}$, that satisfies the Yang–Baxter equation in $\mathfrak{H}\otimes\mathfrak{H}\otimes\mathfrak{H}$,

$$\check{\mathbf{R}}_{12}(\lambda)\,\check{\mathbf{R}}_{13}(\lambda+\mu)\,\check{\mathbf{R}}_{23}(\mu) = \check{\mathbf{R}}_{23}(\mu)\,\check{\mathbf{R}}_{13}(\lambda+\mu)\,\check{\mathbf{R}}_{12}(\lambda)\,. \tag{8}$$

Relation (2) is then a particular case of (8) with the first and second spaces evaluated in the fundamental representation. Evaluating (8) in the $V\otimes\mathfrak{H}\otimes\mathfrak{H}$ representation (and interchanging λ with μ), we obtain

$$r(\lambda)\,L(\lambda+\mu)\dot{\otimes}L(\mu)=L(\mu)\dot{\otimes}L(\lambda+\mu)\,r(\lambda)\,, \tag{9}$$

with $r(\lambda)\equiv\check{\mathbf{R}}(\lambda)\mathbf{P}$, where $\mathbf{P}$ is the permutation in $\mathfrak{H}\otimes\mathfrak{H}$. For a given L-operator, (9) can be regarded as a defining equation on the element $r(\lambda)\in[U_q(sl_2)]^{\otimes 2}$ which we will call the universal r-matrix. Using (5), Eq. (9) can be equivalently rewritten as follows:

$$r(\lambda)\;\;L_{\pm}\dot{\otimes}L_{\pm}=L_{\pm}\dot{\otimes}L_{\pm}\;\;r(\lambda)\,, \tag{10}$$

$$r(\lambda)\,(e^{\gamma\lambda}L_+\dot{\otimes}L_-+e^{-\gamma\lambda}L_-\dot{\otimes}L_+)=(e^{-\gamma\lambda}L_+\dot{\otimes}L_-+e^{\gamma\lambda}L_-\dot{\otimes}L_+)\,r(\lambda)\,. \tag{11}$$

In view of (6), the first line implies that for any element $\xi\in U_q(sl_2)$ we have

$$r(\lambda)\,\Delta(\xi)=\Delta(\xi)\,r(\lambda)\,. \tag{12}$$

Recall that, for a generic q, the tensor product of two irreducible highest weight $U_q(sl_2)$-representations of spin S is completely reducible and decomposes into the sum

$$D_S\otimes D_S=\sum_{j=0}^{2S}D_j\,, \tag{13}$$

where each subspace D_j is a highest weight $U_q(sl_2)$-module with respect to the action of the operators $\Delta(S^{\pm})$ and $\Delta(S^3)$.

Equation (12) implies that $r(\lambda)$ is a function of an operator J such that

$$J\,|j,m\rangle=j\,|j,m\rangle \tag{14}$$

for any vector $|j,m\rangle$ from D_j. In other words,

$$r(\lambda)=\sum_{j=0}^{2S}r_j(\lambda)\,\mathcal{P}_j\,, \tag{15}$$

where $\mathcal{P}_j$ is the projector onto D_j, i.e., $\mathcal{P}_k|j,m\rangle=\delta_{jk}\,|j,m\rangle$. Taking (15) into account, one can solve Eq. (11) explicitly (Refs. 6 and 7 and see also Appendix A),

$$r(\lambda)=\mathcal{P}_0+\sum_{j=1}^{2S}\left(\prod_{k=1}^{j}\frac{\sin[\,\gamma(k-i\lambda)\,]}{\sin[\,\gamma(k+i\lambda)\,]}\right)\mathcal{P}_j\,. \tag{16}$$

Two obvious consequences of this formula are

$$r(\lambda)\,r(-\lambda)=1\otimes 1\,,\quad r(\lambda)\,r(\mu)=r(\mu)\,r(\lambda)\,. \tag{17}$$

Introduce a q-analogue of the gamma function satisfying the relation

$$(q^x-q^{-x})\,\Gamma_q(x)=(q-q^{-1})\,\Gamma_q(x+1)$$

and normalized such that $\Gamma_q(1)=1$. If $|q|\neq 1$, this equation can be solved in terms of a convergent infinite product. For instance, for $|q|<1$, the solution is given by

$$\Gamma_q(x)=q^{1/2\,x(1-x)}(q^{-1}-q)^{1-x}\prod_{n=0}^{\infty}\frac{1-q^{2n+2}}{1-q^{2n+2x}}\,. \tag{18}$$

In terms of the q-gamma function Eq. (16) can be rewritten as follows:

$$r(\lambda)=\frac{\Gamma_q(J+1-i\lambda)}{\Gamma_q(J+1+i\lambda)}\,\frac{\Gamma_q(1+i\lambda)}{\Gamma_q(1-i\lambda)} \tag{19}$$

with J defined by (14). Equations (16) and (19) are q-deformations of their XXX counterparts found in (Refs. 8 and 4) (see also Ref. 9). [Actually, Refs. 8 and 4 dealt with the XXX analogue of $\check{\mathbf{R}}(\lambda)$. In the XXZ case, $\mathbf{P}$ and $\check{\mathbf{R}}(\lambda)$ do not commute with Δ and therefore cannot be represented as combinations of the projectors $\mathcal{P}_j$.]

III. HAMILTONIAN

Having a solution $\check{\mathbf{R}}(\lambda)$ to Eq. (8) such that $\check{\mathbf{R}}(0)=\mathbf{P}$ [equivalently, $r(0)=1\otimes 1$], one can construct an integrable Hamiltonian for a closed chain in the following way[10,4,7,9] (the normalization is chosen for later convenience):

$$\mathcal{H}=i\,\frac{\sin\gamma}{2\gamma}\sum_{n=1}^{N}\mathbf{P}_{n,n+1}\frac{\mathrm{d}}{\mathrm{d}\lambda}\check{\mathbf{R}}_{n,n+1}(\lambda)\bigg|_{\lambda=0}=\sum_{n=1}^{N}\mathbf{P}_{n,n+1}H_{n,n+1}\mathbf{P}_{n,n+1}=\sum_{n=1}^{N}H_{n+1,n}\,,$$
$$H_{n,n+1}=i\,\frac{\sin\gamma}{2\gamma}\,\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln r_{n,n+1}(\lambda)\bigg|_{\lambda=0} \tag{20}$$

with $H_{N,N+1}\equiv H_{N,1}$ (the periodic boundary conditions). Although $H_{n,n+1}\neq H_{n+1,n}$, we will show in the following that for the total Hamiltonian we have

$$\mathcal{H}=\sum_{n=1}^{N}H_{n+1,n}=\sum_{n=1}^{N}H_{n,n+1}\,. \tag{21}$$

The Hamiltonian $\mathcal{H}$ commutes with the higher quantum integrals of motion which are constructed as higher derivatives of $\ln r(\lambda)$. Moreover, if the reference state ω for an L-operator in question is such that $\omega\otimes\omega$ is an eigenvector of $r(\lambda)$, then the corresponding Bethe vectors are eigenvectors of the Hamiltonian.[11,10,4,9] In particular, this is the case for the L-operator (3), for which the reference state ω is just the highest weight vector.

Combining (19) with (20), we obtain a compact formula for the Hamiltonian,

$$H_{n,n+1}=\frac{\sin\gamma}{\gamma}\left(\Psi_q(J_{n,n+1}+1)-\Psi_q(1)\right), \tag{22}$$

where $\Psi_q(x)$ stands for the logarithmic derivative of $\Gamma_q(x)$.

In order to find the Hamiltonian explicitly in terms of the spin generators we first substitute Eq. (16) into Eq. (20) and derive

$$H_{n,n+1}=(\sin\gamma)\sum_{j=1}^{2S}\left(\sum_{k=1}^{j}\frac{\cos\gamma k}{\sin\gamma k}\right)\mathcal{P}_j\,. \tag{23}$$

Next, we have to construct the projectors $\mathcal{P}_j$ explicitly. Recall that the Casimir operator of the algebra (1) is given by

$$C=S^-S^+ +\frac{\sin\gamma S^3\sin\gamma(S^3+1)}{\sin^2\gamma}\,. \tag{24}$$

Its value in the highest weight representation of spin S is

$$C_S=\frac{\sin\gamma S\sin\gamma(S+1)}{\sin^2\gamma}=\frac{\cos\gamma-\cos\gamma(2S+1)}{2\sin^2\gamma}.$$

Applying the co-multiplication (7) to the Casimir operator (24), we obtain an operator that acts in the tensor product $D_S\otimes D_S$,

$$\begin{aligned}\mathbf{X}_S&=\frac{1}{2}\Delta C\\&=\frac{1}{2}(q^{S^3}S^+)\otimes(S^-q^{-S^3})+\frac{1}{2}(q^{S^3}S^-)\otimes(S^+q^{-S^3})\\&\quad+\frac{1}{4\sin^2\gamma}((1\otimes1+q^{2S^3}\otimes q^{-2S^3})\cos\gamma-(1\otimes q^{-2S^3}+q^{2S^3}\otimes1)\cos(\gamma(2S+1))).\end{aligned}\tag{25}$$

Here we employed the commutation relations (1) and used (as reflected in the subscript of $\mathbf{X}_S$) that on $D_S\otimes D_S$ we have $C\otimes1=1\otimes C=(1\otimes1)C_S$. It is now easy to see that

$$\mathbf{X}_S=\frac{\sin\gamma J\sin\gamma(J+1)}{2\sin^2\gamma}\tag{26}$$

with J defined by (14). Indeed, by construction, $\mathbf{X}_S$ commutes with $\Delta(S^\pm)$. Bearing this in mind, (26) follows from computing the action of $\mathbf{X}_S$ on highest weight vectors.

For a generic q, the eigenvalues of (26) on different subspaces D_j in (13) do not coincide. Therefore, we can utilize (26) to construct the projectors $\mathcal{P}_j$ by means of the Lagrange interpolation,

$$\mathcal{P}_j=\prod_{\substack{l=0\\l\neq j}}^{2S}\frac{2\mathbf{X}_S-[l]_q[l+1]_q}{[j-l]_q[j+l+1]_q}.\tag{27}$$

Here we used the q-numbers defined as

$$[k]_q\equiv(q^k-q^{-k})/(q-q^{-1})=\frac{\sin(\gamma k)}{\sin\gamma}.$$

Note that the denominator in (27) can be written differently with the help of the identity $[j-l]_q[j+l+1]_q=[j]_q[j+1]_q-[l]_q[l+1]_q$. We have chosen the first expression to indicate singularities that can occur if q is a root of unity.

Combining (27) with (23), we obtain a local integrable Hamiltonian for the XXZ spin chain (we call $H_{n,n+1}$ local because it is a lattice analogue of the Hamiltonian density. But $H_{n,n+1}$ is also local in the sense that it involves spines only at two nearest sites of the lattice. We hope that this mixed terminology will not lead to a confusion):

$$H_{n,n+1}=(\sin\gamma)\sum_{j=1}^{2S}\left[\left(\sum_{k=1}^{j}\frac{\cos\gamma k}{\sin\gamma k}\right)\prod_{\substack{l=0\\l\neq j}}^{2S}\frac{2(\sin\gamma)^2\mathbf{X}_S-\sin\gamma l\sin\gamma(l+1)}{\sin\gamma(j-l)\sin\gamma(j+l+1)}\right]\tag{28}$$

with $\mathbf{X}_S\in\mathfrak{H}_n\otimes\mathfrak{H}_{n+1}$ given by (25) which can also be rewritten as follows:

$$\begin{aligned}\mathbf{X}_S=e^{i\gamma S_n^3}\Bigg(&\frac{1}{2}S_n^+S_{n+1}^-+\frac{1}{2}S_n^-S_{n+1}^++\sin\gamma S_n^3\sin\gamma S_{n+1}^3\frac{\cos\gamma S\cos\gamma(S+1)}{\sin^2\gamma}\\&+\cos\gamma S_n^3\cos\gamma S_{n+1}^3\frac{\sin\gamma S\sin\gamma(S+1)}{\sin^2\gamma}\Bigg)e^{-i\gamma S_{n+1}^3}.\end{aligned}\tag{29}$$

We remark that $2\mathbf{X}_S$ is a q-deformation of square of the sum of two spins in the sense that in the $\gamma\to 0$ limit Eq. (29) simplifies to

$$\mathbf{X}_S^0 = S(S+1) + \mathbf{S}_n^0 \cdot \mathbf{S}_{n+1}^0 = \tfrac{1}{2}(\mathbf{S}_n^0 + \mathbf{S}_{n+1}^0)^2 ,$$

where S_a^0 are the generators of sl_2. In this limit Eq. (28) turns into the integrable *XXX* Hamiltonian constructed in Refs. 12 and 4.

Let us consider the large spin S asymptotics of the Hamiltonian (22)–(23) in terms of the spin operator J defined by (14). Recall first that for the logarithmic derivative of the (nondeformed) gamma function we have

$$\Psi(j+1) = \Psi(1) + \sum_{k=1}^{j} \frac{1}{k} = \ln\left(j + \frac{1}{2}\right) + O(j^{-2}) .$$

Therefore the large spin approximation of the *XXX* Hamiltonian is

$$H_{n,n+1} = \ln(J + \tfrac{1}{2}) + \text{const} . \tag{30}$$

In the *XXZ* case, if q is real, Eq. (18) (or its counterpart for $|q|>1$) yields $\Psi_q(x) \approx x\,|\gamma|$ for large x. More precisely, we infer from (22) and (23) that

$$\Psi_q(j+1) = \Psi_q(1) + |\gamma| \sum_{k=1}^{j} \tanh(k|\gamma|) = |\gamma|\, j + \varkappa_\gamma + O(e^{-2|\gamma| j}) , \tag{31}$$

where $\varkappa_\gamma$ is a γ-dependent constant. Hence the large spin asymptotics of the *XXZ* Hamiltonian is

$$H_{n,n+1} = J \sinh|\gamma| + \text{const} . \tag{32}$$

Here we should remind that the spin operator in (32) is not the same as in (30), Indeed, it is always given by $J = \Sigma_j\, j\mathcal{P}_j$ but the projectors are different for different γ. Notice also that the correction to the leading order in (31) decays very fast [because $\tanh(x) = 1 + O(e^{-2x})$]. So, if $|\gamma| S$ is not too small, (32) is a good approximation even for not too large S.

Thus, the large spin asymptotics of $H_{n,n+1}$ in the *XXZ* case differs from that in the *XXX* case. Moreover, for real γ, i.e., when $|q| = 1$, the function $\Psi_q(x)$ is not monotonous [as seen from (23)] and does not have an asymptotics at all.

IV. PROPERTIES

Global symmetry: Recall that the co-associativity property, $(\Delta \otimes 1)\Delta = (1 \otimes \Delta)\Delta$, leads to a natural notion of an nth power of the co-multiplication: $\Delta^{(n+1)} \equiv (\Delta \otimes 1^{\otimes n})\Delta^{(n)}$ with $\Delta^{(1)} \equiv \Delta$. Then the global spin generators for a chain with N nodes are naturally introduced[6] as $\mathcal{S}^{\pm} = \Delta^{(N-1)}(S^{\pm})$ and $\mathcal{S}^3 = \Delta^{(N-1)}(S^3)$; which in explicit form reads

$$\mathcal{S}^3 = \sum_{n=1}^{N} S_n^3 , \quad \mathcal{S}^{\pm} = \sum_{n=1}^{N} q^{S_1^3} \cdots q^{S_{n-1}^3} S_n^{\pm} q^{-S_{n+1}^3} \cdots q^{-S_N^3} . \tag{33}$$

By construction [see (12) and (23)], the local Hamiltonian $H_{n,n+1}$ is $U_q(sl_2)$-symmetric, i.e., it commutes with $\Delta(\xi)$ for any $\xi \in U_q(sl_2)$. Furthermore, it is easy to check that

$$[\, H_{n,n+1}, \mathcal{S}^3 \,] = 0 \quad \text{for } n = 1,\ldots,N , \tag{34}$$

$$[\, H_{n,n+1}, \mathcal{S}^{\pm} \,] = 0 \quad \text{for } n = 1,\ldots,N-1 . \tag{35}$$

Since $H_{N,1}$ does not satisfy (35), the total Hamiltonian enjoys only the $U(1)$-symmetry,

$$[\,\mathcal{H},\mathcal{S}^3\,]=0\,. \tag{36}$$

Actually, the higher quantum integrals of motion also commute with $\mathcal{S}^3$. Therefore in the presence of a constant magnetic field h the corresponding Hamiltonian, $\mathcal{H}_h=\mathcal{H}+h\mathcal{S}^3$, remains integrable and $U(1)$-symmetric.

C and P symmetries: Recall that $\mathbf{P}$ denotes the permutation in $\mathfrak{H}\otimes\mathfrak{H}$. Since the comultiplication Δ does not commute with $\mathbf{P}$, neither does $r(\lambda)$, $\mathbf{X}_S$ or $H_{n,n+1}$. However, we observe that (here and in the following dependence on γ is shown explicitly only if it is affected by a transformation)

$$\mathbf{P}\,\mathbf{X}_S(\gamma)\,\mathbf{P}=\mathbf{X}_S(-\gamma)\,,\quad \mathbf{P}\,r(\lambda,\gamma)\,\mathbf{P}=r(\lambda,-\gamma)\,. \tag{37}$$

The first relation is obvious from (29) and yields the second one upon noticing that both the projectors $\mathcal{P}_j(x,\gamma)$ and the coefficients $r_j(\lambda,\gamma)$ in (15) are even functions in γ. Further, the second relation in (37) implies readily that

$$\mathbf{P}_{n,n+1}\,H_{n,n+1}(\gamma)\,\mathbf{P}_{n,n+1}=H_{n,n+1}(-\gamma)\,. \tag{38}$$

Thus $H_{n,n+1}$ does not have the P (reflection) symmetry. But, if q is real, it has the C-symmetry (invariance with respect to the complex conjugation). If $|q|=1$, then Eq. (38) shows that $H_{n,n+1}$ has no C- or P-symmetry separately but it has the CP-symmetry.

Local bulk and boundary terms: As we will see in the following, $H_{n,n+1}$ decomposes into two parts (which we will refer to as the local bulk term and the local boundary term):

$$H_{n,n+1}=\hat{H}_{n,n+1}+i\,\frac{\sin\gamma}{2}(S^3_n-S^3_{n+1})\,. \tag{39}$$

The local bulk term, $\hat{H}_{n,n+1}$, has the following properties (see Sec. VII):

$$\mathbf{P}_{n,n+1}\hat{H}_{n,n+1}\mathbf{P}_{n,n+1}=\hat{H}_{n,n+1}\,,\quad \hat{H}_{n,n+1}(\gamma)=\hat{H}_{n,n+1}(-\gamma)\,. \tag{40}$$

Thus, $\hat{H}_{n,n+1}$ is P- and C-symmetric for real q as well as for $|q|=1$. In fact (see Sec. VII), $\hat{H}_{n,n+1}$ is a local Hamiltonian associated with the L-operator

$$\hat{L}(\lambda)=\frac{1}{\sin\gamma}\begin{pmatrix}\sinh[\,\gamma(\lambda+iS^3)\,] & i\,S^-\sin\gamma\\ i\,S^+\sin\gamma & \sinh[\,\gamma(\lambda-iS^3)\,]\end{pmatrix}. \tag{41}$$

Notice that $\hat{H}_{n,n+1}$ is not $U_q(sl_2)$-symmetric but only $U(1)$-symmetric.

The local boundary term in (39) has the same form for all positive (half-) integer spins. In the total Hamiltonian of a closed chain all these boundary terms mutually cancel, hence

$$\mathcal{H}=\sum_{n=1}^{N}H_{n,n+1}=\sum_{n=1}^{N}\hat{H}_{n,n+1}\,. \tag{42}$$

This together with (40) explains why the two sums in (21) coincide.

Properties with respect to $*$-operation: The $*$-structure on $U_q(sl_2)$ corresponding to the compact real form $U_q(su(2))$ is defined as an antiautomorphism such that

$$(S^\pm)^*=\eta^{\pm1}S^\mp\,,\quad (S^3)^*=S^3 \tag{43}$$

with some real η. Of course, the prefactor $\eta^{\pm1}$ can be eliminated by rescaling the generators. However it may be convenient to keep it. For instance, we saw in Sec. II that, in the spin-$\frac{1}{2}$ case,

it is natural to put $S^{\pm}=q^{\pm 1/2}\sigma^{\pm}$. Then $\eta=1$ if $|q|=1$ but $\eta=q$ if q is real. In fact, the choice of η is not important for our purposes since $H_{n,n+1}$ and $\hat{H}_{n,n+1}$ contain $S^{\pm}$ only in homogeneous combinations like $(S^{+}\otimes S^{-})$.

The action of the $*$-operation extends on a tensor product as $(\xi\otimes\zeta)^*=\xi^*\otimes\zeta^*$. It must be remarked that properties of the co-multiplication with respect to the action of the $*$-operation depend on the choice of q, namely we infer from (7) and (43) that [a $*$-structure satisfying $(\Delta(\xi))^*=\Delta(\xi^*)$ for $|q|=1$ is the *noncompact* real form $U_q(sl(2,\mathbb{R}))$, see Ref. 13]

$$(\Delta(\xi))^*=\Delta(\xi^*) \quad \text{if } q\in\mathbb{R} \quad \text{but} \quad (\Delta(\xi))^*=\mathbf{P}\Delta(\xi^*)\mathbf{P} \quad \text{if } |q|=1\,.$$

Therefore the local Hamiltonian (28) has the following properties:

$$(H_{n,n+1})^*=H_{n,n+1} \quad \text{for } q\in\mathbb{R}, \tag{44}$$

$$(H_{n,n+1})^*=\mathbf{P}_{n,n+1}H_{n,n+1}\mathbf{P}_{n,n+1} \quad \text{for } |q|=1\,. \tag{45}$$

Nevertheless, we see from Eq. (23) that the eigenvalues of $H_{n,n+1}$ are real in the both cases. Furthermore, it follows from (39)–(40) and (44)–(45) that

$$(\hat{H}_{n,n+1})^*=\hat{H}_{n,n+1} \tag{46}$$

for both regimes of q. In combination with (42) this implies that the relation

$$\mathcal{H}^*=\mathcal{H} \tag{47}$$

holds also in the both regimes of q.

It is worth emphasizing that, for $|q|=1$, objects which have the global $U_q(sl_2)$-symmetry, like $H_{n,n+1}$ for $n\neq N$, are in general not self-conjugate with respect to the $*$-operation (43). Indeed, if $\mathcal{O}^*=\mathcal{O}$ and it commutes with the global spin generators $\mathcal{S}^{\pm}$ given by (33), then it must also commute with $(\mathcal{S}^{\pm})^*$. This imposes a strong extra condition on the structure of $\mathcal{O}$ since for $|q|=1$ the conjugate of $\mathcal{S}^{\pm}$ belongs to $U_{q^{-1}}(sl_2)$ rather than to $U_q(sl_2)$. Conversely, objects that are self-conjugate for $|q|=1$ are in general not $U_q(sl_2)$-symmetric, for instance $\hat{H}_{n,n+1}$ and $\mathcal{H}$.

T symmetry: The definition $(\xi\otimes\zeta)^*=\xi^*\otimes\zeta^*$ is consistent with the property of the matrix transposition, $(\xi\otimes\zeta)^t=\xi^t\otimes\zeta^t$, if ξ and ζ are regarded as matrices. Thus the $*$-operation can be realized as the matrix Hermitian conjugation, $\xi^*=\overline{\xi^t}$ (bar denotes the complex conjugation).

From (44), (45), and (38) we deduce that $(H_{n,n+1})^*=\overline{H}_{n,n+1}$ in both regimes of q. Therefore finite dimensional matrix representations of the above-considered Hamiltonians are symmetric matrices,

$$(H_{n,n+1})^t=H_{n,n+1}\,, \quad (\hat{H}_{n,n+1})^t=\hat{H}_{n,n+1}\,, \quad (\mathcal{H})^t=\mathcal{H}\,. \tag{48}$$

Here the first equality leads to the second and the third due to (39) and (42), respectively.

V. EXAMPLES ($S=\frac{1}{2},1,\frac{3}{2}$)

For the spin $S=\frac{1}{2}$, the Hamiltonian (28) is very simple:

$$H_{n,n+1}=(\cos\gamma)\,\mathcal{P}_1=\mathbf{X}_{1/2}\,, \tag{49}$$

and the spin generators are given by $S^{\pm}=q^{\pm 1/2}\sigma^{\pm}$ and $S^3=\frac{1}{2}\sigma^3$. Using the relations

$$e^{t\sigma^3}\sigma^{\pm}=\sigma^{\pm}e^{-t\sigma^3}=e^{\pm t}\sigma^{\pm}\,, \quad e^{it\sigma^3}=\cos t+i\sigma^3\sin t\,, \tag{50}$$

it is easy to check that (49) acquires the following form:

$$H_{n,n+1}=\frac{1}{2}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)+(\cos\gamma)\,S_n^3S_{n+1}^3+\frac{3}{4}\cos\gamma+i\,\frac{\sin\gamma}{2}(S_n^3-S_{n+1}^3)\,. \tag{51}$$

The bulk term here is the well-known XXZ deformation of the Heisenberg spin chain.

For $S=1$ the Hamiltonian (28) looks as follows:

$$H_{n,n+1}=(\cos\gamma)\,\mathcal{P}_1+\frac{\sin 3\gamma}{\sin 2\gamma}\mathcal{P}_2=\frac{1}{4(\cos\gamma)^3}((\cos\gamma+4\cos^3\gamma)\,\mathbf{X}_1-(\mathbf{X}_1)^2)\,. \tag{52}$$

In this case the spin generators are given by (B1); they are related to the spin-1 sl_2-generators as $S^{\pm}=(\cos\gamma)^{1/2}S_0^{\pm}$, $S^3=S_0^3$. Rewriting $\mathbf{X}_1$ and its square as polynomials in the spin generators (see Appendix B), we obtain

$$H_{n,n+1}=\frac{1}{4\cos\gamma}(\mathbf{\Omega}_1-(\mathbf{\Omega}_1)^2+\mathbf{F}_1)+i\,\frac{\sin\gamma}{2}(S_n^3-S_{n+1}^3)\,, \tag{53}$$

where

$$\mathbf{\Omega}_1=\frac{1}{2\cos\gamma}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)+(2\cos\gamma-1)\,S_n^3S_{n+1}^3\,, \tag{54}$$

$$\begin{aligned}\mathbf{F}_1=&\,2\cos\gamma(\cos\gamma-1)S_n^3S_{n+1}^3+2(\cos\gamma-1)^2(S_n^3S_{n+1}^3)^2\\&-2(\sin\gamma)^2\,((S_n^3)^2+(S_{n+1}^3)^2)+4+2\cos 2\gamma\,.\end{aligned} \tag{55}$$

The bulk term of the Hamiltonian (53) [i.e., (53) without the last term] coincides (up to a constant) with the Fateev–Zamolodchikov (FZ) Hamiltonian.[2] The FZ Hamiltonian is usually written in a slightly different way in terms of the spin-1 sl_2-generators; we have chosen the above form since it allows for better comparison with the $S=\frac{3}{2}$ case.

In the limit $\gamma\to 0$, (52)–(53) simplifies to the well-know spin-1 XXX Hamiltonian:

$$H_{n,n+1}^0=\tfrac{5}{4}\mathbf{X}_1^0-\tfrac{1}{4}(\mathbf{X}_1^0)^2=\tfrac{1}{4}\mathbf{S}_n^0\cdot\mathbf{S}_{n+1}^0-\tfrac{1}{4}(\mathbf{S}_n^0\cdot\mathbf{S}_{n+1}^0)^2+\tfrac{3}{2}\,.$$

In the $S=\frac{3}{2}$ case the Hamiltonian (23) is given by

$$H_{n,n+1}=(\cos\gamma)\,\mathcal{P}_1+\frac{\sin 3\gamma}{\sin 2\gamma}\mathcal{P}_2+\left(\frac{\sin 3\gamma}{\sin 2\gamma}+(\sin\gamma)\,\frac{\cos 3\gamma}{\sin 3\gamma}\right)\mathcal{P}_3\,. \tag{56}$$

Rewriting the corresponding expression (28) in the polynomial (with respect to the spin generators) form (see Appendix B), we obtain

$$\begin{aligned}H_{n,n+1}=&\frac{1}{12(\cos\gamma)^3(1+2\cos 2\gamma)^3}\Big(12(\cos\gamma)\,(\mathbf{\Omega}_{3/2})^3+(5\cos 4\gamma-\cos 2\gamma+2)\,(\mathbf{\Omega}_{3/2})^2\\&+\frac{1}{2\cos\gamma}(\mathbf{\Omega}_{3/2}\mathbf{Q}+\mathbf{Q}\,\mathbf{\Omega}_{3/2})+\frac{1+2\cos 2\gamma}{64\cos^2\gamma}\mathbf{F}_{3/2}\Big)+i\,\frac{\sin\gamma}{2}(S_n^3-S_{n+1}^3)\,,\end{aligned} \tag{57}$$

where $\mathbf{Q}$ and $\mathbf{F}_{3/2}$ are real symmetric polynomials in S_n^3 and S_{n+1}^3 (see Appendix B) and

$$\mathbf{\Omega}_{3/2}=\frac{1}{2}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)+(1+2\cos 2\gamma)\,\frac{\cos 2\gamma}{3\cos\gamma}S_n^3S_{n+1}^3\,. \tag{58}$$

Let us remark that in both Hamiltonians (53) and (57) the two ''most non-diagonal'' terms are powers of an operator $\mathbf{\Omega}$ which is quadratic in generators. To clarify this fact, we observe that, like for $S=\frac{1}{2}$, the corresponding Casimir operators (24) are actually quadratic:

$$\tfrac{1}{2}(S^+S^-+S^-S^+)+(\cos\gamma)(S^3)^2=2\cos\gamma \quad \text{for } S=1\,, \tag{59}$$

$$\tfrac{1}{2}(S^+S^-+S^-S^+)+(\cos\gamma)^2(S^3)^2=\tfrac{1}{4}(17\cos^2\gamma-2) \quad \text{for } S=\tfrac{3}{2} \tag{60}$$

(the last expression differs from $C_{3/2}$ by a constant). Equation (59) is due to the first relation in (B2); Eq. (60) follows from relation (B10) and the identity $2(\sin\gamma S^3)^2=1-\cos 2\gamma S^3$.

VI. ANOTHER CO-MULTIPLICATION

As we saw in Sec. II, the co-multiplication operation Δ plays a key role in the construction of the Hamiltonian $\mathcal{H}$. However, Eq. (7) does not exhaust possible definitions of Δ for $U_q(sl_2)$. In fact, a homomorphism $\Delta_\alpha: U_q(sl_2)\to[U_q(sl_2)]^{\otimes 2}$ such that

$$\Delta_\alpha(S^\pm)=S^\pm\otimes q^{(\pm\alpha-1)S^3}+q^{(\pm\alpha+1)S^3}\otimes S^\pm\,, \quad \Delta_\alpha(S^3)=S^3\otimes 1+1\otimes S^3 \tag{61}$$

satisfies all the properties of the co-multiplication for any real α. We had before $\alpha=0$, which is the most ''symmetric'' choice. But we may prefer $\alpha=1$ (or $\alpha=-1$) if we want the regime $q<0$ to be on equal footing with $q>0$ in the sense that the terms $q^{(\pm\alpha\pm 1)S^3}$ in (61) take only real values.

Notice that Δ_α is obtained from the co-multiplication (7) by twisting:

$$\Delta_\alpha(\xi)=F_\alpha\,\Delta(\xi)\,(F_\alpha)^{-1}\,, \quad F_\alpha=q^{\alpha S^3\otimes S^3}\in\mathfrak{H}\otimes\mathfrak{H}\,. \tag{62}$$

This twist is rather specific in that it preserves the co-associativity of the co-multiplication (more general twists give rise to the so-called quasi-Hopf algebras;[14] see Ref. 15 for their applications in integrable spin models).

In order to construct an integrable Hamiltonian using the new co-multiplication Δ_α in the same way as we used Δ in Secs. II and III, we should first find an L-operator, $\tilde{L}_\alpha(\lambda)$, that satisfies (6) with Δ_α. For this purpose we observe that

$$F_\alpha=(\phi_\alpha\otimes\phi_\alpha)^{-1}\,\Delta(\phi_\alpha),$$

where

$$\phi_\alpha=q^{(\alpha/2)(S^3)^2}\in\mathfrak{H}\,. \tag{63}$$

Therefore we can rewrite the left-hand side of (6) for $\tilde{L}_\alpha(\lambda)$ as

$$\Delta_\alpha(\tilde{L}_\alpha(\lambda))=(\phi_\alpha\otimes\phi_\alpha)^{-1}\,\Delta(\phi_\alpha\tilde{L}_\alpha(\lambda)\,\phi_\alpha^{-1})\,(\phi_\alpha\otimes\phi_\alpha),$$

which makes it obvious that $\tilde{L}_\alpha(\lambda)$ satisfies (6) with Δ_α if it is related to the L-operator (3) as follows:

$$\tilde{L}_\alpha(\lambda)=\phi_\alpha^{-1}\,L(\lambda)\,\phi_\alpha \tag{64}$$

$$=\frac{1}{\sin\gamma}\begin{pmatrix}\sinh[\,\gamma(\lambda+iS^3)\,] & i\sin\gamma\, e^{\gamma\lambda}q^{\alpha/2}q^{\alpha S^3}S^-\\ i\sin\gamma\, e^{-\gamma\lambda}q^{\alpha/2}q^{-\alpha S^3}S^+ & \sinh[\,\gamma(\lambda-iS^3)\,]\end{pmatrix}. \tag{65}$$

Since the map $\xi \to \phi_\alpha^{-1} \xi \phi_\alpha$ is an automorphism of $U_q(sl_2)$, it is clear that the exchange relation (2) holds for $\widetilde{L}_\alpha(\lambda)$ with the same R-matrix as for $L(\lambda)$. Consequently, the Bethe ansatz equations for $\widetilde{L}_\alpha(\lambda)$ coincide with those for $L(\lambda)$ (the reference state ω has also not changed).

Substituting (64) into (9), we find a universal r-matrix for the new L-operator:

$$\tilde{r}_\alpha(\lambda) = (\phi_\alpha \otimes \phi_\alpha)^{-1}\, r(\lambda)\, (\phi_\alpha \otimes \phi_\alpha) = F_\alpha\, r(\lambda)\, (F_\alpha)^{-1}. \tag{66}$$

The second equality is due to relation (63) and the property (12). The same twists relate the corresponding solutions of the Yang–Baxter equation (8), i.e.,

$$\check{\mathbf{R}}_\alpha(\lambda) = (\phi_\alpha \otimes \phi_\alpha)^{-1} \check{\mathbf{R}}(\lambda) (\phi_\alpha \otimes \phi_\alpha) = F_\alpha\, \check{\mathbf{R}}(\lambda) (F_\alpha)^{-1}. \tag{67}$$

Notice that the first equality is consistent with (64) since ϕ_α in the fundamental representation is just a constant. Further, evaluating the right-hand side of (67) in $V \otimes \mathfrak{H}$ representation, we see that $\widetilde{L}_\alpha(\lambda)$ can be constructed also as a twist by 2×2 matrix,

$$\widetilde{L}_\alpha(\lambda) = f_\alpha L(\lambda)\, f_\alpha^{-1}, \quad f_\alpha = q^{(\alpha/2)\,\sigma^3 \otimes S^3}.$$

Let us underline that existence of the two ways of constructing $\widetilde{L}_\alpha(\lambda)$ and, as a consequence, of the relation

$$[L(\lambda), \phi_\alpha f_\alpha] = 0$$

is due to the property of the universal r-matrix (12) applied to $\xi = \phi_\alpha$ [indeed, $q^{\alpha/2} \phi_\alpha f_\alpha$ is $\Delta(\phi_\alpha)$ evaluated in $V \otimes \mathfrak{H}$].

According to (20), the local Hamiltonian corresponding to the universal r-matrix (66) is

$$\widetilde{H}^{(\alpha)}_{n,n+1} = (\phi_n^\alpha\, \phi_{n+1}^\alpha)^{-1}\, H_{n,n+1}\, (\phi_n^\alpha\, \phi_{n+1}^\alpha) = F^\alpha_{n,n+1}\, H_{n,n+1}\, (F^\alpha_{n,n+1})^{-1}. \tag{68}$$

This transformation does not modify the $S = \frac{1}{2}$ Hamiltonian (49) since in this case ϕ_α is trivial. But already for $S = 1$ we find (see Appendix B)

$$\widetilde{H}^{(\alpha)}_{n,n+1} - H_{n,n+1} = \frac{1 - \cos(\alpha\gamma)}{2\cos\gamma} \{\Upsilon_{n,n+1}, S^3_n S^3_{n+1}\} - i\, \frac{\sin(\alpha\gamma)}{2\cos\gamma} [\Upsilon_{n,n+1}, S^3_n S^3_{n+1}], \tag{69}$$

where $[,]$ and $\{,\}$ stand for commutator and anticommutator, respectively, and $\Upsilon_{n,n+1} \equiv \frac{1}{2}(S^+_n S^-_{n+1} + S^-_n S^+_{n+1})$. Notice that the terms on the right-hand side of (69) are nondiagonal.

Finally, the total Hamiltonian is given by

$$\widetilde{\mathcal{H}}^{(\alpha)} = \sum_{n=1}^{N} \widetilde{H}^{(\alpha)}_{n,n+1} = (\Phi_\alpha)^{-1}\, \mathcal{H}\, \Phi_\alpha = \mathcal{F}_\alpha\, \mathcal{H}\, (\mathcal{F}_\alpha)^{-1}, \quad \Phi_\alpha \equiv \prod_{n=1}^{N} \phi_\alpha, \quad \mathcal{F}_\alpha \equiv q^{\alpha \Sigma_{n<m} S^3_n S^3_m}.$$

The Φ-twist here follows easily from (68). The $\mathcal{F}$-twist yields the same result because $\mathcal{H}$ commutes with $\mathcal{S}^3$ (36) and hence with $\Phi_\alpha \mathcal{F}_\alpha = q^{(\alpha/2)(\mathcal{S}^3)^2}$. Since $\widetilde{\mathcal{H}}^{(\alpha)}$ and $\mathcal{H}$ are related by a twist they have the same set of eigenvalues; this agrees with the fact that the Bethe ansatz equations have not changed.

Let us conclude this section with a remark: Eqs. (66), (67), and (68) may appear to suggest that $\widetilde{L}_\alpha(\lambda)$ and $\tilde{r}_\alpha(\lambda)$ are related to another twisted co-multiplication, $\widetilde{\Delta}_\theta(\xi) \equiv \theta^{-1}\, \Delta(\xi)\, \theta$, where $\theta = \phi_\alpha \otimes \phi_\alpha$. But $\widetilde{\Delta}_\theta$ fails to satisfy the necessary property of a co-multiplication,[14] $(\epsilon \otimes 1)\Delta(\xi) = \xi$, where ϵ is the co-unit. So $\widetilde{\Delta}_\theta$ is not a co-multiplication of a (quasi) Hopf algebra. (Moreover, $\widetilde{\Delta}_\theta$ is not co-associative.)

VII. FROM $H_{n,n+1}$ TO $\hat{H}_{n,n+1}$

Consider now another family of L-operators,

$$\hat{L}_\beta(\lambda)=\frac{1}{\sin\gamma}\begin{pmatrix}\sinh[\gamma(\lambda+iS^3)] & i\sin\gamma\, e^{(\gamma-\beta)\lambda}S^- \\ i\sin\gamma\, e^{(\beta-\gamma)\lambda}S^+ & \sinh[\gamma(\lambda-iS^3)]\end{pmatrix}, \tag{70}$$

which are obtained from the L-operator (3) as twists by certain 2×2 matrices,

$$\hat{L}_\beta(\lambda)=K_\lambda^{-1}L(\lambda)K_\lambda, \quad K_\lambda=e^{(1/2)\beta\lambda\sigma^3}\in V. \tag{71}$$

For $\beta=\gamma$ this gives the L-operator (41) (which is most often used in applications of the Bethe ansatz). The map $S^\pm\to e^{\pm\beta\lambda}S^\pm$, $S^3\to S^3$ is an automorphism of $U_q(sl_2)$ but, unlike the case treated in Sec. VI, it is λ-dependent. Therefore, the $\check{R}$-matrix corresponding to $\hat{L}_\beta(\lambda)$ differs from (4). Namely, as seen from (71), exchange relation (2) holds for $\hat{L}_\beta(\lambda)$ with $R_\beta(\lambda)=(1\otimes K_\lambda^{-1})R(\lambda)(K_\lambda\otimes 1)$, i.e., $R_\beta(\lambda)=P\check{R}_\beta(\lambda)$, where

$$\check{R}_\beta(\lambda)=i\,e^{(\gamma-\beta)\lambda}\,\sigma^+\otimes\sigma^-+i\,e^{(\beta-\gamma)\lambda}\,\sigma^-\otimes\sigma^+ +\frac{1}{\sin\gamma}\sinh\left(\gamma\lambda+\frac{i\gamma}{2}(1\otimes 1+\sigma^3\otimes\sigma^3)\right). \tag{72}$$

In order to find a universal r-matrix for $\hat{L}_\beta(\lambda)$, we will apply the approach which we used in Sec. VI. Namely, we observe that $\varphi_\lambda\equiv e^{\beta\lambda S^3}\in\mathfrak{H}$ is a complementary twist to (71) in the sense that

$$[L(\lambda),K_\lambda\,\varphi_\lambda]=0$$

as follows from the property of the universal r-matrix (12) for $\xi=\varphi_\lambda$ (in fact, K_λ is just φ_λ evaluated in the fundamental representation; hence $K_\lambda\varphi_\lambda$ is $\Delta(\varphi_\lambda)$ evaluated in $V\otimes\mathfrak{H}$).

Thus, instead of the twist (71) in the auxiliary space V, the L-operator (70) can be obtained as a twist in the quantum space $\mathfrak{H}$,

$$\hat{L}_\beta(\lambda)=\varphi_\lambda L(\lambda)\varphi_\lambda^{-1}, \quad \varphi_\lambda=e^{\beta\lambda S^3}\in\mathfrak{H}. \tag{73}$$

Substituting (73) into (9) and taking again into account that $[r(\lambda),\Delta(\varphi_\mu)]=0$, we find a universal r-matrix for $\hat{L}_\beta(\lambda)$,

$$\hat{r}_\beta(\lambda)=(1\otimes\varphi_\lambda)\,r(\lambda)\,(\varphi_\lambda^{-1}\otimes 1). \tag{74}$$

Unlike Eq. (66) this relation is not a twist. Notice however that the corresponding solutions of the Yang–Baxter equation (8) are related by a twist,

$$\check{\mathbf{R}}_\beta(\lambda)=(1\otimes\varphi_\lambda)\check{\mathbf{R}}(\lambda)(1\otimes\varphi_\lambda^{-1}). \tag{75}$$

It must be stressed now that $\hat{L}_\beta(\lambda)$ does not possess a decomposition of the type (5)–(6), and $\hat{r}_\beta(\lambda)$ does not commute with Δ (or Δ_α), i.e., (12) does not hold for $\hat{r}_\beta(\lambda)$ for a generic ξ. As a consequence, $\hat{r}_\beta(\lambda)$ does not have a representation of the type (15). Moreover, for $\beta\neq 0$ we have in general $[\hat{r}_\beta(\lambda),\hat{r}_\beta(\mu)]\neq 0$ (except for the fundamental representation in the case $\beta=\gamma$). Nevertheless, the general recipe for constructing a local integrable Hamiltonian applies [because the Yang–Baxter equation for $\check{\mathbf{R}}_\beta(\lambda)$ is valid]. So we substitute (74) into the formula (20) and derive

$$\hat{H}^{(\beta)}_{n,n+1}=H_{n,n+1}-i\frac{\beta\sin\gamma}{2\gamma}(S^3_n-S^3_{n+1}). \tag{76}$$

Thus the new local Hamiltonian differs from $H_{n,n+1}$ only in the local boundary term. Hence the total Hamiltonian $\hat{\mathcal{H}}=\Sigma_{n=1}^{N}\hat{H}^{\beta}_{n,n+1}$ coincides with $\mathcal{H}$. Note that the Bethe ansatz equations, describing the spectrum of $\hat{\mathcal{H}}$, have also not changed, which is not entirely trivial since the corresponding R-matrix has changed. The reason is that in the derivation of the Bethe ansatz equations the nondiagonal entries of (72) appear only in the so-called ''unwanted terms'' that cancel each other.[10,11,9]

In Sec. IV we asserted that the local Hamiltonian $H_{n,n+1}$ decomposes into a local boundary term and a local bulk term $\hat{H}_{n,n+1}$ which is associated with the L-operator (41). Now this is obvious from (70) and (76) if we put $\beta=\gamma$. Since we have found the corresponding universal r-matrix, we are in a position to prove the properties of $\hat{H}_{n,n+1}$ stated in Sec. IV. For brevity we denote $r_0(\lambda)\equiv\hat{r}_{\gamma}(\lambda)$.

As seen from (72) for $\beta=\gamma$, the auxiliary R-matrix associated with the L-operator (41) is P-symmetric, i.e., it commutes with the 4×4 permutation matrix P_V. The corresponding universal r-matrix, $r_0(\lambda)$, has analogous properties. Namely, (as we prove in Appendix A) $r_0(\lambda)$ satisfies the following relations:

$$\mathbf{P}\,r_0(\lambda)\,\mathbf{P}=r_0(\lambda)\,,\quad r_0(\lambda,\gamma)=r_0(\lambda,-\gamma)\,, \tag{77}$$

$$(r_0(\lambda))^t=r_0(\lambda)\,,\quad r_0(\lambda)\,r_0(-\lambda)=1\otimes1\,, \tag{78}$$

where $\mathbf{P}$ is the permutation in $\mathfrak{H}\otimes\mathfrak{H}$ and t denotes transposition. The last equality follows from the formula (74), the first relation in (17) for $r(\lambda)$, and the relation $[r(\lambda),\Delta(\varphi_\lambda)]=0$. Taking logarithmic derivative of (77) at $\lambda=0$, we establish the symmetries (40) of the local bulk term $\hat{H}_{n,n+1}$. The first relation in (78) yields in the same way the second relation in (48).

VIII. OPEN CHAIN

Integrable *open* spin chains have also been intensively studied,[16–21] in particular, from the point of view of the fusion procedure and quantum group symmetries.

As we saw in Sec. IV, $H_{N,1}$ is the only term in $\mathcal{H}$ which does not commute with the global spin generators $\mathcal{S}^{\pm}$. Omitting it, we obtain a Hamiltonian for an open spin chain,

$$\mathcal{H}'=\sum_{n=1}^{N-1}H_{n,n+1}=\sum_{n=1}^{N-1}\hat{H}_{n,n+1}+i\,\frac{\sin\gamma}{2}(S_1^3-S_N^3), \tag{79}$$

which is apparently $U_q(sl_2)$-symmetric, i.e., $[\mathcal{H}',\mathcal{S}^{\pm}]=[\mathcal{H}',\mathcal{S}^3]=0$. It is however not immediately evident whether the Hamiltonian (79) remains *integrable*.

Let us refer to the sum on the right-hand side of (79) as the bulk Hamiltonian, $\hat{\mathcal{H}}'$. The remaining part can be called the surface term; it is a sum of $(N-1)$ local boundary terms we dealt with before. As we discussed earlier, the bulk Hamiltonian $\hat{\mathcal{H}}'$ corresponds to the L-operator (41) and it is only $U(1)$-symmetric. The fact that adding the surface term to $\hat{\mathcal{H}}'$ restores the $U_q(sl_2)$-symmetry was observed for spin $\frac{1}{2}$ in Ref. 16 and for spin 1 in Ref. 17. Integrability of the corresponding total Hamiltonians was established in Refs. 18–20 in the framework of boundary integrable lattice models. We will prove in the following that $\mathcal{H}'$ is integrable for the higher spins as well.

Let us briefly recall the construction of an integrable Hamiltonian for a chain with boundaries.[18] Let $\check{\mathbf{R}}(\lambda)$ be a solution of the Yang–Baxter equation (8), and $T(\lambda)$ be a monodromy matrix obeying the exchange relation (2) with R-matrix $\mathbf{P}\check{\mathbf{R}}(\lambda)$. Introduce a boundary monodromy matrix, $Z(\lambda)\equiv T(\lambda)\mathcal{K}^-(\lambda)(T(-\lambda))^{-1}$. The boundary matrix, $\mathcal{K}^-(\lambda)\in\mathfrak{H}$, represents nonperiodic boundary conditions ($\check{\mathbf{R}}$ and $\mathcal{K}^-$ are close analogues of the bulk and boundary scattering

matrices[22]). [Strictly speaking, $\mathcal{K}^-(\lambda)$ is an element of $\mathfrak{H}\otimes\mathfrak{H}$ but with trivial second component. We had a similar situation in Sec. VII where the twist φ_λ had trivial first component, see Eq. (73).] Now, if $\mathcal{K}^-(\lambda)$ satisfies the so-called reflection equation, namely,

$$\begin{aligned}&\check{\mathbf{R}}(\lambda-\mu)\,(\mathcal{K}^-(\lambda)\otimes 1)\,(\check{\mathbf{R}}(-\lambda-\mu))^{-1}\,(1\otimes\mathcal{K}^-(\mu))\\&\quad=(1\otimes\mathcal{K}^-(\mu))\,\check{\mathbf{R}}(\lambda+\mu)\,(\mathcal{K}^-(\lambda)\otimes 1)\,(\check{\mathbf{R}}(-\lambda+\mu))^{-1},\end{aligned}\tag{80}$$

then $Z(\lambda)$ also satisfies this equation. Using this fact one can show that a special trace of $Z(\lambda)$, $\tau(\lambda)=\mathrm{tr}_0\mathcal{K}^+(\lambda)Z(\lambda)$, is a generating function for quantum integrals of motion if the boundary matrix $\mathcal{K}^+(\lambda)\in\mathfrak{H}$ satisfies a "dual" reflection equation,[18,23]

$$\begin{aligned}&\check{\mathbf{R}}(-\lambda+\mu)\,((\mathcal{K}^+)^t(\lambda)\otimes 1)\,\check{\mathbf{R}}(-\lambda-\mu-2\delta)\,(1\otimes(\mathcal{K}^+)^t(\mu))\\&\quad=(1\otimes(\mathcal{K}^+)^t(\mu))\,\check{\mathbf{R}}(-\lambda-\mu-2\delta)\,((\mathcal{K}^+)^t(\lambda)\otimes 1)\,\check{\mathbf{R}}(-\lambda+\mu),\end{aligned}\tag{81}$$

and $\check{\mathbf{R}}$ has the following properties:

$$\mathbf{P}\,\check{\mathbf{R}}(\lambda)\,\mathbf{P}=\check{\mathbf{R}}(\lambda),\quad \check{\mathbf{R}}(\lambda)\,\check{\mathbf{R}}(-\lambda)=\rho_1(\lambda)\,(1\otimes 1),\quad (\check{\mathbf{R}}(\lambda))^t=\check{\mathbf{R}}(\lambda),\tag{82}$$

$$(\check{\mathbf{R}}(\lambda))^{t_1}\,(\check{\mathbf{R}}(-\lambda-2\delta))^{t_1}=\rho_2(\lambda)\,(1\otimes 1),\tag{83}$$

where δ is a constant, and $\rho_1(\lambda)$ and $\rho_2(\lambda)$ are scalar functions.

With all these conditions, an integrable Hamiltonian is given Ref. 18 by the following analogue of the formula (20) [we keep the same normalization as in (20)]:

$$\begin{aligned}&\mathcal{H}''=\sum_{n=1}^{N-1}h_{n,n+1}+i\,\frac{\sin\gamma}{4\gamma}\,\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathcal{K}_1^-(\lambda)\Big|_{\lambda=0}+\frac{\mathrm{tr}_0(\mathcal{K}_0^+(0)\,h_{0,N})}{\mathrm{tr}\,\mathcal{K}^+(0)},\\&h_{n,n+1}=i\,\frac{\sin\gamma}{2\gamma}\,\mathbf{P}_{n,n+1}\frac{\mathrm{d}}{\mathrm{d}\lambda}\check{\mathbf{R}}_{n,n+1}(\lambda)\Big|_{\lambda=0}.\end{aligned}\tag{84}$$

Deriving (84) one assumes that $\check{\mathbf{R}}_{n,n+1}(0)=\mathbf{P}$ and $\mathcal{K}^-(0)=1$, which is consistent with (80).

Let us try to identify the Hamiltonian (79) as a particular case of (84). First, we can put $h_{n,n+1}=\hat{H}_{n,n+1}$ if we choose $\check{\mathbf{R}}(\lambda)=\check{\mathbf{R}}_\gamma(\lambda)$, where $\check{\mathbf{R}}_\gamma(\lambda)=r_0(\lambda)\mathbf{P}$ is given by (75) with $\beta=\gamma$. For this R-matrix the properties (82) follow from (77); in particular, the second relation (unitarity) holds with $\rho_1(\lambda)=1$. The crossing unitarity (83) holds for $\check{\mathbf{R}}_\gamma(\lambda)$ with $\delta=i$.

The derivation of the reflection equation (80) for $\mathcal{K}^-$ does not use the conditions (82) and (83). So, let us look first for an R-matrix for which the reflection equation has a trivial solution, $\mathcal{K}^-(\lambda)=1$. In this case (80) turns into

$$\check{\mathbf{R}}(\lambda-\mu)\,(\check{\mathbf{R}}(-\lambda-\mu))^{-1}=\check{\mathbf{R}}(\lambda+\mu)\,(\check{\mathbf{R}}(-\lambda+\mu))^{-1}.\tag{85}$$

A solution to this equation is given by $\check{\mathbf{R}}(\lambda)=r(\lambda)\mathbf{P}$, where $r(\lambda)$ is the universal r-matrix we discussed in Sec. II. Indeed, (85) follows from the second relation in (17). Using this observation, we can find a solution to the reflection equation for any R-matrix $\check{\mathbf{R}}_\beta(\lambda)$ given by (75). Indeed, substituting (75) in (85), we derive

$$\begin{aligned}&\check{\mathbf{R}}_\beta(\lambda-\mu)\,(1\otimes\varphi_\lambda^2)\,(\check{\mathbf{R}}_\beta(-\lambda-\mu))^{-1}\,(1\otimes\varphi_{-\mu}^2)\\&\quad=(1\otimes\varphi_{-\mu}^2)\,\check{\mathbf{R}}_\beta(\lambda+\mu)\,(1\otimes\varphi_\lambda^2)\,(\check{\mathbf{R}}_\beta(-\lambda+\mu))^{-1}.\end{aligned}\tag{86}$$

Multiplying this relation by $\Delta(\varphi_\lambda^{-2})=(\varphi_\lambda\otimes\varphi_\lambda)^{-2}$ [which commutes with $\check{\mathbf{R}}_\beta(\lambda)$], we bring it to the form of (80). Thus, a solution of the reflection equation for $\check{\mathbf{R}}_\beta$ is

$$\mathcal{K}^-_\beta(\lambda)=(\varphi_\lambda)^{-2}=e^{-2\beta\lambda S^3}.$$

Notice that for $\beta=\gamma$ the R-matrix $\check{\mathbf{R}}$ is symmetric with respect to γ [the second relation in (77)]. Therefore in this case we have another solution [which can be derived directly from (86) by applying the permutation and then multiplying by $(\varphi_\mu\otimes\varphi_\mu)^2$],

$$\mathcal{K}^-(\lambda)=e^{2\gamma\lambda S^3}. \tag{87}$$

This is the boundary matrix we need since its derivative in (84) gives exactly the S_1^3 term in (79).

In general, solutions of the reflection equation and of its ''dual'' are independent of each other. However, as was noted already in Ref. 18, there exist several isomorphisms that allow us to construct $\mathcal{K}^+$ if we know $\mathcal{K}^-$. In particular, it is easy to see that a possible solution for (81) is $\mathcal{K}^+(\lambda)=(\mathcal{K}^-(-\lambda-\delta))^t$. For $\mathcal{K}^-$ given by (87) this yields

$$\mathcal{K}^+(\lambda)=e^{-2\gamma(\lambda+i)S^3}. \tag{88}$$

It turns out that substitution of $\mathcal{K}^+(0)=q^{-2S^3}$ into (84) gives exactly the S_N^3 term in (79). To prove this assertion, we first observe (see Appendix C) that for the q-trace of the local Hamiltonian $H_{n,n+1}$ we have

$$\mathrm{tr}_n(q^{2S_n^3}H_{n,n+1})=\tilde{\rho}_S\,1_{n+1}, \tag{89}$$

where $\tilde{\rho}_S$ is a scalar constant.

Taking into account the relation (39) between $H_{n,n+1}$ and $\hat{H}_{n,n+1}$, we infer from (89) that

$$\mathrm{tr}_0(q^{2S_0^3}\hat{H}_{0,N})=(\mathrm{tr}\,q^{2S^3})\,i\,\frac{\sin\gamma}{2}S_N^3+\mathrm{const}.$$

Now replacing q with q^{-1} and using that $\hat{H}_{n,n+1}$ is an even function of γ (40), we find that

$$\frac{\mathrm{tr}_0(\mathcal{K}^+(0)\,\hat{H}_{0,N})}{\mathrm{tr}\,\mathcal{K}^+(0)}=\frac{\mathrm{tr}_0(q^{-2S_0^3}\hat{H}_{0,N})}{\mathrm{tr}\,q^{-2S^3}}=-\,i\,\frac{\sin\gamma}{2}S_N^3 \tag{90}$$

holds (up to an additive constant). Thus, the boundary matrix (88) gives the S_N^3 term in (79). This completes the proof that the $U_q(sl_2)$-symmetric open chain Hamiltonian (79) is integrable for all (half-) integer spins.

IX. CONCLUSION

In summary, we have constructed explicitly (in terms of the spin generators) higher spin closed chain Hamiltonians for two families of XXZ-type L-operators including the two L-operators most often used in the literature. We have investigated properties of these Hamiltonians, described their interrelations, and discussed the connection with $U_q(sl_2)$-symmetric open chain Hamiltonians.

We have emphasized a key role of the underlying quantum algebraic structure, especially the universal r-matrix and the co-multiplication, for constructing integrable Hamiltonians and investigating their symmetries. The technique presented in this paper can be applied also for constructing the higher quantum integrals of motion. Also, with certain modifications, this technique can be extended to models based on (the quantum deformation of) the superalgebra $osp(1|2)$; the corresponding basic ingredients are known.[24]

The presented construction applies also to the case of q being a root of unity, $q^p=1$, if p is sufficiently large in comparison with the spin S. Indeed, the denominator of (27) does not vanish if $p>8S$ and therefore the projectors $\mathcal{P}_j$ can be used in the usual way. For $p\leqslant 8S$ the construction needs to be modified because eigenvalues of the tensor Casimir operator become degenerate and the so-called cyclic representations appear.

ACKNOWLEDGMENTS

I am grateful to H.M. Babujian for useful discussions and to L.D. Faddeev, P.P. Kulish, and J. Teschner for valuable comments. This work was supported by Alexander von Humboldt Foundation.

APPENDIX A

Here we give some technical details on the universal r-matrices used in the text. First we recall the derivation of the universal r-matrix (16) along the lines of Refs. 6 and 7 (see also Refs. 9 and 25). The explicit form of the off-diagonal entries of Eq. (11) is

$$r(\lambda)\,(e^{\mp\gamma\lambda}S^{\pm}\otimes q^{S^3}+e^{\pm\gamma\lambda}q^{-S^3}\otimes S^{\pm})=(e^{\pm\gamma\lambda}S^{\pm}\otimes q^{S^3}+e^{\mp\gamma\lambda}q^{-S^3}\otimes S^{\pm})\,r(\lambda)\,. \tag{A1}$$

A solution to this equation is unique up to a scalar factor.[7] Notice that the co-multiplication (7) satisfies the following relations:

$$[S^{\varepsilon}\otimes q^{S^3},\Delta(S^{\varepsilon})]=[q^{-S^3}\otimes S^{\varepsilon},\Delta(S^{\varepsilon})]=0\,,\quad \varepsilon=\pm\,.$$

Therefore, for the highest/lowest weight vectors we deduce that

$$S^{\pm}\otimes q^{S^3}\,|j,\pm j\rangle=g_{\pm}(j)|j+1,\pm(j+1)\rangle\,,\quad q^{-S^3}\otimes S^{\pm}\,|j,\pm j\rangle=h_{\pm}(j)|j+1,\pm(j+1)\rangle\,, \tag{A2}$$

where $g_{\pm}(j)$ and $h_{\pm}(j)$ are scalar functions. Furthermore, we have

$$\begin{aligned}&(S^{\pm}\otimes q^{S^3}+q^{\pm(2+2j)}q^{-S^3}\otimes S^{\pm})\,|j,\pm j\rangle\\&\quad=((1\otimes q^{2S^3})\,S^{\pm}\otimes q^{-S^3}+q^{\pm(2+2j)}(q^{S^3}\otimes S^{\pm}q^{2S^3})q^{-2S^3}\otimes q^{-2S^3})\,|j,\pm j\rangle\\&\quad=(1\otimes q^{2S^3})\,\Delta(S^{\pm})\,|j,\pm j\rangle=0\,.\end{aligned} \tag{A3}$$

Applying now (A1) to $|j,j\rangle$ (for the upper signs) or to $|j,-j\rangle$ (for the lower signs) and using (15), (A2), and (A3), we deduce that

$$r_{j+1}(\lambda)\,(e^{\pm\gamma\lambda}-q^{\pm(2+2j)}e^{\mp\gamma\lambda})=(e^{\mp\gamma\lambda}-q^{\pm(2+2j)}e^{\pm\gamma\lambda})\;\;r_j(\lambda)\,. \tag{A4}$$

Both relations in (A4) yield the same functional equation on $r_j(\lambda)$ (which arises also for universal r-matrices in the lattice sine-Gordon model[26] and in the lattice Virasoro algebra[27])

$$r_{j+1}(\lambda)=\frac{\sin[\,\gamma(j+1-i\lambda)]}{\sin[\,\gamma(j+1+i\lambda)]}\,r_j(\lambda)\,. \tag{A5}$$

Upon imposing the normalization condition $r(0)=1$, we obtain expression (16). A proof that this $r(\lambda)$ does satisfy all the relations in (11) is given in Refs. 6 and 7. Of course, one is still free to multiply $r(\lambda)$ by a scalar function, $\rho(\lambda)$, such that $\rho(0)=1$. For instance, the spin-$\frac{1}{2}$ representation of $\check{R}(\lambda)$ given by (4) corresponds to $\rho(\lambda)=\sin[\gamma(1+i\lambda)]/\sin\gamma$.

Consider now the universal r-matrix $r_0(\lambda)$ introduced in Sec. VII. It is a solution to Eq. (9) for the L-operator (41). Unlike the previous case, this L-operator does not have a Borel decomposition of the type (5). Therefore the off-diagonal entries of (9) give us four λ-dependent relations:

$$r_0(\lambda)\,(S^{\pm}\otimes q^{S^3}+e^{\pm\gamma\lambda}q^{-S^3}\otimes S^{\pm})=(e^{\pm\gamma\lambda}S^{\pm}\otimes q^{S^3}+q^{-S^3}\otimes S^{\pm})\,r_0(\lambda)\,, \tag{A6}$$

$$r_0(\lambda)\,(S^{\pm}\otimes q^{-S^3}e^{\pm\gamma\lambda}+q^{S^3}\otimes S^{\pm})=(e^{\pm\gamma\lambda}q^{S^3}\otimes S^{\pm}+S^{\pm}\otimes q^{-S^3})\,r_0(\lambda)\,. \tag{A7}$$

It can be proven along the lines of Ref. 7 that solution to this equation is unique up to a scalar factor. As we have already shown in Sec. VII, this solution is given by $r_0(\lambda)=(1\otimes e^{\gamma\lambda S^3})r(\lambda)\times(e^{-\gamma\lambda S^3}\otimes 1)$, where $r(\lambda)$ solves (A1).

Now we observe that $r_1(\lambda)\equiv\mathbf{P}r_0(\lambda)\mathbf{P}$ and $r_2(\lambda)\equiv(r_0(\lambda))^t$ solve the same set of equations (A6) and (A7). By the above-mentioned uniqueness, this implies that $r_i(\lambda)=c_i(\lambda)r_0(\lambda)$, where $c_i(\lambda)$, $i=1,2$ are scalar functions. Since $\mathbf{P}^2=1\otimes 1$, and $((r_0)^t)^t=r_0$, we conclude that $c_i(\lambda)=\pm 1$. Imposing the condition $r_0(0)=1\otimes 1$, we have to put $c_i(\lambda)=1$. Thus, we have proven the relations on the left-hand side of (77) and (78). Employing the first of them and the property (37) of $r(\lambda)$, we prove the second relation in (77) as follows:

$$\begin{aligned}
r_0(\lambda,-\gamma)&=(1\otimes e^{-\gamma\lambda S^3})r(\lambda,-\gamma)(e^{\gamma\lambda S^3}\otimes 1)\\
&=(1\otimes e^{-\gamma\lambda S^3})\mathbf{P}r(\lambda,\gamma)\mathbf{P}(e^{\gamma\lambda S^3}\otimes 1)\\
&=\mathbf{P}(e^{-\gamma\lambda S^3}\otimes 1)r(\lambda,\gamma)(1\otimes e^{\gamma\lambda S^3})\mathbf{P}\\
&=\mathbf{P}(1\otimes e^{\gamma\lambda S^3})r(\lambda,\gamma)(e^{-\gamma\lambda S^3}\otimes 1)\mathbf{P}\\
&=\mathbf{P}r_0(\lambda,\gamma)\mathbf{P}=r_0(\lambda,\gamma)\,.
\end{aligned}$$

In the fourth line we used that $[r(\lambda),\Delta(e^{\gamma\lambda S^3})]=0$.

APPENDIX B

Here we provide some details on computation of the Hamiltonians in the cases of spin 1 and spin $\frac{3}{2}$. For $S=1$, a matrix representation of the spin generators is (as was discussed in Sec. IV, one has a freedom of rescaling $S^{\pm}\to\eta^{\mp 1/2}S^{\pm}$ with any real $\eta\neq 0$)

$$S^+=\begin{pmatrix}0&a&0\\0&0&a\\0&0&0\end{pmatrix},\quad S^-=(S^+)^t,\quad S^3=\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}, \tag{B1}$$

where t denotes transposition and $a=\sqrt{2\cos\gamma}$. Since $(S^3)^3=S^3$, any function of S^3 is a polynomial in S^3 of a degree not exceeding two. In particular, we have

$$\sin(tS^3)=S^3\sin t\,,\quad \cos(tS^3)=1-2(S^3)^2\sin^2\frac{t}{2}\,. \tag{B2}$$

Denote $\Upsilon=\frac{1}{2}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)$. With the help of formulas (B2) we rewrite (29) as follows:

$$\begin{aligned}
\mathbf{X}_1&=q^{S_n^3}\Upsilon\,q^{-S_{n+1}^3}+(\cos\gamma)\,(\Lambda+\tfrac{1}{2}+2(\cos\gamma)^2)\,,\\
\Lambda&=\tfrac{3}{2}-2(\cos\gamma)^2+(\cos\gamma)^2(S_n^3S_{n+1}^3)+(\sin\gamma)^2((S_n^3S_{n+1}^3)^2-2(S_n^3)^2-2(S_{n+1}^3)^2)\\
&\quad+i(\sin 2\gamma)(S_n^3-S_{n+1}^3+\tfrac{1}{2}(S_n^3)^2S_{n+1}^3-\tfrac{1}{2}S_n^3(S_{n+1}^3)^2)\,.
\end{aligned} \tag{B3}$$

Substituting (B3) into (52), applying several times formulas (B2) and (59), we obtain the Hamiltonian in the following form:

$$\begin{aligned}
H_{n,n+1}=\frac{1}{4\cos\gamma}\Bigg(&-\frac{1}{\cos^2\gamma}(\Upsilon)^2-\frac{1}{\cos\gamma}q^{S_n^3}(\Upsilon\,\Lambda+\Lambda\,\Upsilon)\,q^{-S_{n+1}^3}+4+2\cos 2\gamma+(\cos 2\gamma)\\
&\times(S_n^3S_{n+1}^3-(S_n^3S_{n+1}^3)^2)-2(\sin\gamma)^2((S_n^3)^2+(S_{n+1}^3)^2)\Bigg)+i\frac{\sin\gamma}{2}(S_n^3-S_{n+1}^3)\,.
\end{aligned} \tag{B4}$$

Deriving the first term here we used the following analogue of relation (50):

$$e^{tS^3}(S^{\pm})^2=(S^{\pm})^2 e^{-tS^3}=e^{\pm t}(S^{\pm})^2 . \tag{B5}$$

Next, we observe that the following identity holds (as can be checked directly in terms of matrices):

$$-F_\alpha (q^{S_n^3}(\Upsilon\,\Lambda+\Lambda\,\Upsilon)\,q^{-S_{n+1}^3})\,(F_\alpha)^{-1}=\Theta_\alpha^-\,\Upsilon+\Upsilon\,\Theta_\alpha^+ , \tag{B6}$$

with F_α as in (62) and

$$\Theta_\alpha^{\pm}=\tfrac{1}{2}(1\otimes 1)+(1-2q^{\pm\alpha}\cos\gamma)\,S_n^3 S_{n+1}^3 . \tag{B7}$$

Substituting (B6) and (B7) with $\alpha=0$ into (B4), we obtain the Hamiltonian (53).

The Hamiltonian $\widetilde{H}_{n,n+1}^{(\alpha)}$ discussed in Sec. VI is obtained from (B4) by the twist (68). Notice that the term $(\Upsilon)^2$ in (B4) is not affected due to (B5). The diagonal part of Hamiltonian apparently commutes with the twist. So the only part of (B4) which changes is the second term. It transforms according to (B6), which yields the Hamiltonian (69).

Consider now the case $S=\frac{3}{2}$. The spin generators are given by

$$S^+=\begin{pmatrix} 0 & a_1 & 0 & 0\\ 0 & 0 & a_2 & 0\\ 0 & 0 & 0 & a_1\\ 0 & 0 & 0 & 0 \end{pmatrix},\quad S^-=(S^+)^t,\quad S^3=\begin{pmatrix} \frac{3}{2} & 0 & 0 & 0\\ 0 & \frac{1}{2} & 0 & 0\\ 0 & 0 & -\frac{1}{2} & 0\\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}, \tag{B8}$$

with $a_1=(2\cos 2\gamma+1)^{1/2}$ and $a_2=2\cos\gamma$. Any function of S^3 is a polynomial in S^3 of a degree not exceeding three. In particular,

$$\sin(tS^3)=\left(2\sin\frac{t}{2}+\frac{1}{3}\sin^3\frac{t}{2}\right)S^3-\frac{4}{3}\left(\sin^3\frac{t}{2}\right)(S^3)^3 , \tag{B9}$$

$$\cos(tS^3)=\cos\frac{t}{2}+\frac{1}{4}\sin\frac{t}{2}\sin t-\left(\sin\frac{t}{2}\sin t\right)(S^3)^2 . \tag{B10}$$

The Hamiltonian (56) for $S=\frac{3}{2}$ takes the following form in terms of $\mathbf{X}_{3/2}$:

$$H_{n,n+1}=\frac{1}{4(\cos\gamma)^3(1+2\cos 2\gamma)^3}(4(\cos\gamma)(\mathbf{X}_{3/2})^2-(\mathbf{X}_{3/2})^2(13+20\cos 2\gamma+8\cos 4\gamma +2\cos 6\gamma)+\mathbf{X}_{3/2}(68\cos\gamma+48\cos 3\gamma+23\cos 5\gamma+7\cos 7\gamma+\cos 9\gamma)) . \tag{B11}$$

This Hamiltonian can be rewritten in the same way as we did for $S=1$ using, in particular, relations (60), (B9) and (B10), and appropriate analogues of (B5) and (B6). The final form is given by (57), with

$$\mathbf{Q}=\frac{1}{192}(1\otimes 1)\,(815-5832\cos\gamma+2352\cos 2\gamma-3888\cos 3\gamma+2542\cos 4\gamma-1620\cos 5\gamma$$
$$+1600\cos 6\gamma-324\cos 7\gamma+467\cos 8\gamma)+\frac{2}{3}\left(\sin\frac{\gamma}{2}\right)^2 S_n^3S_{n+1}^3\,(106+37\cos\gamma+186\cos 2\gamma$$
$$+29\cos 3\gamma+88\cos 4\gamma+13\cos 5\gamma+28\cos 6\gamma+5\cos 7\gamma)+\left(\sin\frac{\gamma}{2}\right)^2 (S_n^3S_{n+1}^3)^2\,(28$$
$$-53\cos\gamma+54\cos 2\gamma-31\cos 3\gamma+28\cos 4\gamma-11\cos 5\gamma+10\cos 6\gamma-\cos 7\gamma)$$
$$+\frac{1}{12}\left(\sin\frac{\gamma}{2}\right)^2 ((S_n^3)^2+(S_{n+1}^3)^2)\,(412+1687\cos\gamma+606\cos 2\gamma+1085\cos 3\gamma+268\cos 4\gamma$$
$$+433\cos 5\gamma+58\cos 6\gamma+83\cos 7\gamma)\,,$$

$$\mathbf{F}_{3/2}=\frac{\cos^2\gamma}{4}(1\otimes 1)\,(10328+17080\cos 2\gamma+9071\cos 4\gamma+3220\cos 6\gamma+621\cos 8\gamma)$$
$$-\frac{1}{9}\left(\sin\frac{\gamma}{2}\right)^2 S_n^3S_{n+1}^3\,(8364+5020\cos\gamma+12752\cos 2\gamma+2499\cos 3\gamma+7150\cos 4\gamma$$
$$+1023\cos 5\gamma+3320\cos 6\gamma+447\cos 7\gamma+814\cos 8\gamma+83\cos 9\gamma)$$
$$-\frac{4}{3}\left(\sin\frac{\gamma}{2}\right)^2 (S_n^3S_{n+1}^3)^2\,(536-472\cos\gamma+864\cos 2\gamma-347\cos 3\gamma+650\cos 4\gamma$$
$$-163\cos 5\gamma+272\cos 6\gamma-65\cos 7\gamma+78\cos 8\gamma-9\cos 9\gamma)-\frac{64}{9}\left(\sin\frac{\gamma}{2}\right)^4 (S_n^3S_{n+1}^3)^3\,(50$$
$$-200\cos\gamma+48\cos 2\gamma-168\cos 3\gamma+45\cos 4\gamma-76\cos 5\gamma+28\cos 6\gamma-20\cos 7\gamma$$
$$+13\cos 8\gamma)-(\sin 2\gamma)^2\,((S_n^3)^2+(S_{n+1}^3)^2)\,(169+274\cos 2\gamma+106\cos 4\gamma+27\cos 6\gamma)$$
$$+\frac{4}{9}\left(\sin\frac{\gamma}{2}\right)^2 ((S_n^3)^3S_{n+1}^3+S_n^3(S_{n+1}^3)^2)\,(444-2516\cos\gamma+560\cos 2\gamma-2037\cos 3\gamma$$
$$+334\cos 4\gamma-1137\cos 5\gamma+200\cos 6\gamma-417\cos 7\gamma+46\cos 8\gamma-85\cos 9\gamma)\,.$$

The equivalence of (B11) and (57) as 16×16 matrices has been verified with the help of the program MATHEMATICA.

APPENDIX C

Here we explain the origin of Eq. (89) that was important for our discussion on the open chain Hamiltonian in Sec. VIII.

Recall that, by definition (see, e.g., Refs. 14 and 28), a Hopf algebra $\mathcal{A}$ possesses the antipode map $s:\mathcal{A}\to\mathcal{A}$ which is an antihomomorphism consistent with the co-multiplication and the co-unit in the sense that $m((s\otimes id)\Delta(\xi))=m((id\otimes s)\Delta(\xi))=\epsilon(\xi)\cdot 1$ (here $m:\mathcal{A}^{\otimes 2}\to\mathcal{A}$ is the multiplication). Assume that there exists an element $\chi\in\mathcal{A}$ which realizes the square of the antipode (which is a homomorphism) as an inner automorphism, i.e., $s(s(\xi))=\chi\,\xi\,\chi^{-1}$ for any $\xi\in\mathcal{A}$. Then, as was proven in Ref. 28,

$$\mathrm{tr}_1((\chi^{-1}\otimes 1)\,b) \tag{C1}$$

belongs to the center of $\mathcal{A}$ if an element $b\in\mathcal{A}^{\otimes 2}$ satisfies $[b,\Delta(\xi)]=0$ for any $\xi\in\mathcal{A}$.

For $\mathcal{A}=U_q(sl_2)$ the antipode consistent with the co-multiplication (7) is given by

$$s(S^{\pm}) = -q^{\mp 1} S^{\pm}, \quad s(S^3) = -S^3.$$

It is easy to see that in this case $\chi = q^{-2S^3}$. Since the universal r-matrix $r(\lambda)$ has the property (12), we can apply (C1) and infer that its q-trace, $\mathrm{tr}_1((q^{2S^3} \otimes 1)\, r(\lambda))$, belongs to the center of $U_q(sl_2)$. Consequently, the same holds for the local Hamiltonian $H_{n,n+1}$ constructed as in (20). Being evaluated in an irreducible representation, the q-trace of $H_{n,n+1}$ becomes just a constant, as was stated in Eq. (89).

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Quantum mechanics of damped systems

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(Received 21 January 2003; accepted 16 May 2003)

We show that the quantization of a simple damped system leads to a self-adjoint Hamiltonian with a family of complex generalized eigenvalues. It turns out that they correspond to the poles of energy eigenvectors when continued to the complex energy plane. Therefore, the corresponding generalized eigenvectors may be interpreted as resonant states. We show that resonant states are responsible for the irreversible quantum dynamics of our simple model. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599074]

I. INTRODUCTION

Standard textbooks on quantum mechanics investigate mainly the Hamiltonian system, i.e., by a quantum system one usually means a Hilbert space $\mathcal{H}$ which describes physical quantum states and a self-adjoint operator (Hamiltonian) in $\mathcal{H}$ which governs dynamics of the system. However, most of the classical systems are not Hamiltonian and the quantum mechanics of such systems is poorly understood. In the present paper we are going to investigate one of the simplest non-Hamiltonian systems corresponding to a damped motion in one dimension:

$$\dot{x} = -\gamma x, \tag{1.1}$$

where $x \in \mathbb{R}$, and $\gamma > 0$ stands for the damping constant. Classically, the damping behavior is described by the exponential law

$$x(t) = e^{-\gamma t} x. \tag{1.2}$$

As is well known[1] (see also Ref. 2), within the standard Hilbert space formulation of quantum mechanics there is no room for such behavior on a quantum level. Therefore, in order to deal with this problem, we shall use the rigged Hilbert space approach to quantum mechanics which generalizes the standard Hilbert space version.[3–5] A rigged Hilbert space (or a Gelfand triplet) is a collection of spaces:[6,7]

$$\Phi \subset \mathcal{H} \subset \Phi', \tag{1.3}$$

where $\mathcal{H}$ is a Hilbert space, Φ is a dense nuclear subspace of $\mathcal{H}$, and Φ' denotes its dual, i.e., the space of continuous functionals on Φ (see Sec. II for a brief review).

The quantization of our simple model (1.1) leads to a self-adjoint Hamiltonian $\hat{H}$ in $\mathcal{H} = L^2(\mathbb{R})$. Interestingly, $\hat{H}$ being self-adjoint, gives rise to the family of generalized complex eigenvalues. Clearly, these eigenvalues are not elements of the spectrum $\sigma(\hat{H}) = (-\infty, \infty)$. The corresponding eigenvectors do not belong to $L^2(\mathbb{R})$ but to Φ' for an appropriately chosen Φ. We show that these complex eigenvalues have many remarkable properties analogous to the point spectrum of a self-adjoint operator. In particular, they give rise to the spectral decomposition of $\hat{H}$. Moreover, they are closely related to the continuous spectrum of $\hat{H}$. It turns out that they corre-

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spond to the poles of the energy eigenvectors ψ^E when continued to the complex energy plane.[8] Physicists usually called the corresponding eigenvectors resonant states[3,9,10] (see also Ref. 11). It is widely believed that resonant states are responsible for the irreversible dynamics of physical systems (see, e.g., the recent collection of papers[3]). Indeed, it is true in our simple model. To see this we construct two Gelfand triples:

$$\Phi_{\pm} \subset L^2(\mathbb{R}) \subset \Phi'_{\pm}, \tag{1.4}$$

such that $\Phi_+ \cap \Phi_- = \{\varnothing\}$. Obviously, the time evolution is perfectly reversible when considered on $L^2(\mathbb{R})$. It is given by the one-parameter group of unitary transformations $U(t) = e^{-i\hat{H}t}$. However, when restricted to $\Phi_{\pm}$, it defines only two semigroups: $U(t \geqslant 0)$ on Φ_-, and $U(t \leqslant 0)$ on Φ_+. Therefore, the evolution on $\Phi_{\pm}$ is irreversible. This irreversibility is caused by quantum damping, or, equivalently, by the presence of resonances.

II. RIGGED HILBERT SPACE

Consider a rigged Hilbert space, i.e., the following collection (Gelfand triplet):

$$\Phi \subset \mathcal{H} \subset \Phi', \tag{2.1}$$

where $\mathcal{H}$ is a Hilbert space with the standard norm topology $\tau_{\mathcal{H}}$, Φ is a topological vector space with a topology, τ_{Φ}, stronger than $\tau_{\mathcal{H}}$, and Φ' is the dual space of continuous linear functionals on Φ.[6,7] We denote the action of Φ' on Φ using Dirac notation, i.e., for any $\phi \in \Phi$ and $F \in \Phi'$,

$$\langle \phi | F \rangle := F(\phi). \tag{2.2}$$

Any self-adjoint operator $\hat{A}$ in $\mathcal{H}$ may be extended to an operator on Φ':

$$\hat{A}: \Phi' \to \Phi', \tag{2.3}$$

by

$$\langle \phi | \hat{A} F \rangle := \langle \hat{A}\phi | F \rangle. \tag{2.4}$$

Now, if for any $\phi \in \Phi$,

$$\langle \phi | \hat{A} F_{\lambda} \rangle = \lambda \langle \phi | F_{\lambda} \rangle, \tag{2.5}$$

then $F_{\lambda} \in \Phi'$ is called a generalized eigenvector corresponding to a generalized eigenvalue λ. Omitting ϕ one simply writes

$$\hat{A} | F_{\lambda} \rangle = \lambda | F_{\lambda} \rangle. \tag{2.6}$$

Note that a generalized eigenvalue λ may be complex. Now, if the spectrum of $\hat{A}$,

$$\sigma(\hat{A}) = \sigma_p(\hat{A}) \cup \sigma_c(\hat{A}) \subset \mathbb{R}, \tag{2.7}$$

with $\sigma_p(\hat{A}) = \{\lambda_1, \lambda_2, \ldots\}$, then the Gelfand–Maurin theorem[6,7] implies the following spectral decompositions:

$$\mathbb{1}_{\Phi} = \sum_n |F_n\rangle\langle F_n| + \int_{\sigma_c(\hat{A})} d\lambda \, |F_{\lambda}\rangle\langle F_{\lambda}|, \tag{2.8}$$

and of $\hat{A}$ itself:

$$\hat{A}=\sum_n \lambda_n |F_n\rangle\langle F_n| + \int_{\sigma_c(\hat{A})} d\lambda\, \lambda |F_\lambda\rangle\langle F_\lambda|. \tag{2.9}$$

This way the rigged Hilbert space approach fully justifies the standard Dirac notation.

The choice of Φ depends on the particular problem one deals with. In the present paper we shall consider the following functional spaces: $\mathcal{D}$—the space of $C^\infty(\mathbb{R})$ functions with compact supports equipped with the convex Schwartz topology,[12] $\mathcal{S}$—the space of $C^\infty(\mathbb{R})$ functions vanishing at infinity faster than any polynomial.[12] Moreover, let us define

$$\mathcal{Z} := \{F[\phi] \mid \phi \in \mathcal{D}\}, \tag{2.10}$$

where $F[\phi]$ denotes the Fourier transform of ϕ. It turns out[13] that $\mathcal{Z}$ is isomorphic to the space of entire functions of fast decrease along $\mathbb{R}$. More precisely, let

$$F_L[\phi](z) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{izx}\phi(x)\, dx, \tag{2.11}$$

be the Fourier–Laplace transform of $\phi \in \mathcal{D}$. One proves[12,13] the following

Theorem 1: *(Paley–Wiener–Schwartz) Let $a>0$. An entire function $U(z)$ is a Fourier–Laplace transform of a function $u \in \mathcal{D}$ with support*

$$\mathrm{supp}(u) = \{x \in \mathbb{R} \mid |x| \leqslant a\},$$

if and only if

$$|z|^n |U(z)| \leqslant C_n e^{a|\mathrm{Im}\, z|}, \quad n = 1,2,\ldots .$$

Now, for $z=x \in \mathbb{R}$, i.e., $\mathrm{Im}\, z=0$, $F_L[\phi]=F[\phi]$, and the above theorem implies

$$|x|^n |F[\phi](x)| \leqslant C_n, \qquad n = 1,2,\ldots . \tag{2.12}$$

Clearly, $\mathcal{Z} \cap \mathcal{D} = \{\varnothing\}$. Moreover, one has

$$\mathcal{D} \subset \mathcal{S} \subset L^2(\mathbb{R}), \tag{2.13}$$

and

$$\mathcal{Z} \subset \mathcal{S} \subset L^2(\mathbb{R}), \tag{2.14}$$

and both $\mathcal{D}$ and $\mathcal{Z}$ are dense in $\mathcal{S}$. One proves[13] that the Fourier transformation which defines the unitary operator

$$F : L^2(\mathbb{R}) \to L^2(\mathbb{R}), \tag{2.15}$$

establishes an isomorphism between $\mathcal{D}$ and $\mathcal{Z}$.

III. QUANTIZATION OF DAMPED SYSTEMS

Let us quantize a classical damped system described by (1.1). Clearly this system is not Hamiltonian. However, it is well known (cf. Ref. 14) that any dynamical system may be rewritten in a Hamiltonian form. Consider a dynamical system on n-dimensional configuration space Q:

$$\dot{x} = X(x)\ , \tag{3.1}$$

where X is a vector field on Q. Now, define the following Hamiltonian on the cotangent bundle $\mathcal{P}=T^*Q$:

$$H(\alpha_x) := \alpha_x(X(x)), \tag{3.2}$$

where $\alpha_x \in T_x^*Q$. Using canonical coordinates $(x^1,\ldots,x^n,p_1,\ldots,p_n)$ one obtains

$$H(x,p) = \sum_{k=1}^{n} p_k X^k(x), \tag{3.3}$$

where X^k are components of X in the coordinate basis $\partial/\partial x^k$. The corresponding Hamilton equations take the following form:

$$\dot{x}^k = \{x^k, H\} = X^k(x), \tag{3.4}$$

$$\dot{p}_k = \{p_k, H\} = -\sum_{l=1}^{n} p_l \frac{\partial X^l(x)}{\partial x^k}, \tag{3.5}$$

for $k=1,\ldots,n$. In the above formulas $\{\ ,\ \}$ denotes the canonical Poisson bracket on T^*Q:

$$\{F,G\} = \sum_{k=1}^{n} \left(\frac{\partial F}{\partial x^k}\frac{\partial G}{\partial p_k} - \frac{\partial G}{\partial x^k}\frac{\partial F}{\partial p_k} \right). \tag{3.6}$$

Clearly, the formula (3.4) reproduces our initial dynamical system (3.1) on Q.

Let us apply the above procedure to the damped system (1.1). One obtains for the Hamiltonian

$$H(x,p) = -\gamma x p, \tag{3.7}$$

and hence the corresponding Hamilton equations

$$\dot{x} = -\gamma x, \quad \dot{p} = \gamma p, \tag{3.8}$$

give rise to the following Hamiltonian flow on $\mathbb{R}^2$:

$$(x,p) \to (e^{-\gamma t}x, e^{t\gamma}p). \tag{3.9}$$

Now, the quantization is straightforward: one has for the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$, and for the Hamiltonian

$$\hat{H} = -\frac{\gamma}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}). \tag{3.10}$$

It is evident that (3.10) defines a symmetric operator on $L^2(\mathbb{R})$. In Sec. IV we show that $\hat{H}$ is self-adjoint and hence it gives rise to a well-defined quantum mechanical problem. Actually, this Hamiltonian is well known in quantum optics in connection with the squeezed states of light.[15] Introducing $\hat{a}$ and $\hat{a}^*$: $\hat{x} = (\hat{a} + \hat{a}^*)/\sqrt{2}$, $\hat{p} = (\hat{a} - \hat{a}^*)/\sqrt{2}i$, the Hamiltonian (3.10) may be rewritten as follows: $\hat{H} = (\gamma/2i)(\hat{a}^{*2} - \hat{a}^2)$, which is exactly a generator of squeezing.

Let us observe that performing the canonical transformation

$$x = \frac{-1}{\sqrt{2\gamma}}(P + \gamma X), \quad p = \frac{1}{\sqrt{2\gamma}}(P - \gamma X), \tag{3.11}$$

the classical Hamiltonian (3.10) takes the following form:

$$\hat{H} = \tfrac{1}{2}(\hat{P}^2 - \gamma^2 \hat{X}^2), \tag{3.12}$$

that is, it corresponds to the so-called reversed harmonic oscillator. This system was analyzed in Ref. 16 and recently in Refs. 17–19 (see also Refs. 20 and 21).

IV. PROPERTIES OF THE HAMILTONIAN

Let us investigate the basic properties of the Hamiltonian defined in (3.10).

Proposition 1: The operator $\hat{H}=-(\gamma/2)(\hat{x}\hat{p}+\hat{p}\hat{x})$ *is self-adjoint in* $L^2(\mathbb{R})$.

Proof: To prove that $\hat{H}$ is self-adjoint we show that $e^{-i\hat{H}}$ is unitary in $L^2(\mathbb{R})$. One has

$$\hat{H}=-\frac{\gamma}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})=i\gamma\left(x\frac{\mathrm{d}}{\mathrm{d}x}+\frac{1}{2}\right). \tag{4.1}$$

Let us define

$$U=e^{-i\hat{H}}=e^{\gamma/2}e^{\gamma x\partial_x}. \tag{4.2}$$

Clearly,

$$U\psi(x)=e^{\gamma/2}\psi(e^{\gamma}x), \tag{4.3}$$

for any $\psi\in L^2(\mathbb{R})$. The operator U defines an isometry:

$$\langle U\psi|U\phi\rangle=\int_{-\infty}^{\infty}\overline{U\psi(x)}U\phi(x)\,\mathrm{d}x=\int_{-\infty}^{\infty}e^{\gamma}\overline{\psi(e^{\gamma}x)}\phi(e^{\gamma}x)\,\mathrm{d}x=\int_{-\infty}^{\infty}\overline{\psi(y)}\phi(y)\,\mathrm{d}y=\langle\psi|\phi\rangle. \tag{4.4}$$

Moreover, due to (4.3), U is onto, and hence it is unitary in $L^2(\mathbb{R})$. Therefore, Stone's theorem implies that $\hat{H}$ is self-adjoint (see, e.g., Ref. 12). □

Obviously, $\hat{H}$ is parity invariant:

$$\mathbf{P}\hat{H}\mathbf{P}^{-1}=\hat{H}, \tag{4.5}$$

where the parity operator P is defined by

$$\mathbf{P}\hat{x}\mathbf{P}^{-1}=-\hat{x},\quad \mathbf{P}\hat{p}\mathbf{P}^{-1}=-\hat{p}. \tag{4.6}$$

Now, let us turn to the time reversal operator $\mathbf{T}$. The theory invariant under the time reversal has the following property: if $\psi(t)$ is a solution of the Schrödinger equation given by

$$\psi(t)=U(t)\psi, \tag{4.7}$$

with $U(t)=e^{-i\hat{H}t}$, then $\mathbf{T}\psi$ evolves into

$$(\mathbf{T}\psi)(-t)=U(t)(\mathbf{T}\psi), \tag{4.8}$$

or, equivalently

$$\mathbf{T}(U(t)\psi)=U(-t)(\mathbf{T}\psi), \tag{4.9}$$

for any $\psi\in\mathcal{H}$. Now, following Wigner,[22] $\mathbf{T}$ is either unitary or anti-unitary. If $\mathbf{T}$ is unitary, then (4.9) implies

$$\mathbf{T}\hat{H}+\hat{H}\mathbf{T}=0\,. \tag{4.10}$$

It means that if

$$\hat{H}\psi^E = E\psi^E, \tag{4.11}$$

then

$$\hat{H}\,\mathbf{T}\psi^E = -E\,\mathbf{T}\psi^E, \tag{4.12}$$

that is, any eigenvector ψ^E with the energy E is accompanied by $\mathbf{T}\psi^E$ with energy $-E$. Usually, this case is excluded since one expects that the Hamiltonian is bounded from below. If this is the case, then $\mathbf{T}$ is anti-unitary and (4.9) implies:

$$\mathbf{T}\hat{H} - \hat{H}\mathbf{T} = 0. \tag{4.13}$$

However, the Hamiltonian defined in (3.10) is not bounded from below, and, as we show in Sec. VI its spectrum $\sigma(\hat{H}) = (-\infty, \infty)$. Therefore, we take $\mathbf{T}$ to be unitary in $L^2(\mathbb{R})$.

Proposition 2: The time reversal operator $\mathbf{T}$ *is realized by the Fourier transformation:*

$$\mathbf{T}\psi := F[\psi], \tag{4.14}$$

i.e.,

$$F^{-1}\hat{H}F\psi = -\hat{H}\psi, \tag{4.15}$$

for all $\psi \in L^2(\mathbb{R})$. *Moreover,*

$$\mathbf{T}^2\psi(x) = \mathbf{P}\phi(x) = \psi(-x). \tag{4.16}$$

Denoting by $\mathbf{C}$ the complex conjugation $\mathbf{C}\psi = \overline{\psi}$, one immediately finds

Proposition 3: The Hamiltonian (3.10) is $\mathbf{CT}$ *and* $\mathbf{PCT}$ *invariant, i.e.,*

$$[\hat{H}, \mathbf{CT}] = [\hat{H}, \mathbf{PCT}] = 0\,. \tag{4.17}$$

Therefore, if

$$\hat{H}\psi^E = E\psi^E, \tag{4.18}$$

then

$$\hat{H}F[\overline{\psi^E}] = EF[\overline{\psi^E}]. \tag{4.19}$$

Clearly, $\mathbf{CT}$ invariance does not produce any conserved quantity since $\mathbf{CT}$ is anti-unitary.

V. COMPLEX EIGENVALUES

Interestingly, $\hat{H}$ being self-adjoint admits generalized eigenvectors with complex eigenvalues.[19,23,20,21] Let $f_0^{\pm}$ be distributions satisfying

$$\hat{x}\,f_0^- = 0, \quad \hat{p}\,f_0^+ = 0. \tag{5.1}$$

Clearly,

$$f_0^-(x) = \delta(x), \quad f_0^+(x) = 1. \tag{5.2}$$

Its easy to see that

$$\hat{H}\,f_0^{\pm} = \pm i\frac{\gamma}{2}f_0^{\pm}. \tag{5.3}$$

Let us define two families:

$$f_n^- := \frac{(-i)^n}{\sqrt{n!}}\hat{p}^n f_0^-, \quad f_n^+ := \frac{1}{\sqrt{n!}}\hat{x}^n f_0^+. \tag{5.4}$$

One finds

$$f_n^-(x) = \frac{(-1)^n}{\sqrt{n!}}\delta^{(n)}(x), \quad f_n^+(x) = \frac{x^n}{\sqrt{n!}}. \tag{5.5}$$

Moreover,

$$\hat{H} f_n^\pm = \pm E_n f_n^\pm, \tag{5.6}$$

where

$$E_n := i\gamma(n+\tfrac{1}{2}). \tag{5.7}$$

Clearly, both f_n^- and f_n^- are tempered distributions, i.e., $f_n^\pm \in \mathcal{S}'$. Evidently, they are related by the Fourier transformation:

$$F[f_n^+] = \sqrt{2\pi} i^n f_n^-, \quad F[f_n^-] = \frac{i^n}{\sqrt{2\pi}} f_n^+. \tag{5.8}$$

Let us observe that these two families of generalized eigenvectors have two remarkable properties:

$$\int_{-\infty}^{\infty} f_n^+(x)\, f_m^-(x)\, \mathrm{d}x = \delta_{nm}, \tag{5.9}$$

and

$$\sum_{n=0}^{\infty} f_n^+(x)\, f_n^-(x') = \delta(x-x'). \tag{5.10}$$

These formulas remind one of the basic properties of proper (Hilbert space) eigenvectors: if $\hat{A}$ is a self-adjoint operator in $\mathcal{H}$ and

$$\hat{A}\psi_k = \lambda_k \psi_k, \tag{5.11}$$

where ψ_k are normalized vectors in $\mathcal{H}$, then

$$\int \overline{\psi_n}(x)\psi_m(x)\, \mathrm{d}x = \delta_{nm}, \tag{5.12}$$

and

$$\sum_n \overline{\psi_n}(x)\psi_n(x')\, \mathrm{d}x = \delta(x-x'). \tag{5.13}$$

Obviously, there is no complex conjugation in (5.9) and (5.10) since $f_n^\pm$ are real functions.

Now, for any $\phi \in \mathcal{Z}$ one has

$$\phi(x)=\sum_n \frac{\phi^{(n)}(0)}{n!}(-1)^n x^n=\sum_n f_n^+(x)\langle f_n^-|\phi\rangle. \tag{5.14}$$

On the other hand, for any $\phi\in\mathcal{D}$, its Fourier transform $F[\phi]\in\mathcal{Z}$, and

$$\begin{aligned}\phi(x)&=\frac{1}{\sqrt{2\pi}}\int e^{ikx}F[\phi](k)\mathrm{d}k\\&=\frac{1}{\sqrt{2\pi}}\int e^{ikx}\sum_n \frac{F[\phi]^{(n)}(0)}{n!}(-1)^n k^n\,\mathrm{d}k\\&=\sum_n F[f_n^+](x)\langle f_n^-|F[\phi]\rangle\\&=\sum_n F[f_n^+](x)\langle F[f_n^-]|\phi\rangle\\&=\sum_n f_n^-(x)\langle f_n^+|\phi\rangle.\end{aligned} \tag{5.15}$$

Hence, we have two spectral decompositions:

$$|\phi\rangle=\sum_n |f_n^+\rangle\langle f_n^-|\phi\rangle \quad \text{in} \quad \mathcal{Z}, \tag{5.16}$$

and

$$|\psi\rangle=\sum_n |f_n^-\rangle\langle f_n^+|\psi\rangle \quad \text{in} \quad \mathcal{D}. \tag{5.17}$$

In Sec. VII we derive (5.16) and (5.17) from the spectrum of $\hat{H}$. So let us look for $\sigma(\hat{H})$.

VI. SPECTRUM

The Hamiltonian (3.10) has a continuous spectrum $\sigma(\hat{H})=(-\infty,\infty)$. Since the Hamiltonian (3.10) is parity invariant each generalized eigenvalue $E\in\mathbb{R}$ is doubly degenerated:

$$\hat{H}\psi_\pm^E=E\psi_\pm^E. \tag{6.1}$$

The above equation may be rewritten as the following differential equation for $\psi_\pm^E$:

$$x\frac{\mathrm{d}}{\mathrm{d}x}\psi_\pm^E(x)=-\left(i\frac{E}{\gamma}+\frac{1}{2}\right)\psi_\pm^E. \tag{6.2}$$

To solve (6.2) let us introduce the following distributions[13] (see also Ref. 24):

$$x_+^\lambda:=\begin{cases}x^\lambda, & x\geqslant 0,\\ 0, & x<0,\end{cases}\qquad x_-^\lambda:=\begin{cases}0, & x\geqslant 0,\\ |x|^\lambda, & x<0,\end{cases} \tag{6.3}$$

with $\lambda\in\mathbb{C}$ (basic properties of $x_\pm^\lambda$ are collected in the Appendix). It is, therefore, clear that the generalized eigenvectors $\psi_\pm^E$ may be written as follows:

$$\psi_{\pm}^{E}(x) := \frac{1}{\sqrt{2\pi\gamma}} x_{\pm}^{-(iE/\gamma+1/2)}. \tag{6.4}$$

It turns out that $\psi_{\pm}^{E}$ are well-defined tempered distributions for all $E \in \mathbb{R}$. Actually, instead of $\psi_{\pm}^{E}$ one may work with eigenvectors of the parity operator **P**:

$$\psi_{\text{even}}^{E} = \tfrac{1}{2}(\psi_{+}^{E} + \psi_{-}^{E}), \tag{6.5}$$

$$\psi_{\text{odd}}^{E} = \tfrac{1}{2}(\psi_{+}^{E} - \psi_{-}^{E}). \tag{6.6}$$

Obviously

$$\mathbf{P}\,\psi_{\text{even}}^{E} = \psi_{\text{even}}^{E}, \quad \mathbf{P}\,\psi_{\text{odd}}^{E} = -\psi_{\text{odd}}^{E}. \tag{6.7}$$

These distributions of definite parity are given by

$$\psi_{\text{even}}^{E} = \frac{1}{\sqrt{2\pi\gamma}} |x|^{-(iE/\gamma+1/2)}, \quad \psi_{\text{odd}}^{E} = \frac{1}{\sqrt{2\pi\gamma}} \operatorname{sign}(x)|x|^{-(iE/\gamma+1/2)} \tag{6.8}$$

(see Refs. 13 and 24 for the properties of $|x|^{\lambda}$ and $\operatorname{sign}(x)|x|^{\lambda}$).

With the normalization used in (6.4) one proves[25] orthonormality:

$$\int \overline{\psi_{\pm}^{E_1}(x)}\,\psi_{\pm}^{E_2}(x)\,dx = \delta(E_1 - E_2), \tag{6.9}$$

and completeness:

$$\int \overline{\psi_{\pm}^{E}(x)}\,\psi_{\pm}^{E}(x')\,dE = \delta(x - x'). \tag{6.10}$$

Therefore, due to the Gelfand–Maurin spectral theorem one has

$$\phi(x) = \sum_{\pm} \int dE\; \psi_{\pm}^{E}(x) \langle\, \psi_{\pm}^{E} | \phi \,\rangle, \tag{6.11}$$

for any $\phi \in \mathcal{S}$, and the corresponding spectral resolution of the Hamiltonian has the following form:

$$\hat{H} = \sum_{\pm} \int dE\; E\, |\psi_{\pm}^{E}\rangle\langle\, \psi_{\pm}^{E}|. \tag{6.12}$$

There is another family of energy eigenvectors directly related to $\psi_{\pm}^{E}$. Due to (4.19) one has

$$\hat{H}\, F[\psi_{\pm}^{-E}] = E F[\psi_{\pm}^{-E}]. \tag{6.13}$$

The Fourier transform of $\psi_{\pm}^{E}$ is given by (cf. Ref. 13 and the Appendix):

$$F[\psi_{\pm}^{-E}](k) = \pm \frac{i}{2\pi\sqrt{\gamma}} \exp\left[\pm \frac{i\pi}{2}\left(i\frac{E}{\gamma} - \frac{1}{2}\right)\right] \Gamma\left(i\frac{E}{\gamma} + \frac{1}{2}\right)(k \pm i0)^{-(iE/\gamma+1/2)}. \tag{6.14}$$

One shows[13] that $F[\psi_{\pm}^{E}]$ are well-defined tempered distributions for any $E \in \mathbb{R}$. Moreover,

$$\int \overline{F[\psi_{\pm}^{E_1}]}(x)\, F[\psi_{\pm}^{E_2}](x)\,dx = \delta(E_1 - E_2), \tag{6.15}$$

and

$$\int \overline{F[\psi_{\pm}^{E}]}(x)\, F[\psi_{\pm}^{E}](x')\, \mathrm{d}E = \delta(x-x'). \tag{6.16}$$

Hence, following the Gelfand–Maurin theorem, we have further spectral decompositions: for any $\psi \in \mathcal{S}$,

$$\psi(x) = \sum_{\pm} \int \mathrm{d}E\, F[\psi_{\pm}^{-E}](x) \langle F[\psi_{\pm}^{-E}] | \psi \rangle, \tag{6.17}$$

and for the Hamiltonian itself:

$$\hat{H} = \sum_{\pm} \int \mathrm{d}E\, E |F[\psi_{\pm}^{-E}]\rangle\langle F[\psi_{\pm}^{-E}]|. \tag{6.18}$$

VII. ANALYTICITY OF ENERGY EIGENVECTORS

Let us continue the energy eigenvectors $\psi_{\pm}^{E}$ and $F[\psi_{\pm}^{-E}]$ into the energy complex plane $E \in \mathbb{C}$. It turns out[13] (see also the Appendix) that $\psi_{\pm}^{E}$ has simple poles at $E = -E_n$, whereas $F[\psi_{\pm}^{-E}]$ has simple poles at $E = +E_n$, with E_n defined in (5.7). Therefore, the poles of energy eigenvectors considered as functions of the complex energy correspond exactly to the complex eigenvalues of $\hat{H}$ which we found in Sec. V. One easily computes the corresponding residues:

$$\mathrm{Res}(\psi_{\pm}^{E}(x); -E_n) = i\sqrt{\frac{\gamma}{2\pi}} \frac{\delta^{(n)}(x)}{n!} \begin{cases} (-1)^n & (+) \\ 1 & (-), \end{cases} \tag{7.1}$$

and

$$\mathrm{Res}(F[\psi_{\pm}^{-E}(x)]; +E_n) = \pm \frac{\sqrt{\gamma}}{2\pi} (\mp i)^{n+1} \frac{(-1)^n}{n!} x^n. \tag{7.2}$$

Hence, residues of $\psi_{\pm}^{E}$ and $F[\psi_{\pm}^{-E}]$ correspond, up to numerical constants, to the eigenvectors $f_n^{\pm}$ (5.5):

$$\mathrm{Res}(\psi_{\pm}^{E}(x); -E_n) \sim f_n^{-}, \tag{7.3}$$

and

$$\mathrm{Res}(F[\psi_{\pm}^{-E}(x)]; +E_n) \sim f_n^{+}. \tag{7.4}$$

Any function $\phi \in \mathcal{S} \subset L^2(\mathbb{R})$ gives rise to the following functions of energy:

$$\mathbb{R} \ni E \to \langle \psi_{\pm}^{E} | \phi \rangle \in \mathbb{C},$$

and

$$\mathbb{R} \ni E \to \langle F[\psi_{\pm}^{-E}] | \phi \rangle \in \mathbb{C}.$$

Let us introduce two important classes of functions:[26] a smooth function $f = f(E)$ is in the Hardy class from above $\mathcal{H}_{+}^{2}$ (from below $\mathcal{H}_{-}^{2}$) if $f(E)$ is a boundary value of an analytic function in the upper, i.e., $\mathrm{Im}\, E \geqslant 0$ (lower, i.e., $\mathrm{Im}\, E \leqslant 0$) half complex E-plane vanishing faster than any power of E at the upper (lower) semi-circle $|E| \to \infty$. Now, define

$$\Phi_{-} := \{\phi \in \mathcal{S} \,|\, \langle \psi_{\pm}^{E} | \phi \rangle \in \mathcal{H}_{-}^{2}\}, \tag{7.5}$$

and

$$\Phi_+ := \{\phi \in \mathcal{S} \,|\, \langle F[\psi_\pm^{-E}] | \phi \rangle \in \mathcal{H}_+^2\}. \tag{7.6}$$

Proposition 4: $\Phi_+ \cap \Phi_- = \{\varnothing\}$.

Proof: Clearly, if $\phi \in \Phi_-$, then $\langle \psi_\pm^E | \phi \rangle$ is a smooth function of $E \in \mathbb{R}$. Suppose that $\phi \in \Phi_+$, that is

$$\langle F[\psi_\pm^{-E}] | \phi \rangle = \langle \psi_\pm^{-E} | F[\phi] \rangle \in \mathcal{H}_+^2. \tag{7.7}$$

Now, due to the Paley–Wiener theorem[12] the inverse Fourier transform of $F[\phi]$,

$$F^{-1}[F[\phi]](E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F[\phi](t)\, e^{-itE}\, \mathrm{d}t, \tag{7.8}$$

vanishes for $E>0$. Therefore, $\phi(E)=0$ for $E>0$, and hence $f(E)$ cannot be a smooth function of E. □

Our main result consists in the following.

Theorem 2: *For any* $\phi^\pm \in \Phi_\pm$ *one has*

$$\phi^-(x) = \sum_n f_n^-(x) \langle f_n^+ | \phi^- \rangle, \tag{7.9}$$

and

$$\phi^+(x) = \sum_n f_n^+(x) \langle f_n^- | \phi^+ \rangle. \tag{7.10}$$

Proof: Due to the spectral formula (6.11) one has, for $\phi^- \in \Phi_- \subset \mathcal{S}$:

$$\phi^-(x) = \sum_\pm \int_{-\infty}^{\infty} \mathrm{d}E\, \psi_\pm^E(x) \langle \psi_\pm^E | \phi^- \rangle\ . \tag{7.11}$$

Now, since $\langle \psi_\pm^E | \phi^- \rangle \in \mathcal{H}_-^2$, we may close the integration contour along the lower semi-circle $|E| \to \infty$. Hence, due to the residue theorem one obtains

$$\phi^-(x) = -2\pi i \sum_\pm \sum_n \mathrm{Res}(\psi_\pm^E(x); -E_n) \langle \psi_\pm^E | \phi^- \rangle |_{E=-E_n}. \tag{7.12}$$

Using the definition of $\psi_\pm^E$,

$$\langle \psi_\pm^E | \phi^- \rangle = \frac{1}{\sqrt{2\pi\gamma}} \int \overline{x_\pm^{-(iE/\gamma+1/2)}}\, \phi^-(x) dx = \frac{1}{\sqrt{2\pi\gamma}} \int x_\pm^{-(-iE/\gamma+1/2)}\, \phi^-(x)\, \mathrm{d}x, \tag{7.13}$$

one finds

$$\langle \psi_\pm^E | \phi^- \rangle |_{E=-E_n} = \frac{1}{\sqrt{2\pi\gamma}} \int x_\pm^n \phi^-(x)\, \mathrm{d}x. \tag{7.14}$$

Therefore, inserting into (7.12) the value of the residue given in (7.1) one gets finally

$$\phi^-(x)=\sum_n \frac{\delta^{(n)}(x)}{n!}\int [(-1)^n x_+^n + x_-^n]\phi^-(x)\,\mathrm{d}x$$

$$=\sum_n (-1)^n \frac{\delta^{(n)}(x)}{n!}\int x^n \phi^-(x)\,\mathrm{d}x$$

$$=\sum_n f_n^-(x)\langle f_n^+|\phi^+\rangle. \tag{7.15}$$

To prove (7.10) let us use another spectral formula (6.17): for any $\phi^+\in\Phi_+\subset\mathcal{S}$,

$$\phi^+(x)=\sum_{\pm}\int_{-\infty}^{\infty}\mathrm{d}E\, F[\psi_\pm^{-E}](x)\langle F[\psi_\pm^{-E}]|\phi^-\rangle. \tag{7.16}$$

Now, since $\langle F[\psi_\pm^{-E}]|\phi^-\rangle\in\mathcal{H}_+^2$, we may close the integration contour along the upper semicircle $|E|\to\infty$. Hence the residue theorem implies

$$\phi^+(x)=+2\pi i\sum_{\pm}\sum_n \mathrm{Res}(F[\psi_\pm^{-E}(x)];+E_n)\,\langle F[\psi_\pm^{-E}]|\phi^+\rangle|_{E=+E_n}. \tag{7.17}$$

Now, using once more the formula for $\psi_\pm^E$ one finds

$$\langle F[\psi_\pm^{-E}]|\phi^+\rangle|_{E=+E_n}=\frac{1}{\sqrt{2\pi\gamma}}\langle F[x_\pm^n]|\phi^+\rangle. \tag{7.18}$$

Hence, inserting the values of residues (7.2) into (7.17) and using the formula for $F[x_\pm^n]$ [see (A9)] one has

$$\phi^+(x)=\frac{i}{\sqrt{2\pi}}\sum_n (-1)^n\frac{x^n}{n!}[(-i)^{n+1}\langle F[x_+^n]|\phi^+\rangle - i^{n+1}\langle F[x_-^n]|\phi^+\rangle]$$

$$=\frac{i}{\sqrt{2\pi}}\sum_n (-1)^n\frac{x^n}{n!}\int [(-i)^{n+1}\overline{F[x_+^n](k)}-i^{n+1}\overline{F[x_-^n](k)}]\phi^+(k)\,\mathrm{d}k$$

$$=\frac{i}{2}\sum_n (-1)^n\frac{x^n}{n!}[(-i)^{n+1}i^n - i^{n+1}(-i)^n]\int \delta^{(n)}(k)\phi^+(k)\,\mathrm{d}k$$

$$=\sum_n f_n^+(x)\langle f_n^-|\phi^+\rangle, \tag{7.19}$$

which ends the proof. □

This way we have recovered (5.16) and (5.17). It is not surprising, due to the following.

Proposition 5: $\Phi_+=\mathcal{Z}$ *and* $\Phi_-=\mathcal{D}$.

Corollary 1: We have two spectral decomposition of $\hat{H}$*:*

$$\hat{H}=\sum_n \overline{E_n}|f_n^-\rangle\langle f_n^+| \quad \text{on} \quad \Phi_-, \tag{7.20}$$

and

$$\hat{H}=\sum_n E_n|f_n^+\rangle\langle f_n^-| \quad \text{on} \quad \Phi_+. \tag{7.21}$$

VIII. RESONANCES AND THE QUANTUM DAMPING

Finally, let us turn to the evolution generated by the Hamiltonian (3.10). Obviously, it generates a one-parameter unitary group

$$U(t)=e^{-i\hat{H}t}, \tag{8.1}$$

on $L^2(\mathbb{R})$. It follows from (4.3) that

$$\psi_t(x)=U(t)\psi(x)=e^{\gamma t/2}\psi(e^{\gamma t}x). \tag{8.2}$$

The above formula is well defined for any $t\in\mathbb{R}$ and clearly, as we already showed, the theory is time-reversal invariant: if $\psi(t)$ solves the Schrödinger equation so does $\mathbf{T}\psi(t):=\psi(-t)$. Therefore, working in $L^2(\mathbb{R})$ we do not see any damping at all. Now, let us construct two natural Gelfand triplets:

$$\Phi_{\pm}\subset L^2(\mathbb{R})\subset\Phi_{\pm}'. \tag{8.3}$$

If $\phi^-\in\Phi_-$, then

$$\langle\,\psi_{\pm}^E|U(t)\phi^-\,\rangle=\langle\,U^*(t)\,\psi_{\pm}^E|\phi^-\,\rangle=e^{-iEt}\langle\,\psi_{\pm}^E|\phi^-\,\rangle. \tag{8.4}$$

Hence $\phi^-(t)\in\Phi_-$ only for $t\geqslant 0$. Similarly, if $\phi^+\in\Phi_+$, then $\phi^+(t)\in\Phi_+$ only for $t\leqslant 0$. Therefore, the restriction of the unitary group $U(t)$ on $L^2(\mathbb{R})$ to $\Phi_{\pm}$ no longer defines a group. It gives rise to two semigroups:

$$U_-(t):\Phi_-\to\Phi_- \quad \text{for } t\geqslant 0,$$

and

$$U_+(t):\Phi_+\to\Phi_+ \quad \text{for } t\leqslant 0.$$

Due to (7.20) and (7.21) one has

$$\phi^+(t)=U(t)\phi^+=\sum_n e^{\gamma(n+1/2)t}|f_n^+\,\rangle\langle\,f_n^-|\phi^+\,\rangle, \tag{8.5}$$

for $t\leqslant 0$, and

$$\phi^-(t)=U(t)\phi^-=\sum_n e^{-\gamma(n+1/2)t}|f_n^-\,\rangle\langle\,f_n^+|\phi^-\,\rangle, \tag{8.6}$$

for $t\geqslant 0$. We stress that ϕ_t^- (ϕ_t^+) does belong to $L^2(\mathbb{R})$ also for $t<0$ ($t>0$). However, $\phi_t^-\in\Phi_-$ ($\phi_t^+\in\Phi_+$) only for $t\geqslant 0$ ($t\leqslant 0$). This way the irreversibility enters on a purely Hamiltonian level by restricting dynamics to the dense subspace $\Phi_{\pm}$ of $L^2(\mathbb{R})$.

Formulas (8.5) and (8.6) are quantum analogues of the classical damping laws:

$$x(t)=e^{-\gamma t}x\ , \quad p(t)=e^{+\gamma t}p. \tag{8.7}$$

Finally, let us recall that the time reversal operator $\mathbf{T}$ establishes an isomorphism between Φ_- and Φ_+. Therefore, each solution

$$\phi_t^- = U_-(t)\phi^-, \tag{8.8}$$

with $\phi^- \in \Phi_-$ is mapped into

$$\mathbf{T}(\phi_t^-) = U_-(-t)\mathbf{T}(\phi^-) = U_+(t)\mathbf{T}(\phi^-), \quad t \leqslant 0. \tag{8.9}$$

Conversely, any solution

$$\phi_t^+ = U_+(t)\phi^+, \tag{8.10}$$

with $\phi^+ \in \Phi_+$ is mapped into

$$\mathbf{T}(\phi_t^+) = U_+(-t)\mathbf{T}(\phi^+) = U_-(t)\mathbf{T}(\phi^+), \quad t \geqslant 0. \tag{8.11}$$

Summarizing, quantum dynamics is irreversible on Φ_- and Φ_+. This irreversibility is caused by quantum damping, or, equivalently, by the presence of resonant states $f_n^{\pm}$ (5.5). It should be stressed that it is not an energy that is dissipated. Clearly, the Hamiltonian (3.10) cannot be interpreted as a system energy—it was used to define a Hamiltonian dynamics of the enlarged system on $L^2(\mathbb{R})$. The quantum damped system is not defined on the entire $L^2(\mathbb{R})$ but rather on a dense subset $\Phi_- \subset L^2(\mathbb{R})$. As we saw it imposes the restriction upon the time evolution such that it is defined only for positive t. Another aspect of dissipation may be seen as follows: let $\phi_0^- \in \Phi_-$ be an initial state then the probability of finding a particle in the interval $[-a,a]$ at time t is given by

$$\mathcal{P}_t([-a,a]) = \int_{-a}^{a} p_t(x)\,\mathrm{d}x, \tag{8.12}$$

where

$$p_t(x) = |\phi_t^-(x)|^2 = e^{+\gamma t}|\phi_0^-(e^{+\gamma t}x)|^2 = e^{+\gamma t}p_0(e^{+\gamma t}x). \tag{8.13}$$

Therefore,

$$\mathcal{P}_t([-a,a]) \to 1, \tag{8.14}$$

in the limit $t \to +\infty$. Hence $p_t(x) \to \delta(x)$.

In a forthcoming paper we are going to show that also more complicated damped systems, e.g., the damped harmonic oscillator, give rise to irreversible dynamics.

ACKNOWLEDGMENTS

I would like to thank Jędrzej Śniatycki for very interesting discussions and his warm hospitality during my stay in Calgary and Andrzej Kossakowski for introducing this problem to me and for many interesting and stimulating discussions. This work was partially supported by the Polish State Committee for Scientific Research (KBN) Grant No. 2P03B01619.

APPENDIX

The regular tempered distribution x_+^λ (with $\lambda \in \mathbb{C}$) given by

$$\langle \phi | x_+^\lambda \rangle := \int_0^\infty x^\lambda \phi(x) \mathrm{d}x, \tag{A1}$$

for any $\phi \in \mathcal{S}$, is well defined for $\mathrm{Re}\,\lambda > -1$. However, it may be easily extended to the region $\mathrm{Re}\,\lambda > -2$ due to the following regularization formula:

$$\int_0^\infty x^\lambda \phi(x) \mathrm{d}x = \int_0^1 x^\lambda [\phi(x) - \phi(0)] \mathrm{d}x + \int_1^\infty x^\lambda \phi(x) \mathrm{d}x + \frac{\phi(0)}{\lambda+1}, \tag{A2}$$

which holds for $\lambda \neq -1$. In the same way one may extend the distribution x_+^λ to the region $\mathrm{Re}\,\lambda > -n-1$ using the formula

$$\int_0^\infty x^\lambda \phi(x) \mathrm{d}x = \int_0^1 x^\lambda \left[\phi(x) - \phi(0) - x\phi'(0) - \cdots - \frac{x^{n-1}}{(n-1)!} \phi^{(n-1)}(0) \right] \mathrm{d}x + \int_1^\infty x^\lambda \phi(x) \mathrm{d}x + \sum_{k=1}^n \frac{\phi^{(k-1)}(0)}{(k-1)!(\lambda+k)}, \tag{A3}$$

which holds for $\lambda \neq -1, -2, \ldots, -n$. The above formula shows that $\langle \phi | x_+^\lambda \rangle$ as a function of $\lambda \in \mathbb{C}$ has simple poles at $\lambda = -1, -2, \ldots$, and the corresponding residue at $\lambda = -k$ equals $\phi^{(k-1)}(0)/(k-1)!$.

Using the same arguments one shows that the distribution x_-^λ may be extended to the region $\mathrm{Re}\,\lambda > -n-1$ via

$$\int_{-\infty}^0 x^\lambda \phi(x) \mathrm{d}x = \int_0^\infty x^\lambda \phi(-x) \mathrm{d}x = \int_1^\infty x^\lambda \left[\phi(-x) - \phi(0) + x\phi'(0) - \cdots - \frac{(-1)^{n-1} x^{n-1}}{(n-1)!} \phi^{(n-1)}(0) \right] \mathrm{d}x + \int_1^\infty x^\lambda \phi(x) \mathrm{d}x + \sum_{k=1}^n \frac{(-1)^{k-1} \phi^{(k-1)}(0)}{(k-1)!(\lambda+k)}, \tag{A4}$$

which holds for $\lambda \neq -1, -2, \ldots, -n$. Hence, $\langle \phi | x_-^\lambda \rangle$ has simple poles at $\lambda = -1, -2, \ldots$, and the corresponding residue at $\lambda = -k$ equals $(-1)^{k-1} \phi^{(k-1)}(0)/(k-1)!$.

The Fourier transforms of $x_\pm^\lambda$,

$$F[x_\pm^\lambda](k) = \frac{1}{\sqrt{2\pi}} \int e^{ikx} x_\pm^\lambda \, \mathrm{d}x, \tag{A5}$$

are given by the following formula:[13]

$$F[x_\pm^\lambda](k) = \pm \frac{i}{\sqrt{2\pi}} e^{\pm i\lambda\pi/2} \Gamma(\lambda+1)(k+i0)^{-\lambda-1}, \tag{A6}$$

where $(k \pm i0)^\alpha$ is a distribution defined by

$$(k \pm i0)^\alpha = k_+^\alpha + e^{\pm i\alpha\pi} k_-^\alpha. \tag{A7}$$

Due to the Euler Γ-function the formula (A6) has single poles at $\lambda=-1,-2,\ldots$. Note, that although both k_+^α and k_-^α have poles at $\alpha=-1,-2,\ldots$, the distribution $(k\pm i0)^\alpha$ is well defined for all $\alpha\in\mathbb{C}$. Indeed

$$\lim_{\alpha\to -n}(k\pm i0)^\alpha=\lim_{\alpha\to -n}(k_+^\alpha+(-1)^n k_-^\alpha), \tag{A8}$$

and, due to (A3) and (A4), the singular parts of k_+^α and k_-^α, at $\alpha=-n$, cancel out. In particular, for $\lambda=n\in\mathbb{N}$, one obtains (cf. Ref. 13)

$$F[x_\pm^n](k)=\frac{1}{\sqrt{2\pi}}[(\pm i)^{n+1}n!k^{-n-1}+(\mp i)^n\pi\delta^{(n)}(k)]. \tag{A9}$$

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Extended edge states in finite Hall systems

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(Received 18 July 2002; accepted 6 May 2003)

We study edge states of a random Schrödinger operator for an electron submitted to a magnetic field in a finite macroscopic two dimensional system of linear dimensions equal to L. The y direction is L-periodic and in the x direction the electron is confined by two smoothly increasing parallel boundary potentials. We prove that, with large probability, for an energy range in the first spectral gap of the bulk Hamiltonian, the spectrum of the full Hamiltonian consists only on two sets of eigenenergies whose eigenfuntions have average velocities which are strictly positive/negative, uniformly with respect to the size of the system. Our result gives a well defined meaning to the notion of edge states for a finite cylinder with two boundaries, and extends previous studies on systems with only one boundary. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598642]

I. INTRODUCTION

In this paper we investigate spectral properties of random Hamiltonians describing the dynamics of a spinless quantum particle on a cylinder of circumference L and confined along the cylinder axis by two boundaries separated by the distance L. The particle is subject to an external homogeneous magnetic field and a weak random potential. A precise statement of the model is given in Sec. II. The physical interest of the model comes from the integral quantum Hall effect occurring in disordered two dimensional electronic systems subject to a uniform magnetic field, for example, in the interface of a heterojunction [v. Klitzing (1980), Prange (1987)]. In his treatment of this effect, Halperin (1982) pointed out the fundamental role played by edge states carrying boundary diamagnetic currents, and it is therefore important to understand the spectral properties of finite but macroscopic quantum Hall samples with boundaries. A short review of the spectral properties of finite quantum Hall systems can be found in Ferrari (2001).

Random Landau Hamiltonians on an infinite plane have been analyzed in the last decade [Dorlas (1995), Dorlas (1996), Combes (1996), Barbaroux (1997), Wang (1997), Dorlas (1997), Dorlas (1999), and Germinet (2002)].

The study of random magnetic Hamiltonians with boundaries is more recent and, before we address the case of a (finite) cylinder, we wish to briefly discuss a few existing results. The case of a semi-infinite plane with one planar boundary, modeled by a smooth confining potential U or a Dirichlet condition at $x=0$, is satisfactorily understood. In this case it is proven that the spectrum of the Hamiltonian $H_\omega^e = H_0 + U + V_\omega$, H_0 being the Landau Hamiltonian for a uniform magnetic field B and V_ω an Anderson-type random potential, has absolutely continuous components inside the complement of Landau bands, for $\|V_\omega\|_\infty \ll B$ [Fröhlich (2000), de Bièvre (1999), and Macris (1999)]. The proof of this statement is essentially based on Mourre theory with conjugate operator y. The positivity of $i[H_\omega^e, y]$ in suitable spectral subspaces of H_ω^e leads to the absolutely continuous nature of the spectrum. Since this commutator is equal to the velocity v_y this means that states in the corresponding spectral subspaces propagate in the y-direction along the edge with positive velocity.

For the case of an infinite strip with two boundaries, separated by a distance L, few results are

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known. For a general (random) potential we expect that there is no absolutely continuous component in the spectrum, because the impurities may induce a tunneling (or backscattering) between the two boundaries and thus propagating edge states along each boundary cannot persist for an infinite time. In Combes (2002), the authors have shown that such states survive, for a finite time related to the quantum tunneling time between the two edges. In Exner (2001), the authors consider a parabolic channel in the y-direction. They show that if the perturbation V is periodic, or if V is small enough and decays fast enough in the y-direction, then the absolutely continuous spectrum survives in certain intervals, but their analysis does not cover true Anderson like potentials.

In this work, as in our previous work [Ferrari (2002)], we address the case of a macroscopic finite systems with two confining walls separated by a distance L along the x-direction and with the y-direction of length L made periodic (i.e., the geometry is that of a cylinder). The *left* (resp., *right*) *walls* are modeled by a smooth confining potential U_ℓ (resp., U_r) separated by a distance L, and the *bulk* between them contains impurities modeled by a random Anderson-like potential V_ω. Although the spectrum consists of discrete isolated eigenvalues, we show that there is a well defined notion of edge states associated to each boundary.

Let us explain our main new result expressed in Theorem 1 and compare it with that of Ferrari (2002). We show that, with large probability, the spectrum of the random Hamiltonian,

$$H_\omega = H_0 + V_\omega + U_\ell + U_r,$$

in an energy interval $\Delta \subset (\frac{1}{2}B + \|V_\omega\|_\infty, \frac{3}{2}B - \|V_\omega\|_\infty)$ consists in the union of two sets Σ_ℓ and Σ_r, which are small perturbations of the spectra $\sigma(H_0 + U_\ell + V_\omega^\ell)$ and $\sigma(H_0 + U_r + V_\omega^r)$, of the two edge random Hamiltonians (see Sec. II for their precise definition). The eigenvalues in Σ_ℓ and Σ_r are characterized by their average velocity along the periodic direction $J_E = (\psi_E, v_y \psi_E)$: the eigenfunctions corresponding to the eigenvalues in Σ_ℓ (resp., Σ_r) have a uniformly, negative (resp., positive) velocity, with respect to L. These are the so-called edge states and from the constructions in the proofs it is possible to see that the eigenvalues in Σ_ℓ (resp., Σ_r) correspond to eigenfunctions localized in the x-direction near the left (resp., right) boundary. The number of eigenvalues in Σ_ℓ and Σ_r is of order $O(L)$.

We briefly comment about our paper [Ferrari (2002)] where energies inside the Landau bands are considered. We proved that with large probability, for a similar model (where no disorder is present in a thin strip along the boundaries) the spectrum of H_ω in $\Delta_\varepsilon = [\frac{1}{2}B + \varepsilon, \frac{1}{2}B + V_0]$ is given by $\Sigma_\ell \cup \Sigma_b \cup \Sigma_r$. The eigenfunctions corresponding to the eigenvalues in $\Sigma_\ell \cup \Sigma_r$ have strictly positive/negative velocity, and Σ_b is intermixed in between $\Sigma_\ell \cup \Sigma_r$ and the corresponding eigenfunctions have an infinitesimal velocity of order $O(e^{-B(\log L)^2})$. The number of eigenvalues in Σ_ℓ and Σ_r is $O(L)$ while that in Σ_b is $O(L^2)$.

Although our analysis is presented for a sample of size $L \times L$ the same results can be straightforwardly extended to all geometries where the two boundaries are separated by any distance D at least $O(\ln L)$ (assuming the length of the periodic direction is fixed to L) [Ferrari (2003)]. For distances $D = O(1)$ our analysis does not hold, a fact which is consistent with Combes (2002). In fact, we expect that by using the results in the present paper one could prove that a wave packet localized on the left boundary and with appropriate energy, will propagate along the left boundary up to a finite tunneling time and, then, backscatter and propagate along the right boundary and so forth. The tunneling time is set by V_ω and the distance D between the two boundaries. Thus, if $D = O(1)$ with respect to L, this tunneling time is also $O(1)$, and always remains much smaller than $O(L)$ which is the time needed for a ballistic flight around the whole periodic direction y. In Combes (2002) the randomness of the potential is not needed. We suspect that this may also be the case in the present problem, but in order to study the nonrandom situation one should appeal to other arguments not relying on the Wegner estimate.

The paper is organized as follows. In Sec. II we present the precise definition of the model and state the main theorem. Section III is concerned with the main mathematical tools used in our

analysis: a Wegner estimate and a decoupling scheme of the cylinder into two semi-infinite ones. The proof of the main theorem is then completed in Sec. IV. Some useful estimates and more technical material are collected in the Appendixes.

II. THE MODEL AND MAIN RESULT

We study the spectral properties of the family of random Hamiltonians,

$$H_\omega = H_0 + U_\ell + U_r + V_\omega, \quad \omega \in \Omega_\Lambda, \tag{2.1}$$

acting in the Hilbert space $L^2(\mathbb{R}\times[-L/2, L/2])$ with periodic boundary conditions along y: $\psi(x,-L/2)=\psi(x,L/2)$. The Hamiltonians H_ω, and all the Hamiltonians defined below, are densely defined self-adjoint operators.

We choose the Landau gauge in which the kinetic part has the form $H_0=\frac{1}{2}p_x^2+\frac{1}{2}(p_y-Bx)^2$ with a spectrum given by the Landau levels: $\sigma(H_0)=\{(n+\frac{1}{2})B; n\in\mathbb{N}\}$. The potentials U_ℓ and U_r representing the confinement along the x-direction at $x=\pm L/2$ are independent of y and are supposed strictly monotonic, twice differentiable and satisfy

$$c_1\left|x+\frac{L}{2}\right|^{m_1} \leqslant U_\ell(x) \leqslant c_2\left|x+\frac{L}{2}\right|^{m_2}, \quad \text{for } x\leqslant -\frac{L}{2}, \tag{2.2}$$

$$c_1\left|x-\frac{L}{2}\right|^{m_1} \leqslant U_r(x) \leqslant c_2\left|x-\frac{L}{2}\right|^{m_2}, \quad \text{for } x\geqslant \frac{L}{2}, \tag{2.3}$$

for some constants $0<c_1<c_2$, $2\leqslant m_1<m_2<\infty$ and $U_\ell(x)=0$ for $x\geqslant -L/2$, $U_r(x)=0$ for $x\leqslant L/2$. The random potential V_ω is given by the sum of local perturbations located at the sites of a finite lattice $\Lambda=\{(n,m)\in\mathbb{Z}^2; n\in[-L/2, L/2], m\in[-L/2, L/2]\}$. Let $V\geqslant 0$, with $V\in C^2$, $\|V\|_\infty\leqslant V_0$, $\mathrm{supp}V\subset\mathbb{B}(\mathbf{0},\frac{1}{4})$ (the open ball centered at (0,0) of radius $\frac{1}{4}$) and $X_{n,m}$ i.i.d. random variables with common bounded density $h\in C^2([-1,1])$ representing the random strength of each local perturbation. Then V_ω has the form

$$V_\omega(x,y)=\sum_{(n,m)\in\Lambda} X_{n,m}(\omega)V(x-n,y-m). \tag{2.4}$$

We denote by $\mathbb{P}_\Lambda$ the product measure defined on the set of all possible realizations $\Omega_\Lambda=[-1,1]^\Lambda$. Clearly for each realization $\omega\in\Omega_\Lambda$ we have $\|V_\omega\|\leqslant V_0$ and we suppose $V_0\ll B$.

For future use we collect some properties of three simpler random Hamiltonians. Let us first consider the pure edge Hamiltonians,

$$H_\alpha^0 = H_0 + U_\alpha, \quad \alpha=\ell, r. \tag{2.5}$$

In the half-plane case studied in Macris (1999) [H_α^0 acting in $L^2(\mathbb{R}^2)$ with U_α a confining wall at $x=0$] we deduce, from translation invariance along y, that the spectrum consists of analytic and monotone decreasing (resp., increasing) branches $\varepsilon_n^\ell(k)$ [resp., $\varepsilon_n^r(k)$] where $k\in\mathbb{R}$ is the quantum number associated to p_y. One has $\lim_{k\to+\infty}\varepsilon_n^\ell(k)=\lim_{k\to-\infty}\varepsilon_n^r(k)=(n+\frac{1}{2})B$ and $\lim_{k\to-\infty}\varepsilon_n^\ell(k)=\lim_{k\to+\infty}\varepsilon_n^r(k)=+\infty$. For the present case (2.5) because of periodic boundary conditions along y the quantum number k takes discrete values $2\pi m/L$, $m\in\mathbb{Z}$. For L finite the spectrum consists of discrete eigenvalues $E_{n,m}^\alpha=\varepsilon_n^\alpha(2\pi m/L)$ on the spectral branches. Moreover from the mean value theorem we deduce

$$|E^{\alpha}_{0,m+1}-E^{\alpha}_{0,m}|\geqslant \frac{C_0}{L}, \quad \alpha=\ell,r, \tag{2.6}$$

for each m such that $E^{\alpha}_{0,m}\in\Delta_{\varepsilon}=(\frac{1}{2}B+V_0+\varepsilon,\frac{3}{2}B-V_0-\varepsilon)$, where $C_0>0$ is independent of m and depends only on the spectral branch ε^{α}_0.

We will suppose that the following hypothesis is fulfilled.

Hypothesis 1: *There exists L_0 and $d_0>0$ such that for all $L>L_0$,*

$$\mathrm{dist}(\sigma(H^0_{\ell})\cap\Delta_{\varepsilon},\sigma(H^0_r)\cap\Delta_{\varepsilon})\geqslant \frac{d_0}{L}. \tag{2.7}$$

In order to fulfill this hypothesis one must take nonsymmetric boundary potentials U_{ℓ} and U_r. We expect that in fact our result still holds for $U_{\ell}(x)=U_r(-x)$ because physically the random potential V_{ω} removes with high probability any degeneracy, but in order to control this case one should improve the Wegner estimate in Sec. III. In Appendix C we give an example for a situation where this hypothesis is satisfied.

We will make use of the random edge Hamiltonians,

$$H_{\alpha}=H_0+U_{\alpha}+V^{\alpha}_{\omega}, \tag{2.8}$$

where $V^{\alpha}_{\omega}=V_{\omega}|_{\Lambda_{\alpha}}$ with $\Lambda_r=\{(n,m)\in\mathbb{Z}^2;n\in[L/2-3D/4-1,L/2],m\in[-L/2,L/2]\}$ and $\Lambda_{\ell}=\{(n,m)\in\mathbb{Z}^2;n\in[-L/2,-L/2+3D/4+1],m\in[-L/2,L/2]\}$, where $D=\sqrt{L}$. This choice of D turns out to be convenient in the next sections, but (2.9) and (2.10) below are still true for $D=O(L)$.

Since the perturbation has compact support and the essential spectrum of H^0_{α} is given by the Landau levels, the spectrum of H_{α} is discrete with the Landau levels as only accumulation points. We denote it by $\sigma(H_{\alpha})=\{E^{\alpha}_{\kappa}\}$. One can prove [Macris (2003)] that, for each $\omega\in\Omega_{\Lambda_{\alpha}}=[-1,1]^{\Lambda_{\alpha}}$ (the restriction of the configurations ω to the sublattice Λ_{α}) and for each κ such that $E^{\alpha}_{\kappa}\in\Delta=(B-\delta,B+\delta)\subset\Delta_{\varepsilon}$, for L large enough and V_0/B small but independent of L, the distance between two consecutive eigenvalues satisfies

$$|E^{\alpha}_{\kappa+1}-E^{\alpha}_{\kappa}|\geqslant \frac{C}{L}, \quad \alpha=\ell,r, \tag{2.9}$$

where $C>0$ is uniform in κ, ω. Moreover for each $E^{\ell}_{\kappa}\in\Delta$ (resp., $E^{r}_{\kappa}\in\Delta$) the average velocity associated to the corresponding eigenfunctions is strictly negative (resp., positive) uniformly in L,

$$|J_{E^{\alpha}_{\kappa}}|\geqslant C'>0, \quad \alpha=\ell,r. \tag{2.10}$$

The constant C' is estimated in Appendix B (B17) in terms of the parameters of the model.

Finally we remark that the Hamiltonian $H_0+V_{\omega}|_{\tilde{\Lambda}}$ ($\tilde{\Lambda}\subset\Lambda$) has a point spectrum contained in Landau bands (since $V_{\omega}|_{\tilde{\Lambda}}$ has bounded support and $\|V_{\omega}|_{\tilde{\Lambda}}\|=V_0$),

$$\sigma(H_0+V_{\omega}|_{\tilde{\Lambda}})\subset\bigcup_{n\geqslant 0}[(n+\tfrac{1}{2})B-V_0,(n+\tfrac{1}{2})B+V_0]. \tag{2.11}$$

When $\tilde{\Lambda}$ is given by

$$\Lambda_b\equiv\tilde{\Lambda}=\left\{(n,m)\in\mathbb{Z}^2;n\in\left[-\frac{L}{2}+\left(\frac{D}{4}-1\right),\frac{L}{2}-\left(\frac{D}{4}-1\right)\right],m\in\left[-\frac{L}{2},\frac{L}{2}\right]\right\},$$

we call the Hamiltonian $H_b\equiv H_0+V_{\omega}|_{\Lambda_b}$ the bulk Hamiltonian.

We now state the main result of this paper.

Theorem 1: *Let V_0 small enough, fix $\varepsilon>0$ and let $0<\delta<B/2-V_0-\varepsilon$. Suppose that $(H1)$ hold. Then there exists $\mu>0$, $\overline{L}$ such that if $L>\overline{L}$ one can find a set $\hat{\Omega}\subset\Omega_\Lambda$ of realizations of the random potential V_ω with $\mathbb{P}_\Lambda(\hat{\Omega})\geqslant 1-L^{-\nu}$ $(\nu\gg 1)$ such that for all $\omega\in\hat{\Omega}$ the spectrum of H_ω in $\Delta=(B-\delta,B+\delta)$ is the union of two sets Σ_ℓ and Σ_r with the following properties:*

(a) *$\mathcal{E}_\kappa^\alpha\in\Sigma_\alpha(\alpha=\ell,r)$ are a small perturbation of $E_\kappa^\alpha\in\sigma(H_\alpha)\cap\Delta$ with*

$$|\mathcal{E}_\kappa^\alpha-E_\kappa^\alpha|\leqslant e^{-\mu\sqrt{B}\sqrt{L}}. \tag{2.12}$$

(b) *For $\mathcal{E}_\kappa^\alpha\in\Sigma_\alpha$ the average velocity $J_{\mathcal{E}_\kappa^\alpha}$ of the associated eigenstate satisfies*

$$|J_{\mathcal{E}_\kappa^\alpha}-J_{E_\kappa^\alpha}|\leqslant e^{-\mu\sqrt{B}\sqrt{L}}. \tag{2.13}$$

That is, the eigenfunctions associated to the eigenvalues (of H_ω) *in Δ have an $\mathcal{O}(1)$ velocity.*

The main tools for the proof of Theorem 1 are developed in Sec. III. Basically they consist of a Wegner estimate for the random Hamiltonians H_α $(\alpha=\ell,r)$ and a decoupling scheme that links the resolvent of the full Hamiltonian H_ω with those of H_ℓ, H_r and H_b. In Sec. IV we prove two propositions that lead to parts (a) and (b) of Theorem 1. Finally in Appendix A we prove some technical results; in Appendix B we prove (2.10) and in Appendix C we discuss the Hypothesis 1.

Let $\mathbf{x},\mathbf{x}'\in\mathbb{R}\times[-L/2,L/2]$, then one can check that

$$|\mathbf{x}-\mathbf{x}'|_\star\equiv\inf_{n\in\mathbb{Z}}\sqrt{(x-x')^2+(y-y'-nL)^2} \tag{2.14}$$

has the properties of a distance on $\mathbb{R}\times\mathbb{S}_L$ ($\mathbb{S}_L$ being the circle of circumference L) and that it is related to the Euclidian distance $|\mathbf{x}-\mathbf{x}'|\equiv\sqrt{(x-x')^2+(y-y')^2}$ by

$$|\mathbf{x}-\mathbf{x}'|_\star\leqslant|\mathbf{x}-\mathbf{x}'|. \tag{2.15}$$

The interest of $|\cdot|_\star$ is that, since we are working with a cylindrical geometry, all decay estimates are naturally expressed in terms of this distance. In particular, it permits us to express in a convenient way decay in the y-direction that occurs on a scale much smaller than L.

III. WEGNER ESTIMATES AND DECOUPLING SCHEME

We first give a Wegner estimate for the Hamiltonians H_α $(\alpha=\ell,r)$. Denote by $P_{0,m}^\alpha$ the projector of H_α^0 onto the eigenvalue $E_{0,m}^\alpha$ and by $P_\alpha(I)$ the projector of H_α on an interval I. Let $I_m=(E_{0,m-1}^\alpha+\delta_0,E_{0,m}^\alpha-\delta_0)$ and $\Delta_\alpha=\cup_{m_0\leqslant m\leqslant m_1}I_m$, for some $-\infty\ll m_0<m_1\ll\infty$ and $\delta_0\ll C_0/L$, where C_0 is the constant defined in (2.6). The local potentials $V(x-n,y-m)$ will also be denoted by $V_\mathbf{i}$, $\mathbf{i}=(m,n)\in\Lambda$.

Proposition 1: Let $V_0=\|V_\omega\|$ sufficiently small with respect to B, $E\in\Delta_\alpha\cap\Delta_\varepsilon$ and $I=[E-\overline{\delta},E+\overline{\delta}]\subset I_m$. Then

$$\mathbb{P}_{\Lambda_\alpha}\{\mathrm{dist}(\sigma(H_\alpha),E)<\overline{\delta}\}\leqslant\|h\|_\infty\overline{\delta}\,\mathrm{dist}(I,E_{0,\overline{m}}^\alpha)^{-2}V_0^2L^4, \tag{3.1}$$

where $E_{0\overline{m}}^\alpha$ is the closest eigenvalue of $\sigma(H_\alpha^0)$ to the interval I.

Proof: We first observe that $V_\mathbf{i}^{1/2}P_{0,m}^\alpha V_\mathbf{j}^{1/2}$ is trace class. Indeed, using $\|AB\|_i\leqslant\|A\|\|B\|_i$ $(i=1,2)$ and $\|AB\|_1\leqslant\|A\|_2\|B\|_2$ we get $\|V_\mathbf{i}^{1/2}P_{0,m}^\alpha V_\mathbf{j}^{1/2}\|_1\leqslant\|V_\mathbf{i}^{1/2}P_{0,m}^\alpha\|_2\|P_{0,m}^\alpha V_\mathbf{j}^{1/2}\|_2\leqslant V_0\|P_{0,m}^\alpha\|_1^2\leqslant V_0$.

We have $E \in \Delta_\alpha \cap \Delta_\varepsilon$, and $I=[E-\overline{\delta},E+\overline{\delta}]$ for $\overline{\delta}$ small enough (we require that $I \subset \Delta_\alpha \cap \Delta_\varepsilon$). By the Chebyshev inequality we have

$$\mathbb{P}_{\Lambda_\alpha}\{\mathrm{dist}(\sigma(H_\alpha),E)<\overline{\delta}\}=\mathbb{P}_{\Lambda_\alpha}\{\mathrm{Tr}P_\alpha(I)\geqslant 1\}\leqslant \mathbb{E}_{\Lambda_\alpha}\{\mathrm{Tr}P_\alpha(I)\}, \tag{3.2}$$

where $\mathbb{E}_{\Lambda_\alpha}$ is the expectation with respect to the random variables in Λ_α.

We first give an estimate on $\mathrm{Tr}P_\alpha(I)$. Let $E^\alpha_{0,\overline{m}}$ the closest eigenvalue of $\sigma(H^0_\alpha)$ to I and m_i $(i=0,1)$ s.t. $\mathrm{dist}(E^\alpha_{0,\overline{m}},E^\alpha_{0,m_i})=\mathcal{O}(B)$. Let also $P^\alpha_>=\Sigma_{m>m_1}P^\alpha_{0,m}$ and $P^\alpha_<=\Sigma_{m<m_0}P^\alpha_{0,m}$.

Using $P^\alpha_>(H^0_\alpha-E)P^\alpha_>\geqslant 0$ and $P^\alpha_>R^0_\alpha(E)P^\alpha_>\leqslant \mathrm{dist}(E^\alpha_{0,m_1+1},E)^{-1}P^\alpha_>$ we can write

$$\begin{aligned} P_\alpha(I)P^\alpha_>P_\alpha(I)&=P_\alpha(I)P^\alpha_>(H^0_\alpha-E)^{1/2}R^0_\alpha(E)(H^0_\alpha-E)^{1/2}P^\alpha_>P_\alpha(I)\\ &\leqslant \mathrm{dist}(E^\alpha_{0,m_1+1},E)^{-1}[P_\alpha(I)(H_\alpha-E)P^\alpha_>P_\alpha(I)-P_\alpha(I)V^\alpha_\omega P^\alpha_>P_\alpha(I)], \end{aligned} \tag{3.3}$$

and thus

$$\|P_\alpha(I)P^\alpha_>P_\alpha(I)\|\leqslant \mathrm{dist}(E^\alpha_{0,m_1+1},E)^{-1}\left(\frac{|I|}{2}+V_0\right)\leqslant\frac{1}{4}, \tag{3.4}$$

if, as we can suppose, V_0 is sufficiently small $[\mathrm{dist}(E^\alpha_{0,m_1+1},E)^{-1}V_0=\mathcal{O}(V_0/B)]$. In a similar way we get

$$\|P_\alpha(I)P^\alpha_<P_\alpha(I)\|\leqslant \mathrm{dist}(E^\alpha_{0,m_0-1},E)^{-1}\left(\frac{|I|}{2}+V_0\right)\leqslant\frac{1}{4}. \tag{3.5}$$

Now

$$\mathrm{Tr}\ P_\alpha(I)P^\alpha_<=\mathrm{Tr}\ P_\alpha(I)P^\alpha_<P_\alpha(I)\leqslant\|P_\alpha(I)P^\alpha_<P_\alpha(I)\|\mathrm{Tr}\ P_\alpha(I), \tag{3.6}$$

and similarly for $\mathrm{Tr}P_\alpha(I)P^\alpha_>$. Therefore, using $1=P^\alpha_<+P^\alpha_>+\Sigma_{m_0\leqslant m\leqslant m_1}P^\alpha_{0,m}$, together with (3.4) and (3.5), we obtain

$$\mathrm{Tr}\ P_\alpha(I)\leqslant 2\sum_{m_0\leqslant m\leqslant m_1}\mathrm{Tr}P_\alpha(I)P^\alpha_{0,m}P_\alpha(I). \tag{3.7}$$

Since

$$\mathrm{dist}(I,E^\alpha_{0,m})^2P_\alpha(I)^2\leqslant(P_\alpha(I)(H_\alpha-E^\alpha_{0,m})P_\alpha(I))^2, \tag{3.8}$$

and $\mathrm{dist}(I,E^\alpha_{0,m})^{-1}\leqslant\mathrm{dist}(I,E^\alpha_{0,\overline{m}})^{-1}$ for all $m_0\leqslant m\leqslant m_1$, it follows that

$$\begin{aligned} \mathrm{Tr}\ P^\alpha_{0,m}P_\alpha(I)P^\alpha_{0,m}&\leqslant\mathrm{dist}(I,E^\alpha_{0,\overline{m}})^{-2}\mathrm{Tr}(P^\alpha_{0k}P_\alpha(I)(H_\alpha-E^\alpha_{0,m})P_\alpha(I)(H_\alpha-E^\alpha_{0,m})P_\alpha(I)P^\alpha_{0,m})\\ &=\mathrm{dist}(I,E^\alpha_{0,\overline{m}})^{-2}\mathrm{Tr}(P^\alpha_{0,m}V^\alpha_\omega P_\alpha(I)V^\alpha_\omega P^\alpha_{0,m}). \end{aligned} \tag{3.9}$$

Thus, taking the expectation value in (3.7) and using that there are $\mathcal{O}(L)$ m's between m_0 and m_1, we get

$$\mathbb{E}_{\Lambda_\alpha}\{\mathrm{Tr}\ P_\alpha(I)\}\leqslant 2\cdot\mathcal{O}(L)\cdot\mathrm{dist}(I,E^\alpha_{0,\overline{m}})^{-2}\sup_{m_0\leqslant m\leqslant m_1}\mathbb{E}_{\Lambda_\alpha}\{\mathrm{Tr}(P^\alpha_{0,m}V^\alpha_\omega P_\alpha(I)V^\alpha_\omega P^\alpha_{0,m})\}. \tag{3.10}$$

It remains to estimate the expectation value on the right hand side of (3.10). Here we follow a method of Combes and Hislop (1996). Writing $V^\alpha_\omega=\Sigma_{\mathbf{i}\in\Lambda_\alpha}X_{\mathbf{i}}(\omega)V_{\mathbf{i}}$,

$$\begin{aligned}\mathrm{Tr}\ P^{\alpha}_{0,m}V^{\alpha}_{\omega}P_{\alpha}(I)V^{\alpha}_{\omega}P^{\alpha}_{0,m} &= \sum_{\mathbf{i},\mathbf{j}\in\Lambda^2_{\alpha}} X_{\mathbf{i}}(\omega)X_{\mathbf{j}}(\omega)\mathrm{Tr}\ P^{\alpha}_{0,m}V_{\mathbf{i}}P_{\alpha}(I)V_{\mathbf{j}}P^{\alpha}_{0,m}\\ &= \sum_{\mathbf{i},\mathbf{j}\in\Lambda^2_{\alpha}} X_{\mathbf{i}}(\omega)X_{\mathbf{j}}(\omega)\mathrm{Tr}V^{1/2}_{\mathbf{j}}P^{\alpha}_{0,m}V^{1/2}_{\mathbf{i}}V^{1/2}_{\mathbf{i}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}}. \end{aligned} \tag{3.11}$$

Since $V^{1/2}_{\mathbf{j}}P^{\alpha}_{0,m}V^{1/2}_{\mathbf{i}}$ is trace class, we can introduce the singular value decomposition,

$$V^{1/2}_{\mathbf{j}}P^{\alpha}_{0,m}V^{1/2}_{\mathbf{i}} = \sum_{n=0}^{\infty}\mu_n(u_n,.)v_n, \tag{3.12}$$

where $\Sigma^{\infty}_{n=0}\mu_n = \|V^{1/2}_{\mathbf{j}}P^{\alpha}_{0,m}V^{1/2}_{\mathbf{i}}\|_1$. Then

$$\begin{aligned}\mathrm{Tr}\,V^{1/2}_{\mathbf{j}}P^{\alpha}_{0k}V^{1/2}_{\mathbf{i}}V^{1/2}_{\mathbf{i}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}} &= \sum_{n=0}^{\infty}\mu_n(u_n,V^{1/2}_{\mathbf{i}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}}v_n)\\ &\leqslant \sum_{n=0}^{\infty}\mu_n(v_n,V^{1/2}_{\mathbf{j}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}}v_n)^{1/2}(u_n,V^{1/2}_{\mathbf{i}}P_{\alpha}(I)V^{1/2}_{\mathbf{i}}u_n)^{1/2}\\ &\leqslant \frac{1}{2}\sum_{n=0}^{\infty}\mu_n\{(v_n,V^{1/2}_{\mathbf{j}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}}v_n)+(u_n,V^{1/2}_{\mathbf{i}}P_{\alpha}(I)V^{1/2}_{\mathbf{i}}u_n)\}. \end{aligned} \tag{3.13}$$

An application of the spectral averaging theorem [see Combes and Hislop (1996)] shows that

$$\mathbb{E}_{\Lambda_{\alpha}}\{(v_n,V^{1/2}_{\mathbf{j}}P_{\alpha}(I)V^{1/2}_{\mathbf{j}}v_n)\}\leqslant\|h\|_{\infty}2\overline{\delta}, \tag{3.14}$$

as well as for the term with $\mathbf{j}$ replacing $\mathbf{i}$ and v_n replacing u_n. Combining (3.10), (3.13), (3.14), and (3.11) we get

$$\begin{aligned}\mathbb{E}_{\Lambda_{\alpha}}\{\mathrm{Tr}\ P_{\alpha}(I)\} &\leqslant 4\cdot\mathcal{O}(L)\cdot\|h\|_{\infty}\overline{\delta}\,\mathrm{dist}(I,E^{\alpha}_{0,\overline{m}})^{-2}V_0^2\sum_{\mathbf{i},\mathbf{j}\in\Lambda^2_{\alpha}}\|V^{1/2}_{\mathbf{j}}P^{\alpha}_{0,m}V^{1/2}_{\mathbf{i}}\|_1\\ &\leqslant 4\cdot\mathcal{O}(L)\cdot\|h\|_{\infty}\overline{\delta}\,\mathrm{dist}(I,E^{\alpha}_{0,\overline{m}})^{-2}V_0^2|\Lambda_{\alpha}|^2. \end{aligned} \tag{3.15}$$

□

We now turn to the decoupling scheme. By a decoupling formula [Bentosela (1991), Briet (1989)] the resolvent $R(z)=(z-H_{\omega})^{-1}$ can be expressed, up to a small term, as the sum of $R_{\alpha}(z)=(z-H_{\alpha})^{-1}$ $(\alpha=\ell,r)$ and $R_b(z)=(z-H_b)^{-1}$. We set $D=\sqrt{L}$ and introduce the characteristic functions

$$\tilde{J}_{\ell}(x)=\chi_{]-\infty,-L/2+D/2]}(x),\quad \tilde{J}_b(x)=\chi_{[-L/2+D/2,L/2-D/2]}(x),$$

$$\tilde{J}_r(x)=\chi_{[L/2-D/2,+\infty[}(x). \tag{3.16}$$

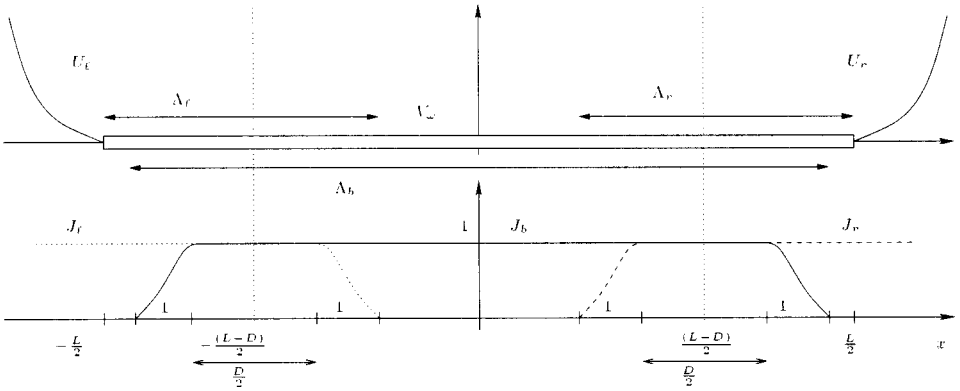

FIG. 1. The system of decoupling functions J_i ($i \in \mathcal{I}$).

We will also use three bounded $C^\infty(\mathbb{R})$ functions $|J_i(x)| \leqslant 1$, $i \in \mathcal{I} \equiv \{\ell, b, r\}$ (see Fig. 1), with bounded first and second derivatives $\sup_x |\partial_x^n J_i(x)| \leqslant 2$, $n = 1,2$, and such that

$$J_\ell(x) = \begin{cases} 1 & \text{if } x \leqslant -\dfrac{L}{2} + \dfrac{3D}{4}, \\ 0 & \text{if } x \geqslant -\dfrac{L}{2} + \dfrac{3D}{4} + 1, \end{cases} \qquad J_b(x) = \begin{cases} 1 & \text{if } |x| \leqslant \dfrac{L}{2} - \dfrac{D}{4}, \\ 0 & \text{if } |x| \geqslant \dfrac{L}{2} - \dfrac{D}{4} + 1, \end{cases}$$

$$J_r(x) = \begin{cases} 1 & \text{if } x \geqslant \dfrac{L}{2} - \dfrac{3D}{4}, \\ 0 & \text{if } x \leqslant \dfrac{L}{2} - \dfrac{3D}{4} - 1. \end{cases} \tag{3.17}$$

For $i \in \mathcal{I}$ we have $H_\omega J_i = H_i J_i$ and the decoupling formula is [Bentosela (1991)]

$$R(z) = \left(\sum_{i \in \mathcal{I}} J_i R_i(z) \tilde{J}_i \right) (1 - \mathcal{K}(z))^{-1}, \tag{3.18}$$

where

$$\mathcal{K}(z) = \sum_{i \in \mathcal{I}} K_i(z) = \sum_{i \in \mathcal{I}} \frac{1}{2} [p_x^2, J_i] R_i(z) \tilde{J}_i. \tag{3.19}$$

The main result of this part is a lemma about $\|\mathcal{K}(z)\|$ for z such that $\operatorname{dist}(z, \sigma(H_\alpha)) \geqslant e^{-\bar{\mu}\sqrt{B}\sqrt{L}}$, for a suitable $\bar{\mu} > 0$ and $\operatorname{dist}(z, \sigma(H_b)) \geqslant \varepsilon$.

Proposition 2: Let $\varepsilon > 0$, *and* $z \in \Delta_\varepsilon$ *such that* $\operatorname{dist}(z, \sigma(H_\ell) \cup \sigma(H_r)) \geqslant e^{-\bar{\mu}\sqrt{B}\sqrt{L}}$ *with* $\bar{\mu} < 1/192$. *Then for* L *large enough there exists* $C(B, V_0, \varepsilon) > 0$ *and* $\tilde{\gamma} > 0$ *independent of* L *such that*

$$\|\mathcal{K}(z)\| \leqslant C(B, V_0, \varepsilon) e^{-\tilde{\gamma}\sqrt{B}\sqrt{L}}. \tag{3.20}$$

Proof: Computing the commutator in the definition of $K_i(z)$ we have

$$K_i(z) = -\tfrac{1}{2} (\partial_x^2 J_i) R_i(z) \tilde{J}_i - (\partial_x J_i) \partial_x R_i(z) \tilde{J}_i. \tag{3.21}$$

Then

$$\|K_b(z)\| \leqslant \tfrac{1}{2}\|(\partial_x^2 J_b)R_b(z)\widetilde{J}_b\| + \|(\partial_x J_b)\partial_x R_b(z)\widetilde{J}_b\|, \tag{3.22}$$

$$\|K_\alpha(z)\| \leqslant \tfrac{1}{2}\|(\partial_x^2 J_\alpha)R_\alpha^b(z)\widetilde{J}_\alpha\| + \tfrac{1}{2}\|(\partial_x^2 J_\alpha)R_\alpha^b(z)U_\alpha\|\,\mathrm{dist}(z,\sigma(H_\alpha))^{-1} + \|(\partial_x J_\alpha)\partial_x R_\alpha^b(z)\widetilde{J}_\alpha\| + \|(\partial_x J_\alpha)\partial_x R_\alpha^b(z)U_\alpha\|\,\mathrm{dist}(z,\sigma(H_\alpha))^{-1}, \tag{3.23}$$

where for the second term we used the second resolvent identity and where $R_\alpha^b(z)=(z-[H_0+V_\omega^\alpha])^{-1}$.

We have to estimate norms of the form $\|f\partial_x^\alpha \widetilde{R}(z)g\|$ ($\alpha=0,1$) where here $\widetilde{R}(z)$ is $R_b(z)$ or $R_\alpha^b(z)$, $f=\partial_x^m J_i$ and $g=\widetilde{J}_i$ or $g=U_\alpha$.

Using the second resolvent formula we develop $\widetilde{R}(z)$ in its Neumann series, denote $V_\omega|_{\tilde{\Lambda}} \equiv W$ ($\tilde{\Lambda}=\Lambda_b$ or Λ_α),

$$\widetilde{R}(z)=\sum_{n=0}^{\infty} R_0(z)[WR_0(z)]^n, \tag{3.24}$$

where $R_0(z)=(z-H_0)^{-1}$. The norm convergence is ensured since we are in a spectral gap, indeed

$$\|WR_0(z)\| \leqslant V_0\ \mathrm{dist}(z,\sigma(H_0))^{-1} \leqslant \frac{V_0}{V_0+\varepsilon} < 1. \tag{3.25}$$

Therefore

$$\|f\partial_x^\alpha \widetilde{R}(z)g\| \leqslant \sum_{n=1}^{\infty} \|f\partial_x^\alpha R_0(z)[WR_0(z)]^n g\|, \tag{3.26}$$

and we have to control the operator norms $\|f\partial_x^\alpha R_0(z)[WR_0(z)]^n g\|$.

For any vector $\varphi \in L^2(\mathbb{R}\times[-L/2, L/2])$ with $\|\varphi\|=1$,

$$\|f\partial_x^\alpha R_0(z)[WR_0(z)]^n g\varphi\|^2 = \int_{\mathrm{supp}\, f} |f(\mathbf{x})|^2 |(\partial_x^\alpha R_0(z)[WR_0(z)]^n g\varphi)(\mathbf{x})|^2\, \mathrm{d}\mathbf{x}. \tag{3.27}$$

For the integrand in (3.27) we have

$$\begin{aligned}\mathcal{T} &\equiv |(\partial_x^\alpha R_0(z)[WR_0(z)]^n g\varphi)(\mathbf{x})| \\ &\leqslant \int_{\mathrm{supp}\, g} \mathrm{d}\mathbf{x}' \int \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_n \\ &\quad \times |\partial_x^\alpha R_0(\mathbf{x},\mathbf{x}_1;z)||W(\mathbf{x}_1)||R_0(\mathbf{x}_1,\mathbf{x}_2;z)|\cdots|W(\mathbf{x}_n)||R_0(\mathbf{x}_n,\mathbf{x}';z)||g(\mathbf{x}')||\varphi(\mathbf{x}')|.\end{aligned} \tag{3.28}$$

Now, taking out $\|W\|_\infty$ and using Lemma 1, Appendix A, we get

$$\begin{aligned}\mathcal{T} &\leqslant \left(cB^2\frac{V_0}{V_0+\varepsilon}\right)^n \int_{\mathrm{supp}\, g} \mathrm{d}\mathbf{x}' \int \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_n \exp\Big(-\overline{\gamma}\sqrt{B}\sum_{i=0}^{n} |\mathbf{x}_i-\mathbf{x}_{i+1}|_\star\Big) \\ &\quad \times |\Phi^1(|\mathbf{x}-\mathbf{x}_1|_\star)|\cdots|\Phi^0(|\mathbf{x}_n-\mathbf{x}'|_\star)||g(\mathbf{x}')||\varphi(\mathbf{x}')|,\end{aligned} \tag{3.29}$$

where $\mathbf{x}_0=\mathbf{x}$ and $\mathbf{x}_{n+1}=\mathbf{x}'$. Splitting the exponential and making the change of variables $\mathbf{x}-\mathbf{x}_1=-\mathbf{z}_1,\ldots,\ \mathbf{x}_{n-1}-\mathbf{x}_n=-\mathbf{z}_n$, we get [with $\mathbf{x}_n=\mathbf{x}_n(\{\mathbf{z}_i\},\mathbf{x})$ and $A=cB^2[V_0/(V_0+\varepsilon)]$

$$\mathcal{T}\leqslant A^n \sup_{\mathbf{z}_1\cdots\mathbf{z}_n}\left\{\int_{\operatorname{supp} g} e^{-2/3\overline{\gamma}\sqrt{B}|\mathbf{x}-\mathbf{x}'|_\star}|g(\mathbf{x}')||\varphi(\mathbf{x}')||\Phi^0(|\mathbf{x}_n-\mathbf{x}'|_\star)|e^{-(1/3)\overline{\gamma}\sqrt{B}|\mathbf{x}_n-\mathbf{x}'|_\star}\,d\mathbf{x}'\right\}$$
$$\times\left[\int_{\mathbb{R}^2}|\Phi^1(|\mathbf{z}|)|e^{-(1/3)\overline{\gamma}\sqrt{B}|\mathbf{z}|}\,d\mathbf{z}\right]\left[\int_{\mathbb{R}^2}|\Phi^0(|\mathbf{z}|)|e^{-(1/3)\overline{\gamma}\sqrt{B}|\mathbf{z}|}\,d\mathbf{z}\right]^{n-1} \tag{3.30}$$

$$\equiv A^n \sup_{\mathbf{z}_1\cdots\mathbf{z}_n}\{\mathcal{X}\}[\mathcal{Y}][\mathcal{Z}]^{n-1}. \tag{3.31}$$

Splitting the exponential and using the Schwartz inequality we have the estimate

$$\sup_{\mathbf{z}_1\cdots\mathbf{z}_n}\mathcal{X}\leqslant \sup_{\mathbf{x}'\in\operatorname{supp} g} e^{-(1/3)\overline{\gamma}\sqrt{B}|\mathbf{x}-\mathbf{x}'|_\star}\left\{\int_{\mathbb{R}^2}|\Phi^0(|\mathbf{w}|)|^2e^{-(2/3)\overline{\gamma}\sqrt{B}|\mathbf{w}|}\,d\mathbf{w}\right\}^{1/2}$$
$$\times\left(\sup_{\mathbf{x}'\in\operatorname{supp} g} e^{-(2/3)\overline{\gamma}\sqrt{B}|x-x'|}|g(x')|^2\right)^{1/2}\|\varphi\|. \tag{3.32}$$

Now, since U_α do not grow too fast [see (2.2), (2.3)] $(\sup_{\mathbf{x}'\in\operatorname{supp} g}e^{-(2/3)\overline{\gamma}\sqrt{B}|x-x'|}|g(x')|^2)^{1/2}$ is bounded by a numerical constant. On the other hand the term $\int_{\mathbb{R}^2}|\Phi^0(|\mathbf{w}|)|^2e^{-(2/3)\overline{\gamma}\sqrt{B}|\mathbf{w}|}\,d\mathbf{w}$ is bounded by a constant depending only on B.

Moreover, the terms $\mathcal{Y}$ and $\mathcal{Z}$ are also bounded by a constant depending only on B and not on L. This leads to

$$\|f\partial_x^\alpha[R_0(z)]^n g\varphi\|\leqslant\|f\|_\infty\hat{C}(B)(\tilde{C}(B)A)^n e^{-(1/2)\overline{\gamma}\sqrt{B}D}\|\varphi\|. \tag{3.33}$$

Therefore, if V_0 is small enough the series (3.26) converges and

$$\|f\partial_x^\alpha\tilde{R}(z)g\|\leqslant\tilde{C}(B,V_0)\sqrt{L}e^{-(1/12)\overline{\gamma}\sqrt{B}D}. \tag{3.34}$$

This implies

$$\|K_b(z)\|\leqslant\varepsilon^{-1}\sqrt{L}C(B,V_0)e^{-(1/12)\overline{\gamma}\sqrt{B}\sqrt{L}}, \tag{3.35}$$

$$\|K_\alpha(z)\|\leqslant\sqrt{L}e^{\overline{\mu}\sqrt{B}\sqrt{L}}C(B,V_0)e^{-(1/12)\overline{\gamma}\sqrt{B}\sqrt{L}},\quad \alpha=\ell,r; \tag{3.36}$$

thus $\|\mathcal{K}(z)\|\leqslant C(B,V_0,\varepsilon)e^{-\tilde{\gamma}\sqrt{B}\sqrt{L}}$, where $2\tilde{\gamma}=\overline{\gamma}/12-\overline{\mu}$. Since $\overline{\gamma}=1/16$ in Lemma 1, Appendix A, we must take $\overline{\mu}<1/192$. □

We remark that in the proof above we have proved the following statement [see (3.34)] that will be useful in the next section,

$$\|(1-\tilde{J}_\alpha)\tilde{R}_b(z)g\|\leqslant\overline{C}(B,V_0,\varepsilon)e^{-\tilde{\gamma}\sqrt{B}\sqrt{L}}, \tag{3.37}$$

where $g=U_\alpha$ or $g=\chi_B$ ($B\subset\mathbb{R}\times[-L/2,L/2]$) with $\operatorname{dist}(\operatorname{supp} g,\operatorname{supp}(1-\tilde{J}_\alpha))=\mathcal{O}(D)$ and $\tilde{R}_b(z)$ a resolvent associated to a generic bulk Hamiltonian $(H_0+V_\omega|_{\tilde{\Lambda}})$.

IV. PROJECTOR ESTIMATES AND THE PROOF OF THEOREM 1

In this section we prove two propositions that lead to Theorem 1. Let $\mathcal{D}'=\{\kappa:E_\kappa^\alpha\in\Delta,\alpha=\ell,r\}$, $\operatorname{card}(\mathcal{D}')=\mathcal{O}(L)$, where $\Delta\subset\Delta_\varepsilon$ is given in Sec. II.

Proposition 3: For L large enough, with probability greater than $1-L^{-\nu}$ $(\nu\gg1)$, *we have for all* $\kappa\in\mathcal{D}'$,

$$\|P-P_\alpha(E_\kappa^\alpha)\|\leqslant e^{-\gamma\sqrt{B}\sqrt{L}}, \tag{4.1}$$

where $P_\alpha(E_\kappa^\alpha)$ is the projector associated to H_α onto E_κ^α and P is the projector associated to H_ω onto $\{z\in\mathbb{C}:|z-E_\kappa^\alpha|\leqslant e^{-\overline{\mu}\sqrt{B}\sqrt{L}}\}$.

Proof: (1) Let $\mathcal{E}=\{m:E_{0,m}^\alpha\in\Delta,\alpha=\ell,r\}$, $\mathrm{card}(\mathcal{E})=\mathcal{O}(L)$, and let

$$\hat{\Omega}_\ell=\{\omega\in\Omega_{\Lambda_\ell}:\mathrm{dist}(E_{0,m}^r,\sigma(H_\ell))\geqslant L^{-\sigma},\forall m\in\mathcal{E}\},\tag{4.2}$$

with $\sigma>11$, this set has probability

$$\mathbb{P}_{\Lambda_\ell}(\hat{\Omega}_\ell)\geqslant 1-L^{-(\sigma-8)}.\tag{4.3}$$

Indeed, for a fixed $m\in\mathcal{E}$, using Proposition 1 and $(H1)$ one gets

$$\begin{aligned}&\mathbb{P}_{\Lambda_\ell}\{\omega\in\Omega_{\Lambda_\ell}:\mathrm{dist}(E_{0,m}^r,\sigma(H_\ell))\geqslant L^{-\sigma},\ \text{for one } m\in\mathcal{E}\}\\&\quad\geqslant 1-C'(h,V_0)L^{-\sigma}L^4\left(\frac{d_0}{L}-L^{-\sigma}\right)^{-2}\geqslant 1-C(h,V_0)L^{6-\sigma}.\end{aligned}\tag{4.4}$$

For a given realization $\omega_\ell\in\hat{\Omega}_\ell$ let

$$\hat{\Omega}_r(\omega_\ell)=\{\omega\in\Omega_{\Lambda_r}:\mathrm{dist}(E_\kappa^\ell,\sigma(H_r))\geqslant L^{-3\sigma},\quad\forall\kappa\in\mathcal{D}'\},\tag{4.5}$$

this set has the probability

$$\mathbb{P}_{\Lambda_r}(\hat{\Omega}_r(\omega_\ell)|\omega_\ell)\geqslant 1-L^{-(\sigma-6)}\tag{4.6}$$

uniformly with respect to the realizations of $\hat{\Omega}_\ell$. Indeed,

$$\begin{aligned}&\mathbb{P}_{\Lambda_r}\{\omega\in\Omega_{\Lambda_r}:\mathrm{dist}(E_\kappa^\ell,\sigma(H_r))\geqslant L^{-3\sigma},\ \text{for one } \kappa\in\mathcal{D}'\}\\&\quad\geqslant 1-C'(h,V_0)L^{-3\sigma}L^4(L^{-\sigma}-L^{-3\sigma})^{-2}\geqslant 1-C(h,V_0)L^{4-\sigma}.\end{aligned}\tag{4.7}$$

It follows that the set

$$\hat{\Omega}^{(\ell)}=\{\omega=(\omega_\ell,\omega_b,\omega_r)\in\Omega:\omega_\ell\in\hat{\Omega}_\ell,\omega_b\in\Omega_b,\omega_r\in\hat{\Omega}_r(\omega_\ell)\}\tag{4.8}$$

$\Omega_b=\Omega|_{\Lambda_b\setminus(\Lambda_\ell\cup\Lambda_r)}$ has probability

$$\mathbb{P}_\Lambda(\hat{\Omega}^{(\ell)})=\mathbb{P}_{\Lambda_b}(\hat{\Omega}_b)\mathbb{E}_{\Lambda_\ell}\{\mathbb{P}_{\Lambda_r}(\hat{\Omega}_r|\omega_\ell)|\omega_\ell\in\hat{\Omega}_\ell\}\geqslant(1-L^{-(\sigma-6)})\mathbb{P}_{\Lambda_\ell}(\hat{\Omega}_\ell)\geqslant 1-L^{-(\sigma-9)}.\tag{4.9}$$

(2) We now work with a given $\omega\in\hat{\Omega}^{(\ell)}$. Take $\overline{\mu}>0$ as in Proposition 2 and L large enough such that for all $\kappa\in\mathcal{D}'$ $\Gamma_\kappa=\{z\in\mathbb{C}:|z-E_\kappa^\ell|\leqslant e^{-\overline{\mu}\sqrt{B}\sqrt{L}}\}\cap\sigma(H_r)=\varnothing$, and remark that $\mathrm{Tr}\,P_b(\Delta)=0$ (P_b the projector associated to H_b).

We need to introduce two auxiliary Hamiltonians H_1 and H_2 defined as follows:

$$H_1=H_0+V_\omega^\ell|_{\Lambda_1},\tag{4.10}$$

$$H_2=H_0+V_\omega^\ell|_{\Lambda_2}+U_\ell,\tag{4.11}$$

where $\Lambda_2=\{(n,m)\in\mathbb{Z}^2;n\in[-L/2,-L/2+(D/4-1)],m\in[-L/2,L/2]\}$, and $\Lambda_1=\Lambda_\ell\setminus\Lambda_2$, of course, $H_\ell=H_2+V_\omega^\ell|_{\Lambda_1}$.

From the decoupling formula (3.18) we have

$$R(z)-R_\ell(z)=\left(\sum_{i\in\mathcal{I}} J_i R_i(z)\tilde{J}_i\right)\left(\sum_{n=1}^{\infty}\mathcal{K}(z)^n\right)-(1-J_\ell)R_\ell(z)$$
$$-J_\ell R_\ell(z)(1-\tilde{J}_\ell)+J_b R_b(z)\tilde{J}_b+J_r R_r(z)\tilde{J}_r, \tag{4.12}$$

integrating over $\partial\Gamma_\kappa$ and taking the operator norm we get

$$\|P-P_\ell(E_\kappa^\ell)\|\leqslant e^{-\bar{\mu}\sqrt{B}\sqrt{L}}\left(\sum_{i\in\mathcal{I}}\sup_{z\in\partial\Gamma_\kappa}\|R_i(z)\|\right)\frac{\sup_{z\in\partial\Gamma_\kappa}\|\mathcal{K}(z)\|}{1-\sup_{z\in\partial\Gamma_\kappa}\|\mathcal{K}(z)\|}+\|(1-J_\ell)P_\ell(E_\kappa^\ell)\|$$
$$+\|J_\ell P_\ell(E_\kappa^\ell)(1-\tilde{J}_\ell)\|=a+b+c. \tag{4.13}$$

For the first term we note that for L large enough $e^{-\bar{\mu}\sqrt{B}\sqrt{L}}\sup_{z\in\partial\Gamma_\kappa}\|R_i(z)\|\leqslant 1$ $(i\in\mathcal{I})$. Indeed, for $i=\ell$ we have $\sup_{z\in\partial\Gamma_\kappa}\|R_\ell(z)\|=e^{\bar{\mu}\sqrt{B}\sqrt{L}}$ by construction, for $i=b$ we have $\sup_{z\in\partial\Gamma_\kappa}\|R_b(z)\|=\varepsilon^{-1}$ and for $i=r$ $\sup_{z\in\partial\Gamma_\kappa}\|R_r(z)\|=(L^{-3\sigma}-e^{-\bar{\mu}\sqrt{B}\sqrt{L}})^{-1}$. Then, applying Proposition 2 we get

$$a\leqslant 2C(B,V_0,\varepsilon)e^{-\tilde{\gamma}\sqrt{B}\sqrt{L}}. \tag{4.14}$$

For the second and third terms we first observe that by the second resolvent formula,

$$\frac{P_\ell(E_\kappa^\ell)}{(z-E_\kappa^\ell)}=(z-H_1)^{-1}P_\ell(E_\kappa^\ell)+(z-H_1)^{-1}[V_\omega^\ell|_{\Lambda_2}+U_\ell]\frac{P_\ell(E_\kappa^\ell)}{(z-E_\kappa^\ell)}, \tag{4.15}$$

and integrating (4.15) along $\partial\Gamma_\kappa$ we obtain [using $\sigma(H_1)\cap\Delta_\varepsilon=\varnothing$]

$$P_\ell(E_\kappa^\ell)=R_1(E_\kappa^\ell)[V_\omega^\ell|_{\Lambda_2}+U_\ell]P_\ell(E_\kappa^\ell) \tag{4.16}$$
$$=P_\ell(E_\kappa^\ell)[V_\omega^\ell|_{\Lambda_2}+U_\ell]R_1(E_\kappa^\ell). \tag{4.17}$$

Therefore, using (4.16) for b and (4.17) for c we get

$$b\leqslant\|(1-J_\ell)R_1(E_\kappa^\ell)[V_\omega^\ell|_{\Lambda_2}+U_\ell]\|\leqslant\|(1-\tilde{J}_\ell)R_1(E_\kappa^\ell)[V_\omega^\ell|_{\Lambda_2}+U_\ell]\|, \tag{4.18}$$

$$c\leqslant\|(1-\tilde{J}_\ell)R_1(E_\kappa^\ell)[V_\omega^\ell|_{\Lambda_2}+U_\ell]\|. \tag{4.19}$$

Using (3.37) we get

$$b+c\leqslant 2(V_0L^2\|(1-\tilde{J}_\ell)R_1(E_\kappa^\ell)\chi_{\Lambda_2}\|+\|(1-\tilde{J}_\ell)R_1(E_\kappa^\ell)U_\ell\|)\leqslant 2\bar{C}(B,V_0,\varepsilon)L^2e^{-\tilde{\gamma}\sqrt{B}\sqrt{L}}. \tag{4.20}$$

Thus

$$\|P-P_\ell(E_\kappa^\ell)\|\leqslant e^{-\gamma\sqrt{B}\sqrt{L}}. \tag{4.21}$$

By repeating the above proof in a symmetrical way we get for ω in a set $\hat{\Omega}^{(r)}$ similar to $\hat{\Omega}^{(\ell)}$,

$$\|P-P_r(E_\kappa^r)\|\leqslant e^{-\gamma\sqrt{B}\sqrt{L}}. \tag{4.22}$$

Finally we have both (4.21) and (4.22) for $\omega\in\hat{\Omega}=\hat{\Omega}^{(\ell)}\cap\hat{\Omega}^{(r)}$ with $\mathbb{P}_\Lambda\geqslant 1-L^{-\nu}$, $\nu=\sigma-10$. Note that we can take $\nu'\gg 1$ by taking $\sigma\gg 11$. □

The estimate on the norm difference of the projectors implies that their dimensions are the same and that $\mathcal{E}_\kappa^\alpha\in\sigma(H_\omega)$ is a small perturbation of E_κ^α: this gives part (a) of Theorem 1.

Proposition 4: Let $\omega \in \hat{\Omega}$. Then there exists $\hat{\mu} > 0$ such that the velocity associated to each eigenvalue $\mathcal{E}_\kappa^\alpha$ of H_ω in Δ satisfies

$$|J_{\mathcal{E}_\kappa^\alpha} - J_{E_\kappa^\alpha}| \leq e^{-\hat{\mu}\sqrt{B}\sqrt{L}}. \tag{4.23}$$

Proof: Let $J_{\mathcal{E}_\kappa^\alpha} = \mathrm{Tr}\, v_y P(\mathcal{E}_\kappa^\alpha)$ the average velocity associated to the eigenvalue $\mathcal{E}_\kappa^\alpha \in \sigma(H_\omega)$ and $J_{E_\kappa^\alpha} = \mathrm{Tr}\, v_y P_\alpha(E_\kappa^\alpha)$ that associated to the eigenvalue E_κ^α of H_α. First we observe that $v_y P(\mathcal{E}_\kappa^\alpha)$ is trace class. Indeed, $v_y P(\mathcal{E}_\kappa^\alpha) = v_y P(\mathcal{E}_\kappa^\alpha) P(\mathcal{E}_\kappa^\alpha)$ with $v_y P(\mathcal{E}_\kappa^\alpha)$ bounded and $\|P(\mathcal{E}_\kappa^\alpha)\|_1 = \mathrm{Tr}\, P(\mathcal{E}_\kappa^\alpha) = \mathrm{Tr}\, P_\alpha(E_\kappa^\alpha) = 1$:

$$\|v_y P(\mathcal{E}_\kappa^\alpha)\|_1^2 \leq \|v_y P(\mathcal{E}_\kappa^\alpha)\|^2 \leq \|P(\mathcal{E}_\kappa^\alpha) v_y^2 P(\mathcal{E}_\kappa^\alpha)\| \leq 2\|P(\mathcal{E}_\kappa^\alpha)(H_\omega - V_\omega) P(\mathcal{E}_\kappa^\alpha)\| \leq (3B + 2V_0). \tag{4.24}$$

To get the second inequality one has simply added positive terms to v_y^2. Similarly,

$$\|v_y P_\alpha(E_\kappa^\alpha)\|_1^2 \leq (3B + 2V_0). \tag{4.25}$$

With the help of the identity

$$\begin{aligned} P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha) = {} & [P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)]^2 + [P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)] P_\alpha(E_\kappa^\alpha) \\ & + P_\alpha(E_\kappa^\alpha)[P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)], \end{aligned} \tag{4.26}$$

we get

$$\begin{aligned} |J_{\mathcal{E}_\kappa^\alpha} - J_{E_\kappa^\alpha}| &= |\mathrm{Tr}\, v_y [P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)]| \\ &\leq |\mathrm{Tr}\, v_y [P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)]^2| + |\mathrm{Tr}\, v_y [P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)] P_\alpha(E_\kappa^\alpha)| \\ &\quad + |\mathrm{Tr}\, v_y P_\alpha(E_\kappa^\alpha)[P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)]|, \end{aligned} \tag{4.27}$$

and then, from (4.24) and (4.25), we get

$$\begin{aligned} |J_{\mathcal{E}_\kappa^\alpha} - J_{E_\kappa^\alpha}| &\leq 2(\|v_y P(\mathcal{E}_\kappa^\alpha)\|_1 + \|v_y P_\alpha(E_\kappa^\alpha)\|_1)\|P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)\| \\ &\leq 4(3B + 2V_0)^{1/2}\|P(\mathcal{E}_\kappa^\alpha) - P_\alpha(E_\kappa^\alpha)\|. \end{aligned} \tag{4.28}$$

Combining this last inequality with Proposition 3 we get the result. □

From Proposition 4 and the result of Appendix B given in (2.10) we obtain part (*b*) of Theorem 1.

ACKNOWLEDGMENTS

We wish to thank F. Bentosela, J. M. Combes, P. Exner, J. Fröhlich, and P. A. Martin for helpful discussions. The work of C. F. was supported by a grant from the Fonds National Suisse de la Recherche Scientifique No. 20-55654.98.

APPENDIX A: ESTIMATE OF THE GREEN'S FUNCTION $R_0(\mathbf{x},\mathbf{x}';z)$

In this appendix we give the necessary decay property of the kernel $R_0(\mathbf{x},\mathbf{x}';z)$ with periodic boundary conditions along y. The exact formula for $R_0(\mathbf{x},\mathbf{x}';z)$ can be found in Ferrari (2002). We introduce the following notation:

$$\Phi^{\alpha}(|\mathbf{x}-\mathbf{x}'|_{\star})=\begin{cases}1+\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|_{\star}^{2}\right)\right|, & \alpha=0,\\ 1+\left[\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|_{\star}^{2}\right)\right|+\left(1+\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|_{\star}^{2}\right)\right|\right)|\mathbf{x}-\mathbf{x}'|_{\star}^{-1}\right], & \alpha=1.\end{cases} \tag{A1}$$

Lemma 1: If $|\mathcal{I}m\, z|\leqslant 1$, $\mathcal{R}e\, z\in\,]\frac{1}{2}B,\frac{3}{2}B[$ *then, for* L *large enough, there exists* $C(z,B)$ *positive constant independent of* L *such that* $(\alpha=0,1)$

$$|\partial_x^{\alpha}R_0(\mathbf{x},\mathbf{x}';z)|\leqslant C'(z,B)e^{-(B/8)|\mathbf{x}-\mathbf{x}'|_{\star}^{2}}\Phi^{\alpha}(|\mathbf{x}-\mathbf{x}'|_{\star})\leqslant C(z,B)e^{-\overline{\gamma}\sqrt{B}|\mathbf{x}-\mathbf{x}'|_{\star}}\Phi^{\alpha}(|\mathbf{x}-\mathbf{x}'|_{\star}), \tag{A2}$$

where $C(z,B)=cB^{2}\mathrm{dist}(z,\sigma(H_0))^{-1}$ *with* c *a numerical positive constant and* $\overline{\gamma}=\frac{1}{16}$.

Proof: As in Ferrari (2002) we can prove that (for L large enough the logarithmic divergences appear only for $|m|\leqslant 1$ and the sum over $|m|>1$ converge)

$$|\partial_x^{\alpha}R_0(\mathbf{x},\mathbf{x}';z)|\leqslant\frac{C'(z,B)}{3}e^{-(B/8)|\mathbf{x}-\mathbf{x}'|^{2}}+\sum_{|m|\leqslant 1}|\partial_x^{\alpha}R_0^{\infty}(xy-mL,\mathbf{x}';z)|, \tag{A3}$$

with

$$|\partial_x^{\alpha}R_0^{\infty}(\mathbf{x},\mathbf{x}';z)|\leqslant\begin{cases}\frac{C'(z,B)}{3}e^{-(B/8)|\mathbf{x}-\mathbf{x}'|^{2}}\left\{1+\mathbf{1}_{\mathbb{B}(\mathbf{0},\sqrt{2B^{-1}})}(|\mathbf{x}-\mathbf{x}'|)\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|^{2}\right)\right|\right\}, & \alpha=0,\\ \frac{C'(z,B)}{3}e^{-B/8|\mathbf{x}-\mathbf{x}'|^{2}}\left\{1+\mathbf{1}_{\mathbb{B}(\mathbf{0},\sqrt{2B^{-1}})}(|\mathbf{x}-\mathbf{x}'|)\left[\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|^{2}\right)\right|\right.\right.\\ \quad\left.\left.+\left(1+\left|\ln\left(\frac{B}{2}|\mathbf{x}-\mathbf{x}'|^{2}\right)\right|\right)|\mathbf{x}-\mathbf{x}'|^{-1}\right]\right\}, & \alpha=1.\end{cases} \tag{A4}$$

Now, using $|\mathbf{x}-\mathbf{x}'|_{\star}\leqslant|\mathbf{x}-\mathbf{x}'|$, we can replace the Euclidean distance with the distance $|\cdot|_{\star}$ in all the terms on the rhs of (A3), since all these functions are decreasing. To obtain the same bound for the terms $|m|\leqslant 1$ in the sum we just drop the characteristic functions $\mathbf{1}_{\mathbb{B}(\mathbf{0},\sqrt{2B^{-1}})}$. □

APPENDIX B: AVERAGE VELOCITY OF THE EIGENSTATE ASSOCIATED TO E_{κ}^{α}

In this appendix we prove following Ferrari (1999) that the eigenstates corresponding to the eigenvalues of H_{α} $(\alpha=\ell,r)$ in a energy interval $\Delta=(B-\delta,B+\delta)\subset\Delta_{\varepsilon}$ have an average velocity that is strictly positive/negative uniformly in L, that is, if we have $H_{\alpha}\psi_{\kappa}^{\alpha}=E_{\kappa}^{\alpha}\psi_{\kappa}^{\alpha}$ then

$$|(\psi_{\kappa}^{\alpha},v_y\psi_{\kappa}^{\alpha})|\geqslant C'>0. \tag{B1}$$

From the eigenvalue equation we have

$$\|(H_{\alpha}^{0}-E_{\kappa}^{\alpha})\psi_{\kappa}^{\alpha}\|^{2}=\|V_{\omega}^{\alpha}\psi_{\kappa}^{\alpha}\|^{2}\leqslant V_0^{2}. \tag{B2}$$

We now expand ψ_{κ}^{α} on the eigenfunctions of H_{α}^{0} denoted $\{\phi_{n,m}(x,y)=(e^{iky}/\sqrt{L})\,\varphi_{nk}(x)\}_{n\in\mathbb{N},k\in(2\pi/L)\mathbb{Z}}$ where φ_{nk} is the solution on the eigenvalue problem $[\frac{1}{2}p_x^{2}+\frac{1}{2}(k-Bx)^{2}+U_{\alpha}]\varphi_{nk}=E_{nk}^{\alpha}\varphi_{nk}$:

$$\psi_{\kappa}^{\alpha}(x,y)=\sum_{n=0}^{\infty}\sum_{m\in\mathbb{Z}}\psi_n(m)\,\phi_{n,m}(x,y), \tag{B3}$$

and of course,

$$\|\psi_\kappa^\alpha\|^2=\sum_{n=0}^{\infty}\sum_{m\in\mathbb{Z}}|\psi_n(m)|^2=1. \tag{B4}$$

From (B3) the equation (B2) becomes

$$\sum_{n=0}^{\infty}\sum_{m\in\mathbb{Z}}|\psi_n(m)|^2(E_{n,m}^\alpha-E_\kappa^\alpha)^2\leqslant V_0^2, \tag{B5}$$

thus since each term in the sum is positive we have

$$\sum_{m\in\mathbb{Z}}|\psi_0(m)|^2(E_{0,m}^\alpha-E_\kappa^\alpha)^2\leqslant V_0^2. \tag{B6}$$

We remark that for $n\geqslant 1$ one has $|E_{n,m}^\alpha-E_\kappa^\alpha|\geqslant B/2-\delta$, this leads to

$$\|\psi_\star\|^2\equiv\sum_{n=1}^{\infty}\sum_{m\in\mathbb{Z}}|\psi_n(m)|^2\leqslant\frac{V_0^2}{\left(\frac{B}{2}-\delta\right)^2}. \tag{B7}$$

Let $m^\star$ such that $|E_{0,m^\star}^\alpha-E_\kappa^\alpha|$ is minimal, and for a fixed a independent of L let $\mathcal{A}=[m^\star-a,m^\star+a]$. Then from (B5),

$$\begin{aligned}V_0^2&\geqslant\sum_{m\in\mathbb{Z}}|\psi_0(m)|^2(E_{0,m}^\alpha-E_\kappa^\alpha)^2\\&\geqslant\sum_{m\in\mathcal{A}^c}|\psi_0(m)|^2(E_{0,m}^\alpha-E_\kappa^\alpha)^2\geqslant\inf_{m\in\mathcal{A}^c}(E_{0,m}^\alpha-E_\kappa^\alpha)^2\sum_{m\in\mathcal{A}^c}|\psi_0(m)|^2,\end{aligned} \tag{B8}$$

thus

$$\sum_{m\in\mathcal{A}^c}|\psi_0(m)|^2\leqslant V_0^2\sup_{m\in\mathcal{A}^c}(E_{0,m}^\alpha-E_\kappa^\alpha)^{-2}. \tag{B9}$$

From (B4) and (B7) we get

$$1\geqslant\sum_{m\in\mathbb{Z}}|\psi_0(m)|^2\geqslant 1-\frac{V_0^2}{\left(\frac{B}{2}-\delta\right)^2}. \tag{B10}$$

Combining the last equation and (B9) we get

$$\sum_{m\in\mathcal{A}}|\psi_0(m)|^2\geqslant 1-V_0^2\left[\frac{1}{\left(\frac{B}{2}-\delta\right)^2}+\sup_{m\in\mathcal{A}^c}(E_{0,m}^\alpha-E_\kappa^\alpha)^{-2}\right]. \tag{B11}$$

Decompose now ψ_κ^α as $\psi_\kappa^\alpha=\psi_0+\psi_\star$; then

$$|(\psi_\kappa^\alpha,v_y\psi_\kappa^\alpha)|\geqslant|(\psi_0,v_y\psi_0)|-|(\psi_\star,v_y\psi_\star)|-2|(\psi_\star,v_y\psi_0)|; \tag{B12}$$

the first term can be written as

$$\int_{\mathbb{R}} \mathrm{d}x \int_{-L/2}^{L/2} \mathrm{d}y \left\{ \sum_{m' \in \mathbb{Z}} \psi_0^*(m') \frac{e^{-i(2\pi m'/L)y}}{\sqrt{L}} \varphi_{0,m'}^*(x) \sum_{m \in \mathbb{Z}} \psi_0(m) v_y \frac{e^{i(2\pi m/L)y}}{\sqrt{L}} \varphi_{0,m}(x) \right\}$$

$$= \sum_{m \in \mathbb{Z}} |\psi_0(m)|^2 \int_{\mathbb{R}} \mathrm{d}x (k - Bx) |\varphi_{0,m}(x)|^2 = \sum_{m \in \mathbb{Z}} |\psi_0(m)|^2 \partial_k E_0^\alpha(k)|_{k=2\pi m/L}. \tag{B13}$$

The partial derivative of E_0^α is the average velocity $\partial_k E_0^\alpha(k)|_{k=2\pi m/L} = J_{E_{0,m}^\alpha}$; thus

$$|(\psi_0, v_y \psi_0)| \geqslant \left| \sum_{m \in \mathbb{Z}} |\psi_0(m)|^2 J_{E_{0,m}^\alpha} \right| \geqslant |J_{E_{0\overline{m}}^\alpha}| \left\{ 1 - V_0^2 \left[\frac{1}{\left(\frac{B}{2} - \delta \right)^2} + \sup_{m \in \mathcal{A}^c} (E_{0,m}^\alpha - E_\kappa^\alpha)^{-2} \right] \right\}, \tag{B14}$$

for a suitable $\overline{m} \in \mathcal{A}$, and we have $|J_{E_{0,\overline{m}}^\alpha}| > 0$. The second term can be bounded as follows: $|(\psi_\star, v_y \psi_\star)| \leqslant \|\psi_\star\| \|v_y \psi_\star\| \leqslant V_0 / B/2 - \delta \|v_y \psi_\star\|$ and

$$\begin{aligned} \|v_y \psi_\star\|^2 &= 2(\psi_\star, \tfrac{1}{2}(p_y - Bx)^2 \psi_\star) \\ &\leqslant 2(\psi_\star, [\tfrac{1}{2}p_x^2 + \tfrac{1}{2}(p_y - Bx)^2 + U_\alpha]\psi_\star) + 2(\psi_0, [\tfrac{1}{2}p_x^2 + \tfrac{1}{2}(p_y - Bx)^2 + U_\alpha]\psi_0) \\ &= 2(\psi_\kappa^\alpha, H_\alpha^0 \psi_\kappa^\alpha) = 2(\psi_\kappa^\alpha, H_\alpha \psi_\kappa^\alpha) - 2(\psi_\kappa^\alpha, V_\omega^\alpha \psi_\kappa^\alpha) \leqslant 2(E_\kappa^\alpha + V_0). \end{aligned} \tag{B15}$$

This leads to the bound

$$|(\psi_\star, v_y \psi_\star)| \leqslant \frac{V_0}{\frac{B}{2} - \delta} \sqrt{2(E_\kappa^\alpha + V_0)}. \tag{B16}$$

A similar argument gives the same bound for the third term.

Finally,

$$|(\psi_\kappa^\alpha, v_y \psi_\kappa^\alpha)| \geqslant |J_{E_{0,\overline{m}}^\alpha}| \left\{ 1 - V_0^2 \left[\frac{1}{\left(\frac{B}{2} - \delta \right)^2} + \sup_{m \in \mathcal{A}^c} (E_{0,m}^\alpha - E_\kappa^\alpha)^{-2} \right] \right\} - 3 \frac{V_0}{\frac{B}{2} - \delta} \sqrt{2(E_\kappa^\alpha + V_0)}. \tag{B17}$$

The right hand side of (B17) is greater than

$$J \left[1 - O\left(\frac{V_0^2}{B^2} \right) \right] - \sqrt{B} O\left(\frac{V_0}{B} \right), \tag{B18}$$

where the strictly positive constant J depends only on B and U_α. For a sufficiently small $V_0 > 0$ the right hand side of (B17) is strictly positive.

APPENDIX C: DISCUSSION OF HYPOTHESIS 1

In this section we indicate a way in which hypothesis $(H1)$ can be achieved explicitly. We thank Bentosela for pointing out this possibility to one of us. We take two symmetric confining walls $U_\ell(-x) = U_r(x) \equiv U(x)$ and add a magnetic flux tube of intensity $0 \leqslant \Phi \leqslant 2\pi$ along the cylinder axis. Below we check that the magnetic flux lifts the degeneracy of the levels on the two sides of the sample. In this case the pure edge Hamiltonians are

$$H_\ell^0[\Phi]=\frac{1}{2}p_x^2+\frac{1}{2}\left(p_y-Bx+\frac{\Phi}{L}\right)^2+U(-x), \tag{C1}$$

$$H_r^0[\Phi]=\frac{1}{2}p_x^2+\frac{1}{2}\left(p_y-Bx+\frac{\Phi}{L}\right)^2+U(x). \tag{C2}$$

The spectra of these Hamiltonians are

$$\sigma(H_\alpha^0[\Phi])=\{E_{n,m}^\alpha(\Phi):n\in\mathbb{N},m\in\mathbb{Z}\}, \tag{C3}$$

with $E_{n,m}^\alpha(\Phi)=\varepsilon_n^\alpha(2\pi m/L+\Phi/L)$. We consider here only the first spectral branches and note that from the symmetry of the walls, for $\Phi=0$,

$$\varepsilon_0^\ell\left(-\frac{2\pi}{L}m\right)=\varepsilon_0^r\left(\frac{2\pi}{L}m\right),\quad \forall\quad m\in\mathbb{Z}. \tag{C4}$$

We have

$$\varepsilon_0^\ell\left(-\frac{2\pi m}{L}+\frac{\Phi}{L}\right)=\varepsilon_0^\ell\left(-\frac{2\pi m}{L}\right)+\partial_k\varepsilon_0^\ell(k_\ell)\frac{\Phi}{L}, \tag{C5}$$

$$\varepsilon_0^r\left(\frac{2\pi m}{L}+\frac{\Phi}{L}\right)=\varepsilon_0^r\left(\frac{2\pi m}{L}\right)+\partial_k\varepsilon_0^r(k_r)\frac{\Phi}{L}, \tag{C6}$$

for a suitable $(2\pi/L)(-m)\leqslant k_\ell\leqslant(2\pi/L)(-m)+\Phi/L$ and $(2\pi/L)m\leqslant k_r\leqslant(2\pi/L)m+\Phi/L$. Thus

$$\left|\varepsilon_0^\ell\left(-\frac{2\pi m}{L}+\frac{\Phi}{L}\right)-\varepsilon_0^r\left(\frac{2\pi m}{L}+\frac{\Phi}{L}\right)\right|=\frac{\Phi}{L}|\partial_k\varepsilon_0^r(k_r)-\partial_k\varepsilon_0^\ell(k_\ell)|\geqslant 2\frac{\Phi}{L}|\partial_k\varepsilon_0^\ell(k_\ell)|\geqslant 2\mathcal{C}\frac{\Phi}{L}, \tag{C7}$$

where $\mathcal{C}>0$. A similar argument shows that

$$\begin{aligned}\left|\varepsilon_0^\ell\left(-\frac{2\pi(m+1)}{L}+\frac{\Phi}{L}\right)-\varepsilon_0^r\left(\frac{2\pi m}{L}+\frac{\Phi}{L}\right)\right|&=\left|\frac{\Phi}{L}[\partial_k\varepsilon_0^\ell(k_\ell)-\partial_k\varepsilon_0^r(k_r)]-\frac{2\pi}{L}\partial_k\varepsilon_0^\ell(k_\ell)\right|\\&\geqslant\left|2\frac{\Phi}{L}\left|\partial_k\varepsilon_0^\ell(k_\ell)\right|-\frac{2\pi}{L}\left|\partial_k\varepsilon_0^\ell(k_\ell)\right|\right|\geqslant 2\mathcal{C}\frac{|\Phi-\pi|}{L}.\end{aligned} \tag{C8}$$

Then, by fixing $\Phi^\star$ such that $0<\Phi^\star<\pi$ or $\pi<\Phi^\star<2\pi$ we achieve (2.7).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Wigner–Yanase information on quantum state space: The geometric approach

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(Received 10 April 2003; accepted 3 May 2003)

In the search of appropriate Riemannian metrics on quantum state space, the concept of statistical monotonicity, or contraction under coarse graining, has been proposed by Chentsov. The metrics with this property have been classified by Petz. All the elements of this family of geometries can be seen as quantum analogs of Fisher information. Although there exists a number of general theorems shedding light on this subject, many natural questions, also stemming from applications, are still open. In this paper we discuss a particular member of the family, the Wigner–Yanase information. Using a well-known approach that mimics the classical pull-back approach to Fisher information, we are able to give explicit formulas for the geodesic distance, the geodesic path, the sectional and scalar curvatures associated to Wigner–Yanase information. Moreover, we show that this is the only monotone metric for which such an approach is possible. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598279]

I. INTRODUCTION

The notion of information proposed by Fisher is fundamental in probability and statistics for a number of reasons; here we mention only the Cramer–Rao inequality and the asymptotic behavior of maximum lilkelihood estimators for exponential models (one can see Ref. 5 for unexpected features and applications of Fisher information). In classical statistics Rao was the first to point out that Fisher information can be seen as a Riemannian metric on the space of probability densities. This point of view was nicely complemented by the results of Chentsov, saying that (on the simplex of probability vectors) Fisher information is the unique Riemannian metric contracting under Markov morphisms. This can be rephrased in a more suggestive way. Markov morphisms, or positive mappings, are the mathematical counterpart of the notion of noise. Now suppose that we want to use a distance to distinguish different states (probability densities) in a statistically relevant way. Then the effect of noise must be that of contracting the metric. Chentsov theorem says therefore that in the classical case there is only one choice, the Fisher information (another argument producing Fisher information can be found in Ref. 43).

In the quantum case one deals with density operators instead of density vectors and completely positive mappings play the role of Markov morphisms. As often happens in the quantum counterpart of a classical theory, instead of a uniqueness result, one has a classification theorem, due to Petz. This result states that there is bijection between statistically monotone metrics on quantum state space and the operator monotone functions: we have therefore a rich ''garden'' of candidates for the role of Fisher information in quantum physics. Among the elements of this family of metrics one can find, in a certain sense, the most relevant Riemannian metrics appeared in the literature.[35,37]

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Despite the existence of general results for the theory[13,17,19,26,27,28,30,40,41] a number of open problems resists investigation. For example, it does not exist yet a general formula for the geodesic path and the geodesic distance associated to an arbitrary monotone metric. For the use of this kind of distances see, for example Ref. 32. Because of the absence of a general formula, inequalities (giving bounds for the geodesic distance) have been proved.[38]

In this paper we discuss the Wigner–Yanase skew information. To find the formulas for geodesic path and geodesic distance we mimic the classical approach to Fisher information via sphere geometry (one should note the importance of determining the geodesic path in the study of the 2-Wasserstein metric[6]). Indeed Wigner–Yanase information appears as the pull-back of the square root map.[18] Next we prove the formula for the scalar curvature. One proof, due to Dittmann, uses the general formula[13] and requires a long calculation. The second one just uses the pull-back approach. One should emphasize that, since the scalar curvature determines the asymptotic behavior of the volume (for a Riemannian metric) then it has also a statistical meaning in relation to the quantum analog of Jeffrey's rule for determining prior probability distributions (see Ref. 35). Finally we prove, as a corollary of the results in Refs. 25, 26, and 19 that the Wigner–Yanase information is the only monotone metric that can be seen as a pull-back metric.

The paper is organized as follows. In Sec. II we review the geometric approach to Fisher information. Sec. III one finds an introduction to the general theory of statistical monotone metrics. Sec. IV shows how the Wigner–Yanase information can be seen as a monotone Riemannian metric. In Sec. V we show that the Wigner–Yanase geometry can be seen as the sphere geometry transposed on the space of density matrices; moreover, we characterize it as the unique pull-back metric. Section VI contains some comments on the main results and on some open problems.

II. FISHER INFORMATION AND ITS GEOMETRY

The classical definition of Fisher information for an indexed family of densities p_θ is given by the variance of the score. In the case of a family indexed by only one parameter θ it is the number

$$I(\theta)=\mathrm{E}_\theta\left[\left(\frac{\partial}{\partial\theta}\log p_\theta\right)^2\right], \tag{2.1}$$

assigned to the parameter θ. For n parameters, say $\theta=(\theta^1,\ldots,\theta^n)$, it is a matrix defined on the parameter manifold given by

$$I(\theta)_{ij}=\mathrm{E}_\theta\left[\left(\frac{\partial}{\partial\theta^i}\log p_\theta\right)\left(\frac{\partial}{\partial\theta^j}\log p_\theta\right)\right]. \tag{2.2}$$

Geometrically this means that $I(\theta)$ is a symmetric bilinear form on the tangent spaces of the parameter manifold. In a coordinate free language it reads as

$$I(\theta)(U,V)=\mathrm{E}_\theta[U(\log p_\theta)\,V(\log p_\theta)], \tag{2.3}$$

where U and V are vectors tangent to the parameter manifold and $U(\log p_\theta)$ is the derivative of $\log p_\theta$ along the direction U, which means $U(\log p_\theta)=(\mathrm{d}/\mathrm{d}t)\log p_{\theta+tU|_{t=0}}$.

$I(\theta)$ is a measure for the statistical distinguishabilty of distribution parameters. Under certain regularity conditions for $\theta\mapsto p_\theta$ the image of this mapping is a manifold of distributions. This manifold is the actual object of interest in information geometry rather than the space of distribution parameters and formula (2.3) defines a Riemannian metric g on it (for a general reference see Ref. 1). Indeed, a vector u tangent to this manifold is of the form

$$u=\frac{\mathrm{d}}{\mathrm{d}t}p_{\theta+tU|_{t=0}},$$

and the right hand side of (2.3) now reads as

$$g(u,v) := \mathrm{E}_p\left[\frac{u}{p}\,\frac{v}{p}\right], \tag{2.4}$$

defining the Fisher metric on the manifold of densities.

We restrict now to $\mathcal{P}_n \subset \mathbb{R}^n$, the simplex of strictly positive probability vectors, that is, $\mathcal{P}_n := \{\rho \in \mathbb{R}^n : \Sigma_{i=1}^n \rho_i = 1, \rho_i > 0, i = 1,\ldots,n\}$. An element $\rho \in \mathcal{P}_n$ is a density on the n-point set $\{1,\ldots,n\}$ with $\rho(i) = \rho_i$. We regard an element u of the tangent space $\mathrm{T}_\rho \mathcal{P}_n \equiv \{u \in \mathbb{R}^n : \Sigma_{i=1}^n u_i = 0\}$ as a function u on $\{1,\ldots,n\}$ with $u(i) = u_i$.

Definition 2.1: The Fisher–Rao Riemannian metric on $\mathrm{T}_\rho \mathcal{P}_n$ is given by

$$\langle u,v \rangle_\rho^F := \sum_{i=1}^n \frac{u_i v_i}{\rho_i}, \tag{2.5}$$

for $u,\ v \in \mathrm{T}_\rho \mathcal{P}_n$.

To see the relation between this metric and the Fisher metric, let $u,v \in \mathrm{T}_\rho \mathcal{P}_n$. We obtain from (2.4),

$$g(u,v) = \sum_{i=1}^n \frac{u(i)}{\rho_i}\,\frac{v(i)}{\rho_i}\,\rho_i = \sum_{i=1}^n \frac{u_i v_i}{\rho_i},$$

in accordance with (2.5).

The following result is well known and is a very special case of a far more general situation (see Ref. 15, for example).

Theorem 2.2: *The manifold $\mathcal{P}_n$ equipped with the Fisher–Rao Riemannian metric $\langle \cdot,\cdot \rangle^F$ is isometric with an open subset of the sphere of radius 2 in $\mathbb{R}^n$.*

Proof: We consider the mapping $\varphi : \mathcal{P}_n \to S_2^{n-1} \subset \mathbb{R}^n$,

$$\varphi(\rho) := 2(\sqrt{\rho_1}, \ldots, \sqrt{\rho_n}).$$

Then $D_\rho \varphi(u) = (u_1/\sqrt{\rho_1}, \ldots, u_n/\sqrt{\rho_n})$ and we get

$$D_\rho \varphi(\langle \cdot,\cdot \rangle^F)(u,v) := \langle D_\rho \varphi(u), D_\rho \varphi(v) \rangle^{\mathbb{R}^n} = \sum_{i=1}^n \frac{u_i v_i}{\rho_i} = \langle u,v \rangle_\rho^F.$$

Hence the standard metric on the sphere of radius 2 is pulled back to the Fisher–Rao Riemannian metric. □

This identification of $\mathcal{P}_n$ with an open subset of a radius 2 sphere allows for obtaining differential geometrical quantities of the Riemannian manifold $(\mathcal{P}_n, \langle \cdot,\cdot \rangle^F)$. From the very definition of geodesic distance, geodesic path and scalar curvature, one has for S_r^{n-1}, with $P_1, P_2 \in S_r^{n-1}$, the following:

(1) geodesic distance,

$$d(P_1,P_2) = r \cdot \arccos\left(\frac{\langle P_1,P_2 \rangle}{r^2}\right);$$

(2) geodesic path connecting P_1 and P_2,

$$\gamma^{P_1,P_2}(t) = r\,\frac{(1-t)P_1 + tP_2}{\|(1-t)P_1 + tP_2\|}$$

(of course, t is not the arc length parameter);

(3) scalar curvature,

$$\mathrm{Scal}(v)=\frac{1}{r^2}(n-1)(n-2),$$

because S_r^{n-1} has constant sectional curvature equal to $1/r^2$.

Let us denote by d_F, γ_F, Scal_F, respectively, the corresponding quantities for the Fisher information. The above considerations give, for $\rho,\sigma\in\mathcal{P}_n$, the following:

(1) Bhattacharya distance,

$$d_{\mathrm{F}}(\rho,\sigma)=2\arccos\left(\sum_i \rho_i^{1/2}\sigma_i^{1/2}\right);$$

(2) geodesic path connecting ρ and σ,

$$\gamma_{\mathrm{F}}^{\rho,\sigma}(t)=2\frac{((1-t)\sqrt{\rho}+t\sqrt{\sigma})^2}{\sum_i ((1-t)\sqrt{\rho_i}+t\sqrt{\sigma_i})^2};$$

(3) scalar curvature,

$$\mathrm{Scal}_{\mathrm{F}}(\rho)=\frac{1}{4}(n-1)(n-2),\quad \forall\rho\in\mathcal{P}_n.$$

The Levi–Civita connection associated to Fisher metric can be decomposed using the geometry of mixture and exponential models. In the rest of the section we explain how.

Definition 2.3: A dualistic structure on a manifold $\mathcal{M}$ is a triple $(\langle\cdot,\cdot\rangle,\nabla,\tilde{\nabla})$, where $\langle\cdot,\cdot\rangle$ is a Riemannian metric on $\mathcal{M}$ and $\nabla,\tilde{\nabla}$ are affine connections on $\mathcal{M}$ such that

$$X\langle Y,Z\rangle=\langle\nabla_X Y,Z\rangle+\langle Y,\tilde{\nabla}_X Z\rangle,$$

where X,Y,Z are vector fields. If $U^{\nabla},U^{\tilde{\nabla}}$ are the parallel transport associated to $\nabla,\tilde{\nabla}$ then the above equation is equivalent to

$$\langle U^{\nabla}(u),U^{\tilde{\nabla}}(v)\rangle=\langle u,v\rangle.$$

A divergence on a manifold is a smooth non-negative function $D:\mathcal{M}\times\mathcal{M}\to\mathbb{R}$ such that $D(\rho,\sigma)=0$ iff $\rho=\sigma$. To each divergence D one may associate a dualistic structure $(\langle\cdot,\cdot\rangle,\nabla,\tilde{\nabla})$ (see Refs. 1 and 14).

Let ∇^2 be the Levi–Civita connection of Fisher information. The Kullback–Leibler relative entropy $K(\rho,\sigma)=\Sigma_i\rho_i(\log\rho_i-\log\sigma_i)$ gives a dualistic structure $(\langle\cdot,\cdot\rangle^F,\nabla^m,\nabla^e)$ such that

$$\nabla^2=\tfrac{1}{2}(\nabla^m+\nabla^e),$$

where ∇^m,∇^e are the mixture and exponential connections. These connections are torsion free and flat: once the representation by scores is used for the tangent spaces, the associated parallel transports are given by

$$U^m_{\rho\sigma}:T_\rho\mathcal{P}\to T_\sigma\mathcal{P},\quad U^m_{\rho\sigma}(u)=\frac{\rho}{\sigma}u,$$

$$U^e_{\rho\sigma}:T_\rho\mathcal{P}\to T_\sigma\mathcal{P},\quad U^e_{\rho\sigma}(u)=u-\mathrm{E}_\sigma(u).$$

The geodesics of ∇^m,∇^e are, respectively, the mixture and exponential models.

III. METRIC CONTRACTION UNDER COARSE GRAINING

In the commutative case a Markov morphism (or stochastic map) is a stochastic matrix $T:\mathbb{R}^n\to\mathbb{R}^k$. In the noncommutative case a stochastic map is a completely positive and trace preserving operator $T:M_n\to M_k$ where M_n denotes the space of n by n complex matrices. We shall denote by $\mathcal{D}_n$ the manifold of strictly positive elements of M_n and by $\mathcal{D}_n^1\subset\mathcal{D}_n$ the submanifold of density matrices.

In the commutative case a monotone metric is a family of Riemannian metrics $g=\{g^n\}$ on $\{\mathcal{P}_n\}$, $n\in\mathbb{N}$ such that

$$g^m_{T(\rho)}(TX,TX)\leqslant g^n_\rho(X,X)$$

holds for every stochastic mapping $T:\mathbb{R}^n\to\mathbb{R}^m$ and all $\rho\in\mathcal{P}_n$ and $X\in T_\rho\mathcal{P}_n$.

In perfect analogy, a monotone metric in the noncommutative case is a family of Riemannian metrics $g=\{g^n\}$ on $\{\mathcal{D}_n^1\}$, $n\in\mathbb{N}$ such that

$$g^m_{T(\rho)}(TX,TX)\leqslant g^n_\rho(X,X)$$

holds for every stochastic mapping $T:M_n\to M_m$ and all $\rho\in\mathcal{D}_n^1$ and $X\in T_\rho\mathcal{D}_n^1$.

Let us recall that a function $f:(0,\infty)\to\mathbb{R}$ is called operator monotone if for any $n\in\mathbb{N}$, any A, $B\in M_n$ such that $0\leqslant A\leqslant B$, the inequalities $0\leqslant f(A)\leqslant f(B)$ hold. An operator monotone function is said to be symmetric if $f(x):=xf(x^{-1})$ and normalized if $f(1)=1$. In what follows by operator monotone we mean normalized symmetric operator monotone. With each operator monotone function f one associates also the so-called Chentsov–Morotzova function (see Ref. 8),

$$c_f(x,y):=\frac{1}{yf\left(\frac{x}{y}\right)},\quad \text{for } x,y>0.$$

Define $L_\rho(A):=\rho A$, and $R_\rho(A):=A\rho$. Since L_ρ,R_ρ commute we may define $c(L_\rho,R_\rho)$. Now we can state the fundamental theorems about monotone metrics (uniqueness and classification are up to scalars).

Theorem 3.1: (Ref. 7) *There exists a unique monotone metric on $\mathcal{P}_n$ given by the Fisher information.*

Theorem 3.2: (Ref. 34) *There exists a bijective correspondence between monotone metrics on $\mathcal{D}_n^1$ and operator monotone functions given by the formula*

$$\langle A,B\rangle_{\rho,f}:=\mathrm{Tr}(A\cdot c_f(L_\rho,R_\rho)(B)).$$

The tangent space to $\mathcal{D}_n^1$ at ρ is given by $T_\rho\mathcal{D}_n^1\equiv\{A\in M_n:A=A^*,\mathrm{Tr}(A)=0\}$, and can be decomposed as $T_\rho\mathcal{D}_n^1=(T_\rho\mathcal{D}_n^1)^c\oplus(T_\rho\mathcal{D}_n^1)^o$, where $(T_\rho\mathcal{D}_n^1)^c:=\{A\in T_\rho\mathcal{D}_n^1:[A,\rho]=0\}$, and $(T_\rho\mathcal{D}_n^1)^o$ is the orthogonal complement of $(T_\rho\mathcal{D}_n^1)^c$, with respect to the Hilbert–Schmidt scalar product $\langle A,B\rangle:=\mathrm{Tr}(A^*B)$. Each statistically monotone metric has a unique expression (up to a constant) given by $\mathrm{Tr}(\rho^{-1}A^2)$, for $A\in(T_\rho\mathcal{D}_n^1)^c$. The following result will be used in Sec. V.

Proposition 3.3: (see Ref. 3) *Let $A\in T_\rho\mathcal{D}_n^1$ be decomposed as $A=A^c+i[\rho,U]$ where $A^c\in(T_\rho\mathcal{D}_n^1)^c$ and $i[\rho,U]\in(T_\rho\mathcal{D}_n^1)^o$. Suppose $\varphi\in\mathcal{C}^1(0,+\infty)$. Then*

$$(D_\rho\varphi)(A)=\varphi'(\rho)A^c+i[\varphi(\rho),U].$$

As proved by Lesniewski and Ruskai each monotone metric is the Hessian of a suitable relative entropy; to state this result more precisely, we introduce some notation. In what follows g is an operator convex function defined on $(0,+\infty)$ and such that $g(1)=0$. The formula

$$f(x)\equiv f_g(x):=\frac{(x-1)^2}{g(x)+xg(x^{-1})},$$

associates a normalized, symmetric operator monotone function $f=f_g$ to each g. We denote by $\Delta_{\sigma,\rho}=L_\sigma R_\rho^{-1}$ the relative modular operator. The relative g–entropy of ρ and σ is defined as

$$H_g(\rho,\sigma):=\mathrm{Tr}(\rho^{1/2}g(\Delta_{\sigma,\rho})(\rho^{1/2})).$$

H_g is a divergence on $\mathcal{D}_n$ in the sense of Refs. 14, and 1. If ρ,σ are diagonal, H_g reduces to the commutative relative g–entropy (see Ref. 9).

Theorem 3.4: (Ref. 30) *Let g be operator convex, $g(1)=0$, $f=f_g$ and $\rho\in\mathcal{D}_n$. Then*

$$-\frac{\partial}{\partial t}\frac{\partial}{\partial s}H_g(\rho+tA,\rho+sB)\Big|_{t=s=0}=\mathrm{Tr}(A\cdot c_f(L_\rho,R_\rho)(B)).$$

To state the general formula for the scalar curvature of a monotone metric we need some auxiliary functions. In what follows c',$(\log c)'$ denote derivatives with respect to the first variable, and $c=c_f$:

$$\begin{aligned}
h_1(x,y,z)&:=\frac{c(x,y)-z\,c(x,z)\,c(y,z)}{(x-z)(y-z)c(x,z)c(y,z)},\\
h_2(x,y,z)&:=\frac{(c(x,z)-c(y,z))^2}{(x-y)^2c(x,y)c(x,z)c(y,z)},\\
h_3(x,y,z)&:=z\,\frac{(\ln c)'(z,x)-(\ln c)'(z,y)}{x-y},\\
h_4(x,y,z)&:=z\,(\ln c)'(z,x)\quad(\ln c)'(z,y),\\
h&:=h_1-\tfrac{1}{2}h_2+2h_3-h_4.
\end{aligned}\tag{3.1}$$

The functions h_i have no essential singularities if arguments coincide.

Note that $\langle A,B\rangle_\rho^f:=\mathrm{Tr}(A\cdot c_f(L_\rho,R_\rho)(B))$ defines a Riemannian metric also over $\mathcal{D}_n$ ($\mathcal{D}_n^1$ is a submanifold of codimension 1). Let $\mathrm{Scal}_f(\rho)$ be the scalar curvature of $(\mathcal{D}_n,\langle\cdot,\cdot\rangle_\rho^f)$ at ρ and $\mathrm{Scal}_f^1(\rho)$ be the scalar curvature of $(\mathcal{D}_n^1,\langle\cdot,\cdot\rangle_\rho^f)$.

Theorem 3.5: (Ref. 13) *Let $\sigma(\rho)$ be the spectrum of ρ. Then*

$$\begin{aligned}
\mathrm{Scal}_f(\rho)&=\sum_{x,y,z\in\sigma(\rho)}h(x,y,z)-\sum_{x\in\sigma(\rho)}h(x,x,x),\\
\mathrm{Scal}_f^1(\rho)&=\mathrm{Scal}_f(\rho)+\tfrac{1}{4}(n^2-1)(n^2-2).
\end{aligned}\tag{3.2}$$

IV. WIGNER–YANASE INFORMATION AS A RIEMANNIAN METRIC

Let $\rho\in\mathcal{D}_n^1$ be a density matrix and let A be a self-adjoint matrix. The Wigner–Yanase information (or skew information, information content relative to A) was defined as

$$I(\rho,A):=-\mathrm{Tr}([\rho^{1/2},A]^2),$$

where $[\cdot,\cdot]$ denotes the commutator (see Ref. 42). Consider now $g(x):=g_{wy}(x):=4(1-\sqrt{x})$. In this case

$$H_g(\rho,\sigma)=4(1-\mathrm{Tr}(\rho^{1/2}\sigma^{1/2})).$$

The associated operator monotone and Chentsov–Morotzova functions are

$$f_{wy}(x) := \frac{1}{4}(\sqrt{x}+1)^2, \quad c_{wy}(x,y) := \frac{1}{y f_{wy}\left(\frac{x}{y}\right)} = \frac{4}{(\sqrt{x}+\sqrt{y})^2}.$$

Let us consider the monotone metric,

$$\langle A,B\rangle_\rho^{wy} := \mathrm{Tr}(A\, c_{wy}(L_\rho,R_\rho)(B)).$$

A typical element of $(T_\rho D_n)^o$ has the form $\mathrm{i}[\rho,A]$, where A is self-adjoint. We have

$$\begin{aligned}
\langle \mathrm{i}[\rho,A],\mathrm{i}[\rho,A]\rangle_\rho^{wy} &= \mathrm{Tr}\,(\mathrm{i}[\rho,A]4(L_\rho^{1/2}+R_\rho^{1/2})^{-2}(\mathrm{i}[\rho,A])) \\
&= -4\,\mathrm{Tr}\,((L_\rho^{1/2}+R_\rho^{1/2})^{-1}([\rho,A])\ \ (L_\rho^{1/2}+R_\rho^{1/2})^{-1}([\rho,A])) \\
&= -4\,\mathrm{Tr}\,((L_\rho^{1/2}+R_\rho^{1/2})^{-1}\circ(L_\rho-R_\rho)(A)\ \ (L_\rho^{1/2}+R_\rho^{1/2})^{-1}\circ(L_\rho-R_\rho)(A)) \\
&= -4\,\mathrm{Tr}\,((L_\rho^{1/2}-R_\rho^{1/2})(A)\ \ (L_\rho^{1/2}-R_\rho^{1/2})(A)) \\
&= -4\,\mathrm{Tr}([\rho^{1/2},A]^2) \\
&= 4I(\rho,A),
\end{aligned}$$

and this explains why the monotone metric associated with the function $\frac{1}{4}(\sqrt{x}+1)^2$ is called the Wigner–Yanase monotone metric.

V. THE MAIN RESULT

First of all, we calculate the scalar curvature of Wigner–Yanase information using Theorem 3.5. If $f_{wy}(x) := \frac{1}{4}(\sqrt{x}+1)^2$, we write Scal^1_{wy} for Scal^1_f.

Theorem 5.1:

$$\mathrm{Scal}^1_{wy}(\rho) = \tfrac{1}{4}(n^2-1)(n^2-2).$$

Proof: Let us calculate the auxiliary functions for $c_{wy}(x,y) := 4(\sqrt{x}+\sqrt{y})^{-2}$. We get

$$h_1(x,y,z) = \frac{\sqrt{x}\,\sqrt{y}+3\,\sqrt{x}\,\sqrt{z}+3\,\sqrt{y}\,\sqrt{z}+z}{4\,(\sqrt{x}+\sqrt{y})^2\,(\sqrt{x}+\sqrt{z})\,(\sqrt{y}+\sqrt{z})},$$

$$h_2(x,y,z) = \frac{(\sqrt{x}+\sqrt{y}+2\,\sqrt{z})^2}{4\,(\sqrt{x}+\sqrt{z})^2\,(\sqrt{y}+\sqrt{z})^2},$$

$$h_3(x,y,z) = \frac{\sqrt{z}}{(\sqrt{x}+\sqrt{y})\,(\sqrt{x}+\sqrt{z})\,(\sqrt{y}+\sqrt{z})},$$

$$h_4(x,y,z) = \frac{1}{(\sqrt{x}+\sqrt{z})\,(\sqrt{y}+\sqrt{z}).}$$

Now one can verify by calculation that the symmetrization of $h_1-\frac{1}{2}h_2$ and the symmetrization of $2\,h_3-h_4$ vanish. Hence, by (3.1), the symmetrization of h vanishes, too. Since we sum up in formula (3.2) over all triples of eigenvalues we may replace h with its symmetrization without changing the summation result. Therefore

$$\mathrm{Scal}_{wy}(\rho)=0\,, \quad \mathrm{Scal}^1_{wy}(\rho) = \tfrac{1}{4}(n^2-1)(n^2-2), \quad \forall \rho \in \mathcal{D}_n^1.$$

□

Remark 5.2: The fact that $\mathrm{Scal}_{wy}(\rho)=0$ can be seen by a different approach (look at the Wigner–Yanase metric over $\mathcal{D}_n$ as the 0-geometry; see Refs. 21 and 27).

In what follows we use the pull-back approach to derive (and explain) the above formula in a direct way. Furthermore we deduce the geodesic distance and geodesic equation.

Let us denote by $\mathcal{S}$ the manifold $\{A \in M_n : \mathrm{Tr}\, A\, A^* = 4,\ A = A^*\}$. Clearly, since $\mathcal{S}$ is the intersection of the radius 2 sphere in $\mathbb{C}^{n\times n}$ and the subspace of Hermitian matrices, it is isometric with a radius 2 sphere $S_2^{n^2-1}$.

Now, let $\varphi : \mathcal{D}_n^1 \to \mathcal{S} \subset \mathbb{C}^{n\times n}$, $\varphi(\rho) := 2\sqrt{\rho}$. Then we have the following result (see Refs. 25, 18, 27, and 21).

Theorem 5.3: *The pull-back by the map φ of the natural metric on $\mathcal{S} \equiv S_2^{n^2-1}$ coincides with the Wigner–Yanase monotone metric.*

Proof: Let A and B be vectors tangent to $\mathcal{D}_n^1$ at ρ. Because $\varphi(\rho)\,\varphi(\rho) = 4\,\rho$ we get from the Leibniz rule $D_\rho\varphi(A)\sqrt{\rho} + \sqrt{\rho}\, D_\rho\varphi(A) = 2A$. Thus, the differential of φ at the point ρ is given by

$$D_\rho\varphi(A) = 2(L_\rho^{1/2} + R_\rho^{1/2})^{-1}(A)\,.$$

Therefore the pull-back of the real part of the Hilbert–Schmidt metric yields

$$\begin{aligned} D_\rho\varphi(\mathrm{Re}\langle\cdot,\cdot\rangle)(A,B) &= \mathrm{Re}\,\langle D_\rho\varphi(A), D_\rho\varphi(B)\rangle \\ &= 4\,\mathrm{Re}\langle (L_\rho^{1/2} + R_\rho^{1/2})^{-1}(A), (L_\rho^{1/2} + R_\rho^{1/2})^{-1}(B)\rangle \\ &= 4\,\langle A, (L_\rho^{1/2} + R_\rho^{1/2})^{-2}(B)\rangle \\ &= 4\,\mathrm{Tr}\, A\, (L_\rho^{1/2} + R_\rho^{1/2})^{-2}(B) \\ &= \mathrm{Tr}\, A\, c_{wy}(L_\rho, R_\rho)(B) = \langle A, B\rangle_\rho^{wy}\,, \end{aligned}$$

which was to be proved. □

From this result one can deduce the following.

Theorem 5.4: *For the geodesic distance, the geodesic path and the scalar curvature of Wigner–Yanase information the following formulas hold:*

(1) geodesic distance,

$$d_{wy}(\rho,\sigma) = 2\,\arccos(\mathrm{Tr}(\rho^{1/2}\sigma^{1/2}))\,; \tag{5.1}$$

(2) geodesic path,

$$\gamma_{wy}^{\rho,\sigma}(t) = 2\,\frac{((1-t)\sqrt{\rho} + t\sqrt{\sigma})^2}{\mathrm{Tr}(((1-t)\sqrt{\rho} + t\sqrt{\sigma})^2)}\,; \tag{5.2}$$

(3) scalar curvature

$$\mathrm{Scal}_{wy}^1(\rho) = \tfrac{1}{4}(n^2-1)(n^2-2). \tag{5.3}$$

Proof: The formulas are immediate consequences of the preceding theorem and of sphere geometry. Indeed by the pull-back argument the Wigner–Yanase metric looks locally like a sphere of radius 2 of dimension (n^2-1). But for a sphere of this kind the sectional curvatures are all equal to $\frac{1}{4}$ and therefore the scalar curvature is given by $\frac{1}{4}(n^2-1)(n^2-2)$. □

One may ask if other monotone metrics are the pull-back of some function φ different from the square root. The rest of the section answers this question.

Definition 5.5: A monotone metric $\langle\cdot,\cdot\rangle_{\rho,f}$ is a pull-back metric if there exists a manifold $\mathcal{S} \subset M_n$ and a function $\varphi \in \mathcal{C}^1(0,+\infty)$ such that the pull-back metric of $\varphi : \mathcal{D}_n^1 \to \mathcal{S} \subset M_n$ coincides with $\langle\cdot,\cdot\rangle_{\rho,f}$.

Proposition 5.6: Let $\langle\cdot,\cdot\rangle_{\rho,f}$ be a monotone metric, let $c = c_f$ be the associated CM-function and let $\varphi \in \mathcal{C}^1(0,+\infty)$. We have that $\langle\cdot,\cdot\rangle_{\rho,f}$ is a pull-back metric by φ if and only if

$$\left(\frac{\varphi(x)-\varphi(y)}{x-y}\right)^2 = c(x,y). \tag{5.4}$$

Proof: Apply the proposition (3.3) to tangent vectors in $(T_\rho \mathcal{D}_n^1)^o$. □

Definition 5.7: Let $\varphi,\chi \in \mathcal{C}^1(0,+\infty)$. We say that (φ,χ) is a dual pair if there exists an operator monotone f such that

$$\frac{\varphi(x)-\varphi(y)}{x-y}\cdot\frac{\chi(x)-\chi(y)}{x-y} = c(x,y), \tag{5.5}$$

where $c=c_f$ is the CM-function associated with f.

In such a case we say that f (or c_f) is a dual function. If (φ,φ) is a dual pair with respect to f (or c_f) we say that f (or c_f) is self-dual. Obviously one has the following.

Proposition 5.8: To say that $\langle\cdot,\cdot\rangle_{\rho,f}$ is a pull-back metric by φ it is equivalent to say that f (or c_f) is self-dual with respect to φ.

Definition 5.9: Two dual pairs $(\varphi,\chi),(\tilde{\varphi},\tilde{\chi})$ are equivalent if there exist constants A_1,A_2,B_1,B_2 such that $A_1A_2=1$,

$$\tilde{\varphi}=A_1\varphi+B_1,$$

$$\tilde{\chi}=A_2\chi+B_2.$$

Obviously equivalent pairs define the same CM-function. In what follows we consider dual pairs up to this equivalence relation with the traditional abuse of language. We are ready to state the fundamental result of the theory that classifies dual pairs.

Theorem 5.10: (Refs. 23, 24, 25, 26, 36, and 19) *Let $\varphi,\chi \in \mathcal{C}^1(0,+\infty)$. Then (φ,χ) is a dual pair if and only if one of the following two possibilities hold:*

$$(\varphi(x),\chi(x)) = \left(\frac{x^p}{p},\frac{x^{1-p}}{1-p}\right), \quad p\in[-1,2]\backslash\{0,1\},$$

$$(\varphi(x),\chi(x)) = (x,\log(x)).$$

Corollary 5.11: The function $f(x)=\frac{1}{4}(\sqrt{x}+1)^2$ is the only self-dual operator monotone function, that is: the Wigner–Yanase metric is the only pull-back metric among statistically monotone metrics.

VI. CONCLUSIONS

Remark 6.1: Note that the formula (5.1) implies $d^{wy}(\rho,\sigma)\leqslant 2\pi$. An analogous inequality holds for the Bures metric (see Ref. 10, p. 311), also known as the SLD-metric: this is the monotone metric associated with $f(x)=\frac{1}{2}(1+x)$. Indeed the formula,

$$d_{\text{Bures}}(\rho,\sigma) = \sqrt{2-2\,\text{Tr}(\rho^{1/2}\sigma\rho^{1/2})^{1/2}}, \tag{6.1}$$

seems to be the only other explicit formula for a geodesic distance (in the family of statistically monotone metrics).

Remark 6.2: In general it is difficult to give explicit formulas for geodesic paths of monotone metrics. In the case of the Bures metric these geodesics can be given because they are projections of large circles on a sphere in the purifying space (see Ref. 10, p. 311 and Refs. 12, 4, and 39). For a discussion of geodesics for α-connections see Refs. 27, 28.

Remark 6.3: A classical theorem classifies the spaces of costant curvature.[29] It is not known at the moment if there are other monotone metrics of costant sectional and scalar curvature.

Remark 6.4: We have seen in the commutative case that for the Levi–Civita connection of the pull-back of the square root the decomposition is available,

$$\nabla^2=\frac{1}{2}(\nabla^m+\nabla^e).$$

In the noncommutative case an analogous decomposition for the pull-back of the square root no longer holds. Indeed, on one hand, the use of Umegaki relative entropy $H(\rho,\sigma)=\mathrm{Tr}(\rho(\log\rho-\log\sigma))$ produces a similar decomposition, but for the Bogoliubov–Kubo–Mori metric.[31,1,22,33] On the other hand, if one uses $H_{wy}(\rho,\sigma)=4(1-\mathrm{Tr}(\rho^{1/2}\sigma^{1/2}))$ as a divergence on $\mathcal{D}_n^1$ and constructs the associated dualistic structure $(\langle\cdot,\cdot\rangle^{H_{wy}},\nabla^{H_{wy}},\nabla^{H_{wy}})$ (again following the lines of Refs. 14 and 1), then the construction is trivial, namely, the dual connections both coincide with the Levi–Civita connection of the Wigner–Yanase information. This is easily seen on $\mathcal{P}_n$ where $H_g(\rho,\sigma)$ reduces to Csiszar relative g-entropy: it is known that such an entropy induces the α-geometry where α is given by the formula $\alpha=3+2g'''(1)/g''(1)$ (see Ref. 1, p. 57). For $g=4(1-\sqrt{x})$ this gives $\alpha=0$, that is, the Fisher information case (see also Ref. 21).

ACKNOWLEDGMENTS

This research has been supported by the italian MIUR program ''Quantum Probability and Infinite Dimensional Analysis'' 2001–2002. It is a pleasure to thank J. Dittmann for a number of valuable conversations on this subject and for permitting us to reproduce in this paper the proof of Theorem 5.1.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Quantum four-body system in *D* dimensions

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(Received 11 March 2003; accepted 6 May 2003)

By the method of generalized spherical harmonic polynomials, the Schrödinger equation for a four-body system in *D*-dimensional space is reduced to the generalized radial equations where only six internal variables are involved. The problem on separating the rotational degrees of freedom from the internal ones for a quantum *N*-body system in *D* dimensions is generally discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599956]

I. INTRODUCTION

Recent years have witnessed a flurry of investigations into the arbitrary *D*-dimensional problems[1–5] in many branches of physical chemistry and chemical physics. The problems associated with the *D*-dimensional hydrogen atom,[6–8] the *D*-dimensional harmonic oscillator,[9–11] and the connection between the two[12–16] have been thoroughly discussed. During the past few years, with the application of dimensional scaling to the quantum theory of atomic and molecular structure, large-*D* helium problem has also been studied by many authors.[17–21] This approach requires solving the few-body Schrödinger equation in a *D*-dimensional coordinate space and has been applied to a large number of physically interesting problems.[22–25] Due to the complexity of the problem for an *N*-body system in *D* dimensions, so far there is no complete theoretical solution when $N>3$.

In our recent work,[26] a new method for separating the rotational degrees of freedom from the internal ones in a few-body system was proposed. The power of this new approach is in its ability of great simplification in calculation of energy levels of a few-body system in terms of the generalized radial equations involving only internal variables, which are derived from the Schrödinger equation without any approximation. Some typical three-body system in three-dimensional space, such as a helium atom[27–29] and a positronium negative ion[30] have been solved numerically with high precision. The key to the approach is that we have found a complete set of independent eigenfunctions of angular momentum for the system, which are homogeneous polynomials in the components of Jacobi coordinate vectors and satisfy the Laplace equation, and chosen a suitable set of internal variables. Any wave function with a given angular momentum can be expanded with respect to the basis functions where the coefficients, called the generalized radial functions, depend only upon the internal variables. The generalized radial equations satisfied by the generalized radial functions are easily derived owing to the nice property of the basis functions.[26] This method has been generalized to the arbitrary dimensional space for a three-body system.[31] The exact interdimensional degeneracies in the system can be obtained directly from the generalized radial equations.[32]

To further this study, we expect to apply this approach to an *N*-body system in *D* dimensions. As noticed in our previous paper,[31] the cases with $N<D$ are very different from the cases with

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$N \geqslant D$. The general formulas are hard to express uniformly due to arbitrariness of D and N. However, the main characters are manifested fully in a four-body system of D dimensions, but not fully in a three-body system. The four-body problems also play a fundamental role in nuclear and hypernuclear physics.[33–35] In this paper we will study the problem of separating the rotational degrees of freedom from the internal ones for a quantum four-body system in D dimensions in some detail. The general case (N-body system) will be summarized.

The plan of this paper is as follows: In Sec. II, after separating the motion of the center of mass by Jacobi coordinate vectors, we will define the generalized spherical harmonic polynomials for a four-body system in D dimensions and prove that they constitute a complete set of independent basis functions for a given total orbital angular momentum in the system. Some new features in comparison with the three-body case are also discussed in this section. The generalized radial equations satisfied by the generalized radial functions are established in Sec. III. In Sec. IV, we will generalize this method to separate the rotational degrees of freedom from the internal ones for an N-body system in D dimensions. Some conclusions will be given in Sec. V.

II. THE GENERALIZED SPHERICAL HARMONIC POLYNOMIALS

For a quantum N-body system in an arbitrary D-dimensional space, we denote the position vectors and the masses of N particles by $\mathbf{r}_k$ and by m_k, $k=1, 2,\ldots, N$, respectively. $M=\Sigma_k m_k$ is the total mass. The Schrödinger equation for the N-body system with a pair potential V, depending upon the distance of each pair of particles, $|\mathbf{r}_j-\mathbf{r}_k|$, is

$$-\frac{1}{2}\nabla^2\Psi+V\Psi=E\Psi, \quad \nabla^2=\sum_{k=1}^{N} m_k^{-1}\nabla_{\mathbf{r}_k}^2, \tag{1}$$

where $\nabla_{\mathbf{r}_k}^2$ is the Laplace operator with respect to the position vector $\mathbf{r}_k$. For simplicity, the natural units $\hbar=c=1$ are employed throughout this paper. The total orbital angular momentum operators L_{ab} in D dimensions are defined as[21,36]

$$L_{ab}=-L_{ba}=-i\sum_{k=1}^{N}\left\{r_{ka}\frac{\partial}{\partial r_{kb}}-r_{kb}\frac{\partial}{\partial r_{ka}}\right\}, \quad a,b=1,2,\ldots,D, \tag{2}$$

where r_{ka} denotes the ath component of the position vector $\mathbf{r}_k$. Now, we replace the position vectors $\mathbf{r}_k$ with the Jacobi coordinate vectors $\mathbf{R}_j$,

$$\mathbf{R}_0=M^{-1/2}\sum_{k=1}^{N} m_k\mathbf{r}_k, \quad \mathbf{R}_j=\left(\frac{m_{j+1}M_j}{M_{j+1}}\right)^{1/2}\left(\mathbf{r}_{j+1}-\sum_{k=1}^{j}\frac{m_k\mathbf{r}_k}{M_j}\right),$$

$$1\leqslant j\leqslant(N-1), \quad M_j=\sum_{k=1}^{j} m_k, \quad M_N=M, \tag{3}$$

where $\mathbf{R}_0$ describes the position of the center of mass, $\mathbf{R}_1$ describes the mass-weighted separation from the second particle to the first particle, $\mathbf{R}_2$ describes the mass-weighted separation from the third particle to the center of mass of the first two particles, and so on. It is straightforward to illustrate that the potential V is a function of $\mathbf{R}_j\cdot\mathbf{R}_k$ and is rotationally invariant.

In the center-of-mass frame, $\mathbf{R}_0=0$. A straightforward calculation by replacement of variables shows that the Laplace operator in Eq. (1) and the total orbital angular momentum operator L_{ab} in Eq. (2) are directly expressed in $\mathbf{R}_j$,

$$\nabla^2=\sum_{j=1}^{N-1}\nabla_{\mathbf{R}_j}^2, \quad L_{ab}=\sum_{j=1}^{N-1}L_{ab}^{(j)}=-i\sum_{j=1}^{N-1}\left\{R_{ja}\frac{\partial}{\partial R_{jb}}-R_{jb}\frac{\partial}{\partial R_{ja}}\right\},$$

$$\mathbf{L}^2=\sum_{a<b=2}^{D} L_{ab}^2, \quad (\mathbf{L}^{(j)})^2=\sum_{a<b=2}^{D} (L_{ab}^{(j)})^2. \tag{4}$$

For a four-body system, there are three Jacobi coordinate vectors $\mathbf{R}_1$, $\mathbf{R}_2$, and $\mathbf{R}_3$, which will be denoted for simplicity by $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$, respectively,

$$\begin{aligned}
\mathbf{x}&=\left[\frac{m_1m_2}{m_1+m_2}\right]^{1/2}\{\mathbf{r}_2-\mathbf{r}_1\},\\
\mathbf{y}&=\left[\frac{(m_1+m_2)m_3}{m_1+m_2+m_3}\right]^{1/2}\left\{\mathbf{r}_3-\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2}{m_1+m_2}\right\},\\
\mathbf{z}&=\left[\frac{(m_1+m_2+m_3+m_4)m_4}{m_1+m_2+m_3}\right]^{1/2}\mathbf{r}_4.
\end{aligned} \tag{5}$$

Hence,

$$\begin{aligned}
&\nabla^2=\nabla_{\mathbf{x}}^2+\nabla_{\mathbf{y}}^2+\nabla_{\mathbf{z}}^2, \quad L_{ab}=L_{ab}^{(x)}+L_{ab}^{(y)}+L_{ab}^{(z)},\\
&\mathbf{L}^2=\sum_{a<b=2}^{D} L_{ab}^2, \quad [\mathbf{L}^{(x)}]^2=\sum_{a<b=2}^{D} [L_{ab}^{(x)}]^2,\\
&[\mathbf{L}^{(y)}]^2=\sum_{a<b=2}^{D} [L_{ab}^{(y)}]^2, \quad [\mathbf{L}^{(z)}]^2=\sum_{a<b=2}^{D} [L_{ab}^{(z)}]^2.
\end{aligned} \tag{6}$$

The Schrödinger equation (1) for $D\geqslant N=4$ reduces to

$$\begin{aligned}
&\{\nabla_{\mathbf{x}}^2+\nabla_{\mathbf{y}}^2+\nabla_{\mathbf{z}}^2\}\Psi(\mathbf{x},\mathbf{y},\mathbf{z})=-2\{E-V(\xi_j,\eta_j,\zeta_j)\}\Psi(\mathbf{x},\mathbf{y},\mathbf{z}),\\
&\xi_1=\mathbf{x}\cdot\mathbf{x}, \quad \xi_2=\eta_1=\mathbf{x}\cdot\mathbf{y}, \quad \xi_3=\zeta_1=\mathbf{x}\cdot\mathbf{z},\\
&\eta_2=\mathbf{y}\cdot\mathbf{y}, \quad \eta_3=\zeta_2=\mathbf{y}\cdot\mathbf{z}, \quad \zeta_3=\mathbf{z}\cdot\mathbf{z},
\end{aligned} \tag{7}$$

where ξ_j, η_j, and ζ_j are internal variables. It is worth noticing that for the cases $3=D<N$ two Jacobi coordinate vectors $\mathbf{x}$ and $\mathbf{y}$ can determine the body-fixed frame and this set of internal variables is not complete because two configurations with different directions of $\mathbf{z}$ reflecting to the plane spanned by $\mathbf{x}$ and $\mathbf{y}$ are described by the same internal variables. As pointed in Ref. 26, the variable ζ_3 has to be changed to $(\mathbf{x}\times\mathbf{y})\cdot\mathbf{z}$. We will further discuss this problem in Sec. IV.

Since Eq. (7) is rotational invariant, the total orbital angular momentum is conserved. As discussed in Ref. 31, in D-dimensional space, the wave function $\Psi(\mathbf{x},\mathbf{y},\mathbf{z})$ with a given total angular momentum has to belong to an irreducible representation of SO(D), and the angular momentum is also denoted by the representation. For a four-body system, there are only three Jacobi coordinate vectors so that the possible irreducible representation is described by a three-row Young pattern $[\mu,\nu,\tau]$ of SO(D), or its highest weight $\mathbf{M}=(M_1,M_2,M_3,0,\ldots,0)$, where

$$M_1=\mu-\nu, \quad M_2=\nu-\tau, \quad M_3=\tau. \tag{8}$$

We only need to consider the highest weight state $\Psi_{\mathbf{M}}^{[\mu,\nu,\tau]}(\mathbf{x},\mathbf{y},\mathbf{z})$ because its partners can be calculated from it by the lowering operators. In this paper the highest weight state will be simply called the wave functions with the given angular momentum $[\mu,\nu,\tau]$ for simplicity.

Now we are going to find a complete set of independent eigenfunctions of total orbital angular momentum, where ''independent'' means that each one in the set cannot be expressed as a combination of the remaining with coefficients only depending on the internal variables. As discussed

in our previous paper,[31] the spherical harmonic polynomials $\mathcal{Y}^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ are homogeneous polynomials in the components of $\mathbf{x}$ of degree l, spanning an irreducible traceless tensor space described by the Young pattern $(l)\equiv[l,0,0]$. When $D>6$, the explicit forms for some polynomials with higher weights $\mathbf{m}$ are as follows:[37]

$$\begin{aligned}
\mathcal{Y}^{(l)}_{(l)}(\mathbf{x}) &= N_{D,l}(x_1+ix_2)^l,\\
\mathcal{Y}^{(l)}_{(l-2,1,0,\ldots,0)}(\mathbf{x}) &= -\sqrt{l}N_{D,l}(x_1+ix_2)^{l-1}(x_3+ix_4),\\
\mathcal{Y}^{(l)}_{(l-4,2,0,\ldots,0)}(\mathbf{x}) &= \sqrt{l(l-1)/2}N_{D,l}(x_1+ix_2)^{l-2}(x_3+ix_4)^2,
\end{aligned} \tag{9}$$

where the last equality holds for $l>1$, and $N_{D,l}$ denotes the normalization factor given in Ref. 37. The product of two spherical harmonic polynomials $\mathcal{Y}^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ and $\mathcal{Y}^{(l')}_{\mathbf{m}'}(\hat{\mathbf{y}})$ belongs to the direct product of two representation (l) and (l'), which is a reducible representation. It can be reduced by the Littlewood–Richardson rule and contraction of a pair of x_a and y_a, where the latter relates to the internal variables,

$$(l)\otimes(l')\simeq \bigoplus_{s=0}^{\min\{l,l'\}} \bigoplus_{t=0}^{\min\{l,l'\}-s} [l+l'-s-2t,s,0]. \tag{10}$$

Since a basis function containing a factor depending on internal variables is not independent, only those representations $[l+l'-s,s,0]$ [$t=0$ in Eq. (10)] calculated by the Littlewood–Richardson rule are related to the independent basis functions.[31] Calculating by the Clebsch–Gordan coefficients and removing the normalization factor, we obtain the independent basis functions for the representations $[l+l'-s,s,0]$, called the generalized spherical harmonic polynomial $Q_l^{(l+l'-s)s}(\mathbf{x},\mathbf{y})$. Changing the parameters $\mu=l+l'-s$, $\nu=s$, and $q=l$, we define the generalized spherical harmonic polynomial $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ for the representation $[\mu,\nu]$ (Ref. 31) as

$$\begin{aligned}
Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}) &= \frac{X_{12}^{q-\nu}Y_{12}^{\mu-q}}{(q-\nu)!(\mu-q)!}(X_{12}Y_{34}-Y_{12}X_{34})^{\nu}, \quad 0\leqslant\nu\leqslant q\leqslant\mu,\\
X_{12} &= x_1+ix_2, \quad X_{34}=x_3+ix_4, \quad Y_{12}=y_1+iy_2, \quad Y_{34}=y_3+iy_4.
\end{aligned} \tag{11}$$

For the product of three spherical harmonic polynomials, Eq. (10) is generalized to

$$(l)\otimes(l')\otimes(l'')\simeq \bigoplus_{r=0}^{\min\{l,l'\}} \bigoplus_{\nu=r}^{\min\{(l+l'-r),(r+l'')\}} \bigoplus_{\tau=0}^{\min\{r,(l''-\nu+r)\}} [l+l'+l''-\nu-\tau,\nu,\tau]\oplus\cdots. \tag{12}$$

The ellipsis denotes those representations related to the basis functions which are not independent.

Filling the digits 1, 2, and 3 arbitrarily into a given Young pattern $[\mu,\nu,\tau]$ ($\mu\geqslant\nu\geqslant\tau$) we obtain a young tableau. A Young tableau is called standard if the digit in every column of the tableau increases downwards and the digit in every row does not decrease from left to right. In fact, the digits "1," "2," and "3" denote the components of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$, respectively. Obviously, the representation $[l+l'+l''-\nu-\tau,\nu,\tau]$ listed in Eq. (12) corresponds to a standard Young tableau, where the number of digit "1" in the first row is l, the numbers of digit "2" in the first and the second rows are respectively $(l'-r)$ and r, and the numbers of digit "3" in the first, second, and third rows are, respectively, $(l''+r-\nu-\tau)$, $\nu-r$, and τ. The basis functions in the remaining representation spaces, which correspond to nonstandard Young tableaux, are not independent.

For a given pattern $[\mu,\nu,\tau]$, each standard Young tableau is determined by three parameters q, p, and r, where q is the number of digit "1" in the first row, p and r are the numbers of digit "2"

in the first and the second rows, respectively. q, p, and r should satisfy the constraints, $\tau \leqslant r \leqslant q$ and $r \leqslant \nu \leqslant q+p \leqslant \mu$. The number of standard Young tableaux for the given Young pattern $[\mu,\nu,\tau]$ is equal to the dimension of the representation $[\mu,\nu,\tau]$ of the SU(3) group,

$$d_{[\mu,\nu,\tau]}(\mathrm{SU}(3)) = \tfrac{1}{2}(\mu-\tau+2)(\nu-\tau+1)(\mu-\nu+1). \tag{13}$$

For a given representation $[\mu,\nu,\tau]$ of SO(D), each standard Young tableau denoted by (q,p,r) corresponds to a representation space. The highest weight state in the representation space (q,p,r) is the generalized spherical harmonic polynomial $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$,

$$Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z}) = \begin{cases} \dfrac{X_{12}^{q-\nu} Y_{12}^{p} Z_{12}^{\mu-q-p} T_{12}^{r-\tau} T_{13}^{\nu-r} T^{\tau}}{(q-\nu)!\,p!\,(\mu-q-p)!\,(r-\tau)!\,(\nu-r)!}, & \text{when } q \geqslant \nu, \\ \dfrac{Y_{12}^{q+p-\nu} Z_{12}^{\mu-q-p} T_{12}^{r-\tau} T_{13}^{q-r} T_{23}^{\nu-q} T^{\tau}}{(q+p-\nu)!\,(\mu-q-p)!\,(r-\tau)!\,(q-r)!\,(\nu-q)!}, & \text{when } q < \nu, \end{cases}$$

$$\tau \leqslant r \leqslant q, \quad r \leqslant \nu \leqslant q+p \leqslant \mu,$$

$$X_{12} = x_1 + i x_2, \quad Y_{12} = y_1 + i y_2, \quad Z_{12} = z_1 + i z_2,$$

$$X_{34} = x_3 + i x_4, \quad Y_{34} = y_3 + i y_4, \quad Z_{34} = z_3 + i z_4,$$

$$X_{56} = x_5 + i x_6, \quad Y_{56} = y_5 + i y_6, \quad Z_{56} = z_5 + i z_6,$$

$$T_{12} = X_{12}Y_{34} - X_{34}Y_{12}, \quad T_{13} = X_{12}Z_{34} - X_{34}Z_{12}, \quad T_{23} = Y_{12}Z_{34} - Y_{34}Z_{12},$$

$$T = X_{12}Y_{34}Z_{56} + X_{34}Y_{56}Z_{12} + X_{56}Y_{12}Z_{34} - X_{12}Y_{56}Z_{34} - X_{34}Y_{12}Z_{56} - X_{56}Y_{34}Z_{12}. \tag{14}$$

It is evident that $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ do not contain a function of the internal variables as a factor, nor do their partners due to the rotational symmetry. Therefore, $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ are independent basis functions for the given angular momentum described by $[\mu,\nu,\tau]$. Due to Eq. (12), the set of $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ is complete. The reason why the generalized spherical harmonic polynomial denoted by a nonstandard Young tableau is not independent can be seen from the following identity:

$$T_{23}X_{12} = T_{13}Y_{12} - T_{12}Z_{12}, \quad \begin{array}{|c|c|}\hline 2 & 1 \\ \hline 3 \\ \cline{1-1} \end{array} = \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1} \end{array} - \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1} \end{array}. \tag{15}$$

This identity is similar to the Fock's cyclic symmetry condition.[38] The left-hand side of Eq. (15) corresponds to a nonstandard Young tableau, and two terms in the right-hand side correspond to two standard Young tableaux, respectively.

Since the problem on completeness of the set is very important, we are going to prove this problem by another method. On the one hand, because the basis function $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ is a homogeneous polynomial of degree $\mu+\nu+\tau$ in the components of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$, we calculate the number $R_D(l)$ of basis functions in the sets for the representations $[\mu,\nu,\tau]$ with $\mu+\nu+\tau=l$. Namely, we want to calculate how many homogeneous polynomials of degree l exist in the sets of the independent basis functions. We first calculate how many basis functions exist in the set for a given representation $[\mu,\nu,\tau]$. The dimension of the representation $[\mu,\nu,\tau]$ of SO(D) is $d_D([\mu,\nu,\tau])$,

$$\begin{aligned} d_D([\mu,\nu,\tau]) = {} & (D+2\mu-2)(D+\mu+\nu-3)(D+\mu+\tau-4)(D+2\nu-4) \\ & \times (D+\nu+\tau-5)(D+2\tau-6)(\mu-\tau+2)(\mu-\nu+1)(\nu-\tau+1) \\ & \times \frac{(D+\mu-5)!\,(D+\nu-6)!\,(D+\tau-7)!}{(D-2)!\,(D-4)!\,(D-6)!\,(\mu+2)!\,(\nu+1)!\,\tau!}. \end{aligned} \tag{16}$$

Thus, the number of basis functions in the set for the representation $[\mu,\nu,\tau]$ is $d_{[\mu,\nu,\tau]}(\mathrm{SU}(3))d_D(\mu,\nu,\tau)$. Then, the number $R_D(l)$ of basis functions in the sets for the representation $[\mu,\nu,\tau]$ with $\mu+\nu+\tau=l$ is

$$R_D(l)=\sum_{\tau=0}^{[l/3]}\sum_{\nu=\tau}^{[(l-\tau)/2]} d_{[(l-\nu-\tau),\nu,\tau]}(\mathrm{SU}(3))d_D([(l-\nu-\tau),\nu,\tau]), \tag{17}$$

where $[x]$ denotes the largest integer less than or equal to x.

On the other hand, the number of linear independent homogeneous polynomials of degree l in the components of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ is $M_D(l)$,

$$M_D(l)=\begin{pmatrix} l+3D-1 \\ 3D-1 \end{pmatrix}.$$

After removing those polynomials in the form $\xi_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, $\eta_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, and $\zeta_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, where $f(\mathbf{x},\mathbf{y},\mathbf{z})$ is a polynomial of degree $(l-2)$, the number $M_D(l)$ reduces to $K_D(l)$,

$$\begin{aligned} K_D(l)=&\ M_D(l)-6M_D(l-2)+15M_D(l-4)-20M_D(l-6)+15M_D(l-8) \\ &-6M_D(l-10)+M_D(l-12) \\ =&\{(3D-7)(3D-8)(3D-9)(3D-10)(3D-11)(3D-12)+12l(D-4) \\ &\times[72+(3D-10)(3D-11)(27D^2-153D+236)]+4l^2[184+45(D-4)(3D-11) \\ &\times(9D^2-57D+98)]+480l^3(D-4)(9D^2-63D+126)+80l^4(27D^2-207D+404) \\ &+576l^5(D-4)+64l^6\}\frac{(l+3D-13)!}{l!(3D-7)!}, \end{aligned} \tag{18}$$

where $l+3D\geqslant 13$ and $K_4(0)=1$. It is checked by MATHEMATICA that

$$R_D(l)=K_D(l). \tag{19}$$

Thus, we have proved again that $d_{[\mu,\nu,\tau]}(\mathrm{SU}(3))$ polynomials $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ construct a complete set of independent basis functions for the angular momentum $[\mu,\nu,\tau]$.

The generalized spherical harmonic polynomial $Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})$ is a homogeneous polynomial of degrees q, $(p+r)$ and $(\mu+\nu+\tau-q-p-r)$ in the components of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$, respectively. It is a simultaneous eigenfunction of $\nabla^2_{\mathbf{x}}$, $\nabla^2_{\mathbf{y}}$, $\nabla^2_{\mathbf{z}}$, $\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}$, $\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{z}}$, $\nabla_{\mathbf{y}}\cdot\nabla_{\mathbf{z}}$, and the angular momentum operators $\mathbf{L}^2$, $[\mathbf{L}^{(x)}]^2$, $[\mathbf{L}^{(y)}]^2$, $[\mathbf{L}^{(z)}]^2$,

$$\nabla^2_{\mathbf{x}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=\nabla^2_{\mathbf{y}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=\nabla^2_{\mathbf{z}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=0,$$

$$\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{z}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=\nabla_{\mathbf{y}}\cdot\nabla_{\mathbf{z}}Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=0,$$

$$\mathbf{L}^2Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=C_2([\mu,\nu,\tau])Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z}),$$

$$C_2([\mu,\nu,\tau])=\mu(\mu+D-2)+\nu(\nu+D-4)+\tau(\tau+D-6), \tag{20}$$

$$[\mathbf{L}^{(x)}]^2Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=q(q+D-2)Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z}),$$

$$[\mathbf{L}^{(y)}]^2Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=(p+r)(p+r+D-2)Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z}),$$

$$[\mathbf{L}^{(z)}]^2Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z})=(\mu+\nu+\tau-q-p-r)(\mu+\nu+\tau-q-p-r+D-2)\times Q^{\mu\nu\tau}_{qpr}(\mathbf{x},\mathbf{y},\mathbf{z}),$$

where $C_2([\mu,\nu])$ is the Casimir invariant calculated by a general formula [see (1.131) in Ref. 39]. The parity of $Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ is obviously equal to $(-1)^{\mu+\nu+\tau}$.

Now, we turn to discuss the case $D\leqslant 6$. As is well known, the irreducible traceless tensor space of SO(D) described by a Young pattern has the following properties. It is a null space if sum of the lengths of the first two columns of the Young pattern is larger than D. It reduces into the selfdual and antiselfdual tensor spaces if the row number of the Young pattern is equal to $D/2$. Two representations are equivalent if their Young patterns are the same as each other except for the first column and the sum of their row numbers is equal to D. Those properties cause the situation for $D\leqslant 6$ different from that for $D>6$.

When $D=6$, there is no problem for the representation $[\mu,\nu,\tau]$ with $\tau=0$, but when $\tau\neq 0$, the representation is reducible. We denote the generalized spherical harmonic polynomials for the self-dual and anti-self-dual representations by $Q_{qpr}^{(S)\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ and $Q_{qpr}^{(A)\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$, respectively. $Q_{qpr}^{(S)\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ is the same as that given in Eq. (14), and $Q_{qpr}^{(A)\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ can be obtained from $Q_{qpr}^{(S)\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ by replacing X_{56}, Y_{56}, and Z_{56} with X'_{56}, Y'_{56}, and Z'_{56},

$$X'_{56}=x_5-ix_6,\quad Y'_{56}=y_5-iy_6,\quad Z'_{56}=z_5-iz_6. \tag{21}$$

The formula (16) for the dimension of the representation $[\mu,\nu,\tau]$ of SO(D) holds for $D=6$ when $\tau=0$. When $\tau\neq 0$, $d_D([\mu,\nu,\tau])$ in Eq. (16) is equal to the sum of the dimensions of the self-dual and antiselfdual representations such that the equality (19) still holds for $D=6$.

When $D=5$, in the possible Young pattern $[\mu,\nu,\tau]$, τ has to be 0 or 1. The representation $[\mu,\nu,1]$ is equivalent to the representation $[\mu,\nu,0]$. Their dimensions calculated from Eq. (16) are also the same. The generalized spherical harmonic polynomials $Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ given in Eq. (14) hold for $D=5$ except for $x_6=y_6=z_6=0$ and $\tau=0$ or 1. Therefore, the equality (19) holds for $D=5$.

For $D=3$, two Jacobi coordinate vectors, say $\mathbf{x}$ and $\mathbf{y}$, can completely determine the body-fixed frame so that the variables ζ_3 has to be changed as $(\mathbf{x}\times\mathbf{y})\cdot\mathbf{z}$ in order to distinguish two configurations with different directions of $\mathbf{z}$. We have discussed in detail the four-body system in three dimensions in our previous paper.[26]

The case of $D=4$ is quite complicated because SO(4) is not a simple group. The representation $[\mu,\nu,0]$ reduces to a direct sum of a self-dual representation $[(S)\mu,\nu,0]$ and an anti-self-dual one $[(A)\mu,\nu,0]$. The generalized spherical harmonic polynomials $Q_{qpr}^{(S)\mu\nu 0}(\mathbf{x},\mathbf{y},\mathbf{z})$ for the self-dual representations is the same as $Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ with $\tau=0$ given in Eq. (14). The generalized spherical harmonic polynomials $Q_{qpr}^{(A)\mu\nu 0}(\mathbf{x},\mathbf{y},\mathbf{z})$ for the anti-self-dual representation can be obtained from $Q_{qpr}^{(S)\mu\nu 0}(\mathbf{x},\mathbf{y},\mathbf{z})$ by replacing X_{34}, Y_{34}, and Z_{34} with X'_{34}, Y'_{34}, and Z'_{34},

$$X'_{34}=x_3-ix_4,\quad Y'_{34}=y_3-iy_4,\quad Z'_{34}=z_3-iz_4. \tag{22}$$

If $\tau=1$, then $\nu=1$ and the representation $[\mu,1,1]$ is equivalent to the representation $[\mu,0,0]$. The standard Young tableau is described by the parameters q and p $(r=1)$, where q and p are, respectively, the numbers of digits ''1'' and ''2'' in the first row of the Young tableau. The generalized spherical harmonic polynomials for two representations $[\mu,\lambda,\lambda]$, $\lambda=0$, or 1, are

$$Q_{qp}^{\mu\lambda\lambda}(\mathbf{x},\mathbf{y},\mathbf{z})=\frac{X_{12}^{q-\lambda}Y_{12}^{p}Z_{12}^{\mu-q-p}T^{\lambda}}{(q-\lambda)!p!(\mu-q-p)!},$$

$$T=X_{12}Y_{34}Z'_{34}+X_{34}Y'_{34}Z_{12}+X'_{34}Y_{12}Z_{34}-X_{12}Y'_{34}Z_{34}-X_{34}Y_{12}Z'_{34}-X'_{34}Y_{34}Z_{12}. \tag{23}$$

The surprising thing is that Eq. (19) is not satisfied for $D=4$ and $l\geqslant 6$. For example,

$l=$	6	7	8	9	10
$R_4(l)$	5346	10908	20550	36332	60996
$K_4(l)$	5336	10836	20256	35436	58728.

(24)

The reason is that the formula (18) for $K_D(l)$ does not hold for $D=4$ and $l\geqslant 6$. For $D=4$ we find an identity with respect to the polynomials of degree 6 checked by MATHEMATICA,

$$\xi_1 T_{23}^2+\eta_2 T_{13}^2+\zeta_3 T_{12}^2-2\xi_2 T_{13}T_{23}+2\xi_3 T_{12}T_{23}-2\eta_3 T_{12}T_{13}=0. \tag{25}$$

The identity obtained from Eq. (25) by replacing X_{34}, Y_{34}, and Z_{34}, respectively, with X'_{34}, Y'_{34}, and Z'_{34} still holds. Those equalities obtained by applying the lowering operators and (or) by multiplying a factor to above two identities are also identities. Thus, the forms $\xi_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, $\eta_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, and $\zeta_j f(\mathbf{x},\mathbf{y},\mathbf{z})$, where $f(\mathbf{x},\mathbf{y},\mathbf{z})$ is a homogeneous polynomial of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ of degree $(l-2)$, are not independent when $l\geqslant 6$. It is easy to count by MATHEMATICA that the revised $K_4(l)$ by considering the identities coincides with $R_4(l)$.

III. GENERALIZED RADIAL EQUATIONS

In the preceding section we proved that $d_{[\mu,\nu,\tau]}(\mathrm{SU}(3))$ polynomials $Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$ construct a complete set of independent basis functions for the angular momentum $[\mu,\nu,\tau]$. Thus, any function $\Psi_{\mathbf{M}}^{[\mu,\nu,\tau]}(\mathbf{x},\mathbf{y},\mathbf{z})$ with angular momentum $[\mu,\nu,\tau]$ in the system can be expanded with respect to the basis functions $Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z})$, where the coefficients are functions of internal variables,

$$\Psi_{\mathbf{M}}^{[\mu,\nu,\tau]}(\mathbf{x},\mathbf{y},\mathbf{z})=\sum_{q=\tau}^{\mu}\sum_{p=\max\{(\nu-q),0\}}^{\mu-q}\sum_{r=\tau}^{\min\{q,\nu\}}\psi_{qpr}^{\mu\nu\tau}(\xi_j,\eta_j,\zeta_j)Q_{qpr}^{\mu\nu\tau}(\mathbf{x},\mathbf{y},\mathbf{z}), \tag{26}$$

where the coefficients $\psi_{qpr}^{\mu\nu\tau}(\xi_j,\eta_j,\zeta_j)$ are called the generalized radial functions. When substituting Eq. (26) into the Schrödinger equation (5), the main calculation is to apply the Laplace operator (4) to the function $\Psi_{\mathbf{M}}^{[\mu,\nu,\tau]}(\mathbf{x},\mathbf{y},\mathbf{z})$. The calculation consists of three parts. In the following, we remove the arguments (ξ_j,η_j,ζ_j) and $(\mathbf{x},\mathbf{y},\mathbf{z})$ for simplicity. The first is to apply the Laplace operator to the generalized radial functions $\psi_{qpr}^{\mu\nu\tau}(\xi_j,\eta_j,\zeta_j)$, which can be calculated by replacement of variables,

$$\begin{aligned}\nabla^2\psi_{qpr}^{\mu\nu\tau}=&\{4\xi_1\partial_{\xi_1}^2+4\eta_2\partial_{\eta_2}^2+4\zeta_3\partial_{\zeta_3}^2+2D(\partial_{\xi_1}+\partial_{\eta_2}+\partial_{\zeta_3})+(\xi_1+\eta_2)\partial_{\xi_2}^2\\&+(\xi_1+\zeta_3)\partial_{\xi_3}^2+(\eta_2+\zeta_3)\partial_{\eta_3}^2+4\xi_2(\partial_{\xi_1}+\partial_{\eta_2})\partial_{\xi_2}+4\xi_3(\partial_{\xi_1}+\partial_{\zeta_3})\partial_{\xi_3}\\&+4\eta_3(\partial_{\eta_2}+\partial_{\zeta_3})\partial_{\eta_3}+2\eta_3\partial_{\xi_2}\partial_{\xi_3}+2\xi_3\partial_{\xi_2}\partial_{\eta_3}+2\xi_2\partial_{\xi_3}\partial_{\eta_3}\}\psi_{qpr}^{\mu\nu\tau},\end{aligned} \tag{27}$$

where ∂_ξ denotes $\partial/\partial\xi$ and so on. The second is to apply the Laplace operator to the generalized spherical harmonic polynomials $Q_{qpr}^{\mu\nu\tau}$. This part is vanishing because $Q_{qpr}^{\mu\nu\tau}$ satisfies the Laplace equation. The last is the mixed application

$$\begin{aligned}&2\{(\partial_{\xi_1}\psi_{qpr}^{\mu\nu\tau})2\mathbf{x}+(\partial_{\xi_2}\psi_{qpr}^{\mu\nu\tau})\mathbf{y}+(\partial_{\xi_3}\psi_{qpr}^{\mu\nu\tau})\mathbf{z}\}\cdot\nabla_{\mathbf{x}}Q_{qpr}^{\mu\nu\tau}+2\{(\partial_{\xi_2}\psi_{qpr}^{\mu\nu\tau})\mathbf{x}+(\partial_{\eta_2}\psi_{qpr}^{\mu\nu\tau})2\mathbf{y}\\&+(\partial_{\eta_3}\psi_{qpr}^{\mu\nu\tau})\mathbf{z}\}\cdot\nabla_{\mathbf{y}}Q_{qpr}^{\mu\nu\tau}+2\{(\partial_{\xi_3}\psi_{qpr}^{\mu\nu\tau})\mathbf{x}+(\partial_{\eta_3}\psi_{qpr}^{\mu\nu\tau})\mathbf{y}+(\partial_{\zeta_3}\psi_{qpr}^{\mu\nu\tau})2\mathbf{z}\}\cdot\nabla_{\mathbf{z}}Q_{qpr}^{\mu\nu\tau}.\end{aligned} \tag{28}$$

From the definition (14) for $Q_{qpr}^{\mu\nu\tau}$ we have

$$\mathbf{x}\cdot\nabla_{\mathbf{x}}Q_{qpr}^{\mu\nu\tau}=qQ_{qpr}^{\mu\nu\tau},\quad \mathbf{y}\cdot\nabla_{\mathbf{y}}Q_{qpr}^{\mu\nu\tau}=(p+r)Q_{qpr}^{\mu\nu\tau},$$

$$\mathbf{z}\cdot\nabla_{\mathbf{z}}Q_{qpr}^{\mu\nu\tau}=(\mu+\nu+\tau-q-p-r)Q_{qpr}^{\mu\nu\tau},$$

$$\mathbf{y}\cdot\nabla_{\mathbf{x}}Q_{qpr}^{\mu\nu\tau}=\begin{cases}\dfrac{(p+1)(q-r)}{q-\nu}Q_{(q-1)(p+1)r}^{\mu\nu\tau}-\dfrac{(\mu-q-p+1)(r-\tau+1)}{q-\nu}Q_{(q-1)p(r+1)}^{\mu\nu\tau},\\ \quad\text{when}\quad q>\nu,\\ (\nu-q+1)Q_{(q-1)(p+1)r}^{\mu\nu\tau},\quad\text{when}\quad q\leqslant\nu,\end{cases}$$

$$\mathbf{x}\cdot\nabla_{\mathbf{y}}Q^{\mu\nu\tau}_{qpr}=\begin{cases}(q-\nu+1)Q^{\mu\nu\tau}_{(q+1)(p-1)r}, & \text{when } q\geqslant\nu,\\ \dfrac{p(q-r+1)}{\nu-q}Q^{\mu\nu\tau}_{(q+1)(p-1)r}-\dfrac{(\mu-q-p+1)(r-\tau+1)}{\nu-q}Q^{\mu\nu\tau}_{(q+1)(p-2)(r+1)}, & \text{when } q<\nu,\end{cases}$$

$$\mathbf{z}\cdot\nabla_{\mathbf{x}}Q^{\mu\nu\tau}_{qpr}=\begin{cases}\dfrac{(\mu-q-p+1)(q-\nu+r-\tau)}{q-\nu}Q^{\mu\nu\tau}_{(q-1)pr}-\dfrac{(p+1)(\nu-r+1)}{q-\nu}\\ \quad\times Q^{\mu\nu\tau}_{(q-1)(p+1)(r-1)}, & \text{when } q>\nu,\\ -(\nu-q+1)Q^{\mu\nu\tau}_{(q-1)(p+1)(r-1)}, & \text{when } q\leqslant\nu,\end{cases}$$

$$\mathbf{x}\cdot\nabla_{\mathbf{z}}Q^{\mu\nu\tau}_{qpr}=\begin{cases}(q-\nu+1)Q^{\mu\nu\tau}_{(q+1)pr}, & \text{when } q\geqslant\nu,\\ \dfrac{(q+p-\nu+1)(q-r+1)}{\nu-q}Q^{\mu\nu\tau}_{(q+1)pr}-\dfrac{(r-\tau+1)(\mu+\nu-2q-p)}{\nu-q}\\ \quad\times Q^{\mu\nu\tau}_{(q+1)(p-1)(r+1)}, & \text{when } q<\nu,\end{cases}$$

$$\mathbf{z}\cdot\nabla_{\mathbf{y}}Q^{\mu\nu\tau}_{qpr}=\begin{cases}(\mu-q-p+1)Q^{\mu\nu\tau}_{q(p-1)r}+(\nu-r+1)Q^{\mu\nu\tau}_{qp(r-1)}, & \text{when } q\geqslant\nu,\\ (\mu-q-p+1)Q^{\mu\nu\tau}_{q(p-1)r}+(q-r+1)Q^{\mu\nu\tau}_{qp(r-1)}, & \text{when } q<\nu,\end{cases}$$

$$\mathbf{y}\cdot\nabla_{\mathbf{z}}Q^{\mu\nu\tau}_{qpr}=\begin{cases}(p+1)Q^{\mu\nu\tau}_{q(p+1)r}+(r-\tau+1)Q^{\mu\nu\tau}_{qp(r+1)}, & \text{when } q\geqslant\nu,\\ (q+p-\nu+1)Q^{\mu\nu\tau}_{q(p+1)r}+(r-\tau+1)Q^{\mu\nu\tau}_{qp(r+1)}, & \text{when } q<\nu.\end{cases}\tag{29}$$

Hence, we obtain the generalized radial equation, satisfied by the functions $\psi^{\mu\nu\tau}_{qpr}(\xi,\eta,\zeta)$,

$$\begin{aligned}&\nabla^2\psi^{\mu\nu\tau}_{qpr}+4q\partial_{\xi_1}\psi^{\mu\nu\tau}_{qpr}+4(p+r)\partial_{\eta_2}\psi^{\mu\nu\tau}_{qpr}+4(\mu+\nu+\tau-p-q-r)\partial_{\zeta_3}\psi^{\mu\nu\tau}_{qpr}\\ &\quad+\frac{2p(q-r+1)}{q-\nu+1}\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q+1)(p-1)r}-\frac{2(\mu-q-p)(r-\tau)}{q-\nu+1}\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q+1)p(r-1)}\\ &\quad+2(q-\nu)\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q-1)(p+1)r}+\frac{2(\mu-q-p)(q-\nu+r-\tau+1)}{q-\nu+1}\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q+1)pr}-\frac{2p(\nu-r)}{q-\nu+1}\\ &\quad\times\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q+1)(p-1)(r+1)}+2(q-\nu)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q-1)pr}+2(\mu-q-p)\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p+1)r}+2(\nu-r)\\ &\quad\times\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r+1)}+2p\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p-1)r}+2(r-\tau)\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r-1)}=-2(E-V)\psi^{\mu\nu\tau}_{qpr},\quad\text{for } q>\nu,\end{aligned}\tag{30a}$$

$$\begin{aligned}&\nabla^2\psi^{\mu\nu\tau}_{qpr}+4q\partial_{\xi_1}\psi^{\mu\nu\tau}_{qpr}+4(p+r)\partial_{\eta_2}\psi^{\mu\nu\tau}_{qpr}+4(\mu+\tau-p-r)\partial_{\zeta_3}\psi^{\mu\nu\tau}_{qpr}+2p(q-r+1)\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q+1)(p-1)r}\\ &\quad-2(\mu-q-p)(r-\tau)\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q+1)p(r-1)}+2(p+1)(q-r)\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q-1)(p+1)r}-2(\mu-q-p)(r-\tau)\\ &\quad\times\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q-1)(p+2)(r-1)}+2(\mu-q-p)(r-\tau+1)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q+1)pr}-2p(q-r)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q+1)(p-1)(r+1)}\\ &\quad+2p(q-r)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q-1)pr}-2(r-\tau)(\mu-q-p+1)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q-1)(p+1)(r-1)}+2(\mu-q-p)\\ &\quad\times\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p+1)r}+2(q-r)\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r+1)}+2p\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p-1)r}+2(r-\tau)\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r-1)}\\ &\quad=-2(E-V)\psi^{\mu\nu\tau}_{qpr},\quad\text{for } q=\nu,\end{aligned}\tag{30b}$$

$$\nabla^2\psi^{\mu\nu\tau}_{qpr}+4q\partial_{\xi_1}\psi^{\mu\nu\tau}_{qpr}+4(p+r)\partial_{\eta_2}\psi^{\mu\nu\tau}_{qpr}+4(\mu+\nu+\tau-p-q-r)\partial_{\zeta_3}\psi^{\mu\nu\tau}_{qpr}+2(\nu-q)$$
$$\times\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q+1)(p-1)r}+\frac{2(p+1)(q-r)}{\nu-q+1}\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q-1)(p+1)r}-\frac{2(\mu-q-p)(r-\tau)}{\nu-q+1}$$
$$\times\partial_{\xi_2}\psi^{\mu\nu\tau}_{(q-1)(p+2)(r-1)}-2(\nu-q)\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q+1)(p-1)(r+1)}+\frac{2(q+p-\nu)(q-r)}{\nu-q+1}$$
$$\times\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q-1)pr}-\frac{2(r-\tau)(\mu+\nu-2q-p+1)}{\nu-q+1}\partial_{\xi_3}\psi^{\mu\nu\tau}_{(q-1)(p+1)(r-1)}+2(\mu-q-p)$$
$$\times\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p+1)r}+2(q-r)\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r+1)}+2(q+p-\nu)\partial_{\eta_3}\psi^{\mu\nu\tau}_{q(p-1)r}+2(r-\tau)\partial_{\eta_3}\psi^{\mu\nu\tau}_{qp(r-1)}$$
$$=-2(E-V)\psi^{\mu\nu\tau}_{qpr},\quad \text{for } q<\nu, \tag{30c}$$

where $\nabla^2\psi^{\mu\nu\tau}_{qpr}$ is given in Eq. (27). Only six internal variables ξ_1, ξ_2, ξ_3, η_2, η_3, and ζ_3 are involved both in the equations and in the functions. Equation (30) holds either for $D>6$ or for $4\leqslant D\leqslant 6$. For the latter cases some self-dual representation, anti-self-dual representation, or equivalent representations may occur. Especially, for a four-body system in $D=4$ dimensions, the representation $[\mu,1,1]$ is equivalent to the representation $[\mu,0,0]$, but the generalized radial equations for them are decoupled. They will be coupled for the N-body system with $N>D=4$.

IV. QUANTUM *N*-BODY SYSTEM IN *D* DIMENSIONS

It is hard to write unified formulas of the generalized radial equations for an N-body system in arbitrary D-dimensions. However, from the study of the three-body[26,31] and four-body system, we are able to summarize the main features on separating the rotational degrees of freedom from the internal ones for an N-body Schrödinger equation in D dimensions.

First, after removing the motion of the center of mass, there are $(N-1)$ Jacobi coordinate vectors $\mathbf{R}_j$ for an N-body system. On the other hand, in a D-dimensional space one needs $(D-1)$ vectors to determine the body-fixed frame. When $D\geqslant N$, all Jacobi coordinate vectors are used to determine the body-fixed frame, and all internal variables can be chosen as $\mathbf{R}_j\cdot\mathbf{R}_k$. The numbers of the rotational variables and the internal variables are $(N-1)(2D-N)/2$ and $N(N-1)/2$, respectively. When $D<N$, only $(D-1)$ Jacobi coordinate vectors are involved to determine the body-fixed frame, and the remaining can be expressed by the first $(D-1)$ Jacobi coordinate vectors and the internal variables. The set of internal variables $\mathbf{R}_j\cdot\mathbf{R}_k$ is no longer complete because it could not distinguish two configurations, say with different $\mathbf{R}_D$ reflecting to the superplane spanned by the first $(D-1)$ Jacobi coordinate vectors. The correct choice for the internal variables are

$$\xi_{jk}=\mathbf{R}_j\cdot\mathbf{R}_k,\quad \zeta_\alpha=\sum_{a_1\cdots a_D}\epsilon_{a_1\cdots a_D}R_{1a_1}\cdots R_{(D-1)a_{D-1}}R_{\alpha a_D},$$
$$1\leqslant j\leqslant D-1,\quad j\leqslant k\leqslant N-1,\quad D\leqslant\alpha\leqslant N-1. \tag{31}$$

The numbers of the rotational variables and the internal variables are $D(D-1)/2$ and $D(2N-D-1)/2$, respectively.

Second, for an N-body system in D-dimensions $(D\geqslant N)$, the angular momentum is described by an irreducible representation of SO(D) denoted by an $(N-1)$-row Young pattern $[\mu]\equiv[\mu_1,\mu_2,\ldots,\mu_{N-1}]$, $\mu_1\geqslant\mu_2\geqslant\cdots\geqslant\mu_{N-1}$. Due to the rotational symmetry, one only needs to discuss the eigenfunctions of angular momentum with the highest weight. The complete set of independent basis functions with the highest weight consists of the eigenfunctions $Q^{[\mu]}_{(q)}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ identified by the standard Young tableau (q). Filling the digits 1, 2, ..., $N-1$ arbitrarily into a given Young pattern $[\mu]$ we obtain a Young tableau. A Young tableau is called standard if the digit in every column of the tableau increases downwards and the digit in

every row does not decrease from left to right. Any standard Young tableau is described by a set of parameters (q) which contains $(N-1)(N-2)/2$ parameters q_{jk}, $1\leqslant k\leqslant j\leqslant N-1$, denoting the number of the digit j in the kth row in the standard Young tableau. The number of independent basis functions $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ in the complete set is equal to the dimension $d_{[\mu]}[\mathrm{SU}(N-1)]$ of the irreducible representation $[\mu]$ of the SU$(N-1)$ group. $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ is a homogeneous polynomial of degree $\Sigma\mu_k$ with respect to the components of $(N-1)$ Jacobi coordinate vectors $\mathbf{R}_j$, and satisfies the generalized Laplace equations [see Eq. (20)]. The explicit form of $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ for the given standard Young tableau (q) is very easy to write. In the Young tableau, for each column with the length t, filled by digits $j_1<j_2<\cdots<j_t$, $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ contains a determinant as a factor. The rth row and sth column in the determinant is $R_{j_r(2s-1)}+iR_{j_r(2s)}$ if $D>2(N-1)$. $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ also contains a numerical coefficient for convenience. When $N\leqslant D\leqslant 2(N-1)$, some self-dual representation, anti-self-dual representation and equivalent representations have to be considered just like the discussion given in the end of Sec. II. When $D<N$, only the first $(D-1)$ Jacobi coordinate vectors are involved in the basis functions $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{D-1})$, which are the same as those for smaller $N=D$.

At last, when $D\geqslant N$, any wave function $\Psi_{\mathbf{M}}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ with the given angular momentum $[\mu]$ can be expanded with respect to the complete and independent basis functions $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$,

$$\Psi_{\mathbf{M}}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})=\sum_{(q)}\psi_{(q)}^{[\mu]}(\xi)Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1}), \tag{32}$$

where the coefficients $\psi_{(q)}^{[\mu]}(\xi)$, called the generalized radial functions, only depend upon the internal variables. When $D<N$, $\psi_{(q)}^{[\mu]}(\xi)$ and $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$ in Eq. (32) have to be replaced with $\psi_{(q)}^{[\mu]}(\xi,\zeta)$ and $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{D-1})$, respectively. Substituting Eq. (32) into the N-body Schrödinger equation in the center-of-mass frame,

$$\sum_{j=1}^{N-1}\nabla_{\mathbf{R}_j}^2\Psi_{\mathbf{M}}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})=-2\{E-V(\xi)\}\Psi_{\mathbf{M}}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1}), \tag{33}$$

one is able to obtain the generalized radial equations. The main calculation is to apply the Laplace operator to the function $\Psi_{\mathbf{M}}^{[\mu,\nu,\tau]}(\mathbf{x},\mathbf{y},\mathbf{z})$. The calculation consists of three parts. The first is to apply the Laplace operator to the generalized radial functions $\psi_{(q)}^{[\mu]}(\xi)$, which can be calculated by replacement of variables. When $D\geqslant N$ we have

$$\begin{aligned}\nabla^2\psi_{(q)}^{[\mu]}(\xi)=\Bigg\{&\sum_{j=1}^{N-1}(4\xi_{jj}\partial_{\xi_{jj}}^2+2D\partial_{\xi_{jj}})+\sum_{j=1}^{N-1}\sum_{k=j+1}^{N-1}[(\xi_{jj}+\xi_{kk})\partial_{\xi_{jk}}^2+4\xi_{jk}(\partial_{\xi_{jj}}+\partial_{\xi_{kk}})\partial_{\xi_{jk}}]\\&+2\sum_{j=1}^{N-1}\sum_{j\neq k=1}^{N-1}\sum_{j\neq t=k+1}^{N-1}\xi_{kt}\partial_{\xi_{jk}}\partial_{\xi_{jt}}\Bigg\}\psi_{(q)}^{[\mu]}(\xi),\end{aligned} \tag{34}$$

where $\xi_{jk}=\xi_{kj}$ and ∂_ξ denotes $\partial/\partial\xi$ and so on. The second is to apply the Laplace operator to the generalized spherical harmonic polynomials. This part is vanishing because the polynomials satisfy the Laplace equation. The last is the mixed application. When $D\geqslant N$ we have

$$2\sum_{j=1}^{N-1}\left\{(\partial_{\xi_{jj}}\psi_{(q)}^{[\mu]})2\mathbf{R}_j+\sum_{j\neq k=1}^{N-1}(\partial_{\xi_{jk}}\psi_{(q)}^{[\mu]})\mathbf{R}_k\right\}\cdot\nabla_{\mathbf{R}_j}Q_{(q)}^{[\mu]}, \tag{35}$$

where the formulas for $\mathbf{R}_j\cdot\nabla_{\mathbf{R}_j}Q_{(q)}^{[\mu]}$ and $\mathbf{R}_k\cdot\nabla_{\mathbf{R}_j}Q_{(q)}^{[\mu]}$ can be calculated from the property of the polynomial $Q_{(q)}^{[\mu]}(\mathbf{R}_1,\ldots,\mathbf{R}_{N-1})$. When $D<N$, the internal variables have to be chosen as those given in Eq. (31) so that Eq. (34) becomes more complicated and Eq. (35) contains more terms of $(\partial\zeta_\alpha/\partial\mathbf{R}_j)\cdot\nabla_{\mathbf{R}_j}Q_{(q)}^{[\mu]}$.[26]

V. CONCLUSIONS

In this paper, the problem of separating the rotational degrees of freedom from the internal ones for the Schrödinger equation of a four-body system in D dimensions is studied in detail by the method of the generalized spherical harmonic polynomials. We have found a complete set of independent basis functions with the given angular momentum described by an irreducible representation $[\mu,\nu,\tau]$ of SO(D). This set of basis functions have different form for the case $D>6$, $4\leqslant D\leqslant 6$, and $D=3$. We have provided an appropriate choice of internal variables for this system and derived the generalized radial equations depending solely on internal variables. The main features on the problem of separating the rotational degrees of freedom from the internal ones for the Schrödinger equation of a N-body system in D dimensions is summarized.

ACKNOWLEDGMENTS

This work is supported by the National Natural Science Foundation of China.

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Global symmetries of time-dependent Schrödinger equations

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(Received 28 October 2002; accepted 27 April 2003)

Some symmetries of time-dependent Schrödinger equations for inverse quadratic, linear, and quadratic potentials have been systematically examined by using a method suitable to the problem. Especially, the symmetry group for the case of the linear potential turns out to be a semidirect product $SL(2,R)\circledS T_2(R)$ of the $SL(2,R)$ with a two-dimensional real translation group $T_2(R)$. Here, the time variable t transforms as $t\to t'=(ct+d)/(at+b)$ for real constants a, b, c, and d satisfying $bc-ad=1$ with an accompanying transformation for the space coordinate x. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1591992]

I. FORMULATION

Many solutions of Schrödinger equations are known (Refs. 1–4 and earlier references quoted therein) to possess dynamical (or hidden) symmetries which are not apparent at first glance.

In a different approach, Eastwood[5] in his study of symmetry of Laplace equation has observed the following: Suppose that a pair of functions $U(\mathbf{x},\boldsymbol{\partial})$ and $W(\mathbf{x},\boldsymbol{\partial})$ of the coordinate $\mathbf{x}$ and its derivative $\boldsymbol{\partial}$ satisfies

$$W(\mathbf{x},\boldsymbol{\partial})\Delta=\Delta U(\mathbf{x},\boldsymbol{\partial}),\quad \left(\Delta=\sum_{j=1}^{n}\frac{\partial^2}{\partial x_j^2}\right)$$

for the Laplacian Δ. Then, if $\psi(\mathbf{x})$ is a solution of the Laplace equation $\Delta\psi(\mathbf{x})=0$, then so will be

$$\psi'(\mathbf{x})=U(\mathbf{x},\boldsymbol{\partial})\psi(\mathbf{x}).$$

The purpose of this note is to utilize an analogous method to systematically find global symmetries of time-independent Schrödinger equations. We consider the equation of motion of the form:

$$\frac{\partial}{\partial t}\psi(t,\mathbf{x})=k\{\Delta-V(\mathbf{x})\}\psi(t,\mathbf{x}). \tag{1.1}$$

If k is purely imaginary with $k=-i\hbar/2m$, then it describes the standard Schrödinger equation, while the case of k being real implies a diffusion-type equation. In what follows, we will always assume that the parameter k is either real or purely imaginary with t and $\mathbf{x}$ being real unless it is stated otherwise.

Consider now a vector space of all suitably smooth functions of t and $\mathbf{x}$, which may be complex. Suppose that we can find a pair of linear operators U and W in this space to satisfy the condition

$$W\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}=\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}U. \tag{1.2}$$

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Then, if $\psi(t,\mathbf{x})$ satisfies Eq. (1.1), the new function given by

$$\psi'(t,\mathbf{x}) = (U\psi)(t,\mathbf{x}) \equiv U\psi(t,\mathbf{x}) \tag{1.3}$$

will also obey the same relation, i.e., we have

$$\frac{\partial}{\partial t}\psi'(t,\mathbf{x}) = k\{\Delta - V(\mathbf{x})\}\psi'(t,\mathbf{x}). \tag{1.4}$$

Some explicit forms of U and W can be found as follows. Let us consider the coordinate transformation of form for $\mathbf{x}=(x_1,x_2,\ldots,x_n)$,

$$t \to t' = \phi(t), \tag{1.5a}$$

$$x_j \to x_j' = F_j(t,\mathbf{x}) \quad (j=1,2,\ldots,n) \tag{1.5b}$$

for some differentiable functions $\phi(t)$ and $F_j(t,\mathbf{x})$ to be determined. The action of the linear operator U to a function $\psi(t,\mathbf{x})$ is then assumed to be given as a multiplication of a function after the coordinate transformation, i.e.,

$$\psi'(t,\mathbf{x}) = U\psi(t,\mathbf{x}) = K(t,\mathbf{x})\psi(t',\mathbf{x}'), \tag{1.6}$$

where $K(t,\mathbf{x})$ is a function of t and $\mathbf{x}$ to be determined. When we note

$$\frac{\partial}{\partial t} = \dot{\phi}(t)\frac{\partial}{\partial t'} + \sum_{j=1}^{n}\frac{\partial F_j(t,\mathbf{x})}{\partial t}\frac{\partial}{\partial x_j'},$$

$$\frac{\partial}{\partial x_j} = \sum_{k=1}^{n}\frac{\partial F_k(t,\mathbf{x})}{\partial x_j}\frac{\partial}{\partial x_k'},$$

then we calculate

$$\begin{aligned}
\left\{\frac{\partial}{\partial t} - k\Delta + kV(\mathbf{x})\right\}\psi'(t,\mathbf{x}) &= \left\{\frac{\partial}{\partial t} - k\Delta + kV(\mathbf{x})\right\}[K(t,\mathbf{x})\psi(t',\mathbf{x}')] \\
&= \left\{\left[\frac{\partial}{\partial t} - k\Delta + kV(\mathbf{x})\right]K(t,\mathbf{x})\right\}\psi(t',\mathbf{x}') \\
&\quad + K(t,\mathbf{x})\sum_{j=1}^{n}\left\{\frac{\partial F_j(t,\mathbf{x})}{\partial t} - k\Delta F_j(t,\mathbf{x})\right. \\
&\quad \left. - 2k\sum_{\ell=1}^{n}\frac{\partial \log K(t,\mathbf{x})}{\partial x_\ell}\frac{\partial F_j(t,\mathbf{x})}{\partial x_\ell}\right\}\frac{\partial}{\partial x_j'}\psi(t',\mathbf{x}') \\
&\quad + K(t,\mathbf{x})\left\{\dot{\phi}(t)\frac{\partial}{\partial t'} - k\sum_{j,\ell=1}^{n}\left(\sum_{i=1}^{n}\frac{\partial F_j}{\partial x_i}\frac{\partial F_\ell}{\partial x_i}\right)\frac{\partial^2}{\partial x_j'\partial x_\ell'}\right\}\psi(t',\mathbf{x}').
\end{aligned} \tag{1.7}$$

If $F_j(t,\mathbf{x})$, and $K(t,\mathbf{x})$ satisfy relations:

$$\text{(i)} \quad \sum_{i=1}^{n}\frac{\partial F_j(t,\mathbf{x})}{\partial x_i}\frac{\partial F_\ell(t,\mathbf{x})}{\partial x_i} = \delta_{j\ell}\dot{\phi}(t)\left(\equiv \delta_{j\ell}\frac{\mathrm{d}}{\mathrm{d}t}\phi(t)\right), \tag{1.8a}$$

$$\text{(ii)} \quad \left(\frac{\partial}{\partial t}-k\Delta\right)F_j(t,\mathbf{x})=2k\sum_{\ell=1}^{n}\frac{\partial \log K(t,\mathbf{x})}{\partial x_\ell}\,\frac{\partial F_j(t,\mathbf{x})}{\partial x_\ell}, \tag{1.8b}$$

$$\text{(iii)} \quad \left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}K(t,\mathbf{x})=k\dot{\phi}(t)V(\mathbf{x}')K(t,\mathbf{x}), \tag{1.8c}$$

then Eq. (1.7) becomes

$$\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}\psi'(t,\mathbf{x})=\dot{\phi}(t)K(t,\mathbf{x})\left\{\frac{\partial}{\partial t'}-k\Delta'+kV(\mathbf{x}')\right\}\psi(t',\mathbf{x}'), \tag{1.9}$$

which reproduces Eq. (1.2) with actions of U and W given by

$$U\psi(t,\mathbf{x})=K(t,\mathbf{x})\psi(t',\mathbf{x}'), \tag{1.10a}$$

$$W\hat{\psi}(t,\mathbf{x})=\dot{\phi}(t)K(t,\mathbf{x})\hat{\psi}(t',\mathbf{x}'), \tag{1.10b}$$

for any two functions ψ and $\hat{\psi}$. For the present problem, we have

$$\hat{\psi}(t,\mathbf{x})=\left(\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right)\psi(t,\mathbf{x}).$$

Summarizing, we have proved the following Theorem.

Theorem 1.1: Let functions $\phi(t)$, $F_j(t,\mathbf{x})$, and $K(t,\mathbf{x})$ satisfy Eq. (1.8) with t' and x_j' being given by Eq. (1.5). Then for any function $\psi(t,\mathbf{x})$ which satisfies Eq. (1.1), i.e.,

$$\frac{\partial}{\partial t}\psi(t,\mathbf{x})=k\{\Delta-V(\mathbf{x})\}\psi(t,\mathbf{x}),$$

the new function given by

$$\psi'(t,\mathbf{x})=K(t,\mathbf{x})\psi(t',\mathbf{x}')=K(t,\mathbf{x})\psi(\phi(t),F_j(t,\mathbf{x}))$$

is also a solution of the same generalized Schrödinger equation, Eq. (1.1).

Remark 1.2: We may call the pair of linear operators (U,W) satisfying Eq. (1.2) admissible. Then, for the second admissible pair (U',W') their product (UU',WW') is clearly also admissible. Moreover, the special pair (1,1) acts as the identity. Therefore, a set of all admissible pairs form a semigroup. If the pair is invertible, then they present a symmetry group of Eq. (1.1). More explicitly, if the transformation with certain $V(\mathbf{x})$ are chosen as in Eq. (1.16), one gets a set S of possible ϕ, F, and K with elements $s \in S$ parametrized by real numbers a, $b,\ldots,$ i.e., $s=s(a,b,\ldots)$ and a set of solutions $\psi(t,\mathbf{x};a,b,\ldots)$. It will be shown in subsequent sections that the $s \in S$ and hence the corresponding solutions can be transformed into each other formally via e.g., $SL(2,R)$ depending upon $V(\mathbf{x})$.

We can modify Theorem 1.1 slightly as follows. Let $V_0(\mathbf{x})$ and $V(\mathbf{x})$ be two potentials, and suppose that the pair of linear operators (U,W) now satisfies

$$W\left\{\frac{\partial}{\partial t}-k\Delta+kV_0(\mathbf{x})\right\}=\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}U \tag{1.11}$$

instead Eq. (1.2). We can proceed exactly in the same way as in the previous case, and we prove the following theorem.

Theorem 1.3: Let functions $\phi(t)$, $F_j(t,\mathbf{x})$, and $K(t,\mathbf{x})$, as in Theorem 1.1 except that Eq. (1.8c) is now replaced by

$$\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}K(t,\mathbf{x})=k\dot{\phi}(t)V_0(\mathbf{x}')K(t,\mathbf{x}). \tag{1.12}$$

Then, for any function $\psi_0(t,\mathbf{x})$ satisfying

$$\left\{\frac{\partial}{\partial t}-k\Delta+kV_0(\mathbf{x})\right\}\psi_0(t,\mathbf{x})=0, \tag{1.13}$$

the function given by

$$\psi(t,\mathbf{x})=U\psi_0(t,\mathbf{x})=K(t,\mathbf{x})\psi_0(t',\mathbf{x}') \tag{1.14}$$

satisfies

$$\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}\psi(t,\mathbf{x})=0. \tag{1.15}$$

Remark 1.4: Examples satisfying Theorem 1.3 for $V_0(\mathbf{x})=0$ will be given in Secs. III and IV. If U^{-1} and W^{-1} exist, then we can conversely express $\psi_0(t,\mathbf{x})$ in terms of $\psi(t,\mathbf{x})$.

Returning now to the original discussion of Theorem 1.1, it is in general difficult to find solutions of differential equations, Eq. (1.8). However, for three cases of $V(\mathbf{x})$ being inverse square, linear, and quadratic potentials, we can solve them as follows. The explicit forms of $F_j(t,\mathbf{x})$ and $K(t,\mathbf{x})$ can then be assumed to be

$$t'=\phi(t), \tag{1.16a}$$

$$x_j'=F_j(t,\mathbf{x})=\xi(t)x_j+f_j(t), \tag{1.16b}$$

$$K(t,\mathbf{x})=\exp\left\{A(t)+\sum_{j=1}^{n}B_j(t)x_j+C(t)\mathbf{x}^2\right\}, \tag{1.16c}$$

for some functions $\phi(t)$, $\xi(t)$, $f_j(t)$, $A(t)$, $B_j(t)$, and $C(t)$ of t to be determined as in the following Proposition.

Proposition 1.5: Equation (1.8) will be satisfied for the ansatz Eq. (1.16), if we have

$$\text{(i)}\quad \dot{\phi}(t)=\xi^2(t), \tag{1.17a}$$

$$\text{(ii)}\quad B_j(t)=\frac{1}{2k}\,\frac{\dot{f}_j(t)}{\xi(t)}, \tag{1.17b}$$

$$\text{(iii)}\quad C(t)=\frac{1}{4k}\,\frac{\dot{\xi}(t)}{\xi(t)}, \tag{1.17c}$$

provided that $K(t,\mathbf{x})$ satisfies Eq. (1.8c), i.e.,

$$\left\{\frac{\partial}{\partial t}-k\Delta+kV(\mathbf{x})\right\}K(t,b)=k\dot{\phi}(t)V(\mathbf{x}')K(t,\mathbf{x}). \tag{1.18}$$

We will solve these differential equations, Eqs. (1.17) and (1.18), in subsequent sections. The simplest case of the inverse quadratic potential will be discussed in Sec. II, where the symmetry group is $SL(2,R)$. By contrast, the symmetry of the linear potential is a larger one of $SL(2,R)\,\textcircled{S}\,T_2(R)$ which is the semidirect product of $SL(2,R)$ with a real two-dimensional translation group $T_2(R)$. This will be presented in Sec. III. For the case of the quadratic potential in

Sec. IV, the symmetry is now either a semigroup or a subgroup of $SL(2,C)\,\textcircled{S}\,T_2(C)$, depending upon choices of parameters involved in theory. In Sec. V, we will discuss the associated Lie algebras of these groups.

Last, we simply remark that the present method will also be applicable when the potential is time-dependent. In that case, we simply replace all $V(\mathbf{x})$, $V(\mathbf{x}')$, $V_0(\mathbf{x})$, and $V_0(\mathbf{x}')$ in Theorem 1.1 and 1.3, respectively, by $V(t,\mathbf{x})$, $V(t',\mathbf{x}')$, $V_0(t,\mathbf{x})$, and $V_0(t',\mathbf{x}')$. Also, we may generalize the present method by replacing $K(t,\mathbf{x})$ by $K(t,\mathbf{x},\boldsymbol{\partial},\partial_t)$ which may depend upon both space and time derivatives, $\boldsymbol{\partial}$ and $\partial_t(\equiv \partial/\partial t)$.

II. INVERSE QUADRATIC POTENTIAL

In this section, we assume that the potential $V(\mathbf{x})$ is a homogeneous function of $\mathbf{x}$ of degree -2, i.e., it satisfies an identity

$$V(\lambda\mathbf{x})=\frac{1}{\lambda^2}V(\mathbf{x}) \tag{2.1}$$

for any nonzero real number λ. For example, we may assume

$$V(\mathbf{x})=\frac{\alpha}{x_1^2+x_2^2+\cdots+x_n^2}+\sum_{j=1}^{n}\frac{a_j}{(x_j)^2}+\sum_{j,k=1}^{n}\frac{b_{jk}}{(x_j-x_k)^2},$$

etc., for some constants α, a_j, and b_{jk}.

We must choose $f_j(t)=0$ with $x_j'=\xi(t)x_j$ in this case. Then Eq. (2.1) implies the validity of

$$V(\mathbf{x})=\xi^2(t)V(\mathbf{x}')=\dot{\phi}(t)V(\mathbf{x}')$$

for $\lambda=\xi(t)$ so that Eq. (1.18) becomes

$$\left\{\frac{\partial}{\partial t}-k\Delta\right\}K(t,\mathbf{x})=0,$$

which gives

$$\dot{A}(t)=2nkC(t),$$

$$\dot{C}(t)=4k(C(t))^2.$$

Solving these with Eq. (1.17) for $\xi(t)$ and $\phi(t)$, we find:

Proposition 2.1: For any function $\psi(t,\mathbf{x})$ satisfying

$$\frac{\partial}{\partial t}\psi(t,\mathbf{x})=k\{\Delta-V(\mathbf{x})\}\psi(t,\mathbf{x}) \tag{2.2}$$

with the condition Eq. (2.1) for $V(\mathbf{x})$, a new function given by

$$\psi'(t,\mathbf{x})=\left(\frac{1}{at+b}\right)^{n/2}\exp\left\{-\frac{a}{4k(at+b)}\mathbf{x}^2\right\}\psi(t',\mathbf{x}') \tag{2.3}$$

also satisfies the same equation, i.e.,

$$\frac{\partial}{\partial t}\psi'(t,\mathbf{x})=k\{\Delta-V(\mathbf{x})\}\psi'(t,\mathbf{x}), \tag{2.4}$$

where t' and $\mathbf{x}'$ are given by

$$t' = \frac{ct+d}{at+b}, \quad \mathbf{x}' = \frac{1}{at+b}\mathbf{x}. \tag{2.5}$$

Here, a, b, c, and d are arbitrary real constants satisfying the condition

$$bc - ad = 1. \tag{2.6}$$

We will show next that the admissible pair (U,W) of Sec. I will offer infinite dimensional realizations of the $SL(2,R)$ group. For this purpose, it is more convenient to consider 2×2 $SL(2,R)$ matrix M by

$$M = \begin{pmatrix} c & d \\ a & b \end{pmatrix}, \quad \det M = 1. \tag{2.7}$$

Moreover, we collectively write the coordinates as

$$Z = \{t, \mathbf{x}\} \tag{2.8}$$

on which M is assumed to act as

$$MZ = M\{t,\mathbf{x}\} = \{t',\mathbf{x}'\} = \left\{ \frac{ct+d}{at+b} \ , \ \frac{\mathbf{x}}{at+b} \right\}. \tag{2.9}$$

Since $K(t,\mathbf{x})$ depends upon parameters a, b, c, and d, we will write it as $K(t,\mathbf{x}|M)$ so that

$$K(t,\mathbf{x}|M) \equiv K(Z|M) = \left(\frac{1}{at+b} \right)^{n/2} \exp\left\{ -\frac{a}{4k(at+b)}\mathbf{x}^2 \right\}. \tag{2.10}$$

It is then easy to verify.

Proposition 2.2: For any two $SL(2,R)$ matrices M and M', we have

$$\text{(i)} \quad M(M'Z) = (MM')Z, \tag{2.11a}$$

$$\text{(ii)} \quad K(Z|M')K(M'Z|M) = K(Z|MM'), \tag{2.11b}$$

where MM' implies the standard matrix product of M and M'.

The linear operators U and W introduced in Sec. I also depend upon M. However, it is more convenient to rewrite them as $U(M^{-1})$ and $W(M^{-1})$ instead of $U(M)$ and $W(M)$ for a reason which will become clear shortly, so that Eq. (2.3) is rewritten as

$$U(M^{-1})\psi(Z) = K(Z|M)\psi(MZ). \tag{2.12}$$

Note that

$$M^{-1} = \begin{pmatrix} b & -d \\ -a & c \end{pmatrix} \quad \text{for} \quad M = \begin{pmatrix} c & d \\ a & b \end{pmatrix}.$$

Then, Eq. (2.11) is immediately translated into the following:

Proposition 2.3: Linear operators $U(M)$ and $W(M)$ satisfy

$$U(MM') = U(M)U(M'), \tag{2.13a}$$

$$W(MM') = W(M)W(M'). \tag{2.13b}$$

In other words, they offer (infinite dimensional) realizations of the $SL(2,R)$ group.

In ending this section, it may be of interest to note the following:

Remark 2.4: The transformation, Eq. (2.5), contains both time translation and dilatation as special cases. If we choose

$$M=\begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix},$$

then Eq. (2.5) gives the time translation,

$$t\to t'=t+\lambda, \quad \mathbf{x}\to\mathbf{x}'=\mathbf{x}.$$

On the other side, the choice of

$$M=\begin{pmatrix} c & 0 \\ 0 & \dfrac{1}{c} \end{pmatrix} \quad (c\neq 0) \tag{2.14a}$$

leads to the dilatation

$$t\to t'=c^2 t, \quad \mathbf{x}\to\mathbf{x}'=c\mathbf{x}. \tag{2.14b}$$

Remark 2.5: For some subgroup of $SL(2,R)$, the linear operator $U(M)$ may possess a non-trivial fixed point in the function space. Consider the one-dimensional case of $n=1$ with $V(\mathbf{x})=0$. The Jacobi's theta function $\theta_1(x|t)$ is given[6] by

$$\theta_1(x|t)=i\sum_{n=-\infty}^{\infty}(-1)^n \exp\left\{ i\pi\left(n-\frac{1}{2}\right)^2 t+i\pi(2n-1)x\right\}, \tag{2.15}$$

which satisfies the one-dimensional Schrödinger equation

$$4\pi i\frac{\partial}{\partial t}\theta_1(x|t)=\frac{\partial^2}{\partial x^2}\theta_1(x|t) \tag{2.16}$$

with $k=-i/4\pi$. Moreover, if a, b, c, d are all integers with $bc-ad=1$, we then have the identity[6]

$$\theta_1\left(\frac{x}{at+b}\,\middle|\,\frac{ct+d}{at+b}\right)=\epsilon(at+b)^{1/2}\exp\left(\frac{i\pi a x^2}{at+b}\right)\theta_1(x|t), \tag{2.17}$$

where ϵ is a constant satisfying $\epsilon^8=1$, whose particular value depends upon the specification of branches of $(at+b)^{1/2}$ in the complex t plane. Setting $\epsilon=1$. Eq. (2.17) is rewritten as

$$U(M_0)\theta_1(x|t)=\theta_1(x|t) \tag{2.18}$$

for any modular matrix M_0. Therefore, the $SL(2,R)$ orbit of $\theta_1(x|t)$ is the homogeneous space

$$SL(2,R)/SL(2,Z),$$

where $SL(2,Z)$ is the modular subgroup of $SL(2,R)$ in which all a, b, c, and d are integers.

Remark 2.6: For the one-dimensional case with $V(\mathbf{x})=0$, the symmetry group is actually a larger one of $SL(2,R)\,\textcircled{S}\,T_2(R)$ which is a semidirect product of $SL(2,R)$ with a two-dimensional translation group $T_2(R)$. This will be shown as a special case of $\alpha=\beta=0$ in Eqs. (3.5)–(3.10) in the following.

III. LINEAR POTENTIAL

In this section, we will consider the case of the linear potential. For a while, we restrict ourselves to one-dimensional space and set

$$V(x)=\alpha+\beta x \tag{3.1}$$

for constants α and β. Dropping all subindices such as j's in $f_j(t)$, $B_j(t)$, etc. (since $n=1$), Eqs. (1.18) and (1.16c) then gives [with $\dot{A}(t)\equiv(\mathrm{d}/\mathrm{d}t)\,A(t)$, etc.]

$$\text{(i)}\quad \dot{C}(t)=4kC^2(t), \tag{3.2a}$$

$$\text{(ii)}\quad \dot{B}(t)=4kB(t)C(t)+k\beta[\xi^3(t)-1], \tag{3.2b}$$

$$\text{(iii)}\quad \dot{A}(t)=k\{B^2(t)+2C(t)\}+k\alpha(\xi^2(t)-1)+k\beta\xi^2(t)f(t). \tag{3.2c}$$

Together with Eq. (1.17), which gives $2kB(t)=\dot{f}(t)/\xi(t)$ and $4kC(t)=\dot{\xi}(t)/\xi(t)$, we can solve these equations. In this case, the general solution contains five independent real parameters. It is convenient for our purpose to parametrize them as

$$\Lambda=\left\{M,\begin{pmatrix}\mu\\ \nu\end{pmatrix}\right\}, \tag{3.3a}$$

$$M=\begin{pmatrix}c & d\\ a & b\end{pmatrix},\quad \det M=1, \tag{3.3b}$$

where M is the real 2×2 unimodular matrix just as in Sec. II, which acts now on a two-dimensional real vector $\binom{\mu}{\nu}$ in the parameter space. We write $C(t)$, $B(t)$, etc., now as $C(t|\Lambda)$, $B(t|\Lambda)$, etc., in order to indicate their dependence on parameters involved in Λ. We also rewrite $K(t,x)$ of Sec. I as

$$K(t,x|\Lambda)=\frac{1}{\sqrt{at+b}}\exp\{A(t|\Lambda)+B(t|\Lambda)x+C(t|\Lambda)x^2\}, \tag{3.4}$$

where we changed however $A(t)$ there into $A(t|\Lambda)-\frac{1}{2}\log(at+b)$ for simplicity. Then, their explicit forms are found to be

$$\text{(i)}\quad C(t|\Lambda)=-\frac{1}{4k}\,\frac{a}{at+b}, \tag{3.5a}$$

$$\text{(ii)}\quad B(t|\Lambda)=-\frac{\nu}{2k}\,\frac{1}{at+b}+\frac{k\beta}{2}\left\{\frac{2(ct+d)}{(at+b)^2}-t-\frac{bt}{at+b}\right\}, \tag{3.5b}$$

$$\begin{aligned}\text{(iii)}\quad A(t|\Lambda)=&-\frac{1}{4k}\mu\nu+\alpha k\left(\frac{ct+d}{at+b}-t\right)+\frac{\nu^2}{4k}\,\frac{ct+d}{at+b}+k\beta\left\{\mu\,\frac{ct+d}{at+b}-\nu\left[\left(\frac{ct+d}{at+b}\right)^2\right.\right.\\ &\left.\left.-\frac{1}{2}\,\frac{t^2}{at+b}\right]\right\}+k^3\beta^2\left\{\frac{2}{3}\left(\frac{ct+d}{at+b}\right)^3+\frac{1}{12}t^3+\frac{b}{4}\,\frac{t^3}{at+b}-\frac{t^2(ct+d)}{(at+b)^2}\right\}.\end{aligned} \tag{3.5c}$$

In Eq. (3.5c), the constant term $-\mu\nu/4k$ has been added to simplify the expression of $\omega(\Lambda,\Lambda')$ given in Eq. (3.16) shortly. We then have the following Proposition.

Proposition 3.1: For any function $\psi(t,x)$ satisfying

$$\frac{\partial}{\partial t}\psi(t,x)=k\left\{\frac{\partial^2}{\partial x^2}-\alpha-\beta x\right\}\psi(t,x), \tag{3.6}$$

the new wave function given by

$$\psi'(t,x)=K(t,x|\Lambda)\psi(t',x') \tag{3.7}$$

satisfies the same, i.e.,

$$\frac{\partial}{\partial t}\psi'(t,x)=k\left\{\frac{\partial^2}{\partial x^2}-\alpha-\beta x\right\}\psi'(t,x), \tag{3.8}$$

where t' and x' are defined by

$$t'=\frac{ct+d}{at+b}, \tag{3.9a}$$

$$x'=\frac{x}{at+b}+\mu-\nu\frac{ct+d}{at+b}+k^2\beta\left\{\left(\frac{ct+d}{at+b}\right)^2-\frac{t^2}{at+b}\right\}. \tag{3.9b}$$

Next we will show that the underlying symmetry group is now the semidirect product

$$G=SL(2,R)\ \ \textcircled{S}T_2(R). \tag{3.10}$$

Let $\Lambda' \in G$ with

$$\Lambda'=\left\{M',\begin{pmatrix}\mu'\\ \nu'\end{pmatrix}\right\},\quad \det M'=1$$

be the second generic element of G in addition to Λ given by Eq. (3.3). We introduce the product $\Lambda\circ\Lambda'$ by

$$\Lambda\circ\Lambda'=\left\{MM',\begin{pmatrix}\mu\\ \nu\end{pmatrix}+M\begin{pmatrix}\mu'\\ \nu'\end{pmatrix}\right\}, \tag{3.11}$$

which can easily be verified to be associative and defines the desired group product of the group G. Note that the unit element 1 and the inverse Λ^{-1} are then given by

$$1=\left\{\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad\begin{pmatrix}0\\0\end{pmatrix}\right\}, \tag{3.12a}$$

$$\Lambda^{-1}=\left\{M^{-1},-M^{-1}\begin{pmatrix}\mu\\ \nu\end{pmatrix}\right\}, \tag{3.12b}$$

respectively. Again, it is convenient to write

$$Z=\{t,x\} \tag{3.13}$$

collectively for coordinates and assume the action of $\Lambda \in G$ to Z to be given by

$$\Lambda Z=\Lambda\{t,x\}=\{t',x'\}, \tag{3.14}$$

in terms of t' and x' given by Eqs. (3.9). We then find

Proposition 3.2: We have

$$\text{(i)}\quad \Lambda\{\Lambda' Z\}=(\Lambda\circ\Lambda')Z, \tag{3.15a}$$

$$\text{(ii)} \quad K(Z|\Lambda')K(\Lambda' Z|\Lambda) = \exp\{\omega(\Lambda,\Lambda')\}K(Z|\Lambda\circ\Lambda'). \tag{3.15b}$$

Here, $\omega(\Lambda,\Lambda')$ is a constant given by

$$\omega(\Lambda,\Lambda') = \frac{1}{4k}\{(\mu a - \nu c)\mu' + (\mu b - \nu d)\nu'\}, \tag{3.16}$$

which satisfies the cycle condition

$$\omega(\Lambda_1,\Lambda_2) + \omega(\Lambda_1\circ\Lambda_2,\Lambda_3) = \omega(\Lambda_2,\Lambda_3) + \omega(\Lambda_1,\Lambda_2\circ\Lambda_3) \tag{3.17a}$$

as well as

$$\omega(\Lambda_2^{-1},\Lambda_1^{-1}) = -\omega(\Lambda_1,\Lambda_2) \tag{3.17b}$$

for $\Lambda_j \in G$ $(j=1,2,3)$.

The proof of this Proposition requires unfortunately long computations, although it is straightforward. First, we set

$$\Lambda' Z = \Lambda'\{t,x\} \equiv \{\overline{t},\overline{x}\}$$

so that

$$\overline{t} = \phi(t|\Lambda') = \frac{c't+d'}{a't+b'},$$

$$\overline{x} = \xi(t|\Lambda')x + f(t|\Lambda')$$

with

$$\xi(t|\Lambda') = \frac{1}{a't+b'},$$

$$f(t|\Lambda') = \mu' - \nu'\frac{c't+d'}{a't+b'} + k^2\beta\left\{\left(\frac{c't+d'}{a't+b'}\right)^2 - \frac{t^2}{a't+b'}\right\}.$$

Since

$$K(Z|\Lambda') = \frac{1}{\sqrt{a't+b'}}\exp\{A(t|\Lambda') + B(t|\Lambda')x + C(t|\Lambda')x^2\}$$

and

$$K(\Lambda' Z|\Lambda) = \frac{1}{\sqrt{a\overline{t}+b}}\exp\{A(\overline{t}|\Lambda) + B(\overline{t}|\Lambda)\overline{x} + C(\overline{t}|\Lambda)\overline{x}^2\},$$

we must now evaluate the product

$$K(Z|\Lambda')K(\Lambda' Z|\Lambda) = \frac{1}{\sqrt{a''t+b''}}\exp\{A_0(t) + B_0(t)x + C_0(t)x^2\},$$

with

$$A_0(t) = A(t|\Lambda') + A(\overline{t}|\Lambda) + B(\overline{t}|\Lambda)f(t|\Lambda') + C(\overline{t}|\Lambda)[f(t|\Lambda')]^2,$$

$$B_0(t)=B(t|\Lambda')+B(\overline{t}|\Lambda)\xi(t|\Lambda')+2C(\overline{t}|\Lambda)\xi(t|\Lambda')f(t|\Lambda'),$$

$$C_0(t)=C(t|\Lambda')+C(\overline{t}|\Lambda)[\xi(t|\Lambda')]^2.$$

Using expressions given in Eq. (3.5), we can then verify the validity of Eq. (3.15b) after long calculations. For its computation, the following identities are however quite useful to simplify the proof. Let us set

$$M''=MM'=\begin{pmatrix} c & d \\ a & b \end{pmatrix}\begin{pmatrix} c' & d' \\ a' & b' \end{pmatrix}=\begin{pmatrix} c'' & d'' \\ a'' & b'' \end{pmatrix} \tag{3.18}$$

for $M,\ M'\in SL(2,R)$. We then find

$$\text{(i)}\quad a\left(\frac{c't+d'}{a't+b'}\right)+b=\frac{a''t+b''}{a't+b'},\quad c\left(\frac{c't+d'}{a't+b'}\right)+d=\frac{c''t+d''}{a't+b'}, \tag{3.19a}$$

$$\text{(ii)}\quad \frac{a}{(a't+b')(a''t+b'')}=\frac{a''}{a''t+b''}-\frac{a'}{a't+b'}, \tag{3.19b}$$

$$\text{(iii)}\quad a't+b'=c(a''t+b'')-a(c''t+d''),$$

$$c't+d'=-d(a''t+b'')+b(c''t+d''). \tag{3.19c}$$

Also, for the proof at Eq. (3.17), it is more convenient to rewrite Eq. (3.16) in the matrix notation of

$$4k\omega(\Lambda,\Lambda')=\begin{pmatrix} \mu \\ \nu \end{pmatrix}^T JM\begin{pmatrix} \mu' \\ \nu' \end{pmatrix}, \tag{3.20}$$

where $\binom{\mu}{\nu}^T$ is the transpose of $\binom{\mu}{\nu}$, and J is given by

$$J=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{3.21a}$$

which satisfies

$$M^TJM=MJM^T=J \tag{3.21b}$$

for any $M\in SL(2,R)$ and its transpose matrix M^T.

Rewriting U and W of Sec. I as $U(\Lambda^{-1})$ and $W(\Lambda^{-1})$ so that

$$U(\Lambda^{-1})\psi(Z)=\psi'(Z)=K(Z|\Lambda)\psi(Z'), \tag{3.22}$$

Proposition 3.2 immediately leads to:

Corollary 3.3: We have

$$U(\Lambda\circ\Lambda')=\exp\{-\omega(\Lambda,\Lambda')\}U(\Lambda)U(\Lambda'), \tag{3.23a}$$

$$W(\Lambda\circ\Lambda')=\exp\{-\omega(\Lambda,\Lambda')\}W(\Lambda)W(\Lambda'). \tag{3.23b}$$

In other words, both $U(\Lambda)$ and $W(\Lambda)$ offer projective representations of $G=SL(2,R)\circledS T_2(R)$. We note here that the cycle condition, Eq. (3.17a), ensures the compatibility of Eq. (3.23) with the associativity of products $U(\Lambda)U(\Lambda')$ and $W(\Lambda)W(\Lambda')$.

Before going into further detail, it may be worthwhile to make the following remark.

Remark 3.4: The group $G=SL(2,R)\circledS T_2(R)$ contains, in some sense, the Galilean group. Consider a set of all $\Lambda \in G$ of form

$$\Lambda=\left\{\begin{pmatrix}1 & \lambda\\ 0 & 1\end{pmatrix},\ \begin{pmatrix}\mu\\ \nu\end{pmatrix}\right\}, \tag{3.24}$$

which causes the coordinate transformation,

$$\begin{aligned} t&\to t'=t+\lambda,\\ x&\to x'=x+\sigma+vt \end{aligned} \tag{3.25a}$$

with

$$\begin{aligned} \sigma&=\mu-\nu\lambda+k^2\beta\lambda^2,\\ v&=2k^2\beta\lambda-\nu \end{aligned} \tag{3.25b}$$

by Eq. (3.9). We note that the classical Newton's equation $m\ddot{x}=F$ is invariant under the Galilean transformation since the Newtonian force F is constant for the linear potential. Therefore, in some sense, the group $G=SL(2,R)\circledS T_2$ together with Eq. (3.9) may be said to be a quantum-mechanical generalization of the Galilean transform.

We will next give examples of Theorem 1.3 for the case of $V_0(\mathbf{x})=0$ and $V(\mathbf{x})=\alpha+\beta x$. For simplicity, we set

$$\mathcal{H}_0=\left\{\psi_0(t,x)\middle|\left(\frac{\partial}{\partial t}-k\Delta\right)\psi_0(t,x)=0\right\}, \tag{3.26a}$$

$$\mathcal{H}=\left\{\psi(t,x)\middle|\left(\frac{\partial}{\partial t}-k\Delta+k\alpha+k\beta x\right)\psi(t,x)=0\right\}. \tag{3.26b}$$

First, we note that Eq. (1.12) for $V_0(\mathbf{x})=0$ implies $K(t,x)\in\mathcal{H}$. Solving conditions stated in Theorem 1.3, we then have two distinct solutions, corresponding to $C(x)=0$ or $\neq 0$. Rewriting these $K(t,x)$ now as $f_j(t,x)$ $(j=1,2)$. We have:

Proposition 3.5: Let us set

$$f_1(t,x)=\exp\{-k(\alpha+\beta x)t+\tfrac{1}{3}k^3\beta^2t^3\}, \tag{3.27a}$$

$$f_2(t,x)=\sqrt{\frac{1}{t}}\exp\left\{-kt\left(\alpha+\frac{\beta}{2}x\right)+\frac{1}{12}k^3\beta^2t^3-\frac{x^2}{4kt}\right\}, \tag{3.27b}$$

both of which are elements of $\mathcal{H}$. Then, for any $\psi_0(t,x)\in\mathcal{H}_0$, the functions defined by

$$\psi_j(t,x)=f_j(t,x)\psi_0(t_j',x_j') \quad (j=1,2) \tag{3.28}$$

are elements of $\mathcal{H}$, where

$$t_1'=t, \quad x_1'=x-k^2\beta t^2, \tag{3.29a}$$

$$t_2'=-\frac{1}{t}, \quad x_2'=\frac{x}{t}-k^2\beta t. \tag{3.29b}$$

Conversely, suppose $\psi(t,x)\in\mathcal{H}$. Then, new functions defined by

$$\psi_0^{(j)}(t,x)=\phi_j(t,x)\psi(\tilde{t}_j,\tilde{x}_j) \quad (j=1,2) \tag{3.30}$$

are elements of $\mathcal{H}_0$, where we have set

$$\phi_1(t,x)=\exp\{k[\alpha+\beta x]t+\tfrac{2}{3}k^2\beta^3t^3\}, \tag{3.31a}$$

$$\phi_2(t,x)=\frac{1}{\sqrt{t}}\exp\left\{-\frac{k\alpha}{t}-\frac{2}{3}\frac{k^2\beta^3}{t^3}-\frac{k\beta x}{t^2}-\frac{x^2}{4kt}\right\}, \tag{3.31b}$$

with

$$\tilde{t}_1=t, \quad \tilde{x}_1=x+k^2\beta t^2, \tag{3.32a}$$

$$\tilde{t}_2=-\frac{1}{t}, \quad \tilde{x}_2=\frac{x}{t}+\frac{k^2\beta}{t^2}. \tag{3.32b}$$

So far, we have considered only one-dimensional problems. However, we can find some examples for multidimensional cases with the same symmetry group $G=SL(2,R)\,\textcircled{S}\,T_2(R)$.

Example 3.6: Suppose that $\psi(t,\mathbf{x})$ with $\mathbf{x}=(x_1,x_2,\ldots,x_n)$ satisfy

$$\frac{\partial}{\partial t}\psi(t,\mathbf{x})=k\left\{\Delta-\sum_{j=1}^{n}(\alpha+\beta x_j)-\sum_{j,k=1}^{n}\frac{a_{jk}}{(x_j-x_k)^2}\right\}\psi(t,\mathbf{x}), \tag{3.33}$$

where a_{jk} with $a_{jj}=0$ are some constants. We also set

$$\tilde{K}(t,\mathbf{x}|\Lambda)=\prod_{j=1}^{n}K(t,x_j|\Lambda), \tag{3.34}$$

where $K(t,x|\Lambda)$ is given by Eqs. (3.4) and (3.5). Moreover, we consider the transformation

$$\psi(t,\mathbf{x})\to\psi'(t,\mathbf{x})=\tilde{K}(t,\mathbf{x}|\Lambda)\psi(t',\mathbf{x}'), \tag{3.35}$$

where t' and x_j' are given by Eq. (3.9) by replacing x there by x_j' for each $j=1,2,\ldots,n$. When we note

$$x_j'-x_k'=\frac{1}{at+b}(x_j-x_k),$$

for $j,k=1,2,\ldots,n$, we can readily verify the validity of Eq. (1.9) so that $\psi'(t,\mathbf{x})$ is another solution of Eq. (3.33).

Example 3.7: As we will see in the following, the two-dimensional nonlinear Schrödinger equation (see Refs. 4 and 7–9 on the subject)

$$\frac{\partial}{\partial t}\psi(t,x_1,x_2)=k\left\{\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\lambda|\psi(t,x_1,x_2)|^2\right\}\psi(t,x_1,x_2) \tag{3.36}$$

possesses also $G=SL(2,R)\,\textcircled{S}\,T_2(R)$ symmetry in spite of the nonlinearity of Eq. (3.36), provided that the parameter k is purely imaginary. Let $\tilde{K}(t,x_1,x_2)$ be given again by Eq. (3.34) with $\alpha=\beta=0$ for $n=2$ so that

$$\tilde{K}(t,x_1,x_2|\Lambda)=\frac{1}{at+b}\exp\left\{-\frac{1}{2k}\mu\nu+\frac{\nu^2}{2k}\,\frac{ct+d}{at+b}-\frac{\nu}{2k}\,\frac{1}{at+b}(x_1+x_2)-\frac{1}{4k}\,\frac{a}{at+b}(x_1^2+x_2^2)\right\}. \tag{3.37}$$

We note then that we have

$$|\tilde{K}(t,x_1,x_2|\Lambda)|^2=\frac{1}{(at+b)^2}$$

if k is purely imaginary. Then, the new function $\psi'(t,x_1,x_2)$ given by Eq. (3.35) for $n=2$ also satisfies

$$|\psi'(t,x_1,x_2)|^2=\frac{1}{(at+b)^2}|\psi(t',x_1',x_2')|^2.$$

As the consequence, it satisfies the analog of Eq. (1.9), i.e.,

$$\left\{\frac{\partial}{\partial t}-k\Delta+k\lambda|\psi'(t,x_1,x_2)|^2\right\}\psi'(t,x_1,x_2)$$
$$=\frac{1}{(at+b)^2}\tilde{K}(t,x_1,x_2)\left\{\frac{\partial}{\partial t'}-k\Delta'+k\lambda|\psi(t',x_1',x_2')|^2\right\}\psi(t',x_1',x_2')=0.$$

Remark 3.8: Let us return now to the function $f_1(t,x)$ given by Eq. (3.27a). One thing interesting about this function is that it is intimately related to a bound state problem. Consider the eigenvalue problem of

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\beta x\right\}u(x)=Eu(x) \tag{3.38}$$

with the boundary condition $u(0)=0$ at $x=0$ for some eigenfunction $u(x)\in L^2(0,\infty)$. To see the connection, we first note

$$\frac{\partial}{\partial t}f_1(t,x)=k\left\{\frac{\partial^2}{\partial x^2}-(\alpha+\beta x)\right\}f_1(t,x) \tag{3.39}$$

since $f_1(t,x)\in\mathcal{H}$. We next choose $k=-i$, and observe

$$\lim_{t\to\pm\infty}f_1(t+i\delta,x)=0,$$

for any $\delta>0$. Therefore, if we set

$$u(x)=\int_{-\infty}^{\infty}\mathrm{d}t\,f_1(t+i\delta,x) \tag{3.40}$$

and integrate Eq. (3.39) in t, $u(x)$ satisfies Eq. (3.38) with $E=-\alpha$. Moreover, letting $\delta\to+0$, we calculate

$$u(x)=2\int_0^{\infty}\mathrm{d}t\cos\left\{(\alpha+\beta x)t+\frac{1}{3}\beta^2t^3\right\}, \tag{3.41}$$

which is the Airy's function[10] with $u(x)\in L^2(0,\infty)$ for $\beta>0$. Therefore, if we set $x=0$ with $\alpha=-E$, the boundary condition $u(0)=0$ leads to

$$\int_0^\infty dt \cos\left(\frac{1}{3}\beta^2 t^3 - Et\right) = 0. \tag{3.42}$$

The relevance of this solution to the quarquonium spectra for the S-wave bound states of the three-dimensional confining linear potential can be found in Ref. 11.

Remark 3.9: Another interesting property of the function $f_1(t,x)$ is that it is invariant under the following two-dimensional Abelian subgroup G_0 of G, which consists of all elements of form:

$$\Lambda_0 = \left\{ \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} \mu \\ 0 \end{pmatrix} \right\}. \tag{3.43}$$

Then, it is straightforward to show the validity of

$$U(\Lambda_0) f_1(t,x) = f_1(t,x)$$

so that the G-orbit of $f_1(t,x)$ is the symmetric space G/G_0. Note that under Λ_0, the coordinate transform as a special Galilean transformation of

$$t \to t' = t + \lambda,$$

$$x \to x' = x + (\mu + k^2 \beta \lambda^2) + 2k^2 \beta \lambda t$$

by Eq. (3.25).

Remark 3.10: If we set $\mu = \nu = 0$, then the group G reduces to $SL(2,R)$. Consider now the following time-dependent potential

$$V(t,x) = \alpha + \beta x + \frac{\lambda}{(x - k^2 \beta t^2)^2} \tag{3.44}$$

for a constant λ. Then, the wave function $\psi(t,x)$ satisfying

$$\frac{\partial}{\partial t}\psi(t,x) = k\left\{\frac{\partial^2}{\partial x^2} - V(t,x)\right\}\psi(t,x) \tag{3.45}$$

is still invariant under the $SL(2,R)$ symmetry, since we will have

$$x' - k^2 \beta t'^2 = \frac{1}{at+b}(x - k^2 \beta t^2) \tag{3.46}$$

under Eq. (3.9) with $\mu = \nu = 0$. In sec. V, we will also show that any function $\psi(t,x)$ satisfying Eq. (3.45) is an eigenstate of the Casimir invariant I_2 of the $s\ell(2)$ Lie algebra.

IV. QUADRATIC POTENTIAL

The same method given in the previous sections is also applicable to the case of the quadratic potential

$$\frac{\partial}{\partial t}\psi(t,x) = k\left\{\frac{\partial^2}{\partial x^2} - (\alpha + \omega^2 x^2)\right\}\psi(t,x), \tag{4.1}$$

for real constants α and ω^2. The value of ω^2 could also assume a negative value in what follows. However, in order to avoid the question of the reality constraint for t' and x', we will temporarily suppose that variables t, x, t', and x' as well as other parameters are allowed to assume complex values. We now perform the coordinate transformation

$$t \to t' = \phi(t), \tag{4.2a}$$

$$x \to x' = \xi(t)x + f(t) \tag{4.2b}$$

as before with

$$\psi(t,x) \to \psi'(t,x) = K(t,x)\psi(t',x'), \tag{4.3a}$$

$$K(t,x) = \exp\{A(t) + B(t)x + C(t)x^2\} \tag{4.3b}$$

as in Sec. I. Then Eqs. (1.17) and (1.18) for $n=1$ give differential equations

$$\text{(i)} \quad \xi(t)\ddot{\xi}(t) - 2\dot{\xi}(t)\dot{\xi}(t) = 4k^2\omega^2\xi^2(t)\{\xi^4(t) - 1\}, \tag{4.4a}$$

$$\text{(ii)} \quad \xi(t)\ddot{f}(t) - 2\dot{\xi}(t)\dot{f}(t) = 4k^2\omega^2\xi^5(t)f(t), \tag{4.4b}$$

$$\text{(iii)} \quad \dot{\phi}(t) = \xi^2(t), \tag{4.4c}$$

among many others.

First, the solution of Eq. (4.4a) leads to

$$\xi^2(t) = \pm \frac{\exp(4k\omega t)}{\{b + a\exp(4k\omega t)\}\{d + c\exp(4k\omega t)\}} \tag{4.5}$$

for constants a, b, c, and d satisfying $bc - ad = 1$. At first glance, this appears rather peculiar, since the second-order differential equation, Eq. (4.4a), admits solutions containing three instead of two arbitrary parameters. However, in writing Eq. (4.5), we took advantage of the translation invariance of Eq. (4.4a) under

$$t \to t' = t + \text{ constant},$$

which adds one more parameter in theory. Then, the general solution of Eq. (4.4b) is found to be

$$f(t) = \nu\left[\frac{d + c\exp(4k\omega t)}{b + a\exp(4k\omega t)}\right]^{1/2} - \mu\left[\frac{b + a\exp(4k\omega t)}{d + c\exp(4k\omega t)}\right]^{1/2}, \tag{4.6}$$

for additional constant μ and ν. Therefore, the solution contains five parameters which we specify by

$$\Lambda = \left\{M, \begin{pmatrix}\mu \\ \nu\end{pmatrix}\right\}, \tag{4.7a}$$

$$M = \begin{pmatrix} c & d \\ a & b \end{pmatrix} \quad \text{at} \quad M = 1 \tag{4.7b}$$

just as Eq. (3.3). If we allow complex values for all these parameters, then the present theory remarkably gives the same symmetry group of $SL(2,C)\,\textcircled{S}\,T_2(C)$ also as we will see in the following. However if we restrict ourselves to real values for t, x, t', and x', then we will have the following complications. Because of the square roots operations for $\xi(t)$ in Eq. (4.5) as well as in $f(t)$ of Eq (4.6), x' given by Eq. (4.2b) will not remain real for arbitrary real values of a, b, c, d, μ, and ν. We will discuss the problem later.

Since all functions $\xi(t)$, $f(t)$, etc., depend upon the parameters of Λ, we rewrite them again as $\xi(t|\Lambda)$, $f(t|\Lambda)$, etc. However, the formulas become simpler, if we use the new variable

$$u = \exp(4k\omega t), \tag{4.8a}$$

$$u' = \exp(4k\omega t') \tag{4.8b}$$

instead of t and t'.

We can then rewrite Eq. (4.2) as

$$u' = \frac{cu+d}{au+b}, \quad bc-ad=1, \tag{4.9a}$$

$$x' = \xi(t|\Lambda)x + f(t|\Lambda), \tag{4.9b}$$

where

$$\xi(t|\Lambda) = \left[\frac{u}{(au+b)(cu+d)}\right]^{1/2}, \tag{4.10a}$$

$$f(t|\Lambda) = \nu\left[\frac{cu+d}{au+b}\right]^{1/2} - \mu\left[\frac{au+b}{cu+d}\right]^{1/2}. \tag{4.10b}$$

Calculating now explicit forms of $A(t|\Lambda)$, $B(t|\Lambda)$, and $C(t|\Lambda)$ as in the previous section, we find:

Proposition 4.1: For any $\psi(t,x)$ satisfying Eq. (4.1), the new function given by

$$\psi'(t,x) = K(t,x|\Lambda)\psi(t',x')(=U(\Lambda^{-1})\psi(t,x)) \tag{4.11}$$

is also a solution of the same differential equation, Eq. (4.1). Here, we have set

$$K(t,x|\Lambda) = \exp\{A(t|\Lambda) + B(t|\Lambda)x + C(t|\Lambda)x^2\}, \tag{4.12a}$$

$$A(t|\Lambda) = \frac{1}{4}\log\frac{u}{(au+b)(cu+d)} + \frac{\alpha}{4\omega}\left\{\log\left(\frac{cu+d}{au+b}\right) - \log u\right\} + \frac{\omega}{2}\left\{\nu^2\frac{cu+d}{au+b} - \mu^2\frac{au+b}{cu+d}\right\}, \tag{4.12b}$$

$$B(t|\Lambda) = \omega\left\{\frac{\nu\sqrt{u}}{au+b} + \frac{\mu\sqrt{u}}{cu+d}\right\}, \tag{4.12c}$$

$$C(t|\Lambda) = \frac{\omega}{2}\left\{-1 + \frac{b}{au+b} + \frac{d}{cu+d}\right\}. \tag{4.12d}$$

We introduce the product $\Lambda\circ\Lambda'$ for two Λ and Λ' again by Eq. (3.11), which defines the group $G = SL(2,C)\,\textcircled{S}\,T_2(C)$ for complex Λ and Λ'. We also assume the action of Λ to the coordinate $Z=\{t,x\}$ to be given by Eq. (3.14) so that

$$\Lambda Z = \Lambda\{t,x\} = \{t',x'\}. \tag{4.13}$$

We then discover after some calculations that the exact analog of Proposition 3.2 also holds valid for the present case except for the fact that $\omega(\Lambda,\Lambda')$ there is now replaced by

$$\omega(\Lambda,\Lambda') \to \tilde{\omega}(\Lambda,\Lambda') = \omega\{(\mu a - \nu c)\mu' + (\mu b - \nu a)\nu'\}. \tag{4.14}$$

For the proof of these facts, the identities (3.19) (with $t\to u$) as well as

$$\frac{b}{a''u+b''}\,\frac{a'u+b'}{c'u+d'} = \frac{1}{c'u+d'} - \frac{a}{a''u+b''}, \tag{4.15a}$$

$$\frac{d}{c''u+d''}\,\frac{a'u+b'}{c'u+d'}=\frac{1}{c'u+d'}-\frac{c}{c''u+d''} \tag{4.15b}$$

are useful, although we will not go into detail. However, we do not understand the reason why both cases of linear and quadratic potentials give at least formally the identical final results.

Remark 4.2: In contrast to the case of linear potential, the special transformation Eq. (3.24) of $G=SL(2,R)\,\textcircled{S}\,T_2(R)$ with Eq. (4.9) does not give the Galilean formula (3.25) for the present problem. This is, of course, expected since the classical Newton's formula $m\ddot{x}=F=\lambda x$ (sor some constant λ) is no longer invariant under the Galilean transformation.

So far we have ignored the question of the reality for variables t, x, t', and x'. Let us discuss the problem in some detail in the following. Since both constants k and ω are assumed to be either real or purely imaginary, so will be the product $k\omega$. Suppose first that $k\omega$ is real. Then, $u=\exp(4k\omega t)$ is real and positive for real t. The condition that both x' and t' are real requires that $au+b$ and $cu+d$ be real with $(au+b)(cu+d)>0$ for any $u>0$. This can be possible in general only in a neighborhood of the unit element $E=\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$ of the $SL(2,R)$ matrix M. Moreover, the allowed values for M depend upon the time t. In other words, the symmetry group of the theory is not in general global $SL(2,R)$ group, but is the so-called local group (or group germ). Alternatively we may better consider a subset of $SL(2,R)$ such that all a, b, c, d are non-negative. Then, the reality condition for t' and u' is readily maintained. However, the inverse matrix M^{-1} does not satisfy the requirement, then. In this case, the symmetry is not a group but a global semigroup consisting of all non-negative matrices in $SL(2,R)$, when $k\omega$ is real. Note that μ and ν are chosen to be real in the present case in order to make x' to be real in Eq. (4.9b).

On the other side, suppose now that $k\omega$ is purely imaginary. Then, we have $|u|=|u'|=1$. In that case, instead of the parametrization Eq. (4.7b) for M, we may use the conformal mapping in the complex u plane by

$$u\to u'=e^{2i\theta}\frac{u-\lambda}{1-\lambda^{*}u}, \tag{4.16}$$

for real θ and any complex λ with $|\lambda|\neq=1$. The condition $|u'|=1$ whenever we have $|u|=1$ is automatically guaranteed by Eq. (4.16) for arbitrary complex number λ. In terms of θ and λ, we can express a, b, c, d as

$$\begin{gathered}a=-\frac{\lambda^{*}}{\sqrt{1-|\lambda|^2}}e^{i\theta},\quad b=\frac{1}{\sqrt{1-|\lambda|^2}}e^{-i\theta},\\ c=\frac{1}{\sqrt{1-|\lambda|^2}}e^{i\theta}=b^{*},\quad d=-\frac{\lambda}{\sqrt{1-|\lambda|^2}}e^{-i\theta}=a^{*}\end{gathered} \tag{4.17}$$

for $|\lambda|<1$. This especially gives an identity

$$cu+d=(au+b)^{*}u \tag{4.18}$$

for $|u|=1$. Then, Eq. (4.10a) gives the desired result of the reality constraint of

$$\xi(t|\Lambda)=\frac{1}{|au+b|}>0.$$

If we next rewrite Eq. (4.10b) as

$$f(t|\Lambda)=\nu\left[\frac{(au+b)^{*}u}{au+b}\right]^{1/2}-\mu\left[\frac{(au+b)u^{*}}{(au+b)^{*}}\right]^{1/2} \tag{4.19}$$

for $|u|=1$, then the reality of $f(t|\Lambda)$ can also be maintained as long as we have

$$\mu^* = -\nu. \tag{4.20}$$

We can verify that both Eq. (4.20) and

$$M = \begin{pmatrix} b^*, & a^* \\ a, & b \end{pmatrix}$$

given by Eq. (4.17) remains invariant under the composition law Eq. (3.11). In conclusion, if $k\omega$ is purely imaginary, the symmetry group of the problem is a particular global subgroup of $G = SL(2,C) \circledS T_2(C)$, where we use the parametrization of $SL(2,C)$ and $T_2(C)$ as in Eqs. (4.17) and (4.20). Especially, it contains a group of conformal mappings of transforming the unit circle onto itself in the complex u plane.

Last, we would like to present another example for Theorem 1.3 for the present problem with $V_0(\mathbf{x})=0$. Let us set

$$\mathcal{H}_0 = \left\{ \psi_0(t,x) \left| \left(\frac{\partial}{\partial t} - k \frac{\partial^2}{\partial x^2} \right) \psi_0(t,x) = 0 \right. \right\}, \tag{4.21a}$$

$$\mathcal{H}_1 = \left\{ \psi(t,x) \left| \left(\frac{\partial}{\partial t} - k \frac{\partial^2}{\partial x^2} - k(\alpha + \omega^2 x^2) \right) \psi(t,x) = 0 \right. \right\}. \tag{4.21b}$$

Solving conditions given in Theorem 1.3, we then find:

Proposition 4.2: For any $\psi_0(t,x) \in \mathcal{H}_0$, the function given by

$$\psi(t,x) = K_0(t,x)\psi_0(t',x') \tag{4.22}$$

is an element of $\mathcal{H}$, where

$$t' = -\frac{\sigma^2}{4k\omega} \frac{1}{u+\lambda}, \tag{4.23a}$$

$$x' = \sigma \frac{\sqrt{u}}{u+\lambda} x - \frac{\sigma\tau}{2\omega} \frac{1}{u+\lambda}, \tag{4.23b}$$

with

$$K_0(t,x) = \frac{u^{1/4}}{(\lambda+u)^{1/2}} \exp\{A_0(t) + B_0(t)x + C_0(t)x^2\}, \tag{4.24a}$$

$$A_0(t) = -\frac{\tau^2}{4\omega} \frac{1}{u+\lambda} - k\alpha t, \tag{4.24b}$$

$$B_0(t) = \tau \frac{\sqrt{u}}{u+\lambda}, \tag{4.24c}$$

$$C_0(t) = \frac{\omega(\lambda-u)}{2(u+\lambda)}. \tag{4.24d}$$

Here, σ, λ, τ are arbitrary constants and

$$u = \exp\{4k\omega t\}. \tag{4.25}$$

Remark 4.3: Unfortunately, the variables t' and x' given by Eq. (4.23) can be real only for the case of $k\omega$ being real. For that case, we can construct solutions of Eq. (4.21b) from that of $\psi(t,x)$ satisfying Eq. (3.26b) by combining Eqs. (3.30) and (4.22).

V. LIE ALGEBRAS AND LOCAL SYMMETRY

In the preceding sections, we found that the time-dependent Schrödinger equation for some potentials has global groups as symmetry of the theory. However, much larger local symmetry could emerge, if we consider its Lie algebraic structure as follows.

Let us first set for simplicity

$$K \equiv \frac{\partial}{\partial t} - k\left\{\frac{\partial^2}{\partial x^2} - V(x)\right\} \tag{5.1}$$

and

$$\mathcal{H} = \{\psi(t,x) | K\psi(t,x) = 0\}. \tag{5.2}$$

Consider now, as an example, the symmetry group $G = SL(2,R) \circledS T_2(R)$ of Sec. III for the linear potential. We know that for any $\psi(t,x) \in \mathcal{H}$, we have $U(\Lambda)\psi(t,x) \in \mathcal{H}$ for any $\Lambda \in G$. Since G is a Lie group, we can associate a Lie algebra L by considering infinitesimal Λ's. It is then evident that we have

$$g\psi(t,x) \in \mathcal{H}, \quad g \in L. \tag{5.3}$$

Let $\tilde{U}(L)$ be the universal enveloping algebra of L. Also, we will then have

$$\tilde{U}(L)\psi(t,x) \in \mathcal{H} \tag{5.4}$$

whenever $\psi(t,x)$ is a sufficiently smooth function of t and x. Since K is invariant under the time translation $t \to t' = t + \lambda$ for any constant λ, the Lie algebra L always contain a special element

$$D \equiv \frac{\partial}{\partial t} \in L \tag{5.5}$$

so that this implies the validity of

$$D^n\psi(t,x) \in \mathcal{H} \tag{5.6}$$

for any positive integer n. This can be, of course, more directly verified from $[D^n, K] = 0$. For the case of the linear potential of Sec. III, the Lie algebra L consists now of six elements (instead of five with the additional unit element 1);

$$L = \{L_\pm, L_3, T_1, T_2, 1\}, \tag{5.7}$$

which forms the Abelian-extended Lie algebra of

$$L = s\ell(2) \oplus t(2) \oplus u(1), \tag{5.8}$$

where $u(1)$ is the extra one-dimensional Abelian algebra in conformity with the projective representation nature of $U(\Lambda)$ in Eq. (3.23). Their explicit forms are easily calculated from Eqs. (3.4), (3.5), (3.7), and (3.9) to be given by

$$-L_3 = t\frac{\partial}{\partial t} + \frac{1}{2}(x + 3k^2\beta t^2)\frac{\partial}{\partial x} + k\left(\alpha + \frac{3}{2}\beta x\right)t + \frac{1}{2}k^3\beta^2 t^3 + \frac{1}{4}, \tag{5.9a}$$

$$L_+ = \frac{\partial}{\partial t} + 2k^2\beta t\frac{\partial}{\partial x} + k(\alpha+\beta x) + k^3\beta^2 t^2, \tag{5.9b}$$

$$L_- = t^2\frac{\partial}{\partial t} + (tx + k^2\beta t^3)\frac{\partial}{\partial x} + \frac{1}{2}t + \alpha k t^2 + \frac{1}{4}k^3\beta^2 t^4 + \frac{3}{2}k\beta t^2 x + \frac{1}{4k}x^2, \tag{5.9c}$$

and

$$T_1 = \frac{\partial}{\partial x} + k\beta t, \tag{5.10a}$$

$$T_2 = t\frac{\partial}{\partial x} + \frac{1}{2k}x + \frac{k\beta}{2}t^2. \tag{5.10b}$$

They satisfy commutation relations:

$$[L_3, L_\pm] = \pm L_\pm, \quad [L_+, L_-] = -2L_3, \tag{5.11a}$$

$$[L_3, T_1] = \frac{1}{2}T_1, \quad [L_3, T_2] = -\frac{1}{2}T_2, \tag{5.11b}$$

$$[L_+, T_1] = [L_-, T_2] = 0, \tag{5.11c}$$

$$[L_+, T_2] = T_1, \quad [L_-, T_1] = -T_2, \tag{5.11d}$$

$$[T_1, T_2] = \frac{1}{2k}. \tag{5.11e}$$

Note that $[T_1, T_2] = 1/2k \neq 0$, reflecting the projective representation of Eq. (3.23). We note that T_1 and T_2 play the role of creation and annihilation operators.

Since $W(\Lambda)$ is also a representation of G, we can perform the same analysis to find that the corresponding Lie algebra $\tilde{L}$ consisting of

$$\tilde{L} = \{\tilde{L}_\pm, \tilde{L}_3, \tilde{T}_1, \tilde{T}_2, 1\} \tag{5.12}$$

has the form

$$\begin{gathered} \tilde{L}_3 = L_3 - 1, \quad \tilde{L}_+ = L_+, \quad \tilde{L}_- = L_- + 2t, \\ \tilde{T}_1 = T_1, \quad \tilde{T}_2 = T_2 \end{gathered} \tag{5.13}$$

with the same commutation relation, Eq. (5.11). When we write

$$K_1 = \frac{\partial}{\partial t} - k\left\{\frac{\partial^2}{\partial x^2} - \alpha - \beta x\right\}, \tag{5.14}$$

then Eq. (1.11) becomes

$$\tilde{L}K_1 = K_1 L. \tag{5.15}$$

This especially implies $[L_+, K_1] = [T_1, K_1] = [T_2, K_1] = 0$ and $[L_3, K_1] = K_1$. Moreover, we can easily find that K_1 is rewritten as a element of $\tilde{U}(L)$ as

$$K_1 = L_+ - kT_1^2 \tag{5.16}$$

while the time derivative $D = \partial/\partial t$ is expressed as

$$D = L_+ - 2k^2\beta T_2 - k\alpha.$$

Before going into further details, we note first that the second-order Casimir invariant of the $s\ell(2)$ sub-Lie algebra of L is given by

$$I_2 = L_+L_- - L_3^2 + L_3. \tag{5.17}$$

In contrast, the larger Lie algebra L possesses not the second- but third-order Casimir invariant

$$I_3 = -I_2 + k\{L_3(T_1T_2 + T_2T_1) + L_+T_2T_2 + L_-T_1T_1\}. \tag{5.18}$$

For our particular form of generators given by Eqs. (5.9) and Eq. (5.10), we find that I_3 is purely a constant

$$I_3 = \tfrac{3}{16}, \tag{5.19}$$

while I_2 is rewritten as

$$I_2 = \frac{3}{16} + \frac{1}{4k}(x - k^2\beta t^2)^2 K_1. \tag{5.20}$$

Especially for any function $\psi = \psi(t,x)$ satisfying $K_1\psi = 0$, we have $I_2\psi = \frac{3}{16}\ \psi$. In this connection, two special functions $f_1(t,x)$ and $f_2(t,x)$ given in Eq. (3.27) have the following interesting property. They satisfy

$$L_+ f_1(t,x) = T_1 f_1(t,x) = 0, \quad L_3 f_1(t,x) = -\tfrac{1}{4}\ f_1(t,x), \tag{5.21a}$$

$$L_- f_2(t,x) = T_2 f_2(t,x) = 0, \quad L_3 f_2(t,x) = \tfrac{1}{4}\ f_2(t,x). \tag{5.21b}$$

Therefore, the function $f_1(t,x)$ corresponds to the highest weight state of simultaneous representations of both $s\ell(2)$ and L, while $f_2(t,x)$ plays the role of the lowest weight state of another representation. They are infinite dimensional and irreducible but *not* unitary. Moreover, they satisfy $K_1 f_j(t,x) = 0$ for $j = 1,2$ so that we have

$$I_2 f_j(t,x) = I_3 f_j(t,x) = \tfrac{3}{16}\ f_j(t,x) \quad (j = 1,2). \tag{5.22}$$

Also, in view of Eq. (5.20), the wave function $\psi(t,x)$ satisfying Eqs. (3.44) and (3.45) is the eigenstate of I_2 with

$$I_2\psi(t,x) = \left\{\frac{3}{16} - \frac{\lambda}{4}\right\}\psi(t,x).$$

The same analysis is readily applicable for the quadratic potential of Sec. IV. In this case, the Lie algebras L and $\tilde{L}$ are specified by

$$-L_3 = u\frac{\partial}{\partial u} + \frac{\alpha}{4\omega}, \tag{5.23a}$$

$$L_+ = \frac{\partial}{\partial u} - \frac{1}{2u}x\frac{\partial}{\partial x} + \left(\frac{\alpha}{4\omega} - \frac{1}{4}\right)\frac{1}{u} + \frac{\omega}{2}\ \frac{x^2}{u}, \tag{5.23b}$$

$$L_- = u^2\frac{\partial}{\partial u} + \frac{1}{2}ux\frac{\partial}{\partial x} + \left(\frac{\alpha}{4\omega} + \frac{1}{4}\right)\ u + \frac{\omega}{2}ux^2, \tag{5.23c}$$

$$T_1 = \frac{1}{\sqrt{u}}\ \frac{\partial}{\partial x} - \frac{\omega}{\sqrt{u}}x, \tag{5.23d}$$

$$T_2 = \sqrt{u}\ \frac{\partial}{\partial x} + \omega\sqrt{u}x, \tag{5.23e}$$

with $u = \exp(4k\omega t)$, and

$$\tilde{L}_3 = L_3, \quad \tilde{L}_+ = L_+ - \frac{1}{u}, \quad \tilde{L}_- = L_- + u, \tag{5.24a}$$

$$\tilde{T}_1 = T_1, \quad \tilde{T}_2 = T_2. \tag{5.24b}$$

They satisfy the same commutation relations. Eqs. (5.11a)–(5.11d) while Eq. (5.11e) is now replaced by

$$[T_1, T_2] = 2\omega. \tag{5.25}$$

Writing

$$K_2 = \frac{\partial}{\partial t} - k\left\{\frac{\partial^2}{\partial x^2} - \alpha - \omega^2 x^2\right\}, \tag{5.26}$$

the analogs of Eqs. (5.15), and (5.16), are now given by

$$\tilde{L}K_2 = K_2 L, \tag{5.27a}$$

$$K_2 = -4k\omega L_3 - \frac{k}{2}(T_1T_2 + T_2T_1), \tag{5.27b}$$

$$D = \frac{\partial}{\partial t} = -4k\omega L_3 - k\alpha. \tag{5.27c}$$

Especially, Eqs. (5.24) and (5.27a) lead to

$$[L_3, K_2] = [T_1, K_2] = [T_2, K_2] = 0.$$

For this case, the second-order Casimir invariant I_2 is still given by Eq. (5.17), while Eq. (5.18) for I_3 must now be replaced by

$$I_3 = -I_2 + \frac{1}{4\omega}\{L_3(T_1T_2 + T_2T_1) + L_-T_1T_1 + L_+T_2T_2\}. \tag{5.28}$$

We still have the validity of $I_3 = 3/16$ but Eq. (5.20) is now replaced by

$$I_2 = \frac{3}{16} + \frac{1}{4k}x^2K_2. \tag{5.29}$$

Especially, if $\psi(t,x)$ now satisfies

$$\left\{\frac{\partial}{\partial t}-k\left(\frac{\partial^2}{\partial x^2}-\alpha-\omega^2x^2-\frac{\lambda}{x^2}\right)\right\}\psi(t,x)=0$$

for some constant λ, then Eq. (5.29) now implies

$$I_2\psi(t,x)=\left(\frac{3}{16}-\frac{\lambda}{4}\right)\psi(t,x).$$

There exist relations analogous to Eqs. (5.21). Setting

$$g_1(t,x)=\exp\left\{k(\omega-\alpha)t+\frac{\omega}{2}x^2\right\}, \tag{5.30a}$$

$$g_2(t,x)=\exp\left\{-k(\omega+\alpha)t-\frac{\omega}{2}x^2\right\}, \tag{5.30b}$$

it is easy to verify

$$K_2g_1(t,x)=L_+g_1(t,x)=T_1g_1(t,x)=0,\quad L_3g_1(t,x)=-\tfrac{1}{4}\,g_1(t,x), \tag{5.31a}$$

$$K_2g_2(t,x)=L_-g_2(t,x)=T_2g_2(t,x)=0,\quad L_3g_2(t,x)=\tfrac{1}{4}\,g_2(t,x). \tag{5.31b}$$

Note that $g_2(t,x)$ given by Eq. (5.30b) corresponds to the ground state wave function of the familiar harmonic potential. It is again the lowest weight state of representations of both $s\ell(2)$ and L. Another interesting function is obtained by setting $\tau=\lambda=0$, and $\sigma=1$ with appropriate choice for $\psi_0(t,x)$ in Proposition 4.3. In this way, the function

$$g_3(t,x)=\exp\left\{-k(\alpha+\omega)t-\frac{\omega}{2}x^2-\gamma\frac{x}{\sqrt{u}}-\frac{\gamma^2}{4\omega}\frac{1}{u}\right\} \tag{5.32}$$

for an arbitrary constant γ turns out to be a simultaneous eigenfunction of K_2, T_2, and L_- as in

$$\text{(i)}\quad K_2g_3(t,x)=0, \tag{5.33a}$$

$$\text{(ii)}\quad T_2g_3(t,x)=\gamma g_3(t,x), \tag{5.33b}$$

$$\text{(iii)}\quad L_-g_3(t,x)=\frac{\gamma^2}{4\omega}g_3(t,x). \tag{5.33c}$$

Especially, Eq. (5.33b) implies that $g_3(t,x)$ plays a role of coherent state as in the quantum optics,[12] since T_2 may be regarded as the analog of the annihilation operator.

ACKNOWLEDGMENT

This paper is supported in part by U.S. Department of Energy Contract No. DE-FG02-91ER40685.

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Nonlinear transforms of momenta and Planck scale limit

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(Received 28 November 2002; accepted 28 April 2003)

Starting with the generators of the Poincaré group for arbitrary mass (m) and spin (s), a nonunitary transformation is implemented to obtain momenta with an absolute Planck scale limit. In the rest frame (for $m>0$) the transformed energy coincides with the standard one, both being m. As the latter tends to infinity under Lorentz transformations the former tends to a finite upper limit $m\coth(lm)=l^{-1}+O(l)$, where l is the Planck length and the mass-dependent nonleading terms vanish exactly for zero rest mass. The invariant m^2 is conserved for the transformed momenta. The speed of light continues to be the absolute scale for velocities. We study various aspects of the kinematics in which two absolute scales have been introduced in this specific fashion. The precession of polarization and transformed position operators are among them. A deformation of the Poincaré algebra to the $SO(4,1)$ de Sitter one permits the implementation of our transformation in the latter case. A supersymmetric extension of the Poincaré algebra is also studied in this context. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1593225]

I. INTRODUCTION

Possible modifications of special relativity introducing, in addition to the velocity of light, a second invariant scale corresponding to the Planck energy (the inverse of the Planck length) have been studied in numerous recent papers exploring various aspects.[1–11] The titles of these papers (citing other relevant sources) convey some idea of the topics addressed. Among the papers cited above, our work can be compared most directly, concerning both analogies and crucial differences, with the work of Magueijo and Smolin.[4,5] Like them, we introduce the nonlinear constructions via a nonunitary transformation. But (unlike all the foregoing studies) we introduce spin at the outset. To be able to do so adequately, we start with an irreducible representation $[m,s]$ of the Poincaré group of positive rest mass ($m>0$) and an arbitrary integer or half-integer spin s. The momentum generators are thus constrained to satisfy

$$P^{\mu}P_{\mu}=P_0^2-\vec{P}^2=m^2. \tag{1}$$

It will be implicit henceforth that (with a positive square root and ∇_i denoting the derivative with respect to P_i),

$$P_0=\sqrt{\vec{P}^2+m^2},\quad \vec{\nabla}P_0=\frac{\vec{P}}{P_0}. \tag{2}$$

Introducing $(2s+1)\times(2s+1)$ spin matrices $\vec{S}$, satisfying

$$[S_i,S_j]=i\epsilon_{ijk}S_k, \tag{3}$$

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the generators of pure rotations ($\vec{J}$) and those of pure Lorentz transformations ($\vec{K}$) can be represented as

$$\vec{J}=-i\vec{P}\times\vec{\nabla}+\vec{S}, \tag{4}$$

$$\vec{K}=-iP_0\vec{\nabla}-\frac{\vec{P}\times\vec{S}}{P_0+m}. \tag{5}$$

Let us briefly note the following points[12] for later use.

(a) The first term of $\vec{K}$ should *not* be symmetrized. The hermiticity of $\vec{K}$ and the relation to Newton–Wigner position operators are discussed in Ref. 12 [from Eq. (2.18) onward].

(b) For $m=0$, the last term of $\vec{K}$ is not well defined only for energy momenta (0,0,0,0), namely, at the tip of the light cone that is never in the same orbit with

$$p^2=0, \quad p_0\neq 0.$$

Hence, excluding massless particles with strictly zero energy, one can consistently use (5) with $m=0$. We will present below results for $m=0$ obtained systematically in this fashion. An explicit unitary transformation to Wigner's construction in terms of the little group E_2 has been presented elsewhere (see the discussion and the references in Ref. 12 from Eq. (2.21) onward). There it is explained how, in spite of the presence of three spin components in (4) and (5), one finally deals with only one conserved helicity component for $m=0$.

(c) The canonical form given by (4) and (5) is valid for any spin. The Pauli–Lubansky 4-vector is obtained by contracting the dual of the tensor ($\vec{J},\vec{K}$) by P_μ, or equivalently as

$$W_\mu=-i[P_\mu,\vec{K}\cdot\vec{J}] \tag{6}$$

$$=(\vec{P}\cdot\vec{J},P_0\vec{J}-\vec{P}\times\vec{K}) \tag{7}$$

$$=(\vec{P}\cdot\vec{S},m\vec{S}+(P_0+m)^{-1}(\vec{P}\cdot\vec{S})\vec{P}). \tag{8}$$

This satisfies

$$W_\mu W^\mu=-m^2\vec{S}^2. \tag{9}$$

The relation, for $s=1/2$, with the the Dirac representation and the Dirac equation, are indicated in Ref. 12 [from Eq. (2.49) onward]. The relevant transformation relating the two representations diagonalizes the Dirac mass operator ($\gamma\cdot p$).

Before introducing the explicit form of the transformation V (to be presented below) let us note the following aspect.

Having explicitly constructed all the transforms,

$$V(P_0,\vec{P},\vec{J},\vec{K})V^{-1}, \tag{10}$$

one can study the set

$$V(\vec{J},\vec{K})V^{-1},(P_0,\vec{P}),$$

or, in a complementary fashion, the set

$$(\vec{J},\vec{K}),V(P_0,\vec{P})V^{-1}.$$

In the latter case one conserves the explicit representation of the Lorentz algebra and associates physical significance with the transformed momenta. We will adopt the latter approach below

[providing, however, complete results for (10)]. This will furnish, in the terminology of Ref. 7, an example of DSR2 theories with bounded energy and momenta. The inverse formulas, giving the standard momenta in terms of the transformed ones, are obtained very simply.

II. THE TRANSFORMATION

Let

$$V=\exp(-lP_0\vec{P}\cdot\vec{\nabla}), \tag{11}$$

where $0<l\ll 1$, and $P_0=\sqrt{\vec{P}^2+m^2}$.

In fact, one may assume that in our chosen units ($c=1$), l is the Planck length, which is, more generally,

$$l_P=\sqrt{(\hbar G/c^3)}. \tag{12}$$

As compared to the corresponding operator,

$$U^{-1}=\exp(-l_P p_0 p^\mu \partial_\mu), \tag{13}$$

of Ref. 4, we have kept only the three space components in the scalar product, but still with the factor P_0 rather than $P=|\vec{P}|$. This is crucial for the remarkable properties obtained below for arbitrary spin.

Implementing, consistently with (2), for any f,

$$[\vec{\nabla},P_0]f=\frac{\vec{P}}{P_0}f,$$

one obtains

$$\vec{\mathsf{P}}\equiv V\vec{P}V^{-1}=\frac{m\vec{P}}{\sinh(lm)P_0+\cosh(lm)m}, \tag{14}$$

$$\mathsf{P}_0\equiv VP_0V^{-1}=m\frac{\cosh(lm)P_0+\sinh(lm)m}{\sinh(lm)P_0+\cosh(lm)m}, \tag{15}$$

satisfying

$$\mathsf{P}_0^2-\vec{\mathsf{P}}^2=P_0^2-\vec{P}^2=m^2, \tag{16}$$

$$V\vec{J}V^{-1}=\vec{J}=-i\vec{P}\times\vec{\nabla}+\vec{S}, \tag{17}$$

$$V\vec{K}V^{-1}=-i\cosh(lm)P_0\vec{\nabla}-i\sinh(lm)(m\vec{\nabla}+m^{-1}\vec{P}(\vec{P}\cdot\vec{\nabla}))-e^{-lm}\frac{\vec{P}\times\vec{S}}{P_0+m}. \tag{18}$$

Note the simplicity of the spin-dependent part on the right of (18). This corresponds to

$$V\frac{\vec{P}}{P_0+m}V^{-1}=e^{-lm}\frac{\vec{P}}{P_0+m}. \tag{19}$$

Hence, squaring each side and using (1), one obtains

$$V\frac{P_0-m}{P_0+m}V^{-1}=e^{-2lm}\frac{P_0-m}{P_0+m}. \tag{20}$$

Thus, one readily obtains (15) and hence also (14). If, without knowing (15) beforehand, one proceeds directly to compute the power series,

$$\mathsf{P}_0 = VP_0V^{-1} = P_0 - l[P_0(\vec{P}\cdot\vec{\nabla}),P_0] + l^2[P_0(\vec{P}\cdot\vec{\nabla})[P_0(\vec{P}\cdot\vec{\nabla}),P_0]] - \cdots, \tag{21}$$

one obtains

$$\mathsf{P}_0 = P_0 - l(P_0^2 - m^2) + l^2 P_0(P_0^2 - m^2) - \cdots. \tag{22}$$

The series is difficult to sum up. On the other hand, developing (15) in powers of l, one easily reproduces (22). One similarly obtains for the modulus of the momentum,

$$\mathsf{P} = P - lPP_0 + \tfrac{1}{2}l^2P(P_0^2 + P^2) - \cdots. \tag{23}$$

It is easy to verify that (14) and (15) can be inverted by simply changing the sign of l. Thus,

$$P_0 = m\frac{\cosh(lm)\mathsf{P}_0 - \sinh(lm)m}{-\sinh(lm)\mathsf{P}_0 + \cosh(lm)m}, \tag{24}$$

and so on. This is consistent with the invariance of $(P_0(\vec{P}\cdot\vec{\nabla}))$ under the transformation.

Let us now consider momentum eigenstates and denote the eigenvalues of P_μ and P_μ by p_μ and p'_μ, respectively. Then

$$p'_0 = m\frac{\coth(lm)p_0 + m}{p_0 + \coth(lm)m}. \tag{25}$$

Hence, since we are considering positive p_0, m, and l,

$$p'_0 < \coth(lm)m.$$

Similarly, for the modulus of the momentum, one obtains

$$p' < \frac{m}{\sinh(lm)}.$$

Thus our transformation, valid for arbitrary spin, indeed leads to an invariant energy scale. This is the crucial property. For

$$p_0 = m, \quad p'_0 = m,$$

and as

$$p_0 \to \infty, \quad p'_0 \to \coth(lm)m,$$

from below. *For all observers, p'_0 remains bounded.* Starting together with p_0 in the rest frame p'_0 lags progressively behind as the former increases to finally encounter the barrier $m\coth(lm)$. In powers of l, one obtains

$$p'_0 < l^{-1} + \tfrac{1}{3}m^2 l + O(l^2), \tag{26}$$

and

$$p' < l^{-1} - \tfrac{1}{6}m^2 l + O(l^2). \tag{27}$$

The modulus of the transformed velocity, quite consistently with our chosen units ($c=1$), has the high-energy limit, for $p_0\to\infty$, given by

$$\frac{p'}{p_0'}\to\frac{1}{\cosh(lm)}=1-\frac{1}{2}l^2m^2<1. \tag{28}$$

The limit 1 is attained exactly for for $m=0$. This will be seen more precisely immediately below.

III. ZERO REST MASS

As explained in (b) following Eq. (5), the essential results for $m=0$ can be obtained (rather than starting again with $m=0$ in V) easily and directly from our previous ones. Thus for $m\to 0$ one obtains from (14) and (15),

$$\vec{\mathsf{P}}=\frac{\vec{P}}{lP_0+1} \tag{29}$$

and

$$\mathsf{P}_0=\frac{P_0}{lP_0+1}, \tag{30}$$

satisfying evidently (like P_0 and $\vec{P}$)

$$\mathsf{P}_0^2-\vec{\mathsf{P}}^2=0.$$

Now, as compared to the inequality following (25), again for all parameters positive,

$$p_0'=\frac{p_0}{lp_0+1}<l^{-1}. \tag{31}$$

As

$$p_0\to\infty,\quad p_0'\to l^{-1},$$

from below. And as compared to (28),

$$\frac{p'}{p_0'}=\frac{p}{p_0}=1. \tag{32}$$

Thus, considering all masses and the system

$$(\vec{J},\vec{K},\mathsf{P}_0,\vec{\mathsf{P}}),$$

one indeed implements *two absolute scales: one for velocity* ($c=1$) *and one for energy*. The leading term for the limiting energy is always l^{-1}. This becomes exact for zero rest mass. For positive mass the exact result is provided by (25).

IV. PRECESSION OF POLARIZATION

Since V commutes with $\vec{S}$ the standard results for precession of polarization are conserved. (See the complete discussion in Ref. 12.) They can, however, be reexpressed in terms of $(\mathsf{P}_0,\vec{\mathsf{P}})$, if so desired. Thus, under an infinitesimal Lorentz transformation of velocity $\tanh\chi\,(\to\chi)$ parallel to the unit vector $\hat{n}$, the change

$$\delta\vec{S}=i[\chi\hat{n}\cdot\vec{K},\vec{S}]=-\chi\frac{(\hat{n}\times\vec{P})\times\vec{S}}{P_0+m}=-\chi e^{lm}\frac{(\hat{n}\times\vec{\mathsf{P}})\times\vec{S}}{\mathsf{P}_0+m}. \tag{33}$$

Thus, the formal expression is altered by a simple overall factor $e^{lm}(=1+O(l))$. In Ref. 12, it is explained how (33) leads to the famous Thomas factor $\frac{1}{2}$. We will not go further into such topics in the present study.

We indicate below very briefly possible generalizations of our study in two different directions.

V. DEFORMATION OF POINCARÉ TO *SO*(4,1) de SITTER ALGEBRA

The Lorentz algebra has two invariants:

$$(\vec{K},\vec{J}),\quad (\vec{K}^2-\vec{J}^2).$$

As pointed out before [see Eqs. (6)–(9)], commuting P_μ with the first one leads to W_μ giving the spin. The commutation of P_μ with the second leads to the homogenous $SO(4,1)$ algebra, where [along with the Lorentz $SO(3,1)$ generators and $\mu=(0,1,2,3)$]

$$L_{\mu 5}=\frac{i}{M}[(\vec{K}^2-\vec{J}^2),P_\mu]+\lambda P_\mu. \tag{34}$$

Here $M=(P^\mu P_\mu)^{1/2}$ is the mass operator and λ is an arbitrary parameter. Starting with an irreducible space $[m,s]$ (with $m>0$, say) one can compute explicitly the actions of $L_{\mu 5}$ on the states using (34). Elsewhere,[13] we have studied (34) in a more general context using, however, the Lorentz basis. Here we only point out that $(VL_{\mu 5}V^{-1})$ is obtained directly from our foregoing results. A detailed study is beyond the scope of this paper.

VI. A SUPERSYMMETRIC EXTENSION

A simple supersymmetric extension[14] permitting a ready implementation of our transformation can be obtained as follows. (Previous sources are cited in Ref. 14.) One starts with two fermionic operators satisfying (for $i=1,2$)

$$[a_i,a_j]_+=0=[a_i^\dagger,a_j^\dagger]_+,\quad [a_i,a_j^\dagger]_+=\delta_{ij}.$$

One defines $Q=(Q_1,Q_2)$ and the adjoint $Q^\dagger$ (a column with two rows) as

$$Q^\dagger=\frac{1}{\sqrt{2(P_0+M)}}[(P_0+M)+\vec{\tau}\cdot\vec{P}]a^\dagger. \tag{35}$$

Then in terms of Pauli matrices,

$$[Q^\dagger,Q]_+=\tau_0 P_0+\vec{\tau}\cdot\vec{P}. \tag{36}$$

This compact notation implies symmetrization of each term of the 2×2 matrix $Q^\dagger Q$. Thus, for example, at the top right one obtains

$$Q_1^\dagger Q_2+Q_2Q_1^\dagger=P_1-iP_2.$$

A Majorana spinor is provided by $(Q_1,Q_2,Q^\dagger{}_2,-Q^\dagger{}_1)$.

Next, one defines

$$\vec{\Sigma}=\tfrac{1}{2}(a\vec{\tau}a^\dagger). \tag{37}$$

Adding the spin operator $\vec{\Sigma}$ to $\vec{S}$, define

$$\vec{J}=-i\vec{P}\times\vec{\nabla}+(\vec{S}+\vec{\Sigma}), \tag{38}$$

$$\vec{K}=-iP_0\vec{\nabla}-\frac{\vec{P}\times(\vec{S}+\vec{\Sigma})}{P_0+m}. \tag{39}$$

Now $(P_\mu,\vec{K},\vec{J})$ continue to satisfy the Poincaré algebra along with

$$[\vec{J},Q^\dagger]=-\tfrac{1}{2}\vec{\tau}Q^\dagger, \tag{40}$$

$$[\vec{K},Q^\dagger]=-\frac{i}{2}\vec{\tau}Q^\dagger. \tag{41}$$

Thus, (36), (40), (41) together complete the supersymmetric extension. Various aspects are studied in Ref. 14, citing other sources. Here we only note that $\vec{\Sigma}$ commutes with V and denoting

$$\tilde{Q}=VQV^{-1},$$

$$\tilde{Q}^\dagger=\frac{1}{\sqrt{2(\mathsf{P}^0+M)}}[(\mathsf{P}_0+M)+\vec{\tau}\cdot\vec{\mathsf{P}}]a^\dagger, \tag{42}$$

and

$$[\tilde{Q}^\dagger,\tilde{Q}]_+=\tau_0\mathsf{P}_0+\vec{\tau}\cdot\vec{\mathsf{P}}. \tag{43}$$

Thus, our transformation can be readily implemented for such an extension. A more detailed study is beyond the scope of this paper.

VII. GRADIENT OPERATORS FOR $\vec{\mathsf{P}}$

One obtains for transforms of $\vec{\nabla}$, consistently with (15) and (18) and with P_0 given by (15),

$$\vec{\xi}=\frac{1}{\mathsf{P}_0}((\cosh(lm)P_0+\sinh(lm)m)\vec{\nabla}+m^{-1}\sinh(lm)\vec{P}(\vec{P}\cdot\vec{\nabla})), \tag{44}$$

where

$$\vec{\xi}\equiv V\vec{\nabla}V^{-1}.$$

Hence, for such ξ_i,

$$[\xi_i,\mathsf{P}_j]=\delta_{ij} \tag{45}$$

and

$$[\xi_i,\xi_j]=0. \tag{46}$$

Substituting for ξ_i,

$$\xi_i'=\xi_i+Vf_iV^{-1},$$

where f_i depends only on the momenta conserves (45) but not necessarily (46) unless

$$(\partial_i f_j - \partial_j f_i) = 0.$$

In particular, starting with the localizing and Hermitian Newton–Wigner position operators [Ref. 12 from Eq. (2.18) onward], namely,

$$\vec{X} = i\vec{\nabla} - \frac{\vec{P}}{2P_0^2}, \tag{47}$$

one obtains

$$V\vec{X}V^{-1} = i\vec{\xi} - \frac{\vec{\mathsf{P}}}{2\mathsf{P}_0^2}. \tag{48}$$

The components continue to satisfy (45) and (46) (with a factor i).

We will not attempt to explore here whether other choices can lead to interesting noncommutative Hopf algebras for the coordinates. Both noncommutative (Ref. 9 and sources cited) and commutative[5] space–times have been proposed in the context of Planck scale limits of momenta. In our formalism, apart from the commutativity of (46), the time t remains a parameter [P_0 being given by (2)].

VIII. CONCLUSION

For all mass and spin we have obtained nonlinear functions of the standard momenta possessing a Planck scale limit. Our construction exhibits that such a property is quite consistent with a fixed velocity of light, time remaining a parameter and commuting position operators corresponding to those for the nonlinear momenta. Even if one deliberately seeks a different formalism violating such properties, a comparison with our formalism will provide a deeper understanding.

Due to the fact that the new momenta are introduced via a relatively simple conjugation, by our V, all relevant properties are obtained fairly easily and systematically. This has permitted a ready passage to de Sitter $SO(4,1)$ and to a supersymmetric extension as well.

Elsewhere[15] we have presented explicit constructions for the generators of the Poincaré group for spacelike momenta and for lightlike momenta with continuous spin. We just mention that they have strong analogies with those introduced here for the timelike case and thus may suggest how our transformation can be adapted to those cases.

We add the following notes.

(1) In this paper we try to clarify further the properties of the transformed momenta. We repeat that in our case equivalence with the standard (untransformed) case would have persisted had one used (10), namely,

$$V(P_0, \vec{P}, \vec{J}, \vec{K})V^{-1}.$$

But implementing, as we choose to do,

$$V(P_0, \vec{P})V^{-1}, \vec{J}, \vec{K},$$

one obtains fundamentally different properties. *Leaving untouched* the realization of the Lorentz algebra and the base space, we attribute direct physical significance to the transformed momenta. One can legitimately explore other, different postulates. Here we have tried to indicate the remarkable consequences of adopting this one, along with our specific transformation.

The simplicity of the inverse transformation [see (24) and related comments] permits quite straightforward derivations of the nonlinear Lorentz transformation properties of the new mo-

menta and the new addition law for velocities. For brevity, we give only one example.

Consider a pure Lorentz transformation along the unit vector $\hat{n}$ and denote $\vec{K}\cdot\hat{n}=K_n$ and so on. Now

$$e^{i\chi K_n}P_0e^{-i\chi K_n}=\cosh\chi P_0+\sinh\chi P_n$$

and

$$e^{i\chi K_n}\mathsf{P}_0e^{-i\chi K_n}=m\,\frac{f_1(\mathsf{P}_0-m\coth(lm))+\coth(lm)\sinh\chi(\sinh(lm)\mathsf{P}_n+m\coth\chi)}{f_2(\mathsf{P}_0-m\coth(lm))+\sinh\chi(\sinh(lm)\mathsf{P}_n+m\coth\chi)},$$

where

$$f_1=(\cosh\chi(\cosh(lm))^2-(\sinh(lm))^2),\quad f_2=\cosh(lm)\sinh(lm)(\cosh\chi-1).$$

It is evident that the eigenvalue $m\coth(lm)$ of P_0 is invariant under Lorentz transformation. Thus the Planck scale limit presented below (25) is encapsulated in the nonlinear Lorentz transformation laws for P_μ. In form and also in content, the two transformation laws exhibited avove are, to say the least, distinguishable.

(2) A paper by Ahluwalia, Kirchbach, and Dadhich (gr-qc/0212128) has been brought to our notice. There also spin has been taken into consideration. In contrast to our canonical generators [(4),(5)] spinor equations are introduced starting with the Dirac equation. We have indicated [below (9)] references to transformations relating spinor and canonical representations.

ACKNOWLEDGMENT

I thank D. V. Ahluwalia for an exchange of information and comments.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Determination of quantum symmetries for higher *ADE* systems from the modular *T* matrix

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(Received 26 March 2002; accepted 24 April 2003)

We show that the Ocneanu algebra of quantum symmetries, for an *ADE* diagram (or for higher Coxeter–Dynkin systems, like the Di Francesco–Zuber system) can be, in most cases, deduced from the structure of the modular *T* matrix in the *A* series. We recover in this way the (known) quantum symmetries of su(2) diagrams and illustrate our method by studying those associated with the three genuine exceptional diagrams of type su(3), namely, $\mathcal{E}_5$, $\mathcal{E}_9$, and $\mathcal{E}_{21}$. This also provides the shortest way to the determination of twisted partition functions in boundary conformal field theory with defect lines. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1592609]

I. INTRODUCTION

This article provides a simple tool for the determination, in most cases, of the algebra of quantum symmetries associated with *ADE* Dynkin diagrams [considered as quantum su(2) objects] or with their generalizations to higher systems [Di Francesco–Zuber diagrams in the case of su(3)].

Although a precise general definition of extended Coxeter–Dynkin systems is still lacking, the known examples always contain a ''principal'' series (the $\mathcal{A}$ series) and a finite number of ''genuine exceptional'' cases.[24] The other diagrams of the system are obtained as orbifolds of the genuine diagrams (exceptional or not) and as twists or conjugates (sometimes both) of the genuine diagrams and of their orbifolds. In the case of su(2) (the usual *ADE* system), we have the principal *A* series, and the two genuine exceptional cases E_6 and E_8; the D_{2n} diagrams are orbifolds of the A_{4n-3} diagrams; and the D_{2n+1} diagrams are orbifolds of the A_{4n-1} diagrams and E_7 is a twist of the D_{10} diagram (itself an orbifold of A_{17}). In the case of su(3) (the Di Francesco–Zuber system, slightly amended by A. Ocneanu in Ref. 25), we have the principal series $\mathcal{A}_k$, and three genuine exceptional diagrams: $\mathcal{E}_5$, $\mathcal{E}_9$, and $\mathcal{E}_{21}$; the others (in particular the other four exceptionals) of the system are obtained from these genuine diagrams by orbifolding, twisting and conjugating.

In some cases, the vector space spanned by the vertices of a given diagram *G* admits ''self-fusion,'' [27,28] i.e., it possesses an associative algebra structure with positive integral structure constants [like A_n, D_{2n}, E_6 and E_8 for the su(2) system]. Sometimes it does not (like D_{2n+1} and E_7). In all cases, this vector space is a module over the associative algebra of the particular diagram *A* of the $\mathcal{A}$ series which has the same Coxeter number (whose definition has to be suitably generalized for the higher systems).

The $\mathcal{A}$ series is always modular: one can define a representation of $\mathrm{SL}(2,\mathbb{Z})$ on the vector space of every diagram of this class (actually this representation factors to a finite group, but we

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shall not need this information here). The standard generators of this group are called S and T. The vector space of the chosen diagram comes with a particular basis, where the basis vectors are associated with graph vertices. The operator T is diagonal on the vertices.

Take G to be a diagram and A to be the corresponding member of the $\mathcal{A}$ series. Being a module over the algebra of A, there exist induction-restriction maps between G and A and one can try to define an action of $\mathrm{SL}(2,\mathbb{Z})$ on the vector space of G, in a way that would be compatible with those maps; this is not necessarily possible. In plain terms, suppose that the vertex σ of G appears both in the branching rules (restriction map from A to G) of vertices τ_p and τ_q of A; one could think of defining the value of the modular generator T on σ either as $T(\tau_p)$ or as $T(\tau_q)$, but this is ambiguous, unless these two values are equal. In general, there is only a subset J of the vertices of G for which T can be defined: a vertex σ will belong to this subset whenever T is constant along the vertices of A whose restriction to G contains σ.

Following Ocneanu,[23] to every diagram G (with or without self-fusion) belonging to a Coxeter–Dynkin system, one can associate a bialgebra $\mathcal{B}G$. This bialgebra should be, technically, a weak Hopf algebra—or quantum groupoid—and we have checked this in a few cases, but we are not aware of any general proof (see our comments in the final section). By using a particular scalar product, one can trade the comultiplication for a multiplication and think that $\mathcal{B}G$ is a di-algebra rather than a bialgebra. There are two—usually distinct—block decompositions for this di-algebra. Blocks of the first type are labeled by points of a diagram A (the member of the $\mathcal{A}$ series that has same Coxeter number as G). Blocks of the second type are labeled by points of another diagram that we call $\mathrm{Oc}(G)$. The two sets of orthogonal projectors associated with these two block decompositions can be multiplied with either of these two associative multiplications and this allows one to define associative algebra structures on the vector spaces spanned by the vertices of the two graphs A and $\mathrm{Oc}(G)$. We denote these algebras by the same symbol as the graphs themselves. In the particular case where G is a member of the $\mathcal{A}$ series, these algebras coincide. In all cases, A is an algebra with a single generator and it is commutative. $\mathrm{Oc}(G)$, also called "algebra of quantum symmetries of G," is in general an algebra with two generators (only one if $G=A$) and it is not always commutative.

In the cases where $\mathrm{Oc}(G)$ is commutative, we observe that this algebra of quantum symmetries can be written in terms of a tensor product of appropriate graph algebras, but the tensor product should be taken above some subalgebra determined by the modular properties of the graph G and we refer to Sec. III for a discussion of the several ADE cases. Paradoxically, the simplest cases (besides the A_n) are those where the diagram G is an exceptional diagram equal to E_6 or E_8 (notice that E_7 does not enjoy self-fusion); in those simple cases $\mathrm{Oc}(G)$ is isomorphic with $G \otimes_J G$, where J is the particular subalgebra of the graph algebra of G whose determination (using modular considerations) was sketched previously. The tensor product sign, taken "above J," means that we identify $au \otimes b$ and $a \otimes ub$ whenever $u \in J \subset G$. When $\mathrm{Oc}(G)$ is not commutative, the method is not fully satisfactory, as we shall see.

The structure of our article is as follows. The first section reminds the reader of several useful (but not necessarily widely known) facts about graph algebras and their quantum symmetries. It also precises our notations. The reader already familiar with quantum symmetries of graphs may skip this part. In the second section, we consider the su(2) Coxeter–Dynkin system, i.e., the usual ADE diagrams. For every one of them we simply recover the structure of $\mathrm{Oc}(G)$ by our method (which is not fully satisfactory for D_{2n}, since the algebra of quantum symmetries of the later is non commutative). We give more details on the E_6 case because it is both nice and pedagogical. In the third section, we move to the su(3) Coxeter–Dynkin system. After some generalities on these Di Francesco–Zuber graphs and a short description of the cases associated with diagrams of $\mathcal{A}$ type (which are relatively trivial), we study, in detail, also because it is simple enough to be pedagogical, the quantum symmetries of the diagram $\mathcal{E}_5$ (the David star), which is one of the three genuine exceptional cases and is a module over $\mathcal{A}_5$. The technique being now clear, we list only the results for the other two genuine exceptional diagrams $\mathcal{E}_9$ and $\mathcal{E}_{21}$, i.e., we give their induction-restriction graphs, the values of the modular operator T and, for $\mathcal{E}_5$ and $\mathcal{E}_{21}$, the structure of their Ocneanu graph. To every point of such a graph, one may associate a "toric matrix,"[7,23] or,

equivalently, a twisted partition function in boundary conformal field theory with defect lines;[31] we also give their explicit expressions for the studied su(3) cases, at least those associated with the so-called ambichiral points (to keep the size of this article reasonable). The list of Di Francesco–Zuber graphs being quite long, we stop at this point, but all the other associated Ocneanu graphs should be obtained by proper generalizations of the study made for su(2); the details can, admittedly, be quite intricate, in particular for those graphs for which $\mathrm{Oc}(G)$ is not commutative.

Many topics discussed in the present article are already known to experts. We believe, however, that a systematic discussion of the correspondence between the eigenvalues of the T operators and the determination of quantum symmetries is not available elsewhere. Our explicit results concerning the Ocneanu graphs of several exceptional diagrams of the su(3) system seem also to be new, and, we hope, of interest for the reader.

II. ABOUT COXETER–DYNKIN GRAPH ALGEBRAS AND THEIR QUANTUM SYMMETRIES

A. Generalities

To a diagram G belonging to a (possibly higher) Coxeter–Dynkin system, one can associate[23] a bialgebra $\mathcal{B}(G)$ that we call Ocneanu–Racah–Wigner bialgebra (the precise definition of this bialgebra uses the notion of essential paths on the graph G: see our discussion in the Appendix). According to A. Ocneanu (unpublished), this object, also called ''algebra of double triangles,'' is a semi-simple weak Hopf algebra (or quantum groupoid)—see Refs. 3 and 21 for general properties of quantum groupoids. We shall not use it explicitly in our article and it is enough to say that, as a bialgebra, it possesses two associative algebra structures (say ''composition $\circ$'' and ''convolution $\star$''), for which the underlying vector space can be block diagonalized (i.e., decomposed as a sum of matrix algebras) in two different ways. Diagonalization of the convolution product is encoded by a finite dimensional algebra $\mathrm{Oc}(G)$ called ''algebra of quantum symmetries.'' As a vector space, $\mathrm{Oc}(G)$ contains one linear generator for every single block of $(\mathcal{B}(G),\star)$. As an algebra, it has a unit called $\underline{0}$ and two generators called $\underline{1}_L$ and $\underline{1}_R$, which, when G is a member of an $\mathcal{A}$ series, coincide. Like the graph algebra of G (when it exists), the algebra $\mathrm{Oc}(G)$ comes with a preferred basis. Even when the vector space of G does not admit self-fusion, so that it is only a module over the corresponding $\mathcal{A}$, the associated object $\mathrm{Oc}(G)$ is always both an associative algebra and a bimodule over $\mathcal{A}\otimes\mathcal{A}$. This last structure is encoded by a set of matrices that we call ''toric matrices''; there is one such matrix for every point of the Ocneanu graph. The multiplicative structure of $\mathrm{Oc}(G)$ is fully determined by the two Cayley graphs of multiplication by the generators; the union of these two graphs is called the Ocneanu graph of G and is denoted by the same symbol. In most cases, $\mathrm{Oc}(G)$ is isomorphic with a tensor product—over a particular subalgebra J—of two associative and commutative algebras; we write $\dot{\otimes}\equiv\otimes_J$ this tensor product; in these cases, $\mathrm{Oc}(G)$ is commutative. When it is not commutative [the case of D_{2n} for the su(2) system], one has also to add some matrix algebra component to this tensor product, in order to take the non-commutativity into account (see Ref. 8 for explicit formulas for D_{2n} cases). The two generators of $\mathrm{Oc}(G)$ read $\underline{1}_L=1\dot{\otimes}0$ and $\underline{1}_R=0\dot{\otimes}1$. Their algebraic span are respectively the ''left chiral'' and ''right chiral'' parts. The intersection of chiral subalgebras is called ''ambichiral'' and the vector space spanned by those (preferred) linear generators which belong to none of the chiral parts is called ''the supplementary part.'' All these structures lead to ''nimreps'' (non-negative integer valued matrix representations) of certain algebras.[30]

From the point of view of conformal field theory, we are interested in partition functions on a torus with defect lines. When there are no defects these partition functions are modular invariant; this is usually not so in the presence of defects. In all cases, they are sesquilinear forms with non-negative integer entries defined on the vector space spanned by the characters of an affine Lie algebra $\hat{\mathcal{G}}$. Here we forget this interpretation and replace these characters by vertices of a diagram of type $\mathcal{A}$. Partition functions are therefore square matrices indexed by these vertices. It was recognized more than 7 years ago by A. Ocneanu (published reference is Ref. 23) that ''the'' modular invariant of Cappelli–Itzykson–Zuber,[4,26,33] for a given ADE diagram G, was given by

the toric matrix W_0 associated with the origin $\underline{0}$ of the graph $\mathrm{Oc}(G)$. To see an example of how all this works, the reader may look at Ref. 7, where toric matrices W_x associated with the 12 points x of the graph $\mathrm{Oc}(E_6)$ are calculated. In Ref. 29 it was shown (among other things) that to the other points—other than the origin—of a graph $\mathrm{Oc}(G)$ can be associated partition functions in boundary conformal field theory (BCFT) with one defect line; these functions are not modular invariant. More general toric matrices (or partition functions) $W_{x,y}$, associated to BCFT with two defect lines, were also introduced in the same paper (note: $W_x \equiv W_{x,\underline{0}}$). Fully explicit expressions for the twisted partition functions W_x are given in Ref. 8, for all ADE cases, by using the formalism introduced in Ref. 7. This was done independently of Ref. 31. It should probably be stressed that all these expressions were already obtained (but unpublished) almost 8 years ago by A. Ocneanu himself.

The direct determination of the algebra $\mathrm{Oc}(G)$, with the definition provided by A. Ocneanu, is not an easy task and the associated graphs are only known (published) for the su(2) Coxeter–Dynkin system. One of the purposes of Refs. 7 and 8, besides the calculation of the toric matrices, was actually to give an algebraic construction providing a realization of the *algebra* $\mathrm{Oc}(G)$ in terms of graph algebras associated with appropriated Dynkin diagrams.

In the simple cases (paradoxically, for Dynkin diagrams, besides the A_n themselves, the ''simple'' cases happen to be those where G is an exceptional diagram equal to E_6 or E_8), the algebra of quantum symmetries is isomorphic with $G \otimes_J G$, where J is a particular subalgebra of the algebra of G (we refer to Ref. 8 for a discussion of all ADE cases). The tensor product sign, taken ''above J,'' means that we identify $au \otimes b$ and $a \otimes ub$ whenever $u \in J \subset G$. In the last quoted reference, the Ocneanu *graphs*, determined by Ocneanu himself, had to be taken as an input. This was a weak point in our approach.

For the su(2) Dynkin system, i.e., for ADE diagrams, one purpose of the present article is to show that the structure of $\mathrm{Oc}(G)$, can be, in most cases, determined from the eigenvalues of the modular T matrix in the Hurwitz-Verlinde representation,[1,15,34] associated with the graph algebra of A_n. The method is general but its implementation depends about the type of diagram considered, i.e., whether it is a member of the $\mathcal{A}$ series, a genuine exceptional, or if it is obtained as an orbifold or by twisting. In any case, one has first to select a particular subspace J by using the list of eigenvalues of the modular operator T acting on the vertices belonging to the corresponding $\mathcal{A}$ diagram. In the case of E_6, for instance, the subset J, obtained as explained in the introduction, by using a modular constraint on the induction-restriction rules coming from the A_{11} action, is isomorphic with an A_3 subalgebra of E_6 and the Ocneanu algebra $\mathrm{Oc}(E_6)$ is recognized as $E_6 \dot{\otimes}_{A_3} E_6$. Warning: everywhere in this article, the symbol denoting the diagram also denotes its corresponding associative graph algebra, when it exists; it never refers to the corresponding Lie algebra with the same name (for the higher Coxeter–Dynkin systems, this would not even be an algebra in the usual sense!). The analysis of the D_{2n} cases, where $\mathrm{Oc}(G)$ is not commutative, is more subtle.

For the su(3) system, a direct diagonalization of the convolution law $\star$ of the bialgebra $\mathcal{B}(G)$ was never performed explicitly (or maybe by A. Ocneanu, but this information is not available), and the algebras $\mathrm{Oc}(G)$—or their Cayley graphs—have never been calculated (published) or even properly defined; therefore our method, which can indeed be generalized in a straightforward manner to this more general setting, has a conjectural flavor since we do not compare our results with those that would be obtained by a direct approach. Nevertheless, we have checked, in the case of exceptional graphs of su(3) type, that partition functions (toric matrices) associated with the origin of ''our'' Ocneanu graphs indeed coincide with the modular invariant partition functions calculated by Ref. 13 and that expected sum rules also hold (nontrivial equalities between two sums of squares coming from the diagonalization of the two associative structures for a given bialgebra). We obtain also, as a by product, the list of twisted partition functions corresponding to a given diagram G [there are 24 of them for the exceptional $\mathcal{E}_5$ case of the su(3) system].

B. Useful formulas and notations

For Dynkin diagrams, i.e., the su(2) system, κ is the (dual) Coxeter number of the diagram itself. It can be defined, without any reference to the theory of Lie algebras, from the norm β of the graph (biggest eigenvalue of the adjacency matrix): β is equal to $2\cos(\pi/\kappa)$. Note that $1<\beta<2$ (see also Ref. 14). For Di Francesco–Zuber graphs, i.e., the su(3) system, the norm β is equal to $1+2\cos(2\pi/\kappa)$. Note that $2<\beta<3$. This again defines the integer κ. We call it the "generalized Coxeter number of the graph" or "altitude" (like in Ref. 10). We also define $q=\exp(i\pi/\kappa)$, so that $q^{2\kappa}=1$. Another integer h characterizes the system of diagrams. For Dynkin diagrams, $h=2$, the (dual) Coxeter number of su(2). For Di Francesco–Zuber graphs, $h=3$, the (dual) Coxeter number of su(3).

The level k of a *diagram* is defined by the relation $k=\kappa-h$. Notation for graphs: we keep the standard notation for usual Dynkin diagrams, with subscript referring to the number of vertices, i.e., the rank of the corresponding Lie algebra. However, for consistency with the notation used for higher Coxeter–Dynkin systems, it would be better for this subscript to refer to the level k or to the altitude κ. We may use both notations, but with script capitals in the latter case, for instance (Dynkin diagrams), $\mathcal{A}_{\kappa-2}=A_{\kappa-1}$, $\mathcal{E}_{10}=E_6$, $\mathcal{E}_{16}=E_7$, $\mathcal{E}_{28}=E_8$. In the case of the Di Francesco–Zuber system of graphs, our subscript will always refer to the level. Since $h=3$ for su(3), we have $k=\kappa-3$ for all diagrams of this family. The reader should be warned that this notation is not universally accepted, and some authors may prefer to use the altitude (as an upper index) rather than the level. For instance, the graphs that we call $\mathcal{E}_5$, $\mathcal{E}_9$ and $\mathcal{E}_{21}$ (like in Ref. 25) were called respectively $\mathcal{E}^{(8)}$, $\mathcal{E}_2^{(12)}$ and $\mathcal{E}^{(24)}$ in Ref. 10.

In the case of su(N), there are $N-1$ fundamental representations f, and therefore $N-1$ graphs G^f (see Ref. 10), representing tensor multiplication of irreps by f. Since we shall work only with su(2) or su(3), we need only one graph. In the case of su(2), this is clear. In the case of su(3), this graph is associated with one fundamental irrep (say 3), the other graph associated with its conjugate (say $\overline{3}$) is obtained by reversing all the arrows; adjacency matrices corresponding to the fundamental and to its conjugate are denoted by G and by its transpose G^T.

For a diagram of type su(N), the graph algebra, when it exists, is faithfully represented (regular representation) by $r\times r$ matrices G_a. In all cases, G_0 is the identity matrix and G_1 is the adjacency matrix. We denote by r the number of vertices of the diagram G. The r linear generators σ_a of G, with dual Coxeter number (or altitude) κ, are then represented by r commuting matrices G_a.

In the particular case where G is a member of the A system, the generators will be called τ_i and the corresponding matrices will be called N_i. For a diagram of type A belonging to a given su(N) system, writing down matrices N_0 (identity) and N_1 (adjacency matrix) is immediate, and there are always simple recurrence formulas that allow one to compute the matrices N_i for all vertices of the A system in terms of N_0 and N_1 (thought as the basic representation). These standard recurrence formulas can be obtained, for instance, by making products of Young frames [see later sections for su(2) and su(3)].

The module property (external multiplication) of the vector space associated with a diagram G, of level k and possessing r vertices, with respect to an action of the corresponding algebra $\mathcal{A}_k$ is encoded by a set of s matrices F_i, $i=0,\ldots,s-1$, of dimension $r\times r$, sometimes called "fused graph matrices" (a misleading terminology!): $\tau_i\sigma_a=\Sigma_b(F_i)_{ab}\sigma_b$. The number s of vertices of $\mathcal{A}_k$ depends on the system: for Dynkin diagrams ($\mathcal{A}_k=A_{k+1}$), $s=k+1$; for Di Francesco–Zuber graphs, $s=(k+1)(k+2)/2$. Matrix F_0 is the identity and matrix $F_1=G_1$ is also the adjacency matrix of G. The other F matrices are determined by imposing that they should obey the same recurrence relation as the N matrices; this ensures compatibility with left multiplication by the algebra $\mathcal{A}_k$. The sets of matrices F_i, N_i and G_a of course coincide when G is a diagram of type A. The r essential matrices E_a are rectangular matrices of dimension $s\times r$ defined by setting $(E_a)_{ib}=(F_i)_{ab}$ (the reader should be cautious about the meaning of indices: our indices i or a refer to actual vertices of the graphs but the numbers chosen for labeling rows and columns depend on some arbitrary ordering on these sets of vertices). The particular matrix E_0 is usually

called ''intertwiner,'' in the statistical physics literature; it also describes ''essential paths'' emanating from the origin (we shall not need this notion in the present article). One can check that, for graphs with self-fusion, $E_a = E_0 G_a$.

Vertices of the diagram G should be thought of as an analog of irreducible representations for a subgroup of a group; the irreducible representations of the bigger group are themselves represented by vertices of the graph A. In this analogy, the first column of each matrix F_i describes the branching rule of τ_i with respect to the chosen subgroup (restriction mechanism). In the same way, the columns of the particular essential matrix E_0 describe the induction mechanism: the nonzero matrix elements of the column labeled by σ_b tell us what are those representations τ_i that contain σ_b in their decomposition (for the branching $A \to G$).

Let us recall how we compute the (twisted) partition functions $Z_{x,y}$, at least, in the cases where $\mathrm{Oc}(G) \simeq G \otimes_J G$. Again, we follow the method explained in Ref. 7 and refer to Ref. 8 for a discussion of all the ADE cases, but another formalism for calculating these quantities was described in Ref. 31. The bimodule structure of $\mathrm{Oc}(G)$ with respect to the corresponding $\mathcal{A}_k$ algebra is encoded by matrices $W_{x,y}$ defined as $\tau_i . x . \tau_j = \Sigma_y (W_{x,y})_{ij} . y$. One sets $W_x = W_{x,\underline{0}}$ and obtain the corresponding twisted partition functions as sesquilinear forms $Z_{x,y} = \overline{\chi} W_{x,y} \chi$, or $Z_x = Z_{x,\underline{0}}$. Here χ is a vector in the complex vector space $\mathbb{C}^s$. The modular invariant partition function is $Z_{\underline{0}}$ with $\underline{0} = 0 \dot{\otimes} 0$. The $W_{x,y}$ can be simply obtained from the W_x by working out the multiplication table of $\mathrm{Oc}(G)$ and decomposing the product $x \times y$ on the basis generators [one of us (RC) acknowledges discussions with M. Huerta about this]. Practically, once we have the r rectangular matrices E_a, of dimension $s \times r$ (with $s = \kappa - 1$ for ADE diagrams), we first replace by 0 all the matrix elements of the columns labeled by vertices b that *do not* belong to the subset J of the graph G, call E_a^{red} these ''reduced'' matrices, and obtain, for each point $x = a \dot{\otimes} b$ of the Ocneanu graph $\mathrm{Oc}(G)$ (in some cases, x may be a linear combination of such elements), a ''toric matrix'' $W_x = E_a (E_b^{red})^T$ of size $s \times s$.

The usual partition function on a torus is calculated by identifying the states at the end of a cylinder through the trace operation. One may incorporate the action of an operator X attached to a nontrivial cycle of the cylinder before identifying the two ends. This operator should commute with the Virasoro generators and its effect is basically to twist the boundary conditions. An explicit expression, in the presence of two twists X and Y, was written for such a twisted partition function by Refs. 29 and 31; it involves matrix elements of the modular operator S. Our own determination of the toric matrices (and corresponding twisted partition functions) uses directly the fusion algebra—i.e., the graph algebra of the A_n diagrams. Of course we could, by using the Verlinde formula, express the fusion rule coefficients through the matrix S, but in our approach, the diagrams themselves are taken as primary data and we do not need to use this operator at all, at least for the determination of the $W_{x,y}$.

III. *ADE* DIAGRAMS: THE su(2) SYSTEM

A. Preliminary remarks

ADE Dynkin diagrams are well known. Their norm (highest eigenvalue of the adjacency matrix) is $2\cos(\pi/\kappa) = \beta$. Diagrams $A_{\kappa-1}$ have r points τ_j, $j = 0, \ldots, \kappa - 2$, with $r = \kappa - 1 = k + 1$ (this defines the level k). In the light of McKay correspondance,[20] these diagrams appear as quantum analog of binary polyhedral groups.[6,17,18] For su(2), the recurrence formula for adjacency matrices associated with irreps is very well known: we have $N_0 N_j = N_j$, $N_1 N_j = N_{j-1} + N_{j+1}$, for $1 \leqslant j \leqslant \kappa - 2$. This is the usual multiplication of spin $j/2$ representation by the fundamental (spin $\frac{1}{2}$). For the diagram $A_{\kappa-1}$, we also have a truncation of the spin rule: $N_1 N_{\kappa-2} = N_{\kappa-3}$.

Left action of the algebra $A_{\kappa-1}$ on the vector space of a diagram G is defined by setting $F_0 = G_0 = \mathbf{1}_{r \times r}$, $F_1 = G_1$, and compatiblility with left multiplication in $A_{\kappa-1}$ is ensured by imposing the spin rule $F_1 F_i = F_{i-1} + F_{i+1}$, a relation that determines the F_i's iteratively.

The modular generator T, in the Hurwitz–Verlinde representation, is given by

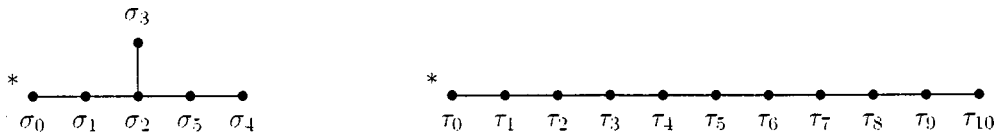

FIG. 1. The E_6 and A_{11} Dynkin diagrams.

$$T_{jj'}=\exp\left[2i\pi\left(\frac{(j+1)^2}{4\kappa}-\frac{1}{8}\right)\right]\delta_{jj'},$$

where j,j' run from 0 to $\kappa-2$.

The value of T on the vertex τ_j of $A_{\kappa-1}$ is therefore determined, up to a global phase, by the quantity $\hat{T}=(j+1)^2 \bmod 4\kappa$, which we will call the "modular exponent" (see also the Appendix). The algebras of quantum symmetries $\mathrm{Oc}(G)$, for diagrams G of type ADE, are already known, and the corresponding Ocneanu graphs can be found, for instance, in Refs. 5, 7, 8, 23, 30, and 31, or also, in the context of the theory of induction of sectors, in Ref. 2. In the present section, the overlap with Ref. 8 is important: in the later reference, an algebraic realization of the algebras $\mathrm{Oc}(G)$ was given, but the primary data was the Ocneanu graph itself, taken from Ref. 23. In the present section, our aim is neither to describe the algebras of quantum symmetries nor their corresponding graphs, since this is known already, but to show how the modular properties of the diagrams (in particular the table of eigenvalues for the operator T), together with the induction-restriction pattern, can be used to recover the known algebras of quantum symmetries. This section also provides a kind of introduction to Sec. IV where the same techniques will be used to determine the structure of $\mathrm{Oc}(G)$ for several diagrams belonging to the su(3) system.

B. First example: The E_6 case

1. Graphs

The vector space of E_6 is both an associative (and commutative) algebra with positive integral structure constants (in other words, it admits self-fusion), and it is a module over A_{11}. This example is fully studied in Ref. 7 (see also Ref. 6); in particular its graph algebra matrices, essential matrices, Ocneanu graph and toric matrices are given there. The E_6 Dynkin diagram and the corresponding A diagram with same norm (i.e., A_{11}) are displayed in Fig. 1.

For trees with one branching point (for instance, E_6, E_7 and E_8 diagrams), we label (one of) the longest branches with increasing integers starting from 0, up to the branching point, then we jump to the extremity of the next (clockwise) branch and so on. This is the ordering consistently chosen in Refs. 7 and 8.

2. Restriction mechanism

We look at E_6 as a module over A_{11}. For this, we define an action of A_{11} on E_6:

$$A_{11}\times E_6\to E_6$$

$$\tau_0.\sigma_i=\sigma_i$$

$$\tau_1.\sigma_i=\sum{}'\ \sigma_j$$

where Σ' runs over the neighbors of σ_i on the diagram E_6.

We have obvious restrictions: $\tau_0\hookrightarrow\sigma_0$, $\tau_1\hookrightarrow\sigma_1$. To obtain the others, we impose the compatibility condition: $(\tau_1)^n.\sigma_i=(\sigma_1)^n.\sigma_i$. We therefore calculate the powers of the fundamentals τ_1 and σ_1 and compare the results:

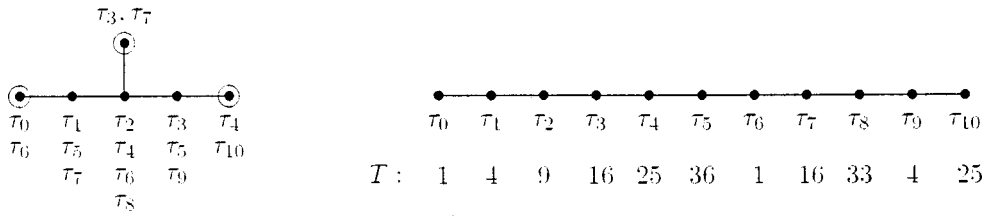

FIG. 2. The $E_6 \hookleftarrow A_{11}$ induction graph and the values of $\hat{T}$ on irreps of A_{11}.

$$(\tau_1)^2 = \tau_0 + \tau_2, \quad (\sigma_1)^2 = \sigma_0 + \sigma_2, \quad \text{so} \quad \tau_2 \hookrightarrow \sigma_2;$$

$$(\tau_1)^3 = 2\tau_1 + \tau_3, \quad (\sigma_1)^3 = 2\sigma_1 + \sigma_3 + \sigma_5, \quad \text{so} \quad \tau_3 \hookrightarrow \sigma_3 + \sigma_5;$$

and so on. In this way, we get the following branching rules $\tau_i \hookrightarrow \oplus E^0_{ij}\sigma_j$ (essential matrix E_0):

$$\tau_0 \hookrightarrow \sigma_0 \quad \tau_1 \hookrightarrow \sigma_1 \quad \tau_2 \hookrightarrow \sigma_2 \quad \tau_3 \hookrightarrow \sigma_3 + \sigma_5$$

$$\tau_4 \hookrightarrow \sigma_2 + \sigma_4 \quad \tau_5 \hookrightarrow \sigma_1 + \sigma_5 \quad \tau_6 \hookrightarrow \sigma_0 + \sigma_2 \quad \tau_7 \hookrightarrow \sigma_1 + \sigma_3$$

$$\tau_8 \hookrightarrow \sigma_2 \quad \tau_9 \hookrightarrow \sigma_5 \quad \tau_{10} \hookrightarrow \sigma_4.$$

The rectangular 11×6 matrix E_0 encodes this result, i.e., the above branching rules give us the lines of this matrix. Notice that this determination of E_0 does not require any calculation involving essential paths (this notion, although extremely nice and useful, is not required at this level).

Once the adjacency matrix G_1 is known (read it from the graph), and the essential matrix E_0 (or intertwiner) determined, we can use the general formulas given in the Introduction to determine the 6 graph matrices G_a, the 11 matrices F_i and the other essential matrices E_a (six of them, including E_0). Notice that, from the very beginning, we could have proceeded differently, determining first the F_i by using both the equation $F_1 = G_1$ and the su(2) rule of composition of spins (recurrence relation); these matrices, in turn, determine the E_a's (in particular E_0).

3. Induction mechanism

We now look at these previous branching rules, but in the opposite direction: for instance, σ_3 *comes from* τ_3 and τ_7, so we can write $\sigma_3 \hookleftarrow (\tau_3, \tau_7)$. We get the induction correspondence $E_6 \hookleftarrow A_{11}$ displayed in Fig. 2. This is only another way to write the columns of the E_0 matrix. We also plot the values of the modular exponent $\hat{T}$ for the vertices τ_i's of A_{11}.

From the induction graph we have $\sigma_0 \hookleftarrow (\tau_0, \tau_6)$, and we notice that the value of the modular matrix T on τ_0 and τ_6 is the same (also for τ_3 and τ_7, and for τ_4 and τ_{10}). This allows one to assign a fixed value of T to three particular vertices of E_6: $\hat{T}(\sigma_0) = 1$, $\hat{T}(\sigma_3) = 16$ and $\hat{T}(\sigma_4) = 25$. For every other point of the E_6 graph, the value of T that would be inherited from the A_{11} graph by this induction mechanism is not uniquely determined (for instance, in the case of σ_1, the values of $\hat{T}$ obtained from A_{11} would be associated with τ_1, τ_5 and τ_7 but these values are not all equal). These elements $\{\sigma_0, \sigma_4, \sigma_3\}$ span the subalgebra $J = A_3$. This subalgebra is known to admit an invariant supplement in the graph algebra of E_6.

4. Quantum symmetries

The Ocneanu graph of E_6 given in Refs. 7, 8, 23, and 31 is the Cayley graph of multiplication by the two generators of an associative algebra $\mathrm{Oc}(E_6)$ which can be realized (see Refs. 7 and 8) as $E_6 \otimes_{A_3} E_6$. It has $12 = 6 \times \frac{6}{3}$ vertices, three of them being ambichiral, namely $\sigma_0 \dot{\otimes} \sigma_0$, $\sigma_0 \dot{\otimes} \sigma_3$ and $\sigma_0 \dot{\otimes} \sigma_4$. We introduce the symbol $\dot{\otimes}$ to denote $\otimes_{A_3}$ to stress the fact that the tensor product is taken not above the complex numbers but above the subalgebra $J = A_3$. This means that

$a\,u\dot{\otimes}b=a\dot{\otimes}u\,b$ whenever $u\in\{\sigma_0,\sigma_4,\sigma_3\}$ and $a,b\in E_6$. The point that we make, here, is that this subalgebra A_3 is actually *determined* as above, by induction, from the eigenvalues of the T operator.

5. Dimensions of blocks

Diagonalization of the two algebra structures of $\mathcal{B}E_6$ leads to the quadratic sum rule

$$dim(\mathcal{B}E_6)=\sum_{i\in A_{11}} d_i^2=\sum_{x\in Oc(E_6)} d_x^2=2512=(2)^4(157)^1,$$

where $d_i=\Sigma_{a,b\in G}(F_i)_{ab}$ runs in the list (6,10,14,18,20,20,20,18,14,10,6) and where, for $x=a\dot{\otimes}b$, $d_x=\Sigma_{i,j\in A_{11}}(G_a.G_b)_{ij}$ runs in the list (6,8,6,10,14,10,10,14,10,20,28,20). This identity follows directly from the fact that $\mathcal{B}E_6$ can be written in two different ways as a direct sum of matrix algebras ($\mathcal{B}E_6$ is semi-simple for both structures).

We have also the linear sum rule $\Sigma d_i=\Sigma d_x=720=(2)^4(3)^2(5)^1$. Such a linear sum rule also holds "experimentally" in almost all ADE cases (for the D_{2n} cases one has actually to introduce a simple correcting factor, as explained in Ref. 31). In general, there is no reason, for a general bialgebra—even semi-simple for both structures—to give rise to such a linear sum rule. The interpretation of this property is therefore still mysterious. As we shall see in the next part, it also holds for the several examples of diagrams of type su(3) that we have analyzed so far.

There are also quantum sum rules ("mass relations"): define $o(G)\doteq\Sigma_{a\in G}qdim_a^2$, where $qdim_a$ are the quantum dimensions of the vertices a of G [for example, $o(E_6)=4(3+\sqrt{3})$, $o(A_{11})=24(2+\sqrt{3})$, $o(A_3)=(1+(\sqrt{2}))^2=4$]; then, if the diagonalizations of the two algebra structures of $\mathcal{B}(G)$ are described respectively by $\mathcal{A}_k$, for some k, and by $\mathrm{Oc}(G)=G\otimes_J G$ for some J, one can check that $o(\mathrm{Oc}(G))$ defined as $o(G)\times o(G)/o(J)$ is equal to $o(\mathcal{A}_k)$. In the present case, $o(E_6)\times o(E_6)/o(A_3)=o(A_{11})$. This observational fact, properly generalized, holds for all ADE diagrams. Indeed, $o(D_n)=\frac{1}{2}o(A_{2n-3})$ and $o(E8)\times o(E8)/o(J)=o(A_{29})$, where $o(J)=[1]_q^2+([5]_q/[3]_q)^2$ since the quantum dimensions of vertices σ_0 and σ_6 spanning the subspace J of E_8 are respectively equal to the q-numbers $[1]_q$ and $[5]_q/[3]_q$ (here $q=\exp(i\pi/30)$). In the case of E_7, we found that $o(\mathrm{Oc}(E_7))$ defined as $o(D_{10})\times o(D10)/o(J)$, where J is the subalgebra of D_{10}, is equal to $o(A_{17})$. We found also empirically the relation $o(A_{17})=o(E_7)\times o(D_{10})/o(J)$, where $o(J)=[2]_q^2+[4]_q^2+([4]_q/[3]_q)^2$ and where the q-numbers $[2]_q$, $[4]_q$ and $[4]_q/[3]_q$ are the q-dimensions of the vertices σ_1, σ_3 and σ_5 of E_7 [here $q=\exp(i\pi/18)$]. Analogous quantum sum rules hold for the several examples of diagrams of type su(3) that we have analyzed so far. We do not know any general formal proof of these quantum relations.

C. The *ADE* diagrams

We show in this section how all cases relative to the su(2) system can be studied in the same manner.

1. E_6 case

It was studied in the last section.

2. E_8 case

The cases of E_6 and E_8 are very similar. The Dynkin diagram of the A series with same Coxeter number ($\kappa=30$) as E_8 is A_{29}. Like E_6, the vector space of the diagram E_8 admits self-fusion (associative algebra structure with positive integral structure constants). The induction graph $E_8\hookleftarrow A_{29}$ is displayed in Fig. 3.

The value of $\hat{T}$ on irreps $(\tau_0,\tau_1,\tau_2,\ldots,\tau_{28})$ of A_{29} [equal for τ_j to $(j+1)^2$ mod 120] gives

$$(\underline{1},4,9,16,25,36,\underline{\underline{49}},64,81,100,\underline{1},22,\underline{\underline{49}},76,105,16,\underline{\underline{49}},84,\underline{1},40,81,4,\underline{\underline{49}},96,25,76,9,64,\underline{1}).$$

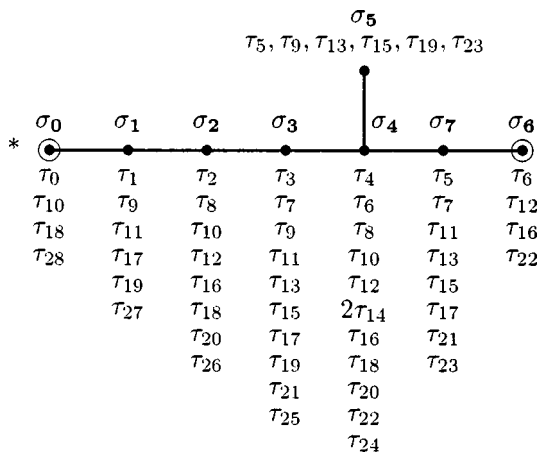

FIG. 3. The $E_8 \hookleftarrow A_{29}$ induction graph.

We see that T has the same value on vertices τ_j that correspond to σ_0 ($\hat{T}=1$). Same comment for σ_6 ($\hat{T}=49$). We therefore take $J=\{\sigma_0,\sigma_6\}$; this generates a subalgebra which is isomorphic with the algebra of the A_2 graph. We have indeed $\mathrm{Oc}(E_8)=E_8 \otimes_{A_2} E_8$ and the Ocneanu graph has $32=8\times\frac{8}{2}$ vertices, two of them being ambichiral, namely, $\sigma_0 \dot{\otimes} \sigma_0$ and $\sigma_0 \dot{\otimes} \sigma_6$. Notice that $\sigma_6 \dot{\otimes} \sigma_6 = \sigma_0 \dot{\otimes} \sigma_0$. Dimensions of blocks can be computed as before (see, for instance, Ref. 8). One writes $dim(\mathcal{B}E_8)=63\,136=(2)^5(1973)^1$ in two different ways as a sum of 29 or 32 squares. The linear sum rule gives $\Sigma d_i = \Sigma d_x = 1240 = (2)^3(5)^1(31)^1$.

3. $A_{\kappa-1}$ cases

The induction-restriction rules from $A_{\kappa-1}$ to itself are of course trivial and the subalgebra J determined by the constancy of T on preimages is equal to the algebra $A_{\kappa-1}$ itself. The algebra $\mathrm{Oc}(A_{\kappa-1})$ equal to $A_{\kappa-1} \otimes_{A_{\kappa-1}} A_{\kappa-1}$ is therefore isomorphic with $A_{\kappa-1}$ itself. The Ocneanu graph coincides with the original Dynkin diagram.

4. D_{2n+1} cases

The Dynkin diagram of the A series with same Coxeter number ($\kappa=4n-2$) as D_{2n+1} is A_{4n-1}. Actually (see Ref. 19). D diagrams are $\mathbb{Z}_2$ orbifolds of A diagrams.

Let's first have a look at the A_7 case. Its Dynkin diagram and the values of $\hat{T}$ on irreps τ_i's are given in Fig. 4.

The algebra of quantum symmetries of A_7, as we saw, is $A_7 \otimes_{A_7} A_7 \simeq A_7$, but there is also another way to quotient the tensor product if we want T to be well defined in the quotient. We see that the values of T are the same ($\hat{T}=4$) for τ_1 and τ_5, so we define therefore a map (twist) $\rho: A_7 \to A_7$ such that

$$\rho(\tau_i)=\tau_i \quad \text{for } i \in \{0,2,3,4,6\} \quad \text{and} \quad \rho(\tau_1)=\tau_5, \quad \rho(\tau_5)=\tau_1.$$

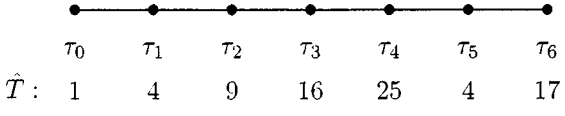

FIG. 4. The A_7 diagram and the values of $\hat{T}$.

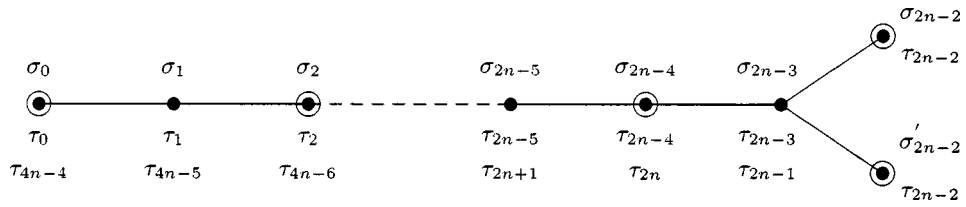

FIG. 5. The $D_{2n} \hookleftarrow A_{4n-3}$ induction graph.

Defining then $\mathrm{Oc}(D_5) = A_7 \otimes_{\rho(A_7)} A_7$ we recover the algebra of quantum symmetry of D_5. This can be generalized for all D_{2n+1} cases. These diagrams do not enjoy self-fusion displayed in Fig. 5.

5. D_{2n} cases

Starting with the D_{2n} diagram and graph algebra, we obtain the induction graph with respect to the corresponding A diagram with the same norm (A_{4n-3}) displayed in Fig. 5.

The value of $\hat{T}$ on the irreps $\{\tau_0, \tau_1, \tau_2, \ldots, \tau_{2n-1}, \tau_{2n}, \tau_{2n+1}, \ldots, \tau_{4n-6}, \tau_{4n-5}, \tau_{4n-4}\}$ of A_{4n-3} gives

$$T(\tau_0) = T(\tau_{4n-4}) \quad T(\tau_2) = T(\tau_{4n-6}) \quad \cdots \quad T(\tau_{2n-4}) = T(\tau_{2n}).$$

These last values are symmetric with respect to the central vertex τ_{2n}.

We can assign a fixed value of T for the irreps $\{\sigma_0, \sigma_2, \ldots, \sigma_{2n-4}, \sigma_{2n-2}, \sigma'_{2n-2}\}$ for D_{2n} (marked with a circle in the induction diagram). They span the subalgebra J. However, we notice immediately that something special happens here: the two ends of the fork (vertices σ_{2n-2} and σ'_{2n-2}) are not distinguished by the values of T. Actually, the determination of the graph matrices G_a for the Dynkin diagram D_{2n} is not as straightforward as for some other cases: looking for an associative algebra determined by this diagram leads to a two-parameter family of solutions, but there is only one solution (up to permutation $G_{2n-2} \leftrightarrow G'_{2n-2}$) that has correct self fusion, i.e., integrality and positivity of structure constants [a similar phenomenon appears, for example, for the $\mathcal{E}_9$ diagram of the su(3) system]. Since T may be defined on any linear combination of these two vertices, it is natural to expect that this arbitrariness is encoded, at the level of the algebra of quantum symmetries, in a "noncommutative geometrical spirit," by an algebra of 2×2 matrices. $\mathrm{Oc}(D_{2n})$ consists indeed of two separate components: the first (usual) is given by $D_{2n}^{trunc} \otimes_{J'} D_{2n}^{trunc}$, where D_{2n}^{trunc} is the vector space corresponding to the subdiagram spanned by $\{\sigma_0, \sigma_1, \sigma_2, \ldots, \sigma_{2n-3}\}$, obtained by removing the fork, and $J' = \{\sigma_0, \sigma_2, \ldots, \sigma_{2n-4}\}$ is the corresponding truncated subset of J. The second component is a noncommutative 2×2 matrix algebra reflecting the indistinguishability of σ_{2n-2} and σ'_{2n-2}. Ambichiral points are associated with the $n+1$ vertices of J (i.e., $n-1$ for the linear branch and 2 for the fork); we expect therefore that the Ocneanu graph of D_{2n} will have $(2n-2)(2n-2)/n - 1 + 4 = 4n$ vertices. We could as well say that the number of "effective" points of J is n, rather than $n+1$ and notice that $4n = 2n \times 2n/n$. This is indeed correct (see Refs. 8, 23, and 31). One way to realize the algebra $\mathrm{Oc}(D_{2n})$ is to write it as a quotient of the semi-direct product, by $\mathbb{Z}_2 = \{-, +\}$ of the tensor square of the graph algebra D_{2n}. The noncommutativity of the multiplication can be seen, for instance, from the fact that $(2 \dot{\otimes} 0, +)(0 \dot{\otimes} 0, -) = (2 \dot{\otimes} 0, -)$, but $(0 \dot{\otimes} 0, -)(2 \dot{\otimes} 0, +) = (2' \dot{\otimes} 0, -)$. The reader may refer to Ref. 8 for another explicit realization of this algebra. In any case, the method followed so far, which is based on the eigenvalues of the T operator, seems to be insufficient to fully determine the Ocneanu graph in that example.

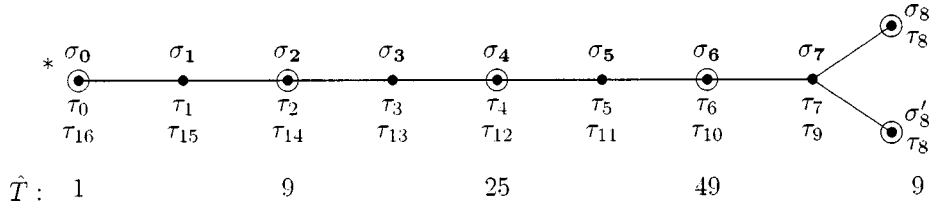

FIG. 6. The $D_{10} \hookleftarrow A_{17}$ induction graph and the values of $\hat{T}$.

6. E_7 case (related to the D_{10} case)

For the D_{10} case, something special happens. The corresponding A diagram with the same norm is A_{17}, the induction graph is displayed in Fig. 6, and the value of T in irreps $\{\tau_0, \tau_1, \ldots, \tau_8, \ldots, \tau_{15}, \tau_{16}\}$ of A_{17} are

$$(1,4,\underline{9},16,25,36,49,64,\underline{9},28,49,0,25,52,\underline{9},40,1).$$

These values are symmetric with respect to the central vertex, as in all A_{4n-3} case. For A_{17}, the value of T on the central vertex (τ_8) is equal to the value of T on other vertices, namely τ_2 and τ_{14}. This gives us another way to define a twist ρ acting on the vertices of D_{10} (this is "the" exceptional twist of the su(2) Coxeter–Dynkin system; existence of this twist is not new, but what we discuss here is its relation with the modular T operator). In other words, we form the tensor product $D_{10} \otimes D_{10}$, but identify $au \otimes b$ with $a \otimes \rho(u) b$ when $u \in \{\sigma_0, \sigma_2, \sigma_4, \sigma_6, \sigma_8, \sigma'_8\}$ and

$$\rho(\sigma_0) = \sigma_0, \quad \rho(\sigma_4) = \sigma_4, \quad \rho(\sigma_8) = \sigma_2,$$

$$\rho(\sigma_2) = \sigma_8, \quad \rho(\sigma_6) = \sigma_6, \quad \rho(\sigma'_8) = \sigma'_8.$$

We obtain the algebra $D_{10} \otimes_\rho D_{10}$ which is isomorphic with the algebra of quantum symmetries of the E_7 diagram. The diagram E_7 does not enjoy self-fusion.

Remark 1. The reader will have noticed that we do not necessarily *start* from a given graph G (for instance, E_7), for which we want to deduce $\mathrm{Oc}(G)$. Rather, we first consider all those graphs G which admit a good algebra structure (self-fusion), i.e., A, D_{2n}, E_6 and E_8; we then determine, for every one of them, the induced pattern of T eigenvalues by looking at the well determined $A \to G$ restriction; finally, we build all the possible quotients of $G \otimes G$ over the subalgebras—and possibly twists—determined by the pattern of T values. For example, if we assume that E_7 is already known to "exist" (as a module over A_{17}), and since it does not admit self-fusion, the only thing that we expect *a priori* is that its algebra of quantum symmetries $\mathrm{Oc}(E_7)$ will be obtained as a quotient of a tensor product of the algebras A_{17} or D_{10}. Therefore, $\mathrm{Oc}(E_7)$ is only the *name* given to $D_{10} \otimes_\rho D_{10}$; the graph E_7 itself can then be recognized as one of the two subsets of vertices of $\mathrm{Oc}(E_7)$ that linearly generates a module over one of the two chiral parts of the Ocneanu graph (each one being isomorphic with the algebra of D_{10}).

Remark 2. As discussed previously, the method that we follow seems to be insufficient to fully determine $\mathrm{Oc}(G)$ when the later is not commutative (cases when a coefficient strictly larger than 1 appears in the corresponding expression of the modular invariant partition function). These is only one example of this kind for the su(2) system (the D_{2n} diagrams), but there are several such examples for the su(3) system.

IV. DI FRANCESCO–ZUBER DIAGRAMS: THE su(3) SYSTEM

A. Preliminary remarks

In the su(2) case, the classification follows an ADE pattern. For su(n), $n \geqslant 2$ cases, there was no at-hand diagrams to start with, but the list of su(3) diagrams ("generalized Coxeter Dynkin diagrams") was obtained in 1989 (with CAF = computer-aided flair) by Di Francesco and Zuber in

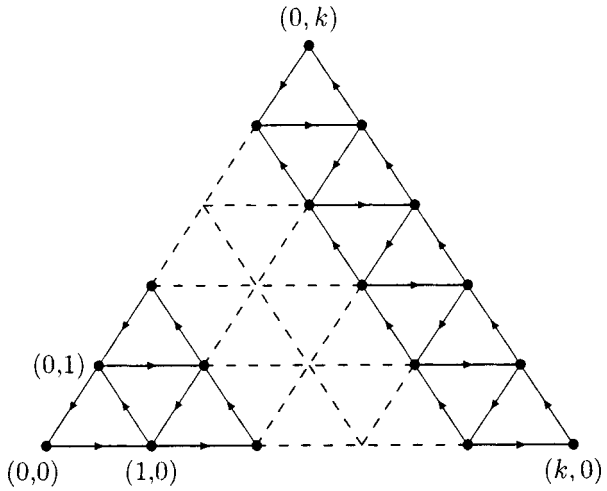

FIG. 7. The $\mathcal{A}_k$ diagram for su(3) with $(k+1)(k+2)/2$ vertices.

Ref. 10; this list was later shown to be complete by A. Ocneanu, during the Bariloche school at the very beginning of 2000 (actually one of their graphs—the one called $\mathcal{E}_3^{(12)}$ in Ref. 10—had to be removed).

Pictures of the graphs belonging to the Coxeter–Dynkin system of su(3) can be found in Refs. 10, 11, and 35–37; we refer to Refs. 25 and 38 or to the school web page *www.univ−mrs.fr/∼coque/Bariloche.html* for the final list. We do not discuss the su(4) system in this article, but these graphs can also be found in the Ocneanu contribution to the same Bariloche school[25] and on the corresponding web pages.

As recalled earlier, this system contains the principal $\mathcal{A}$ series and three genuine exceptional cases: $\mathcal{E}_5$, $\mathcal{E}_9$ and $\mathcal{E}_{21}$. The other diagrams of this system (and in particular the four other exceptional ones) are obtained as twists or as orbifolds of the former list (the ''genuine graphs''), or by using conjugation and twisting on the genuine graphs or on their orbifolds. A member of the $\mathcal{A}$ series (a Weyl alcove) is obtained by truncation of the diagram (Weyl chamber) of tensorization of irreps of su(3) by one of the two—conjugate—fundamentals 3 or $\overline{3}$; for this reason the graphs are oriented (see Fig. 7).

The index refers to the level k of the graph *defined* by $k=\kappa-h=\kappa-3$. Here $h=3$ is the Coxeter number of *the group* SU(3) and κ is the generalized Coxeter number of *the graph* (also called ''altitude'').

We label the vertices j of the $\mathcal{A}_\kappa$ diagram as (λ_1,λ_2), with $\lambda_1,\lambda_2\geqslant 0$ and $\lambda_1+\lambda_2\leqslant k$. Warning: our labels start from 0 and not from 1; many authors follow a different convention. Diagrams $\mathcal{A}_k$ have r points with $r=(k+1)(k+2)/2$.

The action of the modular matrix T on vertices $\tau_j\equiv\tau_{(\lambda_1,\lambda_2)}$ of $\mathcal{A}_k$ is diagonal and given by

$$(T^{(k)})_{\lambda\mu}=e_\kappa[-(\lambda_1+1)^2-(\lambda_1+1).(\lambda_2+1)-(\lambda_2+1)^2+\kappa]\delta_{\lambda\mu},$$

where $\lambda\doteq(\lambda_1,\lambda_2)$, $\mu\doteq(\mu_1,\mu_2)$, $e_\kappa[x]\doteq\exp(-2i\pi x/3\kappa)$, and $\kappa=k+3$. We call ''modular exponent'' the quantity $\hat{T}=-(\lambda_1+1)^2-(\lambda_1+1).(\lambda_2+1)-(\lambda_2+1)^2+\kappa \bmod 3\kappa$.

For su(3), the recurrence formula for adjacency matrices N_i associated with irreps is

$$N_{\lambda,\mu}=0 \qquad \text{if } \lambda<0 \text{ or } \mu<0,$$

$$N_{\lambda,0}=N_{1,0}N_{\lambda-1,0}-N_{\lambda-2,1},$$

$$N_{\lambda,\mu}=N_{1,0}N_{\lambda-1,\mu}-N_{\lambda-1,\mu-1}-N_{\lambda-2,\mu+1} \quad \text{if } \mu\neq 0,$$

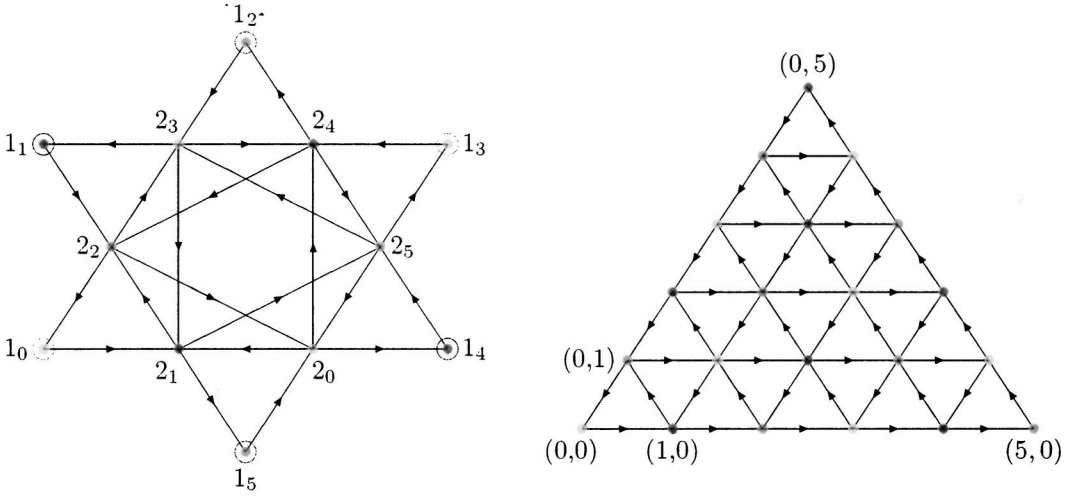

FIG. 8. The $\mathcal{E}_5$ and $\mathcal{A}_5$ generalized Dynkin diagrams.

$$N_{0,\lambda}=N_{\lambda,0}^{T}.$$

Remember that fused adjacency matrices F_i, associated with any graph G of the same level, are determined by the same recurrence relations (but the seed is different: $F_1=G_1$, the adjacency matrix of G).

In some cases the vector space generated by the vertices of a Di Francesco–Zuber graph is an algebra with positive integral structure constants (self-fusion). In all cases it is a module over the algebra of type $\mathcal{A}$ with the same Coxeter number. For an $\mathcal{A}$ graph, the identity element is (0,0); vertices (1,0) and (0,1), corresponding classically to the two representations of dimension 3, are the two complex conjugated generators. As always, a given diagram encodes the multiplication by the generators in the following sense: multiplication of an irrep (λ_1,λ_2) by the left generator (1,0) is given by the sum of the irreps which are connected to (λ_1,λ_2) by an incoming arrow, whereas multiplication by the right generator (0,1) is given by the sum of the irreps which are connected to (λ_1,λ_2) by an outgoing arrow. To label vertices, some readers may prefer Young frames (diagrams) rather than a notation using weights. The correspondance is as follows: (λ_1,λ_2) correspond to Young diagrams $Y(p=\lambda_1+\lambda_2,q=\lambda_2)$ with two rows, p boxes on the first row, and q boxes on the second row. Graphs whose vector space possesses self-fusion have a unit, and one of the two generators is located at the extremity of the (single) oriented edge that leaves the origin (reverse the arrows to get the other generator). Triality, i.e., $\{0,1,2\in\mathbb{Z}/3\mathbb{Z}\}$, is well defined and compatible with internal multiplication (if it exists) or with external multiplication by vertices of the corresponding $\mathcal{A}$ graph; it is represented by different choices of ''colors'' of vertices on the pictures. There is also a conjugacy transformation $\sigma\rightarrow\sigma^c$. At the level of graph matrices, it corresponds to transposition. For $\mathcal{A}$ graphs, it is represented by symmetry with respect to the inner bissectrix of the graph. The adjacency matrix is not symmetric, but it is normal, so that it can always be diagonalized.

In the following we illustrate the construction of the Ocneanu graphs of quantum symmetries, using our method based on the eigenvalues of the T operator, for the three genuine exceptional cases. Going through the whole list of Di Francesco–Zuber graphs would constitute a giant outgrowth of this article. We shall give some more details on the $\mathcal{E}_5$ case than on the two others.

Notice that the genuine diagrams $\mathcal{E}_5,\mathcal{E}_9$ and $\mathcal{E}_{21}$ are the only ones among exceptionals to admit self-fusion; this was first observed in Ref. 9.

B. First example: The $\mathcal{E}_5$ case

The $\mathcal{E}_5$ diagram is illustrated in Fig. 8, together with the corresponding $\mathcal{A}_5$ diagram, with same

norm, equal to $1+\sqrt{2}$, since the altitude is $\kappa=8$. Their respective adjacency matrices G_1 and N_1 are immediately determined (the adjacency matrix given in Ref. 11 is not typed correctly).

The $\mathcal{E}_5$ diagram admits self-fusion; 1_0 is the identity, 2_1 and 2_2 are the left and right generators. The multiplication table of the graph algebra of $\mathcal{E}_5$ reads

$$1_j.1_k=1_{j+k},$$

$$1_j.2_k=2_{j+k},$$

$$2_j.2_k=2_{j+k}+2_{j+k-3}+1_{j+k-3}.$$

This multiplication table allows one to compute easily the 12 square matrices G_a of the graph. The subset 1_i clearly forms a subalgebra of the graph algebra.

1. Restriction mechanism

We define an action of $\mathcal{A}_5$ on $\mathcal{E}_5$ in the same way as for the previous cases (see the discussion for E_6), getting the following restrictions: $(0,0)\hookrightarrow 1_0$, $(1,0)\hookrightarrow 2_1$ and $(0,1)\hookrightarrow 2_2$. For the others points, we compute the powers $(1,0)^\alpha(0,1)^\beta$ of the two fundamentals as well as the powers $(2_1)^\alpha(2_2)^\beta$ and compare them:

$$(1,0)^2=(2,0)+(0,1),\quad (2_1)^2=2_2+2_5+1_5,\quad \text{so}\quad (2,0)\hookrightarrow 1_5+2_5;$$

$$(0,1)^2=(1,0)+(0,2),\quad (2_2)^2=2_1+2_4+1_1,\quad \text{so}\quad (0,2)\hookrightarrow 1_1+2_4;$$

$$(1,0).(0,1)=(0,0)+(1,1),\quad 2_1.2_2=1_0+2_0+2_3,\quad \text{so}\quad (1,1)\hookrightarrow 2_0+2_3;$$

$$(1,0)^3=2(1,1)+(3,0)+(0,0),\quad (2_1)^3=1_0+32_0+22_3+1_3,\quad \text{so}\quad (3,0)\hookrightarrow 2_0+1_3;$$

and so on.

From these restriction rules, we obtain immediately the lines of essential matrix E_0 (intertwiner): it is a rectangular matrix with 12 columns, indexed by vertices of $\mathcal{E}_5$ and 21 rows indexed by vertices of $\mathcal{A}_5$ [i.e., by pairs of integers (λ_1,λ_2) with $\lambda_1+\lambda_2\leqslant 5$ or by Young frames $Y(p,q)$ with $5\geqslant p\geqslant q$].

We could have, as well, calculated directly the 21 fused matrices F_i from G_1 alone by using the su(3) recurrence relations; these matrices, in turn, determine the 12 essential (rectangular) matrices E_a.

2. Induction mechanism

From the branching rules $\mathcal{A}_5\rightarrow\mathcal{E}_5$, we get the following induction rules:

$$1_0\hookleftarrow(0,0),(2,2),\quad 2_1\hookleftarrow(1,0),(2,1),(1,3),(3,2),$$

$$1_1\hookleftarrow(0,2),(3,2),\quad 2_2\hookleftarrow(0,1),(1,2),(3,1),(2,3),$$

$$1_2\hookleftarrow(1,2),(5,0),\quad 2_3\hookleftarrow(1,1),(0,3),(2,2),(4,1),$$

$$1_3\hookleftarrow(3,0),(0,3),\quad 2_4\hookleftarrow(0,2),(2,1),(4,0),(1,3),$$

$$1_4\hookleftarrow(2,1),(0,5),\quad 2_5\hookleftarrow(2,0),(1,2),(3,1),(0,4),$$

$$1_5\hookleftarrow(2,0),(2,3),\quad 2_0\hookleftarrow(1,1),(3,0),(2,2),(1,4).$$

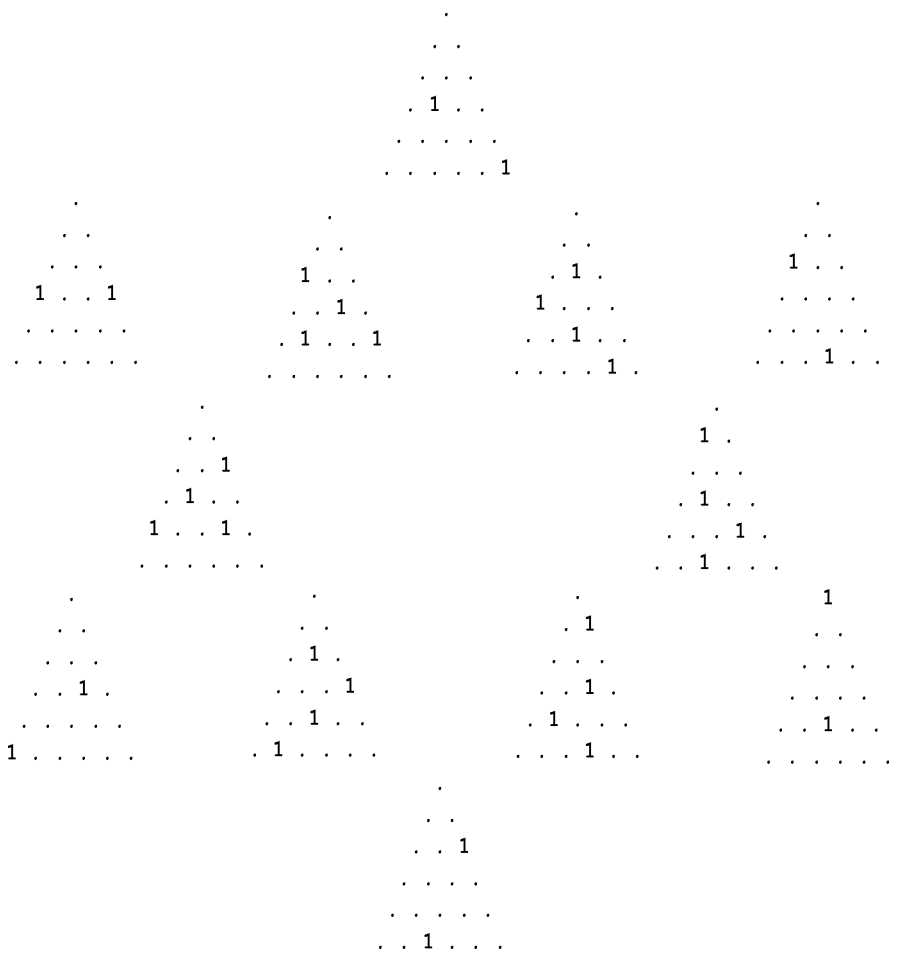

FIG. 9. Matrix E_0 for $\mathcal{E}_5$.

The same information can be gathered from the columns of matrix E_0 (see Fig. 9: each triangle corresponds to a single column). The first rule can be interpreted as a manifestation of the existence of a nontrivial quantum invariant of ''degree'' (2,2).

3. Quantum symmetries

For each 1_i, we can verify that the values of T on the two corresponding (λ_1,λ_2) coming from the induction are the same (see Table I). This allows us to assign a fixed value of T to the 1_i's. We can also verify that we can not do the same for the other vertices 2_i's. We get in this way a characterization of the subalgebra J, spanned by the elements 1_i's.

We therefore expect the algebra of quantum symmetries of $\mathcal{E}_5$ to be $\mathrm{Oc}(\mathcal{E}_5)=\mathcal{E}_5\otimes_J\mathcal{E}_5$. Its dimension is $12.12/6=24$. The left and right subalgebras are respectively spanned by $L=\{a\dot{\otimes}1_0\}$ and $R=\{1_0\dot{\otimes}a\}$, with a equal to 2_j or 1_j. Both left and right chiral subgraphs have 12 points. The ambichiral subalgebra (of dimension 6) is spanned by $A=\{1_j\dot{\otimes}1_0=1_0\dot{\otimes}1_j\}$ and the

TABLE I. Values of $\hat{T}$ on the vertices of the $\mathcal{A}_5$ graph.

(λ_1,λ_2)	(0,0)	(1,0)	(2,0)	(3,0)	(4,0)	(5,0)	(1,1)	(2,1)	(3,1)	(4,1)	(2,2)	(3,2)
		(0,1)	(0,2)	(0,3)	(0,4)	(0,5)		(1,2)	(1,3)	(1,4)		(2,3)
$\hat{T}$	5	1	19	11	1	13	20	13	4	17	5	19

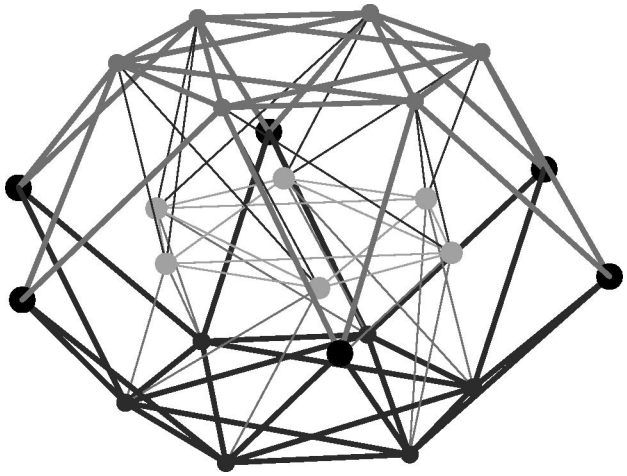

FIG. 10. The $\mathcal{E}_5$ Ocneanu graph.

supplementary subspace (also 6 points) is spanned by $C=\{2_j\dot{\otimes}2_k=2_0\dot{\otimes}2_{j+k}\}$. The Ocneanu graph can be displayed on the (three dimensional) picture (Fig. 10) as two superposed stars kissing each other along the six ambichiral points, with the vertices spanning the supplement displayed ''inside'' the others. As usual, bold lines—of two different colors—refer to the chiral parts and thin lines to the corresponding quotients. This graph is oriented but we have not displayed the orientation of the edges in order not to clutter the picture; the interested reader should do it for himself.

4. Dimensions of blocks

The two multiplicative structures $\circ$ and $\star$ of the bialgebra $\mathcal{BE}_5$ can be diagonalized. Blocks corresponding to the first structure are labeled by the 21 points of the $\mathcal{A}_5$ diagram. Dimension d_i of the block i is obtained by summing the matrix elements of F_i. We order the blocks $i=(\lambda,\mu)$ according to the level, i.e., $(\lambda,\mu)<(\lambda',\mu')$ if $\lambda<\lambda'$ or $\lambda=\lambda'$ and $\mu<\mu'$, and find

$$\{12\},\{24,24\},\{36,48,36\},\{36,60,60,36\},\{24,48,60,48,24\},\{12,24,36,36,24,12\}.$$

Dimension of the bialgebra is obtained by summing the square of these 21 integers d_i: $dim(\mathcal{BE}_5)=29\,376$. Dimension of the vector space of essential paths (graded by the Young frames of $\mathcal{A}_5$) is $\Sigma_i d_i=720$.

Blocks corresponding to the second structure are labeled by the 24 points of the Ocneanu graph $\mathrm{Oc}(\mathcal{E}_5)$. Dimension d_x of the block x is obtained by summing the matrix elements of matrices $S_x=G_aG_b$ when $x=a\dot{\otimes}b$ runs over the points of $\mathrm{Oc}(\mathcal{E}_5)$. One finds the following: the six ambichiral blocks have dimension 12, the six left chiral and the six right chiral blocks which are not ambichiral have dimension 24, the six complementary blocks have dimension 60. Dimension of the bialgebra is also obtained by summing the square of these 24 integers d_x and one finds the same total as before. Notice that writing 29 376 in two different ways as a sum of 21 or 24 squares constitutes, of course, a rather nontrivial check. Notice that we find also $\Sigma_x d_x=720$.

We summarize the discussion as follows:

$$dim(\mathcal{BE}_5)=\sum_{i\in\mathcal{A}_5}d_i^2=\sum_{x\in\mathrm{Oc}(\mathcal{E}_5)}d_x^2=(2)^6(3)^3(17)^1 \quad\text{and}\quad \sum_{i\in\mathcal{A}_5}d_i=\sum_{x\in\mathrm{Oc}(\mathcal{E}_5)}d_x=(2)^4(3)^2(5)^1.$$

5. Toric matrices and twisted partition functions

From the essential matrices E_a, we easily calculate the toric matrices (square matrices of dimension 21) and the corresponding partition functions by the method described earlier. There is one such function for each point of the Ocneanu graph $\mathrm{Oc}(\mathcal{E}_5)$. The one obtained from the identity $1_0 \dot{\otimes} 1_0$ of the graph is the modular-invariant and agrees with the expression of Ref. 13 (there is a global shift of (1,1) due to our conventions):

$$\mathcal{Z}_{\mathcal{E}_5} \doteq \mathcal{Z}_{1_0 \dot{\otimes} 1_0} = |\chi_{(0,0)} + \chi_{(2,2)}|^2 + |\chi_{(0,2)} + \chi_{(3,2)}|^2 + |\chi_{(2,0)} + \chi_{(2,3)}|^2 + |\chi_{(2,1)} + \chi_{(0,5)}|^2 + |\chi_{(3,0)} + \chi_{(0,3)}|^2 + |\chi_{(1,2)} + \chi_{(5,0)}|^2.$$

The others are interpreted as twisted partition functions (one defect line, in the interpretation of Ref. 31). We give only the twisted partition functions associated with ambichiral points $1_0 \dot{\otimes} 1_i$, for $i \in \{1,2,3,4,5\}$:

$$\mathcal{Z}_{1_0 \dot{\otimes} 1_1} = (\chi_{(0,3)} + \chi_{(3,0)}).(\overline{\chi}_{(0,5)} + \overline{\chi}_{(2,1)}) + (\chi_{(2,0)} + \chi_{(2,3)}).(\overline{\chi}_{(0,0)} + \overline{\chi}_{(2,2)}) + (\chi_{(0,5)} + \chi_{(2,1)}).(\overline{\chi}_{(2,0)} + \overline{\chi}_{(2,3)}) + (\chi_{(1,2)} + \chi_{(5,0)}).(\overline{\chi}_{(0,3)} + \overline{\chi}_{(3,0)}) + (\chi_{(0,0)} + \chi_{(2,2)}).(\overline{\chi}_{(0,2)} + \overline{\chi}_{(3,2)}) + (\chi_{(0,2)} + \chi_{(3,2)}).(\overline{\chi}_{(1,2)} + \overline{\chi}_{(5,0)}),$$

$$\mathcal{Z}_{1_0 \dot{\otimes} 1_2} = (\chi_{(1,2)} + \chi_{(5,0)}).(\overline{\chi}_{(0,5)} + \overline{\chi}_{(2,1)}) + (\chi_{(0,5)} + \chi_{(2,1)}).(\overline{\chi}_{(0,0)} + \overline{\chi}_{(2,2)}) + (\chi_{(0,3)} + \chi_{(3,0)}).(\overline{\chi}_{(2,0)} + \overline{\chi}_{(2,3)}) + (\chi_{(0,2)} + \chi_{(3,2)}).(\overline{\chi}_{(0,3)} + \overline{\chi}_{(3,0)}) + (\chi_{(2,0)} + \chi_{(2,3)}).(\overline{\chi}_{(0,2)} + \overline{\chi}_{(3,2)}) + (\chi_{(0,0)} + \chi_{(2,2)}).(\overline{\chi}_{(1,2)} + \overline{\chi}_{(5,0)}),$$

$$\mathcal{Z}_{1_0 \dot{\otimes} 1_3} = (\chi_{(0,2)} + \chi_{(3,2)}).(\overline{\chi}_{(0,5)} + \overline{\chi}_{(2,1)}) + (\chi_{(0,3)} + \chi_{(3,0)}).(\overline{\chi}_{(0,0)} + \overline{\chi}_{(2,2)}) + (\chi_{(1,2)} + \chi_{(5,0)}).(\overline{\chi}_{(2,0)} + \overline{\chi}_{(2,3)}) + (\chi_{(0,0)} + \chi_{(2,2)}).(\overline{\chi}_{(0,3)} + \overline{\chi}_{(3,0)}) + (\chi_{(0,5)} + \chi_{(2,1)}).(\overline{\chi}_{(0,2)} + \overline{\chi}_{(3,2)}) + (\chi_{(2,0)} + \chi_{(2,3)}).(\overline{\chi}_{(1,2)} + \overline{\chi}_{(5,0)}),$$

$$\mathcal{Z}_{1_0 \dot{\otimes} 1_4} = (\chi_{(0,0)} + \chi_{(2,2)}).(\overline{\chi}_{(0,5)} + \overline{\chi}_{(2,1)}) + (\chi_{(1,2)} + \chi_{(5,0)}).(\overline{\chi}_{(0,0)} + \overline{\chi}_{(2,2)}) + (\chi_{(0,2)} + \chi_{(3,2)}).(\overline{\chi}_{(2,0)} + \overline{\chi}_{(2,3)}) + (\chi_{(2,0)} + \chi_{(2,3)}).(\overline{\chi}_{(0,3)} + \overline{\chi}_{(3,0)}) + (\chi_{(0,3)} + \chi_{(3,0)}).(\overline{\chi}_{(0,2)} + \overline{\chi}_{(3,2)}) + (\chi_{(0,5)} + \chi_{(2,1)}).(\overline{\chi}_{(1,2)} + \overline{\chi}_{(5,0)}),$$

$$\mathcal{Z}_{1_0 \dot{\otimes} 1_5} = (\chi_{(2,0)} + \chi_{(2,3)}).(\overline{\chi}_{(0,5)} + \overline{\chi}_{(2,1)}) + (\chi_{(0,2)} + \chi_{(3,2)}).(\overline{\chi}_{(0,0)} + \overline{\chi}_{(2,2)}) + (\chi_{(0,0)} + \chi_{(2,2)}).(\overline{\chi}_{(2,0)} + \overline{\chi}_{(2,3)}) + (\chi_{(0,5)} + \chi_{(2,1)}).(\overline{\chi}_{(0,3)} + \overline{\chi}_{(3,0)}) + (\chi_{(1,2)} + \chi_{(5,0)}).(\overline{\chi}_{(0,2)} + \overline{\chi}_{(3,2)}) + (\chi_{(0,3)} + \chi_{(3,0)}).(\overline{\chi}_{(1,2)} + \overline{\chi}_{(5,0)}).$$

C. Second example: The $\mathcal{E}_9$ case

This diagram is illustrated on Fig. 11 (notice that it would be better drawn three-dimensionally as a small starwars spaceship with two wings and a cockpit, because of the existing symmetries between the two wings, reminiscent of what happens for the D_{2n} Dynkin diagrams).

The corresponding diagram of the A series is $\mathcal{A}_9$. Altitude of both is $\kappa = 9+3 = 12$. Their respective adjacency matrices are immediately read from the graphs. Their number of vertices are 12 and $10 \times \frac{11}{2} = 55$. Restriction and induction is studied as usual, and imposing constancy of the modular operator T singles out the three circled vertices of Fig. 11 as elements of the vector

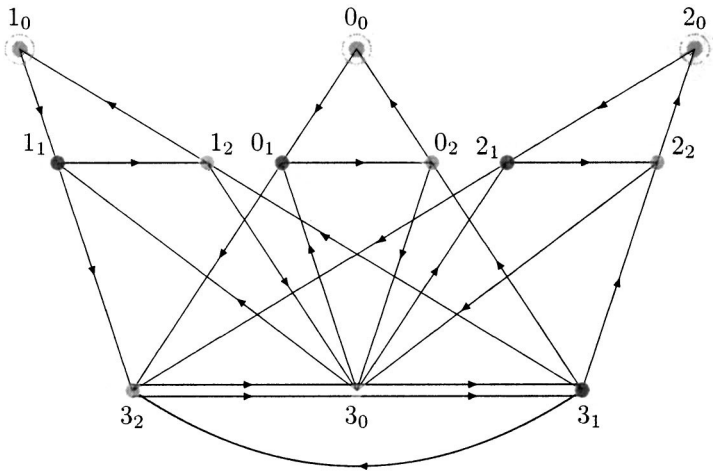

FIG. 11. The $\mathcal{E}_9$ generalized Dynkin diagram.

subspace J that is used to characterize the ambichiral points of the Ocneanu graph. The fused adjacency matrices F_i are obtained from the su(3) recurrence formula; this determines the essential matrices E_a. We give on Fig. 12 the columns of the E_0 matrix indexed by the three special points (these are the ''ambichiral columns'' of the intertwiner E_0); a consistent value of T can be defined for these three points (and these three points only), one finds $\hat{T}=9$ for the vertex 0_0 and $\hat{T}=21$ for 1_0 and 2_0.

Blocks of the bialgebra $\mathcal{BE}_9$, for its first associative law ($\circ$), are labeled by the 55 vertices of $\mathcal{A}_9$ and their dimensions are given on Fig. 13. The total dimension is the sum of corresponding squares: $dim(\mathcal{BE}_9)=\Sigma_i d_i^2=518976=(2)^6(3)^2(17)^1(53)^1$.

Something special happens however for this graph (again reminiscent of a similar situation in the D_{2n} case of Dynkin diagrams): first of all, the diagram itself is not sufficient to determine a unique associative algebra structure, and one has to impose positivity and integrality of the structure constants in order to determine a self-fusion structure (it is unique up to permutation of the two wings). Since the determination of the corresponding graph matrices is not totally straightforward, we give below the two matrices corresponding to the endpoints 1_0 and 2_0. We choose the following order for the vertices: $0_0,1_0,2_0,3_0;0_1,1_1,2_1,3_1;0_2,1_2,2_2,3_2$. We also give the adjacency matrix G_{0_1} whose determination *is* straightforward.

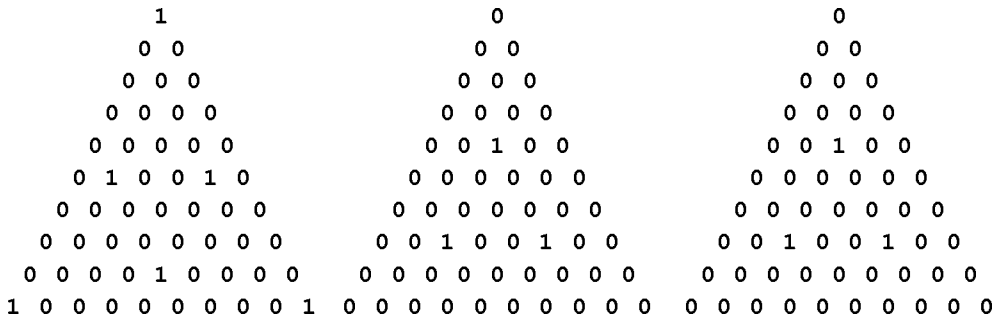

FIG. 12. Induction corresponding to the three upper vertices of $\mathcal{E}_9$.

$$G_{0_1}=\begin{pmatrix}
. & . & . & . & . & . & . & . & 1 & . & . & . \\
. & . & . & . & . & . & . & . & . & 1 & . & . \\
. & . & . & . & . & . & . & . & . & . & 1 & . \\
. & . & . & . & . & . & . & . & 1 & 1 & 1 & 2 \\
1 & . & . & 1 & . & . & . & . & . & . & . & . \\
. & 1 & . & 1 & . & . & . & . & . & . & . & . \\
. & . & 1 & 1 & . & . & . & . & . & . & . & . \\
. & . & . & 2 & . & . & . & . & . & . & . & . \\
. & . & . & . & 1 & . & . & 1 & . & . & . & . \\
. & . & . & . & . & 1 & . & 1 & . & . & . & . \\
. & . & . & . & . & . & 1 & 1 & . & . & . & . \\
. & . & . & . & 1 & 1 & 1 & 1 & . & . & . & .
\end{pmatrix},$$

$$G_{1_0}=\begin{pmatrix}
. & 1 & . & . & . & . & . & . & . & . & . & . \\
. & . & 1 & . & . & . & . & . & . & . & . & . \\
1 & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & 1 & . & . & . & . & . & . & . & . \\
. & . & . & . & . & 1 & . & . & . & . & . & . \\
. & . & . & . & . & . & 1 & . & . & . & . & . \\
. & . & . & . & 1 & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & 1 & . & . & . & . \\
. & . & . & . & . & . & . & . & 1 & . & . & . \\
. & . & . & . & . & . & . & . & . & 1 & . & . \\
. & . & . & . & . & . & . & . & 1 & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & 1
\end{pmatrix},$$

$$G_{2_0}=\begin{pmatrix}
. & . & 1 & . & . & . & . & . & . & . & . & . \\
1 & . & . & . & . & . & . & . & . & . & . & . \\
. & 1 & . & . & . & . & . & . & . & . & . & . \\
. & . & . & 1 & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & 1 & . & . & . & . & . \\
. & . & . & . & 1 & . & . & . & . & . & . & . \\
. & . & . & . & . & 1 & . & . & . & . & . & . \\
. & . & . & . & . & . & . & 1 & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & 1 & . \\
. & . & . & . & . & . & . & . & 1 & . & . & . \\
. & . & . & . & . & . & . & . & . & 1 & . & . \\
. & . & . & . & . & . & . & . & . & . & . & 1
\end{pmatrix}.$$

Next, and as expected, the operator T does not distinguish between these two points, and we therefore expect, as in the D_{2n} case of the su(2) system, that the algebra $\mathrm{Oc}(\mathcal{E}_9)$ of quantum symmetries will possess a noncommutative 2×2 matrix component, encoding, in a ''noncommu-

12
26 26
42 60 42
60 94 94 60
68 120 144 120 68
68 132 162 162 132 68
60 120 162 180 162 120 60
42 94 144 162 162 144 94 42
26 60 94 120 132 120 94 60 26
12 26 42 60 68 68 60 42 26 12

FIG. 13. Dimension of space of blocks (law $\circ$) for $\mathcal{E}_9$.

tative geometrical spirit,'' this indistinguishability. The presence of such a noncommutative piece is also reflected in the presence of a coefficient 2 in the (known) modular invariant partition function. We note, however, that ambichiral points are bound to be, in any case, $0_0\dot{\otimes}0_0$, $1_0\dot{\otimes}0_0=0_0\dot{\otimes}1_0$ and $2_0\dot{\otimes}0_0=0_0\dot{\otimes}2_0$. The corresponding toric matrices W and partition functions $\mathcal{Z}$ are computed as usual. We define the linear combination U and V of characters

$$U=\chi_{(2,2)}+\chi_{(2,5)}+\chi_{(5,2)},$$

$$V=\chi_{(0,0)}+\chi_{(0,9)}+\chi_{(9,0)}+\chi_{(1,4)}+\chi_{(4,1)}+\chi_{(4,4)},$$

and find

$$\mathcal{Z}_{0_0\dot{\otimes}0_0}=2\,U.\overline{U}+V.\overline{V},$$

$$\mathcal{Z}_{1_0\dot{\otimes}0_0}=\mathcal{Z}_{2_0\dot{\otimes}0_0}=U.\overline{V}+V.\overline{U}.$$

The first one is modular invariant and agrees with the expression of Gannon.[13] The other one should be interpreted as a twisted partition function in a BCFT with defect lines.

Unfortunately, in this case, as it was for D_{2n}, the data provided by the eigenvalues of the modular operator T does not seem to be sufficient to determine the full (noncommutative in this case) structure of $\mathrm{Oc}(\mathcal{E}_9)$ or the Ocneanu graph itself, and we decide to stop at this point.

D. Third example: The $\mathcal{E}_{21}$ case

The $\mathcal{E}_{21}$ diagram is illustrated in Fig. 14. The corresponding $\mathcal{A}$ diagram with same norm is $\mathcal{A}_{21}$. The altitude of both is $\kappa=21+3=24$. Their respective adjacency matrices G_1 and N_1 are immediately obtained from the diagrams. The number of vertices of the two diagrams are respectively equal to 24 and $22\times\frac{23}{2}=253$.

1. Restriction and induction mechanism

The easiest method is to determine first the fused matrices F_i by using the recurrence formula for su(3). Essential matrices E_a—and in particular E_0—are then obtained in the usual way from the F_i's. The first column of E_0 gives the quantum invariants; it is displayed on the left array of Fig. 15.

One can check that the values of the modular operator T, calculated for $\mathcal{A}_{21}$, are equal for all nonzero entries of this table. The same property is also true for the column of E_0 associated with the rightmost point of the $\mathcal{E}_{21}$ graph (right array of Fig. 15). However, T, when evaluated on nonzero entries of the 22 other columns of E_0, is not constant. We conclude that the set J

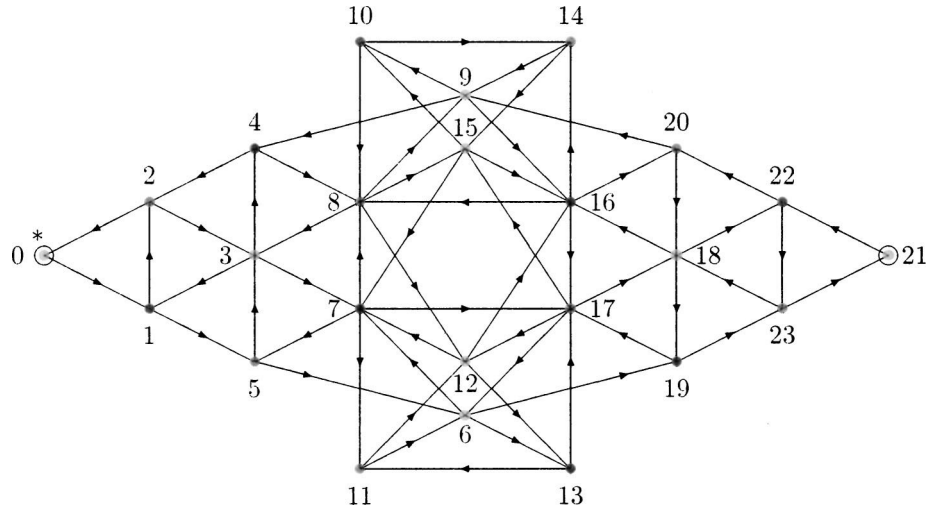

FIG. 14. The $\mathcal{E}_{21}$ generalized Dynkin diagram.

characterizing the ambichiral points of $\mathrm{Oc}(\mathcal{E}_{21})$ is a set with two elements: the two extreme vertices of $\mathcal{E}_{21}$. The values of the modular exponent T obtained for these two points are $\hat{T}=21$ and $\hat{T}=39$.

The dimensions d_j, with $j=(\lambda_1,\lambda_2)$ of the 253 blocks of the bialgebra $\mathcal{BE}_{21}$, for the first law determined by composition of endomorphisms, are obtained by summing matrix elements of matrices F_j. They are displayed in Fig. 16. We obtain $dim(\mathcal{BE}_{21})=\Sigma_j d_j^2=480\,701\,952=(2)^9(3)^4(67)^1(173)^1$, and also $\Sigma_j d_j=288\,576=(2)^6(3)^3(167)^1$.

2. Determination of the graph algebra and of matrices G_a

The determination of graph matrices G_a comes from the graph $\mathcal{E}_{21}$ itself. To ease the calculation, it is worth noticing that graph matrices associated with points symmetric with respect to the horizontal symmetry axis of the graph are transposed. We have, for example, $G_5=G_1.G_1-G_2$ so that $G_4=(G_5)^t=G_2.G_2-G_1$. Their determination is straightforward from vertices 1 to 9. We then use the fact that $G_6.G_{21}=G_9$ to compute the matrix G_{21} associated with the rightmost point of the graph. Multiplying a vertex k by the vertex 21 gives a vertex which is the symmetric of k

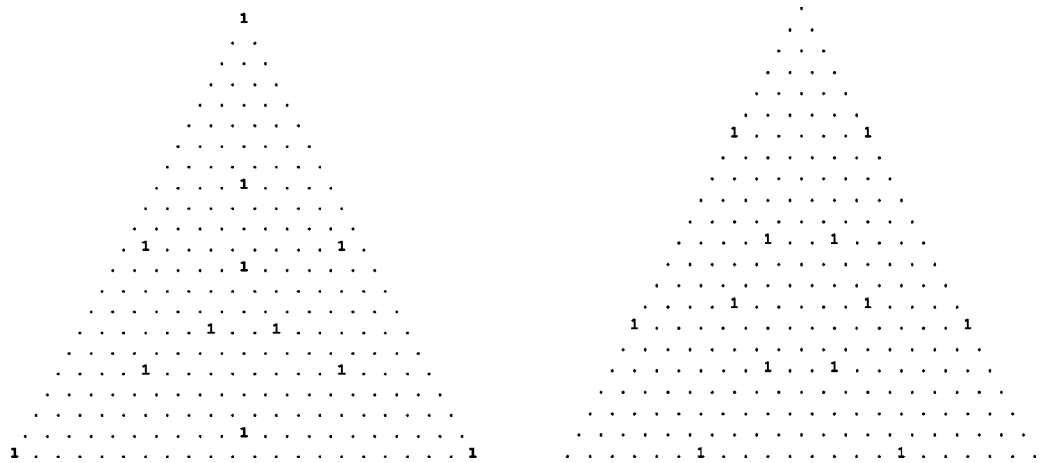

FIG. 15. Induction corresponding to the two extreme points of $\mathcal{E}_{21}$.

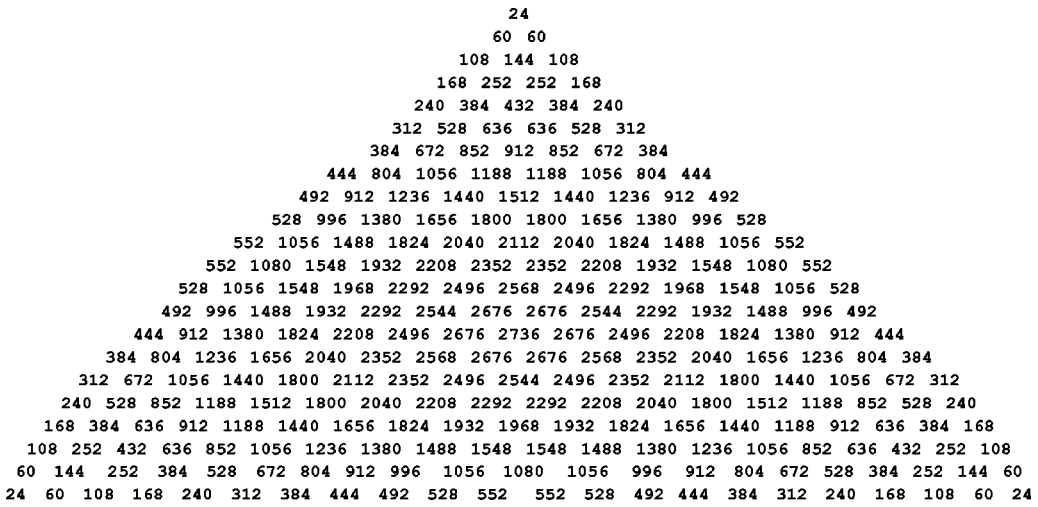

FIG. 16. Dimension of space of blocks (law $\circ$).

with respect to the center of the graph (the center of a star). In graph algebra terms, we get, for example, $G_5.G_{21}=G_{20}$ and $G_8.G_{21}=G_{17}$. It is then easy to compute the matrices associated with all the other vertices of the graph. The most important result, for what follows, is that $G_{21}.G_{21}=G_0$.

3. Quantum symmetries

As already discussed, the subspace J of $\mathcal{E}_{21}$ determining the algebra of quantum symmetries is spanned by 0 and 21; we set $\mathrm{Oc}(\mathcal{E}_{21})=\mathcal{E}_{21}\otimes_J\mathcal{E}_{21}$. This is a commutative algebra. The left and right subalgebras L and R are respectively spanned by $a\dot{\otimes}0$ and by $0\dot{\otimes}a$, where $a=0,1,\ldots,23$. Both left and right chiral subgraphs have 24 points. The ambichiral subalgebra A, of dimension 2 is spanned by $\{0\dot{\otimes}0=21\dot{\otimes}21\}$ and by $\{0\dot{\otimes}21=21\dot{\otimes}0\}$. The supplementary subspace C is spanned by $u\dot{\otimes}a$, where $u\in\{1,2,3,4,5,6,7,8,10,11,12\}$ and a takes all possible values (but neither 0 nor 21). The total number of vertices of the Ocneanu graph is therefore $22+22+2+11\times22=288$, as expected from the naive dimension count $24\times\frac{24}{2}=288$. As usual, blocks corresponding to the second structure of the bialgebra $\mathcal{B}\mathcal{E}_{21}$ are labeled by the 288 points of the Ocneanu graph, and the dimension d_x of the block x is obtained by summing the matrix elements of matrices $S_x=G_aG_b$ when $x=a\dot{\otimes}b$ runs over the points of $\mathrm{Oc}(\mathcal{E}_{21})$. We find (subscript give multiplicities of the blocks)

$$\text{Ambichiral: } (24)_2$$

$$\text{Left (not ambichiral): } (60)_4(108)_4(132)_4(144)_2(168)_2(216)_2(252)_4$$

$$\text{Right (not ambichiral): } (60)_4(108)_4(132)_4(144)_2(168)_2(216)_2(252)_4$$

$$\text{Supplement: } (168)_8(312)_{16}(384)_{16}(420)_8(492)_8(600)_8(636)_8(744)_{32}(804)_8(936)_8(948)_8(996)_8$$

$$(1080)_2(1188)_8(1236)_8(1272)_4(1440)_{16}(1512)_2(1548)_8(1656)_4(1800)_{16}(1932)_8$$

$$(1968)_4(2292)_8(2568)_2(2988)_8(3480)_8$$

The quadratic and linear sum rules read

$$\sum d_x = \sum d_i = 288\,576 = (2)^6(3)^3(167)^1,$$

$$\sum d_x^2 = \sum d_i^2 = 480\,701\,952 = (2)^9(3)^4(67)^1(173)^1.$$

4. Toric matrices and twisted partition functions

We define the linear combination U and V of characters as follows:

$$U = \chi_{(0,0)} + \chi_{(0,21)} + \chi_{(1,10)} + \chi_{(4,4)} + \chi_{(4,13)} + \chi_{(6,6)} + \chi_{(6,9)} + \chi_{(9,6)} + \chi_{(10,1)} + \chi_{(10,10)} + \chi_{(13,4)} + \chi_{(21,0)},$$

$$V = \chi_{(0,6)} + \chi_{(0,15)} + \chi_{(4,7)} + \chi_{(4,10)} + \chi_{(6,0)} + \chi_{(6,15)} + \chi_{(7,4)} + \chi_{(7,10)} + \chi_{(10,4)} + \chi_{(10,7)} + \chi_{(15,0)} + \chi_{(15,6)}.$$

The modular-invariant partition function $\mathcal{Z}_{\mathcal{E}_5}$ (associated with the vertex $0\dot{\otimes}0$) and the one associated with the vertex $0\dot{\otimes}21$, that we call $\mathcal{Z}'_{\mathcal{E}_5}$, are

$$\mathcal{Z}_{\mathcal{E}_5} \doteq \mathcal{Z}_{0\dot{\otimes}0} = U.\overline{U} + V.\overline{V},$$

$$\mathcal{Z}'_{\mathcal{E}_5} \doteq \mathcal{Z}_{0\dot{\otimes}21} = U.\overline{V} + V.\overline{U}.$$

The first one agrees with the expression of Ref. 13, the other, as explained in Sec. II B, should be interpreted as a twisted partition function in a BCFT with one defect line.[29] There are 286 other such functions for the $\mathcal{E}_{21}$ diagram, but these two are the only ones that are ambichiral.

ACKNOWLEDGMENTS

We thank the referee for his careful reading of the manuscript and for his questions and comments. One of us (R.C.) wants to thank the Centro Brasileiro de Pesquisas Físicas (CBPF, Rio de Janeiro), where part of this work was done, for its hospitality. G.S. would like to thank the Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, and the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, CAPES, Brazilian Research Agencies, for financial support.

APPENDIX A: ABOUT MODULAR INVARIANCE

The expressions for S and T can be taken from the theory of quantum groups $\mathcal{U}_q(\mathcal{G})$ at roots of unity, i.e., when $q = e^{i\pi/\mu\kappa}$. Here μ is half the length of a long root, so it is equal to 1 when the Lie algebra $\mathcal{G}$ is simply laced, which is the case in particular for su(2) and su(3), and κ is an arbitrary positive integer, larger or equal to h, the dual Coxeter number of $\mathcal{G}$. The equation $\kappa = h + k$ defines the "level" k. One should consider a particular category whose objects are the so-called tilting modules of $\mathcal{U}_q(\mathcal{G})$ and whose morphisms are defined up to "negligible morphisms" (see, for instance, Ref. 1); this is a semisimple ribbon and modular category. This implies, in particular, that a (projective) representation of $\mathrm{SL}(2,\mathbb{Z})$ can be defined on the simple objects, thanks to two matrices s and t and a phase ζ which are such that $(st)^3 = \zeta^3 s^2$, $s^2 = C$, $Ct = tC$ and $C^2 = 1$. The matrix C is called "conjugation matrix" and t is the "modular twist." For this category, $\zeta = e^{2i\pi c/24}$ with $c = (\kappa - h)dim(\mathcal{G})/\kappa$. The expression for the t matrix, in the case of an arbitrary Lie algebra $\mathcal{G}$ is $t_{mn} = \delta_{mn} q^{\langle\langle n, n+2\rho\rangle\rangle}$ where ρ is half the sum of positive roots and m, n are elements of the weight lattice of $\mathcal{G}$ characterizing the representation τ_m and τ_n. Here $\langle\langle .,. \rangle\rangle$ is

an invariant bilinear form on $\mathcal{G}$ normalized by $\langle\langle\alpha,\alpha\rangle\rangle=2$ for a short root α. The corresponding general expression for the s matrix is more involved and we do not need it in our article. The same expressions for the modular generators can be obtained from the Kac–Peterson formulas[16] for the modular transformations of characters of the affine Lie algebra $\hat{\mathcal{G}}$, evaluated at the same value $q=e^{i\pi/\mu\kappa}$. Here $k=\kappa-h$ is indeed equal to the usual level.

In the case of su(2), the modular generators S, T, are as follows: $S=s$ and $T=t/\zeta$. The SL(2,$\mathbb{Z}$) relations read then $(ST)^3=S^2=1$, with $s_{mn}=\sqrt{2/\kappa}\sin(\pi(m+1)(n+1)/\kappa)$, for $0\leqslant m,n\leqslant\kappa-2$ and $t_{mn}=e^{(i\pi/2\kappa)\,n(n+2)}\delta_{mn}$. Still for su(2) we have $c=3-6/\kappa$, so that $\zeta=e^{i\pi/4}e^{-i\pi/2\kappa}$ and therefore

$$T_{mn}=\exp\left[2i\pi\left(\frac{(n+1)^2}{4\kappa}-\frac{1}{8}\right)\right]\delta_{mn},$$

which is the expression used in the text. One can explicitly see that the previous SL(2,$\mathbb{Z}$) relations hold. It can be checked, from this expression that, $T^{8\kappa}=1$ when κ is odd and $T^{4\kappa}=1$ when κ is even. This, by itself, is not enough to imply the following property, which is nevertheless true, and was proven more than 100 years ago:[15] the above representation of SL(2,$\mathbb{Z}$) factorizes over the finite group SL(2,$\mathbb{Z}/8\kappa\mathbb{Z}$) when κ is odd, and factorizes over SL(2,$\mathbb{Z}/4\kappa\mathbb{Z}$) when κ is even. So, in particular, $T^{40}=1$ for the A_4 graph ($40=8\times5$), but $T^{48}=1$ for the A_{11} graph ($48=4\times12$). In the text, we use [for su(2)] a "modular exponent" defined by $\hat{T}=(n+1)^2 \bmod 4\kappa$, but it is clear that we could use as well $n(n+2) \bmod 4\kappa$ or any other expression differing by a constant shift.

APPENDIX B: THE GENERAL NOTION OF ESSENTIAL PATHS ON A GRAPH *G* OF TYPE *ADE*

The following definitions are not needed if we only want to count the number of essential paths on a graph. They are necessary if we want to obtain explicit expressions for them. These definitions are adapted from Ref. 23, see also several comments made in Refs. 7 and 6. Call β the norm of the graph G (the biggest eigenvalue of its adjacency matrix $\mathcal{G}$) and D_i the components of the (normalized) Perron Frobenius eigenvector. Call σ_i the vertices of G and, if σ_j is a neighbor of σ_i, call ξ_{ij} the oriented edge from σ_i to σ_j. If G is unoriented (the case for ADE and affine ADE diagrams), each edge should be considered as carrying both orientations. An elementary path can be written either as a finite sequence of consecutive (i.e., neighbors on the graph) vertices, $[\sigma_{a_1}\sigma_{a_2}\sigma_{a_3}\cdots]$, or, better, as a sequence $(\xi(1)\xi(2)\cdots)$ of consecutive edges, with $\xi(1)=\xi_{a_1a_2}=\sigma_{a_1}\sigma_{a_2}$, $\xi(2)=\xi_{a_2a_3}=\sigma_{a_2}\sigma_{a_3}$, etc. Vertices are considered as paths of length 0. The length of the (possibly backtracking) path $(\xi(1)\xi(2)\cdots\xi(p))$ is p. We call $r(\xi_{ij})=\sigma_j$ the range of ξ_{ij}, and $s(\xi_{ij})=\sigma_i$ the source of ξ_{ij}. For all edges $\xi(n+1)=\xi_{ij}$ that appear in an elementary path, we set $\xi(n+1)^{-1}\doteq\xi ji$. For every integer $n>0$, the annihilation operator C_n, acting on the vector space generated by elementary paths of length p, is defined as follows: if $p\leqslant n$, C_n vanishes, whereas if $p\geqslant n+1$, then

$$C_n(\xi(1)\xi(2)\cdots\xi(n)\xi(n+1)\cdots)=\sqrt{\frac{D_{r(\xi(n))}}{D_{s(\xi(n))}}}\,\delta_{\xi(n),\xi(n+1)^{-1}}(\xi(1)\xi(2)\cdots\hat{\xi}(n)\hat{\xi}(n+1)\cdots).$$

Here, the symbol "hat" (like in $\hat{\xi}$) denotes omission. The result is therefore either 0 or a linear combination of paths of length $p-2$. Intuitively, C_n chops the round trip that possibly appears at positions n and $n+1$.

A path is called essential if it belongs to the intersection of the kernels of the anihilators C_n's.

The following is an example of calculation for the E_6 diagram (square brackets enclose q-numbers),

$$C_3(\xi_{01}\xi_{12}\xi_{23}\xi_{32}) = \sqrt{\frac{1}{[2]}}(\xi_{01}\xi_{12}),$$

$$C_3(\xi_{01}\xi_{12}\xi_{25}\xi_{52}) = \sqrt{\frac{[2]}{[3]}}(\xi_{01}\xi_{12}).$$

The following difference of nonessential paths of length 4 starting at σ_0 and ending at σ_2 is an essential path of length 4 on E_6:

$$\sqrt{[2]}(\xi_{01}\xi_{12}\xi_{23}\xi_{32}) - \sqrt{\frac{[3]}{[2]}}(\xi_{01}\xi_{12}\xi_{25}\xi_{52}) = \sqrt{[2]}[0,1,2,3,2] - \sqrt{\frac{[3]}{[2]}}[0,1,2,5,2].$$

Remember the values of the q-numbers: $[2]=\sqrt{2}/(\sqrt{3}-1)$ and $[3]=2/(\sqrt{3}-1)$.

Acting on elementary path of length p, the creating operators $C_n^\dagger$ are defined as follows: if $n>p+1$, $C_n^\dagger$ vanishes and, if $n\leqslant p+1$, then, setting $j=r(\xi(n-1))$,

$$C_n^\dagger(\xi(1)\cdots\xi(n-1)\cdots) = \sum_{d(j,k)=1} \sqrt{\left(\frac{D_k}{D_j}\right)}(\xi(1)\cdots\xi(n-1)\xi_{jk}\xi_{kj}\cdots).$$

The above sum is taken over the neighbors σ_k of σ_j on the graph. Intuitively, this operator adds one (or several) small round trip(s) at position n. The result is therefore either 0 or a linear combination of paths of length $p+2$. For instance, on paths of length zero (i.e., vertices),

$$C_1^\dagger(\sigma_j) = \sum_{d(j,k)=1} \sqrt{\left(\frac{D_k}{D_j}\right)}\xi_{jk}\xi_{kj} = \sum_{d(j,k)=1} \sqrt{\left(\frac{D_k}{D_j}\right)}[\sigma_j\sigma_k\sigma_j].$$

Jones' projectors e_k can be realized (as endomorphisms of Path^p) by

$$e_k \doteq \frac{1}{\beta} C_k^\dagger C_k .$$

The reader can check that all Jones–Temperley–Lieb relations between the e_i are satisfied. Essential paths can also be defined as elements of the intersection of the kernels of the Jones projectors e_i's.

APPENDIX C: THE STRUCTURE OF $\mathcal{BG}$

Paths on G generate a vector space Paths(G) which comes with a grading: paths of homogeneous grade j are associated with Young diagrams of SU(N). In the case of su(2) this grading is just an integer (to be thought of as a length or as a point of a diagram of type $\mathcal{A}$).

What turns out to be most interesting is a particular vector subspace $\mathcal{E}=$EssPaths(G) of Paths whose elements are called "essential paths" (see above definition). This subspace is is itself graded in the same way as Paths.

We then consider the graded algebra of endomorphisms of essential paths

$$\mathcal{BG} = \mathrm{End}_\sharp(\mathrm{EssPaths}) = \bigoplus_{j=0,r-1} \mathrm{End}(\mathrm{EssPaths}^j),$$

which, by definition, is an associative algebra. By using the fact that paths on the chosen diagram can be concatenated, one may define[23] *another* multiplicative associative structure on $\mathcal{BG}$ that we call convolution product (see our comments in the next subsection). This vector space with two algebra structures is called, by A. Ocneanu, the "algebra of double triangles."

Existence of a scalar product allows one to transmute one of the multiplications (for instance, the convolution product) into a co-multiplication and it happens that the coproduct Δ is compatible

with the product [in the sense that we have the homomorphism property $\Delta(uv)=\Delta u\otimes\Delta v$]. $\mathcal{B}G$ is therefore a bialgebra. However, $\mathcal{B}G$ is not a Hopf algebra but a weak Hopf algebra (or quantum groupoid). This statement should be taken with a grain of salt: see our comments in the next appendix. General axioms for weak Hopf algebras are given in Ref. 3. In the present case, the following axiom for Hopf algebras fails to be satisfied: the coproduct of the unit $\Delta\mathbb{1}=\mathbb{1}_1\otimes\mathbb{1}_2$ is not equal to $\mathbb{1}\otimes\mathbb{1}$ (as usual, a summation is understood); several other axioms for Hopf algebras are also modified: the counit is not an homomorphism ($\epsilon(xy)=\epsilon(x\mathbb{1}_1)\epsilon(y\mathbb{1}_2)$) and, if $\Delta^2x=x_1\otimes x_2\otimes x_3$, the compatibility axiom for the antipode is modified as follows $S(x_1)x_2\otimes x_3=\mathbb{1}_1\otimes x\mathbb{1}_2$.

APPENDIX D: REMARKS AND OPEN QUESTIONS

Essential paths for *ADE* diagrams [i.e., the su(2) system] have been defined in several published papers but their analog for higher systems (for instance, the Di Francesco–Zuber diagrams), although reasonably well understood by a few people, have never been described, as far as we know, in the literature.

The general definition of the convolution product of $\mathcal{B}G$, for *ADE* diagrams, was given "explicitly" by A. Ocneanu in Ref. 23 by a rather difficult formula involving several types of generalized quantum $6j$ symbols. It is certainly interesting to know this general formula, but, in our opinion, this expression is not very helpful for a practical investigation of the different cases.

The fact that $\mathcal{B}G$ is a weak Hopf algebra is a claim that belongs to the folklore, but we are not aware of any general reference showing that all the axioms of Ref. 3 are indeed verified in this situation. The authors (together with A. Garcia and R. Trinchero) have, however, checked that it is so in a number of particular cases belonging to the *ADE* series and are working on a general proof.

Another possibility for defining the convolution product of $\mathcal{B}G$ is to make use of the notion of cell systems. This general notion was defined in Ref. 22; it is also described in Ref. 12 and it is used, in a particular context, by Ref. 32. We cannot summarize this theory here. Let us just mention that a cell system involves four graphs (top, bottom, left and right) with matching properties and that, in the present case, the top and bottom graphs are the same *ADE* diagram G. Cells are rectangles with top and bottom edges which are also edges of the given graph(s). Macrocells have top and bottom edges (or "horizontal paths") that coincide with the essential paths on G; their left and right edges are called "vertical paths." To every cell system one can associate "'connections" which are particular maps associating complex numbers with cells or macrocells. These numbers, in turn, can be used to define the structure constants of the algebra we are looking for. For every point of the graph Oc(G) there is an irreducible connection on the cell system (or an irreducible quantum symmetry). Although it seems to provide (at the time of this writing) the shortest road to the explicit construction of the bialgebra $\mathcal{B}G$, this construction is unfortunately not explicitly available in the literature.

Among other results, and in the framework of statistical mechanics, Ref. 31 gives many useful relations between the vertical product of $\mathcal{B}G$ [the product of endomorphisms acting on EssPaths(G)] and its horizontal product (or convolution product). There are indeed several families of numeral constants that appear as structure constants for these two products, or that appear as coefficients of a kind of Fourier transform relating the two. These constants look like generalized quantum $6j$ symbols and obey different types of (mixed) pentagon equations which themselves generalize the quantum group version of the Biedenharn–Elliot identity. As discussed in Ref. 3, any solution of this "big pentagon equation" (involving six different types of generalized $6j$ symbols) determines the structural maps of a weak C^* Hopf algebra. Unfortunately, we do not know a single reference that describes a practical implementation of this general construction (and gives the values of these structure constants) for the bialgebras $\mathcal{B}G$ associated with specific *ADE* diagrams or with their higher generalizations.

Graphs Oc(G), encoding the structure of the algebra of quantum symmetries of the diagram G, have been "conceptually" defined by A. Ocneanu in terms of the block structure of $\mathcal{B}G$ for its convolution product, but it is interesting to notice that, to our knowledge, they were never obtained

in this way. Clearly, it would be interesting to do so. We repeat that our modest purpose, in the present article, was to observe that known Ocneanu graphs (or algebras), in the ADE cases, could be recovered, in most cases, from the modular properties of the T matrix; we then used this observation to study several cases belonging to the su(3) system. The problem of deducing Ocneanu graphs from the explicit structure of the bialgebra $\mathcal{B}G$, in the different cases, is a much more difficult and interesting program that it would be nice to investigate.

Here comes a short list of open questions that, we hope, may trigger the interest of the reader:

(i) Give a simple definition—valid in all cases—of the convolution product of $\mathcal{B}G$.
(ii) Show that this bialgebra is indeed a weak Hopf algebra in all cases.
(iii) Is it possible to find a kind of multiplication on EssPaths(G) that would allow one to construct $\mathcal{B}G$ in a functorial (and simple) way?
(iv) Determine explicitly the graphs Oc(G) directly from the study of the corresponding bialgebra $\mathcal{B}G$.
(v) Find a simple algorithm allowing one to calculate all irreducible connections on cell systems (i.e., the values of cells) in all ADE or generalized ADE cases.
(vi) Precise the relation (if any) between the generalized Coxeter–Dynkin systems and the finite subgroups of Lie groups.
(vii) What is the interpretation of all these contructions in terms of the finite dimensional Hopf quotients of $U_q(\mathrm{SL2})$ at roots of unity?
(viii) Can one, in some sense, ''supersymmetrize'' these constructions?
(ix) What is the origin of the linear sum rules?
(x) What is the origin of the quantum sum rules?
(xi) As we know, toric matrices (twisted or not) described in the text can be interpreted as partition functions (with or without defect lines) on a torus, at the critical point, for affine models (WZW models). Clearly this framework can be generalized in several directions: one may consider more general correlation functions, replace affine models by (generalized) minimal models, and replace the torus by higher genus surfaces.
(xii) We know explicitly how to generalize the ADE diagrams in the cases of su(3) and su(4) and a definition of what are the ''generalized Coxeter-Dynkin systems'' was briefly mentionned in Ref. 24 but a detailed description of this notion is clearly needed.
(xiii) What kind of algebraic structures (generalizing the notion of Lie algebras) can one associate with a diagram belonging to such a generalized system?

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

"Massive" spin-2 field in de Sitter space

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(Received 4 February 2003; accepted 24 April 2003)

In this paper we present a covariant quantization of the ''massive'' spin-2 field on de Sitter (dS) space. By ''massive'' we mean a field which carries a specific principal series representation of the dS group. The work is in the direct continuation of previous ones concerning the scalar, the spinor, and the vector cases. The quantization procedure, independent of the choice of the coordinate system, is based on the Wightman-Gärding axiomatic and on analyticity requirements for the two-point function in the complexified pseudo-Riemanian manifold. Such a construction is necessary in view of preparing and comparing with the dS conformal spin-2 massless case (dS linear quantum gravity) which will be considered in a forthcoming paper and for which specific quantization methods are needed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599055]

I. INTRODUCTION

As recent observational data clearly favors a positive acceleration of the present universe, the de Sitter (dS) model represents an appealing first approximation of the background space–time. In two previous papers,[1,2] quantizations of ''massive'' spinor fields and vector fields on the dS space have been considered. The spin-2 case is of great importance since the massless tensor field (spin-2) is among the central objects in quantum cosmology and quantum gravity on dS space (dS linear quantum gravity). It has been found that the corresponding propagator (in the usual linear approximation for gravitational field) exhibits a pathological behavior for large separated points (infrared divergence).[3–5]

On one hand, this behavior may originate from the gauge invariance of the field equation and so should have no physical consequences. Antoniadis, Iliopoulos and Tomaras[6] have shown that the large-distance pathological behavior of the graviton propagator on dS background does not manifest itself in the quadratic part of the effective action in the one-loop approximation. This means the pathological behavior of the graviton propagator may be gauge dependent and so should not appear in an effective way as a physical quantity.

On the other hand, some authors argue that infrared divergence could be exploited in order to create instability of dS space.[7,8] Tsamis and Woodard have considered the field operator for linear gravity in dS space along the latter line in terms of flat coordinates, which cover only one-half of the dS hyperboloid.[9] Hence they have found a quantum field which breaks dS invariance, and they have examined the resulting possibility of quantum instability.

Nevertheless, a fully covariant quantization of the linear gravitational field without infrared divergence in dS space–time may reveal to be of extreme importance for further developments. It

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will be considered in a forthcoming paper.[10] Such a quantization requires preliminary covariant quantizations of the minimally coupled scalar field and the "massive" spin-2 field respectively.

Recently, de Vega *et al.*[11] have shown that, in flat coordinates (not global) on de Sitter space–time, the infrared divergence does not appear in the "massless" minimally coupled scalar field. The question of the covariant minimally coupled scalar field has been completely answered in Ref. 12 after introducing a specific Krein QFT. We have shown that the effect of that quantization, without changing the physical content of the theory, appears as an automatic renormalization of the ultraviolet divergence in the stress tensor and of the infrared divergence in the two-point function.[13] By using this method for linear gravity (the traceless rank-2 "massless" tensor field) the two-point function is free of any infrared divergence.[14] This result has been also obtained by Refs. 15–17.

Here, we present a fully covariant quantization of the "massive" spin-2 field. Our method is based on a rigorous group-theoretical approach combined with a suitable adaptation of the Wightman–Gärding axiomatic, which is carried out in terms of coordinate independent dS waves. The whole procedure originated by Ref. 18 is based on analyticity requirements in the complexified pseudo-Riemanian manifold. The SO(1,N) unitary irreducible representations (UIRs) acting on symmetric, traceless and divergence-free tensor eigenfunctions of the Laplace–Beltrami operator have been investigated in Ref. 19. Previous studies of the "massive" spin-2 field have been carried out in Ref. 20 with a specific choice of coordinates (flat coordinates) covering only one-half of the dS hyperboloid, and in Ref. 21 where the forbidden mass range for spin-2 fields has been clarified, and the null-mass limit considered. The mentioned forbidden mass range is closely related to a novel gauge invariance occurring for a specific representation of the dS group. This phenomena has first been observed in Refs. 22 and 23 in the general framework of constant curvature spaces. Recently, various aspects of higher spin physics have been considered in a series of papers by S. Deser and A. Waldron. Among these, a stability analysis of the massive spin-2 field[24] is given as well as detailed discussions about the richness of the plane defined by the mass parameter and the cosmological constant.[25–27] It is notably shown how this plane is divided by partially massless lines in various regions with different properties (null propagation, stability,...). The null-mass limit has also been analyzed in Ref. 28 and a consistent theory for a massive spin-2 field in a general gravitational background has been presented in Refs. 29 and 30. Pioneering works concerning propagators in a general curved background are due to A. Lichnerowicz (see, for instance, Ref. 31).

In Sec. II, we describe the dS tensor field equation as an eigenvalue equation of the SO(1,4) Casimir operators. The notations and the two independent Casimir operators are introduced. It will be convenient to use ambient space notations in order to express the spin-2 field equation in terms of the coordinate independent Casimir operators. The latter carry the group-theoretical content of the theory and it will be reminded how they enable us to classify the dS group UIR[32,33] according to two parameters p and q which behave like a spin (s) and a mass (m) in the Minkowskian limit, depending on the nature of the involved group representation.

Section III is devoted to the field equation and its solutions. The dS tensor modes are written in terms of a scalar field ϕ and a generalized polarization tensor $\mathcal{E}$,

$$\mathsf{K}_{\alpha\beta}(x)=\mathcal{E}_{\alpha\beta}(x,\xi)\,\phi(x).$$

As for spinor and vector fields, the tensor $\mathcal{E}(x,\xi)$ is a space–time function in dS space–time. There is a certain extent of arbitrariness in the choice of this tensor and we fix it in such a way that, in the limit $H=0$, one obtains the polarization tensor in Minkowski space–time.

In Sec. IV we derive the Wightman two-point function $\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')$. This function fulfills the conditions of (a) positiveness, (b) locality, (c) covariance, (d) normal analyticity, (e) transversality, (f) divergencelessness and (g) permutational index symmetries. The four conditions (c), (e), (f), and (g) allow one to associate this field with a spin-2 unitary irreducible representation of the dS group. The positivity condition permits us to construct a Hilbert space structure. The locality is related to the causality principle, which is a well defined concept in dS space. The normal analy-

ticity allows one to view $\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')$ as the boundary value of an analytic two-point function $W_{\alpha\beta\alpha'\beta'}(z,z')$ from the tube domains. The analytic kernel $W_{\alpha\beta\alpha'\beta'}(z,z')$ is defined in terms of dS waves in their tubular domains. Then, the Hilbert space structure is made explicit and the field operator $\mathcal{K}(f)$ is derived. We also give a coordinate-independent formula for the unsmeared field operator $\mathcal{K}(x)$. Brief conclusion and outlook are given in Sec. V. It is in particular asserted that the extension of our approach to ''massless'' tensor field (gravitational field in a dS background in the linear approximation) requires an indecomposable representation of the dS group in view of the construction of the corresponding covariant quantum field. Finally, we have detailed the classification of the unitary irreducible representation of $SO_0(1,4)$ in Appendix A. In Appendix B we relate our construction to the maximally symmetric bitensors introduced in Ref. 34. In Appendixes C and D we respectively present the ''massive'' vector and tensor two-point functions.

II. FIELD EQUATIONS ON de SITTER SPACE

A. Ambient space notations and Casimir operators

The de Sitter space is a solution of the cosmological Einstein equation with positive cosmological constant Λ. It is conveniently described as a hyperboloid embedded in a five-dimensional Minkowski space

$$X_H=\left\{x\in\mathbb{R}^5; x^2=\eta_{\alpha\beta}x^\alpha x^\beta=-H^{-2}=-\frac{3}{\Lambda}\right\},\quad \alpha,\beta=0,1,2,3,4, \tag{2.1}$$

where $\eta_{\alpha\beta}=\mathrm{diag}(1,-1,-1,-1,-1)$. The de Sitter metrics reads

$$ds^2=\eta_{\alpha\beta}dx^\alpha dx^\beta=g^{dS}_{\mu\nu}dX^\mu dX^\nu,\quad \mu=0,1,2,3,$$

where the X^μ's are four space–time intrinsic coordinates of the dS hyperboloid.

An immediate realization of field space is made of a second-rank intrinsic tensor field $h_{\mu\nu}$ satisfying the conditions of divergenceless, tracelessness, and index permutational symmetry respectively:

$$\nabla\cdot h(X)=0,\quad h^\mu_\mu(X)=0,\quad h_{\mu\nu}=h_{\nu\mu}. \tag{2.2}$$

The wave equation for such fields propagating in de Sitter space can be written as[20]

$$(\Box_H+2H^2+m_H^2)h_{\mu\nu}(X)=0, \tag{2.3}$$

where $\Box_H=\nabla_\mu\nabla^\mu$ is the d'Alembertian operator.

Let us now adopt ambient space notations (for details, see Ref. 35), namely, $\mathcal{K}_{\alpha\beta}(x)$ for the field. With these notations, the relationship with unitary irreducible representations of the dS group becomes straightforward because the Casimir operators are easy to identify. The tensor field $\mathcal{K}_{\alpha\beta}(x)$ has to be viewed as a homogeneous function of the $\mathbb{R}^5$-variables x^α with homogeneous degree λ and thus satisfies

$$x^\alpha\frac{\partial}{\partial x^\alpha}\mathcal{K}_{\gamma\beta}(x)=x\cdot\partial\mathcal{K}_{\gamma\beta}(x)=\lambda\,\mathcal{K}_{\gamma\beta}(x). \tag{2.4}$$

The direction of $\mathcal{K}_{\alpha\beta}(x)$ lies in the de Sitter space if we require the condition of transversality[36]

$$x\cdot\mathcal{K}(x)=0. \tag{2.5}$$

With these notations, the conditions (2.2) read as

$$\overline{\partial}\cdot\mathcal{K}=0,\quad \mathcal{K}^\alpha_\alpha=\mathcal{K}'=0,\quad \mathcal{K}_{\alpha\beta}=\mathcal{K}_{\beta\alpha}, \tag{2.6}$$

where $\overline{\partial}$ is the tangential (or transverse) derivative on dS space,

$$\overline{\partial}_\alpha = \theta_{\alpha\beta}\partial^\beta = \partial_\alpha + H^2 x_\alpha x\cdot\partial, \quad \text{with} \quad x\cdot\overline{\partial}=0. \tag{2.7}$$

The tensor with components $\theta_{\alpha\beta}=\eta_{\alpha\beta}+H^2x_\alpha x_\beta$ is the so-called transverse projector.

In order to express Eq. (2.3) in terms of the ambient coordinates, we use the fact that the "intrinsic" field $h_{\mu\nu}(X)$ is locally determined by the transverse tensor field $\mathcal{K}_{\alpha\beta}(x)$ through

$$h_{\mu\nu}(X)=\frac{\partial x^\alpha}{\partial X^\mu}\frac{\partial x^\beta}{\partial X^\nu}\mathcal{K}_{\alpha\beta}(x(X)). \tag{2.8}$$

For instance, it is easily shown that the metric $\eta_{\mu\nu}$ corresponds to the transverse projector $\theta_{\alpha\beta}$. Covariant derivatives acting on a l-rank tensor are transformed according to

$$\nabla_\mu\nabla_\nu\cdots\nabla_\rho h_{\lambda_1\cdots\lambda_l}=\frac{\partial x^\alpha}{\partial X^\mu}\frac{\partial x^\beta}{\partial X^\nu}\cdots\frac{\partial x^\gamma}{\partial X^\rho}\frac{\partial x^{\eta_1}}{\partial X^{\lambda_1}}\cdots\frac{\partial x^{\eta_l}}{\partial X^{\lambda_l}}\mathrm{Trpr}\overline{\partial}_\alpha\mathrm{Trpr}\overline{\partial}_\beta\cdots\mathrm{Trpr}\overline{\partial}_\gamma\mathcal{K}_{\eta_1..\eta_l}, \tag{2.9}$$

where the transverse projection defined by

$$(\mathrm{Trpr}\,\mathcal{K})_{\lambda_1\cdots\lambda_l}\equiv\theta^{\eta_1}_{\lambda_1}\cdots\theta^{\eta_l}_{\lambda_l}\mathcal{K}_{\eta_1..\eta_l}$$

guarantees the transversality in each index. Applying this procedure to a transverse second rank, symmetric tensor field, leads to

$$\begin{aligned}\nabla_\mu\nabla_\nu h_{\rho\lambda}&=\frac{\partial x^\alpha}{\partial X^\mu}\frac{\partial x^\beta}{\partial X^\nu}\frac{\partial x^\gamma}{\partial X^\rho}\frac{\partial x^\eta}{\partial X^\lambda}\mathrm{Trpr}\overline{\partial}_\alpha\mathrm{Trpr}\overline{\partial}_\beta\mathcal{K}_{\gamma\eta}\\&=\frac{\partial x^\alpha}{\partial X^\mu}\frac{\partial x^\beta}{\partial X^\nu}\frac{\partial x^\gamma}{\partial X^\rho}\frac{\partial x^\eta}{\partial X^\lambda}(\overline{\partial}_\alpha\overline{\partial}_\beta\mathcal{K}_{\gamma\eta}-H^2\theta_{\alpha\gamma}\mathcal{K}_{\beta\eta}-H^2\theta_{\alpha\eta}\mathcal{K}_{\beta\gamma}).\end{aligned} \tag{2.10}$$

The kinematical group of the de Sitter space is the ten-parameter group $SO_0(1,4)$ [connected component of the identity in SO(1,4)], which is one of the two possible deformations of the Poincaré group. There are two Casimir operators

$$Q_2^{(1)}=-\tfrac{1}{2}L_{\alpha\beta}L^{\alpha\beta}, \quad Q_2^{(2)}=-W_\alpha W^\alpha, \tag{2.11}$$

where

$$W_\alpha=-\tfrac{1}{8}\epsilon_{\alpha\beta\gamma\delta\eta}L^{\beta\gamma}L^{\delta\eta}, \quad \text{with ten infinitesimal generators} \quad L_{\alpha\beta}=M_{\alpha\beta}+S_{\alpha\beta}. \tag{2.12}$$

The subscript 2 in $Q_2^{(1)}$, $Q_2^{(2)}$ reminds that the carrier space is constituted by second rank tensors. The orbital part $M_{\alpha\beta}$ and the action of the spinorial part $S_{\alpha\beta}$ on a tensor field $\mathcal{K}$ defined on the ambient space read respectively[37]

$$\begin{aligned}M_{\alpha\beta}&=-i(x_\alpha\partial_\beta-x_\beta\partial_\alpha),\\S_{\alpha\beta}\mathcal{K}_{\gamma\delta}&=-i(\eta_{\alpha\gamma}\mathcal{K}_{\beta\delta}-\eta_{\beta\gamma}\mathcal{K}_{\alpha\delta}+\eta_{\alpha\delta}\mathcal{K}_{\beta\gamma}-\eta_{\beta\delta}\mathcal{K}_{\alpha\gamma}).\end{aligned} \tag{2.13}$$

The symbol $\epsilon_{\alpha\beta\gamma\delta\eta}$ holds for the usual antisymmetrical tensor. The action of the Casimir operator $Q_2^{(1)}$ on $\mathcal{K}$ can be written in the more explicit form

$$Q_2^{(1)}\mathcal{K}(x)=(Q_0^{(1)}-6)\mathcal{K}(x)+2\,\eta\mathcal{K}'+2\mathcal{S}x\partial\cdot\mathcal{K}(x)-2\mathcal{S}\partial x\cdot\mathcal{K}(x), \tag{2.14}$$

In the latter, $Q_0^{(1)}=-\frac{1}{2}M_{\alpha\beta}M^{\alpha\beta}$, and the vector symmetrizer $\mathcal{S}$ is defined for two vectors ξ_α and ω_β by $\mathcal{S}(\xi_\alpha\omega_\beta)=\xi_\alpha\omega_\beta+\xi_\beta\omega_\alpha$.

We are now in position to express the wave equation (2.3) by using the Casimir operators. This can be done with the help of Eq. (2.10) since $Q_0^{(1)}=-H^{-2}(\overline{\partial})^2$. The d'Alembertian operator becomes

$$\Box_H h_{\mu\nu}=\nabla^\lambda\nabla_\lambda h_{\mu\nu}=-\frac{\partial x^\alpha}{\partial X^\mu}\frac{\partial x^\beta}{\partial X^\nu}[Q_0^{(1)}H^2+2H^2]\mathcal{K}_{\alpha\beta}\quad, \tag{2.15}$$

and the wave equation (2.3) is rewritten as

$$(Q_0^{(1)}-H^{-2}m_H^2)\mathcal{K}_{\alpha\beta}(x)=0. \tag{2.16}$$

Finally, using formula (2.14) for the tensor field $\mathcal{K}_{\alpha\beta}(x)$ which satisfies the conditions (2.6), the field equation becomes

$$(Q_2^{(1)}-(m_H^2H^{-2}-6))\mathcal{K}_{\alpha\beta}(x)=0. \tag{2.17}$$

As expected, this formulation of the field equation has now a clear group-theoretical content. In fact, using the representation classification given by the eigenvalues of the Casimir operator, we will be able to identify the involved field. At this point let us clarify what we mean by ''massive'' spin-2 de Sitter field. Inasmuch as mass and spin are well-defined Poincaré concepts, we will consider exclusively the de Sitter elementary systems (in the Wigner sense) associated to a UIR of $SO_0(1,4)$ that admit a nonambiguous massive spin-2 UIR of the Poincaré group at the $H=0$ contraction limit. This contraction is performed with respect to the subgroup $SO_0(1,3)$ which is identified as the Lorentz subgroup in both relativities, and the concerned de Sitter representations are precisely those ones which are induced by the *minimal parabolic*[38] subgroup $SO(3)\times SO(1,1)\times$ (a certain nilpotent subgroup), where SO(3) is the space rotation subgroup of the Lorentz subgroup in both cases. This fully clarifies the concept of spin in de Sitter since it is issued from the *same* SO(3).

B. "Massive" spin-2 unitary representation of the de Sitter group $SO_0(1,4)$

The operator $Q_2^{(1)}$ commutes with the action of the group generators and, as a consequence, it is constant in each unitary irreducible representation (UIR). Thus the eigenvalues of $Q_2^{(1)}$ can be used to classify the UIR's, i.e.,

$$(Q_2^{(1)}-\langle Q_2^{(1)}\rangle)\mathcal{K}(x)=0. \tag{2.18}$$

Following Dixmier[32] we get a classification scheme using a pair (p,q) of parameters involved in the following possible spectral values of the Casimir operators:

$$Q^{(1)}=(-p(p+1)-(q+1)(q-2))I_d,\quad Q^{(2)}=(-p(p+1)q(q-1))I_d. \tag{2.19}$$

Three types of scalar, tensorial or spinorial UIR are distinguished for $SO_0(1,4)$ according to the range of values of the parameters q and p,[32,33] namely, the principal, the complementary and the discrete series. In the following, we shall restrict the list to the unitary representations which have a Minkowskian physical spin-2 interpretation in the limit $H=0$ (for the general situation see Ref. 39 and Appendix A). The flat limit tells us that for the principal and the complementary series it is the value of p which has a spin meaning, and that, in the case of the discrete series, the only representations which have a physically meaningful Minkowskian counterpart are those with $p=q$ (details about the mathematics of the group contraction and the physical principles underlying the relationship between de Sitter and Poincaré groups can be found in Refs. 40 and 41, respectively). The spin-2 tensor representations relevant to the present work are the following:

(i) The UIR's $U^{2,\nu}$ in the principal series where $p=s=2$ and $q=\frac{1}{2}+i\nu$ correspond to the Casimir spectral values:

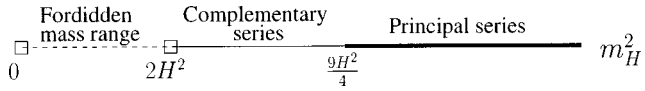

FIG. 1. Mass range and spin-2 $SO_0(1,4)$ unitary irreducible representations.

$$\langle Q_2^{(1)} \rangle = \nu^2 - \tfrac{15}{4}, \tag{2.20}$$

with parameter $\nu \in \mathbb{R}$ (note that $U^{2,\nu}$ and $U^{2,-\nu}$ are equivalent).

(ii) The UIR's $V^{2,q}$ in the complementary series where $p=s=2$ and $q-q^2=\mu$ correspond to

$$\langle Q_2^{(1)} \rangle = q - q^2 - 4 \equiv \mu - 4, \quad 0 < \mu < \tfrac{1}{4}. \tag{2.21}$$

(iii) The UIR's $\Pi^{\pm}_{2,2}$ in the discrete series where $q=p=s=2$ correspond to

$$\langle Q_2^{(1)} \rangle = -6. \tag{2.22}$$

The spin-2 "massless" field in de Sitter space corresponds to the latter case in which the sign $\pm$ in $\Pi^{\pm}_{2,2}$ stands for the helicity. A forthcoming paper will be entirely devoted to this specific field.

Equation (2.17) leads to $H^2(\langle Q_2^{(1)} \rangle + 6) = m_H^2$ which enables us to write the respective "mass" relations for the three types of UIR previously described:

$$m_H^2 = \begin{cases} m_p^2 = H^2(\nu^2 + \frac{9}{4}), & \nu \geqslant 0 \quad \text{(for the principal series)}, \\ m_c^2 = H^2(\mu + 2), & 0 < \mu < \frac{1}{4} \quad \text{(for the complementary series)}, \\ m_d^2 = 0 \quad \text{(for the discrete series)}. \end{cases} \tag{2.23}$$

The spin-2 "mass" range is represented in Fig. 1. The forbidden mass range phenomenon has been discussed by Higuchi in Ref. 21 and largely developed by S. Deser and A. Waldron in Refs. 25–27. It has in particular been shown that for (A)dS space times and for fields with $s>1$, the plane (m_H^2, Λ) is divided in different phases which correspond to unitary or nonunitary regions. These regions are separated "by lines of novel partially massless gauge theories" which correspond to specific representations of the involved group. In the case of the dS group and the spin-2 field, theses lines are given by the values $m_H^2 = 2\Lambda/3 = 2H^2$ and $m_H^2 = 0$. They belong to the discrete series of unitary irreducible representations with the values $p=2$ with $q=1$ $(m_H^2 = 2H^2)$ or $q=2$ $(m_H^2 = 0)$. They are represented by the symbol $\square$ in Fig. 1. Both cases are characterized by a certain gauge invariance which allows us to reduce the degrees of freedom of the corresponding fields. One gets two helicities in the case $m_H^2 = 0$ and four degrees of freedom for the field with $m_H^2 = 2H^2$.

As it is explained above, the case $m_H^2 = 0$ with $p=q=2$ corresponding to the spin-2 linearized gravity admits a Minkowskian interpretation in the flat limit. On the other hand, we do not consider the values of m_H in the range of the complementary series and the discrete series case $m_H^2 = 2H^2$ as acceptable values of a "mass." This is because neither the complementary series with $p=2$ nor the discrete series with $p \neq q$ are linked to any physical representation in the Poincaré flat limit sense. The crucial points are for the complementary series that m_c^2 (unlike m_p^2!) is confined between the values 0 and $\frac{1}{4}$ and therefore simply vanishes in the limit $H=0$ and for the discrete series that in the case $p \neq q$ p and q lose their spin meaning. On the contrary, for the principal series, the contraction limit has to be understood through the constraint $m = H\nu$. The quantity m_H, supposed to depend on H, goes to the Minkowskian mass m when the curvature goes to zero. In short, we only consider as "massive" tensor fields those ones for which the values assumed by the parameter m_H are in the range m_p which corresponds to the principal series of representations. Equation (2.17) then gives

$$(\Box_H + 2H^2 + m_p^2)\mathcal{K}_{\alpha\beta}(x) = 0. \tag{2.24}$$

In order to be more precise, let us recall at this point the physical content of the principal series representation from the point of view of a Minkowskian observer (at the limit $H=0$). The principal series UIR $U^{2,\nu}$, $\nu \geqslant 0$, contracts toward the tensor massive Poincaré UIR's $P^<(m,2)$ and $P^>(m,2)$ with negative and positive energies, respectively. Actually, the group representation contraction procedure is not unique and it has been shown that the principal series UIR can contract either toward the direct sum of the two tensor massive Poincaré UIRs,[42]

$$U^{2,\nu} \frac{H\to 0, \nu\to\infty}{H\nu = m} \to P^<(m,2) \oplus P^>(m,2), \tag{2.25}$$

or simply[43]

$$U^{2,\nu} \frac{H\to 0, \nu\to\infty}{H\nu = m} \to P^>(m,2) \quad \text{or} \quad U^{2,-\nu} \frac{H\to 0, \nu\to\infty}{H\nu = m} \to P^<(m,2). \tag{2.26}$$

In contrast, in the massless spin-2 case, only the two aforementioned representations $\Pi^{\pm}_{2,2}$, in the discrete series with $p=q=2$, have a Minkowskian interpretation. The representation $\Pi^{+}_{2,2}$ has a unique extension to a direct sum of two UIRs $C(3;2,0)$ and $C(-3;2,0)$ of the conformal group $SO_0(2,4)$ with positive and negative energies, respectively.[39,44] The latter restricts to the tensor massless Poincaré UIRs $P^>(0,2)$ and $P^<(0,2)$ with positive and negative energies, respectively. The following diagrams illustrate these connections:

$$\begin{array}{ccccccc} & & \mathcal{C}(3,2,0) & & \mathcal{C}(3,2,0) & \hookleftarrow & \mathcal{P}^>(0,2) \\ \Pi^{+}_{2,2} & \hookrightarrow & \oplus & \overset{H=0}{\to} & \oplus & & \oplus \\ & & \mathcal{C}(-3,2,0) & & \mathcal{C}(-3,2,0) & \hookleftarrow & \mathcal{P}^<(0,2), \end{array} \tag{2.27}$$

$$\begin{array}{ccccccc} & & \mathcal{C}(3,0,2) & & \mathcal{C}(3,0,2) & \hookleftarrow & \mathcal{P}^>(0,-2) \\ \Pi^{-}_{2,2} & \hookrightarrow & \oplus & \overset{H=0}{\to} & \oplus & & \oplus \\ & & \mathcal{C}(-3,0,2) & & \mathcal{C}(-3,0,2) & \hookleftarrow & \mathcal{P}^<(0,-2), \end{array} \tag{2.28}$$

where the arrows $\hookrightarrow$ designate unique extension, and $\mathcal{P}^{\gtrless}(0,2)$ [resp. $\mathcal{P}^{\gtrless}(0,-2)$] are the massless Poincaré UIRs with positive and negative energies and positive (resp. negative) helicity.

III. de SITTER TENSOR WAVES

A. Field equation solution

Our aim is now to solve the "massive" spin-2 wave equation for the dS mode $\mathsf{K}(x)$

$$(Q_2^{(1)} - \langle Q_2^{(1)} \rangle)\mathsf{K}(x) = 0 \quad \text{with} \quad \langle Q_2^{(1)} \rangle = \nu^2 - \tfrac{15}{4}. \tag{3.1}$$

In ambient space notations, the most general transverse, symmetric field $\mathsf{K}_{\alpha\beta}(x)$ can be written in terms of two vector fields K, K_g and a scalar field ϕ through the following recurrence formula:[37]

$$\mathsf{K} = \theta\phi + \mathcal{S}\overline{Z}_1 K + D_2 K_g, \tag{3.2}$$

with K satisfying the conditions (2.6). The symbol Z_1 denotes a constant vector and $\overline{Z}_{1\alpha} = \theta_{\alpha\beta} Z_1^{\beta}$, $x \cdot \overline{Z}_1 = 0$. The operator D_2 is the generalized gradient $D_2 K = H^{-2}\mathcal{S}(\overline{\partial} - H^2 x)K$ which makes a symmetric transverse tensor field from the transverse vector K. The algebraic machinery

valid for describing fields in anti-de Sitter space can be easily transferred *mutatis mutendis* to dS space formalism by the substitutions (see, for instance, Refs. 35, 37, and 45):

$$Q_s^{AdS} \to -Q_s^{dS}, \qquad (H^2)^{AdS} \to -(H^2)^{dS}.$$

Reference 45 provides the following useful relations:

$$\begin{gathered} Q_2\theta\phi = \theta Q_0\phi, \quad Q_2 D_2 K_g = D_2 Q_1 K_g, \\ Q_2 \mathcal{S}\overline{Z}_1 K = \mathcal{S}\overline{Z}_1 (Q_1 - 4)K - 2H^2 D_2 (x\cdot Z_1)K + 4\theta(Z_1\cdot K). \end{gathered} \tag{3.3}$$

Defining the generalized divergence $\partial_2\cdot \mathsf{K} = \partial\cdot\mathsf{K} - H^2 x\mathsf{K}' - \frac{1}{2}\overline{\partial}\mathsf{K}'$ and $D_1 = H^{-2}\overline{\partial}$, one also has

$$\begin{gathered} \partial_2\cdot\theta\phi = -H^2 D_1\phi, \quad \partial_2\cdot D_2 K_g = -(Q_1+6)K_g, \\ \partial_2\cdot\mathcal{S}\overline{Z}_1 K = \overline{Z}_1\partial\cdot K - H^2 D_1(Z_1\cdot K) - H^2 x(Z_1\cdot K) + Z_1\cdot\overline{\partial}K + 5H^2(Z_1\cdot x)K. \end{gathered} \tag{3.4}$$

Putting $\mathsf{K}_{\alpha\beta}(x)$ given by (3.2) into (3.1) and from the linear independence of the terms in (3.2) one gets

$$(Q_1 - \langle Q_1^{(1)}\rangle)K = 0 \quad \text{with} \quad \langle Q_1^{(1)}\rangle = \langle Q_2^{(1)}\rangle + 4\ , \tag{3.5}$$

$$(Q_0 - \langle Q_2^{(1)}\rangle)\phi = -4(Z_1\cdot K)\ , \tag{3.6}$$

$$(Q_1 - \langle Q_2^{(1)}\rangle)K_g = 2H^2(x\cdot Z_1)K\ . \tag{3.7}$$

Note that in these formulas, $\langle Q_s^{(1)}\rangle$ corresponds to the principal series of representation with spin s and that K is chosen to be divergenceless. Using the equations (3.4), the divergenceless condition combined with Eq. (3.7) leads to

$$K_g = \frac{1}{\langle Q_0^{(1)}\rangle}[-H^2 D_1(\phi + Z_1\cdot K) + Z_1\cdot\overline{\partial}K - H^2 x Z_1\cdot K + 3H^2 x\cdot Z_1 K], \tag{3.8}$$

where $\langle Q_0^{(1)}\rangle = \langle Q_2^{(1)}\rangle + 6$. Finally, the traceless condition which yields

$$\overline{\partial}\cdot K_g = -2H^2\phi - H^2 Z_1\cdot K, \tag{3.9}$$

compared to the divergence of Eq. (3.8) allows us to express ϕ in terms of K:

$$\phi = -\tfrac{2}{3}(Z_1\cdot K). \tag{3.10}$$

Thus, the fields K and ϕ are respectively "massive" vector field (e.g., transforming under the vector UIR $U^{1,\nu}$ of the principal series)[1] and "massive" scalar field (e.g., transforming under the scalar UIR $U^{0,\nu}$ of the principal series):[18]

$$(Q_1 - \langle Q_1^{(1)}\rangle)K = 0 \quad \text{and} \quad (Q_0 - \langle Q_0^{(1)}\rangle)\phi = 0. \tag{3.11}$$

Note that the equations for K and ϕ are compatible with the relation $\phi = -\frac{2}{3}Z_1\cdot K$. The equations (3.8) and (3.10) show that the massive vector K determines completely the tensor field K which can now be written

$$\mathsf{K}(x) = \left(-\frac{2}{3}\theta Z_1\cdot + \mathcal{S}\overline{Z}_1 + \frac{1}{\langle Q_0^{(1)}\rangle} D_2\left[Z_1\cdot\overline{\partial} - H^2 x Z_1\cdot + 3H^2 x\cdot Z_1 - \frac{1}{3}H^2 D_1 Z_1\cdot \right]\right) K. \tag{3.12}$$

As explained in Ref. 1 the solutions to Eq. (3.5) are defined on connected open subsets of X_H such that $x\cdot\xi\neq 0$, where $\xi\in\mathbb{R}^5$ lies on the null cone $\mathcal{C}=\{\xi\in\mathbb{R}^5;\quad \xi^2=0\}$. They are homogeneous with degree $-\frac{3}{2}\mp i\nu$ on $\mathcal{C}$ and thus are entirely determined by specifying their values on a well chosen curve (the orbital basis) γ of $\mathcal{C}$. They can be written[1] as a product of a generalized polarization vector $\mathcal{E}_\alpha(x,\xi,Z_2)$ with the so-called[46] (scalar) dS waves $(Hx\cdot\xi)^\sigma$ where $\sigma=-\frac{3}{2}-i\nu\in\mathbb{C}$. The dS wave equations solutions, as functions on de Sitter space, are only locally defined since they are singular on specific lower dimensional subsets of X_H and multivalued on dS space–time. The physical relevance of such waves can be questioned of course, because of their singular behavior and multivaluedness; however their mathematical existence and properties are rigorously justified within the framework of distribution theory.[46,47] Moreover physical de Sitter entities like square integrable states can be built as superpositions of such waves exactly like wave packets are built by superposition of non-square-integrable plane waves in Minkowskian or Galilean quantum mechanics.

The solutions to Eq. (3.5) read

$$K_\alpha(x)=\left(\frac{\sigma}{\sigma+1}\right)\mathcal{E}_\alpha(x,\xi,Z_2)(Hx\cdot\xi)^\sigma,\quad \text{with}\quad \sigma=-\frac{3}{2}-i\nu, \tag{3.13}$$

where Z_2 is another constant vector. Note that contrary to the Minkowskian case, the polarization tensor is a function of space–time. The simplest form of $\mathcal{E}_\alpha(x,\xi,Z_2)$ compatible with the Minkowski polarization vector in the flat limit (see Ref. 1) is obtained through the choice $\xi\cdot Z_2=0$ and reads

$$\mathcal{E}(x,\xi,Z_2)=\left(\overline{Z_2^\lambda}-\frac{Z_2^\lambda\cdot x}{x\cdot\xi}\overline{\xi}\right)\quad \text{with}\quad \mathcal{E}^\lambda(x,\xi,Z_2)\cdot\overline{\xi}=Z_2^\lambda\cdot\xi=0\,. \tag{3.14}$$

It is easy to see (flat limit) that the three Minkowski polarization four-vectors ϵ_μ^λ with $\mu=0,1,2,3$ are linked to Z_2^λ by

$$\lim_{H\to 0}\mathcal{E}_\alpha^\lambda(x,\xi,Z_2)=Z_{2\mu}^\lambda-\frac{Z_{24}^\lambda}{\xi_4}\xi_\mu\equiv\epsilon_\mu^\lambda\,. \tag{3.15}$$

We demand that the Minkowski polarization vectors satisfy the usual relations

$$\epsilon^\lambda\cdot k=0,\quad \epsilon^\lambda\cdot\epsilon^{\lambda'}=\eta^{\lambda\lambda'},\quad \sum_{\lambda=1}^{3}\epsilon_\mu^\lambda(k)\,\epsilon_\nu^\lambda(k)=-\left(\eta_{\mu\nu}-\frac{k_\mu k_\nu}{m^2}\right)\equiv\Pi_{\mu\nu}(k), \tag{3.16}$$

which is achieved if the Z_2^λ's are such that

$$Z_2^\lambda\cdot\xi=0,\quad Z_2^\lambda\cdot Z_2^{\lambda'}=\eta^{\lambda\lambda'},\quad \sum_{\lambda=1}^{3}Z_{2\alpha}^\lambda Z_{2\beta}^\lambda=-\eta_{\alpha\beta}\quad\text{and}\quad \sum_{\lambda=1}^{3}Z_{24}^\lambda Z_{2\mu}^\lambda=0\ \ \forall\ \ \mu\,. \tag{3.17}$$

These conditions are easily derived by working with a well adapted (to the flat limit) orbital basis. This basis, characterized by the values ± 1 of the component ξ_4, will be discussed later on. A remarkable feature connected with the use of ambient space notations is that with Eq. (3.17) one shows that the properties of the dS polarization vector are very similar to the Minkowskian case:

$$\begin{aligned}&\sum_{\lambda=1}^{3}\mathcal{E}_\alpha^\lambda(x,\xi,Z_2)\,\mathcal{E}_\beta^\lambda(x,\xi,Z_2)=-\left(\theta_{\alpha\beta}-\frac{\overline{\xi}_\alpha\overline{\xi}_\beta}{(Hx\cdot\xi)^2}\right)\equiv\Pi_{\alpha\beta}(x,\xi)\,,\\ &\mathcal{E}^\lambda(x,\xi,Z_2)\cdot\mathcal{E}^{\lambda'}(x,\xi,Z_2)=Z_2^\lambda\cdot\mathcal{E}^{\lambda'}(x,\xi,Z_2)=\mathcal{E}^\lambda(x,\xi,Z_2)\cdot\mathcal{E}^{\lambda'}(x',\xi,Z_2)=\eta^{\lambda\lambda'}\,.\end{aligned} \tag{3.18}$$

The last equality involves different space–time points x,x' and will be useful on the level of the two-point function. It follows from Eq. (3.12) that the two spin-2 families of solutions to Eq. (3.1) read

$$\mathsf{K}(x)=\theta\phi+\mathcal{S}\overline{Z_1}K+D_2K_g\equiv\mathcal{D}(x,\partial,Z_1,Z_2)(Hx\cdot\xi)^{-(3/2)\mp i\nu},$$

where the operator $\mathcal{D}(x,\partial,Z_1,Z_2)$ is given by

$$\left(\frac{\sigma}{\sigma+1}\right)\left(-\frac{2}{3}\theta Z_1\cdot+\mathcal{S}\overline{Z_1}+\frac{1}{\langle Q_0^{(1)}\rangle}D_2\left[Z_1\cdot\overline{\partial}-H^2xZ_1\cdot+3H^2x\cdot Z_1-\frac{1}{3}H^2D_1Z_1\cdot\right]\right)\mathcal{E}(x,\xi,Z_2). \tag{3.19}$$

These spin-2 solutions can be brought into the form

$$\mathsf{K}_{\alpha\beta}(x)=a_\nu\mathcal{E}_{\alpha\beta}(x,\xi,Z_1,Z_2)(Hx\cdot\xi)^\sigma \quad\text{and}\quad \mathsf{K}^*_{\alpha\beta}(x) \quad\text{with}\quad a_\nu=c_\nu\left(\frac{2(\sigma-1)}{\sigma+1}\right), \tag{3.20}$$

where the $\mathcal{E}_{\alpha\beta}$'s are the generalized polarization tensor components, c_ν is a normalization constant and where we have again omitted the superscript λ. Because of the conditions $\mathsf{K}_{\alpha\beta}=\mathsf{K}_{\beta\alpha}$, $\partial\cdot\mathsf{K}=0$, and $x\cdot\mathsf{K}=0$, the 25 components $\mathcal{E}_{\alpha\beta}$ reduce to 5 independent components which correspond precisely to the $2s+1=5$ degrees of freedom of a spin-2 field.

The arbitrariness due to the introduction of the constant vectors Z_1,Z_2 in our solution has partly been removed in (3.17) by comparison with the Minkowski polarization vector one eventually reaches by going to the flat limit [see (3.15)]. We now apply the same procedure in order to fix the value of Z_1, that is we investigate the behavior of Eq. (3.19) in the $H=0$ limit. More precisely, we show that $\mathcal{E}_{\alpha\beta}(x,\xi,Z_1,Z_2)$ contracts toward the usual Minkowski tensor polarization and takes a simple form if Z_1 is chosen to be equal to Z_2 and denoted by Z in the following. It is a matter of simple calculation to get the de Sitter polarization tensor starting with formula (3.19):

$$\mathcal{E}_{\alpha\beta}(x,\xi,Z)\equiv\mathcal{E}^{\lambda\lambda'}_{\alpha\beta}(x,\xi)=\frac{1}{2}\left[\mathcal{S}\mathcal{E}^\lambda_\alpha(x,\xi)\mathcal{E}^{\lambda'}_\beta(x,\xi)-\frac{2}{3}\left(\theta_{\alpha\beta}-\frac{\overline{\xi}_\alpha\overline{\xi}_\beta}{(Hx\cdot\xi)^2}\right)\mathcal{E}^\lambda(x,\xi)\cdot\mathcal{E}^{\lambda'}(x,\xi)\right], \tag{3.21}$$

where $\mathcal{E}^\lambda(x,\xi)=\mathcal{E}^\lambda(x,\xi,Z_2)$. In view of (3.18) one obtains

$$\mathcal{E}^{\lambda\lambda'}_{\alpha\beta}(x,\xi)=\frac{1}{2}\left[\mathcal{S}\mathcal{E}^\lambda_\alpha(x,\xi)\mathcal{E}^{\lambda'}_\beta(x,\xi)+\frac{2}{3}\eta^{\lambda\lambda'}\sum_\rho\mathcal{E}^\rho_\alpha(x,\xi)\mathcal{E}^\rho_\beta(x,\xi)\right]. \tag{3.22}$$

It is easy to check that the tensor polarization (3.22) satisfies the properties $\eta^{\alpha\beta}\mathcal{E}_{\alpha\beta}(x,\xi,Z)=0$ (tracelessness), $\overline{\xi}\cdot\mathcal{E}_{\alpha\beta}(x,\xi,Z)=0$ and the relation

$$\mathcal{E}^{\lambda\lambda'}(x,\xi)\cdot\cdot\,\mathcal{E}^{\lambda''\lambda'''}(x,\xi)=\mathcal{E}^{\lambda\lambda'}(x',\xi)\cdot\cdot\,\mathcal{E}^{\lambda''\lambda'''}(x,\xi)=[\eta^{\lambda\lambda''}\eta^{\lambda'\lambda'''}+\eta^{\lambda\lambda'}\eta^{\lambda''\lambda'''}]. \tag{3.23}$$

The dS tensor waves $\mathsf{K}_{\alpha\beta}(x)$ are homogeneous with degree σ on the null cone $\mathcal{C}$ and on the dS submanifold X_H characterized by $x\cdot x=-H^{-2}$ with H being constant. This is due to

$$\mathcal{E}^\lambda(x,a\xi)=\mathcal{E}^\lambda(x,\xi) \quad\text{and}\quad \mathcal{E}^\lambda(ax,\xi)=\mathcal{E}^\lambda(x,\xi),$$

which is obvious from the definition of $\mathcal{E}^\lambda(x,\xi)$

$$\mathcal{E}^\lambda(x,\xi)=\left(\overline{Z^\lambda}-\frac{Z^\lambda\cdot x}{\xi\cdot x}\overline{\xi}\right)=\left(Z^\lambda-\frac{Z^\lambda\cdot x}{\xi\cdot x}\xi\right). \tag{3.24}$$

Note that as a function of $\mathbb{R}^5$, the wave $\mathsf{K}_{\alpha\beta}(x)$ is homogeneous with degree zero $[H(x)=-1/\sqrt{-x\cdot x}]$.

B. Flat limit and analytic tensor wave

It order to compute the flat limit of the polarization tensor, it is useful to precise the notion of orbital basis γ for the future null cone $\mathcal{C}^+=\{\xi\in\mathcal{C};\ \ \xi^0>0\}$.[46] Let us choose a unit vector e in $\mathbb{R}^5$ and let H_e be its stabilizer subgroup in $SO_0(1,4)$. Then two types of orbits are interesting in the present context.

(i) The spherical type γ_0 corresponds to $e\in V^+\equiv\{x\in\mathbb{R}^5;\quad x^0>\sqrt{\|\vec{x}\|^2+(x^4)^2}\}$, and is an orbit of $H_e\approx \mathrm{SO}(4)$,

$$\gamma_0=\{\xi;e\cdot\xi=a>0\}\cap\mathcal{C}^+\quad .$$

(ii) The hyperbolic type γ_4 corresponds to $e^2=-1$. It is divided into two hyperboloid sheets, both being orbits of $H_e\approx \mathrm{SO}_0(1,3)$.

The most suitable parametrization when one has in view the link with massive Poincaré UIRs is to work with the orbital basis of the second type,

$$\gamma_4=\{\xi\in C^+,\xi^{(4)}=1\}\cup\{\xi\in C^+,\xi^{(4)}=-1\},$$

with the null vector ξ given in terms of the four-momentum $(k^0,\vec{k})$ of a Minkowskian particle of mass m:

$$\xi_\pm=\left(\frac{k^0}{mc}=\sqrt{\frac{\vec{k}^2}{m^2c^2}+1},\frac{\vec{k}}{mc},\pm 1\right). \tag{3.25}$$

An appropriate choice of global coordinates is given by

$$\begin{aligned} x^0&=H^{-1}\sinh(HX^0)\,,\\ \vec{x}&=(H\|\vec{X}\|)^{-1}\vec{X}\cosh(HX^0)\sin(H\|\vec{X}\|)\,,\\ x^4&=H^{-1}\cosh(HX^0)\cos(H\|\vec{X}\|)\,, \end{aligned} \tag{3.26}$$

where the dS point is expressed in terms of the Minkowskian variables $X=(X_0=ct,\vec{X})$ measured in units of the dS radius H^{-1}.

The Minkowskian limit of the dS waves at point x can be written as[18]

$$\begin{aligned} &\lim_{H\to 0}(Hx\cdot\xi_-)^\sigma=\exp[-ik\cdot X]\quad\ \ (\text{positive energy}),\\ &\lim_{H\to 0}e^{-i\pi\sigma}(Hx\cdot\xi_+)^\sigma=\exp[ik\cdot X]\quad\ \ (\text{negative energy}). \end{aligned} \tag{3.27}$$

Since the contraction is done with respect to the Lorentz subgroup $\mathrm{SO}_0(1,3)$ [γ_4 is invariant under $\mathrm{SO}_0(1,3)$] the equations (3.27) indicate that with the orbital basis γ_4, dS waves can contract toward the sum of two solutions with opposite energies (see Ref. 43).

The polarization tensor limit is easily obtained with the help of

$$\lim_{H\to 0}H^2\sigma^2=-m^2,\quad \lim_{H\to 0}\mathcal{E}^\lambda_\alpha(x,\xi)=\epsilon^\lambda_\mu(k)\,,\quad \lim_{H\to 0}\theta_{\alpha\beta}=\eta_{\mu\nu}\,,\quad \lim_{H\to 0}\overline{\xi}_\alpha=\frac{k_\mu}{m}\forall\,\xi\in\gamma_4.$$

Finally, one recovers the Minkowskian massive spin-2 polarization tensor:[48]

$$\lim_{H\to 0}\mathcal{E}^{\lambda\lambda'}_{\alpha\beta}(x,\xi)=\epsilon^{\lambda\lambda'}_{\mu\nu}(k)=\frac{1}{2}\mathcal{S}\epsilon^\lambda_\mu(k)\epsilon^{\lambda'}_\nu(k)+\frac{1}{3}\eta^{\lambda\lambda'}\sum_\lambda\ \epsilon^\lambda_\mu(k)\epsilon^\lambda_\nu(k)\,,$$

which satisfies $\eta^{\mu\nu}\epsilon_{\mu\nu}^{\lambda\lambda'}(k)=k^{\mu}\epsilon_{\mu\nu}^{\lambda\lambda'}(k)=0$ and

$$\sum_{\lambda\lambda'}\epsilon_{\mu\nu}^{\lambda\lambda'}(k)\epsilon_{\rho\pi}^{\lambda\lambda'}(k)=\frac{1}{2}[\Pi_{\mu\rho}(k)\Pi_{\nu\pi}(k)+\Pi_{\nu\rho}(k)\Pi_{\mu\pi}(k)]-\frac{1}{3}[\Pi_{\mu\nu}(k)\Pi_{\rho\pi}(k)]. \quad (3.28)$$

Hence, we have shown that in the limit $H=0$, $(Hx\cdot\xi)^{\sigma}$ and $\mathcal{E}_{\alpha\beta}(x,\xi,Z)$ behave like the plane wave $e^{ik\cdot X}$ and the polarization tensor in Minkowski space–time, respectively.

Although the "massive" field equation solutions $\mathsf{K}_{\alpha\beta}(x)$ and $\mathsf{K}^{*}_{\alpha\beta}(x)$ are complex conjugated, they cannot be associated with the positive and negative energies respectively as in the Minkowskian situation. Actually, despite the fact that the solutions are globally defined (in a distributional sense) in dS space, the concept of energy is not (absence of global timelike killing vector field). As a result, concepts like "particle" and "antiparticle" are rather unclear and the differences between these two solutions is not really explained or understood. In terms of group representation these two solutions are equivalent, because the two representations $U^{2,\nu}$ and $U^{2,-\nu}$ are. Note that the minimally coupled scalar field requires both sets of solutions in order to achieve a covariant quantization.[12] This will certainly also be the case for the spin-2 massless field in dS space since it is constructed from a minimally coupled scalar field as it will be shown in Ref. 10.

In the present case, the "massive" free field covariant quantization can be constructed from the positive norm states alone since $\mathsf{K}_{\alpha\beta}(x)$ transforms under the group action in a closed way:

$$\begin{aligned}(U(g)\,\mathsf{K})_{\alpha\beta}(x)&=g_{\alpha}^{\gamma}g_{\beta}^{\delta}\mathsf{K}_{\gamma\delta}(g^{-1}x)\\&=g_{\alpha}^{\gamma}g_{\beta}^{\delta}\,a_{\nu}\mathcal{E}_{\gamma\delta}(g^{-1}x,\xi,Z)(Hg^{-1}x\cdot\xi)^{\sigma}\\&=a_{\nu}\mathcal{E}_{\alpha\beta}(x,g\xi,gZ)(Hx\cdot g\xi)^{\sigma}.\end{aligned} \quad (3.29)$$

This is easily proved since the vector polarization satisfies

$$\mathcal{E}_{\alpha}(g^{-1}x,\xi,Z)=\left(Z_{\alpha}-\frac{g^{-1}x\cdot Z}{g^{-1}x\cdot\xi}\xi_{\alpha}\right)=\left(Z_{\alpha}-\frac{x\cdot gZ}{x\cdot g\xi}\xi_{\alpha}\right)=(g^{-1})_{\alpha}^{\delta}\mathcal{E}_{\delta}(x,g\xi,gZ). \quad (3.30)$$

We have mentioned that the dS waves solutions, as functions on de Sitter space, are only locally defined since they are singular on specific lower dimensional subsets of X_H and multivalued on dS space–time. In order to get a global definition, they have to be viewed as distributions[47] which are boundary values of analytic continuations of the solutions to tubular domains in the complexified de Sitter space $X_H^{(c)}$. The latter is defined as follows:

$$\begin{aligned}X_H^{(c)}&=\{z=x+iy\in\mathbb{C}^5;\ \ \eta_{\alpha\beta}z^{\alpha}z^{\beta}=(z^0)^2-\vec{z}\cdot\vec{z}-(z^4)^2=-H^{-2}\}\\&=\{(x,y)\in\mathbb{R}^5\times\mathbb{R}^5;\ \ x^2-y^2=-H^{-2},\ \ x\cdot y=0\}.\end{aligned}$$

For an univalued determination, we must introduce the forward and backward tubes of $X_H^{(c)}$. First of all, let $T^{\pm}=\mathbb{R}^5-iV^{\pm}$ be the forward and backward tubes in $\mathbb{C}^5$. The domain V^{+} (resp. V^{-}) stems from the causal structure on X_H:

$$V^{\pm}=\{x\in\mathbb{R}^5;\quad x^0\gtrless\sqrt{\|\vec{x}\|^2+(x^4)^2}\}. \quad (3.31)$$

We then introduce their respective intersections with $X_H^{(c)}$,

$$\mathcal{T}^{\pm}=T^{\pm}\cap X_H^{(c)}, \quad (3.32)$$

which are the tubes of $X_H^{(c)}$. Finally, we define the "tuboid" above $X_H^{(c)}\times X_H^{(c)}$ by

$$\mathcal{T}_{12}=\{(z,z');\quad z\in\mathcal{T}^{+},z'\in\mathcal{T}^{-}\}. \quad (3.33)$$

Details are given in Ref. 46. When z varies in $\mathcal{T}^+$ (or $\mathcal{T}^-$) and ξ lies in the positive cone $\mathcal{C}^+$ the wave solutions are globally defined because the imaginary part of $(z\cdot\xi)$ has a fixed sign and $z\cdot\xi\neq 0$.

We define the de Sitter tensor wave $\mathsf{K}_{\alpha\beta}(x)$ as the boundary value of the analytic continuation to the future tube of Eq. (3.20). Hence, for $z\in\mathcal{T}^+$ and $\xi\in\mathcal{C}^+$ one gets the two solutions

$$\mathsf{K}_{\alpha\beta}(z)=a_\nu\,\mathcal{E}^{\lambda\lambda'}_{\alpha\beta}(z,\xi)(Hz\cdot\xi)^\sigma \quad \text{and} \quad \mathsf{K}^*_{\alpha\beta}(z^*)=a^*_\nu\,\mathcal{E}^{*\lambda\lambda'}_{\alpha\beta}(z^*,\xi)(Hz\cdot\xi)^{\sigma^*}. \tag{3.34}$$

IV. TWO-POINT FUNCTION AND QUANTUM FIELD

A. The two-point function

As explained in Ref. 46, the dS axiomatic field theory is based on the Wightman two-point double tensor-valued function

$$\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x') \quad \alpha',\beta'=0,1,...,4. \tag{4.1}$$

Indeed, this kernel entirely encodes the theory of the generalized free fields on dS space–time X_H, at least for the massive case. For this, it has to satisfy the following requirements:

(a) **Positiveness:** For any test function $f_{\alpha\beta}\in\mathcal{D}(X_H)$, we have

$$\int_{X_H\times X_H} f^{*\alpha\beta}(x)\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')f^{\alpha'\beta'}(x')d\sigma(x)d\sigma(x')\geqslant 0, \tag{4.2}$$

where $d\sigma(x)$ denotes the dS-invariant measure on X_H.[46] $\mathcal{D}(X_H)$ is the space of functions C^∞ with compact support in X_H.

(b) **Locality:** For every spacelike separated pair (x,x'), i.e., $x\cdot x'>-H^{-2}$,

$$\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')=\mathcal{W}_{\alpha'\beta'\alpha\beta}(x',x). \tag{4.3}$$

(c) **Covariance:**

$$(g^{-1})^\gamma_\alpha(g^{-1})^\delta_\beta\mathcal{W}_{\gamma\delta\gamma'\delta'}(gx,gx')g^{\gamma'}_{\alpha'}g^{\delta'}_{\beta'}=\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x'), \tag{4.4}$$

for all $g\in \mathrm{SO}_0(1,4)$.

(d) **Index symmetrizer:**

$$\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')=\mathcal{W}_{\alpha\beta\beta'\alpha'}(x,x')=\mathcal{W}_{\beta\alpha\alpha'\beta'}(x,x'). \tag{4.5}$$

(e) **Transversality:**

$$x^\alpha\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')=0=x'^{\alpha'}\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x'). \tag{4.6}$$

(f) **Divergencelessness:**

$$\partial^\alpha_x\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')=0=\partial^{\alpha'}_{x'}\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x'). \tag{4.7}$$

(g) **Normal analyticity:** $\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')$ is the boundary value (bv) in the distributional sense of an analytic function $W_{\alpha\beta\alpha'\beta'}(z,z')$.

Concerning the last requirement, $W_{\alpha\beta\alpha'\beta'}(z,z')$ is actually maximally analytic, i.e., can be analytically continued to the ''cut domain''

$$\Delta=\{(z,z')\in X_H^{(c)}\times X_H^{(c)}:(z-z')^2<0\}.$$

The Wightman two-point function $\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')$ is the boundary value of $W_{\alpha\beta\alpha'\beta'}(z,z')$ from $\mathcal{T}_{12}$ and the "permuted Wightman function" $\mathcal{W}_{\alpha'\beta'\alpha\beta}(x',x)$ is the boundary value of $W_{\alpha\beta\alpha'\beta'}(z,z')$ from the domain

$$\mathcal{T}_{21}=\{(z,z');\quad z\in\mathcal{T}^-,z'\in\mathcal{T}^+\}.$$

Once these properties are satisfied, the reconstruction theorem[49] allows us to recover the corresponding quantum field theory. Our present task is therefore to find a doubled tensor valued analytic function of the variable (z,z') satisfying the properties (a)–(g). Following Ref. 46 (in which the construction has been done for the scalar case), the analytic two-point function $W_{\alpha\beta\alpha'\beta'}(z,z')\equiv W^{\nu}_{\alpha\beta\alpha'\beta'}(z,z')$ is obtained from the dS tensor waves (3.34). The parameter ν refers to the principal series. The two-point function is given in terms of the following class of integral representations,

$$W^{\nu}_{\alpha\beta\alpha'\beta'}(z,z')=|a_\nu|^2\int_\gamma (Hz\cdot\xi)^\sigma (Hz'\cdot\xi)^{\sigma^*}\sum_{\lambda\lambda'}\mathcal{E}^{\lambda\lambda'}_{\alpha\beta}(z,\xi)\,\mathcal{E}^{*\lambda\lambda'}_{\alpha'\beta'}(z'^*,\xi)\,d\sigma_\gamma(\xi),\quad (4.8)$$

where $d\sigma_\gamma(\xi)$ is the natural $\mathcal{C}^+$ invariant measure on γ, induced from the $\mathbb{R}^5$ Lebesgue measure,[46] and the normalization constant a_ν is fixed by local Hadamard condition. The latter selects a unique vacuum state for quantum tensor fields which satisfies the dS field equation. In order to check whether conditions (a)–(g) are satisfied by Eq. (4.8), let us first rewrite the two-point function in a more explicit way. This will be done by using the scalar and the vector "massive" analytic two-point functions $W^\nu_0(z,z')$, $W^\nu_1(z,z')$ (where $\mathcal{Z}=-H^2z\cdot z'$). The latter satisfy the complex versions of the Casimir equations:

$$(Q_1-\langle Q_1^{(1)}\rangle)W^\nu_1(z,z')=0\ \text{ and }\ (Q_0-\langle Q_0^{(1)}\rangle)W^\nu_0(z,z')=0\,.\quad (4.9)$$

In Appendix C and in Ref. 1 it is shown how $W^\nu_1(z,z')$ can be written in terms of the scalar analytic two-point function:

$$W^\nu_1(z,z')=\frac{\langle Q_0\rangle}{\langle Q_1\rangle}\left(-\theta_\alpha\cdot\theta'_{\alpha'}+\frac{H^2\sigma(\theta\cdot z')D'_1}{\langle Q_0\rangle}+\frac{H^2\sigma^*(\theta'\cdot z)D_1}{\langle Q_0\rangle}+\frac{H^2\mathcal{Z}D_1D'_1}{\langle Q_0\rangle}\right)W^\nu_0(z,z').\quad (4.10)$$

The Wightman scalar two-point function $\mathcal{W}^\nu_0(x,x')$ is given by[46]

$$\mathcal{W}^\nu_0(x,x')=\mathrm{bv}\ \ W_0(z,z')\quad\text{with}\quad W^\nu_0(z,z')=c^2_\nu\int_\gamma (Hz\cdot\xi)^\sigma(Hz'\cdot\xi)^{\sigma^*}\,d\sigma_\gamma(\xi)\,.\quad (4.11)$$

The normalization constant c^2_ν is determined by imposing the Hadamard condition on the two-point function. This has been done in Ref. 46 where the scalar two-point function has been rewritten in terms of the generalized Legendre function for well chosen spacelike separated points z and z'. It has been established that $W_0(z,z')=C_\nu P^{(5)}_\sigma(-\mathcal{Z})$ with $C_\nu=2\pi^2e^{-\pi\nu}c^2_\nu$ and

$$c^2_\nu=\frac{H^2e^{\pi\nu}\Gamma(-\sigma)\Gamma(-\sigma^*)}{2^5\pi^4m^2}.\quad (4.12)$$

This normalization corresponds to the Euclidean vacuum[46] and $P^{(5)}_\sigma(\mathcal{Z})$ is the generalized Legendre function of the first kind. There are several reasons which explain the appearance of $W^\nu_0(z,z')$ and $W^\nu_1(z,z')$. First of all, both correspond to the commonly used two-point functions (see, for instance, Ref. 34) as it is checked in Appendix C. Moreover, since the vector two-point function, is written in terms of the scalar two-point function it exhibits the two building blocks of the tensor expression which are well known and simple to manipulate. As a matter of fact, the flat limit is very easy to compute in this framework.

We have seen that the spin-2 analytic two-point function (4.8) is obtained from the tensor waves (3.34). Let us cast the latter into the more suitable form

$$\mathcal{K}(z)=\frac{a_\nu}{2}\left[\mathcal{S}\mathcal{E}^{\lambda}(z,\xi)\mathcal{E}^{\lambda'}(z,\xi)-\frac{2\sigma g^{\lambda\lambda'}}{3(\sigma-1)}\left(\theta-\frac{H^2D_2D_1}{2\sigma^2}\right)\right](Hz\cdot\xi)^{\sigma} \tag{4.13}$$

by using the property

$$\sum_{\lambda}\mathcal{E}^{\lambda}(z,\xi)\,\mathcal{E}^{\lambda}(z,\xi)(Hz\cdot\xi)^{\sigma}=-\left(\theta-\frac{\overline{\xi\xi}}{(Hz\cdot\xi)^2}\right)(Hz\cdot\xi)^{\sigma}=-\frac{\sigma}{\sigma-1}\left[\theta-\frac{H^2D_2D_1}{2\sigma^2}\right](Hz\cdot\xi)^{\sigma}. \tag{4.14}$$

We then simply develop the two-point function and obtain

$$\begin{aligned}W^{\nu}(z,z')=\frac{|a_\nu|^2}{4}\int_{\gamma}\mathcal{S}\mathcal{S}'&\left(\sum_{\lambda}\mathcal{E}^{\lambda}(z,\xi)\,\mathcal{E}^{*\lambda}(z'^{*},\xi)\right)\left(\sum_{\lambda'}\mathcal{E}^{\lambda'}(z,\xi)\,\mathcal{E}^{*\lambda'}(z'^{*},\xi)\right)\\&\times(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}\,d\sigma_{\gamma}(\xi)-\frac{4}{3}\frac{\langle Q_0\rangle}{\langle Q_1\rangle}\left[\theta-\frac{H^2D_2D_1}{2\sigma^2}\right]\left[\theta'-\frac{H^2D_2'D_1'}{2\sigma^{*2}}\right]\\&\times c_\nu^2\int_{\gamma}(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}\,d\sigma_{\gamma}(\xi).\end{aligned} \tag{4.15}$$

From the property

$$\sum_{\lambda}\mathcal{E}^{\lambda}(z)\mathcal{E}^{*\lambda}(z'^{*})=\left[-\theta\cdot\theta'+\frac{(\theta\cdot z')\overline{\xi'}}{z'\cdot\xi}+\frac{(\theta'\cdot z)\overline{\xi}}{z\cdot\xi}+\frac{\mathcal{Z}\,\overline{\xi\xi'}}{H^2z\cdot\xi z'\cdot\xi}\right], \tag{4.16}$$

and the relation $H^2D_2K(x)=(\sigma-1)\,\mathcal{S}\overline{\xi}K(x)/(z\cdot\xi)$, it is clear that the analytic two-point function can be written in the general form:

$$W^{\nu}(z,z')=M(z,z')\,W_1^{\nu}(z,z')+N(z,z')\,W_0^{\nu}(z,z'). \tag{4.17}$$

The differential operators $M(z,z')$ and $N(z,z')$ are given by

$$\begin{aligned}M(z,z')&=\frac{\langle Q_0\rangle+4}{\langle Q_0\rangle}\left[-\mathcal{S}\mathcal{S}'\,\theta\cdot\theta'+\frac{H^2\mathcal{S}(\theta\cdot z')D_2'}{\sigma^*-1}+\frac{H^2\mathcal{S}'(\theta'\cdot z)D_2}{\sigma-1}+\frac{\mathcal{Z}H^2D_2D_2'}{(\sigma-1)(\sigma^*-1)}\right],\\N(z,z')&=\frac{4}{3}\frac{\langle Q_0\rangle}{\langle Q_1\rangle}\left[\theta-\frac{H^2D_2D_1}{2\sigma^2}\right]\left[\theta'-\frac{H^2D_2'D_1'}{2\sigma^{*2}}\right].\end{aligned} \tag{4.18}$$

Eventually, the analytic tensor two-point function is given in terms of the scalar analytic two-point function by

$$W^{\nu}_{\alpha\beta\alpha'\beta'}(z,z')=D(z,z')W_0^{\nu}(z,z'),$$

with $D(z,z')$ a differential operator discussed in Appendix D. The boundary value of $W^{\nu}(z,z')$ gives the following integral representation for the Wightman two-point function:

$$\mathcal{W}(x,x')=|a_\nu|^2\sum_{\lambda\lambda'}\int_{\gamma}d\sigma_{\gamma}(\xi)\mathcal{E}^{\lambda\lambda'}(x,\xi)\mathcal{E}^{*\lambda\lambda'}(x',\xi)\,\mathrm{bv}(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}, \tag{4.19}$$

with

$$\mathrm{bv}(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}=|Hx\cdot\xi|^{\sigma}|Hx'\cdot\xi|^{\sigma^*}[\,\theta(Hx\cdot\xi)+\theta(-Hx\cdot\xi)\,e^{-i\pi\sigma}]$$
$$\times[\,\theta(Hx'\cdot\xi)+\theta(-Hx'\cdot\xi)\,e^{+i\pi\sigma^*}]. \tag{4.20}$$

This relation defines the two-point function in terms of global waves on the real hyperboloid X_H.

Let us now check if this kernel fulfills the conditions (a)–(g) required in order to get a Wightman two-point function. We recall that the existence of the latter which is requested by dS axiomatic field theory.

(i) The positiveness property follows from the relation

$$\int_{X_H\times X_H} f^{*\alpha\beta}(x)\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')f^{\alpha'\beta'}(x')d\sigma(x)d\sigma(x')=|a_\nu|^2\int_\gamma d\sigma_\gamma(\xi)\sum_{\lambda\lambda'} g^{*\lambda\lambda'}(\xi)\,g^{\lambda\lambda'}(\xi)\,, \tag{4.21}$$

where

$$g^{\lambda\lambda'}(\xi)=\int_{X_H} d\sigma(x)f^{\alpha\beta}(x)\mathcal{E}^{*\lambda\lambda'}_{\alpha\beta}(x,\xi)[\,\theta(Hx\cdot\xi)+\theta(-Hx\cdot\xi)\,e^{+i\pi\sigma^*}]|Hx\cdot\xi|^{\sigma^*}\,. \tag{4.22}$$

The hermiticity property is obtained by considering boundary values of the following identity,

$$W_{\alpha\beta\alpha'\beta'}(z,z')=W^*_{\alpha'\beta'\alpha\beta}(z'^*,z^*), \tag{4.23}$$

which is easily checked on Eq. (4.8).

(ii) In order to prove the locality condition, we use the hermiticity condition and the following relation:

$$W^*_{\alpha'\beta'\alpha\beta}(z'^*,z^*)=W_{\alpha'\beta'\alpha\beta}(z',z).$$

This easily follows from the form of the two-point function for spacelike separated points given in Appendix D:

$$W^{\nu}(z,z')=C_\nu D(z,z')P^{(5)}_{\sigma}(-\mathcal{Z}) \quad \text{with} \quad D^*(z^*,z'^*)=D(z,z'),$$

and from the relation[50]

$$P^{(5)}_{\sigma}(-\mathcal{Z})=P^{(5)}_{\sigma^*}(-\mathcal{Z}).$$

One finally gets

$$W_{\alpha\beta\alpha'\beta'}(z,z')=W^*_{\alpha'\beta'\alpha\beta}(z'^*,z^*)=W_{\alpha'\beta'\alpha\beta}(z',z).$$

It should be noticed that the spacelike separated pair (x,x') lies in the same orbit of the complex dS group as the pairs (z,z') and (z'^*,z^*). Therefore the locality condition $\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')=\mathcal{W}_{\alpha'\beta'\alpha\beta}(x',x)$ holds.

(iii) The group action on the dS modes (3.29) and the independence of the integral (4.8) with respect to the selected orbital basis entail the covariance property

$$(g^{-1})^{\gamma}_{\alpha}(g^{-1})^{\delta}_{\beta}\mathcal{W}_{\gamma\delta\gamma'\delta'}(gx,gx')g^{\gamma'}_{\alpha'}g^{\delta'}_{\beta'}=\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x'). \tag{4.24}$$

(iv) The symmetry with respect to the indices α, β and α', β' and the transversality with respect to x and x' are guaranteed by construction. So is the divergencelessness condition.

(v) The analyticity properties of the tensor Wightman two-point function follow from the expression of the dS tensor waves (3.34).

Remark: A massive spin-2 two-point function had already been proposed in Ref. 20. Although the approach we have used here is very different (in Ref. 20 the coordinates are nonglobal, the modes have a spin-0 and spin-2 content,...), it has been possible to check that our vector two-point function is in agreement with the one presented in Ref. 20. This is of importance since it confirms for tensor fields the validity of the integral representation method (4.8) originated in Ref. 46 for the scalar case. However, explicit comparison for the spin-2 case would be a rather tedious task given the differences between both formalisms and the involved expression of the spin-2 two-point function given in Ref. 20. It seems that one can at least say that the ambient space formalism presents the advantage of simplicity. This is again verified by performing the flat limit as it is seen in the next paragraph and this was already the case when the unitary irreducible representations had to be identified in Sec. II.

B. The flat limit

The flat limit is straightforward to compute with the help of the orbital basis γ_4. The measure $d\sigma_{\gamma_4}(\xi)$ is chosen to be m^2 times the natural one induced from the $\mathbb{R}^5$ Lebesgue measure. This yields $d\sigma_{\gamma_4}(\xi)=d^3\vec{k}/k_0$ and the constant $|a_\nu|^2$ reads

$$|a_\nu|^2=4\,\frac{\langle Q_0\rangle+4}{\langle Q_1\rangle}\left[\frac{H^2e^{\pi\nu}\Gamma(-\sigma)\Gamma(-\sigma^*)}{2^5\pi^4m^2}\right]=4\,\frac{\langle Q_0\rangle+4}{\langle Q_1\rangle}\left[\frac{H^2\nu^2+H^2/4}{2^4\pi^3m^2}\right]. \tag{4.25}$$

One finds the massive spin-2 Minkowski two-point function:

$$\lim_{H\to 0}\frac{1}{4}\mathcal{W}^\nu(x,x')=\frac{1}{2(2\pi)^3}\int\sum_{\lambda\lambda'}\epsilon^{\lambda\lambda'}(k)\epsilon^{\lambda\lambda'}(k)\exp(-ik(x-x'))d^3\vec{k}/k_0\,, \tag{4.26}$$

where the factor 1/4 is due to our definition of the operators $\mathcal{S}$ and $\mathcal{S}'$. This limit can also be computed (more explicitly) starting with Formula (4.17). The flat limit for the scalar and vector two-point functions have been computed in Refs. 1 and 46, one obtains:

$$\lim_{H\to 0}\mathcal{W}_0^\nu(x,x')=\mathcal{W}^P(X,X'),\quad \lim_{H\to 0}\mathcal{W}_1(x,x')=-\left[\eta_{\mu\nu}+\frac{1}{m^2}\frac{\partial}{\partial X^\mu\partial X^\nu}\right]\mathcal{W}^P(X,X')\equiv\mathcal{W}^P_{\mu\nu}(X,X')\,, \tag{4.27}$$

where $\mathcal{W}^P(X,X')$ and $\mathcal{W}^P_{\mu\nu}(X,X')$ are the scalar and vector massive Minkowskian two-point functions respectively. Under the constraint $H\nu=m$, which implies

$$\lim_{H\to 0}H^2\langle Q_s\rangle=m^2\quad\text{and}\quad\lim_{H\to 0}H^2\sigma^2=-m^2\,, \tag{4.28}$$

one finally gets the massive spin-2 Minkowski two-point function (see, for instance, Ref. 19)

$$\begin{aligned}\lim_{H\to 0}\frac{1}{4}\mathcal{W}(x,x')=&+\frac{1}{3}\left[\eta_{\mu\nu}+\frac{1}{m^2}\frac{\partial}{\partial X^\mu\partial X^\nu}\right]\mathcal{W}^P_{\mu'\nu'}(X,X')\\&-\frac{1}{2}\mathcal{S}\left[\eta_{\mu\nu'}+\frac{1}{m^2}\frac{\partial}{\partial X^\mu\partial X^{\nu'}}\right]\mathcal{W}^P_{\mu'\nu}(X,X')\,.\end{aligned} \tag{4.29}$$

C. The quantum field

The explicit knowledge of $\mathcal{W}^\nu(x,x')$ allows us to make the QF formalism work. The tensor field $\mathcal{K}(x)$ is expected to be an operator-valued distributions on X_H acting on a Hilbert space $\mathcal{H}$. In terms of Hilbert space and field operator, the properties of the Wightman two-point functions are equivalent to the following conditions:[49]

(1) **Existence of an unitary irreducible representation of the dS group**

$$U=U^{2,\nu}, \quad (\text{and possibly} \quad V^{2,q}).$$

(2) **Existence of at least one "vacuum state"** Ω, cyclic for the polynomial algebra of field operators and invariant under the above representation of the dS group.

(3) **Existence of a Hilbert space** $\mathcal{H}$ with positive definite metric that can be described as the Hilbertian sum

$$\mathcal{H}=\mathcal{H}_0\oplus[\oplus_{n=1}^{\infty}\mathcal{SH}_1^{\otimes n}],$$

where $\mathcal{H}_0=\{\lambda\Omega, \quad \lambda\in\mathbb{C}\}$.

(4) **Covariance** of the field operators under the representation U,

$$U(g)\mathcal{K}_{\alpha\beta}(x)U(g^{-1})=g_{\alpha}^{\gamma}g_{\beta}^{\delta}\mathcal{K}_{\gamma\delta}(gx).$$

(5) **Locality** for every spacelike separated pair (x,x')

$$[\mathcal{K}_{\alpha\beta}(x),\mathcal{K}_{\alpha'\beta'}(x')]=0.$$

(6) **KMS condition or geodesic spectral condition**[46] which means the vacuum is defined as a physical state with the temperature $T=H/2\pi$.

(7) **Transversality**

$$x\cdot\mathcal{K}(x)=0.$$

(8) **Divergencelessness**

$$\partial\cdot\mathcal{K}(x)=0.$$

(9) **Index symmetrizer**

$$\mathcal{K}_{\alpha\beta}=\mathcal{K}_{\beta\alpha}.$$

Given the two-point function, one can realize the Hilbert space as functions on X_H as follows. For any test function $f_{\alpha\beta}\in\mathcal{D}(X_H)$, we define the vector valued distribution taking values in the space generated by the modes $\mathsf{K}_{\alpha\beta}(x,\xi)\equiv \mathrm{bv}\,\mathsf{K}_{\alpha\beta}(z,\xi)$ by

$$x\to p_{\alpha\beta}(f)(x)=\int_{X_H}\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')f^{\alpha'\beta'}(x')d\sigma(x')=\sum_{\lambda\lambda'}\int_{\gamma}d\sigma_{\gamma}(\xi)\mathsf{K}_{\xi}^{\lambda\lambda'}(f)\,\mathsf{K}_{\alpha\beta}^{\lambda\lambda'}(x,\xi), \tag{4.30}$$

where $\mathsf{K}_{\xi}^{\lambda\lambda'}(f)$ is the smeared form of the modes:

$$\mathsf{K}_{\xi}^{\lambda\lambda'}(f)=\int_{X_H}\mathsf{K}_{\alpha\beta}^{*\lambda\lambda'}(x,\xi)f^{\alpha\beta}(x)d\sigma(x). \tag{4.31}$$

The space generated by the $p(f)$'s is equipped with the positive invariant inner product

$$\langle p(f),p(g)\rangle=\int_{X_H\times X_H}f^{*\alpha\beta}(x)\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x')g^{\alpha'\beta'}(x')d\sigma(x')d\sigma(x). \tag{4.32}$$

As usual, the field is defined by the operator valued distribution

$$\mathcal{K}(f)=a(p(f))+a^{\dagger}(p(f)), \tag{4.33}$$

where the operators $a(\mathsf{K}^{\lambda\lambda'}(\xi))\equiv a^{\lambda\lambda'}(\xi)$ and $a^{\dagger}(\mathsf{K}^{\lambda\lambda'}(\xi))\equiv a^{\dagger\lambda\lambda'}(\xi)$ are respectively antilinear and linear in their arguments. One gets

$$\mathcal{K}(f)=\sum_{\lambda\lambda'}\int_{\gamma}d\sigma_{\gamma}(\xi)[\mathsf{K}_{\xi}^{*\lambda\lambda'}(f)\,a^{\lambda\lambda'}(\xi)+\mathsf{K}_{\xi}^{\lambda\lambda'}(f)\,a^{\dagger\lambda\lambda'}(\xi)]. \tag{4.34}$$

The unsmeared operator reads

$$\mathcal{K}_{\alpha\beta}(x)=\sum_{\lambda\lambda'}\int_{\gamma}d\sigma_{\gamma}(\xi)[\mathsf{K}_{\alpha\beta}^{\lambda\lambda'}(x,\xi)\,a^{\lambda\lambda'}(\xi)+\mathsf{K}_{\alpha\beta}^{*\lambda\lambda'}(x,\xi)\,a^{\dagger\lambda\lambda'}(\xi)], \tag{4.35}$$

where $a^{\lambda\lambda'}(\xi)$ satisfies the canonical commutation relations (ccr) and is defined by

$$a^{\lambda\lambda'}(\xi)|\Omega>=0.$$

The measure satisfies $d\sigma_{\gamma}(l\xi)=l^{3}d\sigma_{\gamma}(\xi)$ and $\mathsf{K}_{\alpha\beta}^{\lambda\lambda'}(x,l\xi)=l^{\sigma}\mathsf{K}_{\alpha\beta}^{\lambda\lambda'}(x,\xi)$ yields the homogeneity condition

$$a^{\lambda\lambda'}(l\xi)\equiv a(\mathsf{K}^{\lambda\lambda'}(l\xi))=a(l^{\sigma}\mathsf{K}^{\lambda\lambda'}(\xi))=l^{\sigma*}a^{\lambda\lambda'}(\xi).$$

The integral representation (4.35) is independent of the orbital basis γ as explained in Ref. 46. For the hyperbolic type submanifold γ_4 the measure is $d\sigma_{\gamma_4}(\xi)=d^{3}\vec{\xi}/\xi_0$ and the ccr are represented by

$$[a^{\lambda\lambda'}(\xi),a^{\dagger\lambda''\lambda'''}(\xi')]=[\eta^{\lambda\lambda''}\eta^{\lambda'\lambda'''}+\eta^{\lambda\lambda'}\eta^{\lambda''\lambda'''}]\xi^{0}\delta^{3}(\vec{\xi}-\vec{\xi}'). \tag{4.36}$$

The field commutation relations are

$$[\mathcal{K}_{\alpha\beta}(x),\mathcal{K}_{\alpha'\beta'}(x')]=2i\,\mathrm{Im}\langle p_{\alpha\beta}(x),p_{\alpha'\beta'}(x')\rangle=2i\,\mathrm{Im}\mathcal{W}_{\alpha\beta\alpha'\beta'}(x,x'). \tag{4.37}$$

V. CONCLUSION

In this article we have considered the ''massive'' spin-2 tensor field that is associated to the principal series of the dS group $\mathrm{SO}_0(1,4)$ with $\langle Q_{\nu}\rangle=\nu^{2}-\frac{15}{4}\geqslant 0$, and corresponding to the nonzero ''mass'' $m_p^{2}=H^{2}(\nu^{2}+\frac{9}{4})$. In our view, the use of the ''mass'' concept is more forced by tradition than relevant to our analysis. The use of ambient space formalism endowed the de Sitter physics with a Minkowskian-type appearance. The main differences hold in the space time dependence of the de Sitter polarization tensor. This formalism yields simple expressions and makes de Sitter QFT look almost like standard QFT in flat space–time.

The group theoretical point of view allows a systematic and complete study of the spin-2 field theory and legitimizes the restriction of ''massive'' fields to those which carry principal series representations. Indeed, in the case of the complementary series ($\langle Q_{\mu}\rangle=\mu-4,\quad 0<\mu<\frac{1}{4}$), although the associated ''mass'' $m_c^{2}=H^{2}(\mu+2),\quad 0<\mu<\frac{1}{4}$ is strictly positive, the physical meaning of their carrier fields remains unclear since the $H=0$ limits of these representations in the complementary series do not correspond to any physical representation of the Poincaré group.

Since m_p^{2} and m_c^{2} are strictly nonzero, ''massless'' spin-2 fields must belong to the discrete series among which only $\Pi_{s,s}^{\pm}$ have a physically meaningful Poincaré limit. Now since the associated ''mass'' is $m_d^{2}=H^{2}\{6-2(s^{2}-1)\},\quad s\geqslant 2$, and is expected to be real, the only possible value of s is 2 with $m_d^{2}=0$. Hence $\Pi_{2,2}^{\pm}$ correspond precisely to ''massless'' tensor fields (linear quantum gravity in dS space) in perfect agreement with the fact that, on one hand, these representations have nonambiguous extensions to the conformal group SO(4,2) and, on the other hand, the latter are precisely the unique extensions of the massless Poincaré group representations with helicity ± 2. In this case ν should be replaced by $\pm 3i/2$ in the formulas of the present article.[14] The projection operator $\mathcal{D}$ [Eq. (3.19) on the classical level] and the normalization constant c_{ν}^{2}

[Eq. (4.12) on the quantum level] then become singular. This singularity is actually due to the divergencelessness condition needed to associate the tensor field with a specific UIR of the dS group. To solve this problem, the divergencelessness condition must be dropped. Then the field equation becomes gauge invariant, i.e., $\mathcal{K}^{gt}=\mathcal{K}+D_2\Lambda_g$ is a solution of the field equation for any vector field Λ_g as far as $\mathcal{K}$ is. As a result, the general solutions transform under indecomposable representations of the dS group. By fixing the gauge, the field can eventually be quantized.

A second type of singularity appears. It is due to the zero mode problem of the Laplace–Beltrami operator on dS space inherited from the minimally coupled scalar field.[12] Accordingly, we feel that a Krein space quantization along the lines presented in Ref. 12 can be successfully carried out in the spin-2 massless case in dS space. This situation will be considered in a forthcoming paper.[10]

ACKNOWLEDGMENTS

We are grateful to U. Moschella, J. Renaud and S. Rouhani for helpful discussions and we thank S. Deser and A. Waldron for useful suggestions concerning references.

APPENDIX A: CLASSIFICATION OF THE UNITARY IRREDUCIBLE REPRESENTATIONS OF THE de SITTER GROUP $SO_0(1,4)$

Unitary irreducible representations (UIRs) of $SO_0(1,4)$ are characterized by the eigenvalues of the two Casimir operators $Q^{(1)}$ and $Q^{(2)}$ introduced in Sec. II. In fact the UIRs may be labeled by a pair of parameters $\Delta=(p,q)$ with $2p\in\mathbb{N}$ and $q\in\mathbb{C}$, in terms of which the eigenvalues of $Q^{(1)}$ and $Q^{(2)}$ are expressed as follows:[2,32,33]

$$Q^{(1)}=[-p(p+1)-(q+1)(q-2)]\mathbf{Id},\quad Q^{(2)}=[-p(p+1)q(q-1)]\mathbf{Id}.$$

According to the possible values for p and q, three series of inequivalent representations may be distinguished: the principal, complementary and discrete series. We write s when p or q have spin meaning.

(1) Principal series representations $U_{s,\nu}$, also called "massive" representations: $\Delta=(s,\frac{1}{2}+i\nu)$ with

$$s=0,1,2,\ldots\quad\text{and}\quad\nu\geqslant 0\quad\text{or}\quad s=\tfrac{1}{2},\tfrac{3}{2},\ldots\quad\text{and}\quad\nu>0.$$

The operators $Q^{(1)}$ and $Q^{(2)}$ take respectively the following forms:

$$Q^{(1)}=[(\tfrac{9}{4}+\nu^2)-s(s+1)]\,\mathbf{Id},\quad Q^{(2)}=[(\tfrac{1}{4}+\nu^2)s(s+1)]\,\mathbf{Id}.$$

They are called the massive representations of the dS group because they contract toward the massive spin s representations of the Poincaré group.

(2) Complementary series representations $V_{s,\nu}$: $\Delta=(s,\frac{1}{2}+\nu)$ with

$$s=0\quad\text{and}\quad\nu\in\mathbb{R}\ ,\ 0<|\nu|<\tfrac{3}{2}\quad\text{or}\quad s=1,2,3,\ldots\quad\text{and}\quad\nu\in\mathbb{R}\ ,0<|\nu|<\tfrac{1}{2}.$$

The operators $Q^{(1)}$ and $Q^{(2)}$ take the forms

$$Q^{(1)}=[(\tfrac{9}{4}-\nu^2)-s(s+1)]\,\mathbf{Id},\quad Q^{(2)}=[(\tfrac{1}{4}-\nu^2)s(s+1)]\,\mathbf{Id}.$$

Here, the only physical representation in the sense of the Poincaré limit is the scalar case corresponding to $\Delta=(0,1)$ and also called the conformally coupled massless case.

(3) Discrete series $\Pi_{p,0}$ and $\Pi^{\pm}_{p,q}$: $\Delta=(p,q)$ with

$$p=1,2,3,\ldots\quad\text{and}\quad q=0\quad\text{or}\quad p=\tfrac{1}{2},1,\tfrac{3}{2},2,\ldots\quad\text{and}\quad q=p,p-1,\ldots,1\ \text{or}\ \tfrac{1}{2}.$$

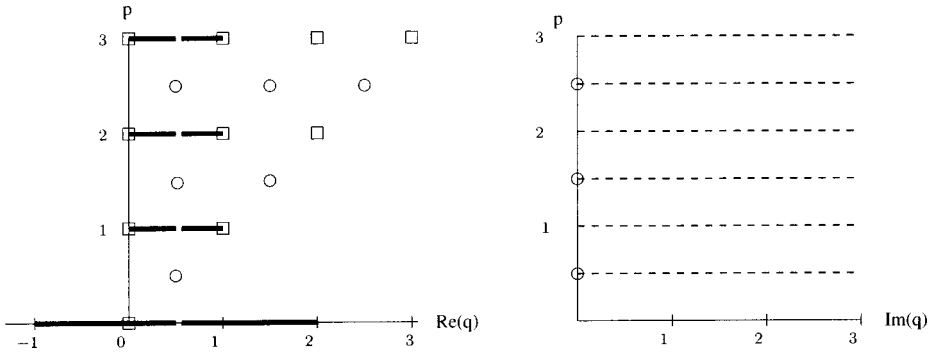

FIG. 2. $SO_0(1,4)$ unitary irreducible representation diagrams.

In this case, the only physical representations in the sense of Poincaré limit are those with $p=q=s$. They are called the massless representations of the dS group.

Note that the substitution $q\rightarrow(1-q)$ does not alter the eigenvalues; the representations with labels $\Delta=(p,q)$ and $\Delta=(p,1-q)$ can be shown to be equivalent. Finally, we have pictured some of these representations in terms of p and q in Fig. 2. The symbols ○ and □ stand for the discrete series with semi-integer and integer values of p, respectively. The complementary series is represented in the same frame by bold lines. The principal series is represented in the $\mathrm{Re}\,(q)=\frac{1}{2}$ plane by dashed lines. We have represented the three discrete series of representation with values $p=\frac{1}{2},\frac{3}{2},\frac{5}{2}$, $\mathrm{Re}\,(q)=\frac{1}{2}$ and $\mathrm{Im}\,(q)=0$ with the principal series in order to show how these two diagrams fit together.

APPENDIX B: MAXIMALLY SYMMETRIC BITENSORS IN AMBIENT SPACE

Following Allen and Jacobson in Ref. 34 we will write the two-point functions in de Sitter space (maximally symmetric) in terms of bitensors. These are functions of two points (x,x') which behave like tensors under coordinate transformations at either point. The bitensors are called maximally symmetric if they respect the de Sitter invariance.

As shown in Ref. 34, any maximally symmetric bitensor can be expressed as a sum of products of three basic tensors. The coefficients in this expansion are functions of the geodesic distance $\mu(x,x')$, that is the distance along the geodesic connecting the points x and x' [note that $\mu(x,x')$ can be defined by unique analytic extension also when no geodesic connects x and x']. In this sense, these fundamental tensors form a complete set. They can be obtained by differentiating the geodesic distance:

$$n_a=\nabla_a\mu(x,x'),\quad n_{a'}=\nabla_{a'}\mu(x,x'),$$

and the parallel propagator

$$g_{ab'}=-c^{-1}(\mathcal{Z})\nabla_a n_{b'}+n_a n_{b'}.$$

The geodesic distance is implicitly defined[46] for $\mathcal{Z}=-H^2x\cdot x'$ by

$$\mathcal{Z}=\cosh(\mu H)\quad \text{for } x \text{ and } y \text{ timelike separated,}$$

$$\mathcal{Z}=\cos(\mu H)\quad \text{for } x \text{ and } y \text{ spacelike separated such that } |x\cdot x'|<H^{-2}.$$

The basic bitensors in ambient space notations are found through

$$\overline{\partial}_\alpha\mu(x,x'),\quad \overline{\partial}'_{\beta'}\mu(x,x'),\quad \overline{\partial}_\alpha\overline{\partial}'_{\beta'}\mu(x,x'),$$

restricted to the hyperboloid by

$$T_{ab'}(x,x')=\frac{\partial x^{\alpha}}{\partial X^{a}}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}T_{\alpha\beta'}\quad .$$

For $\mathcal{Z}=\cos(\mu H)$, one finds

$$n_a=\frac{\partial x^{\alpha}}{\partial X^{a}}\overline{\partial}_{\alpha}\mu(x,x')=\frac{\partial x^{\alpha}}{\partial X^{a}}\ \frac{H(\theta_{\alpha}\cdot x')}{\sqrt{1-\mathcal{Z}^2}},\quad n_b=\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\overline{\partial}'_{\beta'}\mu(x,x')=\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\ \frac{H(\theta'_{\beta'}\cdot x)}{\sqrt{1-\mathcal{Z}^2}},$$

and

$$\nabla_a n_{b'}=\frac{\partial x^{\alpha}}{\partial X^{a}}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\theta^{\sigma}_{\alpha}\theta'^{\gamma'}_{\beta'}\overline{\partial}_{\sigma}\overline{\partial}'_{\gamma'}\mu(x,x')=c(\mathcal{Z})\left[\mathcal{Z}n_a n_{b'}-\frac{\partial x^{\alpha}}{\partial X^{a}}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\theta_{\alpha}\cdot\theta'_{\beta'}\right],$$

with $c(\mathcal{Z})=-H/\sqrt{1-\mathcal{Z}^2}$. For $\mathcal{Z}=\cosh(\mu H)$, n_a, $n_{b'}$ are multiplied by i and $c(\mathcal{Z})$ becomes $-iH/\sqrt{1-\mathcal{Z}^2}$. In both cases we have

$$\frac{\partial x^{\alpha}}{\partial X^{a}}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\theta_{\alpha}\cdot\theta'_{\beta'}=g_{ab'}+(\mathcal{Z}-1)n_a n_{b'}.$$

APPENDIX C: "MASSIVE" VECTOR TWO-POINT FUNCTION

Given the important role played by the "massive" vector Wightman two-point function in the construction of the spin-2 two-point function we briefly present here a derivation of it (for details see Ref. 1). In addition we compare our two-point function with the one given in Ref. 34. We consider the "massive" vector Wightman two-point function which corresponds to the principal series of representation of $SO_0(1,4)$ and satisfies

$$(Q_1-\langle Q_1\rangle)\mathcal{W}^{\nu}_{1\alpha\beta'}(x,x')=0,\quad \text{where}\quad \langle Q_1\rangle=\nu^2+\tfrac{1}{4}\quad \text{with}\quad \nu\in\mathbb{R}.$$

This bivector is obtained as the boundary value of the analytic bivector two-point function obtained with the modes (3.13):

$$W^{\nu}_{1\alpha\beta'}(z,z')=c_{\nu}^2\frac{\langle Q_1\rangle}{\langle Q_0\rangle}\int_{\gamma}\sum_{\lambda}\mathcal{E}^{\lambda}_{\alpha}(z,\xi)\,\mathcal{E}^{*\lambda}_{\beta'}(z'^{*},\xi)(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}\,d\sigma_{\gamma}(\xi).$$

With the help of Eq. (4.16) and the relation $H^2D_1(Hz\cdot\xi)^{\sigma}=\sigma\overline{\xi}(Hz\cdot\xi)^{\sigma}/(z\cdot\xi)$ it is easy to expand the transverse bivector in terms of the analytic scalar two-point function $W_0(z,z')$:

$$W^{\nu}_{1}(z,z')=\frac{\langle Q_0\rangle}{\langle Q_1\rangle}\left(-\theta_{\alpha}\cdot\theta'_{\alpha'}+\frac{H^2\sigma(\theta\cdot z')D'_1}{\langle Q_0\rangle}+\frac{H^2\sigma^*(\theta'\cdot z)D_1}{\langle Q_0\rangle}+\frac{H^2\mathcal{Z}D_1D'_1}{\langle Q_0\rangle}\right)W^{\nu}_{0}(z,z').$$

The analytic "massive " scalar two-point function is

$$W^{\nu}_{0}(z,z')=c_{\nu}^2\int_{\gamma}(Hz\cdot\xi)^{\sigma}(Hz'\cdot\xi)^{\sigma^*}\,d\sigma_{\gamma}(\xi)\quad \text{with}\quad c_{\nu}^2=H^2e^{+\pi\nu}\Gamma(-\sigma)\Gamma(-\sigma^*)/(2^5\pi^4m^2),$$

which satisfies

$$(Q_0-\langle Q_0\rangle)W^{\nu}_{0}(z,z')=0,\quad \text{where}\quad \langle Q_0\rangle=\nu^2+\tfrac{9}{4}\quad \text{with}\quad \nu\in\mathbb{R}.$$

The choice of normalization corresponds to the Euclidean vacuum and $W_0(z,z')$ can be written as a hypergeometric function (see Ref. 46):

$$W_0^{\nu}(z,z')=C_{\nu}\ {}_2F_1\left(-\sigma,-\sigma^*;2;\frac{1+\mathcal{Z}}{2}\right)=C_{\nu}P_{\sigma}^{5}(-\mathcal{Z}) \qquad \text{with} \quad C_{\nu}=\frac{H^2\Gamma(-\sigma)\ \ \Gamma(-\sigma^*)}{2^4\pi^2m^2}.$$

In order to show that our vector two-point function is the same two-point function as the one given by Allen and Jacobson in Ref. 34, we develop $W_1^{\nu}(z,z')$ using essentially $\bar{\partial}_{\alpha}\phi(\mathcal{Z})=-(\theta_{\alpha}\cdot z')H^2\,(d/d\mathcal{Z})\,\phi(\mathcal{Z})$. One finds

$$\mathcal{W}_{1\alpha\beta'}^{\nu}(x,x')=\mathrm{bv}\,W_1^{\nu}(z,z')=\theta_{\alpha}\cdot\theta'_{\beta'}U(\mathcal{Z})+H^2\frac{(\theta'_{\beta'}\cdot z)(\theta_{\alpha}\cdot z')}{1-\mathcal{Z}^2}V(\mathcal{Z}),$$

with

$$U(\mathcal{Z})=-\frac{1}{\langle Q_1\rangle}\left[Q_0+\mathcal{Z}\frac{d}{d\mathcal{Z}}\ \right]W_0^{\nu}(z,z')\ \ ,\quad V(\mathcal{Z})=\frac{1}{\langle Q_1\rangle}\left[3\frac{d}{d\mathcal{Z}}+\mathcal{Z}^2\frac{d}{d\mathcal{Z}}+\mathcal{Z}Q_0\right]W_0^{\nu}(z,z'),$$

where

$$Q_0=(1-\mathcal{Z}^2)\frac{d^2}{d\mathcal{Z}^2}-4\mathcal{Z}\frac{d}{d\mathcal{Z}}$$

is the second order differential operator deduced from the Casimir operator expressed with the variable $\mathcal{Z}$ in place of (z,z'). The functions $U(\mathcal{Z})$ and $V(\mathcal{Z})$ satisfy the property

$$\mathcal{Z}U(\mathcal{Z})+V(\mathcal{Z})=\frac{3}{\langle Q_1\rangle}\frac{d}{d\mathcal{Z}}W_0^{\nu}(z,z')\equiv\Lambda(\mathcal{Z}),$$

with

$$\Lambda(\mathcal{Z})=3H^2\frac{\Gamma(1-\sigma)\ \ \Gamma(1-\sigma^*)}{2^6\langle Q_1\rangle\pi^2m^2}\,{}_2F_1\left(1-\sigma,1-\sigma^*;3;\frac{1+\mathcal{Z}}{2}\right),$$

which is the solution of the equation

$$\left[Q_0-2\mathcal{Z}\frac{d}{d\mathcal{Z}}-6-\langle Q_1\rangle\right]\Lambda(\mathcal{Z})=0.$$

Finally, let us write the intrinsic expression of the two-point function $\mathcal{W}_1^{\nu}(x,x')$ obtained as the boundary value of $W_1^{\nu}(z,z')$. The intrinsic expression is

$$Q_{ab'}\equiv\frac{\partial x^{\alpha}}{\partial X^a}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\ \ \mathcal{W}_{1\alpha\beta'}^{\nu}(x,x').$$

Since

$$\frac{\partial x^{\alpha}}{\partial X^a}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\theta_{\alpha}\cdot\theta'_{\beta'}=g_{ab'}+(\mathcal{Z}-1)n_an_{b'}\,,\quad \frac{\partial x^{\alpha}}{\partial X^a}\frac{\partial x'^{\beta'}}{\partial X'^{b'}}\ \ \frac{H^2(\theta'_{\beta'}\cdot x)(\theta_{\alpha}\cdot x')}{1-\mathcal{Z}^2}=n_an_{b'}\,,$$

one gets

$$Q_{ab}=g_{ab'}U(\mathcal{Z})+n_a\,n_{b'}(\Lambda(\mathcal{Z})-U(\mathcal{Z})),$$

and in the case of $SO_0(4,1)$:

$$Q_{ab} = -g_{ab'}U(\mathcal{Z}) - n_a n_{b'}(U(\mathcal{Z}) - \Lambda(\mathcal{Z})).$$

This is the expression given by Allen and Jacobson in Refs. 20 and 34.

APPENDIX D: ANOTHER EXPRESSION FOR THE SPIN-2 TWO-POINT FUNCTION

We present another form of the spin-2 two-point function, which is useful for the proof of the locality condition. We begin with the term $M(z,z')W_1^\nu(z,z')$:

$$\frac{\langle Q_0\rangle + 4}{\langle Q_0\rangle}\left[-\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' + \frac{H^2\mathcal{S}(\theta\cdot z')D_2'}{\sigma^*-1} + \frac{H^2\mathcal{S}'(\theta'\cdot z)D_2}{\sigma-1} + \frac{\mathcal{Z}H^2D_2D_2'}{(\sigma-1)(\sigma^*-1)}\right]W_1^\nu(z,z').$$

We rewrite this equation using the relations

$$H^2\mathcal{S}(\theta\cdot z')D_2'W_1^\nu = -\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + 2\,\theta'\mathcal{S}\theta\cdot W_1^\nu + \tfrac{1}{2}D_2D_2'W_2,$$

$$H^2\mathcal{S}'(\theta'\cdot z)D_2W_1^\nu = -\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + 2\,\theta\mathcal{S}'\,\theta'\cdot W_1^\nu + \tfrac{1}{2}D_2D_2'W_2,$$

$$H^2\mathcal{Z}D_2D_2'W_1^\nu = -\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + 2\,\theta\mathcal{S}'\,\theta'\cdot W_1^\nu + 2\,\theta'\mathcal{S}\theta\cdot W_1^\nu + D_2D_2'(W_2 + H^2\mathcal{Z}W_1^\nu),$$

where $D_2D_2'W_2 = 2H^2D_2\mathcal{S}'(\theta'\cdot z)W_1 - 4\,\theta\mathcal{S}'\,\theta'\cdot W_1$. This is obtained by simple calculation of

$$(Q_2 - \langle Q_2\rangle)(\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + D_2D_2'W_3) = 0,$$

with the help of Eq. (3.3) and where we have written $W_2 = (Q_1 - \langle Q_2\rangle)W_3$. One gets

$$M(z,z')W_1^\nu(z,z') = -\mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + \frac{2\,\theta\sigma^*\mathcal{S}'\,\theta'\cdot W_1^\nu}{\langle Q_0\rangle} + \frac{2\,\theta'\sigma\mathcal{S}\theta\cdot W_1^\nu}{\langle Q_0\rangle} + D_2D_2'\left(\frac{H^2\mathcal{Z}W_1^\nu}{\langle Q_0\rangle} - \frac{3W_2}{2\langle Q_0\rangle}\right).$$

Now, given that

$$\mathcal{S}\theta\cdot W_1^\nu = \frac{2}{3}\left[\theta + \frac{H^2D_2D_1}{2\langle Q_0\rangle}\right](W_1^\nu)' \quad \text{and} \quad \mathcal{S}'\,\theta'\cdot W_1^\nu = \frac{2}{3}\left[\theta' + \frac{H^2D_2'D_1'}{2\langle Q_0\rangle}\right](W_1^\nu)',$$

where $(W_1^\nu)'$ is the trace of the vector two-point function given by

$$(W_1^\nu)' = \eta\cdot\cdot\, W_1^\nu = 3U(\mathcal{Z}) + \mathcal{Z}\Lambda(\mathcal{Z}) = -3\frac{\langle Q_0\rangle}{\langle Q_1\rangle}W_0^\nu(z,z'),$$

we find the following form for the spin-2 two-point function:

$$\begin{aligned} W^\nu(z,z') &= M(z,z')W_1^\nu(z,z') + N(z,z')W_0^\nu(z,z') \\ &= q[\,\theta\theta'(W_1^\nu)' - \tfrac{3}{2}\,\theta\mathcal{S}'\,\theta'\cdot W_1^\nu - \tfrac{3}{2}\,\theta'\mathcal{S}\theta\cdot W_1^\nu] - \mathcal{S}\mathcal{S}'\,\theta\cdot\theta' W_1^\nu + D_2D_2'W_4, \end{aligned}$$

where $q = -\frac{4}{9}(\langle Q_0\rangle - 9)/\langle Q_0\rangle$ and

$$D_2D_2'W_4 = \frac{6\,\theta\mathcal{S}'\,\theta'\cdot W_1^\nu}{\langle Q_0\rangle} - \frac{3H^2D_2\mathcal{S}'(\theta'\cdot z)W_1^\nu}{\langle Q_0\rangle} + D_2D_2'\left(\frac{H^2\mathcal{Z}W_1^\nu}{\langle Q_0\rangle} + \frac{H^4D_1D_1'(W_1^\nu)'}{9\langle Q_0\rangle^2}\right).$$

The two-point function can be rewritten as

$$W^{\nu}(z,z')=D(z,z')W_0^{\nu}(z,z'),$$

where the differential operator $D(z,z')$ obviously satisfies $D^*(z^*,z'^*)=D(z,z')$. This property serves to prove the locality condition.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Improved Epstein–Glaser renormalization. II. Lorentz invariant framework

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(Received 9 January 2003; accepted 22 April 2003)

The Epstein–Glaser type T-subtraction introduced by one of the authors in a previous paper is extended to the Lorentz invariant framework. The advantage of using our subtraction instead of the Epstein and Glaser standard W-subtraction method is especially important when working in Minkowski space, as then the counterterms necessary to keep Lorentz invariance are simplified. We show how T-renormalization of primitive diagrams in the Lorentz invariant framework directly relates to causal Riesz distributions. A covariant subtraction rule in momentum space is found, sharply improving upon the BPHZL method for massless theories. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1597420]

I. INTRODUCTION

According to the spirit of Epstein–Glaser theory,[1] the physical process of renormalization is mathematically expressed as an extension of functionals, v.gr. (convolutions of) powers of Feynman propagators, to well defined distributions. This paper is a continuation of Ref. 2 by the second named author, in which an extension on configuration space was presented. By modifying the use of, and relaxing the conditions on, the infrared regulators w introduced by Epstein and Glaser, very useful results on the distributions at the crossroads of mathematics and quantum field theory have been obtained; the relationship of this improved Epstein–Glaser subtraction, dubbed ''T-renormalization,'' with Hadamard regularization, the minimal subtraction scheme in analytical regularization, and differential renormalization, has been treated there at length. Hereinafter that paper[2] will be denoted by Paper I.

The discussion in Paper I took place in the Euclidean framework introduced by Stora[3] in the realm of the Epstein–Glaser construction. We tackle in this paper the problem of going to the ''physical world'' with its symmetry group of transformations, namely the Minkowski space and the Lorentz group, respectively.

The Lorentz covariance properties of extensions for powers of propagators are deeply related to the S-matrix covariance. Prima facie, Epstein–Glaser procedures are not covariant. A proof of existence of covariant time ordered products was first given in Ref. 1, working on momentum space. About 10 years later, the problem was translated into a group cohomological question on configuration space by Popineau and Stora in Ref. 4—another work which has remained at the status of preprint. The latter analysis is available in textbook form.[5] In relatively recent (also apparently unpublished) preprints,[6,7] explicit computations for ''counterterms'' re-establishing Lorentz invariance of the extensions have been performed.

A perfectly covariant method for the extension of distributions employed in quantum field theory exists, although it is rarely used: the ''analytical regularization'' method[8] of Bollini, Giam-

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biagi, and Gonzales Domínguez. It leads to quantum versions of the Riesz distributions of classical field theory.[9–11]

In this paper we extend T-renormalization of primitive diagrams to the Lorentz-invariant framework, and show that it generalizes directly the causal or quantum Riesz distributions.

The proof that all difficulties in renormalization theory can be overcome through exclusive use of the T operation is work in progress; the third paper of the series[12]—from now on denoted Paper III—deals with renormalization of nonprimitive diagrams and the Hopf algebra of Feynman graphs.[13–15] It is of course not claimed that the simplicity of the class of extensions envisaged in this work guarantees that it is the physically relevant one in all circumstances; as a rule, the latter will be singled out by appropriate renormalization prescriptions.

We do not suppose the reader to be familiar with causal Riesz distributions. Thus we turn to them in Sec. III, after recalling the main properties of our ''natural'' extension method in Sec. II. The covariance properties of T-renormalization are then addressed in Sec. IV. To fix ideas, we mainly consider in Sec. V the basic primitively divergent graphs in massless φ_4^4 theory, and demonstrate by way of example the link to analytical regularization and causal Riesz distributions. Section VI shows how T-renormalization improves upon the BPHZL formalism. We conclude with a brief discussion and outlook.

II. MAIN FEATURES OF *T*-RENORMALIZATION

Let us begin by fixing some conventions. The scalar functionals we shall be dealing with (coming from the Wick theorem) are to be extended to the main diagonal of $\mathbb{R}^{4(n+1)}$. The latter can be regarded as the origin in $\mathbb{R}^{4n}$ thanks to translation invariance, allowing to set $x_{n+1}=0$, for instance.

For fixed $j\in\{1,\ldots,n\}$, to each four coordinate x_j (a point in $\mathbb{R}^4$) let $\alpha^j=(\alpha_0^j,\alpha_1^j,\alpha_2^j,\alpha_3^j)$ be a quadri-index, where α_μ^j is a non-negative integer for each j and each Lorentz index μ. One has, according to Schwartz's notation,[16] $\alpha^j!=\alpha_0^j!\,\alpha_1^j!\,\alpha_2^j!\,\alpha_3^j!$ and $|\alpha^j|=\alpha_0^j+\alpha_1^j+\alpha_2^j+\alpha_3^j$, as well as

$$x_j^{\alpha^j}:=\prod_{\mu=0}^{3}(x_j^\mu)^{\alpha_\mu^j},\quad \partial_{\alpha^j}:=\left(\frac{\partial}{\partial x_j}\right)^{\alpha^j}=\prod_{\mu=0}^{3}\left(\frac{\partial}{\partial x_j^\mu}\right)^{\alpha_\mu^j}=:\prod_{\mu=0}^{3}(\partial_\mu^j)^{\alpha_\mu^j}.$$

We also use a multiquadri-index $\alpha=(\alpha_\mu^j)$ notation: $\alpha!=\alpha^1!\,\alpha^2!\cdots\alpha^n!$ and $|\alpha|=|\alpha^1|+|\alpha^2|+\cdots+|\alpha^n|$, as well as

$$x^\alpha:=\prod_{j=1}^{n}x_j^{\alpha^j},\quad \partial_\alpha:=\prod_{j=1}^{n}\partial_{\alpha^j}.$$

We assume that the reader is familiar with the basic concepts of distribution theory. In this paper, operators (Fourier transforms, actions of the Lorentz group, subtractions, ...) are defined on distributions always by transposition (or adjoint mapping), and we denote them by the *same* letter denoting the original action on test functions.

Consider scalar functionals $f(x_j)$ defined on $M_4^{n+1}\setminus D_{n+1}$, where $D_{n+1}:=\{x_1=\cdots=x_{n+1}\}$ is the full diagonal; thus we assume that the diagram is primitive or that Bogoliubov's[17] disentangling operation $\overline{R}$ corresponding to all subgraphs (see Paper III) has been performed. Those will be considered as functionals of the difference variables in $\mathbb{R}^{4n}\setminus\{0\}$. A tempered distribution $\tilde{f}\in\mathcal{S}'(\mathbb{R}^{4n})$ is an *extension* or *renormalization* of f if

$$\tilde{f}[\phi]\equiv\langle\tilde{f},\phi\rangle=\int_{\mathbb{R}^{4n}}f(x)\,\phi(x)\,\mathrm{d}^{4n}x$$

holds whenever ϕ belongs to $\mathcal{S}(\mathbb{R}^{4n}\setminus\{0\})$. In QFT one considers a generalized homogeneity degree, the *scaling degree*.[18] The scaling degree σ of a scalar distribution f at the origin of $\mathbb{R}^d$ is defined to be

$$\sigma(f)=\inf\{\, s:\lim_{\lambda\to 0}\lambda^s f(\lambda x)=0\,\}\quad \text{for } f\in\mathcal{S}'(\mathbb{R}^{4n}),$$

where the limit is taken in the sense of distributions. Essentially this means that $f(x)=O(|x|^{-\sigma(f)})$ as $x\to 0$ in the Cesàro or distributional average sense.[19]

Let then $\sigma(f)=a$, with a an integer, and $k=a-4n\geqslant 0$. Then, $f\notin L^1_{\mathrm{loc}}(\mathbb{R}^{4n})$. The simplest way to get an extension of f would appear to be standard Taylor series surgery: throw away the k-jet $j_0^k\phi$ of ϕ at the origin, and define $\tilde{f}$ by transposition:

$$\langle\tilde{f},\phi\rangle=\langle R_0^k f,\phi\rangle:=\langle f,R_0^k\phi\rangle,$$

where $R_0^k\phi:=\phi-j_0^k\phi$ is the Taylor remainder. Using Lagrange's integral formula for R_0^k, and exchanging integrations, one appears to obtain an explicit integral formula for $R_0^k f$:

$$R_0^k f(x)\equiv T_1 f(x):=(-)^{k+1}(k+1)\sum_{|\beta|=k+1}\partial_\beta\left[\frac{x^\beta}{\beta!}\int_0^1 dt\,\frac{(1-t)^k}{t^{k+4n+1}}f\left(\frac{x}{t}\right)\right]. \tag{1}$$

The trouble with (1) is that the remainder $R_0^k\phi$ is not a test function and therefore, unless the infrared behavior of f is good, we can end up with an undefined integral. Actually, for the needs of theories with only massive fields, formula (1) is largely sufficient. However in theories with massless particles, f is typically an homogeneous function with an algebraic singularity, the infrared behavior is pretty bad, and $-4n$ is also the critical degree. A way to avoid the problem is to *weigh* the Taylor subtraction. Epstein and Glaser[1] introduced infrared regulators w with the properties $w(0)=1$ and $w^{(\alpha)}(0)=0$ for $0<|\alpha|\leqslant k$, as well as projector maps $\phi\mapsto W_w\phi$ on $\mathcal{S}(\mathbb{R}^d)$ given by

$$W_w\phi(x):=\phi(x)-w(x)j_0^k\phi(x). \tag{2}$$

There is a considerable amount of overkill in (2). We argued in Paper I that one can, and should, weigh only the *last* term of the Taylor expansion. This leads to the definition used in this paper, at variance with Epstein and Glaser:

$$T_w\phi(x):=\phi(x)-j_0^{k-1}(\phi)(x)-w(x)\sum_{|\alpha|=k}\frac{x^\alpha}{\alpha!}\phi^{(\alpha)}(0). \tag{3}$$

Just $w(0)=1$ is now required in principle for the weight function. T_w is also a projector. To obtain an integral formula for it, start from

$$T_w\phi=(1-w)R_0^{k-1}\phi+wR_0^k\phi.$$

By transposition, using (1), we derive

$$\begin{aligned}T_w f(x)=&(-)^k k\sum_{|\alpha|=k}\partial_\alpha\left[\frac{x^\alpha}{\alpha!}\int_0^1 dt\,\frac{(1-t)^{k-1}}{t^{k+d}}f\left(\frac{x}{t}\right)\left(1-w\left(\frac{x}{t}\right)\right)\right]\\&+(-)^{k+1}(k+1)\sum_{|\beta|=k+1}\partial_\beta\left[\frac{x^\beta}{\beta!}\int_0^1 dt\,\frac{(1-t)^k}{t^{k+d+1}}f\left(\frac{x}{t}\right)w\left(\frac{x}{t}\right)\right].\end{aligned} \tag{4}$$

Consider the functional variation of the renormalized amplitudes with respect to w. One has

$$\left\langle\frac{\delta}{\delta w}T_w f,\psi\right\rangle:=\frac{d}{d\lambda}T_{w+\lambda\psi}f\Big|_{\lambda=0}.$$

Equation (3) yields

$$\frac{\delta}{\delta w} T_w f[\cdot] = (-)^{k+1} \sum_{|\alpha|=k} f[x^\alpha \cdot] \frac{\partial_\alpha \delta}{\alpha!}, \tag{5}$$

independently of w. The combination $(-)^{|\alpha|}/\alpha!\ \partial_\alpha \delta$ is rebaptized δ_α. A central fact of renormalization theory, under its distributional guise, is that there is no unique way to construct the renormalized amplitudes, the inherent ambiguity being represented by the undetermined coefficients of the δ and its derivatives, describing how the chosen extension acts on the (finite codimension) space of test functions which do *not* vanish to some order in a neighborhood of 0. There is, however, a more natural way—in which the ambiguity is reduced to terms in the higher-order derivatives of δ, as seen in (5), exclusively. This is guaranteed by our choice of T_w.

A word on the space of infrared regulators w is in order. In Paper I it was shown that, for the extension of homogeneous f of the kind found in massless field models, any element of the space $\mathcal{K}'$ (dual of the Grossmann–Loupias–Stein function space) of distributions rapidly decreasing in the Cesàro sense,[20] taking the value 1 at zero, qualifies as a weight "function." The space $\mathcal{K}'$ is a kind of distributional analogue of the Schwartz space $\mathcal{S}$. Elements of $\mathcal{K}'$ have moments of all orders. In particular, exponential functions e^{iqx} do qualify; this was realized by Prange, at the heuristical level.[21] See the consequences in Sec. VI. The usefulness of $\mathcal{K}'$ has appeared by now in many different contexts.[22] The regulator $w(\mu x) = H(1-\mu|x|)$ of Paper I, with H the Heaviside function, will be mainly used here. Call T_μ the corresponding renormalization.

The results just summarized go a long way to justify the conjecture (made by Connes and independently by Estrada) that Hadamard's finite part theory is in principle enough to deal with quantum field theory divergences. At least in the Euclidean context. When going from there to the physical signature for the space–time, both the ultraviolet and the infrared problems immediately turn nastier, in a tangled sort of way. For the first, since the singular support of the Feynman propagator lies on the whole light cone, it would appear that we have to worry about singularities supported on the entire cone, and not just at the origin. For the second, it is easy to see that if we approach infinity in directions parallel to the light cone, the Feynman propagator decays as $1/|x|$ and not "naïvely" anymore as $1/|x|^2$.

Both kinds of trouble are a bit less ferocious than they seem. There are techniques for dealing with the worsened infrared problem, conjuring at need combinations of diagrams.[23] Microlocal analysis (Ref. 24, Sec. 8.2) can be invoked[25] to argue that the ultraviolet troubles remain concentrated at the origin, just as in the Euclidean case. In the next section, we show the same for the square and the cube of the Feynman propagator (i.e., the basic four-point and two-point divergent graphs in the φ_4^4 model), by a direct calculation.

Whereas T_1 of (1) ostensibly preserves the Lorentz covariance properties of f, the operator T_w of (4) in general does not. Our main task is to fix this problem.

III. CAUSAL RIESZ DISTRIBUTIONS

Riesz's method consists in generalizing to the Lorentz-invariant context the well-known holomorphic family of distributions on $\mathbb{R}$,

$$\Phi^\lambda(x) := \frac{x_+^{\lambda-1}}{\Gamma(\lambda)}$$

for complex λ, which have the properties

$$\Phi^\lambda * \Phi^\mu = \Phi^{\lambda+\mu}, \quad \frac{d\Phi^\lambda}{dx} = \Phi^{\lambda-1}, \quad \Phi^0(x) = \delta(x),$$

where $*$ denotes convolution of distributions. In fact, Riesz only dealt with the (advanced and) retarded propagators. He was able to show that the holomorphic family of distributions G_{ret}^λ defined on $\mathbb{R}^4$ as follows:

$$G^{\lambda}_{\mathrm{ret}}(x)=C_{\lambda}\,x_{+}^{2(\lambda-2)},$$

with x_{+}^{2} equal to $t^2-|\vec{x}|^2=t^2-r^2$ on the forward light cone and to 0 anywhere else, and

$$C_{\lambda}=\frac{1}{2^{2\lambda-1}\pi\,\Gamma(\lambda)\Gamma(\lambda-1)},$$

fulfills

$$G^{\lambda}_{\mathrm{ret}}*G^{\mu}_{\mathrm{ret}}=G^{\lambda+\mu}_{\mathrm{ret}},\quad \Box G^{\lambda}_{\mathrm{ret}}=G^{\lambda-1}_{\mathrm{ret}},\quad G^{0}_{\mathrm{ret}}=\delta.$$

In particular, $x_{+}^{2(\lambda-2)}$ is at once seen to have (generally double) poles with residues concentrated at the origin as the only singularities. The $G^{\lambda}_{\mathrm{ret}}$ constitute a set of convolution inverse powers of the d'Alembertian, verifying $\Box^{\lambda}G^{\lambda}_{\mathrm{ret}}=\delta(x)$.

In quantum field theory, as stressed in Ref. 8, the relevant set of inverse powers is related to the Feynman propagator

$$D_F(x)=\frac{-i}{4\pi^2(t^2-r^2-i\epsilon)}.$$

We therefore focus on $(t^2-r^2\pm i\epsilon)^{\alpha-2}$, with poles at $\alpha=0,-1,\ldots$, with the aim of studying the renormalization by analytic regularization in the variable α of the functionals $(t^2-r^2\pm i\epsilon)^{-2}$, $(t^2-r^2\pm i\epsilon)^{-3}$, and so on, ill-defined as distributions. For a start, we need to compute the residues at the poles.

It is instructive and convenient for the purpose of looking at the spirit of analytic regularization at the Euclidean $\mathbb{R}^4$ first, in a somewhat unconventional manner. Consider $\rho^2:=|x|^2=t^2+r^2$. The singularities of ρ^{α} are well known (see Paper I): simple poles in the regularizing variable α at $-4-2k$, for $k=0,1,\ldots$, with residues

$$\operatorname*{Res}_{\alpha=-4-2k}\rho^{\alpha}=\frac{\Omega_4\,\Delta^k\delta}{2^k k!\;4.6.8\cdots(2+2k)},\tag{6}$$

the denominator in the case $k=0$ being 1; here $\Omega_4=2\pi^2$ is the area of the sphere in dimension 4, and Δ the Laplacian in dimension 4. It is possible, and usually done, to define a holomorphic family of distributions that encodes the pole structure of ρ^{α} in the same way that Φ^{λ} encodes that of x_{+}^{λ}. However, we consider instead the following *meromorphic* family:

$$G^{\alpha}_{\mathrm{eucl}}(x)=C_{\alpha}\,\rho^{2(\alpha-2)},$$

with

$$C_{\alpha}=\frac{e^{-i\pi\alpha}\Gamma(2-\alpha)}{4^{\alpha}\pi^2\Gamma(\alpha)}.$$

Notice that G^{1}_{eucl} is the Green function for the Laplace equation on $\mathbb{R}^4$; that $\Delta G^{\alpha}_{\mathrm{eucl}}=G^{\alpha-1}_{\mathrm{eucl}}$, which is quickly seen from $\Delta\rho^{\mu}=\mu(\mu+2)\rho^{\mu-2}$; and that $G^{-m}_{\mathrm{eucl}}(x)=\Delta^m\delta(x)$; the latter of course is just another way of writing (6).

It is also true that $G^{\alpha}_{\mathrm{eucl}}*G^{\beta}_{\mathrm{eucl}}=G^{\alpha+\beta}_{\mathrm{eucl}}$. For that, define the Fourier transforms on test functions by

$$F[\phi](p)\equiv\hat{\phi}(p):=\int\frac{\mathrm{d}^4x}{(2\pi)^2}\,e^{-ipx}\phi(x),\quad F^{-1}[\phi](p)\equiv\check{\phi}(p):=\int\frac{\mathrm{d}^4x}{(2\pi)^2}\,e^{ipx}\phi(x),$$

and on distributions by transposition. Then $Ff\,Fg=(2\pi)^{-2}F(f*g)$ for convolvable distributions. It turns out (Ref. 26, Theorem 5.9) that

$$\hat{G}^{\alpha}_{\mathrm{eucl}}(p)=(2\pi)^{-2}e^{-i\pi\alpha}|p|^{-2\alpha}, \tag{7}$$

a most interesting duality. From this the convolution identity follows.

Now we obtain the poles of $(x^2\pm i\epsilon)^{\alpha}$ from the poles of $\rho^{2\alpha}$. We follow Gelfand and Shilov (Ref. 27, Chap. III, Secs. 2.3 and 2.4) in this. Consider the quadratic forms $g_{\pm}(x):=\pm i\rho^2$. Then $g^{\alpha}_{\pm}=e^{\pm i\pi\alpha/2}\rho^{2\alpha}$. Rewrite equation (6) as

$$\operatorname*{Res}_{\alpha=-2-l} g^{\alpha}_{\pm}=\frac{-\pi^2\,\Delta^{l}_{g_{\pm}}\delta}{4^l l!(l+1)!\sqrt{(\mp i)^4\det g_{\pm}}},$$

with $\Delta_{g_{\pm}}$ the Laplacian canonically associated to $g_{\pm}$, which is $\mp i\Delta$ on this occasion. To be precise, if $\tilde{g}^{ij}$ is the inverse matrix of the quadratic form g, then

$$\Delta_g:=\sum_{i,j}\tilde{g}^{ij}\,\partial_i\,\partial_j\,.$$

For the forms $g(x)=t^2-r^2\pm i\epsilon(t^2+r^2)$, we find then by analytic continuation:

$$\operatorname*{Res}_{\alpha=-2-l}(x^2\pm i\epsilon)^{\alpha}=\frac{\pm i\pi^2\,\Box^l\delta}{4^l l!(l+1)!}.$$

(This analytic continuation is not to be confused with the one involved in the definition of the G^{α} for α complex.)

The information on the singularity structure of $(x^2\pm i\epsilon)^{\alpha}$—and of its Fourier transform—can now be codified in *causal Riesz distributions* $G^{\alpha}_{\pm}$. To wit, we define

$$G^{\alpha}_{\pm}(x):=\frac{\mp ie^{\mp i\pi\alpha}\Gamma(2-\alpha)}{4^{\alpha}\pi^2\Gamma(\alpha)}(t^2-r^2\pm i\epsilon)^{\alpha-2}, \tag{8}$$

and, sure enough,

$$G^{1}_{-}(x)=D_F(x),\quad G^{-l}_{\pm}(x)=\Box^l\delta(x)$$

for $l\geqslant 0$. Also, $\Box G^{\alpha}_{\pm}(x)=G^{\alpha-1}_{\pm}(x)$, just as for the ordinary Riesz distributions. This is clear from

$$\Box(t^2-r^2\pm i\epsilon)^{\alpha-2}=4(\alpha-1)(\alpha-2)(t^2-r^2\pm i\epsilon)^{\alpha-3}$$

valid for $1<\Re\alpha<2$, and then analytically extended. It follows that $\Box^l f=G^{-l}_{\pm}*f$ for appropriately convolvable f; and $\Box^{\alpha}$ for complex α can be defined by $\Box^{\alpha}f=G^{-\alpha}_{\pm}*f$.

We can perform the (covariant, if one wishes) Fourier transforms by the same method of analytic prolongation from the Fourier transforms of the $r^{2\alpha}$. The result is

$$\hat{G}^{\alpha}_{\pm}(p)=(2\pi)^{-2}e^{\mp i\pi\alpha}(p^2\mp i\epsilon)^{-\alpha}, \tag{9}$$

where $p^2=E^2-|\vec{p}|^2$. For instance,

$$\hat{G}^{0}_{-}(p)=1/4\pi^2,\quad \hat{G}^{1}_{-}(p)=\hat{D}_F(p)=\frac{-1}{4\pi^2(p^2+i\epsilon)},$$

as expected.[17] There is still an interesting duality at work here. Moreover,

$$G_{\pm}^{\alpha} * G_{\pm}^{\beta} = G_{\pm}^{\alpha+\beta}.$$

In summary, thanks to (rigorous) "Wick rotation," the structure of the causal Riesz distributions $G_{\pm}^{\alpha}$ is remarkably simpler than the structure of the retarded Riesz distributions $G_{\mathrm{ret}}^{\alpha}$. It largely parallels the positive signature case, vindicating Schwinger's contention on the "Euclidean" character of quantum field theory.[28]

We turn finally to the renormalization of the functionals $(t^2-r^2-i\epsilon)^{-l}$ with $l \geqslant 2$ from G_{-}^{α}. We may define the extension $[(t^2-r^2-i\epsilon)^{-2}]_{\mathrm{AR}}$, as a distribution, to be the second term on the right-hand side of the expansion

$$(t^2-r^2-i\epsilon)^{\kappa-2} =: \frac{-i\pi^2\delta(x)}{\kappa} + [(t^2-r^2-i\epsilon)^{-2}]_{\mathrm{AR}} + O(\kappa).$$

That is to say,

$$[(t^2-r^2-i\epsilon)^{-2}]_{\mathrm{AR}} = \lim_{\kappa\to 0} \frac{d}{d\kappa}[\kappa(t^2-r^2-i\epsilon)^{\kappa-2}].$$

Analogously,

$$(t^2-r^2-i\epsilon)^{\kappa-3} =: \frac{-i\pi^2\Box\delta(x)}{8\kappa} + [(t^2-r^2-i\epsilon)^{-3}]_{\mathrm{AR}} + O(\kappa), \tag{10}$$

as $\kappa\to 0$ defines $[(t^2-r^2-i\epsilon)^{-3}]_{\mathrm{AR}}$, and so on.

IV. LORENTZ COVARIANCE OF THE *T*-RENORMALIZATION

The action of an element Λ of the Lorentz group on $\mathbb{R}^{4n}$ is given by the tensorial representation

$$\Lambda^{\otimes n} x := (\Lambda x_1, \ldots, \Lambda x_n),$$

to be denoted Λ as well, according to custom. The action of the Lorentz group on functionals is defined by

$$\langle \Lambda f(x), \phi(x)\rangle \equiv \langle f(\Lambda x), \phi(x)\rangle := \langle f(x), \Lambda\phi(x)\rangle, \quad \text{with } \Lambda\phi(x) := \phi(\Lambda^{-1}x).$$

It follows that $\langle \Lambda f(x), \Lambda^{-1}\phi(x)\rangle = \langle f(x), \phi(x)\rangle$.

A Lorentz invariant functional fulfills

$$f(\Lambda x) = f(x). \tag{11}$$

[More generally, in the nonscalar case, f would have tensorial and/or spinorial character and one would have a covariant transformation

$$f(\Lambda x) = [D(\Lambda)f](x)$$

with $D(\Lambda)$ a finite dimensional representation of SL(2, $\mathbb{C}$)—making no notational distinction between belonging to the Lorentz group and to its cover—acting on functionals in the obvious way.]

Derivatives will transform according to the (tensor powers of the) contragredient representation: one has

$$x^{\alpha}\,\partial_{\alpha}(\Lambda\phi) = x^{\alpha}\,\partial_{\alpha}(\phi\circ\Lambda^{-1}) = x^{\alpha}[\Lambda^{-1}]^{\beta}{}_{\alpha}(\partial_{\beta}\phi)\circ\Lambda^{-1} = (\Lambda x)^{\beta}(\partial_{\beta}\phi)\circ\Lambda^{-1}.$$

In particular,

$$x^\alpha \partial_\alpha(\Lambda\phi)(0)=[\Lambda^{-1}x]^\beta \partial_\beta\phi(0), \tag{12}$$

that is to say $R_0^k\Lambda=\Lambda R_0^k$, and

$$\delta_\alpha(\Lambda x)=[\Lambda^{-1}x]_\alpha^\beta \delta_\beta(x). \tag{13}$$

Suppose that f is Lorentz invariant and a particular extension $T_w f$ to the whole of $\mathbb{R}^{4n}$ has been constructed, according to our scheme. *All* the extensions of f are given by

$$T_w f+\sum_{|\alpha|\leqslant k} a^\alpha \delta_\alpha, \tag{14}$$

with $\binom{4n+k}{k}$ coefficients a^α. Our goal is to show that a Lorentz invariant extension $T_w^{\mathrm{cov}} f$ can be obtained within the class of T extensions, advocated in this series of papers. Namely,

$$T_w^{\mathrm{cov}} f(\Lambda x)=T_w^{\mathrm{cov}} f(x),$$

with

$$T_w^{\mathrm{cov}} f=T_w f+\sum_{|\alpha|=k} a^\alpha \delta_\alpha, \tag{15}$$

for at most $\binom{4n-1+k}{k}$ coefficients a^α; so that the ambiguity (14) in all the smaller orders drops out.

By a theorem of Gårding and Lions,[29] the difference between two covariant extensions must be of the form $P(\Box)\delta$, where $P(\Box)$ is a polynomial in $\Box$; in our case, a monomial.

The proof is by direct computation; since $\Lambda f=f$, we get

$$\begin{aligned}
\langle\Lambda(T_w f)-T_w f,\phi\rangle &=\langle T_w f,\Lambda\phi\rangle-\langle T_w f,\phi\rangle\\
&=\langle f,T_w\Lambda\phi\rangle-\langle f,T_w\phi\rangle\\
&=\langle f,(1-w)R_0^{k-1}\Lambda\phi+wR_0^k\Lambda\phi\rangle-\langle f,(1-w)R_0^{k-1}\phi+wR_0^k\phi\rangle\\
&\overset{(12)}{=}\langle f,(1-w)\Lambda R_0^{k-1}\phi+w\Lambda R_0^k\phi\rangle-\langle f,(1-w)R_0^{k-1}\phi+wR_0^k\phi\rangle\\
&=\langle\Lambda f,(1-\Lambda^{-1}w)R_0^{k-1}\phi+\Lambda^{-1}wR_0^k\phi\rangle-\langle f,(1-w)R_0^{k-1}\phi+wR_0^k\phi\rangle\\
&\overset{(11)}{=}\langle f,(1-\Lambda^{-1}w)R_0^{k-1}\phi+\Lambda^{-1}wR_0^k\phi\rangle-\langle f,(1-w)R_0^{k-1}\phi+wR_0^k\phi\rangle\\
&=\langle f,(w-\Lambda^{-1}w)(R_0^{k-1}\phi-R_0^k\phi)\rangle=\sum_{|\alpha|=k}\langle f,(w-\Lambda^{-1}w)x^\alpha\rangle\frac{\partial_\alpha\phi(0)}{\alpha!}.
\end{aligned}$$

The integral $\langle f,(w-\Lambda^{-1}w)x^\alpha\rangle$ exists under the hypothesis we have made.

This shows that

$$\Lambda(T_w f)-T_w f=\sum_{|\alpha|=k} b^\alpha(\Lambda)\delta_\alpha,$$

with coefficients

$$b^\alpha(\Lambda)=(-)^k\langle f,(w-\Lambda^{-1}w)x^\alpha\rangle,$$

with $|\alpha|=k$. One also has

$$\sum_{|\alpha|=k} b^{\alpha}(\Lambda)\,\delta_{\alpha}=k\sum_{|\alpha|=k}\partial^{\alpha}\left[\frac{x^{\alpha}}{\alpha!}\int_0^1 \mathrm{d}t\,\frac{(1-t)^{k-1}}{t^{k+4n}}f\left(\frac{x}{t}\right)\left(w\left(\frac{x}{t}\right)-w\left(\frac{\Lambda x}{t}\right)\right)\right]$$
$$+(k+1)\sum_{|\beta|=k+1}\partial^{\beta}\left[\frac{x^{\beta}}{\beta!}\int_0^1 \mathrm{d}t\,\frac{(1-t)^{k}}{t^{k+4n+1}}f\left(\frac{x}{t}\right)\left(w\left(\frac{\Lambda x}{t}\right)-w\left(\frac{x}{t}\right)\right)\right].$$

The rest of the proof just follows the steps of the cohomological argument in Ref. 4: applying two Lorentz transformations, on use of (13)—and omitting indices—one obtains

$$b(\Lambda_1\Lambda_2)=\Lambda_2^{-1}b(\Lambda_1)+b(\Lambda_2), \tag{16}$$

where Λ_2^{-1} denotes the tensor antirepresentation. A solution for this equation is given by

$$b(\Lambda)=(1-\Lambda^{-1})a \tag{17}$$

with $a\in\mathbb{R}^{4k}$ independent of Λ. Actually (16) is a group 1-cocycle equation, for SL(2, $\mathbb{C}$), with values in the space carrying the contragredient representation, and because of the vanishing of the the first cohomology group $H^1(\mathrm{SL}(2,\mathbb{C});\mathbb{R}^{4k})$[30] its only solutions are of the trivial form (17).

Now, we conclude that, if a satisfies (17), then, in view of (13), formula (15) gives indeed a Lorentz invariant renormalization of f.

For logarithmic divergences, $b=0$, and, as $[\Lambda^{-1}]^{\otimes 0}=1$, one can take a arbitrary (this is *a priori* obvious in view of the Lorentz invariance of δ). The choice $a=0$ commends itself.

For higher order divergences, in principle one solves (17) for a and plugs the (in general nonunique) solution in (15). However, following a suggestion in Ref. 25, a wiser course can be devised. For simplicity, we take $n=1$ from now on. Then we can assume that f depends only on x^2.[31] It will be seen that only the symmetric part of the Lorentz content of a^{α} counts. Consider $\sigma(f)=6$, i.e., $k=2$, a quadratic divergence. We revert to a Lorentz quadri-index notation: $|\alpha|=2$, $\alpha\leftrightarrow(\mu_1\mu_2)$. It is found[6] that the totally symmetric part

$$a^{(\mu_1\mu_2)}=-\tfrac{1}{4}\langle f,(x^{\mu_1}x^{\mu_2}x^{\rho}\partial_{\rho}-x^2x^{(\mu_1}\partial^{\mu_2)})w\rangle,$$

is a possible choice for a; this choice is canonical in that $a^{\mu}_{\mu}=0$. Integrating by parts the previous expression, on account of $\partial_{\mu}f=2x_{\mu}f'$, we obtain

$$a^{(\mu_1\mu_2)}=\langle f,(x^{\mu_1}x^{\mu_2}-\tfrac{1}{4}x^2g^{\mu_1\mu_2})w\rangle.$$

In (15) with use of (3) we see cancellation of the first term on the right-hand side of this equation, and finally the canonical expression

$$\langle T_w^{\mathrm{cov}}f(x),\phi(x)\rangle=\left\langle f(x),\phi(x)-\phi(0)-w(x)\frac{\Box\phi(0)}{8}x^2\right\rangle,$$

emerges for the Lorentz-invariant distribution extending a quadratically divergent Lorentz-invariant functional f. This formula supplants the case $k=2$ of (3) in practice.

More generally, from the formulas in Ref. 6, we can derive, for $\sigma(f)=2m+4$ or $2m+5$:

$$\langle T_w^{\mathrm{cov}}f(x),\phi(x)\rangle=\left\langle f(x),\phi(x)-\phi(0)-\frac{\Box\phi(0)}{8}x^2-\cdots-w(x)\xi_m x^{2m}\right\rangle, \tag{18}$$

where

$$\xi_m:=\frac{2(2m-1)!!}{(2m+2)!!(2m)!}.$$

Concentrate now in T_μ^{cov}. In Sec. IV B of Paper I we proved that the Euclidean $\langle[\rho^{-4-2m}]_{\mathrm{AR}},\phi(x)\rangle$ is given by

$$\left\langle \rho^{-4-2m},\phi(x)-\phi(0)-\frac{\Delta\phi(0)}{8}\rho^2-\cdots-H(1-\rho)\xi_m\Delta^m\phi(0)\rho^{2m}\right\rangle.$$

This expression Wick-rotates into $\langle[(x^2\pm i\epsilon)^{-2-m}]_{\mathrm{AR}},\phi(x)\rangle$, which therefore is given by

$$\left\langle (x^2\pm i\epsilon)^{-2-m},\phi(x)-\phi(0)-\frac{\Box\phi(0)}{8}x^2-\cdots-H(1-\rho)\xi_m\Box^m\phi(0)(x^2)^m\right\rangle.$$

The conclusion is that $[(x^2\pm i\epsilon)^{-2-m}]_{\mathrm{AR}}=T^{\mathrm{cov}}_{\mu=1}(x^2\pm i\epsilon)^{-2-m}$. For negative powers of the Feynman propagator, the Bollini, Giambiagi, and Gonzales Domínguez analytic regularization and our canonical covariant renormalization using the *improved* subtraction $T_{\mu=1}$ give one and the same result.

This coincidence is extended to T_μ for all values of μ by introduction of a 't Hooft factor in the definition of $[(x^2\pm i\epsilon)^{-2-m}]_{\mathrm{AR}}$. The procedure will be clear from the examples in the next section.

V. COMPUTING EXAMPLES

The singularities of the powers of D_F are concentrated at the origin, so that the improved method of Epstein and Glaser is directly applicable here. Consider first the T_μ renormalization of $(t^2-r^2-i\epsilon)^{-2}$, corresponding to the "fish" diagram in the φ_4^4 model. We use the notations $[f]_{\mathrm{R}}:=[f]_{\mathrm{R},\mu}:=T_\mu^{\mathrm{cov}}f$. From (4) we obtain, in full analogy with the Euclidean case (see Sec. III of Paper I):

$$[(x^2-i\epsilon)^{-2}]_{\mathrm{R},\mu}=\tfrac{1}{2}\partial_\nu\left[x^\nu\frac{\log\mu^2(x^2-i\epsilon)}{(x^2-i\epsilon)^2}\right].$$

This is the very same result coming from analytical regularization: just check

$$\mu^{2\kappa}(x^2-i\epsilon)^{\kappa-2}=\frac{\mu^{2\kappa}}{2\kappa}\partial_\nu[x^\nu(x^2-i\epsilon)^{\kappa-2}],$$

and expand in κ the right-hand side. In conclusion,

$$[(t^2-r^2-i\epsilon)^{-2}]_{\mathrm{R},\mu}=[(t^2-r^2-i\epsilon)^{-2}]_{\mathrm{AR},\mu},$$

or $[(D_F)^2]_{\mathrm{R}}=[(D_F)^2]_{\mathrm{AR}}$, with this generalized definition of $[\,\cdot\,]_{\mathrm{AR}}$.

Consider now the "sunset" diagram in the same model. Have another look at Sec. III of Paper I; one obtains

$$[(x^2-i\epsilon)^{-3}]_{\mathrm{R},\mu}=3\sum_{|\beta|=3}\partial_\beta\left[\frac{x^\beta}{\beta!}\frac{\log(\mu^2(x^2-i\epsilon))}{(x^2-i\epsilon)^3}\right]-\frac{3i\pi^2}{8}\Box\delta(x).$$

Analogously, one checks by a longer but straightforward calculation,

$$\mu^{2\kappa}(x^2-i\epsilon)^{\kappa-3}=\frac{3\mu^{2\kappa}}{2\kappa(1-3\kappa+2\kappa^2)}\sum_{|\beta|=3}\partial_\beta\left(\frac{x^\beta(x^2-i\epsilon)^{\kappa-3}}{\beta!}\right).$$

It is clear from (10) that

$$3\,\partial_\beta\left(\frac{x^\beta(x^2-i\epsilon)^{\kappa-3}}{\beta!}\right)=-\frac{i\pi^2}{4}\Box\delta(x),$$

from which

$$\mu^{2\kappa}(x^2-i\epsilon)^{\kappa-3}=\frac{-i\pi^2\Box\delta(x)}{8\kappa}+[(x^2-i\epsilon)^{-3}]_{\mathrm{R},\mu}+O(\kappa).$$

Therefore $[(D_F)^3]_{\mathrm{R}}=[(D_F)^3]_{\mathrm{AR}}$.

For higher order powers of G_F similar arguments show that

$$[(D_F)^l]_{\mathrm{R}}=[(D_F)^l]_{\mathrm{AR}}$$

is true generally for $l\geqslant 2$.

Powers of the massive propagator D_F^m are renormalizable in our standard way, by use of (1), now applicable, and automatically Lorentz-covariance preserving. The scaling degree of the (powers of) propagators is the same in the massive and in the massless cases. One routinely finds, for instance,

$$[(D_F^m)^2]_{\mathrm{R}}(x)=-\frac{m^2}{32\pi^4}\partial_\mu x^\mu\left(\frac{K_1^2(m\sqrt{-x^2+i\epsilon})-K_0(m\sqrt{-x^2+i\epsilon})K_2(m\sqrt{-x^2+i\epsilon})}{-x^2+i\epsilon}\right).$$

VI. BPHZ RENORMALIZATION REVISITED

It is well known that for zero-mass models, the basic BPHZ scheme runs into trouble. This is due to the failure of $\partial^\mu\hat{f}(0)$ to exist for $|\mu|=k$, on account of the infrared problem. Now, one can try subtraction at some suitable external momentum $q\neq 0$, providing a mass scale. It is patent that this last subtraction will introduce in the Minkowskian context a noncovariance. This prompted Lowenstein and Zimmermann to introduce their ''soft mass insertions;'' [32] but that BPHZL method is quite awkward in practice.

A far simpler solution to the problem is now available to us. It comes from the observation in Paper I that the BPHZ method is ancillary to the Epstein and Glaser: from the definitions

$$\langle F[R_0^k f],F^{-1}[\phi]\rangle=\langle F[f],F^{-1}[R_0^k\phi]\rangle. \tag{19}$$

An expression such as $F[f]$ is *not a priori* meaningless: it is a well-defined functional on the linear subspace of Schwartz functions ϕ whose first moments $\int p^\alpha\phi(p)\,\mathrm{d}^d p$ up to order $k+1$ happen to vanish: this is the Fourier counterpart of the space of distributions on configuration space acting on Schwartz test functions vanishing up to order $k+1$ at the origin.

Now, one has

$$(x^\mu\phi)\check{}\,(p)=(-i)^{|\mu|}\,\partial^\mu\check{\phi}(p),$$

where μ denotes a multi-index; so that, in particular,

$$(x^\mu)\check{}\,(p)=(-i)^{|\mu|}(2\pi)^{d/2}\,\partial^\mu\delta(p).$$

Also,

$$\partial_\mu\phi(0)=(-i)^{|\mu|}(2\pi)^{-d/2}\langle p^\mu,\check{\phi}\rangle.$$

From this, with an integration by parts in the right-hand side of (19), we conclude

$$\langle F[R_0^k f],F^{-1}[\phi]\rangle=\langle R_0^k F[f],F^{-1}[\phi]\rangle;$$

that is to say, F and R_0^k *commute*. Thus the BPHZ subtraction rule in momentum space is equivalent to (1).

Now use (18) instead of (1), with employment of $w(x)=\exp(-iqx)$, with $q\neq 0$, which, as discussed earlier, is a perfectly good infrared regulator. From that follows the simple, obviously covariant, rule:

$$T_q^{\mathrm{cov}} f(p) = f(p) - \frac{\Box f(0) p^2}{8} - \cdots - \xi_m \Box^m f(q)\,(p^2)^m$$

for a Feynman amplitude f in momentum space. Note $\Box^m T_q^{\mathrm{cov}} f(q)=0$. The difference between two of these recipes is, as it should be, a Lorentz-invariant polynomial in p, of degree the divergence index.

VII. OUTLOOK

The ''missing link'' between the Epstein–Glaser subtraction method and the literature on prolongation of distributions found in Paper I has here been extended to the Minkowskian context. Before rendering in the language of T renormalization the full complexity of the construction of time-ordered products, and the main result of perturbative renormalization theory, one needs to handle the combinatorial aspects of diagrams with subdivergences. This we do in the next paper of the series (Paper III), using a variant of the Connes–Kreimer Hopf algebraic paradigm.

ACKNOWLEDGMENTS

We thank Christian Brouder and Joe Várilly for helpful comments. Support from the Vicerrectoría de Investigación of the Universidad de Costa Rica is gratefully acknowledged, as well as from Université de Provence in the early stage of this work.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Dynamical structure of irregular constrained systems

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(Received 5 February 2003; accepted 2 May 2003)

Hamiltonian systems with functionally dependent constraints (irregular systems), for which the standard Dirac procedure is not directly applicable, are discussed. They are classified according to their behavior in the vicinity of the constraint surface into two fundamental types. If the irregular constraints are multilinear (type I), then it is possible to regularize the system so that the Hamiltonian and Lagrangian descriptions are equivalent. When the constraints are power of a linear function (type II), regularization is not always possible and the Hamiltonian and Lagrangian descriptions may be dynamically inequivalent. It is shown that the inequivalence between the two formalisms can occur if the kinetic energy is an indefinite quadratic form in the velocities. It is also shown that a system of type I can evolve in time from a regular configuration into an irregular one, without any catastrophic changes. Irregularities have important consequences in the linearized approximation to nonlinear theories, as well as for the quantization of such systems. The relevance of these problems to Chern–Simons theories in higher dimensions is discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1601299]

I. INTRODUCTION

Dirac's Hamiltonian analysis provides a systematic method for finding the gauge symmetries and the physical degrees of freedom of constrained systems like gauge theories and gravity.[1] Constraints arise through conditions of the form

$$\phi^r(z)\approx 0 \quad (r=1,\ldots,R), \tag{1}$$

where z are local coordinates in phase space Γ. In the most common cases of physical interest the ϕ's are functionally independent; these are the regular constrained systems. There are some exceptional cases in which functional independence is violated. In these *irregular systems* it is not always clear how to identify symmetries and true degrees of freedom. Moreover, the Hamiltonian and Lagrangian descriptions may not be equivalent in irregular systems.

Irregular systems are not necessarily intractable nor exotic. A common example is a relativistic massless particle ($p^\mu p_\mu=0$), which is irregular at the origin of momentum space ($p^\mu=0$). There are other physical circumstances in which regularity is violated, and not only for isolated states but on large portions of phase space where the system evolves. This is the case in Chern–Simons (CS) theories for dimensions $D\geqslant 5$ where, for some initial configurations, regularity can fail at all times and one is forced to live with this problem.

A CS Lagrangian describes a gauge theory for a certain Lie group G in a space–time of odd dimension. The construction is naturally invariant under diffeomorphisms and provides a nonstandard but otherwise acceptable description of gravity as a gauge theory.[2–5] Furthermore, CS theories are highly nonlinear, possess propagating degrees of freedom,[6] and have a very rich phase space structure with many different sectors, some of which describe irregular systems.[7]

In five-dimensional CS supergravity, it was observed that the linearized action around a certain anti–de Sitter background seems to have *one more degree of freedom* than the fully

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nonlinear system.[8] This paradoxical behavior can be seen to arise from a violation of the regularity conditions among the symmetry generators of the theory in the region of phase space defined by the selected background.

Here we address different scenarios in which regularity conditions can be violated, how such systems can be handled in some cases, and why linearization may fail to approximate a nonlinear system faithfully. It is found that there are two main types of irregular constraints, multilinear (type I) and nonlinear (type II). The constraints of the first type can always be regularized, while type II constraints (of the form f^k, where f has a simple zero and $k>1$) can be regularized only if f is a second class function.

Constraints satisfying regularity conditions are sometimes referred to as *effective* constraints.[9] The issue of regularity (*effectiveness*) and its relevance for the equivalence between the Lagrangian and Hamiltonian formalisms has also been discussed in Refs. 10 and 11.

II. REGULARITY CONDITIONS

Consider a dynamical system in a phase space Γ with local coordinates $z^i \equiv (q,p)$ $(i=1,\ldots,2n)$. Conditions (1) define the constraint surface

$$\Sigma = \{\overline{z} \in \Gamma \,|\, \phi^r(\overline{z}) = 0 \;\; (r=1,\ldots,R)(R \leqslant 2n)\}. \tag{2}$$

Dirac's procedure guarantees that the system remains on the constraint surface during its evolution (for reviews, see Refs. 1,12–16). Choosing different coordinates on Γ may lead to different forms for the constraint functions whose functional independence is not obvious. The *regularity conditions* were designed by Dirac to test this.[17]

Regularity conditions (RCs): The constraints $\phi^r \approx 0$ are regular if and only if their small variations $\delta\phi^r$ evaluated on Σ define R linearly independent functions of δz^i.

To first order in δz^i, the variations of the constraints have the form

$$\delta\phi^r = J^r_i \delta z^i \quad (r=1,\ldots,R), \tag{3}$$

where $J^r_i \equiv \partial\phi^r/\partial z^i\,|_\Sigma$ is the Jacobian evaluated on the constraint surface. An equivalent definition of the RCs is:[13] *The set of constraints $\phi^r \approx 0$ is regular if and only if the Jacobian $J^r_i = \partial\phi^r/\partial z^i\,|_\Sigma$ has maximal rank, $\mathfrak{R}(\mathbf{J}) = R$.*

A simple classical mechanical example of functionally *dependent* constraints occurs in a two-dimensional phase space with coordinates (q,p) and constraints $\phi^1 \equiv q \approx 0$ and $\phi^2 \equiv pq \approx 0$. In this case, $\mathbf{J} = \left[\begin{smallmatrix} 1 & p \\ 0 & q \end{smallmatrix}\right]_{q=0}$ and $\mathfrak{R}(\mathbf{J}) = 1$.

A system of just one constraint can also fail the test of regularity. Consider, for example, the constraint $\phi = q^2 \approx 0$ in a two-dimensional phase space. In this case, $\mathbf{J} = (2q,0)_{q^2=0} = 0$ and $\mathfrak{R}(\mathbf{J}) = 0$. The same problem occurs with the constraint $q^k \approx 0$, for $k>1$, which has a zero of kth order on the constraint surface. This example illustrates that one *constraint* may be dependent on itself, while one *function* is, by definition, always functionally independent.

Equivalence: Different sets of constraints are said to be equivalent if they define the same constraint surface.

Note that this definition refers to the locus of constraints, not to equivalence of the resulting dynamics. Since the surface Σ is defined by the zeros of the constraints, while the regularity conditions depend on their derivatives, it is possible to replace a set of irregular ϕ's by an *equivalent* set of *regular* constraints $\tilde{\phi}$.

In the classification of irregular systems, two questions present themselves: what is the *nature* of the constraints that give rise to irregularity, and *where* the irregularities can occur. These issues are addressed in the following sections. A third question is whether a system can evolve from an initial state in which regularity holds, into an irregular configuration. This will be discussed in the last section.

A. Basic types of irregular constraints

Irregular constraints can be classified according to their behavior in the vicinity of the surface Σ. For example, linearly dependent constraints have Jacobian with constant rank R' throughout Σ, and

$$\phi^r \equiv J_i^r(\overline{z})(z^i - \overline{z}^i) \approx 0, \quad \mathfrak{R}(\mathbf{J}) = R' < R. \tag{4}$$

These constraints are regular systems in disguise simply because $R - R'$ constraints are redundant and should be discarded. The subset with R' linearly independent constraints gives the correct description. For example, the linearly dependent constraints $\phi^1 = z$ and $\phi^2 = 2z$ are clearly in this category. Apart from this trivial case, two main types of truly irregular constraints, which do not possess a linear approximation in the vicinity of some points of Σ, can be distinguished.

Type I. Multilinear constraints: Consider the constraint

$$\phi \equiv \prod_{i=1}^{M} f_i(z) \approx 0, \tag{5}$$

where the functions f_i have simple zeros. Each factor defines a surface of codimension 1,

$$\Sigma_i \equiv \{\overline{z} \in \Gamma \,|\, f_i(\overline{z}) = 0\}, \tag{6}$$

and Σ is the collection of all surfaces, $\Sigma = \cup \Sigma_i$. The rank of Jacobian of ϕ is reduced at intersections

$$\Sigma_{ij} \equiv \Sigma_i \cap \Sigma_j . \tag{7}$$

Thus, the RCs hold everywhere on Σ, except at the intersections Σ_{ij}, where ϕ has zeros of higher order. Note that the intersections (7) also include the points where more than two Σ's overlap.

Type II. Nonlinear constraints: Consider the constraint of the form

$$\phi \equiv [f(z)]^k \approx 0 \quad (k > 1), \tag{8}$$

where the function $f(z)$ has a simple zero. This constraint has a zero order k in the vicinity of Σ, its Jacobian vanishes on the constraint surface and, therefore, the RCs fail (here we assume $k > 1$ in order to avoid infinite values for $\partial\phi/\partial z^i$ on Σ). It could seem harmless to replace ϕ by the equivalent regular constraint $f(z) \approx 0$, but it turns out that this may change the dynamics of original system, as we show below.

Types I and II are the two fundamental generic classes of irregular constraints. In general, there can be combinations of them occurring simultaneously near a constraint surface, as in constraints of the form $\phi = [f_1(z)]^2 f_2(z) \approx 0$, etc.

B. Classification of constraint surfaces

The previous classification refers to the way in which ϕ approaches zero. Now we will discuss *where* regularity can be violated. The rank of the Jacobian $\partial\phi^r/\partial z^i$ need not be constant throughout Σ: suppose one eigenvalue of the Jacobian vanishes on a submanifold $\Sigma_0 \subset \Sigma$. On Σ_0 regularity is violated, while it still holds on the rest of Σ. Thus, barring accidental degeneracies such as linearly dependent constraints, one of these three situation may present themselves.

(A) *The RCs are satisfied everywhere on the constraint surface:* $\mathbf{J}$ has maximal rank throughout Σ (regular systems).

(B) *The RCs fail everywhere on the constraint surface:* $\mathbf{J}$ has constant rank $R' < R$ on Σ.

(C) *The RCs fail on* Σ_0: $\mathfrak{R}(\mathbf{J})|_{\Sigma_0} = R' < R$, while $\mathfrak{R}(\mathbf{J}) = R$ elsewhere on Σ.

In the last case, the constraint surface can be decomposed into two nonoverlapping sets Σ_0 and Σ_R. Then, the rank of the Jacobian jumps from $\mathfrak{R}(\mathbf{J})=R$ on Σ_R, to $\mathfrak{R}(\mathbf{J})=R'$ on Σ_0. Although the functions ϕ^r are continuous and differentiable, this is not sufficient for regularity. Irregular cases are illustrated by the following examples.

In a $(2+N)$-dimensional phase space $(q,p,z^1,\ldots,z^N)$, the constraints $\phi^1\equiv q-p\approx 0$ and $\phi^2\equiv qp\approx 0$ are irregular on the whole constraint surface $\{(0,0,z^1,\ldots,z^N)\}$, where the Jacobian has rank $\mathfrak{R}(\mathbf{J})=1$. Note that these constraints are always irregular, although the functions $q+p$ and qp are functionally independent everywhere except for $q=p$, which happens to be the case at the constraint surface.

An example having both regular and irregular sectors is a massless relativistic particle in Minkowski space with phase space (q^μ,p_ν). The constraint $\phi\equiv p^\mu p_\mu\approx 0$ has Jacobian $\mathbf{J}=(0,2p^\mu)_{\phi=0}$, and its rank is one everywhere, except at the apex of the cone, $p^\mu=0$, where the light cone is not differentiable and the Jacobian has rank zero.

The lack of regularity, however, is not necessarily due to the absence of a well-defined smooth tangent space for Σ. Consider, for example, the multilinear constraint

$$\phi(x,y,z)=(x-1)(x^2+y^2-1)\approx 0. \tag{9}$$

Here the constraint surface Σ is composed of two submanifolds: the plane $\Pi=\{(x,y,z)|x-1\approx 0\}$, and the cylinder $C=\{(x,y,z)|x^2+y^2-1\approx 0\}$, which are tangent to each other along the line $L=\{(x,y,z)|x=1,y=0,z\in\mathbb{R}\}$. The Jacobian on Σ is

$$\mathbf{J}=(3x^2+y^2-2x-1,2y(x-1),0)_{\phi=0} \tag{10}$$

and its rank is 1 everywhere, except on L, where it is zero. The constraint ϕ is irregular on this line. However, the tangent vectors to Σ are well defined there. The irregularity arises because ϕ is a multilinear constraint of the type described by (5) and has two simple zeros overlapping on L. The equivalent set of regular constraints on L is $\{\phi_\Pi=x-1\approx 0,\phi_C=x^2+y^2-1\approx 0\}$, as we will see below.

III. TREATMENT OF IRREGULAR SYSTEMS

In what follows regular systems and linearly dependent constraints will not be discussed. They are either treated in standard texts, or they can be trivially reduced to the regular case.

A. Multilinear constraints

Consider a system of type I, as in Eq. (5). In the vicinity of an irregular point where only two surfaces (6) intersect, say Σ_1 and Σ_2, the constraint $\phi\approx 0$ is equivalently described by the set of regular constraints

$$f_1\approx 0,\quad f_2\approx 0. \tag{11}$$

This replacement generically changes the Lagrangian of the system, and the orbits, as well. Suppose the original canonical Lagrangian is

$$L(q,u)=p_i\dot{q}^i-H(q,p)-u\phi(q,p), \tag{12}$$

where H is the Hamiltonian containing all regular constraints. Replacing ϕ by (11), gives rise to an effective Lagrangian

$$L_{12}(q,v)=p_i\dot{q}^i-H(q,p)-v^1f_1(q,p)-v^2f_2(q,p) \tag{13}$$

defined on Σ_{12}. Thus, instead of the *irregular* Lagrangian (12) defined on the whole Σ, there is a collection of *regularized* effective Lagrangians defined in the neighborhood of the different intersections of Σ_i's. For each of these regularized Lagrangians, the Dirac procedure can be carried out to the end.

Let us illustrate this with the example of a Lagrangian in a $(2+N)$-dimensional configuration space $(x,y,q^1,\ldots,q^N)$,

$$L=\frac{1}{2}\sum_{k=1}^{N}(\dot{q}^k)^2+\frac{1}{2}(\dot{x}^2+\dot{y}^2)-\lambda xy. \tag{14}$$

This Lagrangian describes a free particle moving on the set

$$\{(x,y,q^k)\in\mathbb{R}^{N+2}|xy=0\}\subset\mathbb{R}^{N+2}, \tag{15}$$

which is the union of two $(N+1)$-dimensional planes where x and y vanish, respectively. The constraint surface defined by $xy=0$ can be divided into the following sets:

$$\begin{aligned}\Sigma_1&=\{(x,0,q^k;p_x,p_y,p_k)|x\neq 0\},\\ \Sigma_2&=\{(0,y,q^k;p_x,p_y,p_k)|y\neq 0\},\\ \Sigma_{12}&=\{(0,0,q^k;p_x,p_y,p_k)\}.\end{aligned} \tag{16}$$

The constraint is regular on $\Sigma_1\cup\Sigma_2$, while on Σ_{12} it is irregular and can be exchanged by $\{\phi_1=x\approx 0,\ \phi_2=y\approx 0\}$. The corresponding regularized Lagrangians are

$$\begin{aligned}L_1&=\frac{1}{2}\sum_{k=1}^{N}(\dot{q}^k)^2+\frac{1}{2}\dot{x}^2,\\ L_2&=\frac{1}{2}\sum_{k=1}^{N}(\dot{q}^k)^2+\frac{1}{2}\dot{y}^2,\\ L_{12}&=\frac{1}{2}\sum_{k=1}^{N}(\dot{q}^k)^2,\end{aligned} \tag{17}$$

and the Lagrange multipliers have dropped out, so the regularized Lagrangians describe physical degrees of freedom only—as expected.

The corresponding regularized Hamiltonians are

$$\begin{aligned}H_1&=\frac{1}{2}\sum_{k=1}^{N}p_k^2+\frac{1}{2}p_x^2,\\ H_2&=\frac{1}{2}\sum_{k=1}^{N}p_k^2+\frac{1}{2}p_y^2,\\ H_{12}&=\frac{1}{2}\sum_{k=1}^{N}p_k^2,\end{aligned} \tag{18}$$

which are defined in the corresponding reduced manifolds of phase space (obtained after completing the Dirac procedure):

$$\tilde{\Sigma}_1=\{(x,0,q^k;p_x,0,p_k)|x\neq 0\},$$

$$\tilde{\Sigma}_2=\{(0,y,q^k;0,p_y,p_k)|y\neq 0\}, \tag{19}$$

$$\tilde{\Sigma}_{12}=\{(0,0,q^k;0,0,p_k)\}.$$

It is straightforward to generalize the proposed treatment when more than two surfaces Σ_i overlap.

Evolution of a multilinearly constrained system: Since in the presence of a multilinear constraint there are regions of the phase space where the Jacobian has different rank, a question arises about the evolution of this system. Can the system evolve from a generic configuration in a region of maximal rank, reaching a configuration of lower rank in finite time? In the case that that were possible, what happens with the system afterwards? (This problem should not be confused with the issues arising in degenerate systems.[18–20])

To answer this question let us consider the simple example discussed above (14), for $N=1$,

$$L=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2)-\lambda xy. \tag{20}$$

In the regions Σ_1 and Σ_2 [see Eqs. (16)], the rank is maximal and the free particle can move freely along the x- or y-axis, respectively.

Suppose that the initial state is

$$x(0)=a>0, \quad y(0)=0, \quad z(0)=0, \quad \dot{x}(0)=-v<0, \quad \dot{y}(0)=0, \quad \dot{z}(0)=0, \tag{21}$$

so that the particle is moving on Σ_1, with finite speed along the x-axis towards $x=0$ on Σ_{12}. The evolution is given by $\overline{x}(t)=a-vt$, $\overline{y}(t)=0$, $\overline{z}(t)=0$ and the particle clearly reaches $x=0$ in a finite time ($T=a/v$). What happens then? According to the evolution equation, for $x<0$ the trajectory takes the form $\overline{x}(t)=a'-v't$, $\overline{y}(t)=0$, $\overline{z}(t)=0$, however the action would be infinite unless $a=a'$ and $v=v'$. Therefore, the particle continues unperturbed past beyond the point where the RCs fail. So, the irregular surface is not only reachable in a finite time, but it is crossed without any observable effect on the trajectory.

From the point of view of the trajectory in phase space, it is clear that the initial state $(a,0,0;-v,0,0)$ lies on the surface $\tilde{\Sigma}_1$, and at $t=T$ the system reaches the point $(0,0,0;-v,0,0)$, which *does not lie on* the surface $\tilde{\Sigma}_{12}=\{(0,0,z;0,0,p_z)\}$.

While it is true that at $t=T$ the Jacobian changes rank, it would be incorrect to conclude that the evolution suffers a jump since the dynamical equations are perfectly valid there. In order to have significant change in dynamics, the Jacobian should change its rank in an open set.

B. Nonlinear constraints

Let us now turn to the case of irregular systems of type II. As we will show, it is possible to replace a nonlinear irregular constraint by an equivalent linear one without changing the dynamical contents of the theory, provided the linear constraint is second class. Otherwise, the resulting Hamiltonian dynamics will be, in general, inequivalent to that of the original Lagrangian system.

In order to illustrate this point, consider a system given by the Lagrangian

$$L(q,u)=\tfrac{1}{2}\gamma_{ij}\dot{q}^i\dot{q}^j-u[f(q)]^k, \tag{22}$$

where $k>1$ and

$$f(q)\equiv c_i q^i \neq 0, \quad i=1,\ldots,N. \tag{23}$$

Here we assume the metric γ_{ij} to be constant and invertible, and the coefficients c_i are also constant. The Euler–Lagrange equations describe a free particle in an N-dimensional space, with time evolution $\overline{q^i}(t)=v_0^i t+q_0^i$, where $u(t)$ is a Lagrange multiplier. This solution is determined by $2N$ initial conditions, $q^i(0)=q_0^i$ and $\dot{q}^i(0)=v_0^i$ subject to the constraints $c_i q_0^i=0$ and $c_i v_0^i=0$. Thus, the system possesses $N-1$ physical degrees of freedom.

In the Hamiltonian approach this system has a primary constraint $\pi\equiv \partial L_2/\partial \dot{u}\approx 0$ whose preservation in time leads to the secondary constraint

$$\phi\equiv[f(q)]^k\approx 0. \tag{24}$$

According to (8), this is a nonlinear constraint and there are no further constraints. As a consequence, the system has only two first class constraints $\{\pi\approx 0,\ f^k\approx 0\}$, and $N-1$ degrees of freedom, as found in the Lagrangian approach.

On the other hand, if one chooses instead of (24), the equivalent linear constraint

$$f(q)=c_i q^i\approx 0, \tag{25}$$

then its time evolution yields a *new* constraint,

$$\chi(p)\equiv \gamma^{ij}c_i p_j\approx 0. \tag{26}$$

Now, since

$$\{f,\chi\}=\gamma^{ij}c_i c_j\equiv\|c\|^2, \tag{27}$$

two cases can be distinguished.

(1) If $\|c\|=0$, there are three first class constraints, $\pi\approx 0$, $f\approx 0$, and $\chi\approx 0$, which means that the system has $N-2$ physical degrees of freedom. In this case, substitution of (24) by the equivalent linear constraint (25), yields a *dynamically inequivalent* system.
(2) If $\|c\|\neq 0$, then $f\approx 0$ and $\chi\approx 0$ are second class, while $\pi\approx 0$ is first class, which leaves $N-1$ physical degrees of freedom and the substitution does not change the dynamics of the system.

Thus, if $f^k\approx 0$ is irregular, replacing it by the regular constraint $f\approx 0$ changes the dynamics if f is a first class function, but it gives the correct result if it is a second class function.

Note that in the Lagrangian description there is no room to distinguish first and second class constraints, so it would seem like the value of $\|c\|$ did not matter. However, the inequivalence of the substitution can be understood in the Lagrangian analysis as well. Suppose that it were permissible to exchange the constraint $f^k\approx 0$ by $f\approx 0$ in the Lagrangian. Then, instead of (22), one would have

$$\tilde{L}(q,u)=\tfrac{1}{2}\gamma_{ij}\dot{q}^i\dot{q}^j-uf(q). \tag{28}$$

It can be easily checked that (28) yields $N-2$ degrees of freedom when $\|c\|=0$, and $N-1$ degrees of freedom when $\|c\|\neq 0$, which agrees with the results obtained in the Hamiltonian analysis. Note that the substitution of f^k by f modifies the dynamics only if $\gamma^{ij}c_i c_j=0$, but this can happen nontrivially only if the metric γ_{ij} is not positive definite.

In general, a nonlinear irregular constraint $\phi\approx 0$ has a multiple zero on the constraint surface Σ, which means that its gradient vanishes on Σ as well. An immediate consequence of $(\partial\phi/\partial z^i)\approx 0$, is that ϕ commutes with all *finite* functions on Γ,

$$\{\phi,F(z)\}\approx 0. \tag{29}$$

As a consequence, $\phi \approx 0$ is first class and is always preserved in time,

$$\dot{\phi} \approx 0. \tag{30}$$

On the other hand, a nonlinear constraint cannot be viewed as a symmetry generator simply because it does not generate any transformation,

$$\delta_\varepsilon z^i = \{z^i, \varepsilon \phi\} \approx 0. \tag{31}$$

Consistently with this, ϕ cannot be gauge-fixed, as there is no finite function $\mathcal{P}$ on Γ such that

$$\{\phi, \mathcal{P}\} \neq 0. \tag{32}$$

In this sense, a nonlinear first class constraint that cannot be gauge-fixed, cancels only half a degree of freedom. The other half degree of freedom cannot be cancelled because the gauge-fixing function does not exist and, in particular, it cannot appear in the Hamiltonian. Although the features (29)–(32) allow counting the degrees of freedom in a theory, these systems are pathological and their physical relevance is questionable since their Lagrangians cannot be regularized.

When a nonlinear constraint $\phi \approx 0$ can be exchanged by a regular one, the Lagrangian is regularized as in the case of multilinear constraints. For example, the system (22) with $\|c\| \neq 0$ has Hamiltonian

$$H = \tfrac{1}{2}\gamma^{ij} p_i p_j + \lambda \pi + u f(q), \tag{33}$$

where $f = c_i q^i$ will turn out to be a second class constraint. The corresponding regularized Lagrangian is

$$L_{\text{reg}} = \tfrac{1}{2}\gamma_{ij}\dot{q}^i \dot{q}^j - u f(q), \tag{34}$$

which coincides with $\tilde{L}$, Eq. (28), as expected.

In Refs. 10 and 11 irregular systems of the type II were discussed. It was pointed out that there was a possible loss of dynamical information in some cases. From our point of view, it is clear that this would occur when f is a first class function.

IV. LINEARIZATION OF IRREGULAR SYSTEMS

It has been observed in five-dimensional Chern–Simons theory, that the effective action for the linearized perturbations of the system around certain backgrounds seems to have more degrees of freedom than the fully nonlinear theory.[8] This is puzzling since the heuristic picture is that the degrees of freedom of a system correspond to the small perturbations around a local minimum of the action, and therefore the number of degrees of freedom should not change when the linearized approximation is used.

In view of the discussion in the preceding section, it is clear that a possible solution of the puzzle lies in the fact that substituting a nonlinear constraint by a linear one may change the dynamical features of the theory. But the problem with linear approximations is more serious: the linearized approximation retains only up to quadratic and bilinear terms in the Lagrangian, which give linear equations for the perturbations. Thus, irregular constraints in the vicinity of the constraint surface are erased in the linearized action. The smaller number of constraints in the effective theory can lead to the wrong conclusion that the effective system possess more degrees of freedom than the unperturbed theory. The lesson to be learned is that the linear approximation is not valid in the part of the phase space where the RCs fail.

This is illustrated by the same example discussed earlier (22). One can choose as a background the solution $(\overline{q}^1, \ldots, \overline{q}^N, \overline{u})$, where $\overline{q}^i(t) = q_0^i + v_0^i t$ satisfies the constraint

$$c_i \overline{q}^i = 0, \tag{35}$$

and $\overline{u}(t)$ is an arbitrarily given function. This describes a free particle moving in the $(N-1)$-dimensional plane defined by (35). The linearized effective Lagrangian, to second order in the small perturbations $s^i=q^i-\overline{q}^i(t)$ and $w=u-\overline{u}(t)$, has the form

$$L_{\text{eff}}(s,w)=\tfrac{1}{2}\gamma_{ij}(v_0^i+\dot{s}^i)(v_0^j+\dot{s}^j)-\overline{u}(c_is^i)^2, \tag{36}$$

and the equations of motion are

$$\ddot{s}^i+\Gamma^i_j(t)\,s^j=0, \quad i=1,\ldots,N, \tag{37}$$

where $\Gamma^i_j\equiv 2\overline{u}\,\gamma^{ik}c_kc_j$ is the eigenfrequency matrix. Since $\overline{u}$ is not a dynamical variable, it is not varied and the nonlinear constraint $(c_is^i)^2=0$ is absent from the linearized equations. The system described by (37) possesses N physical degrees of freedom, that is, one degree of freedom more than the original nonlinear theory (22).

The only indication that one of these degrees of freedom has a nonphysical origin is the following: If $\|c\|\neq 0$, splitting the components of s^i along c_i and orthogonal to c_i as

$$s^i(t)\equiv s(t)\,\gamma^{ij}c_j+s^i_\perp(t), \tag{38}$$

gives rise to the projected equations

$$\ddot{s}^i_\perp=0, \tag{39}$$

$$\ddot{s}+2\overline{u}(t)\|c\|^2s=0. \tag{40}$$

The $N-1$ components of $s^i_\perp(t)$ obey a deterministic second order equation, whereas $s(t)$ satisfies an equation which depends on an indeterminate arbitrary function $\overline{u}(t)$. The dependence of $s=\overline{s}(t,\overline{u}(t))$ on the background Lagrange multiplier $\overline{u}$ is an indication that s is a nonphysical degree of freedom, since u was an arbitrary function to begin with. This is not manifest in Eq. (40), where $\overline{u}$ is a fixed function and, from a naive point of view, $s(t)$ is determined by the same equation, regardless of the physically obscure origin of the function $\overline{u}$. It is this naive analysis that leads to the wrong conclusion indicated above.

Let us emphasize that a linearized theory may be consistent by itself, but it is not necessarily a faithful approximation of a nonlinear theory.

One way to avoid the inconsistencies between the original theory and the linearized one would be to first regularize the constraints (if possible) and then linearize the corresponding regular Lagrangian.

V. CHERN–SIMONS THEORIES

Hamiltonian structure of CS theories has been studied in Ref. 6. The phase space of a CS theory in $D=2n+1$ space–time dimensions, invariant under N-parameter gauge group, is defined by canonically conjugate pairs of fields $(A^a_i(x,t),\pi^i_a(x',t))$, where $a=1,\ldots,N$ and x^i $(i=1,\ldots,2n)$ are the local coordinates on a spatial section. The CS Hamiltonian density is given by

$$\mathcal{H}=A^a_0\,\tilde{G}_a+u^a_i\phi^i_a, \tag{41}$$

where $u^a_i(x,t)$ and $A^a_0(x,t)$ are Lagrange multipliers for the constraints

$$\phi^i_a\equiv\pi^i_a-\mathcal{L}^{\,i}_a(A^b_j)\approx 0, \tag{42}$$

$$G_a=g_{aa_1\cdots a_n}F^{a_1}\wedge\cdots\wedge F^{a_n}\approx 0. \tag{43}$$

Here $G_a\equiv \mathrm{d}^{2n}x\,\tilde{G}_a$, g is a symmetric tensor of rank $n+1$, invariant under action of a gauge group, and $F=\mathrm{d}A+A\wedge A$ is the curvature two-form associated to the gauge field one-form A.

Constraints ϕ_a^i are regular because they are linear in momenta. Thus, the regularity of CS theories is determined by momentum-independent constraints G_a. Their small variations, $\delta G_a = \mathbf{J}_{ab} D \delta A^b$, evaluated at $G_a = 0$, give the $(2n-2)$-form $\mathbf{J}_{ab}$, which can be identified as the Jacobian,

$$\mathbf{J}_{ab} \equiv n\, g_{aba_2\cdots a_n} F^{a_2} \wedge \cdots \wedge F^{a_n}. \tag{44}$$

According to Dirac's definition, sufficient and necessary condition for G_a to be regular is

$$\mathfrak{R}(\mathbf{J}_{ab}) = N. \tag{45}$$

Since $\mathbf{J}_{ab}$ is field dependent, its rank may change in space. In particular, for a pure gauge configuration $F=0$, and $\mathbf{J}_{ab}$ has rank zero. For other configurations, the rank of Jacobian can range from zero to N, and the irregularities are always of multilinear type because in the expression (43) the phase space coordinates A_i^a occur only linearly.

In general, a non-Abelian CS theory for $D \geqslant 5$ possesses a nonvanishing number of physical degrees of freedom[6]

$$f_{2n+1}(N) = nN - n - N \quad (N \geqslant 2) \tag{46}$$

in regular and *generic* cases.[20] Therefore, in CS theories, the study of dynamics requires not only the analysis of regularity, but also of genericity. In spite of the fact that both conditions are expressed in terms of the same matrix Ω_{ab}^{ij}, they are independent. For example, the extreme case of $F=0$ is both irregular and degenerate, but there are examples in CS supergravity which are generic and irregular.[8] The opposite case occurs in a five-dimensional CS theory based on $G_1 \times G_2$ for particular choice of invariant tensor. In this case, there exist configurations which are regular but degenerate. Take the group indices as $a=(r,\alpha)$ corresponding to G_1 and G_2, respectively, and invariant tensor as $g_{rs1} = g_{rs}$ and $g_{\alpha\beta\bar{1}} = g_{\alpha\beta}$ (both invertible). Then the configuration $F^a = (f^1\, \mathrm{d}x^1 \wedge \mathrm{d}x^2, h^{\bar{1}}\, \mathrm{d}x^3 \wedge \mathrm{d}x^4)$ is regular and degenerate. Indeed, $\mathbf{J}_{ab} = \begin{pmatrix} g_{rs} f^1 & 0 \\ 0 & g_{\alpha\beta} h^{\bar{1}} \end{pmatrix}$ is regular, while Ω_{ab}^{ij} with nonvanishing components $\Omega_{rs}^{34} = g_{rs} f^1$ and $\Omega_{\alpha\beta}^{12} = g_{\alpha\beta} h^{\bar{1}}$ has $2N$ zero modes and is therefore degenerate.

As a consequence of existence of both regularity and genericity issues, the regularization problem is much more delicate in CS theories.

VI. COMMENTS

A. Dirac conjecture

Dirac conjectured that *all* first class constraints generate gauge symmetries.[17] It was shown that Dirac's conjecture is not true for first class constraints of the form f^k $(k>1)$, and following from $\dot{f} \approx 0$.[14,15] Therefore, for systems with nonlinear constraints, the conjecture does not work and they generically provide counterexamples of it.[13,21,22]

From the point of view of irregular systems, it is clear that Dirac's conjecture fails for nonlinear constraints because they do not generate any local transformation, cf. Eq. (31). In Refs. 10 and 11 it was observed that Dirac's conjecture may not hold in the presence of irregular constraints of type II.

In the case of multilinear constraints, however, Dirac's conjecture holds. The fact that at irregular points the constraints do not generate any transformation only means that these are fixed points of the gauge transformation.

B. Quantization

Although, in view of the above discussion, it is possible to deal systematically with classical theories containing irregular constraints, there may be severe problems in their quantum description. Consider a path integral of the form

$$Z \sim \int [\mathrm{d}q][\mathrm{d}p][\mathrm{d}u] \exp i[p\dot{q} - H(q,p) - u\phi(q,p)], \tag{47}$$

where $\phi = [f(q,p)]^k$ is a nonlinear constraint. Integration on u yields to $\delta(f^k)$, which is not well defined for a zero of order $k>1$, making the quantum theory ill defined. Only if the nonlinear constraint could be exchanged by the regular one, $f(q,p)\approx 0$, the quantum theory could be saved. An example of this occurs in the standard approach for QED, where it is usual practice to introduce the nonlinear gauge fixing term $u(\partial_i A^i)^2$ in order to fix the primary constraint $\pi^0 \equiv (\delta I_{ED}/\delta \dot{A}_0) \approx 0$. Since the gauge condition $f(A) = \partial_i A^i(x) \approx 0$ is a second class constraint, its substitution by a regular constraint does not change its dynamical structure.

VII. SUMMARY

We have discussed the dynamics and evolution of a system possessing constraints which may violate the regularity conditions (functional independence) on some subsets of the constraint surface Σ. These so-called irregular systems are seen to arise generically because of nonlinearities in the constraints and can be classified into two families: multilinear (type I) and nonlinear (type II).

Type I constraints are of the form $\phi = \Pi f_i(z)$, where f_i possess simple zeros. These constraints violate the regularity conditions (RCs) on sets of measure zero on the constraint surface Σ.

Type I constraints can be exchanged by equivalent constraints which are regular giving an equivalent dynamical system.

Type II constraints are of the form $\phi = f^k$ $(k>1)$ where f has a simple zero. They violate the RCs on sets of nonzero measure on Σ.

A type II constraint can be replaced by an equivalent linear one only if the latter is second class; if the equivalent linear constraint is first class, substituting it for the original constraint would change the system.

In general, the orbits can cross the configurations where the RCs are violated without any catastrophic effect for the system. If the symplectic form degenerates at the irregular points, additional analysis is required.

The naive linearized approximation of an irregular constrained system generically changes it by erasing the irregular constraints. In order to study the perturbations around a classical orbit in an irregular system, it would be necessary to first regularize it (if possible) and only then do the linearized approximation.

Chern–Simons theories possess irregular and regular sectors. This problem is independent of the presence of degeneracies in the symplectic form, making the regularization problem much more complex.

ACKNOWLEDGMENTS

We are grateful to Milutin Blagojević, Marc Henneaux, and Claudio Teitelboim for enlightening and helpful comments, and specially to Ricardo Troncoso for many useful discussions, insights, and friendly criticisms. We would also like to thank Josep María Pons and Antonio García-Zenteno for bringing their work to our attention and for indicating its relevance to ours. This work is partially funded by grants FONDECYT 1020629, 7020629, 1010450, 2010017 and the grant MECESUP USA 9930. One of us (O.M.) thanks the Abdus Salam ICTP for hospitality during the completion of this work. The generous support of Empresas CMPC to CECS is also acknowledged. CECS is a Millennium Science Institute and is funded in part by grants from Fundación Andes and the Tinker Foundation.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Detecting ill posed boundary conditions in general relativity

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(Received 18 March 2003; accepted 5 May 2003)

A persistent challenge in numerical relativity is the correct specification of boundary conditions. In this work we consider a many-parameter family of symmetric hyperbolic initial-boundary value formulations for the linearized Einstein equations and analyze its well posedness using the Laplace–Fourier technique. By using this technique ill posed modes can be detected and thus a necessary condition for well posedness is provided. We focus on the following types of boundary conditions: (*i*) boundary conditions that have been shown to preserve the constraints, (*ii*) boundary conditions that result from setting the ingoing constraint characteristic fields to zero, and (*iii*) boundary conditions that result from considering the projection of Einstein's equations along the normal to the boundary surface. While we show that in case (*i*) there are no ill posed modes, our analysis reveals that, unless the parameters in the formulation are chosen with care, there exist ill posed constraint violating modes in the remaining cases. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599056]

I. INTRODUCTION

Obtaining a long time convergent numerical simulation of a binary black hole space–time in domains with artificial boundaries continues to be a challenge in numerical relativity and one which has recently received a substantial amount of attention, notably in the case of hyperbolic formulations (see Refs. 1 and 2 for reviews). The challenge remains in part because of the difficulty in specifying boundary conditions. It has been recognized[3–12] that the boundary conditions have to satisfy two important requirements. First, they have to preserve the constraints. By this we mean that they must guarantee that if the constraints are satisfied initially they are also satisfied at later times. We refer to boundary conditions that satisfy this property as constraint preserving boundary conditions (CPBCs). Second, the boundary conditions have to be such that the resulting initial-boundary value problem (IBVP) is well posed. This means that given initial and boundary data a unique solution exists and that at each fixed time the solution depends continuously on the data. Well posedness is a necessary condition for the construction of consistent and stable finite difference schemes.[13,14]

When the evolution equations are in symmetric hyperbolic form one usually specifies maximal dissipative boundary conditions.[15] Under certain technical assumptions, these conditions guarantee that the resulting IBVP is well posed.[16,17] Using maximal dissipative boundary conditions, Friedrich and Nagy[3] were able to find well posed CPBCs for a particular formulation of the full nonlinear vacuum equations. However, most of the hyperbolic formulations used in numerical relativity are based on evolution equations that use a different set of variables than in Ref. 3. For these formulations, the derivation of well posed CPBCs seems to be more difficult. Part of the problem stems from the fact that CPBCs result in a set of partial differential equations that must hold at the boundary surface, and it is not always possible to cast these equations into the form of maximal dissipative boundary conditions. This is probably the reason why current well posed CPBCs for formulations other than that used in Ref. 3 are either limited to homogeneous boundary data[9] or to linearizations around a Minkowski background.[7–9] Even in those cases, the CPBCs obtained so far might be too restrictive in the sense that they do not allow the specification of the

physical quantities at the boundary with the freedom one would like to have. For example, the well posed boundary conditions obtained in Ref. 7 involve a coupling between the in- and outgoing variables and, likely, this coupling will introduce reflections at the boundary. Therefore, more general techniques are desirable in order to show well posedness for more generic CPBCs.

In this article, we use the Laplace–Fourier technique to analyze boundary conditions in linearized general relativity. This technique is very useful when the evolution equations are linear and have constant coefficients since it can be applied to boundary conditions that are more general than the maximal dissipative ones. Specifically, it can be applied to boundary conditions which have the form of differential equations at the boundary. Furthermore, the method is capable of detecting the presence of ill posed modes analytically. Ill posed modes are solutions to the IBVP that grow exponentially in time with an exponential factor that can be arbitrarily large, and their existence makes it impossible for the solution to depend continuously on the data. The Laplace–Fourier technique therefore provides us with a necessary condition for well posedness. However, it should be emphasized that the absence of ill posed modes (as defined in this article) does not automatically guarantee well posedness. Although more complicated in this case, results for the variable coefficient case are available by freezing the coefficients at the boundary (see Refs. 18 and 19).

This article is organized as follows: The conditions under which the specification of nonmaximal dissipative boundary conditions for symmetric hyperbolic systems with constant coefficients yields ill posed modes are reviewed in Sec. II. In Sec. III we discuss the boundary conditions that have been considered for the generalized Einstein–Christoffel formulation of Einstein's equations[20,21] when linearized around flat space–time. The generalized Einstein–Christoffel system is a family of symmetric hyperbolic formulations that is parametrized by a constant η. The boundary conditions we are considering are (i) the CPBCs that were considered in Ref. 7 and that are based on solving a closed evolution system at the boundary and on maximal dissipative boundary conditions, (ii) boundary conditions that are obtained by setting the ingoing constraint characteristic fields to zero, and (iii) boundary conditions that are obtained by considering the projection of Einstein's equations along the normal to the boundary surface, as recently proposed by Frittelli and Gomez.[10,11] In Sec. IV we apply the techniques discussed in Sec. II and show that the cases (ii) and (iii) suffer from the presence of ill posed modes unless the parameter η in the generalized Einstein–Christoffel formulation lies in a specific range. We also show that there are no ill posed modes in case (i) which is consistent with the well posedness estimates derived in Ref. 7. In Sec. V we show that the ill posed modes we have found in cases (ii) and (iii) do, in fact, all violate the constraints. This means that the evolution system for the constraint variables is ill posed in those cases. Since this system is always strongly hyperbolic and since our boundary conditions are constructed from specifying maximal dissipative conditions for this system, this also illustrates that maximal dissipative boundary conditions do not necessarily yield a well posed formulation if the evolution equations are strongly hyperbolic (but not symmetrizable). In particular, our calculations show that the boundary conditions that are constructed following schemes (ii) and (iii) do not necessarily lead to CPBCs and that one should always check the evolution system for the constraint variables. Our results and their implications on deriving well posed CPBCs are discussed in Sec. VI. A similar analysis for the Frittelli–Reula[22] system has been undertaken by Stewart.[4]

II. DETECTING ILL POSED MODES

In this section, we review the techniques that can reveal the presence of ill posed modes. They are based on a Laplace transformation in time and on a Fourier transformation in the spatial directions that are tangential to the boundaries and are described in more detail in Refs. 13 and 23. For simplicity, we restrict the following discussion to the 2D case; the generalization to 3D is straightforward.

Consider a 2D first order in time and space linear evolution equation of the form

$$\partial_t u = A\partial_x u + B\partial_y u, \tag{1}$$

where $u=u(t,x,y)$ is a vector-valued function and the matrices A and B are constant and symmetric. We consider solutions to Eq. (1) on the domain $t>0$, $x>0$, $-\pi<y<+\pi$ with initial data

$$u(0,x,y)=f(x,y) \tag{2}$$

and boundary conditions at $x=0$ of the form

$$L(\partial_t,\partial_y)u(t,0,y)=g(t,y), \tag{3}$$

where L is a linear operator with constant coefficients that only involves derivatives which are tangential to the boundary. For technical reasons, we assume that $L(\partial_t,\partial_y)$ is homogeneous in the sense that $L(\mu\partial_t,\mu\partial_y)=\mu L(\partial_t,\partial_y)$ for all positive μ. We also assume periodic boundary conditions in the y-direction (similar conclusions hold for the case $-\infty<y<+\infty$).

The IBVP (1)–(3) is said to be well posed,[24] if given smooth square integrable data f, g, there exists a unique smooth solution. Furthermore, there are constants C, a such that

$$\|u(t,.)\|^2\leqslant Ce^{at}\left[\|f\|^2+\int_0^t\|g(\tau,.)\|^2d\tau\right], \tag{4}$$

for all $t>0$ and all square integrable data f and g. Here, $\|u(t,.)\|$ denotes the L^2 norm of u defined by $\|u(t,.)\|^2=\int_{x>0}|u(t,x,y)|^2dxdy$ and, similarly, $\|f\|^2=\int_{x>0}|f(x,y)|^2dxdy$ and $\|g(\tau,.)\|^2=\int|g(\tau,y)|^2dy$. The estimate (4) implies that for each fixed t, the solution depends continuously on the data f and g.

A first step in checking if a given initial-boundary formulation satisfies a well posedness inequality of the type (4) is to look for solutions of the problem with homogeneous data ($g=0$) which are of the form

$$u(t,x,y)=e^{st+i\omega y}\tilde{u}(x), \tag{5}$$

where ω is an integer, s is complex with $\mathrm{Re}(s)>0$ and $\tilde{u}(x)$ is a smooth function that lies in $L^2(0,\infty)$. If such a solution exists, the problem cannot be well posed. In order to see this we notice that the functions

$$u_m(t,x,y)=e^{m(st+i\omega y)}\tilde{u}(mx), \tag{6}$$

where $m=1,2,3,\ldots$ can be arbitrarily large, are also solutions and since $\|u_m(t,.)\|/\|u_m(0,.)\|=\exp(m\,\mathrm{Re}(s)t)$ the estimate (4) cannot hold with constants C and a that are independent of the initial data. Therefore, an obvious check for well posedness is to see whether or not Eqs. (1) and (3) admit nontrivial solutions of the form (5) with homogeneous boundary data.

Using expression (5) in Eqs. (1) and (3), we obtain (for $g=0$)

$$s\tilde{u}=A\partial_x\tilde{u}+i\omega B\tilde{u}, \tag{7}$$

$$L(s,i\omega)\tilde{u}(0)=0. \tag{8}$$

These equations form a system of ordinary differential equations and can be solved analytically. In order to do so, we first bring A to diagonal form through an orthonormal transformation. Thus, the matrix B is still symmetric and we can write

$$A=\begin{pmatrix}0 & 0\\ 0 & A_1\end{pmatrix},$$

where $A_1=\mathrm{diag}(\lambda_1,\ldots,\lambda_p,\lambda_{p+1},\ldots,\lambda_{p+q})$ with $\lambda_1,\ldots\lambda_p$ real and negative and $\lambda_{p+1},\ldots,\lambda_{p+q}$ real and positive. Here, p and q are the number of in- and outgoing modes, respectively. Accordingly, we write

$$B=\begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix}, \quad L=(L_0,L_1), \quad \tilde{u}=\begin{pmatrix} \tilde{u}_0 \\ \tilde{u}_1 \end{pmatrix}.$$

Now the zero components of Eq. (7) yield the following algebraic relation between $\tilde{u}_0$ and $\tilde{u}_1$:

$$S_{00}\tilde{u}_0=-S_{01}\tilde{u}_1, \tag{9}$$

where we have introduced the matrix $S=S(s,\omega)=sI-i\omega B$. Since the matrix B is symmetric, the matrix $S_{00}=sI-i\omega B_{00}$ is invertible for all $\mathrm{Re}(s)>0$ and all integer ω, and we can express $\tilde{u}_0$ in terms of $\tilde{u}_1$:

$$\tilde{u}_0=-S_{00}^{-1}S_{01}\tilde{u}_1. \tag{10}$$

Inserting this into the remaining equations of the system (7) and (8), we obtain the reduced problem

$$\partial_x\tilde{u}_1=M(s,\omega)\tilde{u}_1, \tag{11}$$

$$\tilde{L}\tilde{u}_1=0, \tag{12}$$

where

$$M(s,\omega)=A_1^{-1}(S_{11}(s,\omega)-S_{10}S_{00}^{-1}S_{01}(s,\omega)),$$

$$\tilde{L}(s,\omega)=L_1-L_0S_{00}^{-1}S_{01}.$$

One can show[19] that for $\mathrm{Re}(s)>0$ the matrix $M(s,\omega)$ has exactly p eigenvalues with negative real parts and exactly q eigenvalues with positive real parts (the eigenvalues are counted according to their algebraic multiplicity).

The eigenvalues of M that have positive real part lead to exponential growth in x. Since the solution $\tilde{u}$ has to be in $L^2(0,\infty)$, the integration constants have to be chosen such that there is no such growth in x. In order to achieve this, we choose, for each (s,ω), a unitary matrix $U=U(s,\omega)$ that brings $M(s,\omega)$ in upper triangular form:

$$U(s,\omega)^{-1}M(s,\omega)U(s,\omega)=\begin{pmatrix} M_-(s,\omega) & M_0(s,\omega) \\ 0 & M_+(s,\omega) \end{pmatrix}. \tag{13}$$

Here, M_- (M_+) is an upper triangular matrix whose eigenvalues have negative (positive) real parts. If we introduce the new variable $v(x)=U(s,\omega)^{-1}\tilde{u}_1(x)$, system (11) and (12) becomes

$$\partial_x v_-(x)=M_-(s,\omega)v_-(x)+M_0(s,\omega)v_+(x),$$

$$\partial_x v_+(x)=M_+(s,\omega)v_+(x),$$

$$L_-v_-(0)+L_+v_+(0)=0,$$

where $(L_-,L_+)=\tilde{L}U$. It follows that v_+ must vanish for v to be in $L^2(0,\infty)$. This implies that $v_-(x)=\exp(M_-x)\sigma_-$ where σ_- has to satisfy the boundary condition $L_-\sigma_-=0$. We conclude that the system (7) and (8) has only the trivial solution if and only if the determinant condition[25]

$$\det L_-(s,\omega)\neq 0, \quad \mathrm{Re}(s)>0, \tag{14}$$

is satisfied. (In particular, L_- must be a square matrix of dimension p. This means that we need exactly as many independent boundary conditions as there are ingoing modes.) If the determinant condition is violated at some point $(s,\omega)=(s_0,\omega_0)$, it is also violated for $(s,\omega)=m(s_0,\omega_0)$ with

$m=1,2,3,\ldots$ and the initial-boundary formulation admits solutions of the form (5) that grow exponentially in time where the exponential factor s can have arbitrarily large real part.

In Sec. IV we will discuss the determinant condition for the case of the linearized Einstein equations with boundaries.

III. BOUNDARY CONDITIONS FOR THE LINEARIZED EINSTEIN–CHRISTOFFEL SYSTEM

In this section we discuss boundary conditions for a linearization of the generalized Einstein–Christoffel vacuum equations.[20] This formulation has the attractive feature that when linearized around flat space–time written in Minkowski coordinates it simply reduces to a set of six wave equations, written in first order form:

$$\partial_t K_{ij} = -\delta^{kl}\partial_k f_{lij}, \tag{15}$$

$$\partial_t f_{kij} = -\partial_k K_{ij}. \tag{16}$$

Here, K_{ij} denotes the linearized extrinsic curvature and the symbols f_{kij} represent linear combinations of the linearized Christoffel symbols Γ_{kij}:

$$f_{kij} = \Gamma_{(ij)k} + \delta^{rs}\left(\delta_{ki}\Gamma_{[sj]r} + \delta_{kj}\Gamma_{[si]r} + \frac{\eta-4}{2\eta}\delta_{ij}\Gamma_{[sk]r}\right). \tag{17}$$

The value of η (which has to be different from zero) parametrizes the family of formulations. The particular case with $\eta=4$ corresponds to the original Einstein–Christoffel system derived by Anderson and York.[21] We set the shift to zero, and the lapse is linearized in such a way that it satisfies the densitized lapse gauge condition $\alpha=\sqrt{g}$ up to second order corrections, where g denotes the determinant of the three metric. A solution to the system (15) and (16) is a solution to the linearized Einstein equations if and only if the constraints are satisfied. In terms of the constraint variables

$$C = \frac{\eta}{4}\delta^{rs}\partial_r v_s, \tag{18}$$

$$C_j = \delta^{rs}(\partial_r K_{sj} - \partial_j K_{rs}), \tag{19}$$

$$C_{lkij} = 2\partial_{[l}f_{k]ij} + \eta\,\partial_{[l}\delta_{k](i}v_{j)} + \frac{\eta-4}{4}\delta_{ij}\partial_{[l}v_{k]}, \tag{20}$$

where $v_k = \delta^{ij}(f_{kij} - f_{ijk})$, the constraints are given by $C=0$, $C_j=0$, $C_{lkij}=0$.

We consider the evolution system (15) and (16) on the domain $t>0$, $x>0$, $-\pi<y, z, <+\pi$ and introduce the characteristic variables in the x direction,[26]

$$u^{(-)}_{ij} = \frac{1}{\sqrt{2}}(K_{ij} + f_{xij}), \tag{21}$$

$$u^{(+)}_{ij} = \frac{1}{\sqrt{2}}(K_{ij} - f_{xij}), \tag{22}$$

$$u^{(0)}_{Aij} = f_{Aij}\ . \tag{23}$$

Here and in the following, capital Latin indices stand for the tangential directions y and z. When written in terms of these variables the evolution equations (15) and (16) take the form

$$\partial_t u_{ij}^{(-)} = -\partial_x u_{ij}^{(-)} - \frac{1}{\sqrt{2}} \delta^{AB} \partial_A u_{Bij}^{(0)}, \tag{24}$$

$$\partial_t u_{ij}^{(+)} = +\partial_x u_{ij}^{(+)} - \frac{1}{\sqrt{2}} \delta^{AB} \partial_A u_{Bij}^{(0)}, \tag{25}$$

$$\partial_t u_{Aij}^{(0)} = -\frac{1}{\sqrt{2}} \partial_A (u_{ij}^{(-)} + u_{ij}^{(+)}), \tag{26}$$

and we see that the matrix A in Eq. (1) is diagonal.

For the constraints to be satisfied everywhere, when boundaries are present, one has to ensure that they are satisfied initially and that no constraint violating mode enters the domain. In order to ensure this, we follow the analysis in Ref. 7 and first consider the evolution of the constraint variables with respect to the flux defined by the main evolution equations (15) and (16). One can show[7] that the traceless part of C_{lkij} is constant in time, while the remaining constraints propagate according to

$$\partial_t C = \frac{\eta}{4} \delta^{ij} \partial_i C_j, \tag{27}$$

$$\partial_t C_j = \frac{4-2\eta}{\eta} \partial_j C - \delta^{rs} \partial_r T_{sj}, \tag{28}$$

$$\partial_t T_{ij} = -\partial_i C_j + \left(1 - \frac{3\eta}{4}\right) \partial_j C_i + \frac{\eta}{4} \delta_{ij} \delta^{rs} \partial_r C_s, \tag{29}$$

$$\partial_t V_{ij} = \left(\frac{7\eta}{4} - 3\right) \partial_{[i} C_{j]}, \tag{30}$$

where $T_{ij} = \delta^{rs}(C_{rijs} + C_{ijrs})$, and $V_{ij} = \delta^{rs} C_{ijrs}$. Introducing $\kappa = 1 - 3\eta/4$ and the variables

$$C_{ij} = T_{ij} + \frac{2\eta - 4}{\eta} \delta_{ij} C = \delta^{rs}(\partial_r f_{ijs} - \partial_j f_{irs}) + \kappa \partial_j v_i - \kappa \delta_{ij} \delta^{rs} \partial_r v_s, \tag{31}$$

the characteristic fields can be written as[27]

$$V_j^{(-)} = \frac{1}{\sqrt{2}}(C_j + C_{xj}), \tag{32}$$

$$V_j^{(+)} = \frac{1}{\sqrt{2}}(C_j - C_{xj}), \tag{33}$$

$$V_{Aj}^{(0)} = C_{Aj} + \kappa(\delta_{xj} C_{xA} - \delta_{Aj} C_{xx}), \tag{34}$$

$$\tilde{V}_{ij}^{(0)} = -\frac{7\kappa + 2}{3} C_{[ij]} + (\kappa + 1) V_{ij}. \tag{35}$$

If the system (27)–(30) is symmetric (or symmetrizable) hyperbolic, one can guarantee that if the constraints are satisfied initially and if homogeneous maximal dissipative boundary conditions are given, the constraints will be satisfied everywhere. Therefore, we consider boundary conditions at $x = 0$ which are of the form

$$V_x^{(-)} - a V_x^{(+)} = 0, \quad V_A^{(-)} - b V_A^{(+)} = 0, \tag{36}$$

$$u_{xx}^{(-)} - c\, u_{xx}^{(+)} = g_{xx}, \quad \hat{u}_{AB}^{(-)} - d\, \hat{u}_{AB}^{(+)} = \hat{g}_{AB}, \tag{37}$$

where the magnitudes of a, b, c and d are smaller or equal to 1 and $\hat{u}_{AB}^{(\mp)} = u_{AB}^{(\mp)} - \frac{1}{2}\delta_{AB}\delta^{CD}u_{CD}^{(\mp)}$ denotes the traceless part of $u_{AB}^{(\mp)}$. In order to express the conditions (36) in terms of the main variables K_{ij}, f_{kij}, we use the definition of the constraint variables, Eqs. (18), (19), and (31), and the evolution equations (15) and (16) in order to trade x-derivatives by time and tangential derivatives:

$$V_x^{(\mp)} = \delta^{AB}\left[\pm \partial_t u_{AB}^{(\mp)} + \partial_A u_{xB}^{(\mp)} \pm \frac{\delta^{CD}}{\sqrt{2}}\partial_C u_{DAB}^{(0)} \pm \frac{\kappa}{2}\partial_A(\sqrt{2}\,\delta^{CD}u_{CDB}^{(0)} - \sqrt{2}\,\delta^{ij}u_{Bij}^{(0)} + u_{xB}^{(-)} - u_{xB}^{(+)})\right],$$

$$V_A^{(\mp)} = \mp \partial_t u_{xA}^{(\mp)} + \delta^{CD}\partial_C u_{AD}^{(\mp)} - \delta^{ij}\partial_A u_{ij}^{(\mp)} \mp \frac{\delta^{CD}}{\sqrt{2}}\partial_C u_{DxA}^{(0)} \mp \frac{\kappa}{2}\delta^{CD}\partial_A(\sqrt{2}u_{CDx}^{(0)} - u_{CD}^{(-)} + u_{CD}^{(+)}).$$

It follows from the energy estimates derived in Ref. 7 that when $0 < \eta < 2$ the conditions (36) guarantee that the constraints are satisfied everywhere if they are satisfied initially. In the following, we will also consider other values of η and show that one might have ill posed modes if the parameter η lies outside the interval (0, 2). Notice that the conditions (36) do not involve derivatives normal to the boundary (∂_x). They can be interpreted as evolution equations for the variables $\delta^{AB}(u_{AB}^{(-)} + a u_{AB}^{(+)})$ and $u_{xA}^{(-)} + b u_{xA}^{(+)}$ at the boundary. The functions g_{xx} and $\hat{g}_{AB}$ are data that can be given freely for a combination of the in- and outgoing gauge and physical variables, respectively.[7]

In the next section, we will analyze the following choices of parameters:

(1) $a = -1$, $b = 1$, $c = d = 1$:
This corresponds to the Neumann boundary conditions that we have discussed in Ref. 7. In this case the boundary conditions can be recast in a closed evolution system at the boundary. Its solutions provide boundary data for the main evolution system in the form of maximal dissipative boundary conditions. When $0 < \eta < 2$ one can derive well posedness estimates for the resulting IBVP and the boundary conditions can indeed be called CPBCs.

(2) $a = 1$, $b = -1$, $c = d = -1$:
This corresponds to the Dirichlet conditions specified in Ref. 7. They can also be recast in a closed evolution system at the boundary, and for $0 < \eta < 2$ one has a well-posed IBVP with CPBCs.

(3) $a = 0$, $b = 0$:
This corresponds to setting the ingoing constraint variables to zero and might be the most obvious choice for obtaining CPBCs. However, we will show in the next section that the resulting IBVP possesses ill posed modes unless the parameter η is chosen appropriately.

(4) $a = 0$, $b = 1$:
These are the conditions that one obtains after linearizing the boundary conditions that were recently proposed in Ref. 11. There, the Einstein–Christoffel formulation ($\eta = 4$) is considered and the boundary conditions (36) are obtained by projecting Einstein's equations along the normal to the boundary rather than by analyzing the evolution of the constraints. In fact, one can show that setting G_{xA} to zero and rewriting[28] the resulting equations in terms of the variables K_{ij} and f_{kij} is equivalent to the second equation in (36) with $b = 1$, while setting G_{xx} (G_{tx}) to zero is equivalent to the first equation in (36) with $a = 1$ ($a = -1$). In Ref. 11, the authors propose to set the linear combination $G_{xx} - G_{tx}$ to zero which would correspond to using $a = 0$ in (36). In the next section, we show that the resulting boundary conditions yield an ill posed formulation if the parameter η is not chosen appropriately.

IV. LAPLACE–FOURIER ANALYSIS

Following the analysis described in Sec. II, we look for solutions to Eqs. (15), (16), (36), and (37) with homogeneous boundary data ($g_{xx}=0$, $\hat{g}_{AB}=0$) and which are of the form

$$u_{ij}^{(\mp)}(t,x,y,z)=e^{st+i\omega_y y+i\omega_z z}\tilde{u}_{ij}^{(\mp)}(x), \tag{38}$$

$$u_{Aij}^{(0)}(t,x,y,z)=e^{st+i\omega_y y+i\omega_z z}\tilde{u}_{Aij}^{(0)}(x), \tag{39}$$

where s is a complex number with positive real part and ω_y and ω_z are integers. For the solution to be square integrable, we require the functions $\tilde{u}_{ij}^{(\mp)}(x)$ and $\tilde{u}_{Aij}^{(0)}(x)$ to be in $L^2(0,\infty)$. From Eqs. (38), (39), and (26) we obtain an algebraic condition

$$s\tilde{u}_{Aij}^{(0)}=-\frac{i}{\sqrt{2}}\omega_A(\tilde{u}_{ij}^{(-)}+\tilde{u}_{ij}^{(+)}) \tag{40}$$

that can be used to eliminate the variable $\tilde{u}_{Aij}^{(0)}$ from the remaining equations. Inserting Eqs. (38)–(40) into Eqs. (24) and (25) yields the ordinary differential equation

$$\partial_x\begin{pmatrix}\tilde{u}_{ij}^{(-)}\\ \tilde{u}_{ij}^{(+)}\end{pmatrix}=M(s,\underline{\omega})\begin{pmatrix}\tilde{u}_{ij}^{(-)}\\ \tilde{u}_{ij}^{(+)}\end{pmatrix}, \tag{41}$$

where

$$M(s,\underline{\omega})=\begin{pmatrix}-s-\dfrac{\underline{\omega}^2}{2s} & -\dfrac{\underline{\omega}^2}{2s}\\ \dfrac{\underline{\omega}^2}{2s} & s+\dfrac{\underline{\omega}^2}{2s}\end{pmatrix} \tag{42}$$

and $\underline{\omega}=(\omega_y,\omega_z)$. The matrix $M(s,\underline{\omega})$ has the eigenvalues $\pm\sqrt{s^2+\underline{\omega}^2}$.

We first look at the case $\underline{\omega}=0$, which corresponds to solutions that have trivial y and z dependence. For those, the matrix $M(s,\underline{\omega})$ is diagonal and since $\mathrm{Re}(s)>0$ we see that we must have $\tilde{u}_{ij}^{(+)}=0$ for the solution to be in L^2. The boundary conditions (36) and (37) yield

$$\tilde{u}_{xx}^{(-)}(0)=0,\ \ \hat{\tilde{u}}_{AB}^{(-)}(0)=0,\ \ s\delta^{AB}\tilde{u}_{AB}^{(-)}(0)=0,\ \ s\tilde{u}_{xA}^{(-)}(0)=0, \tag{43}$$

therefore we have only the trivial solution. There are no ill posed modes with trivial dependence on the variables that are tangential to the boundary. We show now that the situation becomes rather more complicated when one considers modes that have a nontrivial tangential dependence.

Assume that $\underline{\omega}\neq 0$. Following the analysis of Sec. II we introduce a unitary matrix $U=U(s,\underline{\omega})$ that brings the matrix $M(s,\underline{\omega})$ into upper triangular form. To lighten the notation we introduce the quantities $\zeta=s/|\underline{\omega}|$, $\lambda=\sqrt{1+\zeta^2}$, $\psi(\zeta)=(\lambda-\zeta)^2$ and $N=1+|\psi(\zeta)|^2$. One can then verify that the matrix (a star denotes complex conjugation)

$$U(\zeta)=N^{-1/2}\begin{pmatrix}-\dfrac{|\zeta|}{\zeta} & \dfrac{|\zeta|}{\zeta^*}\psi^*\\ \dfrac{|\zeta|}{\zeta}\psi & \dfrac{|\zeta|}{\zeta^*}\end{pmatrix} \tag{44}$$

is unitary and satisfies

$$U(\zeta)^{-1}MU(\zeta)=|\underline{\omega}|\begin{pmatrix}-\lambda & M_0(\zeta)\\ 0 & \lambda\end{pmatrix},\quad M_0(\zeta)=\frac{1+\psi^*(2+4\zeta^2+\psi^*)}{2\zeta^*N}, \tag{45}$$

where in λ the branch is chosen such that for $\mathrm{Re}(\zeta)>0$, $\mathrm{Re}(\lambda)>0$. In terms of the new variables $(v_{ij}^{(-)},v_{ij}^{(+)})^T=U^{-1}(\tilde{u}_{ij}^{(-)},\tilde{u}_{ij}^{(+)})^T$ Eq. (41) yields

$$|\underline{\omega}|^{-1}\partial_x v_{ij}^{(-)}=-\lambda v_{ij}^{(-)}+M_0(\zeta)v_{ij}^{(+)}, \tag{46}$$

$$|\underline{\omega}|^{-1}\partial_x v_{ij}^{(+)}=\lambda v_{ij}^{(+)}. \tag{47}$$

For the solution to be in L^2, we must have $v_{ij}^{(+)}=0$. This implies that $v_{ij}^{(-)}=e^{-\lambda|\underline{\omega}|x}\sigma_{ij}$, where σ_{ij} are constants which describe the value that $v_{ij}^{(-)}$ takes at the boundary. Using the matrix $U(\zeta)$ we can express the $\tilde{u}$ variables at the boundary as

$$\tilde{u}_{ij}^{(-)}(0)=-N^{-1/2}\frac{|\zeta|}{\zeta}\sigma_{ij}, \tag{48}$$

$$\tilde{u}_{ij}^{(+)}(0)=N^{-1/2}\frac{|\zeta|}{\zeta}\psi(\zeta)\sigma_{ij}, \tag{49}$$

$$\tilde{u}_{Aij}^{(0)}(0)=\frac{i}{\sqrt{2}}\frac{\hat{\omega}_A}{\zeta}N^{-1/2}\frac{|\zeta|}{\zeta}(1-\psi(\zeta))\sigma_{ij}, \tag{50}$$

where $\hat{\omega}_A=\omega_A/|\underline{\omega}|$.

Using Eqs. (38), (48), and (49) in the boundary condition (37), we find that

$$(1+c\psi(\zeta))\sigma_{xx}=0,\ \ (1+d\psi(\zeta))\hat{\sigma}_{AB}=0, \tag{51}$$

where $\hat{\sigma}_{AB}$ denotes the tracefree part of σ_{AB}. Since the function $\psi(\zeta)$ maps the half plane $\mathrm{Re}(\zeta)>0$ to the interior of the unit circle and since $|c|\leqslant 1$, $|d|\leqslant 1$, it follows that $\sigma_{xx}=0$ and $\hat{\sigma}_{AB}=0$.

Next, we insert all of this into the boundary conditions (36). The result is more conveniently expressed if one introduces a normalized vector $\hat{\xi}_A$ that is orthogonal to $\hat{\omega}_A$ and considers the components $\sigma_{x\omega}=\delta^{AB}\sigma_{xA}\hat{\omega}_B$ and $\sigma_{x\xi}=\delta^{AB}\sigma_{xA}\hat{\xi}_B$. The projection of the second equation in (36) along $\hat{\xi}$ implies that $\sigma_{x\xi}$ must vanish, while the remaining equations in (36) imply that $\sigma\equiv\delta^{AB}\sigma_{AB}$ and $\sigma_{x\omega}$ must satisfy the following 2×2 system:

$$\begin{gathered}L_-(\zeta)\begin{pmatrix}\sigma\\ \sigma_{x\omega}\end{pmatrix}=0,\\ L_-(\zeta)=\begin{pmatrix}2\lambda(1+a\psi)-\kappa(1+a)(\lambda-\zeta) & 2i(1+a\psi)+i\kappa(1+a)(1+\psi)\\ i(1+b\psi)-i\kappa(1+b)(1+\psi) & 2\lambda(1+b\psi)+2\kappa(1+b)(\lambda-\zeta)\end{pmatrix}.\end{gathered} \tag{52}$$

The determinant of $L_-(\zeta)$ is given by

$$\det L_-(\zeta)=(6+4\zeta^2)[(1+a\psi(\zeta))(1+b\psi(\zeta))-\kappa^2(1+a)(1+b)\psi(\zeta)]. \tag{53}$$

Clearly, the first factor cannot be zero since $\mathrm{Re}(\zeta)>0$. Therefore, $\det L_-(\zeta)$ can only vanish if the term inside the square brackets does.

We now focus on the different cases discussed in the previous section:

(1) $a=-1$, $b=1$, $c=d=1$:
In this case, the second term inside the square brackets vanishes and the first term is never zero since $|\psi(\zeta)|<1$. Therefore, the resulting formulation possesses no ill posed modes. Of course, when $0<\eta<2$ this is consistent with our calculation in Ref. 7 where the estimates we have derived exclude the presence of ill posed modes.

(2) $a=1$, $b=-1$, $c=d=-1$:
The result is the same as in the previous case.
(3) $a=0$, $b=0$:
In this case, the terms inside the square brackets simplify to $1-\kappa^2\psi(\zeta)$. A small calculation reveals that this can only be zero if $\zeta=(\kappa^2-1)/2|\kappa|$ and $\kappa\neq 0$. Therefore, $\det L_-(\zeta)$ has a zero with $\mathrm{Re}(\zeta)>0$ if and only if $\kappa^2>1$. This is equivalent to $\eta<0$ or $\eta>\frac{8}{3}$. Therefore, setting the ingoing constraint variables to zero in the family of generalized Einstein–Christoffel systems does indeed yield ill posed boundary conditions if the parameter η lies outside the interval [0, 8/3].
(4) $a=0$, $b=1$:
Here the terms inside the square brackets reduce to $1+(1-2\kappa^2)\psi(\zeta)$. Since the function ψ maps the positive real axis onto the open interval (0, 1) it follows that this expression never vanishes if and only if $\kappa^2\leqslant 1$. In particular, one has ill posed modes when $\eta=4$ and the boundary conditions that were proposed in Ref. 11 yield, at least when linearized around flat space–time, an ill posed initial-boundary formulation. On the other hand, if at the boundary one considers the equations $G_{xy}=G_{xz}=0$ and the equation $G_{xt}=0$ instead of the combination $G_{xx}-G_{xt}=0$, one has $a=-1$ and the resulting formulation does not in fact suffer from possessing ill posed modes.

V. VIOLATIONS OF THE CONSTRAINTS

In this section, we show that the ill posed modes we have found in the previous section violate the constraints. In order to see this, we use these ill posed modes to compute the constraint variables C_j. From $K_{ij}=(u_{ij}^{(-)}+u_{ij}^{(+)})/\sqrt{2}$, Eqs. (19), (48), and (49), and $\sigma_{xx}=0$, $\hat{\sigma}_{AB}=0$, we have

$$C_x=-\frac{|\underline{\omega}|}{\sqrt{2N}}\frac{|\zeta|}{\zeta}(1-\psi(\zeta))(\lambda\sigma+i\sigma_{x\omega})\exp[|\underline{\omega}|(\zeta t-\lambda x+i\hat{\omega}_A x^A)], \tag{54}$$

$$\omega^A C_A=\frac{|\underline{\omega}|}{\sqrt{8N}}\frac{|\zeta|}{\zeta}(1-\psi(\zeta))(i\sigma+2\lambda\sigma_{x\omega})\exp[|\underline{\omega}|(\zeta t-\lambda x+i\hat{\omega}_A x^A)], \tag{55}$$

where $(\sigma,\sigma_{x\omega})$ is a nontrivial solution to Eq. (52). Since $|\psi(\zeta)|<1$ for $\mathrm{Re}(\zeta)>0$, and since

$$\det\begin{pmatrix}\lambda & i\\ i & 2\lambda\end{pmatrix}=3+2\zeta^2\neq 0, \tag{56}$$

we see that the variables C_x and $\omega^A C_A$ cannot simultaneously vanish. Therefore, all the ill posed modes we have found are *constraint violating* modes. This means that under generic small perturbations of the initial data these modes will be excited and the constraint variables will grow exponentially with an exponential factor that can be arbitrarily large. In this sense, the boundary conditions that lead to ill posed modes do *not* preserve the constraints. We point out that the constraint variables constructed from any solution of the main evolution system (15) and (16) with boundary conditions (36) and (37) provide a solution of the evolution of the constraint variables, Eqs. (27)–(30) with boundary conditions (36). Since we have shown that the constraint variables constructed from ill posed modes are ill posed modes themselves [see Eqs. (54) and (55)], the IBVP for the constraint variables cannot be well posed. This emphasizes the importance of looking at the evolution system for the constraints and checking its well posedness when deriving CPBCs for Einstein's equations.

We conclude this section with two remarks. First, one can check that the evolution system for the constraint variables, Eqs. (27)–(30), is strongly hyperbolic for any nonvanishing value of the parameter η. On the other hand, our analysis above shows the existence of ill posed modes when η lies outside of the interval $[0,\frac{8}{3}]$ and the coupling constants a and b are chosen as in cases (3)

and (4) of the previous section. This illustrates that applying maximal dissipative boundary conditions to evolution systems that are strongly hyperbolic (but not symmetrizable) does not necessarily yield a well posed problem.

The second remark concerns the choice $a=b=-1$ for the coupling constants in Eq. (36). In this case it follows that the determinant condition is always satisfied, regardless of the value for the parameter η. In fact, one can show that the resulting boundary conditions are constraint preserving: The evolution equations imply that the constraint variable C_j satisfies the wave equation:

$$\partial_t^2 C_j = \delta^{rs}\partial_r\partial_s C_j. \tag{57}$$

On the other hand, the choice $a=b=-1$ corresponds to imposing the momentum constraint at the boundary. Since C_j satisfies the wave equation, this implies that $C_j=0$ everywhere, if C_j is satisfied initially. It then follows from Eqs. (27), (29), and (30) that the remaining constraints are also satisfied if they are satisfied initially. This explains why one has CPBCs for all $\eta\neq 0$ when $a=b=-1$. However, the above argumentation is expected to break down when one considers the nonlinear regime since in this case lower order terms might prevent one from obtaining a closed system for C_j alone. In this case, one has to rely on the symmetrizer for the system (27)–(30) which was constructed in Ref. 7, and one might not be able to show that the constraints propagate when η lies outside the interval $[0, 2)$, even when $a=b=-1$.

VI. CONCLUSIONS

We have analyzed ill posed modes in the family of the generalized Einstein–Christoffel formulation of Einstein's equations with boundaries. We considered boundary conditions which result from coupling the ingoing characteristic constraint variables to the outgoing ones. Specifically, the cases we have studied include the boundary conditions we have obtained in Ref. 7 and the boundary conditions that originate from considering the projection of Einstein's equations along the normal to the boundary. When linear fluctuations around Minkowski space are considered, we have shown that the formulation is subject to constraint violating ill posed modes unless the parameters in the equations and the coupling between the in- and outgoing constraint variables are chosen carefully. In fact, it is not difficult to show that if the coupling constants a and b are real and satisfy $-1<a\leqslant 1$ and $-1<b\leqslant 1$ there are always ill posed modes as long as the parameter η lies outside the interval $[0,\frac{8}{3}]$. In particular, this is the case when the ingoing constraint variables are set to zero. Furthermore, there are ill posed modes for the boundary conditions that were obtained in Ref. 11 when applied to the linearized Einstein–Christoffel system ($\eta=4$). However, our analysis also reveals that these ill posed modes could easily be avoided by imposing a different linear combination of Einstein's equations at the boundary or by changing the parameter η such that it lies in the interval $0<\eta\leqslant\frac{8}{3}$. In any case, our analysis highlights the importance of studying the evolution system for the constraint variables and ensuring its well posedness since all the ill posed modes we have found are constraint violating. In particular, the formulations we have studied in this article show that even though the main evolution system is symmetric hyperbolic, the evolution equations for the constraint variables is not necessarily symmetrizable. For the cases in which the propagation of the constraints is described by a system that is strongly hyperbolic (but not symmetrizable) we have shown that specifying maximal dissipative boundary conditions can lead to an ill posed system.

It is interesting to note that all the ill posed modes that appear have a nontrivial dependence in the spatial directions that are tangential to the boundary surface. Therefore, such modes would not be present in the one-dimensional case. This might explain why the numerical simulations in Ref. 6, where the Einstein–Christoffel system ($\eta=4$) was evolved using boundary conditions obtained by setting the ingoing constraints to zero, did not show any ill posed modes.

The simple analytic method we have used in this article, which is based on the determinant condition (14), should be used to test the well posedness of the boundary conditions before numerically evolving any evolution system since the presence of ill posed modes would detrimen-

tally affect numerical stability. However, we also stress that more work is required to derive sufficient conditions for well posedness for the choices of parameters when the determinant condition is satisfied. In particular, it would be worthwhile to analyze CPBCs where the incoming physical variables can be freely specified.

ACKNOWLEDGMENTS

We particularly thank Gabriel Nagy for many valuable discussions. We also thank L. Lehner, J. Pullin, O. Reula, and M. Tiglio for useful comments. This work was supported in part by Grant Nos. NSF-PHY-9800973 and NSF-INT-0204937, and the Horace C. Hearne Jr. Institute of Theoretical Physics.

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[24] When discussing initial-boundary value problems one sometimes demands a slightly stronger estimate that also bounds the norm of the solution at the boundary surface. For the purpose of the present article, it is sufficient to consider the weaker estimate (4) since we will show that when the determinant condition is violated, the inequality (4) cannot hold for all initial data.
[25] This condition is weaker than the uniform Kreiss condition[18] that requires that $|\det L_-|$ must be bounded away from zero. The reason why here we do not require the uniform Kreiss condition is that it might be too strong for the case of CPBCs in general relativity. As we will see in Sec. IV the well posed CPBCs that were derived in Ref. 7 do not satisfy the uniform Kreiss condition.
[26] Notice that the characteristic variables defined here are related with the ones $v_{ij}^{(\pm)}$ defined in Ref. 7 according to $u_{ij}^{(\pm)} = v_{ij}^{(\mp)}/\sqrt{2}$.
[27] For $\eta=2$ or $\eta=\frac{8}{3}$ these fields are not complete. When $\eta=2$ it follows that C_{ij} is traceless and as a consequence, $\delta^{AB}V_{AB}^{(0)}=0$. But in this case one has the additional field $2C+C_{xx}$ that propagates with zero speed. When $\eta=\frac{8}{3}$, $\tilde{V}_{ij}=0$ can be replaced by the fields V_{AB} and $6V_{xA}+5C_{xA}$.
[28] Actually this procedure is not unique since there is an ambiguity when first derivatives of the variables K_{ij} and f_{kij} are substituted for second derivatives of the three-metric. This ambiguity stems from the fact that one can always change the resulting expression by using the constraints $C_{lkij}=0$. For definiteness, we take the choice that leads to the same boundary conditions as in Ref. 7.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Dynamical system approach to FRW models in higher-order gravity theories

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(Received 18 March 2003; accepted 30 April 2003)

We study the late time evolution of positively curved FRW models with a scalar field which arises in the conformal frame of the $R+\alpha R^2$ theory. The resulted three-dimensional dynamical system has two equilibrium solutions corresponding to a de Sitter space and an ever expanding closed universe. We analyze the structure of the first equilibrium with the methods of the center manifold theory and, for the second equilibrium, we apply the normal form theory to obtain a simplified system, which we analyze with special phase plane methods. It is shown that an initially expanding closed FRW space–time avoids recollapse. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1602161]

I. INTRODUCTION

A central question in relativistic cosmology is that of deciding about the past and future asymptotic states of cosmological models.[1] However, general relativity leads to singularities in the space–times of all known cosmological models with ordinary matter. Higher order curvature corrections in the gravitational action may rectify the problem and lead to cosmological models free from such pathologies, at the cost of diverging from a FRW behavior at late times.[2] There is a resurgence of interest in such theories which naturally arise in string-theoretic considerations (cf. brane models with Gauss–Bonett terms[3–6]). An interesting feature of higher order theories is that inflation emerges in these theories in a most direct way. In one of the first inflationary models, proposed in 1980 by Starobinsky,[7] inflation is due to the R^2 correction term in a gravitational Lagrangian $L=R+\alpha R^2$ where α is a constant. The dynamics of higher order cosmologies is closely related to scalar-field cosmologies in general relativity because of their conformal equivalence.[8,9] There are certain limitations to this procedure related to the issue of physical reality of the two metrics involved[10] and to the fact that the conformal transformation may fail to be regular at all points of the space–time. Nevertheless, it is practically useful and investigations in the conformal frame have given some interesting results, e.g., the cosmic no-hair theorem in quadratic cosmologies.[11,12]

Most of the studies of scalar-field cosmologies with the dynamical systems methods are restricted to FRW models (see, for example, Refs. 13 and 14, and references therein), although there are important investigations in spatially homogeneous Bianchi cosmologies with an exponential potential.[15] In particular, for flat FRW models with a scalar field there are some general results which do not rely on the particular properties of the potential.[16,17] However, the situation is more delicate for positively curved FRW models with a scalar field having a potential with a zero local minimum. The main problem which confronts us is the following: Can a closed universe filled with ordinary matter and a scalar field avoid recollapse?

In this article we investigate the evolution of positively curved FRW models with a scalar field having the potential which arises in the conformal frame of the $R+\alpha R^2$ theory in vacuum.[8,11] The motivation for this choice is presented in Sec. III. The dimension of the dynamical systems involved in such models is greater than two and the usual methods of phase plane analysis cannot

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be applied. In particular, for nonhyperbolic equilibrium points the linearization theorem does not yield any information about the stability of the equilibria and, therefore, more powerful methods are needed. The center manifold theorem shows that the qualitative behavior in a neighborhood of a nonhyperbolic equilibrium point **q** is determined by its behavior on the center manifold near **q**. Since the dimension of the center manifold is generally smaller than the dimension of the dynamical system, this greatly simplifies the problem. The other general method for simplifying the dynamical system is the normal form theory, which consists in a nonlinear coordinate transformation that allows us to simplify the nonlinear part of the system. Both methods are used in Secs. III and IV, respectively.

The plan of the article is as follows. In the next section we write down the field equations assuming an arbitrary potential, as a constrained four-dimensional dynamical system. In Sec. III, we use the constraint equation to reduce the dimension of the system to three and after a suitable change of variables we find the equilibrium points of the system and discuss the physical meaning of these particular solutions. In particular we show using the methods of the center manifold theory that the equilibrium corresponding to the de Sitter solution is asymptotically unstable. In Sec. IV we find the so-called normal form of the dynamical system, which greatly simplifies the problem, since two of the equations decouple. We study the qualitative behavior of the resulted two-dimensional system and analyze the late time evolution of the model. We show that an initially expanding universe avoids recollapse. In Sec. V we apply the same techniques to flat FRW spaces filled with a barotropic fluid in the conformal frame of the $R+\alpha R^2$ theory and study the detailed evolution of the models.

II. SCALAR-FIELD COSMOLOGIES

In general relativity the evolution of FRW models with a scalar field (ordinary matter is described by a perfect fluid with energy density ρ and pressure p) are governed by the Friedmann equation,

$$\left(\frac{\dot{a}}{a}\right)^2+\frac{k}{a^2}=\frac{1}{3}\left(\rho+\frac{1}{2}\dot{\phi}^2+V(\phi)\right), \tag{1}$$

the Raychaudhuri equation,

$$\frac{\ddot{a}}{a}=-\frac{1}{6}(\rho+3p+2\dot{\phi}^2-2V), \tag{2}$$

the equation of motion of the scalar field,

$$\ddot{\phi}+3\frac{\dot{a}}{a}\dot{\phi}+V'(\phi)=0, \tag{3}$$

and the conservation equation,

$$\dot{\rho}+3(\rho+p)\frac{\dot{a}}{a}=0. \tag{4}$$

We adopt the metric and curvature conventions of Ref. 1. Here, $a(t)$ is the scale factor, an overdot denotes differentiation with respect to time t and units have been chosen so that $c=1=8\pi G$.

From Eqs. (1)–(4) we see that the state $(a,\dot{a},\rho,\phi,\dot{\phi})\in\mathbb{R}^5$ of the system lies on the hypersurface defined by the constraint, (1), and the remaining field equations can be written as a five-dimensional dynamical system. In vacuum, $\rho=0$, the dimension of the dynamical system reduces to four.

In the literature of scalar-field cosmologies the exponential potential function, viz., $V(\phi)=V_0e^{-\lambda\phi}$, is the most popular not only because of the variety of alternative theories of gravity

which predict exponential potentials, but also due to the fact that this potential has the nice property that $V' \propto V$, which allows the introduction of normalized variables according to the formalism of Wainwright *et al.*[1] In flat $k=0$ FRW models, for example, with a scalar field having an exponential potential, introducing the variables $x \sim \dot{\phi}/H$, $y \sim \sqrt{V}/H$ and the time coordinate $\tau = \ln(a/a_0)$ enables the evolution equations to be written as a two-dimensional dynamical system (cf. Ref. 18) and in more general homogeneous cosmologies associated with a scalar field, the dimension of the dynamical system reduces by one if the potential function is exponential.

If we set $\dot{\phi}=y$, $\dot{a}/a=H$, the evolution equations (2)–(4) in vacuum become

$$\begin{aligned} \dot{a} &= Ha, \\ \dot{\phi} &= y, \\ \dot{y} &= -3Hy - V'(\phi), \\ \dot{H} &= -\tfrac{1}{2}y^2 + k/a^2, \end{aligned} \tag{5}$$

subject to the constraint

$$3H^2 + 3k/a^2 = \tfrac{1}{2}y^2 + V(\phi). \tag{6}$$

Therefore, the phase space of the dynamical system (5) is the set

$$\{(a,\phi,y,H) \in \mathbb{R}^4 : 3H^2 + 3k/a^2 = \tfrac{1}{2}y^2 + V(\phi)\}.$$

III. CURVED FRW IN $R+\alpha R^2$ THEORY: EQUILIBRIA

In the remainder of the article we assume that the potential function of the scalar field is

$$V(\phi) = V_\infty (1 - e^{-\sqrt{2/3}\phi})^2, \tag{7}$$

which arises in the conformal frame of the $R+\alpha R^2$ theory.[8,11] This potential has a long and flat plateau. For large values of ϕ, the potential, V, is almost constant, $V_\infty = \lim_{\phi \to +\infty} V(\phi)$, thus V has the general properties for inflation to commence. In Ref. 12 it was proved a cosmic no-hair theorem, i.e., Bianchi models with ordinary matter satisfying the strong energy condition and a scalar field with potential (7), asymptotically isotopize. According to this picture, the universe started in a homogeneous state and during inflation it had enough time to isotropize.

In order to reduce the dimension of the dynamical system (5) we use the constraint (6) to eliminate a. The evolution equations become

$$\begin{aligned} \dot{\phi} &= y, \\ \dot{y} &= -3Hy - V'(\phi), \\ \dot{H} &= -H^2 - \tfrac{1}{3}y^2 + \tfrac{1}{3}V(\phi). \end{aligned} \tag{8}$$

Linearization of (8) near the equilibrium point (0,0,0) shows that the Jacobian matrix at that point has one zero and two purely imaginary eigenvalues. Consequently the Hartman–Grobman theorem does not apply. Therefore, we cannot draw any conclusions about the stability of the equilibrium from an examination of the Jacobian.

We simplify the system by rescaling the variables by the equations

$$\phi \to \sqrt{\tfrac{2}{3}}\phi,$$

$$y \to \sqrt{4V_\infty/3}\, y,$$

$$H \to \frac{\sqrt{2V_\infty}}{3} H,$$

$$t \to \frac{1}{\sqrt{2V_\infty}} t.$$

In order to take account of the equilibrium point corresponding to the point at ''infinity'' and to remove the transcendental functions, it is convenient to introduce the variable u defined by

$$u := e^{-\phi}, \tag{9}$$

to obtain finally

$$\begin{aligned} \dot{u} &= -uy, \\ \dot{y} &= -Hy - u(1-u), \\ \dot{H} &= -\tfrac{1}{3}H^2 - \tfrac{2}{3}y^2 + \tfrac{1}{2}(1-u)^2. \end{aligned} \tag{10}$$

Note that under the transformation (9), the resulted three-dimensional dynamical system (10) is quadratic. In view of (6) we have $3H^2 - \frac{1}{2}y^2 - V(\phi) > 0$, hence, the phase space of the system (10) is the set

$$\Sigma := \{(u,y,H) \in \mathbb{R}^3 : H^2 - y^2 - \tfrac{3}{2}(1-u)^2 > 0\}. \tag{11}$$

The equilibrium points of (10) are

A: $(u=1, y=0, H=0)$. This corresponds to the limiting state of an ever-expanding universe with $H \to 0$ while the scalar field approaches the minimum of the potential and the scale factor goes to infinity. Equality in (11) which arises from the flat, $k=0$, case defines a set on the boundary of Σ. We conclude that the point A, which corresponds to the Minkowski solution, is located on this boundary. The detailed structure of this equilibrium will be analyzed in the next section.

B: $(u=0, y=\pm\sqrt{3}/2, H=0)$. These lie outside of the phase space and, therefore, are unphysical.

C: $(u=0, y=0, H=\pm\sqrt{\frac{3}{2}})$. In the next section we show that only the point with the $+$ sign can be approached by a trajectory starting with a $H>0$. It corresponds to the de Sitter universe with a cosmological constant equal to $\sqrt{V_\infty}$. Regarding the stability of this equilibrium, it is easy to see that the Jacobian matrix of (10) at $\mathbf{q}=(0,0,\sqrt{\frac{3}{2}})$ has one zero and two negative eigenvalues. The center manifold theorem implies that there exists a local two-dimensional stable manifold through $\mathbf{q}$ (see, for example, Ref. 19). That means that all trajectories asymptotically approaching $\mathbf{q}$ as $t \to \infty$ lie on a two-dimensional invariant manifold. Since $\mathbf{q}$ is a nonhyperbolic fixed point, the topology of the flow near $\mathbf{q}$ is nontrivial and is characterized by a one-dimensional local center manifold intersecting $\mathbf{q}$. In the Appendix we prove the following result.

Proposition 1: The equilibrium point $\mathbf{q}=(0,0,\sqrt{\frac{3}{2}})$ *of* (10) *is locally asymptotically unstable.*

IV. LATE TIME EVOLUTION

It is easy to see that at the equilibrium point, $(u=1, y=0, H=0)$, the eigenvalues of the Jacobian of (10) are $\pm i, 0$ and, therefore, we cannot infer about the stability of the equilibrium. Nevertheless, it is the most interesting case, because in all other equilibria the scalar field reaches the flat plateau, which is impossible if we restrict ourselves to initial values of H smaller than

$\sqrt{V_\infty}$. The study of the qualitative behavior of a dynamical system near a nonhyperbolic equilibrium point is difficult even in two dimensions. We find the so-called normal form (cf. Ref. 19 for a brief introduction) of the system (10) near the equilibrium point $(u=1, y=0, H=0)$. The idea of the normal form theory is the following: Given a dynamical system with equilibrium point at the origin, $\dot{\mathbf{x}}=A\mathbf{x}+\mathbf{f}(\mathbf{x})$, where A is the Jordan form of the linear part and $\mathbf{f}(\mathbf{0})=\mathbf{0}$, perform a nonlinear transformation $\mathbf{x}\to\mathbf{x}+\mathbf{h}(\mathbf{x})$, where $\mathbf{h}(\mathbf{x})=O(|\mathbf{x}|^2)$ as $|\mathbf{x}|\to 0$, such that the system becomes "as simple as possible."

To write the system in a form suitable for the application of the normal form theory, we shift the fixed point to (0,0,0) by setting $x=u-1$ and the system becomes

$$\dot{x}=-y-xy,$$

$$\dot{y}=x+x^2-Hy, \tag{12}$$

$$\dot{H}=\tfrac{1}{2}x^2-\tfrac{2}{3}y^2-\tfrac{1}{3}H^2.$$

We now perform the nonlinear transformation

$$x\to x-y^2+\tfrac{1}{4}Hy,$$

$$y\to y+xy+\tfrac{1}{4}Hx,$$

$$H\to H+\tfrac{7}{12}xy,$$

and keeping only terms up to second order we obtain the system

$$\dot{x}=-y-\tfrac{1}{2}Hx,$$

$$\dot{y}=x-\tfrac{1}{2}Hy, \tag{13}$$

$$\dot{H}=-\tfrac{1}{12}(x^2+y^2)-\tfrac{1}{3}H^2.$$

Note that the results are valid only near the origin.

Passing to cylindrical coordinates $(x=r\cos\theta, y=r\sin\theta, H=H)$, we have

$$\dot{r}=-\tfrac{1}{2}rH,$$

$$\dot{\theta}=1, \tag{14}$$

$$\dot{H}=-\tfrac{1}{12}r^2-\tfrac{1}{3}H^2 \quad .$$

We note that the θ dependence of the vector field has been eliminated, so that we can study the system on the $r-H$ plane. The equation $\dot{\theta}=1$ means that the trajectory in the $x-y$ plane spirals with angular velocity 1. It is convenient to rescale the variables by

$$r\to 6r, \quad H\to 3H, \tag{15}$$

so that the projection of (14) on the $r-H$ plane is

$$\dot{r}=-\tfrac{3}{2}rH,$$

$$\dot{H}=-r^2-H^2 \quad . \tag{16}$$

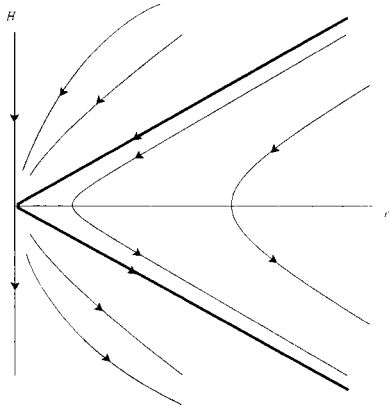

FIG. 1. The phase portrait of (16). The invariant trajectories $H=\pm\sqrt{2}r$ are shown with thicker lines. For expanding models only trajectories above the line $H=\sqrt{6}r$ belong to the phase space of the system.

This system belongs to a family of systems studied in 1974 by Takens.[20]

It is easy to obtain the phase portrait of (16) via numerical integration. However, we can analyze the qualitative behavior of the trajectories using theoretical arguments. First, (16) is invariant under the transformation $t\to -t$, $H\to -H$ (which implies that all trajectories are symmetric with respect to the r axis) and the line $r=0$ is invariant. Second, the system (16) has invariant lines $H=cr$. To see this, write

$$\frac{dH}{dr}=c=\frac{-r^2-c^2r^2}{-\frac{3}{2}cr^2}=\frac{-1-c^2}{-\frac{3}{2}c}\Rightarrow c=\pm\sqrt{2}. \tag{17}$$

Taking the dot product of the vector field $(-\frac{3}{2}rH,-r^2-H^2)^T$ with the radial vector $(r,H)^T$ along the line $H=cr$ we find that it is negative for $H>0$ and positive for $H<0$. Therefore, the direction of the flow along $H=cr$ in the first quadrant is towards the origin and goes away from the origin in the second quadrant. Note that H is always decreasing along the orbits while r is decreasing in the first quadrant. Since no trajectory can cross the line $H=cr$, all trajectories starting above this line approach the origin asymptotically. On any orbit starting in the first quadrant below the line $H=cr$, H becomes zero at some time and the trajectory vertically crosses the r-axis. Once the trajectory enters the second quadrant, r increases and H decreases. The phase portrait is shown in Fig. 1.

At first sight, it seems probable that an initially expanding universe may recollapse. However, the phase space of the dynamical system (16) is not the whole $r-H$ plane, because of the constraint (11), which in terms of the variables (15) becomes

$$H^2>6r^2. \tag{18}$$

Therefore, for an expanding universe we should consider only trajectories starting above the line $H=\sqrt{6}r$ and according to the previous discussion all these trajectories asymptotically approach the origin.

We now turn to the relation of the dynamics in the $r-H$ plane to the full three-dimensional system (14), or the equivalent (13) in Cartesian coordinates. Any trajectory spirals clockwise in the $x-y$ plane while both H and x^2+y^2 are decreasing. In physical terms this means that the scalar field oscillates around the minimum of the potential with a decreasing amplitude, H is always decreasing and, in view of (6), the curvature decreases. A typical trajectory of (13) is shown in Fig. 2.

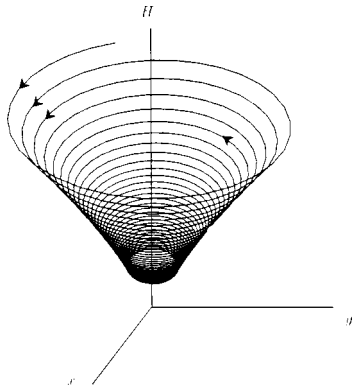

FIG. 2. Trajectories of the full three-dimensional system spiral approaching the origin.

V. COMMENT ON FLAT FRW MODELS

Consider a flat FRW model containing a barotropic fluid with an equation of state $p=(\gamma-1)\rho$, where $0\leqslant\gamma\leqslant 2$, and a scalar field having the potential (7). Then the system (2)–(4) reduces again to a four-dimensional dynamical system, namely,

$$\begin{aligned}\dot{\phi}&=y,\\ \dot{y}&=-3Hy-V'(\phi),\\ \dot{\rho}&=-3\gamma\rho H,\\ \dot{H}&=-\frac{1}{2}y^2-\frac{\gamma}{2}\rho,\end{aligned}\tag{19}$$

subject to the constraint

$$3H^2=\rho+\tfrac{1}{2}y^2+V(\phi).\tag{20}$$

In contrast to (5d), the fourth of (19) implies that H is always decreasing. If we use the constraint (20) to eliminate ρ, the evolution equations become

$$\begin{aligned}\dot{\phi}&=y,\\ \dot{y}&=-3Hy-V'(\phi),\\ \dot{H}&=-\frac{3\gamma}{2}H^2-\frac{2-\gamma}{4}y^2+\frac{\gamma}{2}V(\phi).\end{aligned}\tag{21}$$

We see that the structure of (21) describing a flat FRW model with a perfect fluid and a scalar field, apart from being parameter dependent, has a striking similarity to the dynamical system (8) for the vacuum positively curved FRW with a scalar field. Proceeding as in Sec. IV, we end up with the following system in cylindrical coordinates:

$$\begin{aligned}\dot{r}&=-\tfrac{1}{2}rH,\\ \dot{\theta}&=1,\end{aligned}\tag{22}$$

$$\dot{H}=\frac{5\gamma-4}{8}r^2-\frac{\gamma}{2}H^2 \quad .$$

Although the system (22) depends only on one parameter, it is convenient to rescale the variables by

$$r\to\lambda r, \quad H\to\mu H \tag{23}$$

with

$$\mu=\frac{2}{\gamma}, \quad \lambda=\sqrt{\left|\frac{16}{\gamma(5\gamma-4)}\right|},$$

so that the projection of (22) on the $r-H$ plane is

$$\begin{aligned}\dot{r}&=-\frac{1}{\gamma}rH,\\ \dot{H}&=br^2-H^2 \quad ,\end{aligned} \tag{24}$$

where

$$b=+1 \text{ for } \gamma>\tfrac{4}{5}, \quad b=-1 \text{ for } \gamma<\tfrac{4}{5}.$$

Note that (24) has a first integral, viz.,

$$I(r,H)=-\frac{1}{2\gamma}r^{-2\gamma}\left(\frac{br^2}{1-1/\gamma}-H^2\right). \tag{25}$$

In fact, it is straightforward to verify that $(\partial I/\partial r)\dot{r}+(\partial I/\partial H)\dot{H}=0$ along the solution curves of (24). The level curves of I are the trajectories of the system.

Invariant lines $H=cr$ exist for certain values of the parameter γ. We find [cf. (17)]

$$c=\pm\sqrt{\frac{b}{1-1/\gamma}}.$$

Case I. For $b=+1$, invariant lines exist if $\gamma>1$. We find that the direction of the flow along $H=cr$ in the first quadrant is towards the origin and goes away from the origin in the second quadrant. Note that in the first quadrant r is decreasing along the orbits and that $\dot{H}$ vanishes along the line $H=r$, which lies below the invariant line $H=cr$. It can be shown that in the first quadrant a level curve of $I(r,H)$ may intersect the line $H=r$ only once [it is sufficient to consider the level curve passing through an arbitrary point $(r_1,0)$ and compute the r coordinate at the intersection with the line $H=r$]. We conclude that once a trajectory crosses the line $H=r$, it is trapped between the lines $H=r$ and $H=cr$ and, since $\dot{r}<0$, it approaches the origin asymptotically.

Case II. $b=+1$ and $\frac{4}{5}<\gamma<1$. There are no invariant lines. Similar arguments as in case I yield the phase portrait shown in Fig. 3.

Case III. $\gamma<\frac{4}{5}$ $(\Rightarrow b=-1)$. The analysis is exactly the same as in Sec. IV.

In all cases we must remember that the phase space of the dynamical system (24) is not the whole $r-H$ plane, because of the constraint (11), which in terms of the variables (23) reads

$$H^2>\frac{6\gamma}{|5\gamma-4|}r^2. \tag{26}$$

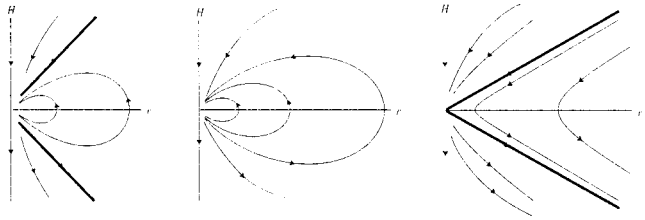

FIG. 3. The phase portrait of (24) for $1<\gamma<2$, $\frac{4}{5}<\gamma<1$, and $0<\gamma<\frac{4}{5}$, respectively.

Therefore, for an expanding universe, we should consider only trajectories starting above the line $H=\sqrt{6\gamma/|5\gamma-4|}r$, which in case III lies always above the line $H=cr$ and, according to the previous discussion, all these trajectories asymptotically approach the origin.

We conclude that, in the conformal frame of the $R+aR^2$ theory, an initially expanding flat universe with a barotropic fluid as matter source remains ever-expanding and eventually the quadratic curvature corrections become negligible. This result, established by stability analysis, is in accordance with the general properties of all flat FRW models with a scalar field having a potential with a unique zero minimum.[17]

VI. DISCUSSION

We have analyzed the qualitative behavior of a positively curved FRW model containing a scalar field with the potential (7). This model is conformally equivalent to the positively curved FRW space–time in the simplest higher order gravity theory, namely the $R+\alpha R^2$ theory. We have shown that an initially expanding closed universe avoids recollapse provided that the initial value of H is less than $\sqrt{V_\infty}$. This result should be compared to a counterexample of the closed universe recollapse conjecture (cf. Ref. 21, where it is shown that initially expanding vacuum diagonal Bianchi IX models in purely quadratic gravity are ever-expanding). It should be of interest to investigate if a closed FRW universe filled with ordinary matter satisfying the usual energy conditions and a scalar field with the potential (7) can avoid recollapse. This is equivalent to the analysis of the qualitative behavior of the full five-dimensional system (2)–(4). A partial answer to this question for an arbitrary non-negative potential having a unique minimum $V(0)=0$ is given in Ref. 17.

ACKNOWLEDGMENTS

I thank P. G. L. Leach and S. Cotsakis for fruitful discussions during the preparation of this work. I wish to thank an anonymous referee for useful suggestions, especially for pointing out to me the remarks regarding the equilibrium A after Eq. (11).

APPENDIX: PROOF OF PROPOSITION 1

In order to determine the local center manifold of (10) at $\mathbf{q}$, we have to transform the system into a form suitable for the application of the center manifold theorem. The procedure is fairly systematic and will be accomplished in the following steps.

(1) The Jacobian of (10) at $\mathbf{q}=(0,0,\sqrt{\frac{3}{2}})$ has eigenvalues 0, $-\sqrt{\frac{2}{3}}$ and $-\sqrt{\frac{3}{2}}$ with corresponding eigenvectors $(-\sqrt{\frac{2}{3}},\frac{2}{3},1)^T$, $(0,0,1)^T$ and $(0,1,0)^T$. Let T be the matrix having as columns these eigenvectors. We shift the fixed point to (0,0,0) by setting $\tilde{H}=H-\sqrt{\frac{3}{2}}$ and write (10) in vector notation as

$$\dot{\mathbf{z}}=A\mathbf{z}+\mathbf{F}(\mathbf{z}), \tag{A1}$$

where A is the linear part of the vector field and $\mathbf{F}(\mathbf{0})=\mathbf{0}$.

(2) Using the matrix T which transforms the linear part of the vector field into Jordan canonical form, we define new variables, $(x,y_1,y_2)\equiv\mathbf{x}$, by the equations

$$u=-\sqrt{\tfrac{2}{3}}x,$$

$$y=\tfrac{2}{3}x+y_2,$$

$$\tilde{H}=x+y_1,$$

or in vector notation $\mathbf{z}=T\mathbf{x}$, so that (A1) becomes

$$\dot{\mathbf{x}}=T^{-1}AT\mathbf{x}+T^{-1}\mathbf{F}(T\mathbf{x}).$$

Denoting the canonical form of A by B we finally obtain the system

$$\dot{\mathbf{x}}=B\mathbf{x}+\mathbf{f}(\mathbf{x}), \tag{A2}$$

where $\mathbf{f}(\mathbf{x})\coloneqq T^{-1}\mathbf{F}(T\mathbf{x})$. In components system (A2) is

$$\begin{pmatrix}\dot{x}\\ \dot{y}_1\\ \dot{y}_2\end{pmatrix}=\begin{pmatrix}0 & 0 & 0\\ 0 & -\sqrt{\frac{2}{3}} & 0\\ 0 & 0 & -\sqrt{\frac{3}{2}}\end{pmatrix}\begin{pmatrix}x\\ y_1\\ y_2\end{pmatrix}+\begin{pmatrix}-\frac{2}{3}x^2-xy_2\\ \frac{10}{27}x^2-\frac{1}{3}y_1^2-\frac{2}{3}y_2^2-\frac{2}{3}xy_1+\frac{1}{9}xy_2\\ \frac{4}{9}x^2-\frac{2}{3}xy_1-\frac{1}{3}xy_2-y_1y_2\end{pmatrix}. \tag{A3}$$

(3) The system (A3) is written in diagonal form

$$\begin{aligned}\dot{x}&=Cx+f(x,\mathbf{y}),\\ \dot{\mathbf{y}}&=P\mathbf{y}+\mathbf{g}(x,\mathbf{y}),\end{aligned} \tag{A4}$$

where $(x,\mathbf{y})\in\mathbb{R}\times\mathbb{R}^2$, C is the zero 1×1 matrix, P is a square matrix with negative eigenvalues and $f,\mathbf{g}$ vanish at $\mathbf{0}$ and have vanishing derivatives at $\mathbf{0}$. The center manifold theorem asserts that there exists a one-dimensional invariant local center manifold $W^c(\mathbf{0})$ of (A4) tangent to the center subspace (the $\mathbf{y}=\mathbf{0}$ space) at $\mathbf{0}$. Moreover, $W^c(\mathbf{0})$ can be represented as

$$W^c(\mathbf{0})=\{(x,\mathbf{y})\in\mathbb{R}\times\mathbb{R}^2:\mathbf{y}=\mathbf{h}(x),\ \ |x|<\delta\};\qquad \mathbf{h}(0)=0,\ D\mathbf{h}(0)=\mathbf{0},$$

for δ sufficiently small (cf. Ref. 19, p. 155). The restriction of (A4) to the center manifold is

$$\dot{x}=Cx+f(x,\mathbf{h}(x)). \tag{A5}$$

According to Theorem 3.2.2 in Ref. 22, if the origin $x=0$ of (A5) is stable (resp. unstable), then the origin of (A4) is also stable (resp. unstable). Therefore, we have to find the local center manifold, i.e., the problem reduces to the computation of $\mathbf{h}(x)$.

(4) Substituting $\mathbf{y}=\mathbf{h}(x)$ in the second component of (A4) and using the chain rule, $\dot{\mathbf{y}}=D\mathbf{h}(x)\dot{x}$, one can show that the function $\mathbf{h}(x)$ that defines the local center manifold satisfies

$$D\mathbf{h}(x)[Cx+f(x,\mathbf{h}(x))]-P\mathbf{h}(x)-\mathbf{g}(x,\mathbf{h}(x))=0. \tag{A6}$$

This condition allows for an approximation of $\mathbf{h}(x)$ by a Taylor series at $x=0$. Since $\mathbf{h}(0)=0$, $D\mathbf{h}(0)=\mathbf{0}$, it is obvious that $\mathbf{h}(x)$ commences with quadratic terms. We substitute

$$\mathbf{h}(x)\coloneqq\begin{pmatrix}h_1(x)\\ h_2(x)\end{pmatrix}=\begin{pmatrix}a_1x^2+a_2x^3+O(x^4)\\ b_1x^2+b_2x^3+O(x^4)\end{pmatrix}$$

into (A6) and set the coefficients of like powers of x equal to zero to find the unknowns $a_1, b_1, \ldots$.

(5) Since y_1 is absent from the first of (A3), we give only the result for $h_2(x)$. We find $b_1 = \frac{4}{9}\sqrt{\frac{2}{3}}$, $b_2 = \frac{4}{81}$. Therefore, (A5) yields

$$\dot{x} = -\tfrac{2}{3}x^2 - \tfrac{4}{9}\sqrt{\tfrac{2}{3}}x^3 - \tfrac{4}{81}x^4 + O(x^5). \tag{A7}$$

It is obvious that the origin $x=0$ of (A7) is asymptotically unstable (saddle point). The theorem mentioned after (A5) implies that the origin $\mathbf{x}=\mathbf{0}$ of the full three-dimensional system is unstable. This completes the proof.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Generalized variational principle of Herglotz for several independent variables. First Noether-type theorem

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(Received 25 July 2002; accepted 28 April 2003)

This paper extends the generalized variational principle of Herglotz to one with several independent variables and derives the corresponding generalized Euler–Lagrange equations. The extended principle contains the classical variational principle with several independent variables and the variational principle of Herglotz as special cases. A first Noether-type theorem is proven for the new variational principle, which gives the conserved quantities corresponding to symmetries of the associated functional. This theorem contains the classical first Noether theorem as a special case. As examples for applications we calculate a conserved quantity for the damped nonlinear Klein–Gordon equation and we show that the equations which describe the propagation of electromagnetic fields in a conductive medium can be derived from the generalized variational principle of Herglotz (but not from a classical variational principle). © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1597419]

I. INTRODUCTION

The generalized variational principle, proposed by Herglotz,[1,2] defines the functional whose extrema are sought by a differential equation rather than by an integral. It contains as a special case the classical variational principle with one independent variable.

The Herglotz principle gives a variational description of nonconservative as well as conservative processes involving one independent variable. The solutions of the equations providing the extrema of the functional determine a one-parameter group of contact transformations. See Guenther *et al.*[3] From the paper of Furta[4] we see that there is a close link between the Herglotz variational principle and control and optimal control theories. Through contact transformations the Herglotz principle is also related to thermodynamics. See Mrugala.[5] Georgieva *et al.*[6] prove a Noether-type theorem which yields conservation laws corresponding to the symmetries of the functional defined by the Herglotz variational principle.

In this paper we extend the generalized variational principle of Herglotz to one with several independent variables. This new variational principle can give a variational description of nonconservative processes involving physical fields. It reduces to the Herglotz generalized variational principle when only one independent variable, the time-variable, is present. It also reduces to the classical variational principle with several independent variables. Thus, it contains both the Herglotz's variational principle and the classical variational principle with several independent variables as special cases. One valuable characteristic of the new variational principle is that it gives a variational description of nonconservative processes even when the *Lagrangian is not an explicit*

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function of time, which is not possible with the classical variational principle. This is shown in Sec. VII.

The classical first Noether theorem applies only to functionals defined by integrals, see Noether.[7,8] Thus, a need arises for a Noether-type theorem which does apply to functionals defined by differential or integro-differential equations. In this paper we formulate and prove a first Noether-type theorem for the generalized variational principle with several independent variables, i.e., when the functional is defined by an integro-differential equation. One of its corollaries provides an explicit procedure for finding the conserved quantities corresponding to symmetries of this functional.

A criterion for a transformation to be a symmetry of the functional defined by the generalized variational principle with several independent variables is proven. This criterion contains as a special case the criterion for a transformation to be a symmetry of a variational integral due to Lie.

Six corollaries of the first Noether-type theorem are proven. Five of them provide conserved quantities in systems described by the generalized Euler–Lagrange equations with several independent variables. The significance of the first Noether-type theorem in the several independent variables case is further demonstrated by applying it to the equations describing the propagation of electromagnetic fields in conductive media and to the damped nonlinear Klein–Gordon equation.

II. THE GENERALIZED VARIATIONAL PRINCIPLE WITH SEVERAL INDEPENDENT VARIABLES

In the variational principle of Herglotz the functional $z=z[x;s]$ of $x\equiv(x^1,\ldots,x^n)$ is defined by a differential equation of the form

$$\frac{\mathrm{d}z}{\mathrm{d}t}=L(t,x,\dot{x},z), \quad 0\leqslant t\leqslant s,$$

where t is the only independent variable and $\dot{x}=\mathrm{d}x/\mathrm{d}t$. Herglotz showed that the value of this functional is an extremum when its argument functions $x^k(t)$ are solutions of the generalized Euler–Lagrange equations

$$\frac{\partial L}{\partial x^k}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}^k}+\frac{\partial L}{\partial z}\frac{\partial L}{\partial \dot{x}^k}=0, \quad k=1,\ldots,n.$$

In this section we generalize the Herglotz variational principle to one involving several independent variables.

For the remainder of this paper, the independent variables will be the time variable t and the spatial coordinates $x\equiv(x^1,\ldots,x^n)$. The argument function of the functional $z[u;s]$ defined by the new variational principle will be $u=u(t,x)=(u^1(t,x),\ldots,u^m(t,x))$. The standard abbreviations $u^i_t=\partial u^i/\partial t$ and $u^i_{x^k}=\partial u^i/\partial x^k$ will be used. The summation convention is assumed for the entire paper.

The generalized variational principle with several independent variables is as follows:

Let the functional $z=z[u;s]$ of $u=u(t,x)$ be given by an integro-differential equation of the form

$$\frac{\mathrm{d}z}{\mathrm{d}t}=\int_\Omega \mathcal{L}(t,x,u,u_t,u_x,z)\,\mathrm{d}^n x, \quad 0\leqslant t\leqslant s, \tag{2.1}$$

where $x\equiv(x^1,\ldots,x^n)$, $\mathrm{d}^n x\equiv \mathrm{d}x^1\cdots\mathrm{d}x^n$, $u\equiv(u^1,\ldots,u^m)$, $u_x\equiv(u^1_x,\ldots,u^m_x)$, $u_t\equiv(u^1_t,\ldots,u^m_t)$, and $u^i_x\equiv(u^i_{x^1},\ldots,u^i_{x^n})$, $i=1,\ldots,m$, and where the function $\mathcal{L}$ is at least twice differentiable with respect to u_x, u_t and once differentiable with respect to t,x,z. Let $\eta\equiv(\eta^1(t,x),\ldots,\eta^m(t,x))$ have continuous first derivatives and otherwise be arbitrary except for the boundary conditions:

$$\eta(0,x)=\eta(s,x)=0,$$

$$\eta(t,x)=0 \qquad \text{for} \quad x\in\partial\Omega, \quad 0\leqslant t\leqslant s,$$

where $\partial\Omega$ is the boundary of Ω. Then, the value of the functional $z[u;s]$ is an extremum for functions u which satisfy the condition

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} z[u+\varepsilon\,\eta;s]\big|_{\varepsilon=0}=0. \tag{2.2}$$

The function $\mathcal{L}$ will be called, just as in the classical case, the *Lagrangian density*. It should be observed that when a variation $\varepsilon\,\eta$ is applied to u the equation (2.1), defining the functional z, must be solved with the same fixed initial condition $z(0)$ at $t=0$ and the solution evaluated at the same fixed final time $t=s$ for all varied argument functions $u+\varepsilon\,\eta$.

III. GENERALIZED EULER–LAGRANGE EQUATIONS WITH SEVERAL INDEPENDENT VARIABLES

In this section we derive the equations which provide the extrema of the functional $z[u;s]$ defined by the integro-differential equation (2.1). Because of the obvious correspondence with the classical case, we call these equations the *generalized Euler–Lagrange equations with several independent variables*.

Theorem 3.1.: *Every function $u\equiv(u^1,\ldots,u^m)$, for which the functional z defined by the integro-differential equation (2.1) has an extremum, is a solution of*

$$\frac{\partial\mathcal{L}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial u^i_t}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}+\frac{\partial\mathcal{L}}{\partial u^i_t}\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\,\mathrm{d}x=0\,, \quad i=1,\ldots,m. \tag{3.1}$$

Proof: We will show that equations (3.1) are a consequence of condition (2.2). For this purpose let $\varepsilon\,\eta$ be the variation of the argument of the functional z and denote by $\zeta=\zeta(t)$ the quantity

$$\zeta(t)=\frac{\mathrm{d}}{\mathrm{d}\varepsilon} z[u+\varepsilon\,\eta;t]\big|_{\varepsilon=0}. \tag{3.2}$$

To find the differential equation for ζ we apply the variation $\varepsilon\,\eta$ to the argument function in the defining equation (2.1), i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t} z[u+\varepsilon\,\eta;t]=\int_\Omega\mathcal{L}(t,x,u+\varepsilon\,\eta,u_t+\varepsilon\,\eta_t,u_x+\varepsilon\,\eta_x,z)\,\mathrm{d}^n x \tag{3.3}$$

and differentiate the result with respect to ε. Then, we set $\varepsilon=0$ to obtain

$$\frac{\mathrm{d}\zeta}{\mathrm{d}t}=\int_\Omega\left(\frac{\partial\mathcal{L}}{\partial u^i}\,\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\,\eta^i_t+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\,\eta^i_{x^k}\right)\mathrm{d}^n x+\zeta\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\,\mathrm{d}^n x, \quad i=1,\ldots,m, \tag{3.4}$$

where in the last term we have used the fact that ζ does not depend on x. For convenience we denote by $A(t)$ and $B(t)$ the quantities

$$A(t)=\int_\Omega\left(\frac{\partial\mathcal{L}}{\partial u^i}\,\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\,\eta^i_t+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\,\eta^i_{x^k}\right)\mathrm{d}^n x, \quad B(t)=\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\,\mathrm{d}^n x.$$

With this notation Eq. (3.4) becomes

$$\frac{\mathrm{d}\zeta(t)}{\mathrm{d}t}=A(t)+B(t)\,\zeta(t)$$

which is the sought equation for $\zeta(t)$. Its solution $\zeta(s)$, evaluated at the end of the time interval $t=s$, is the variation of $z[u;s]$ and is given by

$$\exp\left(-\int_0^s B(\theta)\,\mathrm{d}\theta\right)\zeta(s)=\int_0^s \exp\left(-\int_0^t B(\theta)\,\mathrm{d}\theta\right)A(t)\,\mathrm{d}t \tag{3.5}$$

since $\zeta(0)=0$. We are interested in those functions u which leave the functional $z[u;s]$ stationary, i.e., those for which the variation $\zeta(s)$ is identically zero. Hence, (3.5) becomes

$$\int_0^s \exp\left(-\int_0^t B(\theta)\,\mathrm{d}\theta\right)A(t)\,\mathrm{d}t=0. \tag{3.6}$$

Inserting expressions $A(t)$ and $B(t)$ into (3.6), denoting the exponential function by

$$E(t)\equiv\exp\left(-\int_0^t B(\theta)\,\mathrm{d}\theta\right)$$

and integrating by parts the terms containing $\eta^i_{x^k}$ produces the equation

$$\int_0^s E(t)\int_\Omega\left(\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\eta^i_t+\frac{\mathrm{d}}{\mathrm{d}x^k}\left(\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\eta^i\right)-\eta^i\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\right)\mathrm{d}^nx\,\mathrm{d}t=0. \tag{3.7}$$

By Gauss' theorem the space integral of the third term in (3.7)

$$\int_\Omega\frac{\mathrm{d}}{\mathrm{d}x^k}\left(\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\eta^i\right)\mathrm{d}^nx=\int_{\partial\Omega}\eta^i\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\mathrm{d}a_k=0$$

vanishes because $\eta=0$ on $\partial\Omega$, by definition. Here, $\mathrm{d}a_k$ stands for the k-component of the surface element $\mathrm{d}a=(\mathrm{d}a_1,\ldots,\mathrm{d}a_n)$ of $\partial\Omega$. Next, we integrate by parts (with respect to t) the terms involving η^i_t in (3.7) to obtain

$$\int_0^s E(t)\int_\Omega\left(\frac{\partial\mathcal{L}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\right)\eta^i\,\mathrm{d}^nx\,\mathrm{d}t-\int_\Omega\int_0^s\eta^i\frac{\mathrm{d}}{\mathrm{d}t}\left(E(t)\frac{\partial\mathcal{L}}{\partial u^i_t}\right)\mathrm{d}t\,\mathrm{d}^nx=0$$

because $\eta(0,x)=0$ and $\eta(s,x)=0$, by definition. Finally, expanding the second integrand in the last equation and collecting terms, we get

$$\int_0^s\int_\Omega E(t)\left(\frac{\partial\mathcal{L}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial u^i_t}+\frac{\partial\mathcal{L}}{\partial u^i_t}\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx\right)\eta^i\,\mathrm{d}^nx\,\mathrm{d}t=0\,.$$

Taking in consideration that η is arbitrary and that $E(t)>0$ for all t, we obtain equation (3.1), which concludes the proof. □

It is important to observe that the generalized Euler–Lagrange equations (3.1) reduce to the classical Euler–Lagrange equations when $\mathcal{L}$ does not depend on z, i.e., when the functional z defined by the integro-differential equation (2.1) reduces to the classical definition of a functional by an integral. Also, Eqs. (3.1) reduce to the generalized Euler–Lagrange equations for the generalized variational principle of Herglotz when t is the only independent variable involved.

IV. INFINITESIMAL CRITERION FOR INVARIANCE

In this section we give an infinitesimal criterion for the invariance of the functional z defined by Eq. (2.1) under the action of a one-parameter group of transformations of the independent variables t, $x\equiv(x^1,\ldots,x^n)$ and the dependent variables $u\equiv(u^1,\ldots,u^m)$, i.e.,

$$\overline{t}=\phi(t,x,u;\varepsilon),$$

$$\overline{x^k}=\varphi^k(t,x,u;\varepsilon),\quad k=1,\ldots,n, \tag{4.1}$$

$$\overline{u^i}=\psi^i(t,x,u;\varepsilon),\quad i=1,\ldots,m\,.$$

To find the transformed functions $\overline{u^i}=\overline{u^i}(\overline{t},\overline{x};\varepsilon)$ of the functions $u^i=u^i(t,x)$ we insert the latter into ϕ and φ^k of (4.1) to get a system of $n+1$ equations with $n+1$ unknowns $t,x^1,\ldots,x^n$ and a parameter ε. We invert this system to obtain t and $x^1,\ldots,x^n$ as functions of $\overline{t}$ and $\overline{x^1},\ldots,\overline{x^n}$. These we substitute into the last m equations of (4.1) to get $\overline{u^i}$ as a function of $\overline{t}$ and $\overline{x^1},\ldots,\overline{x^n}$ and ε, which we denote by $\overline{u^i}=\overline{u^i}(\overline{t},\overline{x};\varepsilon)$.

Definition 4.1: The transformed functional $\overline{z}$ of a functional z defined by (2.1), is the solution of the transformed integro-differential equation

$$\frac{\mathrm{d}\overline{z}}{\mathrm{d}\overline{t}}=\int_{\overline{\Omega}}\mathcal{L}(\overline{t},\overline{x},\overline{u}(\overline{t},\overline{x}),\overline{u_t},\overline{u_x},\overline{z})\,\mathrm{d}^n\overline{x}, \tag{4.2}$$

where $\overline{\Omega}$ is the transformed domain of the domain Ω.

Observation: The most general one-parameter group of transformations of the independent and dependent variables admitted by equation (2.1) is

$$\overline{t}=\phi(t;\varepsilon),$$

$$\overline{x^k}=\varphi^k(t,x,u;\varepsilon),\quad k=1,\ldots,n, \tag{4.3}$$

$$\overline{u^i}=\psi^i(t,x,u;\varepsilon),\quad i=1,\ldots,m.$$

Proof: For a given $u=u(x,t)$ the solution z of the nontransformed equation (2.1) and it's derivative $\mathrm{d}z/\mathrm{d}t$ are functions of t only. Assume that we transform (2.1) with (4.1) where ϕ *does* depend on either x or u or both. Then, from the transformed equation (4.2) follows that $\mathrm{d}\overline{z}/\mathrm{d}\overline{t}$, and hence $\overline{z}$, are functions of $\overline{t}$ only. On the other hand, if we apply the transformation (4.1) directly to the solution z the result will depend on x. Clearly, this is a contradiction. To avoid it, we must restrict the transformation of the t-variable as shown in (4.3). □

Definition 4.2: Let Φ, Ω, and Ψ^i be the sets on which t, x, and $u^i(t,x)$ vary. A local group of transformations G acting on the independent and dependent variables is a *symmetry group* of the functional z defined by the integro-differential equation (2.1) if whenever D is a subdomain with closure $D^{cl}\subset\Omega$ and $u^i=u^i(t,x)$ are functions defined over $\Phi\times D$ whose graphs lie in $\Phi\times\Omega\times\Psi^i$ with continuous second partial derivatives, and $g\in G$ is such that

$$\overline{u^i}=\overline{u^i}(\overline{t},\overline{x})=g\circ u^i(t,x),\quad i=1,\ldots,m$$

are single valued functions defined over $\overline{\Phi}\times\overline{D}\subset\Phi\times\Omega$, then the functional defined by the transformed integro-differential equation

$$\frac{\mathrm{d}\overline{z}}{\mathrm{d}\overline{t}}=\int_{\overline{D}}\mathcal{L}(\overline{t},\overline{x},\overline{u}(\overline{t},\overline{x}),\overline{u_t},\overline{u_x},\overline{z})\,\mathrm{d}^n\overline{x} \tag{4.4}$$

is equal to the functional defined by the original integro-differential equation

$$\frac{\mathrm{d}z}{\mathrm{d}t}=\int_D\mathcal{L}(t,x,u(t,x),u_t,u_x,z)\,\mathrm{d}^nx \tag{4.5}$$

for all t. Here $\overline{D}$ denotes the transformed D under G.

Proposition 4.3: The one-parameter group of transformations G in (4.3) is a symmetry group of the functional defined by the integro-differential equation (2.1) if and only if

$$\frac{\mathrm{d}\tau}{\mathrm{d}t}\mathcal{L}+\left.\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\right|_{\varepsilon=0}(\,\mathrm{pr}^{(1)}v(\,\mathcal{L})+\,\mathcal{L}\,\mathrm{Div}\,\xi)=0 \tag{4.6}$$

for all t,x,u,u_t, and u_x in the domain of definition, where

$$v=\tau(t)\frac{\partial}{\partial t}+\,\xi^k(t,x,u)\frac{\partial}{\partial x^k}+\,\eta^i(t,x,u)\frac{\partial}{\partial u^i} \tag{4.7}$$

is the infinitesimal generator of the group G, $\mathrm{Div}\,\xi$ denotes the total divergence of the n-tuple $\xi\equiv(\xi^1,\ldots,\xi^n)$, and $\mathrm{pr}^{(1)}v$ is the first prolongation of v.

Proof: The functions τ, ξ^k, and η^i in (4.7) are

$$\tau\equiv\left.\frac{\mathrm{d}\phi}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0},\quad \xi^k\equiv\left.\frac{\mathrm{d}\varphi^k}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0},\quad k=1,\ldots,n,\quad \eta^i\equiv\left.\frac{\mathrm{d}\psi^i}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0},\quad i=1,\ldots,m.$$

For each $g\in G$ the group transformation $(\overline{t},\overline{x},\overline{u})=g\circ(t,x,u)$ can be regarded as a change of variables, so that we can rewrite the transformed equation (4.4) as

$$\frac{\mathrm{d}\overline{z}}{\mathrm{d}t}=\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\int_D\mathcal{L}(\overline{t},\overline{x},\mathrm{pr}^{(1)}(g\circ u)(\overline{t},\overline{x}),\overline{z})\,\det J_g(t,x,\mathrm{pr}^{(1)}u(t,x))\,\mathrm{d}^nx, \tag{4.8}$$

where the Jacobi matrix has the entries

$$J_g^{kj}(t,x,u^{(1)})=\frac{\mathrm{d}}{\mathrm{d}x^k}\varphi_g^j(t,x,u^{(1)}),$$

and $u^{(1)}=(u,u_t,u_x)$. If G is a symmetry group of the functional z defined by (2.1), then the functional z defined by (4.5) is identical with the functional $\overline{z}$ defined by (4.8). Hence

$$\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\int_D\mathcal{L}(\overline{t},\overline{x},\mathrm{pr}^{(1)}(g\circ u)(\overline{t},\overline{x}),\overline{z})\,\det J_g(t,x,\mathrm{pr}^{(1)}u(t,x))\,\mathrm{d}^nx=\int_D\mathcal{L}(t,x,u(t,x),u_t,u_x,z)\,\mathrm{d}^nx$$

holds for all subdomains D of Ω, all functions u^i and all t in the domain of definition. Since $\overline{t}=\phi(t;\varepsilon)$ does not depend on $x^1,\ldots,x^n$, the arbitrariness of D implies that

$$\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\mathcal{L}(\overline{t},\overline{x},\mathrm{pr}^{(1)}(g\circ u)(\overline{t},\overline{x}),\overline{z})\,\det J_g(t,x,\mathrm{pr}^{(1)}u(t,x))=\mathcal{L}(t,x,u(t,x),u_t,u_x,z) \tag{4.9}$$

holds for all t,x,u,u_t,u_x in the domain of definition. The infinitesimal version of (4.9) is obtained by setting $g=g_\varepsilon=\exp(\varepsilon v)$ and differentiating with respect to ε which produces

$$\left(\frac{\mathrm{d}\tau}{\mathrm{d}t}\mathcal{L}+\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}(\,\mathrm{pr}^{(1)}v\,(\mathcal{L})+\,\mathcal{L}\,\mathrm{Div}\,\xi)\right)\det J_{g_\varepsilon}=0, \tag{4.10}$$

the expression in parentheses being evaluated at $(\overline{t},\overline{x},\overline{u}_\varepsilon^{(1)})$. In particular, when $\varepsilon=0$, g_ε is the identity map and we obtain (4.6). Conversely, if (4.6) holds for all (t,x,u,u_t,u_x) in the domain of definition, then (4.10) holds for ε sufficiently small. The left-hand side of (4.10) is just the derivative of the left-hand side of (4.9) with respect to ε. Thus, integrating from 0 to ε we get (4.9)

for g sufficiently near the identity. The usual connectivity arguments complete the proof for all $g \in G$. □

We observe that the infinitesimal criterion which the above proposition provides reduces to the infinitesimal criterion for the invariance of the classical variational integral under a group of transformations, when the generalized variational principle with several independent variables reduces to the classical variational principle.

V. FIRST NOETHER-TYPE THEOREM FOR THE GENERALIZED VARIATIONAL PRINCIPLE WITH SEVERAL INDEPENDENT VARIABLES

In this section we formulate and prove a theorem which provides an identity corresponding to each symmetry of the functional z defined by the integro-differential equation (2.1). We call it a first Noether-type theorem for the generalized variational principle with several independent variables because this theorem contains as a special case the classical first Noether theorem.

As corollaries to this theorem we show that there is a correspondence between the symmetries of the functional z defined by Eq. (2.1) and conserved quantities of the corresponding generalized Euler–Lagrange equations.

Theorem 5.1: *Let (4.3) be a given symmetry group with infinitesimal generator*

$$v = \tau(t)\frac{\partial}{\partial t} + \xi^k(t,x,u)\frac{\partial}{\partial x^k} + \eta^i(t,x,u)\frac{\partial}{\partial u^i}, \quad k=1,\ldots,n, \quad i=1,\ldots,m. \tag{5.1}$$

of the functional $z[u;s]$ defined by (2.1). Then the identity

$$\int_D \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(E\left((\tau u_t^i + \xi^j u_{xj}^i - \eta^i)\frac{\partial \mathcal{L}}{\partial u_t^i} - \tau\mathcal{L}\right)\right) + \frac{\mathrm{d}}{\mathrm{d}x^k}\left(E\left((\tau u_t^i + \xi^j u_{xj}^i - \eta^i)\frac{\partial \mathcal{L}}{\partial u_{x^k}^i} - \xi^k\mathcal{L}\right)\right)\right) \mathrm{d}^n x = 0 \tag{5.2}$$

holds on solutions of the generalized Euler–Lagrange equations (3.1). Here D is any subdomain of Ω, including Ω itself, whose closure $D^{cl} \subset \Omega^{cl}$ and $E = E(t)$ is

$$E = \exp\left(-\int_0^t \int_D \frac{\partial \mathcal{L}}{\partial z}\mathrm{d}^n x\, d\theta\right). \tag{5.3}$$

Proof: We write the integro-differential equation (2.1) for any subdomain D of Ω and apply the transformation (5.1) to it, i.e.,

$$\frac{\mathrm{d}\overline{z}}{\mathrm{d}\overline{t}} = \int_{\overline{D}} \mathcal{L}(\overline{t},\overline{x},\overline{u}(\overline{t},\overline{x}),\overline{u_t},\overline{u_x},\overline{z})\,\mathrm{d}^n\overline{x}, \quad \phi(0;\varepsilon) \leqslant \overline{t} \leqslant \phi(s;\varepsilon). \tag{5.4}$$

Here $\mathrm{d}^n\overline{x} = \mathrm{d}\overline{x^1}\cdots\mathrm{d}\overline{x^n}$ and $\overline{D} = \overline{D}(\overline{t},\overline{u},\varepsilon)$ denotes the result of transforming D with (5.1) which, in general, depends on $\overline{t}$, $\overline{u}$, and ε. Now we change the independent variables $\overline{t}$ and $\overline{x^k}$ in (5.4) (but not the dependent variables) back to the original independent variables t and x^k. The resulting equation is

$$\frac{\mathrm{d}\overline{z}}{\mathrm{d}t} = \frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\int_D \mathcal{L}(\overline{t},\overline{x},\overline{u}(\overline{t},\overline{x}),\overline{u_t},\overline{u_x},\overline{z})\det\left(\frac{\partial\overline{x}}{\partial x}\right)\mathrm{d}^n x, \quad 0 \leqslant t \leqslant s, \tag{5.5}$$

where $\partial\overline{x}/\partial x$ stands for the Jacobian matrix of the transformation of the x variables. Differentiating equation (5.5) with respect to ε,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{d}\overline{z}}{\mathrm{d}\varepsilon} = \frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\int_D \left(\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\det\left(\frac{\partial\overline{x}}{\partial x}\right) + \mathcal{L}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\frac{\partial\overline{x}}{\partial x}\right)\right)\mathrm{d}^n x + \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\int_D \mathcal{L}\det\left(\frac{\partial\overline{x}}{\partial x}\right)\mathrm{d}^n x, \tag{5.6}$$

and observing that

$$\left.\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\right|_{\varepsilon=0}=1,\quad \det\left(\left.\frac{\partial\overline{x}}{\partial x}\right)\right|_{\varepsilon=0}=1,\quad \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\right|_{\varepsilon=0}=\frac{\mathrm{d}\tau}{\mathrm{d}t}$$

produces

$$\frac{\mathrm{d}\zeta}{\mathrm{d}t}=\int_D\left.\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\mathrm{d}^nx+\int_D\mathcal{L}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\left.\frac{\partial\overline{x}}{\partial x}\right)\right|_{\varepsilon=0}\mathrm{d}^nx+\frac{\mathrm{d}\tau}{\mathrm{d}t}\int_D\mathcal{L}\,\mathrm{d}^nx, \tag{5.7}$$

where, by definition, the variation $\zeta=\zeta(t)$ of $\overline{z}$ is

$$\zeta(t)\equiv\left.\frac{\mathrm{d}\overline{z}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}.$$

Now, we need to express the first and the second integrands in (5.7) in terms of known functions. The calculations are lengthy and are given in the Appendix. When the results

$$\left.\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u^i_t\frac{\mathrm{d}\tau}{\mathrm{d}t}-u^i_{x^k}\frac{\mathrm{d}\xi^k}{\mathrm{d}t}\right)+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u^i_{x^j}\frac{\mathrm{d}\xi^j}{\mathrm{d}x^k}\right)+\frac{\partial\mathcal{L}}{\partial z}\zeta, \tag{5.8}$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\left.\frac{\partial\overline{x}}{\partial x}\right)\right|_{\varepsilon=0}=\frac{\mathrm{d}\xi^k}{\mathrm{d}x^k} \tag{5.9}$$

are inserted into (5.7) we obtain the equation for the variation $\zeta(t)$, namely,

$$\begin{aligned}\frac{\mathrm{d}\zeta(t)}{\mathrm{d}t}=\int_D\Bigg(&\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u^i_t\frac{\mathrm{d}\tau}{\mathrm{d}t}-u^i_{x^k}\frac{\mathrm{d}\xi^k}{\mathrm{d}t}\right)\\&+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u^i_{x^j}\frac{\mathrm{d}\xi^j}{\mathrm{d}x^k}\right)+\mathcal{L}\frac{\mathrm{d}\xi^j}{\mathrm{d}x^j}\Bigg)\mathrm{d}^nx+\frac{\mathrm{d}\tau}{\mathrm{d}t}\int_D\mathcal{L}\,\mathrm{d}^nx+\zeta(t)\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx.\end{aligned} \tag{5.10}$$

Its solution $\zeta(s)$, evaluated at $t=s$, is given by

$$\begin{aligned}E(s)\,\zeta(s)-\zeta(0)=\int_0^s\int_D E(t)\Bigg(&\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u^i_t\frac{\mathrm{d}\tau}{\mathrm{d}t}-u^i_{x^k}\frac{\mathrm{d}\xi^k}{\mathrm{d}t}\right)\\&+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u^i_{x^j}\frac{\mathrm{d}\xi^j}{\mathrm{d}x^k}\right)+\mathcal{L}\left(\frac{\mathrm{d}\xi^j}{\mathrm{d}x^j}+\frac{\mathrm{d}\tau}{\mathrm{d}t}\right)\Bigg)\mathrm{d}^nx\,\mathrm{d}t,\end{aligned} \tag{5.11}$$

where $E(t)$ is the expression (5.3) and s is the value of t at which the solution $z(t)$ of Eq. (2.1) was evaluated in order to obtain the functional $z[u;s]$. By definition, $\zeta(0)=0$. By hypothesis, the transformation group (4.3) leaves the functional $\overline{z}$ invariant, so $\zeta(s)=0$. Thus, (5.11) becomes

$$\begin{aligned}\int_0^s\int_D E\Bigg(&\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u^i_t\frac{\mathrm{d}\tau}{\mathrm{d}t}-u^i_{x^k}\frac{\mathrm{d}\xi^k}{\mathrm{d}t}\right)\\&+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u^i_{x^j}\frac{\mathrm{d}\xi^j}{\mathrm{d}x^k}\right)+\mathcal{L}\left(\frac{\mathrm{d}\xi^j}{\mathrm{d}x^j}+\frac{\mathrm{d}\tau}{\mathrm{d}t}\right)\Bigg)\mathrm{d}^nx\,\mathrm{d}t=0.\end{aligned} \tag{5.12}$$

Next we form total derivatives with respect to t and x^k in the integrand I of (5.12). A tedious but straightforward calculation yields

$$I=-\frac{\mathrm{d}}{\mathrm{d}t}\left(E\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)\right)-\frac{\mathrm{d}}{\mathrm{d}x^k}\left(E\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}-\xi^k\mathcal{L}\right)\right)$$
$$-E(\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\left(\frac{\partial\mathcal{L}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial u_t^i}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}+\frac{\partial\mathcal{L}}{\partial u_t^i}\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx\right)$$
$$+\tau E\left(\mathcal{L}\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx-\frac{\partial\mathcal{L}}{\partial z}\int_D\mathcal{L}\,\mathrm{d}^nx\right). \tag{5.13}$$

We evaluate the above expression on a solution of the generalized Euler–Lagrange equation (3.1) (hence the third term becomes zero) and insert it into (5.12). Then, recognizing that the space-integral of the last term in (5.13) vanishes, i.e.,

$$\int_D\left(\mathcal{L}\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx-\frac{\partial\mathcal{L}}{\partial z}\int_D\mathcal{L}\,\mathrm{d}^nx\right)\mathrm{d}^nx'=\int_D\mathcal{L}\,\mathrm{d}^nx'\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx-\int_D\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx'\int_D\mathcal{L}\,\mathrm{d}^nx=0$$

and that the limit s of the time integral is arbitrary, we obtain

$$\int_D\left(\frac{\mathrm{d}}{\mathrm{d}t}\left(E\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)\right)+\frac{\mathrm{d}}{\mathrm{d}x^k}\left(E\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}-\xi^k\mathcal{L}\right)\right)\right)\mathrm{d}^nx=0,$$

which concludes the proof. □

Corollary 5.2: Theorem 5.1 reduces to the classical first Noether theorem when the generalized variational principle with several independent variables reduces to the classical variational principle.

Proof: The generalized variational principle with several independent variables reduces to the classical variational principle if the Lagrangian density $\mathcal{L}$, in the defining equation (2.1), does not depend on z. This is so because, then, the functional $z[u;s]$ becomes a space–time integral of $\mathcal{L}$, i.e.,

$$z[u;s]=\int_0^s\int_\Omega\mathcal{L}(t,x,u,u_t,u_x)\,\mathrm{d}^nx\,\mathrm{d}t \tag{5.14}$$

and the generalized Euler–Lagrange equation (3.1) becomes the classical Euler–Lagrange equation. On the other hand, when $\mathcal{L}$ does not depend on z the integrand in (5.2) is independent of D since, in this case, $E=1$ as seen from (5.3). Then, the arbitrariness of D in the identity (5.2) implies that the integrand is identically zero and we obtain the conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t}\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)+\frac{\mathrm{d}}{\mathrm{d}x^k}\left((\tau u_t^i+\xi^j u_{xj}^i-\eta^i)\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}-\xi^k\mathcal{L}\right)=0, \tag{5.15}$$

which holds on solutions of the classical Euler–Lagrange equations. This is precisely the conservation law of the classical first Noether theorem. □

VI. CONSERVED QUANTITIES IN DISSIPATIVE AND GENERATIVE SYSTEMS WITH SEVERAL INDEPENDENT VARIABLES

Systems described by the generalized Euler–Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial u_t^i}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}+\frac{\partial\mathcal{L}}{\partial u_t^i}\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^nx=0,\quad i=1,\ldots,m \tag{6.1}$$

are in general not conservative. In this section we show how Theorem 5.1 can be used to find conserved quantities in such systems. To carry out this procedure, we must find the symmetries of

the functional $z[u,s]$ defined by Eq. (2.1). Each one-parameter symmetry provides one conserved quantity. To test whether a one-parameter group of transformations of the independent and dependent variables is a symmetry group of the functional z we use the infinitesimal criterion which Proposition 4.3 provides.

Theorem 6.1: *Let (4.3) be a symmetry group, with infinitesimal generator (4.7), of the functional z defined by (2.1). If the equations*

$$(\tau u_t^i+\xi^j u_{x^j}^i-\eta^i)\frac{\partial \mathcal{L}}{\partial u_{x^k}^i}-\xi^k\mathcal{L}=0, \quad k=1,\ldots,n, \quad i=1,\ldots,m$$

hold on the boundary $\partial\Omega$ of Ω, then the quantity

$$E(t)\int_\Omega\left((\tau u_t^i+\xi^j u_{x^j}^i-\eta^i)\frac{\partial \mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)\mathrm{d}^n x=\text{const} \tag{6.2}$$

is conserved on solutions of the generalized Euler–Lagrange equations (6.1), where

$$E(t)\equiv\exp\left(-\int_0^t\int_\Omega\frac{\partial \mathcal{L}}{\partial z}\mathrm{d}^n x\,\mathrm{d}\theta\right). \tag{6.3}$$

Proof: From Gauss divergence theorem and the hypothesis of the theorem follows that the second term in the identity (5.2) of Theorem 5.1 is zero, that is

$$\int_\Omega\frac{\mathrm{d}}{\mathrm{d}x^k}\left(E\left((\tau u_t^i+\xi^j u_{x^j}^i-\eta^i)\frac{\partial \mathcal{L}}{\partial u_{x^k}^i}-\xi^k\mathcal{L}\right)\right)\mathrm{d}^n x=0.$$

Hence, identity (5.2) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega E\left((\tau u_t^i+\xi^j u_{x^j}^i-\eta^i)\frac{\partial \mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)\mathrm{d}^n x=0,$$

which is the statement of the theorem. □

The following corollary is an important special case of Theorem 6.1.

Corollary 6.2: Let (4.3) be a symmetry group, with infinitesimal generator (5.1), of the functional z defined by (2.1) with $\Omega=\mathbb{R}^n$. If

$$\left|\int_{\mathbb{R}^n}\mathcal{L}(t,x,u(t,x),u_t,u_x,z)\,\mathrm{d}^n x\right|<\infty \tag{6.4}$$

over the entire time domain, then the quantity

$$E(t)\int_{\mathbb{R}^n}\left((\tau u_t^i+\xi^j u_{x^j}^i-\eta^i)\frac{\partial \mathcal{L}}{\partial u_t^i}-\tau\mathcal{L}\right)\mathrm{d}^n x=\text{const} \tag{6.5}$$

is conserved on solutions of the generalized Euler–Lagrange equations (6.1), where

$$E(t)\equiv\exp\left(-\int_0^t\int_{\mathbb{R}^n}\frac{\partial \mathcal{L}}{\partial z}\mathrm{d}^n x\,d\theta\right). \tag{6.6}$$

Proof: The requirement (6.4) implies that $\lim_{|x|\to\infty}\mathcal{L}=0$. Then $\partial\mathcal{L}/\partial u_{x^k}^i$, $k=1,\ldots,n$, $i=1,\ldots,m$ are also zero at infinity. Thus, the hypotheses of Theorem 6.1 are satisfied and (6.5) follows from (6.2). □

VII. SOME APPLICATIONS

The generalized variational principle with several independent variables gives a variational description of nonconservative as well as conservative processes involving physical fields. The next three corollaries give conserved quantities which correspond in the classical case to the total energy, linear momentum, and angular momentum of the field $u(t,x)=(u^1(t,x),\ldots,u^m(t,x))$ defined on $\mathbb{R}^n$. See Goldstein,[9] Chap. 12.

Corollary 7.1: Let the condition (6.4) hold and let the functional z, defined by the equation (2.1), be invariant with respect to translations in time. Then the quantity

$$E(t)\int_{\mathbb{R}^n}\left(u_t^i\frac{\partial\mathcal{L}}{\partial u_t^i}-\mathcal{L}\right)\mathrm{d}^n x=\text{const},\quad i=1,\ldots,m \tag{7.1}$$

with $E(t)$ given by (6.6), is conserved on solutions of the generalized Euler–Lagrange equations (6.1).

Proof: Time-translations are the transformations

$$\overline{t}=t+\varepsilon,\quad \overline{x^k}=x^k,\quad k=1,\ldots,n,\quad \overline{u}=u$$

from which we have

$$\tau=\left.\frac{\mathrm{d}\overline{t}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=1,\quad \xi^k=0,\quad k=1,\ldots,n,\quad \eta=0.$$

Inserting these into (6.5) produces (7.1). □

If, following the classical field theory, we interpret the expression

$$\mathcal{E}=u_t^i\frac{\partial\mathcal{L}}{\partial u_t^i}-\mathcal{L} \tag{7.2}$$

as the energy density of the field $u(t,x)$, then (7.1) states that the total field energy changes in time proportional to $1/E(t)$.

Corollary 7.2: Let the condition (6.4) hold and let the functional z, defined by the equation (2.1), be invariant with respect to space translations along the x^k coordinate. Then the quantity

$$E(t)\int_{\mathbb{R}^n}\frac{\partial u^i}{\partial x^k}\frac{\partial\mathcal{L}}{\partial u_t^i}\mathrm{d}^n x=\text{const} \tag{7.3}$$

with $E(t)$ given by (6.6), is conserved on solutions of the generalized Euler–Lagrange equations (6.1).

Proof: Space translations along the x^k coordinate are the transformations

$$\overline{t}=t,\quad \overline{x^k}=x^k+\varepsilon,\quad \overline{x^j}=x^j\quad \text{for } j\neq k,\quad \overline{u}=u,\quad j=1,\ldots,n$$

from which we get

$$\xi^k=\left.\frac{\mathrm{d}\overline{x^k}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=1,\quad \xi^j=0\quad \text{for } j\neq k,\quad \tau=\eta=0.$$

Then, (7.3) follows from (6.5). □

If, following the classical field theory, we interpret the expression

$$\mathcal{P}_k=-\frac{\partial u^i}{\partial x^k}\frac{\partial\mathcal{L}}{\partial u_t^i},\quad i=1,\ldots,m \tag{7.4}$$

as the k component of the linear momentum density, then (7.3) states that the kth component of the field's total linear momentum changes in time proportional to $1/E(t)$.

Corollary 7.3: Let the condition (6.4) hold and let the functional z, defined by the equation (2.1), be invariant with respect to rotations in the ij-coordinate plane. Then the quantity

$$E(t)\int_{\mathbb{R}^n}\left(x^j\frac{\partial u^l}{\partial x^i}-x^i\frac{\partial u^l}{\partial x^j}\right)\frac{\partial \mathcal{L}}{\partial u^l_t}\,\mathrm{d}^n x=\text{const} \tag{7.5}$$

with $E(t)$ given by (6.6), is conserved on solutions of the generalized Euler–Lagrange equations (6.1).

Proof: The rotations in the ij plane are the transformations

$$\overline{x}^i=x^i\cos\varepsilon+x^j\sin\varepsilon,\quad \overline{x}^j=-x^i\sin\varepsilon+x^j\cos\varepsilon,\quad \overline{x}^k=x^k\quad \text{for}\ \ k\neq i,j$$

from which we obtain

$$\xi^i=\left.\frac{\mathrm{d}\overline{x}^i}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=x^j,\quad \xi^j=\left.\frac{\mathrm{d}\overline{x}^j}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=-x^i,\quad \xi^k=0\quad \text{for}\ \ k\neq i,j,\quad \tau=\eta=0.$$

Inserting these into (6.5) of Corollary 6.2 produces (7.5). □

If, following the classical field theory, we interpret the expression

$$\mathcal{M}_{ij}=\left(x^j\frac{\partial u^l}{\partial x^i}-x^i\frac{\partial u^l}{\partial x^j}\right)\frac{\partial \mathcal{L}}{\partial u^l_t}=x^i\mathcal{P}_j-x^j\mathcal{P}_i \tag{7.6}$$

as the ij component of the angular momentum density of the field $u(t,x)$, then (7.5) states that the ij component of the field's total angular momentum changes in time proportionally to $1/E(t)$.

An observation: Let $\mathcal{F}=\mathcal{F}(u,u_x,u_t,x,t)$ be any real-valued function which is, at least, twice differentiable with respect to u, u_x, u_t and once differentiable with respect to x, t. Then, all equations, linear and nonlinear, of the form

$$\frac{\partial \mathcal{F}}{\partial u^i}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial \mathcal{F}}{\partial u^i_{x^k}}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{F}}{\partial u^i_t}+a\frac{\partial \mathcal{F}}{\partial u^i_t}=0\,,\quad i=1,\ldots,m \tag{7.7}$$

are generalized Euler–Lagrange equations (3.1) derivable from the generalized variational principle with Lagrangian density

$$\mathcal{L}=\mathcal{F}+\alpha\, z,$$

where $\alpha=\alpha(x,t)$ and

$$a(t)=\int_\Omega \alpha(x,t)\,\mathrm{d}^n x.$$

Hence, we can apply the Noether-type theorems to any equation of the form (7.7). It should be noticed that due to the presence of the term $a\,\partial\mathcal{F}/\partial u^i_t$ these equations describe generative or dissipative processes and cannot be derived from the classical variational principle.

Here, we give two illustrative examples of equations from the family (7.7). The first is the set of equations which describe the propagation of electromagnetic fields in a conductive medium,

$$c^2\,\nabla^2\mathbf{E}-\frac{\partial^2\mathbf{E}}{\partial t^2}-\frac{\sigma}{\varepsilon}\frac{\partial\mathbf{E}}{\partial t}=0, \tag{7.8}$$

where $\mathbf{E}=(E^1,E^2,E^3)$ is the electric field vector, c is the velocity of the electromagnetic waves, σ is the electrical conductivity, and ε is the dielectric constant of the medium. Exactly the same equation holds for the magnetic field vector $\mathbf{B}=(B^1,B^2,B^3)$. These equations are a direct consequence of the Maxwell's equations in conjunction with the medium's property equations $\mathbf{J}=\sigma\mathbf{E}$ and $\rho=0$, where $\mathbf{J}=(J^1,J^2,J^3)$ is the current density and ρ is the charge density.

One can easily verify that Eq. (7.8) belongs to the family (7.7) by inserting

$$\mathcal{L}=c^2\frac{\partial E^i}{\partial x^j}\frac{\partial E^i}{\partial x^j}-\frac{\partial E^i}{\partial t}\frac{\partial E^i}{\partial t}+\alpha(x)\,z, \quad i,j=1,2,3 \tag{7.9}$$

into the generalized Euler–Lagrange equations (3.1) and setting

$$\frac{\sigma}{\varepsilon}=\int_\Omega \alpha(x)\,\mathrm{d}^3x=\text{const.}$$

Thus, the Noether-type theorem can be applied and, with the appropriate boundary conditions and function $\alpha(x)$, we obtain the conserved quantities of the Corollaries 7.1, 7.2, and 7.3.

As a second example consider the equation

$$\nabla^2 u-\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}+G(uu^*)\,u=0 \tag{7.10}$$

describing the real or complex field $u=u(x,t)$, where u^* denotes the complex conjugate of u, G is a differentiable function and v is a constant. This equation is known as the nonlinear Klein–Gordon equation. Its linear version, with $G=\text{const}$ plays an important role in relativistic field theories. The one-dimensional version of (7.10) with real u and $G(u^2)u=\sin u$ is the sine-Gordon equation. The field equations of the form (7.10) can be derived from the Lagrangian density

$$\mathcal{L}(u,u_t,\nabla u)=\nabla u\cdot\nabla u^*-\frac{1}{v^2}\frac{\partial u}{\partial t}\frac{\partial u^*}{\partial t}-F(uu^*), \tag{7.11}$$

where

$$\frac{\mathrm{d}F(\rho)}{\mathrm{d}\rho}=G(\rho) \quad \text{and} \quad F(0)=0.$$

We consider as physically meaningful only those solutions of (7.10) which are free of singularities and for which

$$\left|\int_\Omega \mathcal{L}(t,x,u,u_t,u_x)\,\mathrm{d}x\right|<\infty$$

holds over the entire time domain. The processes described with an equation of the form (7.10) are conservative since the Lagrangian (7.11) does not explicitly depend on time.

One is also interested in nonconservative processes involving fields. The simplest modification of (7.10) which makes it suitable to describe nonconservative processes is to include in it a term proportional to the time derivative of the field. Thus, a physically meaningful nonconservative version of (7.10) is

$$\nabla^2 u-\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}+k\frac{\partial u}{\partial t}+G(uu^*)\,u=0, \tag{7.12}$$

where k is a constant. With $k>0$ the process described by (7.12) is generative, and with $k<0$ it is dissipative. When u is a real field, equations of the form (7.12) belong to the family (7.7) and can be derived via the present generalized variational principle from the Lagrangian density

$$\mathcal{L}=\nabla u\cdot\nabla u-\frac{1}{v^2}\left(\frac{\partial u}{\partial t}\right)^2-F(u^2)+\alpha(x)\,z, \tag{7.13}$$

where $\partial F(\rho)/\partial\rho=G(\rho)$, and $\alpha=\alpha(x)$ is a given function of the coordinates $x=(x^1,\ldots,x^n)$ which satisfies the condition

$$\left|\int_\Omega \alpha(x)\,\mathrm{d}^n x\right|<\infty.$$

Indeed, inserting the Lagrangian (7.13) into the generalized Euler–Lagrange equations (3.1),

$$\frac{\partial\mathcal{L}}{\partial u}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial u_t}-\frac{\mathrm{d}}{\mathrm{d}x^k}\frac{\partial\mathcal{L}}{\partial u_{x^k}}+\frac{\partial\mathcal{L}}{\partial u_t}\int_\Omega\frac{\partial\mathcal{L}}{\partial z}\mathrm{d}^n x$$
$$=-2u\frac{\partial F}{\partial(u^2)}+\frac{2}{v^2}\frac{\partial^2 u}{\partial t^2}-2\nabla^2 u-\frac{2}{v^2}\frac{\partial u}{\partial t}\int_\Omega\alpha(x)\,\mathrm{d}^n x=0,$$

we see that the last expression is the same as (7.12) with

$$k=\frac{1}{v^2}\int_\Omega\alpha(x)\,\mathrm{d}^n x=\text{const}. \tag{7.14}$$

Consequently, we may apply the first Noether-type theorem 5.1 to obtain conserved quantities. In particular, observing that the Lagrangian (7.13) is invariant under translations in time we may apply Corollary 7.1 to obtain the conserved quantity

$$\exp(-kv^2t)\int_\Omega\left(\frac{1}{v^2}\left(\frac{\partial u}{\partial t}\right)^2+\nabla u\cdot\nabla u-F(u^2)+\alpha(x)\,z\right)\mathrm{d}x=\text{const}, \tag{7.15}$$

where z is the solution of the defining equation (2.1). In accordance with the conservative case, we can interpreted the quantity

$$\frac{\partial\mathcal{L}}{\partial u_t}u_t-\mathcal{L}=-\frac{1}{v^2}\left(\frac{\partial u}{\partial t}\right)^2-\nabla u\cdot\nabla u+F(u^2)-\alpha(x)\,z$$

as the energy density of the field $u(t,x)$. Then Eq. (7.15) states that the total field energy exponentially increases when $k>0$ and decreases when $k<0$.[10–20]

APPENDIX

Derivation of the relation (5.8): We differentiate the transformed Lagrangian density $\mathcal{L}(\overline{t},\overline{x},\overline{u},\overline{u_t},\overline{u_x},\overline{z})$ in Eq. (5.5) with respect to ε and set $\varepsilon=0$,

$$\left.\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=\left.\left(\frac{\partial\mathcal{L}}{\partial\overline{t}}\frac{\mathrm{d}\phi}{\mathrm{d}\varepsilon}+\frac{\partial\mathcal{L}}{\partial\overline{x}^k}\frac{\mathrm{d}\varphi^k}{\mathrm{d}\varepsilon}+\frac{\partial\mathcal{L}}{\partial\overline{u}^i}\frac{\mathrm{d}\psi^i}{\mathrm{d}\varepsilon}+\frac{\partial\mathcal{L}}{\partial\overline{u}^i_t}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial\overline{t}}+\frac{\partial\mathcal{L}}{\partial\overline{u}^i_{\overline{x}^k}}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial\overline{x}^k}+\frac{\partial\mathcal{L}}{\partial\overline{z}}\frac{\mathrm{d}\overline{z}}{\mathrm{d}\varepsilon}\right)\right|_{\varepsilon=0},$$

which when written with ζ and the infinitesimal generators of the group becomes

$$\left.\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}=\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u^i_t}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{u}^i}{\partial\overline{t}}\right)\Bigg|_{\varepsilon=0}+\frac{\partial\mathcal{L}}{\partial u^i_{x^k}}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{u}^i}{\partial\overline{x}^k}\right)\Bigg|_{\varepsilon=0}+\frac{\partial\mathcal{L}}{\partial z}\zeta. \quad \text{(A1)}$$

To calculate

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{u}^i}{\partial\overline{t}}\right)\Bigg|_{\varepsilon=0}$$

differentiate the equation $\overline{u}^i(\overline{t},\overline{x};\varepsilon)=\psi^i(t,x,u;\varepsilon)=\overline{u}^i(t,x,u;\varepsilon)$ with respect to t,

$$\frac{\partial\overline{u}^i}{\partial\overline{t}}\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}+\frac{\partial\overline{u}^i}{\partial\overline{x}^k}\left(\frac{\partial\overline{x}^k}{\partial t}+\frac{\partial\overline{x}^k}{\partial u^j}u^j_t\right)=\frac{\partial\overline{u}^i}{\partial t}+\frac{\partial\overline{u}^i}{\partial u^j}u^j_t. \quad \text{(A2)}$$

Set $\varepsilon=0$ and take into account the identities

$$\left.\frac{\partial\overline{u}^i}{\partial t}\right|_{\varepsilon=0}=0,\quad \left.\frac{\partial\overline{u}^i}{\partial u^j}\right|_{\varepsilon=0}=\delta^i_j,\quad \left.\frac{\partial\overline{t}}{\partial t}\right|_{\varepsilon=0}=1,\quad \left.\frac{\partial\overline{x}^k}{\partial t}\right|_{\varepsilon=0}=0,\quad \left.\frac{\partial\overline{x}^k}{\partial u^j}\right|_{\varepsilon=0}=0.$$

Substitute these in (A2) and solve the resulting equation for $\overline{u}^i_{\overline{t}}|_{\varepsilon=0}$ to find

$$\overline{u}^i_{\overline{t}}|_{\varepsilon=0}=u^i_t. \quad \text{(A3)}$$

Differentiate the equation $\overline{u}^i(\overline{t},\overline{x};\varepsilon)=\psi^i(t,x,u;\varepsilon)\equiv\overline{u}^i(t,x,u;\varepsilon)$ with respect to x^k,

$$\frac{\partial\overline{u}^i}{\partial\overline{x}^k}\left(\frac{\partial\overline{x}^k}{\partial x^k}+\frac{\partial\overline{x}^k}{\partial u^j}u^j_{x^k}\right)=\frac{\partial\overline{u}^i}{\partial x^k}+\frac{\partial\overline{u}^i}{\partial u^j}u^j_{x^k}. \quad \text{(A4)}$$

Set $\varepsilon=0$ and substitute the identities

$$\left.\frac{\partial\overline{u}^i}{\partial x^k}\right|_{\varepsilon=0}=0,\quad \left.\frac{\partial\overline{u}^i}{\partial u^j}\right|_{\varepsilon=0}=\delta^i_j,\quad \left.\frac{\partial\overline{x}^k}{\partial x^k}\right|_{\varepsilon=0}=\delta^l_k,\quad \left.\frac{\partial\overline{x}^k}{\partial u^j}\right|_{\varepsilon=0}=0$$

in (A4). Then solve the resulting equation for $\overline{u}^i_{\overline{x}^k}|_{\varepsilon=0}$ to obtain

$$\overline{u}^i_{\overline{x}^k}|_{\varepsilon=0}=u^i_{x^k}. \quad \text{(A5)}$$

Differentiate (A2) with respect to ε to get

$$\begin{aligned}\overline{u}^i_{\overline{t}}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}+\frac{\mathrm{d}\overline{t}}{\mathrm{d}t}\frac{\mathrm{d}\overline{u}^i_{\overline{t}}}{\mathrm{d}\varepsilon}+\overline{u}^i_{\overline{x}^k}\left(\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^k}{\partial t}+\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{x}^k}{\partial u^j}\right)u^j_t\right)+\left(\frac{\partial\overline{x}^k}{\partial t}+\frac{\partial\overline{x}^k}{\partial u^j}u^j_t\right)\frac{\mathrm{d}\overline{u}^i_{\overline{x}^k}}{\mathrm{d}\varepsilon}\\ =\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{u}^i}{\partial t}+\frac{\partial\overline{u}^i}{\partial u^j}u^j_t\right).\end{aligned} \quad \text{(A6)}$$

Set $\varepsilon=0$ in (A6) and substitute (A3) and (A5) in it. Then take into account the identities

$$\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial t}\right|_{\varepsilon=0}=\frac{\partial\eta^i}{\partial t},\quad \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial u^j}\right|_{\varepsilon=0}=\frac{\partial\eta^i}{\partial u^j},\quad \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{t}}{\partial t}\right|_{\varepsilon=0}=\frac{\partial\tau}{\partial t},\quad \left.\frac{\partial\overline{t}}{\partial t}\right|_{\varepsilon=0}=1,$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^k}{\partial t}\bigg|_{\varepsilon=0}=\frac{\partial\xi^k}{\partial t},\quad \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^k}{\partial u^j}\bigg|_{\varepsilon=0}=\frac{\partial\xi^k}{\partial u^j},\quad \frac{\partial\overline{x}^k}{\partial t}\bigg|_{\varepsilon=0}=0,\quad \frac{\partial\overline{x}^k}{\partial u^j}\bigg|_{\varepsilon=0}=0.$$

Consequently, Eq. (A6) becomes

$$\frac{\partial\eta^i}{\partial t}+\frac{\partial\eta^i}{\partial u^j}u_t^j=u_t^i\frac{\partial\tau}{\partial t}+\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\overline{u}_{\overline{t}}^i\bigg|_{\varepsilon=0}+u_{x^k}^i\left(\frac{\partial\xi^k}{\partial t}+\frac{\partial\xi^k}{\partial u^j}u_t^j\right) \tag{A7}$$

from which we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\overline{u}_{\overline{t}}^i\bigg|_{\varepsilon=0}=\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u_t^i\frac{\mathrm{d}\tau}{\mathrm{d}t}-u_{x^k}^i\frac{\mathrm{d}\xi^k}{\mathrm{d}t}. \tag{A8}$$

We must now calculate

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{u}^i}{\partial\overline{x}^k}\right)\bigg|_{\varepsilon=0},$$

which appears in (A1). For this purpose differentiate (A4) with respect to ε,

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial x^k}+\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial u^j}u_{x^k}^j=\frac{\mathrm{d}}{\mathrm{d}\varepsilon}(\overline{u}_{\overline{x}^l}^i)\left(\frac{\partial\overline{x}^l}{\partial x^k}+\frac{\partial\overline{x}^l}{\partial u^j}u_{x^k}^j\right)+\overline{u}_{\overline{x}^l}^i\left(\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^l}{\partial x^k}+u_{x^k}^j\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^l}{\partial u^j}\right). \tag{A9}$$

Set $\varepsilon=0$ in (A9), substitute (A3) and (A5) into (A9) and observe that

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial x^k}\bigg|_{\varepsilon=0}=\frac{\partial\eta^i}{\partial x^k},\quad \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{u}^i}{\partial u^j}\bigg|_{\varepsilon=0}=\frac{\partial\eta^i}{\partial u^j},\quad \frac{\partial\overline{x}^l}{\partial x^k}\bigg|_{\varepsilon=0}=\delta_k^l,$$

$$\frac{\partial\overline{x}^l}{\partial u^j}\bigg|_{\varepsilon=0}=0,\quad \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^l}{\partial x^k}\bigg|_{\varepsilon=0}=\frac{\partial\xi^l}{\partial x^k},\quad \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\partial\overline{x}^l}{\partial u^j}\bigg|_{\varepsilon=0}=\frac{\partial\xi^l}{\partial u^j}.$$

Then (A9) becomes

$$\frac{\partial\eta^i}{\partial x^k}+\frac{\partial\eta^i}{\partial u^j}u_{x^k}^j=\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\overline{u}_{\overline{x}^l}^i\bigg|_{\varepsilon=0}\delta_k^l+u_{x^l}^i\left(\frac{\partial\xi^l}{\partial x^k}+\frac{\partial\xi^l}{\partial u^j}u_{x^k}^j\right), \tag{A10}$$

from which we get

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\overline{u}_{\overline{x}^k}^i\bigg|_{\varepsilon=0}=\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u_{x^l}^i\frac{\mathrm{d}\xi^l}{\mathrm{d}x^k}. \tag{A11}$$

Substituting (A8) and (A11) into (A1) produces the relation (5.8),

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0}=\frac{\partial\mathcal{L}}{\partial t}\tau+\frac{\partial\mathcal{L}}{\partial x^k}\xi^k+\frac{\partial\mathcal{L}}{\partial u^i}\eta^i+\frac{\partial\mathcal{L}}{\partial u_t^i}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}t}-u_t^i\frac{\mathrm{d}\tau}{\mathrm{d}t}-u_{x^k}^i\frac{\mathrm{d}\xi^k}{\mathrm{d}t}\right)+\frac{\partial\mathcal{L}}{\partial u_{x^k}^i}\left(\frac{\mathrm{d}\eta^i}{\mathrm{d}x^k}-u_{x^l}^i\frac{\mathrm{d}\xi^l}{\mathrm{d}x^k}\right)+\frac{\partial\mathcal{L}}{\partial z}\zeta.$$

Derivation of the relation (5.9): We use the formula for the derivative of a determinant, according to which

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\frac{\partial\overline{x}}{\partial x}\right)=A_k^j\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{x}^k}{\partial x^j}\right), \tag{A12}$$

where A_k^j is the cofactor of the determinant's entry $\partial\overline{x}^k/\partial x^j$. Next,

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{\partial\overline{x}^k}{\partial x^j}\right)=\frac{\partial}{\partial x^j}\frac{\mathrm{d}\overline{x}^k}{\mathrm{d}\varepsilon}=\frac{\partial^2\overline{x}^k}{\partial x^j\,\partial\varepsilon}+\frac{\partial^2\overline{x}^k}{\partial u^i\,\partial\varepsilon}\frac{\partial u^i}{\partial x^j},$$

because $\overline{x}^k=\overline{x}^k(t,x,u(t,x);\varepsilon)$. Hence (A12) becomes

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\frac{\partial\overline{x}}{\partial x}\right)=A_k^j\left(\frac{\partial^2\overline{x}^k}{\partial x^j\,\partial\varepsilon}+\frac{\partial^2\overline{x}^k}{\partial u^i\,\partial\varepsilon}\frac{\partial u^i}{\partial x^j}\right).$$

Setting $\varepsilon=0$ in the above expression and observing that $A_k^j|_{\varepsilon=0}=\delta_k^j$ is a cofactor of the identity matrix, we get the relation (5.9),

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\det\left(\frac{\partial\overline{x}}{\partial x}\right)\Bigg|_{\varepsilon=0}=\left(\frac{\partial\xi^k}{\partial x^j}+\frac{\partial\xi^k}{\partial u^i}\frac{\partial u^i}{\partial x^j}\right)\delta_k^j=\frac{\mathrm{d}\xi^k}{\mathrm{d}x^j}\,\delta_k^j=\frac{\mathrm{d}\xi^k}{\mathrm{d}x^k}.$$

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Two choices of the gauge transformation for the AKNS hierarchy through the constrained KP hierarchy

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(Received 25 February 2003; accepted 31 March 2003)

On the basis of the equivalence between the AKNS hierarchy and the cKP hierarchy with the constraint $k=1$, we point out that there exist two choices to keep the form of the Lax operator when we perform the gauge transformation for the AKNS hierarchy, which results in two classes of functions to trigger the gauge transformation. For the second choice, two theorems for two types of gauge transformation are established. Several new and more general forms of tau-functions for the AKNS hierarchy are obtained by means of gauge transformations of both types. The union of the two choices leads to new forms of τ-functions. We generate the AKNS hierarchy from the "free" Lax operator $L^{(0)}=\partial$ via a chain of gauge transformations. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1581973]

I. INTRODUCTION

The AKNS hierarchy and its generalizations[1,2] are very important and basic in the theory of PDEs. They yields the generalized nonlinear Schrödinger equation (including nonlinear Schrödinger equation and the derivative Schrödinger equation), the KdV equation, the mKdV equation, the sine-Gordon equation, the sinh-Gordon equation, the Harry–Dym equation, etc. This hierarchy is also equivalent to the constrained KP hierarchy (cKP) with constraint $k=1$.[3–5] Explicitly, the AKNS hierarchy can be expressed as

$$\frac{\partial L^{(0)}}{\partial t_k}=[B_k^{(0)},L^{(0)}] \tag{1.1}$$

by means of a pseudodifferential operator having the following form:

$$L^{(0)}=\partial+\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)},\quad B_k^{(0)}\equiv(L^{(0)})_+^k. \tag{1.2}$$

Here A_+, respectively, A_- denote the differential, respectively, integral part of the pseudodifferential operator $A=A_++A_-$. For $L^{(0)}$, $L_+^{(0)}=\partial$, $L_-^{(0)}=\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)}$, where $\phi^{(0)}$ and $\psi^{(0)}$ in $L^{(0)}$ are the solutions of the equations

$$\frac{\partial\phi^{(0)}}{\partial t_k}=B_k^{(0)}\cdot\phi^{(0)},\quad \frac{\partial\psi^{(0)}}{\partial t_k}=-B_k^{*(0)}\cdot\psi^{(0)}. \tag{1.3}$$

Here the symbol "$\circ$" denotes product of operators and the symbol "$\cdot$" indicates that the operator acts the function just following. For example, $\partial^2\circ f=f_{xx}+2f_x\circ\partial+f\circ\partial^2$ is a sum of operators; $\partial^{-1}\circ f=f\circ\partial^{-1}-f_x\circ\partial^{-2}+f_{xx}\circ\partial^{-2}+\cdots$ is also an operator. But $\partial^2\cdot f=f_{xx}$ is a function; $\partial^{-1}\cdot f=\int f\,dx$ is a function. Of course, $f\circ\partial=f\cdot\partial, f\circ g=f\cdot g$; the functions f and g can be regarded as the zeroth order operators. The symbol * indicates the operation of conjugation; $(A\circ B)^*=B^*$

$\circ A^*, \partial^* = -\partial, f^*(x) = f(x), (f \circ \partial^{-1} \circ g)^* = -g \circ \partial^{-1} \circ f$ (here A, B are differential operators, f, g are functions). It can be shown that (1.3) are consistent with (1.1). For simplicity, we adopt the notation of Ref. 6. The solutions of (1.3), $\phi^{(0)}$, respectively, $\psi^{(0)}$ are called the ''eigenfunction,'' respectively, the ''adjoint eigenfunction'' of the AKNS hierarchy. For example, the first two flows of the AKNS hierarchy $(t_1 = x)$ are

$$\phi^{(0)}_{t_2} = \phi^{(0)}_{xx} + 2(\phi^{(0)})^2 \psi^{(0)}, \quad \psi^{(0)}_{t_2} = -\psi^{(0)}_{xx} - 2\phi^{(0)}(\psi^{(0)})^2, \tag{1.4}$$

and

$$\phi^{(0)}_{t_3} = \phi^{(0)}_{xxx} + 6\phi^{(0)}\psi^{(0)}\phi^{(0)}_x, \quad \psi^{(0)}_{t_3} = \psi^{(0)}_{xxx} + 6\phi^{(0)}\psi^{(0)}\psi^{(0)}_x. \tag{1.5}$$

The Baker–Akhiezer (BA) function $\chi^{(0)}(\lambda, x)$ is defined by the equation

$$L^{(0)} \cdot \chi^{(0)}(\lambda, x) = \lambda \cdot \chi^{(0)}(\lambda, x), \quad \frac{\partial \chi^{(0)}(\lambda, x)}{\partial t_k} = B^{(0)}_k \cdot \chi^{(0)}(\lambda, x). \tag{1.6}$$

The adjoint BA function $\mu^{(0)}(\lambda, x)$ is defined by the equation

$$L^{*(0)} \mu^{(0)}(\lambda, x) = \lambda \cdot \mu^{(0)}(\lambda, x), \quad \frac{\partial \mu^{(0)}(\lambda, x)}{\partial t_k} = -B^{*(0)}_k \cdot \mu^{(0)}(\lambda, x). \tag{1.7}$$

On the other hand, we can rewrite $L^{(0)}$ as

$$L^{(0)} = \partial + u^{(0)}_2 \circ \partial^{-1} + u^{(0)}_3 \circ \partial^{-2} + u^{(0)}_4 \circ \partial^{-3} + \cdots, \tag{1.8}$$

so that the coordinates $u^{(0)}_2, u^{(0)}_3, u^{(0)}_4, \ldots$ are expressed uniquely by the dynamical variables $\phi^{(0)}, \psi^{(0)}$ and their derivatives

$$u^{(0)}_2 = \phi^{(0)} \cdot \psi^{(0)}, \quad u^{(0)}_3 = -\phi^{(0)} \cdot \psi^{(0)}_x, \quad u^{(0)}_4 = \phi^{(0)} \cdot \psi^{(0)}_{xx}, \quad \ldots. \tag{1.9}$$

It is easy to find via $u = u_2, t_1 = x, t_2 = y, t_3 = t$ the KP equation

$$(4u_t - 12uu_x - u_{xxx})_x - 3u_{yy} = 0. \tag{1.10}$$

From Sato's KP theory (see, for example, Refs. 7 and 8), the set $\{u^{(0)}_i\}$ can be generated by the τ-function $\tau^{(0)}$,

$$u^{(0)}_2 = \frac{\partial^2 \ln \tau^{(0)}}{\partial x^2}, \tag{1.11}$$

$$u^{(0)}_3 = \tfrac{1}{2}(\partial_x \partial_{t_2} - \partial_x^2) \cdot \ln \tau^{(0)}, \tag{1.12}$$

etc. Through (1.11) and (1.12), $\{\phi^{(0)}, \psi^{(0)}\}$ can be expressed by the same $\tau^{(0)}$, which provides an alternative to representing the solution to the AKNS hierarchy via its corresponding τ-function.

Recently several peoples have been devoted to solving the cKP hierarchy by gauge transformations.[6,9–18] Two types of gauge transformation operators

$$\text{Type } \mathbf{I}: \quad T_D(\chi) = \chi \circ \partial \circ \chi^{-1},$$

$$\text{Type } \mathbf{II}: \quad T_I(\mu) = \mu^{-1} \circ \partial^{-1} \circ \mu,$$

for the KP hierarchy were proposed first by Ref. 19; they were then shown to be also able to deal with the cKP hierarchy.[6,9–12,18] Here χ and μ are the ''eigenfunction'' and the ''adjoint eigenfunction'' of the KP hierarchy, respectively. On the other hand, there are two classes of functions (we

call them the generating functions of the gauge transformation, denoted shortly by GFGT) appropriate to produce the above-mentioned transformations. The first is the BA function,[9] the other is the ''eigenfunction'' (or the ''adjoint-eigenfunction'').[6,10–12,18] However, the discussion for the two types of gauge transformations with the two classes of GFGT is neither complete nor systematic. In addition, the transformed function $\tau^{(n)}$ of Ref. 6 does not hold for the cKP with $k=1$ and one component (i.e., in the AKNS case). So we provide a unified frame to deal with the AKNS hierarchy and we discuss some explicit solutions of the KP equation as examples.

The organization of the present paper is as follows. In Sec. II, we deduce the transformed Lax operator $L^{(1)}$ from the $L^{(0)}$ in (1.2) under the gauge transformations of Type **I** and Type **II**. In this process, we point out that there are two choices of gauge transformation for the AKNS hierarchy in order to keep the form of the Lax operator, which results in two classes of GFGT. Particularly, the second choice for Type **I** and Type **II** is discussed in detail, respectively. Then, in Sec. III, we study the successive applications of the gauge transformation with the second choice. This is followed by the Sec. IV, which treats the union of the two choices in one chain of gauge transformations. The generation of the AKNS hierarchy from the ''free'' Lax operator $L^{(0)}=\partial$ is the main content of the Sec. V. The last Sec. VI contents some concluding remarks.

Before ending this section, let us list some identities, which are used repeatedly in the following sections:

$$\partial\circ f = f\circ\partial + f_x, \tag{1.13}$$

$$\partial^{-1}\circ f = f\circ\partial^{-1} - \partial^{-1}\circ f_x\circ\partial^{-1}, \tag{1.14}$$

$$T_I(\chi) = -(T_D^{-1}(\chi))^* = -(T_D^*(\chi))^{-1}, \tag{1.15}$$

$$T_D(\mu) = -(T_I^{-1}(\mu))^* = -(T_I^*(\mu))^{-1}, \tag{1.16}$$

$$(T_D(\chi)\circ A_-\circ T_D^{-1}(\chi))_+ = 0. \tag{1.17}$$

In addition, because the τ-function can be only determined up to a constant factor, we always omit the global minus of τ-function for AKNS hierarchy in this paper.

II. TWO CHOICES OF GAUGE TRANSFORMATION FOR THE AKNS HIERARCHY

Let us begin with a brief summary about the gauge transformation for the AKNS hierarchy. Suppose T is a pseudodifferential operator, and

$$L^{(1)} = T\circ L^{(0)}\circ T^{-1}, \quad B_n^{(1)} \equiv (L^{(1)})_+^n, \tag{2.1}$$

so that

$$\frac{\partial}{\partial t_n}L^{(1)} = [B_n^{(1)}, L^{(1)}] \tag{2.2}$$

still holds for the transformed Lax operator $L^{(1)}$; then T is called a gauge transformation operator. According to the definition of gauge transformation, we have

Lemma 2.1: The operator T is a gauge transformation operator, if

$$(T\circ B_n^{(0)}\circ T^{-1})_+ = T\circ B_n^{(0)}\circ T^{-1} + \frac{\partial T}{\partial t_n}\circ T^{-1}, \tag{2.3}$$

or

$$(T\circ B_n^{(0)}\circ T^{-1})_- = -\frac{\partial T}{\partial t_n}\circ T^{-1}. \tag{2.4}$$

Proof: By using (2.1) we have

$$\frac{\partial L^{(1)}}{\partial t_n}=\frac{\partial T}{\partial t_n}\circ T^{-1}\circ T\circ L^{(0)}\circ T^{-1}+T\circ B_n^{(0)}\circ T^{-1}\circ T\circ L^{(0)}\circ T^{-1}-T\circ L^{(0)}$$
$$\circ T^{-1}\circ T\circ B_n^{(0)}\circ T^{-1}-T\circ L^{(0)}\circ T^{-1}\circ\frac{\partial T}{\partial t_n}\circ T^{-1},$$
$$[B_n^{(1)},L^{(1)}]=B_n^{(1)}\circ T\circ L^{(0)}\circ T^{-1}-T\circ L^{(0)}\circ T^{-1}\circ B_n^{(1)}.$$

Taking these back into (2.2), one gets

$$B_n^{(1)}=T\circ B_n^{(0)}\circ T^{-1}+\frac{\partial T}{\partial t_n}\circ T^{-1}.$$

On the other hand, we have

$$B_n^{(1)}\equiv(L^{(1)})_+^n=(T\circ B_n^{(0)}\circ T^{-1})_+.$$

from the definition of the gauge transformation. The lemma is then proved by comparing the two expressions of $B_n^{(1)}$. □

This is concordant with the statement of Refs. 6 and 19, where it is given in the contest of the Zakharov–Shabat (ZS) equation. Our proof is independent of the concrete form of the Lax operator $L^{(0)}$, so it also hold for the generalized KP hierarchy.[14,20] In order to prove the existence of the two types of gauge transformation, we need to discuss first the following lemma.

Lemma 2.2: (Ref. 21) *Let f be a well defined function, A a pseudodifferential operator; then*

$$(1)\quad (f\circ\partial\circ f^{-1}\circ A\circ f\circ\partial^{-1}\circ f^{-1})_+=f\circ\partial\circ f^{-1}\circ A_+\circ f\circ\partial^{-1}\circ f^{-1}-f^{-1}$$
$$\circ[\partial_x(f^{-1}\cdot(A_+\cdot f))]\circ\partial^{-1}\circ f^{-1}. \tag{2.5}$$

$$(2)\quad (f^{-1}\circ\partial^{-1}\circ f\circ A\circ f^{-1}\circ\partial\circ f)_-=f^{-1}\circ\partial^{-1}\circ f\circ A_-\circ f^{-1}\circ\partial\circ f-f^{-1}$$
$$\circ\partial^{-1}\circ f\circ\partial_x(f^{-1}\cdot(A_+^*\cdot f)). \tag{2.6}$$

Theorem 2.1: *(Ref. 6) For the AKNS hierarchy, there exist two types of gauge transformation operators:*

$$\text{Type I:}\quad T_D(\chi)=\chi\circ\partial\circ\chi^{-1}, \tag{2.7}$$

$$\text{Type II:}\quad T_I(\mu)=\mu^{-1}\circ\partial^{-1}\circ\mu. \tag{2.8}$$

Here χ and μ are the eigenfunction and the adjoint eigenfunction of the Lax operator $L^{(0)}$ in (1.2), respectively.

Proof: First, for the Type **I** case [see (2.7)],

$$\begin{aligned}B_n^{(1)}\equiv(L^{(1)})_+^n&=(T_D\circ(L^{(0)})^n\circ T_D^{-1})_+\\&=T_D\circ(L^{(0)})_+^n\circ T_D^{-1}-\chi\cdot\partial_x(\chi^{-1}\cdot((L^{(0)})_+^n\cdot\chi)))\circ\partial^{-1}\circ\chi^{-1}\\&=T_D\circ B_n^{(0)}\circ T_D^{-1}-\chi\cdot\partial_x(\chi^{-1}\cdot(B_n^{(0)}\cdot\chi))\circ\partial^{-1}\circ\chi^{-1}\\&=T_D\circ B_n^{(0)}\circ T_D^{-1}-\left(\chi\circ\partial\circ\frac{\chi_{t_n}}{\chi}\circ\partial^{-1}\circ\chi^{-1}-\chi\circ\frac{\chi_{t_n}}{\chi}\circ\partial\circ\partial^{-1}\circ\chi^{-1}\right)\end{aligned}$$

$$=T_D\circ B_n^{(0)}\circ T_D^{-1}+\frac{\chi_{t_n}}{\chi}-\chi\circ\partial\circ\frac{\chi_{t_n}}{\chi}\circ\partial^{-1}\circ\chi^{-1}.$$

Here the relations (2.5), $B_n^{(0)}=(L^{(0)})_+^n$, $\chi_{t_n}=B_n^{(0)}\cdot\chi$ and (1.13) have been used. On the other hand,

$$\begin{aligned}\frac{\partial T_D}{\partial t_n}\circ T_D^{-1}&=(\chi\circ\partial\circ\chi^{-1})_{t_n}\circ T_D^{-1}\\&=\chi_{t_n}\circ\partial\circ\chi^{-1}\circ\chi\circ\partial^{-1}\circ\chi^{-1}-\chi\circ\partial\circ\frac{\chi_{t_n}}{\chi^2}\circ\chi\circ\partial^{-1}\circ\chi^{-1}\\&=\frac{\chi_{t_n}}{\chi}-\chi\circ\partial\circ\frac{\chi_{t_n}}{\chi}\circ\partial^{-1}\circ\chi^{-1}.\end{aligned}$$

Hence

$$B_n^{(1)}\equiv(L^{(1)})_+^n=T_D\circ B_n^{(0)}\circ T_D^{-1}+\frac{\partial T_D}{\partial t_n}\circ T_D^{-1},$$

and this indicates that $T_D(\chi)$ is indeed a gauge transformation operator via Lemma 2.1. Second, we want to prove that the equation (2.4) hold for Type **II** case [see (2.8)],

$$\begin{aligned}(T_I\circ B_n^{(0)}\circ T_I^{-1})_-&=(\mu^{-1}\circ\partial^{-1}\circ\mu\circ B_n^{(0)}\circ\mu^{-1}\circ\partial\circ\mu)_-\\&=\mu^{-1}\circ\partial^{-1}\circ\mu\circ(B_n^{(0)})_-\circ\mu^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\partial^{-1}\circ\mu\circ\partial_x(\mu^{-1}\cdot((B^{*(0)}_n)_+\cdot\mu))\\&=\mu^{-1}\circ\partial^{-1}\circ\mu\circ\partial_x(\mu^{-1}\cdot\mu_{t_n}).\end{aligned}$$

In the above destination, the relations (2.6), $(B_n^{(0)})_-=0$, $\mu_{t_n}=-B_n^{*(0)}\cdot\mu$ have been used. Moreover, with the help of (1.14), we have

$$\begin{aligned}-\frac{\partial T_I}{\partial t_n}\circ T_I^{-1}&=-\frac{\partial}{\partial t_n}((\mu^{-1}\circ\partial^{-1}\circ\mu))\circ\mu^{-1}\circ\partial\circ\mu\\&=\frac{\mu_{t_n}}{\mu^2}\circ\partial^{-1}\circ\mu\circ\mu^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\partial^{-1}\circ\mu_{t_n}\circ\mu^{-1}\circ\partial\circ\mu\\&=\frac{\mu_{t_n}}{\mu}-\mu^{-1}(\mu_{t_n}\circ\mu^{-1}\circ\partial^{-1}-\partial^{-1}\circ(\mu_{t_n}\cdot\mu^{-1})_x\circ\partial^{-1})\circ\partial\circ\mu\\&=\frac{\mu_{t_n}}{\mu}-\frac{\mu_{t_n}}{\mu}+\mu^{-1}\circ\partial^{-1}\circ\partial_x(\mu_{t_n}\circ\mu^{-1})\circ\mu\\&=\mu^{-1}\circ\partial^{-1}\circ\mu\circ\partial_x(\mu_{t_n}\circ\mu^{-1}).\end{aligned}$$

The above two equations show that $T_I(\mu)$ satisfies (2.4), so $T_I(\mu)$ is also a gauge transformation operator according to Lemma 2.1. □

Although the gauge transformation operators in Theorem 2.1 guarantee the validity of the Lax equation, it is not enough to ensure that the $\phi^{(0)}$ and $\psi^{(0)}$ are transformed to be the new solutions of the AKNS hierarchy. To this end, the gauge transformation operators, must be moreover re-

quired to keep the form of Lax operator. Let us now introduce n BA functions $\{\chi_i^{(0)}=\chi(\lambda_i,x), i=1,2,\ldots,n\}$ and n adjoint BA functions $\{\mu_i^{(0)}=\mu(\lambda_i,x), i=1,2,\ldots,n\}$, besides the "eigenfunction" $\phi^{(0)}$ and the "adjoint eigenfunction" $\psi^{(0)}$ of $L^{(0)}$.

Lemma 2.3: Via the gauge transformation of Type **I** *[see (2.7)], $L^{(0)}$ becomes $L^{(1)}$, which is given by*

$$\begin{aligned} L^{(1)} &= \partial+\chi\cdot(\ln\chi)_{xx}\circ\partial^{-1}\circ\chi^{-1}+\chi\cdot\left(\chi^{-1}\cdot\phi^{(0)}\cdot\int\psi^{(0)}\cdot\chi\right)_x\circ\partial^{-1}\circ\chi^{-1}-\chi \\ &\quad\cdot(\chi^{-1}\cdot\phi^{(0)})_x\circ\partial^{-1}\circ\left(\int\psi^{(0)}\cdot\chi\right)\circ\chi^{-1} \\ &= \partial+\phi_0^{(1)}\circ\partial^{-1}\circ\psi_0^{(1)}+\widetilde{\phi^{(1)}}\circ\partial^{-1}\circ\widetilde{\phi^{(1)}}, \end{aligned} \tag{2.9}$$

$$\phi_0^{(1)}=\chi\cdot(\ln\chi)_{xx}+\chi\cdot\left(\chi^{-1}\cdot\psi^{(0)}\cdot\left(\int\phi^{(0)}\cdot\chi\right)\right)_x=(T_D(\chi)\circ L^{(0)})\cdot\chi, \tag{2.10}$$

$$\psi_0^{(1)}=\chi^{-1}, \tag{2.11}$$

$$\widetilde{\phi^{(1)}}=\chi\cdot(\chi^{-1}\cdot\phi^{(1)})_x=T_D(\chi)\cdot\phi^{(0)}, \tag{2.12}$$

$$\widetilde{\phi^{(0)}}=-\chi^{-1}\cdot\left(\int\psi^{(0)}\cdot\chi\right)=-T_I(\chi)\cdot\psi^{(0)}. \tag{2.13}$$

Proof: The transformed Lax operator $L^{(1)}=T_D(\chi)\circ L^{(0)}\circ(T_D(\chi))^{-1}$ can be written in two parts. (a) The first part is

$$\begin{aligned} L_A &= T_D(\chi)\circ\partial\circ(T_D(\chi))^{-1} \\ &= \left(\partial-\frac{\chi_x}{\chi}\right)\circ\partial\circ\chi\circ\partial^{-1}\circ\chi^{-1} \\ &= \partial^2\circ\chi\circ\partial^{-1}\circ\chi^{-1}-\frac{\chi_x}{\chi}\circ\partial\circ\chi\circ\partial^{-1}\circ\chi^{-1} \\ &= (\chi_{xx}+2\chi_x\circ\partial+\chi\circ\partial^2)\circ\partial^{-1}\circ\chi^{-1}-\frac{\chi_x}{\chi}\circ(\chi_x+\chi\circ\partial)\circ\partial^{-1}\circ\chi^{-1} \\ &= (\chi_{xx}+2\chi_x\circ\partial)\circ\partial^{-1}\circ\chi^{-1}+\chi\circ\partial\circ\chi^{-1}-\frac{\chi_x^2}{\chi}\circ\partial^{-1}\circ\chi^{-1}-\chi_x\cdot\chi^{-1} \\ &= \partial+\left(\chi_{xx}+2\chi_x\circ\partial-\frac{\chi_x^2}{\chi}\right)\circ\partial^{-1}\circ\chi^{-1}-2\frac{\chi_x}{\chi} \\ &= \partial+\left(\chi_{xx}-\frac{\chi_x^2}{\chi}\right)\circ\partial^{-1}\circ\chi^{-1} \\ &= \partial+\chi\cdot(\ln\chi)_{xx}\circ\partial^{-1}\circ\chi^{-1}. \end{aligned}$$

In above destination, the relation (1.13) is used repeatedly. (b) The second part, L_B, comes from

$$
\begin{aligned}
L_B &= T_D(\chi)\circ\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)}\circ(T_D(\chi))^{-1}\\
&= \chi\circ\partial\circ\chi^{-1}\circ\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)}\circ\chi\circ\partial^{-1}\circ\chi^{-1}\\
&= \chi\circ\partial\circ\chi^{-1}\circ\phi^{(0)}\circ\left(\left(\int\psi^{(0)}\cdot\chi\right)\circ\partial^{-1}-\partial^{-1}\circ\left(\int\psi^{(0)}\cdot\chi\right)\right)\circ\chi^{-1}\\
&= \chi\cdot\left(\chi^{-1}\cdot\phi^{(0)}\cdot\left(\int\psi^{(0)}\cdot\chi\right)\right)_x\circ\partial^{-1}\circ\chi^{-1}+\chi\cdot\chi^{-1}\cdot\phi^{(0)}\cdot 1\cdot\left(\int\psi^{(0)}\cdot\chi\right)\cdot\chi^{-1}\\
&\quad -\chi\cdot(\chi^{-1}\phi^{(0)})_x\circ\partial^{-1}\circ\left(\int\psi^{(0)}\cdot\chi\right)\circ\chi^{-1}-\chi\cdot\chi^{-1}\phi^{(0)}\cdot 1\cdot\left(\int\psi^{(0)}\cdot\chi\right)\circ\chi^{-1}\\
&= \chi\cdot\left(\chi^{-1}\cdot\phi^{(0)}\cdot\left(\int\psi^{(0)}\cdot\chi\right)\right)_x\circ\partial^{-1}\circ\chi^{-1}-\chi\cdot(\chi^{-1}\phi^{(0)})_x\circ\partial^{-1}\circ\left(\int\psi^{(0)}\cdot\chi\right)\circ\chi^{-1},
\end{aligned}
$$

with the help of (1.13) and (1.14). From (a) and (b), $L^{(1)}$ in (2.9) is obtained. Then

$$
\begin{aligned}
\phi_0^{(1)} &= \chi\cdot(\ln\chi)_{xx}+\chi\cdot\left(\chi^{-1}\cdot\phi^{(0)}\cdot\left(\int\psi^{(0)}\cdot\chi\right)\right)_x\\
&= \chi\cdot\left[(\ln\chi)_x+\chi^{-1}\cdot\phi^{(0)}\cdot\left(\int\psi^{(0)}\cdot\chi\right)\right]_x\\
&= \chi\cdot\left[\frac{1}{\chi}\left(\chi_x+\phi^{(0)}\cdot\left(\int\psi^{(0)}\cdot\chi\right)\right)\right]_x\\
&= \chi\cdot\left[\frac{L^{(0)}\cdot\chi}{\chi}\right]_x=(T_D(\chi)\circ L^{(0)})\cdot\chi.
\end{aligned}
$$

It is easy to deduce the other equations Lemma 2.3.

This lemma shows that, there are two choices to keep the form of $L^{(1)}$: the first choice is characterized by the formula $\widetilde{\phi^{(1)}}\circ\partial^{-1}\circ\widetilde{\phi^{(1)}}=0$; the second choice by the formula $\psi_0^{(1)}\circ\partial^{-1}\circ\psi_0^{(1)}=0$. So we have the following.

Theorem 2.2: *(A) The GFGT of the first choice is the "eigenfunction" of* $L^{(0)}$*, i.e.,* $\chi=\phi^{(0)}$*, which results in* $T_D(\phi^{(0)})=\phi^{(0)}\circ\partial\circ(\phi^{(0)})^{-1}$*, then*

$$
\phi^{(1)}=\phi^{(0)}\cdot((\ln\phi^{(0)})_{xx}+\phi^{(0)}\cdot\psi^{(0)})=(T_D(\phi^{(0)})\circ L^{(0)})\cdot\phi^{(0)},\quad \frac{\partial\phi^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\phi^{(1)}, \tag{2.14}
$$

$$
\psi^{(1)}=(\phi^{(0)})^{-1},\quad \frac{\partial\psi^{(1)}}{\partial t_n}=-B_n^{*(1)}\cdot\psi^{(1)}. \tag{2.15}
$$

Moreover, from $\{\chi_i^{(0)},\mu_i^{(0)},i=1,2,\ldots,n\}$*, if we define*

$$
\chi_i^{(1)}=T_D(\phi^{(0)})\cdot\chi_i^{(0)}=\phi^{(0)}\circ\partial\circ(\phi^{(0)})^{-1}\cdot\chi_i^{(0)}, \tag{2.16}
$$

$$
\mu_i^{(1)}=-T_I(\phi^{(0)})\cdot\mu_i^{(0)}=-(\phi^{(0)})^{-1}\circ\partial^{-1}\circ\phi^{(0)}\cdot\mu_i^{(0)}, \tag{2.17}
$$

then $\{\chi_i^{(1)},\mu_i^{(1)}\}$ *statisfy*

$$
\frac{\partial\chi_i^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\chi_i^{(1)},\quad L^{(1)}\cdot\chi_i^{(1)}=\lambda_i\cdot\chi_i^{(1)}, \tag{2.18}
$$

$$\frac{\partial \mu_i^{(1)}}{\partial t_n} = -B_n^{*(1)} \cdot \mu_i^{(1)}, \quad L^{*(1)} \mu_i^{(1)} = \lambda_i \cdot \mu_i^{(1)}. \tag{2.19}$$

The transformed τ-function $\tau^{(1)}$ related to $L^{(1)}$ reads

$$\tau^{(1)} = \phi^{(0)} \cdot \tau^{(0)}, \tag{2.20}$$

where $\tau^{(0)}$ is the τ-function of $L^{(0)}$. (B) For the second choice, the corresponding $GFGT$ is one of the BA functions, for example, $\chi = \chi_k^{(0)}$, then $T_D(\chi_k^{(0)}) = \chi_k^{(0)} \circ \partial \circ (\chi_k^{(0)})^{-1}$,

$$\phi^{(1)} = T_D(\chi_k^{(0)}) \cdot \phi^{(0)} = \chi_k^{(0)} \circ \partial \circ (\chi_k^{(0)})^{-1} \cdot \phi^{(0)}, \quad \frac{\partial \phi^{(1)}}{\partial t_n} = B_n^{(1)} \cdot \phi^{(1)}, \tag{2.21}$$

$$\psi^{(1)} = -T_I(\chi_k^{(0)}) \cdot \psi^{(0)} = -(\chi_k^{(0)})^{-1} \circ \partial^{-1} \circ \chi_k^{(0)} \cdot \psi^{(0)}, \quad \frac{\partial \psi^{(1)}}{\partial t_n} = -B_n^{*(1)} \cdot \psi^{(1)}. \tag{2.22}$$

From $\{\chi_l^{(0)}, \mu_l^{(0)}, l = 1,2,\ldots,n, l \neq k,\}$, if we define

$$\chi_l^{(1)} = T_D(\chi_k^{(0)}) \cdot \chi_l^{(0)} = \chi_k^{(0)} \circ \partial \circ (\chi_k^{(0)})^{-1} \cdot \chi_l^{(0)}, \quad \chi_k^{(1)} = 0, \tag{2.23}$$

$$\mu_l^{(1)} = -T_I(\chi_k^{(0)}) \cdot \mu_l^{(0)} = -(\chi_k^{(0)})^{-1} \circ \partial^{-1} \circ \chi_k^{(0)} \cdot \mu_l^{(0)}, \quad \mu_k^{(1)} = -T_I(\chi_k^{(0)}) \cdot \mu_k^{(0)} \neq 0, \tag{2.24}$$

then the $\{\chi_l^{(1)}, \mu_l^{(1)}\}$ satisfy

$$\frac{\partial \chi_l^{(1)}}{\partial t_n} = B_n^{(1)} \cdot \chi_l^{(1)}, \quad L^{(1)} \cdot \chi_l^{(1)} = \lambda_l \cdot \chi_l^{(1)}, \tag{2.25}$$

$$\frac{\partial \mu_l^{(1)}}{\partial t_n} = -B_n^{*(1)} \cdot \mu_l^{(1)}, \quad L^{*(1)} \mu_l^{(1)} = \lambda_l \cdot \mu_l^{(1)}. \tag{2.26}$$

The transformed τ-function $\tau^{(1)}$ of $L^{(1)}$ is

$$\tau^{(1)} = \chi_k^{(0)} \cdot \tau^{(0)}, \tag{2.27}$$

in which $\tau^{(0)}$ is the τ-function of $L^{(0)}$.

Furthermore, for the gauge transformation of Type **II** $T_I(\mu) = \mu^{-1} \circ \partial^{-1} \circ \mu$, see (2.8), the transformed Lax operator is given by the following.

Lemma 2.4:

$$\begin{aligned} L^{(1)} &= T_I(\mu) \circ L^{(0)} \circ T_I^{-1}(\mu) \\ &= \partial + \mu^{-1} \circ \partial^{-1} \circ (\mu_x \cdot \mu^{-1})_x \circ \mu + \mu^{-1} \circ \partial^{-1} \\ &\quad \circ \left(\left(\int \mu \cdot \phi^{(0)} \right) \cdot \psi^{(0)} \cdot \mu^{-1} \right)_x \circ \mu - \mu^{-1} \cdot \left(\int \mu \cdot \phi^{(0)} \right) \circ \partial^{-1} \circ (\psi^{(0)} \cdot \mu^{-1})_x \circ \mu \\ &= \partial + \phi_0^{(1)} \circ \partial^{-1} \circ \psi_0^{(1)} + \widetilde{\phi^{(1)}} \circ \partial^{-1} \circ \widetilde{\phi^{(1)}}, \end{aligned} \tag{2.28}$$

in which

$$\psi_0^{(1)} = \mu^{-1}, \tag{2.29}$$

$$\psi_0^{(1)} = (\mu_x \cdot \mu^{-1})_x \cdot \mu + \left(\left(\int \mu \cdot \phi^{(0)} \right) \cdot \psi^{(0)} \cdot \mu^{-1} \right)_x \cdot \mu, \tag{2.30}$$

$$\widetilde{\phi^{(1)}}=T_I(\mu)\cdot\psi^{(0)}=\frac{1}{\mu}\cdot\int\mu\cdot\phi^{(0)}, \tag{2.31}$$

$$\widetilde{\phi^{(1)}}=-T_D(\mu)\cdot\phi^{(0)}=-\mu\cdot\left(\frac{\phi^{(0)}}{\mu}\right)_x. \tag{2.32}$$

Proof: As in Lemma 2.3, it is convenient to express the transformed Lax operator in two parts.
(a) The first part needs

$$\begin{aligned}
L_A&=T_I(\mu)\circ\partial\circ(T_I(\mu))^{-1}\\
&=\mu^{-1}\circ\partial^{-1}\circ\mu\circ\partial\circ\mu^{-1}\circ\partial\circ\mu\\
&=\mu^{-1}\circ(\mu\circ\partial^{-1}-\partial^{-1}\circ\mu_x\circ\partial^{-1})\circ\partial\circ\mu^{-1}\circ\partial\circ\mu\\
&=\mu^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\partial^{-1}\circ\mu_x\circ 1\circ\mu^{-1}\circ\partial\circ\mu\\
&=\partial+\mu^{-1}\cdot\mu_x-\mu^{-1}((\mu_x\cdot\mu^{-1})\circ\partial^{-1}-\partial^{-1}\circ(\mu_x\cdot\mu^{-1})_x\circ\partial^{-1})\circ\partial\circ\mu\\
&=\partial+\mu^{-1}\cdot\mu_x-\mu^{-1}\cdot(\mu_x\cdot\mu^{-1})\circ\partial^{-1}\circ\partial\circ\mu+\mu^{-1}\circ\partial^{-1}\circ(\mu_x\cdot\mu^{-1})_x\circ\partial^{-1}\circ\partial\circ\mu\\
&=\partial+\mu^{-1}\cdot\mu_x-\mu_x\cdot\mu^{-1}+\mu^{-1}\circ\partial^{-1}\circ(\mu_x\cdot\mu^{-1})_x\circ\partial^{-1}\circ\partial\circ\mu\\
&=\partial+\mu^{-1}\circ\partial^{-1}\circ(\mu_x\cdot\mu^{-1})_x\circ\mu.
\end{aligned}$$

Obviously, we used the relation (1.14) repeatedly.

(b) With the same method of (a), on direct computation the second part become

$$\begin{aligned}
L_B&=T_I(\mu)\circ\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)}\circ(T_I(\mu))^{-1}\\
&=\mu^{-1}\circ\partial^{-1}\circ\mu\circ\phi^{(0)}\circ\partial^{-1}\circ\psi^{(0)}\circ\mu^{-1}\circ\partial\circ\mu\\
&=\mu^{-1}\circ\left(\left(\int\mu\cdot\phi^{(0)}\right)\circ\partial^{-1}-\partial^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\right)\circ\psi^{(0)}\circ\mu^{-1}\circ\partial\circ\mu\\
&=\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\partial^{-1}\circ\psi^{(0)}\circ\mu^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\partial^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\psi^{(0)}\circ\mu^{-1}\circ\partial\circ\mu\\
&=\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ((\psi^{(0)}\cdot\mu^{-1})\circ\partial^{-1}-\partial^{-1}\circ(\psi^{(0)}\cdot\mu^{-1})\circ\partial^{-1})\circ\partial\circ\mu\\
&\quad-\mu^{-1}\circ\left(\left(\left(\int\mu\cdot\phi^{(0)}\right)\cdot\psi^{(0)}\cdot\mu^{-1}\right)\circ\partial^{-1}-\partial^{-1}\circ\left(\left(\int\mu\cdot\phi^{(0)}\right)\cdot\psi^{(0)}\cdot\mu^{-1}\right)_x\circ\partial^{-1}\right)\circ\partial\circ\mu\\
&=\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\psi^{(0)}\circ\mu^{-1}\circ\partial^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\partial^{-1}\circ(\psi^{(0)}\cdot\mu^{-1})_x\\
&\quad\circ\partial^{-1}\circ\partial\circ\mu-\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\psi^{(0)}\circ\mu^{-1}\circ\partial^{-1}\circ\partial\circ\mu\\
&\quad+\mu^{-1}\circ\partial^{-1}\circ\left(\left(\int\mu\cdot\phi^{(0)}\right)\cdot\psi^{(0)}\cdot\mu^{-1}\right)_x\circ\partial^{-1}\circ\partial\circ\mu\\
&=-\mu^{-1}\circ\left(\int\mu\cdot\phi^{(0)}\right)\circ\partial^{-1}\circ(\psi^{(0)}\cdot\mu^{-1})_x\circ\mu+\mu^{-1}\circ\partial^{-1}\circ\left(\left(\int\mu\cdot\phi^{(0)}\right)\cdot\psi^{(0)}\cdot\mu^{-1}\right)_x\circ\mu.
\end{aligned}$$

The sum of L_A and L_B provides $L^{(1)}$. In view of its use in the following section, we rewrite $\psi_0^{(1)}$ as

$$\psi_0^{(1)}=(\mu_x\cdot\mu^{-1})_x\cdot\mu+\left(\left(\int\mu\cdot\phi^{(0)}\right)\cdot\psi^{(0)}\cdot\mu^{-1}\right)_x\cdot\mu,$$

$$=-\mu\cdot\left(-\frac{\mu_x}{\mu}-\frac{1}{\mu}\cdot\psi^{(0)}\cdot\left(\int\mu\cdot\phi^{(0)}\right)\right)_x$$

$$=-\mu\cdot\left(\frac{-\mu_x-\psi^{(0)}\cdot(\int\mu\cdot\phi^{(0)})}{\mu}\right)_x=-\mu\cdot\left(\frac{L^{*(0)}\mu}{\mu}\right)_x.$$

$$=-(T_D(\mu)\circ L^{*(0)})\cdot\mu.$$

□

Lemma 2.4 indicates that there are two choices of gauge transformation in order to keep the form of Lax operator. The first choice is $\widetilde{\phi^{(1)}}\circ\partial^{-1}\circ\widetilde{\phi^{(1)}}=0$. The second choice is $\psi^{(1)}\circ\partial^{-1}\circ\psi^{(1)}=0$. Then we have

Theorem 2.3: *(A) Under the gauge transformation with the first choice, characterized by the relation* $\widetilde{\phi^{(1)}}\circ\partial^{-1}\circ\widetilde{\phi^{(1)}}=0$, *the corresponding GFGT is the "adjoint eigenfunction" (of the first class), i.e.,* $\mu=\psi^{(1)}$. *Then* $T_I(\psi^{(1)})=(\psi^{(0)})^{-1}\circ\partial^{-1}\circ\psi^{(0)}$,

$$\psi^{(1)}=(\psi^{(0)})^{-1},\quad \frac{\partial\phi^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\phi^{(1)}, \tag{2.33}$$

$$\psi^{(1)}=\psi^{(0)}\cdot((\ln\psi^{(0)})_{xx}+\psi^{(0)}\cdot\phi^{(0)})=-(T_D(\psi^{(0)})\circ L^{*(0)})\cdot\psi^{(0)}, \tag{2.34}$$

$$\frac{\partial\psi^{(1)}}{\partial t_n}=-B_n^{*(1)}\cdot\psi^{(1)}. \tag{2.35}$$

From $\{\chi_i^{(0)},\mu_i^{(0)},i=1,2,\ldots,n\}$, *if we define*

$$\chi_i^{(1)}=T_I(\psi^{(0)})\cdot\chi_i^{(0)}=\frac{1}{\psi^{(0)}}\cdot\int\psi^{(0)}\cdot\chi_i^{(0)}, \tag{2.36}$$

$$\mu_i^{(1)}=-T_D(\psi^{(0)})\cdot\mu_i^{(0)}=-\psi^{(0)}\cdot\left(\frac{\mu_i^{(0)}}{\psi^{(0)}}\right)_x, \tag{2.37}$$

then $\{\chi_i^{(1)},\mu_i^{(1)}\}$ *satisfy*

$$\frac{\partial\chi_i^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\chi_i^{(1)},\quad L^{(1)}\cdot\chi_i^{(1)}=\lambda_i\cdot\chi_i^{(1)}, \tag{2.38}$$

$$\frac{\partial\mu_i^{(1)}}{\partial t_n}=-B_n^{*(1)}\cdot\mu_i^{(1)},\quad L^{*(1)}\mu_i^{(1)}=\lambda_i\cdot\mu_i^{(1)}. \tag{2.39}$$

The transformed τ*-function* $\tau^{(1)}$ *of* $L^{(1)}$ *becomes*

$$\tau^{(1)}=\psi^{(0)}\cdot\tau^{(0)}, \tag{2.40}$$

where $\tau^{(0)}$ *is the* τ*-function of* $L^{(0)}$.

(B) For the gauge transformation with the second choice, characterized by the relation $\phi^{(1)}\circ\partial^{-1}\circ\psi^{(1)}=0$, *the corresponding GFGT is the adjoint-BA function (of the second class). For example, if* $\mu=\mu_k^{(0)}$, *then* $T_I((\mu_k^{(0)})=(\mu_k^{(0)})^{-1}\circ\partial^{-1}\circ\mu_k^{(0)})$,

$$\phi^{(1)}=T_I(\mu_k^{(0)})\cdot\phi^{(0)}=(\mu_k^{(0)})^{-1}\cdot\left(\int \mu_k^{(0)}\cdot\phi^{(0)}\right),\quad \frac{\partial\phi^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\phi^{(1)}, \tag{2.41}$$

$$\psi^{(1)}=-T_D(\mu_k^{(0)})\cdot\psi^{(0)}=-\mu_k^{(0)}\cdot\left(\frac{\psi^{(0)}}{\mu_k^{(0)}}\right)_x,\quad \frac{\partial\psi^{(1)}}{\partial t_n}=-B_n^{*(1)}\psi^{(1)}. \tag{2.42}$$

Let $l\neq k$, *for* $\{\chi_l^{(0)},\mu_l^{(0)},l=1,2,\ldots,n\}$, *we can then define*

$$\chi_l^{(1)}=T_I(\mu_k^{(0)})\cdot\chi_l^{(0)}=\frac{1}{\mu_k^{(0)}}\cdot\left(\int \mu_k^{(0)}\cdot\chi_l^{(0)}\right),\quad \chi_k^{(1)}=\frac{1}{\mu_k^{(0)}}\cdot\left(\int \mu_k^{(0)}\cdot\chi_k^{(0)}\right)\neq 0, \tag{2.43}$$

$$\mu_l^{(1)}=-T_D(\mu_k^{(0)})\cdot\mu_l^{(0)}=-\mu_k^{(0)}\cdot\left(\frac{\mu_l^{(0)}}{\mu_k^{(0)}}\right)_x,\quad \mu_k^{(1)}=0, \tag{2.44}$$

and then $\{\chi_l^{(1)},\mu_l^{(1)}\}$ *satisfy*

$$\frac{\partial\chi_l^{(1)}}{\partial t_n}=B_n^{(1)}\cdot\chi_l^{(1)},\quad L^{(1)}\cdot\chi_l^{(1)}=\lambda_l\cdot\chi_l^{(1)}, \tag{2.45}$$

$$\frac{\partial\mu_l^{(1)}}{\partial t_n}=-B_n^{*(1)}\mu_l^{(1)},\quad L^{*(1)}\mu_l^{(1)}=\lambda_l\cdot\mu_l^{(1)}. \tag{2.46}$$

The transformed τ*-function* $\tau^{(1)}$ *corresponding to the* $L^{(1)}$ *is*

$$\tau^{(1)}=\mu_k^{(0)}\cdot\tau^{(0)}, \tag{2.47}$$

where $\tau^{(0)}$ *is the* τ *function of* $L^{(0)}$.

Remark 2.1: There is a main difference between the results of Refs. 6, 10–12 and this paper. Their GFGT (i.e., of the first class) can come only from the integral part of $L^{(0)}$, but ours (i.e., of the second class) can come only from the outside of $L^{(0)}$, which implies that the second class of GFGT (which is a BA function of $L^{(0)}$) can't come from $L^{(0)}$. So there exist an essential difference between the two choices, Theorem 2.2 and Theorem 2.3 can not be on obtained results of the Refs. 6, 10–12, although it has a similar form to those results. But let us note that Theorem 2.2 agrees with Ref. 9, which is obtained from the matrix hierarchy.

Remark 2.2: Theorem 2.2 and Theorem 2.3 can be the generalized to the case of the general cKP hierarchy.

Remark 2.3: One can find from Theorem 2.2 and Theorem 2.3 that all the gauge transformations keep the eigenvalue equation of the *BA* functions and the adjoint BA functions $\{\chi_l^{(0)},\mu_l^{(0)},l=1,2,\ldots,n\}$. This observation indicates that we can make gauge transformations with the union of the two choices. This union will be discussed in Sec. IV.

III. SUCCESSIVE APPLICATION OF GAUGE TRANSFORMATIONS WITH THE SECOND CHOICE FOR THE AKNS HIERARCHY

In Refs. 6, 10–12, the gauge transformation with the first choice has been studied clearly and completely. So we will not consider this case in the following. Our main aim is to analyze the successive applications of the gauge transformations with the second choice. To simplify our presentation, we introduce the following notations for the Wronskian $W_n=W_n(\chi_1^{(0)},\chi_2^{(0)},\chi_3^{(0)},\ldots,\chi_n^{(0)})$, and the generalized Wronskian determinant:[22]

$$IW_{k,n}\equiv IW_{k,n}(\mu_k^{(0)},\mu_{k-1}^{(0)},\ldots,\mu_1^{(0)};\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)})$$

$$=\begin{vmatrix} \int \mu_k^{(0)}\cdot\chi_1^{(0)} & \int \mu_k^{(0)}\cdot\chi_2^{(0)} & \int \mu_k^{(0)}\cdot\chi_3^{(0)} & \cdots & \int \mu_k^{(0)}\cdot\chi_n^{(0)} \\ \int \mu_{k-1}^{(0)}\cdot\chi_1^{(0)} & \int \mu_{k-1}^{(0)}\cdot\chi_2^{(0)} & \int \mu_{k-1}^{(0)}\cdot\chi_3^{(0)} & \cdots & \int \mu_{k-1}^{(0)}\cdot\chi_n^{(0)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \int \mu_1^{(0)}\cdot\chi_1^{(0)} & \int \mu_1^{(0)}\cdot\chi_2^{(0)} & \int \mu_1^{(0)}\cdot\chi_3^{(0)} & \cdots & \int \mu_1^{(0)}\cdot\chi_n^{(0)} \\ \chi_1^{(0)} & \chi_2^{(0)} & \chi_3^{(0)} & \cdots & \chi_n^{(0)} \\ \chi_{1,x}^{(0)} & \chi_{2,x}^{(0)} & \chi_{3,x}^{(0)} & \cdots & \chi_{n,x}^{(0)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ (\chi_1^{(0)})^{(n-k-1)} & (\chi_2^{(0)})^{(n-k-1)} & (\chi_3^{(0)})^{(n-k-1)} & \cdots & (\chi_n^{(0)})^{(n-k-1)} \end{vmatrix}, \tag{3.1}$$

$$IW_{0,n}\equiv W_n(\chi_1^{(0)},\chi_2^{(0)},\chi_3^{(0)},\ldots,\chi_n^{(0)}). \tag{3.2}$$

$$\widehat{IW}_{k,n}\equiv\widehat{IW}_{k,n}(\chi_k^{(0)},\chi_{k-1}^{(0)},\ldots,\chi_1^{(0)};\mu_1^{(0)},\ldots,\mu_n^{(0)})$$

$$=\begin{vmatrix} \int \chi_k^{(0)}\cdot\mu_1^{(0)} & \int \chi_k^{(0)}\cdot\mu_2^{(0)} & \int \chi_k^{(0)}\cdot\mu_3^{(0)} & \cdots & \int \chi_k^{(0)}\cdot\mu_n^{(0)} \\ \int \chi_{k-1}^{(0)}\cdot\mu_1^{(0)} & \int \chi_{k-1}^{(0)}\cdot\mu_2^{(0)} & \int \chi_{k-1}^{(0)}\cdot\mu_3^{(0)} & \cdots & \int \chi_{k-1}^{(0)}\cdot\mu_n^{(0)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \int \chi_1^{(0)}\cdot\mu_1^{(0)} & \int \chi_1^{(0)}\cdot\mu_2^{(0)} & \int \chi_1^{(0)}\cdot\mu_3^{(0)} & \cdots & \int \chi_1^{(0)}\cdot\mu_n^{(0)} \\ \mu_1^{(0)} & \mu_2^{(0)} & \mu_3^{(0)} & \cdots & \mu_n^{(0)} \\ \mu_{1,x}^{(0)} & \mu_{2,x}^{(0)} & \mu_{3,x}^{(0)} & \cdots & \mu_{n,x}^{(0)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ (\mu_1^{(0)})^{(n-k-1)} & (\mu_2^{(0)})^{(n-k-1)} & (\mu_3^{(0)})^{(n-k-1)} & \cdots & (\mu_n^{(0)})^{(n-k-1)} \end{vmatrix}, \tag{3.3}$$

$$\widehat{IW}_{0,n}\equiv W_n(\mu_1^{(0)},\mu_2^{(0)},\mu_3^{(0)},\ldots,\mu_n^{(0)}). \tag{3.4}$$

Here, $(f_i^{(0)})^{(k)}=\partial^k f_i^{(0)}/\partial x^n$, $\int f=\int f\,\mathrm{d}x$ with the integration constant sets to zero.

Now let us discuss several interesting chains of gauge transformations through the following n-step gauge transformations. We first consider the successive application of T_D in the ith channel (we adopt the notation of Ref. 6). For the chain of gauge transformations, we have the following:

$$L^{(0)}\xrightarrow{T_D^{(1)}(\chi_i^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\mu_i^{(1)})}L^{(2)}\xrightarrow{T_D^{(3)}(\chi_i^{(2)})}L^{(3)}\xrightarrow{T_I^{(4)}(\mu_i^{(3)})}\cdots\to\cdots, \tag{3.5}$$

we have the following.

Lemma 3.1: Let $\chi_i^{(0)}\neq 0,\mu_i^{(0)}\neq 0$, *then*

$$\chi_i^{(1)}=T_D^{(1)}(\chi_i^{(0)})\cdot\chi_i^{(0)}=0,\quad \mu_i^{(1)}=-T_I^{(1)}(\chi_i^{(0)})\cdot\mu_i^{(0)}=-\frac{1}{\chi_i^{(0)}}\int\chi_i^{(0)}\mu_i^{(0)},$$

$$\chi_i^{(2)}=\frac{1}{\mu_i^{(1)}},\quad \mu_i^{(2)}=0,$$

$$\chi_i^{(3)}=0,\quad \mu_i^{(3)}=\frac{1}{\chi_i^{(2)}}=\mu_i^{(1)},$$

$$\chi_i^{(4)}=\frac{1}{\mu_i^{(3)}}=\frac{1}{\mu_i^{(1)}},\quad \mu_i^{(4)}=0,$$

$$\vdots\vdots$$

$$\chi_i^{(2k+1)}=0,\quad \mu_i^{(2k+1)}=\mu_i^{(1)};\quad k\geqslant 1,$$

$$\chi_i^{(2k+2)}=\frac{1}{\mu_i^{(1)}},\quad \mu_i^{(2k+2)}=0,\quad k\geqslant 0. \tag{3.6}$$

Lemma 3.2: Let $\chi_i^{(0)}\neq 0,\mu_i^{(0)}\neq 0$, *then*

$$T_I^{(2)}(\mu_i^{(1)})\circ T_D^{(1)}(\chi_i^{(0)})=1-\frac{\chi_i^{(0)}}{\int \chi_i^{(0)}\cdot\mu_i^{(0)}}\circ\partial^{-1}\circ\mu_i^{(0)}\neq I, \tag{3.7}$$

and

$$T_I^{(2k)}(\mu_i^{(2k-1)})\circ T_D^{(2k-1)}(\chi_i^{(2k-2)})=I\quad (k\geqslant 2), \tag{3.8}$$

$$T_D^{(2k-1)}(\chi_i^{(2k-2)})\circ T_I^{(2k-2)}(\mu_i^{(2k-3)})=I\quad (\geqslant 2). \tag{3.9}$$

Proof:

$$\begin{aligned}T_I^{(2)}(\mu_i^{(1)})\circ T_D^{(1)}(\chi_i^{(0)})&=(\mu_i^{(1)})^{-1}\circ\partial^{-1}\circ\mu_i^{(1)}\circ\chi_i^{(0)}\circ\partial\circ(\chi_i^{(0)})^{-1}\\&=-(\mu_i^{(1)})^{-1}\circ\partial^{-1}\circ\left(\int\mu_i^{(0)}\cdot\chi_i^{(0)}\right)\circ\partial\circ(\chi_i^{(0)})^{-1}\\&=(\mu_i^{(1)})^{-1}\circ\left[\left(-\int\mu_i^{(0)}\cdot\chi_i^{(0)}\right)\circ\partial^{-1}+\partial^{-1}\circ(\mu_i^{(0)}\cdot\chi_i^{(0)})\circ\partial^{-1}\right]\circ\partial\circ(\chi_i^{(0)})^{-1}\\&=1+\frac{1}{\mu_i^{(1)}}\circ\partial^{-1}\circ\mu_i^{(0)}=1-\frac{\chi_i^{(0)}}{\int\chi_i^{(0)}\cdot\mu_i^{(0)}}\circ\partial^{-1}\circ\mu_i^{(0)}\neq I.\end{aligned}$$

Using Lemma 3.1, the left-hand side of (3.8) and (3.9) can be written explicitly as

$$\begin{aligned}T_I^{(2k)}(\mu_i^{(2k-1)})\circ T_D^{(2k-1)}(\chi_i^{(2k-2)})&=(\mu_i^{(2k-1)})^{-1}\circ\partial^{-1}\circ\mu_i^{(2k-1)}\circ\chi_i^{(2k-2)}\circ\partial\circ(\chi_i^{(2k-2)})^{-1}\\&=(\mu_i^{(2k-1)})^{-1}\circ\partial^{-1}\circ 1\circ\partial\circ(\chi_i^{(2k-2)})^{-1}=I\end{aligned}$$

and

$$\begin{aligned}T_D^{(2k-1)}(\mu_i^{(2k-2)})\circ T_I^{(2k-2)}(\chi_i^{(2k-3)})&=\chi_i^{(2k-2)}\circ\partial\circ(\chi_i^{(2k-2)})^{-1}\circ(\mu_i^{(2k-3)})^{-1}\circ\partial^{-1}\circ\mu_i^{(2k-3)}\\&=\chi_i^{(2k-2)}\circ\partial\circ 1\circ\partial^{-1}\circ\mu_i^{(2k-3)}=I.\end{aligned}$$

□

Theorem 3.1:

$$\tau^{(2k)}=\tau^{(2k-2)}=\cdots=\tau^{(2)}=-\left(\int \chi_i^{(0)}\cdot\mu_i^{(0)}\right)\cdot\tau^{(0)}, \tag{3.10}$$

$$\tau^{(2k-1)}=\tau^{(2k-3)}=\cdots=\tau^{(1)}=\chi_i^{(0)}\cdot\tau^{(0)}. \tag{3.11}$$

Proof: From Theorem 2.2 and Theorem 2.3, the tau-function of $L^{(2k)}$ is $\tau^{(2k)}=\mu_i^{(2k-1)}\cdot\tau^{(2k-1)}$. Then, according to Lemma 3.1,

$$\begin{aligned}\tau^{(2k)}&=\mu_i^{(2k-1)}\cdot\tau^{(2k-1)}=\mu_i^{(2k-1)}\cdot\chi_i^{(2k-2)}\tau^{(2k-2)}=\tau^{(2k-2)}=\mu_i^{(2k-3)}\cdot\chi_i^{(2k-4)}\tau^{(2k-4)}=\tau^{(2k-4)}\\ &\vdots\\ &=\tau^{(2)}=\mu_i^{(1)}\cdot\chi_i^{(0)}\cdot\tau^{(0)}=-\left(\int\chi_i^{(0)}\cdot\mu_i^{(0)}\right)\tau^{(0)}.\end{aligned}$$

And (3.11) is obtained by a similar way. □

Remark 3.1: The property of the tau-function in the above theorem is different from the case of the first choice.[6] For the first choice, if we construct one chain of gauge transformations such as (3.5), obviously we can only obtain two tau-functions: $\tau^{(2k)}=\cdots=\tau^{(2)}=\tau^{(0)}, \tau^{(2k-1)}=\cdots=\tau^{(1)}$. In particular, the alternative application of Type **I** and Type **II** can be obtained via the single channel. Meanwhile, this novel property of the τ-function results in the periodical transformation with respect to the number of steps in the chain of gauge transformations, when we consider the multichannel (mixed) case (see below).

We now consider another chain of gauge transformations in the ith channel, in which the first step is a gauge transformation of Type **II**,

$$L^{(0)}\xrightarrow{T_I^{(1)}(\mu_i^{(0)})}L^{(1)}\xrightarrow{T_D^{(2)}(\chi_i^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\mu_i^{(2)})}L^{(3)}\xrightarrow{T_D^{(4)}(\chi_i^{(3)})}\cdots\rightarrow\cdots. \tag{3.12}$$

For this chain of gauge transformations, we have the following.

Lemma 3.3: Let $\chi_i^{(0)}\neq 0, \mu_i^{(0)}\neq 0$, *then*

$$\chi_i^{(1)}=\frac{1}{\mu_i^{(0)}}\circ\partial^{-1}\circ\mu_i^{(1)}\cdot\chi_i^{(0)}=\frac{1}{\mu_i^{(0)}}\cdot\int(\mu_i^{(0)}\cdot\chi_i^{(0)}),\quad \mu_i^{(1)}=0,$$

$$\chi_i^{(2)}=0,\quad \mu_i^{(2)}=\frac{1}{\chi_i^{(1)}},$$

$$\chi_i^{(3)}=\frac{1}{\mu_i^{(2)}}=\chi_i^{(1)},\quad \mu_i^{(3)}=0,$$

$$\chi_i^{(4)}=0,\quad \mu_i^{(4)}=\frac{1}{\chi_i^{(3)}}=\frac{1}{\chi_i^{(1)}},$$

$$\vdots\qquad\vdots$$

$$\chi_i^{(2k)}=0,\quad \mu_i^{(2k)}=\frac{1}{\chi_i^{(2k-1)}}=\frac{1}{\chi_i^{(1)}},\quad k\geqslant 1,$$

$$\chi_i^{(2k+1)}=\frac{1}{\mu_i^{(2k)}}=\chi_i^{(1)},\quad \mu_i^{(2k+1)}=0,\quad k\geqslant 0. \tag{3.13}$$

Lemma 3.4: Let $\chi_i^{(0)} \neq 0, \mu_i^{(0)} \neq 0$, *then*

$$T_D^{(2)}(\chi_i^{(1)}) \circ T_I^{(1)}(\mu_i^{(0)}) = 1 - \frac{\chi_i^{(0)}}{\int \chi_i^{(0)} \cdot \mu_i^{(0)}} \circ \partial^{-1} \circ \mu_i^{(0)} \neq I \tag{3.14}$$

and

$$T_D^{(2k)}(\chi_i^{(2k-1)}) \circ T_I^{(2k-1)}(\mu_i^{(2k-2)}) = I \quad (k \geqslant 2), \tag{3.15}$$

$$T_I^{(2k-1)}(\mu_i^{(2k-2)}) \circ T_D^{(2k-2)}(\chi_i^{(2k-3)}) = I \quad (k \geqslant 2). \tag{3.16}$$

Proof:

$$\begin{aligned} T_D^{(2)}(\chi_i^{(1)}) \circ T_I^{(1)}(\mu_i^{(0)}) &= \chi_i^{(1)} \circ \partial \circ (\chi_i^{(1)})^{-1} \circ (\mu_i^{(0)})^{-1} \circ \partial^{-1} \circ \mu_i^{(0)} \\ &= \chi_i^{(1)} \circ \partial \circ \frac{1}{\int \mu_i^{(0)} \cdot \chi_i^{(0)}} \circ \partial^{-1} \circ \mu_i^{(0)} \\ &= \chi_i^{(1)} \circ \left(\frac{\partial}{\int \mu_i^{(0)} \cdot \chi_i^{(0)}} + \left(\frac{1}{\int \mu_i^{(0)} \cdot \chi_i^{(0)}} \right)_x \right) \circ \partial^{-1} \circ \mu_i^{(0)} \\ &= \frac{\int \mu_i^{(0)} \cdot \chi_i^{(0)}}{\mu_i^{(0)}} \circ \left(- \frac{\mu_i^{(0)} \cdot \chi_i^{(0)}}{(\int \mu_i^{(0)} \cdot \chi_i^{(0)})^2} + \frac{1}{\int \mu_i^{(0)} \cdot \chi_i^{(0)}} \circ \partial \right) \circ \partial^{-1} \circ \mu_i^{(0)} \\ &= 1 - \frac{\chi_i^{(0)}}{\int \mu_i^{(0)} \cdot \chi_i^{(0)}} \circ \partial^{-1} \circ \mu_i^{(0)} \neq = I. \end{aligned}$$

Using Lemma 3.3, then

$$\begin{aligned} T_D^{(2k)}(\chi_i^{(2k-1)}) \circ T_I^{(2k-1)}(\mu_i^{(2k-2)}) &= \chi_i^{(2k-1)} \circ \partial \circ (\chi_i^{(2k-1)})^{-1} \circ (\mu_i^{(2k-2)})^{-1} \circ \partial^{-1} \circ \mu_i^{(2k-2)} \\ &= \chi_i^{(2k-1)} \circ \partial \circ 1 \circ \partial^{-1} \circ \mu_i^{(2k-2)} = I \end{aligned}$$

and

$$\begin{aligned} T_I^{(2k-1)}(\mu_i^{(2k-2)}) \circ T_I^{(2k-2)}(\chi_i^{(2k-3)}) &= (\mu_i^{(2k-2)})^{-1} \circ \partial^{-1} \circ \mu_i^{(2k-2)} \circ \chi_i^{(2k-3)} \circ \partial \circ (\chi_i^{(2k-3)})^{-1} \\ &= \mu_i^{(2k-2)} \circ \partial^{-1} \circ 1 \circ \partial \circ (\chi_i^{(2k-3)})^{-1} = I. \end{aligned}$$

□

Theorem 3.2:

$$\tau^{(2k)} = \tau^{(2k-2)} = \cdots = \tau^{(2)} = \left(\int \chi_i^{(0)} \cdot \mu_i^{(0)} \right) \cdot \tau^{(0)}, \tag{3.17}$$

$$\tau^{(2k-1)} = \tau^{(2k-3)} = \cdots = \tau^{(1)} = \mu_i^{(0)} \cdot \tau^{(0)}. \tag{3.18}$$

Proof: Lemma 3.4 shows that $\tau^{(2k)} = \tau^{(2k-2)} = \cdots = \tau^{(2)}, \tau^{(2k-1)} = \tau^{(2k-3)} = \cdots = \tau^{(1)}$. From Theorem 2.2 and Theorem 2.3, we have $\tau^{(1)} = \mu_i^{(0)} \cdot \tau^{(0)}$ and $\tau^{(2)} = (\int \chi_i^{(0)} \cdot \mu_i^{(0)}) \cdot \tau^{(0)}$. □

In order ot obtain the explicit form of $\phi^{(n)}, \psi^{(n)}, \tau^{(n)}$ after a n-step gauge transformation, we give the determinant representation of the gauge transformation operators.

Lemma 3.5: (Ref. 22) *For* $n > k$, *there are two gauge transformation operators*

$$T_{n+k}=T_I^{(n+k)}(\mu_k^{(n+k-1)})\circ T_I^{(n+k-1)}(\mu_{k-1}^{(n+k-2)})\cdots T_I^{(n+1)}(\mu_1^{(n)})\circ T_D^{(n)}(\chi_n^{(n-1)})$$
$$\circ T_D^{(n-1)}(\chi_{n-1}^{(n-2)})\cdots T_D^{(1)}(\chi_1^{(0)})$$
$$=\frac{1}{IW_{k,n}}\cdot\begin{vmatrix} \int \chi_1^{(0)}\cdot\mu_k^{(0)} & \int \chi_2^{(0)}\cdot\mu_k^{(0)} & \cdots & \int \chi_n^{(0)}\cdot\mu_k^{(0)} & \partial^{-1}\circ\mu_k^{(0)} \\ \int \chi_1^{(0)}\cdot\mu_{k-1}^{(0)} & \int \chi_2^{(0)}\cdot\mu_{k-1}^{(0)} & \cdots & \int \chi_n^{(0)}\cdot\mu_{k-1}^{(0)} & \partial^{-1}\circ\mu_{k-1}^{(0)} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \int \chi_1^{(0)}\cdot\mu_1^{(0)} & \int \chi_2^{(0)}\cdot\mu_1^{(0)} & \cdots & \int \chi_n^{(0)}\cdot\mu_1^{(0)} & \partial^{-1}\circ\mu_1^{(0)} \\ \chi_1^{(0)} & \chi_2^{(0)} & \cdots & \chi_n^{(0)} & 1 \\ \chi_{1,x}^{(0)} & \chi_{2,x}^{(0)} & \cdots & \chi_{n,x}^{(0)} & \partial \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ (\chi_1^{(0)})^{(n-k)} & (\chi_2^{(0)})^{(n-k)} & \cdots & (\chi_n^{(0)})^{(n-k)} & \partial^{n-k} \end{vmatrix}, \quad (3.19)$$

and

$$T_{n+k}^{-1}=\begin{vmatrix} \chi_1^{(0)}\circ\partial^{-1} & \int \mu_k^{(0)}\cdot\chi_1^{(0)} & \cdots & \int \mu_1^{(0)}\cdot\chi_1^{(0)} & \chi_1^{(0)} & \chi_{1,x}^{(0)} & \cdots & (\chi_1^{(0)})^{(n-k-2)} \\ \chi_2^{(0)}\circ\partial^{-1} & \int \mu_k^{(0)}\cdot\chi_2^{(0)} & \cdots & \int \mu_1^{(0)}\cdot\chi_2^{(0)} & \chi_2^{(0)} & \chi_{2,x}^{(0)} & \cdots & (\chi_2^{(0)})^{(n-k-2)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \chi_{n-1}^{(0)}\circ\partial^{-1} & \int \mu_k^{(0)}\cdot\chi_{n-1}^{(0)} & \cdots & \int \mu_1^{(0)}\cdot\chi_{n-1}^{(0)} & \chi_{n-1}^{(0)} & \chi_{n-1,x}^{(0)} & \cdots & (\chi_{n-1}^{(0)})^{(n-k-2)} \\ \chi_n^{(0)}\circ\partial^{-1} & \int \mu_k^{(0)}\cdot\chi_n^{(0)} & \cdots & \int \mu_1^{(0)}\cdot\chi_n^{(0)} & \chi_n^{(0)} & \chi_{n,x}^{(0)} & \cdots & (\chi_n^{(0)})^{(n-k-2)} \end{vmatrix}$$
$$\cdot\frac{(-1)^{n-1}}{IW_{k,n}}. \quad (3.20)$$

Let us to discuss the multichannel (pure) case. For the chain of gauge transformations,

$$L^{(0)}\xrightarrow{T_D^{(1)}(\chi_1^{(0)})}L^{(1)}\xrightarrow{T_D^{(2)}(\chi_2^{(1)})}L^{(2)}\xrightarrow{T_D^{(3)}(\chi_3^{(2)})}L^{(3)}\xrightarrow{T_D^{(4)}(\chi_4^{(3)})}\cdots\to\cdots L^{(n-1)}\xrightarrow{T_D^{(n)}(\chi_n^{(n-1)})}L^{(n)}, \quad (3.21)$$

we have

Theorem 3.3:

$$\phi^{(n)}=T_D^{(n)}(\chi_n^{(n-1)})\circ T_D^{(n-1)}(\chi_{n-1}^{(n-2)})\cdots\circ T_D^{(2)}(\chi_2^{(1)})\circ T_D^{(1)}(\chi_1^{(0)})\cdot\phi^{(0)}$$
$$=\frac{W_{n+1}(\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)},\phi^{(0)})}{W_n(\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)})}, \quad (3.22)$$

$$\psi^{(n)}=-T_I^{(n)}(\chi_n^{(n-1)})\cdot\psi^{(n-1)}$$
$$=(-1)^n T_I^{(n)}(\chi_n^{(n-1)})\circ T_I^{(n-1)}(\chi_{n-1}^{(n-2)})\cdots T_I^{(2)}(\chi_2^{(1)})\circ T_I^{(1)}(\chi_1^{(0)})\cdot\psi^{(0)}$$
$$=(-1)^n\frac{IW_{1,n}(\psi^{(0)};\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)})}{W_n}, \quad (3.23)$$

$$\tau^{(n)}=W_n(\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)})\cdot\tau^{(0)}, \tag{3.24}$$

$$\chi_i^{(j)}=\begin{cases}0, & n\geqslant j\geqslant i,\\ \dfrac{W_{j+1}(\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_j^{(0)},\chi_i^{(0)})}{W_j(\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_j^{(0)})}, & j<i\leqslant n,\end{cases} \tag{3.25}$$

$$\begin{aligned}\mu_i^{(n)}&=-T_I^{(n)}(\chi_n^{(n-1)})\cdot\mu_i^{(n-1)}\\&=(-1)^nT_I^{(n)}(\chi_n^{(n-1)})\circ T_I^{(n-1)}(\chi_{n-1}^{(n-2)})\cdots T_I^{(2)}(\chi_2^{(1)})\circ T_I^{(1)}(\chi_1^{(0)})\cdot\mu_i^{(0)}\\&=(-1)^n\frac{IW_{1,n}(\mu_i^{(0)};\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_n^{(0)})}{W_n}.\end{aligned} \tag{3.26}$$

Proof: This can be obtained by direct calculation with the help of successive applications of Theorem 2.2, and by using Lemma 3.5. □

Similarly, for the gauge transformation of Type **II**, the following chain of gauge transformations:

$$L^{(0)}\xrightarrow{T_I^{(1)}(\mu_1^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\mu_2^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\mu_3^{(2)})}L^{(3)}\xrightarrow{T_I^{(4)}(\mu_4^{(3)})}\cdots\rightarrow L^{(n-1)}\xrightarrow{T_I^{(n)}(\mu_n^{(n-1)})} \tag{3.27}$$

implies the following.

Theorem 3.4:

$$\begin{aligned}\phi^{(n)}&=T_I^{(n)}(\mu_n^{(n-1)})\circ T_I^{(n-1)}(\mu_{n-1}^{(n-2)})\cdots T_I^{(2)}(\mu_2^{(1)})\circ T_I^{(1)}(\mu_1^{(0)})\cdot\phi^{(0)},\\&=\frac{IW_{1,n}(\phi^{(0)};\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)})}{W_n(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)})},\end{aligned} \tag{3.28}$$

$$\begin{aligned}\psi^{(n)}&=(-1)^nT_D^{(n)}(\mu_n^{(n-1)})\circ T_D^{(n-1)}(\mu_{n-1}^{(n-2)})\cdots T_D^{(2)}(\mu_2^{(1)})\circ T_D^{(1)}(\mu_1^{(0)})\cdot\psi^{(0)}\\&=(-1)^n\frac{W_{n+1}(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)},\psi^{(0)})}{W_n(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)})},\end{aligned} \tag{3.29}$$

$$\tau^{(n)}=W_n(\mu_n^{(0)},\mu_{n-1}^{(0)},\ldots\mu_2^{(0)},\mu_1^{(0)})\cdot\tau^{(0)}, \tag{3.30}$$

$$\begin{aligned}\chi_i^{(n)}=T_I^{(n)}(\mu_n^{(n-1)})\cdot\chi_i^{(n-1)}&=T_I^{(n)}(\mu_n^{(n-1)})\circ T_I^{(n-1)}(\mu_{n-1}^{(n-2)})\cdots T_I^{(2)}(\mu_2^{(1)})\circ T_I^{(1)}(\mu_1^{(0)})\cdot\chi_i^{(0)},\\&=\frac{IW_{1,n}(\chi_i^{(0)};\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)})}{W_n(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_n^{(0)})}\end{aligned} \tag{3.31}$$

$$\mu_i^{(j)}=\begin{cases}0, & n\geqslant j\geqslant i,\\ (-1)^j\cdot\dfrac{W_{j+1}(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_j^{(0)},\mu_i^{(0)})}{W_j(\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_j^{(0)})}, & j<i\leqslant n.\end{cases} \tag{3.32}$$

Remark 3.2: This formula, (3.22), is the same as the result of Ref. 21, and (3.24) also equals with those result [although Ref. 21 does not include the explicit form as (3.24)]. Because the GFGT will be lost after the gauge transformation, cannot do the $(n+1)$th step of gauge transformation in the multichannel (pure) case according to (3.21) and (3.27) if we only use n BA functions or n adjoint BA functions.

Finally, we would like to discuss the more complicated case: the multichannel (mixed). First of all, there is an important lemma exactly similar to the result of Ref. 6 [see (67) and (68) there].

Lemma 3.6: Suppose the BA function $\chi_i^{(k-1)}$ and the adjoint BA function $\mu_j^{(k-1)}$ of $L^{(k-1)}$ lied in a chain of gauge transformations, and $\chi_i^{(k-1)} \neq 0, \mu_i^{(k-1)} \neq 0, i \neq j$. For the two chains,

$$(A): L^{(k-1)} \xrightarrow{T_D(\chi_i^{(k-1)})} L^{(k)} \xrightarrow{T_I(\mu_j^{(k)})} L^{(k+1)}, \tag{3.33}$$

$$(B): L^{(k-1)} \xrightarrow{T_I(\mu_j^{(k-1)})} L^{(k)} \xrightarrow{T_D(\chi_i^{(k)})} L^{(k+1)}, \tag{3.34}$$

we have

$$T_I(\mu_j^{(k)}) \circ T_D(\chi_i^{(k-1)}) = T_D(\chi_i^{(k)}) \circ T_I(\mu_j^{(k-1)}) = 1 - \frac{\chi_i^{(k-1)}}{\int \mu_j^{(k-1)} \cdot \chi_i^{(k-1)}} \circ \partial^{-1} \circ \mu_j^{(k-1)}. \tag{3.35}$$

Meanwhile, the $\tau_A^{(k+1)}$ is generated by A and $\tau_B^{(k+1)}$ is generated by B, which are of the form

$$\tau_A^{(k+1)} = -\left(\int \chi_i^{(k-1)} \cdot \mu_j^{(k-1)} \right) \cdot \tau^{(k-1)}, \tag{3.36}$$

$$\tau_B^{(k+1)} = \left(\int \chi_i^{(k-1)} \cdot \mu_j^{(k-1)} \right) \cdot \tau^{(k-1)}, \tag{3.37}$$

and $\tau_A^{(k+1)}$ is equivalent to $\tau_B^{(k+1)}$.

Proof: Formula (3.35) is proved in a similar way to (3.7) and (3.14). $\tau_A^{(k+1)}$ and $\tau_B^{(n+k)}$ are obtained by successive applications of Theorem 2.2 and Theorem 2.3 with two steps. □

This lemma is very important to study the τ-function generated by gauge transformations in the multichannel (mixed) case. The $\tau^{(n+k)}$ is determined uniquely up to an unimportant minus sign. It leads us to neglect the order of the channel adopted in one chain of gauge transformations. However, in order to understand and calculate easily the transformation of the τ-function, we still discuss firstly the chain of gauge transformations with a fixed ordering of the channels. For the chain of gauge transformations with $n \geqslant k > 1$,

$$\begin{aligned} L^{(0)} &\xrightarrow{T_D^{(1)}(\chi_1^{(0)})} L^{(1)} \xrightarrow{T_D^{(2)}(\chi_2^{(1)})} L^{(2)} \xrightarrow{T_D^{(3)}(\chi_3^{(2)})} L^{(3)} \cdots \\ &\to L^{(n-1)} \xrightarrow{T_D^{(n)}(\chi_n^{(n-1)})} L^{(n)} \xrightarrow{T_I^{(n+1)}(\mu_1^{(n)})} L^{(n+1)} \xrightarrow{T_I^{(n+2)}(\mu_2^{(n+1)})} L^{(n+2)} \cdots \\ &\to L^{(n+k-1)} \xrightarrow{T_I^{(n+k)}(\mu_k^{(n+k-1)})} L^{(n+k)}, \end{aligned} \tag{3.38}$$

we want to obtain the $\phi^{(n+k)}, \psi^{(n+k)}, \tau^{(n+k)}$ of $L^{(n+k)}$ transformed from the $L^{(0)}$ by the above chain of gauge transformations.

Theorem 3.5:

$$\begin{aligned} \phi^{(n+k)} &= T_I^{(n+k)}(\mu_k^{(n+k-1)}) \circ T_I^{(n+k-1)}(\mu_{k-1}^{(n+k-2)}) \cdots T_I^{(n+1)}(\mu_1^{(n)}) \circ T_D^{(n)}(\chi_n^{(n-1)}) \\ &\circ T_D^{(n-1)}(\chi_{n-1}^{(n-2)}) \cdots T_D^{(1)}(\chi_1^{(0)}) \cdot \phi^{(0)} = \frac{IW_{k,n+1}(\mu_k^{(0)}, \ldots, \mu_1^{(0)}; \chi_1^{(0)}, \ldots, \chi_n^{(0)}, \phi^{(0)})}{IW_{k,n}}, \end{aligned} \tag{3.39}$$

$$\psi^{(n+k)} = (T_{n+k}^{-1})^* \cdot \psi^{(0)} = (-1)^n \frac{IW_{k+1,n}(\psi^{(0)}, \mu_k^{(0)}, \mu_{k-1}^{(0)}, \ldots, \mu_1^{(0)}; \chi_1^{(0)}, \ldots, \chi_n^{(0)})}{IW_{k,n}}, \tag{3.40}$$

$$\tau^{(n+k)}=IW_{k,n}\cdot\tau^{(0)}, \tag{3.41}$$

Proof: $\phi^{(n+k)}=T_{n+k}\cdot\phi^{(0)}$ is obtained by the successive applications of Theorem 2.2, Theorem 2.3, then taking the expression of T_{n+k} into it yields the explicit form of $\psi^{(n+k)}$ as a determinant. Meanwhile, using Theorem 2.2, Theorem 2.3 and the definition of operation of conjugation, we have

$$\begin{aligned}\psi^{(n+k)}&=(-1)^{n+k}T_D^{(n+k)}(\mu_k^{(n+k-1)})\circ T_D^{(n+k-1)}(\mu_{k-1}^{(n+k-2)})\cdots T_D^{(n+1)}(\mu_k^{(n+k-1)})T_I^{(n)}(\chi_n^{(n-1)})\\&\quad\circ T_I^{(n)}(\chi_{n-1}^{(n-2)})\cdots T_I^{(n)}(\chi_1^{(0)})\cdot\psi^{(0)}=(T_{n+k}^{-1})^*\cdot\psi^{(0)}.\end{aligned}$$

The formal determinantal expression of $\psi^{(n+k)}$ follows from the above lemma. Theorem 2.2 and Theorem 2.3 imply

$$\tau^{(n+k)}=\mu_k^{(n+k-1)}\cdot\mu_{k-1}^{(n+k-2)}\cdots\mu_1^{(n)}\cdot\tau^{(n)},$$

in which $\mu_i^{(j)}$ given by

$$\begin{aligned}\mu_i^{(n+j)}&=(T_{n+j}^{-1})^*\cdot\mu_i^{(0)}\\&=\begin{cases}0, & j\geqslant i\\ (-1)^n\dfrac{IW_{j+1,n}(\mu_i^{(0)},\mu_j^{(0)},\mu_{j-1}^{(0)},\ldots,\mu_1^{(0)};\chi_1^{(0)},\ldots,\chi_n^{(0)})}{IW_{j,n}(\mu_j^{(0)},\mu_{j-1}^{(0)},\ldots,\mu_1^{(0)};\chi_1^{(0)},\ldots,\chi_n^{(0)})}, & k\geqslant i>j\geqslant 1.\end{cases}\end{aligned}$$

Specially, the $\mu_i^{(n)}$ and the $\tau^{(n)}$ are given by Theorem 3.3. So taking these expressions back into $\tau^{(n+k)}$ finishes the proof of theorem. □

Moreover, for

$$\begin{aligned}&L^{(0)}\xrightarrow{T_I^{(1)}(\mu_1^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\mu_2^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\mu_3^{(2)})}L^{(3)}\cdots\\&\to L^{(n-1)}\xrightarrow{T_I^{(n)}(\mu_n^{(n-1)})}L^{(n)}\xrightarrow{T_D^{(n+1)}(\chi_1^{(n)})}L^{(n+1)}\xrightarrow{T_D^{(n+2)}(\chi_2^{(n+1)})}L^{(n+2)}\cdots L^{(n+k-1)}\xrightarrow{T_D^{(n+k)}(\chi_k^{(n+k-1)})}L^{(n+k)},\end{aligned} \tag{3.42}$$

the $\phi^{(n+k)}$, $\psi^{(n+k)}$, $\tau^{(n+k)}$ are written as follows.

Theorem 3.6:

$$\phi^{(n+k)}=(-1)^k\frac{\widehat{IW}_{k+1,n}(\phi^{(0)},\chi_k^{(0)},\chi_{k-1}^{(0)},\ldots,\chi_1^{(0)};\mu_1^{(0)},\ldots,\mu_n^{(0)})}{\widehat{IW}_{k,n}}, \tag{3.43}$$

$$\begin{aligned}\psi^{(n+k)}&=(-)^{n+k}T_I^{(n+k)}(\chi_k^{(n+k-1)})\circ T_I^{(n+k-1)}(\chi_{k-1}^{(n+k-2)})\cdots T_I^{(n+1)}(\chi_1^{(n)})\circ T_D^{(n)}(\mu_n^{(n-1)})\\&\quad\circ T_D^{(n-1)}(\mu_{n-1}^{(n-2)})\cdots T_D^{(1)}(\mu_1^{(0)})\cdot\psi^{(0)}\\&=(-1)^{n+k}\frac{IW_{k,n+1}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\mu_1^{(0)},\ldots,\mu_n^{(0)},\psi^{(0)})}{\widehat{IW}_{k,n}},\end{aligned} \tag{3.44}$$

$$\tau^{(n+k)}=\widehat{IW}_{k,n}\tau^{(0)}. \tag{3.45}$$

Proof: Its proof is similar to way of Theorem 3.5, hence we omit it.

Theorem 3.7: *For the following chain of gauge transformations with* $k<n$,

$$
\begin{aligned}
&L^{(0)} \xrightarrow{T_D^{(1)}(\chi_1^{(0)})} L^{(1)} \xrightarrow{T_D^{(2)}(\chi_2^{(1)})} L^{(2)} \xrightarrow{T_D^{(3)}(\chi_3^{(2)})} L^{(3)}\cdots\\
&\to L^{(n-1)} \xrightarrow{T_D^{(n)}(\chi_n^{(n-1)})} L^{(n)} \xrightarrow{T_I^{(n+1)}(\mu_1^{(n)})} L^{(n+1)} \xrightarrow{T_I^{(n+2)}(\mu_2^{(n+1)})} L^{(n+2)}\cdots\\
&\to L^{(2n-1)} \xrightarrow{T_I^{(2n)}(\mu_n^{(2n-1)})} L^{(2n)} \xrightarrow{T_D^{(2n+1)}(\chi_1^{(2n)})} L^{(2n+1)} \xrightarrow{T_D^{(2n+2)}(\chi_2^{(2n+1)})} L^{(2n+2)}\cdots\\
&\to L^{(3n-1)} \xrightarrow{T_D^{(2n)}(\chi_n^{(3n-1)})} L^{(3n)} \xrightarrow{T_I^{(3n+1)}(\mu_1^{(3n)})} L^{(3n+1)} \xrightarrow{T_I^{(3n+2)}(\mu_2^{(3n+1)})} L^{(3n+2)}\cdots\\
&\to L^{(4n-1)} \xrightarrow{T_I^{(4n)}(\mu_n^{(4n-1)})} L^{(4n)} \xrightarrow{T_D^{(4n+1)}(\chi_1^{(4n)})} \cdots,
\end{aligned}
\tag{3.46}
$$

the final form of $\tau^{(mn+k)}$ $(m=0,1,2,\ldots;\ k=0,1,2,\ldots,n-1)$ *for* $L^{(mn+k)}$ *is*

$$
\tau^{(mn+k)}=\begin{cases}
\tau^{(k)}=W_k(\chi_1^{(0)},\cdots,\chi_k^{(0)})\cdot\tau^{(0)}, & \text{if } m=0.\\
\tau^{(n+k)}=IW_{k,n}\cdot\tau^{(0)}, & \text{if } m \text{ is odd.}\\
\tau^{(2n+k)}=IW_{n-k,n}(\mu_n^{(0)},\cdots,\mu_{k+1}^{(0)};\chi_1^{(0)},\cdots,\chi_n^{(0)})\cdot\tau^{(0)}, & \text{if } m \text{ is even.}
\end{cases}
\tag{3.47}
$$

Proof: First of all, Lemma 3.2, Lemma 3.4, and Lemma 3.6 imply directly

$$
\tau^{(mn+k)}=\begin{cases}
\tau^{(n+k)}, & \text{if } m \text{ is odd}\\
\tau^{(2n+k)}, & \text{if } m \text{ is even.}
\end{cases}
$$

On the other hand, $\tau^{(k)}$ is given by Theorem 3.3, and $\tau^{(n+k)}$ is given by Theorem 3.5. In fact, according to Lemma 3.2, Lemma 3.4, and Lemma 3.6, $\tau^{(2n+k)}$ is equivalent to τ-function obtained by the following chain:

$$
\begin{aligned}
&L^{(0)} \xrightarrow{T_D^{(1)}(\chi_1^{(0)})} L^{(1)} \xrightarrow{T_D^{(2)}(\chi_2^{(1)})} L^{(2)} \xrightarrow{T_D^{(3)}(\chi_3^{(2)})} L^{(3)}\cdots\\
&\to L^{(n-1)} \xrightarrow{T_D^{(n)}(\chi_n^{(n-1)})} L^{(n)} \xrightarrow{T_I^{(n+1)}(\mu_{k+1}^{(n)})} L^{(n+1)} \xrightarrow{T_I^{(n+2)}(\mu_{k+2}^{(n+1)})} L^{(n+2)}\cdots\\
&\to L^{(n+n-k-1)} \xrightarrow{T_I^{(n+n-k)}(\mu_n^{(n+n-k-1)})} L^{(n+n-k)}.
\end{aligned}
$$

So Theorem 3.5 yields $\tau^{(n+n-k)}$ with a corresponding modification of the GFGTs. □

Moreover,

Theorem 3.8: *For the chain of gauge transformations*

$$
\begin{aligned}
&L^{(0)} \xrightarrow{T_I^{(1)}(\mu_1^{(0)})} L^{(1)} \xrightarrow{T_I^{(2)}(\mu_2^{(1)})} L^{(2)} \xrightarrow{T_I^{(3)}(\mu_3^{(2)})} L^{(3)}\cdots\\
&\to L^{(n-1)} \xrightarrow{T_I^{(n)}(\mu_n^{(n-1)})} L^{(n)} \xrightarrow{T_D^{(n+1)}(\chi_1^{(n)})} L^{(n+1)} \xrightarrow{T_D^{(n+2)}(\chi_2^{(n+1)})} L^{(n+2)}\cdots\\
&\to L^{(2n-1)} \xrightarrow{T_D^{(2n)}(\chi_n^{(2n-1)})} L^{(2n)} \xrightarrow{T_I^{(2n+1)}(\mu_1^{(2n)})} L^{(2n+1)} \xrightarrow{T_I^{(2n+2)}(\mu_2^{(2n+1)})} L^{(2n+2)}\cdots\\
&\to L^{(3n-1)} \xrightarrow{T_I^{(2n)}(\mu_n^{(3n-1)})} L^{(3n)} \xrightarrow{T_D^{(3n+1)}(\chi_1^{(3n)})} L^{(3n+1)} \xrightarrow{T_D^{(3n+2)}(\chi_2^{(3n+1)})} L^{(3n+2)}\cdots
\end{aligned}
$$

$$\rightarrow L^{(4n-1)} \xrightarrow{T_D^{(4n)}(\chi_n^{(4n-1)})} L^{(4n)} \xrightarrow{T_I^{(4n+1)}(\mu_1^{(4n)})} \cdots, \tag{3.48}$$

the final form of $\tau^{(mn+k)}$ $(m=0,1,2,\ldots;\ k=0,1,2,\ldots,n-1)$ *for* $L^{(mn+k)}$ *is*

$$\tau^{(mn+k)}=\begin{cases}\tau^{(k)}=W_k(\mu_1^{(0)},\ldots,\mu_k^{(0)})\cdot\tau^{(0)}, & \text{if } m=0\\ \tau^{(n+k)}=\widehat{IW}_{k,n}\cdot\tau^{(0)}, & \text{if } m \text{ is odd}\\ \tau^{(2n+k)}=\widehat{IW}_{n-k,n}(\chi_n^{(0)},\cdots,\chi_{k+1}^{(0)};\mu_1^{(0)},\ldots,\mu_n^{(0)})\cdot\tau^{(0)}, & \text{if } m \text{ is even.}\end{cases} \tag{3.49}$$

Proof: The proof of this theorem is similar to way of Theorem 3.8. □

IV. THE UNION OF THE TWO CHOICES OF GAUGE TRANSFORMATIONS

In the previous part of this paper, all chains of gauge transformations include only one choice. It is natural to explore the case of the union of two choices. To our knowledge, this has not been done so far in literature. We consider the following four chains. For the chain with $k<n$,

$$\begin{aligned}&L^{(0)} \xrightarrow{T_D^{(1)}(\phi^{(0)})} L^{(1)} \xrightarrow{T_D^{(2)}(\phi^{(1)})} L^{(2)} \xrightarrow{T_D^{(3)}(\phi^{(2)})} L^{(3)}\cdots\\ &\rightarrow L^{(n-1)} \xrightarrow{T_D^{(n)}(\phi^{(n-1)})} L^{(n)} \xrightarrow{T_D^{(n+1)}(\chi_1^{(n)})} L^{(n+1)} \xrightarrow{T_D^{(n+2)}(\chi_2^{(n+1)})} L^{(n+2)}\cdots\\ &\rightarrow L^{(n+k-1)} \xrightarrow{T_D^{(n+k)}(\chi_k^{(n+k-1)})} L^{(n+k)},\end{aligned} \tag{4.1}$$

we have the following.

Theorem 4.1:

$$\phi^{(n)}=\frac{W_{n+1}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\eta^{(n)})}{W_n(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})}, \tag{4.2}$$

$$\psi^{(n)}=(\phi^{(n-1)})^{-1}, \tag{4.3}$$

$$\phi^{(n+k)}=\frac{W_{n+k+1}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_k^{(0)},\eta^{(n)})}{W_{n+k}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_k^{(0)})}, \tag{4.4}$$

$$\begin{aligned}\psi^{(n+k)}&=(-1)^k T_I^{(n+k)}(\chi_k^{(n+k-1)})\circ T_I^{(n+k-1)}(\chi_{k-1}^{(n+k-2)})\cdots T_I^{(n+2)}(\chi_2^{(n+1)})\circ T_I^{(n+1)}(\chi_1^{(n)})\cdot\psi^{(n)},\\ &=(-1)^k\frac{IW_{1,k}(\psi^{(n)};\chi_1^{(n)},\ldots,\chi_k^{(n)})}{W_k(\chi_1^{(n)},\ldots,\chi_k^{(n)})},\end{aligned} \tag{4.5}$$

$$\chi_i^{(n+j)}=\begin{cases}0, & k\geqslant j\geqslant i,\\ \dfrac{W_{n+j+1}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_j^{(0)},\chi_i^{(0)})}{W_{n+j}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_j^{(0)})}, & j<i\leqslant k,\end{cases} \tag{4.6}$$

$$\begin{aligned}\mu_i^{(n+j)}&=(-1)^{n+j}T_I^{(n+j)}(\chi_j^{(n+j-1)})\circ T_I^{(n+j-1)}(\chi_{j-1}^{(n+j-2)})\cdots T_I^{(n+1)}(\chi_1^{(n)})\circ T_I^{(n)}(\phi^{(n-1)})\\ &\quad\circ T_I^{(n-1)}(\phi^{(n-2)})\cdots T_I^{(1)}(\phi^{(0)})\cdot\mu_i^{(0)}\\ &=(-1)^{n+j}\frac{IW_{1,n+j}(\mu_i^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\ldots,\chi_j^{(0)})}{W_{n+j}(\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\ldots,\chi_j^{(0)})},\end{aligned} \tag{4.7}$$

$$\tau^{(n+k)}=W_{n+k}(\phi^{(0)},\eta^{(1)},\eta^{(2)},\ldots,\eta^{(n-1)},\chi_1^{(0)},\chi_2^{(0)},\ldots,\chi_k^{(0)})\tau^{(0)}. \tag{4.8}$$

Here $\eta^{(k)}=(L^{(0)})^k\cdot\phi^{(0)}$.

Proof: This is a straightforward calculation via the repeated use of Theorem 2.2 and Lemma 3.5. We only point that, in the above chain, the first n steps are gauge transformations of Type **I** with the first choice, while the latter **k** steps use the second choice. □

The second chain is

$$\begin{aligned}
&L^{(0)}\xrightarrow{T_D^{(1)}(\phi^{(0)})}L^{(1)}\xrightarrow{T_D^{(2)}(\phi^{(1)})}L^{(2)}\xrightarrow{T_D^{(3)}(\phi^{(2)})}L^{(3)}\cdots\\
&\to L^{(n-1)}\xrightarrow{T_D^{(n)}(\phi^{(n-1)})}L^{(n)}\xrightarrow{T_I^{(n+1)}(\mu_1^{(n)})}L^{(n+1)}\xrightarrow{T_I^{(n+2)}(\mu_2^{(n+1)})}L^{(n+2)}\cdots\\
&\to L^{(n+k-1)}\xrightarrow{T_I^{(n+k)}(\mu_k^{(n+k-1)})}L^{(n+k)}.
\end{aligned} \tag{4.9}$$

If $k<n$, we have

Theorem 4.2:

$$\phi^{(n+k)}=\frac{IW_{k,n+1}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\eta^{(n)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})}, \tag{4.10}$$

$$\psi^{(n+k)}=(-1)^k\frac{W_{k+1}(\mu_1^{(n)},\ldots,\mu_k^{(n)},\psi^{(n)})}{W_k(\mu_1^{(n)},\ldots,\mu_k^{(n)})}, \tag{4.11}$$

$$\chi_i^{(n+k)}=\frac{IW_{k,n+1}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)},\chi_i^{(0)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})}, \tag{4.12}$$

$$\mu_i^{(n+k)}=(-1)^n\frac{IW_{k+1,n}(\mu_i^{(0)},\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})}, \tag{4.13}$$

$$\tau^{(n+k)}=IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\eta^{(1)},\ldots,\eta^{(n-1)})\tau^{(0)}. \tag{4.14}$$

Here $\psi^{(n)}$, $\mu_i^{(n)}$ and $\eta^{(n)}$ are given by Theorem 4.1.

We also like to consider the analogous treatment for the Type **II** case. For the chain with $k<n$,

$$\begin{aligned}
&L^{(0)}\xrightarrow{T_I^{(1)}(\psi^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\psi^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\psi^{(2)})}L^{(3)}\cdots\\
&\to L^{(n-1)}\xrightarrow{T_I^{(m)}(\psi^{(n-1)})}L^{(n)}\xrightarrow{T_I^{(n+1)}(\mu_1^{(n)})}L^{(n+1)}\xrightarrow{T_I^{(n+2)}(\mu_2^{(n+1)})}L^{(n+2)}\cdots\\
&\to L^{(n+k-1)}\xrightarrow{T_I^{(n+k)}(\mu_k^{(n+k-1)})}L^{(n+k)},
\end{aligned} \tag{4.15}$$

we have the following.

Theorem 4.3:

$$\phi^{(n)}=(\psi^{(n-1)})^{-1}, \tag{4.16}$$

$$\psi^{(n)}=(-1)^n\frac{W_{n+1}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\xi^{(n)})}{W_n(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})}, \tag{4.17}$$

$$\phi^{(n+k)}=T_I^{(n+k)}(\mu_k^{(n+k-1)})\circ T_I^{(n+k-1)}(\mu_{k-1}^{(n+k-2)})\cdots T_I^{(n+2)}(\mu_2^{(n+1)})\circ T_I^{(n+1)}(\mu_1^{(n)})\cdot\phi^{(n)},$$
$$=\frac{IW_{1,k}(\phi^{(n)};\mu_1^{(n)},\ldots,\mu_k^{(n)})}{W_k(\mu_1^{(n)},\ldots,\mu_k^{(n)})}, \tag{4.18}$$

$$\psi^{(n+k)}=(-)^{n+k}\frac{W_{n+k+1}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_k^{(0)},\xi^{(n)})}{W_{n+k}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_k^{(0)})}, \tag{4.19}$$

$$\chi_i^{(n+j)}=T_I^{(n+j)}(\mu_j^{(n+j-1)})\circ T_I^{(n+j-1)}(\mu_{j-1}^{(n+j-2)})\cdots T_I^{(n+1)}(\mu_1^{(n)})\circ T_I^{(n)}(\psi^{(n-1)})$$
$$\circ T_I^{(n-1)}(\psi^{(n-2)})\cdots T_I^{(1)}(\psi^{(0)})\cdot\chi_i^{(0)}=\frac{IW_{1,n+j}(\chi_i^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\ldots,\mu_j^{(0)})}{W_{n+j}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\ldots,\mu_j^{(0)})}, \tag{4.20}$$

$$\mu_i^{(n+j)}=\begin{cases}0, & k\geqslant j\geqslant i,\\ (-1)^{n+j}\dfrac{W_{n+j+1}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_j^{(0)},\mu_i^{(0)})}{W_{n+j}(\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_j^{(0)})}, & j<i\leqslant k,\end{cases} \tag{4.21}$$

$$\tau^{(n+k)}=W_{n+k}(\psi^{(0)},\xi^{(1)},\xi^{(2)},\ldots,\xi^{(n-1)},\mu_1^{(0)},\mu_2^{(0)},\ldots,\mu_k^{(0)})\tau^{(0)}. \tag{4.22}$$

Here $\xi^{(k)}=(L^{*(0)})^k\cdot\psi^{(0)}$.

Proof: This is obtained by a straightforward calculation via the repeated use of Theorem 2.3 and Lemma 3.5. We only point that, in the above chain, the first m steps are gauge transformations of Type **II** with the first choice, while in the latter k steps with second choice is used. □

The fourth chain is

$$L^{(0)}\xrightarrow{T_I^{(1)}(\psi^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\psi^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\psi^{(2)})}L^{(3)}\cdots$$
$$\to L^{(n-1)}\xrightarrow{T_I^{(m)}(\psi^{(n-1)})}L^{(n)}\xrightarrow{T_D^{(n+1)}(\chi_1^{(n)})}L^{(n+1)}\xrightarrow{T_D^{(n+2)}(\chi_2^{(n+1)})}L^{(n+2)}\cdots$$
$$\to L^{(n+k-1)}\xrightarrow{T_D^{(n+k)}(\chi_k^{(n+k-1)})}L^{(n+k)}. \tag{4.23}$$

We then have the following.

Theorem 4.4:

$$\phi^{(n+k)}=\frac{W_{k+1}(\chi_1^{(n)},\ldots,\chi_k^{(n)},\phi^{(n)})}{W_k(\chi_1^{(n)},\ldots,\chi_k^{(n)})}, \tag{4.24}$$

$$\psi^{(n+k)}=(-1)^{n+k}\frac{\widehat{IW}_{k,n+1}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\xi^{(n)})}{\widehat{IW}_{k,n}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})}, \tag{4.25}$$

$$\chi_i^{(n+k)}=(-1)^k\frac{\widehat{IW}_{k+1,n}(\chi_i^{(0)},\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})}{\widehat{IW}_{k,n}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})}, \tag{4.26}$$

$$\mu_i^{(n+k)}=(-1)^{n+k}\frac{\widehat{IW}_{k,n+1}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)},\mu_i^{(0)})}{\widehat{IW}_{k,n}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})}, \tag{4.27}$$

$$\tau^{(n+k)}=\widehat{IW}_{k,n}(\chi_k^{(0)},\ldots,\chi_1^{(0)};\psi^{(0)},\xi^{(1)},\ldots,\xi^{(n-1)})\tau^{(0)}. \tag{4.28}$$

Here, $\xi^{(k)}$, $\chi_i^{(n)}$ and $\phi^{(n)}$ are given by Theorem 4.3.

Remark 4.1: The main characteristic of the τ-functions, $\phi^{(n+k)}$ and $\psi^{(n+k)}$, in the four chains mentioned above is that there are ''eigenfunctions'' and BA functions of $L^{(0)}$ in their Wronskians or the generalized Wronskians at the same time.

V. GENERATION OF THE AKNS HIERARCHY FROM THE "FREE" LAX OPERATOR $L^{(0)}=\partial$

In Refs. 10–12, Aratyn *et al.* have performed the following gauge transformation with the first choice,

$$T_D^{(1)}(\phi^{(0)})=\phi^{(0)}\circ\partial\circ(\phi^{(0)})^{-1}, \tag{5.1}$$

$$L^{(1)}=T_D^{(0)}(\phi^{(0)})\circ\partial\circ(T_D^{(0)}(\phi^{(0)}))^{-1}=\partial+\phi^{(0)}\cdot(\ln\phi^{(0)})_{xx}\circ\partial^{-1}\circ(\phi^{(0)})^{-1}, \tag{5.2}$$

where $\phi^{(0)}$ is an ''eigenfunction'' of $L^{(0)}=\partial$, i.e., it satisfies

$$\frac{\partial\phi^{(0)}}{\partial t_n}=(L^{(0)})_+^n\cdot\phi^{(0)}=\partial^n\cdot\phi^{(0)}. \tag{5.3}$$

They showed

Theorem 5.1: *(Refs. 10–12) For the successive k-step gauge transformations,*

$$L^{(0)}\xrightarrow{T_D^{(1)}(\phi^{(0)})}L^{(1)}\xrightarrow{T_D^{(2)}(\phi^{(1)})}L^{(2)}\xrightarrow{T_D^{(3)}(\phi^{(2)})}L^{(3)}\xrightarrow{T_D^{(4)}(\phi^{(3)})}\cdots\to\cdots, \tag{5.4}$$

starting with the initial "free" Lax operator $L^{(0)}=\partial$,

$$L^{(n)}=T_D^{(n)}(\phi^{(n-1)})\circ\partial\circ(T_D^{(n)}(\phi^{(n-1)}))^{-1}=\partial+\phi^{(n)}\circ\partial^{-1}\circ\psi^{(n)}, \tag{5.5}$$

where

$$\phi^{(n)}=\frac{W_{n+1}\left(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,\frac{\partial^{n-1}\phi^{(0)}}{\partial x^{n-1}},\frac{\partial^n\phi^{(0)}}{\partial x^n}\right)}{W_n\left(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,\frac{\partial^{n-1}\phi^{(0)}}{\partial x^{n-1}}\right)}, \tag{5.6}$$

$$\psi^{(n)}=(\phi^{(n-1)})^{-1}, \tag{5.7}$$

$$\tau^{(n)}=W_n\left(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,\frac{\partial^{n-1}\phi^{(0)}}{\partial x^{n-1}}\right),\quad \tau^{(0)}=1. \tag{5.8}$$

Proof: See Refs. 10–12. In fact, this result is the corollary of Theorem 4.1 in the case $\eta^{(i)}=\partial^i\phi^{(0)}/\partial x^i, i=1,2,\ldots,n$. □

This theorem indicates that one can construct the AKNS hierarchy from the ''free'' Lax operator $L^{(0)}=\partial$. And it is also suggested formula in the following.

Theorem 5.2: *Let* $L^{(0)}=\partial$*; for the chain of n-step gauge transformations with the operator of Type* **II**,

$$L^{(0)} \xrightarrow{T_I^{(1)}(\psi^{(0)})} L^{(1)} \xrightarrow{T_I^{(2)}(\psi^{(1)})} L^{(2)} \xrightarrow{T_I^{(3)}(\psi^{(2)})} L^{(3)} \xrightarrow{T_I^{(4)}(\psi^{(3)})} \cdots \to \cdots, \tag{5.9}$$

we obtain

$$L^{(n)} = T_D^{(n)}(\phi^{(n-1)}) \circ \partial \circ (T_D^{(n)}(\phi^{(n-1)}))^{-1} = \partial + \phi^{(n)} \circ \partial^{-1} \circ \psi^{(n)}, \tag{5.10}$$

where

$$\phi^{(n)} = (\psi^{(n-1)})^{-1}, \tag{5.11}$$

$$\psi^{(n)} = \frac{W_{n+1}\left(\psi^{(0)}, \psi_x^{(0)}, \psi_{xx}^{(0)}, \ldots, \frac{\partial^{n-1}\psi^{(0)}}{\partial x^{n-1}}, \frac{\partial^n \psi^{(0)}}{\partial x^n}\right)}{W_n\left(\psi^{(0)}, \psi_x^{(0)}, \psi_{xx}^{(0)}, \ldots, \frac{\partial^{n-1}\psi^{(0)}}{\partial x^{n-1}}\right)}, \tag{5.12}$$

$$\tau^{(n)} = W_n\left(\psi^{(0)}, \psi_x^{(0)}, \psi_{xx}^{(0)}, \ldots, \frac{\partial^{n-1}\psi^{(0)}}{\partial x^{n-1}}\right), \quad \tau^{(0)} = 1. \tag{5.13}$$

Here $\psi^{(0)}$ is the "adjoint eigenfunction" of $L^{(0)} = \partial$.

Proof: One states by noting that

$$L^{(0)} = \partial \equiv \partial + \phi^{(0)} \circ \partial^{-1} \circ \psi^{(0)}\big|_{\phi^{(0)}=0}.$$

So we can regard $\psi^{(0)}$ as the "adjoint eigenfunction" of $L^{(0)}$, i.e.,

$$\frac{\partial \psi^{(0)}}{\partial t_n} = -(L^{*(0)})_+^n \cdot \psi^{(0)}, \quad \psi_{t_n}^{(0)} = (-1)^{n+1}\partial^n \cdot \psi^{(0)}.$$

Using the gauge transformation with the first choice in Theorem 2.3 (or see Ref. 6), we have

$$T_I^{(1)}(\psi^{(0)}) = (\psi^{(0)})^{-1} \circ \partial^{-1} \circ \psi^{(0)},$$

$$L^{(1)} = T_I^{(1)}(\psi^{(0)}) \circ L^{(0)} \circ (T_I^{(1)}(\psi^{(0)}))^{-1} = T_I^{(1)}(\psi^{(0)}) \circ \partial \circ (T_I^{(1)}(\psi^{(0)}))^{-1} = \partial + \psi^{(1)} \circ \partial^{-1} \circ \psi^{(1)},$$

$$\phi^{(1)} = (\psi^{(0)})^{-1},$$

$$\psi^{(1)} = -T_D^{(1)}(\psi^{(0)}) \cdot (L^{*(0)}\psi^{(0)}) = \frac{W_2(\psi^{(0)}, \psi_x^{(0)})}{W_1(\psi^{(0)})}.$$

Then using the property of the Wronskian, and applying successively T_I with the first choice, this theorem is proven. □

The two chains of gauge transformations mentioned in above refer to single-channel (pure) case. There is no multichannel possibility in the present case (i.e., with the first choice), hence we only need to discuss the single-channel (mixed) case.

Theorem 5.3: *Let one chain of n-step gauge transformations start with $L^{(0)} = \partial$, the let p of them be of Type* **I**, *q of them of Type* **II**, *$W_0 = 1$.*

(A) If the first step is of Type **I**, *$\phi^{(0)} \neq 0$, $\psi^{(0)} = 0$, then*

$$\tau^{(n)} = W_{p-q}\left(\phi^{(0)}, \phi_x^{(0)}, \phi_{xx}^{(0)}, \ldots, \frac{\partial^{p-q}\phi^{(0)}}{\partial x^{p-q}}\right) \tag{5.14}$$

in which $p \geqslant q$.

(B) If the first step is of Type **II**, *$\psi^{(0)} \neq 0$, $\phi^{(0)} = 0$, then*

$$\tau^{(n)}=W_{q-p}\left(\psi^{(0)},\psi_x^{(0)},\psi_{xx}^{(0)},\ldots,\frac{\partial^{q-p}\psi^{(0)}}{\partial x^{q-p}}\right) \tag{5.15}$$

in which $q\geqslant p$.

Proof: There is an obvious identity

$$T_I^{(k+1)}(\psi^{(k+1)})\circ T_D^{(k)}(\phi^{(k)})=T_D^{(k+1)}(\phi^{(k+1)})\circ T_I^{(k)}(\psi^{(k)})=I,$$

which is similar to the equation (61) of Ref. 6. Using this identity and the Theorem 5.1 and Theorem 5.2, theorem is proved. □

Since the AKNS hierarchy can be produced from $L^{(0)}=\partial$ with the first choice, we would like to introduce an analogous procedure for the chain of gauge transformations with the second choice, i.e.,

$$L^{(0)}\xrightarrow{T_D^{(1)}(\chi_1^{(0)})}L^{(1)}\xrightarrow{T_D^{(2)}(\chi_2^{(1)})}L^{(2)}\xrightarrow{T_D^{(3)}(\chi_3^{(2)})}L^{(3)}\xrightarrow{T_D^{(4)}(\chi_4^{(3)})}\cdots\rightarrow\cdots,$$

$$L^{(0)}\xrightarrow{T_I^{(1)}(\mu_1^{(0)})}L^{(1)}\xrightarrow{T_I^{(2)}(\mu_2^{(1)})}L^{(2)}\xrightarrow{T_I^{(3)}(\mu_3^{(2)})}L^{(3)}\xrightarrow{T_I^{(4)}(\mu_4^{(3)})}\cdots\rightarrow\cdots.$$

Unfortunately, these two chains of gauge transformations cannot produce the AKNS hierarchy, because they keep $L^{(k)}=\partial$. However, the union of the two choices is very interesting. Each of the theorems given in the preceding section can supply an explicit approach to generate the AKNS hierarchy from "free" Lax operator $L^{(0)}=\partial$. To save space, we only discuss the gauge transformation chain (4.9) with $L^{(0)}=\partial=\partial+\phi^{(0)}\cdot\partial^{-1}\cdot\psi^{(0)}|_{\psi^{(0)}=0}$, which leads to the following theorem.

Theorem 5.4:

$$\chi_i^{(n)}=\frac{W_{n+1}(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)},\chi_i^{(0)})}{W_n(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}, \tag{5.16}$$

$$\mu_i^{(n)}=(-1)^n\frac{IW_{1,n}(\mu_i^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}{W_n(\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}, \tag{5.17}$$

$$\phi^{(n+k)}=\frac{IW_{k,n+1}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)},(\phi^{(0)})^{(n)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}, \tag{5.18}$$

$$\psi^{(n+k)}=(-1)^k\frac{W_{k+1}(\mu_1^{(n)},\ldots,\mu_k^{(n)},\psi^{(n)})}{W_k(\mu_1^{(n)},\ldots,\mu_k^{(n)})}, \tag{5.19}$$

$$\chi_i^{(n+k)}=\frac{IW_{k,n+1}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)},\chi_i^{(0)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}, \tag{5.20}$$

$$\mu_i^{(n+k)}=(-1)^n\frac{IW_{k+1,n}(\mu_i^{(0)},\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}{IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)})}, \tag{5.21}$$

$$\tau^{(n+k)}=IW_{k,n}(\mu_k^{(0)},\ldots,\mu_1^{(0)};\phi^{(0)},\phi_x^{(0)},\phi_{xx}^{(0)},\ldots,(\phi^{(0)})^{(n-1)}). \tag{5.22}$$

Here $\phi^{(0)}$ is the eigenfunction of $L^{(0)}=\partial$, hence it satisfies $\partial\phi^{(0)}/\partial t_n=(L^{(0)})_+^n\cdot\phi^{(0)}=\partial^n\cdot\phi^{(0)}$; and $\partial\mu_i^{(0)}/\partial t_n=-(L^{(0)*})_+^n\mu_i^{(0)}=(-1)^{n+1}\partial^n\cdot\mu_i^{(0)}$, $(L^{(0)})^*\cdot\mu_i^{(0)}=-\partial\mu_i^{(0)}=\lambda_i\mu_i^{(0)}$. $\psi^{(n)}$ and $\phi^{(n)}$ are given by Theorem 5.1.

Now we consider some concrete examples of Theorem 5.4 with $n=2,k=1$. Let $\lambda_i(i=1,2,\ldots,5)$ and η_1 be constants, $\theta_i=\lambda_i t_1+\lambda_i^2 t_2+\lambda_i^3 t_3$, $\hat{\theta}_1=-\eta_1 t_1-\eta_1^2 t_2-\eta_1^3 t_3$.

(1) Let

$$\phi^{(0)}=e^{\theta_1}+e^{\theta_2}+e^{\theta_3},\quad \psi^{(0)}=0,\quad \mu_1^{(0)}=e^{\hat{\theta}_1}.$$

Then Theorem 5.4 yields

$$\phi^{(2+1)}=\frac{e^{\theta_1+\theta_2+\theta_3}(\lambda_1-\lambda_2)^2(\lambda_1-\lambda_3)^2(\lambda_2-\lambda_3)^2}{e^{\theta_1+\theta_3}(-\eta_1+\lambda_2)(\lambda_1-\lambda_3)^2+e^{\theta_2+\theta_3}(-\eta_1+\lambda_1)(\lambda_2-\lambda_3)^2+e^{\theta_1+\theta_2}(-\eta_1+\lambda_3)(\lambda_1-\lambda_2)^2},\tag{5.23}$$

$$\psi^{(2+1)}=\frac{e^{\theta_3}(-\eta_1+\lambda_1)(-\eta_1+\lambda_2)+e^{\theta_2}(-\eta_1+\lambda_1)(-\eta_1+\lambda_3)+e^{\theta_1}(-\eta_1+\lambda_2)(-\eta_1+\lambda_3)}{e^{\theta_1+\theta_3}(-\eta_1+\lambda_2)(\lambda_1-\lambda_3)^2+e^{\theta_2+\theta_3}(-\eta_1+\lambda_1)(\lambda_2-\lambda_3)^2+e^{\theta_1+\theta_2}(-\eta_1+\lambda_3)(\lambda_1-\lambda_2)^2},\tag{5.24}$$

$$\tau^{(2+1)}=e^{\hat{\theta}_1}\frac{e^{\theta_1+\theta_3}(\eta_1-\lambda_2)(\lambda_1-\lambda_3)^2+e^{\theta_2+\theta_3}(\eta_1-\lambda_1)(\lambda_2-\lambda_3)^2+e^{\theta_1+\theta_2}(\eta_1-\lambda_3)(\lambda_1-\lambda_2)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_2)(\eta_1-\lambda_3)}.\tag{5.25}$$

$\phi^{(2+1)}$ and $\psi^{(2+1)}$ satisfy equations (1.4) and (1.5). Furthermore, a solution of the KP equation (1.10) is given by $u=\phi^{(2+1)}\psi^{(2+1)}$ or (1.11). In Figs. 1(a)–1(c), $-\phi^{(2+1)},\psi^{(2+1)},u$, respectively, are plotted.

(2) Let

$$\phi^{(0)}=e^{\theta_1}+e^{\theta_2+\theta_3}+e^{\theta_4},\quad \psi^{(0)}=0,\quad \mu_1^{(0)}=e^{\hat{\theta}_1}.$$

With the help of the *MATHEMATICA*, we got

$$\begin{aligned}\phi^{(2+1)}=&\Bigg\{(e^{\theta_1}\lambda_1^3+e^{\theta_2}\lambda_2^3+e^{\theta_3}\lambda_3^3+e^{\theta_4}\lambda_4^3)\Bigg[(e^{\theta_1}\lambda_1+e^{\theta_2}\lambda_2+e^{\theta_3}\lambda_3+e^{\theta_4}\lambda_4)\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}\\&+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\Bigg)-(e^{\theta_1}+e^{\theta_2}+e^{\theta_3}+e^{\theta_4})\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}\lambda_1\\&+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}\lambda_2+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}\lambda_3+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\lambda_4\Bigg)\Bigg]-(e^{\theta_1}\lambda_1^2+e^{\theta_2}\lambda_2^2+e^{\theta_3}\lambda_3^2+e^{\theta_4}\lambda_4^2)\\&\times\Bigg[(e^{\theta_1}\lambda_1^2+e^{\theta_2}\lambda_2^2+e^{\theta_3}\lambda_3^2+e^{\theta_4}\lambda_4^2)\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\Bigg)\\&-(e^{\theta_1}+e^{\theta_2}+e^{\theta_3}+e^{\theta_4})\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}\lambda_1^2+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}\lambda_2^2+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}\lambda_3^2+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\lambda_4^2\Bigg)\Bigg]\\&+(e^{\theta_1}\lambda_1+e^{\theta_2}\lambda_2+e^{\theta_3}\lambda_3+e^{\theta_4}\lambda_4)\Bigg[(e^{\theta_1}\lambda_1^2+e^{\theta_2}\lambda_2^2+e^{\theta_3}\lambda_3^2+e^{\theta_4}\lambda_4^2)\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}\lambda_1\\&+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}\lambda_2+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}\lambda_3+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\lambda_4\Bigg)-(e^{\theta_1}\lambda_1+e^{\theta_2}\lambda_2+e^{\theta_3}\lambda_3+e^{\theta_4}\lambda_4)\\&\times\Bigg(\frac{e^{\theta_1}}{-\eta_1+\lambda_1}\lambda_1^2+\frac{e^{\theta_2}}{-\eta_1+\lambda_2}\lambda_2^2+\frac{e^{\theta_3}}{-\eta_1+\lambda_3}\lambda_3^2+\frac{e^{\theta_4}}{-\eta_1+\lambda_4}\lambda_4^2\Bigg)\Bigg]\Bigg\}\Bigg\{\frac{e^{\theta_1+\theta_2}(\lambda_1-\lambda_2)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_2)}\end{aligned}$$

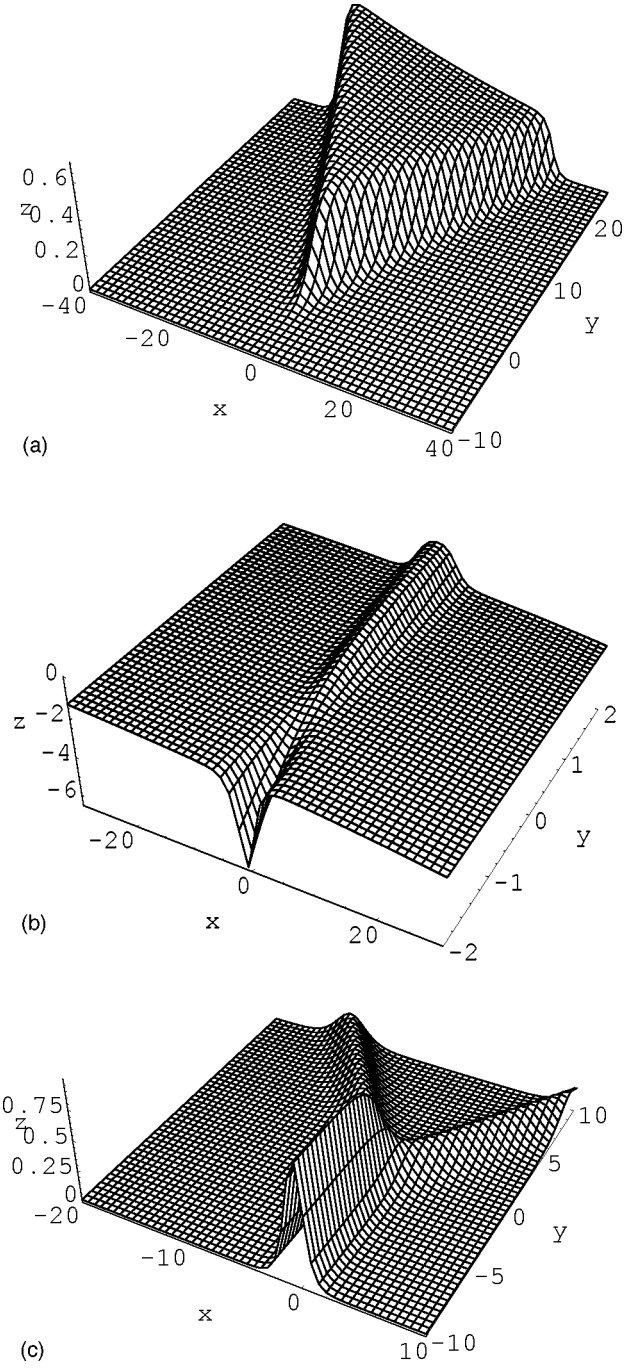

FIG. 1. Parameters in (a)–(c) are $t=0$, $\lambda_1=-1$, $\lambda_2=-0.015$, $\lambda_3=1$, $\eta_1=2$. (a) Minus times solution $\phi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (b) solution $\psi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (c) solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10).

$$+\frac{e^{\theta_1+\theta_3}(\lambda_1-\lambda_3)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_3)}+\frac{e^{\theta_2+\theta_3}(\lambda_2-\lambda_3)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_3)}+\frac{e^{\theta_1+\theta_4}(\lambda_1-\lambda_4)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_4)}+\frac{e^{\theta_2+\theta_4}(\lambda_2-\lambda_4)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_4)}$$
$$+\frac{e^{\theta_3+\theta_4}(\lambda_3-\lambda_4)^2}{(\eta_1-\lambda_3)(\eta_1-\lambda_4)}\Bigg\}, \tag{5.26}$$

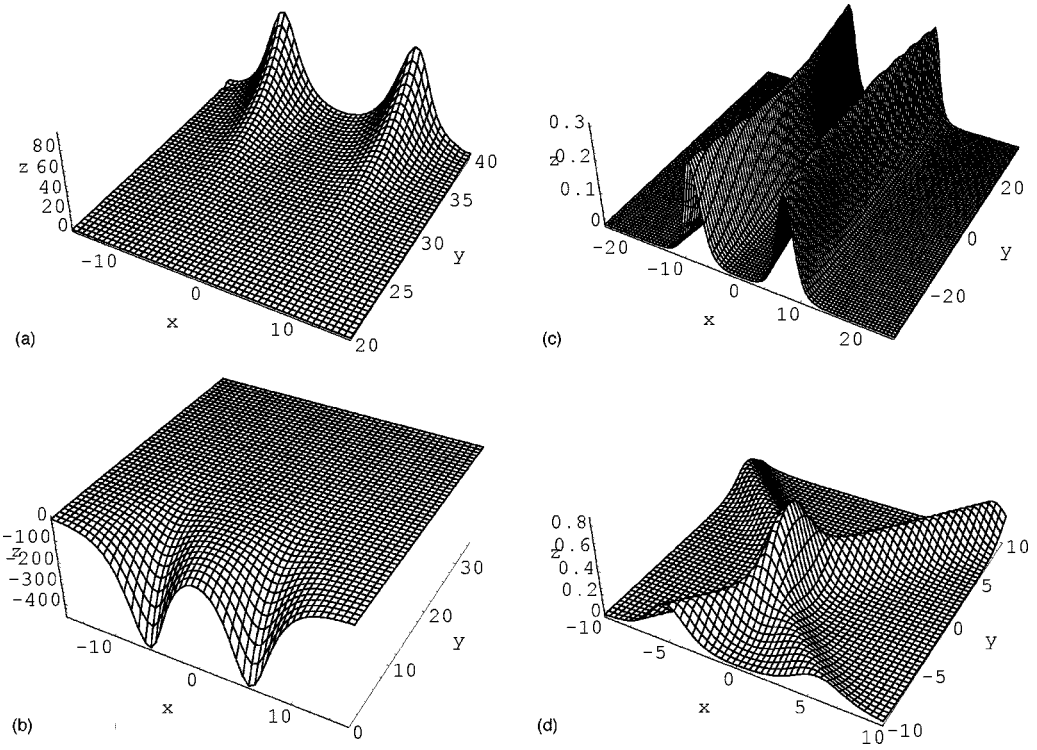

FIG. 2. Parameters in (a)–(c) are $t=0$, $\lambda_1=-0.5$, $\lambda_2=0.5$, $\lambda_3=-0.6$, $\lambda_4=0.6$, $\eta_1=100$. (a) Minus times solution $\phi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (b) solution $\psi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (c) solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10); (d) solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10) with parameters $t=0$, $\lambda_1=-1$, $\lambda_2=0.2$, $\lambda_3=1$, $\lambda_4=0.05$, $\eta_1=2$.

$$
\begin{aligned}
\psi^{(2+1)}=\{&e^{\theta_1+2\theta_4}(-\eta_1+\lambda_1)(\eta_1-\lambda_2)(\eta_1-\lambda_3)(\lambda_1-\lambda_4)^2+e^{\theta_2+2\theta_4}(\eta_1-\lambda_1)(-\eta_1+\lambda_2)(\eta_1\\
&-\lambda_3)(\lambda_2-\lambda_4)^2+e^{\theta_3+2\theta_4}(\eta_1-\lambda_1)(\eta_1-\lambda_2)(-\eta_1+\lambda_3)(\lambda_3-\lambda_4)^2+e^{\theta_1+2\theta_3}(-\eta_1\\
&+\lambda_1)(\eta_1-\lambda_2)(\eta_1-\lambda_4)(\lambda_1-\lambda_3)^2+e^{\theta_2+2\theta_3}(\eta_1-\lambda_1)(-\eta_1+\lambda_2)(\eta_1-\lambda_4)(\lambda_2-\lambda_3)^2\\
&+e^{\theta_4+2\theta_3}(\eta_1-\lambda_1)(\eta_1-\lambda_2)(-\eta_1+\lambda_4)(\lambda_3-\lambda_4)^2+e^{\theta_1+2\theta_2}(-\eta_1+\lambda_1)(\eta_1-\lambda_3)(\eta_1\\
&-\lambda_4)(\lambda_1-\lambda_2)^2+e^{\theta_3+2\theta_2}(\eta_1-\lambda_1)(-\eta_1+\lambda_3)(\eta_1-\lambda_4)(\lambda_3-\lambda_2)^2+e^{\theta_4+2\theta_2}(\eta_1-\lambda_1)\\
&\times(\eta_1-\lambda_3)(-\eta_1+\lambda_4)(\lambda_4-\lambda_2)^2+e^{\theta_2+2\theta_1}(-\eta_1+\lambda_2)(\eta_1-\lambda_3)(\eta_1-\lambda_4)(\lambda_1-\lambda_2)^2\\
&+e^{\theta_3+2\theta_1}(\eta_1-\lambda_2)(-\eta_1+\lambda_3)(\eta_1-\lambda_4)(\lambda_1-\lambda_3)^2+e^{\theta_4+2\theta_1}(\eta_1-\lambda_2)(\eta_1-\lambda_3)(-\eta_1\\
&+\lambda_4)(\lambda_1-\lambda_4)^2-e^{\theta_1+\theta_2+\theta_3}(\eta_1-\lambda_4)[\lambda_2(\lambda_2-\lambda_3)^2\lambda_3+\lambda_1^3(\lambda_2+\lambda_3)-2\lambda_1^2(\lambda_2^2+\lambda_3^2)\\
&+\lambda_1(\lambda_2^3+\lambda_3^3)+2\eta_1^2(\lambda_1^2+\lambda_2^2-\lambda_2\lambda_3+\lambda_3^2-\lambda_1(\lambda_2+\lambda_3))+\eta_1(-2\lambda_1^3-2\lambda_2^3+\lambda_2^2\lambda_3\\
&+\lambda_2\lambda_3^2-2\lambda_3^3+\lambda_1^2(\lambda_2+\lambda_3)+\lambda_1(\lambda_2^2+\lambda_3^2))]-e^{\theta_1+\theta_2+\theta_4}(\eta_1-\lambda_3)[\lambda_2(\lambda_2-\lambda_4)^2\lambda_4\\
&+\lambda_1^3(\lambda_2+\lambda_4)-2\lambda_1^2(\lambda_2^2+\lambda_4^2)+\lambda_1(\lambda_2^3+\lambda_4^3)+2\eta_1^2(\lambda_1^2+\lambda_2^2-\lambda_2\lambda_4+\lambda_4^2-\lambda_1(\lambda_2+\lambda_4))\\
&+\eta_1(-2\lambda_1^3-2\lambda_2^3+\lambda_2^2\lambda_4+\lambda_2\lambda_4^2-2\lambda_4^3+\lambda_1^2(\lambda_2+\lambda_4)+\lambda_1(\lambda_2^2+\lambda_4^2))]-e^{\theta_1+\theta_3+\theta_4}(\eta_1\\
&-\lambda_2)[\lambda_3(\lambda_3-\lambda_4)^2\lambda_4+\lambda_1^3(\lambda_3+\lambda_4)-2\lambda_1^2(\lambda_3^2+\lambda_4^2)+\lambda_1(\lambda_3^3+\lambda_4^3)+2\eta_1^2(\lambda_1^2+\lambda_3^2\\
&-\lambda_3\lambda_4+\lambda_4^2-\lambda_1(\lambda_3+\lambda_4))+\eta_1(-2\lambda_1^3-2\lambda_3^3+\lambda_3^2\lambda_4+\lambda_3\lambda_4^2-2\lambda_4^3+\lambda_1^2(\lambda_3+\lambda_4)\\
&+\lambda_1(\lambda_3^2+\lambda_4^2))]-e^{\theta_2+\theta_3+\theta_4}(\eta_1-\lambda_1)[\lambda_3(\lambda_3-\lambda_4)^2\lambda_4+\lambda_2^3(\lambda_3+\lambda_4)-2\lambda_2^2(\lambda_3^2+\lambda_4^2)
\end{aligned}
$$

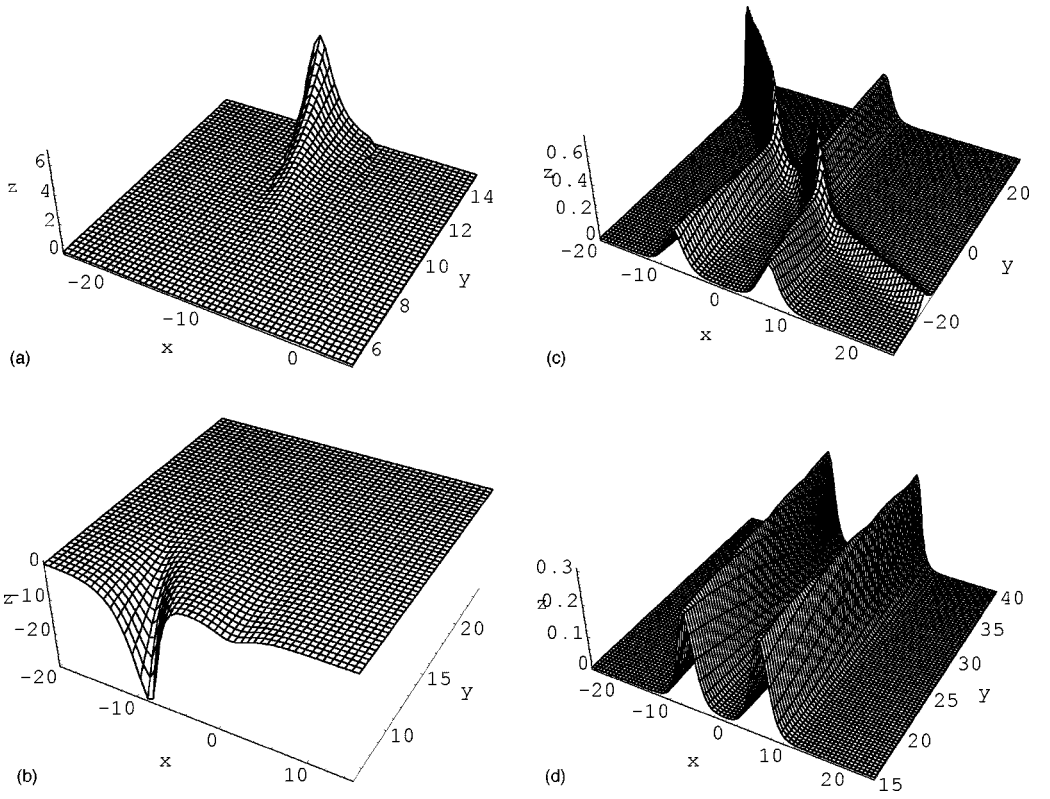

FIG. 3. Parameters in (a)–(c) are $t=0$, $\lambda_1=-0.5$, $\lambda_2=0.5$, $\lambda_3=-0.6$, $\lambda_4=0.6$, $\lambda_5=1.2$, $\eta_1=100$. (a) Minus times solution $\phi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (b) solution $\psi^{(2+1)}$ to the first two flows (1.4) and (1.5) of AKNS hierarchy; (c) solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10); (d) solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10) with parameters $t=0$, $\lambda_1=-0.5$, $\lambda_2=0.5$, $\lambda_3=-0.6$, $\lambda_4=0.6$, $\lambda_5=0$, $\eta_1=100$.

$$
\begin{aligned}
&+\lambda_2(\lambda_3^3+\lambda_4^3)+2\eta_1^2(\lambda_2^2+\lambda_3^2-\lambda_3\lambda_4+\lambda_4^2-\lambda_2(\lambda_3+\lambda_4))+\eta_1(-2\lambda_2^3-2\lambda_3^3+\lambda_3^2\lambda_4 wz\\
&+\lambda_3\lambda_4^2-2\lambda_4^3+\lambda_2^2(\lambda_3+\lambda_4)+\lambda_2(\lambda_3^2+\lambda_4^2))]\}\Big/\Big\{(\eta_1-\lambda_1)(\eta_1-\lambda_2)(\eta_1-\lambda_3)(\eta_1\\
&-\lambda_4)(e^{\theta_1+\theta_2}(\lambda_1-\lambda_2)^2+e^{\theta_1+\theta_3}(\lambda_1-\lambda_3)^2+e^{\theta_1+\theta_4}(\lambda_1-\lambda_4)^2+e^{\theta_2+\theta_3}(\lambda_2-\lambda_3)^2\\
&+e^{\theta_2+\theta_4}(\lambda_2-\lambda_4)^2+e^{\theta_3+\theta_4}(\lambda_3-\lambda_4)^2)\Big(\frac{e^{\theta_1+\theta_2}(\lambda_1-\lambda_2)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_2)}+\frac{e^{\theta_1+\theta_3}(\lambda_1-\lambda_3)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_3)}\\
&+\frac{e^{\theta_2+\theta_3}(\lambda_2-\lambda_3)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_3)}+\frac{e^{\theta_1+\theta_4}(\lambda_1-\lambda_4)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_4)}+\frac{e^{\theta_2+\theta_4}(\lambda_2-\lambda_4)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_4)}\\
&+\frac{e^{\theta_3+\theta_4}(\lambda_3-\lambda_4)^2}{(\eta_1-\lambda_3)(\eta_1-\lambda_4)}\Big)\Big\},
\end{aligned}
\tag{5.27}
$$

$$
\begin{aligned}
\tau^{(2+1)}=e^{\hat{\theta}_1}\Big[&\frac{e^{\theta_1+\theta_2}(\lambda_1-\lambda_2)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_2)}+\frac{e^{\theta_1+\theta_3}(\lambda_1-\lambda_3)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_3)}+\frac{e^{\theta_2+\theta_3}(\lambda_2-\lambda_3)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_3)}\\
&+\frac{e^{\theta_1+\theta_4}(\lambda_1-\lambda_4)^2}{(\eta_1-\lambda_1)(\eta_1-\lambda_4)}+\frac{e^{\theta_2+\theta_4}(\lambda_2-\lambda_4)^2}{(\eta_1-\lambda_2)(\eta_1-\lambda_4)}+\frac{e^{\theta_3+\theta_4}(\lambda_3-\lambda_4)^2}{(\eta_1-\lambda_3)(\eta_1-\lambda_4)}\Big].
\end{aligned}
\tag{5.28}
$$

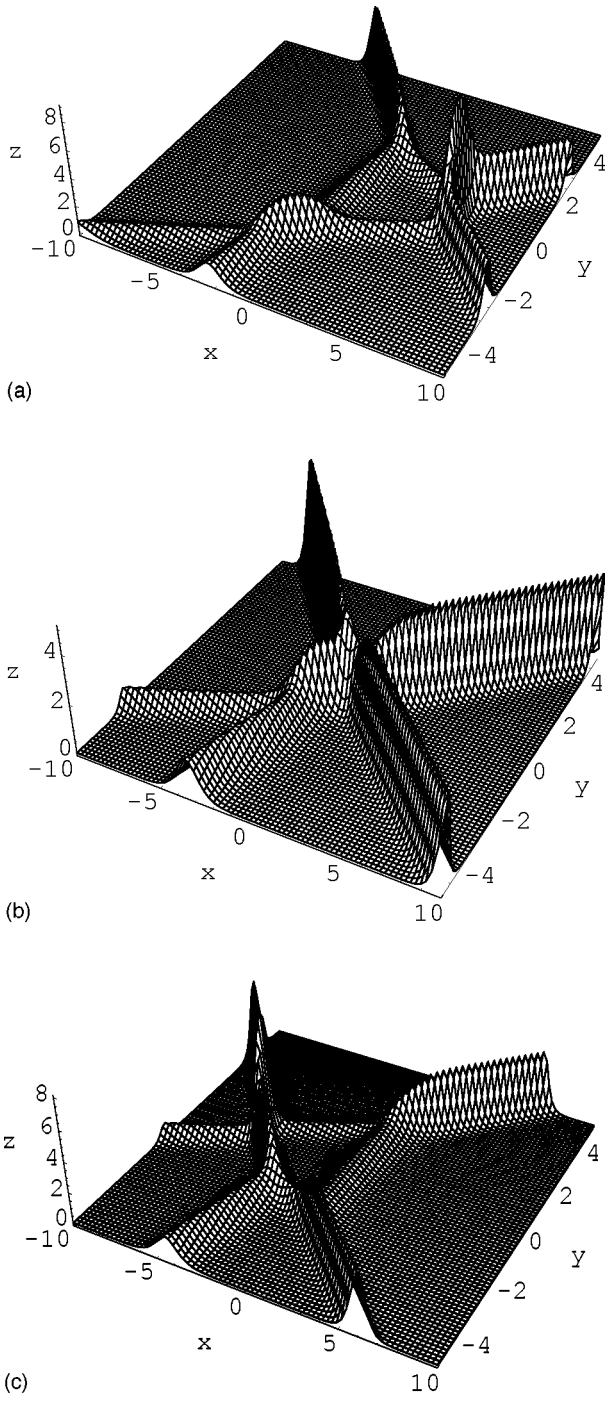

FIG. 4. Solution $u=\phi^{(2+1)}\psi^{(2+1)}$ to the KP equation (1.10) with parameters $\lambda_1=-1$, $\lambda_2=-1.5$, $\lambda_3=1$, $\lambda_4=3$, $\lambda_5=-3$, $\eta_1=-4$. (a) $t=-0.6$; (b) $t=0$; (c) $t=0.6$.

The graphs of $-\phi^{(2+1)},\psi^{(2+1)},u$ are plotted in Figs. 2(a)–2(c) for this case. Additionally, we also give in Fig. 2(d) another graph of u with a different parameter.

(3) Take

$$\phi^{(0)}=e^{\theta_1}+e^{\theta_2}+^{\theta_3}+e^{\theta_4}+e^{\theta_5},\quad \psi^{(0)}=0,\quad \mu_1^{(0)}=e^{\hat{\theta}_1}.$$

We give the graphs [Figs. 3(a)–3(c)] of $-\phi^{(2+1)}, \psi^{(2+1)}, u$, and in Fig. 3(d) the graph of u for a different parameter. Specifically, in order to explore approximately the evolution of the solution of KP equation, we also display in Figs. 4(a)–4(c) u at $t_3 = -0.6, 0, 0.6$.

VI. CONCLUSION AND DISCUSSION

In this paper we point out that there exist two choices that keep the form of the Lax operator when we perform gauge transformations for the AKNS hierarchy, which naturally leads to two classes of GFGT—eigenfunction and BA function of $L^{(0)}$. The second choice automatically implies that the GFGT χ must come from outside of $L^{(0)}$, in contrast to the first choice.[6,10–12] On the basis of these facts, we obtain Theorem 2.2 and Theorem 2.3 about the two choices of Type **I** and Type **II**, respectively. We study systematically the successive application of gauge transformation with the second choice for the AKNS hierarchy. The union of the two choices is also discussed, which results in a new τ-function. Finally, starting with the ''free'' Lax operator $L^{(0)} = \partial$, the AKNS hierarchy has been constructed via gauge transformation, and its several τ-functions are obtained. Our results also show that the generalized Wronskian of the τ function of the AKNS can not be of the binary type if $k > 1$, the latter is defined by Ref. 6 Obviously, $\tau^{(n+k)}$ is still of binary type when $k = 1$.

Finally we would like to re-emphasize that the functions in the elements of the Wronskian of the τ-functions presented in this paper (with the second choice) are different from those in the previous literature.[6,10–12] So the final τ-function are as well essentially different. The figures in Fig. 1 are similar to the results of Ref. 23, which are obtained from the Wronskian solution of the KP hierarchy. The relation between the gauge transformation given here and the known Darboux transformation[24] for the AKNS hierarchy is an interesting question, the discussion of which is left for future publications. Moreover, it will be interesting to consider the analogue of our results for the matrix constrained KP hierarchy, see Ref. 9. For chains of gauge transformations including two choices, there also exist other more complicated cases that shall have to be discussed. Finally, we also would like to generalize our results to the supersymmetric KP and cKP hierarchy.[25–27]

ACKNOWLEDGMENTS

One of the authors (Jingsong He) would like to thank sincerely Professor F. Calogero for his encouragement and friendly help to improve the English presentation of this paper. This work was supported by the National Natural Science Foundation of China (19725104,10101025), the Chinese National Basic Research Project(973)—''Nonlinear Science.''

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Tri-Hamiltonian formulation for certain integrable lattice equations

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(Received 5 May 2003; accepted 8 May 2003)

A systematic investigation of integrable differential–difference equations with two independent variables admitting multi-Hamiltonian structure is presented. Considering the Volterra (VL), Toda (TL), Relativistic Toda (RT), Belov–Chaltikian (BC) and Blaszak–Marciniak both three (BM3) and four (BM4) coupled lattice equations it is shown that they admit a sequence of operators out of which only three are Hamiltonian ones and so they are tri-Hamiltonian systems only. It is observed that the constructed third operator for VL and BC lattice equations is Hamiltonian only if the field variable is periodic with even period. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1601300]

I. INTRODUCTION

The study of discrete nonlinear systems governed by both ordinary and partial differential–difference and pure difference equations including lattice equations has aroused increasing interest in the last few years particularly from the point of view of complete integrability. It is well known that the completely integrable nonlinear partial differential equations (PDEs) admitting solitons possess a variety of mathematical structures such as Lax representation, Painlevé property, a sequence of generalized symmetries and conservation laws, master symmetries, multi-Hamiltonians, etc.[1–11]

The discovery of solitons started with an investigation of the solution of nonlinear PDEs and the soliton solution could be explained by the existence of conservation laws. It is known that every conservation law of a PDE comes from a corresponding symmetry property. This basic principle constitutes the first fundamental result in the study of classical or quantum mechanical systems with prescribed groups of symmetries. In a classic work, Emmy Noether has devised a procedure to derive conservation laws and explicitly shown that there exists a one to one correspondence between symmetry groups and conservation laws for the Euler Lagrange equations. This resulted in the search for hidden symmetries called generalized symmetries, which are groups whose infinitesimal generators depend not only on the independent and dependent variables of the PDEs but also on the derivatives of the dependent variables.

Considering nonlinear evolution equations with $(1+1)$ dimensions, Olver[12] has shown remarkably that, how a sequence of generalized symmetries can be derived recursively through an operator known as recursion operator, if one nontrivial generalized symmetry is known. In late 1980s Shabat[13] and his school using the basic principles have classified a complete list of nonlinear evolution equations with $(1+1)$ dimension demanding that under what conditions the given equation admits a sequence of generalized symmetries and conservation laws. The possession of a sequence of generalized and conservation laws is characterizing property of integrable nonlinear PDEs.[3] Also the existence of generalized symmetries often helps to derive other integrability properties: recursion operator, hereditary operator, bi-Hamiltonian formulation, etc., of nonlinear PDEs. This fact has been verified for a large number of nonlinear evolution equations with $(1+1)$ and $(2+1)$ dimensions possessing solitons by different researchers during the past few decades. Recent development in discrete nonlinear systems reveals that the above-mentioned results appear to hold for nonlinear PDDEs with two independent variables ($t \in \mathbb{R}$, $n \in \mathbb{Z}$) as well.[14–22] Given a PDDE with two independent variables we have shown that how to construct (i)

a sequence of generalized symmetries and conserved densities[17] and (ii) a factorizable recursion operator using its generalized symmetries.[21] As illustrations, in Ref. 21 we have considered BC, BM3, and RT lattice equations and derived factorizable recursion operators using their generalized symmetries and shown explicitly that they are bi-Hamiltonian systems. It is known that VL, TL, and BM4 lattice equations are bi-Hamiltonian systems.[18,20] In this paper, we wish to investigate whether RT, VL, TL, BC, BM3, and BM4 lattice equations, respectively, governed by

$$v_{nt}=v_n(u_{n-1}-u_n), \quad u_{nt}=u_n(u_{n-1}-u_{n+1}+v_n-v_{n+1}), \tag{1}$$

$$u_{nt}=u_n(u_{n+1}-u_{n-1}), \tag{2}$$

$$u_{nt}=v_{n+1}-v_n, \quad v_{nt}=v_n(u_n-u_{n-1}), \tag{3}$$

$$u_{nt}=u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n, \quad v_{nt}=v_n(u_{n+2}-u_{n-1}), \tag{4}$$

$$u_{nt}=w_{n+1}-w_{n-1}, \quad v_{nt}=u_{n-1}w_{n-1}-u_nw_n, \quad w_{nt}=w_n(v_n-v_{n+1}), \tag{5}$$

$$u_{nt}=u_n(v_n-v_{n-1}), \quad v_{nt}=w_nu_{n+1}-w_{n-1}u_n, \quad w_{nt}=q_nu_{n+2}-u_nq_{n-1}, \quad q_{nt}=u_{n+3}-u_n, \tag{6}$$

where

$$u_{nt}=\frac{du_n}{dt}, \quad v_{nt}=\frac{dv_n}{dt}, \quad w_{nt}=\frac{dw_n}{dt}, \quad q_{nt}=\frac{dq_n}{dt},$$

$$u_n=u(n,t), \quad v_n=v(n,t), \quad w_n=w(n,t), \quad q_n=q(n,t),$$

t is a continuous variable and n is a discrete variable, admit multi-Hamiltonian structures or not and show explicitly that they are tri-Hamiltonian systems only.

The plan of the article is as follows: In Sec. II, we briefly outline the basic notations and definitions required for this paper. In Sec. III, we explain how to construct a sequence of operators $\{H_3,H_4,\ldots\}$ for an integrable nonlinear PDDE if it admits two distinct and invertible Hamiltonian operators H_1 and H_2. Also for each of the above lattice Eqs. (1)–(6) we construct a sequence of operators and show that only three of them are Hamiltonian ones. In Sec. IV, we give brief details of our results.

II. PRELIMINARIES AND BASIC RESULTS

We recall the following notations and definitions which are required for further discussion. Consider, a first order PDDE with two independent variables (one-continuous, one-discrete) of the form

$$\frac{\partial \mathbf{U}_n}{\partial t}=\mathbf{U}_{nt}=\mathbf{F}(\ldots,\mathbf{U}_{n-1},\mathbf{U}_n,\mathbf{U}_{n+1},\ldots), \tag{7}$$

where $\mathbf{U}_n=\mathbf{U}(n,t)$ and $\mathbf{F}(\cdots)$ are vector quantities with same number of components, say m. The vector function $\mathbf{F}$ is assumed to be a polynomial in the dependent variable and their shifts. There is no restriction on the level of shifts or the degree of nonlinearity. Define the shift operators E and E^{-1} by

$$E\mathbf{U}_n=\mathbf{U}_{n+1}, \quad E^{-1}\mathbf{U}_n=\mathbf{U}_{n-1}.$$

Let Δ and Δ^+ being the difference operators are defined by

$$\Delta\mathbf{U}_n=(E-1)\mathbf{U}_n, \quad \Delta^+\mathbf{U}_n=(E^{-1}-1)\mathbf{U}_n.$$

We then define the linear operator $(E-E^{-1})^{-1}=(\Delta-\Delta^{+})^{-1}$, $(E-1)^{-1}=\Delta^{-1}$, and $(E^{-1}-1)^{-1}=(\Delta^{+})^{-1}$ by

$$(\Delta-\Delta^{+})^{-1}\mathbf{U}_n=\frac{1}{2}\left[\sum_{k=-\infty}^{-1}\mathbf{U}_{n+1+2k}-\sum_{k=1}^{\infty}\mathbf{U}_{n-1+2k}\right],$$

$$\Delta^{-1}\mathbf{U}_n=\frac{1}{2}\left[\sum_{k=-\infty}^{-1}[\mathbf{U}_{n+1+2k}+\mathbf{U}_{n+2k}]-\sum_{k=1}^{\infty}[\mathbf{U}_{n-1+2k}+\mathbf{U}_{n-2+2k}]\right],$$

$$(\Delta^{+})^{-1}\mathbf{U}_n=-\frac{1}{2}\left[\sum_{k=-\infty}^{-1}[\mathbf{U}_{n+2+2k}+\mathbf{U}_{n+1+2k}]-\sum_{k=1}^{\infty}[\mathbf{U}_{n+2k}+\mathbf{U}_{n-1+2k}]\right].$$

Note that $(\Delta-\Delta^{+})^{-1}((\Delta-\Delta^{+})^{-1})^{-1}=((\Delta-\Delta^{+})^{-1})^{-1}(\Delta-\Delta^{+})^{-1}=1$. Let $H:\mathcal{L}^q\to\mathcal{L}^q$ be a linear operator and V_H be a formal evolutionary vector field with characteristic is the q-tuple,

$$(H\theta)_\alpha=\sum_{\beta=1}^{q}H_{\alpha\beta}\theta^{\beta}$$

of vertical univector. Then the prolongation of the vector field is given by

$$PrV_{H\theta}=\sum_{\alpha,J}E^{J}\left(\sum_{\beta}H_{\alpha\beta}\theta^{\beta}\right)\frac{\partial}{\partial E^{J}\mathbf{U}^{\alpha}}.$$

Definition 2.1: A linear operator H_1 of Eq. (7) is said to be a Hamiltonian operator if it is skew symmetric and satisfies Jacobi identity.[4]

Definition 2.2: Equation (7) is said to be a bi-Hamiltonian and tri-Hamiltonian system, if it can be written as

$$\mathbf{U}_{nt}=H_2\frac{\delta\mathcal{H}_0}{\delta\mathbf{U}_n}=H_1\frac{\delta\mathcal{H}_1}{\delta\mathbf{U}_n},\tag{8a}$$

and

$$\mathbf{U}_{nt}=H_3\frac{\delta\mathcal{H}_0}{\delta\mathbf{U}_n}=H_2\frac{\delta\mathcal{H}_1}{\delta\mathbf{U}_n}=H_1\frac{\delta\mathcal{H}_2}{\delta\mathbf{U}_n},\tag{8b}$$

where H_1, H_2, and H_3 are Hamiltonian operators while $\mathcal{H}_0[\mathbf{U}_n]$, $\mathcal{H}_1[\mathbf{U}_n]$, and $\mathcal{H}_2[\mathbf{U}_n]$ are appropriate Hamiltonian functionals.

Definition 2.3: An operator valued function $\mathcal{R}$ is said to be a recursion operator of Eq. (7) if it satisfies

$$\tilde{G}(n)=\mathcal{R}G(n),\tag{9}$$

where $\mathbf{G}(n)=(G_1(n),G_2(n),\ldots,G_m(n))$ and $\tilde{\mathbf{G}}(n)=(\tilde{G}_1(n),\tilde{G}_2(n),\ldots,\tilde{G}_m(n))$ are generalized symmetries of Eq. (7). In other words, $\mathcal{R}$ maps symmetries to new symmetries.

A. Construction of the second operator H_2

Let us assume that the given PDDE (7) can be written as

$$\mathbf{U}_{nt}=H_1\frac{\delta\mathcal{H}_0}{\delta\mathbf{U}_n},\tag{10}$$

where H_1 is an $(m\times m)$ invertible matrix Hamiltonian operator which can be expressed in terms of the difference operators of the dependent variables while $\mathcal{H}_0$ is the associated $(1\times m)$ matrix Hamiltonian functional. We further assume that the entries $(H_{ij}^{(1)})$, $(\mathcal{H}_{1j}^{(0)})$, $(\mathcal{H}_{1j}^{(1)})$ of the Hamiltonian operator H_1, the Hamiltonian functionals $\mathcal{H}_0$ and $\mathcal{H}_1$, respectively, having ranks p_{ij}, r_{1j}, and s_{1j}, $i,j=1,2,\ldots,m$ which may be integers or rational numbers.

The second operator H_2, if exists, for Eq. (7) satisfying the relation

$$H_2\frac{\delta\mathcal{H}_0}{\delta\mathbf{U}_n}=H_1\frac{\delta\mathcal{H}_1}{\delta\mathbf{U}_n} \tag{11}$$

can be constructed in the following way. Let H_2 be a $(m\times m)$ invertible matrix operator of the form

$$H_2=\begin{bmatrix} H_{11}^{(2)} & H_{12}^{(2)} & \ldots & H_{1\mathrm{m}}^{(2)} \\ H_{21}^{(2)} & H_{22}^{(2)} & \ldots & H_{2\mathrm{m}}^{(2)} \\ \vdots & & \vdots & \\ H_{\mathrm{m}1}^{(2)} & H_{\mathrm{m}2}^{(2)} & \ldots & H_{\mathrm{mm}}^{(2)} \end{bmatrix}.$$

Then the rank of the entries $(H_{ij}^{(2)})$ of H_2 must satisfy the following relations:

$$\begin{aligned} &\mathrm{rank}\ \ H_{11}^{(1)}+\mathrm{rank}\frac{\delta\mathcal{H}_1}{\delta U_1}+\cdots+\mathrm{rank}\ \ H_{1\mathrm{m}}^{(1)}+\mathrm{rank}\frac{\delta\mathcal{H}_1}{\delta U_m} \\ &\quad=\mathrm{rank}\ \ H_{11}^{(2)}+\mathrm{rank}\frac{\delta\mathcal{H}_0}{\delta U_1}+\cdots+\mathrm{rank}\ \ H_{1\mathrm{m}}^{(2)}+\mathrm{rank}\frac{\delta\mathcal{H}_0}{\delta U_m}, \\ &\vdots \\ &\mathrm{rank}\ \ H_{\mathrm{m}1}^{(1)}+\mathrm{rank}\frac{\delta\mathcal{H}_1}{\delta U_1}+\cdots+\mathrm{rank}\ \ H_{\mathrm{mm}}^{(1)}+\mathrm{rank}\frac{\delta\mathcal{H}_1}{\delta U_m} \\ &\quad=\mathrm{rank}\ \ H_{\mathrm{m}1}^{(2)}+\mathrm{rank}\frac{\delta\mathcal{H}_0}{\delta U_1}+\cdots+\mathrm{rank}\ \ H_{\mathrm{mm}}^{(2)}+\mathrm{rank}\frac{\delta\mathcal{H}_0}{\delta U_m}. \end{aligned}$$

Accordingly, we choose the entries $(H_{ij}^{(2)})$ of the matrix operator H_2 written in terms of the difference and inverse difference operators of the dependent variables and their inverse. Substituting the operator H_2 in Eq. (11) and then solving yields the explicit form of the operator H_2 with the required ranks.

If the constructed operator H_2 for Eq. (7) is also a Hamiltonian operator, then the recursion operator $\mathcal{R}$ usually can be written as

$$\mathcal{R}=H_2H_1^{-1}.$$

B. Application

We consider the VL lattice equation (2) which can be written as

$$u_{nt}=H_1\frac{\delta\mathcal{H}_1}{\delta u_n}=u_n(E-E^{-1})u_n, \tag{12}$$

where the Hamiltonian operator $H_1=u_n(E-E^{-1})u_n$, while the Hamiltonian functional $\mathcal{H}_1$ takes the form $\mathcal{H}_1=\Sigma_n u_n$. Obviously the rank of the right-hand side of Eq. (12) is 2. We know that the

Hamiltonian functional of VL lattice Eq. (2) is $\mathcal{H}_0=\Sigma_n \log u_n$ and so rank of $\delta\mathcal{H}_0/\delta u_n=-1$. Then the left-hand side of Eq. (11) demands that the rank of H_2 must be equal to 3 and so we consider H_2 having the form[21]

$$H_2=au_n^2Eu_n+bu_nEu_n^2+cu_nEu_nEu_n+a_1u_n^2E^{-1}u_n+b_1u_nE^{-1}u_n^2+c_1u_nE^{-1}u_nE^{-1}u_n+\mathrm{d}_1u_n^3,$$

where a, b, c, a_1, b_1, c_1, and d_1 are arbitrary constants to be determined. Substituting the Hamiltonian operator H_1, Hamiltonian functionals $\mathcal{H}_0$ and $\mathcal{H}_1$ along with the operator H_2 in Eq. (11), we find that the consistency condition holds only for the following parametric restrictions:

$$a=b=c=-a_1=-b_1=-c_1=1$$

and so the operator H_2 becomes

$$H_2=u_n(Eu_n+u_nE+Eu_nE-E^{-1}u_n-u_nE^{-1}u_n-u_nE^{-1})u_n. \tag{13}$$

It is straightforward to check that the skew symmetric operator H_2 is Hamiltonian (see Sec. III). Thus the recursion operator $\mathcal{R}=H_2H_1^{-1}$ for the VL lattice equation (2) is

$$\mathcal{R}=u_n[u_nE-u_nE^{-1}+Eu_n+Eu_nE-E^{-1}u_n-E^{-1}u_nE^{-1}](E-E^{-1})^{-1}\frac{1}{u_n}. \tag{14}$$

It is appropriate to mention here that there exists a link between Lax operators and some of the integrability properties of the nonlinear PDEs (see Ref. 3) and PDDEs.[23,24]

III. TRI-HAMILTONIAN SYSTEM

It is known that if an integrable partial differential–difference equation with two independent variables admit two invertible Hamiltonian operators H_1 and H_2, then it is possible to construct a sequence of operators H_n satisfying the relation

$$H_n=\mathcal{R}^{n-2}H_2, \quad n\geqslant 3, \tag{15}$$

where $\mathcal{R}=H_2H_1^{-1}$ is a recursion operator. It is appropriate to mention here that the constructed operators $H_n, n\geqslant 3$ need not be Hamiltonian, in general. We show below that the integrable lattice Eqs. (1)–(6) possessing bi-Hamiltonian structure admits a sequence of operators $H_n, n\geqslant 3$ out of which the operator H_3 alone Hamiltonian and the remaining operators $H_n, n\geqslant 4$ are non-Hamiltonian ones. For clarity of presentation, we furnish below the computational details of the RT and VL equations and for the remaining lattice equations only brief details are given.

A. RT lattice equation

1. Construction of a sequence of operators

In Ref. 21 we have shown that the RT lattice equation (1) can be written as

$$\begin{bmatrix} v_t \\ u_t \end{bmatrix}=H_2\begin{bmatrix} \dfrac{\delta\mathcal{H}_0}{\delta u} \\ \dfrac{\delta\mathcal{H}_0}{\delta v} \end{bmatrix}=H_1\begin{bmatrix} \dfrac{\delta\mathcal{H}_1}{\delta u} \\ \dfrac{\delta\mathcal{H}_1}{\delta v} \end{bmatrix} \tag{16}$$

associated with the Hamiltonian functionals, $\mathcal{H}_0(u,v)=-\Sigma_n[u+v]$ and $\mathcal{H}_1(u,v)=\Sigma_n\left[\frac{1}{2}(u^2+v^2)+uv+\overline{v}\,u+u\,\overline{u}\right]$, where $u=u_n$, $v=v_n$, $\overline{u}=u_{n+1}$, $\overline{v}=v_{n+1}$. Here the Hamiltonian operators H_1 and H_2 take the form

$$H_1=\begin{bmatrix} uE-E^{-1}u & -(1-E^{-1})u \\ -u(E-1) & 0 \end{bmatrix}, \tag{17a}$$

$$H_2=\begin{bmatrix} 0 & v(E^{-1}-1)u \\ u(E-1)v & u(E-E^{-1})u \end{bmatrix} \tag{17b}$$

and so the recursion operator $\mathcal{R}$ becomes

$$\mathcal{R}=\begin{bmatrix} v & v+v(1-E^{-1})u(E-1)^{-1}\dfrac{1}{u} \\ u(1+E) & u(1+E)+u(E-1)v(E-1)^{-1}\dfrac{1}{u}+u(E-E^{-1})u(E-1)^{-1}\dfrac{1}{u} \end{bmatrix}. \tag{18}$$

Making use of the Hamiltonian operators H_1 and H_2 in Eq. (15) we construct a sequence of operators $(H_n, n\geqslant 3)$:

$$H_3=\begin{bmatrix} v(E^{-1}u-uE)v & v(-v-u-uE+E^{-1}u \\ & \quad +vE^{-1}+E^{-1}uE^{-1})u \\ u(v+u+E^{-1}u-uE-Ev-EuE)v & u(-Eu+uE^{-1}-uE+E^{-1}u \\ & \quad -2Ev+2vE^{-1}-EuE+E^{-1}uE^{-1})u \end{bmatrix}, \tag{19}$$

$$H_4=\mathcal{R}^2H_2=\begin{bmatrix} H_{11}^{(4)} & H_{12}^{(4)} \\ H_{21}^{(4)} & H_{22}^{(4)} \end{bmatrix}, \tag{20}$$

where

$$\begin{aligned} H_{11}^{(4)}&=v^2(E^{-1}u-uE)v+vu(v+u+E^{-1}u-uE-Ev-EuE)v \\ &\quad +v(1-E^{-1})u(E-1)^{-1}(v+u+E^{-1}u-uE-Ev-EuE)v, \end{aligned}$$

$$\begin{aligned} H_{12}^{(4)}&=v^2(-v-u-uE+E^{-1}u+vE^{-1}+E^{-1}uE^{-1})u+vu(-Eu+uE^{-1}-uE+E^{-1}u-2Ev \\ &\quad +2vE^{-1}-EuE+E^{-1}uE^{-1})u+v(1-E^{-1})u(E-1)^{-1}(-Eu+uE^{-1}-uE+E^{-1}u-2Ev \\ &\quad +2vE^{-1}-EuE+E^{-1}uE^{-1})u, \end{aligned} \tag{20a}$$

$$\begin{aligned} H_{21}^{(4)}&=u(1+E)v(E^{-1}u-uE)v+u(1+E)u(v+u+E^{-1}u-uE-Ev-EuE)v \\ &\quad +u(E-1)v(E-1)^{-1}(v+u+E^{-1}u-uE-Ev-EuE)v \\ &\quad +u(E-E^{-1})u(E-1)^{-1}(v+u+E^{-1}u-uE-Ev-EuE)v, \end{aligned}$$

$$\begin{aligned} H_{22}^{(4)}&=u(1+E)v(-v-u-uE+E^{-1}u+vE^{-1}+E^{-1}uE^{-1})u+u(1+E)u(-Eu+uE^{-1}-uE \\ &\quad +E^{-1}u-2Ev+2vE^{-1}-EuE+E^{-1}uE^{-1})u+u(E-1)v(E-1)^{-1}(-Eu+uE^{-1}-uE \\ &\quad +E^{-1}u-2Ev+2vE^{-1}-EuE+E^{-1}uE^{-1})u+u(E-E^{-1})u(E-1)^{-1}(-Eu+uE^{-1} \\ &\quad -uE+E^{-1}u-2Ev+2vE^{-1}-EuE+E^{-1}uE^{-1})u, \end{aligned} \tag{20b}$$

and so on. Since the entries of the remaining operators $H_n, n\geqslant 5$ involves lengthy expressions we refrain from presenting their explicit form.

2. Tri-Hamiltonian structure

For completeness we briefly present the computational details of the operators H_1 and H_2 as Hamiltonian ones. In order to prove that the skew symmetric operators H_1 and H_2 are Hamil-

tonian it remains to prove that they satisfy the Jacobi identity. Let us first consider the skew symmetric operator H_1. It is appropriate to mention the following theorem for a system of nonlinear partial differential equations $\partial \mathbf{u}/\partial t = K(\mathbf{u})$ due to Olver.[4]

Theorem: Let $\mathcal{D}$ be a skew-adjoint $q \times q$ matrix differential operator of the system of partial differential equations, $\partial \mathbf{u}/\partial t = K(\mathbf{u})$ and $\Theta = \frac{1}{2}\int\{\Theta \wedge \mathcal{D}\Theta\}\mathrm{d}x$, the corresponding functional bi-vector. Then $\mathcal{D}$ is Hamiltonian if and only if

$$PrV_{\mathcal{D}\theta}(\Theta) = 0. \tag{21}$$

Here $\theta = \theta(x,t,\mathbf{u})$. Recent investigations by Sanders and Wang[25] suggest that the above result, Eq. (21), holds good for nonlinear PDDEs as well. For nonlinear PDDEs, the prolongation of the vector field takes the form

$$PrV_{\mathcal{D}\theta} = \sum_{\alpha,J} E^J\left(\sum_{\beta} \mathcal{D}_{\alpha\beta}\theta^{\beta}\right)\frac{\partial}{\partial E^J u^{\alpha}},$$

where E^J is the shift operator.

Let $\theta_1 = (\theta, \varsigma)^T$. Then

$$H_1\theta_1 = H_1\begin{bmatrix}\theta\\ \varsigma\end{bmatrix} = \begin{bmatrix}(uE - E^{-1}u)\theta + (E^{-1}-1)u\varsigma\\ -u\Delta\theta\end{bmatrix} = \begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix}.$$

Next, define a bi-vector Θ of H_1 by

$$\Theta_{H_1} = \frac{1}{2}\sum[\theta \wedge \Phi_1 + \varsigma \wedge \Phi_2]$$

$$= \frac{1}{2}\sum[u\ \theta \wedge \overline{\theta} - u\ \overline{\theta} \wedge \theta + u\ \overline{\theta} \wedge \varsigma - u\ \theta \wedge \varsigma - u\ \varsigma \wedge \overline{\theta} + u\ \varsigma \wedge \theta]$$

which can be simplified, using the property of the wedge product, ($\theta \wedge \overline{\theta} = -\overline{\theta} \wedge \theta$, $\overline{\theta} \wedge \varsigma = -\varsigma \wedge \overline{\theta}$, $\theta \wedge \theta = 0$), into

$$\Theta_{H_1} = \sum[u\ \theta \wedge \overline{\theta} + u\overline{\theta} \wedge \varsigma + u\ \varsigma \wedge \theta],$$

where $\overline{\varsigma} = \varsigma_{n+1}, \overline{\theta} = \theta_{n+1}$. Now

$$PrV_{H_1\theta_1}(\Theta_{H_1}) = \sum[(-u\ \overline{\theta} + u\theta) \wedge (\theta \wedge \overline{\theta} + \overline{\theta} \wedge \varsigma + \varsigma \wedge \theta)] = 0$$

and so the skew symmetric operator H_1 is Hamiltonian. Here Σ is used to denote the equivalence classes after dividing the image of $(1-E)$. In a similar manner, we have checked that the skew symmetric operators H_2 and H_3 satisfy

$$PrV_{H_2\theta_1}(\Theta_{H_2}) = 0, \quad PrV_{H_3\theta_1}(\Theta_{H_3}) = 0$$

indicating they are Hamiltonian operators.

Next consider the skew symmetric operator H_4. Now

$$H_4\theta_1 = H_4\begin{bmatrix}\theta\\ \varsigma\end{bmatrix} = \begin{bmatrix}H_{11}^{(4)}\theta + H_{12}^{(4)}\varsigma\\ H_{21}^{(4)}\theta + H_{22}^{(4)}\varsigma\end{bmatrix} = \begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix},$$

where $H_{11}^{(4)}$, $H_{12}^{(4)}$, $H_{21}^{(4)}$, and $H_{22}^{(4)}$ are given in Eqs. (20a) and (20b). As before we define a bi-vector Θ of H_4 as

$$\Theta_{H_4}=\frac{1}{2}\sum\ [\theta\wedge\Phi_1+\varsigma\wedge\Phi_2].$$

Proceeding further along the lines described above we find that $PrV_{H_4\theta_1}(\Theta_{H_4})$ reduce into

$$PrV_{H_4\theta_1}(\Theta_{H_4})=\sum\ (E-1)(\cdots)+\sum\ (E-E^{-1})^{-1}(\cdots). \tag{22}$$

Obviously the expression in the first summation becomes zero while the expression in the second summation does not vanish due to the presence of the inverse difference operator $(E-E^{-1})^{-1}$ and so

$$PrV_{H_4\theta_1}(\Theta_{H_4})\neq 0$$

proving that the operator H_4 is not a Hamiltonian operator. Similar conclusions can be arrived at for the remaining skew symmetric operators $H_n, n\geqslant 5$.

It is appropriate to mention here that a similar feature has been observed in the case of integrable nonlinear partial differential equations. For example, Fordy and Antonwicz[8] have shown that the two coupled Korteweg–de Vries equation admits *four* distinct operators H_1, H_2, H_3, and H_4 and pointed out that the first three operators are Hamiltonian while H_4 is not a Hamiltonian operator because the associated $PrV_{H_4\theta_1}(\Theta_{H_4})\neq 0$ since it involves integro differential operator.

Thus we conclude that the RT lattice equation (1) is only a tri-Hamiltonian system. Using a different approach Fuchssteiner *et al.*[19] have also shown that RT is a tri-Hamiltonian system.

B. VL lattice equation

1. Construction of a sequence of operators

Here

$$H_1=u(E-E^{-1})u,\quad H_2=u(Eu+uE+EuE-uE^{-1}-E^{-1}u-E^{-1}uE^{-1})u.$$

Using the operators H_1 and H_2 in Eq. (15) we obtain the following operators:

$$\begin{aligned}H_3&=\mathcal{R}H_2\\&=u(1+E+E^{-1})u[Eu+uE+EuE-E^{-1}u-uE^{-1}-E^{-1}uE^{-1}]u+u[Eu^2+EuE^{-1}u\\&\quad+Eu^2E+EuE^{-1}uE-E^{-1}u^2-E^{-1}uEu-E^{-1}u^2E-E^{-1}uEuE]u+u[Eu(E-1)^{-1}E^{-1}u\\&\quad+Eu(E-1)^{-1}u-E^{-1}u(1-E^{-1})^{-1}E^{-1}u-E^{-1}u(1-E^{-1})^{-1}u](E-E^{-1})u,\end{aligned} \tag{23}$$

$$\begin{aligned}H_4&=\mathcal{R}^2H_2\\&=[u(1+E+E^{-1})u+uEu(E-1)^{-1}-uE^{-1}u(1-E^{-1})^{-1}]\{(1+E+E^{-1})\\&\quad\times u[Eu+uE+EuE-E^{-1}u-uE^{-1}-E^{-1}uE^{-1}]u+Eu(1+E^{-1})u^2\\&\quad+Eu(1+E^{-1})uEu+Eu(E-1)^{-1}E^{-1}u(E-E^{-1})u+Eu(E-1)^{-1}u(E-E^{-1})u\\&\quad-E^{-1}u(E+1)u^2-E^{-1}u(E+1)uEu-E^{-1}u(1-E^{-1})^{-1}E^{-1}u(E-E^{-1})u\\&\quad-E^{-1}u(1-E^{-1})^{-1}u(E-E^{-1})u\},\end{aligned} \tag{24}$$

and so on.

2. Tri-Hamiltonian structure

First consider the skew symmetric operator H_1. Let

$$H_1\theta = u\ \overline{u}\ \overline{\theta} - u\ \underline{u}\ \underline{\theta},$$

where $\underline{\theta} = \theta_{n-1}$, etc. As before we define a bi-vector Θ of H_1 by

$$\Theta_{H_1} = \frac{1}{2}\sum [\theta \wedge H_1\theta] = \frac{1}{2}\sum [\theta \wedge u\ \overline{u}\,\overline{\theta} - \theta \wedge \underline{u}\ \underline{\theta}] = \frac{1}{2}\sum [u\ \overline{u}\ \theta \wedge \overline{\theta} - u\ \overline{u}\ \overline{\theta} \wedge \theta]. \tag{25}$$

Making use of the property of wedge product, the above equation can be written as

$$\Theta_{H_1} = \sum [\ u\ \overline{u}\ \theta \wedge \overline{\theta}\ ]$$

and hence

$$\begin{aligned} PrV_{H_1\theta_1}(\Theta_{H_1}) &= \sum [\ \overline{u}\ (u\overline{u}\ \overline{\theta} - u\ \underline{u}\ \underline{\theta}) \wedge \theta \wedge \overline{\theta} + u\ (\overline{u}\overline{\bar{u}}\ \bar{\bar{\theta}} - u\ \overline{u}\ \theta) \wedge \theta \wedge \overline{\theta}\ ] \\ &= \sum [\ u\ \overline{u}\ \bar{u}\ \theta \wedge \overline{\theta} \wedge \bar{\bar{\theta}} - \underline{u}\ u\ \overline{u}\ \underline{\theta} \wedge \theta \wedge \overline{\theta}\ ] \\ &= \sum [\ (E-1)\underline{u}\ u\ \overline{u}\ \underline{\theta} \wedge \theta \wedge \overline{\theta}\ ] = 0 \end{aligned}$$

and so the operator H_1 is Hamiltonian. In a similar manner, we have checked that the skew symmetric operator H_2 satisfy

$$PrV_{H_2\theta_1}(\Theta_{H_2}) = 0 \tag{26}$$

indicating that it is a Hamiltonian operator.

Next consider the skew symmetric operator H_3. As before we define a bi-vector Θ of H_3 by

$$\begin{aligned} \Theta_{H_3} = \sum [&u^3\ \overline{u}\ \overline{\theta} + u^2\ \overline{u}\overline{\bar{u}}\ \bar{\bar{\theta}} - u^2\ \underline{u}^2\ \underline{\theta} - u^3\ \underline{u}\ \underline{\theta} - u^2\ \underline{u}\ \underline{\underline{u}}\ \underline{\underline{\theta}} + u\ \overline{u\bar{u}}^2\ \bar{\bar{\theta}} + u\ \overline{u}^2\ \bar{u}\ \bar{\bar{\theta}} \\ &+ u\ \overline{u}\ \bar{\bar{\theta}} u\ \overline{\overline{\theta}} - u\ \underline{u}\ \underline{\underline{u}}^2\ \underline{\underline{\theta}} - u\ \underline{u}^2\ \underline{\underline{u}}\ \underline{\underline{\theta}} - u\underline{u}\ \underline{\underline{u}}\ \underline{\underline{\underline{u}}}\ \underline{\underline{\underline{\theta}}} + u\ \overline{u}^3\ \overline{\theta} + u^2\ \overline{u}^2\ \overline{\theta} - u\ \underline{u}^3\underline{\theta} \\ &+ uEu(E-1)^{-1}u(E-E^{-1})u\theta + uEu(E-1)^{-1}Eu(E-E^{-1})u\theta \\ &- uE^{-1}u(1-E^{-1})^{-1}E^{-1}u(E-E^{-1})u\theta - uE^{-1}u(1-E^{-1})^{-1}u(E-E^{-1})u\theta]. \end{aligned}$$

Making use of the property of wedge product and then computing the related prolongation, after a tedious calculation, we find that

$$PrV_{H_3\theta_1}(\Theta_{H_3}) = \sum (E-1)(\cdots) = 0 \tag{27}$$

provided if the field variable u is periodic with even period. Furthermore we have checked that the prolongation associated with the operators $H_n, n \geqslant 4$ does not vanish, that is

$$PrV_{H_4\theta_1}(\Theta_{H_4}) \neq 0,\ \ PrV_{H_5\theta_1}(\Theta_{H_5}), \neq 0, \ldots \tag{28}$$

even if the field variable u is periodic with even period.

Hence Vl lattice equation is a tri-Hamiltonain system only if the field variable is periodic with even period.

Using the Poisson structure technique Wadati *et al.*[22] have also shown that the VL lattice equation (2) is a tri-Hamiltonian system.

C. TL lattice equation

We have checked that the TL lattice equation (3) admits a tri-Hamiltonian structure and thus can be written as

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = H_3 \begin{bmatrix} \frac{1}{2v} \\ 0 \end{bmatrix} = H_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} = H_1 \begin{bmatrix} 1 \\ u \end{bmatrix}.$$

Here the operators

$$H_1 = \begin{bmatrix} (E-1)v & 0 \\ 0 & v(1-E^{-1}) \end{bmatrix}, \quad H_2 = \begin{bmatrix} u(E-1)v & Ev - vE^{-1} \\ v(E-E^{-1})v & v(1-E^{-1})u \end{bmatrix} \tag{29}$$

and

$$H_3 = \mathcal{R} H_2 = \begin{bmatrix} (E-1)v^2 + (EvE - vE^{-1})v + u^2(E-1)v & u(Ev - vE^{-1}) + (Ev - vE^{-1})u \\ 2v(uE - E^{-1}u)v & v(Ev - E^{-1}vE^{-1}) + v(1-E^{-1})u^2 + v^2(1-E^{-1}) \end{bmatrix} \tag{30}$$

with the recursion operator $\mathcal{R} = H_2 H_1^{-1}$ as

$$\mathcal{R} = \begin{bmatrix} u & (Ev - vE^{-1})(1-E^{-1})^{-1}\frac{1}{v} \\ v(1+E^{-1}) & v(1-E^{-1})u(1-E^{-1})^{-1}\frac{1}{v} \end{bmatrix}. \tag{31}$$

Proceeding in a similar manner we construct a sequence of operators $(H_n,\ n \geqslant 4)$. For example, the operator H_4 is

$$H_4 = \mathcal{R}^2 H_2 = \begin{bmatrix} H_{11}^{(4)} & H_{12}^{(4)} \\ H_{21}^{(4)} & H_{22}^{(4)} \end{bmatrix}, \tag{32}$$

where

$$H_{11}^{(4)} = 2(Ev - vE^{-1})(1-E^{-1})^{-1}(uE - E^{-1}u)v + u(E-1)v^2 + u(EvE - vE^{-1})v + u^3(E-1)v,$$

$$\begin{aligned} H_{12}^{(4)} &= (Ev - vE^{-1})(1-E^{-1})^{-1}(Ev - E^{-1}vE^{-1}) + (Ev - vE^{-1})u^2 \\ &\quad + (Ev - vE^{-1})(1-E^{-1})^{-1}v(1-E^{-1}) + u^2(Ev - vE^{-1}) + u(Ev - vE^{-1})u, \end{aligned} \tag{32a}$$

$$\begin{aligned} H_{21}^{(4)} &= 2v(1-E^{-1})u(1-E^{-1})^{-1}(uE - E^{-1}u)v + v(1+E^{-1})(E-1)v^2 \\ &\quad + v(1+E^{-1})(EvE - vE^{-1})v + v(1+E^{-1})u^2(E-1)v, \end{aligned}$$

$$\begin{aligned} H_{22}^{(4)} &= v(1-E^{-1})u(1-E^{-1})^{-1}(Ev - E^{-1}vE^{-1}) + v(1-E^{-1})u^3 + v(1-E^{-1}) \\ &\quad \times u(1-E^{-1})^{-1}v(1-E^{-1}) + v(1+E^{-1})(uEv - uvE^{-1}) + v(1+E^{-1})(Ev - vE^{-1})u. \end{aligned} \tag{32b}$$

The operators $H_n, n \geqslant 5$ involve lengthy expressions; we have not presented their explicit forms here.

In order to investigate the nature of the operator H_4 Hamiltonian or not let

$$H_4 \theta_1 = H_4 \begin{bmatrix} \theta \\ \varsigma \end{bmatrix} = \begin{bmatrix} H_{11}^{(4)} \theta + H_{12}^{(4)} \varsigma \\ H_{21}^{(4)} \theta + H_{22}^{(4)} \varsigma \end{bmatrix} = \begin{bmatrix} \Phi_1 \\ \Phi_2 \end{bmatrix},$$

where $H_{11}^{(4)}$, $H_{12}^{(4)}$, $H_{21}^{(4)}$, and $H_{22}^{(4)}$ are given in Eqs. (32a) and (32b). Define a bivector Θ of H_4 as

$$\Theta_{H_4} = \frac{1}{2} \sum [\theta \wedge \Phi_1 + \varsigma \wedge \Phi_2].$$

Proceeding as before for the RT lattice equation (1) we find that the prolongation associated with H_4 does not vanish due to the presence of the inverse difference operator $(E - E^{-1})^{-1}$ and so H_4 is not a Hamiltonian operator. Similar conclusions can be arrived at for the remaining skew symmetric operators $H_n, n \geqslant 5$.

Thus we conclude that the TL lattice equation (3) is only a tri-Hamiltonian system. Similar observation has also pointed out by Oevel *et al.* using a different approach.[18]

D. BC lattice equation

A detailed but cumbersome calculation shows that BC lattice equation (4) possesses tri-Hamiltonian structure and hence can be written as

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = H_3 \begin{bmatrix} u + \overline{u} + \underline{u} \\ -1 \end{bmatrix} = H_2 \begin{bmatrix} 0 \\ \dfrac{1}{3v} \end{bmatrix} = H_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{33}$$

where the Hamiltonian operators H_1, H_2, and H_3 take the form

$$H_1 = \begin{bmatrix} H_{11}^{(1)} & H_{12}^{(1)} \\ H_{21}^{(1)} & H_{22}^{(1)} \end{bmatrix}, \quad H_2 = \begin{bmatrix} H_{11}^{(2)} & H_{12}^{(2)} \\ H_{21}^{(2)} & H_{22}^{(2)} \end{bmatrix}$$

and

$$H_3 = \begin{bmatrix} R_{11} H_{11}^{(2)} + R_{12} H_{21}^{(2)} & R_{11} H_{12}^{(2)} + R_{12} H_{22}^{(2)} \\ R_{13} H_{11}^{(2)} + R_{14} H_{21}^{(2)} & R_{13} H_{12}^{(2)} + R_{14} H_{22}^{(2)} \end{bmatrix}$$

with the recursion operator $\mathcal{R}$

$$\mathcal{R} = H_2 H_1^{-1} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix},$$

where

$$H_{11}^{(1)} = uEu - uE^{-1}u + E^{-1}v - vE,$$

$$H_{12}^{(1)} = -uE^{-2}v + uEv,$$

$$H_{21}^{(1)} = vE^2u - vE^{-1}u,$$

$$H_{22}^{(1)} = vE^2v + vEv - vE^{-2}v - vE^{-1}v, \tag{34}$$

$$H_{11}^{(2)}=u(uE+Eu+EuE-uE^{-1}-E^{-1}u-E^{-1}uE^{-1})u+uE^{-1}v-uEvE+E^{-1}vE^{-1}u-vE^{2}u$$
$$-uvE-vEu+E^{-1}uv+uE^{-2}v,$$

$$H_{12}^{(2)}=-u(-uE-Eu-EuE+uE^{-2}+E^{-1}uE^{-2}+E^{-1}uE^{-1})v-v(1+E+E^{2})v$$
$$+E^{-1}v(1+E^{-1}+E^{-2})v-(uE^{-1}u-uEuE^{-1})v,$$

$$H_{21}^{(2)}=-v(uE^{-1}+E^{-1}u+E^{-1}uE^{-1}-EuE-E^{2}u-E^{2}uE)u-v[(1+E+E^{2})vE$$
$$-(1+E^{-1}+E^{-2})v]-v[-uE+EuE^{-1}]u,$$

$$H_{22}^{(2)}=-v[E^{-1}uE^{-2}+uE^{-2}-uE-E^{2}uE+E^{-1}u+E^{-1}uE^{-1}$$
$$-E^{2}uE^{-1}-EuE+EuE^{-2}-E^{2}u]v, \tag{35}$$

$$R_{11}=[u(EuE-E^{-1}uE^{-1})u+uE^{-1}(1+E^{-1})v-u(1+E)vE+(E^{-1}uv-vEu)$$
$$+(u^{2}(1-E^{-1})+uE^{-1}uE^{-2}-uEuE+(1-E^{-1}))v^{2}(1+E^{-1})^{-1}u]$$
$$\times(E^{-1}v-vE-u(E^{-1}-1)(1+E^{-1})^{-1}u)^{-1}, \tag{36a}$$

$$R_{12}=\Bigg\{[u(uE+Eu+EuE-uE^{-1}-E^{-1}u-E^{-1}uE^{-1})u+uE^{-1}v-uEvE+E^{-1}vE^{-1}u-vE^{2}u$$
$$-uvE-vEu+E^{-1}uv+uE^{-2}v]+[u(-uE-Eu-EuE+uE^{-2}+E^{-1}uE^{-2}+E^{-1}uE^{-1})$$
$$+v(1+E+E^{2})-E^{-1}v(1+E^{-1}+E^{-2})v+(uE^{-1}u-uEuE^{-1})]\Bigg[(E-E^{-2})^{-1}(E-E^{-1})u$$
$$+(E-E^{-2})^{-1}\frac{1}{u}(E^{-1}v-vE)\Bigg]\Bigg\}\Bigg(v(1-E)u-(1+E)\frac{1}{u}(E^{-1}v-vE)\Bigg)^{-1}, \tag{36b}$$

$$R_{13}=\{[v(EuE-E^{-1}uE^{-1}+E^{2}uE-EuE^{-1})u-(1+E+E^{2})vE+(1+E^{-1}+E^{-2})v$$
$$+[u((1-E^{-1})+(E+E^{-1})uE^{-2}-(1+E)EuE)\}(1+E^{-1})^{-1}u](E^{-1}v-vE$$
$$-u(E^{-1}-1)(1+E^{-1})^{-1}u)^{-1}, \tag{37a}$$

$$R_{14}=\Bigg\{[-v(uE^{-1}+E^{-1}u+E^{-1}uE^{-1}-EuE-E^{2}u-E^{2}uE)v-v(1+E+E^{2})vE+v(1+E^{-1}$$
$$+E^{-2})v+v(uE-EuE^{-1})u+v(E^{-1}uE^{-2}+uE^{-2}-uE-E^{2}uE+E^{-1}u+E^{-1}uE^{-1}$$
$$-E^{2}uE^{-1}-EuE+EuE^{-2}-E^{2}u)]\Bigg[(E-E^{-2})^{-1}(E-E^{-1})u+(E-E^{-2})^{-1}\frac{1}{u}(E^{-1}v$$
$$-vE)\Bigg]\Bigg\}\Bigg(v(1-E)u-(1+E)\frac{1}{u}(E^{-1}v-vE)\Bigg)^{-1}. \tag{37b}$$

Making use of the operators H_1 and H_2 in Eq. (15) we have constructed a sequence of operators $\{H_4,H_5,H_6,\ldots\}$ which involve lengthy expressions.

We observe that the prolongation corresponding to the operator H_3 vanishes only if the field variables u and v are periodic with even period like for VL equation. Further we have checked that the prolongation associated with the operators $H_n, n\geqslant 4$ does not vanish even if the field variables are periodic with even period and so they are not Hamiltonian ones.

Thus the BC lattice equation (4) is a tri-Hamiltonian system provided if the field variables are periodic.

We find after detailed calculations that, both BM3 and BM4 lattice equations (5) and (6) admit only three distinct Hamiltonian operators and so they are tri-Hamiltonian system (brief details are given in Appendixes A and B).

IV. CONCLUSION

A systematic investigation of multi-Hamiltonian structure of certain integrable nonlinear partial differential–difference equations with two independent variables is presented. It is shown that the RT, TL, BM3, and BM4 lattice equations admit only three Hamiltonian operators while the well-known VL and BC lattice equations possess three Hamiltonian operators only if the filed variable is periodic with even period and hence they are tri-Hamiltonian systems only. It is observed that the presence of the inverse difference operators prevents one to show that the operator H_N, $N \geqslant 4$ is not Hamiltonian. A similar feature was observed for two coupled Korteweg–de Vries equations by Fordy and Antonwicz.[8]

ACKNOWLEDGMENT

One of the authors (S.K.) would like to thank the University of Madras for providing University Research Fellowship.

APPENDIX A: BM3 LATTICE EQUATION

The BM3 lattice equation (5) can be written as

$$\begin{bmatrix} u_t \\ v_t \\ w_t \end{bmatrix} = H_3 \begin{bmatrix} 0 \\ 0 \\ \dfrac{1}{w} \end{bmatrix} = H_2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = H_1 \begin{bmatrix} w \\ v \\ u \end{bmatrix}, \tag{A1}$$

where $w = w_n$ and the Hamiltonian operators H_1, H_2, H_3 takes

$$H_1 = \begin{bmatrix} (E-E^{-1}) & 0 & 0 \\ 0 & 0 & (E^{-1}-1)w \\ 0 & -w(E-1) & 0 \end{bmatrix},$$

$$H_2 = \begin{bmatrix} H_{11}^{(2)} & H_{12}^{(2)} & H_{13}^{(2)} \\ H_{21}^{(2)} & H_{22}^{(2)} & H_{23}^{(2)} \\ H_{31}^{(2)} & H_{32}^{(2)} & H_{33}^{(2)} \end{bmatrix} \quad \text{and} \quad H_3 = \begin{bmatrix} H_{11}^{(3)} & H_{12}^{(3)} & H_{13}^{(3)} \\ H_{21}^{(3)} & H_{22}^{(3)} & H_{23}^{(3)} \\ H_{31}^{(3)} & H_{32}^{(3)} & H_{33}^{(3)} \end{bmatrix}, \tag{A2}$$

where

$$H_{11}^{(2)} = Ev - vE^{-1} - u(E-1)(E-E^{-1})^{-1}(E^{-1}-1)u, \quad H_{12}^{(2)} = EwE - E^{-1}w,$$

$$H_{13}^{(2)} = u(E-1)(E-E^{-1})^{-1}(E^{-1}-1)w,$$

$$H_{21}^{(2)} = wE - E^{-1}wE^{-1}, \quad H_{22}^{(2)} = E^{-1}uw - uwE, \quad H_{23}^{(2)} = v(E^{-1}-1)w,$$

$$H_{31}^{(2)} = w(E-1)(E-E^{-1})^{-1}(E^{-1}-1)u, \quad H_{32}^{(2)} = -w(E-1)v,$$

$$H_{33}^{(2)} = w(-(E-E^{-1}) - (E-1)(E-E^{-1})^{-1}(E^{-1}-1))w, \tag{A2a}$$

$$H_{11}^{(3)} = uwE^{-1} + E^{-1}wu - wuE - Ewu + v^2E^{-1} - Ev^2,$$

$$H_{12}^{(3)}=-EwvE-EwEv+vE^{-1}w+E^{-1}wv,$$

$$H_{13}^{(3)}=(EwE-E^{-1}wE^{-1})w,$$

$$H_{21}^{(3)}=E^{-1}wvE^{-1}+vE^{-1}wE^{-1}-wEv-vwE,$$

$$H_{22}^{(3)}=E^{-1}wE^{-1}w-wEwE+uwvE+uwEv-E^{-1}uwv-vE^{-1}uw,$$

$$H_{23}^{(3)}=v^2(1-E^{-1})w+(-E^{-1}uwE^{-1}+uwE)w,$$

$$H_{31}^{(3)}=wE^{-1}wE^{-1}-wEwE-wE^{-1}uv+wEuv,$$

$$H_{32}^{(3)}=wEv^2-wv^2+wEuwE-wE^{-1}wuE-uw^2+uw^2E,$$

$$H_{33}^{(3)}=wEvw-wvE^{-1}w \tag{A2b}$$

with the recursion operator $\mathcal{R}$ for the BM3 lattice equation (5) takes the form

$$\mathcal{R}=\begin{bmatrix} (E-E^{-1})^{-1}[Ev-vE^{-1} & (E-E^{-1})^{-1}[EwE-E^{-1}w] & (E-E^{-1})^{-1}[u(E-1) \\ -u(E-1)(E-E^{-1})^{-1} & & (E-E^{-1})^{-1}(E^{-1}-1)]w \\ (E^{-1}-1)u] & & \\ -(E-E^{-1})^{-1}(E^{-1}-1)u & v & [1+E^{-1}+(E-E^{-1})^{-1} \\ & & (E^{-1}-1)]w \\ \frac{1}{w}(E^{-1}-1)^{-1} & \frac{1}{w}(E^{-1}-1)^{-1} & \frac{1}{w}(E^{-1}-1)^{-1} \\ [wE-E^{-1}wE^{-1}] & [E^{-1}uw-uwE] & [v(E^{-1}-1)w] \end{bmatrix}.$$

Making use of the operators H_1 and H_2 in Eq. (10) we have constructed a sequence of operators H_n, $n\geqslant 4$ and checked that the required prolongation does not vanish in each of the operators indicating that they are not Hamiltonian.

APPENDIX B: BM4 LATTICE EQUATION

A detailed calculation shows that the BM4 lattice equation (6) possesses a tri-Hamiltonian structure and thus can be written as

$$\begin{bmatrix} u_t \\ v_t \\ w_t \\ q_t \end{bmatrix}=H_3\begin{bmatrix} \frac{1}{u} \\ 0 \\ 0 \\ 0 \end{bmatrix}=H_2\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}=H_1\begin{bmatrix} \underline{w} \\ \frac{v}{u} \\ 0 \end{bmatrix}, \tag{B1}$$

where $q=q_n$, $\underline{w}=w_{n-1}$,

$$H_1=\begin{bmatrix} 0 & u(1-E^{-1}) & 0 & 0 \\ (E-1)u & 0 & 0 & 0 \\ 0 & 0 & qE-E^{-1}q & E-E^{-2} \\ 0 & 0 & E^2-E^{-1} & 0 \end{bmatrix},$$

$$H_2=\begin{bmatrix} H_{11}^{(2)} & H_{12}^{(2)} & H_{13}^{(2)} & H_{14}^{(2)} \\ H_{21}^{(2)} & H_{22}^{(2)} & H_{23}^{(2)} & H_{24}^{(2)} \\ H_{31}^{(2)} & H_{32}^{(2)} & H_{33}^{(2)} & H_{34}^{(2)} \\ H_{41}^{(2)} & H_{42}^{(2)} & H_{43}^{(2)} & H_{44}^{(2)} \end{bmatrix} \quad \text{and} \quad H_3=\begin{bmatrix} H_{11}^{(3)} & H_{12}^{(3)} & H_{13}^{(3)} & H_{14}^{(3)} \\ H_{21}^{(3)} & H_{22}^{(3)} & H_{23}^{(3)} & H_{24}^{(3)} \\ H_{31}^{(3)} & H_{32}^{(3)} & H_{33}^{(3)} & H_{34}^{(3)} \\ H_{41}^{(3)} & H_{42}^{(3)} & H_{43}^{(3)} & H_{44}^{(3)} \end{bmatrix},$$

where

$$H_{11}^{(2)}=u(E^3-E^{-1})u,\quad H_{12}^{(2)}=u(1-E^{-1})v,$$

$$H_{13}^{(2)}=u(1-E^2)w,\quad H_{14}^{(2)}=u(1+E^{-2}-E-E^2)q,$$

$$H_{21}^{(2)}=v(E^3-1)u,\quad H_{22}^{(2)}=wEu-uE^{-1}w,$$

$$H_{23}^{(2)}=vw-vE^2w+qEu-uE^{-2}q,$$

$$H_{24}^{(2)}=-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q,$$

$$H_{31}^{(2)}=-wE^3u+wE^2u,\quad H_{32}^{(2)}=qE^2u-uE^{-1}q,$$

$$H_{33}^{(2)}=wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u,$$

$$H_{34}^{(2)}=wE^2q-vE^{-2}+Ev-wE^{-1}q,$$

$$H_{41}^{(2)}=-qE^3u+qE^2u,\quad H_{42}^{(2)}=E^3u-uE^{-1},$$

$$H_{43}^{(2)}=qE^2w-qEw+E^2v-vE^{-1},\quad H_{44}^{(2)}=qE^2q-q^2+Ew-wE^{-1},$$

$$\begin{aligned} H_{11}^{(3)}=&u(1-E^{-1})v(E+1)(E^2+1)u+u(E^3-E^{-1})(E-1)^{-1}v(E^3-1)u+u(1+E^{-2}-E\\ &-E^2)q(E-E^{-2})^{-1}wE^2(1-E)u+[u(1-E^2)w-u(1-E^{-2}-E-E^2)q(E-E^{-2})^{-1}\\ &\times(qE-E^{-1}q)](E^2-E^{-1})^{-1}qE^2(1-E)u, \end{aligned}$$

$$\begin{aligned} H_{12}^{(3)}=&u(1-E^{-1})v^2+u(E^2+1)(1+E^{-1})(wEu-uE^{-1}w)+u(1+E^{-2}-E-E^2)q\\ &\times(E-E^{-2})^{-1}(qE^2u-uE^{-1}q)+[u(1-E^2)w-u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}\\ &\times(qE-E^{-1}q)](E^2-E^{-1})^{-1}(E^3u-uE^{-1}), \end{aligned}$$

$$\begin{aligned} H_{13}^{(3)}=&-u(1-E^{-1})vE(1+E)w+u(E^2+1)(1+E^{-1})(vw-vE^2w+qEu-uE^{-2}q)\\ &+u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)\\ &+[u(1-E^2)w-u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}\\ &\times(qE^2w-qEw+E^2v-vE^{-1}), \end{aligned}$$

$$\begin{aligned} H_{14}^{(3)}=&u(E^{-1}-1)v(1+E^2+2E+E^{-1})q+u(E^3-E^{-1})(E-1)^{-1}(-vEq+qv-uE^{-3}+Eu\\ &-vE^2q+vE^{-1}q)+u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}(wE^2q-wE^{-1}q-vE^{-2}+Ev)\\ &+[u(1-E^2)w-u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}\\ &\times(qE^2q-q^2+Ew-wE^{-1}), \end{aligned}$$

$$H_{21}^{(3)}=(wEu-uE^{-1}w)(E+1)(E^2+1)u+v(E^3-1)(E-1)^{-1}v(E^3-1)u+(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}wE^2(1-E)u+[vw-vE^2w+qEu-uE^{-2}q-(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)]\times(E^2-E^{-1})^{-1}qE^2(1-E)u,$$

$$H_{22}^{(3)}=(wEu-uE^{-1}w)v+v(E^3-1)(E-1)^{-1}(wEu-uE^{-1}w)+(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}(qE^2u-uE^{-1}q)+[vw-vE^2w+qEu-uE^{-2}q-(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)]\times(E^2-E^{-1})^{-1}(E^3u-uE^{-1}),$$

$$H_{23}^{(3)}=(uE^{-1}w-wEu)E(1+E)w+v(E^3-1)(E-1)^{-1}(vw-vE^2w+qEu-uE^{-2}q)+(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)+[(vw-vE^2w+qEu-uE^{-2}q)-(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)\times(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(qE^2w-qEw+E^2v-vE^{-1}),$$

$$H_{24}^{(3)}=(wEu-uE^{-1}w)(1-E^{-1})^{-1}(1+E^{-2}-E-E^2)q+v(E^3-1)(E-1)^{-1}(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)+(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)\times(E-E^{-2})^{-1}(wE^2q-vE^{-2}+Ev-wE^{-1}q)+[(vw-vE^2w+qEu-uE^{-2}q)-(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(qE^2q-q^2+Ew-wE^{-1}),$$

$$H_{31}^{(3)}=(qE^2u-uE^{-1}q)(E+1)(E^2+1)u-wE^2v(E^3-1)u+(wE^2q-vE^{-2}+Ev-wE^{-1}q)\times(E-E^{-2})^{-1}wE^2(1-E)u+[(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)-(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}qE^2(1-E)u,$$

$$H_{32}^{(3)}=(qE^2u-uE^{-1}q)v-wE^2(wEu-uE^{-1}w)+(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(qE^2u-uE^{-1}q)+[(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)-(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(E^3u-uE^{-1}),$$

$$H_{33}^{(3)}=(qE^2u-uE^{-1}q)(1-E^{-1})^{-1}(1-E^2)w-wE^2(wv-vE^2w+qEu-uE^{-2}q)+(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)+[(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)-(wE^2q-vE^{-2}+Ev-wE^{-1}q)\times(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(qE^2w-qEw+E^2v-vE^{-1}),$$

$$H_{34}^{(3)}=(qE^2u-uE^{-1}q)(1-E^{-1})^{-1}(1+E^{-2}-E-E^2)q-wE^2(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)+(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(wE^2q-vE^{-2}+Ev-wE^{-1}q)+[(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)-(wE^2q-vE^{-2}+Ev-wE^{-1}q)\times(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(qE^2q-q^2+Ew-wE^{-1}),$$

$$H_{41}^{(3)}=(E^3u-uE^{-1})(E+1)(E^2+1)u-qE^2v(E^3-1)u+(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}wE^2(1-E)u+[(qE^2w-qEw+E^2v-vE^{-1})-(qE^2q-q^2+Ew-wE^{-1})\times(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}qE^2(1-E)u,$$

$$H_{42}^{(3)}=(E^3u-uE^{-1})v-qE^2(wEu-uE^{-1}w)+(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}(qE^2u-uE^{-1}q)+[(qE^2w-qEw+E^2v-vE^{-1})-(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}\times(qE-E^{-1}q)](E^2-E^{-1})^{-1}(E^3u-uE^{-1}),$$

$$H_{43}^{(3)}=(E^3u-uE^{-1})(1-E^{-1})^{-1}(1-E^2)w-qE^2(vw-vE^2w+qEu-uE^{-2}q)+(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)+[(qE^2w-qEw+E^2v-vE^{-1})-(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}(qE-E^{-1}q)](E^2-E^{-1})^{-1}(qE^2w-qEw+E^2v-vE^{-1}),$$

$$H_{44}^{(3)}=(E^3u-uE^{-1})(1-E^{-1})^{-1}(1+E^{-2}-E-E^2)q-qE^2(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)+(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}(wE^2q-vE^{-2}+Ev-wE^{-1}q)+[(qE^2w-qEw+E^2v-vE^{-1})-(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1}(qE-E^{-1}q)]\times(E^2-E^{-1})^{-1}(qE^2q-q^2+Ew-wE^{-1})$$

with the recursion operator $\mathcal{R}$ for the BM4 lattice equation is

$$\mathcal{R}=\begin{bmatrix} R_{11} & R_{12} & R_{13} & R_{14} \\ R_{21} & R_{22} & R_{23} & R_{24} \\ R_{31} & R_{32} & R_{33} & R_{34} \\ R_{41} & R_{42} & R_{43} & R_{44} \end{bmatrix},$$

where

$$R_{11}=u(1-E^{-1})v(1-E^{-1})^{-1}u^{-1},$$

$$R_{12}=u(E^3-E^{-1})(E-1)^{-1},$$

$$R_{13}=u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1},$$

$$R_{14}=u(1-E^2)w(E^2-E^{-1})^{-1}-u(1+E^{-2}-E-E^2)q(E-E^{-2})^{-1}(qE-E^{-1}q)(E^2-E^{-1})^{-1}, \tag{B2a}$$

$$R_{21}=(wEu-uE^{-1}w)(1-E^{-1})^{-1}u^{-1},$$

$$R_{22}=v(E^3-1)(E-1)^{-1},$$

$$R_{23}=(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)(E-E^{-2})^{-1},$$

$$R_{24}=(vw-vE^2w+qEu-uE^{-2}q)(E^2-E^{-1})^{-1}-(-vEq+qv-uE^{-3}+Eu-vE^2q+vE^{-1}q)\times(E-E^{-2})^{-1}(qE-E^{-1}q)(E^2-E^{-1})^{-1}, \tag{B2b}$$

$$R_{31}=(qE^2u-uE^{-1}q)(1-E^{-1})^{-1}u^{-1},$$

$$R_{32}=-wE^2,$$

$$R_{33}=(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1},$$

$$R_{34}=(wE^2w-vE^{-1}q-wEw+qEv-uE^{-2}+E^2u)(E^2-E^{-1})^{-1}-(wE^2q-vE^{-2}+Ev-wE^{-1}q)(E-E^{-2})^{-1}(qE-E^{-1}q)(E^2-E^{-1})^{-1}, \tag{B2c}$$

$$R_{41}=(E^3u-uE^{-1})(1-E^{-1})^{-1}u^{-1},$$

$$R_{42}=-qE^2,$$

$$R_{43}=(qE^2q-q^2+Ew-wE^{-1})(E-E^{-2})^{-1},$$

$$R_{44}=(qE^2w-qEw+E^2v-vE^{-1})(E^2-E^{-1})^{-1}-(qE^2q-q^2+Ew-wE^{-1})(E-E^{-1})^{-1}\times(qE-E^{-1}q)(E^2-E^{-1})^{-1}. \tag{B2d}$$

Here again we have constructed a sequence of operators $H_4, H_5, \ldots$ and verified that none of them is Hamiltonian ones.

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Spectral curve and Hamiltonian structure of isomonodromic SU(2) Calogero–Gaudin system

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(Received 25 November 2001; accepted 8 May 2003)

This paper presents a new approach to the Hamiltonian structure of isomonodromic deformations of a matrix system of ordinary differential equations (ODEs) on a torus. An isomonodromic analogue of the SU(2) Calogero–Gaudin system is used for a case study of this approach. A clue of this approach is a mapping to a finite number of points on the spectral curve of the isomonodromic Lax equation. The coordinates of these moving points give a new set of Darboux coordinates called the spectral Darboux coordinates. The system of isomonodromic deformations is thereby converted to a nonautonomous Hamiltonian system in the spectral Darboux coordinates. The Hamiltonians turn out to resemble those of a previously known isomonodromic system of a second-order scalar ODE. The two isomonodromic systems are shown to be linked by a simple relation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1591053]

I. INTRODUCTION

The notion of isomonodromic deformations originates in the celebrated work of Fuchs.[1] Fuchs studied isomonodromic deformations of a second-order linear ordinary differential equation (ODE) of the form

$$\frac{\mathrm{d}^2y}{\mathrm{d}z^2}+\left(\frac{a}{z^2}+\frac{b}{(z-1)^2}+\frac{c}{(z-t)^2}+\frac{\mathrm{d}}{z(z-1)}-\frac{3}{4(z-\lambda)^2}-\frac{t(t-1)K}{z(z-1)(z-t)}+\frac{\lambda(\lambda-1)\nu}{z(z-1)(z-\lambda)}\right)y=0$$

with five regular singular points $z=0,1,\infty,t,\lambda$ on the Riemann sphere, and discovered a nonlinear ODE that is nowadays called the sixth Painlevé equation. His work was soon generalized by Garnier[2] and Schlesinger[3] in two different directions. Whereas Garnier extended the work of Fuchs to a second-order linear ODE with more singularities (including irregular ones as well), Schlesinger studied a matrix system of the form

$$\frac{\mathrm{d}Y}{\mathrm{d}z}=\sum_{j=1}^{N}\frac{A_j}{z-t_j}Y,$$

and obtained the so-called Schlesinger system

$$\frac{\partial A_k}{\partial t_j}=(1-\delta_{jk})\frac{[A_k,A_j]}{t_k-t_j}-\delta_{jk}\sum_{l\neq k}\frac{[A_k,A_l]}{t_k-t_l}$$

that characterizes isomonodromic deformations. It turned out afterwards[4] that Garnier's isomonodromic deformations with an arbitrary number of regular singular points can be reconstructed from the 2×2 Schlesinger system.

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The next stage of generalization is, naturally, isomonodromic deformations on a torus. This issue was first tackled by Okamoto,[5] who obtained a system of isomonodromic deformations of a second-order scalar ODE on a torus. One of his remarkable results is that the isomonodromic system on a torus can be formulated as a Hamiltonian system in much the same way as Garnier's isomonodromic system on a sphere was converted to a Hamiltonian system.[6] Iwasaki[7] extended Okamoto's work to scalar ODEs of an arbitrary order on an arbitrary compact Riemann surface, and elucidated the geometric origin of the Hamiltonian structure that Okamoto derived. The study of isomonodromic systems on a torus was further refined by Okamoto himself[8] and Kawai.[9]

As regards matrix systems, Korotkin and Samtleben[10] constructed an example of isomonodromic deformations of a 2×2 matrix system on a torus. Levin and Olshanetsky[11] developed a general framework in which the Schlesinger system and Korotkin and Samtleben's isomonodromic system are placed, along with generalizations to higher genus Riemann surfaces, in a unified way. Some more examples of matrix systems with different structures are also known.[12–15] Compared with Okamoto and Iwasaki's formulation, these ''elliptic analogues of the Schlesinger system'' are obtained on an entirely different ground, such as conformal field theories, vector bundles on a torus, KZ equations, and (classical or quantum) integrable systems. This can be seen in the structure of the matrix linear system

$$\frac{\mathrm{d}Y}{\mathrm{d}z}=L(z)Y$$

for which isomonodromic deformations are constructed. Namely, the matrix $L(z)$ (''L-matrix'') in these examples is borrowed from the isospectral Lax equation of an integrable system, though the Lax equation of isomonodromic deformations takes the nonisospectral form

$$\frac{\partial L(z)}{\partial t_j}=[L(z),M_j(z)]-\frac{\partial M_j(z)}{\partial z}.$$

Each of those isomonodromic systems is thus accompanied by an isospectral partner.

The correspondence between isospectral and isomonodromic systems will have a number of significant implications. Among them, we are particularly interested in the role of ''spectral Darboux coordinates.'' The notion of spectral Darboux coordinates was introduced by the Montreal group for isospectral systems with a rational L-matrix,[16] and extended to isomonodromic systems on a sphere.[17,18] As they demonstrated for those cases, one can construct a mapping from the Lax equation of this type of systems to a dynamical system of a finite number of points $P_1,\ldots,P_N$ on the spectral curve

$$\Gamma=\{(z,w)|\det(wI-L(z))=0\},$$

though the spectral curve itself becomes dynamical in the case of isomonodromic deformations. Spectral Darboux coordinates are the coordinates $\lambda_1,\ldots,\lambda_N,\mu_1,\ldots,\mu_N$ of the moving points $P_k=(\lambda_k,\mu_k)$. These coordinates lead to ''separation of variables'' of isospectral systems. The most classical case is the so-called Moser systems;[19] separation of variable of those systems was worked out by Moser himself. Remarkably, as Harnad and Wisse pointed out,[18] almost the same story repeats on the isomonodromic side, except that separability is lost there. In particular, this shows an algebro-geometric interpretation of Okamoto's reformulation[6] of Garnier's work[4] on the 2×2 Schlesinger system.

This paper presents a similar approach to one of the ''elliptic analogues'' of the Schlesinger systems, namely, the aforementioned isomonodromic system of Korotkin and Samtleben (in a slightly modified form). The isospectral partner of this isomonodromic system is the Calogero–Gaudin system[20,21] for the SU(2) group. Separation of variables of the usual SU(2) Calogero–Gaudin system has been developed by Brzeziński[22] and Enriquez *et al.*[23] (including ''quantum separation of variables'' in the sense of Sklyanin[24]). Our method is more or less parallel to theirs, in particular, that of Brzeziński. Actually, it is a rational (rather than elliptic) model of the SU(2)

Calogero–Gaudin system that he considered. Thus we are to extend his method in two ways—first, to an elliptic model (which is the subject of the work of Enriquez *et al.* as well), and second, to an isomonodromic system.

A main outcome of our consideration (summarized in Theorem 1, Sec. V) is that the isomonodromic SU(2) Calogero–Moser system can be converted to a nonautonomous Hamiltonian system in the spectral Darboux coordinates. The Hamiltonians of this non-autonomous system turn out to be a considerably intricate functions of the Darboux coordinates and the time variables. Remarkably, however, a very similar Hamiltonian system has been discovered by Okamoto[8] for isomonodromic deformations of a second-order scalar ODE on a torus. We shall show a natural explanation of this coincidence from our point of view.

This paper is organized as follows. Sections II and III are for preparation. In Sec. II, the Poisson structure of the L-matrix of the Calogero–Gaudin systems is reviewed. In Sec. III, the isomonodromic system is formulated in terms of two canonically conjugate ''Calogero variables'' and a set of ''spin variables.'' Sections IV and V are the main part of this paper. In Sec. IV, the spectral curve and the spectral Darboux coordinates are introduced. In Sec. V, the nonautonomous Hamiltonian system is derived. Section VI deals with the relation to isomonodromic deformations of a second-order scalar ODE. Section VII is for conclusion and supplementary remarks. Part of the technical details are collected in Appendixes.

II. *L*-MATRIX AND POISSON STRUCTURE

A. *L*-matrix

Following the idea of Korotkin and Samtleben,[10] we start from the L-matrix

$$L(z)=\begin{pmatrix} p & 0 \\ 0 & -p \end{pmatrix}+\sum_{j=1}^{N}\begin{pmatrix} \zeta(z-t_j)A_j^3 & \phi(q,z-t_j)A_j^- \\ \phi(-q,z-t_j)A_j^+ & -\zeta(z-t_j)A_j^3 \end{pmatrix}, \tag{1}$$

where q and p are Calogero variables, $A_j^{\pm}$ and A_j^3 are spin variables, $\zeta(z)$ denotes the Weierstrass ζ function, and $\phi(u,z)$ the auxiliary function that is widely used in the study of systems of the Calogero type:

$$\zeta(z)=\frac{\sigma'(z)}{\sigma(z)}, \quad \phi(u,z)=\frac{\sigma(u-z)}{\sigma(u)\sigma(z)}. \tag{2}$$

Here $\sigma(z)$ is the Weierstrass sigma function, and the prime stands for a derivative, i.e., $\sigma'(z)=\mathrm{d}\sigma(z)/\mathrm{d}z$. Let $2\omega_1$ and $2\omega_3$ denote the primitive periods of the Weierstrass functions. Throughout this paper, we assume that $t_j\neq t_k$ if $j\neq k$.

This L-matrix is slightly different from that of Korotkin and Samtleben.[10] They use Jacobi's elliptic theta function ϑ_1 rather than Weierstrass' sigma function σ. Their L-matrix is thereby more suited for formulating isomonodromic deformations against the modulus τ. We dare to modify Korotkin and Samtleben's L-matrix because this simplifies the use of interpolation formulas of elliptic functions. It should be possible to start from the L-matrix of Korotkin and Samtleben and to derive substantially the same results, though we shall not pursue it in this paper.

The Poisson structure of the dynamical variables is a standard one. The Calogero variables q,p are, in fact, the relative coordinate q_1-q_2 and momentum $(p_1-p_2)/2$ of a two body system with canonical variables (q_1,q_2,p_1,p_2), and become a canonically conjugate pair $\{q,p\}=1$ in themselves. The spin variables $A_j^{\pm},A_j^3$ obey the su(2) relations

$$\{A_j^3,A_k^{\pm}\}=\pm\delta_{jk}A_k^{\pm}, \quad \{A_j^+,A_k^-\}=2\delta_{jk}A_k^3 \tag{3}$$

with respect to the Poisson bracket.

The Poisson bracket of the spin variables is nothing but the Kostant–Killilov bracket for the residue matrix

$$A_j=\begin{pmatrix} A_j^3 & A_j^- \\ A_j^+ & -A_j^3 \end{pmatrix} \tag{4}$$

of $L(z)$ at $z=t_j$. The conjugacy class

$$\mathcal{O}_j=\{A_j|A_j\sim\mathrm{diag}(\theta_j/2,-\theta_j/2)\} \tag{5}$$

of semi-simple matrices with fixed eigenvalues $\pm\theta_j/2$ is a maximal (two-dimensional) symplectic leaf of this Poisson structure. One can use a canonically conjugate pair (x_j,ξ_j), $\{x_j,\xi_j\}=1$, to parametrize this symplectic leaf as follows:

$$A_j^+=-\frac{\xi_j^2}{2}+\frac{\theta_j^2}{2x_j^2},\quad A_j^-=\frac{x_j^2}{2},\quad A_j^3=\frac{x_j\xi_j}{2}. \tag{6}$$

Note that this parametrization is consistent with the Poisson bracket of $A_j^{\pm,3}$.

B. Poisson bracket of *L*-matrix elements

Let us write the matrix elements of $L(z)$ as

$$L(z)=\begin{pmatrix} A(u) & B(u) \\ C(u) & -A(u) \end{pmatrix}. \tag{7}$$

More explicitly,

$$A(u)=p+\sum_{j=1}^{N}\zeta(z-t_j)A_j^3,$$

$$B(u)=\sum_{j=1}^{N}\phi(q,z-t_j)A_j^-,$$

$$C(u)=\sum_{j=1}^{N}\phi(-q,z-t_j)A_j^+.$$

The nonzero Poisson brackets of these matrix elements take the form

$$\{A(z),B(w)\}=B(z)\phi(-q,z-w)-B(w)\zeta(z-w), \tag{8}$$

$$\{A(z),C(w)\}=-C(z)\phi(q,z-w)+C(w)\zeta(z-w), \tag{9}$$

$$\{B(z),C(w)\}=2(A(z)-A(w))\phi(q,z-w)+2\phi_u(q,z-w)\sum_{j=1}^{N}A_j^3, \tag{10}$$

where

$$\phi_u(u,z)=\frac{\partial\phi(u,z)}{\partial u}.$$

Thus the Poisson algebra of the matrix elements of $L(z)$ *almost closes* up to the extra term proportional to $\Sigma_{j=1}^{N}A_j^3$, which is later set to zero in order to derive the Lax equation.

These Poisson commutation relations can be easily verified by direct calculations using the functional identity

$$\phi(u,z)\phi(-u,w)+\phi(u,z-w)(\zeta(z)-\zeta(w))+\phi_u(u,z-w)=0 \tag{11}$$

of the auxiliary functions. This functional identity is a consequence of the more general one

$$\phi(u,z)\phi(v,w)+\phi(u+v,z)\phi(-v,z-w)-\phi(u+v,w)\phi(u,z-w)=0, \tag{12}$$

from which the former identity can be derived by letting $v\to -u$.

The Poisson structure of the $L(z)$-matrix elements can be cast into the compact form

$$\begin{aligned}\{L(z)\overset{\otimes}{,}L(w)\}&=\sum_{a,b,c,d}\{L_{ab}(z),L_{cd}(w)\}E_{ab}\otimes E_{cd}\\&=[L(z)\otimes I+I\otimes L(w),\ r(z-w)]+2\frac{\partial r(z-w)}{\partial q}\sum_{j=1}^{N}A_j^3,\end{aligned} \tag{13}$$

where E_{ab} denotes the matrix with the (a,b) element equal to 1 and the other elements vanishing. The r-matrix takes the form

$$\begin{aligned}r(z-w)&=\zeta(z-w)E_{11}\otimes E_{11}+\phi(q,z-w)E_{12}\otimes E_{21}+\phi(-q,z-w)E_{21}\otimes E_{12}+\zeta(z-w)E_{22}\otimes E_{22}\\&=\begin{pmatrix}\zeta(z-w)&0&0&0\\0&0&\phi(q,z-w)&0\\0&\phi(-q,z-w)&0&0\\0&0&0&\zeta(z-w)\end{pmatrix},\end{aligned} \tag{14}$$

which is a special case of the well-known dynamical r-matrix of the elliptic Calogero–Moser system.[25–27]

III. HAMILTONIANS AND LAX EQUATIONS

A. Hamiltonians

We now introduce the Hamiltonians

$$\mathcal{H}_j=\operatorname*{Res}_{z=t_j}\frac{1}{2}\operatorname{Tr}L(z)^2, \tag{15}$$

which can be written, more explicitly, as

$$\mathcal{H}_j=pA_j^3+2\sum_{k\neq j}\zeta(t_j-t_k)A_j^3A_k^3+\sum_{k\neq j}\phi(-q,t_j-t_k)A_j^-A_k^++\sum_{k\neq j}\phi(q,t_j-t_k)A_j^+A_k^-.$$

Note that these Hamiltonians depend on the time variables explicitly; the associated Hamiltonian system is thus nonautonomous. As we show in the following, these Hamiltonians *almost commute* up to a term proportional to the factor $\Sigma_j A_j$.

To this end, we use the general formula

$$\left\{\frac{1}{m}\operatorname{Tr}L(z)^m,\ \frac{1}{k}\operatorname{Tr}L(n)^n\right\}=\operatorname{Tr}(\{L(z)\overset{\otimes}{,}L(w)\}L(z)^{m-1}\otimes L(w)^{n-1}). \tag{16}$$

Inserting the Poisson commutation relations (13) into the right-hand side, we obtain the identity

$$\left\{\frac{1}{2}\operatorname{Tr}L(z)^2,\ \frac{1}{2}\operatorname{Tr}L(w)^2\right\}=2\operatorname{Tr}\left(\frac{\partial r(z-w)}{\partial q}L(z)\otimes L(w)\right)\sum_{j=1}^{N}A_j^3, \tag{17}$$

which implies that the Poisson brackets of the Hamiltonians are proportional to $\Sigma_{j=1}^N A_j^3$:

$$\{\mathcal{H}_j,\mathcal{H}_k\}\propto\sum_{j=1}^N A_j^3. \tag{18}$$

Moreover, as direct calculations show, the factor $\Sigma_{j=1}^N A_j^3$ itself commutes with the Hamiltonians:

$$\left\{\sum_{j=1}^N A_j^3,\ \mathcal{H}_k\right\}=0. \tag{19}$$

These relations ensure that one can consistently impose the constraint

$$\sum_{j=1}^N A_j^3=0, \tag{20}$$

which is preserved by the Hamiltonian flows

$$\frac{\partial q}{\partial t_j}=\{q,\mathcal{H}_j\},\quad \frac{\partial p}{\partial t_j}=\{p,\mathcal{H}_j\},\quad \frac{\partial A_k}{\partial t_j}=\{A_k,\mathcal{H}_j\}. \tag{21}$$

This constrained nonautonomous Hamiltonian system is our elliptic analogue of the Schesinger system.

B. Calculating $\{L(z),\mathcal{H}_j\}$

Our next task is to calculate the Poisson bracket

$$\{L(z),\mathcal{H}_j\}=\sum_{a,b}\{L_{ab}(z),\mathcal{H}_j\}E_{ab}$$

of the L-matrix with the Hamiltonians. To this end, one can use another general formula

$$\left\{L(z),\ \frac{1}{n}\mathrm{Tr}L(w)^n\right\}=\mathrm{Tr}_2(\{L(z)\overset{\otimes}{,}L(w)\}I\otimes L(w)^{n-1}), \tag{22}$$

where Tr_2 denotes the trace over the second component of the tensor product:

$$\mathrm{Tr}_2\left(\sum_{a,b,c,d}X_{abcd}E_{ab}\otimes E_{cd}\right)=\sum_{a,b}\left(\sum_c X_{abcc}\right)E_{ab}.$$

Plugging the Poisson commutation relation (13) into this formula, one obtains the identity

$$\left\{L(z),\ \frac{1}{2}\mathrm{Tr}L(w)^2\right\}=[L(z),\ \mathrm{Tr}_2(r(z-w)I\otimes L(w))]+2\,\mathrm{Tr}_2\left(\frac{\partial r(z-w)}{\partial q}I\otimes L(w)\right)\sum_{j=1}^N A_j^3. \tag{23}$$

The residue at $w=t_j$ should give the Poisson bracket that we have sought. The residues of the quantities on the right-hand side can be easily evaluated:

$$\operatorname*{Res}_{w=t_j}\mathrm{Tr}_2(r(z-w)I\otimes L(w))=\begin{pmatrix}\zeta(z-t_j)A_j^3 & \phi(q,z-t_j)A_j^-\\ \phi(-q,z-t_j)A_j^+ & -\zeta(z-t_j)A_j^3\end{pmatrix},$$

$$\operatorname*{Res}_{w=t_j} \mathrm{Tr}_2\left(\frac{\partial r(z-w)}{\partial q} I\otimes L(w)\right)=\begin{pmatrix} 0 & \phi_u(q,z-t_j)A_j^- \\ -\phi_u(-q,z-t_j)A_j^+ & 0 \end{pmatrix}.$$

One thus ends up with the identity

$$\{L(z),\mathcal{H}_j\}=[L(z),M_j(z)]+\text{term proportional to } \Sigma_{j=1}^N A_j^3, \tag{24}$$

where

$$M_j(z)=\begin{pmatrix} \zeta(z-t_j)A_j^3 & \phi(q,z-t_j)A_j^- \\ \phi(-q,z-t_j)A_j^+ & -\zeta(z-t_j)A_j^3 \end{pmatrix}. \tag{25}$$

C. Isomonodromic Lax equation

We are now ready to rewrite the constrained Hamiltonian system (20) and (21) into an isomonodromic Lax equation.

Let us examine what occurs if the matrix elements of $L(z)$ are differentiated against t_j. For instance, the (1,2) element reads

$$L_{12}(z)=\sum_{k=1}^N \phi(q,z-t_k)A_k^-,$$

hence the Leibniz rule yields

$$\frac{\partial L_{12}(z)}{\partial t_j}=\sum_{k=1}^N \left(\phi_u(q,z-t_k)\frac{\partial q}{\partial t_j}A_k^- + \phi(q,z-t_k)\frac{\partial A_k^-}{\partial t_j}\right)-\phi'(q,z-t_j)A_j^-,$$

where

$$\phi'(u,z)=\frac{\partial \phi(q,z)}{\partial z}.$$

Note here that the last term on the right-hand side is equal to $\partial M_{j,12}(z)/\partial z$. Since the t_j-derivatives of the dynamical variables can be expressed as the Poisson bracket with $\mathcal{H}_j$ [see (21)], the foregoing equation can be rewritten

$$\frac{\partial L_{12}(z)}{\partial t_j}=\{L_{12}(z),\mathcal{H}_j\}-\frac{\partial M_{j,12}(z)}{\partial z}.$$

Repeating similar calculations for the other matrix elements, we can eventually confirm that

$$\frac{\partial L(z)}{\partial t_j}=\{L(z),\mathcal{H}_j\}-\frac{\partial M_j(z)}{\partial z}.$$

We now turn on the constraint (20) and apply the previous calculation converting the Poisson bracket $\{L(z),\mathcal{H}_j\}$ to the commutator $[L(z),M_j(z)]$. The outcome is the isomonodromic Lax equation

$$\frac{\partial L(z)}{\partial t_j}=[L(z),M_j(z)]-\frac{\partial M_j(z)}{\partial z} \tag{26}$$

with an extra term on the right-hand side that breaks isospectrality of the L-matrix.

IV. SPECTRAL CURVE AND DARBOUX COORDINATES

A. Spectral curve

The spectral curve is defined by the eigenvalue equation

$$\det(wI - L(z)) = 0. \tag{27}$$

Since $L(z)$ is trace-free, the left-hand side can be rewritten as

$$\det(wI - L(z)) = w^2 + \det L(z) = w^2 - \tfrac{1}{2}\mathrm{Tr}\, L(z)^2. \tag{28}$$

Under the constraint (20), the matrix elements of $L(z)$ enjoy the following quasi-periodicity along the period lattice of the torus:

$$L(z + 2m\omega_1 + 2n\omega_3) = e^{-(2m\eta_1 + 2n\eta_3)Q} L(z) e^{(2m\eta_1 + 2n\eta_3)Q}, \tag{29}$$

where Q is the diagonal matrix $Q = \mathrm{diag}(q, -q)$, and η_1 and η_3 are the values of $\zeta(z)$ at $z = \omega_1, \omega_3$. The quasiperiodicity of $L(z)$ is a consequence of the quasiperiodicity of $\zeta(z)$ and $\phi(u,z)$,

$$\zeta(z + 2m\omega_1 + 2n\omega_3) = \zeta(z) + 2m\eta_1 + 2n\omega_3, \tag{30}$$

$$\phi(u, z + 2m\omega_1 + 2m\omega_3) = e^{-2m\eta_1 - 2n\eta_3} \phi(u,z), \tag{31}$$

which are easy to confirm from the property of the sigma function.

The quasiperiodicity of $L(z)$, in particular, implies the double periodicity of $\mathrm{Tr}\, L(z)^2/2$, which thereby becomes an elliptic function with poles at $z = t_1, \ldots, t_N$. Since

$$L(z) = \frac{A_j}{z - t_j} + O(1)$$

as $z \to t_j$, this elliptic function has a double pole at $z = t_j$ with the leading coefficient equal to the quadratic Casimir

$$C_j = \frac{1}{2}\mathrm{Tr}\, A_j^2 = \frac{\theta_j^2}{4} \tag{32}$$

of A_j. The residue is nothing but the Hamiltonian $\mathcal{H}_j$. Thus $\mathrm{Tr}\, L(z)^2/2$ can be expressed as

$$\frac{1}{2}\mathrm{Tr}\, L(z)^2 = \sum_{j=1}^{N} C_j \wp(z - t_j) + \sum_{j=1}^{N} \mathcal{H}_j \zeta(z - t_j) + \mathcal{H}_0, \tag{33}$$

where $\mathcal{H}_0$ is a constant term (which however depends on ω_1 and ω_3). Also note that the Hamiltonians are not linearly independent, but obey the linear constraint

$$\sum_{j=1}^{N} \mathcal{H}_j = 0. \tag{34}$$

This is a consequence of the the double periodicity of $\mathrm{Tr}\, L(z)^2/2$.

The spectral curve thus turns out to be a double covering of the torus. The branch points are located above the (possibly multiple) $2N$ zeros of $\mathrm{Tr}\, L(z)^2/2$. If these zeros are all simple, the genus of the spectral curve is equal to $N+1$. The spectral curve is time-dependent because of the extra term $\partial M_j(z)/\partial z$ on the right-hand side of the Lax equation.

B. Spectral Darboux coordinates

The construction of spectral Darboux coordinates is parallel to the case of the rational (and isospectral) model.[22] The "coordinate part" $\lambda_1,\ldots,\lambda_N$ are defined as the N zeros (modulo the period lattice) of $L_{12}(z)$,

$$L_{12}(\lambda_j)=0, \tag{35}$$

and the "momentum part" $\mu_1,\ldots,\mu_N$ are defined to be the value of $L_{11}(z)$ at these points,

$$\mu_j=L_{11}(\lambda_j)=p+\sum_{k=1}^{N}\zeta(\lambda_j-t_k)A_k^3. \tag{36}$$

In order to avoid a delicate problem, we assume throughout the following consideration that $\lambda_j \neq \lambda_k$ if $j\neq k$. It is easy to see that (λ_j,μ_j) sits on the spectral curve; $L(\lambda_j)$ takes the triangular form

$$L(\lambda_j)=\begin{pmatrix} \mu_k & 0 \\ L_{21}(\lambda_j) & -\mu_k \end{pmatrix},$$

which implies that $\pm\mu_j$ are eigenvalues of $L(\lambda_j)$.

The λ_j's are constrained by a linear relation. To see this, let us note that $L_{12}(z)$ can be factorized as

$$L_{12}(z)=\kappa\frac{\Pi_{j=1}^{N}\sigma(z-\lambda_j)}{\Pi_{j=1}^{N}\sigma(z-t_j)}, \tag{37}$$

where κ is a constant that does not depend on z. The quasiperiodicity

$$L_{12}(z+2m\omega_1+2n\omega_3)=e^{-(2m\eta_1+2n\eta_3)q}L_{12}(z)$$

of $L_{12}(z)$ implies that its zeros $\lambda_1,\ldots,\lambda_N$ are constrained as

$$\sum_{j=1}^{N}\lambda_j-\sum_{j=1}^{N}t_j\equiv q \quad \mathrm{mod}\, 2\omega_1\mathbf{Z}+2\omega_3\mathbf{Z}. \tag{38}$$

Since each λ_j is defined only up to a difference by an element of the period lattice, let us redefine λ_j's, if necessary, such that this holds without "$\mathrm{mod}\, 2\omega_1\mathbf{Z}+2\omega_3\mathbf{Z}$":

$$\sum_{j=1}^{N}\lambda_j-\sum_{j=1}^{N}t_j=q. \tag{39}$$

Of course this will be valid only for a *local* study of the system; this naive prescription has to be modified if one considers a global problem.

C. Time-dependent canonical transformation

In order to prove the canonicity of these variables λ_j,μ_j, we now restrict the spin variables onto the direct product $\mathcal{O}_1\times\cdots\times\mathcal{O}_N$ of the symplectic leaves and use the parametrization (6) by (x_j,ξ_j). Moreover, we tentatively relax the constraint (20), which now takes the form

$$\sum_{j=1}^{N}x_j\xi_j=0, \tag{40}$$

and restore it in the final stage.

The factorization relation (37) of $L_{12}(z)$ now reads

$$\frac{1}{2}\sum_{j=1}^{N}\phi(q,z-t_j)x_j^2=\kappa\frac{Q(z)}{P(z)}, \tag{41}$$

where we have introduced the two functions

$$Q(z)=\prod_{j=1}^{N}\sigma(z-\lambda_j),\quad P(z)=\prod_{j=1}^{N}\sigma(z-t_j). \tag{42}$$

This reduces to the relations

$$\frac{1}{2}x_j^2=\kappa\frac{Q(t_j)}{P'(t_j)}=\kappa\frac{\Pi_{k=1}^{N}\sigma(t_j-\lambda_k)}{\Pi_{k\neq j}\sigma(t_j-t_k)} \tag{43}$$

of the residues of both sides at $z=t_j$. These relations show how the old variables x_j are connected with the new variables λ_j (and κ). By logarithmic differentiation, these relations can be further converted to the linear relations

$$\begin{aligned}2\,\mathrm{d}\log x_j&=\mathrm{d}\log\kappa+\sum_{k=1}^{N}\mathrm{d}\log\sigma(t_j-\lambda_k)-\sum_{k\neq j}\mathrm{d}\log\sigma(t_j-t_k)\\&=\mathrm{d}\log\kappa+\sum_{k=1}^{N}\zeta(t_j-\lambda_k)(\mathrm{d}t_j-\mathrm{d}\lambda_k)-\sum_{k\neq j}\zeta(t_j-t_k)(\mathrm{d}t_j-\mathrm{d}t_k)\end{aligned} \tag{44}$$

of differential forms.

Our goal is to derive a relation between the canonical one-forms $\Sigma_{j=1}^{N}\xi_j\mathrm{d}x_j+p\,\mathrm{d}q$ and $\Sigma_{j=1}^{N}\mu_j\mathrm{d}\lambda_j$. We first multiply the both sides of the last relation by $x_j\xi_j/2$, sum over $j=1,\ldots,N$, and add $p\,\mathrm{d}q$ to both sides. We then obtain the linear relation

$$\begin{aligned}\sum_{j=1}^{N}\xi_j\,\mathrm{d}x_j+p\,\mathrm{d}q&=\frac{1}{2}\sum_{j=1}^{N}x_j\xi_j\mathrm{d}\log\kappa+\frac{1}{2}\sum_{j,k=1}^{N}x_j\xi_j\zeta(t_j-\lambda_k)(\mathrm{d}t_j-\mathrm{d}\lambda_k)\\&\quad-\frac{1}{2}\sum_{j\neq k}x_j\xi_j\zeta(t_j-t_k)(\mathrm{d}t_j-\mathrm{d}t_k)+p\,\mathrm{d}q.\end{aligned}$$

On the other hand, by differentiating (39), we have the relation

$$\mathrm{d}q=\sum_{j=1}^{N}\mathrm{d}\lambda_j-\sum_{j=1}^{N}\mathrm{d}t_j,$$

which we can use to eliminate the differential $\mathrm{d}q$ on the right-hand side of the foregoing linear relation of one-forms. The right-hand side thereby becomes a linear combination of $\mathrm{d}\log\kappa$, $\mathrm{d}\lambda_j$'s, and $\mathrm{d}t_j$'s, and the coefficient of $\mathrm{d}\lambda_j$ turns out to be equal to μ_j by (36). We thus eventually find that

$$\begin{aligned}\sum_{j=1}^{N}\xi_j\mathrm{d}x_j+p\,\mathrm{d}q&=\frac{1}{2}\sum_{j=1}^{N}x_j\xi_j\mathrm{d}\log\kappa+\sum_{j=1}^{N}\mu_j\mathrm{d}\lambda_j-p\sum_{j=1}^{N}\mathrm{d}t_j+\frac{1}{2}\sum_{j,k=1}^{N}x_j\xi_j\zeta(t_j-\lambda_k)\mathrm{d}t_j\\&\quad-\frac{1}{2}\sum_{j\neq k}x_j\xi_j\zeta(t_j-t_k)(\mathrm{d}t_j-\mathrm{d}t_k).\end{aligned} \tag{45}$$

Equation (45) shows that λ_j and μ_j are Darboux coordinates of the canonical one-form $\Sigma_{j=1}^{N}\xi_j\,dx_j+p\,dq$, and that $\log\kappa$ is a conjugate variable of the left-hand side of constraint (40). This interpretation is fully parallel to the spectral description of rational isospectral systems.[16–18]

An essential difference lies in the fact that the time variables explicitly enter the relation between the two canonical one-forms. This means that the spectral Darboux coordinates are connected with the old variables (x_j,ξ_j,q,p) by a *time-dependent* canonical transformation. Accordingly, the Hamiltonians (which is denoted by H_j in the following) in the spectral Darboux coordinates differ from the Hamiltonians $\mathcal{H}_j$ in the old variables (x_j,ξ_j,q,p). Their relation is to be determined by the fundamental formula

$$\sum_{j=1}^{N}\xi_j dx_j+p\,dq-\sum_{j=1}^{N}\mathcal{H}_j dt_j=\sum_{j=1}^{N}\mu_j d\lambda_j-\sum_{j=1}^{N}H_j dt_j, \tag{46}$$

in which we have imposed the constraint (40). More explicitly, the new Hamiltonians are defined as

$$H_j=\mathcal{H}_j+p-\frac{1}{2}x_j\xi_j\left(\sum_{k=1}^{N}\zeta(t_j-\lambda_k)-\sum_{k\neq j}\zeta(t_j-t_k)\right)+\frac{1}{2}\sum_{k\neq j}\zeta(t_j-t_k)x_k\xi_k. \tag{47}$$

The goal of Sec. V is to rewrite the right-hand side in terms of the spectral Darboux coordinates.

V. HAMILTONIAN SYSTEM IN SPECTRAL DARBOUX COORDINATES

A. Linear equations characterizing Hamiltonians

Let us recall that the pairs (λ_j,μ_j) of the spectral Darboux coordinates all sit on the spectral curve. Therefore the equations

$$\mu_k^2=\sum_{j=1}^{N}C_j\wp(\lambda_k-t_j)+\sum_{j=1}^{N}\mathcal{H}_j\zeta(\lambda_k-t_j)+\mathcal{H}_0$$

are satisfied for $k=1,\ldots,N$. These equations, along with the linear constraint (34), may be thought of as a system of linear equations that determine $\mathcal{H}_j$'s. In fact, as we shall discuss afterwards, these linear equations can be solved for $\mathcal{H}_j$'s, which thereby becomes an explicit function of the spectral Darboux coordinates (and of the time variables).

If the system in consideration were an isospectral system (such as the Moser system or the usual Calogero–Gaudin system), the time variables would not appear here explicitly, and $\mathcal{H}_j$'s would be the Hamiltonians that we have sought. The only problem would have been to solve the foregoing linear equations for $\mathcal{H}_j$. This is, actually, what Brzeziński[22] and Enriquez *et al.*[23] did in their work on separation of variables of the SU(2) Calogero–Gaudin system.

In the present case, the true Hamiltonians are *not* $\mathcal{H}_j$'s *but* H_j's. We have to rewrite the extra terms on the right-hand side of (47), too, as a function of the spectral Darboux coordinates. This is another problem that we have to solve.

To this end, let us note that the defining equation (36) of μ_j, which can be rewritten as

$$\mu_k=\sum_{j=1}^{N}\zeta(\lambda_k-t_j)\frac{x_j\xi_j}{2}+p,$$

may be thought of as a system of linear equations for p and $x_j\xi_j/2$. If one can solve these equations for p and $x_j\xi_j/2$, the solution should be an expression of p and $x_j\xi_j/2$ as a function of the spectral Darboux coordinates. Remarkably, these linear equations have the same coefficients as the foregoing linear equations for $\mathcal{H}_0$ and $\mathcal{H}_j$. Moreover, $x_j\xi_j/2$ obey the linear constraint (40), in perfect analogy with the linear constraint (34) for $\mathcal{H}_j$.

Thus the two problems, one for $\mathcal{H}_j$ and the other for the extra terms in (47), can be reduced to a single problem, namely, solving a system of linear equations of the form

$$\sum_{j=1}^{N} \zeta(\lambda_k - t_j) X_j + X_0 = b_k \quad (k=1,\dots,N),$$
$$\sum_{j=1}^{N} X_j = 0. \tag{48}$$

As we shall show in the following, this system of linear equations has a unique and explicit solution.

B. Solution of linear equations

We assume that $q \not\equiv 0 \bmod 2\omega_1\mathbf{Z} + 2\omega_3\mathbf{Z}$ or, equivalently, $\sigma(q) \neq 0$. The following ensures the uniqueness of solution of (48).

Lemma 1: If $b_j = \cdots = b_N = 0$, *then* $X_0 = X_1 = \cdots = X_N = 0$.

Proof: Consider the function

$$f(z) = \sum_{j=1}^{N} \zeta(z - t_j) X_j + X_0.$$

The first N equations of (48) imply that $f(z)$ has zeros at $z = \lambda_1, \dots, \lambda_N$. The remaining one ensures that $f(z)$ is a doubly periodic meromorphic function on the z plane. All possible poles are obviously simple and confined to $z = t_1, \dots, t_N$ and their translations by the period lattice. Therefore, if $f(z)$ is not identically zero, the zeros λ_j and the poles t_j are constrained as

$$\sum_{j=1}^{N} \lambda_j - \sum_{j=1}^{N} t_j \equiv 0 \mod 2\omega_1\mathbf{Z} + 2\omega_3\mathbf{Z},$$

but this contradicts the assumption that $q \not\equiv 0$; recall the constraint (39). Thus $f(z)$ is identically zero, and all the coefficients $X_0, X_1, \dots, X_N$ have to be zero. Q.E.D.

Having proven the uniqueness, the problem is to find a solution by any means. This can be done with the aid of an elliptic analogue of Lagrange's interpolation formula (see Appendix A).

Lemma 2: A solution of (48) is given by

$$X_j = \sum_{k=1}^{N} \frac{Q(t_j) P(\lambda_k) \sigma(t_j - \lambda_k + q) b_k}{P'(t_j) Q'(\lambda_k) \sigma(t_j - \lambda_k) \sigma(q)}, \tag{49}$$

$$X_0 = -\sum_{j,k=1}^{N} \frac{Q(t_j) P(\lambda_k) \sigma(t_j - \lambda_k + q) \zeta(\lambda_k - t_j - q) b_k}{P'(t_j) Q'(\lambda_k) \sigma(t_j - \lambda_k) \sigma(q)}. \tag{50}$$

Proof: We have only to confirm that these X_j and X_0 do satisfy (48). The last equation of (48) is indeed satisfied as (A1) shows. As regards the other equations of (48), the main task is to calculate

$$\sum_{j=1}^{N} \zeta(\lambda_l - t_j) X_j = \sum_{k=1}^{N} \left(\sum_{j=1}^{N} \frac{Q(t_j) \sigma(t_j - \lambda_k + q)}{P'(t_j) \sigma(t_j - \lambda_k)} \zeta(\lambda_l - t_j) \right) \frac{P(\lambda_k) b_k}{Q'(\lambda_k) \sigma(q)}.$$

We can use the two identities (A3) and (A4) to rewrite the sum over j on the right-hand side, and find that

$$\sum_{j=1}^{N}\zeta(\lambda_l-t_j)X_j=\sum_{k,j=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)\zeta(\lambda_k-t_j-q)b_k}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)}+b_l=-X_0+b_l,$$

which is nothing but the first N equations of (48). Q.E.D.

C. Writing H_j explicitly

Let us apply the foregoing formulas (49) and (50) of solution of (48) to the problem of deriving an explicit form of H_j as a function of the spectral Darboux coordinates.

If we use the formulas to the case where

$$X_j=\mathcal{H}_j,\quad X_0=\mathcal{H}_0,\quad b_k=\mu_k^2-\sum_{l=1}^{N}C_l\wp(\lambda_k-t_l),$$

we find the following expression of $\mathcal{H}_j$ and $\mathcal{H}_0$:

$$\mathcal{H}_j=\sum_{j=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)}\left(\mu_k^2-\sum_{l=1}^{N}C_l\wp(\lambda_k-t_l)\right),\tag{51}$$

$$\mathcal{H}_0=-\sum_{j,k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)\zeta(\lambda_k-t_j-q)}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)}\left(\mu_k^2-\sum_{l=1}^{N}C_l\wp(\lambda_k-t_l)\right).\tag{52}$$

Similarly, if we use the formulas in the case where

$$X_j=\tfrac{1}{2}x_j\xi_j,\quad X_0=p,\quad b_k=\mu_k,$$

we find the following expression of $x_j\xi_j/2$ and p as a function of the spectral Darboux coordinates:

$$\frac{1}{2}x_j\xi_j=\sum_{k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)\mu_k}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)},\tag{53}$$

$$p=-\sum_{j,k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)\zeta(\lambda_k-t_j-q)\mu_k}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)}.\tag{54}$$

Thus we have been able to rewrite each term on the right-hand side of (47) to an explicit function of the spectral Darboux coordinates.

Although the extra terms on the right-hand side of (47) still appear to be in disorder, one can see by straightforward calculations (see Appendix B) that the sum of these terms boils down to a form similar to the foregoing expression of $\mathcal{H}_j$:

$$\begin{aligned}p-\frac{1}{2}x_j\xi_j\left(\sum_{k=1}^{N}\zeta(t_j-\lambda_k)-\sum_{k\neq j}\zeta(t_j-t_k)\right)+\frac{1}{2}\sum_{k\neq j}\zeta(t_j-t_k)x_k\xi_k\\=\sum_{k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)}(\zeta(t_j-\lambda_k+q)-\zeta(t_j-\lambda_k))\mu_k.\end{aligned}\tag{55}$$

Combining these results, we obtain the following expression of H_j in terms of the spectral Darboux coordinates:

$$H_j=\sum_{k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(t_j-\lambda_k+q)}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(q)}$$
$$\times\left(\mu_k^2+(\zeta(t_j-\lambda_k+q)-\zeta(t_j-\lambda_k))\mu_k-\sum_{l=1}^{N}C_l\wp(\lambda_k-t_l)\right). \tag{56}$$

Eliminating q by (39), we eventually obtain a final expression of the Hamiltonians:

$$H_j=\sum_{k=1}^{N}\frac{Q(t_j)P(\lambda_k)\sigma(\Sigma_{l\neq k}\lambda_l-\Sigma_{l\neq j}t_l)}{P'(t_j)Q'(\lambda_k)\sigma(t_j-\lambda_k)\sigma(\Sigma_{l=1}^{N}\lambda_l-\Sigma_{l=1}^{N}t_l)}$$
$$\times\left(\mu_k^2+(\zeta(t_j-\lambda_k+q)-\zeta(t_j-\lambda_k))\mu_k-\sum_{l=1}^{N}C_l\wp(\lambda_k-t_l)\right). \tag{57}$$

In summary, we have proven the following.

Theorem 1: *The isomonodromic* SU(2) *Calogero–Gaudin system can be converted to the nonautonomous Hamiltonian system*

$$\frac{\partial\lambda_k}{\partial t_j}=\frac{\partial H_j}{\partial\mu_k},\quad \frac{\partial\mu_k}{\partial t_j}=-\frac{\partial H_j}{\partial\lambda_j} \tag{58}$$

in the spectral Darboux coordinates λ_j,μ_j. *The Hamiltonians are given by (57).*

VI. RELATION TO SECOND-ORDER SCALAR ODE

A. Deriving second-order ODE

The structure of the Hamiltonians H_j is very similar to Okamoto's Hamiltonians for isomonodromic deformations of a scalar ODE on a torus.[8] This is not a coincidence, but can be explained in the same way as the case of the 2×2 Schlesinger system.[6]

A clue is the fact that any 2×2 matrix system

$$\frac{\mathrm{d}Y}{\mathrm{d}z}=L(z)Y,\quad Y=\begin{pmatrix}y_1\\y_2\end{pmatrix},$$

yields a second-order scalar ODE of the form

$$\frac{\mathrm{d}^2y_1}{\mathrm{d}z^2}+p_1(z)\frac{\mathrm{d}y_1}{\mathrm{d}z}+p_2(z)y_1=0. \tag{59}$$

The coefficients $p_1(z)$ and $p_2(z)$ of the latter are determined by the matrix $L(z)$ as follows:

$$p_1(z)=-\operatorname{Tr}L(z)-(\log L_{12}(z))', \tag{60}$$

$$p_2(z)=\det L(z)-L_{11}'(z)+L_{11}(z)(\log L_{12}(z))'. \tag{61}$$

In our case, $L(z)$ is trace-free, so that the foregoing formulas of $p_1(z)$ and $p_2(z)$ become slightly simpler: First, $p_1(z)$ can be written explicitly as

$$p_1(z)=-(\log L_{12}(z))'=-\sum_{j=1}^{N}\zeta(z-\lambda_j)+\sum_{j=1}^{N}\zeta(z-t_j), \tag{62}$$

which implies that $p_1(z)$ is doubly periodic. Second, $p_2(z)$ is also doubly periodic (as the quasiperiodicity of the matrix elements of $L(z)$ implies), and given by

$$p_2(z) = -\tfrac{1}{2}\mathrm{Tr}\, L(z)^2 - L_{11}'(z) + L_{11}(z)(\log L_{12}(z))'.$$

One can see from this formula that $p_2(z)$ has simple poles at $z=\lambda_j$ and double poles at $z=t_j$. Let us express $p_2(z)$ as

$$p_2(z) = \sum_{j=1}^{N} \alpha_j \wp(z-t_j) + \sum_{j=1}^{N} \beta_j \zeta(z-t_j) + \sum_{j=1}^{N} \gamma_j \zeta(z-\lambda_j) + \delta \tag{63}$$

and determine the coefficients by Laurent expansion at the poles.

(1) The first coefficient α_j can be read off from the $(z-t_j)^{-2}$ term of the Laurent expansion of $-\mathrm{Tr}\, L(z)^2/2$:

$$\alpha_j = -C_j = -\mathrm{Tr}\, A_j^2/2. \tag{64}$$

(2) The second coefficient β_j is the residue of $p_2(z)$ at $z=t_j$. The term $L_{11}'(z)$ does not contribute to the residue. The residue of the other terms at $z=t_j$ can be expressed as

$$-\operatorname*{Res}_{z=t_j} \tfrac{1}{2}\mathrm{Tr}\, L(z)^2 = -\mathcal{H}_j$$

and

$$\operatorname*{Res}_{z=t_j} L_{11}(z)(\log L_{12}(z))' = -p - \frac{1}{2}\sum_{k\neq j} \zeta(t_j-t_k)x_k\xi_k + \frac{1}{2}x_j\xi_j\left(\sum_{k=1}^{N} \zeta(t_j-\lambda_k) - \sum_{k\neq j} \zeta(t_j-t_k)\right).$$

As (47) shows, the sum of these two quantities is equal to $-H_j$. Therefore

$$\beta_j = \operatorname*{Res}_{z=t_j} p_2(z) = -H_j. \tag{65}$$

(3) The thrid coefficient γ_j is the residue of $p_2(z)$ at $z=\lambda_j$. Since

$$-\operatorname*{Res}_{z=\lambda_j} \tfrac{1}{2}\mathrm{Tr}\, L(z)^2 = 0$$

and

$$\operatorname*{Res}_{z=\lambda_j} L_{11}(z)(\log\, L_{12}(z))' = L_{11}(\lambda_j) = \mu_j,$$

γ_j can be expressed as

$$\gamma_j = \operatorname*{Res}_{z=\lambda_j} p_2(z) = \mu_j. \tag{66}$$

Thus the Hamiltonians H_j and the ''momenta'' μ_j can be identified with the residues of $p_2(z)$. Exactly the same relation can be seen in the case of Garnier's isomonodromic system on a sphere.[6]

B. Another form of second-order ODE

Strictly speaking, however, the second-order ODE above differs from that of Okamoto[8] and Kawai,[9] who consider a linear ODE of the form

$$\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + p(z)y = 0. \tag{67}$$

At least formally, this discrepancy can be removed by the ''gauge transformation''

$$y_1 = \exp\left(-\tfrac{1}{2}\int^z p_1(z)\mathrm{d}z \right) y. \tag{68}$$

The coefficient $p(z)$ is given by

$$p(z) = -\tfrac{1}{2}p_1'(z) - \tfrac{1}{4}p_1(z)^2 + p_2(z). \tag{69}$$

Note, however, that this is actually a delicate procedure, because the gauge transformation might spoil the isomonodromic property. Fortunately, the present case is free from this problem: The gauge transformation takes the form

$$y_1 = \left(\frac{\Pi_{j=1}^N \sigma(z-\lambda_j)}{\Pi_{j=1}^N \sigma(z-t_j)} \right)^{1/2} y, \tag{70}$$

and since the factor in front of y has constant monodromy, the isomonodromic property is preserved by the gauge transformation.

The zeroth order term $p(z)$ of the transformed ODE is a doubly periodic meromorphic function with second-order poles at $z=\lambda_j, t_j$. The residues of $p(z)$ at these poles can be readily determined:

$$\operatorname*{Res}_{z=\lambda_j} p(z) = \mu_j - 2\sum_{k=1}^N \zeta(\lambda_j - t_k) + 2\sum_{k\neq j} \zeta(\lambda_j - \lambda_k), \tag{71}$$

$$\operatorname*{Res}_{z=t_j} p(z) = -H_j - 2\sum_{k=1}^N \zeta(t_j - \lambda_k) + 2\sum_{k\neq j} \zeta(t_j - t_k). \tag{72}$$

It is rather these quantities that Okamoto[8] and Kawai[9] use as Hamiltonians and conjugate variables of λ_j's. We can indeed reformulate our Hamiltonian system in that way. Namely, if we define

$$\nu_j = \operatorname*{Res}_{z=\lambda_j} p(z), \quad K_j = -\operatorname*{Res}_{z=t_j} p(z), \tag{73}$$

these quantities satisfy

$$\sum_{j=1}^N \mu_j \mathrm{d}\lambda_j - \sum_{j=1}^N H_j \mathrm{d}t_j = \sum_{j=1}^N \nu_j \mathrm{d}\lambda_j - \sum_{j=1}^N K_j \mathrm{d}t_j + \text{exact form}. \tag{74}$$

This implies that λ_j's and ν_j's are a new set of Darboux coordinates, and that the previous Hamiltonian system is now converted to the new Hamiltonian system

$$\frac{\partial \lambda_k}{\partial t_j} = \frac{\partial K_j}{\partial \nu_k}, \quad \frac{\partial \nu_k}{\partial t_j} = -\frac{\partial K_j}{\partial \lambda_j}. \tag{75}$$

C. Reconstructing 2×2 matrix system

Let us now consider the inverse problem. Namely, given the isomonodromic deformations of the second-oder scalar ODE above, the problem is to reconstruct a 2×2 matrix system. A similar problem is discussed by Okamoto (Ref. 6, Sec. 3) in the case of isomonodromic deformations on a sphere. One can mostly follow his method. As it turns out, the L-matrix $L(z)$ can be reconstructed by an algebraic procedure once the factor κ is determined. The factor κ, on the other hand, has to be determined by a set of differential equations.

Suppose that κ has been determined. The first step of reconstruction of $L(z)$ is to reconsider (37) and (39) as *definition* of $L_{12}(z)$ and q. A_j^- and q are thus reproduced. Second, let $L_{11}(z)$ be a function of the form

$$L_{11}(z)=p+\sum_{j=1}^{N}\phi(q,z-t_j)A_j^3 \tag{76}$$

that satisfies the interpolation relations $L_{11}(\lambda_j)=\mu_j$ for $j=1,\ldots,N$. As we have seen in Sec. V, these relations can be solved for A_j^3 and p under the constraint $\Sigma_{j=1}^N A_j^3=0$. The remaining variables A_j^+ can be reproduced by

$$A_j^+=\frac{\theta_j^2-4(A_j^3)^2}{4A_j^-} \tag{77}$$

as (6) shows. One can thus reconstruct $L(z)$ from the fundamental variables λ_j,μ_j,t_j of the isomonodromic deformations of the second-order scalar ODE.

To derive a set of differential equations for κ, we start from the differential equations

$$\frac{\partial A_k}{\partial t_j}=[A_k,M_j(t_k)]\quad(j\neq k), \tag{78}$$

which is a consequence of the Lax equation (26). The (1,2) component of this matrix equation reads

$$\frac{\partial A_k^-}{\partial t_j}=2\phi(q,t_k-t_j)A_j^-A_k^3-2\zeta(t_k-t_j)A_j^3A_k^- . \tag{79}$$

After long and messy calculations (which we omit), one can derive the following intricate differential equation for κ:

$$\frac{\partial\log\kappa}{\partial t_j}=\frac{Q(t_j)}{P'(t_j)}\sum_{\ell=1}^{N}\frac{P(\lambda_\ell)\sigma(t_j-\lambda_\ell+q)}{Q'(\lambda_\ell)\sigma(t_j-\lambda_\ell)\sigma(q)}(2(\zeta(t_j-\lambda_\ell+q)-\zeta(q))\mu_\ell$$
$$+\zeta(t_j-\lambda_\ell)(\zeta(t_j-\lambda_\ell+q)-\zeta(t_j-\lambda_\ell)))-\sum_{\ell\neq j}\zeta(t_j-t_\ell)+\sum_{\ell=1}^{N}\zeta(t_j-\lambda_\ell). \tag{80}$$

VII. CONCLUSION

We have applied the method of spectral Darboux coordinates to Korotkin and Samtleben's isomonodromic system on a torus.[10] The isomonodromic system has thus been converted to a nonautonomous Hamiltonian system in the spectral Darboux coordinates. Although the Hamiltonians turn out to be a considerably intricate function, the method we have used is a rather straightforward analogue of the usual method for isomonodromic deformations on a sphere.

Our nonautonomous Hamiltonian system may be thought of as an elliptic analogue of Garnier's isomonodromic systems.[2,4,6] Almost the same system has been derived by Okamoto from isomonodromic deformations of a second-order scalar ODE on a torus.[8] We have seen how these two systems are related. Speaking differently, our approach from a 2×2 matrix system reveals a hidden algebro-geometric meaning of the Hamiltonian structure in Okamoto's work.[6]

An important lesson of the present work is that the notions of spectral curve and spectral Darboux coordinates persist to be useful and essential beyond isospectral deformations. This observation lies in the heart of the work of Harnad and Wisse.[18] We have confirmed it for an example of isomonodromic deformations on a torus.

In this respect, an interesting problem is to describe the isomonodromic SU(2) pure Gaudin system[12,14] from the same point of view. Separation of variables of the isospectral partner has been studied by Sklyanin and Takebe[28] (see also the paper of Hurtubise and Kjiri[29] for geometric aspects). The work of Sklyanin and Takebe shows that separation of variables of this system is technically far more complicated than the Calogero–Gaudin system. This will be also the case for the isomonodromic analogue.

Let us conclude the present consideration with a remark on trigonometric and rational analogues. The trigonometric and rational analogues of Korotkin and Samtleben's isomonodromic deformations can be obtained by replacing the basic functions $\sigma(z)$, $\zeta(z)$, and $\phi(u,z)$ by the following trigonometric or rational functions.

(1) Trigonometric model:

$$\sigma(z)=\sin z, \quad \zeta(z)=\frac{\cos z}{\sin z}, \quad \phi(u,z)=\frac{\cos z}{\sin z}-\frac{\cos u}{\sin u}. \tag{81}$$

(2) Rational model:

$$\sigma(z)=z, \quad \zeta(z)=\frac{1}{z}, \quad \phi(u,z)=\frac{1}{z}-\frac{1}{u}. \tag{82}$$

A hyperbolic model will be obtained if one replaces the trigonometric functions by the corresponding hyperbolic functions. These are nothing but the well-known pattern of degeneration of the Calogero–Moser systems; the Calogero–Gaudin systems, too, obey this pattern. In fact, it is the rational model in this list that Brzeziński considered in his work.[22] One can formulate an isomonodromic partner of these degenerate Calogero–Gaudin systems as in the case of the elliptic model. Presumably, those isomonodromic systems will not be known in the literature.

ACKNOWLEDGMENTS

I am grateful to Shingo Kawai and Takashi Takebe for many useful comments. This work is partially supported by the Grant-in-Aid for Scientific Research (No. 12640169) from the Ministry of Education, Culture, Sports and Technology.

APPENDIX A: INTERPOLATION FORMULA

Let us examine the auxiliary function

$$f_k(z)=\frac{Q(z)\sigma(z-\lambda_k+q)}{P(z)\sigma(z-\lambda_k)}.$$

This is a doubly periodic meromorphic function with simple zeros at λ_j $(j\neq k)$ and λ_k-q and simple poles at t_j $(j=1,\ldots,N)$. By the residue theorem, the residues

$$\operatorname*{Res}_{z=t_j} f_k(z)=\frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}$$

at the poles $z=t_j$ obey the sum-to-zero constraint

$$\sum_{j=1}^{N}\frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}=0. \tag{A1}$$

Let us consider the linear combination

$$\sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}\zeta(z-t_j)$$

of $\zeta(z-t_j)$ weighted by these residues. Since this function is a doubly periodic meromorphic function with the same set of simple poles and residues as $f_k(z)$, it differs from $f_k(z)$ by at most a constant:

$$\frac{Q(z)\sigma(z-\lambda_k+q)}{P(z)\sigma(z-\lambda_k)} = \sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}\zeta(z-t_j) + \text{constant}.$$

Moreover, since the left-hand side vanishes at $z=\lambda_k-q$, the constant term on the right-hand side can be easily determined as follows:

$$\text{constant} = -\sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}\zeta(\lambda_k-t_j-q).$$

We thus obtain the interpolation formula

$$\frac{Q(z)\sigma(z-\lambda_k+q)}{P(z)\sigma(z-\lambda_k)} = \sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}(\zeta(z-t_j)-\zeta(\lambda_k-t_j-q)). \tag{A2}$$

One can derive the following three identities from this interpolation formula.

(1) Since the left-hand side of the interpolation formula vanishes at $z=\lambda_l$ $(l\neq k)$,

$$\sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}(\zeta(\lambda_l-t_j)-\zeta(\lambda_k-t_j-q)) = 0 \quad (l\neq k). \tag{A3}$$

(2) By letting $z\to\lambda_k$ in the interpolation formula,

$$\sum_{j=1}^{N} \frac{Q(t_j)\sigma(t_j-\lambda_k+q)}{P'(t_j)\sigma(t_j-\lambda_k)}(\zeta(\lambda_k-t_j)-\zeta(\lambda_k-t_j-q)) = \frac{Q'(\lambda_k)\sigma(q)}{P'(\lambda_k)}. \tag{A4}$$

(3) By replacing $k\to l$, $j\to k$ and separating a term from the sum, the interpolation formula takes the form

$$\sum_{k\neq j} \frac{Q(t_k)\sigma(t_k-\lambda_l+q)}{P'(t_k)\sigma(t_k-\lambda_l)}\zeta(z-t_k) = \frac{Q(z)\sigma(z-\lambda_l+q)}{P(z)\sigma(z-\lambda_l)} - \frac{Q(t_j)\sigma(t_j-\lambda_l+q)}{P'(t_j)\sigma(t_j-\lambda_l)}\zeta(z-t_j) + \sum_{k=1}^{N} \frac{Q(t_k)\sigma(t_k-\lambda_l+q)}{P'(t_k)\sigma(t_k-\lambda_l)}\zeta(\lambda_l-t_k-q).$$

By letting $z\to t_j$,

$$\begin{aligned}\sum_{k\neq j} &\frac{Q(t_k)\sigma(t_k-\lambda_l+q)}{P'(t_k)\sigma(t_k-\lambda_l)}\zeta(t_j-t_k) \\ &= \frac{Q(t_j)\sigma(t_j-\lambda_l+q)}{P'(t_j)\sigma(t_j-\lambda_\ell)}\left(-\frac{1}{2}\frac{P''(t_j)}{P'(t_j)} + \frac{Q'(t_j)}{Q(t_j)} - \zeta(t_j-\lambda_l) + \zeta(t_j-\lambda_l+q)\right) \\ &\quad + \sum_{k=1}^{N} \frac{Q(t_k)\sigma(t_k-\lambda_l+q)}{P'(t_k)\sigma(t_k-\lambda_l)}\zeta(\lambda_l-t_k-q).\end{aligned} \tag{A5}$$

APPENDIX B: CALCULATION OF EXTRA TERMS IN (47)

Let us use (53) to rewrite the last piece on the right-hand side of (47) as

$$\frac{1}{2}\sum_{k=1}^{N}\zeta(t_j-t_k)x_k\xi_k=\sum_{l=1}^{N}\left(\sum_{k\neq j}\frac{Q(t_k)\sigma(t_k-\lambda_l+q)}{P'(t_k)\sigma(t_k-\lambda_l)}\zeta(t_j-t_k)\right)\frac{P(\lambda_l)\mu_l}{Q'(\lambda_l)\sigma(q)}.$$

The sum over $k\neq j$ arising here has been partially calculated in (A5). Using the identities

$$\frac{1}{2}\frac{P''(t_j)}{P'(t_j)}=\sum_{k\neq j}\zeta(t_j-t_k),\quad \frac{Q'(t_j)}{Q(t_j)}=\sum_{k=1}^{N}\zeta(t_j-\lambda_k)$$

on the right-hand side of (A5), one can rewrite the foregoing quantity as

$$\begin{aligned}\frac{1}{2}\sum_{k=1}^{N}\zeta(t_j-t_k)x_k\xi_k=&\sum_{l=1}^{N}\frac{Q(t_j)P(\lambda_l)\sigma(t_k-\lambda_l+q)\mu_\ell}{P'(t_j)Q'(\lambda_l)\sigma(t_j-\lambda_l)\sigma(q)}\left(-\sum_{k\neq j}\zeta(t_j-t_k)+\sum_{k=1}^{N}\zeta(t_j-\lambda_k)\right)\\&+\sum_{l=1}^{N}\frac{Q(t_j)P(\lambda_l)\sigma(t_k-\lambda_l+q)}{P'(t_j)Q'(\lambda_l)\sigma(t_j-\lambda_l)\sigma(q)}(\zeta(t_j-\lambda_l+q)-\zeta(t_j-\lambda_l))\mu_\ell\\&+\sum_{k,l=1}^{N}\frac{Q(t_k)P(\lambda_l)\sigma(t_k-\lambda_l+q)\zeta(\lambda_l-t_k-q)\mu_l}{P'(t_k)Q'(\lambda_l)\sigma(t_k-\lambda_l)\sigma(q)}.\end{aligned}$$

By (53) and (54), the first and third lines on the right-hand side turn into the following form:

$$\text{first line}=-\frac{1}{2}x_j\xi_j\left(\sum_{\neq j}\zeta(t_j-t_k)-\sum_{k=1}^{N}\zeta(t_j-\lambda_k)\right),$$

$$\text{third line}=-p.$$

Since the sum of these two cancels the second and third pieces on the right-hand side of (47), we eventually obtain the identity

$$\begin{aligned}&p-\frac{1}{2}x_j\xi_j\left(\sum_{k=1}^{N}\zeta(t_j-\lambda_k)-\sum_{k\neq j}\zeta(t_j-t_k)\right)+\frac{1}{2}\sum_{k\neq j}\zeta(t_j-t_k)x_k\xi_k\\&\quad=\sum_{l=1}^{N}\frac{Q(t_j)P(\lambda_l)\sigma(t_j-\lambda_l+q)}{P'(t_j)Q'(\lambda_l)\sigma(t_j-\lambda_l)\sigma(q)}(\zeta(t_j-\lambda_l+q)-\zeta(t_j-\lambda_l))\mu_l,\end{aligned}$$

which is nothing but (55).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Extended multilinear variable separation approach and multivalued localized excitations for some (2+1)-dimensional integrable systems

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(Received 22 January 2003; accepted 20 May 2003)

The multilinear variable separation approach and the related ''universal'' formula have been applied to many $(2+1)$-dimensional nonlinear systems. Starting from the universal formula, abundant $(2+1)$-dimensional localized excitations have been found. In this paper, the universal formula is extended in two different ways. One is obtained for the modified Nizhnik–Novikov–Veselov equation such that two universal terms can be combined linearly and this type of extension is also valid for the $(2+1)$-dimensional symmetric sine-Gordon system. The other is for the dispersive long wave equation, the Broer–Kaup–Kupershmidt system, the higher order Broer–Kaup–Kupershmidt system, and the Burgers system where arbitrary number of variable separated functions can be involved. Because of the existence of the arbitrary functions in both the original universal formula and its extended forms, the multivalued functions can be used to construct a new type of localized excitations, folded solitary waves (FSWs) and foldons. The FSWs and foldons may be ''folded'' in quite complicated ways and possess quite rich structures and multiplicate interaction properties. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598619]

I. INTRODUCTION

In nonlinear science, soliton theory plays an essential role and has been applied in almost all the natural sciences especially in all the physical branches such as fluid physics, condensed matter, biophysics, plasma physics, nonlinear optics, quantum field theory and particle physics, etc.[1–7] Most of the previous studies on soliton theory especially in high dimensions are restricted in the single valued situations. However, in various cases, the real natural phenomena are too intricate to describe only by virtue of the single valued functions. For instance, in nature, there exist very complicated folded phenomena such as the folded protein,[8] folded brain and skin surfaces, and many other kinds of folded biologic systems.[9] The simplest multivalued (folded) waves may be the bubbles on (or under) a fluid surface. Various ocean waves are really folded waves, too. Of course, at present stage, it is impossible (and we have no ambitions) to make satisfactory analytic descriptions for such complicated folded natural phenomena. But, it is still worth starting with some simpler cases.

Similar to the single valued cases, the primary question we should (and we can) ask is: Are there any stable multivalued (folded) localized excitations? For convenience later, we define the multivalued localized excitations as folded solitary waves (FSWs). Furthermore, if the interactions

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among FSWs are completely elastic, we call them foldons. In $(1+1)$-dimensional case, the simplest foldons are so-called loop solitons[10] which have been found in many $(1+1)$-dimensional integrable systems[10] and applied in some possible physical fields like the string interaction with external field,[11] quantum field theory,[12] and particle physics.[13] Nonetheless, within our knowledge, there is no study at all for the possible higher dimensional foldons.

Lately, the multilinear variable separation approach (MLVSA) has been developed well for many $(2+1)$-dimensional integrable systems[14] such as the Davey–Stewartson (DS) equation,[15,16] the Nizhnik–Novikov–Veselov (NNV) equation,[17] the asymmetric NNV (ANNV) equation,[18] the asymmetric DS (ADS) equation,[19] the dispersive long wave equation (DLWE),[20,21] the Broer–Kaup–Kupershmidt (BKK) system,[22] the higher order BKK system,[23] the nonintegrable $(2+1)$-dimensional Korteweg–de Vries (KdV) equation,[24] the long wave–short wave interaction model (LWSWIM),[25] the Maccari system,[26] the Burgers equation,[27] the $(2+1)$-dimensional sine-Gordon (2DsG) system,[28] and the general $(N+M)$-component AKNS system.[29] We call all these models the MLVSA solvable models. Using the MLVSA results, we have found that the formula,

$$U \equiv \frac{-2\Delta q_y p_x}{(a_0+a_1 p+a_2 q+a_3 pq)^2}, \quad \Delta \equiv a_0 a_3 - a_1 a_2, \tag{1}$$

is valid for suitable fields or potentials of all the above-mentioned models. In Eq. (1), $p \equiv p(x, t)$ is an arbitrary function of $\{x, t\}$, $q \equiv q(y, t)$ may be either an arbitrary function for some kinds of models such as the DS system, the NNV system, and the 2DsG system or an arbitrary solution of a Riccati equation (or heat conduction equation) for some other systems, a_0, a_1, a_2, and a_3 are constants. One of the most important results obtained from (1) is that all the known MLVSA solvable models possess quite rich localized excitations such as the solitoffs, dromions, lumps, breathers, instantons, ring solitons, peakons, compactons, localized chaotic and fractal patterns, and so on.[14]

In the universal formula (1), the appearance of the arbitrary function p (and q for some of the MLVSA solvable models) is closely related to the arbitrary boundary conditions of some types of the quantities for the related models. In some celebrated papers, the effects of arbitrary boundary conditions have been considered for some $(2+1)$-dimensional integrable systems.[30–34] For instance, Fokas and Santini[30–32] had investigated the exact solutions of the DS system with arbitrary boundary data by means of the most powerful and fruitful method, the inverse scattering transformation. The similar treatment for the 2DsG system was given by Konopelchenko and Dubrovsky.[33,34] One of the interesting results obtained by Fokas and Santini is worth mentioning again here: The localized traveling solutions, say, dromions, do not preserve their form upon interaction and hence exchange energy. Only for a special choice of the spectral parameters do these solutions preserve their forms. This kind of result had been found also for other $(2+1)$-integrable models. In fact, the non-complete elastic interaction property among the $(2+1)$-dimensional localized excitations is correct for all the MLVSA solvable models because of the validity of (1). In this paper, the necessary and sufficient conditions on the selections of the arbitrary functions appearing in the universal formula (1) (and its extended forms) for the completely elastic interaction will be given.

On the other hand, following the general ideas introduced in Ref. 30, one could, in principle, investigate the stability properties of the solutions presented in this paper and their relevance as asymptotic states for suitable initial boundary value problems. However, here, we study only the interaction behavior among the localized solutions by studying the asymptotic property of the universal formula (1) and its extensions because these formulas are valid for more than one system.

In Sec. II of this paper, the MLVSA is extended for the modified NNV (MNNV) system and the 2DsG system. Compared with the other known MLVSA solvable models, the variable separation solutions of these two systems display a new phenomenon, Two solutions expressed by the universal quantity (1) can be added linearly to generate a new solution under some special conditions. In the linear case, any number of variable separation solutions can be linearly superposed

to yield new solutions of the same system. Thus, naturally, there comes another important question, whether the ''universal'' formula can be extended in a way that more variable separated functions are included. In Sec. III A, we extend the ansatz of the MLVSA to get an extended form of the universal formula (1) for the $(2+1)$-dimensional DLWE. Whence the universal formula is extended to a general form for a particular system, one will ask whether the extended formula is valid for the other systems. In the Secs. III B, III C, and III D, the extended formula is demonstrated valid at least for three other nonlinear systems, the BKK system, the higher order BKK system, and the $(2+1)$-dimensional Burgers system. In Sec. IV, starting from the universal formula and its extended forms, a new type of localized excitations, FSWs and foldons, are discussed in detail. Section V is devoted to investigating the interaction properties both for the general localized excitations and the particular types of FSWs and foldons. The last section is a short summary and discussion. Some special results of this paper have already been reported in our previous brief report.[35]

II. THE FIRST TYPE OF EXTENSION OF THE MLVSA

A. The variable separation solution for the MNNV system

In this section, we apply the MLVSA to a new example, the MNNV system,[36]

$$u_t+u_{xxx}+u_{yyy}+\sigma^2u_x^3+\sigma^2u_y^3+3u_xv_{xx}+3u_yv_{yy}=0, \tag{2}$$

$$v_{xy}+\sigma^2u_xu_y=0, \tag{3}$$

which is a main member of the MNNV hierarchy associated with the generalized Lamé system.[37] In (2) and (3), $\sigma^2=\pm1$. We call the system (2)–(3) the MNNV I for $\sigma^2=-1$ and the MNNV II for $\sigma^2=1$. The 2DsG system is just the negative member of the MNNV I hierarchy.[38] In Ref. 39, the geometrical significance of the MNNV I system is established. The binary Darboux transformation of the MNNV I is constructed in Ref. 40.

The first step of the MLVSA is to transform the original model into a general multilinear form by means of the Painlevé Bäcklund transformation. For the MNNV system, through the standard leading order analysis and the truncated expansion approach of the Weiss–Tabor–Carnevale Painlevé analysis,[41] we find that the following Painlevé Bäcklund transformation

$$u=\pm\sigma\ln\frac{f}{g}+u_0, \tag{4}$$

$$v=-\ln(fg)+v_0, \tag{5}$$

where $\{u_0,v_0\}$ is an arbitrary known seed solution of the MNNV system, changes the model to a bilinear equation system

$$(D_t+D_x^3+D_y^3+3v_{0xx}D_x+3v_{0yy}D_y)f\cdot g+[\sigma^2(u_{0x}^2D_x+u_{0y}^2D_y)\pm\sigma^{-1}(u_{0x}D_x^2\pm u_{0y}D_y^2)]f\cdot g=0, \tag{6}$$

$$[\sigma D_xD_y\pm u_{0y}D_x\pm u_{0x}D_y]f\cdot g=0, \tag{7}$$

where the Hirota's bilinear operators D_x, D_y, D_t are defined by

$$D_x^nD_y^mD_t^kf\cdot g\equiv\partial_{\epsilon_1}^n\partial_{\epsilon_2}^m\partial_{\epsilon_3}^kf(x+\epsilon_1,y+\epsilon_2,t+\epsilon_3)g(x-\epsilon_1,y-\epsilon_2,t-\epsilon_3)|_{\epsilon_1=0,\epsilon_2=0,\epsilon_3=0}. \tag{8}$$

The second key step of the MLVSA is to take a suitable variable separation ansatz such that the space variable can be separated into different functions.

Compared with the universal formula (1) of the other MLVSA solvable models, the variable separation ansatz for the bilinear MNNV system (6) and (7) can be taken as

$$f=a_0+a_1p+a_2q+a_3pq, \tag{9}$$

$$g=b_0+b_1p+b_2q+b_3pq, \tag{10}$$

where $p\equiv p(x,\ t)$ is y-independent, $q\equiv q(y,\ t)$ is x-independent, and $a_i,\ b_i\ (i=0,\ \ldots,\ 3)$ are taken as constants here though they may be t-dependent.

The third step of the MLVSA is to select some types of seed solutions for the sake of including as many arbitrary functions as possible. It is straightforward that, for the MNNV system (2) and (3),

$$u_0=0,\quad v_0=v_1(x,\ t)+v_2(y,\ t) \tag{11}$$

with arbitrary functions $v_1(x,\ t)\equiv v_1,\ v_2(y,\ t)\equiv v_2$ is one of the appropriate seed solutions.

Now we come to the final step of obtaining the variable separation solution to the MNNV system. Substituting (9)–(11) into Eq. (7) yields a simple relation among constants $a_i,\ b_i,\ i=0,\ \ldots,\ 3$,

$$b_3a_0+a_3b_0-a_1b_2-a_2b_1=0. \tag{12}$$

Thereafter, due to (9)–(12), Eq. (6) becomes

$$\frac{q_t+q_{yyy}+3v_{2yy}q_y}{(a_3b_2-a_2b_3)q^2+2(a_3b_0-a_2b_1)q+a_1b_0-a_0b_1}$$
$$=-\frac{p_t+p_{xxx}+3v_{1xx}p_x}{(a_3b_1-a_1b_3)p^2+2(a_3b_0-a_1b_2)p+a_2b_0-a_0b_2}. \tag{13}$$

Because the left of (13) is x-independent and the right is y-independent, (13) is correct iff (if and only if)

$$p_t+p_{xxx}+3v_{1xx}p_x=-c(t)[(a_1b_3-a_3b_1)p^2+2(a_1b_2-a_3b_0)p+a_0b_2-a_2b_0], \tag{14}$$

$$q_t+q_{yyy}+3v_{2yy}q_y=c(t)[(a_3b_2-a_2b_3)q^2+2(a_3b_0-a_2b_1)q+a_1b_0-a_0b_1], \tag{15}$$

where $c(t)$ is an arbitrary function of t.

For any fixed v_1 and v_2, to solve (14) and (15) is still very difficult since the terms, q^2 and p^2, imply the nonintegrability.[42] However, thanks to the arbitrariness of the functions v_1 and v_2, we can treat the problem in an alternative way: considering p and q to be arbitrary functions, then v_1 and v_2 can be solved from (14) and (15),

$$v_{1xx}=-\frac{1}{3p_x}\{p_t+p_{xxx}+c(t)[(a_3b_1-a_1b_3)p^2+2(a_3b_0-a_1b_2)p+a_2b_0-a_0b_2]\}, \tag{16}$$

$$v_{2yy}=-\frac{1}{3q_y}\{q_t+q_{yyy}-c(t)[(a_3b_2-a_2b_3)q^2+2(a_3b_0-a_2b_1)q+a_1b_0-a_0b_1]\}. \tag{17}$$

Till now, the variable separation solution of the MNNV system is obtained

$$u=\pm\sigma\ln\frac{a_0+a_1p+a_2q+a_3pq}{b_0+b_1p+b_2q+b_3pq}, \tag{18}$$

$$v=-\ln[(a_0+a_1p+a_2q+a_3pq)(b_0+b_1p+b_2q+b_3pq)]+v_1+v_2 \tag{19}$$

with arbitrary functions p and q, the constant relation (12), and the functions v_1 and v_2 determined by (16) and (17).

It is known that the localized excitations and the universal quantity U expressed by (1) are related to the different quantities for different models. For instance, for the DS system,

$$iu_t+\tfrac{1}{2}(u_{xx}+u_{yy})+\alpha|u|^2u-uv=0, \tag{20}$$

$$v_{xx}-v_{yy}-2\alpha(|u|^2)_{xx}=0, \tag{21}$$

the universal quantity (1) is valid for the quantity $\alpha|u|^2$, i.e., $\alpha|u|^2=U$, whereas, for the NNV equation,

$$u_t-au_{xxx}-bu_{yyy}+3a(uv)_x+3b(uw)_y=0, \tag{22}$$

$$u_x=v_y, \tag{23}$$

$$u_y=w_x, \tag{24}$$

the field u itself can be expressed by the universal quantity, say, $u=U$.

As for the MNNV system (2) and (3), it is interesting to consider the potentials $F(\equiv -2u_{xy}/\sigma)$ and $G(\equiv -2v_{xy})$,

$$F=\pm\left\{\frac{2(a_1a_2-a_0a_3)p_xp_y}{(a_0+a_1p+a_2q+a_3pq)^2}-\frac{2(b_1b_2-b_0b_3)p_xp_y}{(b_0+b_1p+b_2q+b_3pq)^2}\right\}\equiv\pm(U_a-U_b), \tag{25}$$

$$G=\left\{\frac{2(a_1a_2-a_0a_3)p_xp_y}{(a_0+a_1p+a_2q+a_3pq)^2}+\frac{2(b_1b_2-b_0b_3)p_xp_y}{(b_0+b_1p+b_2q+b_3pq)^2}\right\}\equiv U_a+U_b. \tag{26}$$

In Eqs. (25) and (26), each one of U_a and U_b is rightly the universal quantity (1), which reveals two universal terms (every term is a solution of the MNNV system) can be combined linearly for the potentials F and G. The nonlinearity of the model is implied by the relation (12) among the constants in U_a and U_b and the opposite sign of the term, U_b, in Eqs. (25) and (26).

B. The variable separation solution for the 2DsG system

In Ref. 28, one of the present authors (S.-Y.L.) has shown that the variable separation solution of the 2DsG system[43,44]

$$u_{xyt}+u_yv_{xt}+u_xv_{yt}=0, \tag{27}$$

$$v_{xy}=u_xu_y, \tag{28}$$

is completely similar to that of the MNNV system. To compare the results of two models, we outline the variable separation solution of the 2DsG system here. Using the Painlevé Bäcklund transformation,

$$u=\pm i\ln\frac{f}{g}, \tag{29}$$

$$v=\ln(fg)+v_1+v_2, \tag{30}$$

where we also fix the seed solution as $\{u_0=0,\ v_0=v_1(x,t)+v_2(y,\ t)\}$ similar to the case of the MNNV system, the 2DsG system is changed to a bilinear form

$$[D_xD_yD_t+v_{1xt}D_y+v_{2yt}D_x]f\cdot g=0, \tag{31}$$

$$D_xD_yf\cdot g=0. \tag{32}$$

Adopting the ansatz (9)–(10) with the seed solution simultaneously, Eq. (32) gives the constant relation (12) and Eq. (31) becomes

$$\{[A_1p^2+2A_2p+a_2b_0-b_2a_0]v_{1xt}+2[A_1p-A_2]p_{xt}\}p_x^{-1}-2A_1p_t$$
$$=\{[B_1q^2-2A_2q+b_1a_0-a_1b_0]v_{2yt}+2[B_1q-A_2]q_{yt}\}q_y^{-1}-2B_1q_t, \tag{33}$$

where

$$A_1=a_3b_1-a_1b_3, \quad A_2=a_3b_0-b_2a_1, \quad B_1=a_2b_3-a_3b_2.$$

Likewise, taking p and q as arbitrary functions, then Eq. (33) is valid iff v_1 and v_2 satisfy

$$v_{1xt}=\frac{(c(t)+2A_1p_t)p_x-2(A_1p-A_2)p_{xt}}{A_1p^2+2A_2p+a_2b_0-b_2a_0}, \tag{34}$$

$$v_{2yt}=\frac{(c(t)+2B_1q_t)q_y-2(B_1q-A_2)q_{yt}}{B_1q^2-2A_2q+b_1a_0-a_1b_0}, \tag{35}$$

with an arbitrary function $c(t)$.

Now defining

$$F\equiv 2iu_{xy}, \quad G\equiv -2v_{xy} \tag{36}$$

for the 2DsG system, then we obtain the completely same results (25) and (26).

For the real 2DsG system and the real MNNV I system, the field u itself is important. The real condition of u tells one that g should be a complex conjugate of f,

$$g=f^*. \tag{37}$$

Under the real condition (37), the expression of u for the real MNNV I system and the 2DsG system becomes

$$u=2\arctan\frac{(a_{1r}+Aq_r-a_{3i}q_i)p_i+(a_{2r}+Ap_r)q_i+p_r(a_{1i}+a_{3i}q_r)+a_{0i}+a_{2i}q_r}{(a_{1i}+Aq_i+a_{3i}q_r)p_i+(a_{3i}p_r+a_{2i})q_i-p_r(a_{1r}+Aq_r)-a_{0r}-a_{2r}q_r}, \tag{38}$$

where the subscripts r and i express the real and imaginary parts of the related quantities, say,

$$a_{1r}=\Re(a_1), \quad a_{1i}=\Im(a_1). \tag{39}$$

Actually, expressions (4), (5), and (11) hint that for the real MNNV I system and the real 2DsG system, f and g can be simply taken as[28]

$$f=1+ipq, \quad g=1-ipq \tag{40}$$

with arbitrary real $p=p(x,t)$ and $q=q(y,t)$ by redefining the functions p, q, v_1, and v_2. Under this observation, (38) is simplified to

$$u=2\arctan(pq). \tag{41}$$

In Ref. 28, various single valued localized excitations with and without completely elastic interaction property have been discussed for quantities F, G, and u of the 2DsG system. It has also been pointed out that the variable separation solution of the real 2DsG system is equivalent to that obtained by the Moutard transformation.[28,33,34,45]

III. THE SECOND TYPE OF EXTENSIONS OF THE MLVSA

A. Extension of the variable separation solution of the DLWE

In Sec. II, we have extended the MLVSA to the MNNV and the 2DsG systems such that two universal terms can be combined linearly. However, except for some functions of time t, there are no further space variable separated functions included. In this section, we will extend the MLVSA in a quite different way for the DLWE, the BKK system, the higher order BKK system, and the Burgers equation so as to include more variable separated functions.

For the $(2+1)$-dimensional DLWE,

$$u_{yt}+\eta_{xx}+u_x u_y+u u_{xy}=0, \tag{42}$$

$$\eta_t+u_x+\eta u_x+u\eta_x+u_{xxy}=0, \tag{43}$$

the basic variable separation solution reads

$$v\equiv-\eta-1=U, \tag{44}$$

$$u=\pm\frac{2p_x(a_1+a_3q)}{a_0+a_1p+a_2q+a_3pq}+u_0, \tag{45}$$

where p is an arbitrary functions of $\{x,\ t\}$, $q=q(y,t)$ is an arbitrary solution of the Riccati equation,

$$q_t-a_0c_0-(a_1c_1+a_2c_0-a_0c_2)q-(a_3c_1-a_2c_2)q^2=0, \tag{46}$$

and the seed function u_0 is linked to p by

$$u_0=-p_x^{-1}[p_t\pm p_{xx}-a_0c_1-(a_1c_1+a_2c_0+a_0c_2)p-(a_1c_2+a_3c_0)p^2]. \tag{47}$$

The $(1+1)$-dimensional DLWE [$y=x$ of (42)–(43)] is also called the classical Boussinesq equation. There are lots of papers discussing its possible applications and exact solutions.[46] The $(2+1)$-dimensional DLWE was first obtained by Boiti *et al.*[20] as a compatibility condition for a "weak" Lax pair. In Ref. 47, Paquin and Winternitz showed that the symmetry algebra of (42)–(43) possesses the infinite-dimensional Kac–Moody–Virasoro structure. Some special similarity solutions are given in Ref. 47 by using symmetry algebra and the classical theoretical analysis. The more general symmetry algebra, W_∞ symmetry algebra, is given in Ref. 48. In Ref. 49, nine types of two-dimensional similarity reductions and thirteen types of ordinary differential equation reductions are given. Though the model is Lax or IST integrable, it does not pass the Painlevé test.[50]

To extend the universal formula to a more general form, we use the MLVSA again. For completeness, we repeat the first two steps of the MLVSA for the DLWE (42)–(43) though they have been given in our previous papers.[14,21]

To change the system to a multilinear form, by using the standard truncated Painlevé expansion, we have the following Bäcklund transformation:

$$u=\pm 2\frac{f_x}{f}+u_0, \tag{48}$$

$$\eta=2\frac{f_{xy}}{f}-2\frac{f_x f_y}{f^2}+\eta_0, \tag{49}$$

with $\{u_0,\ \eta_0\}$ being its arbitrary solution. Substituting Eqs. (48) and (49) into Eqs. (42) and (43) leads to

$$(f_{xxxx}\pm f_{xyt})f^2-[f_{xx}f_{xy}+f_yf_{xxx}+f_xf_{xxy}\pm(f_tf_{xy}+f_yf_{x,t}+f_xf_{yt})]f+2f_xf_y(f_{xx}\pm f_t)$$
$$\pm[u_0(f^2f_{xxy}-ff_yf_{xx}-2ff_xf_{xy}+2f_yf_x^2)+f(ff_{xy}-f_xf_y)u_{0x}+f(ff_{xx}-f_x^2)u_{0y}+f^2f_xu_{0xy}]=0. \tag{50}$$

$$(\eta_0+1\mp u_{0y})(ff_{xx}-f_x^2)+ff_x(\eta_{0x}\mp u_{0xy})=0. \tag{51}$$

From the DLWE (42)–(43), it is easy to see that

$$u_0=u_0(x,t), \tag{52}$$

$$\eta_0=-1, \tag{53}$$

is a trivial seed solution with u_0 being an arbitrary function of $\{x, t\}$. Under the selections (52)–(53), the bilinear equation (51) satisfies identically.

In order to solve the trilinear equation (50) with (52)–(53), one has to use some prior ansatz. The basic variable separation solution (44)–(45) results from the ansatz

$$f=a_0+a_1p+a_2q+a_3pq. \tag{54}$$

It is known that for the DLWE (42)–(43), there are two sets of infinitely many symmetries, and every symmetry possesses an arbitrary function of y or t.[48] That means infinitely many arbitrary functions of y and t can enter into the solution of (42)–(43). So, it is probable to extend the solution (44) to a more general form with more arbitrary functions. After finishing the detailed calculations, we find that the following variable separation ansatz,

$$f=q_0+\sum_{i=1}^{N}p_iq_i, \tag{55}$$

where $\{q_i, i=0, 1, 2, \ldots, N\}$, and $\{p_i, i=1, 2,\ldots, N\}$ are functions of $\{y, t\}$ and $\{x, t\}$, respectively, solves the trilinear equation (51) with (52)–(53) under the conditions

$$q_{it}=\sum_{j=0}^{N}(c_{ij}+q_iC_j)q_j, \quad i=0, 1, \ldots, N, \tag{56}$$

$$p_{it}=(c_{00}-u_0\partial_x-\partial_x^2)p_i-c_{0i}+\sum_{j=1}^{N}(c_{j0}p_i-c_{ji})p_j, \quad i=1, 2, \ldots, N, \tag{57}$$

where $\{c_{ij}, C_j, i,j=0, 1, 2, \ldots, N\}$ are arbitrary functions of t. Obviously, the general ansatz (55) will return back to the known one, Eq. (54), when $N=3, q_0=a_0, q_1=a_1, q_2=a_2q, q_3=a_3q, p_1=p_3=p, p_2=1$.

The corresponding solution for the field $v(\equiv-\eta-1)$ now reads

$$v=\frac{-2\Sigma_{i=1}^{N}p_{ix}q_{iy}}{q_0+\Sigma_{i=1}^{N}p_iq_i}+\frac{2\Sigma_{i=1}^{N}p_{ix}q_i(q_{0y}+\Sigma_{j=1}^{N}p_jq_{jy})}{(q_0+\Sigma_{i=1}^{N}p_iq_i)^2}\equiv U_E \tag{58}$$

while the quantity u is given by

$$u=\pm\frac{2\Sigma_{i=1}^{N}p_{ix}q_i}{q_0+\Sigma_{i=1}^{N}p_iq_i}+u_0. \tag{59}$$

It is clear that in addition to one $(1+1)$-dimensional arbitrary function of $\{x, t\}$ (one of u_0 and p_i), $(N+1)(N+2)-1$ arbitrary functions of t, c_{ij}, C_j have been included in the general solution. Furthermore, various arbitrary functions of y and $\{x, t\}$ will enter into (58) after the

coupled systems of (56) and (57) are solved. Because of the complexity, we have to leave these problems for our future studies. Here we just write down the simplest nontrivial case for later use. Fixing $N=1$, $c_{ij}=C_i=0$, $p_1=p$, and $q_0\to a_0+q_0$, the formula (58) is simplified to

$$v=\frac{2p_x(q_1q_{0y}-(a_0+q_0)q_{1y})}{(a_0+q_0+pq_1)^2}\equiv V \tag{60}$$

with q_0 and q_1 being arbitrary functions of y and p being an arbitrary function of $\{x,\ t\}$. It has been proven that the simplified quantity expressed by (60) does work for many other known models which allow the universal formula (1).[24,51,52]

B. Extension of the variable separation solution of the BKK system

It should be mentioned that though we have not yet proven the validity of (58) for all the models listed in Sec. I, the extended form (58) is really valid at least for some of them like the BKK system, the higher order BKK system, and the (2+1)-dimensional Burgers system.

In this section, we extend the universal formula (1) to (58) for the BKK system

$$H_{ty}-H_{xxy}+2(HH_x)_y+2G_{xx}=0, \tag{61}$$

$$G_t+G_{xx}+2(HG)_x=0. \tag{62}$$

The variable separation solution (1) for the quantity $U=-2G$ of the BKK system has been given in Ref. 22. From Ref. 22, we know that for the BKK system the corresponding Painlevé Bäcklund transformation

$$H=(\ln f)_x+H_0, \tag{63}$$

$$G=(\ln f)_{xy}+G_0, \tag{64}$$

where $\{H_0,G_0\}$ is an arbitrary known seed solution, transforms Eqs. (61) and (62) to the following trilinear and bilinear forms, respectively,

$$\begin{aligned}&2H_0(2f_x^2f_y+f^2f_{xxy}-ff_yf_{xx}-2ff_xf_{xy})+2H_{0x}f(ff_{xy}-f_xf_y)+2f^2f_xH_{0xy}-f(f_xf_{ty}+f_yf_{tx}\\&\quad+f_tf_{xy}+f_xf_{xxy}+f_yf_{xxx}+f_{xx}f_{xy})+f^2(f_{txy}+f_{xxxy})+2f_xf_y(f_t+f_{xx})+2H_{0y}f(ff_{xx}-f_x^2)=0,\end{aligned} \tag{65}$$

$$(ff_{xx}-f_x^2+ff_x\partial_x)(G_0-H_{0y})=0. \tag{66}$$

For the BKK system, the seed solution can be taken as

$$G_0=0, \tag{67}$$

$$H_0\equiv h(x,\ t)=h, \tag{68}$$

with an arbitrary function h with respect to the indicated arguments.

Now, using the ansatz (54), we can retrieve the results in Ref. 22. Whereas, taking advantage of the general ansatz (55), we have

$$q_{it}=\sum_{j=0}^{N}(c_{i,j}+q_iC_j)q_j,\quad i=0,\ 1,\ \ldots,\ N, \tag{69}$$

$$p_{it}=(c_{00}-2h\partial_x-\partial_x^2)p_i-c_{0i}+\sum_{j=1}^{N}(c_{j0}p_i-c_{ji})p_j,\quad i=1,\ 2,\ \ldots,\ N \tag{70}$$

with $\{c_{ij},\ C_j,\ i,j=0,\ 1,\ 2,\ \ldots,\ N\}$ being arbitrary functions of t. Therefore, the corresponding solutions for the fields G and H read

$$G=-\frac{1}{2}U_E, \tag{71}$$

$$H=\frac{2\Sigma_{i=1}^{N}p_{ix}q_i}{q_0+\Sigma_{i=1}^{N}p_iq_i}+h, \tag{72}$$

where the expression of U_E is exactly same as that of the DLWE expressed by (58).

C. Extension of the variable separation solution of the higher order BKK system

Though not proved yet, it is rather reasonable to believe that if one member of an integrable hierarchy is (generalized) MLVSA solvable, then the whole hierarchy may be (generalized) MLVSA solvable. For instance, in Ref. 14, the ANNV system and the ADS system, which belong to the same system, are solved by the similar MLVSA. The MLVSA solvable systems NNV and DS also belong to the same hierarchy. In Sec. II, two models, the MNNV system and the 2DsG system, existing in the same hierarchy, are MLVSA solvable in a similar way. To confirm the conclusion further, in this section, we work on the generalized MLVSA solvability of the next member of the BKK hierarchy, the higher order BKK system,[53]

$$H_{yt}+4(H_{xx}+H^3-3HH_x+3Hg_y)_{xy}+12(Hg_y)_{xx}=0, \tag{73}$$

$$g_{yt}+4(g_{xxy}+3H^2g_y+3Hg_{xy}+3g_yg_x)_x=0. \tag{74}$$

The details of the MLVSA solvability of an equivalent form of the higher order BKK system can be found in Ref. 23 and the generalized MLVSA solvability of the equivalent higher order BKK system has been given by Lin and Qian.[54]

Obviously, the higher order BKK system has a trivial seed solution

$$H=H_0\equiv H_0(x,t),\quad g=g_0\equiv g_0(x,t), \tag{75}$$

with H_0 and g_0 being arbitrary functions of $\{x,\ t\}$.

The following Painlevé Bäcklund transformation,

$$H=(\ln f)_x+H_0,\quad g=(\ln f)_x+g_0, \tag{76}$$

degenerates two equations of the higher order BKK system to a single trilinear equation

$$\begin{aligned}&12f(ff_{xy}-f_xf_y)(g_{0x}+H_0^2)_x+12[2\,f_x(f_xf_y-ff_{xy})+f^2f_{xxy}-ff_yf_{xx}](H_0^2+g_{0x})+12[2\,f_xf_yf_{xx}\\&\quad+f(ff_{xxxy}-f_yf_{xxx}-(f_xf_{xy})_x)]H_0+12f(ff_{xxy}-f_yf_{xx})H_{0x}-f(f_yf_{xt}+4f_yf_{xxxx}+4f_{xy}f_{xxx}\\&\quad+4f_xf_{xxxy}+f_tf_{xy}+f_xf_{yt})+f^2(4f_{xxxxy}+f_{xyt})+2\,f_xf_y(f_t+4f_{xxx})=0.\end{aligned} \tag{77}$$

To solve the trilinear equation (77), we use the generalized variable separation ansatz (55) again. After finishing some detailed calculations, one can find that the general variable separation ansatz (55) really solves Eq. (77) under the conditions

$$q_{it}=\sum_{j=0}^{N}(c_{ji}+C_jq_i)q_j,\quad i=0,\ 1,\ \ldots,\ N, \tag{78}$$

$$p_{it}=-4p_{ixxx}-12H_0p_{ixx}-12(g_{0x}+H_0^2)p_{ix}+c_{00}p_i-c_{0i}+\sum_{j=1}^{N}(c_{j0}p_i-c_{ji})p_j,$$

$$i=1,\ 2,\ \ldots,\ N, \tag{79}$$

where $\{c_{ij},\ C_j,\ i,j=0,\ 1,\ 2,\ \ldots,\ N\}$ are arbitrary functions of t.

For the higher order BKK system (73)–(74), the extended expression of the universal quantity U_E expressed by (58) is valid for the potential $G_1\equiv 2H_y=2g_y$, i.e.,

$$G_1=2H_y=2g_y=U_E. \tag{80}$$

D. Extension of the variable separation solution of the Burgers equation

In this section, we discuss another generalized MLVSA solvable system, the $(2+1)$-dimensional Burgers equation,

$$v_{yt}=v_yv_{yy}+av_xv_{xy}+bv_{yyy}+abv_{xxy}, \tag{81}$$

in its potential form, where a and b are arbitrary constants. An equivalent form of the potential Burgers equation (81) is derived from the generalized Painlevé integrable classification.[27]

The following transformation

$$v=2b\ln f+v_0, \tag{82}$$

with arbitrary seed solution v_0 changes the potential Burgers equation (81) to a bilinear form

$$v_{0y}(ff_{yy}-f_y^2)+av_{0x}(ff_{xy}-f_xf_y)+v_{0yy}ff_y+av_{0xy}ff_x-(f\partial_y-f_y)(f_t-bf_{yy}-abf_{xx})=0. \tag{83}$$

Evidently, Eq. (81) possesses a trivial seed solution

$$v_0=v_0(x,t) \tag{84}$$

with v_0 being an arbitrary function of the indicated variables.

The simple and direct calculations show that the generalized variable separation ansatz (55) solves the bilinear equation (83) under the conditions

$$p_{it}=\left(ab\partial_x^2+av_0\partial_x-\alpha_i+\sum_{j=1}^{N}\beta_jp_j\right)p_i,\quad i=1,\ 2,\ \ldots,\ N, \tag{85}$$

$$q_{it}=bq_{iyy}+(\alpha_0+\alpha_i)q_i,\quad i=0,\ 1,\ \ldots,\ N, \tag{86}$$

where $\{\alpha_i,\ i=0,\ 1,\ 2,\ \ldots,\ N,\ \beta_j,\ j=1,\ 2,\ldots,\ N\}$ are all arbitrary functions of t.

For the Burgers equation, the quantity $w\equiv(1/b)\,v_{xy}$ possesses the same form as the extended universal formula, i.e.,

$$w=\frac{1}{b}v_{xy}=U_E. \tag{87}$$

IV. FSWs AND FOLDONS

Starting from the ''universal'' formula (1) and using many kinds of single valued functions for p and q, plenty of localized excitations such as the solitoffs, dromions, lumps, breathers, instantons, ring solitons, peakons, and compactons have been obtained. Using $(1+1)$-dimensional chaotic and fractal functions, some kinds of $(2+1)$-dimensional localized chaotic and fractal patterns have also been found.[14]

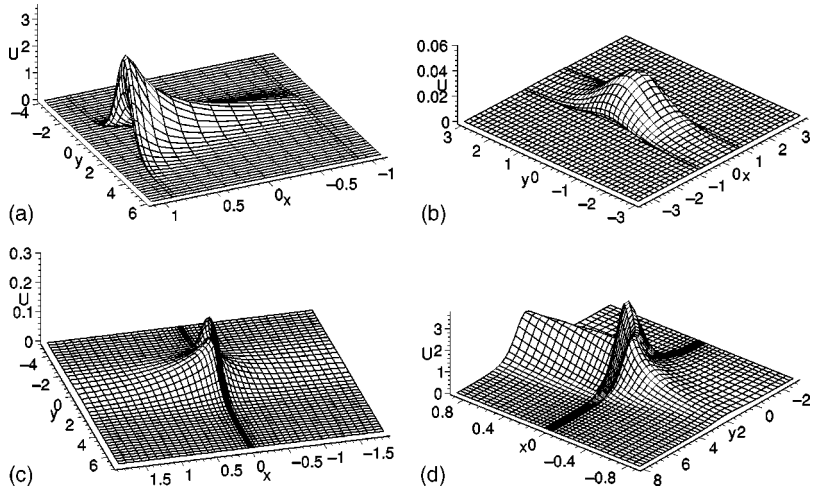

FIG. 1. Four typical FSWs for the field U expressed by (92) at $t=0$ with (93)–(98) and the related concrete parameter selections are given in (99) for the ''tent'' shape FSW (a), (100) for the ''worm'' shape FSW (b), (101) for the ''worm-dromion'' shape FSW (c), and (102) for the ''worm-solitoff'' shape FSW (d), respectively.

In this section, we focus our attention on the possible multivalued localized excitations, FSWs and foldons, constructed on the basis of the universal formula (1) and extended forms, especially, the quantity v expressed by (60) and the field u shown in (41) for the real MNNV I and 2DsG systems.

First of all, we write down a $(1+1)$-dimensional localized function, p_f, in the form

$$p_f \equiv \sum_{j=1}^{M} f_j(\xi - c_j t), \tag{88}$$

$$x = \xi + \sum_{j=1}^{M} g_j(\xi - c_j t), \tag{89}$$

where $c_1 < c_2 < \cdots < c_M$ are all arbitrary constants and $\{f_j, g_j\}$, $\forall j$ are all localized functions with the properties

$$f_j(\pm\infty) = F^{\pm}, \quad g_j(\pm\infty) = G_j^{\pm} = \text{constant}. \tag{90}$$

Judged from expression (89), ξ may be a multivalue function in certain regions of x by selecting the functions g_j suitably. Therefore, the function p_f may be a multivalue function of x in these regions though it is a single valued function of ξ. Besides, p_f is an interaction traveling solution of M localized excitations due to the property

$$\xi|_{x\to\infty} \to x \to \infty. \tag{91}$$

Indeed, most of the known $(1+1)$-dimensional multiloop solutions are the special cases of (89). Now, if all the arbitrary functions in the universal formula (1) and/or its slightly general one (60) [and/or its even more general extended one (58)] possess the forms similar to (88) with (89)–(90), then we can get various $(2+1)$-dimensional FSWs and/or foldons.

In Fig. 1, four typical FSWs are plotted for the universal quantity U expressed in its special form

$$U = \frac{2p_x q_y}{(p+q+a_0)^2}, \tag{92}$$

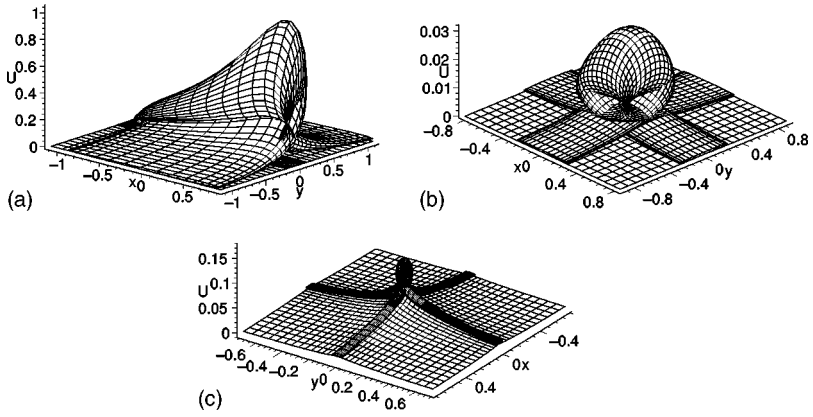

FIG. 2. Another three typical FSWs for the field U expressed by (92) at $t=0$ with (93)–(98) and the detailed parameter selections are shown in (a) (103), (b) (104), and (c) (105), respectively.

i.e., $a_3=a_1-1=a_2-1=0$ of (1), with the function selections

$$p_x=-k_1\,\mathrm{sech}^2(k_2\xi-k_3t), \tag{93}$$

$$p=-\frac{k_1}{3k_2}[3+2k_2k_4+k_2k_4\,\mathrm{sech}^2(k_2\xi-k_3t)]\tanh(k_2\xi-k_3t), \tag{94}$$

$$x=\xi+k_4\tanh(k_2\xi-k_3t), \tag{95}$$

$$q_y=-l_1\,\mathrm{sech}^2(l_2\xi), \tag{96}$$

$$q=-\frac{l_1}{3l_2}[3+2l_2l_3+l_2l_3\,\mathrm{sech}^2(l_2\eta)]\tanh(l_2\eta), \tag{97}$$

$$y=\eta+l_3\tanh(l_2\eta), \tag{98}$$

while the parameters k_1, k_2, k_3, k_4, l_1, l_2, and l_3 are selected such that p is multivalued in a small region of k_2x-k_3t and q is single valued in the whole region of y.

The detailed selections of the parameters are

$$k_1=k_2=k_3=l_1=l_2=1,\quad l_3=0,\quad k_4=-2.5,\quad a_0=1.9 \tag{99}$$

for the ''tent'' shape FSW shown in Fig. 1(a),

$$k_1=k_2=k_3=l_1=l_2=1,\quad l_3=0,\quad k_4=-2.5,\quad a_0=8 \tag{100}$$

for the ''worm'' shape FSW plotted in Fig. 1(b),

$$k_1=10,\quad k_2=k_3=l_1=l_2=l_3=1,\quad k_4=-1.15,\quad a_0=10 \tag{101}$$

for the ''worm-dromion'' shape FSW (which looks like a ''worm'' riding on a dromion) given in Fig. 1(c), and

$$k_1=k_2=k_3=l_1=l_2=l_3=1,\quad k_4=-1.15,\quad a_0=1.9 \tag{102}$$

for the ''worm-solitoff'' shape FSW (which looks like a ''worm'' riding on a solitoff's head) exhibited in Fig. 1(d).

Figure 2 shows another three typical FSWs for the same universal quantity expressed by (92)

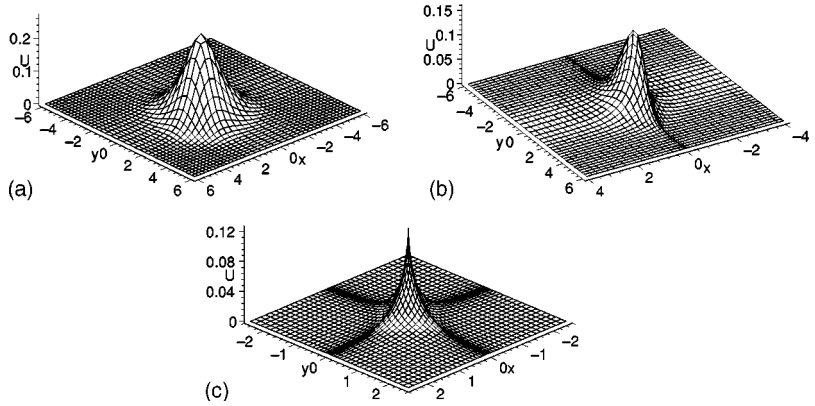

FIG. 3. Three novel single valued localized excitations for the universal quantity U shown by (92) at $t=0$ with (93)–(98) while the corresponding parameters are fixed as in (106) for the dromion (a), (110) for the first type of peakon (b), and (111) for the second type of peakon (c), respectively.

with (93)–(98). However, the parameters are chosen such that both p and q are multivalued.

For Fig. 2(a), the corresponding parameters are

$$k_1=k_2=k_3=l_1=l_2=1, \quad l_3=-1.4, \quad k_4=-2.5, \ a_0=1.9. \tag{103}$$

For Fig. 2(b), we have

$$k_1=k_2=k_3=l_1=l_2=1, \quad l_3=k_4=-1.6, \quad a_0=8. \tag{104}$$

The parameter selections

$$k_1=k_2=k_3=l_1=l_2=1, \quad l_3=k_4=-1.15, \quad a_0=4 \tag{105}$$

are related to Fig. 2(c).

In fact, the expression (92) with (93)–(98) also includes some interesting new types of single valued localized excitations by selecting the parameters appropriately such that both p and q are single valued.

In Fig. 3, three types of single valued localized excitations are plotted. Figure 3(a) shows a dromion structure and the corresponding parameters read

$$k_1=k_2=k_3=l_1=l_2=l_3=k_4=1, \quad a_0=4. \tag{106}$$

Because of the arbitrariness of the functions p and q, some types of piecewise continuous functions can be used to produce some types of $(2+1)$-dimensional peakons[14,55] and compactons.[22,56] Three special critical cases,

$$k_2k_4=-1, \quad l_2l_3\langle\ \rangle-1, \tag{107}$$

$$k_2k_4\langle\ \rangle-1, \ l_2l_3=-1, \tag{108}$$

and

$$k_2k_4=-1, \quad l_2l_3=-1, \tag{109}$$

of the expression (92) with (93)–(98) display some new types of peakon solutions.

Figure 3(b) shows a peakon structure of (92) with (93)–(98) and (107) at time $t=0$. The detailed parameters read

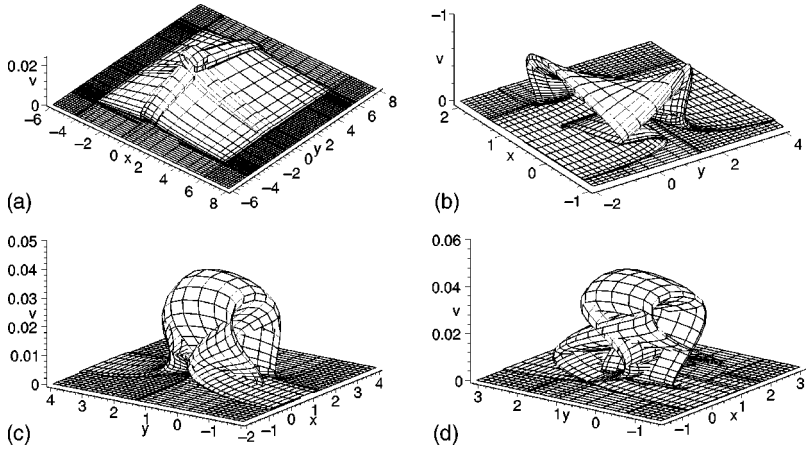

FIG. 4. Plots of the FSWs for the field v expressed by (60) at $t=0$ with (112)–(119) and the related concrete parameter selections are (120) for (a), (121) for (b), (122) for (c), and (123) for (d).

$$k_1=k_2=k_3=l_1=l_2=l_3=1, \quad k_4=-1,\ a_0=4. \tag{110}$$

Figure 3(c) shows the structure of another kind of peakon solution expressed by (92) with (93)–(98) and (109) at $t=0$ while the related parameters are

$$k_1=k_2=k_3=l_1=l_2=1, \quad l_3=-1, \quad k_4=-1, \quad a_0=4. \tag{111}$$

The more complicated FSWs and/or foldons can be constructed in two ways, selecting more complicated multivalue functions for the universal formula or using the extended forms of the universal formula with more arbitrary functions. In Fig. 4, some slightly more complex FSWs are plotted for the quantity v expressed by (60) with

$$p_x=-k_1\,\mathrm{sech}^2(k_2\xi-k_3t), \tag{112}$$

$$p=\frac{1}{2}k_1k_5(\mathrm{sech}^4(k_2\xi-k_3t)-1)-\frac{k_1}{15k_2}\{15+k_2[6k_6+10k_4+(5k_4+3k_6)\mathrm{sech}^2(k_2\xi-k_3t) -9k_6\,\mathrm{sech}^4(k_2\xi-k_3t)]\tanh(k_2\xi-k_3t)\}, \tag{113}$$

$$x=\xi+k_4\tanh(k_2\xi-k_3t)+k_5\tanh^2(k_2\xi-k_3t)+k_6\tanh^3(k_2\xi-k_3t), \tag{114}$$

$$q_{0y}=-l_1\,\mathrm{sech}^2(l_2\eta), \tag{115}$$

$$q_0=\frac{1}{2}l_1l_5[\mathrm{sech}^4(l_2\eta)-1]-\frac{l_1}{15l_2}[15+6l_2l_6+10l_2l_4+l_2(5l_4+3l_6)\mathrm{sech}^2(l_2\xi) -9l_2l_6\,\mathrm{sech}^4(l_2\xi)]\tanh(l_2\eta), \tag{116}$$

$$q_{1y}=-l_3\,\mathrm{sech}(l_2\eta), \tag{117}$$

$$q_1=\frac{l_3}{8}\mathrm{sech}(l_2\eta)\tanh(l_2\eta)[6l_6\,\mathrm{sech}^2(l_2\eta)-3l_6-4l_4]-\frac{l_3}{4l_2}(8+4l_2l_4+3l_2l_6)\arctan\exp(l_2\eta) +\frac{2}{3}l_3l_5\,\mathrm{sech}^3(l_2\eta), \tag{118}$$

$$y=\eta+l_4\tanh(l_2\eta)+l_5\tanh^2(l_2\eta)+l_6\tanh^3(l_2\eta), \tag{119}$$

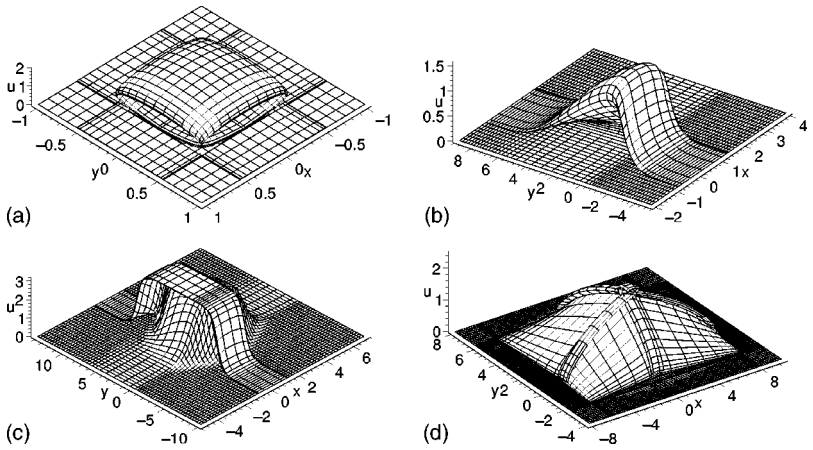

FIG. 5. Plots of the FSWs for the field u (41) with (124)–(127) for the real MNNV I and 2DsG systems at $t=0$ while the corresponding parameters are (128) for (a), (129) for (b), (130) for (c), and (131) for (d).

at time $t=0$.

The detailed selections of the parameters are

$$-k_1=k_2=k_3=k_5=l_1=l_2=l_3=l_5=1,\quad k_4=l_5=2,\quad k_6=l_6=-4,\quad a_0=50 \tag{120}$$

for Fig. 4(a),

$$k_1=72,\quad k_2=k_3=k_5=l_1=l_2=l_3=l_5=1,\quad k_4=l_4=2,\quad k_6=l_6=-4,\quad a_0=250 \tag{121}$$

for Fig. 4(b),

$$k_1=-\tfrac{6}{5},\quad k_2=k_3=k_5=l_1=l_2=l_3=l_5=1,\quad k_4=l_4=2,\quad k_6=l_6=-\tfrac{27}{5},\quad a_0=50 \tag{122}$$

for Fig. 4(c), and

$$k_1=-3,\quad k_2=k_3=k_5=l_1=l_2=l_3=l_5=1,\quad k_4=l_4=2,\quad k_6=l_6=-10,\quad a_0=250 \tag{123}$$

for Fig. 4(d).

As mentioned in Sec. II the field u is very important for the real MNNV I system and the real 2DsG system. Similar FSWs and foldons can also be constructed for the field u expressed by (38) and/or (41).

In Fig. 5, four types of FSWs are plotted for the field u of the MNNV I system and the 2DsG system expressed by (41) and the functions p and q are taken as

$$p=k_1\,\mathrm{sech}^2(k_2\xi-k_3t), \tag{124}$$

$$x=\xi+k_4\tanh(k_2\xi-k_3t)+k_5\tanh^2(k_2\xi-k_3t)+k_6\tanh^3(k_2\xi-k_3t), \tag{125}$$

$$q=l_1\,\mathrm{sech}^2(l_2\eta), \tag{126}$$

$$y=\eta+l_3\tanh(l_2\eta)+l_4\tanh^2(l_2\eta)+l_5\tanh^3(l_2\eta). \tag{127}$$

For Fig. 5(a), the related parameters are fixed as

$$k_1=1.2,\quad l_1=l_2=k_2=k_3=1,\quad l_3=k_4=-2,\quad l_4=l_5=k_5=k_6=0. \tag{128}$$

The details on the parameters of Fig. 5(b) read

$$k_1=k_2=k_3=k_5=l_1=l_2=l_3=l_5=1, \quad k_4=l_4=2, \quad k_6=-4. \tag{129}$$

For Fig. 5(c), we select

$$k_1=120, \quad k_2=k_3=k_5=l_2=l_3=l_5=1, \quad l_1=6, \; k_4=l_4=2, \quad k_6=-4. \tag{130}$$

The parameter selections

$$k_1=3, \quad k_2=k_3=k_5=l_1=l_2=l_3=1, \quad l_5=-8, \quad k_4=l_4=2, \quad k_6=-12, \tag{131}$$

are responsible for Fig. 5(d).

Fortunately, owing to the arbitrariness of the functions in the universal formula and its extension forms, we have constructed not only the single valued localized excitations but also quite rich FSWs. Now, one of the most important problems which should be discussed in the first place is whether these types of localized excitations are solitons. Particularly, are these FSWs foldons? To find the answer, we have to study the interaction properties among these types of localized excitations.

V. INTERACTION PROPERTIES OF (2+1)-DIMENSIONAL LOCALIZED EXCITATIONS

In Ref. 14, we have plotted some special interaction figures for two special types of localized excitations (saddle type of ring solitons and peakons) with and without completely interaction properties. In Ref. 22, a method is proposed to construct compact solitary waves and compactons on the basis of the universal formula (1). In Ref. 28, the method has been developed to generate general $(2+1)$-dimensional solitary waves and solitons for the quantity F expressed by (25). The complete interaction properties of the plateau type, basin type, and bowl type ring solitons for the 2DsG system are discussed in Ref. 28. In our previous short report,[35] a possible way is provided to construct foldons for the quantity given by (60) with static q_0 and q_1. In this section, as a summary and extension, we first discuss the interaction property of the localized excitations related to the universal quantity (1) and the field v (60). The possible foldon excitations are specified both for the quantities v and u expressed by (60) and (41), respectively. Then we give some concrete interaction examples of FSWs and foldons.

A. Asymptotic behaviors of the localized excitations produced from (1)

In general, if the functions p and q are selected as multi-localized solitonic excitations with

$$p|_{t\to\mp\infty}=\sum_{i=1}^{M} f_i^{\mp}, f_i^{\mp}\equiv f_i(x-c_it+\delta_i^{\mp}), \tag{132}$$

$$q|_{t\to\mp\infty}=\sum_{j=1}^{N} h_j^{\mp}, \quad h_j^{\mp}\equiv h_j(y-C_jt+\Delta_j^{\mp}), \tag{133}$$

where $\{f_i, h_j\}$ $\forall i$ and j are localized functions, then the universal quantity U expressed by (1) delivers $M\times N$ $(2+1)$-dimensional localized excitations with the asymptotic behavior

$$U|_{t\to\mp\infty}\to\sum_{i=1}^{M}\sum_{j=1}^{N}\frac{2(a_1a_2-a_3a_0)f_{ix}^{\mp}h_{jy}^{\mp}}{(a_0+a_1(f_i^{\mp}+F_i^{\mp})+a_2(h_j^{\mp}+H_j^{\mp})+a_3(f_i^{\mp}+F_i^{\mp})(h_j^{\mp}+H_j^{\mp}))^2}\equiv\sum_{i=1}^{M}\sum_{j=1}^{N}U_{ij}^{\mp}, \tag{134}$$

where

$$F_i^{\mp}=\sum_{j<i} f_j(\mp\infty)+\sum_{j>i} f_j(\pm\infty), \tag{135}$$

$$H_i^{\mp}=\sum_{j<i} h_j(\mp\infty)+\sum_{j>i} h_j(\pm\infty), \tag{136}$$

and we have assumed, without loss of generality, $C_i>C_j$ and $c_i>c_j$ if $i>j$.

It can be deduced from expression (134) that the ijth localized excitation U_{ij} preserves its shape during the interaction iff

$$F_i^{+}=F_i^{-}, \tag{137}$$

$$H_j^{+}=H_j^{-}. \tag{138}$$

Meanwhile, the phase shift of the ijth localized excitation F_{ij} reads

$$\delta_i^{+}-\delta_i^{-} \tag{139}$$

in the x direction and

$$\Delta_j^{+}-\Delta_j^{-}. \tag{140}$$

in the y direction.

The above discussions demonstrate that multiple localized solitonic excitations for the universal quantity U can be constructed without difficulties via the $(1+1)$-dimensional multiple localized excitations with the properties (132), (133), (137), and (138). As a matter of fact, any multiple localized solutions (or their derivatives) with completely elastic interaction behaviors of any known $(1+1)$-dimensional integrable models can be utilized to construct $(2+1)$-dimensional multiple localized solitonic solutions with completely elastic interaction properties for all the MLVSA models. Some detailed examples have been given in Ref. 28 for the 2DsG system based on the multi-soliton solutions of the $(1+1)$-dimensional sine-Gordon equation and the KdV equation.

If f_i and h_j of (132) and (133) are taken as $(1+1)$-dimensional localized multivalue functions (say, loop solitons), then (1) becomes multiple FSWs ($F_i^{+}\neq F_i^{-}$, $H_j^{+}\neq H_j^{-}$ at least for one of i,j) or multiple foldons ($F_i^{+}=F_i^{-}$, $H_j^{+}=H_j^{-}$ for all i, j).

B. Asymptotic properties of the localized excitations generated via (60)

If the function p is in the form (132) while q_0 and p_0 are taken as arbitrary static functions, then the field v expressed by (60) possesses the following asymptotic behavior:

$$v|_{t\to\mp\infty}\to\sum_{i=1}^{M}\frac{2f_{ix}^{\mp}[q_1q_{0y}-(a_0+q_0)q_{1y}]}{(a_0+q_0+(f_i^{\mp}+F_i^{\mp})q_1)^2}\equiv\sum_{i=1}^{M} v_j^{\mp}. \tag{141}$$

If condition (137) is satisfied, then the asymptotic property (141) reveals the solitonic property for the field v given by (60).

To get the multiple FSWs and/or foldons from (60) with p selected as (132), we have to require p and then f_i be localized multivalue functions again.

More concretely, selecting the multivalue function p of (60) as (88)–(90), $v_j^{\mp}$ of (141) will be ($z_j\equiv\xi-c_jt$),

$$v_j^{\mp}=\frac{2f_{jz_j}^{\mp}[q_1q_{0y}-(a_0+q_0)q_{1y}]}{(1+g_{jz_j}^{\mp})[a_0+q_0+q_1(f_j^{\mp}(z_j)+F_j^{\mp})]^2}, \tag{142}$$

$$x=\xi+\delta_j^{\mp}+g_j^{\mp}(z_j), \tag{143}$$

where the phase factors $\delta_j^{\mp}$ read

$$\delta_j^{\mp}=\sum_{i<j} G_i^{\mp}+\sum_{i>j} G_i^{\pm}. \tag{144}$$

From the asymptotic results (142)–(144), we discover four important facts.

(i) The jth localized excitation given by (60) with (88)–(90) is a traveling wave moving in the velocity c_j along the negative ($c_j<0$) or positive ($c_j>0$) x direction.

(ii) The multivalued properties of the jth localized excitation is only determined by g_j of (89).

(iii) The shape of the jth excitation will change if

$$F_j^{+}\neq F_j^{-}, \tag{145}$$

following the interaction. Contrarily, if

$$F_j^{+}=F_j^{-}, \tag{146}$$

it will preserve its shape.

(iv) The total phase shift for the jth excitation is

$$\delta_j^{+}-\delta_j^{-}. \tag{147}$$

C. Interaction properties of the localized excitations for the field u (41) of the real MNNV I system and the 2DsG system

For the real MNNV I system and the 2DsG systems, the important localized excitations for the field u come from (41). Selecting the functions p and q as (132) and (133) leads to

$$u|_{t\to\mp\infty}\to 2\arctan\sum_{i=1}^{M}\sum_{j=1}^{N}(f_i^{\mp}+F_i^{\mp})(h_j^{\mp}+H_j^{\mp}). \tag{148}$$

Furthermore, the most important selections for p and q may be

$$f_i(\pm\infty)=0,\ \ h_j(\pm\infty)=0,\forall i,j. \tag{149}$$

Under condition (149), we have

$$f_i^{\mp}h_j^{\mp}|_{x^2+y^2\to\infty}\to 0, \tag{150}$$

and then (148) can be simplified to

$$u|_{t\to\mp\infty}\to\sum_{i=1}^{M}\sum_{j=1}^{N}2\arctan(f_i^{\mp}h_j^{\mp})\equiv\sum_{i=1}^{M}\sum_{j=1}^{N}u_{ij}. \tag{151}$$

The asymptotic property (151) gives rise to a conclusion that when p and q possess the property (132) and (133) with (149), the interactions among the localized excitations for the field u of the MNNV I and 2DsG systems are completely elastic no matter whether the functions p and q are single valued or multivalued. In Ref. 28, some special examples for the complete interactions of the plateau type and basin type ring solitons are given.

D. Examples of the foldon interactions

In this section, we give some concrete examples on the foldon and FSW interactions.

Example 1: *Two foldon interaction of the MNNV I system and the 2DsG system.*

For the real MNNV I and 2DsG systems, a special type of multiple foldon solutions for the field u (41) can be obtained by taking

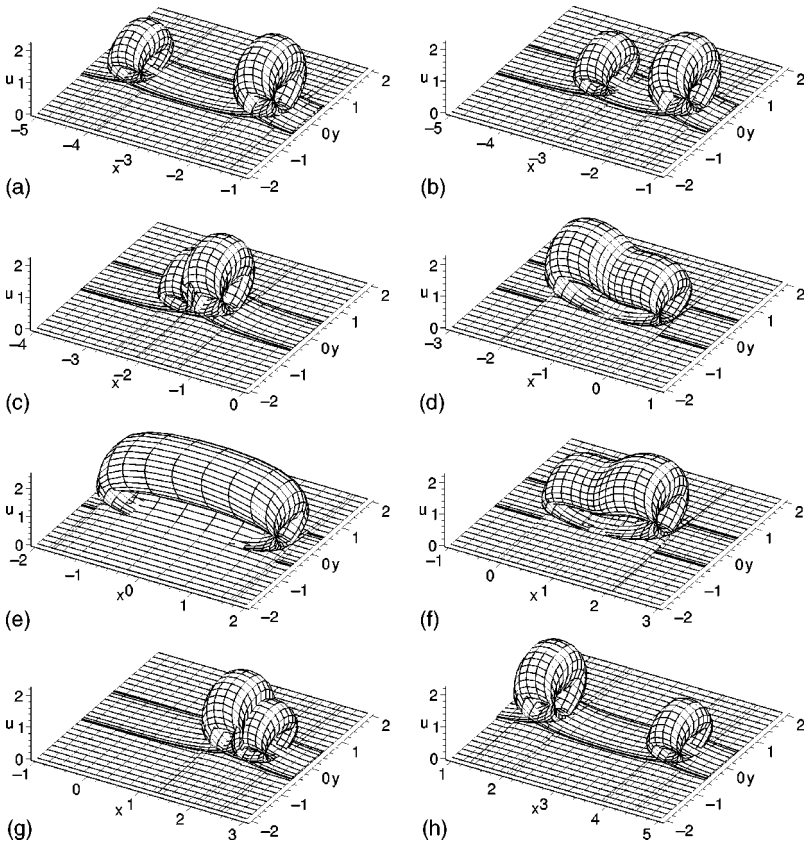

FIG. 6. Evolution plots of two foldons for the field u expressed by (41) for the MNNV I and 2DsG systems with the selections (156)–(159) at the times (a) $t=-24$, (b) $t=20$, (c) $t=-16$, (d) $t=-8$, (e) $t=0$, (f) $t=8$, (g) $t=16$, and (h) $t=24$, respectively.

$$p=\sum_{i=1}^{N} s_i \operatorname{sech}^{m_i}(k_i(\xi-c_i t)), \tag{152}$$

$$x=\xi+\sum_{i=1}^{N} y_i \tanh^{n_i}(k_i(\xi-c_i t)), \tag{153}$$

$$q=\sum_{i=1}^{M} S_i \operatorname{sech}^{M_i}(K_i(\eta-C_i t)), \tag{154}$$

$$y=\eta+\sum_{i=1}^{M} Y_i \tanh^{N_i}(K_i(\eta-C_i t)), \tag{155}$$

where s_i, y_i, S_i, Y_i, c_i, C_i, k_i, and K_i are all arbitrary constants, M, N, m_i, n_i, M_i, and N_i are positive integers.

Figure 6 shows the two-foldon interaction with

$$p=2\operatorname{sech}^2\xi+\operatorname{sech}^2(\xi-\tfrac{1}{4}t), \tag{156}$$

$$x=\xi-1.8\tanh\xi-1.7\tanh(\xi-\tfrac{1}{4}t), \tag{157}$$

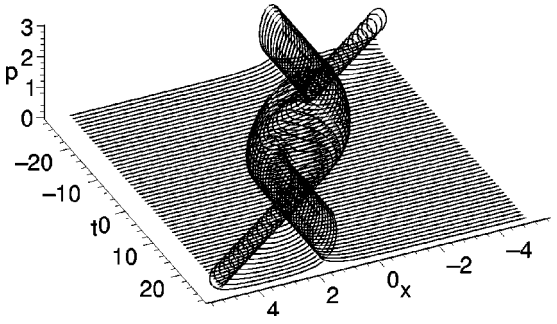

FIG. 7. Evolution plot of two loop solitons for the quantity p expressed by (156) with (157) regarding Fig. 6.

$$q=\operatorname{sech}^2\,\eta, \tag{158}$$

$$y=\eta-2\tanh\,\eta. \tag{159}$$

From Figs. 6(a)–6(h), we can see that the interaction between two foldons is completely elastic. One of the velocities of two foldons is fixed as zero, which makes it easy to survey their phase shifts. Clearly, before the interaction, the static foldon (the large one) is located at $x=-1.7$ while after the interaction, it shifts to $x=1.7$. Actually, once the conditions (149) are satisfied, the completely elastic interaction property of the multiple localized excitations for the field u expressed (41) with (132)–(133) of the MNNV I and 2DsG systems is entirely guaranteed by the completely elastic interaction property of the $(1+1)$-dimensional fields p and q. For instance, the completely elastic interaction property of the two-loop solution p expressed by (156) with (157) ensures the completely elastic interaction property of two dromions shown in Fig. 6. Figure 7 is an evolution plot of two $(1+1)$-dimensional loop solitons expressed by (156) with (157).

Example 2: Interaction among Four foldons of the MNNV I system and the 2DsG system.

Figure 8 shows a special four-foldon interaction of u expressed by (41) for the MNNV I and 2DsG systems where the functions p and q are taken as

$$p=0.6\operatorname{sech}^2\,\xi+\operatorname{sech}^2(\xi-t), \tag{160}$$

$$x=\xi-1.15\tanh\,\xi-1.15\tanh(\xi-t), \tag{161}$$

$$q=\operatorname{sech}^2\,\eta+2\operatorname{sech}^2(\eta-t), \tag{162}$$

$$y=\eta-1.15\tanh\,\eta-1.15\tanh(\eta-t). \tag{163}$$

Similar to the example shown in Fig. 6, in addition to the completely elastic interaction property among four foldons, phase shifts are observed from Fig. 8. To reveal phase shifts, it is convenient and sufficient to set the velocity of one loop soliton (either for p or q) to zero. Seen from Figs. 8(a) to 8(h), prior to interaction, the smallest foldon is static and situated at $\{x=-1.15,\ y=-1.15\}$, the largest foldon is moving with its center located at $\{x=t+1.15,\ y=t+1.15\}$, while for the other two foldons, they are static in one direction and moving in the other direction and their centers are located at $\{x=-1.15,\ \eta=t+1.15\}$ and $\{x=t+1.5,\ y=-1.15\}$, respectively; after the interaction, the static foldon remains static with shape unchanged and its center shifts to $\{x=1.15,\ y=1.15\}$, the largest foldon recovers its shape and its center shifts to $\{\xi=t-1.15,\ y=t-1.15\}$, the others preserve their shapes and velocities (static in one case) but have their centers shifted to $\{x=1.15,y=t-1.15\}$ and $\{x=t-1.15,\ y=1.15\}$, respectively.

Example 3: Interaction between two FSWs for all the MLVSA solvable systems.

The last two special examples are responsible for the real MNNV I system and the real 2DsG system. For the other MLVSA models studied in Ref. 14 and also mentioned in Sec. I, the

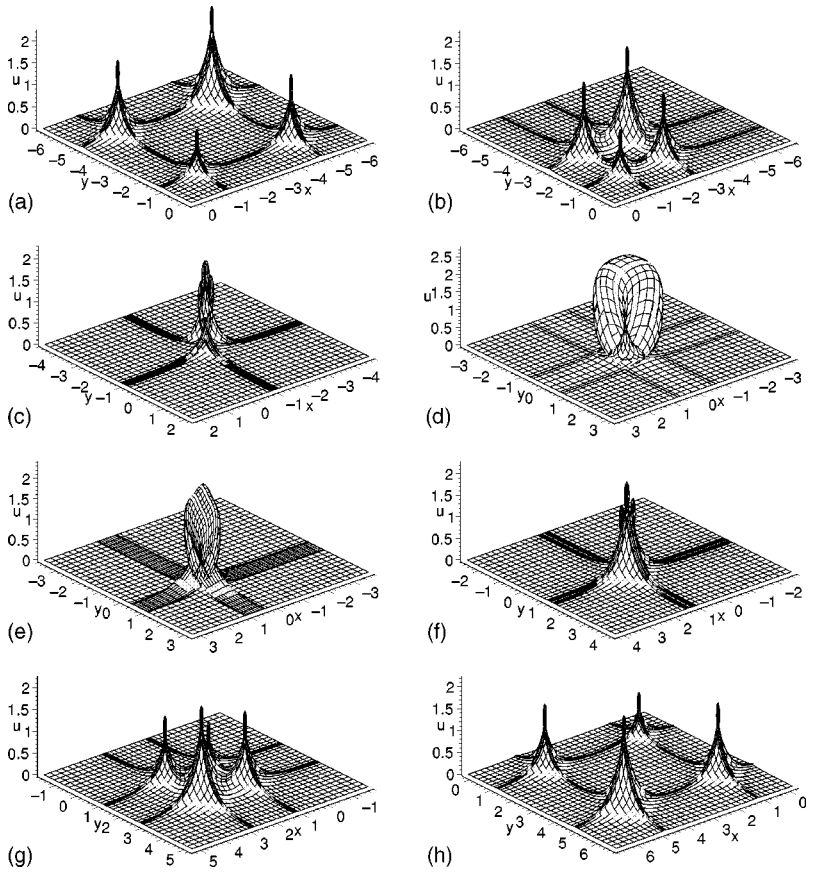

FIG. 8. Evolution plot of four foldons for the field u expressed by (41) for the MNNV I and 2DsG systems with the selections (160)–(163) at the times (a) $t=-6$, (b) $t=-4$, (c) $t=-2$, (d) $t=0$, (e) $t=1.5$, (f) $t=2.5$, (g) $t=4$, and (h) $t=6$, respectively.

universal quantity (1) [or its extend form (58)] is of more importance. Some examples of the single FSW have been discussed in the last section and the general aspect of the related multiple FSWs and foldons has been given in Secs. V A and V B. Here we write and plot down two more special two-FSW (example 3) and two-foldon (example 4) solutions for the universal quantity U.

Figure 9 is a pre- and post-interaction plot of the two FSWs for the quantity U expressed by (92) with the selections

$$p_x=-12\,\mathrm{sech}^2\,\xi-10\,\mathrm{sech}^2(\xi-t), \tag{164}$$

$$\begin{aligned} p=\frac{253}{5}\coth t\,\mathrm{csch}^2\,t\ln\frac{\alpha+1}{\alpha+\beta}+\frac{2}{15(\beta+1)^3(\beta+\alpha)^3(\alpha-1)^2}\{&(150\alpha^3+1398\alpha^2+1308\alpha\\ &+180)\beta^5+(4116\alpha^3+4134\alpha-45\alpha^4+7029\alpha^2-54)\beta^4+(35\alpha^5+1853\alpha^4+13\,175\alpha^3\\ &+13\,533\alpha^2+1722\alpha+42)\beta^3+3\alpha(1735\alpha^3+92+95\alpha^4+6457\alpha^2+1741\alpha)\beta^2\\ &+3\alpha^2(27+2493\alpha+2523\alpha^2+17\alpha^3)\beta+11\alpha^3(262\alpha+7+7\alpha^2)\}, \end{aligned} \tag{165}$$

$$\alpha\equiv\exp(2\xi),\quad \beta\equiv\exp(2t), \tag{166}$$

$$x=\xi-1.15\tanh\xi-1.15\tanh(\xi-t), \tag{167}$$

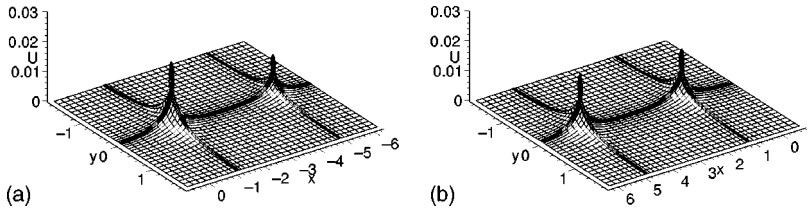

FIG. 9. Pre- and post-interaction of two FSWs at times (a) $t=-4.5$, and (b) $t=4.5$ for the universal quantity U (92) with (164)–(171).

$$q_y=-\operatorname{sech}^2\,\eta, \tag{168}$$

$$q=-\tfrac{1}{30}\tanh\,\eta(7-\tfrac{23}{2}\operatorname{sech}^2\,\eta), \tag{169}$$

$$y=\eta-1.15\tanh\,\eta, \tag{170}$$

$$a_0=30. \tag{171}$$

From Figs. 9(a) and 9(b), we know that the quantity U (92) with (164)–(171) expresses a special two-FSW solution in that the interaction between them is nonelastic. Actually, the completely elastic interaction condition (137) is not satisfied for the solution (92) with (164)–(171). For the static FSW,

$$F_1^+-F_1^-=\tfrac{14}{3}\neq 0, \tag{172}$$

and for the moving FSW,

$$F_2^+-F_2^-=-\tfrac{28}{5}\neq 0. \tag{173}$$

Though the singular factors (at $t=0$), $\coth t$, $\operatorname{csch} t$, and $1/(\alpha-1)$ appear in the expression of p (165), there is no singularity for the interaction solution (92) with (164)–(171) inasmuch

$$p|_{t=0}=\lim_{t\to 0}p=\frac{44(15\alpha^2-39\alpha-8)}{15(\alpha+1)^3}, \tag{174}$$

and

$$\max|p+q|\leqslant\max|p|+\max|q|=\tfrac{359}{30}+\tfrac{286}{345}\sqrt{299}\approx 26.3<a_0=30. \tag{175}$$

Example 4: Interaction between two foldons for the MLVSA solvable systems.

According to the general discussions in Secs. V A and V B, in order to find foldons, the functions p and q must be selected in a way that the conditions (137)–(138) or (146) are satisfied.

Figure 10 is a pre- and post-interaction plot of two foldons for the field U expressed by (92) with the selections $[\alpha\equiv\exp(2\xi),\ \beta\equiv\exp(2t)]$

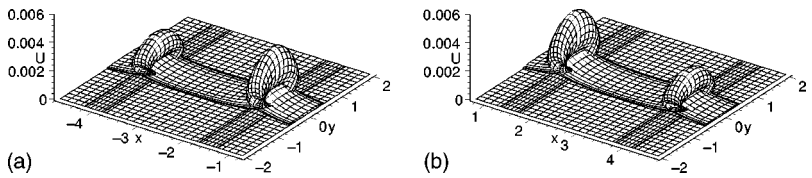

FIG. 10. Pre- and post-interaction of two foldons at times (a) $t=-5.5$, and $t=5.5$ for the universal quantity U (92) with (176)–(182).

$$p_x = -\tfrac{4}{5}\operatorname{sech}^2\xi - \tfrac{1}{2}\operatorname{sech}^2(\xi - t), \tag{176}$$

$$p = \frac{39}{10}\coth t\,\operatorname{csch}^2 t \ln\frac{\alpha+1}{\alpha+\beta} + \frac{1}{5(\beta+1)^3(\beta+\alpha)^3(\alpha-1)^2}\{(67\alpha+76\alpha^2+5\alpha^3+8)\beta^5 - (8 - 211\alpha - 205\alpha^3 - 377\alpha^2 + 5\alpha^4)\beta^4 + 3\alpha(23+243\alpha+225\alpha^2+29\alpha^3)\beta^3 + \alpha\beta^2(8\alpha^4+257\alpha^3 + 1027\alpha^2+263\alpha+5) - \alpha^2(5-401\alpha^2-392\alpha+8\alpha^3)\beta + 156\alpha^4\}, \tag{177}$$

$$x = \xi - 1.5\tanh\xi - 1.5\tanh(\xi - t), \tag{178}$$

$$q_y = -\operatorname{sech}^2\eta, \tag{179}$$

$$q = \tfrac{1}{3}\tanh\eta(1 + 2\operatorname{sech}^2\eta), \tag{180}$$

$$y = \eta - 2\tanh\eta, \tag{181}$$

$$a_0 = 20. \tag{182}$$

Since the completely elastic interaction condition (137) is really satisfied for both the static excitation and the moving one, the solution (92) with (176)–(182) is genuinely a two-foldon solution. Likewise, there is no singularity for the solution (92) with (176)–(182) thanks to

$$p|_{t=0} = \lim_{t\to 0} p = \frac{13(\alpha^2-4\alpha-1)}{5(\alpha+1)^3} \tag{183}$$

and

$$\max|p+q| \leqslant \max|p| + \max|q| = \frac{13}{10} + \frac{26}{45}\sqrt{6} + \frac{\sqrt{2}}{3} \approx 3.12 < a_0 = 20. \tag{184}$$

VI. SUMMARY AND DISCUSSIONS

The MLVSA has been successfully applied to many $(2+1)$-dimensional nonlinear systems. Utilizing the MLVSA, a universal formula is derived for all the known MLVSA solvable models. Simultaneously, a diversity of localized excitations are obtained from this universal formula via the appropriate selections of the arbitrary functions included in the formula.

In this paper, the MLVSA and the universal formula have been extended in two directions. First, the MLVSA is extended for the MNNV system and the 2DsG system where two universal terms with some suitable conditions can be superposed to generate a new exact solution of the same models. Second, by changing the basic ansatz of the MLVSA, the universal formula is extended at least for the DLWE, the BKK system, the higher order BKK system, and the Burgers system such that arbitrary number of variable separated functions are included in the variable separation solutions. The MLVSA and the universal formula may also be extended in some other ways. For instance, the MLVSA has been successfully extended to the differential-difference systems,[57] and arbitrary number of the variable separated functions can also be introduced by means of the Darboux transformations and the Bäcklund transformations[58] and so on.

Starting from the ''universal'' formula and/or its extended forms, all sorts of localized excitations with and without completely elastic interaction properties are constructed readily by suitably selecting the arbitrary functions according to the asymptotic results (134), (141), (142), and (151). Especially, a new kind of localized excitations, FSWs and foldons, is investigated both analytically and graphically. Foldons may be folded quite freely and complicatedly and then possess quite rich structures and interaction properties. The explicit phase shifts for all the localized excitations offered by the universal formula and its extended forms have also been given.

On the one hand, there are a large number of complicated ''folded'' and/or the multivalued phenomena in the real natural world. Nonetheless, there is no good analytical way to treat these kinds of complicated phenomena. This paper is only a beginning attempt to looking for some types of possible stable multivalued localized excitations, FSWs and foldons, for some real physical models including some quite ''universal'' systems like the well-known DS systems[59–61] and the DLWE.

In Refs. 30 and 62, the authors pointed out that the localized solutions of the DS equation, say, dromions, can be remote controlled by choosing a suitable motion of the boundaries. In Ref. 14, we also pointed out that though the localized excitations such as the dromions, lumps, ring solitons, peakons and foldons proposed here possess zero boundary conditions for the quantity U and its extended forms, the boundary conditions for other quantities, say, the mean flow for the DS model and v for the MNNV system, are not identically zero. The different selections of the arbitrary functions p and q in (1) correspond to the different selections of boundary conditions of those fields (or potentials) with nonzero boundary conditions and vice versa. That means, in some sense, the dromions, foldons, and other types of localized excitations for some physical quantities are remote controlled by some other quantities (or potentials). This fact hints that it is possible for one to observe the dromions, foldons, and other kinds of localized excitations from the systems governed by the MLVSA solvable models via inputting suitable boundary conditions. For foldons, the input boundaries may be selected as $(1+1)$-dimensional loop solitons.

Because the formula (60) is valid for various $(2+1)$-dimensional interesting models which are widely applied in many physical fields, we do believe that foldons are useful in the studies on the complicated ''folded'' natural world. The more about both the (extended) ''universal'' formula and the general (or special) foldons especially their possible real applications should be studied further.

ACKNOWLEDGMENTS

We acknowledge helpful discussions with Professor C. Rogers, Dr. W. Schief, Professor C-z Qu, and Dr. H-c Hu. The work is supported by the National Outstanding Youth Foundation of China (No. 19925522), the National Natural Science Foundation of China (No. 90203001), and the Research Fund for the Doctoral Program of Higher Education of China (Grant. No. 2000024832).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Vavilov–Cherenkov and transition radiations on the dielectric and metallic spheres

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(Received 2 April 2003; accepted 20 May 2003)

Closed expressions are obtained for angular and frequency radiation intensities produced by a charge moving inside the dielectric sphere S, with observations made outside S (in fact, this is a typical experimental situation when a charge moves in one medium while measurements are made in the other one). It is shown that the difference in media properties inside and outside S drastically affects angular and frequency distributions. Also, a charge motion is considered which begins and terminates in medium 2 and which passes either through the dielectric sphere filled with medium 1 or through the metallic one. The energy flux in medium 2 involves the Vavilov–Cherenkov, transition radiation and the one arising from the charge instantaneous beginning and termination of motion. The evaluated angular and frequency distributions for various charge velocities and medium properties inside and outside S show that the standard identification of the charge velocity by its radiation on the part of the charge trajectory where $\beta n > 1$ is not always valid. We analyze also the frequently used interpretation of the transition radiation in terms of instantaneous charge deceleration in one medium and its sudden acceleration in another one, and find them as to be insufficient. On the other hand, attempts to interpret the transition radiation in terms of semi-infinite motions terminating in one medium and beginning in the other one turn out to be correct if one takes into account the terms corresponding to the Vavilov–Cherenkov radiation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1602162]

I. INTRODUCTION

This paper has a twofold aim.

First, usually, a charge moves in the one medium (1) while the measurements are made in the other one (2). For example, in the original Cherenkov experiments,[1] the electron moved in the vessel filled with water, while measurements were made outside this vessel, in air. The radiation of a charge moving inside the infinite cylindrical sample C was considered by Frank and Ginsburg[2] who shown that there is no radiation outside C if the Tamm–Frank radiation condition is not fulfilled there. It should be recalled that Frank and Ginsburg evaluated the energy flux in the direction perpendicular to the motion axis. The energy flux in the direction parallel to the motion axis was evaluated in Ref. 3. It was shown there that this component of radiation is infinitely small for all frequencies except for the infinite discrete sequence of frequencies where it is infinite.

In the same reference,[3] the geometrical optics consideration has been applied to the radiation of charge moving in the finite space interval lying completely inside the sphere S filled with a substance 1 with refractive index n_1. Observations are made outside S, in medium 2 with refractive index n_2. It was shown there that the angular spectrum broadens if $n_2 < n_1$. One of the goals of the present treatment is to make the quantitative analysis of this problem. For this, we evaluated angular and frequency radiation intensities for a number of charge velocities and media properties. In general, the presence of medium 2 outside S different from medium 1 inside S leads to the

broadening of the angular spectrum and to the appearance of additional maxima at large angles. Calculations predict the oscillations of the frequency spectrum. This could be observed experimentally.

The second problem which will be studied here is the transition and Vavilov–Cherenkov (VC) radiations on the dielectric and metallic spheres. The notion of the transition radiation was introduced by Frank and Ginsburg[4] who studied radiation arising from the uniformly moving charge passing from one medium to another. They considered the plane boundary between media 1 and 2. A thorough exposition of the transition radiation may be found in Ref. 5. In this consideration, we consider a charge motion which begins and terminates in medium 2 and which passes through the dielectric sphere filled with medium 1. The energy flux is evaluated in medium 2. As far as we know, the transition radiation only for plane interfaces was considered in physical literature. For the treated problem the angular and frequency radiation intensities are evaluated for a number of charge velocities and media properties. These expressions contain transition and VC radiations as well as the radiation from the charge instantaneous beginning and termination of motion. It is proved that the identification (frequently used by experimentalists) of the charge velocity by the Cherenkov radiation on the part of the charge trajectory where $\beta n>1$ is not always valid in the presence of boundaries.

There are analyzed attempts to explain transition radiation in terms of the charge instantaneous termination of motion in one medium and the instantaneous charge beginning of motion in another medium. It is proved that their contribution to the radiation intensity disappears if the charge motion with instantaneous velocity jumps can be considered as a limiting case of the charge smooth motion. It is considered also the interpretation of the transition radiation in terms of semi-infinite charge motions with instantaneous termination of the charge motion in one medium and with its instantaneous beginning of motion in the other one. It is shown that if the charge velocity is greater than the light velocity in medium, the terms corresponding to the VC radiation should be taken into account.

The plan of our exposition is as follows. The mathematical preliminaries are collected in Sec. II. The expansion of the electromagnetic field in terms of Legendre polynomials for the Tamm problem is given in Sec. III. In Sec. IV, a charge moving inside the dielectric sphere S filled with the substance 1 is considered. The radiation intensity is evaluated outside S, in medium 2. In Sec. V, a charge whose motion begins and terminates in the medium 2 and which passes through the dielectric sphere filled with medium 1 or through the metallic one. The energy flux is evaluated in medium 2. In Sec. VI, the review of attempts to interpret the transition radiation in terms of sudden termination of the charge motion in one medium and its sudden beginning in the other one is given. A short resume of the results obtained is presented in Sec. VII.

II. MATHEMATICAL PRELIMINARIES

We consider the charge motion in medium as to be given and intend to evaluate the electromagnetic field arising from such a motion. The solving of Maxwell equations grounds on the use of the Green functions.

For the charge motion in medium with refractive index n, the Green function is equal to

$$G_n=\exp(ik_nR)/R, \quad R=|\vec{r}-\vec{r}\,'|. \tag{2.1}$$

Here $k_n=kn$, $k=\omega/c$ and n is the medium refractive index. Its expansion in spherical coordinates is given by (see, e.g., Ref. 6)

$$G_n=2\sum_{m\geqslant 0}\epsilon_m(2l+1)\frac{(l-m)!}{(l+m)!}\cos m(\phi-\phi')G_l(r,r')P_l^m(\cos\theta)P_l^m(\cos\theta'), \tag{2.2}$$

where

$$G_l(r,r')=ik_n j_l(k_n r_<)h_l(k_n r_>), \quad j_l(x)=\sqrt{\frac{\pi}{2x}}J_{l+1/2}(x), \quad h_l(x)=\sqrt{\frac{\pi}{2x}}H^{(1)}_{l+1/2}(x),$$

$\epsilon_m=1/(1+\delta_{m,0})$; $r_>=r, r_<=r'$ if $r>r'$; $r_>=r', r_<=r$ if $r<r'$.

These equations are no longer valid if medium consists of two pieces with different refractive indices. We consider a particular case when space regions inside and outside the sphere S of the radius a are filled with the substances 1 and 2 with parameters ϵ_1,μ_1 and ϵ_2,μ_2, respectively. The Green function satisfying equations

$$(\Delta+k_1^2)G_n=-4\pi\delta^3(\vec{r}-\vec{r}')$$

for $r<a$ and

$$(\Delta+k_2^2)G_n=-4\pi\delta^3(\vec{r}-\vec{r}')$$

for $r>a$ has the same form as (2.2) but with $G_l(r,r')$ given by

$$\begin{aligned}G_l=&ik_1\Theta(a-r)\Theta(a-r')j_l(k_1r_<)h_l(k_1r_>)+ik_2\Theta(r-a)\Theta(r'-a)j_l(k_2r_<)h_l(k_2r_>)\\&+ik_1D_l\Theta(a-r)\Theta(r'-a)j_l(k_1r)h_l(k_2r')+ik_2C_l\Theta(r-a)\Theta(a-r')j_l(k_1r')h_l(k_2r).\end{aligned} \tag{2.3}$$

Here $k_1=kn_1$ and $k_2=kn_2$ ($n_1=\sqrt{\epsilon_1\mu_1}$ and $n_2=\sqrt{\epsilon_2\mu_2}$ are the refractive indices of media 1 and 2, respectively). The constants C_l and D_l are defined by the boundary conditions at $r=a$. The vector potential (VP) in the spectral representation for a charge moving along the z axis is found from the equation

$$A_z=\frac{1}{c}\int G(\vec{r},\vec{r}')\mu(r')j_z(\vec{r}')dV', \tag{2.4}$$

where $\mu=\mu_1$ for $r<a$ and $\mu=\mu_2$ for $r>a$. The integration is performed over space points where the spectral current density $j_z(\vec{r}')$ differs from zero.

III. PEDAGOGICAL EXAMPLE: THE TAMM PROBLEM IN A SPHERICAL BASIS

A. The original Tamm problem

Tamm considered the following problem.[7] A point charge is at rest at the point $z=-z_0$ of the z axis up to a moment $t=-t_0$ and at the point $z=z_0$ after the moment $t=t_0$. In the time interval $-t_0<t<t_0$, it moves uniformly along the z axis with the velocity v greater than the light velocity in medium $c_n=c/n$. The nonvanishing z component of the VP in the spectral representation is given by

$$A_z(x,y,z)=\frac{e\mu}{2\pi c}\alpha_T, \tag{3.1}$$

where

$$\alpha_T=\int_{-z_0}^{z_0}\frac{dz'}{R}\exp\left[ik\left(\frac{z'}{\beta}+nR\right)\right], \quad R=[\rho^2+(z-z')^2]^{1/2}, \quad \rho^2=x^2+y^2.$$

Imposing the conditions: (i) $R\gg z_0$ (this means that the observation distance is much larger than the motion interval); (ii) $k_nR\gg 1$, $k_n=\omega/c_n$ (this means that the observations are made in the wave zone); (iii) $nz_0^2/2R\lambda\ll 1$, $\lambda=2\pi c/\omega$ [this means that the second-order terms in the expansion of R should be small compared with π since they enter as a phase in (3.1); λ is the observed wavelength], Tamm obtained the following expression for the magnetic VP:

$$A_z=\frac{e\mu}{\pi n\omega r}\exp(iknr)q,\quad q=\frac{1}{1/\beta_n-\cos\theta}\sin\left[\frac{kLn}{2}\left(\frac{1}{\beta_n}-\cos\theta\right)\right]. \tag{3.2}$$

Here $L=2z_0$ is the motion interval and $\beta_n=\beta n$. In the limit $kL\to\infty$, one gets

$$q\to\pi\delta\left(\frac{1}{\beta_n}-\cos\theta\right),\quad A_z\to\frac{e\mu}{\omega nr}\exp(iknr)\,\delta(\cos\theta-1/\beta_n). \tag{3.3}$$

Using the vector potential (3.2), Tamm evaluated the electromagnetic field strengths and the energy flux through the sphere of the radius r for the whole time of observation

$$\mathcal{E}=R_0^2\int S_r\,\mathrm{d}\Omega\,\mathrm{d}t=\int\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\Omega\,\mathrm{d}\omega}\mathrm{d}\Omega\,\mathrm{d}\omega,\quad \mathrm{d}\Omega=\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi,\quad S_r=\frac{c}{4\pi}E_\theta H_\phi,$$

where

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\Omega\,\mathrm{d}\omega}=\frac{e^2\mu}{\pi^2nc}q^2\sin^2\theta \tag{3.4}$$

is the energy emitted into the solid angle $\mathrm{d}\Omega$, in the frequency interval $\mathrm{d}\omega$. This famous formula obtained by Tamm is frequently used by experimentalists for the identification of the charge velocity. Equation (3.4), being integrated over the solid angle, defines the frequency distribution of the radiation

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=\int\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\Omega\,\mathrm{d}\omega}\mathrm{d}\Omega.$$

It is given by[8,9]

$$\begin{aligned}\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=&\frac{2e^2\beta}{\pi c}\left(1-\frac{1}{\beta_n^2}\right)\left\{\frac{\sin^2[kL(1-\beta_n)/2\beta]}{1-\beta_n}-\frac{\sin^2\omega[kL(1+\beta_n)/2\beta]}{1+\beta_n}-\frac{kL}{2\beta}\left[si\left(\frac{kL}{\beta}(1-\beta_n)\right)\right.\right.\\&\left.\left.-si\left(\frac{kL}{\beta}(1+\beta_n)\right)\right]\right\}-\frac{2e^2}{\pi cn^2\beta}\left[\ln\frac{|1-\beta_n|}{1+\beta_n}-ci\left(\frac{kL}{\beta}|1-\beta_n|\right)+ci\left(\frac{kL}{\beta}(1+\beta_n)\right)\right]\\&-\frac{e^2}{\pi cn^2}\left\{2n+\frac{1}{kL}\left[\sin\left(\frac{kL}{\beta}(1-\beta_n)\right)-\sin\left(\frac{kL}{\beta}(1+\beta_n)\right)\right]\right\}.\end{aligned} \tag{3.5}$$

Here $si(x)$ and $ci(x)$ are the integral sine and cosine defined by equations

$$si(x)=-\int_x^\infty\frac{\sin t}{t}dt,\quad ci(x)=-\int_x^\infty\frac{\cos t}{t}dt.$$

For $kL\gg1$, Eq. (3.5) reduces to the form given by Tamm:

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=W_{BS} \tag{3.6}$$

for $v<c_n$ and

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=W_{BS}+W_{Ch} \tag{3.7}$$

for $v>c_n$. Here

$$W_{BS}=\frac{2e^2\mu}{\pi c\beta n^2}\left(\ln\frac{1+\beta_n}{|1-\beta_n|}-2\beta_n\right) \quad \text{and} \quad W_{Ch}=\frac{e^2\mu kL}{c}\left(1-\frac{1}{\beta_n^2}\right).$$

Tamm identified W_{BS} with the spectral distribution of the bremsstrahlungs, arising from the charge instantaneous acceleration and deceleration at the moments $\pm t_0$, respectively. On the other hand, W_{Ch} was identified with the spectral distribution of the VC radiation. This is supported by the fact that W_{Ch} related to the charge motion interval coincides with the famous Frank-Tamm formula describing the energy radiated per unit length and per unit frequency for the charge unbounded motion[10]

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\omega\,\mathrm{d}L}=\frac{e^2}{c^2}\left(1-\frac{1}{\beta_n^2}\right).$$

The typical experimental situations described by the Tamm formula are (i) the β decay of a nucleus at one space point accompanied by a subsequent absorption of the emitted electron at another point; (ii) a high energy electron consequently moves in vacuum, enters into the dielectric slab, leaves the slab and propagates again in vacuum. Since the electron moving uniformly in vacuum does not radiate (apart from the transition radiation arising at the boundaries of the dielectric slab), the experimentalists describe this situation via the Tamm formula, assuming that the electron is created at one side of the slab and is absorbed at the other (see, e.g., Refs. 8, 11–15).

B. Expansion of the Tamm problem in terms of Legendre polynomials

Let a charge moves in medium in a finite interval $(-z_0,z_0)$ (this corresponds to the so-called Tamm problem). Then, the current density corresponding to the Tamm problem, in the spherical coordinates, is given by

$$j_z(\omega)=\frac{e}{4\pi^2r^2\sin\theta}\left[\delta(\theta)\exp\left(\frac{ikr}{\beta}\right)+\delta(\theta-\pi)\exp\left(-\frac{ikr}{\beta}\right)\right]\Theta(z_0-r). \tag{3.8}$$

Then, using (2.2), one gets on the observation sphere of the radius $r>z_0$,

$$A_z(\omega)=\frac{ie\mu kn}{2\pi c}\sum\,(2l+1)P_l h_l(knr)J_l(0,z_0),$$

$$H_\phi(\omega)=-\frac{iek^2n^2}{2\pi c}\sum\,P_l^1 h_l(knr)\tilde{J}_l(0,z_0), \quad E_\theta(\omega)=-\frac{ek^2\mu n}{2\pi c}\sum\,P_l^1 H_l(knr)\tilde{J}_l(0,z_0). \tag{3.9}$$

Here

$$J_l(0,z_0)=\int_0^{z_0} j_l(knr')f_l(r')\mathrm{d}r', \quad \tilde{J}_l(0,z_0)=J_{l-1}(0,z_0)+J_{l+1}(0,z_0),$$

$$H_l(x)=\dot{h}_l(x)+\frac{h_l(x)}{x},$$

$$f_l(r')=\exp\left(\frac{ikr'}{\beta}\right)+(-1)^l\exp\left(-\frac{ikr'}{\beta}\right), \quad k_1=kn_1, \quad k_2=kn_2.$$

In obvious cases, we omit the arguments of the Legendre polynomials if they equal cos θ. At large distances ($kr\gg 1$) one can replace Hankel functions by their asymptotic values:

$$A_z \sim \frac{e\mu}{2\pi cr}\exp(iknr)\sum\ (2l+1)i^{-l}P_l J_l(0,z_0),$$

$$H_\phi \sim -\frac{ekn}{2\pi cr}\exp(iknr)\sum\ i^{-l}P_l^1 \tilde{J}_l(0,z_0), \quad E_\theta \sim -\frac{ek\mu}{2\pi cr}\exp(iknr)\sum\ i^{-l}P_l^1 \tilde{J}_l(0,z_0).$$

The angular radiation intensity on the sphere of the radius r

$$\frac{d^2\mathcal{E}}{d\omega\, d\Omega} = \frac{1}{2}cr^2(E_\theta H_\phi^* + \text{c.c.}) = \frac{e^2k^2n\mu}{4\pi^2 c}\left|\sum\ i^{-l}P_l^1 \tilde{J}_l(0,z_0)\right|^2$$
$$= \frac{e^2k^2n\mu\sin^2\theta}{4\pi^2 c}\left|\sum\ (2l+1)i^{-l}P_l J_l(0,z_0)\right|^2. \tag{3.10}$$

Or, in a manifest form,

$$\frac{d^2\mathcal{E}}{d\omega\, d\Omega} = \frac{e^2\mu n}{\pi^2 c}\sin^2\theta(S_1+S_2)^2, \tag{3.11}$$

where

$$S_1 = \sum_{l=0}^{\infty}(-1)^l(4l+1)P_{2l}(\cos\theta)I_{2l}^c, \quad S_2 = \sum_{l=0}^{\infty}(-1)^l(4l+3)P_{2l+1}(\cos\theta)I_{2l+1}^s,$$
$$I_{2l}^c = \int_0^{kz_0} j_{2l}(nx)\cos\left(\frac{x}{\beta}\right)dx, \quad I_{2l+1}^s = \int_0^{kz_0} j_{2l+1}(nx)\sin\left(\frac{x}{\beta}\right)dx. \tag{3.12}$$

Integrating (3.11) over the solid angle, one obtains the frequency distribution of the radiation

$$\frac{d\mathcal{E}}{d\omega} = \frac{e^2k^2n\mu}{\pi c}\sum\ \frac{l(l+1)}{2l+1}|\tilde{J}_l(0,z_0)|^2$$
$$= \frac{8e^2n\mu}{\pi c}\left[\sum\ \frac{(l+1)(2l+1)}{4l+3}(I_{2l}^c + I_{2l+2}^c)^2 + \sum\ \frac{l(2l+1)}{4l+1}(I_{2l+1}^s + I_{2l-1}^s)^2\right]. \tag{3.13}$$

These equations are valid if the radius r of the observation sphere is larger than z_0.

Numerical calculations show that Eqs. (3.11) and (3.13) coincide with the corresponding Tamm equations (3.4) and (3.5).

We concentrate now on the vector potential. For this, we rewrite it as

$$A_z = \frac{ie\mu n}{\pi c}\sum_{l=0}^{\infty}(4l+1)h_{2l}(knr)P_{2l}(\cos\theta)I_{2l}^c - \frac{e\mu n}{\pi c}\sum_{l=0}^{\infty}(4l+3)h_{2l+1}(knr)P_{2l+1}(\cos\theta)I_{2l+1}^s. \tag{3.14}$$

Usually, observations are made on large distances. For example, for $\lambda = 4\times10^{-5}$ cm and $r = 1$ m, $kr = 2\pi r/\lambda \sim 10^7$. Replacing the Hankel functions by their asymptotic values, one gets

$$A_z = \frac{e\mu}{kr\pi c}\exp(iknr)(S_1+S_2). \tag{3.15}$$

Obviously, (3.2) and (3.15) should coincide (since the same assumptions are involved in their derivation). Equating them, one gets

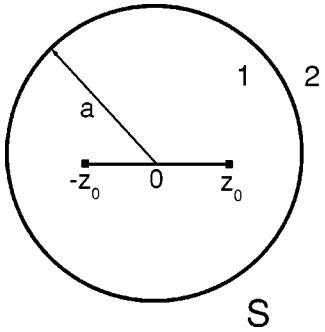

FIG. 1. A charge moves inside the dielectric sphere S filled with the medium 1. The radiation of intensity is measured outside S, in medium 2.

$$S_1+S_2=\frac{1}{n}\,\frac{\sin[kz_0n(\cos\theta-1/\beta_n)}{\cos\theta-1/\beta_n}. \tag{3.16}$$

Now we consider the coefficients I^c_{2l} and I^s_{2l+1}. In the limit $kz_0\to\infty$, the integrals

$$I^c_{2l}=\int_0^\infty j_{2l}(nx)\cos\left(\frac{x}{\beta}\right)\mathrm{d}x,\quad I^s_{2l+1}=\int_0^\infty j_{2l+1}(nx)\sin\left(\frac{x}{\beta}\right)\mathrm{d}x$$

can be evaluated in a closed form (see, e.g., Ref. 6). They are given 0 for $\beta n<1$ and

$$I^c_{2l}=\frac{\pi}{2n}(-1)^l P_{2l}(1/\beta n),\quad I^s_{2l+1}=\frac{\pi}{2n}(-1)^l P_{2l+1}(1/\beta n)$$

for $\beta n>1$. Substituting this into (3.15), one gets

$$\begin{aligned}A_\omega&=\frac{e\mu}{2nkrc}\exp(iknr)\left[\sum_{l=0}^{\infty}(4l+1)P_{2l}(\cos\theta)P_{2l}(1/\beta n)\right.\\&\quad\left.+\sum_{l=0}^{\infty}(4l+3)P_{2l+1}(\cos\theta)P_{2l+1}(1/\beta n)\right]\\&=\frac{e\mu}{2nkrc}\exp(iknr)\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)P_l(1/\beta n)\\&=\frac{e\mu}{nkrc}\exp(iknr)\,\delta(\cos\theta-1/\beta n).\end{aligned} \tag{3.17}$$

In deriving this, we used the completeness relation

$$\sum_{l=0}^{\infty}(l+1/2)P_l(x)P_l(x')=\delta(x-x').$$

Vector potential (3.17) coincides with the one entering into (3.3).

IV. THE TAMM PROBLEM FOR A CHARGE MOVING INSIDE THE SPHERICAL SAMPLE

A. Main formulas

Let a charge move in a finite space interval $(-z_0,z_0)$ lying entirely inside the sphere S of the radius a (Fig. 1). The sphere is filled by a substance 1 with parameters ϵ_1 and μ_1. The observa-

tions are made in the medium 2 with parameters ϵ_2 and μ_2 surrounding S. The EMF strengths contributing to the radial energy flux are equal to (see Appendix A)

$$H_\phi = -\frac{iek^2n_2^2}{2\pi c}\sum \tilde{C}_l P_l^1 h_l(k_2 r),$$

$$E_\theta = -\frac{i}{\epsilon_2 kr}\frac{\mathrm{d}}{\mathrm{d}r}(rH_\phi) = -\frac{e\mu_2 n_2 k^2}{2\pi c}\sum H_l(k_2 r) P_l^1 \tilde{C}_l \tag{4.1}$$

for $r>a$ and

$$H_\phi = -\frac{iek^2n_1^2}{2\pi c}\sum P_l^1[\tilde{D}_l j_l(k_1 r)+\tilde{J}_l^{(1)}(0,z_0)h_l(k_1 r)],$$

$$E_\theta = -\frac{e\mu_1 n_1 k^2}{2\pi c}\sum P_l^1[\tilde{D}_l J_l(k_1 r)+\tilde{J}_l^{(1)}(0,z_0)H_l(k_1 r)] \tag{4.2}$$

for $z_0<r<a$. Here

$$\tilde{J}_l^{(1)}(x,y)=J_{l-1}^{(1)}(x,y)+J_{l+1}^{(1)}(x,y), \quad J_l^{(1)}(x,y)=\int_x^y j_l(k_1 r')f_l(r')\mathrm{d}r',$$

$$J_l(x)=\frac{\mathrm{d}j_l(x)}{\mathrm{d}x}+\frac{j_l(x)}{x}=\frac{1}{2l+1}[(l+1)j_{l-1}-lj_{l+1}],$$

$$H_l(x)=\frac{\mathrm{d}h_l(x)}{\mathrm{d}x}+\frac{h_l(x)}{x}=\frac{1}{2l+1}[(l+1)h_{l-1}-lh_{l+1}].$$

Imposing the continuity of H_ϕ and E_θ at $r=a$, one finds the following equations for $\tilde{C}_l$ and $\tilde{D}_l$:

$$n_2^2\tilde{C}_l h_l(2)-n_1^2\tilde{D}_l j_l(1)=n_1^2 h_l(1)\tilde{J}_l^{(1)}(0,z_0),$$

$$\mu_2 n_2\tilde{C}_l H_l(2)-\mu_1 n_1\tilde{D}_l J_l(1)=\mu_1 n_1 H_l(1)\tilde{J}_l^{(1)}(0,z_0), \tag{4.3}$$

where $1=k_1 a$ and $2=k_2 a$. From this one easily finds $\tilde{C}_l$,

$$\tilde{C}_l=\frac{i\mu_1}{n_2 k^2 a^2 \delta u p_l}\tilde{J}_l^{(1)}(0,z_0), \tag{4.4}$$

where

$$\Delta_l=\mu_2 n_1 j_l(1)H_l(2)-\mu_1 n_2 J_l(1)h_l(2).$$

At large distances ($kr\gg 1$) one can replace Hankel function by its asymptotic value. Then,

$$H_\phi = -\frac{ekn_2}{2\pi c}\frac{\exp(ik_2 r)}{r}S, \quad E_\theta = -\frac{ek\mu_2}{2\pi c}\frac{\exp(ik_2 r)}{r}S, \tag{4.5}$$

where

$$S=\sum i^{-l}P_l^1\tilde{C}_l. \tag{4.6}$$

The radiation intensity per unit frequency unit and per unit solid angle is

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\Omega\,\mathrm{d}\omega}=\frac{1}{2}cr^2(E_\theta H_\phi^*+\text{c.c.})=\frac{e^2k^2n_2\mu_2}{4\pi^2c}|S|^2. \tag{4.7}$$

The integration over the solid angle gives the frequency distribution of radiation

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=\frac{e^2k^2n_2\mu_2}{\pi c}\sum\frac{l(l+1)}{2l+1}|\tilde{C}_l|^2. \tag{4.8}$$

When the media inside and outside S are the same ($\epsilon_1=\epsilon_1=\epsilon,\ \mu_1=\mu_2=\mu$), one gets

$$\Delta_l=\frac{i\mu}{nk^2a^2}\quad\text{and}\quad\tilde{C}_l=\tilde{J}_l^{(1)}(0,z_0),$$

that is, one arrives at the one-medium Tamm problem for the space interval $(-z_0,z_0)$.

B. Numerical results

In Fig. 2, there are shown angular radiation intensities (solid lines) evaluated according (4.7) for $kz_0=10$, $ka=20$, $n_1=2$ and $n_2=1$ (that is, there is a vacuum outside S) for a number of charge velocities. Side by side with them, the Tamm angular intensities (3.4) (dotted lines) corresponding to $n=n_1$, $L=2z_0$ are shown. The distinction of (4.7) from (3.4) is due to the presence of the medium 2 outside S not coinciding with medium 1. This results in the broadening of the angular intensity distribution and in its rise at large observation angles.

The corresponding frequency distributions (4.8) (solid lines) together with the Tamm frequency distributions (3.5) (dotted lines) are shown in Fig. 3. It is seen that the frequency distribution (4.8) oscillates around the Tamm one (3.5). When evaluating $\mathrm{d}\mathcal{E}/\mathrm{d}\omega$, we implicitly assumed that the refractive index n_1 does not depend on ω in the treated frequency interval. In fact, this is a common thing in refractive media. For example, for the usual water the refractive index is almost constant in the frequency interval $6\times10^{14}<\omega<6\times10^{15}\ \mathrm{s}^{-1}$ encompassing the visible light region.

In Fig. 4, there are shown angular radiation intensities (solid lines) evaluated according (4.7) for $kz_0=10$, $ka=20$, $n_1=1$ and $n_2=2$ (that is, there is a vacuum inside S) for a number of charge velocities. Side by side with them, the Tamm angular intensities (3.4) (dotted lines) corresponding to $n=n_1$, $L=2z_0$ are shown. It is seen that the presence of medium outside S affects not so strongly as in Fig. 2.

The corresponding frequency distributions are shown in Fig. 5. Again, oscillations around the Tamm frequency distribution (3.5) are observed.

Probably, the rise of angular intensities at large angles shown in Figs. 2 and 4 is due to the reflection of the VC radiation from the internal side of S.

V. THE TAMM PROBLEM FOR A CHARGE PASSING THROUGH THE SPHERE

A. Dielectric sphere

1. Main formulas

Let a charge move with a constant velocity v in the interval $(-z_0,z_0)$. There is a sphere S of the radius $a<z_0$ with its center at the origin (Fig. 6).

The space inside S is filled by the substance with parameters ϵ_1, μ_1. Outside S there is substance with parameters ϵ_2, μ_2. The EMF strengths contributing to the radial energy flux are (see Appendix B)

$$H_\phi=-\frac{iek_2^2}{2\pi c}\sum\tilde{C}_lP_l^1h_l(k_2r),\quad E_\theta=-\frac{ek^2\mu_2n_2}{2\pi c}\sum H_l(k_2r)P_l^1\tilde{C}_l \tag{5.1}$$

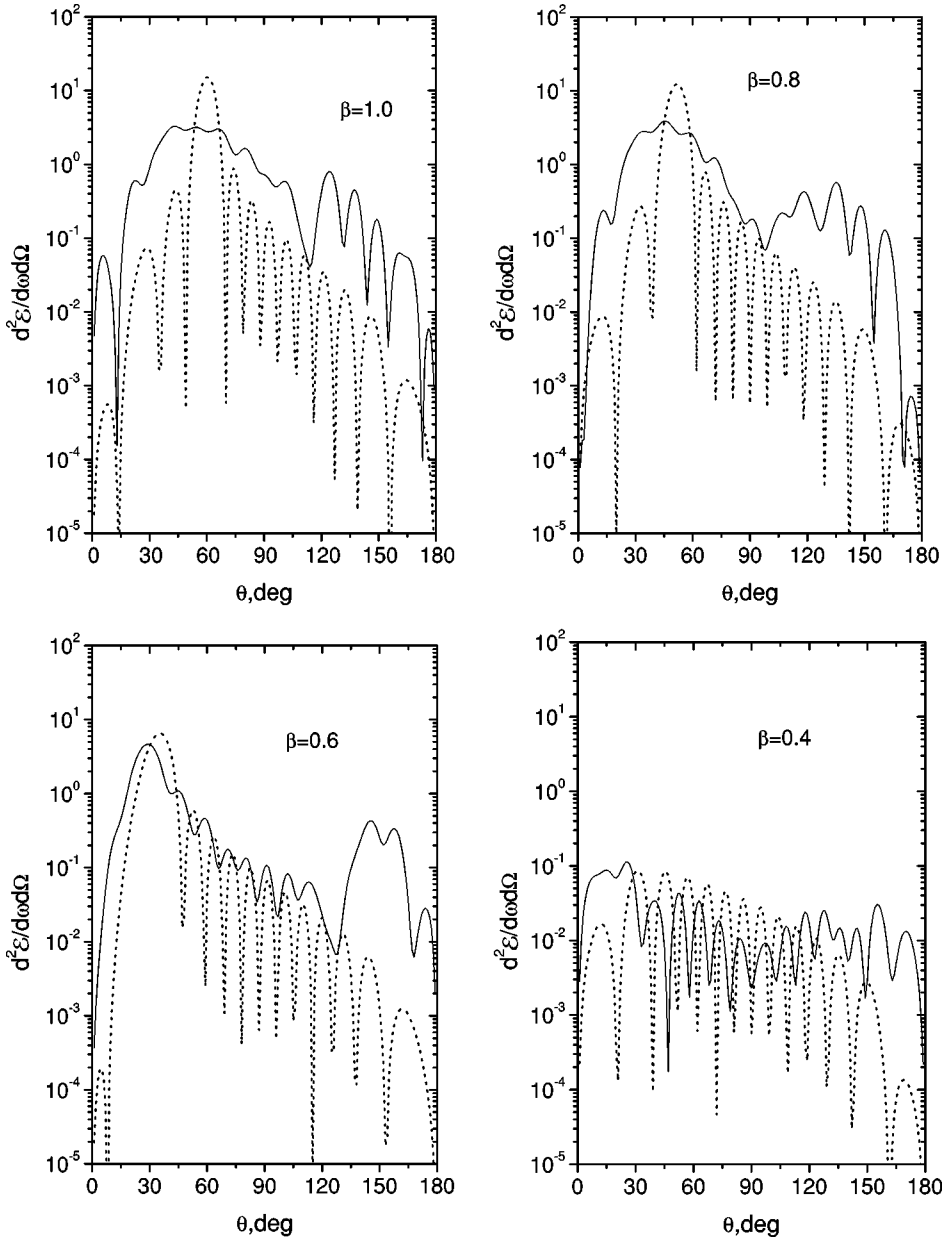

FIG. 2. Angular radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 1 and various charge velocities. The media parameters are $n_1=2$, $n_2=1$ (that is, there is vacuum outside the sphere S). Further, $kz_0=10$, $ka=20$. The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2kz_0$ and $n=n_1$. The difference between these two curves is due to the fact that the medium outside S is not the same as inside S. The exact angular intensities are much broader than the corresponding Tamm ones. Probably, the rise of angular intensities at large angles is due to the reflection of the VC radiation from the internal side of S.

for $r>z_0$,

$$H_\phi=-\frac{iek_2^2}{2\pi c}\sum\ \tilde{P}_l^1[\tilde{C}_l h_l(k_2r)-h_l(k_2r)\tilde{J}_l^{(2)}(r,z_0)+j_l(k_2r)\tilde{H}_l^{(2)}(r,z_0)],$$

$$E_\theta=-\frac{ek^2\mu_2 n_2}{2\pi c}\sum\ \tilde{P}_l^1[\tilde{C}_l H_l(k_2r)-H_l(k_2r)\tilde{J}_l^{(2)}(r,z_0)+J_l(k_2r)\tilde{H}_l^{(2)}(r,z_0)] \tag{5.2}$$

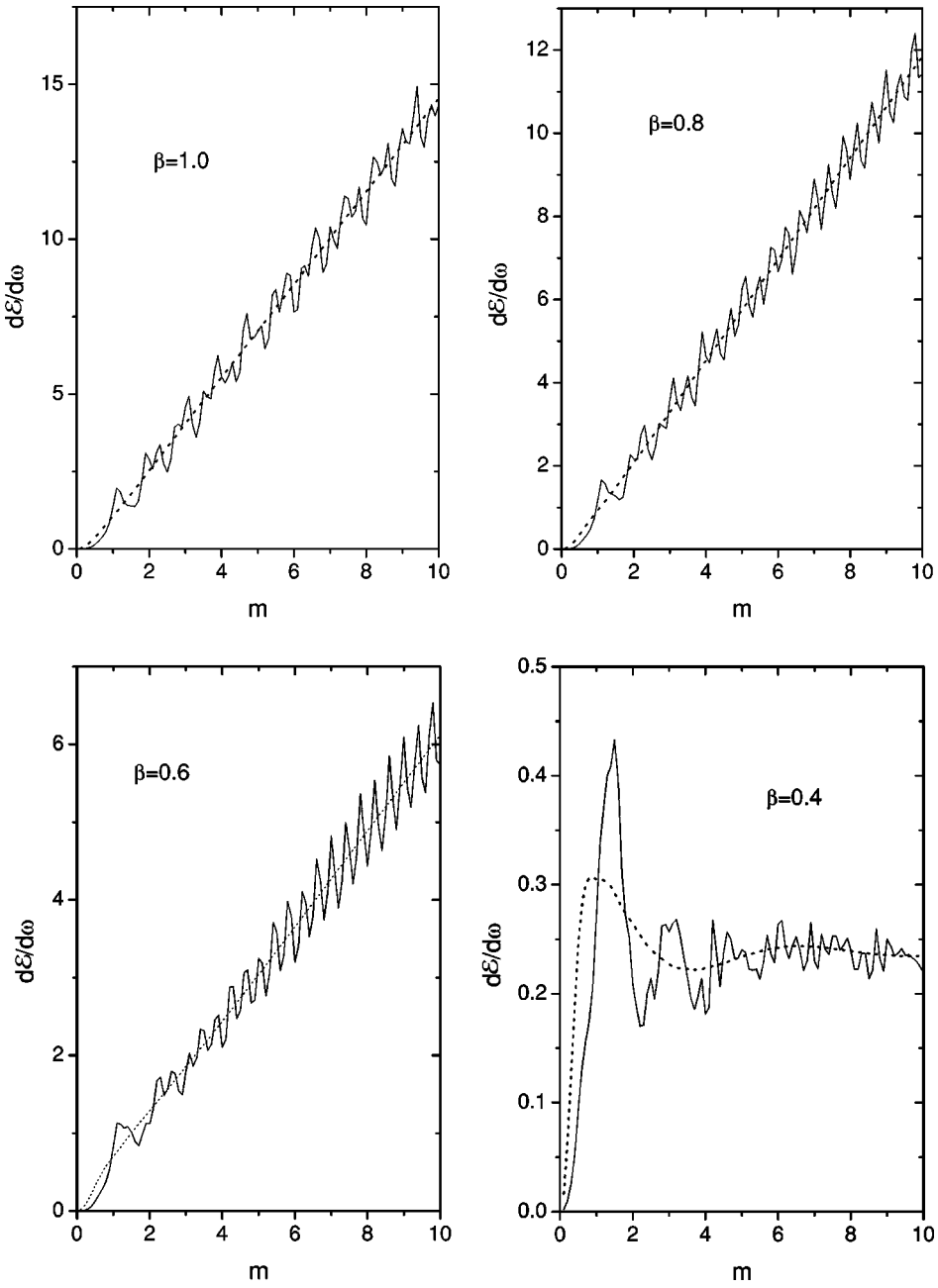

FIG. 3. Frequency radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 1 and various charge velocities. The media parameters are the same as in Fig. 2. Further, $kz_0=m$, $ka=2m$. The dotted curves are the Tamm frequency intensities (3.5) evaluated for $kL=2kz_0$ and $n=n_1$. It is seen that frequency intensities (4.8) oscillate around the Tamm ones.

for $a<r<z_0$ and

$$H_\phi=-\frac{iek_1^2}{2\pi c}\sum\ \tilde{P}_l^1[\tilde{D}_l j_l(k_1r)+h_l(k_1r)\tilde{J}_l^{(1)}(0,r)+j_l(k_1r)\tilde{H}_l^{(1)}(r,a)],$$

$$E_\theta=-\frac{ek^2\mu_1 n_1}{2\pi c}\sum\ \tilde{P}_l^1[\tilde{D}_l J_l(k_1r)+H_l(k_1r)\tilde{J}_l^{(1)}(0,r)+J_l(k_1r)\tilde{H}_l^{(1)}(r,a)] \tag{5.3}$$

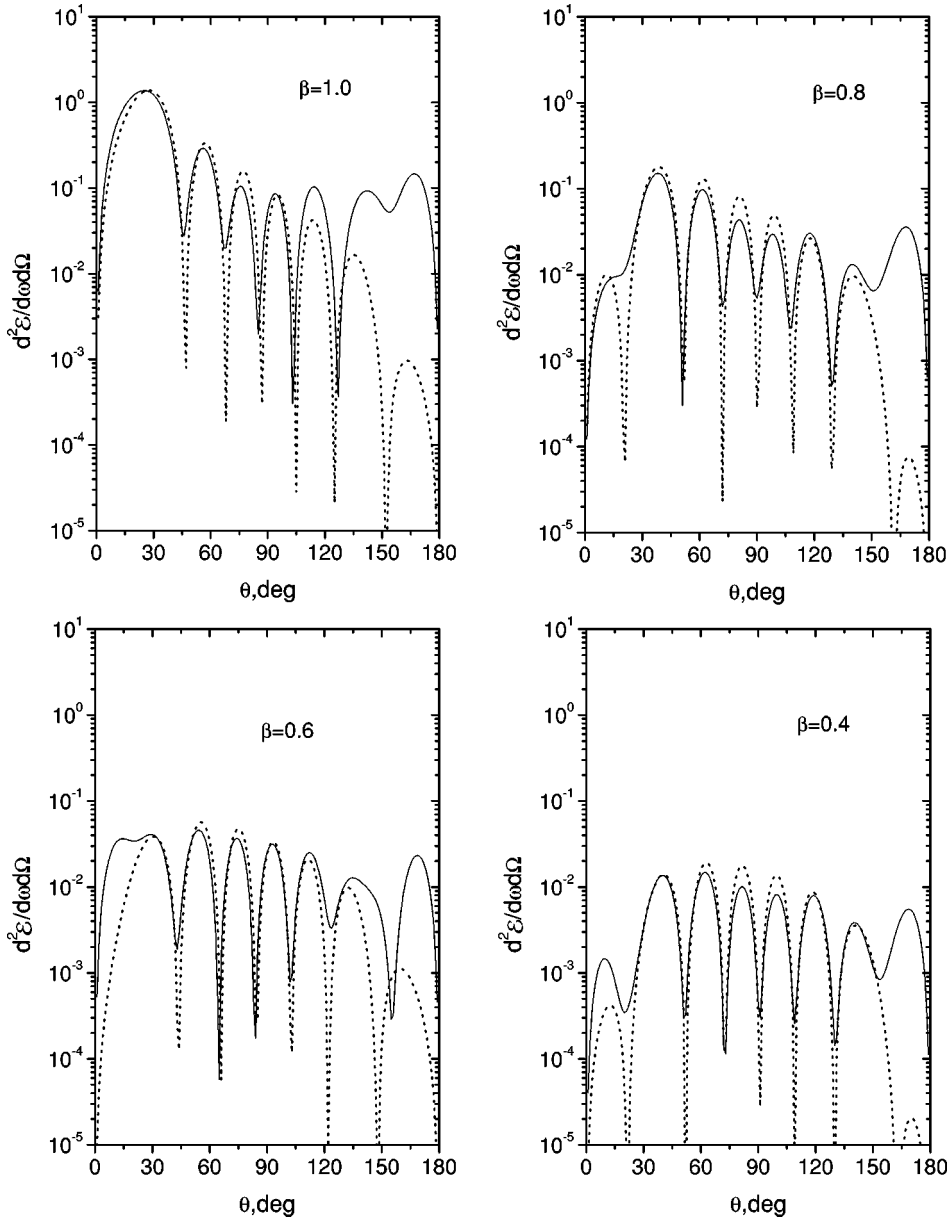

FIG. 4. The same as in Fig. 2 but for $n_1=1$, $n_2=2$ (that is, there is vacuum inside S). The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2kz_0$ and $n=n_1$.

for $r<a$. Here

$$\tilde{H}_l^{(1)}(x,y)=H_{l-1}^{(1)}(x,y)+H_{l+1}^{(1)}(x,y), \quad \tilde{J}_l^{(2)}(x,y)=J_{l-1}^{(2)}(x,y)+J_{l+1}^{(2)}(x,y),$$

$$\tilde{H}_l^{(2)}(x,y)=H_{l-1}^{(2)}(x,y)+H_{l+1}^{(2)}(x,y), \quad H_l^{(1)}(x,y)=\int_x^y h_l(k_1r')f_l(r')\mathrm{d}r',$$

$$J_l^{(2)}(x,y)=\int_x^y j_l(k_2r')f_l(r')\mathrm{d}r', \quad H_l^{(2)}(x,y)=\int_x^y h_l(k_2r')f_l(r')\mathrm{d}r'.$$

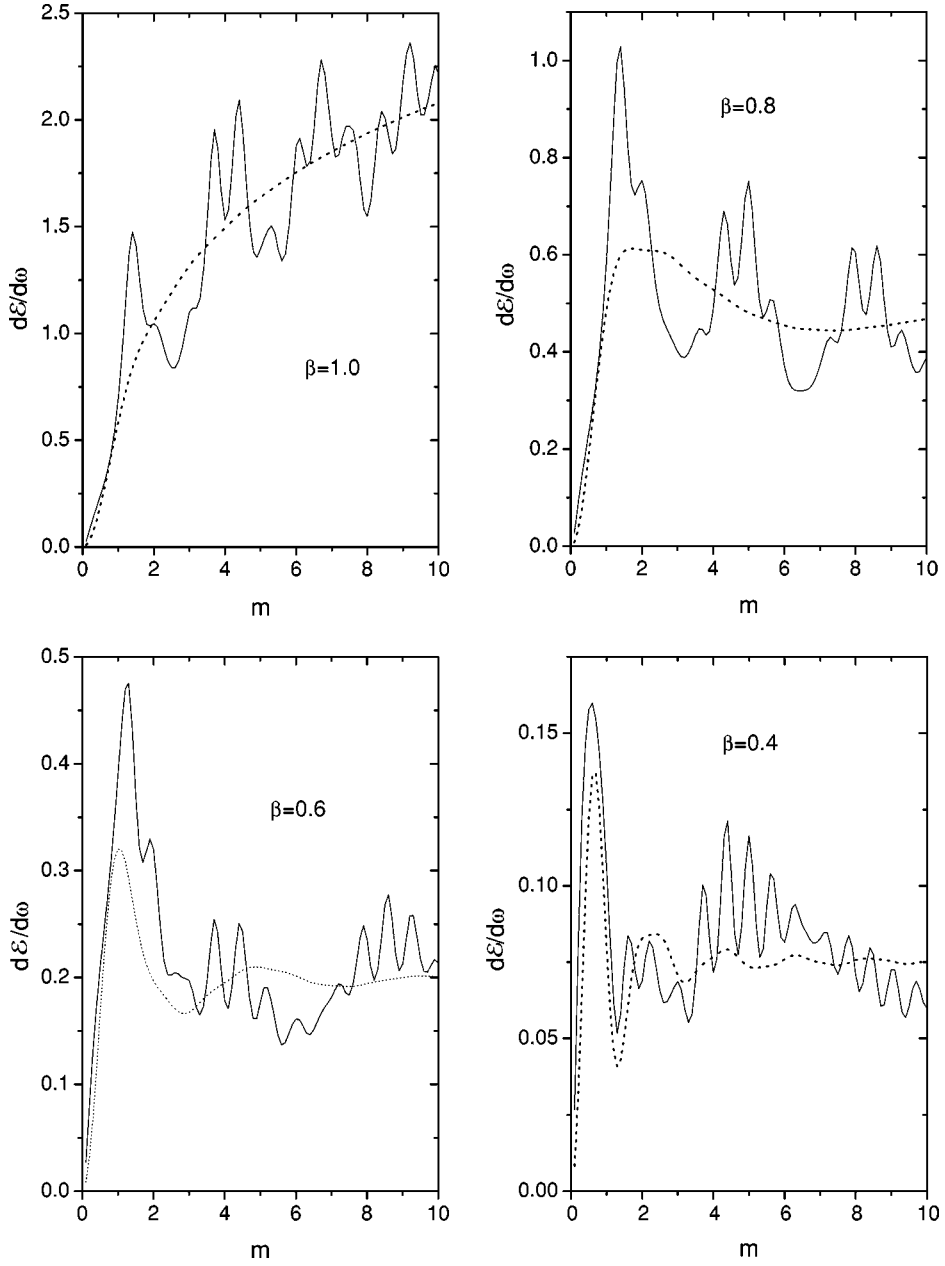

FIG. 5. The same as in Fig. 3 but for $n_1=1$, $n_2=2$ (vacuum inside S). The Tamm frequency intensities (3.5) are evaluated for $kL=2kz_0$ and $n=n_1$.

Equating E_θ and H_ϕ at $r=a$, one obtains the following equations for $\tilde{C}_l$ and $\tilde{D}_l$:

$$n_2^2 h_l(2)\tilde{C}_l - n_1^2 j_l(1)\tilde{D}_l = n_1^2 h_l(1)\tilde{J}_l^{(1)}(0,a) + n_2^2[h_l(2)\tilde{J}_l^{(2)}(a,z_0) - j_l(2)\tilde{H}_l^{(2)}(a,z_0)],$$
$$\mu_2 n_2 H_l(2)\tilde{C}_l - \mu_1 n_1 J_l(1)\tilde{D}_l = \mu_1 n_1 H_l(1)\tilde{J}_l^{(1)}(0,a) + n_2\mu_2[H_l(2)\tilde{J}_l^{(2)}(a,z_0) - J_l(2)\tilde{H}_l^{(2)}(a,z_0)]. \tag{5.4}$$

Here we set $1=k_1a$ and $2=k_2a$. For example, $j_l(1)\equiv j_l(k_1a)$, etc. From this one easily obtains $\tilde{C}_l$:

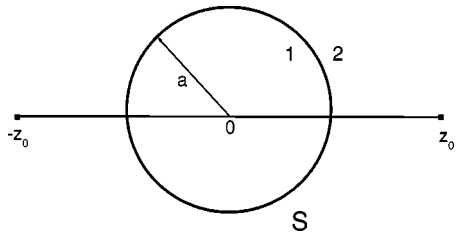

FIG. 6. A charge motion begins and terminates in medium 2. It passes through sphere S filled with the medium 1. The radiation of intensity is measured outside S, in medium 2.

$$\tilde{C}_l=\frac{1}{\Delta_l}\left\{\frac{i\mu_1}{n_2k^2a^2}\tilde{J}_l^{(1)}(0,a)+\tilde{J}_l^{(2)}(a,z_0)[\mu_2n_1j_l(1)H_l(2)-\mu_1n_2J_l(1)h_l(2)]\right.$$
$$\left.-\tilde{H}_l^{(2)}(a,z_0)[\mu_2n_1j_l(1)J_l(2)-\mu_1n_2J_l(1)j_l(2)]\right\}$$
$$=\frac{i}{\Delta_l}\left\{\frac{\mu_1}{n_2k^2a^2}\tilde{J}_l^{(1)}(0,a)+\tilde{J}_l^{(2)}(a,z_0)[\mu_2n_1j_l(1)N_l(2)-\mu_1n_2J_l(1)n_l(2)]\right.$$
$$\left.-\tilde{N}_l^{(2)}(a,z_0)[\mu_2n_1j_l(1)J_l(2)-\mu_1n_2J_l(1)j_l(2)]\right\}. \tag{5.5}$$

Here $\Delta_l=n_1\mu_2j_l(1)H_l(2)-\mu_1n_2J_l(1)h_l(2)$. At large distances ($kr\gg1$), one has

$$H_\phi\approx-\frac{ekn_2}{2\pi cr}\exp(ikn_2r)S,\quad E_\theta\approx-\frac{ek\mu_2}{2\pi cr}\exp(ikn_2r)S, \tag{5.6}$$

where

$$S=\sum\ i^{-l}\tilde{C}_lP_l^1. \tag{5.7}$$

Correspondingly, the energy flux through the sphere of the radius r is

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\omega\,\mathrm{d}\Omega}=\frac{1}{2}cr^2(E_\theta H_\phi^*+\text{c.c.})=\frac{e^2k^2n_2\mu_2}{4\pi^2c}|S|^2. \tag{5.8}$$

Integration over the solid angle gives the frequency distribution of radiation

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\omega}=\frac{e^2k^2n_2\mu_2}{\pi c}\sum\ \frac{l(l+1)}{2l+1}|\tilde{C}_l|^2. \tag{5.9}$$

The one-medium Tamm problem is obtained either in the limit $ka\to0$ or when media 1 and 2 are the same.

2. Numerical results

In Fig. 7, there are shown angular radiation intensities (solid lines) evaluated according (5.8) for $kz_0=20$, $ka=10$, $n_1=2$ and $n_2=1$ (that is, there is a vacuum outside the sphere S and a substance with $n_1=2$ inside it) for a number of charge velocities. Side by side with them, the Tamm angular intensities (3.4) (dotted lines) corresponding to $n=n_1$, $L=2a$ are shown. It is the usual thing in the VC radiation theory to associate the observed radiation with the part of the charge trajectory where $\beta n>1$ [see, e.g., Ref. 10 and (ii) item at the end of Sec. III A]. It the treated case, it lies within the sphere S. We observe a rather poor agreement of the exact

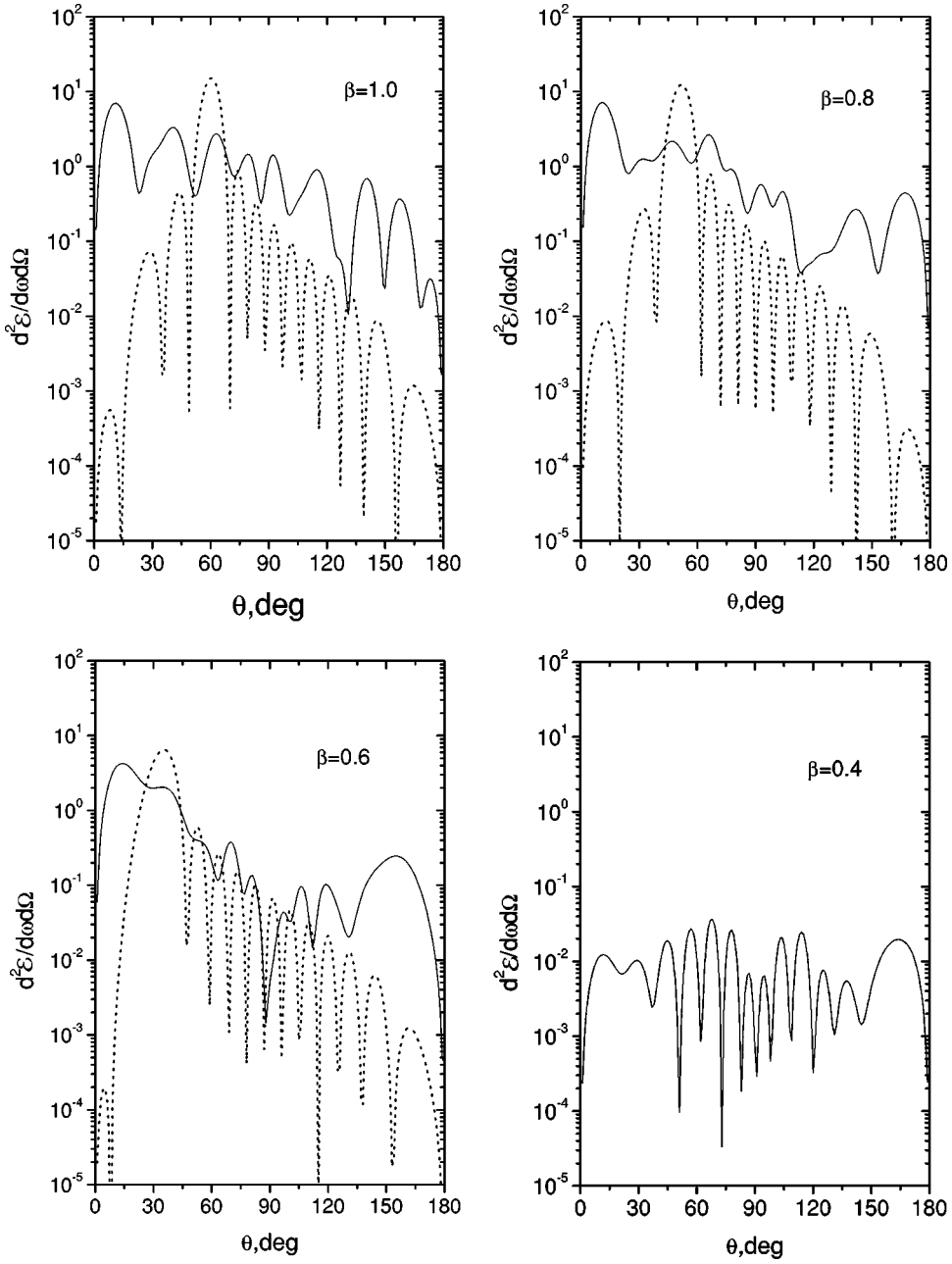

FIG. 7. Angular radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 6 and various charge velocities. The medium inside S is dielectric with $n_1=2$. Outside S there is vacuum ($n_2=1$). Further, $ka=10$, $kz_0=20$. The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2ka$ and $n=n_1$. The noncoincidence of exact angular intensities with the corresponding Tamm ones and, in particular, the absence of the pronounced maximum at $\cos\theta=1/\beta n$ (especially for $\beta=1$ and $\beta=0.8$) demonstrates that the applicability of the Tamm formula for describing the radiation arising from the charge passage through the dielectric sample is rather limited.

intensity (5.8) with the Tamm one (3.4). Experimentalist studying, e.g., electron passing through the dielectric sphere S, will not see the pronounced Cherenkov maximum at $\theta=\theta_c$ ($\cos\theta_c=1/\beta n$) and, on these grounds, will not identify the charge velocity. For $\beta=0.4$ we did not present the Tamm intensity since for this velocity the Tamm intensities arising from the charge motion in $0<r<a$ (medium 1) and $a<r<z_0$ (medium 2) intervals are of the same order. It is not clear to us

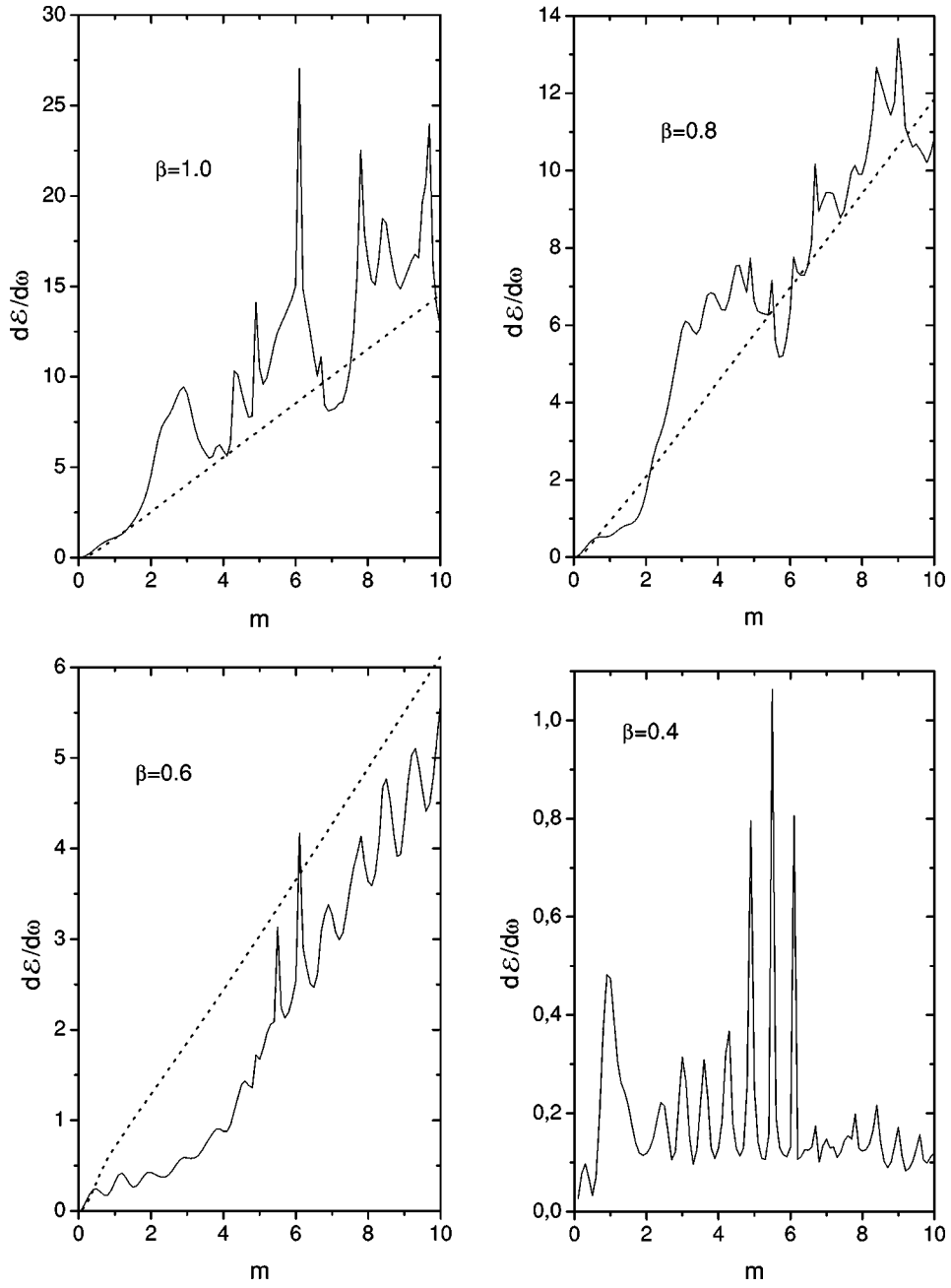

FIG. 8. Frequency radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 6 and various charge velocities. The media parameters are the same as in Fig. 7. Further, $ka=m$, $kz_0=2m$. The dotted curves are the Tamm frequency intensities (3.5) evaluated for $kL=2ka$ and $n=n_1$.

how to combine the corresponding Tamm amplitudes. In any case, Eqs. (5.8) and (5.9) give the exact solution of the treated problem, while the Tamm intensities are needed only for the interpretation purposes. The corresponding frequency distribution (5.9) also differs appreciably from the Tamm one (3.5) (Fig. 8).

In Fig. 9, there are shown angular radiation intensities (solid lines) evaluated according to (5.2) for $kz_0=20$, $ka=10$, $n_1=1$ and $n_2=2$ (that is, the vacuum bubble inside S surrounded by

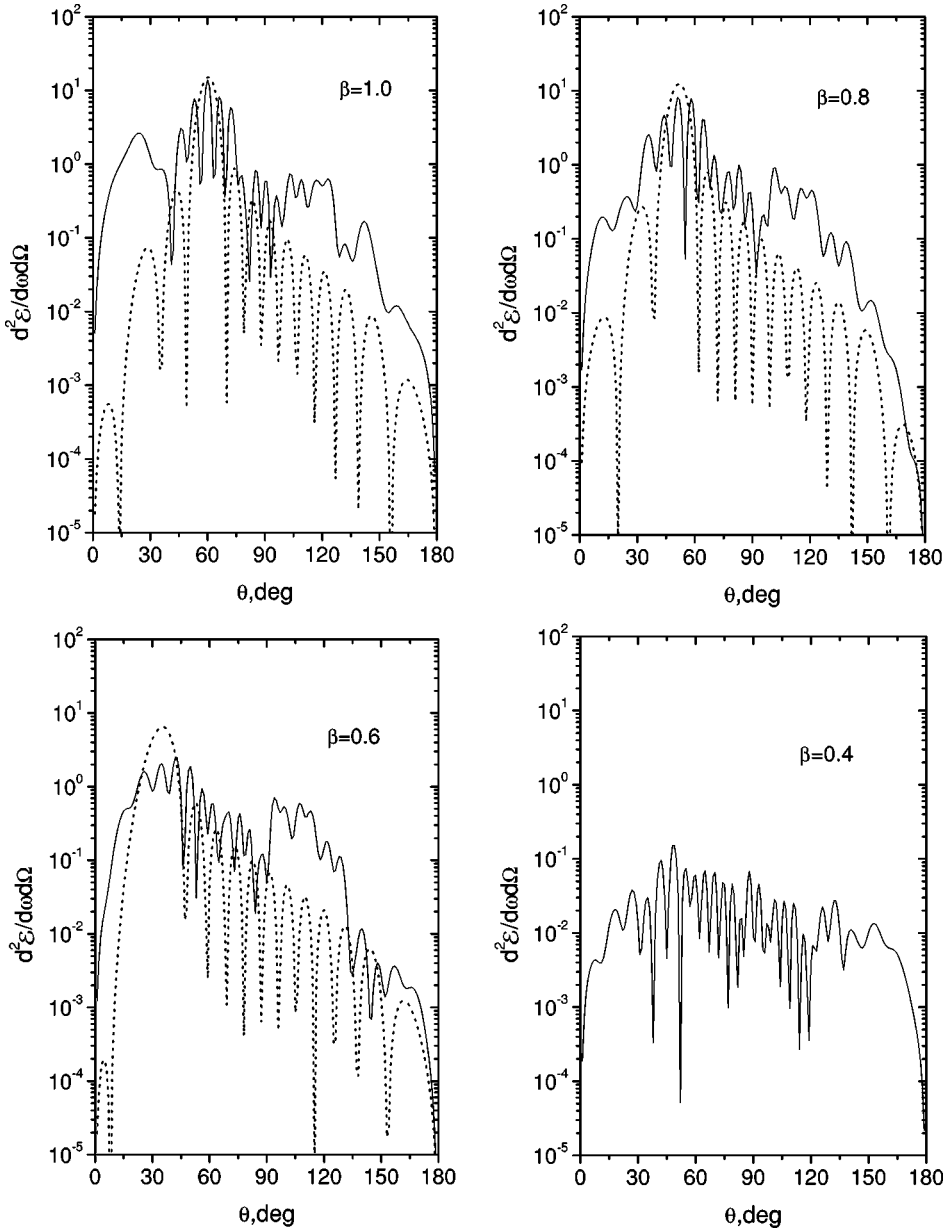

FIG. 9. The same as in Fig. 7 but for $n_1=1$, $n_2=2$ (that is, there is vacuum inside S). The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

a substance with $n_2=2$) for a number of charge velocities. Side by side with them, the Tamm angular intensities (3.4) (dotted lines) corresponding to $n=n_2$, $L=2(z_0-a)$ are shown. In the treated case, the part of the charge trajectory where $\beta n>1$ lies outside the sphere S. We observe a satisfactory agreement of the exact intensity (5.8) with the Tamm intensity (3.4). Experimentalist studying, e.g., the electron passing through the dielectric sphere S, will see the pronounced Cherenkov maximum at $\theta=\theta_c$ ($\cos\theta_c=1/\beta n$). The corresponding frequency distribution (5.3) does not differ appreciably from the Tamm one (3.5) (Fig. 10).

B. Metallic sphere

On the surface of ideal metal, tangential components of the electric field strength vanish.[16] For the metallic sphere of the radius a, this leads to the disappearance of E_θ. This defines $\tilde{C}_l$:

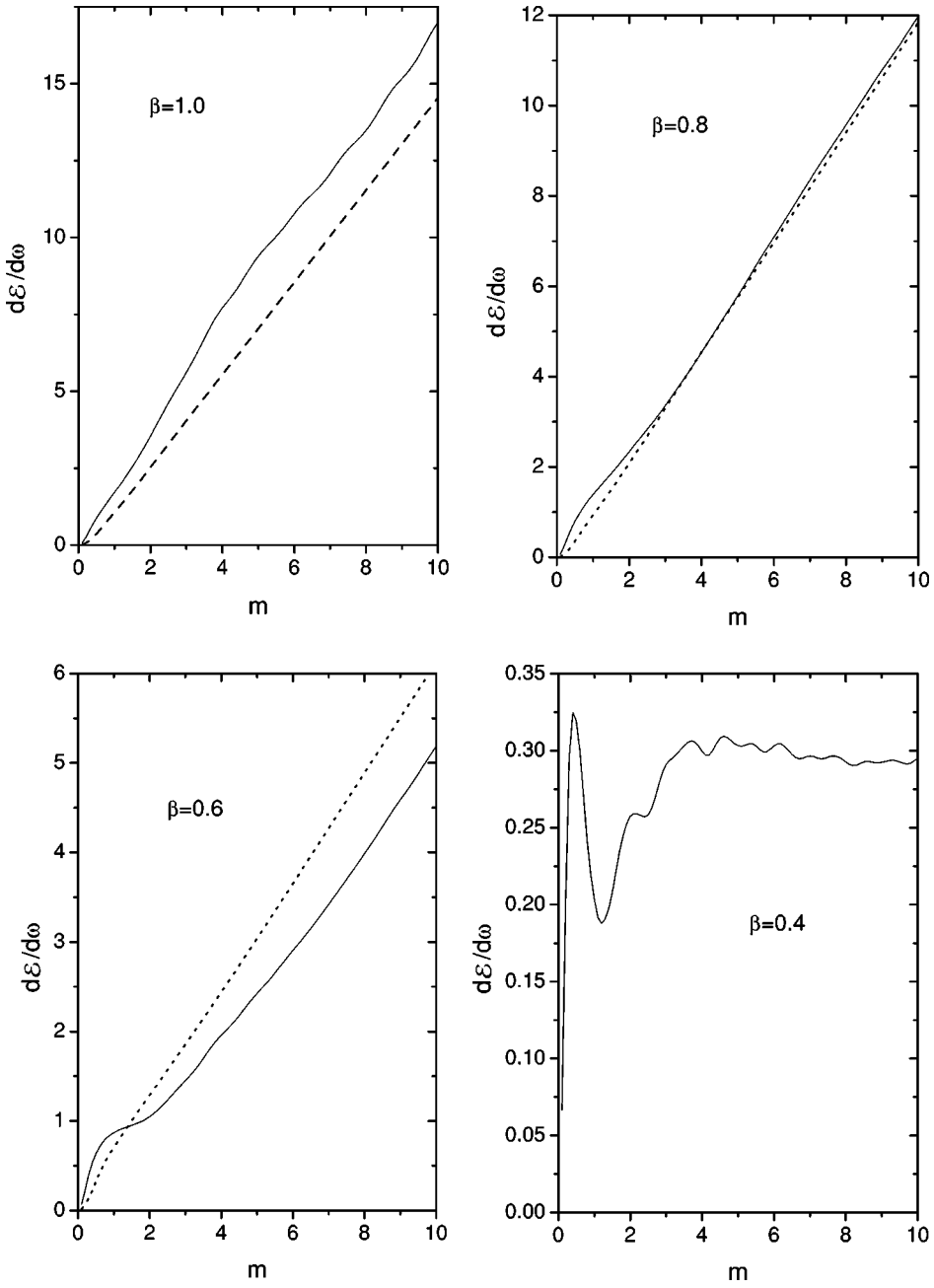

FIG. 10. The same as in Fig. 8 but for $n_1=1$, $n_2=2$ (there is vacuum inside S). The dotted curves are the Tamm frequency intensities (3.5) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

$$\widetilde{C}_l=\widetilde{J}_l^{(2)}(a,z_0)-\frac{J_l(2)}{H_l(2)}\widetilde{H}_l^{(2)}(a,z_0)=\frac{i}{H_l(2)}[N_l(2)\widetilde{J}_l^{(2)}(a,z_0)-J_l(2)\widetilde{N}_l^{(2)}(a,z_0)]. \quad (5.10)$$

Then, angular and frequency distributions are given by (5.8), (5.9) but with $\widetilde{C}_l$ defined by (5.10).

Numerical results: Let outside S be vacuum. The corresponding angular distributions (5.8) (solid lines) are compared in Fig. 11 with the Tamm angular intensities (3.4) (dotted lines) evaluated for $L=2(z_0-a)$ and $n=n_2$. Since $\beta n\leqslant 1$ outside the sphere S, the angular intensities are rather small.

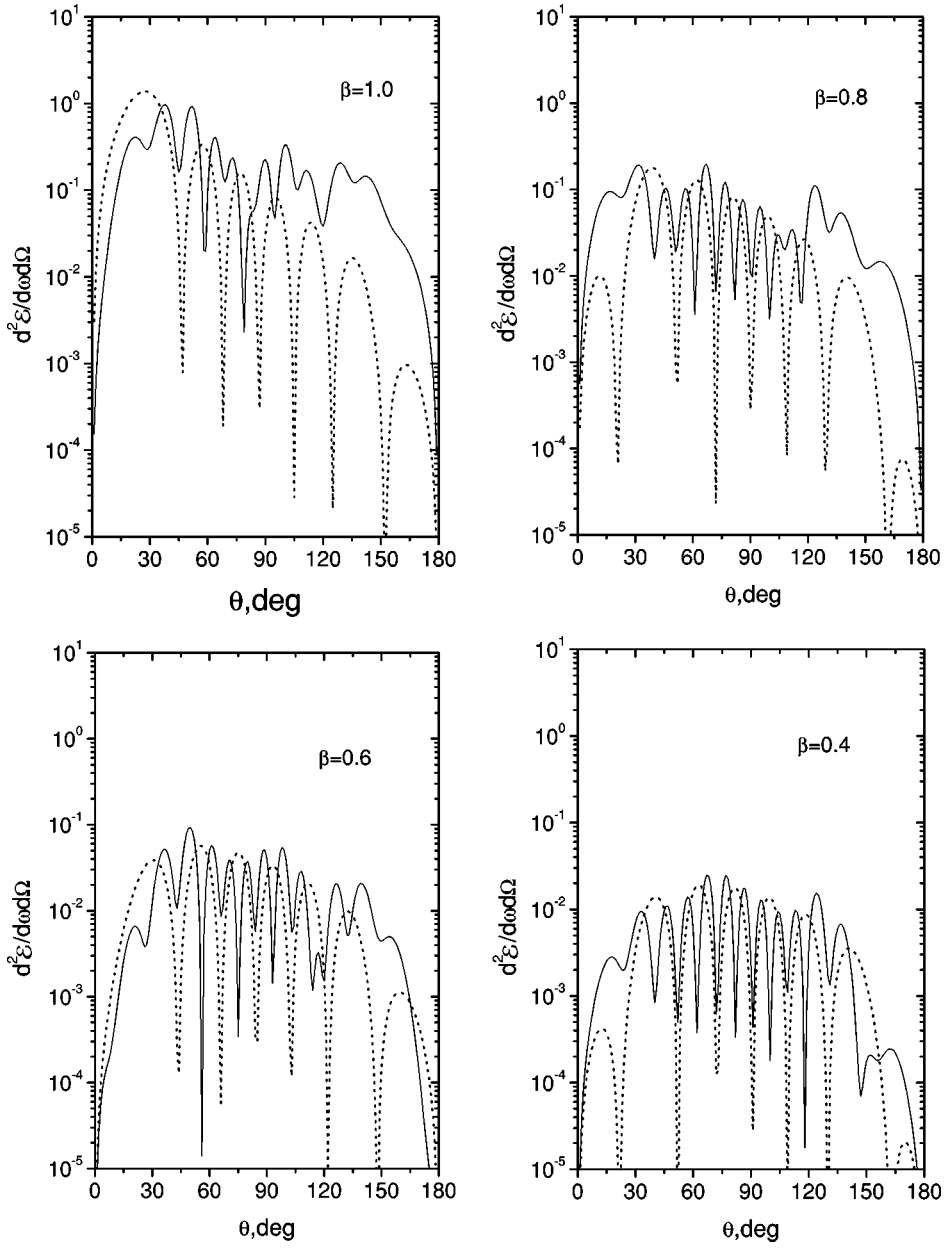

FIG. 11. Angular radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 6 and various charge velocities. The medium inside S is ideal metallic substance. The medium refractive index outside S is $n_2=1$ (vacuum). Further, $ka=10, kz_0=20$. The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

The corresponding frequency distributions (5.9) (solid lines) and the Tamm ones (3.5) (dotted lines) are shown in Fig. 12. Their agreement is rather poor.

Let outside S be the medium with the refractive index $n_2=2$. The corresponding angular and frequency distributions are shown in Figs. 13 and 14, respectively. We observe the satisfactory agreement with the Tamm intensities evaluated for $L=2(z_0-a)$ and $n=n_2$.

VI. DISCUSSION

Formulas obtained in the preceding two sections describe the VC radiation, the radiation arising from the charge instantaneous acceleration and deceleration and the transition radiation arising from a charge passing from one medium to another.

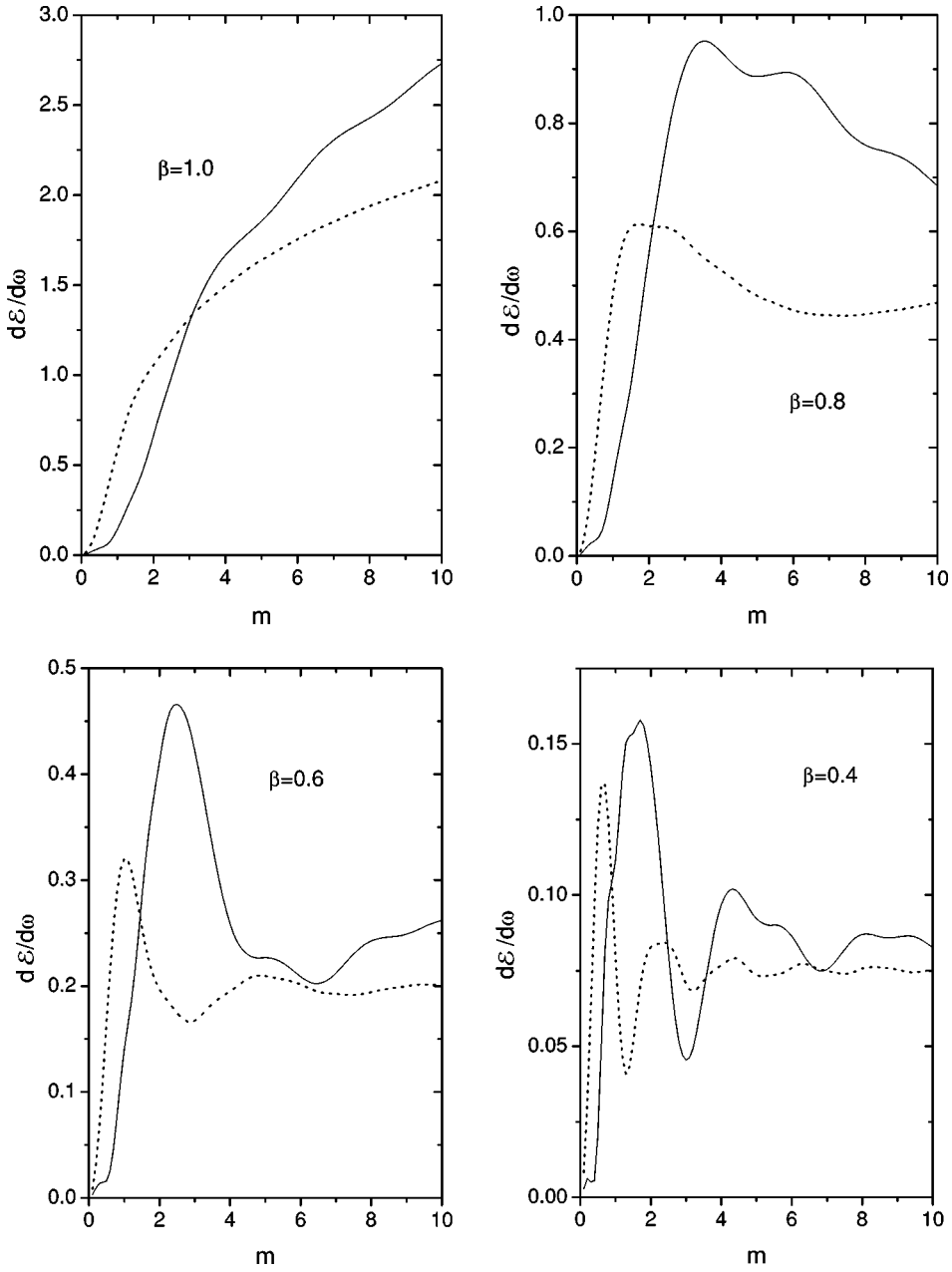

FIG. 12. Frequency radiation intensities in e^2/c units (solid curves) for the charge motion shown in Fig. 6 and various charge velocities. The medium inside S is ideal metallic substance. The medium refractive index outside S is $n_2=1$ (vacuum). Further, $ka=m, kz_0=2m$. The dotted curves are the Tamm frequency intensities (3.5) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

To separate contribution of the transition radiation, one should subtract (according, e.g., to Ref. 5 or Ref. 17) the field strengths corresponding to the inhomogenuous solution of the Maxwell equations from the total field strengths. In the treated case, the field strengths corresponding to the Tamm problem should be subtracted (they are written out in Sec. III B). This leads to the following redefinition of the $\tilde{C}_l$ coefficients:

$$\tilde{C}_l \to \tilde{C}_l - \sqrt{\frac{n_1\mu_1}{n_2\mu_2}}\tilde{J}_l^{(1)}(0,z_0)$$

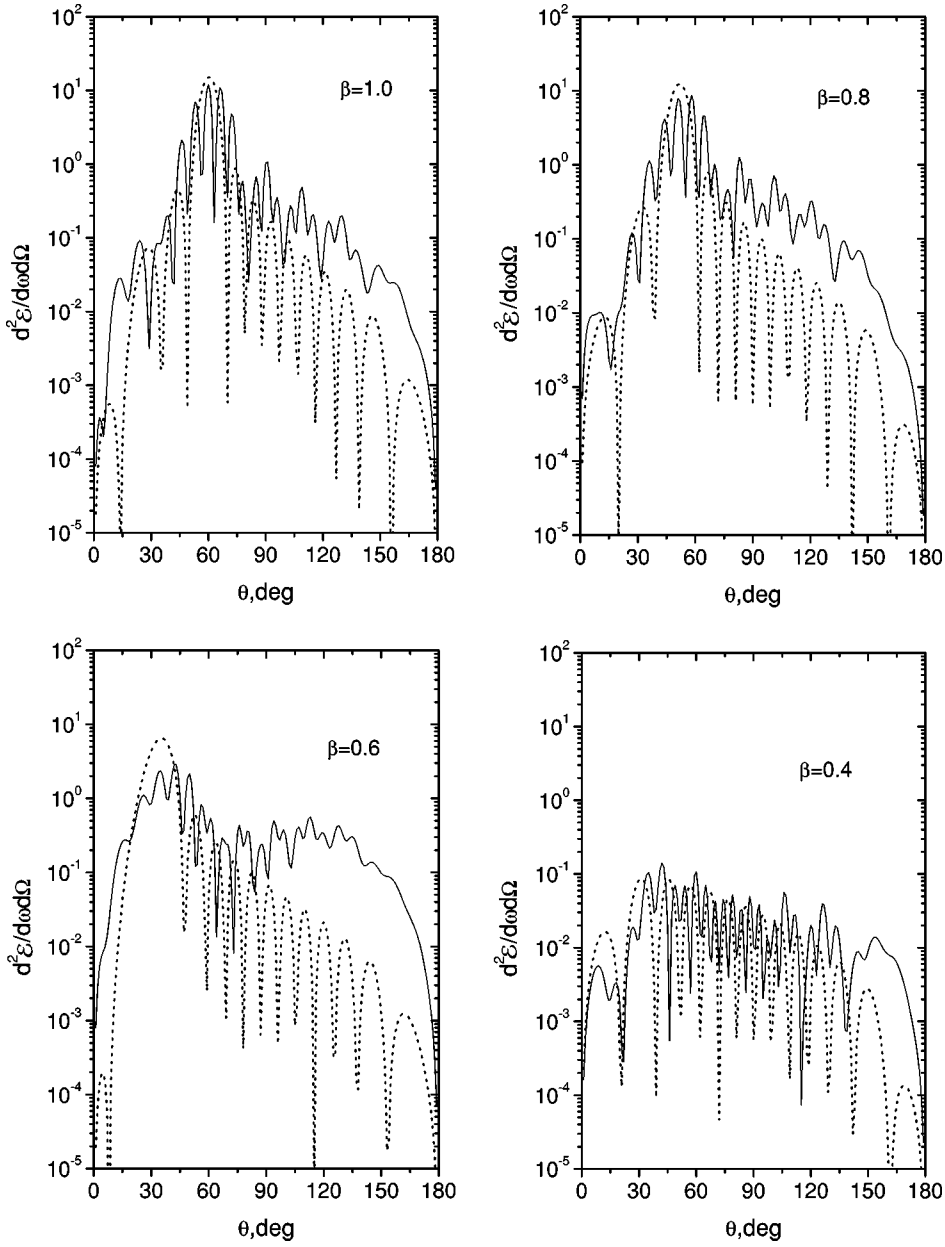

FIG. 13. The same as in Fig. 11 but for metallic substance. The medium refractive index outside S is $n_2=2$. The dotted curves are the Tamm angular intensities (3.4) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

for the motion shown in Fig. 1,

$$\tilde{C}_l \to \tilde{C}_l - \sqrt{\frac{n_1\mu_1}{n_2\mu_2}}\tilde{J}_l^{(1)}(0,a) - J_l^{(2)}(a,z_0)$$

for the charge motion through the dielectric sphere (Fig. 7) and

$$\tilde{C}_l \to \tilde{C}_l - J_l^{(2)}(a,z_0)$$

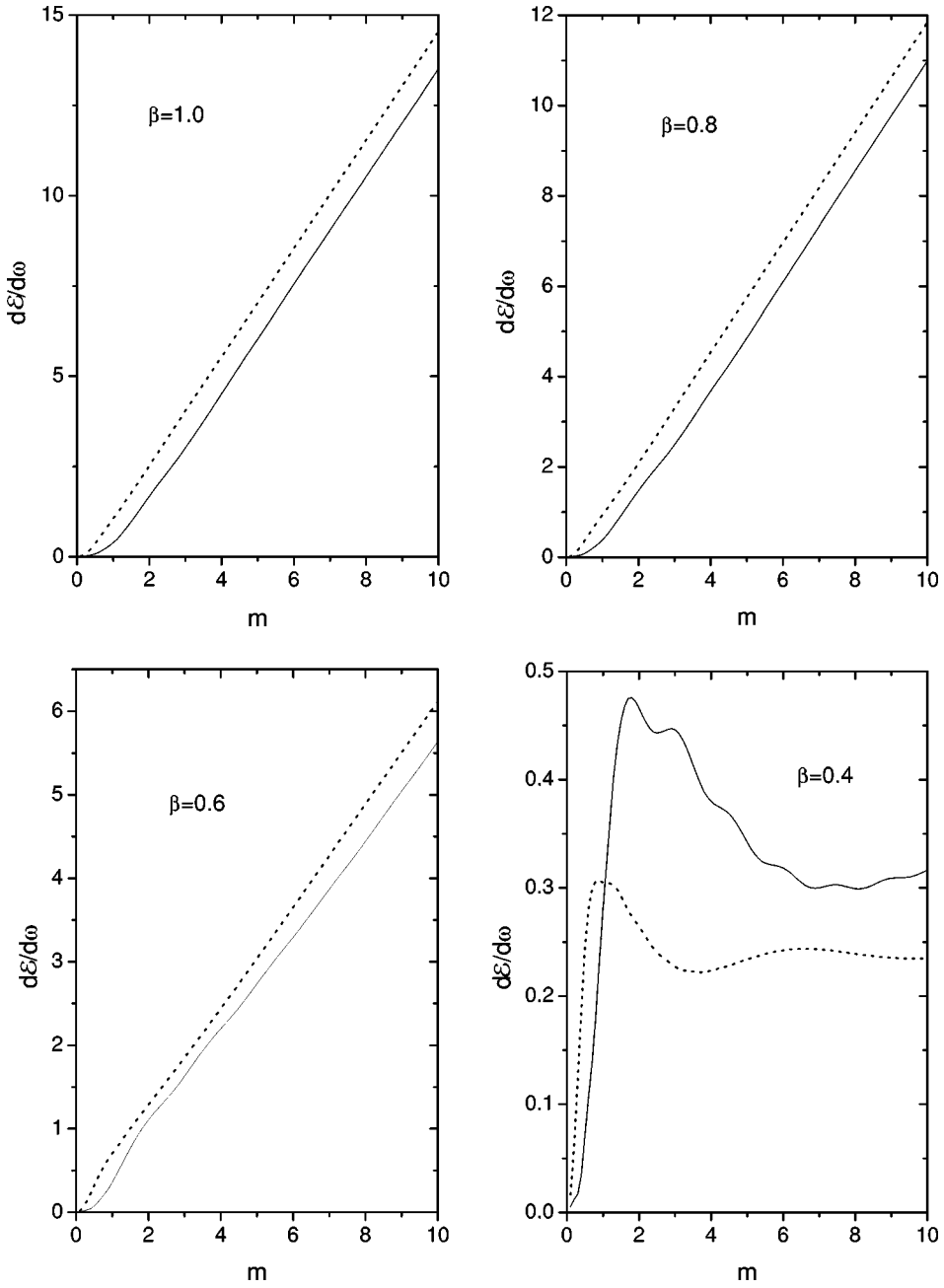

FIG. 14. The same as in Fig. 12 but for $n_2=2$. The dotted curves are the Tamm frequency intensities (3.5) evaluated for $kL=2k(z_0-a)$ and $n=n_2$.

for the charge motion through the metallic sphere (Fig. 7). These newly defined $\tilde{C}_l$ being substituted into (4.7), (4.8), (5.8), and (5.9) give transition radiation intensities. Due to the lack of space and since the observable radiation intensities are the total ones presented in Figs. 2–5 and 7–14, we do not evaluate transition radiation intensities in this paper.

In the physical literature there are semi-intuitive interpretations of the transition radiation and the one arising in the Tamm problem in terms of instantaneous acceleration and deceleration, and in terms of semi-infinite charge motion terminating at one side of the media interface and beginning at the other one. Their insufficiencies (discussed below) prevent us from their applying to the

consideration of VC and transition radiation on the spherical sample. In any case, exact solutions and numerical calculations presented in Secs. IV and V contain all necessary information for the analysis of experimental data.

A. Comment on the transition radiation

1. Interpretation of the transition radiation in terms of instantaneous velocity jumps

Sometimes the transition radiation is interpreted as a charge uniform motion with the velocity v in medium 1, its sudden stop in medium 1 at the border with medium 2, the sudden start of motion in medium 2 and the charge uniform motion in medium 2 with the velocity v (see, e.g., Refs. 18–20). It is suggested that the main contribution to the radiation intensity give the mentioned above instantaneous jumps of the charge velocity. The radiation intensity arising from the charge sudden stop in medium 1 is taken in the form

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\omega\,\mathrm{d}\Omega}=\frac{e^2}{4\pi^2 c}\left[\frac{\vec{\beta}\times\vec{n}_r}{1-n_1(\vec{\beta}\vec{n}_r)}\right]^2, \tag{6.1}$$

where $\vec{\beta}=\vec{v}/c$, $\vec{n}_r$ is the unit radius vector of the observation point and n_1 is the refractive index of the medium 1.

On the other hand, the exact calculations were made in Ref. 21 for the following decelerated motion along the z axis:

$$z(t)=z_1+v_1(t-t_1)-\tfrac{1}{2}a(t-t_1)^2,\quad v(t)=v_1-a(t-t_1),\quad t_1<t<t_2, \tag{6.2}$$

which begins at the moment t_1 at the space point z_1 with the velocity v_1 and ends at the moment t_2 at the space point z_2 with the velocity v_2. The time motion interval t_2-t_1 and deceleration a are easily expressed through z_1, z_2, v_1, and v_2,

$$t_2-t_1=2\frac{z_2-z_1}{v_1+v_2},\quad a=\frac{1}{2}\frac{v_1^2-v_2^2}{z_2-z_1}. \tag{6.2$'$}$$

It was shown in Ref. 21 that for the fixed wavelength λ, the intensity of radiation tends to zero for $k(z_2-z_1)\to 0$ $(k=2\pi/\lambda)$. This certainly disagrees with (6.1) which differs from zero for any motion interval. To clarify the situation, we turn to the derivation of (6.1).

2. The derivation of (6.1)

For simplicity, we consider at first a charge motion in vacuum closely following Landau and Lifshitz treatise.[22] Its authors begin with the equations

$$\vec{H}=(\vec{n}_r\times\vec{E}),\quad \vec{E}=-\frac{1}{c}\dot{\vec{A}},$$

which are valid in the wave zone (the dot above the vector potential $\vec{A}$ means the differentiation over the laboratory time). For the Fourier transform of $\vec{H}$ one gets

$$\vec{H}_\omega=-\frac{1}{2\pi c}\int_{-\infty}^{\infty}(\vec{n}_r\times\dot{\vec{A}})\exp(i\omega t)\mathrm{d}t. \tag{6.3}$$

Now, if $\vec{A}\neq 0$ for $t_1<t<t_2$, then for $\omega(t_2-t_1)\ll 1$ one can set $\exp(i\omega t)\approx 1$, thus obtaining

$$\vec{H}_\omega=-\frac{1}{2\pi c}\int\vec{n}_r\times\frac{\partial\vec{A}}{\partial t}\mathrm{d}t=-\frac{1}{2\pi c}\vec{n}_r\times(\vec{A}_2-\vec{A}_1). \tag{6.4}$$

Here $\vec{A}_2=\vec{A}(t=t_2)$ and $\vec{A}_1=\vec{A}(t=t_1)$. Further, authors of Ref. 22 change $\vec{A}_1$ and $\vec{A}_2$ by the Lienard–Wiechert potentials. This gives

$$\vec{H}_\omega=\frac{e}{2\pi cr}\left[\frac{\beta_2\times n_r}{1-(\vec{\beta}_2\vec{n}_r)}-\frac{\beta_1\times n_r}{1-(\vec{\beta}_1\vec{n}_r)}\right]. \tag{6.5}$$

The radiation intensity per unit frequency and per unit solid angle is

$$\frac{\mathrm{d}^2\mathcal{E}}{\mathrm{d}\omega\,\mathrm{d}\Omega}=cr^2|\vec{H}_\omega|^2=\frac{e^2}{4\pi^2c}\left[\frac{\beta_2\times n_r}{1-(\vec{\beta}_2\vec{n}_r)}-\frac{\beta_1\times n_r}{1-(\vec{\beta}_1\vec{n}_r)}\right]^2. \tag{6.6}$$

Now if the final velocity is zero, (6.6) coincides with (6.1).

3. Resolution of paradox

We rewrite the integral entering into (6.4) in the form

$$\int\frac{\partial\vec{A}}{\partial t}\mathrm{d}t=\int\frac{\partial\vec{A}(t(t'))}{\partial t'}\mathrm{d}t'=\vec{A}_2-\vec{A}_1, \tag{6.7}$$

where t' is the charge retarded (proper) time. The laboratory times t_1 and t_2 being expressed through the retarded times for the one dimensional motion along the z axis are given by

$$t_1=t_1'+\frac{1}{c}[\rho^2+(z-z_1')^2]^{1/2},\quad t_2=t_2'+\frac{1}{c}[\rho^2+(z-z_2')^2]^{1/2}, \tag{6.8}$$

where $z_1'=z'(t_1')$ and $z_2'=z'(t_2')$ are the charge positions at the times t_1' and t_2'. Now, let the charge proper time t' be uniquely related to its position z'. Then, for $z_1'=z_2'$, one gets $t_1'=t_2'$, $t_1=t_2$ and, therefore, $\vec{A}_2=\vec{A}_1$, $\vec{H}_\omega=0$, and $\mathrm{d}^2\mathcal{E}/\mathrm{d}\omega\,\mathrm{d}\Omega=0$.

We illustrate this using the motion law (6.2) as an example [note that t and z entering into (6.2) are the charge proper time t' and its position z']. For this motion law, t' is uniquely related to z',

$$t'=t_1+2v_1\frac{z_2-z_1}{v_1^2-v_2^2}\left[1-\left(1-\frac{z'-z_1}{z_2-z_1}\,\frac{v_1^2-v_2^2}{v_1^2}\right)^{1/2}\right]. \tag{6.9}$$

According to (6.2′), $t_2=t_1$ for $z_2=z_1$. Therefore, $\vec{A}_2=\vec{A}_1$ for $t_2=t_1$ and $\vec{H}_\omega$ given by (6.4) vanishes in the $k(z_2-z_1)\to 0$ limit, in accordance with Ref. 21.

The main assumptions for the vanishing of $\vec{H}_\omega$ are (i) the discontinuous charge motion with the velocity jumps can be viewed as a limiting case of the continuous motion without the velocity jumps when the length along which the velocity changes from v_1 to v_2 tends to zero; (ii) the retarded (proper) charge time is uniquely related to its position.

We conclude the interpretation of the transition radiation in terms of the charge instantaneous acceleration and deceleration at the border of two media is not sufficient if the discontinuous charge motion can be treated as a limiting case of the continuous charge motion. In any case, the discontinuous charge motion cannot be realized in nature: it is the suitable idealization of some continuous charge motion.

In general, $\vec{A}(t_2)$ does not coincide with $\vec{A}(t_1)$ if the charge proper time is not uniquely related to its position. Consider, for example, the immovable elementary (infinitesimal) time dependent source. Then, $\vec{A}(t_2)\neq\vec{A}(t_1)$ and $\vec{H}_\omega\neq 0$. Another possibility to obtain $\vec{A}(t_2)\neq\vec{A}(t_1)$ is to take into account the internal degrees of freedom of a moving charged particle [for example, its spin flip at the fixed space point can give $\vec{A}(t_2)\neq\vec{A}(t_1)$].

4. On the interpretation of the transition radiation in terms of the charge semi-infinite motions

In Refs. 4 and 5, the transition radiation was associated with the charge radiation on the semi-infinite intervals $(-\infty,0)$ and $(0,\infty)$ lying in media 1 and 2, respectively. We analyze this situation using the vector potential as an example. VP corresponding to the charge motion in medium 1 is given by

$$A_z=\frac{e\mu_1}{2\pi c}\int_{-\infty}^{0}\frac{dz'}{R}\exp(i\psi), \tag{6.10}$$

where $\psi=kz'/\beta+k_1R$, $k_1=kn_1$, $R=\sqrt{\rho^2+(z-z')^2}$. In the quasiclassical approximation one gets

$$A_z^{(1)}=\frac{e\mu_1}{2\pi cr}\frac{1}{1-\beta_1\cos\theta} \tag{6.11}$$

for $\beta<\beta_1=1/n_1$. For $\beta>\beta_1$,

$$A_z^{(1)}=(6.11)\quad\text{for}\quad\theta<\theta_1\ ,$$

$$A_z^{(1)}=(6.11)+A_T^{(1)}\quad\text{for}\quad\theta>\theta_1.$$

Here

$$A_T^{(1)}=\frac{e\mu_1}{2\pi c}\exp\left(\frac{i\pi}{4}\right)\sqrt{\frac{2\pi\beta\gamma_1}{kr\sin\theta}}\exp\left[\frac{ikr}{\beta}\left(\cos\theta+\frac{\sin\theta}{\gamma_1}\right)\right],\quad \gamma_1=\frac{1}{\sqrt{|1-\beta_1^2|}},\quad \cos\theta_1=\frac{1}{\beta_1}. \tag{6.12}$$

Since $A_T(1)$ decreases like $1/\sqrt{kr}$, the radiation intensity is large in the $\theta>\theta_1$ angular region.

Similarly, the vector potential corresponding to the charge motion in medium 2 is given by

$$A_z^{(2)}=-\frac{e\mu_2}{2\pi cr}\frac{1}{1-\beta_2\cos\theta}\quad\text{for}\quad\beta<\beta_2=1/n_2. \tag{6.13}$$

For $\beta>\beta_2$,

$$A_z^{(2)}=(6.13)\quad\text{for}\quad\theta>\theta_2,$$

$$A_z^{(2)}=(6.13)+A_T^{(2)}\quad\text{for}\quad\theta<\theta_2.$$

Here

$$A_T^{(2)}=\frac{e\mu_2}{2\pi c}\exp\left(\frac{i\pi}{4}\right)\sqrt{\frac{2\pi\beta\gamma_2}{kr\sin\theta}}\exp\left[\frac{ikr}{\beta}\left(\cos\theta+\frac{\sin\theta}{\gamma_2}\right)\right],\quad \gamma_2=\frac{1}{\sqrt{|1-\beta_2^2|}},\quad \cos\theta_2=\frac{1}{\beta_2}. \tag{6.14}$$

Usually, the terms $A_T^{(1)}$ and $A_T^{(2)}$ are dropped in standard considerations of the transition radiation. Their interference with $A_z^{(1)}$ and $A_z^{(2)}$ given by (6.12) and (6.13), respectively, leads to the oscillations of the radiation intensity in the $\theta>\theta_1$ angular region for the charge semi-infinite motion $(-\infty,0)$ in medium 1, and in the $\theta<\theta_2$ angular region for the charge semi-infinite motion $(0,\infty)$ in medium 2.

A further procedure in obtaining the transition radiation intensities is the evaluation of EMF strengths corresponding to vector potentials in media 1 and 2 and their superposition with corresponding Fresnel coefficients. Sometimes the secondary photon rescatterings at the boundaries of media 1 and 2 (for the dielectric plate) are taken into account.

Since we have at hand the exact solution for the charge moving inside and outside the dielectric or metallic sphere, these tricks are not needed: they are automatically taken into account in closed expressions for radiation intensities.

5. On the physical meaning of $A_T^{(1)}$ and $A_T^{(2)}$ terms

To clarify the physical meaning of $A_T^{(1)}$ and $A_T^{(2)}$ terms, we consider the case when media 1 and 2 are the same. Then, the vector potential corresponding to the infinite motion $(-\infty,\infty)$ reduces to the sum of vector potentials corresponding to semi-infinite motions in media 1 and 2:

$$A_z=A_z^{(1)}+A_z^{(2)}=0$$

for $\beta<1/n$ and

$$A_z=A_T^{(1)}+A_T^{(2)}=\frac{e\mu}{2\pi c}\exp\left(\frac{i\pi}{4}\right)\sqrt{\frac{2\pi\beta\gamma_n}{kr\sin\theta}}\exp\left[\frac{ikr}{\beta}\left(\cos\theta+\frac{\sin\theta}{\gamma_n}\right)\right],\quad \gamma_n=\frac{1}{\sqrt{|1-\beta_n^2|}} \tag{6.15}$$

for $\beta>1/n$. But this is the asymptotic form $(\rho\to\infty)$ of the VC vector potential corresponding to the charge infinite motion in unbounded medium

$$A_z=\frac{e\mu}{\pi c}K_0\left(\frac{k\rho}{\beta\gamma_n}\right)\quad \text{for}\quad \beta<\frac{1}{n}\quad \text{and}\quad A_z=\frac{ie\mu}{2c}\exp\left(\frac{ikz}{\beta}\right)H_0^{(1)}\left(\frac{k\rho}{\beta\gamma_n}\right)\quad \text{for}\quad \beta>\frac{1}{n}.$$

This means that $A_T^{(1)}$ and $A_T^{(2)}$ terms describe the VC radiation for the semi-infinite charge motions in media 1 and 2. This is also confirmed by the exact solution corresponding to the semi-infinite charge motion in dispersion free medium found in Refs. 23 and 24 in the time representation. Indeed, the space regions where the VC radiation differs from zero are just the same where $A_T^{(1)}$ and $A_T^{(2)}$ terms differ from zero.

It is easy to check that the values of $A_z^{(1)}$ and $A_z^{(2)}$ are defined by the boundary point $z'=0$, while the values of $A_T^{(1)}$ and $A_T^{(2)}$ terms are defined by stationary points z' lying in the intervals $(-\infty,0)$ and $(0,\infty)$, respectively.

We see that the interpretation of the transition radiation in terms of semi-infinite motions in the intervals $(-\infty,0)$ and $(0,\infty)$ is sufficient only for $\beta<1/n$. On the other hand, for $\beta>1/n$, the Cherenkov terms $A_T^{(1)}$ and $A_T^{(2)}$ should be taken into account.

B. Comment on the Tamm problem

For the Tamm problem (uniform charge motion in a restricted space interval), the vector potential is given by (3.1). It is easily evaluated in the quasiclassical approximation. For $z<\rho\gamma_n-z_0$ and $z>\rho\gamma_n+z_0$ one gets

$$A_z^{\text{out}}=-\frac{ie\mu\beta}{2\pi ck}\left\{\frac{1}{r_2-\beta_n(z-z_0)}\exp\left[\frac{ik}{\beta}(\beta n r_2+z_0)\right]-\frac{1}{r_1-\beta_n(z+z_0)}\exp\left[\frac{ik}{\beta}(\beta n r_1-z_0)\right]\right\}. \tag{6.16}$$

Here $r_1=\sqrt{\rho^2+(z+z_0)^2}$ and $r_2=\sqrt{\rho^2+(z-z_0)^2}$. Inside the interval $\rho\gamma_n-z_0<z<\rho\gamma_n+z_0$, the vector potential equals

$$A_z^{\text{in}}=A_z^{\text{out}}+A_z^{Ch}, \tag{6.17}$$

where

$$A_z^{Ch}=\frac{e\mu}{2\pi c}\exp\left(\frac{ikz}{\beta}\right)\sqrt{\frac{2\pi\beta\gamma_n}{kr\sin\theta}}\exp\left(i\frac{\pi}{4}\right)\exp\left(\frac{ikr\sin\theta}{\beta\gamma_n}\right).$$

It is seen that A_z^{out} is infinite at $z=\rho\gamma_n\pm z_0$ (this is due to the quasiclassical approximation used). Therefore, the radiation intensity should have maxima at $z=\rho\gamma_n\pm z_0$, with a kind of plateau for $\rho\gamma_n-z_0<z<\rho\gamma_n+z_0$ and a sharp decreasing for $z<\rho\gamma_n-z_0$ and $z>\rho\gamma_n+z_0$. At the observation distances much larger than the motion length

$$r_1-\beta_n(z+z_0)\approx r(1-\beta_n\cos\theta),\quad r_2-\beta_n(z-z_0)\approx r(1-\beta_n\cos\theta),$$

$$\beta_n r_1-z_0=\beta_n r-z_0(1-\beta_n\cos\theta),\quad \beta_n r_2+z_0=\beta_n r+z_0(1-\beta_n\cos\theta).$$

Then,

$$A_z^{\text{out}}=\frac{e\mu\beta}{\pi ckr}\exp(iknr)\frac{\sin[\omega t_0(1-\beta n\cos\theta)]}{1-\beta n\cos\theta},\tag{6.18}$$

that coincides with the Tamm vector potential A_z^T entering into (3.2). Thus, inside the interval $\rho\gamma_n-z_0<z<\rho\gamma_n+z_0$,

$$A_z^{\text{in}}=A_z^T+A_z^{Ch}.\tag{6.19}$$

We observe that infinities of A_z^{out} disappeared due to the approximations involved. It is seen that for $kr\gg1$, A_z^{Ch} and A_z^T behave like $1/\sqrt{kr}$ and $1/kr$, respectively. It follows from this that the radiation intensity in space regions $z>\rho\gamma_n+z_0$ and $z<\rho\gamma_n-z_0$ is described by the Tamm formula (3.4). On the other hand, inside the space region $\rho\gamma_n-z_0<z<\rho\gamma_n+z_0$, the radiation intensity differs appreciably from the Tamm one. In fact, the second term in A_z^{in} is much larger than the first one (A_z^T) for $kr\gg1$ (since they decrease like $1/\sqrt{kr}$ and $1/kr$ for $kr\to\infty$, respectively). It is easy to check that on the surface of the sphere of the radius r, the intervals $z<\rho\gamma_n-z_0$, $\rho\gamma_n-z_0<z<\rho\gamma_n+z_0$ and $z>\rho\gamma_n+z_0$ correspond to angular intervals $\theta>\theta_1$, $\theta_2<\theta<\theta_1$ and $\theta<\theta_2$, where θ_1 and θ_2 are defined by

$$\cos\theta_1=-\frac{\epsilon_0}{\beta_n^2\gamma_n^2}+\frac{1}{\beta_n}\left[1-\left(\frac{\epsilon_0}{\beta_n\gamma_n}\right)^2\right]^{1/2}$$

and

$$\cos\theta_2=\frac{\epsilon_0}{\beta_n^2\gamma_n^2}+\frac{1}{\beta_n}\left[1-\left(\frac{\epsilon_0}{\beta_n\gamma_n}\right)^2\right]^{1/2}.\tag{6.20}$$

Here $\epsilon_0=z_0/r$. For $r\gg z_0$,

$$\theta_1=\theta_c+\frac{\epsilon_0}{\beta_n\gamma_n},\quad \theta_2=\theta_c-\frac{\epsilon_0}{\beta_n\gamma_n},$$

where θ_c is defined by $\cos\theta_c=1/\beta n$. Therefore, inside the angular interval $\theta_2<\theta<\theta_1$ the radiation intensity should have plateau with its height proportional to the observation distance r. In the limit $r\to\infty$, the above θ interval diminishes and for the radiation intensity one gets the δ-type singularity at $\cos\theta=1/\beta n$ (in addition to A_z^T). However, the θ integral from it is finite. Although $\Delta\theta=\theta_1-\theta_2=2\epsilon_0/\beta_n\gamma_n$ is very small for $r\gg z_0$, the length of arc on the observation sphere on

which the radiation intensity differs from the Tamm one is finite: it is given by $2z_0/\beta_n\gamma_n$. It would be interesting to observe this deviation experimentally (there are recent experimental indications for the existence of this plateau[25]).

From the previous consideration it follows that A_z^{Ch} is a part of the Cherenkov shock wave enclosed between straight lines $z=-z_0+\rho\gamma_n$ and $z=z_0+\rho\gamma_n$ with its normal inclined under the angle θ_c towards the motion axis. In the quasiclassical approximation, the stationary point $z'=z-\rho\gamma_n$ of the integral α_T entering in (3.1) lies inside the motion interval $(-z_0,z_0)$ and defines the value of A_z^{Ch}. On the other hand, for the A_z^{out} the stationary point of α_T lies outside the charge motion interval and the value of α_T is defined by initial and final points of the motion interval. Therefore, A_z^{out} is somehow related to the beginning and the end of motion. In Refs. 26 and 27 the radiation intensity in the Tamm problem was associated with the interference of bremsstrahlung shock waves arising from the instantaneous velocity jumps at the beginning and the end of motion. However, if one replaces the instantaneous velocity jumps by the smoothed ones and then tends the width of the transition region (where the velocity smoothly changes) to zero then the contribution of this region to the radiation intensity also tends to zero.[21] There are no velocity jumps for this smoothed motion and, therefore, the radiation intensity in the Tamm problem cannot be attributed to them. However, there are acceleration jumps at the beginning and the end of motion and at the moments when the accelerated motion meets the uniform one. Thus, the above intensity can be still associated with acceleration jumps. To clarify the situation, the Tamm problem with absolutely continuous charge motion (for which the velocity itself and all its time derivatives are absolutely continuous functions of time) was considered in Ref. 28. It was shown that the relatively slow decreasing of the radiation intensity outside the plateau is replaced by its exponential damping. This means that the discontinuities of higher derivatives of the charge velocity contribute to the asymptotic behavior of the radiation intensities as well. Formerly, for the charge motion in vacuum, the exponential damping for all angles was recognized in Refs. 29–32. We conclude: the instantaneous velocity jumps at the beginning and the end of motion do not contribute to the radiation intensity provided they can be viewed as the limiting cases of the smooth charge motion in the limit when the lengths of accelerated (decelerated) pieces of the charge trajectory tend to zero. This means that attempts to interpret the radiation intensity given by the Tamm formula (3.4) in terms of the charge instantaneous acceleration and deceleration are insufficient.

We summarize:

(1) The interpretation of the transition radiation and the Tamm problem in terms of instantaneous acceleration and deceleration is not sufficient;
(2) the usual interpretation of the transition radiation arising when the charge crosses the boundary between two media in terms of semi-infinite charge motions is valid only if $\beta<1/n_1$ and $\beta<1/n_2$. Otherwise, this interpretation should be supplemented by the Cherenkov-type terms;
(3) there is no need in artificial means mentioned in previous two items in the treated exactly solvable case corresponding to the transition and VC radiations on a spherical sample.

VII. CONCLUSION

We briefly review the main results obtained.

(1) The electromagnetic field strengths and angular radiation intensity corresponding to the Tamm problem are developed in terms of Legendre polynomials. The corresponding representation for the frequency distributions is also found.

(2) We found closed expressions for the electromagnetic field arising from the charge motion confined to the dielectric sphere S which is surrounded by another dielectric medium with dielectric properties different from those inside S. It is studied how differences of media properties inside and outside S affect the angular and frequency radiation intensities for various charge velocities. In general, these differences lead to the broadening of the angular spectrum, to the rise of angular intensities at large angles, and to the appearance of oscillations in the frequency spectrum.

(3) It is considered how radiates a charge whose motion begins and terminates in medium 2 and which passes through the dielectric sphere S filled with medium 1 or through the metallic sphere. The evaluated energy flux includes the VC and transition radiations as well as ones originating from the beginning and termination of motion. It is shown that when the medium 2 outside S is vacuum and medium 1 inside S has refractive index n_1 satisfying $\beta n_1 > 1$, the angular and frequency radiation intensities cannot be always interpreted in terms of the Tamm formula (3.4) corresponding to the charge motion inside S (as it is usually believed).

(4) It is proved that the interpretation of the transition radiation in terms of the instantaneous termination of the charge motion in one medium and its instantaneous beginning in the other one is not valid if the above motion with sudden velocity jumps can be considered as a limiting case of the smooth charge motion. It is shown that the interpretation of the transition radiation in terms of semi-infinite motions with instantaneous termination of the charge motion in one medium and with its instantaneous beginning in the other one, should be supplemented with the VC radiation terms. Certainly, these remarks are related only to the interpretation of the transition radiation, not to the exact solutions obtained for the plane interface, e.g., in Refs. 5 and 17.

APPENDIX A

Using (2.3), (2.4), and (3.8) we find that the magnetic vector potential corresponding to Fig. 1 equals

$$A_z = \frac{iek_2\mu_2}{2\pi c} \sum (2l+1) P_l(\cos\theta) h_l(k_2 r) C_l$$

for $r > a$,

$$A_z = \frac{iek_1\mu_1}{2\pi c} \sum (2l+1) P_l(\cos\theta) [j_l(k_1 r) D_l + h_l(k_1 r) J_l^{(1)}(0, z_0)]$$

for $z_0 < r < a$, and

$$A_z = \frac{iek_1\mu_1}{2\pi c} \sum (2l+1) P_l(\cos\theta) [j_l(k_1 r) D_l + h_l(k_1 r) J_l^{(1)}(0, r) + j_l(k_1 r) H_l^{(1)}(r, z_0)]$$

for $r < z_0$. Here we set

$$J_l^{(1)}(x,y) = \int_x^y j_l(k_1 r') f_l(r') \mathrm{d}r', \quad H_l^{(1)}(x,y) = \int_x^y h_l(k_1 r') f_l(r') \mathrm{d}r'.$$

Differentiating A_z, one finds EMF strengths (4.1), (4.2) in which

$$\tilde{C}_l = C_{l-1} + C_{l+1} \quad \text{and} \quad \tilde{D}_l = D_{l-1} + D_{l+1}.$$

Since EMF strengths contain only $\tilde{C}_l$ and $\tilde{D}_l$, the coefficients C_l and D_l entering into electromagnetic potentials are not needed.

APPENDIX B

The magnetic vector potential satisfying equations $(\Delta + k_2^2) A_z = 0$ for $r > z_0$, $(\Delta + k_2^2) A_z = -4\pi\mu_2 j_z / c$ for $a < r < z_0$ and $(\Delta + k_1^2) A_z = -4\pi\mu_1 j_z / c$ for $r < a$ is given by

$$A_z = \frac{iek_2\mu_2}{2\pi c} \sum (2l+1) P_l h_l(k_2 r) \left[C_l \frac{\mu_1}{\mu_2} J_l^{(1)}(0, a) + J_l^{(2)}(a, z_0) \right]$$

for $r > z_0$,

$$A_z=\frac{iek_2\mu_2}{2\pi c}\sum\ (2l+1)P_l\left[h_l(k_2r)C_l\frac{\mu_1}{\mu_2}J_l^{(1)}(0,a)+h_l(k_2r)J_l^{(2)}(a,r)+j_l(k_2r)H_l^{(2)}(r,z_0)\right]$$

for $a<r<z_0$, and

$$A_z=\frac{iek_1\mu_1}{2\pi c}\sum\ (2l+1)P_l(\cos\theta)\left[j_l(k_1r)\frac{\mu_2}{\mu_1}D_lH_l^{(2)}(a,z_0)+h_l(k_1r)J_l^{(1)}(0,r)\right.$$
$$\left.+j_l(k_1r)H_l^{(1)}(r,a)\right]$$

for $r<a$. Here

$$J_l^{(2)}(x,y)=\int_x^y j_l(k_2r')f_l(r')\mathrm{d}r',\quad H_l^{(2)}(x,y)=\int_x^y h_l(k_2r')f_l(r')\mathrm{d}r'.$$

It is convenient to redefine C_l and D_l:

$$C_l'=C_l\frac{\mu_1}{\mu_2}J_l^{(1)}(0,a)+J_l^{(2)}(a,z_0),\quad D_l'=D_l\frac{\mu_2}{\mu_1}H_l^{(2)}(a,z_0).$$

Then,

$$A_z=\frac{iek_2\mu_2}{2\pi c}\sum\ (2l+1)P_lh_l(k_2r)C_l'$$

for $r>z_0$,

$$A_z=\frac{iek_2\mu_2}{2\pi c}\sum\ (2l+1)P_l(\cos\theta)[C_l'h_l(k_2r)-h_l(k_2r)J_l^{(2)}(r,z_0)+j_l(k_2r)H_l^{(2)}(r,z_0)]$$

for $a<r<z_0$, and

$$A_z=\frac{iek_1\mu_1}{2\pi c}\sum\ (2l+1)P_l(\cos\theta)[D_l'j_l(k_1r)+h_l(k_1r)J_l^{(1)}(0,r)+j_l(k_1r)H_l^{(1)}(r,a)]$$

for $r<a$. Differentiating A_z, one recovers EMF strengths (5.1)–(5.3) where

$$\tilde{C}_l=C_{l-1}'+C_{l+1}',\quad \tilde{D}_l=D_{l-1}'+D_{l+1}'.$$

Again, we do not need coefficients C_l and D_l entering into the vector potential since EMF field strengths (and the radiation intensity) depend only on $\tilde{C}_l$ and $\tilde{D}_l$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Classical transport of charged particles in a magnetic field

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(Received 8 September 2002; accepted 23 April 2003)

We examine the traditional transport equation for classical, charged particles diffusing in a cold, absorbing medium subject to a uniform magnetic field and in which scattering is isotropic. Steady-state solutions in plane geometry are examined in some detail; we make no expansion about an isotropic angular distribution. Restricting the motion to two dimensions captures most of the interesting features; there is some discussion of the three-dimensional case. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1591994]

I. INTRODUCTION

The motion of ions and electrons in a weakly ionized gas subjected to external electric and magnetic fields is an ancient and ''classical'' problem in kinetic theory.[1,2] The analysis of these systems (''swarms'') is based, almost always, upon a linear ''Boltzmann,'' or transport equation. The equation is treated in its most general form so that one can be as faithful as possible to the experiments. Most often the velocity variation of the distribution function is expressed in terms of a series of tensorial spherical harmonics, and the evolution of the density described in ''hydrodynamic'' and ''nonhydrodynamic'' terms. (Here, the interested reader should consult the impressive publications of Australian physicists.[3–6]) Such expansions—which may be viewed as a generalization of the traditional, Chapman–Enskog treatment of Boltzmann's equation—generate an infinite hierarchy of ''moment-equations,'' a hierarchy which is truncated at some level, for reasons which are physical or practical. This procedure, with its advantages and its limitations, has been part of transport theory almost since its creation. Since these expansions are usually asymptotic, at best, one welcomes comparison with exact solutions of related transport equations which are not trivial.

This paper is concerned with the solution of such a relevant model—it describes the time-independent transport of charged test-particles in a cold medium which scatters isotropically, may capture particles, and is immersed in a uniform magnetic field. Since no electric field is present, the distribution in velocity is simpler, but still interesting. In the solution, the most important dimensionless parameter is ω, the ratio of cyclotron frequency to collision frequency. If one wishes to go beyond treating the analysis as a mathematical exercise, merely, one notes that ω is trivially small for ions in realistic situations, but can be interestingly large for electrons. Then, the (asymptotic) velocity distribution deviates considerably from the isotropic form about which the simplest ''hydrodynamic'' models are centered. Other results are—apart from an array of attractive equations involving Bessel functions—(1) that the magnetic field shatters the famous continuous spectrum associated with the ''one-speed transport equation[7]'' into an infinity of discrete eigenvalues. (We discuss the behavior of these eigenvalues as field and absorption strength are varied; the limit $\omega \to 0$ is quite singular.) (2) The magnetic field induces a flow parallel to the source plane. This ''diamagnetic drift'' is well known to plasma physicists.[8] Here we treat it in some detail. Most important is that none of our results rely upon an assumption of ''small gradients.''

Justifying the irreversible, transport—rather than the reversible, Liouville treatment of a problem in kinetic theory—poses famous and delicate problems. In the case of an isolated and simple gas one justifies mathematically the transition from Liouville to transport by a limiting

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process—by invoking the ''Grad-limit.[9]'' To the physicist, this means, roughly, that the gas should be sufficiently dilute for transport theory to be useful. When the system is subject to external fields, matters become more difficult. Recently, a group of scholars[10] has analyzed the limiting process for the Lorentz model—which describes charged particles diffusing through a static array of scatterers—immersed in a magnetic field. Their analysis considers how unusual trajectories—a particle whirling in circular orbit in the space between two scatterers, for example—are to be treated in the construction of the ''correct,'' coarse-grained transport equation. Our paper avoids these difficult issues. We simply study the ''traditional'' transport equation as a mathematical object, acknowledging that it describes the physics correctly in some regime where the magnetic field is not too strong and that often, continuing results obtained from a sanctioned region, say $\omega<1$, into a questionable one, say $\omega\gg 1$, has some value.

Most of the paper is devoted to motion in two dimensions (2D)—in a plane perpendicular to the uniform magnetic field. We give, briefly, expressions for densities and currents in the three-dimensional case as well. In treating the equation, its features and consequences, we allow the strength of the uniform magnetic field to vary arbitrarily. The fact that a steady source of particles in an absorbing medium produces a steady distribution indicates that the traditional equation gives no weight to particles whirling, collisionless in tight circles,

II. ANALYSIS OF A SIMPLE MODEL

We begin with a simple model: noninteracting charged particles of fixed kinetic energy move in a plane perpendicular to an uniform magnetic field. The particles scatter elastically and isotropically from host atoms (''neutrals.'') We are in steady state, there is a plane source ($y-z$ plane) at the origin, and the medium, which is unbounded, may absorb particles. The distribution function for position and velocity, $F(x,\phi)$, depends then upon two variables, and we face the kinetic equation

$$\mu\frac{\partial}{\partial x}F(x,\phi)-\omega\frac{\partial}{\partial\phi}F(x,\phi)=\frac{c}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,F(x,\phi)-F(x,\phi)+Q(\phi)\,\delta(x). \tag{1}$$

This familiar equation, with $(v\cdot x)=\mu=\cos\phi$, is written in dimensionless variables. The constant speed is taken to be unity, distance is scaled by the total mean-free-path for encounters, time by the corresponding mean-free-time, and ω represents the cyclotron frequency qB/mc divided by the collision frequency. ω may also be seen as the ratio of mean-free-path to Larmor radius. c, the number of secondaries produced per collision, is limited to $1>c\geqslant 0$. As we see later, transport in three dimensions—with plane symmetry—is not that much more difficult.

After Fourier transformation in x we have

$$\mathcal{O}f(k,\phi)=-\omega\frac{\partial}{\partial\phi}f(k,\phi)+(1+ik\mu)f(k,\phi)=\frac{c}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,f(k,\phi)+Q(\phi) \tag{2}$$

or

$$(\mathcal{O}-c\mathcal{P})f(k,\phi)=Q(\phi).$$

A new notation, Dirac-like, helps. Our operators act in function spaces whose elements are distribution functions $|f\rangle$. and $\langle g|$. There is a complex inner product. Thus,

$$\langle g|f\rangle\equiv\int_0^{2\pi}\mathrm{d}\phi\,g^*(\phi)f(\phi)=\langle f|g\rangle^*$$

and

$$(\mathcal{O}-c\mathcal{P})|f\rangle=|Q\rangle. \tag{3}$$

$\mathcal{P}$ is the projection operator,

$$\mathcal{P}|f\rangle \equiv |a\rangle\langle a|f\rangle, \quad \langle a|a\rangle = 1$$

with

$$|a\rangle = \frac{1}{\sqrt{2\pi}}, \quad \langle a|f\rangle = \int_0^{2\pi} \mathrm{d}\phi \frac{1}{\sqrt{2\pi}} f(\phi).$$

We may also use $|1\rangle = \sqrt{2\pi}|a\rangle$, so that $\langle 1|f\rangle = \int_0^{2\pi} \mathrm{d}\phi\, f(k,\phi)$ gives $n(k)$, the angle-integrated density. The particle currents are

$$\mathcal{J}_{x,y}(k) = \int_0^{2\pi} \mathrm{d}\phi [\cos\phi, \sin\phi] \;\; f(k,\phi).$$

We use the special notation $\mathcal{J}_{x,y}(k) = \langle j_{x,y}|f\rangle$ for the currents.

Two results follow quickly; the solution to the kinetic equation, Eq. (3), is

$$|f\rangle = \frac{1}{\mathcal{O}}|Q\rangle + c\frac{1}{\mathcal{O}}|a\rangle \frac{\langle a|\dfrac{1}{\mathcal{O}}|Q\rangle}{\left[1 - c\langle a|\dfrac{1}{\mathcal{O}}|a\rangle\right]}, \tag{4}$$

and if we take the particularly simple case of an isotropic source of strength $|Q\rangle = |a\rangle$ we find

$$\begin{aligned} |f\rangle &= \frac{1}{\left[1 - c\langle a|\dfrac{1}{\mathcal{O}}|a\rangle\right]} \frac{1}{\mathcal{O}}|a\rangle = \frac{1}{\mathcal{D}(k,c)} \frac{1}{\mathcal{O}}|a\rangle, \\ \langle a|f\rangle &= \frac{1}{\left[1 - c\langle a|\dfrac{1}{\mathcal{O}}|a\rangle\right]} \langle a|\frac{1}{\mathcal{O}}|a\rangle = \frac{1}{\mathcal{D}(k,c)}\langle a|\frac{1}{\mathcal{O}}|a\rangle. \end{aligned} \tag{5}$$

The last equation also states that with unit source, $|Q_1\rangle = 1/2\pi$,

$$n(k) = \frac{1}{\mathcal{D}(k,c)}\langle a|\frac{1}{\mathcal{O}}|a\rangle = \frac{\mathcal{K}(k)}{\mathcal{D}(k,c)} = \frac{\mathcal{K}(k)}{1 - c\mathcal{K}(k)}.$$

There are corresponding expressions for the currents,

$$\mathcal{J}_{x,y}(k) = \frac{1}{\mathcal{D}(k,c)}\langle j_{x,y}|\frac{1}{\mathcal{O}}|a\rangle$$

for source $|Q\rangle = |a\rangle$.

An alternative expression for $\mathcal{J}_x(k)$ appears if we integrate Eq. (1) directly, to get the equation of continuity,

$$\frac{\partial}{\partial x}\mathcal{J}_x(x) + (1-c)n(x) = Q\delta(x).$$

We find

$$ik\mathcal{J}_x(k,c)=\frac{1-\mathcal{K}(k)}{1-c\mathcal{K}(k)}=\frac{\mathcal{D}(k,1)}{\mathcal{D}(k,c)}, \tag{6}$$

for unit source $|Q_1\rangle$. That the various expressions are related by partial integration will be evident later, as will the expression

$$i\mathcal{J}_y(k,c)=\frac{\omega}{2}\frac{1}{\mathcal{D}(k,c)}\frac{\partial}{\partial k}\mathcal{K}(k). \tag{7}$$

The quantity

$$\mathcal{K}(k)=\langle a|\frac{1}{\mathcal{O}}|a\rangle$$

contains the essence of the system, generating the relaxation lengths, for example. This kernel is the Fourier transform of the kernel controlling the Peierls integral equation[11] for $n(x)$ (see the following). We shall refer to $\mathcal{D}(k,c)=1-c\mathcal{K}$ as the dispersion function. This article is concerned with the features of density and current. To get at them, we learn as much as we can about $\mathcal{K}(k)$ and $\mathcal{D}(k,c)$.

A. Evaluating the kernel

Of the several ways to evaluate the kernel; two are particularly helpful. In the first, we make use of the eigen-vectors of the operator $\mathcal{O}$,

$$\mathcal{O}|n\rangle=\lambda_n|n\rangle.$$

One finds

$$|n\rangle=\frac{1}{\sqrt{2\pi}}\exp[in\phi]\exp\left[i\frac{k}{\omega}\sin\phi\right],$$
$$\lambda_n=1-in\omega. \tag{8}$$

The $|n\rangle$ are complete and orthonormal, with the usual complex inner product. The wave number k appears parametrically in the eigenvector but not in the eigenvalue. The $|n\rangle$ form a useful basis for expansion. Since

$$\langle a|n\rangle=\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\exp[in\phi]\exp\left[i\frac{k}{\omega}\sin\phi\right]=(-)^nJ_n\left(\frac{k}{\omega}\right)=\langle n|a\rangle. \tag{9}$$

Bessel functions make their expected appearance. A quite straightforward calculation leads then to the first of several expressions for the kernel,

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle=\left[J_0\left(\frac{k}{\omega}\right)\right]^2+2\sum_{n=1}^{\infty}\left[J_n\left(\frac{k}{\omega}\right)\right]^2\Big/(1+n^2\omega^2). \tag{10}$$

(In the following text, we may denote k/ω by κ, which is proportional to the ratio of cyclotron radius to wavelength of the k mode.)

Another straightforward calculation, making use of $\mathcal{J}_{\pm}=\mathcal{J}_x\pm i\mathcal{J}_y$ and recursion relations, leads to Eq. (7) for the transverse current—the ''diamagnetic drift'' of the plasma physicists. We note an alternate derivation ahead.

A more powerful and elastic representation of the kernel stems from an ''algebraic'' method, which is a simplified version of the method of characteristics.

Write

$$\frac{1}{\mathcal{O}}|f\rangle=\int_0^\infty \mathrm{d}t\, e^{-t}e^{-t(A+B)}|f\rangle,$$
$$(A+B)=ik\cos\phi-\omega\frac{\partial}{\partial\phi}=e^{i\kappa\sin\phi}\left(-\omega\frac{\partial}{\partial\phi}\right)e^{-i\kappa\sin\phi}. \tag{11}$$

Multiplication by t and constructing the exponential series gives

$$e^{-t(A+B)}=e^{i\kappa\sin\phi}\exp\left(\omega t\frac{\partial}{\partial\phi}\right)e^{-i\kappa\sin\phi},$$

and we can write, quite generally,

$$\langle g|\frac{1}{\mathcal{O}}|Q\rangle=\int_0^\infty \mathrm{d}t\, e^{-t}\int_0^{2\pi}\mathrm{d}\phi\, g(\phi)^* e^{i\kappa[\sin\phi-\sin(\phi+\omega t)]}Q(\phi+\omega t). \tag{12}$$

In particular, our kernel is

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{2\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\int_0^{2\pi}\mathrm{d}\phi\, e^{i\kappa[\sin\phi-\sin(\phi+\omega t)]}, \tag{13}$$

and inversion of the Fourier transform gives the Peierls integral equation which corresponds to Eq. (1). One finds—for an isotropic source—

$$n(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\,\mathcal{K}(x-x')[n(x')+q(x')]$$

with

$$\mathcal{K}(x-x')=\int_0^\infty \mathrm{d}t\, e^{-t}\int_0^{2\pi}\mathrm{d}\phi\,\delta(x-x'+[\sin\phi-\sin(\phi+\omega t)]).$$

After some reduction, using the fact that the integral of a periodic function over its period is unaltered by a shift in the variable of integration, we find

$$\mathcal{K}(x-x')=\frac{1}{1-e^{-4\pi/\omega}}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\, e^{-2\theta/\omega}\delta\left(\frac{\omega}{2}(x-x')-\sin\theta\sin\phi\right).$$

$\mathcal{K}$ is even, in its argument. In our dimensionless units ω, the ratio of cyclotron frequency to collision frequency is the reciprocal of the ratio of cyclotron radius to mean-free-path. Thus, the constraint expressed by the δ-function, that $|x-x'|\leqslant 2/\omega$, is precisely the statement that the farthest-ranging particle is found at one ''cyclotron-diameter'' from a plane source, having left the source traveling parallel to it. The Peierls' kernel, $\mathcal{K}(x)$, has ''compact support''; it has no exponential tail. Further reduction will be remarked upon later. [See Eq. (24).]

Returning to the kernel, note the limit $\omega\to 0$ when

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle\to\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,\frac{1}{1+ik\cos\phi}=\frac{1}{\sqrt{1+k^2}}. \tag{14}$$

In the field-free case, the kernel and the dispersion function are analytic in a cut, complex-k plane, and spatial relaxation is described by a discrete and a continuous spectrum of relaxation lengths. The Fourier inverse of the kernel,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ikx}\langle a|\frac{1}{\mathcal{O}}|a\rangle = \frac{1}{\pi}K_0(|x|),$$

expresses the density of uncollided particles as a Bessel function. Another useful limiting expression holds when $\omega \gg 1$. Then Eq. (10) informs us that

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle \to \left[J_0\left(\frac{k}{\omega}\right)\right]^2. \tag{15}$$

The kernel, as expressed by Eq. (13), may be simplified if we expand the exponential, noting that only even powers survive the angle-averaging. One finds that when $n=2m$,

$$\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\phi[\sin\phi - \sin(\phi+\omega t)]^n = \binom{2m}{m}\left[\sin\left(\frac{\omega t}{2}\right)\right]^{2m}.$$

Now, two paths are open; one can use

$$\frac{1}{(2m)!}\int_0^{\infty} \mathrm{d}t\, e^{-t}\left(\sin\frac{\omega}{2}t\right)^{2m} = \omega^{2m}\prod_{r=1}^{m}\frac{1}{1+r^2\omega^2},$$

to get the useful series

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle = 1+\sum_{m=1}^{\infty}(-)^m\binom{2m}{m}\left(\frac{k^2}{4}\right)^m\prod_{r=1}^{m}\frac{1}{1+r^2\omega^2}, \tag{16}$$

or eschew the t-integration, recognizing the series as generating the Bessel function J_0, and hence that

$$\mathcal{K}(k) = \langle a|\frac{1}{\mathcal{O}}|a\rangle = \int_0^{\infty}\mathrm{d}t\, e^{-t}J_0\left(2\frac{k}{\omega}\sin\frac{\omega t}{2}\right). \tag{17}$$

(The Appendix contains a shorter derivation of this result.)

Equation (17) may be rearranged by exploiting periodicity, and using

$$\int_0^{\pi}\mathrm{d}\phi\, g(\phi)F(\sin\phi) = \int_0^{\pi/2}\mathrm{d}\phi\left[g\left(\frac{\pi}{2}-\phi\right)+g\left(\frac{\pi}{2}+\phi\right)\right]F(\cos\phi),$$

to get

$$\mathcal{K}(k) = \frac{2}{\omega}\frac{1}{1-e^{-2\pi/\omega}}\int_0^{\pi}\mathrm{d}\phi\, e^{-2\phi/\omega}J_0\left(2\frac{k}{\omega}\sin\phi\right) \tag{18}$$

$$= \frac{2}{\omega}\frac{1}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\pi/2}\mathrm{d}\phi\cosh\left(\frac{2\phi}{\omega}\right)J_0\left(2\frac{k}{\omega}\cos\phi\right), \tag{19}$$

all of which have been found useful. A nice connection with the eigenfunction expansion, Eq. (10), is made via Neumann's addition formula

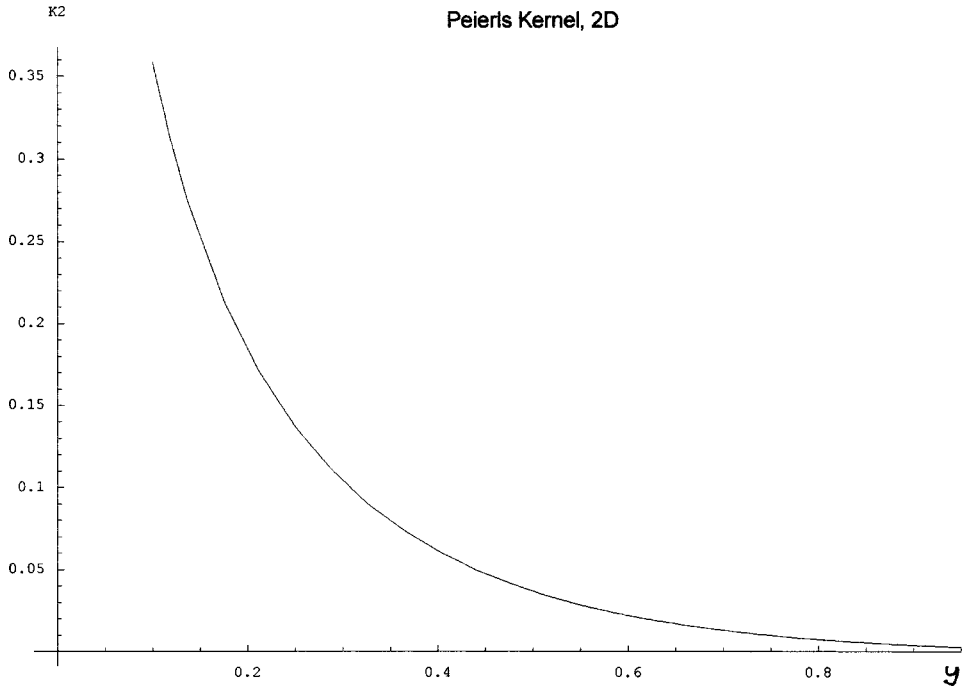

FIG. 1. $\mathcal{K}_2$, the 2D kernel (Peierls) for the integral equation for density, $n(x)$, with $\omega=0.5$, shown as a function of its argument, $y=\omega|x|/2$. The kernel is zero when $y>1$ while $\mathcal{K}_2(1^-)=1/[2\sinh(\pi/\omega)]$.

$$J_0(2t\sin\psi)=J_0(t)^2+2\sum_{n=1}^{\infty}J_n(t)^2\cos 2n\psi$$

in concert with Eq. (17).

Finally, we may Fourier-invert Eq. (19) to get another representation of the Peierls kernel, namely

$$\mathcal{K}(x)=\frac{1}{\pi}\frac{1}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\phi_*(\omega x)}d\phi\,\frac{\cosh\left(\frac{2\phi}{\omega}\right)}{\sqrt{\cos^2\phi-\cos^2\phi_*(\omega x)}},\quad 0<x<\frac{2}{\omega}$$

$$=0,\quad x>\frac{2}{\omega},\tag{20}$$

where ϕ_* is defined through $\cos\phi_*=(\omega/2)x$. (See Fig. 1.)

A final comment for this section: There is still another way to solve our transport equation, Fourier expansion in ϕ. That approach, which is more natural when the scattering is anisotropic, leads to difference equations, to solutions in terms of continued fractions and to the traditional, truncated solutions which we wish to avoid.

B. The complex *k* plane

The Fourier inversion of $\langle a|f\rangle$ and $\langle j_{x,y}|f\rangle$ will be controlled by singularities in the complex k plane. The series in Eq. (16) converges throughout the k plane for all nonzero ω, assuring us that our kernel is an entire function of k. Thus, the only singularities are the zeros of the dispersion function. The magnetic field has shattered the continuous spectrum and it is to the zeros that we turn. They will describe the relaxation lengths which characterize the system. Since their location

depends upon both magnetic field and absorption, $0 \leqslant \omega < \infty$ and $0 \leqslant c \leqslant 1$, the picture, overall, is complicated. But the analysis is eased somewhat by the fact that c and ω occur separately in the dispersion function. We begin by observing the following.

(1) Since $\mathcal{D}$ is a real function of k^2, a complex root of the dispersion equation will generate four zeros in the k plane, of the form $\pm(\xi \pm i\eta)$. Thus we may limit our discussion to a single quadrant of the complex k plane, with the understanding that the other three will be filled by reflection.

(2) If the particle distribution is to be bounded at infinity we expect that $\mathcal{D}$ has no zeros on the real axis of k. (The exceptional case $c=1$ produces a second-order zero at the origin, and is "physical" when the source is moved to infinity—the Milne case.) And inspection of the series for $\mathcal{D}$ shows that when $c=1$, there are no zeros (poles) on the imaginary axis.

(3) *The dominant zero*. When $0<c<1$ there is a dominant zero (pole) on the positive (and the negative) sections of the imaginary axis, where $k=i\eta$. This pole, with its associated residue, describes the dominant, large-x, "asymptotic" behavior of the distribution. There is no other zero on the axis because the kernel is a function of η which increases smoothly. (The zeros which are off-axis and are discussed later, give oscillatory contributions which cannot dominate, asymptotically.) Then, for the dominant zero, we have four regimes as follows.

(i) *Strong field* ($\omega \gg 1$, c arbitrary). Here, Eq. (15) enables us to write

$$\eta_0 = \omega y(c),$$

where

$$1 - cI_0(y)^2 = 0 \tag{21}$$

for all c. (In practice, the estimate is valuable even at $\omega \approx 1$.)

(ii) *Weak absorption* ($1-c \ll 1$, ω arbitrary). Here, the zero lies close to the origin, and the series, Eq. (16) yields

$$\eta_0 \simeq \sqrt{2(1-c)(1+\omega^2)}, \tag{22}$$

a result which emerges from Eq. (21), too. It describes a simple, exponential attenuation, which has been increased by the magnetic field. In the field-free case $\eta_0 = \sqrt{1-c^2}$ exactly.

(iii) *Strong absorption* ($c \to 0$, ω arbitrary). When field is absent the kernel displays branch points, and the zero falls into the branch singularity when $c=0$. With field present, there are no branch points and matters are quite different. The dominant zero moves along the imaginary axis to infinity as $c \to 0$, the dominant relaxation length becoming arbitrarily small. It is the magnetic field, rather than the mean free-path, which is in control. Equation (21) yields an easy estimate, when the field is large,

$$\eta_0 \simeq \frac{\omega}{2} \log\left(\frac{1}{c}\right). \tag{23}$$

In the limit, $c=0$, the distribution becomes that of uncollided particles proceeding from a plane, isotropic source. It is simply the Peierls kernel, Eq. (20). It helps to write the symmetric distribution as ($x>0$)

$$n_0(x)=\mathcal{K}(x)=\frac{1}{\pi}\frac{\cosh\left(\frac{2\phi_*(\omega x)}{\omega}\right)}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\phi_*(\omega x)}d\phi\,\frac{1}{\sqrt{\cos^2\phi-\cos^2\phi_*(\omega x)}}$$

$$+\frac{1}{\pi}\frac{1}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\phi_*(\omega x)}d\phi\,\frac{\cosh\left(\frac{2\phi}{\omega}\right)-\cosh\left(\frac{2\phi_*(\omega x)}{\omega}\right)}{\sqrt{\cos^2\phi-\cos^2\phi_*(\omega x)}},\quad 0<x<\frac{2}{\omega}$$

$$=0,\quad x>\frac{2}{\omega}. \tag{24}$$

The key quantity in its description is $\phi_*(\omega x)$, which descends from $(\pi/2)$ at the plane source to zero at the edge of the distribution. We note further that (a) the second term in Eq. (24) is bounded for all $\phi_*(x)$, vanishing at the edge of the distribution, while (b) the integral appearing in the first term may be transformed into the complete elliptical integral $K(\sin^2\phi_*)$. It diverges, logarithmically at the source plane, and is $(\pi/2)$ at the edge. Thus, the distribution of uncollided particles is discontinuous at its edge. We have the limits (see Fig. 1)

$$n_0(x)=\mathcal{K}(x)\to\frac{1}{2\sinh\left(\frac{\pi}{\omega}\right)},\quad x\to\frac{2}{\omega},$$

$$n_0(x)=\mathcal{K}(x)\sim\frac{1}{\pi}\coth\left(\frac{\pi}{\omega}\right)\log\left(\frac{1}{x}\right)+\cdots,\quad x\to 0. \tag{25}$$

The size of the step-discontinuity vanishes, conveniently, as $\omega\to 0$, while the leading behavior at the source plane coincides with that of the field-free case.

(iv) *Weak field* ($\omega\to 0$, c arbitrary). While the large-ω limit is relatively simple, the small-ω limit is not. Since singularities which are absent when $\omega\neq 0$ appear (at $\eta=\pm 1$) when $\omega=0$, the behavior in the neighborhood of these points cannot be analytic. The simple expression, Eq. (22), does not tell the full story. We begin by studying

$$\mathcal{I}(\phi,\eta)=\cosh\left(\frac{2}{\omega}\phi\right)I_0\left(\frac{2}{\omega}\eta\cos\phi\right),$$

the integrand appearing in Eq. (19), in the regime $(2/\omega)\equiv\lambda\gg 1$. At the limits of integration we have

$$\mathcal{I}(0,\eta)=I_0(\lambda\eta),\quad \mathcal{I}\left(\frac{\pi}{2},\eta\right)=\cosh\left(\lambda\frac{\pi}{2}\right),$$

and behavior will be different in different intervals of η, for absorption may cause η_0 to be large. It is no surprise that $\eta=1$, and $\eta=\pi/2$, play important roles in the analysis.

(a) When $\eta<1$, $\mathcal{I}(\phi,\eta)$ is seen to be an increasing function of ϕ in $(0,\pi/2)$ and the integral is controlled by the behavior of $\mathcal{I}$ near its maximum—at the edge. If we rearrange Eq. (19) to place the maximum at the origin we obtain

$$\mathcal{K}(i\eta)=\frac{1}{2}\int_0^{\Lambda}dt\,I_0\left(\lambda\eta\sin\left(\frac{t}{\lambda}\right)\right)\{(\coth(\Lambda)-1)e^{t}+(\coth(\Lambda)+1)e^{-t}\},$$

where

TABLE I. $1/\eta_0$ is the relaxation length, in units of mean-free-path, for the particle distribution far from its plane source, in the presence of various amounts of capture and various magnetic field strengths.

	Dominant zero, η_0				
ω	$c=0.9$	$c=0.7$	$c=0.5$	$c=0.3$	$c=0.1$
0.25	0.46	0.78	1.0	1.2	1.5
0.5	0.50	0.89	1.2	1.5	2.0
1	0.65	1.2	1.6	2.1	3.0

$$\Lambda=\frac{\pi}{\omega}=\frac{\pi}{2}\lambda.$$

A little consideration shows that when λ is very large we may write

$$\mathcal{K}(i\eta)\simeq\int_0^\infty \mathrm{d}t\, I_0\left(\lambda\eta\sin\left(\frac{t}{\lambda}\right)\right)e^{-t}$$

with exponentially small error, $O(e^{-(1-\eta)\Lambda})$. Then, expansion about $t=0$, aided by the relation

$$\frac{1}{n!}\int_0^\infty \mathrm{d}t\, e^{-t}t^n J_0(kt)=\frac{1}{(1+k^2)^{(n+1/2)}}P_n\left(\frac{1}{\sqrt{1+k^2}}\right) \tag{26}$$

(P_n is the Legendre polynomial) yields

$$\mathcal{K}(i\eta)=\langle a|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{\sqrt{1-\eta^2}}\left[1-\frac{1}{2}\left(\frac{\omega}{2}\right)^2\eta^2\frac{4+\eta^2}{(1-\eta^2)^3}+\cdots\right], \tag{27}$$

in which the singular nature of the small-ω behavior is displayed.

In the complimentary situation, when $\eta>1$, $\mathcal{I}(\phi,\eta)$ posesses a maximum inside the interval $(0,\pi/2)$. When that sharp maximum dominates the contribution from the edge, expansion produces

$$\mathcal{K}(i\eta)\simeq\frac{1}{\sqrt{\eta^2-1}}\exp\left[\left(\frac{2}{\omega}\right)\left(\sin^{-1}\frac{1}{\eta}-\frac{\pi}{2}+\sqrt{\eta^2-1}\right)\right], \tag{28}$$

as $(2/\omega)\to\infty$. Thus, when $\eta\gg1$ as well,

$$\mathcal{K}(i\eta)\simeq\frac{1}{\eta}\exp\left[\frac{2}{\omega}\left(\eta-\frac{\pi}{2}\right)\right], \tag{29}$$

which leads easily to the estimate

$$\eta_0\simeq\frac{\omega}{2}\log\left(\frac{1}{c}\right)\quad\text{for } c\to0\quad\text{and }\omega\text{ ``small,''} \tag{30}$$

familiar, and in agreement with Eq. (23).

Some dominant zeros are displayed in Table I.

(4) *Transients*. The other zeros, or relaxation lengths, form a complex pattern. They produce transient, oscillating terms in the spatial distribution. We would like a picture of the pattern, and how it alters as the magnetic field is altered. In particular, we are interested in the limit $\omega\to0$. Ultimately, we rely on the summation, numerically, of Eq. (16). But the search for zeros is helped greatly by asymptotic estimates, to which we turn.

(i) *Strong field* ($\omega \gg 1$, $|\kappa|$ arbitrary) ($\kappa \equiv k/\omega$). We begin with the simplest estimate, $\omega \gg 1$, when a different approach yields a familiar result,

$$\mathcal{K}(k) \simeq 1 + \sum_{m=1}^{\infty} \binom{2m}{m} \left(-\frac{k^2}{4\omega^2} \right)^m \frac{1}{(m!)^2} = \frac{2}{\pi} \int_0^{\pi/2} d\phi \, J_0\left(2\frac{k}{\omega} \sin\phi \right) = J_0\left(\frac{k}{\omega} \right)^2. \tag{31}$$

Then, the ω dependence is simple, $k_n = \omega \kappa_n$, where $\kappa_n(c)$ is one of the complex zeros of $1 - cJ_0(\kappa)^2$. (In practice, the estimate is valuable even at $\omega \approx 1$.) Among these, the "higher harmonics" ($|\kappa| \gg 1$) obey

$$\frac{\sin 2x}{2x} e^{2y} = \frac{\pi}{c}, \quad \cos 2x = 2y e^{-2y} \frac{\pi}{c}, \tag{32}$$

where $\kappa = x + iy$. From these, we infer

$$k_n \approx \omega \left\{ n\pi + i\frac{1}{2} \log\left[\left(2n + \frac{1}{2} \right) \frac{\pi^2}{c} \right] \right\}, \quad n = 0,1,2,... \tag{33}$$

for the regime $\omega \gg 1$ and $|k| \gg \omega$. The real parts of the relaxation constants increase only logarithmically, the imaginary parts linearly. Note that the dominant zero is contained here, associated with $c \ll 1$, and behaves as

$$k_0 \simeq i\frac{\omega}{2} \log\left(\frac{1}{c} \right).$$

(ii) *Weak field* is included in the regime ($|\kappa| \gg 1$, ω arbitrary). We begin with the estimate

$$\int_0^{\pi} d\phi \, e^{-2\phi/\omega} J_0(2\kappa \sin\phi) \sim \frac{1}{2\kappa} [1 + e^{-2\pi/\omega} + 2e^{-\pi/\omega} \sin 2\kappa], \quad |\kappa| \to \infty, \tag{34}$$

derived by the method of stationary phase, including end-point corrections. The derivation proceeds with the assumption that k is real, but suggests strongly that the result holds throughout the quadrant when $\mathrm{Re}(\kappa) > 0$. This conjecture is supported by the fact that Eqs. (34) and (31) are identical, namely,

$$\mathcal{K}(k) \approx \frac{i}{2\pi\kappa} e^{-2i\kappa}$$

when their domains overlap, and by numerical experience. We have, then, the approximate dispersion equation,

$$1 + \left(\frac{2e^{-\pi/\omega}}{1 + e^{-2\pi/\omega}} \right) \sin 2\kappa = \frac{\kappa\omega}{c} \left(\frac{1 - e^{-2\pi/\omega}}{1 + e^{-2\pi/\omega}} \right). \tag{35}$$

For field strengths $e^{-2\pi/\omega} \ll 1$, and for κ large, further simplification enables us to write the estimate as

$$\begin{aligned} c\xi &= 1 + \exp\left[\frac{2}{\omega} \left(\eta - \frac{\pi}{2} \right) \right] \sin\frac{2\xi}{\omega}, \\ c\eta &= \exp\left[\frac{2}{\omega} \left(\eta - \frac{\pi}{2} \right) \right] \cos\frac{2\xi}{\omega} \end{aligned} \tag{36}$$

(recall that $k=\xi+i\,\eta$).

When ω is small these expressions are useful when $\eta>\pi/2$. Then, with

$$\eta=\frac{\pi}{2}+\frac{\omega}{2}\,\eta_1(\omega)$$

and

$$\xi=\frac{\omega}{2}\,\xi_1(\omega).$$

the new functions assumed to be regular, we are led to

$$k_n=\omega[n\pi-\xi_*]+i\left[\frac{\pi}{2}+\frac{\omega}{4}\log\left\{1+\left(\frac{\pi c}{2}\right)^2\right\}\right]+o(\omega),$$

where $(n\pi-\xi_*)=2\xi_1(0)$ is the solution to

$$\tan\{2\xi_1(0)\}=-\frac{2}{\pi c},$$

and $n=1,2,...$ is not too large. This pattern of zeros, differing little in their imaginary parts, and marching into a point on the imaginary axis, is roughly (''semiquantitatively'') correct. The numerical values it yields are helpful, even though the true point of accumulation is $k=i$ rather than $k=i(\pi/2)$. Of course, the asymptotic expansion fails on the imaginary axis. There, and in an unknown strip containing it, we return to the expansion used in connection with Eq. (27) to obtain

$$\mathcal{K}(k)=\langle a|\,\frac{1}{\mathcal{O}}\,|a\rangle=\frac{1}{\sqrt{k^2+1}}\left[1-\frac{1}{2}\left(\frac{\omega}{2}\right)^2 k^2\frac{k^2-4}{(k^2+1)^3}+\cdots\right], \tag{37}$$

a complicated series which exhibits clearly the branch-point singularity and omits exponentially small terms (in ω). Before Eq. (37) is used to estimate zeros computation of the winding-number suggests that if we consider a small circular region about $k=i$, the number of zeros (poles) present in the region increases without limit as $\omega\to 0$. Analysis of the series suggests that the zeros do not follow distinct, ray-like paths as they fall into the (nascent) branch point. Rather, their paths merge. For example the first few terms of Eq. (37) yield a pair of roots and a merged path described by

$$k-i\approx\alpha\omega^{2/3}\exp\left(\frac{\pi}{6}i\right)\left[1\mp\frac{1}{3}\sqrt{2\alpha}\;\omega^{1/3}\exp\left(\frac{\pi}{3}i\right)\right], \tag{38}$$

$$\alpha=\frac{1}{4}(5)^{1/3}$$

in the first quadrant. The dependence upon $\omega^{2/3}$ is borne out to a fraction of a percent by numerical calculation, and the $\pi/6$, which characterizes the asymptote, appears to be correct, but the numerical coefficients need improvement. Overall the dependence upon ω is quite singular, for we have omitted exponentially singular factors. See Fig. 2.

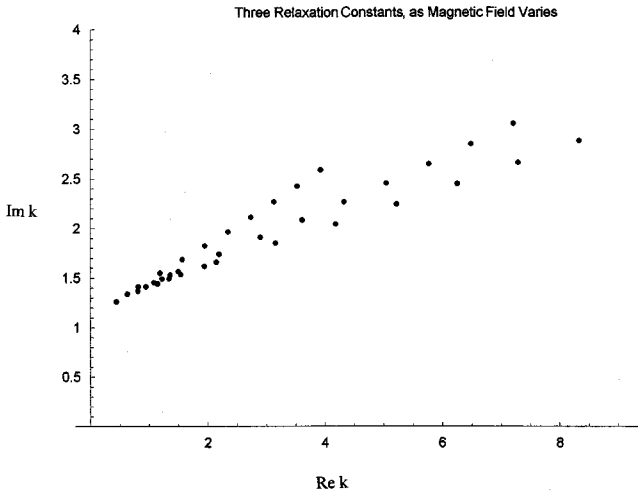

FIG. 2. Three zeros (poles) and their "motion" in the k plane as the magnetic field (ω) is altered. $\omega\to 0$ brings them to $k=i$.

C. Densities and currents

The currents $\mathcal{J}_{x,y}(k)$ may be obtained from the kernel via Eqs. (6) and (7) or directly, from

$$\frac{1}{\sqrt{2\pi}}\langle j_{\pm}|\frac{1}{\mathcal{O}}|a\rangle=\int_0^{\infty}\mathrm{d}t\,e^{-t}\int_0^{2\pi}\frac{\mathrm{d}\phi}{2\pi}e^{\pm i\phi}e^{i\kappa[\sin\phi-\sin(\phi+\omega t)]},$$

which yields, for $|Q_1\rangle$ (unit source),

$$\begin{aligned} i\mathcal{J}_x(k)&=\frac{1}{\mathcal{D}(k,c)}\int_0^{\infty}\mathrm{d}t\,e^{-t}\cos\frac{\omega t}{2}J_1\left(2\kappa\sin\frac{\omega t}{2}\right),\\ -i\mathcal{J}_y(k)&=\frac{1}{\mathcal{D}(k,c)}\int_0^{\infty}\mathrm{d}t\,e^{-t}\sin\frac{\omega t}{2}J_1\left(2\kappa\sin\frac{\omega t}{2}\right), \end{aligned} \tag{39}$$

as symmetric alternatives to Eqs. (6) and (7). Also, there is Eq. (17),

$$n(k)=\frac{1}{\mathcal{D}(k,c)}\int_0^{\infty}\mathrm{d}t\,e^{-t}J_0\left(2\frac{k}{\omega}\sin\frac{\omega t}{2}\right).$$

Equations (6) and (7) follow easily from Eq. (39) by integration by parts.

Since $\mathcal{D}(k,c)$ is even in k, we conclude that the components of current change sign when x is replaced by $-x$. Since $\mathcal{D}(k,c)$ diminishes with increasing k [see Eq. (34)], the behavior of density and current near the source is linked to the behavior of the integrals in Eq. (39). These, which describe the uncollided particles, may be inverted and reduced to

$$\begin{aligned} \mathcal{J}_{0x}(x)&=\frac{1}{\pi}\frac{\cos\phi_*(x)}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\phi_*(x)}\mathrm{d}\phi\,\sinh\left(\frac{2\phi}{\omega}\right)\frac{\tan\phi}{\sqrt{\cos^2\phi-\cos^2\phi_*(x)}}\\ &=\tfrac{1}{2}-(1-c)x\;n_0(x)+\cdots, \end{aligned} \tag{40}$$

$$\mathcal{J}_{0y}(x)=-\frac{1}{\pi}\frac{\cos\phi_*(x)}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\phi_*(x)}d\phi\frac{\cosh\left(\frac{2\phi}{\omega}\right)}{\sqrt{\cos^2\phi-\cos^2\phi_*(x)}}$$

$$=-\frac{\omega}{2}x\,n_0(x) \tag{41}$$

near the source-plane. For the behavior (''asymptotic'') far from the plane, we turn to inversion by contour integration to get

$$\mathcal{J}_y(x)=-\frac{\omega}{2c}\sum_n e^{ik_nx},$$

$$\mathcal{J}_x(x)=-\left(\frac{1-c}{c}\right)\sum_n\frac{1}{k_nD_n}e^{ik_nx}, \tag{42}$$

$$n(x)=\frac{i}{c}\sum_n\frac{1}{D_n}e^{ik_nx},$$

with $D_n\equiv(\partial/\partial k)D(k_n,c)$. Though the summation is over all zeros in the upper half-plane, we are most interested in the contribution from the dominant zero. Note that the equation of continuity is satisfied, ''mode by mode,'' and observe the strangely simple expression for $\mathcal{J}_y(x)$, as well as the singular behavior at $x=0$.

The transverse current, $\mathcal{J}_y(x)$, which is zero at the source plane, grows as one proceeds away. The ratio $\mathcal{J}_y(x)/\mathcal{J}_x(x)$ is then of some interest. The ratio assumes the value $\frac{1}{2}[k_0D_0/(1-c)]\omega$ asymptotically. One may compute the quantity easily in two limiting cases. In the first, very weak capture, $c\gg1-c$, the ratio is simply $(-\omega)$. In the second, very high frequency, $\omega\gg1$ [see Eqs. (16) and (31)] the ratio is $(-\omega\mathcal{F}(c))$, where

$$\mathcal{F}(c)=\frac{\sqrt{c}}{1-c}\kappa_0J_1(\kappa_0),\quad J_0(\kappa_0)=\frac{1}{\sqrt{c}}. \tag{43}$$

Diffusion: $(k_0=i\eta_0=\omega\kappa_0)$. The question of diffusion and diffusion constant may be viewed in two ways. One can note that far from the source the density follows $n_{xx}+k_0^2n=0$, an equation suggesting steady-state diffusion with diffusion coefficient

$$\mathbb{D}_{xx}=\frac{(1-c)}{\eta_0^2}.$$

More generally,

$$\mathbb{D}_{xx}=\mathbb{D}_{yy}=\frac{(1-c)}{\eta_0^2},\quad \mathbb{D}_{yx}=-\mathbb{D}_{xy}=\frac{\omega}{2k_0}\frac{\partial}{\partial k}\mathcal{D}(k,\omega)|_{k_0}, \tag{44}$$

the tensor components depending upon field strength and capture. This view is surely more helpful to the experimenter than is the traditional attitude that ''Fick's law'' holds throughout, that there is everywhere a proportionality between density gradient and current. In fact, the law holds only when spatial variations are so gentle (''long-ranged'') that only the lowest powers in an expansion in k need be retained. Then, Eq. (16) leads to

$$\begin{pmatrix} \mathcal{J}_x \\ \mathcal{J}_y \end{pmatrix} = -\frac{1}{2}(ik)\frac{1}{1-c}\frac{1}{1+\omega^2}\begin{pmatrix} 1 \\ -\omega \end{pmatrix}, \tag{45}$$

describing ''classical'' anisotropic diffusion, with diffusion tensor

$$\mathbb{D}_{ij} = \frac{1}{2}\frac{1}{1+\omega^2}\begin{pmatrix} 1 & \omega \\ -\omega & 1 \end{pmatrix}. \tag{46}$$

This simple picture, found in most textbooks, displays a ''normal'' diffusion, inhibited by the magnetic field, and transverse diffusion, induced by the field. The tensor multiplication may also be written

$$\mathbb{D}\cdot\nabla n = \frac{1}{2}\frac{1}{1+\omega^2}[1-\omega\hat{z}\times]\nabla n.$$

The two treatments differ little when capture is almost negligible and k_0 is small. The case of large field (''high frequency'') is accessible through Eqs. (16) and (31) when Eq. (44) yields

$$\mathbb{D}_{yx} = -\mathbb{D}_{xy} = -\frac{1}{\omega\sqrt{c}}\frac{J_1(\kappa_0)}{\kappa_0}.$$

Thus, for fixed capture, the transverse diffusion is—again—inhibited by the magnetic field when the field is large. D_{yx} rises, proportionally to ω when ω is small, reaches some peak value, then decreases, as $1/\omega$.

D. The distribution in angle

The angular distribution in the dominant, asymptotic mode is of particular interest. In the notation of Eq. (44) that quantity, $F_\infty(x,\phi)$, is

$$F_\infty(x,\phi) = \frac{i}{D_0}e^{ik_0x}\Phi_0(\phi)$$

with

$$\Phi_0(\phi) = \frac{1}{2\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\exp\left(i\left(\frac{k_0}{\omega}\right)[\sin\phi - \sin(\phi+\omega t)]\right) \tag{47}$$

for unit source. The transient modes have a similar appearance. One of the many possible rearrangements brings us to the convenient form,

$$\Phi_0(\phi) = \frac{1}{2\pi\omega}\frac{1}{1-e^{-2\pi/\omega}}e^{(1/\omega)\mathcal{F}(\phi)}\int_\phi^{\phi+2\pi}\mathrm{d}\alpha\, e^{-(1/\omega)\mathcal{F}(\alpha)} \tag{48}$$

with $\mathcal{F}(\phi) = \phi - \eta_0\sin\phi$ $[k_0 = i\eta_0(\omega,c)]$. And there is always the differential equation

$$-\omega\frac{\partial}{\partial\phi}z(\phi) + (1-\eta_0\cos\phi)z(\phi) = \frac{1}{2\pi}$$

which, when solved (numerically) under the condition that $z(\phi) = z(\phi+2\pi)$, yields a function proportional to $\Phi_0(\phi)$.

Once again, the question of $\eta_0 < 1$ or $\eta_0 > 1$ enters. In the former case $\mathcal{F}(\phi)$ is positive and increasing, in the latter, not so, and one encounters more dramatic behavior. Analytical information

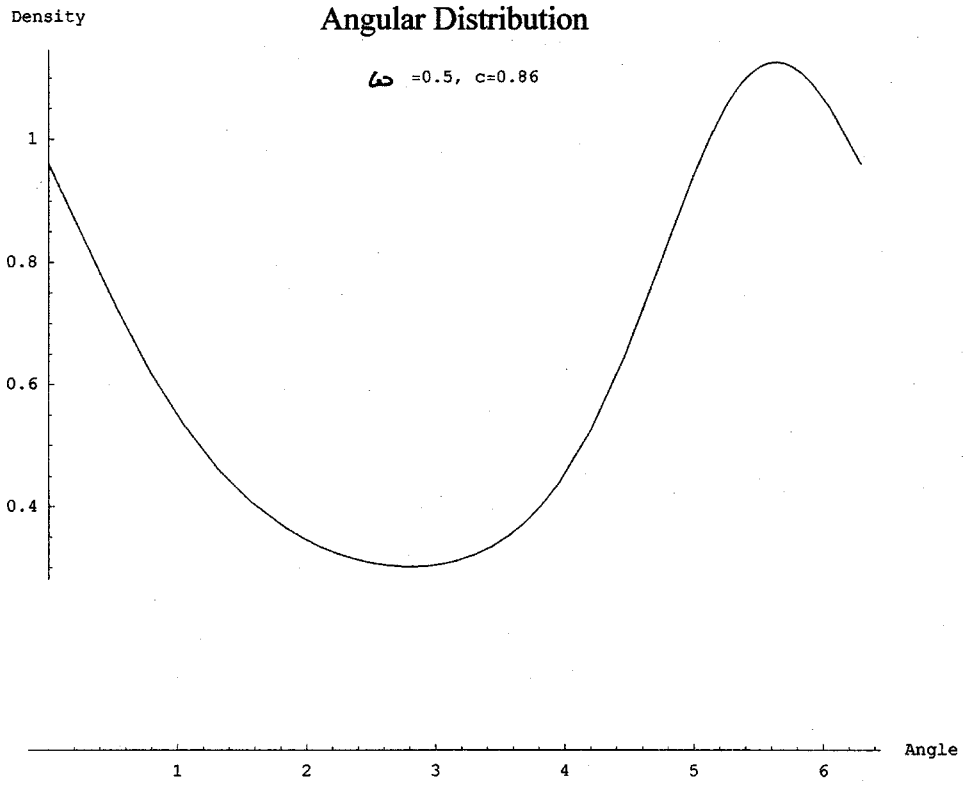

FIG. 3. Asymptotic angular distribution (2D) for $\omega=0.5$, $c=0.86$. Arbitrary normalization. Capture moderate, field strong.

is available when ω is small, when familiar ideas from ''asymptotics'' enter.[12] For example, as $\omega\to 0$ the dominant contribution from the integral in Eq. (48) comes from the interval where $\mathcal{F}(\alpha)$ is minimum. In the case $\eta_0<1$ the minimum is at $\alpha=\phi$ and expansion about that (edge-) value yields

$$\Phi_0(\phi)=\frac{1}{2\pi}\,\frac{1}{(1-\eta_0\cos\phi)}\left[1-\omega\,\frac{\eta_0\sin\phi}{(1-\eta_0\cos\phi)^2}+\cdots\right],$$

precisely the ''outer expansion'' of the solution to the differential equation. Since the outer solution satisfies the boundary condition, there is no need for a boundary layer. This simple expression displays an interesting feature of the angular distribution—a small peak centered at a small angle. The disturbance, vanishing with ω, generates the transverse current.

When $\eta_0>1$ the situation is different. $\mathcal{F}(\alpha)$ is oscillatory, and has a single minimum, at $0\leqslant\phi_*<\pi/2$ where $\cos\phi_*=(1/\eta_0)$. In a subinterval of $(-\pi<\phi\leqslant\pi)$, namely, $(\phi_{**}<0<\phi<\phi_*)$, where $\mathcal{F}(\phi_{**})=\mathcal{F}(\phi_*)$, the minimum lies inside the integration of Eq. (48) and produces boundary layer behavior. $\Phi(\phi)$ rises rapidly, proportional to $\exp[(1/\omega)(\mathcal{F}(\phi)-\mathcal{F}(\phi_*))]$ then falls and passes to the nonexponential ''outer''-behavior for the remainder of the interval. These features are displayed in Figs. 3 and 4. Clearly, these angular distributions are not represented well by an expansion-in-angle that is near-isotropic. The distributions associated with $\eta_0>1$ become quite singular in the limit of vanishing field—the continuum limit.

E. Transport in three dimensions (3D)

Since the key features are captured in the 2D case, we treat 3D briefly. We remain with plane symmetry. Then, the modifications are relatively minor. It is convenient to use two sets of angle variables. In one, the x axis is the polar axis and the polar and azimuthal angles are denoted (θ,ψ);

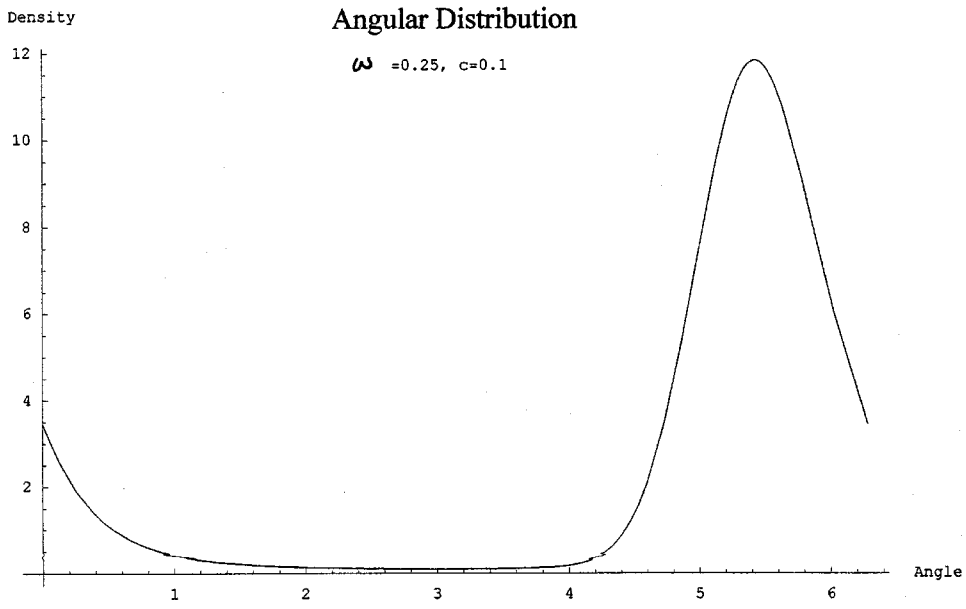

FIG. 4. Asymptotic angular distribution (2D) for $\omega=0.25$, $c=0.1$. Arbitrary normalization. Capture very strong, field moderate.

in the other, the z axis, to which the field is parallel, is the polar axis and the angles are (χ,ϕ). The streaming portion of the transport equation is altered only in that "$\mu=\cos\phi$" is replaced by $\mu=\sin\chi\cos\phi$. Since χ enters the equation only "parametrically," it may be absorbed through much of the subsequent calculation by simply replacing the Fourier transform variable "k" by $k_\perp=k\sin\chi$. The density is now a function of two angles, (χ,ϕ). The in-scattering term is altered through the replacement,

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi \rightarrow \frac{1}{4\pi}\int d\Omega = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} d\chi \sin\chi.$$

The vector space is now a space of functions defined on the unit sphere, and we may use (θ,ψ) or (χ,ϕ) in place of the variable, ϕ. The inner product is now

$$\langle g|f\rangle \equiv \int d\Omega\, g^*(\Omega) f(\Omega) = \langle f|g\rangle^*$$

and the ubiquitous

$$\langle \phi|a\rangle = \frac{1}{\sqrt{2\pi}}, \quad \langle a|f\rangle = \int_0^{2\pi} d\phi \frac{1}{\sqrt{2\pi}} f(\phi)$$

become

$$\langle \Omega|a\rangle = \frac{1}{\sqrt{4\pi}}, \quad \langle a|f\rangle = \int d\Omega \frac{1}{\sqrt{4\pi}} f(\Omega).$$

With these reinterpretations, most of the equations of the 2D case may be carried over, easily, to 3D, turning Bessel functions into spherical Bessel functions. We begin with the kernel,

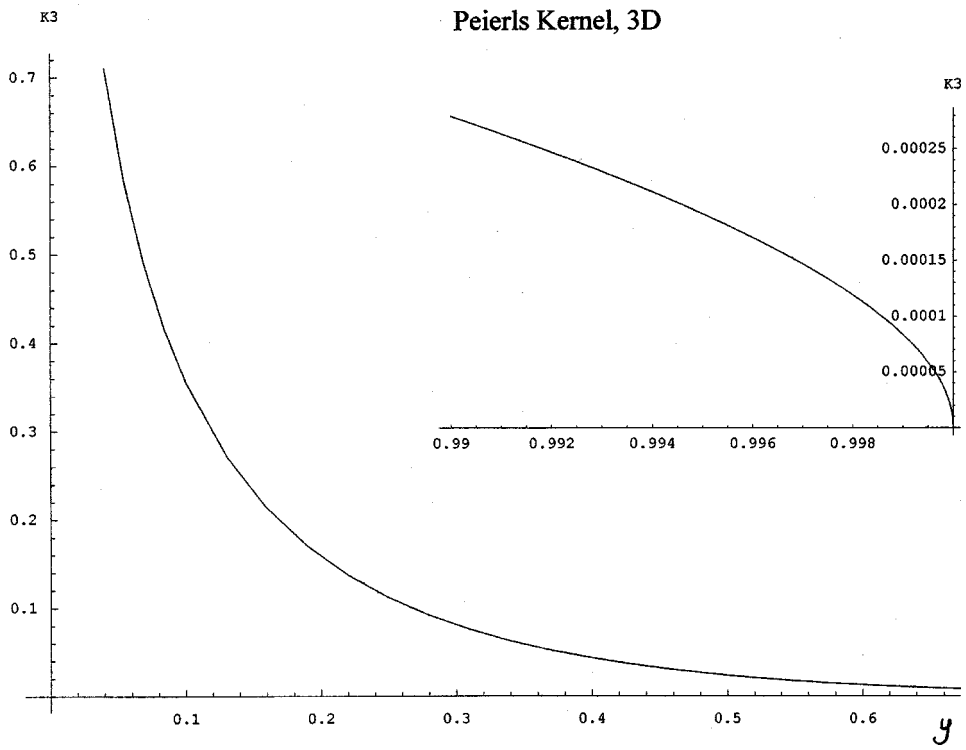

FIG. 5. $\mathcal{K}_3$, the 3D kernel (Peierls) for the integral equation for density, $n(x)$, with $\omega=0.5$, shown as a function of its argument, $y=\omega|x|/2$. The kernel is zero when $y\geqslant 1$.

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle \to \frac{1}{4\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\int \mathrm{d}\Omega\, e^{i\kappa_\perp[\sin\phi-\sin(\phi+\omega t)]}$$
$$=\int_0^\infty \mathrm{d}t\, e^{-t}\frac{1}{2}\int_0^\pi \mathrm{d}\chi \sin\chi \;\; J_0\left(2\kappa\sin\frac{\omega t}{2}\sin\chi\right). \tag{49}$$

Here, and in the discussion of currents, the relation

$$\int_0^{\pi/2}\mathrm{d}\chi \sin^{n+1}\chi \;\; J_n(z\sin\chi)=j_n(z),$$

between ordinary and spherical Bessel functions is useful. Then,

$$\mathcal{K}_3(k,\omega)\equiv\langle a|\frac{1}{\mathcal{O}}|a\rangle=\int_0^\infty \mathrm{d}t\, e^{-t}j_0\left(2\kappa\sin\frac{\omega t}{2}\right)=\frac{2}{\omega}\frac{1}{\sinh\left(\frac{\pi}{\omega}\right)}\int_0^{\pi/2}\mathrm{d}\phi\cosh\left(\frac{2\phi}{\omega}\right)j_0\left(2\frac{k}{\omega}\cos\phi\right), \tag{50}$$

with $j_0(z)=\sin z/z$.

Upon expansion to produce a power series in k, one finds

$$\mathcal{K}_3(k,\omega)=\left[1+\sum_{m=1}^{\infty}\frac{(-k^2)^m}{2m+1}\prod_{r=1}^{m}\frac{1}{1+r^2\omega^2}\right]. \tag{51}$$

Setting $\omega=0$ gives the familiar logarithm of the field-free case, and expanding for small ω in the manner given earlier [e.g., Eqs. (27) and (37)] yields the singular and asymptotic sequence

$$\mathcal{K}_3(k,\omega)=\frac{1}{2ik}\log\frac{1+ik}{1-ik}+\frac{1}{3}\omega^2\frac{k^2}{(k^2+1)^3}+\cdots+\text{exponentially small terms.} \tag{52}$$

The regime $\omega\gg 1$ is dealt with best via the series, Eq. (49), giving

$$\mathcal{K}_3(k,\omega)\asymp\frac{\omega}{2k}\int_0^{2k/\omega}\mathrm{d}z\,J_0(z). \tag{53}$$

These expressions are helpful in determining the zeros of $\mathcal{D}_3(k,\omega,c)$, which, like its predecessor, is entire-in-k. The behavior of these zeros is quite similar to their 2D counterparts. Turning to the picture in x coordinates, we note that the Peierls kernel may be obtained by Fourier-inverting Eq. (49) to get a pretty, ''3-Sine'' formula for the even function,

$$\mathcal{K}_3(x-x',\omega)=\frac{1}{1-e^{-4\pi/\omega}}\int_0^{2\pi}\mathrm{d}\theta\int\mathrm{d}\Omega\,e^{-2\theta/\omega}\delta\left(\frac{\omega}{2}(x-x')-\sin\theta\sin\phi\sin\chi\right). \tag{54}$$

Comments made earlier about its compact support continue to hold. On the other hand, we may Fourier-invert Eq. (50) to get quite a different compact form,

$$\mathcal{K}_3(x,\omega)=\frac{1}{2\sinh\left(\dfrac{\pi}{\omega}\right)}\int_0^{\phi_*(\omega x)}\frac{\mathrm{d}\phi}{\cos\phi}\cosh\frac{2\phi}{\omega} \tag{55}$$

($\cos\phi_*=(\omega/2)x$, and $|(\omega/2)x|<1$). In fact, $\mathcal{K}_3$ may be shown to vanish with vertical tangent. (See Fig. 5.) That this rather peculiar expression does become the familiar exponential integral when $\omega\to 0$ may be seen by setting

$$\phi=\left(\frac{\pi}{2}-\psi\right),$$

expanding the cosh, and passing to the limit.

Currents. We have, generally,

$$\mathcal{J}_{x,y,z}(k)\equiv\mathcal{J}(k)=\langle j|\frac{1}{\mathcal{O}}|Q\rangle+\frac{c}{\mathcal{D}(k,c)}\langle j|\frac{1}{\mathcal{O}}|a\rangle\langle a|\frac{1}{\mathcal{O}}|Q\rangle. \tag{56}$$

When the source is isotropic, and normalized to $\sqrt{4\pi}$,

$$\mathcal{J}(k)=\frac{1}{\mathcal{D}(k,c)}\langle j|\frac{1}{\mathcal{O}}|a\rangle, \tag{57}$$

and we discuss the numerator of this expression,

$$\frac{1}{\sqrt{4\pi}}\langle j_{x,y}|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{4\pi}\int_0^\infty\mathrm{d}t\,e^{-t}\int\mathrm{d}\Omega\sin\chi[\cos\phi,\sin\phi]e^{i\kappa_\perp[\sin\phi-\sin(\phi+\omega t)]}, \tag{58}$$

$$\frac{1}{\sqrt{4\pi}}\langle j_z|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{4\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\int \mathrm{d}\Omega\cos\chi e^{i\kappa_\perp[\sin\phi-\sin(\phi+\omega t)]}$$

$$=\int_0^\infty \mathrm{d}t\, e^{-t}\frac{1}{2}\int_0^\pi \mathrm{d}\chi\sin\chi\cos\chi J_0\left(2\kappa\sin\chi\sin\frac{\omega t}{2}\right)=0,\quad \text{by symmetry.} \tag{59}$$

Thus, quite generally,

$$\mathcal{J}_z(k)=\langle j_z|\frac{1}{\mathcal{O}}|Q\rangle,$$

an expression which is, at first sight, puzzling, for the current appears to be independent of capture. A moment's thought convinces one of its correctness, and that J_z is, in any case, trivial. We merely note that with isotropic scattering, a beam becomes distributed isotropically at the first collision. After that collision, only a density gradient will drive a current. But in our problem, there are no gradients in the z direction; J_z exists only in the interval from birth to first collision when the value of "c" is irrelevant. This argument holds for particles immersed in an arbitrary external field that is independent of z. The z current is carried only by uncollided particles. Adding a bit of anisotropy to the scattering changes the result significantly.

The current components, $\mathcal{J}_{x,y}(k)$, are simply the weighted χ average of their counterparts in two dimensions, Eq. (39). The connection between ordinary and spherical Bessel functions then gives the concise result,

$$i\mathcal{J}_x(k)=\frac{1}{\mathcal{D}_3(k,c)}\int_0^\infty \mathrm{d}t\, e^{-t}\cos\frac{\omega t}{2}\; j_1\left(2\kappa\sin\frac{\omega t}{2}\right),$$

$$-i\mathcal{J}_y(k)=\frac{1}{\mathcal{D}_3(k,c)}\int_0^\infty \mathrm{d}t\, e^{-t}\sin\frac{\omega t}{2}\; j_1\left(2\kappa\sin\frac{\omega t}{2}\right), \tag{60}$$

for currents in three dimensions.

Angular distributions. Expressions for the angular distribution associated with dominant and transient modes may be obtained easily. One simply replaces k_0 with $k_0\sin\chi$ in Eq. (47). The distributions are then symmetric with respect to the $(x-y)$ plane and fixing a value of χ is equivalent to selecting one of the 2D distributions we have described earlier. As χ decreases from its in-plane value of $\pi/2$, the effective η_0 diminishes and the corresponding distribution is smoother. Overall, angular distributions in 3D appear to be smoother than those in 2D.

One can proceed further with details of the 3D case, in a manner similar to that of 2D but it is clear that the 2D case displays almost everything that is interesting about the problem. The next step should be an attack upon the time-dependent problem, which is simple enough after Laplace-transform, but whose inversion is a complicated matter.

ACKNOWLEDGMENTS

The author is grateful for a friendly and helpful correspondence with Professor R. E Robson and Professor K. Kumar, during the early phase of this research.

APPENDIX

An alternative, easier way to evaluate the key quantity,

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{2\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\int_0^{2\pi}\mathrm{d}\phi\, e^{i\kappa[\sin\phi-\sin(\phi+\omega t)]}$$

is to notice that $[\sin\phi-\sin(\phi+\omega t)]=-2\sin(\omega t/2)\cos(\phi+\omega t/2)$, and that the replacement of $(\phi+\omega t/2)$ by ϕ does not alter the value of the integral. The expression

$$\langle a|\frac{1}{\mathcal{O}}|a\rangle=\int_0^\infty \mathrm{d}t\, e^{-t}J_0\left(2\kappa\sin\frac{\omega t}{2}\right)$$

follows at once. In fact, evaluation of the matrix element in the expression for the current induced by an isotropic source

$$J_{x,y}(k)=\frac{1}{\mathcal{D}(k)}\langle j_{x,y}|\frac{1}{\mathcal{O}}|a\rangle,$$

$$\frac{1}{\sqrt{2\pi}}\langle j_{x,y}|\frac{1}{\mathcal{O}}|a\rangle=\frac{1}{2\pi}\int_0^\infty \mathrm{d}t\, e^{-t}\int_0^{2\pi}\mathrm{d}\phi[\cos\phi,\sin\phi]e^{i\kappa[\sin\phi-\sin(\phi+\omega t)]}$$

is made easy by the same approach. The change of variable $(\phi+\omega t/2)\rightarrow\phi$ and integration by parts produces the results noted earlier.

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The three-body problem with an inverse square law potential

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(Received 2 April 2003; accepted 14 April 2003)

We study the motion of three masses in a plane interacting with a central potential proportional to $1/r^2$ using the coordinates introduced recently by Piña. We show that this problem with four degrees of freedom (three angles and a distance related to the inertia moment of the system in these coordinates) is partially separable, and can be reduced to a problem with two degrees of freedom (two angles) with a new constant of motion. We find a symmetry of reflection (an involution) for this system and we use the symmetry lines to find periodic orbits in the angular coordinates. These orbits will not be periodic in general on the whole phase space because the coordinate of distance type grows as t when $t\to\infty$ and it is unbounded. However, if the inertia moment of the system remains constant, they will be periodic on the whole phase space. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1597948]

I. INTRODUCTION

We consider three masses $m_1 \geqslant m_2 \geqslant m_3$ moving in a plane and interacting with a central potential k/r^2, k constant. Poincaré studied this problem at the end of the 19th century[1] and he showed by the minimum action principle that there exist periodic orbits for this problem. Sbano[2] consider Newtonian-type potentials k/r^n when the total angular momentum vanishes, and he proves the existence of a periodic orbit. We use the coordinates introduced in Ref. 3 in the way of Ref. 4 to show that for a potential k/r^2 there is an extra constant of motion that allows us to separate the motion of the total inertia moment. We then introduce appropriate dimensionless variables in order to reduce the number of parameters, and we give a global description of the total inertia moment variable. We then reduce the problem to an equivalent two degrees of freedom one with a constant of motion, and we obtain a symmetry of involution. By means of the symmetry lines of the problem we find explicitly periodic orbits.

The main idea introducing the new coordinates is to choose the origin of coordinates at the center of mass, and to select the frame of principal axes of the three particles. Since the motion is in a plane, it is sufficient to take into account only one rotation angle ψ (instead of three Euler angles) in order to transform from the principal axes frame to the inertial one. Two distances R_1 and R_2 (associated with the two independent inertia moments), and an extra angle σ are defined in these coordinates. In the Appendix we show explicitly the change of coordinates from the six coordinates (x_i, y_i), $i=1,2,3$ to the four generalized coordinates ψ, R_1, R_2, σ and the relation of the last three with the distances between particles.

II. EQUATIONS OF MOTION

The Hamiltonian $\mathcal{H}=T+V$ of these problem results in[5]

$$\mathcal{H}=\frac{1}{2\mu}\left(P_1^2+P_2^2+\frac{(R_1^2+R_2^2)(P_\sigma^2+P_\psi^2)+4R_1R_2P_\sigma P_\psi}{(R_1^2-R_2^2)^2}\right)-\frac{k}{2}\left(\frac{1}{r_{23}^2}+\frac{1}{r_{13}^2}+\frac{1}{r_{12}^2}\right),$$

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where $\mu=\sqrt{(m_1 m_2 m_3)/(m_1+m_2+m_3)}$, P_i, $i=1,2,\sigma,\psi$ are the canonical momenta, r_{jl}, $j,l=1,2,3$ are the distances between m_j and m_l, k is a constant and the two independent inertia moments are related with R_1 and R_2 by $I_1=\mu R_1^2$ and $I_2=\mu R_2^2$. Note that if $R_1=R_2$, the Hamiltonian is not well defined, because the change of variables is not well defined there, then we will avoid those values.

It is convenient to change the variables R_1 and R_2 for the polar variables R, θ,

$$R_1=R\cos\theta,$$

$$R_2=R\sin\theta$$

with $R\in\mathbb{R}^+$, $\theta\in\mathbb{S}^1$. Now $\mu R^2=I$ is the inertia moment of the system, $I=\Sigma_{i=1}^3 m_i\mathbf{r}_i^2$. The Hamiltonian goes over to

$$\mathcal{H}=\frac{1}{2\mu}\left(P_R^2+\frac{P_\theta^2}{R^2}+\frac{(P_\sigma^2+P_\psi^2)+2\sin 2\theta P_\sigma P_\psi}{R^2\cos^2 2\theta}\right)-\frac{k}{2}\left(\frac{1}{r_{23}^2}+\frac{1}{r_{13}^2}+\frac{1}{r_{12}^2}\right),$$

where the distances between particles r_{jl} become

$$\begin{pmatrix} r_{23}^2 \\ r_{13}^2 \\ r_{12}^2 \end{pmatrix}=\mathbf{B}\,R^2\begin{pmatrix} \cos^2\theta\sin^2\sigma+\sin^2\theta\cos^2\sigma \\ \cos^2\theta\cos^2\sigma+\sin^2\theta\sin^2\sigma \\ -\cos 2\theta\sin 2\sigma \end{pmatrix}, \tag{1}$$

with $\mathbf{B}$ being the constant dimensionless matrix, depending only on the masses, given in the appendix, Eq. (A8). If we define the dimensionless distances $s_{ij}=r_{ij}/R$, divide (1) by R^2 and simplify, we obtain

$$\begin{pmatrix} s_{23}^2 \\ s_{13}^2 \\ s_{12}^2 \end{pmatrix}=\mathbf{B}\begin{pmatrix} (1-\cos 2\sigma\cos 2\theta)/2 \\ (1+\cos 2\sigma\cos 2\theta)/2 \\ -\sin 2\sigma\cos 2\theta \end{pmatrix}, \tag{2}$$

and then the Hamiltonian results in

$$\mathcal{H}=\frac{P_R^2}{2\mu}+\frac{1}{2\mu R^2}\left(P_\theta^2+\frac{(P_\sigma^2+P_\psi^2)+2\sin 2\theta P_\sigma P_\psi}{\cos^2 2\theta}-\mu k\left[\frac{1}{s_{23}^2}+\frac{1}{s_{13}^2}+\frac{1}{s_{12}^2}\right]\right). \tag{3}$$

The equations of motion derived from this Hamiltonian function have three constants of motion: the energy with the value E,

$$\mathcal{H}=T+V=E, \tag{4}$$

the angular momentum with the value p_ψ,

$$P_\psi=\mu R^2[\dot{\psi}-\sin 2\theta\dot{\sigma}]=p_\psi, \tag{5}$$

and a third constant,

$$\mathcal{K}=\frac{P_\theta^2}{2}+\frac{P_\sigma^2+P_\psi^2+2\sin 2\theta P_\sigma P_\psi}{2\cos^2 2\theta}-\frac{\mu k}{2}\left[\frac{1}{s_{23}^2}+\frac{1}{s_{13}^2}+\frac{1}{s_{12}^2}\right]=K. \tag{6}$$

III. SEPARATION OF VARIABLES

The Hamiltonian (3) is separable in t, ψ, and R variables, with constants of separation $\mathcal{H}=E$, $P_\psi=p_\psi$ and $\mathcal{K}=K$, respectively. The Hamiltonian reduces to

$$\mathcal{H}=\frac{P_R^2}{2\mu}+\frac{\mathcal{K}}{\mu R^2}, \tag{7}$$

then the $R(t)$ variable can be solved independently of the other ones by using the first integrals $\mathcal{H}=E$ and $\mathcal{K}=K$ with the solution

$$\mu R^2=2Et^2+At+B, \tag{8}$$

A, B constants of integration.

For the angular variables the Hamilton equations are given by

$$-\frac{\partial\mathcal{H}}{\partial\beta}=-\frac{1}{\mu R^2}\frac{\partial\mathcal{K}}{\partial\beta}=\frac{dP_\beta}{dt},$$

$$\frac{\partial\mathcal{H}}{\partial P_\beta}=\frac{1}{\mu R^2}\frac{\partial\mathcal{K}}{\partial P_\beta}=\frac{d\beta}{dt}$$

with $\beta=\theta,\sigma,\psi$. These equations suggest that we introduce a new time rescaled by R^{-2} to obtain Hamilton equations, with $\mathcal{K}$ the ''Hamiltonian'' of a reduced system without the R variable. Before doing this, we introduce dimensionless variables in order to reduce the number of parameters.

IV. DIMENSIONLESS VARIABLES

We simplify the study of this problem introducing dimensionless variables denoted by a prime. This reduces the study to a few cases depending on whether E or K are equal or different from zero.

We first define

$$\mathcal{K}'=\frac{\mathcal{K}}{\mu k},\quad P_i'=\frac{P_i}{\sqrt{\mu k}},\quad i=\theta,\sigma,\psi,$$

where we are assuming an attractive potential, i.e., $k>0$, but this is not restrictive. Equation (6) becomes

$$\mathcal{K}'=\frac{P_\theta'^2}{2}+\frac{P_\sigma'^2+P_\psi'^2+2\sin 2\theta P_\sigma' P_\psi'}{2\cos^2 2\theta}+\mathcal{V}(\theta,\sigma), \tag{9}$$

where the ''potential'' $\mathcal{V}$ is

$$\mathcal{V}(\theta,\sigma)=-\frac{1}{2}\left[\frac{1}{s_{23}^2}+\frac{1}{s_{13}^2}+\frac{1}{s_{12}^2}\right],$$

and the dimensionless square distances are given by (2). Now we consider the energy equation (7) with two cases.

(1) $E\neq 0$. Now let

$$\mathcal{H}'=\frac{\mathcal{H}}{|E|},\quad P_R'=\frac{P_R}{\sqrt{\mu|E|}},\quad R'=R\sqrt{\frac{|E|}{k}},\quad t'=t\frac{|E|}{\sqrt{\mu k}}, \tag{10}$$

be the dimensionless Hamiltonian, momentum, distance, and time, respectively. Then we have only two values for $\mathcal{H}'=\pm 1$, depending on whether E is positive or negative. The first integral of energy reduces to

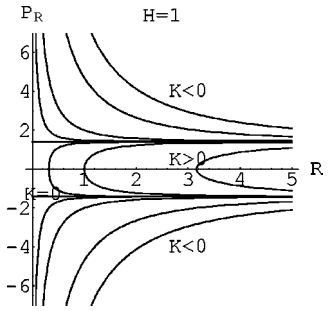

FIG. 1. Motion on the (R, P_R) plane for $\mathcal{H}=1$, $\mathcal{K}\in\mathbb{R}$.

$$\mathcal{H}'=\frac{P_R'^2}{2}+\frac{\mathcal{K}'}{R'^2}=\pm 1\,. \tag{11}$$

(2) $E=0$. We define $R_0=R(0)$ and

$$\mathcal{H}'=\frac{\mathcal{H}R_0^2}{k},\quad P_R'=\frac{P_R R_0}{\sqrt{\mu k}},\quad R'=\frac{R}{R_0},\quad t'=\frac{t}{R_0^2}\sqrt{\frac{k}{\mu}}. \tag{12}$$

Then the energy equation is the same as that in the $E\neq 0$ case but now it has the numerical value zero,

$$\mathcal{H}'=\frac{P_R'^2}{2}+\frac{\mathcal{K}'}{R'^2}=0\,, \tag{13}$$

and then

$$P_R'=\pm\frac{\sqrt{-2\mathcal{K}'}}{R'},$$

with $\mathcal{K}'\leqslant 0$.

In this way, we have to consider essentially three cases for the energy: $\mathcal{H}'=-1$, $\mathcal{H}'=0$ and $\mathcal{H}'=1$. From now on, we will work with the dimensionless variables but we drop the prime in order to make easier the notation.

V. SOLUTION OF THE *R* VARIABLE

As we have shown in Sec. IV, the dimensionless energy equation (11) or (13) gives the solution for the R variable

$$\mathcal{H}=\frac{P_R^2}{2}+\frac{\mathcal{K}}{R^2} \tag{14}$$

with $\mathcal{H}=\pm 1$ in case (1) and $\mathcal{H}=0$ in case (2). Solving for P_R^2 we have

$$\mathcal{H}R^2\geqslant\mathcal{K}$$

then the total inertia moment must be greater or equal to $\mathcal{K}/\mathcal{H}$. In Figs. 1, 2, and 3 we show the projection of the phase portrait on the (R, P_R) plane when $\mathcal{H}=1$, $\mathcal{H}=0$ and $\mathcal{H}=-1$, respectively. Now we consider these three values separately.

(a) $\mathcal{H}=1$. From Eq. (14), we see that $\mathcal{K}\in\mathbb{R}$. When $\mathcal{K}=0$, the solution has constant momentum $P_R=\pm\sqrt{2}$. The R variable comes from infinity, and then the system goes to total collision R

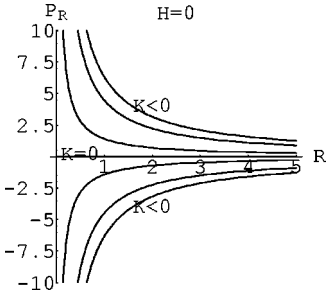

FIG. 2. Motion on the (R, P_R) plane for $\mathcal{H}=0$, $\mathcal{K}\leqslant 0$.

$=0$, or the system comes from total collision and then R escapes to infinity hyperbolically. Note that $R\to\infty$ means that at least two of the particles escape to infinity. This solution gives the asymptote that divides the other two cases $\mathcal{K}>0$ or $\mathcal{K}<0$. If $\mathcal{K}>0$, the inertia moment comes from infinity with $P_R<0$, reaches a minimum value at $R=\sqrt{K}$ when $P_R=0$, and then escapes to infinity with $P_R>0$ (hyperbolic solutions). If $\mathcal{K}<0$, then the system goes out from total collision and escapes to infinity with $P_R>0$, or comes from infinity and goes to total collision. See Fig. 1.

(b) $\mathcal{H}=0$. Then we have that $\mathcal{K}\leqslant 0$. If $\mathcal{K}=0$, all the solutions are equilibrium points. Then, if we find periodic solutions in the angular variables when $\mathcal{K}=0$, they will be periodic also in R if we put $\mathcal{H}=0$. If $\mathcal{K}<0$, the system goes out from total collision and escapes to infinity with $P_R=0$ (parabolic solutions), or comes from infinity and goes to total collision. See Fig. 2.

(c) $\mathcal{H}=-1$. Then $\mathcal{K}<0$ and all the solutions come from total collision, reach a maximum value of the inertia moment at $R=\sqrt{-K}$, and then return to total collision. See Fig. 3.

VI. THE ANGULAR MOTION

We have seen that the R variable can be separated and the study of this problem reduced to a few cases: (a) $\mathcal{H}=1$, $\mathcal{K}\in\mathbb{R}$; (b) $\mathcal{H}=0$, $\mathcal{K}\leqslant 0$; (c) $\mathcal{H}=-1$, $\mathcal{K}\in\mathbb{R}^-$ (remember we are using the dimensionless variables of Sec. IV dropping the primes). At any rate, the Hamilton equations for the angular variables result in

$$-\frac{\partial\mathcal{H}}{\partial\beta}=-\frac{1}{R^2}\frac{\partial\mathcal{K}}{\partial\beta}=\frac{dP_\beta}{dt}, \tag{15}$$

$$\frac{\partial\mathcal{H}}{\partial P_\beta}=\frac{1}{R^2}\frac{\partial\mathcal{K}}{\partial P_\beta}=\frac{d\beta}{dt}, \tag{16}$$

with $\beta=\theta,\sigma,\psi$. These equations suggest that we define a new (dimensionless) time

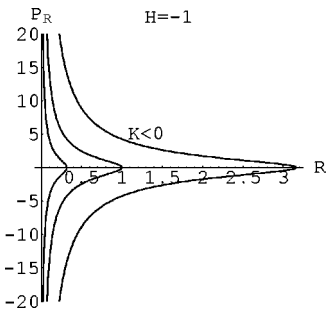

FIG. 3. Motion on the (R, P_R) plane for $\mathcal{H}=-1$, $\mathcal{K}<0$.

$$d\tau = \frac{dt}{R^2}$$

and consider $\mathcal{K}$ as a "Hamiltonian," with τ its canonical coordinate

$$\frac{dP_\beta}{d\tau} = -\frac{\partial \mathcal{K}}{\partial \beta},$$

$$\frac{d\beta}{d\tau} = \frac{\partial \mathcal{K}}{\partial P_\beta},$$

where $\beta = \theta, \sigma, \psi$.

As P_ψ is a first integral, we will assume it to be a constant parameter with value p_ψ in all the calculations. Coordinate ψ can be ignored until the other coordinates are known as functions of time, then the quadrature for ψ can be used to obtain the complete solution

$$\dot{\psi} = \frac{p_\psi + \sin 2\theta P_\sigma}{\mu R^2 \cos^2 2\theta}. \tag{17}$$

This quadrature reduces the number of variables from three to two. From now on, $P_\psi = p_\psi$ will be an extra constant parameter.

For θ and σ variables we obtain

$$\begin{aligned} \frac{dP_\theta}{d\tau} &= -\frac{2(P_\sigma^2 + p_\psi^2 + 2\sin 2\theta P_\sigma p_\psi)\tan 2\theta}{\cos^2 2\theta} - \frac{2P_\sigma p_\psi}{\cos 2\theta} - \frac{\partial \mathcal{V}}{\partial \theta}, \\ \frac{dP_\sigma}{d\tau} &= -\frac{\partial \mathcal{V}}{\partial \sigma}, \\ \frac{d\theta}{d\tau} &= P_\theta, \\ \frac{d\sigma}{d\tau} &= \frac{P_\sigma + \sin 2\theta p_\psi}{\cos^2 2\theta}. \end{aligned} \tag{18}$$

This Hamiltonian system is not defined at $\theta = \pm \pi/4, \pm 3\pi/4$, because the change of variables is not well defined there. Furthermore, the potential $\mathcal{V}(\theta, \sigma)$ is a function of 2θ and 2σ. Thus the dominium of σ and θ is $\sigma \in [0, \pi)$ and $\theta \in (-\pi/4, \pi/4) \cup (\pi/4, 3\pi/4)$.

We have reduced the original problem with four degrees of freedom and Hamiltonian (3) to a two degrees of freedom problem with Hamiltonian $\mathcal{K}$ and a parameter p_ψ.

VII. SYMMETRIES AND POINCARÉ MAPS

The Hamiltonian system obtained by (3) is invariant under the involution

$$(R, \theta, \sigma, \psi, P_R, P_\theta, P_\sigma, p_\psi, t) \to (R, -\theta, \sigma, -\psi, -P_R, P_\theta, -P_\sigma, p_\psi, -t).$$

Upon restricting it to two degrees of freedom and calling it I_0, we get

$$I_0(\theta, \sigma, P_\theta, P_\sigma, \tau) = (-\theta, \sigma, P_\theta, -P_\sigma, -\tau).$$

Let $\Pi = \{(\theta, \sigma) : \theta \in (-\pi/4, \pi/4) \cup (\pi/4, 3\pi/4)$ and $\sigma \in [0, \pi)\}$ and $\Omega = \{(\theta, \sigma, P_\theta, P_\sigma) : (\theta, \sigma) \in \Pi, (P_\theta, P_\sigma) \in \mathbb{R}^2\}$ be the configuration and phase space in the reduced problem, respectively. Let $\mathcal{E} = \{x \in \Omega : \mathcal{K} = K\}$, $K \in \mathbb{R}$ be the level of constant "energy." We introduce a Poincaré section $\Sigma = \{x \in \mathcal{E} : \theta = 0\}$ and the Poincaré map $T : \Sigma \to \Sigma$ induced by the Hamiltonian flow. We observe

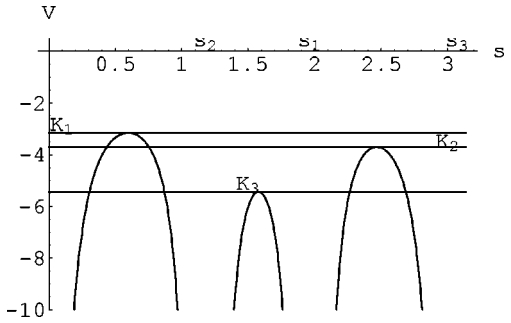

FIG. 4. The potential $\mathcal{V}(0,\sigma)$ (we used s instead of σ in the graph) for $m_1=3$, $m2=2$, $m_3=1$, and $p_\psi=0$. We also show its maximum values $K_1=-3.1561$, $K_2=-3.7003$, and $K_3=-5.4352$, and the values $\sigma_1=1.963\,49$, $\sigma_2=1.178\,09$, $\sigma_3=3.070\,64$ where a double collision takes place and the potential tends to $-\infty$.

that $I_0\Sigma=\Sigma$, i.e., the Poincaré section is invariant under the involution I_0. From Eq. (9) with $\theta=0$ we see that every point in Σ and their iterations with T must be in the interior of the region

$$P_\sigma^2 \leqslant 2K-2\mathcal{V}(0,\sigma)-p_\psi^2, \tag{19}$$

We next fix the values $p_\psi=0$, $m_1=3$, $m_2=2$, and $m_3=1$ to show some numerical results. The vectors **a** and **b** become $\mathbf{a}=(0.377\,172,-0.533\,402,-0.064\,712\,5)$ and $\mathbf{b}=(0.156\,230,0.220\,942,-0.910\,574)$; then relation (19) implies $K\geqslant\mathcal{V}(0,\sigma)$. In Fig. 4 we plot $\mathcal{V}(0,\sigma)$. The three values $\sigma_1=1.963\,495$, $\sigma_2=1.178\,097$, and $\sigma_3=3.070\,644$ correspond to the double collisions $s_{23}=0$, $s_{13}=0$ and $s_{12}=0$ on the Σ section, respectively, where $\mathcal{V}(0,\sigma_i)\to-\infty$, $i=1,2,3$. The potential has three maximum values $K_1=-3.156\,102$, $K_2=-3.700\,327$, and $K_3=-5.435\,221$. For values $K>K_1$, all the values of σ are allowed in the Poincaré region. If $K_1>K>K_2$, there is a forbidden region of σ. If $K_2>K>K_3$, there are two forbidden regions and if $K<K_3$, there are three forbidden regions in the Poincaré region.

The Poincaré maps for $\mathcal{K}=-1,0$ do not seem to have islands. In Fig. 5 the Poincaré map for $\mathcal{K}=10$ is shown, where two islands are evident. For this value of $\mathcal{K}$ there are stable periodic orbits at the center of the islands.

In what follows, symmetrical periodic orbits will be found.

VIII. PERIODIC ORBITS

A survey of the state of the art on the theory of reversible dynamical systems and the results on symmetrical periodic orbits is given in Ref. 6. Here we use the symmetry lines to find periodic orbits. Let $\Gamma_0=\{x\in\Sigma: I_0x=x\}=\{x\in\Sigma: P_\sigma=0\}$ be the set of invariant points of I_0, called the

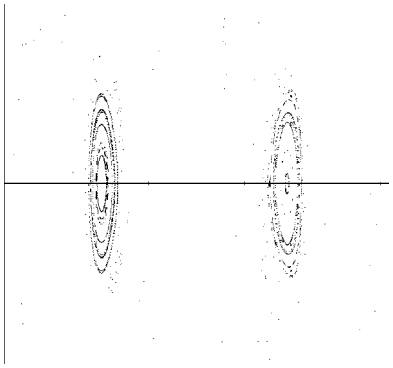

FIG. 5. Poincaré map for $m_1=3$, $m2=2$, $m_3=1$, $p_\psi=0$, and $\mathcal{K}=10$. The horizontal axis is $\sigma\in[0,\pi]$, and the vertical one is $P_\sigma\in[-\pi,\pi]$.

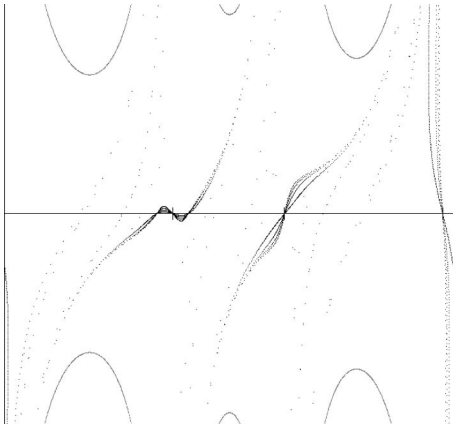

FIG. 6. Γ_0, Γ_2, Γ_4, Γ_6, and Γ_8 symmetry lines for $m_1=3$, $m2=2$, $m_3=1$, $p_\psi=0$, and $\mathcal{K}=-1$. The horizontal axis is $\sigma\in[0,\pi]$, and the vertical one is $P_\sigma\in[-\pi,\pi]$.

fundamental symmetry line, and $\Gamma_{2j}=T^j\Gamma_0$, $j\in\mathbb{Z}$ the symmetry lines obtained by the Poincaré map of Γ_0. It can be shown[7,8] that the intersections of these symmetry lines are periodic orbits, i.e., if

$$x\in\Gamma_{2j}\cap\Gamma_{2i} \quad \text{then} \quad T^{2|j-i|}x=x, \quad i\neq j \ .$$

If x is at the intersection of Γ_{2j} and Γ_{2i}, then it is a periodic orbit of T and its period divides $2|j-i|$, $j,i\in\mathbb{Z}$.

We have integrated the Hamiltonian system (18) by a Runge–Kutta method order 7–8 with initial conditions $(\sigma,P_\sigma)=(\sigma,0)$ on the fundamental symmetry line Γ_0 and we calculated the Γ_2, Γ_4, Γ_6, and Γ_8 lines. In Figs. 6, 7, and 8 are shown these lines for $p_\psi=0$, $m_1=3$, $m_2=2$, $m_3=1$ and $\mathcal{K}=-1,0,10$, respectively. The intersections of the symmetry lines are periodic orbits in Σ. We show in Fig. 9 three periodic orbits in the configuration space Π, obtained by the intersection of the symmetry lines for three different values of $\mathcal{K}=-1,0,10$, and in Figs. 10, 11, and 12 the respective orbits of the three bodies in the Cartesian rotating frame moving with ψ for each case of $\mathcal{K}$. In general, they will not be periodic in all the variables because R is not a periodic variable, except for the case $\mathcal{K}=0$ and $\mathcal{H}=0$ where R becomes constant. In addition we must choose the p_ψ parameter properly to have a periodic orbit with the same frequency of the ψ

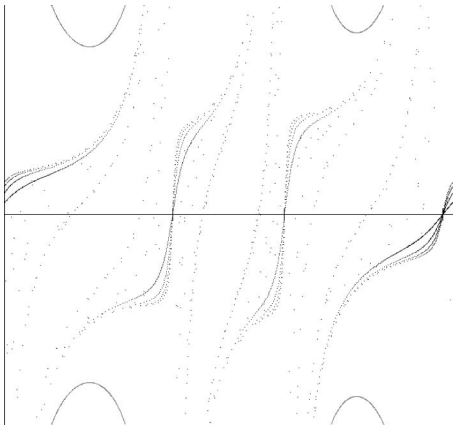

FIG. 7. Γ_0, Γ_2, Γ_4, Γ_6, and Γ_8 symmetry lines for $m_1=3$, $m2=2$, $m_3=1$, $p_\psi=0$, and $\mathcal{K}=0$. The horizontal axis is $\sigma\in[0,\pi]$, and the vertical one is $P_\sigma\in[-\pi,\pi]$.

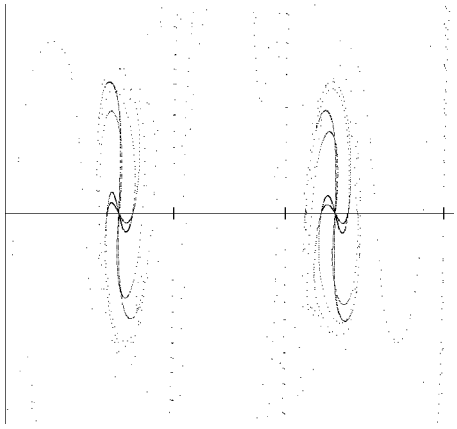

FIG. 8. Γ_0, Γ_2, Γ_4, Γ_6, and Γ_8 symmetry lines for $m_1=3$, $m2=2$, $m_3=1$, $p_\psi=0$, and $\mathcal{K}=10$. The horizontal axis is $\sigma\in[0,\pi]$, and the vertical one is $P_\sigma\in[-\pi,\pi]$.

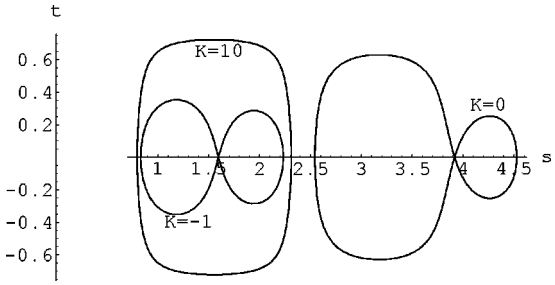

FIG. 9. Three different periodic orbits in the reduced configuration space (σ,θ) for $\mathcal{K}=-1,0,10$ (we used s and t instead of σ and θ in the graph). The respective periodic orbits of the three bodies in Cartesian coordinates are shown in Figs. 10–12.

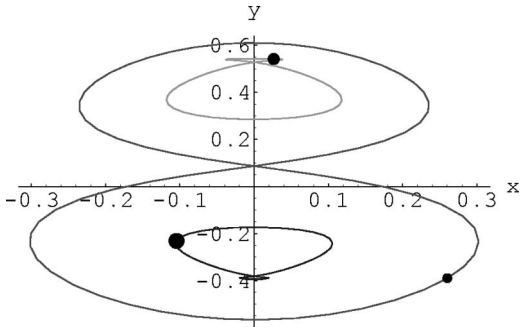

FIG. 10. Periodic orbits in Cartesian coordinates for $\mathcal{K}=-1$. m_1 corresponds to the biggest dot and m_3 corresponds to the smallest dot.

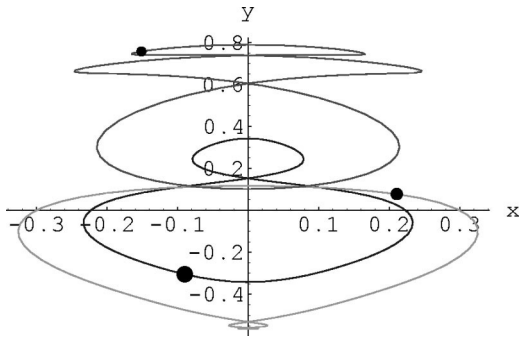

FIG. 11. Periodic orbits in Cartesian coordinates for $\mathcal{K}=0$. m_1 corresponds to the biggest dot and m_3 corresponds to the smallest dot.

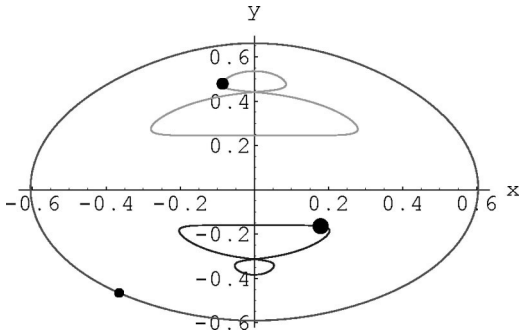

FIG. 12. Periodic orbits in cartesian coordinates for $\mathcal{K}=10$. m_1 corresponds to the biggest dot and m_3 corresponds to the smallest dot.

motion, which we are not describing here. The periodic solutions here obtained are in general periodic up to a rotation and a homothetic transformation by ψ and R variables, respectively.

IX. CONCLUSIONS

We have introduced suitable coordinates to separate partially the problem of four degrees of freedom by means of three first integrals. We thus studied the motion in the (R,P_R) plane and we showed that generically, at least two particles will escape to infinity increasing continuously their inertia moment, or the three particles will collide.

We therefore have reduced the problem to a two degrees of freedom one with an extra constant of motion $\mathcal{K}$, and we have been able to find periodic orbits for these reduced problems. These solutions will be in general periodic up to a rotation and homothetic transformation in the whole space. For special values of the constants of motion ($E=0$, $K=0$), the periodic orbits will also be periodic in the R variable. If we properly select p_ψ, the solution will be completely periodic.

Generically, the three bodies either collide, or their total inertia moment tends to infinity, which means that at least two of them escape to infinity.

ACKNOWLEDGMENTS

We thank Professor Jaume Llibre for important remarks and also for providing us with the subroutine developed by his group at the University of Barcelona that makes the numerical integration by the Runge–Kutta 7–8 method. We also thank Professor Florin Diacu for providing us the reference of Poincaré and Dr. Teresa de la Selva for helpful discussions.

APPENDIX

In this appendix we give the explicit change of coordinates from the coordinates in Ref. 4 to the Cartesian inertial frame. First, we put the origin of coordinates at the center of mass of the three particles, and we choose the third coordinate of each particle to be zero. In addition to the ψ coordinate that rotates from the principal axes frame to the inertial frame, three other coordinates are introduced: σ, R_1, and R_2. The last two are distances closely related to the two independent inertia moments $I_1=\mu R_1^2$ and $I_2=\mu R_2^2$, where μ is the mass

$$\mu=\sqrt{\frac{m_1 m_2 m_3}{m_1+m_2+m_3}}.$$

The Cartesian inertial coordinates in the plane of motion (x_i,y_i) for each m_i, written in terms of the new coordinates are

$$\mathbf{r}_j=\begin{pmatrix} x_j \\ y_j \end{pmatrix}=\mathbf{C}\begin{pmatrix} a_j \\ b_j \end{pmatrix}, \quad i=1,2,3, \tag{A1}$$

where

$$\mathbf{C}=\begin{pmatrix} R_2\cos\sigma\cos\psi+R_1\sin\sigma\sin\psi & R_2\sin\sigma\cos\psi-R_1\cos\sigma\sin\psi \\ R_2\cos\sigma\sin\psi-R_1\sin\sigma\cos\psi & R_2\sin\sigma\sin\psi+R_1\cos\sigma\cos\psi \end{pmatrix}.$$

The vectors **a** and **b** are constant, perpendicular, and orthogonal to the vector $\mathbf{m}=(m_1,m_2,m_3)$ in the mass space,

$$\mathbf{a}\cdot\mathbf{m}=\mathbf{b}\cdot\mathbf{m}=\mathbf{a}\cdot\mathbf{b}=0\,. \tag{A2}$$

If we denote the matrix $\mathbf{M}=\mathrm{diag}\{m_1,m_2,m_3\}$, we can complete the definition of vectors **a** and **b** assuming

$$\mathbf{b}\,\mathbf{M}\,\mathbf{a}^T=0, \tag{A3}$$

and the normalization conditions

$$\mathbf{a}\,\mathbf{M}\,\mathbf{a}^T=\mathbf{b}\,\mathbf{M}\,\mathbf{b}^T=\mu\,, \tag{A4}$$

that define the vectors **a** and **b** with no dimensions. The transformation (A1) is well defined when $(a_ib_j-a_jb_i)(R1^2-R_2^2)\neq 0$, $i\neq j$. In the case of $m_1>m_2>m_3$ the **a** and **b** vectors result in[4]

$$\mathbf{a}=y_a\left(\frac{m_1}{m_1-x_a},\frac{m_2}{m_2-x_a},\frac{m_3}{m_3-x_a}\right) \tag{A5}$$

and

$$\mathbf{b}=y_b\left(\frac{m_1}{m_1-x_b},\frac{m_2}{m_2-x_b},\frac{m_3}{m_3-x_b}\right), \tag{A6}$$

where x_a and x_b are the roots (with $x_a>x_b$) of the quadratic equation

$$x^2(m_1^2+m_2^2+m_3^2)-x[(m_1+m_2+m_3)(m_1m_2+m_1m_3+m_2m_3)-3m_1m_2m_3]$$
$$+(m_1+m_2+m_3)m_1m_2m_3=0\,,$$

and y_a and y_b are normalization factors given by

$$y_i^2\left(\frac{m_1^3}{(m_1-x_i)^2}+\frac{m_2^3}{(m_2-x_i)^2}+\frac{m_3^3}{(m_3-x_i)^2}\right)=\mu\,,$$

with $i=a,b$.

If two or three masses are equal, vectors **a** and **b** must be redefined and constructed by using the properties (A2)–(A4). For instance, for $m1\geqslant m2=m3$ we choose

$$\mathbf{a}=\frac{1}{\sqrt{2}}(0,1,-1)\,,$$

and

$$\mathbf{b}=\frac{1}{\sqrt{2(1+2m_2/m_1)}}(-2m_2/m_1,1,1)\,,$$

where the factor of normalization is m_2 instead of μ in (A4).

Finally, the relation among the distance between particles and the new coordinates is

$$\begin{pmatrix} r_{23}^2 \\ r_{13}^2 \\ r_{12}^2 \end{pmatrix} = \mathbf{B} \begin{pmatrix} R_1^2 \sin^2\sigma + R_2^2 \cos^2\sigma \\ R_1^2 \cos^2\sigma + R_2^2 \sin^2\sigma \\ (R_2^2 - R_1^2) 2 \sin\sigma \cos\sigma \end{pmatrix}, \tag{A7}$$

where **B** is the constant matrix, depending only on the masses,

$$\mathbf{B} = \frac{1}{\mu^2} \begin{pmatrix} m_1^2 b_1^2 & m_1^2 a_1^2 & -m_1^2 a_1 b_1 \\ m_2^2 b_2^2 & m_2^2 a_2^2 & -m_2^2 a_2 b_2 \\ m_3^2 b_3^2 & m_3^2 a_3^2 & -m_3^2 a_3 b_3 \end{pmatrix}. \tag{A8}$$

In the case of two or three equal masses, the factor $1/\mu^2$ in B must be changed by

$$\frac{1}{m_2^2} + \frac{2}{m_1 m_2}.$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

The Ermanno–Bernoulli constants and representations of the complete symmetry group of the Kepler problem

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(Received 12 July 2002; accepted 28 March 2003)

The expression of the components of the equation of motion of the classical Kepler problem in terms of the natural variables associated with the Ermanno–Bernoulli constants leads naturally to the same equations as are obtained by the technique of reduction of order developed by Nucci [J. Math. Phys. **37**, 1772 (1996)], reported by Nucci and Leach [J. Math. Phys. **42**, 746 (2001)]. Three representations of the complete symmetry group of the Kepler problem are obtained from the three standard representations of the complete symmetry group of the simple harmonic oscillator. The algebra of the complete symmetry group of the two-dimensional Kepler problem is identified to be $A_1 \oplus \{A_{3,3}\}$. The applicability of the results to other classes of problem, such as the Kepler problem with drag, which possess a conserved vector of Laplace–Runge–Lenz type, is indicated. The three-dimensional Kepler problem is shown to be completely specified by six symmetries rather than the eight previously reported by Krause [J. Math. Phys. **35**, 5734 (1994)]. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1576903]

I. INTRODUCTION

When studies of the Lie point symmetries of various ordinary differential equations and systems of ordinary differential equations were being reported in the late 1970s, it was customary to describe the set of point symmetries obtained by the Lie method as the complete symmetry group of the differential equation (or system of differential equations). This was a reaction to some earlier results obtained using Noether's theorem for which, in the case of a linear second order ordinary differential equation, five point symmetries were reported. The expression fell out of use during the 1980s. In 1994 Krause[15] revived the usage of the expression in a context for which it was a much more suitable descriptor. Krause's concept of a complete symmetry group of a differential equation is the group associated with the set of symmetries, be they point, contact, generalized or nonlocal, required to specify the equation or system completely. Specifically he required that the elements of the group have the two properties that the manifold of solutions be an homogeneous space of the group and the group be specific to the system, i.e., no other system admits it. Subsequently a requirement of minimality was added after Andriopoulos *et al.*[1,2] showed that not only was the group not unique but also the dimensionality could vary. The completeness of the specification was up to a scaling factor in the example used by Krause as the vehicle for his discussion and up to an arbitrary translation in an example discussed by Leach *et al.*[21]

As a vehicle to illustrate the concept of a complete symmetry group Krause used the Kepler problem, which is probably the central paradigm of mechanics. The Kepler problem possesses the first integrals of the conservation of the scalar energy, the vector of angular momentum and

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vectors in the plane of the orbit known as Hamilton's vector[13] and the Laplace–Runge–Lenz vector.[5,14,3,16,31,22] The invariance Lie algebra of the first integrals under the operation of taking the Poisson bracket is so(4) (in the case of negative energy) and the Lie algebra of the five Lie point symmetries of the equation of motion $A_2 \oplus \mathrm{so}(3)$. The algebra of the complete symmetry group has not been given. The elements of the five-dimensional algebra are

$$X_1=\partial_t, \quad X_3=x_2\partial_{x_3}-x_3\partial_{x_2},$$

$$X_2=t\partial_t+\tfrac{2}{3}r\partial_r, \quad X_4=x_3\partial_{x_1}-x_1\partial_{x_3}, \tag{1.1}$$

$$X_5=x_1\partial_{x_2}-x_2\partial_{x_1}$$

in which x_1, x_2, and x_3 are the usual Cartesian components of the position vector $\mathbf{r}$ of magnitude r. These five point symmetries of the equation of motion are insufficient to specify the equation completely. To overcome the deficiency in the number of symmetries Krause introduced a nonlocal symmetry of specific structure defined by

$$Y=\left[\int \xi(t,x_1,\ldots,x_N)\mathrm{d}t\right]\partial_t+\sum_{i=1}^{N} \eta_i(t,x_1,\ldots,x_N)\partial_{x_i} \tag{1.2}$$

and obtained three symmetries of this form, *videlicet*

$$Y_1=2\left(\int x_1\mathrm{d}t\right)\partial_t+x_1r\partial_r,$$

$$Y_2=2\left(\int x_2\mathrm{d}t\right)\partial_t+x_2r\partial_r, \tag{1.3}$$

$$Y_1=2\left(\int x_3\mathrm{d}t\right)\partial_t+x_3r\partial_r,$$

which has the compact form

$$\mathbf{Y}=2\left(\int \mathbf{r}\,\mathrm{d}t\right)\partial_t+\mathbf{r}\,r\partial_r, \tag{1.4}$$

in which $r^2=x_1^2+x_2^2+x_3^2$, for the Kepler problem. With these three additional symmetries he was able to specify completely the three second order equations of the equation of motion, up to the value of the gravitational constant in the radial equation which, as was noted above, is scalable.

Despite Krause's belief that the necessary number of symmetries for the complete symmetry group of the Kepler problem could not the obtained by means of the standard Lie point symmetry analysis, Nucci[28] was able to obtain all of the elements of the complete symmetry group by means of Lie point symmetry analysis—to be fair to Krause one must omit the word standard—so that the determination of the symmetries could be determined by the use of her interactive code.[26,27] The technique of reduction of order introduced by Nucci[28] was successfully used by Nucci and Leach[29] on a number of problems, both real and imaginary, for which conserved vectors of the type of the Laplace–Runge–Lenz had been found, mainly in the 1980s.[7,8,10,11,18,17] Just as the Laplace–Runge–Lenz vector provides a direct route to the equation of the orbit of the classical Kepler problem, the corresponding vectors of the generalized Kepler problems provide the same direct route to the equations of their orbits.

Nucci and Leach[29] showed that there were more nonlocal symmetries of the structure adopted by Krause (1.2), obtainable as point symmetries by the reduction method of Nucci, than Krause had reported. One of the intentions of this paper is to show that these additional nonlocal sym-

metries have a place in the discussion of the complete symmetry group. We find that there are three equivalent representations of the complete symmetry group, which we also described, for the Kepler problem. All symmetries are found by point methods. We find that there is no need to use the method of reduction of order introduced by Nucci since there is a natural variable available—its existence was demonstrated using the method of reduction of order in Nucci and Leach[29]—to write the system as the equation of a one-dimensional simple harmonic oscillator plus a conservation law. (This is in the case of a two-dimensional treatment. For three dimensions the corresponding result is one differential equation plus two conservation laws. We confine our attention to two dimensions for purposes of simplicity of presentation.) The equivalence of the Kepler problem to the simple harmonic oscillator plus a conservation law is carried over in the group properties. Some years ago Mahomed and Leach[20] showed that the three first integrals of the simple harmonic oscillator, $\ddot{x}+x=0$,

$$I_1=x\cos t-\dot{x}\sin t,$$

$$I_2=x\sin t+\dot{x}\cos t, \tag{1.5}$$

$$I_3=\frac{x\cos t-\dot{x}\sin t}{x\sin t+\dot{x}\cos t}$$

each possessed three Lie point symmetries with the same algebra. More recently Andriopoulos *et al.*[1] showed that this very algebra provided the elements of the complete symmetry group of the equation of motion for the simple harmonic oscillator. We see that these three equivalent representations lead to three equivalent representations of the complete symmetry group of the Kepler problem.

By analogy these results apply to all other systems for which one can obtain a Laplace–Runge–Lenz vector.

In the next section we summarize the determination and properties of the integrals of the Kepler problem, show how this leads naturally to the simple harmonic oscillator and consider the properties of the symmetries of the latter. In the following section we provide an explicit demonstration that the sets of symmetries obtained are indeed the elements of the complete symmetry group of the two-dimensional Kepler problem. In Sec. IV we consider the connection between the simple harmonic oscillator and the Kepler problem in three dimensions. We present some observations in Sec. V.

II. THE CONSERVATION LAWS OF THE KEPLER PROBLEM

The reduced equation for the Kepler problem is

$$0=\ddot{\mathbf{r}}+\frac{\mu\mathbf{r}}{r^3}. \tag{2.1}$$

The vector product of $\mathbf{r}$ with (2.1), *videlicet*

$$0=\mathbf{r}\times\ddot{\mathbf{r}}+\frac{\mu\mathbf{r}\times\mathbf{r}}{r^3}, \tag{2.2}$$

gives that

$$\mathbf{L}:=\mathbf{r}\times\dot{\mathbf{r}} \tag{2.3}$$

is a conserved vector, essentially the angular momentum. (One could imagine that we set the effective mass of the system at unity by rescaling.)

The vector product of (2.1) with $\mathbf{L}$ gives

$$0=(\dot{\mathbf{r}}\times\mathbf{L})^{\cdot}+\frac{\mu\mathbf{r}\times\mathbf{L}}{r^3}. \tag{2.4}$$

With the use of the decomposition

$$\dot{\mathbf{r}}=\dot{r}\hat{\mathbf{r}}+r\dot{\hat{\mathbf{r}}} \tag{2.5}$$

we may write the vector product in the numerator of the second term of (2.4) as

$$\mathbf{r}\times\mathbf{L}=r\dot{r}\mathbf{r}-r^2(\dot{r}\hat{\mathbf{r}}+r\dot{\hat{\mathbf{r}}})=-r^3\dot{\hat{\mathbf{r}}} \tag{2.6}$$

so that (2.4) becomes

$$0=(\dot{\mathbf{r}}\times\mathbf{L})^{\cdot}-\mu\dot{\hat{\mathbf{r}}} \tag{2.7}$$

and we obtain a second conserved vector, *videlicet*

$$\mathbf{J}:=\dot{\mathbf{r}}\times\mathbf{L}-\mu\hat{\mathbf{r}} \tag{2.8}$$

which is the renowned Laplace–Runge–Lenz vector, presumably so-called because it was discovered by Ermanno and Bernoulli at the beginning of the eighteenth century.

There is a third conserved vector which was obtained by Hamilton in 1845. Trivially it may be obtained by taking the vector product of **L** and **J**. However, as it arises from a direct integration of the equation of motion (2.1), such a derivation from integrals which require the use of integrating factors applied to the equation of motion does seem to be a little lacking in fundamentalism. We define a unit vector, $\hat{\boldsymbol{\omega}}$, as the unit vector in the instantaneous direction of the angular velocity, i.e., in the direction of $\dot{\hat{\mathbf{r}}}$. With $\hat{\mathbf{r}}$ and $\hat{\mathbf{L}}$ it forms an orthogonal triad. Specifically we have

$$\hat{\boldsymbol{\omega}}=\hat{\mathbf{L}}\times\hat{\mathbf{r}}, \tag{2.9}$$

so that

$$\dot{\hat{\boldsymbol{\omega}}}=\hat{\mathbf{L}}\times\dot{\hat{\mathbf{r}}}, \tag{2.10}$$

since the direction of **L** is constant. We consider the vector product on the right of (2.10). From the definition of the angular momentum we have

$$\hat{\mathbf{L}}\frac{L}{r^2}=\hat{\mathbf{r}}\times\dot{\hat{\mathbf{r}}}. \tag{2.11}$$

Taking the vector product of this with $\dot{\hat{\mathbf{r}}}$ we have

$$\hat{\mathbf{L}}\times\dot{\hat{\mathbf{r}}}\,\frac{L}{r^2}=-\dot{\hat{\mathbf{r}}}.\dot{\hat{\mathbf{r}}}\hat{\mathbf{r}}$$

$$\Leftrightarrow\quad \hat{\mathbf{r}}=-\frac{L}{r^2}\frac{1}{\dot{\hat{\mathbf{r}}}.\dot{\hat{\mathbf{r}}}}\hat{\mathbf{L}}\times\dot{\hat{\mathbf{r}}}$$

$$=-\frac{L}{r^2}\frac{1}{\dot{\hat{\mathbf{r}}}.\dot{\hat{\mathbf{r}}}}\dot{\hat{\boldsymbol{\omega}}} \tag{2.12}$$

and so the equation of motion (2.1) becomes

$$0=\ddot{\mathbf{r}}-\frac{\mu}{r^2}\frac{L}{r^2}\frac{1}{\dot{\hat{\mathbf{r}}}.\dot{\hat{\mathbf{r}}}}\dot{\hat{\boldsymbol{\omega}}}. \tag{2.13}$$

Since $\mathbf{L}=r^2\hat{\mathbf{r}}\times\dot{\hat{\mathbf{r}}}$, Eq. (2.13) is trivially integrated to give

$$\mathbf{K}:=\dot{\mathbf{r}}-\frac{\mu\hat{\boldsymbol{\omega}}}{L}, \tag{2.14}$$

which is Hamilton's vector.

We note that in the above derivation we have not made use of the fact that the orbit is in a plane due to the conservation of the angular momentum. When we reduce the motion to motion in a plane, we may use plane polar coordinates, (r,θ), and replace $\hat{\boldsymbol{\omega}}$ with $\hat{\boldsymbol{\theta}}$.

The vectors **J**, **K**, and **L** constitute an orthogonal triad.

The explicit expression for **J** in plane polar coordinates is

$$\mathbf{J}=(r^3\dot{\theta}^2-\mu)\hat{\mathbf{r}}-r^2\dot{r}\dot{\theta}\hat{\boldsymbol{\theta}}. \tag{2.15}$$

Since $\hat{\mathbf{r}}=\hat{\mathbf{i}}\cos\theta+\hat{\mathbf{j}}\sin\theta$ and $\hat{\boldsymbol{\theta}}=-i\sin\theta+\hat{\mathbf{j}}\cos\theta$, the Cartesian components of **J** are

$$J_x=(r^3\dot{\theta}^2-\mu)\cos\theta+r^2\dot{r}\dot{\theta}\sin\theta, \tag{2.16}$$

$$J_y=(r^3\dot{\theta}^2-\mu)\sin\theta-r^2\dot{r}\dot{\theta}\cos\theta. \tag{2.17}$$

From the combination

$$J_x\pm iJ_y=(r^3\dot{\theta}^2-\mu)e^{\pm i\theta}\pm ir^2\dot{r}\dot{\theta}e^{\pm i\theta}=L^2\left(\frac{1}{r}-\frac{\mu}{L^2}\pm i\frac{\dot{r}}{r^2\dot{\theta}}\right)=\mp iL^2\left(\left(\frac{1}{r}\right)'\pm i\left(\frac{1}{r}-\frac{\mu}{L^2}\right)\right)e^{\pm i\theta}, \tag{2.18}$$

where $L:=r^2\dot{\theta}$ is the magnitude of the angular momentum and the prime denotes differentiation with respect to θ, we define the Ermanno–Bernoulli constants as

$$J_\pm=(v_1'\pm iv_1)e^{\pm i\theta}, \tag{2.19}$$

where $v_1=1/r-\mu/L^2$. The reason for the rescaling is to be found in the radial equation of motion which has the simple form

$$v_1''+v_1=0, \tag{2.20}$$

i.e., the equation for a one-dimensional simple harmonic oscillator. Of course, the reduction of the radial equation to that of a linear oscillator equation is scarcely novel [see, for example, Whitaker (Ref. 32, p. 83)], but its group theoretical derivation and the identification of the new variable as being derived from the Laplace–Runge–Lenz vector is more recent.[29] Note that we can write the Laplace–Runge–Lenz vector in terms of v_1 as

$$\mathbf{J}=L^2(v_1\hat{\mathbf{r}}+v_1'\hat{\boldsymbol{\theta}}). \tag{2.21}$$

For the sake of completion we note that the scalar product of $\dot{\mathbf{r}}$ with (2.1) is easily integrated to give the energy integral, *videlicet*

$$E:=\frac{1}{2}\dot{\mathbf{r}}.\dot{\mathbf{r}}-\frac{\mu}{r}. \tag{2.22}$$

The various first integrals are related according to

$$L^4 J_+ J_- = 2L^2 E + \mu^2. \tag{2.23}$$

III. THE THREE REPRESENTATIONS OF THE COMPLETE SYMMETRY GROUP OF THE KEPLER PROBLEM

In terms of the dependent variables v_1 and v_2 and the independent variable θ the two-dimensional Kepler problem is defined by the system of differential equations

$$v_1'' + v_1 = 0, \tag{3.1}$$

$$v_2' = 0, \tag{3.2}$$

which correspond to the radial and angular components of the equation of motion (2.1). As a linear second order ordinary differential equation (3.1) possesses eight Lie point symmetries. The Lie point symmetries of the system (3.1) and (3.2) can be written as

$$\begin{gathered}\Gamma_1 = \partial_{v_2}, \quad \Gamma_{4\pm} = e^{\pm i\theta}\partial_{v_1}, \\ \Gamma_2 = \partial_\theta, \quad \Gamma_{5\pm} = e^{\pm 2i\theta}(\partial_\theta \pm i v_1 \partial_{v_1}), \\ \Gamma_3 = v_1 \partial_{v_1}, \quad \Gamma_{6\pm} = e^{\pm i\theta}(v_1 \partial_\theta \pm i v_1^2 \partial_{v_1}).\end{gathered} \tag{3.3}$$

These nine point symmetries plus ∂_t which is implicit in the change of independent variable from t to θ constitute the set of symmetries at our disposal for the determination of the complete symmetry group of the Kepler problem.

In 1988 Mahomed and Leach[20] showed that to each of three specific invariants of a second order equation possessing eight Lie point symmetries there were three point symmetries with the same algebra, *videlicet* $D \oplus_s T_2$. Recently, Andriopoulos *et al.*[1] showed that the same three symmetries completely specified the equation and so the complete symmetry group was the semidirect product of dilations and translations in the plane. In our format, which differs somewhat from the earlier literature, the invariants, I_A, I_B, and I_C, and the symmetries A_i, B_i, and C_i, $i=1,3$, are

$$I_A = (v_1 + i v_1') e^{i\theta} \begin{cases} A_1 = e^{i\theta}\partial_{v_1}, \\ A_2 = \partial_\theta - i v_1 \partial_{v_1}, \\ A_3 = e^{2i\theta}(\partial_\theta + i v \partial_{v_1}), \end{cases} \tag{3.4}$$

$$I_B = (v_1 - i v_1') e^{-i\theta} \begin{cases} B_1 = e^{-i\theta}\partial_{v_1}, \\ B_2 = \partial_\theta + i v_1 \partial_{v_1}, \\ B_3 = e^{-2i\theta}(\partial_\theta - i v \partial_{v_1}), \end{cases} \tag{3.5}$$

$$I_C = \frac{v_1 + i v_1'}{v_1 - i v_1'} e^{2i\theta} \begin{cases} C_1 = v_1 \partial_{v_1}, \\ C_{2\pm} = e^{\pm i\theta}(v_1 \partial_\theta \pm i v_1^2 \partial_{v_1}). \end{cases} \tag{3.6}$$

We note the typical variation of the appearance of combinations of Γ_2 and Γ_3, both of which are rescaling symmetries, in the algebras of the invariants.[6,19]

Proposition: The complete symmetry group of the two-dimensional Kepler problem given by the equation of motion (2.1) has three (equivalent) representations given by the sets A, B or C plus ∂_t.

To demonstrate the correctness of the proposition we first express the symmetries in terms of the variables found in (2.1). A (t, r, θ) symmetry becomes a (θ, v_1, v_2) symmetry according to

$$\tau\partial_t+\eta\partial_r+\zeta\partial_\theta\rightarrow\zeta\partial_\theta+\Omega\partial_{v_1}+\Sigma\partial_{v_2}, \tag{3.7}$$

where

$$v_2=r^2\dot{\theta},\quad v_1=\frac{1}{r}-\frac{\mu}{v_2^2},$$

$$\Sigma=2\eta r\dot{\theta}+r^2(\dot{\zeta}-\dot{\theta}\dot{\tau}), \tag{3.8}$$

$$\Omega=-\frac{\eta}{r^2}+\frac{2\mu}{v_2^3}\Sigma.$$

For A_1 we have $\zeta=0$, $\Omega=e^{i\theta}$ and $\Sigma=0$. We use the relations in (3.8) to determine that $\eta=-r^2e^{i\theta}$ and $\tau=-2\int re^{i\theta}\,\mathrm{d}t$. The same procedure is followed for A_2 and A_3. In (t,r,θ) coordinates we obtain

$$A_1=\left(2\int re^{i\theta}\,\mathrm{d}t\right)\partial_t+r^2e^{i\theta}\partial_r,$$

$$A_2=2\left(t-\frac{\mu}{L^2}\int r\,\mathrm{d}t\right)+r\left(1-\frac{\mu r}{L^2}\right)\partial_r-i\partial_\theta, \tag{3.9}$$

$$A_3=\left(\frac{2i\mu}{L^2}\int re^{2i\theta}\,\mathrm{d}t\right)\partial_t-ir\left(1-\frac{\mu r}{L^2}\right)e^{2i\theta}\partial_r+e^{2i\theta}\partial_\theta.$$

The general radial and angular components of the equation of motion can be written as the system

$$\ddot{r}=f(t,r,\theta,\dot{r},\dot{\theta}),$$

$$\ddot{\theta}=g(t,r,\theta,\dot{r},\dot{\theta}),$$

and invariance under the symmetry ∂_t immediately enables us to write this in the simpler form

$$\ddot{r}=f(r,\theta,\dot{r},\dot{\theta}), \tag{3.10}$$

$$\ddot{\theta}=g(r,\theta,\dot{r},\dot{\theta}). \tag{3.11}$$

The actions of the second extensions of A_1, A_2, and A_3 on (3.10) and (3.11) give, respectively,

$$r\frac{\partial f}{\partial r}+ir\dot{\theta}\frac{\partial f}{\partial\dot{r}}-2\dot{\theta}\frac{\partial f}{\partial\dot{\theta}}=irg-2f+2i\dot{r}\dot{\theta}-r\dot{\theta}^2, \tag{3.12}$$

$$r\frac{\partial g}{\partial r}+ir\dot{\theta}\frac{\partial g}{\partial\dot{r}}-2\dot{\theta}\frac{\partial g}{\partial\dot{\theta}}=-4g-\frac{2\dot{r}\dot{\theta}}{r}-2i\dot{\theta}^2, \tag{3.13}$$

$$r\left(1-\frac{\mu r}{L^2}\right)\frac{\partial f}{\partial r}-i\frac{\partial f}{\partial\theta}-\dot{r}\frac{\partial f}{\partial\dot{r}}-2\dot{\theta}\left(1-\frac{\mu r}{L^2}\right)\frac{\partial f}{\partial\dot{\theta}}=-3f+2\frac{\mu r}{L^2}f, \tag{3.14}$$

$$r\left(1-\frac{\mu r}{L^2}\right)\frac{\partial g}{\partial r}-i\frac{\partial g}{\partial\theta}-\dot r\frac{\partial g}{\partial\dot r}-2\dot\theta\left(1-\frac{\mu r}{L^2}\right)\frac{\partial g}{\partial\dot\theta}=-4g\left(1-\frac{\mu r}{L^2}\right)+\frac{2\mu\dot r\dot\theta}{L^2}, \tag{3.15}$$

$$-r\left(1-\frac{\mu r}{L^2}\right)\frac{\partial f}{\partial r}+\frac{\partial f}{\partial\theta}-\left[\dot r+2ir\dot\theta\left(1-\frac{\mu r}{L^2}\right)\right]\frac{\partial f}{\partial\dot r}+2\dot\theta\left(1-\frac{\mu r}{L^2}\right)\frac{\partial f}{\partial\dot\theta}$$
$$=-f\left(1+\frac{2\mu r}{L^2}\right)-2igr\left(1-\frac{\mu r}{L^2}\right)+4r\dot\theta^2\left(1-\frac{\mu r}{L^2}\right)-4i\dot r\dot\theta\left(1-\frac{\mu r}{L^2}\right), \tag{3.16}$$

$$-r\left(1-\frac{\mu r}{L^2}\right)\frac{\partial g}{\partial r}+\frac{\partial f}{\partial\theta}-\left[\dot r+2ir\dot\theta\left(1-\frac{\mu r}{L^2}\right)\right]\frac{\partial g}{\partial\dot r}+2\dot\theta\left(1-\frac{\mu r}{L^2}\right)\frac{\partial g}{\partial\dot\theta}$$
$$=2g\left(1-\frac{2\mu r}{L^2}\right)+4i\dot\theta^2\left(1-\frac{\mu r}{L^2}\right)-\frac{2\mu\dot r\dot\theta}{L^2}, \tag{3.17}$$

after division by $e^{i\theta}$ in (3.12) and (3.13) and $e^{2i\theta}$ in (3.16) and (3.17), respectively.

We observe that the right-hand sides of the angular equations contain only g whereas those of the radial equations contained both f and g. We work with the former set of equations. Adding (3.15) and (3.17) we obtain

$$-2\left[\dot r+ir\dot\theta\left(1-\frac{\mu r}{L^2}\right)\right]\frac{\partial g}{\partial\dot r}=-2g+4i\dot\theta^2\left(1-\frac{\mu r}{L^2}\right). \tag{3.18}$$

The combination $-(1-\mu r/L^2)$ (3.13) and (3.15) gives

$$-\left[\dot r+ir\dot\theta\left(1-\frac{\mu r}{L^2}\right)\right]\frac{\partial g}{\partial\dot r}=\frac{2\mu\dot r\dot\theta}{L^2}+2\left(1-\frac{\mu r}{L^2}\right)\left(\frac{\dot r\dot\theta}{r}+i\dot\theta^2\right). \tag{3.19}$$

We eliminate all derivatives of g by means of the combination (3.18) and (3.19) to obtain

$$g=-\frac{2\dot r\dot\theta}{r}. \tag{3.20}$$

We further observe that the left-hand sides of the radial equations contain the same terms as those of the angular equations with f in place of g and take the same combinations as in the preceding paragraph to obtain

$$f=r\dot\theta^2\left(1-\frac{\mu r}{L^2}\right) \tag{3.21}$$

which, on the replacement of L by $r^2\dot\theta$ becomes

$$f=r\dot\theta^2-\frac{\mu}{r^2}. \tag{3.22}$$

Hence the A-set of symmetries, together with ∂_t, provides a representation of the complete symmetry group of the Kepler problem in the two-dimensional form considered here. As the B-set of symmetries is the complex conjugate of the A-set, it is evident that this set also leads to a representation of the complete symmetry group. We need only consider now the C-set.

In terms of (t,r,θ) coordinates the C-set symmetries are

$$C_1=\left(-2\int x\,\mathrm{d}t\right)\partial_t-rx\partial_r, \tag{3.23}$$

$$C_{2\pm}=\left[\int\left(-\frac{\dot r}{L}\pm\frac{ix}{r}\mp 2i\frac{x^2}{r}\right)e^{\pm i\theta}\,\mathrm{d}t\right]\partial_t\mp ix^2e^{\pm i\theta}\partial_r+\frac{x}{r}e^{\pm i\theta}\partial_\theta, \tag{3.24}$$

in which we have introduced the notation

$$x=1-\frac{\mu r}{L^2},\quad \dot x=-\frac{\mu\dot r}{L^2} \tag{3.25}$$

in an attempt to compactify the expressions.

From our experience with the A-set of symmetries we know that the right-hand sides of the equations will be the same, apart from an interchange of f and g, for both the radial and angular components of (3.10) and (3.11). We also expect the angular equation to be simpler and so commence with these. We obtain

$$C_1,\quad -rx\frac{\partial g}{\partial r}+(\dot r x-r\dot x)\frac{\partial g}{\partial\dot r}+2x\dot\theta\frac{\partial g}{\partial\dot\theta};$$

$$C_{2\pm},\quad \left[\mp ix^2\frac{\partial g}{\partial r}+\frac{x}{r}\frac{\partial g}{\partial\theta}+\left(\mp 2ix\dot x+x^2\dot\theta+\frac{\dot r^2}{L}\mp\frac{i\dot r x}{r}\pm\frac{2i\dot r x^2}{r}\right)\frac{\partial g}{\partial\dot r}\pm 2i\frac{x^2\dot\theta}{r}\frac{\partial g}{\partial\dot\theta}\right]e^{\pm i\theta}. \tag{3.26}$$

By means of some obvious manipulations we find that

$$2ixC_1-r(C_{2+}e^{-i\theta}-C_{2-}e^{i\theta})=0 \tag{3.27}$$

and so must use this combination on the left-hand sides to obtain g. The left-hand sides are

$$\begin{aligned}&C_1,\quad 4gx+2\dot x\dot\theta;\\ &C_{2\pm},\quad \pm\frac{4ix\dot x\dot\theta}{r}\mp\frac{2ix^2\dot r\dot\theta}{r^2}+g\left(\frac{\dot r}{L}\mp\frac{ix}{r}\pm\frac{4ix^2}{r}\right);\end{aligned} \tag{3.28}$$

from the latter of which a common factor of $\exp[\pm i\theta]$ has been removed. After a little manipulation of these expressions in (3.27) we regain (3.20).

The left-hand sides of the radial equations are

$$C_1,\quad f\left(3x+\frac{\mu r}{L^2}\right);$$

$$\begin{aligned}C_{2\pm},\quad &f\left(3\frac{\dot r}{L}\pm 2i\frac{\mu x}{L^2}\mp 2i\frac{x}{r}\pm 4i\frac{x^2}{r}\right)\mp 2i\dot x^2+4x\dot x\dot\theta+x^2g\pm ix^2\dot\theta^2\pm i\frac{\dot r^2\dot\theta}{L}\\ &-\dot r\left(\pm\frac{i\dot x}{r}\mp\frac{ix\dot r}{r^2}\mp\frac{4ix\dot x}{r}\pm\frac{2ix^2\dot r}{r^2}-\frac{x\dot\theta}{r}+\frac{2x^2\dot\theta}{r}\right);\end{aligned}$$

and, when we substitute these expressions in (3.27) and simplify, we obtain

$$2ix\left(f-r\dot\theta^2+\frac{\mu}{r^2}\right) \tag{3.29}$$

and so the radial equation of motion is regained.

Thus we have proven the proposition by explicit demonstration.

We observe that the symmetry, ∂_t, is necessary to enable the manipulations with the terms in $e^{\pm i\theta}$ above. Without this symmetry we would have to include the nonlocal coefficients of the ∂_t and so the exponential terms could not be eliminated. *A priori* one would have expected five symmetries from general considerations of the number of symmetries needed for an nth order system[1] and it is evident that the first order equation, representing the conservation of angular momentum, does not lead to the requirement of an additional symmetry.

It remains to consider the algebra of these representations of the complete symmetry group. The Lie brackets of the three representations are

$$\begin{gathered}
[A_1,A_2]_{\mathrm{LB}}=-2iA_1,\quad [B_1,B_2]_{\mathrm{LB}}=2iB_1,\quad [C_1,C_{2\pm}]_{\mathrm{LB}}=C_{2\pm},\\
[A_1,A_3]_{\mathrm{LB}}=0,\quad [B_1,B_3]_{\mathrm{LB}}=0,\quad [C_{2+},C_{2-}]_{\mathrm{LB}}=0,\\
[A_2,A_3]_{\mathrm{LB}}=2iA_3,\quad [B_2,B_3]_{\mathrm{LB}}=-2iB_3,\\
[\partial_t,A_i]_{\mathrm{LB}}=0,\quad [\partial_t,B_i]_{\mathrm{LB}}=0,\quad [\partial_t,C_i]_{\mathrm{LB}}=0.
\end{gathered}\tag{3.30}$$

The differences in the brackets can be rectified by suitable rescaling of the symmetries and renumbering. We note that ∂_t has zero Lie brackets with all other symmetries. Taking the C-set as an example we see that subalgebra C_1 acts semidirectly on the pair, $C_{2\pm}$, which is an Abelian subalgebra. Thus the structure of the algebra is $A_1\oplus\{A_1\oplus_s 2A_1\}$, where we use the standard notation of the Mubarakzyanov classification,[23–25] in which the algebras within braces constitute the semidirect sum of dilations and translations in the plane, also known as $A_{3,3}$.

The reduction of (2.1) to (3.1) and (3.2) is essentially a reduction of order using the symmetry ∂_t of the system (2.1). We have noted that all of the elements of the algebra of the complete symmetry group have zero Lie bracket with this symmetry. It is a commonplace [see, for example, Olver (Ref. 30, p. 185)] that, if a point symmetry has zero Lie bracket with the symmetry used for the reduction, it remains as a point symmetry of the reduced system. If it does not, then it becomes an exponential nonlocal symmetry of the reduced system. Here we have an interesting situation in that a nonlocal symmetry having zero Lie bracket with the reducing symmetry becomes a point symmetry of the reduced system. This is a hitherto unexplored aspect of the subject of nonlocal symmetries and may well bear fruitful investigation.

As a final point in connection with the representations of the complete symmetry group of the two-dimensional Kepler problem we note that it is not necessary to express these in terms of nonlocal symmetries. If we consider the three A symmetries by way of example, we have

$$\begin{aligned}
A_1&=\left(2\int re^{i\theta}\,\mathrm{d}t\right)\partial_t+r^2e^{i\theta}\partial_r,\\
A_2&=2\left(t-\frac{\mu}{L^2}\int r\,\mathrm{d}t\right)\partial_t+r\left(1-\frac{\mu r}{L^2}\right)\partial_r-i\partial_\theta,\\
A_3&=\left(\frac{2i\mu}{L^2}\int re^{2i\theta}\,\mathrm{d}t\right)\partial_t-ir\left(1-\frac{\mu r}{L^2}\right)e^{2i\theta}\partial_r+e^{2i\theta}\partial_\theta.
\end{aligned}\tag{3.31}$$

In each case the nonlocality comes from the integral in the coefficient function of ∂_t. In the case of A_2 we may manipulate the integral as follows:

$$\int r\,\mathrm{d}t=\int r\frac{\mathrm{d}\theta}{\dot\theta}=\int\frac{r^3}{L}\mathrm{d}\theta=L^5\int\frac{\mathrm{d}\theta}{(\mu+J\cos\theta)^3},\tag{3.32}$$

in which we have used the equation, $r(\theta)$, of the orbit. Similarly we have

$$\int re^{i\theta}\,\mathrm{d}t = L^5\int\frac{e^{i\theta}\,\mathrm{d}\theta}{(\mu+J\cos\theta)^3},$$
$$\int re^{2i\theta}\,\mathrm{d}t = L^5\int\frac{e^{2i\theta}\,\mathrm{d}\theta}{(\mu+J\cos\theta)^3}, \tag{3.33}$$

for A_1 and A_3, respectively. The integrals may be evaluated using standard integrals (Ref. 12, pp. 179, 180). In the case of negative energy as generalized symmetries we have

$$A_1=\left[\frac{ir^2L}{J}+\frac{\mu r^2\sin\theta}{2(-2E)L}+\frac{r(\mu^2+2J^2)\sin\theta}{2(-2E)^2L}-\frac{6\mu J}{(-2E)^{5/2}}\arctan\left(\frac{\mu-J}{\mu+J}\right)^{1/2}\tan\frac{\theta}{2}\right]\partial_t+r^2e^{i\theta}\partial_r,$$

$$A_2=2\left[t-\frac{\mu}{L^2}\left(\frac{r^2J\sin\theta}{4EL}-\frac{3\mu rJ\sin\theta}{8E^2L}+\frac{2\mu^2+J^2}{(-2E)^{5/2}}\arctan\left(\frac{\mu-J}{\mu+J}\right)^{1/2}\tan\frac{\theta}{2}\right)\right]\partial_t+r\left(1-\frac{\mu r}{L^2}\right)\partial_r$$
$$+\partial_\theta, \tag{3.34}$$

$$A_3=\frac{2i\mu}{L^2}\left[\frac{(2\mu^2-J^2)\mu r^2\sin\theta}{2J^2(-2E)L}+\frac{2\mu^4+3\mu^2J^2-2J^4-8\mu J^3+8\mu^3J}{2J^2L(-2E)^2}r\sin\theta\right.$$
$$\left.-\frac{4\mu^4+12\mu^3J-6\mu J^3-4J^4}{J^2(-2E)^{5/2}}\arctan\sqrt{\frac{\mu-J}{\mu+J}}\tan\frac{1}{2}\theta\right]\partial_t-ir\left(1-\frac{\mu r}{L^2}\right)e^{2i\theta}\partial_r+e^{2i\theta}\partial_\theta,$$

in which we have used the well-known relationship $J^2=2EL^2+\mu^2$. (The forms of the symmetries for the cases of positive and zero energy are calculated similarly.) The symmetries are generalized since L, E, and J are functions of $\dot r$ and $\dot\theta$. We note that the appearances of the generalized symmetries are complicated and not particularly intuitive. One is inclined to the opinion that the nonlocal representation is to be preferred.

IV. THE KEPLER PROBLEM IN THREE DIMENSIONS

The radial, polar and azimuthal components of the equation of motion for the Kepler problem, (2.1), are

$$\ddot r-r\dot\theta^2-r\sin^2\theta\dot\phi^2=-\frac{\mu}{r^2}, \tag{4.1}$$

$$r\ddot\theta+2\dot r\dot\theta-r\dot\phi^2\sin\theta\cos\theta=0, \tag{4.2}$$

$$(r\ddot\phi+2\dot r\dot\phi)\sin\theta+2r\dot\theta\dot\phi\cos\theta=0, \tag{4.3}$$

respectively. The Laplace–Runge–Lenz vector, (2.8), has the three Cartesian components

$$J_x=\left(\frac{L^2}{r}-\mu\right)\sin\theta\cos\phi-r^2\dot r(\dot\theta\cos\theta\cos\phi-\dot\phi\sin\theta\sin\phi), \tag{4.4}$$

$$J_y=\left(\frac{L^2}{r}-\mu\right)\sin\theta\sin\phi-r^2\dot r(\dot\theta\cos\theta\sin\phi+\dot\phi\sin\theta\cos\phi), \tag{4.5}$$

$$J_z=\left(\frac{L^2}{r}-\mu\right)\cos\theta+r^2\dot r\dot\theta\sin\theta, \tag{4.6}$$

and we combine the first two to obtain

$$J_{\pm}=J_x\pm iJ_y=\left[\left(\frac{L^2}{r}-\mu\right)\sin\theta-r^2\dot{r}\dot{\theta}\cos\theta\mp ir^2\dot{r}\dot{\phi}\sin\theta\right]e^{\pm i\phi}. \tag{4.7}$$

By analogy with the two-dimensional Kepler problem the real part of the expression within the crochets is the obvious candidate for one of the new variables.

The matter of identifying a third variable—the z-component of the angular momentum which comes from direct integration of the azimuthal inflation makes an obvious second variable—requires a little ingenuity. From the azimuthal equation, (4.3), we have

$$\dot{r}=-r\dot{\theta}\cot\theta-\frac{r\ddot{\phi}}{2\dot{\phi}}. \tag{4.8}$$

With this and following division by the common r the polar equation becomes

$$\ddot{\theta}-2\dot{\theta}^2\cot\theta-\frac{\ddot{\phi}\dot{\theta}}{\dot{\phi}}-\dot{\phi}^2\sin\theta\cos\theta=0. \tag{4.9}$$

We take ϕ to be the new independent variable. Then (4.9) is

$$\theta''-2\theta'^2\cot\theta-\sin\theta\cos\theta=0, \tag{4.10}$$

where the prime denotes differentiation with respect to the new independent variable ϕ. A second oscillator is obtained after the change of variable $v_2=\cot\theta$.

Thus we obtain a two-dimensional oscillator plus a conservation law, *videlicet*

$$\begin{gathered}v_1''+v_1=0,\quad v_1=\left(\frac{L^2}{r}-\mu\right)\sin\theta-r^2\dot{r}\dot{\theta}\cos\theta,\\ v_2''+v_2=0,\quad v_2=\cot\theta,\\ v_3'=0,\quad v_3=r^2\dot{\phi}\sin^2\theta,\end{gathered} \tag{4.11}$$

where the independent variable is ϕ.

The Lie point symmetries of (4.11) are those of the two-dimensional linear system plus ∂_{v_3} and are[9]

$$\begin{gathered}\Gamma_{1\pm}=e^{\pm i\phi}\partial_{v_1},\quad \Gamma_{2\pm}=e^{\pm i\phi}\partial_{v_2},\\ \Gamma_{3\pm}=v_1e^{\pm i\phi}[\partial_\phi\pm(v_1\partial_{v_1}+v_2\partial_{v_2})],\quad \Gamma_{4\pm}=v_2e^{\pm i\phi}[\partial_\phi\pm(v_1\partial_{v_1}+v_2\partial_{v_2})],\\ \Gamma_{5\pm}=e^{\pm i\phi}[\partial_\phi\pm(v_1\partial_{v_1}+v_2\partial_{v_2})],\\ \Gamma_6=v_1\partial_{v_1},\quad \Gamma_7=v_1\partial_{v_2},\\ \Gamma_8=v_2\partial_{v_1},\quad \Gamma_9=v_2\partial_{v_2},\\ \Gamma_{10}=\partial_\phi,\quad \Gamma_{11}=\partial_{v_3}.\end{gathered} \tag{4.12}$$

The algebra of these 16 symmetries is $A_1\oplus\mathrm{sl}(4,R)$, where the $\mathrm{sl}(4,R)$ is the algebra of the point symmetries of the two-dimensional simple harmonic oscillator.

The two-dimensional oscillator is completely specified by the five symmetries[2] $\Gamma_{1\pm}$, $\Gamma_{2\pm}$, and $\Gamma_6+\Gamma_9$ which has the algebra $A_1\oplus_s\{2A_1\oplus 2A_1\}$, being a representation of the semidirect product of dilations and translations in the four-plane. This algebra completely specifies the system (4.11). Consequently the three-dimensional Kepler problem is completely specified by the six-dimensional algebra $A_1\oplus\{A_1\oplus_s\{2A_1\oplus 2A_1\}\}$.

Krause[15] reported that eight symmetries were needed to specify the three-dimensional Kepler problem. Evidently he did not make the correct choice of symmetries. If one considers the representation of, say, $\Gamma_{1\pm}$ in terms of spherical polar coordinates, one obtains

$$\Gamma_{1\pm}=\left\{\int 2r\cos\theta\exp\left[-\int\frac{\dot\phi^2\sin^3\theta}{\dot\theta\cos\theta}\mathrm{d}t\right]\left[\int\frac{\exp(\pm i\phi)}{r^4\dot\theta\cos^2\theta}\exp\left(\int\frac{\dot\phi^2\sin^3\theta}{\dot\theta\cos\theta}\mathrm{d}t\right)\mathrm{d}t\right]\mathrm{d}t\right\}\partial_t$$
$$+\left\{r^2\cos\theta\exp\left[-\int\frac{\dot\phi^2\sin^3\theta}{\dot\theta\cos\theta}\mathrm{d}t\right]\left[\int\frac{\exp(\pm i\phi)}{r^4\dot\theta\cos^2\theta}\exp\left(\int\frac{\dot\phi^2\sin^3\theta}{\dot\theta\cos\theta}\mathrm{d}t\right)\mathrm{d}t\right]\right\}\partial_r. \tag{4.13}$$

The structure of this symmetry is scarcely intuitive and it is unlikely that anyone could make an Anzatz for a structure of this type.

V. CONCLUSION

In this paper we have shown that there are three representations of the complete symmetry group for the Kepler problem. These three representations followed directly from the three representations of the complete symmetry group for the simple harmonic oscillator. As Nucci and Leach[29] have shown that a number of related problems, all characterized by the possession of a conserved vector of Laplace–Runge–Lenz type, may be reduced to the simple harmonic oscillator, we may infer that these systems also have three representations for their complete symmetry groups. Indeed, one expects that the algebra be the same.

Given that the algebra is the same, there should exist a transformation of coordinates between any two of these systems. We illustrate this in the case of the Kepler problem with drag, the problem of a low altitude satellite modelled by Danby,[4] with the equation of motion

$$\ddot r+\frac{\alpha}{r^2}\dot r+\frac{\mu}{r^3}r=0, \tag{5.1}$$

where α and μ are constants. Since the direction of the angular momentum is a constant, we may analyze the problem in two dimensions using plane polar coordinates, (r,θ). The radial and angular components of the equation of motion are

$$\ddot r-r\dot\theta^2+\frac{\alpha\dot r}{r^2}+\frac{\mu}{r^2}=0, \tag{5.2}$$

$$r\ddot\theta+2\dot r\dot\theta+\frac{\alpha\dot\theta}{r}=0. \tag{5.3}$$

The reduction to the simple harmonic oscillator and a first-order conservation law is achieved by the change of variables

$$v_1=\frac{1}{r}-\mu z(\theta),$$
$$v_2=r^2\dot\theta+\alpha\theta, \tag{5.4}$$

where the function $z(\theta)$ is defined by

$$z(\theta)=\int^{\theta}\frac{\sin(\theta-\eta)\,\mathrm{d}\eta}{(\beta-\alpha\eta)^2}$$

$$\Leftrightarrow z''(\theta)+z(\theta)=\frac{1}{(\beta-\alpha\eta)^2} \tag{5.5}$$

and β is the value of the conservation law $L+\alpha\theta$ which replaces the conservation of the magnitude of the angular momentum found for the standard Kepler problem. The Ermanno–Bernoulli constants are

$$J_{\pm}=\left[\left(\frac{1}{r}-\mu z\right)'\pm i\left(\frac{1}{r}-\mu z\right)\right]. \tag{5.6}$$

In line with the treatment of the Kepler problem we would expect the system (5.2) and (5.3) to be completely specified by the symmetry ∂_t plus any one of the triplets which completely specify the equation for the oscillator, say the A-set. We can incorporate the symmetry ∂_t into the definition of the system to be tested, *videlicet*

$$\ddot{r}=f(r,\theta,\dot{r},\dot{\theta}), \tag{5.7}$$

$$\ddot{\theta}=g(r,\theta,\dot{r},\dot{\theta}). \tag{5.8}$$

In terms of the variables t, r, and θ the three A symmetries are

$$A_1=\left(2\int re^{i\theta}\,\mathrm{d}t\right)\partial_t+r^2e^{i\theta}\partial_r, \tag{5.9}$$

$$A_2=\left[\int\left(2i-2\mu r(z'+iz)\frac{\alpha}{L}\right)\mathrm{d}t\right]\partial_t+ir[1+i\mu r(z'+iz)]\partial_r+\partial_\theta, \tag{5.10}$$

$$A_3=\left[\int\left(-2\mu r(z'-iz)+\frac{\alpha}{L}\right)e^{2i\theta}\,\mathrm{d}t\right]\partial_t-ir[1-\mu ir(z'-iz)]e^{2i\theta}\partial_r+e^{2i\theta}\partial_\theta. \tag{5.11}$$

The actions of the second extensions of these three symmetries on the pair of equations (5.7) and (5.8) produce the following set of equations to be solved to determine f and g. The equations alternate from radial to angular in turn,

$$ir^2g+2ir\dot{r}\dot{\theta}-r^2\dot{\theta}^2-2rf=r^2\frac{\partial f}{\partial r}+ir^2\dot{\theta}\frac{\partial f}{\partial\dot{r}}-2r\dot{\theta}\frac{\partial f}{\partial\dot{\theta}}, \tag{5.12}$$

$$-4rf-2r\dot{\theta}-2ir\dot{\theta}^2=r^2\frac{\partial g}{\partial r}+ir^2\dot{\theta}\frac{\partial g}{\partial\dot{r}}-2r\dot{\theta}\frac{\partial g}{\partial\dot{\theta}}, \tag{5.13}$$

$$-3if-2\frac{\alpha}{L}f-\mu(r^2g+2r\dot r\dot\theta)(z''+iz')-\mu r^2\dot\theta^2(z'''+iz'')+2\mu rf(z'+iz)$$
$$=ir[1+\mu ir(z'+iz)]\frac{\partial f}{\partial r}+\frac{\partial f}{\partial\theta}+\left[-i\dot r-\mu r^2\dot\theta(z''+iz')-\frac{\alpha\dot r}{L}\right]\frac{\partial f}{\partial\dot r}$$
$$+\left[-2i\dot\theta+2\mu r\dot\theta(z'+iz)-\frac{\alpha\dot\theta}{L}\right]\frac{\partial f}{\partial\dot\theta}, \tag{5.14}$$

$$-4ig+2\mu(2rg+\dot r\dot\theta)(z'+iz)+2\mu r\dot\theta^2(z''+iz')+\frac{2\alpha\dot r}{r^3}-\frac{\alpha g}{L}$$
$$=ir[1+\mu ir(z'+iz)]\frac{\partial g}{\partial r}+\frac{\partial g}{\partial\theta}+\left[-i\dot r-\mu r^2\dot\theta(z''+iz')-\frac{\alpha\dot r}{L}\right]\frac{\partial g}{\partial\dot r}$$
$$+\left[-2i\dot\theta+2\mu r\dot\theta(z'+iz)-\frac{\alpha\dot\theta}{L}\right]\frac{\partial g}{\partial\dot\theta}, \tag{5.15}$$

$$-if-\mu(r^2g+2r\dot r\dot\theta)(z''+iz'+2z)+2(r\ddot\theta+2\dot r\dot\theta)-\mu r^2\dot\theta^2(z'''-iz'')-4i\mu r^2\dot\theta^2(z''-iz')$$
$$-\frac{\alpha f}{L}+\frac{\alpha\dot rL}{L^2}+4ir\dot\theta^2+2\mu(rf+2r^2\dot\theta^2)(z'-iz)-\frac{2i\alpha\dot r\dot\theta}{L}-\frac{\alpha f}{L}$$
$$=-ir[1-\mu ir(z'-iz)]\frac{\partial f}{\partial r}+\frac{\partial f}{\partial\theta}+\left[2r\dot\theta-\mu r\dot\theta(z''+iz'+2z)-\frac{\alpha\dot r}{L}\right]\frac{\partial f}{\partial\dot r}$$
$$+\left[2i\dot\theta+2\mu r\dot\theta(z'-iz)-\frac{\alpha\dot\theta}{L}\right]\frac{\partial f}{\partial\dot\theta}, \tag{5.16}$$

$$2ig+2\mu(2rg+\dot r\dot\theta)(z'-iz)+2\mu r\dot\theta^2(z''+iz'+2z)+\frac{2\alpha\dot r}{r^3}-4\dot\theta^2-\frac{2i\alpha\dot\theta}{r^2}\frac{\alpha g}{L}$$
$$=-ir[1-\mu ir(z'-iz)]\frac{\partial g}{\partial r}+\frac{\partial g}{\partial\theta}+\left[2r\dot\theta-\mu r\dot\theta(z''+iz'+2z)-\frac{\alpha\dot r}{L}\right]\frac{\partial g}{\partial\dot r}$$
$$+\left[2i\dot\theta+2\mu r\dot\theta(z'-iz)-\frac{\alpha\dot\theta}{L}\right]\frac{\partial g}{\partial\dot\theta}. \tag{5.17}$$

We observe that the combinations $r[(5.17)-(5.15)]+2i(1-\mu rz)(5.13)$ and the same with (5.16), (5.14), and (5.12) give zero on the right-hand side and so the system of partial differential equations to determine f and g reduces to an algebraic equation. From the combination of the angular equations we verify that

$$g=-\frac{2\dot r\dot\theta}{r}-\frac{\alpha\dot\theta}{r^2}. \tag{5.18}$$

With this and the combination of the radial equations we then verify that

$$f = r\dot{\theta}^2 - \frac{\alpha \dot{r}}{r^2} - \frac{\mu}{r^2} \tag{5.19}$$

provided the function $z(\theta)$ is a solution of the equation

$$z'' + z = \frac{1}{L^2}. \tag{5.20}$$

Since the sets of symmetries B and C are related to those of A by means of a point transformation which preserves the differential equation, it is evident that the same result applies for the sets B and C.

In this paper we have demonstrated that the Kepler problem can be recast as a simple harmonic oscillator plus a conservation law. By contrast with other literature on the relationship between the Kepler problem and the simple harmonic oscillator in which the Kepler problem is embedded in an oscillator of higher dimension we have shown that the Kepler problem in two dimensions has a natural representation in terms of a one-dimensional oscillator plus a first-order equation which represents the conservation of angular momentum. In the case of the Kepler problem in three dimensions the natural representation is in terms of a two-dimensional oscillator and the conservation of the z component of the angular momentum. Because of this relationship between the Kepler problem and the simple harmonic oscillator and the well-established results for the complete symmetry group of the latter it has been a relatively easy matter to determine the complete symmetry group for the Kepler problem in its two- and three-dimensional forms. The former requires four symmetries to specify it completely and the latter six. In both cases the number of symmetries required is one less than would have been expected, that being five for the two-dimensional case and seven for the three-dimensional case.

We recall that Krause[15] reported that the complete symmetry group of the three-dimensional Kepler problem consists of eight elements which is considerably in excess of the number reported here. It is known[1] that an inappropriate choice of symmetries can result in more symmetries being required to specify the equation than the minimal number. Apparently this is what happened in the case of Krause's work. That it should happen is quite understandable since he was working in a vacuum, as it were. In the case of the present work we had the advantage of the results for oscillator systems[2] and the relationship between the Kepler problem and the oscillator which we have shown for the three-dimensional problem. Furthermore, as we saw in the case of the three-dimensional Kepler problem, the representation of the elements of the complete symmetry algebra in terms of the original variables of the Kepler problem is extremely nonlocal and most nonintuitive.

ACKNOWLEDGMENTS

P.G.L.L. expresses his appreciation of the hospitality of GEODYSYC, Department of Mathematics, University of the Aegean, during the period in which this work was undertaken and acknowledges the support of the National Research Foundation of South Africa and the University of Natal. K.A. acknowledges the support of the Municipality of Samos through its award of a scholarship.

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Lorenz integrable system moves à la Poinsot

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(Received 12 February 2003; accepted 20 May 2003)

A transformation is derived which takes the Lorenz integrable system into the well-known Euler equations of a torque-free rigid body about a fixed point, i.e., the famous motion à la Poinsot. The proof is based on Lie group analysis applied to two third-order ordinary differential equations admitting the same two-dimensional Lie symmetry algebra. Lie's classification of two-dimensional symmetry algebras in the plane is used. If the same transformation is applied to the Lorenz system with any values of the parameters, then one obtains Euler equations of a rigid body about a fixed point subjected to a torsion depending on time and angular velocity. The numerical solution of this system yields a three-dimensional picture which looks like a ''tornado'' the cross-section of which has a butterfly-shape. Thus Lorenz's *butterfly* has been transformed into a *tornado*. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599955]

I. INTRODUCTION

The motion of a heavy rigid body about a fixed point is one of the most famous problems of classical mechanics.[1] In 1750 Euler[2] derived the equations of motion, which now bear his name, and described what is nowadays known as the Euler–Poinsot case because of the geometrical description given by Poinsot about 100 years later.[3] It was Jacobi[4] who integrated this case by using the elliptic functions which he had developed (along with Legendre, Abel, and Gauss[5]) and mastered[6]—we have translated this fundamental text into Italian and commented extensively.[7]

More than 200 years later, in 1963, a paper was published[8] in which was presented a system of three ordinary differential equations. The author considered a hydrodynamical system developed by Rayleigh[9] and reduced it by applying a double Fourier series as in Ref. 10. Thus he obtained what nowadays is the famous Lorenz system.[11] Three parameters are part of the Lorenz system. For particular values of those parameters the Lorenz system can be integrated in closed form by means of Jacobi elliptic functions.[12] We call this system the Lorenz integrable system.

In January 2001 the first Whiteman prize for notable exposition on the history of mathematics was awarded to Thomas Hawkins by the American Mathematical Society. In the citation, published in the Notices of AMS **48**, 416-417 (2001), one reads that Thomas Hawkins ''... has written extensively on the history of Lie groups. In particular he has traced their origins to [Lie's] work in the 1870s on differential equations ... the *idée fixe* guiding Lie's work was the development of a Galois theory of differential equations ... (Hawkins's book[13]) highlights the fascinating interaction of geometry, analysis, mathematical physics, algebra and topology ...'' Also Hawkins had established ''the nature and extent of Jacobi's influence upon Lie.'' [14]

In the Introduction of his book[15] Olver wrote that ''it is impossible to overestimate the importance of Lie's contribution to modern science and mathematics. Nevertheless anyone who is already familiar with [it] ... is perhaps surprised to know that its original inspirational source was the field of differential equations.''

Lie's monumental work on transformation groups,[16–18] and in particular contact transformations,[19] led him to achieve his goal.[20]

Many books have been dedicated to this subject and its generalizations (Refs. 21–23, 15, 24–29).

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Lie group analysis is indeed the most powerful tool to find the general solution of ordinary differential equations. Any known integration technique can be shown to be a particular case of a general integration method based on the derivation of the continuous group of symmetries admitted by the differential equation, i.e., the Lie symmetry algebra. In particular Bianchi's theorem (Refs. 30 and 15) states that, if an admitted n-dimensional solvable Lie symmetry algebra is found, then the general solution of the corresponding nth-order system of ordinary differential equations can be obtained by quadratures. The admitted Lie symmetry algebra can be easily derived by a straightforward although lengthy procedure. As computer algebra software becomes widely used, the integration of systems of ordinary differential equations by means of Lie group analysis is becoming easier to perform. A major drawback of Lie's method is that it is useless when applied to systems of n first-order equations, because they admit an infinite number of symmetries, and there is no systematic way to find even a one-dimensional Lie symmetry algebra, apart from trivial groups like translations in time admitted by autonomous systems. One may try to derive an admitted n-dimensional solvable Lie symmetry algebra by making an ansatz on the form of its generators.

However, in Ref. 31 we have remarked that any system of n first-order equations could be transformed into an equivalent system where at least one of the equations is of second order. Then the admitted Lie symmetry algebra is no longer infinite-dimensional, and nontrivial symmetries of the original system could be retrieved.[31] This idea has been successfully applied in several instances (Refs. 31–34). Also in Ref. 35 we have have shown that first integrals can be obtained by Lie group analysis, even if the system under study does not come from a variational problem, i.e., without making use of Noether's theorem.[36] If we consider a system of first-order equations and, by eliminating one of the dependent variables, derive an equivalent system which has one equation of second-order, then Lie group analysis applied to that equivalent system yields the first integral(s) of the original system which do(es) not contain the eliminated dependent variable. Of course this requires that such first integrals exist. The procedure should be repeated as many times as there are dependent variables in order to find all such first integrals. The first integrals correspond to the characteristic curves of determining equations of parabolic type which are constructed by the method of Lie group analysis. We remark that interactive (not automatic) programs for calculating Lie symmetries such as Refs. 37 and 38 are more appropriate for performing this task.

We have briefly sketched three apparently unrelated subjects. In this paper we show that the Lorenz system and the Euler equations are actually related by means of Lie group analysis. In Ref. 39 we applied Lie group analysis to a third-order differential equation, which is equivalent to the Lorenz integrable system, and obtained a two-dimensional Lie symmetry algebra, which we then used to integrate the Lorenz integrable system in terms of Jacobi elliptic functions. Here we show that the same Lie symmetry algebra is admitted by a third-order differential equation which is equivalent to the Euler equations of a torque-free rigid body moving about a fixed point. Then a transformation is easily derived by which the Lorenz integrable system becomes the Euler equations of a torque-free rigid body moving about a fixed point. Thus, it can be stated that ''the Lorenz integrable system moves à la Poinsot.'' If the same transformation is applied to the Lorenz system with any value of parameters, then one obtains the Euler equations of a rigid body moving about a fixed point and subjected to a torsion depending on time and angular velocity. The numerical solution of this system yields a three-dimensional picture which resembles a ''tornado'' the cross-section of which has a butterfly-shape. By means of our transformation Lorenz's *butterfly* becomes a *tornado*.

In the last section the relationship between Lie group analysis and first integrals[35] is exemplified by considering the Euler equations of a torque-free rigid body about a fixed point and the Lorenz integrable system.

II. BUTTERFLIES AND TORNADOES

Consider the Lorenz system:[8]

$$x' = \tilde{\sigma}(y-x), \tag{1}$$

$$y' = -xz + \tilde{r}x - y, \tag{2}$$

$$z' = xy - \tilde{b}z, \tag{3}$$

where $\tilde{\sigma}$, $\tilde{b}$, and $\tilde{r}$ are parameters (a prime denotes differentiation with respect to τ). This system can be reduced to a single third-order ordinary differential equation for x,[41] which admits a two-dimensional Lie symmetry algebra if $\tilde{\sigma}=1/2$, $\tilde{b}=1$, and $\tilde{r}=0$. System (1)–(3) becomes

$$x' = \frac{(y-x)}{2}, \tag{4}$$

$$y' = -xz - y, \tag{5}$$

$$z' = xy - z. \tag{6}$$

The corresponding third-order equation is

$$2xx''' - 2x'x'' + 5xx'' - 3x'^2 + 2x^3x' + 3xx' + x^4 + x^2 = 0, \tag{7}$$

and admits a two-dimensional Lie symmetry algebra L_2 with basis:

$$X_1 = \partial_\tau, \qquad X_2 = e^{\tau/2}\left(\partial_\tau - \frac{1}{2}x\partial_x\right). \tag{8}$$

A basis of its differential invariants of-order $\leqslant 2$ is given by

$$\phi = \left(x' + \frac{x}{2}\right)x^{-2}, \qquad \psi = \left(x'' + \frac{3}{2}x' + \frac{x}{2}\right)x^{-3}. \tag{9}$$

Equation (7) is reduced to the following first-order equation:

$$(\psi - 2\phi^2)\frac{\mathrm{d}\psi}{\mathrm{d}\phi} = -2\psi\phi - \phi, \tag{10}$$

which can be easily integrated[40] to give

$$\frac{1+4\psi-4\phi^2}{(1+2\psi)^2} = c_1, \tag{11}$$

where c_1 is an arbitrary constant. The substitution of x and its derivatives into (11) yields a second-order ordinary differential equation,

$$\frac{1+4\left(x''+\frac{3}{2}x'+\frac{1}{2}x\right)x^{-3}-4\left(x'+\frac{1}{2}x\right)^2x^{-4}}{(x^3+2x''+3x'+x)^2x^{-6}} = c_1, \tag{12}$$

which admits the Lie symmetry algebra L_2. Lie's classification of two-dimensional algebras into four canonical types[20] allows us to integrate (12) by quadrature if we introduce the canonical variables:

$$v=-2e^{-\tau/2}, \qquad u=\frac{e^{-\tau/2}}{x}, \tag{13}$$

which transform Eq. (12) into

$$\frac{1+4\left(\frac{du}{dv}\right)^2-4u\frac{d^2u}{dv^2}}{\left[2u\frac{d^2u}{dv^2}-4\left(\frac{du}{dv}\right)^2-1\right]^2}=c_1, \tag{14}$$

and operators (8) into

$$\overline{X}_1=\partial_v, \qquad \overline{X}_2=v\partial_v+u\partial_u. \tag{15}$$

Then the general solution of (14) can be easily derived[20] to be

$$\int (-c_1\mp 2c_2u^2-c_2^2u^4)^{-1/2}du=\pm\frac{v}{2\sqrt{c_1}}+c_3, \tag{16}$$

with c_2 and c_3 arbitrary constants. This solution which involves an elliptic integral has already been obtained by Sen and Tabor[41] by means of a lengthier analysis.

The Euler equations describing the motion of a heavy rigid body about a fixed point with no torsion are

$$\dot{p}=\frac{(B-C)}{A}qr, \tag{17}$$

$$\dot{q}=\frac{(C-A)}{B}pr, \tag{18}$$

$$\dot{r}=\frac{(A-B)}{C}pq, \tag{19}$$

with A, B, and C being the principal moments of inertia, and $p(t)$, $q(t)$, and $r(t)$ the components of the angular velocity (a dot denotes differentiation with respect to t). This system can be reduced to a single third-order ordinary differential equation for, say, p, viz.,

$$p\frac{d^3p}{dt^3}-\frac{dp}{dt}\frac{d^2p}{dt^2}-\frac{4(C-A)(A-B)}{BC}p^3\frac{dp}{dt}=0, \tag{20}$$

which admits a two-dimensional Lie symmetry algebra $\mathcal{L}_2$ with basis:

$$\Gamma_1=\partial_t, \qquad \Gamma_2=t\partial_t-p\partial_p. \tag{21}$$

The two Lie symmetry algebras L_2 and $\mathcal{L}_2$ that we have found are actually the same, i.e., Type IV in Lie's classification.[20] Therefore they are linked by a transformation which takes (τ,x) into (t,p). Prolongation to the second-order of the two equivalent Lie symmetry algebras yields a transformation which takes the system (17)–(19) into the system (4)–(6) as

$$\tau=\log\left(\frac{4}{t^2}\right),$$

$$x=\frac{p\,t}{2},$$

$$y=\frac{C-B}{2A}qrt^2, \tag{22}$$

$$z=\frac{C-B}{2A}\left[\frac{(C-A)}{B}r^2+\frac{(A-B)}{C}q^2\right]t^2,$$

with the following condition on the momenta of inertia:

$$\frac{(A-B)(A-C)}{BC}=\frac{1}{4}. \tag{23}$$

A slightly more general condition could have been considered if one replaces 1/4 with $k/4$ (k an arbitrary parameter). If one derives B from (23) by assuming $A-C>0$ and $4A-3C>0$, i.e.,

$$B=\frac{4A(A-C)}{4A-3C}, \tag{24}$$

then the transformation (22) turns into the following:

$$\tau=\log\left(\frac{4}{t^2}\right),$$

$$x=\frac{p\,t}{2},$$

$$y=-\frac{(2A-C)(2A-3C)}{2A(4A-3C)}qrt^2, \tag{25}$$

$$z=-\frac{(2A-C)(2A-3C)[4A^2q^2-(4A-3C)^2r^2]}{8A^2(4A-3C)^2}t^2,$$

and the system (17)–(19) assumes the form

$$\dot{p}=\frac{(2A-C)(2A-3C)}{A(4A-3C)}qr, \tag{26}$$

$$\dot{q}=\frac{3C-4A}{4A}pr, \tag{27}$$

$$\dot{r}=\frac{A}{4A-3C}pq. \tag{28}$$

We also derive the inverse transformation, i.e.,

$$t=2e^{-\tau/2},$$

$$p=xe^{\tau/2}, \tag{29}$$

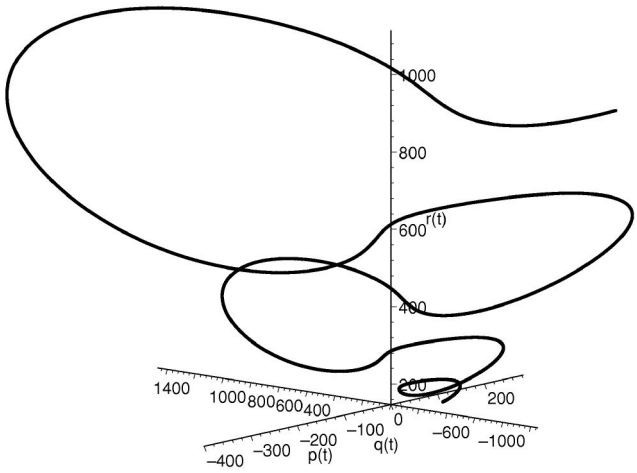

FIG. 1. The 3-dim plot of the ''tornado.''

$$q=-\frac{(4A-3C)ye^{\tau/2}}{2\sqrt{(2A-C)(2A-3C)(\sqrt{y^2+z^2}+z)}},$$

$$r=\frac{Ae^{\tau/2}\sqrt{\sqrt{y^2+z^2}+z}}{\sqrt{(2A-C)(2A-3C)}},$$

which takes the system (4)–(6) into the system (17)–(19) after substituting B as in (24).

If one applies the transformation (29) to the general Lorenz system (1)–(3), then the following equations are obtained:

$$\dot{p}=\frac{2(2A-C)(2A-3C)\tilde{\sigma}}{A(4A-3C)}qr+(2\tilde{\sigma}-1)\frac{p}{t}, \tag{30}$$

$$\dot{q}=\frac{3C-4A}{4A}pr+(\tilde{b}-1)\frac{4A^2q^2-(4A-3C)^2r^2}{4A^2q^2+(4A-3C)^2r^2}\frac{q}{t}+\tilde{r}\frac{2(4A-3C)^3A}{(2A-C)(2A-3C)[4A^2q^2+(4A-3C)^2r^2]}\frac{pr}{t^2}, \tag{31}$$

$$\dot{r}=\frac{A}{4A-3C}pq-(\tilde{b}-1)\frac{4A^2q^2-(4A-3C)^2r^2}{4A^2q^2+(4A-3C)^2r^2}\frac{r}{t}+\tilde{r}\frac{8(4A-3C)A^3}{(2A-C)(2A-3C)[4A^2q^2+(4A-3C)^2r^2]}\frac{pq}{t^2}. \tag{32}$$

They can be interpreted as the Euler equations of a rigid body moving about a fixed point and subjected to a torsion which depends on time t and angular velocity (p,q,r) in the body-frame reference. Also the momenta of inertia are linked by relation (24). To our knowledge such a system has never been described.

If we use Maple V in order to draw a three-dimensional plot of system (30)–(32), then a ''tornado,'' the cross-section of which resembles a butterfly, is obtained (Fig. 1). The usual values

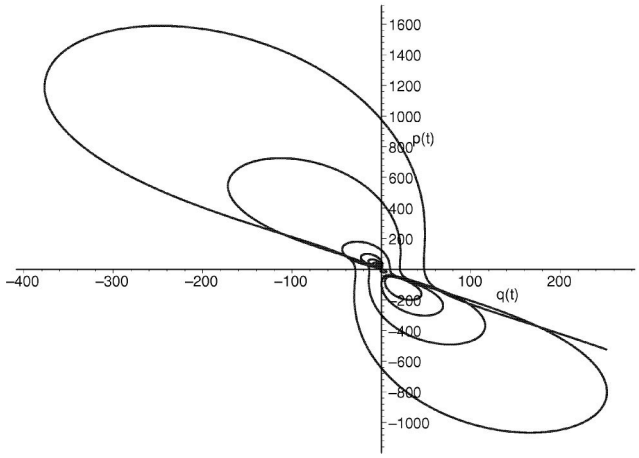

FIG. 2. The 2-dim plot of p vs q.

for the Lorenz parameters, $\tilde{\sigma}=10$, $\tilde{b}=8/3$, $\tilde{r}=28$, are imposed. Also we assume $A=2$ and $C=1$. We consider t as it varies in the interval $[2,0.015]$, which corresponds to $\tau\in[0,9.8]$ approximately. The step size used is 0.00005.

The butterfly-shape curve is better seen in Fig. 2, which shows the two-dimensional plot of p versus q.

A clearer view of the ''tornado'' is given in Fig. 3, which shows the two-dimensional plot of r versus q. Another view can be found in Fig. 4 which shows the two-dimensional plot of r versus p.

In Figs. 5 and 6 the plot of p versus t is given for two different but close initial values (1 and 1.01). For relatively large values of t, say $t\in[2,0.5]$, the solutions are the same (Fig. 5). For small t, say $t\in[0.05,0.015]$, a dramatic difference appears (Fig. 6).

In Ref. 42 it was found that one could explicitly derive a first integral of the Lorenz system (1)–(3) in six different instances which correspond to particular values of the Lorenz parameters. It is a trivial task to apply those findings to system (30)–(32) by using the transformation (22). The following is the list of the six cases with a relative first integral F for the system (30)–(32).

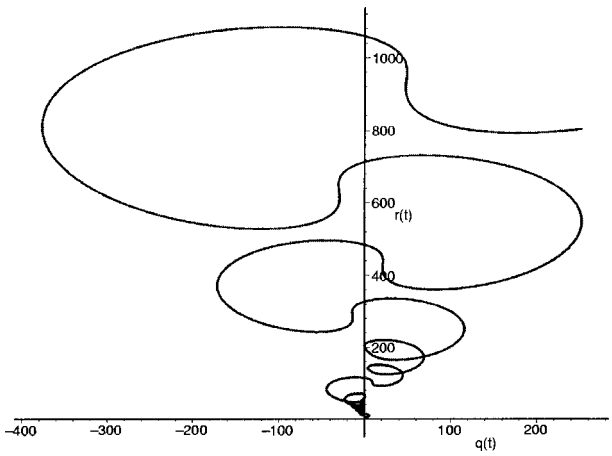

FIG. 3. The 2-dim plot of r vs q.

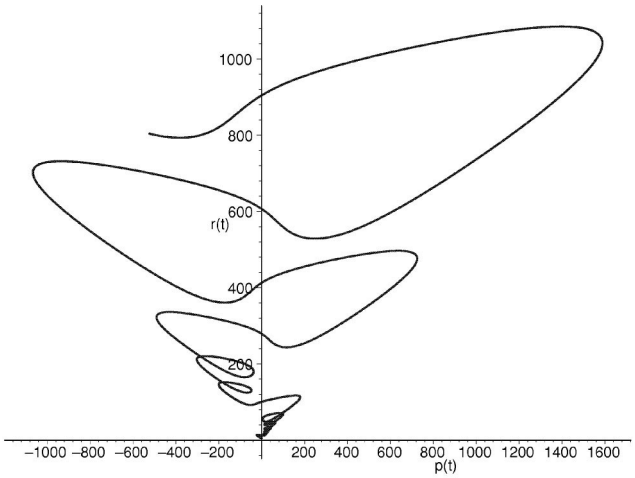

FIG. 4. The 2-dim plot of r vs p.

(1) $\tilde{b}=2\tilde{\sigma}$, $\tilde{r}$ arbitrary,

$$F=4^{2\tilde{\sigma}-1}t^{2(1-2\tilde{\sigma})}\left(p^2+\frac{[4A^2q^2-(4A-3C)^2r^2](2A-C)(2A-3C)\tilde{\sigma}}{A^2(4A-3C)^2}\right).$$

(2) $\tilde{b}=0$, $\tilde{\sigma}=1/3$, $\tilde{r}$ arbitrary,

$$F=4^{1/3}t^{-2/3}\left(-p^2\tilde{r}-2\frac{(2A-C)(2A-3C)}{3A(4A-3C)}pqrt-\frac{3}{16}p^4t^2\right.$$
$$\left.-\frac{(4A^2q^2-(4A-3C)^2r^2)(2A-C)(2A-3C)}{8A^2(4A-3C)^2}p^2t^2+\frac{(2A-C)^2(2A-3C)^2}{3A^2(4A-3C)^2}q^2r^2t^2\right).$$

(3) $\tilde{b}=1$, $\tilde{r}=0$, $\tilde{\sigma}$ arbitrary,

$$F=\frac{(4A^2q^2+(4A-3C)^2r^2)^2(2A-C)^2(2A-3C)^2}{4A^4(4A-3C)^4}.$$

(4) $\tilde{b}=4$, $\tilde{\sigma}=1$, $\tilde{r}$ arbitrary,

$$F=4t^{-6}\left(16p^2\tilde{r}+32\tilde{r}\frac{(4A^2q^2-(4A-3C)^2r^2)(2A-C)(2A-3C)}{A^2(4A-3C)^2}-p^4t^2\right.$$

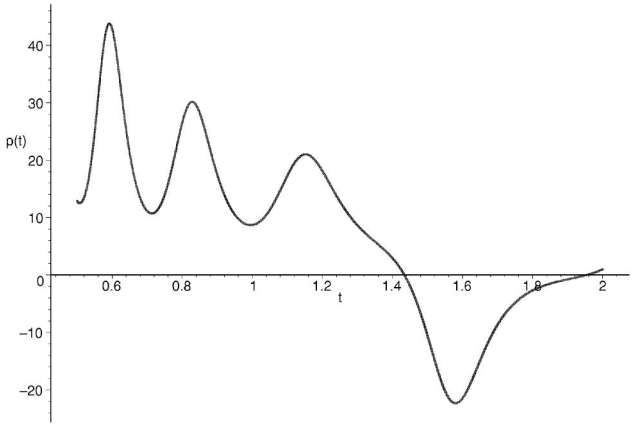

FIG. 5. Varying the initial condition of p in $t=2$ by 0.01. The two plots of $p(t), t\in[2,0.5]$ are indistinguishable.

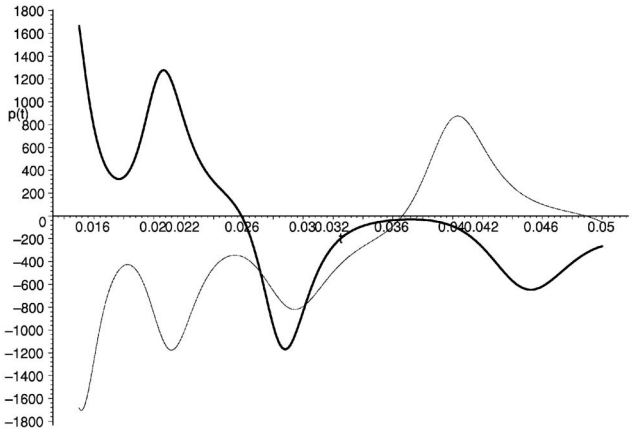

FIG. 6. Varying the initial condition of p in $t=2$ by 0.01. There are two different plots of $p(t), t\in[0.05,0.015]$: the darker line represents the plot of $p(t)$ with initial condition $p=1$ in $t=2$, and the lighter line the plot of $p(t)$ with initial condition $p=1.01$ in $t=2$.

$$-2\frac{(4A^2q^2-(4A-3C)^2r^2)(2A-C)(2A-3C)}{A^2(4A-3C)^2}p^2t^2+32\frac{(2A-C)(2A-3C)}{A(4A-3C)}pqrt$$
$$+16\frac{(2A-C)^2(2A-3C)^2}{A^2(4A-3C)^2}q^2r^2t^2-32\frac{(4A^2q^2-(4A-3C)^2r^2)(2A-C)(2A-3C)}{A^2(4A-3C)^2}\Bigg).$$

(5) $\tilde{b}=1$, $\tilde{\sigma}=1$, $\tilde{r}$ arbitrary,

$$F=-\frac{4}{t^2}p^2\tilde{r}+\frac{(4A^2q^2+(4A-3C)^2r^2)^2(2A-C)^2(2A-3C)^2}{4A^4(4A-3C)^4}.$$

(6) $\tilde{b}=6\tilde{\sigma}-2$, $\tilde{r}=2\tilde{\sigma}-1$

$$F=4^{4\tilde{\sigma}}t^{2(1-4\tilde{\sigma})}\Bigg(-\frac{p^4t^2}{64\tilde{\sigma}}-\tilde{\sigma}\frac{(4A^2q^2-(4A-3C)^2r^2)(2A-C)(2A-3C)}{32A^2(4A-3C)^2}p^2t^2+\frac{(2\tilde{\sigma}-1)^2}{4\tilde{\sigma}}p^2$$
$$+\frac{(2A-C)(2A-3C)(2\tilde{\sigma}-1)}{2A(4A-3C)}pqrt+\frac{(2A-C)^2(2A-3C)^2\tilde{\sigma}}{4A^2(4A-3C)^2}q^2r^2t^2\Bigg).$$

III. LIE GROUP ANALYSIS AND FIRST INTEGRALS

In Ref. 35 we showed the application of Lie group analysis in order to obtain first integrals with at least one missing variable. Consider Euler equations (17)–(19). There exist two well-known first integrals, i.e., the conservation of kinetic energy and the conservation of angular momentum:

$$Ap^2+Bq^2+Cr^2=I_1, \tag{33}$$

$$A^2p^2+B^2q^2+C^2r^2=I_2. \tag{34}$$

We derive p from (19) (the method works independently of the chosen equation) as

$$p=\frac{C\dot{r}}{(A-B)q},$$

in order to obtain the following two differential equations in q and r, one of first-order and one second-order, respectively:

$$\dot{q}=\frac{C(C_A)r\dot{r}}{B(A-B)q}, \tag{35}$$

$$\ddot{r}=\frac{C(C-A)}{B(A-B)q^2}r\dot{r}^2+\frac{(B-C)(A-B)}{AC}rq^2. \tag{36}$$

When Lie group analysis of the system (35)–(36) is performed, a linear partial differential equation of a parabolic structure is generated. Its characteristic curve is given by

$$B(A-B)q^2+C(A-C)r^2,$$

which is a combination of the two first integrals (33) and (34). Consequently we introduce the new dependent variable s such that

$$q=\sqrt{\frac{C(C-A)r^2+s}{B(A-B)}}, \tag{37}$$

in order to obtain the following system:

$$\dot{s}=0, \tag{38}$$

$$\ddot{r}=\frac{C(C-A)r\dot{r}^2}{C(C-A)r^2+s}+\frac{(C-A)(B-C)r^3}{AB}+\frac{(B-C)sr}{ABC}. \tag{39}$$

Equation (39) admits an eight-dimensional Lie symmetry algebra (i.e., it is linearizable) if either $A=C$ or $B=C$, i.e., the case of the torque-free Lagrange top (uniform precession). If either q or r, one at a time, is eliminated from system (17)–(19), then a similar result is obtained, i.e., the other two combinations of the first integrals (33) and (34). Indeed the elimination of q yields the first integral,

$$A(A-B)p^2+C(B-C)r^2,$$

and the elimination of r yields the first integral

$$B(B-C)q^2+A(A-C)p^2.$$

If the same method is applied to the Lorenz integrable system (4)–(6), then the following two first integrals are obtained:

$$(y^2+z^2)\,e^{2\tau}, \tag{40}$$

$$(z-x^2)\,e^{\tau}. \tag{41}$$

Those first integrals were found in Ref. 12 by using the Painlevé analysis.

From (6) we have

$$x=\frac{z'+z}{y},$$

in order to obtain the following two differential equations in y and z: one of first-order and one second-order, respectively:

$$y'=-\frac{y^2+z^2+zz'}{y}, \tag{42}$$

$$z''=\frac{y^4-3y^2z-5y^2z'-2z^3-4z^2z'-2zz'^2}{2y^2}. \tag{43}$$

When the Lie group analysis of the system (42)–(43) is performed, a linear partial differential equation of a parabolic structure is generated. Its characteristic curve is given by

$$y^2+z^2.$$

Consequently we introduce the new dependent variable Y such that

$$y=\sqrt{Y-z^2}, \tag{44}$$

in order to obtain the following system:

$$Y'=-2Y, \tag{45}$$

$$z''=\frac{Y^2-2Yz^2-3Yz-5Yz'+z^4+z^3+z^2z'-2zz'^2}{2(Y-z^2)}. \tag{46}$$

The first equation can be easily integrated to yield the first integral (40). If we eliminate y from system (4)–(6), a similar procedure provides the first integral (41).

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Asymptotic behavior of the centroids of a family of vortices

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(Received 2 February 2003; accepted 24 April 2003)

In this article we consider a family of minimization problems whose solutions represent the vortices of two dimensional flows. We prove that if we consider an admissible sequence of vortices, then the corresponding centroids converge to the global minimizer of the Routh function associated with an appropriate energy functional. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1597947]

I. INTRODUCTION

It is well known that for isochoric (volume-preserving) plane motion of a fluid, the velocity field $\mathbf{u}(x_1,x_2)$ satisfies the continuity equation $\nabla\cdot\mathbf{u}=0$, which is identically satisfied if we write

$$\mathbf{u}=\left(\frac{\partial\psi}{\partial x_2},-\frac{\partial\psi}{\partial x_1}\right),$$

where ψ is the stream function, which is constant on any curve everywhere tangent to the velocity field. It is also well known that for an incompressible fluid, the dynamical equations of plane motion can be reduced to the vorticity equation

$$\frac{\partial\omega}{\partial t}+\mathbf{u}\cdot\nabla\omega=0,$$

where $\omega=-\Delta\psi$ is the (scalar) vorticity (i.e., the nonzero component of $\nabla\times\mathbf{u}$). Note that when $\omega=0$, the flow is said to be irrotational. It follows that for steady motion (no time dependence) the Jacobian determinant of ψ and ω vanishes; that is,

$$[\psi,\omega]=0, \tag{1}$$

and so ψ and ω are functionally dependent. Inserting $\omega=-\Delta\psi$ into (1) we derive

$$[\psi,-\Delta\psi]=0. \tag{2}$$

Therefore, if ϕ is any real valued function and ψ is a solution of the semilinear equation

$$-\Delta\psi=\phi(\psi), \tag{3}$$

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then ψ is also a solution of (2). So, a solution of (3) would represent the stream function of a two dimensional ideal fluid. For the mathematical background in fluid dynamics the reader is referred to Ref. 15.

In Ref. 11, it was proved that the following inverse (the nonlinearity ϕ was not known *a priori*) problem,

$$\begin{gathered} -\Delta\psi=\phi(\psi) \quad \text{in } \Omega, \\ \psi=0 \quad \text{on } \partial\Omega, \\ -\Delta\psi\in\mathcal{F}, \\ \psi\to\lambda x_1x_2 \quad \text{at infinity,} \end{gathered} \tag{4}$$

has a solution, where Ω was a set obtained by excluding a region containing the origin and $\mathcal{F}$ was the set of rearrangements of a given function (see the next section for definition). Any solution of (4), recalling the above discussion, represents a planar ideal fluid in Ω which is tangential to $\partial\Omega$ ($\psi=0$ on $\partial\Omega$), its vorticity belongs to $\mathcal{F}$, and behaves as an irrotational flow at long range points ($\psi\to\lambda x_1x_2$). The proof was based on the extensively developed rearrangement variational principles for strictly convex functionals which are weakly sequentially continuous. More precisely, it was shown that for $\Psi_\lambda=\Psi-\lambda\mathcal{I}$, the difference of a quadratic and a linear integral functional over Ω, the variational problem

$$P_\lambda: \quad \sup_{\zeta\in\mathcal{F}}\Psi_\lambda(\zeta) \tag{5}$$

is solvable for small positive values of λ. The corresponding Euler–Lagrange equation at a solution of (5) would then provide a solution for (4). It was shown that using a standard rescaling $[\zeta(x)\to c\zeta(c^{1/2}x)]$, one converts (5) into a new parametrized family of variational problems

$$\hat{P}_c: \quad \sup_{\zeta\in\mathcal{F}_c}\hat{\Psi}_c(\zeta), \tag{6}$$

which are easier to deal with essentially because the rescaling would elliminate the λ in front of the linear part of Ψ_λ at the price of having all the integrals involved in $\hat{\Psi}_c$ over the rescaled Ω, denoted Ω_c (see the next section for definitions). It was proved in Ref. 11 that (6) is solvable provided $c\gg1$; this implies that (5) is solvable when λ is small enough. Since solutions of (6) also represent steady flows, in this article we would like to consider (6) independent of (5), and prove an asymptotic result concerning the centroids of the solutions of (6). We will show that if c_n is an admissible sequence, and if ζ_{c_n} is any solution of $\hat{P}_{c_n}$, then the sequence of centroids of ζ_{c_n} will converge to the global maximizer of the Routh function

$$H(x)=\frac{1}{4\pi}\log\frac{|x|}{2x_1x_2}+x_1x_2.$$

This result is stated in Theorem 3 of the next section.

Badiani[1] considered a similar situation where Ω in his case was the upper half plane excluding a region containing the origin. Since the upper half plane is symmetric with respect to the x_2-axis, the author of Ref. 1 could make effective use of Steiner symmetrization techniques. However, in our case, due to lack of symmetry of the quarter plane, we are unable to use Steiner symmetrization, so we need to obtain novel estimates in order to make up for this deficiency. Moreover, these estimates can be similarly reproduced for the upper half plane case and in fact for any wedge type domains in general.

The main mathematical difficulty in proving solvability of problems like $\hat{P}_c$ is the unboundedness of the domain of the problem which makes the usual direct method of calculus of variations *unavailable*. However, it is well known that essential information can be extracted from considering $\hat{P}_c$ first on bounded domains (see Ref. 2). Therefore, for the convenience of the reader we end this section with a brief review of the variational principle suitable for proving solvability of variational problems similar to $\hat{P}_c$. For a complete treatment the reader is referred to Ref. 11.

Let Ω be a bounded domain in $\mathbb{R}^2$; let p and q be conjugate exponents, that is, $1/p+1/q=1$, for $2<p<\infty$. Suppose that $\Phi: L^p(\Omega)\to\infty$ is a convex functional and $\mathcal{F}(\Omega)$ is the set of rearrangements of a given function $f_0\in L^p(\Omega)$. Then the following result was obtained by Burton:[4] *If Φ is weakly sequentially continuous, then Φ attains a maximum relative to $\mathcal{F}(\Omega)$. In addition, if Φ is strictly convex and f^* is a maximizer relative to $\mathcal{F}(\Omega)$ and $g\in\partial\Phi(f^*)$, subdifferential of Φ at f^*, then*

$$f^*=\phi\circ g, \tag{7}$$

almost everywhere in Ω for some increasing function ϕ.

Note that in case Φ is differentiable, which is indeed the case we are interested in, then $\partial\Phi(f^*)=\{\Phi'(f^*)\}$. Therefore (7) turns into

$$f^*=\phi\circ\Phi'(f^*), \tag{8}$$

almost everywhere in Ω. Equation (8) will prove to be the main ingredient in our analysis; in particular it is very helpful in deriving essential estimates.

Rearrangement variational problems have been an active field of research in recent years; see Refs. 1, 5, 6, and 9–12 for theoretical results and Refs. 7 and 8 for numerical results.

II. NOTATION, DEFINITIONS AND THE STATEMENT OF THE MAIN RESULTS

Henceforth p is an arbitrary fixed number in $(2,\infty)$. For any number $r\geqslant 1$, r^* denotes the conjugate exponent, $1/r+1/r^*=1$. For a measurable set $E\subseteq\mathbb{R}^2$, $|E|$ denotes the Lebesgue measure of E. The ball centered at x with radius ξ is denoted $B_\xi(x)$; in the case where the center is the origin we write B_ξ. Given a measurable set $A\subseteq\mathbb{R}^2$, $x\in\mathbb{R}^2$ is called a density point of A whenever

$$|B_\epsilon(x)\cap A|>0,$$

for every $\epsilon>0$. The set of all density points of A is denoted $\mathrm{den}(A)$. The essential diameter of A, denoted $\mathrm{diam}(A)$, is defined by

$$\mathrm{diam}(A)=\sup\{|x-y|:\ \ x,y\in\mathrm{den}(A)\}.$$

Let D be an open, bounded, simply connected set containing the origin and assume $\overline{D}\subset B_1$. Let Π_+ denote the open first quadrant; let $\Omega=\Pi_+\backslash\overline{D}$ such that $\partial\Omega\in C^2$. For $c>0$ we set

$$\Omega_c=\{x\in\Pi_+|\ \ c^{1/2}x\in\Omega\}.$$

The symbols G_+, G, G_B and G_c denote the Green's functions for $-\Delta$ with homogeneous Dirichlet boundary conditions in Π_+, Ω, $\Pi_+\backslash\overline{B_1}$ and Ω_c, respectively. It is well known that

$$G_+(x,y)=\frac{1}{2\pi}\log\frac{|x-\overline{y}|\ \ |x-\underline{y}|}{|x-y|\ \ |x-\underline{\overline{y}}|},\qquad x,y\in\Pi_+,\ \ x\neq y,$$

where the overline and the underline signs designate the reflections with respect to x_1 and x_2 axes, respectively. We also have the following identity:

$$G_c(x,y)=G(c^{1/2}x,c^{1/2}y), \quad x,y\in\Omega_c, \quad x\neq y.$$

By applying the maximum principle we readily obtain

$$G_B(x,y)\leqslant G_c(x,y)\leqslant G_+(x,y), \tag{9}$$

where each inequality holds in the positive domain. For a measurable function ζ and $x\in\mathbb{R}^2$ we define

$$K_+\zeta(x)=\int_{\Pi_+} G_+(x,y)\quad \zeta(y)dy,$$

$$K\zeta(x)=\int_{\Omega} G(x,y)\quad \zeta(y)dy,$$

$$K_c\zeta(x)=\int_{\Omega_c} G_c(x,y)\quad \zeta(y)dy,$$

whenever the integrals exist.

We let $\eta\in C^2(\Omega)\cap C^1(\overline{\Omega})$ be a function satisfying

$$\Delta\eta=0 \quad \text{in} \quad \Omega,$$

$$\eta=0 \quad \text{on} \quad \partial\Omega,$$

$$\eta=x_1x_2+O(|x|^{-2}) \quad \text{as} \quad |x|\to\infty,$$

$$\nabla\eta=(x_2,x_1)+O(|x|^{-3}), \quad \text{as} \quad |x|\to\infty,$$

and

$$x_1x_2-\frac{x_1x_2}{|x|^4}\leqslant\eta\leqslant x_1x_2, \quad x\in\Omega. \tag{10}$$

Let us fix $\zeta_0\in L^p(\Omega)$, a non-negative, nontrivial function with compact support and assume $|\text{supp}(\zeta_0)|=\pi a^2$, for some $a>0$. In addition, we suppose that $\|\zeta_0\|_1=1$. A measurable function ζ is said to be a rearrangement of ζ_0 on Ω whenever

$$|\{x\in\Omega|\quad \zeta(x)\geqslant\alpha\}|=|\{x\in\Omega|\quad \zeta_0(x)\geqslant\alpha\}|,$$

for every $\alpha\in\mathbb{R}$. The set of all rearrangements of ζ_0 on Ω, with compact support, is denoted $\mathcal{F}$. For $c>0$ and a measurable function ζ we define

$$\mathcal{C}_c(\zeta)(x)=c\,\zeta(c^{1/2}x), \quad x\in\Omega_c. \tag{11}$$

The mapping $\mathcal{C}_c$ as defined in (11) takes measurable functions on Ω to measurable functions on Ω_c. By $\mathcal{F}_c$ we denote the set of all rearrangements of $\mathcal{C}_c(\zeta_0)$ on Ω_c with compact support. Given a measurable function ζ on Ω_c, $c>0$, we define the energy functional

$$\hat{\Psi}_c(\zeta)=\frac{1}{2}\int_{\Omega_c}\zeta\quad K_c\zeta-\int_{\Omega_c}\eta_c\zeta, \tag{12}$$

where $\eta_c(x)=c^{-1}\quad \eta(c^{1/2}x)$, whenever the integrals exist. For $c>0$ we set

$$\hat{P}_c: \quad \sup_{\zeta \in \mathcal{F}_c} \hat{\Psi}_c(\zeta).$$

The solution set for $\hat{P}_c$ is denoted Σ_c. Let us note that from (10) we infer

$$x_1x_2 - \frac{x_1x_2}{c^2|x|^4} \leqslant \eta_c(x) \leqslant x_1x_2, \qquad x \in \Omega_c. \tag{13}$$

We end this section with a result from Ref. 11 (Theorem 1) followed by the main results of this article (Theorems 2 and 3).

Theorem 1: *There exists $c^0>0$ such that for $c \geqslant c^0$, $\hat{P}_c$ is solvable. Moreover, if $\zeta \in \Sigma_c$, then*

$$\mathrm{supp}(\zeta) \subset B_{R(c)},$$

where $R(c)$ is a constant merely depending on c which satisfies

$$R(c) \leqslant Ac^{1/2}, \tag{14}$$

for some $A>0$. In addition we have

$$\mathrm{supp}(\zeta) = \{x \in \Omega_c : K_c\zeta(x) - \eta_c(x) \geqslant \gamma_c\}, \tag{15}$$

where γ_c is a constant depending on c satisfying the following inequality:

$$\gamma_c \geqslant \frac{1}{2\pi} \log \frac{c^{1/2}}{2a} + C. \tag{16}$$

Theorem 2: *There exist $c^1 \geqslant c^0$ and $R>0$ such that if $c \geqslant c^1$ and $\zeta \in \Sigma_c$, then*

$$\mathrm{supp}(\zeta) \subseteq B_R, \tag{17}$$

modulo a set of measure zero.

Before stating our last result we need the following definitions.

Definition 1: For a measurable function f on $S \subseteq \mathbb{R}^2$, the centroid of f, denoted $\mathrm{cent}(f)$, is defined by

$$\mathrm{cent}(f) = \int_S x \quad f(x)dx.$$

Definition 2: Suppose $\{c_j\}$ is a sequence of real numbers and ζ_{c_j} is a measurable function on Ω_{c_j}, for $j \in \mathbb{N}$. We say the sequence $\{\zeta_{c_j}\}$ is admissible whenever $\{\mathrm{cent}(\zeta_{c_j})\}$ is a convergent sequence in $\mathbb{R}^2$.

Remark: Let us point out that if $\{c_j\}$ is a sequence with $c_j \geqslant c^1$, and $\zeta_{c_j} \in \Sigma_{c_j}$, $j \in \mathbb{N}$, then by Theorem 2, $\{\zeta_{c_j}\}$ contains a subsequence which is admissible.

Theorem 3: *Suppose $\{c_j\}$ is a sequence of real numbers tending to infinity. Suppose $\zeta_{c_j} \in \Sigma_{c_j}$, and $\{\zeta_{c_j}\}$ is admissible. Then*

$$\mathrm{cent}(\zeta_{c_j}) \to \hat{x}, \tag{18}$$

as $j \to \infty$.

Throughout the article the symbol C always indicates a universal constant which may appear in consecutive steps with different values.

III. PRELIMINARIES

In this section we recall some results from Ref. 11. We begin with the following identities:

$$G(x,y)=\frac{1}{2\pi}\log\frac{1}{|x-y|}-h(x,y),$$

$$G_+(x,y)=\frac{1}{2\pi}\log\frac{1}{|x-y|}-h_+(x,y),$$

$$G_B(x,y)=\frac{1}{2\pi}\log\frac{1}{|x-y|}-h_B(x,y),$$

where h, h_+, and h_B are harmonic functions, for fixed y, in their respective domains. From (9) it follows that

$$h_+(x,y)\leqslant h(x,y)\leqslant h_1(x,y), \tag{19}$$

where the inequalities are understood to hold in the positive domains. We set $\hat{h}=h-h_+$ and $\hat{h}_1=h_1-h_+$. Then from (19) we infer $0\leqslant\hat{h}\leqslant\hat{h}_1$; also elementary calculations verify that

$$\hat{h}_1(x,y)\leqslant\frac{x_2y_2}{\pi(|x||y|-1)^2}\ , \tag{20}$$

provided $x,y\in\Pi_+\backslash\overline{B}_1$. Similarly, we obtain

$$0\leqslant\hat{h}_1(x,y)\leqslant\frac{x_1y_1}{\pi(|x||y|-1)^2}\ , \tag{21}$$

provided $x,y\in\Pi_+\backslash\overline{B}_1$.

Let $\zeta\in L^p(\Omega)$ have compact support. Then $K_+\zeta(x)$ is defined at every point $x\in\mathbb{R}^2$ (see Ref. 9). Thus from

$$|K\zeta(x)|\leqslant K|\zeta|(x)\leqslant K_+|\zeta|(x),$$

it follows that $K\zeta(x)$ is defined at every $x\in\mathbb{R}^2$.

For $c>0$, let $\mathcal{C}_c:\mathcal{F}\to\mathcal{F}_c$ be defined as in (11). Then $\mathcal{C}_c$ is a bijection. Moreover, if $\zeta\in\mathcal{F}$, then

(i) $\|\mathcal{C}_c(\zeta)\|_p=c^{1/p^*}\ \|\zeta\|_p$ and
(ii) $|\mathrm{supp}(\mathcal{C}(\zeta))|=c^{-1}\ |\mathrm{supp}(\zeta)|$, where $\mathrm{supp}(\cdot)$ denotes the usual support of a function.

The Routh function associated with $\hat{P}_c$ is denoted $H(x)=H_1(x)+H_2(x)$, $x\in\Pi_+$, where

$$H_1(x)=\frac{1}{4\pi}\log\frac{|x|}{2x_1x_2},$$

$$H_2(x)=x_1x_2.$$

Observe that for $z\in\partial\Pi_+$ we have $\lim_{x\to z}H(x)=\infty$. Elementary calculations prove that H has a unique global minimum at $\hat{x}=(\hat{x}_1,\hat{x}_2):=(1/(2\sqrt{2\pi}),1/(2\sqrt{2\pi}))$. For more information on the Routh function the reader is referred to the classic monograph, Ref. 14.

IV. AN AUXILIARY LEMMA

The main feature of this section is the following support lemma which is a crucial tool in the analysis to follow. We first need the following result from Ref. 1.

Proposition: Suppose $Q \geqslant 1$ and $c \geqslant 4a^2$. Let $v \in L^p(\Pi_+)$ be a non-negative function vanishing outside a set of measure πa^2 and define $v_c(x) = C_c(v)(x)$. For $x \in \Pi_+$, we set $\hat{B}(x) = B_{Qa/c^{1/2}}(x)$ and

$$I(x) = \int_{\hat{B}(x)} \log\left(\frac{2a|x-\overline{y}|}{c^{1/2}|x-y|}\right) \; v_c(y)dy,$$

$$\overline{I}(x) = \int_{\hat{B}(x)} \log\left(\frac{2a|x-\underline{y}|}{c^{1/2}|x-y|}\right) \; v_c(y)dy.$$

Then there exist constants N_1, N_2, N_3, N_1', N_2' and N_3' such that

$$I(x) \leqslant \begin{cases} (N_1 + N_2|\log x_2|)\|v\|_p, & x_2 \geqslant a, \\ N_3\|v\|_p, & 0 < x_2 \leqslant a, \end{cases} \tag{22}$$

and

$$\overline{I}(x) \leqslant \begin{cases} (N_1' + N_2'|\log x_1|)\|v\|_p, & x_1 \geqslant a, \\ N_3'\|v\|_p, & 0 < x_1 \leqslant a. \end{cases} \tag{23}$$

Lemma (support lemma): Let c^0 be as in Theorem 1. Then there exist $\check{c} > c^0$ and $d > 0$ such that if $c \geqslant \check{c}$, then

$$\operatorname{diam}(\operatorname{supp}(\check{\zeta}_c)) \leqslant d, \tag{24}$$

for all $\check{\zeta}_c \in \Sigma_c$.

Proof: It suffices to set $\check{c} = \max\{c^0, 4a^2\}$. Fix $c \geqslant \check{c}$ and $\check{\zeta}_c \in \Sigma_c$. From (15) and (16) we infer

$$K_c\check{\zeta}_c(x) - \eta_c(x) \geqslant \frac{1}{2\pi}\log\frac{c^{1/2}}{2a} + C,$$

for almost every $x \in \operatorname{supp}(\check{\zeta}_c)$. Since $K_c\check{\zeta}_c(x) \leqslant K_+\check{\zeta}_c(x)$ we deduce

$$\eta_c(x) + C \leqslant K_+\check{\zeta}_c(x) - \frac{1}{2\pi}\log\frac{c^{1/2}}{2a} = \frac{1}{2\pi}\int_{\Omega_c} \log\frac{2a|x-\overline{y}||x-\underline{y}|}{c^{1/2}|x-y||x-\overline{\underline{y}}|}\,\check{\zeta}_c(y)dy, \tag{25}$$

for almost every $x \in \operatorname{supp}(\check{\zeta}_c)$. Let us set $S = \{x \in \Pi_+ \mid \min\{x_1, x_2\} > a\}$ and for $x \in \Pi_+$ define

$$J(x) = \frac{1}{2\pi}\int_{\hat{B}(x)} \log\frac{2a|x-\overline{y}||x-\underline{y}|}{c^{1/2}|x-y||x-\overline{\underline{y}}|}\;\check{\zeta}_c(y)dy,$$

where $\hat{B}(x)$ is defined as in the proposition. Observe that for x, $y \in \Pi_+$ we have $|x-\overline{y}|/|x-\overline{\underline{y}}| < 1$ and $|x-\underline{y}|/|x-\overline{\underline{y}}| < 1$. Hence, for $x \in \Pi_+ \backslash S$ we can apply (22) and (23) to obtain

$$J(x) \leqslant N_3''\|\zeta_0\|_p, \tag{26}$$

where $N'' = \max\{N_3, N_3'\}$. Also, for $x \in S$ we have

$$J(x) \leqslant I(x) \leqslant (N_1 + N_2|\log x_2|) \;\; \|\zeta_0\|_p. \tag{27}$$

Therefore, from (25)–(27) we infer that for almost every $x \in \mathrm{supp}(\check{\zeta}_c)$ we have

$$\eta_c(x)+C \leqslant \frac{1}{2\pi}\int_{\Omega_c\setminus\hat{B}(x)} \log\left(\frac{2a|x-\overline{y}|}{c^{1/2}|x-y|}\right)\ \check{\zeta}_c(y)dy+\begin{cases}(N_1+N_2|\log x_2|)\|\zeta_0\|_p, & x\in S,\\ N_3''\|\zeta_0\|_p, & x\in \Pi_+\setminus S.\end{cases} \tag{28}$$

Since $\mathrm{supp}(\check{\zeta}_c)$ is essentially contained in $B_{R(c)}$ and $R(c)\leqslant Ac^{1/2}$, by (14), we obtain

$$\frac{1}{2\pi}\int_{\Omega_c\setminus\hat{B}(x)} \log\left(\frac{2a|x-\overline{y}|}{c^{1/2}|x-y|}\right)\ \check{\zeta}_c(y)dy \leqslant \frac{1}{2\pi}\log\frac{4R(c)}{Q}\int_{\Omega_c\setminus\hat{B}(x)}\check{\zeta}_c(y)dy, \tag{29}$$

for every $x\in\Pi_+$. Therefore by (29) and rearranging the terms in (28) we infer that for almost every $x\in\mathrm{supp}(\check{\zeta}_c)$ we have

$$\frac{1}{2\pi}\log\frac{Q}{4R(c)}\int_{\Omega_c\setminus\hat{B}(x)}\check{\zeta}_c(y)dy\leqslant\begin{cases}N_3''\|\zeta_0\|_p+C-\eta_c(x), & x\in\Pi_+-S,\\ (N_1+N_2|\log x_2|)\|)\|\zeta_0\|_p+C-\eta_c(x), & x\in S.\end{cases}$$

From this we deduce the existence of a positive constant ν such that

$$\log\frac{Q}{4R(c)}\int_{\Omega_c\setminus\hat{B}(x)}\check{\zeta}_c(y)dy<\nu. \tag{30}$$

Let us now set $Q=4R(c)e^{2\nu}$. Then, from (30) we obtain

$$\int_{\Omega_c\setminus\hat{B}(x)}\check{\zeta}_c(y)dy<\frac{1}{2}, \tag{31}$$

for almost every $x\in\mathrm{supp}(\check{\zeta}_c)$. We now claim that

$$\mathrm{diam}(\mathrm{supp}(\check{\zeta}_c))\leqslant 8aR(c)e^{2\nu}/c^{1/2}. \tag{32}$$

To seek a contradiction suppose this is not true, that is, $\mathrm{diam}(\mathrm{supp}(\check{\zeta}_c))>8aR(c)e^{2\nu}/c^{1/2}$. In this case, there exist x and y in $\mathrm{den}(\mathrm{supp}(\check{\zeta}_c))$ such that $|x-y|>8aR(c)e^{2\nu}/c^{1/2}$. Hence $B_{8aR(c)e^{2\nu}/c^{1/2}}(x)$ and $B_{8aR(c)e^{2\nu}/c^{1/2}}(y)$ are disjoint. Thus, by (31), we obtain

$$1<\int_{B_{8aR(c)e^{2\nu}/c^{1/2}}(x)}\check{\zeta}_c(w)dw+\int_{B_{8aR(c)e^{2\nu}/c^{1/2}}(y)}\check{\zeta}_c(w)dw\leqslant 1,$$

which is a contradiction, hence from (14) and (32) we obtain (24). □

V. PROOFS OF THEOREMS 2 AND 3

Proof of Theorem 2: The proof consists of three assertions.

Assertion 1: Let $\check{c}$ be as in the lemma. Then there exist $c_1'\geqslant\check{c}$ and $\overline{R}>0$ such that if $c\geqslant c_1'$ and $\check{\zeta}_c\in\Sigma_c$, then

$$\mathrm{supp}(\check{\zeta}_c)\subset L(2d)\cup(\Pi_+\cap B_{\overline{R}}), \tag{33}$$

modulo a set of measure zero. Here

$$L(2d)=\{x\in\Pi_+|\ \ \min\{x_1,x_2\}\leqslant 2d\}, \tag{34}$$

where d is the bound stated in the lemma.

Proof of Assertion 1: Suppose the assertion is false. Hence there exist sequences $\{c_j\}$, $\{\check{\zeta}_{c_j}\}$ and $\{x_j\}$ such that

(a) $\check{c} \leqslant c_j \to \infty$, as $j \to \infty$,
(b) $\check{\zeta}_{c_j} \in \Sigma_{c_j}$, for all j, and
(c) $x_j = (x_{j,1}, x_{j,2}) \in \mathrm{den}(\mathrm{supp}(\check{\zeta}_{c_j}))$, for all j, and $|x_j| \to \infty$, as $j \to \infty$.

For simplicity, when appropriate, we replace c_j by j, thus we write $\hat{\Psi}_j$ for $\hat{\Psi}_{c_j}$, $\check{\zeta}_j$ for $\check{\zeta}_{c_j}$. The Schwarz-symmetrization of $\check{\zeta}_j$ with respect to $\hat{x}$ is denoted by ζ_j^*. Without loss of generality we may assume that $\mathrm{supp}(\zeta_j^*) \subset B_{1/4\sqrt{2\pi}}(\hat{x})$ for all j. Fixing j, we observe, from the lemma, that $\mathrm{supp}(\check{\zeta}_j)$ is essentially contained in $\Pi_+ \backslash L(d)$, where

$$L(d) = \{x \in \Pi_+ | \quad \min\{x_1, x_2\} \leqslant d\}.$$

Therefore

$$\begin{aligned}\hat{\Psi}_j(\zeta_j^*) - \hat{\Psi}_j(\check{\zeta}_j) \geqslant & \int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + \eta_j(x)\right) \quad \check{\zeta}_j(x)\check{\zeta}_j(y)dxdy \\ & - \int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + \eta_j(x)\right) \quad \zeta_j^*(x)\zeta_j^*(y)dxdy,\end{aligned} \tag{35}$$

where we have applied an n-dimensional generalization of an inequality of F. Riesz on rearrangements to the logarithmic parts (see, for example, Ref. 3). Since $h \geqslant h_+$ we infer

$$\begin{aligned}\frac{1}{2}h(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + \eta_j(x) &\geqslant \frac{1}{4\pi}\log\frac{|x-\overline{y}|}{c_j^{1/2}|x-\overline{y}||x-\underline{y}|} - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + x_1x_2 - \frac{x_1x_2}{c_j^2|x|^4} \\ &\geqslant \frac{1}{4\pi}\log\frac{|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}|} + \frac{1}{2}x_1x_2,\end{aligned} \tag{36}$$

for all x, $y \in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$. Also, note that for x, $y \in \mathrm{supp}(\zeta_j^*) \subset B_{1/4\sqrt{2\pi}}(\hat{x})$ we have

$$\begin{aligned}\frac{1}{2}h(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + \eta_j(x) &\leqslant \frac{1}{2}\hat{h}(c_j^{1/2}x, c_j^{1/2}y) + \frac{1}{2}h_+(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c^{1/2}} + x_1x_2 \\ &\leqslant \frac{1}{2}\hat{h}_1(c_j^{1/2}x, c_j^{1/2}y) + \frac{1}{4\pi}\log\frac{|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}|} + x_1x_2 \\ &\leqslant \frac{c_jx_1x_2}{2\pi(c_j|x||y|-1)^2} + \frac{1}{4\pi}\log\frac{|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}|} + x_1x_2 \leqslant K_1,\end{aligned} \tag{37}$$

provided j is sufficiently large; here, K_1 is positive constant.

Let us assume that $x_{j,2} \to \infty$, as $j \to \infty$ (the case where $x_{j,1} \to \infty$ can be treated similarly); moreover we may assume that for almost every $x = (x_1, x_2) \in \mathrm{supp}(\check{\zeta}_j)$ we have $x_2 \leqslant x_{j,2}$. Therefore, by (36), for x, $y \in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$ we find

$$\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}+\eta_j(x)\geqslant\frac{1}{4\pi}\log\frac{1}{|x-\bar{y}|}+\frac{1}{2}d(x_{j,2}-d)$$
$$\geqslant\frac{1}{4\pi}\log\frac{1}{2x_{j,2}}+\frac{1}{2}d(x_{j,2}-d)\to\infty, \tag{38}$$

as $j\to\infty$. Hence from (35), (37), and (38) we deduce

$$\hat{\Psi}_{j_0}(\zeta_{j_0}^*)-\hat{\Psi}_{j_0}(\check{\zeta}_{j_0})>0,$$

for some j_0 sufficiently large. This contradicts the maximality of $\check{\zeta}_{j_0}$. Hence the assertion is proved.

Assertion 2: Let c_1' be as in Assertion 1. Then there exists $\mu>0$ such that if $c\geqslant c_1'$ and $\check{\zeta}_c\in\Sigma_c$, then

$$\mathrm{supp}(\check{\zeta}_c)\subset\{x\in\Pi_+|\ \ x_1x_2<\mu\}, \tag{39}$$

modulo a set of measure zero.

Proof of Assertion 2: Let us fix $c\geqslant c_1'$ and consider $\check{\zeta}_c\in\Sigma_c$. From Assertion 1 it follows that there exists $\tau>a$ such that $\mathrm{supp}(\check{\zeta}_c)$ is essentially contained in $\mathbb{R}^+\times(0,\tau)$ or $(0,\tau)\times\mathbb{R}^+$. Let us first suppose that $\mathrm{supp}(\check{\zeta}_c)$ is essentially contained in $\mathbb{R}^+\times(0,\tau)$. Then for almost every $x=(x_1,x_2)\in\mathrm{supp}(\check{\zeta}_c)$, with $x_1>\tau$, we can apply the estimate (13) to obtain

$$K_+\check{\zeta}_c(x)-\frac{1}{2}x_1x_2\geqslant K_c\check{\zeta}_c(x)-\eta_c(x)\geqslant\frac{1}{2\pi}\log\frac{c^{1/2}}{2a}-C. \tag{40}$$

Therefore from (40) we infer

$$x_1x_2\leqslant 2K_+\check{\zeta}_c(x)-\frac{1}{\pi}\log\frac{c^{1/2}}{2a}+C=\frac{1}{\pi}\int_{\Omega_c}\log\frac{2a|x-\bar{y}||x-y|}{c^{1/2}|x-y||x-\bar{y}|}\check{\zeta}_c(y)dy+C. \tag{41}$$

The integral in (41) is dominated by $\int_{\Omega_c}\log(2a|x-\bar{y}|/c^{1/2}|x-y|)\ \ \check{\zeta}_c(y)dy$. Now we write

$$\int_{\Omega_c}\log\frac{2a|x-\bar{y}|}{c^{1/2}|x-y|}\check{\zeta}_c(y)dy=\int_{B_{a/c^{1/2}}(x)}\log\frac{2a|x-\bar{y}|}{c^{1/2}|x-y|}\check{\zeta}_c(y)dy$$
$$+\int_{\Omega_c\setminus B_{a/c^{1/2}}(x)}\log\frac{2a|x-\bar{y}|}{c^{1/2}|x-y|}\check{\zeta}_c(y)dy.$$

Applying (22), with $Q=1$, we find $\bar{\eta}>0$ such that

$$\int_{B_{a/c^{1/2}}(x)}\log\frac{2a|x-\bar{y}|}{c^{1/2}|x-y|}\check{\zeta}_c(y)dy\leqslant\bar{\eta}. \tag{42}$$

We also have

$$\int_{\Omega_c\setminus B_{a/c^{1/2}}(x)}\log\frac{2a|x-\bar{y}|}{c^{1/2}|x-y|}\check{\zeta}_c(y)dy\leqslant\log(4\tau). \tag{43}$$

Hence from (42) and (43) we conclude that for almost every $x\in\mathrm{supp}(\check{\zeta}_c)$ we have

$$x_1 x_2 \leqslant \frac{1}{\pi}(\overline{\eta}+\log(4\tau))+C. \tag{44}$$

From (44) we readily deduce (39).

The case where $\mathrm{supp}(\check{\zeta}_c)$ is essentially contained in $(0,\tau)\times\mathbb{R}^+$ can be treated similarly [in the proof we make use of (23)]. Therefore the proof of Assertion 2 is complete.

Assertion 3: Let c_1' be as in Assertion 1. Then there exist $c^1 \geqslant c_1'$, $R>0$, such that if $c \geqslant c^1$ and $\check{\zeta}_c \in \Sigma_c$, then

$$\mathrm{supp}(\check{\zeta}_c) \subset B_R,$$

modulo a set of measure zero.

Proof of Assertion 3: To seek a contradiction, suppose the assertion is false. Then by Assertion 2, there exist sequences $\{c_j\}$, $\{\check{\zeta}_j\}$ and $\{x_j\}$ such that the following hold.

(i) $c_1' \leqslant c_j \to \infty$, as $j \to \infty$.

(ii) $\check{\zeta}_j \in \Sigma_j$ such that $\mathrm{supp}(\check{\zeta}_j)$ is essentially contained in $\mathbb{R}^+\times(0,1/j)$, for all j; the case where $\mathrm{supp}(\check{\zeta}_j)$ is essentially contained in $(0,1/j)\times\mathbb{R}^+$ can be treated similarly.

(iii) $x_j \in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$, for every j, and $|x_j| \to \infty$ as $j \to \infty$.

Notice that we have again replaced c_j by j, when appropriate.

We claim that $\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j)) \to 0$, as $j \to \infty$. To prove the claim we fix j. Then for almost every $x \in \mathrm{supp}(\check{\zeta}_j)$ we have

$$\frac{1}{2\pi}\log\frac{c_j^{1/2}}{2a}+C \leqslant K_j\check{\zeta}_j(x)-\eta_j(x) \leqslant K_+\check{\zeta}_j(x) \leqslant \frac{1}{2\pi}\int_{\Omega_j}\log\frac{|x-\overline{y}|}{|x-y|}\check{\zeta}_j(y)dy,$$

since η_j is positive and $K_j\check{\zeta}_j(x) \leqslant K_+\check{\zeta}_j(x)$ for almost every $x \in \Omega_j$. Therefore,

$$C \leqslant \frac{1}{2\pi}\int_{\Omega_j}\log\frac{2a|x-\overline{y}|}{c_j^{1/2}|x-y|}\check{\zeta}_j(y)dy.$$

Let $Q>1$ and set $\hat{B}(x) := B_{Qa/c_j^{1/2}}(x)$. Then

$$C \leqslant \frac{1}{2\pi}\int_{\hat{B}(x)}\log\frac{2a|x-\overline{y}|}{c_j^{1/2}|x-y|}\check{\zeta}_j(y)dy+\frac{1}{2\pi}\int_{\Omega_j\setminus\hat{B}(x)}\log\frac{2a|x-\overline{y}|}{c_j^{1/2}|x-y|}\check{\zeta}_j(y)dy.$$

Applying (22) we find that

$$\frac{1}{2\pi}\int_{\hat{B}(x)}\log\frac{2a|x-\overline{y}|}{c_j^{1/2}|x-y|}\check{\zeta}_j(y)dy \leqslant K_2,$$

where K_2 is a positive constant. Also

$$\frac{1}{2\pi}\int_{\Omega_j\setminus\hat{B}(x)}\log\frac{2a|x-\overline{y}|}{c_j^{1/2}|x-y|}\check{\zeta}_j(y)dy \leqslant \frac{1}{2\pi}\log\frac{2(d+2)}{Q}\int_{\Omega_j\setminus\hat{B}(x)}\check{\zeta}_j(y)dy,$$

where we have used the fact that for $x,\ y \in \mathrm{supp}(\check{\zeta}_j)$,

$$|x-\overline{y}| \leqslant |x-y|+|y-\overline{y}| \leqslant \mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+2y_2 \leqslant \mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+2/j, \tag{45}$$

and that $\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+2/j \leqslant d+2$. Therefore, we obtain

$$C \leqslant K_2 + \frac{1}{2\pi}\log\frac{2(d+2)}{Q}\int_{\Omega_j \setminus \hat{B}(x)} \check{\zeta}_j(y)\,dy.$$

Hence by rearranging we derive

$$\log\frac{Q}{2(d+2)}\int_{\Omega_j \setminus \hat{B}(x)} \check{\zeta}_j(y)\,dy \leqslant 2\pi(C+K_2) < \hat{\nu},$$

for some $\hat{\nu} > 0$. Let us now set $Q = 2(d+2)e^{2\hat{\nu}}$ to obtain

$$\int_{\Omega_j \setminus \hat{B}(x)} \check{\zeta}_j(y)\,dy < \frac{1}{2}, \tag{46}$$

for almost every $x \in \mathrm{supp}(\check{\zeta}_j)$. From (46), applying the same argument as in the lemma, we find

$$\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j)) < \frac{4a(d+2)e^{2\hat{\nu}}}{c_j^{1/2}}. \tag{47}$$

The proof of the claim is complete when we let $j \to \infty$ in (47).

Let ζ_j^* denote the Schwarz symmetrization of $\check{\zeta}_j$ with respect to $\hat{x}$. We intend to show that $\hat{\Psi}_{j_1}(\zeta_{j_1}^*) - \hat{\Psi}_{j_1}(\check{\zeta}_{j_1}) > 0$, for some j_1, which is a contradiction to the maximality of $\check{\zeta}_{j_1}$, and hence the desired result follows. However, this is easily proved using the same method employed in Assertion 1, the key step being a result similar to (38) which is explained here. For x, $y \in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$ we have

$$\begin{aligned}\frac{1}{2}h(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} + \eta_j(x) &\geqslant \frac{1}{2}h_+(c_j^{1/2}x, c_j^{1/2}y) - \frac{1}{4\pi}\log\frac{1}{c_j^{1/2}} \\ &= \frac{1}{4\pi}\log\frac{|x-\overline{y}|}{|x-\overline{y}||\bar{x}-\underline{y}|} \\ &\geqslant \frac{1}{4\pi}\log\frac{1}{|x-\overline{y}|};\end{aligned} \tag{48}$$

now by using (45) we obtain

$$\frac{1}{4\pi}\log\frac{1}{|x-\overline{y}|} \geqslant \frac{1}{4\pi}\log\frac{1}{\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j)) + 2/j} \to 0, \tag{49}$$

as $j \to \infty$. This finishes the proof of Assertion 3, hence the proof of the theorem is complete. □

Proof of Theorem 3: We again replace c_j by j to simplify notation. Let us also set $\mathrm{cent}(\zeta_j) = z_j = (z_{j,1}, z_{j,2})$ and assume that $z_j \to z$, as $j \to \infty$. By maximality of $\check{\zeta}_j$ we have

$$\hat{\Psi}_j(\check{\zeta}_j) \geqslant \hat{\Psi}_j(\zeta_j^*), \tag{50}$$

where ζ_j^* denotes the Schwarz symmetrization of $\check{\zeta}_j$ with respect to $\hat{x}$. From (50) and an application of Riesz's inequality we obtain

$$T_j(\check{\zeta}_j) := \int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}+\eta_j(x)\right)\check{\zeta}_j(x)\check{\zeta}_j(y)dxdy$$
$$\leqslant \int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}+\eta_j(x)\right)\zeta_j^*(x)\zeta_j^*(y)dxdy = T_j(\zeta_j^*). \quad (51)$$

We now fix $0<\epsilon<1/(2\sqrt{2\pi})$. Then there exists $j_0(\epsilon)\in\mathbb{N}$ such that if $j\geqslant j_0(\epsilon)$, then $\mathrm{supp}(\zeta_j^*)\subset B_\epsilon(\hat{x})$. For $j\geqslant j_0(\epsilon)$ and $x,\ y\in B_\epsilon(\hat{x})$ we have

$$\left|\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}-H_1(\hat{x})\right|$$
$$\leqslant \frac{1}{2}\hat{h}_1(c_j^{1/2}x,c_j^{1/2}y)+\frac{1}{4\pi}\left|\log\frac{2\hat{x}_1\hat{x}_2|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}||\hat{x}|}\right|$$
$$\leqslant \frac{c_jx_2y_2}{2\pi(c_j|x||y|-1)^2}+\frac{1}{4\pi}\left|\log\frac{2\hat{x}_1\hat{x}_2|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}||\hat{x}|}\right|$$
$$\leqslant \frac{c_j(\hat{x}_1+\epsilon)(\hat{x}_2+\epsilon)}{2\pi(c_j(|\hat{x}|-\epsilon)^2-1)^2}+\frac{1}{4\pi}\sup_{x,y\in B_\epsilon(\hat{x})}\left|\log\frac{2\hat{x}_1\hat{x}_2|x-\overline{y}|}{|x-\overline{y}||x-\underline{y}||\hat{x}}\right|\to 0,$$

as $j\to\infty$. This implies

$$\int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}\right)\zeta_j^*(x)\zeta_j^*(y)dxdy\to H_1(\hat{x}), \quad (52)$$

as $j\to\infty$. Also, from (13), we have

$$|\eta_j(x)-H_2(\hat{x})|\leqslant|x_1x_2-\hat{x}_1\hat{x}_2|+\frac{1}{c_j^2|x|^2},$$

for $x\in B_\epsilon(\hat{x})$,

$$\sup_{x\in B_\epsilon(\hat{x})}|\eta_j(x)-H_2(\hat{x})|\to 0, \quad (53)$$

as $j\to\infty$. From (52) and (53) we deduce that $T_j(\zeta_j^*)\to H(\hat{x})$, as $j\to\infty$.

We now claim that

$$T_j(\check{\zeta}_j)\to H(z), \quad \text{as } j\to\infty. \quad (54)$$

Note that by proving (54) we will have completed the proof of the theorem; indeed, if (54) is true, then from (51) we infer $H(z)\leqslant H(\hat{x})$, hence $\hat{z}=\hat{x}$. To prove the claim we first show that $z\notin\partial\Pi_+$. Seeking a contradiction we suppose $z\in\partial\Pi_+$. Setting $z=(z_1,z_2)$, we may assume that $z_2=0$. Fix $\epsilon>0$; then there exists $\overline{j}(\epsilon)\in\mathbb{N}$ such that if $j\geqslant\overline{j}(\epsilon)$, then

$$|x-z|\leqslant|x-z_j|+|z_j-z|\leqslant\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+\epsilon, \quad (55)$$

for almost every $x\in\mathrm{supp}(\check{\zeta}_j)$. Now, similarly to (48) and (49) we derive

$$\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}+\eta_j(x)\geqslant\frac{1}{4\pi}\log\frac{1}{|x-\overline{y}|}\geqslant\frac{1}{4\pi}\log\frac{1}{\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+2y_2},$$

for $x,\ y\in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$ and $j\geqslant \overline{j}(\epsilon)$. If $j\geqslant \overline{j}(\epsilon)$ and $y\in \mathrm{supp}(\check{\zeta}_j)$, we can apply (55) to derive

$$y_2\leqslant |y-z|\leqslant \mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+\epsilon.$$

Therefore if $j\geqslant \overline{j}(\epsilon)$ and $x,\ y\in \mathrm{den}(\mathrm{supp}(\check{\zeta}_j))$, then

$$\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}+\eta_j(x)\geqslant \frac{1}{4\pi}\log\frac{1}{3\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+2\epsilon}.$$

This in conjunction with the fact that $\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))\to 0$, as $j\to\infty$, implies

$$\limsup_{j\to\infty} T_j(\check{\zeta}_j)\geqslant \frac{1}{4\pi}\log\frac{1}{2\epsilon},$$

hence $\limsup_{j\to\infty} T_j(\check{\zeta}_j)=\infty$, since $\epsilon>0$ was arbitrary. However, this contradicts (51), since $T_j(\zeta_j^*)$ is bounded from above for all sufficiently large j [see (37)]. Hence, $z\notin \partial\Pi_+$.

We now set $\varepsilon=\mathrm{dist}(z,\partial\Pi_+)$, the distance from z to $\partial\Pi_+$. We showed above that $\varepsilon>0$. Observe that there exists $\check{j}(\varepsilon)\in\mathbb{N}$ such that if $j\geqslant \check{j}(\varepsilon)$, then $\mathrm{supp}(\check{\zeta}_j)$ is essentially contained in $B_{\varepsilon/2}(z)$. We next define the real valued function D on $\Omega\times\Omega\subset\mathbb{R}^4$ by

$$D(x,y)=D(x_1,x_2,y_1,y_2)=h_+(x,y).$$

Note that ∇D is bounded on $B_{\varepsilon/2}(z)\times B_{\varepsilon/2}(z)$, hence, there exists a positive constant, say K_3, such that $\|\nabla D\|_{\infty,B_{\varepsilon/2}(z)\times B_{\varepsilon/2}(z)}\leqslant K_3$. Now, for $j\geqslant \check{j}(\varepsilon)$ and $x,\ y\in B_{\varepsilon/2}(z)$ we can apply the mean value inequality to deduce

$$\begin{aligned}\left|\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}-H_1(z)\right| &\leqslant \frac{1}{2}\hat{h}_1(c_j^{1/2}x,c_j^{1/2}y)+\frac{1}{4\pi}|D(x,y)-D(z,z)|\\ &\leqslant \frac{1}{2}\hat{h}_1(c_j^{1/2}x,c_j^{1/2}y)+\frac{1}{4\pi}K_3|(x,y)-(z,z)|_{\mathbb{R}^4}\\ &= o(1)+\frac{1}{4\pi}K_3|(x,y)-(z,z)|_{\mathbb{R}^4},\end{aligned}\tag{56}$$

as $j\to\infty$, uniformly in x and y, where $|\cdot|_{\mathbb{R}^4}$ denotes the usual Euclidean distance in $\mathbb{R}^4$. Note that for $j\geqslant \check{j}(\varepsilon)$ and $x,\ y\in B_{\varepsilon/2}(z)$ we have

$$|(x,y)-(z,z)|_{\mathbb{R}^4}\leqslant 4(\mathrm{diam}(\mathrm{supp}(\check{\zeta}_j))+|\hat{z}_j-z|)=o(1),\tag{57}$$

as $j\to\infty$. Whence by (56) and (57) we obtain

$$\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}-H_1(z)=o(1),$$

as $j\to\infty$, uniformly in $x,\ y\in B_{\varepsilon/2}(z)$. This, in turn, shows that

$$\int_{\Omega_j}\int_{\Omega_j}\left(\frac{1}{2}h(c_j^{1/2}x,c_j^{1/2}y)-\frac{1}{4\pi}\log\frac{1}{c_j^{1/2}}\right)\check{\zeta}_j(x)\check{\zeta}_j(y)dxdy\to H_1(z),$$

as $j\to\infty$. To complete the proof it remains to show that

$$\eta_j(x)-H_2(z)=o(1),\tag{58}$$

as $j\to\infty$, uniformly in $x\in B_{\varepsilon/2}(z)$. So let us fix $x\in B_{\varepsilon/2}(z)$ and suppose $j\geqslant\check{j}(\varepsilon)$. Then

$$|\eta_j(x)-H_2(z)|\leqslant|x_1x_2-z_1z_2|+\frac{1}{c_j^2|x|^2}.$$

It is easy to verify that

$$|x_1x_2-z_1z_2|\leqslant|x_2|\mathrm{diam}(\mathrm{supp}(\check{\xi}_j))+|z_{j,1}|\mathrm{diam}(\mathrm{supp}(\check{\xi}_j))+|z_{j,1}z_{j,2}-z_1z_2|\to 0,$$

as $j\to\infty$, uniformly in x. Therefore (58) follows, so we infer

$$\int_{\Omega_j}\eta_j(x)\check{\xi}_j(x)dx\to H_2(z),$$

as $j\to\infty$. Thus the proof of the theorem is complete. □

ACKNOWLEDGMENT

The first author acknowledges partial financial support from the Institute for Studies in Theoretical Physics and Mathematics, Tehran, Iran.

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Integrable hydrodynamic chains

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(Received 16 January 2003; accepted 17 April 2003)

A new approach for derivation of Benney-type moment chains and integrable hydrodynamic type systems is presented. New integrable hydrodynamic chains are constructed; all their hydrodynamical reductions are described and integrated. New $(2+1)$ integrable hydrodynamic type systems are found. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1597946]

I. INTRODUCTION

The integrable hydrodynamic chain

$$\partial_t A_k = \partial_x A_{k+1} + k A_{k-1} A_{0,x}, \quad k = 0,1,\ldots, \tag{1}$$

for the first time was introduced by D. J. Benney in a theory of finite-depth fluid (see Ref. 5). Here the moments A_k are an infinite number of field variables. Later, it was shown that these moments satisfy a dispersionless limit of KP hierarchy determined by the Sato pseudo-differential operator

$$\hat{L} = \partial_x + A_0 \partial_x^{-1} + A_1 \partial_x^{-2} + \cdots,$$

which in dispersionless limit is reduced to

$$\lambda = \mu + \frac{A_0}{\mu} + \frac{A_1}{\mu^2} + \cdots. \tag{2}$$

The Benney moment chain can be written in the equivalent form (see Ref. 20)

$$\lambda_t - \mu \lambda_x = \frac{\partial \lambda}{\partial \mu}\left[\mu_t - \partial_x\left(\frac{\mu^2}{2} + A_0\right)\right]. \tag{3}$$

If $\lambda = \text{const}$, then μ is a generating function (with respect to the parameter λ) of the conservation law densities

$$\mu_t = \partial_x\left(\frac{\mu^2}{2} + A_0\right). \tag{4}$$

In the case, when only the first N moments A_k are functionally independent ($k = 0, 1, \ldots, N-1$), all A_k with $k \geqslant N$ can be consistently expressed as functions of the first N moments. This is called a hydrodynamical reduction. More generally, we can define ''differential reductions,'' in which all A_k with $k \geqslant N$ can be consistently expressed as functions of the first N moments and their derivatives. However, we are only concerned with hydrodynamical reductions here (in the spirit of Ref. 21). Then these hydrodynamical reductions are the hydrodynamic type systems written in Riemann invariants r^i,

$$r_t^i = \mu_i(\mathbf{r}) r_x^i, \quad i = 1,2,\ldots,N, \tag{5}$$

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i.e., a hydrodynamic type system has diagonal form in these field variables and there is no summation over each repeated index (see, for instance, Ref. 36). The Riemann invariants r^i and the characteristic velocities $\mu_i(\mathbf{r})$ are determined by conditions

$$r^i=\mu_i+\frac{A_0}{\mu_i}+\frac{A_1}{\mu_i^2}+\frac{A_2}{\mu_i^3}+\cdots, \quad 1=\frac{A_0}{\mu_i^2}+2\frac{A_1}{\mu_i^3}+3\frac{A_2}{\mu_i^4}+\cdots.$$

[See (2) and (3). Of course, defining the Riemann invariants and characteristic speeds in terms of formal series is apparently risky—at least we should emphasize that these series will converge to analytic functions in all cases considered, see Ref. 21.] These hydrodynamic type systems are integrable, too (all moments A_k are some functions of r^i, which are determined by compatibility conditions with whole Benney moment chain, see Ref. 21). These hydrodynamic type systems have the same generating functions of conservation laws [see (4)] and the commuting flows (see Ref. 33; the "commuting flows" means that the Riemann invariants r^i simultaneously are functions of an infinite number of independent variables t_k, $k=0,1,\ldots$, here $t_0\equiv x$, $t_1\equiv t$),

$$\mu(\lambda)_{\tau(\tilde{\lambda})}=\partial_x \ln[\mu(\lambda)-\mu(\tilde{\lambda})], \tag{6}$$

where

$$\partial_{\tau(\tilde{\lambda})}=\partial_{t_0}+\frac{1}{\tilde{\lambda}}\partial_{t_1}+\frac{1}{\tilde{\lambda}^2}\partial_{t_2}+\cdots.$$

Moreover, the generating function (with respect to the parameter $\tilde{\lambda}$) of solutions for any reduction (5) can be found by the Tsarev generalized hodograph method (Ref. 36, also see Ref. 33)

$$x+\mu_i(\mathbf{r})t=\frac{1}{\mu_i(\mathbf{r})-\mu(\tilde{\lambda})}, \quad i=1,2,\ldots,N. \tag{7}$$

Thus, if some hydrodynamic type system is recognized as a reduction of the Benney moment chain, it means that this system has most properties of the Benney moment chain.

The idea presented in this article is the following: if one can introduce the moments A_k for given integrable hydrodynamic type system (5), then **one can ignore the origin** (i.e., given hydrodynamic type system) of this *hydrodynamic chain*

$$\partial_t A=F(\mathbf{A})A_x,$$

where A is an infinite-number component vector and $F(\mathbf{A})$ is an infinite-number component matrix. The next step is a description of all possible integrable hydrodynamical reductions [one of them, of course, must be the original hydrodynamic type system (5)],

$$r^i_t=V_i(\mathbf{r})r^i_x, \quad i=1,2,\ldots,M, \tag{8}$$

where M is not connected with N [see (5)], and V_i satisfy some nonlinear system of partial differential equations (PDE's) (see below). Also, we assume that $V_i\neq V_k$ for any $i\neq k$ (this is a necessary condition for the application of the Tsarev generalized hodograph method). Thus, every hydrodynamic chain constructed in this way can be regarded as a *huge box* for some variety of the integrable hydrodynamic type systems.

For instance, the particular case of gas dynamics

$$u_t=\partial_x\left[\frac{u^2}{2}+\frac{\eta^{\gamma-1}}{\gamma-1}\right], \quad \eta_t=\partial_x(u\eta), \tag{9}$$

for $\gamma=2$ (shallow water equations),

$$u_t=\partial_x\left[\frac{u^2}{2}+\eta\right],\quad \eta_t=\partial_x(u\eta), \tag{10}$$

satisfies the Benney moment chain (1) if one introduces the moments $A_k=u^k\eta$.

It is easy to check that the Benney moment chain has a more general (the Zakharov) reduction $A_k=\Sigma_{i=1}^N u_i^k\eta_i$ (see Ref. 38), which creates the dispersionless limit of the vector nonlinear Schrödinger equation (VNLS)

$$\partial_t u_i=\partial_x\left[\frac{u_i^2}{2}+\sum_{k=1}^N \eta_k\right],\quad \partial_t\eta_i=\partial_x(u_i\eta_i),\quad i=1,2,\ldots,N. \tag{11}$$

Remark: Under this Zakharov reduction infinite series (2) yields a more compact expression (see Ref. 38)

$$\lambda=\mu+\sum_{k=1}^N \frac{\eta_k}{\mu-u_k}. \tag{12}$$

It is easy to check that the dispersionless limit of VNLS satisfies equation (3) with respect to the equation of Riemann surface (12).

Obviously, in both above-mentioned cases, corresponding hydrodynamic type systems (10) and (11) have the same generating functions of conservation law densities (4) and commuting flows (6) as whole Benney moment chain (1). Here we demonstrate this approach on an example of a new hydrodynamic chain, which contains some important reductions well known in mathematics, fluid dynamics, nonlinear optics, biology and chemistry.

The main classification problem in the theory of integrable hydrodynamic type systems can be reformulated as the problem of description of all possible integrable hydrodynamic chains. For simplicity, we restrict our consideration to the case, when any hierarchy of the hydrodynamic chains can be written in a conservative form [see, for instance, (30) below]:

$$\partial_{t_n}A_k=\partial_x F_{k,n}(A_{k+n},A_{k+n-1},\ldots,A_0),\quad k,n=0,1,2\ldots$$

If one can classify all possible functions F_k, it means that all the hydrodynamic type systems embedded in such hydrodynamic chains by different reductions are classified, too. In the simplest case $(N=2)$,

$$\partial_t A_0=\partial_x F_{01}(A_0,A_1),\quad \partial_t A_1=\partial_x F_{11}(A_0,A_1,A_2),$$

where $A_2(A_0,A_1)$ is a conservation law density of the reduced hydrodynamic type system. Then the governing equation for function A_2 is quasilinear,

$$f_v w_{uu}=[f_u-\varphi_v-\varphi_w w_v]w_{uv}+[\varphi_u+\varphi_w w_u]w_{vv},$$

where

$$u\equiv A_0,\quad v\equiv A_1,\quad w\equiv A_2,\quad f\equiv F_{01},\quad \varphi\equiv F_{11}.$$

When $F_{01}=v$ and $F_{11}=w(u,v)-u^2/2$, this is the two-component reduction of the Benney moment chain (see Ref. 21),

$$w_{uu}=-w_v w_{uv}+(w_u-u)w_{vv}.$$

If $F_{01}=v-u^2$ and $F_{11}=w(u,v)-uv$, then the corresponding equation,

$$w_{uu}=-(u+w_v)w_{uv}+(w_u-v)w_{vv},$$

can be solved in the parametric form

$$w=\tfrac{1}{6}[A''(s)+B''(r)]^3+[A''(s)+B''(r)][A'(s)-sA''(s)+B'(r)-rB''(r)]+s^2A''(s)-2sA'(s)$$
$$+2A(s)+r^2B''(r)-2rB'(r)+2B(r),$$

$$v=\tfrac{1}{2}[A''(s)+B''(r)]^2+A'(s)-sA''(s)+B'(r)-rB''(r),\quad u=A''(s)+B''(r),$$

where $A(s)$ and $B(r)$ are arbitrary functions. Thus, the two-component reduced (hydrodynamic type) system in Riemann invariants is

$$r_t=(A''(s)+B''(r)+r)r_x,\quad s_t=(A''(s)+B''(r)+s)s_x.$$

This system is the natural two-parametric generalization of gas dynamics (9) (see below).

The goal of this article is a complete description of the N-component generalization of the above-mentioned formulas.

In Sec. II of this paper, so-called the "ε-systems" are introduced. All their properties such as conservation laws and commuting flows are described. The corresponding hydrodynamic chain is found by the natural introduction of moments.

In Sec. III, some properties of such transformations between different representations of this hydrodynamic chain are obtained.

In Sec. IV, all possible hydrodynamical reductions are found. Particular and important reductions of this hydrodynamic chain are emphasized.

In Sec. V, generating functions of conservation law densities, commuting flows and solutions (by the Tsarev generalized hodograph method) for these hydrodynamical reductions are constructed.

In Sec. VI, a general solution of these hydrodynamic type systems is presented.

In Sec. VII, new $(2+1)$ integrable hydrodynamic type systems are found.

In Sec. VIII, another hydrodynamic chain is presented and all its hydrodynamical reductions are described.

In Sec. IX, we discuss some still open problems: Hamiltonian structures and integrable dispersive extensions of hydrodynamic chains and their reductions.

In Sec. X (Conclusion), we describe a general situation in a theory of hydrodynamic chains.

II. "ε-SYSTEMS"

This class of integrable hydrodynamic type systems

$$r^i_t=\left[r^i-\varepsilon\sum_{m=1}^{N}r^m\right]r^i_x,\quad i=1,2,\ldots,N, \tag{13}$$

where ε is an arbitrary constant, was established in Ref. 29 (also see Refs. 17 and 30–32). These hydrodynamic type systems (13) and its commuting flows (see below) we shall call the "ε-systems." The particular case $N=2$ plays an important role in gas dynamics [see (9), where the adiabatic index $\gamma=(3-2\varepsilon)/(1-2\varepsilon)$], in field theory ($\gamma=-1$, the Born–Infeld equation), in nonlinear optics [$\gamma=2$, the dispersionless limit of the nonlinear Schrödinger equation, see (9)] and in fluid dynamics ($\gamma=4$, the dispersionless limit of the second commuting flow to the Boussinesq equation). Also, the "ε-systems" (for arbitrary N) are well known in differential geometry ($\varepsilon=-\frac{1}{2}$, elliptic coordinates, see, for instance, Ref. 32; the dispersionless limit of Coupled KdV, see, for instance, Ref. 16), in soliton theory ($\varepsilon=1$, some particular solutions of linearly degenerated systems are multi-gap solutions of KdV, see Ref. 11), in biology and chemistry ($\varepsilon=-1$, chromatography, electrophoresis, isotahophoresis). Moreover, a general solution can be found explicitly (see Ref. 31), for instance, in one-atomic ($\gamma=\frac{5}{3}$, $\varepsilon=-1$) and two-atomic ($\gamma=\frac{7}{5}$, $\varepsilon=-2$) gases

[see (13)] and their generalization for an arbitrary N and an arbitrary **integer** ε. Thus, the obvious aim is to extend a class of integrable hydrodynamic type systems starting from (13) with preservation of some properties.

The hydrodynamic type system (13) has a generation function μ of conservation law densities; when $\lambda \to \infty$,

$$\mu \equiv \prod_{m=1}^{N} (1 - r_m/\lambda)^{-\varepsilon} = 1 + a_1/\lambda + a_2/\lambda^2 + \cdots, \tag{14}$$

when $\lambda \to 0$ (up to constant multiplier)

$$\mu \equiv \prod_{m=1}^{N} (r_m - \lambda)^{-\varepsilon} = b_0 + b_1\lambda + b_2\lambda^2 + \cdots. \tag{15}$$

The first series (14) is a series of polynomial conservation law densities a_k with respect to Riemann invariants (this is analog of the Kruskal series of conservation law densities for integrable dispersive systems like the Korteweg–de Vries equation). We shall call them as ''higher'' (or ''positive'') conservation law densities and correspondingly their homogeneity. The coefficients b_k we shall call as ''lower'' (or ''negative'') conservation law densities (they play a role as ''new'' conservation law densities appearing under Miura type transformation in the theory of integrable dispersive systems).

It is easy to check that any commuting flow (so, every Riemann invariant r^i is a function of three independent variables x, t, τ)

$$r^i_\tau = w^i_{(\varepsilon)}(\mathbf{r}) r^i_x \tag{16}$$

to hydrodynamic type system (13) has velocities

$$w^i_{(\varepsilon)}(\mathbf{r}) = \partial_i h_{(-\varepsilon)}, \tag{17}$$

where $h_{(-\varepsilon)}$ is some conservation law density of the ''$(-\varepsilon)$-system,''

$$r^i_t = \left[r^i + \varepsilon \sum_{m=1}^{N} r^m \right] r^i_x, \quad i = 1,2,\ldots,N.$$

Since the ''ε-systems'' and ''$(-\varepsilon)$-systems'' have generating functions of conservation law densities such that

$$\mu_{(\varepsilon)} \cdot \mu_{(-\varepsilon)} = 1, \tag{18}$$

then a generating function of commuting flows to (13) in Riemann invariants is [see (16) and (17)]

$$r^i_{\tau(\tilde{\lambda})} = \frac{1}{(1 - r^i/\tilde{\lambda})\tilde{\mu}} r^i_x, \tag{19}$$

and in the conservative form [cf. (6)] is

$$\mu_{\tau(\tilde{\lambda})} = \frac{\tilde{\lambda}}{\tilde{\lambda} - \lambda} \partial_x \left(\frac{\mu}{\tilde{\mu}} \right), \tag{20}$$

where $\tilde{\mu} \equiv \mu(\tilde{\lambda})$ [see (14) and (15)].

Higher commuting flows can be obtained from [see (14)]

$$\tilde{\mu}\equiv\prod_{m=1}^{N}(1-r_m/\tilde{\lambda})^{-\varepsilon}=1+a_1/\tilde{\lambda}+a_2/\tilde{\lambda}^2+\cdots$$

and formal series

$$\partial_{\tau(\tilde{\lambda})}=\partial_{t_0}+\frac{1}{\tilde{\lambda}}\partial_{t_1}+\frac{1}{\tilde{\lambda}^2}\partial_{t_2}+\cdots$$

when $\tilde{\lambda}\to\infty$. The corresponding generating functions of conservation laws are

$$\partial_{t_k}\mu=\partial_x\left[\mu\sum_{m=0}^{k}\tilde{a}_m\lambda^{k-m}\right],\qquad k=0,1,2,\ldots, \tag{21}$$

where

$$\tilde{a}_0=a_0=1,\quad \tilde{a}_1=-a_1,\quad \tilde{a}_n=-a_n-\sum_{m=1}^{n-1}\tilde{a}_m a_{n-k},\quad n=2,3,\ldots.$$

The corresponding *higher* commuting flows (in Riemann invariants) are

$$\partial_{t_k}r^i=\left[\sum_{m=0}^{k}\tilde{a}_m(r^i)^{k-m}\right]r_x^i,\qquad k=0,1,2,\ldots. \tag{22}$$

Lower commuting flows can be obtained from [see (15)]

$$\tilde{\mu}\equiv\prod_{m=1}^{N}(r_m-\tilde{\lambda})^{-\varepsilon}=b_0+b_1\tilde{\lambda}+b_2\tilde{\lambda}^2+\cdots$$

and formal series

$$\partial_{\tau(\tilde{\lambda})}=\tilde{\lambda}\partial_{t_{-1}}+\tilde{\lambda}^2\partial_{t_{-2}}+\tilde{\lambda}^3\partial_{t_{-3}}+\cdots,$$

when $\tilde{\lambda}\to 0$. The corresponding generating functions of conservation laws are

$$\partial_{t_{-k-1}}\mu=\partial_x\left[\mu\sum_{m=0}^{k}\tilde{b}_m\lambda^{m-k-1}\right],\quad k=0,1,2,\ldots, \tag{23}$$

where

$$\tilde{b}_0=\frac{1}{b_0},\quad \tilde{b}_k=-\frac{1}{b_0}\sum_{m=0}^{k-1}\tilde{b}_m b_{k-m},\quad k=1,2,\ldots.$$

The corresponding *lower* commuting flows (in Riemann invariants) are

$$\partial_{t_{-k-1}}r^i=\left[\sum_{m=0}^{k}\tilde{b}_m(r^i)^{m-k-1}\right]r_x^i,\quad k=0,1,2,\ldots. \tag{24}$$

If $\lambda\to\infty$ and $\tilde{\lambda}\to\infty$, all the *higher* conservation laws for the *higher* commuting flows are

$$\partial_{t_k}a_m=\partial_x\left[\sum_{s=0}^{k}\tilde{a}_s a_{k+m-s}\right],\quad k=0,1,2,\ldots. \tag{25}$$

If $\lambda\to 0$ and $\tilde{\lambda}\to\infty$, all the *lower* conservation laws for the *higher* commuting flows are

$$\partial_{t_n} b_k=\partial_x\left[\sum_{s=0}^{k} b_s\tilde{a}_{n+s-k}\right],\quad k\leqslant n,\quad \partial_{t_n} b_k=\partial_x\left[\sum_{s=0}^{n}\tilde{a}_s b_{k+s-n}\right],\quad k\geqslant n. \tag{26}$$

If $\lambda\to 0$ and $\tilde{\lambda}\to 0$, all the *lower* conservation laws for the *lower* commuting flows are

$$\partial_{t_{-n-1}} b_m=\partial_x\left[\sum_{k=0}^{n}\tilde{b}_k b_{n+m+1-k}\right],\quad n=0,1,2,\ldots. \tag{27}$$

If $\lambda\to\infty$ and $\tilde{\lambda}\to 0$, all the *higher* conservation laws for the *lower* commuting flows are

$$\partial_{t_{-n-1}} a_{m+1}=\partial_x\left[\sum_{k=0}^{m} a_s\tilde{b}_{n+s-m}\right],\ m\leqslant n,\ \partial_{t_{-n-1}} a_{m+1}=\partial_x\left[\sum_{k=0}^{n}\tilde{b}_s a_{m+s-n}\right],\ m\geqslant n. \tag{28}$$

All these above formulas can be easily checked by direct calculations.

For instance, the initial system (13) has the generating function of conservation laws

$$\partial_t\mu=\partial_x[(\lambda-a_1)\mu], \tag{29}$$

where an infinite set of the *positive* (polynomial) conservation laws is

$$\partial_{t_1} a_k=\partial_x[a_{k+1}-a_1 a_k],\quad k=1,2,\ldots, \tag{30}$$

and an infinite set of the *negative* conservation laws is

$$\partial_{t_1} b_0=\partial_x(-a_1 b_0),\quad \partial_{t_1} b_k=\partial_x[b_{k-1}-a_1 b_k],\quad k=1,2,\ldots. \tag{31}$$

The second commuting flow [see (13) and (22)]

$$r^i_{t_2}=\left[(r^i)^2-\varepsilon r^i\sum_{m=1}^{N} r^m+\frac{\varepsilon^2}{2}\left(\sum_{m=1}^{N} r^m\right)^2-\frac{\varepsilon}{2}\sum_{m=1}^{N}(r^m)^2\right]r^i_x,\quad i=1,2,\ldots,N,$$

has the generating function of conservation laws [see (21)]

$$\mu_{t_2}=\partial_x[(\lambda^2-a_1\lambda+a_1^2-a_2)\mu],$$

where an infinite set of the *positive* (polynomial) conservation laws is [see (25)]

$$\partial_{t_2} a_k=\partial_x[a_{k+2}-a_1 a_{k+1}+(a_1^2-a_2)a_k]. \tag{32}$$

An infinite set of the *negative* conservation laws is [see (26)]

$$\partial_{t_2} b_0=\partial_x[b_0(a_1^2-a_2)],\quad \partial_{t_2} b_1=\partial_x[b_1(a_1^2-a_2)-a_1 b_0],$$

$$\partial_{t_2} b_k=\partial_x[b_k(a_1^2-a_2)-a_1 b_{k-1}+b_{k-2}],\quad k=2,3,\ldots.$$

The first *negative* ($\tilde{\lambda}\to 0$) commuting flow is [see (24)]

$$r^i_{t_{-1}}=\frac{1}{b_0 r^i}r^i_x=\frac{\Pi_{m=1}^{N}(r^m)^{\varepsilon}}{r^i}r^i_x, \tag{33}$$

where the generating function of conservation laws is [see (23)]

$$\mu_{t_{-1}}=\partial_x\frac{\mu}{\lambda b_0}, \tag{34}$$

where an infinite set of *negative* conservation laws is [see (27)]

$$\partial_{t_{-1}}b_k=\partial_x\frac{b_{k+1}}{b_0},\quad k=0,1,2,\ldots, \tag{35}$$

and an infinite set of *positive* conservation laws is [see (28)]

$$\partial_{t_{-1}}a_1=\partial_x\frac{1}{b_0},\quad \partial_{t_{-1}}a_{k+1}=\partial_x\frac{a_k}{b_0},\quad k=1,2,\ldots. \tag{36}$$

Remark: The reciprocal transformation [see the first equation in (31)]

$$dy_{-1}=b_0dx-a_1b_0dt_1,\quad dz=dt_1,$$

connects system (13) [also, see (30) and (31)] and its commuting flow (33) [also, see (35) and (36)].

The reciprocal transformation [see (29)]

$$dy=\mu[dx+(\lambda-a_1)dt_1],\quad dz=dt_1,$$

connects system (13) and the generating function of its commuting flows [see (16)–(20)]

$$\partial_t a_1=-\lambda\partial_x(1/\mu).$$

III. NEW HYDRODYNAMIC CHAIN

The hydrodynamic type system (13) can be rewritten as the infinite moment chain

$$\partial_t c_k=\partial_x c_{k+1}-c_1\partial_x c_k,\quad k=0,\pm1,\pm2,\ldots, \tag{37}$$

where the first N moments c_k $(k=1,2,\ldots,N)$ are functionally independent:

$$c_0=\varepsilon\sum_{m=1}^{N}\ln r^m,\quad c_k=\frac{\varepsilon}{k}\sum_{m=1}^{N}(r^m)^k,\quad k=\pm1,\pm2,\ldots. \tag{38}$$

Thus, all a_k, b_k and c_k can be expressed via each other (see below). This is an invertible transformation.

However, now we can start our investigation namely from a hydrodynamic chain written in form (37) or, for instance, in form (30) without any reference on the original hydrodynamic type system (13) [and the explicit expressions (38)]. If now we restrict our infinite moment chain to the N-component case, then just one particular solution obviously is exactly the hydrodynamic type system (13) [also, see (38)]. How to find all other possible reductions? The answer will be done in next section.

Remark: For the first time, this hydrodynamic chain (30) has been derived (in another terms) by S. J. Alber (see Ref. 2; also it has been independently obtained in another context by V. G. Mikhalev, see Ref. 27), and recently by L. M. Alonso and A. B. Shabat (see Ref. 4; they describe mostly differential reductions and very particular hydrodynamical reductions; in our article we describe all possible hydrodynamical reductions). Actually, the starting point of their investigations was the hydrodynamic type "ε-system," when $\varepsilon=-\frac{1}{2}$, related by generalized reciprocal transformation with averaged (by the Whitham method) integrable systems (determined by scalar second order spectral transform with energy-dependent potential, see also mentioned references) related with hyperelliptic surfaces.

The generating function of conservation laws for the hydrodynamic chain (37) is exactly (29), where [cf. (14)]

$$\mu=1+\sum_{k=1}^{\infty} a_k\lambda^{-k}=\exp\left[\sum_{k=1}^{\infty} c_k\lambda^{-k}\right], \quad c_1\equiv a_1, \tag{39}$$

and $\lambda\to\infty$. The hydrodynamic chain (31) satisfies the same generating function (29), where [cf. (15)]

$$\mu=\sum_{k=0}^{\infty} b_k\lambda^{k}=\exp\left[-\sum_{k=0}^{\infty} c_{-k}\lambda^{k}\right], \quad c_0\equiv-\ln b_0, \tag{40}$$

and $\lambda\to 0$.

All the *positive* commuting flows in field variables c_k are

$$\partial_{t_n} c_k=\sum_{m=0}^{n} \tilde{a}_m c_{k+n-m,x}, \quad k=0,\pm 1,\pm 2,\ldots,$$

where the generating function of conservation law densities for an arbitrary *positive* commuting flow is (21); all *negative* flows are

$$\partial_{t_{-n-1}} c_k=\sum_{m=0}^{n} \tilde{b}_m c_{k+m-n,x}, \quad k=0,\pm 1,\pm 2,\ldots,$$

where the generating function of conservation law densities for an arbitrary *negative* commuting flow is (23). All these *negative* flows can be obtained from *positive* commuting flows (see above) by the reciprocal transformation (see the Remark of the previous section). For instance, the first *negative* flow is

$$\partial_{t_{-1}} c_k=e^{c_0}\partial_x c_{k-1}, \quad k=0,\pm 1,\pm 2,\ldots. \tag{41}$$

Remark: Obviously, the values $\tilde{a}_k$ and $\tilde{b}_k$ can be expressed from analogs of (39) and (40) [see (20)],

$$\frac{1}{\mu}=1+\sum_{k=1}^{\infty} \tilde{a}_k\lambda^{-k}=\exp\left[-\sum_{k=1}^{\infty} c_k\lambda^{-k}\right], \quad \tilde{a}_1\equiv -c_1, \quad \lambda\to\infty.$$

$$\frac{1}{\mu}=\sum_{k=0}^{\infty} \tilde{b}_k\lambda^{k}=\exp\left[\sum_{k=0}^{\infty} c_{-k}\lambda^{k}\right], \quad \tilde{b}_0\equiv e^{c_0}, \quad \lambda\to 0.$$

Thus, the hydrodynamic chain (37) can be expressed via the different moments (a_k, b_k), see, for instance, the Remark in Sec. VI.

The relationship (39) between the *positive* moments c_k and the *positive* conservation law densities a_k can be expressed explicitly by the next four recursive formulas, where the first of them,

$$da_{k+1}=\sum_{m=1}^{k} a_m dc_{k+1-m}+dc_{k+1}, \quad k=0,1,2,\ldots,$$

is a consequence of the three local symmetry operators acting on a space of the conservation law densities a_k: the shift operator

$$\hat{\delta}a_{k+1}=\frac{\partial a_{k+1}}{\partial c_1}=a_k, \quad k=0,1,2,\ldots;$$

the scaling operator

$$\hat{R}a_k=\sum_{m=1}^{\infty} mc_m\frac{\partial a_k}{\partial c_m}=ka_k, \quad k=0,1,2,\ldots;$$

and the projective operator

$$\hat{S}a_k=\left[c_1+\sum_{m=1}^{\infty}(m+1)c_{m+1}\frac{\partial}{\partial c_m}\right]a_k=(k+1)a_{k+1}, \quad k=0,1,2,\ldots.$$

IV. FINITE-COMPONENT REDUCTIONS

Theorem 1: *The hydrodynamic type system (8) with an arbitrary number of components is embedded into the hydrodynamic chain (37) if and only if*

$$V_i=f_i(r^i)-c_1, \quad c_1=\sum_{m=1}^{N}\psi_m(r^m), \tag{42}$$

where $f_i(r^i)$ *and* $\psi_k(r^k)$ *are arbitrary functions.*

Proof: Any reductions are compatible with given hydrodynamic chain (37) if every moment c_k can be expressed as a function of just N independent Riemann invariants r^i. Then one obtains

$$V_i\partial_i c_k=\partial_i c_{k+1}-c_1\partial_i c_k, \quad i=1,2,\ldots,,N,k=0,\pm 1,\pm 2,\ldots,$$

It is easy to see, that

$$\partial_i c_{k+1}=(V_i+c_1)^k\partial_i c_1, \quad i=1,2,\ldots,N, \quad k=0,\pm 1,\pm 2,\ldots.$$

Thus, the second derivatives

$$\partial_j[(V_i+c_1)^k\partial_i c_1]=\partial_i[(V_j+c_1)^k\partial_j c_1], \quad i=1,2,\ldots,N, \quad k=0,\pm 1,\pm 2,\ldots,$$

yield the general reduction (42). ■

Thus, all moments are

$$c_k=\sum_{m=1}^{N}\int^{r^m}[f_m(\lambda)]^{k-1}d\psi_m(\lambda), \quad k=0,\pm 1,\pm 2,\ldots.$$

Remark: The hydrodynamic type systems

$$r^i_{t_{-1}}=W^i(\mathbf{r})r^i_x, \quad i=1,2,\ldots,N, \tag{43}$$

embedded into first negative flow (41) [see (37)] can be found in the same way [see (42)]: from $W^i\partial_i c_k=e^{c_0}\partial_i c_{k-1}$ *one can obtain* $\partial_i c_k=(e^{c_0}/W^i)^k\partial_i c_0$. *In comparison with* $\partial_i c_k=(V_i+c_1)^k\partial_i c_0$ *one can obtain*

$$W^i=\frac{1}{f_i(r^i)}\exp\left[\sum_{m=1}^{N}\int^{r^m}\frac{d\psi_m(\lambda)}{f_m(\lambda)}\right]. \tag{44}$$

The next task is how to write hydrodynamical reductions in *closed* form via special variables like conservation law densities [see, e.g., (30)]. It means that all higher moments a_{N+k} (k

$=1,2,\dots$) must be expressed via lower moments a_k ($k=1,2,\dots,N$). In the particular case (13), all higher moments a_{N+k} are polynoms, which can be found from the relations [see (14)]

$$0=[(1+\lambda a_1+\lambda^2 a_2+\cdots+\lambda^N a_N+\lambda^{N+1}a_{N+1}+\cdots)^{-1/\varepsilon}]^{(N+k)}, \quad k=1,2,\dots.$$

For example, the first higher moment a_{N+1} can be found from the more compact recursive relation

$$\sum_{k=1}^{N+1}\frac{\Gamma(1-1/\varepsilon)z_k^{(N+1)}}{\Gamma(1-k-1/\varepsilon)\Gamma(k+1)}=0,$$

where $z_k^{(N+1)}$ is a coefficient of the series

$$[a_1+a_2\lambda+a_3\lambda^2+\cdots+a_{N+2-k}\lambda^{N+1-k}]^k=a_1^k+\lambda k a_1^{k-1}a_2+\cdots+\lambda^{N+1-k}z_k^{(N+1)}+\cdots.$$

All higher moments a_{N+k} are polynoms of lower moments a_k, e.g.,

$$a_3=\frac{1+\varepsilon}{\varepsilon}a_1a_2-\frac{(1+\varepsilon)(1+2\varepsilon)}{6\varepsilon^2}a_1^3, \quad N=2,$$

$$a_4=\frac{1+\varepsilon}{2\varepsilon}(2a_1a_3+a_2^2)-\frac{(1+\varepsilon)(1+2\varepsilon)}{2\varepsilon^2}a_1^2a_2+\frac{(1+\varepsilon)(1+2\varepsilon)(1+3\varepsilon)}{24\varepsilon^3}a_1^4, \quad N=3,$$

$$a_5=\frac{1+\varepsilon}{\varepsilon}(a_1a_4+a_2a_3)-\frac{(1+\varepsilon)(1+2\varepsilon)}{2\varepsilon^2}(a_1^2a_3+a_1a_2^2)+\frac{(1+\varepsilon)(1+2\varepsilon)(1+3\varepsilon)}{6\varepsilon^3}a_1^3a_2$$
$$-\frac{(1+\varepsilon)(1+2\varepsilon)(1+3\varepsilon)(1+4\varepsilon)}{120\varepsilon^4}a_1^5, \quad N=4,$$

and so on. The first exceptional case is the chromatography phenomena ($\varepsilon=-1$). Then

$$a_3=-a_1a_2+\tfrac{1}{6}a_1^3, \quad N=2,$$

$$a_4=-\tfrac{1}{2}(2a_1a_3+a_2^2)+\tfrac{1}{2}a_1^2a_2-\tfrac{1}{12}a_1^4, \quad N=3,$$

$$a_5=-(a_1a_4+a_2a_3)+\tfrac{1}{2}(a_1^2a_3+a_1a_2^2)-\tfrac{1}{3}a_1^3a_2+\tfrac{1}{20}a_1^5, \quad N=4;$$

the second exceptional case is (dispersionless limits of coupled KdV and coupled Harry Dym) $\varepsilon=-\frac{1}{2}$, then first higher moment a_{N+1} is just a quadratic expression via lower moments a_k. It means that corresponding hydrodynamic type systems have at least one local Hamiltonian structure (see Ref. 34); actually, the largest number of local Hamiltonian structures is $(N+1)$, *iff* $\varepsilon=-\frac{1}{2}$, see Ref. 16. The third exceptional case is $\varepsilon=-1/M$, where $M=3,4,\dots$. Then all expressions for the higher moments a_k will be quickly truncated (see above; it means that just few terms will survive in corresponding sums).

V. COMMUTING FLOWS AND REDUCTIONS

The corresponding linear system for conservation law densities (see Ref. 36) is

$$\partial_{ik}h=\frac{\psi_k'(r^k)}{f_i(r^i)-f_k(r^k)}\partial_i h-\frac{\psi_i'(r^i)}{f_i(r^i)-f_k(r^k)}\partial_k h, \quad i\neq k. \tag{45}$$

The general solution of such a system is determined by N functions of a single variable (also, see Ref. 36). In a particular, but very important, case of the "ε-systems" [see, for example, (13)] this linear system (45) is exactly the N-component generalization of the Euler–Darboux–Poisson system (see Ref. 31)

$$\partial_{ik}h=\frac{\varepsilon}{r^i-r^k}[\partial_i h-\partial_k h],\quad i\neq k. \tag{46}$$

At first, it is necessary to find a generating function of conservation law densities μ, which can be found in comparison with (29) and (42)

$$\mu(\mathbf{r},\lambda)=\exp\left(\sum_{k=1}^{N}\int^{r^k}\frac{d\psi_k(\tilde{\lambda})}{\lambda-f_k(\tilde{\lambda})}\right). \tag{47}$$

This formula (47) simplifies in the case of the "ε-systems" [see (14) and (15), that was well known in the case $N=2$, for example, see Ref. 7]. The velocities w^i of the commuting flows (i.e., Riemann invariants r^i are considered as the functions simultaneously of three independent variables x, t, τ),

$$r^i_\tau=w^i(\mathbf{r})r^i_x,\quad i=1,2,\ldots,N, \tag{48}$$

can be found as the solutions of another linear system (also see Ref. 36):

$$\partial_i w^k=-\frac{\psi_i'}{f_i(r^i)-f_k(r^k)}(w^i-w^k),\quad i\neq k. \tag{49}$$

Theorem 2: *Any solutions of the linear system (49) are connected with the solutions of another linear system [cf. (45)],*

$$\partial_{ik}\tilde{h}=-\frac{\psi_k'(r^k)}{f_i(r^i)-f_k(r^k)}\partial_i\tilde{h}+\frac{\psi_i'(r^i)}{f_i(r^i)-f_k(r^k)}\partial_k\tilde{h},\quad i\neq k,$$

by the differential substitution of the first order

$$w^i=\frac{1}{\psi_i'}\partial_i\tilde{h}.$$

Thus, the generating function of solutions [for the hydrodynamic type systems (8) and (42)–(44); cf. (13) and (33)] by the Tsarev generalized hodograph method (also see Ref. 36) is

$$\begin{aligned}x+\left[f_i(r^i)-\sum_{k=1}^{N}\psi_k(r^k)\right]t_1+\frac{1}{f_i(r^i)}\exp\left[\sum_{m=1}^{N}\int^{r^m}\frac{d\psi_m(\lambda)}{f_m(\lambda)}\right]t_{-1}\\ =-\frac{1}{\lambda-f_i(r^i)}\exp\left[-\sum_{k=1}^{N}\int^{r^k}\frac{d\psi_k(\tilde{\lambda})}{\lambda-f_k(\tilde{\lambda})}\right],\end{aligned} \tag{50}$$

where the generating function of commuting flows [see (19)] in Riemann invariants is

$$r^i_{\tau(\tilde{\lambda})}=\frac{1}{(1-f_i(r^i)/\tilde{\lambda})\tilde{\mu}}r^i_x.$$

Remark: If one selects the monoms

$$\psi_i(r^i)=\varepsilon_i r^i,$$

where ε_k are arbitrary constants, then the generalized "ε-systems"

$$r_t^i=\left[r^i-\sum_{m=1}^{N}\varepsilon_m r^m\right]r_x^i \tag{51}$$

have the generating function of conservation law densities [cf. (14) and (47)]

$$\mu=\prod_{m=1}^{N}(1-r_m/\lambda)^{-\varepsilon_m}.$$

In the general case (N *is arbitrary) the hydrodynamic type system (51) is the natural* N*-parametric reduction of the hydrodynamic chain (37). When* $N=2$ *this system (51) is the natural two-parametric generalization of gas dynamics (9). If we choose [cf. (38)]*

$$c_0=\sum_{m=1}^{N}\varepsilon_m\ln r^m,\quad c_k=\frac{1}{k}\sum_{m=1}^{N}\varepsilon_m(r^m)^k,\quad k=\pm1,\pm2,\ldots,$$

then the hydrodynamic type system (51) satisfies hydrodynamic chain (37).

Remark: In the particular case $f_i(r^i)=\varepsilon_i$ (ε_i *are arbitrary constants and* $\varepsilon_i\neq\varepsilon_k$ *for* $i\neq k$; *this is the* N*-component generalization of gas dynamics, when the adiabatic index* $\gamma=1$*) the hydrodynamic type system (42)*

$$r_t^i=\left[\varepsilon_i-\sum_{m=1}^{N}\psi_m(r^m)\right]r_x^i$$

is "trivial" [also $\psi_i(r^i)\neq\text{const}$*]. In this case, the linear system (45) has constant coefficients*

$$\frac{\partial^2 h}{\partial R^i\partial R^k}=\frac{1}{\varepsilon_i-\varepsilon_k}\left[\frac{\partial h}{\partial R^i}-\frac{\partial h}{\partial R^k}\right],\quad i\neq k,$$

where $R^i=\psi_i(r^i)$.

VI. GENERAL SOLUTION

Description of the general solution for the linear system (45) is a very complicated task. Construction of the general solution has been made only in the case of the "ε-systems" (see Ref. 31), when N is arbitrary; cases $N=2$ and $N=3$ were completely investigated by G. Darboux, L. P. Eisenhart, and T. H. Gronwall (see Refs. 7 and 10). The basic idea of how to construct a general solution (parametrized by N functions of a single variable, see Ref. 36) of any overdetermined linear systems like (45) was presented in Ref. 36 by recursive application of symmetry operators compatible with such systems. However, here we establish an alternative approach in the spirit of G. Darboux (see Ref. 36; also, see the section concerning elliptic coordinates in Ref. 7). Elliptic coordinates μ_α ($\alpha=1,2,\ldots,N$) appear in the theory of integrable hydrodynamic type systems associated with hyperelliptic curves, i.e., with the "ε-systems," where $\varepsilon=-\frac{1}{2}$. G. Darboux suggested to introduce special variables r^k ($k=1,2,\ldots,N$) for separation of coordinates in the Laplace equation by the following rule [see (15), when $\varepsilon=-\frac{1}{2}$]

$$\mu_\alpha^2=\frac{\Pi_{k=1}^{N}(\gamma_\alpha-r^k)}{\Pi_{\beta\neq\alpha}(\gamma_\alpha-\gamma_\beta)},\quad g^{ii}=\frac{\Pi_{\beta=1}^{N}(r^i-\gamma_\beta)}{\Pi_{k\neq i}(r^i-r^k)},$$

where γ_α are arbitrary constants [the denominator $\Pi_{\beta\neq\alpha}(\gamma_\alpha-\gamma_\beta)$ in the first expression is just a constant multiplier, which does not affect the property to be a conservation law density, also see (29)] and the flat (not constant) metric $g^{ii}(\mathbf{r})$ determined by

$$ds^2=\sum_{\alpha=1}^{N}(d\mu_\alpha)^2=\sum_{k=1}^{N}g_{kk}(dr^k)^2.$$

Thus, elliptic coordinates coincide with the Riemann invariants for "ε-systems," where $\varepsilon=-\frac{1}{2}$. It is easy to generalize the Darboux coordinates μ_α to an arbitrary ε:

$$(\mu_\alpha)^{-1/\varepsilon}=\frac{\Pi_{k=1}^{N}(\gamma_\alpha-r^k)}{\Pi_{\beta\neq\alpha}\Pi(\gamma_\alpha-\gamma_\beta)},\quad \alpha=1,2,\ldots,N.$$

In this case, all the "ε-systems," for instance, (13) and (33), can be written explicitly via μ_α in the conservative form [see (30) and (35) in the particular case $\varepsilon=-\frac{1}{2}$]

$$\begin{aligned}&\partial_t\mu_\alpha=\partial_x\left[\left(\varepsilon\sum_{\beta=1}^{N}(\mu_\beta)^{-1/\varepsilon}+\gamma_\alpha-\varepsilon\sum_{\beta=1}^{N}\gamma_\beta\right)\mu_\alpha\right],\\ &\partial_{t_{-1}}\mu_\alpha=\frac{\Pi_{\beta=1}^{N}(\gamma_\beta)^{\varepsilon}}{\gamma_\alpha}\partial_x\left[\left(1-\sum_{\beta=1}^{N}\frac{(\mu_\beta)^{-1/\varepsilon}}{\gamma_\beta}\right)^{\varepsilon}\mu_\alpha\right],\quad \alpha=1,2,\ldots,N.\end{aligned}\tag{52}$$

Remark: The hydrodynamic type systems (13) and (33) for another set of the moments $E_k=\Sigma_{\beta=1}^{N}(\gamma_\beta)^k(\mu_\beta)^{-1/\varepsilon}$ *[see (52)] can be written as the following hydrodynamic chains:*

$$\partial_{t_1}E_k=\partial_xE_{k+1}+\varepsilon\left[E_0-\sum_{\beta=1}^{N}\gamma_\beta\right]E_{k,x}-E_kE_{0,x},\quad k=0,\pm1,\pm2,\ldots,\tag{53}$$

$$\partial_{t_{-1}}E_k=\prod_{\beta=1}^{N}(\gamma_\beta)^{\varepsilon}[(1-E_{-1})^{\varepsilon}\partial_xE_{k-1}+(1-E_{-1})^{\varepsilon-1}E_{k-1}E_{-1,x}],\tag{54}$$

where

$$a_1=\varepsilon\left(\sum_{\beta=1}^{N}\gamma_\beta-E_0\right),\quad b_0=\prod_{\beta=1}^{N}(\gamma_\beta)^{-\varepsilon}(1-E_{-1})^{-\varepsilon}.$$

Remark: The hydrodynamic chain (53) is the same as the hydrodynamic chain (30), because these two chains are connected by the invertible transformation [see (29) and (39)]

$$\mu^{-1/\varepsilon}=1+\sum_{k=0}^{\infty}E_k\lambda^{-(k+1)},\tag{55}$$

where $\lambda\to\infty$. *The hydrodynamic chain (54) is the same as the hydrodynamic chain (35), because these two chains are connected by the invertible transformation [see (34) and (40)]*

$$\mu^{-1/\varepsilon}=1-\sum_{k=1}^{\infty}E_{-k}\lambda^{k-1},$$

where $\lambda\to0$.

Thus, our approach is the following: we mark N arbitrary points $\lambda=\gamma_\alpha$ (N distinct punctures) on the Riemann surface $F(\lambda,\mu)=0$ [see (47) and cf. (12)]; then we obtain special set of coordinates

$$\mu_\alpha=\exp\left(\sum_{k=1}^{N}\int_{\gamma_\alpha}^{r^k}\frac{d\psi_k(\tilde\lambda)}{\gamma_\alpha-f_k(\tilde\lambda)}\right),\tag{56}$$

which in fact is *the fundamental basis of linearly independent solutions* for the corresponding linear system (45). It means that any solution of the linear system (45) can be presented as a linear combination of the basis solutions (56) with some coefficients. Finally, we just mention that any overdetermined linear system like (45) must have a general solution which depends on N arbitrary parameters γ_α. In our case, we should take N infinite series of the conservation law densities $\mu_{\alpha,k}$ $(k=1,2,\dots)$ starting near already fixed punctures γ_α:

$$\mu^{(\alpha)}=\mu_\alpha+(\lambda-\gamma_\alpha)\mu_{\alpha,1}+(\lambda-\gamma_\alpha)^2\mu_{\alpha,2}+\cdots, \quad \lambda\to\gamma_\alpha, \quad \alpha=1,2,\dots,N.$$

Thus, the general solution of the linear system (45) is

$$h(\mathbf{r})=\sum_{\beta=1}^{N}\int_{\gamma_\beta}^{r^\beta}\varphi_\beta(\lambda)\mu^{(\beta)}(\lambda)d\lambda,$$

where $\varphi_\beta(\lambda)$ are arbitrary functions, and the general solution of the hydrodynamic type systems is given in the implicit form [see (8), (42)–(44), and (50)]:

$$x+\left[f_i(r^i)-\sum_{k=1}^{N}\psi_k(r^k)\right]t_1+\frac{1}{f_i(r^i)}\exp\left[\sum_{m=1}^{N}\int^{r^m}\frac{d\psi_m(\lambda)}{f_m(\lambda)}\right]t_{-1}$$
$$=\frac{1}{\psi_i'(r^i)}\partial_i\left[\sum_{\beta=1}^{N}\int_{\gamma_\beta}^{r^\beta}\varphi_\beta(\lambda)\tilde{\mu}^{(\beta)}(\lambda)d\lambda\right], \tag{57}$$

where

$$\tilde{\mu}_\alpha=\exp\left[-\sum_{k=1}^{N}\int_{\gamma_\alpha}^{r^k}\frac{d\psi_k(\tilde{\lambda})}{\gamma_\alpha-f_k(\tilde{\lambda})}\right], \quad \tilde{\mu}(\mathbf{r},\lambda)=\exp\left[-\sum_{k=1}^{N}\int^{r^k}\frac{d\psi_k(\tilde{\lambda})}{\lambda-f_k(\tilde{\lambda})}\right],$$

$$\tilde{\mu}^{(\alpha)}=\tilde{\mu}_\alpha+(\lambda-\gamma_\alpha)\tilde{\mu}_{\alpha,1}+(\lambda-\gamma_\alpha)^2\tilde{\mu}_{\alpha,2}+\cdots, \quad \lambda\to\gamma_\alpha, \quad \alpha=1,2,\dots,N.$$

The general solution of the linear system (45) can be presented in the most possible explicit form in special case, when values ε are *integers* for the "ε-systems." The case $N=2$ (namely, Euler–Darboux–Poisson equation) was completely investigated (see, for instance, Ref. 35). Its generalization on the N-component case (46), or moreover on the case of arbitrary *integers* ε_m [see (51)],

$$\partial_{ik}h=\frac{1}{r^i-r^k}[\varepsilon_k\partial_i h-\varepsilon_i\partial_k h], \quad i\neq k, \tag{58}$$

can be made in the same way as in Ref. 35. For simplicity, here we shall restrict our consideration to the case of (46) (see Ref. 31).

The general solution of (46) (if $\varepsilon=\pm n$, $n=1,2,\dots$) is

$$h_{(n)}=\sum_{k=1}^{N}\frac{d^n}{d(r^k)^n}\left[\frac{\varphi_k(r^k)}{\sum_{m\neq k}(r^k-r^m)^n}\right], \quad h_{(-n)}=\sum_{k=1}^{N}\int^{r^k}\varphi_k(\lambda)\prod_{m=1}^{N}(\lambda-r^m)^n d\lambda,$$

where $\varphi_k(r^k)$ are N arbitrary functions of a single variable [if we replace $\varphi_k(\lambda)\to\varphi_k^{(nN+1)}(\lambda)$ in second *negative* case, then all integrals can be expressed via finite number of derivatives only]. Thus, indeed, these solutions are general (see Ref. 36) for *positive* and *negative integers* ε [see (13) and (46)]. The general solutions for (58) can be obtained by recursive application of Laplace transformations (see Ref. 11) to the above formulas (also, see Ref. 1).

If ε is negative and $\varepsilon\neq -n$, $n=1,2,\dots$, then the above-mentioned solution (right) easily generalizes to

$$h_\varepsilon=\sum_{k=1}^{N}\int_{\gamma_k}^{r^k}\varphi_k(\lambda)\prod_{m=1}^{N}(\lambda-r^m)^{-\varepsilon}d\lambda,$$

where γ_k $(k=1,2,\ldots,N)$ are arbitrary constants. If ε is positive and $\varepsilon\neq n$, $n=1,2,\ldots$, then the above-mentioned solution (left) easily generalizes to just the case when εN is integer. Then

$$h_\varepsilon=\sum_{k=1}^{N}\oint_{C_k}\frac{\varphi_k(\lambda)d\lambda}{\Pi_{m=1}^{N}(\lambda-r^m)^{\varepsilon}},$$

where C_k $(k=1,2,\ldots,N)$ are simple small contours surrounding the points $\lambda=r^k$ $(k=1,2,\ldots,N)$. However, in a general case (when ε is positive and εN is not integer) these contours C_k could not be closed on corresponding Riemann surface, because a sum of all phase shifts (for every point) will not be proportional to $2\pi M$, where M is some integer. For avoiding this problem one can introduce another set of contour-dumbbell-shaped figures $C_{k,k+1}$ surrounding every two neighbor points $\lambda=r^k$ and $\lambda=r^{k+1}$ $(k=1,2,\ldots,N)$. So, the integration must change sign twice from clockwise to anticlockwise, then every time a phase shift will be 2π exactly. However, the number of contours must be equal to $N-1$, because in the opposite case (if the number is N) all contours became linearly dependent. Thus, in this general case a general solution of (46) parametrized by the N arbitrary functions of a single variable is

$$h_\varepsilon=\sum_{k=1}^{N-1}\oint_{C_{k,k+1}}\frac{\varphi_k(\lambda)d\lambda}{\Pi_{m=1}^{N}(\lambda-r^m)^{\varepsilon}}+\int_{-\infty}^{0}\frac{\varphi_N(\lambda)d\lambda}{\Pi_{m=1}^{N}(\lambda-r^m)^{\varepsilon}},$$

where for simplicity we assume (without lost of generacy) that real parts of Riemann invariants r^k (branch points on a complex Riemann surface) are numerated as follows:

$$0<\mathrm{Re}r^1<\mathrm{Re}r^2<\cdots<\mathrm{Re}r^N.$$

VII. (2+1)-INTEGRABLE HYDRODYNAMIC TYPE SYSTEMS

The Benney moment chain (1) is equivalent to the hierarchy of $(2+1)$ hydrodynamic type systems embedded in the dispersionless KP hierarchy as the Khohlov–Zabolotskaya equation

$$(u_{t_2}-uu_x)_x=u_{t_1t_1}, \tag{59}$$

which can be obtained from the coupled equations of the Benney moment chain (1) and one equation of its first nontrivial commuting flow (see Sec. IX)

$$\partial_{t_2}A_k=\partial_xA_{k+2}+A_0A_{k,x}+(k+1)A_kA_{0,x}+kA_{k-1}A_{1,x},\quad k=0,1,2,\ldots, \tag{60}$$

by eliminating the moments A_1 and A_2:

$$\partial_{t_1}A_0=\partial_xA_1,\quad \partial_{t_1}A_1=\partial_x[A_2+\tfrac{1}{2}A_0^2],\quad \partial_{t_2}A_0=\partial_x[A_2+A_0^2],$$

where $u=A_0$.

Let us start now with the hydrodynamic chains (30) and (32), eliminate the field variable a_3 from couple equations from the first hydrodynamic chain (30) and one equation from the second hydrodynamic chain (60),

$$\partial_{t_1}a_1=\partial_x[a_2-a_1^2],\quad \partial_{t_1}a_2=\partial_x[a_3-a_1a_2],\quad \partial_{t_2}a_1=\partial_x[a_3-2a_1a_2+a_1^3].$$

Then we came to the new integrable $(2+1)$ hydrodynamic type system

$$u_{t_1}=w_x, \quad u_{t_2}=w_{t_1}+uw_x-wu_x, \tag{61}$$

where

$$u=a_1, \quad w=a_2-a_1^2.$$

It is easy to check that all possible hydrodynamical reductions of this system (61) (see, for instance, the approach in Ref. 15):

$$r^i_{t_1}=\mu_i(\mathbf{r})r^i_x, \quad r^i_{t_2}=\zeta_i(\mathbf{r})r^i_x, \quad i=1,2,\ldots,N,$$

are exactly the same as those found already [see (42)], where

$$\zeta_i=f_i^2(r^i)-f_i(r^i)\sum_{k=0}^{N}\psi_m(r^m)+\frac{1}{2}\left(\sum_{k=0}^{N}\psi_m(r^m)\right)^2-\sum_{k=0}^{N}\int^{r^k}f_k(\lambda)d\psi_k(\lambda).$$

Moreover, one can obtain a whole hierarchy of such integrable $(2+1)$ hydrodynamic type systems like (61) by eliminating some other field variables a_k in combination with other commuting flows of the hydrodynamic chain (30). For example, two other equations [see (37) and (41)],

$$\partial_{t_1}e^{-c_0}=\partial_x[-c_1e^{-c_0}], \quad \partial_{t_{-1}}c_1=\partial_x e^{c_0}, \tag{62}$$

yield a new integrable $(2+1)$ hydrodynamic type system [its $(1+1)$ hydrodynamical reductions are exactly (43) and (44)].

VIII. ANOTHER HYDRODYNAMIC CHAIN

Now we start with the integrable hydrodynamic type system[18]

$$r^i_t=\left[\sum_{m=1}^{N}\varepsilon_m r^m-\varepsilon_i\sum_{m=1}^{N}r^m\right]r^i_x, \quad i=1,2,\ldots,N, \tag{63}$$

when ε_k are arbitrary constants. This system can be rewritten as the hydrodynamic chain

$$\partial_t c_k=c_1\partial_x c_k-c_0\partial_x c_{k+1}, \quad k=0,\pm1,\pm2,\ldots, \tag{64}$$

where the moments

$$c_k=\sum_{m=1}^{N}r^m(\varepsilon_m)^k.$$

Theorem 3: *Under the reciprocal transformation*

$$dz=\frac{1}{c_0}dx+\frac{c_1}{c_0}dt, \quad dy=dt,$$

this hydrodynamic chain linearizes

$$\partial_y c_k+\partial_z c_{k+1}=0, \quad k=0,\pm1,\pm2,\ldots. \tag{65}$$

It means that any reductions such as (63) of the hydrodynamic chain (64) linearizes under above reciprocal transformation. The solution of the hydrodynamic chain (65) is a set of the separate Riemann–Monge–Hopf equations

$$r^i_y+f_i(r^i)r^i_z=0, \quad i=1,2,\ldots,N,$$

where $f_i(r^i)$ are arbitrary functions. Thus, every integrable reduction of hydrodynamic chain (64) has the simple form

$$r^i_t=[c_0 f_i(r^i)-c_1]r^i_x,$$

where

$$c_k=\sum_{m=1}^{N}\int^{r^m}[f_m(\lambda)]^k d\psi_m(\lambda),\quad k=0,\pm 1,\pm 2,\ldots,$$

and $\psi_m(r^m)$ are arbitrary functions [by scaling $\psi_m(r^m)\to R_m$ integrable hydrodynamical reductions are parametrized by N arbitrary functions of a single variable only].

IX. OPEN PROBLEMS

The Benney moment chain (the Zakharov reduction) is a dispersionless limit of the vector nonlinear Schrödinger equation [see (11), (12), and Ref. 38]. The inverse problem is how to reconstruct a *dispersive* integrable analog of given hydrodynamic type system. A *dispersive* analog is known [coupled KdV is a *dispersive* analog of system (13); couple Harry Dym is a *dispersive* analog of system (33), see, e.g., Refs. 22 and 16] just in the case of the "ε-systems" with $\varepsilon=-\frac{1}{2}$. The KP hierarchy is a *dispersive* analog for the *whole* Benney moment chain (1) [as the KP equation is a *dispersive* analog of the Khohlov–Zabolotzkaya system (59)], but similar *dispersive* $(2+1)$ analogs for the whole hydrodynamic chain (37) or for the $(2+1)$ hydrodynamic type systems (61) or (62) still are unknown.

Local Hamiltonian structures for the hydrodynamic type system (13) were completely investigated in Ref. 29 and 16. It was proved that, if $N=2$, then the hydrodynamic type system (13) for any ε has three local Hamiltonian structures (also, see Refs. 28 and 12); if $N=3$ and $\varepsilon=-\frac{1}{2}$, then it has four local Hamiltonian structures; if $N=3$ and $\varepsilon=1$, then it has two-parametric family of local Hamiltonian structures (also see Refs. 30 and 17); if $N>3$, then $\varepsilon=-\frac{1}{2}$ and it has $(N+1)$-local Hamiltonian structures.

Hamiltonian structures of integrable hydrodynamic type systems are determined by a metric g_{ii} (see, Ref. 9). The metric

$$g^{ii}=\zeta_i(r^i)\exp\left[-2\sum_{k\neq i}\int^{r^k}\frac{d\psi_k(\lambda)}{f_i(r^i)-f_k(\lambda)}\right]$$

with arbitrary functions $\zeta_i(r^i)$ determines a nonlocal Hamiltonian formalism (see Ref. 13 and 36) of hydrodynamic type systems (8) and (42)–(44) and their commuting flows. Unfortunately, local and nonlocal Hamiltonian formalism has been done just for the hydrodynamic type systems (13) when $\varepsilon=\pm 1$ and $\varepsilon=-\frac{1}{2}$ (see, for instance Refs. 17 and 13). However, the problem of a description of local and nonlocal Hamiltonian structures in general case (42) still is open. Nevertheless, this problem can be solved by the Dirac restriction of a Hamiltonian structure (see for the beginning Ref. 13) known for the whole hydrodynamic chain, as it was already done in Ref. 6 for other hydrodynamic chains.

The starting point of such an investigation is a Lax-type representation. For instance, the Lax-type representation [see (2)] for the dispersionless KP hierarchy [i.e., the Benney moment chain (1)] is well known (see Ref. 26)

$$\partial_{t_n}\lambda=\{Q_n,\lambda\}=\frac{\partial Q_n}{\partial\mu}\frac{\partial\lambda}{\partial x}-\frac{\partial Q_n}{\partial x}\frac{\partial\lambda}{\partial\mu},\quad n=0,1,2,\ldots, \tag{66}$$

where Q_n is the part, polynomial in μ, of λ^n. Also, the first local Hamiltonian structure for whole Benney moment chain (1),

$$\partial_{t_n} A_k = \sum_{m \geqslant 0} \left[k A_{k+m-1} \partial_x \frac{\delta H_{n+1}}{\delta A_m} + \left(m A_{k+m-1} \frac{\delta H_{n+1}}{\delta A_m} \right)_x \right], \tag{67}$$

where the Hamiltonian is $H_2 = \frac{1}{2}\int [A_2 + A_0^2] dx$, was constructed in Ref. 25 [the relationship between formulas (66) and (67) was found in Ref. 26, too; first nontrivial commuting flow [see (60)] is determined by the next Hamiltonian $H_3 = \frac{1}{3}\int [A_3 + 3A_0 A_1] dx$; functional $H_0 = \int A_0 dx$ is a Casimir of this Hamiltonian structure, the functional $H_1 = \int A_1 dx$ is a momentum of this Hamiltonian structure].

Similar Lax type representation for the hydrodynamic chain (37) was established in Ref. 4 [cf. (66)]

$$\partial_{t_n} L = \langle Q_n, L \rangle = Q_n \frac{\partial L}{\partial x} - \frac{\partial Q_n}{\partial x} L, \quad n = 0,1,2,\ldots, \tag{68}$$

where

$$Q_n = (\lambda^n L)_+, \quad L = 1 + G_0/\lambda + G_1/\lambda^2 + G_2/\lambda^3 + \cdots.$$

The corresponding first hydrodynamic chain

$$\partial_{t_1} G_k = \partial_x G_{k+1} + G_0 G_{k,x} - G_k G_{0,x}, \quad k = 0,1,2,\ldots,$$

is exactly the hydrodynamic chain (53), where $\varepsilon = 1$, and the linear term $-\varepsilon(\Sigma_{\beta=1}^N \gamma_\beta) E_{k,x}$ is removed by a shift of the independent variable $[x \to x - \varepsilon(\Sigma_{\beta=1}^N \gamma_\beta) t]$. Thus, a generating function of these moments is [see (53), (55), and (68)]

$$\mu^{-1} \equiv L = 1 + \sum_{k=0}^{\infty} G_k \lambda^{-(k+1)}.$$

The alternative Lax type representations are

$$\partial_{t_k} \rho = \left[\sum_{m=0}^{k} \tilde{a}_m \lambda^{k-m} \partial_x, \rho \right], \quad \partial_{t_{-k-1}} \rho = \left[\sum_{m=0}^{k} \tilde{b}_m \lambda^{m-k-1} \partial_x, \rho \right], \quad k = 0,1,2,\ldots,$$

where $\mu = \rho_x$ [see (21) and (23)].

We suppose that the hydrodynamic chain (37) and its commuting flows have local Hamiltonian structure [cf. (67)]

$$\partial_{t_n} c_k = \sum_{k=1}^{\infty} [\beta_{k,m}(\mathbf{c}) \partial_x + \partial_x \beta_{m,k}(\mathbf{c})] \frac{\delta H_{n+1}}{\delta c_m},$$

where $\beta_{k,m}$ are some functions.

The Hamiltonian structures of integrable hydrodynamic type systems can be successfully investigated by application of methods from the differential (see, for example, Refs. 36, 29–33, 12,16, 13, and 17) and algebraic geometries (see, for instance, Refs. 8 and 24). An alternative way is following: assume that our given integrable hydrodynamic type system (N components) is a some reduction of some ''bigger'' integrable hydrodynamic type system ($N+M$ components); assume that Hamiltonian structure of such ''bigger'' integrable hydrodynamic type system is already known. Then the direct application of the Dirac restriction to this Hamiltonian structure [the first step in such procedure (see Ref. 13) is the choice of some Riemann invariants $r^k = \text{const}$, $k = 1,2,\ldots,M$] yields the transformed Hamiltonian structure of a ''restricted'' hydrodynamic type system. The Dirac restriction of Hamiltonian structures (in algebraic language) was developed in application to hydrodynamic chains and their reductions (see Ref. 6). The first step

in such a procedure is the recalculation of the Lax type representation [such as (66) or (68)] to the Hamiltonian structure of a whole hydrodynamic chain [see, for instance, (67)].

X. CONCLUSION

In this article we present a recipe: how to construct a hydrodynamic chain starting from any given hydrodynamic type system with *polynomial* (or *rational*) velocities with respect to their field variables [for simplicity we have mentioned just two cases: namely Benney moment chain, whose moments are connected directly with some *conservation law densities* (u_k, η_k) and the hydrodynamic chain (37), whose moments are connected directly with *Riemann invariants*]. In fact, it means that **any integrable hydrodynamic type system (written in Riemann invariants) with such *polynomial* velocities is embedded in hydrodynamic chain (37) or its higher (or lower) commuting flows**. Any integrable hydrodynamic type system written in Riemann invariants with *rational* velocities

$$r^i_t = g_0 \frac{(r^i)^M + g_1 (r^i)^{M-1} + \cdots + g_M}{(r^i)^K + e_1 (r^i)^{K-1} + \cdots + e_K} r^i_x, \quad i = 1,2,\ldots,N, \tag{69}$$

has the generating function of conservation laws

$$\mu_t = \partial_x \left[g_0 \frac{\lambda^M + g_1 \lambda^{M-1} + \cdots + g_M}{\lambda^K + e_1 \lambda^{K-1} + \cdots + e_K} \mu \right]. \tag{70}$$

For simplicity we assume that the coefficients e_k and g_k of such *rational* velocities are some *symmetric* (not necessary to be *polynomials*!) functions of Riemann invariants; K, M, and N are arbitrary natural numbers. As example, we can take any integrable systems embedded into 2×2 spectral transform like the Korteweg–de Vries equation, the Bonnet equation (the sine-Gordon equation) and the nonlinear Schrödinger equation. All their Whitham deformations [i.e., hydrodynamic type systems, see, for instance, Refs. 8 and 24] have such representation (69) as consequence (70) written in Abelian differentials on hyperelliptic surfaces

$$\partial_t dp = \partial_x dq,$$

where

$$dp = \frac{\lambda^K + e_1 \lambda^{K-1} + \cdots + e_K}{\sqrt{\Pi_{m=1}^N (r_m - \lambda)}} d\lambda, \quad dq = g_0 \frac{\lambda^M + g_1 \lambda^{M-1} + \cdots + g_M}{\sqrt{\Pi_{m=1}^N (r_m - \lambda)}} d\lambda,$$

and velocities of (69) are

$$g_0 \frac{(r^i)^M + g_1 (r^i)^{M-1} + \cdots + g_M}{(r^i)^K + e_1 (r^i)^{K-1} + \cdots + e_K} = \left. \frac{dq}{dp} \right|_{\lambda = r^i}.$$

Substituting [cf. (39)]

$$\mu = 1 + \sum_{k=1}^{\infty} a_k \lambda^{-k}$$

into the generating function (70) one can obtain similar formulas and results as it was done in this article. The next step is a *replication* of integrable hydrodynamic type systems as different hydrodynamical reductions of hydrodynamic chains. The *main advantage* of such *replicated* systems is a *preservation* of some properties of original hydrodynamic type systems like *generating functions of conservation laws and commuting flows* [see (2), (4), and (6) for the Benney moment chain (1); see (14), (29), and (20) for the hydrodynamic chain (37)]. Thus, a problem of integrability is much

simpler—all that necessary to do: to construct a general solution [starting from already obtained generating function, see (7), (50), and (57)], parametrized by N functions of a single variable (see Ref. 36) and to solve Cauchy problem, that in fact is done to this moment just for four cases (the Zakharov reduction of the Benney moment chain, see Ref. 19; linearly degenerate system, see Ref. 37; this particular class is the "ε-systems" with $\varepsilon=1$; hydrodynamic type systems of the Tample class, this particular class is the "ε-systems" with $\varepsilon=-1$, see Ref. 29; Whitham hydrodynamic type systems related with hyperelliptic surfaces such averaged N-phase solutions of Korteweg–de Vries equation (KdV) or nonlinear Schrödinger equation (NLS), it was done in articles of G. El, T. Grava, B.A. Dubrovin, F. R. Tian, J. Gibbons and many others).

Moreover, any two commuting flows of (29), for example, (21),

$$dz=\mu\left[dx+\sum_{m=0}^{k}\tilde{a}_m\lambda^{k-m}dt^k+\sum_{m=0}^{n}\tilde{a}_m\lambda^{n-m}dt^n\right],\qquad k,n=1,2,\ldots,$$

yield the hydrodynamic type systems with *rational* velocities

$$r^i_{t_k}=\frac{\sum_{m=0}^{k}\tilde{a}_m(r^i)^{k-m}}{\sum_{m=0}^{n}\tilde{a}_m(r^i)^{n-m}}r^i_{t_n},\quad k\neq n,\qquad i=1,2,\ldots,N.$$

A more complicated *rational* dependence can be obtained by application of a generalized reciprocal transformation (see, for instance, Ref. 11 and 17), starting from (29) and its commuting flows.

Thus, this is a *powerful tool for classification* of integrable hydrodynamic type systems and their *integrability*. Moreover, if any given hydrodynamic type system has a generating function of conservation laws [see, for instance, (4) or (29)], it means that the corresponding hydrodynamic chain has the same generating function. For example, if a some hydrodynamic type system has the same generating function as the Benney moment chain (4), it means that this hydrodynamic type system is some reduction of the Benney moment chain. Thus, this is a wonderful symptom in a recognition of an immersion of any unknown hydrodynamic type systems into already known hydrodynamic chains. Thus, *if one can construct a generating function of conservation laws for some hydrodynamic type system, it means that, in fact, the hydrodynamic chain is already constructed* (and may be recognized, because, obviously, the number of hydrodynamic chains is much smaller than the number of integrable hydrodynamic type systems).

However, the problem of a description of all possible reductions is very complicated. For instance, this problem for the Benney moment chain is still open (see Ref. 21). However, this problem for the Boyer–Finley moment chain (continuum limit of the Darboux–Laplace chain, which also is known as two-dimensional Toda lattice, see Refs. 3, 15, and 24) in fact does *not exist*, because both mentioned hydrodynamic chains are related by special exchange of independent variables (see Ref. 23). Thus, we are lucky to solve this problem for the hydrodynamic chain (37).

ACKNOWLEDGMENTS

I am grateful to my friends and colleagues Eugeni Ferapontov for his suggestions in improvement of my calculations and Yuji Kodama for useful discussions. Also I would like to thank Gennady El' and Anatoly Kamchatnov for carefully reading the manuscript.

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Random matrix averages and the impenetrable Bose gas in Dirichlet and Neumann boundary conditions

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(Received 30 January 2003; accepted 12 May 2003)

The density matrix for the impenetrable Bose gas in Dirichlet and Neumann boundary conditions can be written in terms of $\langle \Pi_{l=1}^{n} |\cos\phi_1 - \cos\theta_l||\cos\phi_2 - \cos\theta_l| \rangle$, where the average is with respect to the eigenvalue probability density function for random unitary matrices from the classical groups $\mathrm{Sp}(n)$ and $\mathrm{O}^+(2n)$, respectively. In the large n limit log-gas considerations imply that the average factorizes into the product of averages of the form $\langle \Pi_{l=1}^{n} |\cos\phi - \cos\theta_l| \rangle$. By changing variables this average in turn is a special case of the function of t obtained by averaging $\Pi_{l=1}^{n} |t - x_l|^{2q}$ over the Jacobi unitary ensemble from random matrix theory. The latter task is accomplished by a duality formula from the theory of Selberg correlation integrals, and the large n asymptotic form is obtained. The corresponding large n asymptotic form of the density matrix is used, via the exact solution of a particular integral equation, to compute the asymptotic form of the low lying effective single particle states and their occupations, which are proportional to $\sqrt{N}$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1599954]

I. INTRODUCTION

The probability density functions (p.d.f.'s)

$$\frac{1}{n!}\left(\frac{1}{2\pi}\right)^n \prod_{l=1}^{n} 4\sin^2(\theta_l) \prod_{1\leqslant j<k\leqslant n} 4(\cos\theta_k - \cos\theta_j)^2, \tag{1}$$

$$\frac{2}{n!}\left(\frac{1}{2\pi}\right)^n \prod_{1\leqslant j<k\leqslant n} 4(\cos\theta_k - \cos\theta_j)^2, \tag{2}$$

where $0 \leqslant \theta_j \leqslant \pi$ $(j=1,\ldots,n)$ occur in both random matrix theory and the quantum many body problem. In the former they are eigenvalue p.d.f.'s for classical groups with the Haar (uniform) measure—the group $\mathrm{Sp}(n)$ of $n\times n$ unitary matrices with real quaternion elements (which are themselves 2×2 matrices), and the group $\mathrm{O}^+(2n)$ of $2n\times 2n$ unitary matrices with real elements (real orthogonal matrices) and determinant equal to $+1$, for (1) and (2), respectively. A self-contained derivation of these facts can be found in Ref. 1, Chap. 2. In the latter they are the absolute value squared of the ground state wave function for n free fermions on the interval $[0, \pi]$ with Dirichlet and Neumann boundary conditions, respectively. As is similarly well known, and revised from first principles in our work,[2] they are also the absolute value squared of the ground

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state wave function for n impenetrable bosons on the interval $[0, \pi]$—in one-dimension the ground state wave function of the impenetrable Bose system is equal to the absolute value of the corresponding free Fermi system.

In studies relating to both these seemingly disparate interpretations of the p.d.f.'s (1) and (2) there is cause to investigate the function of (ϕ, m, n) defined by averaging

$$\prod_{l=1}^{n} (\cos\phi - \cos\theta_l)^m \tag{3}$$

with respect to these p.d.f.'s. In the random matrix interpretation this comes about in applications to L-function theory.[3–5] Briefly, there are families of L-functions with special symmetries which are known to have their nontrivial zeros well described by eigenvalues of random matrices from the classical group corresponding to that symmetry. For $\cos\phi = 1$ and small values of m the expected value of (3) can be computed with $\{\theta_l\}$ corresponding to the zeros of particular families of L-functions, and it can also be computed—with m a general non-negative integer—for the random matrix ensembles. This then allows for both a test of the original hypothesis relating L-functions to random matrices, and provides specific conjectures for the statistical properties of the zeros of the L-function families.

In the quantum many body interpretation the immediate interest is not in the average of (3), but rather the average of

$$\prod_{l=1}^{n} |\cos\phi_1 - \cos\theta_l||\cos\phi_2 - \cos\theta_l|. \tag{4}$$

This gives the ground state density matrix of the corresponding impenetrable Bose gas system (if the absolute value signs are removed, the average gives the ground state density matrix for the free Fermi system).[2] However the study of (4) leads back to the computation of (3). Thus as noted in Refs. 6 and 7 for the problem of computing the asymptotic behavior of the ground state density matrix for the impenetrable bosons in the bulk and in an harmonic trap respectively, for large n and ϕ_1 and ϕ_2 fixed the average (4) is expected to factorize, and be proportional to the average of the product involving ϕ_1 times the average of the product involving ϕ_2. The latter are then the continuation in m of (3) from the even positive integers to the value $m = 1$ [this being a way to effectively study the average of the absolute value of (3)].

We remark that in the case of the density matrix for the impenetrable bosons in periodic boundary conditions the analogous task is to compute the average of

$$\prod_{l=1}^{n} |e^{i\phi_1} - e^{i\theta_l}|\,|e^{i\phi_2} - e^{i\theta_l}| \tag{5}$$

with respect to the p.d.f.,

$$\frac{1}{n!}\left(\frac{1}{2\pi}\right)^n \prod_{1 \leqslant j < k \leqslant n} |e^{i\theta_k} - e^{i\theta_j}|^2, \tag{6}$$

where $-\pi < \theta_j \leqslant \pi$ $(j = 1, \ldots, n)$. In this case the asymptotic form for large n with ϕ_1 and ϕ_2 fixed is a special case of known asymptotic forms for Toeplitz determinants with singular generating functions of the so-called Fisher–Hartwig-type (for an extended discussion on this point and references to the relevant literature, see Ref. 2). The average of (4) with respect to (1) or (2) can readily be written as a Hankel determinant, but there is no known analog of the Fisher–Hartwig asymptotic form.

In Sec. II we show how, for m an even positive integer, the average of (3) with respect to the p.d.f.'s (1) and (2), which is by definition an n-dimensional integral, can be written as an m-dimensional integral. From the latter the large n asymptotic form of the average is deduced. In

Sec. III the result of Sec. II is used to deduce the large n asymptotic form of the average (4) with respect to the p.d.f.'s (1) and (2) and thus of the ground state density matrix. We conclude in Sec. IV by applying our result for the asymptotic form of the density matrix to the computation of the occupations of the effective single particle states. We also make some remarks in relation to the wider setting of our asymptotic analysis, in which we use Coulomb gas arguments to formulate an analog of the Fisher–Hartwig asymptotic form for a class of Jacobi unitary ensemble averages.

II. DUALITY FORMULAS FOR MULTIPLE INTEGRALS AND ASYMPTOTIC ANALYSIS

A. The duality formula

The change of variables,

$$x_j=\tfrac{1}{2}(\cos\theta_j+1) \quad (0\leqslant x_j\leqslant 1, \quad j=1,\dots,n) \tag{7}$$

transforms (1) and (2) into p.d.f.'s which are proportional to

$$\prod_{l=1}^{n}(x_l(1-x_l))^{1/2}\prod_{1\leqslant j<k\leqslant n}(x_k-x_j)^2, \tag{8}$$

$$\prod_{l=1}^{n}(x_l(1-x_l))^{-1/2}\prod_{1\leqslant j<k\leqslant n}(x_k-x_j)^2, \tag{9}$$

respectively. These p.d.f.'s in turn are special cases of the class of p.d.f.'s proportional to

$$\prod_{l=1}^{n}x_l^{\lambda_1}(1-x_l)^{\lambda_2}\prod_{1\leqslant j<k\leqslant n}(x_k-x_j)^2 \tag{10}$$

known in random matrix theory as the Jacobi unitary ensemble. Also, under the change of variables (7) the task of computing the average of (3) becomes the task of computing the average of

$$\prod_{l=1}^{n}(t-x_l)^m \tag{11}$$

with respect to (8) and (9), or more generally with respect to (10).

In fact there is an advantage in further generalizing the setting of the computation of the average of (11) and considering the class of multiple integrals known as Selberg correlation integrals, defined by

$$\begin{aligned}S_{n,m}(\lambda_1,\lambda_2,\lambda;t_1,\dots,t_m)&:=\frac{1}{C}\int_{[0,1]^n}dx_1\cdots dx_n\prod_{l=1}^{n}\left(x_l^{\lambda_1}(1-x_l)^{\lambda_2}\prod_{i=1}^{m}(t_i-x_l)\right)\\&\quad\times\prod_{1\leqslant j<k\leqslant n}|x_k-x_j|^{2\lambda}\\&=\left\langle\prod_{l=1}^{n}\prod_{i=1}^{m}(t_i-x_l)\right\rangle_{\mathrm{J}(2\lambda)\mathrm{E}_n}.\end{aligned} \tag{12}$$

Here,

$$C=S_n(\lambda_1,\lambda_2,\lambda)=\int_{[0,1]^n}dx_1\cdots dx_n\prod_{l=1}^{n}x_l^{\lambda_1}(1-x_l)^{\lambda_2}\prod_{1\leqslant j<k\leqslant n}|x_k-x_j|^{2\lambda}, \tag{13}$$

known as the Selberg integral, is the normalization chosen so that the coefficient of $\Pi_{i=1}^m t_i^n$ is unity, and the average over $\mathrm{J}(2\lambda)\mathrm{E}_n$ refers to the p.d.f.,

$$\frac{1}{S_n(\lambda_1,\lambda_2,\lambda)}\prod_{l=1}^n x_l^{\lambda_1}(1-x_l)^{\lambda_2}\prod_{1\leqslant j<k\leqslant n}|x_k-x_j|^{2\lambda} \tag{14}$$

[the notation $\mathrm{J}(2\lambda)\mathrm{E}_n$ denotes the Jacobi-(2λ) ensemble, which with $\lambda=1$ corresponds to the Jacobi unitary ensemble (10)]. Setting $t_1=\cdots=t_m=t$ in (12) gives the average of (11) with respect to (14). The advantage in studying (12) is that we can put to use the discovery of Ref. 8, relating the Selberg correlation integrals to the theory of Jack polynomials (in the case $\lambda=1$ the Jack polynomials coincide with the Schur polynomials[9]). In particular the Selberg correlation integrals were evaluated in terms of a generalization of the Gauss hypergeometric function ${}_2F_1$ based on the Jack polynomials. It was realized by one of the present authors[10–15] that theory initiated in Ref. 8 could be further developed and used to express the average of (9) with respect to (14) and its limiting forms as the Laguerre—(2λ) ensemble and the Gaussian—(2λ) ensemble, as m-dimensional integrals. Because the role of n and m is effectively interchanged, these integration identities have been referred to as duality formulas.[16–18] One of their uses, as we will demonstrate in the case of the average of (11) with respect to (10), is in the computation of the large n asymptotics.

The particular duality formula of interest to us is given explicitly in Ref. 15. To state the result we must introduce the generalized circular ensemble, $\mathrm{C}\beta\mathrm{E}_N$, as the p.d.f. proportional to

$$\prod_{1\leqslant j<k\leqslant N}|z_k-z_j|^\beta \quad (z_j=e^{i\theta_j},\ -\pi<\theta_j<\pi,\ j=1,\dots,N). \tag{15}$$

With this notation, we read off from Ref. 15, Eq. (3.41) that

$$\left\langle\prod_{l=1}^N z_l^{(\eta_1-\eta_2)/2}|1+z_l|^{\eta_1+\eta_2}(1+tz_l)^m\right\rangle_{\mathrm{C}\beta\mathrm{E}_N}\propto\left\langle\prod_{l=1}^m[1-(1-t)x_l]^N\right\rangle_{\mathrm{J}(4/\beta)\mathrm{E}_m}\Bigg|_{\substack{\lambda_1=2(\eta_2-m+1)/\beta-1\\ \lambda_2=2(\eta_1+1)/\beta-1}}. \tag{16}$$

But we want to make $\langle\Pi_{l=1}^n(t-x_l)^m\rangle_{\mathrm{J}(2\lambda)\mathrm{E}_n}$ the quantity being transformed, so (16) requires manipulation. For this we write

$$t\mapsto 1-\frac{1}{t},\quad m\leftrightarrow N,\quad \frac{2}{\beta}=\lambda,\quad N=n. \tag{17}$$

Noting that then

$$\eta_1=\frac{1}{\lambda}(\lambda_2+1)-1,\quad \eta_2=\frac{1}{\lambda}(\lambda_1+1)+n-1, \tag{18}$$

multiplying both sides of (16) by t^{mN} and taking the complex conjugate of the left-hand side of (16) shows

$$\left\langle\prod_{l=1}^n(t-x_l)^m\right\rangle_{\mathrm{J}(2\lambda)\mathrm{E}_n}$$
$$=A\left\langle\prod_{l=1}^m z_l^{([(\lambda_1-\lambda_2)/\lambda]-n)/2}|1+z_l|^{[(\lambda_1+\lambda_2+2)/\lambda]+n-2}[t(1+z_l)-1]^n\right\rangle_{\mathrm{C}(2/\lambda)\mathrm{E}_m}, \tag{19}$$

where A, the proportionality constant, is independent of t. To specify A requires, in addition to the Selberg integral (13), the so-called Morris integral,

$$M_n(a,b,\lambda) := \left(\frac{1}{2\pi}\right)^n \int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_n \prod_{l=1}^{n} z_l^{(a-b)/2} |1+z_l|^{a+b} \prod_{1\le j<k\le n} |z_k - z_j|^{2\lambda}. \quad (20)$$

Then setting $t=1$ in (19) shows that

$$A = \frac{S_n(\lambda_1,\lambda_2+m,\lambda)}{S_n(\lambda_1,\lambda_2,\lambda)} \frac{M_m(0,0,1/\lambda)}{M_m(\eta_2,\eta_1,1/\lambda)}, \quad (21)$$

where η_1 and η_2 are given by (18). Both the Selberg integral and Morris integral have exact evaluations in terms of products of gamma functions (see, e.g., Ref. 1). In the case $\lambda=1$ these read

$$\begin{aligned} S_n(a,b,1) &= \prod_{j=0}^{n-1} \frac{\Gamma(a+1+j)\Gamma(b+1+j)\Gamma(2+j)}{\Gamma(a+b+1+n+j)} \\ &= \frac{G(n+1+a)}{G(1+a)} \frac{G(n+1+b)}{G(1+b)} \frac{G(n+1+a+b)}{G(2n+1+a+b)} G(n+2), \end{aligned} \quad (22)$$

$$\begin{aligned} M_n(a,b,1) &= \prod_{j=0}^{n-1} \frac{\Gamma(a+b+1+j)\Gamma(2+j)}{\Gamma(a+1+j)\Gamma(b+1+j)} \\ &= \frac{G(n+1+a+b)}{G(1+a+b)} \frac{G(1+a)}{G(n+1+a)} \frac{G(1+b)}{G(n+1+b)} G(n+2), \end{aligned} \quad (23)$$

where $G(z)$ denotes the Barnes G-function, related to the gamma function by the functional equation,

$$G(z+1) = \Gamma(z) G(z). \quad (24)$$

B. Asymptotics

Our interest is in the asymptotic form of the $\mathrm{J}(2\lambda)\mathrm{E}_n$ average in (19) in the case $\lambda=1$ and m even. The experience of our previous study,[7] in which we studied the same product averaged over the Gaussian unitary ensemble (eigenvalue p.d.f. of complex Hermitian matrices with Gaussian entries) using a result known in the literature[19] (see also Ref. 20), tells us the related quantity,

$$\frac{Z_{n,\lambda_1,\lambda_2}((X,q))}{Z_{n+q,\lambda_1,\lambda_2}((\cdot,0))}, \quad (25)$$

where

$$\begin{aligned} Z_{n,\lambda_1,\lambda_2}((X,q)) &= X^{\lambda_1 q}(1-X)^{\lambda_2 q} \int_0^1 dX_1 \cdots \int_0^1 dX_n \prod_{l=1}^{n} X_l^{\lambda_1} (1-X_l)^{\lambda_2} |X-X_l|^{2q} \\ &\times \prod_{1\le j<k\le n} |X_k - X_j|^2 \end{aligned} \quad (26)$$

is better suited for the purpose. In addition to multiplying the JUE_n average in (19) by the t-dependent factor $t^{\lambda_1 m/2}(1-t)^{\lambda_2 m/2}$, a key feature of (25) is the normalization chosen so that in the interpretation of (26) as the configuration integral for a log-potential Coulomb gas the normalization has the same total charge.

It follows from (19), (21), and noting

$$Z_{n+q,\lambda_1,\lambda_2}((\cdot,0))=S_{n+q}(\lambda_1,\lambda_2,1), \tag{27}$$

that we have the duality formula for (25) with $q=m/2$, m even

$$\begin{aligned}
&\frac{Z_{n,\lambda_1,\lambda_2}((t,m/2))}{Z_{n+m/2,\lambda_1,\lambda_2}((\cdot,0))} \\
&\quad=\frac{S_n(\lambda_1,\lambda_2+m,1)}{S_{n+m/2}(\lambda_1,\lambda_2,1)M_m(\lambda_1+n,\lambda_2,1)}t^{\lambda_1 m/2}(1-t)^{\lambda_2 m/2} \\
&\quad\quad\times\left(\frac{1}{2\pi}\right)^m\int_{-\pi}^{\pi}d\theta_1\cdots\int_{-\pi}^{\pi}d\theta_m\prod_{l=1}^{m}z_l^{(\lambda_1-\lambda_2-n)/2}|1+z_l|^{\lambda_1+\lambda_2+n}[t(1+z_l)-1]^n \\
&\quad\quad\times\prod_{1\le j<k\le m}|z_k-z_j|^2 \\
&\quad=\frac{S_n(\lambda_1,\lambda_2+m,1)}{(2\pi)^m S_{n+m/2}(\lambda_1,\lambda_2,1)M_m(\lambda_1+n,\lambda_2,1)}I_n(t),
\end{aligned} \tag{28}$$

where

$$\begin{aligned}
I_n(t)&:=t^{\lambda_1 m/2}(1-t)^{\lambda_2 m/2}\int_{\mathcal{C}^m}dx_1\cdots dx_m\prod_{l=1}^{m}(x_l)^{\lambda_1+\lambda_2+n}(x_l-1)^{-(\lambda_2+n+m)}(tx_l-1)^n \\
&\quad\times\prod_{1\le j<k\le m}(x_k-x_j)^2.
\end{aligned} \tag{29}$$

In (29), $\mathcal{C}$ is any simple closed contour starting at $x_j=0$ in the complex plane and encircling $x_j=1$ anticlockwise without crossing the interval $x_j\in(0,1)$. We obtain the second equality in (28) by writing the integrand in a form without absolute value signs, changing variables

$$d\theta_j=\frac{1}{iz_j}dz_j, \tag{30}$$

then changing variables $z_j\mapsto x_j-1$.

The large n, fixed $t\in(0,1)$ asymptotic analysis of an integral very similar to (29) has been detailed in Ref. 14, and that analysis in turn follows the stationary phase analysis of a related multiple integral given in Ref. 11. Now, the n-dependent terms in the integrand of $I_n(t)$ are

$$x_j^n(1-x_j)^{-n}(1-tx_j)^n=\exp[n(\log x_j-\log(1-x_j)+\log(1-tx_j))]. \tag{31}$$

As noted in Ref. 14, a simple calculation shows that the stationary point of the exponent occurs when

$$x_j=1\pm i\left[\frac{1}{t}(1-t)\right]^{1/2}=:x_\pm. \tag{32}$$

This suggests we deform the contours so that $m/2$ integration variables, $(x_1,\ldots,x_{m/2})$ say, pass through x_+, and the remaining pass through x_-. We must then expand the integrand in the neighborhood of these stationary points. Because we have made a definite choice of the $m/2$ variables, we must multiply by the combinatorial factor $\binom{m}{m/2}$. Another factor of $(-1)^{m/2}$ comes from the sense of the deformed contour being opposite for x_+ and x_-. From Ref. 14 we know that expanding the exponent in (31) to second order in $(x_\pm-x_j)$ gives

$$\exp[n(\log x_j-\log(1-x_j)+\log(1-tx_j))]\sim\exp\left[-\frac{n\alpha}{2}(x_j-x_\pm)^2\right], \tag{33}$$

where

$$\alpha = \frac{t^2}{(1-tx_\pm)^2} + \frac{1}{x_\pm^2} - \frac{1}{(1-x_\pm)^2}. \tag{34}$$

Regarding the leading order expansion of the other terms in the integrand we have

$$\prod_{1\leqslant j<k\leqslant m} (x_k - x_j)^2 \sim (x_+ - x_-)^{2(m/2)^2} \prod_{1\leqslant j<k\leqslant m/2} (x_k - x_j)^2 \prod_{m/2+1\leqslant j<k\leqslant m} (x_k - x_j)^2, \tag{35}$$

$$\prod_{j=1}^{m} (x_j)^{\lambda_1+\lambda_2} (x_j - 1)^{-(\lambda_2+m)} \sim |x_+|^{(\lambda_1+\lambda_2)m} |1-x_+|^{-(\lambda_2+m)m}. \tag{36}$$

Hence,

$$\begin{aligned} I_n(t) &\sim (-1)^{m/2} \binom{m}{m/2} [t^{\lambda_1}(1-t)^{\lambda_2}]^{m/2} (x_+ - x_-)^{2(m/2)^2} |x_+|^{(\lambda_1+\lambda_2)m} |1-x_+|^{-(\lambda_2+m)m} \\ &\quad \times \left| \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{m/2} \prod_{l=1}^{m/2} \exp\left[\frac{-n\alpha}{2} x_l^2 \right] \prod_{1\leqslant j<k\leqslant m/2} (x_k - x_j)^2 \right|^2 \\ &= (-1)^{m/2} \binom{m}{m/2} [t^{\lambda_1}(1-t)^{\lambda_2}]^{m/2} (x_+ - x_-)^{2(m/2)^2} |x_+|^{(\lambda_1+\lambda_2)m} |1-x_+|^{-(\lambda_2+m)m} \\ &\quad \times |n\alpha|^{-(m/2)^2} (V_{m/2})^2, \end{aligned} \tag{37}$$

where

$$V_{m/2} := \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{m/2} \prod_{l=1}^{m/2} \exp\left[-\frac{1}{2} x_l^2 \right] \prod_{1\leqslant j<k\leqslant m/2} (x_k - x_j)^2. \tag{38}$$

From Ref. 14,

$$|x_+| = \sqrt{\frac{1}{t}}, \quad |1-x_+| = \sqrt{\frac{1-t}{t}}, \quad |x_+ - x_-| = 2\sqrt{\frac{1-t}{t}}, \quad |\alpha| = \frac{2t^{3/2}}{(1-t)^{1/2}}, \tag{39}$$

so (37) simplifies to read

$$I_n(t) \sim \binom{m}{m/2} 2^{(m/2)^2} n^{-(m/2)^2} [t(1-t)]^{-m^2/8} (V_{m/2})^2. \tag{40}$$

Furthermore, we recognize $V_{m/2}$ as a limiting case of the Selberg integral known as the Mehta integral,[21] which has the evaluation,

$$V_{m/2} = (2\pi)^{m/4} \prod_{j=0}^{m/2-1} \Gamma(2+j) = (2\pi)^{m/4} G(m/2+2). \tag{41}$$

Recalling (28), our remaining task is to compute the asymptotic form of the combination of Selberg integrals and the Morris integral therein. According to (22) and (23), for this we require knowledge of the asymptotic expansion of the Barnes G-function. In fact Barnes himself showed[22]

$$\log\left(\frac{G(n+a+1)}{G(n+b+1)} \right) \underset{n\to\infty}{\sim} (b-a)n + \frac{a-b}{2} \log(2\pi) + \left((a-b)n + \frac{a^2-b^2}{2} \right) \log n + o(1). \tag{42}$$

Using this we find

$$\frac{S_n(\lambda_1,\lambda_2+m,1)}{S_{n+m/2}(\lambda_1,\lambda_2,1)M_m(\lambda_1+n,\lambda_2,1)}\sim\frac{n^{m^2/2-m/2}}{G(m+2)}. \tag{43}$$

Substituting (41) in (40), then substituting the result together with (43) in (28) we obtain the sought asymptotic formula,

$$\frac{Z_{n,\lambda_1,\lambda_2}((t,q))}{Z_{n+q,\lambda_1,\lambda_2}((\cdot,0))}\sim\frac{1}{\pi^q}\frac{G^2(q+1)}{G(2q+1)}(2n)^{-q+q^2}[t(1-t)]^{-q^2/2}, \tag{44}$$

where we have set $m/2=q$ and use has been made of the functional equation (24). We note that the right-hand side of (44) is independent of the parameters λ_1 and λ_2.

A check on our workings to this stage is the special case $q=1$. Then (25) coincides with the eigenvalue density in the JUE, $\rho^{\mathrm{JUE}}(X)$, normalized so that its integral on $[0, 1]$ is unity. Setting $q=1$ in (44) we read off that

$$\rho^{\mathrm{JUE}}(X)\sim\frac{1}{\pi}(X(1-X))^{-1/2}, \tag{45}$$

which is indeed the known functional form (see, e.g., Ref. 1).

III. ASYMPTOTIC FORM OF THE DENSITY MATRICES

Consider the impenetrable Bose gas of $N+1$ particles confined to the interval $[0,L]$ with Dirichlet boundary conditions. We know from Ref. 2 that the ground state density matrix $\rho^D_{N+1}(x,y)$ is given by

$$\rho^D_{N+1}(x,y)=\frac{(N+1)}{C}\left(\sin\frac{\pi x}{L}\right)\left(\sin\frac{\pi y}{L}\right)\int_0^L dx_1\cdots\int_0^L dx_N\prod_{l=1}^{N}\sin^2\frac{\pi x_l}{L}$$
$$\times\left|\cos\frac{\pi x}{L}-\cos\frac{\pi x_l}{L}\right|\left|\cos\frac{\pi y}{L}-\cos\frac{\pi x_l}{L}\right|\prod_{1\le j<k\le N}\left|\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right|^2, \tag{46}$$

where

$$C=\int_0^L dx_1\cdots\int_0^L dx_{N+1}\prod_{l=1}^{N+1}\sin^2\frac{\pi x_l}{L}\prod_{1\le j<k\le N+1}\left|\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right|^2. \tag{47}$$

Let us now change variables,

$$\cos\frac{\pi x_j}{L}=2X_j-1 \tag{48}$$

in both (46) and (47), and let us define

$$\rho^D_{N+1}(X,Y):=\rho^D_{N+1}(x,y)\big|_{\substack{\cos \pi x/L=2X-1\\ \cos \pi y/L=2Y-1}}. \tag{49}$$

Then in terms of the generalization of (26),

$$Z_{n,\lambda_1,\lambda_2}((X,q_1),(Y,q_2))=|X-Y|^{2q_1q_2}X^{\lambda_1q_1}(1-X)^{\lambda_2q_1}Y^{\lambda_1q_2}(1-Y)^{\lambda_2q_2}\int_0^1 dX_1\cdots\int_0^1 dX_n$$
$$\times\prod_{l=1}^{n} X_l^{\lambda_1}(1-X_l)^{\lambda_2}|X-X_l|^{2q_1}|Y-X_l|^{2q_2}\prod_{1\leq j<k\leq n}|X_k-X_j|^2 \quad (50)$$

we have

$$\rho^D_{N+1}(X,Y)=\frac{\pi\rho}{|X-Y|^{1/2}}[X(1-X)]^{1/4}[Y(1-Y)]^{1/4}\frac{Z_{N,1/2,1/2}((X,1/2),(Y,1/2))}{Z_{N+1,1/2,1/2}((\cdot,0),(\cdot,0))}, \quad (51)$$

where $\rho:=N/L$.

Similar considerations apply to the impenetrable Bose gas of $N+1$ particles confined to the interval $[0,L]$ with Neumann boundary conditions. Again from Ref. 2 we know that the ground state density matrix $\rho^N_{N+1}(x,y)$ is given by

$$\rho^N_{N+1}(x,y)=\frac{(N+1)}{C}\int_0^L dx_1\cdots\int_0^L dx_N\prod_{l=1}^{N}\left|\cos\frac{\pi x}{L}-\cos\frac{\pi x_l}{L}\right|\left|\cos\frac{\pi y}{L}-\cos\frac{\pi x_l}{L}\right|$$
$$\times\prod_{1\leq j<k\leq N}\left|\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right|^2, \quad (52)$$

where

$$C=\int_0^L dx_1\cdots\int_0^L dx_{N+1}\prod_{1\leq j<k\leq N+1}\left|\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right|^2. \quad (53)$$

Defining

$$\rho^N_{N+1}(X,Y):=\rho^N_{N+1}(x,y)\big|_{\substack{\cos \pi x/L=2X-1\\ \cos \pi y/L=2Y-1}} \quad (54)$$

and changing variables according to (48) in (52) and (53) shows

$$\rho^N_{N+1}(X,Y)=\frac{\pi\rho}{|X-Y|^{1/2}}[X(1-X)]^{1/4}[Y(1-Y)]^{1/4}\frac{Z_{N,-1/2,-1/2}((X,1/2),(Y,1/2))}{Z_{N+1,-1/2,-1/2}((\cdot,0),(\cdot,0))}. \quad (55)$$

As already noticed in Refs. 6, 7, the log-gas interpretation of (50) allows us to predict that for large n it factorizes into a function of X and the same function of Y, which are themselves of the form (26). Explicitly, we expect

$$\frac{Z_{n,\lambda_1,\lambda_2}((X,q_1),(Y,q_2))}{Z_{n+q_1+q_2,\lambda_1,\lambda_2}((\cdot,0),(\cdot,0))}\sim\frac{Z_{n,\lambda_1,\lambda_2}((X,q_1))}{Z_{n+q_1,\lambda_1,\lambda_2}((\cdot,0))}\frac{Z_{n,\lambda_1,\lambda_2}((Y,q_2))}{Z_{n+q_2,\lambda_1,\lambda_2}((\cdot,0))}. \quad (56)$$

As in (26), the key to choosing the correct normalizations is to balance the total charge in the log-gas interpretation. Setting $q_1=q_2=q$ as required by (51) and (55) it follows from (56) that

$$\frac{Z_{n,\lambda_1,\lambda_2}((X,q),(Y,q))}{Z_{n+2q,\lambda_1,\lambda_2}((\cdot,0),(\cdot,0))}\sim\left(\frac{1}{\pi^q}\frac{G^2(q+1)}{G(2q+1)}(2n)^{-q+q^2}\right)^2[X(1-X)]^{-q^2/2}[Y(1-Y)]^{-q^2/2}. \quad (57)$$

Substituting this asymptotic form with $q=1/2$ in (51) and (55) we obtain that for large N and fixed $X,Y\in(0,1)$,

$$\rho_{N+1}^{D}(X,Y)\sim\rho_{N+1}^{N}(X,Y)\sim\rho\frac{G^4(3/2)}{\sqrt{2N}}\frac{[X(1-X)]^{1/8}[Y(1-Y)]^{1/8}}{|X-Y|^{1/2}}. \tag{58}$$

It is of interest to compare the asymptotic formula (58) against a numerical determination of say $\rho_{N+1}^{D}(X,Y)$ or more conveniently $\rho_{N+1}^{D}(X,1-X)$. To compute the latter we write it as a random matrix average. Thus it follows from the various definitions that

$$\rho_{N+1}^{D}(X,1-X)=\frac{8\rho}{N+1}X(1-X)\left\langle\prod_{l=1}^{N}(|4(1-X)-4X_l|)(|4X-4X_l|)\right\rangle_{\mathrm{JUE}_N}\Bigg|_{\lambda_1=\lambda_2=1/2}. \tag{59}$$

For each $k=1,2,\ldots,M$ suppose we sample from $\mathrm{JUE}_N|_{\lambda_1=\lambda_2=1/2}$ obtaining the N-tuple $(X_1^{(k)},X_2^{(k)},\ldots,X_N^{(k)})$. Then the method of Monte Carlo integration tells us that

$$\rho_{N+1}^{D}(X,1-X)=\frac{8\rho}{N+1}X(1-X)\frac{1}{M}\sum_{k=1}^{M}\prod_{l=1}^{N}(|4(1-X)-4X_l^{(k)}|)(|4X-4X_l^{(k)}|)+O\left(\frac{1}{\sqrt{M}}\right). \tag{60}$$

Fortuitously, we have available a recently discovered[23] random three term recurrence which generates a polynomial, the zeros of which have the p.d.f. $\mathrm{J}(2\lambda)\mathrm{E}_n$. In the case of interest ($\lambda_1=\lambda_2=1/2$, $\lambda=1$) the recurrence states

$$A_0(x)=1,$$

$$A_1(x)=x-\mathrm{BD}[n+1/2,n+1/2],$$

$$A_j(x)=(w_2(x-1)+w_0x)A_{j-1}(x)+w_1x(x-1)A_{j-2}(x)\quad(j=2,\ldots,n), \tag{61}$$

where with

$$a\in\mathrm{GD}[n+1-j+1/2,1],\quad b\in\mathrm{GD}[j-1,1/2],\quad c\in\mathrm{GD}[n+1-j+1/2,1], \tag{62}$$

and $d:=a+b+c$ we have

$$w_0=\frac{a}{d},\quad w_1=\frac{b}{d},\quad w_2=1-w_0-w_1. \tag{63}$$

Here $\mathrm{BD}[a,b]$ denotes the classical beta distribution, while $\mathrm{GD}[m,\sigma]$ denotes the classical gamma distribution. The theory of Ref. 23 tells us that $A_n(x)$ has its zeros distributed according to $\mathrm{JUE}_n|_{\lambda_1=\lambda_2=\lambda}$. Implementing (61) for fixed n we thus computed the samples required in (60) for the Monte Carlo evaluation of $\rho_{N+1}^{D}(X,1-X)$. Forming the ratio then with the asymptotic form (58) gave the data in Table I.

IV. PHYSICAL AND MATHEMATICAL IMPLICATIONS

A. Ground state occupation of effective single particle states

The ground state density matrix is the theoretical quantity which quantifies the condensation of a Bose system. Thus if we decompose the density matrix

$$\rho_N(x,y)=\sum_{j=0}^{\infty}\lambda_j\phi_j(x)\phi_j(y), \tag{64}$$

where the λ_j,ϕ_j are the eigenvalues and normalized eigenfunctions in the eigenvalue problem

TABLE I. The ratio $\rho_{N+1}^{D,\mathrm{MC}}(X,1-X)/\rho_{N+1}^{D}(X,1-X)$ where $\rho_{N+1}^{D,\mathrm{MC}}(X,1-X)$ refers to the Monte Carlo expression (60), while $\rho_{N+1}^{D}(X,1-X)$ is the asymptotic form (58). We chose $N=14$, and evaluated (60) with $M=5000$.

X	$\rho_{N+1}^{D,\mathrm{MC}}(X,1-X)/\rho_{N+1}^{D}(X,1-X)$
0.025	1.0958
0.075	1.0039
0.125	1.0363
0.175	1.0098
0.225	0.9439
0.275	1.0080
0.325	0.9692
0.375	1.0338
0.425	0.9706
0.475	1.1309

$$\int \rho_N(x,y)\phi_j(y)\,dy=\lambda_j\phi_j(x), \tag{65}$$

then by analogy with the free Fermi system in which (64) holds with $\lambda_j=1$ $(j=0,\ldots,N-1)$, $\lambda_j=0$ $(j\geqslant N)$, we see that the λ_j have the physical interpretation as the occupation numbers of effective single particle states $\phi_j(x)$. For Bose–Einstein condensation to occur we must have λ_0 proportional to N.

To study (65) in the case of the impenetrable Bose gas in Dirichlet or Neumann boundary conditions we restrict ourselves to large N where use can be made of the asymptotic form of the density matrices (58). Before making the substitution, recalling the definitions (49) and (54) we must first change variables in (65) and redefine the eigenfunctions so that

$$\cos \pi y/L=2Y-1, \quad \phi_j(Y)=\phi_j(y)|_{\cos \pi y/L=2Y-1}, \quad \phi_j(X)=\phi_j(x)|_{\cos \pi x/L=2X-1}. \tag{66}$$

Doing this we obtain, for large N, the integral equation

$$\sqrt{\frac{N}{2}}\frac{G^4(3/2)}{\pi}\int_0^1 \frac{[X(1-X)]^{1/8}[Y(1-Y)]^{1/8}}{|X-Y|^{1/2}}\phi_j(Y)\frac{dY}{\sqrt{Y(1-Y)}}=\lambda_j\phi_j(X). \tag{67}$$

It follows immediately that

$$\lambda_j\propto\sqrt{N}. \tag{68}$$

As noted in Ref. 7 this conclusion requires that j be fixed—for $j\geqslant N$ we expect $\lambda_j\propto(N/j)^4$ in keeping with the corresponding result in periodic boundary conditions, since in this regime the boundary conditions are not expected to play a role.

Setting

$$\lambda_j=\frac{G^4(3/2)}{\sqrt{2}\pi}\sqrt{N}\overline{\lambda}_j \tag{69}$$

and rearranging, (67) reads

$$\int_0^1 \frac{\phi_j(Y)}{|X-Y|^{1/2}}\frac{dY}{[Y(1-Y)]^{3/8}}=\overline{\lambda}_j\frac{\phi_j(X)}{[X(1-X)]^{1/8}}. \tag{70}$$

Remarkably the effective single particle ground state $\phi_0(X)$, and the corresponding scaled occupation number $\overline{\lambda}_0$ can be computed exactly from (70). To see this requires knowledge of a piece of integral equation theory presented in Porter and Stirling.[24] The relevant theory tells us that the solution of the integral equation,

$$\int_0^1 \frac{\phi(t)}{|x-t|^\nu} dt = 1, \qquad \nu < 1 \tag{71}$$

is

$$\phi(x) = \frac{1}{\pi}\left(\cos\frac{\pi\nu}{2}\right)[x(1-x)]^{(\nu-1)/2}. \tag{72}$$

Setting $\nu = 1/2$, it follows immediately that

$$\phi_0(X) = \frac{1}{\sqrt{A}}[X(1-X)]^{1/8}, \quad \overline{\lambda}_0 = \pi\sqrt{2} \tag{73}$$

satisfies (71), where the normalization A is determined by the requirement that

$$\frac{L}{\pi}\int_0^1 (\phi_0(X))^2 \frac{dX}{\sqrt{X(1-X)}} = 1, \tag{74}$$

and so

$$A = \frac{L}{\pi}B(3/4,3/4), \tag{75}$$

where $B(a,b)$ denotes the beta function. Substituting the exact evaluation of $\overline{\lambda}_0$ in (69) shows that in the large N limit,

$$\lambda_0 = G^4(3/2)\sqrt{N} = 1.3069\sqrt{N}. \tag{76}$$

To compute the higher order single particle states and their corresponding occupations we make the ansatz,

$$\phi_j(X) \propto \phi_0(X) p_j(X), \tag{77}$$

where $p_j(X)$ is a polynomial of degree j. Now $\{\phi_j(X)\}$ can always be chosen to be orthogonal (note that the measure is $dX/\sqrt{X(1-X)}$ on [0, 1]) so recalling (73) we require

$$\int_0^1 \frac{p_j(X)p_k(X)}{(X(1-X))^{1/4}} dX = 0, \quad j \neq k. \tag{78}$$

Up to normalization, the unique polynomials with this property are the particular Gegenbauer polynomials

$$p_j(X) = C_j^{1/4}(2X-1), \tag{79}$$

which we note are proportional to the particular Jacobi polynomials $P_j^{-1/4,-1/4}(2X-1)$. Normalizing (77) with the substitution (79) as in (74) shows

$$\phi_j(X) = \sqrt{\frac{1}{L}}\sqrt{\frac{j!(j+1/4)\Gamma^2(1/4)}{\Gamma(j+1/2)}}(X(1-X))^{1/8}C_j^{1/4}(2X-1). \tag{80}$$

Now substituting (80) in (70) and setting $X=1$ we obtain a definite integral for $\overline{\lambda_j}$ which can be found in Ref. 25, giving us the evaluation

$$\overline{\lambda_j}=\sqrt{2\pi}\frac{\Gamma(j+1/2)}{j!} \tag{81}$$

and hence

$$\lambda_j=G^4(3/2)\frac{\Gamma(j+1/2)}{\sqrt{\pi}j!}\sqrt{N}. \tag{82}$$

To arrive at (80) we have made the ansatz (77). In fact a different approach can be taken to the problem, in which it is shown that an integral operator following from (70) commutes with the differential operator determining the polynomials $\{C_j^{1/4}(2X-1)\}_{j=0,1,2,\ldots}$. This is done in the Appendix.

Finally, we note that substituting (58), (80), and (81) in (64) gives the following interesting identity:

$$\frac{1}{|X-Y|^{1/2}}=\sqrt{\frac{2}{\pi}}\Gamma^2(1/4)\sum_{j=0}^{\infty}(j+1/4)C_j^{1/4}(2X-1)C_j^{1/4}(2Y-1). \tag{83}$$

B. Generalized Fisher–Hartwig-type asymptotics

One viewpoint of our asymptotic analysis of multiple integrals of the form (50) is that we are studying asymptotic problems of the Fisher–Hartwig class. Let us recall that the latter refers literally to Toeplitz determinants with both zeros and jump discontinuities is its generating function,

$$D_N[e^{a(\theta)}]:=\det[a_{i-j}]_{i,j=1,\ldots,N},\quad e^{a(\theta)}=\sum_{p=-\infty}^{\infty}a_p e^{ip\theta}, \tag{84}$$

where

$$a(\theta)=g(\theta)-i\sum_{r=1}^{R}b_r[\pi-(\theta-\phi_r)]\bmod 2\pi+\sum_{r=1}^{R}a_r\log|2-2\cos(\theta-\phi_r)| \tag{85}$$

with

$$g(\theta)=\sum_{p=-\infty}^{\infty}g_p e^{ip\theta},\qquad \sum_{p=-\infty}^{\infty}|p||g_p|^2<\infty. \tag{86}$$

Thus $g(\theta)$ is a regular term, while at ϕ_r $(r=1,\ldots,R)$ there is a jump discontinuity of strength b_r and a zero of order a_r. To see the relationship with (50) we set $b_r=0$ $(r=1,\ldots,R)$ thus eliminating the jump discontinuities, and recall the general formula relating a Toeplitz determinant to a multiple integral,

$$\begin{aligned}D_N[e^{a(\theta)}]&=\frac{1}{N!}\int_0^{2\pi}d\theta_1\cdots\int_0^{2\pi}d\theta_N\prod_{l=1}^{N}e^{a(\theta_l)}\prod_{1\leqslant j<k\leqslant N}|e^{i\theta_k}-e^{i\theta_j}|^2\\&=\frac{1}{N!}\int_0^{2\pi}d\theta_1\cdots\int_0^{2\pi}d\theta_N\prod_{l=1}^{N}e^{g(\theta_l)}\left(\prod_{r=1}^{R}|e^{i\theta_l}-e^{i\phi_r}|^{2a_r}\right)\prod_{1\leqslant j<k\leqslant N}|e^{i\theta_k}-e^{i\theta_j}|^2.\end{aligned} \tag{87}$$

Fisher and Hartwig[26] conjectured that in the case (87),

$$D_N[e^{a(\theta)}] \sim e^{g_0 N} e^{\sum_{r=1}^R a_r^2 \log N} E, \tag{88}$$

where E is independent of N. This was subsequently proved, and it was furthermore shown

$$E = e^{\sum_{k=1}^\infty k g_k g_{-k}} \prod_{r=1}^R e^{-a_r(g(\phi_r)-g_0)} \prod_{1\le j<k\le R} |e^{i\phi_k} - e^{i\phi_j}|^{-2a_k a_j} \prod_{r=1}^R \frac{G^2(1+a_r)}{G(1+2a_r)} \tag{89}$$

(see, for example, the monograph[27] and references therein).

As noted by one of the present authors some years ago,[28] it is straightforward to reproduce the structure of (88) using the analogous log-gas argument to that used here in the analysis of (50). Now the (normalized) multiple integral corresponding to (87) which relates to (50) is

$$\frac{H_{n,\lambda_1,\lambda_2}[e^{h(x)} \Pi_{r=1}^R |y_r - x|^{2q_r}]}{H_{n,\lambda_1,\lambda_2}[1]}, \tag{90}$$

$$H_{n,\lambda_1,\lambda_2}[f(x)] := \int_0^1 dx_1 \cdots \int_0^1 dx_n \prod_{l=1}^n f(x_l) x_l^{\lambda_1} (1-x_l)^{\lambda_2} \prod_{1\le j<k\le n} |x_k - x_j|^2, \tag{91}$$

where $h(x)$ is analytic on (0,1). As our final issue, we would like to extend the log-gas argument used in the analysis of (50) to predict the large n asymptotic form of (90).

From the log-gas perspective, the natural quantity to analyze is

$$\prod_{1\le j<k\le r} |y_k - y_j|^{2q_j q_k} \frac{H_{n,\lambda_1,\lambda_2}[e^{h(x)} \Pi_{r=1}^R |y_r - x|^{2q_r}]}{H_{n+\sum_{r=1}^R q_r,\lambda_1,\lambda_2}[e^{h(x)}]}. \tag{92}$$

Analogous to (56) we expect for large n (92) to factorize as

$$\frac{H_{n,\lambda_1,\lambda_2}[e^{h(x)} \Pi_{r=1}^R |y_r - x|^{2q_r}]}{H_{n+\sum_{r=1}^R q_r,\lambda_1,\lambda_2}[e^{h(x)}]} \sim \prod_{r=1}^R e^{-q_r h(y_r)} \frac{H_{n,\lambda_1,\lambda_2}[|y_r - x|^{2q_r}]}{H_{n+q_r,\lambda_1,\lambda_2}[1]}, \tag{93}$$

where the second expression is motivated by inspection of the known results (88) and (89) for (87).

Thus we expect

$$\frac{H_{n,\lambda_1,\lambda_2}[e^{h(x)} \Pi_{r=1}^R |y_r - x|^{2q_r}]}{H_{n,\lambda_1,\lambda_2}[1]} \sim \prod_{1\le j<k\le r} |y_k - y_j|^{-2q_j q_k} \frac{H_{n+\sum_{r=1}^R q_r,\lambda_1,\lambda_2}[e^{h(x)}]}{H_{n,\lambda_1,\lambda_2}[1]} \times \prod_{r=1}^R e^{-q_r h(y_r)} \frac{H_{n,\lambda_1,\lambda_2}[|y_r - x|^{2q_r}]}{H_{n+q_r,\lambda_1,\lambda_2}[1]}. \tag{94}$$

But according to (44),

$$\frac{H_{n,\lambda_1,\lambda_2}[|y_r-x|^{2q_r}]}{H_{n+q_r,\lambda_1,\lambda_2}[1]} \sim \frac{1}{\pi^{q_r}} \frac{G^2(q_r+1)}{G(2q_r+1)} (2n)^{-q_r+q_r^2} (y_r(1-y_r))^{-q_r^2/2}. \tag{95}$$

Also, for the first ratio on the right hand side of (94) we have available both rigorous results[29,30] as well as log-gas type arguments[31] which together tell us that

$$\frac{H_{n+Q,\lambda_1,\lambda_2}[e^{h(x)}]}{H_{n,\lambda_1,\lambda_2}[1]} \sim \exp\left[\frac{n+Q+(\lambda_1+\lambda_2)/2}{\pi} \int_0^1 \frac{h(x)}{[x(1-x)]^{1/2}} dx\right] \exp\left[-\frac{\lambda_1+\lambda_2}{4}(h(0)+h(1))\right]$$
$$\times \exp\left[\frac{1}{4\pi^2} \int_0^1 dx \frac{h(x)}{[x(1-x)]^{1/2}} \int_0^1 dy \frac{h'(y)[y(1-y)]^{1/2}}{x-y}\right]. \tag{96}$$

Substituting (95) and (96) in (93) gives the analog of (88),

$$\frac{H_{n,\lambda_1,\lambda_2}[e^{h(x)} \Pi_{r=1}^R |y_r-x|^{2q_r}]}{H_{n,\lambda_1,\lambda_2}[1]} \sim \exp\left[\frac{n+\Sigma_{r=1}^R q_r+(\lambda_1+\lambda_2)/2}{\pi} \int_0^1 \frac{h(x)}{[x(1-x)]^{1/2}} dx\right]$$
$$\times \exp\left[\sum_{r=1}^R (-q_r+q_r^2)\log 2n\right] K, \tag{97}$$

where

$$K = \prod_{1\leqslant j<k\leqslant R} |y_k-y_j|^{-2q_jq_k} e^{-(\lambda_1+\lambda_2)[h(0)+h(1)]/4} e^{-\Sigma_{r=1}^R q_r h(y_r)}$$
$$\times \exp\left[\frac{1}{4\pi^2} \int_0^1 dx \frac{h(x)}{[x(1-x)]^{1/2}} \int_0^1 dy \frac{h'(y)[y(1-y)]^{1/2}}{x-y}\right]$$
$$\times \prod_{r=1}^R [y_r(1-y_r)]^{-q_r^2/2} \prod_{r=1}^R \frac{1}{\pi^{q_r}} \frac{G^2(q_r+1)}{G(2q_r+1)}. \tag{98}$$

C. Concluding remarks

In our first paper on the impenetrable Bose gas[2] we set ourselves the goal of providing the leading asymptotic form of the density matrix for the impenetrable Bose gas in a harmonic trap and in Dirichlet and Neumann boundary conditions. It was noted in Ref. 2 that for the impenetrable Bose gas in periodic boundary conditions, the Fisher–Hartwig formula gave the asymptotic form,

$$\rho_{N+1}^C(x;0) \sim \rho \frac{G^4(3/2)}{\sqrt{2\pi}} \left(\frac{\pi}{N \sin(\pi\rho x/N)}\right)^{1/2}. \tag{99}$$

In Ref. 7, it was shown that for the harmonic well

$$(2N)^{1/2} \rho_{N+1}^H(\sqrt{2N}X, \sqrt{2N}Y) \sim N^{1/2} \frac{G^4(3/2)}{\pi} \frac{(1-X^2)^{1/8}(1-Y^2)^{1/8}}{|X-Y|^{1/2}}, \tag{100}$$

while in the present paper, after changing variables according to (49), the asymptotic form of the density matrix is shown to have the leading asymptotic form (58). As a consequence of the scaling properties of these asymptotic forms, the occupation number of the low lying effective single particle states are all proportional to $\sqrt{N}$, but with a proportionality constant dependent on the particular system.

To obtain the asymptotic forms we have used a combination of exact analysis, made possible by the theory of Selberg correlation integrals, and physical reasoning based on log-gas analogies. Taking this argument to its logical conclusion leads to a conjectured exact asymptotic formula, given by (97) and (98) for a Jacobi weight analog of the Fisher–Hartwig formula.

ACKNOWLEDGMENT

The authors would like to thank the Australian Research Council for funding this work.

APPENDIX: PROOF THAT $\{\phi_0(X)C_j^{1/4}(2X-1)\}_{j=0,1,2,\ldots}$ ARE SOLUTIONS OF THE INTEGRAL EQUATION (70)

The assertion that the $\phi_j(X)$ given by (77) are solutions of (70) is equivalent to stating that the Gegenbauer polynomials are eigenfunctions of the integral operator,

$$K[f(\xi)] := \int_{-1}^{1} \frac{d\psi}{|\xi-\psi|^{1/2}(1-\psi^2)^{1/4}} f(\psi), \tag{A1}$$

where for convenience we are working on the interval $-1 \leqslant \xi \leqslant 1$. In this appendix we prove that K commutes with the differential operator, L, which determines the Gegenbauer polynomials,

$$L := (1-\xi^2)\frac{d^2}{d\xi^2} - \frac{3}{2}\xi\frac{d}{d\xi}, \tag{A2}$$

with

$$LC_j^{1/4}(\xi) = -j(j+1/2)C_j^{1/4}(\xi). \tag{A3}$$

We begin by identifying $K[C_j^{1/4}(\xi)]$ with the following finite sum of hypergeometric functions:

$$\begin{aligned} K[C_j^{1/4}(\xi)] = {} & \Omega_j \sum_{k=0}^{j} \frac{(-j)_k (j+1/2)_k}{k!(3/4)_k} \left(\frac{1+\xi}{2}\right)^{1/4} {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; \frac{1+\xi}{2}\right) \\ & + (-1)^j \Omega_j \sum_{k=0}^{j} \frac{(-j)_k (j+1/2)_k}{k!(3/4)_k} \left(\frac{1-\xi}{2}\right)^{1/4} {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; \frac{1-\xi}{2}\right), \end{aligned} \tag{A4}$$

where

$$\Omega_j := \frac{\Gamma(3/4)}{\Gamma(5/4)} \frac{\Gamma(j+1/2)}{j!}. \tag{A5}$$

To derive (A4) we break up the interval of integration in $K[C_j^{1/4}(\xi)]$ into two regions, thus removing the need for the modulus, which gives

$$\begin{aligned} K[C_j^{1/4}(\xi)] &= \int_{\xi}^{1} (1-\psi^2)^{-1/4} C_j^{1/4}(\psi) \frac{d\psi}{\sqrt{\psi-\xi}} + (-1)^j \int_{-\xi}^{1} (1-\psi^2)^{-1/4} C_j^{1/4}(\psi) \frac{d\psi}{\sqrt{\psi+\xi}} \\ &= z_-^{1/4} \int_0^1 d\psi\, \psi^{-1/4} (1-\psi)^{-1/2} (1-z_-\psi)^{-1/4} C_j^{1/4}(1-2z_-\psi) \\ &\quad + (-1)^j z_+^{1/4} \int_0^1 d\psi\, \psi^{-1/4} (1-\psi)^{-1/2} (1-z_+\psi)^{-1/4} C_j^{1/4}(1-2z_+\psi), \end{aligned} \tag{A6}$$

where we have defined

$$z_{\pm} := \frac{1 \pm \xi}{2} \tag{A7}$$

and in obtaining the second equality we have changed integration variables from ψ to $(1-\psi)/(1-\xi)$ and $(1-\psi)/(1+\xi)$ in the first and second integrals respectively. Substituting the following known[25] expansion for the Gegenbauer polynomials

$$C_j^{1/4}(\psi) = \frac{(-1)^j \Gamma(j+1/2)}{j!\sqrt{\pi}} \sum_{k=0}^{j} \frac{(-j)_k (j+1/2)_k}{k!(3/4)_k} \left(\frac{1+\psi}{2} \right)^k \tag{A8}$$

into (A6), and using the standard integral representation of the ${}_2F_1$ function,

$$\int_0^1 d\psi \frac{\psi^{-1/4}(1-\psi)^{-1/2}}{(1-z\psi)^{-k+1/4}} = B(3/4,1/2)\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; z \right), \tag{A9}$$

then results in (A4).

We can now utilize known hypergeometric identities to facilitate the operation of the differential operator L on the expression for $K[C_j^{1/4}(\xi)]$ given by (A4). We note that the structure of (A4) is of the form,

$$K[C_j^{1/4}(\xi)] = \Omega_j S_j(z_+) + (-1)^j \Omega_j S_j(z_-), \tag{A10}$$

where

$$S_j(z) := \sum_{k=0}^{j} \frac{(-j)_k (j+1/2)_k}{k!(3/4)_k} z^{1/4}\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; z \right). \tag{A11}$$

In terms of both the variables $z = z_+$ and $z = z_-$ the differential operator L has the form

$$L = z(1-z)\frac{d^2}{dz^2} - \frac{3}{4}(2z-1)\frac{d}{dz}. \tag{A12}$$

Utilizing the identity[32]

$$\frac{d^n}{dz^n}\left[z^{\delta}\, {}_pF_q\left(\begin{matrix} \alpha_1, \ldots, \alpha_p \\ \rho_1, \ldots, \rho_q \end{matrix} \middle| z \right) \right] = (\delta - n + 1)_n z^{\delta - n}\, {}_{p+1}F_{q+1}\left(\begin{matrix} \delta+1, \alpha_1, \ldots, \alpha_p \\ \delta+1-n, \rho_1, \ldots, \rho_q \end{matrix} \middle| z \right), \tag{A13}$$

we find that

$$\begin{aligned} L z^{1/4}\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; z \right) &= \frac{z^{1/4}}{z}\left(-\frac{3}{16} \right)(1-z)\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; -\frac{3}{4}; z \right) \\ &\quad + \frac{z^{1/4}}{z}\left(-\frac{3}{16} \right)(2z-1)\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{1}{4}; z \right), \end{aligned} \tag{A14}$$

$$L z^{1/4}\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; z \right) = -\frac{1}{2} z^{1/4} k\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{5}{4}; z \right) - \frac{1}{4} z^{1/4} k\, {}_2F_1\left(\frac{1}{4}-k, \frac{3}{4}; \frac{1}{4}; z \right), \tag{A15}$$

$$Lz^{1/4}{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right)=-z^{1/4}k\left(k+\frac{1}{2}\right)\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right)$$
$$-z^{1/4}k\left(\frac{1}{4}-k\right)\,{}_2F_1\left(\frac{1}{4}-(k-1),\frac{3}{4};\frac{5}{4};z\right), \tag{A16}$$

where the equalities in (A15) and (A16), respectively, follow from the two particular contiguity relations,[32]

$$\left(-\frac{3}{16}\right)(1-z)_2F_1\left(\frac{1}{4}-k,\frac{3}{4};-\frac{3}{4};z\right)=\frac{1}{16}[(6-4k)z-3]_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{1}{4};z\right)$$
$$-\frac{kz}{2}\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right), \tag{A17}$$

and

$$-\frac{1}{4}\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{1}{4};z\right)=-k\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right)-\left(\frac{1}{4}-k\right)\,{}_2F_1\left(\frac{1}{4}-(k-1),\frac{3}{4};\frac{5}{4};z\right). \tag{A18}$$

Hence from (A16) we obtain

$$LS_j(z)=-z^{1/4}\sum_{k=0}^{j}\frac{(-j)_k(j+1/2)_k}{k!(3/4)_k}k\left(\frac{1}{2}+k\right)\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right)$$
$$-z^{1/4}\sum_{k=0}^{j}\frac{(-j)_k(j+1/2)_k}{k!(3/4)_k}k\left(\frac{1}{4}-k\right)\,{}_2F_1\left(\frac{1}{4}-(k-1),\frac{3}{4};\frac{5}{4};z\right). \tag{A19}$$

Changing summation index in the second sum in (A19) from k to $k-1$ and simplifying we deduce finally that

$$LS_j(z)=-j(j+1/2)\sum_{k=0}^{j}\frac{(-j)_k(j+1/2)_k}{k!(3/4)_k}z^{1/4}\,{}_2F_1\left(\frac{1}{4}-k,\frac{3}{4};\frac{5}{4};z\right)=-j(j+1/2)S_j(z), \tag{A20}$$

which then implies that

$$LKC_j^{1/4}(\xi)=-j(j+1/2)KC_j^{1/4}(\xi) \tag{A21}$$
$$=KLC_j^{1/4}(\xi)\qquad(j=0,1,2,\dots) \tag{A22}$$

and so

$$[K,L]=0. \tag{A23}$$

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Entropy production fluctuations of finite Markov chains

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(Received 6 September 2002; accepted 14 April 2003)

For almost every trajectory segment over a finite time span of a finite Markov chain with any given initial distribution, the logarithm of the ratio of its probability to that of its time-reversal converges exponentially to the entropy production rate of the Markov chain. The large deviation rate function has a symmetry of Gallavotti–Cohen type, which is called the fluctuation theorem. Moreover, similar symmetries also hold for the rate functions of the joint distributions of general observables and the logarithmic probability ratio. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1581971]

I. INTRODUCTION

Stationary nonequilibrium states play an important role in statistical physics and have been studied since Boltzmann's time. In 1993, Evans, Cohen, and Morriss[1] found in computer simulations that the natural invariant measure of a stationary nonequilibrium system has a symmetry which, being called later the fluctuation theorem by Gallavotti and Cohen,[2–5] gives a general formula for the probability ratio of observing trajectories that satisfy or violate the second law of thermodynamics. Since then there have been many derivations and generalizations of the fluctuation theorem. Motivated by the result in Ref. 1, Gallavotti and Cohen[6] gave the first mathematical presentation of the fluctuation theorem for stationary nonequilibrium systems modelled by hyperbolic dynamical systems: Provided that the dynamics is invariant under time reversal and is sufficiently chaotic, the probability distributions of the phase space contraction averaged over large time spans have a large deviation property and the large deviation rate function has a symmetry. Evans and Searles[7–13] considered transient, rather than stationary, nonequilibrium systems and employed a known equilibrium state (such as the Liouville measure) as the initial distribution to derive a transient fluctuation theorem. Gallavotti[14] and Evans *et al.*[13,15] proposed a local version of the fluctuation theorem. Kurchan[16] pointed out that the fluctuation theorem also holds for certain diffusion processes. Lebowitz and Spohn[17] extended Kurchan's results to general Markov processes, and Maes[18] thought of the fluctuation theorem as a property of space–time Gibbs measures. Searles and Evans[19] derived the transient fluctuation theorem for non-stationary stochastic systems.

For systems close to equilibrium, the distribution of trajectories over a finite time interval has little difference from that of their time reversals, and the fluctuation theorem yields the well-known Green–Kubo formula and the Onsager reciprocity relations,[3,17,18,20,21] i.e., the symmetry of the transport coefficients matrix which relate thermodynamic ''forces'' and ''fluxes.'' Surprisingly, the fluctuation theorem is also valid for systems in the nonlinear response regime far from equilibrium. In this sense, the fluctuation theorem can be thought of as an extension of the fluctuation-dissipation theorem, which holds for systems in the linear response regime close to equilibrium.

The concept of entropy production was first put forward in nonequilibrium statistical physics to describe how far a specific state of a system is away from its equilibrium state.[22–24] In Refs. 25–27, a measure-theoretic definition of entropy production rate is proposed for stochastic processes, unifying different entropy production formulas in various concrete cases. Suppose that ξ

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$=\{\xi_n\}_{n\in\mathbf{Z}}$ is a stationary, irreducible and positive recurrent Markov chain with finite state space S, transition probability matrix $P=(p_{ij})_{i,j\in S}$, and invariant distribution $\Pi=\{\pi_i\}_{i\in S}$. Let $\mathbf{P}$ and $\mathbf{P}^-$ be the distributions of the Markov chain and its time-reversal respectively, and denote their restrictions on $\mathcal{F}_0^n=\sigma(\xi_i,0\leqslant i\leqslant n)$ by $\mathbf{P}_{[0,n]}$ and $\mathbf{P}^-_{[0,n]}$. The entropy production rate of ξ is defined as

$$e_p \overset{\text{def}}{=} \lim_{n\to+\infty}\frac{1}{n}H(\mathbf{P}_{[0,n]},\mathbf{P}^-_{[0,n]}),$$

where $H(\mathbf{P}_{[0,n]},\mathbf{P}^-_{[0,n]})$ is the relative entropy of $\mathbf{P}_{[0,n]}$ with respect to $\mathbf{P}^-_{[0,n]}$. A sufficient and necessary condition for $\mathbf{P}_{[0,n]}$ and $\mathbf{P}^-_{[0,n]}$ being mutually absolutely continuous is that $p_{ij}>0\Leftrightarrow p_{ji}>0$ for any i,j. Under this assumption,

$$e_p=E^{\mathbf{P}_{[0,n]}}\log\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}=\frac{1}{2}\sum_{i,j\in S}(\pi_i p_{ij}-\pi_j p_{ji})\log\frac{\pi_i p_{ij}}{\pi_j p_{ji}}. \tag{1}$$

For a stationary Markov process, its entropy production rate can be defined similarly. In Refs. 25 and 28–30, the entropy production rate e_p of a stationary finite Markov chain is expressed in terms of cycles, which occur along almost all sample paths, and their weights. Recently, Jiang *et al.*[31] gave a measure-theoretic exposition of the entropy production rate for hyperbolic dynamical systems, which was defined by Ruelle[32] from the physical point of view. Maes *et al.*[33] presented a definition of entropy production rate for some classes of deterministic and stochastic dynamics in the context of Gibbs measures.

In this paper, we prove the following strong limit theorem for a stationary irreducible finite Markov chain with discrete or continuous time parameter:

$$\lim_{t\to+\infty}\frac{1}{t}\log\frac{d\mathbf{P}_{[0,t)}}{d\mathbf{P}^-_{[0,t)}}(\omega)=e_p,\quad \mathbf{P}-\text{a.s.}$$

Furthermore, the convergence of the corresponding distributions is shown to be exponential, and the large deviation rate function $I(z)$ satisfies a symmetry: $I(z)=I(-z)-z$ for any $z\in\mathbf{R}$; this is actually the fluctuation theorem of Gallavotti–Cohen type for finite Markov chains. The proof is based on the well-known Perron–Frobenius theorem.[34–37] The statement of the theorem appeared in the pioneering paper Lebowitz and Spohn,[17] which also contained a proof. Here we present a mathematically strict proof. Part of the idea and techniques in our paper comes from Ref. 17, to which it is sincerely acknowledged. Moreover, we give a strict but very simple proof to the fluctuation theorem for the logarithmic probability ratios and for the joint distributions of them with general observables. We also discuss the transient fluctuation theorem for nonstationary Markov chains with discrete or continuous time parameter.

II. FINITE MARKOV CHAINS WITH DISCRETE TIME PARAMETER

To bring the main ideas into eminence, in this section we first treat the simplest case. $\xi=\{\xi_n:n\in\mathbf{Z}\}$ will be from now on a stationary irreducible discrete time Markov chain on probability space $(\Omega,\mathcal{F},\mathbf{P})$ with finite state space $S=\{1,2,\ldots,d\}$, transition probability matrix $P=(p_{ij})_{i,j\in S}$, and invariant probability distribution $\Pi=\{\pi_i\}_{i\in S}$. Without loss of generality, we assume that ξ is a coordinate process on its canonical trajectory space $(\Omega,\mathcal{F},\mathbf{P})$. That is, $\Omega=S^{\mathbf{Z}}$, $\mathcal{F}=\sigma\{\xi_n:n\in\mathbf{Z}\}$ and $\mathbf{P}$ is the distribution of ξ. Now we introduce two transformations: the time-reversal transformation

$$r:\Omega\to\Omega,\quad \xi_n(r\omega)=\xi_{-n}(\omega),\quad \forall n\in\mathbf{Z};$$

and the shift operator

$$\theta:(\Omega,\mathcal{F})\to(\Omega,\mathcal{F}),\quad \xi_n(\theta\omega)=\xi_{n+1}(\omega),\quad \forall n\in\mathbf{Z}.$$

It is easy to see that r and θ are $\mathcal{F}$-measurable and invertible with $r^{-1}=r$. Since ξ is stationary, $\theta^n\mathbf{P}=\mathbf{P}$, which yields $\theta^n\mathbf{P}^-=\mathbf{P}^-$ because $r\theta=\theta^{-1}r$, where $\mathbf{P}^-=r\mathbf{P}$ is the distribution of ξ's time reversal. The stationary Markov chain ξ is said to be reversible if $\mathbf{P}=\mathbf{P}^-$. As is well known, ξ is reversible if and only if the entropy production rate e_p of ξ vanishes, or iff $\pi_i p_{ij}=\pi_j p_{ji}$ for any $i,j\in S$, i.e. ξ is in detailed balance.[25–27]

For each $n\in\mathbf{Z}$ and $k\in\mathbf{N}$, denote by $\mathbf{P}_{[n,n+k]}$ and $\mathbf{P}^-_{[n,n+k]}$, respectively, the restrictions of $\mathbf{P}$ and $\mathbf{P}^-$ on $\mathcal{F}_n^{n+k}=\sigma(\xi_m:n\leqslant m\leqslant n+k)$. We assume that the transition matrix P satisfies the condition

$$p_{ij}>0\Leftrightarrow p_{ji}>0,\quad \forall i,j\in S. \tag{2}$$

Otherwise, $\mathbf{P}_{[0,n]}$ is not absolutely continuous with respect to $\mathbf{P}^-_{[0,n]}$, and by the definition of relative entropy, $H(\mathbf{P}_{[0,n]},\mathbf{P}^-_{[0,n]})$ is infinite for all $n\in\mathbf{N}$, hence $e_p=+\infty$. This is a trivial case.

Proposition 2.1: Under the condition (2), $\mathbf{P}_{[n,n+k]}$ and $\mathbf{P}^-_{[n,n+k]}$ are absolutely continuous with respect to each other, and the Radon–Nikodym derivative is given by

$$\frac{\mathrm{d}\mathbf{P}_{[n,n+k]}}{\mathrm{d}\mathbf{P}^-_{[n,n+k]}}(\omega)=\frac{\pi_{\xi_n(\omega)}p_{\xi_n(\omega)\xi_{n+1}(\omega)}\cdots p_{\xi_{n+k-1}(\omega)\xi_{n+k}(\omega)}}{\pi_{\xi_{n+k}(\omega)}p_{\xi_{n+k}(\omega)\xi_{n+k-1}(\omega)}\cdots p_{\xi_{n+1}(\omega)\xi_n(\omega)}},\quad \mathbf{P}-\text{a.s.}$$

Notice that $(1/n)\,E^{\mathbf{P}}\log(\mathrm{d}\mathbf{P}_{[0,n]}/\mathrm{d}\mathbf{P}^-_{[0,n]})$ converges to the entropy production rate e_p of ξ, which is given in (1). In fact, we can get a stronger result.

Proposition 2.2: Under the condition (2),

$$\lim_{n\to+\infty}\frac{1}{n}\log\frac{\mathrm{d}\mathbf{P}_{[0,n]}}{\mathrm{d}\mathbf{P}^-_{[0,n]}}(\omega)=e_p,\quad \mathbf{P}-\text{a.s. or } L^1(\mathrm{d}\mathbf{P}).$$

Proof: Let

$$f(\omega)=\log\frac{\pi_{\xi_0(\omega)}p_{\xi_0(\omega)\xi_1(\omega)}}{\pi_{\xi_1(\omega)}p_{\xi_1(\omega)\xi_0(\omega)}},$$

then

$$\begin{aligned}\frac{1}{n}\log\frac{\mathrm{d}\mathbf{P}_{[0,n]}}{\mathrm{d}\mathbf{P}^-_{[0,n]}}(\omega)&=\frac{1}{n}\log\frac{\pi_{\xi_0(\omega)}p_{\xi_0(\omega)\xi_1(\omega)}\cdots p_{\xi_{n-1}(\omega)\xi_n(\omega)}}{\pi_{\xi_n(\omega)}p_{\xi_n(\omega)\xi_{n-1}(\omega)}\cdots p_{\xi_1(\omega)\xi_0(\omega)}}\\&=\frac{1}{n}\sum_{k=0}^{n-1}\log\frac{\pi_{\xi_k(\omega)}p_{\xi_k(\omega)\xi_{k+1}(\omega)}}{\pi_{\xi_{k+1}(\omega)}p_{\xi_{k+1}(\omega)\xi_k(\omega)}}\\&=\frac{1}{n}\sum_{k=0}^{n-1}f(\theta^k\omega),\quad \mathbf{P}-\text{a.s.}\end{aligned}$$

By the Birkhoff ergodic theorem,[38]

$$\lim_{n\to+\infty}\frac{1}{n}\log\frac{\mathrm{d}\mathbf{P}_{[0,n]}}{\mathrm{d}\mathbf{P}^-_{[0,n]}}(\omega)=\lim_{n\to+\infty}\frac{1}{n}\sum_{k=0}^{n-1}f(\theta^k\omega)=\int f\,\mathrm{d}\mathbf{P}=e_p,\quad \mathbf{P}-\text{a.s. or } L^1(\mathrm{d}\mathbf{P}).\qquad\square$$

There will naturally arise the question what is the convergence rate. The large deviation theory provides us a way to calculate this rate. Let $W_n(\omega)=\log(\mathrm{d}\mathbf{P}_{[0,n]}/\mathrm{d}\mathbf{P}^-_{[0,n]})(\omega)$ and $c_n(\lambda)=(\log Ee^{\lambda W_n})/n$. It is not difficult to see that W_n/n takes finitely many values and $e^{\lambda W_n(\omega)}>0$,

$\mathbf{P}-$a.s. Thus, according to Theorem II.6.1 in Ellis,[39] in order to verify $\{\mu_n : n \in \mathbf{Z}^+\}$, where μ_n is the distribution of W_n/n, has a large deviation property, we only need to verify the free energy function $c(\lambda) \overset{\text{def}}{=} \lim_{n\to+\infty} c_n(\lambda)$ of $\{W_n : n \in \mathbf{Z}^+\}$ exists and is differentiable.

Theorem 2.3: *For all* $\lambda \in \mathbf{R}$, $\lim_{n\to+\infty} c_n(\lambda)$ *exists and the free energy function* $c(\lambda)$ *of* $\{W_n : n \in \mathbf{Z}^+\}$ *is differentiable.*

Proof: From Proposition 2.1,

$$Ee^{\lambda W_n} = \sum_{\substack{i_0,i_1,\cdots,i_n: \\ p_{i_0i_1}\cdots p_{i_{n-1}i_n}>0}} \pi_{i_0} p_{i_0i_1}\cdots p_{i_{n-1}i_n} \left(\frac{\pi_{i_0} p_{i_0i_1}\cdots p_{i_{n-1}i_n}}{\pi_{i_n} p_{i_1i_0}\cdots p_{i_ni_{n-1}}}\right)^{\lambda}$$

$$= \sum_{i_0,i_1,\cdots,i_n} \pi_{i_0} a_{i_0i_1}(\lambda)\cdots a_{i_{n-1}i_n}(\lambda)\left(\frac{\pi_{i_0}}{\pi_{i_n}}\right)^{\lambda},$$

where

$$a_{ij}(\lambda) = \begin{cases} p_{ij}^{1+\lambda} p_{ji}^{-\lambda}, & p_{ij}>0, \\ 0, & p_{ij}=0. \end{cases}$$

It is obvious that $p_{ij}>0 \Leftrightarrow a_{ij}(\lambda)>0$. Hence $\mathbf{A}(\lambda)=(a_{ij}(\lambda))$ is an irreducible nonnegative matrix. By the Perron–Frobenius theorem, the spectral radius $e(\lambda)$ of $\mathbf{A}(\lambda)$ is a positive eigenvalue of $\mathbf{A}(\lambda)$ with one-dimensional eigenspace $\{k\vec{\alpha} : k \in \mathbf{R}\}$, where $\vec{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_d)^T$ and $\alpha_i>0$ for all $i \in S$.

For any given $\lambda>0$, denote

$$C_0 = \max_{i,j}\left(\frac{\pi_i}{\pi_j}\right)^{\lambda}, \quad \alpha_{\min} = \min_i \alpha_i, \quad \alpha_{\max} = \max_i \alpha_i.$$

Then

$$\frac{1}{C_0\alpha_{\max}} \vec{\pi}\mathbf{A}(\lambda)^n\vec{\alpha} \leqslant Ee^{\lambda W_n} \leqslant \frac{C_0}{\alpha_{\min}} \vec{\pi}\mathbf{A}(\lambda)^n\vec{\alpha},$$

where $\vec{\pi}=(\pi_1,\pi_2,\ldots,\pi_d)$. Hence

$$\lim_{n\to+\infty}\frac{1}{n}\log Ee^{\lambda W_n} = \lim_{n\to+\infty}\frac{1}{n}\log \vec{\pi}\mathbf{A}(\lambda)^n\vec{\alpha} = \log e(\lambda),$$

where $e(\lambda)$ is differentiable because it is the simple eigenvalue of a differentiable matrix $\mathbf{A}(\lambda)$ (see Ref. 37 for details). □

By now, we have verified the fact that $\{\mu_n : n \in \mathbf{Z}^+\}$ has a large deviation property with rate function $I(z)=\sup_{\lambda\in\mathbf{R}}\{\lambda z - c(\lambda)\}$. Since $c_n(\cdot)$, $n \in \mathbf{N}$, and $c(\cdot)$ are all finite, and $c(\cdot)$ is differentiable at $\lambda=0$, by Theorem II.6.3 in Ellis,[39] W_n/n converges exponentially to the constant $c'(0)$. From Proposition 2.2, $c'(0)$ equals the entropy production rate e_p of the stationary Markov chain ξ. Furthermore, the innate symmetry of $\{W_n\}$ implies the symmetry of its free energy function and rate function.

Theorem 2.4: *(Fluctuation theorem) The free energy function* $c(\lambda)$ *and the large deviation rate function* $I(z)$ *of* $\{W_n : n \in \mathbf{Z}^+\}$ *have the following properties:*

$$c(\lambda) = c(-(1+\lambda)), \ \forall \lambda \in \mathbf{R}, \quad I(z) = I(-z) - z, \ \forall z \in \mathbf{R}.$$

Proof: Since $\mathbf{P}$ and $\mathbf{P}^-$ are reciprocal under the time-reversal transformation,

$$\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(r\omega)=\frac{d\mathbf{P}^-_{[-n,0]}}{d\mathbf{P}_{[-n,0]}}(\omega)=\frac{d\mathbf{P}^-_{[0,n]}}{d\mathbf{P}_{[0,n]}}(\theta^{-n}\omega)=\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(\theta^{-n}\omega)\right)^{-1}.$$

Thus

$$\begin{aligned}Ee^{\lambda W_n}&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(\omega)\right)^{\lambda}d\mathbf{P}(\omega)\\&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(r\omega)\right)^{\lambda}d\mathbf{P}^-(\omega)\\&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(\theta^{-n}\omega)\right)^{-\lambda}d\mathbf{P}^-(\omega)\\&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^-_{[0,n]}}(\omega)\right)^{-(1+\lambda)}d\mathbf{P}(\omega)=Ee^{-(1+\lambda)W_n}.\end{aligned}$$

This yields $c(\lambda)=c(-(1+\lambda))$, and hence

$$\begin{aligned}I(z)&=\sup_{\lambda\in\mathbf{R}}\{\lambda z-c(\lambda)\}=\sup_{\lambda\in\mathbf{R}}\{\lambda z-c(-(1+\lambda))\}\\&=\sup_{\lambda\in\mathbf{R}}\{-(1+\lambda)z-c(\lambda)\}=\sup_{\lambda\in\mathbf{R}}\{\lambda\cdot(-z)-c(\lambda)\}-z=I(-z)-z.\end{aligned}$$ □

We could regard $W_n(\omega)/n=(1/n)\log(d\mathbf{P}_{[0,n]}/d\mathbf{P}^-_{[0,n]})(\omega)$ as the time-averaged entropy production rate of the sample trajectory ω of the stochastic system modelled by the Markov chain ξ. Roughly speaking, the fluctuation theorem gives a formula for the probability ratio that the sample entropy production rate W_n/n takes a value z to that of $-z$, and the ratio is roughly e^{nz}. If the Markov chain ξ is reversible, $I(0)=0$ and $I(z)=+\infty$ for any $z\neq 0$. In this case the fluctuation theorem gives a trivial result. However, if the Markov chain ξ is not reversible, for $z>0$ in a certain range, the sample entropy production rate W_n/n has a positive probability to take the value $z>0$ as well as the value $-z$. The fluctuation theorem tells that the former probability is greater, which accords with the second law of thermodynamics.

Now we discuss the transient fluctuation theorem for non-stationary Markov chains. Assume that $\tilde{\xi}=\{\tilde{\xi}_n:n\in\mathbf{Z}^+\}$ is an irreducible finite Markov chain on its canonical trajectory space $(\tilde{\Omega},\tilde{\mathcal{F}},\tilde{\mathbf{P}})$ with finite state space S and transition probability matrix $P=(p_{ij})_{i,j\in S}$ as ξ. Suppose that the initial distribution ν (not necessarily invariant) satisfies $\nu_i>0$ for any $i\in S$. Denote the distributions of the trajectory segments of ξ over a finite time interval $[0,n]$ and their time reversals by $\tilde{\mathbf{P}}_{[0,n]}$ and $\tilde{\mathbf{P}}^-_{[0,n]}$, respectively. Let $\tilde{W}_n=\log(d\tilde{\mathbf{P}}_{[0,n]}/d\tilde{\mathbf{P}}^-_{[0,n]})$. From the above presentation, one can easily see that $\{\tilde{\mu}_n:n\geqslant 0\}$, the family of distributions of $\{\tilde{W}_n/n:n\geqslant 0\}$, also has a large deviation property and $\{\tilde{W}_n\}$ has the same free energy function as $\{W_n\}$, which yields that $\{\tilde{\mu}_n\}$ has the same large deviation rate function as $\{\mu_n\}$ and thus the rate function has a symmetry. Moreover, for any $n>0,z\in\mathbf{R}$, it holds that

$$\begin{aligned}\tilde{\mathbf{P}}\left(\frac{\tilde{W}_n}{n}=z\right)&=\tilde{\mathbf{P}}\left(\frac{d\tilde{\mathbf{P}}_{[0,n]}}{d\tilde{\mathbf{P}}^-_{[0,n]}}=e^{nz}\right)=\tilde{\mathbf{P}}_{[0,n]}\left(\frac{d\tilde{\mathbf{P}}_{[0,n]}}{d\tilde{\mathbf{P}}^-_{[0,n]}}=e^{nz}\right)=e^{nz}\tilde{\mathbf{P}}^-_{[0,n]}\left(\frac{d\tilde{\mathbf{P}}_{[0,n]}}{d\tilde{\mathbf{P}}^-_{[0,n]}}=e^{nz}\right)\\&=e^{nz}\tilde{\mathbf{P}}_{[0,n]}\left(\frac{d\tilde{\mathbf{P}}^-_{[0,n]}}{d\tilde{\mathbf{P}}_{[0,n]}}=e^{nz}\right)=e^{nz}\tilde{\mathbf{P}}\left(\frac{\tilde{W}_n}{n}=-z\right).\end{aligned}$$

Since S is finite, $\tilde{W}_n/n$ only takes a finite number of values and both sides of the above equality may simultaneously be equal to zero. However, in case one can divide over, the above equality can be written as

$$\frac{\tilde{\mathbf{P}}\left(\frac{\tilde{W}_n}{n}=z\right)}{\tilde{\mathbf{P}}\left(\frac{\tilde{W}_n}{n}=-z\right)}=e^{nz}.$$

Such an equality is called the transient fluctuation theorem by Evans *et al.*[7–13,19]

III. FINITE MARKOV CHAINS WITH CONTINUOUS TIME PARAMETER

In this section, we will discuss the same problem in the case of continuous time. The emphasis is much more oriented to detailed mathematical analysis and estimates. Let $\xi=\{\xi_t:t\in\mathbf{R}\}$ be a stationary, irreducible Markov chain on a probability space $(\Omega,\mathcal{F},\mathbf{P})$ with finite state space $S=\{1,\ldots,d\}$, conservative Q-matrix $Q=(q_{ij})_{i,j\in S}$, and invariant distribution $\Pi=\{\pi_i\}_{i\in S}$. Without loss of generality, we suppose that $(\Omega,\mathcal{F},\mathbf{P})$ is the canonical trajectory space of ξ, and its trajectories are right continuous having left limits. Since the time-reversed trajectories are left continuous having right limits, we should modify them. Define the time-reversal transformation and the shift operator as

$$r:(\Omega,\mathcal{F})\to(\Omega,\mathcal{F}),\quad \xi_t(r\omega)=\lim_{s\uparrow -t}\xi_s(\omega),\quad \forall t\in\mathbf{R},$$

$$\theta^t:(\Omega,\mathcal{F})\to(\Omega,\mathcal{F}),\quad \xi_s(\theta^t\omega)=\xi_{s+t}(\omega),\quad \forall s,t\in\mathbf{R}.$$

r,θ^t are $\mathcal{F}$-measurable and invertible with $r^{-1}=r$, $r\theta^t=\theta^{-t}r$, $\theta^t\mathbf{P}=\mathbf{P}$ and $\theta^t\mathbf{P}^-=\mathbf{P}^-$, where $\mathbf{P}^-=r\mathbf{P}$. The stationary Markov chain ξ is said to be reversible if $\mathbf{P}=\mathbf{P}^-$. As is well known, ξ is reversible if and only if the entropy production rate e_p of ξ vanishes, or iff $\pi_i q_{ij}=\pi_j q_{ji}$ for any $i,j\in S$.[26,27,29] Similarly as in the discrete time case, we assume that the Q-matrix satisfies the condition

$$q_{ij}>0\Leftrightarrow q_{ji}>0,\quad \forall i,j\in S. \tag{3}$$

For each $s\in\mathbf{R}$ and $t\in\mathbf{R}^+$, denote by $\mathbf{P}_{[s,s+t)}$ and $\mathbf{P}^-_{[s,s+t)}$, respectively, the restrictions of $\mathbf{P}$ and $\mathbf{P}^-$ on $\mathcal{F}_s^{s+t}=\sigma(\xi_u:s\leqslant u<s+t)$, then we have the following proposition.

Proposition 3.1: Under the condition (3), $\mathbf{P}_{[s,s+t)}$ and $\mathbf{P}^-_{[s,s+t)}$ are absolutely continuous with respect to each other, and the Radon–Nikodym derivative is given by

$$\left.\frac{\mathrm{d}\mathbf{P}_{[s,s+t)}}{\mathrm{d}\mathbf{P}^-_{[s,s+t)}}\right|_{A_{i_0i_1\cdots i_n}(t)}=\frac{\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}}{\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_1i_0}},\quad \mathbf{P}-\text{a.s.},$$

where

$$A_{i_0i_1\cdots i_n}(t)=\{\omega\in\Omega:\omega \textit{ jumps } n \textit{ times in } [s,s+t),\ \textit{and the states are } i_0,\ldots,i_n \textit{ in turn}\}.$$

Proof: Denote $T_0=s$ and the jump times in the interval $[s,s+t)$ by $T_1(\omega),T_2(\omega),\ldots$ in turn. For any $n\geqslant 0$, $i_0,i_1,\ldots,i_n\in S$, $0<s_1<\cdots<s_n<s_{n+1}=t$ and small $\delta s_1,\ldots,\delta s_n>0$ (such that $s_k+\delta s_k<s_{k+1}$, $k=1,\ldots,n$), denote

$$A=\{\omega\in A_{i_0i_1\cdots i_n}(t):s_k\leqslant T_k(\omega)<s_k+\delta s_k,\ k=1,\ldots,n\}.$$

Then

$$\begin{aligned}\mathbf{P}(A)=&\int_{s_1}^{s_1+\delta s_1}\mathrm{d}t_1\int_{s_2}^{s_2+\delta s_2}\mathrm{d}t_2\cdots\int_{s_n}^{s_n+\delta s_n}\mathrm{d}t_n\\&\times\int_t^{+\infty}\mathrm{d}t_{n+1}\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}q_{i_n}e^{-q_{i_0}t_1}e^{-q_{i_1}(t_2-t_1)}\cdots e^{-q_{i_n}(t_{n+1}-t_n)}\\=&\int_{s_1}^{s_1+\delta s_1}\mathrm{d}t_1\int_{s_2}^{s_2+\delta s_2}\mathrm{d}t_2\cdots\int_{s_n}^{s_n+\delta s_n}\mathrm{d}t_n\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}\\&\times e^{-q_{i_0}t_1}e^{-q_{i_1}(t_2-t_1)}\cdots e^{-q_{i_{n-1}}(t_n-t_{n-1})}e^{-q_{i_n}(t-t_n)}.\end{aligned}$$

Since

$$rA=\{\omega\in A_{i_ni_{n-1}\cdots i_0}(t):t-(s_{n+1-k}+\delta s_{n+1-k})\leqslant T_k(\omega)<t-s_{n+1-k},\ \ k=1,\ldots,n\},$$

it follows that

$$\begin{aligned}\mathbf{P}^-(A)=\mathbf{P}(rA)=&\int_{t-(s_n+\delta s_n)}^{t-s_n}\mathrm{d}t_1\int_{t-(s_{n-1}+\delta s_{n-1})}^{t-s_{n-1}}\mathrm{d}t_2\cdots\int_{t-(s_1+\delta s_1)}^{t-s_1}\mathrm{d}t_n\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_1i_0}\\&\times e^{-q_{i_n}t_1}e^{-q_{i_{n-1}}(t_2-t_1)}\cdots e^{-q_{i_1}(t_n-t_{n-1})}e^{-q_{i_0}(t-t_n)}\\=&\int_{s_1}^{s_1+\delta s_1}\mathrm{d}t_1\int_{s_2}^{s_2+\delta s_2}\mathrm{d}t_2\cdots\int_{s_n}^{s_n+\delta s_n}\mathrm{d}t_n\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_1i_0}\\&\times e^{-q_{i_0}t_1}e^{-q_{i_1}(t_2-t_1)}\cdots e^{-q_{i_{n-1}}(t_n-t_{n-1})}e^{-q_{i_n}(t-t_n)}\\=&\frac{\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_1i_0}}{\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}}\mathbf{P}(A).\end{aligned}$$

Notice that such A's as above generate $\mathcal{F}_{[s,s+t)}$, then one obtains the desired result immediately. □

The entropy production rate e_p of the stationary Markov chain ξ can be defined by

$$e_p\overset{\text{def}}{=}\lim_{t\to+\infty}\frac{1}{t}H(\mathbf{P}_{[0,t)},\mathbf{P}^-_{[0,t)})=\lim_{t\to+\infty}\frac{1}{t}E^{\mathbf{P}}\log\frac{\mathrm{d}\mathbf{P}_{[0,t)}}{\mathrm{d}\mathbf{P}^-_{[0,t)}},$$

or equivalently, as in Refs. 26 and 27, by

$$e_p\overset{\text{def}}{=}\lim_{t\downarrow0+}\frac{1}{t}H(\mathbf{P}_{[s,s+t)},\mathbf{P}^-_{[s,s+t)})=\lim_{t\downarrow0+}\frac{1}{t}E^{\mathbf{P}}\log\frac{\mathrm{d}\mathbf{P}_{[s,s+t)}}{\mathrm{d}\mathbf{P}^-_{[s,s+t)}},$$

where $s\in\mathbf{R}$. The equivalence is a direct consequence of Theorem 10.4 in Varadhan.[40] In Refs. 26, 28, and 29, an entropy production formula was given for ξ:

$$e_p=\frac{1}{2}\sum_{i,j\in S}(\pi_iq_{ij}-\pi_jq_{ji})\log\frac{\pi_iq_{ij}}{\pi_jq_{ji}}.\tag{4}$$

Employing Proposition 3.1 and (6), (7) below, it is not difficult to prove this formula strictly.

Proposition 3.2: Under the condition (3),

$$\lim_{t\to+\infty}\frac{1}{t}\log\frac{d\mathbf{P}_{[s,s+t)}}{d\mathbf{P}^{-}_{[s,s+t)}}(\omega)=e_p,\quad \mathbf{P}-\text{a.s.}$$

Proof: Let $N_t(\omega)$ be the number of jumps of ω in the interval $[s,s+t)$, $N_t(i,j,\omega)$ be the number of jumps from i to j of ω in the interval $[s,s+t)$ and $\{X_k\}_{k\in\mathbf{Z}^+}$ be the embedded chain of ξ defined by $X_k=\xi_{T_k}$. By Proposition 3.1,

$$\begin{aligned}\frac{1}{t}\log\frac{d\mathbf{P}_{[s,s+t)}}{d\mathbf{P}^{-}_{[s,s+t)}}(\omega)&=\frac{1}{t}\sum_{n=0}^{+\infty}\left(\log\frac{\pi_{X_0(\omega)}}{\pi_{X_n(\omega)}}+\sum_{k=0}^{n-1}\log\frac{q_{X_k(\omega)X_{k+1}(\omega)}}{q_{X_{k+1}(\omega)X_k(\omega)}}\right)1_{\{N_t=n\}}(\omega)\\&=\frac{1}{t}\sum_{n=0}^{+\infty}1_{\{N_t=n\}}(\omega)\log\frac{\pi_{X_0(\omega)}}{\pi_{X_n(\omega)}}\\&\quad+\sum_{i,j\in S}\sum_{n=0}^{+\infty}\sum_{k=0}^{n-1}\frac{1}{t}1_{\{N_t=n\}}(\omega)1_{\{X_k=i,X_{k+1}=j\}}(\omega)\log\frac{q_{ij}}{q_{ji}}\\&=\frac{1}{t}\sum_{n=0}^{+\infty}1_{\{N_t=n\}}(\omega)\log\frac{\pi_{X_0(\omega)}}{\pi_{X_n(\omega)}}+\sum_{i,j\in S}\frac{1}{t}N_t(i,j,\omega)\log\frac{q_{ij}}{q_{ji}},\end{aligned}\tag{5}$$

where $1_A(\cdot)$ is the indicator function of the event $A\in\mathcal{F}$. For any $t_1,t_2\geqslant 0$ and $i,j\in S$, $N_{t_1+t_2}(i,j,\omega)=N_{t_1}(i,j,\omega)+N_{t_2}(i,j,\theta^{t_1}\omega)$, $\mathbf{P}-$a.s. By the subadditive ergodic theorem,[38] for any $\delta>0$, it holds that

$$\lim_{n\to+\infty}\frac{1}{n\delta}N_{n\delta}(i,j,\omega)=\inf_n\frac{1}{n\delta}EN_{n\delta}(i,j,\cdot)=\frac{1}{\delta}EN_\delta(i,j,\cdot),\quad \mathbf{P}-\text{a.s.}$$

For any t, there exist $n(t)\in\mathbf{Z}^+$ and $r(t)\in[0,\delta)$ such that $t=n(t)\delta+r(t)$, thus

$$\frac{1}{t}N_t(i,j,\omega)=\frac{1}{t}N_{n(t)\delta}(i,j,\omega)+\frac{1}{t}N_{r(t)}(i,j,\theta^{n(t)\delta}\omega),\quad \mathbf{P}-\text{a.s.}$$

Consequently,

$$\lim_{t\to+\infty}\frac{1}{t}N_{n(t)\delta}(i,j,\omega)=\frac{1}{\delta}EN_\delta(i,j,\cdot),\quad \mathbf{P}-\text{a.s.}$$

Now we would like to prove that $\lim_{t\to+\infty}N_{r(t)}(i,j,\theta^{n(t)\delta}\omega)/t=0$, $\mathbf{P}-$a.s. For any given $i_0,i_1,\ldots,i_n\in S$,

$$\begin{aligned}\mathbf{P}(A_{i_0i_1\cdots i_n}(t))&=\int_0^t dt_n\int_{0<t_1<t_2<\cdots<t_n}dt_1\,dt_2\cdots dt_{n-1}\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}e^{-q_{i_n}t}\prod_{k=1}^{n}e^{(q_{i_k}-q_{i_{k-1}})t_k}\\&\leqslant\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}\frac{t^n}{n!}.\end{aligned}\tag{6}$$

Hence for any n,

$$\mathbf{P}(N_t(\omega)=n)\leqslant\sum_{\substack{i_0,\cdots,i_n\\ i_k\neq i_{k+1}}}\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}\frac{t^n}{n!}\leqslant\frac{(\max_i q_i t)^n}{n!}.\tag{7}$$

For any $\varepsilon>0$,

$$\begin{aligned}\sum_{n=0}^{+\infty}\mathbf{P}(N_\delta(i,j,\omega)>n\varepsilon)&\leqslant\sum_{n=0}^{+\infty}\mathbf{P}(N_\delta(\omega)>n\varepsilon)\\&=\sum_{n=0}^{+\infty}\sum_{k>n\varepsilon}\mathbf{P}(N_\delta(\omega)=k)\\&=\sum_{k=1}^{+\infty}\sum_{0\leqslant n<k\varepsilon^{-1}}\mathbf{P}(N_\delta(\omega)=k)\\&\leqslant\sum_{k=1}^{+\infty}\mathbf{P}(N_\delta(\omega)=k)(k\varepsilon^{-1}+1)<+\infty.\end{aligned}$$

Since the process is stationary, $\mathbf{P}(N_\delta(i,j,\theta^{n\delta}\omega)>n\varepsilon)=\mathbf{P}(N_\delta(i,j,\omega)>n\varepsilon)$ for any $n>0$. This together with the Borel–Cantelli lemma yields that

$$\begin{aligned}&\mathbf{P}\left(\exists\ \text{a sequence}\ \{t_k\geqslant 0\}_{k\in\mathbf{N}}\ \text{s.t.}\ t_k\uparrow+\infty\ \text{and}\ \frac{1}{t_k}N_{r(t_k)}(i,j,\theta^{n(t_k)\delta}\omega)>\varepsilon,\forall k\in\mathbf{N}\right)\\&\qquad\leqslant\mathbf{P}[N_\delta(i,j,\theta^{n\delta}\omega)>n\varepsilon\ \text{ infinitely often}]=0.\end{aligned}$$

Hence $\mathbf{P}-$a.s., $\lim_{t\to+\infty}(1/t)\,N_{r(t)}(i,j,\theta^{n(t)\delta}\omega)=0$. So for any given $\delta>0$, it holds that

$$\lim_{t\to+\infty}\frac{1}{t}N_t(i,j,\omega)=\frac{1}{\delta}EN_\delta(i,j,\cdot),\quad\mathbf{P}-\text{a.s.},\tag{8}$$

where $EN_\delta(i,j,\cdot)=\Sigma_{n=1}^{+\infty}EN_\delta(i,j,\cdot)1_{\{N_\delta=n\}}(\cdot)$. On one hand,

$$\begin{aligned}\frac{1}{\delta}EN_\delta(i,j,\cdot)1_{\{N_\delta=1\}}(\cdot)&=\frac{1}{\delta}P(N_\delta(\omega)=1,N_\delta(i,j,\omega)=1)\\&=\frac{1}{\delta}\int_0^\delta\pi_iq_{ij}e^{-q_j\delta}e^{(q_j-q_i)\tau}\,\mathrm{d}\tau\to\pi_iq_{ij},\quad\text{as}\ \ \delta\to0+.\end{aligned}$$

On the other hand, from (7)

$$\frac{1}{\delta}\sum_{n=2}^{+\infty}EN_\delta(i,j,\cdot)1_{\{N_\delta=n\}}(\cdot)\leqslant\frac{1}{\delta}\sum_{n=2}^{+\infty}nP(N_\delta(\omega)=n)\to0,\quad\text{as}\ \ \delta\to0+.$$

Hence $(1/\delta)\,EN_\delta(i,j,\cdot)=\pi_iq_{ij}$, which together with (5) and (8) yields that

$$\lim_{t\to+\infty}\frac{1}{t}\log\frac{\mathrm{d}\mathbf{P}_{[s,s+t)}}{\mathrm{d}\mathbf{P}^-_{[s,s+t)}}(\omega)=\sum_{i,j}\pi_iq_{ij}\log\frac{\pi_iq_{ij}}{\pi_jq_{ji}}=e_p,\quad\mathbf{P}-\text{a.s.}\qquad\square$$

Let $W_t(\omega)=\log(\mathrm{d}\mathbf{P}_{[0,t)}/\mathrm{d}\mathbf{P}^-_{[0,t)})(\omega)$, μ_t be the distribution of W_t/t and $c_t(\lambda)=(\log Ee^{\lambda W_t})/t$. According to Theorem II.6.1 in Ellis[39] (modified for continuous time parameter), in order to verify $\{\mu_t:t\in\mathbf{R}^+\}$ has a large deviation property, we only need to prove $c_t(\lambda)$ is finite and the free energy function $c(\lambda)\overset{\text{def}}{=}\lim_{t\to+\infty}c_t(\lambda)$ of $\{W_t:t\in\mathbf{R}^+\}$ exists and is differentiable.

Proposition 3.3: For any $t>0$ and $\lambda\in\mathbf{R}$, $c_t(\lambda)$ is finite.

Proof: For any $i\in S$, by Proposition 3.1, it holds that

$$E_i(t,\lambda)\overset{\text{def}}{=}E(e^{\lambda W_t}|\xi_0=i)=\sum_{n=0}^{+\infty}\sum_{\substack{i_1,\cdots,i_n:\\ q_{ii_1}q_{i_1i_2}\cdots q_{i_{n-1}i_n}>0}}\left(\frac{\pi_i q_{ii_1}q_{i_1i_2}\cdots q_{i_{n-1}i_n}}{\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_2i_1}q_{i_1i}}\right)^{\lambda}\mathbf{P}(A_{ii_1\ldots i_n}(t)|\xi_0=i). \tag{9}$$

From (6) and (7),

$$\sum_{\substack{i_1,\cdots,i_n:\\ q_{ii_1}q_{i_1i_2}\cdots q_{i_{n-1}i_n}>0}}\left(\frac{\pi_i q_{ii_1}q_{i_1i_2}\cdots q_{i_{n-1}i_n}}{\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_2i_1}q_{i_1i}}\right)^{\lambda}\mathbf{P}(A_{ii_1\ldots i_n}(t)|\xi_0=i)\leqslant B^{\lambda}\frac{(C^{\lambda}Dt)^n}{n!},$$

where $B=\max_{i,j}\pi_i/\pi_j$, $C=\max\{q_{ij}/q_{ji}:q_{ij}>0\}$ and $D=\max_i q_i$. Hence $E_i(t,\lambda)<+\infty$ and $Ee^{\lambda W_t}=\Sigma_i\pi_iE_i(t,\lambda)<+\infty$. On the other hand, it is easy to see $Ee^{\lambda W_t}>0$. Thus $c_t(\lambda)=(1/t)\log Ee^{\lambda W_t}$ is finite. □

Theorem 3.4: *For all* $\lambda\in\mathbf{R}$, $\lim_{t\to+\infty}c_t(\lambda)$ *exists and the free energy function* $c(\lambda)$ *of* $\{W_t:t\in\mathbf{R}^+\}$ *is differentiable.*

Proof: From (6),

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P}(A_{i_0i_1\cdots i_n}(t))=-q_{i_n}\mathbf{P}(A_{i_0i_1\cdots i_n}(t))+q_{i_{n-1}i_n}\mathbf{P}(A_{i_0i_1\cdots i_{n-1}}(t)). \tag{10}$$

By Proposition 3.1 and $\mathbf{P}^-=r\mathbf{P}$, it holds that

$$\mathbf{P}(A_{i_0i_1\cdots i_n}(t))=\frac{\pi_{i_0}q_{i_0i_1}\cdots q_{i_{n-1}i_n}}{\pi_{i_n}q_{i_ni_{n-1}}\cdots q_{i_1i_0}}\mathbf{P}(A_{i_ni_{n-1}\cdots i_0}(t)).$$

This together with (10) yields that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P}(A_{i_0i_1\cdots i_n}(t))=-q_{i_0}\mathbf{P}(A_{i_0i_1\cdots i_n}(t))+\frac{\pi_{i_0}q_{i_0i_1}}{\pi_{i_1}}\mathbf{P}(A_{i_1i_2\cdots i_n}(t)),$$

and it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P}(A_{i_0i_1\cdots i_n}(t)|\xi_0=i_0)=-q_{i_0}\mathbf{P}(A_{i_0i_1\cdots i_n}(t)|\xi_0=i_0)+q_{i_0i_1}\mathbf{P}(A_{i_1\cdots i_n}(t)|\xi_0=i_1).$$

Taking differentials on both sides of (9) with respect to t, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}E_i(t,\lambda)=-q_iE_i(t,\lambda)+\sum_{j:q_{ij}>0}q_{ij}\left(\frac{\pi_iq_{ij}}{\pi_jq_{ji}}\right)^{\lambda}E_j(t,\lambda). \tag{11}$$

Let

$$\mathbf{E}(t,\lambda)=\begin{pmatrix}E_1(t,\lambda)\\ \cdots\\ E_d(t,\lambda)\end{pmatrix},\quad l_{ij}(\lambda)=\begin{cases}-q_i, & \text{if } i=j,\\ q_{ij}\left(\dfrac{\pi_iq_{ij}}{\pi_jq_{ji}}\right)^{\lambda}, & \text{if } q_{ij}>0,\\ 0, & \text{if } q_{ij}=0.\end{cases}\quad \mathbf{1}=\begin{pmatrix}1\\ \vdots\\ 1\end{pmatrix}.$$

Since $\mathbf{E}(0,\lambda)=\mathbf{1}$, (11) yields $\mathbf{E}(t,\lambda)=e^{\mathbf{L}(\lambda)t}\mathbf{1}$, where $\mathbf{L}(\lambda)=(l_{ij}(\lambda))$. Thus

$$c_t(\lambda)=\frac{1}{t}\log Ee^{\lambda W_t}=\frac{1}{t}\log\sum_i\pi_iE_i(t,\lambda)=\frac{1}{t}\log\vec{\pi}e^{\mathbf{L}(\lambda)t}\mathbf{1}, \tag{12}$$

where $\vec{\pi}=(\pi_1,\pi_2,\ldots,\pi_d)$. It is easy to see that $q_{ij}>0\Leftrightarrow l_{ij}(\lambda)>0$ and $q_{ij}=0\Leftrightarrow l_{ij}(\lambda)=0$. Since Q is irreducible, the Taylor expansion of $e^{\mathbf{L}(\lambda)t}$ at $t=0$,

$$e^{\mathbf{L}(\lambda)t}=\mathbf{I}+\mathbf{L}(\lambda)t+\frac{1}{2!}\mathbf{L}(\lambda)^2t^2+\cdots+\frac{1}{n!}\mathbf{L}(\lambda)^nt^n+\mathbf{o}(t^n),$$

tells that for any $i,j\in S$, there is a $\delta(i,j)>0$ such that $[e^{\mathbf{L}(\lambda)t}]_{ij}>0$ for any $t\in(0,\delta(i,j)]$. Hence $e^{\mathbf{L}(\lambda)\delta}>0$ for any sufficiently small δ, which yields that it holds for all $\delta>0$. For a fixed $\delta>0$, by the Perron–Frobenius theorem, the spectral radius $e(\lambda,\delta)$ of $e^{\mathbf{L}(\lambda)\delta}$ is a positive eigenvalue of $e^{\mathbf{L}(\lambda)\delta}$ with one-dimensional eigenspace. This together with (12) yields that

$$c(\lambda)=\lim_{t\to+\infty}c_t(\lambda)=\delta^{-1}\log e(\lambda,\delta).$$

$c(\lambda)$ is differentiable because $\mathbf{L}(\lambda)$ is differentiable and so are $e^{\mathbf{L}(\lambda)\delta}$ and $e(\lambda,\delta)$. □

Also the innate symmetry of $\{W_t\}$ implies symmetries of its free energy function and rate function. The proof is exactly the same as that of Theorem 2.4.

Theorem 3.5: *(Fluctuation theorem) The free energy function $c(\cdot)$ and the large deviation rate function $I(\cdot)$ of $\{W_t:t\in\mathbf{R}^+\}$ satisfy*

$$c(\lambda)=c(-(1+\lambda)),\quad \forall\lambda\in\mathbf{R},\quad I(z)=I(-z)-z,\quad \forall z\in\mathbf{R}.$$

As in the discrete-time case, the transient fluctuation theorem holds for nonstationary Markov chains with continuous-time parameter. Suppose that $\tilde{\xi}=\{\tilde{\xi}_t:t\geqslant 0\}$ is a Markov chain on its canonical trajectory space $(\tilde{\Omega},\tilde{\mathcal{F}},\tilde{\mathbf{P}})$ with the same state space S and the same Q-matrix Q as those of ξ. Assume that the initial distribution ν (may not invariant) satisfies $\nu_i>0$ for all $i\in S$. Denote the distributions of the trajectory segments of ξ over a finite time interval $[0,t)$ and their time reversals by $\tilde{\mathbf{P}}_{[0,t)}$ and $\tilde{\mathbf{P}}^-_{[0,t)}$, respectively. Let $\tilde{W}_t=\log(\mathrm{d}\tilde{\mathbf{P}}_{[0,t)}/\mathrm{d}\tilde{\mathbf{P}}^-_{[0,t)})$. From the above presentation, one can see that $\{\tilde{\mu}_t:t\geqslant 0\}$, the family of the distributions of $\{\tilde{W}_t/t:t\geqslant 0\}$, also has a large deviation property and $\{\tilde{W}_t\}$ has the same free energy function as $\{W_t\}$, which yields that $\{\tilde{\mu}_t\}$ has the same large deviation rate function as $\{\mu_t\}$ and thus the rate function has a symmetry. We also have

$$\tilde{\mathbf{P}}\left(\frac{\tilde{W}_t}{t}=z\right)=e^{tz}\tilde{\mathbf{P}}\left(\frac{\tilde{W}_t}{t}=-z\right),\quad \forall t>0,z\in\mathbf{R}.$$

IV. FLUCTUATIONS OF GENERAL OBSERVABLES

With the assumptions and notation of the stationary case in Sec. II, let $\varphi:S\to\mathbf{R}$ be an observable and $\Phi_n(\omega)=\Sigma_{k=0}^n\varphi(\xi_k(\omega))=\Sigma_{k=0}^n\varphi(\xi_0(\theta^k\omega))$. Clearly, Φ_n satisfies $\Phi_n(r\omega)=\Phi_n(\theta^{-n}\omega)$ for any $\omega\in\Omega$. From the Birkhoff ergodic theorem, it follows that $\lim_{n\to+\infty}\Phi_n/n=E^{\mathrm{II}}\varphi$. Use the Perron–Frobenius theorem, then one sees that

$$c(\lambda_1,\lambda_2)\overset{\text{def}}{=}\lim_{n\to+\infty}\frac{1}{n}\log Ee^{\lambda_1W_n+\lambda_2\Phi_n}$$

exists and is differentiable with respect to λ_1,λ_2. Thus $\{\mu_n:n\geqslant 0\}$, the family of the distributions of $\{(W_n/n,\Phi_n/n):n\geqslant 0\}$, has a large deviation property with rate function $I(z_1,z_2)=\sup_{\lambda_1,\lambda_2\in\mathbf{R}}\{\lambda_1z_1+\lambda_2z_2-c(\lambda_1,\lambda_2)\}$. It is not difficult to find that $c(\lambda_1,\lambda_2)=c(-(1+\lambda_1),\lambda_2)$ and $I(z_1,z_2)=I(-z_1,z_2)-z_1$. In general, let $\{\vec{\Phi}_n:n\geqslant 0\}$ and $\{\vec{\Psi}_n:n\geqslant 0\}$ be two sets of random vectors on $(\Omega,\mathcal{F},\mathbf{P})$, where $\vec{\Phi}_n$ and $\vec{\Psi}_n$ are $\mathcal{F}_0^n$ measurable. Provided that the free energy function

$$c(\lambda,\vec{\nu},\vec{\gamma})\overset{\text{def}}{=}\lim_{n\to+\infty}\frac{1}{n}\log Ee^{\lambda W_n+\langle\vec{\nu},\vec{\Phi}_n\rangle+\langle\vec{\gamma},\vec{\Psi}_n\rangle}$$

exists and is differentiable, it holds that $\{\mu_n:n\geqslant 0\}$, the family of the distributions of $\{(1/n)(W_n,\vec{\Phi}_n,\vec{\Psi}_n):n\geqslant 0\}$, has a large deviation property with rate function $I(z,\vec{u},\vec{v})=\sup_{\lambda,\vec{\nu},\vec{\gamma}}\{\lambda z+\langle\vec{\nu},\vec{u}\rangle+\langle\vec{\gamma},\vec{v}\rangle-c(\lambda,\vec{\nu},\vec{\gamma}\}$.

Theorem 4.1: *If* $\vec{\Phi}_n(r\omega)=\vec{\Phi}_n(\theta^{-n}\omega)$ *and* $\vec{\Psi}_n(r\omega)=-\vec{\Psi}_n(\theta^{-n}\omega)$ *for any* $n\geqslant 0$ *and* $\omega\in\Omega$, *it holds that*

$$c(\lambda,\vec{\nu},\vec{\gamma})=c(-(1+\lambda),\vec{\nu},-\vec{\gamma}),\quad I(z,\vec{u},\vec{v})=I(-z,\vec{u},-\vec{v})-z.$$

Proof: For any given $\lambda,\vec{\nu},\vec{\gamma}$,

$$\begin{aligned}Ee^{\lambda W_n+\langle\vec{\nu},\vec{\Phi}_n\rangle+\langle\vec{\gamma},\vec{\Psi}_n\rangle}&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^{-}_{[0,n]}}(\omega)\right)^{\lambda}e^{\langle\vec{\nu},\vec{\Phi}_n(\omega)\rangle+\langle\vec{\gamma},\vec{\Psi}_n(\omega)\rangle}\,d\mathbf{P}(\omega)\\&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^{-}_{[0,n]}}(r\omega)\right)^{\lambda}e^{\langle\vec{\nu},\vec{\Phi}_n(r\omega)\rangle+\langle\vec{\gamma},\vec{\Psi}_n(r\omega)\rangle}\,d\mathbf{P}^{-}(\omega)\\&=\int\left(\frac{d\mathbf{P}_{[0,n]}}{d\mathbf{P}^{-}_{[0,n]}}(\theta^{-n}\omega)\right)^{-\lambda}e^{\langle\vec{\nu},\vec{\Phi}_n(\theta^{-n}\omega)\rangle+\langle\vec{\gamma},-\vec{\Psi}_n(\theta^{-n}\omega)\rangle}\,d\mathbf{P}^{-}(\omega)\\&=Ee^{-(1+\lambda)W_n+\langle\vec{\nu},\vec{\Phi}_n\rangle+\langle-\vec{\gamma},\vec{\Psi}_n\rangle}.\end{aligned}$$

The desired result follows immediately. □

Remark: The same result still holds for the continuous time case.

ACKNOWLEDGMENTS

This work is supported by the SFMSBRP, the 973 Funds of China for Nonlinear Science, the NSFC 10271008 and the Doctoral Program Foundation of Institute Higher Education.

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A direct calculation of the free energy from the Bethe ansatz equation for the Heisenberg model

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(Received 18 November 2002; accepted 14 April 2003)

Thermodynamics of the XXX Heisenberg model is studied. The trace of the Boltzmann weight with respect to the Hilbert space is taken in the thermodynamic limit with the number of up-spins being fixed. The expression of the trace gives an explanation why the correct thermodynamic quantities are derived from the string hypothesis. A combination of this with the previous result leads to a conclusion that the free energy can be calculated only from the Bethe ansatz equation. The method is more direct than other known methods which were used to derive the free energy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1592610]

I. INTRODUCTION

There are two well-known methods to calculate the free energy for quantum integrable systems. One is the thermodynamic Bethe ansatz (TBA) method,[1] and the other is the quantum transfer matrix (QTM) method.[2–6] Both methods, however, are still unsatisfactory. In TBA case, we assume the form of the entropy. And we use the string hypothesis[7,8] for some models, whose validity is not yet proved. While QTM is a general formulation, it is difficult to analyze the resultant equations. We solve them asymptotically or numerically. In this paper, we present a direct method whereby the free energy is derived without logical jumps, assumptions and numerical supports.

We treat the spin-half XXX Heisenberg chain. The Hamiltonian of the system is

$$H=-J\sum_{j=1}^{L}(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+S_j^zS_{j+1}^z)-h\sum_{j=1}^{L}S_j^z+\text{constant}, \tag{1.1}$$

where L is the total number of sites, J is the coupling constant and h expresses the external field. This model is interesting since it has bound states, and correspondingly the Bethe equations have complex solutions. Throughout the paper, we assume periodic boundary condition, and use a unit which makes $J=1$.

We briefly summarize our previous work[9] on this system. We suppose the expression of Z_M, the trace of the Boltzmann weight with respect to the Hilbert space in which the number of up-spins is fixed to be M. An infinite sum $\Sigma_M Z_M$ defined by the expression is analyzed by use of combinatorial relations. Then, it is proved that the free energy $-k_BT\log\Sigma_M Z_M$ can be expressed in term of the function which satisfies an integral equation. The result perfectly agrees with the free energy derived from a different method.[10]

Our purpose is to derive directly the expression

$$Z_M\equiv\mathrm{Tr}\,e^{-\beta H_M},\quad \beta=1/k_BT \tag{1.2}$$

$$=\frac{e^{hM}}{M!}\sum_{\theta\in\Theta_M}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\mu(\hat{0}_\theta,\zeta)\left[\prod_{\theta'\in\zeta}\int_{-\infty}^{\infty}\mathrm{d}x_{\theta'}\right]\left|\frac{\partial I}{\partial x}\right|_{L,\zeta}e^{-\beta E(\zeta)} \tag{1.3}$$

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in the thermodynamic limit $L\to\infty$. All the notation in (1.3) are explained in the following sections. Here, H_M denotes the Hamiltonian (1.1) acting on the Hilbert space in which the number of up-spins is restricted to a constant M. In this paper, we use only the Bethe ansatz; the eigenenergy E of H_M is given by

$$E+hM=\sum_{m=1}^{M}\frac{2}{x_m^2+1}, \tag{1.4}$$

where $\{x_m\}$ satisfies the Bethe equations,

$$\left[\frac{x_m+i}{x_m-i}\right]^L=\prod_{m'\neq m}\frac{x_m-x_{m'}+2i}{x_m-x_{m'}-2i}, \tag{1.5}$$

which are due to periodic boundary condition. Note that (1.3) is the expression of Z_M supposed in the previous paper.[9] We thus complete a new method to derive the free energy of this system independent of TBA and QTM.

The derivation goes as follows. First, we express the trace in a series with respect to solutions of the Bethe equations, which constitute a complete set of the system. Next, the series are replaced by integrals over pseudomomenta. The replacement, however, has a difficulty, because the Bethe equations have complex solutions. The difficulty is resolved by taking a ''good'' integral path. Finally, changing the integral path into a straight line on the complex plane, Z_M in (1.3) is obtained.

We also show that the expression of Z_M gives a reason why the string hypothesis, that is, the substitution of the Bethe equations for string center equations, is appropriate. The substitution is a critical procedure when we apply the thermodynamic Bethe ansatz to an integrable system which has bound states.

The outline of this paper is the following. In Sec. II, we derive the expression (1.3) under the condition $M=2$ only from the Bethe ansatz. In Sec. III, we outline the derivation of Z_M in arbitrary M case. In Sec. IV, we reformulate the results in graphical expressions. In Sec. V, we examine the string hypothesis by use of thus proved expression of Z_M. The last section is devoted to the concluding remarks. Technical details of calculations and proofs are very complicated and therefore we write them in a separate paper.

II. DERIVATION OF Z_2 FROM BETHE EQUATIONS

To explain the essence of the method, we consider the $M=2$ case. With the eigenenergies E (1.4) for $M=2$, Z_2 becomes

$$2Z_2e^{-\beta h2}=\sum\ \exp\left(-\beta\sum_{m=1}^{2}\frac{2}{x_m^2+1}\right). \tag{2.1}$$

Here, Σ without subscript means a summation over all the different physical solutions of the Bethe equations. It is interpreted as a summation with respect to a set of integers $\{I_1,I_2\}$ corresponding to a physical solution, where $\{I_1,I_2\}$ is related to $\{x_1,x_2\}$ by

$$\left[\frac{x_1+i}{x_1-i}\right]^L=e^{-2\pi iI_1}\left[\frac{x_1-x_2+2i}{x_1-x_2-2i}\right]\quad\text{and}\qquad(1\leftrightarrow2). \tag{2.2}$$

Note that I_1, I_2 are so-called quantum numbers and they are usually used when Eqs. (2.2) are written in logarithm forms. They are included in (2.2) to show explicitly I_1, I_2-dependences of x_1, x_2. We say that a solution of the Bethe equations is a ''physical solution'' if and only if the two

pseudomomenta x_1, x_2 of the solution do not have ''same value.'' The words ''different'' and ''same value'' will be explained later.

Equation (2.1) can be written as

$$2Z_2 e^{-\beta h 2} = \sum_{I_1, I_2} \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2 + 1} \right) - \sum_{I} \exp\left(-\beta \frac{4}{x^2+1} \right), \tag{2.3}$$

where $x_1 = x_1(I_1, I_2)$, $x_2 = x_2(I_1, I_2)$ are functions of I_1 and I_2. The first double summations are over all the solutions of the Bethe equations (2.2) and the second summation is over the solutions of the following equation:

$$\left[\frac{x+i}{x-i} \right]^L = -e^{-2\pi i I}. \tag{2.4}$$

In (2.3), extinction of nonphysical states from the sum is realized by the subtraction of the second term.

By using the Poisson formula

$$\sum_n f(n) = \sum_{m=-\infty}^{\infty} \int f(n) e^{2\pi i n m} \, \mathrm{d}n, \tag{2.5}$$

we express (2.3) as

$$\begin{aligned} 2Z_2 e^{-\beta h 2} = & \sum_{m_1, m_2 = -\infty}^{\infty} \int \int \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2+1} + 2\pi i (m_1 I_1 + m_2 I_2) \right) \mathrm{d}I_1 \, \mathrm{d}I_2 \\ & - \sum_{m=-\infty}^{\infty} \int \exp\left(-\beta \frac{4}{x^2+1} + 2\pi i (mI) \right) \mathrm{d}I. \end{aligned} \tag{2.6}$$

The most important matter in (2.6) is the definition of the paths of the multiple integrals. For the Poisson formula we define the paths as follows: The paths are manifolds on which I_1, I_2, I is a set of real numbers and x_1, x_2, x are continuously distributed. The orientation of the integral paths are chosen so that the values of integrals $\int \mathrm{d}I_1 \, \mathrm{d}I_2$ and $\int \mathrm{d}I$ for any part of the integral path are positive. The above definition explicitly characterizes the second integral in (2.6): we may take the integral path with respect to x to be $(-\infty, \infty)$.

For rewriting (2.1) into (2.6), it is necessary to define the words ''different'' and ''same value.'' We regard $\{x_1, x_2 \in \mathbb{C} \text{ or } \infty\}$ in Eq. (2.2) as a multivalued vector function of $\{e^{2\pi i I_1}, e^{2\pi i I_2} \neq 0, \infty\}$. Whether x_1 and x_2 take the ''same value'' or not depends on neighborhoods of the point $\{x_1, x_2\}$ on the Riemann surface defined by the function. We call that x_1 and x_2 take the ''same value'' if and only if there is a point $\{x_1', x_2'\}$ in any neighborhood where $x_1' = x_2'$ and $x_{1,2} \neq x_{1,2}'$. In case $x_1 = x_2 \neq \infty, \pm i$, this definition indicates that x_1 and x_2 take the ''same value.'' Therefore, in almost all the region of variables $\{x_1, x_2\}$, this definition leads to a valid definition of the ''physical solution.'' Next, ''different'' is defined as follows. Solutions of (2.2) corresponding to different points on the Riemann surface are ''different,'' where we regard (2.2) as an equation for $\{x_1, x_1\}$ fixing $\{e^{2\pi i I_1}, e^{2\pi i I_2}\}$ to be constants. At any point on the Riemann surface, the number of ''different'' solutions is estimated by

$$\lim_{\epsilon \to 0} \max \text{ number of points on } R_\epsilon \text{ corresponding to the same } \{e^{2\pi i I_1'}, e^{2\pi i I_2'}\}, \tag{2.7}$$

where R_ϵ is an ϵ-neighborhood of the point on the Riemann surface. Summarizing the above

considerations, we can say that the point on the Riemann surface $x_1, x_2 = \infty$, $I_1, I_2 =$ integer corresponds to two ''different'' solutions, and to two ''physical solutions.'' But, there is only one eigenstate corresponding to the point. We interpret this as follows. The ''values'' x_1 and x_2 are not the ''same value,'' and one of the ''physical solutions'' is given by exchanging the ''values'' x_1, x_2 of the other ''physical solution.''

We consider an integral, that is the first term in (2.6),

$$\sum_{m_1,m_2=-\infty}^{\infty} \int\int \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2+1} + 2\pi i(m_1 I_1 + m_2 I_2) \right) \mathrm{d}I_1 \, \mathrm{d}I_2 \tag{2.8}$$

along the integral path

$$\left| \left(\frac{x_1 - i}{x_1 + i} \right)^L \left(\frac{x_1 - x_2 + 2i}{x_1 - x_2 - 2i} \right) \right| = A_1 \quad \text{and} \ (1 \leftrightarrow 2), \tag{2.9}$$

where A_1 and A_2 are constants. The integral (2.8) does not depend on $A_{1,2}$ in case $0 < A_{1,2} < \infty$. The reason is that the integrand on the path is bounded, and the dimension of the nonanalytic region, i.e., $x_1, x_2 = \pm i$ or ∞, on the Riemann surface $\{e^{2\pi i I_1}, e^{2\pi i I_2}\}$ is sufficiently small. It is to be noted that we define the orientation of the path so that an integral $\int\int \mathrm{d}I_1 \, \mathrm{d}I_2$ for any part of the path is positive.

Using the above fact, we can change the integral path of the multiple integral (2.8) into the path (2.9). Defining $A_{1,2}$ as a set of sufficiently small real numbers, we have

$$\begin{aligned} (2.8) = \sum_{m_1,m_2=-\infty}^{\infty} & \int_{|x_2 - i| = 0+} \int_{|x_1 - i| = 0+} \left| \frac{\partial(I_1, I_2)}{\partial(x_1, x_2)} \right| \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2+1} \right) \\ & \times \left(\frac{x_1 - i}{x_1 + i} \right)^{m_1 L} \left(\frac{x_2 - i}{x_2 + i} \right)^{m_2 L} \left(\frac{x_1 - x_2 + 2i}{x_1 - x_2 - 2i} \right)^{m_1 - m_2} \mathrm{d}x_1 \, \mathrm{d}x_2, \end{aligned} \tag{2.10}$$

where $|x_{1,2} - i| = 0+$ indicates the integral path that $x_{1,2}$ turns around a point i anticlockwise. The Jacobian from (I_1, I_2) to (x_1, x_2) is denoted by $|\partial(I_1, I_2)/\partial(x_1, x_2)|$. This expression (2.10) enables us to evaluate the upper bound for the absolute value of the sum without the term corresponding to $m_1, m_2 = 0$. The upper bound is estimated as Ce^{-cL} where C and c do not depend on L. Then, in the thermodynamic limit the terms corresponding to $m_1 \neq 0$ or $m_2 \neq 0$ can be neglected. Hereafter, we drop these terms.

We change the integral path from $|x_\sigma - i| = 0+$ into $(-\infty, \infty)$. From (2.10), we have

$$\begin{aligned} (2.8) = & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left| \frac{\partial(I_1, I_2)}{\partial(x_1, x_2)} \right| \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2+1} \right) \mathrm{d}x_1 \, \mathrm{d}x_2 + \int_{-\infty}^{\infty} \left(\frac{8L}{(x+i)^2+4} \right) \\ & \times \exp\left(-\beta \frac{4}{(x+i)^2+4} \right) \frac{\mathrm{d}x}{2\pi}. \end{aligned} \tag{2.11}$$

The second term in the above represents a residue which the modification of the integral path generates.

We shift the integral path of the variables x in (2.11) from $(-\infty, \infty)$ to $(-\infty - i, \infty - i)$, and rewrite variables x into $x - i$,

$$(2.8) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left| \frac{\partial(I_1, I_2)}{\partial(x_1, x_2)} \right| \exp\left(-\beta \sum_{m=1}^{2} \frac{2}{x_m^2+1} \right) \mathrm{d}x_1 \, \mathrm{d}x_2 + \int_{-\infty}^{\infty} \left(\frac{8L}{x^2+4} \right) \exp\left(-\beta \frac{4}{x^2+4} \right) \frac{\mathrm{d}x}{2\pi}. \tag{2.12}$$

We purposely write this obvious modification in order to compare this procedure with that in case $M \geqslant 3$.

Using the expression (2.12) in (2.6) and substituting the Jacobian explicitly, we obtain

$$2Z_2 e^{-\beta h 2} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\frac{\partial(I_1,I_2)}{\partial(x_1,x_2)}\right|\exp\left(-\beta\sum_{m=1}^{2}\frac{2}{x_m^2+1}\right)dx_1\,dx_2+\int_{-\infty}^{\infty}\left(\frac{8L}{x^2+4}\right)\exp\left(-\beta\frac{4}{x^2+4}\right)\frac{dx}{2\pi}$$
$$-\int_{-\infty}^{\infty}\left(\frac{2L}{x^2+1}\right)\exp\left(-\beta\frac{4}{x^2+1}\right)\frac{dx}{2\pi}.$$

$$=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{2L}{x_1^2+1}\,\frac{2L}{x_2^2+1}\exp\left(-\beta\sum_{m=1}^{2}\frac{2}{x_m^2+1}\right)dx_1\,dx_2+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{2L}{x_1^2+1}\right.$$
$$\left.+\frac{2L}{x_2^2+1}\right)\frac{-4L}{(x_1^2-x_2^2)+4}\exp\left(-\beta\sum_{m=1}^{2}\frac{2}{x_m^2+1}\right)dx_1\,dx_2+2\int_{-\infty}^{\infty}\left(\frac{4L}{x^2+4}\right)$$
$$\times\exp\left(-\beta\frac{4}{x^2+4}\right)\frac{dx}{2\pi}-\frac{1}{2}\int_{-\infty}^{\infty}\left(\frac{4L}{x^2+1}\right)\exp\left(-\beta\frac{4}{x^2+1}\right)\frac{dx}{2\pi}. \tag{2.13}$$

This formula corresponds to (1.3) for $M=2$. A remark is in order: Because of the same reason as we neglect the terms corresponding to $m_1 \neq 0$ or $m_2 \neq 0$, we drop the terms corresponding to $m \neq 0$ in the second term of (2.6) by taking the thermodynamic limit.

III. DERIVATION OF Z_M FROM BETHE EQUATIONS

In order to explain our analysis of (1.2) for arbitrary M case, we need several symbols and notations. Definitions of symbols are placed before we first use them. To make clear the extension from $M=2$, we refer to the corresponding expression by writing, for instance, cf. (2.8).

With the eigenenergies E (1.4), Z_M is written as

$$M!Z_M e^{-\beta h M} = \sum \exp\left(-\beta\sum_{m=1}^{M}\frac{2}{x_m^2+1}\right) \tag{3.1}$$

[cf. (2.1)]. Here, Σ without subscript means a summation over all the different physical solutions of the Bethe equations (1.5). It is interpreted as a summation with respect to a set of integers $\{I_m\}$ corresponding to a physical solution, where $\{I_m\}$ is related to $\{x_m\}$ by

$$\left[\frac{x_m+i}{x_m-i}\right]^L = e^{-2\pi i I_m}\prod_{m'\neq m}\left[\frac{x_m-x_{m'}+2i}{x_m-x_{m'}-2i}\right] \tag{3.2}$$

[cf. (2.2)]. We call that a solution of the Bethe equation is a physical solution if and only if any two pseudomomenta x_m of the solution do not take same value. The words different, and same value are defined in the same way as in $M=2$ case.

Definition $\Theta(\sigma)$*:* Let σ be a set which has a finite number of elements. $\Theta(\sigma)$ denotes all the patterns of division of a set σ. A pattern of division θ is a set with elements each of which is a cluster. The cluster σ' is one of the pieces into which a set σ is divided, and the cluster is also regarded as a set

$$\Theta(\sigma)=\left\{\ \theta\ \middle|\ \sigma=\bigoplus_{\sigma'\in\theta}\sigma'\ \right\}. \tag{3.3}$$

In case of $\sigma=\{1,2,\ldots,n\}$, we write Θ_n for $\Theta(\{1,2,\ldots,n\})$ for simplicity.

Definition N_σ*:* Let σ be a set or a sequence which has a finite number of elements. The number of elements of a set or a sequence σ is denoted by N_σ.

By use of the above symbols, (3.1) can be rewritten as

$$M!Z_M e^{-\beta hM} = \sum_{\theta \in \Theta_M} \mu(\hat{0}_M, \theta) \sum_{\{I_\sigma\}} e^{-\beta E_\theta} \tag{3.4}$$

[cf. (2.3)], where $\mu(\hat{0}_M, \theta)$ and E_θ are, respectively, defined as

$$\mu(\hat{0}_M, \theta) \equiv \prod_{\sigma \in \theta} (-)^{N_\sigma - 1}(N_\sigma - 1)!, \tag{3.5}$$

$$E_\theta \equiv \sum_{\sigma \in \theta} \frac{2N_\sigma}{x_\sigma^2 + 1}, \quad \theta \in \Theta_M. \tag{3.6}$$

In (3.4), $\Sigma_{\{I_\sigma\}}$ means a summation over all the solutions of equations

$$\left[\frac{x_\sigma + i}{x_\sigma - i}\right]^L = e^{-2\pi i I_\sigma} \prod_{\sigma' \in \theta, \neq \sigma} \left[\frac{x_\sigma - x_{\sigma'} + 2i}{x_\sigma - x_{\sigma'} - 2i}\right]^{N_{\sigma'}}, \quad \sigma \in \theta. \tag{3.7}$$

We note that Eqs. (3.7) are Eqs. (3.2) with the restrictions

$$x_m = x_\sigma, \quad I_m = I_\sigma, \quad m \in \sigma. \tag{3.8}$$

In other words, (3.7) for θ which satisfies $N_\theta = M$ is equivalent to (3.2). Then, the difference between (3.1) and the term corresponding to the θ in (3.4) is the sum over nonphysical states with respect to (3.2). And, extinction of nonphysical states from the sum is realized by the coefficients $\Sigma_{\theta \in \Theta_M} \mu(\hat{0}_M, \theta)$. The function $\mu(\hat{0}_M, \theta)$ is a special case of the Möbius function $\mu(\theta', \theta)$ which comes from a natural definition of partial order among elements in Θ_M. In this way, the equivalence of (3.1) and (3.4) can be regarded as the Möbius inversion formula.[11,12]

The sum in (3.4) is replaced by integrals

$$M!Z_M e^{-\beta hM} = \sum_{\theta \in \Theta_M} \mu(\hat{0}_M, \theta) \int e^{-\beta E_\theta} \prod_{\sigma \in \theta} \mathrm{d}I_\sigma \tag{3.9}$$

[cf. (2.6)]. Here, we have applied the Poisson formula, and neglected higher order terms of the form e^{-cL} which do not contribute to Z_M in the thermodynamic limit. It is important to pay attention to the integral paths. We define the path of the multiple integral in (3.9) depending on θ. The integral path is a manifold on which $\{I_\sigma\}$ is a set of real numbers and $\{x_\sigma\}$ are continuously distributed. Concretely, the integral path for θ is an N_θ-dimensional surface defined by conditions,

$$\left| \left(\frac{x_\sigma - i}{x_\sigma + i}\right)^L \prod_{\sigma' \in \theta, \neq \sigma} \left(\frac{x_\sigma - x_{\sigma'} + 2i}{x_\sigma - x_{\sigma'} - 2i}\right)^{N_{\sigma'}} \right| = 1. \tag{3.10}$$

The orientation of the integral path is chosen so that the value of an integral $\int \Pi \mathrm{d}I_\sigma$ for any part of the integral path is positive.

We introduce integrals

$$\int e^{-\beta E_\theta} \prod_{\sigma \in \theta} \mathrm{d}I_\sigma, \tag{3.11}$$

along the integral path

$$\left|\left(\frac{x_\sigma - i}{x_\sigma + i}\right)^L \prod_{\sigma' \in \theta, \neq \sigma} \left(\frac{x_\sigma - x_{\sigma'} + 2i}{x_\sigma - x_{\sigma'} - 2i}\right)^{N_{\sigma'}}\right| = A_\sigma, \quad \sigma \in \theta \tag{3.12}$$

[cf. (2.8) and (2.9)]. The relation between x_σ and I_σ is defined by (3.7) and E_θ is defined by (3.6). The integrals (3.11) do not depend on A_σ in case $0 < A_\sigma < \infty$ due to the same reason as in the case $M = 2$. Note again that we define the orientation of the path so that an integral $\int \Pi \mathrm{d}I_\sigma$ for any part of the path is positive.

Therefore, we can change the integral path (3.10) in the multiple integral (3.9) into the path (3.12). By defining A_σ as a set of sufficiently small real numbers, we can rewrite (3.9) as

$$(3.9) = \sum_{\theta \in \Theta_M} \mu(\hat{0}_M, \theta) \left[\prod_{\sigma \in \theta} \int_{|x_\sigma - i| = 0+} \mathrm{d}x_\sigma\right] \left|\frac{\partial I_\sigma}{\partial x_\sigma}\right|_{L,\theta} e^{-\beta E_\theta} \tag{3.13}$$

[cf. (2.10)], where $|x_\sigma - i| = 0+$ indicates the integral path that x_σ turns around a point i anticlockwise. To be precise, there remain other integral paths in the limit $A_\sigma \to 0$, but all the integrals for these paths cancel out each other.

Definition $\Lambda(\theta)$: Let θ be a set with a finite number of elements. We denote by $\Lambda(\theta)$ all the patterns of connection of the set θ. What we call a pattern of connection satisfies the following two conditions. (1) Any two elements of θ are connected or not. Simply, there is no multiple connection. (2) There is no closed path in the connections. Then, a pattern of connection λ is a set of elements each of which corresponds to a connection η. To summarize, $\Lambda(\theta)$ satisfies conditions,

$$\text{if} \quad \eta \in \lambda \in \Lambda(\theta), \quad \text{then} \quad \eta = \{\sigma, \sigma'\}, \quad \sigma, \sigma' \in \theta,$$

$$\text{if} \quad \{\sigma_1, \sigma_2\}, \{\sigma_2, \sigma_3\}, \ldots, \{\sigma_{m-1}, \sigma_m\} \in \lambda \in \Lambda(\theta), \quad \text{then} \quad \{\sigma_1, \sigma_m\} \notin \lambda, \tag{3.14}$$

and has the most elements of all sets which satisfy the above conditions.

Definition $G_\theta(\lambda)$: Let θ be a set with a finite number of elements, and $\lambda \in \Lambda(\theta)$. $G_\theta(\lambda)$ is an element of $\Theta(\theta)$. In other words, $G_\theta(\lambda)$ is a pattern of division of θ. We call that σ and σ' in θ are indirectly connected by λ when σ is linked to σ' through one or some connections in λ. Two elements in θ are indirectly connected by λ if and only if there is a cluster $\theta' \in G_\theta(\lambda)$ containing the two elements. Precisely, $G_\theta(\lambda)$ satisfies the conditions,

$$G_\theta(\lambda) \in \quad \Theta(\theta)$$

$$\text{if} \quad \{\sigma, \sigma'\} \in \lambda, \quad \text{then} \quad \sigma, \sigma' \in \theta' \in G_\theta(\lambda), \tag{3.15}$$

and has the most elements of all sets which satisfy the conditions.

Definition $\tilde{\Theta}(\theta)$: Let θ be a set with a finite number of elements. A set $\tilde{\Theta}(\theta)$ consists of all elements $\tilde{\zeta}$ satisfying the following conditions. First, $\tilde{\zeta}$ is a set of sequences as elements. Second, all the elements in the sequences are in θ. Third, a set of sets ζ derived from $\tilde{\zeta}$ is in $\Theta(\theta)$. Here, ζ is derived from $\tilde{\zeta}$ when we replace sequences in $\tilde{\zeta}$ with sets by ignoring the order of the sequences. Note that the number of $\tilde{\zeta}$'s which become a ζ by the above procedure is $\Pi_{\theta' \in \zeta} N_{\theta'}!$.

Using these symbols, we can change the integral path in (3.13) from $|x_\sigma - i| = 0+$ into $[-\infty + i \min(\sigma_1)\delta, \infty + i \min(\sigma_1)\delta]$;

$$
\begin{aligned}
(3.9)=&\sum_{\theta\in\Theta_M}\sum_{\tilde{\zeta}\in\tilde{\Theta}(\theta)}\sum_{\lambda\in\Lambda(\tilde{\zeta})}\left[\prod_{(\sigma_1,\sigma_2,\ldots)=\tilde{\theta}\in\tilde{\zeta}}\int_{-\infty+i\min(\sigma_1)\delta}^{+\infty+i\min(\sigma_1)\delta}\frac{dx_{\tilde{\theta}}}{2\pi}\right]\\
&\times\left[\prod_{\tilde{\zeta}'\in G_{\tilde{\zeta}}(\lambda)}\left(\sum_{\tilde{\theta}\in\tilde{\zeta}'}\sum_{\sigma_m\in\tilde{\theta}=(\sigma_1,\ldots)}\frac{2N_{\sigma_m}L}{(x_{\tilde{\theta}}+2(m-1)i)^2+1}\right)\right]\\
&\times\left[\prod_{\{\tilde{\theta},\tilde{\theta}'\}\in\lambda}\left(\sum_{\sigma_m\in\tilde{\theta}=(\sigma_1,\ldots)}\sum_{\sigma'_{m'}\in\tilde{\theta}'=(\sigma'_1,\ldots)}\frac{-4N_{\sigma_m}N_{\sigma'_{m'}}}{(x_{\tilde{\theta}}-x_{\tilde{\theta}'}+2(m-m')i)^2+4}\right)\right]\\
&\times\exp\left(-\beta\sum_{\tilde{\theta}\in\tilde{\zeta}}\sum_{\sigma_m\in\tilde{\theta}=(\sigma_1,\ldots)}\frac{2N_{\sigma_m}}{(x_{\tilde{\theta}}+2(m-1)i)^2+1}\right)\\
&\times\prod_{(\sigma_1,\ldots)=\tilde{\theta}\in\tilde{\zeta}}\left[(-)^{N_{\sigma_1}-1}(N_{\sigma_1}-1)!N_{\sigma_1}^{-1}\prod_{\sigma_{m>1}\in\tilde{\theta}}\right.\\
&\left.\times\left[\sum_{\theta'\in\Theta(\sigma_m)}N_{\sigma_{m-1}}^{N_{\theta'}}\prod_{\sigma'\in\theta'}(-)^{N_{\sigma'}-1}(N_{\sigma'}-1)!\right]\right]
\end{aligned}
\tag{3.16}
$$

[cf. (2.11)], where $\min(\sigma_1)$ means the smallest integer in the set σ_1. In (3.16), we have substituted an explicit expression of the Jacobian,

$$
(2\pi)^{N_\theta}\left|\frac{\partial I_\sigma}{\partial x'_\sigma}\right|_{L,\theta}\equiv\left[\prod_{\sigma\in\theta}N_\sigma\right]^{-1}\sum_{\lambda\in\Lambda(\theta)}\left[\prod_{\{\sigma,\sigma'\}\in\lambda}-\frac{4N_\sigma N_{\sigma'}}{(x_\sigma-x_{\sigma'})^2+4}\right]\prod_{\theta'\in G_\theta(\lambda)}\left[\sum_{\sigma\in\theta'}\frac{2N_\sigma L}{x_\sigma^2+1}\right].
\tag{3.17}
$$

A remark is in order. In (3.16), the series $\Sigma_{\tilde{\zeta}\ldots}$ with respect to $\tilde{\zeta}$ can be divided into two parts. One is a set in which all elements have only one element, and the other contains the rest. The former is a set of terms corresponding to (3.13) with an integral path $(-\infty,\infty)$. The latter is a set of terms corresponding to residues which the modification of the integral path generates.

Definition $\bar{\Theta}(\theta)$*:* Let θ be a set which has a finite number of sets as elements. $\bar{\Theta}(\theta)$ consists of all elements ζ satisfying the following two conditions. First, ζ is in $\Theta(\theta)$. Second, any set θ' in ζ satisfies the condition that all sets as elements in the set θ' have the same number of elements. Then,

$$
\bar{\Theta}(\theta)=\{\zeta\in\Theta(\zeta)|N_\sigma=N_{\sigma'},\quad \sigma,\sigma'\in\theta'\in\zeta\}.
\tag{3.18}
$$

We transform the integral path of a variable $x_{\tilde{\theta}}$ in (3.16) from $[-\infty+i\min(\sigma_1)\delta,+\infty+i\min(\sigma_1)\delta]$ to $[-\infty-(N_{\tilde{\theta}}-1)i,+\infty-(N_{\tilde{\theta}}-1)i]$, and change variables $x_{\tilde{\theta}}$ into $x_{\tilde{\theta}}-(N_{\tilde{\theta}}-1)i$. Then, we obtain

$$
M!Z_M e^{-hM}=\sum_{\theta\in\Theta_M}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\mu(\hat{0}_\theta,\zeta)\left[\prod_{\theta'\in\zeta}\int_{-\infty}^{\infty}dx_{\theta'}\right]\left|\frac{\partial I}{\partial x}\right|_{L,\zeta}e^{-\beta E(\zeta)}
\tag{3.19}
$$

[cf. (2.12)] and then [cf. (2.13)] where

$$
\mu(\hat{0}_\theta,\zeta)\equiv\prod_{\theta'\in\zeta}(-)^{N_{\theta'}-1}(N_{\theta'}-1)!,
\tag{3.20}
$$

$$
E(\zeta)\equiv\sum_{\theta'\in\zeta}\frac{2N_{\theta'}M_{\theta'}}{x_{\theta'}^2+M_{\theta'}^2},
\tag{3.21}
$$

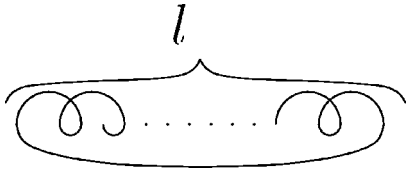

FIG. 1. l-toron.

$$(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{L,\zeta} \equiv \left[\prod_{\theta'\in\zeta} N_{\theta'}^{-1}\right]\sum_{\lambda\in\Lambda(\zeta)}\left[\prod_{\zeta'\in G_\zeta(\lambda)}\left(\sum_{\theta'\in\zeta'}\frac{2N_{\theta'}M_{\theta'}L}{x_{\theta'}^2+M_{\theta'}^2}\right)\right] \times\left[\prod_{\{\theta',\theta''\}\in\lambda}(-N_{\theta'}N_{\theta''})K_{M_{\theta'},M_{\theta''}}(x_{\theta'}-x_{\theta''})\right], \tag{3.22}$$

with

$$K_{n,m}(x)\equiv\begin{cases}\kappa_{|n-m|}(x)+2\kappa_{|n-m|+2}(x)+\cdots+2\kappa_{n+m-2}(x)+\kappa_{n+m}(x), & n\neq m,\\ 2\kappa_2(x)+\cdots+2\kappa_{2n-2}(x)+\kappa_{2n}(x), & n=m,\end{cases} \tag{3.23}$$

and

$$\kappa_n(x)\equiv\frac{2n}{x^2+n^2}. \tag{3.24}$$

Contrary to the $M=2$ case, this modification of the integral paths is not trivial in general M case, because many residues are generated by the modification. In this way, we have shown the equivalence of (3.9) and (3.19), and therefore have proved (1.3). This completes the main purpose of this paper. We remark that (3.19) is the expression which we suppose Z_M to be in the previous paper.[9]

IV. GRAPH REPRESENTATION

We further develop a graphical representation of Z_M. We call an l times rolled coil an *l-toron* (Fig. 1), and call an m times repeated l-toron an l^m-toron (Fig. 2). Therefore, l^1-toron is simply an l-toron. The terminology ''toron'' has been introduced in the theory of quantum cluster expansions.[13,14] We call a connection of two torons a *branch*. The *tree* consists of a toron or torons connected by branches. The *forest* consists of the trees. We denote by $\mathcal{W}_M$ a set of all the forests which satisfy the condition that M is the sum of the number of rolls multiplied by the number of repetitions for torons. Figure 3 illustrates all the elements in $\mathcal{W}_2$. Remark that there are four types of forest in $\mathcal{W}_2$. It turns out that each forest in $\mathcal{W}_2$ corresponds to a term in (2.13).

In terms of these terminologies, we may rewrite (3.19) as

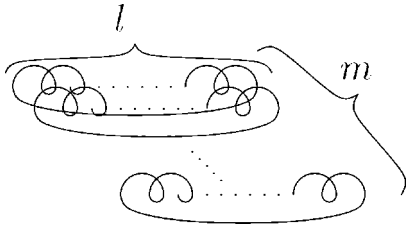

FIG. 2. l^m-toron.

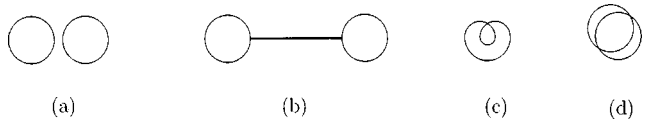

FIG. 3. A set of the forests, $\mathcal{W}_2$. (a) Two trees each of which consists of a 1-toron. (b) A tree where two 1-torons are connected by a branch. (c) A 2-toron, (d) 1^2-toron.

$$Z_M e^{-\beta h M} = \sum_{f \in \mathcal{W}_M} \frac{\mathrm{Sym}(f)}{M!} \prod_{t \text{ in the forest } f} \mathcal{S}(t). \tag{4.1}$$

Here, $\mathrm{Sym}(f)$ indicates a symmetrical factor of the forest. That is, $\mathrm{Sym}(f)$ means the number of different ways in which a set $\{1,\ldots,M\}$ can be distributed to all the torons of f at a time, on the condition that ml elements are placed in an l^m-toron. For example,

$$\mathrm{Sym}(\circ) = 1, \quad \mathrm{Sym}(\circ\!-\!\circ) = 1, \quad \mathrm{Sym}(\text{⊙}) = 1, \quad \mathrm{Sym}(\text{◎}) = 1. \tag{4.2}$$

From (3.19), we can show that $\mathcal{S}(t)$ in (4.1) is given as follows:

$$\mathcal{S}(t) \equiv \left(\prod_{\omega} (M_\omega N_\omega)! (-1)^{N_\omega - 1} N_\omega^{n(\omega,t)-2} \right) \int \prod_{\omega} \frac{dx_\omega}{2\pi} L \left(\sum_{\omega} \frac{2N_\omega M_\omega}{x_\omega^2 + M_\omega^2} \right) \left(\prod_{b \in \Xi(t)} - K_{M_{\omega_\alpha(b)}, M_{\omega_\beta(b)}} (x_{\omega_\alpha(b)} - x_{\omega_\beta(b)}) \right) e^{-\beta(\Sigma_\omega [2N_\omega M_\omega / (x_\omega^2 + M_\omega^2)])}. \tag{4.3}$$

We explain notations in (4.3): M_ω denotes the number of repetitions for toron ω, N_ω the number of rolls for toron ω, and $\Xi(t)$ a set of all the branches contained in a tree t. $n(\omega,t)$ is the number of branches with which the toron ω is connected in the tree t. $\omega_\alpha(b)$ and $\omega_\beta(b)$ denote two end-torons connected by a branch b. And Σ_ω (or Π_ω) indicates a sum (or a product) with respect to all the torons ω in the tree t. For example,

$$\text{(a)} \quad [\mathcal{S}(\text{●})]^2 = \left[((1\times 1)!(-1)^0 1^{-2}) \times \int \frac{dx_\omega}{2\pi} L \times \frac{2}{x_\omega^2 + 1} \times e^{-\beta[2/(x_\omega^2+1)]} \right]^2, \tag{4.4}$$

$$\text{(b)} \quad \mathcal{S}(\circ\!-\!\circ) = ((1\times 1)!(-1)^0 1^{-1} \times (1\times 1)!(-1)^0 1^{-1}) \times \int \frac{dx_{\omega_1}}{2\pi} \frac{dx_{\omega_2}}{2\pi} L \times \left(\frac{2}{x_{\omega_1}^2 + 1} + \frac{2}{x_{\omega_2}^2 + 1} \right) \times (-K_{11}(x_{\omega_1} - x_{\omega_2})) e^{-\beta([2/(x_{\omega_1}^2+1)] + [2/(x_{\omega_2}^2+1)])}, \tag{4.5}$$

$$\text{(c)} \quad \mathcal{S}(\text{⊙}) = ((1\times 2)!(-1)^1 2^{-2}) \times \int \frac{dx_\omega}{2\pi} L \times \frac{4}{x_{\omega_1}^2 + 1} \times e^{-\beta([4/(x_{\omega_1}^2+1)])}, \tag{4.6}$$

$$\text{(d)} \quad \mathcal{S}(\text{◎}) = ((2\times 1)!(-1)^0 1^{-2}) \times \int \frac{dx_\omega}{2\pi} L \times \frac{4}{x_{\omega_1}^2 + 4} \times e^{-\beta([4/(x_{\omega_1}^2+4)])}. \tag{4.7}$$

Substitution of (4.2) and the above expressions into (4.1) gives Eq. (2.13).

As examples, we list graphical representations of $Z_1 \sim Z_4$,

$$Z_1 e^{-\beta h} = \bigcirc, \tag{4.8}$$

$$Z_2 e^{-\beta h 2} = \tfrac{1}{2}\bigcirc\bigcirc + \tfrac{1}{2}\bigcirc\!\!-\!\!\bigcirc - \tfrac{1}{4}\,\textcircled{\scriptsize 0} + \textcircled{\scriptsize 0}, \tag{4.9}$$

$$Z_3 e^{-\beta h 3} = \tfrac{1}{6}\,\bigcirc\bigcirc\bigcirc + \tfrac{1}{2}\,\bigcirc\!\!-\!\!\bigcirc\bigcirc - \tfrac{1}{4}\,\textcircled{\scriptsize 0}\bigcirc + \textcircled{\scriptsize 0}\textcircled{\scriptsize 0} + \tfrac{1}{2}$$
$$- \tfrac{1}{2}\,\textcircled{\scriptsize 0}\!\!-\!\!\bigcirc + \textcircled{\scriptsize 0}\!\!-\!\!\bigcirc + \tfrac{1}{9}\,\textcircled{\scriptsize 00} + \textcircled{\scriptsize 0}\textcircled{\scriptsize 0}\ . \tag{4.10}$$

The coefficients of trees are $\mathrm{Sym}(f)/M!$ multiplied by the coefficients of $\mathcal{S}(t)$, i.e.,

$$\left(\prod_{\omega} (M_\omega N_\omega)! (-1)^{N_\omega - 1} N_\omega^{n(\omega,t)-2} \right). \tag{4.11}$$

V. A RELATION BETWEEN Z_M AND THE STRING HYPOTHESIS

The function (3.22) is the Jacobian between $\{x_\theta\}$ and $\{I_\theta\}$ defined by the relations,

$$\left[\frac{x_{\theta'} + M_{\theta'} i}{x_{\theta'} - M_{\theta'} i} \right]^L = e^{-2\pi i I_{\theta'}} \prod_{\theta'' \in \zeta, \neq \theta'} E_{M_{\theta'}, M_{\theta''}}(x_{\theta'} - x_{\theta''})^{N_{\theta''}}, \tag{5.1}$$

where $\theta \in \Theta_M$, $\zeta \in \overline{\Theta}(\theta)$, and

$$E_{n,m}(x) \equiv \frac{[x-(n+m)i][x-|n-m|i]}{[x+(n+m)i][x+|n-m|i]} \prod_{k=1}^{\min(n,m)} \left[\frac{x+(n+m-2k)i}{x-(n+m-2k)i} \right]^2. \tag{5.2}$$

We emphasize the following: We regard the variable I_θ as an integer and interpret the value $x_{\theta'}$ as an $M_{\theta'}$-string center. The relations (5.1) are indeed the equations which are introduced by the string hypothesis on condition that all $N_{\theta' \in \zeta} = 1$. And, each term of (3.21) is the energy corresponding to an $M_{\theta'}$-string in the string hypothesis.

Now, we study Eq. (3.19) again. As we have shown in the previous paper,[9] the expression (3.19) can be derived by summing up the string center equation formally. The derivation is summarized as follows. From the string hypothesis, we have

$$M! Z_M e^{-hM} = \sum_{\theta \in \Theta_M} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \overline{\Theta}(\theta)} \mu(\hat{0}_\theta, \zeta) \sum_{\{I_\theta\}} e^{-\beta E(\zeta)}, \tag{5.3}$$

where $\Sigma_{\{I_\theta\}}$ means a summation over all the real number solutions of (5.1) on condition that $\{I_\theta\}$ are integers. Note that the coefficients are derived from the symmetry of the quasiparticles. We can derive

$$\begin{aligned} M! Z_M e^{-hM} &= \sum_{\theta \in \Theta_M} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \overline{\Theta}(\theta)} \mu(\hat{0}_\theta, \zeta) \left[\prod_{\theta' \in \zeta} \int \mathrm{d}I_{\theta'} \right] e^{-\beta E(\zeta)} \\ &= \sum_{\theta \in \Theta_M} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \overline{\Theta}(\theta)} \mu(\hat{0}_\theta, \zeta) \left[\prod_{\theta' \in \zeta} \int_{-\infty}^{\infty} \mathrm{d}x_{\theta'} \right] \left| \frac{\partial I}{\partial x} \right| e^{-\beta E(\zeta)}, \end{aligned} \tag{5.4}$$

from (5.3) by formally using the formula (2.5), and neglecting the terms which correspond to $m \neq 0$ in the formula (2.5) in the thermodynamic limit, i.e., replacing the sum $\Sigma_{\{I_\theta\}}$ into the integral $\Pi_{\theta' \in \zeta} \int \mathrm{d}I_{\theta'}$. We usually do such a replacement in the thermodynamic limit: e.g., in case of the free Fermion, we use the relation

$$\sum_k \log(1+e^{-\beta k^2}) = L \int \frac{\mathrm{d}k}{2\pi} \log(1+e^{-\beta k^2}). \tag{5.5}$$

The relation (5.4) is obviously equivalent to (3.19). But, there remains a problem with this derivation of (5.4) from the string hypothesis. When we use the Poisson formula (2.5), the orientation of the integral path on the right-hand side of (2.5) should have the following property: the value of an integral $\int \Pi \mathrm{d}I$ for any part of the integral path is positive. Recall that we have defined the orientation of the integral path (3.9) by this condition. The integral path in (5.4), however, does not have this property since the Jacobian $|\partial I/\partial x|$ is not necessarily positive definite. The value of the integral is $O(L^M)$ and the difference between the right-hand side of (5.4) and the value of the integral using the truly oriented integral path is $O(L^{M-1.5})$, where M is the number of up-spins. The solution of this problem is one of the followings: (1) The difference $O(L^{M-1.5})$ does not have any effect on the free energy. (2) The sum of the terms we have dropped in (5.4) is $O(L^{M-1.5})$, i.e., we must not neglect the terms. Note that such neglect in (3.9) has been proved to be valid. (3) The string hypothesis is not true, and a formal replacement of Σ into $\int \mathrm{d}x$ in the thermal Bethe ansatz cancels the error of the string hypothesis.

Note that in the previous paper,[9] we do not claim that the derivation of (3.19) using the string hypothesis is complete, but claim that (3.19) is related to the string hypothesis and the free energy is properly derived when we assume the relation (3.19). On the contrary, in this paper, we have derived (3.19) step by step only assuming the Bethe ansatz equations.

VI. CONCLUSION

In this paper, we have explicitly calculated $\mathrm{Tr}\, e^{-\beta H_M}$ for the one-dimensional XXX Heisenberg model, which is the trace of the Boltzmann weight under the restriction that the number of up-spin M is fixed. This method relies only on the Bethe ansatz equations. Using this method and the result in Ref. 9, we have obtained the free energy, whose expression perfectly agrees with TBA. In a sense, we have generalized the direct method or the Bethe ansatz cluster expansion method[11,12,15] into models with bound states. We emphasize that this derivation of the free energy is independent of QTM, TBA and is free from the string hypothesis. We can replace the Boltzmann weight with some other functions in case that the Boltzmann weight and the functions have the same analyticity. Therefore, it may be possible to calculate some other thermodynamic quantities $\langle A \rangle$ in the same way by replacing the Boltzmann weight $e^{-\beta H}$ with $Ae^{-\beta H}$. A further application of the method to other integrable models is also one of the future problems.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Symmetry and pattern formation for a planar layer of nematic liquid crystal

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(Received 6 February 2003; accepted 12 May 2003)

Using equivariant bifurcation theory, and on the basis of symmetry considerations independent of the model, we classify square and hexagonally periodic patterns that typically arise when a homeotropic or planar isotropic nematic state becomes unstable, perhaps as a consequence of an applied magnetic or electric field. We relate this to a Landau–de Gennes model for the free energy, and derive dispersion relations in sufficient generality to illustrate the role of up/down symmetry in determining which patterns can arise as a stable bifurcation branch from either initial state. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598620]

I. INTRODUCTION

There is an extensive amount of literature on spatially periodic pattern-formation in physical and biological systems: see for example the surveys by Cross and Hohenberg (1993) and Cladis and Palffy-Muhoray (1995). The mathematical techniques to analyze the creation and interactions of such patterns often involve reduction of the governing partial differential equations to a finite-dimensional system that captures the essential dynamics near a bifurcation point of a fundamental equilibrium state, followed by a bifurcation analysis to classify the branching of multiple solutions.

The crucial role of *symmetry* in organizing pattern-forming bifurcations has been recognized for some time: see Busse (1962); Buzano and Golubitsky (1983); Golubitsky *et al.* (1984), for example. Indeed, on the basis of symmetry considerations alone, and with some natural nondegeneracy assumptions, a classification of branching behavior for systems with symmetry can be given that is independent of the actual mathematical model. This insight, with the associated technical machinery of group theory and group actions, is the inspiration for the texts such as Golubitsky *et al.* (1988); Chossat and Lauterbach (2000); Golubitsky and Stewart (2002). The general theory provides a framework: in order to make specific predictions of physical behavior exerimental numerical values (or sometimes just their signs) need to be determined, unfortunately not necessarily an easy task.

In this paper we generalize methods that have been previously and successfully applied in other fields (Buzano and Golubitsky, 1983; Golubitsky *et al.*, 1984; Golubitsky *et al.*, 1988; Bressloff *et al.*, 2001a; Golubitsky and Stewart, 2002) to the context of pattern formation in planar liquid crystals. A preliminary version of our results appears in Golubitsky and Chillingworth (2003). We consider periodic planar patterns with square or hexagonal symmetry that can bifurcate from a homeotropic or planar isotropic state. We do not claim to predict experimental conditions under which these states can be observed; rather we set out a dictionary of possibilities on the basis of natural mathematical assumptions. Numerous patterns similar to those we describe have indeed been observed in liquid crystal experiments, see, e.g., de Gennes (1974); Huh *et al.* (2000), but under conditions often quite different from ours. The question of how to detect experimentally

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the variety of director-field patterns predicted here is one that we are not yet in a position to answer. However, we do give some pointers on dealing with this issue by calculating key aspects of branching behavior for an explicit Landau–de Gennes type model.

II. THE GENERAL STRATEGY

In the Landau theory of phase transitions for a liquid crystal the degree of coherence of alignment of molecules is usually represented by a *tensor order parameter*, a field of symmetric 3×3 tensors $Q(\mathbf{x})$, $\mathbf{x}\in\mathbf{R}^3$ with $\mathrm{tr}(Q)=0$ (Sluckin, 2000). We think of Q as the second moment of a probability distribution for the directional alignment of a rod-like molecule. In a spatially uniform system, Q is independent of $\mathbf{x}\in\mathbf{R}^3$. When $Q=0$ the system is *isotropic*, with molecules not aligned in any particular direction. If there is a preferred direction along which the molecules tend to lie (but with no positional constraints) the liquid crystal is in *nematic* phase. There are many other types of phase involving local and global structures, see Sluckin (2000).

In this paper we consider a thin planar layer of nematic liquid crystal where the top and bottom boundary conditions on this layer are identical. In this situation the symmetries of any liquid crystal model will include planar Euclidean symmetries $\mathbf{E}(2)$ as well as up/down reflection symmetry.

A configuration or *state* of a liquid crystal is often described by a director field (a unit length vector field) that assigns to each point $\mathbf{x}$ in the planar layer a unit vector $\mathbf{n}(\mathbf{x})$ in the direction in $\mathbf{R}^3$ along which molecules tend to align. In this description $\mathbf{n}(\mathbf{x})$ and $-\mathbf{n}(\mathbf{x})$ are not distinguished. We approximate a planar layer by a plane—so for us a liquid crystal state consists of a three-dimensional director field $\mathbf{n}$ defined on $\mathbf{R}^2$.

In the Landau theory the direction of $\mathbf{n}(\mathbf{x})$ is just an eigenvector corresponding to the largest eigenvalue of $Q(\mathbf{x})$—the direction in which a molecule has the ''maximum probability'' of aligning. We shall refer to $Q(\mathbf{x})$ also as the *state* of the system. If $Q(\mathbf{x})$ has two (or three) equal maximum eigenvalues then $\mathbf{n}(\mathbf{x})$ is undefined (a dislocation occurs), whereas the tensor field $Q(\mathbf{x})$ is everywhere defined, continuous and in our case analytic.

In our discussion we assume an initial equilibrium state Q_0 that is $\mathbf{E}(2)$-invariant. Because of translation symmetry such states are spatially uniform and because of rotation symmetry they have the form

$$Q_0=\eta\begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 2\end{bmatrix}$$

for some nonzero $\eta\in\mathbf{R}$. For $\eta>0$ the state Q_0 represents a *homeotropic* phase (the state has constant alignment in the vertical direction), whereas for $\eta<0$ it represents a planar *isotropic* liquid crystal (a molecule is equally likely to align in any horizontal direction). The state Q_0 is also invariant under up/down reflection, that is conjugacy by the matrix

$$\tau=\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}.$$

We consider models for equilibria that are determined internally by a free energy rather than externally by, say, a magnetic field. Thus, the symmetry group for our discussion is

$$\Gamma=\mathbf{E}(2)\times\mathbf{Z}_2(\tau),$$

since these are the symmetries of both the initial state Q_0 and the model.

Our aim in this paper is to study local bifurcation from Q_0 to states that have spatially varying alignment along the plane. Specifically, we consider bifurcation to states exhibiting spatial peri-

odicity with respect to some planar lattice. Following Golubitsky *et al.* (1988) and Golubitsky and Stewart (2002) we use group representation theory to extract information about nonlinear behavior near bifurcation that is independent of the model.

There is a common approach to all lattice bifurcation problems, which we now describe. This discussion, adapted from Bressloff *et al.* (2001a), will be familiar to anyone who has studied pattern formation in Bénard convection models, although there are minor differences due to the change in context. See Golubitsky *et al.* (1988); Golubitsky and Stewart (2002).

Let λ be a bifurcation parameter and assume that the equations have Q_0 as an equilibrium for all λ. Let L denote the equations linearized about Q_0. In the models, λ is the temperature and bifurcation occurs as λ is decreased.

(1) A linear analysis about Q_0 leads to a *dispersion curve*.

Translation symmetry in a given direction implies that (complex) eigenfunctions have a *plane wave factor* $w_{\mathbf{k}}(\mathbf{x})=e^{2\pi i\mathbf{k}\cdot\mathbf{x}}$ where $\mathbf{k}\in\mathbf{R}^2$. Rotation symmetry implies that the linearized equations have infinite-dimensional eigenspaces; instability occurs simultaneously to all functions $w_{\mathbf{k}}(\mathbf{x})$ with constant $k=|\mathbf{k}|$. The number k is called the *wave number*. Points (k,λ) on the dispersion curve are defined by the maximum values of λ for which an instability of the solution Q_0 to an eigenfunction with wave number k occurs.

(2) Often, the dispersion curve has a unique maximum, that is, there is a *critical* wave number k_* at which the first instability of the homogeneous solution occurs as λ is decreased.

Bifurcation analyses near such points are difficult since the kernel of the linearization is infinite-dimensional. This difficulty can be side-stepped by restricting solutions to the class of possible solutions that are doubly periodic with respect to a planar lattice $\mathcal{L}$.

(3) The symmetries of the bifurcation problem restricted to $\mathcal{L}$ change from Euclidean symmetry in two ways.

First, translations act on the restricted problem modulo $\mathcal{L}$; that is, translations act as a torus $\mathbf{T}^2$. Second, only a finite number of rotations and reflections remain as symmetries. Let the *holohedry* $H_{\mathcal{L}}$ be the group of rotations and reflections that preserve the lattice. The symmetry group $\Gamma_{\mathcal{L}}$ of the lattice problem is then generated by $H_{\mathcal{L}}$, $\mathbf{T}^2$, as well as (in our case) $\mathbf{Z}_2(\tau)$.

(4) The restricted bifurcation problem must be further specialized. First, a *lattice type* needs to be chosen (in this paper square or hexagonal). Second, the *size* of the lattice must be chosen so that a plane wave with critical wave number k_* is an eigenfunction in the space $\mathcal{F}_{\mathcal{L}}$ of matrix functions periodic with respect to $\mathcal{L}$.

Those $\mathbf{k}\in\mathbf{R}^2$ for which the scalar plane wave $e^{2\pi i\mathbf{k}\cdot\mathbf{x}}$ is $\mathcal{L}$-periodic are called *dual wave vectors*. The set of dual wave vectors is a lattice, called the *dual lattice*, and is denoted by $\mathcal{L}^*$. In this paper we consider only those lattice sizes where the critical dual wave vectors are vectors of shortest length in $\mathcal{L}^*$. Therefore, generically, we expect $\ker L=\mathbf{R}^n$ where n is 4 and 6 on the square and hexagonal lattices, respectively.

(5) Since $\ker L$ is finite-dimensional, we can use Liapunov–Schmidt or center manifold reduction to obtain a system of reduced bifurcation equations on $\mathbf{R}^n$ whose zeros are in 1:1 correspondence with the steady states of the original equation. Moreover, this reduction can be performed so that the reduced bifurcation equations are $\Gamma_{\mathcal{L}}$-equivariant.

(6) Solving the reduced bifurcation equations is still difficult. A partial solution can be found as follows. A subgroup $\Sigma\subset\Gamma_{\mathcal{L}}$ is *axial* if $\dim \mathrm{Fix}(\Sigma)=1$ where

$$\mathrm{Fix}(\Sigma)=\{x\in\ker L:\sigma x=x \quad \forall\sigma\in\Sigma\}.$$

The Equivariant Branching Lemma (Golubitsky *et al.*, 1988) states that generically there exists a branch of solutions corresponding to each axial subgroup. These solution types are then classified by finding all axial subgroups, up to conjugacy.

On general grounds, when restricting attention to bifurcations corresponding to shortest wavelength vectors, we may assume the representation (action) of $\Gamma_{\mathcal{L}}$ to be irreducible: see Golubitsky *et al.* (1988); Chossat and Lauterbach (2000). In Sec. III we show that there are four distinct types of irreducible representation of $\Gamma_{\mathcal{L}}$ that can occur in bifurcations from Q_0. These representations

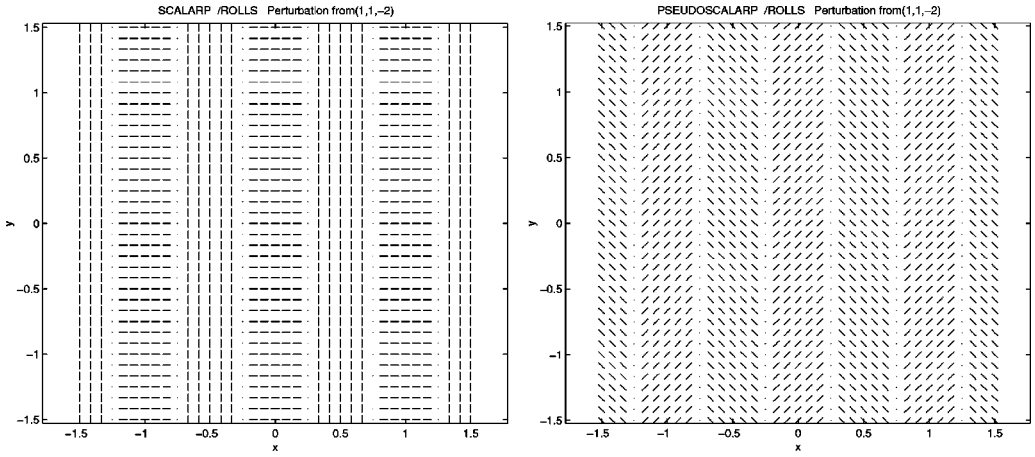

FIG. 1. Stripes from isotropic ($\eta<0$) state with $\tau=+1$ representations: scalar ''martensite'' (left); pseudoscalar ''chevron'' (right). Note that $\cdot$ in the figures indicates points where $Q(\mathbf{x})$ has a double maximum eigenvalue.

are the four combinations of (i) scalar or pseudoscalar (see Bosch Vivancos *et al.*, 1995; Bressloff *et al.*, 2001a; Golubitsky and Stewart, 2002) and (ii) preserve or break τ symmetry. In Sec. III we also compute the axial subgroups for each of these representations and draw pictures of each of the relevant planforms on the square and hexagonal lattices.

Note that line fields near hometropic are almost vertical, whereas line fields near isotropic are almost horizontal. In our figures, where we view the perturbed line fields from above, we see the planar projections of the line field in all cases. We also see the deviation from vertical and, through foreshortening of the line field elements, the deviation from horizontal. However, in this presentation, we cannot distinguish the ''up'' and ''down'' ends of the line field elements. It is an elementary yet curious observation that in Landau models restricted to a planar layer, bifurcations from the homeotropic phase ($\eta>0$) do not lead to clear new patterns unless τ symmetry is broken: the τ symmetry ''freezes'' the director field to the vertical. This point is discussed in more detail in Sec. III. Therefore we present pictures of the four bifurcations from the isotropic case ($\eta<0$) and only the two bifurcations when τ acts as -1 in the homeotropic case ($\eta>0$). The $\tau=+1$ bifurcations in the homeotropic case can lead to patterns in a theory posed on a thickened planar layer. In such a theory, which goes beyond what we present here, the precise form of boundary conditions on the upper and lower boundaries of the layer will determine the pattern types. In the other bifurcations, the contributions to pattern selection of these boundary conditions should be less important.

In fact, the bifurcation theory for each of these four representations of $\Gamma_{\mathcal{L}}$ has been discussed previously in different contexts. It is only the interpretation of eigenfunctions in the context of $Q(\mathbf{x})$ that needs to be computed, along with the pictures of the resulting planforms. More specifically, when τ acts trivially on $\ker \mathsf{L}$ the scalar representation has been used in the study of pattern formation in Rayleigh–Bénard convection by Busse (1962) and Buzano and Golubitsky (1983), and the pseudoscalar representation has been studied by Bosch-Vivancos, Chossat, and Melbourne (1995) and also in the context of geometric visual hallucinations by Bressloff *et al.* (2001b); (2001a). When τ acts nontrivially the two representations have the same matrix generators and although the planforms are different for these two representations the bifurcation theory is identical. Indeed, this theory is just the one studied for Rayleigh–Bénard convection with a midplane reflection by Golubitsky, Swift, and Knobloch (1984).

Perhaps the most interesting patterns that appear from our analysis are the stripes or ''rolls'' (from convection studies) type patterns that bifurcate from the isotropic state when τ symmetry is not broken, that is $\tau=+1$. The scalar pattern is a ''martensite'' pattern whereas the pseudoscalar pattern is a ''chevron'' pattern. See Fig. 1. The fact that such patterns do occur in liquid crystal layers is well known: see, for example, de Gennes (1974), and also Huh *et al.* (2000) from which

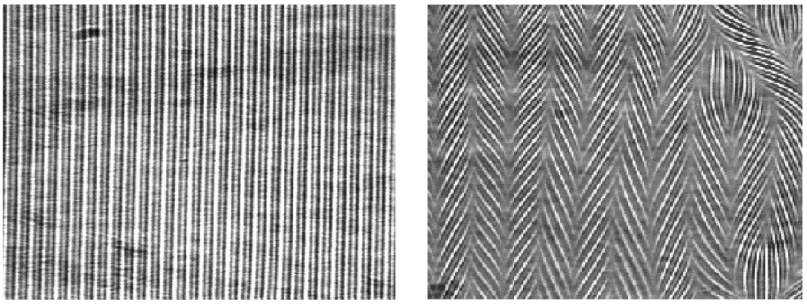

FIG. 2. Rolls (left) and chevrons (right). (Pictures courtesy of J.-H. Huh.)

the pictures in Fig. 2 are taken. However, it is important to emphasize that these patterns were observed under experimental conditions far removed from those to which our theoretical model applies. Moreover, the observed chevrons exhibit additional fine periodic structure (which renders them visible as chevrons and not stripes) that we do not discuss here. We recall that patterns described in this paper are those that can arise close to homeotropic or planar isotropic states.

In Sec. IV we introduce free energies that illustrate that all four representations can be encountered as λ is decreased, although in our model only two of them can be the first bifurcation from homeotropy while only the other two can be the first bifurcation from isotropy. (It is likely that different models will allow other variations.) It then follows from the Equivariant Branching Lemma that each of the axial equilibrium types that we describe in Sec. III is an equilibrium solution to the nonlinear model equations.

III. SPATIALLY PERIODIC EQUILIBRIUM STATES

In this section we list the axial subgroups for each of the four representations of $\Gamma_{\mathcal{L}}$ on the square and hexagonal lattices, and then plot the planforms for the associated bifurcating branches from both the isotropic ($\eta<0$) and homeotropic ($\eta>0$) states. We emphasize that these results depend only on symmetry and can be obtained independently of any particular model. First, we describe the form of the eigenspaces for each of these four representations. Second, we discuss the group actions and the axial subgroups for each of these representations. Finally, we plot the associated direction fields.

A. Linear theory

Let L denote the linearization of the governing system of differential equations at Q_0 [for the free energy model with free energy $\mathcal{F}$ we have $\mathsf{L}=d^2F(Q_0)$]. Bifurcation occurs at parameter values where L has nonzero kernel. We prove that generically, at bifurcation to shortest dual wave vectors, $\ker \mathsf{L}$ has the form given in Theorem 3.1. Let

$$Q^{++}=\begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -a-b \end{bmatrix}, \quad Q^{+-}=\begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix},$$
$$Q^{-+}=\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad Q^{--}=\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & i & 0 \end{bmatrix}. \tag{1}$$

In the double superscript on Q, the first $\pm$ refers to scalar or pseudoscalar representation and the second $\pm$ refers to the action of τ. In Table I we also fix the generators of the lattice and its dual lattice.

TABLE I. Generators for the planar lattices and their dual lattices.

Lattice	ℓ_1	ℓ_2	$\mathbf{k}_1$	$\mathbf{k}_2$	$\mathbf{k}_3=-(\mathbf{k}_1+\mathbf{k}_2)$
Square	(1,0)	(0,1)	(1,0)	(0,1)	—
Hexagonal	$\left(1,\frac{1}{\sqrt{3}}\right)$	$\left(0,\frac{2}{\sqrt{3}}\right)$	(1,0)	$\frac{1}{2}(-1,\sqrt{3})$	$\frac{1}{2}(-1,-\sqrt{3})$

Theorem 3.1: *On the square lattice, let ξ be rotation counterclockwise by $\pi/2$. Then, in each irreducible representation,* $\ker \mathsf{L}$ *is four-dimensional and its elements have the form*

$$z_1 e^{2\pi i \mathbf{k}_1\cdot\mathbf{x}} Q^{\pm\pm} + z_2\, e^{2\pi i \mathbf{k}_2\cdot\mathbf{x}}\, \xi\cdot Q^{\pm\pm} + \text{c.c.} \tag{2}$$

for $z_1, z_2 \in \mathbf{C}$, where $Q^{\pm\pm}$ is the appropriate matrix specified in (1), $\xi\cdot Q$ denotes $\xi Q \xi^{-1}$, and c.c. *denotes complex conjugate.*

On the hexagonal lattice, let ξ be rotation counterclockwise by $\pi/3$. Then, in each irreducible representation, $\ker \mathsf{L}$ *is six-dimensional and its elements have the form*

$$z_1 e^{2\pi i \mathbf{k}_1\cdot\mathbf{x}} Q^{\pm\pm} + z_2\, e^{2\pi i \mathbf{k}_2\cdot\mathbf{x}}\, \xi^2\cdot Q^{\pm\pm} + z_3\, e^{2\pi i \mathbf{k}_3\cdot\mathbf{x}}\, \xi^4\cdot Q^{\pm\pm} + \text{c.c.} \tag{3}$$

for $z_1, z_2, z_3 \in \mathbf{C}$.

Proof: Let V and $V_{\mathbf{C}}$ denote the space of (respectively) real and complex 3×3 symmetric matrices with zero trace. Planar translation symmetry implies that eigenfunctions (nullvectors) of L are linear combinations of matrices that have the plane wave form

$$e^{2\pi i \mathbf{k}\cdot\mathbf{x}} Q + \text{c.c.}, \tag{4}$$

where $Q \in V_{\mathbf{C}}$ is a constant matrix and $\mathbf{k} \in \mathbf{R}^2$ is a wave vector. For fixed $\mathbf{k}$ let

$$W_{\mathbf{k}} = \{e^{2\pi i \mathbf{k}\cdot\mathbf{x}} Q + \text{c.c.} : Q \in V_{\mathbf{C}}\} \tag{5}$$

be the ten-dimensional L-invariant real linear subspace consisting of such functions.

Rotations and reflections $\gamma \in \mathbf{O}(2)\times\mathbf{Z}_2(\tau) \subset \mathbf{O}(3)$ act on $W_{\mathbf{k}}$ by

$$\gamma(e^{2\pi i \mathbf{k}\cdot\mathbf{x}} Q) = e^{2\pi i (\gamma\mathbf{k})\cdot\mathbf{x}}\, \gamma Q \gamma^{-1}. \tag{6}$$

When looking for nullvectors we can assume, after rotation, that $\mathbf{k} = k(1,0)$. We can also rescale length so that the dual wave vectors of shortest length have length 1; that is, we can assume that $k=1$.

Bosch Vivancos, Chossat, and Melbourne (1995) observed that reflection symmetries can further decompose $W_{\mathbf{k}}$ into two L-invariant subspaces. To see why, consider the reflection

$$\kappa(x,y,z) = (x,-y,z).$$

Note that the action (6) of κ on $W_{\mathbf{k}}$ (dropping the $+$c.c.) is

$$\kappa(e^{2\pi i \mathbf{k}\cdot\mathbf{x}} Q) = e^{2\pi i \kappa(\mathbf{k})\cdot\mathbf{x}}\, \kappa Q \kappa^{-1} = e^{2\pi i \mathbf{k}\cdot\mathbf{x}}\, \kappa Q \kappa^{-1}.$$

Since $\kappa^2 = 1$, the subspace $W_{\mathbf{k}}$ itself decomposes as

$$W_{\mathbf{k}} = W_{\mathbf{k}}^{+} \oplus W_{\mathbf{k}}^{-}, \tag{7}$$

where κ acts trivially on $W_{\mathbf{k}}^+$ and as minus the identity on $W_{\mathbf{k}}^-$, and each of $W_{\mathbf{k}}^+$ and $W_{\mathbf{k}}^-$ are L invariant. We call functions in $W_{\mathbf{k}}^+$ *even* and functions in $W_{\mathbf{k}}^-$ *odd*. Bifurcations based on even eigenfunctions are called *scalar* and bifurcations based on odd eigenfunctions are called *pseudoscalar*.

A further simplification in the form of Q can be made. Consider $\rho \in \mathbf{SO}(2) \subset \mathbf{O}(3)$ given by $(x,y,z) \mapsto (-x,-y,z)$. Since (dropping the $+$c.c.)

$$\rho(e^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q) = e^{2\pi i \rho\mathbf{k}\cdot\mathbf{x}}\rho Q\rho^{-1} = e^{-2\pi i \mathbf{k}\cdot\mathbf{x}}\rho Q\rho^{-1} = e^{2\pi i \mathbf{k}\cdot\mathbf{x}}\overline{\rho Q\rho^{-1}}$$

the associated action of ρ on $V_{\mathbf{C}}$ is related to the conjugacy action by

$$\rho(Q) = \overline{\rho Q \rho^{-1}}. \tag{8}$$

Since L commutes with ρ and $\rho^2 = 1$, the subspaces of the kernel of L where $\rho(Q) = Q$ and $\rho(Q) = -Q$ are L-invariant. Therefore, we can assume that Q is in one of these two subspaces. Note moreover that translation by $\frac{1}{4}\mathbf{k}$ implies that if $e^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q$ is an eigenfunction then $ie^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q$ is a (symmetry related) eigenfunction. It follows from (8) that if ρ acts as minus the identity on Q, then ρ acts as the identity on iQ. Thus we can assume without loss of generality that up to translational symmetry Q is ρ-invariant, that is Q has the form

$$Q = \begin{bmatrix} a & g & ic \\ g & b & ih \\ ic & ih & -a-b \end{bmatrix},$$

where $a,b,c,g,h \in \mathbf{R}$. Therefore we have proved

Lemma 3.2: Up to symmetry eigenfunctions in $W_{\mathbf{k}}$ have the form

$$e^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q + \text{c.c.}$$

where Q is nonzero, ρ-invariant, and either even or odd.

Lemma 3.2 implies that typically eigenfunctions in $W_{\mathbf{k}}$ lie in one of the two-dimensional subspaces $V_{\mathbf{k}}^+, V_{\mathbf{k}}^-$ of $W_{\mathbf{k}}^+, W_{\mathbf{k}}^-$ that have the form

$$V_{\mathbf{k}}^+ = \{ze^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q^+ : z \in \mathbf{C}\},$$

$$V_{\mathbf{k}}^- = \{ze^{2\pi i \mathbf{k}\cdot\mathbf{x}}Q^- : z \in \mathbf{C}\},$$

where

$$Q^+ = \begin{bmatrix} a & 0 & ic \\ 0 & b & 0 \\ ic & 0 & -a-b \end{bmatrix} \quad \text{and} \quad Q^- = \begin{bmatrix} 0 & g & 0 \\ g & 0 & hi \\ 0 & hi & 0 \end{bmatrix} \tag{9}$$

with the specific values $a,b,c,g,h \in \mathbf{R}$ being chosen by L (cf. Golubitsky and Stewart, 2002, Sec. 5.7).

Moreover, since L commutes with τ we can further split

$$V_{\mathbf{k}}^+ = V_{\mathbf{k}}^{++} \oplus V_{\mathbf{k}}^{+-} \quad \text{and} \quad V_{\mathbf{k}}^- = V_{\mathbf{k}}^{-+} \oplus V_{\mathbf{k}}^{--}$$

into subspaces on which τ acts trivially and by minus the identity, and each of these subspaces is L-invariant. Since

TABLE II. (Left) $\mathbf{D}_4 \dotplus \mathbf{T}^2$ action on square lattice; (right) $\mathbf{D}_6 \dotplus \mathbf{T}^2$ action on hexagonal lattice. Here $[\theta_1,\theta_2]=\theta_1\ell_1+\theta_2\ell_2$ as in Table I. For scalar representation $\epsilon=+1$; for pseudoscalar representation $\epsilon=-1$.

$\mathbf{D}_4$	Action	$\mathbf{D}_6$	Action
$\mathbf{1}$	(z_1,z_2)	$\mathbf{1}$	(z_1,z_2,z_3)
ξ	(z_2,z_1)	ξ	(z_2,z_3,z_1)
ξ^2	(z_1,z_2)	ξ^2	(z_3,z_1,z_2)
ξ^3	(z_2,z_1)	ξ^3	(z_1,z_2,z_3)
κ	$\epsilon(z_1,z_2)$	ξ^4	(z_2,z_3,z_1)
$\kappa\xi$	$\epsilon(z_2,z_1)$	ξ^5	(z_3,z_1,z_2)
$\kappa\xi^2$	$\epsilon(z_1,z_2)$	κ	$\epsilon(z_1,z_3,z_2)$
$\kappa\xi^3$	$\epsilon(z_2,z_1)$	$\kappa\xi$	$\epsilon(z_2,z_1,z_3)$
		$\kappa\xi^2$	$\epsilon(z_3,z_2,z_1)$
		$\kappa\xi^3$	$\epsilon(z_1,z_3,z_2)$
		$\kappa\xi^4$	$\epsilon(z_2,z_1,z_3)$
		$\kappa\xi^5$	$\epsilon(z_3,z_2,z_1)$
$[\theta_1,\theta_2]$	$(e^{-2\pi i\theta_1}z_1,e^{-2\pi i\theta_2}z_2)$	$[\theta_1,\theta_2]$	$(e^{-2\pi i\theta_1}z_1,e^{-2\pi i\theta_2}z_2,e^{2\pi i(\theta_1+\theta_2)}z_3)$

$$\tau Q\tau=\begin{bmatrix} a & g & -ic \\ g & b & -ih \\ -ic & -ih & -a-b \end{bmatrix}$$

we see that $V_{\mathbf{k}}^{\pm\pm}=\{ze^{2\pi i\mathbf{k}\cdot\mathbf{x}}Q^{\pm\pm}:z\in\mathbf{C}\}$, where the matrices $Q^{\pm\pm}$ are as given in (1).

Finally, note that $\ker \mathsf{L}$ is invariant under the action of ξ. It follows that on the square lattice

$$\ker \mathsf{L}=V_{\mathbf{k}}^{\pm\pm}\oplus\xi(V_{\mathbf{k}}^{\pm\pm})$$

whereas on the hexagonal lattice

$$\ker \mathsf{L}=V_{\mathbf{k}}^{\pm\pm}\oplus\xi^2(V_{\mathbf{k}}^{\pm\pm})\oplus\xi^4(V_{\mathbf{k}}^{\pm\pm})$$

thus verifying (2), (3) and completing the proof of Theorem (3.1). □

B. Axial subgroups

The scalar and pseudoscalar actions of $\mathbf{E}(2)$ on the eigenfunctions on the square and hexagonal lattices are computed in Bressloff *et al.* (2001a). The results are given in Table II in terms of the coefficients z_j in (2) and (3).

The axial subgroups for each of the four irreducible representations of $\Gamma_{\mathcal{L}}$ are given in Table III, together with generators $(z_1,z_2)\in\mathbf{C}^2$ or $(z_1,z_2,z_3)\in\mathbf{C}^3$ (fixed vectors) of the corresponding one-dimensional fixed-point subspaces (axial eigenspaces) in $\ker \mathsf{L}$, and descriptions of the associated patterns (planforms).

The results in Table III summarize known results for scalar actions with and without the midplane reflection (Buzano and Golubitsky, 1983; Golubitsky *et al.*, 1984) and the less well known results for pseudoscalar actions (Bosch Vivancos *et al.*, 1995; Bressloff *et al.*, 2001a). See also Golubitsky and Stewart (2002). More precisely, on the hexagonal lattice, the scalar$^+$ action is identical to the action studied in Bénard convection (Busse, 1962; Buzano and Golubitsky, 1983) and the scalar$^-$ action is identical to the one studied in Bénard convection with the midplane reflection (Golubitsky *et al.*, 1984). The pseudoscalar$^+$ action is identical to that studied in Bosch Vivancos *et al.* (1995) and Bressloff *et al.* (2001a), whereas the pseudoscalar$^-$ action is again the same as the one in Bénard convection with the midplane reflection—but with different isotropy subgroups, as Figs. 5 and 6 show.

TABLE III. Summary of axial subgroups. On the hexagonal lattice in the scalar case with $\tau=+1$ the points (1,1,1) and $(-1,-1,-1)$ have the same isotropy subgroup $[\mathbf{D}_6(\kappa,\xi)\oplus\mathbf{Z}_2(\tau)]$—but are not conjugate by any element of $\Gamma_{\mathcal{L}}$. Therefore, the associated eigenfunctions generate different planforms.

Lattice	Planform	Axial isotropy subgroup	Fixed vector
		Scalar representation ($\epsilon=+1$); $\tau=+1$	
Square	Squares	$\mathbf{D}_4(\kappa,\xi)\oplus\mathbf{Z}_2(\tau)$	(1,1)
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^2,\tau)\oplus\mathbf{O}(2)[\theta_2,\kappa]$	(1,0)
Hexagonal	Hexagons$^+$	$\mathbf{D}_6(\kappa,\xi)\oplus\mathbf{Z}_2(\tau)$	(1,1,1)
	Hexagons$^-$	$\mathbf{D}_6(\kappa,\xi)\oplus\mathbf{Z}_2(\tau)$	$(-1,-1,-1)$
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^3,\tau)\oplus\mathbf{O}(2)[\theta_2,\kappa]$	(1,0,0)
		Pseudoscalar representation ($\epsilon=-1$); $\tau=+1$	
Square	Squares	$\mathbf{D}_4(\kappa[\frac{1}{2},\frac{1}{2}],\xi)\oplus\mathbf{Z}_2(\tau)$	(1,1)
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^2[\frac{1}{2},0],\tau)\oplus\mathbf{O}(2)[\theta_2,\kappa[\frac{1}{2},0]]$	(1,0)
Hexagonal	Hexagons	$\mathbf{Z}_6(\xi)\oplus\mathbf{Z}_2(\tau)$	(1,1,1)
	Triangles	$\mathbf{D}_3(\kappa\xi,\xi^2)\oplus\mathbf{Z}_2(\tau)$	(i,i,i)
	Rectangles	$\mathbf{Z}_2^3(\kappa,\xi^3,\tau)$	$(0,1,-1)$
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^3[\frac{1}{2},0],\tau)\oplus\mathbf{O}(2)[\theta_2,\kappa[\frac{1}{2},0]]$	(1,0,0)
		Scalar representation ($\epsilon=+1$); $\tau=-1$	
Square	Squares	$\mathbf{D}_4(\kappa,\xi)\oplus\mathbf{Z}_2(\tau[\frac{1}{2},\frac{1}{2}])$	(1,1)
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^2,\tau[\frac{1}{2},0])\oplus\mathbf{O}(2)[\theta_2,\kappa]$	(1,0)
Hexagonal	Hexagons	$\mathbf{D}_6(\kappa,\xi)$	(1,1,1)
	Triangles	$\mathbf{D}_6(\kappa,\tau\xi)$	(i,i,i)
	Rectangles	$\mathbf{Z}_2^3(\tau\kappa,\xi^3,\tau[0,\frac{1}{2}])$	$(0,1,-1)$
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^3,\tau[\frac{1}{2},0])\oplus\mathbf{O}(2)[\theta_2,\kappa]$	(1,0,0)
		Pseudoscalar representation ($\epsilon=-1$); $\tau=-1$	
Square	Squares	$\mathbf{D}_4(\tau\kappa,\xi)\oplus\mathbf{Z}_2(\tau[\frac{1}{2},\frac{1}{2}])$	(1,1)
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^2[\frac{1}{2},0],\tau[\frac{1}{2},0])\oplus\mathbf{O}(2)[\theta_2,\kappa[\frac{1}{2},0]]$	(1,0)
Hexagonal	Hexagons	$\mathbf{D}_6(\tau\kappa,\xi)$	(1,1,1)
	Triangles	$\mathbf{D}_6(\tau\kappa,\tau\xi)$	(i,i,i)
	Rectangles	$\mathbf{Z}_2^3(\kappa,\xi^3,\tau[0,\frac{1}{2}])$	$(0,1,-1)$
	Stripes	$\mathbf{Z}_2^2(\kappa\xi^3[\frac{1}{2},0],\tau[\frac{1}{2},0])\oplus\mathbf{O}(2)[\theta_2,\kappa[\frac{1}{2},0]]$	(1,0,0)

C. The planforms

We now consider two-dimensional patterns by disregarding the z coordinate in $\mathbf{x}$ (but not in Q) and restricting attention to equilibrium states that are periodic with respect to a square or hexagonal lattice in the xy plane.

To visualize the patterns of bifurcating solutions we assume a layer of liquid crystal material in the xy plane that to first order has the form

$$Q(\mathbf{x})=Q_0+\varepsilon E(\mathbf{x}),$$

where E is an axial eigenfunction, ε is small, and Q_0 is either isotropic ($\eta=-1$) or homeotropic ($\eta=+1$). At each point (x,y) we represent the director field by a standard-length interval in the eigendirection corresponding to the largest eigenvalue of the symmetric 3×3 matrix $Q(\mathbf{x})$ at $\mathbf{x}=(x,y)$ and we plot only the projection of that interval in the xy plane. In this picture, a line element that degenerates to a point corresponds to a vertical eigendirection.

Suppose first that Q_0 is homeotropic. In this case the associated pattern is an array of points. Moreover, in our simulations no pattern will appear in bifurcations for which $Q(\mathbf{x})$ is fixed by the action of τ. For, if $E(\mathbf{x})\in V_{\mathbf{k}}^{++}$ or $V_{\mathbf{k}}^{-+}$ then

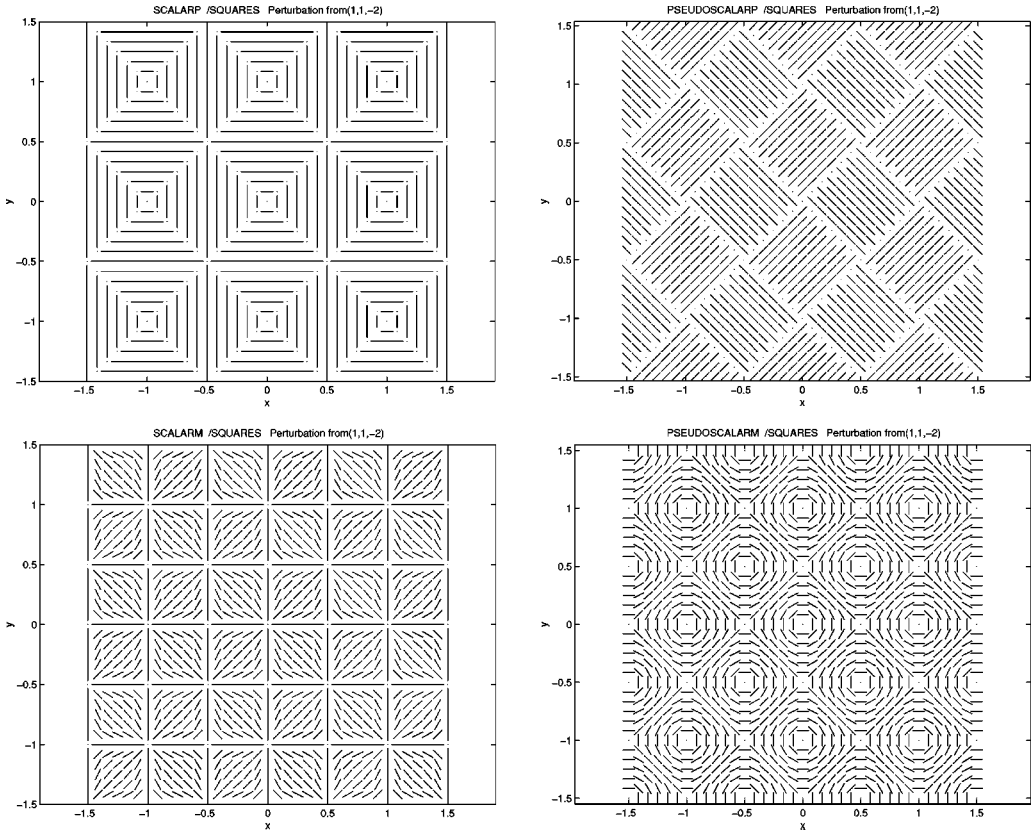

FIG. 3. Square lattice bifurcations from isotropic ($\eta<0$) liquid crystal to square patterns: (upper left) scalar $\tau=+1$; (upper right) pseudoscalar $\tau=+1$; (lower left) scalar $\tau=-1$; (lower right) pseudoscalar $\tau=-1$. Corresponding stripes patterns can be found in Figs. 1 and 7–10.

$$Q(\mathbf{x})=\begin{bmatrix} A & 0 \\ 0 & b \end{bmatrix},$$

where A is a 2×2 block and b is a scalar. Since b is close to 2 (the largest eigenvalue of Q_0) it is also the largest eigenvalue for $Q(\mathbf{x})$ for ε small. Hence, the leading eigendirection (corresponding to the largest eigenvalue) is always vertical and no patterns appear that are determined by changes in eigendirection. Nevertheless, since variation in the vertical eigenvalue of $Q(\mathbf{x})$ represents variation in the propensity of molecules to align vertically it is plausible that indistinct patterns could nevertheless be observed in practice.

Next suppose that Q_0 is planar isotropic. For small ε the director field is nearly horizontal (exactly horizontal if $\tau=+1$) and so our figures represent the pattern fairly accurately. When $\tau=-1$ there are small sinusoidal oscillations in the vertical component of the director field.

Bifurcations from isotropy exhibit lines or points of dislocation (where the director field is undefined) whereas bifurcations from homeotropy do not. In the latter case the director field is near vertical and there are small sinusoidal variations in the horizontal components. In this context the standard ''rolls'' terminology is misleading, as the director field is never horizontal: rather it oscillates about the vertical in a vertical plane and so generates ''stripes.''

In Figs. 3 and 4 we plot solutions corresponding to scalar and pseudoscalar square lattice patterns. In Figs. 5–10 we plot those for a hexagonal lattice. In the planforms obtained by bifurcation from homeotropy $\cdot$ indicates a vertical line element; whereas in the planforms obtained by bifurcation from isotropy $\cdot$ indicates points where $Q(\mathbf{x})$ has a double maximum eigenvalue,

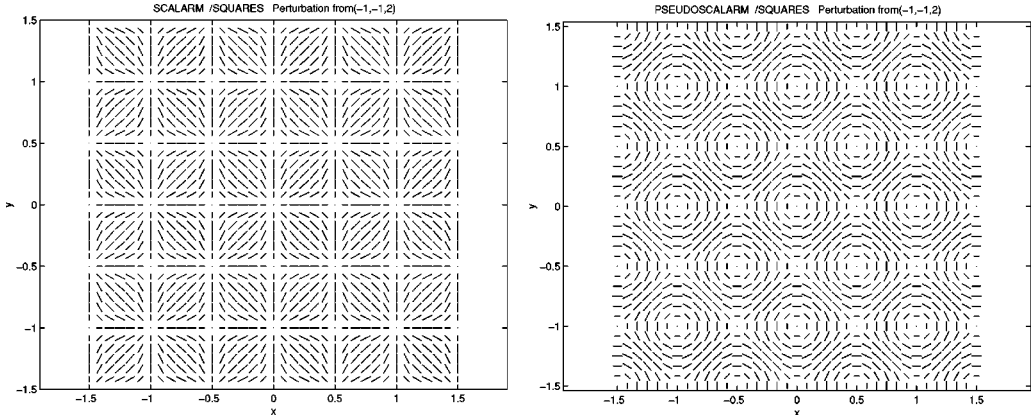

FIG. 4. Square lattice bifurcations from homeotropic ($\eta>0$) to squares with $\tau=-1$: (left) scalar; (right) pseudoscalar. Corresponding stripes patterns can be found in Figs. 5 and 6.

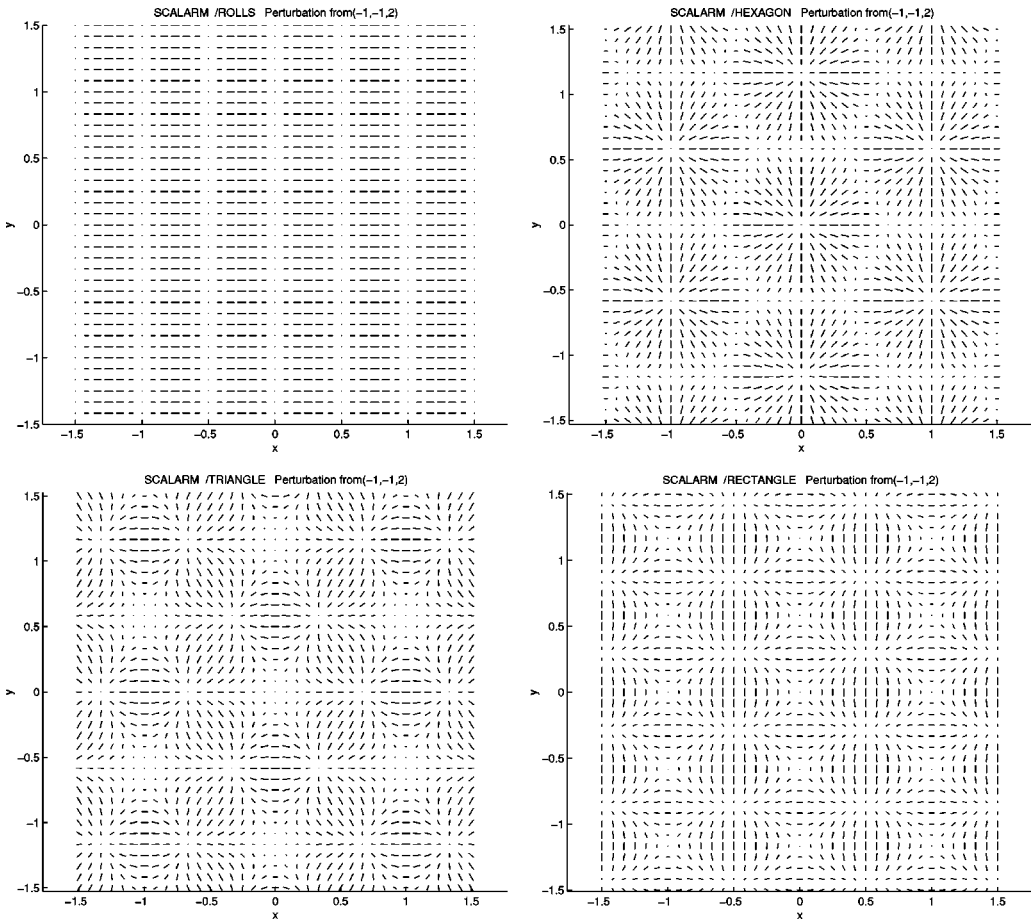

FIG. 5. Hexagonal lattice bifurcations from homeotropic ($\eta>0$) with scalar $\tau=-1$ representation: (upper left) stripes; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

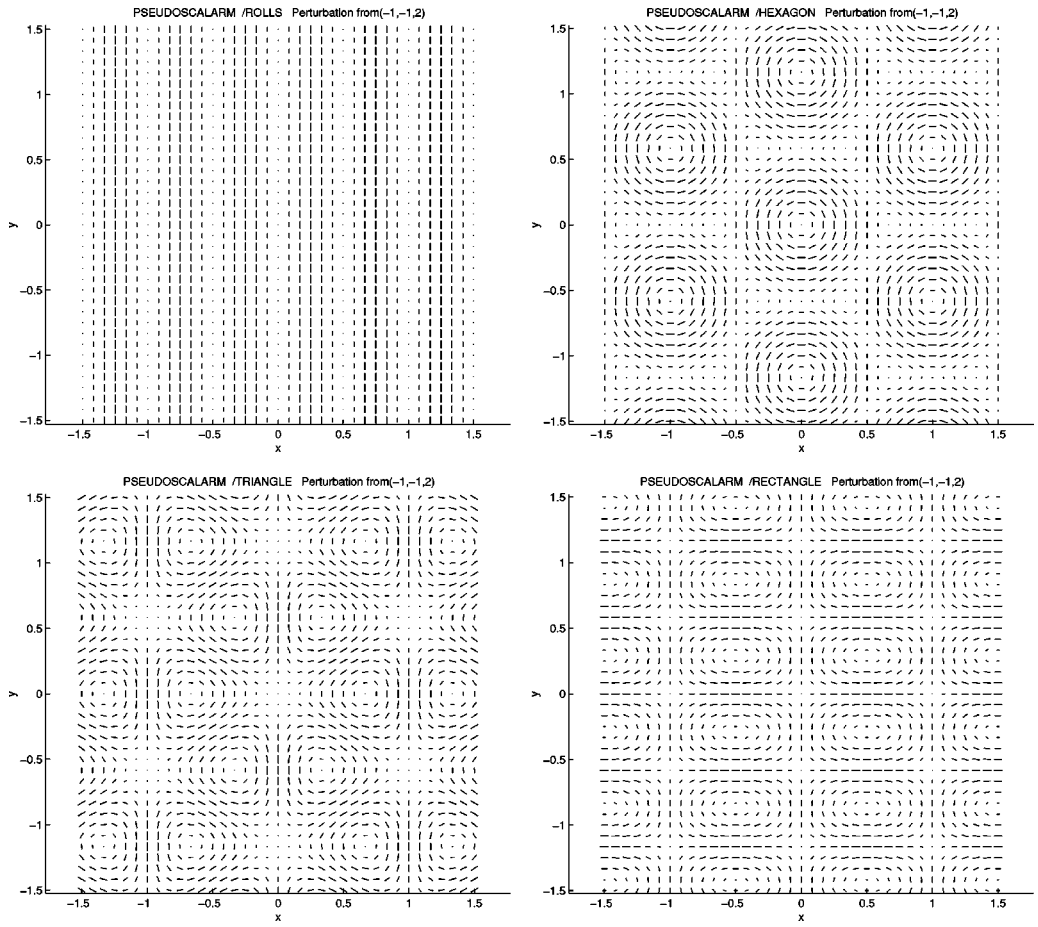

FIG. 6. Hexagonal lattice bifurcations from homeotropic ($\eta>0$) with pseudoscalar $\tau=-1$ representation: (upper left) stripes; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

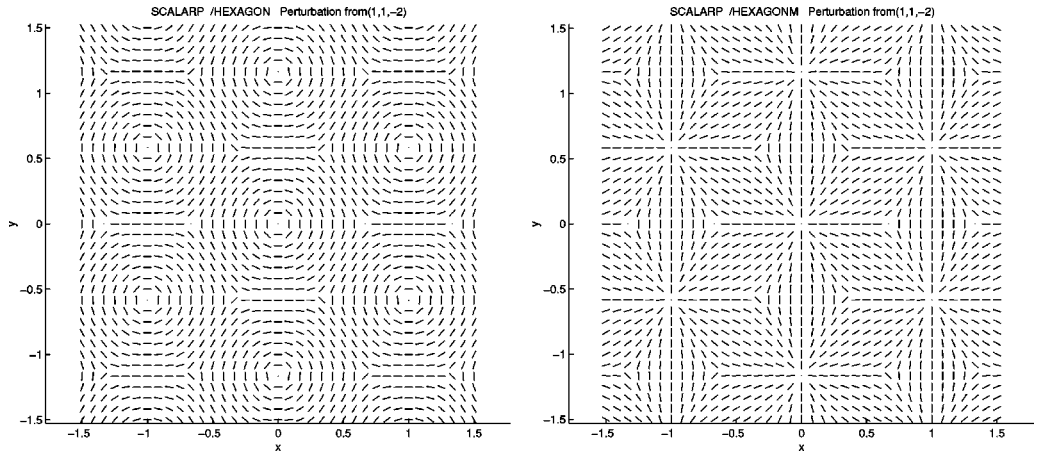

FIG. 7. Hexagonal lattice bifurcations from isotropic ($\eta<0$) with scalar $\tau=+1$ representation: stripes in Fig. 1; (left) hexagons^{+}; (right) hexagons^{-}.

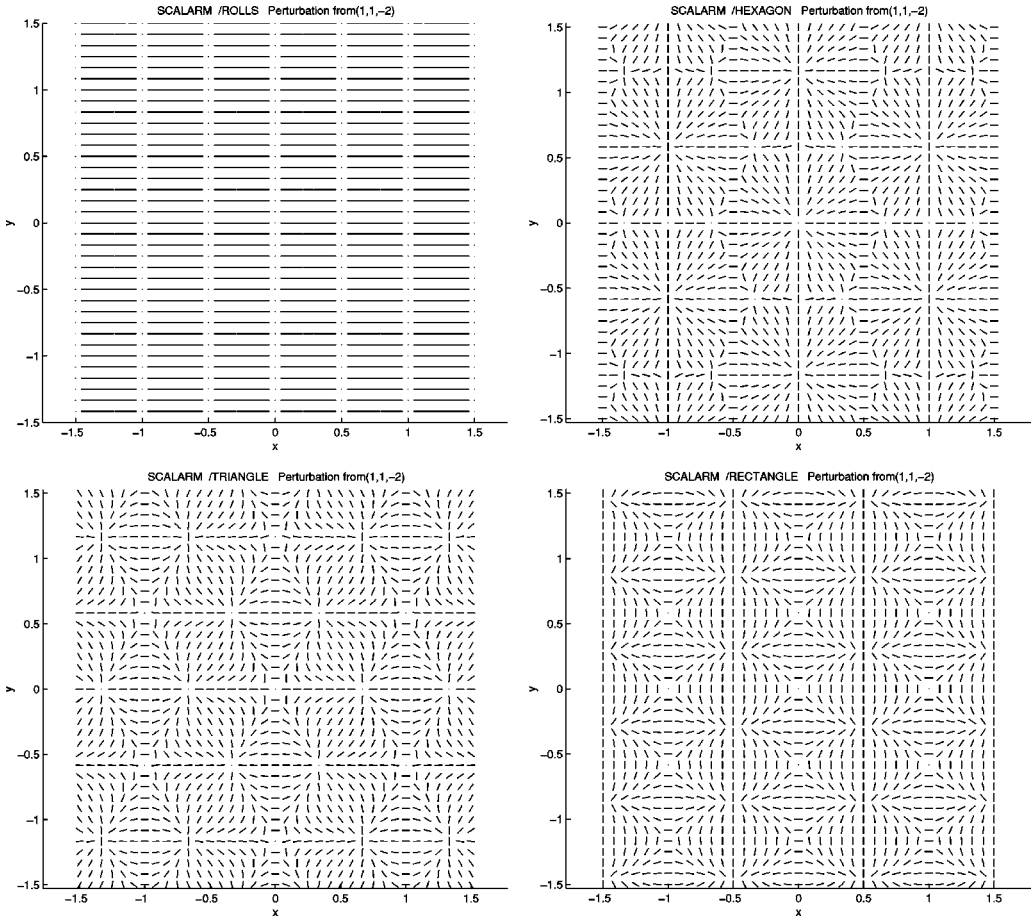

FIG. 8. Hexagonal lattice bifurcations from isotropic ($\eta<0$) with scalar $\tau=-1$ representation: (upper left) stripes; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

that is, a dislocation. Observe that across lines of dislocation the two competing directions are necessarily orthogonal in $\mathbf{R}^3$.

IV. FREE ENERGY MODELS

These results imply that for a planar liquid crystal there are four types of steady-state bifurcations, scalar, pseudoscalar, and $\tau=\pm 1$ of each type, that can occur from a spatially homogeneous equilibrium to spatially periodic equilibria. Whichever bifurcation occurs, then generically all of the planforms that we listed in the relevant section of Table III will be solutions. We have not discussed the difficult issue of stability of these solutions since these are model dependent results, whereas the classification of equilibria that we have given is independent of the model.

What remains is to complete a linear calculation to determine when a steady-state bifurcation occurs and whether it is scalar or pseudoscalar. The outline of such a calculation goes as follows. We first compute a *dispersion curve* for both scalar and pseudoscalar eigenfunctions. That is, for each wavelength $k=|\mathbf{k}|$ we determine the first value λ_k of the bifurcation parameter λ where L has a nonzero kernel. The curve (k,λ_k) is called the dispersion curve. We then find the minimum value $\lambda_*=\lambda_{k_*}$ on the dispersion curve; the corresponding wavelength k_* is the *critical* wavelength. We expect the first instability of the spatially homogeneous equilibrium to occur at the value λ_* of the bifurcation parameter. A bifurcating branch can consist of stable solutions only if the branch emanates from the first bifurcation (at λ_*).

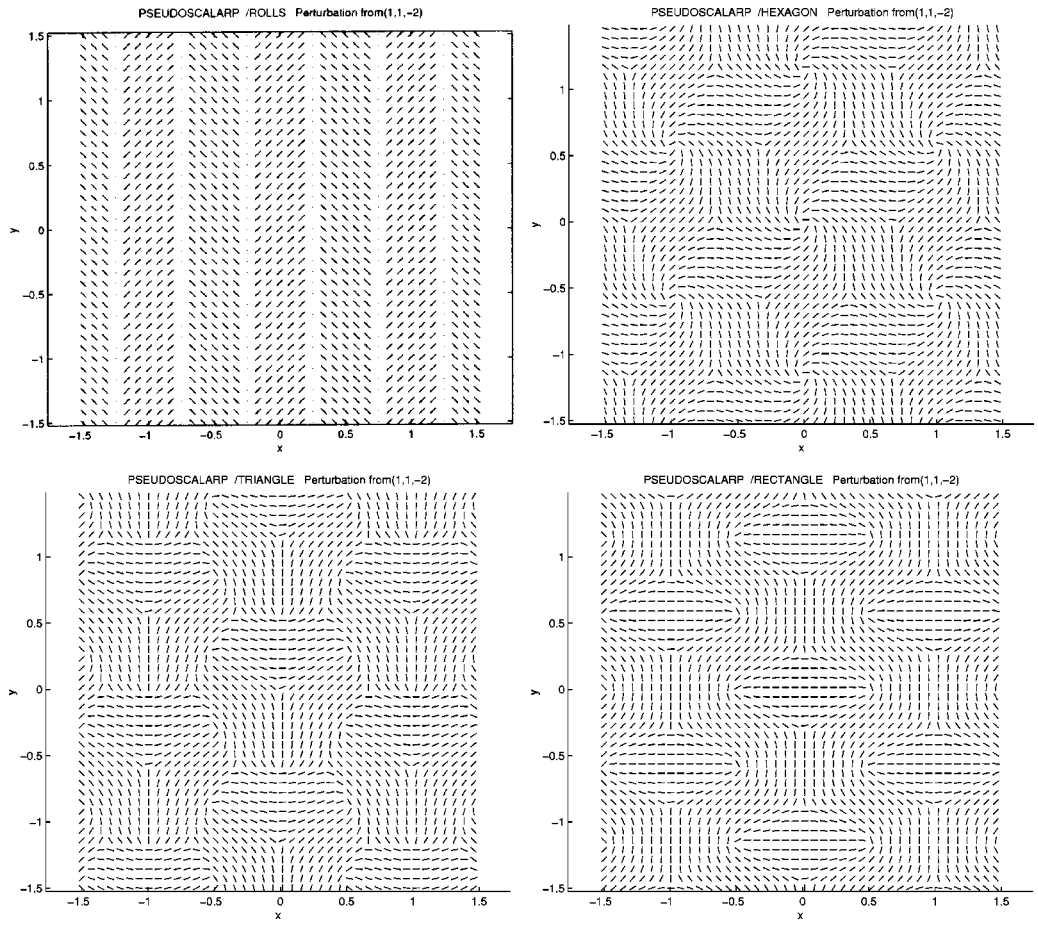

FIG. 9. Hexagonal lattice bifurcations from isotropic ($\eta<0$) with pseudoscalar $\tau=+1$ representation: (upper left) stripes; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

As an illustration we now carry out these calculations for a Landau–de Gennes type model with appropriate planar symmetry. Related calculations were carried out for bifurcation from the three-dimensional isotropic phase in Grebel *et al.* (1983). In this model we show that there are bifurcations corresponding to each of the four irreducible representations of $\Gamma_{\mathcal{L}}$, and which of them occurs first depends on the action of τ.

A. Dispersion curves for a two-dimensional Landau–de Gennes model

The free energy F is expressed as an integral per unit volume of a *free energy density* $\mathcal{F}$ which has two principal components $\mathcal{F}_0$ and $\mathcal{F}_d$ corresponding to *bulk terms* and *deformation terms*, respectively: we write F accordingly as $F=F_0+F_d$. For a system in three dimensions these typically [see, e.g., Grebel *et al.* (1983)] take the form

$$\mathcal{F}_0(Q)=\tfrac{1}{2}\lambda|Q|^2-\tfrac{1}{3}B\,\mathrm{tr}Q^3+\tfrac{1}{4}C|Q|^4,$$

$$\mathcal{F}_d(Q)=c_1|\nabla Q|^2+c_2|\nabla\cdot Q|^2+c_3|Q\cdot\nabla\wedge Q|,$$

respectively, where $|R|^2$ denotes the sum of the squares of the coefficients of the tensor R. The expression for $\mathcal{F}_0$ represents the simplest $\mathbf{SO}(3)$-invariant function on V exhibiting nontrivial interaction of local minima close to $Q=0$, while $\mathcal{F}_d$ consists of those $\mathbf{SO}(3)$-invariant terms of at most order 2 in spatial first derivatives (the chiral term $|Q\cdot\nabla\wedge Q|$ is not reflection-invariant).

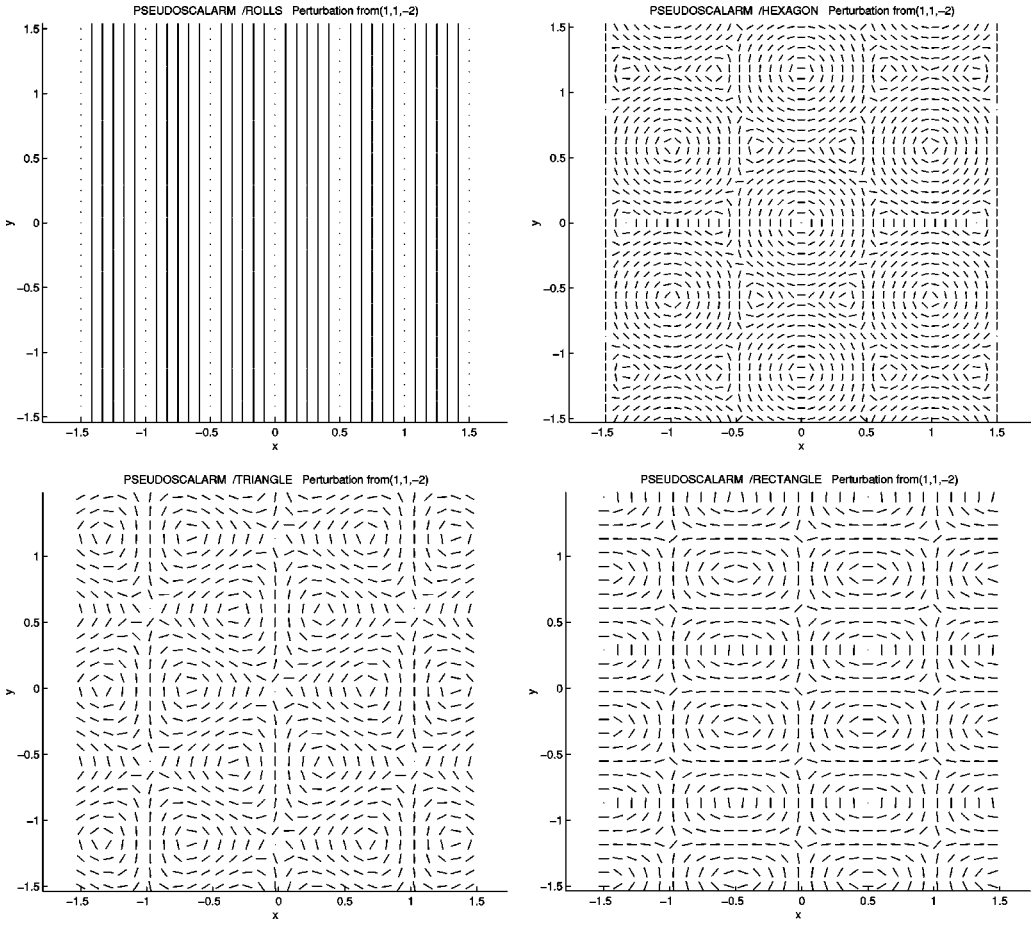

FIG. 10. Hexagonal lattice bifurcations from isotropic ($\eta<0$) with pseudoscalar $\tau=-1$ representation: (upper left) stripes; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

For a two-dimensional problem this choice of free energy function is not fully appropriate: the relevant symmetry group is now $\Gamma=\mathbf{E}(2)\times\mathbf{Z}_2(\tau)$. Consequently a wider range of terms can appear in $\mathcal{F}_0$, while the $|Q\cdot\nabla\wedge Q|$ term will no longer appear in $\mathcal{F}_d$.

We are interested in planforms that bifurcate from either the bulk homeotropic state or isotropic state, represented by Q_0 with $\eta>0$ or $\eta<0$, respectively. An example of a bulk term with $\mathbf{E}(2)\times\mathbf{Z}_2(\tau)$ invariance is $(Q_0\cdot Q)^2$, and a candidate for a deformation term to replace the chiral term is $|\Delta Q|^2$ representing longer range interactions of molecules. Accordingly we consider a free energy density $\mathcal{F}=\mathcal{F}_0+\mathcal{F}_d$ where now

$$\mathcal{F}_0(Q)=\tfrac{1}{2}\lambda|Q|^2-\tfrac{1}{3}B\mathrm{tr}Q^3+\tfrac{1}{4}C|Q|^4+\tfrac{1}{12}D(Q_0\cdot Q)^2,$$

$$\mathcal{F}_d(Q)=c_1|\nabla Q|^2+c_2|\nabla\cdot Q|^2+c_4|\Delta Q|^2.$$

Equilbrium states are critical points of F, and for $\mathcal{F}_0$ we have

$$d\mathcal{F}_0(Q)R=\lambda Q\cdot R-BQ^2\cdot R+C|Q|^2Q\cdot R+\tfrac{1}{6}D(Q_0\cdot Q)(Q_0\cdot R)$$

for arbitrary 3×3 real symmetric matrices Q,R; thus restricted to Q with trace zero we have $dF_0(Q)=0$ when

$$\lambda Q-B(Q^2-\tfrac{1}{3}|Q|^2I)+C|Q|^2Q+\tfrac{1}{6}D(Q_0\cdot Q)Q_0=0$$

TABLE IV. Computation of $d^2F(Q_0)R^2$.

R	$d^2F_0(Q_0)R^2$	$d^2F_d(Q_0)R^2$
$V_{\mathbf{k}}^{++}$	$\lambda(a^2+b^2-2ab)$ $-B(a^2+b^2+10ab)\eta$ $+6C(7(a^2+b^2)+10ab)\eta^2$	$2k^2(c_2a^2+$ $(a^2+b^2+(a+b)^2)(c_1+c_4k^2))$
$V_{\mathbf{k}}^{+-}$	$4(\lambda-B\eta+6C\eta^2)$ $=-4D\eta^2$ by (10)	$(4c_1+2c_2)k^2+4c_4k^4$
$V_{\mathbf{k}}^{-+}$	$4(\lambda+2B\eta+6C\eta^2)$	$(4c_1+2c_2)k^2+4c_4k^4$
$V_{\mathbf{k}}^{--}$	$4(\lambda-B\eta+6C\eta^2)$ $=-4D\eta^2$	$4c_1k^2+4c_4k^4$

and we easily verify the following:

$$dF_0(Q_0)=0\Leftrightarrow\lambda-B\eta+(6C+D)\eta^2=0. \tag{10}$$

Observe that $dF(Q)R=0$ automatically for any spatially periodic state R with zero mean, as the integral of an expression linear in R or its derivatives remains bounded as the volume tends to infinity. Therefore (10) is the condition for Q_0 to be an equilibrium state in our free energy model.

To study stability of the state Q_0 we evaluate the second derivative of the free energy at Q_0. For $R\in V$ we find

$$d^2F_0(Q_0)R^2=\lambda|R|^2-2BQ_0\cdot R^2+C(2(Q_0\cdot R)^2+|Q_0|^2|R|^2)+\tfrac{1}{6}D(Q_0\cdot R)^2$$

and (integrating over unit area)

$$d^2F_d(Q_0)R^2=c_1\int|\nabla R|^2+c_2\int|\nabla\cdot R|^2+c_4\int|\Delta R|^2$$

since Q_0 is spatially constant and terms linear in R integrate to zero.

We have already seen from Theorem 3.1 that the $\mathbf{E}(2)\times\mathbf{Z}_2(\tau)$ invariance of the free energy implies that generically the eigenfunctions of $d^2F(Q_0)$ on the space of $\mathcal{L}$-periodic matrix functions are linear combinations of functions belonging to one of the four subspaces $V_{\mathbf{k}}^{\pm\pm}$ and their rotations under $\pi/2$ (square lattice) or $\pm2\pi/3$ (hexagonal lattice). We next seek dispersion relations for each of the spaces $V_{\mathbf{k}}^{\pm\pm}$ in turn. When $R=e^{2\pi i\mathbf{k}\cdot\mathbf{x}}Q+\text{c.c.}$ it is easy to check that

$$\frac{1}{4\pi^2}\int|\nabla R|^2=2k^2|Q|^2,\quad\frac{1}{4\pi^2}\int|\nabla\cdot R|^2=2|Q\mathbf{k}|^2,\quad\frac{1}{16\pi^4}\int|\Delta R|^2=2k^4|Q|^2,$$

where $k=|\mathbf{k}|$. Without loss of generality we can take $\mathbf{k}=(k,0,0)$ and then after rescaling k by a factor of 2π the evaluations of $d^2F_0(Q_0)R^2$ and $d^2F_d(Q_0)R^2$ are given in Table IV.

If we normalize by choosing D so that (10) is satisfied by $\eta=1$ (corresponding to homeotropy) then we find the conditions for a zero eigenvalue in each of the last three (one-dimensional) eigenspaces are, respectively,

$$\begin{aligned}\lambda-B+6C+(c_1+\tfrac{1}{2}c_2)k^2+c_4k^4=0,\\ \lambda+2B+6C+(c_1+\tfrac{1}{2}c_2)k^2+c_4k^4=0,\\ \lambda-B+6C+c_1k^2+c_4k^4=0\end{aligned} \tag{11}$$

with the analogous expressions for $\eta=-1$ (bifurcation from two-dimensional isotropy) obtained by merely reversing the sign of B in these equations.

Stationary values of λ as a function of k occur where

$$k^2 = -(c_1 + \tfrac{1}{2}c_2)/2c_4$$

for $V_{\mathbf{k}}^{+-}$ and $V_{\mathbf{k}}^{-+}$, or

$$k^2 = -c_1/2c_4$$

for $V_{\mathbf{k}}^{--}$, giving values

$$\lambda = \begin{cases} B - 6C + (c_1 + \frac{1}{2}c_2)^2/4c_4 & \text{for } V_{\mathbf{k}}^{+-} \\ -2B - 6C + (c_1 + \frac{1}{2}c_2)^2/4c_4 & \text{for } V_{\mathbf{k}}^{-+} \\ B - 6C + c_1^2/4c_4 & \text{for } V_{\mathbf{k}}^{--}. \end{cases} \tag{12}$$

Finally, if $R \in V_{\mathbf{k}}^{++}$ then the matrix for $d^2F_0(Q_0)R^2$ as a quadratic form in a,b is

$$\begin{bmatrix} \lambda - B + 42C & -\lambda - 5B + 30C \\ -\lambda - 5B + 30C & \lambda - B + 42C \end{bmatrix}$$

and for $d^2F_d(Q_0)R^2$ is

$$\begin{bmatrix} 4c_1k^2 + 2c_2k^2 + 4c_4k^4 & 2c_1k^2 + 2c_4k^4 \\ 2c_1k^2 + 2c_4k^4 & 4c_1k^2 + 4c_4k^4 \end{bmatrix}$$

and so $d^2F(Q_0)|V_{\mathbf{k}}^{++}$ has a nontrivial kernel when the determinant of the sum of these two matrices vanishes.

With $c_2 = 0$ (that is, in physical terms, with no energy cost to the molecules for ''splay'') the algebra simplifies to yield the dispersion relation

$$\lambda = -2B - 6C + \frac{c_1^2}{4c_4}. \tag{13}$$

From (11) and (13) we therefore see that with $c_2 = 0$ the values of λ for $V_{\mathbf{k}}^{\pm\pm}$ depend only on the second $\pm$, that is on whether bifurcating solutions have vertical reflection symmetry ($\tau = +1$) or not ($\tau = -1$) and are the same for the scalar and the pseudoscalar representations. Moreover, as λ decreases, the first bifurcation from the homeotropic state ($\eta > 0$) has $\tau = -1$ while the first bifurcation from the isotropic state ($\eta < 0$) has $\tau = +1$. These statements remain true for sufficiently small $|c_2|$.

B. Plausibility and applications

The models that we have described are of course mathematical idealizations of any real physical situation. In particular

(i) full two-dimensional Euclidean lattice symmetry (by its nature infinite) cannot exist in practice, and
(ii) the question of stability of the patterns has not been addressed.

Issue (i) arises in many areas of pattern formation, and it is a common observation that, despite the meaninglessness of full Euclidean lattice symmetry, the types of pattern that such symmetry predicts are indeed seen in physical situations over even fairly small regions. Moreover, attempts to force a planar solution into a sphere or other geometrical surface naturally lead to dislocations in the pattern. For liquid crystals these questions become particularly important in the context of membranes and other structures in biology [Brown and Wolken (1979)] where hexagonal patterns, for example, are not uncommon (although we make no claim to connect them directly

with the hexagonal planforms that we discuss). Our planar idealization may thus form a starting point for understanding two-dimensional pattern formation in more realistic contexts.

The very interesting question of stability of solutions (ii) is a mathematical issue that needs to be addressed on two levels. First, stability restricted to perturbations within the lattice should be considered. The general analysis has been worked out for the scalar representations (Buzano and Golubitsky, 1983; Golubitsky *et al.*, 1984) and discussed for the pseudoscalar $\tau=1$ (Bressloff *et al.*, 2001a), but has not been completed for the pseudoscalar $\tau=-1$ representation (though the analysis should be similar to the pseudoscalar $\tau=1$ case). A full treatment of this stability (based on symmetry and otherwise independent of the equations) will, even for our simplified model, require a long calculation and is beyond the scope of this work. We note that with the extra assumption of a free energy function it might be feasible to address even more general stability issues. However, we again believe that such efforts should be reserved for models more physically realistic than ours.

V. CONCLUSION

We have classified those square and hexagonally periodic patterns that are predicted to arise in the director field of a planar layer of a nematic liquid crystal when a homeotropic or planar isotropic state loses stability via the simplest spatially doubly periodic steady-state bifurcations. The techniques are those of group theory and representation theory, and are valid for any PDE model under various reasonable assumptions. If such patterns are observed experimentally, under conditions consistent with our assumptions, then our analysis provides the explanation: what remains is to evaluate relevant constants (on the basis of physical data) in order to determine *which* of the patterns is to occur. We have investigated some aspects of this for a Landau–de Gennes free energy model. Analogous methods to these have been used for some time in related fields such as Bénard convection, but for liquid crystal models the extra complexity of the matrix order parameter here gives a richer geometric structure.

ACKNOWLEDGMENTS

We are grateful to Tim Sluckin for instructive conversations on the mathematical physics of liquid crystals. We also wish to thank Greg Forest, Steve Morris, Axel Rossberg, and Ian Stewart for helpful conversations. The research of M.G. was supported in part by NSF Grant No. DMS-0071735 and ARP Grant No. 003652-0032-2001.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Riemannian geometry of bicovariant group lattices

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(Received 18 December 2002; accepted 14 May 2003)

Group lattices (Cayley digraphs) of a discrete group are in natural correspondence with differential calculi on the group. On such a differential calculus geometric structures can be introduced following general recipes of noncommutative differential geometry. Despite the noncommutativity between functions and (generalized) differential forms, for the subclass of ''bicovariant'' group lattices considered in this work it is possible to understand central geometric objects like metric, torsion and curvature as ''tensors'' with (left) covariance properties. This ensures that tensor components (with respect to a basis of the space of 1-forms) transform in the familiar homogeneous way under a change of basis. There is a natural compatibility condition for a metric and a linear connection. The resulting (pseudo-) Riemannian geometry is explored in this work. It is demonstrated that the components of the metric are indeed able to properly describe properties of discrete geometries like lengths and angles. A simple geometric understanding of torsion and curvature in particular is achieved. The formalism has much in common with lattice gauge theory. For example, the Riemannian curvature is determined by parallel transport of vectors around a plaquette (which corresponds to a biangle, a triangle or a quadrangle). © *2003 American Institute of Physics.* [DOI: 10.1063/1.1594820]

I. INTRODUCTION

In a previous paper[1] we started to develop a general formalism of differential geometry of group lattices (Cayley digraphs), based on elementary notions of noncommutative geometry. The present work extends the latter to a formalism of discrete (pseudo-) Riemannian geometry of the subclass of *bicovariant* group lattices, as defined in Ref. 1. A group lattice, which is determined by a *discrete* group G and a *finite* subset S (not containing the unit element e), naturally defines a first-order differential calculus (which extends to higher orders) over the algebra $\mathcal{A}$ of functions on G. If S generates G, bicovariance of the group lattice (G,S) is equivalent to bicovariance of the first-order differential calculus in the sense of Ref. 2.

''Riemannian geometry'' of discrete groups in the context of noncommutative geometry has already been considered in several publications.[3–5] The present approach differs from those in particular by introducing a metric tensor as an element of a left-covariant tensor product of the space of 1-forms with itself. This tensor product is obtained from the *a priori* given tensor product over $\mathcal{A}$ by using the special structure of group lattices and the bicovariance condition. Though this formalism has ideas in common with the approach of Ref. 6, it crucially differs from the latter, where a left-covariant tensor product for arbitrary differential calculi on finite sets was constructed making use of a connection. The present approach is simpler and geometrically more transparent, but restricted to bicovariant group lattices and thus a subclass of *regular*[7] digraphs. One should keep in mind that extensions of geometric structures from ordinary differential geometry to the

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framework of noncommutative geometry may be carried out in various ways and only applications can decide on their usefulness. For our choice, we will demonstrate that it leads to simple and convenient rules of discrete geometry. It is also this last aspect, namely the fact that we establish a geometric interpretation of the *a priori* abstract formalism, which distinguishes the present work from some previous publications on noncommutative geometry of discrete groups.

The reason why we define a metric as a left-covariant tensor is that in this case its components are ''local'' objects (see Sec. II A). More generally, the components of left-covariant tensors obey a homogeneous local transformation law under a change of basis. In this sense they are really counterparts of tensors in ordinary differential geometry. This is quite in the spirit of Wilson's lattice gauge theory: discretization *a priori* moves local fields to nonlocal objects, but via parallel transport around a plaquette local objects are obtained. This is important in order to maintain gauge invariance, which is the main principle behind it. Similarly, we may postulate the preservation of the tensor transformation principle. This also allows us to consider coordinate transformations on group lattices very much in analogy with continuum differential geometry (see Sec. VI). The idea of constructing left- or alternatively right-covariant tensors in a noncommutative differential calculus already appeared in Ref. 8. Viewed as a map between left $\mathcal{A}$-modules, a left-covariant tensor is left $\mathcal{A}$-linear.

Discrete (pseudo-) Riemannian geometry is of relevance for numerical evaluation and also path integral quantization of classical physical models based on continuum Riemannian geometry, like mechanical and general relativistic systems (see Ref. 9, for example). The approach based on concepts of noncommutative geometry is an alternative to Regge calculus.[10] It has the advantage, however, that its formal structure is much closer to continuum differential geometry. Similarities with previous approaches to gravity using concepts of lattice gauge theory exist,[11] but there is little overlap when it comes to the details of the formalism. Of course, discrete geometry is an old subject (see Ref. 12, for example) and relations between the present work and earlier approaches can certainly be established to some extent. This will not be attempted in this work. Rather, we concentrate on what the machinery of algebraic noncommutative geometry applied in a natural way to (bicovariant) group lattices gives us and we reveal the geometric significance of discrete analogs of metric, metric-compatible linear connections, torsion and curvature.

Section II discusses the nonlocality of the tensor product over $\mathcal{A}$ and introduces the left-covariant tensor product for bicovariant group lattices, which induces a left-covariant product in the space of forms Ω. Left-covariant metrics are then introduced and a compatibility condition with a linear connection is formulated. The geometric meaning of the parallel transport determined by a metric-compatible linear connection is explored. Furthermore, we introduce the notion of a ''discrete Killing vector field.'' Section III elaborates the torsion and the curvature of linear connections on bicovariant group lattices and also provides corresponding expressions in terms of basic vector fields (which constitute a subclass of discrete vector fields, see Ref. 1). The Appendix presents expressions of basic formulas with respect to an orthonormal coframe field. Section IV deals with group lattices which carry a metric and a torsion-free compatible linear connection.

A metric-compatible linear connection provides us with a parallel transport which maps part of the group lattice isometrically into the tangent space at some site. Torsion and curvature of the connection are, respectively, corresponding first and second order obstructions. It turns out that torsion plays a much more fundamental role in this discrete framework than in ordinary continuum differential geometry. Linear connections with torsion are needed to describe even simple group lattice geometries in this framework (see Sec. V).

In Sec. VI we introduce the concept of coordinates on group lattices and elaborate in particular the geometry of hypercubic lattices based on the Abelian group $\mathbb{Z}^n$. Some concluding remarks are collected in Sec. VII.

The present work relies on the notation and results of Ref. 1. It is *not* self-contained. We refer to an equation in Ref. 1 in the form $(I.a.b)$ where $(a.b)$ is the equation number in Ref. 1. In the following we restrict our considerations to bicovariant group lattices (G,S), i.e., S is assumed to be closed under the adjoint action of all elements of S and their inverses.

II. TENSOR PRODUCTS, METRICS, AND LINEAR CONNECTIONS

In this section we first briefly discuss the consequences of the nonlocality of the usual tensor product over $\mathcal{A}$. Then we make use of the special structure of bicovariant group lattices in order to construct a new tensor product which is left-covariant so that the corresponding tensor components are ''local'' and able to carry a geometric meaning. The left-covariant tensor product of forms induces a left-covariant (generalized wedge) product in the space of forms. Left-covariant metrics are introduced and a compatibility condition with a linear connection is formulated. The latter involves an extension of the linear connection from the space of 1-forms to a left-covariant tensor product. This is a familiar procedure in the tensor calculus on manifolds, but in general not at all straightforward in noncommutative geometries (see also Ref. 3). Of particular importance for an understanding of the formalism is the observation that a metric-compatible linear connection determines an isometric map of parts of the group lattice into the tangent space at a (fixed) site. In the last subsection we define discrete Killing vector fields and invariant metrics on a (bicovariant) group lattice.

A. Nonlocality of the tensor product over $\mathcal{A}$

For the differential calculus (Ω,d) determined by a group lattice (G,S) there is a distinguished (left and right) $\mathcal{A}$-module basis $\{\theta^h \mid h\in S\}$ of the space of 1-forms Ω^1 which satisfies $\theta^h f = R_h^* f\, \theta^h$ for all elements f of the space of functions $\mathcal{A}$ on G, where R_h is the right action on G by an element $h\in S$. As a consequence,

$$(f\theta^h)\otimes_{\mathcal{A}}(f'\theta^{h'}) = f\,(R_h^* f')\;\theta^h\otimes_{\mathcal{A}}\theta^{h'} \tag{2.1}$$

for all $f,f'\in\mathcal{A}$. For each $g\in G$ there is a function e^g such that $e^g(g')=\delta_{g,g'}$ for all $g'\in G$. For this function we obtain

$$e^g(\,\theta^h\otimes_{\mathcal{A}}\theta^{h'}) = (e^g\theta^h)\otimes_{\mathcal{A}}(e^{gh}\theta^{h'}), \tag{2.2}$$

which shows that the tensor product $\otimes_{\mathcal{A}}$ is nonlocal since the two factors ''sit'' at different (though neighboring) points. Let us consider an object

$$\mathrm{g} = \sum_{h,h'\in S}\gamma_{h,h'}\;\theta^h\otimes_{\mathcal{A}}\theta^{h'} \quad (\gamma_{h,h'}\in\mathcal{A}). \tag{2.3}$$

Under a linear change of basis $\theta^h\mapsto\tilde{\theta}^h := \Sigma_{h'\in S}\,a^h{}_{h'}\;\theta^{h'}$ with coefficients $a^h{}_{h'}\in\mathcal{A}$ we find

$$\mathrm{g} = \sum_{h_1,h_2,h_1',h_2'\in S}\gamma_{h_1',h_2'}\,(a^{-1})^{h_1'}{}_{h_1}\,(R_{h_1}^* a^{-1})^{h_2'}{}_{h_2}\,\tilde{\theta}^{h_1}\otimes_{\mathcal{A}}\tilde{\theta}^{h_2} = \sum_{h_1,h_2\in S}\tilde{\gamma}_{h_1,h_2}\,\tilde{\theta}^{h_1}\otimes_{\mathcal{A}}\tilde{\theta}^{h_2} \tag{2.4}$$

from which we read off the coefficients with respect to the new cobasis:

$$\tilde{\gamma}_{h_1,h_2} = \sum_{h_1',h_2'\in S}\gamma_{h_1',h_2'}\,(a^{-1})^{h_1'}{}_{h_1}\,(R_{h_1}^* a^{-1})^{h_2'}{}_{h_2}. \tag{2.5}$$

Here we see again the nonlocal character of the tensor product $\otimes_{\mathcal{A}}$.

B. Left-covariant tensor product for bicovariant group lattices

By acting on each component, the maps R_h^* and $R_{h^{-1}}^*$ for $h\in S$ extend to tensor products of Ω^1 and to Ω as automorphisms. Then there is another tensor product with a local transformation rule. This ''left-covariant'' tensor product is defined via

$$(\,\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\otimes_L T := \theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r}\otimes_{\mathcal{A}}R_{h_r^{-1}}^*\cdots R_{h_1^{-1}}^* T, \tag{2.6}$$

where T is an arbitrary element of a tensor product of Ω^1 over $\mathcal{A}$. The inverse relation is

$$(\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\otimes_{\mathcal{A}}T=(\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\otimes_L R^*_{h_1}\cdots R^*_{h_r}T. \tag{2.7}$$

Using $R^*_h\,\theta^{h'}=\theta^{\mathrm{ad}(h)h'}$ we find in particular

$$\theta^h\otimes_L\theta^{h'}=\theta^h\otimes_{\mathcal{A}}\theta^{\mathrm{ad}(h^{-1})h'},\quad \theta^h\otimes_{\mathcal{A}}\theta^{h'}=\theta^h\otimes_L\theta^{\mathrm{ad}(h)h'}. \tag{2.8}$$

Note also that

$$(\theta^{h_1}\otimes_L\cdots\otimes_L\theta^{h_r})\otimes_L T=(\theta^{h_1}\otimes_L\cdots\otimes_L\theta^{h_r})\otimes_{\mathcal{A}}R^*_{h_1^{-1}}\cdots R^*_{h_r^{-1}}T, \tag{2.9}$$

$$(\theta^{h_1}\otimes_L\cdots\otimes_L\theta^{h_r})\otimes_{\mathcal{A}}T=(\theta^{h_1}\otimes_L\cdots\otimes_L\theta^{h_r})\otimes_L R^*_{h_r}\cdots R^*_{h_1}T. \tag{2.10}$$

A local transformation law is indeed obtained since the new tensor product satisfies

$$(f_1T_1)\otimes_L(f_2T_2)=f_1f_2\,T_1\otimes_L T_2 \tag{2.11}$$

for all $f_1,f_2\in\mathcal{A}$ and elements T_1,T_2 of tensor products of Ω^1.

Lemma 2.1: The left-covariant tensor product $\otimes_L$ is associative:

$$(T_1\otimes_L T_2)\otimes_L T_3=T_1\otimes_L(T_2\otimes_L T_3) \tag{2.12}$$

for all T_i in tensor products of Ω^1.

Proof: In particular, we find

$$\begin{aligned}(\theta^{h_1}\otimes_L\theta^{h_2})\otimes_L T&=(\theta^{h_1}\otimes_{\mathcal{A}}R^*_{h_1^{-1}}\theta^{h_2})\otimes_L T\\&=(\theta^{h_1}\otimes_{\mathcal{A}}\theta^{\mathrm{ad}(h_1^{-1})h_2})\otimes_L T\\&=\theta^{h_1}\otimes_{\mathcal{A}}\theta^{\mathrm{ad}(h_1^{-1})h_2}\otimes_{\mathcal{A}}R^*_{[\mathrm{ad}(h_1^{-1})h_2]^{-1}}R^*_{h_1^{-1}}T\\&=\theta^{h_1}\otimes_{\mathcal{A}}\theta^{\mathrm{ad}(h_1^{-1})h_2}\otimes_{\mathcal{A}}R^*_{h_1^{-1}}R^*_{h_2^{-1}}T\\&=\theta^{h_1}\otimes_{\mathcal{A}}R^*_{h_1^{-1}}(\theta^{h_2}\otimes_{\mathcal{A}}R^*_{h_2^{-1}}T)=\theta^{h_1}\otimes_L(\theta^{h_2}\otimes_L T).\end{aligned}$$

Our more general assertion is proved in the same way. ■

Lemma 2.2: For all T_1,T_2 in tensor products of Ω^1,

$$R^*_h(T_1\otimes_L T_2)=(R^*_hT_1)\otimes_L(R^*_hT_2). \tag{2.13}$$

Proof:

$$\begin{aligned}R^*_h[(f\,\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\otimes_L T]&=R^*_h(f\,\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\,R^*_hR^*_{h_r^{-1}}\cdots R^*_{h_1^{-1}}R^*_{h^{-1}}R^*_hT\\&=R^*_h(f\,\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\,R^*_{[\mathrm{ad}(h)h_r]^{-1}}\cdots R^*_{[\mathrm{ad}(h)h_1]^{-1}}R^*_hT\\&=R^*_h(f\,\theta^{h_1}\otimes_{\mathcal{A}}\cdots\otimes_{\mathcal{A}}\theta^{h_r})\otimes_L R^*_hT\end{aligned}$$

for all $f\in\mathcal{A}$ and all T in a tensor product of Ω^1. Now the assertion follows by linearity. ■

C. A left-covariant product in the space of forms

The nonlocality of the tensor product $\otimes_{\mathcal{A}}$ discussed above is inherited by the product in Ω. For a bicovariant group lattice we can define a left-covariant product in Ω via

$$\omega_1 \cap \omega_2 = \pi(\omega_1 \otimes_L \omega_2), \tag{2.14}$$

where π is the projection $\Omega \otimes_{\mathcal{A}} \Omega \to \Omega$. The new product inherits from $\otimes_L$ left-covariance and associativity. From the definition we obtain

$$(\theta^{h_1} \cdots \theta^{h_r}) \cap \omega = \theta^{h_1} \cdots \theta^{h_r} R^*_{h_r^{-1}} \cdots R^*_{h_1^{-1}} \omega, \tag{2.15}$$

$$\theta^{h_1} \cdots \theta^{h_r} \omega = (\theta^{h_1} \cdots \theta^{h_r}) \cap R^*_{h_1} \cdots R^*_{h_r} \omega, \tag{2.16}$$

and also

$$(\theta^{h_1} \cap \cdots \cap \theta^{h_r}) \cap \omega = (\theta^{h_1} \cap \cdots \cap \theta^{h_r})\, R^*_{h_1^{-1}} \cdots R^*_{h_r^{-1}} \omega, \tag{2.17}$$

$$(\theta^{h_1} \cap \cdots \cap \theta^{h_r})\, \omega = (\theta^{h_1} \cap \cdots \cap \theta^{h_r}) \cap R^*_{h_r} \cdots R^*_{h_1} \omega. \tag{2.18}$$

In particular,

$$\theta^h \cap \theta^{h'} = \theta^h\, \theta^{\mathrm{ad}(h^{-1})h'}, \quad \theta^h\, \theta^{h'} = \theta^h \cap \theta^{\mathrm{ad}(h)h'}. \tag{2.19}$$

The 2-form relations (see Sec. IV of Ref. 1) now read

$$\sum_{h,h' \in S} \delta^g_{h'h}\, \theta^h \cap \theta^{h'} = 0 \quad \forall\, g \in S_{(2)} \tag{2.20}$$

and a 2-form can be decomposed using the projections

$$\begin{aligned} p_{(e)}(\theta^h \cap \theta^{h'}) &= \delta^e_{hh'}\, \theta^h \cap \theta^{h'}, \\ p_{(h)}(\theta^{h'} \cap \theta^{h''}) &= \delta^h_{h''h'}\, \theta^{h'} \cap \theta^{h''}, \quad h \in S_{(1)}, \\ p_{(g)}(\theta^h \cap \theta^{h'}) &= \delta^g_{h'h}\, \theta^h \cap \theta^{h'}, \quad g \in S_{(2)}, \end{aligned} \tag{2.21}$$

where $S_{(1)} = S^2 \cap S$, $S_{(2)} = S^2 \backslash S_e$ and $S_e = S \cup \{e\}$. For a cycle $h_1 h_2 = h_2 h_3 = \cdots = h_r h_1$ we obtain

$$\theta^{h_1} \theta^{h_2} + \theta^{h_2} \theta^{h_3} + \cdots + \theta^{h_r} \theta^{h_1} = \theta^{h_1} \cap \theta^{h_r} + \theta^{h_2} \cap \theta^{h_1} + \cdots + \theta^{h_r} \cap \theta^{h_{r-1}}. \tag{2.22}$$

Hence the structure of 2-form relations is preserved by the $\cap$-product.

Since R^*_h commutes with π, (2.13) leads to

$$R^*_h(\omega_1 \cap \omega_2) = (R^*_h \omega_1) \cap (R^*_h \omega_2). \tag{2.23}$$

In Ref. 1 a map $\Delta : \Omega \to \Omega$ has been introduced which is a graded derivation with respect to the ordinary product in Ω and satisfies

$$\Delta(\theta^h) := \sum_{h',h'' \in S} \delta^h_{h''h'}\, \theta^{h'} \cap \theta^{h''}. \tag{2.24}$$

Lemma 2.3: Δ *is a graded derivation with respect to the* $\cap$*-product in* Ω.

Proof: Using (I.4.11) and (I.4.20) we obtain

$$\begin{aligned}\Delta(\theta^h \cap \omega) &= \Delta(\theta^h R^*_{h^{-1}}\omega)\\ &= \Delta(\theta^h)\, R^*_{h^{-1}}\omega - \theta^h\, \Delta(R^*_{h^{-1}}\omega)\\ &= \Delta(\theta^h)\, R^*_{h^{-1}}\omega - \theta^h\, R^*_{h^{-1}}\Delta(\omega)\\ &= \sum_{h',h''\in S} \delta^h_{h''h'}\, \theta^{h'} \cap \theta^{h''} \cap R^*_{h''h'}\, R^*_{h^{-1}}\omega - \theta^h \cap \Delta(\omega)\\ &= \Delta(\theta^h)\cap\omega - \theta^h \cap \Delta(\omega)\end{aligned}$$

for all $\omega \in \Omega$. This in turn implies the general derivation rule

$$\Delta(\omega' \cap \omega) = \Delta(\omega')\cap\omega + (-1)^r\, \omega' \cap \Delta(\omega),$$

where ω' is an arbitrary r-form. ■

The map d is *not* a derivation with respect to the $\cap$-product. For an r-form ω we obtain from (I.4.12) the formula

$$\mathrm{d}\omega = \sum_{h\in S} \theta^h \cap R^*_h \omega - (-1)^r\, \omega \cap \theta - \Delta(\omega), \tag{2.25}$$

where

$$\theta = \sum_{h\in S} \theta^h. \tag{2.26}$$

This allows us to evaluate d applied to any form in terms of expressions which only involve the $\cap$-product (instead of the original product in Ω). In fact, we could have defined the left-covariant product of forms (and moreover the left-covariant tensor product) by its basic properties (without reference to the tensor product over $\mathcal{A}$) and the action of d directly in terms of (2.25). Reversing some of the arguments would then demonstrate that there is a product in Ω with respect to which d becomes a derivation.

D. Fixing the ambiguity of 2-form components

Given a 2-form

$$\psi = \sum_{h,h'\in S} \psi_{h,h'}\, \theta^h \cap \theta^{h'}, \tag{2.27}$$

the biangle and triangle coefficient functions $\psi_{h,h'}$ are uniquely determined, but there is an ambiguity in the quadrangle coefficients as a consequence of the 2-form relations (2.20). Indeed, writing

$$\psi_{(g)} = p_{(g)}\psi = \sum_{h,h'\in S} \check{\psi}_{(g)\,h,h'}\, \theta^h \cap \theta^{h'} \tag{2.28}$$

for $g \in S_{(2)}$, there is a freedom of gauge transformations $\check{\psi}_{(g)\,h,h'} \mapsto \check{\psi}_{(g)\,h,h'} + \Psi_{(g)}\, \delta^g_{h'h}$ with an arbitrary function $\Psi_{(g)}$ on G.[13] For any two members h,h' and $\hat{h},\hat{h}'$ of the chain $h_1 h_1{}' = \cdots = h_r h_r{}' = g \in S_{(2)}$, the difference

$$\psi_{(g)\,h,h';\hat{h},\hat{h}'} := \check{\psi}_{(g)\,h,h'} - \check{\psi}_{(g)\,\hat{h},\hat{h}'} \tag{2.29}$$

and thus also

$$\psi_{(g)\,h',h} := \sum_{\hat{h},\hat{h}' \in S} \psi_{(g)\,h',h;\hat{h}',\hat{h}} = |g|\,\breve{\psi}_{(g)\,h',h} - \sum_{\hat{h},\hat{h}' \in S} \delta^{g}_{\hat{h}\hat{h}'}\,\breve{\psi}_{(g)\,\hat{h}',\hat{h}} \tag{2.30}$$

is gauge invariant and hence independent of the choice of the coefficient functions $\breve{\psi}_{(g)\,h,h'}$ (from their gauge equivalence class). Here $|g|$ denotes the length of the chain which belongs to g, i.e., $|g| = r$. Furthermore, we obtain $\Sigma_{h,h'} \delta^{g}_{h'h}\,\psi_{(g)\,h,h'} = 0$ and

$$\psi_{(g)} = \frac{1}{|g|} \sum_{h,h' \in S} \delta^{g}_{h'h}\,\psi_{(g)\,h,h'}\,\theta^{h} \cap \theta^{h'}, \tag{2.31}$$

which suggests to *define* the functions (2.30) as the *quadrangle components* of the 2-form ψ (with respect to the $\cap$-product). The equation $\psi_{(g)} = 0$ (for a 2-form ψ) is equivalent to the vanishing of all the differences $\psi_{(g)\,h,h';\hat{h},\hat{h}'}$.

Of course, also in the case of higher than 2-forms there is an ambiguity in the choice of coefficients and a corresponding way of fixing it.

E. Left-covariant metric and compatibility with a linear connection

Let us express g given in (2.3) as

$$\mathrm{g} = \sum_{h,h' \in S} \mathfrak{g}_{h,h'}\,\theta^{h} \otimes_{L} \theta^{h'} \tag{2.32}$$

with $\mathfrak{g}_{h,h'} \in \mathcal{A}$. By comparison with (2.3), we obtain

$$\gamma_{h,h'} = \mathfrak{g}_{h,hh'h^{-1}}. \tag{2.33}$$

We say that g is *symmetric* if $\mathfrak{g}_{h,h'} = \mathfrak{g}_{h',h}$, which corresponds to $\gamma_{h,h^{-1}h'h} = \gamma_{h',h'^{-1}hh'}$. Furthermore, g is said to be *invertible* if the matrix $\mathfrak{g} = (\mathfrak{g}_{h,h'})$ is invertible (at all sites).

An object g as considered above is a candidate for a ''metric tensor.'' Its components should then be expected to determine lengths of vectors and angles between vectors at a site. This interpretation clearly distinguishes the components $\mathfrak{g}_{h,h'}$ and thus the left-covariant tensor product (see also the corresponding remarks in the Introduction). Hence we define a *metric tensor* as an object g of the form (2.32) such that the coefficient matrix $\mathfrak{g}$ is real, symmetric and invertible.

A metric g is called *left-invariant* if $L_h^{*}\mathrm{g} = \mathrm{g}$ for all $h \in S$, where L_h denotes the left action by h on G. This is equivalent to a ''constant metric,'' i.e., $\mathfrak{g}_{h,h'} \in \mathbb{R}$. A left-invariant metric is called *bi-invariant* if it is also *right-invariant*, i.e., $R_h^{*}\mathrm{g} = \mathrm{g}$ for all $h \in S$. This means that the metric is constant and satisfies $\mathfrak{g}_{h_1,h_2} = \mathfrak{g}_{\mathrm{ad}(h)h_1,\mathrm{ad}(h)h_2}$ for all $h, h_1, h_2 \in S$.

Let $\{\ell_h \mid h \in S\}$ be the vector fields dual to $\{\theta^h \mid h \in S\}$, so that $\ell_h f = R_h^{*} f - f$ for $f \in \mathcal{A}$. Let $\mathcal{V}_{\ell_h}$ be the parallel transport along the vector field ℓ_h with respect to a linear connection on Ω^1 (see Ref. 1). We write

$$\mathcal{V}_{\ell_{h'}}\theta^{h} = \sum_{h'' \in S} (R^{*}_{h'^{-1}} V^{h}{}_{h',h''})\,\theta^{h''}, \tag{2.34}$$

where $V_h = (V^{h''}{}_{h,h'})$ are matrices with entries in $\mathcal{A}$. $\mathcal{V}$ extends to $\Omega^1 \otimes_L \Omega^1$ via

$$\mathcal{V}_{\ell_h}(\alpha \otimes_L \beta) = \mathcal{V}_{\ell_h}\alpha \otimes_L \mathcal{V}_{\ell_h}\beta. \tag{2.35}$$

Then $\mathcal{V} := \Sigma_{h \in S} \theta^{h} \otimes_{\mathcal{A}} \mathcal{V}_{\ell_h}$ has the property $\mathcal{V}(f\,\alpha \otimes_L \beta) = f\,\mathcal{V}(\alpha \otimes_L \beta)$ and thus defines a connection according to Lemma 6.1 of Ref. 1.

An element $\mathrm{g} \in \Omega^1 \otimes_L \Omega^1$ is said to be *compatible* with the linear connection ∇ if

$$\nabla \mathrm{g} = 0, \tag{2.36}$$

which in terms of the parallel transport operators takes the form

$$\mathcal{V}_{\ell_h} \mathrm{g} = \mathrm{g} \quad \forall h \in S. \tag{2.37}$$

In components, this reads

$$\sum_{h_1, h_2 \in S} V^{h_1}{}_{h,h'_1} V^{h_2}{}_{h,h'_2} \mathfrak{g}_{h_1,h_2} = R^*_h \mathfrak{g}_{h'_1,h'_2} \tag{2.38}$$

and in matrix form

$$R^*_h \mathfrak{g} = V_h^T \mathfrak{g} V_h. \tag{2.39}$$

If g is a metric, this condition requires that the matrices V_h, $h \in S$, are invertible. For a given metric, there are not always matrices V_h satisfying (2.39).

Lemma 2.4: A linear connection compatible with a metric on a connected component of a bicovariant group lattice exists if and only if the metric has the same signature at all sites.

Proof: This is a direct consequence of the fact that two real symmetric matrices A, B with the same rank are related by $B = V^T A V$ with an invertible matrix V if and only if both have the same signature. ■

A bicovariant group lattice supplied with a metric of constant signature will be called a *Riemannian group lattice* in the following. Since we require a metric to be nondegenerate, a Riemannian group lattice (G, S, g) should be regarded as an $|S|$-dimensional structure.

The metric-compatibility condition determines the transport matrices, and thus the connection, only up to transformations $V_h \mapsto J_h V_h$ with arbitrary isometries J_h, which are matrices of functions on G such that

$$J_h^T \mathfrak{g} J_h = \mathfrak{g}. \tag{2.40}$$

F. Backward parallel transport of vector fields and geometric interpretation of metric-compatible linear connections

Vector fields are elements of the $\mathcal{A}$-bimodule generated by $\{\ell_h \mid h \in S\}$.[1] A linear connection determines a backward parallel transport of vector fields along a vector field:

$$\tilde{\mathcal{V}}_{\ell_h} X := \sum_{h', h'' \in S} (R^*_h X^{h'}) V^{h''}{}_{h,h'} \cdot \ell_{h''}, \quad \tilde{\mathcal{V}}_X := \sum_{h \in S} X^h \tilde{\mathcal{V}}_{\ell_h} \tag{2.41}$$

(see Ref. 1 for details). The vectors

$$V_{h,h'} := \tilde{\mathcal{V}}_{\ell_h} \ell_{h'} = \sum_{h'' \in S} V^{h''}{}_{h,h'} \cdot \ell_{h''} \tag{2.42}$$

are the images in the tangent space at g of the vectors $\ell_{h'}$ at gh. If the transport is metric-compatible, the vectors $V_{h,h'}$ at g carry the metric properties of $\ell_{h'}$ at gh, i.e.,

$$\mathfrak{g}_{h',h''}(gh) = \mathrm{g}(\ell_{h'}, \ell_{h''})(gh) = \mathrm{g}(V_{h,h'}, V_{h,h''})(g). \tag{2.43}$$

Of course, we can also transport tangent vectors from more remote sites to the tangent space at g by iterated application of the operators $\tilde{\mathcal{V}}_{\ell_h}$:

$$V_{h_1,\ldots,h_{r+1}} := \tilde{\mathcal{V}}_{\ell_{h_1}} \cdots \tilde{\mathcal{V}}_{\ell_{h_r}} \ell_{h_{r+1}}. \tag{2.44}$$

The results will, however, be path-dependent in general. But here we see very clearly the geometric significance of a metric-compatible linear connection. It maps part of the group lattice into the tangent space at a site in such a way that the metric relations are preserved, i.e., isometrically. In general, this cannot be done for the whole group lattice. Torsion and curvature are obstructions. We have already shown in Ref. 1 that in the case of vanishing torsion at least the next-neighbor part of the group lattice is mapped isometrically into the tangent space in this way, i.e., the backward parallel transport preserves the group lattice geometry to first order. Curvature is a second order obstruction. Its biangle, triangle and quadrangle parts are given, respectively, by

$$(\tilde{\mathcal{V}}_{\ell_{h_1}}\tilde{\mathcal{V}}_{\ell_{h_2}}-I)\,\ell_h=\sum_{h'\in S}(V_{h_1}R^*_{h_1}V_{h_2}-I)^{h'}{}_h\,\ell_{h'}\quad\text{if } h_1h_2=e,$$

$$(\tilde{\mathcal{V}}_{\ell_{h_1}}\tilde{\mathcal{V}}_{\ell_{h_2}}-\tilde{\mathcal{V}}_{\ell_{h_3}})\,\ell_h=\sum_{h'\in S}(V_{h_1}R^*_{h_1}V_{h_2}-V_{h_3})^{h'}{}_h\,\ell_{h'}\quad\text{if } h_1h_2=h_3\in S_{(1)},$$

$$(\tilde{\mathcal{V}}_{\ell_{h_1}}\tilde{\mathcal{V}}_{\ell_{h_2}}-\tilde{\mathcal{V}}_{\ell_{\hat{h}_1}}\tilde{\mathcal{V}}_{\ell_{\hat{h}_2}})\,\ell_h=\sum_{h'\in S}(V_{h_1}R^*_{h_1}V_{h_2}-V_{\hat{h}_1}R^*_{\hat{h}_1}V_{\hat{h}_2})^{h'}{}_h\,\ell_{h'}\quad\text{if } h_1h_2=\hat{h}_1\hat{h}_2\in S_{(2)}. \tag{2.45}$$

An equivalent curvature definition will be presented in Sec. III. The last formula of (2.45) is a discrete version of a familiar formula of continuum differential geometry: the quadrangle curvature is determined by parallel transport of a vector field around a quadrangle. There are no counterparts of biangle and triangle curvature in continuum differential geometry.

Let us make more precise how an isometric tangent space picture of (part of) a group lattice is obtained if a metric-compatible linear connection is given. If S has n different elements, let $(\,,\,)$ be an inner product in $\mathbb{R}^n$ with the same signature as g. At the origin in $\mathbb{R}^n$ we choose an n-bein $\{\mathbf{u}_h \mid h\in S\}$ such that

$$(\mathbf{u}_h,\mathbf{u}_{h'})=\mathrm{g}(\ell_h,\ell_{h'})(g). \tag{2.46}$$

Then $\iota:\ell_h\mapsto\mathbf{u}_h$ extends to an isomorphism of metric linear spaces. Furthermore, $\mathbf{V}_{h,h'}:=\iota(V_{h,h'})=\Sigma_{h''\in S}V^{h''}{}_{h,h'}\,\mathbf{u}_{h''}$ represents the vector $V_{h,h'}$ in $\mathbb{R}^n$. We attach it at the tip of $\mathbf{u}_h$. More generally, the vector

$$\mathbf{V}_{h_1,\ldots,h_{r+1}}:=\iota(V_{h_1,\ldots,h_{r+1}})=\sum_{h\in S}\mathbf{u}_h\,[V_{h_1}(g)\,V_{h_2}(gh_1)\cdots V_{h_r}(gh_1\cdots h_{r-1})]^h{}_{h_{r+1}} \tag{2.47}$$

has to be attached at the tip of $\mathbf{u}_{h_1}+\mathbf{V}_{h_1,h_2}+\cdots+\mathbf{V}_{h_1,\ldots,h_r}$.

The isometries J_h act on the vectors $\mathbf{V}_{h,h'}$ as follows:

$$J_h(\mathbf{V}_{h,h'}):=\sum_{h_1,h_2}\mathbf{u}_{h_1}J^{h_1}{}_{h,h_2}V^{h_2}{}_{h,h'}. \tag{2.48}$$

The isometry property of the J_h then implies

$$(J_h(\mathbf{V}_{h,h'}),J_h(\mathbf{V}_{h,h''}))=(\mathbf{V}_{h,h'},\mathbf{V}_{h,h''}). \tag{2.49}$$

The backward parallel transport and the isomorphism ι provide us with a convenient way to describe the action of a (metric-compatible) linear connection in $\mathbb{R}^n$ (supplied with a standard inner product). This will be used extensively in Secs. IV and V.

G. Contravariant metric and compatibility with a linear connection

A left-covariant tensor product of vector fields X,Y is defined as follows:

$$X\otimes_L Y:=\sum_{h\in S}X^h\,\ell_h\otimes_{\mathcal{A}}R_{h*}Y\,. \tag{2.50}$$

Given a metric tensor in the sense of Sec. II E, there is also a "contravariant" metric tensor,

$$\mathsf{h}=\sum_{h,h'\in S}\mathfrak{h}^{h,h'}\cdot\ell_h\otimes_L\ell_{h'}=\sum_{h,h'\in S}\mathfrak{h}^{h,\mathrm{ad}(h)h'}\cdot\ell_h\otimes_{\mathcal{A}}\ell_{h'}, \tag{2.51}$$

where $(\mathfrak{h}(g)^{h,h'})$ is the inverse of the matrix $\mathfrak{g}$ at $g\in G$.

If the matrices V_h are invertible for all $h\in S$, the corresponding linear connection on Ω^1 induces a connection on the space $\mathcal{X}$ of vector fields (see Ref. 1). An element $\mathsf{h}\in\mathcal{X}\otimes_L\mathcal{X}$ is *compatible* with the connection ∇ if $\nabla\mathsf{h}=0$, where ∇ has been extended to $\mathcal{X}\otimes_L\mathcal{X}$ following the procedure in Sec. II E. This is

$$R_h^*\mathfrak{h}^{h_1,h_2}=\sum_{h_1',h_2'\in S}(U_h)^{h_1}{}_{h_1'}(U_h)^{h_2}{}_{h_2'}\mathfrak{h}^{h_1',h_2'} \tag{2.52}$$

or $R_h^*\mathfrak{h}=U_h\,\mathfrak{h}\,U_h^T$ in matrix form, where $U_h:=V_h^{-1}$.

H. Discrete Killing vector fields

Let $X=\Sigma_{h\in S}X^h\cdot\ell_h$ be a discrete vector field for which the map $\phi_X:G\to G$, which is determined by $\phi_X^*=I+X$ on functions, is differentiable (see Ref. 1). X will be called a *Killing vector field* of a metric g if $\pounds_X\mathrm{g}=\phi_X^*\mathrm{g}-\mathrm{g}=0$ (with the Lie derivative $\pounds$ introduced in Ref. 1). For $X=\ell_h$ this becomes $R_h^*\mathrm{g}=\mathrm{g}$, i.e.,

$$\mathfrak{g}(gh)_{h_1,h_2}=\mathfrak{g}(g)_{\mathrm{ad}(h)h_1,\mathrm{ad}(h)h_2} \tag{2.53}$$

for all $g\in G$. The right hand side of (2.53) can be expressed in the form $(P_h^T\,\mathfrak{g}(g)\,P_h)_{h_1,h_2}$ where the matrix P_h represents a permutation.

A metric g on a bicovariant group lattice (G,S) is thus right-invariant if it satisfies $\pounds_{\ell_h}\mathrm{g}=0$ for all $h\in S$. A right-invariant metric is completely determined by its values at one site (e.g., at the unit element e).

$V_h:=P_h$ defines a linear connection which is compatible with every right-invariant metric. Each other linear connection compatible with a right-invariant metric is then obtained as $V_h:=J_hP_h$, where J_h is at each lattice site an isometry of the metric.

Example 2.1: Let G be a discrete group and $S\subset G\backslash\{e\}$ finite and *Abelian*. If $\pounds_{\ell_h}\mathrm{g}=0$ for some $h\in S$, the condition (2.53) becomes $\mathfrak{g}(gh)=\mathfrak{g}(g)$, which means that the functions $\mathfrak{g}_{h_1,h_2}$, $h_1,h_2\in S$, are constant on the orbits in G under the right action R_h. Let $G=\mathbb{Z}_n$ or $G=\mathbb{Z}$, and $1\in S$. If ℓ_1 is a Killing vector field, the metric coefficients $\mathfrak{g}_{h_1,h_2}$ are constant on the whole group. The corresponding natural linear connection is then given by $V_h=I$. ■

Example 2.2: Let $G=\mathcal{S}_3$ and $S=\{(12),(13),(23)\}$. We introduce the matrices

$$P_{(12)}=\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix},\quad P_{(13)}=\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix},\quad P_{(23)}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}. \tag{2.54}$$

If $\ell_{(12)}$ is a Killing vector field of a metric g on this group lattice, then $\mathfrak{g}(g\,(12))=P_{(12)}\,\mathfrak{g}(g)\,P_{(12)}$ which determines the metric at the sites $(12),(13),(23)$ in terms of the metric at the sites $e,(132),(123)$, respectively. If $\ell_{(13)}$ and $\ell_{(23)}$ are Killing vector fields of g, then $\mathfrak{g}(g\,(13))=P_{(13)}\,\mathfrak{g}(g)\,P_{(13)}$ and $\mathfrak{g}(g\,(23))=P_{(23)}\,\mathfrak{g}(g)\,P_{(23)}$. The right-invariant metrics on $(\mathcal{S}_3,\{(12),(13),(23)\})$ are then given by

$$\mathfrak{g}(e)=\begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix},\quad \mathfrak{g}((12))=\begin{pmatrix} a & c & b \\ c & f & e \\ b & e & d \end{pmatrix},\quad \mathfrak{g}((13))=\begin{pmatrix} f & e & c \\ e & d & b \\ c & b & a \end{pmatrix},$$
$$\mathfrak{g}((23))=\begin{pmatrix} d & b & e \\ b & a & c \\ e & c & f \end{pmatrix},\quad \mathfrak{g}((123))=\begin{pmatrix} d & e & b \\ e & f & c \\ b & c & a \end{pmatrix},\quad \mathfrak{g}((132))=\begin{pmatrix} f & c & e \\ c & a & b \\ e & b & d \end{pmatrix}, \tag{2.55}$$

with constants a,b,c,d,e,f. A linear connection compatible with this family of metrics is obtained by choosing $V_h=P_h$. The family of right-invariant metrics includes

$$\mathfrak{g}(h)=\begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix}, \tag{2.56}$$

which is bi-invariant. ■

III. TORSION AND CURVATURE AS LEFT-COVARIANT TENSORS

The torsion 2-forms

$$\Theta^h=\mathrm{d}\theta^h-\pi(\nabla\theta^h)=\mathrm{d}\theta^h-\theta\,\theta^h-\sum_{h',h''\in S} V^h{}_{h',h''}\,\theta^{h'}\theta^{h''} \tag{3.1}$$

can be rewritten in terms of the $\cap$-product and then decomposed into biangle, triangle and quadrangle parts as follows:

$$\begin{aligned}\Theta^h&=\sum_{h_1,h_2\in S} Q^h{}_{h_1,h_2}\,\theta^{h_1}\cap\theta^{h_2}\\ &=\sum_{h_1,h_2\in S}\left(Q^h_{(e)\,h_1,h_2}+\sum_{h_0\in S_{(1)}} Q^h_{(h_0)\,h_1,h_2}+\sum_{g\in S_{(2)}}\check{Q}^h_{(g)\,h_1,h_2}\right)\theta^{h_1}\cap\theta^{h_2}.\end{aligned} \tag{3.2}$$

In this way we find the biangle components

$$Q^h_{(e)\,h_1,h_2}=\delta^e_{h_1h_2}(\delta^h_{h_1}+V^h{}_{h_1,h_2}) \tag{3.3}$$

and the triangle components

$$Q^h_{(h_0)\,h_1,h_2}=\delta^{h_0}_{h_2h_1}(\delta^h_{h_1}-\delta^h_{h_0}+V^h{}_{h_1,h_1^{-1}h_2h_1}). \tag{3.4}$$

In the case of the quadrangle components, one has to take the 2-form relations (2.20) into account. As a consequence of the latter, the functions $Q^h_{(g)\,h_1,h_2}$ are not uniquely determined. Following the discussion in Sec. II D, it is convenient to introduce the differences

$$Q^h_{(g)\,h_1,h_2;\hat{h}_1,\hat{h}_2}:=\check{Q}^h_{(g)\,h_1,h_2}-\check{Q}^h_{(g)\,\hat{h}_1,\hat{h}_2}=\delta^g_{h_2h_1}(\delta^h_{h_1}-\delta^h_{\hat{h}_1}+V^h{}_{h_1,h_1^{-1}h_2h_1}-V^h{}_{\hat{h}_1,\hat{h}_1^{-1}\hat{h}_2\hat{h}_1}) \tag{3.5}$$

[cf. (2.29)] where $\hat{h}_2,\hat{h}_1$ is any pair of elements of S which belongs to the same chain as h_2,h_1 (so that $\hat{h}_2\hat{h}_1=g=h_2h_1$). In particular, the vanishing of the quadrangle part of the torsion 2-form is equivalent to the vanishing of all the quantities (3.5). According to Sec. II D, the quadrangle torsion components should be defined as follows,

$$Q^{h}_{(g)\,h_i',h_i}:=|g|\,\check{Q}^{h}_{(g)\,h_i',h_i}-\sum_{h',h''\in S}\delta^{g}_{h'h''}\,\check{Q}^{h}_{(g)\,h'',h'}=\sum_{\substack{h',h''\in S\\ h'h''=g}}Q^{h}_{(g)\,h_i',h_i;h'',h'},\quad i=1,\dots,|g|, \tag{3.6}$$

if $h_1h_1'=\cdots=h_rh_r'=g$ is the corresponding chain. This does not depend on the choice of the coefficient functions $\check{Q}^{h}_{(g)\,h',h}$ which is ambiguous as a consequence of the 2-form relations.

After some manipulations like

$$\begin{aligned}
&\sum_{h',h''\in S}\theta^{h'}\theta^{h''}\otimes_{\mathcal{A}}\mathcal{V}_{\ell_{h''}}\mathcal{V}_{\ell_{h'}}\theta^{h}\\
&\quad=\sum_{h_1,h''\in S}(\theta^{h_1}\theta^{h''})\otimes_L R^{*}_{h_1}R^{*}_{h''}\mathcal{V}_{\ell_{h''}}\mathcal{V}_{\ell_{h_1}}\theta^{h}\\
&\quad=\sum_{h_1,h''\in S}(\theta^{h_1}\cap\theta^{\mathrm{ad}(h_1)h''})\otimes_L R^{*}_{h_1}R^{*}_{h''}\mathcal{V}_{\ell_{h''}}\mathcal{V}_{\ell_{h_1}}\theta^{h}\\
&\quad=\sum_{h_1,h_2\in S}(\theta^{h_1}\cap\theta^{h_2})\otimes_L R^{*}_{h_2h_1}\mathcal{V}_{\ell_{\mathrm{ad}(h_1^{-1})h_2}}\mathcal{V}_{\ell_{h_1}}\theta^{h}\\
&\quad=\sum_{h_1,h_2\in S}(\theta^{h_1}\cap\theta^{h_2})\otimes_L R^{*}_{h_2h_1}\sum_{h',h''}(R^{*}_{(h_2h_1)^{-1}}V^{h}_{h_1,h''})\\
&\qquad\times(R^{*}_{h_1^{-1}h_2^{-1}h_1}V^{h''}_{h_1^{-1}h_2h_1,h'})\,\theta^{h''}\\
&\quad=\sum_{h_1,h_2,h',h''\in S}(\theta^{h_1}\cap\theta^{h_2})\otimes_L V^{h}_{h_1,h''}(R^{*}_{h_1}V^{h''}_{h_1^{-1}h_2h_1,h'})\,\theta^{\mathrm{ad}(h_2h_1)h''}\\
&\quad=\sum_{h_1,h_2,h',h''\in S}(\theta^{h_1}\cap\theta^{h_2})\otimes_L V^{h}_{h_1,h''}(R^{*}_{h_1}V^{h''}_{\mathrm{ad}(h_1^{-1})h_2,\mathrm{ad}[(h_2h_1)^{-1}]h'})\,\theta^{h'}
\end{aligned}\tag{3.7}$$

the definition of the curvature, see (I.7.4), leads to

$$\begin{aligned}
\mathcal{R}(\theta^{h})=\sum_{h',h_1,h_2\in S}\Bigg(&\sum_{h''\in S}V^{h}{}_{h_1,h''}(R^{*}_{h_1}V^{h''}{}_{h_1^{-1}h_2h_1,\mathrm{ad}[(h_2h_1)^{-1}]h'})-\delta^{h}_{h'}\,\delta^{e}_{h_2h_1}\\
&-\sum_{h''\in S}\delta^{h''}_{h_2h_1}V^{h}{}_{h'',\mathrm{ad}[(h_2h_1)^{-1}]h'}\Bigg)\,\theta^{h_1}\cap\theta^{h_2}\otimes_L\theta^{h'}.
\end{aligned}\tag{3.8}$$

Writing

$$\mathcal{R}(\theta^h) = \sum_{h',h_1,h_2} \mathcal{R}^{h}{}_{h',h_1,h_2}\, \theta^{h_1} \cap \theta^{h_2} \otimes_L \theta^{h'}$$

$$= \sum_{h_1,h_2 \in S} \left(\mathcal{R}^{h}{}_{(e)\,h',h_1,h_2} + \sum_{h_0 \in S_{(1)}} \mathcal{R}^{h}{}_{(h_0)\,h',h_1,h_2} + \sum_{g \in S_{(2)}} \check{\mathcal{R}}^{h}_{(g)\,h',h_1,h_2} \right) \theta^{h_1} \cap \theta^{h_2} \otimes_L \theta^{h'} \tag{3.9}$$

we obtain the biangle components

$$\mathcal{R}^{h}{}_{(e)\,h',h_1,h_2} = \delta^{e}_{h_2 h_1} (V_{h_1} R^{*}_{h_1} V_{h_2} - I)^{h}{}_{h'}, \tag{3.10}$$

the triangle components

$$\mathcal{R}^{h}{}_{(h_0)\,h',h_1,h_2} = \delta^{h_0}_{h_2 h_1} (V_{h_1} R^{*}_{h_1} V_{h_1^{-1} h_2 h_1} - V_{h_0})^{h}{}_{h_0^{-1} h' h_0}, \tag{3.11}$$

and the differences of quadrangle components

$$\mathcal{R}^{h}{}_{(g)\,h',h_1,h_2;\hat{h}_1,\hat{h}_2} := \check{\mathcal{R}}^{h}_{(g)\,h',h_1,h_2} - \check{\mathcal{R}}^{h}_{(g)\,h',\hat{h}_1,\hat{h}_2}$$

$$= \delta^{g}_{h_2 h_1} (V_{h_1} R^{*}_{h_1} V_{h_1^{-1} h_2 h_1} - V_{\hat{h}_1} R^{*}_{\hat{h}_1} V_{\hat{h}_1^{-1} \hat{h}_2 \hat{h}_1})^{h}{}_{g^{-1} h' g}. \tag{3.12}$$

Again, $\hat{h}_2, \hat{h}_1$ is any pair with $\hat{h}_2 \hat{h}_1 = g \in S_{(2)}$.

According to Sec. II D, the quadrangle curvature components should be defined as follows,

$$\mathcal{R}^{h}{}_{(g)\,h',h_i',h_i} := |g|\, \check{\mathcal{R}}^{h}_{(g)\,h',h_i',h_i} - \sum_{h'',h''' \in S} \delta^{g}_{h'' h'''}\, \check{\mathcal{R}}^{h}_{(g)\,h',h''',h''}$$

$$= \sum_{\substack{h'',h''' \in S \\ h'' h''' = g}} \mathcal{R}^{h}{}_{(g)\,h',h_i',h_i;h''',h''},$$

$$i = 1, \ldots, |g|, \tag{3.13}$$

if $h_1 h_1' = \cdots = h_r h_r' = g$ is the corresponding chain. Understanding that the quadrangle part of $\mathcal{R}^{h}{}_{h',h'',h'''}$ is given by the above expression, the components of a *Ricci tensor* can be defined without ambiguity as follows:

$$\mathrm{Ric}_{h,h'} := \sum_{h'' \in S} \mathcal{R}^{h''}{}_{h,h'',h'}. \tag{3.14}$$

With the help of a metric, a *curvature scalar* can be built:

$$R := \sum_{h,h' \in S} (\mathfrak{g}^{-1})^{h,h'} \mathrm{Ric}(\ell_h, \ell_{h'}). \tag{3.15}$$

There is, however, another contraction of the curvature tensor, namely,

$$\widetilde{\mathrm{Ric}}_{h,h'} := \sum_{h'' \in S} \mathcal{R}^{h''}{}_{h,h',h''}, \tag{3.16}$$

which leads in general to a different Ricci tensor and curvature scalar. Moreover, also the contraction $\Sigma_{h'' \in S} \mathcal{R}^{h''}{}_{h'',h,h'}$ is in general different from zero. This complicates finding a suitable analog of the Einstein equation, for example.

A. Bianchi identities

According to Ref. 1, the first Bianchi identity can be expressed as follows:

$$\mathrm{d}\Theta^h+\Theta(\nabla\theta^h)=\pi\circ\mathcal{R}(\theta^h)=\sum_{h',h_1,h_2\in S}\mathcal{R}^h{}_{h',h_1,h_2}\,\theta^{h_1}\cap\theta^{h_2}\cap\theta^{h'}. \tag{3.17}$$

Using $\theta\,\omega=\Sigma_{h\in S}\theta^h\cap R^*_h\omega$ we find

$$\Theta(\nabla\theta^h)=-\theta\,\Theta^h+\sum_{h',h''\in S}V^h{}_{h',h''}\,\theta^{h''}\,\Theta^{h'}=-\sum_{h'\in S}\theta^{h'}\cap R^*_{h'}\Theta^h+\sum_{h',h''\in S}V^h{}_{h',h''}\,\theta^{h''}\cap R^*_{h''}\Theta^{h'}, \tag{3.18}$$

and, thus, with the help of (2.25),

$$\mathrm{d}\Theta^h+\Theta(\nabla\theta^h)=-\Theta^h\cap\theta-\Delta(\Theta^h)+\sum_{h',h''}V^h{}_{h',h''}\theta^{h''}\cap(R^*_{h''}\Theta^{h'}). \tag{3.19}$$

Replacing the left hand side of (3.17) with the last expression, we obtain the first Bianchi identity in terms of the $\cap$-product. In the case of vanishing torsion, it reduces to

$$\sum_{h',h_1,h_2\in S}\mathcal{R}^h{}_{h',h_1,h_2}\,\theta^{h_1}\cap\theta^{h_2}\cap\theta^{h'}=0. \tag{3.20}$$

Using $V^h{}_{h'}:=\Sigma_{h''\in S}V^h{}_{h'',h'}\,\theta^{h''}$ and

$$\mathcal{R}^h{}_{h'}:=\sum_{h_1,h_2\in S}\mathcal{R}^h{}_{\mathrm{ad}(h_2h_1)h',h_1,h_2}\,\theta^{h_1}\cap\theta^{h_2} \tag{3.21}$$

the second Bianchi identity (I.7.15) reads

$$\begin{aligned}\Delta(\mathcal{R}^h{}_{h'})&=\sum_{h''\in S}(V^h{}_{h''}\mathcal{R}^{h''}{}_{h'}-\mathcal{R}^h{}_{h''}V^{h''}{}_{h'})\\&=\sum_{h_1,h_2\in S}V^h{}_{h_1,h_2}\,\theta^{h_1}\cap R^*_{h_1}\mathcal{R}^{h_2}{}_{h'}-\sum_{h_1,h_2,h_3\in S}\mathcal{R}^h{}_{\mathrm{ad}(h_3h_2)h_1,h_2,h_3}\,\theta^{h_2}\cap\theta^{h_3}\cap R^*_{h_3h_2}V^{h_1}{}_{h'}.\end{aligned} \tag{3.22}$$

Evaluating the left hand side with the help of Lemma 2.3, this yields a 3-form expression which only involves the $\cap$-product.

B. Integrability conditions of the metric-compatibility equation

The integrability condition for the metric-compatibility of a linear connection is $\nabla^2\mathrm{g}=0$ and thus involves the curvature. After some manipulations we obtain the conditions

$$V_{h_1}R^*_{h_1}V_{h_2}=B_{h_1,h_2}\quad\text{for a biangle}\quad h_1h_2=e, \tag{3.23}$$

$$V_{h_1}R^*_{h_1}V_{h_2}=T_{h_1,h_2}V_h\quad\text{for a triangle}\quad h_1h_2=h\in S_{(1)}, \tag{3.24}$$

$$V_{h_1}R^*_{h_1}V_{h_2}=K_{h_1,h_2;\hat h_1\hat h_2}V_{\hat h_1}R^*_{\hat h_1}V_{\hat h_2}\quad\text{for a quadrangle}\quad h_1h_2=\hat h_1\hat h_2\in S_{(2)}, \tag{3.25}$$

where for all $g \in G$ the matrices $B_{h_1,h_2}(g)$, $T_{h_1,h_2}(g)$, $K_{h_1,h_2;\hat{h}_1\hat{h}_2}(g)$ are elements of the isometry group of $\mathfrak{g}(g)$. Now we obtain for biangles

$$\mathcal{R}^{h}{}_{(e)\,h',h_1,h_2} = \delta^{e}_{h_2 h_1} (B_{h_1,h_2} - I)^{h}{}_{h'}\,, \tag{3.26}$$

for triangles

$$\mathcal{R}^{h}{}_{(h_0)\,h',h_1,h_2} = \delta^{h_0}_{h_2 h_1} ((T_{h_1,h_2} - I) V_{h_0})^{h}{}_{h_0^{-1} h' h_0}\,, \tag{3.27}$$

and for quadrangles

$$\mathcal{R}^{h}{}_{(g)\,h',h_1,h_2;\hat{h}_1,\hat{h}_2} = \delta^{g}_{h_2 h_1} ((K_{h_1,h_2;\hat{h}_1,\hat{h}_2} - I)\, V_{\hat{h}_1} R^{*}_{\hat{h}_1} V_{\hat{h}_1^{-1}\hat{h}_2\hat{h}_1})^{h}{}_{g^{-1}h'g}\,, \tag{3.28}$$

where $\hat{h}_2\hat{h}_1 = g \in S_{(2)}$. As a consequence, the essential part of the curvature tensor is given by the isometries B, T, K.

C. Torsion and curvature as maps on vector fields

Let (G,S) be a bicovariant group lattice and $Q^{h}{}_{h_1,h_2}$ be the torsion tensor components introduced in (3.2) with the quadrangle part defined in (3.6). For vector fields X, Y we introduce the *torsion tensor*

$$Q(X,Y) := \sum_{h \in S,\ h_1,h_2 \in S_e} X^{h_1} Y^{h_2}\, Q^{h}{}_{h_1,h_2} \cdot \ell_h. \tag{3.29}$$

This expression obviously satisfies $Q(f \cdot X, f' \cdot Y) = f f'\, Q(X,Y)$ and is therefore a (left) tensor. In the following we consider in more detail the case where X, Y are basic. The torsion tensor can then be written as

$$Q(X,Y) = \sum_{h \in S} Q^{h}{}_{s_X, s_Y} \cdot \ell_h\,, \tag{3.30}$$

where the map $s_X : G \to S$ is determined by $X^h(g) = \delta^{h}_{s_X(g)}$ (see also Ref. 1).

Below we will need the following expression for basic vector fields X, Y,

$$\begin{aligned} \tilde{\mathcal{V}}_X R_{X*} Y &= \sum_{h_1,h_2 \in S} X^{h_1}\, Y^{\mathrm{ad}(h_1)h_2}\, \tilde{\mathcal{V}}_{\ell_{h_1}} \ell_{h_2} \\ &= \sum_{h_1,h_2 \in S} \delta^{h_1,s_X}\, \delta^{h_2,\mathrm{ad}(s_X)^{-1} s_Y}\, \tilde{\mathcal{V}}_{\ell_{h_1}} \ell_{h_2} \\ &= \sum_{h \in S} V^{h}{}_{s_X,\mathrm{ad}(s_X)^{-1} s_Y} \cdot \ell_h\,, \end{aligned} \tag{3.31}$$

where we used (I.5.21), (I.7.17), and (I.5.12).

If X, Y form a biangle, so that $s_Y s_X = e$, then

$$Q(X,Y)=\sum_{h\in S} Q^{h}_{(e)s_X,s_Y}\cdot \ell_h$$

$$=\sum_{h\in S} \delta^{e}_{s_Xs_Y}(\delta^{h}_{s_X}+V^{h}_{s_X,s_Y})\cdot \ell_h$$

$$=X+\sum_{h\in S} V^{h}{}_{s_X,s_Y}\cdot \ell_h=X+\tilde{\mathcal{V}}_X R_{X*}Y. \tag{3.32}$$

If X,Y,Z form a triangle, so that $s_Ys_X=s_Z$, we obtain

$$Q(X,Y)=\sum_{h\in S,h_1\in S_{(1)}} Q^{h}_{(h_1)s_X,s_Y}\cdot \ell_h$$

$$=\sum_{h\in S,h_1\in S_{(1)}} \delta^{h_1}_{s_Ys_X}(\delta^{h}_{s_X}-\delta^{h}_{h_1}+V^{h}{}_{s_X,\mathrm{ad}(s_X)^{-1}s_Y})\cdot \ell_h$$

$$=X+\tilde{\mathcal{V}}_X R_{X*}Y-Z. \tag{3.33}$$

Finally, for a quadrangle $X,Y,\hat{X},\hat{Y}$ (which satisfies $s_Ys_X=s_{\hat{Y}}s_{\hat{X}}\notin S_e$) we find

$$Q(X,Y;\hat{X},\hat{Y}):=Q(X,Y)-Q(\hat{X},\hat{Y})$$

$$=\sum_{h\in S,g\in S_{(2)}} Q^{h}_{(g)s_X,s_Y;s_{\hat{X}},s_{\hat{Y}}}\cdot \ell_h$$

$$=\sum_{h\in S,g\in S_{(2)}} \delta^{g}_{s_Ys_X}(\delta^{h}_{s_X}-\delta^{h}_{s_{\hat{X}}}+V^{h}{}_{s_X,\mathrm{ad}(s_X)^{-1}s_Y}-V^{h}{}_{s_{\hat{X}},\mathrm{ad}(s_{\hat{X}})^{-1}s_{\hat{Y}}})\cdot \ell_h$$

$$=X+\tilde{\mathcal{V}}_X R_{X*}Y-\hat{X}-\tilde{\mathcal{V}}_{\hat{X}} R_{\hat{X}*}\hat{Y}\,. \tag{3.34}$$

For arbitrary vector fields X,Y,Z we define the *curvature tensor*

$$\mathcal{R}(X,Y)(Z)=\sum_{h\in S,\ h_1,h_2,h_3\in S_e} X^{h_1}Y^{h_2}Z^{h_3}\,\mathcal{R}^{h}{}_{h_3,h_1,h_2}\cdot \ell_h\,, \tag{3.35}$$

where the ambiguity in the quadrangle components is fixed by (3.13). If X,Y,Z are basic, we obtain

$$\mathcal{R}(X,Y)(Z)=\sum_{h\in S}\mathcal{R}^{h}{}_{s_Z,s_X,s_Y}\cdot \ell_h. \tag{3.36}$$

For further evaluation we need the following expressions,

$$\tilde{\mathcal{V}}_{R_{X*}Y}Z=\sum_{h_1}(R_{X*}Y)^{h_1}\,\tilde{\mathcal{V}}_{\ell_{h_1}}Z$$

$$=\sum_{h_1,h_2}(R_{X*}Y)^{h_1}(R^{*}_{h_1}Z^{h_2})\,\tilde{\mathcal{V}}_{\ell_{h_1}}\ell_{h_2}$$

$$=\sum_{h_1,h_2,h}(R_{X*}Y)^{h_1}(R^{*}_{h_1}Z^{h_2})\,V^{h}{}_{h_1,h_2}\cdot \ell_h \tag{3.37}$$

and

$$\tilde{\mathcal{V}}_X \tilde{\mathcal{V}}_{R_{X*Y}} Z = \sum_{h_1} X^{h_1} \tilde{\mathcal{V}}_{\ell_{h_1}} (\tilde{\mathcal{V}}_{R_{X*Y}} Z) = \sum_{h,h_1,h_2,h_3} X^{h_1} Y^{\mathrm{ad}(h_1)h_2} (R^*_{h_1 h_2} Z^{h_3}) (V_{h_1} R^*_{h_1} V_{h_2})^h{}_{h_3} \cdot \ell_h \tag{3.38}$$

using (I.5.21) and (I.5.12). With the help of these formulas we obtain

$$\mathcal{R}(X,Y)(Z) = \tilde{\mathcal{V}}_X \tilde{\mathcal{V}}_{R_{X*Y}} Z - Z \quad \text{for a biangle } X,Y, \tag{3.39}$$

$$\mathcal{R}(X,Y)(Z) = (\tilde{\mathcal{V}}_X \tilde{\mathcal{V}}_{R_{X*Y}} - \tilde{\mathcal{V}}_W) R_{W*} Z \quad \text{for a triangle } X,Y,W, \tag{3.40}$$

and

$$\begin{aligned} \mathcal{R}(X,Y;\hat{X},\hat{Y})(Z) &:= \mathcal{R}(X,Y)(Z) - \mathcal{R}(\hat{X},\hat{Y})(Z) \\ &= (\tilde{\mathcal{V}}_X \tilde{\mathcal{V}}_{R_{X*Y}} - \tilde{\mathcal{V}}_{\hat{X}} \tilde{\mathcal{V}}_{R_{\hat{X}*\hat{Y}}}) R_{(R_{X*Y})*} R_{X*} Z \\ &\quad \text{for a quadrangle } X,Y,\hat{X},\hat{Y}. \end{aligned} \tag{3.41}$$

The *Ricci tensor* defined in (3.14) can also be expressed as follows:

$$\mathrm{Ric}(X,Y) := \sum_{h \in S} \langle \mathcal{R}(\ell_h, Y)(X), \theta^h \rangle. \tag{3.42}$$

IV. RIEMANNIAN GROUP LATTICES ADMITTING A TORSION-FREE COMPATIBLE LINEAR CONNECTION

Let (G,S) be a bicovariant group lattice and (Ω,d) be the associated differential calculus. The formalism developed in the previous sections enables us to carry familiar constructions of continuum differential geometry over to group lattices. In particular, we may look for an analog of the *Levi-Civita connection* of a metric g. This means we should look for torsion-free linear connections which are compatible with g.

In Sec. II E a (bicovariant) group lattice supplied with a metric tensor g of constant signature has been called a ''Riemannian group lattice.'' In this section we further demand that it admits a *torsion-free* metric-compatible linear connection. Unlike the continuum case, on most group lattices not every metric admits such a connection. As we shall see below, this condition indeed places severe restrictions on the components of a metric. This should not come as a big surprise. In continuum differential geometry the requirement of a smooth metric on a smooth manifold guarantees that the metric components at ''neighboring'' points fit together. On the other hand, given a set of points in a Euclidean space, for example, and prescribing metric components at every point, a corresponding embedded digraph does not exist, in general. This is not the whole story, however. In the case of a maximal group lattice (complete digraph), which corresponds to a maximal set S, vanishing torsion already determines a unique linear connection, so that no freedom is left to satisfy the metric-compatibility conditions for a ''nontrivial'' geometry (see Sec. IV A). Reducing S to smaller sets allows for more freedom in a torsion-free connection and thus for more solutions of the metric-compatibility conditions.

If a metric-compatible linear connection is found for a given metric, it is only determined up to transformations $V_h \mapsto J_h V_h$ of the transport matrices with isometry matrices J_h (see Sec. II E) with coefficients $J^{h'}{}_{h,h''}$. Requiring vanishing torsion restricts this freedom, but in general does not fix it completely. In the following we elaborate this in more detail. More generally, we look separately at the consequences of vanishing biangle, triangle and quadrangle torsion together with the metric-compatibility condition. In the following, the matrices J_h are always constrained by the isometry condition (2.40).

(*a*) *Vanishing biangle torsion.* The biangle torsion vanishes for a biangle $h_1h_2=e$ (at some lattice site) if and only if

$$V^h{}_{h_1,h_2}=-\delta^h_{h_1} \quad \forall\, h\in S, \tag{4.1}$$

which is $V_{h_1,h_2}=-\ell_{h_1}$. Together with the compatibility condition (2.39), this leads to

$$R^*_{h_1}\mathfrak{g}_{h_2,h}=-\sum_{h'\in S}\mathfrak{g}_{h_1,h'}\,V^{h'}{}_{h_1,h} \quad \forall\, h\in S \tag{4.2}$$

and in particular

$$R^*_{h_1}\mathfrak{g}_{h_2,h_2}=\mathfrak{g}_{h_1,h_1} \quad (h_1h_2=e). \tag{4.3}$$

It is natural to assign to $\mathfrak{g}_{h_1,h_1}$ the interpretation of the square of the distance from g to gh_1. Then (4.3) tells us that this distance is equal to the reverse distance, i.e., that from gh_1 to g.

Remark: For making contact with ordinary discrete geometry, this suggests to demand vanishing biangle torsion. It should be noticed, however, that (4.3) does not necessarily require vanishing biangle torsion (see Sec. V B). Furthermore, in a communication network it is natural to allow the possibility of assigning different lengths (routing distances) to a direction and its inverse. ■

As a consequence of (4.1), only transformations of V_{h_1} are allowed with an isometry matrix J_{h_1} subject to

$$J^h{}_{h_1,h_1}=\delta^h_{h_1} \quad \forall\, h\in S. \tag{4.4}$$

This means $J_{h_1}\ell_{h_1}=\ell_{h_1}$, which restricts the freedom to isometries leaving the vector $V_{h_1,h_2}=-\ell_{h_1}$ invariant. These are rotations (including reflections) about V_{h_1,h_2}.

(*b*) *Vanishing triangle torsion.* The vanishing of the triangle torsion for a triangle $h_1h_2=h_0$ (at some lattice site) amounts to

$$V^h{}_{h_1,h_2}=\delta^h_{h_0}-\delta^h_{h_1} \quad \forall\, h\in S, \tag{4.5}$$

which is $V_{h_1,h_2}=\ell_{h_0}-\ell_{h_1}$. Together with (2.39) this implies

$$R^*_{h_1}\mathfrak{g}_{h_2,h}=\sum_{h'\in S}(\mathfrak{g}_{h_0,h'}-\mathfrak{g}_{h_2,h'})\,V^{h'}{}_{h_1,h} \quad \forall\, h\in S \tag{4.6}$$

and in particular

$$R^*_{h_1}\mathfrak{g}_{h_2,h_2}=\mathfrak{g}_{h_1,h_1}+\mathfrak{g}_{h_0,h_0}-2\,\mathfrak{g}_{h_0,h_1} \quad (h_1h_2=h_0). \tag{4.7}$$

Using the standard interpretation of the metric components, this is a well-known law of Euclidean geometry, the cosine law of triangles. Hence, the requirement of a metric-compatible and triangle-torsion-free linear connection restricts the metric in such a way that triangles are always flat. If triangle torsion is admitted, then it is possible to curve a triangle in such a way that the parallel transport is that of a spherical triangle, for example, see Sec. V A.

Equation (4.5) restricts the freedom of isometries in the transport matrices by

$$J^h{}_{h_1,h_0}-J^h{}_{h_1,h_1}=\delta^h_{h_0}-\delta^h_{h_1} \quad \forall\, h\in S, \tag{4.8}$$

which is $J_{h_1}(\ell_{h_0}-\ell_{h_1})=\ell_{h_0}-\ell_{h_1}$. Hence J_{h_1} corresponds to a ''rotation'' which leaves the vector $V_{h_1,h_2}=\ell_{h_0}-\ell_{h_1}$ fixed.

(*c*) *Vanishing quadrangle torsion*. The vanishing of the quadrangle torsion associated with a quadrangle $h_1h_2=\hat{h}_1\hat{h}_2=g\notin S_e$ (at some lattice site) means

$$V^h{}_{h_1,h_2}+\delta^h_{h_1}=V^h{}_{\hat{h}_1,\hat{h}_2}+\delta^h_{\hat{h}_1}\quad\forall\, h\in S \tag{4.9}$$

and thus $V_{h_1,h_2}-V_{\hat{h}_1,\hat{h}_2}=\ell_{\hat{h}_1}-\ell_{h_1}$. Together with the metric-compatibility condition this imposes restrictions on the metric components. In particular, for a positive definite metric the triangle inequalities lead to

$$|\|V_{h_1,h_2}\|-\|V_{\hat{h}_1,\hat{h}_2}\||\leqslant\|\ell_{h_1}-\ell_{\hat{h}_1}\|\leqslant\|V_{h_1,h_2}\|+\|V_{\hat{h}_1,\hat{h}_2}\|, \tag{4.10}$$

where $\|V_{h_1,h_2}\|=\sqrt{g(V_{h_1,h_2},V_{h_1,h_2})}$. Using (2.39), this restricts the metric components by

$$|\sqrt{R^*_{h_1}\mathfrak{g}_{h_2,h_2}}-\sqrt{R^*_{\hat{h}_1}\mathfrak{g}_{\hat{h}_2,\hat{h}_2}}|\leqslant\sqrt{\mathfrak{g}_{h_1,h_1}+\mathfrak{g}_{\hat{h}_1,\hat{h}_1}-2\,\mathfrak{g}_{h_1,\hat{h}_1}}\leqslant\sqrt{R^*_{h_1}\mathfrak{g}_{h_2,h_2}}+\sqrt{R^*_{\hat{h}_1}\mathfrak{g}_{\hat{h}_2,\hat{h}_2}}\,. \tag{4.11}$$

The isometries J_h have to satisfy the equation

$$\sum_{h'\in S}(J^h{}_{h_1,h'}-J^h{}_{\hat{h}_1,h'})\,V^{h'}{}_{h_1,h_2}=J^h{}_{\hat{h}_1,h_1}-\delta^h_{h_1}-J^h{}_{\hat{h}_1,\hat{h}_1}+\delta^h_{\hat{h}_1}\quad\forall\, h\in S, \tag{4.12}$$

which is $J_{h_1}V_{h_1,h_2}-J_{\hat{h}_1}V_{\hat{h}_1,\hat{h}_2}=\ell_{\hat{h}_1}-\ell_{h_1}$. In particular, a rotation which leaves V_{h_1,h_2} fixed, so that $J_{h_1}V_{h_1,h_2}=V_{h_1,h_2}$, together with a rotation which leaves $V_{\hat{h}_1,\hat{h}_2}$ fixed, so that $J_{\hat{h}_1}V_{\hat{h}_1,\hat{h}_2}=V_{\hat{h}_1,\hat{h}_2}$, preserves the quadrangle and thus solves the above constraint. Another possibility is given by combined rotations J_{h_1} and $J_{\hat{h}_1}$ which leave the vector $V_{h_1,h_2}-V_{\hat{h}_1,\hat{h}_2}$ and thus $\ell_{\hat{h}_1}-\ell_{h_1}$ fixed, so that $J_{h_1}(\ell_{h_1}-\ell_{\hat{h}_1})=\ell_{h_1}-\ell_{\hat{h}_1}$ and $J_{\hat{h}_1}(\ell_{h_1}-\ell_{\hat{h}_1})=\ell_{h_1}-\ell_{\hat{h}_1}$.

The following subsections provide examples of Riemannian group lattices which admit torsion-free linear connections. In the discussions we make use of the fact that a linear connection determines a tangent space picture of the group lattice, as described in Sec. II F.

A. Maximal group lattices

A group lattice (G,S) with $S=G\backslash\{e\}$ is called *maximal*. It is bicovariant and carries the universal differential calculus. There are only biangles and triangles, but no quadrangles. The condition of vanishing torsion determines a unique linear connection which is given by

$$V^h{}_{h_1,h_2}=\begin{cases}-\delta^h_{h_1} & \text{if } h_1h_2=e,\\ \delta^h_{h_0}-\delta^h_{h_1} & \text{if } h_0:=h_1h_2\neq e,\end{cases} \tag{4.13}$$

and thus constant. This implies $V_hV_{h^{-1}}=I$ and $V_{h_1}V_{h_2}=V_{h_0}$ if $h_1h_2=h_0$. As a consequence, the curvature of the connection vanishes.[14]

The metric compatibility condition evaluated for this connection becomes

$$R^*_h\mathfrak{g}_{h_1,h_2}=\begin{cases}\mathfrak{g}_{h,h}-\mathfrak{g}_{h,hh_2}-\mathfrak{g}_{hh_1,h}+\mathfrak{g}_{hh_1,hh_2} & \text{if } hh_1\neq e,\ hh_2\neq e,\\ \mathfrak{g}_{h,h}-\mathfrak{g}_{h,hh_2} & \text{if } hh_1=e,\ hh_2\neq e,\\ \mathfrak{g}_{h,h} & \text{if } h_1=h_2,\ hh_1=e.\end{cases} \tag{4.14}$$

Example 4.1: Let G be $\mathbb{Z}_3$, the cyclic group consisting of the three elements 0,1,2 with addition modulo 3 as the group composition. We choose the group lattice determined by S

$=\{1,2\}$ which is the complete digraph with three vertices. There are two biangles, $1+2=0=2+1$ (modulo 3), and two triangles, $1+1=2$ and $2+2=1$ (modulo 3). The unique torsion-free linear connection is determined by the two matrices

$$V_1=\begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \quad V_2=\begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}. \tag{4.15}$$

A metric is given by

$$\mathfrak{g}=\begin{pmatrix} a & b \\ b & c \end{pmatrix} \tag{4.16}$$

with functions a,b,c, and the compatibility condition with the above connection reduces to

$$R_1^*\begin{pmatrix} a & b \\ b & c \end{pmatrix}=\begin{pmatrix} a-2b+c & a-b \\ a-b & a \end{pmatrix}. \tag{4.17}$$

This means that one can specify arbitrary values of the metric functions a,b,c at *one* point. The metric at the other points is then determined by the last equation and the resulting metric on $\mathbb{Z}_3$ is compatible with the above torsion-free connection. Assigning the usual interpretation in terms of Euclidean distances and angles to the metric components, one recovers the rules of Euclidean trigonometry. In particular, in case of a constant metric, the compatibility condition restricts $\mathfrak{g}$ to

$$\mathfrak{g}=a\begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \tag{4.18}$$

with a constant a. This expresses metric properties of a regular Euclidean triangle. The parallel transport determined by the torsion-free connection coincides with that of the Euclidean plane. Indeed, from (2.41) we infer

at $k+1$ mod 3			at k mod 3	at $k+2$ mod 3			at k mod 3
$\tilde{\mathcal{V}}_{\ell_1}$:	ℓ_1	$\mapsto$	$\ell_2-\ell_1$	$\tilde{\mathcal{V}}_{\ell_2}$:	ℓ_1	$\mapsto$	$-\ell_2$
	ℓ_2		$-\ell_1$		ℓ_2		$\ell_1-\ell_2$

which maps the Riemannian group lattice isometrically onto a Euclidean triangle in the tangent space at a site. ■

Example 4.2: Let $G=\mathbb{Z}_4$, $S=\{1,2,3\}$. The torsion-free linear connection is then given by

$$V_1=\begin{pmatrix} -1 & -1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad V_2=\begin{pmatrix} 0 & 0 & 1 \\ -1 & -1 & -1 \\ 1 & 0 & 0 \end{pmatrix}, \quad V_3=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & -1 & -1 \end{pmatrix}. \tag{4.19}$$

Assuming the metric to be constant, the compatibility condition restricts it to the form

$$\mathfrak{g}=\begin{pmatrix} a & b & a-b \\ b & 2b & b \\ a-b & b & a \end{pmatrix}. \tag{4.20}$$

For $b=a/2$ we recover the geometry of a regular tetrahedron in Euclidean $\mathbb{R}^3$. Since we deal with a three-dimensional Riemannian group lattice, we are actually describing the tetrahedron volume. Furthermore, in the limit $b\to a$ the above geometry tends to that of a quadrate in the Euclidean

plane where the vector associated with $2 \in S$ corresponds to the diagonal. Accordingly, in this limit the determinant of $\mathfrak{g}$ vanishes, so that $\mathfrak{g}$ no longer defines a metric according to our definition in Sec. II E. ■

B. Two-dimensional Riemannian group lattices

Let G be a discrete group and $S=\{a,b\}$ be a subset consisting of two different elements of G which generate G such that (G,S) is a bicovariant group lattice. Then either $aba^{-1}=a$, which contradicts $a\neq b$, or $aba^{-1}=b$, which is $ab=ba$. Hence, bicovariance requires that G is Abelian. By a fundamental theorem, every finite Abelian group is isomorphic to a direct product of cyclic groups of prime power order.

The following examples in particular demonstrate that, for a given metric on a group lattice, there may not exist a metric-compatible linear connection with vanishing torsion, i.e., a Levi-Civita connection. Moreover, in contrast to ordinary continuum differential geometry, if such a connection exists, then is not unique in general.

1. $\mathbb{Z}_4$ lattices

(a) Let $G=\mathbb{Z}_4$ and $S=\{1,2\}$. There is one biangle, $2+2=0$ (modulo 4), one triangle, $1+1=2$, and one quadrangle, $1+2=3=2+1$, which implies the 2-form relation $\theta^1\cap\theta^2=-\theta^2\cap\theta^1$. Vanishing torsion restricts the matrices V_i of the linear connection to

$$V_1=\begin{pmatrix} -1 & p \\ 1 & 1+q \end{pmatrix}, \quad V_2=\begin{pmatrix} 1+p & 0 \\ q & -1 \end{pmatrix} \tag{4.21}$$

with arbitrary functions p and q. For a metric of the form (4.16), the metric-compatibility condition $R_1^*\mathfrak{g}=V_1^T\mathfrak{g}V_1$ reads

$$\begin{gathered} R_1^*a=a-2\,b+c\,, \quad R_1^*b=p\,(b-a)+(1+q)(c-b)\,, \\ R_1^*c=p^2\,a+2\,p\,(1+q)\,b+(1+q)^2\,c. \end{gathered} \tag{4.22}$$

With the help of $R_2^*=(R_1^*)^2$, the second condition $R_2^*\mathfrak{g}=V_2^T\mathfrak{g}V_2$ leads to $V_1\,(R_1^*V_1)\,V_2^{-1}=J$, where J is an arbitrary element of the isometry group of the metric (at each site of the group lattice). A lengthy computation, aided by computer algebra, reveals that *every Levi-Civita connection on* $(\mathbb{Z}_4,\{1,2\})$ *is flat, i.e., its curvature vanishes*.[15] The integrability condition (3.27) then enforces $J=I$ so that $V_2=V_1\,R_1^*V_1$. As a consequence, we obtain the following representation of $\mathbb{Z}_4$: $R_1^*p=-p/(1+p+q)$, $R_1^*q=-(2+p+q)/(1+p+q)$. This implies $R_2^*p=-p/(1+p)$ and $R_2^*q=q/(1+p)$ and thus $(R_1^*)^4p=(R_2^*)^2p=p$, $(R_1^*)^4q=(R_2^*)^2q=q$.

Excluding special values of $q(0)$ and $p(0)$, the geometries with a Levi-Civita connection are given by

$$\begin{aligned} &a(1)=a(0)-2\,b(0)+c(0)\,, \quad b(1)=-p(0)\,a(0)+[p(0)-1-q(0)]\,b(0)+[1+q(0)]\,c(0), \\ &c(1)=p(0)^2\,a(0)+2\,p(0)\,[1+q(0)]\,b(0)+[1+q(0)]^2\,c(0), \\ &a(2)=[1+p(0)]^2\,a(0)+2\,q(0)\,[1+p(0)]\,b(0)+q(0)^2\,c(0), \\ &b(2)=-[1+p(0)]\,b(0)-q(0)\,c(0)\,, \quad c(2)=c(0), \\ &a(3)=[1+p(0)]^2\,a(0)+2\,[1+p(0)]\,[1+q(0)]\,b(0)+[1+q(0)]^2\,c(0), \\ &b(3)=p(0)\,[1+p(0)]\,a(0)+[1+2\,p(0)]\,[1+q(0)]\,b(0)+[1+q(0)]^2\,c(0), \\ &c(3)=p(0)^2\,a(0)+2\,p(0)\,[1+q(0)]\,b(0)+[1+q(0)]^2\,c(0), \end{aligned} \tag{4.23}$$

and

$$q(1)=-[2+p(0)+q(0)]/[1+p(0)+q(0)], \quad p(1)=-p(0)/[1+p(0)+q(0)],$$
$$q(2)=q(0)/[1+p(0)], \quad p(2)=-p(0)/[1+p(0)], \tag{4.24}$$
$$q(3)=-[2+p(0)+q(0)]/[1+q(0)], \quad p(3)=p(0)/[1+q(0)].$$

(*b*) Let $G=\mathbb{Z}_4$ again, but now we choose $S=\{1,3\}$. In this case, there are two biangles, $1+3=0=3+1$ (modulo 4), no triangle and a quadrangle corresponding to $1+1=2=3+3$ (modulo 4). The latter leads to the 2-form relation $\theta^1\cap\theta^1+\theta^3\cap\theta^3=0$. The condition of vanishing torsion imposes the following restrictions on a linear connection,

$$V_1=\begin{pmatrix} u & -1 \\ 1+v & 0 \end{pmatrix}, \quad V_3=\begin{pmatrix} 0 & 1+u \\ -1 & v \end{pmatrix}, \tag{4.25}$$

with arbitrary functions u and v. For a metric of the form (4.16) the compatibility condition $R_1^*\mathfrak{g}=V_1^T\mathfrak{g}V_1$ reads

$$R_1^*a=u^2\,a+2u(1+v)\,b+(1+v)^2\,c\,, \quad R_1^*b=-u\,a-(1+v)\,b\,, \quad R_1^*c=a, \tag{4.26}$$

and, with the help of $R_3^*=(R_1^*)^3$, the second metric-compatibility condition $R_3^*\mathfrak{g}=V_3^T\mathfrak{g}V_3$ leads to $V_1\,(R_1^*V_1)[(R_1^*)^2V_1]\,V_3^{-1}=J$ where J is an element of the isometry group of the metric. Further exploration with the help of computer algebra shows that *every Levi-Civita connection on* $(\mathbb{Z}_4,\{1,3\})$ *has vanishing curvature.*

Since the only metric-compatible torsion-free linear connections on the above $\mathbb{Z}_4$ lattices have vanishing curvature, via backward parallel transport they are isometrically mapped to a closed lattice in $\mathbb{R}^2$ which represents the tangent space at a site. In particular, this means that we cannot model something like a tetrahedron surface in this way. To supply the $\mathbb{Z}_4$ group lattices with nonvanishing curvature is only possible if the condition of vanishing torsion is dropped (see Sec. V B).

2. $\mathbb{Z}^2$ lattices

Let us consider the group lattice $(\mathbb{Z}^2,\{\hat{1},\hat{2}\})$ where $\hat{1}:=(1,0)$ and $\hat{2}:=(0,1)$. It has no biangles or triangles, but a quadrangle corresponding to $\hat{1}+\hat{2}=\hat{2}+\hat{1}$. The condition of vanishing torsion restricts the parallel transport matrices $V_i:=V_{\hat{i}}$ to

$$V_1=\begin{pmatrix} p & u \\ q & 1+v \end{pmatrix}, \quad V_2=\begin{pmatrix} 1+u & r \\ v & s \end{pmatrix} \tag{4.27}$$

with arbitrary functions p,q,r,s,u,v. The following example demonstrates that there are torsion-free and metric-compatible parallel transports with *non*vanishing curvature even on a two-dimensional lattice carrying the metric properties of a regular quadratic lattice in Euclidean $\mathbb{R}^2$.

Example 4.3: Let us choose the metric to be

$$\mathfrak{g}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.28}$$

at all sites. The metric-compatibility condition for the above torsion-free linear connection then leads to the following two classes of solutions. The first class is given by

$$V_1=\begin{pmatrix} \epsilon_1 & 0 \\ 0 & 1 \end{pmatrix}, \quad V_2=\begin{pmatrix} 1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} \tag{4.29}$$

with functions ϵ_i with values in $\{\pm 1\}$. The curvature only vanishes if ϵ_1 and ϵ_2 are constant in the $\hat{1}$ and $\hat{2}$ direction, respectively.

If the curvature vanishes, the (backward) parallel transport does not depend on the path in the lattice, see (2.45). It can thus be used to map the whole group lattice into the tangent space at one point, which is isomorphic to $\mathbb{R}^2$ in the case under consideration. Let us choose the lattice point (0,0). The tangent vectors ℓ_h at this site may then be identified with the vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ pointing from (0,0) to (1,0) and (0,1), respectively, in $\mathbb{R}^2$. Then $\ell_{\hat{1}}$ at the group lattice site (1,0) is mapped to the vector $\mathbf{V}_{1,1}$ which we attach at the tip of $\mathbf{u}_1$ in $\mathbb{R}^2$ according to the prescription of Sec. II F. If $\epsilon_1 = -1$, this vector points into the "wrong direction," i.e., its tip coincides with (0,0). This means that the resulting lattice in $\mathbb{R}^2$ gets *folded*. Similarly, if $\epsilon_2 = -1$, the lattice gets folded in the other direction.

A particular solution is given by $V_h = I$, the unit matrix, at all sites. It corresponds to the ordinary Euclidean parallel transport. This solution certainly has a nice continuum limit. Introducing a lattice spacing parameter, we may write $V_h = I + \kappa \Gamma_h + O(\kappa^2)$. Some of the other solutions V_h given above have negative determinant at some sites and cause folding in the sense described above. They are related to the above solution at those sites by an isometry J_h with determinant -1. As a consequence, they cannot have a continuum limit. The requirement of a continuum limit may thus distinguish a certain connection and eliminate connections with folding.

The second class of solutions is given by

$$V_1 = \begin{pmatrix} 0 & -1 \\ \epsilon_1 & 0 \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 & \epsilon_2 \\ -1 & 0 \end{pmatrix}. \tag{4.30}$$

The curvature only vanishes if at all sites $R_2^* \epsilon_1 = \epsilon_2$ and $R_1^* \epsilon_2 = \epsilon_1$. An orientation-preserving connection is obtained if $\epsilon_1 = \epsilon_2 = 1$. The corresponding transports in the two directions act with rotations. ■

There are metrics (with constant signature) on $(\mathbb{Z}^2, \{\hat{1}, \hat{2}\})$ which do *not* admit a Levi-Civita connection, although the constraints are by far not as stringent as in our previous examples. Counterexamples are easily constructed. A geometric condition for the existence of a Levi-Civita connection is given by (4.11) in the case of a positive definite metric. Let us recall its origin in the case under consideration. The tangent space at a site a is isomorphic to $\mathbb{R}^2$ with the Euclidean inner product of vectors (see Sec. II F). The tangent vectors $\ell_{\hat{i}}$ are then represented by vectors $\mathbf{u}_i \in \mathbb{R}^2$, $i = 1,2$, such that $\mathbf{u}_i \cdot \mathbf{u}_j = \mathfrak{g}_{ij}(a)$ where $\mathfrak{g}_{ij} := \mathfrak{g}_{\hat{i},\hat{j}}$. The parallel transport $\widetilde{\mathcal{V}}_{\ell_{\hat{i}}}$ maps the tangent space at the site $a + \hat{i}$ into the tangent space at a. Metric-compatibility of the connection means

$$\mathbf{V}_{ij} \cdot \mathbf{V}_{ik} = \mathfrak{g}_{jk}(a + \hat{i}), \tag{4.31}$$

where $\mathbf{V}_{ij}$ represents $\widetilde{\mathcal{V}}_{\ell_{\hat{i}}} \ell_{\hat{j}}$ at the site a. If the connection is (quadrangle) torsion free, then adjacent quadrangles are preserved by the backward parallel transport, so that $\mathbf{u}_i + \mathbf{V}_{ij} = \mathbf{u}_j + \mathbf{V}_{ji}$. The last equation has solutions if and only if $\|\mathbf{V}_{12}| - |\mathbf{V}_{21}\| \leq |\mathbf{u}_2 - \mathbf{u}_1| \leq |\mathbf{V}_{12}| + |\mathbf{V}_{21}|$, where $|\mathbf{V}_{12}|$ denotes the Euclidean norm of $\mathbf{V}_{12}$ in $\mathbb{R}^2$. This is illustrated in Fig. 1. Using (4.31), this condition is expressed as

$$|\sqrt{\mathfrak{g}_{22}(a+\hat{1})} - \sqrt{\mathfrak{g}_{11}(a+\hat{2})}| \leq \sqrt{\mathfrak{g}_{11}(a) + \mathfrak{g}_{22}(a) - 2\,\mathfrak{g}_{12}(a)} \leq \sqrt{\mathfrak{g}_{22}(a+\hat{1})} + \sqrt{\mathfrak{g}_{11}(a+\hat{2})} \tag{4.32}$$

in terms of the metric at the sites a, $a + \hat{1}$ and $a + \hat{2}$ [see also (4.11)]. If this condition is not fulfilled, a Levi-Civita connection does not exist. If the condition is satisfied, a Levi-Civita connection exists, but it is not unique. Even if equality holds in the last part of (4.32), so that the circles in Fig. 1 have exactly one point in common, we still have the freedom to choose $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$ in two possible ways, as illustrated in Fig. 2.

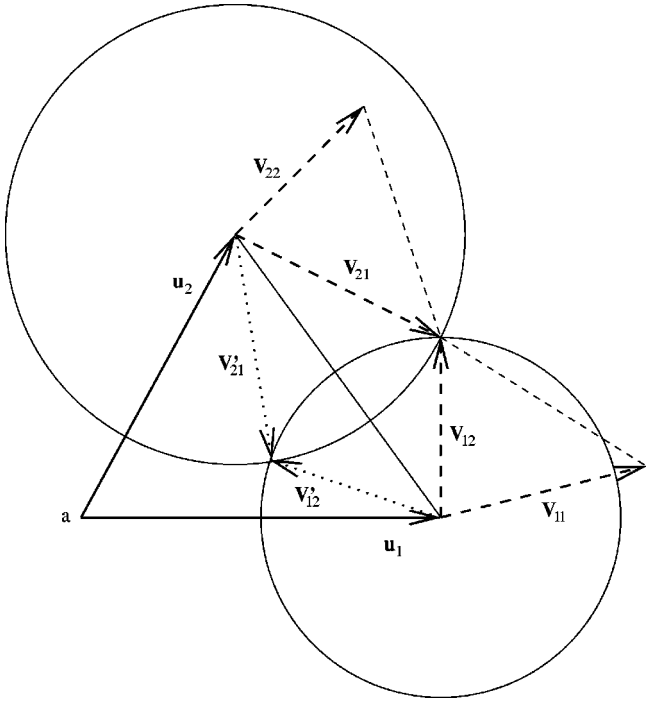

FIG. 1. Levi-Civita connections on a $\mathbb{Z}^2$ lattice exist iff at each lattice site the circle with radius $|\mathbf{V}_{12}|$ around the tip of $\mathbf{u}_1$ intersects the circle with radius $|\mathbf{V}_{21}|$ around the tip of $\mathbf{u}_2$.

The freedom in the parallel transport left by the conditions of metric-compatibility and vanishing torsion is a freedom of reflections about some axes. In Fig. 2 it shows up as reflections about the three axes AC, BC and AB. In Sec. IV C we show that reflections about AB and BC and their composition comprise the whole freedom left for V_1 and V_2 by the conditions of vanishing torsion and metric-compatibility. Such reflections lead to folding of the tangent space lattice obtained by backward parallel transport of the group lattice to the tangent space at a. Moreover, the orientation of some of the frames at a obtained by backward parallel transport of frames of basic tangent vectors at $a+\hat{\imath}$, $i=1,2$, gets changed. This can be excluded by demanding that $\det V_i>0$. But we should also require that the dyad $(\mathbf{V}_{21},\mathbf{V}_{12})$ has positive orientation, which is necessary in order to avoid reflections about the axis AB. This amounts to $V^1{}_{12}+V^2{}_{12}>0$. In higher dimensions, the determination of the ambiguities in the Levi-Civita connections and their reduction appears to be a difficult task (see also Sec. IV C).

Whereas torsion is a first order quantity, curvature is of second order since it expresses features of the geometry determined by the composition of *two* (backward) parallel transports. In the case under consideration, the components of the curvature tensor are given in matrix form by $\mathcal{R}_{ij}:=V_i R_{\hat{i}}^{*} V_j - V_j R_{\hat{j}}^{*} V_i$. In Fig. 3 the vector $\mathbf{z}$ represents $\tilde{\mathcal{V}}_{\ell_1}\tilde{\mathcal{V}}_{\ell_2} Z$ where $Z=\Sigma_i Z^i\cdot \ell_{\hat{\imath}}$. Hence

$$\mathbf{z}=\sum_{i,j}\ \mathbf{u}_i\,[V_1(a)V_2(a+\hat{1})]^i{}_j\,Z^j(a+\hat{1}+\hat{2}). \tag{4.33}$$

The vector $\mathbf{z}'$ represents $\tilde{\mathcal{V}}_{\ell_2}\tilde{\mathcal{V}}_{\ell_1} Z$, so that

$$\mathbf{z}'=\sum_{i,j}\ \mathbf{u}_i\,[V_2(a)V_1(a+\hat{2})]^i{}_j\,Z^j(a+\hat{2}+\hat{1}). \tag{4.34}$$

The difference gives a measure of the curvature at a [see also (2.45)]:

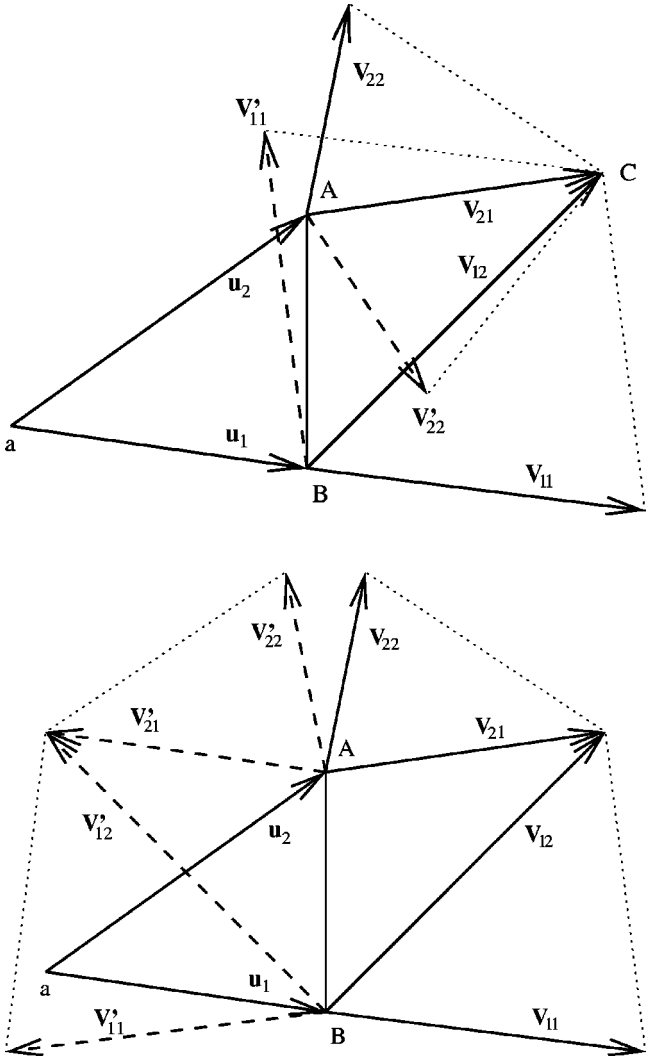

FIG. 2. The vectors $\mathbf{V}_{ij}$ and $\mathbf{V}'_{ij}$ result from torsion-free metric-compatible (backward) parallel transports which differ by a reflection about some axis.

$$\mathbf{z}-\mathbf{z}'=\sum_{i,j}\mathbf{u}_i\,\mathcal{R}^{i}{}_{j12}(a)\,Z^j(a+\hat{1}+\hat{2}). \tag{4.35}$$

If the torsion vanishes at a site a, one can draw an isometric picture of the geometry in the tangent space at a to first order. This represents the site a, its first order neighbors $a+\hat{\imath}$, and the basic tangent vectors at these sites while preserving the metric properties at all these sites and preserving biangles, triangles and quadrangles at a. If, moreover, the curvature vanishes at a, then we can draw an isometric picture to second order.

C. Freedom of Levi-Civita connections on a hypercubic $\mathbb{Z}^n$ lattice

We already learned that, in general, there is no Levi-Civita connection for a given metric on a group lattice. If such a connection exists, it need not be unique. The corresponding freedom will be explored in this section for the case of hypercubic $\mathbb{Z}^n$ lattices given by $G=\mathbb{Z}^n$ and $S=\{\hat{\imath}\mid i=1,\ldots,n\}$, where $\hat{\imath}:=(0,\ldots,1,\ldots,0)$ with the 1 in the ith position. We consider only positive

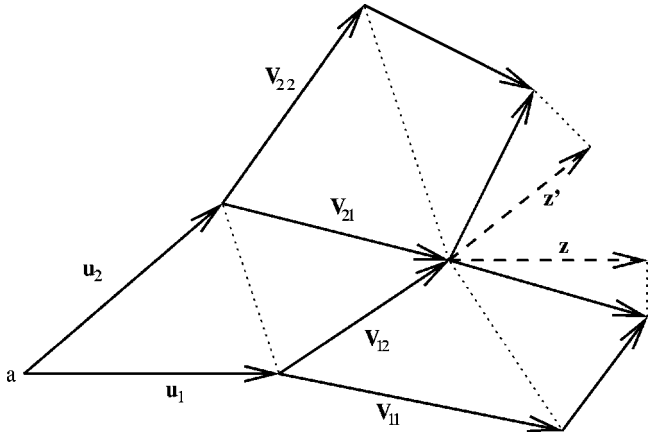

FIG. 3. The familiar effect of curvature: backward parallel transport along different paths results in different vectors in the tangent space at a point.

definite metrics and choose the standard inner product $(\mathbf{u},\mathbf{v})=\mathbf{u}\cdot\mathbf{v}$ for $\mathbf{u},\mathbf{v}\in\mathbb{R}^n$ (cf. Sec. II F). In the case of a hypercubic group lattice the condition of vanishing torsion can be expressed as

$$\mathbf{u}_i+\mathbf{V}_{ij}=\mathbf{u}_j+\mathbf{V}_{ji}\,. \tag{4.36}$$

Together with the metric-compatibility, this determines a Levi-Civita connection up to isometries J_i which preserve the above conditions, i.e.,

$$\mathbf{u}_i+J_i(\mathbf{V}_{ij})=\mathbf{u}_j+\mathbf{J}_j(\mathbf{V}_{ji}) \tag{4.37}$$

[see also (2.48)]. Subtracting (4.36) from (4.37), we find

$$\mathbf{A}_{ij}=\mathbf{A}_{ji}\quad\text{where}\quad\mathbf{A}_{ij}:=J_i(\mathbf{V}_{ij})-\mathbf{V}_{ij}\,. \tag{4.38}$$

Using the isometry condition (2.49) and the last equation, we obtain

$$\mathbf{V}_{ij}\cdot\mathbf{V}_{ij}=J_i(\mathbf{V}_{ij})\cdot J_i(\mathbf{V}_{ij})=\mathbf{V}_{ij}\cdot\mathbf{V}_{ij}+\mathbf{A}_{ij}\cdot(\mathbf{A}_{ij}+2\,\mathbf{V}_{ij}) \tag{4.39}$$

so that

$$\mathbf{A}_{ij}\cdot(\mathbf{A}_{ij}+2\,\mathbf{V}_{ij})=0 \tag{4.40}$$

and because of (4.38) also

$$\mathbf{A}_{ij}\cdot(\mathbf{A}_{ij}+2\,\mathbf{V}_{ji})=0. \tag{4.41}$$

Subtracting the last two equations and using (4.36) leads to

$$\mathbf{A}_{ij}\cdot(\mathbf{u}_j-\mathbf{u}_i)=0. \tag{4.42}$$

For $i\neq j$ and if $\mathbf{A}_{ij}\neq 0$, we set $\mathbf{A}_{ij}=\alpha_{ij}\,\mathbf{a}_{ij}$ with a unit vector $\mathbf{a}_{ij}$ orthogonal to $\mathbf{u}_j-\mathbf{u}_i$. From (4.40) we then obtain $\alpha_{ij}=-2\,\mathbf{a}_{ij}\cdot\mathbf{V}_{ij}=0$, so that

$$\mathbf{A}_{ij}=-2\,(\mathbf{a}_{ij}\cdot\mathbf{V}_{ij})\,\mathbf{a}_{ij} \tag{4.43}$$

and thus

$$J_i(\mathbf{V}_{ij})=\mathbf{V}_{ij}-2\,(\mathbf{a}_{ij}\cdot\mathbf{V}_{ij})\,\mathbf{a}_{ij}\,,\quad J_j(\mathbf{V}_{ji})=\mathbf{V}_{ji}-2\,(\mathbf{a}_{ij}\cdot\mathbf{V}_{ji})\,\mathbf{a}_{ij}. \tag{4.44}$$

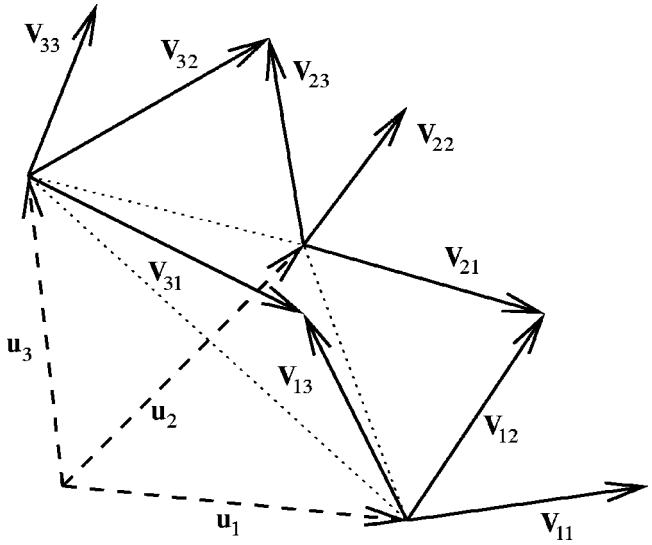

FIG. 4. Tangent space picture of the nearest neighborhood for the cubic $\mathbb{Z}^3$ lattice, as determined by a Levi-Civita connection. The freedom in the choice of such a connection is due to reflections with respect to hyperplanes through $\mathbf{u}_i - \mathbf{u}_j$, $i \neq j$.

As a consequence, the effect of J_i on $\mathbf{V}_{ij}$ is that of a reflection with respect to the hyperplane orthogonal to $\mathbf{a}_{ij}$ (which in turn is orthogonal to $\mathbf{u}_j - \mathbf{u}_i$). If $\mathbf{A}_{ij} \neq 0$ for all $j \neq i$, then J_i for a fixed i reflects all the $n-1$ vectors $\mathbf{V}_{ij}$, $j \neq i$, with respect to the respective hyperplane (orthogonal to $\mathbf{a}_{ij}$). Of course, we still have to respect the remaining conditions which arise from the isometry conditions (2.49), i.e., $J_i(\mathbf{V}_{ik}) \cdot J_i(\mathbf{V}_{il}) = \mathbf{V}_{ik} \cdot \mathbf{V}_{il}$.

Let us look at the two-dimensional case. If $\mathbf{A}_{12} = 0$, we have $J_1(\mathbf{V}_{12}) = \mathbf{V}_{12}$ and $J_2(\mathbf{V}_{21}) = \mathbf{V}_{21}$, so J_1 and J_2 are reduced to reflections about $\mathbf{V}_{12}$ and $\mathbf{V}_{21}$, respectively. If $\mathbf{A}_{12} \neq 0$, then we have $J_1(\mathbf{V}_{12}) = \mathbf{V}_{12} - 2\,(\mathbf{a}_{12} \cdot \mathbf{V}_{12})\,\mathbf{a}_{12}$, $J_2(\mathbf{V}_{21}) = \mathbf{V}_{21} - 2\,(\mathbf{a}_{12} \cdot \mathbf{V}_{21})\,\mathbf{a}_{12}$. The effect of both is a reflection about the axis along $\mathbf{u}_2 - \mathbf{u}_1$. If H_{12} is such a reflection, then $H_{12} J_1(\mathbf{V}_{12}) = \mathbf{V}_{12}$ and $H_{12} J_2(\mathbf{V}_{21}) = \mathbf{V}_{21}$ which reduces the problem to the case $\mathbf{A}_{12} = 0$ for $H_{12} J_i$. In three dimensions (see Fig. 4) a classification of the various possibilities already turns out to be quite involved.

V. GROUP LATTICE GEOMETRIES WITH TORSION

Section IV demonstrated that Riemannian group lattices in general do not possess a Levi-Civita connection. In some cases only *flat* Levi-Civita connections exist so that one has to allow for nonvanishing torsion in order to get nonvanishing curvature and thus enough flexibility to assign a nontrivial geometry to the group lattice. Relaxing the previous requirement of vanishing torsion clearly opens more possibilities for modeling discrete surfaces. In fact, the following examples demonstrate that linear connections with torsion naturally appear as properties of Riemannian group lattice geometries. The first subsection below shows how in the presence of torsion a triangle can be curved so that it fits on the surface of a sphere. The remaining subsection treats a $\mathbb{Z}_4$ lattice example.

A. A $\mathbb{Z}_3$ lattice geometry with torsion

Let $G = \mathbb{Z}_3$ and $S = \{1,2\}$. According to Sec. III the components of the torsion tensor are

$$
\begin{aligned}
&Q^1{}_{1,1} = 1 + V^1{}_{1,1}, \quad Q^1{}_{1,2} = 1 + V^1{}_{1,2}, \quad Q^1{}_{2,1} = V^1{}_{2,1}, \quad Q^1{}_{2,2} = -1 + V^1{}_{2,2}, \\
&Q^2{}_{1,1} = -1 + V^2{}_{1,1}, \quad Q^2{}_{1,2} = V^2{}_{1,2}, \quad Q^2{}_{2,1} = 1 + V^2{}_{2,1}, \quad Q^2{}_{2,2} = 1 + V^2{}_{2,2}.
\end{aligned}
\tag{5.1}
$$

If we do not require the vanishing of the whole torsion, but only of the biangle part, i.e., $Q^h_{(0)\,1,2}=Q^h_{(0)\,2,1}=0$, then we can simulate the geometry of a spherical triangle. Setting

$$\mathfrak{g}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{5.2}$$

a particular solution of the metric-compatibility conditions is

$$V_1=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \quad V_2=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}. \tag{5.3}$$

Now (2.41) leads to

	at $k+1$ mod 3		at k mod 3		at $k+2$ mod 3		at k mod 3
$\tilde{\mathcal{V}}_{\ell_1}$:	ℓ_1 ℓ_2	$\mapsto$	ℓ_2 $-\ell_1$	$\tilde{\mathcal{V}}_{\ell_2}$:	ℓ_1 ℓ_2	$\mapsto$	$-\ell_2$ ℓ_1

which matches the parallel transport along a spherical triangle. The curvature tensor has only triangle components. Using the matrix notation $\mathcal{R}_{h_1,h_2}=(\mathcal{R}^h{}_{h',h_1,h_2})$, we obtain

$$\mathcal{R}_{(2)\,1,1}=\begin{pmatrix}-1 & -1\\ 1 & -1\end{pmatrix}, \quad \mathcal{R}_{(1)\,2,2}=\begin{pmatrix}-1 & 1\\ -1 & -1\end{pmatrix}, \tag{5.4}$$

and $\mathcal{R}_{(0)\,1,2}=\mathcal{R}_{(0)\,2,1}=0$ (vanishing biangle curvature). The Ricci tensor $\mathrm{Ric}_{h,h'}=\mathcal{R}^1{}_{h,1,h'}+\mathcal{R}^2{}_{h,2,h'}$ is given by

$$\mathrm{Ric}=-\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} \tag{5.5}$$

in matrix notation, and the curvature scalar is $R=-2$. The torsion 2-form is given by

$$\Theta^1=\theta^1\cap\theta^1, \quad \Theta^2=\theta^2\cap\theta^2. \tag{5.6}$$

This is an example of a geometry which cannot be isometrically embedded in a Euclidean space $\mathbb{R}^n$ for any $n\in\mathbb{N}$, simply due to the fact that with the choice of metric (5.2) the sum of the angles of the triangle is $3\pi/2$ and not π as in Euclidean geometry. This fact is taken care of by the torsion of the connection which causes the backward parallel transport of the group lattice triangle not to close to a triangle in the tangent space at a site. The resulting picture in $\mathbb{R}^2$, which represents the tangent space at the unit element, is drawn in Fig. 5. Here we used $\mathbf{V}_{11}=-\mathbf{V}_{21}=\mathbf{u}_2$, $\mathbf{V}_{12}=-\mathbf{V}_{22}=-\mathbf{u}_1$ which follows from (5.3). The triangle torsion satisfies

$$\sum_i \mathbf{u}_i Q^i{}_{1,1}=\mathbf{u}_1+\mathbf{V}_{11}-\mathbf{u}_2=\mathbf{u}_1, \quad \sum_i \mathbf{u}_i Q^i{}_{2,2}=\mathbf{u}_2+\mathbf{V}_{22}-\mathbf{u}_1=\mathbf{u}_2. \tag{5.7}$$

From (2.47) we obtain $\mathbf{V}_{111}=\mathbf{V}_{221}=-\mathbf{u}_1$, $\mathbf{V}_{112}=\mathbf{V}_{222}=-\mathbf{u}_2$ and, using (2.45) and (3.11), the following curvature expressions:

$$\begin{aligned}&\sum_i \mathbf{u}_i \mathcal{R}^i{}_{(2)\,1,1,1}=-\mathbf{u}_1+\mathbf{u}_2, \quad \sum_i \mathbf{u}_i \mathcal{R}^i{}_{(2)\,2,1,1}=-\mathbf{u}_2-\mathbf{u}_1,\\ &\sum_i \mathbf{u}_i \mathcal{R}^i{}_{(1)\,1,2,2}=-\mathbf{u}_1-\mathbf{u}_2, \quad \sum_i \mathbf{u}_i \mathcal{R}^i{}_{(1)\,2,2,2}=-\mathbf{u}_2+\mathbf{u}_1.\end{aligned} \tag{5.8}$$

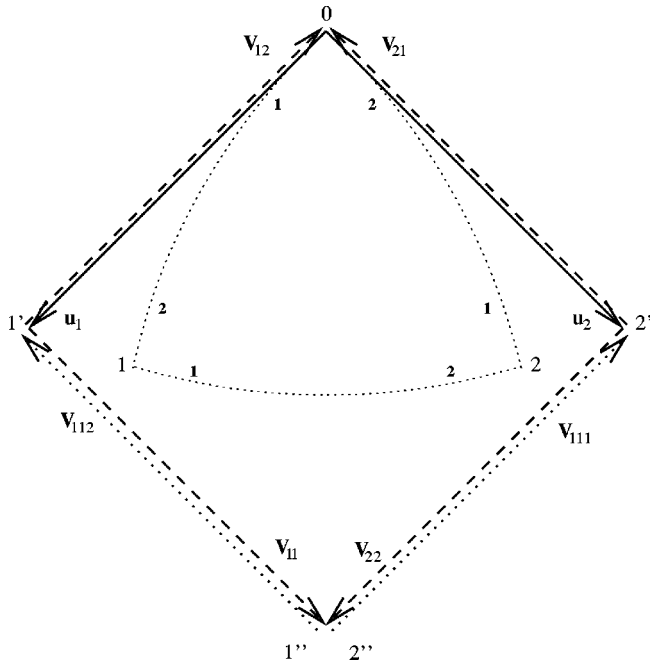

FIG. 5. The result of backward parallel transport of the group lattice $(\mathbb{Z}_3,\{1,2\})$ into the tangent space at 0, using the connection given by (5.3). The points $1'$ and $1''$, and also $2'$ and $2''$, do not coincide because of nonvanishing torsion.

B. The group lattice $(\mathbb{Z}_4,\{1,2\})$

Let $G=\mathbb{Z}_4$ and $S=\{1,2\}$. The torsion of a linear connection has the following components:

$$
\begin{aligned}
&Q^h{}_{2,2}=V^h{}_{2,2}+\delta^h_2 \quad \text{for the biangle } 2+2=0,\\
&Q^h{}_{1,1}=V^h{}_{1,1}-\delta^h_2+\delta^h_1 \quad \text{for the triangle } 1+1=2,\\
&Q^h{}_{2,1}=-Q^h{}_{1,2}=Q^h{}_{1,2;2,1}=V^h{}_{1,2}-V^h{}_{2,1}-\delta^h_2+\delta^h_1 \quad \text{for the quadrangle } 1+2=2+1=3\,.
\end{aligned}
\tag{5.9}
$$

(a) If we require vanishing biangle and triangle torsion, but nonvanishing quadrangle torsion, the coefficient matrices of the parallel transport have the form

$$
V_1=\begin{pmatrix} -1 & p \\ 1 & 1+q \end{pmatrix}, \quad V_2=\begin{pmatrix} 1+r & 0 \\ s & -1 \end{pmatrix} \tag{5.10}
$$

with functions p,q,r,s. As an example, choosing the constant metric

$$
\mathfrak{g}(k)=\begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}, \quad k=0,1,2,3 \tag{5.11}
$$

(which is the metric of a regular tetrahedron surface immersed in three-dimensional Euclidean space), and assuming also constant transport matrices, the compatibility conditions with the connection given by (5.10) take the form

$$
q=p\,, \quad p(p+1)=0, \quad s=-1-r/2\,, \quad r(r+2)=0, \tag{5.12}
$$

so that there are four different connections which are compatible with the metric. All solutions have vanishing biangle curvature. The solution with $p=-1,\ r=0$ has nonvanishing triangle and

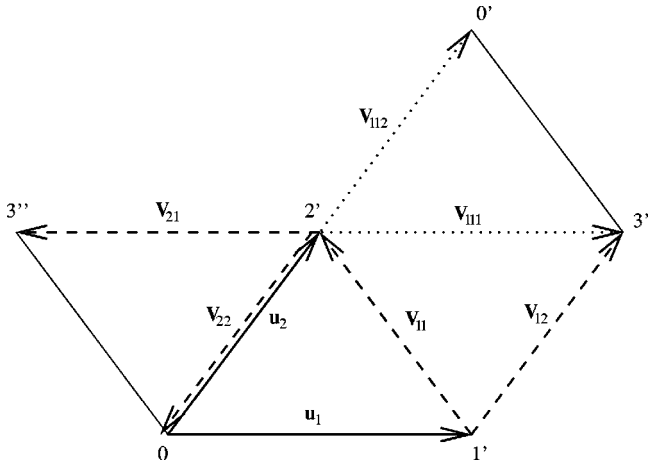

FIG. 6. The result of backward parallel transport of the group lattice $(\mathbb{Z}_4,\{1,2\})$ into the tangent space at 0, using the connection given by (5.13).

quadrangle curvature. The solutions with $(p,r)=(0,0)$, $(p,r)=(-1,-2)$ and $(p,r)=(0,-2)$ possess only nonvanishing triangle curvature. In the latter case $(p=0,r=-2)$ we have

$$V_1=\begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}, \quad V_2=\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.13}$$

The only nonvanishing part of the curvature 2-form is the triangle part

$$\mathcal{R}_{(2)\,1,1}=V_1V_1-V_2=\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}. \tag{5.14}$$

The development of this group lattice in the tangent space at 0 is shown in Fig. 6. Here we used $\mathbf{V}_{11}=\mathbf{u}_2-\mathbf{u}_1$, $\mathbf{V}_{12}=\mathbf{u}_2$, $\mathbf{V}_{21}=-\mathbf{u}_1$ and $\mathbf{V}_{22}=-\mathbf{u}_2$ which follows from (5.13). The resulting surface does not exhibit folding. The quadrangle torsion is given by

$$\sum_i \mathbf{u}_i Q^i{}_{(3)\,1,2}=\mathbf{u}_1+\mathbf{V}_{12}-\mathbf{u}_2-\mathbf{V}_{21}=2\,\mathbf{u}_1. \tag{5.15}$$

Using (2.47) we obtain $\mathbf{V}_{111}=\mathbf{u}_1$, $\mathbf{V}_{112}=\mathbf{u}_2$ and thus the following curvature expressions:

$$\sum_i \mathbf{u}_i \mathcal{R}^i{}_{(2)\,1,1,1}=\mathbf{V}_{111}-\mathbf{V}_{21}=2\,\mathbf{u}_1, \quad \sum_i \mathbf{u}_i \mathcal{R}^i{}_{(2)\,2,1,1}=\mathbf{V}_{112}-\mathbf{V}_{22}=2\,\mathbf{u}_2. \tag{5.16}$$

Remark: In general, the compatibility condition for a constant metric does not enforce a constant connection, i.e., constant transport matrices. Conversely, a constant connection may be compatible with nonconstant metrics. As an example, all metrics of the form

$$\mathfrak{g}(0)=\mathfrak{g}(2)=\begin{pmatrix} a & b \\ b & c \end{pmatrix}, \quad \mathfrak{g}(1)=\mathfrak{g}(3)=\begin{pmatrix} a-2b+c & c-b \\ c-b & c \end{pmatrix} \tag{5.17}$$

are compatible with the connection (5.13). ■

(*b*) If only nonvanishing *biangle torsion* is admitted, the coefficient matrices of the parallel transport take the form

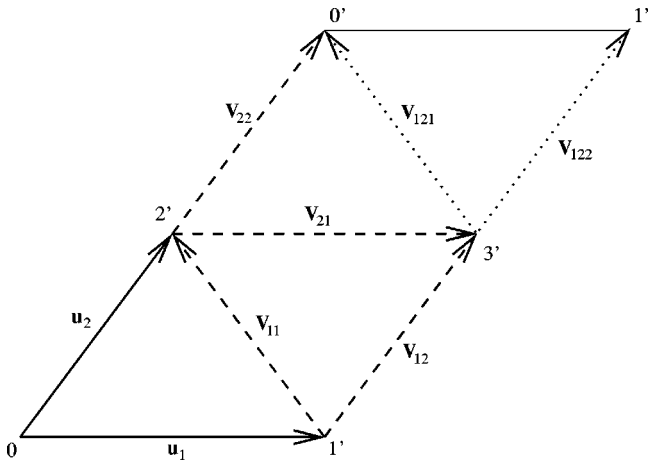

FIG. 7. The group lattice $(\mathbb{Z}_4,\{1,2\})$ mapped to the tangent space at 0 using a connection with nonvanishing biangle torsion, but vanishing triangle and quadrangle torsion.

$$V_1=\begin{pmatrix} -1 & p \\ 1 & 1+q \end{pmatrix}, \quad V_2=\begin{pmatrix} 1+p & u \\ q & v \end{pmatrix} \tag{5.18}$$

with functions p,q,u,v. If these are taken to be constants, the compatibility conditions with the metric (5.11) reduce to

$$\begin{matrix} p=q=0 \\ u=0, v=1 \ \text{ or } \ u=1, v=-1 \end{matrix} \quad \text{or} \quad \begin{matrix} p=q=-1 \\ u=1, v=-1 \ \text{ or } \ u=-1, v=0 \end{matrix}$$

which determines four different connections. The solution with $(p,q,u,v)=(0,0,0,1)$ has the transport matrices

$$V_1=\begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}, \quad V_2=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.19}$$

for which the curvature 2-form vanishes. The corresponding tangent space picture obtained by backward parallel transport of the group lattice into the tangent space at 0 is drawn in Fig. 7. Indeed, from the figure we read off $\mathbf{V}_{22}=\mathbf{u}_2$, $\mathbf{u}_1+\mathbf{V}_{11}=\mathbf{u}_2$, $\mathbf{u}_1+\mathbf{V}_{12}=\mathbf{u}_2+\mathbf{V}_{21}$, which determines the above transport matrices. The biangle torsion satisfies $\Sigma_i \mathbf{u}_i\, Q^i{}_{(2)\,1,1}=\mathbf{u}_2+\mathbf{V}_{22}=2\,\mathbf{u}_2$. Furthermore, we have $\mathbf{V}_{121}=\mathbf{V}_{211}=\mathbf{u}_2-\mathbf{u}_1$ and $\mathbf{V}_{122}=\mathbf{V}_{212}=\mathbf{u}_2$.

The solution with $(p,q,u,v)=(-1,-1,1,-1)$ has the properties $V_1V_1=V_2$, $V_2V_2=V_1$ and $[V_1,V_2]=0$, so again the whole curvature 2-form vanishes. The remaining two solutions have vanishing biangle curvature, but nonvanishing triangle and quadrangle curvature.

(c) If only triangle torsion is allowed, there is no connection compatible with the metric (5.11).

VI. GROUP LATTICE GEOMETRY AND COORDINATES

In order to explore discrete structures in close analogy with the continuum it should be of interest to consider analogs of coordinates and coordinate transformations, as well as the associated properties of geometric objects. Moreover, if there is a continuum limit, as in the case of a hypercubic $\mathbb{Z}^n$ lattice, one should recover the corresponding continuum structures.

Let (G,S) be a group lattice with $|S|=n$. Real functions x^μ, $\mu=1,\ldots,n$, are said to be *coordinates* on G if $(x^\mu):G\to\mathbb{R}^n$ is injective and the matrix $(\ell_h x^\mu)$ is invertible at all $g\in G$. If coordinates do not exist globally, they can still be introduced on subsets of G.

The first subsection below presents an example of a coordinate system on a $\mathbb{Z}_4$ lattice. In particular, it demonstrates a relation between discrete structures and noncommutative differential calculi on the algebra of functions on $\mathbb{R}^n$ which has not yet been sufficiently explored. The second subsection then treats in some detail Riemannian geometry of a hypercubic $\mathbb{Z}^n$ lattice in terms of adapted coordinates.

A. Coordinates on $(\mathbb{Z}_4,\{1,2\})$

The two functions

$$x=e^0-e^1+e^2-e^3, \quad y=e^0+e^1-e^2-e^3 \tag{6.1}$$

are coordinates on $\mathbb{Z}_4$ with $S=\{1,2\}$. Since $(x(0),y(0))=(1,1)$, $(x(1),y(1))=(-1,1)$, $(x(2),y(2))=(1,-1)$ and $(x(3),y(3))=(-1,-1)$, the map $(x,y):\mathbb{Z}_4\to\mathbb{R}^2$ is obviously injective. Using $R_1^*x=-x$, $R_2^*x=x$, $R_1^*y=xy$, $R_2^*y=-y$, we obtain the Jacobian

$$(\ell_h x^\mu)=\begin{pmatrix} -2x & 0 \\ (x-1)y & -2y \end{pmatrix}, \tag{6.2}$$

which is indeed invertible at each lattice site. Every function on $\mathbb{Z}_4$ can be expressed as a function of x and y. They satisfy $x^2=y^2=\mathbf{1}$. The coordinates x,y then constitute a representation of $\mathbb{Z}_4$. For the differentials we obtain the expressions

$$\mathrm{d}x=[\theta,x]=-2x\,\theta^1, \quad \mathrm{d}y=[\theta,y]=(x-1)y\,\theta^1-2y\,\theta^2, \tag{6.3}$$

and, thus, using $x^2=\mathbf{1}$,

$$\theta^1=-\frac{1}{2x}\mathrm{d}x, \quad \theta^2=\frac{1}{4}(x-1)\,\mathrm{d}x-\frac{1}{2y}\mathrm{d}y. \tag{6.4}$$

Furthermore, using $\theta^h f=R_h^* f\,\theta^h$ we obtain the following commutation relations between the coordinates x,y and their differentials:

$$[\mathrm{d}x,x]=-2x\,\mathrm{d}x, \quad [\mathrm{d}y,y]=-2y\,\mathrm{d}y, \quad [\mathrm{d}x,y]=[\mathrm{d}y,x]=(x-1)y\,\mathrm{d}x. \tag{6.5}$$

We have thus reached a formulation of the differential calculus on $(\mathbb{Z}_4,\{1,2\})$ as a noncommutative differential calculus on $\mathbb{R}^2$. Indeed, imposing the relations (6.5) on two real functions x,y, the group lattice $(\mathbb{Z}_4,\{1,2\})$ can be essentially recovered. The first two relations imply $\mathrm{d}(x^2)=0=\mathrm{d}(y^2)$. As a consequence, x^2 and y^2 are "constants" for this differential calculus and commute with differentials. Using (6.5) this implies

$$\begin{aligned} 0&=[\mathrm{d}(y^2),x]=[\mathrm{d}x,y^2]=[\mathrm{d}x,y]\,y+y\,[\mathrm{d}x,y]=(x-1)\,y\,(\mathrm{d}x)\,y+(x-1)\,y^2\,\mathrm{d}x \\ &=(x-1)\,y\,xy\,\mathrm{d}x+(x-1)\,y^2\,\mathrm{d}x=(x^2-1)\,y^2\,\mathrm{d}x, \end{aligned} \tag{6.6}$$

and, thus, $x^2=\mathbf{1}$, assuming $y^2\neq 0$ and that Ω^1 is free with basis $\mathrm{d}x,\mathrm{d}y$. The equations (6.5) are homogeneous in y, so that they are not able to fix the value of y^2. But the calculus is obviously consistent with the constraint $y^2=\mathbf{1}$. Passing over to the algebra $\mathcal{A}$ of functions generated by the variables x,y modulo the relations $x^2=y^2=\mathbf{1}$ and setting

$$e^0=\frac{(1+x)(1+y)}{4}, \quad e^1=\frac{(1-x)(1+y)}{4}, \quad e^2=\frac{(1+x)(1-y)}{4}, \quad e^3=\frac{(1-x)(1-y)}{4}, \tag{6.7}$$

we find $e^ie^j=\delta^{i,j}e^i$ and $\Sigma_i e^i=\mathbf{1}$. These are the primitive idempotents of $\mathcal{A}$.

Let us deduce some more consequences from the commutation relations (6.5). They are equivalent to

$$\mathrm{d}x\, x = -x\, \mathrm{d}x\,, \quad \mathrm{d}x\, y = x\, y\, \mathrm{d}x\,, \quad \mathrm{d}y\, y = -y\, \mathrm{d}y\,, \quad \mathrm{d}y\, x = x\, \mathrm{d}y + (x-1)\, y\, \mathrm{d}x, \tag{6.8}$$

so that

$$\mathrm{d}x f(x,y) = f(-x,xy)\, \mathrm{d}x, \tag{6.9}$$

$$\mathrm{d}y f(x,y) = f(x,-y)\, \mathrm{d}y + \frac{f(x,xy)-f(-x,xy)}{2\,x}(x-1)\, y\, \mathrm{d}x\,. \tag{6.10}$$

Introducing (left) partial derivatives of a function f via

$$\mathrm{d}f = \partial_x f \mathrm{d}x + \partial_y f \mathrm{d}y, \tag{6.11}$$

we find

$$\mathrm{d}y f(x,y) - f(x,y)\, \mathrm{d}y = [\mathrm{d}f, y] = (\partial_x f)\, [\mathrm{d}x, y] + (\partial_y f)\, [\mathrm{d}y, y], \tag{6.12}$$

which together with (6.5) and (6.10) leads to

$$\partial_x f = \frac{1}{2x}(f(x,xy) - f(-x,xy))\,, \quad \partial_y f = \frac{1}{2y}(f(x,y) - f(x,-y)). \tag{6.13}$$

A similar calculation starting with $\mathrm{d}x\, f(x,y) - f(x,y)\, \mathrm{d}x = [\mathrm{d}f, x]$ leads to an apparently different expression for $\partial_x f$. It reduces to the above formula with the help of

$$f(x,xy) = \tfrac{1}{2}((x+1)\, f(x,y) - (x-1)\, f(x,-y)), \tag{6.14}$$

which holds as a consequence of $x^2 = \mathbf{1}$. Of course, all geometric structures on $(\mathbb{Z}_4, \{1,2\})$ can now be expressed in terms of the coordinates and their differentials.

B. Hypercubic group lattice geometry in coordinates

Let G be the additive group $\mathbb{Z}^n$ and $S = \{\hat{\mu} \mid \mu = 1,\ldots,n\}$ be the standard basis of $\mathbb{Z}^n$, i.e., $\hat{\mu} = (0,\ldots,0,1,0,\ldots,0)$ with the 1 at the μth position. There are no biangles or triangles, but only quadrangles. The group lattice is the oriented hypercubic lattice and for $a \in \mathbb{Z}^n$ the functions e^a form a basis over $\mathbb{C}$ of $\mathcal{A}$. Then $(\ell_{\hat{\mu}} f)(a) = f(a+\hat{\mu}) - f(a)$ defines a basis $\{\ell_{\hat{\mu}}\}$ of the space $\mathcal{X}$ of vector fields. The dual basis of Ω^1 is given by

$$\theta^{\hat{\mu}} = \sum_{a \in \mathbb{Z}^n} e^a\, \mathrm{d}e^{a+\hat{\mu}}\,. \tag{6.15}$$

The functions $x^\mu = \kappa \sum_{a \in \mathbb{Z}^n} a^\mu e^a$, $\mu = 1,\ldots,n$, with a constant κ, are coordinates on the space. Every function can be written as $f(x)$ with $x = (x^1,\ldots,x^n)$. Furthermore, we find

$$\theta^{\hat{\mu}} = \frac{1}{\kappa}\mathrm{d}x^\mu, \quad \mu = 1, \ldots, n\,. \tag{6.16}$$

Since $\hat{\mu} + \hat{\nu} = \hat{\nu} + \hat{\mu}$, the 2-form relations $\mathrm{d}x^\mu\, \mathrm{d}x^\nu = -\mathrm{d}x^\nu\, \mathrm{d}x^\mu$ hold for all pairs $\mu, \nu = 1,\ldots,n$. As a consequence, every product of the form $\mathrm{d}x^{\mu_1}\cdots\mathrm{d}x^{\mu_r}$ is totally antisymmetric. Since the group is Abelian, $\mathrm{d}x^{\mu_1} \cap \cdots \cap \mathrm{d}x^{\mu_r} = \mathrm{d}x^{\mu_1}\cdots\mathrm{d}x^{\mu_r}$. This implies that $\alpha_1 \cap \cdots \cap \alpha_r$ is totally antisymmetric for arbitrary 1-forms α_i. It should be noticed, however, that $\alpha_1 \cdots \alpha_r$ is not antisymmetric, in general.

Introducing (left) partial derivatives of a function $f(x)$ via

$$\mathrm{d}f=\sum_{\mu=1}^{n}(\partial_{+\mu}f)\,\mathrm{d}x^{\mu}, \tag{6.17}$$

we find

$$\partial_{+\mu}f=\frac{R_{\hat{\mu}}^{*}f-f}{\kappa},\quad (R_{\hat{\mu}}^{*}f)(x)=f(x+\kappa\hat{\mu}). \tag{6.18}$$

The backward parallel transport of a linear connection with transport matrices $V_{\mu}=(V^{\rho}{}_{\mu\sigma})$ acts as follows:

$$\tilde{\mathcal{V}}_{\partial_{+\mu}}\partial_{+\nu}=\frac{1}{\kappa}\sum_{\rho}V^{\rho}{}_{\mu\nu}\cdot\partial_{+\rho}. \tag{6.19}$$

Let us write

$$\nabla\mathrm{d}x^{\mu}=\theta\otimes_{\mathcal{A}}\mathrm{d}x^{\mu}-\sum_{\nu=1}^{n}V^{\mu}{}_{\nu}\otimes_{\mathcal{A}}\mathrm{d}x^{\nu}=-\sum_{\nu=1}^{n}\Gamma^{\mu}{}_{\nu}\otimes_{\mathcal{A}}\mathrm{d}x^{\nu}, \tag{6.20}$$

where

$$V^{\mu}{}_{\nu}=\frac{1}{\kappa}\sum_{\rho=1}^{n}V^{\mu}{}_{\rho\nu}\,\mathrm{d}x^{\rho},\quad \Gamma^{\mu}{}_{\nu}=\sum_{\rho=1}^{n}\Gamma^{\mu}{}_{\rho\nu}\,\mathrm{d}x^{\rho}. \tag{6.21}$$

Using $\theta=\Sigma_{\mu=1}^{n}\theta^{\hat{\mu}}=(1/\kappa)\Sigma_{\mu=1}^{n}\vartheta_{\mu}\,\mathrm{d}x^{\mu}$ with $\vartheta_{\mu}=1$ for $\mu=1,\ldots,n$, we obtain

$$\Gamma^{\mu}{}_{\rho\nu}=\frac{1}{\kappa}[V^{\mu}{}_{\rho\nu}-\vartheta_{\rho}\,\delta^{\mu}_{\nu}]. \tag{6.22}$$

The components of the torsion 2-form $\Theta^{\mu}=\frac{1}{2}\Sigma_{\nu,\rho=1}^{n}Q^{\mu}{}_{\nu\rho}\,\mathrm{d}x^{\nu}\cap\mathrm{d}x^{\rho}$ are

$$Q^{\mu}{}_{\nu\rho}=\frac{1}{\kappa}(V^{\mu}{}_{[\nu\rho]}-\vartheta_{[\nu}\,\delta^{\mu}_{\rho]})=\Gamma^{\mu}{}_{[\nu\rho]} \tag{6.23}$$

and the components of the curvature 2-form $\mathcal{R}(\mathrm{d}x^{\mu})=\frac{1}{2}\Sigma_{\nu,\rho,\sigma=1}^{n}\mathcal{R}^{\mu}{}_{\nu\rho\sigma}\,\mathrm{d}x^{\rho}\cap\mathrm{d}x^{\sigma}\otimes_{L}\mathrm{d}x^{\nu}$ are given by

$$\mathcal{R}^{\mu}{}_{\nu\rho\sigma}=(\mathcal{R}_{\rho\sigma})^{\mu}{}_{\nu}=\frac{1}{\kappa^{2}}(V_{\rho}\,R_{\hat{\rho}}^{*}V_{\sigma}-V_{\sigma}\,R_{\hat{\sigma}}^{*}V_{\rho})^{\mu}{}_{\nu}. \tag{6.24}$$

The two Bianchi identities take the form

$$\sum_{\lambda=1}^{n}V^{\mu}{}_{[\nu|\lambda|}R_{\hat{\nu}}^{*}Q^{\lambda}{}_{\rho\sigma]}-Q^{\mu}{}_{[\nu\rho}R_{\hat{\nu}+\hat{\rho}}^{*}\vartheta_{\sigma]}=\kappa\,\mathcal{R}^{\mu}{}_{[\nu\rho\sigma]},\quad V_{[\nu}R_{\hat{\nu}}^{*}\mathcal{R}_{\rho\sigma]}=\mathcal{R}_{[\nu\rho}R_{\hat{\nu}+\hat{\rho}}^{*}V_{\sigma]}. \tag{6.25}$$

The compatibility condition for the linear connection and a metric tensor

$$\mathrm{g}=\sum_{\mu,\nu=1}^{n}\mathfrak{g}_{\mu\nu}(x)\,\mathrm{d}x^{\mu}\otimes_{L}\mathrm{d}x^{\nu} \tag{6.26}$$

with symmetric components, i.e., $\mathfrak{g}_{\mu\nu}=\mathfrak{g}_{\nu\mu}$, reads

$$R^*_{\hat{\rho}}(\mathfrak{g}_{\mu\nu}) = V^T_\rho(\mathfrak{g}_{\mu\nu})\, V_\rho. \tag{6.27}$$

The integrability condition of this equation (iteration around a plaquette) implies that the matrices $K_{\mu\nu}$, which are defined by

$$V_\mu R^*_{\hat{\mu}} V_\nu = K_{\mu\nu}\, V_\nu R^*_{\hat{\nu}} V_\mu, \tag{6.28}$$

are isometries of $\mathfrak{g}$ at every point of the lattice. The curvature tensor, in matrix form, can now be written as follows:

$$\mathcal{R}_{\mu\nu} = \frac{1}{\kappa^2}(K_{\mu\nu} - I)\, V_\nu R^*_{\hat{\nu}} V_\mu. \tag{6.29}$$

If the torsion vanishes, the first Bianchi identity reduces to $\mathcal{R}^\mu{}_{[\nu\rho\sigma]} = 0$. Then there is (up to the global sign) only one definition of a Ricci tensor:

$$\mathrm{Ric}_{\mu\nu} = \sum_{\rho=1}^{n} \mathcal{R}^\rho{}_{\mu\rho\nu}. \tag{6.30}$$

The curvature scalar is given by

$$\mathcal{R} = \sum_{\mu,\nu=1}^{n} \mathfrak{g}^{\mu\nu}\, \mathrm{Ric}_{\mu\nu} \tag{6.31}$$

involving the components of the inverse metric $\mathrm{g}^{-1} = \Sigma^n_{\mu,\nu=1} \mathfrak{g}^{\mu\nu}\, \partial_{+\mu} \otimes_L \partial_{+\nu}$.

Let $y^\mu(x)$ be a set of n real-valued functions which can be inverted to express x^ν in terms of the functions y^μ and for which the Jacobian

$$\mathcal{J}^\mu{}_\nu := \partial_{+\nu} y^\mu \tag{6.32}$$

is invertible. The functions y^μ are then new coordinates and we have

$$\mathrm{d}y^\mu = \sum_{\nu=1}^{n} \mathcal{J}^\mu{}_\nu\, \mathrm{d}x^\mu, \quad \mathrm{d}x^\mu = \sum_{\nu=1}^{n} (\mathcal{J}^{-1})^\mu{}_\nu\, \mathrm{d}y^\nu. \tag{6.33}$$

Note that $\mathrm{d}y^\mu \cap \mathrm{d}y^\nu + \mathrm{d}y^\nu \cap \mathrm{d}y^\mu = 0$, while $\mathrm{d}y^\mu\, \mathrm{d}y^\nu + \mathrm{d}y^\nu\, \mathrm{d}y^\mu \neq 0$, in general. Introducing (left) partial derivatives with respect to the basis $\mathrm{d}y^\mu$ via

$$\mathrm{d}f = \sum_{\nu=1}^{n} \partial^y_{+\nu} f\, \mathrm{d}y^\nu, \tag{6.34}$$

we obtain

$$\partial^y_{+\nu} f = \sum_{\mu=1}^{n} (\mathcal{J}^{-1})^\mu{}_\nu\, \partial_{+\mu} f \tag{6.35}$$

and, in particular,

$$(\mathcal{J}^{-1})^\mu{}_\nu = \partial^y_{+\nu} x^\mu. \tag{6.36}$$

Using the coordinates x^μ, the basic commutation relations of the differential calculus are

$$[\mathrm{d}x^\mu, x^\nu] = \kappa\, \delta^{\mu\nu}\, \mathrm{d}x^\mu. \tag{6.37}$$

In terms of y^μ they read

$$[\mathrm{d}y^\mu, y^\nu] = \kappa \sum_{\rho=1}^{n} C^{\mu\nu}{}_{\rho}\, \mathrm{d}y^\rho, \quad C^{\mu\nu}{}_{\rho} := \sum_{\sigma=1}^{n} \mathcal{J}^\mu{}_\sigma \mathcal{J}^\nu{}_\sigma (\mathcal{J}^{-1})^\sigma{}_\rho. \tag{6.38}$$

In the limit as $\kappa \to 0$ we obtain in both coordinate systems the ordinary continuum differential calculus, as long as the coordinate transformation does not involve κ. If f and y^μ are differentiable functions of x^μ, then in this limit $\mathrm{d}f$ becomes $\Sigma_\mu (\partial f/\partial x^\mu)\mathrm{d}x^\mu$ and also $\Sigma_\mu (\partial f/\partial y^\mu)\mathrm{d}y^\mu$ with the help of the chain rule. Although the lattice differential calculus becomes particularly simple when expressed in terms of the coordinates x^μ, in the continuum limit all coordinate systems are on an equal footing. The discrete calculus also allows κ-dependent coordinate transformations. But exploring the continuum limit we should require that such a transformation remains a coordinate transformation in the limit $\kappa \to 0$.

Since the metric is defined using the left-covariant tensor product, the metric components transform homogeneously with the Jacobi matrix:

$$\mathfrak{g}'_{\mu\nu}(y) = \sum_{\rho,\sigma=1}^{n} (\mathcal{J}^{-1})^\rho{}_\mu (\mathcal{J}^{-1})^\sigma{}_\nu\, \mathfrak{g}_{\rho\sigma}(x), \tag{6.39}$$

where $\mathrm{g} = \Sigma_{\mu,\nu} \mathfrak{g}'_{\mu\nu}(y)\mathrm{d}y^\mu \otimes_L \mathrm{d}y^\nu$. This local tensor transformation property is shared by the components of the torsion and curvature, in particular. A linear connection and the associated transport matrices have a nonlocal character. With the help of (2.41) and (6.19) we find

$$V'_\mu(y) = \sum_{\nu=1}^{n} (\mathcal{J}^{-1})^\nu{}_\mu(x)\, \mathcal{J}(x)\, V_\nu(x)\, \mathcal{J}^{-1}(x + \kappa\hat{\nu}). \tag{6.40}$$

For an appropriate Levi-Civita connection, (6.22) should tend to the Christoffel symbols in the continuum limit. Expressing V_ρ in (6.27) in terms of $\Gamma^\rho{}_{\mu\nu}$, we find

$$\partial_{+\rho} g_{\mu\nu} = g_{\mu\lambda} \Gamma^\lambda{}_{\rho\nu} + g_{\lambda\nu} \Gamma^\lambda{}_{\rho\mu} + \kappa\, g_{\kappa\lambda} \Gamma^\kappa{}_{\rho\mu} \Gamma^\lambda{}_{\rho\nu}. \tag{6.41}$$

If torsion vanishes, so that $\Gamma^\lambda{}_{\mu\nu} = \Gamma^\lambda{}_{\nu\mu}$, this implies

$$2\Gamma_{\rho\mu\nu} = \partial_{+\mu}\mathfrak{g}_{\rho\nu} + \partial_{+\nu}\mathfrak{g}_{\rho\mu} - \partial_{+\rho}\mathfrak{g}_{\mu\nu} + \kappa(\Gamma_{\lambda\rho\mu}\Gamma^\lambda{}_{\rho\nu} - \Gamma_{\lambda\mu\rho}\Gamma^\lambda{}_{\mu\nu} + \Gamma_{\lambda\nu\rho}\Gamma^\lambda{}_{\nu\mu}), \tag{6.42}$$

so that indeed the Christoffel symbols, which express $\Gamma^\rho{}_{\mu\nu}$ in terms of the metric functions, are obtained in the continuum limit. There is no such expression in the discrete framework.

VII. CONCLUSIONS

Starting from basic formulas of noncommutative geometry, we developed a formalism of Riemannian geometry of group lattices. More precisely, we restricted our considerations to the subclass of bicovariant group lattices. Only for this subclass there is a simple conversion between the ordinary tensor product $\otimes_{\mathcal{A}}$ and the left-covariant tensor product $\otimes_L$. The latter played a crucial role in making contact with classical geometry. In particular, it allows us to introduce a discrete analog of a metric tensor with a natural geometric interpretation and, more technically, to formulate a compatibility condition with a linear connection.

In particular in the case of a $\mathbb{Z}^n$ group lattice, the discrete geometry obtained has much in common with lattice gauge theory. It yields a discretization of continuum geometry via plaquettes where the curvature results from parallel transport around a plaquette (see also the various approaches[11] to ''lattice gravity'' in this context). In contrast, in Regge calculus the curvature is concentrated at a hinge (which in two dimensions is a vertex).

Given a metric, the compatibility condition for a linear connection leaves us with the freedom of torsion. This is analogous to continuum differential geometry where the additional requirement

of vanishing torsion uniquely determines a particular linear connection, the Levi-Civita connection (which is expressed via the Christoffel symbols in terms of the metric coefficients). The situation is much more complicated for group lattices, however.

A Levi-Civita connection need not exist for a given Riemannian group lattice. Furthermore, if such a connection exists, then it is not unique in general. We achieved a geometric understanding of this ambiguity through the elaboration of several examples. The deeper origin is the fact that our connections have values in a group algebra rather than a Lie algebra. The latter only feels the part of a (continuous) group which is connected with the identity.

The requirement of a Levi-Civita connection for a Riemannian group lattice strongly restricts the metric, in general. On the other hand, we learned from our examples that metric-compatible linear connections with nonvanishing torsion show up quite naturally. A convenient condition which replaces that of vanishing torsion is not available. A few general statements can nevertheless be made. Vanishing triangle torsion means assigning Euclidean properties to the respective triangle. Of course, a group lattice with Euclidean triangles, but more than three sites, may still be curved. Nonvanishing biangle torsion allows for an anisotropy of the distance relation between the respective two lattice sites, adhering to a simple interpretation of the metric coefficients. The requirement of vanishing biangle torsion would rule out this feature. But it would also eliminate geometries without such an anisotropy as we saw in Sec. V B.

On the other hand, a distance anisotropy may indeed appear in communication networks (with a group lattice structure), a relation which should be elaborated elsewhere.[16] The design of a communication network determines its efficiency. The broadcast time, for example, clearly depends on its geometry.[17] For such problems the geometric formalism developed in this work could be of help.

Our examples demonstrate that torsion quite naturally enters the stage. The more we depart from the continuum, the more we get away from the familiar condition of vanishing torsion of continuum (pseudo-) Riemannian geometry. Hypercubic group lattices, which only consist of quadrangles, are rather close to the continuum in this sense. Biangles and triangles add to the rigidity of a lattice, so that torsion becomes necessary in order to curve it. The conclusion is that, in contrast to ordinary continuum differential geometry, (nonzero) torsion is an essential ingredient of our discrete geometric formalism. Interesting field equations will have to take care of this fact and describe the dynamics of metric *and* torsion.

Is there a distinguished geometry associated with a (bicovariant) group lattice? Indeed, a direct consequence of the definition of a group lattice is the existence of a family of vector fields $\ell_h, h \in S$. Requiring that these are Killing vector fields of the metric, so that their flows preserve the metric, restricts the *a priori* possible metrics to the class of right-invariant metrics which are completely determined by the components at one site. If S is Abelian, these are simply the constant metrics, i.e., the components are the same at all sites (which correspond to the group elements). Associated with the class of right-invariant metrics is a distinguished metric-compatible linear connection. Moreover, we have the notion of bi-invariance of a metric which determines a subclass of right-invariant metrics. Interesting relations between group structure and geometry are expected to emerge from this.

Even in the familiar hypercubic lattice case the (pseudo-) Riemannian geometry derived from the general framework of group lattice geometry appears to be new. In particular in the form presented in Sec. VI B, using coordinates on the lattice, the close analogy with continuum Riemannian geometry becomes transparent. This provides an alternative to the existing discretizations of gravity theories.

Representations of ''intrinsic'' group lattice geometries via immersions in a Euclidean space will be treated in a separate work. For two-dimensional Riemannian group lattices (where S consists of two different elements), the bicovariance condition restricts to Abelian groups, and a relatively simple formalism of immersions can be developed in analogy with that of continuum differential geometry. For immersions of higher than two-dimensional Riemannian group lattices in Euclidean $\mathbb{R}^n$ the formalism is more complex and new features will show up.

APPENDIX: ORTHONORMAL COFRAME FIELDS

Let g be a metric on a group lattice (G,S) which has Euclidean (or Lorentzian) signature at each point. An *orthonormal coframe field* is a set of $|S|$ linearly independent 1-forms E^a (at each point of G) such that

$$\mathrm{g}=\sum_{a,b=1}^{|S|}\eta_{ab}\,E^a\otimes_L E^b, \tag{A1}$$

where $\eta=(\eta_{ab})$ has entries ± 1 on the diagonal and zeros otherwise (according to the signature of g). Writing

$$E^a=\sum_{h\in S}E^a{}_h\,\theta^h, \quad a=1,\ldots,|S|, \tag{A2}$$

it follows that the matrix $(E^a{}_h)$ is invertible at all sites $g\in G$. Let $(\overline{E}^h{}_a)$ denote its inverse. In the following, for (η_{ab}) we may take more generally an arbitrary constant symmetric matrix. Using (I.6.5) and (2.34), we find

$$\mathcal{V}_{\ell_h}E^a=\sum_{b=1}^{|S|}(R^*_{h^{-1}}L^a{}_{h,b})\,E^b \tag{A3}$$

with

$$L^a{}_{h,b}:=\sum_{h',h''\in S}E^a{}_{h'}\,V^{h'}{}_{h,h''}\,R^*_h\overline{E}^{h''}{}_b, \tag{A4}$$

or $L_h=E\,V_h\,R^*_h\overline{E}$ in an obvious matrix notation. As a consequence,

$$\nabla E^a=\theta\otimes_{\mathcal{A}}E^a-\sum_b L^a{}_b\otimes_{\mathcal{A}}E^b, \quad L^a{}_b:=\sum_{h\in S}L^a{}_{h,b}\,\theta^h. \tag{A5}$$

Let us introduce the dual frame field

$$\overline{E}_a:=\sum_{h\in S}\overline{E}^h{}_a\cdot\ell_h \tag{A6}$$

which satisfies $\langle\overline{E}_a,E^b\rangle=\delta^b_a$. As a consequence of (I.7.17) and (2.41), we find

$$\tilde{\mathcal{V}}_{\ell_h}\overline{E}_a=\sum_b L^b{}_{h,a}\cdot\overline{E}_b. \tag{A7}$$

The metric-compatibility condition for the connection takes the form

$$L_h^T\,\eta\,L_h=\eta. \tag{A8}$$

The matrices L_h are thus isometries of η, they have values in the orthogonal group $O(\eta)$ of η. This shows that if an orthonormal coframe field is chosen, *an η-compatible linear connection is equivalent to a map $G\times S\to O(\eta)$*.

The components of the torsion 2-form with respect to the coframe E^a are

$$\Theta^a:=\Theta(E^a)=E^a\,\theta-\Delta(E^a)+\sum_{b=1}^{|S|}L^a{}_b\,E^b. \tag{A9}$$

Here we used (I.7.6), $\Delta(f\,\omega)=f\,\Delta(\omega)$, (I.6.5) and (A3). Writing this as

$$\Theta^a=\sum_{h_1,h_2\in S}\left(E^a{}_{h_1}-\sum_{h\in S}E^a{}_h\,\delta^h_{h_1h_2}+\sum_b L^a{}_{h_1,b}\,R^*_{h_1}E^b{}_{h_2}\right)\theta^{h_1}\,\theta^{h_2} \tag{A10}$$

the condition of vanishing torsion $\Theta^a=0$ yields for biangles ($h_1h_2=e, h_1,h_2\in S_{(0)}$)

$$L_{h_1}R^*_{h_1}E_{h_2}=-E_{h_1}, \tag{A11}$$

where, for example, E_{h_1} denotes the column with entries $E^a{}_{h_1}$. For triangles $[h_1h_2=h\in S_{(1)}]$ it yields

$$L_{h_1}R^*_{h_1}E_{h_2}=E_h-E_{h_1}, \tag{A12}$$

and for quadrangles ($h_1h_2=\hat{h}_1\hat{h}_2=g\in S_{(2)}$)

$$L_{h_1}R^*_{h_1}E_{h_2}-L_{\hat{h}_1}R^*_{\hat{h}_1}E_{\hat{h}_2}=E_{\hat{h}_1}-E_{h_1}\,. \tag{A13}$$

The components of the curvature with respect to the coframe E^a are

$$\mathcal{R}(E^a)=\sum_{b=1}^{|S|}\mathcal{R}^a{}_b\otimes_{\mathcal{A}}E^b, \tag{A14}$$

where

$$(\mathcal{R}^a{}_b)=L^2-\Delta(L)-I\,\Delta^e\,,\quad L:=\sum_{h\in S}L_h\,\theta^h. \tag{A15}$$

With the help of the Leibniz rule and (I.2.15), we obtain the first Bianchi identity (I.7.11) in the following form,

$$\mathrm{d}\Theta(E)+(L-\theta)\,\Theta(E)=\left(\sum_b\mathcal{R}^a{}_bE^b\right)=-\Delta^eE-\Delta(L)\,E+L^2\,E, \tag{A16}$$

where E stands for the column with entries E^a. From

$$0=\nabla(\mathcal{R}(E^a))-\mathcal{R}(\nabla E^a)=\sum_b\left(-\Delta(\mathcal{R}^a{}_b)+\sum_c(L^a{}_c\,\mathcal{R}^c{}_b-\mathcal{R}^a{}_cL^c{}_b)\right)\otimes_{\mathcal{A}}E^b \tag{A17}$$

we obtain the following version of the second Bianchi identity:

$$\Delta(\mathcal{R}^a{}_b)=\sum_c(L^a{}_c\,\mathcal{R}^c{}_b-\mathcal{R}^a{}_cL^c{}_b). \tag{A18}$$

Writing

$$\mathcal{R}(E^a)=\sum_{b=1}^{|S|}\sum_{h_1,h_2\in S}\mathcal{R}^a{}_{b,h_1,h_2}\,\theta^{h_1}\cap\theta^{h_2}\otimes_LE^b, \tag{A19}$$

we find the biangle part of the curvature

$$\mathcal{R}_{(e)\,h_1,h_2}=\delta^e_{h_2h_1}(L_{h_1}R^*_{h_1}L_{h_1^{-1}h_2h_1}-I), \tag{A20}$$

the triangle part ($h\in S_{(1)}$)

$$\mathcal{R}_{(h)\,h_1,h_2} = \delta^h_{h_2 h_1}(L_{h_1} R^*_{h_1} L_{h_1^{-1}h_2 h_1} - L_h)\,\mathcal{E}_{(h)}\,, \tag{A21}$$

and the quadrangle curvature ($g \in S_{(2)}$)

$$\mathcal{R}_{(g)\,h_1,h_2;\hat{h}_1,\hat{h}_2} = \delta^g_{h_2 h_1}(L_{h_1} R^*_{h_1} L_{h_1^{-1}h_2 h_1} - L_{\hat{h}_1} R^*_{\hat{h}_1} L_{\hat{h}_1^{-1}\hat{h}_2 \hat{h}_1})\,\mathcal{E}_{(g)}\,. \tag{A22}$$

Here we have introduced

$$\mathcal{E}^a_{(g)\,b} := \sum_{h' \in S} (R^*_g E^a{}_{h'})\,\overline{E^{g h' g^{-1}}}{}_b. \tag{A23}$$

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[14] Here the vanishing of the curvature is a special case of a much more general well-known result. If the torsion of a linear connection with respect to a differential calculus on some associative algebra vanishes, then $\pi \circ \nabla = d \circ \pi$. In the case of the universal differential calculus this reduces to $\nabla = \mathrm{d}$ and the vanishing of the curvature follows from $\mathrm{d}^2 = 0$.
[15] A corresponding Mathematica notebook is available at the authors' homepages. Mathematica is a registered trademark of *Wolfram, Research*. See S. Wolfram, *The Mathematica Book*, (Cambridge University Press, Cambridge, 1999).
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Continuous wavelet transform on a special homogeneous space

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(Received 22 July 2002; accepted 23 April 2003)

We consider a semidirect product of two locally compact groups S and T, with S Abelian, denoted by $S\sigma T$. An action of $S\sigma T$ on S is introduced to make S a homogeneous space of $S\sigma T$. Then we define a unitary representation from $S\sigma T$ into the unitary group of $L^2(S)$ which is our main tool for defining the continuous wavelet transform on $L^2(S)$. Also the main properties of the transform are discussed. We prove the Plancherel and inversion formulas and reproducing kernel's formula for this transform. This is finally specialized to the case of the continuous wavelet transform on $L^2(R^d)$. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1591055]

I. INTRODUCTION AND NOTATIONS

Let G be a locally compact topological group. We denote by $d\mu_G$ a fixed left Haar measure on G and by Δ_G the modular function. By $C_c(G)$ we mean the space of continuous functions of compact support on G. An action of a locally compact group G on a locally compact Hausdorff space S is a continuous map $(x,s)\mapsto xs$ from $G\times S$ to S such that $s\mapsto xs$ is a homeomorphism of S for each $x\in G$, and $x(ys)=(xy)s$, for all $x,y\in G$ and $s\in S$. S is called a transitive G-space if for every $s,t\in S$ there exists $x\in G$ such that $xs=t$. A homogeneous space is a transitive G-space that is isomorphic to a quotient space G/H for some closed subgroup H of G [for more information see Folland (1995), Chap. 2].

Let G/H be a homogeneous space. A rho-function for the pair (G,H) is a continuous function $\rho:G\mapsto(0,\infty)$ such that

$$\rho(x\xi)=\frac{\Delta_H(\xi)}{\Delta_G(\xi)}\rho(x),\quad x\in G,\xi\in H.$$

For any locally compact group G and any closed subgroup H of G, (G,H) admits a rho-function [see Folland (1995), Proposition 2.54].

Any homogeneous space G/H has a strongly quasi-invariant measure which arises from a rho-function and for any rho-function for the pair (G,H) there is a strongly quasi-invariant measure [see Folland (1995), Chap. 2, or Reiter (1968), Chap. 8]. But here we meet a special case of a homogeneous space which has more familiar measure than strongly quasi-invariant measures.

Let G be of the form $G=G_1H$ where G_1 and H are closed subgroups and $G_1\cap H=\{e\}$, so every $x\in G$ could be written uniquely in the form $x=gh$ with $g\in G_1,h\in H$. Suppose further that the map $x\mapsto(g,h)$ of G onto the product $G_1\times H$ is continuous and hence a homeomorphism. Now, the function

$$\rho(x)=\frac{\Delta_H(h)}{\Delta_G(h)},\quad x=gh,g\in G_1,h\in H \tag{1}$$

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is a rho-function for the pair (G,H). By Reiter (1968), Chap. 8, Sec. 1.4, there is a relatively invariant positive measure $d_\rho \dot{x}$ on G/H such that for all $f \in C_c(G/H)$:

$$\int_{G/H} f(y^{-1}\dot{x})\, \mathrm{d}_\rho(\dot{x}) = \rho(y) \int_{G/H} f(\dot{x})\, \mathrm{d}_\rho(\dot{x}), \quad y \in G, \tag{2}$$

But G/H is isomorphic to G_1 as a topological space, so by Reiter (1968), Chap. 8, Sec. 1.5, $\mathrm{d}_\rho \dot{x}$ is a left Haar measure on G_1, which will be shown by $\mathrm{d}\mu_{G_1}$, and for all $f \in C_c(G)$ we have

$$\int_{G_1} \int_H f(gh) \mathrm{d}\mu_H(h)\, \mathrm{d}\mu_{G_1}(g) = \int_G f(x)\rho(x)\, \mathrm{d}\mu_G(x), \tag{3}$$

or if we replace f by f/ρ we obtain

$$\int_{G_1} \int_H f(gh) \frac{\Delta_G(h)}{\Delta_H(h)} \mathrm{d}\mu_H(h)\, \mathrm{d}\mu_{G_1}(g) = \int_G f(x)\, \mathrm{d}\mu_G(x). \tag{4}$$

Also we can rewrite (2) as follows, which is valid for all $f \in L^1(G_1)$,

$$\int_{G_1} f(y^{-1}x)\, \mathrm{d}\mu_{G_1}(x) = \rho(y) \int_{G_1} f(x)\, \mathrm{d}\mu_{G_1}(x), \quad y \in G. \tag{5}$$

By Reiter (1968), Chap. 8, Sec. 2.3, formula (3) holds for all $f \in L^1(G)$. Later we approach a homogeneous space which has the above properties.

Let S and T be groups and suppose that there is a homomorphism $t \mapsto \sigma_t$ from T into the group of automorphisms of S. For (s,t), $(\acute{s},\acute{t}) \in S \times T$, define

$$(s,t)(\acute{s},\acute{t}) = (s\sigma_t(\acute{s}), t\acute{t}).$$

Then $S \times T$ is a group, it is called a semidirect product of S and T and is denoted by $S\sigma T$. Its identity is (e_1,e_2), where e_1 and e_2 are the identities of S and T, respectively. The inverse of (s,t) is $(\sigma_{t^{-1}}(s^{-1}), t^{-1})$.

Let $\tilde{S} = \{(s,e_2); s \in S\}$ and $\tilde{T} = \{(e_1,t); t \in T\}$. Then $\tilde{S} \trianglelefteq G$ and $\tilde{T} \leqslant G$, $\tilde{S} \cap \tilde{T} = \{(e_1,e_2)\}$, and $G = \tilde{S}\tilde{T}$. If S and T are locally compact groups and $(s,t) \mapsto \sigma_t(s)$ is continuous then G is a locally compact group and $\tilde{S}$ and $\tilde{T}$ are closed in G.

We denote by $\hat{G}$ the dual group of a locally compact Abelian group G and by $\hat{f}$ Fourier transform of a function f. For more information about the properties of $\hat{G}$, the definition of Fourier transform and related theorems, we refer the reader to Rudin (1960), Chap. 1 or Folland (1995), Chap. 4.

By a (unitary) representation we mean a homomorphism π from a locally compact group G into the group $\mathcal{U}(\mathcal{H})$ of unitary operators on some nonzero Hilbert space $\mathcal{H}$ that is continuous with respect to the strong operator topology. A vector $\phi \in \mathcal{H}$ is said to be admissible if

$$\int_G |\langle \phi, \pi(x)\phi \rangle|^2 \mathrm{d}\mu_G(x) < +\infty.$$

A representation π is called irreducible if $\{0\}$ and $\mathcal{H}$ are the only closed linear subspaces that are invariant under the unitary operators $\pi(x); x \in G$. An irreducible representation which has at least one admissible vector is called a square integrable representation. If there exists a vector $\phi \in \mathcal{H}$ such that the closed linear span of $\{\pi(x)\phi, x \in G\}$ is equal to $\mathcal{H}$, then ϕ is called a cyclic vector and π is called a cyclic representation.

In this paper we study the continuous wavelet transform on $L^2(S)$ using a unitary representation from $S\sigma T$ into the unitary group of $L^2(S)$. In particular we extend the results of Koorn-

winder (1993). The idea of working on semidirect product of groups in the framework of wavelet analysis is not new. In Grossman *et al.* (1985), which is one of the first papers of wavelet analysis, the continuous wavelet transform on $L^2(R)$ was defined by means of a certain square integrable representation of the semidirect product $R\sigma R^+$ on the unitary group of $L^2(R)$. The square integrability of this representation guarantees the existence of an inverse wavelet transform and admissibility condition. However, we prove them without square integrability's assumption, instead we use the fact that S is a homogeneous space of $S\sigma T$. In recent years, this kind of result to other groups has been extended, especially the construction of wavelet transform and discrete frames from semidirect product of R^k and a closed matrix group has been considered [see, e.g., Aniello *et al.* (2001), Aniello *et al.* (1998), Fuehr and Meyer (2002)]. Also some authors have concerned the wavelet transform in the context of square integrable representations of locally compact groups on infinite dimensional separable Hilbert spaces [see Wong (2002)]. These wavelet transforms are based on coherent states parametrized by elements in the group G. The book by Ali *et al.* (2000) presents the more general theory of coherent states associated with homogeneous space and contains an extensive list of references on coherent states parametrized by points in a homogeneous space. Torresani (1995) and Antoine and Vandergheynst (1999) have presented some applications of coherent states on manifolds.

II. MAIN RESULTS

Let G be semidirect product of two locally compact groups S and T, that S is Abelian, and let $\cdot: G\times S\mapsto S$ be as follows:

$$(a,b).s = a\sigma_b(s).$$

It is easy to check that "." is an action of G on S. Since for each s_1, $s_2\in S$, $(s_2 s_1^{-1}, e_2).s_1 = s_2$, S is a transitive G-space. Also S is a homogeneous space of G, since $\Phi: G/\tilde{T}\mapsto S$ defined by $\Phi((s,t)\tilde{T}) = s$ is a homeomorphism. Let

$$\rho(s,t) = \rho(e_1,t) = \frac{\Delta_{\tilde{T}}(e_1,t)}{\Delta_G(e_1,t)}.$$

Clearly, ρ is a rho-function for the pair $(G,\tilde{T})$. From now on, we use $\rho(t)$ instead of $\rho(e_1,t)$. ρ satisfies Eq. (1), so there is a left Haar measure $d\mu_{\tilde{S}}(s,e_2)$ on $\tilde{S}$ such that (4) and (5) hold, hence there is a left Haar measure $d\mu_S$ on S, that (4) and (5) could be rewritten as follows:

$$\int_S\int_T \frac{f(s,t)}{\rho(t)}\mathrm{d}\mu_T(t)\mathrm{d}\mu_S(s) = \int_G f(g)\mathrm{d}\mu_G(g), \quad f\in L^1(G), \tag{6}$$

$$\int_S f((a,b)^{-1}.s)\mathrm{d}\mu_S(s) = \rho(b)\int_S f(s)\mathrm{d}\mu_S(s), \quad f\in L^1(S). \tag{7}$$

Now we define π from G into $\mathcal{U}(L^2(S))$, the unitary group of $L^2(S)$ such that

$$[\pi(a,b)f](s) = \rho(b)^{-1/2} f((a,b)^{-1}.s). \tag{8}$$

It can be easily checked that π is a unitary representation.

Definition 1: We say $\Psi\in L^1\cap L^2(S)$ is a *wavelet* if $\|\Psi\|_{L^2(S)} = 1$ and there is a constant C_Ψ such that $0 < C_\Psi < +\infty$ and for any $\gamma\in\hat{S}$,

$$C_\Psi := \int_T |\hat{\Psi}(\gamma\circ\sigma_t)|^2 \mathrm{d}\mu_T(t).$$

For a wavelet Ψ we put

$$\Psi_{s,t} := \pi(s,t)\Psi, \quad (s,t) \in G.$$

Definition 2: For any $f \in L^2(S)$, the *continuous wavelet transform* of f is defined as follows:

$$Wf(s,t) = \langle f, \Psi_{s,t} \rangle_{L^2(S)}.$$

By Parseval's formula [see Rudin (1960), Sec. 1.6.2] we also have

$$Wf(s,t) = \langle \hat{f}, \hat{\Psi}_{s,t} \rangle_{L^2(\hat{S})}, \quad f \in L^2(S).$$

Using the Schwarz inequality it is easy to see that Wf is a bounded and continuous function on G.

Lemma 3: Let $\Psi \in L^2(S)$, then

$$\hat{\Psi}_{s,t}(\gamma) = \rho(t)^{1/2} \overline{\gamma(s)} \hat{\Psi}(\gamma \circ \sigma_t), \quad \gamma \in \hat{S}. \tag{9}$$

Proof: First we assume $\Psi \in L^1 \cap L^2(S)$. Since $\Psi_{s,t} \in L^1 \cap L^2(S)$ by definition of Fourier transform [Rudin (1960), Sec. 1.2.3] and using (7) and (8) we have

$$\hat{\Psi}_{s,t}(\gamma) = \int_S \Psi_{s,t}(x) \overline{\gamma(x)}\, d\mu_S(x) = \rho(t)^{1/2} \int_S \Psi(x) \overline{\gamma((s,t).x)}\, d\mu_S(x) = \rho(t)^{1/2} \overline{\gamma(s)} \hat{\Psi}(\gamma \circ \sigma_t).$$

Now, if $\Psi \in L^2(S)$, by definition of Fourier transform of functions in $L^2(S)$ [see the proof of Theorem 1.6.1 in Rudin (1960)] formula (9) obtains. □

Theorem 4: Let Ψ be a wavelet and $f, g \in L^2(S)$. Then we have

(i) *(Plancherel formula)* $\|Wf\|^2_{L^2(G)} = C_\Psi \|f\|^2_{L^2(S)}$,

(ii) *(Parseval formula)* $\langle Wf, Wg \rangle_{L^2(G)} = C_\Psi \langle f, g \rangle_{L^2(S)}$.

Proof: Put

$$F_t(\gamma) = \hat{f}(\gamma)\, \overline{\hat{\Psi}}(\gamma \circ \sigma_t), \quad t \in T, \gamma \in \hat{S}.$$

By Holder's inequality $F_t \in L^1(\hat{S})$. Also we can easily check that

$$F_t(\gamma) = \rho(t^{-1}) [f \star (\Psi \circ \sigma_{t^{-1}})^\star]\, \hat{}\, (\gamma),$$

where $\Psi^\star(s) = \Psi(s^{-1})$. Since $f \in L^2(S)$ and $(\Psi \circ \sigma_{t^{-1}})^\star \in L^1 \cap L^2(S)$ by Folland (1995), Proposition 2.39, $f \star (\Psi \circ \sigma_{t^{-1}})^\star \in L^2(S)$, thus its Fourier transform is defined, so $F_t \in L^2(\hat{S})$ and by Pontriagin Duality Theorem [Rudin (1960), Theorem 1.7.2], $\hat{F}_t \in L^2(S)$. Also we put $G_t(\gamma) = \hat{g}(\gamma)\, \overline{\hat{\Psi}}(\gamma \circ \sigma_t)$, so G_t satisfies the above results about F_t. Therefore by (9)

$$Wf(s,t) = \langle \hat{f}, \hat{\Psi}_{s,t} \rangle_{L^2(\hat{S})} = \rho(t)^{1/2} \int_{\hat{S}} F_t(\gamma)\, \gamma(s)\, d\mu_{\hat{S}}(\gamma) = \rho(t)^{1/2}\, \hat{F}_t(s^{-1}).$$

Similarly, $Wg(s,t) = \rho(t)^{1/2}\, \hat{G}_t(s^{-1})$. So we have

$$\begin{aligned} \int_T \int_S Wf(s,t) \overline{Wg(s,t)}\, \rho(t)^{-1}\, d\mu_S(s) d\mu_T(t) &= \int_T \langle \hat{F}_t, \hat{G}_t \rangle_{L^2(S)}\, d\mu_T(t) \\ &= \int_T \int_{\hat{S}} F_t(\gamma) \overline{G_t}(\gamma)\, d\mu_{\hat{S}}(\gamma) d\mu_T(t) \\ &= C_\Psi \langle \hat{f}, \hat{g} \rangle_{L^2(\hat{S})} = C_\Psi \langle f, g \rangle_{L^2(S)}. \end{aligned}$$

So by (6) we obtain

$$\int_G Wf(s,t)\overline{Wg(s,t)}\,d\mu_G(s,t)=C_\Psi\langle f,g\rangle_{L^2(S)}. \tag{10}$$

If $f=g$, then

$$\|Wf\|^2_{L^2(G)}=C_\Psi\|f\|^2_{L^2(S)}.$$

That means $Wf\in L^2(G)$, so we have the Parseval formula by (10). □

Remark 5: For a moment, let us define the continuous wavelet transform as follows:

$$Wf(s,t)=\frac{1}{\sqrt{C_\Psi}}\langle f,\Psi_{s,t}\rangle,\quad f\in L^2(S). \tag{11}$$

By Theorem 4 we can easily conclude that W is an isometry of $L^2(S)$ into its range. Theorem 7 will specify the range of continuous wavelet transform which is a closed subspace of $L^2(G)$. The following lemma will be used for proving Theorem 6, we refer the reader to Koornwinder (1993), Lemma 4.1, for its proof.

Lemma 6: Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces and let $\Phi:\mathcal{H}_1\to\mathcal{H}_2$ be an isometry into $\mathcal{H}_2$. Then $\Phi\Phi^\star:\mathcal{H}_2\to\mathcal{H}_2$ is the orthogonal projection of $\mathcal{H}_2$ onto $\Phi(\mathcal{H}_2)$.

Theorem 7: *(Reproducing kernel formula)* Let $h\in L^2(G)$. Then $h=Wf$, for some $f\in L^2(S)$ if and only if

$$h(\acute{s},\acute{t})=1/C_\Psi\int_G h(s,t)\,\langle\Psi_{s,t},\Psi_{\acute{s},\acute{t}}\rangle_{L^2(S)}\,d\mu_G(s,t).$$

Proof: Let us consider W as in (11), so by Lemma 6, $WW^\star$ is an orthogonal projection of $L^2(G)$ onto $W(L^2(S))$. Now, if $h\in L^2(G)$ we have

$$\begin{aligned}(WW^\star h)(\acute{s},\acute{t})&=\frac{1}{\sqrt{C_\Psi}}\langle W^\star h,\Psi_{\acute{s},\acute{t}}\rangle_{L^2(S)}\\&=\frac{1}{\sqrt{C_\Psi}}\langle h,W\Psi_{\acute{s},\acute{t}}\rangle_{L^2(G)}\\&=1/C_\Psi\int_G h(s,t)\,\langle\Psi_{s,t},\Psi_{\acute{s},\acute{t}}\rangle_{L^2(S)}\,d\mu_G(s,t).\end{aligned}$$

□

Lemma 8: Let f and $\Psi\in L^1\cap L^2(S)$. Put $h_t(s)=Wf(s,t)$, for a fixed $t\in T$, then

$$\hat{h}_t(\gamma)=\rho(t)^{1/2}\hat{f}(\gamma)\overline{\hat{\Psi}}(\gamma\circ\sigma_t),\quad \gamma\in\hat{S}. \tag{12}$$

Proof: By (9) we have

$$\begin{aligned}h_t(s)=Wf(s,t)&=\rho(t)^{1/2}\int_{\hat{S}}\hat{f}(\gamma)\overline{\hat{\Psi}}(\gamma\circ\sigma_t)\,\gamma(s)\,d\mu_{\hat{S}}(\gamma)\\&=\rho(t)^{-1/2}\int_{\hat{S}}[f\star(\Psi\circ\sigma_{t^{-1}})^\star]\,\hat{}\,(\gamma)\,\gamma(s)\,d\mu_{\hat{S}}(\gamma)\\&=\rho(t)^{-1/2}[f\star(\Psi\circ\sigma_{t^{-1}})^\star](s).\end{aligned}$$

In the last equality we applied Fourier Inversion formula [see Folland (1995), Theorem 2.40] which is valid here because $[f\star(\Psi\circ\sigma_{t^{-1}})^{\star}]\in L^1\cap L^2(S)\cap C_0(S)$, also $[f\star(\Psi\circ\sigma_{t^{-1}})^{\star}]\hat{}\in L^1(\hat{S})$. Therefore $h_t\in L^1\cap L^2(S)$ and (12) obtains. □

Theorem 9: *(Inversion formula)* Let $f\in L^1\cap L^2(S)$ and $\hat{f}\in L^1(\hat{S})$, then for each $u\in S$,

$$f(u)=1/C_\Psi\int_G Wf(s,t)\,\Psi_{s,t}(u)\,\mathrm{d}\mu_G(s,t).$$

Proof: By Lemma 8 we have

$$\int_S Wf(s,t)\,\gamma(s^{-1})\,\mathrm{d}\mu_S(s)=\rho(t)^{1/2}\hat{f}(\gamma)\overline{\hat{\Psi}}(\gamma\circ\sigma_t).$$

Multiplying both sides of the above equality by $\rho(t)^{-1/2}\hat{\Psi}(\gamma\circ\sigma_t)$ and integrating over T we get

$$\hat{f}(\gamma)=1/C_\Psi\int_T\int_S\rho(t)^{-1/2}\,Wf(s,t)\hat{\Psi}(\gamma\circ\sigma_t)\,\gamma(s^{-1})\,\mathrm{d}\mu_S(s)\mathrm{d}\mu_T(t).$$

Now, by the inverse Fourier transform, Lemma 3 and (6) we have

$$\begin{aligned}f(u)=\int_{\hat{S}}\hat{f}(\gamma)\,\gamma(u)\,d\mu_{\hat{S}}(\gamma)&=\frac{1}{C_\Psi}\int_T\rho(t)^{-1}\int_S Wf(s,t)\int_{\hat{S}}\hat{\Psi}_{s,t}(\gamma)\,\gamma(u)\,d\mu_{\hat{S}}(\gamma)\mathrm{d}\mu_S(s)\mathrm{d}\mu_T(t)\\&=\frac{1}{C_\Psi}\int_T\int_S\rho(t)^{-1}Wf(s,t)(u)\Psi_{s,t}(u)\,\mathrm{d}\mu_S(s)\mathrm{d}\mu_T(t)\\&=\frac{1}{C_\Psi}\int_G Wf(s,t)\Psi_{s,t}(u)\,\mathrm{d}\mu_G(s,t).\end{aligned}$$

□

III. EXAMPLE AND REMARKS

As an example of the continuous wavelet transform discussed in Sec. II we consider semidirect product of the additive group R^d and the multiplicative group $R_+:=(0,\infty)$ under homomorphism $\sigma:R^+\to Aut(R^d)$ defined by

$$\sigma_a(b)=ab,\quad a\in R^+,b\in R^d.$$

In order to compare our result with Koornwinder (1993), we reverse the order of R^d and R^+ and we put $G=R^+\sigma R^d$ with the following multiplication and inversion;

$$(a,b)(\acute{a},\acute{b})=(a\acute{a},b+a\acute{b}),\quad (a,b)^{-1}=(a^{-1},-ba^{-1}).$$

Since $(a,b)\to ab$ is continuous so G is a locally compact group with modular function $\Delta_G(a,b)=a^{-d}$ and with Haar measure $a^{-d-1}\mathrm{d}a\,\mathrm{d}b$, where d$a$ is the Lebesgue measure on R and db is the Lebesgue measure on R^d [for more information about computing the Haar measure for semidirect product of two locally compact groups see Hewitt and Ross (1985), Chap. 5, Sec. 15.29]. G acts on R^d with the following action:

$$G\times R^d\to R^d,\quad (a,b).x=ax+b,$$

that are the affine transformations. With this action R^d is a homogeneous space of G. Now formulas (6) and (7) are valid with the rho-function $\rho(a)=a^d,a\in R^+$ and $\mathrm{d}\mu_{R^d}$ appearing in them is equal to the Lebesgue measure on R^d. The representation π defined by (8) is as follows:

$$[\pi(a,b)f](x)=a^{-d/2}f\left(\frac{x-b}{a}\right),\quad (a,b)\in G,x\in R^d,f\in L^2(R^d).$$

Let Ψ be a wavelet as in Definition 1, so

$$C_\Psi = \int_{R^d} |\hat{\Psi}(a\xi)|^2 \frac{da}{a}, \quad \forall \xi \in R^+,$$

and

$$\Psi_{a,b}(x) = a^{-d/2}\Psi\left(\frac{x-b}{a}\right), \quad (a,b) \in G, x \in R^d.$$

We refer the reader to Theorems 2.2, 2.3, 2.5 and Proposition 4.4 in Koornwinder (1993) to compare them with properties of this transform that we obtained in Sec. II.

Remark 10: Theorem 4 implies that any wavelet Ψ is an admissible and cyclic vector for the representation π defined by (8).

Remark 11: If $G = R\sigma R^\star$ where $R^\star = R - \{0\}$, then the representation π defined by (8) is irreducible [see Koornwinder (1993), Sec. 5]; however, if $G = R\sigma R^+$ then

$$\{f \in L^2(R); \text{support } \hat{f} \subseteq [0,\infty)\}$$

is a proper closed invariant subspace for π, so in this case π is not irreducible. Therefore, it is not possible to say anything about irreducibility of π defined by (8).

Remark 12: Let G be a locally compact group, $\mathcal{H}$ a Hilbert space, and π a square integrable representation of G on $\mathcal{U}(\mathcal{H})$ and g be an admissible vector for it. In Grossman *et al.* (1985), the continuous wavelet transform of any $f \in \mathcal{H}$ is defined by

$$W_g f(x) = \langle f, \pi(x) g \rangle,$$

which satisfies in plancherel formula, inversion formula, and reproducing kernel formula because of irreducibility of π [the latest results in this context could be found in Wong (2002)]. We defined the continuous wavelet transform in the same way, but without irreducibility's assumption.

ACKNOWLEDGMENT

The authors wish to express their gratitude to the referee for his helpful comments and suggestions.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Angular Gelfand–Tzetlin coordinates for the supergroup UOSp($k_1/2k_2$)

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(Received 15 December 2002; accepted 20 May 2003)

We construct Gelfand–Tzetlin coordinates for the unitary orthosymplectic supergroup UOSp($k_1/2k_2$). This extends a previous construction for the unitary supergroup U(k_1/k_2). We focus on the angular Gelfand–Tzetlin coordinates, i.e., our coordinates stay in the space of the supergroup. We also present a generalized Gelfand pattern for the supergroup UOSp($k_1/2k_2$) and discuss various implications for representation theory. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1594819]

I. INTRODUCTION

If the symmetries of a physical problem are simple enough, proper coordinates are easy to find. However, already the Schrödinger equation for a particle in a potential with spherical symmetry leads to nontrivial group theory, such as parametrization of the Lie group SO(3) with Euler angles, spherical harmonics, Wigner representation functions and, in the case of the hydrogen atom, additional symmetries and the Lie group SO(4). The coordinates mostly used distinguish, for a good physics reason, certain directions and thus do not treat all coordinates on an equal footing. Group theoretically, such parametrizations are called noncanonical. The Euler angles, for example, describe three subsequent rotations, first, about the z-axis, second, about the new y-axis, and, third, about the new z-axis. Nevertheless, there are many problems, particularly in statistical mechanics, in many-body physics and in matrix models, where one does not want to distinguish certain directions. Rather, all variables parametrizing the group should be treated on an equal footing. Gelfand–Tzetlin coordinates[1–3] are such a coordinate system. Their construction is based on a group chain or coset decomposition. Thus Gelfand–Tzetlin coordinates have a clear recursive structure. From a physics point of view, it is important that matrix elements, measures and other quantities reflect this clear recursive structure and can be given very explicitly. The generality of this group chain construction makes Gelfand–Tzetlin coordinates powerful tools in applications (see, for example, Refs. 4 and 5), but also for conceptual studies (see, for example, Refs. 6–8). A particularly intriguing aspect is the intimate and direct connection between Gelfand–Tzetlin coordinates on the group manifold and representations of this group. Their rich features and their relevance for different types of studies ranging from physics applications to pure mathematics render Gelfand–Tzetlin coordinates important objects in their own right.

In Ref. 5, Gelfand–Tzetlin coordinates were constructed for the unitary supergroup U(k_1/k_2). In the present contribution, we further extend this and construct Gelfand–Tzetlin coordinates for the unitary orthosymplectic supergroup UOSp($k_1/2k_2$). As this supergroup appears in the theory of disordered systems,[9] our construction of Gelfand–Tzetlin coordinates might be of direct use for future physics applications. The unitary orthosymplectic supergroup UOSp($k_1/2k_2$) contains the symplectic group USp($2k_2$) and the orthogonal group SO(k_1) as subgroups. Thus, our construction also includes coordinate systems for these two groups in ordinary space. The construction for

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the orthogonal group was implicitly also done in Ref. 8.

For the sake of clarity, an important remark is in order: We distinguish between *angular* and *radial* Gelfand–Tzetlin coordinates. In the present work, we construct angular ones. By that we mean that they never leave the space of the group and its algebra. In previous contributions,[10–13] we constructed radial Gelfand–Tzetlin coordinates to study certain types of group integrals. These radial Gelfand–Tzetlin coordinates are capable of mapping the integral over a group onto integrals over the radial part of a different symmetric space. Hence, in this sense, these coordinates leave the space of the group and its algebra. Here, we always stay with the angular Gelfand–Tzetlin coordinates.

The appreciated explicit formulas resulting from the Gelfand–Tzetlin construction imply the unavoidable disadvantage that a reader, not familiar with the subject, can quickly lose his orientation. Therefore, we decided to skip several detailed calculations if, in our opinion, it would not be too cumbersome for the reader to recover the missing steps by properly adjusting the corresponding ones in Ref. 5. In any case, we recommend that an interested but unexperienced reader studies first Refs. 4 and 8 and then Ref. 5 before reading the present contribution.

The article is organized as follows: In Sec. II, we construct the angular Gelfand–Tzetlin coordinates. We state the generalized Gelfand pattern in Sec. III and discuss some issues related to representation theory. Summary and conclusions are given in Sec. IV.

II. CONSTRUCTION OF THE COORDINATE SYSTEM

In Sec. II A, we collect some properties of the supergroup $\mathrm{UOSp}(k_1/2k_2)$ needed in the sequel. We set up the proper Gelfand–Tzetlin equations and their recursion to all levels in Secs. II B and II C, respectively. We solve these equations in Sec. II D. We summarize the construction of the Gelfand–Tzetlin coordinates for the ordinary unitary symplectic group in Sec. II E. The invariant measure of the supergroup is worked out in Sec. II F. The matrix elements of the supergroup are obtained in Sec. II G.

A. The supergroup $\mathrm{UOSp}(k_1/2k_2)$

The classification of superalgebras and supergroups can be found in Refs. 14–16. Here, we restrict ourselves to summarizing features of the supergroups $\mathrm{OSp}(k_1/2k_2)$ and $\mathrm{UOSp}(k_1/2k_2)$. We will refer to k_1 and $2k_2$ as the bosonic and fermionic dimensions, respectively. We introduce the notation $(k_1/2k_2)$ for the resulting superdimension. The elements of $\mathrm{OSp}(k_1/2k_2)$ are those elements u of the general linear supergroup $\mathrm{GL}(k_1/2k_2)$ which satisfy $u^{\dagger}Lu=L$. The metric L is given by

$$L=\mathrm{diag}(1_{k_1},1_{k_2}\otimes\tau^{(2)}), \tag{1}$$

where 1_{k_1} and 1_{k_2} are the $k_1\times k_1$ and the $k_2\times k_2$ unit matrices and where $\tau^{(2)}$ is one of the two by two matrices,

$$\begin{aligned}\tau^{(0)} &= \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \quad \tau^{(1)} = \begin{bmatrix}0 & -i\\ -i & 0\end{bmatrix},\\ \tau^{(2)} &= \begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}, \quad \tau^{(3)} = \begin{bmatrix}+i & 0\\ 0 & -i\end{bmatrix}.\end{aligned} \tag{2}$$

The supergroup $\mathrm{UOSp}(k_1/2k_2)$ is the compact subgroup of $\mathrm{OSp}(k_1/2k_2)$. By construction, the direct product $\mathrm{SO}(k_1)\otimes\mathrm{USp}(2k_2)$ of the ordinary orthogonal and the ordinary unitary symplectic group is a subgroup of $\mathrm{UOSp}(k_1/2k_2)$. As is well known, the ordinary orthogonal group $\mathrm{SO}(k_1)$ has slightly different features for even and odd dimension k_1. Thus, these differences are also present in the supergroup $\mathrm{UOSp}(k_1/2k_2)$.

The group elements act on a graded space, which we denote by $\mathcal{L}={}^0\mathcal{L}\oplus{}^1\mathcal{L}$. It decomposes into a sum of an even ${}^0\mathcal{L}$ and an odd ${}^1\mathcal{L}$ subspace according to its transformation properties under the parity automorphism.[17] We define a basis $e_j=e_{j1}, j=1,\ldots,k_1$, for ${}^0\mathcal{L}$, and $e_{k_1+j}=e_{j2}, j=1,\ldots,2k_2$, for ${}^1\mathcal{L}$, respectively.

The supergroup $\mathrm{UOSp}(k_1/2k_2)$ can be obtained by the exponential mapping of the superalgebra $\mathrm{uosp}(k_1/2k_2)$, such that $\sigma\in\mathrm{uosp}(k_1/2k_2)$ leads to $u=\exp(\sigma)\in\mathrm{UOSp}(k_1/2k_2)$. The construction of the angular Gelfand–Tzetlin coordinates uses as the starting point the Cartan subalgebra $\mathrm{uosp}^{(0)}(k_1/2k_2)$ of $\mathrm{uosp}(k_1/2k_2)$. For even bosonic dimension $2k_1$, the elements of $\mathrm{uosp}^{(0)}(2k_1/2k_2)$ are the matrices

$$s=\mathrm{diag}(is_{11}\tau^{(2)},\ldots,is_{k_11}\tau^{(2)},s_{12}\tau^{(3)},\ldots,s_{k_21}\tau^{(3)}), \tag{3}$$

while for odd bosonic dimension $2k_1+1$, the $\mathrm{uosp}^{(0)}(2k_1+1/2k_2)$ consists of the matrices

$$s=\mathrm{diag}(is_{11}\tau^{(2)},\ldots,is_{k_11}\tau^{(2)},0,s_{12}\tau^{(3)},\ldots,s_{k_21}\tau^{(3)}). \tag{4}$$

Naturally, $\mathrm{uosp}^{(0)}(k_1/2k_2)$ is the direct sum of the Cartan subalgebras of $\mathrm{so}(k_1)$ and $\mathrm{usp}(2k_2)$.

B. Derivation of the angular Gelfand–Tzetlin equations

Gelfand–Tzetlin coordinates are based on a group chain or, equivalently, on a coset decomposition. The coset decomposition needed for the supergroup $\mathrm{UOSp}(k_1/2k_2)$ is

$$\mathrm{UOSp}(k_1/2k_2)=\frac{\mathrm{UOSp}(k_1/2k_2)}{\mathrm{UOSp}((k_1-1)/2k_2))}\otimes\frac{\mathrm{UOSp}((k_1-1)/2k_2)}{\mathrm{UOSp}((k_1-2)/2k_2))}\otimes\cdots\otimes\frac{\mathrm{UOSp}(1/2k_2)}{\mathrm{USp}(2k_2)}$$
$$\otimes\frac{\mathrm{USp}(2k_2)}{\mathrm{USp}(2k_2-2)}\otimes\cdots\otimes\frac{\mathrm{USp}(4)}{\mathrm{SU}(2)}\otimes\mathrm{SU}(2). \tag{5}$$

Every coset space describes a unit sphere. The first coset $\mathrm{UOSp}(k_1/2k_2)/\mathrm{UOSp}((k_1-1)/2k_2))$ is a sphere in a superspace with dimension $(k_1/2k_2)$. The dimension of the space in which the sphere lives is lowered by one in every step. The sphere $\mathrm{UOSp}(1/2k_2)/\mathrm{USp}(2k_2)$ is the last one living in a superspace; the following spheres in the second line of Eq. (5) are spheres in ordinary spaces. Coordinate systems will be constructed on all these spheres under the nontrivial requirement that the orthogonality, more precisely the equation $u^\dagger Lu=L$, is always respected. Thus, once the coordinate system on one sphere has been obtained, the orthogonal complement to every fixed vector on this sphere has to be constructed, the next sphere lives in this smaller space. Hence, loosely speaking, the spheres in the coset decomposition are orthogonal to each other. The construction to follow is an extension of the one in Ref. 5 for the unitary supergroup. For simplicity, we consider the case of even k_1 first. The differences occurring for odd k_1 will be dealt with in Sec. II C.

To project onto a smaller subspace, we write $u\in\mathrm{UOSp}(k_1/2k_2)$ as $u=[u_1\,u_2\cdots u_{k_1+2k_2}]$ where the columns u_i are normalized supervectors. We denote by u_{ji} their entries in the basis $e_{j1}, j=1,\ldots,k_1$, and $e_{j2}, j=1,\ldots,2k_2$. The orthogonality condition requires the vectors u_i, $i\leqslant k_1$, to be real:

$$u_{ji}=u_{ji}^*,\quad \text{for}\quad 1\leqslant j\leqslant k_1,\quad \text{and}\quad u_{(k_1+2j)i}=u_{(k_1+2j-1)i}^*,\quad \text{for}\quad 1\leqslant j\leqslant k_2. \tag{6}$$

We consider the first vector. It is parametrized by k_1 real commuting variables u_{j1} and $2k_2$ complex anticommuting variables. For the latter we write

$$u_{(k_1+2j)i}=\alpha_j^*,\quad 1\leqslant j\leqslant k_2. \tag{7}$$

We also define $|\alpha_j|^2=\alpha_j^*\alpha_j$. The supervector u_1 describes the coset space $\mathrm{UOSp}(k_1/2k_2)/\mathrm{UOSp}((k_1-1)/2k_2)$ which is—similar to ordinary spaces—isomorphic to the surface of the $(k_1/2k_2)$ dimensional sphere $S^{(k_1-1)/2k_2}$. We go from Cartesean coordinates to a new set of coordinates for u_1 by projecting a fixed element s of the Cartan subalgebra on a space of superdimension $((k_1-1)/2k_2)$ orthogonal to u_1,

$$s^{(1)}=(1_{k_1+2k_2}-u_1u_1^\dagger)s(1_{k_1+2k_2}-u_1u_1^\dagger). \tag{8}$$

The eigenvalues and eigenvectors of this projected matrix are obtained by solving the supersymmetric Gelfand–Tzetlin equation

$$s_p^{(1)}e_p^{(1)}=(1_{k_1+2k_2}-u_1u_1^\dagger)s(1_{k_1+2k_2}-u_1u_1^\dagger)e_p^{(1)}=(1_{k_1+2k_2}-u_1u_1^\dagger)se_p^{(1)}, \tag{9}$$

which extends the equation in Ref. 5 for the unitary supergroup to $\mathrm{UOSp}(k_1/2k_2)$. It is convenient to rotate the basis in such a way that s becomes diagonal before solving Eq. (9). We introduce the primed basis

$$e'_{(2i-1)1}=\frac{1}{\sqrt{2}}(e_{(2i-1)1}+ie_{(2i)1}),$$

$$e'_{(2i)1}=\frac{1}{\sqrt{2}}(ie_{(2i-1)1}+e_{(2i)1}),\quad i=1...,k_1/2, \tag{10}$$

$$e'_{i2}=e_{i2},\quad i=k_1+1,\ldots,k_1+2k_2.$$

The rotation only affects the bosonic degrees of freedom, not the fermionic ones. Due to this rotation, the bosonic entries of u_1' are now complex variables which we write in the form

$$u'_{(2j)1}=iu'^*_{(2j-1)1}=\frac{i}{\sqrt{2}}|v_j^{(1)}|\exp(-i\vartheta_j^{(1)}),\quad j=1,\ldots,k_1/2. \tag{11}$$

The fermionic entries are, also in the primed basis, given by Eq. (7). To calculate the eigenvalues, we need the characteristic function of the eigenvalue equation (9),

$$z(s_p^{(1)})=\mathrm{detg}\,((1_{k_1+2k_2}-u_1u_1^\dagger)s-s_p^{(1)})=-s_p^{(1)}\mathrm{detg}\,(s-s_p^{(1)})u_1^\dagger\frac{1_{k_1+2k_2}}{s-s_p^{(1)}}u_1. \tag{12}$$

Importantly, the function $z(s_p^{(1)})$ behaves differently for the k_1 bosonic eigenvalues, i.e., for those in the boson–boson block $s_p^{(1)}=s_{p1}^{(1)}$, $p=1,\ldots,k_1$, and for the $2k_2$ fermionic eigenvalues, i.e., for those in the fermion–fermion block $s_{k_1+p}^{(1)}=is_{p2}^{(1)}$, $p=1,\ldots,2k_2$. The equation above has therefore to be discussed in the limits

$$z(s_p^{(1)})\to\begin{cases}0 & \text{for } p=1,\ldots,k_1,\\ \infty & \text{for } p=k_1+1,\ldots,\ k_1+2k_2.\end{cases} \tag{13}$$

Together with the normalization condition $u_1^\dagger u_1=1$ we find the following set of equations:

$$1=\sum_{p=1}^{k_1/2}|v_p^{(1)}|^2+\sum_{p=1}^{k_2}|\alpha_p^{(1)}|^2, \tag{14}$$

$$0=(s_{p1}^{(1)})^2\left(\sum_{q=1}^{k_1/2}\frac{|v_q^{(1)}|^2}{(s_{q1})^2-(s_{p1}^{(1)})^2}+\sum_{q=1}^{k_2}\frac{|\alpha_q^{(1)}|^2}{(is_{q2})^2-(s_{p1}^{(1)})^2}\right),\quad p=1,\ldots,(k_1-1), \tag{15}$$

$$z_p=(is_{p2}^{(1)})^2\frac{\Pi_{q=1}^{k_1/2}((s_{q1})^2-(is_{p2}^{(1)})^2)}{\Pi_{q=1}^{k_2}((is_{q2})^2-(is_{p2}^{(1)})^2)}\left(\sum_{q=1}^{k_1/2}\frac{|v_q^{(1)}|^2}{(s_{q1})^2-(is_{p2}^{(1)})^2}+\sum_{q=1}^{k_2}\frac{|\alpha_q^{(1)}|^2}{(is_{q2})^2-(is_{p2}^{(1)})^2}\right),$$

$$z_p\to\infty,\quad p=1,\ldots,2k_2. \tag{16}$$

This is a system of equations in the variables $(s_{p1}^{(1)})^2$ and $(is_{p2}^{(1)})^2$. The second equation has a twofold degenerate solution at $s_{p1}^{(1)}=0$. If $s_{p1}^{(1)}, is_{p2}^{(1)}$ are solutions of the above equations, $-s_{p1}^{(1)}$ and $-is_{p2}^{(1)}$ are solutions as well. Hence the projected matrix (8) is of the form (4) in the proper basis $e_j^{(1)}$ and belongs itself to the Cartan subalgebra $\mathrm{uosp}^{(0)}((k_1-1)/2k_2)$. This is crucial for the recursion. The system (14)–(16) is overdetermined; out of the k_1+2k_2+1 equations in (14)–(16), only $k_1/2+k_2$ are independent. The system yields the moduli squared of the entries of the vector u_1' expressed in terms of the eigenvalues $s^{(1)}$. We call the latter bosonic eigenvalues if they satisfy Eq. (15), and fermionic eigenvalues if they satisfy Eq. (16). With the substitutions $s_{q1}^{(j)}\to(s_{q1}^{(j)})^2$ and $is_{q2}^{(j)}\to(is_{q2}^{(j)})^2$, $j=1,2$, the set of independent equations is equivalent to the corresponding set of equations for the unitary supergroup. Thus, we can directly read off the solutions from Ref. 5. They will be stated in Sec. II D.

C. Recursion to all levels in superspace

The construction just outlined for the first coset space has to be continued recursively to cover the entire group manifold. For the ordinary groups, this recursion can be found in Refs. 1–3. In the present case, we extend the recursion for the unitary supergroup in Ref. 5. As the Cartan subalgebra $\mathrm{uosp}^{(0)}(k_1/2k_2)$ is slightly different for even and odd bosonic dimension k_1 according to Eqs. (3) and (4), we have to distinguish these two cases for the recursion. For brevity, we refer to a level as even, if (k_1-n+1) is even, and as odd otherwise.

In the nth step the vector u_n' is expanded in a set of $k_1-n+1+2k_2$ basis vectors $e_j'^{(n-1)}$, which span the subspace of $\mathcal{L}$ orthogonal to $u=[u_1\,u_2\cdots u_{n-1}]$. This set splits into two disjoint subsets. The first subset contains k_1-n+1 vectors $e_{j1}'^{(n-1)}$ spanning some subspace of ${}^0\mathcal{L}$. The second one contains $2k_2$ basis vectors $e_{j2}'^{(n-1)}$ spanning ${}^1\mathcal{L}$. The entries of u_n in this basis are complex variables

$$e_{(2p)1}'^{(n-1)\dagger}u_n=i(e_{(2p-1)1}'^{(n-1)\dagger}u_n)^*=\frac{i}{\sqrt{2}}|v_p^{(n)}|\exp(-i\vartheta_p^{(n)}),$$

$$p\leqslant\begin{cases}(k_1-n+1)/2 & \text{for } k_1-n+1 \text{ even},\\ (k_1-n)/2 & \text{for } k_1-n+1 \text{ odd},\end{cases} \tag{17}$$

$$e_{(2p)2}'^{(n-1)\dagger}u_n=(e_{(2p-1)2}'^{(n-1)\dagger}u_n)^*=\alpha_p^{(n)*},\quad p\leqslant k_2.$$

For k_1-n+1 odd, the remaining entry is parametrized by a real variable and an integer $r\in\{0,1\}$ as

$$e_{(k_1-n+1)1}'^{(n-1)\dagger}u_n=(-1)^r v_{(k_1-n)/2+1}^{(n)}. \tag{18}$$

Thus, we can write down the rotated nth eigenvector on the $(n-1)$th level,

$$u_n'^{(n-1)}=\sum_{j=1}^{k_1+2k_2-n+1}e_j'^{(n-1)\dagger}u_n e_j'^{(n-1)}. \tag{19}$$

The projection of s onto this subspace after the nth step is given by

$$s^{(n-1)}=\left(\sum_{i=n}^{k_1+2k_2} u_i u_i^\dagger\right) s \left(\sum_{i=n}^{k_1+2k_2} u_i u_i^\dagger\right) = \left(1_{k_1+2k_2}-\sum_{i=1}^{n-1} u_i u_i^\dagger\right) s \left(1_{k_1+2k_2}-\sum_{i=1}^{n-1} u_i u_i^\dagger\right) \quad (20)$$

and belongs to the Cartan subalgebra of $\mathrm{UOSp}((k_1-n)/2k_2)$. The new coordinates are obtained by projecting $s^{(n-1)}$ on the subspace orthogonal to u_n by

$$s_p^{(n)} e_p^{(n)} = (1_{k_1+2k_2}-u_n u_n^\dagger) s^{(n-1)} (1_{k_1+2k_2}-u_n u_n^\dagger) e_p^{(n)} = (1_{k_1+2k_2}-u_n u_n^\dagger) s^{(n-1)} e_p^{(n)}. \quad (21)$$

For k_1-n+1 even, this leads to a system of equations as in (14)–(16) reduced by $(n-1)/2$ unknown variables. For (k_1-n+1) odd, the equations have a slightly different form,

$$1=\sum_{p=1}^{(k_1-n)/2} |v_p^{(n)}|^2+|v_{(k_1-n)/2+1}^{(n)}|^2+\sum_{p=1}^{k_2} |\alpha_p^{(n)}|^2, \quad (22)$$

$$0=s_{p1}^{(n)}\left(\sum_{q=1}^{(k_1-n)/2} \frac{(s_{p1}^{(n)})^2 |v_q^{(n)}|^2}{(s_{q1}^{(n-1)})^2-(s_{p1}^{(n)})^2}+|v_{(k_1-n)/2+1}^{(n)}|^2+\sum_{q=1}^{k_2} \frac{(s_{p1}^{(n)})^2 |\alpha_q^{(n)}|^2}{(is_{q2}^{(n-1)})^2-(s_{p1}^{(n)})^2}\right),$$
$$p=1,\ldots,(k_1-n), \quad (23)$$

$$z_p=-is_{p2}^{(n)} \frac{\prod_{q=1}^{(k_1-n)/2}((s_{q1}^{(n-1)})^2-(is_{p2}^{(n)})^2)}{\prod_{q=1}^{k_2}((is_{q2}^{(n-1)})^2-(is_{p2}^{(n)})^2)} \left(\sum_{q=1}^{(k_1-n)/2} \frac{(s_{p1}^{(n)})^2 |v_q^{(n)}|^2}{(s_{q1}^{(n-1)})^2-(is_{p2}^{(n)})^2}+|v_{(k_1-n)/2+1}|^2 \right.$$
$$\left.+\sum_{q=1}^{k_2} \frac{(s_{p1}^{(n)})^2 |\alpha_q^{(n)}|^2}{(is_{q2}^{(n-1)})^2-(is_{p2}^{(n)})^2}\right), \quad z_p\to\infty, \quad p=1,\ldots,2k_2. \quad (24)$$

The difference between Eqs. (22)–(24) and the corresponding equations (14)–(16) for the even levels is due to the isolated entry (18), which has to be treated separately. This reflects the difference between the even orthogonal group and the odd orthogonal group in ordinary space.

The new basis vectors $e_j'^{(n)}$ are related to the basis vectors of the foregoing level by a $(k_1-n+2k_2)\times(k_1-n+1+2k_2)$ rectangular supermatrix $\hat{b}'^{(n)}$. The moduli squared of its entries $\hat{b}_{pm}'^{(n)}$ are determined by rewriting Eq. (21) and multiplying it from the left hand side with $e_m'^{(n-1)\dagger}$:

$$e_m'^{(n-1)\dagger} s^{(n-1)} e_p'^{(n)} = s_p^{(n)} e_m'^{(n-1)\dagger} e_p'^{(n)} + e_m'^{(n-1)\dagger} u_n b_p^{(n)}, \quad (25)$$

where we defined $b_p^{(n)}=u_n^\dagger s^{(n-1)} e_p'^{(n)}$. On the other hand, we have

$$e_m'^{(n-1)\dagger} s^{(n-1)} e_p'^{(n)} = s_m^{(n-1)} e_m'^{(n-1)} e_p'^{(n)}, \quad (26)$$

which yields for the matrix elements of $\hat{b}'^{(n)}$ the expression

$$\hat{b}_{pm}'^{(n)}=\frac{1}{s_m^{(n-1)}-s_p^{(n)}} u_{mn}'^{(n-1)} b_p^{(n)}. \quad (27)$$

The modulus squared of $b_p^{(n)}$ is determined by the normalization of the rotated basis vectors $e_m'^{(n)\dagger} e_p'^{(n)}=\delta_{mp}$, i.e., by the condition that the matrix $\hat{b}'^{(n)}\hat{b}'^{(n)\dagger}$ is unity in the k_1-n+2k_2 dimensional subspace orthogonal to $u=[u_1\, u_2\cdots u_n]$. Due to the block structure of the supermatrix $\hat{b}'^{(n)}$, the vector $b^{(n)}$ has commuting and anticommuting elements. For k_1-n+1 even we define $|w_p^{(n)}|^2=|b_{2p}^{(n)}|^2=|b_{2p-1}^{(n)}|^2, p=1,\ldots,(k_1-n+1)/2$, for the commuting elements and $|\beta_p^{(n)}|^2=|b_{k_1-n+1+2p}^{(n)}|^2=|b_{k_1-n+2p}^{(n)}|^2, p=1,\ldots,k_2$, for the anticommuting elements. For k_1-n

$+1$ odd we define $|w_p^{(n)}|^2$ and $|\beta_p^{(n)}|^2$ correspondingly. Again, there is a difference in the determining equations of $|w_p^{(n)}|^2$ and $|\beta_p^{(n)}|^2$ between the even and the odd levels of the recursion. For k_1-n+1 even we have

$$\frac{1}{|w_p^{(n)}|^2}=\sum_{m=1}^{(k_1-n+1)/2}\frac{(s_{m1}^{(n-1)})^2+(s_{p1}^{(n)})^2}{((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)^2}|v_m^{(n)}|^2+\sum_{m'=1}^{k_2}\frac{(is_{m'2}^{(n-1)})^2+(s_{p1}^{(n)})^2}{((is_{m'2}^{(n-1)})^2-(s_{p1}^{(n)})^2)^2}|\alpha_{m'}^{(n)}|^2,$$
$$p=1,\ldots,(k_1-n-1)/2. \tag{28}$$

For the remaining modulus squared we obtain

$$\frac{1}{|w_{(k_1-n+1)/2}^{(n)}|^2}=\sum_{m=1}^{(k_1-n+1)/2}\frac{1}{(s_{m1}^{(n-1)})^2}|v_m^{(n)}|^2+\sum_{m'=1}^{k_2}\frac{1}{(is_{m'2}^{(n-1)})^2}|\alpha_{m'}^{(n)}|^2. \tag{29}$$

The moduli squared of the anticommuting coordinates of $b^{(n)}$ fulfill a formally similar equation. However, it is mathematically more precise to write it in the inverted form to avoid the appearance of purely nilpotent variables in the denominator,

$$1=|\beta_p^{(n)}|^2\left(\sum_{m=1}^{(k_1-n+1)/2}\frac{(s_{m1}^{(n-1)})^2+(is_{p2}^{(n)})^2}{((s_{m1}^{(n-1)})^2-(is_{p2}^{(n)})^2)^2}|v_m^{(n)}|^2+\sum_{m'=1}^{k_2}\frac{(is_{m'2}^{(n-1)})^2+(s_{p1}^{(n)})^2}{((is_{m'2}^{(n-1)})^2-(s_{p1}^{(n)})^2)^2}|\alpha_{m'}^{(n)}|^2\right),$$
$$p=1,\ldots,k_2. \tag{30}$$

The corresponding equations for the odd levels are obtained from Eqs. (28) and (30) by making the following formal replacements. In Eq. (28), the sum over m runs only to $(k_1-n)/2$ and, in addition, the term $|v_{(k_1-n)/2+1}^{(n)}|^2/(s_{p1}^{(n)})^2$ is subtracted. In Eq. (30), the first sum runs only to $(k_1-n)/2$ and the term $|v_{(k_1-n)/2+1}^{(n)}|^2/(is_{p2}^{(n)})^2$ is subtracted. Moreover, Eq. (29) does not exist for the odd levels.

D. Solution of the angular Gelfand–Tzetlin equations

Up to the k_1th level both sets of equations (14)–(16) and (28)–(30) have to be solved for even and odd levels separately. For the even levels, there is, as already mentioned above, a direct correspondence to the case of the unitary supergroup. Thus, we find employing the results of Ref. 5,

$$|v_p^{(n)}|^2=\frac{\Pi_{q=1}^{(k_1-n-1)/2}((s_{p1}^{(n-1)})^2-(s_{q1}^{(n)})^2)\Pi_{q=1}^{k_2}((s_{p1}^{(n-1)})^2-(is_{q2}^{(n-1)})^2)}{\Pi_{q=1,q\neq p}^{(k_1-n+1)/2}((s_{p1}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)\Pi_{q=1}^{k_2}((s_{p1}^{(n-1)})^2-(is_{q2}^{(n)})^2)},$$
$$p=1,\ldots,(k_1-n+1)/2,\quad k_1-n+1 \text{ even},$$
$$|\alpha_p^{(n)}|^2=((is_{p2}^{(n)})^2-(is_{p2}^{(n-1)})^2)\times\frac{\Pi_{q=1}^{(k_1-n-1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n)})^2)\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n-1)})^2)}{\Pi_{q=1}^{(k_1-n+1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n)})^2)},$$
$$p=1,\ldots,k_2. \tag{31}$$

We have included the first level by setting $s=s^{(0)}$. To find the solution of Eqs. (28)–(30), one cannot directly make use of the results in the unitary case. An explicit calculation is necessary which is given in Appendix A. It yields

$$|w_p^{(n)}|^2=\frac{-\prod_{m=1}^{(k_1-n+1)/2}((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n)})^2-(is_{q2}^{(n)})^2)}{2(s_{p1}^{(n)})^2\prod_{q=1,q\neq p}^{(k_1-n-1)/2}((s_{p1}^{(n)})^2-(s_{q1}^{(n)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n)})^2-(is_{q2}^{(n-1)})^2)},$$

$$p=1,\ldots,(k_1-n-1)/2\ ,$$

$$|w_{(k_1-n+1)/2}^{(n)}|^2=\frac{\prod_{m=1}^{(k_1-n+1)/2}(s_{m1}^{(n-1)})^2\prod_{q=1}^{k_2}(is_{q2}^{(n)})^2}{\prod_{m=1}^{(k_1-n-1)/2}(s_{m1}^{(n)})^2\prod_{q=1}^{k_2}(is_{q2}^{(n-1)})^2}, \tag{32}$$

$$|\beta_p^{(n)}|^2=((is_{p2}^{(n)})^2-(is_{p2}^{(n-1)})^2)$$

$$\times\frac{\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n)})^2-(is_{q2}^{(n)})^2)\prod_{q=1}^{(k_1-n+1)/2}((is_{p2}^{(n)})^2-(s_{q1}^{(n)})^2)}{2(is_{p2}^{(n)})^2\prod_{q=1}^{(k_1-n-1)/2}((is_{p2}^{(n)})^2-(s_{q1}^{(n)})^2)\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n)})^2-(is_{q2}^{(n-1)})^2)},$$

$$p=1,...,k_2\,.$$

We observe that the squares of the fermionic eigenvalues of the different levels $(is_{p2}^{(n)})^2$ differ only by a nilpotent variable. Hence, we introduce complex anticommuting variables $\xi_p^{(n)}$ such that

$$|\xi_p^{(n)}|^2=(is_{p2}^{(n)})^2-(is_{p2}^{(n-1)})^2. \tag{33}$$

We emphasize that this feature is highly nontrivial: the difference of the squared fermionic eigenvalues for two neighboring levels can be expressed as the modulus squared of one anticommuting variable.

The solutions of Eqs. (22)–(24) for the odd levels, i.e., for k_1-n+1 odd, cannot directly be obtained by adjusting the results of Ref. 5. However, as the necessary modifications are intuitively clear, we do not derive the solutions for the odd levels in detail. We simply state the results,

$$|v_p^{(n)}|^2=\frac{\prod_{q=1}^{(k_1-n)/2}((s_{p1}^{(n-1)})^2-(s_{q1}^{(n)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n-1)})^2-(is_{q2}^{(n-1)})^2)}{(s_{p1}^{(n-1)})^2\prod_{q=1,q\neq p}^{(k_1-n)/2}((s_{p1}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n-1)})^2-(is_{q2}^{(n)})^2)},$$

$$p=1,\ldots,(k_1-n)/2,$$

$$|v_{(k_1-n)/2+1}^{(n)}|^2=\frac{\prod_{q=1}^{(k_1-n)/2}(s_{q1}^{(n)})^2\prod_{q=1}^{k_2}(is_{q2}^{(n-1)})^2}{\prod_{q=1}^{(k_1-n)/2}(s_{q1}^{(n-1)})^2\prod_{q=1}^{k_2}(is_{q2}^{(n)})^2}, \tag{34}$$

$$|\alpha_p^{(n)}|^2=((is_{p2}^{(n)})^2-(is_{p2}^{(n-1)})^2)$$

$$\times\frac{\prod_{q=1}^{(k_1-n)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n)})^2)\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n-1)})^2)}{(is_{p2}^{(n-1)})^2\prod_{q=1}^{(k_1-n)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n)})^2)},$$

$$p=1,\ldots,k_2.$$

The solutions of Eqs. (28)–(30) for the odd levels read

$$|w_p^{(n)}|^2=\frac{1}{2}\,\frac{\prod_{m=1}^{(k_1-n)/2}((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n)})^2-(is_{q2}^{(n)})^2)}{\prod_{q=1,q\neq p}^{(k_1-n)/2}((s_{p1}^{(n)})^2-(s_{q1}^{(n)})^2)\prod_{q=1}^{k_2}((s_{p1}^{(n)})^2-(is_{q2}^{(n-1)})^2)},\quad p=1,\ldots,(k_1-n)/2, \tag{35}$$

$$|\beta_p^{(n)}|^2=\frac{1}{2}((is_{p2}^{(n)})^2-(is_{p2}^{(n-1)})^2)\,\frac{\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n)})^2-(is_{q2}^{(n)})^2)\prod_{q=1}^{(k_1-n)/2}((is_{p2}^{(n)})^2-(s_{q1}^{(n-1)})^2)}{\prod_{q=1}^{(k_1-n)/2}((is_{p2}^{(n)})^2-(s_{q1}^{(n)})^2)\prod_{q=1,q\neq p}^{k_2}((is_{p2}^{(n)})^2-(is_{q2}^{(n-1)})^2)},$$

$$p=1,\ldots,k_2.$$

From the solutions stated in Eqs. (31)–(35) one derives the corresponding formulas for the group $SO(k_1)$ in ordinary space by setting all anticommuting variables to zero.

A comparison with the results for the unitary supergroup $U(k_1/2k_2)$ in Ref. 5 reveals an interesting formal connection. The Cartan subalgebras $u^{(0)}(k_1-n+1/2k_2)$ and $u^{(0)}(k_1-n/2k_2)$ of $U(k_1-n+1/2k_2)$ and $U(k_1-n/2k_2)$, respectively, are all diagonal matrices:

$$s^{(n-1)}=\mathrm{diag}(s_{11}^{(n-1)},\ldots,s_{(k_1-n+1)1}^{(n-1)},is_{12}^{(n-1)},\ldots,is_{2k_2 2}^{(n-1)}),$$
$$s^{(n)}=\mathrm{diag}(s_{11}^{(n)},\ldots,s_{(k_1-n)1}^{(n)},is_{12}^{(n)},\ldots,is_{2k_2 2}^{(n)}). \tag{36}$$

If one now formally replaces, in the results for the unitary supergroup, these matrices $s^{(n-1)}$ and $s^{(n)}$ with elements of the Cartan subalgebra of $\mathrm{uosp}^{(0)}(k_1-n+1/2k_2)$ and $\mathrm{uosp}^{(0)}(k_1-n/2k_2)$ according to

$$s^{(n-1)}\leftrightarrow\mathrm{diag}(is_{11}^{(n-1)}\tau^{(3)},\ldots,is_{[(k_1-n+1)/2]1}^{(n-1)}\tau^{(3)},-s_{12}^{(n-1)}\tau^{(3)},\ldots,-s_{k_2 2}^{(n-1)}\tau^{(3)}),$$
$$s^{(n)}\leftrightarrow\mathrm{diag}(is_{11}^{(n)}\tau^{(3)},\ldots,is_{[(k_1-n-1)/2]1}^{(n-1)}\tau^{(3)},0,-s_{12}^{(n)}\tau^{(3)},\ldots,-s_{k_2 2}^{(n)}\tau^{(3)}),\quad k_1-n+1\ \text{even}, \tag{37}$$

the results in Eqs. (31) and (32) and in Eqs. (34) and (35) are recovered. This formal connection between the unitary supergroup and the unitary orthosymplectic one is natural and plausible. Unfortunately, we could not make a sound mathematical reasoning out of the replacement (37) which would go beyond the *a posteriori* observation. However, the formal connection stated above illustrates the deep relationship between the groups which will become even more apparent in the generalized Gelfand pattern given in Sec. IV.

E. Ordinary unitary symplectic group

The k_1th step of the recursion is the last one in a superspace. We now approach the second line of Eq. (5). The following steps do not involve anticommuting variables anymore. We are left with the ordinary unitary symplectic group $USp(2k_2)$ and its coset decomposition. We make use of the isomorphism[18] $USp(2k_2)\cong U(k_2;4)$ where $U(k_2;4)$ is the unitary group in k_2 dimensions parametrized over the quaternions. Since $U(k_2;4)$ can be parametrized analogously to $U(k_2;2)=U(k_2)$, i.e., to the unitary group over the complex numbers, we simply have to adjust the results of Refs. 1 and 4 where Gelfand–Tzetlin coordinates for the ordinary unitary group were constructed. We write $U\in U(k_2;4)$ as $U=[U_1\,U_2\cdots U_{k_2}]$. The normalized vectors U_i have quaternionic entries:

$$U_{mi}=U_{mi0}\tau^{(0)}+U_{mi1}\tau^{(1)}+U_{mi2}\tau^{(2)}+U_{mi3}\tau^{(3)}. \tag{38}$$

The quantities U_{mik}, $k=0,...,3$, are real numbers. As basis vectors in Eq. (38), one can use the 2×2 matrices defined in Eq. (2).[18] Thus, we stay with the notation $\tau^{(i)}, i=0,\ldots,3$. The Cartan subalgebra is of the form $s_2^{(k_1)}=\mathrm{diag}\,(s_{12}^{(k_1)}\tau^{(3)},\ldots,s_{k_2 2}^{(k_1)}\tau^{(3)})$. The Gelfand–Tzetlin eigenvalue equation reads for the first level of the $USp(2k_2)$ recursion, i.e., for the level k_1+1 of the $UOSp(k_1/2k_2)$ recursion,

$$(1_{k_2}-U_1U_1^{\dagger})is_2^{(k_1)}(1_{k_2}-U_1U_1^{\dagger})E_n^{(1)}=is_{n2}^{(k_1+1)}E_n^{(1)}. \tag{39}$$

We introduced the notation $U_1=u_{k_1+1}$ and $E_n^{(1)}=e_n^{(k_1+1)}$ to highlight that the vectors and matrices used here span an ordinary vector space. Equation (39) can be viewed either as an eigenvalue equation for a $k_2\times k_2$ matrix over the quaternion field or for a $2k_2\times 2k_2$ matrix over the field of complex numbers. For a comprehensive account on matrices with quaternionic entries see Ref. 19. The eigenvalues on the right hand side of Eq. (39) are in principle still quaternionic. We now can proceed by multiplying Eq. (39) on both sides with $1_{k_2}\otimes\tau^{(3)}$ from the left. This renders the matrix

on the left hand side of Eq. (39) Hermitian self-dual.[19] Employing the Pauli matrices as quaternion basis a Hermitian self-dual $2k_2\times 2k_2$ matrix B is characterized by entries of the form

$$B_{ij}=\begin{bmatrix} z_{ij} & w_{ij}^* \\ -w_{ij} & z_{ij}^* \end{bmatrix}, \quad i\neq j, \quad i,j=1,\ldots,k_2, \quad \text{and} \quad B_{ii}=\begin{bmatrix} z_{ii} & 0 \\ 0 & z_{ii}^* \end{bmatrix}, \quad i=1,\ldots,k_2. \tag{40}$$

It is easy to see that $\tau^{(3)}((1_{k_2}-U_1U_1^\dagger)is_2^{(k_1)}(1_{k_2}-U_1U_1^\dagger))_{ij}$ has exactly this property. In physics, Hermitian self-dual matrices describe systems with Kramers degeneracy. We now use a standard result for matrices with quaternionic entries: A Hermitian self-dual matrix has k_2 scalar eigenvalues $s_{p2}^{(k_1+1)}\tau^{(0)}$.[19] In order to keep the notation simple, we also denote them by $s_{p2}^{(k_1+1)}$. After this adjustment, we can proceed along the same lines which led to Eq. (12). The equation reduces to the well known Gelfand–Tzetlin equations[1,4] of the unitary group $\mathrm{U}(k_2;2)=\mathrm{U}(k_2)$,

$$\begin{aligned} 1&=\sum_{n=1}^{k_2}|U_{n1}|^2, \\ 0&=\sum_{m=1}^{k_2}\frac{|U_{m1}|^2}{is_{m2}^{(k_1)}-is_{p2}^{(k_1+1)}}, \quad p=1,\ldots,k_2-1. \end{aligned} \tag{41}$$

This establishes a one-to-one correspondence between the (k_2-1) eigenvalues $is_{p2}^{(k_1+1)}$ and the moduli squared of the quaternionic entries

$$|U_{m1}|^2=\sum_{k=0}^{3}U_{m1k}^2. \tag{42}$$

All formulas derived in Refs. 1 and 4 for the unitary group can now be adopted to the unitary symplectic one.

F. Invariant measure

According to the coset decomposition (5), the invariant measure $d\mu(u)$ of $u\in\mathrm{UOSp}(k_1/2k_2)$ is the product of all measures on the cosets, i.e., on the spheres described by them. Of course, these measures are conditioned, because the orthogonality of the vectors u_n in $u=[u_1\,u_2\cdots u_{k_1+2k_2}]$ has to be respected. As we will see, the Gelfand–Tzetlin coordinates take care of this condition in a most convenient way. We evaluate the squared invariant length element $du_n^\dagger du_n$. For (k_1-n+1) even, it reads,

$$\begin{aligned} du_n'^\dagger du_n' &= du_n^\dagger du_n \\ &= \sum_{m=1}^{(k_1-n+1)/2}\frac{1}{4|v_m^{(n)}|^2}(d|v_m^{(n)}|^2)^2+\sum_{m=1}^{(k_1-n+1)/2}|v_m^{(n)}|^2(d\vartheta_m^{(n)})^2+\sum_{m'=1}^{k_2}d(\alpha_{m'}^{(n)})^*d\alpha_{m'}^{(n)}, \end{aligned} \tag{43}$$

where we use the parametrization (11). The first equality is due to the basis independence of the invariant length element. It is a highly welcomed feature of the Gelfand–Tzetlin coordinates for the unitary group in ordinary space[1,4] and in superspace[5] that the metric remains diagonal. This holds also in the present problem. Extending the corresponding calculation of Ref. 5, we find for the even levels, i.e., for k_1-n+1 even,

$$d\mu(u_n)=2^{k_2}\prod_{p=1}^{(k_1-n-1)/2} s_{p1}^{(n)}\frac{B_{[(k_1-n-1)/2]\,k_2}((s^{(n)})^2)}{B_{[(k_1-n+1)/2]\,k_2}((s^{(n-1)})^2)}d[s_1^{(n)}]d[\vartheta^{(n)}]d[\xi^{(n)}],$$

$$n\leqslant k_1,\quad k_1-n+1 \text{ even}, \tag{44}$$

and for the odd levels, i.e., for k_1-n+1 odd, we have

$$d\mu(u_n)=2^{k_2}\frac{\Pi_{p=1}^{k_2} is_{p2}^{(n)}is_{p2}^{(n-1)}}{\Pi_{p=1}^{(k_1-n)/2}s_{p1}^{(n-1)}}\frac{B_{[(k_1-n)/2]\,k_2}((s^{(n)})^2)}{B_{[(k_1-n)/2]\,k_2}((s^{(n-1)})^2)}d[s_1^{(n)}]d[\vartheta^{(n)}]d[\xi^{(n)}],$$

$$n\leqslant k_1,\quad k_1-n+1 \text{ odd}. \tag{45}$$

Here, we introduced the function

$$B_{nm}(s)=\frac{\Pi_{p>q}^{n}(s_{p1}-s_{q1})\Pi_{p>q}^{m}(is_{p2}-is_{q2})}{\Pi_{p,q}(s_{p1}-is_{q2})}=\frac{\Delta_n(s_1)\Delta_m(is_2)}{\Pi_p^n\Pi_q^m(s_{p1}-is_{q2})}. \tag{46}$$

It contains the ordinary Vandermonde determinants $\Delta_n(s_1)$ and $\Delta_m(is_2)$ and can be viewed as the supersymmetric generalization of the Vandermonde determinant.[5,20,21] Furthermore, we defined

$$d[s_1^{(n)}]=\prod_{p=1}^{(k_1-n+1)/2} ds_{p1}^{(n)},\quad d[\vartheta^{(n)}]=\prod_{p=1}^{(k_1-n+1)/2} d\vartheta_p^{(n)},\quad \text{and}\quad d[\xi^{(n)}]=\prod_{p=1}^{k_2} d\xi_p^{(n)*}d\xi_p^{(n)}. \tag{47}$$

Remarkably, Eqs. (44) and (45) imply that the measures on all cosets factorize. Collecting all these measures up to the k_1th step, we obtain the invariant measure of $u\in \mathrm{UOSp}(k_1/2k_2)$ in the form

$$d\mu(u)=2^{k_1k_2}\frac{\Delta_{k_2}((is_2^{(k_1)})^2)}{B_{k_1/2\,k_2}(s^2)}\prod_{i=1}^{k_1}\prod_{p=1}^{k_2} is_{p2}^{(i)}d[s_1^{(i)}]d[\vartheta^{(i)}]d[\xi^{(i)}]d\mu(U), \tag{48}$$

where $d\mu(U)$ is the invariant measure on $U\in \mathrm{USp}(2k_2)$. We mention in passing that the measure of the orthogonal group in ordinary space can be obtained by setting all anticommuting variables to zero in the invariant length (43), and skipping all couplings between the bosonic and fermionic eigenvalues in Eq. (48).

The measure (48) on $\mathrm{UOSp}(k_1/2k_2)$ has an important feature: Most conveniently, it is, apart from $d\mu(U)$, flat. This follows directly from the factorization of the measures (44) and (45) on the coset spaces. This is also true for the Gelfand–Tzetlin coordinates of the unitary group in ordinary[1,4] and in superspace[5] as well as for the ones of the orthogonal group in ordinary space. However, this important feature does not continue beyond the k_1th level. We will see that now in working out the measure $d\mu(U)$ for $U\in \mathrm{USp}(2k_2)$. We write $u=[U_1\,U_2\cdots U_{k_2}]$ and decompose the entry U_{nm} as $U_{nm}=|U_{nm}|\hat{U}_{nm}$, with $\hat{U}_{nm}$ a unimodular quaternion. We introduce a parametrization of the unimodular quaternion,

$$\hat{U}_{nm}=\begin{bmatrix}\cos\psi_n^{(m)}\exp(-i\gamma_{n1}^{(m)}) & -\sin\psi_n^{(m)}\exp(i\gamma_{n2}^{(m)})\\ \sin\psi_n^{(m)}\exp(-i\gamma_{n2}^{(m)}) & \cos\psi_n^{(m)}\exp(i\gamma_{n1}^{(m)})\end{bmatrix}, \tag{49}$$

which allows us to write the invariant length element squared as

$$\mathrm{Tr}\,dU_m^{\dagger}dU_m=\sum_{n=1}^{k_2}\left(\frac{1}{4|U_{nm}|^2}(d|U_{nm}|^2)^2+\sum_{i=1}^{2}|U_{nm}|^2(d\gamma_{ni}^{(m)})^2+|U_{nm}|^2(d\cos\psi_n^{(m)})^2\right),$$

$$m=1,\ldots,k_2. \tag{50}$$

Employing and properly adjusting the results of Refs. 1 and 4, one finds the measure of the coset in the mth level

$$d\mu(U_m)=\frac{\Delta_{k_2-m}(is_2^{(k_1+m)})}{2^{k_2-m}\Delta^3_{k_2-m+1}(is_2^{(k_1+m-1)})}\prod_{p,q}\,(is_{p2}^{(k_1+m-1)} - is_{q2}^{(k_1+m)})d[s_2^{(k_1+m)}]d[\cos\psi^{(m)}]d[\gamma^{(m)}], \tag{51}$$

with the definitions

$$d[s_2^{(k_1+m)}]=\prod_{p=1}^{k_2-m+1} ds_{p2}^{(k_1+m)}, \quad d[\cos\psi^{(m)}]=\prod_{p=1}^{k_2-m+1} d\cos\psi_p^{(m)}, \quad \text{and}$$

$$d[\gamma^{(m)}]=\prod_{p=1}^{k_2-m+1} d\gamma_{p1}^{(m)}d\gamma_{p2}^{(m)}. \tag{52}$$

One clearly sees that the factorization property does not hold for the unitary symplectic group. This is a peculiarity of the Gelfand–Tzetlin parametrization for the unitary symplectic group. Collecting all levels we arrive at the invariant measure on $U\in \mathrm{USp}(2k_2)$,

$$d\mu(U)=\frac{1}{2^{k_2(k_2-1)/2}\Delta^3_{k_2}(is_2^{(k_1)})}\prod_{m=1}^{k_2}\prod_{n=1}^{k_2-m+1}\prod_{n'=1}^{k_2-m}\frac{is_{n2}^{(k_1+m-1)}-is_{n'2}^{(k_1+m)}}{\Delta^2_{k_2-m}(is_2^{(k_1+m)})} \times d[s_2^{k_1+m}]d[\cos\psi^{(m)}]d[\gamma^{(m)}], \tag{53}$$

which combines with Eq. (48) to the full measure on $\mathrm{UOSp}(k_1/2k_2)$.

G. Matrix elements

With the results of the previous sections, we can express an arbitrary column u_p of a matrix $u=[u_1\,u_2\cdots u_{k_1+2k_2}]$ in the unitary orthosymplectic supergroup $\mathrm{UOSp}(k_1/2k_2)$ in terms of our angular Gelfand–Tzetlin coordinates. In the rotated primed basis (10), we have

$$u'_p=\hat{b}'^{(1)^T}\hat{b}'^{(2)^T}\cdots\hat{b}'^{(n-1)^T}u_p'^{(n-1)}, \tag{54}$$

where $\hat{b}^{(n)}$ and the scalar products are defined in Eqs. (17)–(19) and in Eqs. (25) and (27). So far, we have constructed a unitary representation of $\mathrm{UOSp}(k_1/2k_2)$. We also wish to obtain an orthosymplectic representation. To this end, we have to assure that the vectors u_j, $j\leqslant k_1$, become real, when the matrix $u'=[u'_1\,u'_2\cdots u'_{k_1+k_2}]$ is rotated back into the unprimed basis. We only discuss the case k_1-n+1 even; the odd case is treated analogously. We recall that the vector $b^{(n)}$ entering in the projection matrix in Eq. (27) has been determined only up to a phase. There is an ambiguity in choosing the phase of $b^{(n)}$. The Gelfand–Tzetlin coordinates parametrize the vector u_n only up to some phases associated with the action of the Cartan subgroup of $\mathrm{UOSp}((k_1-n+1)/2k_2)$. Thus, the projection matrix $\hat{b}^{(n)}$ is as well invariant under the action of this Cartan subgroup. We may multiply $\hat{b}^{(n)}$ with an arbitrary element of the Cartan subgroup without changing its projection properties. We set $b^{(n)}_{2p}=ib^{(n)}_{2p-1}$, $p\leqslant(k_1-n-1)/2$, and $b^{(n)}_{k_1-n}=i|w_{(k_1-n+1)/2}|$ in the commuting sector and $b^{(n)}_{k_1-n+1+2p}=-b^{(n)*}_{k_1-n+2p}$, $p=1,\ldots,k_2$, in the anticommuting one. The remaining phases may be set to zero. With this choice of phases and after undoing the basis rotation, the columns as well as the rows of $\hat{b}^{(n)T}$ fulfill the reality condition (6). The vectors $u_n^{(n-1)}$ become real, too. An explicit form of the real matrices $\hat{b}^{(n)}$ is given in Appendix B.

III. GENERALIZED GELFAND PATTERN

The unitary Lie group $U(k;\beta)$ over the real ($\beta=1$) and complex ($\beta=2$) numbers and over the quaternions ($\beta=4$) is isomorphic to the orthogonal, unitary and unitary symplectic group, $SO(k)\cong U(k;1)$, $U(k)\cong U(k;2)$, and $USp(2k)\cong U(k;4)$. The Gelfand–Tzetlin representation scheme are obtained from the following procedure.[3] An irreducible representation is defined by an ordered set of integers or half integers called highest weights. This irreducible representation can be decomposed in irreducible representations of $U(k-1;\beta)$. In the decomposition each irreducible representation of $U(k-1;\beta)$ occurs either exactly once or never. Only those irreducible representations appear whose highest weights satisfy certain betweenness conditions depending on the group under consideration. Going through all steps of the group chain or, equivalently, the coset decomposition,

$$U(k;\beta)=\frac{U(k;\beta)}{U(k-1;\beta)}\otimes\frac{U(k-1;\beta)}{U(k-2;\beta)}\otimes\cdots\otimes\frac{U(2;\beta)}{U(1;\beta)}\otimes U(1;\beta), \tag{55}$$

one has labeled all states in the irreducible representation of $U(k;\beta)$ by a set of integers or half integers, arranged in a Gelfand pattern.

The analog for the coordinates is as follows. We consider the adjoint group action $\mathcal{O}_k=U^\dagger xU$ on an element x of the Cartan subalgebra $u^{(0)}(k;\beta)$ with $U\in U(k;\beta)$. Here, in this one instance, we use the symbol x for an element in the algebra, because we want to emphasize that the present discussion so far applies to ordinary groups and because we want to avoid confusion with the discussion to follow on the supergroups. This subset $\mathcal{O}_k=U^\dagger xU$ of the complete algebra is called *orbit*. We can map the $U(k;\beta)$ orbit labeled by an ordered set of eigenvalues $x_i>x_{i+1}$ onto many different $U(k-1;\beta)$ orbits by projecting $\mathcal{O}_k$ onto a $k-1$ dimensional subspace. But only those $U(k-1;\beta)$ orbits $\mathcal{O}_{k-1}$ can be reached, whose eigenvalues interlace two neighboring eigenvalues of $\mathcal{O}_k$. This is the so called minimax principle for self-adjoint operators.[22] The Gelfand–Tzetlin method uses the eigenvalues of the projected matrix as coordinates of the coset $U(k;\beta)/U(k-1;\beta)$. However, x is a fixed point of the action of the Cartan subgroup $\exp(ix_0)$, $x_0\in u^{(0)}(k;\beta)$. Hence, the coset $U(k;\beta)/U(k-1;\beta)$ is parametrized by the eigenvalues of $\mathcal{O}_{k-1}$ only up to equivalence classes with respect to the action of the Cartan subgroup of $U(k;\beta)$, parametrized by x_0. In this way the set of variables describing the coset is split into two parts: One part consists of the eigenvalues of $\mathcal{O}_{k-1}$, the other one of the independent elements of x_0. Guillemin and Sternberg[6] introduced the concept of complete integrability by interpreting the entries of x as action and the elements of x_0 as angle coordinates of a generalized mechanical system. We emphasize that this usage of the term angles is different from the one introduced previously. We distinguish between radial and angular Gelfand–Tzetlin coordinates. However, both Gelfand–Tzetlin coordinates, the radial and the angular ones, allow for a further distinction between action and angle degrees of freedom, although the interpretation is slightly different in the two cases. The Guillemin–Sternberg theory applies only to the groups $U(k;\beta)$ for $\beta=1,2$ but not to the unitary symplectic group. This can be considered as the reason for the relatively complicated expression of the measure for $USp(2k)\cong U(k;4)$.

The generalized Gelfand pattern for $UOSp(k_1/2k_2)$ can be extracted from the positive definiteness of the moduli squared of the bosonic matrix elements $|v_i^{(n)}|^2$. If one restricts oneself to the subgroup, which consists of the direct product $SO(k_1)\otimes USp(2k_2)$, the pattern of the $SO(k_1)$ and $USp(2k_2)$ are rederived which are well known from representation theory.[3] We state them here in a different form which emphasizes the relation to the pattern of the unitary group $U(k)$ which is the famous triangle[23]

$$
\begin{array}{ccccccccc}
\underline{x_1^{(0)}} & & \underline{x_2^{(0)}} & & \cdots & & \underline{x_k^{(0)}} & & \underline{x_{k+1}^{(0)}} \\
& x_1^{(1)} & & x_2^{(1)} & \cdots & x_{k-2}^{(1)} & & x_k^{(1)} & \\
& & & \vdots & & & & & \\
& & x_1^{(k-1)} & & & & x_2^{(k-1)} & & \\
& & & & x_1^{(k)} & & & &
\end{array}
\tag{56}
$$

with the betweenness conditions

$$
x_{i+1}^{(j-1)} \leqslant x_i^{(j)} \leqslant x_i^{(j-1)}. \tag{57}
$$

The first row in the pattern (56) labels the orbit which was used as the starting point for the construction of the parametrization. We underline them to distinguish them from the coordinates of the group. From this pattern the pattern of the orthogonal group can be derived by the substitution rule (37), i.e., by assigning to the Cartan subalgebra $\mathrm{u}^{(0)}(k)$ of the unitary group $\mathrm{U}(k)$ the corresponding one $\mathrm{so}^{(0)}(k)$ of the orthogonal group $\mathrm{SO}(k)$. We restrict ourselves to the case of even k. The pattern (56) acquires the form

$$
\begin{array}{ccccccccccccc}
\underline{+x_1^{(0)}} & & \underline{+x_2^{(0)}} & & \cdots & & \underline{+x_{k+1}^{(0)}} & & \underline{-x_{k+1}^{(0)}} & & \cdots & & \underline{-x_2^{(0)}} & & \underline{-x_1^{(0)}} \\
& x_1^{(1)} & & x_2^{(1)} & \cdots & x_k^{(1)} & & 0 & & \underline{-x_k^{(1)}} & \cdots & \underline{-x_2^{(1)}} & & \underline{-x_1^{(1)}} & \\
& & & & & \vdots & & & & & & & & & \\
& & x_1^{(2k-2)} & & x_2^{(2k-2)} & & \underline{-x_2^{(2k-2)}} & & & & \underline{-x_1^{(2k-2)}} & & & & \\
& & & x_1^{(2k-1)} & & 0 & & & \underline{-x_1^{(2k-1)}} & & & & & & \\
& & & & x_1^{(2k)} & & \underline{-x_1^{(2k)}} & & & & & & & & \\
& & & & & 0 & & & & & & & & &
\end{array}
\tag{58}
$$

with the betweenness conditions

$$
\begin{aligned}
x_{i+1}^{(j-1)} &\leqslant x_i^{(j)} \leqslant x_i^{(j-1)}, \\
\left|x_j^{(2k-2j+2)}\right| &\leqslant x_j^{(2k-2j+1)}.
\end{aligned}
\tag{59}
$$

We notice the symmetry along the middle axis. The variable space of the $\mathrm{SO}(2k+2)$ is already covered by the left half of the triangle. The other half is shown to indicate its relation to the unitary case (56). This symmetry in the pattern is due to the presence of an anti-unitary invariance (see the discussion in Ref. 24). In most physics applications, this is time reversal invariance: A system which is not invariant under time reversal is modeled by Hermitian operators. One can go to a time reversal invariant system by replacing these operators with real symmetric ones. Restricting the pattern (58) to the left half of the triangle, the patterns appear in their traditional form.[2] By construction, the pattern of the unitary symplectic group $\mathrm{USp}(2k)$ coincides with the one of the unitary group $\mathrm{U}(k)$; this is due to the fact that only the action variables are used in the pattern. The unitary group has only one, but the unitary symplectic group has three angle variables coming with every action.

The two patterns of the orthogonal and the unitary symplectic groups together represent the subgroup $\mathrm{SO}(k_1)\otimes\mathrm{USp}(2k_2)$ of $\mathrm{UOSp}(k_1/2k_2)$. What represents the coset $\mathrm{UOSp}(k_1/2k_2)/(\mathrm{SO}(k_1)\otimes\mathrm{USp}(2k_2))$? We observe that the lengths squared $|\xi_p^{(n)}|^2$ of the anticommuting variables $\xi_p^{(n)}$ introduced in Eq. (33) have a distinguished meaning. We may identify these lengths of the anticommuting variables as the analogs of the actions stemming from the commuting degrees of freedom. We can organize the lengths squared $|\xi_p^{(n)}|^2$ in a rectangular pattern. Thus, the generalized Gelfand pattern for the unitary orthosymplectic supergroup $\mathrm{UOSp}(k_1/2k_2)$ are obtained,

$$
\begin{array}{ccccccccccccc}
\underline{+s_{11}^{(0)}} & & \underline{+s_{21}^{(0)}} & & \cdots & & \underline{+s_{k+11}^{(0)}} & & \underline{-s_{k+11}^{(0)}} & & \cdots & & \underline{-s_{21}^{(0)}} \quad \underline{-s_{11}^{(0)}} \\
& s_{11}^{(1)} & & s_{21}^{(1)} & \cdots & s_{k1}^{(1)} & & 0 & & \underline{-s_{k1}^{(1)}} & \cdots & \underline{-s_{21}^{(1)}} \quad \underline{-s_{11}^{(1)}} & \\
& & & & & \vdots & & & & & & & \\
& & s_{11}^{(2k-2)} & & s_{21}^{(2k-2)} & & & \underline{-s_{21}^{(2k-2)}} & & \underline{-s_{11}^{(2k-2)}} & & & \\
& & & s_{11}^{(2k-1)} & & 0 & & \underline{-s_{11}^{(2k-1)}} & & & & & \\
& & & & s_{11}^{(2k)} & & \underline{-s_{11}^{(2k)}} & & & & & & \\
& & & & & & 0 & & & & & & \\
& & & & & |\xi_1^{(1)}|^2 & & |\xi_2^{(1)}|^2 & \cdots & |\xi_{k_2-1}^{(1)}|^2 & & |\xi_{k_2}^{(1)}|^2 & \\
& & & & & |\xi_1^{(2)}|^2 & & |\xi_2^{(2)}|^2 & \cdots & |\xi_{k_2-1}^{(2)}|^2 & & |\xi_{k_2}^{(2)}|^2 & \\
& & & & & & \vdots & & & & & & & \\
& & & & & |\xi_1^{(k_1)}|^2 & & |\xi_2^{(k_1)}|^2 & \cdots & |\xi_{k_2-1}^{(k_1)}|^2 & & |\xi_{k_2}^{(k_1)}|^2 & \\
& & & & s_{12}^{(k_1)} & & s_{22}^{(k_1)} & & \cdots & & s_{(k_2-1)2}^{(k_1)} & & s_{k_2 2}^{(k_1)} \\
& & & s_{12}^{(k_1+1)} & & s_{22}^{(k_1+1)} & & \cdots & & s_{(k_2-2)2}^{(k_1+1)} & & s_{(k_2-1)2}^{(k_1+1)} & \\
& & & & & & \vdots & & & & & & & \\
& & & & s_{12}^{(k_1+k_2-1)} & & & & s_{22}^{(k_1+k_2-1)} & & & & \\
& & & & & & s_1^{(k_1+k_2)} & & & & & &
\end{array}
\tag{60}
$$

with the betweenness conditions

$$
\begin{gathered}
s_{(i+1)1}^{(m-1)} \leqslant s_{i1}^{(m)} \leqslant s_{i1}^{(m-1)}, \\
s_{(i+1)2}^{(k_1+l)} \leqslant s_{i2}^{(k_1+l+1)} \leqslant s_{i2}^{(k_1+l)}, \\
-s_{j1}^{(k_1-2j-1)} \leqslant s_{j1}^{(k_1-2j)} \leqslant s_{j1}^{(k_1-2j-1)},
\end{gathered}
\tag{61}
$$

where $1\leqslant j\leqslant k_1/2-1$, $1\leqslant m\leqslant k_1-2$, and $0\leqslant l\leqslant k_2-1$. It was shown in Ref. 25 that the unitary supergroup U(1/1) can be represented by supersymmetric generalizations of Wigner functions.

This representation of the supergroup U(1/1) is labeled by the length of an anticommuting variable. Therefore, we want to interpret the generalized Gelfand pattern (60) as labeling another kind of representation which involves anticommuting variables as labels. The two triangles label the basis of an irreducible representation of the product $\mathrm{SO}(k_1)\otimes\mathrm{USp}(2k_2)$, whereas the remaining coset $\mathrm{UOSp}(k_1/2k_2)/(\mathrm{SO}(k_1)\otimes\mathrm{USp}(2k_2))$ is represented by the rectangular block of the lengths squared of anticommuting variables. This extends the corresponding considerations for the unitary supergroup in Ref. 5. It is challenging to find a further interpretation of these new representations of supergroups, possibly by generalizing the Guillemin–Sternberg theory.

IV. SUMMARY AND CONCLUSIONS

We constructed Gelfand–Tzetlin coordinates for the unitary orthosymplectic supergroup $\mathrm{UOSp}(k_1/2k_2)$. To this end, we further extended the construction for the unitary supergroup $\mathrm{U}(k_1/k_2)$. We obtained *angular* Gelfand–Tzetlin coordinates, which always live in the space of the unitary orthosymplectic supergroup. They ought to be distinguished from *radial* Gelfand–Tzetlin which map group degrees of freedom onto those of another space. We also calculated the invariant Haar measure on $\mathrm{UOSp}(k_1/2k_2)$ and obtained an expression that is fairly simple due to the recursive structure of the coordinates. As the orthogonal and the unitary symplectic groups are subgroups of the unitary orthosymplectic supergroup, our construction also includes *angular* Gelfand–Tzetlin coordinates on these ordinary groups.

The Gelfand–Tzetlin coordinates can be arranged in a generalized Gelfand pattern. A remarkable feature of this pattern is the appearance of moduli squared of anticommuting variables. We argued that an interpretation of these anticommuting variables as eigenvalues of a set of invariant operators is likely to exist. It is an interesting task to clarify the rôle of these anticommuting variables in the representation theory for supergroups.

So far, Gelfand–Tzetlin coordinates were only constructed for compact groups. But there is no apparent obstacle to construct them also for noncompact groups. It would be interesting to see if such a construction is indeed possible and how the noncompactness of some variables is reflected in the corresponding Gelfand pattern, in ordinary and in superspace.

ACKNOWLEDGMENTS

T.G. and H.K. acknowledge financial support from the Swedish Research Council and from the RNT Network of the European Union with Grant No. HPRN-CT-2000-00144, respectively. H.K. also thanks the division of Mathematical Physics, LTH, for its hospitality during his visits to Lund.

APPENDIX A: SOLUTION OF EQS. (28)–(30)

We consider Eq. (28) and insert the solutions for $|v_m^{(n)}|^2$ and $|\alpha_m^{(n)}|^2$ given in (31). The right hand side of Eq. (28) can then be expanded in a sum of monomials in the nilpotent Gelfand–Tzetlin variables $|\xi_q^{(n)}|^2$, $q=1,\ldots,k_2$. Since each of the $|\xi_q^{(n)}|^2$ only appears linearly, the rank of the monomials cannot exceed k_2. Thus, we can rewrite Eq. (28) in the form

$$\frac{1}{|w_p^{(n)}|^2}=\sum_{r=0}^{k_2} M^{(r)}\ , \tag{A1}$$

where $M^{(r)}$ is the nilpotent part of $1/|w_p^{(n)}|^2$, consisting of monomials in $|\xi_q^{(n)}|^2$ with rank r. Explicitly we have

$$M^{(r)}=\sum_{j_1\leqslant j_2\leqslant\cdots\leqslant j_r}^{k_2}\sum_{m}^{(k_1-n+1)/2}\frac{\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((s_{m1}^{(n-1)})^2-(s_{q1}^{(n)})^2)}{\Pi_{q=1,q\neq m}^{(k_1-n+1)/2}((s_{m1}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\frac{(s_{m1}^{(n-1)})^2+(s_{p1}^{(n)})^2}{(s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2}$$
$$\times\frac{\Pi_{i=1}^{r}|\xi_{j_i}|^2}{\Pi_{i=1}^{r}((s_{m1}^{(n-1)})^2-(is_{j_i2}^{(n-1)})^2)}$$
$$+\sum_{\substack{j_2\leqslant\cdots\leqslant j_r\\ j_1\neq j_i}}^{k_2}\frac{\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((is_{j_12}^{(n-1)})^2-(s_{q1}^{(n)})^2)}{\Pi_{q=1}^{(k_1-n+1)/2}((is_{j_12}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\frac{(is_{j_12}^{(n-1)})^2+(s_{p1}^{(n)})^2}{(is_{j_12}^{(n-1)})^2-(s_{p1}^{(n)})^2}$$
$$\times\frac{\Pi_{i=1}^{r}|\xi_{j_i}|^2}{\Pi_{i=2}^{r}((is_{j_12}^{(n-1)})^2-(is_{j_i2}^{(n-1)})^2)}, \tag{A2}$$

for $r=1,\ldots,k_2$. The sum over m is the Laplace expansion of a determinant. For its evaluation we use the formula

$$\frac{1}{\Pi_{i=1}^{r}((s_{m1}^{(n-1)})^2-(is_{i2}^{(n-1)})^2)}=\sum_{i=1}^{r}\frac{1}{(s_{m1}^{(n-1)})^2-(is_{i2}^{(n-1)})^2}\frac{1}{\Pi_{i'\neq i}^{r}((is_{i2}^{(n-1)})^2-(is_{i'2}^{(n-1)})^2)}, \tag{A3}$$

which is well known from complex analysis. After symmetrizing the second sum in the indices, $j_i, i=1,\ldots,r$, we arrive at the following expression for $M^{(r)}$:

$$M^{(r)}=\sum_{j_1\leqslant j_2\leqslant\cdots\leqslant j_r}^{k_2}\sum_{i=1}^{r}\frac{1}{\Pi_{i'\neq i}^{r}((is_{j_i2}^{(n-1)})^2-(is_{j_{i'}2}^{(n-1)})^2)}$$
$$\times\sum_{m}^{(k_1-n+1)/2}\frac{\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((s_{m1}^{(n-1)})^2-(s_{q1}^{(n)})^2)}{\Pi_{q=1,q\neq m}^{(k_1-n+1)/2}((s_{m1}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\left[\frac{(s_{m1}^{(n-1)})^2+(s_{p1}^{(n)})^2}{((s_{p1}^{(n)})^2-(is_{j_i2}^{(n-1)})^2)((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)}\right.$$
$$\left.-\frac{(s_{m1}^{(n-1)})^2+(s_{p1}^{(n)})^2}{((s_{p1}^{(n)})^2-(is_{j_i2}^{(n-1)})^2)((s_{m1}^{(n-1)})^2-(is_{j_i2}^{(n-1)})^2)}\right]\prod_{i=1}^{r}|\xi_{j_i}|^2$$
$$+\sum_{j_1\leqslant j_2\leqslant\cdots\leqslant j_r}^{k_2}\sum_{i=1}^{r}\frac{1}{\Pi_{i'\neq i}^{r}((is_{j_i2}^{(n-1)})^2-(is_{j_{i'}2}^{(n-1)})^2)}$$
$$\times\frac{\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((is_{j_12}^{(n-1)})^2-(s_{q1}^{(n)})^2)}{\Pi_{q=1}^{(k_1-n+1)/2}((is_{j_12}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\frac{(is_{j_12}^{(n-1)})^2+(s_{p1}^{(n)})^2}{(is_{j_12}^{(n-1)})^2-(s_{p1}^{(n)})^2}\prod_{i=1}^{r}|\xi_{j_i}|^2. \tag{A4}$$

Now the determinant mentioned above can be evaluated by using the translational invariance of the differences. The second term in the squared bracket cancels completely; we are left with

$$M^{(r)}=\sum_{j_1\leqslant j_2\leqslant\cdots\leqslant j_r}^{k_2}\sum_{i=1}^{r}\frac{1}{\Pi_{i'\neq i}^{r}((is_{j_i2}^{(n-1)})^2-(is_{j_{i'}2}^{(n-1)})^2)}$$
$$\times\frac{2(s_{p1}^{(n)})^2\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((s_{q1}^{(n)})^2-(s_{p1}^{(n)})^2)}{((s_{p1}^{(n)})^2-(is_{j_i2}^{(n-1)})^2)\Pi_{m=1}^{(k_1-n+1)/2}((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)}\prod_{i=1}^{r}|\xi_{j_i}|^2. \tag{A5}$$

Using identity (A3) once more and summing over r gives

$$\frac{1}{|w_p^{(n)}|^2}=\frac{-2(s_{p1}^{(n)})^2\Pi_{q=1,q\neq p}^{(k_1-n-1)/2}((s_{p1}^{(n)})^2-(s_{q1}^{(n)})^2)}{\Pi_{m=1}^{(k_1-n+1)/2}((s_{m1}^{(n-1)})^2-(s_{p1}^{(n)})^2)}\left(\sum_{r=0}^{k_2}\sum_{j_1\leqslant j_2\leqslant\cdots t\leqslant j_r}^{k_2}\prod_{i=1}^{r}\frac{|\xi_{j_i}|^2}{(s_{p1}^{(n)})^2-(is_{j_i2}^{(n-1)})^2}\right). \tag{A6}$$

The double sum in Eq. (A6) simply amounts to

$$\prod_{q=1}^{k_2}\left(1+\frac{|\xi_q^{(n)}|^2}{(s_{p1}^{(n)})^2-(is_{q2}^{(n-1)})^2}\right). \tag{A7}$$

Employing the definition (33) of $|\xi_q^{(n)}|^2$, we arrive at the final result for $|w_p^{(n)}|^2$ in Eq. (32). Equation (29) and the corresponding equation for the odd levels are evaluated similarly, yielding the results stated in Sec. II D. Equation (30) has to be treated differently due to the Grassmann singularities, occurring on the left hand side. Inserting the expressions Eq. (31) into Eq. (30) we have

$$\begin{aligned}1=|\beta_p^{(n)}|^2\Bigg(&\sum_{m}^{(k_1-n+1)/2}\frac{(s_{m1}^{(n-1)})^2+(is_{p2}^{(n)})^2}{((s_{m1}^{(n-1)})^2-(is_{p2}^{(n)})^2)^2}|v_m^{(n)}|^2+\sum_{\substack{m'=1\\m'\neq p}}^{k_2}\frac{(is_{m'2}^{(n-1)})^2+(is_{p2}^{(n)})^2}{((is_{m'2}^{(n-1)})^2-(is_{p2}^{(n)})^2)^2}|\alpha_{m'}^{(n)}|^2\\&+\frac{\Pi_{q=1}^{(k_1-n-1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n)})^2)\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n-1)})^2)}{\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n)})^2)\Pi_{q=1}^{(k_1-n+1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\\&\times\frac{(is_{p2}^{(n-1)})^2+(is_{p2}^{(n)})^2}{|\xi_p^{(n)}|^2}\Bigg).\end{aligned} \tag{A8}$$

To cancel the singularity, $|\beta_p^{(n)}|^2$ has to be expanded in terms of $c_p^{(n)}|\xi_p^{(n)}|^2$. The expansion coefficient $c_p^{(n)}$ now contains a nonzero part and its inverse is therefore well defined. Dividing both sides by $c_p^{(n)}$ and ordering the right hand side by powers of $|\xi_p^{(n)}|^2$, one finds

$$\begin{aligned}\frac{1}{c_p^{(n)}}=&2(is_{p2}^{(n-1)})^2\frac{\Pi_{q=1}^{(k_1-n-1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n)})^2)\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n-1)})^2))}{\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n)})^2)\Pi_{q=1}^{(k_1-n+1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\\&+\Bigg(\sum_{m}^{(k_1-n+1)/2}\frac{(s_{m1}^{(n-1)})^2+(is_{p2}^{(n)})^2}{((s_{m1}^{(n-1)})^2-(is_{p2}^{(n)})^2)^2}|v_m^{(n)}|^2+\sum_{\substack{m'=1\\m'\neq p}}^{k_2}\frac{(is_{m'2}^{(n-1)})^2+(is_{p2}^{(n)})^2}{((is_{m'2}^{(n-1)})^2-(is_{p2}^{(n)})^2)^2}|\alpha_{m'}^{(n)}|^2\\&-\frac{\Pi_{q=1}^{(k_1-n-1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n)})^2)\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n-1)})^2))}{\Pi_{q=1,q\neq p}^{k_2}((is_{p2}^{(n-1)})^2-(is_{q2}^{(n)})^2)\Pi_{q=1}^{(k_1-n+1)/2}((is_{p2}^{(n-1)})^2-(s_{q1}^{(n-1)})^2)}\Bigg)|\xi_p^{(n)}|^2.\end{aligned} \tag{A9}$$

Since $c_p^{(n)}$ and thus $1/c_p^{(n)}$ are of order zero in $|\xi_p^{(n)}|^2$, the whole term in round brackets can be neglected. It can be shown by straightforward manipulations that this term leads just to a shift of $(is_{p2}^{(n-1)})^2\rightarrow(is_{p2}^{(n)})^2$ in the resulting expression for $c_p^{(n)}$. This does not affect $|\beta_p^{(n)}|^2$. Hence, we immediately arrive at the result for $|\beta_p^{(n)}|^2$ given in Eq. (32). The equations for the odd levels are treated accordingly.

APPENDIX B: REAL FORM OF THE PROJECTION MATRICES $\hat{b}^{(n)}$

We restrict ourselves to the case $n\leqslant k_1$, (k_1-n+1) even. The odd case can be treated accordingly. The rectangular $(k_1-n+1+k_2)\times(k_1-n+k_2)$ matrix $\hat{b}^{(n)T}$ can schematically be written as

$$\hat{b}^{(n)}=\begin{bmatrix} \tilde{b}_{11}^{(n)} & \tilde{b}_{1}^{(n)} & \tilde{b}_{12}^{(n)} \\ \tilde{b}_{21}^{(n)} & \tilde{b}_{2}^{(n)} & \tilde{b}_{22}^{(n)} \end{bmatrix}. \tag{B1}$$

Here, $\tilde{b}_{11}^{(n)}$ is a $(k_1-n+1)/2\times(k_1-n-1)/2$ matrix with entries

$$(\tilde{b}_{11}^{(n)})_{ij}=\sqrt{2}\,\frac{|v_i^{(n)}||w_j^{(n)}|}{(s_{i1}^{(n-1)})^2-(s_{j1}^{(n)})^2}\begin{bmatrix} s_{j1}^{(n)}\cos\vartheta_i^{(n)} & s_{j1}^{(n-1)}\sin\vartheta_i^{(n)} \\ -s_{j1}^{(n)}\sin\vartheta_i^{(n)} & s_{j1}^{(n-1)}\cos\vartheta_i^{(n)} \end{bmatrix}. \tag{B2}$$

The matrix $\tilde{b}_{12}^{(n)}$ has dimension $(k_1-n+1)/2\times k_2$ and entries

$$\begin{aligned}(\tilde{b}_{12}^{(n)})_{ij}=&\frac{|v_i^{(n)}|}{(s_{i1}^{(n-1)})^2-(is_{j2}^{(n)})^2}\\ &\times\begin{bmatrix} \beta_j^{(n)*}(is_{j2}^{(n)}\cos\vartheta_i^{(n)}+s_{j1}^{(n-1)}i\sin\vartheta_i^{(n)}) & -i\beta_j^{(n)*}(s_{i1}^{(n-1)}\cos\vartheta_i^{(n)}+is_{j2}^{(n)}i\sin\vartheta_i^{(n)}) \\ -\beta_j^{(n)}(is_{j2}^{(n)}\cos\vartheta_i^{(n)}-s_{j1}^{(n-1)}i\sin\vartheta_i^{(n)}) & -i\beta_j^{(n)}(s_{i1}^{(n-1)}\cos\vartheta_i^{(n)}-is_{j2}^{(n)}i\sin\vartheta_i^{(n)}) \end{bmatrix}.\end{aligned} \tag{B3}$$

Moreover, $\tilde{b}_{21}^{(n)}$ is a $k_2\times(k_1-n+1)/2$ matrix with entries

$$(\tilde{b}_{21}^{(n)})_{ij}=\frac{|w_j^{(n)}|}{(is_{i2}^{(n-1)})^2-(s_{j1}^{(n)})^2}\begin{bmatrix} \alpha_i^{(n)}s_{j1}^{(n)} & i\alpha_i^{(n)}is_{i2}^{(n-1)} \\ \alpha_i^{(n)*}s_{j1}^{(n)} & -i\alpha_i^{(n)*}is_{i2}^{(n-1)} \end{bmatrix}, \tag{B4}$$

and $\tilde{b}_{22}^{(n)}$ is a $k_2\times(k_1-n+1)/2$ matrix with entries

$$(\tilde{b}_{22}^{(n)})_{ij}=\sqrt{2}\begin{bmatrix} \alpha_i^{(n)}\beta_j^{(n)*}/(is_{i2}^{(n-1)}-is_{j2}^{(n)}) & \alpha_i^{(n)}\beta_j^{(n)}/(is_{i2}^{(n-1)}+is_{j2}^{(n)}) \\ -\alpha_i^{(n)*}\beta_j^{(n)*}/(is_{i2}^{(n-1)}+is_{j2}^{(n)}) & -\alpha_i^{(n)*}\beta_j^{(n)}/(is_{i2}^{(n-1)}-is_{j2}^{(n)}) \end{bmatrix}. \tag{B5}$$

Finally, the entries of $\tilde{b}_1^{(n)}$ and $\tilde{b}_2^{(n)}$ are given by

$$\begin{aligned}(\tilde{b}_1^{(n)})_i&=\sqrt{2}\,\frac{|v_i^{(n)}||w_{(k_1-n+1)/2}^{(n)}|}{s_{i1}^{(n-1)}}\begin{bmatrix}\sin\vartheta_i^{(n)}\\ \cos\vartheta_i^{(n)}\end{bmatrix},\quad i=1,\ldots,\frac{k_1-n+1}{2},\\ (\tilde{b}_2^{(n)})_i&=\frac{1}{\sqrt{2}}\,\frac{|w_{(k_1-n+1)/2}^{(n)}|}{s_{i1}^{(n-1)}}\begin{bmatrix} i\alpha_i^{(n)} \\ -i\alpha_i^{(n)*}\end{bmatrix},\quad i=1,\ldots,k_2.\end{aligned} \tag{B6}$$

We notice that all elements of $\hat{b}^{(n)}$ are real.

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On the construction of self-polar and self-polar Hilbertian norms on Minkowski space of dimension 2

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(Received 12 February 2003; accepted 15 April 2003)

Considering the real Minkowski space $\mathcal{M}^2$ endowed with the indefinite inner product $(\vec{a},\vec{b})=x_a x_b - y_a y_b$, $\vec{a}=(x_a,y_a)$, $\vec{b}=(x_b,y_b)\in\mathcal{M}^2$, we give a general construction for the boundary $\partial U_p=\{\vec{a}\in\mathcal{M}^2; p(\vec{a})=1\}$ of the unit ball U_p of some self-polar norm p on $\mathcal{M}^2$. We show further that every self-polar norm p on $\mathcal{M}^2$ is obtained by our construction. A detailed investigation of the possible choices of the ingredients of our construction (two points P_j, $j=1,2$, and a convex arc connecting P_1 and P_2) yields a complete classification of all self-polar norms on $\mathcal{M}^2$. Our results are finally applied to the special case of Hilbertian self-polar norms. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1597421]

I. INTRODUCTION AND SOME PRELIMINARIES

For a pre-Hilbert (unitary) space $E,[.,.]$ (i.e., the inner product $[.,.]$ is positive definite), a canonical norm

$$p(x)=\sqrt{[x,x]}, \tag{1}$$

$x\in E$, exists on E. Now it is of interest to find the corresponding substitutes when the pre-Hilbert space is replaced by some nondegenerate inner product space $E,(.,.)$, [i.e., E is a real or complex vector space equipped with a bilinear symmetric respective sesquilinear Hermitian form $(.,.)$ which is nondegenerate, see Refs. 4 and 3].

If the inner product $(.,.)$ is indefinite, then (1) does not define a norm, and thus, no canonical norm is available. As explained in Refs. 8 and 9, the role of the canonical norm (1) is now played by Hilbertian self-polar norms q satisfying

$$q(x)=\sup_{0\neq y\in E}\frac{|(x,y)|}{q(y)}, \tag{2}$$

and furthermore, given by

$$q(x)=\sqrt{[x,x]}, \tag{3}$$

$x\in E$, in terms of a positive definite inner product $[.,.]$ on $E\times E$.

In generalization of the positive definite case, where the canonical norm is uniquely defined, the following is possible in the general case of an inner product space:

(i) there is no self-polar norm on $E,(.,.)$, (cf. Ref. 4, Example III.3.2).
(ii) there is exactly one self-polar norm on $E,(.,.)$, (cf. Ref. 10, and references cited there).
(iii) there is a whole family of self-polar norms defining nonequivalent topologies on E, (such a family of self-polar norms was explicitely constructed by Araki in Ref. 1).

If (iii) applies to some inner product space $E,(.,.)$, it is of interest to have a complete classification of all self-polar norms as well as Hilbertian self-polar norms on $E,(.,.)$. Along these lines, the present paper is aimed at such a classification in the easiest instance of an indefinite inner

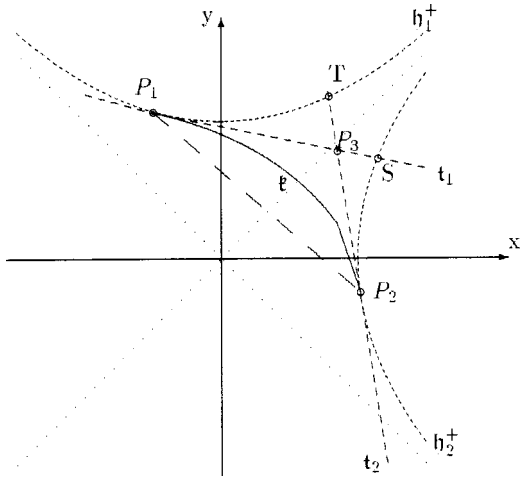

FIG. 1. Steps I and II of the construction.

product space, namely, the real Minkowski space $\mathcal{M}^2$ of dimension 2. Let us mention that a special example of such a self-polar norm on $\mathcal{M}^2$, which is different from the well-known Euclidean norm, is given in Ref. 6, Example 2.9. Furthermore, the self-polar and Hilbertian self-polar norms on $\mathcal{M}^2$ are also of some interest, since they serve as building blocks for the construction of self-polar and Hilbertian self-polar norms, respectively, on inner product spaces of higher dimensions, including the case of infinitely many dimensions, where those norms define nonequivalent locally convex topologies (see Ref. 10, Sec. 6.2).

In order to obtain such a classification, we give a general construction which explicitly yields all self-polar and Hilbertian self-polar norms, respectively, on $\mathcal{M}^2$. It turns out that in contrast to the positive definite case, where exactly one Hilbertian self-polar norm exists, on $\mathcal{M}^2$ there are as well nondenumerably many self-polar as nondenumerably many Hilbertian self-polar norms.

Remembering that on the one hand the unit ball $U_p=\{a\in\mathcal{M}^2;\, p(a)\leqslant 1\}$ of some norm p is a symmetric, convex, compact set containing the origin O as an inner point, and on the other hand, p is the gauge of U_p, we have a one-to-one correspondence between the norms p and the convex curves $\partial U_p=\{a\in\mathcal{M}^2;\, p(a)=1\}$ (see Lemma 4.1 for more details). The idea of our construction is to construct those curves ∂U_p for which the norm p is self-polar and Hilbertian self-polar, respectively.

In all what follows let a connected piece of the boundary of some convex, compact set containing O as an inner point be denoted as *convex arc*. Roughly speaking, we show that every convex arc $\mathfrak{k}$, which connects the two halfs of hyperbolae

$$\mathfrak{h}_1^+=\{\vec{a}=(x_a,y_a)\in\mathcal{M}^2;\;\; x_a^2-y_a^2=-1, y_a>0\}\,,$$

$$\mathfrak{h}_2^+=\{\vec{a}=(x_a,y_a)\in\mathcal{M}^2;\;\; x_a^2-y_a^2=-1, x_a>0\}$$

from some point $P_1\in\mathfrak{h}_1^+$ to a point $P_2\in\mathfrak{h}_2^+$ and lies completely between them (see Fig. 1), extends to a convex curve ∂U_p related to some self-polar norm p (see Theorem 4.11). On the other hand, we show that every convex curve ∂U_q related to a given self-polar norm q on $\mathcal{M}^2$ is obtained by that construction (see Theorem 4.13).

Let us mention that the well-known Aronszajn–Schatten construction of self-polar norms (Ref. 2 and Ref. 4, Chap. IV.4) is completely different from our construction, because our construction completes some convex arc $\mathfrak{k}$ to the boundary of the unit ball of a self-polar norm, while

the Aronszajn–Schatten construction starts with some norm q satisfying $q' \leqslant q$ (q' denotes the polar norm of q) and then constructs a self-polar norm q_∞ by an iteration process.

The pattern of the present paper is as follows. While the three steps I, II, III of the construction of ∂U_p of some self-polar norm p is described in Sec. II, Sec. III is aimed at the determination of this construction. More precisely, the possible choices of $P_j \in \mathfrak{h}_j^+$, $j=1,2$, are characterized in Lemma 3.1, and then all the possible constructions of Sec. II are parametrized in Corollary 3.3. Our main results are contained in Sec. IV. While Theorem 4.11 shows that self-polar norms are obtained by our construction, Theorem 4.13 proves that every self-polar norm on $\mathcal{M}^2$ is given by our construction. Using those results, a complete classification of all self-polar norms on $\mathcal{M}^2$ is contained in Corollary 4.14. In Sec. V, the above results on self-polar norms are applied to the interesting case of Hilbertian self-polar norms. Along these lines all self-polar Hilbertian norms are explicitely given in Proposition 5.2, and those constructions of Sec. II, which yield Hilbertian self-polar norms, are characterized in Corollary 5.6. Let us mention that some ideas of the present paper are taken from Ref. 11.

II. THE CONSTRUCTION

In the present section the construction of the boundary ∂U_p of the unit ball

$$U_p = \{\vec{a} \in \mathcal{M}^2; p(\vec{a}) \leqslant 1\}$$

of some self-polar norm p on the real Minkowski space $\mathcal{M}^2$ is given. Using Cartesian (x,y)-coordinates, remember that the inner product on $\mathcal{M}^2$ is given by

$$(\vec{a},\vec{b}) = x_a x_b - y_a y_b\,,$$

where $\vec{a}=(x_a,y_b), \vec{b}=(x_b,y_b) \in \mathcal{M}^2$, $x_a, y_a, x_b, y_b \in \mathbb{R}$.

Let us consider the following four halfs of hyperbolae:

$$\mathfrak{h}_1^+ = \{\vec{a} \in \mathcal{M}^2; x_a^2 - y_a^2 = -1, y_a > 0\}, \tag{4}$$

$$\mathfrak{h}_1^- = \{\vec{a} \in \mathcal{M}^2; x_a^2 - y_a^2 = -1, y_a < 0\}, \tag{5}$$

$$\mathfrak{h}_2^+ = \{\vec{a} \in \mathcal{M}^2; x_a^2 - y_a^2 = 1, x_a > 0\}, \tag{6}$$

$$\mathfrak{h}_2^- = \{\vec{a} \in \mathcal{M}^2; x_a^2 - y_a^2 = 1, x_a < 0\}. \tag{7}$$

The construction proceeds through the following steps I–III.

Step I:

(1) Choosing an arbitrary $x_1 \in \mathbb{R}$, consider the point
$$P_1 = (x_1, \sqrt{1+x_1^2}) \in \mathfrak{h}_1^+\,.$$

(2) Consider the tangent $\mathfrak{t}_1$ on $\mathfrak{h}_1^+$ at P_1 given by
$$\mathfrak{t}_1: \quad y = \sqrt{1+x_1^2} + \frac{x_1}{\sqrt{1+x_1^2}}(x - x_1)\,. \tag{8}$$

(3) Consider the intersection point $S = \mathfrak{t}_1 \cap \mathfrak{h}_2^+$ with coordinates x_S, y_S, which are explicitly given by
$$\begin{aligned} x_S &= x_1 + \sqrt{2}\,\sqrt{1+x_1^2}\,, \\ y_S &= \sqrt{2}\,x_1 + \sqrt{1+x_1^2}\,. \end{aligned} \tag{9}$$

Step II:

(1) Choose a point $P_2 \in \mathfrak{h}_2^+$ with coordinates $P_2=(x_2,y_2)$ such that

$$\text{(i)}\quad y_2 \leqslant \sqrt{2}\, x_1 + \sqrt{1+x_1^2}\,, \tag{10}$$

$$\text{(ii)}\quad x_1 \leqslant \sqrt{2}\, y_2 + \sqrt{1+y_2^2} \tag{11}$$

are satisfied.

(2) Choose a convex arc $\mathfrak{k}$ with the properties

$$\begin{aligned} &\text{(i)} \quad \mathfrak{k} \text{ connects } P_2 \text{ with } P_1\,, \\ &\text{(ii)} \quad \mathfrak{k} \text{ does not contain any points of } \mathfrak{h}_1^+ \text{ or } \mathfrak{h}_2^+ \text{ other than } P_1 \text{and } P_2\,. \end{aligned} \tag{12}$$

(See Fig. 1.)

Remark 2.1: (a) Using polar coordinates, the above conditions (10), (11) upon P_2 are more transparently described in (30). Especially, it will be shown in Remark 3.2(b) that P_2 satisfying (10), (11) always exists.

(b) The geometric interpretation of (10), (11) is the following. Considering the tangent $\mathfrak{t}_2$ on $\mathfrak{h}_2^+$ at P_2, given by

$$\mathfrak{t}_2\colon\ \frac{x-x_2}{y-y_2} = \frac{y_2}{\sqrt{1+y_2^2}}\ , \tag{13}$$

and the intersection point $P_3=\mathfrak{t}_1 \cap \mathfrak{t}_2$, we get that (10), (11) are equivalent to the property that the triangle $\Delta(P_1P_2P_3)$ is either positively orientated or it collapses to the straight line $\overline{P_1P_2}$.

[*Proof:* Consider the intersection point $T=\mathfrak{t}_2 \cap \mathfrak{h}_1^+$ with coordinates

$$\begin{aligned} x_T &= \sqrt{2}\, y_2 + \sqrt{1+y_2^2}\,, \\ y_T &= \sqrt{2}\, \sqrt{1+y_2^2} + y_2\,. \end{aligned} \tag{14}$$

Notice that the triangle $\Delta(P_1P_2P_3)$ is positively orientated or it collapses to the straight line $\overline{P_1P_2}$ if and only if

$$y_2 \leqslant y_S\,, \tag{15}$$

$$x_1 \leqslant x_T\,, \tag{16}$$

are satisfied. Inserting (9) and (14) in (15) and (16), respectively, the proof is completed.] □

(c) Considering the triangle $\Delta(P_1P_2P_3)$ given above, we get that a convex arc $\mathfrak{k}$ connecting P_2 with P_1 satisfies (12) if and only if $\mathfrak{k}$ is inside or at the boundary of $\Delta(P_1P_2P_3)$. Hence, such an arc $\mathfrak{k}$ always exists by Remark 2.1(b).

Step III: Introducing polar coordinates $r=\sqrt{x^2+y^2}$, $\varphi=\arctan(y/x)$ on $\mathcal{M}^2$, let the convex arc $\mathfrak{k}$ be given by the function

$$\varphi \to r_{\mathfrak{k}}(\varphi) \quad \text{with} \quad \varphi_2 \leqslant \varphi \leqslant \varphi_1\,,$$

where $\varphi_j=\arctan(y_j/x_j)$ denote the polar angles of P_j, $j=1,2$. Then,

$$r(\varphi)=\begin{cases} r_{\mathfrak{k}}(\varphi) \quad \text{for } \varphi_2 \leqslant \varphi \leqslant \varphi_1\,, \\ \left(\sup\limits_{\varphi_2 \leqslant \psi \leqslant \varphi_1} r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi-\pi)\right)^{-1} \quad \text{for } \varphi_1 < \varphi \leqslant \varphi_2+\pi, \\ r_{\mathfrak{k}}(\varphi+\pi) \quad \text{for } \varphi_2+\pi < \varphi \leqslant \varphi_1+\pi, \\ \left(\sup\limits_{\varphi_2 \leqslant \psi \leqslant \varphi_1} r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi)\right)^{-1} \quad \text{for } \varphi_1+\pi < \varphi < \varphi_2+2\pi \end{cases} \tag{17}$$

describes the boundary ∂U_p of the unit ball U_p of some self-polar norm p on $\mathcal{M}^2$.

While the proof that $\varphi \to r(\varphi)$ given in (17) describes the boundary of the unit ball of some norm p [which especially implies that $\varphi \to r(\varphi)$ is continuous at $\varphi_1, \varphi_2, \varphi_1+\pi, \varphi_2+\pi$] will be given in Lemmas 4.1a and 4.2, the self-polarity of p will be shown in Theorem 4.11.

The suprema used in (17) are considered next.

Lemma 2.2: (a) The suprema considered in (17) are positive.

(b) The following relations hold:

$$r(\varphi) = \inf_{\substack{\varphi_2 \leqslant \psi \leqslant \varphi_1, \\ \pi/2 < \psi+\varphi < 3/2\,\pi}} (r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi-\pi))^{-1}$$

$$\text{for} \quad \varphi_1 < \varphi \leqslant \varphi_2 + \pi, \tag{18}$$

$$r(\varphi) = \inf_{\substack{\varphi_2 \leqslant \psi \leqslant \varphi_1, \\ 3/2\,\pi < \psi+\varphi < 5/2\,\pi}} (r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi))^{-1}$$

$$\text{for} \quad \varphi_1 + \pi < \varphi \leqslant \varphi_2 + 2\,\pi. \tag{19}$$

Proof: (a) Let us consider the first sup in (17):

$$\left(\sup_{\varphi_2 \leqslant \psi \leqslant \varphi_1} r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi-\pi) \right)^{-1} \quad \text{for} \quad \varphi_1 < \varphi \leqslant \varphi_2 + \pi\,. \tag{20}$$

For proving that this sup is positive, it is enough to show that for each $\varphi \in (\varphi_1, \varphi_2+\pi]$ there is a $\psi_0 \in [\varphi_2, \varphi_1]$ such that

$$\frac{\pi}{2} < \psi_0 + \varphi < \frac{3}{2}\,\pi \tag{21}$$

are satified, since then $\cos(\psi_0+\varphi-\pi) > 0$ follows. Notice first that

$$-\frac{\pi}{4} < \varphi_2 < \frac{\pi}{4}, \quad \frac{\pi}{4} < \varphi_1 < \frac{3}{4}\,\pi$$

by construction. We consider now two cases. (i) If $\varphi \in (\varphi_1, \varphi_2 + (\pi/2)]$, then choose $\psi_0 = \varphi_1$. (21) now follows from $\psi_0 + \varphi = \varphi_1 + \varphi$ and

$$\frac{\pi}{2} < 2\varphi_1 < \varphi_1 + \varphi \leqslant \varphi_1 + \varphi_2 + \frac{\pi}{2} < \frac{\pi}{4} + \frac{3}{4}\,\pi + \frac{\pi}{2} = \frac{3}{2}\,\pi\,.$$

(ii) If $\varphi \in (\varphi_2 + (\pi/2), \varphi_2 + \pi]$, then choose $\psi_0 = \varphi_2$. (21) then follows from $\psi_0 + \varphi = \varphi_2 + \varphi$ and

$$0 < 2\varphi_2 + \frac{\pi}{2} < \varphi_2 + \varphi < 2\varphi_2 + \pi < \frac{3}{2}\,\pi\,.$$

The proof for the second sup in (17) is analogous.

(b) Equation (18) follows from (a) and the fact that this sup is positive if and only if (21) is satisfied with $\psi_0 = \psi$ modulo 2π. If we take $\varphi' = \varphi + \pi$ in (18) then (19) follows. □

The following is aimed at a geometric intepretation of (17) which yields a construction of the curve $\varphi \to r(\varphi)$. For each $\psi \in [\varphi_2, \varphi_1]$, consider

$$\chi \to g_\psi(\chi) = (r_{\mathfrak{k}}(\psi)\cos(\psi+\chi-\pi))^{-1} \quad \text{for} \quad \frac{\pi}{2} - \psi < \chi < \frac{3}{2}\,\pi - \psi\,, \tag{22}$$

and notice that (22) describes in polar coordinates a straight line $\mathfrak{g}_\psi$ through the point

$$P_\psi \equiv ((r_{\mathfrak{k}}(\psi))^{-1}, \pi - \psi)$$

and with normal direction $\pi-\psi$ in polar coordinates [see also Remark 2.5(b)]. Let G_ψ be the half-plane which is defined by the straight line $\mathfrak{g}_\psi$ and contains O. The equation (18) readily yields the following.

Proposition 2.3: The curve $\varphi \to r(\varphi)$, $\varphi_1 < \varphi \leqslant \varphi_2 + \pi$, *given in (17) coincides with the boundary of the figure* $\cap_{\psi \in [\varphi_2, \varphi_1]} G_\psi$ *in the sector with polar angles* $\varphi_1 < \varphi \leqslant \varphi_2 + \pi$. □

Corollary 2.4: The curve $\varphi \to r(\varphi)$, $\varphi_1 < \varphi \leqslant \varphi_2 + \pi$, *given in (17) is a convex arc in* $\mathcal{M}^2$.

Proof: Due to Proposition 2.3, the curve under consideration arrises as the inner boundary of that part of the sector with polar angles beween φ_1 and $\varphi_2+\pi$ which is enveloped by the lines $\mathfrak{g}_\psi$, $\psi \in [\varphi_2, \varphi_1]$, given in (22). Consequently, the curve under consideration is a convex arc (see Ref. 7, Example 1.2.2). □

Remark 2.5: (a) Since $\varphi \to r(\varphi), \varphi_2 \leqslant \varphi < \varphi_2 + 2\pi$, given in (17) is π-periodic by construction, analogues statements to Proposition 2.3 and Corollary 2.4 apply to $\varphi \to r(\varphi)$ with $\varphi_1 + \pi < \varphi < \varphi_2 + 2\pi$, too.

(b) We confirm for all what follows that the normal direction of a straight line $\mathfrak{g}$ not containing O points into the half plane which is defined by $\mathfrak{g}$ and does not contain O.

III. DETERMINATION OF THE CONSTRUCTION

The aim of the present section is to describe all possible choices of the ingredients of the construction given in Sec. II, and then to parametrize all the constructions in Corollary 3.3.

For later use, let us describe the geometric objects considered in Sec. II in polar coordinates (see Fig. 1).

(1) The hyperbolae,

$$\mathfrak{h}_1^+ : \; r_{\mathfrak{h}_1^+}(\varphi) = (\sqrt{|\cos 2\varphi|})^{-1} \quad \text{for } \frac{\pi}{4} < \varphi < \frac{3\pi}{4}; \tag{23}$$

$$\mathfrak{h}_2^+ : \; r_{\mathfrak{h}_2^+}(\varphi) = (\sqrt{\cos 2\varphi})^{-1} \quad \text{for } -\frac{\pi}{4} < \varphi < \frac{\pi}{4}. \tag{24}$$

(2) The points,

$$P_1 : \; (r_1, \varphi_1) \quad \text{with } \; r_1 = r_{\mathfrak{k}}(\varphi_1) = (\sqrt{|\cos 2\varphi_1|})^{-1}; \tag{25}$$

$$P_2 : \; (r_2, \varphi_2) \quad \text{with } \; r_2 = r_{\mathfrak{k}}(\varphi_2) = (\sqrt{\cos 2\varphi_2})^{-1}. \tag{26}$$

(3) The tangents $\mathfrak{t}_j$ on $\mathfrak{h}_j^+$ at P_j, $j=1,2$,

$$\mathfrak{t}_1 : \; r_{\mathfrak{t},1}(\varphi) = (r_1 \cos(\pi - \varphi_1 - \varphi))^{-1} \quad \text{for } \frac{\pi}{2} - \varphi_1 < \varphi < \frac{3}{2}\pi - \varphi_1, \tag{27}$$

$$\mathfrak{t}_2 : \; r_{\mathfrak{t},2}(\varphi) = (r_2 \cos(\varphi_2 + \varphi))^{-1} \quad \text{for } -\frac{\pi}{2} - \varphi_2 < \varphi < \frac{\pi}{2} - \varphi_2. \tag{28}$$

Let us also consider the half-lines $\mathfrak{s}_j = \{\lambda \vec{OP}_j ; \; \lambda > 0\}$, $j=1,2$, and the intersection points

$$Q_1 = \mathfrak{s}_1 \cap \mathfrak{t}_2 \quad \text{and} \quad Q_2 = \mathfrak{s}_2 \cap \mathfrak{t}_1 . \tag{29}$$

The possible choices of the points P_j, $j=1,2$, considered in Sec. II, steps I, II, are characterized next.

Lemma 3.1: Let the Cartesian and polar coordinates of P_j, $j=1,2$, be given by

$$P_j \equiv (x_j, y_j) \equiv (r_j, \varphi_j),$$

respectively. Then the following are equivalent.

(i) *The Cartesian coordinates of P_j, $j=1,2$, satisfy the inequalities (10) and (11).*

(ii) *The triangle $\Delta(P_1P_2P_3)$ [see Remark 2.1(b)] is either positively orientated or it collapses to the straight line $\overline{P_1P_2}$.*

(iii) *The following two properties hold:*
(α) either the origin O and P_1 are in the same half-plane relative to the tangent $\mathfrak{t}_2$ or $P_1 \in \mathfrak{t}_2$;
(β) either the origin O and P_2 are in the same half-plane relative to the tangent $\mathfrak{t}_1$ or $P_2 \in \mathfrak{t}_1$.

(iv) *The following two properties hold:*
(α) if Q_1 exists, then $|\overline{OP_1}| \leqslant |\overline{OQ_1}|$; (e.g., here $|\overline{OP_1}|$ denotes the Euclidean length of the straight line segment $\overline{OP_1}$);
(β) if Q_2 exists, then $|\overline{OP_2}| \leqslant |\overline{OQ_2}|$;

(v) *The polar angles φ_j of P_j satisfy*

$$\cos^2(\varphi_1+\varphi_2) \leqslant |\cos(2\varphi_1)| \cos(2\varphi_2), \tag{30}$$

where

$$-\frac{\pi}{4} < \varphi_2 < \frac{\pi}{4}, \quad \frac{\pi}{4} < \varphi_1 < \frac{3}{4}\pi.$$

Proof: (i)$\Leftrightarrow$(ii) The proof is given in Remark 2.1(b). (ii)$\Leftrightarrow$(iii) is obvious. (iii)$\Leftrightarrow$(iv), First we prove the following:

$$Q_1 = \mathfrak{s}_1 \cap \mathfrak{t}_2 \quad \text{exists if and only if} \quad \varphi_1+\varphi_2 < \frac{\pi}{2}, \tag{31}$$

$$Q_2 = \mathfrak{s}_2 \cap \mathfrak{t}_1 \quad \text{exists if and only if} \quad \varphi_1+\varphi_2 > \frac{\pi}{2}. \tag{32}$$

Noticing that the normal direction of the tangent $\mathfrak{t}_2$ is $-\varphi_2$ by (28) [see also Remark 2.5(b)], we get that Q_1 exists if and only if $(\pi/2)-\varphi_2 > \varphi_1$, and so (31) applies. The proof of (32) is analogous.

In view of (31) and (32), we consider the following three cases separately.

Case 1: Let $\varphi_1+\varphi_2 < (\pi/2)$. Note first that if Q_1 (respectively, Q_2) does not exist, then (iii)(α) [respectively, (iii)(β)] is satisfied. In the case under consideration we have that Q_1 exists, and Q_2 does not exist. Hence, both (iii)(β) and (iv)(β) hold. Furthermore, (iii)(α) is obviously satisfied if and only if $|\overline{OP_1}| \leqslant |\overline{OQ_1}|$, i.e., (iv)($\alpha$) holds.

Case 2: Let $\varphi_1+\varphi_2 > (\pi/2)$. The proof is analogous to case 1.

Case 3: Let $\varphi_1+\varphi_2 = (\pi/2)$. Now, neither Q_1 nor Q_2 exist by (31), (32). Consequently (iii)(α),(β) and (iv)(α),(β) are satisfied.

(iv)$\Leftrightarrow$(v): The above three cases are again considered.

Case 1: $\varphi_1+\varphi_2 < (\pi/2)$. (28) and (31) now yield

$$|\overline{OQ_1}| = r_{\mathfrak{t},2}(\varphi_1) = \frac{1}{r_2 \cos(\varphi_1+\varphi_2)}.$$

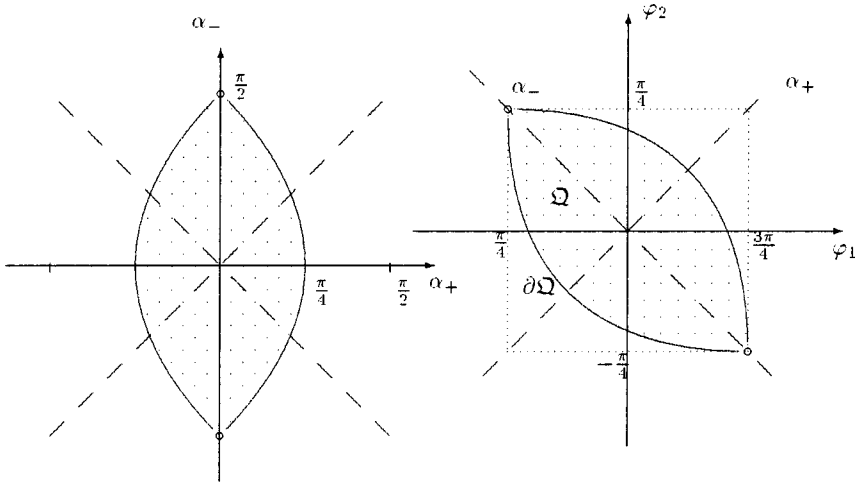

FIG. 2. The admissible values for (α_+,α_-) and (φ_1,φ_2).

Then (iv)(α) is satisfied if and only if

$$r_1 \leqslant \frac{1}{r_2 \cos(\varphi_1+\varphi_2)}. \tag{33}$$

Inserting (25), (26) in (33), we get that (iv) holds if and only if (30) is satisfied.

Case 2: $\varphi_1+\varphi_2>(\pi/2)$. The proof is analogous to case 1.

Case 3: $\varphi_1+\varphi_2=(\pi/2)$. Because (30) as well as (iv) are obviously satisfied, the proof is completed. □

Motivated by (30), let us put

$$\Omega=\left\{(\varphi_1,\varphi_2);\ \frac{\pi}{4}<\varphi_1<\frac{3\pi}{4},-\frac{\pi}{4}<\varphi_2<\frac{\pi}{4},\cos^2(\varphi_1+\varphi_2)<|\cos(2\varphi_1)|\cos(2\varphi_2)\right\}, \tag{34}$$

$$\partial\Omega=\left\{(\varphi_1,\varphi_2);\ \frac{\pi}{4}<\varphi_1<\frac{3\pi}{4},-\frac{\pi}{4}<\varphi_2<\frac{\pi}{4},\cos^2(\varphi_1+\varphi_2)=|\cos(2\varphi_1)|\cos(2\varphi_2)\right\}, \tag{35}$$

see Fig. 2.

Remark 3.2: (a) Introducing new variables

$$\alpha_\pm=\varphi_2\pm\left(\varphi_1-\frac{\pi}{2}\right),$$

we get $\cos^2(\varphi_1+\varphi_2)=\sin^2(\alpha_+)$ and

$$\begin{aligned}|\cos(2\varphi_1)|\cos(2\varphi_2)&=(\cos\alpha_+\cos\alpha_-)^2-(\sin\alpha_+\sin\alpha_-)^2\\&=-1+\cos^2\alpha_++\cos^2\alpha_-\\&=\cos^2\alpha_--\sin^2\alpha_+.\end{aligned}$$

Inserting the above in (30), we obtain

$$\sin^2(\alpha_+)\leqslant\tfrac{1}{2}\cos^2(\alpha_-).$$

Hence the polar angles φ_j of P_j, $j=1,2$, satisfy (30) if and only if (φ_1,φ_2) belongs to the shaded area given in Fig. 2. Especially, it is now obvious that for each $\pi/4<\varphi_1<3\pi/4$, there is some $-\pi/4<\varphi_2<\pi/4$ such that (30) holds.

(b) A slight modification of the above proof yields the following refinement of Lemma 3.1, (ii)$\Leftrightarrow$(v):

(α) the triangle $\Delta(P_1,P_2,P_3)$ is positively orientated if and only if

$$(\varphi_1,\varphi_2)\in\mathfrak{Q};$$

(β) the triangle $\Delta(P_1,P_2,P_3)$ collapses to the straight line $\overline{P_1P_2}$ if and only if $(\varphi_1,\varphi_2)\in\partial\mathfrak{Q}$.

A parametrization of all the constructions of self-polar norms given in Sec. II is given next.

Corollary 3.3: Let $\mathcal{Z}$ denote the set of all convex arcs connecting A_1 with A_2, and lying inside or at the border of the triangle $\Delta(A_1A_2A_3)$, where $A_1=(0,1),A_2=(1,0),A_3=(1,1)$ in Cartesian coordinates, we have a bijection from

$$\mathfrak{P}=(\mathfrak{Q}\times\mathcal{Z})\cup\partial\mathfrak{Q}\quad(\cup\ \textit{denotes disjoint union})$$

onto the set of (self-polar) norms constructed in Sec. II.

Proof: Using Lemma 3.1, (i)$\Leftrightarrow$(v), and (34), (35), the ingredients $\{P_1,P_2,\mathfrak{k}\}$ of our construction given in Sec. II are determined by a pair $(\varphi_1,\varphi_2)\in\mathfrak{Q}\cup\partial\mathfrak{Q}$ and a convex arc $\mathfrak{k}$ satisfying the requirements of step II of our construction. Assume first that $(\varphi_1,\varphi_2)\in\mathfrak{Q}$. For each $(\varphi_1,\varphi_2)\in\mathfrak{Q}$ let us now introduce an affine mapping $\Xi_{(\varphi_1,\varphi_2)}:\mathbb{R}^2\to\mathbb{R}^2$ defined by

$$\Xi_{(\varphi_1,\varphi_2)}(P_j)=A_j,\quad j=1,2,3, \tag{36}$$

and notice that $\Xi_{(\varphi_1,\varphi_2)}$ is regular (i.e., one-to-one) since P_1,P_2,P_3 are affinely independent by Remark 3.2(b), (α). Note then that a convex arc $\mathfrak{k}$ satisfies the requirements of step II [see Remark 2.1(c)] if and only if $\Xi_{(\varphi_1,\varphi_2)}(\mathfrak{k})\in\mathcal{Z}$ due to elementary geometric properties of affine mappings (Ref. 5. Kap. E2). Otherwise, if $(\varphi_1,\varphi_2)\in\partial\mathfrak{Q}$ then the triangle $\Delta(P_1P_2P_3)$ collapses to the straight line P_1P_2 [see Remark 3.2 (b), (β)], and consequently, we get $\mathfrak{k}=P_1P_2$. Finally, because on the one hand a unit ball U_p uniquely defines the ingredients $(P_1,P_2,\mathfrak{k})$ of our constuction by $P_j=\partial U_p\cap\mathfrak{h}_j$, $j=1,2$, and $\mathfrak{k}$ is that part of ∂U_p which connects P_2 with P_1, and on the other hand, equal choices of the ingredients give the same norm by (17), the map from $\mathfrak{P}$ onto the set of norms constructed in (17) is a bijection. □

IV. PROOF OF THE CONSTRUCTION

The aim of the present section is to show that $\varphi\to r(\varphi)$, $\varphi_2\leqslant\varphi<\varphi_2+2\pi$, given in (17) describes the boundary ∂U_p of some self-polar norm p on $\mathcal{M}^2$. The proof is based on the following five Lemmata 4.1, 4.2, 4.5, 4.9, 4.10. While Lemmata 4.1, 4.2 are concerned with general properties of a norm p, its polar norm p' will be considered in Lemmata 4.5, 4.9, 4.10.

Throughout the present section let us use polar coordinates (r,φ) on $\mathcal{M}^2$.

While (a) of the following lemma characterizes those functions $\varphi\to r(\varphi)$ which describe the boundary ∂U_p of some norm p, part (b) gives a relation between a norm p and the function $\varphi\to r_p(\varphi)$ which describes ∂U_p in polar coordinates.

Lemma 4.1: (a) A function $\varphi\to r_p(\varphi)$, $\varphi_0\leqslant\varphi<\varphi_0+2\pi$, with some $\varphi_0\in\mathbb{R}$ describes the boundary $\partial U_p=\{\vec{a}\in\mathcal{M}^2;\ p(\vec{a})=1\}$ of a norm p on $\mathcal{M}^2$ if and only if

(i) $\varphi\to r_p(\varphi)$, $\varphi_0\leqslant\varphi<\varphi_0+2\pi$, with some $\varphi_0\in\mathbb{R}$ describes the outer boundary of a convex figure in $\mathcal{M}^2$, which contains O,

(ii) r_p is π-periodic, i.e.,

$$r_p(\varphi_0+\varphi+\pi)=r_p(\varphi_0+\varphi)\quad\text{for}\ \varphi_0\leqslant\varphi<\varphi_0+\pi.$$

(iii) There are reals c_j *with* $0<c_j<\infty$, $j=1,2$, *such that*

$$c_1 \leqslant r_p(\varphi) \leqslant c_2$$

for $\varphi_0 \leqslant \varphi < \varphi_0 + 2\pi$.

(b) If $\varphi \to r_p(\varphi)$, $0 \leqslant \varphi < 2\pi$, *describes the boundary* ∂U_p *of some norm* p *on* $\mathcal{M}^2$, *then for* $\vec{a}=(x_a, y_a) \in \mathcal{M}^2$, $a_x = \varrho \cos\varphi$, $a_y = \varrho \sin\varphi$, *we have*

$$p(\vec{a}) = \frac{\varrho}{r_p(\varphi)}. \tag{37}$$

Proof: The above assertions are immedeate consequences of the defining properties of a norm which yield that the unit ball $U_p = \{\vec{a} \in \mathcal{M}^2;\ \ p(\vec{a}) \leqslant 1\}$ associated with p is a symmetric, convex, compact set containing the origin O as an inner point, and vice versa, p is the gauge of U_p (e.g., see Ref. 7, C, Sec. 1.2), (Ref. 12, Sec. 14.1). □

Under the situation of Lemma 4.1, let the π-periodic extension of the above r_p also be denoted by the same symbol r_p.

Lemma 4.2: Properties (i), (ii), (iii) of the above Lemma 4.1 are satisfied by $\varphi \to r(\varphi)$, $\varphi_2 \leqslant \varphi < \varphi_2 + 2\pi$, *given in (17).*

Proof: Setting $\varphi_0 = \varphi_2$ in Lemma 4.1(a), property (ii) is obviously satisfied by the construction given in (17).

For verifying (i), let us consider the curve $\mathfrak{l}$ defined by

$$\mathfrak{l}: \quad \varphi \to r_{\mathfrak{l}}(\varphi) = \inf_{\substack{\varphi_2 \leqslant \psi \leqslant \varphi_1 \\ \pi/2 < \psi + \varphi < 3/2\,\pi}} (r_{\mathfrak{k}}(\psi)\cos(\psi + \varphi - \pi))^{-1}, \quad \varphi_1 \leqslant \varphi \leqslant \varphi_2 + \pi. \tag{38}$$

Due to Corollary 2.4, $\mathfrak{l}$ is a convex arc. Noticing now that both curves $\mathfrak{k}$ and $\mathfrak{l}$ are continuous due to their convexity, it is enough to show the following (1) and (2) for verifying that $\mathfrak{k}$ and $\mathfrak{l}$ "glue" together to one convex arc $\mathfrak{k} \cup \mathfrak{l}$:

(1) $\mathfrak{k} \cup \mathfrak{l}$ is continuous at φ_1, i.e.,

$$\inf_{\substack{\varphi_2 \leqslant \psi \leqslant \varphi_1 \\ \pi/2 < \psi + \varphi_1 < 3/2\,\pi}} (r_{\mathfrak{k}}(\psi)\cos(\psi + \varphi_1 - \pi))^{-1} = r_{\mathfrak{k}}(\varphi_1), \tag{39}$$

(2) the tangent $\mathfrak{t}_1$ touches $\mathfrak{k} \cup \mathfrak{l}$ at P_1, and $\mathfrak{t}_1$ does not have any further points of $\mathfrak{k} \cup \mathfrak{l}$ in common, i.e.,

$$\mathfrak{t}_1 \cap (\mathfrak{k} \cup \mathfrak{l}) = P_1. \tag{40}$$

Noticing that $\pi/2 < 2\,\varphi_1 < \frac{3}{2}\pi$, we insert $\varphi = \varphi_1$ in (38) and then use (25):

$$\begin{aligned} r_{\mathfrak{l}}(\varphi_1) &= \inf_{\substack{\varphi_2 \leqslant \psi \leqslant \varphi_1 \\ \pi/2 < \varphi_1 + \psi < 3/2\,\pi}} (r_{\mathfrak{k}}(\psi)\cos(\psi + \varphi_1 - \pi))^{-1} \\ &\leqslant (r_{\mathfrak{k}}(\varphi_1)\cos(2\varphi_1 - \pi))^{-1} \\ &= (r_{\mathfrak{k}}(\varphi_1)\,|\cos(2\varphi_1)|)^{-1} = (r_{\mathfrak{k}}(\varphi_1)\,(r_1)^{-2})^{-1} = r_1. \end{aligned} \tag{41}$$

For showing the converse estimation, remember first that the tangent $\mathfrak{t}_1$ lies above arc $\mathfrak{k}$ by Remark 2.1(c), i.e.,

$$(r_1 \cos(\pi - \varphi_1 - \psi))^{-1} \geqslant r_{\mathfrak{k}}(\psi) \quad \text{for } \psi \in [\varphi_2, \varphi_1] \cap \left(\frac{\pi}{2} - \varphi_1, \frac{3}{2}\pi - \varphi_1\right)$$

by (27). Hence,

$$(r_{\mathfrak{k}}(\psi)\cos(\pi-\varphi_1-\psi))^{-1}\geqslant r_1 \quad \text{for } \psi\in[\varphi_2,\varphi_1]\cap\left(\frac{\pi}{2}-\varphi_1,\frac{3}{2}\pi-\varphi_1\right),$$

and thus

$$r_{\mathfrak{l}}(\varphi_1)=\inf_{\substack{\varphi_2\leqslant\psi\leqslant\varphi_1\\ \pi/2<\varphi+\psi<3/2\,\pi}}(r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi_1-\pi))^{-1}\geqslant r_1. \tag{42}$$

(39) is now a consequence of (41), (42), and (25). Because $\mathfrak{g}_{\varphi_1}=\mathfrak{t}_1$, (40) follows from (38) and Remark 2.1(c). Hence $\mathfrak{k}\cup\mathfrak{l}$ is a convex arc.

Considering now the curve $\mathfrak{m}$ given by

$$\varphi\to r_{\mathfrak{m}}(\varphi)=\inf_{\substack{\varphi_2\leqslant\psi\leqslant\varphi_1,\\ 3/2\,\pi<\psi+\varphi<5/2\,\pi}}(r_{\mathfrak{k}}(\psi)\cos(\psi+\varphi))^{-1}$$
$$\text{for } \varphi_1+\pi<\varphi\leqslant\varphi_2+2\,\pi,$$

and arguing as above, we get that $\mathfrak{k}\cup\mathfrak{m}$ is a convex arc, too. Finally using π-periodicity of $\varphi\to r(\varphi)$, we obtain (ii).

In order to verify (iii), note first that the construction of $\mathfrak{k}$ implies that there are constants $0<d_j<\infty$, $j=1,2$, such that

$$d_1<r_{\mathfrak{k}}(\varphi)<d_2 \quad \text{for } \varphi\in[\varphi_2,\varphi_1]$$

[see Remark 2.1(c)]. Because the convex arc $\mathfrak{l}$ connects the points P_1 and

$$P_4\equiv(r_2,\varphi_2+\pi),$$

it is obvious that the straight line through P_1,P_3 does not contain the origin O, and the triangle $\Delta(P_1,P_3,0)$ is positively orientated. For the distance $0<d_3<\infty$ of O to the straight line through P_1,P_3, the convexity of $\mathfrak{l}$ yields

$$r(\varphi)>d_3 \quad \text{for } \varphi\in[\varphi_1,\varphi_2+\pi].$$

The continuity of $\mathfrak{l}$ then implies that there is a $0<d_4<\infty$ with

$$r(\varphi)<d_4 \quad \text{for } \varphi\in[\varphi_1,\varphi_2+\pi].$$

Again using (i), we finally obtain

$$c_1<r(\varphi)<c_2 \quad \text{for } \varphi\in[\varphi_2,\varphi_2+2\pi],$$

where $0<c_1=\min\{d_1,d_3\}<\infty$, $0<c_2=\max\{d_2,d_4\}<\infty$. □

The polar norm

$$p'(\vec{a})=\sup_{0\neq\vec{b}\in\mathcal{M}^2}\frac{|x_a x_b-y_a y_b|}{p(\vec{b})} \tag{43}$$

of some norm p on $\mathcal{M}^2$ is considered next, where $\vec{a}=(x_a,y_a)$, $\vec{b}=(x_b,y_b)$.

Definition 4.3: Let $\varphi\to r_p(\varphi)$, $0\leqslant\varphi<2\pi$, describe the boundary ∂U_p of the unit ball of some norm p on $\mathcal{M}^2$. Then let us consider $\varphi\to r_p^*(\varphi)$, $0\leqslant\varphi<2\pi$, where

$$r_p^*(\varphi)=\left(\sup_{0\leqslant\vartheta<2\pi}r_p(\vartheta)\cos(\vartheta-\varphi)\right)^{-1}. \tag{44}$$

Remark 4.4: Using π-periodicity of r_p and $\cos(\vartheta-\varphi\pm\pi)=-\cos(\vartheta-\varphi)$, we get

$$r_p^*(\varphi)=\left(\sup_{0\leqslant\vartheta<2\pi} r_p(\vartheta)\,|\cos(\vartheta-\varphi)|\right)^{-1}=\left(\sup_{\vartheta\in} r_p(\vartheta)\,|\cos(\vartheta-\varphi)|\right)^{-1}. \tag{45}$$

Lemma 4.5: For every norm p on $\mathcal{M}^2$, the boundary

$$\partial U_{p'}=\{\vec{a}\in\mathcal{M}^2;\ \ p'(\vec{a})=1\}$$

of the unit ball of its polar norm p' is given by $\varphi\to r_{p'}(\varphi)$, $0\leqslant\varphi<2\pi$, where

$$r_{p'}(\varphi)=r_p^*(-\varphi)\,. \tag{46}$$

Proof: For $\vec{a}=(x_a,y_a)=(\varrho\cos\varphi,\varrho\sin\varphi$, $\vec{b}=(x_b,y_b)=(\sigma\cos\psi,\sigma\sin\psi)$, Eqs. (37), (43), (45) imply

$$\begin{aligned}\frac{\varrho}{r_{p'}(\varphi)}&=p'(\vec{a})\\&=\sup_{\substack{\sigma>0\\0\leqslant\psi<2\pi}}\frac{\varrho\,\sigma|\cos\varphi\cos\psi-\sin\varphi\sin\psi|}{\dfrac{\sigma}{r_p(\psi)}}\\&=\varrho\sup_{0\leqslant\psi<2\pi}\{r_p(\psi)\,|\cos(\varphi+\psi)|\}\\&=\frac{\varrho}{r_p^*(-\varphi)},\end{aligned}$$

and consequently, $r_{p'}(\varphi)=r_p^*(-\varphi)$. □

Remark 4.6: (a) Since p' is a norm on $\mathcal{M}^2$ (e.g., see Ref. 4, Chap. III.4), (46) implies that properties (i), (ii), (iii) of Lemma 4.1(a) are satisfied by $\varphi\to r_p^*(\varphi)$, too.

(b) For a construction of the polar norm in case of Euclidean metric, the reader is referred to Ref. 7, C, Sec. 3.2.

In order to get relations between r_p and r_p^*, we need the following prerequisites. Remembering the following properties of a convex curve $\varphi\to r(\varphi)$, $0\leqslant\varphi<2\pi$:

(i) $\varphi\to r(\varphi)$ is continuous for $\varphi\in[0,2\pi)$, and

$$\lim_{\varphi\to 2\pi-0} r(\varphi)=\lim_{\varphi\to+0} r(\varphi)=r(0)\,.$$

(ii) The left and right derivative,

$$(\partial^{\pm}r)(\varphi_0)=\lim_{h\to\pm 0}\frac{r(\varphi_0+h)-r(\varphi_0)}{h} \tag{47}$$

exits for each $\varphi_0\in[0,2\pi)$.

(iii) $\varphi\to r(\varphi)$ is everywhere differentiable (i.e., $\partial^+=\partial^-$) exept on a countable set of points.

Let us introduce the notion of a support line, its normal direction, extremal support lines, and functions assigning the normal directions of all the support lines and of the extremal support lines, respectively, at a given point.

Definition 4.7: Let ∂U_p: $\varphi\to r_p(\varphi)$, $0\leqslant\varphi<2\pi$, be a convex curve satisfying (i), (ii), (iii) of Lemma 4.1(a).

(a) A straight line $\mathfrak{g}$ is then called support line *on $\mathfrak{g}$ at point $P_0\equiv(r(\varphi_0),\varphi_0)$ if both $P_0\in\mathfrak{g}\cap\partial U_p$ and U_p lies on one side of $\mathfrak{g}$.*

(b) The normal direction *of a support line $\mathfrak{g}$ on ∂U_p is the direction of a vector being orthogonal on $\mathfrak{g}$ and pointing into that half-plane which is defined by $\mathfrak{g}$ and does not contain the origin O.*

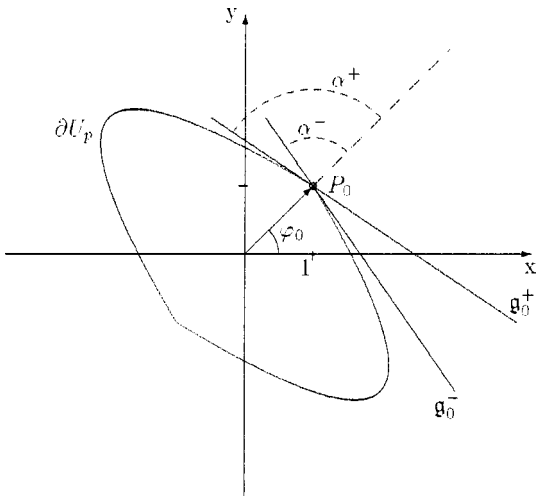

FIG. 3. The extremal support lines on ∂U_p at P_0.

(c) For every point $P_0 \in \partial U_p$, *let us consider the* extremal support lines $\mathfrak{g}_0^{\pm}$ *on* ∂U_p *at* P_0 *defined as the limits of the straight lines* $\mathfrak{s}^{\pm}$ *through the points* P_0 *and*

$$P^{\pm} \equiv (r_p(\varphi_0 \pm h), \varphi_0 \pm h)$$

as $h \to 0$.

(d) Let $\Theta_r : \mathbb{R} \to \{\text{intervals of } S^1\}$ *denote the* 2π*-periodic function which assigns to each* $\varphi_0 \in \mathbb{R}$ *the set of the normal directions of all the support lines on* ∂U_p *at* $P_0 \equiv (r_p(\varphi_0), \varphi_0)$. *(Here* S^1 *denotes the unit sphere in two dimensions.)*

(e) Let $\Phi_r^{\pm} : \mathbb{R} \to \mathbb{R}$ *be the* 2π*-periodic functions which assigns to each* $\varphi_0 \in \mathbb{R}$ *the normal directions of the extremal support lines* $\mathfrak{g}_0^{\pm}$ *[cf. (c)].*

If it is clear from the context, then let us write Θ and $\Phi^{\pm}$ instead of Θ_r and $\Phi_r^{\pm}$, respectively.

Remark 4.8: (a) Obviously, a support line exists at every point $P \equiv (r_p(\varphi), \varphi)$. (b) If $\varphi \to r_p(\varphi)$ is differentiable at $\varphi = \varphi_0$, then the tangent on ∂U_p at P_0 is the unique support line at P_0. (c) Recall that the angles $\alpha^{\pm}$ between the extremal support lines $\mathfrak{g}_0^{\pm}$ and the vector $\overrightarrow{OP}_0$ are given by

$$\tan \alpha^{\pm} = \frac{r_p(\varphi_0)}{(\partial^{\pm} r_p)(\varphi_0)}, \tag{48}$$

where $\alpha^{\pm} = \pi/2$ is confirmed if $\partial^{\pm} r_p = 0$, see Fig. 3. Since $0 \leqslant \alpha^- \leqslant \alpha^+ < \pi$, here and in the following we make the convention $0 \leqslant \arctan \varrho < \pi$, $\varrho \in \mathbb{R}$, i.e.,

$$\arctan \varrho = \begin{cases} \operatorname{Arctan} \varrho & \text{if } \varrho \geqslant 0, \\ \pi + \operatorname{Arctan} \varrho & \text{if } \varrho < 0, \end{cases} \tag{49}$$

where Arctan denotes the principal branch. The normal directions of $\mathfrak{g}_0^{\pm}$ are then given by

$$\Phi^{\pm}(\varphi_0) = \alpha^{\pm} + \varphi_0 - \frac{\pi}{2} = \left(\arctan \frac{r_p(\varphi_0)}{(\partial^{\pm} r_p)(\varphi_0)} \right) + \varphi_0 - \frac{\pi}{2}. \tag{50}$$

(d) We have $\Theta(\varphi_0) = [\Phi^-(\varphi_0), \Phi^+(\varphi_0)]$, since a straight line $\mathfrak{g}_\vartheta$ with normal direction ϑ through P_0 is a support line on ∂U_p at $P_0 \equiv (r_p(\varphi_0), \varphi_0)$ if and only if

$$\Phi^-(\varphi_0) \leqslant \vartheta \leqslant \Phi^+(\varphi_0). \tag{51}$$

The convexity of ∂U_p readily yields the following.

Lemma 4.9: Let $\varphi \to r_p(\varphi)$ describe the boundary ∂U_p of some norm p on $\mathcal{M}^2$, and $0 \leqslant \chi_1 < \chi_2 < \chi_3 < 2\pi$.

(a) For each $\vartheta \in \Theta(\chi_2)$, we have $\Phi^+(\chi_1) \leqslant \vartheta \leqslant \Phi^-(\chi_3)$.

(b) If $\Phi^+(\chi_1) < \Phi^-(\chi_2)$, then $\Theta(\chi_1) \cap \Theta(\chi_2) = \varnothing$.

(c) If $\Phi^+(\chi_1) = \Phi^-(\chi_2)$, then $\Theta(\chi_1) \cap \Theta(\chi_2) = \Phi^+(\chi_1)$.

(d) It holds $\cup_{\chi \in [0,2\pi)} \Theta(\chi) = S^1$, and

$$\bigcup_{\chi \in [\chi_1, \chi_2]} \Theta(\chi) = [\Phi^-(\chi_1), \Phi^+(\chi_2)]\,. \tag{52}$$

Proof: See Ref. 13. Theorem 24.1. □

In the following the π-periodic extensions of r_p and r_p^* are again denoted by r_p and r_p^*, respectively.

Lemma 4.10: Let $\varphi \to r_p(\varphi)$ describe the boundary ∂U_p of some norm p on $\mathcal{M}^2$. Then,

(a) for each $\varphi, \vartheta \in \mathbb{R}$, we have

$$r_p^*(\vartheta)\, r_p(\varphi)\, |\cos(\varphi - \vartheta)| \leqslant 1\,;$$

(b) the following are equivalent:

(i) the function

$$\chi \to g_\vartheta(\chi) = \frac{r_p(\varphi_0)\cos(\varphi_0 - \vartheta)}{\cos(\chi - \vartheta)}, \quad \chi \in \left(\vartheta - \frac{\pi}{2}, \vartheta + \frac{\pi}{2}\right),$$

defines a support line $\mathfrak{g}_\vartheta$ with normal direction ϑ on ∂U_p at $P_0 \equiv (r(\varphi_0), \varphi_0)$,

(ii) $\vartheta \in \Theta_r(\varphi_0)$,

(iii) $r_p^*(\vartheta)\, r_p(\varphi_0) \cos(\varphi_0 - \vartheta) = 1$,

(iv)

$$\arctan\left(\frac{r_p(\varphi_0)}{(\partial^- r_p)(\varphi_0)}\right) \leqslant \vartheta - \varphi_0 + \frac{\pi}{2} \leqslant \arctan\left(\frac{r_p(\varphi_0)}{(\partial^+ r_p)(\varphi_0)}\right);$$

(c) $r_p(\varphi) = r_p^{**}(\varphi), \varphi \in \mathbb{R}$.

Proof. (a) Using (45), we obtain the estimation under consideration from

$$r_p^*(\vartheta) r_p(\varphi)\, |\cos(\varphi - \vartheta)| = \frac{r_p(\varphi)\, |\cos(\varphi - \vartheta)|}{\sup_{\chi \in} r_p(\chi)\, |\cos(\chi - \vartheta)|} \leqslant \frac{r_p(\varphi)\, |\cos(\varphi - \vartheta)|}{r_p(\varphi)\, |\cos(\varphi - \vartheta)|} = 1\,.$$

(b) *(i)⇔(ii)* readily follows from Definition 4.7 (d).

(i)⇔(iii): Notice first that

$$\mathfrak{g}_\vartheta\colon\ \chi \to g_\vartheta = \frac{r_p(\varphi_0)\cos(\varphi_0 - \vartheta)}{\cos(\chi - \vartheta)},\ \ \chi \in \left(\vartheta - \frac{\pi}{2}, \vartheta + \frac{\pi}{2}\right),$$

is a support line on ∂U_p at $P_0 \equiv (r_p(\varphi_0), \varphi_0)$ if and only if

$$r_p(\chi) \leqslant \frac{r_p(\varphi_0)\cos(\varphi_0 - \vartheta)}{\cos(\chi - \vartheta)}, \quad \chi \in \left(\vartheta - \frac{\pi}{2}, \vartheta + \frac{\pi}{2}\right). \tag{53}$$

Using π-periodizity of r_p, (53) is equivalent to

$$r_p(\varphi)\,|\cos(\varphi-\vartheta)|\leqslant r_p(\varphi_0)\cos(\varphi_0-\vartheta)\,,\quad \varphi\in\mathbb{R}\,. \tag{54}$$

Because (54) is equivalent to

$$r_p^*(\vartheta)=(r_p(\varphi_0)\cos(\varphi_0-\vartheta))^{-1}$$

by (45), the euivalence $(i)\Leftrightarrow(iii)$ follows.

(i)⇔(iv): Considering the extemal support lines $\mathbf{t}_0^{\pm}$ on ∂U_p at P_0, and taking (49), (50) into account, we get the equivalence under consideration by (51).

(c) Let $\varphi\in\mathbb{R}$. We get

$$(r_p^{**}(\varphi))^{-1}\,r_p(\varphi)=\sup_{\vartheta\in} r_p^*(\vartheta)\cos(\varphi-\vartheta)\,r_p(\varphi)\leqslant 1 \tag{55}$$

by Definition 4.3 and Lemma 4.10(a). Furthermore, (52) yields that there is a $\vartheta_0\in\Theta(\varphi)$, and then

$$r_p^*(\vartheta_0)\cos(\varphi-\vartheta_0)\,r_p(\varphi)=1 \tag{56}$$

by Lemma 4.10(b). Now, (55) and (56) yield the assertion under consideration. □

We are now prepared to prove the first main result of this section.

Theorem 4.11: *The curve $\varphi\to r(\varphi)$, $\varphi_2\leqslant\varphi<\varphi_2+2\pi$, given in (17) describes the boundary*

$$\partial U_p=\{\vec{a}\in\mathcal{M}^2;\;\; p(\vec{a})=1\} \tag{57}$$

of some self-polar norm p on Minkowski space $\mathcal{M}^2$.

Proof: Due to Lemmas 4.1 and 4.2, there is some norm p on $\mathcal{M}^2$ such that (57) holds. For showing that p is self-polar, it is enough to verify that

$$r(\varphi)=r^*(-\varphi) \tag{58}$$

for $\varphi\in\mathbb{R}$, by Lemma 4.5. Since both r and r^* are π-periodic, it suffices to show (58) for $\varphi\in[\varphi_1-\pi,\,\varphi_2]\cup[\varphi_2,\varphi_1]$.

Case 1: Let $\varphi\in[\varphi_1-\pi,\,\varphi_2]$. Noticing that the normal directions ϑ_j of the tangents $\mathbf{t}_j$, $j=1,2$, introduced in (8) and (13) are given by

$$\vartheta_1=\pi-\varphi_1\quad\text{and}\quad\vartheta_2=-\varphi_2\,, \tag{59}$$

respectively [see (27), (28)], we get

$$-\varphi\in[\,\vartheta_2,\,\vartheta_1]\,. \tag{60}$$

Furthermore, we have $\vartheta_1\in\Theta_r(\varphi_1)$ since both (1) ϑ_1 is the normal direction of $\mathbf{t}_1$ and (2) $\mathbf{t}_1$ is a support line at φ_1 by (40) and the explanation beforehand of (40). An analogous reasoning yields $\vartheta_2\in\Theta_r(\varphi_2)$.

Because of (52) and Lemma 4.9(a), (60) implies that there is some $\psi_0\in[\varphi_2,\,\varphi_1]$ such that

$$-\varphi\in\Theta(\psi_0)\,. \tag{61}$$

Due to Lemma 4.10(b), *(ii)⇔(iii),* relation (61) yields

$$r^*(-\varphi)r(\psi_0)\cos(\varphi+\psi_0)=1. \tag{62}$$

Now,

$$
\begin{aligned}
r(\varphi) &\overset{(*)}{\leqslant} (r(\psi_0)\cos(\varphi+\psi_0))^{-1} \\
&\overset{(**)}{=} r^*(-\varphi) \\
&\overset{(***)}{=} \left(\sup_{0\leqslant\chi<2\pi}\{r(\chi)\cos(\chi+\varphi)\}\right)^{-1} \\
&\leqslant \left(\sup_{\varphi_2\leqslant\psi\leqslant\varphi_1}\{r(\psi)\cos(\psi+\varphi)\}\right)^{-1} \\
&\overset{(*)}{=} r(\varphi)
\end{aligned}
$$

verifies (58) in case 1, where (*) follows from (17), (**) from (62), and (***) from (44).

Case 2: Let $\varphi\in[\varphi_2,\varphi_1]$. (59) then implies

$$-\varphi\in[-\varphi_1,-\varphi_2]=[\vartheta_1-\pi,\vartheta_2]\,. \tag{63}$$

The same reasoning as in case 1 yields the existence of a $\tilde{\psi}_0\in[\varphi_1-\pi,\varphi_2]$ such that

$$-\varphi\in\Theta_r(\tilde{\psi}_0)\,, \tag{64}$$

and

$$r^*(-\varphi)r(\tilde{\psi}_0)\cos(\tilde{\psi}_0+\varphi)=1\,. \tag{65}$$

As for $\chi\to r^*(\chi),\chi\in\mathbb{R}$, the further proof is based on the assertion

$$\varphi\in\Theta_{r^*}(-\tilde{\psi}_0) \tag{66}$$

which will be verified at the end of the proof. Due to Lemma 4.10(b), *(ii)*⇔*(iii)*, applied to $\chi\to r^*(\chi)$, (66) yields

$$r^{**}(\varphi)r^*(-\tilde{\psi}_0)\cos(\tilde{\psi}_0+\varphi)=1\,. \tag{67}$$

Because of relations $r^{**}(\varphi)=r(\varphi)$ due to Lemma 4.10(c), and $r^*(-\tilde{\psi}_0)=r(\tilde{\psi}_0)$ already proved in case 1 above, (67) implies

$$r(\varphi)r(\tilde{\psi}_0)\cos(\tilde{\psi}_0+\varphi)=1\,.$$

The last equation and (65) now imply $r(\varphi)=r^*(-\varphi)$ in case 2.

Proof of (66): If $\tilde{\psi}_0\in(\varphi_1-\pi,\varphi_2)$, then $r(\tilde{\psi}_0)=r^*(-\tilde{\psi}_0)$ by case 1, and

$$(\partial^{\pm}r^*)(-\tilde{\psi}_0)=-(\partial^{\mp}r)(\tilde{\psi}_0) \tag{68}$$

readily follows from (47). Using (49), (50) and Remark 4.8(d), we get

$$\Theta_{r^*}(-\tilde{\psi}_0)=-\Theta_r(\tilde{\psi}_0)$$

from (68). The last equation and (64) now imply (66).

Assume now $\tilde{\psi}_0=\varphi_2$. Due to (63), (64) and $\vartheta_2\in\Theta_r(\varphi_2)$, we get

$$-\varphi\in[\vartheta_1-\pi,\vartheta_2]\cap\Theta_r(\tilde{\psi}_0)=[\vartheta_1-\pi,\vartheta_2]\cap[\Phi_r^-(\varphi_2),\Phi_r^+(\varphi_2)]=[\Phi_r^-(\varphi_2),\vartheta_2]\,.$$

Then,

$$\varphi \in [-\vartheta_2, -\Phi_r^-(\varphi_2)] = [\varphi_2, \Phi_{r*}^+(-\varphi_2)] \tag{69}$$

by (59), and $r^*(-\varphi_2) = r(\varphi_2)$ (which is a consequence of case 1) yields $\Phi_r^-(\varphi_2) = -\Phi_{r*}^+(-\varphi_2)$ by (68) and (50). Noticing that

$$r^{**}(\varphi_2) r^*(-\varphi_2) \cos 2\varphi_2 = r(\varphi_2) r^*(-\varphi_2) \cos 2\varphi_2 = 1$$

by Lemma 4.10(c), $-\varphi_2 = \vartheta_2 \in \Theta(\varphi_2)$ and Lemma 4.10(b), *(ii)⇔(iii),* we get

$$\varphi_2 \in \Theta_{r*}(-\varphi_2) = [\Phi_{r*}^-(-\varphi_2), \Phi_{r*}^+(-\varphi_2)]$$

from Lemma 4.10(b), *(ii)⇔(iii),* too. The assertion to be shown now follows from

$$\varphi \in [\varphi_2, \Phi_{r*}^+(-\varphi_2)] \subset [\Phi_{r*}^-(-\varphi_2), \Phi_{r*}^+(-\varphi_2)] = \Theta_{r*}(-\varphi_2) = \Theta_{r*}(-\tilde{\psi}_0) .$$

The final case $\tilde{\psi}_0 = \varphi_1 - \pi$ is treated analogously. The proof of Theorem IV is completed. □

The following is aimed at showing that every self-polar norm on $\mathcal{M}^2$ is obtained by our construction given in Sec. II.

Lemma 4.12: Let p be any self-polar norm on $\mathcal{M}^2$, *and* $\partial U_p = \{\vec{x} \in \mathcal{M}^2; p(\vec{x}) = 1\}$ *the boundary of the unit ball* U_p *of p. Then* ∂U_p *touches each of the four hyperbolae* $\mathfrak{h}_j^{\pm}$, $j = 1,2$, *[cf. (4)–(7)] in exactly one point. The tangents of the hyperbolae in these points are support lines on* ∂U_p.

Proof: (Uniqueness). Let $\varphi \to r_p(\varphi)$, $0 \leqslant \varphi < 2\pi$, denote the function describing ∂U_p in polar coordinates. Because the assumption $p = p'$ of the lemma under consideration implies $r_p^*(-\varphi) = r_p(\varphi)$, $0 \leqslant \varphi < 2\pi$, by (46), Lemma 4.10(a) yields

$$1 \geqslant r_p^*(-\varphi) r_p(\varphi) |\cos(2\varphi)| = (r_p(\varphi))^2 |\cos(2\varphi)| ,$$

and consequently, $(r_p(\varphi))^2 \leqslant |\cos(2\varphi)|^{-1}$ for $0 \leqslant \varphi < 2\pi$. Remembering the equations of the hyperbolae $\mathfrak{h}_j^{\pm}$, $j = 1,2$, [see (23), (24), and related equations for $\mathfrak{h}_j^-$], we obtain that the curve ∂U_p must lie between the four hyperbolae. On the other hand, ∂U_p has to be convex, and so there cannot be more than one point of intersection with each of the four hyperbolae.

Existence of intersection points: In analogy to Definition 4.7(d) let us introduce a function $\Theta_{\mathfrak{h}_2^+}: (-\pi/4, \pi/4) \to \mathbb{R}$ given by

$$\Theta_{\mathfrak{h}_2^+}(\varphi) = -\varphi , \quad \varphi \in \left(-\frac{\pi}{4}, \frac{\pi}{4} \right) , \tag{70}$$

and notice that $\Theta_{\mathfrak{h}_2^+}(\varphi_0)$ gives the normal direction of the tangent $\mathfrak{t}$ on $\mathfrak{h}_2^+$ at $P_0 \equiv ((\sqrt{\cos 2\varphi_0})^{-1}, \varphi_0)$ (in polar coordinates). Furthermore, $\varphi \to \Theta_{\mathfrak{h}_2^+}(\varphi)$ is a continuous, strictly monotone decreasing function which satisfies

$$\lim_{\varphi \to -\pi/4 + 0} \Theta_{\mathfrak{h}_2^+}(\varphi) = \frac{\pi}{4}, \tag{71}$$

$$\lim_{\varphi \to \pi/4 - 0} \Theta_{\mathfrak{h}_2^+}(\varphi) = -\frac{\pi}{4}. \tag{72}$$

Since on the one hand the unit ball U_p is a convex figure containing O as an inner point and lying between the four hyperbolae $\mathfrak{h}_j^{\pm}$, $j = 1,2$, and on the other hand, the tangents $\mathfrak{t}_\varphi$ on $\mathfrak{h}_2^+$ at $P_\varphi \equiv ((\sqrt{\cos 2\varphi_0})^{-1}, \varphi_0)$ approach the straight line $y = -x$ from above as $\varphi \to -\pi/4 + 0$ there has to be an angle $-\pi/4 < \beta < 0$ such that $\mathfrak{t}_\beta \cap U_p \neq \varnothing$ and the triangle $\Delta(OP_\beta R)$ is positively orientated for some point $R \in \mathfrak{t}_\beta \cap U_p$. Then

$$\Phi^{+}_{r_p}(\beta)\leqslant\Theta_{\mathfrak{h}^{+}_2}(\beta) \tag{73}$$

since $\Phi^{+}_{r_p}(\beta)$ is the normal direction of the extremal support line $\mathfrak{g}^{+}_{\beta}$ [see Definition 4.7(e)] on ∂U_p at β which cannot intersect the inner of the convex figure U_p. Noticing then that the tangents $\mathfrak{t}_{\varphi}$ considered above approach the straight line $y=x$ from below as $\varphi\to(\pi/4)-0$, we get analogously the existence of some angle $0<\tilde{\beta}<\pi/4$ such that

$$\Phi^{-}_{r_p}(\tilde{\beta})\geqslant\Theta_{\mathfrak{h}^{+}_2}(\tilde{\beta})\,. \tag{74}$$

Because of (52) of Lemma 4.9, the continuity of $\Theta_{\mathfrak{h}^{+}_2}$ and (73), (74) yield the existence of some $\psi_0\in[\beta,\tilde{\beta}]\subset(-\pi/4,\pi/4)$ such that

$$\Theta_{\mathfrak{h}^{+}_2}(\psi_0)\in[\Phi^{-}_{r_p}(\psi_0),\Phi^{+}_{r_p}(\psi_0)]\,. \tag{75}$$

Due to Lemma 4.10(b) [*(ii)*⇔*(iii)*], (75) and (70) with $\varphi_0=\psi_0$ imply

$$1=r^{*}_p(-\psi_0)r_p(\psi_0)\cos(2\psi_0)\overset{(*)}{=}(r_p(\psi_0))^2\cos(2\psi_0)\,, \tag{76}$$

where (*) follows from (46) and the assumption $p=p'$ of the lemma under consideration. Now, (76) and the equation of the hyberbola $\mathfrak{h}^{+}_2$ given in (24) imply

$$C\in\partial U_p\cap\mathfrak{h}^{+}_2\,,$$

where the polar coordinates of the intersection point C are given by $(r_p(\psi_0),\psi_0)$. Furthermore, Lemma 4.10(b) [*(i)*⇔*(ii)*] and (75) imply that the tangent $\mathfrak{t}$ on $\mathfrak{h}^{+}_2$ at C is a support line of ∂U_p.

The remaining three hyperbolae can be treated in the same way. □

Theorem 4.13: *For every self-polar norm p on Minkowski space $\mathcal{M}^2$, there exist ingredients $\{P_1,P_2,\mathfrak{k}\}$ of the construction given in Sec. II such that the boundary ∂U_p of the unit ball of p is obtained by (17).*

Proof: Let p denote a self-polar norm on $\mathcal{M}^2$. We consider the π-periodic function

$$\varphi\to r_p(\varphi)\,,\quad \varphi\in\mathbb{R}\,,$$

which describes ∂U_p in polar coordinates. Due to Lemma 4.12, there are four points

$$C^{\pm}_j=\partial U_p\cap\mathfrak{h}^{\pm}_j\,,\quad j=1,2\,,$$

at which ∂U_p touches the hyperbolae $\mathfrak{h}^{\pm}_j$. Set $P_j=C^{+}_j$. Let φ_j denote the polar angles of P_j, $j=1,2$. Because the tangents $\mathfrak{t}_j$ on $\mathfrak{h}^{+}_j$ at P_j, $j=1,2$, are support lines for ∂U_p by Lemma 4.12 and because ∂U_p is the outer boundary of a convex figure containing O as an inner point, $\{P_1,P_2,\mathfrak{k}\}$ satisfy the requirements of steps I, II of our construction, where $\mathfrak{k}$ is given by $\varphi\to r_p(\varphi)$, $\varphi_2\leqslant\varphi\leqslant\varphi_1$. Let now

$$\varphi\to r(\varphi)\,,\quad \varphi_2\leqslant\varphi<\varphi_2+2\pi\,,$$

denote the function given in (17). Obviously, $r_p(\varphi)=r(\varphi)$ for $\varphi_2\leqslant\varphi\leqslant\varphi_1$. Using the π-periodicity of both r and r_p, it remains to verify that $r_p(\varphi)=r(\varphi)$ for $\varphi_1\leqslant\varphi\leqslant\varphi_2+\pi$. So let $\varphi_0\in[\varphi_1,\varphi_2+\pi]$. Analogously to (60) we obtain

$$-\varphi_0\in[\vartheta_2,\vartheta_1]\,,$$

where ϑ_j denote the normal directions of the tangents $\mathfrak{t}_j$ on $\mathfrak{h}^{+}_j$ at P_j, $j=1,2$. Due to (52), there is a

$$\psi_0 \in [\varphi_2, \varphi_1] \tag{77}$$

such that $-\varphi_0 \in \Theta_r(\psi_0)$. Applying Lemma 4.10(b), $(ii) \Leftrightarrow (iii)$, to both r and r_p, we get

$$1 = r_p^*(-\varphi_0) r_p(\psi_0) \cos(\psi_0 + \varphi_0) \overset{(*)}{=} r_p(\varphi_0) r_p(\psi_0) \cos(\psi_0 + \varphi_0), \tag{78}$$

$$1 = r^*(-\varphi_0) r(\psi_0) \cos(\psi_0 + \varphi_0) \overset{(**)}{=} r(\varphi_0) r_p(\psi_0) \cos(\psi_0 + \varphi_0), \tag{79}$$

where (*) follows from $p = p'$, and (**) from the facts that $r(\varphi)$ describes the boundary ∂U of the unit ball of some self-polar norm by Theorem 4.11 and then $r_p(\psi_0) = r(\psi_0)$ by (77). Now, (78) and (79) imply $r_p(\varphi_0) = r(\varphi_0)$. □

Corollary 3.3 and Theorem 4.13 immedeately yield the following parametrization of all self-polar norms on $\mathcal{M}^2$.

Corollary 4.14: The mapping given in Corollary 3.3 is a bijection between $\mathfrak{P} = (\Omega \times \mathcal{Z}) \cup \partial\Omega$ *and the set of all self-polar norms on* $\mathcal{M}^2$. □

V. HILBERTIAN SELF-POLAR NORMS ON $\mathcal{M}^2$

The aim of the present section is to characterize those self-polar norms on $\mathcal{M}^2$ which are Hilbertian in addition. To do so, we apply the following taken from Ref. 9, Theorem 5.4.

Proposition 5.1: Let q *be a norm on an inner product space* $E, (.,.)$ *with complete Hilbertian majorant* $\tau(p)$, $p(.) = \sqrt{[.,.]}$, *and Gram operator* G, $(x,y) = [x, Gy]$, $x, y \in E$. *Then the following are equivalent:*

(i) q *is Hilbertian and self-polar,*

(ii) a symmetry S $(= S^{-1} = S^*)$ *and a bounded linear operator* B *exist on the Hilbert space* $E, [.,.]$ *such that*

(1) B *is positive on* $E, [.,.]$,

(2) $Gx = BSBx$, $x \in E$,

(3) $q(x) = p(Bx)$, $x \in E$.

In the case at hand we have $E = \mathcal{M}^2$, $[\vec{a}, \vec{b}] = x_a x_b + y_a y_b$, $(\vec{a}, \vec{b}) = x_a x_b - y_a y_b$, $p(\vec{a}) = \sqrt{x_a^2 + y_a^2}$, Gram operator $G = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, $\vec{a} = (x_a, y_a)$, $\vec{b} = (x_b, y_b)$.

Proposition 5.2: All the Hilbertian self-polar norms on $\mathcal{M}^2$ *are given by*

$$q_\alpha(\vec{a}) = \sqrt{\alpha\, \xi_+^2 + \frac{1}{\alpha} \xi_-^2}, \quad \xi_\pm = \frac{1}{\sqrt{2}} (x_a \pm y_a),$$

where $\alpha > 0$.

Proof: Consider the linear operator $A = B^2$, where B is taken from Proposition 5.1(ii), (2). Let $\vec{a}^{(j)} = (x^{(j)}, y^{(j)})$ and $\lambda^{(j)} > 0$, $j = 1,2$, be eigenvectors and eigenvalues of the positive operator A, respectively. Using $G^2 = I$ (identity operator) and $A = B^2 = BSBB^{-2}BSB = GB^{-2}G = GA^{-1}G$, we get

$$A(G\vec{a}^{(1)}) = GA^{-1}G^2\vec{a}^{(1)} = GA^{-1}\vec{a}^{(1)} = \lambda^{-1}(G\vec{a}^{(1)}).$$

Hence $G\vec{a}^{(1)}$ is an eigenvector of A, too, and so

$$\lambda^{(2)} = \frac{1}{\lambda^{(1)}}.$$

If $\lambda^{(1)} = \lambda^{(2)} = 1$, then $A = B = I$. Otherwise, $\vec{a}^{(2)} = G\vec{a}^{(1)} = (x^{(1)}, -y^{(1)})$ and the orthogonality of the eigenvectors $x^{(1)}x^{(2)} + y^{(1)}y^{(2)} = 0$ imply

$$\vec{a}^{(1)}=\frac{1}{\sqrt{2}}(1,1)\,,\quad \vec{a}^{(2)}=\frac{1}{\sqrt{2}}(1,-1)\,.$$

Hence,

$$A=\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}\lambda^{(1)} & 0\\ 0 & (\lambda^{(1)})^{-1}\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

follows. The assertion to be shown now follows from Proposition 5.1 (ii), (3), and

$$\begin{aligned}(q_\alpha(\vec{a}))^2&=[B\vec{a},B\vec{a}]\\ &=\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}x_a\\ y_a\end{pmatrix},\frac{1}{\sqrt{2}}\begin{pmatrix}\lambda^{(1)} & 0\\ 0 & \dfrac{1}{\lambda^{(1)}}\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}x_a\\ y_a\end{pmatrix}\right]\\ &=\frac{\lambda^{(1)}}{2}(x_a+y_a)^2+\frac{1}{2\lambda^{(1)}}(x_a-y_a)^2=\lambda^{(1)}\xi_+^2+(\lambda^{(1)})^{-1}\xi_-^2\end{aligned}$$

with $\alpha=\lambda^{(1)}$, and $\xi_\pm=1/\sqrt{2}\,(a_x\pm a_y)$. □

Proposition 5.2 readily yields the following.

Corollary 5.3: The boundary $\partial U_{q,\alpha}=\{\vec{a}\in\mathcal{M}^2;\,q_\alpha(\vec{a})=1\}$ *of the unit ball* $U_{q,\alpha}$ *is given by the ellipse* $\mathfrak{E}_\alpha$*:*

$$\frac{\alpha^2+1}{2\alpha}(x^2+y^2)+\frac{\alpha^2-1}{\alpha}xy=1\,. \tag{80}$$

Remark 5.4: (a) The semiaxis of the ellipse $\mathfrak{E}_\alpha$ considered in (80) are given by

$$\vec{b}^{(1)}=\frac{1}{\sqrt{2\alpha}}(1,1)\,,\quad \vec{b}^{(2)}=\sqrt{\frac{\alpha}{2}}\,(1,-1)\,.$$

(b) The ellipse $\mathfrak{E}_\alpha$ is given in polar coordinates by

$$r(\varphi)=\left(\sqrt{\frac{\alpha^2+1}{2\alpha}+\frac{\alpha^2-1}{2\alpha}\sin 2\varphi}\;\right)^{-1},\quad 0\leqslant\varphi<2\pi\,. \tag{81}$$

The aim of the following is to derive a relation between the general construction given in Sec. II and $\partial U_{q,\alpha}$ described in (80), (81). More precicely, the ingredients of the general construction P_1,P_2 and $\mathfrak{k}$ will be given for the case at hand.

Lemma 5.5: We have $\mathfrak{E}_\alpha\cap\mathfrak{h}_j^\pm=Q_j^\pm$, $j=1,2$, *where the polar coordinates of the points* $Q_j^\pm$ *are given by*

$$Q_j^\pm\equiv\left(\sqrt{\frac{\alpha^2+1}{2\alpha}},\varphi_{\alpha,j}^\pm\right),$$

with $\varphi_{\alpha,2}^+=-\frac{1}{2}\arcsin(\alpha^2-1)/(\alpha^2+1)$, $\varphi_{\alpha,2}^-=\varphi_{\alpha,2}^++\pi$, $\varphi_{\alpha,1}^+=(\pi/2)-\varphi_{\alpha,2}^+$, *and* $\varphi_{\alpha,1}^-=(3\pi/2)-\varphi_{\alpha,2}^+$.

Proof: Equations (24) and (81) imply

$$\frac{\alpha^2+1}{2\alpha}+\frac{\alpha^2-1}{2\alpha}\sin 2\varphi=\cos 2\varphi\,,\quad -\frac{\pi}{4}<\varphi<\frac{\pi}{4}\,,$$

and a simple calculation yields the polar coordinates of Q_2^+:

$$\varphi^+_{\alpha,2} = -\frac{1}{2}\arcsin\frac{\alpha^2-1}{\alpha^2+1}$$

and

$$r_{\mathfrak{h}_2^+}(\varphi^+_{\alpha,2}) = \left(1-\left(\frac{\alpha^2-1}{\alpha^2+1}\right)^2\right)^{-1/4} = \sqrt{\frac{\alpha^2+1}{2\alpha}}.$$

The second half of the lemma under consideration is now obvious by symmetry. □

Since a self-polar norm on $\mathcal{M}^2$ is uniquely determined by the ingredients $\{P_1, P_2, \mathfrak{k}\}$ of our construction (see Corollary 4.14), we get the following characterization of those constructions which yield Hilbertian self-polar norms on $\mathcal{M}^2$.

Corollary 5.6: The general construction given in Sec. II with the ingredients $P_1 = Q_1^+$, $P_2 = Q_2^+$ *and the convex arc* $\mathfrak{k}$ *given in polar coordinates by*

$$\varphi \to \left(\sqrt{\frac{\alpha^2+1}{2\alpha} + \frac{\alpha^2-1}{2\alpha}\sin 2\varphi}\right)^{-1}, \quad \varphi^+_{\alpha,2} \leqslant \varphi < \varphi^+_{\alpha,1}$$

yields the curve $\partial U_{q,\alpha}$ *described in* (80), (81). □

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The eigenvalue equation on the Eguchi–Hanson space

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(Received 14 December 2002; accepted 23 February 2003)

We consider the eigenvalue equation for the Laplace–Beltrami operator acting on scalar functions on the noncompact Eguchi–Hanson space. The corresponding differential equation is reducible to a confluent Heun equation with Ince symbol $[0,2,1_2]$. We construct approximations for the eigenfunctions and their asymptotic scattering phases with the help of the Liouville–Green approximation (WKB). Furthermore, for specific discrete eigenvalues obtained by a continued T-fraction we construct the solution by the Frobenius method and determine its scattering phase by a monodromy computation. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1579548]

I. INTRODUCTION

The Eguchi–Hanson metric (Eguchi and Hanson, 1979) is a self-dual, asymptotically locally Euclidean (ALE) metric on the cotangent bundle of the 2-sphere T^*S^2. Geometrically, this corresponds to a Ricci-flat metric on the smooth resolution space of an A_1-singularity—such a singularity looks like the origin of $\mathbb{C}^2/\mathbb{Z}_2$, where the $\mathbb{Z}_2$-group acts by point reflection at the origin.

Apart from Euclidean quantum gravity this metric has physical applications in string compactification. In fact, it is well known that the only nontrivial two-dimensional Calabi–Yau manifold—this is a K3-surface—can be obtained from the $\mathbb{Z}_2$-orbifold limit $\mathbb{T}^2_{\mathbb{C}}/\mathbb{Z}_2$ by blowing up its 16 A_1-singularities (where $\mathbb{T}^2_{\mathbb{C}}$ is the complex two-dimensional torus). By gluing the Eguchi–Hanson metric together with the flat torus metric one can explicitly construct an almost Ricci-flat metric on a K3-surface (Bozhkov, 1988) which is related to a Ricci-flat metric on K3 by a gauge transformation (Taubes, 1982).

In this paper we shall examine the eigenvalue equation for the Laplace–Beltrami operator on the Eguchi–Hanson space. The problem is interesting from a mathematical point of view since the differential equation is separable and reduces to an ordinary differential equation which due to its singularities can be identified as confluent Heun equation with corresponding Ince symbol $[0,2,1_2]$ (see Decarreau, Maroni, and Robert, 1978 for definitions). The Heun equation is an ordinary differential equation with four regular singularities on the punctured Riemann sphere. By coalescing two of the regular singularities to one irregular singularity one obtains the confluent Heun equation (analogously to the procedure by which one obtains the confluent hypergeometric differential equation from the hypergeometric one).

The problem is also interesting from a physical point of view since the functions that are obtained by gluing the eigenfunctions on the Eguchi–Hanson space together with the well known eigenfunctions on the flat torus describe the quantum mechanical limit of string fields on K3.

The plan of the paper is as follows: In Sec. II we introduce the ordinary differential equation that describes the radial part of the eigenvalue equation of the Laplace operator on the Eguchi–Hauson space. In Sec. III we construct its solutions and their corresponding scattering phases by the Liouville–Green approximation (WKB). This extends and corrects a result in Mignemi (1991). In Mignemi (1991) the author used the ad hoc version of the Liouville–Green approximation. This version did not give approximations for the wave functions which are valid over the whole range. Furthermore, we give error bounds for the constructed solutions and their scattering phases. The

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explicit calculations can be found in the Appendix (cf. Appendices A and B). In Sec. IV we construct the exact solutions for specific discrete eigenvalues by the Frobenius method. These special values are given by the vanishing condition for a continned fraction. This approach is similar to the treatment of the generalized spheroidal wave equation in Wilson (1928) and Leaver (1986). In addition, we can determine the exact scattering phase by a monodromy computation. Finally, we will show how this information can be used to compute the asymptotic scattering phase for this discrete set of eigenvalues. In Sec. V we present the numerical results obtained by the method of Secs. III and IV and show that they match up to a high accuracy. In Sec. VI we give the conclusions of this article and a brief outlook.

II. THE EIGENVALUE EQUATION

In this section we introduce the eigenvalue equation for the Laplace–Beltrami operator of the Eguchi–Hanson space. Using the SU(2)×U(1) symmetry of the Eguchi–Hanson space this eigenvalue equation will reduce to an ordinary differential equation of second order. A complete derivation of these and similar results can be found in Gibbons and Manton (1986) and Perry (1978).

The Riemannian metric on T^*S^2 that is known as the Eguchi–Hanson metric is Hyperkähler. Moreover, a complex structure which is compatible with the Hyperkähler structure can be introduced by identifying T^*S^2 with the complex manifold $T^*\mathbb{CP}^1$. In particular, the latter can be covered by two coordinate charts $U\cong U'\cong\mathbb{C}^2$ with coordinates (u,ξ), (u',ξ'), respectively. Here, u, u' denote Euclidean coordinates on the base $\mathbb{C}P^1$, and ξ, ξ' parameterize the fiber of the bundle $T^*\mathbb{CP}^1\to\mathbb{CP}^1$. This means that

$$U\cap U'\cong\mathbb{C}^*\times\mathbb{C},\quad (u',\xi')\in U\cap U':(u',\xi')=(u^{-1},u^2\xi). \tag{1}$$

Note that $T^*\mathbb{CP}^1$ describes the minimal resolution $\widetilde{\mathbb{C}^2/\mathbb{Z}_2}$ of $\mathbb{C}^2/\mathbb{Z}_2$, where $\mathbb{Z}_2$ acts on $(z^1,z^2)\in\mathbb{C}^2$ by $(z^1,z^2)\mapsto(-z^1,-z^2)$. To see this, on $U_0:=\{(u,\xi)\in U|\xi\neq 0\}$ use $(u,\xi)=(z^1/z^2,(z^2)^2)$, and analogously for the other chart. Then (1) is given by $z^1\leftrightarrow z^2$, and by the above we identify $\mathbb{C}^2/\mathbb{Z}_2$ with $T^*\mathbb{CP}^1$ with the zero section removed. The exceptional divisor of $\widetilde{\mathbb{C}^2/\mathbb{Z}_2}$ therefore corresponds to the zero section of $T^*\mathbb{CP}^1$. In these coordinates, i.e., outside the exceptional divisor, the Eguchi–Hanson metric takes the form,

$$g^{\mathrm{EH}}_{i\bar{j}}=\frac{\sqrt{c^4+R^4}}{R^2}\left\{\delta_{i\bar{j}}-\frac{c^4 z_i z_{\bar{j}}}{R^2(c^4+R^4)}\right\},$$

where

$$R^2=|z^1|^2+|z^2|^2,$$

and $c>0$ is the parameter of the Eguchi–Hanson metric. Introducing the Euler angles (θ,ϕ,ψ) on S^3 by

$$\begin{pmatrix}z^1\\ z^2\end{pmatrix}=R\begin{pmatrix}\cos\dfrac{\theta}{2}e^{(i/2)(\psi+\phi)}\\ \sin\dfrac{\theta}{2}e^{(i/2)(\psi-\phi)}\end{pmatrix},$$

we can describe coordinates (in the coordinate patch with $z_2\neq 0$) by a radial part $R\in\mathbb{R}_{>0}$ and the angles $\theta\in(0,\pi)$, $\phi\in[0,2\pi)$, $\psi\in[0,4\pi)$. In the following, it will be more convenient to use $r:=\sqrt[4]{R^4+c^4}$ instead of R.

The singularity of $\mathbb{C}^2/\mathbb{Z}_2$ then sits at $r=c$. On the exceptional divisor, the Eguchi–Hanson metric takes the form of the Fubini–Study metric on $\mathbb{CP}^1$, and therefore assigns volume π to the exceptional divisor (Eguchi and Hanson, 1979).

The $\mathbb{Z}_2$-operation mentioned above takes the form

$$\mathbb{Z}_2: \quad \begin{pmatrix} z^1 \\ z^2 \end{pmatrix} \mapsto -\begin{pmatrix} z^1 \\ z^2 \end{pmatrix}$$

$$(\theta, \psi, \phi) \mapsto (\theta, \psi + 2\pi, \phi).$$

In these new coordinates the metric takes the form originally found by Eguchi and Hanson. The Lie group SO(3) acts on itself by multiplication from the left and from the right. Let us call the vector fields that generate the right-multiplication (ξ_1, ξ_2, ξ_3), and the ones that generate the left-multiplication $(\bar{\xi}_1, \bar{\xi}_2, \bar{\xi}_3)$. Since $SO(3) \cong SU(2)/\mathbb{Z}_2 \cong S^3/\mathbb{Z}_2$ we have an action of these vector fields on the Eguchi–Hanson space. In Gibbons and Manton (1986) the authors derive that $\forall i,j: [\xi_i, \bar{\xi}_j] = 0$ and that $(\xi_1, \xi_2, \xi_3, \bar{\xi}_1)$ define Killing vector fields that generate an $su(2)_L \oplus u(1)_R$ symmetry algebra of the Eguchi–Hanson space.

Let Δ denote the Laplace–Beltrami operator on functions that is associated to the Eguchi–Hanson metric. Furthermore, let Ψ denote a smooth function on the Eguchi–Hanson space. We consider the eigenvalue equation for the real positive eigenvalue. (We are considering only the scattering case since we want to glue together the eigenfunctions on the Eguchi–Hanson space and the flat torus. However, eigenfunctions for $E < 0$ would correspond to bounded states.) i.e., $(E + \Delta)\Psi = 0$ for $E > 0$. The operator $E + \Delta$ can be expressed merely in terms of d/dr, $\xi^2 = \Sigma_{i=1}^3 \xi_i^2$, ξ_3^2, i.e.,

$$E + \Delta = E + \left(1 - \frac{c^4}{r^4}\right)\frac{d^2}{dr^2} + \left(\frac{3}{r} + \frac{c^4}{r^5}\right)\frac{d}{dr} + \frac{4\xi^2}{r^2} + \frac{4c^4\xi_3^2}{r^2(r^4 - c^4)}.$$

Due to their commutation relations we can diagonalize the operators ξ_3, $\bar{\xi}_3$, ξ^2 simultaneously and expand the eigenfunctions in terms of Wigner functions $D^j_{qm}(\theta, \psi, \phi)$ [see Abramowitz and Stegun (1955) for definitions], i.e.,

$$\Psi(r, \theta, \psi, \phi) = \sum_{j=0}^{\infty} \sum_{q,m=-j}^{j} \alpha^j_{qm} A(j, q, \beta | z) D^j_{qm}(\theta, \psi, \phi),$$

where $z := r^2/c^2$, $\beta := c^2 E/4$, and α^j_{qm} are complex coefficients, and the $A(j, q, \beta | z)$ are functions that depend only on the coordinate z. The Wigner functions fulfill

$$\bar{\xi}_3 D^j_{qm} = -imD^j_{qm},$$

$$\xi_3 D^j_{qm} = iqD^j_{qm},$$

$$(\xi_1^2 + \xi_2^2 + \xi_3^2) D^j_{qm} = -j(j+1) D^j_{qm},$$

where

$$j \in \mathbb{N}, \quad q, m \in [-j, j]_{\mathbb{N}}.$$

Here, j, q are the quantum numbers that label the SU(2) representation. The eigenvalue equation for Ψ then reduces to an ordinary differential equation for $A(j, q, \beta | .)$,

$$0 = \left[\frac{d^2}{dz^2} + \frac{2z}{z^2 - 1}\frac{d}{dz} + \frac{(\beta z - j(j+1))(z^2 - 1) - q^2}{(z^2 - 1)^2}\right] A(j, q, \beta | z). \tag{2}$$

The differential equation (2) has three singularities which we have summarized in the following table:

z	r	singularity	roots
1	c	regular	$\pm\frac{q}{2}$
-1	ic	regular	$\pm\frac{q}{2}$
∞	∞	irregular	

(for $q=0$ the regular singularities are logarithmic).

One should notice that our differential equation has an irregular singularity at infinity, thus is *not* of Fuchsian-type. More precisely, it is a confluent Heun equation with Ince symbol $[0,2,1_2]$. To construct a continuous solution valid on the whole Eguchi–Hanson sphere we have to choose the regular boundary condition at $z=1$ (then we can extend this solution to $z=1$, i.e., the blown up A_1-singularity). This means that we are looking for the *recessive* solutions that behave like $(z-1)^{q/2}$ for $z\to 1$. This means that all the eigenfunctions obtain a constant value on the entire $\mathbb{CP}^1$ which gives the exceptional divisor of the blow-up. By approaching the singular point of $\mathbb{C}^2/\mathbb{Z}_2$ with different slopes, one reaches different points in the exceptional divisor. But for a well-defined solution of the differential equation, the limit does not depend on the chosen slope.

We remark that the differential equation (2) does not depend on q but only on q^2. Therefore, it suffices to restrict ourselves to $q\geqslant 0$. Then, the function Ψ takes the following form:

$$\Psi(r,\theta,\psi,\phi)=\sum_{j=0}^{\infty}\sum_{q=0}^{j}A(j,q,\beta|z)\sum_{m=-j}^{j}(\alpha^j_{qm}D^j_{qm}(\theta,\psi,\phi)+\alpha^j_{-qm}D^j_{-qm}(\theta,\psi,\phi)).$$

On these functions the differential operator of Eq. (2) is self-adjoint: Since the differential operator in Eq. (2) is already formally self-adjoint the statement follows from the application of the results in [Coddington and Levinson (1955), Sec. 3.9] and a detailed study of the singularity at $z=1$ for $q=0$, where the differential equation is of a *limit-circle* type, and for $q\geqslant 1$, where it is of *limit-point* type; for more details see Coddington and Levinson (1955).

The specific problems that arise in the treatment of the differential Eq. (2) are due to the structure of singularities. In particular, the major issue is to treat *three* singularities—one being an *irregular* singularity—at the same time. The problem is to derive the connection between the different bases which provide expansions of the solutions in the neighborhood of the singular points. Another important question is how given a system of solutions the solutions transform into each other when passing through a cycle around the corresponding singularity.

For the thrice-punctured Riemann sphere with only regular singularities (this is a generalized hypergeometric equation) this can be done in terms of the Meijer transcendental functions—as they were recently applied in Greene and Lazaroiu (2001). Here, the key technique lies in a representation of the solutions in terms of Mellin–Barnes integrals.

For only two singularities—one being regular, one being singular—techniques can be applied which are familiar from the treatment of the Bessel differential equation. This corresponds to the confluent hypergeometric equation, i.e., a hypergeometric equation where two regular singularities are coalescing and forming one irregular singularity. Here, the key technique is a generalized Borel transformation [Gurarii and Matsaev (1994) and Gurarii and Matsaev (1994)] which relates a cycle around the regular singularity at $z=1$ to the irregular one at $z=\infty$.

In the case of two regular and one irregular singularities we cannot apply Mellin–Barnes integrals. Due to the irregular singularity solutions are oscillating at large real values. Thus, the conditions for convergence for the Mellin–Barnes integrals when continuing into the complex plane to close the path of integration to a cycle are not satisfied any more.

On the other hand, due to the third singularity at $z=-1$ a cycle around infinity is also not homologous to a cycle around $z=1$. Thus, an asymptotic expansion of the regular solution cannot be derived by a Borel transformation. However, as we will show in Sec. IV B, in some particular cases one can still use a similar argument.

III. WKB-TYPE SOLUTIONS

In this section we give approximations to the recessive solutions of differential equation (2) that can be obtained by the Liouville–Green approximation (WKB). The explicit derivation of the results can be found in Appendices A.1–A.4.

From now on we suppress the labels β, j, q in $A(\beta,j,q|z)$. Substituting $A(z)=(z^2-1)^{-(1/2)}w(u,z)$ in Eq. (2) we find

$$\frac{d^2}{dz^2}w(u,z)=[-u^2f(z)+g(z)]w(u,z), \tag{3}$$

where $u^2=\beta$, $g(z)=-(z^2-1)^{-2}$, $a=j(j+1)/\beta$, $b=q^2/\beta$, and

$$f(z)=\frac{(z-a)(z^2-1)-b}{(z^2-1)^2}.$$

We remark that due to the possible values for j, q, β we will always have $1\leqslant b+1<a$ and $0\leqslant a$.

Equation (3) is the standard form of a differential equation of second order considered for Liouville–Green approximation (WKB). Following the discussion in Olver (1974), the specific approximation depends on the order of the pole at $z=1$ as well as the number of *simple transition points* (tps), i.e., simple zeros, in the region $z>1$ which is of interest in connection with the geometry discussed in Sec. II. A simple analysis of the function f shows that we have to deal with the four different cases (I–IV) which are summarized in the table below.

case	condition	order of pole at $z=1$	tp for $z>1$
I	$1<b+1<a$	2	yes
II	$b=0$, $1<a$	1	yes
III	$b=0$, $a=1$	0	no
IV	$b=0$, $0\leqslant a<1$	1	no

For the different cases one can then apply the Liouville–Green approximation. First, one performs a Liouville-transformation of the variable z to the new variable ζ. The transformation is given by an integral equation of the form,

$$\forall z\geqslant z_0: G(\zeta)=\int_{z_0}^{z}\sqrt{|f(t)|}dt$$

such that ζ and z are analytic functions of each other, and where the function G and the point z_0 depend on the case (I–IV) we are dealing with. Simultaneously, we replace the function w by a function W according to $w(u,z)=\sqrt{|dz/d\zeta|}W(u,\zeta)$. The choices are as follows:

case	$G(\zeta)$	z_0
I	$\frac{2}{3}(-\zeta)^{2/3}$	>1 such that $f(z_0)=0$
II	$\zeta^{1/2}(\zeta-\alpha)^{1/2}-\frac{\alpha}{2}\ln\left(\frac{2\zeta-\alpha+2\zeta^{1/2}(\zeta-\alpha)^{1/2}}{\alpha}\right)$	a
III	ζ	1
IV	$(-\zeta)^{1/2}$	1

and

$$\alpha := \frac{2}{\pi}\int_1^a dt\sqrt{-f(t)}.$$

The aim of this transformation is to transform the differential equation (3) to a differential equation of the form,

$$\frac{d^2}{d\zeta^2}W(u,\zeta) = (T_1(u,\zeta)+T_2(\zeta))W(u,\zeta),$$

where T_1 and T_2 are real-valued functions such that the approximating differential equation obtained by omitting T_2 has solutions which are functions of a single variable. However, this transformation has been done in a way that the approximate solution will still reflect the right behavior of the solution at the singularity at $z=1$ and for $z\to\infty$. From now on we suppress the dependence of u in w and W.

We have found the following approximations for the solutions of differential equation (2) that are regular at $z=1$:

case	approx. function	form
I	Airy	$w(z)=\sqrt[4]{-\frac{\zeta}{f(z)}}\,\mathrm{Ai}(u^{2/3}\zeta)$
II	Whittaker	$w(z)=\sqrt[4]{\frac{\zeta-\alpha}{2u\zeta f(z)}}\,e^{-i\pi/4}\mathrm{M}_{iu\alpha/2,0}(2iu\zeta)$
III	Bessel	$w(z)=\frac{\zeta^{1/2}}{\sqrt[4]{f(z)}}\,\mathrm{J}_0(u\zeta)$
IV	Bessel	$w(z)=\frac{\lvert\zeta\rvert^{1/2}}{\sqrt[4]{4\lvert\zeta\rvert f(z)}}\,\mathrm{J}_0(u\lvert\zeta\rvert^{1/2})$

Asymptotically, the Eguchi–Hanson metric becomes the flat metric. Therefore, the solutions of the differential equation (2) must have the following behavior:

$$A(z) \overset{z\to\infty}{\sim} \frac{1}{z^{3/4}}\sin(2\sqrt{\beta z}+\Delta_{j,q}), \tag{4}$$

where $\Delta_{j,q}$ is called the scattering phase. Based on the results of Olver *et al.* (see Appendices A.1–A.4 for details), for the scattering phase we obtain the results listed below, where in the last column we give the equation number for the error bounds that are determined in Appendix A,

case	$\Delta_{j,q}(\beta)$	error
I	$\sqrt{\beta}\lim_{z\to\infty}\left(\int_{z_0}^{z}\sqrt{f(t)}dt-2\sqrt{z}\right)+\frac{\pi}{4}$	(22)
II	$-2\sqrt{\beta}\sqrt{1+a}\,\mathrm{E}\left[\sqrt{\frac{2}{1+a}}\right]+\frac{\alpha\sqrt{\beta}}{2}$ $-\frac{\alpha\sqrt{\beta}}{2}\ln\left(\frac{\alpha\sqrt{\beta}}{2}\right)+\arg\Gamma\left(\frac{1}{2}+\frac{i\alpha\sqrt{\beta}}{2}\right)+\frac{\pi}{4}$	(24)
III	$-\sqrt{8\beta}+\frac{\pi}{4}$	(27)
IV	$(1-a)\sqrt{2\beta}\,\mathrm{K}\left[\sqrt{\frac{1+a}{2}}\right]-2\sqrt{2\beta}\,\mathrm{E}\left[\sqrt{\frac{1+a}{2}}\right]+\frac{\pi}{4}.$	(30)

Here, $F(\phi,m)$, $E(\phi,m)$ denote elliptic integrals of the first and second kind, and $K(m)=F(\pi/2,m)$ and $E(m)=E(\pi/2,m)$ are the corresponding complete elliptic integrals [cf. Abramowitz and Stegun (1955), Sec. 17]. This corrects a result in Mignemi (1991).

IV. SOLUTIONS RELATED TO CONTINUED FRACTIONS

In this section we determine for which values of β, j, q the exact solution of the differential equation (2) can be obtained by a formal power series expansion (Frobenius method) around the singularity at $z=1$.

For an expansion around the regular singularity at $z=1$ a transformation according to $\zeta=\frac{1}{2}(z-1)$ is suitable. Substitution of

$$A(z)=(z^2-1)^{q/2}u(\zeta) \tag{5}$$

in Eq. (2) yields

$$0=\zeta(\zeta+1)u''(\zeta)+(q+1)(2\zeta+1)u'(\zeta)+(\beta(2\zeta+1)+\mu)u(\zeta), \tag{6}$$

where $\mu=q(q+1)-j(j+1)$. In a neighborhood of $z=1$ the two linearly independent solutions can be represented by the series,

$$\begin{aligned} u_{\mathrm{reg}}(\zeta)&=\sum_{k=0}^{\infty} a_k(\beta,j,q)\zeta^k,\\ u_{\mathrm{sing}}(\zeta)&=u_{\mathrm{reg}}(\zeta)(\ln\zeta+B_u)+\frac{1}{\zeta^q}\sum_{k=0}^{\infty} b_k(\beta,j,q)\zeta^k, \end{aligned} \tag{7}$$

where B_u is a real number. Since the singular solution is not unique (one can always add a multiple of the regular solution), the parameter B_u is not uniquely determined. However, the parameter can be fixed by fixing the asymptotic scattering phase of the singular solution.

By the Frobenius method [cf. Rabenstein (1972), Chap. 3.6] we obtain the coefficients $(a_k)_{k\geqslant -1}$ as solutions of the following three-term recurrence relation:

$$\begin{aligned} &a_{-1}=0,\\ \forall k\geqslant 0:\quad &a_{k+1}=-\frac{k(k+2q+1)+\mu+\beta}{(k+1)(k+q+1)}a_k-\frac{2\beta}{(k+1)(k+q+1)}a_{k-1}. \end{aligned} \tag{8}$$

Notice that a rescaling of the parameter a_0 results in a general rescaling of all the coefficients $(a_k)_{k\geqslant -1}$ since Eq. (8) is linear. However, the crucial information, i.e., the ratio of a_1 and a_0 is fixed by the recurrence relation (8). By standard methods one can show that there are only two types of solutions for $(a_k)_{k\in\mathbb{N}}$ in (8) depending on the radius of convergence r_c of the series $\Sigma_{k=0}^{\infty}a_k\zeta^k$,

$$\lim_{k\to\infty}\frac{a_{k+1}}{a_k}=\begin{cases}-1 & r_c=1,\\ 0 & r_c=\infty.\end{cases}$$

A solution with $r_c=1$ corresponds to a solution of the recurrence relation for generic values of (β,j,q), whereas the solution with $r_c=\infty$ is the *minimal solution*. [A minimal solution $(g_n)_{n\in\mathbb{N}}$ is defined by the universal property that for any other solution $(h_n)_{n\in\mathbb{N}}$ one obtains $\lim_{n\to\infty} g_n/h_n=0$.] The question for which values of the parameters (β,j,q) this minimal solution exists will be considered in Sec. IV A. One should mention that it is possible to derive an explicit representation of the coefficients $(a_k)_{k\in\mathbb{N}}$ by the use of Babister's inhomogeneous hypergeometric functions (Exton, 1991). However, this approach did not enable us to derive the asymptotic behavior in the

case of a minimal solution. To solve the differential equation (6) by a Laplace transformation as in Exton (1991) for similar differential equations or an Euler transformation as in Kazakov (1998) is not possible due to the structure of the coefficients in Eq. (6).

To gain a better understanding of solutions to (6), let us take a look at the solution u_{reg} which is regular at $z=1$ ($\zeta=0$) in terms of the singularity at $z=-1$ ($\zeta=-1$). Let $v_{\mathrm{reg}}(\zeta)$ be the solution regular at $z=-1$ ($\zeta=-1$). Its continuation to $\zeta\to\infty$ shall have an asymptotic scattering phase of γ, which by (4) and (5) gives an asymptotic expansion,

$$v_{\mathrm{reg}}(\zeta)\overset{\zeta\to\infty}{\sim}\frac{\sin(2\sqrt{2\beta\zeta}+\gamma)}{\zeta^{q+(3/4)}}\left(1+O\left(\frac{1}{\zeta}\right)\right).$$

We fix a solution singular at $z=-1$ ($\zeta=-1$) by the requirement that its asymptotic scattering phase differs from the regular solution by a phase of $\pi/2$, giving an asymptotic expansion,

$$v_{\mathrm{sing}}(\zeta)\overset{\zeta\to\infty}{\sim}\frac{\cos(2\sqrt{2\beta\zeta}+\gamma)}{\zeta^{q+(3/4)}}\left(1+O\left(\frac{1}{\zeta}\right)\right).$$

To resume, looking for the nontrivial solutions of the differential equation (2) we have already found two contributions: for a generic set of parameters (β,j,q) the solution regular at $z=1$ ($\zeta=0$) has a regular singularity at $z=-1$ ($\zeta=-1$). This means that it is a linear combination of v_{reg} and v_{sing}, without loss of generality,

$$u_{\mathrm{reg}}(\zeta)=\cos(\alpha)v_{\mathrm{reg}}(\zeta)+\sin(\alpha)v_{\mathrm{sing}}(\zeta)$$

$$\overset{\zeta\to\infty}{\sim}\frac{1}{\zeta^{q+(3/4)}}\sin(2\sqrt{2\beta\zeta}+\underbrace{\gamma+\alpha}_{=\Delta_{j,q}(\beta)})\left(1+O\left(\frac{1}{\zeta}\right)\right).$$

Because of the singularity at $z=-1$ ($\zeta=-1$) the representation of u_{reg} by a power series expansion must break down for all values $|\zeta|>1$. Therefore, the asymptotic scattering phase of u_{reg} can in general not be obtained from (7).

Only for those values $(\beta_n)_{n\in\mathbb{N}}$ that lead to a minimal solution of the recurrence relation (8) the solution regular at $z=1$ is regular at $z=-1$ as well, and therefore of class $C^\infty(\mathbb{R})$. This means $\sin\alpha=0$ and therefore

$$\Delta_{j,q}(\beta_n)=\gamma \bmod \pi. \tag{9}$$

Since we can always change the sign of the solution by an overall factor the scattering phase is only determined up to an integer multiple of π. In Sec. IV B we will eventually determine γ.

A. Minimal solutions and continued fractions

According to Pincherle's Theorem (see Jones and Thron (1980), Sec. 5.3) a three-term recurrence relation,

$$\forall_{n\geqslant 1}\quad y_{n+1}=-\delta_n y_n+\gamma_n y_{n-1}$$

has a minimal solution if and only if the following continued fraction converges,

$$\sum_{k=1}^{\infty}\frac{\gamma_k|}{|\delta_k}=\frac{\gamma_1}{\delta_1+\dfrac{\gamma_2}{\delta_2+\dfrac{\gamma_3}{\delta_3+\cdots}}}.$$

In particular, if $(a_n)_{n\in\mathbb{N}}$ is the minimal solution it follows that $a_0\neq 0$ and

$$-\frac{a_1}{a_0}+\sum_{k=1}^{\infty}\frac{\gamma_k|}{|\delta_k}=0.$$

For any set of parameters (j,q), where as before $q\geqslant 0$, we now define the function $\tilde{\mathcal{M}}(j,q|x)$ by the continued fraction of *Thron* type (or T-fraction),

$$\tilde{\mathcal{M}}(j,q|x):=\delta_0+\sum_{k=1}^{\infty}\frac{\gamma_k|}{|\delta_k},$$

where

$$\forall_{k\geqslant 0}\quad \delta_k:=\frac{k(k+2q+1)+\mu-x}{(k+1)(k+q+1)},$$

$$\forall_{k\geqslant 1}\quad \gamma_k:=\frac{2x}{(k+1)(k+q+1)}.$$

Using the Umordnungssatz [Perron, 1977, Kap. 6.42, Satz 2] and [Jones and Thron (1980), Sec. 7.3, Th. 7.23], we can conclude that the function $\tilde{\mathcal{M}}(j,q|x)$ is a meromorphic function on $\mathbb{C}$. Moreover, by the above its real zeros determine the values of $x=-\beta$ for which the recurrence relation (8) has a minimal solution, i.e., the radius of convergence of the power series expansion (7) becomes infinite.

The corresponding solution u_{reg} is then of class $C^{\infty}(\mathbb{R})$. Since the relation $A(\beta,j,q|z)=A(-\beta,j,q|-z)$ holds for the differential Eq. (2), it follows that any such smooth solution for β,j,q in z is simultaneously a smooth solution for $-\beta,j,q$ in the variable $-z$. Therefore, $x=\beta$ must be another zero of $\tilde{\mathcal{M}}(j,q|x)$. This is,

$$\tilde{\mathcal{M}}(j,q|\beta)=0\Leftrightarrow\tilde{\mathcal{M}}(j,q|-\beta)=0.$$

Using the Umordnungssatz [Perron (1977), Kap. 6.42, Satz 2], one can see that one can cancel the factor $(k+1)(k+q+1)$ in γ_k, δ_k. Namely, it is equivalent to calculate the zeros of the meromorphic function $\mathcal{M}(j,q|x)$ instead of $\tilde{\mathcal{M}}(j,q|x)$, where $\mathcal{M}(j,q|x)$ is defined by the continued fraction,

$$\mathcal{M}(j,q|x):=d_0+\sum_{k=1}^{\infty}\frac{c_k|}{|d_k},\tag{10}$$

where

$$\forall_{k\geqslant 0}\quad d_k:=k(k+2q+1)+\mu-x,$$

$$\forall_{k\geqslant 1}\quad c_k:=2k(k+q)x.$$

For this continued fraction one can even prove separate convergence [see Thron (1991) for definitions]. To see this, recall that $\mu=(q-j)(j+q+1)$, and rewrite the continued fraction in the following way:

$$\forall_{j-q\geqslant 1}\quad \mathcal{M}(j,q|x)=d_0+\sum_{k=1}^{j-q-1}\frac{c_k|}{|d_k}+\frac{2j(j-q)}{-1+\dfrac{m(j,q|x)}{x}},$$

$$\forall_{j\geqslant 0}\ \ \mathcal{M}(j,j|x)=x\left(-1+\frac{m(j,j|x)}{x}\right).$$

Here,

$$m(j,q|x):=\sum_{k=j-q+1}^{\infty}\frac{c_k|}{|d_k}$$

can be written as a T-fraction using again the Umordnungssatz [Perron (1977), Kap. 6.42, Satz 2], i.e.,

$$m(j,q|x)=\sum_{k=j-q+1}^{\infty}\frac{F_k x|}{|1+G_k x}, \tag{11}$$

where

$$\forall_{k\geqslant j-q+1}\ \ G_k:=-\frac{1}{(k-j+q)(k+j+q+1)},$$

$$\forall_{k\geqslant j-q+2}\ \ F_k:=\frac{2k(k+q)}{(k-j+q-1)(k-j+q)(k+j+q)(k+j+q+1)},$$

$$F_{j-q+1}:=j-q+1.$$

Since we have both $\Sigma_{k=j-q+1}^{\infty}|F_k|<\infty$ and $\Sigma_{k=j-q+1}^{\infty}|G_k|<\infty$ we can apply [Thron (1991), Sec. 3, Th. 3.1] to the T-fraction (11): let $A_k(x)$ and $B_k(x)$ be the numerators and denominators, respectively, of the nth approximant of the T-fraction (11). Then the sequences $(A_k(x))_{k\geqslant j-q+1}$ and $(B_k(x))_{k\geqslant j-q+1}$ converge, uniformly on compact subsets of $\mathbb{C}$, to entire functions $A(x)$ and $B(x)$ of order at most one. Further $B(0)=1$, $A(0)=0$, $A'(0)=F_{j-q+1}$ so that neither function is identically zero, and $(1/x)m(j,q|x)$ is well defined at $x=0$.

B. The determination of the scattering phase and the monodromy

In this section we calculate the scattering phase of the regular solution u_{reg} in the case that it is also regular at $\zeta=-1$.

Let us first look at the asymptotic expansion of the solutions of Eq. (6). For an asymptotic expansion a Fabry transformation (Olver, 1974) is suitable, i.e., a change of the variable according to $x^2=\zeta$. With $u(\zeta)=U(x)$, Eq. (6) becomes

$$(x^2+1)U''(x)+\left(-\frac{x^2+1}{x}+\frac{2(q+1)(2x^2+1)}{x}\right)U'(x)+(4\beta(2x^2+1)+4\mu)U(x)=0.$$

By standard methods, [cf. Coddington and Levinson (1955)] one finds that this equation has two linearly independent solutions H_1, H_2, such that for some $\delta>0$ the following asymptotic expansions hold,

$$\begin{aligned}
&\forall_x\ \ -2\pi+\delta\leqslant\arg x\leqslant\pi-\delta:\ \ H_1(x)\sim\frac{1}{x^{2q+(3/2)}}e^{-2i\sqrt{2\beta}x}\sum_{k=0}^{\infty}\frac{(-1)^k p_k}{(4i\sqrt{2\beta}x)^k},\\
&\forall_x\ \ -\pi+\delta\leqslant\arg x\leqslant 2\pi-\delta:\ \ H_2(x)\sim\frac{1}{x^{2q+(3/2)}}e^{-2i\sqrt{2\beta}x}\sum_{k=0}^{\infty}\frac{p_k}{(4i\sqrt{2\beta}x)^k},
\end{aligned} \tag{12}$$

where the coefficients $(p_k)_{k\in\mathbb{N}}$ fulfill the following four-term recurrence relation:

$$
\begin{aligned}
&p_{-2}=p_{-1}=0,\\
\forall k\geqslant 0:\quad &p_{k+1}=\frac{k(k+1)-4\beta-4j(j+1)-\frac{3}{4}}{k+1}p_k+32\beta\frac{k+q}{k+1}p_{k-1}\\
&-32\beta\frac{k^2+(2q-1)k-q+\frac{1}{4}}{k+1}p_{k-2}.
\end{aligned}
\tag{13}
$$

It follows from this recurrence relation that for $p_0\in\mathbb{R}$ the coefficients $(p_k)_{k\in\mathbb{N}}$ are real. In particular, we have $H_1(x)=\overline{H_2(\bar{x})}$. This property remains true not only asymptotically, but also for the actual solutions: Since all the coefficients in the differential equation are real, the complex conjugate of any solution is again a solution.

The Stokes phenomenon will lead to a nontrivial monodromy of the solutions if we pass through a cycle around infinity (Olde Daalhuis, 1995). However, since the solutions H_1, H_2 are a complete system of solutions the new solutions can be expressed as linear combinations of them. These are the connection formulas. In the case of a second order differential equation they had been explicitly calculated, namely in Olde Daalhuis and Olver (1994). We obtain for $|x|\gg 0$,

$$
\begin{aligned}
&\lim_{\theta\to 1} H_1(xe^{-2\pi i\theta})=-H_1(x)+2\pi iPH_2(x),\\
&\lim_{\theta\to 1} H_2(xe^{2\pi i\theta})=-2\pi iPH_1(x)-H_2(x).
\end{aligned}
\tag{14}
$$

The parameter P can be determined by a generalized Borel transformation of the asymptotic solution as pointed out in Gurarii and Matsaev (1994) and Gurarii and Matsaev (1994). For ordinary differential equations of second order this has been done explicitly by Olde Daalhuis and Olver (1994). Applying these results we can determine the parameter P from the coefficients in the asymptotic expansion (13), i.e.,

$$
P=\lim_{k\to\infty}\frac{1}{(k-1)!}\frac{p_k}{p_0}. \tag{15}
$$

In particular, the parameter P is real. We subsume the solutions H_1, H_2 in the vector $\mathbf{H}:={}^t(H_1,H_2)$. We are interested in the matrix $\mathbf{C}$ which describes the behavior if we go around the singularity at $x=\infty$, i.e.,

$$
\begin{aligned}
&\lim_{\theta\to 1}\mathbf{H}(xe^{2\pi i\theta})=\mathbf{C}\cdot\mathbf{H}(x),\\
&\lim_{\theta\to 1}\mathbf{H}(xe^{-2\pi i\theta})=(\mathbf{C})^{-1}\cdot\mathbf{H}(x).
\end{aligned}
$$

From the connection formulas (14) we obtain

$$
\mathbf{C}=-\begin{pmatrix} 1-4\pi^2P^2 & 2\pi iP\\ 2\pi iP & 1\end{pmatrix}. \tag{16}
$$

Notice that this matrix describes the monodromy by passing through a cycle around infinity (in the x-variable). In the original variable ζ this describes a cycle that winds up twice around infinity.

As a last step we need to calculate the linear combination of the regular solution $u_{\mathrm{reg}}(\zeta)$ in terms of the solutions $\mathbf{H}(x)$ derived earlier. This amounts to determining a complex parameter $\lambda\in U(1)$ such that

$$u_{\mathrm{reg}}(\zeta)=(\lambda\ \ \overline{\lambda})\cdot\mathbf{H}(x).$$

The occurrence of λ and $\overline{\lambda}$ is due to the fact that $u_{\mathrm{reg}}(\zeta)$ is real, i.e., $\overline{u_{\mathrm{reg}}(\zeta)}=u_{\mathrm{reg}}(\zeta)$, and $\overline{H_1(\overline{x})}=H_2(x)$.

Now, the representation of $u_{\mathrm{reg}}(\zeta)$ by the power series (7) is valid for $|\zeta|>1$ iff the coefficients $(a_k)_{k\geqslant 1}$ constitute a minimal solution of the recurrence relation (8). Therefore, $u_{\mathrm{reg}}(\zeta)$ has a trivial monodromy around both of the regular singularities iff the $(a_k)_{k\geqslant 1}$ constitute a minimal solution of Eq. (8). Hence, iff for any set of parameters (β,j,q) the equation $\mathcal{M}(j,q|\beta)=0$ holds, then the following equation must hold:

$$u_{\mathrm{reg}}(\zeta)=\lim_{\theta\to 1}u_{\mathrm{reg}}(\zeta e^{4\pi i\theta})=(\lambda\ \ \overline{\lambda})\cdot\lim_{\theta\to 1}\mathbf{H}(xe^{2\pi i\theta})=(\lambda\ \ \overline{\lambda})\cdot\mathbf{C}\cdot\mathbf{H}(x).$$

Thus, the equation $\mathcal{M}(j,q|\beta)=0$ holds iff

$$(\lambda\ \ \overline{\lambda})=(\lambda\ \ \overline{\lambda})\cdot\mathbf{C},$$

or equivalently (since P is real),

$$P^2=\frac{1}{\pi^2},$$

$$\overline{\lambda}=-i\pi P\lambda.$$

If we set $\lambda=ie^{-i\gamma}$ with $\gamma\in\mathbb{R}$ we obtain

$$\gamma=\begin{cases}\dfrac{\pi}{4} & \text{if } P=\dfrac{1}{\pi}\\[2ex] \dfrac{3\pi}{4} & \text{if } P=-\dfrac{1}{\pi}\end{cases}\quad \mathrm{mod}\ \pi. \tag{17}$$

Thus, λ encodes the crucial information for the asymptotic expansion of the regular solution, i.e.,

$$u_{\mathrm{reg}}(\zeta)=\frac{1}{i}(e^{i\gamma}H_2(x)-e^{-i\gamma}H_1(x))\sim\frac{2p_0}{\zeta^{q+(3/4)}}\left(\sin(2\sqrt{2\beta\zeta}+\gamma)+O\left(\frac{1}{\sqrt{\zeta}}\right)\right).$$

This is the desired formula for the scattering phase in the case that the set of parameters (β,j,q) induces a minimal solution of the recurrence relation (8).

By standard methods one can show that there are only the following two types of asymptotic behavior for solutions $(p_k)_{k\in\mathbb{N}}$ of the recurrence relation (13),

$$\frac{p_{k+1}}{p_k}=\begin{cases}k+O\left(\dfrac{1}{k}\right)\\[2ex] \pm 4\sqrt{2\beta}+O\left(\dfrac{1}{k}\right).\end{cases} \tag{18}$$

Therefore, if $P_k:=1/(k-1)!(p_k/p_0)$ converges to σ/π [cf. Eqs. (15) and (17)] i.e.,

$$P_k=\frac{\sigma}{\pi}+\frac{m}{k^n}+o\left(\frac{1}{k^n}\right),$$

where σ is either -1 or 1 and $m \in \mathbb{R}$, $n \in \mathbb{R}_{>0}$, the ratio of the coefficients p_{k+1} and p_k must behave asymptotically as

$$\frac{p_{k+1}}{p_k} = k - \frac{nm\sigma\pi}{k^n} + o\left(\frac{1}{k^n}\right).$$

A comparison with (18) then gives $n \geqslant 1$, and by expanding the RHS of (13) we finally obtain

$$\frac{p_{k+1}}{p_k} = k - \frac{m\sigma\pi}{k} + O\left(\frac{1}{k^2}\right),$$

$$m\sigma\pi = 4\beta + 4j(j+1) + \tfrac{3}{4}.$$

Therefore, the coefficients $(p_k)_{k\in\mathbb{N}}$ must be a dominant solution of Eq. (13) if P_k converges to σ/π.

C. Computation

The numerical determination of the scattering phase consists of two steps: First, we have to determine the successive zeros of the function $\mathcal{M}(j,q|x)$. However, one should mention that for the necessary evaluation of the continued fraction one has to use a backward algorithm since any forward algorithm must be numerically instable as shown in Gautschi (1967).

We have determined the positive zeros $(\beta_n)_{n\in\mathbb{N}}$ of $\mathcal{M}(j,q|x)$ by a simple bisection algorithm where the evaluation of the continued fraction was accomplished by the Gautschi algorithm. It is essential to use the function $\mathcal{M}(j,q|x)$ instead of the earlier defined $\tilde{\mathcal{M}}(j,q|x)$: Because of the structure of the coefficients in the continued fraction the typical values of $\tilde{\mathcal{M}}(j,q|x)$ become very small, and the determination of its zeros unstable.

Second, for those values of β_n for which the recurrence relation (8) has a minimal solution by (17) the asymptotic scattering phase is either $\pi/4$ or $3\pi/4$ depending on the sign of P. P is determined by a solution of the four-term recurrence relation (13). We have proven in Sec. IV B that for the parameters (β_n, j, q) this must be a dominant solution of the recurrence relation (13). Thus, P can be determined by a simple forward algorithm which will be numerically stable. With the set $(\beta_n, j, q, \operatorname{sign} P)$ we then have the data needed for a numerical interpolation of the scattering phase over the whole range of β.

V. NUMERICAL RESULTS

A. Numerical results for the WKB approximation

The figures below show the scattering phases for different quantum numbers j and q with varying parameter β obtained by the WKB approximation from Sec. III. In Figs. 1–4 we have applied the WKB approximation of case I. Figure 1 shows (from the top to the bottom) the graphs for $\Delta_{j,q}$ for $j=1,...,10$ and $q=1$. Figure 2 shows (from the top to the bottom) the graphs for $\Delta_{j,q}$ for $j=3,...,10$ and $q=3$. Figure 3 shows (from the top to the bottom) the graphs for $\Delta_{j,q}$ for $j=4,...,10$ and $q=4$. Figure 4 shows (from the top to the bottom) the graphs for $\Delta_{j,q}$ for $j=5$ and $q=1,3,5$. In Figs. 5 and 6 we have compared the WKB approximation of case II–IV (left) with the WKB approximation of case I (right) for the values $j=9$, $q=0$. The vertical line in Fig. 5 is indicating the transition from case II–IV. Figure 7 shows (from the top to the bottom) the graphs for $\Delta_{j,0}$ for $j=1,3,5$. Figure 8 shows the graph for $\Delta_{12,0}$.

B. Comparison between WKB and Frobenius method

In this section we compare the numerical results for the asymptotic scattering phase obtained by the WKB approximation (already shown in Sec. V A) with the numerical data obtained by the Frobenius/continued-fraction method as described in Sec. IV C.

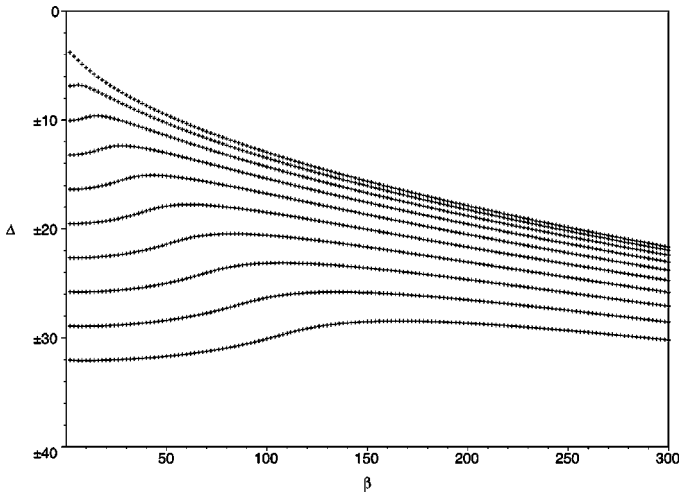

FIG. 1. $\Delta_{j,q}$ for $j=1,...,10;\ q=1$.

The figures below show the scattering phases for different quantum numbers j and q with varying parameter β. Each figure will show the graph $[\beta,\Delta_{j,q}^{\mathrm{WKB}}(\beta)]$ of the corresponding WKB approximation, and crosses will mark the points $[\beta_n,\Delta_{j,q}^{\mathrm{Fr}}(\beta_n)]_{n\geqslant 1}$ obtained by the Frobenius/continued-fraction method where β_n is the nth zero of $\mathcal{M}(j,q|\beta)$ and

$$\Delta_{j,q}^{\mathrm{Fr}}(\beta_n)=-\frac{\pi}{4}(2+\sigma)-l_{j,q}(n)\,\pi-\max(0,j-1)\,\pi \tag{19}$$

with $\sigma=\mathrm{sign}(P)$ (cf. Sec. IV B) and $\forall_{n\geqslant 1}: l_{j,q}(n)\in\mathbb{N}_0$. Notice that the scattering phase is only determined up to a multiple of π since we can always change the sign of a solution by an overall factor. Therefore, Eq. (19) is equivalent to Eq. (17). We will also present an additional and more significant diagram of $(\Delta_{j,q}(\beta)\mathrm{mod}\,\pi)$ and varying parameter β.

Figures 9, 11, 13, 15 show $\Delta_{j,0}(\beta)$ with varying β. For all j and $q=0$ we have found $\sigma=\mathrm{sign}(P)=-1$. For $j\leqslant 6$ it is $l(n):=n$ and all $\beta_n>j(j+1)$, i.e., $1>a\geqslant 0$ and we have to compare it to case IV of the WKB approximation. $j=7$ is the lowest value where for $q=0$ we

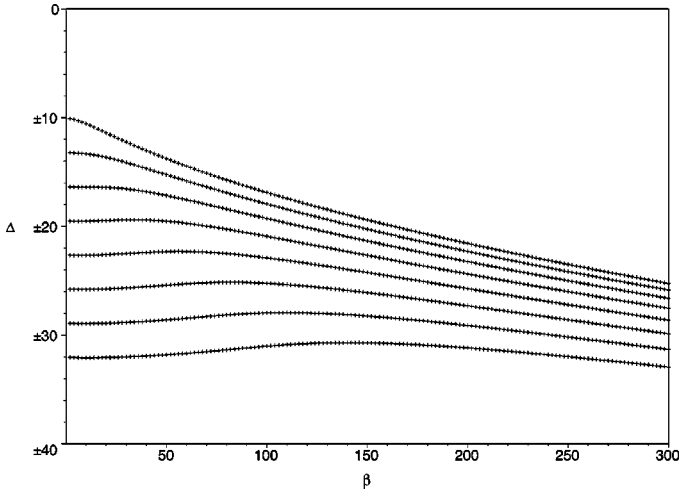

FIG. 2. $\Delta_{j,q}$ for $j=3,...,10;\ q=3$.

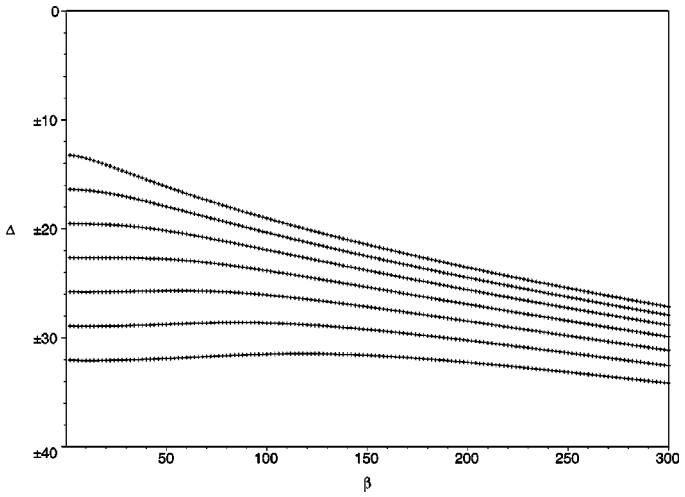

FIG. 3. $\Delta_{j,q}$ for $j=4,\ldots,10$; $q=4$.

have $\beta_1<j(j+1)$, i.e., $1<a$, and we have to compare it to case II of the WKB approximation; we have to relabel the β_n. This can be done by setting $\forall_{j\geqslant 7}: l(n):=|n-\frac{3}{2}|-\frac{1}{2}$.

However, since the phase can be obtained only up to multiples of π the function $l(n)$ is irrelevant for the comparison of $\Delta_{j,q}^{\mathrm{WKB}}(\beta)$ and $\Delta_{j,0}^{\mathrm{Fr}}(\beta_n)$. For this purpose one can look at Figs. 10–16, which are independent of $l(n)$. These figures show an exact match of the data sets obtained by the WKB approximation and the Frobenius/continued-fraction method.

Figures 17–24 show $\Delta_{j,1}(\beta)$ with varying β. For all j and $q=1$ we have found $\sigma=\mathrm{sign}(P)=-1$. For $j\leqslant 8$ it is $l(n):=n$. $j=9$ is the lowest value where for $q=1$ we have $\beta_1<\beta_{\max}$, where $\beta_{\max}$ denotes the local maximum of the WKB approximation: We have to relabel the β_n. This can be done by setting $\forall_{j\geqslant 9}: l(n):=|n-\frac{3}{2}|-\frac{1}{2}$. Figures 17–24 show an exact match of the data sets obtained by the WKB approximation and the Frobenius/continued-fraction method.

Figures 25–32 show $\Delta_{j,2}(\beta)$ with varying β. For all j and $q=2$ we have found $\sigma=\mathrm{sign}(P)=-1$. For $j\leqslant 11$ it is $l(n):=n$. Figures 25–32 show an exact match of the data sets obtained by the WKB approximation and the Frobenius/continued-fraction method.

The accuracy of the WKB approximation can be explained as follows: from the error bound in Eq. (30) we can deduce the following numerical result for the error $\delta_{j,q}(\beta)$ of $\Delta_{j,q}(\beta)$;

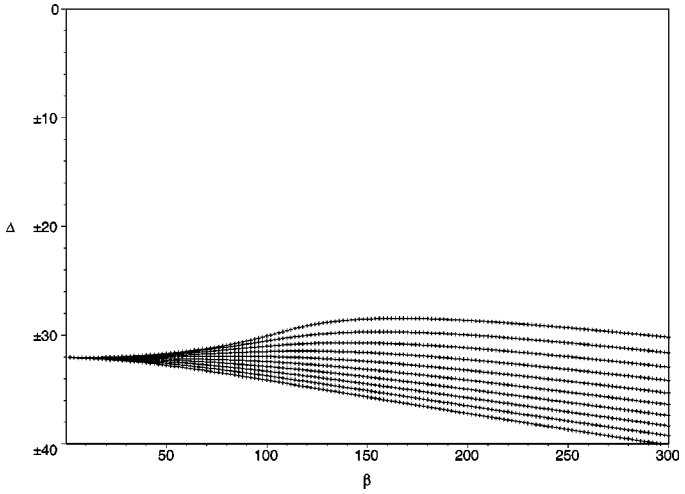

FIG. 4. $\Delta_{j,q}$ for $j=10$, $q=1,\ldots,10$.

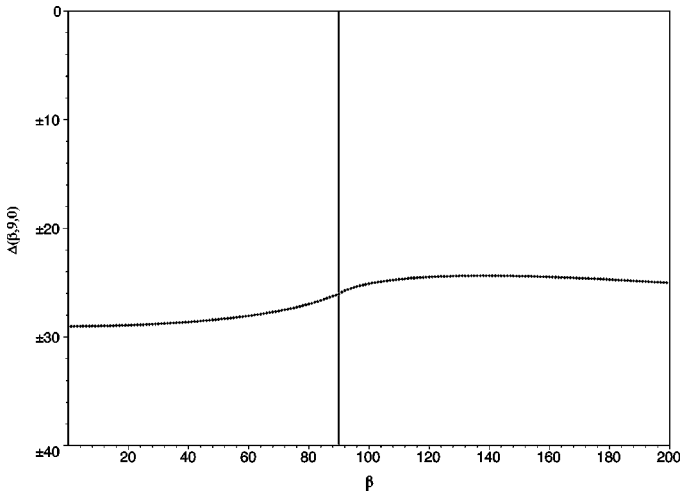

FIG. 5. $\Delta_{9,0}$ for cases II, III, IV.

$$|\delta_{j,q=0}(\beta)| \leqslant \frac{\pi}{2}\min(1,1.1e^{(1.2/\sqrt{\beta})}-1).$$

This means that for $\beta>4$ we already have

$$|\delta_{j,q=0}(\beta)| \leqslant \frac{\pi}{2}(e^{(1.2/\sqrt{\beta})}-1),$$

and for $\beta>100$ we find $|\delta_{j,q=0}(\beta)| \leqslant \pi/10$.

The same computations can be made for $q \geqslant 1$ with similar results since we also have a similar error bound for the general $\delta_{j,q}(\beta)$ in Eq. (22).

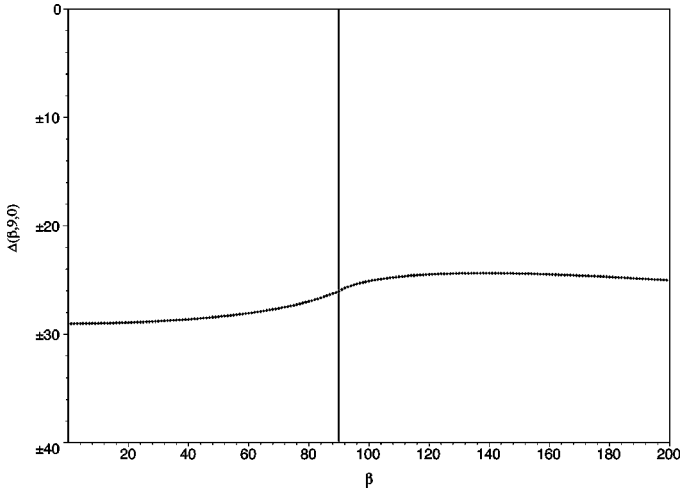

FIG. 6. $\Delta_{9,0}$ for case I.

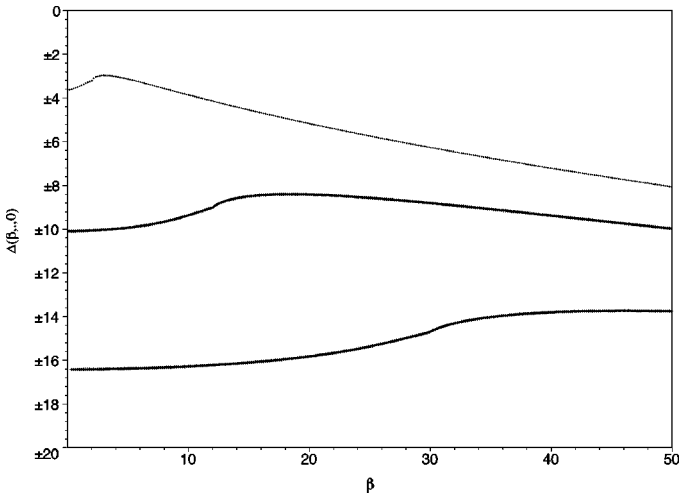

FIG. 7. $\Delta_{j,0}$ for $j=1, 3, 5$.

VI. CONCLUSIONS AND OUTLOOK

The eigenvalue equation for the Laplace–Beltrami operator acting on scalar functions on the noncompact Eguchi–Hanson space reduces to a confluent Heun equation [(2) or after a suitable substitution (6)] with the Ince symbol $[0,2,1_2]$.

With the help of the Liouville–Green approximation (WKB) we have constructed approximations for the eigenfunctions by special functions in Sec. III. Depending on the quantum numbers that label the SU(2)-representation the approximating functions are either Airy, Whittaker, or Bessel functions. Furthermore, we have derived the scattering phases and error bounds in these cases.

Moreover, for specific discrete values of the eigenvalue in Sec. IV we have constructed the exact solutions by the Frobenius methods. These eigenvalues are given by the zeros of a meromorphic function defined by the infinite continuous fraction (10). Together with a monodromy computation this has provided us with the data needed for a numerical interpolation of the scattering phases.

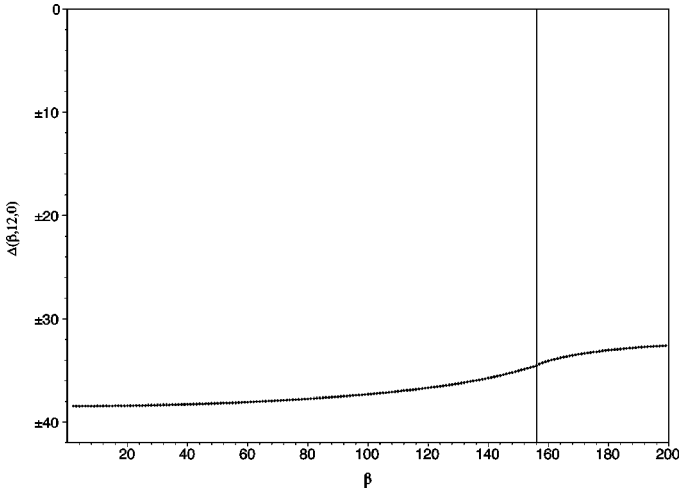

FIG. 8. $\Delta_{12,0}$.

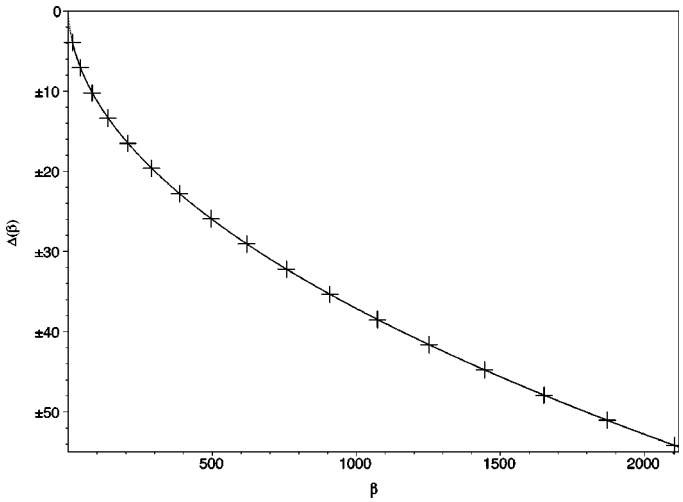

FIG. 9. $\Delta_{0,0}^{\mathrm{WKB}}$ and $\Delta_{0,0}^{\mathrm{Fr}}$.

Finally, in Sec. V we have shown that these two sets of data (obtained by the WKB approximation and the Frobenius/continued-fraction method) agree to a high accuracy. This shows that one can find a discrete set of exact values for the spectral density of the Laplace–Beltrami operator by the method described in Sec. IV C. Conversely, it shows that the expressions for the eigenfunctions and scattering phases which were derived in Sec. III and which have the advantage of being given in terms of explicit functions are very accurate approximations and can be used for all numerical purposes.

It is now interesting to ask whether the meromorphic function defined by the continued fraction (10) can be expressed explicitly as a ratio of special functions. If so we could obtain the discrete eigenvalues—for which we have already calculated the exact scattering phase and which we have also computed numerically by the continued fraction—as zeros of this ratio of special functions. A first step towards an explicit representation of the continued fraction might arise from the method of Pincherle. If we apply Perron (1977) (Kap. 21.84, Satz 8) to the continued fraction (10) we obtain the following result: a representation of the meromorphic function defined by the T-fraction (10) is given by

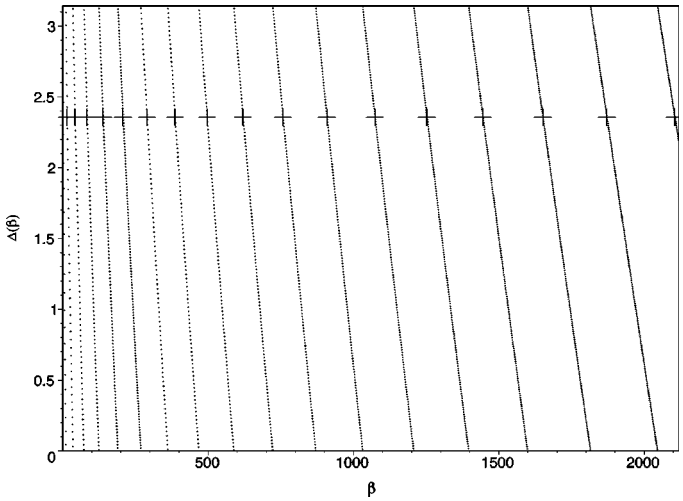

FIG. 10. $\Delta_{0,0}^{\mathrm{WKB}}$ and $\Delta_{0,0}^{\mathrm{Fr}}$ modulo π.

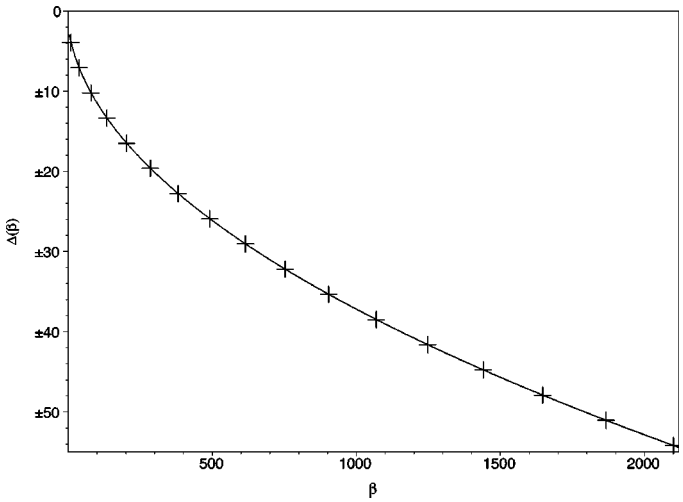

FIG. 11. $\Delta_{1,0}^{\mathrm{WKB}}$ and $\Delta_{1,0}^{\mathrm{Fr}}$.

$$\mathcal{M}(j,q|x)=q(q+1)-j(j+1)+x+\frac{\delta_{q0}16\pi x^3\phi\left(\frac{1}{2x}\right)+\int_{1/2x}^{\infty}dz\,\phi(z)z^{-3}}{\delta_{q0}8\pi x^2\phi\left(\frac{1}{2x}\right)+\int_{1/2x}^{\infty}dz\,\phi(z)z^{-2}}.$$

Here, ϕ is the solution of the differential equation,

$$\left\{z^3\left(z-\frac{1}{2x}\right)\frac{d^2}{dz^2}+z^2\left((q+1)z-\frac{q}{x}\right)\frac{d}{dz}+\left(\frac{x-q(q+1)+j(j+1)}{2x}z-\frac{1}{2x}\right)\right\}\phi(z)=0$$

that behaves as $(z-(1/2x))^q$ at the regular singularity $z=1/2x$. An analysis of the differential equation shows that such a solution always exists. A further analysis of the behavior at the irregular singularity $z=\infty$ then shows that all the appearing integrals also exist.

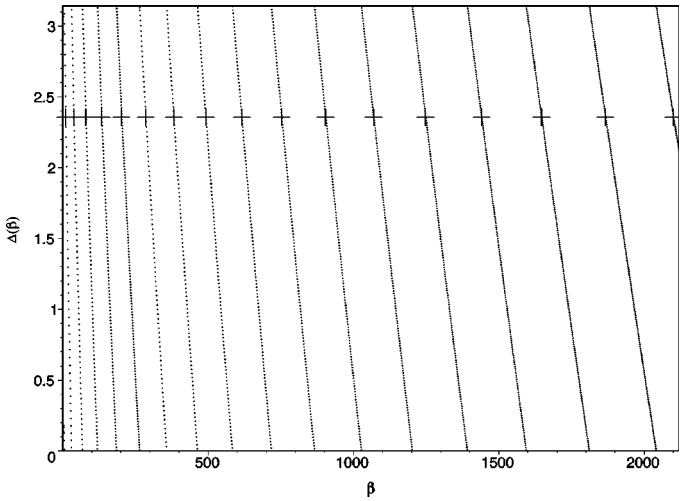

FIG. 12. $\Delta_{1,0}^{\mathrm{WKB}}$ and $\Delta_{1,0}^{\mathrm{Fr}}$ modulo π.

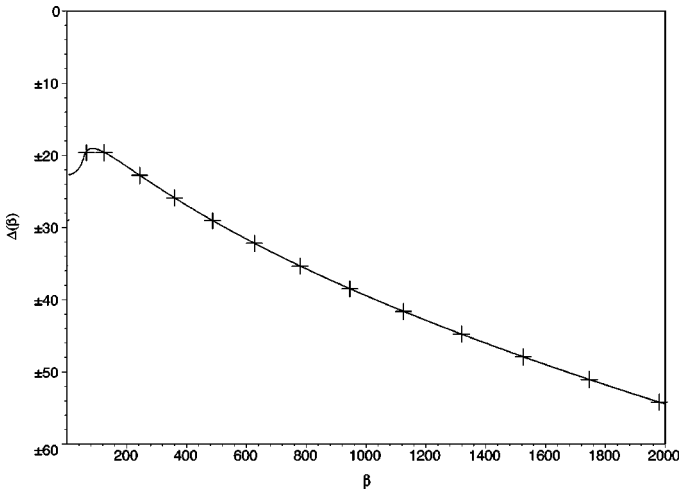

FIG. 13. $\Delta_{7,0}^{\mathrm{WKB}}$ and $\Delta_{7,0}^{\mathrm{Fr}}$.

A closer investigation of the meromorphic function $\mathcal{M}(j,q|x)$ is subject of our ongoing research.

ACKNOWLEDGMENTS

I would like to thank Professor W. Nahm for suggesting the problem and some useful discussions. Moreover, I wish to thank Professor F. W. J. Olver and Professor W. B. Jones for bringing the articles Dunster (1994) and Thron (1991) to my attention. In particular, I would like to thank Katrin Wendland for many helpful discussions and a lot of encouragement. I also wish to thank the Physics Department of the UNC at Chapel Hill for hospitality, and the *Studienstiftung des deutschen Volkes* and the *Deutschen Akademischen Austauschdienst* (DAAD) for financial support.

APPENDIX A: THE DIFFERENT CASES IN THE WKB APPROXIMATION

In this Appendix we show the explicit construction of the approximate solutions of the differential equation (3) by the Liouville–Green approximation (WKB) in cases I–IV (cf. Sec. III).

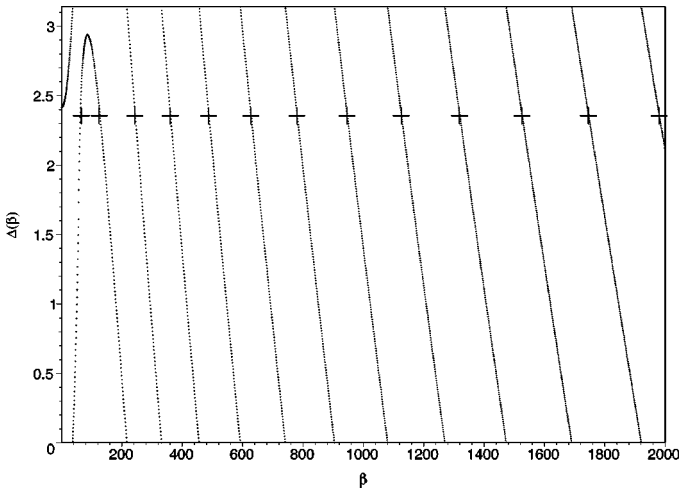

FIG. 14. $\Delta_{7,0}^{\mathrm{WKB}}$ and $\Delta_{7,0}^{\mathrm{Fr}}$ modulo π.

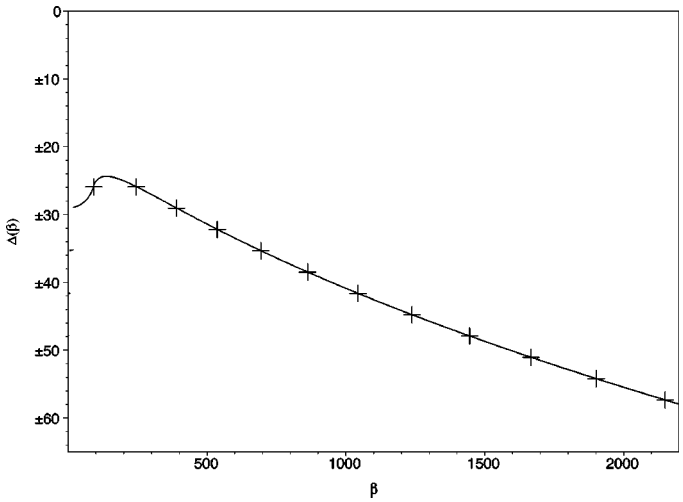

FIG. 15. $\Delta_{9,0}^{\mathrm{WKB}}$ and $\Delta_{9,0}^{\mathrm{Fr}}$.

The construction of an error bound in cases I–III can be found in the references. The construction of the bound in case IV is given in Appendix B and might explain the construction and philosophy behind these error bounds.

To give bounds for the different cases I–IV we need the notion of auxiliary weight, modulus, and phase function E, M, and θ: If X, Y are solutions of the respective differential equation of the first and second kind, then $X=ME^{-1}\sin\theta$ and $Y=EM\cos\theta$.

In particular, in case I we will need E, M, θ for the Airy function [see Olver (1974), Sec. 11.2] for more details),

$$\mathrm{Ai}(x)=\frac{M(x)}{E(x)}\sin\theta(x),\quad \mathrm{Bi}(x)=E(x)M(x)\cos\theta(x).$$

In cases III and IV, we will use the functions E_0, M_0, θ_0 for the Bessel function [see Olver (1974), Secs. 12.1 and 12.3 for more details],

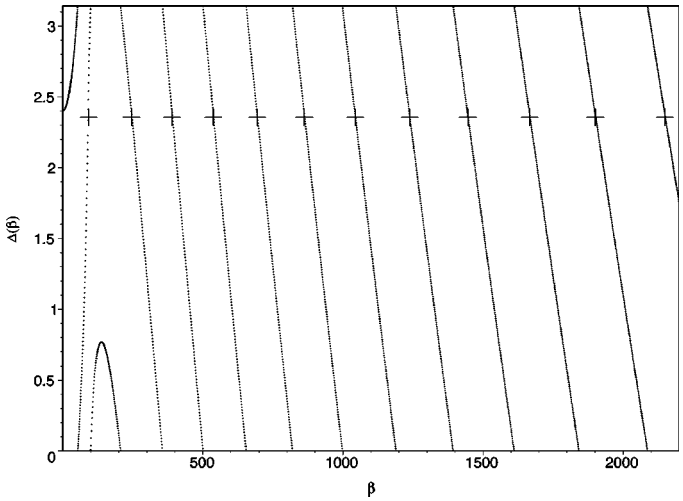

FIG. 16. $\Delta_{9,0}^{\mathrm{WKB}}$ and $\Delta_{9,0}^{\mathrm{Fr}}$ modulo π.

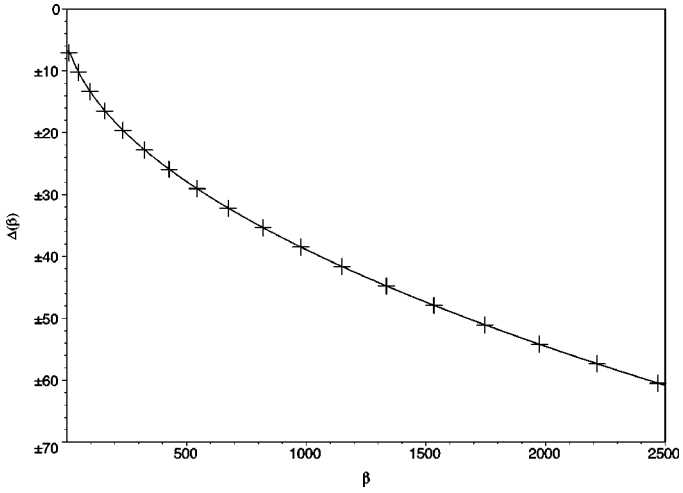

FIG. 17. $\Delta_{2,1}^{\mathrm{WKB}}$ and $\Delta_{2,1}^{\mathrm{Fr}}$.

$$\mathrm{J}_0(x)=\frac{M_0(x)}{E_0(x)}\cos\theta_0(x),\quad \mathrm{Y}_0(x)=E_0(x)M_0(x)\sin\theta_0(x).$$

For case II, the definition of modulus and weight function is the most complicated. Therefore, we refer to [Dunster (1994), Chap. 2, Th. 1] for quite extensive definitions in this case.

1. Case I

In case I it is easy to prove that the function f has a transition point (i.e., simple zero) at $z>1$ which we denote by z_0. The idea is now to perform the transformation of the variable z and the function $w(z)$ to ζ, $W(\zeta)$ according to

$$\begin{cases} \forall\ z\geqslant z_0: & \frac{2}{3}(-\zeta)^{3/2}=\displaystyle\int_{z_0}^{z}\sqrt{f(t)}dt, \\ \forall\ z\leqslant z_0: & \frac{2}{3}\zeta^{3/2}=\displaystyle\int_{z}^{z_0}\sqrt{-f(t)}dt, \end{cases}$$

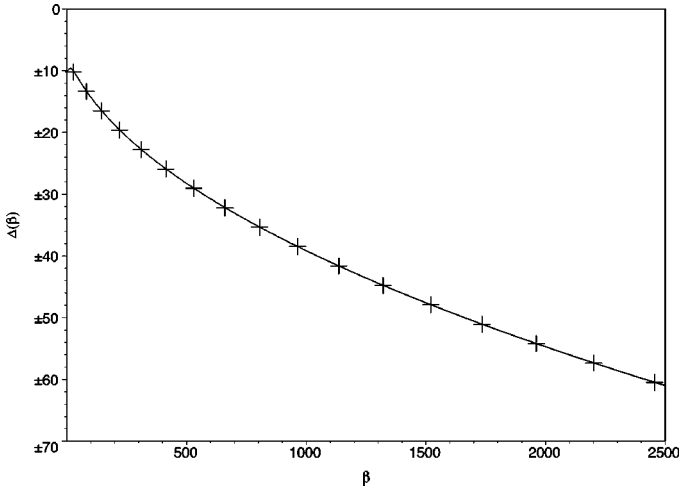

FIG. 18. $\Delta_{3,1}^{\mathrm{WKB}}$ and $\Delta_{3,1}^{\mathrm{Fr}}$.

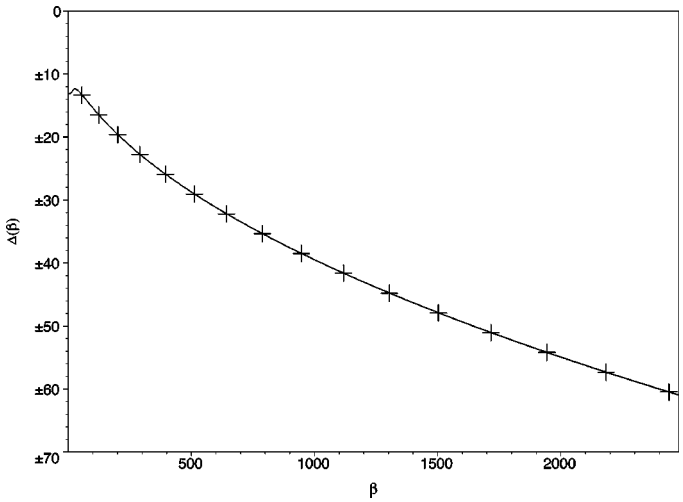

FIG. 19. $\Delta_{4,1}^{\mathrm{WKB}}$ and $\Delta_{4,1}^{\mathrm{Fr}}$.

and $w(z)=\sqrt{-(dz/d\zeta)}W(\zeta)$. Note that $\zeta\to-\infty$ corresponds to $z\to\infty$, $\zeta\to 0-$ to $z\to z_0+$, and $\zeta\to\infty$ to $z\to 1$. Equation (3) becomes

$$\frac{d^2}{d\zeta^2}W(\zeta)=[u^2\zeta+\psi(\zeta)]W(\zeta),$$
$$\psi(\zeta)=\frac{5}{16\zeta^2}-[4f(z)f''(z)-5f'(z)^2]\frac{\zeta}{16f(z)^3}-\frac{\zeta g(z)}{f(z)}. \tag{A1}$$

Approximate solutions of (3), i.e., solutions of (A1) with $\psi=0$, that are regular at $z=1$, are given by Olver (1974) (Sec. 11.3, Th. 3.1),

$$w(z)=\sqrt[4]{-\frac{\zeta}{f(z)}}[\mathrm{Ai}(u^{2/3}\zeta)+\epsilon(u,\zeta)], \tag{A2}$$

with

$$|\epsilon(u,\zeta)|\leqslant\frac{1}{\lambda}\frac{M(u^{2/3}\zeta)}{E(u^{2/3}\zeta)}[e^{(2\lambda/u)\mathcal{V}_{\zeta,\infty}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))}-1].$$

The constant λ and the function $\mathcal{B}_0$ are defined as follows:

$$\lambda:=\sup_x\left\{\pi|x|\frac{1}{2}M^2(x)\right\},$$

$$\mathcal{B}_0(\zeta):=\frac{1}{2\sqrt{|\zeta|}}\int_\zeta^\infty\frac{dv}{|v|^{1/2}}\psi(u,v),$$

and $\mathcal{V}$ is the variational operator, i.e.,

$$\mathcal{V}_{\zeta,\infty}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))=\frac{1}{2}\int_\zeta^\infty\frac{dv}{|v|^{1/2}}|\psi(u,v)|.$$

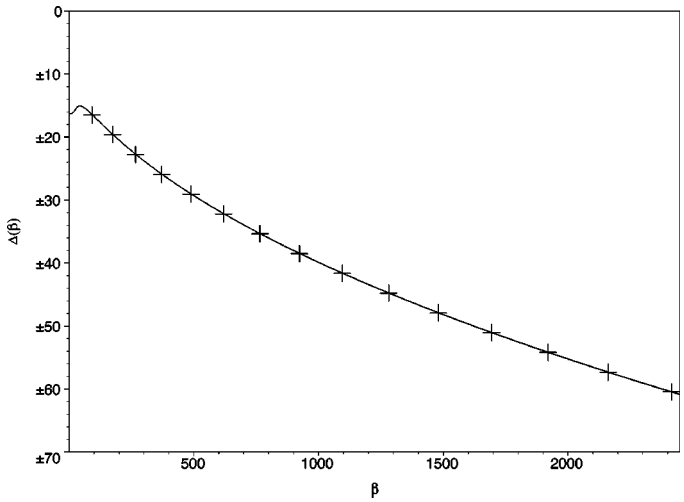

FIG. 20. $\Delta_{5,1}^{\mathrm{WKB}}$ and $\Delta_{5,1}^{\mathrm{Fr}}$.

Following the discussion in Olver (1974) (Sec. 13.7.2) we can determine the behavior for $z\to 1$ and $z\to\infty$,

$$A(z) \xrightarrow{z\to 1} \frac{\sqrt[4]{\beta}}{2\sqrt{\pi q}}(z-1)^{q/2},$$

$$A(z) \overset{z\to\infty}{\sim} \frac{1}{\sqrt{\pi}z^{3/4}}\sin\left(u\int_{z_0}^{z}\sqrt{f(t)}dt+\frac{\pi}{4}+\delta\right),$$

where we have used $\lim_{\zeta\to\infty}\epsilon(u,\zeta)=0$, and the phase δ is determined by $\lim_{\zeta\to\infty}\epsilon(u,\zeta)$. We know that the argument of the sin-function equals $2\sqrt{\beta z}+\Delta_{j,q}$ for large z, i.e.,

$$A(z) \overset{z\to\infty}{\sim} \frac{1}{\sqrt{\pi}z^{3/4}}\sin(2\sqrt{\beta z}+\Delta_{j,q}).$$

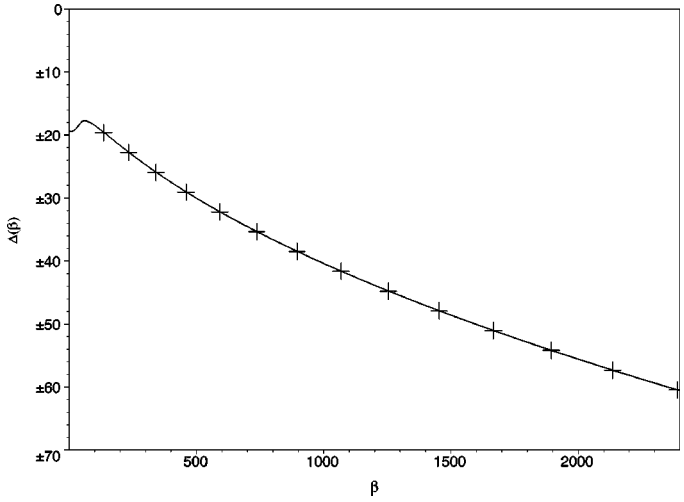

FIG. 21. $\Delta_{6,1}^{\mathrm{WKB}}$ and $\Delta_{6,1}^{\mathrm{Fr}}$.

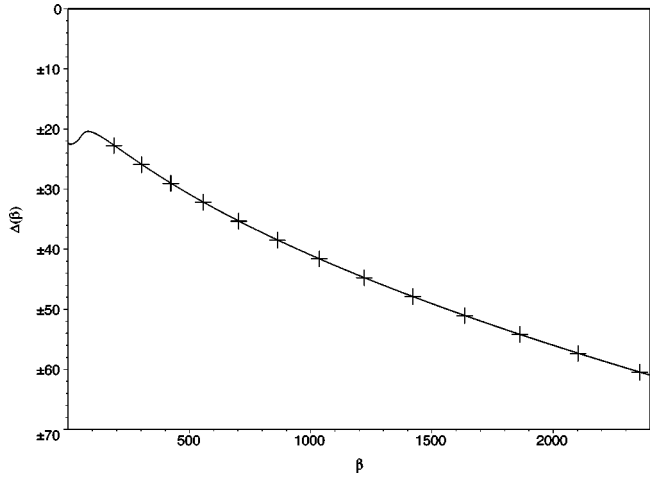

FIG. 22. $\Delta_{7,1}^{\mathrm{WKB}}$ and $\Delta_{7,1}^{\mathrm{Fr}}$.

Therefore, for the scattering phase we obtain

$$\Delta_{j,q} = u \lim_{z\to\infty}\left(\int_{z_0}^{z} \sqrt{f(t)}\,dt - 2\sqrt{z}\right) + \frac{\pi}{4} + \delta,$$

and with the help of Olver (1974) (Sec. 11.2) it follows that

$$\frac{2|\delta|}{\pi} \leqslant \min\left\{ 1, \frac{1}{\lambda}\left[e^{(2\lambda/u)\mathcal{V}_{-\infty,\infty}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))} - 1\right]\right\}. \tag{A3}$$

To resume, the solution (A2) can be considered as relation between the recessive solution and its asymptotic expansion. In this sense, the solution is a *connection formula* and it is known as the *Gans–Jeffreys* formula.

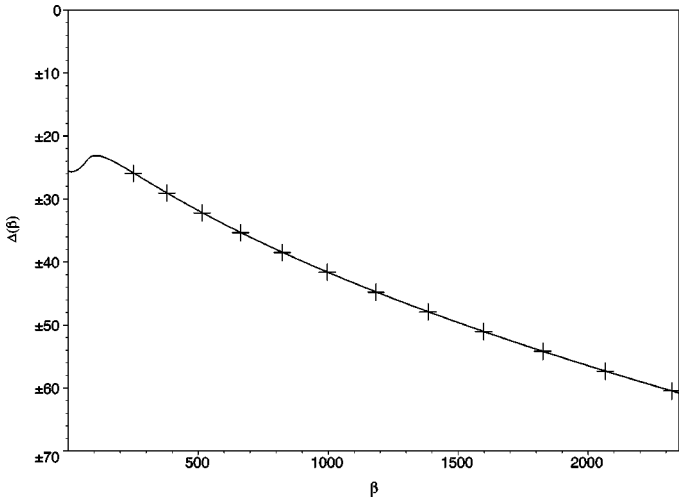

FIG. 23. $\Delta_{8,1}^{\mathrm{WKB}}$ and $\Delta_{8,1}^{\mathrm{Fr}}$.

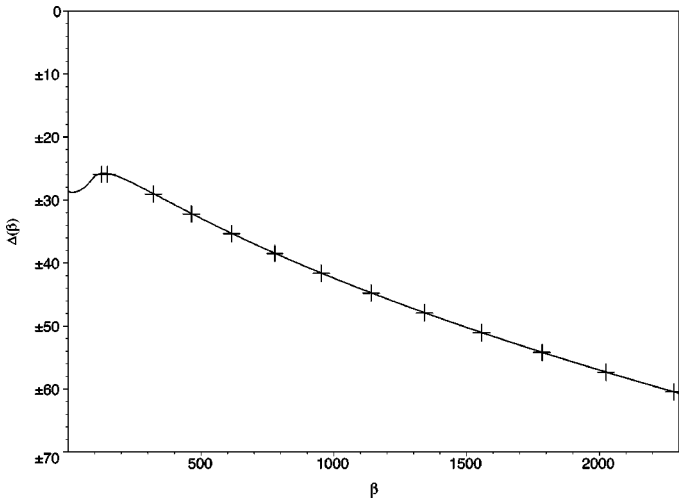

FIG. 24. $\Delta_{9,1}^{\mathrm{WKB}}$ and $\Delta_{9,1}^{\mathrm{Fr}}$.

2. Case II

In case II, $f(z)=(z-a)/(z^2-1)$, we can apply a result of Olver and Nestor that has been generalized in Dunster (1994). The Liouville transformation takes the form,

$$\int_{\alpha}^{\zeta}\left(\frac{\tau-\alpha}{\tau}\right)^{1/2}d\tau=\int_{a}^{z}dt\sqrt{f(t)}$$

with

$$\alpha:=\frac{2}{\pi}\int_{1}^{a}\sqrt{-f(t)}dt.$$

Therefore, we perform the transformation of the variable z and the function $w(z)$ to ζ, $W(\zeta)$ according to

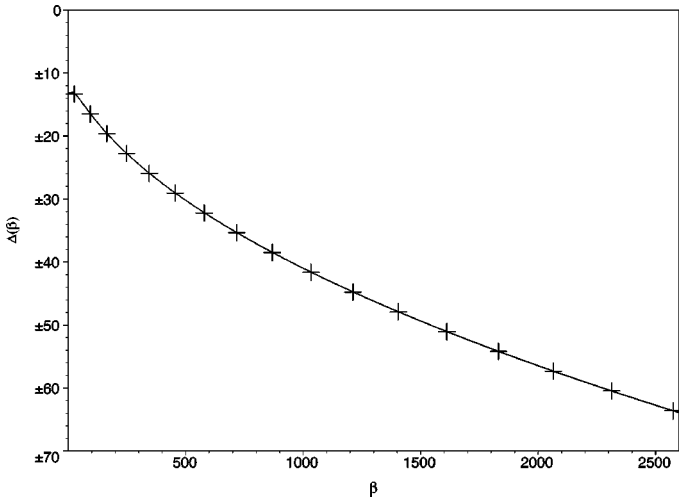

FIG. 25. $\Delta_{4,2}^{\mathrm{WKB}}$ and $\Delta_{4,2}^{\mathrm{Fr}}$.

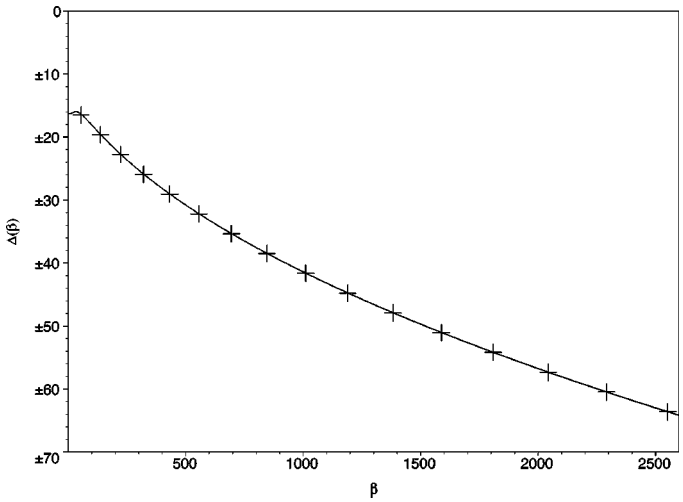

FIG. 26. $\Delta^{\mathrm{WKB}}_{5,2}$ and $\Delta^{\mathrm{Fr}}_{5,2}$.

$$\zeta^{1/2}(\zeta-\alpha)^{1/2}-\frac{\alpha}{2}\ln\left(\frac{2\zeta-\alpha+2\zeta^{1/2}(\zeta-\alpha)^{1/2}}{\alpha}\right)=\int_a^z\sqrt{f(t)}dt$$

and $w(z)=\sqrt{dz/d\zeta}W(\zeta)$. The integral can be expressed through an elliptic integral of the second kind;

$$\int_a^z\sqrt{f(t)}dt=2\sqrt{\frac{(z-a)(z+1)}{z-1}}-2\sqrt{1+a}\,\mathrm{E}\left[\arcsin\left(\sqrt{\frac{z-a}{z-1}}\right),\sqrt{\frac{2}{1+a}}\right].$$

Note that $\zeta\to\alpha$ corresponds to $z\to a$, $\zeta\to 0$ to $z\to 1$, where branches of ζ must be chosen such that it is an analytic function at both values. Moreover, $\zeta\to\infty$ corresponds to $z\to\infty$. Equation (3) becomes

$$\frac{d^2}{d\zeta^2}W(\zeta)=\left[u^2\frac{\alpha-\zeta}{\zeta}-\frac{1}{4\zeta^2}+\frac{\psi(\zeta)}{\zeta}\right]W(\zeta),$$

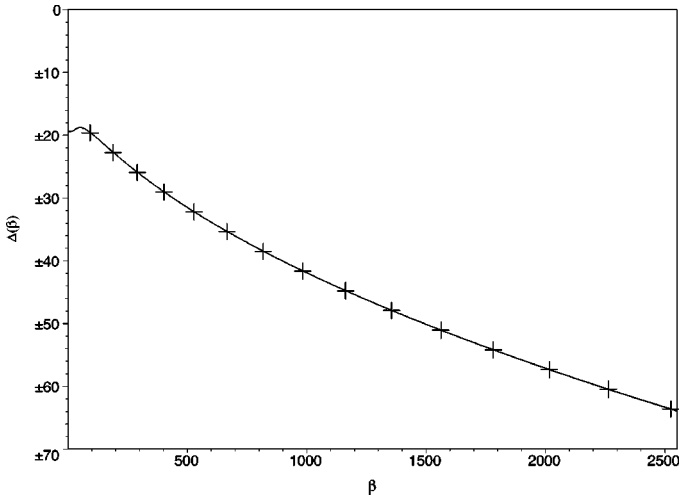

FIG. 27. $\Delta^{\mathrm{WKB}}_{6,2}$ and $\Delta^{\mathrm{Fr}}_{6,2}$.

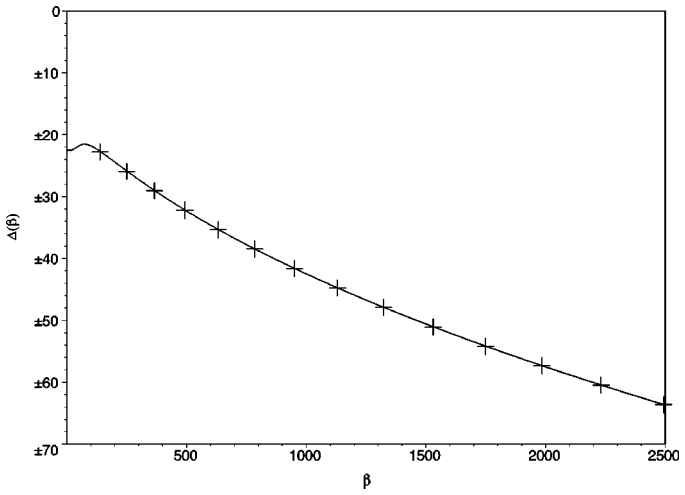

FIG. 28. $\Delta_{7,2}^{\mathrm{WKB}}$ and $\Delta_{7,2}^{\mathrm{Fr}}$.

$$\psi(\zeta)=\frac{4\zeta^2+\alpha^2}{16\zeta(\alpha-\zeta)^2}+[4f(z)f''(z)-5f'(z)^2]\frac{\zeta-\alpha}{16f(z)^3}+\frac{(\zeta-\alpha)g(z)}{f(z)}.$$

Approximate solutions of (3), i.e., solutions of (20) with $\psi=0$, that are regular at $z=1$, are given in Dunster (1994) (Chap. 2, case 1, $m=0$) in terms of the Whittaker function M, i.e.,

$$w(z)=\sqrt[4]{\frac{\zeta-\alpha}{\zeta f(z)}}\left[e^{-(i\pi/4)}\sqrt{\frac{2\pi}{1+e^{\pi u\alpha}}}\,\mathrm{M}_{iu\alpha/2,0}(2iu\zeta)+\epsilon(u,\zeta)\right] \tag{A4}$$

with

$$|\epsilon(u,\zeta)|\leqslant\frac{M^{(1)}_{u\alpha/2,0}(2u\zeta)}{E^{(0)}_{u\alpha/2,0}(2u\zeta)}[e^{\kappa_0(u\alpha/2+1)^{1/3}/2u\mathcal{V}_{\mathcal{P}^{(0)}}(F)}-1].$$

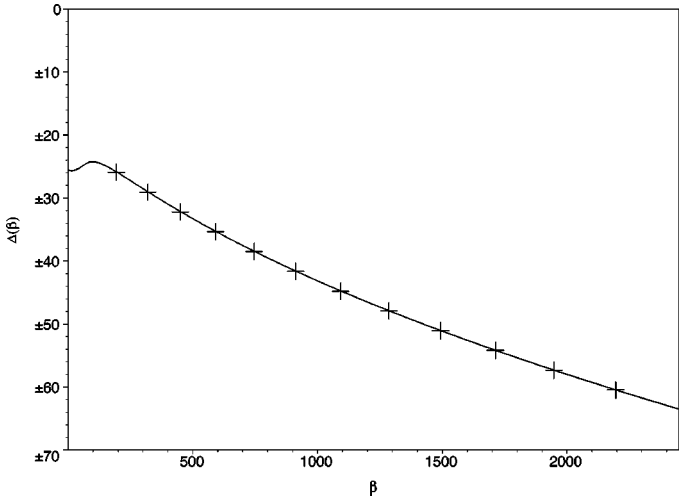

FIG. 29. $\Delta_{8,2}^{\mathrm{WKB}}$ and $\Delta_{8,2}^{\mathrm{Fr}}$.

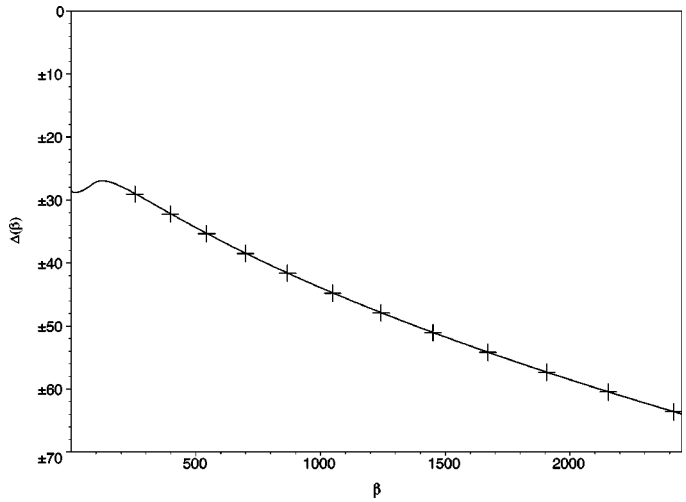

FIG. 30. $\Delta_{9,2}^{\mathrm{WKB}}$ and $\Delta_{9,2}^{\mathrm{Fr}}$.

For the error bound we have adopted the notation of Dunster (1994) (Chap. 2, Th. 1). Using formula (2.19) in Dunster (1994) we determine the behavior of the solution for $z\to 1$,

$$A(z) \xrightarrow{z\to 1} \sqrt{\frac{2\pi}{1+e^{\pi u\alpha}}}\sqrt[4]{\frac{2\alpha u^2}{a-1}}\left(\frac{\zeta}{z-1}\right)^{1/4},$$

where we have used $\lim_{\zeta\to 0}\epsilon(u,\zeta)=0$. A close examination of the Liouville transformation then shows that $\zeta/(z-1)\to(a-1)/(2\alpha)$ for $\zeta\to 0$ and $z\to 1$. Using Dunster (1994) [(2.16)–(2.18)] we obtain for $z\to\infty$,

$$A(z) \overset{z\to\infty}{\sim} \frac{2}{z^{3/4}}\sin\left(u\zeta-\frac{u\alpha}{2}\ln(2u\zeta)+\frac{\pi}{4}+\gamma+\delta\right),$$

where

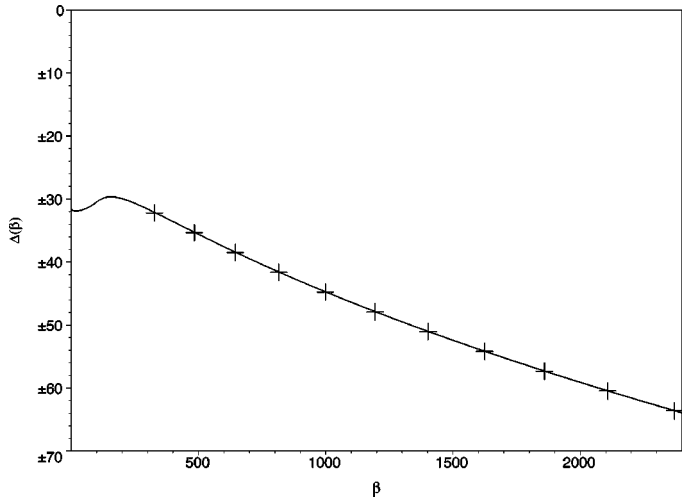

FIG. 31. $\Delta_{10,2}^{\mathrm{WKB}}$ and $\Delta_{10,2}^{\mathrm{Fr}}$.

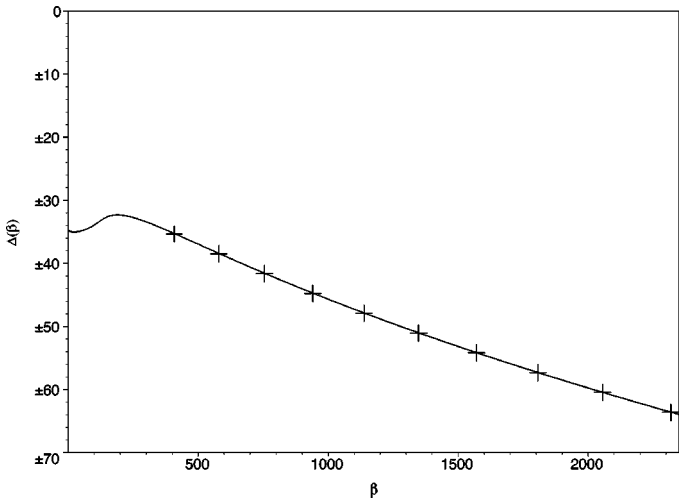

FIG. 32. $\Delta_{11,2}^{\mathrm{WKB}}$ and $\Delta_{11,2}^{\mathrm{Fr}}$.

$$\gamma = \arg\Gamma\left(\frac{1}{2}+\frac{iu\alpha}{2}\right)$$

and the phase δ is determined by $\lim_{\zeta\to\infty}\epsilon(u,\zeta)$. We know that the argument in the sin-function equals $2\sqrt{\beta z}+\Delta_{j,0}$ for large z, i.e.,

$$A(z) \overset{z\to\infty}{\sim} \frac{1}{z^{3/4}}\sin(2\sqrt{\beta z}+\Delta_{j,0}|_{a>1}).$$

A careful examination of the Liouville transformation reveals the following relation between large ζ and z,

$$\zeta-\frac{\alpha}{2}-\frac{\alpha}{2}\ln(\zeta)+\frac{\alpha}{2}\ln\left(\frac{\alpha}{4}\right)+O(\zeta^{-1})=2\sqrt{z}-2\sqrt{1+a}\,\mathrm{E}\left[\sqrt{\frac{2}{1+a}}\right]+O(z^{-(1/2)}).$$

Therefore, for the scattering phase we obtain

$$\begin{aligned}\Delta_{j,0}|_{a>1} &= u\lim_{z\to\infty}\left(\zeta-\frac{\alpha}{2}\ln(2u\zeta)-2\sqrt{z}\right)+\frac{\pi}{4}+\gamma+\delta\\ &= -2u\sqrt{1+a}\,\mathrm{E}\left[\sqrt{\frac{2}{1+a}}\right]+\frac{\alpha u}{2}-\frac{\alpha u}{2}\ln\left(\frac{\alpha u}{2}\right)+\frac{\pi}{4}+\gamma,\end{aligned}$$

$$\gamma = \arg\Gamma\left(\frac{1}{2}+\frac{iu\alpha}{2}\right), \tag{A5}$$

$$\frac{2|\delta|}{\pi} \leqslant \min\{1,[e^{\kappa_0(u\alpha/2+1)^{1/3}/2u\mathcal{V}_{\mathcal{P}^{(0)}}(F)}-1]\}.$$

The phase $\Delta_{j,0}|_{a>1}$ differs from the one obtained in Mignemi (1991).

3. Case III

In case III, the function f has neither a transition point nor a pole for $z \geqslant 1$. This case can be understood as the limit $a \to 1$ of case II, and applying further results of Olver's (1977), in this limit the Whittaker function will become the Bessel function J_0.

The idea is to perform the transformation of the variable z and the function $w(z)$ to ζ, $W(\zeta)$ according to

$$\zeta = \int_1^z \sqrt{f(t)}\,dt = 2\sqrt{z+1} - 2\sqrt{2}$$

and $w(z) = \sqrt{dz/d\zeta}\,W(\zeta)$. Note that $\zeta \to \infty$ corresponds to $z \to \infty$ and $\zeta \to 0$ to $z \to 1$. Equation (3) becomes

$$\begin{aligned} \frac{d^2}{d\zeta^2} W(\zeta) &= \left[-u^2 - \frac{1}{4\zeta^2} + \frac{\psi(\zeta)}{\zeta} \right] W(\zeta), \\ \psi(\zeta) &= \frac{1}{4\zeta} + [4f(z)f''(z) - 5f'(z)^2] \frac{\zeta}{16 f(z)^3} + \frac{\zeta g(z)}{f(z)}. \end{aligned} \tag{A6}$$

Approximate solutions of (3), i.e., solutions of (A6) with $\psi = 0$, that are regular at $z = 1$, are given by Olver (1977) (Chap. 5, Th. 2, case 2, $\nu = 0$, $\mu = 0$), i.e.,

$$w(z) = \frac{1}{\sqrt[4]{f(z)}} [\zeta^{1/2} \mathrm{J}_0(u\zeta) + \epsilon(u,\zeta)], \tag{A7}$$

with

$$|\epsilon(u,\zeta)| \leqslant \frac{l_{0,1}}{l_{0,0}} \frac{M_0(u\zeta)}{E_0(u\zeta)} [e^{l_{0,0} \mathcal{V}_{0,\zeta}(H)} - 1].$$

The constants $l_{0,0}$, $l_{0,1}$, and the function H are defined as follows:

$$l_{0,0} := \sup_x \{\pi \Omega_0(x) M_0^2(x)\},$$

$$l_{0,1} := \sup_x \{\pi \Omega_0(x) |J_0(x)| E_0(x) M_0(x)\},$$

$$H(u,\zeta) := \frac{1}{2} \int \frac{\psi(u,\zeta)}{\Omega_0(\zeta)}\,d\zeta,$$

$$\Omega_0(x) := \frac{1+x}{\ln\left(e + \frac{1}{x}\right)},$$

and $\mathcal{V}$ is the variational operator, i.e.,

$$\mathcal{V}_{0,\zeta}(H) = \frac{1}{2} \int_0^\zeta \frac{dv}{\Omega_0(uv)} |\psi(u,v)|.$$

We determine the behavior of the solutions for $z \to 1$ and $z \to \infty$,

$$A(z) \xrightarrow{z\to 1} \frac{1}{\sqrt{2}} J_0\left(u\,\frac{z-1}{\sqrt{2}}\right) \to \frac{1}{\sqrt{2}},$$

$$A(z) \overset{z\to\infty}{\sim} \frac{\sqrt{2}}{\sqrt{\pi u} z^{3/4}} \sin\left(u \int_1^z \sqrt{f(t)}\,dt + \frac{\pi}{4} + \delta\right),$$

where we have used $\lim_{\zeta\to 0+} \epsilon(u,\zeta)=0$, and the phase δ is determined by $\lim_{\zeta\to\infty} \epsilon(u,\zeta)$. We know that the argument of the sin-function equals $2\sqrt{\beta z}+\Delta_{j,0}|_{a=1}$ for large z, i.e.,

$$A(z) \overset{z\to\infty}{\sim} \frac{\sqrt{2}}{\sqrt{\pi u} z^{3/4}} \sin(2\sqrt{\beta z}+\Delta_{j,0}|_{a=1}).$$

Therefore, for the scattering phase we obtain

$$\Delta_{j,0}|_{a=1} = u \lim_{z\to\infty}\left(\int_1^z \sqrt{f(t)}\,dt - 2\sqrt{z}\right) + \frac{\pi}{4} + \delta = -\sqrt{8\beta} + \frac{\pi}{4} + \delta$$

and with the help of Olver (1977) (Chap. 5) and analogous to Appendix B the bound for ϵ in (A7) gives a bound for the phase δ. It follows that

$$\frac{2|\delta|}{\pi} \leqslant \min\left\{ 1, \frac{l_{0,1}}{l_{0,0}} [e^{l_{0,0}/u \mathcal{V}_{0,\infty}(H)} - 1]\right\}. \tag{A8}$$

The phase $\Delta_{j,0}$ differs from the one obtained in Mignemi (1991) by $\pi/4$.

4. Case IV

In case IV the function f has no transition point for $z \geqslant 1$ and takes the form $f(z)=(z-a)/(z^2-1)$. The idea is now to perform the transformation of the variable z and the function $w(z)$ to ζ, $W(\zeta)$ according to

$$(-\zeta)^{1/2} = \int_1^z \sqrt{f(t)}\,dt$$

and $w(z)=\sqrt{-(dz/d\zeta)}W(\zeta)$. The integral can be expressed through elliptic integrals of the first and second kind,

$$\int_1^z \sqrt{f(t)}\,dt = 2\sqrt{\frac{z^2-1}{z-a}} + (1-a)\sqrt{2}\,\mathrm{F}\left[\arcsin\left(\sqrt{\frac{z-1}{z-a}}\right), \sqrt{\frac{1+a}{2}}\right]$$
$$-2\sqrt{2}\,\mathrm{E}\left[\arcsin\left(\sqrt{\frac{z-1}{z-a}}\right), \sqrt{\frac{1+a}{2}}\right].$$

Note that $\zeta\to-\infty$ corresponds to $z\to\infty$ and $\zeta\to 0-$ to $z\to 1+$. Equation (3) becomes

$$\frac{d^2}{d\zeta^2} W(\zeta) = \left[\frac{u^2}{4\zeta} - \frac{1}{4\zeta^2} + \frac{\psi(\zeta)}{\zeta}\right] W(\zeta),$$
$$\psi(\zeta) = \frac{1}{16\zeta} - \frac{g(z)}{4f(z)} - \frac{4f(z)f''(z) - 5f'(z)^2}{64 f(z)^3}. \tag{A9}$$

Approximate solutions of (3), i.e., solutions of (A9) with $\psi=0$, that are regular at $z=1$, are then given by Olver (1974) (Sec. 12.4, Th. 4.1, $\nu=0$, $n=0$), i.e.,

$$\omega(z)=\frac{1}{\sqrt[4]{4|\zeta|f(z)}}[|\zeta|^{1/2}J_0(u|\zeta|^{1/2})+\epsilon(u,\zeta)] \tag{A10}$$

with

$$|\epsilon(u,\zeta)|\leqslant\frac{\lambda_{0,1}}{\lambda_{0,0}}|\zeta|^{1/2}\frac{M_0(u\zeta)}{E_0(u\zeta)}[e^{\lambda_{0,0}/u\mathcal{V}_{\zeta,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))}-1].$$

The bound for the error ϵ is derived in Appendix B. The constants $\lambda_{0,0},\lambda_{0,1}$, as well as the function $\mathcal{B}_0$ are defined as follows:

$$\lambda_{0,0}:=\sup_{x\geqslant 0}\{\pi x M_0^2(x)\},$$

$$\lambda_{0,1}:=\sup_{x\geqslant 0}\{\pi x M_0^2(x),\cos\theta_0(x)\},$$

$$\mathcal{B}_0(\zeta):=\frac{1}{|\zeta|^{1/2}}\int_\zeta^0\frac{dv}{|v|^{1/2}}\psi(v),$$

and $\mathcal{V}$ is the variational operator, i.e.,

$$\mathcal{V}_{\zeta,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))=\int_\zeta^0\frac{dv}{|v|^{1/2}}|\psi(v)|,$$

We determine the behavior of the solutions for $z\to 1$ and $z\to\infty$,

$$A(z)\xrightarrow{z\to 1}\frac{1}{\sqrt{2}}J_0(u\sqrt{2(1-a)}\sqrt{z-1})\to\frac{1}{\sqrt{2}},$$

$$A(z)\overset{z\to\infty}{\sim}\frac{1}{\sqrt{\pi u}z^{3/4}}\sin\left(u\int_1^z\sqrt{f(t)}dt+\frac{\pi}{4}+\delta\right),$$

where we have used that $\lim_{\zeta\to 0-}\epsilon(u,\zeta)=0$ and the phase δ is determined by $\lim_{\zeta\to-\infty}\epsilon(u,\zeta)$. We know that the argument of the sin-function equals $2\sqrt{\beta z}+\Delta_{j,0}$ for large z, i.e.,

$$A(z)\sim\frac{1}{\sqrt{\pi u}z^{3/4}}\sin(2\sqrt{\beta z}+\Delta_{j,0}).$$

Therefore, we obtain for the scattering phase,

$$\begin{aligned}\Delta_{j,0}|_{a<1}&=u\lim_{z\to\infty}\left(\int_1^z\sqrt{f(t)}dt-2\sqrt{z}\right)+\frac{\pi}{4}+\delta\\&=(1-a)\sqrt{2\beta}\,\mathrm{K}\left[\sqrt{\frac{1+a}{2}}\right]-2\sqrt{2\beta}\,\mathrm{E}\left[\sqrt{\frac{1+a}{2}}\right]+\frac{\pi}{4}+\delta.\end{aligned}$$

In addition, we will derive in Appendix B,

$$\frac{2|\delta|}{\pi} \leqslant \min\left\{1, \frac{\lambda_{0,1}}{\lambda_{0,0}}\left[e^{(\lambda_{0,0}/u)\mathcal{V}_{-\infty,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))} - 1\right]\right\}. \tag{A11}$$

The phase $\Delta_{j,0}|_{a<1}$ differs from the one obtained in Mignemi (1991) by $\pi/4$ and the factor in front of the elliptic integral of the first kind.

APPENDIX B: ERROR BOUNDS

In this Appendix we apply the construction of error bounds presented in Olver (1974) (Sec. 11.3) to case IV [cf. Olver (1974) (Sec. 12.4, Ex. 4.4)]. In case IV the Bessel functions $|\zeta|^{1/2}\mathrm{J}_0(u|\zeta|^{1/2})$ and $|\zeta|^{1/2}\mathrm{Y}_0(u|\zeta|^{1/2})$ of the first and second type, are first approximations for W. They are exact solutions if $\psi \equiv 0$. Substituting $W(\zeta) = |\zeta|^{1/2}\mathrm{J}_0(u|\zeta|^{1/2}) + \epsilon(u,\zeta)$, the differential equation becomes

$$\frac{d^2}{d\zeta^2}\epsilon(u,\zeta) - \left[\frac{u^2}{4\zeta} - \frac{1}{4\zeta^2}\right]\epsilon(u,\zeta) = \frac{\psi(\zeta)}{\zeta}\left[\epsilon(u,\zeta) + |\zeta|^{1/2}\mathrm{J}_0(u|\zeta|^{1/2})\right].$$

If we rewrite it as an integral equation we obtain a Volterra integral equation,

$$\epsilon(u,\zeta) = \int_{\zeta}^{0} \mathrm{K}(\zeta,v)\frac{\psi(v)}{|v|^{1/2}}\left[\epsilon(v) + |v|^{1/2}\mathrm{J}_0(u|v|^{1/2})\right]dv,$$

where

$$\mathrm{K}(\zeta,v) = \pi|v|^{1/2}\left[\mathrm{J}_0(u|\zeta|^{1/2})\mathrm{Y}_0(u|v|^{1/2}) - \mathrm{Y}_0(u|\zeta|^{1/2})\mathrm{J}_0(u|v|^{1/2})\right].$$

Using the fact that E_0 is a nonincreasing function we obtain

$$\forall\, \zeta \leqslant v \leqslant 0: \quad |\mathrm{K}(\zeta,v)| \leqslant \underbrace{\frac{M_0(u|\zeta|^{1/2})}{E_0(u|\zeta|^{1/2})}}_{=:P_0(\zeta)} \underbrace{\pi|v|^{1/2}M_0(u|v|^{1/2})E_0(u|v|^{1/2})}_{=:Q(v)}.$$

We introduce the parameters κ_0, κ by

$$\kappa_0 := \sup_{v\in[\zeta,0]}\{P_0(v)Q(v)\} \leqslant \frac{\lambda_{0,0}}{u},$$

$$\kappa := \sup_{v\in[\zeta,0]}\{Q(v)||v|^{1/2}\mathrm{J}_0(u|v|^{1/2})|\} \leqslant \frac{|\zeta|^{1/2}\lambda_{0,1}}{u}.$$

With the help of Olver (1974) (Sec. 6.10, Th. 10.2) which establishes a bound for the solution of a Volterra integral equation we end up with a bound for ϵ,

$$\frac{|\epsilon(u,\zeta)|}{P_0(\zeta)} \leqslant \frac{\kappa}{\kappa_0}\left[\exp\{\kappa_0\mathcal{V}_{\zeta,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))\} - 1\right] \leqslant |\zeta|^{1/2}\frac{\lambda_{0,1}}{\lambda_{0,0}}\left[\exp\left\{\frac{\lambda_{0,0}}{u}\mathcal{V}_{\zeta,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))\right\} - 1\right]. \tag{B1}$$

We are interested in an error bound for the phase in the asymptotic expansion of the solution. Assume that the solution W takes the following form for large arguments ζ:

$$W(u,\zeta) \overset{\zeta\to\infty}{\sim} \left(\frac{2|\zeta|^{1/2}}{\pi u}\right)^{1/2}\left((1+\rho)\sin\left(u|\zeta|^{1/2} + \frac{\pi}{4} + \delta\right) + o(1)\right).$$

As in Olver (1974) (Sec. 6.7) we rewrite the difference of the exact and the approximate solution as a trigonometric function,

$$\epsilon(u,\zeta)=W(u,\zeta)-|\zeta|^{1/2}\mathrm{J}_0(u|\zeta|^{1/2})$$

$$\overset{\zeta\to\infty}{\sim}\left(\frac{2|\zeta|^{1/2}}{\pi u}\right)^{1/2}\left\{[1+\rho]\sin\left(u|\zeta|^{1/2}+\frac{\pi}{4}+\delta\right)-\sin\left(u|\zeta|^{1/2}+\frac{\pi}{4}\right)\right\}$$

$$=\left(\frac{2|\zeta|^{1/2}}{\pi u}\right)^{1/2}\sigma\sin\left(u|\zeta|^{1/2}+\frac{\pi}{4}+\eta\right),$$

where the new parameters σ (always considered to be positive) and η are related to ρ and δ by

$$(1+\rho)e^{i\delta}=1+\sigma e^{i\eta}.$$

By elementary geometry it follows that $2|\delta|/\pi\leqslant\sigma$. Then, the bound for ϵ in (B1) gives a bound for σ. Now, we choose a sequence (ζ_n) with $\lim_{n\to\infty}\zeta_n=-\infty$ for which $u|\zeta|^{1/2}+(\pi/4)+\eta$ is an odd integer multiple of $\pi/2$. This shows that

$$\sigma_{\zeta\to-\infty}=\lim_{\zeta\to-\infty}\left(\frac{\pi u}{2|\zeta|^{1/2}}\right)^{1/2}|\epsilon(u,\zeta)|.$$

Finally, since

$$M_0(x)\overset{x\to\infty}{\sim}\left(\frac{2}{\pi x}\right)^{1/2},$$

$$E_0(x)\overset{x\to\infty}{=}1,$$

we obtain a bound for δ,

$$\frac{2|\delta|}{\pi}\leqslant\min\left\{1,\frac{\lambda_{0,1}}{\lambda_{0,0}}[e^{(\lambda_{0,0}/u)\mathcal{V}_{-\infty,0}(|\zeta|^{1/2}\mathcal{B}_0(\zeta))}-1]\right\}.$$

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Berezin transform on the quantum unit ball

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(Received 27 November 2002; accepted 21 April 2003)

We introduce and study, in the framework of a theory of quantum Cartan domains, a q-analog of the Berezin transform on the unit ball. We construct q-analogs of weighted Bergman spaces, Toeplitz operators, and covariant symbol calculus. In studying the analytical properties of the Berezin transform we introduce also the q-analog of the SU(n,1)-invariant Laplace operator (the Laplace–Beltrami operator) and present related results on harmonic analysis on the quantum ball. These are applied to obtain an analog of one result by A. Unterberger and H. Upmeier. An explicit asymptotic formula expressing the q-Berezin transform via the q-Laplace–Beltrami operator is also derived. At the end of the article, we give an application of our results to basic hypergeometric q-orthogonal polynomials.
 [DOI: 10.1063/1.1593226]

I. INTRODUCTION

Since the appearance of quantum groups in the middle of the 1980s there have been different attempts to find an appropriate generalization to the q-case of various classical constructions in the analysis and geometry of Lie groups. Recently, it became clear[1] that there should exist a substantial q-analog of the theory of Cartan domains (the most studied class of such domains constitutes the so-called classical domains[2]). In turn, this observation has opened a way to generalization of other important theories about those domains. One of the most fascinating among them is the Berezin quantization.[3] Though Berezin applied his construction to a wide class of Kähler manifolds, the most complete and precise results have been obtained just in the particular case of Cartan domains.[4,5]

It should be noted that first attempts to find q-analogs of some constructions of the Berezin theory were made before the study of q-Cartan domains was initiated. For example, in Ref. 6 the authors studied a two-parameter deformation $\mathcal{P}_{q,\lambda}$ of the polynomial algebra $\mathbb{C}[z,\bar{z}]$ related to certain SU(1,1)-covariant Poisson brackets on the unit disk. They showed, among other things, that for any λ the algebra $\mathcal{P}_{q,\lambda}$ is acted upon by the quantum universal enveloping algebra $U_q\mathfrak{sl}_2$. Also, for each q the authors defined q-analogs of the weighted Bergman spaces $L^2_a((1-|z|^2)^\lambda d\bar{z}dz)$ ($\lambda \geqslant 0$) on the unit disk and showed that $\mathcal{P}_{q,\lambda}$ could be realized as the algebra of Toeplitz operators (with symbols from $\mathcal{P}_{q,0}$) on the q-weighted Bergman space corresponding to λ. This observation suggests that it is reasonable to regard $\mathcal{P}_{q,0}$ as a genuine function algebra on the *quantum* unit disk and $\mathcal{P}_{q,\lambda}$ as a result of the Toeplitz quantization of $\mathcal{P}_{q,0}$ which, in addition, respects the $U_q\mathfrak{sl}_2$-actions in complete analogy with the classical setting.

This point of view was developed in detail in Ref. 7. There, in addition to the results of Ref. 6, q-analogs of covariant symbols and of the Berezin transform on the quantum unit disk were produced (see Ref. 8 for a concise account). Also, in Ref. 7 an explicit asymptotic formula, expressing the q-Berezin transform via a q-Laplace–Beltrami operator on the quantum disk, was

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derived. This allowed the authors to produce an analog of the Berezin star product and thus to obtain a formal deformation of the algebra $\mathcal{P}_{q,0}$.

The present article continues the study of the q-Berezin transform initiated in Ref. 7. Here we investigate the case of the quantum unit ball, whose one-dimensional version is the aforementioned quantum unit disk, and generalize to this case almost all constructions of Ref. 7. Namely, we produce analogs of the weighted Bergman spaces, Toeplitz operators, covariant symbols, and the Berezin transform on the unit ball. Also, we define a q-analog of the SU(n,1)-invariant Laplace operator (the Laplace–Beltrami operator) and derive an explicit asymptotic formula expressing the q-Berezin transform via the q-Laplace–Beltrami operator.

It is appropriate to mention here that in the case of the quantum unit ball we encounter a new phenomenon imperceptible in the case of the quantum unit disk. Namely, there is not any satisfactory analog of coherent states on the ball which are used to define covariant symbols of operators and regarded as a basic ingredient of the Berezin's theory. An appropriate analog for the quantum unit disk was found in Ref. 7. However, that was possible due to commutativity of the algebra of ''holomorphic functions'' on the quantum disk, but the commutativity fails in the case of the quantum ball. Fortunately, even in the classical setting there is an alternative way to define covariant symbols. Namely, the map

$$\begin{array}{c}\text{operator on a}\\ \text{weighted Bergman space}\end{array} \mapsto \begin{array}{c}\text{covariant symbol,}\\ \text{a function on the ball}\end{array}$$

is, roughly speaking, the adjoint of the map

$$\begin{array}{c}\text{function}\\ \text{on the ball}\end{array} \mapsto \begin{array}{c}\text{Toeplitz operator on a}\\ \text{weighted Bergman space}\end{array}$$

with respect to certain SU(n,1)-invariant inner products in the spaces of functions and operators (see Ref. 5). The significance of the Toeplitz and covariant calculi is of course well known and has been intensively studied. We exploit just this idea to define covariant symbols and thus the Berezin transform in the q-setting.

Let us turn now to description of the contents of the article.

Our results rely heavily on function theory in the quantum unit ball. In Sec. II we recall the basic setup and results from that theory obtained earlier by L. Vaksman and his group[9,10] in the more general setting of quantum *matrix* balls. In brief, we define an involutive algebra of ''polynomials'' on the quantum $\mathbb{C}^n$ which generalize the algebra $\mathcal{P}_{q,0}$ mentioned above. The algebra is endowed with an action of the quantum universal enveloping algebra $U_q\mathfrak{su}_{n,1}$. This is a counterpart of the classical SU(n,1)-action on the unit ball. Using the polynomial algebra, we produce the spaces of ''finite functions'' and ''distributions'' on the quantum ball which inherit the $U_q\mathfrak{su}_{n,1}$-action. The crucial property, which justifies our definition of the space of finite functions on the quantum ball, is the existence of a $U_q\mathfrak{su}_{n,1}$-invariant integral on that space, an analog of the integral with respect to the SU(n,1)-invariant measure on the ball. We present an explicit formula for that integral. We note that the existence of the integral allows one to formulate many problems of harmonic analysis on the quantum ball. Though the present article does not deal with harmonic analysis, we develop some partial results (see description of Sec. IV below) which are needed to put our result in a coherent and rigorous mathematics context.

Section III is devoted to find an appropriate algebraic and analytical setting. There we start developing of the q-Berezin's theory and present all necessary definitions. First, we define analogs of the weighted Bergman spaces in the ball and produce the notion of Toeplitz operators with polynomial or finite symbols. Though the finite symbols are of more importance for our exposition, we devote a separate subsection to the study of the algebra of Toeplitz operators with polynomial symbols. This is motivated by the observation that this algebra is a multivariable generalization of the algebra $\mathcal{P}_{q,\lambda}$ studied in Ref. 6. Results of Ref. 6 suggest that the algebra of Toeplitz operators with polynomial symbols might be interesting from the point of view of the theory of operator algebras. In the last subsection we present definitions of covariant symbols and

of the q-Berezin transform. Thus, in Sec. III we define three important maps: the map that sends a function to the corresponding Toeplitz operator, the map that sends an operator to its covariant symbol (a function on the quantum ball), and, finally, their composition—the q-Berezin transform—which sends a function to the covariant symbol of the corresponding Toeplitz operator. We observe also that the three maps intertwine natural $U_q\mathfrak{su}_{n,1}$-actions on the spaces of functions and operators. This quantum group symmetry of the q-Berezin transform simplifies drastically many computations in subsequent sections.

To investigate the q-Berezin transform further, for instance, to find its asymptotic expansion, we need some results on harmonic analysis, particularly on q-spherical transform in the quantum ball. These are presented in Sec. IV. First of all, we define there an analog of the Laplace–Beltrami operator on the ball. At first sight, our definition seems to be somewhat unusual: the q-Laplace–Beltrami operator appears as the first term in the asymptotic expansion of the q-Berezin transform. However, this agrees with the classical Berezin's theory. Besides, we believe that results of Sec. IV provide a sufficient evidence of rationality of such a definition. In particular, a ''radial part'' of our q-Laplace–Beltrami operator turns out to be a second order difference operator which tends to the radial part of the classical Laplace–Beltrami operator as q approaches 1. Moreover, the difference operator turned out to be quite well studied by experts in the theory of q-special functions (see, for instance, Ref. 11). In particular, the problem of expansion in eigenfunctions of that difference operator had been already solved, and we recall explicit formulas in the text. In view of our approach, those eigenfunctions should be regarded as analogs of the spherical functions on the ball while the expansion is an analog of the spherical transform (see Ref. 12). Moreover, the Plancherel measure, which appears in the inverse transform, involves an analog of the Harish–Chandra c-function for the ball.

After we present the results on the q-spherical transform, we turn back in Sec. V to the study of the q-Berezin transform. In the first subsection of Sec. V we consider its ''radial part.'' We prove that the radial part of the transform is extended to a bounded self-adjoint operator on the space of square-integrable radial function on the quantum ball (we mean square-integrability with respect to the invariant q-integral). Moreover, the resulting operator commutes with the radial part of the q-Laplace–Beltrami operator which is also a bounded self-adjoint operator on the same space. Since the latter operator has simple spectrum (this is stated in Sec. IV), the radial part of the q-Berezin transform appears to be a function of the radial part of the q-Laplace–Beltrami operator. We found the function explicitly. We note that in the classical case the corresponding result was obtained in Ref. 5 for any Cartan domain. This computation has a number of consequences, some of which we use further in Sec. VI. In the last subsection of Sec. V, we present an asymptotic formula expressing the q-Berezin transform via the q-Laplace–Beltrami operator.

Section VI is meant for those readers who are interested in various mathematical applications of the Berezin transform. It is, however, nevertheless related to quantization. In the theory of Wick quantization one associates to each function an operator so that the one-dimensional projections onto the coherent state at a point (in the phase space) are assigned to the delta function. However, if the given Hilbert space has an orthogonal basis, the projections onto the basis vectors are also natural subjects so it is interesting to compute their covariant symbols. Here in our setting we show that the spherical transforms of those covariant symbols are, roughly speaking, hypergeometric orthogonal q-polynomials. We derive orthogonality relations for those orthogonal polynomials, the so-called continuous dual q-Hahn polynomials.[13] The entire family of these polynomials depends on three parameters (not counting q) while we treat a two-parameter subfamily which appears naturally in connection with the q-Berezin transform. The idea we use appeared for the first time in Ref. 14 in the classical setting (see also Ref. 15).

Let us make some comments about the most important agreements and notations used in the article. First of all, the quantum-group parameter q is supposed to be a number from the interval (0,1). Next, we put $h:=\log q^{-2}$, so $h>0$; $t:=q^{2\alpha}$ will be the deformation parameter in the Berezin transform. Finally, we describe some convenient multi-index notations. We denote multi-indices by underlined small letters, the zero multi-index by $\underline{0}$. For $\underline{i}=(i_1,\ldots,i_n)$, $\underline{j}=(j_1,\ldots,j_n)$ we put

$|\underline{i}|=i_1+i_2+\cdots+i_n$ and $\underline{i}\times\underline{j}=(i_1\cdot j_1,\ldots,i_n\cdot j_n)$. For noncommuting variables $z_1,z_2,\ldots,z_n$ and $z_1^*,z_2^*,\ldots,z_n^*$ we set

$$\mathbf{z}^{\underline{i}}:=z_n^{i_n}\cdot z_{n-1}^{i_{n-1}}\cdot\ \cdots\ \cdot z_1^{i_1},\quad \mathbf{z}^{*\underline{i}}:=z_1^{*i_1}\cdot\ \cdots\ \cdot z_{n-1}^{*i_{n-1}}\cdot z_n^{*i_n}.$$

Finally, we denote $P(n)=\{\underline{k}\in\mathbb{Z}^n_{\geqslant 0}\ \mid\ k_1\geqslant k_2\geqslant\cdots\geqslant k_n\}$.

II. BASICS OF FUNCTION THEORY IN THE QUANTUM UNIT BALL

The aim of Sec. II is to introduce some notions of function theory in the quantum ball. We define the involutive algebra of finite functions and the space of distributions on the q-ball. These spaces admit actions of certain quantum universal enveloping algebra. Finally, we produce an explicit formula for the invariant integral on the space of finite functions. The material presented in this section is not new: the quantum ball treated here is a particular case of the quantum *matrix* ball considered in details in Refs. 9 and 10. Most results can be found in those papers, however, we reformulate some of them for our particular purpose.

A. Polynomials on the quantum $\mathbb{C}^n$

An initial object in constructing function theory in the quantum ball is the unital involutive algebra given by its generators $z_1,z_2,\ldots,z_n$ and the relations

$$z_iz_j=qz_jz_i,\quad i<j, \tag{2.1}$$

$$z_i^*z_j=qz_jz_i^*,\quad i\neq j, \tag{2.2}$$

$$z_j^*z_j=q^2z_jz_j^*+(1-q^2)\left(1-\sum_{k=j+1}^{n}z_kz_k^*\right). \tag{2.3}$$

We denote this algebra by $\mathcal{P}(\mathbb{C}^n)_q$ and treat it as the polynomial algebra on the quantum $\mathbb{C}^n$. The algebra $\mathcal{P}(\mathbb{C}^n)_q$ is a particular case of the algebra $\mathrm{Pol}(\mathrm{Mat}_{m,n})_q$ of polynomials on the quantum space of $m\times n$ matrices considered in Refs. 9 and 10. Specifically, $\mathcal{P}(\mathbb{C}^n)_q$ coincides with $\mathrm{Pol}(\mathrm{Mat}_{1,n})_q$. [Moreover, it is not hard to show that $\mathcal{P}(\mathbb{C}^n)_q$ is isomorphic to the known twisted CCR-algebra.[16]]

In the sequel we use the algebra $\mathcal{P}(\mathbb{C}^n)_q$ to produce some ''functional'' spaces and algebras on the quantum ball. Those spaces, as well as the algebra $\mathcal{P}(\mathbb{C}^n)_q$ itself, are endowed with structures of $U_q\mathfrak{su}_{n,1}$-modules where $U_q\mathfrak{su}_{n,1}$ is certain $*$-Hopf algebra called the quantized universal enveloping algebra for $\mathfrak{su}_{n,1}$. Let us turn to precise definitions.

We recall first the definition of $U_q\mathfrak{su}_{n,1}$. It is a ''real form'' of the Drinfeld–Jimbo quantum universal enveloping algebra $U_q\mathfrak{sl}_{n+1}$. The latter algebra is the unital algebra given by the generators $E_i,F_i,K_i^{\pm 1}$, $i=1,2,\ldots,n$, and the following relations:

$$K_iK_j=K_jK_i,\ \ K_iK_i^{-1}=K_i^{-1}K_i=1,\ \ K_iE_j=q^{a_{ij}}E_jK_i,$$

$$K_iF_j=q^{-a_{ij}}F_jK_i,\quad E_iF_j-F_jE_i=\delta_{ij}(K_i-K_i^{-1})/(q-q^{-1}),$$

$$E_i^2E_j-(q+q^{-1})E_iE_jE_i+E_jE_i^2=0,\quad |i-j|=1,$$

$$F_i^2F_j-(q+q^{-1})F_iF_jF_i+F_jF_i^2=0,\quad |i-j|=1,$$

$$[E_i,E_j]=[F_i,F_j]=0,\quad |i-j|\neq 1,$$

with (a_{ij}) being the Cartan matrix of type A_n. Moreover, $U_q\mathfrak{sl}_{n+1}$ is a Hopf algebra. The comultiplication Δ, the antipode S, and the counit ε are determined by

$$\Delta(E_i)=E_i\otimes 1+K_i\otimes E_i,\quad \Delta(F_i)=F_i\otimes K_i^{-1}+1\otimes F_i,\quad \Delta(K_i)=K_i\otimes K_i,$$

$$S(E_i)=-K_i^{-1}E_i,\quad S(F_i)=-F_iK_i,\quad S(K_i)=K_i^{-1},$$

$$\varepsilon(E_i)=\varepsilon(F_i)=0,\quad \varepsilon(K_i)=1.$$

The quantum universal enveloping algebra $U_q\mathfrak{su}_{n,1}$ is defined as the $*$-Hopf algebra $(U_q\mathfrak{sl}_{n+1},*)$ with $*$ being the involution in $U_q\mathfrak{sl}_{n+1}$ given by

$$E_n^*=-K_nF_n,\quad F_n^*=-E_nK_n^{-1},\quad (K_n^{\pm 1})^*=K_n^{\pm 1},$$

$$E_j^*=K_jF_j,\quad F_j^*=E_jK_j^{-1},\quad (K_j^{\pm 1})^*=K_j^{\pm 1},\quad \text{for}\quad j\neq n$$

(see Ref. 17 for basic definitions concerning $*$-Hopf algebras).

We need also the notion of $U_q\mathfrak{su}_{n,1}$-module algebra. Let A be a Hopf algebra. An algebra F is said to be an A-module algebra if F carries a structure of A-module and multiplication in F agrees with the A-action, i.e., the multiplication $F\otimes F\to F$ is a morphism of A-modules. (We recall that for any A-modules V_1, V_2 their tensor product is endowed with an A-module structure via the comultiplication $\Delta:A\to A\otimes A$.) If A or F has some extra structures this definition includes natural additional requirements. For example, in the case of a unital algebra F one adds the requirement of A-invariance of the unit: $\xi(1)=\varepsilon(\xi)\cdot 1$, $\xi\in A$. In the case of an involutive algebra F and a $*$-Hopf algebra A one imposes the requirement of agreement of the involutions:

$$(\xi(f))^*=S(\xi)^*(f^*),\quad \xi\in A, f\in F. \tag{2.4}$$

Some natural examples of module algebras appear in the classical setting. Suppose X is a smooth G-space with G being a Lie group. The G-action induces an action of the universal enveloping algebra $U\mathfrak{g}$ in the space $C^\infty(X)$ via differential operators. The usual Leibnitz rule for the differentiation of product of two functions means that $C^\infty(X)$ is a $U\mathfrak{g}$-module algebra. This example suggests the use of the language of module algebras for description of algebras of functions on *quantum* G-spaces.

The structure of $U_q\mathfrak{su}_{n,1}$-module algebra in $\mathcal{P}(\mathbb{C}^n)_q$ which we are going to present has the following classical counterpart. The unit ball $U_n=\{\mathbf{z}\in\mathbb{C}^n|\|\mathbf{z}\|<1\}$ is a homogeneous space of the group SU$(n,1)$ whose elements act via (biholomorphic) linear-fractional transformations. Elements of the universal enveloping algebra $U\mathfrak{su}_{n,1}$ act on the space $C^\infty(U_n)$ via differential operators with polynomial coefficients and thus keep the subspace of polynomials invariant. This induces a $U\mathfrak{su}_{n,1}$-module algebra structure in the polynomial algebra on $\mathbb{C}^n$. We turn now to the quantum case.

To describe the $U_q\mathfrak{su}_{n,1}$-module algebra structure in $\mathcal{P}(\mathbb{C}^n)_q$ we consider the action of the elements $E_i,F_i,K_i^{\pm 1}$ on the generators z_i,z_i^*. Moreover, by (2.4) it is sufficient to present formulas for the action of $E_i,F_i,K_i^{\pm 1}$ on the "holomorphic" part $z_1,\ldots,z_n$ of generators of $\mathcal{P}(\mathbb{C}^n)_q$. These are given in the following:

Proposition 2.1: There exists a unique structure of $U_q\mathfrak{su}_{n,1}$-module algebra in $\mathcal{P}(\mathbb{C}^n)_q$ such that, for $k\neq n$,

$$K_kz_i=\begin{cases} qz_i, & i=k,\\ q^{-1}z_i, & i=k+1,\\ z_i, & \text{otherwise,}\end{cases} \tag{2.5}$$

$$F_kz_i=q^{1/2}\cdot\begin{cases} z_{i+1}, & i=k,\\ 0, & \text{otherwise,}\end{cases} \tag{2.6}$$

$$E_k z_i = q^{-1/2} \cdot \begin{cases} z_{i-1}, & i = k+1, \\ 0, & \text{otherwise}, \end{cases} \tag{2.7}$$

and

$$K_n z_i = \begin{cases} q^2 z_i, & i = n, \\ q z_i, & \text{otherwise}, \end{cases} \tag{2.8}$$

$$F_n z_i = q^{1/2} \cdot \begin{cases} 1, & i = n, \\ 0, & \text{otherwise}, \end{cases} \tag{2.9}$$

$$E_n z_i = -q^{1/2} \cdot \begin{cases} z_n^2, & i = n, \\ z_n z_i, & \text{otherwise}. \end{cases} \tag{2.10}$$

This statement may be deduced from Proposition 2.1 and Corollary 5.6 in Ref. 9 by easy computations. In the next subsection we will introduce some other important $U_q\mathfrak{su}_{n,1}$-module algebras.

B. Finite functions on the quantum ball

It should be noted that in the classical case the space of polynomials does not suit purposes of harmonic analysis in the ball because the volume of the ball with respect to the SU(n,1)-invariant measure

$$d\nu(\mathbf{z}) = \frac{dm(\mathbf{z})}{(1-\|\mathbf{z}\|^2)^{n+1}} \tag{2.11}$$

[where $dm(\mathbf{z})$ is the normalized Lebesgue measure] is infinite. One observes the same problem in the quantum setting: there is no $U_q\mathfrak{su}_{n,1}$-invariant integral on $\mathcal{P}(\mathbb{C}^n)_q$, i.e., a linear positive functional $\nu:\mathcal{P}(\mathbb{C}^n)_q \to \mathbb{C}$ such that $\nu(\xi(f)) = \varepsilon(\xi)\cdot\nu(f)$ for any $\xi \in U_q\mathfrak{su}_{n,1}$ (ε is the counit of $U_q\mathfrak{su}_{n,1}$). Thus it is reasonable to look for a quantum counterpart of the space of finite functions on the ball (functions with compact supports inside the ball). The following construction for such a counterpart was proposed in Ref. 9, Sec. 7.

Let us add to the algebra $\mathcal{P}(\mathbb{C}^n)_q$ one more generator f_0 which satisfies the relations

$$f_0^* = f_0^2 = f_0, \quad z_i^* f_0 = f_0 z_i = 0, \quad i = 1,2,\ldots,n. \tag{2.12}$$

The resulting involutive algebra will be denoted by $\mathcal{F}(U_n)_q$. It is demonstrated in Ref. 9, Sec. 7, that one may extend the structure of $U_q\mathfrak{su}_{n,1}$-module algebra in $\mathcal{P}(\mathbb{C}^n)_q$ to one in $\mathcal{F}(U_n)_q$ as follows:

$$K_k f_0 = f_0, \quad F_k f_0 = E_k f_0 = 0, \tag{2.13}$$

with $k \neq n$ and

$$K_n f_0 = f_0, \quad F_n f_0 = -\frac{q^{1/2}}{q^{-2}-1} f_0 \cdot z_n^*, \quad E_n f_0 = -\frac{q^{1/2}}{1-q^2} z_n \cdot f_0. \tag{2.14}$$

The involutive algebra $\mathcal{D}(U_n)_q$ of finite functions on the quantum ball is defined as the two-sided ideal $\mathcal{F}(U_n)_q \cdot f_0 \cdot \mathcal{F}(U_n)_q$ in $\mathcal{F}(U_n)_q$. Due to (2.13) and (2.14), $\mathcal{D}(U_n)_q$ is a $U_q\mathfrak{su}_{n,1}$-module subalgebra in $\mathcal{F}(U_n)_q$. In the next subsection we present an explicit formula for a $U_q\mathfrak{su}_{n,1}$-invariant integral on $\mathcal{D}(U_n)_q$.

The above definition of $\mathcal{D}(U_n)_q$ is convenient for many purposes but performing computations. We present therefore an alternative description of $\mathcal{D}(U_n)_q$. For that purpose we let H be the $\mathcal{P}(\mathbb{C}^n)_q$-module given by its unique generator e_0 such that $z_i^* e_0 = 0$, $i = 1,2,\ldots,n$. By the formulas

(2.2) and (2.3), $H=\mathcal{P}(\mathbb{C}^n)_q\cdot e_0=\mathbb{C}[\mathbb{C}^n]_q\cdot e_0$ with $\mathbb{C}[\mathbb{C}^n]_q$ being the unital (noninvolutive) subalgebra in $\mathcal{P}(\mathbb{C}^n)_q$ generated by z_i, $i=1,2,\ldots,n$. Moreover, the elements $\{\mathbf{z}^{\underline{m}}\cdot e_0\}_{\underline{m}\in\mathbb{Z}^n_{\geqslant 0}}$ constitute a basis in H. The following statement may be deduced from known results concerning the twisted CCR-algebra (see, for instance, Ref. 18).

Proposition 2.2: (i) There exists a (unique up to a positive multiplier) scalar product in H such that

$$(f\cdot e_1,e_2)=(e_1,f^*\cdot e_2)$$

for any $f\in\mathcal{P}(\mathbb{C}^n)_q$ *and* $e_1,e_2\in H$.

(ii) The corresponding $*$*-representation T of* $\mathcal{P}(\mathbb{C}^n)_q$ *in the completion* $\overline{H}$ *of the pre-Hilbert space H* (*the so-called Fock representation*) *is a faithful irreducible representation by bounded operators*.

We let $C^*(\mathcal{P}(\mathbb{C}^n)_q)$ be the C^*-algebra generated by $\mathcal{P}(\mathbb{C}^n)_q$ via the representation T. We describe now an embedding of $\mathcal{D}(U_n)_q$ in $C^*(\mathcal{P}(\mathbb{C}^n)_q)$.

The representation T can be extended to a faithful $*$-representation of the algebra $\mathcal{F}(U_n)_q$ by setting

$$T(f_0)=\text{orthogonal projection onto } \mathbb{C}\cdot e_0.$$

It is easy to show that the subalgebra $\{T(f)\mid f\in\mathcal{D}(U_n)_q\}$ of the algebra of bounded operators on $\overline{H}$ coincides with the subalgebra of those operators whose matrices in the basis $\{\mathbf{z}^{\underline{m}}\cdot e_0\}_{\underline{m}\in\mathbb{Z}^n_{\geqslant 0}}$ have only finitely many nonzero entries. Thus the algebra $\mathcal{D}(U_n)_q$ can be realized as a subalgebra of $C^*(\mathcal{P}(\mathbb{C}^n)_q)$. It admits the following transparent description.

Let $y_i=1-z_iz_i^*-\cdots-z_nz_n^*\in\mathcal{P}(\mathbb{C}^n)_q$, $i=1,2,\ldots,n$. Then $(y_1,\ldots,y_n)$ is a tuple of pairwise commuting positive operators on $\overline{H}$. The joint spectrum of the tuple $(y_1,\ldots,y_n)$ in $C^*(\mathcal{P}(\mathbb{C}^n)_q)$ is the closure in $\mathbb{R}^n$ of the "q-simplex"

$$\mathfrak{M}=\{(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})\mid \underline{k}\in P(n)\} \tag{2.15}$$

[$P(n)$ is defined in the Introduction]. This is a consequence of the commutation relations

$$z_iy_j=\begin{cases}q^{-2}y_jz_i, & i\leqslant j,\\ y_jz_i, & \text{otherwise,}\end{cases}\qquad z_i^*y_j=\begin{cases}q^2y_jz_i^*, & i\leqslant j,\\ y_jz_i^*, & \text{otherwise.}\end{cases} \tag{2.16}$$

We will henceforth identify a function $f(y_1,\ldots,y_n)$ with a function f on the set $\mathfrak{M}$ via the spectral calculus.

Using the definition of y_i's and (2.16), one can write an arbitrary element $f\in\mathcal{P}(\mathbb{C}^n)_q$ uniquely in the form

$$f=\sum_{\underline{i}\times\underline{j}=0}\mathbf{z}^{\underline{i}}f_{\underline{i},\underline{j}}(y_1,y_2,\ldots,y_n)\mathbf{z}^{*\underline{j}}. \tag{2.17}$$

The subalgebra $\mathcal{D}(U_n)_q\subset C^*(\mathcal{P}(\mathbb{C}^n)_q)$ may be identified with the algebra of finite sums of the form (2.17) whose coefficients are functions on $\mathfrak{M}$ with finite supports.

We will use both descriptions of $\mathcal{D}(U_n)_q$. It is clear that the "distinguished" finite function f_0 which appears in the definition of $\mathcal{D}(U_n)_q$ may be described, in those terms, as follows: $f_{\underline{i},\underline{j}}\equiv 0$ provided $\underline{i}\neq\underline{0}$ or $\underline{j}\neq\underline{0}$, and

$$f_{\underline{0},\underline{0}}(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})=\begin{cases}1, & \underline{k}=\underline{0},\\ 0, & \text{otherwise.}\end{cases}$$

The following crucial property of f_0 will simplify proofs of many results.

Proposition 2.3: f_0 generates $\mathcal{D}(U_n)_q$ as a $U_q\mathfrak{su}_{n,1}$-module.
A proof can be found in Ref. 9, Sec. 7.

C. Invariant integral

In this subsection we present an explicit formula for the $U_q\mathfrak{su}_{n,1}$-invariant integral on the quantum ball. This formula was found in Ref. 9, Sec. 9.

Keep in mind the notation T for the Fock representation of $\mathcal{P}(\mathbb{C}^n)_q$ and H for a $\mathcal{P}(\mathbb{C}^n)_q$-module, a dense linear subspace in the Hilbert space $\overline{H}$ of the representation T (see the previous subsection). It is easy to observe that $T(f)(H)\subset H$ for any finite function f. Thus H becomes a $\mathcal{D}(U_n)_q$-module. It is convenient to identify the $\mathcal{D}(U_n)_q$-module H with the left ideal $\mathbb{C}[\mathbb{C}^n]_q\cdot f_0$ [this is possible due to (2.12)], with which we may equip H with some extra structures. In particular, the isomorphism of $\mathcal{D}(U_n)_q$-modules

$$H\simeq\mathbb{C}[\mathbb{C}^n]_q\cdot f_0\subset\mathcal{D}(U_n)_q$$

and formulas (2.5), (2.8), (2.13), and (2.14) define H as a $U_q\mathfrak{h}$-module where $U_q\mathfrak{h}$ is the Hopf subalgebra in $U_q\mathfrak{sl}_{n+1}$ generated by $K_i^{\pm 1}$, $i=1,2,\ldots,n$. Denote the corresponding representation of $U_q\mathfrak{h}$ in H by Γ. The following statement was proved in Ref. 9.

Proposition 2.4: The linear functional on $\mathcal{D}(U_n)_q$ given by

$$f\mapsto\nu(f)=\mathrm{tr}\left(T(f)\Gamma\left(\prod_{j=1}^{n}K_j^{-j(n+1-j)}\right)\right)$$

is a $U_q\mathfrak{su}_{n,1}$-invariant integral, i.e., $\nu(f^*f)>0$, $f\neq 0$, and $\nu(\xi(f))=\varepsilon(\xi)\cdot\nu(f)$, $\xi\in U_q\mathfrak{su}_{n,1}$.

We shall use the normalized integral

$$\int_{U_n}f d\nu_q=(q^2;q^2)_n\cdot\nu(f)$$

with $(q^2;q^2)_n=(1-q^2)(1-q^4)\cdots(1-q^{2n})$.

The invariant integral is unique up to a positive scalar. This is an immediate consequence of Proposition 2.3.

We can rewrite now the formula for the invariant integral in a more convenient form. Suppose $f\in\mathcal{D}(U_n)_q$ is written in the form (2.17). Then one checks easily that

$$\int_{U_n}f d\nu_q=(q^2;q^2)_n\cdot\sum_{\underline{k}\in P(n)}f_{\underline{0},\underline{0}}(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})\cdot q^{-2nk_1}\cdot q^{2k_2}\cdot\ldots\cdot q^{2k_n}. \tag{2.18}$$

In the next proposition we explain how the $U_q\mathfrak{su}_{n,1}$-invariant integral makes $\mathcal{D}(U_n)_q$ into a unitary $U_q\mathfrak{su}_{n,1}$-module and thus provides a setup for harmonic analysis in the quantum ball.

Proposition 2.5: The scalar product in $\mathcal{D}(U_n)_q$ given by

$$(\varphi_1,\varphi_2)=\int_{U_n}\varphi_2^*\cdot\varphi_1 d\nu_q$$

is $U_q\mathfrak{su}_{n,1}$-invariant, i.e., $(\xi(\varphi_1),\varphi_2)=(\varphi_1,\xi^*(\varphi_2))$ for any $\varphi_1,\varphi_2\in\mathcal{D}(U_n)_q$ and any $\xi\in U_q\mathfrak{su}_{n,1}$.

Proof: This follows from the condition (2.4) in $\mathcal{D}(U_n)_q$ and the following formula of "integrating by parts:" for any $\varphi_1,\varphi_2\in\mathcal{D}(U_n)_q$ and $\xi\in U_q\mathfrak{su}_{n,1}$ one has

$$\int_{U_n}\xi(\varphi_1)\cdot\varphi_2 d\nu_q=\int_{U_n}\varphi_1\cdot S(\xi)(\varphi_2)d\nu_q \tag{2.19}$$

with S being the antipode of $U_q\mathfrak{su}_{n,1}$. To prove the latter formula, it is sufficient to verify the equality on generators $E_i, F_i, K_i^{\pm 1}$ of $U_q\mathfrak{su}_{n,1}$. In this particular case the equality is equivalent to the $U_q\mathfrak{su}_{n,1}$-invariance of the integral. ■

D. Distributions on the quantum ball

The aim of this subsection is to define the space $\mathcal{D}(U_n)_q'$ of distributions on the quantum ball. We follow ideas in Ref. 19, Sec. 1, where the simplest case $n=1$ is treated.

Equip the vector space $\mathcal{D}(U_n)_q$ with the weakest topology so that all the linear functionals

$$l^{\underline{k}}_{\underline{i},\underline{j}}: f \mapsto f_{\underline{i},\underline{j}}(q^{2k_1}, q^{2k_2}, \ldots, q^{2k_n})$$

are continuous [here $\underline{i},\underline{j} \in \mathbb{Z}^n_{\geqslant 0}$ satisfy $\underline{i} \times \underline{j} = \underline{0}$, $\underline{k} \in P(n)$, and $f_{\underline{i},\underline{j}}$ is the corresponding coefficient in the expansion (2.17) of f].

The following results can be proved by direct, however tedious, computations, which we omit.

Proposition 2.6: For a fixed $f \in \mathcal{D}(U_n)_q$ the operator in $\mathcal{D}(U_n)_q$ of the right multiplication by f is continuous. Also, the $U_q\mathfrak{su}_{n,1}$-action in $\mathcal{D}(U_n)_q$ is continuous.

Let $\mathcal{D}(U_n)_q'$ be the completion of the topological vector space $\mathcal{D}(U_n)_q$. We shall use the concrete realization of $\mathcal{D}(U_n)_q'$ as the space of infinite sums of the form (2.17) whose coefficients $f_{\underline{i},\underline{j}}$ are arbitrary functions on the q-simplex $\mathfrak{M}$ [see (2.15)]. The above proposition, by continuity, implies that $\mathcal{D}(U_n)_q'$ is a right $\mathcal{D}(U_n)_q$-module and a $U_q\mathfrak{su}_{n,1}$-module. Moreover, these structures agree: the multiplication map $\mathcal{D}(U_n)_q' \otimes \mathcal{D}(U_n)_q \to \mathcal{D}(U_n)_q'$ is a morphism of $U_q\mathfrak{su}_{n,1}$-modules. This is a consequence of $U_q\mathfrak{su}_{n,1}$-moduleness of the algebra $\mathcal{D}(U_n)_q$.

Let us construct a nondegenerate pairing $\mathcal{D}(U_n)_q' \times \mathcal{D}(U_n)_q \to \mathbb{C}$ which will justify the term "distribution." Let $\{\psi_\beta\}_\beta$ be a convergent net in $\mathcal{D}(U_n)_q$ and suppose $\lim_\beta \psi_\beta = \psi$, $\psi \in \mathcal{D}(U_n)_q'$. Then for any $\varphi \in \mathcal{D}(U_n)_q$ the limit $\lim_\beta \int_{U_n} \psi_\beta \varphi \, d\nu_q$ exists and depends only on ψ and φ (i.e., independent of a choice of ψ_β). Indeed, let us prove existence of $\lim \int_{U_n} \psi_\beta \varphi \, d\nu_q$. Proposition 2.3 implies that there exists $\xi_\varphi \in U_q\mathfrak{su}_{n,1}$ such that $\varphi = \xi_\varphi(f_0)$. By (2.19)

$$\int_{U_n} \psi_\beta \varphi \, d\nu_q = \int_{U_n} S^{-1}(\xi_\varphi)(\psi_\beta) f_0 \, d\nu_q .$$

Since the $U_q\mathfrak{su}_{n,1}$-action is continuous, it is sufficient now to prove existence of the limit in the particular case $\varphi := f_0$. But in this case existence is equivalent to continuity of the functional $l^{\underline{0}}_{\underline{0}\underline{0}}$ and thus is obvious. Independence of the limit on a particular choice of the net $\{\psi_\beta\}$ can be proved by the same arguments.

Thus we get a well defined pairing

$$\mathcal{D}(U_n)_q' \times \mathcal{D}(U_n)_q \to \mathbb{C}, \quad (\psi, \varphi) \mapsto \int_{U_n} \psi \varphi \, d\nu_q ,$$

and, due to (2.19), it satisfies the property

$$\int_{U_n} \xi(\psi) \cdot \varphi \, d\nu_q = \int_{U_n} \psi \cdot S(\xi)(\varphi) \, d\nu_q \tag{2.20}$$

for any $\psi \in \mathcal{D}(U_n)_q'$, $\varphi \in \mathcal{D}(U_n)_q$, and $\xi \in U_q\mathfrak{su}_{n,1}$. In other words, we have constructed a morphism of $U_q\mathfrak{su}_{n,1}$-modules,

$$\mathcal{D}(U_n)_q' \to \text{dual of } \mathcal{D}(U_n)_q .$$

[For an A-module V the dual space V^* is endowed with an A-module structure via the antipode: $\xi f(\cdot) = f(S(\xi)\cdot)$.] In fact, this is an isomorphism. This can be proved by computation just as it was done in Ref. 19, Sec. 1, in the case $n=1$.

III. q-BEREZIN TRANSFORM

The aim of this section is to construct a q-analog of the Berezin transform in the unit ball. For that purpose we define also q-analogs of the weighted Bergman spaces, Toeplitz operators, and covariant symbols.

A. q-weighted Bergman spaces

In the classical case the weighted Bergman space is defined as the closure of the space of holomorphic polynomials with respect to the norm

$$\|f\|_\alpha=\left(\frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}\int_{U_n}|f(\mathbf{z})|^2(1-\|\mathbf{z}\|^2)^\alpha dm(\mathbf{z})\right)^{1/2}. \tag{3.1}$$

Here $\alpha>-1$, dm is the normalized Lebesgue measure, and the multiplier $\Gamma(n+\alpha+1)/\Gamma(n+1)\Gamma(\alpha+1)$ normalizes the measure $dm_\alpha=(1-\|\mathbf{z}\|^2)^\alpha dm(\mathbf{z})$. Let us define a q-analog of dm_α.

Suppose $\alpha\in\mathbb{Z}_{\geqslant 0}$. The formula (3.1), along with (2.11), suggests the following definition of the q-weighted integral,

$$\int_{U_n} f dm_{\alpha,q}=\frac{\Gamma_{q^2}(n+\alpha+1)}{\Gamma_{q^2}(n+1)\Gamma_{q^2}(\alpha+1)}\int_{U_n} f\cdot y_1^{\alpha+n+1} d\nu_q \tag{3.2}$$

with $y_1=1-z_1z_1^*-\cdots-z_nz_n^*\in\mathcal{P}(\mathbb{C}^n)_q$ (see Sec. II B). Here we use the standard notation:[20]

$$\Gamma_q(x)=\frac{(q;q)_\infty}{(q^x;q)_\infty}(1-q)^{1-x}$$

with

$$(a;q)_\infty=(1-a)(1-aq)(1-aq^2)\cdots,\quad (a;q)_\gamma=\frac{(a;q)_\infty}{(aq^\gamma;q)_\infty},\quad \gamma\in\mathbb{C}.$$

Using (2.18) and the definition of Γ_{q^2}, we may rewrite the integral in the following way:

$$\int_{U_n} f dm_{\alpha,q}=(q^{2\alpha+2};q^2)_n\sum_{\underline{k}\in P(n)} f_{\underline{0},\underline{0}}(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})\cdot q^{2k_1(\alpha+1)}\cdot q^{2k_2}\cdot\ldots\cdot q^{2k_n}. \tag{3.3}$$

The latter formula can be used to define the q-weighted integral for arbitrary $\alpha\in\mathbb{R}$.

We define $L^2(dm_{\alpha,q})$ as the completion of $\mathcal{D}(U_n)_q$ with respect to the norm

$$\|f\|_{\alpha,q}=\left(\int_{U_n} f^*\cdot f dm_{\alpha,q}\right)^{1/2}.$$

We shall use the concrete realization of $L^2(dm_{\alpha,q})$ as the subspace in $\mathcal{D}(U_n)_q'$ of those distributions for which the right-hand side is finite.

From now on we suppose α is a positive real number. In this case, we have $\mathcal{P}(\mathbb{C}^n)_q\subset L^2(dm_{\alpha,q})$ [this may be checked by direct computations using formula (3.3)]. By analogy with the classical case, we define the q-weighted Bergman space $L_a^2(dm_{\alpha,q})$ as the closure in $L^2(dm_{\alpha,q})$ of the subspace $\mathbb{C}[\mathbb{C}^n]_q$ of "holomorphic" polynomials.

Proposition 3.1: The monomials $\mathbf{z}^{\underline{m}}$ constitute an orthogonal basis in $L_a^2(dm_{\alpha,q})$ and

$$\|\mathbf{z}^{\underline{m}}\|_{\alpha,q}^2=\frac{\Gamma_{q^2}(n+\alpha+1)\Gamma_{q^2}(m_1+1)\cdots\Gamma_{q^2}(m_n+1)}{\Gamma_{q^2}(m_1+\cdots+m_n+n+\alpha+1)}.$$

Proof: By the above definitions

$$(\mathbf{z}^{\underline{m}},\mathbf{z}^{\underline{l}})_{\alpha,q}=(q^{2\alpha+2};q^2)_n\sum_{\underline{k}\in P(n)} f_{\underline{0},\underline{0}}(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})\cdot q^{2k_1(\alpha+1)}\cdot q^{2k_2}\cdot\ \ldots\ \cdot q^{2k_n},$$

where $f_{\underline{0},\underline{0}}$ is the corresponding term in the expansion (2.17) of the polynomial $\mathbf{z}^{*\underline{l}}\mathbf{z}^{\underline{m}}$. Obviously, the $f_{\underline{0},\underline{0}}$-term vanishes for $\underline{m}\neq\underline{l}$. This implies the pairwise orthogonality of the monomials. Suppose $\underline{m}=\underline{l}$. It is easy to show that

$$\mathbf{z}^{*\underline{m}}\mathbf{z}^{\underline{m}}=y_2^{m_1}y_3^{m_2}\cdots y_n^{m_{n-1}}\left(q^2\frac{y_1}{y_2};q^2\right)_{m_1}\left(q^2\frac{y_2}{y_3};q^2\right)_{m_2}\cdots\left(q^2\frac{y_{n-1}}{y_n};q^2\right)_{m_{n-1}}(q^2y_n;q^2)_{m_n}. \tag{3.4}$$

Denote by $f(y_1,y_2,\ldots,y_n)$ the right-hand side of the latter equality. One has

$$\sum_{\underline{k}\in P(n)} f(q^{2k_1},q^{2k_2},\ldots,q^{2k_n})\cdot q^{2k_1(\alpha+1)+2k_2+\cdots+2k_n}$$
$$=\frac{1}{(1-q^2)^n}\prod_{j=0}^{n-1}\int_0^1 t^{\alpha+m_1+\cdots+m_j+j}(q^2t;q^2)_{m_{j+1}}d_{q^2}t$$

where $\int_0^1 f(t)d_{q^2}t$ is the Jackson integral given by

$$\int_0^1 f(t)d_{q^2}t=(1-q^2)\sum_{l=0}^{\infty} f(q^{2l})q^{2l}. \tag{3.5}$$

What remains is to use the following well known formula:[20]

$$\int_0^1 t^a(q^2t;q^2)_b d_{q^2}t=\frac{\Gamma_{q^2}(a+1)\Gamma_{q^2}(b+1)}{\Gamma_{q^2}(a+b+2)}.$$

■

In the classical case the Hilbert space $L^2(dm_\alpha)$ admits a natural unitary $\widetilde{\mathrm{SU}(n,1)}$-action, where $\widetilde{\mathrm{SU}(n,1)}$ is the universal covering of $\mathrm{SU}(n,1)$. The invariant subspace $L_a^2(dm_\alpha)$ of holomorphic functions is called the representation of the holomorphic discrete series.[21,22] The corresponding infinitesimal $U\mathfrak{su}_{n,1}$-action is obtained by a simple twisting of the natural action. Below, we produce an analog of the twisted $U\mathfrak{su}_{n,1}$-action.

It was proved in Ref. 10, Sec. 6, that there exists a unique representation π_α of $U_q\mathfrak{su}_{n,1}$ in $\mathcal{P}(\mathbb{C}^n)_q$ and $\mathcal{D}(U_n)_q$ such that for all $f\in\mathcal{P}(\mathbb{C}^n)_q$ [or $f\in\mathcal{D}(U_n)_q$]

$$\pi_\alpha(E_j)f=\begin{cases}E_jf, & j\neq n,\\ E_nf-q^{1/2}\dfrac{1-q^{2\alpha+2n+2}}{1-q^2}(K_nf)z_n, & j=n,\end{cases} \tag{3.6}$$

$$\pi_\alpha(F_j)f=\begin{cases}F_jf, & j\neq n,\\ q^{-\alpha-n-1}F_nf, & j=n,\end{cases} \tag{3.7}$$

$$\pi_\alpha(K_j^{\pm1})f=\begin{cases}K_j^{\pm1}f, & j\neq n,\\ q^{\pm(\alpha+n+1)}K_n^{\pm1}f, & j=n,\end{cases} \tag{3.8}$$

where E_jf,F_jf,K_jf are defined in Proposition 2.1 [(2.13) and (2.14) for $f\in\mathcal{D}(U_n)_q$]. In order to not consider the polynomials and finite functions separately, it will be convenient sometimes to regard π_α as a representation of $U_q\mathfrak{su}_{n,1}$ in $\mathcal{F}(U_n)_q$.

The following statement is proved in Ref. 10, Sec. 6.

Proposition 3.2: For any $\varphi_1, \varphi_2 \in \mathcal{F}(U_n)_q$ *and any* $\xi \in U_q\mathfrak{su}_{n,1}$

$$(\pi_\alpha(\xi)\varphi_1, \varphi_2)_{\alpha,q} = (\varphi_1, \pi_\alpha(\xi^*)\varphi_2)_{\alpha,q}$$

with $(\cdot,\cdot)_{\alpha,q}$ *being the scalar product in* $L^2(dm_{\alpha,q})$.

Note that the subspace $\mathbb{C}[\mathbb{C}^n]_q \subset \mathcal{F}(U_n)_q$ is actually a $U_q\mathfrak{su}_{n,1}$-submodule. It should be treated as a module of the holomorphic discrete series for $U_q\mathfrak{su}_{n,1}$.

Before we proceed further, let us fix more notation. The space $\mathbb{C}[\mathbb{C}^n]_q$ [as well as $\mathcal{F}(U_n)_q$] admits two different $U_q\mathfrak{su}_{n,1}$-actions, namely, the original one which was introduced earlier in Proposition 2.1 and the twisted one which appeared in this subsection. In order to emphasize that a space is considered together with the twisted $U_q\mathfrak{su}_{n,1}$-action π_α we shall add the subscript α in the notation, for example, $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$. The subscript will also indicate the pre-Hilbert space structure given by the scalar product $(\cdot,\cdot)_{\alpha,q}$.

The following important observation relates the usual and the twisted $U_q\mathfrak{su}_{n,1}$-actions: the multiplication map $\mathcal{F}(U_n)_q \otimes \mathcal{F}(U_n)_{q,\alpha} \to \mathcal{F}(U_n)_{q,\alpha}$ is a morphism of $U_q\mathfrak{su}_{n,1}$-modules. This can be proved by direct computations.

B. Toeplitz operators

In this subsection we produce q-analogs of Toeplitz operators with polynomial and finite symbols. As in the previous subsection, it is convenient to consider symbols from the algebra $\mathcal{F}(U_n)_q$ when there is no necessity to consider the cases of polynomial and finite symbols separately.

Let $P_{\alpha,q}$ be the orthogonal projection in $L^2(dm_{\alpha,q})$ onto $L^2_a(dm_{\alpha,q})$. The Toeplitz operator T_f with the symbol $f \in \mathcal{F}(U_n)_q$ is defined as follows:

$$T_f : \mathbb{C}[\mathbb{C}^n]_{q,\alpha} \to \mathbb{C}[\mathbb{C}^n]_{q,\alpha}, \quad T_f(\psi) = P_{\alpha,q}(f \cdot \psi).$$

To formulate the principal result of the present subsection, we recall the following well known construction. Let A be a Hopf algebra and V an A-module. Then the space $\mathrm{End}(V)$ admits the following "canonical" structure of the A-module: for $\xi \in A$, $T \in \mathrm{End}(V)$,

$$\xi(T) = \sum_j \xi'_j \cdot T \cdot S(\xi''_j),$$

where S is the antipode of A, $\Delta(\xi) = \Sigma_j \xi'_j \otimes \xi''_j$ (with Δ being the comultiplication), and the elements on the right-hand side are multiplied within the algebra $\mathrm{End}(V)$. This action of A in $\mathrm{End}(V)$ makes $\mathrm{End}(V)$ into an A-module algebra.

Proposition 3.3: The linear map

$$\mathcal{F}(U_n)_q \to \mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha}), \quad f \mapsto T_f,$$

is a morphism of $U_q\mathfrak{su}_{n,1}$*-modules.*

Proof: In the classical case the projection $P_{\alpha,q}$ intertwines the twisted $\widetilde{\mathrm{SU}(n,1)}$-action in $L^2(dm_\alpha)$ and $L^2_a(dm_\alpha)$. In the quantum case the $U_q\mathfrak{su}_{n,1}$-action π_α is not defined on the entire $L^2(dm_{\alpha,q})$. Nevertheless, the intertwining property may be formulated due to the equality

$$P_{\alpha,q}(\mathcal{F}(U_n)_{q,\alpha}) = \mathbb{C}[\mathbb{C}^n]_{q,\alpha}.$$

To prove the equality, we endow the space $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ with the obvious $\mathbb{Z}_{\geqslant 0}$-grading by powers of monomials and observe that each $f \in \mathcal{F}(U_n)_{q,\alpha}$ is orthogonal to all but finitely many homogeneous components of $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$. Now it is evident that the operator $P_{\alpha,q} : \mathcal{F}(U_n)_{q,\alpha} \to \mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ is a morphism of $U_q\mathfrak{su}_{n,1}$-modules: this follows from $U_q\mathfrak{su}_{n,1}$-invariance of the orthogonal complement of $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ in $\mathcal{F}(U_n)_{q,\alpha}$.

Let $f \in \mathcal{F}(U_n)_q$. Denote by $\hat{f} = \hat{f}_\alpha$ the endomorphism of $\mathcal{F}(U_n)_{q,\alpha}$ given by $\hat{f}_\alpha(\varphi) = f \cdot \varphi$. The map

$$\mathcal{F}(U_n)_q \to \mathrm{End}(\mathcal{F}(U_n)_{q,\alpha}), \quad f \mapsto \hat{f}_\alpha,$$

is a morphism $U_q\mathfrak{su}_{n,1}$-modules (see the remark at the end of the previous subsection). It remains to use the equality $T_f = P_{q,\alpha} \cdot \hat{f}_\alpha|_{\mathbb{C}[\mathbb{C}^n]_{q,\alpha}}$. ■

Remark: One can use the above observation to show that the projection $P_{\alpha,q}$ is a q-integral operator with a simple kernel which is a q-analog of the so-called Bergman kernel; see Ref. 10. But this result is not needed in the present article.

C. On the case of polynomial symbols

For purposes of this article we need mostly Toeplitz operators with finite symbols. However, we present some results about the polynomial case which seem to be interesting by themselves.

Let $\hat{z}_i$ stand for the operator in $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ of the left multiplication by z_i, $\hat{z}_i^*$ for the adjoint operator. The following observation is straightforward: for a polynomial $f = \Sigma a_{\underline{l},\underline{m}} \mathbf{z}^{*\underline{l}} \mathbf{z}^{\underline{m}}$ one has $T_f = \Sigma a_{\underline{l},\underline{m}} \hat{\mathbf{z}}^{*\underline{l}} \hat{\mathbf{z}}^{\underline{m}}$. Thus all Toeplitz operators with polynomial symbols belong to the unital subalgebra in $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ generated by $\hat{z}_i$ and $\hat{z}_i^*$, $i = 1,2,\ldots,n$. Denote this subalgebra by $\mathcal{P}_{n,q,\alpha}$. It is an involutive algebra with the involution given by $*: \hat{z}_i \mapsto \hat{z}_i^*$.

Proposition 3.4: The $U_q\mathfrak{su}_{n,1}$-action in $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ *induces a $U_q\mathfrak{su}_{n,1}$-module algebra structure in $\mathcal{P}_{n,q,\alpha}$.*

Proof: First we have to establish $U_q\mathfrak{su}_{n,1}$-invariance of the subspace $\mathcal{P}_{n,q,\alpha}$ in $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$, that is, to show that $\xi(\hat{z}_i^{*a} \hat{z}_j^b)$ belong to $\mathcal{P}_{n,q,\alpha}$ for any $a,b \in \mathbb{Z}_{\geqslant 0}$, $i,j = 1,2,\ldots,n$, and $\xi \in U_q\mathfrak{su}_{n,1}$. According to Proposition 3.3

$$\xi(\hat{z}_i^{*a} \hat{z}_j^b) = \xi(T_{z_i^{*a} z_j^b}) = T_{\xi(z_i^{*a} z_j^b)}.$$

By the remark preceding the present proposition, $T_{\xi(z_i^{*a} z_j^b)} \in \mathcal{P}_{n,q,\alpha}$. It remains to prove module algebra property (2.4) for $\mathcal{P}_{n,q,\alpha}$. But it may be derived easily from Proposition 3.2. ■

Proposition 3.5: The following commutation relations hold:

$$\hat{z}_i \hat{z}_j = q \hat{z}_j \hat{z}_i, \quad i < j,$$

$$\hat{z}_i^* \hat{z}_j = q \hat{z}_j \hat{z}_i^* + q^{2\alpha+2n} \left(\hat{z}_i^* \hat{z}_j \left(q^2 + (1-q^2) \sum_{k=1}^{n} \hat{z}_k \hat{z}_k^* \right) - q \hat{z}_j \hat{z}_i^* \right), \quad i \neq j,$$

$$\hat{z}_j^* \hat{z}_j = q^2 \hat{z}_j \hat{z}_j^* + (1-q^2) \left(1 - \sum_{k=j+1}^{n} \hat{z}_k \hat{z}_k^* \right)$$
$$+ q^{2\alpha+2n} \left(\hat{z}_j^* \hat{z}_j \left(q^2 + (1-q^2) \sum_{k=1}^{n} \hat{z}_k \hat{z}_k^* \right) - q^2 \hat{z}_j \hat{z}_j^* - (1-q^2) \sum_{k=1}^{j} \hat{z}_k \hat{z}_k^* \right).$$

Proof: The relations may be deduced from the formulas

$$\hat{z}_i(\mathbf{z}^{\underline{m}}) = q^{m_n + m_{n-1} + \cdots + m_{i+1}} \mathbf{z}^{\underline{m}'}$$

[where $\underline{m}' = (m_1, \ldots, m_i + 1, \ldots, m_n)$],

$$\hat{z}_i^*(\mathbf{z}^{\underline{m}}) = 0, \quad m_i = 0,$$

$$\hat{z}_i^*(\mathbf{z}^{\underline{m}}) = \frac{q^{m_n + m_{n-1} + \cdots + m_{i+1}} (1 - q^{2m_i})}{1 - q^{2m_1 + 2m_2 + \cdots + 2m_n + 2n + 2\alpha}} \mathbf{z}^{\underline{m}''}$$

[where $\underline{m}''=(m_1,\ldots,m_i-1,\ldots,m_n)$]. The first equality is obvious, the other follows from Proposition 3.1. ■

Note that for $\alpha=\infty$ the above relations coincide with the defining relations for $\mathcal{P}(\mathbb{C}^n)_q$.

The unital involutive algebra given by the above commutation relations can be viewed as a two-parameter deformation of the polynomial algebra on $\mathbb{C}^n$. It is easy to show that for $n=1$ the algebra is isomorphic to the one considered in details in Ref. 6 (see the Introduction).

D. Covariant symbols and *q*-Berezin transform

In this subsection, we define the notion of covariant symbols of operators on the q-weighted Bergman spaces and use it to define a q-analog of the Berezin transform.

To define covariant symbols we need a certain inner product in the space of operators on a q-weighted Bergman space (see the Introduction). This product is defined via the so-called q-trace. So we recall first its definition.

Let V be a finite-dimensional $U_q\mathfrak{sl}_{n+1}$-module. The q-trace is the linear functional on $\mathrm{End}(V)$ given by

$$\mathrm{tr}_q : T \mapsto \mathrm{tr}\left(T \cdot \prod_{j=1}^{n} K_j^{-j(n+1-j)} \right). \tag{3.9}$$

The following well known observation explains the importance of this functional (see Ref. 17): the q-trace is an invariant linear functional on $\mathrm{End}(V)$, i.e., $\mathrm{tr}_q(\xi(T))=\varepsilon(\xi)\cdot\mathrm{tr}_q(T)$ for any $\xi \in U_q\mathfrak{sl}_{n+1}$ and $T\in\mathrm{End}(V)$.

We will modify the definition slightly for the infinite-dimensional space $V=\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$. Let $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ be the subspace in $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ of those automorphisms whose matrices in the basis $\{\mathbf{z}^{\underline{m}}\}$ have only finitely many nonzero entries. The q-trace (3.9) is a well defined linear functional on $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$. The invariance property still holds in this case.

Proposition 3.6: The q-trace is an invariant linear functional on $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$.

Sketch of a proof: A standard proof in the finite-dimensional case uses the canonical isomorphism of $U_q\mathfrak{sl}_{n+1}$-modules $\mathrm{End}(V)\simeq V\otimes V^*$ with V^* being the dual $U_q\mathfrak{sl}_{n+1}$-module.[17] The statement of Proposition 3.6 can be proved by the same argument since $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha}) \simeq \mathbb{C}[\mathbb{C}^n]_{q,\alpha}\otimes\mathbb{C}[\mathbb{C}^n]^*_{q,\alpha}$. ■

Remarks: (i) The formula (3.9) is the same as the one which defines the invariant integral on the quantum ball (see Proposition 2.4). But Proposition 2.4 does not follow formally from the above statement since the $\mathcal{D}(U_n)_q$-module H is not a $U_q\mathfrak{sl}_{n+1}$-module.

(ii) Using the equality (3.12) below and the same idea as in the proof of Proposition 2.5 one can show that the scalar product in $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ given by $(T_1,T_2)=\mathrm{tr}_q(T_2^*\cdot T_1)$ is $U_q\mathfrak{su}_{n,1}$-invariant. The unitary representation of $U_q\mathfrak{su}_{n,1}$ in $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ should be treated as a q-analog of the canonical representation of $\mathrm{SU}(n,1)$.[23]

For a particular α, we shall use the modified q-trace Tr_q on $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ which differs from tr_q by a constant:

$$\mathrm{Tr}_q = q^{n(n+\alpha+1)} \frac{(q^2;q^2)_n}{(q^{2+2\alpha};q^2)_n} \mathrm{tr}_q .$$

It is easy to deduce the following explicit formula for Tr_q. Let $A\in\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ be the endomorphism given by $A(\mathbf{z}^{\underline{m}})=\Sigma_{\underline{k}}A^{\underline{m}}_{\underline{k}}\cdot\mathbf{z}^{\underline{k}}$. Then

$$\mathrm{Tr}_q(A)=\frac{(q^2;q^2)_n}{(q^{2+2\alpha};q^2)_n}\cdot\sum_{\underline{m}} A^{\underline{m}}_{\underline{m}}\cdot q^{-2n(m_1+m_2+\cdots+m_n)}\cdot q^{2m_2+\cdots+2m_n}\cdot\ \cdots\ \cdot q^{2m_n}. \tag{3.10}$$

Now we are ready to define the notion of covariant symbols. Let $T\in\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$. A distribution $\sigma(T)\in\mathcal{D}(U_n)'_q$ is said to be the covariant symbol of T if for any $f\in\mathcal{D}(U_n)_q$

$$\int_{U_n} \sigma(T)\cdot f d\nu_q = \mathrm{Tr}_q(T\cdot T_f). \tag{3.11}$$

Note that for $f\in\mathcal{D}(U_n)_q$ one has $T_f\in \mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$. Thus the right-hand side of (3.11) is well defined. The arguments cited at the end of Sec. II D imply existence and uniqueness of the covariant symbol of an arbitrary endomorphism F. Actually, the map $T\mapsto\sigma(T)$ is conjugated to the map $f\mapsto T_f$.

We have the following elementary property of the q-trace, which can be proved by the same arguments as the formula of integrating by parts (see the proof of Proposition 2.5): for any $T\in\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$, $T_0\in\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$, and $\xi\in U_q\mathfrak{su}_{n,1}$,

$$\mathrm{Tr}_q(\xi(T)\cdot T_0)=\mathrm{Tr}_q(T\cdot S(\xi)(T_0)). \tag{3.12}$$

This implies the following.

Proposition 3.7: The map

$$\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})\to\mathcal{D}(U_n)'_q,\quad T\mapsto\sigma(T),$$

is a morphism of $U_q\mathfrak{su}_{n,1}$-modules.

Proof: The equality (3.12) gives an identification of the $U_q\mathfrak{su}_{n,1}$-module $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ with the dual of $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ (see the definition of the dual module in Sec. II D). What remains is to use Proposition 3.3 and the observation that the map $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})\to\mathcal{D}(U_n)'_q$, $T\mapsto\sigma(T)$ is conjugated to $\mathcal{D}(U_n)_q\to\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$, $f\mapsto T_f$. ■

We are in position to define the q-Berezin transform $B_{q,\alpha}$. It is defined as the linear map from $\mathcal{D}(U_n)_q$ to $\mathcal{D}(U_n)'_q$ which sends a finite function to the covariant symbol of the corresponding Toeplitz operator:

$$B_{q,\alpha}: f\mapsto\sigma(T_f).$$

The following crucial statement is straightforward.

Proposition 3.8: The q-Berezin transform is a morphism of $U_q\mathfrak{su}_{n,1}$-modules.

Due to Proposition 2.3, any morphism of $U_q\mathfrak{su}_{n,1}$-modules $T:\mathcal{D}(U_n)_q\to\mathcal{D}(U_n)'_q$ is completely determined by the element $T(f_0)\in\mathcal{D}(U_n)'_q$. Thus it would be very useful to compute $B_{q,\alpha}(f_0)$.

Proposition 3.9:

$$B_{q,\alpha}(f_0)=(q^{2\alpha+2};q^2)_n\cdot y_1^{\alpha+n+1}.$$

Proof: We have to check that for any $f\in\mathcal{D}(U_n)_q$

$$(q^{2\alpha+2};q^2)_n\int_{U_n} y_1^{\alpha+n+1}\cdot f d\nu_q=\mathrm{Tr}_q(T_{f_0}\cdot T_f). \tag{3.13}$$

Let us denote by $f^{\underline{k}}_{\underline{i},\underline{j}}$ ($\underline{k}\in P(n)$, $\underline{i},\underline{j}\in\mathbb{Z}^n_{\geqslant 0}$, $\underline{i}\times\underline{j}=\underline{0}$) the finite function given by $f^{\underline{k}}_{\underline{i},\underline{j}}=\mathbf{z}^{\underline{i}}f_{\underline{k}}(y_1,y_2,\ldots,y_n)\mathbf{z}^{*\underline{j}}$ with

$$f_{\underline{k}}(q^{2l_1},q^{2l_2},\ldots,q^{2l_n})=\begin{cases}1, & \underline{k}=\underline{l}\\ 0, & \text{otherwise.}\end{cases}$$

For example, $f^{\underline{0}}_{\underline{0},\underline{0}}=f_0$. Evidently, the functions $f^{\underline{k}}_{\underline{i},\underline{j}}$ constitute a basis in $\mathcal{D}(U_n)_q$.

It follows from the definitions that both sides of (3.13) vanish for $f:=f^{\underline{k}}_{\underline{i},\underline{j}}$ provided $\underline{i}\neq\underline{0}$ or $\underline{j}\neq\underline{0}$. Thus we have to verify (3.13) for $f:=f_{\underline{k}}$. It follows from (2.18) that

$$(q^{2\alpha+2};q^2)_n \int_{U_n} y_1^{\alpha+n+1} \cdot f_{\underline{k}} d\nu_q = (q^{2\alpha+2};q^2)_n \cdot (q^2;q^2)_n \cdot q^{2k_1(\alpha+1)} \cdot q^{2k_2} \cdot \ldots \cdot q^{2k_n}.$$

Let us compute the right-hand side of (3.13) with $f := f_{\underline{k}}$. Evidently,

$$f_0 \cdot \mathbf{z}^{\underline{m}} = \begin{cases} f_0, & \underline{m} = \underline{0}, \\ 0, & \text{otherwise.} \end{cases}$$

Besides, $\int_{U_n} f_0 dm_{\alpha,q} = (q^{2\alpha+2};q^2)_n$. These equalities mean that

$$T_{f_0}(\mathbf{z}^{\underline{m}}) = \begin{cases} (q^{2\alpha+2};q^2)_n, & \underline{m} = \underline{0}, \\ 0, & \text{otherwise.} \end{cases}$$

Clearly, the vector $f_{\underline{k}} \cdot \mathbf{z}^{\underline{m}} \in L^2(dm_{\alpha,q})$ is orthogonal to any monomial $\mathbf{z}^{\underline{l}}$ except the case $\underline{l} = \underline{m}$. In particular, the monomials are eigenvectors of $T_{f_{\underline{k}}}$. Thus

$$\begin{aligned} \mathrm{Tr}_q(T_{f_0} \cdot T_{f_{\underline{k}}}) &= (q^2;q^2)_n (T_{f_{\underline{k}}}(1),1)_{\alpha,q} \\ &= (q^2;q^2)_n \int_{U_n} f_{\underline{k}} dm_{\alpha,q} \\ &= (q^{2\alpha+2};q^2)_n \cdot (q^2;q^2)_n \cdot q^{2k_1(\alpha+1)} \cdot q^{2k_2} \cdot \ldots \cdot q^{2k_n}. \end{aligned}$$

■

IV. *q*-LAPLACE–BELTRAMI OPERATOR AND ASSOCIATED *q*-SPHERICAL TRANSFORM

In this section we define a q-analog of the SU(n.1)-invariant Laplace operator (the Laplace–Beltrami operator) on the unit ball and study a q-analog of the spherical transform in the unit ball. Namely, we calculate the ''radial part'' of the q-Laplace-Beltrami operator, find q-spherical functions, and present an inversion formula for the q-spherical transform.

A. *q*-Laplace–Beltrami operator

In this subsection, we consider the asymptotic expansion of the q-Berezin transform $B_{q,\alpha}$ at the limit $t = q^{2\alpha} \to 0$. A q-analog of the Laplace–Beltrami operator on the ball is defined as the coefficient at t in that expansion.

Recall (see the proof of Proposition 3.9) the notation $f^{\underline{k}}_{\underline{i},\underline{j}}$ ($\underline{k} \in P(n)$, $\underline{i},\underline{j} \in \mathbb{Z}^n_{\geqslant 0}$, $\underline{i} \times \underline{j} = \underline{0}$). Suppose T is the linear map from $\mathcal{D}(U_n)_q$ to $\mathcal{D}(U_n)'_q$. The numbers

$$T^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}} = \int_{U_n} T(f^{\underline{k}}_{\underline{i},\underline{j}}) \cdot f^{\underline{s}}_{\underline{p},\underline{r}} d\nu_q$$

will be called the matrix entries of T. Due to nondegeneracy of the pairing $\mathcal{D}(U_n)'_q \times \mathcal{D}(U_n)_q \to \mathbb{C}$ (Sec. II D), the matrix entries determine T completely.

Let us denote the matrix entries of the q-Berezin transform $B_{q,\alpha}$ by $B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(\alpha)$. Introduce the new variable $t = q^{2\alpha}$. We will regard the matrix entries $B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(\alpha)$ as functions of t and use the notation $B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(t) := B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(\alpha)$, $B_{q,t} := B_{q,\alpha}$.

Proposition 4.1: There exists a sequence $\{B_{q,j}\}_{j \in \mathbb{N}}$ *of linear endomorphisms of* $\mathcal{D}(U_n)_q$ *such that*

(i) $B_{q,j}$ *are independent of t (i.e., their matrix entries are independent of t);*

(ii) each $B_{q,j}$ *is a* $U_q\mathfrak{su}_{n,1}$*-module morphism; and*

(iii) for any $f \in \mathcal{D}(U_n)_q$

$$B_{q,t}(f)=f+\sum_{j=1}^{\infty} B_{q,j}(f)\cdot t^j, \tag{4.1}$$

where the series is convergent in $\mathcal{D}(U_n)_q'$.

Proof: First of all, we will construct a sequence $\{B_{q,j}\}_{j\in\mathbb{Z}_{\geqslant 0}}$ of linear operators from $\mathcal{D}(U_n)_q$ to $\mathcal{D}(U_n)_q'$ such that each $B_{q,j}$ is independent of t and $B_{q,t}(f)=\Sigma_{j=0}^{\infty}B_{q,j}(f)\cdot t^j$ for any $f\in\mathcal{D}(U_n)_q$ (the series is convergent in the sense that all the corresponding series of matrix entries are convergent). For that purpose we need the following.

Lemma 4.2: The matrix entries $B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(t)$ *are polynomials in* t.

Proof of the lemma: Due to Proposition 2.3, for any $\underline{k},\underline{i},\underline{j}\in\mathbb{Z}^n_{\geqslant 0}$ ($\underline{i}\times\underline{j}=\underline{0}$) there exists $\xi^{\underline{k}}_{\underline{i},\underline{j}}\in U_q\mathfrak{su}_{n,1}$ such that $f^{\underline{k}}_{\underline{i},\underline{j}}=\xi^{\underline{k}}_{\underline{i},\underline{j}}(f_0)$. Then,

$$B^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(t)=\int_{U_n}B_{q,t}(f^{\underline{k}}_{\underline{i},\underline{j}})\cdot f^{\underline{s}}_{\underline{p},\underline{r}}d\nu_q=\int_{U_n}B_{q,t}(\xi^{\underline{k}}_{\underline{i},\underline{j}}(f_0))\cdot f^{\underline{s}}_{\underline{p},\underline{r}}d\nu_q=\int_{U_n}B_{q,t}(f_0)\cdot S(\xi^{\underline{k}}_{\underline{i},\underline{j}})(f^{\underline{s}}_{\underline{p},\underline{r}})d\nu_q,$$

where the last equality is due to Proposition 3.8 and the equality (2.20). Thus to prove the lemma it suffices to establish that the entries $B^{\underline{0},\underline{s}}_{\underline{0},\underline{0};\underline{p},\underline{r}}(t)=\int_{U_n}B_{q,t}(f_0)\cdot f^{\underline{s}}_{\underline{p},\underline{r}}d\nu_q$ are polynomials.

Recall (Proposition 3.9) that $B_{q,\alpha}(f_0)=(q^{2\alpha+2};q^2)_n\cdot y_1^{\alpha+n+1}$. Thus

$$\int_{U_n}B_{q,t}(f_0)\cdot f^{\underline{s}}_{\underline{p},\underline{r}}d\nu_q=(q^{2\alpha+2};q^2)_n\int_{U_n}y_1^{\alpha+n+1}\cdot f^{\underline{s}}_{\underline{p},\underline{r}}d\nu_q.$$

The latter integral vanishes with $\underline{p}\neq\underline{0}$ or $\underline{r}\neq\underline{0}$. Consider the integral $(q^{2\alpha+2};q^2)_n\int_{U_n}y_1^{\alpha+n+1}\cdot f_{\underline{k}}d\nu_q$ ($f_{\underline{k}}$ are defined in the proof of Proposition 3.9). Obviously,

$$\begin{aligned}(q^{2\alpha+2};q^2)_n\int_{U_n}y_1^{\alpha+n+1}\cdot f_{\underline{k}}d\nu_q&=(q^{2\alpha+2};q^2)_n(q^2;q^2)_n q^{2k_1(\alpha+1)}q^{2k_2}\cdots q^{2k_n}\\&=(q^2t;q^2)_n(q^2;q^2)_n q^{2k_1}t^{k_1}q^{2k_2}\cdots q^{2k_n}.\end{aligned}$$

■

Now we can define $\{B_{q,m}\}_{m\in\mathbb{Z}_{\geqslant 0}}$ by their matrix coefficients

$$(B_{q,m})^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}=\frac{1}{m!}\left.\frac{d^mB^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}(t)}{dt^m}\right|_{t=0}.$$

This definition implies the $U_q\mathfrak{su}_{n,1}$-invariance of the maps $B_{q,m}$. Indeed, we should prove coincidence of the maps $B_{q,m}\cdot\xi$ and $\xi\cdot B_{q,m}$ for any $\xi\in U_q\mathfrak{su}_{n,1}$, or, equivalently, equality of all matrix entries $(B_{q,m}\cdot\xi)^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}$ and $(\xi\cdot B_{q,m})^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}$. Due to $U_q\mathfrak{su}_{n,1}$-invariance of $B_{q,t}$, one has

$$(B_{q,t}\cdot\xi)^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}=(\xi\cdot B_{q,t})^{\underline{k},\underline{s}}_{\underline{i},\underline{j};\underline{p},\underline{r}}$$

for any $\underline{i},\underline{j},\underline{p},\underline{r},\underline{k},\underline{s}$. What remains is to differentiate the latter equality.

Let us show that the image of the map $B_{q,m}:\mathcal{D}(U_n)_q\to\mathcal{D}(U_n)_q'$ is contained in $\mathcal{D}(U_n)_q$. Since all $B_{q,m}$ are morphisms of $U_q\mathfrak{su}_{n,1}$-modules, we need to verify that $B_{q,m}(f_0)\in\mathcal{D}(U_n)_q$. This can be easily deduced from the following equivalent formulation of Proposition 3.9:

$$B_{q,t}(f_0)=(q^2t;q^2)_n\cdot\sum_{k=0}^{\infty}f_kq^{2k(n+1)}t^k, \tag{4.2}$$

where f_k, $k\in\mathbb{Z}_{\geqslant 0}$, are the finite functions given by

$$f_k = f_k(y_1, y_2, \ldots, y_n) = \begin{cases} 1, & y_1 = q^{2k}, \\ 0, & \text{otherwise}, \end{cases} \tag{4.3}$$

and the series (4.2) is convergent in $\mathcal{D}(U_n)'_q$. Differentiating with respect to t proves $B_{q,m}(f_0) \in \mathcal{D}(U_n)_q$.

The equality (4.2) and continuity of the $U_q\mathfrak{su}_{n,1}$-action in $\mathcal{D}(U_n)'_q$ prove also statement (iii) of Proposition 4.1. ■

Proposition 4.1 implies, in particular, that $B_{q,t} = \mathrm{id} + o(1)$ when $t \to 0$. By analogy with the classical case we call the first term of the asymptotic series (4.1) the q-Laplace–Beltrami operator on the quantum ball:

$$\Delta_{n,q} = \frac{q^{-2n}}{1-q^2} \frac{dB_{q,t}}{dt}\bigg|_{t=0}. \tag{4.4}$$

Clearly, $\Delta_{n,q}: \mathcal{D}(U_n)_q \to \mathcal{D}(U_n)_q$ is a morphism of $U_q\mathfrak{su}_{n,1}$-modules.

There are many evidences that this operator should indeed be treated as a q-analog of the classical Laplace-Beltrami operator in the unit ball. The results of the present section provide an example of such an evidence.

In conclusion, we make also the following remark. The operator $\Delta_{n,q}$ appeared as the first term of asymptotic of the q-Berezin transform. It turns out that other terms can be explicitly expressed via $\Delta_{n,q}$. This will be shown in the next section (Sec. V B).

B. Radial part of the *q*-Laplace–Beltrami operator

In the classical case the Laplace–Beltrami operator in the unit ball keeps invariant the space of smooth radial functions, i.e., functions depending on the radius only. The reason is that the radial functions are precisely the $\mathrm{S}(\mathrm{U}(n)\times\mathrm{U}(1))$-invariant functions with $\mathrm{S}(\mathrm{U}(n)\times\mathrm{U}(1)) \subset \mathrm{SU}(n,1)$ being the isotropy group of the center of the ball. Thus the "right" q-analog of the radial functions are functions on the quantum ball which are $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-invariant where $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$ is the $*$-Hopf subalgebra in $U_q\mathfrak{su}_{n,1}$ generated by E_i, F_i, $i = 1,2,\ldots,n-1$, and all $K_j^{\pm 1}$, s.

It can be proved that any $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-invariant element in $\mathcal{P}(\mathbb{C}^n)_q$ is a polynomial in $z_1 z_1^* + z_2 z_2^* + \cdots + z_n z_n^*$. The idea of the proof is as follows. $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-invariance of a polynomial, in particular, implies its $U_q\mathfrak{h}$-invariance, i.e., K_j-invariance for any j. Obviously, the latter means that the polynomial depends on $z_1 z_1^*, z_2 z_2^*, \ldots, z_n z_n^*$ only. One can write down without difficulties explicit formulas for the action of the generators E_i, F_i, $i = 1,2,\ldots,n-1$, on an arbitrary element which depends on $z_1 z_1^*, z_2 z_2^*, \ldots, z_n z_n^*$ and find the invariant elements.

In many computations it is convenient to use the element $y_1 = 1 - z_1 z_1^* - \cdots - z_n z_n^*$ instead of $z_1 z_1^* + z_2 z_2^* + \cdots + z_n z_n^*$ since the former quasicommutes with all the generators z_i, z_i^* [see (2.16)]:

$$z_i y_1 = q^{-2} y_1 z_i, \quad z_i^* y_1 = q^2 y_1 z_i^*.$$

In the sequel we omit the subscript 1 in the notation for y_1.

Using precisely the same arguments, one can show that any $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-invariant finite function or distribution on the quantum ball depends on $y = y_1$ only.

Recall the notation f_k, $k \in \mathbb{Z}_{\geqslant 0}$, from the previous subsection:

$$f_k(y) = \begin{cases} 1, & y = q^{2k}, \\ 0, & \text{otherwise}. \end{cases}$$

These functions constitute a basis in the space of radial finite functions on the quantum ball. They have the following obvious properties: first, $f_k \cdot f_l = \delta_{kl} f_k$ with δ_{kl} being the Kronecker symbol, and, second, for any distribution $f(y)$,

$$f=\sum_{k=0}^{\infty} f(q^{2k})\cdot f_k,$$

where the series converges in $\mathcal{D}(U_n)'_q$.

Our aim now is to compute the action of the q-Laplace–Beltrami operator $\Delta_{n,q}$ on radial finite functions. We would determine the action completely if we find $\Delta_{n,q}(f_k)$.

Proposition 4.3: The operator $\Delta_{n,q}$ has the following matrix form:

$$\Delta_{n,q}(f_k)=\frac{q^2}{(1-q^2)^2}\cdot((1-q^{2k+2})f_{k+1}-(1+q^{-2n}-2q^{2k})f_k+(q^{-2n}-q^{2k-2})f_{k-1})$$

(we assume $f_k\equiv 0$ for $k<0$).

The proof of the proposition will be given in Sec. IV D.

Proposition 4.3 allows us to apply the q-Laplace–Beltrami operator to any radial function $f=f(y)$. We call the restriction of the operator to the space of radial functions the radial part of the q-Laplace–Beltrami operator and denote it by $\Delta^{(\mathrm{r})}_{n,q}$. Using the explicit formula from Proposition 4.3, one can show that the radial part is given by the following second-order difference operator

$$\Delta^{(\mathrm{r})}_{n,q}=\frac{q^{-n}y^{n+1}}{(yq^2;q^2)_{n-1}}Dy^{-n+1}(yq;q^2)_nD \tag{4.5}$$

with $Df(y)=[f(q^{-1}y)-f(qy)]/(q^{-1}y-qy)$.

C. *q*-spherical transform

In this subsection we describe eigenfunctions of the operator $\Delta^{(\mathrm{r})}_{n,q}$ and present an explicit formula for expansion in these functions. The associated q-spherical transform should be viewed as a q-analog of the spherical transform in the unit ball.[12] The eigenfunctions of $\Delta^{(\mathrm{r})}_{n,q}$ appear to be closely related to certain one-parameter family of the Al-Salam-Chihara polynomials,[13] and this observation simplifies proofs of many statements.

Recall the definition of the basic hypergeometric series ${}_3\phi_2$:[20]

$${}_3\phi_2\left(\begin{matrix}a_1, & a_2, & a_3\\ b_1, & b_2\end{matrix}\,q,\quad z\right)=\sum_{n=0}^{\infty}\frac{(a_1;q)_n\cdot(a_2;q)_n\cdot(a_3;q)_n}{(b_1;q)_n\cdot(b_2;q)_n\cdot(q;q)_n}z^n.$$

Recall also the notation $h=\log q^{-2}$ (see the Introduction). We define the element $\phi_\rho(y)\in\mathcal{D}(U_n)'_q$ as follows:

$$\phi_\rho(y)={}_3\phi_2\left(\begin{matrix}y^{-1}, & q^{n+i\rho}, & q^{n-i\rho}\\ & q^{2n}, & 0\end{matrix}\,q^2,\quad q^2\right),\qquad \rho\in\left[0;\frac{2\pi}{h}\right]. \tag{4.6}$$

Obviously, $\phi_\rho(1)=1$. It is a q-analog of the spherical function in the unit ball as one can see from the following.

Proposition 4.4: The distribution $\phi_\rho(y)$ is an eigenvector of the operator $\Delta^{(\mathrm{r})}_{n,q}$:

$$\Delta^{(\mathrm{r})}_{n,q}(\phi_\rho(y))=\lambda(\rho)\cdot\phi_\rho(y)$$

with $\lambda(\rho)=-q^{2-2n}(1-q^{n+i\rho})(1-q^{n-i\rho})/(1-q^2)^2$, $\rho\in[0;2\pi/h]$.

Proof: Recall the notation $Q_m(x;a,b|q)$ for the Al-Salam-Chihara polynomials (Ref. 13, Sec. 3.8). It is straightforward that

$$\phi_\rho(q^{2m})=\frac{q^{nm}}{(q^{2n};q^2)_m}\cdot Q_m\left(\cos\frac{h\rho}{2};q^n,q^n\middle|q^2\right). \tag{4.7}$$

The statement of Proposition 4.4 is just another formulation of the recurrence relation for the Al-Salam-Chihara polynomials [Ref. 13, (3.8.4)]. ■

Let us compute restriction of the invariant integral in the quantum ball onto the space of radial finite functions:

$$\begin{aligned}\int_{U_n} f(y)\,d\nu_q &= (q^2;q^2)_n\cdot\sum_{\underline{k}\in P(n)} f(q^{2k_1})\cdot q^{-2nk_1}\cdot q^{2k_2}\cdot\ \dots\ \cdot q^{2k_n}\\ &= (q^2;q^2)_n\cdot\sum_{k=0}^{\infty} f(q^{2k})\cdot q^{-2nk}\sum_{0\leqslant k_n\leqslant\dots\leqslant k_2\leqslant k} q^{2k_2}\cdot\ \dots\ \cdot q^{2k_n}.\end{aligned}$$

Using the formula (4.15) and the Jackson integral (3.5), we finally get

$$\int_{U_n} f(y)\,d\nu_q=\frac{1-q^{2n}}{1-q^2}\int_0^1 f(y)y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y. \tag{4.8}$$

Let us denote by $\mathcal{L}_{n,q}$ and $\mathcal{L}'_{n,q}$ the spaces of radial finite functions and radial distributions on the quantum ball, respectively. Elements of these spaces can be treated as functions on the geometric progression $q^{2\mathbb{Z}_{\geqslant 0}}$. We also impose the notation $\mathcal{L}^2_{n,q}$ for the Hilbert space of ''square integrable'' radial distributions:

$$\mathcal{L}^2_{n,q}=\left\{ f(y)\in\mathcal{L}'_{n,q}\ \middle|\ \|f\|^2_{\mathcal{L}^2}=\frac{1-q^{2n}}{1-q^2}\int_0^1|f(y)|^2y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y<\infty\right\}.$$

We define the q-spherical transform as the map $\mathcal{F}:\mathcal{L}_{n,q}\to C^\infty(0;2\pi/h)$ given by

$$f(y)\mapsto\mathcal{F}f(\rho)=\frac{1-q^{2n}}{1-q^2}\int_0^1 f(y)\phi_\rho(y)y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y. \tag{4.9}$$

It is clear (see the proof of Proposition 4.4) that

$$\begin{aligned}\mathcal{F}f_k(\rho)&=(1-q^{2n})\cdot q^{-2kn}\cdot(q^{2k+2};q^2)_{n-1}\cdot\phi_\rho(q^{2k})\\ &=(1-q^{2n})\cdot q^{-kn}\cdot\frac{(q^{2k+2};q^2)_{n-1}}{(q^{2n};q^2)_k}\cdot Q_k\left(\cos\frac{h\rho}{2};q^n,q^n\middle|q^2\right).\end{aligned} \tag{4.10}$$

Hence the image of $\mathcal{F}$ is the space of polynomials in $\cos h\rho/2$.

The following proposition can be derived from the spectral decomposition of the operator $\Delta^{(\mathrm{r})}_{n,q}$, and a special case of a general result of Ref. 11, Sec. 5.

Proposition 4.5: (i) The operator $\Delta^{(\mathrm{r})}_{n,q}$ on $\mathcal{L}_{n,q}$ can be extended to a bounded self-adjoint operator on $\mathcal{L}^2_{n,q}$. It has simple purely continuous spectrum which coincides with the segment $[\lambda(2\pi/h);\lambda(0)]$ (with λ being defined in Proposition 4.4).

(ii) For any finite function $f(y)$

$$f(y)=\frac{1}{4\pi}\cdot\frac{h}{1-q^{2n}}\cdot\int_0^{2\pi/h}\mathcal{F}f(\rho)\phi_\rho(y)\frac{d\rho}{|c(\rho)|^2}, \tag{4.11}$$

where $c(\rho)$ (a q-analog of the Harish–Chandra function) is given by

$$c(\rho)=\frac{\Gamma_{q^2}(n)\Gamma_{q^2}(i\rho)}{\Gamma^2_{q^2}(n/2+i\rho/2)}.$$

(iii) The q-spherical transform $\mathcal{F}:\mathcal{L}_{n,q}\to C^\infty(0;2\pi/h)$ *can be extended to a unitary linear operator* $\mathcal{F}:\mathcal{L}^2_{n,q}\to L^2(d\rho/|c(\rho)|^2)$:

$$\frac{1-q^{2n}}{1-q^2}\int_0^1|f(y)|^2y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y=\frac{1}{4\pi}\cdot\frac{h}{1-q^{2n}}\cdot\int_0^{2\pi/h}|\mathcal{F}f(\rho)|^2\frac{d\rho}{|c(\rho)|^2} \quad (4.12)$$

(the Plancherel formula).

Note that, due to (4.10), statement (*iii*) can be rewritten as the orthogonality relations for the Al-Salam-Chihara polynomials (Ref. 13, Sec. 3.8):

$$\frac{1}{4\pi}\int_0^{2\pi/h}Q_k\left(\cos\frac{h\rho}{2};q^n,q^n\middle|q^2\right)Q_m\left(\cos\frac{h\rho}{2};q^n,q^n\middle|q^2\right)\frac{d\rho}{|c(\rho)|^2}=\delta_{km}\cdot\frac{(q^{2n};q^2)^2_k}{h(q^{2k+2};q^2)_{n-1}}. \quad (4.13)$$

D. Proof of Proposition 4.3

It suffices, due to (4.4), to verify that

$$B_{q,t}(f_k)=f_k+t\frac{q^{2n+2}}{(1-q^2)}\cdot((1-q^{2k+2})f_{k+1}-(1+q^{-2n}-2q^{2k})f_k+(q^{-2n}-q^{2k-2})f_{k-1}) \quad (4.14)$$

modulo t^2. For that purpose we compute first T_{f_k}.

Recall the notation $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ (Sec. III A). Define a $\mathbb{Z}_{\geqslant 0}$-grading in the space $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ as follows:

$$\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}=\text{linear span of } \mathbf{z}^{\underline{m}},\ |\underline{m}|=m.$$

We need first the following lemma.

Lemma 4.6:

$$T_{f_k}|_{\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}}=q^{2(k-m)(\alpha+1)}\cdot\frac{(q^{2\alpha+2};q^2)_{n+m}\cdot(q^{2k-2m+2};q^2)_{n+m-1}}{(q^2;q^2)_{n+m-1}}.$$

Proof of the lemma: Using the same arguments as in the classical case, it can be proved that $\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}$, $m\in\mathbb{Z}_{\geqslant 0}$, are pairwise non-isomorphic irreducible $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-modules [we mean restriction of the representation π_α onto $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$]. Due to the $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-invariance of f_k [with respect to the untwisted $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-action], Proposition 3.3, and the Schur lemma,

$$T_{f_k}|_{\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}}=c_k^m.$$

[Since $\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}$ is an irreducible $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-module, the algebra homomorphism $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)\to\mathrm{End}(\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha})$ is surjective, however the only operators commuting with the full matrix algebra are constants.] To compute the constant c_k^m we apply T_{f_k} to a distinguished vector in $\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}$, for example, z_n^m:

$$c_k^m=\frac{(T_{f_k}z_n^m,z_n^m)_{\alpha,q}}{(z_n^m,z_n^m)_{\alpha,q}}=\frac{(f_kz_n^m,z_n^m)_{\alpha,q}}{(z_n^m,z_n^m)_{\alpha,q}}.$$

By Proposition 3.1 the denominator is equal to $(q^2;q^2)_m/(q^{2n+2\alpha+2};q^2)_m$. What remains is to compute the numerator:

$$
\begin{aligned}
(T_{f_k} z_n^m, z_n^m)_{\alpha,q} &= \int_{U_n} z_n^{*m} f_k z_n^m dm_{\alpha,q} \\
&= \int_{U_n} f_{k-m}(q^2 y_n; q^2)_m dm_{\alpha,q} \\
&= (q^{2\alpha+2};q^2)_n \sum_{\underline{k}\in P(n)} f_{k-m}(q^{2k_1})(q^{2+2k_n};q^2)_m q^{2k_1(\alpha+1)} q^{2k_2}\cdots q^{2k_n} \\
&= (q^{2\alpha+2};q^2)_n q^{2(k-m)(\alpha+1)} \sum_{0\leqslant k_n\leqslant\cdots\leqslant k_2\leqslant k-m} (q^{2+2k_n};q^2)_m q^{2k_2}\cdots q^{2k_n}.
\end{aligned}
$$

To continue computation we need the following simple formula which can be proved by induction:

$$
\sum_{a\leqslant l_n\cdots\leqslant l_1\leqslant b} q^{2l_1}\cdots q^{2l_n} = q^{2an}\frac{(q^{2b-2a+2};q^2)_n}{(q^2;q^2)_n}. \tag{4.15}
$$

By this formula $(q^{2+2k_n};q^2)_m = (q^2;q^2)_m \Sigma_{0\leqslant l_m\leqslant\cdots\leqslant l_1\leqslant k_n} q^{2l_1}\cdots q^{2l_m}$. Applying (4.15) one more time, we finally get

$$
(T_{f_k} z_n^m, z_n^m)_{\alpha,q} = (q^{2\alpha+2};q^2)_n q^{2(k-m)(\alpha+1)} (q^2;q^2)_m \frac{(q^{2k-2m+2};q^2)_{n+m-1}}{(q^2;q^2)_{n+m-1}}.
$$

■

Let P_m denote the orthogonal projection in $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ onto $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}^{(m)}$. The above lemma says that

$$
T_{f_k} = \sum_{m=0}^{k} q^{2(k-m)(\alpha+1)} \cdot \frac{(q^{2\alpha+2};q^2)_{n+m}\cdot(q^{2k-2m+2};q^2)_{n+m-1}}{(q^2;q^2)_{n+m-1}} \cdot P_m. \tag{4.16}
$$

Lemma 4.7: The covariant symbol $\sigma(P_m)$ is given by

$$
\sigma(P_m) = q^{-2m(\alpha+n+1)} \cdot \frac{(q^{2\alpha+2n+2};q^2)_m}{(q^2;q^2)_m} \cdot y^{\alpha+n+1} \cdot (yq^{-2m+2};q^2)_m.
$$

Proof of the lemma: Since $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}^{(m)}$, $m\in\mathbb{Z}_{\geqslant 0}$, are pairwise non-isomorphic irreducible $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-modules, the projections P_m are $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_1)$-module morphisms. Thus by Proposition 3.7 $\sigma(P_m)$ should be a function of y. Denote it by $p_m(y)$. Recall that $p_m(y) = \Sigma_{k=0}^{\infty} p_m(q^{2k}) f_k(y)$. The coefficients $p_m(q^{2k})$ can be derived from the equalities

$$
\int_{U_n} p_m(y)\cdot f_l d\nu_q = \mathrm{Tr}_q(P_m\cdot T_{f_l}), \quad l\in\mathbb{Z}_{\geqslant 0}.
$$

Using the property $f_k\cdot f_l = \delta_{kl} f_k$ and Lemma 4.6, we can rewrite the latter equality as follows:

$$
\begin{aligned}
& p_m(q^{2l})\cdot(q^2;q^2)_n\cdot q^{-2nl}\cdot \sum_{0\leqslant k_n\leqslant\cdots\leqslant k_2\leqslant l} q^{2k_2}\cdots q^{2k_n} \\
&\quad = q^{2(l-m)(\alpha+1)}\cdot \frac{(q^{2\alpha+2};q^2)_{n+m}\cdot(q^{2l-2m+2};q^2)_{n+m-1}}{(q^2;q^2)_{n+m-1}}\cdot \mathrm{Tr}_q(P_m).
\end{aligned}
$$

By (3.10) $\mathrm{Tr}_q(P_m) = [(q^2;q^2)_n/(q^{2\alpha+2};q^2)_n]\cdot q^{-2nm}\cdot\Sigma_{0\leqslant k_n\leqslant\cdots\leqslant k_2\leqslant m} q^{2k_2}\cdots q^{2k_n}$. Using (4.15) we obtain $p_m(q^{2l}) = [(q^{2\alpha+2n+2};q^2)_m\cdot(q^{2l-2m+2};q^2)_m/(q^2;q^2)_m]\cdot q^{2(l-m)(\alpha+n+1)}$. ■

We continue the proof of our proposition. Lemmas 4.6 and 4.7 now imply

$$B_{q,\alpha}(f_k)=q^{2k(\alpha+1)}\cdot y^{\alpha+n+1}\cdot\sum_{m=0}^{k}q^{-4m(\alpha+1)-2mn}\cdot\frac{(q^{2\alpha+2};q^2)_{n+m}(q^{2k-2m+2};q^2)_{n+m-1}(q^{2\alpha+2n+2};q^2)_m}{(q^2;q^2)_{n+m-1}(q^2;q^2)_m}\cdot(yq^{-2m+2};q^2)_m.\tag{4.17}$$

Note that $(yq^{-2m+2};q^2)_m=\Sigma_{l=0}^{\infty}(q^{2l-2m+2};q^2)_m\cdot f_l=\Sigma_{l=m}^{\infty}(q^{2l-2m+2};q^2)_m\cdot f_l$. Consequently,

$$y^{\alpha+n+1}\cdot(yq^{-2m+2};q^2)_m=\sum_{l=m}^{\infty}q^{2l(\alpha+n+1)}\cdot(q^{2l-2m+2};q^2)_m\cdot f_l=\sum_{r=0}^{\infty}q^{2(m+r)(\alpha+n+1)}\cdot(q^{2r+2};q^2)_m\cdot f_{m+r},$$

and

$$B_{q,\alpha}(f_k)=\sum_{m=0}^{k}\sum_{r=0}^{\infty}q^{2\alpha(k-m+r)}\cdot q^{2k-2m+2rn+2r}\cdot\frac{(q^{2\alpha+2};q^2)_{n+m}(q^{2k-2m+2};q^2)_{n+m-1}(q^{2\alpha+2n+2};q^2)_m(q^{2r+2};q^2)_m}{(q^2;q^2)_{n+m-1}(q^2;q^2)_m}\cdot f_{m+r}.$$

The substitution $t=q^{2\alpha}$ gives

$$B_{q,t}(f_k)=\sum_{m=0}^{k}\sum_{r=0}^{\infty}t^{k-m+r}\cdot q^{2k-2m+2rn+2r}\cdot\frac{(tq^2;q^2)_{n+m}(q^{2k-2m+2};q^2)_{n+m-1}(tq^{2n+2};q^2)_m(q^{2r+2};q^2)_m}{(q^2;q^2)_{n+m-1}(q^2;q^2)_m}\cdot f_{m+r}.$$

To finish the proof of (4.14) we have to compute the coefficient at t in the last series. Due to presence of t^{k-m+r} in the sum, the only terms which might give a nonzero contribution to this coefficient correspond to the values $(m,r)=(k,0)$, $(m,r)=(k,1)$, or $(m,r)=(k-1,0)$ which we treat separately.

(1) $(m,r)=(k,0)$: the corresponding term is equal to

$$(tq^2;q^2)_{n+k}(tq^{2n+2};q^2)_k f_k=\left(1-t\frac{q^{2n+2}}{(1-q^2)}(1+q^{-2n}-2q^{2k})\right)f_k+o(t).$$

(2) $(m,r)=(k,1)$: the corresponding term is equal to

$$t\cdot q^{2n+2}\cdot(tq^2;q^2)_{n+k}(tq^{2n+2};q^2)_k\frac{1-q^{2k+2}}{1-q^2}f_{k+1}=t\cdot\frac{q^{2n+2}}{(1-q^2)}\cdot(1-q^{2k+2})f_{k+1}+o(t).$$

(3) $(m,r)=(k-1,0)$: the corresponding term is equal to

$$t\cdot q^2\cdot(tq^2;q^2)_{n+k-1}(tq^{2n+2};q^2)_{k-1}\frac{1-q^{2n+2k-2}}{1-q^2}f_{k-1}=t\cdot\frac{q^{2n+2}}{(1-q^2)}\cdot(q^{-2n}-q^{2k-2})f_{k-1}+o(t).$$

This finishes the proof.

V. FURTHER PROPERTIES OF THE *q*-BEREZIN TRANSFORM

In this section we study further the q-Berezin transform. Namely, we consider its restriction $B^{(\mathrm{r})}_{q,\alpha}$ onto the space of radial functions. We prove that $B^{(\mathrm{r})}_{q,\alpha}$ is extended to a bounded self-adjoint operator on $\mathcal{L}^2_{n,q}$ which commutes with the radial part $\Delta^{(\mathrm{r})}_{n,q}$ of the q-Laplace–Beltrami operator. Since the latter has a simple spectrum, $B^{(\mathrm{r})}_{q,\alpha}$ is a function of $\Delta^{(\mathrm{r})}_{n,q}$. We find the function explicitly. In the classical case this is computed in Ref. 24 We also present an asymptotic expansion for the q-Berezin transform at the limit $t=q^{2\alpha}\to 0$ mentioned at the end of Sec. IV A.

A. Boundedness of the *q*-Berezin transform

Let $B^{(\mathrm{r})}_{q,\alpha}:\mathcal{L}_{n,q}\to\mathcal{L}'_{n,q}$ be restriction of the q-Berezin transform onto the space $\mathcal{L}_{n,q}$ of finite radial functions on the quantum ball.

Proposition 5.1: $B^{(\mathrm{r})}_{q,\alpha}$ can be extended to a bounded self-adjoint operator on $\mathcal{L}^2_{n,q}$. It is a function of $\Delta^{(\mathrm{r})}_{n,q}$. The operator $\mathcal{F}\cdot B^{(\mathrm{r})}_{q,\alpha}\cdot\mathcal{F}^{-1}$ on $L^2(d\rho/|c(\rho)|^2)$ is the multiplication by the (bounded) function

$$b_{q,\alpha}(\rho)=\frac{(q^{2+2\alpha};q^2)_\infty\cdot(q^{2n+2+2\alpha};q^2)_\infty}{(q^{n+2+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty}. \tag{5.1}$$

Proof: We divide the proof into three lemmas.

Lemma 5.2: $B^{(\mathrm{r})}_{q,\alpha}(\mathcal{L}_{n,q})\subset\mathcal{L}^2_{n,q}$ and one has the equality

$$\Delta^{(\mathrm{r})}_{n,q}\cdot B^{(\mathrm{r})}_{q,\alpha}=B^{(\mathrm{r})}_{q,\alpha}\cdot\Delta^{(\mathrm{r})}_{n,q} \tag{5.2}$$

of linear maps from $\mathcal{L}_{n,q}$ to $\mathcal{L}^2_{n,q}$.

Sketch of a proof: The inclusion is due to the formula (4.17). Indeed, one has to show that $y^{\alpha+n+1}\cdot(yq^{-2m+2};q^2)_m\in\mathcal{L}^2_{n,q}$ for any m, and this is clear by the definition.

To prove the equality (5.2), we have to show that $\Delta^{(\mathrm{r})}_{n,q}\cdot B^{(\mathrm{r})}_{q,\alpha}(f_k)=B^{(\mathrm{r})}_{q,\alpha}\cdot\Delta^{(\mathrm{r})}_{n,q}(f_k)$ for any k. The left-hand side may be computed by successive application of (4.17) and (4.5) while the right-hand one may be computed via Proposition 4.3 and (4.17). ■

Lemma 5.3: Suppose B is a linear operator from $\mathcal{L}_{n,q}$ to $\mathcal{L}^2_{n,q}$ which satisfies the properties

$$\Delta^{(\mathrm{r})}_{n,q}\cdot B=B\cdot\Delta^{(\mathrm{r})}_{n,q};$$

$$Bf_0=(q^{2\alpha+2};q^2)_n\cdot y^{\alpha+n+1}.$$

Then $B=B^{(\mathrm{r})}_{q,\alpha}$.

Proof: The statement is a simple consequence of the equality

$$\mathcal{L}_{n,q}=\text{linear span of }\{(\Delta^{(\mathrm{r})}_{n,q})^m f_0\}_{m\in\mathbb{Z}_{\geqslant 0}},$$

which in turn may be deduced easily from Proposition 4.3. ■

Lemma 5.4: The bounded self-adjoint operator $\mathcal{F}^{-1}\cdot b_{q,\alpha}(\rho)\cdot\mathcal{F}$ [$b_{q,\alpha}$ is given by (5.1)] on $\mathcal{L}^2_{n,q}$ possesses the properties from the previous lemma.

Proof: The first property holds trivially. Let us prove the second one.

Let $(\cdot,\cdot)_{L^2}$, $(\cdot,\cdot)_{\mathcal{L}^2}$ be the inner products in $L^2(d\rho/|c(\rho)|^2)$ and $\mathcal{L}^2_{n,q}$, respectively. It is sufficient to show that

$$(b_{q,\alpha}(\rho)\cdot\mathcal{F}f_0,\ \mathcal{F}f_k)_{L^2}=(q^{2\alpha+2};q^2)_n\cdot(y^{\alpha+n+1},\ f_k)_{\mathcal{L}^2}$$

for any $k\in\mathbb{Z}_{\geqslant 0}$. Recall (4.10) that $\mathcal{F}f_k(\rho)=(1-q^{2n})\cdot q^{-kn}\cdot[(q^{2k+2};q^2)_{n-1}/(q^{2n};q^2)_k]\cdot Q_k(\rho)$ with $Q_k(\rho):=Q_k(\cos(h\rho/2);q^n,q^n|q^2)$. We rewrite the condition as follows:

$$(b_{q,\alpha}(\rho),\ Q_k(\rho))_{L^2}=q^{k(n+2+2\alpha)}\cdot\frac{(q^{2\alpha+2};q^2)_n}{(q^2;q^2)_n}. \tag{5.3}$$

Keep in mind the following formula for the generating function of the Al-Salam-Chihara polynomials [Ref. 13 formula (3.8.13)]:

$$\sum_{j=0}^{\infty} \frac{z^j}{(q^2;q^2)_j} \cdot Q_j(\rho) = \frac{(q^n z;q^2)_\infty \cdot (q^n z;q^2)_\infty}{(q^{i\rho} z;q^2)_\infty \cdot (q^{-i\rho} z;q^2)_\infty}.$$

Substitution $z := q^{2\alpha+2+n}$ gives $(q^{2\alpha+2};q^2)_n \Sigma_{j=0}^{\infty} [q^{j(2\alpha+n+2)}/(q^2;q^2)_j] \cdot Q_j(\rho) = b_{q,\alpha}(\rho)$. Now validity of (5.3) follows from the latter equality and the orthogonality relations (4.13) for the Al-Salam-Chihara polynomials. ■

Proposition 5.1 follows directly from the last two lemmas.

B. Asymptotic expansion of the *q*-Berezin transform

Proposition 5.5: For any $f \in \mathcal{D}(U_n)_q$

$$B_{q,t}(f) = (q^2 t;q^2)_n \cdot \sum_{j=0}^{\infty} t^j \cdot q^{2j} \cdot \frac{(q^{2j+2};q^2)_{n-1}}{(q^2;q^2)_{n-1}} \cdot p_j(\Delta_{n,q}) f$$

with

$$p_j(\Delta_{n,q}) = \sum_{l=0}^{j} \frac{(q^{-2j};q^2)_l \cdot q^{2l}}{(q^{2n};q^2)_l \cdot (q^2;q^2)_l} \cdot \prod_{m=0}^{l-1} ((1-q^{2m})(1-q^{2m+2n}) - q^{2m+2n-2}(1-q^2)^2 \Delta_{n,q}).$$

Proof: Recall [see (3.9)] that

$$B_{q,\alpha}(f_0) = (q^{2\alpha+2};q^2)_n \cdot y^{\alpha+n+1} = (q^{2\alpha+2};q^2)_n \cdot \sum_{j=0}^{\infty} q^{2j(\alpha+n+1)} \cdot f_j$$

or, in terms of $t = q^{2\alpha}$,

$$B_{q,t}(f_0) = (tq^2;q^2)_n \cdot \sum_{j=0}^{\infty} t^j q^{2j(n+1)} \cdot f_j.$$

Since any morphism of $U_q\mathfrak{su}_{n,1}$-modules is determined uniquely by its value on the vector f_0, it suffices to prove that $p_j(\Delta_{n,q}) f_0 = q^{2jn} \cdot [(q^2;q^2)_{n-1}/(q^{2j+2};q^2)_{n-1}] \cdot f_j$ or, equivalently,

$$p_j(\Delta_{n,q}^{(r)}) f_0 = q^{2jn} \cdot \frac{(q^2;q^2)_{n-1}}{(q^{2j+2};q^2)_{n-1}} \cdot f_j.$$

Let us apply the q-spherical transform $\mathcal{F}$ to both sides of the latter equality. We get

$$p_j(\lambda(\rho)) \mathcal{F} f_0(\rho) = q^{2jn} \cdot \frac{(q^2;q^2)_{n-1}}{(q^{2j+2};q^2)_{n-1}} \cdot \mathcal{F} f_j(\rho). \tag{5.4}$$

Recall [see (4.10)] that $\mathcal{F} f_k(\rho) = (1-q^{2n}) \cdot q^{-2kn} \cdot (q^{2k+2};q^2)_{n-1} \cdot \phi_\rho(q^{2k})$. This formula reduces proving (5.4) to proving the equality

$$p_j(\lambda(\rho)) = \phi_\rho(q^{2j}), \tag{5.5}$$

and the latter is just a straightforward computation. ■

VI. AN APPLICATION: ORTHOGONALITY RELATIONS FOR CONTINUOUS DUAL *q*-HAHN POLYNOMIALS

The aim of this section is to describe one application of our results to the theory of basic orthogonal polynomials. Namely, we use the q-Berezin and the q-spherical transform to obtain orthogonality relations for certain two-parameter family of the so-called continuous dual q-Hahn polynomials (see Ref. 13). Of course, this result is not new. However, we believe that our approach might be interesting.

Throughout this section $\alpha > -1$ is a fixed number.

A. Auxiliary results

The aim of this subsection is to derive some useful consequences of Proposition 5.1.

Proposition 6.1: $B^{(\mathrm{r})}_{q,\alpha}$ is extended to an invertible operator on $\mathcal{L}^{\,2}_{n,q}$.

Proof: It suffices to observe that the "symbol" $b_{q,\alpha}(\rho)$ is invertible:

$$b_{q,\alpha}(\rho) \geqslant \frac{(q^{2+2\alpha};q^2)_\infty \cdot (q^{2n+2+2\alpha};q^2)_\infty}{(-q^{n+2+2\alpha};q^2)_\infty \cdot (-q^{n+2+2\alpha};q^2)_\infty} > 0.$$

■

To go further, we introduce some auxiliary notations. Denote by $\mathcal{L}_{\mathrm{Op}}$ and $\mathcal{L}'_{\mathrm{Op}}$ the subspaces of $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-module morphisms in $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ and $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$, respectively. Since the subspaces $\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}$, $m \in \mathbb{Z}_{\geqslant 0}$, in $\mathbb{C}[\mathbb{C}^n]_{q,\alpha}$ are pairwise non-isomorphic irreducible $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_1)$-modules (see the proof of Lemma 4.6), the vector space $\mathcal{L}_{\mathrm{Op}}$ is generated by the orthogonal projections P_m onto the subspaces $\mathbb{C}[\mathbb{C}^n]^{(m)}_{q,\alpha}$. $\mathcal{L}'_{\mathrm{Op}}$ is the space of infinite series of the form

$$T = \sum_m a_m P_m, \quad a_m \in \mathbb{C}.$$

Elements of $\mathcal{L}_{\mathrm{Op}}$ and $\mathcal{L}'_{\mathrm{Op}}$ play the role of "radial" elements in $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ and $\mathrm{End}(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$.

Let $\mathcal{L}^{\,2}_{\mathrm{Op}}$ be the subspace in $\mathcal{L}'_{\mathrm{Op}}$ of "q-Hilbert–Schmidt" operators:

$$\mathcal{L}^{\,2}_{\mathrm{Op}} = \{T \in \mathcal{L}'_{\mathrm{Op}} \mid \mathrm{Tr}_q(T^* \cdot T) < \infty\}.$$

Note that the triple $(\mathcal{L}_{\mathrm{Op}}, \mathcal{L}'_{\mathrm{Op}}, \mathcal{L}^{\,2}_{\mathrm{Op}})$ is very similar to the triple $(\mathcal{L}_{n,q}, \mathcal{L}'_{n,q}, \mathcal{L}^{\,2}_{n,q})$ introduced in Sec. IV C.

Recall (Sec. III D) the notation σ for the linear map from $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ to $\mathcal{D}(U_n)'_q$ which sends endomorphisms to their covariant symbols. Due to Proposition 3.7 $\sigma(\mathcal{L}_{\mathrm{Op}}) \subset \mathcal{L}'_{n,q}$. Let us denote restriction of σ onto $\mathcal{L}_{\mathrm{Op}}$ by $\sigma^{(\mathrm{r})}$.

Proposition 6.2: The image of operator $\sigma^{(\mathrm{r})}$ lies in $\mathcal{L}^{\,2}_{n,q}$. Moreover, $\sigma^{(\mathrm{r})}$ can be extended to a bounded invertible operator from $\mathcal{L}^{\,2}_{\mathrm{Op}}$ to $\mathcal{L}^{\,2}_{n,q}$.

Proof: Recall (Sec. III D) that the map σ is defined via the equality

$$\int_{U_n} \sigma(T) \cdot f \, d\nu_q = \mathrm{Tr}_q(T \cdot T_f),$$

which should be fulfilled for any $f \in \mathcal{D}(U_n)_q$. Let $T^{(\mathrm{r})}$ be restriction onto $\mathcal{L}_{n,q}$ of the operator from $\mathcal{D}(U_n)_q$ to $\mathrm{End}_0(\mathbb{C}[\mathbb{C}^n]_{q,\alpha})$ which sends finite functions to the corresponding Toeplitz operators. By Proposition 3.3 $T^{(\mathrm{r})}(\mathcal{L}_{n,q}) \subset \mathcal{L}'_{\mathrm{Op}}$. More precisely, by Lemma 4.6,

$$T^{(\mathrm{r})}(\mathcal{L}_{n,q}) \subset \mathcal{L}_{\mathrm{Op}}. \tag{6.1}$$

In particular, $T^{(r)}$ can be considered as a densely defined operator from $\mathcal{L}^2_{n,q}$ into $\mathcal{L}^2_{\mathrm{Op}}$. The above definition of σ implies the following equivalent definition of $\sigma^{(r)}$: for an element $T\in\mathcal{L}_{\mathrm{Op}}$ one has $\sigma^{(r)}(T)=t(y)$ iff

$$\frac{1-q^{2n}}{1-q^2}\int_0^1 t(y)f(y)y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y=\mathrm{Tr}_q(T\cdot T^{(r)}(f(y))) \tag{6.2}$$

for any $f(y)\in\mathcal{L}_{n,q}$. Let us prove that $T^{(r)}$ can be extended up to a bounded operator from $\mathcal{L}^2_{n,q}$ to $\mathcal{L}^2_{\mathrm{Op}}$. Suppose $f(y)\in\mathcal{L}_{n,q}$. Then, by (6.1) and (6.2)

$$\begin{aligned}\mathrm{Tr}_q((T^{(r)}(f(y)))^*\cdot T^{(r)}(f(y)))&=\frac{1-q^{2n}}{1-q^2}\int_0^1\sigma^{(r)}\cdot T^{(r)}(f(y))\overline{f(y)}y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y\\&=\frac{1-q^{2n}}{1-q^2}\int_0^1 B^{(r)}_{q,\alpha}(f(y))\overline{f(y)}y^{-n-1}(yq^2;q^2)_{n-1}d_{q^2}y\\&=(B^{(r)}_{q,\alpha}f,f)_{\mathcal{L}^2}\leqslant\|B^{(r)}_{q,\alpha}\|(f,f)_{\mathcal{L}^2}.\end{aligned}$$

To prove boundedness of $\sigma^{(r)}$ it remains to observe that, by (6.2), $\sigma^{(r)}$ coincides on $\mathcal{L}_{\mathrm{Op}}$ with $(T^{(r)})^*$. Invertibility of $\sigma^{(r)}$ may be deduced using similar arguments and Proposition 6.1. ■

B. Orthogonality relations

First we describe an idea of producing the orthogonality relations. It is based on the following statement.

Proposition 6.3: The operator

$$U_\alpha:\mathcal{L}^2_{\mathrm{Op}}\to L^2\left(\frac{d\rho}{|c(\rho)|^2}\right),\quad T\mapsto\frac{1}{\sqrt{b_{q,\alpha}(\rho)}}\cdot\mathcal{F}\sigma^{(r)}(T)$$

is unitary.

Remark: In the classical case the operator U_α (the product of the spherical transform with the unitary part of the covariant symbol map) was studied in Ref. 14.

Proof: By Proposition 5.1

$$\frac{1}{b_{q,\alpha}(\rho)}\cdot\mathcal{F}=\mathcal{F}(B^{(r)}_{q,\alpha})^{-1}.$$

Keep in mind the notation $(\cdot,\cdot)_{L^2}$, $(\cdot,\cdot)_{\mathcal{L}^2}$ for the inner products in $L^2(d\rho/|c(\rho)|^2)$ and $\mathcal{L}_{n,q}$, respectively. Then

$$\begin{aligned}&\left(\frac{1}{\sqrt{b_{q,\alpha}(\rho)}}\cdot\mathcal{F}\sigma^{(r)}(T),\ \frac{1}{\sqrt{b_{q,\alpha}(\rho)}}\cdot\mathcal{F}\sigma^{(r)}(T)\right)_{L^2}\\&\quad=\left(\frac{1}{b_{q,\alpha}(\rho)}\cdot\mathcal{F}\sigma^{(r)}(T),\ \mathcal{F}\sigma^{(r)}(T)\right)_{L^2}\\&\quad=(\mathcal{F}(B^{(r)}_{q,\alpha})^{-1}\sigma^{(r)}(T),\ \mathcal{F}\sigma^{(r)}(T))_{L^2}=((B^{(r)}_{q,\alpha})^{-1}\sigma^{(r)}(T),\ \sigma^{(r)}(T))_{\mathcal{L}^2}.\end{aligned}$$

The result then follows since $(B^{(r)}_{q,\alpha})^{-1}=(\sigma^{(r)*})^{-1}\cdot(\sigma^{(r)})^{-1}$. ■

Recall that the projections P_m, $m\in\mathbb{Z}_{\geqslant 0}$, constitute an orthogonal basis in the Hilbert space $\mathcal{L}^2_{Op}$. Proposition 6.3 implies that $\mathcal{F}\sigma^{(r)}(P_m)$, $m\in\mathbb{Z}_{\geqslant 0}$, constitute an orthogonal basis in

$L^2(d\rho/b_{q,\alpha}(\rho)|c(\rho)|^2)$. Our intention now is to show that $\mathcal{F}\sigma^{(r)}(P_m)$ are very close to certain continuous dual q-Hahn polynomials, and the above observations will give us the orthogonality relations for these polynomials.

Proposition 6.4: Let $P_m(\rho)=\mathcal{F}\sigma^{(r)}(P_m)(\rho)$. *Then*

$$P_m(\rho)=\frac{(q^2;q^2)_n\cdot(q^{2n+2+2\alpha};q^2)_\infty^2}{(q^{n+2+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty}\cdot q^{-2m(n+\alpha)}\cdot\frac{(q^{2n+2+2\alpha};q^2)_m}{(q^2;q^2)_m}$$
$$\cdot{}_3\phi_2\left(\begin{matrix}q^{-2m}, & q^{n+2+2\alpha+i\rho}, & q^{n+2+2\alpha-i\rho},\\ & q^{2n+2+2\alpha}, & q^{2n+2+2\alpha}\end{matrix}\;\begin{matrix}\\ q^2, & q^2\end{matrix}\right).$$

Proof: Keep in mind (Lemma 4.7) that we have already computed $\sigma^{(r)}(P_m)$

$$\sigma^{(r)}(P_m)=q^{-2m(\alpha+n+1)}\cdot\frac{(q^{2\alpha+2n+2};q^2)_m}{(q^2;q^2)_m}\cdot y^{\alpha+n+1}\cdot(yq^{-2m+2};q^2)_m.$$

By the q-binomial formula[20] the equality can be rewritten as follows:

$$\sigma^{(r)}(P_m)=q^{-2m(\alpha+n+1)}\cdot\frac{(q^{2\alpha+2n+2};q^2)_m}{(q^2;q^2)_m}\cdot\sum_{l=0}^{m}\frac{(q^2;q^2)_m}{(q^2;q^2)_l(q^2;q^2)_{m-l}}\cdot(-1)^m$$
$$\cdot q^{l(l-2m+1)}\cdot y^{n+1+l+\alpha}$$
$$=q^{-2m(\alpha+n+1)}\cdot\sum_{l=0}^{m}\frac{(q^{2\alpha+2n+2};q^2)_m}{(q^2;q^2)_l(q^2;q^2)_{m-l}}\cdot(-1)^m\cdot q^{l(l-2m+1)}\cdot y^{n+1+l+\alpha}. \quad (6.3)$$

Hence it remains to compute $\mathcal{F}y^{n+1+l+\alpha}$ for any $l\geqslant 0$. Let us apply the q-spherical transform to both sides of the formula $B_{q,\alpha}(f_0)=(q^{2\alpha+2};q^2)_n\cdot y^{\alpha+n+1}$. Due to Proposition 5.1

$$\frac{(q^{2+2\alpha};q^2)_\infty\cdot(q^{2n+2+2\alpha};q^2)_\infty}{(q^{n+2+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty}\cdot\mathcal{F}f_0=(q^{2+2\alpha};q^2)_n\cdot\mathcal{F}y^{n+1+\alpha},$$

or, equivalently,

$$\mathcal{F}y^{n+1+\alpha}=\frac{(q^2;q^2)_n\cdot(q^{2n+2+2\alpha};q^2)_\infty^2}{(q^{n+2+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty}.$$

Let us make the substitution $N:=n+1+\alpha$ $(N>n+1)$:

$$\mathcal{F}y^{N}=\frac{(q^2;q^2)_n\cdot(q^{2N};q^2)_\infty^2}{(q^{2N-n+i\rho};q^2)_\infty\cdot(q^{2N-n-i\rho};q^2)_\infty}.$$

Thus,

$$\mathcal{F}y^{n+1+l+\alpha}=\frac{(q^2;q^2)_n\cdot(q^{2n+2+2l+2\alpha};q^2)_\infty^2}{(q^{n+2+2l+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2l+2\alpha-i\rho};q^2)_\infty}.$$

The latter equality, together with (6.3) and simple computations, gives our formula. ■

Recall the notation $p_k(x;a,b,c|q)$ for the continuous dual q-Hahn polynomials (Ref. 13, Sec. 3.3). The above proposition implies

$$\mathcal{F}\sigma^{(r)}(P_m)=\frac{q^{-mn}\cdot(q^2;q^2)_n\cdot(q^{2n+2+2\alpha};q^2)_\infty\cdot(q^{2n+2m+2+2\alpha};q^2)_\infty}{(q^{n+2+2\alpha+i\rho};q^2)_\infty\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty\cdot(q^2;q^2)_m}$$
$$\cdot p_m\left(\cos\frac{h\rho}{2};q^{n+2+2\alpha},q^n,q^n\middle|q^2\right).$$

Let $p_m(\rho):=p_m(\cos(h\rho/2);q^{n+2+2\alpha},q^n,q^n|q^2)$. Applying Proposition 6.3 and the above observations, we get

$$\frac{1}{4\pi}\int_0^{2\pi/h}p_m(\rho)p_l(\rho)\frac{d\rho}{(q^{n+2+2\alpha+i\rho};q^2)_\infty^2\cdot(q^{n+2+2\alpha-i\rho};q^2)_\infty^2\cdot b_{q,\alpha}(\rho)|c(\rho)|^2}$$
$$=\frac{q^{2mn}\cdot(1-q^{2n})\cdot(q^2;q^2)_m^2}{h\cdot(q^2;q^2)_n^2\cdot(q^{2n+2+2\alpha};q^2)_\infty^2\cdot(q^{2n+2m+2+2\alpha};q^2)_\infty^2}\cdot\mathrm{Tr}_q(P_m\cdot P_l),$$

or, using the explicit formula for $b_{q,\alpha}$,

$$\frac{1}{4\pi}\int_0^{2\pi/h}p_m(\rho)p_l(\rho)\frac{d\rho}{(q^{n+2+2\alpha+i\rho};q^2)_\infty(q^{n+2+2\alpha-i\rho};q^2)_\infty|c(\rho)|^2}$$
$$=\delta_{ml}\frac{(q^2;q^2)_m(q^2;q^2)_{m+n-1}}{h(q^2;q^2)_{n-1}(q^{2n+2m+2+2\alpha};q^2)_\infty^2}.$$

Recall (Proposition 4.5) that

$$\frac{1}{|c(\rho)|^2}=\left|\frac{\Gamma_{q^2}^2(n/2+i\rho/2)}{\Gamma_{q^2}(n)\Gamma_{q^2}(i\rho)}\right|^2=(q^{2n};q^2)_\infty^2\cdot\frac{(q^{2i\rho};q^2)_\infty(q^{-2i\rho};q^2)_\infty}{(q^{n+i\rho};q^2)_\infty^2(q^{n-i\rho};q^2)_\infty^2}.$$

Finally we have

$$\frac{1}{4\pi}\int_0^{2\pi/h}p_m(\rho)p_l(\rho)\frac{(q^{2i\rho};q^2)_\infty(q^{-2i\rho};q^2)_\infty}{(q^{n+2+2\alpha+i\rho};q^2)_\infty(q^{n+2+2\alpha-i\rho};q^2)_\infty(q^{n+i\rho};q^2)_\infty^2(q^{n-i\rho};q^2)_\infty^2}d\rho$$
$$=\delta_{ml}\frac{1}{h(q^{2n+2m+2+2\alpha};q^2)_\infty^2(q^{2m+2};q^2)_\infty(q^{2n+2m};q^2)_\infty}.$$

The latter equality is a particular case of the orthogonality relations for the entire family of continuous dual q-Hahn polynomials given in Ref. 13 (3.3.2).

VII. CONCLUSION

As it was mentioned in the Introduction, this research is, above all, a part of the general program of studying q-Cartan domains, which we believe is a promising subject in quantum group theory. To our knowledge the results above on finding a mathematical setting for the Toeplitz and covariant calculi, expressing Berezin transform as a function of the q-Laplacian operator, and on computing the covariant symbol of the projections are all new. Those results, in the classical case, are naturally related to finding an expansion of the associate $*$-product $f*_h g$ of covariant symbols as a power series in the Planck constant h (see, e.g., Ref. 25). Thus, the most natural continuation of the present paper would be understanding the expansion of the $*$-product in this case since certain computation might be easier than in the classical case, and generalization of our results to the case of other, more complicated q-Cartan domains, first of all, q-matrix balls.[9,10] We mention Ref. 10 where q-weighted Bergman spaces on q-matrix balls are constructed and studied. Using these results, it is not so difficult to generalize our definition of the q-Berezin transform. However, to obtain more deep results (for instance, an explicit asymptotic formula for the q-Berezin trans-

form) one needs to develop to some extent harmonic analysis on q-matrix balls. This seems to be a difficult problem itself. By now, harmonic analysis is developed quite well for compact quantum homogeneous spaces only. Nevertheless, we are fully confident that all the results we present in this article admit generalization to other q-Cartan domains.

ACKNOWLEDGMENTS

It is our pleasure to thank Leonid Vaksman for many interesting discussions. This research was supported by Royal Swedish Academy of Sciences under the program ''Cooperation between researchers in Sweden and the former Soviet Union.'' We thank also the anonymous referee for expert comments and advice.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 9 SEPTEMBER 2003

Algebraic classification of the curvature of three-dimensional manifolds with indefinite metric

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(Received 25 November 2002; accepted 30 April 2003)

The curvature of a three-dimensional Riemannian manifold with Lorentzian signature is algebraically classified using the fact that the spinor equivalent of the traceless part of the Ricci tensor is a totally symmetric four-index spinor. Following G. S. Hall and M. S. Capocci [J. Math. Phys. **40**, 1466 (1999)] it is shown that at each point of the manifold there exists four, possibly complex, null vectors which are analogous to the Debever–Penrose vectors and also satisfy the condition $R_{ab}l^a l^b = 0$. It is also shown that a similar conclusion holds for the Cotton–York tensor. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1592611]

I. INTRODUCTION

The usefulness of the two-component spinor formalism in general relativity is well established and an illustrative example of it can be found in the algebraic classification of the conformal curvature (see, e.g., Refs. 1 and 2). At each point of the space-time manifold, the spinor equivalent of the conformal curvature tensor is given by a totally symmetric four-index spinor (the Weyl spinor) and its complex conjugate. The Weyl spinor is the symmetrized product of four one-index spinors which define four null directions whose coincidences determine the algebraic type of the conformal curvature.

In the case of a Riemannian manifold of dimension three, the Riemann curvature tensor is determined by the Ricci tensor alone and therefore the curvature can be classified using the Ricci tensor directly. By considering a three-dimensional space with indefinite (Lorentzian) metric, Hall *et al.*[3,4] obtained four canonical forms for symmetric two-index tensors in terms of triads $\{l_a, n_a, x_a\}$ such that $l^a n_a = 1 = x^a x_a$, with all other products equal to zero, which were then applied to classify the Ricci and the Cotton–York tensors. The Cotton–York tensor is analogous to the conformal curvature tensor of a Riemannian manifold of dimension greater than three in the sense that its vanishing is locally equivalent to the conformal flatness of the manifold.

It is noteworthy that a spinor formalism similar to that employed in the four-dimensional space–time can be applied in the case of space–times of $2+1$ dimensions, that is, three-dimensional Riemannian manifolds with indefinite metric. By contrast with the two-component spinors in four dimensions, for which two types of spinor indices are necessary, in a three-dimensional space only one type of spinor indices is required.[5–7]

The traceless symmetric real two-index tensors in three-dimensional spaces have been classified in Ref. 6 making use of the fact that the spinor equivalent of a tensor of this type can be expressed as the symmetrized product of four one-index spinors. The aim of this paper is to apply this classification to the traceless part of the Ricci tensor and to the Cotton–York tensor of a three-dimensional manifold with Lorentzian signature and to establish some properties of the curvature tensors that follow from those of their spinor equivalents. It should be remarked that

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since the Cotton–York and the Ricci tensor are symmetric two-index tensors, the same classification scheme can be applied to both of them. The classification employed here is also of interest in the case of a four-dimensional manifold with ultra-hyperbolic, or Kleinian, signature $(++--)$, since its conformal curvature corresponds to two independent four-index totally symmetric spinors and the spin group is isomorphic to the product of two copies of $SL(2,\mathbb{R})$ or of $SU(1,1)$.

In Sec. II a brief description of the spinor formalism for three-dimensional spaces with indefinite metric is given and in Sec. III this formalism is applied in the classification of the curvature of a three-dimensional manifold with Lorentzian signature.

II. SPINORS IN THREE-DIMENSIONAL SPACES WITH INDEFINITE METRIC

A two-component spinor formalism analogous to that employed in the study of the spin of the electron in nonrelativistic quantum mechanics can be applied in any three-dimensional real vector space, V, with an indefinite metric tensor. A one-index spinor has two complex components which will be denoted by symbols like ψ_A or ψ^A, where the capital italic indices take two values only, e.g., 1 and 2. The spinor indices will be lowered or raised following the rules

$$\psi_A=\varepsilon_{AB}\psi^B, \quad \psi^A=-\varepsilon^{AB}\psi_B, \tag{1}$$

where

$$(\varepsilon_{AB})=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}=(\varepsilon^{AB}). \tag{2}$$

Hence, $\psi_A\phi^A=-\psi^A\phi_A$, for any pair of one-index spinors, $\varepsilon^A{}_B=\delta^A_B$, and $\varepsilon_B{}^A=-\delta^A_B$.

If $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ is an orthogonal basis of V with respect to which the components of the metric tensor are given by $(g_{ab})=\mathrm{diag}(1,1,-1)$, $a,b,\ldots=1,2,3$, and $\sigma^a{}_{AB}$ are (possibly complex) scalars such that

$$\sigma^a{}_{AB}=\sigma^a{}_{BA}, \tag{3}$$

$$\sigma^a{}_{AB}\sigma^b{}_{CD}g_{ab}=-(\varepsilon_{AC}\varepsilon_{BD}+\varepsilon_{AD}\varepsilon_{BC}), \tag{4}$$

then with each vector with components v^a we can associate its spinor equivalent with components

$$v_{AB}=\frac{1}{\sqrt{2}}\sigma^a{}_{AB}v_a. \tag{5}$$

(The tensor indices, $a,b,\ldots$, are raised or lowered by means of g^{ab} and g_{ab} in the usual way.)

Equation (4) is equivalent to

$$\sigma_a{}^{AB}\sigma_{bAB}=-2g_{ab}. \tag{6}$$

Hence, from Eq. (5) we have

$$v_a=-\frac{1}{\sqrt{2}}\sigma_a{}^{AB}v_{AB}. \tag{7}$$

In general, if $t_{ab\cdots d}$ are the components of an n-index tensor, the components of its spinor equivalent are defined by

$$t_{ABCD\cdots GH}=\frac{1}{\sqrt{2}}\sigma^a{}_{AB}\frac{1}{\sqrt{2}}\sigma^b{}_{CD}\cdots\frac{1}{\sqrt{2}}\sigma^d{}_{GH}t_{ab\cdots d}. \tag{8}$$

Then

$$t_{ab\cdots d}=\left(-\frac{1}{\sqrt{2}}\sigma_a{}^{AB}\right)\left(-\frac{1}{\sqrt{2}}\sigma_b{}^{CD}\right)\cdots\left(-\frac{1}{\sqrt{2}}\sigma_d{}^{GH}\right)t_{ABCD\cdots GH} \tag{9}$$

and

$$t_{\cdots a\cdots}\ \ s^{\cdots a\cdots}=-t_{\cdots AB\cdots}\ \ s^{\cdots AB\cdots}. \tag{10}$$

Owing to Eq. (3) the components of the spinor equivalent of a tensor are symmetric on each pair of spinor indices corresponding to a tensor index, $t_{ABCD\cdots GH}=t_{(AB)(CD)\cdots(GH)}$, where the parentheses denote symmetrization on the indices enclosed. The components $t_{ABCD\cdots GH}$ may have additional symmetries depending on those of $t_{ab\ldots d}$. For instance, if t_{ab} are the components of a skewsymmetric two-index tensor then $t_{ABCD}=-t_{CDAB}$ and, therefore, the components t_{ABCD} can be expressed in the form

$$t_{ABCD}=\tau_{BD}\varepsilon_{AC}+\tau_{AC}\varepsilon_{BD}, \tag{11}$$

where τ_{AB} is a symmetric object ($\tau_{AB}=\frac{1}{2}t^R{}_{ARB}$).

Similarly, if the t_{ab} are the components of a symmetric two-index tensor then, in addition to the symmetries $t_{ABCD}=t_{(AB)(CD)}$, we have $t_{ABCD}=t_{CDAB}$, but not necessarily t_{ABCD} will coincide with, e.g., t_{ACBD}; the components t_{ABCD} are totally symmetric iff t_{ab} is symmetric and traceless. In general, $t_{ab\cdots d}$ is symmetric and traceless iff its spinor equivalent $t_{ABCD\cdots GH}$ is totally symmetric.

The *connection symbols*, $\sigma^a{}_{AB}$, are not uniquely defined by Eqs. (3) and (4); a convenient choice is given by the real matrices

$$(\sigma^1{}_{AB})\equiv\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad (\sigma^2{}_{AB})\equiv\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad (\sigma^3{}_{AB})\equiv\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}. \tag{12}$$

Alternatively, we can also make use of

$$(\sigma^1{}_{AB})\equiv\begin{pmatrix}i & 0\\ 0 & i\end{pmatrix},\quad (\sigma^2{}_{AB})\equiv\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad (\sigma^3{}_{AB})\equiv\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}, \tag{13}$$

which satisfy

$$\overline{\sigma^a{}_{AB}}=-\eta_{AC}\eta_{BD}\sigma^{aCD}, \tag{14}$$

where

$$(\eta_{AB})=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{15}$$

The spin transformations will be given by SL(2,$\mathbb{R}$) or SU(1,1) matrices ($U^A{}_B$), depending on whether we employ the connection symbols (12) or (13), respectively.[5] Under a spin transformation the components of an m-index spinor $\psi_{AB\ldots F}$ transform as

$$\psi'^{AB\cdots F}=U^A{}_M U^B{}_N\cdots U^F{}_R\psi^{MN\cdots R}. \tag{16}$$

With any m-index spinor $\psi_{AB\cdots F}$ we can associate another m-index spinor, called the mate, conjugate, or adjoint, of $\psi_{AB\cdots F}$ whose components are given by[5,7]

$$\hat{\psi}_{AB\cdots F}=\begin{cases}\overline{\psi_{AB\cdots F}} & \text{if } \sigma_{aAB} \text{ are given by (12),}\\ i^m \eta_{AM}\eta_{BN}\cdots\eta_{FR}\overline{\psi^{MN\cdots R}} & \text{if the } \sigma_{aAB} \text{ are given by (13).}\end{cases} \tag{17}$$

Then the components $\hat{\psi}_{AB\cdots F}$ also transform according to Eq. (16) (as can be shown noticing that the spin transformations are given by matrices that satisfy the condition $\hat{U}^A{}_B=U^A{}_B$), $\hat{\varepsilon}_{AB}=\varepsilon_{AB}$, $\hat{\hat{\psi}}_{AB\cdots F}=\psi_{AB\cdots F}$, and $t_{AB\cdots GH}$ are the components of the spinor equivalent of a real tensor iff $\hat{t}_{AB\cdots GH}=t_{AB\cdots GH}$. Actually, one can define a spinor as real if it is equal to its mate.

From Eq. (10) it follows that for a vector v^a, $v^a v_a=-v^{AB}v_{AB}=-2\det(v_{AB})$; hence, v^a is null (i.e., $v^a v_a=0$) iff there exists a one-index spinor α_A such that

$$v_{AB}=\alpha_A\alpha_B; \tag{18}$$

the null vector v^a is real iff, additionally, $\hat{\alpha}_A\hat{\alpha}_B=\alpha_A\alpha_B$, which is equivalent to the condition $\hat{\alpha}_A=\pm\alpha_A$. The factorization (18) is a special case of the fact that any totally symmetric m-index spinor $\psi_{AB\cdots F}$ can be expressed as the symmetrized product of m (not necessarily different) one-index spinors

$$\psi_{AB\cdots F}=\alpha_{(A}\beta_B\cdots\delta_{F)}. \tag{19}$$

The spinors α_A, $\beta_A,\ldots,\delta_A$, are defined up to a scalar factor and are called principal spinors of $\psi_{AB\cdots F}$. A one-index spinor ξ_A is a principal spinor of $\psi_{AB\cdots F}$ iff $\psi_{AB\cdots F}\xi^A\xi^B\cdots\xi^F=0$. As in the case of the two-component spinor formalism employed in the four-dimensional space–time, the factorization (19) follows from the fundamental theorem of algebra.[1]

III. ALGEBRAIC CLASSIFICATION OF THE CURVATURE

Let M be a three-dimensional Riemannian manifold with indefinite metric. The components of the curvature tensor R_{abcd} of the Levi–Civita connection of M, with respect to an orthogonal basis of the tangent space of M at a point p such that $(g_{ab})=\mathrm{diag}(1,1,-1)$, satisfy the conditions $R_{abcd}=R_{[ab][cd]}$, where the square brackets denote antisymmetrization on the indices enclosed; hence, applying (11) it follows that the spinor equivalent of R_{abcd} can be expressed in the form[5]

$$R_{ABCDEFHI}=\tfrac{1}{2}(\varepsilon_{AC}\varepsilon_{EH}G_{BDFI}+\varepsilon_{AC}\varepsilon_{FI}G_{BDEH}+\varepsilon_{BD}\varepsilon_{EH}G_{ACFI}+\varepsilon_{BD}\varepsilon_{FI}G_{ACEH}) \tag{20}$$

(the factor 1/2 is introduced for convenience), with

$$G_{ABCD}=G_{(AB)(CD)}. \tag{21}$$

Then, the symmetry $R_{abcd}=R_{cdab}$, is equivalent to $G_{ABCD}=G_{CDAB}$ and from Eq. (20) it follows that

$$G_{ABCD}=R_{ABCD}+\tfrac{1}{4}R(\varepsilon_{AC}\varepsilon_{BD}+\varepsilon_{AD}\varepsilon_{BC}), \tag{22}$$

where R_{ABCD} is the spinor equivalent of the Ricci tensor, $R_{ab}\equiv R^c{}_{acb}$, and R is the scalar curvature, $R=R^a{}_a$. Hence, G_{ABCD} is the spinor equivalent of $G_{ab}=R_{ab}-\frac{1}{2}Rg_{ab}$ and if Φ_{ABCD} denotes the spinor equivalent of the traceless part of the Ricci tensor, $\Phi_{ab}=R_{ab}-\frac{1}{3}Rg_{ab}$, we have

$$G_{ABCD}=\Phi_{ABCD}+\tfrac{1}{12}R(\varepsilon_{AC}\varepsilon_{BD}+\varepsilon_{AD}\varepsilon_{BC}). \tag{23}$$

Thus, the curvature tensor is determined by the totally symmetric spinor Φ_{ABCD} and the scalar curvature R; therefore, the curvature can be classified according to the algebraic structure of Φ_{ABCD}.

In the case of a four-dimensional manifold with Lorentzian signature, at each point of the manifold there exist four (not necessarily different) *real null* vectors l_μ (called Debever–Penrose

vectors) such that $l^{\mu}l_{[\nu}C_{\rho]\mu\sigma[\tau}l_{\lambda]}l^{\sigma}=0$, where $C_{\mu\nu\rho\sigma}$ is the conformal curvature tensor (see Refs. 8 and 9; the existence of these null directions was already implicit in Ref. 10). As we shall show, at each point of a three-dimensional manifold with indefinite metric there exist four, possibly complex, null vectors l_a such that

$$l^a l_{[b}R_{c]ad[e}l_{f]}l^d=0 \tag{24}$$

(see also Ref. 4). In effect, making use of the fact that the spinor equivalent of a null vector is of the form $\alpha_A\alpha_B$ and of the expression (11) for the spinor equivalent of a skewsymmetric two-index tensor, one finds that Eq. (24) amounts to

$$\alpha^A\alpha^M\alpha_{(B}\alpha^N R_{C)NAMDP(E}{}^Q\alpha_{F)}\alpha_Q\alpha^D\alpha^P=0,$$

which, by virtue of Eq. (20), reduces to $G_{NMPQ}\alpha^N\alpha^M\alpha^P\alpha^Q=0$ or, equivalently,

$$\Phi_{NMPQ}\alpha^N\alpha^M\alpha^P\alpha^Q=0, \tag{25}$$

i.e., α_A is a principal spinor of Φ_{ABCD}. Even though Φ_{ABCD} is the spinor equivalent of a real tensor, its principal spinors need not be real. If α_A is a principal spinor of Φ_{ABCD} then so is its mate $\hat{\alpha}_A$; hence, as shown in Ref. 6, $\hat{\Phi}_{ABCD}=\Phi_{ABCD}$ iff Φ_{ABCD} is of one of the following forms:

$$\text{Type I}\quad \Phi_{ABCD}=\alpha_{(A}\beta_B\gamma_C\delta_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,\ \hat{\beta}_A=\beta_A,\ \hat{\gamma}_A=\gamma_A,\ \hat{\delta}_A=\delta_A,$$

$$\text{Type II}\quad \Phi_{ABCD}=\alpha_{(A}\beta_B\gamma_C\hat{\gamma}_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,\ \hat{\beta}_A=\beta_A,$$

$$\text{Type III}\quad \Phi_{ABCD}=\pm\alpha_{(A}\hat{\alpha}_B\beta_C\hat{\beta}_{D)},$$

$$\text{Type IV}\quad \Phi_{ABCD}=\alpha_{(A}\alpha_B\beta_C\gamma_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,\ \hat{\beta}_A=\beta_A,\ \hat{\gamma}_A=\gamma_A,$$

$$\text{Type V}\quad \Phi_{ABCD}=\pm\alpha_{(A}\alpha_B\beta_C\hat{\beta}_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,$$

$$\text{Type VI}\quad \Phi_{ABCD}=\pm\alpha_{(A}\alpha_B\beta_C\beta_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,\ \hat{\beta}_A=\beta_A,$$

$$\text{Type VII}\quad \Phi_{ABCD}=\pm\alpha_{(A}\alpha_B\hat{\alpha}_C\hat{\alpha}_{D)},$$

$$\text{Type VIII}\quad \Phi_{ABCD}=\alpha_{(A}\alpha_B\alpha_C\beta_{D)}\quad \text{with}\quad \hat{\alpha}_A=\alpha_A,\ \hat{\beta}_A=\beta_A,$$

$$\text{Type IX}\quad \Phi_{ABCD}=\pm\alpha_A\alpha_B\alpha_C\alpha_D\quad \text{with}\quad \hat{\alpha}_A=\alpha_A. \tag{26}$$

Thus, α_A is a principal spinor of Φ_{ABCD} iff $\alpha_A\alpha_B$ is the spinor equivalent of a null vector satisfying Eq. (24).

Equation (25) is equivalent to $R_{ABCD}\alpha^A\alpha^B\alpha^C\alpha^D=0$, i.e.,

$$R_{ab}l^a l^b=0 \tag{27}$$

and therefore we conclude that, at each point of M, there are four, possibly complex, null vectors l_a such that $R_{ab}l^a l^b=0$ and that Eq. (24) is equivalent to Eq. (27) if l_a is null (cf. Ref. 4).

On the other hand, the condition $R_{ab}l^a=\lambda l_b$ is equivalent to $\Phi_{ab}l^a=(\lambda-\frac{1}{3}R)l_b$ and, assuming again that l_a is null and possibly complex we have

$$\Phi_{ABCD}\alpha^A\alpha^B=(\tfrac{1}{3}R-\lambda)\alpha_C\alpha_D, \tag{28}$$

where $\alpha_A\alpha_B$ is the spinor equivalent of l_a. If $\frac{1}{3}R-\lambda=0$, Eq. (28) means that α_A is a triple or quadruple principal spinor of Φ_{ABCD} (types VIII and IX), and conversely; then α_A (and hence l_a)

must be real [see Eq. (26)] and its direction is unique [i.e., there is only one linearly independent solution to Eq. (28)]. When $\frac{1}{3}R-\lambda\neq 0$, α_A is a double principal spinor of Φ_{ABCD} (types IV, V, VI, and VII) and, therefore, in this case there are at most two linearly independent solutions of Eq. (28); furthermore, since $\overline{\gamma^A\delta_A}=\hat{\gamma}^A\hat{\delta}_A$ for any pair of one-index spinors, by inspection of the possible cases in (26), one finds that λ must be real. [Actually, there are exactly two real linearly independent solutions of Eq. (28) iff Φ_{ABCD} is of type VI, in which case $\frac{1}{3}R-\lambda>0$ and there are two complex linearly independent solutions of Eq. (28) iff Φ_{ABCD} is of type VII, then $\frac{1}{3}R-\lambda<0$.]

Using Eqs. (20) and (23) one finds that the spinor equivalent of $R_{abcd}l^b l^c$ is

$$R_{ABCDEFHI}\alpha^C\alpha^D\alpha^E\alpha^F=\tfrac{1}{6}R\,\alpha_A\alpha_B\alpha_H\alpha_I-2\,\alpha_{(A}\Phi_{B)DF(H}\alpha_{I)}\alpha^D\alpha^F,$$

which is proportional to $\alpha_A\alpha_B\alpha_H\alpha_I$ iff Eq. (28) holds. Hence, $R_{abcd}l^b l^c$ is proportional to $l_a l_d$ iff $R_{ab}l^a=\lambda l_b$.[4]

It may be noticed that, for instance, the expression $\Phi_{ABCD}=\alpha_{(A}\beta_B\gamma_C\delta_{D)}$ is the spinor equivalent of the traceless part of the symmetrized product of the vector equivalents of $\alpha_{(A}\beta_{B)}$ and $\gamma_{(A}\delta_{B)}$, i.e., of $\Phi_{ab}=v_{(a}w_{b)}-\frac{1}{3}v^c w_c g_{ab}$, where v_a and w_a are the vector equivalents of $\alpha_{(A}\beta_{B)}$ and $\gamma_{(A}\delta_{B)}$, respectively. (However, if the principal spinors of Φ_{ABCD} are not repeated, the vectors v_a and w_a are not defined uniquely by Φ_{ab} since we can combine α_A, β_A, γ_A, and δ_A in three different ways to form a pair of vectors. By contrast, the directions of the principal spinors of Φ_{ABCD} are uniquely defined.)

In a three-dimensional Riemannian manifold M, the Riemann tensor is completely determined by the Ricci tensor and an analog of the conformal curvature tensor is given by the Schouten–Bach–Cotton–York tensor

$$Y_{ab}=\varepsilon_{acd}(\nabla^c R_b{}^d-\tfrac{1}{4}\delta_b^d\partial^c R)=\varepsilon_{acd}(\nabla^c\Phi_b{}^d+\tfrac{1}{12}\delta_b^d\partial^c R), \tag{29}$$

which is symmetric and traceless. M is locally conformally flat iff Y_{ab} vanishes. The spinor equivalent of Y_{ab} is totally symmetric and can be algebraically classified in the same manner as Φ_{ABCD} [see Eq. (26)]. Thus, we conclude that at each point of M there exist four (not necessarily different) complex null vectors l_a such that

$$Y_{ab}l^a l^b=0 \tag{30}$$

(cf. Ref. 4) and the spinor equivalent of a null vector l_a satisfying Eq. (30) is of the form $\alpha_A\alpha_B$, where α_A is a principal spinor of Y_{ABCD}, the spinor equivalent of Y_{ab}. The eigenvalue equation $Y_{ab}l^a=\lambda l_b$, for l_a null, has solution only if Y_{ABCD} has at least one repeated principal spinor.

The principal spinors of Φ_{ABCD} need not coincide with those of Y_{ABCD} and the algebraic types of Φ_{ABCD} and Y_{ABCD} may be different. However, if α_A is a k-fold repeated principal spinor of Φ_{ABCD} with $k\geqslant 3$, then α_A is at least a $(k-2)$-fold repeated principal spinor of Y_{ABCD}, as can be seen using the fact that Eq. (29) amounts to

$$Y_{ABCD}=-\sqrt{2}\,\nabla^R{}_{(A}\Phi_{BCD)R}, \tag{31}$$

where ∇_{AB} denotes the spinor equivalent of the covariant derivative operator ∇_a.

The spinor formalism obtained with the real connection symbols (12) is equivalent to the triad formalism given in Ref. 3. When the complex connection symbols (13) are employed, instead, the number of independent components and equations reduces almost by half, thus obtaining a formalism closer to the Newman–Penrose formalism applied in the case of the four-dimensional space-time.

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Pauli approximations to the self-adjoint extensions of the Aharonov–Bohm Hamiltonian

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(Received 6 January 2003; accepted 8 April 2003)

It is well known that the formal Aharonov–Bohm Hamiltonian operator, describing the interaction of a charged particle with a magnetic vortex, has a four-parameter family of self-adjoint extensions, which reduces to a two-parameter family if one requires that the Hamiltonian commutes with the angular momentum operator. The question we study here is which of these self-adjoint extensions can considered as limits of regularized Aharonov–Bohm Hamiltonians, that is Pauli Hamiltonians in which the magnetic field corresponds to a flux tube of nonzero diameter. We show that not all the self-adjoint extensions in this two-parameter family can be obtained by these approximations, but only two one-parameter subfamilies. In these two cases we can choose the gyromagnetic ratio in the approximating Pauli Hamiltonian in such a way that we get convergence in the norm resolvent sense to the corresponding self-adjoint extension. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1601298]

I. INTRODUCTION

The Aharonov–Bohm Hamiltonian operator, describing the interaction of a charged particle with a magnetic vortex, that is, an infinitely extended, infinitely thin, impenetrable magnetic flux tube, is given by

$$H=\frac{1}{2\mathrm{m}}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2, \tag{1.1}$$

where the vector potential $\mathbf{A}$ is given by

$$\mathbf{A}=\frac{\phi}{2\pi}\frac{\mathbf{k}\times\mathbf{r}}{r^2}, \tag{1.2}$$

ϕ being the flux of the tube. It is well known[1,2] that this formal operator has a four-parameter family of self-adjoint extensions, which reduces to a two-parameter family if one requires that the Hamiltonian commutes with the angular momentum operator. These self-adjoint extensions can be obtained formally by adding a delta function. The question we study in this paper is which of these self-adjoint extensions can considered as limits of regularized Aharonov–Bohm (AB) Hamiltonians, that is Pauli Hamiltonians in which the magnetic field corresponds to a flux tube of nonzero diameter.

This problem has been studied by Bordag and Voropaev[3] and by Moroz.[4] These authors make the connection between the regularized Hamiltonian and the self-adjoint extensions of the AB Hamiltonian and show that the gyromagnetic ratio has to be chosen in a particular way. They do

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this by matching the bound states as the radius of the vortex tends to zero, but do not prove convergence of the operators. Also they do not take into account the second parameter in the two-parameter family of self-adjoint extensions mentioned above. Here we proceed more systematically to extend the results of Refs. 3 and 4. We consider convergence in the norm resolvent sense. We show that not all the self-adjoint extensions in this two-parameter family can be obtained by these approximations, but only two one-parameter subfamilies. Tamura[5] has done related work but with a different emphasis.

When the AB Hamiltonian is decomposed into the subspaces corresponding to the values of the angular momentum $m \in \mathbb{Z}$, it turns out that if N is the integer part of the dimensionless parameter $\alpha = \phi e/hc$, then the Hamiltonians restricted to $m=N$ and $m=N+1$ are not essentially self-adjoint while the ones with other values of m are essentially self-adjoint. The operators corresponding to $m=N$ and $m=N+1$ each have a one-parameter family of self-adjoint extensions. We denote these parameters in $(-\infty,\infty]$ by ν_N and ν_{N+1}, respectively, $\nu_N=\infty$ and $\nu_{N+1}=\infty$ corresponding to the *regular* self-adjoint extension. We prove that for the subfamilies $\nu_N \in (-\infty,\infty)$, $\nu_{N+1}=\infty$ and $\nu_{N+1}\in(-\infty,\infty)$, $\nu_N=\infty$ we can choose the gyromagnetic ratio, g, in the approximating Pauli Hamiltonian in such a way that we get convergence in the norm resolvent sense to the corresponding self-adjoint extension. The approximating Hamiltonian is

$$H_R = \frac{1}{2\mathrm{m}}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}_R\right)^2 - \frac{ge\hbar}{2\mathrm{m}c}\mathbf{k}\cdot\mathbf{B}_R \tag{1.3}$$

with $\mathbf{B}_R = \operatorname{curl}\mathbf{A}_R$. The vector potential $\mathbf{A}_R$ is 0 inside a tube of radius R away from its boundary and given by (1.2) outside the tube away from the boundary. It was shown in Refs. 3 and 4 that to obtain a nontrivial limit, g must depend on R and must tend to 2 in a certain way. For a discussion of the physical significance of this limit we refer the reader to these papers. The same result holds here for the self-adjoint extensions with $\nu_N \in (-\infty,\infty)$, $\nu_{N+1}=\infty$. However, for the self-adjoint extensions with $\nu_{N+1}\in(-\infty,\infty)$, $\nu_N=\infty$, which were not considered in Refs. 3 and 4, g must behave like $-2+4(N+1)/\alpha$.

Two other approximations have been considered, namely, the case when the magnetic field inside the tube is homogeneous[3,4] and the case when it is proportional to $1/r$.[3] The situation in these cases is similar but more complex. We deal with these briefly at the end of the paper.

The paper is set out as follows. In Sec. II we give the basic properties of the AB Hamiltonian. In Sec. III we carry out the approximation to the AB Hamiltonian with an infinitely thin infinitely extended cylindrical shell of nonzero radius R. In Sec. IV we smooth the flux shell to give it a nonzero thickness. In this section we only sketch the proof. In Sec. V we discuss the other two approximations. In the Appendixes A and B we give the asymptotic behavior of the special functions needed for these approximations.

II. THE AB HAMILTONIAN

In the sequel we set $\hbar^2/\mathrm{m}=2$ and $e/c=1$ so that the AB Hamiltonian is formally the operator

$$H = (i\nabla + \mathbf{A})^2, \tag{2.1}$$

in $L^2(\mathbb{R}^2)$, where the vector potential $\mathbf{A}$ is now given by

$$\mathbf{A} = \alpha\frac{\mathbf{k}\times\mathbf{r}}{r^2}. \tag{2.2}$$

We let $\alpha = N+\delta$, where $N\in\mathbb{Z}$ and $0<\delta<1$. Without loss of generality, we shall assume that $\alpha > 0$.

This Hamiltonian is discussed in great detail in Refs. 1 and 2. The analysis proceeds by decomposing the underlying space and studying the radial Hamiltonians

$$h_m = -\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{(m-\alpha)^2}{r^2} \tag{2.3}$$

in $L^2((0,\infty), r\,dr)$. Taking as domain $C_0^\infty((0,\infty), r\,dr)$, these operators are essentially self-adjoint, except for the cases $m=N,N+1$ which have deficiency indices (1,1). These two operators therefore have self-adjoint extensions h_{N,ν_N} and $h_{N+1,\nu_{N+1}}$, parametrized by ν_N and ν_{N+1}, where $-\infty < \nu_N,\ \nu_{N+1} \leqslant \infty$. These self-adjoint extensions can be identified with the boundary conditions

$$\nu_m \phi_0 = \phi_1,$$

where

$$\phi_0 = \lim_{r\downarrow 0} r^{|m-\alpha|}\phi(r)$$

and

$$\phi_1 = \lim_{r\downarrow 0} r^{-|m-\alpha|}[\phi(r) - r^{-|m-\alpha|}\phi_0].$$

A four-parameter family of self-adjoint extensions of H can be constructed from these. If we consider only self-adjoint extensions which commute with the angular momentum operator, this reduces to a two-parameter family. For this particular choice, the self-adjoint extension, $H^{\boldsymbol{\nu}}$, with $\boldsymbol{\nu} \in (-\infty,\infty]^2$, is just the direct sum

$$H^{\boldsymbol{\nu}} = h_{N,\nu_N} \oplus h_{N+1,\nu_{N+1}} \oplus \bigoplus_{\substack{m=-\infty \\ m\neq N,N+1}}^{\infty} h_m .$$

We shall write H^∞ for $H^{\boldsymbol{\nu}}$ with $\boldsymbol{\nu}=(\infty,\infty)$. Let $g_{k,\,m} = (h_m - k^2)^{-1}$. Then

$$g_{k,\,m}(r,r') = \frac{i\pi}{2} J_{|m-\alpha|}(kr_<) H^{(1)}_{|m-\alpha|}(kr_>), \tag{2.4}$$

where $r_< = \min\{r,r'\}$ and $r_> = \max\{r,r'\}$. The resolvents $g^{\nu_m}_{k,m} = (h_{m,\nu_m} - k^2)^{-1}$, $m=N,N+1$, are given by

$$g^{\nu_m}_{k,m}(r,r') = g_{k,\,m}(r,r') + c(m,\nu_m,k) H^{(1)}_{|m-\alpha|}(kr) H^{(1)}_{|m-\alpha|}(kr'), \quad m=N,N+1, \tag{2.5}$$

with

$$c(m,\nu,k) = \frac{-\pi^2}{2\Gamma(1+|m-\alpha|)} \left(\frac{k}{2}\right)^{2|m-\alpha|} \left(e^{-i\pi|m-\alpha|} \frac{\Gamma(1-|m-\alpha|)}{|m-\alpha|} \left(\frac{k}{2}\right)^{2|m-\alpha|} + \nu\Gamma(|m-\alpha|)\right)^{-1}, \tag{2.6}$$

$$c(m,\infty,k) = 0. \tag{2.7}$$

Finally, the resolvent of the Hamiltonian $G^{\boldsymbol{\nu}}_k = (H^{\boldsymbol{\nu}} - k^2)^{-1}$ is given by (see Ref. 1):

$$G^{\boldsymbol{\nu}}_k = g^{\nu_N}_{k,N} \oplus g^{\nu_{N+1}}_{k,N+1} \oplus \bigoplus_{\substack{m=-\infty \\ m\neq N,N+1}}^{\infty} g_{k,m} . \tag{2.8}$$

Note that the operators h_{m,ν_m} have no bound state for $\nu_m \geqslant 0$ and one bound state, E_m, for $\nu_m < 0$ given by

$$\left(i \frac{\sqrt{E_m}}{2} \right)^{2|m-\alpha|} = - \frac{\Gamma(1+|m-\alpha|)}{\Gamma(1-|m-\alpha|)} \nu_m, \quad m = N, N+1. \tag{2.9}$$

III. APPROXIMATION BY FINITE FLUX TUBE

The Aharonov–Bohm Hamiltonian consists of an infinitely thin magnetic flux tube. As a first approximation to H^{AB}, consider a flux tube of radius $R>0$, with a δ-function on a cylindrical shell (following Ref. 3 but see also Refs. 6, 4). That is we take the vector potential

$$\mathbf{A}_R = \begin{cases} 0, & r<R, \\ \alpha \dfrac{\mathbf{k}\times\mathbf{r}}{r^2}, & r>R. \end{cases} \tag{3.1}$$

Then $\mathbf{k}\cdot\mathbf{B}_R = (\alpha/R)\,\delta(r-R)$, so that formally, the Hamiltonian is then given by

$$H_R = (i\nabla + \mathbf{A}_R)^2 + \frac{\beta}{R}\delta(r-R), \tag{3.2}$$

where $\beta = -g\alpha/2$. The components in $L^2((0,\infty), r\,\mathrm{d}r)$ corresponding to the angular momentum m of this formal operator are

$$-\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{(m-\alpha\Theta(r-R))^2}{r^2} + \frac{\beta}{R}\delta(r-R), \tag{3.3}$$

where Θ is the unit step function. The procedure for adding a point interaction at $r=R$ to a radial Hamiltonian is standard (cf. Ref. 7 Sec. I.3.1). The point we make here is that β, the strength of the point interaction, has to depend on R and α in a definite way so that the self-adjoint extensions obtained in this manner converge to the AB self-adjoint extensions as R tends to 0.

Consider the following operator in $L^2((0,\infty), r\,\mathrm{d}r)$:

$$h_{m,R} = -\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{(m-\alpha\Theta(r-R))^2}{r^2} \tag{3.4}$$

with the closure of $C_0^\infty((0,\infty)\backslash\{R\})$ as its domain (Ref. 7, p. 75), i.e.,

$$\mathcal{D}(h_{m,\,R}) = \{g \in H^{2,2}((0,\infty), r\,\mathrm{d}r) \ \text{ s.t. } \ h_{m,\,R} g \in L^2((0,\infty), r\,\mathrm{d}r) \ \text{ and } \ g(R)=0\}. \tag{3.5}$$

Then its adjoint has domain (Ref. 7, p. 75)

$$\mathcal{D}(h^*_{m,\,R}) = \{g \in H^{2,2}((0,\infty)\backslash\{R\}, r\,\mathrm{d}r) \cap H^{2,1}((0,\infty), r\,\mathrm{d}r) \text{ s.t. } h_{m,\,R} g \in L^2((0,\infty), r\,\mathrm{d}r)\}. \tag{3.6}$$

The equation $h^*_{m,\,R}\phi = k^2\phi$, $\Im(k)>0$, has one solution in $\mathcal{D}(h^*_{m,\,R})$ for all values of $m \in \mathbb{Z}$ (see Note 1, Appendix A), given by

$$\phi_{m,k}(r) = \begin{cases} J_{|m|}(kr), & r<R, \\ B_m(k) H^{(1)}_{|m-\alpha|}(kr), & r>R, \end{cases} \tag{3.7}$$

where $B_m(k)$ is chosen so that the condition $\phi_{m,k}(R+) = \phi_{m,k}(R-)$ is satisfied. Thus the operators $h_{m,\,R}$ have deficiency indices (1,1). Self-adjoint extensions $h^\beta_{m,\,R}$ are obtained by imposing the following boundary condition on the domain of $h_{m,\,R}$:

$$\phi'_{m,k}(R+) - \phi'_{m,k}(R-) = \frac{\beta(\alpha,R)}{R}\phi_{m,k}(R), \tag{3.8}$$

where $\beta(\alpha,R)$ is a constant parameter (Ref. 7, p. 76). Note that we do not want the parameter $\beta(\alpha,R)$ to depend on m since it represents $-g\alpha/2$. We shall henceforth be writing β for this parameter to make the notation less cumbersome.

Next we find the resolvent $g^{\beta}_{k,\,m,\,R}=(h^{\beta}_{m,\,R}-k^2)^{-1}$. Note first that $g^{0}_{k,\,m,\,R}=(h_{m,\,R}-k^2)^{-1}$, $\Im(k)>0$, is given by (Note 2, Appendix A)

$$g^{0}_{k,\,m,\,R}(r,r')=\begin{cases}\dfrac{i\pi}{2}J_{|m|}(kr_<)\left(\dfrac{A^{(2)}_{m,R}(k)}{B^{(2)}_{m,R}(k)}J_{|m|}(kr_>)+H^{(1)}_{|m|}(kr_>)\right), & r,r'<R,\\[2ex] \dfrac{i\pi}{2}\left(J_{|m-\alpha|}(kr_<)+\dfrac{B^{(1)}_{m,R}(k)}{A^{(1)}_{m,R}(k)}H^{(1)}_{|m-\alpha|}(kr_<)\right)H^{(1)}_{|m-\alpha|}(kr_>), & r,r'>R,\\[2ex] \dfrac{i\pi}{2A^{(1)}_{m,R}(k)}J_{|m|}(kr_<)H^{(1)}_{|m-\alpha|}(kr_>), & \text{otherwise,}\end{cases} \tag{3.9}$$

where the constants $A^{(1)}_{m,R}(k),A^{(2)}_{m,R}(k),B^{(1)}_{m,R}(k)$, and $B^{(2)}_{m,R}(k)$ are given by

$$A^{(1)}_{m,R}(k)=\frac{W[J_{|m|},H^{(1)}_{|m-\alpha|}](kR)}{W[J_{|m-\alpha|},H^{(1)}_{|m-\alpha|}](kR)}, \tag{3.10}$$

$$B^{(1)}_{m,R}(k)=\frac{W[J_{|m|},J_{|m-\alpha|}](kR)}{W[H^{(1)}_{|m-\alpha|},J_{|m-\alpha|}](kR)}, \tag{3.11}$$

$$A^{(2)}_{m,R}(k)=\frac{W[H^{(1)}_{|m-\alpha|},H^{(1)}_{|m|}](kR)}{W[J_{|m|},H^{(1)}_{|m|}](kR)}, \tag{3.12}$$

$$B^{(2)}_{m,R}(k)=\frac{W[J_{|m|},H^{(1)}_{|m-\alpha|}](kR)}{W[J_{|m|},H^{(1)}_{|m|}](kR)}. \tag{3.13}$$

Here $W[\,\cdot\,,\,\cdot\,]$ denotes the Wronskian. Then the resolvent of $h^{\beta}_{m,\,R}$ is given by (Note 3, Appendix A):

$$g^{\beta}_{k,\,m,\,R}=g^{0}_{k,\,m,\,R}-\frac{\beta}{1+\beta g^{0}_{k,\,m,\,R}(R,R)}g^{0}_{k,\,m,\,R}(\,\cdot\,,R)\otimes\overline{g^{0}_{k,\,m,\,R}(\,\cdot\,,R)}, \tag{3.14}$$

for $\Im(k)>0$. We are interested in the behavior of $g^{\beta}_{k,\,m,\,R}(r,r')$ for small R. We note first that $\lim_{R\to 0}g^{0}_{k,\,m,\,R}(r,r')=g_{k,\,m}(r,r')$, which is the resolvent of the regular operator. For small R,

$$g^{0}_{k,\,m,\,R}(r,R)g^{0}_{k,\,m,\,R}(R,r')\simeq\tilde{c}^{2}_{m}(k)R^{2|m-\alpha|}H^{(1)}_{|m-\alpha|}(kr)H^{(1)}_{|m-\alpha|}(kr'), \tag{3.15}$$

where

$$\tilde{c}_{m}(k)=\frac{i\pi}{(|m-\alpha|+|m|)\Gamma(|m-\alpha|)}\left(\frac{k}{2}\right)^{|m-\alpha|}. \tag{3.16}$$

If $|m-\alpha|>1$ (i.e., if $m\notin\{N,N+1\}$), then the second term will either go to zero, or to a constant multiple of $H^{(1)}_{|m-\alpha|}(kr)H^{(1)}_{|m-\alpha|}(kr')$. Now $H^{(1)}_{|m-\alpha|}(kr)$ is not in $L^2((0,\infty),r\,dr)$ since it behaves like $r^{-|m-\alpha|}$ for small r (see Note 1, Appendix A). So in the latter case, the limit is not the kernel of a rank-one operator in $L^2((0,\infty),r\,dr)$. In particular, this means that it cannot be the kernel of a resolvent operator. Thus a meaningful nonzero limit for the second term in Eq. (3.14) exists only for the cases $m=N,N+1$. It shall be shown later that for small R, we get

$$g^0_{k,\ m,\ R}(R,R)\simeq\frac{1}{|m-\alpha|+|m|}\left(1-\frac{2e^{-i\pi|m-\alpha|}\Gamma(1-|m-\alpha|)}{(|m-\alpha|+|m|)\Gamma(|m-\alpha|)}\left(\frac{kR}{2}\right)^{2|m-\alpha|}\right). \tag{3.17}$$

For the case $r,r'>R$ (the other cases are straightforward), this results in

$$g^\beta_{k,\ m,\ R}(r,r')\simeq g^0_{k,\ m,\ R}(r,r')-\frac{\beta\tilde{c}^2_m(k)R^{2|m-\alpha|}}{1+\dfrac{\beta(1-\tilde{c}'(k)R^{2|m-\alpha|})}{|m-\alpha|+|m|}}H^{(1)}_{|m-\alpha|}(kr)H^{(1)}_{|m-\alpha|}(kr'), \tag{3.18}$$

where

$$\tilde{c}'(k)=\frac{2e^{-i\pi|m-\alpha|}\Gamma(1-|m-\alpha|)}{(|m-\alpha|+|m|)\Gamma(|m-\alpha|)}\left(\frac{k}{2}\right)^{2|m-\alpha|}. \tag{3.19}$$

The second term in (3.18) converges to a nonzero limit if β has the following R-dependence for small R:

$$\beta\simeq-(|m-\alpha|+|m|)\left(1-\frac{2|m-\alpha|\,\nu_m}{|m-\alpha|+|m|}R^{2|m-\alpha|}\right). \tag{3.20}$$

Then we obtain

$$\lim_{R\to0}g^\beta_{k,\ m,\ R}(r,r')=g_{k,\ m}(r,r')+c(m,\nu_m,k)H^{(1)}_{|m-\alpha|}(kr)H^{(1)}_{|m-\alpha|}(kr'). \tag{3.21}$$

This gives the correct expression in (2.5) for the kernel of the resolvent of some self-adjoint extension of h_m, $m=N,N+1$.

The following are the only cases of interest.

(I) If $\beta\simeq-\alpha[1-(2\delta/\alpha)\,\nu_N R^{2\delta}]$, then the second term in Eq. (3.14) approaches

(1) a nonzero limit for $m=N$, corresponding to the self-adjoint extension h_{N,ν_N};
(2) zero limit for $m=N+1$, corresponding to the regular self-adjoint extension $h_{N+1,\infty}$;
(3) zero limit for $m\neq N,N+1$, corresponding to the self-adjoint operators h_m.

(II) If $\beta\simeq(\alpha-2(N+1))(1-(2(1-\delta)/[2(N+1)-\alpha])\,\nu_{N+1}R^{2(1-\delta)})$, then the second term in Eq. (3.14) approaches
(1) a non-zero limit for $m=N+1$, corresponding to the self-adjoint extension $h_{N+1,\nu_{N+1}}$;
(2) zero limit for $m=N$, corresponding to the regular self-adjoint extension $h_{N,\infty}$;
(3) zero limit for $m\neq N,N+1$, as before.

We can state the above results as a Theorem.

Theorem 1: *Let*

$$H^\beta_R=\bigoplus_{m=-\infty}^{\infty}h^\beta_{m,R}. \tag{3.22}$$

Then $H^{\beta(\alpha,R)}_R$ converges, as $R\to0$, to one of the self-adjoint extensions H^ν of the AB Hamiltonian only if either

(I) $\beta(\alpha,R)+\alpha/R^{2\delta})\to2\delta\nu_N$
or
(II) $\beta(\alpha,R)-\alpha+2(N+1)/R^{2(1-\delta)}\to2(1-\delta)\nu_{N+1}$.

In case (I) $H_R^{\beta(\alpha,R)}$ converges in the norm resolvent sense, as $R\to 0$, to $H^{(\nu_N,\,\infty)}$, and in case (II) to $H^{(\infty,\,\nu_{N+1})}$.

Proof: Let us consider case (I), case (II) is similar. Since

$$\|(H_R^{\beta(\alpha,R)}-k^2)^{-1}-G_k^{(\nu_N,\,\infty)}\|=\max\{\|g_{k,\,N,\,R}^{\beta(\alpha,R)}-g_{k,\,N}^{\nu_N}\|,\|g_{k,\,N+1,\,R}^{\beta(\alpha,R)}-g_{k,\,N+1}\|,\ \sup_{\substack{m\in\mathbb{Z}\\ m\neq N,N+1}}\|g_{k,\,m,\,R}^{\beta(\alpha,R)}-g_{k,\,m}\|\},\tag{3.23}$$

we not only have to prove that the the terms in the right-hand side of the above equations tend to zero, but we have to show that $\|g_{k,\,m,\,R}^{\beta(\alpha,R)}-g_{k,\,m}\|$ tends to zero uniformly in m. To do this we need to obtain detailed upper and lower bounds on the special functions J_ν and $H_\nu^{(1)}$. These are given in the Appendix.

The first term in the expressions for $g_{k,\,m,\,R}^{\beta(\alpha,R)}$ is $g_{k,\,m,\,R}^{0}$ and first term in the expressions for $g_{k,\,m}^{\nu}$ is $g_{k,\,m}$. Therefore we start with the following lemma. Here $\|\cdot\|_2$ denotes the Hilbert–Schmidt norm, and of course $\|\cdot\|\leqslant\|\cdot\|_2$.

Lemma 1: For any m, $\lim_{R\to 0}\|g_{k,\,m,\,R}^{0}-g_{k,\,m}\|_2=0$. Furthermore, there exists $M\in\mathbb{N}$ such that for $|m|>M$, there exists a constant $c(R)$, independent of m, such that $\|g_{k,\,m,\,R}^{0}-g_{k,\,m}\|_2\leqslant c(R)$, and $\lim_{R\to 0}c(R)=0$.

Proof:

$$\|g_{k,\,m,\,R}^{0}-g_{k,\,m}\|_2\leqslant\|\tilde g_1\|_2+\|\tilde g_2\|_2+\|\tilde g_3\|_2+\|\tilde g_4\|_2+\|\tilde g_5-g_{k,\,m}\|_2,\tag{3.24}$$

where

$$\tilde g_1(r,r')=\frac{i\pi}{2}\frac{A_{m,R}^{(2)}(k)}{B_{m,R}^{(2)}(k)}J_{|m|}(kr)J_{|m|}(kr')\mathbf{1}_{(0,\,R)\times(0,\,R)}(r,r'),\tag{3.25}$$

$$\tilde g_2(r,r')=\frac{i\pi}{2}J_{|m|}(kr_<)H_{|m|}^{(1)}(kr_>)\mathbf{1}_{(0,\,R)\times(0,\,R)}(r,r'),\tag{3.26}$$

$$\tilde g_3(r,r')=\frac{i\pi}{2}\frac{B_{m,R}^{(1)}(k)}{A_{m,R}^{(1)}(k)}H_{|m-\alpha|}^{(1)}(kr)H_{|m-\alpha|}^{(1)}(kr')\mathbf{1}_{(R,\,\infty)\times(R,\,\infty)}(r,r'),\tag{3.27}$$

$$\tilde g_4(r,r')=\frac{i\pi}{2A_{m,R}^{(1)}(k)}J_{|m|}(kr_<)H_{|m-\alpha|}^{(1)}(kr_<)\mathbf{1}_{(0,\,R]\times[R,\,\infty)\cup[R,\,\infty)\times(0,\,R]}(r,r'),\tag{3.28}$$

$$\tilde g_5(r,r')=\frac{i\pi}{2}J_{|m-\alpha|}(kr_<)H_{|m-\alpha|}^{(1)}(kr_>)\mathbf{1}_{(R,\,\infty)\times(R,\,\infty)}(r,r').\tag{3.29}$$

Using the bounds (B32), (B41), and (B45) in Appendix B and the relation

$$W[J_\nu(z),H_\nu^{(1)}(z)]=\frac{2i}{\pi z},\tag{3.30}$$

we can see that for any $\varepsilon>0$, there exists $R_0>0$ such that if $R<R_0$, then the following bounds hold:

$$\frac{1}{|A_{m,R}^{(1)}(k)|}\leqslant\frac{2\Gamma(|m|+1)}{||m-\alpha|+|m||\Gamma(|m-\alpha|)}\left|\frac{kR}{2}\right|^{|m-\alpha|-|m|}(1+\varepsilon),\tag{3.31}$$

$$\left|\frac{B^{(1)}_{m,R}(k)}{A^{(1)}_{m,R}(k)}\right| \leqslant \frac{\pi||m-\alpha|-|m||}{(|m-\alpha|+|m|)\Gamma(|m-\alpha|)\Gamma(|m-\alpha|+1)}\left|\frac{kR}{2}\right|^{2|m-\alpha|}(1+\varepsilon), \tag{3.32}$$

$$\left|\frac{A^{(2)}_{m,R}(k)}{B^{(2)}_{m,R}(k)}\right| \leqslant \frac{||m-\alpha|-|m||\Gamma(|m|)\Gamma(|m|+1)}{2\pi(|m-\alpha|+|m|)}\left|\frac{kR}{2}\right|^{-2|m|}(1+\varepsilon). \tag{3.33}$$

Now we can find bounds for the terms in Eq. (3.24) for small R,

$$\|\tilde{g}_1\|_2^2 = \int\int |\tilde{g}_1(r,r')|^2\, r\,\mathrm{d}r\, r'\,\mathrm{d}r' = \frac{\pi^2}{4}\left|\frac{A^{(2)}_{m,R}(k)}{B^{(2)}_{m,R}(k)}\right|^2\left(\int_0^R r\,\mathrm{d}r|J_{|m|}(kr)|^2\right)^2.$$

Using (3.33) and (B1) we get

$$\|\tilde{g}_1\|_2^2 \leqslant \begin{cases} \dfrac{(|m-\alpha|-|m|)^2R^4}{64|m|^2(|m|+1)^2(|m-\alpha|+|m|)^2}(1+\varepsilon), & m\neq 0, \\ \dfrac{R^4}{64}(1+\varepsilon), & m=0. \end{cases} \tag{3.34}$$

Next we have

$$\begin{aligned}\|\tilde{g}_2\|_2^2 &= \int |\tilde{g}_2(r,r')|^2\, r\,\mathrm{d}r\, r'\,\mathrm{d}r' \\ &= \frac{\pi^2}{4}\int_0^R r\,\mathrm{d}r\, r'\,\mathrm{d}r'|J_{|m|}(kr_<)|^2|H^{(1)}_{|m|}(kr'_>)|^2 \\ &= \frac{\pi^2}{2}\int_0^R r\,\mathrm{d}r|J_{|m|}(kr)|^2\int_r^R r'\,\mathrm{d}r'|H^{(1)}_{|m|}(kr')|^2.\end{aligned}$$

From (B1), (B18) and (B25), we get

$$\|\tilde{g}_2\|_2^2 \leqslant \begin{cases} \dfrac{R^4}{16|m|^2(1+|m|)}(1+\varepsilon), & |m|>1, \\ \dfrac{R^4}{32}(1+\varepsilon), & |m|=1, \\ \dfrac{R^4}{32}(8(\ln kR)^2+4\ln kR+1)(1+\varepsilon), & m=0. \end{cases} \tag{3.35}$$

From the relations $\overline{K_\nu(z)}=K_\nu(\overline{z})$ and

$$H^{(1)}_\nu(z) = -\frac{2i}{\pi}e^{-1/2\,i\pi\nu}K_\nu(-iz), \tag{3.36}$$

we obtain

$$\begin{aligned}\int_R^\infty r\,\mathrm{d}r\ \ |H^{(1)}_{|m-\alpha|}(kr)|^2 &= \frac{4}{\pi^2}\int_R^\infty \mathrm{d}r\,\frac{r^{2|m-\alpha|+\xi-1}}{r^{2|m-\alpha|+\xi-2}}K_{|m-\alpha|}(i\overline{kr})K_{|m-\alpha|}(-ikr) \\ &\leqslant \frac{4R^{2-2|m-\alpha|-\xi}}{\pi^2}\int_0^\infty \mathrm{d}r\, r^{2|m-\alpha|+\xi-1}K_{|m-\alpha|}(i\overline{kr})K_{|m-\alpha|}(-ikr).\end{aligned}$$

for $2|m-\alpha|+\xi>2$.

Using the formula 6.576 of Ref. 8, we then get

$$\int_R^\infty r\,\mathrm{d}r\ |H^{(1)}_{|m-\alpha|}(kr)|^2 \leqslant \frac{2}{\pi^2}|k|^{-2|m-\alpha|-\xi}\left|\frac{R}{2}\right|^{2-2|m-\alpha|-\xi}\frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)} \times\frac{\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma\left(2|m-\alpha|+\frac{\xi}{2}\right)\left(\Gamma\left(|m-\alpha|+\frac{\xi}{2}\right)\right)^2}{\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)} \tag{3.37}$$

for $|m-\alpha|\geqslant 1$ and $\xi>0$.

So, if $m\neq N,N+1$,

$$\begin{aligned}\|\tilde{g}_3\|_2^2 &= \int |\tilde{g}_3(r,r')|^2\,r\,\mathrm{d}r\,r'\,\mathrm{d}r' = \frac{\pi^2}{4}\left|\frac{B^{(1)}_{m,R}(k)}{A^{(1)}_{m,R}(k)}\right|^2\int_R^\infty r\,\mathrm{d}r|H^{(1)}_{|m-\alpha|}(kr)|^2\int_r^\infty r'\,\mathrm{d}r'|H^{(1)}_{|m-\alpha|}(kr')|^2\\ &\leqslant \frac{\pi^2}{4}\left|\frac{B^{(1)}_{m,R}(k)}{A^{(1)}_{m,R}(k)}\right|^2\left[\int_R^\infty r\,\mathrm{d}r|H^{(1)}_{|m-\alpha|}(kr)|^2\right]^2\\ &\leqslant \frac{(|m-\alpha|-|m|)^2}{(|m-\alpha|+|m|)^2}\left(\frac{R}{2}\right)^{4-2\xi}|k|^{-2\xi}\left(\frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)}\right)^2(1+\varepsilon)\\ &\quad\times\left(\frac{\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma\left(2|m-\alpha|+\frac{\xi}{2}\right)\left(\Gamma\left(|m-\alpha|+\frac{\xi}{2}\right)\right)^2}{\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)\Gamma(|m-\alpha|)\Gamma(|m-\alpha|+1)}\right)^2.\end{aligned} \tag{3.38}$$

For $m=N,N+1$ the following bound is sufficient:

$$\|\tilde{g}_3\|_2^2 \leqslant \left(\frac{\pi^2||m-\alpha|-|m||}{4(|m-\alpha|+|m|)\Gamma(|m-\alpha|)\Gamma(|m-\alpha|+1)}\right)^2\left|\frac{kR}{2}\right|^{4|m-\alpha|}\times\|H^{(1)}_{|m-\alpha|}(kr)\|^4(1+\varepsilon). \tag{3.39}$$

Thus, for fixed m, $\|\tilde{g}_3\|_2\to 0$ as $R\to 0$ provided we choose $\xi<2$.

To make the bound for $\|\tilde{g}_3\|_2$ in (3.38) independent of m, we use the following limit:

$$\lim_{n\to\infty} n^{b-a}\frac{\Gamma(n+a)}{\Gamma(n+b)}=1, \tag{3.40}$$

to deduce that there exists $M_0\in\mathbb{N}$ such that, if $|m|>M_0$, then

$$\frac{\left(\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi/2)\right)^2(\Gamma(|m-\alpha|+\xi/2))^4}{\left(\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)\Gamma(|m-\alpha|)\Gamma(|m-\alpha|+1)\right)^2}\leqslant 2^{-\xi}\overline{m}^{3/2\,\xi-2} \tag{3.41}$$

where $\overline{m}=\lfloor|m-\alpha|\rfloor$, and we must choose $\xi<\frac{4}{3}$.

Similarly, for $m \neq N, N+1$,

$$\|\tilde{g}_4\|_2^2 = \int |\tilde{g}_4(r,r')|^2 r \, \mathrm{d}r \, r' \, \mathrm{d}r' \tag{3.42}$$

$$= \frac{\pi^2}{2|A^{(1)}_{m,R}(k)|^2} \int_0^R r \, \mathrm{d}r |J_{|m|}(kr)|^2 \int_R^\infty r' \, \mathrm{d}r' |H^{(1)}_{|m-\alpha|}(kr')|^2 \tag{3.43}$$

$$\leqslant \frac{2^{\xi-1} R^{4-\xi}}{(|m|+1)(|m-\alpha|+|m|)^2} |k|^{-\xi} \frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)} (1+\varepsilon)$$
$$\times \frac{\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma\left(2|m-\alpha|+\frac{\xi}{2}\right)\left(\Gamma\left(|m-\alpha|+\frac{\xi}{2}\right)\right)^2}{\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)(\Gamma(|m-\alpha|))^2}, \tag{3.44}$$

while for $m = N, N+1$,

$$\|\tilde{g}_4\|_2^2 \leqslant \frac{\pi^2 \left|\frac{k}{2}\right|^{2|m-\alpha|} R^{2|m-\alpha|+2}}{(|m|+1)(|m-\alpha|+|m|)^2 (\Gamma(|m-\alpha|))^2} \|H^{(1)}_{|m-\alpha|}(kr)\|^2 (1+\varepsilon). \tag{3.45}$$

As previously, for fixed m, $\|\tilde{g}_4\|_2 \to 0$ as $R \to 0$ if we choose $\xi < 2$.

To obtain a bound independent of m in (3.44), we again use the limit in (3.40) to show that there exists $M_1 \in \mathbb{N}$ such that, if $|m| > M_1$, then

$$\frac{\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma\left(2|m-\alpha|+\frac{\xi}{2}\right)\left(\Gamma\left(|m-\alpha|+\frac{\xi}{2}\right)\right)^2}{(1+|m|)\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)(\Gamma(|m-\alpha|))^2} \leqslant 2^{\xi/4} M_1^{3/4\,\xi-1}. \tag{3.46}$$

Finally,

$$\tilde{g}_5(r,r') - g_{k,\ m}(r,r') = -\frac{i\pi}{2} J_{|m-\alpha|}(kr_<) H^{(1)}_{|m-\alpha|}(kr_>) \mathbf{1}_{\mathbb{R}^2 \setminus (R,\infty)\times(R,\infty)} \tag{3.47}$$

so

$$\|\tilde{g}_5 - g_{k,\ m}\|_2^2 = \frac{\pi^2}{2} \int_0^R r \, \mathrm{d}r |J_{|m-\alpha|}(kr)|^2 \int_r^R r' \, \mathrm{d}r' |H^{(1)}_{|m-\alpha|}(kr')|^2$$
$$+ \frac{\pi^2}{2} \int_0^R r \, \mathrm{d}r |J_{|m-\alpha|}(kr)|^2 \int_R^\infty r' \, \mathrm{d}r' |H^{(1)}_{|m-\alpha|}(kr')|^2. \tag{3.48}$$

The first term is bounded by $R^4(1+\varepsilon)/16|m-\alpha|^2(1+|m-\alpha|)$, while for the second term we need to consider the cases $m \neq N, N+1$ separately using Eq. (3.37).

Then we deduce that for $m \neq N, N+1$,

$$\|\tilde{g}_5 - g_{k,\,m}\|_2^2 \leqslant \frac{R^4(1+\varepsilon)}{8|m-\alpha|^2(1+|m-\alpha|)} + \frac{\left(\frac{2}{k}\right)^{\xi}\Gamma\left(\frac{1}{2}\right)R^{4-\xi}}{8(1+|m-\alpha|)}(1+\varepsilon) \times \frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(|m-\alpha|+\frac{\xi}{2}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi/2)(\Gamma(|m-\alpha|+\xi/2))^2}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)\Gamma\left(|m-\alpha|+\frac{\xi}{4}+\frac{1}{2}\right)\Gamma(2|m-\alpha|+\xi)(\Gamma(|m-\alpha|+1))^2}, \tag{3.49}$$

while for $m=N,N+1$,

$$\|\tilde{g}_5 - g_{k,\,m}\|_2^2 \leqslant \frac{R^4(1+\varepsilon)}{8|m-\alpha|^2(1+|m-\alpha|)} + \frac{\pi^2\left|\frac{k}{2}\right|^{2|m-\alpha|}R^{2|m-\alpha|+2}}{4(1+|m-\alpha|)(\Gamma(1+|m-\alpha|))^2}\|H^{(1)}_{|m-\alpha|}(kr)\|^2(1+\varepsilon). \tag{3.50}$$

A similar argument to that used previously shows that the bound in (3.49) may be taken to be independent of m. This completes the proof of Lemma 1.

□

Next we shall show that the operator $h^{\beta}_{m,\,R}$ converges in the norm resolvent sense to the appropriate limit provided β obeys condition I or II.

Lemma 2: (a) If condition I (condition II) holds, then for $m\neq N$ ($m\neq N+1$), the operator $h^{\beta}_{m,\,R}$ converges to h_m in the norm resolvent sense as $R\to 0$.

Furthermore, there exists $M\in\mathbb{N}$ such that for $|m|>M$, there exists a constant $c(R)$, independent of m, such that $\|g^{\beta}_{k,\,m,\,R}-g_{k,\,m}\|_2\leqslant c(R)$, and $\lim_{R\to 0}c(R)=0$.

(b) If condition I (condition II) holds, then the operator $h^{\beta}_{N,R}$ converges to h_{N,ν_N} ($h^{\beta}_{N+1,R}$ converges to $h_{N+1,\nu_{N+1}}$) in the norm resolvent sense as $R\to 0$.

Proof: We shall prove the Lemma for the case when condition I holds. The corresponding proof for the case when condition II holds is similar.

First we note the limiting behavior of $g^{0}_{k,\,m,\,R}(R,R)$ for small R,

$$g^{0}_{k,\,m,\,R}(R,R)\simeq\begin{cases}\dfrac{1}{|m-\alpha|+|m|}(1-\tilde{c}'(k)R^{2|m-\alpha|}), & m=N,N+1,\\ \dfrac{1}{|m-\alpha|+|m|}(1-d(k)R^2), & m\neq N,N+1.\end{cases} \tag{3.51}$$

where

$$\tilde{c}'(k)=\frac{2e^{-i\pi|m-\alpha|}\Gamma(1-|m-\alpha|)}{(|m-\alpha|+|m|)\Gamma(|m-\alpha|)}\left(\frac{k}{2}\right)^{2|m-\alpha|} \tag{3.52}$$

and

$$d(k)=\frac{1}{1-|m-\alpha|}\left(1+\frac{|m-\alpha|-|m|}{|m-\alpha|(|m-\alpha|+|m|)}\right)\left(\frac{k}{2}\right)^2. \tag{3.53}$$

(a) Let $m\neq N$ and suppose condition I holds. We need to show that

$$\lim_{R\to 0}\|g^{\beta}_{k,\ m,\ R}-g_{k,\ m}\|_2=0. \tag{3.54}$$

Now

$$\|g^{\beta}_{k,\ m,\ R}-g_{k,\ m}\|_2\leqslant\|g^{0}_{k,\ m,\ R}-g_{k,\ m}\|_2+\left|\frac{\beta}{1+\beta g^{0}_{k,\ m,\ R}(R,R)}\right|\|g^{0}_{k,\ m,\ R}(\ \cdot\ ,R)\|^2. \tag{3.55}$$

In Lemma 1, we have shown that $\lim_{R\to 0}\|g^{0}_{k,\ m,\ R}-g_{k,\ m}\|_2=0$.

The following three cases need to be considered separately:

Case 1. $m=0,1,2,\ldots,N-1$;

Case 2. $m=N+1$;

Case 3. $m\leqslant -1$ or $m\geqslant N+2$.

Case 1. If $m=0,1,2,\ldots,N-1$, then $|m-\alpha|+|m|=\alpha$. For small R,

$$\left|\frac{\beta}{1+\beta g^{0}_{k,\ m,\ R}(R,R)}\right|\simeq\frac{\alpha^2}{2\delta|\nu_N|}R^{-2\delta}, \tag{3.56}$$

while

$$\begin{aligned}\|g^{0}_{k,\ m,\ R}(\ \cdot\ ,R)\|^2&=\int_0^{\infty}r\,\mathrm{d}r|g^{0}_{k,\ m,\ R}(r,R)|^2\\&=\frac{\pi^2}{4|A^{(1)}_{m,R}(k)|^2}\left\{|H^{(1)}_{|m-\alpha|}(kR)|^2\int_0^{R}r\,\mathrm{d}r\left|J_{|m|}(kr)\right|^2\right.\\&\quad\left.+|J_{|m|}(kR)|^2\int_R^{\infty}r\,\mathrm{d}r|H^{(1)}_{|m-\alpha|}(kr)|^2\right\}\\&\leqslant(1+\varepsilon)\left[\frac{R^2}{2\alpha^2(1+|m|)}+\frac{R^{2-\xi}}{2\alpha^2}\left(\frac{2}{k}\right)^{\xi}\frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)}\right.\\&\quad\left.\times\frac{\Gamma\left(|m-\alpha|+\frac{\xi+1}{2}\right)\Gamma(2|m-\alpha|+\xi/2)(\Gamma(|m-\alpha|+\xi/2))^2}{\Gamma\left(|m-\alpha|+\frac{\xi+2}{4}\right)\Gamma(2|m-\alpha|+\xi)(\Gamma(|m-\alpha|))^2}\right],\end{aligned} \tag{3.57}$$

Taking $\xi<2(1-\delta)$ gives the desired limit.

Case 2. If $m=N+1$, then $|m-\alpha|+|m|=N+2-\delta$. Then

$$\lim_{R\to 0}\left|\frac{\beta}{1+\beta g^{0}_{k,N+1,R}(R,R)}\right|=\frac{\alpha(N+2-\delta)}{2(1-\delta)}, \tag{3.58}$$

while

$$\int_0^\infty r\,\mathrm{d}r|g^0_{k,N+1,R}(r,R)|^2$$

$$=\frac{\pi^2}{4|A^{(1)}_{N+1,R}(k)|^2}\left\{|H^{(1)}_{1-\delta}(kR)|^2\int_0^R r\,\mathrm{d}r|J_{N+1}(kr)|^2+|J_{N+1}(kR)|^2\int_R^\infty r\,\mathrm{d}r|H^{(1)}_{1-\delta}(kr)|^2\right\} \tag{3.59}$$

$$\leqslant\frac{R^2}{2(N+2)(N+2-\delta)^2}(1+\varepsilon)+\frac{\pi^2\|H^{(1)}_{1-\delta}(kr)\|^2}{(N+2-\delta)^2(\Gamma(1-\delta))^2}\left|\frac{kR}{2}\right|^{2(1-\delta)}(1+\varepsilon). \tag{3.60}$$

Case 3. If $m\leqslant -1$ or $m\geqslant N+2$, then $|m-\alpha|+|m|=|2m-\alpha|$. The constant term is bounded as follows:

$$\left|\frac{\beta}{1+\beta g^0_{k,\,m,\,R}(R,R)}\right|\leqslant\frac{\alpha|2m-\alpha|}{|2m-\alpha|-\alpha}(1+\varepsilon), \tag{3.61}$$

and

$$\int_0^\infty r\,\mathrm{d}r|g^0_{k,\,m,\,R}(r,R)|^2=\frac{\pi^2}{4|A^{(1)}_{m,R}(k)|^2}\left\{|H^{(1)}_{|m-\alpha|}(kR)|^2\int_0^R r\,\mathrm{d}r|J_{|m|}(kr)|^2\right.$$

$$\left.+|J_{|m|}(kR)|^2\int_R^\infty r\,\mathrm{d}r|H^{(1)}_{|m-\alpha|}(kr)|^2\right\} \tag{3.62}$$

$$\leqslant\left[\frac{R^2}{2|2m-\alpha|^2(1+|m|)}+\frac{R^{2-\xi}}{2|2m-\alpha|^2}\left(\frac{2}{k}\right)^\xi\frac{\Gamma\left(\frac{\xi}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\xi}{4}+\frac{1}{2}\right)}(1+\varepsilon)\right.$$

$$\left.\times\frac{\Gamma\left(|m-\alpha|+\frac{\xi+1}{2}\right)\Gamma(2|m-\alpha|+\xi/2)(\Gamma(|m-\alpha|+\xi/2))^2}{\Gamma\left(|m-\alpha|+\frac{\xi+2}{2}\right)\Gamma(2|m-\alpha|+\xi)(\Gamma(|m-\alpha|))^2}\right], \tag{3.63}$$

An argument similar to that used in (3.46) ensures that the bound is independent of m if $|m|$ is large enough.

(b) Let $m=N$ and suppose condition I holds. Then

$$\|g^\beta_{k,N,R}-g^{\nu_N}_{k,N}\|_2\leqslant\|g^0_{k,N,R}-g_{k,N}\|_2+\|l_{k,N,R}-l_{k,N}\|_2, \tag{3.64}$$

where

$$l_{k,N,R}(r,r')=\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r') \tag{3.65}$$

and

$$l_{k,N}=c(N,\nu_N,k)H^{(1)}_\delta(kr)H^{(1)}_\delta(kr'). \tag{3.66}$$

As noted previously, Lemma 1 proves that $\lim_{R\to 0}\|g^0_{k,N,R}-g_{k,N}\|_2=0$.

Now,

$$\|l_{k,N,R}-l_{k,N}\|_2^2=\int r\,dr\,r'\,dr'\left|\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r')\right.$$
$$\left.-c(N,\nu_N,k)H^{(1)}_\delta(kr)H^{(1)}_\delta(kr')\right|^2 \tag{3.67}$$

$$=l^{(1)}+l^{(2)}-l^{(3)}-\overline{l^{(3)}}, \tag{3.68}$$

where

$$l^{(1)}=\left|\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}\right|^2\int r\,dr\,r'\,dr'|g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r')|^2, \tag{3.69}$$

$$l^{(2)}=|c(N,\nu_N,k)|^2\int r\,dr\,r'\,dr'|H^{(1)}_\delta(kr)H^{(1)}_\delta(kr')|^2, \tag{3.70}$$

and

$$l^{(3)}=\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}\overline{c(N,\nu_N,k)}\int r\,dr\,r'\,dr'g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r')\overline{H^{(1)}_\delta(kr)H^{(1)}_\delta(kr')}. \tag{3.71}$$

For small R,

$$\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}\simeq\frac{-\alpha^2R^{-2\delta}}{2\delta\nu_N+\alpha\tilde{c}'(k)}. \tag{3.72}$$

Then

$$\int r\,dr\,r'\,dr'|g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r')|^2$$
$$=\frac{\pi^4}{16|A^{(1)}_{N,R}(k)|^4}\left\{|H^{(1)}_\delta(kR)|^4\left[\int_0^R r\,dr|J_N(kr)|^2\right]^2+\left|J_N(kR)|^4\left[\int_R^\infty r\,dr|H^{(1)}_\delta(kR)|^2\right]^2\right\}. \tag{3.73}$$

The first term is bounded by $[R^4/(4\alpha^4(N+1)^2)](1+\varepsilon)$, while for small R,

$$\left|\frac{\beta}{1+\beta g^0_{k,N,R}(R,R)}\right|^2\frac{\pi^4|J_N(kR)|^4}{16|A^{(1)}_{N,R}(k)|^4}\left[\int_R^\infty r\,dr|H^{(1)}_\delta(kR)|^2\right]^2$$
$$\simeq\frac{\pi^4\left(\frac{k}{2}\right)^{4\delta}}{(\Gamma(\delta))^4(2\delta\nu_N+\alpha\tilde{c}'(k))^2}\|H^{(1)}_\delta(kr)\mathbf{1}_{(R,\infty)}\|^4=|c(N,\nu_N,k)|^2\|H^{(1)}_\delta(kr)\mathbf{1}_{(R,\infty)}\|^4. \tag{3.74}$$

Then $l^{(1)}\to l^{(2)}$ as $R\to 0$ by dominated convergence.

For $l^{(3)}$ we have

$$\int r\,dr\,r'\,dr'\,g^0_{k,N,R}(r,R)g^0_{k,N,R}(R,r')\overline{H^{(1)}_\delta(kr)H^{(1)}_\delta(kr')}$$

$$=\left[\frac{i\pi}{2A^{(1)}_{N,R}(k)}\left\{H^{(1)}_\delta(kR)\int_0^R r\,dr\,J_N(kr)\overline{H^{(1)}_\delta(kr)}\ +J_N(kR)\int_R^\infty r\,dr|H^{(1)}_\delta(kr)|^2\right\}\right]^2. \quad (3.75)$$

The first term in the brackets goes to $[i\Gamma(\delta)R^{2-\delta}/(\alpha\pi(N+2-\delta))]\,(\overline{k}/2)^{-\delta}$, while for small R,

$$\frac{i\pi}{2A^{(1)}_{N,R}(k)}J_N(kR)\int_R^\infty r\,dr|H^{(1)}_\delta(kr)|^2\simeq\frac{i\pi}{\alpha\Gamma(\delta)}\left|\frac{kR}{2}\right|^\delta\|H^{(1)}_\delta(kr)\mathbf{1}_{(R,\infty)}\|^2. \quad (3.76)$$

Then $l^{(3)}\to l^{(2)}$ as $R\to 0$ by dominated convergence, which completes the proof.

□

IV. APPROXIMATION BY SMOOTH FLUX TUBE

In Sec. III, $\mathbf{A}_R=\alpha\,(\mathbf{k}\times\mathbf{r}/r^2)\,\Theta(r-R)$ so that $\mathbf{B}_R$ is concentrated on a cylindrical shell. Now we replace the Θ-function by a smooth step function which approximates the Θ-function as $R\to 0$. Let $a:\mathbb{R}\mapsto\mathbb{R}$ be a differentiable function with $a(r)=0$ for $r\leqslant 0$ and $a(r)=1$ for $r\geqslant r_0$, where $r_0>0$. Furthermore, let a be such that the function $b(r)=(1/r)(\mathrm{d}/\mathrm{d}r)\,a(r)$ is bounded in absolute value (i.e., there exists $b_0\in\mathbb{R}$ such that $|b(r)|\leqslant b_0$). Then $b(r)$ has support only in $(0,r_0)$, and $\int_0^\infty b(r)\,r\,dr=1$. We take

$$\hat{\mathbf{A}}_R=\alpha\frac{\mathbf{k}\times\mathbf{r}}{r^2}a\left(\frac{r-R}{R^5}\right) \quad (4.1)$$

so that $\mathbf{k}\cdot\hat{\mathbf{B}}_R=R^{-5}\alpha\ b((r-R)/R^5)$. Let

$$\hat{H}_R=(i\nabla+\hat{\mathbf{A}}_R)^2+\frac{\beta}{\alpha}\mathbf{k}\cdot\hat{\mathbf{B}}_R. \quad (4.2)$$

β here depends on α and R. Motivated by the result of Sec. III we shall consider two cases:

(a) $\beta(\alpha,R)\simeq-\alpha(1-2\delta/\alpha\,\nu_N R^{2\delta})$,
(b) $\beta(\alpha,R)\simeq(\alpha-2(N+1))(1-2(1-\delta)/2(N+1)-\alpha\,\nu_{N+1}R^{2(1-\delta)})$.

The component of the operator $\hat{H}_R$ on the space with angular momentum m are

$$\hat{h}_{m,R}=-\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{\left(m-\alpha a\left(\frac{r-R}{R^5}\right)\right)^2}{r^2}+\beta R^{-5}b\left(\frac{r-R}{R^5}\right). \quad (4.3)$$

We shall prove convergence in the norm resolvent sense of the operators $\hat{h}_{m,R}$, and hence of $\hat{H}_R$.

We can rewrite the last equation as

$$\hat{h}_{m,R}=-\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{(m-\alpha\Theta(r-R))^2}{r^2}+\frac{\beta}{R^5 r}V_m\left(\frac{r-R}{R^5}\right) \quad (4.4)$$

where

$$V_m(r)=r\,b(r)+\frac{R^4}{\beta(rR^4+1)}\{-2m\alpha(a(r)-\Theta(r))+\alpha^2(a^2(r)-\Theta(r))\}. \quad (4.5)$$

We note that $V_m(r)$ has support only in $(0,r_0)$, and that

$$|\hat{a}_m(r)| := |-2m\alpha(a(r)-\Theta(r))+\alpha^2(a^2(r)-\Theta(r))| \leqslant mK, \tag{4.6}$$

where K is a constant independent of m and R.

Define the auxiliary operators

$$\tilde{h}_{m,\,R} = -\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\left(m-\alpha\Theta\left(r-\frac{1}{R^4}\right)\right)^2}{r^2} + \frac{R^5\beta}{r} V_m\left(r-\frac{1}{R^4}\right). \tag{4.7}$$

V_m is form compact (Note 4, Appendix A) with respect to

$$-\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{(m-\alpha\Theta(r-R))^2}{r^2},$$

so the form sum (4.7) is well-defined. From Theorem B.1(b) of Ref. 7, the resolvent of $\tilde{h}_{m,\,R}$ for $k^2 \in \rho(\tilde{h}_{m,\,R})$ and $\Im(k)>0$, is given by

$$[\tilde{h}_{m,\,R}-k^2]^{-1} = g^0_{k,\,m,\,R} - R^5\beta g^0_{k,\,m,\,R}\tilde{v}_m[1+\beta\tilde{B}_{m,R}(k)]^{-1}\tilde{u}_m g^0_{k,\,m,\,R}, \tag{4.8}$$

where

$$\tilde{v}_m(r) = \left|\frac{1}{r}V_m\left(r-\frac{1}{R^4}\right)\right|^{1/2}, \quad \tilde{u}_m(r) = \left|\frac{1}{r}V_m\left(r-\frac{1}{R^4}\right)\right|^{1/2} \operatorname{sgn}\left[V_m\left(r-\frac{1}{R^4}\right)\right] \tag{4.9}$$

and

$$\tilde{B}_{m,R}(k) = R^5\tilde{u}_m g^0_{k,\,m,\,R}\tilde{v}_m, \quad \Im(k)>0. \tag{4.10}$$

$\tilde{B}_{m,R}$ extends to a Hilbert–Schmidt operator (Note 4, Appendix A).

Introducing the unitary scaling group $(U_R g)(r) = (1/R^5)\, g(r/R^5)$, we get

$$\hat{h}_{m,R} = \frac{1}{R^{10}} U_R \tilde{h}_{m,\,R} U_R^{-1}. \tag{4.11}$$

Then, noting that

$$R^{10} U_R g^0_{k,\,m,\,R} U_R^{-1} = g^0_{k/R^5,m,R} \tag{4.12}$$

and taking the translation $r \to r + (1/R^4)$, we obtain

$$\begin{aligned}[\hat{h}_{m,R}-k^2]^{-1} &= \left[\frac{1}{R^{10}} U_R \tilde{h}_{m,\,R} U_R^{-1} - k^2\right]^{-1} \\ &= R^{10} U_R [\tilde{h}_{m,\,R} - (R^5k)^2]^{-1} U_R^{-1} \\ &= R^{10} U_R [g^0_{R^5k,\,m,\,R} - R^5\beta g^0_{R^5k,\,m,\,R}\tilde{v}_m[1+\beta\tilde{B}_{m,R}(R^5k)]^{-1}\tilde{u}_m g^0_{R^5k,\,m,\,R}] U_R^{-1}\end{aligned} \tag{4.13}$$

for $k^2 \in \rho(\hat{h})$ and $\Im(k)>0$. For $\Im(k)>0$, define Hilbert–Schmidt operators $A_{m,R}(k)$, $B_{m,R}(k)$, and $C_{m,R}(k)$, with integral kernels

$$A_{m,R}(k,r,r') = g^0_{k,\,m,\,R}(r, R(1+R^4r'))\hat{v}_m(r'), \tag{4.14}$$

$$B_{m,R}(k,r,r') = \hat{u}_m(r) g^0_{k,\,m,\,R}(R(1+R^4r), R(1+R^4r'))\hat{v}_m(r'), \tag{4.15}$$

$$C_{m,R}(k,r,r')=\hat{u}_m(r)g^0_{k,\ m,\ R}(R(1+R^4r),r'), \tag{4.16}$$

where

$$\hat{v}_m(r)=\left|\frac{V_m(r)}{r}\right|^{1/2} \quad \text{and} \quad \hat{u}_m(r)=\left|\frac{V_m(r)}{r}\right|^{1/2}\operatorname{sgn}[V_m(r)]. \tag{4.17}$$

Then (4.13) becomes

$$[\hat{h}_{m,R}-k^2]^{-1}=g^0_{k,\ m,\ R}-\beta A_{m,R}(k)[1+\beta B_{m,R}(k)]^{-1}C_{m,R}(k) \tag{4.18}$$

for $k^2\in\rho(h_{\varepsilon,\ m,\ R})$ and $\Im(k)>0$.

Using this representation we can prove the following result.

Theorem 2: Let

$$\hat{H}_R=\bigoplus_{m=-\infty}^{\infty}\hat{h}_{m,R}. \tag{4.19}$$

Then $\hat{H}_R$ converges, as $R\to 0$, to one of the self-adjoint extensions H^ν of the AB Hamiltonian only if either

(I) $\beta(\alpha,R)+\alpha/R^{2\delta}\to 2\delta\nu_N$
or
(II) $\beta(\alpha,R)-\alpha+2(N+1)/R^{2(1-\delta)}\to 2(1-\delta)\nu_{N+1}$.

In case (I) $\hat{H}_R$ converges in the norm resolvent sense, as $R\to 0$, to $H^{(\nu_N,\ \infty)}$, and in case (II) to $H^{(\infty,\ \nu_{N+1})}$.

The proof of this theorem is fairly standard but by no means trivial. Because again we require uniform convergence in m we need to control the m behavior and this makes the proof very lengthy. We therefore do not give the proof here but only state the two lemmas required in the case when Condition I holds. Once we have these two lemmas, the proof is similar to that of Theorem 1 and the result follows from them.

We have already proved that $g^0_{k,\ m,\ R}\to g_{k,m}$ in norm. Let

$$v(r)=|b(r)|^{1/2}, \quad u(r)=|b(r)|^{1/2}\operatorname{sgn}[b(r)]. \tag{4.20}$$

Lemma 3: If condition I holds, then

(a) for $m<0$ and $m>N$, the operators $A_{m,R}(k),C_{m,R}(k)\to 0$ in norm;
(b) for $m=0,\ldots,N-1$, the operators $R^{-\delta}A_{m,R}(k),R^{-\delta}C_{m,R}(k)\to 0$ in norm;
(c) for $m=N$, $R^{-\delta}A_{m,R}(k)\to A_N(k)$ and $R^{-\delta}C_{m,R}(k)\to C_N(k)$ in norm, where $A_N(k,r,r')=\tilde{c}_N(k)H^{(1)}_\delta(kr)v(r')$ and $C_N(k,r,r')=\tilde{c}_N(k)u(r)H^{(1)}_\delta(kr')$.

Lemma 4: If condition I holds, then

(a) for $m<0$ and $m>N$, $\|\beta(\alpha,R)B_{m,R}(k)\|_2\leq C|\alpha|/(|m-\alpha|+|m|)$, where C is a constant independent of m and R;
(b) for $m=0,\ldots,N$, $R^{2\delta}[1+\beta(\alpha,R)B_{m,R}]^{-1}\to(1/\kappa_m)\langle v,\cdot\rangle u$ in norm as $R\to 0$, where

$$\kappa_m=\begin{cases}-\dfrac{\alpha}{2\delta\nu_N}, & m=0,\ldots,N-1,\\[2ex] \dfrac{\alpha\tilde{c}_N^2(k)}{c(N,\nu_N,k)}, & m=N.\end{cases} \tag{4.21}$$

V. OTHER APPROXIMATIONS

As mentioned in the Introduction, there are two other very natural approximations. These were investigated also in Refs. 3 and 4. Case (1) is when the magnetic field inside the cylinder of radius R is homogeneous, that is,

$$\mathbf{A}_R=\begin{cases}\alpha\dfrac{\mathbf{k}\times\mathbf{r}}{R^2}\ , & r<R\\ \alpha\dfrac{\mathbf{k}\times\mathbf{r}}{r^2}\ , & r>R.\end{cases} \tag{5.1}$$

Here $\mathbf{k}\cdot\mathbf{B}_R=2\alpha/R^2\,\Theta(R-r)$.

Case (2) is when the magnetic field is proportional to $1/r$ inside the cylinder

$$\mathbf{A}_R=\begin{cases}\alpha\dfrac{\mathbf{k}\times\mathbf{r}}{rR}\ , & r<R,\\ \alpha\dfrac{\mathbf{k}\times\mathbf{r}}{r^2}\ , & r>R.\end{cases} \tag{5.2}$$

In this case $\mathbf{k}\cdot\mathbf{B}_R=(\alpha/rR)\,\Theta(R-r)$.

Let

$$\sigma=\begin{cases}\dfrac{1+N}{M(1,2+N,\alpha)}, & \text{in case (1)}\\ \dfrac{1+2N}{M(1,2+2N,2\alpha)}, & \text{in case (2)},\end{cases} \tag{5.3}$$

where $M(a,b,z)$ is Kummer's function. Let η be a solution of the equation

$$\eta=-\frac{(1-\delta)(2+N)M(\eta,2+N,\alpha)}{\alpha M(\eta+1,3+N,\alpha)}, \tag{5.4}$$

in case (1) and of the equation

$$\eta=-\frac{(1-\delta)(3+2N)M(\eta,3+2N,2\alpha)}{\alpha M(\eta+1,4+2N,2\alpha)}, \tag{5.5}$$

in case (2). Note that both these equations have an infinite number of solutions.
Let

$$\phi_{k,\,m,\,R}(r,r')=g^{\beta}_{k,\,m,\,R}(r,r')-g_{k,\,m}(r,r'),$$

where $g^{\beta}_{k,\,m,\,R}(r,r')$ is the resolvent of the approximating Hamiltonian in each case and $g_{k,\,m}(r,r')$ is as in (2.4).

The following are the only cases which give nontrivial results:

(I) if $\beta\simeq-\alpha[1-\sigma(2\delta/\alpha)\,\nu_N R^{2\delta}]$ as $R\to0$, then $\phi_{k,\,m,\,R}(r,r')$ approaches
(1) a nonzero limit for $m=N$, corresponding to the self-adjoint extension h_{N,ν_N},
(2) zero limit for $m=N+1$, corresponding to the regular self-adjoint extension $h_{N+1,\infty}$,
(3) zero limit for $m\neq N,N+1$, corresponding to the self-adjoint operators h_m.

(II) if $\beta\simeq\alpha(2\eta-1)[1-(2\eta/(2\eta-1))\,\nu_{N+1}R^{2(1-\delta)}]$ as $R\to0$, then $\phi_{k,\,m,\,R}(r,r')$ approaches

(1) a nonzero limit for $m=N+1$, corresponding to the self-adjoint extension $h_{N+1,\nu_{N+1}}$,
(2) zero limit for $m=N$, corresponding to the regular self-adjoint extension $h_{N,\infty}$,
(3) zero limit for $m\neq N,N+1$, as before.

ACKNOWLEDGMENT

One of the authors (J.L.B.) would like to thank the University of Malta (Staff Development Fund) for financial support during the course of this work.

APPENDIX A

Note 1

The Bessel functions of the first and third kind have the following limiting and asymptotic properties:[9]

(1) for small z,

$$J_\nu(z)\simeq\frac{1}{\Gamma(\nu+1)}\left(\frac{z}{2}\right)^\nu \quad (\nu\neq -1,-2,-3,\ldots), \tag{A1}$$

$$H_\nu^{(1)}(z)\simeq\frac{-i\Gamma(\nu)}{\pi}\left(\frac{z}{2}\right)^{-\nu} \quad (\mathcal{R}\nu>0); \tag{A2}$$

(2) for large $|z|$,

$$J_\nu(z)=\sqrt{\frac{2}{\pi z}}\left\{\cos\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right)+e^{|\mathcal{I}z|}O(|z|^{-1})\right\}(\,|\arg z|<\pi), \tag{A3}$$

$$H_\nu^{(1)}(z)=\sqrt{\frac{2}{\pi z}}\,e^{i[z-(\nu\pi/2)-(\pi/4)]} \quad (-\pi<\arg z<2\pi). \tag{A4}$$

Two linearly independent solutions of

$$\left(-\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{\nu^2}{r^2}\right)\phi_k(r)=k^2\phi_k(r) \tag{A5}$$

are $J_\nu(kr)$ and $H_\nu^{(1)}(kr)$.

In the given case, the only solution for $r<R$ which lies in $\mathcal{D}(h^*_{m,R})$ is $J_{|m|}(kr)$, while for $r>R$ the only solution is $H^{(1)}_{|m-\alpha|}(kr)$.

Note 2

To obtain the Green's function, consider two solutions of Eq. (A5), one of which is regular at $r=0$ and irregular at $r=\infty$, while the other is irregular at $r=0$ and regular at $r=\infty$.

Consider

$$\phi_{1,m,k}(r)=\begin{cases}J_{|m|}(kr), & r<R,\\ A_m^{(1)}(k)J_{|m-\alpha|}(kr)+B_m^{(1)}(k)H^{(1)}_{|m-\alpha|}(kr), & r>R,\end{cases} \tag{A6}$$

$$\phi_{2,m,k}(r)=\begin{cases}A^{(2)}_{m,R}(k)J_{|m|}(kr)+B^{(2)}_{m,R}(k)H^{\{1\}}_{|m|}(kr), & r<R,\\ H^{(1)}_{|m-\alpha|}(kr), & r>R,\end{cases} \tag{A7}$$

where the constants $A^{(1)}_{m,R}(k),A^{(2)}_{m,R}(k),B^{(1)}_{m,R}(k)$, and $B^{(2)}_{m,R}(k)$ are chosen so that the boundary conditions $\phi_{m,k}(R+)=\phi_{m,k}(R-)$ and $\phi'_{m,k}(R+)=\phi'_{m,k}(R-)$ are satisfied (note that the second boundary condition is the one imposed to obtain the regular self-adjoint extension, i.e., the one with $\beta=0$).

Then $g^0_{k,\,m,\,R}(r,r')=c\,\phi_{1,m,k}(r_<)\,\phi_{2,m,k}(r_>)$, where $r_<=\min\{r,r'\}$ and $r_>=\max\{r,r'\}$. The constant c is determined by considering the boundary condition at $r=r'$:

$$\Delta\,\frac{\partial g^0_{k,\,m,\,R}}{\partial r}\bigg|_{r=r'}\equiv\lim_{r\downarrow r'}\frac{\partial g^0_{k,\,m,\,R}}{\partial r}(r,r')-\lim_{r\uparrow r'}\frac{\partial g^0_{k,\,m,\,R}}{\partial r}(r,r')=-\frac{1}{r'}. \tag{A8}$$

Then we obtain

$$g^0_{k,\,m,\,R}(r,r')=\begin{cases}\dfrac{i\pi}{2B^{(2)}_{m,R}(k)}\,\phi_{1,m,k}(r_<)\,\phi_{2,m,k}(r_>), & r,r'\leqslant R,\\[2ex] \dfrac{i\pi}{2A^{(1)}_{m,R}(k)}\,\phi_{1,m,k}(r_<)\,\phi_{2,m,k}(r_>), & r,r'\geqslant R.\end{cases} \tag{A9}$$

Note that the boundary conditions imply that

$$\lim_{R\to 0}\,(A^{(1)}_{m,R}(k)-B^{(2)}_{m,R}(k))=0. \tag{A10}$$

Note 3

(Compare Theorem I.3.1.2 of Ref. 7) The general structure of Eq. (3.14) follows from Krein's formula. To verify the constant in the second term, define for $g\in L^2((0,\infty),r\,\mathrm{d}r)$ and $\Im(k)>0$,

$$f_\beta(r)=((h_{m,R}-k^2)^{-1}g)(r)-\frac{\beta}{1+\beta g^0_{k,\,m,\,R}(R,R)}\langle\overline{g^0_{k,\,m,\,R}(\cdot,R)},g\rangle g^0_{k,\,m,\,R}(r,R). \tag{A11}$$

$$=\int_0^\infty \mathrm{d}r'\,r'\,g^0_{k,\,m,\,R}(r,r')g(r')-\frac{\beta}{1+\beta g^0_{k,\,m,\,R}(R,R)}$$

$$\times\int_0^\infty \mathrm{d}r'\,r'\,g^0_{k,\,m,\,R}(r,R)g^0_{k,\,m,\,R}(R,r')g(r'). \tag{A12}$$

Then $f_\beta\in H^{2,2}_{\mathrm{loc}}((0,\infty)\backslash\{R\},r\,\mathrm{d}r)\cap H^{2,1}((0,\infty),r\,\mathrm{d}r)$ and

$$f'_\beta(R+)-f'_\beta(R-)=\frac{\beta/R}{1+\beta g^0_{k,\,m,\,R}(R,R)}\int_0^\infty \mathrm{d}r'\,r'\,g^0_{k,\,m,\,R}(R,r')g(r')=\frac{\beta}{R}f_\beta(R). \tag{A13}$$

This means that $f_\beta\in\mathcal{D}(h^\beta_{m,\,R})$. Furthermore, for $\Im(k)>0$,

$$(h^\beta_{m,\,R}-k^2)f_\beta=g(r),\quad r\in(0,\infty)\backslash\{R\} \tag{A14}$$

which proves Eq. (3.14).

Note 4

To show that $\tilde{B}$ extends to a Hilbert–Schmidt operator, we need to show that (cf. Ref. 7, p. 80)

$$\int_{[0,\infty)\times[0,\infty)}\mathrm{d}r\,\mathrm{d}r'\,|V(r)||g^0_{k,\,m,\,R}(r,r')|^2|V(r')|\;<\;\infty,\quad \Im(k)>0. \tag{A15}$$

This follows by considering the behavior of the Bessel functions for small and large arguments, as discussed in Note 1. From the previous estimate we obtain

$$\left|\frac{V(r)}{r}\right|^{1/2}\left(-\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{(m-\alpha\Theta(r-R))^2}{r^2}+E\right)^{1/2}\in\mathcal{B}_\infty(L^2((0,\infty),r\,dr)),\quad E>0. \tag{A16}$$

APPENDIX B

In this section we shall derive bounds for expressions involving the Bessel functions $J_\nu(z)$ and $H_\nu^{(1)}(z)$.

First we shall obtain upper bounds for $|J_\nu(z)|$. If $\nu\geqslant-\frac{1}{2}$, then it follows[10] from Poisson's integral that

$$|J_\nu(z)|\leqslant\frac{\left|\frac{z}{2}\right|^\nu}{\Gamma(\nu+1)}e^{|\Im z|}. \tag{B1}$$

For $\nu<-\frac{1}{2}$, the following series expansion,[9] which is valid for all z and ν, is used:

$$J_\nu(z)=\left(\frac{z}{2}\right)^\nu\sum_{k=0}^{\infty}\frac{\left(-\frac{1}{4}z^2\right)^k}{k!\Gamma(\nu+k+1)} \tag{B2}$$

$$=\frac{\left(\frac{z}{2}\right)^\nu}{\Gamma(\nu+1)}\left(1+\sum_{k=1}^{\infty}\frac{\Gamma(\nu+1)\left(-\frac{1}{4}z^2\right)^k}{k!\Gamma(\nu+k+1)}\right). \tag{B3}$$

For $\nu\neq-1,-2,-3,...,$

$$\frac{|\Gamma(\nu+1)|}{|\Gamma(\nu+k+1)|}\leqslant\frac{1}{|\nu_0+1|^k},$$

where $|\nu_0+1|=\min\{|\nu+1|,|\nu+2|,|\nu+3|,...\}$. Thus we obtain

$$|J_\nu(z)|\leqslant\frac{\left|\frac{z}{2}\right|^\nu}{|\Gamma(\nu+1)|}e^{1/4\,|z|^2/|\nu_0+1|},\quad \nu\neq-1,-2,-3,\ldots. \tag{B4}$$

Next we obtain lower bounds for $|J_\nu(z)|$. Using the series expansion (B2), and the same argument used for (B4), we obtain

$$|J_\nu(z)|\geqslant\frac{\left|\frac{z}{2}\right|^\nu}{|\Gamma(\nu+1)|}(2-e^{1/4\,|z|^2/|\nu_0+1|}),\quad \nu\neq-1,-2,-3,\ldots. \tag{B5}$$

The above bounds imply that, given any $\varepsilon>0$, there exists z_0 such that, for any ν, if $|z|<|z_0|$ then

$$|J_\nu(z)|\leqslant\frac{\left|\frac{z}{2}\right|^\nu}{|\Gamma(\nu+1)|}(1+\varepsilon), \tag{B6}$$

$$|J_\nu(z)|\geqslant\frac{\left|\frac{z}{2}\right|^\nu}{|\Gamma(\nu+1)|}(1-\varepsilon). \tag{B7}$$

If ν is a negative integer, upper and lower bounds may be deduced using

$$J_\nu(z)=(-1)^\nu J_{|\nu|}(z). \tag{B8}$$

Upper and lower bounds for expressions involving the derivatives of $J_\nu(z)$ may be deduced from the recurrence relation

$$J'_\nu(z)=-J_{\nu+1}(z)+\frac{\nu}{z}J_\nu(z). \tag{B9}$$

Now we turn to bounds for $|H_\nu^{(1)}(z)|$. These are obtained using the following relation:

$$H_\nu^{(1)}(z)=i\csc(\nu\pi)\{e^{-\nu\pi i}J_\nu(z)-J_{-\nu}(z)\}. \tag{B10}$$

Note that we are only interested in the case $\nu\geqslant 0$. Thus, when $\nu>0$ and $\nu\notin\mathbb{Z}$,

$$|H_\nu^{(1)}(z)|\leqslant\frac{\Gamma(\nu)}{\pi}\left|\frac{z}{2}\right|^{-\nu}e^{1/4|z|^2/|\nu_1+1|}\left(1+\frac{|\Gamma(1-\nu)|}{\Gamma(1+\nu)}\left|\frac{z}{2}\right|^{2\nu}\right), \tag{B11}$$

$$|H_\nu^{(1)}(z)|\geqslant\frac{\Gamma(\nu)}{\pi}\left|\frac{z}{2}\right|^{-\nu}(2-e^{1/4|z|^2/|\nu_1+1|})\left(1-\frac{|\Gamma(1-\nu)|}{\Gamma(1+\nu)}\left|\frac{z}{2}\right|^{2\nu}\right). \tag{B12}$$

Here $|\nu_1+1|=\min\{|\nu+1|,|\nu+2|,|\nu+3|,\ldots,|-\nu+1|,|-\nu+2|,|-\nu+3|,\ldots\}$.

For $\nu\in\mathbb{Z}^+$, we use the relation

$$H_n^{(1)}(z)=J_n(z)+iY_n(z), \tag{B13}$$

where $Y_n(z)$ is the Bessel function of the second kind with series expansion

$$Y_n(z)=-\frac{\left(\frac{z}{2}\right)^{-n}}{\pi}\sum_{k=0}^{n-1}\frac{(n-k-1)!}{k!}\left(\frac{z^2}{4}\right)^k+\frac{2}{\pi}\ln\left(\frac{z}{2}\right)J_n(z)-\frac{\left(\frac{z}{2}\right)^n}{\pi}\sum_{k=0}^{\infty}\frac{\psi(k+1)+\psi(n+k+1)}{k!(n+k)!}$$
$$\times\left(-\frac{z^2}{4}\right)^k,\quad n\geqslant 1 \tag{B14}$$

with the Digamma function $\psi(n)=\Gamma'(n)/\Gamma(n)$ given by

$$\psi(1)=-\gamma,\quad \psi(n)=-\gamma+\sum_{k=1}^{n-1}\frac{1}{k},\quad n\geqslant 2, \tag{B15}$$

where γ is Euler's constant.

Noting that $(n-k-1)!\leqslant\Gamma(n)$ and $[\psi(k+1)+\psi(n+k+1)]/(n+k)!\leqslant 2\Gamma(n)$ for $n\geqslant 1$, we get the following bounds:

$$|Y_n(z)|\leqslant\frac{\Gamma(n)}{\pi}\left|\frac{z}{2}\right|^{-n}e^{1/4|z|^2}\left\{1+\frac{2}{\Gamma(n)}\left|\frac{z}{2}\right|^{2n}\left(1+\frac{1}{\Gamma(n+1)}\left|\ln\frac{z}{2}\right|e^{|\Im(z)|-1/4|z|^2}\right)\right\},\quad n\geqslant 1, \tag{B16}$$

$$|Y_n(z)|\geqslant\frac{\Gamma(n)}{\pi}\left|\frac{z}{2}\right|^{-n}\left\{(2-e^{1/4|z|^2})-\frac{2}{\Gamma(n)}\left|\frac{z}{2}\right|^{2n}e^{1/4|z|^2}-\frac{2}{\Gamma(n)\Gamma(n+1)}\left|\ln\frac{z}{2}\right|\left|\frac{z}{2}\right|^{2n}e^{|\Im(z)|}\right\},$$
$$n\geqslant 1. \tag{B17}$$

The corresponding inequalities for $H_n^{(1)}(z)$ are

$$|H_n^{(1)}(z)| \leqslant \frac{\Gamma(n)}{\pi}\left|\frac{z}{2}\right|^{-n} e^{1/4|z|^2}\left\{1+\frac{2}{\Gamma(n)}\left|\frac{z}{2}\right|^{2n}\left(1+\left(\left|\ln\frac{z}{2}\right|+\frac{\pi}{2}\right)\frac{1}{\Gamma(n+1)}e^{|\Im(z)|-1/4|z|^2}\right)\right\}, \quad n\geqslant 1, \tag{B18}$$

$$|H_n^{(1)}(z)| \geqslant \frac{\Gamma(n)}{\pi}\left|\frac{z}{2}\right|^{-n}\left\{(2-e^{1/4|z|^2})-\frac{2}{\Gamma(n)}\left|\frac{z}{2}\right|^{2n}e^{1/4|z|^2}\right.$$
$$\left.-\left(2\left|\ln\frac{z}{2}\right|+\pi\right)\frac{1}{\Gamma(n)\Gamma(n+1)}\left|\frac{z}{2}\right|^{2n}e^{|\Im(z)|}\right\}, \quad n\geqslant 1. \tag{B19}$$

The above bounds imply that, given any $\varepsilon>0$, there exists z_0 such that, for any $\nu>0$, if $|z|<|z_0|$ then

$$|H_\nu^{(1)}(z)| \leqslant \frac{\Gamma(\nu)}{\pi}\left|\frac{z}{2}\right|^{-\nu}(1+\varepsilon), \tag{B20}$$

$$|H_\nu^{(1)}(z)| \geqslant \frac{\Gamma(\nu)}{\pi}\left|\frac{z}{2}\right|^{-\nu}(1-\varepsilon). \tag{B21}$$

For $n=0$, we use the following series expansion for $Y_0(z)$:

$$Y_0(z)=\frac{2}{\pi}\left\{\ln\left(\frac{z}{2}\right)+\gamma\right\}J_0(z)+\frac{2}{\pi}\left\{\frac{z^2}{4}-\left(1+\frac{1}{2}\right)\frac{\left(\frac{1}{4}z^2\right)^2}{(2!)^2}-\left(1+\frac{1}{2}+\frac{1}{3}\right)\frac{\left(\frac{1}{4}z^2\right)^3}{(3!)^2}-\cdots\right\}. \tag{B22}$$

Noting that $1+\frac{1}{2}+\cdots+(1/n)\leqslant n!$, we find that the term in the second bracket of (B22) is bounded in absolute value by $e^{1/4|z|^2}-1$. Hence we get the following bounds for $Y_0(z)$:

$$|Y_0(z)| \leqslant \frac{2}{\pi}|\ln z|\left\{|J_0(z)|+\frac{|J_0(z)|}{|\ln z|}(\ln 2+\gamma)+\frac{e^{1/4|z|^2}-1}{|\ln z|}\right\}, \tag{B23}$$

$$|Y_0(z)| \geqslant \frac{2}{\pi}|\ln z|\left\{|J_0(z)|-\frac{|J_0(z)|}{|\ln z|}(\ln 2+\gamma)-\frac{e^{1/4|z|^2}-1}{|\ln z|}\right\}. \tag{B24}$$

Then, using (B4) and (B5) for the case $\nu=0$, we obtain the corresponding bounds for $H_0^{(1)}(z)$:

$$|H_0^{(1)}(z)| \leqslant \frac{2}{\pi}|\ln z|e^{1/4|z|^2}\left\{1+\frac{1}{|\ln z|}\left(\ln 2+\gamma+\frac{\pi}{2}\right)+\frac{1-e^{-1/4|z|^2}}{|\ln z|}\right\}, \tag{B25}$$

$$|H_0^{(1)}(z)| \geqslant \frac{2}{\pi}|\ln z|\left\{(2-e^{1/4|z|^2})-\frac{e^{1/4|z|^2}}{|\ln z|}\left(\ln 2+\gamma+\frac{\pi}{2}\right)-\frac{e^{1/4|z|^2}-1}{|\ln z|}\right\}. \tag{B26}$$

Now, for fixed arg(z), we know that $|\ln z|\geqslant\ln|z|$, and that for any $\varepsilon'>0$, $|\ln z|\leqslant\ln|z|(1+\varepsilon')$ if $|z|$ is small enough. This implies that for any $\varepsilon>0$, there exists z_0 such that, if $|z|<|z_0|$, then

$$|H_0^{(1)}(z)| \leqslant \frac{2}{\pi}\ln|z|(1+\varepsilon), \tag{B27}$$

$$|H_0^{(1)}(z)| \geqslant \frac{2}{\pi}\ln|z|(1-\varepsilon). \tag{B28}$$

Next we obtain bounds for the Wronskians that appear in the expressions for the constants $A_{m,R}^{(1)}(k), A_{m,R}^{(2)}(k), B_{m,R}^{(1)}(k)$, and $B_{m,R}^{(2)}(k)$ which are defined in Note 2 of Appendix A.

Using (B9) and (B10), we can write

$$W[H_\nu^{(1)}(z), J_{\nu'}(z)] = H_\nu^{(1)}(z)J'_{\nu'}(z) - H_\nu^{(1)\prime}(z)J_{\nu'}(z)$$

$$= \frac{i}{\sin(\nu\pi)}(\{e^{-\nu\pi i}J_\nu(z) - J_{-\nu}(z)\}J'_{\nu'}(z) - \{e^{-\nu\pi i}J'_\nu(z) - J'_{-\nu}(z)\}J_\nu(z)) \tag{B29}$$

$$= \frac{i}{\sin(\nu\pi)}\left(-\frac{\nu'+\nu}{z}J_{\nu'}(z)J_{-\nu}(z) + J_{\nu'+1}(z)J_{-\nu}(z) - J_{\nu'}(z)J_{-\nu+1}(z) \right.$$
$$\left. + e^{-i\pi\nu}\left\{ \frac{\nu'-\nu}{z}J_{\nu'}(z)J_\nu(z) - J_{\nu'+1}(z)J_\nu(z) + J_{\nu'}(z)J_{\nu+1}(z) \right\} \right). \tag{B30}$$

From the bounds derived above, we obtain

$$|W[H_\nu^{(1)}(z), J_{\nu'}(z)]| \geqslant \frac{(\nu'+\nu)\Gamma(\nu)}{2\pi\Gamma(\nu'+1)}\left|\frac{z}{2}\right|^{\nu'-\nu-1}\left\{ (2-e^{1/4|z|^2/\nu'+1})(2-e^{1/4|z|^2/|\nu_1+1|}) \right.$$
$$- \frac{2e^{|\Im(z)|}}{\nu'+\nu}\left(\frac{e^{1/4|z|^2/|\nu_1+1|}}{\nu'+1}\left|\frac{z}{2}\right|^2 + \frac{e^{1/4|z|^2/|\nu_1+1|}}{|1-\nu|}\left|\frac{z}{2}\right|^2 + \frac{|\nu'+\nu|e^{|\Im(z)|}}{2\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{2\nu} \right.$$
$$\left. \left. + \frac{|\Gamma(1-\nu)|e^{|\Im(z)|}}{\Gamma(\nu+2)}\left|\frac{z}{2}\right|^{2\nu+2} + \frac{|\Gamma(1-\nu)|e^{|\Im(z)|}}{(\nu'+1)\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{2\nu+2} \right) \right\}, \tag{B31}$$

for $\nu, \nu' > 0$, $\nu \notin \mathbb{Z}$.

Since $\Gamma(1-\nu) = \pi/(\sin(\pi\nu)\Gamma(\nu))$, then for any $\varepsilon_0 > 0$ there exist z_0 and $\tilde{\nu}_0$ such that for $|z| < |z_0|$ and $\nu', \nu > \tilde{\nu}_0$,

$$|W[H_\nu^{(1)}(z), J_{\nu'}(z)]| \geqslant \frac{(\nu'+\nu)\Gamma(\nu)}{2\pi\Gamma(\nu'+1)}\left|\frac{z}{2}\right|^{\nu'-\nu-1}(1-\varepsilon_0). \tag{B32}$$

Using a similar argument to that used in (B30), as well as the relation

$$H_\nu^{(1)\prime}(z) = -H_{\nu+1}^{(1)}(z) + \frac{\nu}{z}H_\nu^{(1)}(z), \tag{B33}$$

we can write

$$W[H_\nu^{(1)}(z), H_n^{(1)}(z)] = H_\nu^{(1)}(z)H_n^{(1)\prime}(z) - H_\nu^{(1)\prime}(z)H_n^{(1)}(z) \tag{B34}$$

$$= \frac{i}{\sin(\nu\pi)}\left(J_{-\nu}(z)H_{n+1}^{(1)}(z) - \frac{n+\nu}{z}J_{-\nu}(z)H_n^{(1)}(z) - J_{1-\nu}(z)H_n^{(1)}(z) \right.$$
$$\left. + e^{-i\pi\nu}\left\{ \frac{n-\nu}{z}J_\nu(z)H_n^{(1)}(z) - J_\nu(z)H_{n+1}^{(1)}(z) + J_{\nu+1}(z)H_n^{(1)}(z) \right\} \right). \tag{B35}$$

Let $n \in \mathbb{Z}^+$, $\nu > 0$, and $\nu \notin \mathbb{Z}$. Using the relation

$$H_{n+1}^{(1)}(z)=\frac{2n}{z}H_n^{(1)}(z)-H_{n-1}^{(1)}(z),$$

and the bounds in (B4) and (B11), one can see that for any $\varepsilon_1>0$ there exist z_1 and n_1 such that for $|z|<|z_1|$ and $\nu,n>n_1$,

$$\left|J_{-\nu}(z)\left(H_{n+1}^{(1)}(z)-\frac{n+\nu}{z}H_n^{(1)}(z)\right)\right|\leqslant\frac{\nu-n}{2\pi}\frac{\Gamma(n)}{|\Gamma(1-\nu)|}\left|\frac{z}{2}\right|^{-n-\nu-1}(1+\varepsilon_1),$$

$$|J_{1-\nu}(z)H_n^{(1)}(z)|\leqslant\frac{\Gamma(n)}{\pi|\Gamma(2-\nu)|}\left|\frac{z}{2}\right|^{-n-\nu+1}(1+\varepsilon_1), \tag{B36}$$

$$\left|\frac{n-\nu}{z}J_\nu(z)H_n^{(1)}(z)\right|\leqslant\frac{|n-\nu|\Gamma(n)}{2\pi\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{-n+\nu-1}(1+\varepsilon_1), \tag{B37}$$

$$|J_\nu(z)H_{n+1}^{(1)}(z)|\leqslant\frac{\Gamma(n+1)}{\pi\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{-n+\nu-1}(1+\varepsilon_1), \tag{B38}$$

$$|J_{\nu+1}(z)H_n^{(1)}(z)|\leqslant\frac{\Gamma(n)}{\pi\Gamma(\nu+2)}\left|\frac{z}{2}\right|^{-n+\nu+1}(1+\varepsilon_1). \tag{B39}$$

The above results imply that for $|z|<|z_1|$ and $\nu,n>n_1$,

$$|W[H_\nu^{(1)}(z),H_n^{(1)}(z)]|\leqslant\frac{|\nu-n|}{2\pi^2}\Gamma(n)\Gamma(\nu)\left|\frac{z}{2}\right|^{-n-\nu-1}\left(1+\frac{2}{|\nu-n||1-\nu|}\left|\frac{z}{2}\right|^2+\frac{|\Gamma(1-\nu)|}{\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{2\nu}\right.$$
$$\left.+\frac{2n|\Gamma(1-\nu)|}{|\nu-n|\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{2\nu}+\frac{2|\Gamma(1-\nu)|}{|\nu-n|\Gamma(\nu+2)}\left|\frac{z}{2}\right|^{2\nu+2}\right)(1+\varepsilon_1). \tag{B40}$$

From this we deduce that for any $\varepsilon_2>0$ there exist z_2 and n_2 such that for $|z|<|z_2|$ and $\nu,n>n_2$,

$$|W[H_\nu^{(1)}(z),H_n^{(1)}(z)]|\leqslant\frac{|\nu-n|}{2\pi^2}\Gamma(n)\Gamma(\nu)\left|\frac{z}{2}\right|^{-n-\nu-1}(1+\varepsilon_2). \tag{B41}$$

Using (B9), we obtain

$$W[J_n(z),J_\nu(z)]=J_n(z)J_\nu'(z)-J_n'(z)J_\nu(z) \tag{B42}$$

$$=\frac{\nu-n}{z}J_n(z)J_\nu(z)-J_n(z)J_{\nu+1}(z)+J_{n+1}(z)J_\nu(z). \tag{B43}$$

Then, for $n\in\mathbb{Z}^+$, and $\nu\geqslant-\frac{1}{2}$,

$$|W[J_n(z),J_\nu(z)]|\leqslant\frac{|\nu-n|e^{|\Im(z)|}}{2\Gamma(n+1)\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{n+\nu-1}\left\{1+\left(\frac{2n}{\nu+1}+\frac{2}{n+1}\right)\left|\frac{z}{2}\right|^2\right\}. \tag{B44}$$

Thus, for any $\varepsilon_3>0$ there exist z_3 and n_3 such that for $|z|<|z_3|$ and $\nu,n>n_3$,

$$|W[J_n(z),J_\nu(z)]| \leqslant \frac{|\nu-n|}{2\Gamma(n+1)\Gamma(\nu+1)}\left|\frac{z}{2}\right|^{n+\nu-1}\{1+\varepsilon_3\}. \tag{B45}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Stratified reduction of many-body kinetic energy operators

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(Received 6 March 2003; accepted 26 May 2003)

The center-of-mass system of many bodies admits a natural action of the rotation group SO(3). According to the orbit types for the SO(3) action, the center-of-mass system is stratified into three types of strata. The principal stratum consists of nonsingular configurations for which the isotropy subgroup is trivial, and the other two types of strata consist of singular configurations for which the isotropy subgroup is isomorphic with either SO(2) or SO(3). Depending on whether the isotropy subgroup is isomorphic with SO(2) or SO(3), the stratum in question consists of collinear configurations or of a single configuration of the multiple collision. It is shown that the kinetic energy operator is expressed as the sum of rotational and vibrational energy operators on each stratum except for the stratum of multiple collision. The energy operator for nonsingular configurations has singularity at singular configurations. However, the singularity is not essential in the sense that both of the rotational and vibrational energy integrals have a finite value. This can be proved by using the boundary conditions of wave functions at singular configurations for three-body systems, for simplicity. It is shown, in addition, that the energy operator for collinear configurations has also singularity at the multiple collision, but the singularity is not essential either in the sense that the kinetic energy integral is not divergent at the multiple collision. Reduction procedure is applied to the respective energy operators for the nonsingular and the collinear configurations to obtain respective reduced operators, both of which are expressed in terms of internal coordinates. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1602160]

I. INTRODUCTION

This article has an aim to study n-body Hamiltonians by means of a transformation group. A key idea is as follows: Consider a quantum system on a manifold on which a compact Lie group acts. The manifold is then stratified into the disjoint union of strata according to the orbit types of the group action. If a Hamiltonian operator defined on the manifold is invariant under the group action, it will be stratified in such a manner that the Hamiltonian operator has a description on each stratum. The restricted Hamiltonian operator on each stratum will be reduced, by using a unitary irreducible representation of the group, to an operator on the orbit space formed from the stratum in question.

The center-of-mass system for n bodies admits the action of the rotation group SO(3) in a natural manner. According to the orbit types for the SO(3) action, the center-of-mass system is stratified into strata. The principal (or maximal) stratum consists of nonsingular configurations for which the isotropy subgroup is trivial, so that it is made into an SO(3) principal fiber bundle.[1] The strata of lower dimension consist of singular configurations for which the isotropy subgroup is not trivial. Practically, singular configurations are collinear ones and simultaneous multiple collision, and nonsingular configurations are planar or spatial ones.

To study quantum systems for nonsingular configurations, one can apply connection theory on the SO(3) bundle, through which the kinetic energy operator is determined to be the sum of

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rotational and vibrational energy operators.[2–5] However, these operators fail to be defined at singular configurations. In contrast with the case of nonsingular configurations, the stratum of collinear configurations is not made into a principal fiber bundle, but it remains to have a bundle structure. The present article shows that one can set up quantum systems on each stratum on the basis of the bundle structure of each stratum. The quantum systems defined on respective strata will be reduced to quantum systems defined on respective orbit spaces formed from the respective strata.

On each stratum except for the multiple collision stratum, the kinetic energy operator is decomposed into the sum of rotational and vibrational energy operators. The energy operator for nonsingular configurations has singularity at singular configuration, but it is shown that the singularity is not essential in the sense that both of the rotational and vibrational energy integrals have a finite value. This can be proved by using the boundary conditions of wave functions at singular configurations, while the proof is given only for three-body systems for simplicity. Furthermore, the energy operator for collinear configurations, which is also expressed as the sum of rotational and vibrational energy operators, has also singularity at the multiple collision, but the singularity is not essential either in the sense that the kinetic energy integral is not divergent at the multiple collision. The description of the kinetic energy operator as the sum of rotational and vibrational energy operators is effectively used to provide reduced kinetic energy operators in terms of internal (or shape) coordinates.

The organization of this article is as follows: In Sec. II, a brief review is made of the center-of-mass system along with the stratification by means of the SO(3) action. Section III is a review of the Fourier analysis of wave functions,[6,7] which is an application of the Peter–Weyl theorem on unitary irreducible representations of compact Lie groups. Section IV is concerned with a geometric setting for nonsingular configurations. A connection form and a metric are defined and expressed in terms of local coordinates. Transformation law for locally defined connection forms is discussed also. In Sec. V, the kinetic energy operator is defined for nonsingular configurations, which is broken up into the sum of rotational and vibrational energy operators. Operating on equivariant functions with these operators, one obtains reduced rotational and vibrational energy operators in terms of local coordinates for the shape of nonsingular configurations. Transformation law for locally defined reduced operators is studied as well. Section VI is specialized to three-body systems. Though the three-body system was already studied in the same manner,[4] this section deals with it in a different coordinate system to discuss the singularity of the kinetic energy operator. It is shown that the rotational and the vibrational energy operators are not singular in the sense that the rotational and vibrational energy integrals are not divergent at singular configurations. Section VII deals with collinear configurations. A (singular) connection form will be defined on the stratum of collinear configurations. In Sec. VIII, the kinetic energy operator for collinear configurations is studied on the basis of the singular connection treated in Sec. VII. Operating on equivariant wave functions with the kinetic energy operator, one obtains a reduced kinetic energy operator, which is defined on the shape space of collinear configurations.

II. THE CENTER-OF-MASS SYSTEM

Let $\mathbf{x}_i$ and m_i with $i=1,\ldots,N$ be position vectors and masses of point particles in $\mathbf{R}^3$, respectively. Then the configurations of the point particles are denoted by $x=(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$. The center-of-mass system M is defined to be

$$M=\left\{ x=(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \,\middle|\, \mathbf{x}_i\in\mathbf{R}^3, \sum_{i=1}^{N} m_i\mathbf{x}_i=0 \right\}. \tag{1}$$

The configuration x is characterized by the linear subspace

$$F_x := \mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\}. \tag{2}$$

According as $\dim F_x = 0,1,2,3$, the configurations of the particles are pointlike, collinear, planar, and spatial, respectively. Thus M is broken up into four subsets:

$$M = \bigcup_{k=0}^{3} M_k, \quad M_k := \{x \in M \mid \dim F_x = k\}, \quad k = 0,1,2,3. \tag{3}$$

The center-of-mass system admits a natural SO(3) action:

$$\Phi_g(x) = gx = (g\mathbf{x}_1, g\mathbf{x}_2, \ldots, g\mathbf{x}_N), \quad g \in \mathrm{SO}(3), \quad x \in M. \tag{4}$$

The isotropy subgroup G_x of $G = \mathrm{SO}(3)$ at $x \in M$ is defined, as usual, to be $G_x = \{g \in G \mid gx = x\}$. Now one can show that the isotropy subgroups are trivial, $G_x = \{e\}$, on $M_2 \cup M_3$, that is, SO(3) acts on $M_2 \cup M_3$ freely. However, on M_1 and on M_0, the isotropy subgroups are nontrivial; at $x \in M_1$ and at $x \in M_0$, they are isomorphic with SO(2) and with SO(3), respectively. Configurations in $M_0 \cup M_1$ are called singular, which are pointlike or collinear. Depending on the dimensionality of the isotropy subgroups G_x, orbits $\mathcal{O}_x$ of G through $x \in M$ are classified into three cases:

$$\mathcal{O}_x \cong \begin{cases} \mathrm{SO}(3) \quad \text{for} \quad x \in M_2 \cup M_3, \\ S^2 \cong \mathrm{SO}(3)/\mathrm{SO}(2) \quad \text{for} \quad x \in M_1, \\ \{0\} \quad \text{for} \quad x \in M_0. \end{cases} \tag{5}$$

According to the orbit types, M is stratified into strata:

$$M = \dot{M} \cup M_1 \cup M_0, \quad \dot{M} := M_2 \cup M_3. \tag{6}$$

On restricting M to $\dot{M} = M_2 \cup M_3$, we can make $\dot{M}$ into a principal fiber bundle $\dot{M} \to \dot{Q} := \dot{M}/\mathrm{SO}(3)$,[1] since SO(3) is compact and since SO(3) acts on $\dot{M}$ freely. However, the total space M cannot be made into a principal fiber bundle. The orbit space $Q := M/\mathrm{SO}(3)$ is not a manifold in general. In fact, in the case of the three-body system, the orbit space is homeomorphic with the closed half space of $\mathbf{R}^3$.[4] In the case of the four-body system, the orbit space is shown to be homeomorphic with $\mathbf{R}^6$.[8] Though M itself is not a principal fiber bundle, we may make M into a stratified fiber bundle with respective projections

$$\dot{M} \to \dot{M}/\mathrm{SO}(3), \quad M_1 \to M_1/S^2, \quad M_0 \to M_0/M_0. \tag{7}$$

It is to be noted that $\dot{M}$ and M_1 are viewed as the configuration spaces for ''nonlinear molecules'' and for ''linear molecules,'' respectively. Equation (7) implies that we can discuss nonlinear and linear molecules separately, but on an equal footing from the viewpoint of transformation group theory.

It is of great use to employ Jacobi vectors in working with the center-of-mass system. The Jacobi vectors $\mathbf{r}_j$, $j = 1,\ldots,N-1$, are defined to be

$$\mathbf{r}_j := \left(\frac{1}{\mu_j} + \frac{1}{m_{j+1}}\right)^{-1/2} \left(\mathbf{x}_{j+1} - \frac{1}{\mu_j} \sum_{i=1}^{j} m_i \mathbf{x}_i\right), \quad \mu_j := \sum_{i=1}^{j} m_i. \tag{8}$$

Since the position vectors $\mathbf{x}_i$ in the center-of-mass system are uniquely described in terms of Jacobi vectors, we can identify the center-of-mass system with the set of collections of Jacobi vectors:

$$M \cong \{x = (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \mid \mathbf{r}_j \in \mathbf{R}^3, \quad j = 1,\ldots,N-1\}. \tag{9}$$

Thus, M is viewed as the linear space formed by $x=(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})$, or as the space of $3\times(N-1)$ matrices. Since $\operatorname{rank} x=\dim F_x$, we can regard $\dot{M}:=M_2\cup M_3$ as the space of $3\times(N-1)$ matrices of rank greater than or equal to two. M_1 and M_0 are the spaces of $3\times(N-1)$ matrices of rank 1 and of rank 0, respectively. The space of singular configurations, M_1 and M_0, forms the boundary of the space of nonsingular configurations, $M_2\cup M_3$. Note that $\dim\dot{M}=3N-3$, $\dim M_1=N+1$, and $\dim M_0=0$. We note, in conclusion, that the SO(3) action is expressed as

$$(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\mapsto(g\mathbf{r}_1,\ldots,g\mathbf{r}_{N-1}). \tag{10}$$

III. FOURIER ANALYSIS OF WAVE FUNCTIONS

To treat wave functions irrespectively of the orbit type of the SO(3) action on the center-of-mass system, it is of great use to apply Fourier analysis on the basis of the Peter–Weyl theorem on unitary irreducible representations of compact Lie groups. To describe this method,[6,7] we put the problem in a general setting. Let M be a manifold on which a compact Lie group G acts. Let μ_M be a G-invariant measure on M. We take the space $L^2(M)$ of square integrable functions on M as the Hilbert space of wave functions, in which the G is represented unitarily through $(U(g)f)(x)=f(g^{-1}x)$, $g\in G$, $x\in M$.

Let μ_G and $L^2(G)$ denote the normalized invariant measure on G and the space of square integrable functions on G with respect to μ_G, respectively. Let $(\mathcal{H}^\chi,\rho^\chi)$ be irreducible unitary representations of G, where χ ranges over all the inequivalent representations. We denote by ρ^χ_{ij} the matrix elements of the representation ρ^χ with respect to some orthonormal basis e^χ_i of $\mathcal{H}^\chi$, where $i,j=1,\ldots,d_\chi$, with $d_\chi=\dim\mathcal{H}^\chi$. The Peter–Weyl theorem states that the set of all the matrix elements $\{\sqrt{d_\chi}\rho^\chi_{ij}\}_{\chi,i,j}$ forms a complete orthonormal system in $L^2(G)$. By this theorem, any function φ of $L^2(G)$ is expanded into

$$\varphi(h)=\sum_{\chi,i,j} d_\chi\rho^\chi_{ij}(h)\int_G\overline{\rho^\chi_{ij}(g)}\varphi(g)d\mu_G(g). \tag{11}$$

We turn to wave functions on M. For a function $f\in L^2(M)$, we may view $f(hx)$ as a function on G with x fixed arbitrarily, $f_x(h):=f(hx)$, and apply the above expansion to f_x to obtain

$$f(hx)=\sum_{\chi,i,j} d_\chi\rho^\chi_{ij}(h)\int_G\overline{\rho^\chi_{ij}(g)}f(gx)d\mu_G(g). \tag{12}$$

We here introduce the operators P^χ_{ij} and P^χ_i on $L^2(M)$ by

$$P^\chi_{ij}:=d_\chi\int_G\rho^\chi_{ij}(g)U(g)d\mu_G(g), \tag{13}$$

$$P^\chi_i:=P^\chi_{ii}, \tag{14}$$

respectively. These operators satisfy that

$$(P^\chi_{ij})^\dagger=P^\chi_{ji},\quad P^\chi_{ij}P^{\chi'}_{k\ell}=\delta^{\chi\chi'}\delta_{jk}P^\chi_{i\ell}, \tag{15}$$

and

$$(P^\chi_i)^\dagger=P^\chi_i,\quad P^\chi_iP^{\chi'}_j=\delta^{\chi\chi'}\delta_{ij}P^\chi_i, \tag{16}$$

respectively. Moreover, one verifies that

$$(P^\chi_{ij})^\dagger P^\chi_{ij}=P^\chi_j,\quad P^\chi_{ij}(P^\chi_{ij})^\dagger=P^\chi_i. \tag{17}$$

It then follows that when restricted to $\mathrm{Im}\,P_j^\chi$, the P_{ij}^χ provides the unitary isomorphism

$$P_{ij}^\chi : \mathrm{Im}\,P_j^\chi \xrightarrow{\sim} \mathrm{Im}\,P_i^\chi . \tag{18}$$

Furthermore, we can show that P_{ij}^χ and $U(g)$ are put together to give

$$P_{ij}^\chi U(g) = \sum_k \rho_{kj}^\chi(g^{-1}) P_{ik}^\chi , \tag{19}$$

$$U(g) P_{ij}^\chi = \sum_k \rho_{ik}^\chi(g^{-1}) P_{kj}^\chi . \tag{20}$$

From (20), it turns out that the map $E_j^\chi : L^2(M) \to \mathcal{H}^\chi \otimes L^2(M)$ defined by

$$E_j^\chi := \frac{1}{\sqrt{d_\chi}} \sum_{i=1}^{d_\chi} e_i^\chi \otimes P_{ij}^\chi \tag{21}$$

satisfies $U(g^{-1})E_j^\chi = \rho^\chi(g) E_j^\chi$, or equivalently

$$(E_j^\chi f)(gx) = \rho^\chi(g)(E_j^\chi f)(x), \quad f \in L^2(M), \tag{22}$$

which implies that the $\mathcal{H}^\chi$-valued function $E_j^\chi f$ is a ρ^χ-equivariant function.

We here introduce the space, $L^2(M;\mathcal{H}^\chi)^G$, of square integrable equivariant $\mathcal{H}^\chi$-valued functions by

$$L^2(M;\mathcal{H}^\chi)^G := \left\{ \psi : M \to \mathcal{H}^\chi \,\middle|\, \int_M \|\psi(x)\|^2 d\mu_M(x) < \infty,\ \psi(gx) = \rho^\chi(g)\psi(g) \right\}, \tag{23}$$

where $g \in G$, $x \in M$, and $\|\cdot\|$ denotes the norm in $\mathcal{H}^\chi$. Then we can view the operator E_j^χ as a map $L^2(M) \to L^2(M;\mathcal{H}^\chi)^G$. The adjoint operator $(E_j^\chi)^\dagger : L^2(M;\mathcal{H}^\chi)^G \to L^2(M)$ is defined, of course, through

$$\langle \psi, E_j^\chi f \rangle_{\mathcal{H}^\chi \otimes L^2(M)} = \langle (E_j^\chi)^\dagger \psi, f \rangle_{L^2(M)}, \quad \psi \in L^2(M;\mathcal{H}^\chi)^G, \quad f \in L^2(M), \tag{24}$$

where the subscripts $\mathcal{H}^\chi \otimes L^2(M)$ and $L^2(M)$ attached to $\langle\,,\rangle$ indicate the spaces on which the respective inner products are defined. Then one can observe that

$$(E_j^\chi)^\dagger E_j^\chi = P_j^\chi, \quad E_j^\chi (E_j^\chi)^\dagger = \mathrm{id}_{L^2(M;\mathcal{H}^\chi)^G}. \tag{25}$$

These relations imply that when restricted to $\mathrm{Im}\,P_j^\chi$, the E_j^χ provides a unitary isomorphism

$$E_j^\chi : \ \mathrm{Im}\,P_j^\chi \xrightarrow{\sim} L^2(M;\mathcal{H}^\chi)^G, \quad j = 1,\ldots,d_\chi . \tag{26}$$

We now apply the above-mentioned Fourier analysis to N-body systems. The manifold M we take is the center-of-mass system for N bodies. We introduce the Euler angles (ϕ, θ, ψ) through

$$g = e^{\phi R(\mathbf{e}_3)} e^{\theta R(\mathbf{e}_2)} e^{\psi R(\mathbf{e}_3)}, \quad g \in \mathrm{SO}(3), \tag{27}$$

where $\mathbf{e}_k$, $k = 1,2,3$, are the standard basis of $\mathbf{R}^3$ and $R(\mathbf{e}_k)$ denote the 3×3 antisymmetric matrices defined through $R(\mathbf{e}_k)\mathbf{a} = \mathbf{e}_k \times \mathbf{a}$ for $\mathbf{a} \in \mathbf{R}^3$. Let $D_{nm}^\ell(g)$ denote the matrix elements of unitary irreducible representations of SO(3) with $\ell = 0,1,2,\ldots$, and $|m|, |n| \leqslant \ell$.[9] They are expressed as

$$D^{\ell}_{nm}(g)=e^{-in\phi}d^{\ell}_{nm}(\theta)e^{-im\psi}, \tag{28}$$

where $d^{\ell}_{nm}(\theta)$ are given by

$$\begin{aligned} d^{\ell}_{nm}(\theta) &= (-1)^{n-m}\sqrt{(\ell+n)(\ell-n)(\ell+m)(\ell-m)} \\ &\times\sum_{k=0}^{\ell-m}\frac{(-1)^k}{k!(\ell-n-k)!(\ell+m-k)!(n-m+k)!}\left(\sin\frac{\theta}{2}\right)^{2k+n-m}\left(\cos\frac{\theta}{2}\right)^{2\ell-2k-(n-m)}. \end{aligned} \tag{29}$$

Let $d\mu(g)$ denote the invariant volume element on SO(3), which is expressed, in terms of the Euler angles, as

$$d\mu(g)=\sin\theta\, d\theta d\phi d\psi \quad \text{with} \quad \int_{\mathrm{SO}(3)} d\mu(g)=8\pi^2. \tag{30}$$

According to (12) with $\rho^{\chi}_{ij}=D^{\ell}_{mn}$, $d_{\chi}=2\ell+1$, and $d\mu_G(g)=d\mu(g)/(8\pi^2)$, a wave function $f(hx)$ on M is expanded into a Fourier series

$$f(hx)=\sum_{\ell=0}^{\infty}\sum_{|m|,|n|\leqslant\ell}\frac{2\ell+1}{8\pi^2}D^{\ell}_{mn}(h)\int_{\mathrm{SO}(3)}\overline{D^{\ell}_{mn}}(g)f(gx)d\mu(g), \quad x\in M. \tag{31}$$

The map $E^{\ell}_{m}: L^2(M)\to\mathcal{H}^{\ell}\otimes L^2(M)$ is defined as in (21):

$$E^{\ell}_{m}f=\frac{1}{\sqrt{2\ell+1}}\sum_{|m'|\leqslant\ell}e^{\ell}_{m'}\otimes P^{\ell}_{m'm}f, \tag{32}$$

where $e^{\ell}_{m'}$, denoted usually by $|\ell\, m'\rangle$, is the basis of the representation space $\mathcal{H}^{\ell}$. The ρ^{χ}-equivariance condition (22) now takes the form

$$(E^{\ell}_{m}f)(hx)=D^{\ell}(h)(E^{\ell}_{m}f)(x). \tag{33}$$

IV. NONSINGULAR CONFIGURATIONS

In this section, we make a brief review of the geometric setting-up for the nonsingular configurations.[4] We note first that the center-of-mass system is now identified with the set of collections of the Jacobi vectors [see (9)]. As is already mentioned, SO(3) acts on $\dot{M}$ freely, so that $\dot{M}$ is made into an SO(3) bundle,

$$\pi:\ \dot{M}\to\dot{Q}:=\dot{M}/\mathrm{SO}(3). \tag{34}$$

The inertia tensor, $A_x:\ \mathbf{R}^3\to\mathbf{R}^3$, is defined for $x\in M$ through

$$A_x(\mathbf{v})=\sum_{j=1}^{N-1}\mathbf{r}_j\times(\mathbf{v}\times\mathbf{r}_j), \quad \mathbf{v}\in\mathbf{R}^3, \tag{35}$$

and the connection form ω is defined for $x\in\dot{M}$ to be

$$\omega_x=R\left(A_x^{-1}\left(\sum_{j=1}^{N-1}\mathbf{r}_j\times d\mathbf{r}_j\right)\right), \tag{36}$$

where $R:\mathbf{R}^3\to\mathrm{so}(3)$ is the isomorphism already mentioned in Sec. III. Note that A_x^{-1} exists only for $x\in\dot{M}$. The connection form ω gives rise to a direct sum decomposition of the tangent space to $\dot{M}$ at $x\in\dot{M}$,

$$T_x(\dot{M})=V_x\oplus H_x, \tag{37}$$

where $V_x:=T_x(\mathcal{O}_x)$ is the tangent space to the SO(3)-orbit $\mathcal{O}_x$ through $x\in\dot{M}$ and $H_x:=\ker\omega_x$ with $\omega_x:T_x(\dot{M})\to\mathrm{so}(3)$. Tangent vectors in V_x and in H_x are called rotational (or vertical) and vibrational (or horizontal), respectively. By definition, rotational vectors are put in the form $R(\mathbf{a})x$ with $\mathbf{a}\in\mathbf{R}^3$. In fact, for a one-parameter group of rotations $e^{tR(\mathbf{a})}$ acting on M, its infinitesimal generator is given by

$$\frac{d}{dt}e^{tR(\mathbf{a})}x\bigg|_{t=0}=R(\mathbf{a})x=(R(\mathbf{a})\mathbf{r}_1,\ldots,R(\mathbf{a})\mathbf{r}_{N-1}). \tag{38}$$

In contrast with this, the definition of H_x implies that

$$u=(\mathbf{u}_1,\ldots,\mathbf{u}_{N-1})\in H_x\Leftrightarrow\sum_{j=1}^{N-1}\mathbf{r}_j\times\mathbf{u}_j=0. \tag{39}$$

Further, it is easy to see that V_x and H_x are orthogonal to each other with respect to the metric

$$ds^2=\sum_{j=1}^{N-1}d\mathbf{r}_j\cdot d\mathbf{r}_j. \tag{40}$$

In fact, for $R(\mathbf{a})x\in V_x$ and $u\in H_x$, one has

$$\sum_j R(\mathbf{a})\mathbf{r}_j\cdot\mathbf{u}_j=\mathbf{a}\cdot\sum_j\mathbf{r}_j\times\mathbf{u}_j=0. \tag{41}$$

For a tangent vector $v=(\mathbf{v}_1,\ldots,\mathbf{v}_{N-1})\in T_x(\dot{M})$, its vertical components $P_x(v)=(P_x(v)_1,\ldots,P_x(v)_{N-1})\in V_x$ are given by

$$P_x(v)_j=\left(A_x^{-1}\left(\sum_{k=1}^{N-1}\mathbf{r}_k\times\mathbf{v}_k\right)\right)\times\mathbf{r}_j. \tag{42}$$

In what follows, we describe the connection form ω and the metric ds^2 in terms of local coordinates. Let σ be a local section defined on an open subset U of $\dot{Q}$, $\sigma:U\to\dot{M}$. Then any point $x\in\pi^{-1}(U)$ is expressed as

$$x=g\sigma(q)=(g\boldsymbol{\sigma}_1(q),\ldots,g\boldsymbol{\sigma}_{N-1}(q)),\quad q\in U. \tag{43}$$

Let $g\in\mathrm{SO}(3)$ and $q\in U$ be assigned by the Euler angles (θ,ϕ,ψ) and by local coordinates q^α, $\alpha=1,\ldots,3N-6$, respectively. Then a straightforward calculation along with (36) and (43) provides

$$\omega_{g\sigma(q)}=dgg^{-1}+g\omega_{\sigma(q)}g^{-1}=g(g^{-1}dg+\omega_{\sigma(q)})g^{-1}, \tag{44}$$

where

$$\omega_{\sigma(q)}:=R\left(A_{\sigma(q)}^{-1}\left(\sum_{j=1}^{N-1}\boldsymbol{\sigma}_j(q)\times d\boldsymbol{\sigma}_j(q)\right)\right). \tag{45}$$

We here express $\omega_{\sigma(q)}$ as

$$\omega_{\sigma(q)}=\sum_{a=1}^{3}\sum_{\alpha=1}^{3N-6}\Lambda^a_\alpha(q)dq^\alpha R(\mathbf{e}_a), \tag{46}$$

and introduce a moving frame $\mathbf{u}_a$, $a=1,2,3$, and the left-invariant one-forms Ψ^a, $a=1,2,3$, on SO(3) by

$$\mathbf{u}_a=g\mathbf{e}_a, \tag{47}$$

$$g^{-1}dg=\sum_{a=1}^{3}\Psi^a R(\mathbf{e}_a), \tag{48}$$

respectively. Then the connection form ω given by (44) is put in the form

$$\omega_{g\sigma(q)}=\sum_a \Theta^a R(\mathbf{u}_a), \quad \Theta^a:=\Psi^a+\sum_\alpha \Lambda^a_\alpha(q)dq^\alpha, \tag{49}$$

where we have used the formula $R(g\mathbf{e}_a)=gR(\mathbf{e}_a)g^{-1}$.

The horizontal lift, $(\partial/\partial q^\alpha)^*$, of a local vector field $\partial/\partial q^\alpha$ on U is defined through

$$\omega_{g\sigma(q)}\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=0, \quad \pi_*\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=\frac{\partial}{\partial q^\alpha}, \tag{50}$$

and proves to be given by

$$\left(\frac{\partial}{\partial q^\alpha}\right)^*=\frac{\partial}{\partial q^\alpha}-\sum_a \Lambda^a_\alpha(q)K_a, \quad \alpha=1,2,\ldots,3N-6, \tag{51}$$

where K_a are the left-invariant vector fields on SO(3), which are dual to Ψ^a:

$$\Psi^a(K_b)=\delta^a_b, \quad a,b=1,2,3. \tag{52}$$

The dq^α, Θ^a and the $(\partial/\partial q^\alpha)^*$, K_a form local bases of one-forms and of vector fields on $\pi^{-1}(U)\cong U\times \mathrm{SO}(3)$, respectively, in accordance with the decomposition (37). They are dual to each other:

$$dq^\alpha\left(\left(\frac{\partial}{\partial q^\beta}\right)^*\right)=\delta^\alpha_\beta, \quad dq^\alpha(K_a)=0, \tag{53}$$

$$\Theta^a\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=0, \quad \Theta^a(K_b)=\delta^a_b. \tag{54}$$

In contrast with left-invariant one-forms and vector fields, right-invariant one-forms Φ^a and vector fields J_a are defined through

$$dgg^{-1}=\sum_{a=1}^{3}\Phi^a R(\mathbf{e}_a), \tag{55}$$

$$\Phi^a(J_b)=\delta^a_b, \quad a,b=1,2,3, \tag{56}$$

respectively. Since $g(g^{-1}dg)g^{-1}=dgg^{-1}$, the right- and left-invariant one-forms are related to each other, and so are the right- and left-invariant vector fields,

$$\Phi^a=\sum_{b=1}^{3} g_{ab}\Psi^b,\quad J_a=\sum_{b=1}^{3} g_{ab}K_b\,, \tag{57}$$

where g_{ab} denote the matrix elements of g.

We here associate the vector fields K_a and J_a with the angular momentum operator. The infinitesimal rotation (38) is put in the form of operator,

$$\sum_{k=1}^{N-1} R(\mathbf{a})\mathbf{r}_k\cdot\frac{\partial}{\partial\mathbf{r}_k}=\mathbf{a}\cdot\left(\sum_{k=1}^{N-1}\mathbf{r}_k\times\frac{\partial}{\partial\mathbf{r}_k}\right)=\mathbf{a}\cdot\mathbf{J}, \tag{58}$$

where we have set

$$\mathbf{J}=\sum_{k=1}^{N-1}\mathbf{r}_k\times\frac{\partial}{\partial\mathbf{r}_k}. \tag{59}$$

Since one has, from (58) with $\mathbf{a}=\mathbf{e}_a$,

$$\mathbf{e}_a\cdot\mathbf{J}=\frac{d}{dt}e^{tR(\mathbf{e}_a)}x\bigg|_{t=0}=\frac{d}{dt}e^{tR(\mathbf{e}_a)}g\,\sigma(q)\bigg|_{t=0}, \tag{60}$$

$\mathbf{e}_a\cdot\mathbf{J}$ can be identified with the right-invariant vector fields J_a on SO(3), $J_a=\mathbf{e}_a\cdot\mathbf{J}$. Further, on account of (47) and (57), we obtain

$$\mathbf{J}=\sum_{a=1}^{3}\mathbf{e}_aJ_a=\sum_{a=1}^{3}\mathbf{u}_aK_a\,. \tag{61}$$

The last equality of the above equation also means that

$$K_a=\mathbf{u}_a\cdot\mathbf{J}=\frac{d}{dt}e^{tR(\mathbf{u}_a)}x\bigg|_{t=0}=\frac{d}{dt}g\,e^{tR(\mathbf{e}_a)}\sigma(q)\bigg|_{t=0}. \tag{62}$$

This implies that K_a can be identified with an infinitesimal rotation with respect to the so-called body frame.

In terms of the Euler angles given by $g=e^{\phi R(\mathbf{e}_3)}e^{\theta R(\mathbf{e}_2)}e^{\psi R(\mathbf{e}_3)}$, the K_a and J_a and the Ψ^a and Φ^a are expressed, respectively, as

$$\begin{aligned}
K_1&=-\frac{\cos\psi}{\sin\theta}\frac{\partial}{\partial\phi}+\sin\psi\frac{\partial}{\partial\theta}+\cot\theta\cos\psi\frac{\partial}{\partial\psi},\\
K_2&=\frac{\sin\psi}{\sin\theta}\frac{\partial}{\partial\phi}+\cos\psi\frac{\partial}{\partial\theta}-\cot\theta\sin\psi\frac{\partial}{\partial\psi},\\
K_3&=\frac{\partial}{\partial\psi},
\end{aligned} \tag{63}$$

$$\begin{aligned}
\Psi^1&=\sin\psi\,d\theta-\sin\theta\cos\psi\,d\phi,\\
\Psi^2&=\cos\psi\,d\theta+\sin\theta\sin\psi\,d\phi,\\
\Psi^3&=d\psi+\cos\theta\,d\phi,
\end{aligned} \tag{64}$$

$$J_1 = -\cos\phi\cot\theta\frac{\partial}{\partial\phi} - \sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\psi},$$

$$J_2 = -\sin\phi\cot\theta\frac{\partial}{\partial\phi} + \cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\psi}, \tag{65}$$

$$J_3 = \frac{\partial}{\partial\phi},$$

$$\Phi^1 = -\sin\phi\, d\theta + \sin\theta\cos\phi\, d\psi,$$

$$\Phi^2 = \cos\phi\, d\theta + \sin\theta\sin\phi\, d\psi, \tag{66}$$

$$\Phi^3 = d\phi + \cos\theta\, d\psi.$$

We now wish to express the metric (40) in terms of dq^α, Θ^a. We first note that the basis vector fields $(\partial/\partial q^\alpha)^*$, K_a are expressed also as

$$\left(\frac{\partial}{\partial q^\alpha}\right)^* = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot \frac{\partial}{\partial \mathbf{r}_j}, \quad K_a = \sum_j K_a \mathbf{r}_j \cdot \frac{\partial}{\partial \mathbf{r}_j}, \tag{67}$$

respectively. Since vibrational and rotational vectors are orthogonal to each other, one has

$$ds^2\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*, K_a\right) = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot K_a \mathbf{r}_j = 0. \tag{68}$$

We further introduce the quantities $a_{\alpha\beta}$ and A_{ab} by

$$a_{\alpha\beta} := ds^2\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*, \left(\frac{\partial}{\partial q^\beta}\right)^*\right) = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot \left(\frac{\partial}{\partial q^\beta}\right)^* \mathbf{r}_j, \tag{69}$$

$$A_{ab} := ds^2(K_a, K_b) = \sum_j K_a \mathbf{r}_j \cdot K_b \mathbf{r}_j. \tag{70}$$

Then the metric ds^2 is put in the form

$$ds^2 = \sum_{\alpha,\beta} a_{\alpha\beta} dq^\alpha dq^\beta + \sum_{a,b} A_{ab}\Theta^a\Theta^b. \tag{71}$$

Since $K_a \mathbf{r}_j = \mathbf{u}_a \times \mathbf{r}_j = g(\mathbf{e}_a \times \boldsymbol{\sigma}_j(q))$, one obtains, from (51),

$$\left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j = g\left(\frac{\partial \boldsymbol{\sigma}_j(q)}{\partial q^\alpha} - \sum_a \Lambda^a_\alpha(q)(\mathbf{e}_a \times \boldsymbol{\sigma}_j(q))\right), \tag{72}$$

and then the quantities $a_{\alpha\beta}$ and A_{ab} are put, respectively, in the form

$$a_{\alpha\beta} = \sum_j \left(\frac{\partial \boldsymbol{\sigma}_j}{\partial q^\alpha} - \sum_a \Lambda^a_\alpha(q)(\mathbf{e}_a \times \boldsymbol{\sigma}_j)\right) \cdot \left(\frac{\partial \boldsymbol{\sigma}_j}{\partial q^\beta} - \sum_b \Lambda^b_\beta(q)(\mathbf{e}_b \times \boldsymbol{\sigma}_j)\right), \tag{73}$$

$$A_{ab} = \sum_j (\mathbf{u}_a \times \mathbf{r}_j) \cdot (\mathbf{u}_b \times \mathbf{r}_j) = \mathbf{u}_a \cdot A_x(\mathbf{u}_b) = \mathbf{e}_a \cdot A_{\sigma(q)}(\mathbf{e}_b). \tag{74}$$

In the remainder of this section, we consider the transformation law for local expressions of the connection form. Let $\tau: V \to \dot{M}$ be another local section defined on an open subset V with $V \cap U \neq \varnothing$. Then the local sections τ and σ are related by $\tau(q) = k(q)\sigma(q)$, $q \in V \cap U$ with $k(q) \in \mathrm{SO}(3)$. From (44), it follows that

$$\omega_{\tau(q)} = dk k^{-1} + k \omega_{\sigma(q)} k^{-1}. \tag{75}$$

Like (46), we describe the connection form $\omega_{\tau(q)}$ as

$$\omega_{\tau(q)} = \sum_a \sum_\alpha \tilde{\Lambda}^a_\alpha(q) dq^\alpha R(\mathbf{e}_a). \tag{76}$$

Then the transformation law (75) brings about

$$\sum_\alpha \tilde{\Lambda}^a_\alpha dq^\alpha = \Phi^a(k) + \sum_b k_{ab} \sum_\alpha \Lambda^b_\alpha dq^\alpha, \tag{77}$$

where $\Phi^a(k)$ are defined through $dk k^{-1} = \Sigma_a \Phi^a(k) R(\mathbf{e}_a)$ and k_{ab} denote the components of $k \in \mathrm{SO}(3)$. Furthermore, we note that the inertia tensor is subject to the transformation $A_{hx} = h A_x h^{-1}$ for any $h \in \mathrm{SO}(3)$, so that the components (A_{ab}) transform according to

$$\tilde{A}_{ab} = \sum_{c,d} k_{ad} A_{dc} k_{bc}, \quad k = (k_{ab}), \tag{78}$$

where

$$\tilde{A}_{ab} = \mathbf{e}_a \cdot A_{\tau(q)}(\mathbf{e}_b). \tag{79}$$

We note also that since the metric ds^2 is SO(3)-invariant, $a_{\alpha\beta}$ are defined independently of the choice of sections, so that the $(a_{\alpha\beta})$ defines a metric tensor on $U \subset \dot{Q}$.

V. KINETIC ENERGY OPERATOR FOR NONSINGULAR CONFIGURATIONS

In this section, we study the kinetic energy operator for nonsingular configurations by using the setup stated in Secs. III and IV, and obtain a reduced kinetic energy operator which is defined on $\dot{Q}$. We begin by considering the gradient vector

$$\nabla = \left(\frac{\partial}{\partial \mathbf{r}_1}, \ldots, \frac{\partial}{\partial \mathbf{r}_{N-1}} \right). \tag{80}$$

For a smooth wave function f, we regard ∇f as a tangent vector to $\dot{M}$, and decompose ∇f according to (37):

$$\nabla f = (\nabla f)_{\mathrm{rot}} + (\nabla f)_{\mathrm{vib}}. \tag{81}$$

The rotational vector $(\nabla f)_{\mathrm{rot}}$ is given by $(\nabla f)_{\mathrm{rot}} := P_x(\nabla f)$, so that its components are expressed, on using (42) with $\mathbf{v}_k = \partial f / \partial \mathbf{r}_k$, as

$$\begin{aligned} P_x(\nabla f)_j &= \left(A_x^{-1} \left(\sum_k \mathbf{r}_k \times \frac{\partial f}{\partial \mathbf{r}_k} \right) \right) \times \mathbf{r}_j \\ &= (A_x^{-1}(\mathbf{J} f)) \times \mathbf{r}_j \\ &= \left(A_x^{-1} \left(\sum_a \mathbf{u}_a K_a f \right) \right) \times \mathbf{r}_j \\ &= \sum_a ((A_x^{-1}(\mathbf{u}_a)) \times \mathbf{r}_j) K_a f. \end{aligned} \tag{82}$$

Then $(\nabla f)_{\mathrm{rot}}$ turns out to have the components

$$\left(\frac{\partial f}{\partial \mathbf{r}_j}\right)_{\mathrm{rot}} = \sum_{a=1}^{3} \mathbf{t}_j^a K_a f, \quad \mathbf{t}_j^a := A_x^{-1}(\mathbf{u}_a) \times \mathbf{r}_j, \quad j = 1, \ldots, N-1. \tag{83}$$

In contrast with this, the components of $(\nabla f)_{\mathrm{vib}}$ can be put in the form

$$\left(\frac{\partial f}{\partial \mathbf{r}_j}\right)_{\mathrm{vib}} = \sum_{\alpha=1}^{3N-6} \mathbf{v}_j^\alpha \left(\frac{\partial}{\partial q^\alpha}\right)^* f, \quad j = 1, \ldots, N-1, \tag{84}$$

where the vectors $\mathbf{v}_j^\alpha$ will be determined as follows: From (67) along with the decomposition $\partial/\partial \mathbf{r}_j = (\partial/\partial \mathbf{r}_j)_{\mathrm{rot}} + (\partial/\partial \mathbf{r}_j)_{\mathrm{vib}}$, the basis tangent vectors can be expressed as

$$K_a = \sum_j K_a \mathbf{r}_j \cdot \left(\sum_b \mathbf{t}_j^b K_b + \sum_\alpha \mathbf{v}_j^\alpha \left(\frac{\partial}{\partial q^\alpha}\right)^* \right), \tag{85}$$

$$\left(\frac{\partial}{\partial q^\beta}\right)^* = \sum_j \left(\frac{\partial}{\partial q^\beta}\right)^* \mathbf{r}_j \cdot \left(\sum_b \mathbf{t}_j^b K_b + \sum_\alpha \mathbf{v}_j^\alpha \left(\frac{\partial}{\partial q^\alpha}\right)^* \right). \tag{86}$$

These equations provide

$$\sum_j K_a \mathbf{r}_j \cdot \mathbf{t}_j^b = \delta_a^b, \quad \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot \mathbf{t}_j^b = 0, \tag{87}$$

$$\sum_j K_a \mathbf{r}_j \cdot \mathbf{v}_j^\alpha = 0, \quad \sum_j \left(\frac{\partial}{\partial q^\beta}\right)^* \mathbf{r}_j \cdot \mathbf{v}_j^\alpha = \delta_\beta^\alpha. \tag{88}$$

Equations (88) are used to determine $\mathbf{v}_j^\alpha$ or the vectors $v^\alpha := \Sigma_j \mathbf{v}_j^\alpha \cdot (\partial/\partial \mathbf{r}_j)$. It then turns out that v^α are expressed as

$$v^\alpha = \sum_\beta a^{\alpha\beta} \left(\frac{\partial}{\partial q^\beta}\right)^*, \tag{89}$$

or

$$\mathbf{v}_j^\alpha = v^\alpha \mathbf{r}_j = \sum_\beta a^{\alpha\beta} \left(\frac{\partial}{\partial q^\beta}\right)^* \mathbf{r}_j, \tag{90}$$

where

$$(a^{\alpha\beta}) := (a_{\alpha\beta})^{-1}. \tag{91}$$

In addition, it is easy to show that

$$\sum_j \mathbf{t}_j^a \cdot \mathbf{t}_j^b = A^{ab}, \tag{92}$$

$$\sum_j \mathbf{t}_j^a \cdot \mathbf{v}_j^\alpha = 0, \tag{93}$$

$$\sum_j \mathbf{v}_j^\alpha \cdot \mathbf{v}_j^\beta = a^{\alpha\beta}, \tag{94}$$

where

$$A^{ab} := \mathbf{u}_a \cdot A_x^{-1}(\mathbf{u}_b) = \mathbf{e}_a \cdot A_{\sigma(q)}^{-1}(\mathbf{e}_b). \tag{95}$$

It is to be noted that A_x^{-1} is defined only for $x \in \dot{M}$.

We are now in a position to study the kinetic energy operator. The kinetic energy integral of our N-body system is given by

$$T = \frac{1}{2} \int_M \sum_j \overline{\frac{\partial f}{\partial \mathbf{r}_j}} \cdot \frac{\partial f}{\partial \mathbf{r}_j} dV, \tag{96}$$

where dV is the standard volume element of M. The energy operator, which is equal to $-\frac{1}{2}$ times the Laplacian Δ, is defined through integration by part as follows:

$$T = \int_M \overline{f} \left(-\frac{1}{2} \sum_j \left(\frac{\partial}{\partial \mathbf{r}_j} \right)^2 f \right) dV = \int_M \overline{f} \left(-\frac{1}{2} \Delta f \right) dV, \tag{97}$$

where f is assumed to be a smooth function with compact support. According to the orthogonal decomposition, $\nabla = \nabla_{\text{rot}} + \nabla_{\text{vib}}$, of the gradient operator, the kinetic energy is also broken up into rotational and vibrational energies,

$$T = T_{\text{rot}} + T_{\text{vib}}, \tag{98}$$

where

$$T_{\text{rot}} = \frac{1}{2} \int_M \sum_j \left(\overline{\frac{\partial f}{\partial \mathbf{r}_j}} \right)_{\text{rot}} \cdot \left(\frac{\partial f}{\partial \mathbf{r}_j} \right)_{\text{rot}} dV, \tag{99}$$

$$T_{\text{vib}} = \frac{1}{2} \int_M \sum_j \left(\overline{\frac{\partial f}{\partial \mathbf{r}_j}} \right)_{\text{vib}} \cdot \left(\frac{\partial f}{\partial \mathbf{r}_j} \right)_{\text{vib}} dV. \tag{100}$$

The rotational and vibrational energy operators will be defined by carrying out the integration by part for the energy integrals T_{rot} and T_{vib}, respectively. Accordingly, the Laplacian Δ is broken up into two,

$$\Delta = \Delta_{\text{rot}} + \Delta_{\text{vib}}. \tag{101}$$

We wish to express Δ_{rot} and Δ_{vib} in terms of local coordinates. From (71) together with (49), the volume element dV proves to be expressed as

$$dV = dQ \wedge d\mu(g), \tag{102}$$

where

$$dQ = \rho(q) dq^1 \wedge \cdots \wedge dq^{3N-6}, \tag{103}$$

$$\rho(q) = \sqrt{\det(A_{ab}) \det(a_{\alpha\beta})}, \tag{104}$$

$$d\mu(g) = \Psi^1 \wedge \Psi^2 \wedge \Psi^3 = \sin\theta \, d\theta \wedge d\phi \wedge d\psi. \tag{105}$$

By using (83) and (92) and performing integration by part, we obtain

$$T_{\text{rot}} = \frac{1}{2} \int_M \sum_j \sum_a \mathbf{t}_j^a \overline{K_a f} \cdot \sum_b \mathbf{t}_j^b K_b f \, dV = -\frac{1}{2} \int_M \overline{f} \sum_{a,b} K_a (A^{ab} K_b f) \, dV, \tag{106}$$

where we have used the fact that K_a are volume-preserving operators on SO(3). In the same manner, it follows from (84) and (94) that

$$T_{\mathrm{vib}}=\frac{1}{2}\int_M \sum_j \sum_\alpha \mathbf{v}_j^\alpha \overline{\left(\frac{\partial}{\partial q^\alpha}\right)^* f}\cdot \sum_\beta \mathbf{v}_j^\beta \left(\frac{\partial}{\partial q^\beta}\right)^* f\, dV$$
$$=-\frac{1}{2}\int_M \overline{f}\frac{1}{\rho(q)}\sum_{\alpha,\beta}\left(\frac{\partial}{\partial q^\alpha}\right)^*\left(a^{\alpha\beta}\rho(q)\left(\frac{\partial}{\partial q^\beta}\right)^* f\right) dV. \tag{107}$$

Thus we have found the respective expressions of Δ_{rot} and Δ_{vib}:

$$\Delta_{\mathrm{rot}}=\sum_{a,b} K_a(A^{ab}K_b), \tag{108}$$

$$\Delta_{\mathrm{vib}}=\frac{1}{\rho(q)}\sum_{\alpha,\beta}\left(\frac{\partial}{\partial q^\alpha}\right)^*\left(a^{\alpha\beta}\rho(q)\left(\frac{\partial}{\partial q^\beta}\right)^*\right). \tag{109}$$

Note that these operators fail to be defined at singular configurations. In fact, for singular configurations, one has $\det(A_{ab})=0$, so that A^{ab} is not defined, and further $\rho(q)=0$.

In the remainder of this section, we show that the rotational and vibrational energy operators, $-\frac{1}{2}\Delta_{\mathrm{rot}}$ and $-\frac{1}{2}\Delta_{\mathrm{vib}}$, will reduce to operators acting on wave functions of internal variables (q^α). To this end, we restrict ourselves to the subspace $\mathrm{Im}\,P_m^\ell$ of $L^2(M)$. Then we obtain, from (26),

$$\langle P_m^\ell f_1, P_m^\ell f_2\rangle_{L^2(M)}=\int_M \langle E_m^\ell f_1, E_m^\ell f_2\rangle_{\mathcal{H}^\ell} dV,\quad f_1, f_2\in L^2(M), \tag{110}$$

where we have used the fact that $E_m^\ell P_m^\ell f=E_m^\ell f$, and $\langle\ ,\ \rangle_{\mathcal{H}^\ell}$ denotes the inner product on the representation space $\mathcal{H}^\ell$ assigned by ℓ. From (33) together with (43), one finds that the $\mathcal{H}^\ell$-valued function $E_m^\ell f$ is locally expressed as

$$(E_m^\ell f)(g\sigma(q))=D^\ell(g)(E_m^\ell f)(\sigma(q)). \tag{111}$$

If f has a compact support in $\pi^{-1}(U)$, Eq. (110) becomes

$$\langle P_m^\ell f_1, P_m^\ell f_2\rangle_{L^2(M)}=8\pi^2\int_{\dot{Q}}\langle (E_m^\ell f_1)(\sigma(q)),(E_m^\ell f_2)(\sigma(q))\rangle_{\mathcal{H}^\ell} dQ, \tag{112}$$

where we have used the fact that $D^\ell(g)$ is a unitary matrix. This equation means that we may view $(E_m^\ell f)(\sigma(q))$ as a (locally defined) $\mathcal{H}^\ell$-valued wave function on the internal space $\dot{Q}$. If f is smooth enough, the projection operator $P_{m'm}^\ell$ and a differential operator such as $(\partial/\partial q^\alpha)^*$ commute, so that we obtain

$$E_m^\ell\left(\frac{\partial}{\partial q^\alpha}\right)^* f=\left(\mathrm{id}_{\mathcal{H}^\ell}\otimes\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)E_m^\ell f, \tag{113}$$

where $\mathrm{id}_{\mathcal{H}^\ell}$ denotes the identity of $\mathcal{H}^\ell$. The right-hand side of this equation means that we may differentiate $E_m^\ell f$ componentwise. We recall here that the operator K_a acts on the D-functions[10] as

$$K_a D^\ell(g)=-iD^\ell(g)[\hat{J}_a^{(\ell)}], \tag{114}$$

where $\hat{J}_a$ are the angular momentum operators defined to be $\hat{J}_a=-iJ_a$, and $[\hat{J}_a^{(\ell)}]$ denote their representation matrices which are, as usual, given by

$$[\hat{J}_1^{(\ell)}]_{m-1\,m}=\frac{1}{2}\sqrt{(\ell+m)(\ell-m+1)},\quad [\hat{J}_1^{(\ell)}]_{m+1\,m}=\frac{1}{2}\sqrt{(\ell-m)(\ell+m+1)},$$

$$[\hat{J}_2^{(\ell)}]_{m-1\,m}=-\frac{1}{2i}\sqrt{(\ell+m)(\ell-m+1)},\quad [\hat{J}_2^{(\ell)}]_{m+1\,m}=\frac{1}{2i}\sqrt{(\ell-m)(\ell+m+1)},\quad (115)$$

$$[\hat{J}_3^{(\ell)}]_{mm}=m,\qquad \text{the others vanishing.}$$

Operating on $D^{\ell}(g)(E_m^{\ell}f)(\sigma(q))$ with $\mathrm{id}_{\mathcal{H}^{\ell}}\otimes(\partial/\partial q^{\alpha})^*$ and using (114), we obtain

$$\left(\mathrm{id}_{\mathcal{H}^{\ell}}\otimes\left(\frac{\partial}{\partial q^{\alpha}}\right)^*\right)D^{\ell}(g)(E_m^{\ell}f)(\sigma(q))=D^{\ell}(g)\nabla_{\alpha}(E_m^{\ell}f)(\sigma(q)),\quad (116)$$

where

$$\nabla_{\alpha}=I_{2\ell+1}\otimes\frac{\partial}{\partial q^{\alpha}}+i\sum_a\ \Lambda_{\alpha}^{a}(q)[\hat{J}_a^{(\ell)}],\quad (117)$$

and $I_{2\ell+1}$ denotes the $(2\ell+1)\times(2\ell+1)$ identity matrix.

We have to point out that the operators ∇_{α} may be defined independently of the choice of local sections. We recall here that the $\dot{M}$ is made into the fiber bundle (34). Take a representation space $\mathcal{H}^{\ell}\cong\mathbf{C}^{2\ell+1}$ of SO(3). Then the associated complex vector bundle is defined to be $\dot{M}\times_{\ell}\mathcal{H}^{\ell}:=(\dot{M}\times\mathcal{H}^{\ell})/\mathrm{SO}(3)$, where the SO(3) action on the product space $\dot{M}\times\mathcal{H}^{\ell}$ is defined by $(gx,D^{\ell}(g)v)$ for $(x,v)\in\dot{M}\times\mathcal{H}^{\ell}$. The space of equivariant functions on $\dot{M}$ is in one-to-one correspondence with the space of sections in $\dot{M}\times_{\ell}\mathcal{H}^{\ell}$; $s(\pi(x))=[(x,F(x))]$, where s and F are a section and an equivariant function, respectively, and $[\,\cdot\,]$ denotes the equivalence class. We denote this correspondence by $s=\gamma F$. For a local section σ in $\dot{M}$ and the equivariant function $E_m^{\ell}f$, one has $[(x,(E_m^{\ell}f)(x))]=[(\sigma(q),(E_m^{\ell}f)(\sigma(q)))]$, which means that $(E_m^{\ell}f)(\sigma(q))$ serves as a local expression of the section $s(\pi(x))=[(x,(E_m^{\ell}f)(x))]$. For a section s in $\dot{M}\times_{\ell}\mathcal{H}^{\ell}$, the covariant derivative of s with respect to a vector field X on $\dot{Q}=\dot{M}/\mathrm{SO}(3)$ is defined by

$$\nabla_X s=\gamma X^*(\gamma^{-1}s),\quad (118)$$

where X^* denotes the horizontal lift of X. Equation (117) is a local expression of the covariant differential operator with respect to $\partial/\partial q^{\alpha}$.

For confirmation, we show that locally defined operators (117) can be pieced together to define an operator independently of the choice of sections. For another local section τ in $\dot{M}$, we have another local expression $(E_m^{\ell}f)(\tau(q))$ of the section $s(\pi(x))=[(x,(E_m^{\ell}f)(x))]$. The locally defined $\mathcal{H}^{\ell}$-valued functions $(E_m^{\ell}f)(\tau(q))$ and $(E_m^{\ell}f)(\sigma(q))$ are related by the gauge transformation

$$(E_m^{\ell}f)(\tau(q))=D^{\ell}(k(q))(E_m^{\ell}f)(\sigma(q)),\quad q\in V\cap U.\quad (119)$$

For $(E_m^{\ell}f)(\tau(q))$, we have the covariant differential operator, instead of (117),

$$\tilde{\nabla}_{\alpha}=I_{2\ell+1}\otimes\frac{\partial}{\partial q^{\alpha}}+i\sum_a\ \tilde{\Lambda}_{\alpha}^{a}(q)[\hat{J}_a^{(\ell)}].\quad (120)$$

We show that the locally defined covariant differential operators, ∇_{α} and $\tilde{\nabla}_{\alpha}$, are subject to the transformation law

$$\tilde{\nabla}_{\alpha}(E_m^{\ell}f)(\tau(q))=D^{\ell}(k(q))\nabla_{\alpha}(E_m^{\ell}f)(\sigma(q)),\quad (121)$$

or, equivalently,

$$\sum_{\alpha} \tilde{\nabla}_{\alpha}(E_m^{\ell} f)(\tau(q))dq^{\alpha} = D^{\ell}(k(q)) \sum_{\alpha} \nabla_{\alpha}(E_m^{\ell} f)(\sigma(q))dq^{\alpha}. \tag{122}$$

The transformation law (121) shows that locally defined covariant differential operators are pieced together to define a covariant differential operator acting on sections in $\dot{M} \times_{\ell} \mathcal{H}^{\ell}$;

$$[(\sigma(q), \nabla_{\alpha}(E_m^{\ell} f)(\sigma(q)))] = [(\tau(q), \tilde{\nabla}_{\alpha}(E_m^{\ell} f)(\tau(q)))]. \tag{123}$$

To prove (122), we need some formulas on D-functions. In contrast with (114), we have the formula[10]

$$J_a D^{\ell}(g) = -i[\hat{J}_a^{(\ell)}] D^{\ell}(g). \tag{124}$$

From (114) and (124) together with (57), we obtain the formula

$$[\hat{J}_a^{(\ell)}] D^{\ell}(g) = \sum_{b} g_{ab} D^{\ell}(g)[\hat{J}_b^{(\ell)}]. \tag{125}$$

Using the transformation law (77) along with the above formulas and the equation

$$dD^{\ell}(k) = \sum_{a} K_a D^{\ell}(k) \Psi^a(k), \tag{126}$$

we can verify (122) in a straightforward manner.

We proceed to the operators Δ_{rot} and Δ_{vib}. Operating on $D^{\ell}(g)(E_m^{\ell} f)(\sigma(q))$ with $\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{rot}}$ and $\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{vib}}$, we obtain

$$(\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{rot}}) D^{\ell}(g)(E_m^{\ell} f)(\sigma(q)) = -D^{\ell}(g) \sum_{a,b} A^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}](E_m^{\ell} f)(\sigma(q)), \tag{127}$$

$$(\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{vib}}) D^{\ell}(g)(E_m^{\ell} f)(\sigma(q)) = D^{\ell}(g) \frac{1}{\rho(q)} \sum_{\alpha,\beta} \nabla_{\alpha}(a^{\alpha\beta} \rho(q) \nabla_{\beta}(E_m^{\ell} f)(\sigma(q))), \tag{128}$$

respectively. From these equations, it turns out that the Laplacian $\Delta = \Delta_{\mathrm{vib}} + \Delta_{\mathrm{rot}}$ reduces to the operator acting on vector-valued wave functions $(E_m^{\ell} f)(\sigma(q))$,

$$\Delta^{\mathrm{red}} := \frac{1}{\rho(q)} \sum_{\alpha,\beta} \nabla_{\alpha}(a^{\alpha\beta} \rho(q) \nabla_{\beta}) - \sum_{a,b} A^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}]. \tag{129}$$

We here have to mention the transformation law for the locally defined reduced Laplacians. For $(E_m^{\ell} f)(\tau(q))$, we have the reduced Laplacian expressed as

$$\tilde{\Delta}^{\mathrm{red}} := \frac{1}{\rho(q)} \sum_{\alpha,\beta} \tilde{\nabla}_{\alpha}(a^{\alpha\beta} \rho(q) \tilde{\nabla}_{\beta}) - \sum_{a,b} \tilde{A}^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}]. \tag{130}$$

Using the transformation law (78) and the formula (125) in addition to (121), we can also show that $\tilde{\Delta}^{\mathrm{red}}$ and Δ^{red} are related by

$$\tilde{\Delta}^{\mathrm{red}}(E_m^{\ell} f)(\tau(q)) = D^{\ell}(k(q)) \Delta^{\mathrm{red}}(E_m^{\ell} f)(\sigma(q)). \tag{131}$$

Thus we obtain the following.

Theorem 1: For nonsingular configurations, the Laplacian reduces to an operator acting on the sections in the associated vector bundle $\dot{M}\times_{\ell}\mathcal{H}^{\ell}$, which is expressed locally as Δ^{red} given by (129) or $\tilde{\Delta}^{\mathrm{red}}$ given by (130) according to the choice of local sections in $\dot{M}\to\dot{Q}$. The reduced local operators Δ^{red} and $\tilde{\Delta}^{\mathrm{red}}$ are subject to the transformation law (131).

VI. THREE-BODY SYSTEMS

Our aim in this section is to show that in spite of the singularity of Δ_{rot} and Δ_{vib} at singular configurations, the rotational and vibrational energy integrals are not divergent at singular configurations. To this end, we need to understand the detailed behavior of wave functions at singular configurations. For this reason, we specialize in three-body systems for simplicity. Let us introduce internal coordinates $(\zeta_1,\zeta_2,\zeta_3)$ by

$$\zeta_1=r_1,\quad \zeta_2=r_2\cos\varphi,\quad \zeta_3=r_2\sin\varphi, \tag{132}$$

where

$$r_1=\|\mathbf{r}_1\|,\quad r_2=\|\mathbf{r}_2\|,\quad \mathbf{r}_1\cdot\mathbf{r}_2=r_1r_2\cos\varphi. \tag{133}$$

Using ζ_α, $\alpha=1,2,3$, we define a local section σ by

$$\boldsymbol{\sigma}_1(q)=\zeta_1\mathbf{e}_3,\quad \boldsymbol{\sigma}_2(q)=\zeta_2\mathbf{e}_3+\zeta_3\mathbf{e}_1. \tag{134}$$

We note here that the local section σ is defined originally on an open subset U of $\dot{Q}=\dot{M}/\mathrm{SO}(3)$. If we are strict in using the term "local section," we must pose the restriction that $\zeta_1>0$ and $\zeta_3>0$ to identify the open subset U. However, $(\zeta_1,\zeta_2,\zeta_3)$ can serve as local coordinates beyond U,

$$\{(\zeta_1,\zeta_2,\zeta_3)|\ \zeta_1\geqslant 0,\zeta_3\geqslant 0\}. \tag{135}$$

The coordinates $(\zeta_1,\zeta_2,\zeta_3)$ work well in the orbit space $M/\mathrm{SO}(3)$ for describing singular configurations. In fact, we have collinear configurations if $\zeta_3=0$, and the configurations that two of three particles collide but the remainder is separate, if $\zeta_1=0$. If $\zeta_1=\zeta_2=\zeta_3=0$, we have a triple collision. With this interpretation, we are allowed to make ζ_3 tend to zero, for example.

From the definition (74) along with (134), the inertia tensor and its inverse at $\sigma(q)$ are put, respectively, in the form

$$(A_{ab})=\begin{pmatrix}\zeta_1^2+\zeta_2^2 & 0 & -\zeta_2\zeta_3\\ 0 & \zeta_1^2+\zeta_2^2+\zeta_3^2 & 0\\ -\zeta_2\zeta_3 & 0 & \zeta_3^2\end{pmatrix}, \tag{136}$$

$$(A^{ab})=\begin{pmatrix}\dfrac{1}{\zeta_1^2} & 0 & \dfrac{\zeta_2}{\zeta_1^2\zeta_3}\\ 0 & \dfrac{1}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & 0\\ \dfrac{\zeta_2}{\zeta_1^2\zeta_3} & 0 & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2\zeta_3^2}\end{pmatrix}. \tag{137}$$

From (45), (134), and (137), the connection form proves to be expressed as

$$\omega_{\sigma(q)}=\frac{\zeta_2d\zeta_3-\zeta_3d\zeta_2}{\zeta_1^2+\zeta_2^2+\zeta_3^2}R(\mathbf{e}_2). \tag{138}$$

From (51) together with (138), the horizontal lifts of $\partial/\partial\zeta_\alpha$ are given by

$$\left(\frac{\partial}{\partial\zeta_1}\right)^* = \frac{\partial}{\partial\zeta_1},$$

$$\left(\frac{\partial}{\partial\zeta_2}\right)^* = \frac{\partial}{\partial\zeta_2} + \frac{\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2}K_2, \tag{139}$$

$$\left(\frac{\partial}{\partial\zeta_3}\right)^* = \frac{\partial}{\partial\zeta_3} - \frac{\zeta_2}{\zeta_1^2+\zeta_2^2+\zeta_3^2}K_2.$$

From (73) and (139), the metric tensor and its inverse are calculated, respectively, as

$$(a_{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & \dfrac{\zeta_2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2} \\ 0 & \dfrac{\zeta_2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & \dfrac{\zeta_1^2+\zeta_3^2}{\zeta_1^2+\zeta_2^2+\zeta_3^2} \end{pmatrix}, \tag{140}$$

$$(a^{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{\zeta_1^2+\zeta_3^2}{\zeta_1^2} & -\dfrac{\zeta_2\zeta_3}{\zeta_1^2} \\ 0 & -\dfrac{\zeta_2\zeta_3}{\zeta_1^2} & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2} \end{pmatrix}. \tag{141}$$

Further, the volume density $\rho(q)$ given in (104) is expressed as

$$\rho(q) = \zeta_1^2\zeta_3. \tag{142}$$

Thus we have obtained all the quantities needed for expressing the rotational and the vibrational energy operators given by (108) and (109), respectively. The resultant expression looks singular at the singular configurations, i.e., at the triple collision, $\zeta_1=\zeta_2=\zeta_3=0$, and at the collinear configuration, $\zeta_1=0$ or $\zeta_3=0$.

To investigate how singular the operators are at singular configurations, we treat the rotational and the vibrational energy integrals in detail. The vibrational energy integral for the three-body system is expressed as

$$T_{\text{vib}} = \frac{1}{2}\int_M \left(\left(\left|\frac{\partial f}{\partial\zeta_1}\right|^2 + \frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_2}\right)^* f\right|^2 + \frac{\zeta_1^2+\zeta_2^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_3}\right)^* f\right|^2 - \frac{\zeta_2\zeta_3}{\zeta_1^2}\left(\overline{\left(\frac{\partial}{\partial\zeta_2}\right)^* f}\left(\frac{\partial}{\partial\zeta_3}\right)^* f \right.\right.\right.$$
$$\left.\left.\left. + \overline{\left(\frac{\partial}{\partial\zeta_3}\right)^* f}\left(\frac{\partial}{\partial\zeta_2}\right)^* f\right)\right)\zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{143}$$

From this along with (139), we can observe that the integral T_{vib} is not divergent at singular configurations. In fact, at a glance, we see that no singularity occurs at $\zeta_1=0$. Turning to the singular configuration given by $\zeta_1=\zeta_2=\zeta_3=0$, we pick up one of the terms in the integrand, say,

$$\frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_2}\right)^* f\right|^2 = \frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left(\left|\frac{\partial f}{\partial\zeta_2}\right|^2 + \frac{\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2}\left(\overline{\frac{\partial f}{\partial\zeta_2}}K_2 f + \frac{\partial f}{\partial\zeta_2}\overline{K_2 f}\right) + \frac{\zeta_3^2|K_2 f|^2}{(\zeta_1^2+\zeta_2^2+\zeta_3^2)^2}\right). \tag{144}$$

If we take the spherical polar coordinates for $(\zeta_1,\zeta_2,\zeta_3)$ with the radial variable $r=\sqrt{\zeta_1^2+\zeta_2^2+\zeta_3^2}$, the volume element $dQ=\zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3$ is put in the form $dQ=r^5 dr d\nu$, where $d\nu$ denotes the area element induced on the quarter sphere given by $\zeta_1^2+\zeta_2^2+\zeta_3^2=1$, $\zeta_1\geqslant 0$, and $\zeta_3\geqslant 0$. Now it is easy to see that if f is smooth in a neighborhood of $r=0$, no divergence occurs at $r=0$ in the integral of the above term with respect to $r^5 dr d\nu$. For the other terms of the integrand, the same proof of non-divergence also runs well.

The rotational energy integral for the three-body system is expressed as

$$T_{\mathrm{rot}}=\frac{1}{2}\int_M\left(\frac{1}{\zeta_1^2}|K_1 f|^2+\frac{1}{\zeta_1^2+\zeta_2^2+\zeta_3^2}|K_2 f|^2+\frac{\zeta_1^2+\zeta_2^2}{\zeta_1^2\zeta_3^2}|K_3 f|^2+\frac{\zeta_2}{\zeta_1^2\zeta_3}(\overline{K_1 f}K_3 f+\overline{K_3 f}K_1 f)\right)$$
$$\times\zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{145}$$

It is clear that no divergence occurs at $\zeta_1=0$. We are now interested in the singularity at $\zeta_3=0$. Among the terms of the integrand of the right-hand side of (145), $[(\zeta_1^2+\zeta_2^2)/\zeta_1^2\zeta_3^2]|K_3 f|^2$ might cause the divergence of the integral at $\zeta_3=0$:

$$\int_M\frac{\zeta_1^2+\zeta_2^2}{\zeta_3}|K_3 f|^2 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{146}$$

However, we can show that the integral (146) is not divergent on account of the boundary condition for the wave function f at $\zeta_3=0$. To this end, we may restrict M to $\pi^{-1}(U)$ and use the fact that if f is assumed to be analytic at $\zeta_3=0$, f can be expanded into a Fourier series, with respect to D-functions, of the form

$$f(g\sigma(q))=\sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}\sum_{|n|,|m|\leqslant\ell}D_{mn}^{\ell}(g)\zeta_3^{|n|}\sum_{j=0}^{\infty}\zeta_3^{2j}C_{nmj}(\zeta_1,\zeta_2). \tag{147}$$

We notice here that in Ref. 11 Mitchell and Littlejohn proved that the analyticity assumption for an equivariant function gives rise to a power series in ζ_3 with the exponents of the form $|n|+2j$. By the Fubini theorem, the integral (146) restricted on $\pi^{-1}(U)$ can be written as

$$\int_U d\zeta_1 d\zeta_2 d\zeta_3\frac{\zeta_1^2+\zeta_2^2}{\zeta_3}\int_{\mathrm{SO}(3)}|K_3 f|^2 d\mu(g). \tag{148}$$

Carrying out the integration over SO(3) along with (147), we obtain

$$\int_{\mathrm{SO}(3)}|K_3 f|^2 d\mu(g)=\frac{1}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\sum_{|m|,|n|\leqslant\ell}n^2\zeta_3^{2|n|}F_{nm}(\zeta_1,\zeta_2,\zeta_3), \tag{149}$$

where

$$F_{nm}(\zeta_1,\zeta_2,\zeta_3):=\sum_{j,j'=0}^{\infty}\zeta_3^{2j+2j'}\overline{C_{nmj}}(\zeta_1,\zeta_2)C_{nmj'}(\zeta_1,\zeta_2), \tag{150}$$

and we have used the orthogonality of D-functions,

$$\int_{\mathrm{SO}(3)}\overline{D_{mn}^{\ell}(g)}D_{m'n'}^{\ell'}(g)d\mu(g)=\frac{8\pi^2}{2\ell+1}\delta_{\ell\ell'}\delta_{mm'}\delta_{nn'}, \tag{151}$$

and the fact that $K_3 D_{mn}^{\ell}(g)=-inD_{mn}^{\ell}(g)$. Hence, we obtain

$$\int_U d\zeta_1 d\zeta_2 d\zeta_3 \frac{\zeta_1^2+\zeta_2^2}{\zeta_3} \int_{\mathrm{SO}(3)} |K_3 f|^2 d\mu(g)$$

$$= \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{|m|,|n| \leq \ell} \int_U \frac{\zeta_1^2+\zeta_2^2}{\zeta_3} n^2 \zeta_3^{2|n|} F_{nm}(\zeta_1,\zeta_2,\zeta_3) d\zeta_1 d\zeta_2 d\zeta_3 . \tag{152}$$

From this, we observe that the integral (146) is not divergent at $\zeta_3=0$. We may weaken the analyticity assumption on wave functions at $\zeta_3=0$ to smoothness assumption to some extent.

We turn to the singularity at $\zeta_1=\zeta_2=\zeta_3=0$. In this case, we have to consider whether the integral

$$\int_{\pi^{-1}(U)} \left(\frac{\zeta_1^2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2} |K_2 f|^2 + \frac{\zeta_1^2+\zeta_2^2}{\zeta_3} |K_3 f|^2 \right) d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g) \tag{153}$$

is divergent at $\zeta_1=\zeta_2=\zeta_3=0$ or not. In the spherical polar coordinates for $(\zeta_1,\zeta_2,\zeta_3)$, the three-form $d\zeta_1 d\zeta_2 d\zeta_3$ is expressed as $r^2 dr d\nu$. Hence the integral (153) is not divergent at $\zeta_1=\zeta_2=\zeta_3=0$, if f is smooth in the neighborhood of $r=0$. Thus we conclude that

Theorem 2: While the rotational and the vibrational energy operators look singular at singular configurations, the singularity is not essential in the sense that the rotational and the vibrational energy integrals are not divergent at singular configurations on account of the boundary behavior of wave functions there. The reduced kinetic energy operator looks singular as well, but the singularity is not essential in the same sense.

VII. COLLINEAR CONFIGURATIONS

In this section, we consider the space M_1 of collinear configurations. Though M_1 is a part of the boundary of $\dot{M}$, and the rotational and the vibrational energy operators defined on $\dot{M}$ have singularity at M_1, we will be able to define restricted rotational and vibrational energy operators for collinear configurations, if we restrict ourselves to M_1. The rotation group SO(3) does not act freely on M_1, but it has the isotropy subgroup which is isomorphic with SO(2), so that the orbit of SO(3) through $x \in M_1$ is identified with S^2; $\mathcal{O}_x \cong \mathrm{SO}(3)/\mathrm{SO}(2) \cong S^2$. We can decompose the tangent space to M_1 at $x \in M_1$ into a direct sum of vertical and horizontal subspaces; the vertical subspace $V_x^{(1)}$ is defined to be the tangent space to the orbit $\mathcal{O}_x$ through $x \in M_1$, and the horizontal subspace $H_x^{(1)}$ to be the orthogonal complement of $V_x^{(1)}$:

$$T_x(M_1) = V_x^{(1)} \oplus H_x^{(1)}, \quad V_x^{(1)} := T_x(\mathcal{O}_x), \quad H_x^{(1)} := (V_x^{(1)})^{\perp}, \tag{154}$$

where the metric with respect to which the orthogonality is referred is induced on M_1 from that on the center-of-mass system M.

We are to express basis vectors in $V_x^{(1)}$ in terms of local coordinates. To this end, we recall here the formula (62) which holds for singular configurations as well. However, in the present case, we must take the $\sigma(q)$ as a local section in M_1: $\sigma_0 : U^{(1)} \subset M_1/S^2 \to M_1$. The formula (62) restricted to $x \in M_1$ implies that K_a are tangent vectors in $V_x^{(1)}$. To find an explicit local expression of K_a, we take the section σ_0 to be

$$\sigma_0(q) = (\xi_1 \mathbf{e}_3, \ldots, \xi_{N-1} \mathbf{e}_3), \quad q \in U^{(1)}, \tag{155}$$

where ξ_j are local coordinates in $U^{(1)}$. Then a generic point $x \in \pi^{-1}(U^{(1)})$ is expressed as

$$x = g\sigma_0(q) = (\xi_1 g\mathbf{e}_3, \ldots, \xi_{N-1} g\mathbf{e}_3), \quad g \in \mathrm{SO}(3). \tag{156}$$

We put g in the form $g = e^{\phi R(\mathbf{e}_3)} e^{\theta R(\mathbf{e}_2)} e^{\psi R(\mathbf{e}_3)}$. Then the point x is assigned by the local coordinates $(\theta, \phi, \xi_1, \ldots, \xi_{N-1})$, ψ being eliminated on account of $e^{\psi R(\mathbf{e}_3)} \mathbf{e}_3 = \mathbf{e}_3$. Hence we may take the matrix g as $e^{\phi R(\mathbf{e}_3)} e^{\theta R(\mathbf{e}_2)}$.

We first deal with K_1. Using the formula (62) restricted to M_1, one has

$$K_1=\frac{d}{dt}ge^{tR(\mathbf{e}_1)}\sigma_0(q)\bigg|_{t=0}=-(\xi_j g\mathbf{e}_2)=-(\xi_j(-\sin\phi\,\mathbf{e}_1+\cos\phi\,\mathbf{e}_2)). \tag{157}$$

On the other hand, the curve $x(t)=ge^{tR(\mathbf{e}_1)}\sigma_0(q)$ is put, in terms of (θ,ϕ,ξ_j), in the form

$$x(t)=(\xi_j(\sin\theta\cos\phi\,\mathbf{e}_1+\sin\theta\sin\phi\,\mathbf{e}_2+\cos\theta\,\mathbf{e}_3)), \tag{158}$$

where θ and ϕ are viewed as functions of t. Differentiating this with respect to t at $t=0$, and setting the resultant tangent vector equal to K_1 given by (157), we find that

$$K_1^{(1)}=\frac{-1}{\sin\theta}\frac{\partial}{\partial\phi}, \tag{159}$$

where the superscript $^{(1)}$ indicates that the vector field $K_1^{(1)}$ is defined on M_1. In the same manner as above, we have

$$K_2^{(1)}=\frac{\partial}{\partial\theta}. \tag{160}$$

For K_3, we can easily find that

$$K_3^{(1)}=\frac{d}{dt}ge^{tR(\mathbf{e}_3)}\sigma_0(q)\bigg|_{t=0}=0. \tag{161}$$

The vector fields $K_1^{(1)}$ and $K_2^{(1)}$ form a local basis of vertical vector fields on M_1. We have observed, in the course of the above calculation, that $K_1^{(1)}$ and $K_2^{(2)}$ can also be expressed as

$$K_1^{(1)}=-\sum_{j=1}^{N-1}\xi_j\mathbf{u}_2\cdot\frac{\partial}{\partial\mathbf{r}_j},\quad K_2^{(1)}=\sum_{j=1}^{N-1}\xi_j\mathbf{u}_1\cdot\frac{\partial}{\partial\mathbf{r}_j}, \tag{162}$$

respectively.

We proceed to find a local basis in $H_x^{(1)}$. The local vector fields $\partial/\partial\xi_j$ can be put in the form

$$\frac{\partial}{\partial\xi_j}=\sum_{i=1}^{N-1}\frac{\partial\mathbf{r}_i}{\partial\xi_j}\cdot\frac{\partial}{\partial\mathbf{r}_i}=\mathbf{u}_3\cdot\frac{\partial}{\partial\mathbf{r}_j}. \tag{163}$$

From (162) and (163), it follows that $\partial/\partial\xi_j$ are orthogonal to $K_1^{(1)}, K_2^{(1)}$;

$$ds^2(K_a^{(1)},\partial/\partial\xi_j)=0,\quad a=1,2,\quad j=1,\ldots,N-1. \tag{164}$$

This implies that $\partial/\partial\xi_j$, $j=1,\ldots,N-1$, form a local basis of horizontal vector fields. The inner product among these basis vector fields are given by

$$ds^2(K_a^{(1)},K_b^{(1)})=\sum_{j=1}^{N-1}\xi_j^2\delta_{ab},\quad a,b=1,2, \tag{165}$$

$$ds^2(\partial/\partial\xi_i,\partial/\partial\xi_j)=\delta_{ij},\quad i,j=1,\ldots,N-1. \tag{166}$$

It is easy to see that the basis of one-forms dual to $K_a^{(1)}$ and $\partial/\partial\xi_j$ are given by

$$-\sin\theta\,d\phi,\quad d\theta,\quad d\xi_1,\ldots,d\xi_{N-1}, \tag{167}$$

of which the first two are vertical and the remainder horizontal. From (165)–(167), the induced metric on M_1 proves to be expressed as

$$ds^{2(1)}=\sum_{j=1}^{N-1}\xi_j^2(d\theta^2+\sin^2\theta\, d\phi^2)+\sum_{j=1}^{N-1}d\xi_j^2. \tag{168}$$

The volume element on M_1 is then given by

$$dV^{(1)}=dQ^{(1)}\wedge dS, \tag{169}$$

where

$$dQ^{(1)}=\rho_1(\xi)d\xi_1\wedge\cdots\wedge d\xi_{N-1},\quad \rho_1(\xi)\coloneqq\sum_{j=1}^{N-1}\xi_j^2, \tag{170}$$

$$dS=\sin\theta\, d\theta\wedge d\phi. \tag{171}$$

As was already mentioned in Sec. IV, the inertia tensor A_x is singular at $x\in M_1$. However, to study collinear configurations, we have to know to what extent the A_x is singular at $x\in M_1$. For $x=(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\in M_1$, one has $\operatorname{rank}x=1$. Hence we can express Jacobi vectors as $\mathbf{r}_j=\lambda_j\mathbf{a}$, where $\lambda_j\in\mathbf{R}$ and $\mathbf{a}\neq 0$. Then for $\mathbf{v}$, the inertia tensor takes the value

$$A_x(\mathbf{v})=\sum_{j=1}^{N-1}\lambda_j^2(|\mathbf{a}|^2\mathbf{v}-(\mathbf{a}\cdot\mathbf{v})\mathbf{a}). \tag{172}$$

Suppose now that $\mathbf{v}\in\ker A_x$. Then one has $\mathbf{v}=(\mathbf{a}\cdot\mathbf{v})\mathbf{a}/|\mathbf{a}|^2$, which means that

$$\ker A_x=\operatorname{span}\{\mathbf{a}\},\quad x\in M_1. \tag{173}$$

In contrast with this, for any vector $\mathbf{u}\in\operatorname{span}\{\mathbf{a}\}^{\perp}$, one has

$$A_x(\mathbf{u})=\sum_{j-1}^{N-1}\lambda_j^2|\mathbf{a}|^2\mathbf{u}, \tag{174}$$

which implies that $\operatorname{span}\{\mathbf{a}\}^{\perp}$ is the eigenspace associated with the multiple eigenvalue $\Sigma_{j=1}^{N-1}\lambda_j^2|\mathbf{a}|^2=\Sigma_{j=1}^{N-1}|\mathbf{r}_j|^2$.

If we take $\mathbf{a}=g\mathbf{e}_3=\mathbf{u}_3$ and set $\lambda_j=\xi_j$, and if we restrict the domain of A_x to the subspace $\operatorname{span}\{\mathbf{u}_1,\mathbf{u}_2\}=\operatorname{span}\{\mathbf{u}_3\}^{\perp}$, the restricted A_x becomes invertible:

$$(A_x^{(1)})^{-1}(\mathbf{u}_a)=\left(\sum_{j=1}^{N-1}\xi_j^2\right)^{-1}\mathbf{u}_a,\quad x\in M_1,\quad a=1,2. \tag{175}$$

The connection form (36) fails to be defined for $x\in M_1$, as is easily seen. However, taking (175) into account, we may define a restricted connection form. We recall here that we have obtained the decomposition (154), which allows the interpretation that M_1 admits a "singular" connection, since (154) may be viewed as an analog to the decomposition (37). We now look into the connection form associated with the decomposition (154). By using the local coordinates given in (156), we obtain

$$\mathbf{r}_j\times d\mathbf{r}_j=\xi_j^2(\Psi^{1(1)}\mathbf{u}_1+\Psi^{2(1)}\mathbf{u}_2), \tag{176}$$

where $\Psi^{a(1)}$ are given by

$$\Psi^{1(1)}=-\sin\theta\, d\phi,\quad \Psi^{2(1)}=d\theta. \tag{177}$$

Note that $\Psi^{a(1)}$ are the reduced form of Ψ^a given in (64). Thus the total angular momentum is put in the form

$$\sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j = \sum_{j=1}^{N-1} \xi_j^2 (\Psi^{1(1)}\mathbf{u}_1 + \Psi^{2(1)}\mathbf{u}_2). \tag{178}$$

Since this vector is in the space span$\{\mathbf{u}_1, \mathbf{u}_2\}$, we can apply the restricted inverse operator $(A_x^{(1)})^{-1}$ to (178) to obtain a one-form,

$$\omega^{(1)} := R\left((A_x^{(1)})^{-1} \left(\sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j \right) \right) = \Psi^{1(1)} R(\mathbf{u}_1) + \Psi^{2(1)} R(\mathbf{u}_2). \tag{179}$$

For horizontal and vertical vectors on M_1, the form $\omega^{(1)}$ takes values as follows:

$$\omega^{(1)}(\partial/\partial\xi_j) = 0, \quad j = 1,\ldots,N-1, \tag{180}$$

$$\omega^{(1)}(K_a^{(1)}) = R(\mathbf{u}_a), \quad a = 1,2. \tag{181}$$

Since these equations are in keeping with the decomposition (154), we may call the form $\omega^{(1)}$ a (singular) connection form on M_1. Since $\partial/\partial\xi_i$ form a basis of the horizontal subspace $V_x^{(1)}$ and since $[\partial/\partial\xi_j, \partial/\partial\xi_i] = 0$, the curvature of the connection $\omega^{(1)}$ vanishes.

In conclusion of this section, we show that

$$M_1/S^2 \cong \mathbf{R}_+ \times \mathbf{R}P^{N-2}, \tag{182}$$

where $\mathbf{R}_+ = \{r \in \mathbf{R} \mid r > 0\}$ and $\mathbf{R}P^{N-2}$ denotes the real projective space of dimension $N-2$. Since $x \in M_1$ is of rank 1, we can describe x as $x = (\xi_1\mathbf{u}, \ldots \xi_{N-1}\mathbf{u})$ with $|\mathbf{u}| = 1$ and $(\xi_1, \ldots, \xi_{N-1}) \neq 0$. If $(\xi_1\mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})$ and $(\eta_1\mathbf{v}, \ldots, \eta_{N-1}\mathbf{v})$ are equivalent under the SO(3) action, we have $\eta_k\mathbf{v} = \xi_k g\mathbf{u}$, $k = 1,\ldots,N-1$, for some $g \in \mathrm{SO}(3)$. This implies that $|\eta_k| = |\xi_k|$, hence $\eta_k = \pm\xi_k$, and further the choice of sign should be independent of k. Conversely, if $\eta_k = \pm\xi_k$, then there exist $g \in \mathrm{SO}(3)$ such that $(\eta_1\mathbf{v}, \ldots, \eta_{N-1}\mathbf{v}) = g(\xi_1\mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})$. This is because one has $-\mathbf{u} = e^{\pi R(\mathbf{w})}\mathbf{u}$ for a vector $\mathbf{w}$ such that $\mathbf{w} \perp \mathbf{u}$. It then follows that the map

$$\dot{\mathbf{R}}^{N-1} := \mathbf{R}^{N-1} - \{0\} \to M_1/S^2; \quad (\xi_1, \ldots, \xi_{N-1}) \mapsto [(\xi_1\mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})], \tag{183}$$

where $[(\cdots)]$ denotes the equivalence class, is two-to-one, that is, $\pm(\xi_1, \ldots, \xi_{N-1})$ maps to the same point of M_1/S^2. This results in

$$\dot{\mathbf{R}}^{N-1}/\mathbf{Z}_2 \cong M_1/S^2, \tag{184}$$

where $\mathbf{Z}_2$ acts on $\dot{\mathbf{R}}^{N-1}$ by $(\xi_k) \mapsto \pm(\xi_k)$. Since $\dot{\mathbf{R}}^{N-1} \cong \mathbf{R}_+ \times S^{N-2}$, one obtains

$$M_1/S^2 \cong \mathbf{R}_+ \times S^{N-2}/\mathbf{Z}_2 \cong \mathbf{R}_+ \times \mathbf{R}P^{N-2}. \tag{185}$$

In Ref. 12, they showed that the orbit of the shape, $\pi(x)$, of a collinear configuration $x \in M_1$ by the action of the kinetic group $\mathrm{O}(N-1)$ on $M/\mathrm{SO}(3)$ to the right is diffeomorphic with $\mathbf{R}P^{N-2}$.

VIII. KINETIC ENERGY OPERATOR FOR COLLINEAR CONFIGURATIONS

In the same manner as that used to obtain the kinetic energy operator Δ for nonsingular configurations, we can obtain the kinetic energy operator for singular configurations. From (168), it follows that the kinetic energy integral for collinear configurations is given by

$$\frac{1}{2}\int_{M_1}\left(\frac{1}{\rho_1(\xi)}\left(\left|\frac{\partial f}{\partial\theta}\right|^2+\frac{1}{\sin^2\theta}\left|\frac{\partial f}{\partial\phi}\right|^2\right)+\sum_{j=1}^{N-1}\left|\frac{\partial f}{\partial\xi_j}\right|^2\right)dV^{(1)}, \tag{186}$$

where $dV^{(1)}$ is the volume element given in (169). Integrated by part, this integral is expressed as

$$-\frac{1}{2}\int_{M_1}\overline{f}\left(\frac{1}{\rho_1(\xi)}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}\right)+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial f}{\partial\xi_j}\right)\right)dV^{(1)}. \tag{187}$$

Thus we obtain the kinetic energy operator $-\frac{1}{2}\Delta^{(1)}$ with the Laplacian $\Delta^{(1)}$ on M_1,

$$\Delta^{(1)}=\frac{1}{\rho_1(\xi)}\Lambda+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial}{\partial\xi_j}\right), \tag{188}$$

where Λ is the spherical Laplacian on S^2,

$$\Lambda=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{189}$$

The first and second terms on the right-hand side of (188) are a rotational and a vibrational operator, respectively.

The operator $\Delta^{(1)}$ has singularity at multiple collision for which $\rho_1(\xi)=0$. However, it is clear that the energy integral (186) is not divergent at the multiple collision $\xi_j=0$. Note also that the spherical Laplacian Λ has no singularity at $\theta=0,\pi$, as is well known.

We proceed to show that the Laplacian $\Delta^{(1)}$ will reduce to an operator acting on the wave functions of variables (ξ_j). For $x=\sigma_0(q)$ and $h=e^{tR(\mathbf{e}_3)}$, the equivariance condition (33) specializes to

$$(E^\ell_m f)(\sigma_0(q))=(E^\ell_m f)(e^{tR(\mathbf{e}_3)}\sigma_0(q))=D^\ell(e^{tR(\mathbf{e}_3)})(E^\ell_m f)(\sigma_0(q)). \tag{190}$$

Since

$$D^\ell(e^{tR(\mathbf{e}_3)})=\mathrm{diag}(e^{-i\ell t},\ldots,e^{-it},0,e^{it},\ldots,e^{i\ell t}), \tag{191}$$

the above condition implies that the $\mathcal{H}^\ell$-valued function $(E^\ell_m f)(\sigma_0(q))$ has only one non-zero component $(P^\ell_{0m}f)(\sigma(q))/\sqrt{2\ell+1}$, and hence the $\mathcal{H}^\ell$-valued function $(E^\ell_m f)(g\sigma_0(q))=D^\ell(g)(E^\ell_m f)(\sigma_0(q))$ has the nth ($|n|\leqslant\ell$) component expressed as

$$\frac{1}{\sqrt{2\ell+1}}D^\ell_{n0}(g)(P^\ell_{0m}f)(\sigma_0(q))=\sqrt{4\pi}\ \overline{Y_{\ell n}(g\mathbf{e}_3)}(P^\ell_{0m}f)(\sigma_0(q)), \tag{192}$$

where $Y_{\ell n}$ are the spherical harmonics and $g\mathbf{e}_3$ denotes a point of the unit sphere S^2, which are designated by the variables (θ,ϕ).

Operating on (192) with the Laplacian $\Delta^{(1)}$, we obtain (up to the factor $\sqrt{4\pi}$)

$$\Delta^{(1)}\overline{Y_{\ell n}(g\mathbf{e}_3)}(P^\ell_{0m}f)(\sigma_0(q))=\overline{Y_{\ell n}(g\mathbf{e}_3)}\left(-\frac{\ell(\ell+1)}{\rho_1(\xi)}+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial}{\partial\xi_j}\right)\right)\times(P^\ell_{0m}f)(\sigma_0(q)). \tag{193}$$

Thus we find an operator acting on functions $(P^\ell_{0m}f)(\sigma_0(q))$,

$$\Delta^{(1)\mathrm{red}} := \frac{1}{\rho_1(\xi)} \sum_{j=1}^{N-1} \frac{\partial}{\partial \xi_j} \left(\rho_1(\xi) \frac{\partial}{\partial \xi_j} \right) - \frac{\ell(\ell+1)}{\rho_1(\xi)}. \tag{194}$$

We have to note here that this reduced operator is globally expressed on the orbit space M_1/S^2 on account of (184). In fact, the operator (194) is expressed in terms of $(\xi_1,\ldots,\xi_{N-1}) \in \dot{\mathbf{R}}^{N-1}$ and invariant under the inversion $(\xi_k) \mapsto -(\xi_k)$. Thus we have the following.

Theorem 3: For collinear configurations, the reduced kinetic energy operator $-\frac{1}{2}\Delta^{(1)\mathrm{red}}$ on M_1/S^2 is given by (194). It looks singular at the multiple collision configuration $(\xi_j=0)$, but the singularity is not essential in the sense that the kinetic energy integral is not divergent at the multiple collision.

We note that the Hamiltonian operator for linear molecules was already discussed in an elementary manner.[13] The method taken in this article to derive the kinetic energy operator is quite different from that in Ref. 13. Ours is clear and natural from the viewpoint of differential geometry.

ACKNOWLEDGMENT

This work was partly supported by the Grant-in-Aid for the Scientific Research of the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Dense Dirac combs in Euclidean space with pure point diffraction

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(Received 7 February 2003; accepted 9 July 2003)

Regular model sets, describing the point positions of ideal quasicrystallographic tilings, are mathematical models of quasicrystals. An important result in mathematical diffraction theory of regular model sets, which are defined on locally compact Abelian groups, is the pure pointedness of the diffraction spectrum. We derive an extension of this result, valid for dense point sets in Euclidean space, which is motivated by the study of quasicrystallographic random tilings. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1609032]

I. INTRODUCTION

An important question in mathematical diffraction theory concerns the problem of which distributions of matter diffract [Bombieri and Taylor (1986)]. By now, there are only partial answers to this question which go beyond the crystallographic case. A mathematical idealization of the set of atomic positions of a piece of matter are Delone sets [Lagarias (2000)]. A subset Λ of $\mathbb{R}^d$ is called a *Delone* set if it is uniformly discrete and relatively dense. This means that there are radii $r,R>0$ such that each ball of radius r (respectively, R) contains at most (respectively, at least) one point of Λ. This class, however, is too general to obtain specific results about spectral properties. It includes, for example, ordered structures such as crystals, as well as structures with disorder, and also amorphous systems.

A special class of Delone sets are model sets [see, for example, Moody (1997)], which arise from a cut-and-project scheme. We will repeat their precise definition below. Model sets have strong regularity properties such as uniform point densities. They are mathematical abstractions of ideal quasicrystals, whose diffraction spectrum is experimentally known to consist of Bragg peaks only. By now, the study of model sets is a rather well developing subject, and their diffraction properties are well understood [Hof (1995), Hof (1998), Schlottmann (1998), Schlottmann (2000)]. The most general description is in terms of measures on locally compact Abelian groups, in generalization of Euclidean space [Schlottmann (1998)]. It is known that regular model sets are pure point diffractive. A first proof of this fact was given by Hof (1998) and, in a more general setup, by Schlottmann (1998), where they used a dynamical systems approach together with an argument due to Dworkin (1993). Recently, an alternative proof has been given by Baake and Moody (2002), who considered Delone sets with certain additional properties, which include model sets. For these sets, they explicitly constructed a cut-and-project scheme and were able to prove the pure pointedness of the diffraction spectrum directly. As they showed, their results have a natural interpretation in terms of the theory of almost periodic measures [Gil de Lamadrid and Argabright (1990)]. An important assumption of the approach is the (uniform) discreteness of the point set Λ, arising from the physical motivation.

In this paper, we will show that the diffraction result for regular model sets remains valid for certain dense point sets in Euclidean space, which appropriately generalize model sets. These point sets are not a mathematical curiosity but admit an interpretation in terms of averaged structures derived from *random tilings* with quasicrystallographic symmetries [Henley (1999), Richard *et al.* (1998), Richard (1999)]: Soon after the discovery of quasicrystals, it became clear that there are two competing models for the description of their unusual diffraction properties, namely the ideal tiling model and the random tiling model. Whereas the ideal tiling model (i.e., a

model set) leads to a diffraction spectrum consisting of Bragg peaks only, in the random tiling model a continuous background in addition to Bragg peaks was expected, as has been argued by Henley (1999). There is at present no rigorous treatment of diffraction properties of quasicrystallographic random tilings in $d>1$, apart from the comparatively simple situation of disorder arising from independent random variables [Baake and Moody (1998)] and the investigation Külske (2001). For rigorous results about diffraction of crystallographic random tilings in $d=2$ and random tilings in $d=1$, see Baake and Höffe (2000), Höffe and Baake (2000). The derivation of Henley's prediction rests on nonrigorous arguments and uses an averaged point distribution, which can be regarded as a generalized model set, being dense in Euclidean space. This distribution was assumed to exist in dimensions $d>2$ [Henley (1999)]. In the following, we give a rigorous exposition of a main part of this approach, which is, on the other hand, a generalization of the cut-and-project scheme for regular model sets to dense point sets [see also Höffe (2001), which introduces the setup used in this paper, and the review article Baake *et al.* (2003), where the diffraction formula of Theorem 10 is cited]. After recollecting the basic terminology and central theorems of diffraction theory of regular model sets in Sec. II, we will define generalized model sets in Sec. III and show that they are pure point diffractive. This leads to a generalization of Poisson's summation formula to certain dense point sets. Section IV will apply the results within Henley's framework for the description of diffraction properties of quasicrystallographic random tilings. A discussion of open questions and possible future work concludes the paper.

II. DIFFRACTION OF WEIGHTED REGULAR MODEL SETS

In this section, we recollect and extend results from diffraction theory of weighted regular model sets, which we shall generalize in the following section to the setup of a dense Dirac comb.

Throughout the paper, we consider the situation of a *cut-and-project scheme* [Moody (1997)] with a Euclidean space $\mathbb{R}^d$ and a Euclidean space $\mathbb{R}^m$, called *direct* space and *internal space*.

Let $\tilde{L}\subset\mathbb{R}^d\times\mathbb{R}^m$ be a lattice and denote the volume of its fundamental domain by $|\det(\tilde{L})|$. If π_1 and π_2 are the natural (orthogonal) projections of $\mathbb{R}^d\times\mathbb{R}^m$ onto $\mathbb{R}^d$ and $\mathbb{R}^m$, respectively, then $\pi_1|_{\tilde{L}}$ is assumed to be one-to-one and $\pi_2(\tilde{L})$ is assumed to be dense. Set $L=\pi_1(\tilde{L})$ and let $(\,)^\star: L\to\pi_2(\tilde{L})$ denote the mapping $\pi_2\circ(\pi_1|_{\tilde{L}})^{-1}$, also called the *star-map*. This is summarized in the following diagram:

$$\begin{array}{ccccc} & \pi_1 & & \pi_2 & \\ \mathbb{R}^d & \leftarrow & \mathbb{R}^d\times\mathbb{R}^m & \rightarrow & \mathbb{R}^m \\ \cup & {\scriptstyle 1-1}\nwarrow & \cup & \nearrow_{\text{dense}} & \\ L & & \tilde{L}=\{(x,x^\star)\,|\,x\in L\} & & \end{array} \tag{1}$$

For an open and relatively compact subset $W\subset\mathbb{R}^m$, also called *window*, define the *model set* $\Lambda(W)$ by

$$\Lambda(W):=\{x\in L\mid x^\star\in W\}. \tag{2}$$

Denote the volume of W by $\mathrm{vol}(W)$. Model sets are Delone sets, i.e., they are both uniformly discrete and relatively dense [Moody (1997), Schlottmann (1998)]. The model set $\Lambda(W)$ is called *regular* if $\varnothing\neq W=\overline{\mathrm{int}(W)}$ is compact and if ∂W has zero Lebesgue measure.

Associated with the lattice $\tilde{L}$ is its dual lattice $(\tilde{L})^*$, defined via

$$(\tilde{L})^*=\{y\in\mathbb{R}^d\times\mathbb{R}^m\mid y\cdot x\in\mathbb{Z}\ \text{ for all }\ x\in L\}. \tag{3}$$

Denote its image in $\mathbb{R}^d$ by $L^*=\pi_1((\tilde{L})^*)$. A remarkable property of cut-and-project schemes is duality [Moody (1997), p. 418]. We can dualize the given cut-and-project scheme to obtain a cut-and-project scheme for the dual lattice. By identifying direct and internal space with their

corresponding duals, we can see that the projection π_1, restricted to the dual lattice $(\widetilde{L})^*$, is one-to-one, and that the dual lattice has dense image $\pi_2((\widetilde{L})^*)$ in $\mathbb{R}^m$. The corresponding star-map is defined on the set L^*. We denote it by $(\,)^\star$ again.

Regular model sets have a well-defined density. Throughout the paper, we will consider infinite volume limits to be taken on sequences of balls. Existence of these limits may however be derived for more general van Hove sequences, see Schlottmann (2000) for the example of the density formula. Let $B_n(a)$ denote the closed ball of radius n centered at $a\in\mathbb{R}^d$. We set $B_n = B_n(0)$.

Theorem 1: [Density formula (Schlottmann, 1998)] *Let $\Lambda(W)$ be a regular model set. Then*

$$\lim_{r\to\infty}\frac{1}{\mathrm{vol}(B_r(0))}\left(\sum_{x\in\Lambda(W+u)\cap B_r(a)} 1\right)=\frac{\mathrm{vol}(W)}{|\det(\widetilde{L})|},$$

uniformly in a and in u. □

This result may be used to consider sums over weighted regular model sets. Consider first the situation where the weight of a point $x\in\Lambda(W)$ only depends on x.

Lemma 1: Let $\Lambda(W)$ be a regular model set, $f:\mathbb{R}^d\to\mathbb{C}$ bounded and $|x|^{d+1+\alpha}|f(x)|\leqslant C$ for some constants $C>0$ and $\alpha>0$. Then, for $a\in\mathbb{R}^d$ and $u\in\mathbb{R}^m$, the sums

$$s(u,a):=\sum_{x\in\Lambda(W+u)+a} f(x)$$

are absolutely convergent. Moreover, they are uniformly bounded in u and in a, the bound being proportional to $\mathrm{vol}(W)$.

Proof: For $R\in\mathbb{N}$, consider the sums

$$s_<(u,a,R):=\sum_{\substack{x\in\Lambda(W+u)+a\\ |x|<R}}|f(x)|,\quad s_\geqslant(u,a,R):=\sum_{\substack{x\in\Lambda(W+u)+a\\ |x|\geqslant R}}|f(x)|.$$

In the density formula, the sequence on the left-hand side is certainly bounded by twice its limit for almost all r. This implies for the number of points within a ball of radius n,

$$|(\Lambda(W+u)+a)\cap B_n(0)|=|\Lambda(W+u)\cap B_n(-a)|\leqslant c\,\mathrm{vol}(W)\,n^d\quad (n>n_0(W)),$$

uniformly in u and in a, where $c=2S_d/|\det(\widetilde{L})|$, and $S_d\subset\mathbb{R}^d$ denotes the volume of the unit ball. The number $n_0(W)$ is increasing with decreasing volume of W. Together with f bounded, the above estimate implies that $s_<(u,a,R)$ is uniformly bounded in u and in a with a number proportional to $\mathrm{vol}(W)$. We derive a uniform bound on $s_\geqslant(u,a,R)$. By assumption, we have $|x|^{d+1+\alpha}|f(x)|\leqslant C$. Define $g_n:=\Sigma_{n\leqslant|x|<n+1}|f(x)|$ and estimate g_n by

$$g_n\leqslant|(\Lambda(W+u)+a)\cap B_{n+1}(0)|\,\frac{C}{n^{d+1+\alpha}}\leqslant c\,\mathrm{vol}(W)(n+1)^d\frac{C}{n^{d+1+\alpha}}\leqslant\frac{2c\,C\,\mathrm{vol}(W)}{n^{1+\alpha}}\qquad(4)$$

for $n>n_1(W)$. Thus for $R>n_1(W)$,

$$|s_\geqslant(u,a,R)|\leqslant\sum_{n\geqslant R}g_n\leqslant 2c\,C\,\mathrm{vol}(W)\sum_{n=R}^{\infty}\frac{1}{n^{1+\alpha}}<\infty,\qquad(5)$$

since by assumption $\alpha>0$. The bound is independent of u and of a. Note that we have $\lim_{R\to\infty}s_\geqslant(u,a,R)=0$.

Remark: The above sums $s(u,a)$ are absolutely convergent and bounded uniformly in u and in a under the milder assumption $|x|^{d+\alpha}|f(x)|\leqslant C$ for some constants $C>0$ and $\alpha>0$. This follows already from the uniform discreteness of $\Lambda(W)$ by a standard estimation. The additional

property that there exists a bound proportional to $\mathrm{vol}(W)$, which we will use extensively below, is a result of the density formula. It would be interesting to consider whether the assumptions on f in the above lemma may be weakened, since the estimation in Eq. (4) seems rather crude.

Consider now the situation where the weight of a point $x \in \Lambda(W)$ depends only on its internal coordinate $x^\star$. This leads to Weyl's theorem on uniform distribution in the context of regular model sets [Kuipers and Niederreiter (1974), Schlottmann (1998)].

Theorem 2: [Weyl's theorem for regular model sets (Baake and Moody, 2000)] *Let $\Lambda(W)$ be a regular model set, with compact, Riemann measurable $W \subset \mathbb{R}^m$. Let $f: \mathbb{R}^m \to \mathbb{C}$ be continuous with* $\mathrm{supp}(f) \subset W$. *Then, for all $a \in \mathbb{R}^d$,*

$$\lim_{r\to\infty} \frac{1}{\mathrm{vol}(B_r(0))} \sum_{x \in \Lambda(W)\cap B_r(a)} f(x^\star) = \frac{1}{|\det(\tilde{L})|} \int_W f(y)\, \mathrm{d}y,$$

uniformly in a. □

The fundamental object in diffraction theory of weighted model sets is the *weighted Dirac comb* ω defined by

$$\omega = \sum_{x \in \Lambda(W)} f(x^\star)\, \delta_x, \tag{6}$$

where $\sup_{x\in\Lambda(W)} |f(x^\star)| < \infty$. This defines a complex regular Borel measure on $\mathbb{R}^d$, which is translation bounded, since $\Lambda(W)$, being a model set, is uniformly discrete. Recall that a measure ω is *translation bounded* iff, for all compact $K \subset \mathbb{R}^d$, $\sup_{y\in\mathbb{R}^d} |\omega|(y+K) \leqslant C_K < \infty$ for some constant C_K which only depends on K. Here, $|\omega|$ denotes the total variation measure and $y+K = \{y + x \mid x \in K\}$. In the following, we assume that the function f satisfies the assumption of Weyl's theorem for regular model sets, i.e., we assume that $f: \mathbb{R}^m \to \mathbb{C}$ is continuous with $\mathrm{supp}(f) \subset W$.

Diffraction properties can be expressed using the *Fourier–Bohr coefficient* $c_W(k)$ of the weighted Dirac comb ω, defined by

$$c_W(k) = \lim_{r\to\infty} \frac{1}{\mathrm{vol}(B_r(0))} \sum_{x \in \Lambda(W)\cap B_r(a)} f(x^\star) e^{-2\pi\imath k\cdot x}, \tag{7}$$

where $k \in \mathbb{R}^d$ and $a \in \mathbb{R}^d$. We have the following theorem.

Theorem 3: [Fourier–Bohr coefficients (Bernuau and Duneau, 2000; Hof, 1995)] *Let $\Lambda(W)$ be a regular model set, with compact, Riemann measurable $W \subset \mathbb{R}^m$. Let $f: \mathbb{R}^m \to \mathbb{C}$ be continuous with* $\mathrm{supp}(f) \subset W$. *Then, for all $k \in \mathbb{R}^d$, the Fourier–Bohr coefficient $c_W(k)$ exists and is independent of $a \in \mathbb{R}^d$. Its value is given as follows. For any $k \in L^*$, one has*

$$c_W(k) = \frac{1}{|\det(\tilde{L})|} \int_W e^{2\pi\imath k^\star\cdot u} f(u)\, \mathrm{d}u = \frac{1}{|\det(\tilde{L})|} \widehat{f|_W}(-k^\star),$$

and $c_W(k) = 0$ if k does not belong to the $\mathbb{Z}$-module L^*. □

Remark: In Bernuau and Duneau (2000), the theorem is proved only for the case where $f(u)$ equals unity. The statement can be generalized to the situation described above by the same methods which lead to Weyl's formula, generalizing the density formula. For $k \in L^*$, the theorem is a direct consequence of Weyl's density formula.

For regular model sets, the *weighted density of points* ρ exists, because Weyl's theorem for regular model sets implies

$$\rho := \lim_{r\to\infty} \frac{1}{\mathrm{vol}(B_r)}\, \omega(B_r) = \frac{1}{|\det(\tilde{L})|} \int_W f(u)\, \mathrm{d}u. \tag{8}$$

This identity may be viewed as a particular normalization of admissible functions f, which we employ in the following.

Diffraction is described by properties of the Fourier transform of the *autocorrelation*, which we now define [see also Hof (1995), Baake, Moody, and Pleasants (2000)]. Set $\tilde{\omega}(f)=\overline{\omega(\tilde{f})}$, where $\tilde{f}(x)=\overline{f(-x)}$. Define truncated Dirac combs $\omega_n=\omega|_{B_n}$ and set $\tilde{\omega}_n=(\omega_n)^{\sim}$. The finite autocorrelation measures

$$\gamma_\omega^{(n)}:=\frac{1}{\mathrm{vol}(B_n)}\,\omega_n*\tilde{\omega}_n \tag{9}$$

are well defined, since ω_n has compact support. Recall that the *convolution* of two measures μ, ν is defined as $\mu*\nu(f)=\int_{\mathbb{R}^d\times\mathbb{R}^d} f(x+y)\,\mathrm{d}\mu(x)\,\mathrm{d}\nu(y)$, being well defined if at least one of them has compact support. The finite autocorrelation measures read explicitly

$$\gamma_\omega^{(n)}=\sum_{z\in\Delta}\eta_n(z)\,\delta_z,\quad \eta_n(z)=\frac{1}{\mathrm{vol}(B_n)}\sum_{\substack{x,y\in\Lambda(W)\cap B_n\\ x-y=z}} f(x^\star)\overline{f(y^\star)}, \tag{10}$$

where $\Delta=\Lambda(W)-\Lambda(W)$ is the set of difference vectors of $\Lambda(W)$. It can be shown that the vague limit $n\to\infty$ leads to a unique autocorrelation γ_ω.

Theorem 4: (Autocorrelation) *Let $\Lambda(W)$ be a regular model set, with compact, Riemann measurable $W\subset\mathbb{R}^m$. Let $f:\mathbb{R}^m\to\mathbb{C}$ be continuous with* $\mathrm{supp}(f)\subset W$. *Then, the vague limit $n\to\infty$ of the finite autocorrelation measures $\gamma_\omega^{(n)}$ leads to a unique measure γ_ω, called natural autocorrelation, being a translation bounded, positive definite pure point measure. It is given explicitly by*

$$\gamma_\omega=\sum_{z\in\Delta}\eta(z)\,\delta_z,\quad \eta(z)=\frac{1}{|\det(\tilde{L})|}\int_{W\cap(W+z^\star)} f(u)\overline{f(u-z^\star)}\,\mathrm{d}u. \tag{11}$$

□

Recall that a measure μ is *positive definite* iff $\mu(g*\tilde{g})\geqslant 0$ for all compactly supported continuous functions g.

The proof of the theorem proceeds as follows [Baake, Moody, and Pleasants (2000)]. All autocorrelation coefficients $\eta(z)=\lim_{n\to\infty}\eta_n(z)$ exist due to Weyl's theorem for regular model sets. They are locally summable, since Δ is closed and discrete. Then, γ_ω defines a distribution over the space of all C^∞ functions of compact support. The translation boundedness is inherited from ω [see Hof (1995), Prop. 2.2]. Finally, γ_ω can be written as a certain volume-normalized convolution, which implies that it is a distribution of positive type.

Due to Bochner's theorem [Reed and Simon (1980), p. 331], the Fourier transform $\widehat{\gamma_\omega}$ of γ_ω is a positive measure and also translation bounded [Baake, Moody, and Pleasants (2000)]. Recall that the *Fourier transform* $\hat{\mu}$ of a tempered distribution μ is defined as $\hat{\mu}(\varphi)=\mu(\hat{\varphi})$ for all Schwartz functions φ, where $\hat{\varphi}(y)=\int e^{-2\pi\imath y\cdot x}\varphi(x)\,\mathrm{d}x$. It can be shown that the Fourier transform of the autocorrelation is a pure point measure [Schlottmann (2000), Baake and Moody (2002)].

Theorem 5: [Diffraction formula (Bernuau and Duneau, 2000] *Let $\Lambda(W)$ be a regular model set, with compact, Riemann measurable $W\subset\mathbb{R}^m$. Let $f:\mathbb{R}^m\to\mathbb{C}$ be continuous with* $\mathrm{supp}(f)\subset W$. *The Fourier transform $\widehat{\gamma_\omega}$ of the autocorrelation measure γ_ω is a translation bounded, positive pure point measure. It is explicitly given by*

$$\widehat{\gamma_\omega}=\sum_{k\in L^*}|c_W(k)|^2\,\delta_k,$$

where L^* is the projection of the dual lattice into direct space, and $c_W(k)$ are the Fourier–Bohr coefficients of Theorem 3. □

Recall that a measure μ is *positive* iff $\mu(g)\geqslant 0$ for all compactly supported continuous functions $g\geqslant 0$.

Remark: The pure pointedness of $\widehat{\gamma_\omega}$ has been shown in Hof (1998), Schlottmann (1998), and Baake and Moody (2002). The explicit formula for the discrete part of $\widehat{\gamma_\omega}$ was proved in Hof (1995), but appeared earlier at different places in the physical literature. In the context of deformed model sets, which include regular model sets as a special case, the theorem appears in Bernuau and Duneau (2000). The diffraction formula is often stated for unweighted Dirac combs, but also holds for weighted Dirac combs, as is seen by an approximation of the weight function f by step functions, analogously to the proof of Weyl's theorem for regular model sets in Baake and Moody (2000) using the density formula.

III. DIFFRACTION OF DENSE DIRAC COMBS

We now extend the above results to the situation of a dense Dirac comb. The corresponding proofs will rely on the above results. In the following, we assume a cut-and-project scheme as in the preceding section with the additional property that the canonical projections π_1 and π_2, restricted to $\tilde{L}$, are both one-to-one, and the images of $\tilde{L}$ are both dense in $\mathbb{R}^d$ and $\mathbb{R}^m$, respectively. The star-map is then a bijection between L and $L^\star$. This additional assumption makes it possible to regard subsets $B\subset\mathbb{R}^d$ as windows, leading to model sets in internal space $\mathbb{R}^m$.

Define the *weighted Dirac comb* ω by

$$\omega=\sum_{x\in L} f(x^\star)\,\delta_x. \tag{12}$$

Since the $\mathbb{Z}$-module L is dense in Euclidean space, the above sum is now well defined only under special assumptions on the weight function f.

Theorem 6: (Weighted Dirac combs with dense support) *Let $f:\mathbb{R}^m\to\mathbb{C}$ be bounded, and $|x|^{m+1+\alpha}|f(x)|\leqslant C$ for some constants $C>0$ and $\alpha>0$. Then, the weighted Dirac comb ω is a translation bounded measure.*

Proof: Let a compact $K\subset\mathbb{R}^d$ be given. Cover K with a finite number of translated unit balls W_i such that $K\subset\cup_{i=1}^n W_i=W$. For $y\in\mathbb{R}^d$, the total variation measure of ω is bounded by

$$|\omega|(K+y)\leqslant\sum_{x\in L\cap(W+y)}|f(x^\star)|=\sum_{x^\star\in(L\cap(W+y))^\star}|f(x^\star)|=:a_K(y).$$

The additional assumptions on the cut-and-project setup, introduced at the beginning of this section, imply that $(L\cap(W+y))^\star$ is a regular model set with window $(W+y)\subset\mathbb{R}^d$. Lemma 1 then yields that $a_K(y)<b_K<\infty$, uniformly in y, for some b_K. This implies that ω is a measure, and that ω is translation bounded. □

We derive a generalization of Weyl's theorem on uniform distribution to dense point sets.

Theorem 7: (Weyl's theorem for dense point sets) *Let $f:\mathbb{R}^m\to\mathbb{C}$ be continuous, and $|x|^{d+1+\alpha}|f(x)|\leqslant C$ for some constants $C>0$ and $\alpha>0$. Then*

$$\lim_{r\to\infty}\frac{1}{\mathrm{vol}(B_r(0))}\sum_{x\in L\cap B_r(a)}f(x^\star)=\frac{1}{|\det(\tilde{L})|}\int_{\mathbb{R}^m}f(u)\,\mathrm{d}u,$$

uniformly in a.

Proof: For $s\in\mathbb{N}$, let $B_s\subset\mathbb{R}^m$ denote the ball of radius s centered at 0. The idea of the proof is to approximate the dense set L by the model sets $\Lambda(B_s)$. Let $\chi_s:\mathbb{R}^m\to[0,1]$ be continuous with $\chi_s(x)=1$ for $|x|<s-1$ and $\chi_s(x)=0$ for $|x|\geqslant s$. Define the numbers

$$w_{r,s}=\frac{1}{\mathrm{vol}(B_r(0))}\sum_{x\in\Lambda(B_s)\cap B_r(a)}(\chi_s\cdot f)(x^\star),\quad w'_s=\frac{1}{|\det(\tilde{L})|}\int_{B_s}(\chi_s\cdot f)(u)\,\mathrm{d}u,$$

$$w_r = \frac{1}{\mathrm{vol}(B_r(0))} \sum_{x \in L \cap B_r(a)} f(x^\star), \quad w = \frac{1}{|\det(\tilde{L})|} \int_{\mathbb{R}^m} f(u)\, \mathrm{d}u.$$

We have $\lim_{r\to\infty} w_{r,s} = w_s' < \infty$ due to Weyl's theorem for regular model sets. We also have $\lim_{s\to\infty} w_s' = w < \infty$. This follows from Lebesgue's dominated convergence theorem, since the functions $|(\chi_s \cdot f)(u)|$ are bounded by $|f(u)|$ uniformly in s, and $f(u)$ is by assumption absolutely integrable (the integral being finite).

We now show that $\lim_{s\to\infty} w_{r,s} = w_r$ uniformly in r and in a. We have the estimate

$$\begin{aligned} |w_r - w_{r,s}| &= \frac{1}{\mathrm{vol}(B_r(0))} \left| \sum_{x \in L \cap B_r(a)} f(x^\star) - \sum_{x \in \Lambda(B_s) \cap B_r(a)} (\chi_s \cdot f)(x^\star) \right| \\ &\leqslant \frac{1}{\mathrm{vol}(B_r(0))} \left(\sum_{x^\star \in (L \cap B_r(a))^\star \setminus B_s} |f(x^\star)| + \sum_{\substack{x^\star \in (L \cap B_r(a))^\star \\ s-1 \leqslant |x^\star| < s}} |f(x^\star)| \right) \\ &= \frac{1}{\mathrm{vol}(B_r(0))} \left(\sum_{x^\star \in (L \cap B_r(a))^\star \setminus B_{s-1}} |f(x^\star)| \right). \end{aligned}$$

We estimate the last term using Eq. (5) in Lemma 1. Since $n_1(B_{r_2}) \leqslant n_1(B_{r_1})$ for $r_2 \geqslant r_1$, we get for $s \geqslant n_1(B_1)$ and $r > 1$,

$$|w_r - w_{r,s}| \leqslant \frac{1}{\mathrm{vol}(B_r)} \left(2c\, C\, \mathrm{vol}(B_r) \sum_{n=s-1}^{\infty} \frac{1}{n^{1+\alpha}} \right).$$

Since the bound is independent of r and a and vanishes as $s \to \infty$, the assertion follows.

We now use a 3ε argument to show that $w_r \to w$. Fix $\varepsilon > 0$. We have $|w - w_s'| < \varepsilon$ for $s > s_0(\varepsilon)$. We also have $|w_{r,s} - w_r| < \varepsilon$ for $s > s_1(\varepsilon)$ uniformly in r. Last, we have $|w_s' - w_{r,s}| < \varepsilon$ for $r > r_0(\varepsilon, s)$. Take $s > \max\{s_0(\varepsilon), s_1(\varepsilon)\}$. For $r > r_0(\varepsilon, s)$, we thus have

$$|w - w_r| \leqslant |w - w_s'| + |w_s' - w_{r,s}| + |w_{r,s} - w_r| \leqslant 3\,\varepsilon.$$

This establishes the convergence result of the theorem. □

For applications to diffraction, we restrict the class of admissible functions f in the remainder of this paper. Let $f: \mathbb{R}^m \to \mathbb{C}$ be continuous, and $|f(x)| \leqslant C/|x|^{m+1+\alpha}$ for some constants $C > 0$ and $\alpha > 0$. We can argue as in the preceding section, using Weyl's theorem for dense point sets, that the weighted density of points exists,

$$\rho := \lim_{r\to\infty} \frac{1}{\mathrm{vol}(B_r)}\, \omega(B_r) = \frac{1}{|\det(\tilde{L})|} \int_{\mathbb{R}^m} f(u)\, \mathrm{d}u. \tag{13}$$

This identity may be viewed as a particular normalization of admissible functions f. Given a weighted Dirac comb ω with dense support, we consider its Fourier–Bohr coefficients. We define the finite volume approximations

$$c_r(k) = \frac{1}{\mathrm{vol}(B_r(0))} \sum_{x \in L \cap B_r(a)} f(x^\star) e^{-2\pi \imath k \cdot x}, \tag{14}$$

where $k \in \mathbb{R}^d$ and $a \in \mathbb{R}^d$. The numbers $c_r(k)$ exist (and may depend on a), as is seen by an argument similar to that used for proving the existence of the Dirac comb ω. In the limit $r \to \infty$, we have the following result.

Theorem 8: (Fourier–Bohr coefficients for dense point sets) *Let* $f:\mathbb{R}^m\to\mathbb{C}$ *be continuous, and* $|x|^{m+1+\alpha}|f(x)|\leq C$ *for some constants* $C>0$ *and* $\alpha>0$. *Then, for all* $k\in\mathbb{R}^d$, *the Fourier–Bohr coefficient* $c(k)=\lim_{r\to\infty}c_r(k)$ *exists and is independent of* a. *Its value is given as follows. For any* $k\in L^*$ *and for any* $a\in\mathbb{R}^d$, *one has*

$$c(k)=\frac{1}{|\det(\tilde{L})|}\int_{\mathbb{R}^m}e^{2\pi\imath k^\star\cdot u}f(u)\,\mathrm{d}u=\frac{1}{|\det(\tilde{L})|}\hat{f}(-k^\star),$$

and $c(k)=0$ *if* k *does not belong to the* $\mathbb{Z}$*-module* L^*.

Proof: The proof is analogous to the proof of Weyl's theorem for dense point sets above. For $s\in\mathbb{N}$, let $B_s\subset\mathbb{R}^m$ denote the ball of radius s, centered at 0, and define the numbers

$$c_{r,s}(k)=\frac{1}{\mathrm{vol}(B_r(0))}\sum_{x\in\Lambda(B_s)\cap B_r(a)}(\chi_s\cdot f)(x^\star)e^{-2\pi\imath k\cdot x},$$

$$c_s'(k)=\begin{cases}\dfrac{1}{|\det(\tilde{L})|}\displaystyle\int_{B_s}(\chi_s\cdot f)(u)e^{2\pi\imath k^\star\cdot u}\,\mathrm{d}u, & k\in L^*,\\ 0, & k\notin L^*,\end{cases}$$

$$c'(k)=\begin{cases}\dfrac{1}{|\det(\tilde{L})|}\displaystyle\int_{\mathbb{R}^m}f(u)e^{2\pi\imath k^\star\cdot u}\,\mathrm{d}u, & k\in L^*,\\ 0, & k\notin L^*.\end{cases}$$

We have $\lim_{r\to\infty}c_{r,s}(k)=c_s'(k)<\infty$ due to Theorem 3. We also have $\lim_{s\to\infty}c_s'(k)=c'(k)<\infty$ by Lebesgue's dominated convergence theorem. We show that $\lim_{s\to\infty}c_{r,s}(k)=c_r(k)$ uniformly in r and in a. As in Theorem 7, we can then use a 3ε argument to show that $c_r(k)$ converges to $c'(k)$ as $r\to\infty$. Thus $c(k)=\lim_{r\to\infty}c_r(k)=c'(k)$, and the assertion of the theorem follows.

For every $k\in\mathbb{R}^d$, we have the estimate

$$|c_r(k)-c_{r,s}(k)|\leq\frac{1}{\mathrm{vol}(B_r(0))}\left(\sum_{x^\star\in(L\cap B_r(a))^\star\setminus B_s}|f(x^\star)|+\sum_{\substack{x^\star\in(L\cap B_r(a))^\star\\ s-1\leq|x^\star|<s}}|f(x^\star)|\right).$$

This is the same expression as in the proof of Theorem 7. We can repeat the previous argument and derive a uniform bound in r and in a, which vanishes as $s\to\infty$. □

The finite autocorrelation measures of the dense Dirac comb ω,

$$\gamma_\omega^{(n)}:=\frac{1}{\mathrm{vol}(B_n)}\,\omega_n*\tilde{\omega}_n\,,\tag{15}$$

are well defined, since ω_n has compact support. They read explicitly

$$\gamma_\omega^{(n)}=\sum_{z\in L}\eta_n(z)\,\delta_z\,,\quad \eta_n(z)=\frac{1}{\mathrm{vol}(B_n)}\sum_{\substack{x,y\in L\cap B_n\\ x-y=z}}f(x^\star)\overline{f(y^\star)}.\tag{16}$$

We show that the limit $n\to\infty$ leads to a unique autocorrelation. As a first step, we show that the pointwise limit exists.

Lemma 2: Let $\eta_n(z)$ *denote the finite autocorrelation coefficients of the weighted Dirac comb* ω. *The numbers* $\eta_n(z)$ *have a well-defined limit* $\eta(z)$, *which is a positive definite function. It is given by*

$$\lim_{n\to\infty} \eta_n(z) = \eta(z) = \frac{1}{|\det(\widetilde{L})|} \int_{\mathbb{R}^m} f(u)\overline{f(u-z^\star)}\,\mathrm{d}u. \tag{17}$$

Proof: This is an application of Weyl's theorem for dense point sets. We have

$$\begin{aligned}\eta_n(z) &= \frac{1}{\mathrm{vol}(B_n)} \sum_{\substack{x\in L\cap B_n \\ x-z\in L\cap B_n}} f(x^\star)\overline{f(x^\star-z^\star)} \\ &= \frac{1}{\mathrm{vol}(B_n)} \sum_{x\in L\cap B_n} f(x^\star)\overline{f(x^\star-z^\star)} - \frac{1}{\mathrm{vol}(B_n)} \sum_{\substack{x\in L\cap B_n \\ x-z\notin L\cap B_n}} f(x^\star)\overline{f(x^\star-z^\star)}.\end{aligned}$$

The first term in the last line converges to $\eta(z)$ by Weyl's theorem for dense point sets, and the second one, which we denote by $r_n(z)$, converges to zero, as we now show. Note that $|x|<n-|z|$ implies $|x-z|<n$. Consider for $n>|z|$ the estimate

$$\begin{aligned}|r_n(z)| &\leqslant \frac{1}{\mathrm{vol}(B_n)} \left(\sum_{x\in L\cap B_n} - \sum_{x\in L\cap B_{n-|z|}} \right) |f(x^\star)|\,|f(x^\star-z^\star)| \\ &= \frac{1}{\mathrm{vol}(B_n)} \sum_{x^\star\in (L\cap (B_n\setminus B_{n-|z|}))^\star} |f(x^\star)|\,|f(x^\star-z^\star)|.\end{aligned}$$

This is a summation over a regular model set with window $B_n\setminus B_{n-|z|}$. Due to Lemma 1, the sum is bounded by the volume of the window, which is a shell of thickness $|z|$ of the ball of radius n. Thus, the last expression vanishes like $1/n$ as $n\to\infty$. The limit $\eta(z)$ is a positive definite function, since it is the limit of the positive definite functions $\eta_n(z)$. □

Theorem 9: (Autocorrelation) *Let $f:\mathbb{R}^m\to\mathbb{C}$ be continuous, and $|x|^{m+1+\alpha}|f(x)|\leqslant C$ for some constants $C>0$ and $\alpha>0$. The weighted dense Dirac comb ω has the unique autocorrelation*

$$\gamma_\omega = \sum_{z\in L} \eta(z)\,\delta_z, \quad \eta(z) = \frac{1}{|\det(\widetilde{L})|} \int_{\mathbb{R}^m} f(u)\overline{f(u-z^\star)}\,\mathrm{d}u,$$

where γ_ω is a translation bounded, positive definite pure point measure.

Proof: Consider the regular model set autocorrelation measures

$$\gamma_{\omega,s} = \sum_{z\in\Delta_s} \eta_s(z)\,\delta_z, \quad \eta_s(z) = \frac{1}{|\det(\widetilde{L})|} \int_{B_s\cap(B_s+z^\star)} (\chi_s\cdot f)(u)\overline{(\chi_s\cdot f)(u-z^\star)}\,\mathrm{d}u,$$

where B_s denotes the ball of radius $s\in\mathbb{N}$, and $\Delta_s=\Lambda(B_s)-\Lambda(B_s)$. Note that $\Delta_s\subset\Delta_{s+1}\subset L$ and set $\eta_s(z)=0$ if $z\notin\Delta_s$. Consider the associated finite autocorrelation measures

$$\gamma_{\omega,s}^{(n)} = \sum_{z\in\Delta_s} \eta_{n,s}(z)\,\delta_z, \quad \eta_{n,s}(z) = \frac{1}{\mathrm{vol}(B_n)} \sum_{\substack{x,y\in\Lambda(B_s)\cap B_n \\ x-y=z}} (\chi_s\cdot f)(x^\star)(\chi_s\cdot f)(y^\star).$$

Since these measures arise from regular model sets, we have $\gamma_{\omega,s}^{(n)}\to\gamma_{\omega,s}$ vaguely. The measures $\gamma_{\omega,s}$ converge to γ_ω vaguely, as follows from Lebesgue's dominated convergence theorem: Note that $\eta_s(z)\to\eta(z)$ and $|\eta_s(z)|<|\eta|(z) := [1/|\det(\widetilde{L})|]\int_{\mathbb{R}^m}|f(u)|\,|f(u-z^\star)|\mathrm{d}u$. Note that $\gamma_{|\omega|} := \Sigma_{z\in L}|\eta|(z)\,\delta_z$ defines a measure: For $\gamma_{|\omega|}$ and compact K, we have the estimate

$$\gamma_{|\omega|}(K) \leqslant \sum_{z\in L\cap W} |\eta|(z) = \sum_{z^\star\in(L\cap W)^\star} \frac{1}{|\det(\tilde{L})|} \int_{\mathbb{R}^m} |f(u)|\,|f(u-z^\star)|\,\mathrm{d}u$$
$$= \frac{1}{|\det(\tilde{L})|} \int_{\mathbb{R}^m} |f(u)| \left(\sum_{z^\star\in(L\cap W)^\star} |f(u-z^\star)| \right) \mathrm{d}u < \infty,$$

where $W=\cup_{i=1}^{n} W_i$ is a covering of K with a finite number of translated unit balls W_i. In the last equation, we exchanged summation and integration, which is justified by Lebesgue's dominated convergence theorem, since the terms in brackets are bounded uniformly in u due to Lemma 1. For g continuous with support on K, we then have

$$\lim_{s\to\infty} \gamma_{\omega,s}(g) = \lim_{s\to\infty} \sum_{z\in L\cap K} \eta_s(z)g(z) = \sum_{z\in L\cap K} \lim_{s\to\infty} \eta_s(z)g(z) = \sum_{z\in L\cap K} \eta(z)g(z) = \gamma_\omega(g).$$

We will show below that $\gamma_{\omega,s}^{(n)} \to \gamma_\omega^{(n)}$ vaguely, uniformly in n. The above results may then be used with a 3ε argument as in Theorem 7 to show that $\gamma_\omega^{(n)} \to \gamma_\omega$. Since ω is translation bounded, we further conclude that all finite volume approximations $\gamma_\omega^{(n)}$ are uniformly translation bounded [Hof (1995), Prop. 2.2], hence the limit is translation bounded. As it coincides with the pointwise limit, it is unique. The measures $\gamma_\omega^{(n)}$ are positive definite by construction. Since the positive definite measures are closed in the vague topology, γ_ω is a positive definite measure. The explicit form of the vague limit shows that γ_ω is pure point.

To show the uniform convergence of $\gamma_{\omega,s}^{(n)}$, consider for a compact set $K\subset\mathbb{R}^d$ the estimate

$$|\gamma_\omega^{(n)}(K) - \gamma_{\omega,s}^{(n)}(K)| = \frac{1}{\mathrm{vol}(B_n)} \Bigg| \sum_{z\in L\cap K} \sum_{\substack{x\in L\cap B_n \\ x-z\in L\cap B_n}} f(x^\star)\overline{f(x^\star-z^\star)}$$
$$- \sum_{z\in L\cap K} \sum_{\substack{x\in \Lambda(B_s)\cap B_n \\ x-z\in \Lambda(B_s)\cap B_n}} (\chi_s\cdot f)(x^\star)\overline{(\chi_s\cdot f)(x^\star-z^\star)} \Bigg|$$
$$\leqslant \frac{1}{\mathrm{vol}(B_n)} \Bigg| \sum_{z\in L\cap K} \Bigg(\sum_{x\in L\cap B_n} f(x^\star)\overline{f(x^\star-z^\star)}$$
$$- \sum_{x\in \Lambda(B_s)\cap B_n} (\chi_s\cdot f)(x^\star)\overline{(\chi_s\cdot f)(x^\star-z^\star)} \Bigg) \Bigg|$$
$$+ \frac{1}{\mathrm{vol}(B_n)} \Bigg| \sum_{z\in L\cap K} \Bigg(\sum_{\substack{x\in L\cap B_n \\ x-z\notin L\cap B_n}} f(x^\star)\overline{f(x^\star-z^\star)}$$
$$- \sum_{\substack{x\in \Lambda(B_s)\cap B_n \\ x-z\notin \Lambda(B_s)\cap B_n}} (\chi_s\cdot f)(x^\star)\overline{(\chi_s\cdot f)(x^\star-z^\star)} \Bigg) \Bigg|.$$

Both terms in the last inequality may be estimated by

$$\frac{1}{\mathrm{vol}(B_n)} \sum_{z\in L\cap K} \left(\sum_{x^\star\in(L\cap B_n)^\star\setminus B_s} |f(x^\star)|\,|f(x^\star-z^\star)| + \sum_{\substack{x^\star\in(L\cap B_n)^\star \\ s-1\leqslant|x^\star|<s}} |f(x^\star)|\,|f(x^\star-z^\star)| \right)$$

by the same argument as in the proof of Theorem 7. We may now interchange the summations and use the fact that the sum over z is bounded uniformly in $x^\star$ due to Lemma 1. The remaining term

is of the same form as that in Theorem 7. We conclude that it approaches zero as $s\to\infty$ uniformly in n. Thus $\gamma_{\omega,s}^{(n)}\to\gamma_{\omega}^{(n)}$ vaguely and uniformly in n, which concludes the proof. □

It now follows from the theorem of Bochner–Schwartz [Reed and Simon (1980), p. 331] that the Fourier transform of the autocorrelation is a positive, translation bounded measure. An explicit expression for the discrete part $(\widehat{\gamma_\omega})_{pp}$ of $\widehat{\gamma_\omega}$, which is given in the following theorem, can be deduced from Hof (1995), Theorem 3.4. The theorem states that the Fourier transform of the autocorrelation measure has no continuous component.

Theorem 10: (Diffraction formula) *Let $f:\mathbb{R}^m\to\mathbb{C}$ be continuous and, for some constants $C>0$ and $\alpha>0$, $|x|^{m+1+\alpha}|f(x)|\leqslant C$. The Fourier transform $\widehat{\gamma_\omega}$ of the autocorrelation γ_ω of the weighted dense Dirac comb ω is a positive, translation bounded pure point measure and explicitly given by*

$$\widehat{\gamma_\omega}=\sum_{k\in L^*}|c(k)|^2\delta_k=\frac{1}{|\det(\tilde{L})|^2}\sum_{k\in L^*}|\hat{f}(-k^\star)|^2\delta_k,$$

where the $\mathbb{Z}$-module L^* is the projection of the dual lattice.

Proof: We showed in the proof of Theorem 9 that the autocorrelation measures $\gamma_{\omega,s}$ converge vaguely to γ_ω. Since the Fourier transform is continuous in the vague topology, the Fourier transforms of the autocorrelation measures $\widehat{\gamma_{\omega,s}}$ converge vaguely to $\widehat{\gamma_\omega}$. We will show that the vague limit leads to the above expression.

Take a compact set $K\subset\mathbb{R}^d$ and a covering $W=\cup_{i=1}^n W_i$ of K with a finite number of translated unit balls W_i. Since $(L^*\cap W)^\star$ is, by duality, a Delone set, we may order the numbers $k\in L^*\cap K$ to obtain a sequence $(k_i)_{i\in\mathbb{N}}$ with $|k_j^\star|\geqslant|k_i^\star|$ for $j>i$. Moreover, since $c_s'(k)\to c(k)$ (in the notation of the proof of Theorem 8), we may choose a subsequence $(s_j)_{j\in\mathbb{N}}$ such that $||c_{s_j}'(k_i)|^2-|c(k_i)|^2|<2^{-i}$ on $L^*\cap K$ for all $j\in\mathbb{N}$. For explicity of notation, we will suppress the index j in the following. Fix $\varepsilon>0$. We have

$$\sum_{i=m+1}^{\infty}|c_s'(k_i)|^2+\sum_{i=m+1}^{\infty}|c(k_i)|^2\leqslant\sum_{i=m+1}^{\infty}2^{-i}+2\sum_{i=m+1}^{\infty}|c(k_i)|^2<\varepsilon$$

for $m>m_0(\varepsilon)$. The last sum can be made arbitrarily small, since it arises from the discrete part of the measure $\widehat{\gamma_\omega}$, see Hof (1995), Theorem 3.4. Moreover, we have $\Sigma_{i=1}^m(|c_s'(k_i)|^2-|c(k_i)|^2)<\varepsilon$ for $s>s_0(\varepsilon,m)$, since $|c_s'(k)|^2\to|c(k)|^2$ uniformly in k. Fix now $m>m_0(\varepsilon)$. For $s>s_0(\varepsilon,m)$, we have

$$\left|\sum_{i=1}^{\infty}|c_s'(k_i)|^2-\sum_{i=1}^{\infty}|c(k_i)|^2\right|\leqslant\sum_{i=m+1}^{\infty}|c_s'(k_i)|^2+\left|\sum_{i=1}^{m}(|c_s'(k_i)|^2-|c(k_i)|^2)\right|+\sum_{i=m+1}^{\infty}|c(k_i)|^2$$
$$\leqslant 2\varepsilon.$$

For g continuous and compactly supported on K, this implies

$$\widehat{\gamma_\omega}(g)=\lim_{s\to\infty}\widehat{\gamma_{\omega,s}}(g)=\lim_{s\to\infty}\sum_{k\in L^*\cap K}|c_s'(k)|^2g(k)=\sum_{k\in L^*\cap K}|c(k)|^2g(k).$$

Since K was an arbitrary compact set, our claim follows. □

The above results lead to a generalized Poisson summation formula. Recall that, for a lattice $L\subset\mathbb{R}^d$, the Poisson summation formula is [Córdoba (1989)]

$$\left(\sum_{x\in L}\delta_x\right)\hat{}=\frac{1}{|\det(L)|}\sum_{k\in L^*}\delta_k,\tag{18}$$

where $|\det(L)|$ is the volume of the fundamental domain of the lattice L, and the sum ranges over all points of the dual lattice L^*. For regular model sets $\Lambda(W)\subset\mathbb{R}^d$, a generalized Poisson formula is given by

$$\left(\sum_{z\in\Delta}\eta(z)\,\delta_z\right)\hat{}=\sum_{k\in L^*}|c_W(k)|^2\,\delta_k, \tag{19}$$

as is readily inferred from Theorem 5. This identity is not symmetric because the first sum ranges over the uniformly discrete set $\Delta=\Lambda(W)-\Lambda(W)$, whereas the second sum ranges over the projection of the dual lattice L^*, which is a dense set. For weighted Dirac combs defined on a dense $\mathbb{Z}$-module $L\subset\mathbb{R}^d$, we obtain from Theorem 10 the formula

$$\left(\sum_{z\in L}\eta(z)\,\delta_z\right)\hat{}=\sum_{k\in L^*}|c(k)|^2\,\delta_k, \tag{20}$$

where the sums on both sides are defined on a dense set. Within this symmetric setup, it may be easier to investigate which constraints on an underlying point set an identity of the above type imposes [Lagarias (2000), Problem 4.1].

IV. APPLICATIONS TO RANDOM TILINGS

In this section, we explain how the above results can be used to infer diffraction properties of random tiling ensembles.

A *tiling* of $\mathbb{R}^d$ is a face-to-face space filling with tiles from a finite set of $\mathbb{R}^d$-polytopes called *prototiles*, without any gaps and overlaps [Richard *et al.* (1998)]. There might be a number of additional packing rules specifying the allowed configurations. Associated with a tiling is the set Λ of all vertex positions of the tiling. Take a ball $B_n\subset\mathbb{R}^d$ of radius n and count the number of different patches of B_n, where we identify patches which are equal up to a translation. If the number of allowed patches increases exponentially with the volume of the ball, we call the set of all tilings a *random tiling* ensemble.

The usual ideal quasiperiodic tilings like the Penrose tiling, the Ammann–Beenker tiling, and others, have the special property that the vertex positions of its tiles form a (regular) model set. Essentially, the set of all tilings is given by the collection of the original model set together with model sets of arbitrarily translated window. For tilings of $\mathbb{R}^d$ whose vertex positions constitute a Delone set and are described by a primitive substitution, it can be shown that the number of allowed patches of radius n grows asymptotically proportional to n^d [Lenz (2002)].

Relaxation of the packing rules for these tilings usually results in a random tiling ensemble with strictly positive entropy [Henley (1999)]. Since entropy is an indication of disorder, one should expect a nonvanishing continuous component in the diffraction spectrum in addition to a discrete part. By construction, the set of vertex positions of each random tiling can be mapped into internal space via the star-map, resulting in a distribution, which may be supported on an unbounded domain in internal space. This is different from the distribution of a model set $\Lambda(W)$, which is the characteristic function 1_W of the window.

A natural object to consider is the *averaged distribution*, where we take the average over all random tilings. Here, we adopt the normalization that $0\in\Lambda$ for all random tilings Λ. The averaged distribution defines a weighted point set of $\mathbb{R}^d$ which is supported on a countable, dense subset of $\mathbb{R}^d$.

Henley (1999) gives nonrigorous arguments that the averaged distribution (for infinite tilings) exists in dimensions $d>2$. In dimensions $d\leqslant 2$, the width of the averaged distribution for finite patches on balls should diverge with the radius n of the ball. In $d=1$, the divergence is with the square root of the system size, in $d=2$, the divergence is logarithmic. He concludes that in dimension $d\leqslant 2$ the diffraction spectrum of a random tiling should have a trivial discrete part.

In $d=1$, his arguments can be made rigorous [Baake *et al.* (2003)]. Consider, for example, the Fibonacci model set. Other tilings may be treated similarly. Let $\mathbb{Z}[\tau]=\mathbb{Z}+\mathbb{Z}\tau\subset\mathbb{R}$, where $\tau=(1+\sqrt{5})/2$ is the golden mean. The ring $\mathbb{Z}[\tau]$ is the ring of integers of the quadratic field $\mathbb{Q}(\tau)=\mathbb{Q}(\sqrt{5})$. Let $(\,)^\star$ denote the automorphism of $\mathbb{Q}(\tau)$ that maps $\sqrt{5}\mapsto-\sqrt{5}$. The set $\tilde{L}=\{(x,x^\star)\,|\,x\in\mathbb{Z}[\tau]\}$ is a lattice in $\mathbb{R}\times\mathbb{R}$. The Fibonacci model set is the set $\Lambda(W)=\{x\in\mathbb{Z}[\tau]\,|\,x^\star\in(-1,\tau-1]\}$. Consecutive points of the model set have distances 1 or τ. If we regard the point positions as left endpoints of half-open intervals u, v of length 1 and τ, we get the *Fibonacci tiling*. A *Fibonacci random tiling* is an arbitrary sequence (a.s.) of intervals u, v such that the frequency of u is a.s. equal to $1/\tau$. The averaged distribution for a patch of size N is, to leading order in N, given by [Höffe (2001), Baake *et al.* (2003)]

$$\rho(x^\star)=\sqrt{\frac{\tau}{2N}}f\left(x^\star\sqrt{\frac{\tau}{2N}}\right),\quad f(z)=2\left(\frac{e^{-z^2}}{\sqrt{\pi}}-|z|\,\mathrm{erfc}(|z|)\right),\tag{21}$$

where $\mathrm{erfc}(x)=(2/\sqrt{\pi})\int_x^\infty e^{-t^2}\,dt$ denotes the complementary error function. The distribution width therefore grows with the system size as $\sqrt{N}$. Together with the above analysis, this may lead to a trivial Bragg peak at the origin as $N\to\infty$. This corresponds to the behavior of the Fibonacci random tiling, whose diffraction spectrum has been computed explicitly [Baake and Höffe (2000)]. It consists of an absolutely continuous component in addition to a trivial Bragg peak at the origin. It would be interesting to compute the continuous component of the averaged structure, which may be given by large N corrections to the asymptotic behavior in Eq. (21).

For $d>1$, there are no rigorous results about the averaged distribution of quasicrystalline random tilings, which is due to more restrictive matching rules for the prototiles. (In $d=1$, the only matching rule is the face-to-face condition, resulting in Bernoulli ensembles, which are easy to analyze.) There are however numerical investigations for a number of quasicrystallographic random tilings in $d=2$ and $d=3$.

In $d=2$, the averaged distribution of the Ammann–Beenker random tiling appears to be of Gaussian type, with a distribution width diverging logarithmically with the system size [Höffe (2001)]. Thus, the situation is similar to the $d=1$ case discussed above. A numerical analysis of the diffraction measure indicates a trivial Bragg peak at the origin, together with a singular continuous component [Höffe (2001)]. This behavior is believed to be generic in $d=2$ [Henley (1999)].

In $d\geqslant 3$, the averaged distribution is predicted to exist [Henley (1999)]. Our result then implies that the averaged structure is pure point diffractive, if the distribution function is well-behaved. However, the diffraction picture of a typical random tiling in $d\geqslant 3$ is expected to display an diffuse background in addition to Bragg peaks [Henley (1999)]. The averaging on the level of the Dirac comb thus has the effect of extinguishing continuous components of the diffraction spectrum.

To conclude, it is necessary to prove Henley's statements about the existence of an averaged distribution with finite width in $d\geqslant 3$. Furthermore, it would be interesting to investigate the relation between diffraction properties of the averaged structure and the random tiling, in particular whether the discrete parts of both structures coincide and whether the continuous parts coincide in $d\leqslant 2$. Concerning the results of this paper, a natural question is how they can be extended beyond the Euclidean case towards the setup of locally compact Abelian groups. (The proofs of the pure pointedness of the diffraction spectrum used the fact that $\mathbb{R}^n$ is isomorphic to its dual.) Another aspect concerns the connection to the theory of almost periodic measures [Gil de Lamadrid and Argabright (1990)], which may also be used for a characterization of diffraction spectra with continuous components.

ACKNOWLEDGMENTS

The author thanks Michael Baake and Moritz Höffe for discussions, and Michael Baake and Bernd Sing for a critical reading of the paper. The author is grateful to the Erwin Schrödinger

International Institute for Mathematical Physics in Vienna for supporting a stay in December 2002, where the paper was completed. Financial support from the German Research Council (DFG) is gratefully acknowledged.

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On the pseudo-Hermitian nondiagonalizable Hamiltonians

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(Received 4 December 2002; accepted 23 June 2003)

We consider a class of (possibly nondiagonalizable) pseudo-Hermitian operators with discrete spectrum, and we establish for such a class the equivalence between the pseudo-Hermiticity property and the existence of an antilinear involutory symmetry. Moreover, we prove that this class actually coincides with the one of (possibly nondiagonalizable) weak pseudo-Hermitian operators, and that in no case (unless they are diagonalizable and have a real spectrum) they are Hermitian with respect to a definite inner product. Finally, we show that a typical degeneracy of the real eigenvalues (which reduces to the well-known Kramers degeneracy in the Hermitian case) occurs whenever a fermionic (possibly nondiagonalizable) pseudo-Hermitian Hamiltonian admits an antilinear symmetry like the time-reversal operator T. Some consequences and applications are briefly discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1609031]

I. INTRODUCTION

Non-Hermitian Hamiltonians play by now a relevant role in physics, in that they appear in several completely different problems.[1] Among them, a remarkable subclass is given by the *pseudo-Hermitian operators*,[2] i.e., those operators which satisfy

$$\eta H \eta^{-1} = H^{\dagger} \tag{1}$$

with $\eta = \eta^{\dagger}$ [instead, whenever (1) holds without any constraint on the (linear and invertible) operator η, H is called *weakly pseudo-Hermitian*[3]]. Of course, Hermiticity is a particular case of pseudo-Hermiticity, corresponding to $\eta = \mathbf{1}$. In particular, in the last several years, the concept of pseudo-Hermiticity has given rise to a growing interest, since it allows one to explain the typical features of PT-symmetric quantum mechanics. Pseudo-Hermiticity also represents the mathematical background of a recent proposal on a *complex extension of Quantum Mechanics*.[4,5]

The essential feature of the pseudo-Hermitian operators is the peculiarity of their spectrum, which can be constituted by real as well as complex (but grouped in complex-conjugate pairs) eigenvalues.[3,6] Another characteristic feature of the pseudo-Hermiticity property is its connection with the existence of antilinear symmetries. The idea of such a connection stemmed naturally from the studies on the PT-symmetric quantum mechanics, as we said above, and it has been already proven in the case of diagonalizable operators.[3,7]

The aim of this paper is just to go on a systematic and deep study on nondiagonalizable, pseudo-Hermitian operators. Such Hamiltonians can arise, for instance, for some critical parameter values, whenever a physical system undergoes a perturbation which preserves the pseudo-Hermiticity, but not the diagonalizability, of its Hamiltonian. An example of such a situation, concerning the effective Hamiltonian for a certain closed FRW mini-super-space-quantum cosmological model, is discussed in Ref. 8; another example is shown in Sec. VI. Furthermore, some cases of nondiagonalizable operators also arise in the classification of the real, 4×4 pseudo-Hermitian energy momentum tensor T^{α}_{β}.[1]

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We recall that the peculiarity of the spectrum of pseudo-Hermitian operators, originally stated with reference to diagonalizable operators with discrete spectrum, has been recently extended to a class of nondiagonalizable Hamiltonians.[8] In particular, in this paper we intend to establish the equivalence of the pseudo-Hermiticity property and the existence of antilinear symmetries for such class of operators.

To this end, we recall (and partly refine) in Sec. II the basic results on this subject, and we show that the (possibly broader) class of weakly pseudo-Hermitian operators with a discrete spectrum actually coincides with the class of pseudo-Hermitian operators. Next, we inquire in Sec. III into the definiteness or the indefiniteness of the metric induced by η, concluding that for any pseudo-Hermitian operator H with discrete spectrum, the metric is always indefinite unless H is diagonalizable with real spectrum. This result disproves a recently stated theorem on the subject.[8]

Successively, in Sec. IV, we take into account the connection between the pseudo-Hermiticity property and the existence of antilinear symmetries, showing that such connection holds also for the nondiagonalizable case. Section V is devoted to a discussion on the time-reversal invariance of fermionic Hamiltonians, extending a result on the (generalized) Kramers degeneracy that we have already proven for diagonalizable operators.[9] Finally, some concluding remarks and possible applications of the previous results are briefly presented in Sec. VI.

II. THE SPECTRUM OF NONDIAGONALIZABLE PSEUDO-HERMITIAN OPERATORS

According to Ref. 8 we consider here only linear operators H acting in a separable Hilbert space $\mathfrak{H}$ and having discrete spectrum. Moreover, throughout this paper we shall assume that all the eigenvalues E_n of H have finite algebraic multiplicity g_n and that there is a basis of $\mathfrak{H}$ in which H is block diagonal with finite-dimensional diagonal blocks. Then, a complete biorthonormal basis $\mathfrak{E}=\{|\psi_n,a,i\rangle,|\phi_n,a,i\rangle\}$ exists such that the operator H can be written in the following form:[8]

$$H=\sum_n \sum_{a=1}^{d_n} \left(E_n \sum_{i=1}^{p_{n,a}} |\psi_n,a,i\rangle\langle\phi_n,a,i| + \sum_{i=1}^{p_{n,a}-1} |\psi_n,a,i\rangle\langle\phi_n,a,i+1| \right), \tag{2}$$

where d_n denotes the geometric multiplicity (i.e., the degree of degeneracy) of E_n, a is a degeneracy label and $p_{n,a}$ represents the dimension of the simple Jordan block $J_a(E_n)$ associated with the labels n and a (hence, $\Sigma_{a=1}^{d_n} p_{n,a}=g_n$). Furthermore, we denote by $k(n,a)$ the total number of identical simple blocks $J_a(E_n)$ occurring in the above decomposition of H.

Hence, $|\psi_n,a,1\rangle$ (respectively, $|\phi_n,a,p_{n,a}\rangle$) is an eigenvector of H (respectively, $H^\dagger$):

$$H|\psi_n,a,1\rangle=E_n|\psi_n,a,1\rangle, \quad H^\dagger|\phi_n,a,p_{n,a}\rangle=E_n^*|\phi_n,a,p_{n,a}\rangle, \tag{3}$$

and the following relations hold:

$$H|\psi_n,a,i\rangle=E_n|\psi_n,a,i\rangle+|\psi_n,a,i-1\rangle, \quad i\neq 1, \tag{4}$$

$$H^\dagger|\phi_n,a,i\rangle=E_n^*|\phi_n,a,i\rangle+|\phi_n,a,i+1\rangle, \quad i\neq p_{n,a}. \tag{5}$$

The elements of the biorthonormal basis obey the usual relations

$$\langle\psi_m,a,i|\phi_n,b,j\rangle=\delta_{mn}\delta_{ab}\delta_{ij}, \tag{6}$$

$$\sum_n \sum_{a=1}^{d_n} \sum_{i=1}^{p_{n,a}} |\psi_n,a,i\rangle\langle\phi_n,a,i| = \sum_n \sum_{a=1}^{d_n} \sum_{i=1}^{p_{n,a}} |\phi_n,a,i\rangle\langle\psi_n,a,i| = \mathbf{1}. \tag{7}$$

The following theorem has been proven in Ref. 8:

Theorem 1: *Let H be a linear operator acting in a Hilbert space $\mathfrak{H}$. Suppose that the spectrum of H is discrete, that its eigenvalues have finite algebraic multiplicity, and that (2) holds. Then, the following conditions are equivalent:*

(i) *the eigenvalues of H are either real or come in complex-conjugate pairs and the geometric multiplicity and the Jordan dimensions of the complex-conjugate eigenvalues coincide;*
(ii) *H is pseudo-Hermitian.*

In order to fix our notation, and for the benefit of the reader, we prefer to provide here a (somewhat different) proof of the implication (i)⇒(ii), which allows us to obtain a useful decomposition of η.

Let us therefore assume that condition (i) holds, and use (whenever it is necessary) the subscript "0" to denote real eigenvalues, and the subscripts "±" to denote the complex eigenvalues with positive or negative imaginary part, respectively. Then, H assumes the following form [see Eq. (2)]:

$$\begin{aligned} H=&\sum_{n_0}\sum_{a=1}^{d_{n_0}}\left(E_{n_0}\sum_{i=1}^{p_{n_0,a}}|\psi_{n_0},a,i\rangle\langle\phi_{n_0},a,i|+\sum_{i=1}^{p_{n_0,a}-1}|\psi_{n_0},a,i\rangle\langle\phi_{n_0},a,i+1|\right)\\ &+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\left[\sum_{i=1}^{p_{n_+,a}}(E_{n_+}|\psi_{n_+},a,i\rangle\langle\phi_{n+},a,i|+E_{n_-}|\psi_{n_-},a,i\rangle\langle\phi_{n_-},a,i|)\right.\\ &\left.+\sum_{i=1}^{p_{n_+,a}-1}(|\psi_{n_+},a,i\rangle\langle\phi_{n+},a,i+1|+|\psi_{n_-},a,i\rangle\langle\phi_{n_-},a,i+1|)\right]. \end{aligned} \tag{8}$$

Furthermore, given any complete orthonormal basis $\mathfrak{F}=\{|u_n,a,i\rangle\}$ in our space (that we denote by the same n,a,i labels used for the elements of $\mathfrak{E}$), let us pose

$$S=\sum_n\sum_{a=1}^{d_n}\sum_{i=1}^{p_{n,a}}|\phi_n,a,i\rangle\langle u_n,a,i|, \tag{9}$$

and $\tilde{H}=S^\dagger HS^{\dagger-1}$. By a straightforward calculation one obtains

$$\begin{aligned} \tilde{H}=&\sum_{n_0}\sum_{a=1}^{d_{n_0}}\left(E_{n_0}\sum_{i=1}^{p_{n_0,a}}|u_{n_0},a,i\rangle\langle u_{n_0},a,i|+\sum_{i=1}^{p_{n_0,a}-1}|u_{n_0},a,i\rangle\langle u_{n_0},a,i+1|\right)\\ &+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\left[\sum_{i=1}^{p_{n_+,a}}(E_{n_-}|u_{n_+},a,i\rangle\langle u_{n+},a,i|+E_{n_+}|u_{n_-},a,i\rangle\langle u_{n_-},a,i|)\right.\\ &\left.+\sum_{i=1}^{p_{n_+,a}-1}(|u_{n_+},a,i\rangle\langle u_{n+},a,i+1|+|u_{n_-},a,i\rangle\langle u_{n_-},a,i+1|)\right]. \end{aligned} \tag{10}$$

Then, let us consider the involutory operators U and V defined, respectively, as follows:

$$U|u_{n_\pm},a,i\rangle=|u_{n_\mp},a,i\rangle,\quad U|u_{n_0},a,i\rangle=|u_{n_0},a,i\rangle, \tag{11}$$

and

$$V|u_n,a,i\rangle=|u_n,a,p_{n,a}+1-i\rangle. \tag{12}$$

The explicit forms of U and V are

$$U=U\mathbf{1}=\sum_{n_0,a,i}|u_{n_0},a,i\rangle\langle u_{n_0},a,i|+\sum_{n_+,n_-,a,i}(|u_{n_-},a,i\rangle\langle u_{n_+},a,i|+|u_{n_+},a,i\rangle\langle u_{n_-},a,i|) \tag{13}$$

and

$$V=V\mathbf{1}=\sum_{n_0,a,i}|u_{n_0},a,p_{n_0,a}+1-i\rangle\langle u_{n_0},a,i|$$
$$+\sum_{n_+,n_-,a,i}(|u_{n_+},a,p_{n_+,a}+1-i\rangle\langle u_{n_+},a,i|+|u_{n_-},a,p_{n_-,a}+1-i\rangle\langle u_{n_-},a,i|). \tag{14}$$

Moreover both U and V are clearly Hermitian operators, and (recalling that, by hypothesis, $p_{n_+,a}=p_{n_-,a}$)

$$UV=UV\mathbf{1}=\sum_{n_0}\sum_{a=1}^{d_{n_0}}\sum_{i=1}^{p_{n_0,a}}|u_{n_0},a,p_{n_0,a}+1-i\rangle\langle u_{n_0},a,i|$$
$$+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\sum_{i=1}^{p_{n_+,a}}(|u_{n_+},a,p_{n_+,a}+1-i\rangle\langle u_{n_-},a,i|+|u_{n_-},a,p_{n_-,a}+1-i\rangle\langle u_{n_+},a,i|)$$
$$=VU.$$

Thus, one can easily verify that $\tilde{H}$ is a pseudo-Hermitian operator:

$$\tilde{\eta}\tilde{H}\tilde{\eta}^{-1}=\tilde{H}^\dagger,$$

where $\tilde{\eta}=UV$. Hence, finally,

$$\eta H\eta^{-1}=H^\dagger,$$

where

$$\eta=S\tilde{\eta}S^\dagger=SUVS^\dagger=\sum_{n_0}\sum_{a=1}^{d_{n_0}}\sum_{i=1}^{p_{n_0,a}}|\phi_{n_0},a,p_{n_0,a}+1-i\rangle\langle\phi_{n_0},a,i|$$
$$+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\sum_{i=1}^{p_{n_+,a}}(|\phi_{n_+},a,p_{n_+,a}+1-i\rangle\langle\phi_{n_-},a,i|$$
$$+|\phi_{n_-},a,p_{n_-,a}+1-i\rangle\langle\phi_{n_+},a,i|)$$
$$=\eta^\dagger. \tag{15}$$

In conclusion we see that *the spectrum of a pseudo-Hermitian operator is real if and only if* $U\equiv\mathbf{1}$ *[hence, by Eq. (15),* $\eta=SVS^\dagger$*],* and that *a pseudo-Hermitian operator is diagonalizable if and only if* $V\equiv\mathbf{1}$ *[hence, again by Eq. (15),* $\eta=SUS^\dagger$*].*

Remark: We stress here that in order to prove the implication (ii)⇒(i) only the invertibility of η is needed, while the Hermiticity property $\eta=\eta^\dagger$ does not come into play.[8] Hence, by the same arguments one can prove that even the spectrum of a *weakly pseudo-Hermitian* operator[3] [i.e., an operator which satisfies Eq. (1) without any constraint on the (linear and invertible) operator η],

satisfies condition (i). On the other hand, the above proof shows that condition (i) implies that an Hermitian operator η exists which fulfils Eq. (1). Thus, if we just consider operators having a discrete spectrum, the (possibly broader) class of weakly pseudo-Hermitian operators actually coincides with the one of pseudo-Hermitian operators. (This fact was already pointed out for diagonalizable operators.[3,10]) Nevertheless, we recall that the weak pseudo-Hermiticity is a more useful notion, in that, for instance, it simplifies checking Eq. (1).

III. NONDIAGONALIZABILITY AND METRIC INDEFINITENESS

We have seen in the preceding section that an Hermitian operator η always exists such that a nondiagonalizable operator H [whose spectrum obeys condition (i) in Theorem 1] is pseudo-Hermitian; moreover, it is well known that in this case one can define a new inner product,[8]

$$\langle\langle \psi, \phi \rangle\rangle_\eta := \langle \psi | \eta | \phi \rangle, \tag{16}$$

and, correspondingly, a η-pseudonorm $\langle\langle \psi, \psi \rangle\rangle_\eta$. Then, one may of course inquire into the definiteness or the indefiniteness of the metric induced by $\langle\langle ,\rangle\rangle_\eta$.

Equation (15) in the preceding section clearly shows that the metric associated with such an η cannot be a definite (nor a semidefinite) operator; indeed, being $\tilde{\eta}$ involutory and nonidentical (unless H is a diagonalizable operator with real spectrum), some of its eigenvalues (but not all) must be negative, hence the same happens (by the Sylvester's law of inertia[11]) for the eigenvalues of the operator η. This fact can suggest that in all cases of nondiagonalizable (or else, diagonalizable with complex spectrum) pseudo-Hermitian operators, the metric must be indefinite; however, as Eq. (15) does not provide us the more general form of η, we must resort to some other argument in order to confirm this conjecture.

Let us then consider the simplest 2×2 nondiagonalizable operator A:

$$A = \begin{pmatrix} E & 1 \\ 0 & E \end{pmatrix} (E \in \mathbf{R}).$$

A is clearly pseudo-Hermitian and, by a straightforward calculation, one can easily verify that the *most general* operator η which fulfils Eq. (1) is

$$\eta = \begin{pmatrix} 0 & k \\ k & k' \end{pmatrix} \quad (k \neq 0);$$

moreover $\eta = \eta^\dagger$, if and only if, $k, k' \in \mathbf{R}$, and in this case the eigenvalues of η have with certainty opposite signs. Obviously the same happens for the η-pseudonorm of the corresponding eigenvectors; hence some state exists with a negative η-pseudonorm, besides other states with a positive η-pseudonorm.

This simple example disproves a recently stated theorem according to which "(a nondiagonalizable operator) *H is pseudo-Hermitian if and only if it is Hermitian with respect to a positive semidefinite inner product.*" [8]

Actually, the following theorem holds.

Theorem 2: *Let H be an operator with discrete spectrum. Then, there exists a definite operator η such that H is η-pseudo-Hermitian if and only if H is diagonalizable with real spectrum.*

Proof: Let H be a pseudo-Hermitian operator. We preliminarily observe that, being in any case η an invertible operator, all its eigenvalues must be different from zero, so that the metric induced by the inner product (16) either is definite or is indefinite. Now, let us suppose that a positive (respectively, negative) definite operator η exists which fulfils condition (1); then, an R exists such that $\eta = R^\dagger R$ (respectively, $\eta = -R^\dagger R$),[11] and by Eq. (1) we obtain

$$RHR^{-1} = R^{\dagger -1} H^\dagger R^\dagger = (RHR^{-1})^\dagger,$$

i.e., RHR^{-1} is Hermitian, hence it is diagonalizable and it has a real spectrum. Since the similarity transformations preserve the properties of the spectrum, the same occurs for H. Conversely, if H is diagonalizable with real spectrum, then by Eq. (15) in the preceding section a positive definite metric $\eta=SS^{\dagger}$ exists which fulfils condition (1) (since in this case $U=V\equiv\mathbf{1}$). ■

We recall that the equivalence between the definiteness of a suitable η and the reality of the spectrum of H was already proven for diagonalizable operators.[6]

IV. NONDIAGONALIZABLE OPERATORS AND ANTILINEAR SYMMETRIES

A very intriguing feature of the pseudo-Hermiticity property is its connection with the existence of antilinear symmetries. This connection was already acknowledged to hold in the case of diagonalizable operators with discrete spectrum;[3,7] indeed, the pseudo-Hermiticity property is a necessary and sufficient condition for a (diagonalizable) operator H to admit an antilinear (involutory) symmetry.[3] Considering the great physical interest in the study of such symmetries (we recall that the time-reversal symmetry is associated, in complex quantum mechanics, with an antilinear operator), we intend here to inquire the above-mentioned connection in the case of nondiagonalizable pseudo-Hermitian operators. To this end, let us premise a definition.

Definition (Ref. 12): Given the complete orthonormal basis $\mathfrak{F}=\{|u_m,a,i\rangle\}$ *in a Hilbert space, we call* conjugation *associated with it the involutory antilinear operator*

$$\Theta_{\mathfrak{F}}=\sum_{m,a,i}|u_m,a,i\rangle K\langle u_m,a,i|, \tag{17}$$

where the operator K acts transforming each complex number on the right into its complex conjugate.

Analogously, in the case of a complete biorthonormal basis $\mathfrak{E}=\{|\psi_n,a,i\rangle,|\phi_n,a,i\rangle\}$, we call conjugation associated with it the involutory antilinear operator[3]

$$\Theta_{\mathfrak{E}}=\sum_{n,a,i}|\psi_n,a,i\rangle K\langle\phi_n,a,i|. \tag{18}$$

Then, the following theorem holds.

Theorem 3: *Let H be a linear operator. Suppose that the spectrum of H is discrete, that its eigenvalues have finite algebraic multiplicity and that (2) holds. Then the following conditions are equivalent:*

(i) *an antilinear invertible operator* Ω *exists such that* $[H,\Omega]=0$*;*
(ii) *H is (weakly) pseudo-Hermitian;*
(iii) *an antilinear involutory operator* $\hat{\Omega}$ *exists such that* $[H,\hat{\Omega}]=0$*;*
(iv) *a basis exists in which H assumes a real form.*

Proof: (i)⇒(ii) Let Ω exist such that $[H,\Omega]=0$. This implies that $[\tilde{H},\tilde{\Omega}]=0$, where $\tilde{H}=S^{\dagger}HS^{\dagger-1}$ and $\tilde{\Omega}=S^{\dagger}\Omega S^{\dagger-1}$. Then, the linear operator

$$\tilde{\eta}=V\Theta_{\mathfrak{F}}\tilde{\Omega}$$

[where $\mathfrak{F}$ is the orthonormal basis associated with $\tilde{H}$ [see Eq. (10)], while V and $\Theta_{\mathfrak{F}}$ are defined as in Eqs. (12) and (17), respectively] fulfils the condition stated by Eq. (1), hence $\tilde{H}$ is (weakly) pseudo-Hermitian; indeed,

$$
\begin{aligned}
&V\Theta_{\mathfrak{F}}\tilde{\Omega}\tilde{H}\tilde{\Omega}^{-1}\Theta_{\mathfrak{F}}^{-1}V^{-1}\\
&\quad=V\Theta_{\mathfrak{F}}\tilde{H}\Theta_{\mathfrak{F}}V\\
&\quad=\sum_{n_0}\sum_{a=1}^{d_{n_0}}\left(E_{n_0}\sum_{i=1}^{p_{n_0,a}}|u_{n_0},a,i\rangle\langle u_{n_0},a,i|+\sum_{i=1}^{p_{n_0,a}-1}|u_{n_0},a,i+1\rangle\langle u_{n_0},a,i|\right)\\
&\qquad+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\left[\sum_{i=1}^{p_{n_+,a}}(E_{n_+}^{*}|u_{n_+},a,i\rangle\langle u_{n+},a,i|+E_{n_+}|u_{n_-},a,i\rangle\langle u_{n_-},a,i|)\right.\\
&\qquad\left.+\sum_{i=1}^{p_{n_+,a}-1}(|u_{n_+},a,i+1\rangle\langle u_{n_+},a,i|+|u_{n_-},a,i+1\rangle\langle u_{n_-},a,i|)\right]=\tilde{H}^{\dagger}.
\end{aligned}
$$

Finally, posing $\eta=S\tilde{\eta}S^{\dagger}=SV\Theta_{\mathfrak{F}}S^{\dagger}\Omega$ one obtains

$$\eta H\eta^{-1}=SV\Theta_{\mathfrak{F}}S^{\dagger}\Omega H(SV\Theta_{\mathfrak{F}}S^{\dagger}\Omega)^{-1}=S\tilde{H}^{\dagger}S^{-1}=H^{\dagger}.$$

(ii)⇒(iii). If H is (weakly) pseudo-Hermitian, the eigenvalues of H are either real or come in complex-conjugate pairs and the geometric multiplicity and the Jordan dimensions of the complex-conjugate eigenvalues coincide (see the remark below Theorem 1). Then, one can easily see, recalling the definition of the operator U provided in the proof of Theorem 1 [Eq. (11)] and Eqs. (10) and (17), that

$$\Theta_{\mathfrak{F}}\tilde{H}\Theta_{\mathfrak{F}}=U\tilde{H}U.$$

Hence the antilinear operator

$$
\begin{aligned}
\tilde{\Omega}=\Theta_{\mathfrak{F}}U=U\Theta_{\mathfrak{F}}=&\sum_{n_0}\sum_{a=1}^{d_{n_0}}\sum_{i=1}^{p_{n_0,a}}|u_{n_0},a,i\rangle K\langle u_{n_0},a,i|\\
&+\sum_{n_+,n_-}\sum_{a=1}^{d_{n_+}}\sum_{i=1}^{p_{n_+,a}}(|u_{n_+},a,i\rangle K\langle u_{n_-},a,i|+|u_{n_-},a,i\rangle K\langle u_{n_+},a,i|)
\end{aligned}
$$

commutes with $\tilde{H}$. Moreover, $\tilde{\Omega}$ is involutory, as one can immediately verify by using the explicit expression of $\tilde{\Omega}$ in the previous equation. Then, it follows immediately [recalling Eq. (18) and observing that $\Theta_{\mathfrak{F}}S^{\dagger}=S^{\dagger}\Theta_{\mathfrak{E}}$] that

$$\hat{\Omega}=S^{\dagger-1}\tilde{\Omega}S^{\dagger}=S^{\dagger-1}U\Theta_{\mathfrak{F}}S^{\dagger}=S^{\dagger-1}US^{\dagger}\Theta_{\mathfrak{E}} \tag{19}$$

commutes with H and is involutory.

(iii)⇒(iv). (See Prop. 5 in Ref. 3, where an analogous statement has been proven, referring to diagonalizable operators.)

If we denote by L the linear part of $\hat{\Omega}$, i.e., $\hat{\Omega}=LK$ (where K is the complex conjugation operator), then $\hat{\Omega}^2=\mathbf{1}$ implies $LL^{*}=\mathbf{1}$ and this is possible if and only if an M exists such that $L=MM^{*-1}$.[12] Then $[H,\hat{\Omega}]=0$ implies $HMM^{*-1}=MM^{*-1}H^{*}$, hence

$$M^{-1}HM=(M^{*-1}H^{*}M^{*})=(M^{-1}HM)^{*}.$$

(iv)⇒(i) Trivially, every operator which assumes a real form in some basis $\mathfrak{B}$ commutes with the conjugation associated with $\mathfrak{B}$. ■

Remark: Note that the equivalence (i)⇔(iv) that we prove above clearly restates precisely a similar (seemingly, more general) result in literature, according to which *whenever H commutes with an antiunitary symmetry A such that $A^{2k}=1$ (k odd), it is possible to construct a basis in which the matrix elements of H are real*.[13]

V. THE KRAMERS DEGENERACY

On the basis of the above-stated theorem [in particular, by the implication (i)⇒(ii)] one can conclude that any time-reversal invariant (diagonalizable or not) Hamiltonian H must belong to the class of pseudo-Hermitian Hamiltonians. The converse does not hold in general, since one cannot always interpret the antilinear symmetry Ω of H as the time-reversal operator T; furthermore, it is well known that in case of fermionic systems

$$T^2=-\mathbf{1}$$

and the above theorem, whereas it assures the existence of an involutory antilinear symmetry, does not say anything about the existence of a symmetry like T.

In order to go more deeply into the matter, we can now state the following.

Theorem 4: *Let H be a linear operator with a discrete spectrum. Then, the following conditions are equivalent:*

(i) an antilinear operator $\mathfrak{T}$ exists such that $[H,\mathfrak{T}]=0$, with $\mathfrak{T}^2=-1$;

(ii) H is pseudo-Hermitian and the Jordan blocks associated with any real eigenvalue occur in pair [i.e., for any couple E_{n_0},a, the number $k(n_0,a)$ is even (see Sec. II)].

Proof: Let us assume that condition (i) holds; then, by Theorem 3, H is pseudo-Hermitian, hence its eigenvalues are either real or come in complex-conjugate pairs and the geometric multiplicity and the Jordan dimensions of the complex-conjugate eigenvalues coincide (see Theorem 2).

Let now $|\psi_{n_0},a,1\rangle$ be an eigenvector of H; then, $\mathfrak{T}|\psi_{n_0},a,1\rangle$ too is an eigenvector of H, corresponding to the same eigenvalue E_{n_0}, and linearly independent from $|\psi_{n_0},a,1\rangle$. (Indeed, assume that $\mathfrak{T}\ |\psi_{n_0},a,1\rangle=\alpha|\psi_{n_0},a,1\rangle$ for some $\alpha\in\mathbf{C}$; applying $\mathfrak{T}$ one gets $|\psi_{n_0},a,1\rangle=-|\alpha|^2|\psi_{n_0},a,1\rangle$, which is impossible.)

If $|\psi_{n_0},b,1\rangle$ is another eigenvector of H, linearly independent from $|\psi_{n_0},a,1\rangle$ and $\mathfrak{T}|\psi_{n_0},a,1\rangle$, also $\mathfrak{T}|\psi_{n_0},b,1\rangle$ is linearly independent from all three; otherwise, applying once again $\mathfrak{T}$ to the relation

$$\alpha|\psi_{n_0},a,1\rangle+\beta\mathfrak{T}|\psi_{n_0},a,1\rangle+\gamma|\psi_{n_0},b,1\rangle+\delta\mathfrak{T}|\psi_{n_0},b,1\rangle=0$$

we could eliminate, for instance, $\mathfrak{T}|\psi_{n_0},b,1\rangle$, thus obtaining a linear dependence between $|\psi_{n_0},a,1\rangle$, $\mathfrak{T}|\psi_{n_0},a,1\rangle$, and $|\psi_{n_0},b,1\rangle$, contrary to the previous hypothesis.

We can conclude, iterating this procedure, that the geometric multiplicity d_{n_0} of E_{n_0} must be necessarily even. Moreover, one can always assume that, for a suitable choice of the basis vectors, $\mathfrak{T}|\psi_{n_0},a,1\rangle\equiv|\psi_{n_0},a',1\rangle$ for some a'.

Let us consider now the subset of vectors $\{|\psi_{n_0},a,i\rangle,i=1,\ldots,p_{n_0,a}\}$. They constitute a basis in the subspace associated with the Jordan block $J_a(E_{n_0})$; then by hypothesis one has

$$\sum_{i=1}^{p_{n_0,a}}\alpha_i|\psi_{n_0},a,i\rangle=0\Leftrightarrow\alpha_i=0\ \forall i=1,\ldots,p_{n_0,a}.$$

Applying $\mathfrak{T}$ to the previous equation, one obtains

$$\sum_{i=1}^{p_{n_0,a}} \alpha_i^* \mathfrak{T}|\psi_{n_0},a,i\rangle = 0 \Leftrightarrow \alpha_i = 0 \ \forall i = 1,\ldots,p_{n_0,a},$$

hence, the vectors $\{\mathfrak{T}|\psi_{n_0},a,i\rangle \equiv |\psi_{n_0},a',i\rangle, i=1,\ldots,p_{n_0,a}\}$ too are linearly independent, and $p_{n_0,a} = \dim J_a(E_{n_0}) \leqslant p_{n_0,a'} = \dim J_{a'}(E_{n_0})$. On the other hand, applying $\mathfrak{T}$ to the basis vectors $\{\mathfrak{T}|\psi_{n_0},a,i\rangle\}$ of the subspace associated with $J_{a'}(n_0)$, one obtains that the dimensions of the two blocks must coincide, hence $J_a(n_0)$ and $J_{a'}(n_0)$ are identical.

[Alternatively, the same result can be obtained by applying $\mathfrak{T}$ to both members of Eq. (4).]

Conversely, let condition (ii) hold; then H assumes the form

$$\begin{aligned} H = \sum_{n_0} \sum_{a=1}^{d_{n_0}/2} \Bigg[& E_{n_0} \sum_{i=1}^{p_{n_0,a}} (|\psi_{n_0},a,i\rangle\langle\phi_{n_0},a,i| + |\psi_{n_0},a+d_{n_0,a}/2,i\rangle\langle\phi_{n_0},a+d_{n_0,a}/2,i|) \\ & + \sum_{i=1}^{p_{n_0,a-1}} (|\psi_{n_0},a,i\rangle\langle\phi_{n_0},a,i+1| + |\psi_{n_0},a+d_{n_0,a}/2,i\rangle\langle\phi_{n_0},a+d_{n_0,a}/2,i+1|) \Bigg] \\ & + \sum_{n_+,n_-} \sum_{a=1}^{d_{n+}} \Bigg[\sum_{i=1}^{p_{n_+,a}} (E_{n_+}|\psi_{n_+},a,i\rangle\langle\phi_{n+},a,i| + E_{n_+}^*|\psi_{n_-},a,i\rangle\langle\phi_{n_-},a,i|) \\ & + \sum_{i=1}^{p_{n_+,a-1}} (|\psi_{n_+},a,i\rangle\langle\phi_{n+},a,i+1| + |\psi_{n_-},a,i\rangle\langle\phi_{n_-},a,i+1|) \Bigg]. \end{aligned}$$

Let us denote by $\mathfrak{T}$ the following antilinear operator:

$$\begin{aligned} \mathfrak{T} = \sum_{n_0} \sum_{a=1}^{d_{n_0}/2} \sum_{i=1}^{p_{n_0,a}} & (|\psi_{n_0},a,i\rangle K\langle\phi_{n_0},a+d_{n_0,a}/2,i| - |\psi_{n_0},a+d_{n_0,a}/2,i\rangle K\langle\phi_{n_0},a,i|) \\ & + \sum_{n_+,n_-} \sum_{a=1}^{d_{n+}} \sum_{i=1}^{p_{n_+,a}} (|\psi_{n_-},a,i\rangle K\langle\phi_{n+},a,i| - |\psi_{n_+},a,i\rangle K\langle\phi_{n_-},a,i|), \end{aligned} \tag{20}$$

where the operator K acts transforming each complex number on the right into its complex conjugate. Then, one easily obtains, by inspection, that $[H,\mathfrak{T}]=0$ and $\mathfrak{T}^2 = -\mathbf{1}$. ■

Recalling that the algebraic multiplicity of any E_n is $g_n = \sum_{a=1}^{d_n} p_{n,a}$, from Theorem 4 in particular it follows that whenever *a pseudo-Hermitian operator H admits an antilinear symmetry* $\mathfrak{T}$ *with* $\mathfrak{T}^2 = -1$, *both the geometric and the algebraic multiplicity of any real eigenvalue of H is even*.

The above-mentioned theorem generalizes an analogous theorem stated from the authors (and referring to diagonalizable pseudo-Hermitian operators),[9] which in turn generalizes from various points of view the Kramers theorem on the degeneracy of any fermionic (Hermitian) Hamiltonian. Hence, by an abuse of language, we will continue to denote as "*Kramers degeneracy*" this typical feature of real eigenvalues of pseudo-Hermitian operators admitting a symmetry like $\mathfrak{T}$.

VI. CONCLUDING REMARKS

Basing on Theorem 4, we can quickly test the T-invariance properties of pseudo-Hermitian Hamiltonians. Indeed, let us consider for instance the operator

$$H_{\text{eff}} = \begin{pmatrix} E & ir \\ is & E \end{pmatrix} (E,r,s \in \mathbf{R})$$

which we already discussed elsewhere,[9] and which arises in the modified Mashhoon model,[14] where one introduces a (T-violating) spin-rotation coupling to explain the muon's anomalous g factor.

This Hamiltonian (as long as it is diagonalizable and $rs<0$) is time-reversal violating;[9] however, for some choice of parameter values (for instance, $r\neq s=0$), H_{eff} is no longer diagonalizable. Now, on the basis of Theorem 4 we can conclude that also for such values H_{eff} cannot admit an antilinear symmetry $\mathfrak{T}$ such that $\mathfrak{T}^2=-\mathbf{1}$ (hence, H_{eff} cannot be T-invariant). In fact, being the geometric multiplicity of its eigenvalue E odd, condition (ii) of Theorem 4 does not hold. We recall however that we obtained the same result by a straightforward calculation.[9]

Finally, we note that in a symmetry-adapted basis $\{|\psi_n\rangle,\mathfrak{T}|\psi_n\rangle\}$ the matrix of any pseudo-Hermitian operator H, satisfying condition (ii) of Theorem 4, assumes a symplectic form. This property, in the Hermitian case, is often used in order to simplify some electronic-structure calculations occurring for instance in molecular or solid-state physics.[15]

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Potential and field singularity at a surface point charge

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(Received 14 May 2003; accepted 13 June 2003)

The behavior of the magnetic potential near a point charge (fluxon) located at a curved regular boundary surface is shown to be essentially different from that of a volume point charge. In addition to the usual inverse distance singularity, two singular terms are generally present. The first of them, a logarithmic one, is axially symmetric with respect to the boundary normal at the charge location, and proportional to the sum of the two principal curvatures of the boundary surface at this point, that is, to the local mean curvature. The second term is asymmetric and proportional to the difference of the two principal curvatures in question; it is also bounded at the charge location. Both terms vanish, apparently, if the charge is at a planar point of the boundary, and only in this case. The field in the charge vicinity behaves accordingly, featuring generally two singular terms proportional to the inverse distance, in addition to the main inverse distance squared singularity. This result is significant, in particular, for studying the interaction of magnetic vortices in type II superconductors. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1605497]

Magnetic vortex lines are formed in type II superconductors.[1] When crossing the superconductor boundary, they create strongly localized surface sources of magnetic field (fluxons), which may play an important role in various physical situations. For instance, two space tests of Einstein's General Relativity, Gravity Probe B,[2,3] and STEP (Space Test of the Equivalence Principle),[4] are based on low temperature technology with type II superconductors, and their setup is significantly affected by fluxons.

The size of a surface magnetic spot is about the microscopic London length,[1] i.e., it is typically much smaller than characteristic macroscopic sizes involved. Thus the *point charge* approximation appears naturally and proves to be sufficient for many applications. Within this approximation, the magnetic potential, $\psi=\psi(\mathbf{R})$, satisfies the Neumann boundary value problem

$$\Delta\psi=0, \quad \mathbf{R}\in D, \tag{1}$$

$$\left.\frac{\partial\psi}{\partial n}\right|_S=\sum_{j=1}^{N}\nu_j\Phi_0\delta_S(\mathbf{R}-\mathbf{R}_j), \quad \mathbf{R},\mathbf{R}_j\in S\,. \tag{2}$$

Here the domain D is the empty space, surface S is the superconductor boundary, $\Phi_0=h/2e$ is the

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magnetic flux quantum in SI units, and the magnetic field is $\mathbf{B}=-\nabla\psi$. Moreover, $\delta_S(\mathbf{R}-\mathbf{R}_j)$ denotes the surface delta-function at the position, $\mathbf{R}_j$, of a vortex, and ν_j is either plus or minus one, depending on whether the field line enters the domain D ($\nu_j=+1$), or exits it ($\nu_j=-1$). We assume that the boundary S is smooth enough (at least C^3) near every charge. Outside the charge vicinities it may have any singularities compatible with the finite local energy condition, meaning $(\nabla\psi)^2$ is locally integrable.

If D is bounded, then each vortex line starts and ends at the boundary, the number of charges is even, and the total charge vanishes, $\Sigma_{j=1}^{N}\nu_j\Phi_0=0$, which condition is the solvability criterion of the problem, Eqs. (1) and (2). If the domain D is infinite, some field lines may end at infinity, and this condition may not hold; in any case, we do not use it in the following analysis, which is entirely local.

An immediate question regarding the above boundary value problem is how does its solution behave near a surface charge? For a curved boundary, an answer based on the similarity with the volume point charge turns out incorrect. This is seen from the simplest example, a spherical domain. A closed-form exact solution to Eqs. (1) and (2) in the exterior of a sphere was obtained in Ref. 5. It shows that a new logarithmic singular term, inversely proportional to the radius of the sphere, is added to the main inverse distance singularity in the expansion of the potential near the charge. So, what happens with the singularity for a generally curved smooth surface?

Our search for the answer to this natural and, in fact, classical question covered books and papers in both mathematical physics and in the field of vortices in superconductors, as well as communications with colleagues in both fields. We also talked with high energy theorists expecting to find perhaps some relevant results in view of the discussions of the magnetic monopole. However, no ready answer was found, which might not be so surprising. Indeed, the Neumann boundary value problem with surface charges is not relevant to the design of electrostatic systems. On the other hand, its magnetostatic implementation became available only with the widespread technical use of superconductors in the recent years. Last but not least, the answer proves to be not that simple.

In this paper we fill the gap by deriving a complete singular part of the expansion of the solution to Eqs. (1) and (2) near a charge at an arbitrary curved smooth boundary. As compared to the case of a sphere, one more singular term, proportional to the difference of the two principal curvatures, appears in the general case.

We are interested in the behavior of the potential near a single surface charge at some $\mathbf{R}_j$. For brevity, we thus drop the charge index in the following calculation. We put the origin of a Cartesian coordinate system at $\mathbf{R}_j$, so that $\mathbf{r}\equiv\mathbf{R}-\mathbf{R}_j$. We point the z axis along the outward normal to the surface S (that is, into the superconducting bulk), choosing the x and y axes in the tangent plane, so that the unit vectors $\{\hat{x},\hat{y},\hat{z}\}$ form a right orthogonal triplet. Along with Cartesian $\{x, y, z\}$, we will use the corresponding spherical, $\{r, \theta, \phi\}$, and cylindrical, $\{\rho, \phi, z\}$, coordinate systems (see Fig. 1).

The shape of the smooth boundary surface in the vicinity of the charge can be described by the equation $z=F(x,y)$. The Taylor expansion of the function $F(x,y)$ around $x=y=0$ apparently has no terms linear in x or y, since z is oriented along the normal. Moreover, by an appropriate rotation of the coordinate axes $\hat{x},\hat{y}$ in the tangent plane, we can ensure that the second cross-derivative of F vanishes at the origin, hence the expansion acquires the form

$$z=F(x,y)=\frac{k^{(x)}}{2}x^2+\frac{k^{(y)}}{2}y^2+O(\rho^3)\equiv f(x,y)+O(\rho^3)\,, \tag{3}$$

where

$$k^{(x)}=\left.\frac{\partial^2 F}{\partial x^2}\right|_{x=y=0}\,,\quad k^{(y)}=\left.\frac{\partial^2 F}{\partial y^2}\right|_{x=y=0} \tag{4}$$

are the two principal curvatures of the boundary surface at the charge location.

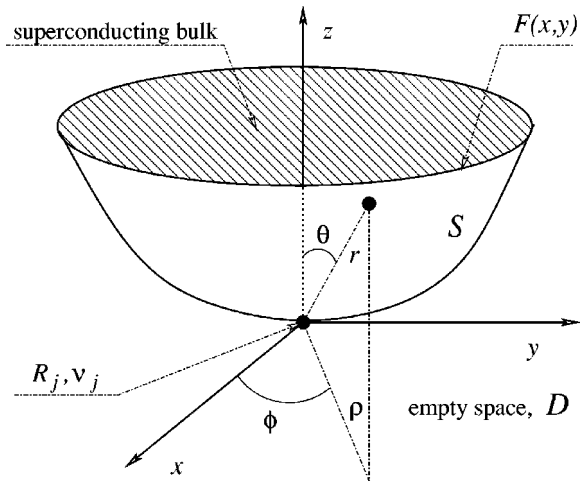

FIG. 1. Definition of coordinate systems near a charge.

Since, near $\mathbf{r}=0$,

$$\delta_S(\mathbf{r})=\delta(x)\,\delta(y)/J,$$

$$\partial/\partial n=\hat{n}\cdot\nabla=(1/J)(\partial/\partial z-F_x\,\partial/\partial x-F_y\,\partial/\partial y),$$

$$J\equiv\sqrt{1+F_x^2+F_y^2},$$

the boundary condition, Eq. (2), in the vicinity of the charge can be written in terms of variables x,y,z as[6]

$$\left.\frac{\partial\psi}{\partial z}\right|_{z=F(x,y)}=\nu\Phi_0\delta(x)\,\delta(y)+\left.\left(F_x\frac{\partial\psi}{\partial x}+F_y\frac{\partial\psi}{\partial y}\right)\right|_{z=F(x,y)}. \tag{5}$$

The partial derivatives of the function $F(x,y)$ near the origin are given, to the order we are interested in, by

$$F_x=k^{(x)}x+O(\rho^2),\quad F_y=k^{(y)}y+O(\rho^2). \tag{6}$$

Once again, we only care about the vicinity of the charge where $z=F(x,y)$ is small, so we can use perturbation of the boundary to move the boundary condition, Eq. (5), to the plane $z=0$. This is done by means of the following Taylor expansion of an arbitrary function $w=w(x,y,z)$:

$$w|_{z=F(x,y)}=w|_{z=0}+F\left.\frac{\partial w}{\partial z}\right|_{z=0}+\frac{F^2}{2}\left.\frac{\partial^2 w}{\partial z^2}\right|_{z=0}+\cdots.$$

Applying this to the derivatives of ψ in Eq. (5) we write it, to the proper order, in the form:

$$\left.\frac{\partial\psi}{\partial z}\right|_{z=0}=\nu\Phi_0\delta(x)\,\delta(y)+\left.\left(F_x\frac{\partial\psi}{\partial x}+F_y\frac{\partial\psi}{\partial y}-F\frac{\partial^2\psi}{\partial z^2}\right)\right|_{z=0}+\cdots. \tag{7}$$

The final step of this derivation is to expand ψ in a series of successively smaller (that is, less singular at the origin) functions $\psi^{(i)}$,

$$\psi=\psi^{(0)}+\psi^{(1)}+\psi^{(2)}+\cdots. \tag{8}$$

Introducing this expansion in the boundary condition Eq. (7) and then matching the terms of the same order, we end up with the following sequence of boundary conditions for $\psi^{(i)}$, $i=0,1,2,\ldots$, at $z=0$:

$$\left.\frac{\partial\psi^{(0)}}{\partial z}\right|_{z=0}=\nu\Phi_0\,\delta(x)\,\delta(y), \tag{9}$$

$$\left.\frac{\partial\psi^{(1)}}{\partial z}\right|_{z=0}=\left[k^{(x)}x\,\frac{\partial\psi^{(0)}}{\partial x}+k^{(y)}y\,\frac{\partial\psi^{(0)}}{\partial y}-f(x,y)\,\frac{\partial^2\psi^{(0)}}{\partial z^2}\right]\Bigg|_{z=0}, \tag{10}$$

and so on. Here we have dropped higher order terms on the right-hand sides by replacing F and F_x, F_y with their main term expressions from Eqs. (3) and (6), respectively. Of course, all functions $\psi^{(i)}$ are subject to the Laplace equation, Eq. (1).

Thus, *locally* we have successfully replaced the boundary value problem of Eqs. (1) and (2) in the domain D by a sequence of problems for functions $\psi^{(i)}$, $i=0,1,2,\ldots$, harmonic in the half-space $z<0$ and satisfying the above boundary conditions, Eqs. (9), (10), etc. We now need to solve these problems for the half-space one by one, until the normal derivative of the solution becomes finite at the boundary.

The zero-order solution $\psi^{(0)}$ obeying the boundary condition of Eq. (9) is, of course,

$$\psi^{(0)}=\frac{\nu\Phi_0}{2\pi}\,\frac{1}{r}. \tag{11}$$

It allows one to immediately calculate the right-hand side of Eq (10). Indeed,

$$f\left.\frac{\partial^2\psi^{(0)}}{\partial z^2}\right|_{z=0}=-\frac{\nu\Phi_0 f}{2\pi}\left(\frac{1}{r^3}-\frac{3z^2}{r^5}\right)\Bigg|_{z=0}=-\frac{\nu\Phi_0}{2\pi}\,\frac{k^{(x)}x^2+k^{(y)}y^2}{2\rho^3},$$

where the second term in the middle expression turns to zero at $z=0$, contributing no δ-like singularities, due to the presence of the factor $f=O(\rho^2)$. Also taking into account that $\partial r^{-1}/\partial x=-x/r^3$, $\partial r^{-1}/\partial y=-y/r^3$, we find the boundary condition for $\psi^{(1)}$ in its final explicit form:

$$\left.\frac{\partial\psi^{(1)}}{\partial z}\right|_{z=0}=-\frac{\nu\Phi_0}{2\pi}\,\frac{k^{(x)}x^2+k^{(y)}y^2}{2\rho^3}=-\frac{\nu\Phi_0}{8\pi}\left[\frac{k^{(x)}+k^{(y)}}{\rho}+\frac{k^{(x)}-k^{(y)}}{\rho}\cos 2\phi\right]. \tag{12}$$

The two terms on the utmost right here have essentially different singularities at the origin. For this reason, we treat them separately by splitting the problem in two in the following way:

$$\psi^{(1)}=\psi_s^{(1)}+\psi_r^{(1)}, \tag{13}$$

$$\left.\frac{\partial\psi_s^{(1)}}{\partial z}\right|_{z=0}=-\frac{\nu\Phi_0}{8\pi}\,\frac{k^{(x)}+k^{(y)}}{\rho}, \tag{14}$$

$$\left.\frac{\partial\psi_r^{(1)}}{\partial z}\right|_{z=0}=-\frac{\nu\Phi_0}{8\pi}\,\frac{k^{(x)}-k^{(y)}}{\rho}\cos 2\phi. \tag{15}$$

The Neumann problem for $\psi_s^{(1)}$ in the half-space does not have solutions bounded at infinity, as one would expect in our investigation (we are actually looking for terms *growing* away from the charge, because a weaker singularity next to the inverse distance is most probably some logarithm tending to infinity at both the charge and the infinite distance from it). For this reason, no solution can be found by means of standard techniques. However, a harmonic and regular in the half-space $z<0$ function

$$\psi_s^{(1)} = K_+ \ln[(r-z)/d] = K_+[\ln(r/d) + \ln(1-\cos\theta)], \tag{16}$$

$$K_\pm \equiv \nu\Phi_0[k^{(x)} \pm k^{(y)}]/8\pi, \tag{17}$$

where $d>0$ is an arbitrary constant of the dimension of length, provides the needed solution. Indeed, it satisfies the boundary condition, Eq. (14), in view of

$$\partial \ln(r-z)/\partial z = (r-z)^{-1}(z/r-1) = -1/r \to -1/\rho, \quad z \to -0.$$

The solution given by Eq. (16) is unique in the class of functions with the logarithmic growth at infinity, namely, those with the asymptotics

$$\psi_s^{(1)} = K_+ \ln(r/d) + K_+ \ln(1-\cos\theta) + o(1), \ \frac{\partial \psi_s^{(1)}}{\partial r} = K_+/r + O(1/r^2), \ r \to \infty.$$

Contrary to the previous one, the Neumann problem for $\psi_r^{(1)}$,

$$\Delta \psi_r^{(1)} = 0, \ z<0, \ \left.\frac{\partial \psi_r^{(1)}}{\partial z}\right|_{z=0} = -\frac{K_-}{\rho}\cos 2\phi, \tag{18}$$

has a unique, up to a constant, solution bounded at infinity [namely, a solution that obeys somewhat unusual conditions $\psi_r^{(1)} = O(1)$, $\partial\psi_r^{(1)}/\partial r = o(1/r^2)$, $r\to\infty$]. The solution is obtained by the standard separation of variables in cylindrical coordinates using the Hankel transform, and it reads:

$$\begin{aligned}\psi_r^{(1)} &= -K_- \cos 2\phi \int_0^\infty J_2(\lambda\rho)\exp(-\lambda|z|)\frac{d\lambda}{\lambda} \\ &= -\frac{K_-\cos 2\phi}{2}\left(\frac{\rho}{r-z}\right)^2 = -\frac{K_-}{2}\frac{x^2-y^2}{(r-z)^2}.\end{aligned} \tag{19}$$

The value of the integral is found in Ref. 7, 4.14.(5), and the constant K_- is defined in Eq. (17). Interestingly, this solution in spherical coordinates does not depend on the radius, being a function of the angles only [singular on the positive semiaxis $z>0$, same as $\psi_s^{(1)}$ in Eq. (16)]:

$$\psi_r^{(1)} = -\frac{K_-}{2}\frac{\sin^2\theta\cos 2\phi}{(1-\cos\theta)^2}, \quad \frac{\partial\psi_r^{(1)}}{\partial r} = 0.$$

It is now straightforward to see that the Neumann boundary data for all higher order corrections to the potential, starting with $\psi^{(2)}$, are finite at the origin (and dropping fast enough at infinity); accordingly, the solutions of the corresponding problems bounded at infinity are unique up to an additive constant. It also means that all the terms in the expansion, Eq. (8), of the potential, whose normal derivative are singular at the location of a surface charge, are given by the solutions already found. Hence, combining the expressions from Eqs. (11), (16), and (19), we find the desired formula for the magnetostatic potential near a surface charge ($r\to 0$):

$$\begin{aligned}\psi &= \psi^{(0)} + \psi_s^{(1)} + \psi_r^{(1)} + \cdots \\ &= \frac{\nu\Phi_0}{2\pi}\left[\frac{1}{r} + \frac{k^{(x)}+k^{(y)}}{4}\ln\frac{r-z}{d} - \frac{k^{(x)}-k^{(y)}}{8}\frac{x^2-y^2}{(r-z)^2}\right] + (\text{nonsingular terms}).\end{aligned} \tag{20}$$

It is easy to rewrite this in our general notations from Eqs. (1) and (2) by replacing $|\mathbf{r}|$ with $|\mathbf{R}-\mathbf{R}_j|$, x with $X-X_j$, etc. Instead, we give the expression of the singular part of the magnetic field near the charge. It can be written in the form:

$$\mathbf{B}=-\nabla\psi=\frac{\nu\Phi_0}{2\pi}\left[\frac{\hat{r}}{r^2}-\frac{k^{(x)}+k^{(y)}}{4r}\left(\hat{r}+\frac{\sin\theta}{1-\cos\theta}\hat{\theta}\right)-\frac{k^{(x)}-k^{(y)}}{4r}\frac{\sin\theta}{(1-\cos\theta)^2}(\cos 2\phi\,\hat{\theta}\right.$$
$$\left.+\sin 2\phi\,\hat{\phi})\right]+(\text{nonsingular terms}). \tag{21}$$

Here are a few concluding remarks regarding the obtained result.

First, notice that the leading order contribution to the potential, Eq. (11), is twice that of the point charge located in a volume away from its boundaries. This is clearly explained by the fact that the field lines and the flux from the surface charge emanate only into the half-space, versus the full space for the volume charge.

The two singular corrections to the usual inverse distance singularity of the potential, Eq. (20), are very different. The first one is logarithmic, axially symmetric about the direction of the normal to the boundary at the charge location, and proportional to the sum of two principal surface curvatures there, i.e., to the mean boundary curvature. Thus, it vanishes if the charge sits at a symmetric saddle point of the boundary. The second additional singularity is asymmetric, proportional to the difference of the principal curvatures, and vanishes thus when the latter are equal, i.e., when the charge is at a spherical point of the boundary. This second term is bounded at the charge location [giving unbounded field components, see Eq. (21)], but is not uniquely defined there, with the limiting values depending on the direction along which the limit is taken. Note that both corrections vanish simultaneously if and only if the charge is at the planar point of the boundary.

In a particular case when the domain D is the exterior of a sphere of the radius a, one has $k^{(x)}=k^{(y)}=1/a$. If there is just one surface charge, $N=j=1$ and $\nu=1$ (so that the incoming vortex line ends at infinity), Eq. (20) becomes

$$\psi=\frac{\Phi_0}{2\pi}\left[\frac{1}{|\mathbf{R}-\mathbf{R}_1|}+\frac{1}{2a}\ln\frac{|\mathbf{R}-\mathbf{R}_1|-\hat{n}\cdot(\mathbf{R}-\mathbf{R}_1)}{d}\right]+(\text{nonconstant nonsingular terms}), \tag{22}$$

in complete agreement with the exact solution obtained in Ref. 5 with $d=2a$.

Finally, the obtained singular expansion of the potential can be used in the derivation of the force acting on a charge in a fashion similar to the one developed in the case of volume point charges,[8] i.e., by means of the geometrical regularization of energy and, henceforth, the force, as the energy gradient in the charge location. However, in a striking contrast with the volume case, the force here is found to depend on the gradient of the curvature at the charge location. Namely, due to the first additional singular term in the potential, Eq. (20), there appears a tangential force on the charge which tries to move it toward the point of the stationary mean curvature of the boundary, and which diverges in the regularization limit. If confirmed, this divergence would mean that either the approximation of the *point* surface charges does not completely describe real microscopic, but finite size fluxons, or, strangely enough, that the fluxons cannot reside at arbitrary points of a curved boundary, or perhaps even something else.

A detailed study of fluxon interactions will be carried out in a separate publication. However, it is clear that it will necessarily use the results of this paper, in view of the relation

$$\psi(\mathbf{r},\mu)=\int_S dS(\boldsymbol{\xi})\,\mu(\boldsymbol{\xi})\,\psi(\mathbf{r}-\boldsymbol{\xi}),$$

where $\psi(\mathbf{r},\mu)$ is the potential created by the surface charge density $\mu(\boldsymbol{\xi})$, $\boldsymbol{\xi}\in S$, and $\psi(\mathbf{r})$ is the potential from Eq. (20). For small, yet finite size fluxons the divergent asymptotics derived above will have an explicit short scale cutoff defined by the spatial extent of the density (presumably, the London length). However, the detailed analysis will require a deeper insight in the real structure of magnetic vortex lines near a boundary. Without such an analysis one cannot, in fact, speculate about the strength and importance of these surface interactions; we will thus limit ourselves to just a few short comments.

First, one compares, naturally, the surface force coming from the logarithmic term in the field potential to the strength of the random pinning force that defines the fluxon's position.[9] The latter depends on the flux tube length and the former does not. So, allowing for a physical regularization of the mathematically divergent surface effects, one will in any case come up with some characteristic length, L, below which the surface force will dominate. The description of the vortex line dynamics that does not account for surface effects at distances from the surface smaller than L is necessarily incomplete.

Second, forces between two vortices in a superconducting bulk are exponentially small if the vortex line separation is larger than the London length (precisely the regime we are discussing). These forces can be neglected. Thus, the surface effects we have found will be the leading interaction terms. Such effects are significant and translate into an experimentally relevant magnetic ''friction'' between superconducting bodies.[10]

We thank Leonid Bakaleinikov, David Gross, Lev Kapitanski, Akakii Melikidze, Andrei Ruckenstein, Andrey Shytov, and Robert Wagoner for discussions and valuable references. A.S. and partly I.M. were supported by NASA Grant No. NAS 8-39225 to Gravity Probe B. I.N. was supported by NSF Grant No. PHY99-07949 to Kavli Institute for Theoretical Physics.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Group theory approach to the Dirac equation with a Coulomb plus scalar potential in $D+1$ dimensions[a)]

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(Received 18 March 2003; accepted 15 May 2003)

We generalize the Dirac equation to $D+1$ space–time. The conserved angular momentum operators and their quantum numbers are discussed. The eigenfunctions of the total angular momentums are calculated for both odd D and even D cases. The exact solutions of the $D+1$-dimensional radial equations of the Dirac equation with a Coulomb plus scalar potential are analytically presented by studying the Tricomi equations obtained from a pair of coupled first-order ones. The eigenvalues are also discussed in some detail. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1604185]

I. INTRODUCTION

The exact solutions of the nonrelativistic and relativistic equations with the Coulomb potential play an important role in quantum mechanics.[1–3] For example, the study of the exact solutions of the Schrödinger equation for a hydrogen atom is an important advance at the beginning of establishment of quantum mechanics. Recently the study of the Dirac equation with the Coulomb plus scalar potential has been investigated. For instance, the bound states of this case have been studied in $3+1$ dimensions.[4,5] Moreover the corresponding S-matrix in the quantum scattering theory has also been carried out by Vaidya and Souza in $3+1$ dimensions.[6] With the interest of the lower-dimensional field theory and condensed matter physics, the lower-dimensional case seems physically relevant since the results obtained in this case exhibit some new features. Therefore, the bound states of the $(2+1)$-dimensional Dirac equation with the Coulomb plus scalar potential have been investigated in our previous work.[7] Similarly with the interest of the higher-dimensional field theory, it is worth studying the exact solutions of this quantum system in $D+1$ dimensional space–time, which is the main purpose of this work.

This article is organized as follows. Section II is devoted to the generalization of the Dirac equation to $D+1$ space–time. In Sec. III, the conserved angular momentum operators and their quantum numbers are discussed. The eigenfunctions of the total angular momentums are calculated for both odd D and even D cases from the view point of the group theory. The radial equations of this quantum system are obtained. In Sec. IV, the exact solutions of the radial equations, which are expressed by the confluent hypergeometric functions, are analytically presented. The energy levels and some special cases are also discussed in great detail. The concluding remarks are given in Sec. V.

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II. THE DIRAC EQUATION IN $D+1$ DIMENSIONS

In this section we review some properties of the Dirac equation in $D+1$ dimensional space–time. The Dirac equation in $D+1$ dimensions can be written as[8]

$$i\sum_{\mu=0}^{D} \gamma^{\mu}(\partial_{\mu}+ieA_{\mu})\Psi(\mathbf{x},t)=M\Psi(\mathbf{x},t), \tag{1}$$

where M is the mass of the particle, and $D+1$ matrices γ_{μ} satisfy the anticommutative relations:

$$\gamma^{\mu}\gamma^{\nu}+\gamma^{\nu}\gamma^{\mu}=2\,\eta^{\mu\nu}\mathbf{1}, \tag{2}$$

with

$$\eta^{\mu\nu}=\eta_{\mu\nu}=\begin{cases}\delta_{\mu\nu} & \text{when} \quad \mu=0,\\ -\delta_{\mu\nu} & \text{when} \quad \mu\neq 0.\end{cases} \tag{3}$$

Throughout this article, the natural units $\hbar=c=1$ are employed if not explicitly stated otherwise. Discuss the special case where only A_0 of A_{μ} is nonvanishing and spherically symmetric:

$$eA_0=V(r), \qquad A_a=0, \qquad \text{when} \quad a\neq 0. \tag{4}$$

The Hamiltonian $H(\mathbf{x})$ of the system is expressed as

$$\begin{gathered} i\partial_0\Psi(\mathbf{x},t)=H(\mathbf{x})\Psi(\mathbf{x},t), \qquad H(\mathbf{x})=\sum_{c=1}^{D}\gamma^0\gamma^c p_c+V(r)+\gamma^0 M,\\ p_c=-i\partial_c=-i\frac{\partial}{\partial x^c}, \quad c\in[1,D]. \end{gathered} \tag{5}$$

The orbital angular momentum operators L_{ab}, the spinor operators S_{ab}, and the total angular momentum operators J_{ab} are defined as follows:

$$\begin{gathered} L_{ab}=-L_{ba}=ix_a\partial_b-ix_b\partial_a, \quad S_{ab}=-S_{ba}=i\frac{\gamma_a\gamma_b}{2},\\ J_{ab}=L_{ab}+S_{ab}, \quad 1\leqslant a<b\leqslant D,\\ J^2=\sum_{a<b=2}^{D}J_{ab}^2, \quad L^2=\sum_{a<b=2}^{D}L_{ab}^2, \quad S^2=\sum_{a<b=2}^{D}S_{ab}^2. \end{gathered} \tag{6}$$

The eigenvalue of J^2 (L^2 or S^2) is denoted by the Casimir $C_2(\mathbf{M})$, where $\mathbf{M}$ is the highest weight of the representation to which the total (orbital or spinor) wave function belongs. We will discuss the Casimir in the next section. It is easy to show by the standard method[8] that J_{ab} and κ are commutative with the Hamiltonian $H(\mathbf{x})$,

$$\kappa=\gamma^0\left(\sum_{a<b} i\gamma^a\gamma^b L_{ab}+\frac{D-1}{2}\right)=\gamma^0\left(J^2-L^2-S^2+\frac{D-1}{2}\right). \tag{7}$$

III. THE RADIAL EQUATIONS

Because of the spherically symmetric potential $V(r)$, the symmetry group of the system is SO(D) group. Erdelyi,[9] Louck[10] and Chatterjee[11] have introduced the hyperspherical coordinates in the real D-dimensional space:

$$
\begin{aligned}
x^1 &= r\cos\theta_1 \sin\theta_2 \cdots \sin\theta_{D-1},\\
x^2 &= r\sin\theta_1 \sin\theta_2 \cdots \sin\theta_{D-1},\\
x^b &= r\cos\theta_{b-1} \sin\theta_k \cdots \sin\theta_{D-1}, \quad b\in[3,D-1],\\
x^D &= r\cos\theta_{D-1},\\
\sum_{a=1}^{D} (x^a)^2 &= r^2.
\end{aligned}
\tag{8}
$$

The unit vector along $\mathbf{x}$ is usually denoted by $\hat{\mathbf{x}}=\mathbf{x}/r$. The volume element of the configuration space is

$$
\prod_{a=1}^{D} dx^a = r^{D-1} dr\, d\Omega, \quad d\Omega = \prod_{a=1}^{D-1} (\sin\theta_a)^{a-1} d\theta_a,
\tag{9}
$$

$$
r\in[0,\infty], \qquad \theta_1\in[-\pi,\pi], \quad \theta_c\in[0,\pi], \qquad c\in[2,D-1].
$$

We now sketch some necessary information of the SO(D) group. From the representation theory of Lie groups,[12–14] the Lie algebras of the groups SO($2N+1$) and SO($2N$) are B_N and D_N, respectively. Their Chevalley bases with the subscript μ, $1\leqslant\mu\leqslant N-1$, are the same:

$$
\begin{aligned}
H_\mu(J) &= J_{(2\mu-1)(2\mu)} - J_{(2\mu+1)(2\mu+2)},\\
E_\mu(J) &= \tfrac{1}{2}(J_{(2\mu)(2\mu+1)} - J_{(2\mu-1)(2\mu+2)} - iJ_{(2\mu-1)(2\mu+1)} - iJ_{(2\mu)(2\mu+2)}),\\
F_\mu(J) &= \tfrac{1}{2}(J_{(2\mu)(2\mu+1)} - J_{(2\mu-1)(2\mu+2)} + iJ_{(2\mu-1)(2\mu+1)} + iJ_{(2\mu)(2\mu+2)}).
\end{aligned}
\tag{10a}
$$

However, the bases with the subscript N are different:

$$
\begin{aligned}
H_N(J) &= 2J_{(2N-1)(2N)},\\
E_N(J) &= -iJ_{(2N-1)(2N+1)} + J_{(2N)(2N+1)},\\
F_N(J) &= iJ_{(2N-1)(2N+1)} + J_{(2N)(2N+1)}
\end{aligned}
\tag{10b}
$$

for SO($2N+1$), and

$$
\begin{aligned}
H_N(J) &= J_{(2N-3)(2N-2)} + J_{(2N-1)(2N)},\\
E_N(J) &= \tfrac{1}{2}(J_{(2N-2)(2N-1)} + J_{(2N-3)(2N)} + iJ_{(2N-2)(2N)} - iJ_{(2N-3)(2N-1)}),\\
F_N(J) &= \tfrac{1}{2}(J_{(2N-2)(2N-1)} + J_{(2N-3)(2N)} + iJ_{(2N-3)(2N-1)} - iJ_{(2N-2)(2N)}),
\end{aligned}
\tag{10c}
$$

for SO($2N$). The operator J_{ab} may be replaced by L_{ab} or S_{ab} depending on the studied wave functions. $H_\mu(J)$ span the Cartan subalgebra, and their eigenvalues for an eigenstate $|\mathbf{m}\rangle$ in a given irreducible representation (IR) are the components of a weight vector $\mathbf{m}=(m_1,\ldots,m_n)$:

$$
H_\mu(J)|\mathbf{m}\rangle = m_\mu|\mathbf{m}\rangle, \qquad \mu\in[1,N].
\tag{11}
$$

If the eigenstates $|\mathbf{m}\rangle$ for a given weight $\mathbf{m}$ are degeneracy, this weight is called a multiple weight, otherwise a simple one. E_μ are called the raising operators and F_μ the lowering ones. For an IR there is a highest weight $\mathbf{M}$, which is a simple weight and is used to describe the IR. Generally, the

irreducible representation is also called the highest weight representation and directly denoted by **M**. The Casimir $C_2(\mathbf{M})$ is calculated by the formula [see (1.131) of Ref. 14]

$$C_2(\mathbf{M})=\mathbf{M}\cdot(\mathbf{M}+2\varrho)=\sum_{\mu,\nu=1}^{N} M_\mu d_\mu (A^{-1})_{\mu\nu}(M_\nu+2), \tag{12}$$

where ϱ is the half sum of the positive roots in the Lie algebra, A^{-1} is the inverse of the Carton matrix, and d_μ are the half square lengths of the simple roots.

The orbital wave functions in D-dimensional space are usually expressed by the spherical harmonics $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$,[10,11] which belong to the weight **m** of the highest weight representation $(l)\equiv(l,0,\ldots,0)$. For the highest weight state, $\mathbf{m}=(l)$, we have

$$Y^{(l)}_{(l)}(\hat{\mathbf{x}})=N_{D,l}\, r^{-l}(x^1+ix^2)^l, \tag{13a}$$

with the normalization factor

$$N_{D,l}=\begin{cases} 2^{-N-l}\sqrt{\dfrac{(2l+2N-1)!}{\pi^N l!(l+N-1)!}} & \text{when} \quad D=2N+1, \\ \sqrt{\dfrac{(l+N-1)!}{2\pi^N l!}} & \text{when} \quad D=2N. \end{cases} \tag{13b}$$

Its partners $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ is calculated from $Y^{(l)}_{(l)}(\hat{\mathbf{x}})$ by lowering operators $F_\mu(L)$. The Casimir for the spherical harmonic $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ can be calculated by Eq. (12):

$$L^2 Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})=C_2[(l)]Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}}), \tag{14}$$

with

$$C_2[(l)]=l(l+D-2).$$

It is known that the spinor wave functions as well as those for the total angular momentum are different for $D=2N+1$ and $D=2N$, as studied in Ref. 15. Nevertheless, for completeness and clearness, it is necessary to review how to calculate these wave functions with the help of the groups SO$(2N+1)$ and SO$(2N)$.

A. The SO$(2N+1)$ case

When $D=2N+1$ we can define

$$\gamma^0=\sigma_3\times\mathbf{1}, \qquad \gamma^a=(i\sigma_2)\times\alpha_a, \qquad a\in[1,2N+1], \tag{15}$$

with the Pauli matrix σ_a, the 2^N-dimensional unit matrix **1** and the $(2N+1)$ matrices α_a satisfying the following anticommutative relations:

$$\alpha_b\alpha_a+\alpha_a\alpha_b=2\delta_{ab}\mathbf{1}, \quad b,\ a=1,\ 2,\ldots,(2N+1). \tag{16}$$

The dimensions of α_a matrices are 2^N. Thus the spinor operator S_{ab} becomes a block matrix

$$S_{ab}=\mathbf{1}\times\overline{S}_{ab}, \quad \overline{S}_{ab}=-i\frac{\alpha_a\alpha_b}{2}. \tag{17}$$

The relation between S_{ab} and $\overline{S}_{ab}$ is very similar to that between the spinor operators for the Dirac spinors and for the Pauli spinors. The operator κ becomes

$$\kappa=\sigma_3\times\overline{\kappa},\quad \overline{\kappa}=-i\sum_{a<b}\ \alpha_a\alpha_b L_{ab}+\frac{D-1}{2}. \tag{18}$$

The spinor $\chi(\mathbf{m})$ belongs to the spinor representation $(s)\equiv(0,\ldots,0,1)$. It is found from Eq. (12) that the Casimir for the representation (s) can be calculated as $C_2[(s)]=(2N^2+N)/4$.

On the other hand, it is well known that the product of $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ and $\chi(\mathbf{m}')$ belongs to the direct product of two representation (l) and (s), which is a reducible representation:

$$(l)\times(s)\simeq(l,0,\ldots,0,1)\oplus(l-1,0,\ldots,0,1). \tag{19}$$

Generally speaking, there are two different ways to construct a wave function belonging to the representation $(j)\equiv(l,0,\ldots,0,1)$, namely, the combination of $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi(\mathbf{m}')$ and that of $Y^{(l+1)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi(\mathbf{m}')$, which are different in eigenvalues of $\overline{\kappa}$. Considering the spherically symmetric system, we only calculate the highest weight state for the representation (j) from the Clebsch–Gordan coefficients

$$\phi_{|K|,(j)}(\hat{\mathbf{x}})=Y^{(l)}_{(l)}(\hat{\mathbf{x}})\chi[(s)]=N_{D,l}r^{-l}(x^1+ix^2)^l\chi[(s)], \tag{20}$$

with

$$|K|=C_2[(j)]-C_2[(l)]-C_2[(s)]+N=l+N,$$

and

$$\begin{aligned}\phi_{-|K|,(j)}(\hat{\mathbf{x}})&=\sum_{\mathbf{m}}\ Y^{(l+1)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi[(j)-\mathbf{m}]\langle(l+1),\mathbf{m},(s),(j)-\mathbf{m}|(j),(j)\rangle\\&=N_{D,l}r^{-l-1}(x^1+ix^2)^l\{x^{2N+1}\chi[(s)]+(x^{2N-1}+ix^{2N})\chi[(0,\ldots,0,1,\overline{1})]\\&\quad+(x^{2N-3}+ix^{2N-2})\chi[(0,\ldots,0,1,\overline{1},1)]+\cdots+(x^3+ix^4)\chi[(1,\overline{1},0,\ldots,0,1)]\\&\quad+(x^1+ix^2)\chi[(\overline{1},0,\ldots,0,1)]\},\end{aligned} \tag{21}$$

with

$$-|K|=C_2[(j)]-C_2[(l+1)]-C_2[(s)]+N=-l-N.$$

The wave functions $\Psi_{K,(j)}(\mathbf{x})$ of the total angular momentum belonging to the IR (j) can be written as

$$\Psi_{K,(j)}(\mathbf{x},t)=r^{-N}e^{-iEt}\begin{pmatrix}F(r)\phi_{K,(j)}(\hat{\mathbf{x}})\\iG(r)\phi_{-K,(j)}(\hat{\mathbf{x}})\end{pmatrix}, \tag{22a}$$

with the following properties:

$$\begin{aligned}&H_1(J)\Psi_{K,(j)}(\mathbf{x})=l\Psi_{K,(j)}(\mathbf{x}),\\&H_N(J)\Psi_{K,(j)}(\mathbf{x})=\Psi_{K,(j)}(\mathbf{x}),\\&H_\mu(J)\Psi_{K,(j)}(\mathbf{x})=0,\qquad \mu\in[2,N-1],\\&\kappa\Psi_{K,(j)}(\mathbf{x})=K\Psi_{K,(j)}(\mathbf{x}),\quad K=\pm(l+N).\end{aligned} \tag{22b}$$

Their partners can be calculated by the lowering operators F_μ.

The radial equation depends on the explicit forms of α_a matrices, which can be expressed by direct products of N Pauli matrices σ_a:[16]

$$\alpha_{2m-1}=\overbrace{\mathbf{1}\times\ldots\times\mathbf{1}}^{m-1}\times\sigma_1\times\overbrace{\sigma_3\times\ldots\times\sigma_3}^{N-m},$$

$$\alpha_{2m-1}=\overbrace{\mathbf{1}\times\ldots\times\mathbf{1}}^{m-1}\times\sigma_2\times\overbrace{\sigma_3\times\ldots\times\sigma_3}^{N-m}, \tag{23}$$

$$\alpha_{2N+1}=\sigma_3\times\sigma_3\times\ldots\times\sigma_3.$$

From the explicit forms of α_a, one can obtain

$$\begin{aligned}(\vec{\alpha}\cdot\hat{\mathbf{x}})\phi_{K,(j)}(\hat{\mathbf{x}})&=r^{-1}\sum_{b=1}^{2N+1}\alpha_b x^b \quad \phi_{K,(j)}(\hat{\mathbf{x}})=\phi_{-K,(j)}(\hat{\mathbf{x}}),\\ (\vec{\alpha}\cdot\vec{\mathbf{p}})r^{-N}\phi_{K,(j)}(\hat{\mathbf{x}})&=\sum_{b=1}^{2N+1}\alpha_b p_b \quad r^{-N}\phi_{K,(j)}(\hat{\mathbf{x}})=iKr^{-N-1}\phi_{-K,(j)}(\hat{\mathbf{x}}).\end{aligned} \tag{24}$$

Substitution of $\Psi_{K(j)}(\mathbf{x})$ into the Dirac equation (5) leads to the following radial equation,

$$\begin{aligned}G'(r)+\frac{K}{r}G(r)&=[E-V(r)-M]F(r),\\ -F'(r)+\frac{K}{r}F(r)&=[E-V(r)+M]G(r),\end{aligned} \tag{25}$$

where and hereafter the prime denotes the first derivative with respect to the variable $r(\rho)$.

B. The SO(2*N*) case

As we know, the reducible spinor representation of SO($2N$) is reduced to two inequivalent fundamental spinor representations $(+s)\equiv(0,0,\ldots,0,1)$ and $(-s)\equiv(0,0,\ldots,1,0)$. Likewise it is shown from Eq. (12) that the Casimir for both spinor representations can be obtained as $C_2[(\pm s)]=(2n^2-n)/4$. From the α_a matrices given in Eq. (23), we define the γ^μ matrices for $D=2N$:

$$\gamma^0=\alpha_{2N+1},\qquad \gamma^a=\alpha_{2N+1}\alpha_a,\qquad a\in[1,2N]. \tag{26}$$

Here the γ^0 is a diagonal matrix where half of the diagonal elements are equal to $+1$ and the remainder to -1. On considering the spinor operator S_{ab} and the operator κ are commutative with γ^0, each of them becomes a direct sum of two matrices, referring to the rows with the eigenvalues $+1$ and -1 of γ^0, respectively. The spinors $\chi_\pm(\mathbf{m})$ belong to the spinor representations $(+s)$ and $(-s)$, respectively, and satisfy

$$\gamma^0\chi_\pm(\mathbf{m})=\pm\chi_\pm(\mathbf{m}). \tag{27}$$

Thus the product of $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})$ and $\chi_\pm(\mathbf{m}')$ belongs to the direct product of two representation (l) and $(\pm s)$, which is a reducible representation:

$$\begin{aligned}(l)\times(+s)&\simeq(l,0,\ldots,0,1)\oplus(l-1,0,\ldots,0,1,0),\\ (l)\times(-s)&\simeq(l,0,\ldots,0,1,0)\oplus(l-1,0,\ldots,0,1).\end{aligned} \tag{28}$$

There exist two kinds of representations for the total angular momentum: the representation $(j_1)\equiv(l,0,\ldots,0,1)$ and the representation $(j_2)\equiv(l,0,\ldots,0,1,0)$. Nevertheless, their Casimirs are equal:

$$C_2[(j_1)]=C_2[(j_2)]=l(l+2N-1)+\frac{N(2N-1)}{4}. \tag{29}$$

Similar to the case of $SO(2N+1)$, there exist two different ways to obtain the wave functions belonging to the representation (j_1): the combination of $Y^{(l)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi_+(\mathbf{m}')$ and that of $Y^{(l+1)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi_-(\mathbf{m}')$. Because of the spherical symmetry, one only calculates the highest weight state for the representation (j_1) by the Clebsch–Gordan coefficients:

$$\phi_{K,(j_1)}(\hat{\mathbf{x}})=Y^{(l)}_{(l)}(\hat{\mathbf{x}})\chi_+[(+s)]=N_{D,l}r^{-l}(x^1+ix^2)^l\chi_+[(+s)], \tag{30a}$$

and

$$\begin{aligned}\phi_{-K,(j_1)}(\hat{\mathbf{x}})&=\sum_{\mathbf{m}}\ Y^{(l+1)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi_-[(j_1)-\mathbf{m}]\langle(l+1),\mathbf{m},(+s),(j_1)-\mathbf{m}|(j_1),(j_1)\rangle\\&=N_{D,l}r^{-l-1}(x^1+ix^2)^l\{x^{2N-1}+ix^{2N}\chi_-[(-s)]+(x^{2N-3}+ix^{2N-2})\\&\quad\times\chi_-[(0,\ldots,0,1,\overline{1},0)]+(x^{2N-5}+ix^{2N-4})\chi_-[(0,\ldots,0,1,\overline{1},0,1)]+\cdots\\&\quad+(x^3+ix^4)\chi_-[(1,\overline{1},0,\ldots,0,1)]+(x^1+ix^2)\chi_-[(\overline{1},0,\ldots,0,1)]\},\end{aligned} \tag{30b}$$

with

$$K=C_2[(j_1)]-C_2[(l+1)]-C_2[(+s)]+N-\tfrac{1}{2}=l+N-\tfrac{1}{2}.$$

However, for the representation $(j_2)\equiv(l,0,\ldots,0,1,0)$ we obtain

$$\phi_{-K,(j_2)}(\hat{\mathbf{x}})=Y^{(l)}_{(l)}(\hat{\mathbf{x}})\chi_-[(-s)]=N_{D,l}r^{-l}(x^1+ix^2)^l\chi_-[(-s)], \tag{31a}$$

and

$$\begin{aligned}\phi_{K,(j_2)}(\hat{\mathbf{x}})&=\sum_{\mathbf{m}}\ Y^{(l+1)}_{\mathbf{m}}(\hat{\mathbf{x}})\chi_+[(j_2)-\mathbf{m}]\langle(l+1),\mathbf{m},(-s),(j_2)-\mathbf{m}|(j_2),(j_2)\rangle\\&=N_{D,l}r^{-l-1}(x^1+ix^2)^l\{x^{2N-1}-ix^{2N}\chi[(+s)]+(x^{2N-3}+ix^{2N-2})\chi_+[(0,\ldots,0,1,0,\overline{1})]\\&\quad+(x^{2N-5}+ix^{2N-4})\chi_+[(0,\ldots,0,1,\overline{1},1,0)]+\cdots+(x^3+ix^4)\chi_+[(1,\overline{1},0,\ldots,0,1,0)]\\&\quad+(x^1+ix^2)\chi_+[(\overline{1},0,\ldots,0,1,0)]\},\end{aligned} \tag{31b}$$

with

$$K=C_2[(j_2)]-C_2[(l+1)]-C_2[(+s)]+N-\tfrac{1}{2}=-(l+N-\tfrac{1}{2}).$$

From the explicit forms of α_a one obtains

$$\begin{aligned}(\vec{\alpha}\cdot\hat{\mathbf{x}})\phi_{K,(j_\omega)}(\hat{\mathbf{x}})&=r^{-1}\sum_{a=1}^{2N}\ \alpha_a x^a\phi_{K,(j_\omega)}(\hat{\mathbf{x}})=\phi_{-K,(j_\omega)}(\hat{\mathbf{x}}),\\(\vec{\alpha}\cdot\vec{\mathbf{p}})r^{-N+1/2}\phi_{K,(j_\omega)}(\hat{\mathbf{x}})&=\sum_{a=1}^{2N}\ \alpha_a p_a\ \ r^{-N+1/2}\phi_{K,(j_\omega)}(\hat{\mathbf{x}})=iKr^{-N-1/2}\phi_{-K,(j_\omega)}(\hat{\mathbf{x}}),\end{aligned} \tag{32}$$

with $\omega=1$ or 2.

The wave functions $\Psi_{K,(j_\omega)}(\mathbf{x})$ of the total angular momentum belonging to the IR (j_ω) are expressed as

$$\Psi_{|K|,(j_1)}(\mathbf{x},t)=r^{-N+1/2}e^{-iEt}\{F(r)\phi_{|K|,(j_1)}(\hat{\mathbf{x}})+iG(r)\phi_{-|K|,(j_1)}(\hat{\mathbf{x}})\},$$

$$\Psi_{-|K|,(j_2)}(\mathbf{x},t)=r^{-N+1/2}e^{-iEt}\{F(r)\phi_{-|K|,(j_2)}(\hat{\mathbf{x}})+iG(r)\phi_{|K|,(j_2)}(\hat{\mathbf{x}})\}, \tag{33a}$$

$$\kappa\Psi_{K,(j_\omega)}(\mathbf{x})=K\Psi_{K,(j_\omega)}(\mathbf{x}), \quad |K|=l+N-\tfrac{1}{2}, \quad \omega=1 \text{ or } 2,$$

with the following properties:

$$H_1(J)\Psi_{K,(j_\omega)}(\mathbf{x})=l\Psi_{K,(j_1)}(\mathbf{x}), \qquad H_{N-1}(J)\Psi_{K,(j_1)}(\mathbf{x})=0, \tag{33b}$$

$$H_N(J)\Psi_{K,(j_1)}(\mathbf{x})=\Psi_{K,(j_1)}(\mathbf{x}), \quad H_{N-1}(J)\Psi_{K,(j_2)}(\mathbf{x})=\Psi_{K,(j_2)}(\mathbf{x}), \tag{33c}$$

$$H_N(J)\Psi_{K,(j_2)}(\mathbf{x})=0, \qquad H_\mu(J)\Psi_{K,(j_\omega)}(\mathbf{x})=0, \qquad \mu\in[2,N-2]. \tag{33d}$$

Their partners can be calculated by the lowering operators F_μ.

Substitution of $\Psi_{K(j_\omega)}(\mathbf{x})$ into the Dirac equation (5) allows us to obtain the radial equations, which are in the same forms as those in $D=2N+1$ case:

$$\begin{aligned} G'(r)+\frac{K}{r}G(r)&=[E-V(r)-M]F(r),\\ -F'(r)+\frac{K}{r}F(r)&=[E-V(r)+M]G(r). \end{aligned} \tag{34}$$

IV. THE EXACT SOLUTIONS OF THE RADIAL EQUATION

Although the wavefunctions and the eigenvalues K are different for the $D=2N+1$ case and the $D=2N$ case, the forms of the radial equations are unified

$$\begin{aligned} G'_{KE}(r)+\frac{K}{r}G_{KE}(r)&=[E-V(r)-M]F_{KE}(r),\\ -F'_{KE}(r)+\frac{K}{r}F_{KE}(r)&=[E-V(r)+M]G_{KE}(r), \end{aligned} \tag{35}$$

$$K=\pm(2l+D-1)/2.$$

We now consider the Dirac equation with a mixed potential including a Coulomb potential and a scalar one. The Coulomb potential is derived from the exchange of massless photons between the nucleus and the lepton orbiting around it, namely,

$$V_c=-\frac{A_1}{r}. \tag{36}$$

However, the scalar potential

$$V_s=-\frac{A_2}{r} \tag{37}$$

is added to the mass term of the Dirac equation, which can be interpreted as an effective, position-dependent mass. It is created by the exchange of the massless scalar meson. The A_1 and A_2 are the electrostatic and the scalar coupling constants, respectively.

It is found that the radial components $F_{KE}(r)$ and $G_{KE}(r)$ satisfy the following first-order differential equations

$$\begin{aligned} G'_{KE}(r)+\frac{K}{r}G_{KE}(r)&=\left(E-M+\frac{A_1+A_2}{r}\right)F_{KE}(r),\\ -F'_{KE}(r)+\frac{K}{r}F_{KE}(r)&=\left(E+M+\frac{A_1-A_2}{r}\right)G_{KE}(r). \end{aligned} \tag{38}$$

It is convenient to introduce ρ for the bound states:

$$\rho=2r\sqrt{M^2-E^2}, \qquad |E|<M. \tag{39}$$

We thus have

$$\begin{aligned} G'_{KE}(\rho)+\frac{K}{\rho}G_{KE}(\rho)&=\left(-\frac{1}{2}\sqrt{\frac{M-E}{M+E}}+\frac{A_1+A_2}{\rho}\right)F_{KE}(\rho),\\ F'_{KE}(\rho)-\frac{K}{\rho}F_{KE}(\rho)&=\left(-\frac{1}{2}\sqrt{\frac{M+E}{M-E}}-\frac{A_1-A_2}{\rho}\right)G_{KE}(\rho). \end{aligned} \tag{40}$$

Define the wave functions $\Phi_{\pm}(\rho)$ with the forms

$$\begin{aligned} G_{KE}(\rho)&=\sqrt{M-E}[\Phi_+(\rho)+\Phi_-(\rho)],\\ F_{KE}(\rho)&=\sqrt{M+E}[\Phi_+(\rho)-\Phi_-(\rho)]. \end{aligned} \tag{41}$$

Substitutions of Eq. (41) into Eq. (40) allow us to write down

$$\begin{aligned} \Phi'_+(\rho)+\Phi'_-(\rho)+\frac{K}{\rho}[\Phi_+(\rho)+\Phi_-(\rho)]&=\left[-\frac{1}{2}+\frac{A_1+A_2}{\rho}\sqrt{\frac{M+E}{M-E}}\right][\Phi_+(\rho)-\Phi_-(\rho)],\\ \Phi'_+(\rho)-\Phi'_-(\rho)-\frac{K}{\rho}[\Phi_+(\rho)-\Phi_-(\rho)]&=\left[-\frac{1}{2}-\frac{A_1-A_2}{\rho}\sqrt{\frac{M-E}{M+E}}\right][\Phi_+(\rho)+\Phi_-(\rho)]. \end{aligned} \tag{42}$$

Their addition and subtraction lead to

$$\begin{aligned} \Phi'_+(\rho)-\left(\frac{A_1E+A_2M}{\rho\sqrt{M^2-E^2}}-\frac{1}{2}\right)\Phi_+(\rho)&=-\left(\frac{K}{\rho}+\frac{A_1M+A_2E}{\rho\sqrt{M^2-E^2}}\right)\Phi_-(\rho),\\ \Phi'_-(\rho)+\left(\frac{A_1E+A_2M}{\rho\sqrt{M^2-E^2}}-\frac{1}{2}\right)\Phi_-(\rho)&=-\left(\frac{K}{\rho}-\frac{A_1M+A_2E}{\rho\sqrt{M^2-E^2}}\right)\Phi_+(\rho). \end{aligned} \tag{43}$$

Taking the following conventions,

$$\tau=\frac{A_1E+A_2M}{\sqrt{M^2-E^2}}, \qquad \tau'=\frac{A_1M+A_2E}{\sqrt{M^2-E^2}}, \tag{44}$$

we have

$$\Phi'_+(\rho)-\left(\frac{\tau}{\rho}-\frac{1}{2}\right)\Phi_+(\rho)=-\frac{\tau'+K}{\rho}\Phi_-(\rho),$$
$$\Phi'_-(\rho)+\left(\frac{\tau}{\rho}-\frac{1}{2}\right)\Phi_-(\rho)=\frac{\tau'-K}{\rho}\Phi_+(\rho), \tag{45}$$

from which we can obtain the following important second-order differential equations:

$$\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}+\left(-\frac{1}{4}+\frac{\tau\pm 1/2}{\rho}-\frac{\eta^2}{\rho^2}\right)\right]\Phi_\pm(\rho)=0,$$
$$\eta^2=K^2-A_1^2+A_2^2. \tag{46}$$

For the weak Coulomb potential, we have

$$\eta=\sqrt{K^2-A_1^2+A_2^2}>0. \tag{47}$$

It is found that Eq. (46) is a special case of the Tricomi equation,[17] which can be expressed as

$$\frac{d^2y}{dx^2}+\left(a+\frac{b}{x}\right)\frac{dy}{dx}+\left(\alpha+\frac{\alpha}{x}+\frac{\xi}{x^2}\right)y=0. \tag{48}$$

From the behaviors of the wave functions at the origin and infinity, we define

$$\Phi_\pm(\rho)=\rho^\eta e^{-\rho/2}R_\pm(\rho). \tag{49}$$

Substitution of this into (47) leads to

$$\frac{d^2}{d\rho^2}R_\pm(\rho)+\left(-1+\frac{1+2\eta}{\rho}\right)\frac{d}{d\rho}R_\pm(\rho)+\frac{\tau-\eta-\frac{1}{2}\pm\frac{1}{2}}{\rho}R_\pm(\rho)=0, \tag{50}$$

whose solutions are the confluent hypergeometric functions

$$R_+(\rho)=a_0\Phi(\eta-\tau,2\eta+1;\rho),$$
$$R_-(\rho)=b_0\Phi(1+\eta-\tau,2\eta+1;\rho), \tag{51}$$

which imply that $G_{KE}(\rho)$ and $F_{KE}(\rho)$ can be directly expressed by the combinations of the confluent hypergeometric functions.

We now study the relation between the coefficients a_0 and b_0. Before proceeding to do so, it is necessary to review the following recursive relations between the confluent hypergeometric functions[17]

$$\gamma\frac{d}{dz}\Phi(\alpha,\gamma;z)=\alpha\,\Phi(\alpha+1,\gamma+1;z),$$
$$z\Phi(\alpha+1,\gamma+1;z)=\gamma\Phi(\alpha+1,\gamma;z)-\gamma\Phi(\alpha,\gamma;z),$$
$$\alpha\Phi(\alpha+1,\gamma+1;z)=(\alpha-\gamma)\Phi(\alpha,\gamma+1;z)+\gamma\Phi(\alpha,\gamma;z), \tag{52}$$
$$\alpha\Phi(\alpha+1,\gamma;z)=(z+2\alpha-\gamma)\Phi(\alpha,\gamma;z)+(\gamma-\alpha)\Phi(\alpha-1,\gamma;z).$$

It is shown from Eqs. (46), (51) and (52) that

$$\left(\frac{\eta-\tau}{\rho}a_0+\frac{\tau'+K}{\rho}b_0\right)\Phi(1+\eta-\tau,2\eta+1;\rho)=0. \tag{53}$$

Since both a_0 and b_0 cannot be vanishing, we obtain

$$b_0=\frac{\tau-\eta}{\tau'+K}a_0. \tag{54}$$

From Eq. (42) we thus have

$$\begin{aligned}
G_{KE}(\rho)&=N_{KE}\sqrt{M-E}\,\rho^{\eta}e^{-\rho/2}\\
&\quad\times[(\tau'+K)\Phi(\eta-\tau,2\eta+1;\rho)+(\tau-\eta)\Phi(1+\eta-\tau,2\eta+1;\rho)],\\
F_{KE}(\rho)&=N_{KE}\sqrt{M+E}\,\rho^{\eta}e^{-\rho/2}\\
&\quad\times[(\tau'+K)\Phi_1(\eta-\tau,2\eta+1;\rho)-(\tau-\eta)\Phi(1+\eta-\tau,2\eta+1;\rho)],
\end{aligned} \tag{55}$$

where the normalization factor $N_{KE}=a_0(\tau'+K)^{-1}(2\sqrt{M^2-E^2})^{-1/2}$ can be determined later.

We now study the eigenvalues of this quantum system. The quantum condition is obtained from the finiteness of the solutions at infinity:

$$\tau-\eta=n'=0,1,2,\ldots, \tag{56}$$

when $n'=0$, $\eta=\tau$, and

$$K^2=\tau^2+A_1^2-A_2^2=(\tau')^2.$$

Therefore K has to be positive in order to avoid the trivial solution.

Introducing the principal quantum number

$$n=|K|-(D-3)/2+n'=|K|-(D-3)/2+\tau-\eta=l+1+n'=1,\ 2,\ldots, \tag{57}$$

we have

$$\frac{EA_1+MA_2}{\sqrt{M^2-E^2}}=n-|K|+\frac{D-3}{2}+\eta=n'+\eta\equiv\kappa. \tag{58}$$

The energy E can be solved from Eq. (58):

$$E(n,K)=M\left\{-\frac{A_1A_2}{A_1^2+\kappa^2}\pm\left[\left(\frac{A_1A_2}{A_1^2+\kappa^2}\right)^2-\frac{A_2^2-\kappa^2}{A_1^2+\kappa^2}\right]^{1/2}\right\}. \tag{59}$$

We now consider a few special cases. First, if $A_1=0$, then $\eta=\sqrt{K^2+A_2^2}$, and

$$E(n,K)=\pm M\left(1-\frac{A_2^2}{\kappa^2}\right)^{1/2}. \tag{60}$$

It implies that there are two branches of solutions symmetric for the positive and negative energies. For a large D, we have

$$E(n,D)\simeq\pm M[1-2A_2^2D^{-2}+4A_2^2(2n-3)D^{-3}-\cdots], \tag{61}$$

which implies that the energy is independent of l for a large D. For a small A_2, we have

$$E(n,l,D)\simeq\pm M\left\{1-\frac{A_2^2}{2[n+(D-3)/2]^2}+\frac{A_2^4}{2[n+(D-3)/2]^4}\left(\frac{2n+D-3}{2l+D-1}-\frac{1}{4}\right)\right\}, \tag{62}$$

where the first term on the right-hand side is the rest energy M ($c^2=1$ in our conventions), the second one is from the solutions of the Schrödinger equation, and the third one is the fine structure energy, which removes the degeneracy between the states with the same n.

Second, if $A_2=0$, then $\eta=\sqrt{K^2-A_1^2}$ and from Eq. (58) E has the same sign as A_1 when $K^2>A_1^2$. For the attractive Coulomb potential ($A_1>0$) we have the positive energy E_{nK}

$$E_{nK}=M\left(1+\frac{A_1^2}{\kappa^2}\right)^{-1/2}. \tag{63}$$

It coincides with the conclusion from the Sturm–Liouville theorem for a weak attractive potential.[18] For a large D similarly we have the same result as Eq. (61).

For a small A_1, we have

$$E(n,l,D)\simeq M\frac{A_1}{|A_1|}\left\{1-\frac{A_1^2}{2[n+(D-3)/2]^2}-\frac{A_1^4}{2[n+(D-3)/2]^4}\left(\frac{2n+D-3}{2l+D-1}-\frac{3}{4}\right)\right\}. \tag{64}$$

Similarly, the physical meanings of three terms are similar to those of Eq. (62) except for the different expansion coefficients.

We are now briefly considering the special case $D=1$ in this case. It is found that there is absence of the bound states since η becomes imaginary regardless of the value of A_1. This can be easily checked from the fact that the eigenvalues and eigenfunctions do not exist at all.

Third, if $A_1=A_2$, we have $\eta=|K|$ and

$$E(n)=M\left[-\frac{A_1^2}{A_1^2+(n+(D-3)/2)^2}\pm\frac{(n+(D-3)/2)^2}{A_1^2+(n+(D-3)/2)^2}\right]. \tag{65}$$

If we choose the negative sign in the result, we have $E=-M$, which is a singular solution of Eq. (58). For the positive sign, we have

$$E(n)=M\left[1-\frac{2A_1^2}{A_1^2+(n+(D-3)/2)^2}\right]. \tag{66}$$

We now determine the normalization factor N_{KE} from the normalization condition

$$\int \Psi_{KE}^{\dagger}\Psi_{KE}dV=1. \tag{67}$$

Noticing $n'=\tau-\eta$ is a non-negative integer, we can express the confluent hypergeometric function by the associated Laguerre polynomial[19]

$$L_n^{\alpha}(\rho)=\frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+1)}{}_1F_1(-n,\alpha+1;\rho), \tag{68}$$

$$\int_0^{\infty}\rho^{\alpha}e^{-\rho}L_n^{\alpha}(\rho)L_m^{\alpha}(\rho)d\rho=\frac{\Gamma(n+\alpha+1)}{n!}\delta_{nm}. \tag{69}$$

Through a direct calculation we obtain

$$N_{KE}=\frac{(M^2-E^2)^{1/4}}{\Gamma(2\eta+1)}\left[\frac{\Gamma(\tau+\eta+1)}{2M\tau'(K+\tau')(\tau-\eta)!}\right]^{1/2}. \tag{70}$$

V. CONCLUDING REMARKS

In this work we have studied the (D+1)-dimensional Dirac equation with a Coulomb plus scalar potential with the interest of higher-dimensional field theory. The eigenfunctions can be analytically obtained by studying the second-order differential equations obtained from the first-order coupled ones. The eigenvalues as well as their special cases are studied. Before ending this article, we give two remarks here. First, in comparison with the 3D case, the angular momentum quantum number K in $D+1$ dimensions plays the role of the good quantum number κ in three dimensions (more strictly, $|K|+\frac{1}{2}\leftrightarrow|\kappa|$). Second, for the special case $D=1$, it is found from Eq. (35) that $K=0$. Therefore, it is shown from Eq. (47) that η becomes imaginary if $|A_2|<|A_1|$, which means that there is absence of the bound states in this case. On the contrary, there exist the bound states if $|A_2|>|A_1|$.

ACKNOWLEDGMENTS

The authors thank Professor M. Lozada-Cassou for the hospitality at IMP. This work is supported by CONACyT, Mexico, under Project Nos. L007E and C086A and NEGROMEX.

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A quantum weak energy inequality for spin-one fields in curved space–time

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(Received 4 April 2003; accepted 22 May 2003)

Quantum weak energy inequalities (QWEI) provide state-independent lower bounds on averages of the renormalized energy density of a quantum field. We derive QWEIs for the electromagnetic and massive spin-one fields in globally hyperbolic space–times whose Cauchy surfaces are compact and have trivial first homology group. These inequalities provide lower bounds on weighted averages of the renormalized energy density as ''measured'' along an arbitrary timelike trajectory, and are valid for arbitrary Hadamard states of the spin-one fields. The QWEI bound takes a particularly simple form for averaging along static trajectories in ultrastatic space–times; as specific examples we consider Minkowski space (in which case the topological restrictions may be dispensed with) and the static Einstein universe. A significant part of the paper is devoted to the definition and properties of Hadamard states of spin-one fields in curved space–times, particularly with regard to their microlocal behavior. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1602554]

I. INTRODUCTION

In common with all observed forms of classical matter, the spin-one fields described by the Maxwell and Proca equations obey the weak energy condition (WEC). That is, the stress-energy tensor T_{ab} obeys $T_{ab}v^a v^b \geqslant 0$ for all timelike vectors v^a. In classical general relativity, energy conditions such as the WEC play a key role in many important results, notably the singularity theorems of Penrose[1] and Hawking.[2] Moreover, since any metric solves the Einstein equations for some choice of stress-energy tensor, it is arguable that general relativity has limited predictive power in the absence of such conditions.

However, all classical energy conditions are violated by quantum fields, as has been known for many years.[3] Typically, the energy density at a given space–time point is unbounded from below as a function of the state. Specific examples of negative energy states are provided by highly squeezed states of light in quantum optics, the Casimir vacuum state for a quantized field between uncharged perfectly conducting parallel planar plates and the Boulware vacuum state outside a black holes. Replacing the classical stress-energy tensor on the right-hand side of Einstein's equation with its quantum expectation value, we must therefore allow for negative energy sources, raising the possibility of exotic phenomena within the realm of semiclassical gravity. For example, negative energy can be used to maintain static traversable wormholes,[4,5] create naked singularities,[6,7] travel faster than light,[8,9] and travel backward through time.[5,10] In negative energy models studied by Parker and Fulling it is even possible to avoid the cosmological singularity,[11] thus threatening to overthrow the classical singularity theorems. One might also expect that negative energy fluxes could lead to macroscopic violations of the second law of thermodynamics.[12]

Of course, macroscopic violations of the second law are not observed in nature. Motivated by these thermodynamic considerations, Ford[12] deduced that the negative fluxes and energy densities

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of quantum fields must be subject to constraints, at least on average. These constraints, known as *quantum inequalities*, or QI, provide state-independent lower bounds on certain weighted averages of the stress-energy tensor. They may therefore be regarded as the remnants of the classical energy conditions after quantization; thus, for example, the analogue of the WEC is sometimes referred to as a *quantum weak energy inequality* or QWEI. Such bounds typically take the form

$$\int \langle :T_{ab}(\gamma(\tau))u^a(\tau)u^b(\tau):\rangle_\omega f(\tau)\mathrm{d}\tau \geqslant -\mathfrak{Q}(\gamma,f)\,, \tag{1}$$

where $f\geqslant 0$ is the weight, or sampling function, γ is a smooth timelike curve, parametrized by proper time τ and with four-velocity $u^a=(\mathrm{d}\gamma/\mathrm{d}\tau)^a$, and $:T_{ab}:$ denotes the stress-energy tensor, normal ordered with respect to some reference state ω_0. The significant point is that the bound $\mathfrak{Q}(\gamma,f)$ is independent of the state ω. The class of states ω for which the bound holds must also be delineated—all bounds in the literature require (at least) that ω and ω_0 be Hadamard states, although this can be weakened slightly. Of course the normal ordered energy density differs from the renormalized energy density by the (renormalized) energy density of the reference state. Accordingly, Eq. (1) may easily be converted into a bound on the renormalized energy density.

As we will shortly describe, various authors have established QWEI's for the scalar and Dirac fields in different circumstances, leading up to general results valid in curved space–times. The main aim of the present paper is to establish similar QWEI's for the Maxwell and Proca fields in general globally hyperbolic space–times. In order to do this, we have also made a detailed study of the field theories concerned, particularly in relation to the class of Hadamard states. Several new results obtained here may therefore be of more general interest.

As already mentioned, the earliest work on quantum inequalities is due to Ford, who established a bound on negative energy fluxes for scalar fields in 1991.[13] The first QWEI was obtained for the massless, minimally coupled scalar field in Minkowski space–time by Ford and Roman,[14] who established the inequality (1) for the case of an inertial worldline γ and with f taking the Lorentzian form $f(\tau)=\tau_0/(\pi(\tau^2+\tau_0^2))$, in which τ_0 sets the characteristic time scale for the averaging. In four dimensions, the resulting bound was

$$\int \langle :T_{ab}(\tau)u^a(\tau)u^b(\tau):\rangle_\omega \frac{\tau_0}{\pi(\tau^2+\tau_0^2)}\,\mathrm{d}\tau \geqslant -\frac{3}{32\pi^2\tau_0^4}\,. \tag{2}$$

These results were then extended by Ford and Roman to the massive scalar field in Minkowski space[14,15] and were further extended by Pfenning and Ford to minimally coupled scalar fields of arbitrary mass in ultrastatic curved space–times.[16–18] In these generalizations, it was found that the dominant term of the QWEI has a form similar to Eq. (2), but with subdominant correction terms due to the curvature and the mass of the field. Pfenning and Ford also showed that one could express the bound on the right-hand side of the QWEI in terms of derivatives of the Euclidean Green's function for the space–time and developed a short sampling time approximation to the QWEI which could be used in space–times where it would be too hard to calculate the exact QWEI bound.

The restriction to the Lorentzian weight $\tau_0/(\pi(\tau^2+\tau_0^2))$ was removed by various authors. By making use of the conformal properties of field theories in two dimensions, Flanagan[19,20] has derived optimal quantum inequalities for the massless scalar field for arbitrary smooth positive sampling functions, and Vollick has done the same for the Dirac field.[21] QWEI's for the minimally coupled scalar field in static curved space–times of any dimension for an arbitrary sampling function were established by Fewster in work with Eveson[22] and Teo.[23]

More recently, techniques drawn from microlocal analysis have been used to considerably generalize previous QWEI's and to put them on a mathematically rigorous footing. Fewster[24] used these techniques to derive a QWEI for minimally coupled scalar fields in general globally hyperbolic space–times (the most general class on which the Klein–Gordon equation is well-posed). In this case, averaging takes place along an arbitrary timelike worldline, using any weight of the form

$f(t)=g(t)^2$ for g smooth, real-valued and compactly supported. Subsequently, Fewster and Verch established similar results for the Dirac and Majorana fields in four-dimensional globally hyperbolic space–times.[25] Averaging over space–time volumes has been considered by Helfer,[26] also in great generality.

Previous work on QWEIs for spin-one fields has focussed on the electromagnetic field, beginning with the work of Ford and Roman,[15] who derived a QWEI for the case of Lorentzian sampling along inertial trajectories in Minkowski space. More recently, Pfenning[27] has derived a QWEI for the electromagnetic field in static curved space–times with arbitrary positive weight sampling functions by using the techniques developed for the scalar field in Refs. 22 and 23. Using similar techniques, Marecki[28] has derived bounds on the fluctuations of the electric field strength, which are of interest in quantum optics.

In this paper we will adapt the methods of Ref. 24 to the Maxwell and Proca fields. This depends crucially on the fact, first discovered by Radzikowski[29] for scalar fields, that the class of Hadamard states may be characterized in terms of a wave-front set condition on the two-point function. Similar reformulations are known for the Dirac field[30–32] but there is as yet no full treatment for the Maxwell and Proca fields in the literature. [See, however, Refs. 33 and 34 for (non microlocal) discussions of Hadamard states for electromagnetism using Faddeev–Popov ghosts.] Our treatment of this issue has been influenced to some extent by the forthcoming work of Junker and Lledó,[35] although it has been conducted largely independently, leading to some technical differences with their approach (Ref. 69).

The paper is structured as follows. The Maxwell and Proca fields are most elegantly described using differential forms; accordingly, we begin in Sec. II with a description of our conventions for differential forms and other geometric objects which will appear in this paper. In particular, we delineate the class of globally hyperbolic space–times to be considered; for technical reasons it is convenient to assume that their Cauchy surfaces are compact and have trivial first homology group. This is followed by a brief introduction to microlocal analysis leading to the definition of the wave-front set for p-form distributions.

In Sec. III we describe the quantization of the Maxwell and Proca fields in globally hyperbolic space–times. We adopt an algebraic approach, giving a direct construction of algebras of observables equivalent to those obtained by Dimock[36] and Furlani.[37] We also define the notion of a Hadamard state for these fields, as a state whose two-point function (Ref. 70) is related in a certain way to a one-form *Klein–Gordon* bisolution of Hadamard form. Such bisolutions and their microlocal properties have been discussed in detail by Sahlmann and Verch;[32] we may therefore read off the microlocal properties of the Maxwell and Proca two-point functions in Hadamard states. This permits us to apply the methods of Ref. 24 to obtain quantum inequalities for these fields in Sec. V. Before this, in Sec. IV, we specialize to the class of ultrastatic space–times in order to gain further insight into the abstract definitions of Sec. III. In particular, we prove the existence of Hadamard states in these space–times and use deformation arguments[38] to deduce from this the existence of Hadamard states in general globally hyperbolic space–times obeying our topological restrictions. We also compare our approach with other quantization schemes, including the Gupta–Bleuler method. As mentioned above, we expect that some of the results obtained here to be of wider interest.

In Sec. VI we investigate our QWEI in Minkowski space, and in general ultrastatic space–times (modulo the usual topological conditions). Simple formulas are obtained for the QWEI bound, which are readily compared with those previously obtained for the scalar field. In Minkowski space, the QWEI bound is weaker by a factor of exactly 2 for the Maxwell field (as already noted in Ref. 27) and by a factor of 3 for the Proca field. This is not very surprising and simply reflects the number of spin degrees of freedom. In curved space–time, however, the spin-one and scalar QWEIs cannot be related in this fashion. To emphasize this, we explicitly determine the QWEI bound in the Einstein static universe, providing a concrete example of our ultrastatic QWEI. Two appendixes contain the proofs of some technical results required in the body of the paper.

II. PRELIMINARIES

Units where $\hbar = c = 1$ are used throughout. The notation $C_0^\infty(\mathbb{R}^n)$ denotes the space of smooth, compactly supported (Ref. 71), complex-valued functions on $\mathbb{R}^n$.

A. Geometry and forms

Spin-one fields on globally hyperbolic space–times are most elegantly formulated in terms of differential forms. We will follow the conventions of Ref. 39, which we now briefly summarize for the benefit of the reader.

Suppose $\mathcal{N}$ is a smooth n-dimensional manifold which is connected, boundaryless, orientable, Hausdorff, paracompact, and equipped with a smooth metric of index s (Ref. 72). We denote the space of smooth, complex-valued p-forms on $\mathcal{N}$ by $\Omega^p(\mathcal{N})$; the subspace of compactly supported p-forms will be written $\Omega_0^p(\mathcal{N})$. Each p-form may be regarded as an antisymmetric covariant p-tensor field and we will occasionally use index notation accordingly. Thus the exterior product $\alpha\wedge\beta \in \Omega^{p+q}(\mathcal{N})$ of $\alpha \in \Omega^p(\mathcal{N})$ and $\beta \in \Omega^q(\mathcal{N})$ is given by

$$(\alpha\wedge\beta)_{a_1\cdots a_{p+q}} = \frac{(p+q)!}{p!q!}\,\alpha_{[a_1\cdots a_p}\beta_{a_{p+1}\cdots a_{p+q}]}, \tag{3}$$

and the exterior derivative $\mathbf{d}:\Omega^p(\mathcal{N})\to\Omega^{p+1}(\mathcal{N})$ is defined by

$$(\mathbf{d}\alpha)_{a_1\cdots a_{p+1}} = (p+1)\nabla_{[a_1}\alpha_{a_2\cdots a_{p+1}]}, \tag{4}$$

where the square brackets denote antisymmetrization and ∇_a is any connection on $\mathcal{N}$ ($\mathbf{d}$ is independent of the choice of connection). The Hodge $*$-operator is defined uniquely as the map $*:\Omega^p(\mathcal{N})\to\Omega^{n-p}(\mathcal{N})$ such that

$$\alpha\wedge *\beta = \frac{1}{p!}\,\alpha_{a_1\ldots a_p}\beta^{a_1\cdots a_p}\mathrm{d}\,\mathrm{vol}_g, \tag{5}$$

where $\mathrm{d}\,\mathrm{vol}_g$ is the positive volume n-form associated with the metric g. In particular, $(*)^2 = (-1)^{p(n-p)+s}$ on p-forms. By combining the Hodge $*$ and exterior derivative, we may define the coderivative $\boldsymbol{\delta}:\Omega^p(\mathcal{N})\to\Omega^{p-1}(\mathcal{N})$ (with the convention that $\boldsymbol{\delta}$ annihilates all zero-forms) by $\boldsymbol{\delta} = (-1)^{n(p-1)+s+1} * \mathbf{d} *$, which reduces to $\boldsymbol{\delta} = *\mathbf{d}*$ in a four-dimensional Lorentzian space–time.

The operations introduced above allow us to define a symmetric pairing $\langle\cdot,\cdot\rangle$ of p-forms under integration: we set

$$\langle\mathcal{U},\mathcal{V}\rangle \equiv \int_{\mathcal{N}} \mathcal{U}\wedge *\mathcal{V} \tag{6}$$

for any $\mathcal{U},\mathcal{V}\in\Omega^p(\mathcal{N})$ for which the integral exists. Since $\mathbf{d}(\mathcal{U}\wedge *\mathcal{V}) = \mathbf{d}\mathcal{U}\wedge *\mathcal{V} - \mathcal{U}\wedge *\boldsymbol{\delta}\mathcal{V}$, Stokes' theorem gives

$$\langle\boldsymbol{\delta}\mathcal{U},\mathcal{V}\rangle = \langle\mathcal{U},\mathbf{d}\mathcal{V}\rangle \tag{7}$$

for smooth $(p+1)$- and p-forms $\mathcal{U}$ and $\mathcal{V}$ whose supports have compact intersection. In this sense the operators $\mathbf{d}$ and $\boldsymbol{\delta}$ are dual.

The Laplace–Beltrami operator is defined as $-(\mathbf{d}\boldsymbol{\delta}+\boldsymbol{\delta}\mathbf{d})$, i.e., it is equal to *minus* the Laplace–de Rahm operator $\mathbf{d}\boldsymbol{\delta}+\boldsymbol{\delta}\mathbf{d}$. Where the manifold $\mathcal{N}$ is a Lorentzian space–time, with signature $+-\cdots-$, the Laplace–Beltrami operator is also known as the D'Alembertian and will be denoted by $\Box$. We wish to point out that Dimock[36] uses $\Box$ to denote the Laplace–de Rahm operator; our usage is determined by the convention that $\Box$ should have principal part $g^{\mu\nu}\partial_\mu\partial_\nu$, in accordance with typical usage in general relativity.

Finally, the spaces $\Omega_0^p(\mathcal{N})$ may be given locally convex topologies (Ref. 73) and the corresponding topological duals $\Omega_0^p(\mathcal{N})'$ will be called the spaces of p-form distributions on $\mathcal{N}$. [The

pairing $\langle \cdot , \cdot \rangle$ provides a natural embedding of $\Omega^p(\mathcal{N})$ in $\Omega_0^p(\mathcal{N})'$.] In the case $p=0$, we will also use $\mathcal{D}(\mathcal{N})$ and $\mathcal{D}'(\mathcal{N})$ for $\Omega_0^0(\mathcal{N})$ and $\Omega_0^0(\mathcal{N})'$, respectively. The exterior derivative and coderivative are defined on these spaces by

$$(\mathbf{d}\mathcal{U})(f)=\mathcal{U}(\boldsymbol{\delta} f) \quad (\mathcal{U}\in\Omega_0^p(\mathcal{N})', \ f\in\Omega_0^{p+1}(\mathcal{N})) \tag{8}$$

and

$$(\boldsymbol{\delta}\mathcal{U})(f)=\mathcal{U}(\mathbf{d} f) \quad (\mathcal{U}\in\Omega_0^p(\mathcal{N})', \ f\in\Omega_0^{p-1}(\mathcal{N})) \tag{9}$$

which extend the definitions given for smooth forms by virtue of the embeddings defined above and the calculation (7). In a similar way, the Hodge $*$-operator may also be extended to a map from p-form distributions to $(n-p)$-form distributions by

$$(*\mathcal{U})(f)=(-1)^{p(n-p)}\mathcal{U}(*f) \quad (\mathcal{U}\in\Omega_0^p(\mathcal{N})', \ f\in\Omega_0^{n-p}(\mathcal{N}))\,; \tag{10}$$

and it is easily checked that the formula $\boldsymbol{\delta}=(-1)^{n(p-1)+s+1}*\mathbf{d}*$ remains true for distributions.

B. Microlocal analysis and the wave-front set

Our proof of the quantum weak energy inequality turns on the detailed singularity properties of various distributions related to the two-point functions of quantum fields in Hadamard states. The information required is encoded in the *wave-front set* of these distributions, which is defined as follows. (See Ref. 40 for a full presentation.)

We will define the Fourier transform $\hat{u}$ of $u\in C_0^\infty(\mathbb{R}^n)$ using the nonstandard convention

$$\hat{u}(k)=\int \mathrm{d}^n y\, u(y) e^{ik\cdot y}, \tag{11}$$

which conforms to the conventions used, e.g., in Ref. 24. The Fourier transform can be extended to scalar distributions of compact support by writing $\hat{u}(k)=u(f_k)$ where $f_k=e^{ik\cdot y}$. Given a cone $V\subset(\mathbb{R}^n\backslash\{0\})$, we will say that $\hat{u}(k)$ is of rapid decrease in V if for each $N\in\mathbb{N}$ there exists a real constant C_N such that

$$|\hat{u}(k)|\leqslant \frac{C_N}{(1+|k|)^N} \quad \forall k\in V, \tag{12}$$

where $|k|$ denotes the Euclidean norm of k.

Smooth compactly supported functions have Fourier transforms which decay faster than any inverse power in the whole of $\mathbb{R}^n$, but the same is not true for arbitrary distributions u of compact support. A well-known example is the Dirac δ-function, whose Fourier transform does not decay at infinity in any direction. We define the set of singular directions $\Sigma(u)$ to be the set of all $k\in\mathbb{R}^n\backslash\{0\}$ having no conical neighborhood V in which $\hat{u}$ is of rapid decrease.

More detailed information about the singularities of u can be gained by localizing the singular directions. In particular, the set of *singular directions* of u at a point x is defined by

$$\Sigma_x(u)=\bigcap_\chi \Sigma(\chi u)\,, \tag{13}$$

where the intersection is taken over all smooth compactly supported test functions $\chi\in C_0^\infty(\mathbb{R}^n)$ with $\chi(x)\neq 0$. The *wave-front set* $\mathrm{WF}(u)$ of u is then defined by

$$\mathrm{WF}(u)=\{(x,k)\in\mathbb{R}^n\times(\mathbb{R}^n\backslash\{0\})\,|\,k\in\Sigma_x(u)\}. \tag{14}$$

The wave-front set can be extended in a natural way to distributions on manifolds. Let $(\mathcal{N},g)$ be a smooth n-dimensional manifold of the type discussed above. Each distribution u in $\mathcal{D}'(\mathcal{N})$ has a representative $u_\kappa \in \mathcal{D}'(\mathbb{R}^n)$ in each coordinate chart (U,κ) [with corresponding coordinates denoted $x^\mu = \kappa(x)^\mu$] defined so that

$$u_\kappa(f\sqrt{-|g|}) = u(f\circ\kappa) \tag{15}$$

holds for every smooth function f compactly supported in $\kappa(U)\subset\mathbb{R}^n$, where $|g|$ is the determinant of $g_{\mu\nu}$. The wave-front set $\mathrm{WF}(u)$ is now a subset of the cotangent bundle $T^*\mathcal{N}$ with the property that $(x,k)\in \mathrm{WF}(u)$ if and only if there is a chart (U,κ) about x so that $(\underline{x},\underline{k}) \in \mathrm{WF}(u_\kappa)$, where $(\underline{x},\underline{k})$ are the coordinates of (x,k) and u_κ is defined as in (15). In fact, it may be shown (see Theorem 8.2.4 and the following discussion in Ref. 40) that the restriction of $\mathrm{WF}(u)$ to U is given by

$$\mathrm{WF}(u)\cap T^*U = \kappa^*\mathrm{WF}(u_\kappa) := \{\kappa^*(\underline{x},\underline{k}) : (\underline{x},\underline{k})\in \mathrm{WF}(u_\kappa)\}\,, \tag{16}$$

where the pull-back κ^* relates $(x,k)\in T^*\mathcal{N}$ to its coordinates by $\kappa^*(\underline{x},\underline{k}) = (x,k)$.

There is a natural extension of the wave-front set to p-form distributions. Let v_i $(i=0,\ldots,n-1)$ be a global orthonormal n-bein on $\mathcal{N}$ (i.e., the vectors v_i obey $g_{ab}v_i^a v_j^b = \eta^{ij}$ and thus $\eta^{ij}v_i^a v_j^b = g^{ab}$, where η^{ij} is diagonal with s entries equal to -1 and the rest equal to $+1$) and let V^i be the dual basis of one-forms: $V_a^i = \eta^{ij}g_{ab}v_j^b$. For each $\mathcal{U}\in\Omega_0^p(\mathcal{N})'$, we may define the component distributions $\mathcal{U}_{i_1\cdots i_p}\in\mathcal{D}'(\mathcal{N})$ by

$$\mathcal{U}_{i_1\cdots i_p}(f) = \eta_{i_1 j_1}\cdots\eta_{i_p j_p}\mathcal{U}(fV^{j_1}\wedge\cdots\wedge V^{j_p}) \tag{17}$$

for $f\in\mathcal{D}(\mathcal{N})$. Then we define the wave-front set of $\mathcal{U}$ to be

$$\mathrm{WF}(\mathcal{U}) = \bigcup_{i_1,\ldots,i_p} \mathrm{WF}(\mathcal{U}_{i_1\ldots i_p})\,, \tag{18}$$

which may be shown to be independent of the particular choice of n-bein v_i.

III. QUANTIZATION OF THE MAXWELL AND PROCA FIELDS

A. Classical theory

We will consider the Maxwell and Proca fields propagating on four-dimensional Lorentzian globally hyperbolic space–times. Each such space–time is a pair $(\mathcal{M},g)$ consisting of a four-dimensional, smooth, real manifold $\mathcal{M}$, with the topological properties listed at the start of Sec. II A, together with a smooth Lorentzian metric g with signature $(+,-,-,-)$. Global hyperbolicity, which will ensure well-posedness of our field equations, requires that $(\mathcal{M},g)$ be time-orientable and that $\mathcal{M}$ contain a Cauchy surface Σ, that is, a smooth spacelike hypersurface intersected precisely once by every inextendible causal curve in $\mathcal{M}$. In fact, one may show[41] that $\mathcal{M}$ is diffeomorphic to $\mathbb{R}\times\Sigma$. We will assume for the most part that Σ (also referred to as the spatial section) is compact and that Σ has trivial first singular homology group with real coefficients, $H_1(\Sigma)$. This is equivalent to the triviality of the compact support de Rahm cohomology group $H_c^3(\mathcal{M})$ (Ref. 74); note that this condition excludes, for example, the 3-torus T^3 as a spatial section. The compactness assumption is made for convenience only; triviality of $H_1(\Sigma)$ is inessential for the Proca field, but appears to be required in order to establish some of our results for the Maxwell field.

The classical uncharged spin-1 field of mass $M>0$ is a real one-form field $\mathcal{A}\in\Omega^1(\mathcal{M})$ obeying the Proca equation

$$(-\boldsymbol{\delta}\mathbf{d}+M^2)\mathcal{A} = 0\,. \tag{19}$$

Applying the coderivative $\boldsymbol{\delta}$ we see that $\boldsymbol{\delta}\mathcal{A}=0$ and so any solution to Eq. (19) also satisfies the one-form Klein–Gordon equation

$$(\Box+M^2)\mathcal{A}=0\,. \tag{20}$$

Conversely, any solution to (20) satisfying the constraint

$$\boldsymbol{\delta}\mathcal{A}=0 \tag{21}$$

solves the Proca equation. The advantage of the system (20) and (21) is that (20) has the hyperbolic principal part $g^{\alpha\beta}\partial_\alpha\partial_\beta$ in local coordinates and therefore admits unique fundamental solutions $E_M^{\pm}:\Omega_0^1(\mathcal{M})\to\Omega^1(\mathcal{M})$, respectively,[37,42] such that

$$(\Box+M^2)E_M^{\pm}=E_M^{\pm}(\Box+M^2)=\mathbb{1} \tag{22}$$

and $\operatorname{supp}(E_M^{\pm}\mathcal{J})\subset J^{\pm}(\operatorname{supp}\mathcal{J})$ for $\mathcal{J}\in\Omega_0^1(\mathcal{M})$. Here, $J^{\pm}(S)$, the causal future $(+)$/past$(-)$ of S, is defined to be the set of points in $(\mathcal{M},g)$ that can be reached from the set $S\subset\mathcal{M}$ by a future $(+)$/past$(-)$ directed causal curve. The operators $E_M^{\pm}$ extend to $\mathcal{J}$ with $\operatorname{supp}\mathcal{J}$ compact to the past/future and for such $\mathcal{J}$, $\mathcal{A}^{\pm}=E_M^{\pm}\mathcal{J}$ is the unique solution of $(\Box+M^2)A^{\pm}=\mathcal{J}$ with $\operatorname{supp}\mathcal{A}$ compact to the past/future. In addition, we introduce the advanced-minus-retarded bisolution[75]

$$E_M=E_M^{-}-E_M^{+}\,, \tag{23}$$

which satisfies the homogenous Klein–Gordon equation

$$(\Box+M^2)E_M=E_M(\Box+M^2)=0\,. \tag{24}$$

We also note that, since $\mathbf{d}$ and $\boldsymbol{\delta}$ commute with the Klein–Gordon operator $\Box+M^2$ (or, more precisely, intertwine its action on zero- and one-forms) these operators also intertwine the action of $E_M^{\pm}$ on zero- and one-forms.

The fundamental solutions for the one-form Klein–Gordon equation allow us to solve the inhomogeneous Proca equation,

$$(-\boldsymbol{\delta}\mathbf{d}+M^2)\mathcal{A}=\mathcal{J}, \tag{25}$$

with advanced $(-)$ or retarded $(+)$ boundary conditions. Assuming the existence of a solution and applying the coderivative, we find $\boldsymbol{\delta}\mathcal{A}=M^{-2}\boldsymbol{\delta}\mathcal{J}$. This allows us to rewrite (25) as

$$(\Box+M^2)\mathcal{A}=(-\boldsymbol{\delta}\mathbf{d}+M^2)\mathcal{A}-\mathbf{d}\boldsymbol{\delta}\mathcal{A}=\mathcal{J}-M^{-2}\,\mathbf{d}\boldsymbol{\delta}\,\mathcal{J}, \tag{26}$$

to which $\mathcal{A}^{\pm}=E_M^{\pm}(\mathcal{J}-M^{-2}\,\mathbf{d}\boldsymbol{\delta}\mathcal{J})$ are the unique solutions with support in $J^{\pm}(\operatorname{supp}\mathcal{J})$. Using the property $\boldsymbol{\delta}E_M^{\pm}=E_M^{\pm}\boldsymbol{\delta}$, these may be shown to be the required solutions to (25). We write

$$\Delta_M^{\pm}=E_M^{\pm}(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta}) \tag{27}$$

for the corresponding solution operators and define

$$\Delta_M=\Delta_M^{-}-\Delta_M^{+}\,, \tag{28}$$

which will later appear in the commutation relations for the quantized Proca field. We will also use the notation Δ_M and E_M for the bidistributions defined by $\Delta_M(f,g)=\langle f,\Delta_M g\rangle$ and $E_M(f,g)=\langle f,E_M g\rangle$ $(f,g\in\Omega_0^1(\mathcal{M}))$.

Turning to electromagnetism, the theory is described by a one-form potential $\mathcal{A}\in\Omega^1(\mathcal{M})$ obeying

$$\boldsymbol{\delta}\mathbf{d}\mathcal{A}=0\,, \tag{29}$$

which entails that the field strength $\mathcal{F}=\mathbf{d}\mathcal{A}$ obeys Maxwell's equations,

$$\mathbf{d}\mathcal{F}=0 \quad \text{and} \quad \boldsymbol{\delta}\mathcal{F}=0\,. \tag{30}$$

Two potentials $\mathcal{A}$ and $\mathcal{A}'$ are gauge equivalent, denoted by $\mathcal{A}\sim\mathcal{A}'$, if $\mathcal{A}=\mathcal{A}'+\mathbf{d}\chi$ for some $\chi\in\Omega^0(\mathcal{M})$. Since gauge equivalent potentials lead to the same field strength, it is really the gauge equivalence classes $[\mathcal{A}]$ of solutions which are of physical significance rather than the potentials themselves. We can partially fix the gauge freedom by passing to the Lorentz gauge $\boldsymbol{\delta}\mathcal{A}=0$, in which the Maxwell equations are expressed by the $M=0$ case of the system (20), (21). Just as with the Proca equation, the fundamental solutions to (20) permit us to solve the inhomogeneous Maxwell equation

$$-\boldsymbol{\delta}\mathbf{d}\mathcal{A}=\mathcal{J}, \tag{31}$$

where, for consistency, the source $\mathcal{J}\in\Omega_0^1(\mathcal{M})$ is required to obey the current conservation equation $\boldsymbol{\delta}\mathcal{J}=0$. Defining $\mathcal{A}^{\pm}=E_0^{\pm}\mathcal{J}$, we note that $\boldsymbol{\delta}\mathcal{A}^{\pm}=\boldsymbol{\delta}E_0^{\pm}\mathcal{J}=E_0^{\pm}\boldsymbol{\delta}\mathcal{J}=0$ and therefore deduce that $\mathcal{A}^{\pm}$ is the unique Lorentz gauge solution to (31) with support in $J^{\pm}(\mathrm{supp}\,\mathcal{J})$.

B. Quantization: Algebras of observables

The canonical quantization of the Maxwell and Proca fields in globally hyperbolic space–times was accomplished by Dimock[36] and Furlani,[37] respectively (see also Ref. 43). Here, we give a direct construction of suitable algebras of (polynomials in) smeared fields for these theories, isomorphic to those emerging from the constructions of Refs. 36 and 37. We begin with the more straightforward Proca case, for which the algebra of observables will be denoted $\mathfrak{A}_M(\mathcal{M},g)$. This algebra is constructed by first using the set of smooth compactly supported complex valued one-form test functions $\Omega_0^1(\mathcal{M})$ to label a set of abstract objects $\{\mathcal{A}(f)|f\in\Omega_0^1(\mathcal{M})\}$ which generate a free unital $*$-algebra over $\mathbb{C}$. These objects are interpreted as smeared one-form fields

$$\mathcal{A}(f)\ \text{`}=\text{'}\ \langle\mathcal{A},f\rangle\,. \tag{32}$$

The algebra $\mathfrak{A}_M(\mathcal{M},g)$ is defined to be the quotient of $\mathfrak{A}_M$ by the following relations:

(P1) Linearity, $\mathcal{A}(\alpha f_1+\beta f_2)=\alpha\mathcal{A}(f_1)+\beta\mathcal{A}(f_2)$ for all $\alpha,\beta\in\mathbb{C}$ and $f_i\in\Omega_0^1(\mathcal{M})$;
(P2) Hermiticity, $\mathcal{A}(f)^*=\mathcal{A}(\overline{f})$ for all $f\in\Omega_0^1(\mathcal{M})$;
(P3) Field equations, $\mathcal{A}([\boldsymbol{\delta}\mathbf{d}-M^2]f)=0$ for all $f\in\Omega_0^1(\mathcal{M})$;
(P4) CCRs, $[\mathcal{A}(f_1),\mathcal{A}(f_2)]=-i\Delta_M(f_1,f_2)\mathbb{1}$ for all $f_i\in\Omega_0^1(\mathcal{M})$.

Here, Δ_M is the propagator defined in (28).

For electromagnetism, quantization is complicated by gauge freedom. Even in Minkowski space this presents serious problems: as shown by Strocchi[44,45] in the Wightman axiomatic approach, the vector potential cannot exist as an operator-valued distribution if it is to transform correctly under the Lorentz group or even display commutativity at spacelike separations in a weak sense. Dimock[36] circumvented such problems by constructing smeared field operators $[\mathcal{A}]\times(f)$ which may be smeared only with co-closed (divergence-free) test functions, i.e., f must satisfy $\boldsymbol{\delta}f=0$. These objects may be interpreted as smeared gauge-equivalence classes of quantum one-form fields: formally,

$$[\mathcal{A}](f)\ \text{`}=\text{'}\ \langle\mathcal{A},f\rangle\,, \tag{33}$$

where $\mathcal{A}$ is a representative of the equivalence class $[\mathcal{A}]$; since $\boldsymbol{\delta}f=0$, we have $\langle\mathbf{d}\chi,f\rangle=\langle\chi,\boldsymbol{\delta}f\rangle=0$ so this interpretation is indeed gauge independent. Adapting this idea to our present setting, we start with a set of abstract objects $\{[\mathcal{A}](f)\,|f\in\Omega_0^1(\mathcal{M})$ with $\boldsymbol{\delta}f=0\}$ labeled only by co-closed test one-forms. As before, we use this set to generate a free unital $*$-algebra over $\mathbb{C}$ and define the algebra of observables $\mathfrak{A}(\mathcal{M},g)$ to be the quotient of this algebra by the following relations:

(M1) Linearity, $[\mathcal{A}](\alpha f_1+\beta f_2)=\alpha[\mathcal{A}](f_1)+\beta[\mathcal{A}](f_2)$ for all $\alpha,\beta\in\mathbb{C}$ and co-closed $f_i \in\Omega^1_0(\mathcal{M})$;
(M2) Hermiticity, $[\mathcal{A}](f)^*=\mathcal{A}(\overline{f})$ for all co-closed $f\in\Omega^1_0(\mathcal{M})$;
(M3) Field equations, $[\mathcal{A}](\boldsymbol{\delta}\mathbf{d}f)=0$ for all $f\in\Omega^1_0(\mathcal{M})$;
(M4) CCRs, $[[\mathcal{A}](f_1),[\mathcal{A}](f_2)]=-iE_0(f_1,f_2)\mathbb{1}$ for all co-closed $f_i\in\Omega^1_0(\mathcal{M})$.

[Note that the one-forms f appearing in axiom (M3) need not be co-closed.]

To see that these algebras are equivalent to those constructed in Refs. 36 and 37, it suffices to observe that, first, the field operators of Refs. 36 and 37 certainly satisfy the relations above (see Proposition 8 of Ref. 36 and Theorem 3 of Ref. 37; note that there are notational differences) and, second, that the algebras we have constructed admit no nontrivial quotients, as may be seen by applying the theory of Sec. 7.1 in Refs. 46 and 76. Accordingly, our algebras are isomorphic to those of Refs. 36 and 37.

C. Quantization: Hadamard states

A *state* on a $*$-algebra $\mathfrak{A}$ is a linear functional $\omega:\mathfrak{A}\to\mathbb{C}$ which is normalized so that $\omega(\mathbb{1})=1$ and has the positivity property $\omega(\mathcal{B}^*\mathcal{B})\geqslant 0$ for all $\mathcal{B}\in\mathfrak{A}$. However, not all states on $\mathfrak{A}_M(\mathcal{M},g)$ and $\mathfrak{A}(\mathcal{M},g)$ are of physical relevance—many are insufficiently regular to permit the definition of the stress-tensor, for example. We will focus attention on the class of *Hadamard* states, for which the stress-tensor may be defined by point-splitting techniques. The Hadamard condition was first stated rigorously for the scalar field by Kay and Wald;[47] more recently, Sahlmann and Verch[32] have studied the Hadamard form for wave equations with metric principal part. This does not immediately cover either the Maxwell or Proca equations (which are not hyperbolic). Nonetheless, we may exploit the close relationship of these equations to the one-form Klein–Gordon equation to define the notion of Hadamard states for these theories.

To be more specific, a distribution $W\in(\Omega^1_0(\mathcal{M})\times\Omega^1_0(\mathcal{M}))'$ is said to be of Hadamard form if its singular part takes a prescribed form in a causal normal neighborhood $\mathcal{N}$ of some Cauchy surface in $\mathcal{M}$. This requirement is implemented by requiring that $W-H_k$ should be C^k for each $k\in\mathbb{N}$, where H_k is a prescribed sequence of distributions on $\mathcal{N}\times\mathcal{N}$. Furthermore—as in the scalar case[47,48]—if W is a bisolution to $\Box+M^2$ (or even a bisolution modulo C^∞) then the Hadamard form propagates in the sense that W will satisfy the above criterion in any causal normal neighborhood of any Cauchy surface in $\mathcal{M}$ (see Theorem 5.5 in Ref. 32). It follows that the difference $W-W'$ between Hadamard form $(\Box+M^2)$-bisolutions W and W' is everywhere smooth on $\mathcal{M}\times\mathcal{M}$. For our purposes, the second crucial property of a Hadamard bisolution W (first noted in the scalar case by Radzikowski[29]) is that its wave-front set is given explicitly by

$$\mathrm{WF}(W)=\mathcal{R}:=\{(x,k;x',-k')\in\dot{T}^*(\mathcal{M}\times\mathcal{M}) : (x,k)\sim(x',k') \text{ and } k\in\overline{V}^+_x\}. \tag{34}$$

Here, $\dot{T}^*(\mathcal{M}\times\mathcal{M})$ denotes the cotangent bundle of $\mathcal{M}\times\mathcal{M}$ with its zero section excised, and $(x,k)\sim(x',k')$ if and only if k' is the parallel transport of k along a null geodesic connecting x and x', to which k is a cotangent vector at x (if $x=x'$ this degenerates to the requirement that $k=k'$ is null). We have also used $\overline{V}^+_x$ to denote the closed cone of future pointing covectors at x. It is also worth noting that the wave-front set condition essentially characterizes the Hadamard form [see Remark 5.9(i) in (Ref. 32)]: if W is a $(\Box+M^2)$-bisolution $(\mathrm{mod}\,C^\infty)$ which obeys Eq. (34) and has $W(f_1,f_2)-W(f_2,f_1)=-iE_M(f_1,f_2)$ $(\mathrm{mod}\,C^\infty)$ then W is of Hadamard form.

We are now in a position to define the notion of a Hadamard state for the Maxwell and Proca fields. Our definitions are similar to those employed by Junker and Lledó[35] and (particularly in the Maxwell case) were influenced by early versions of their work.[49]

Proca: A state ω on $\mathfrak{A}_M(\mathcal{M},g)$ is Hadamard if there exists a Hadamard form $(\Box+M^2)$-bisolution W_M such that

$$\omega(\mathcal{A}(f_1)\mathcal{A}(f_2))=W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2) \tag{35}$$

for all $f_i \in \Omega_0^1(\mathcal{M})$.

Maxwell: A state ω on $\mathfrak{A}(\mathcal{M},g)$ is Hadamard if there exists a Hadamard form $\Box$-bisolution W such that

$$\omega([\mathcal{A}](f_1)[\mathcal{A}](f_2)) = W(f_1,f_2) \tag{36}$$

for all $f_i \in \Omega_0^1(\mathcal{M})$ with $\boldsymbol{\delta} f_i = 0$.

Remarks: (a) In neither case is the Hadamard form bisolution uniquely determined by the state.

(b) As stated, these conditions appear global in nature and it is not clear, *a priori*, that any states satisfying these definitions exist in general space–times. These concerns will be allayed in Sec. IV E, where we show that Hadamard states exist on general globally hyperbolic space–times (subject to our usual topological restrictions on Σ). A key part of this argument is the proof (in Appendix A) that it suffices for Eqs. (35) and (36) to hold for f_i supported in a causal normal neighborhood of a Cauchy surface for them to hold for all f_i. In combination with an explicit construction of a Hadamard state in ultrastatic space–times (in Secs. IV B and IV C) this permits us to apply standard deformation arguments[38] to deduce the existence of Hadamard states in general.

(c) Since the two-point function $\omega^{(2)}(f,f') := \omega(\mathcal{A}(f_1)\mathcal{A}(f_2))$ for a Hadamard state ω of the Proca field is given by acting on a Hadamard $(\Box + M^2)$-bisolution with a partial differential operator, we may use Eq. (34) and the nonexpansion of the wave-front set under such operators to obtain

$$\mathrm{WF}(\omega^{(2)}) \subseteq \mathcal{R}. \tag{37}$$

In the Maxwell case, the two-point function $\omega^{(2)}(f,f') := \omega([\mathcal{A}](f_1)[\mathcal{A}](f_2))$ is not a distribution (because it is only defined on co-closed test one-forms f_i). However, the two-point function of the field strength $\mathcal{F}(f) := [\mathcal{A}](\boldsymbol{\delta} f)$ is a bidistribution on two-forms satisfying

$$\omega(\mathcal{F}(f_1)\mathcal{F}(f_2)) = W(\boldsymbol{\delta} f_1, \boldsymbol{\delta} f_2) \tag{38}$$

and therefore has wave-front set contained in $\mathcal{R}$.

(d) The Hadamard condition for electromagnetism was discussed in Refs. 33 and 34 in the context of a Faddeev–Popov method. Here, the action is modified by the addition of a gauge breaking term and the ghost action, describing the dynamics of a complex, anticommuting scalar field. In that context, the electromagnetic potential may be smeared with arbitrary one-form test fields and so the corresponding two-point function is a distributional bisolution to the massless Klein–Gordon equation (at least in the Feynman gauge). In a Hadamard state (on the algebra generated by the vector potential and the ghost fields), this two-point function is required to be of Hadamard form [thus generalizing (36) to non-co-closed f_i]; in addition, a Ward identity is required to connect this two-point function to that of the ghost field. This ensures that the contributions to the stress-energy tensor arising from the gauge-breaking and ghost actions precisely cancel in Hadamard states.

IV. HADAMARD STATES IN ULTRASTATIC SPACE–TIMES

To provide a concrete example of the foregoing definitions, we now specialize to the class of ultrastatic space–times. Although one may quantize the Maxwell and Proca fields directly in such space–times (see, e.g., Refs. 50 and 51) it appears that no attention has been given to whether the resulting Fock vacua are Hadamard. Our approach is rather to construct a distinguished Hadamard state and then to observe that the corresponding representations coincide with those obtained directly. Our analysis of the ultrastatic case will also lead to a proof of the existence of Hadamard states for the Proca and Maxwell fields in general globally hyperbolic space–times as well as providing explicit two-point functions for particular Hadamard states which will be used in Sec. VI. We recall that a space–time $(\mathcal{M},g)$ is said to be ultrastatic if $\mathcal{M} = \mathbb{R} \times \Sigma$ and $g = 1 \oplus -h$,

where (Σ,h) is a smooth Riemannian manifold. As usual, we will also assume that Σ is compact and the homology group $H_1(\Sigma)$ is trivial. We will often denote a point in $\mathcal{M}$ by the pair $(t,\underline{x})$, with $t\in\mathbb{R}$, $\underline{x}\in\Sigma$.

Our discussion in this section will proceed as follows. We begin with the construction of a one-form Hadamard $(\Box+M^2)$-bisolution W_M on $(\mathcal{M},g)$. Next, we construct Fock representations of the Proca and Maxwell fields on $(\mathcal{M},g)$ with the property that the Fock vacuum in each case is Hadamard according to the definitions of the preceding section. In each case, the W_M plays the role of the required Hadamard $(\Box+M^2)$-bisolution. We also discuss the relationship of our procedure to the Gupta–Bleuler approach and the method of quantization in a fixed gauge. Finally, we explain how these results imply the existence of Hadamard states in general space–times. Some parts of the analysis are relegated to Appendix B.

A. Construction of a Hadamard $(\Box+M^2)$-bisolution

As is well-known, the Klein–Gordon equation in an ultrastatic space–time is readily reduced to the analysis of an elliptic eigenvalue problem. Namely, if $\xi\in\Omega^1(\mathcal{M})$ is a static one-form (i.e., independent of the ultrastatic time parameter t) then $\mathcal{A}(t,\underline{x})=e^{-i\omega t}\xi(\underline{x})$ solves the one-form Klein–Gordon equation if and only if

$$K\xi=\omega^2\xi, \tag{39}$$

where the operator K acts on $\xi(\underline{x})=\xi_0(\underline{x})\mathbf{d}t+\xi_\Sigma(\underline{x})$ $(\xi_0\in\Omega^0(\Sigma),\ \xi_\Sigma\in\Omega^1(\Sigma))$ by

$$K\xi=((-\Delta_\Sigma^s+M^2)\xi_0)\mathbf{d}t+(-\Delta_\Sigma+M^2)\xi_\Sigma\,, \tag{40}$$

with Δ_Σ^s and Δ_Σ denoting the scalar and one-form Laplace–Beltrami operators on (Σ,h).

To analyze K further, it is helpful to have various inner product spaces in mind. For each p, the space $\Omega^p(\Sigma)$ may be endowed with a positive definite inner product

$$(u,v)_{\Lambda^p(\Sigma)}=\int_\Sigma \overline{u}\wedge *_\Sigma v\,, \tag{41}$$

where $*_\Sigma$ is the Hodge operator on (Σ,h). By completing $\Omega^p(\Sigma)$ with respect to the corresponding norm we obtain the Hilbert space $\Lambda^p(\Sigma)$ of square integrable p-forms on Σ. The direct sum $\mathsf{H}=\Lambda^0(\Sigma)\oplus\Lambda^1(\Sigma)$ therefore corresponds to a Hilbert space of static one-forms, on which the K may be defined as a positive self-adjoint operator [by using Eq. (40) to define K on $\Omega^0(\Sigma)\oplus\Omega^1(\Sigma)$ and then forming the Friedrichs extension]. Because Σ is compact, K has a purely discrete spectrum.

From a geometrical viewpoint, however, the Hilbert space inner product is not completely natural. It is therefore convenient to introduce an indefinite inner product on H by

$$\langle\!\langle\xi|\,\eta\rangle\!\rangle=\int_\Sigma \overline{\xi_\mu(\underline{x})}\;\eta^\mu(\underline{x})\,\mathrm{d}\,\mathrm{vol}_h(\underline{x})=(\xi_0,\eta_0)_{\Lambda^0(\Sigma)}-(\xi_\Sigma,\eta_\Sigma)_{\Lambda^1(\Sigma)}\,. \tag{42}$$

We will denote the resulting indefinite inner product space (also known as a *Krein space*) by K. In addition, we will say that a set $\{\xi_j:j\in J\}$ of vectors (labeled by the elements of some set J) in K is *pseudo-orthonormal* if $\langle\!\langle\xi_j|\xi_j\rangle\!\rangle=\pm1$ for each j and $\langle\!\langle\xi_j|\xi_{j'}\rangle\!\rangle=0$ for all $j\neq j'$; the set is said to be complete if

$$\eta=\sum_{j\in J}\langle\!\langle\xi_j|\xi_j\rangle\!\rangle\langle\!\langle\xi_j|\,\eta\rangle\!\rangle\,\xi_j \tag{43}$$

holds for all $\eta\in\mathsf{K}$, with the sum converging in the topology induced by the norm of H. We will refer to $\xi\in\mathsf{K}$ as timelike, spacelike or null depending on whether $\langle\!\langle\xi|\xi\rangle\!\rangle$ is positive, negative or zero, respectively.

The following result is proved in Appendix B.

Theorem IV.1: *Let* ξ_j $(j \in J)$ *be a complete, pseudo-orthonormal basis for* K *such that* $K\xi_j = \omega_j^2 \xi_j$ $(\omega_j \geqslant 0)$ *and set* $\mathcal{A}_j(t,\underline{x}) = e^{-i\omega_j t}\xi_j(\underline{x})$. *Then*

$$W_M(f_1,f_2) = -\sum_{j\in J:\omega_j>0} \frac{1}{2\omega_j} \langle\!\langle \xi_j | \xi_j \rangle\!\rangle \langle \mathcal{A}_j, f_1\rangle \langle \overline{\mathcal{A}_j}, f_2\rangle \quad (f_i \in \Omega^1(\Sigma)) \tag{44}$$

defines a one-form Hadamard $(\Box + M^2)$*-bisolution* W_M *on* $(\mathcal{M},g)$ *which is independent of the particular basis chosen. For* $M>0$, *we have*

$$W_M(f_1,f_2) - W_M(f_2,f_1) = -iE_M(f_1,f_2) \tag{45}$$

for all $f_i \in \Omega_0^1(\mathcal{M})$; *in the case* $M=0$, *this holds provided the* f_i *are both co-closed.*

Our task is now to analyze the eigenproblem (39). We may identify various families of eigenfunctions which are more or less convenient for different purposes and which may be combined to form complete pseudo-orthonormal bases (again, different bases are useful in different contexts). A typical eigenfunction will be denoted $\xi(\lambda,j)$, where λ labels the family to which it belongs and j (which labels eigenfunctions within families) takes values in a labeling set $J(\lambda)$. Because K is manifestly positive, the eigenvalues may be expressed as the squares of non-negative quantities $\omega(\lambda,j)$: thus $K\xi(\lambda,j) = \omega(\lambda,j)^2\xi(\lambda,j)$. The corresponding Klein–Gordon solution is

$$\mathcal{A}(\lambda,j)(t,\underline{x}) = e^{-i\omega(\lambda,j)t}\xi(\lambda,j)(\underline{x})\,. \tag{46}$$

We begin by identifying three eigenfunction families which together form a simultaneously K-pseudo-orthonormal and H-orthonormal basis. The analysis of Eq. (39) is considerably simplified by the fact that it decouples into the two equations

$$(-\Delta_\Sigma^s + M^2)\xi_0 = \omega^2\xi_0\,, \tag{47}$$

$$(-\Delta_\Sigma + M^2)\xi_\Sigma = \omega^2\xi_\Sigma\,. \tag{48}$$

Accordingly, choosing φ_j $(j \in J(S))$ to label a complete orthonormal basis of $(-\Delta_\Sigma^s + M^2)$-eigenfunctions for $\Lambda^0(\Sigma)$ with corresponding eigenvalues $\omega(S,j)^2$, we may identify a family of "scalar" K-eigenfunctions given by

$$\xi(S,j) = \varphi_j\,\mathbf{d}t \quad (j \in J(S))\,. \tag{49}$$

(By elliptic regularity, each φ_j is in fact smooth.) Clearly the $\xi(S,j)$ are pseudo-orthonormal and timelike in K, as well as being H orthonormal. For future reference, we note that there is a unique spatially constant eigenfunction $\mathrm{vol}_h(\Sigma)^{-1/2}\,\mathbf{d}t$ with eigenvalue M^2. Writing $\Phi_j(t,\underline{x}) = e^{-i\omega(S,j)t}\varphi_j(\underline{x})$, the corresponding one-form positive frequency modes are

$$\mathcal{A}(S,j) = \Phi_j\,\mathbf{d}t\,. \tag{50}$$

The remaining pseudo-orthogonal modes must have vanishing $\mathbf{d}t$ component; that is, they must lie in the spacelike subspace $\Lambda^1(\Sigma)$ of H. On this subspace, the inner products of H and K differ by an overall sign only, so K-pseudo-orthonormality and H-orthonormality are again identical. Since $H_1(\Sigma)$ is trivial, the Hodge decomposition (see, e.g., Prop. 11.7 in Ref. 52) gives $\Lambda^1(\Sigma) = \overline{\mathbf{d}_\Sigma\Omega^0(\Sigma)} \oplus \overline{\boldsymbol{\delta}_\Sigma\Omega^2(\Sigma)}$, where the decomposition is orthogonal with respect to $(\cdot,\cdot)_{\Lambda^1}$ and hence $\langle\!\langle\cdot|\cdot\rangle\!\rangle$, and the bars denote closure. As is easily verified, the Laplacian Δ_Σ is block diagonal with respect to this decomposition, thus enabling us to seek eigenfunctions within each subspace in turn. If the restriction on $H_1(\Sigma)$ were removed, there would be a third subspace, consisting of harmonic forms (i.e., the kernel of Δ_Σ). In the Proca case, the resulting modes lead to additional terms in various expansions given below and in the quantum inequality, but do not

significantly alter the formalism. By contrast, the incorporation of the harmonic modes in the Maxwell case raises nontrivial issues, to which we hope to return elsewhere.

Now, the ''longitudinal'' subspace $\overline{\mathbf{d}_\Sigma \Omega^0(\Sigma)}$ is clearly spanned by the set of nonvanishing vectors of the form $\mathbf{d}\xi(S,j)$ $(j \in J(S))$; owing to the relation $\Delta_\Sigma \mathbf{d}_\Sigma = \mathbf{d}_\Sigma \Delta_\Sigma^S$, these must also be eigenvectors for $-\Delta_\Sigma + M^2$ with eigenvalue $\omega(L,j)^2 = \omega(S,j)^2$. As the only vanishing vector of this form is obtained from the spatially constant mode, the appropriate labeling set is $J(L) = \{j \in J(S) : \omega(S,j) > M\}$. Furthermore, the calculation

$$\langle\langle \mathbf{d}_\Sigma \varphi_j | \mathbf{d}_\Sigma \varphi_{j'} \rangle\rangle = -(\mathbf{d}_\Sigma \varphi_j, \mathbf{d}_\Sigma \varphi_{j'})_{\Lambda^1(\Sigma)} = -(\varphi_j, \boldsymbol{\delta}_\Sigma \mathbf{d}_\Sigma \varphi_{j'})_{\Lambda^1(\Sigma)} = -(\omega(S,j)^2 - M^2)\delta_{jj'} \quad (51)$$

shows that the appropriately normalized longitudinal eigenfunctions are

$$\xi(L,j) = (\omega(S,j)^2 - M^2)^{-1/2} \mathbf{d}_\Sigma \varphi_j \quad (j \in J(L)). \quad (52)$$

The corresponding Klein–Gordon modes may also be expressed in the form

$$\mathcal{A}(L,j) = \frac{\mathbf{d}\Phi_j + i\omega(L,j)\Phi_j \mathbf{d}t}{\sqrt{\omega(L,j)^2 - M^2}}. \quad (53)$$

All remaining pseudo-orthonormal modes must lie in the coexact subspace $\boldsymbol{\delta}_\Sigma \Omega^2(\Sigma)$. We will refer to these as the transverse modes $\xi(T,j)$ with labeling set $J(T)$ and eigenfrequencies $\omega(T,j)$; they are necessarily spacelike. In general, the $\omega(T,j)$'s will be distinct from the $\omega(S,j)$'s (even in situations of high symmetry such as the Einstein space–time—see Sec. VI C).

Applying Theorem IV A, we obtain a Hadamard bisolution

$$W_M(f_1,f_2) = -\sum_{\lambda \in \{S,L,T\}} \sum_{j \in J(\lambda)} \frac{s(\lambda)}{2\omega(\lambda,j)} \langle \mathcal{A}(\lambda,j), f_1 \rangle \langle \overline{\mathcal{A}(\lambda,j)}, f_2 \rangle, \quad (54)$$

where $s(S) = 1$, $s(L) = s(T) = -1$.

B. The Proca field

We now construct a state on $\mathfrak{A}_M(\mathcal{M},g)$ whose two-point function is related to W_M by Eq. (35) and is therefore Hadamard. We begin by finding an expression for $W_M(f_1, (\mathbb{1} - M^{-2}\mathbf{d}\boldsymbol{\delta}) f_2)$. To this end, we first note that the transverse modes $\xi(T,j)$, being coexact, are necessarily co-closed: $\boldsymbol{\delta}_\Sigma \xi(T,j) = 0$. It follows that $\boldsymbol{\delta}\mathcal{A}(T,j) = 0$, so transverse modes therefore solve the Proca equation. The same cannot be said of the scalar and longitudinal modes, for which

$$\boldsymbol{\delta}\mathcal{A}(S,j) = i\omega(S,j)\Phi_j \quad (55)$$

for all $j \in J(S)$, and

$$\boldsymbol{\delta}\mathcal{A}(L,j) = -\sqrt{\omega(S,j)^2 - M^2}\Phi_j \quad (56)$$

for all $j \in J(L)$. It is convenient to change basis, introducing

$$\xi(P,j) = \frac{1}{M}[\omega(S,j)\xi(L,j) - i\sqrt{\omega(S,j)^2 - M^2}\xi(S,j)], \quad (57)$$

$$\xi(G,j) = \frac{1}{M}[\sqrt{\omega(S,j)^2 - M^2}\xi(L,j) - i\omega(S,j)\xi(S,j)] \quad (58)$$

with labeling sets $J(P)=J(G)=J(L)$. The two sets are pseudo-orthonormal, with $\xi(P,j)$ and $\xi(G,j)$ being spacelike and timelike, respectively. By construction, the "scalar Proca" modes $\mathcal{A}(P,j)(t,\underline{x})=e^{-i\omega(P,j)t}\xi(P,j)(\underline{x})$ are co-closed and therefore obey the Proca equation. We also note the expressions

$$\mathcal{A}(P,j)=\frac{1}{M}[\,\omega(S,j)\mathcal{A}(L,j)-i\sqrt{\omega(S,j)^2-M^2}\mathcal{A}(S,j)\,]$$

$$=\frac{iM}{\sqrt{\omega(S,j)^2-M^2}}\left[\,\Phi_j\,\mathbf{d}t-i\,\frac{\omega(S,j)}{M^2}\,\mathbf{d}\Phi_j\right]. \tag{59}$$

On the other hand, the corresponding "gradient" modes $\mathcal{A}(G,j)$ have

$$\mathcal{A}(G,j)=M^{-1}\,\mathbf{d}\Phi_j \tag{60}$$

and therefore have nonvanishing coderivative

$$\boldsymbol{\delta}\mathcal{A}(G,j)=M\Phi_j\,. \tag{61}$$

From Theorem IV A, we know that W_M is basis independent and may therefore be expressed in terms of the $\mathcal{A}(P,j)$, $\mathcal{A}(G,j)$, $\mathcal{A}(T,j)$ and the unique spatially constant mode. Of these, the scalar Proca and transverse modes are left invariant by the operator $(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})$, while the spatially constant mode and the gradient modes are annihilated. Accordingly, with W_M expressed in the new basis, we find

$$W_M((\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_1,f_2)=W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2)$$

$$=\sum_{\lambda\in\{T,P\}}\sum_{j\in J(\lambda)}\frac{1}{2\omega(\lambda,j)}\langle\mathcal{A}(\lambda,j),f_1\rangle\,\langle\overline{\mathcal{A}(\lambda,j)},f_2\rangle\,. \tag{62}$$

As a consequence of the first equality and Eq. (45) we see that

$$W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2)-W_M(f_2,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_1)=-iE_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2)$$

$$=-i\Delta_M(f_1,f_2), \tag{63}$$

which in turn leads to the expansion

$$\Delta_M(f_1,f_2)=\sum_{\lambda\in\{T,P\}}\sum_{j\in J(\lambda)}\frac{1}{2\omega(\lambda,j)}(\langle\mathcal{A}(\lambda,j),f_1\rangle\,\langle\overline{\mathcal{A}(\lambda,j)},f_2\rangle-\langle\mathcal{A}(\lambda,j),f_2\rangle\,\langle\overline{\mathcal{A}(\lambda,j)},f_1\rangle)\,. \tag{64}$$

To complete the analysis, we define smeared fields

$$\mathcal{A}(f)=\sum_{\lambda\in\{T,P\}}\sum_{j\in J(\lambda)}\frac{1}{\sqrt{2\omega(\lambda,j)}}(\langle\mathcal{A}(\lambda,j),f\rangle\,a(\lambda,j)+\langle\overline{\mathcal{A}(\lambda,j)},f\rangle\,a(\lambda,j)^*) \tag{65}$$

on the Fock space F_M generated by operators $a(\lambda,j)$ obeying $[a(\lambda,j),a(\lambda',j')^*]=\delta_{\lambda\lambda'}\delta_{jj'}\mathbb{1}$. It is now easily verified that the $\mathcal{A}(f)$ provide a representation of axioms (P1)–(P4) on (a dense domain) F_M. Thus the Fock vacuum $|0\rangle$ defines a state on $\mathfrak{A}_M(\mathcal{M},g)$ with two-point function

$$\langle 0|\mathcal{A}(f_1)\mathcal{A}(f_2)|0\rangle=W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2)\,. \tag{66}$$

Accordingly, this state is Hadamard. Acting on the vacuum with smeared fields, we obtain a dense set of Hadamard states in F_M.

C. The Maxwell field

We now repeat the above analysis for the Maxwell field. In this instance, we begin by finding an expression for $W_0(f_1,f_2)$ for co-closed f_i. Since the $\mathcal{A}(P,j)$ and $\mathcal{A}(G,j)$ diverge as $M\to 0$, we revert to the scalar, longitudinal, and transverse modes of Sec. IV A. Now, from Eqs. (50) and (53), it is simple to show $\langle \mathcal{A}(L,j),F\rangle = i\langle \mathcal{A}(S,j),F\rangle$ for all co-closed F. This has the effect that the contributions to $W_0(f_1,f_2)$ from the scalar and longitudinal modes cancel and so only has contributions from the transverse modes:

$$W_0(f_1,f_2)=\sum_{j\in J(T)}\frac{1}{2\omega(T,j)}\langle \mathcal{A}(T,j),f_1\rangle\,\langle\overline{\mathcal{A}(T,j)},f_2\rangle\,, \tag{67}$$

for any co-closed f_i. Defining

$$[\mathcal{A}](f)=\sum_{j\in J(T)}\frac{1}{\sqrt{2\omega(T,j)}}(\langle \mathcal{A}(T,j),f\rangle\, a(T,j)+\langle\overline{\mathcal{A}(T,j)},f\rangle\, a(T,j)^*) \tag{68}$$

on the Fock space F_0 generated by operators $a(T,j)$ obeying $[a(T,j),a(T,j')^*]=\delta_{jj'}\mathbb{1}$, we may again verify that the $[\mathcal{A}](f)$ provide a representation of axioms (M1)–(M4) on (a dense domain in) F_0. Thus the Fock vacuum $|0\rangle$ defines a state on $\mathfrak{A}(\mathcal{M},g)$ with two-point function

$$\langle 0|[\mathcal{A}](f_1)[\mathcal{A}](f_2)|0\rangle = W_0(f_1,f_2) \tag{69}$$

for all co-closed f_i and is therefore Hadamard, as are states obtained from it by acting with polynomials in smeared fields.

D. Comparison with other quantization methods

It is instructive to compare our approach to two more familiar methods of quantization, in particular, the Gupta–Bleuler formalism[50,53,54] and (for electromagnetism) quantization in a fixed gauge. A detailed presentation of these methods for electromagnetic fields in static space–times can be found in Ref. 27. We will confine our remarks to the Maxwell case, but analogous comments apply to the Proca field.

As is well-known, the Gupta–Bleuler procedure starts by adding a gauge breaking term to the Maxwell Lagrangian. By choosing the coefficient of this term appropriately, the field equations become precisely those of the massless Klein–Gordon equation. (This is sometimes known as the Feynman gauge.) This equation is then quantized using an indefinite inner product space [effectively the symmetric Fock space $\mathsf{F}(\mathsf{K})$ over our Krein space K]. The physical Hilbert space is then selected by the requirement that they be annihilated by the positive frequency part of the divergence of the resulting field operators.

In our approach the various ingredients of the Gupta–Bleuler formalism appear in a different way. We start from the Hadamard bisolution W_0, which is in fact the two-point function of the static vacuum of the Gupta–Bleuler theory in the indefinite space $\mathsf{F}(\mathsf{K})$. In our approach, however, the restriction to the physical state space occurs at the one-particle level: the Hadamard condition and the restriction to co-closed test one-forms pick out a preferred Hilbert subspace of K, namely, the subspace H_{phys} spanned by the transverse modes $\xi(T,j)$. The quantum fields are then given immediately as operators on the symmetric Fock space $\mathsf{F}_0=\mathsf{F}(\mathsf{H}_{\text{phys}})$ over this Hilbert space. The key advantage of our approach over the Gupta–Bleuler method is, of course, that it is not tied to a particular notion of positive frequency and is applicable in general globally hyperbolic space–times.

An alternative to the Gupta–Bleuler approach is to fix a gauge from the outset. Employing the Coulomb gauge,[27] we would seek modes $\mathcal{A}_j$ obeying $\boldsymbol{\delta}\mathcal{A}_j=0$ with vanishing $\mathbf{d}t$ component. These modes are easily seen to constitute the transverse family $\mathcal{A}(T,j)$ and we essentially recover the

field operators of Eq. (68), but without the restriction to co-closed f_i. By contrast, no gauge is ever chosen in our approach and the transverse modes emerge naturally from the Hadamard condition in combination with the restriction to co-closed f_i.

E. Existence of Hadamard states in globally hyperbolic space–times

Once the existence of Hadamard states has been established in ultrastatic space–time, arguments due to Fulling, Narcowich, and Wald[38] may be used to deduce their existence in general globally hyperbolic space–times obeying our usual topological restrictions. We illustrate this for the Proca field, indicating the slight differences required in the Maxwell case.

Let $(\mathcal{M},g)$ and $(\mathcal{M}',g')$ be globally hyperbolic space–times and suppose that there is an isometry $\psi:\mathcal{N}\to\mathcal{N}'$ between causal normal neighborhoods $\mathcal{N}$ and $\mathcal{N}'$ of Cauchy surfaces in $\mathcal{M}$ and $\mathcal{M}'$, respectively. Then any state ω on $\mathfrak{A}_M(\mathcal{M},g)$ determines a state ω' on $\mathfrak{A}_M(\mathcal{M}',g')$ as follows: given any $f_1,\ldots,f_n\in\Omega^1_0(\mathcal{M}')$ choose $\tilde{f}_1,\ldots,\tilde{f}_n\in\Omega^1_0(\mathcal{N}')$ such that $\tilde{f}_k-f_k\in(-\boldsymbol{\delta}\mathbf{d}+M^2)\Omega^1_0(\mathcal{M}')$. [The existence of such $\tilde{f}_k$ follows from Proposition A 3(a).] Now define

$$\omega'(\mathcal{A}'(f_1)\cdots\mathcal{A}'(f_n))=\omega(\mathcal{A}(\psi^*\tilde{f}_1)\cdots\mathcal{A}(\psi^*\tilde{f}_n)), \tag{70}$$

where ψ^* denotes the pull-back, $\psi^*f=f\circ\psi$ and we have used $\mathcal{A}'(f)$ to denote field operators in $\mathfrak{A}_M(\mathcal{M}',g')$. It is easily verified that ω' is a state on $\mathfrak{A}_M(\mathcal{M}',g')$. Moreover, if ω is Hadamard then the isometry ensures that $\omega'(\mathcal{A}(f_1)\mathcal{A}(f_2))=W(f_1,(\mathbb{1}-M^{-1}\mathbf{d}\boldsymbol{\delta})f_2)$ for all $f_i\in\Omega^1_0(\mathcal{N}')$, where W is a $(\Box+M^2)$-bisolution Hadamard bisolution on $\mathcal{N}\times\mathcal{N}$. It then follows from Theorem A.1 that ω' is Hadamard.

Given a globally hyperbolic space–time $(\mathcal{M},g)$, we may now employ a construction described in Ref. 38 to obtain a globally hyperbolic space–times $(\mathcal{M}',g')$ and (M'',g'') so that (i) $(\mathcal{M}'',g'')$ is ultrastatic; (ii) $\mathcal{M}'$ contains Cauchy surfaces Σ'_1 and Σ'_2 with causal normal neighborhoods $\mathcal{N}'_1$ and $\mathcal{N}'_2$ so that $\mathcal{N}'_1$ (respectively, $\mathcal{N}'_2$) is isometric to a causal normal neighborhood of a Cauchy surface in $(\mathcal{M},g)$ [respectively, $(\mathcal{M}'',g'')$]. As all the Cauchy surfaces involved are therefore homeomorphic, $(\mathcal{M}',g')$ and $(\mathcal{M}'',g'')$ will obey our topological restrictions if $(\mathcal{M},g)$ does. Starting with a Hadamard state on the ultrastatic space–time $(\mathcal{M}'',g'')$ we may induce Hadamard states on $(\mathcal{M}',g')$ and hence on $(\mathcal{M},g)$. Thus $\mathfrak{A}_M(\mathcal{M},g)$ admits Hadamard states.

An analogous argument applies in the Maxwell case. The only differences are that all test functions must now be co-closed, we use part (b) of Proposition A instead of part (a), and use the appropriate form of the Hadamard condition.

V. A QUANTUM WEAK ENERGY INEQUALITY

We now proceed to prove our quantum inequality. Let $\tau\mapsto\gamma(\tau)$ be a smooth timelike curve in $\mathcal{M}$ parametrized by its proper time $\tau\in\mathbb{R}$, and let Γ be a tubular neighborhood of γ. Inside Γ let $\{v^\rho_i|i=0,1,2,3\}$ be an orthonormal frame obeying $g^{\rho\sigma}=\eta^{ij}v^\rho_i v^\sigma_j$ and with the property that the restriction of v_0 to γ is the four-velocity $u^\sigma(\tau)=(\mathrm{d}\gamma(\tau)/\mathrm{d}\tau)^\sigma$ of the curve: $v^\sigma_0(\gamma(\tau))=u^\sigma(\tau)$. (See Ref. 25 for an explicit construction of such a frame.)

The first step is to construct the quantized energy density measured along the curve. The starting point is the classical stress-energy tensor, which for the Proca and Maxwell fields, takes the form

$$T_{\mu\nu}=\tfrac{1}{4}g_{\mu\nu}\mathcal{F}_{\rho\sigma}\mathcal{F}^{\rho\sigma}-\mathcal{F}_{\mu\rho}\mathcal{F}^\rho_\nu+M^2(\mathcal{A}_\mu\mathcal{A}_\nu-\tfrac{1}{2}g_{\mu\nu}\mathcal{A}_\rho\mathcal{A}^\rho), \tag{71}$$

with $M=0$ in the Maxwell case. The energy density along the curve is given by $T_{\mu\nu}(\gamma(\tau))u^\mu(\tau)u^\nu(\tau)$; we may extend this quantity off the curve by defining $\mathcal{T}(x)=T_{\mu\nu}(x)v^\mu_0(x)v^\nu_0(x)$. A little manipulation shows that

$$\mathcal{T}(x)=\frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3}(v^\rho_i v^\sigma_j\mathcal{F}_{\rho\sigma})^2+\frac{1}{2}M^2\sum_{i=0}^{3}(v^\rho_i\mathcal{A}_\rho)^2. \tag{72}$$

We may rewrite $\mathcal{T}$ in terms of forms with the aid of the one-form basis $\{V^i : i=0,1,2,3\}$ dual to the v_i, given by $V^i_\mu = \eta^{ij} g_{\mu\nu} v_j^\nu$. Writing $W^{ij} = V^i \wedge V^j$, we find

$$\mathcal{T}(x) = \frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3} [*(\mathcal{F}\wedge *W^{ij})]^2 + \frac{1}{2}M^2 \sum_{i=0}^{3} [*(\mathcal{A}\wedge *V^i)]^2 , \tag{73}$$

which is clearly the restriction to the diagonal $x' = x$ of

$$\begin{aligned} T(x,x') = \frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3} [*(\mathcal{F}\wedge *W^{ij})]|_x [*(\mathcal{F}\wedge *W^{ij})]|_{x'} \\ + \frac{1}{2}M^2 \sum_{i=0}^{3} [*(\mathcal{A}\wedge *V^i)]|_x [*(\mathcal{A}\wedge *V^i)]|_{x'} . \end{aligned} \tag{74}$$

The function $T(x,x')$ provides a point-split classical energy density, related to the true energy density on the curve γ by $\mathcal{T}(\gamma(\tau)) = T(\gamma(\tau),\gamma(\tau))$. Moreover, for $f, f' \in \mathcal{D}(\mathcal{M})$ we see that

$$\begin{aligned} &\int_{\mathcal{M}\times\mathcal{M}} T(x,x') f(x) f'(x') \mathrm{d}\,\mathrm{vol}_g(x) \mathrm{d}\,\mathrm{vol}_g(x') \\ &\quad = \frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3} \langle \mathcal{F}, W^{ij} f\rangle \langle \mathcal{F}, W^{ij} f'\rangle + \frac{1}{2}M^2 \sum_{i=0}^{3} \langle \mathcal{A}, V^i f\rangle \langle \mathcal{A}, V^i f'\rangle \\ &\quad = \frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3} \langle \mathcal{A}, \boldsymbol{\delta}(W^{ij} f)\rangle \langle \mathcal{A}, \boldsymbol{\delta}(W^{ij} f')\rangle + \frac{1}{2}M^2 \sum_{i=0}^{3} \langle \mathcal{A}, V^i f\rangle \langle \mathcal{A}, V^i f'\rangle . \end{aligned} \tag{75}$$

The advantage of this reformulation is that it is easily quantized: given a Hadamard state ω on $\mathfrak{A}_M(\mathcal{M},g)$ for the Proca field, or $\mathfrak{A}(\mathcal{M},g)$ for the Maxwell field we simply replace occurrences of $\langle \mathcal{A},F\rangle\langle \mathcal{A},F'\rangle$ with the two-point function $\omega^{(2)}(F,F')$ thus obtaining a scalar bidistribution $\langle T\rangle_\omega \in \mathcal{D}'(\mathcal{M}\times\mathcal{M})$ given by

$$\langle T\rangle_\omega(f,f') = \frac{1}{4}\sum_{i=0}^{3}\sum_{j=0}^{3} \omega^{(2)}(\boldsymbol{\delta}(W^{ij} f), \boldsymbol{\delta}(W^{ij} f')) + \frac{1}{2}M^2 \sum_{i=0}^{3} \omega^{(2)}(V^i f, V^i f') . \tag{76}$$

(Note that in the Maxwell case, the above expression reduces to its first term, in which the arguments of the two-point function are co-closed.)

Now suppose that a reference Hadamard state ω_0 is specified. Since the difference between Hadamard form $(\Box + M^2)$-bisolutions is smooth,

$$\langle :T: \rangle_\omega = \langle T\rangle_\omega - \langle T\rangle_{\omega_0} \tag{77}$$

is easily seen to be a smooth function on $\mathcal{M}\times\mathcal{M}$. Thus we may unsplit points to define the normal ordered energy density along γ by

$$\langle :\rho: \rangle_\omega(\tau) = \langle :T: \rangle_\omega(\gamma(\tau),\gamma(\tau)) . \tag{78}$$

We will need three further observations. First, $\langle :T: \rangle_\omega$ is symmetric as a consequence of the commutator axiom (P4)/(M4). Second, $\langle T\rangle_\omega$ is a distribution of *positive type*, i.e., $\langle T\rangle_\omega(\overline{f},f) \geqslant 0$ for all $f \in \mathcal{D}(\mathcal{M})$. This is ultimately a consequence of the positivity property $\omega(\mathcal{B}^*\mathcal{B}) \geqslant 0$ and the hermiticity axiom (P2)/(M2). Third, the wave-front set of $\langle T\rangle_\omega$ obeys

$$\mathrm{WF}(\langle T\rangle_\omega) \subseteq \mathcal{R} . \tag{79}$$

In the Proca case, this is a straightforward consequence of the nonexpansion of the wave-front set under partial differential operators. In the electromagnetic case, the key point is that $(F,G)\mapsto\omega^{(2)}(\delta F,\delta G)$ is a distribution (the two-point function of the field strength) whose wave-front set is known to be contained in $\mathcal{R}$.

Now consider the pull-back $\varphi^*\langle T\rangle_\omega$ of the bidistribution $\langle T\rangle_\omega$ induced by the smooth map $\varphi(\tau,\tau')=(\gamma(\tau),\gamma(\tau'))$. This quantity is formally the unrenormalized energy density, with points split along γ. We now claim that $\varphi^*\langle T\rangle_\omega$ is a well-defined distribution of positive type. To verify this, we first note that ${}^t\varphi'(\tau,\tau'):T^*_{(\gamma(\tau),\gamma(\tau'))}(\mathcal{M}\times\mathcal{M})\to\mathbb{R}$ is the linear map

$$ {}^t\varphi'(\tau,\tau'):(k,k')\mapsto(u^\rho(\tau)k_\rho,u^{\sigma'}(\tau')k'_{\sigma'}) \tag{80}$$

from which it follows that φ has the following set of normals:

$$ N_\varphi=\{(\gamma(\tau),k;\gamma(\tau'),k')\in T^*(\mathcal{M}\times\mathcal{M}):u^\rho(\tau)k_\rho=u^{\sigma'}(\tau')k'_{\sigma'}=0\}\,. \tag{81}$$

Second, we note that all the covectors appearing in $\mathrm{WF}(\langle T\rangle_\omega)$ are null, and therefore cannot annihilate any nonzero timelike vector. Accordingly, the intersection $\mathrm{WF}(\langle T\rangle_\omega)\cap N_\varphi$ is empty and the pull-back $\varphi^*\langle T\rangle_\omega$ exists by Theorem 2.5.11′ in Ref. 55 (in which the set of normals is also defined). Theorem 2.2 of Ref. 24 guarantees that it inherits the positive type property.

Theorem 2.5.11′ in Ref. 55 also asserts that the wave-front set of $\varphi^*\langle T\rangle_\omega$ obeys $\mathrm{WF}(\varphi^*\langle T\rangle_\omega)\subset\varphi^*\mathrm{WF}(\langle T\rangle_\omega)$. Thus, we have $(\tau,\zeta;\tau',-\zeta')\in\varphi^*\mathrm{WF}(\langle T\rangle_\omega)$ only if

$$ (\zeta,-\zeta')=({}^t\varphi'(\tau,\tau'))(k,-k')=(u^\rho(\tau)k_\rho,-u^{\sigma'}(\tau')k'_{\sigma'})\,. \tag{82}$$

Since the vectors $u^\sigma(\tau)$, $u^{\sigma'}(\tau')$ and the covectors k_σ, $k'_{\sigma'}$ are all future pointing their contractions will always be positive. It will therefore be the case that $\zeta,\zeta'>0$.

Summarizing, $\varphi^*\langle T\rangle_\omega$ is a well-defined distribution in $\mathcal{D}'(\mathbb{R}^2)$, which is of positive type and has a wave-front set obeying

$$ \mathrm{WF}(\varphi^*\langle T\rangle_\omega)\subset\{(\tau,\zeta;\tau',-\zeta')\,|\,\zeta,\zeta'>0\}\,. \tag{83}$$

We are now in a position to state and prove our quantum weak energy inequality. The proof is in fact essentially identical to that given for the scalar field in Ref. 24; it is given here for completeness.

Theorem V.1: *Let ω and ω_0 be Hadamard states on $\mathfrak{A}_M(\mathcal{M},g)$ for the Proca field, or $\mathfrak{A}(\mathcal{M},g)$ for the electromagnetic field. Define the point-split normal ordered energy density $\langle:T:\rangle_\omega$ relative to ω_0 by Eq. (77) and the normal ordered energy density $\langle:\rho:\rangle_\omega(\tau)$ by Eq. (78). Then the quantum inequality*

$$ \int\mathrm{d}\tau(g(\tau))^2\langle:\rho:\rangle_\omega(\tau)\geqslant-\int_0^\infty\frac{\mathrm{d}\alpha}{\pi}[(g\otimes g)\varphi^*\langle T\rangle_{\omega_0}]\hat{}(-\alpha,\alpha) \tag{84}$$

holds and the right-hand side is finite for all real-valued $g\in C_0^\infty(\mathbb{R})$.

Proof: Letting $g\in C_0^\infty(\mathbb{R})$ be a real valued function of proper time τ, we have

$$\int \mathrm{d}\tau (g(\tau))^2 \langle :\rho: \rangle_\omega(\tau) = \int \mathrm{d}\tau\, (g(\tau))^2 \varphi^* \langle :T: \rangle_\omega(\tau,\tau)$$

$$= \int \mathrm{d}\tau \int \mathrm{d}\tau'\, g(\tau) g(\tau') \delta(\tau-\tau') \varphi^* \langle :T: \rangle_\omega(\tau,\tau')$$

$$= \int_{-\infty}^{\infty} \frac{\mathrm{d}\alpha}{2\pi} \int \mathrm{d}\tau \int \mathrm{d}\tau'\, g_{-\alpha}(\tau) g_\alpha(\tau') \varphi^* \langle :T: \rangle_\omega(\tau,\tau')$$

$$= \int_{-\infty}^{\infty} \frac{\mathrm{d}\alpha}{2\pi} \varphi^* \langle :T: \rangle_\omega (g_{-\alpha} \otimes g_\alpha) = \int_0^{\infty} \frac{\mathrm{d}\alpha}{\pi} \varphi^* \langle :T: \rangle_\omega (\overline{g_\alpha} \otimes g_\alpha), \quad (85)$$

where $g_\alpha(\tau) = g(\tau) e^{i\alpha\tau}$ and we used the symmetry property $\varphi^* \langle :T: \rangle_\omega (\overline{g_\alpha} \otimes g_\alpha) = \varphi^* \langle :T: \rangle_\omega (g_\alpha \otimes \overline{g_\alpha})$ in the last step. Using the definition of $\langle :T: \rangle_\omega$ and the fact that $\varphi^* \langle T \rangle_\omega$ is of positive type we have

$$\int \mathrm{d}\tau (g(\tau))^2 \varphi^* \langle :T: \rangle_\omega(\tau,\tau) \geqslant - \int_0^{\infty} \frac{\mathrm{d}\alpha}{\pi} \varphi^* \langle T \rangle_{\omega_0} (\overline{g_\alpha} \otimes g_\alpha). \quad (86)$$

Setting $e_{(\alpha,\alpha')}(\tau,\tau') = e^{i(\alpha\tau + \alpha'\tau')}$, we note that the integrand in the above expression may be rewritten as

$$\varphi^* \langle T \rangle_{\omega_0} (\overline{g_\alpha} \otimes g_\alpha) = \varphi^* \langle T \rangle_{\omega_0} ((g \otimes g) e_{(-\alpha,\alpha)})$$

$$= [(g \otimes g) \varphi^* \langle T \rangle_{\omega_0}] (e_{(-\alpha,\alpha)})$$

$$= [(g \otimes g) \varphi^* \langle T \rangle_{\omega_0}]\hat{}(-\alpha,\alpha) \quad (87)$$

by our definition for the Fourier transform. Thus we obtain Eq. (84).

The fact that the right-hand side of Eq. (84) is convergent follows from an analysis of the wave-front set. From the definition of the wave-front set, it is obvious that

$$\mathrm{WF}((f_1 \otimes f_2) \varphi^* \langle T \rangle_{\omega_0}) \subseteq \mathrm{WF}(\varphi^* \langle T \rangle_{\omega_0}) \quad (88)$$

for any $f_i \in C_0^\infty(\mathbb{R})$. Thus the singular directions for $(f_1 \otimes f_2) \varphi^* \langle T \rangle_{\omega_0}$ are contained in $\{(\zeta, -\zeta') | \zeta, \zeta' > 0\}$. In consequence, the Fourier transform $[(g \otimes g) \varphi^* \langle T \rangle_{\omega_0}]\hat{}(-\alpha,\alpha)$ decays rapidly as $\alpha \to +\infty$. The integral on the right-hand side of Eq. (84) therefore converges thereby providing a finite bound for all $g \in C_0^\infty(\mathbb{R})$. □

VI. EXAMPLES

A. Minkowski space–time

Although Minkowski space lies outside the discussion of Sec. III because its Cauchy surfaces are noncompact, the arguments presented in Sec. V apply equally well to the two-point functions arising from standard Minkowski quantizations of the Maxwell and Proca fields based on the Poincaré invariant vacua. As we will see, these vacua are Hadamard; furthermore the topology of the Cauchy surface played no role in the proof of our QWEIs. We refer the reader to Ref. 56 (and references therein) for a careful discussion of the quantization of constrained systems in the context of algebraic field theory in Minkowski space.

We illustrate our QWEIs for the case of an inertial worldline γ, using the usual Poincaré invariant vacua as reference states. Boosting to the rest frame of γ, we adopt coordinates in which $\gamma(\tau) = (\tau, x_0, y_0, z_0)$ for some fixed $(x_0, y_0, z_0) \in \mathbb{R}^3$. We also adopt the orthonormal frame $v_i^\mu = (\partial/\partial x^i)^\mu$ for $i = 0, \ldots, 3$.

Let us begin by recalling that the vacuum two-point function for the *scalar* Klein–Gordon equation is given by

$$W_M^{(s)}(x,x') = \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\omega} e^{-ik_l(x-x')^l}, \tag{89}$$

where $k^j=(\omega,\mathbf{k})$ and $\omega=(|\mathbf{k}|^2+M^2)^{1/2}$. This is of course a Hadamard $(\Box+M^2)$-bisolution, and it may be used to define a one-form Hadamard $(\Box+M^2)$-bisolution by

$$W_M(f,f') = -\eta^{ij} W_M^{(s)}(f_i,f_j)\,. \tag{90}$$

[The overall sign is determined by the requirement that—anticipating the commutation relations (P4)/(M4)—the antisymmetric part $W_M(f,f')-W_M(f',f)$ should be equal to $-iE_M(f,f')$ $=-i\eta^{ij}E_M^{(s)}(f_i,f_j)$.]

Turning to the Proca field, the Poincaré invariant vacuum two-point function[57]

$$\omega_0^{(2)}(f,f') = -\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\omega} \left(\eta^{ij} - \frac{k^i k^j}{M^2} \right) \hat{f}_i(-k) \hat{f}_j(k) \tag{91}$$

is easily seen to be of the form

$$\omega_0^{(2)}(f,f') = W_M(f,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f') \tag{92}$$

and is therefore Hadamard. We may also write the vacuum two-point function in terms of its kernel

$$\omega_0^{(2)ij}(x,x') = -\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\omega} \left(\eta^{ij} - \frac{k^i k^j}{M^2} \right) e^{-ik_l(x-x')^l}. \tag{93}$$

It is not a difficult calculation to show that the point-split vacuum energy density along the worldline γ is

$$\varphi^* \langle T \rangle_{\omega_0}(\tau,\tau') = \frac{3}{2} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \omega e^{-i\omega(\tau-\tau')} = \frac{6\pi}{(2\pi)^3} \int_0^\infty \mathrm{d}\kappa\, \kappa^2 \omega(\kappa) e^{-i\omega(\kappa)(\tau-\tau')}\,, \tag{94}$$

where in the last step, we have changed to spherical polar coordinates in the momentum integration, performed the angular integrals, and written $\omega(\kappa)=\sqrt{\kappa^2+M^2}$. This expression can be used to evaluate the right-hand side of Eq. (84), giving

$$\begin{aligned} \int \mathrm{d}\tau \langle :\rho: \rangle_\omega(\tau) g(\tau)^2 &\geqslant -\int_0^\infty \frac{\mathrm{d}\alpha}{\pi} [(g\otimes g)\varphi^* \langle T \rangle_{\omega_0}]\hat{}\,(-\alpha,\alpha) \\ &= -\frac{6}{(2\pi)^3} \int_0^\infty \mathrm{d}\alpha \int_0^\infty \mathrm{d}\kappa\, \kappa^2 \omega(\kappa) |\hat{g}(\alpha+\omega(\kappa))|^2\,. \end{aligned}$$

Before commenting on the above expression, we wish to perform a similar analysis for the electromagnetic field. The vacuum two-point function for electromagnetism in the Coulomb gauge is given by

$$\omega_0^{(2)ij}(x,x') = -\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\omega} h^{ij} e^{-ik_l(x-x')^l}, \tag{95}$$

where $\omega=|\mathbf{k}|$ and

$$h^{ij}=\begin{cases}\eta^{ij}+k^ik^j/\omega^2 & \text{for } i\neq 0\neq j,\\ 0 & \text{otherwise.}\end{cases} \tag{96}$$

It is straightforward to check that, for co-closed test one-forms f,f' [i.e., $k^i\hat{f}_i(k)=0$] we have $\omega_0^{(2)}(f,f')=W_0(f,f')$ and that ω_0 is therefore Hadamard. An identical computation to the above now reveals that

$$\varphi^*\langle T\rangle_{\omega_0}(\tau,\tau')=\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\omega e^{-i\omega(\tau-\tau')}=\frac{4\pi}{(2\pi)^3}\int_0^\infty \mathrm{d}\kappa\,\kappa^2\omega(\kappa)e^{-i\omega(\kappa)(\tau-\tau')}\,, \tag{97}$$

and hence

$$\int \mathrm{d}\tau\langle{:}\rho{:}\rangle_\omega(\tau)g(\tau)^2\geqslant-\frac{4}{(2\pi)^3}\int_0^\infty\mathrm{d}\alpha\int_0^\infty\mathrm{d}\kappa\,\kappa^2\omega(\kappa)|\hat{g}(\alpha+\omega(\kappa))|^2\,. \tag{98}$$

From this point on, the Proca and electromagnetic fields can be treated simultaneously as the two bounds take the common form (setting $M=0$ for electromagnetism)

$$\int \mathrm{d}\tau\langle{:}\rho{:}\rangle_\omega(\tau)g(\tau)^2\geqslant-sI_M(g)\,, \tag{99}$$

where s is the number of spin degrees of freedom for the field, i.e., $s=2$ for Maxwell and $s=3$ for Proca, and

$$I_M(g)=\frac{2}{(2\pi)^3}\int_0^\infty\mathrm{d}\alpha\int_0^\infty\mathrm{d}\kappa\,\kappa^2\omega(\kappa)|\hat{g}(\alpha+\omega(\kappa))|^2\,. \tag{100}$$

This integral can be further simplified by making an additional change of variables,

$$\begin{aligned}u&=\alpha+\omega(\kappa),\\ v&=\omega(\kappa)\,,\end{aligned} \tag{101}$$

whereupon the above integral can be rewritten as

$$I_M(g)=\frac{2}{(2\pi)^3}\int_M^\infty\mathrm{d}u|\hat{g}(u)|^2\int_M^u\mathrm{d}v\,v^2\sqrt{v^2-M^2}. \tag{102}$$

In fact, the scalar field also satisfies Eq. (99) with $s=1$.[22] Thus, in Minkowski space, the QWEI bounds for scalar, Proca and Maxwell fields differ only by a factor equal to the number of spin states (as already noted for the electromagnetic field in Ref. 27). However, in more general curved space–times the scalar and one-form fields can have different eigenfrequency spectra leading to very different quantum weak energy inequalities for each field.

B. Ultrastatic space–times

We now turn to the class of examples in which the space–time is ultrastatic (with compact Cauchy surface obeying our usual requirements) and the energy density is sampled along a static worldline, using the ultrastatic vacua of Sec. IV as reference states. In this case, the quantum inequality Eq. (84) takes a remarkably simple form. Recall that, for both the Proca and the Maxwell fields, the two-point function of the vacuum state can be written compactly as

$$\omega^{(2)}(F,F')=\sum_{\lambda}\sum_{\text{physical}\ j\in J(\lambda)}\frac{1}{2\omega(\lambda,j)}\langle\mathcal{A}(\lambda,j),F\rangle\,\langle\overline{\mathcal{A}(\lambda,j)},F'\rangle, \tag{103}$$

where λ ranges only over the physical families of modes, i.e., $\lambda \in \{T,P\}$ for Proca, but $\lambda = T$ only for Maxwell. In the Maxwell case, we restrict attention to co-closed test one-forms F and F'. Using the mode expansion (103) for the two point function, and recalling that $\mathcal{F} = \mathbf{d}\mathcal{A}$, it is not difficult to show that[77]

$$[(g\otimes g)\varphi^*\langle T\rangle_\omega]\hat{}(-\alpha,\alpha) = \int \mathrm{d}\tau \int \mathrm{d}\tau'\, g(\tau)\, g(\tau')\, e^{-i\alpha(\tau-\tau')} \times \sum_{\lambda}\ \sum_{\text{physical}}\ \sum_{j\in J(\lambda)} N(\lambda,j)(\gamma(\tau),\gamma(\tau'))\,, \tag{104}$$

where

$$N(\lambda,j)(x,x') = \frac{1}{2\omega(\lambda,j)}\left\{ \frac{1}{4}\sum_{p=0}^{3}\sum_{q=0}^{3} [\mathcal{F}_{\mu\nu}(\lambda,j)v_p^\mu v_q^\nu](x)\,[\overline{\mathcal{F}_{\rho\sigma}(\lambda,j)}v_p^\rho v_q^\sigma](x') + \frac{1}{2}M^2\sum_{p=0}^{3}[\mathcal{A}_\mu(\lambda,j)v_p^\mu](x)\,[\overline{\mathcal{A}_\rho(\lambda,j)}v_p^\rho](x')\right\}. \tag{105}$$

Now if we choose a static worldline $\gamma(\tau) = (\tau,\mathbf{x}_0)$, then

$$N(\lambda,j)(\gamma(\tau),\gamma(\tau')) = e^{-i\omega(\lambda,j)(\tau-\tau')}\,\mathfrak{T}(\lambda,j)\,, \tag{106}$$

where

$$\mathfrak{T}(\lambda,j) = \frac{1}{2\omega(\lambda,j)}\left\{\frac{1}{4}\sum_{p=0}^{3}\sum_{q=0}^{3}|[\mathcal{F}_{\mu\nu}(\lambda,j)v_p^\mu v_q^\nu](\gamma(\tau_0))|^2 + \frac{1}{2}M^2\sum_{p=0}^{3}|[\mathcal{A}_\mu(\lambda,j)v_p^\mu](\gamma(\tau_0))|^2\right\} \tag{107}$$

is the classical energy density per mode at the spatial position of the observer's worldline. [Note that the leading factor of $(2\omega(\lambda,j))^{-1}$ appears because our modes were normalized using the L^2-inner product on Σ, rather than the symplectic inner product.] The most notable point to be made here is that $\mathfrak{T}(\lambda,j)$ is τ independent because the $e^{-i\omega_\lambda\tau}$ dependence in the modes is removed by taking the magnitude of the complex functions. Thus Eq. (104) becomes

$$[(g\otimes g)\varphi^*\langle T\rangle_\omega]\hat{}(-\alpha,\alpha) = \sum_{\lambda}\ \sum_{\text{physical}}\ \sum_{j\in J(\lambda)} |\hat{g}(\alpha+\omega(\lambda,j))|^2\mathfrak{T}(\lambda,j)\,, \tag{108}$$

and the quantum weak energy inequality for static observers in ultrastatic space–times becomes

$$\int \mathrm{d}\tau (g(\tau))^2\langle{:}\rho{:}\rangle_\omega(\tau) \geqslant -\int_0^\infty \frac{\mathrm{d}\alpha}{\pi}\sum_{\lambda}\ \sum_{\text{physical}}\ \sum_{j\in J(\lambda)} |\hat{g}(\alpha+\omega(\lambda,j))|^2\mathfrak{T}(\lambda,j). \tag{109}$$

As we will see, the above form turns out to be calculationally convenient in some settings. However, we also note that the quantum weak energy inequality may be written

$$\int \mathrm{d}\tau (g(\tau))^2\langle{:}\rho{:}\rangle_\omega(\tau) \geqslant -\int_0^\infty \mathrm{d}u\, |\hat{g}(u)|^2 Q(u), \tag{110}$$

where

$$Q(u) = \frac{1}{\pi}\sum_{\lambda}\ \sum_{\text{physical}}\ \sum_{\substack{j\in J(\lambda)\\ \text{s.t. } \omega(\lambda,j)\leqslant u}} \mathfrak{T}(\lambda,j) \tag{111}$$

measures the maximum energy density available if no mode with frequency greater than u is excited. The analysis carried out in Sec. 5 of Ref. 24 for the scalar field may be adapted to show that $Q(u)$ is positive and polynomially bounded as $u\to\infty$. Several other systems obey quantum inequalities of this form, which motivated the study of related conditions for general quantum dynamical systems in Ref. 58. In the terminology of that paper, the ultrastatic vacuum states constructed here fulfill a *limiting static QWEI*. We expect that the analysis of Ref. 58 would apply equally well to the Proca and Maxwell fields, thereby establishing links between quantum inequalities and the thermodynamic properties of these fields.

C. Static Einstein universe

A nice example of the ultrastatic quantum inequality is provided by the static Einstein universe $\mathbb{R}\times S^3$ with line element

$$\mathrm{d}s^2=\mathrm{d}t^2-a^2[\mathrm{d}\chi^2+\sin^2\chi(\mathrm{d}\theta^2+\sin^2\theta\mathrm{d}\varphi^2)]. \tag{112}$$

Here a is the radius of the universe and (χ,θ,φ) are spherical polar coordinates on the unit three-sphere. Various authors have studied the electromagnetic mode functions in the Einstein universe[59–61] and it turns out that essentially the same ansatz can be used to obtain the modes of the Proca field.

We know from Sec. IV that the scalar Proca modes are completely specified by finding mode solutions to the massive, minimally coupled scalar wave equation $(\Box^s+M^2)\Phi=0$. A complete set of suitably normalized positive frequency mode solutions in the Einstein universe is given by[62,63]

$$\Phi_{nlm}(x)=a^{-3/2}\Pi_{nl}(\chi)\,Y_{lm}(\theta,\varphi)\,e^{-i\sigma_n t}, \tag{113}$$

where $Y_{lm}(\theta,\varphi)$ are the standard spherical harmonics on a two-sphere,[64] $\Pi_{nl}(\chi)$ can be written in terms of Gegenbauer polynomials $C_\eta^\lambda(x)$[65] as

$$\Pi_{nl}(\chi)=\frac{l!\,2^{l+1/2}\sqrt{(n-l)!(n+1)}}{\sqrt{\pi(n+l+1)!}}\sin^l\chi\,C_{n-l}^{l+1}(\cos\chi), \tag{114}$$

and the frequency of the modes is

$$\sigma_n=\sqrt{\frac{n(n+2)}{a^2}+M^2}. \tag{115}$$

Here, the primary quantum number n ranges over the non-negative integers $n=0,1,2,\ldots$. For a given n there are $(n+1)^2$ harmonic states with the same frequency labeled by the quantum numbers, $l=0,1,\ldots,n$ and $m=-l,-l+1,\ldots,0,\ldots,l-1,l$. However, the case $n=l=m=0$ corresponds to the spatially constant mode; thus the labelling set for the scalar Proca modes given by Eq. (59) is $n=1,2,\ldots$, with l and m as before.

On the other hand, the family of transverse modes breaks up into two subfamilies:[61] the magnetic J-pole modes taking the form

$$\mathcal{A}(M,n,l,m)=*\mathbf{d}(\Psi_{nlm}\,\mathbf{d}t\wedge\mathbf{d}\chi), \tag{116}$$

and the electric J-pole modes,

$$\mathcal{A}(E,n,l,m)=*\mathbf{d}\left(\frac{a}{n}\mathcal{A}(M,n,l,m)\wedge\mathbf{d}t\right), \tag{117}$$

where the scalar functions Ψ_{nlm} obey

$$\left(\Box^s + \frac{2\cos\chi}{a^2\sin\chi}\partial_\chi + M^2\right)\Psi_{nlm} = 0. \tag{118}$$

The positive frequency mode solutions to this partial differential equation are

$$\Psi_{nlm}(x) = \sqrt{2an}\, V_{nl}(\chi)\, Y_{lm}(\theta,\varphi)\, e^{-i\omega_n t}, \tag{119}$$

where

$$V_{nl}(\chi) = \frac{l!\, 2^l\sqrt{(n-l-1)!}}{\sqrt{\pi l(l+1)(n+l)!}}\sin^{l+1}\chi\, C^{l+1}_{n-l-1}(\cos\chi) \tag{120}$$

and the frequency of the modes is given by

$$\omega_n = \sqrt{\frac{n^2}{a^2} + M^2}. \tag{121}$$

Here the quantum numbers range over a different set of allowed values. The primary quantum number n ranges over the integers $n = 2,3,\ldots$. For a given n there are n^2-1 harmonic states with the same frequency labeled by the quantum numbers, $l = 1,2,\ldots,n-1$ and $m = -l,-1+1,\ldots,0,\ldots,l-1,l$. We stress that both transverse subfamilies have an energy spectrum given by Eq. (121), which differs from that of the scalar Proca modes. There is actually a more convenient basis of transverse mode solutions given by

$$\mathcal{A}(\pm,n,l,m) = \frac{1}{\sqrt{2}}[\mathcal{A}(M,n,l,m) \pm \mathcal{A}(E,n,l,m)], \tag{122}$$

which are simultaneous eigenfunctions of $\boldsymbol{\delta}_\Sigma * _\Sigma$ and $-\Delta_\Sigma + M^2$ (which commute). The $\lambda = M$ or E families of modes are, roughly speaking, the linearly polarized solutions of the field while the $\lambda = +$ or $-$ modes are the circularly polarized solutions.

For the interested reader, we also state the component form of the three families of physical modes. The two transverse polarizations of the field are

$$\mathcal{A}_\mu(M,n,l,m) = \frac{1}{a}\left(0, 0, -\frac{1}{\sin\theta}\partial_\varphi, \sin\theta\partial_\theta\right)\Psi_{nlm} \tag{123}$$

and

$$\mathcal{A}_\mu(E,n,l,m) = \frac{1}{an}\left(0, \frac{l(l+1)}{\sin^2\chi}, \partial_\chi\partial_\theta, \partial_\chi\partial_\varphi\right)\Psi_{nlm}, \tag{124}$$

while the scalar Proca modes are

$$\mathcal{A}_\mu(P,n,l,m) = \frac{a\sigma_n^2}{M\sqrt{n(n+2)}}\left(\frac{n(n+2)}{i\sigma_n a^2}, \partial_\chi, \partial_\theta, \partial_\varphi\right)\Phi_{nlm}. \tag{125}$$

One may readily verify that the two transverse modes and the scalar Proca mode all have the property $\boldsymbol{\delta}\mathcal{A}(\lambda,n,l,m) = 0$, for $\lambda = M,E,P$ and therefore solve the Proca equation (19). Moreover, these modes obey the (pseudo)-orthonormality conditions of Sec. IV A.

Since the Einstein space–time is ultrastatic, we can find the quantum weak energy inequality from Eq. (109). To begin, let the worldline for a stationary observer be given by $\gamma(\tau) = (\tau,\chi,\theta,\varphi)$ where (χ,θ,φ) are the coordinates of a fixed point in space. An orthonormal basis in

the neighborhood around γ is given by $v_i^\mu = \sqrt{|g^{\mu\mu}|}(\partial/\partial x^i)^\mu$ (no sum on μ). All of the work is in the evaluation of the classical energy density per mode, $\mathfrak{T}(\lambda,n,l,m)$, defined by Eq. (107), which, in the Einstein space–time takes the form

$$\mathfrak{T}(\lambda,j) = \frac{1}{4\omega(\lambda,j)}\left[\frac{|\mathcal{F}_{01}|^2}{a^2} + \frac{|\mathcal{F}_{02}|^2}{a^2\sin^2\chi} + \frac{|\mathcal{F}_{03}|^2}{a^2\sin^2\chi\sin^2\theta} + \frac{|\mathcal{F}_{12}|^2}{a^4\sin^2\chi} + \frac{|\mathcal{F}_{13}|^2}{a^4\sin^2\chi\sin^2\theta} + \frac{|\mathcal{F}_{23}|^2}{a^4\sin^4\chi\sin^2\theta} + M^2\left(|\mathcal{A}_0|^2 + \frac{|\mathcal{A}_1|^2}{a^2} + \frac{|\mathcal{A}_2|^2}{a^2\sin^2\chi} + \frac{|\mathcal{A}_3|^2}{a^2\sin^2\chi\sin^2\theta}\right)\right]. \tag{126}$$

Beginning with the $\pm$ modes, it is straightforward to calculate the field strength $\mathcal{F}(\pm,n,l,m) = \mathbf{d}\mathcal{A}(\pm,n,l,m)$. Inserting the field strength into the above expression, and using $\partial_\chi \Psi_{nlm} = \partial_\chi \overline{\Psi_{nlm}}$, we arrive at

$$\mathfrak{T}(\pm,n,l,m) = \frac{\omega_n}{4a^4n^2}\left[\left(\frac{l(l+1)}{\sin^2\chi}\right)^2|\Psi_{nlm}|^2 + \frac{1}{\sin^2\chi}\left(|\partial_\chi\partial_\theta\Psi_{nlm}|^2 + \frac{1}{\sin^2\theta}|\partial_\chi\partial_\varphi\Psi_{nlm}|^2\right) + \frac{n^2}{\sin^2\chi}\left(|\partial_\theta\Psi_{nlm}|^2 + \frac{1}{\sin^2\theta}|\partial_\varphi\Psi_{nlm}|^2\right)\right]. \tag{127}$$

Note that the $+$ and $-$ modes have equal energy densities. Next, we use the definition Eq. (119) of the scalar functions Ψ_{nlm} and two identities. The first identity,

$$|\partial_\theta Y_{lm}|^2 + \frac{1}{\sin^2\theta}|\partial_\varphi Y_{lm}|^2 = \frac{1}{2}\Delta_{S^2}|Y_{lm}|^2 + l(l+1)|Y_{lm}|^2 \tag{128}$$

is for the spherical harmonics where

$$\Delta_{S^2} = \frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2 \tag{129}$$

is the two-sphere Laplacian. The second identity is

$$\frac{l(l+1)}{\sin^2\chi}V_{nl}^2 + (\partial_\chi V_{nl})^2 = \left(n^2 + \frac{1}{2}\partial_\chi^2\right)V_{nl}^2, \tag{130}$$

which follows from the ordinary differential equation satisfied by $V_{nl}(\chi)$. Using both of these we arrive at

$$\mathfrak{T}(\pm,n,l,m) = \frac{\omega_n}{2a^3n}\left\{\frac{l(l+1)}{\sin^2\chi}\left(2n^2 + \frac{1}{2}\partial_\chi^2\right)V_{nl}^2|Y_{lm}|^2 + \frac{1}{2\sin^2\chi}[(\partial_\chi V_{nl})^2 + n^2V_{nl}^2]\Delta_{S^2}|Y_{lm}|^2\right\}. \tag{131}$$

Because the frequency ω_n is independent of l and m, we can sum over these labels, obtaining considerable simplification from the summation theorems for the spherical harmonics and Gegenbauer polynomials. In the case of the spherical harmonics it is well-known that[64]

$$\sum_{m=-l}^{l}|Y_{lm}(\theta,\varphi)|^2 = \frac{2l+1}{4\pi}, \tag{132}$$

which reduces the sum over all l and m of $\mathfrak{T}(\pm,n,l,m)$ to

$$\sum_{l=1}^{n-1}\sum_{m=-l}^{+l}\mathcal{T}(\pm,n,l,m)=\frac{\omega_n}{8\pi a^3 n}\sum_{l=1}^{n-1}\frac{(2l+1)l(l+1)}{\sin^2\chi}\left(2n^2+\frac{1}{2}\partial_\chi^2\right)V_{nl}^2$$

$$=\frac{\omega}{8\pi a^3 n}\frac{1}{\sin^2\chi}\left(2n^2+\frac{1}{2}\partial_\chi^2\right)\sin^2\chi\sum_{l=1}^{n-1}\frac{(2l+1)l(l+1)}{\sin^2\chi}V_{nl}^2. \quad (133)$$

Using the summation theorem for the Gegenbauer polynomials,

$$\sum_{l=1}^{n-1}\frac{(2l+1)l(l+1)}{\sin^2\chi}V_{nl}^2(\chi)=\frac{1}{\pi}\left[n-\frac{1}{n}\left(\frac{\sin n\chi}{\sin\chi}\right)^2\right], \quad (134)$$

[(Eq. 8.934.3) of Ref. 65] we finally obtain

$$\sum_{l=1}^{n-1}\sum_{m=-l}^{+l}\mathfrak{T}(\pm,n,l,m)=\frac{(n^2-1)\omega_n}{4\pi^2a^3}. \quad (135)$$

It is noteworthy that this expression is exactly the total zero-point energy of n^2-1 harmonic oscillators at frequency ω_n, divided by the spatial volume $2\pi^2a^3$ of the Einstein universe.

The contribution from the scalar Proca modes is calculated in much the same manner. The only difference is that we make use of the following two identities:

$$(\partial_\chi\Pi_{nl})^2+\frac{l(l+1)}{\sin^2\chi}\Pi_{nl}^2=n(n+2)\Pi_{nl}^2+\frac{1}{2\sin^2\chi}\partial_\chi\sin^2\chi\partial_\chi\Pi_{nl}^2, \quad (136)$$

which follows from the ordinary differential equation satisfied by Π_{nl} and

$$\sum_{l=0}^{n}(2l+1)\Pi_{nl}^2(\chi)=\frac{2(n+1)^2}{\pi}, \quad (137)$$

which again follows from the summation theorem for the Gegenbauer polynomials. For the Proca mode we find

$$\sum_{l=0}^{n}\sum_{m=-l}^{+l}\mathfrak{T}(P,n,l,m)=\frac{(n+1)^2\sigma_n}{4\pi^2a^3}. \quad (138)$$

Again we have found the zero-point energy times the multiplicity divided by the spatial volume.

Finally, let s be the total number of spin degrees of freedom for the field, i.e., $s=2$ for Maxwell and $s=3$ for Proca. Substituting Eqs. (135) and (138) into Eq. (109), we can write the quantum weak energy inequality in the Einstein space–time for an arbitrary real-valued test function $g(\tau)\in C_0^\infty(\mathbb{R})$ as

$$\int \mathrm{d}\tau\langle:\rho:\rangle_\omega(\tau)g(\tau)^2\geqslant-\frac{2}{4\pi^2a^3}\sum_{n=2}^{\infty}(n^2-1)\omega_n\int_0^\infty\frac{\mathrm{d}\alpha}{\pi}|\hat{g}(\alpha+\omega_n)|^2$$

$$-\frac{(s-2)}{4\pi^2a^3}\sum_{n=1}^{\infty}(n+1)^2\sigma_n\int_0^\infty\frac{\mathrm{d}\alpha}{\pi}|\hat{g}(\alpha+\sigma_n)|^2, \quad (139)$$

which holds for all Hadamard states ω.

By suitably restricting the class of allowed states (if necessary) this bound may be extended to noncompactly supported g whose Fourier transforms have sufficiently rapid decay.[78] For electromagnetism, the above bound was evaluated for a Lorentzian test function in Ref. 27; here we will treat the example of a Gaussian test function in both the electromagnetic and Proca cases. Setting

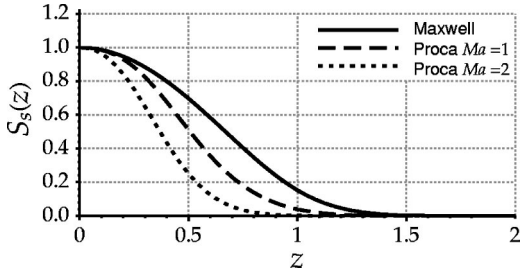

FIG. 1. Plot of the scale function $\mathcal{S}_s(z)$ for the Gaussian sampling function in the Einstein universe. Three different cases are of Eq. (144) are displayed: Electromagnetism (solid line) and two cases of the Proca field for different values of the mass times the radius of universe, Ma$=1$ (dashed line) and Ma$=2$ (dotted line). The plots were produced by evaluating the first 3000 terms in the summation of Eq. (144).

$$g(\tau)=\pi^{-1/4}\tau_0^{-1/2}\exp\left(-\frac{1}{2}\frac{\tau^2}{\tau_0^2}\right), \tag{140}$$

the weight function $g(\tau)^2$ is a normalized Gaussian. Using the Fourier transform of g,

$$\hat{g}(\alpha)=\pi^{1/4}(2\tau_0)^{1/2}\exp\left(-\frac{\alpha^2\tau_0^2}{2}\right), \tag{141}$$

it is now possible to calculate

$$\int_0^\infty \mathrm{d}\alpha|\hat{g}(\alpha+\omega)|^2=\pi\,\mathrm{erfc}(\omega\tau_0), \tag{142}$$

where erfc(x) is the complementary error function. Accordingly, the quantum weak energy inequality for this test function is

$$\int \mathrm{d}\tau\langle:\rho:\rangle_\omega(\tau)g(\tau)^2\geqslant-\frac{3s}{64\pi^2\tau_0^4}\mathcal{S}_s(\tau_0/a), \tag{143}$$

where the scale function

$$\mathcal{S}_s(z)=\frac{16}{3}z^4\left[\frac{2}{s}\sum_{n=2}^{\infty}(n^2-1)\sqrt{n^2+M^2a^2}\,\mathrm{erfc}(\sqrt{n^2+M^2a^2}z)\right.$$
$$\left.+\frac{s-2}{s}\sum_{n=1}^{\infty}(n+1)^2\sqrt{n(n+2)+M^2a^2}\,\mathrm{erfc}(\sqrt{n(n+2)+M^2a^2}z)\right] \tag{144}$$

is plotted in Fig. 1. For very short sampling times the scale function is close to unity and the QWEI bound is the same as that for Minkowski space–time.[27] This is expected because the space–time appears to be flat over time scales which are short relative to the radius of the universe, and we should expect to recover the Minkowski space result. As the sampling time becomes progressively longer, the field has more time to ''sample'' the curvature of the universe, and thus it becomes increasingly difficult to generate negative energy densities. Also, as the mass of the field increases it becomes increasingly difficult to generate negative energy densities. This is seen by the faster decay in the scale functions for larger value of the field mass as seen in previous evaluations of the scale function for scalar fields in other space–times.[15,17,18] As mentioned above, the quantum inequality bound has also been evaluated for electromagnetism with a Lorentzian sampling function[27] and the behavior is very much the same.

APPENDIX A: CONSISTENCY OF THE HADAMARD CONDITION WITH THE CONSTRAINTS

In this appendix we prove the following local-to-global result.

Theorem A.1: *Let ω be a state on either $\mathfrak{A}_M(\mathcal{M},g)$ or $\mathfrak{A}(\mathcal{M},g)$ and suppose that there exists a causal normal neighborhood $\mathcal{N}$ of a Cauchy surface Σ in $\mathcal{M}$, and a Hadamard bisolution W_M (respectively, W) to $\Box+M^2$ (respectively, $\Box$) on $\mathcal{N}\times\mathcal{N}$ such that*

$$\omega(\mathcal{A}(f_1)\mathcal{A}(f_2))=W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2) \tag{A1}$$

for all $f_i\in\Omega_0^1(\mathcal{N})$ (in the Proca case) or

$$\omega([\mathcal{A}](f_1)[\mathcal{A}](f_2))=W(f_1,f_2) \tag{A2}$$

for all $f_i\in\Omega_0^1(\mathcal{N})$ with $\boldsymbol{\delta}f_i=0$ (in the Maxwell case). Then ω is Hadamard.

Thus the Hadamard conditions introduced in Sec. III C respect the Cauchy evolution of the field equations: if they are satisfied near one Cauchy surface, they hold near all others and hence hold globally. As the Hadamard form for Klein–Gordon bisolutions also propagates in this sense (Theorem 5.5 in Ref. 32), our discussion may be regarded as checking the consistency of the definitions of Sec. III C with the Proca and Maxwell constraints. The propagation property is one of the key ingredients used in Sec. IV E, where we established the existence of Hadamard states on general globally hyperbolic space–times obeying our usual topological conditions. Although we will use the fact that Σ is compact for both the Maxwell and Proca fields this condition can probably be dropped; however in the Maxwell case it appears to be necessary [in Lemma A.4(b)] to assume that $H_1(\Sigma)$ is trivial and that the compact support cohomology group $H_c^3(\mathcal{M})$ of the space–time is therefore also trivial.

The proof of Theorem A relies on a number of results concerning the classical Proca, Maxwell, and Klein–Gordon fields. One fact which will be used repeatedly is that, for $f\in\Omega_0^1(\mathcal{M})$, $E_Mf=0$ if and only if $f\in(\Box+M^2)\Omega_0^1(\mathcal{M})$. Indeed, $f=(\Box+M^2)E_M^+f$ and since, by hypothesis, $E_M^+f=E_M^-f$, the support of E_M^+f is contained in the compact set $J^+(\mathrm{supp}\,f)\cap J^-(\mathrm{supp}\,f)$. Our first observation generalizes this fact to the Proca field.

Lemma A.2: Let $M>0$. For $f\in\Omega_0^1(\mathcal{M})$, $\Delta_Mf=0$ if and only if $f\in(-\boldsymbol{\delta}\mathbf{d}+M^2)\Omega_0^1(\mathcal{M})$.

Proof: Since $(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})(-\boldsymbol{\delta}\mathbf{d}+M^2)=\Box+M^2$, sufficiency holds because E_M is a Klein–Gordon bisolution. Conversely, $\Delta_Mf=0$ is equivalent to $E_M(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f=0$; hence, we have

$$(-\mathbf{d}\boldsymbol{\delta}+M^2)f=M^2(\Box+M^2)g \tag{A3}$$

for some $g\in\Omega_0^1(\mathcal{M})$. By applying $\boldsymbol{\delta}\mathbf{d}$ to both sides, we obtain $\boldsymbol{\delta}\mathbf{d}f=(\Box+M^2)\,\boldsymbol{\delta}\mathbf{d}g$, which may be subtracted from the previous expression to yield

$$(\Box+M^2)f=(\Box+M^2)(-\boldsymbol{\delta}\mathbf{d}+M^2)g\,. \tag{A4}$$

Since both f and g are compactly supported, we conclude that $f=(-\boldsymbol{\delta}\mathbf{d}+M^2)g$. □

Proposition A.3: (a) Given any $f\in\Omega_0^1(\mathcal{M})$ there exists $g\in\Omega_0^1(\mathcal{M})$ such that $\tilde{f}=f+(-\boldsymbol{\delta}\mathbf{d}+M^2)g$ is an element of $\Omega_0^1(\mathcal{N})$.

(b) Given any co-closed $f\in\Omega_0^1(\mathcal{M})$ there exists $g\in\Omega_0^1(\mathcal{M})$ such that $\tilde{f}=f-\boldsymbol{\delta}\mathbf{d}g$ is a co-closed element of $\Omega_0^1(\mathcal{N})$.

Proof: (a) Choose smooth functions $\chi^{\pm}$ on $\mathcal{M}$ with $\chi^++\chi^-=1$ and χ^+ equal to unity to the future of $\mathcal{N}$ and vanishing to the past of $\mathcal{N}$. Then

$$\tilde{f}=(-\boldsymbol{\delta}\mathbf{d}+M^2)\chi^+\Delta_Mf \tag{A5}$$

belongs to $\Omega_0^1(\mathcal{N})$ and satisfies $\Delta_M\tilde{f}=\Delta_Mf$. Applying Lemma A.2 to $\tilde{f}-f$, it follows that $\tilde{f}=f+(-\boldsymbol{\delta}\mathbf{d}+M^2)g$ as required.

(b) With $\chi^{\pm}$ as above, set $\tilde{f}=-\boldsymbol{\delta}\mathbf{d}\chi^{+}E_0 f$. Then $\tilde{f}$ belongs to $\Omega^1_0(\mathcal{N})$ and is co-closed; moreover $E_0\tilde{f}$ and $E_0 f$ are gauge equivalent by the proof of Prop. 4(c) in Ref. 36. Accordingly, there exists $\eta\in\Omega^0(\mathcal{M})$ such that $E_0(\tilde{f}-f)=\mathbf{d}\eta$. Taking coderivatives, using $\boldsymbol{\delta}E_0=E_0\boldsymbol{\delta}$ and co-closure of $\tilde{f}$ and f, we have $\boldsymbol{\delta}\mathbf{d}\eta=0$ and hence $\eta=E_0\zeta$ for some $\zeta\in\Omega^0_0(\mathcal{M})$. Substituting back, we see that $E_0(\tilde{f}-f-\mathbf{d}\zeta)=0$, so

$$\tilde{f}-f-\mathbf{d}\zeta=\Box g \tag{A6}$$

for some $g\in\Omega^1_0(\mathcal{M})$. Taking coderivatives again, $\Box(\zeta-\boldsymbol{\delta}g)=0$ and hence (because both ζ and g are compactly supported) $\zeta=\boldsymbol{\delta}g$. Substituting back in Eq. (A6), we have $\tilde{f}=f+\mathbf{d}\boldsymbol{\delta}g+\Box g=f-\boldsymbol{\delta}\mathbf{d}g$ as required. □

Lemma A.4: (a) If $\mathcal{A}$ is a weak one-form $(\Box+M^2)$-solution obeying

$$\mathcal{A}((-\boldsymbol{\delta}\mathbf{d}+M^2)f)=0 \tag{A7}$$

for all $f\in\Omega^1_0(\mathcal{N})$, then Eq. (A7) holds for all $f\in\Omega^1_0(\mathcal{M})$.

(b) If $\mathcal{A}$ is a weak one-form $\Box$-solution vanishing on co-closed $f\in\Omega^1_0(\mathcal{N})$, then $\mathcal{A}$ vanishes on all co-closed $f\in\Omega^1_0(\mathcal{M})$.

Proof: (a) Since, for $f\in\Omega^1_0(\mathcal{N})$, $\mathcal{A}((\Box+M^2)f)=0$, we have by Eq. (A7) that

$$\mathcal{A}(\mathbf{d}\boldsymbol{\delta}f)=0 \tag{A8}$$

for all $f\in\Omega^1_0(\mathcal{N})$. Thus, $\mathcal{A}(\mathbf{d}\cdot)$ is a global weak scalar $(\Box+M^2)$-solution vanishing on $\boldsymbol{\delta}\Omega^1_0(\mathcal{N})$. Now we may fix $f_0\in\Omega^0_0(\mathcal{N})$ such that any $f\in\Omega^0_0(\mathcal{N})$ may be written

$$f=f_0\int f\,\mathrm{d}\,\mathrm{vol}_g+\boldsymbol{\delta}h \tag{A9}$$

for some $h\in\Omega^1_0(\mathcal{N})$. (Since $\mathcal{N}$ is connected, boundaryless and orientable, this follows by de Rahm's theorem: see the remarks following Theorem 7.5.19 in Ref. 39.) Combining Eqs. (A8) and (A9), we have $\mathcal{A}(\mathbf{d}f)=\mathcal{A}(\mathbf{d}f_0)\int f\,\mathrm{d}\,\mathrm{vol}_g$ for all $f\in\Omega^0_0(\mathcal{N})$. Accordingly, $\mathcal{A}(\mathbf{d}\cdot)$ is constant on $\mathcal{N}$ and hence [since it is a $(\Box+M^2)$-solution] on $\mathcal{M}$. It follows that $\mathcal{A}(\mathbf{d}\boldsymbol{\delta}f)=\mathcal{A}(\mathbf{d}f_0)\int\boldsymbol{\delta}f\,\mathrm{d}\,\mathrm{vol}_g=0$ for all $f\in\Omega^1_0(\mathcal{M})$. Since $\mathcal{A}((\Box+M^2)f)=0$, we deduce that Eq. (A7) holds for all $f\in\Omega^1_0(\mathcal{M})$ as required.

(b) $\mathcal{A}(\boldsymbol{\delta}\cdot)$ is a two-form weak $\Box$-solution vanishing on all $h\in\Omega^2_0(\mathcal{N})$ and hence on all $h\in\Omega^2_0(\mathcal{M})$. But since $H^3_c(\mathcal{M})$ is trivial, any $f\in\Omega^1_0(\mathcal{M})$ such that $\boldsymbol{\delta}f=0$ can be written as $f=\boldsymbol{\delta}h$ for some $h\in\Omega^2_0(\mathcal{M})$ and we conclude that $\mathcal{A}(f)=\mathcal{A}(\boldsymbol{\delta}h)=0$. □

After these preliminaries, we may now prove the main result of this section.

Proof of Theorem A.1: The arguments for the two theories run along parallel lines. First one extends the W_M (respectively, W) to be a global bisolution to the appropriate one-form Klein–Gordon equation. Crucially, Theorem 5.5 of Ref. 32 assures us that the Hadamard form propagates and that the resulting bisolution is therefore of Hadamard from on the whole of $\mathcal{M}\times\mathcal{M}$. Thus it suffices to show that Eq. (A1) holds for all $f_i\in\Omega^1_0(\mathcal{M})$ [respectively, that Eq. (A2) holds for all co-closed $f_i\in\Omega^1_0(\mathcal{M})$]. In the Proca case, we apply Proposition A.3(a) together with the field equation axiom (P3) and Eq. (A1) to show that

$$\omega(\mathcal{A}(f_1)\mathcal{A}(f_2))=\omega(\mathcal{A}(\tilde{f}_1)\mathcal{A}(\tilde{f}_2))=W_M(\tilde{f}_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})\tilde{f}_2) \tag{A10}$$

for general $f_i\in\Omega^1_0(\mathcal{M})$. In the Maxwell case, we apply Proposition A.3(b), axiom (M3) and Eq. (A2) to obtain

$$\omega([\mathcal{A}](f_1)[\mathcal{A}](f_2))=\omega([\mathcal{A}](\tilde{f}_1)[\mathcal{A}](\tilde{f}_2))=W(\tilde{f}_1,\tilde{f}_2) \tag{A11}$$

for co-closed $f_i\in\Omega^1_0(\mathcal{M})$. The following claim will be proved below.

Proposition A.5: In the Proca case,

$$W_M((-\boldsymbol{\delta}\mathbf{d}+M^2)f,f')=W_M(f',(-\boldsymbol{\delta}\mathbf{d}+M^2)f)=0 \tag{A12}$$

for all $f,f'\in\Omega_0^1(\mathcal{M})$, *while in the Maxwell case, we have*

$$W(\boldsymbol{\delta}\mathbf{d}f,f')=W(f',\boldsymbol{\delta}\mathbf{d}f)=0 \tag{A13}$$

for all $f,f'\in\Omega_0^1(\mathcal{M})$ *with* f' *co-closed.*

In combination with the explicit form of $\tilde{f}_i-f_i$ [and, in the Proca case, the fact that $(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})$ and $-\boldsymbol{\delta}\mathbf{d}+M^2$ commute], Proposition A.5 allows us to show that

$$W_M(\tilde{f}_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})\tilde{f}_2)=W_M(f_1,(\mathbb{1}-M^{-2}\,\mathbf{d}\boldsymbol{\delta})f_2) \tag{A14}$$

in the Proca case, and that $W(\tilde{f}_1,\tilde{f}_2)=W(f_1,f_2)$ holds for the Maxwell field. Taken together with Eqs. (A10) and (A11), respectively, these relations then establish Eqs. (A1) and (A2). □

The claim made above is proved as follows.

Proof of Proposition A.5: Fix an arbitrary $f'\in\Omega_0^1(\mathcal{N})$ (with the additional requirement that $\boldsymbol{\delta}f'=0$ in the Maxwell case). Then $W_M(\cdot,f')$ and $W_M(f',\cdot)$ [or $W(\cdot,f')$ and $W(f',\cdot)$ in the Maxwell case] obey the hypotheses of Lemma A.4(a) owing to Eq. (A1) and axiom (P3) [respectively, Eq. (A2) and axiom (M3)]. Accordingly, Eq. (A12) [respectively, Eq. (A13)] holds for all $f\in\Omega_0^1(\mathcal{M})$ and the fixed $f'\in\Omega_0^1(\mathcal{N})$. Now fix $f\in\Omega_0^1(\mathcal{M})$ arbitrarily. In the Proca case, $W_M((-\boldsymbol{\delta}\mathbf{d}+M^2)f,\cdot)$ and $W_M(\cdot,(-\boldsymbol{\delta}\mathbf{d}+M^2)f)$ are weak $(\Box+M^2)$-solutions vanishing on $\mathcal{N}$ and hence globally, as required. In the Maxwell case, $W(\boldsymbol{\delta}\mathbf{d}f,\cdot)$ and $W(\cdot,\boldsymbol{\delta}\mathbf{d}f)$ are weak $\Box$-solutions vanishing on co-closed elements of $\Omega_0^1(\mathcal{N})$. Lemma A.4(b) entails that they therefore vanish on all co-closed $f'\in\Omega_0^1(\mathcal{M})$, thereby completing the proof. □

APPENDIX B: CONSTRUCTION OF A HADAMARD $(\Box+M^2)$-BISOLUTION IN ULTRASTATIC SPACE–TIMES

In this appendix we prove Theorem IV.1 by explicitly constructing a Hadamard $(\Box+M^2)$-bisolution W_M on any ultrastatic space–time $(\mathcal{M},g)$ obeying the assumptions stated at the beginning of Sec. IV. For $M>0$, the argument proceeds as follows. First, we use functional calculus on the Hilbert space H to define W_M as a bilinear map from $\Omega_0^1(\mathcal{M})\times\Omega_0^1(\mathcal{M})$ to $\mathbb{C}$. We show that W_M is in fact a one-form bidistributional weak $(\Box+M^2)$-bisolution, with antisymmetric part $-iE_M$, and determine a crude bound on its wave-front set. Next, we appeal to the existence of a *Hadamard* $(\Box+M^2)$-bisolution $\widetilde{W}_M$, also with antisymmetric part $-iE_M$, established in Lemma 5.4(a) of Ref. 32. A simple microlocal argument is used to show that $W_M-\widetilde{W}_M$ is smooth, from which it follows that W_M is itself Hadamard. Finally, we show that W_M may be expanded in terms of any K-pseudo-orthonormal complete set of eigenvectors for the operator K as claimed in Theorem IV.1. The argument is only slightly different in the case $M=0$.

It will be convenient to regard each $\mathcal{A}\in\Omega^1(\mathcal{M})$ as a smooth one-parameter family $t\mapsto\mathcal{A}(t)$ of elements in $\mathsf{H}=\Lambda^0(\Sigma)\oplus\Lambda^1(\Sigma)$, where $\mathcal{A}(t)$ is the restriction of $\mathcal{A}$ to the constant time surface $\{t\}\times\Sigma$. The pairing $\langle\cdot,\cdot\rangle$ of one-forms on $\mathcal{M}$ is related to the inner products of H and K by

$$\langle\mathcal{A},\mathcal{B}\rangle=\int \mathrm{d}t\,\langle\!\langle\overline{\mathcal{A}(t)}|\mathcal{B}(t)\rangle\!\rangle=\int \mathrm{d}t\,(\overline{\mathcal{A}(t)},J\mathcal{B}(t))_{\mathsf{H}}, \tag{B1}$$

where $J=\mathbb{1}_{\Lambda^0(\Sigma)}\oplus-\mathbb{1}_{\Lambda^1(\Sigma)}$. We note that J and $K=(-\Delta_\Sigma^S+M^2)\oplus(-\Delta_\Sigma+M^2)$ commute.

With these conventions, the Klein–Gordon equation $(\Box+M^2)\mathcal{A}=0$ may be written as the Hilbert space ordinary differential equation,

$$-\partial_t^2\mathcal{A}(t)=K\mathcal{A}(t)\,. \tag{B2}$$

Suppose that $M>0$. Because Σ is compact, K has discrete spectrum bounded below by $M^2>0$. Accordingly, the operator $K^{-1/2}$ is well-defined and bounded, and the advanced-minus-retarded solution operator $E_M:\Omega_0^1(\mathcal{M})\to\Omega^1(\mathcal{M})$ may be written

$$(E_M\mathcal{J})(t)=\int \mathrm{d}t'\, K^{-1/2}\sin[K^{1/2}(t'-t)]\mathcal{J}(t')\,, \tag{B3}$$

thus obtaining

$$E_M(\mathcal{J},\mathcal{J}')=\langle\mathcal{J},E_M\mathcal{J}'\rangle=\int \mathrm{d}t\,\mathrm{d}t'\,(\overline{\mathcal{J}(t)},JK^{-1/2}\sin[K^{1/2}(t'-t)]\mathcal{J}'(t'))_{\mathsf{H}}\,. \tag{B4}$$

We define our candidate Hadamard $(\Box+M^2)$-bisolution W_M by taking the positive frequency part of $-iE_M$, i.e., by replacing the sine function by an exponential. To be precise, for $f,f'\in\mathcal{D}(\mathbb{R})$ and $g,g'\in\Omega^0(\Sigma)\oplus\Omega^1(\Sigma)$, we define

$$W_M(f\otimes g,f'\otimes g')=-\tfrac{1}{2}(\hat{\bar{f}}(K^{1/2})\overline{g},K^{-1/2}\hat{f}'(K^{1/2})Jg')_{\mathsf{H}}\,, \tag{B5}$$

in which operators such as $\hat{f}'(K^{1/2})$ are defined by functional calculus. Using the Cauchy–Schwarz inequality and elementary operator norm estimates, we find

$$|W_M(f\otimes g,f'\otimes g')|\leqslant\tfrac{1}{2}\|K^{-1/2}\|\,\|g\|\,\|g'\|\sup_{\omega\in\sigma(K^{1/2})}|\hat{f}(-\omega)|\sup_{\omega\in\sigma(K^{1/2})}|\hat{f}'(\omega)|\,, \tag{B6}$$

from which it follows that W_M extends to a distribution in $(\Omega_0^1(\mathcal{M})\times\Omega_0^1(\mathcal{M}))'$. It is straightforward to check that W_M is a weak $(\Box+M^2)$-bisolution, with antisymmetric part $-iE_M$.

The wave-front set of W_M may be estimated in two ways. First, because it is a $(\Box+M^2)$-bisolution, we have

$$\mathrm{WF}\,(W_M)\subseteq\mathcal{N}\times\mathcal{N}, \tag{B7}$$

where $\mathcal{N}=\{(x,k)\in T^*\mathcal{M}:g^{ab}(x)k_ak_b=0\}$ is the null bundle of $(\mathcal{M},g)$. Second, the explicit bound (B6), coupled with the observation that $\sup_{\omega\in\sigma(K^{1/2})}|\hat{f}(\lambda-\omega)|$ is bounded as $\lambda\to+\infty$, but rapidly decaying for $\lambda\to-\infty$ (and vice versa for $\sup_{\omega\in\sigma(K^{1/2})}|\hat{f}(\lambda+\omega)|$) entails that

$$\mathrm{WF}\,(W_M)\subseteq(\mathcal{T}^+\cup\mathcal{Z})\times(\mathcal{T}^-\cup\mathcal{Z}), \tag{B8}$$

where $\mathcal{T}^\pm=\{(x,k)\in T^*\mathcal{M}:\pm k_0>0\}$ and $\mathcal{Z}=\{(x,k)\in T^*\mathcal{M}:k=0\}$ is the zero section of $T^*\mathcal{M}$. Comparing these two estimates,

$$\mathrm{WF}\,(W_M)\subseteq(\mathcal{N}^+\cup\mathcal{Z})\times(\mathcal{N}^-\cup\mathcal{Z}), \tag{B9}$$

where $\mathcal{N}^\pm=\mathcal{N}\cap\mathcal{T}^\pm$ are the future $(+)$ and past $(-)$ null bundles.

We now appeal to the existence of a Hadamard form $(\Box+M^2)$-bisolution $\tilde{W}_M$ on $(\mathcal{M},g)$ with antisymmetric part $-iE_M$ [Lemma 5.4(a) of Ref. 32]. Since the wave-front set of $\tilde{W}_M$ also obeys (B9), we have

$$\mathrm{WF}\,(W_M-\tilde{W}_M)\subseteq(\mathcal{N}^+\cup\mathcal{Z})\times(\mathcal{N}^-\cup\mathcal{Z})\,. \tag{B10}$$

But $W_M-\tilde{W}_M$ is symmetric, so we also have

$$\mathrm{WF}\,(W_M-\tilde{W}_M)\subseteq(\mathcal{N}^-\cup\mathcal{Z})\times(\mathcal{N}^+\cup\mathcal{Z})\,. \tag{B11}$$

Comparing these two bounds, we see that $\mathrm{WF}(W_M-\widetilde{W}_M)\subseteq\mathcal{Z}\times\mathcal{Z}$ and, since the wave-front set excludes the zero section, we conclude that this wave-front set is in fact empty. Accordingly, $W_M=\widetilde{W}_M \pmod{C^\infty}$ so W_M is of Hadamard form.

The analysis of the massless case is complicated by the existence of a zero eigenvalue mode $\varphi_0=(1,0)$ for K. [Triviality of $H_1(\Sigma)$ precludes the existence of any harmonic one-forms on Σ, so φ_0 is the unique zero mode.] However, the spectrum of K is otherwise bounded away from zero, so $K^{-1/2}$ is well-defined and bounded on $P\mathsf{H}$, where P is the orthogonal projector onto the orthogonal complement of φ_0. In this case, we define

$$W(f\otimes g,f'\otimes g')=-\tfrac{1}{2}(\hat{\bar{f}}(K^{1/2})P\bar{g},K^{-1/2}\hat{f}'(K^{1/2})PJg')_{\mathsf{H}}. \tag{B12}$$

It is easy to check that W is a bi-distributional $\Box$-bisolution, whose antisymmetric part is

$$W(\mathcal{J},\mathcal{J}')-W(\mathcal{J}',\mathcal{J})=-iE_0(\mathcal{J},\mathcal{J}')+i\int \mathrm{d}t\,\mathrm{d}t'\,(t'-t)\,(\overline{\mathcal{J}(t)},\varphi_0)_{\mathsf{H}}(\varphi_0,J\mathcal{J}'(t'))_{\mathsf{H}} \tag{B13}$$

and is therefore equal $(\mathrm{mod}\,C^\infty)$ to $-iE_0$. Appealing as before to the existence of a Hadamard $\Box$-bisolution $\widetilde{W}$ with antisymmetric part $-iE_0$, the argument used above shows that $W=\widetilde{W}$ $(\mathrm{mod}\,C^\infty)$ because $W-\widetilde{W}$ is symmetric $(\mathrm{mod}\,C^\infty)$. It remains to show that the last term in Eq. (B13) vanishes if $\mathcal{J}$ and $\mathcal{J}'$ are both co-closed, as required for consistency with the commutator axiom (M4). Using Eq. (B1) and the fact that $J\varphi_0=\varphi_0$, one may show that the term in question is proportional to $\langle\overline{\mathcal{J}},\mathbf{d}t\rangle\langle t\mathbf{d}t,\mathcal{J}'\rangle-\langle\overline{\mathcal{J}},t\mathbf{d}t\rangle\langle\mathbf{d}t,\mathcal{J}'\rangle$, which vanishes because $\langle\overline{\mathcal{J}},\mathbf{d}t\rangle=\langle\overline{\boldsymbol{\delta}\mathcal{J}},t\rangle=0$ and similarly $\langle\mathbf{d}t,\mathcal{J}'\rangle=0$.

Finally, let ξ_j be a complete set of K-pseudo-orthonormal K-eigenfunctions, with corresponding eigenvalues ω_λ^2 $(\omega_\lambda\geqslant 0)$. Using the completeness relation Eq. (43), we see that

$$\hat{f}'(K^{1/2})^*K^{-1/2}\hat{\bar{f}}(K^{1/2})P\bar{g}=\sum_{j:\omega_j\neq 0}\xi_j\omega_j^{-1}\overline{\hat{f}'(\omega_j)}\hat{\bar{f}}(\omega_j)\langle\!\langle\xi_j|\xi_j\rangle\!\rangle\langle\!\langle\xi_j|\bar{g}\rangle\!\rangle \tag{B14}$$

and hence

$$\begin{aligned}W(\mathcal{J},\mathcal{J}')&=-\sum_{j:\omega_j\neq 0}\frac{1}{2\omega_j}\langle\!\langle\xi_j|\xi_j\rangle\!\rangle\langle\!\langle\hat{\bar{f}}(\omega_j)\bar{g}|\xi_j\rangle\!\rangle\langle\!\langle\xi_j|\hat{f}'(\omega_j)g'\rangle\!\rangle\\&=-\sum_{j:\omega_j\neq 0}\frac{1}{2\omega_j}\langle\!\langle\xi_j|\xi_j\rangle\!\rangle\langle\mathcal{A}_j,\mathcal{J}\rangle\langle\overline{\mathcal{A}_j},\mathcal{J}'\rangle,\end{aligned} \tag{B15}$$

where we have defined the modes $\mathcal{A}_j$ by $\mathcal{A}_j(t)=e^{-i\omega_j t}\xi_\lambda$ and used

$$\langle\!\langle\xi_j|\hat{f}'(\omega_j)g'\rangle\!\rangle=\int \mathrm{d}t\,e^{i\omega_j t}\langle\!\langle\xi_j|f'(t)g'\rangle\!\rangle=\int \mathrm{d}t\,\langle\!\langle\mathcal{A}_j(t)|\mathcal{J}'(t)\rangle\!\rangle=\langle\overline{\mathcal{A}_j},\mathcal{J}'\rangle \tag{B16}$$

and $\langle\!\langle\hat{\bar{f}}(\omega_j)\bar{g}|\xi_j\rangle\!\rangle=\langle\mathcal{J},\mathcal{A}_j\rangle=\langle\mathcal{A}_j,\mathcal{J}\rangle$.

In the case $M>0$, exactly analogous arguments show that the $W_M(\mathcal{J},\mathcal{J}')$ may also be written in the form of the right-hand side of Eq. (B15) (the restriction to $\omega_j>0$ is inessential as all modes obey this condition). This completes the proof of Theorem IV. 1.

ACKNOWLEDGMENTS

Part of this work was conducted at the Erwin Schrödinger Institute for Mathematical Physics, Vienna, during the program on Quantum Field Theory in Curved Space–time. We are grateful to the organisers of this program and to the Institute for its hospitality and financial support. We also thank Atsushi Higuchi, Wolfgang Junker, Fernando Lledó, Ian McIntosh, and Rainer Verch for many illuminating discussions. This work was partially supported by EPSRC Grant No. GR/

R25019/01 to the University of York. M.J.P. also thanks the University of York for a grant awarded under its ''Research Funding for Staff on Fixed Term Contracts'' scheme.

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[69] We also observe that their work is directed towards a construction of Hadamard states in general globally hyperbolic space–times which avoids the use of deformation arguments.
[70] Some care is needed over the definition of the two-point function in the Maxwell case (see Sec. III). In particular, it is not a distribution.
[71] The *support* of a function is the closure of the set of points on which it is nonzero.
[72] The index is the number of spacelike (i.e., negative norm-squared) basis vectors in any g-orthonormal frame.
[73] The topology is defined so that a sequence $\mathcal{U}_n \to 0$ in $\Omega_0^p(\mathcal{N})$ if and only if $*(\mathcal{V}LU*\mathcal{U}_n) \to 0$ in $\mathcal{D}(\mathcal{N})$ for every $\mathcal{V} \in \Omega^p(\mathcal{N})$.
[74] Since Σ is compact, it admits a finite good cover (Theorem 5.1 in Ref. 66) which determines a finite good cover of $\mathcal{M}=\mathbb{R}\times\Sigma$. Accordingly, we may use Poincaré duality (Theorem 5.4 in Ref. 66) to prove that $H_c^3(\mathcal{M})$ is isomorphic to $H^1(\mathcal{M})$ and hence to $H^1(\Sigma)$ (see the remarks following Corollary 5.1.1 in Ref. 66). This is isomorphic to $H_1(\Sigma)$ by de Rahm's theorem (Ref. 67).
[75] Note that Dimock (Ref. 36) uses E for the retarded-minus-advanced bisolution.
[76] For example, $\mathfrak{A}_M(\mathcal{M},g)$ is the infinitesimal Weyl algebra over the real symplectic space $\Omega_0^1(\mathcal{M};\mathbb{R})/\ker \Delta_M$ (with the quotient topology) with the addition of the $*$-operation. This has no nontrivial two-sided $*$-ideals (see Sec. 7.1 in Ref. 46).
[77] Effectively, one is substituting the test function $f(x)=\int \mathrm{d}\tau |h(x)|^{-1/2}\delta^4(x-\gamma(\tau))\overline{g_\alpha(\tau)}$ in Eq. (76). This results in the required expression.
[78] The right-hand side of the bound may be written in the form $-\int_0^\infty \mathrm{d}u\, Q(u)|\hat{g}(u)|^2$, where $Q(u)$ is a polynomially bounded function. Accordingly, the integral will converge provided that the Fourier transform $\hat{g}(u)$ decays sufficiently rapidly as $u\to+\infty$; equivalently, provided that g belongs to a Sobolev space $W^{k,2}(\mathbb{R})$ (see e.g., Ref. 68) of sufficiently high regularity (k sufficiently large). If we restrict the class of states so that $\langle :\rho: \rangle_\omega(\tau)$ belongs to the dual Sobolev space $W^{-k,2}(\mathbb{R})$ then Eq. (139) will continue to hold. To see this, we approximate g in the $W^{k,2}(\mathbb{R})$ norm by a sequence of compactly supported smooth functions [using density of $C_0^\infty(\mathbb{R})$ in $W^{k,2}(\mathbb{R})$] and apply Eq. (139). It is not presently known whether this requires a nontrivial restriction on the class of allowed states.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

A direct derivation of polynomial invariants from perturbative Chern–Simons gauge theory

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(Received 22 April 2003; accepted 1 June 2003)

There have been several methods to show that the expectation values of Wilson loop operators in the SU(N) Chern–Simons gauge theory satisfy the HOMFLY skein relation. We shall give another method from the perturbative method of the SU(N) Chern–Simons gauge theory in the light-cone gauge, which is more direct than already known methods. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1606525]

I. INTRODUCTION

The connection between the three-dimensional Chern–Simons gauge theory and knot theory was established by E. Witten, who showed that the expectation value of Wilson loop operators in the Chern–Simons gauge theory satisfies the HOMFLY skein relation,[10] using certain conformal field theories [see Fig. 1(a)]. Since then the Chern–Simons gauge theory has been studied from a variety of points of view. J. Frohlich and C. King[3] derived the Knizhnik–Zamolodchikov equations from the Chern-Simons gauge theory in the light-cone gauge [Fig. 1, (b_1)]. The solution of this differential equation was shown to be simply related to the HOMFLY skein relation for links [Fig. 1, (b_2)]. On the other hand, J. M. F. Labastida and E. Perez[6] derived the Kontsevich integral from the perturbative analysis of the Chern–Simons gauge theory in the light-cone gauge [Fig. 1(c)]. It is known that the combination of the Kontsevich integral and the weight system of $\mathfrak{su}(N)$ satisfies the HOMFLY skein relation[7,9] [Fig. 1(d)]. We remark that the Kontsevich integral is derived from the Knizhnik–Zamolodchikov equations, using an iterated integral[5] [Fig. 1(e)]. These relations among the three-dimensional Chern–Simons gauge theory, the HOMFLY skein relation, the Knizhnik–Zamolodchikov equations and the Kontsevich integral imply the deep structure of the Chern–Simons gauge theory.

But these already known methods need rather complicated concepts. Therefore, we would like to give a more straightforward and simpler approach. In this article, inspired by the two methods[6,9] [Figs. 1(c) and 1(d)], we give another such method to derive the HOMFLY skein relation from the Chern–Simons gauge theory [Fig. 1(f)] without using any other theory.

We remark that in Refs. 2 and 4 the skein relation was derived at first order in the coupling constant, using a variational method based on the properties of the path integral.

II. THE FORMULATION OF THE CHERN–SIMONS GAUGE THEORY

In this section, we review the Chern–Simons gauge theory as in Refs. 2, 3, 6, and 8.

The Chern–Simons gauge theory is a three dimensional model based on the Lagrangian L which is a differential three-form defined on $\mathbf{R}^3$ parametrized by (x^0,x^1,x^2):

$$L(A)=tr(A\wedge dA+i\ \tfrac{2}{3}A\wedge A\wedge A),$$

where a connection A is $\mathfrak{su}(N)$-valued one form on $\mathbf{R}^3$, and "tr" means the trace.

The generators of $\mathfrak{su}(N)$ are normalized as follows:

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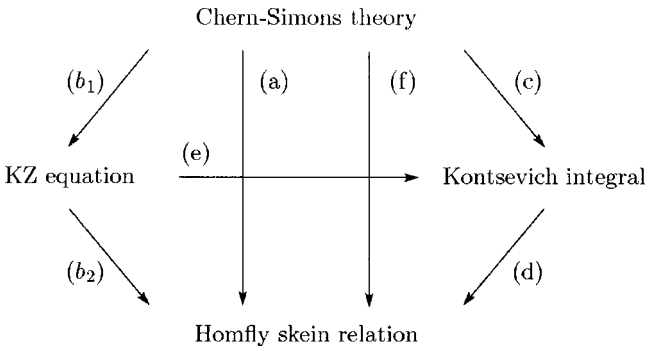

FIG. 1. Illustration of introduction.

$$tr(T_aT_b)=\tfrac{1}{2}\delta_{ab},\ [T_a,T_b]=if^c_{ab}T_c,$$

with the structure constants f^c_{ab}. The action of the Chern–Simons gauge theory is given by

$$S_k(A)=\frac{k}{4\pi}\int_{\mathbf{R}^3}L(A)=\frac{k}{4\pi}\int_{\mathbf{R}^3}dx^0\wedge dx^1\wedge dx^2\epsilon^{\mu\nu\rho}tr\left(A_\mu\partial_\nu A_\rho+i\frac{2}{3}A_\mu A_\nu A_\rho\right)$$
$$=\frac{k}{8\pi}\int_{\mathbf{R}^3}dx^3\epsilon^{\mu\nu\rho}\left(A^a_\mu\partial_\nu A^a_\rho-\frac{1}{3}A^a_\mu A^b_\nu A^c_\rho f^c_{ab}\right),\tag{2.1}$$

where k is a real parameter and

$$A=A_\mu dx^\mu=A^a_\mu T_a dx^\mu.$$

Let us introduce so-called ''Wilson loop operators.'' Let C be a curve parametrized by $\vec{x}(t)$. Define the holonomy of A along a curve C by

$$H_C(A)=P\exp i\oint_C A,\tag{2.2}$$

where the right-hand side of (2.2) means

$$1+\sum_{m=1}^{\infty}i^m\int_{t_{\min}<t_1<\cdots<t_m<t_{\max}}dt_1\cdots dt_m\ \dot{x}^{\mu_m}(t_m)A_{\mu_m}(x(t_m))\cdots\dot{x}^{\mu_1}(t_1)A_{\mu_1}(x(t_1)).$$

The holonomy $H_C(A)$ has the important property as follows. If a curve $C=\{\vec{x}(t)|t_{\min}\leqslant t\leqslant t_{\max}\}$ is divided into n-curves $C_k=\{\vec{x}(s)\ |s_{k-1}\leqslant s\leqslant s_k\}$ $(t_{\min}=s_0<s_1<\cdots<s_n=t_{\max})$, then the holonomy $H_C(A)$ is decomposed as follows:

$$H_C(A)=H_{C_n}(A)\ \cdots\ H_{C_1}(A).\tag{2.3}$$

Let K be a knot (i.e., a closed curve) in $\mathbf{R}^3$. The Wilson loop operator $W_K(A)$ is a special type of functional of connection A defined by

$$W_K(A)=tr(H_K(A)).$$

We extend the above definition to a link. Let $L=\{K_1,\ldots,K_m\}$ be an m-component link which is a union of m knots $K_i(i=1,\ldots,m)$. Then, the definition of the Wilson loop operator can be extended to a link L as follows:

$$W_L(A)=W_{K_1}(A)\cdots W_{K_m}(A). \tag{2.4}$$

We will define the expectation value of the Chern–Simons gauge theory as follows. The expectation value of $W_L(A)$ is defined by

$$\langle W_L\rangle=\frac{1}{Z}\int [DA]e^{iS_k(A)}\ \ W_L(A), \tag{2.5}$$

where

$$Z=\int [DA]e^{iS_k(A)} \tag{2.6}$$

and the symbol $[DA]$ denotes the path integral over all equivalence classes of connections modulo gauge transformations.

It is convenient to introduce new coordinates,

$$z=x^1+ix^2,\ \ \overline{z}=x^1-ix^2,\ \ t=x^0, \tag{2.7}$$

and define also

$$\partial=\frac{1}{2}\left(\frac{\partial}{\partial x_1}-i\frac{\partial}{\partial x_2}\right),\ \ \overline{\partial}=\frac{1}{2}\left(\frac{\partial}{\partial x_1}+i\frac{\partial}{\partial x_2}\right). \tag{2.8}$$

For a connection $A=A_\mu\, dx^\mu$, set

$$A_z=\tfrac{1}{2}(A_1+A_2),\ \ A_{\overline{z}}=\tfrac{1}{2}(A_1-A_2). \tag{2.9}$$

In order to evaluate expectation value (2.5), it is necessary to fix a gauge condition. We introduce the light-cone gauge condition as in Refs. 3 and 6. The light-cone gauge condition is defined by

$$A_{\overline{z}}=\tfrac{1}{2}(A_1-A_2)=0. \tag{2.10}$$

This gauge condition is preferable, since it kills the second term on the right-hand side of (2.1) and greatly simplifies the theory.

Using these new coordinates (2.7)–(2.9) and the light-cone gauge condition (2.10), the action of the Chern–Simons gauge theory (2.1) is transformed into

$$S_k(A)=\frac{k}{4\pi}\int dtd\overline{z}dz\,\frac{1}{2}(A_0^a\overline{\partial}A_z^a-A_z^a\overline{\partial}A_0^a). \tag{2.11}$$

We remark that the above equation is a quadratic form.

Under these conditions, the two-point correlation functions are computed in Refs. 3 and 6. For fixed $\mathbf{x}=(t,z,\overline{z})$, $\mathbf{x}'=(t',z',\overline{z}')$, we can consider $A_0^a(\mathbf{x})A_z^b(\mathbf{x}')$, $A_0^a(\mathbf{x})A_0^b(\mathbf{x}')$ and $A_z^a(\mathbf{x})A_z^b(\mathbf{x}')$ as functionals of A. From the Appendix, their expectation values are given by

$$\langle A_0^a(\mathbf{x})A_z^b(\mathbf{x}')\rangle=-\delta^{ab}\frac{2}{k}\frac{\delta(t-t')}{z-z'}, \tag{2.12}$$

$$\langle A_0^a(\mathbf{x})A_0^b(\mathbf{x}')\rangle=0, \tag{2.13}$$

$$\langle A_z^a(\mathbf{x})A_z^b(\mathbf{x}')\rangle=0. \tag{2.14}$$

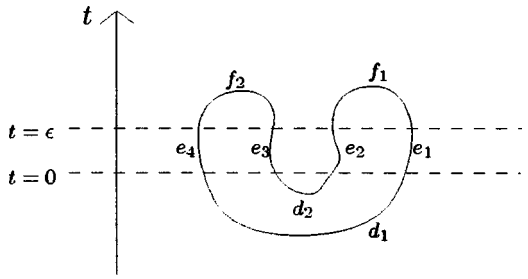

FIG. 2. Division of a knot K.

Under these preparations, we will show that the expectation value of the Wilson loop operator satisfies the HOMFLY skein relation by a direct computation. The main idea of the computation is as follows. First, we decompose $\mathbf{R}^3$ into the three domains $\{t\leqslant 0\}$, $\{0\leqslant t\leqslant \epsilon\}$, $\{\epsilon\leqslant t\}$ called the lower domain, the middle domain and the upper domain, respectively. We will show that the expectation value of the Wilson loop operator is essentially the product of three expectation values corresponding to these three domains. By applying the perturbative method to the expectation value corresponding to the middle domain, we can derive the HOMFLY polynomial.

III. DIVISION OF THE EXPECTATION VALUE OF THE WILSON LOOP OPERATOR

In this section, we divide the expectation value of the Wilson loop operator into three parts. We assume that a knot K is in a special position as follows. We divide a knot K into $4n$ curves

$$C_\alpha=\{\vec{x}(s)\,|\,s_{\alpha-1}\leqslant s\leqslant s_\alpha\},\quad 0=s_0<s_1<\cdots<s_{4n}=1,$$

and set

$$\begin{aligned} d_\alpha &= C_{4\alpha-3}\quad(\alpha=1,2,3,\ldots,n),\\ e_\beta &= C_{2\beta}\quad(\beta=1,2,3,\ldots,2n),\\ f_\alpha &= C_{4\alpha-1}\quad(\alpha=1,2,3,\ldots,n). \end{aligned} \tag{3.1}$$

Moreover, it is assumed that the curves d_α, e_β and f_α are in the region $t\leqslant 0$, $0\leqslant t\leqslant\epsilon$, $\epsilon\leqslant t$, respectively. (See Fig. 2)

Define holonomies $D_K^\alpha(A)$, $E_K^\beta(A)$ and $F_K^\alpha(A)$ for the curves d_α, e_β and f_α by

$$\begin{aligned} D_K^\alpha(A) &= P\exp i\int_{d_\alpha} A,\\ E_K^\beta(A) &= P\exp i\int_{e_\beta} A,\\ F_K^\alpha(A) &= P\exp i\int_{f_\alpha} A. \end{aligned} \tag{3.2}$$

From (2.3), the Wilson loop operator $W_K(A)$ can be expressed as the trace over the product of the matrices D_K^α, E_K^β, and F_K^α $(1\leqslant\alpha\leqslant n,\ 1\leqslant\beta\leqslant 2n)$ as follows:

$$W_K = tr\left(\prod_{\alpha=1}^{4n} H_{C_\alpha}\right) = tr\left(\prod_{\alpha=1}^{n} E_K^{2\alpha} F_K^{\alpha} E_K^{2\alpha-1} D_K^{\alpha}\right)$$

$$= \sum_{i_1\cdots i_{2n}} \sum_{j_1\cdots j_{2n}} \prod_{\alpha=1}^{n} (E_K^{2\alpha})_{j_{2\alpha}}^{i_{2\alpha}} (F_K^{\alpha})_{j_{2\alpha-1}}^{j_{2\alpha}} (E_K^{2\alpha-1})_{i_{2\alpha-1}}^{j_{2\alpha-1}} (D_K^{\alpha})_{i_{2\alpha-2}}^{i_{2\alpha-1}}$$

$$= \sum_{i_1\cdots i_{2n}} \sum_{j_1\cdots j_{2n}} (F_K)_{j_{2n},\cdots,j_1} (E_K)_{i_{2n}\cdots i_1}^{j_{2n}\cdots j_1} (D_K)^{i_{2n}\cdots i_1},$$

where we set $i_{2n}=i_0$ and D_K, E_K and F_K in the last line are defined by

$$(D_K)^{i_{2n}\cdots i_1} = \prod_{\alpha=1}^{n} (D_K^{\alpha})_{i_{2\alpha-2}}^{i_{2\alpha-1}},$$

$$(E_K)_{i_{2n}\cdots i_1}^{j_{2n}\cdots j_1} = \prod_{\alpha=1}^{n} (E_K^{2\alpha})_{j_{2\alpha}}^{i_{2\alpha}} (E_K^{2\alpha-1})_{i_{2\alpha-1}}^{j_{2\alpha-1}},$$

$$(F_K)_{j_{2n},\cdots,j_1} = \prod_{\alpha=1}^{n} (F_K^{\alpha})_{j_{2\alpha-1}}^{j_{2\alpha}}.$$

As a result, we obtain the following lemma.

Lemma 3.1: The Wilson loop operator $W_K(A)$ is decomposed as follows:

$$W_K = F_K \;\; E_K \;\; D_K, \tag{3.3}$$

where the right-hand side of (3.3) means

$$F_K \;\; E_K \;\; D_K = \sum_{i_1\cdots i_{2n}} \sum_{j_1\cdots j_{2n}} (F_K)_{j_{2n},\cdots,j_1} (E_K)_{i_{2n}\cdots i_1}^{j_{2n}\cdots j_1} (D_K)^{i_{2n}\cdots i_1}.$$

Remark: Note that the curves in D_K, E_K, and F_K are in the region $t\leqslant 0$, $0\leqslant t\leqslant \epsilon$, $\epsilon\leqslant t$, respectively.

For a link, we extend the above lemma as follows.

Lemma 3.2: Let $L=\{K_1,\ldots,K_m\}$ be an m-component link. The Wilson loop operator for L is decomposed as follows:

$$W_L = F_L \;\; E_L \;\; D_L, \tag{3.4}$$

where D_L, E_L, and F_L on the right-hand side are defined by

$$D_L = D_{K_1}\cdots D_{K_m},$$

$$E_L = E_{K_1}\cdots E_{K_m},$$

$$F_L = F_{K_1}\cdots F_{K_m}.$$

Proof: From Lemma 3.1, we decompose each Wilson loop operator W_{K_α} $(\alpha=1,2,\ldots,m)$ as follows:

$$W_{K_j} = F_{K_j} \;\; E_{K_j} \;\; D_{K_j} \;\; (j=1,2,\ldots,m).$$

Inserting this into (2.4), we obtain

$$W_L = F_{K_1} \cdots F_{K_m} E_{K_1} \cdots E_{K_m} D_{K_1} \cdots D_{K_m}.$$

This shows (3.4). □

We divide the expectation value of the Wilson loop operator into three parts in the same manner as the Wilson loop operator.

Lemma 3.3: The expectation value of Wilson loop operator for a knot is decomposed as follows:

$$\langle W_K \rangle = \langle F_K \rangle_F \langle E_K \rangle_E \langle D_K \rangle_D, \tag{3.5}$$

where the right-hand side of (3.5) means

$$\langle F_K \rangle_F \langle E_K \rangle_E \langle D_K \rangle_D = \sum_{i_1 \cdots i_{2n}} \sum_{j_1 \cdots j_{2n}} \langle (F_K)_{j_{2n}, \cdots, j_1} \rangle_F \langle (E_K)^{j_{2n} \cdots j_1}_{i_{2n} \cdots i_1} \rangle_E \langle (D_K)^{i_{2n} \cdots i_1} \rangle_D$$

and

$$\langle (D_K)^{i_{2n} \cdots i_1} \rangle_D = \frac{1}{Z_D} \int [DA]_D \exp\left(\frac{ik}{4\pi} \int_{\{-\infty \leqslant t \leqslant 0\}} \right\} L(A) \ \ (D_K(A))^{i_{2n} \cdots i_1},$$

$$\langle (E_K)^{j_{2n} \cdots j_1}_{i_{2n} \cdots i_1} \rangle_E = \frac{1}{Z_E} \int [DA]_E \exp\left(\frac{ik}{4\pi} \int_{\{0 \leqslant t \leqslant \epsilon\}} L(A) \right) (E_K(A))^{j_{2n} \cdots j_1}_{i_{2n} \cdots i_1},$$

$$\langle (F_K)_{j_{2n}, \cdots, j_1} \rangle_F = \frac{1}{Z_F} \int [DA]_F \exp\left(\frac{ik}{4\pi} \int_{\{\epsilon \leqslant t \leqslant \infty\}} L(A) \right) \ \ (F_K(A))_{j_{2n}, \cdots, j_1},$$

where $[DA]_D$, $[DA]_E$ and $[DA]_F$ mean the measure restricted to the region $t \leqslant 0$, $0 \leqslant t \leqslant \epsilon$ and $\epsilon \leqslant t$, respectively. Here, Z_D, Z_E and Z_F are defined as in (2.6), but the regions of the measure and the action are restricted to $t \leqslant 0$, $0 \leqslant t \leqslant \epsilon$ and $\epsilon \leqslant t$, respectively.

Proof: We divide the domain of integration of action (2.1) into three parts:

$$S_k(A) = \frac{k}{4\pi} \int_{\{\infty \leqslant t \leqslant 0\}} L(A) + \frac{k}{4\pi} \int_{\{0 \leqslant t \leqslant \epsilon\}} L(A) + \frac{k}{4\pi} \int_{\{\epsilon \leqslant t \leqslant \infty\}} L(A). \tag{3.6}$$

Next, since the measure of the path integral has the property

$$[DA] = [DA]_F [DA]_E [DA]_D, \tag{3.7}$$

inserting (3.6), (3.7) and (3.4) into (2.5) yields (3.5). □

More generally, Lemma 3.3 can be easily extended for a link L as follows:

Lemma 3.4: $\langle W_L \rangle = \langle F_L \rangle_F \ \langle E_L \rangle_E \ \langle D_L \rangle_D$.

IV. THE MAIN PART OF COMPUTATION

Let L_+, L_- and L_0 be general multi-component links as shown in Fig. 3 which are identical with each other outside the region $0 \leqslant t \leqslant \epsilon$. Especially, we write K_+, K_- and K_0 instead of L_+, L_- and L_0, if L_+, L_- and L_0 are a one-component knot, a one-component knot, and a two-component link, respectively.

From Lemma 3.4, we decompose the expectation value of Wilson loop operators as follows:

$$\langle W_{L_+} \rangle = \langle F_{L_+} \rangle_F \langle E_{L_+} \rangle_E \langle D_{L_+} \rangle_D, \tag{4.1}$$

$$\langle W_{L_-} \rangle = \langle F_{L_-} \rangle_F \langle E_{L_-} \rangle_E \langle D_{L_-} \rangle_D, \tag{4.2}$$

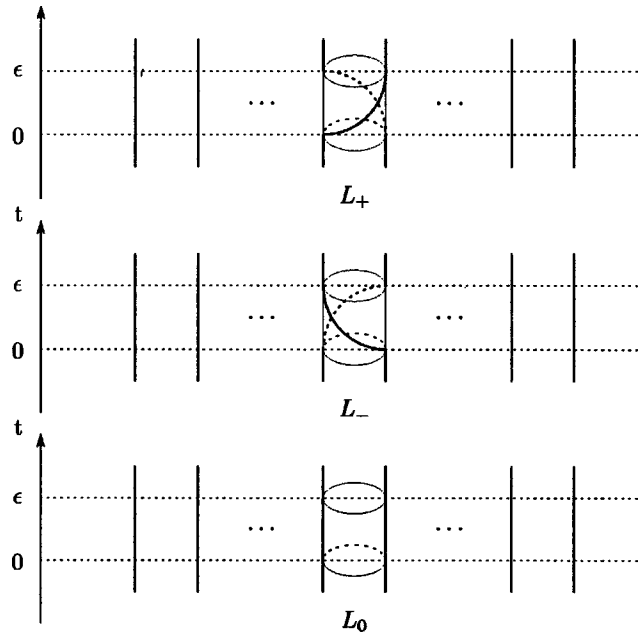

FIG. 3. L_+, L_-, L_0.

$$\langle W_{L_0}\rangle = \langle F_{L_0}\rangle_F \langle E_{L_0}\rangle_E \langle D_{L_0}\rangle_D . \tag{4.3}$$

We will concentrate our attention on the computation of $\langle E_{L_\rho}\rangle_L$ $(\rho = 0, \pm)$, since $\langle D_{L_\rho}\rangle_D$ and $\langle F_{L_\rho}\rangle_F$ take the same value for $\rho = 0, \pm$. But, avoiding unnecessary complexity, we will limit our situation to the case $L_\rho = K_\rho$ $(\rho = 0, \pm)$. Then, decompositions (4.1)–(4.3) become

$$\langle W_{K_+}\rangle = \langle F_{K_+}\rangle_F \langle E_{K_+}\rangle_E \langle D_{K_+}\rangle_D ,$$

$$\langle W_{K_-}\rangle = \langle F_{K_-}\rangle_F \langle E_{K_-}\rangle_E \langle D_{K_-}\rangle_D ,$$

$$\langle W_{K_0}\rangle = \langle F_{K_0}\rangle_F \langle E_{K_0}\rangle_E \langle D_{K_0}\rangle_D .$$

In what follows, we will be mainly concerned with the computation of $\langle E_{K_+}\rangle_E$. Without loss of generality, we may assume that the curves $e_1, e_2, \ldots, e_{2n}$ in K_+ are given as follows. Two curves $e_1(t)$ and $e_3(t)$ are given by

$$e_\alpha(t) = (t, z_\alpha(t)), \qquad \alpha = 1,3 \qquad 0 \leqslant t \leqslant \epsilon,$$

where

$$z_1(t) = -a \exp\left(\frac{i\pi t}{\epsilon}\right), \qquad z_3(t) = a \exp\left(\frac{i\pi t}{\epsilon}\right). \tag{4.4}$$

Here we remark that we have chosen $e_1(t)$ and $e_3(t)$ instead of $e_1(t)$ and $e_2(t)$, since $e_1(t)$ and $e_3(t)$ are upward while $e_2(t)$ is downward [see (3.1)].

The other curves $e_2, e_4, \ldots, e_{2n}$ are straight lines parallel to t-axis

$$e_\alpha(t) = (t, z_\alpha), \qquad \alpha = 2,4,\ldots,2n,$$

where z_α $(\alpha = 2,4,\ldots,2n)$ are fixed points and distinct from each other.

Under these assumptions, we will compute $\langle E_{K_+}\rangle_E$ using the perturbative method.
In new coordinates (2.7) and (2.9), holonomy (3.2) takes the form

$$E^{\alpha}_{K_+}(A)=P\exp i\int_{e_\alpha}A=1+\sum_{m=1}^{\infty}i^m\int_{0<t_1<\cdots<t_m<\epsilon}dt_1\cdots dt_m\quad\prod_{k=1}^{m}(A_0^{a_k}(t_k,z_\alpha(t_k))$$
$$+\dot z_\alpha(t_k)A_z^{a_k}(t_k,z_\alpha(t_k)))\times T^{a_1}\cdots T^{a_m}. \tag{4.5}$$

Let us consider the integrands of (4.5) in the next lemma.
Lemma 4.1:

$$\langle(A_0^a(t,z_\alpha(t))+\dot z_\alpha(t)A_z^a(t,z_\alpha(t)))(A_0^b(s,z_\beta(s))+\dot z_\beta(s)A_z^b(s,z_\beta(s)))\rangle_E$$
$$=\delta^{ab}\quad\delta(t-s)\frac{2}{k}\frac{d}{dt}\log(z_\alpha(t)-z_\beta(t)). \tag{4.6}$$

Proof: The left-hand side of (4.6) is equal to

$$-(\dot z_\alpha(t)-\dot z_\beta(s))\langle A_0^a(t,z_\alpha(t))A_z^b(s,z_\beta(s))\rangle_E\,.$$

Inserting (2.12) into this, we have the right-hand side of (4.6). Here we remark that (2.12) is still valid for $\langle\cdot\rangle_E$, since the argument for deriving (2.12) is independent of the domain of t. See the Appendix. □

Lemma 4.2: For sufficiently small a, $\langle E_{K_+}\rangle_E$ is transformed into the following simple form:

$$\langle(E_{K_+})^{j_{2n}\cdots j_1}_{i_{2n}\cdots i_1}\rangle_E=\delta^{j_{2n}}_{i_{2n}}\cdots\delta^{j_4}_{i_4}\delta^{j_2}_{i_2}\langle(E^3_{K_+}\otimes E^1_{K_+})^{j_3j_1}_{i_3i_1}\rangle_E, \tag{4.7}$$

where

$$(E^3_{K_+}\otimes E^1_{K_+})^{j_3j_1}_{i_3i_1}=(E^3_{K_+})^{j_3}_{i_3}(E^1_{K_+})^{j_1}_{i_1}.$$

Proof: Using (A6) in the Appendix, we can express the left-hand side of (4.7) as the sum of the products of the elements

$$\langle(A_0^a(t,z_\alpha(t))+\dot z_\alpha(t)A_z^a(t,z_\alpha(t)))(A_0^b(s,z_\beta(s))+\dot z_\beta(s)A_z^b(s,z_\beta(s)))\rangle_E\,. \tag{4.8}$$

If a is sufficiently small, for all the combination $(\alpha,\beta)\neq(1,3),(3,1)$, we may consider $z_\alpha(t)$ and $z_\beta(s)$ to be constant. Then, from Lemma 4.1, we find that these elements (4.8) vanish. Hence it is enough to consider the combination $(\alpha,\beta)=(1,3),(3,1)$ only. We can see that this combination directly gives the nontrivial factor $\langle(E^3_{K_+}\otimes E^1_{K_+})^{j_3j_1}_{i_3i_1}\rangle_E$ in (4.7). This completes the proof. □

Next, let us evaluate the nontrivial element $\langle(E^3_{K_+}\otimes E^1_{K_+})^{j_3j_1}_{i_3i_1}\rangle_E$ on the right-hand side of (4.7).

Lemma 4.3: The nontrivial element on the right-hand side of (4.7) is computed as follows:

$$\langle(E^3_{K_+}\otimes E^1_{K_+})^{j_3j_1}_{i_3i_1}\rangle_E=(\exp(\sigma\quad T^a\otimes T^a))^{j_3j_1}_{i_3i_1}, \tag{4.9}$$

where $(\sigma=-2\pi i/k)$.

Proof: Inserting (4.5) into the left-hand side of (4.9) and using Lemma 4.1, we obtain

$$\langle E^3_{K_+}\otimes E^1_{K_+}\rangle_E=1+\sum_{m=1}^{\infty}\left(-\frac{2}{k}T^a\otimes T^a\right)^m\int_{0<t_1<\cdots<t_m<1}\prod_{k=1}^{m}(d\log(z_3(t_k)-z_1(t_k))). \tag{4.10}$$

Here we have used the fact that (4.6) vanishes if $t\neq s$.

Inserting (4.4) into the second term on the right-hand side of (4.10), we have

$$\int_{0<t_1<\cdots<t_m<1}\prod_{k=1}^{m}(d\log(z_3(t_k)-z_1(t_k)))=\frac{1}{m!}(i\pi)^m.$$

Inserting this into the right-hand of (4.10) and summarizing it as an exponential function, we obtain

$$\langle E^3_{K_+}\otimes E^1_{K_+}\rangle_E=\exp(\sigma\ \ T^a\otimes T^a).$$

□

Let $V=\mathbf{R}^n$ be the N-dimensional vector space. Define $P:V\otimes V\to V\otimes V$ by

$$P(v\otimes w)=w\otimes v,$$

where v and w are N-dimensional vectors.

Lemma 4.4:

$$\exp\left(\frac{\sigma}{2N}\right)\langle E^3_{K_+}\otimes E^1_{K_+}\rangle_E-\exp\left(-\frac{\sigma}{2N}\right)\langle E^3_{K_-}\otimes E^1_{K_-}\rangle_E=\left(\exp\left(\frac{\sigma}{2}\right)-\exp\left(-\frac{\sigma}{2}\right)\right)P. \quad (4.11)$$

Proof: Inserting the so-called Fierz identity

$$T^a\otimes T^a=-\frac{1}{2N}1\otimes 1+\frac{1}{2}P$$

into the right-hand side of (4.9), we obtain

$$\langle(E^3_{K_+}\otimes E^1_{K_+})\rangle_E=\exp\left(-\frac{\sigma}{2N}\right)\exp\left(\frac{\sigma}{2}P\right). \quad (4.12)$$

Similarly, we compute the expectation value for K_- in the same manner as K_+ and obtain

$$\langle(E^3_{K_-}\otimes E^1_{K_-})\rangle_E=\exp\left(\frac{\sigma}{2N}\right)\exp\left(-\frac{\sigma}{2}P\right). \quad (4.13)$$

Inserting (4.12) and (4.13) into the left-hand side (4.11) and using

$$\left(\exp\left(\frac{\sigma}{2}P\right)-\exp\left(-\frac{\sigma}{2}P\right)\right)=\left(\exp\left(\frac{\sigma}{2}\right)-\exp\left(-\frac{\sigma}{2}\right)\right)P$$

yields the right-hand side of (4.11). □

Theorem 4.5: The expectation values for L_+, L_- and L_0 satisfy the relation

$$\exp\left(\frac{\sigma}{2N}\right)\langle W_{L_+}\rangle-\exp\left(-\frac{\sigma}{2N}\right)\langle W_{L_-}\rangle=(e^{(1/2)\sigma}-e^{-(1/2)\sigma})\ \langle W_{L_0}\rangle. \quad (4.14)$$

Proof: First, we prove relation (4.14) for K_ρ $(\rho=0,\pm)$, i.e.,

$$\exp\left(\frac{\sigma}{2N}\right)\langle W_{K_+}\rangle-\exp\left(-\frac{\sigma}{2N}\right)\langle W_{K_-}\rangle=(e^{(1/2)\sigma}-e^{-(1/2)\sigma})\langle W_{K_0}\rangle. \quad (4.15)$$

Multiplying both sides of (4.11) by $\delta^{j_{2n}}_{i_{2n}}\cdots\delta^{j_4}_{i_4}\delta^{j_2}_{i_2}$, we have

$$\exp\left(\frac{\sigma}{2N}\right)\langle (E_{K_+})^{j_{2n}\cdots j_1}_{i_{2n}\cdots i_1}\rangle_E - \exp\left(-\frac{\sigma}{2N}\right)\langle (E_{K_-})^{j_{2n}\cdots j_1}_{i_{2n}\cdots i_1}\rangle_E = (e^{\sigma/2}-e^{-\sigma/2})\ \ \delta^{j_{2n}}_{i_{2n}}\cdots\delta^{j_4}_{i_4}\delta^{j_2}_{i_2}P^{j_3 j_1}_{i_3 i_1}.$$

Multiplying this by $\langle (D_{K_\rho})^{i_{2n}\cdots i_1}\rangle_D$ and $\langle (F_{K_\rho})_{j_{2n},\cdots,j_1}\rangle_F$ $(\rho=0,\pm)$, we obtain (4.15).

Next, relation (4.15) can be extended for L_ρ $(\rho=0,\pm)$ in the same way, since the proof of relation (4.15) is focused on two curves $e_1(t)$ and $e_3(t)$ and independent of the other parts. This completes the proof. □

Let $L=\{K_1,\ldots,K_m\}$ be an m-component link which is a union of n knots K_i $(i=1,\ldots,m)$. Define $lk(K_i,K_j)$ to be the linking number between K_i and K_j, and $\psi_f(K_i)$ the framing number, i.e., the linking number between the knot K_i and its framing. For a link L, set

$$w(L)=2\sum_{i<j} lk(K_i,K_j)+\sum_{i=1}^{m}\psi_f(K_i).$$

Next, define $P_L(x,N)$ by

$$P_L(\sigma,N)=\exp\left\{-\sigma\frac{N^2-1}{2N}w(L)\right\}\langle W_L\rangle. \tag{4.16}$$

Then, we easily obtain the following corollary, using standard argument.[2]

Corollary 4.6:

$$\exp\left(\frac{N\sigma}{2}\right)P_{L_+}(\sigma,N)-\exp\left(-\frac{N\sigma}{2}\right)P_{L_-}(\sigma,N)=(e^{(1/2)\sigma}-e^{-(1/2)\sigma})P_{L_0}(\sigma,N). \tag{4.17}$$

Proof: Inserting (4.16) into (4.14) and using

$$w(L_+)-w(L_0)=w(L_0)-w(L_-)=1$$

yield (4.17). □

Remark: Equation (4.17) is called the HOMFLY skein relation.

APPENDIX: THE PERTURBATIVE METHOD

In this section, we review the perturbative method for the Chern–Simons gauge theory for the matter of convenience. See quantum field theory textbooks for more details.

Let $W(A)$ be an arbitrary complex-valued functional of connection A. The expectation value of $W(A)$ is defined by

$$\langle W\rangle=\frac{1}{Z}\int [DA]e^{iS_k(A)}\ \ W(A), \tag{A1}$$

where the symbol $[DA]$ denotes the path integral.

The action of the Chern–Simons gauge theory in light-cone gauge (2.11) is transformed into the matrix form:

$$S_k(A)=\frac{k}{4\pi}\int dtd\bar{z}dz\ \ \frac{1}{2}(A^a_0\overline{\partial}A^a_z-A^a_z\overline{\partial}A^a_0)=-\frac{1}{2}\int dtd\bar{z}dz(A^a_0,A^a_z)\frac{k}{4\pi}\begin{pmatrix}0 & -\overline{\partial}\\ \overline{\partial} & 0\end{pmatrix}\begin{pmatrix}A^a_0\\ A^a_z\end{pmatrix}.$$

We remark that the above equation is a quadratic form. Therefore, for the above equation, we write

$$S_k(A)=-\frac{1}{2}\int d\mathbf{x}\ \ d\mathbf{x}'\ \ {}^t\hat{A}(\mathbf{x})D(\mathbf{x},\mathbf{x}')\hat{A}(\mathbf{x}'),$$

where $\mathbf{x}=(t,z,\overline{z})$, $\mathbf{x}'=(t',z',\overline{z}')$, $\hat{A}={}^t(A_0^a,A_z^a)$,

$$D(\mathbf{x},\mathbf{x}')=\frac{k}{4\pi}\begin{pmatrix}0 & -\overline{\partial}\\ \overline{\partial} & 0\end{pmatrix}\delta(\mathbf{x}-\mathbf{x}')$$

and $\overline{\partial}$ means the derivative with respect to $\overline{z}$.

Then expectation value (A1) is transformed into the following form:

$$\langle W\rangle=\frac{1}{Z}\int [DA_0][DA_z]e^{-(i/2)\int d\mathbf{x}\ d\mathbf{x}'\ {}^t\hat{A}(\mathbf{x})D(\mathbf{x},\mathbf{x}')\hat{A}(\mathbf{x}')}\ W(A). \tag{A2}$$

Unfortunately, A_0 and A_z are infinite dimensional spaces and there is no rigorous method to define the path integral. Instead we know the perturbative analysis, which will be explained as follows.

In order to explain the perturbative method, we start with a finite dimensional situation as in Ref. 1. Let V be an arbitrary complex-valued function on $\mathbf{R}^n$. Let us evaluate

$$\langle V\rangle=\frac{1}{U}\int_{\mathbf{R}^n}d\vec{x}\exp\left(-\frac{i}{2}\sum_{\alpha\beta}\lambda_{\alpha\beta}x^\alpha x^\beta\right)\ V(\vec{x}), \tag{A3}$$

where

$$U=\int_{\mathbf{R}^n}d\vec{x}\ \ e^{-(i/2)\Sigma_{\alpha\beta}\lambda_{\alpha\beta}x^\alpha x^\beta}.$$

This is a finite dimensional analog for infinite dimensional situation (A2). Introducing new variables $J=(J_\alpha)$, we have

$$\begin{aligned}\langle V\rangle&=\frac{1}{U}\int_{\mathbf{R}^n}d\vec{x}\ \ e^{-(i/2)\Sigma_{\alpha\beta}\lambda_{\alpha\beta}x^\alpha x^\beta}V(\vec{x})e^{iJ_\alpha x^\alpha}\big|_{\vec{J}=0},\\ &=V\left(\frac{\partial}{\partial(iJ_\alpha)}\right)\frac{1}{U}\int_{\mathbf{R}^n}d\vec{x}\ \ e^{-(i/2)\Sigma_{\alpha\beta}\lambda_{\alpha\beta}x^\alpha x^\beta}e^{iJ_\alpha x^\alpha}\big|_{\vec{J}=0},\end{aligned}$$

where we set

$$V\left(\frac{\partial}{\partial(iJ_\alpha)}\right)=\sum_{\nu_1\cdots\nu_n}\frac{1}{\nu_1!\cdots\nu_n!}\frac{\partial^{\nu_1+\cdots+\nu_n}V}{(\partial x^1)^{\nu_1}\cdots(\partial x^n)^{\nu_n}}(0)\left(\frac{\partial}{i\partial J_1}\right)^{\nu_1}\cdots\left(\frac{\partial}{i\partial J_n}\right)^{\nu_n}.$$

This integral is Gaussian and easily calculated as follows:

$$\langle V\rangle=V\left(\frac{\partial}{\partial(iJ_\alpha)}\right)e^{-(i/2)\Sigma_{\alpha\beta}\lambda^{\alpha\beta}(iJ_\alpha)(iJ_\beta)}\big|_{\vec{J}=0}, \tag{A4}$$

where $\lambda^{\alpha\beta}$ is the inverse matrix of $\lambda_{\alpha\beta}$. We have the identity

$$F\left(\frac{\partial}{\partial(iJ_\alpha)}\right)G(i\vec{J})\Big|_{\vec{J}=0}=G\left(\frac{\partial}{\partial x^\alpha}\right)F(\vec{x})\Big|_{\vec{x}=0},$$

where F and G are arbitrary functions on $\mathbf{R}^n$. Using this identity, (A4) is transformed into

$$\langle V\rangle=\exp\left(-\frac{i}{2}\sum_{\alpha\beta}\lambda^{\alpha\beta}\frac{\partial}{\partial x^\alpha}\frac{\partial}{\partial x^\beta}\right)V(\vec{x})\big|_{\vec{x}=0}. \tag{A5}$$

This is a final result for the finite dimensional situation.

Now, let us turn our attention to infinite dimensional situation (A2). Let us introduce ''the inverse matrix analog'' of $D(\mathbf{x},\mathbf{x}')$ as follows. Set

$$G(\mathbf{x}-\mathbf{x}')=\begin{pmatrix} 0 & -\frac{2}{k}\frac{\delta(t-t')}{z-z'} \\ \frac{2}{k}\frac{\delta(t-t')}{z-z'} & 0 \end{pmatrix}.$$

Then we have

$$\int d\mathbf{x}' D(\mathbf{x},\mathbf{x}')G(\mathbf{x}'-\mathbf{x}'')=id\ \ \delta(\mathbf{x}-\mathbf{x}''),$$

where ''id'' denotes the identity matrix. Therefore $G(\mathbf{x}-\mathbf{x}')$ is thought to be ''the inverse matrix analog'' of $D(\mathbf{x},\mathbf{x}')$.

Now we can compare infinite dimensional situation (A2) with the finite dimensional one (A3) by the following correspondence:

$$\alpha,\beta\leftrightarrow\mathbf{x}=(t,z,\overline{z}),\mathbf{x}'=(t',z',\overline{z}'),$$

$$\sum_{\alpha\beta}\leftrightarrow\int d\mathbf{x}\ \ d\mathbf{x}',$$

$$x^{\alpha}\leftrightarrow\hat{A}(\mathbf{x})={}^{t}(A_0^a(\mathbf{x}),A_z^a(\mathbf{x})),$$

$$\lambda_{\alpha\beta}\leftrightarrow D(\mathbf{x},\mathbf{x}'),$$

$$\lambda^{\alpha\beta}\leftrightarrow iG(\mathbf{x}-\mathbf{x}').$$

Therefore, comparing (A5), we can evaluate path integral (A2) as follows:

$$\langle W\rangle=\exp\left\{\int dtdzd\overline{z}\int dt'dz'd\overline{z}'\frac{\delta}{\delta A_0^a(\mathbf{x})}\Delta_{0z}^{ab}(\mathbf{x}-\mathbf{x}')\frac{\delta}{\delta A_z^b(\mathbf{x}')}\right\}W(A)|_{A=0},\tag{A6}$$

where $\mathbf{x}=(t,z,\overline{z})$, $\mathbf{x}'=(t',z',\overline{z}')$ and

$$\Delta_{0z}^{ab}(\mathbf{x}-\mathbf{x}')=-\delta^{ab}\frac{2}{k}\frac{\delta(t-t')}{z-z'}.$$

Here we remark that (A6) is still valid for $\langle W\rangle_E$, since the argument for deriving (A6) is independent of the domain of t.

From (A6), we can compute the two-point correlation functions (2.12)–(2.14) as follows:

$$\langle A_0^a(\mathbf{x})A_z^b(\mathbf{x}')\rangle=\Delta_{0z}^{ab}(\mathbf{x}-\mathbf{x}')=-\delta^{ab}\frac{2}{k}\frac{\delta(t-t')}{z-z'},$$

$$\langle A_0^a(\mathbf{x})A_0^b(\mathbf{x}')\rangle=0,$$

$$\langle A_z^a(\mathbf{x})A_z^b(\mathbf{x}')\rangle=0.$$

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Seiberg–Witten monopole equations on noncommutative $\mathbb{R}^4$

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(Received 2 May 2003; accepted 27 May 2003)

It is well known that, due to vanishing theorems, there are no nontrivial finite action solutions to the Abelian Seiberg–Witten (SW) monopole equations on Euclidean four-dimensional space $\mathbb{R}^4$. We show that this is no longer true for the noncommutative version of these equations, i.e., on a noncommutative deformation $\mathbb{R}^4_\theta$ of $\mathbb{R}^4$ there exist smooth solutions to the SW equations having nonzero topological charge. We introduce action functionals for the noncommutative SW equations and construct explicit regular solutions. All our solutions have finite energy. We also suggest a possible interpretation of the obtained solutions as codimension four vortex-like solitons representing $D(p-4)$- and $\overline{D(p-4)}$-branes in a Dp-$\overline{Dp}$ brane system in type II superstring theory. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604454]

I. INTRODUCTION

The Seiberg–Witten (SW) monopole equations[1] have been derived in the context of twisted $\mathcal{N}=2$ supersymmetric Yang-Mills (SYM) theory[2,3] in some limit of the coupling constant. Another limit of this theory yields the anti-self-dual Yang–Mills (ASDYM) equations. Namely, the ASDYM equations correspond to the weak coupling limit while the SW equations are related to the strong coupling regime obtained by the S-dualization (see, e.g., Refs. 1, 4–6 and references therein). Note that the SW equations are associated with the Abelian group $U(1)$ and have a compact moduli space while the ASDYM equations, considered in Donaldson–Witten (DW) theory,[7,2] possess the non-Abelian gauge group $SU(2)$ and a noncompact moduli space. That is why SW theory is much easier to handle compared to DW theory. A bridge between these theories is provided by the non-Abelian SW equations (see, e.g., Refs. 8–11, 6 and references therein) whose moduli space contains both DW and SW moduli spaces as singular submanifolds.

It is well known that, due to a vanishing theorem of the Lichnerowicz–Weitzenböck type, there are no nontrivial finite action solutions to the Abelian SW equations on Riemannian four-manifolds with non-negative scalar curvature and, in particular, on $\mathbb{R}^4$ (cf. Ref. 1). This assertion is also true for lower-dimensional reductions of the SW equations, i.e., these reductions also do not exhibit regular solutions on $\mathbb{R}^{n\leqslant 3}$ with a nonzero topological charge. Nevertheless, one may construct nontrivial non-L^2 solutions, as it has been done, e.g., in Refs. 12–15.

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Note that for the vanishing spinor field the SW equations specialize to the Abelian ASDYM equations which have no nontrivial regular solutions (instantons) on $\mathbb{R}^4$ either. However, Nekrasov and Schwarz have demonstrated in Ref. 16 that smooth Abelian instanton solutions do exist on $\mathbb{R}^4_\theta$, which is a noncommutative deformation of $\mathbb{R}^4$ with constant deformation parameters $\theta=(\theta^{\mu\nu})$. Moreover, they have proven that noncommutativity resolves the singularities of the instanton moduli space. In the present paper we observe a similar phenomenon for the SW equations on $\mathbb{R}^4_\theta$ by constructing nontrivial regular solutions to the noncommutative SW equations.

It is well known that the SW equations on Kähler surfaces are similar to the vortex equations in two dimensions. Motivated by this relation, we interpret regular (vortex-like) solutions to the SW equations on $\mathbb{R}^4_\theta$ as $D(p-4)$- and $\overline{D(p-4)}$-branes in a Dp-$\overline{Dp}$ brane–antibrane system in type II superstring theory. This interpretation can also be extended to the commutative case of the SW equations on Kähler surfaces.

The paper is organized as follows. In the next section we formulate the SW equations on $\mathbb{R}^4$ and fix our notation. In Sec. III we introduce the noncommutatively deformed non-Abelian SW equations. We derive them from properly deformed $U(2)$ self-duality type equations in eight dimensions[17] by a dimensional reduction to four dimensions (cf. Ref. 18). The resulting $U_+(1)\times U_-(1)$, $U_+(1)$ and $U_-(1)$ noncommutative SW equations can also be produced from appropriate action functionals by using a Bogomolny type transformation. We point out that the $U_+(1)\times U_-(1)$, $U_+(1)$ and $U_-(1)$ noncommutative SW equations share the same commutative limit. In Sec. IV we present a number of regular solutions to the noncommutative SW equations and discuss their D-brane interpretation in a string theoretic context. In Sec. V we conclude with a brief summary and open problems. Finally, in an Appendix we perform the Bogomolny type transformation for the noncommutative $U_+(1)\times U_-(1)$ SW action functional.

II. SW MONOPOLE EQUATIONS ON $\mathbb{R}^4$

A. SW action functional

In this paper we consider the SW equations on the Euclidean space $\mathbb{R}^4$, provided with the standard metric $g=(\delta_{\mu\nu})$, where $\mu,\nu,\ldots=1,\ldots,4$. The (energy) functional $E=E(A,\Phi)$ for these equations has the form (cf., e.g., Refs. 19–21)

$$E(A,\Phi)=\int_{\mathbb{R}^4}\mathrm{d}^4x\{|F_A|^2+|D_A\Phi|^2+\tfrac{1}{4}|\Phi|^4\}. \tag{2.1}$$

Here $A\in\Omega^1(\mathbb{R}^4,\mathfrak{u}(1))$ is a connection one-form on $\mathbb{R}^4$ with pure imaginary smooth coefficients and $\Phi\in C^\infty(\mathbb{R}^4,\mathbb{C}^2)$ is a Weyl spinor given by a smooth complex-valued vector function on $\mathbb{R}^4$. We denote by $F_A^+\in\Omega^2_+(\mathbb{R}^4,\mathfrak{u}(1))$ the self-dual part of the curvature F_A of A and by D_A the covariant derivative associated with A. Moreover, we use the abbreviation $|D_A\Phi|^2=D_\mu\phi_i(D_\mu\phi_i)^\dagger$ and set $|F_A|^2=\frac{1}{2}F_{\mu\nu}F^\dagger_{\mu\nu}$.

By exploiting a Bogomolny type formula, the energy functional can be rewritten in the form

$$E(A,\Phi)=\mathrm{SW}(A,\Phi)-8\pi^2Q, \tag{2.2}$$

where

$$\mathrm{SW}(A,\Phi)=\int_{\mathbb{R}^4}\mathrm{d}^4x\{|\mathcal{D}_A\Phi|^2+2|F_A^+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\} \tag{2.3}$$

is the SW action functional and

$$Q=-\frac{1}{8\pi^2}\int_{\mathbb{R}^4}F_A\wedge F_A \tag{2.4}$$

is the topological charge. In the above formula (2.3) we denote by $\mathcal{D}_A$ the Dirac operator associated with A. We also use the notation

$$\sigma^+(\Phi\otimes\Phi^\dagger)_0 := \sigma^+(\Phi\otimes\Phi^\dagger - \tfrac{1}{2}|\Phi|^2\mathrm{id}), \tag{2.5}$$

where

$$\sigma^+ : \mathrm{Herm}_0(\mathbb{C}^2) \to \Omega^2_+(\mathbb{R}^4, \mathfrak{u}(1))$$

is a map identifying the space $\mathrm{Herm}_0(\mathbb{C}^2)$ of traceless Hermitian endomorphisms of $\mathbb{C}^2$ with the space $\Omega^2_+(\mathbb{R}^4,\mathfrak{u}(1))$ of imaginary-valued self-dual two-forms on $\mathbb{R}^4$. The inverse of this map is given by the Clifford multiplication by two-forms (see, e.g., Refs. 19–21).

It is easy to see that the functionals (2.1) and (2.3) are invariant under gauge transformations of the form

$$A \mapsto A + g^\dagger \mathrm{d}g \quad \text{and} \quad \Phi \mapsto g^\dagger \Phi, \tag{2.6}$$

where $g \in C^\infty(\mathbb{R}^4, U(1))$.

B. SW monopole equations

Since the functional $\mathrm{SW}(A,\Phi)$ is positive semi-definite and Q is a topological term, the Bogomolny formula (2.2) implies that the lower bound of the energy $E(A,\Phi)$ is attained on solutions to the equations

$$F_A^+ = \sigma^+(\Phi\otimes\Phi^\dagger)_0, \tag{2.7a}$$

$$\mathcal{D}_A\Phi = 0, \tag{2.7b}$$

which are known as the SW monopole equations. They are differential equations of first order and their solutions, which minimize the energy functional $E(A,\Phi)$, automatically satisfy the (second order) Euler–Lagrange equations for the functionals $E(A,\Phi)$ and $\mathrm{SW}(A,\Phi)$.

Writing ${}^t\Phi = (\phi_1,\phi_2)$, one can see that Eqs. (2.7) are equivalent to (cf. Ref. 19)

$$\begin{aligned} F_{12}+F_{34} &= \frac{i}{2}(\phi_1\overline{\phi}_1 - \phi_2\overline{\phi}_2), \\ F_{13}+F_{42} &= -\tfrac{1}{2}(\phi_2\overline{\phi}_1 - \phi_1\overline{\phi}_2), \\ F_{14}+F_{23} &= \frac{i}{2}(\phi_2\overline{\phi}_1 + \phi_1\overline{\phi}_2) \end{aligned} \tag{2.8a}$$

and

$$\begin{pmatrix} -D_4+iD_3 & D_2+iD_1 \\ -D_2+iD_1 & -D_4-iD_3 \end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} = 0. \tag{2.8b}$$

It is easy to prove that these equations have no nontrivial solutions with finite action. Namely, we have the following theorem (see, e.g., Refs. 1, 19–21):

Theorem: *Suppose* $A \in \Omega^1(\mathbb{R}^4,\mathfrak{u}(1))$ *and* $\Phi \in C^\infty(\mathbb{R}^4,\mathbb{C}^2)$ *satisfy the equations (2.8). Moreover, we assume that* $\Phi \in L^2(\mathbb{R}^4)$ *and* $E(A,\Phi) < \infty$. *Then the only solution to (2.8) is the trivial solution* $(A,\Phi) = (0,0)$ *modulo the gauge transformations (2.6).*

This theorem is also true for lower dimensional reductions of the SW equations (defined on $\mathbb{R}^{n\leqslant 3}$), i.e., these reductions do not exhibit regular nontrivial solutions either. However, as we have already mentioned in the Introduction, one can construct nontrivial non-L^2 solutions.[12–15]

C. Perturbed SW action functional and monopole equations

The gauge group action (2.6) on the space of pairs (A,Φ) is free, unless $\Phi\equiv 0$. In order to avoid solutions of the form $(A,0)$, which may cause singularities in the moduli space of solutions, we perturb the monopole equations by adding an extra term to the first SW equation,

$$F_A^+ + \chi^+ = \sigma^+(\Phi\otimes\Phi^\dagger)_0, \tag{2.9a}$$

$$\mathcal{D}_A\Phi = 0, \tag{2.9b}$$

where χ^+ is the self-dual part of a two-form $\chi\in\Omega^2(\mathbb{R}^4,\mathfrak{u}(1))$ (perturbation). Solutions to these equations minimize the functional

$$\mathrm{SW}_\chi(A,\Phi)=\int_{\mathbb{R}^4}\mathrm{d}^4x\{|\mathcal{D}_A\Phi|^2+2|F_A^+ +\chi^+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\}. \tag{2.10}$$

In components Eq. (2.9a) reads as

$$\begin{aligned} F_{12}+F_{34}+\chi_{12}+\chi_{34}&=\frac{i}{2}(\phi_1\overline{\phi_1}-\phi_2\overline{\phi_2}),\\ F_{13}+F_{42}+\chi_{13}+\chi_{42}&=-\tfrac{1}{2}(\phi_2\overline{\phi_1}-\phi_1\overline{\phi_2}),\\ F_{14}+F_{23}+\chi_{14}+\chi_{23}&=\frac{i}{2}(\phi_2\overline{\phi_1}+\phi_1\overline{\phi_2}). \end{aligned} \tag{2.11}$$

The SW action functional, as in the unperturbed case, is related to an energy functional,

$$E_\chi(A,\Phi)=\int_{\mathbb{R}^4}\mathrm{d}^4x\{|F_A|^2+|D_A\Phi|^2+2|\chi^+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\}, \tag{2.12}$$

via a Bogomolny type formula,

$$\mathrm{SW}_\chi(A,\Phi)=E_\chi(A,\Phi)+16\pi^2K_\chi+8\pi^2Q. \tag{2.13}$$

The topological charge Q is given, as before, by formula (2.4) and the Chern–Simons type term K_χ is defined as

$$K_\chi=-\frac{1}{4\pi^2}\int_{\mathbb{R}^4}F_A^+\wedge\chi^+. \tag{2.14}$$

III. SW MONOPOLE EQUATIONS ON $\mathbb{R}^4_\theta$

A. Non-Abelian SW monopole equations

1. Noncommutative Euclidean space $\mathbb{R}^{2n}_\theta$

Let $\mathcal{A}(\mathbb{R}^{2n})$ be the algebra of polynomial functions on $\mathbb{R}^{2n}$ (which is endowed with the canonical metric $\delta_{\alpha\beta}$) and $\theta=(\theta^{\alpha\beta})$ be a real invertible skew-symmetric $2n\times 2n$ matrix with the inverse matrix $\theta^{-1}=(\theta_{\alpha\beta})$ defined by $\theta_{\alpha\gamma}\theta^{\gamma\beta}=\delta_\alpha^\beta$ for $\alpha,\beta,\ldots=1,\ldots,2n$. Then the deformed algebra $\mathcal{A}_\theta(\mathbb{R}^{2n})$ is defined as

$$\mathcal{A}_\theta(\mathbb{R}^{2n}):=T(\mathbb{R}^{2n})/\langle[x^\alpha,x^\beta]-i\theta^{\alpha\beta}\rangle_{1\leqslant\alpha,\beta\leqslant 2n}, \tag{3.1}$$

where $T(\mathbb{R}^{2n})$ is the tensor algebra of $\mathbb{R}^{2n}$ and $\langle[x^\alpha,x^\beta]-i\theta^{\alpha\beta}\rangle_{1\leqslant\alpha,\beta\leqslant 2n}$ denotes the two-sided ideal generated by $[x^\alpha,x^\beta]-i\theta^{\alpha\beta}\subset T(\mathbb{R}^{2n})$. For brevity we shall denote $\mathcal{A}_\theta(\mathbb{R}^{2n})$ simply by $\mathbb{R}^{2n}_\theta$ and call it the noncommutative Euclidean $2n$-dimensional space.

One way to realize the noncommutative extension (3.1) of the algebra $\mathcal{A}(\mathbb{R}^{2n})$ is by deformation of the pointwise product between functions via the so-called star (Moyal) product,

$$(f\star g)(x) := f(x)\exp\left\{\frac{i}{2}\overleftarrow{\partial}_\alpha\theta^{\alpha\beta}\overrightarrow{\partial}_\beta\right\}g(x), \tag{3.2}$$

where $f,g\in C^\infty(\mathbb{R}^{2n},\mathbb{C})$. In particular, it follows from (3.2) that

$$[x^\alpha,x^\beta]_\star := x^\alpha\star x^\beta - x^\beta\star x^\alpha = i\theta^{\alpha\beta}. \tag{3.3}$$

For later convenience we introduce complex coordinates on $\mathbb{R}^{2n}\cong\mathbb{C}^n$,

$$z^a = x^{2a-1}+ix^{2a} \quad \text{and} \quad \overline{z^a} = x^{2a-1}-ix^{2a}, \quad \text{for} \quad a=1,\ldots,n, \tag{3.4}$$

and derivatives

$$\partial_{z^a} = \tfrac{1}{2}(\partial_{2a-1}-i\partial_{2a}) \quad \text{and} \quad \partial_{\overline{z^a}} = \tfrac{1}{2}(\partial_{2a-1}+i\partial_{2a}). \tag{3.5}$$

Note that by an orthogonal change of coordinates one can always transform $\theta^{\alpha\beta}$ to its canonical (Darboux) form whose only nonzero components are $\theta^{2a-1,2a}$ with $a=1,\ldots,n$. Then the commutation relations (3.3) translate to

$$[z^a,\overline{z^a}]_\star = \theta^{a\overline{a}}, \quad \text{with} \quad \theta^{a\overline{a}} = 2\theta^{2a-1,2a}, \tag{3.6}$$

and all other commutators are equal to zero.

2. Self-duality type equations in eight dimensions

A standard way to obtain a noncommutative generalization of a theory is to replace naively the ordinary commutative product between field variables with the noncommutative star product. However, it is well known that this method of translating a commutative theory into a noncommutative one is not uniquely defined when the matter fields are involved. For instance, the scalar fields in noncommutative $U(1)$ gauge theory on $\mathbb{R}^{2n}$ can be regarded in three different ways, namely as elements of a left module [over the algebra $\mathcal{A}_\theta(\mathbb{R}^{2n})$], or as elements of a right module, or they can transform in the adjoint representation. For this reason we propose deriving the noncommutative SW equations from noncommutative self-duality type Yang–Mills (YM) equations in eight dimensions, which are uniquely defined. Eventually, we will discover the equations corresponding to the above mentioned naive substitution rule by a formal reduction of more general equations. In the commutative case a similar idea has been worked out by the authors of Ref. 18.

Let us consider pure $U(2)$ YM theory on $\mathbb{R}^8_\theta$. In star-product formulation the components $F_{\alpha\beta}$ of the YM curvature F_A read as

$$F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha + [A_\alpha,A_\beta]_\star \tag{3.7}$$

and take values in $\mathfrak{u}(2)$. Here α, β,..., run from 1 to 8. Consider the generalized self-duality equations for YM fields in eight dimensions,

$$F_{\alpha\beta} = \tfrac{1}{2}T_{\alpha\beta\gamma\delta}F_{\gamma\delta}, \tag{3.8}$$

where the totally antisymmetric tensor $T_{\alpha\beta\gamma\delta}$ is determined by the octonionic structure constants f_{ijk} as

$$T_{ijkl} = \tfrac{1}{6}\epsilon_{ijklmnq}f_{mnq} \quad \text{and} \quad T_{8ijk} = f_{ijk}, \quad \text{for} \quad i,j,k,\ldots = 1,\ldots,7. \tag{3.9}$$

(In the commutative case these equations were introduced in Ref. 17 and discussed, e.g., in Refs. 22, 23. We use $f_{127}=f_{347}=f_{567}=f_{163}=f_{246}=f_{253}=f_{154}=1$.) Note that the tensor $T_{\alpha\beta\gamma\delta}$ and there-

fore the equations (3.8) are invariant with respect to the group $Spin(7)$ rather than $SO(8)$. In fact, it is impossible to construct a totally antisymmetric tensor of rank four in eight dimensions which is invariant under $SO(8)$ rotations.

Using the definition (3.9), we can write down the generalized self-duality (3.8) in components as follows:

$$\begin{aligned}
&F_{12}+F_{34}+F_{56}+F_{78}=0,\\
&F_{13}+F_{42}+F_{57}+F_{86}=0,\\
&F_{14}+F_{23}+F_{76}+F_{85}=0,\\
&F_{15}+F_{62}+F_{73}+F_{48}=0,\\
&F_{16}+F_{25}+F_{38}+F_{47}=0,\\
&F_{17}+F_{82}+F_{35}+F_{64}=0,\\
&F_{18}+F_{27}+F_{63}+F_{54}=0.
\end{aligned} \tag{3.10}$$

With the help of (3.4) and the definitions

$$A_{z^a}=\tfrac{1}{2}(A_{2a-1}-iA_{2a}) \quad \text{and} \quad A_{\bar{z}^a}=\tfrac{1}{2}(A_{2a-1}+iA_{2a}), \quad \text{for} \quad a=1,\ldots,4, \tag{3.11}$$

we rewrite (3.10) as

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}+F_{z^3\bar{z}^3}+F_{z^4\bar{z}^4}=0, \tag{3.12a}$$

$$F_{z^1z^2}+F_{\bar{z}^3\bar{z}^4}=0, \tag{3.12b}$$

$$F_{z^2z^4}-F_{\bar{z}^1\bar{z}^3}=0, \tag{3.12c}$$

$$F_{z^1z^4}+F_{\bar{z}^2\bar{z}^3}=0. \tag{3.12d}$$

Note that $A_{\bar{z}^a}=-A^{\dagger}_{z^a}$, since the components A_α are skew-Hermitian.

3. Reduction to four dimensions

Following Baulieu *et al.*,[18] we assume that the gauge potential components A_{z^a} for $a=1,\ldots,4$ do not depend on the coordinates $z^3,z^4,\bar{z}^3,\bar{z}^4$ and define ${}^t\Psi:=(\Psi_1,\Psi_2)$ with $\Psi_1:=A_{\bar{z}^3}$ and $\Psi_2:=A_{z^4}$. Then the equations (3.12) dimensionally reduce to

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}=-([\Psi_1,\Psi_1^{\dagger}]_\star-[\Psi_2,\Psi_2^{\dagger}]_\star), \tag{3.13a}$$

$$F_{z^1z^2}=[\Psi_1,\Psi_2^{\dagger}]_\star, \tag{3.13b}$$

$$D_{\bar{z}^1}\Psi_1-D_{z^2}\Psi_2=0, \tag{3.13c}$$

$$D_{\bar{z}^2}\Psi_1+D_{z^1}\Psi_2=0, \tag{3.13d}$$

where the covariant derivative D_{z^a} is defined by $D_{z^a}\Psi=\partial_{z^a}\Psi+[A_{z^a},\Psi]_\star$. In the commutative limit these equations coincide with a non-Abelian generalization of the SW equations, considered in Ref. 18. Note that the special case of these equations corresponding to $\Psi_2\equiv 0$ was discussed in Refs. 24, 25.

Along with the unperturbed equations (3.13) we shall also consider the perturbed equations (cf. Refs. 8–10). For that we introduce a $\mathfrak{u}(2)$-valued two-form χ and add its self-dual part χ^+ to F_A^+,

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}+\chi_{z^1\bar{z}^1}+\chi_{z^2\bar{z}^2}=-([\Psi_1,\Psi_1^\dagger]_\star-[\Psi_2,\Psi_2^\dagger]_\star), \tag{3.14a}$$

$$F_{z^1z^2}+\chi_{z^1z^2}=[\Psi_1,\Psi_2^\dagger]_\star, \tag{3.14b}$$

$$D_{\bar{z}^1}\Psi_1-D_{z^2}\Psi_2=0, \tag{3.14c}$$

$$D_{\bar{z}^2}\Psi_1+D_{z^1}\Psi_2=0. \tag{3.14d}$$

B. Abelian SW monopole equations

In order to get Abelian SW equations from the non-Abelian ones, we shall consider solutions of a particular type given by a suitable ansatz. This will reduce the gauge group $U(2)$ to $U(1)\times U(1)$ and then, further down to $U(1)$.

1. Noncommutative $U_+(1)\times U_-(1)$ SW monopole equations

Let us consider the $U(1)\times U(1)$ subgroup of $U(2)$ with the generators

$$\begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{3.15}$$

and assume that the components of the gauge potential A_{z^a} for $a=1,2$ take the form

$$A_{z^a}:=\begin{pmatrix} A_{+z^a} & 0 \\ 0 & A_{-z^a} \end{pmatrix}, \quad \text{with} \quad A_{\pm z^a}=\tfrac{1}{2}(\mathcal{B}_{z^a}\pm\mathcal{A}_{z^a}), \tag{3.16}$$

and $\mathcal{A}_{z^a},\mathcal{B}_{z^a}\in C^\infty(\mathbb{R}^4,i\mathbb{R}\otimes\mathbb{C})$. (If not stated differently, $a,b,\ldots$, run always from 1 to 2 in the sequel.) Furthermore, we restrict Ψ_1 and Ψ_2 to the form

$$\Psi_{1,2}:=\begin{pmatrix} 0 & \dfrac{1}{\sqrt{8}}\phi_{1,2} \\ 0 & 0 \end{pmatrix}, \tag{3.17}$$

where $\phi_{1,2}\in C^\infty(\mathbb{R}^4,\mathbb{C})$.

Substituting (3.16) and (3.17) into the equations (3.13), after a straightforward calculation we obtain the equations

$$F_{+z^1\bar{z}^1}+F_{+z^2\bar{z}^2}=-\tfrac{1}{8}(\phi_1\star\phi_1^\dagger-\phi_2\star\phi_2^\dagger) \quad \text{and} \quad F_{+z^1z^2}=\tfrac{1}{8}\phi_1\star\phi_2^\dagger, \tag{3.18a}$$

$$F_{-z^1\bar{z}^1}+F_{-z^2\bar{z}^2}=\tfrac{1}{8}(\phi_1^\dagger\star\phi_1-\phi_2^\dagger\star\phi_2) \quad \text{and} \quad F_{-z^1z^2}=-\tfrac{1}{8}\phi_2^\dagger\star\phi_1, \tag{3.18b}$$

as well as

$$D_{\bar{z}^1}\phi_1-D_{z^2}\phi_2=0 \quad \text{and} \quad D_{\bar{z}^2}\phi_1+D_{z^1}\phi_2=0, \tag{3.19}$$

where we have used the definition

$$D_{z^a}\phi:=\partial_{z^a}\phi+A_{+z^a}\star\phi-\phi\star A_{-z^a}. \tag{3.20}$$

Here $F_{\pm z^a\bar{z}^a}$ are the components of the curvature associated with $A_{\pm z^a}$, i.e.,

$$F_{\pm z^a\bar{z}^a}=\partial_{z^a}A_{\pm\bar{z}^a}-\partial_{\bar{z}^a}A_{\pm z^a}+[A_{\pm z^a},A_{\pm\bar{z}^a}]_\star. \tag{3.21}$$

Analogously, by assuming that $\chi=\mathrm{diag}(\chi_+,\chi_-)$ with $\chi_\pm\in\Omega^2(\mathbb{R}^4,\mathrm{i}\mathbb{R})$ in (3.14), we obtain the perturbed equations

$$F_{+z^1\bar{z}^1}+F_{+z^2\bar{z}^2}+\chi_{+z^1\bar{z}^1}+\chi_{+z^2\bar{z}^2}=-\tfrac{1}{8}(\phi_1\star\phi_1^\dagger-\phi_2\star\phi_2^\dagger), \tag{3.22a}$$

$$F_{+z^1z^2}+\chi_{+z^1z^2}=\tfrac{1}{8}\phi_1\star\phi_2^\dagger, \tag{3.22b}$$

$$F_{-z^1\bar{z}^2}+F_{-z^2\bar{z}^2}+\chi_{-z^1\bar{z}^1}+\chi_{-z^2\bar{z}^2}=\tfrac{1}{8}(\phi_1^\dagger\star\phi_1-\phi_2^\dagger\star\phi_2), \tag{3.22c}$$

$$F_{-z^1z^2}+\chi_{-z^1z^2}=-\tfrac{1}{8}\phi_2^\dagger\star\phi_1. \tag{3.22d}$$

We consider the equations (3.18), (3.19) and (3.22), (3.19) as a noncommutative extension of the unperturbed and perturbed Abelian SW equations, respectively. Since there are two gauge potentials in the equations, we call them the noncommutative unperturbed and perturbed $U_+(1)\times U_-(1)$ SW equations.

It remains to find out what kind of gauge transformations leave the $U_+(1)\times U_-(1)$ SW equations invariant. It is obvious from the explicit form of these equations that ϕ_1 and ϕ_2 are in the bi-fundamental representation of $U_+(1)\times U_-(1)$. Hence, Eqs. (3.18), (3.19) and (3.22) are invariant under gauge transformations of the form

$$A_\pm\mapsto g_\pm^\dagger\star A_\pm\star g_\pm+g_\pm^\dagger\star\mathrm{d}g_\pm,\quad \chi_\pm\mapsto g_\pm^\dagger\star\chi_\pm\star g_\pm\quad\text{and}\quad \Phi\mapsto g_+^\dagger\star\Phi\star g_-, \tag{3.23}$$

where $g_\pm\in C^\infty(\mathbb{R}^4,U_\pm(1))$ and ${}^t\Phi=(\phi_1,\phi_2)$.

In the commutative limit the covariant derivative (3.20) turns into

$$D_{z^a}\phi=\partial_{z^a}\phi+(A_{+z^a}-A_{-z^a})\phi=\partial_{z^a}\phi+\mathcal{A}_{z^a}\phi, \tag{3.24}$$

i.e., the gauge potential $\mathcal{B}$ disappears from the equations (3.19). In other words, one copy of $U(1)$ decouples from $U(2)$ and the matter field Φ interacts only with the $SU(2)$ part. Hence, in the commutative case Φ is charged with respect to the diagonal $U(1)$ subgroup of $U_+(1)\times U_-(1)$ corresponding to the gauge potential $\mathcal{A}=A_+-A_-$. Furthermore, the commutator in the expression for the (Abelian) curvature vanishes and hence as a corollary we have $F_{\pm z^a\bar{z}^a}=\frac{1}{2}(F_{\mathcal{B}z^a\bar{z}^a}\pm F_{\mathcal{A}z^a\bar{z}^a})$. In the commutative limit one may choose the perturbations $\chi_\pm$ so that

$$\chi_{\pm z^a\bar{z}^a}=-\tfrac{1}{2}F_{\mathcal{B}z^a\bar{z}^a}\pm\tfrac{1}{2}\chi_{z^a\bar{z}^a}\quad\text{and}\quad \chi_{\pm z^1z^2}=-\tfrac{1}{2}F_{\mathcal{B}z^1z^2}\pm\tfrac{1}{2}\chi_{z^1z^2}, \tag{3.25}$$

where $\chi\in\Omega^2(\mathbb{R}^4,\mathfrak{u}(1))$ is some other perturbation. Then from Eqs. (3.22) we obtain

$$F_{\mathcal{A}z^1\bar{z}^1}+F_{\mathcal{A}z^2\bar{z}^2}+\chi_{z^1\bar{z}^1}+\chi_{z^2\bar{z}^2}=-\tfrac{1}{4}(\phi_1\bar{\phi}_1-\phi_2\bar{\phi}_2)\quad\text{and}\quad F_{\mathcal{A}z^1z^2}+\chi_{z^1z^2}=\tfrac{1}{4}\phi_1\bar{\phi}_2. \tag{3.26}$$

(Note that in the case of complex valued-functions "$\dagger$" goes to "$-$" in the commutative limit.) Thus, we recover the perturbed SW equations (2.8b) and (2.11) (written in complex coordinates). Of course, the choice $\chi\equiv 0$ corresponds to the unperturbed equations.

Remark: Consider the unperturbed equations (3.18) and (3.19). In the commutative limit we arrive at the standard unperturbed SW equations for configurations $(\mathcal{A},\Phi)$ plus the Abelian ASDYM equations for $\mathcal{B}$, i.e.,

$$F_{\mathcal{B}z^1\bar{z}^1}+F_{\mathcal{B}z^2\bar{z}^2}=0\quad\text{and}\quad F_{\mathcal{B}z^1z^2}=0. \tag{3.27}$$

Taking the trivial solution $\mathcal{B}=0$ (recall that there are no Abelian instantons on $\mathbb{R}^4$) we remain with the standard unperturbed SW equations. More generally, any pure gauge configuration for $\mathcal{B}$ will do the same. The noncommutative version of the latter statement is, however, nontrivial. If we choose $\mathcal{B}_{z^a}$ in (3.16) of the form

$$\mathcal{B}_{z^a}=\tfrac{1}{2}(b^\dagger\star\partial_{z^a}b-b\star\partial_{z^a}b^\dagger), \tag{3.28}$$

with $b\in C^\infty(\mathbb{R}^4,U(1))$, then it will correspond in the commutative limit to a pure gauge configuration but, of course, it is not pure gauge in the noncommutative case. Only in the commutative limit the curvature $F_{\mathcal{B}}$ disappears and we arrive at the unperturbed SW equations (2.8).

2. Noncommutative $U_\pm(1)$ SW monopole equations

In Eqs. (3.18)–(3.23) the field Φ is regarded as an element of a $\mathbb{R}^4_\theta$-bimodule transforming in the bi-fundamental representation of the gauge group $U_+(1)\times U_-(1)$. However, in the noncommutative setup the matter field Φ can also be thought of either as an element of a right $\mathbb{R}^4_\theta$-module [the $U_+(1)$ case] or as an element of a left $\mathbb{R}^4_\theta$-module [the $U_-(1)$ case]. These two cases can easily be read off Eqs. (3.22a), (3.22b) and (3.22c), (3.22d), respectively. Namely, consider the equations

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}+\chi_{z^1\bar{z}^1}+\chi_{z^2\bar{z}^2}=-\tfrac{1}{4}(\phi_1\star\phi_1^\dagger-\phi_2\star\phi_2^\dagger)\quad\text{and}\quad F_{z^1z^2}+\chi_{z^1z^2}=\tfrac{1}{4}\phi_1\star\phi_2^\dagger, \tag{3.29a}$$

as well as

$$D_{\bar{z}^1}\phi_1-D_{z^2}\phi_2=0\quad\text{and}\quad D_{\bar{z}^2}\phi_1+D_{z^1}\phi_2=0, \tag{3.29b}$$

where $\chi\in\Omega^2(\mathbb{R}^4,\mathrm{i}\mathbb{R})$ and the (right) covariant derivative reads as

$$D_{z^a}\phi=\partial_{z^a}\phi+\mathcal{A}_{z^a}\star\phi. \tag{3.29c}$$

[Formally, these equations can be obtained from (3.19)–(3.22) by choosing $\mathcal{B}_{z^a}=\mathcal{A}_{z^a}$ (i.e., $A_{-z^a}=0$), taking $\chi_\pm$ such that $\chi_{+z^a\bar{z}^a}=\chi_{z^a\bar{z}^a}$, $\chi_{+z^1z^2}=\chi_{z^1z^2}$, $\chi_{-z^1\bar{z}^1}+\chi_{-z^2\bar{z}^2}=\frac{1}{8}(\phi_1^\dagger\star\phi_1-\phi_2^\dagger\star\phi_2)$ and $\chi_{-z^1z^2}=-\frac{1}{8}\phi_2^\dagger\star\phi_1$, where $\chi\in\Omega^2(\mathbb{R}^4,\mathrm{i}\mathbb{R})$, and rescaling $\Phi\mapsto\sqrt{2}\Phi$.] Note that the curvature $F_{\mathcal{A}}$ is now computed from $\mathcal{A}$, i.e. $F_{\mu\nu}=\partial_\mu\mathcal{A}_\nu-\partial_\nu\mathcal{A}_\mu+[\mathcal{A}_\mu,\mathcal{A}_\nu]_\star$.

Similarly, we may introduce the equations

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}+\chi_{z^1\bar{z}^1}+\chi_{z^2\bar{z}^2}=\tfrac{1}{4}(\phi_1^\dagger\star\phi_1-\phi_2^\dagger\star\phi_2)\quad\text{and}\quad F_{z^1z^2}+\chi_{z^1z^2}=-\tfrac{1}{4}\phi_2^\dagger\star\phi_1 \tag{3.30a}$$

and

$$D_{\bar{z}^1}\phi_1-D_{z^2}\phi_2=0\quad\text{and}\quad D_{\bar{z}^2}\phi_1+D_{z^1}\phi_2=0, \tag{3.30b}$$

where $\chi\in\Omega^2(\mathbb{R}^4,\mathrm{i}\mathbb{R})$ and

$$D_{z^a}\phi=\partial_{z^a}\phi-\phi\star\mathcal{B}_{z^a} \tag{3.30c}$$

is the (left) derivative. [These equations can formally be obtained from (3.19)–(3.22) by choosing $\mathcal{B}_{z^a}=-\mathcal{A}_{z^a}$ (i.e., $A_{+z^a}=0$) and putting $\chi_{+z^1\bar{z}^1}+\chi_{+z^2\bar{z}^2}=-\frac{1}{8}(\phi_1\star\phi_1^\dagger-\phi_2\star\phi_2^\dagger)$, $\chi_{+z^1z^2}=\frac{1}{8}\phi_1\star\phi_2^\dagger$, $\chi_{-z^a\bar{z}^a}=\chi_{z^a\bar{z}^a}$ and $\chi_{-z^1z^2}=\chi_{z^1z^2}$, where $\chi\in\Omega^2(\mathbb{R}^4,\mathrm{i}\mathbb{R})$. Again we should rescale $\Phi\mapsto\sqrt{2}\Phi$.] Now the curvature $F_{\mathcal{B}}$ is associated with the gauge potential $\mathcal{B}$, i.e., $F_{\mu\nu}=\partial_\mu\mathcal{B}_\nu-\partial_\nu\mathcal{B}_\mu+[\mathcal{B}_\mu,\mathcal{B}_\nu]_\star$.

We shall call (3.29) and (3.30) the perturbed noncommutative $U_+(1)$ and $U_-(1)$ SW equations. Obviously, the unperturbed equations appear for $\chi\equiv0$. Note that the systems (3.29) and (3.30) are totally equivalent and the only difference between them is an artifact of noncommutativity. The commutative limits of both cases are, of course, identical and produce (2.9). Moreover, in the commutative case the gauge transformations (3.23) reduce to the standard ones, i.e., one may choose the identity either for g_- or for g_+.

C. Operator form of the Abelian SW monopole equations

1. Weyl transform

Due to the nonlocal nature of the star product, explicit calculations might be quite tedious. It is therefore convenient to pass over to the operator formalism via the Weyl ordering $\mathcal{W}$ given by

$$\mathcal{W}: \tilde{f}(k) \mapsto \hat{f}(\hat{x}) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}k \, \tilde{f}(k) \, e^{ik\hat{x}}, \tag{3.31a}$$

$$\mathcal{W}^{-1}: \hat{f}(\hat{x}) \mapsto \tilde{f}(k) = |\mathrm{Pf}(2\pi\theta)| \mathrm{Tr}\{e^{-ik\hat{x}} \hat{f}(\hat{x})\}, \tag{3.31b}$$

where $\tilde{f}(k)$ stands for the Fourier transform of $f(x) \in \mathcal{S}(\mathbb{R}^{2n})$,

$$f(x) \mapsto \tilde{f}(k) = \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}x \, f(x) e^{-ikx}. \tag{3.32}$$

Here $\mathcal{S}(\mathbb{R}^{2n})$ is the Schwartz space of fast decreasing functions on $\mathbb{R}^{2n}$, "Tr" denotes the trace in the operator representation of the noncommutative algebra and "Pf$(2\pi\theta)$" is the Pfaffian of $(2\pi\theta^{\alpha\beta})$. (However, in later considerations we shall make suitable choices for f which are weaker.) Also, in these equations kx is a shorthand notation for $k_\alpha x^\alpha$. One can verify (see, e.g., Ref. 26) that the following relations are true:

$$\mathcal{W}: f \star g \mapsto \hat{f}\hat{g} \quad \text{and} \quad \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}x \, f = |\mathrm{Pf}(2\pi\theta)| \mathrm{Tr}\hat{f}. \tag{3.33}$$

We may regard the coordinates $\hat{x}^\alpha$ as operators which act on some Fock space $\mathcal{H}$, specified in Sec. IV, and satisfy the commutation relations $[\hat{x}^\alpha, \hat{x}^\beta] = i\theta^{\alpha\beta}$. With a proper choice of coordinates the parameters $\theta^{\alpha\beta}$ will have the canonical form (3.6). For the complex coordinates $\hat{z}^a$, also considered as operators in $\mathcal{H}$, we then get

$$[\hat{z}^a, \hat{z}^b] = 0 \quad \text{and} \quad [\hat{z}^a, \hat{\bar{z}}^{\bar{a}}] = \theta^{a\bar{a}}, \quad \text{for} \quad a, b = 1, \ldots, n. \tag{3.34}$$

A straightforward calculation shows that coordinate derivatives are now inner derivations of this algebra, i.e.,

$$\hat{\partial}_{z^a} \hat{f} = \theta_{a\bar{a}} [\hat{\bar{z}}^{\bar{a}}, \hat{f}] \quad \text{and} \quad \hat{\partial}_{\bar{z}^{\bar{a}}} \hat{f} = \theta_{\bar{a}a} [\hat{z}^a, \hat{f}]. \tag{3.35}$$

In the operator formulation, the perturbed noncommutative $U_+(1) \times U_-(1)$ SW equations (3.19) and (3.22) retain their form,

$$\hat{F}_{+z^1\bar{z}^1} + \hat{F}_{+z^2\bar{z}^2} + \hat{\chi}_{+z^1\bar{z}^1} + \hat{\chi}_{+z^2\bar{z}^2} = -\tfrac{1}{8}(\hat{\phi}_1 \hat{\phi}_1^\dagger - \hat{\phi}_2 \hat{\phi}_2^\dagger), \tag{3.36a}$$

$$\hat{F}_{+z^1z^2} + \hat{\chi}_{+z^1z^2} = \tfrac{1}{8} \hat{\phi}_1 \hat{\phi}_2^\dagger, \tag{3.36b}$$

$$\hat{F}_{-z^1\bar{z}^1} + \hat{F}_{-z^2\bar{z}^2} + \hat{\chi}_{-z^1\bar{z}^1} + \hat{\chi}_{-z^2\bar{z}^2} = \tfrac{1}{8}(\hat{\phi}_1^\dagger \hat{\phi}_1 - \hat{\phi}_2^\dagger \hat{\phi}_2), \tag{3.36c}$$

$$\hat{F}_{-z^1z^2} + \hat{\chi}_{-z^1z^2} = -\tfrac{1}{8} \hat{\phi}_2^\dagger \hat{\phi}_1, \tag{3.36d}$$

and

$$\hat{D}_{\bar{z}^1} \hat{\phi}_1 - \hat{D}_{z^2} \hat{\phi}_2 = 0 \quad \text{and} \quad \hat{D}_{\bar{z}^2} \hat{\phi}_1 + \hat{D}_{z^1} \hat{\phi}_2 = 0, \tag{3.36e}$$

where

$$\hat{D}_{z^a}\phi=\hat{\partial}_{z^a}\hat{\phi}+\hat{A}_{+z^a}\hat{\phi}-\hat{\phi}\hat{A}_{-z^a}. \tag{3.37}$$

In order to simplify our notation, from now on we omit the hats over the operators.

2. $U_+(1)\times U_-(1)$ SW action functional

Having introduced the $U_+(1)\times U_-(1)$ noncommutative extension of the SW equations (3.36), we shall define an appropriate action functional. For this purpose we switch back to real coordinates.

Let ${}^t\Phi=(\phi_1,\phi_2)$ and ${}^t\Phi^*:=(\phi_2^\dagger,-\phi_1^\dagger)$. (Note that "$*$" is nothing but a spinor conjugation.) Then the noncommutative deformation of the action functional (2.10) will have the form

$$\begin{aligned}\mathrm{SW}_\chi(A_+,A_-,\Phi;\theta)=\tfrac{1}{2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{&|\mathcal{D}_{A_+,A_-}\Phi|^2+|(\mathcal{D}_{A_+,A_-}\Phi)^\dagger|^2+\ 8|F^+_{A_+}\\&+\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2+8|F^+_{A_-}+\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2\},\end{aligned} \tag{3.38}$$

where

$$|\psi|^2:=\psi_1\psi_1^\dagger+\psi_2\psi_2^\dagger \quad\text{and}\quad |\psi^\dagger|^2:=\psi_1^\dagger\psi_1+\psi_2^\dagger\psi_2, \tag{3.39}$$

for any ${}^t\psi=(\psi_1,\psi_2)$. Here, $\mathcal{D}_{A_+,A_-}$ denotes the Dirac operator depending on the two gauge potentials A_+ and A_-, i.e.,

$$\mathcal{D}_{A_+,A_-}\Phi=\begin{pmatrix}-D_4+iD_3 & D_2+iD_1\\ -D_2+iD_1 & -D_4-iD_3\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \tag{3.40}$$

where the covariant derivatives D_μ are given by (3.37). Note that the prefactors in (3.38) are adjusted in such a way that we recover (2.10) in the commutative limit. It is not difficult to see that the (perturbed) $U_+(1)\times U_-(1)$ SW equations following from (3.38) are given by the equations

$$\mathcal{D}_{A_+,A_-}\Phi=0,\quad F^+_{A_+}+\chi^+_+=\sigma^+(\Phi\otimes\Phi^\dagger)_0 \quad\text{and}\quad F^+_{A_-}+\chi^+_-=\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0, \tag{3.41}$$

whose solutions minimize the action functional (3.38). In components these equations coincide with (3.36).

Assuming that $\phi_{1,2}$ and $F_{\pm\mu\nu}$ are of proper trace-class, e.g., $|\mathrm{Tr}\phi_{1,2}|<\infty$ and $|\mathrm{Tr}F_{\pm\mu\nu}|<\infty$, we can show that

$$\mathrm{SW}_\chi(A_+,A_-,\Phi;\theta)=E_\chi(A_+,A_-,\Phi;\theta)+16\pi^2K_\chi-|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\mathcal{T}, \tag{3.42}$$

where the functionals E_χ and K_χ are given by

$$\begin{aligned}E_\chi(A_+,A_-,\Phi;\theta)=|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{&2|F_{A_+}|^2+2|F_{A_-}|^2+\tfrac{1}{2}|D_{A_+,A_-}\Phi|^2+\tfrac{1}{2}|(D_{A_+,A_-}\Phi)^\dagger|^2\\&+\ 4|\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2+4|\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2\}\end{aligned} \tag{3.43}$$

and

$$K_\chi=-\frac{1}{8\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\sum_{i=\pm}\{F^+_{i\mu\nu},\chi^+_{i\mu\nu}\}. \tag{3.44}$$

The topological term $\mathcal{T}$ reads as

$$\mathcal{T}=\sum_{i=\pm}(F_{i\mu\nu}*F_{i\mu\nu}+\nabla_{i\mu}\mathcal{J}_{i\mu}). \tag{3.45a}$$

Here

$$\nabla_{\pm\mu}\cdot := \partial_\mu \cdot + [A_{\pm\mu}, \cdot\ ], \tag{3.45b}$$

"$*$" denotes the Hodge operator and $\{A,B\} := AB + BA$. The currents $\mathcal{J}_{\pm\mu}$ depend in a particular fashion on the fields ϕ_1 and ϕ_2, their derivatives and on the gauge potentials $A_{\pm\mu}$. The explicit derivation of (3.42) and the expressions for the currents $\mathcal{J}_{\pm\mu}$ are given in Appendix A. Note that similarly to the commutative case the functionals $E_\chi + 16\pi^2 K_\chi$ and SW_χ yield the same equations of motion. The integration of (3.45a) yields the topological charge

$$Q = -\frac{1}{8\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\mathcal{T}, \tag{3.46}$$

for the considered field configuration (A_+, A_-, Φ) on $\mathbb{R}^4_\theta$.

3. Generalized coupled vortex equations

Let us put one component of Φ to zero, e.g., consider the case ${}^t\Phi = (\phi_1, \phi_2) =: (\phi, 0)$. [Note that in the case of Kähler manifolds ($\mathbb{R}^4$ is trivially Kähler) the field ϕ can be regarded as a scalar.[20,21]] Moreover, we choose

$$\chi_{\pm z^1 z^2} = 0 \quad \text{and} \quad \chi_{\pm z^1 \bar{z}^1} + \chi_{\pm z^2 \bar{z}^2} = \mp \tfrac{1}{8} v_\pm, \tag{3.47}$$

where $v_\pm$ are some Hermitian operators acting on $\mathcal{H}$. Then the energy functional (3.43) turns into

$$\begin{aligned} E_\chi(A_+, A_-, \Phi; \theta) = |\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{&F_{+\mu\nu}F^\dagger_{+\mu\nu} + F_{-\mu\nu}F^\dagger_{-\mu\nu} + \tfrac{1}{2}D_\mu\phi(D_\mu\phi)^\dagger + \tfrac{1}{2}(D_\mu\phi)^\dagger D_\mu\phi \\ &+ \tfrac{1}{8}(v_+ - \phi\phi^\dagger)^2 + \tfrac{1}{8}(v_- - \phi^\dagger\phi)^2\}, \end{aligned} \tag{3.48a}$$

and K_χ is given by

$$K_\chi = -\frac{i}{32\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{\{F_{+12} + F_{+34}, v_+\} - \{F_{-12} + F_{-34}, v_-\}\}. \tag{3.48b}$$

Also the currents $\mathcal{J}_{\pm\mu}$ have a fairly simple form,

$$\mathcal{J}_{+\mu} = \frac{i}{4}(\epsilon_{\mu\nu 12} + \epsilon_{\mu\nu 34})(\phi(D_\nu\phi)^\dagger - (D_\nu\phi)\phi^\dagger), \tag{3.49a}$$

$$\mathcal{J}_{-\mu} = -\frac{i}{4}(\epsilon_{\mu\nu 12} + \epsilon_{\mu\nu 34})(\phi^\dagger(D_\nu\phi) - (D_\nu\phi)^\dagger\phi), \tag{3.49b}$$

where $\epsilon_{\mu\nu\lambda\sigma}$ is the Levi-Civita symbol with $\epsilon_{1234} = 1$ (see the Appendix).

For our choices of Φ and $\chi_\pm$ the perturbed $U_+(1)\times U_-(1)$ SW equations in complex coordinates read as

$$F_{+z^1\bar{z}^1} + F_{+z^2\bar{z}^2} = \tfrac{1}{8}(v_+ - \phi\phi^\dagger) \quad \text{and} \quad F_{+z^1 z^2} = 0, \tag{3.50a}$$

$$F_{-z^1\bar{z}^1} + F_{-z^2\bar{z}^2} = -\tfrac{1}{8}(v_- - \phi^\dagger\phi) \quad \text{and} \quad F_{-z^1 z^2} = 0, \tag{3.50b}$$

$$D_{\bar{z}^1}\phi = 0 \quad \text{and} \quad D_{\bar{z}^2}\phi = 0. \tag{3.50c}$$

In the commutative case these equations were considered, e.g., in Ref. 9.

4. $U_{\pm}(1)$ SW action functionals

Having introduced the $U_+(1)\times U_-(1)$ SW functionals, we are now interested in proper functionals for the $U_{\pm}(1)$ cases (3.29) and (3.30). Let us first discuss the perturbed $U_+(1)$ SW equations. In this case the SW action functional takes the following form:

$$\mathrm{SW}_\chi(\mathcal{A},\Phi;\theta)=|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{|\mathcal{D}_{\mathcal{A}}\Phi|^2+2|F^+_{\mathcal{A}}+\chi^+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\}. \tag{3.51}$$

Note that now the Dirac operator depends only on $\mathcal{A}$ and the covariant derivatives are given by (3.29c). Also here the prefactors have been chosen such that the correct commutative limit will be obtained. As before, the functional SW_χ may be rewritten as

$$\mathrm{SW}_\chi(\mathcal{A},\Phi;\theta)=E_\chi(\mathcal{A},\Phi;\theta)+16\pi^2K_\chi-|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\mathcal{T}, \tag{3.52}$$

where E_χ turns out to be

$$E_\chi(\mathcal{A},\Phi;\theta)=|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{|F_{\mathcal{A}}|^2+|D_{\mathcal{A}}\Phi|^2+2|\chi^+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\}. \tag{3.53}$$

The Chern–Simons term K_χ reads as

$$K_\chi=-\frac{1}{16\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{F^+_{\mu\nu},\chi^+_{\mu\nu}\}, \tag{3.54}$$

and the topological term $\mathcal{T}$ is given by

$$\mathcal{T}=\tfrac{1}{4}\{F_{\mu\nu},{*F}_{\mu\nu}\}+\nabla_\mu\mathcal{J}_\mu,\quad \text{with}\quad \nabla_\mu\mathcal{J}_\mu=\partial_\mu\mathcal{J}_\mu+[\mathcal{A}_\mu,\mathcal{J}_\mu], \tag{3.55}$$

implying the charge

$$Q=-\frac{1}{8\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\mathcal{T}. \tag{3.56}$$

Again all equations simplify essentially if one chooses ${}^t\Phi=(\phi_1,\phi_2)=(\phi,0)$, $\chi_{z^1z^2}=0$ and $\chi_{z^1\bar{z}^1}+\chi_{z^2\bar{z}^2}=-\frac{1}{4}v$, where v is some Hermitian operator. Then E_χ and K_χ are given by

$$E_\chi(\mathcal{A},\Phi;\theta)=|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{\tfrac{1}{2}F_{\mu\nu}F^\dagger_{\mu\nu}+D_\mu\phi(D_\mu\phi)^\dagger+\tfrac{1}{4}(v-\phi\phi^\dagger)^2\} \tag{3.57a}$$

and

$$K_\chi=-\frac{i}{32\pi^2}|\mathrm{Pf}(2\pi\theta)|\mathrm{Tr}\{F_{12}+F_{34},v\}. \tag{3.57b}$$

The current $\mathcal{J}_\mu$ reduces in this case to

$$\mathcal{J}_\mu=\frac{i}{2}(\epsilon_{\mu\nu12}+\epsilon_{\mu\nu34})(\phi(D_\nu\phi)^\dagger-(D_\nu\phi)\phi^\dagger). \tag{3.58}$$

Finally, the perturbed $U_+(1)$ SW equations read as

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}=\tfrac{1}{4}(v-\phi\phi^\dagger)\quad\text{and}\quad F_{z^1z^2}=0, \tag{3.59a}$$

$$D_{\bar{z}^1}\phi=0\quad\text{and}\quad D_{\bar{z}^2}\phi=0. \tag{3.59b}$$

In the commutative case these v-vortex equations in four dimensions were considered, e.g., in Ref. 9. Note that in a similar manner one can write down the functionals corresponding to the $U_-(1)$ case (3.30). Since they look essentially the same as the above-introduced $U_+(1)$ functionals we refrain from writing down their explicit form.

IV. PARTICULAR SOLUTIONS

A. Operator realization

The form of the Heisenberg algebra type commutation relations (3.34) suggests that the algebra $\mathbb{R}^4_\theta$ may be represented by a pair of harmonic oscillators in the two-oscillator Fock space $\mathcal{H}\cong\mathcal{H}_1\otimes\mathcal{H}_2\cong\oplus_{n_1,n_2}\mathbb{C}|n_1,n_2\rangle$. We introduce, as usual, annihilation and creation operators $\{c_a,c_a^\dagger\}_{a=1,2}$, satisfying $[c_a,c_a^\dagger]=1$. They act on $\mathcal{H}$ and are defined by the relations

$$c_1|n_1,n_2\rangle=\sqrt{n_1}\,|n_1-1,n_2\rangle \quad \text{and} \quad c_1^\dagger|n_1,n_2\rangle=\sqrt{n_1+1}\,|n_1+1,n_2\rangle, \tag{4.1a}$$

$$c_2|n_1,n_2\rangle=\sqrt{n_2}\,|n_1,n_2-1\rangle \quad \text{and} \quad c_2^\dagger|n_1,n_2\rangle=\sqrt{n_2+1}\,|n_1,n_2+1\rangle, \tag{4.1b}$$

where $\{|n_1,n_2\rangle \mid n_1,n_2\in\mathbb{N}_0\}$ form an orthonormal basis in $\mathcal{H}$. The commutation relations (3.34) imply that the operators $\{c_a,c_a^\dagger\}_{a=1,2}$ have the form

$$c_1:=\frac{\hat z^1}{\sqrt{\theta^{\bar 1\bar 1}}}\frac{1+\mathrm{sgn}(\theta^{\bar 1\bar 1})}{2}+\frac{\hat{\bar z}^{\bar 1}}{\sqrt{\theta^{\bar 1\bar 1}}}\frac{1-\mathrm{sgn}(\theta^{\bar 1\bar 1})}{2} \quad \text{and}$$

$$c_1^\dagger:=\frac{\hat{\bar z}^{\bar 1}}{\sqrt{\theta^{\bar 1\bar 1}}}\frac{1+\mathrm{sgn}(\theta^{\bar 1\bar 1})}{2}+\frac{\hat z^1}{\sqrt{\theta^{\bar 1\bar 1}}}\frac{1-\mathrm{sgn}(\theta^{\bar 1\bar 1})}{2}, \tag{4.2a}$$

$$c_2:=\frac{\hat z^2}{\sqrt{\theta^{\bar 2\bar 2}}}\frac{1+\mathrm{sgn}(\theta^{\bar 2\bar 2})}{2}+\frac{\hat{\bar z}^{\bar 2}}{\sqrt{\theta^{\bar 2\bar 2}}}\frac{1-\mathrm{sgn}(\theta^{\bar 2\bar 2})}{2} \quad \text{and}$$

$$c_2^\dagger:=\frac{\hat{\bar z}^{\bar 2}}{\sqrt{\theta^{\bar 2\bar 2}}}\frac{1+\mathrm{sgn}(\theta^{\bar 2\bar 2})}{2}+\frac{\hat z^2}{\sqrt{\theta^{\bar 2\bar 2}}}\frac{1-\mathrm{sgn}(\theta^{\bar 2\bar 2})}{2}. \tag{4.2b}$$

We introduce so-called shift operators $S^{(a)}$ acting on the Fock spaces $\mathcal{H}_a$. They are partially isometric operators sending the Fock space $\mathcal{H}_a$ to its subspace $(\mathbb{1}^{(a)}-P_0^{(a)})\mathcal{H}_a$, where we denote by $P_0^{(a)}=|0\rangle_a\langle 0|_a$ the orthogonal projector onto the ground state of $\mathcal{H}_a$ and $\mathbb{1}^{(a)}-P_0^{(a)}$ is the complement projector. Then

$$S^{(a)}:\mathcal{H}_a\to(\mathbb{1}^{(a)}-P_0^{(a)})\mathcal{H}_a, \quad \text{with} \quad S^{(a)\dagger}S^{(a)}=\mathbb{1}^{(a)} \quad \text{and} \quad S^{(a)}S^{(a)\dagger}=\mathbb{1}^{(a)}-P_0^{(a)}. \tag{4.3}$$

The operator $S^{(a)}$ may be given by the explicit formula

$$S^{(a)}=\sum_{n\geqslant 0}|n+1\rangle_a\langle n|_a. \tag{4.4}$$

We will sometimes drop the index "a" on the state $|n\rangle_a$ in the following if the meaning is clear from the context.

The next step is to construct a shift operator S on $\mathcal{H}\cong\mathcal{H}_1\otimes\mathcal{H}_2$ such that

$$S:\mathcal{H}\to(\mathbb{1}-P_0)\mathcal{H}, \quad \text{with} \quad P_0=|0,0\rangle\langle 0,0|, \tag{4.5}$$

and $S^\dagger S=\mathbb{1}$ and $SS^\dagger=\mathbb{1}-P_0$. A naive idea to take simply the tensor product $S^{(1)}\otimes S^{(2)}$ does not work. One possible realization of the required operator S is given by the formula[27]

$$S=\mathbb{1}+\sum_{n\geqslant 0}\,(|n+1\rangle\langle n|-|n\rangle\langle n|)\otimes P_0^{(2)}=\mathbb{1}+(S^{(1)}-\mathbb{1}^{(1)})\otimes P_0^{(2)}, \tag{4.6}$$

but there are also other realizations (see, e.g., Ref. 28).

For later convenience we introduce the operators

$$X_{\pm z^a} := A_{\pm z^a} + \theta_{a\bar{a}}\bar{z^a} \quad \text{and} \quad X_{\pm \bar{z}^{\bar{a}}} := A_{\pm \bar{z}^{\bar{a}}} + \theta_{\bar{a}a} z^a, \quad \text{for} \quad a = 1,2. \tag{4.7}$$

Then a short calculation of the YM curvature yields

$$F_{\pm z^1 z^2} = [X_{\pm z^1}, X_{\pm z^2}], \quad F_{\pm z^1 \bar{z}^{\bar{2}}} = [X_{\pm z^1}, X_{\pm \bar{z}^{\bar{2}}}], \quad F_{\pm z^2 \bar{z}^{\bar{1}}} = [X_{\pm z^2}, X_{\pm \bar{z}^{\bar{1}}}], \tag{4.8a}$$

$$F_{\pm z^1 \bar{z}^{\bar{1}}} = [X_{\pm z^1}, X_{\pm \bar{z}^{\bar{1}}}] + \theta_{1\bar{1}}, \quad F_{\pm z^2 \bar{z}^{\bar{2}}} = [X_{\pm z^2}, X_{\pm \bar{z}^{\bar{2}}}] + \theta_{2\bar{2}}, \tag{4.8b}$$

and the covariant derivatives become

$$D_{z^a}\phi = X_{+z^a}\phi - \phi X_{-z^a} \quad \text{and} \quad D_{\bar{z}^{\bar{a}}}\phi = X_{+\bar{z}^{\bar{a}}}\phi - \phi X_{-\bar{z}^{\bar{a}}}. \tag{4.9}$$

B. Solutions to the perturbed SW equations

1. $U_+(1)\times U_-(1)$ SW monopole equations

Let us consider Eqs. (3.50) rewritten in operator form. For the operators (4.7) we take (cf., e.g., Refs. 29, 30)

$$X_{\pm z^a} = \theta_{a\bar{a}} S^N \bar{z^a} (S^\dagger)^N + \sum_{n=0}^{N-1} \lambda_{a,n} |n\rangle\langle n| \otimes P_0^{(2)}, \tag{4.10}$$

where the shift operator S is given by (4.6), $\lambda_{a,n} \in \mathbb{C}$ and $N \in \mathbb{N}$. Then the commutator $[X_{\pm z^a}, X_{\pm \bar{z}^{\bar{a}}}]$ is readily computed to be

$$[X_{\pm z^a}, X_{\pm \bar{z}^{\bar{a}}}] = -\theta_{a\bar{a}}(\mathbb{1} - \mathcal{P}_N), \tag{4.11}$$

where $\mathcal{P}_N$ is given by

$$\mathcal{P}_N := \sum_{n=0}^{N-1} |n\rangle\langle n| \otimes P_0^{(2)}. \tag{4.12}$$

It easy to see that the second equations of (3.50a) and (3.50b) are trivially satisfied. Choosing $v_- \equiv 0$ and

$$\phi = \sqrt{8(\theta_{1\bar{1}} + \theta_{2\bar{2}})}\, \mathcal{P}_N, \tag{4.13}$$

we can solve (3.50c) and the first equation of (3.50b) consistently, while the first equation of (3.50a) implies that

$$v_+ = 16(\theta_{1\bar{1}} + \theta_{2\bar{2}})\mathcal{P}_N. \tag{4.14}$$

Note that the moduli $\lambda_{a,n}$ in (4.10) can be interpreted as position parameters (see, e.g., Refs. 29, 31, 32).

Obviously, the components (4.8) of the curvature and the field ϕ are of proper trace-class. Moreover, it can be easily checked that ϕ is covariantly constant, i.e., along with $D_{\bar{z}^{\bar{a}}}\phi = 0$, required by the SW equations, we also have $D_{z^a}\phi = 0$. This means that the currents $\mathcal{J}_{\pm\mu}$ (3.49) vanish identically. Thus, it is straightforward to evaluate the topological charge (3.46) for this configuration. What we find for the topological term (3.45a) is

$$\mathcal{I} = -8\,\frac{1}{\theta^{12}\theta^{\bar{3}\bar{4}}}\,\mathcal{P}_N. \tag{4.15}$$

Using $|\mathrm{Pf}(2\pi\theta)| = 4\pi^2 |\theta^{12}\theta^{\bar{3}\bar{4}}|$, we get immediately a charge,

$$Q=4\epsilon_1\epsilon_2 N, \quad \text{with} \quad \epsilon_1:=\frac{|\theta^{12}|}{\theta^{12}} \quad \text{and} \quad \epsilon_2:=\frac{|\theta^{34}|}{\theta^{34}}. \tag{4.16}$$

[Note that the definition of the charge (3.46) differs by a factor of 2 in comparison with the standard one.] Note that K_χ given by (3.48b) is also finite. Therefore, the considered field configuration has finite energy

$$E_\chi=32\pi^2 f(\theta)N \quad \text{with} \quad f(\theta):=|\theta^{12}\theta^{34}|\left[\left(\frac{1}{\theta^{12}}\right)^2+\frac{1}{\theta^{12}\theta^{34}}+\left(\frac{1}{\theta^{34}}\right)^2\right]. \tag{4.17}$$

Let us now consider a slight generalization of the ansatz (4.10). We take first

$$X_{\pm z^a}=\theta_{a\bar{a}}S^{N_\pm}\overline{z^a}(S^\dagger)^{N_\pm}+\sum_{n=0}^{N_\pm-1}\lambda^\pm_{a,n}|n\rangle\langle n|\otimes P_0^{(2)}, \tag{4.18a}$$

and find that $[X_{\pm z^a},X_{\pm\bar{z}^{\bar{a}}}]=-\theta_{a\bar{a}}(\mathbb{1}-\mathcal{P}_{N_\pm})$. Second, choosing

$$\phi=\sqrt{8(\theta_{1\bar{1}}+\theta_{2\bar{2}})}\,S^{N_+}(S^\dagger)^{N_-} \tag{4.18b}$$

and the perturbations $v_\pm$ such that

$$v_+=8(\theta_{1\bar{1}}+\theta_{2\bar{2}}) \quad \text{and} \quad v_-=8(\theta_{1\bar{1}}+\theta_{2\bar{2}})(1-2\mathcal{P}_{N_-}), \tag{4.19}$$

one can easily show that our equations are solved consistently. Again, all our operators are of proper trace-class for $N_+\neq N_-$. In the case of $N_+=N_-$ one encounters a slight subtlety since the field ϕ is not of trace-class contrary to our assumption. However, potentially dangerous terms, like $\phi F_{-12}\phi^\dagger$ for instance (see the Appendix), which occurred in (3.43), are obviously zero when $N_+=N_-$. Moreover, the field ϕ is covariantly constant, as one can readily check. Therefore, the currents $\mathcal{J}_{\pm\mu}$ (3.49) are identically zero. The topological term (3.45a) for this configuration thus reads as

$$\mathcal{T}=-4\,\frac{1}{\theta^{12}\theta^{34}}(\mathcal{P}_{N_+}+\mathcal{P}_{N_-}), \tag{4.20}$$

which produces a topological charge $Q=2\epsilon_1\epsilon_2(N_++N_-)$. [Note that the definition of the charge (3.46) differs by a factor of 2 in comparison with the standard one.] The functional E_χ for these solutions computes to

$$E_\chi=16\pi^2 f(\theta)(N_++N_-), \tag{4.21}$$

where $f(\theta)$ is given by (4.17).

2. $U_+(1)$ SW monopole equations

Consider now Eqs. (3.59) and choose the ansatz

$$X_{z^a}=\theta_{a\bar{a}}S^N\overline{z^a}(S^\dagger)^N+\sum_{n=0}^{N-1}\lambda_{a,n}|n\rangle\langle n|\otimes P_0^{(2)} \quad \text{and} \quad \phi=\gamma S^N, \tag{4.22}$$

with $\lambda_{a,n}\in\mathbb{C}$ and $\gamma\in\mathbb{R}$. Then the first equation of (3.59a) can be solved by $\theta_{1\bar{1}}+\theta_{2\bar{2}}=\frac{1}{4}\gamma^2=\frac{1}{4}v$, while the other two equations are trivially satisfied. The only nonvanishing components of the curvature are $F_{z^a\bar{z}^{\bar{a}}}=\theta_{a\bar{a}}\mathcal{P}_N$. Note that the expression for ϕ is covariantly constant which implies the vanishing of the current (3.58). The charge (3.56) is equal to $Q=\epsilon_1\epsilon_2 N$ and the energy E_χ is $8\pi^2 f(\theta)N$, where $f(\theta)$ is given by (4.17).

Consider again Eqs. (3.59). Besides the shift type solution for ϕ we can also find a projector type solution. Namely, we choose $\phi=\gamma P_0$ with $\gamma\in\mathbb{R}$,

$$v=(4(\theta_{1\bar{1}}+\theta_{2\bar{2}})+\gamma^2)P_0, \tag{4.23}$$

and the X_{z^a}'s as previously. With this choice the first two equations of (3.59a) are trivially satisfied, while (3.59b) yields the condition $P_0 z^a=0$. Hence, we have to set $\theta^{a\bar{a}}<0$. Again, the only nonvanishing components of the curvature are $F_{z^a\bar{z}^a}=\theta_{a\bar{a}}P_0$. Moreover, we have

$$D_1\phi=-iD_2\phi=-\sqrt{\theta_{1\bar{1}}}\gamma|0,0\rangle\langle 1,0| \quad \text{and} \quad D_3\phi=-iD_4\phi=-\sqrt{\theta_{2\bar{2}}}\gamma|0,0\rangle\langle 0,1|, \tag{4.24}$$

which imply the vanishing of the current $\mathcal{J}_\mu$ (3.58). The topological charge for this configuration is $Q=\epsilon_1\epsilon_2$.

C. Solutions to the unperturbed SW equations

In this section we shall consider solutions to the unperturbed SW equations. We concentrate on the case of the unperturbed $U_+(1)$ equations, i.e., (3.59) with $v\equiv 0$, as an illustrative example.

1. $U_+(1)$ SW monopole equations with $\Phi\equiv 0$

In this case we obtain the noncommutative Abelian ASDYM equations. Solutions to these equations, i.e., noncommutative Abelian instantons, have been known for quite some time.[16] However, for the sake of completeness we briefly review their construction. Note that in the case $\Phi\equiv 0$ the current $\mathcal{J}_\mu$ is identically zero.

In terms of the operators (4.7) the Abelian ASDYM equations read as

$$[X_{z^1},X_{\bar{z}^1}]+[X_{z^2},X_{\bar{z}^2}]+\theta_{1\bar{1}}+\theta_{2\bar{2}}=0 \quad \text{and} \quad [X_{z^1},X_{z^2}]=0. \tag{4.25}$$

Again we consider an ansatz for X_{z^a} of the form (4.22). This ansatz yields solutions to the equations (4.25) if the deformation tensor $\theta^{\mu\nu}$ is anti-self-dual which trivially follows from (4.22). The only nonvanishing components of the curvature are $F_{z^a\bar{z}^a}=\theta_{a\bar{a}}\mathcal{P}_N$ implying that the charge (3.56) is equal to $Q=-N$. The moduli $\lambda_{a,n}$ entering the solution are position parameters showing the location of the noncommutative instantons[33] (see also Ref. 32 for a recent review).

It is also possible to consider the case of ASDYM equations on a self-dual background for which $\theta^{1\bar{1}}=\theta^{2\bar{2}}=:\theta$. Let us assume that $\theta>0$, which leads to the definitions $c_1=z^1/\sqrt{\theta}$ and $c_2=z^2/\sqrt{\theta}$. We choose the ansatz[34,35]

$$X_{z^1}=-\frac{1}{\theta}S^\dagger\bar{z}^{\bar{1}}f(N)S=-\frac{1}{\sqrt{\theta}}S^\dagger c_1^\dagger f(N)S \quad \text{and} \quad X_{z^2}=-\frac{1}{\theta}S^\dagger\bar{z}^{\bar{2}}f(N)S=-\frac{1}{\sqrt{\theta}}S^\dagger c_2^\dagger f(N)S, \tag{4.26}$$

and assume that $f(N)|0\rangle=f(0)|0\rangle=0$, where $N:=N_1+N_2:=c_1^\dagger c_1+c_2^\dagger c_2$. Then the equation $[X_{z^1},X_{z^2}]=0$ is trivially satisfied. A short calculation yields for $f(N)$ the result[34,35]

$$f^2(N)=\frac{N(N+3)}{(N+1)(N+2)}. \tag{4.27}$$

The nonvanishing components of the curvature in this case are

$$F_{z^a\bar{z}^b}=\frac{1}{\theta}S^\dagger c_a^\dagger(f^2(N+1)-f^2(N))c_b S, \tag{4.28a}$$

$$F_{z^a\bar{z}^a}=\frac{1}{\theta}S^\dagger[(N_a+1)f^2(N)-N_a f^2(N-1)-1]S. \tag{4.28b}$$

Using these expressions, we compute the topological charge (3.56) to be -1. A straightforward extension of the above ansatz allows one to construct multi-instanton configurations, as well.[34,35]

2. Fock spaces with indefinite norm

Let us now discuss the case when Φ does not vanish identically. For that we relax the condition of positivity of the norm of the Fock spaces $\mathcal{H}_{1,2}$ and assume instead that at least one of them has an indefinite norm (cf. Ref. 36). For instance, we can introduce a collection of the creation and annihilation operators $\{c_a, c_a^\dagger\}_{a=1,2}$, satisfying $[c_1, c_1^\dagger]=1$, $[c_2, c_2^\dagger]=-1$, and defined by the relations

$$c_1|n_1,n_2\rangle=\sqrt{n_1}\,|n_1-1,n_2\rangle \quad \text{and} \quad c_1^\dagger|n_1,n_2\rangle=\sqrt{n_1+1}\,|n_1+1,n_2\rangle, \tag{4.29a}$$

$$c_2|n_1,n_2\rangle=-\sqrt{n_2}\,|n_1,n_2-1\rangle \quad \text{and} \quad c_2^\dagger|n_1,n_2\rangle=\sqrt{n_2+1}\,|n_1,n_2+1\rangle, \tag{4.29b}$$

substituting (4.1). The normalization condition is modified to $\langle n_1,n_2|m_1,m_2\rangle = (-1)^{n_2}\delta_{n_1m_1}\delta_{n_2m_2}$. The identity operator is given by

$$\mathbb{1}=\sum_{n_1,n_2}(-1)^{n_2}|n_1,n_2\rangle\langle n_1,n_2|. \tag{4.30}$$

Moreover, we have to redefine the relations between $\{c_a, c_a^\dagger\}_{a=1,2}$ and $\{z^a, \bar{z}^{\bar{a}}\}_{a=1,2}$ so that

$$c_1 := \frac{\hat{z}^1}{\sqrt{\theta^{\bar{1}\bar{1}}}}\frac{1+\mathrm{sgn}(\theta^{\bar{1}\bar{1}})}{2}+\frac{\hat{\bar{z}}^{\bar{1}}}{\sqrt{\theta^{\bar{1}\bar{1}}}}\frac{1-\mathrm{sgn}(\theta^{\bar{1}\bar{1}})}{2} \quad \text{and}$$

$$c_1^\dagger := \frac{\hat{\bar{z}}^{\bar{1}}}{\sqrt{\theta^{\bar{1}\bar{1}}}}\frac{1+\mathrm{sgn}(\theta^{\bar{1}\bar{1}})}{2}+\frac{\hat{z}^1}{\sqrt{\theta^{\bar{1}\bar{1}}}}\frac{1-\mathrm{sgn}(\theta^{\bar{1}\bar{1}})}{2}, \tag{4.31a}$$

$$c_2 := \frac{\hat{\bar{z}}^{\bar{2}}}{\sqrt{\theta^{\bar{2}\bar{2}}}}\frac{1+\mathrm{sgn}(\theta^{\bar{2}\bar{2}})}{2}+\frac{\hat{z}^2}{\sqrt{\theta^{\bar{2}\bar{2}}}}\frac{1-\mathrm{sgn}(\theta^{\bar{2}\bar{2}})}{2} \quad \text{and}$$

$$c_2^\dagger := \frac{\hat{z}^2}{\sqrt{\theta^{\bar{2}\bar{2}}}}\frac{1+\mathrm{sgn}(\theta^{\bar{2}\bar{2}})}{2}+\frac{\hat{\bar{z}}^{\bar{2}}}{\sqrt{\theta^{\bar{2}\bar{2}}}}\frac{1-\mathrm{sgn}(\theta^{\bar{2}\bar{2}})}{2}. \tag{4.31b}$$

The definition of the shift operator $S^{(1)}$ remains the same, while for $S^{(2)}$ we obtain

$$S^{(2)}:\mathcal{H}_2\to(\mathbb{1}^{(2)}-P_0^{(2)})\mathcal{H}_2 \quad \text{with} \quad S^{(2)\dagger}S^{(2)}=-\mathbb{1}^{(2)} \quad \text{and} \quad S^{(2)}S^{(2)\dagger}=-(\mathbb{1}^{(2)}-P_0^{(2)}), \tag{4.32}$$

with the representation

$$S^{(2)}=\sum_{n\geqslant 0}(-1)^n|n+1\rangle_2\langle n|_2. \tag{4.33}$$

For an operator $S:\mathcal{H}\to(\mathbb{1}-P_0)\mathcal{H}$ on $\mathcal{H}$ with the properties $SS^\dagger=\mathbb{1}-P_0$ and $S^\dagger S=\mathbb{1}$, we can use the old expression (4.6), since the indefiniteness of the norm does not affect the verification of these properties. Indeed, S contains only the identity $\mathbb{1}$, given by (4.30), and the projector $P_0^{(2)}$ on $\mathcal{H}_2$.

3. $U_+(1)$ SW monopole equations with ${}^t\Phi=(\phi,0)$

We start from (3.59) with $v\equiv 0$. In this case the SW equations read as

$$F_{z^1\bar{z}^1}+F_{z^2\bar{z}^2}=-\tfrac{1}{4}\phi\phi^\dagger, \quad F_{z^1z^2}=0 \quad \text{and} \quad D_{\bar{z}^a}\phi=0, \tag{4.34}$$

where the covariant derivative D_{z^a} acts as $D_{z^a}\phi=-\theta_{a\bar{a}}\phi\bar{z}^{\bar{a}}+X_{z^a}\phi$. Suppose that $\mathcal{H}_1$ is positive normed while $\mathcal{H}_2$ is endowed with an indefinite norm. Using the definition (4.6) and the ansatz $X_{z^a}=\theta_{a\bar{a}}S\bar{z}^{\bar{a}}S^\dagger$, we find again (4.11). Assuming that $\phi=\gamma P_0$ with $\gamma\in\mathbb{R}$, we can solve the last equation of (4.34) if $P_0z^a=0$, i.e., $z^a\sim c_a^\dagger$. For $a=2$ this is satisfied because of our choice $\theta^{2\bar{2}}>0$ and for $a=1$ it implies $\theta^{1\bar{1}}<0$. The second equation of (4.34) is again identically satisfied, while the first one yields the condition $\theta_{1\bar{1}}+\theta_{2\bar{2}}=-\frac{1}{4}\gamma^2$, which makes sense due to the different signs of $\theta_{1\bar{1}}$ and $\theta_{2\bar{2}}$. The nonvanishing components of the curvature are $F_{z^a\bar{z}^a}=\theta_{a\bar{a}}P_0$ and one can readily verify that the current $\mathcal{J}_\mu$ from (3.58) has no contributions to the topological charge (3.56). Moreover, the computation of the topological charge gives -1. Note that the introduction of an indefinite norm on $\mathcal{H}_2$ was needed for having solutions to the equation $\theta_{1\bar{1}}+\theta_{2\bar{2}}=-\frac{1}{4}\gamma^2$ on the components of $\theta_{\mu\nu}$.

4. $U_+(1)$ SW monopole equations and vortices

Finally we discuss a case which is slightly different from the cases described above, in the sense that we fix the explicit form of the solutions on a two-dimensional subspace of $\mathbb{R}^4_\theta$ from the very beginning. This eventually results in the $U_+(1)$ vortex equations on the complementary two-dimensional subspace.

Again, let $\mathcal{H}_1$ be positive normed and $\mathcal{H}_2$ endowed with an indefinite norm, such that $[z^2,\bar{z}^2]=\theta^{2\bar{2}}>0$ and $[c_2,c_2^\dagger]=-1$. Furthermore, we choose an ansatz for X_{z^2} of the form $X_{z^2}=\theta_{2\bar{2}}\mathbb{1}^{(1)}\otimes S^{(2)}\bar{z}^{\bar{2}}S^{(2)\dagger}$. A short calculation yields the result $F_{z^2\bar{z}^2}=\theta_{2\bar{2}}\mathbb{1}^{(1)}\otimes P_0^{(2)}$. Assuming that $\mathcal{A}_{z^1}=\mathfrak{A}_{z^1}\otimes P_0^{(2)}$, we obtain $F_{z^1\bar{z}^1}=\mathfrak{F}_{z^1\bar{z}^1}\otimes P_0^{(2)}$. Similarly, we take $\phi=\psi\otimes P_0^{(2)}$. Then the equation $D_{\bar{z}^2}\phi=0$ implies the condition $P_0^{(2)}z^2=0$, which is identically satisfied due to the relation $z^2\sim c_2^\dagger$. Moreover, the equation $F_{z^1z^2}=0$ is trivially satisfied. Using $\theta_{2\bar{2}}=-1/\theta^{2\bar{2}}$, we finally arrive at the equations

$$\left\{\mathfrak{F}_{z^1\bar{z}^1}-\left(\frac{1}{\theta^{2\bar{2}}}-\frac{1}{4}\psi\psi^\dagger\right)\right\}\otimes P_0^{(2)}=0, \tag{4.35a}$$

$$(\partial_{\bar{z}^1}+\mathfrak{A}_{\bar{z}^1})\psi\otimes P_0^{(2)}=0. \tag{4.35b}$$

(Note that these equations can also be obtained in the context of the perturbed SW equations if one chooses the perturbation proportional to $P_0^{(2)}$. Then there is no necessity to introduce an indefinite normed space.) Rescaling $\psi\mapsto 2\,\tilde{\psi}/\sqrt{\theta^{2\bar{2}}}$ and introducing $\beta:=4/\theta^{2\bar{2}}$, we obtain the equations

$$\mathfrak{F}_{z^1\bar{z}^1}=\frac{\beta}{4}(1-\tilde{\psi}\tilde{\psi}^\dagger) \quad \text{and} \quad (\partial_{\bar{z}^1}+\mathfrak{A}_{\bar{z}^1})\tilde{\psi}=0, \tag{4.36}$$

on $\mathbb{R}^2_\theta\subset\mathbb{R}^4_\theta$. For $\beta=1$ they coincide with the standard $U_+(1)$ vortex equations. The equations (4.36) with $\theta^{1\bar{1}}=2\,\theta^{12}\neq 0$ and their explicit solutions were extensively discussed in the literature (see, e.g., Refs. 37, 38, 30). Note that the choice of the projector $P_0^{(2)}$ on $\mathcal{H}_2$ ensures a finite charge for this solution. To exemplify this case let us rewrite $\mathfrak{A}_{z^1}$ via $\mathfrak{X}_{z^1}=\mathfrak{A}_{z^1}+\theta_{1\bar{1}}\bar{z}^{\bar{a}}$ with $\mathfrak{X}_{z^1}=\theta_{1\bar{1}}(S^{(1)})^N\bar{z}^{\bar{1}}(S^{(1)\dagger})^N$. Moreover, suppose that $\tilde{\psi}=(S^{(1)})^N$. Then one readily verifies that $\theta_{1\bar{1}}=\beta/4=1/\theta^{2\bar{2}}$. Therefore, we end up with $F_{z^1\bar{z}^1}=\theta_{1\bar{1}}\mathcal{P}_N$ and $\phi=(2/\sqrt{\theta^{2\bar{2}}})\,(S^{(1)})^N\otimes P_0^{(2)}$. Note that $\theta^{1\bar{1}}<0$. The topological charge (3.46) for this configuration is $Q=-N$.

To summarize, we have described solutions on $\mathbb{R}^2_{\theta^{12}}\times\mathbb{R}^2_{\theta^{34}}$. It is also allowed to put θ^{12} to zero in order to have solutions on $\mathbb{R}^2\times\mathbb{R}^2_{\theta^{34}}$. Then the second equation of (4.36) reduces to $\mathfrak{A}_{\bar{z}^1}=-\partial_{\bar{z}^1}\log\tilde{\psi}$. Assuming that $\tilde{\psi}=e^{(u+iv)/2}$ has zeros at points z^1_n in the complex plane, we obtain from the first equation of (4.36) with $\beta=1$ (see, e.g., Refs. 39, 21),

$$\Delta u=e^u-1+4\pi\sum_{n=1}^{N}\delta^{(2)}(z^1-z^1_n,\bar{z}^{\dot{1}}-\bar{z}^{\dot{1}}_n), \tag{4.37}$$

i.e., the standard Liouville type equation on $\mathbb{R}^2\cong\mathbb{C}$. The moduli z^1_n are position parameters of the N-vortex solution on the z^1-plane. It is well known that this equation exhibits regular N-vortex solutions.[39]

D. Noncommutative solitons and *D*-branes

Without refering to string theory the $U_+(1)\times U_-(1)$ and $U_\pm(1)$ SW monopole equations are simply understood as noncommutative generalizations of the Abelian SW equations. In this section we shall discuss how one can interpret solutions to the noncommutative SW equations as D-brane configurations in a stringy context.

1. Brane–antibrane effective action

In the simplest case of type II superstrings living in the target space $\mathbb{R}^{9,1}$ a Dp-brane with a world volume $\mathbb{R}^{p,1}\hookrightarrow\mathbb{R}^{9,1}$ may be defined via a relative map,

$$\varphi:(\Sigma_2,\partial\Sigma_2)\to(\mathbb{R}^{9,1},\mathbb{R}^{p,1}), \tag{4.38}$$

where Σ_2 is a string world sheet with boundary $\partial\Sigma_2$. One may also consider $\overline{Dp}$-branes (=anti-Dp-branes) which are Dp-branes with opposite orientation and Ramond–Ramond (RR) charge.

It is well known that there are stable BPS Dp-branes in type IIA (even p) and type IIB (odd p) superstring theory. Besides that, it is also well known that a system consisting of coincident Dp-brane and $\overline{Dp}$-brane is unstable since open strings ending on these branes have a tachyonic mode ($M^2<0$) in the spectrum (see, e.g., Refs. 40–44 and references therein). This instability can be seen in the low energy effective action for the brane–antibrane pair. Namely, the effective field theory describing light excitations of this system contains two Abelian gauge potentials $A_\pm$ and a complex scalar ϕ (tachyon). The latter one is associated with modes of the open string stretched between brane and antibrane, and is believed to be subject to a ''Mexican hat'' potential. The tachyon carries charge one under the diagonal $U(1)$ subgroup of the group $U_+(1)\times U_-(1)$ with the generator diag$(i,-i)$ corresponding to the gauge potential A_+-A_-. After turning on a constant B-field (generating a noncommutativity tensor θ on $\mathbb{R}^{p,1}$ [45]) the theory becomes noncommutative and the tachyon field transforms in the bi-fundamental representation of $U_+(1)\times U_-(1)$.[46]

In perturbative string theory the first computations of the brane-antibrane effective action were performed in Ref. 47. The resulting effective Lagrangian reads as

$$\mathcal{L}^{(2)}=F_{+\hat{\alpha}\hat{\beta}}\overline{F_+^{\hat{\alpha}\hat{\beta}}}+F_{-\hat{\alpha}\hat{\beta}}\overline{F_-^{\hat{\alpha}\hat{\beta}}}+(D^{\hat{\alpha}}\phi)\overline{D_{\hat{\alpha}}\phi}+\frac{1}{4}(\tau^2-\phi\bar{\phi})^2, \tag{4.39}$$

where the covariant derivative is given by $D_{\hat{\alpha}}\phi=\partial_{\hat{\alpha}}\phi+(A_{+\hat{\alpha}}-A_{-\hat{\alpha}})\phi$, the overbar denotes complex conjugation, τ^2 is a constant and $\hat{\alpha},\hat{\beta},\ldots=0,1,\ldots,p$. This is not the full effective Lagrangian since the coupling between closed string RR fields and open strings gives an additional term $\mathcal{L}_{\mathrm{CS}}$ called the Chern–Simons term.[48] For constant components of the RR fields, which we now consider, this term does not contribute to the equations of motion, and therefore we will not discuss it here. Note that the terms given by (2.14) and (3.44) are of such a kind.

The tachyon potential given by (4.39) has the quartic form

$$V(\phi,\overline{\phi})=\tfrac{1}{4}(\tau^2-\phi\overline{\phi})^2. \tag{4.40}$$

Computations in level truncated superstring field theory yield the same result.[49] Any minimum $\phi\overline{\phi}=\tau^2$ of the tachyon potential describes the closed string vacuum (tachyon condensate). The perturbative spectrum around this vacuum is conjectured not to contain any open string excitations. As it was discussed in Refs. 46, 30, 50, in the presence of a B-field background a noncommutative generalization of the effective theory (4.39) might be of the form

$$\mathcal{L}^{(2)}_{\rm nc}=F_{+\hat{\alpha}\hat{\beta}}F_{+}^{\dagger\hat{\alpha}\hat{\beta}}+F_{-\hat{\alpha}\hat{\beta}}F_{-}^{\dagger\hat{\alpha}\hat{\beta}}+\tfrac{1}{2}\{D^{\hat{\alpha}}\phi,(D_{\hat{\alpha}}\phi)^{\dagger}\}+\tfrac{1}{8}(\tau^2-\phi\phi^{\dagger})^2+\tfrac{1}{8}(\tau^2-\phi^{\dagger}\phi)^2, \tag{4.41}$$

where $D_{\hat{\alpha}}\phi=\partial_{\hat{\alpha}}\phi+A_{+\hat{\alpha}}\phi-\phi A_{-\hat{\alpha}}$. Higher order corrections to the quartic tachyon potential are known (see, e.g., Refs. 51, 43). The result is qualitatively similar (''Mexican hat'' form with minima at $\phi\overline{\phi}<\infty$), and (4.40) is the leading order term. Note that a quartic form of the potential was also obtained in Refs. 45, 52–54 for bound states in $D(p-2)$-Dp and $D(p-4)$-Dp systems by using scattering calculations in string theory, level truncated superstring field theory and by analyzing the fluctuation spectrum around (noncommutative) vortex and instanton solutions.

Quite different results have been obtained in boundary string field theory (BSFT) (see, e.g., Refs. 55, 56 and references therein). There (as in Ref. 57) the Lagrangian density is proportional to the tachyon potential itself, and the potential has the form $V\sim\exp(-\phi\overline{\phi})$ with a ring of minima at $\phi\overline{\phi}\to\infty$. It is believed that the level truncation scheme and the BSFT approach can be related by a field redefinition involving all components of the string field.[55] Various ''improved versions'' of the effective action of the brane–antibrane system have been introduced (see, e.g., Refs. 58, 59), and in the literature there is no final agreement on its form. Thus, the action based on the Lagrangian (4.39) [or (4.41) in the presence of a B-field] might be considered as an approximation of the low energy effective action of the brane–antibrane system. In any case the discussed Yang–Mills–Higgs theory provides a simple field theoretic model of the more complicated string field theory description of brane–antibrane systems.

2. Noncommutative vortices and ABS solitons

Recall that branes and antibranes have opposite RR charge and therefore they can annihilate into the closed string vacuum state with $A_{\pm}=0$ and $\phi\phi^{\dagger}=\phi^{\dagger}\phi=\tau^2$. However, instead of taking the vacuum solution, one can choose as the ground state a (tachyon) soliton solution to the equations of motion for the Lagrangian (4.41). Such kinds of solutions are interpreted as bound states of Dp-branes and $\overline{Dp}$-branes, equivalent to D-branes of lower dimensionality. Here we discuss the main example of such solutions obtained via the Atiyah–Bott–Shapiro (ABS) construction.[40,60–62] These ABS (noncommutative) solitons live in $2n\leqslant p$ dimensions, and for $n=1$ they coincide with noncommutative vortices on $\mathbb{R}^2_{\theta}$. For $n=2$ the ABS solitons are non-Abelian and therefore differ from those (Abelian) SW solutions which also solve the field equations following from (4.41).

To describe the ABS solitons on $\mathbb{R}^{2n}_{\theta}$ we consider a non-Abelian generalization of the Lagrangian (4.41) with a $U_{+}(q)\times U_{-}(q)$ gauge group for $q=2^{n-1}$ and the tachyon field ϕ in the bi-fundamental representation $(q,\overline{q})$ of this group. This model describes two Hermitian rank q vector bundles $E_{\pm}\to\mathbb{R}^{p,1}$ with connection one-forms $A_{\pm}$ and $\phi\in\mathrm{Hom}(E_{-},E_{+})$ and is associated with a system of q Dp-branes and q $\overline{Dp}$-branes with common world volume $\mathbb{R}^{p,1}$. We assume that $2n\leqslant p$ and introduce an ansatz for ABS solitons related to Clifford algebras.

Consider the Clifford algebra of the Euclidean space $(\mathbb{R}^{2n},\delta_{\alpha\beta})$, generated by unity and elements Γ_{α} such that

$$\Gamma_{\alpha}\Gamma_{\beta}+\Gamma_{\beta}\Gamma_{\alpha}=-2\,\delta_{\alpha\beta}, \tag{4.42}$$

with $\alpha,\beta,\ldots=1,\ldots,2n$. In the $2^n\times 2^n$ matrix representation of this algebra the generators Γ_α can be chosen of the form

$$\Gamma_\alpha=\begin{pmatrix} 0 & \gamma_\alpha^\dagger \\ -\gamma_\alpha & 0 \end{pmatrix}, \tag{4.43}$$

where the γ_α's are $q\times q$ gamma matrices with $q=2^{n-1}$. In this representation the spinor space $W\cong\mathbb{C}^{2q}$ can be decomposed into a direct sum $W\cong W^+\oplus W^-$ of semi-spinor spaces $W^\pm$ (the spaces of Weyl spinors). Note that for $n=1$ we have $\gamma_1=1$ and $\gamma_2=i$.

Considering the noncommutative deformation $\mathbb{R}^{2n}_\theta$ of $\mathbb{R}^{2n}$ discussed in Secs. III A and III C, we introduce the operators

$$T=\gamma_\alpha^\dagger x^\alpha\frac{1}{\sqrt{(\gamma x)(\gamma x)^\dagger}} \quad \text{and} \quad T^\dagger=\frac{1}{\sqrt{(\gamma x)(\gamma x)^\dagger}}\gamma_\alpha x^\alpha, \tag{4.44}$$

where γx is a short hand notation for $\gamma_\alpha x^\alpha$. The operator T defines a map,

$$\hat{T}:\mathcal{H}\otimes W^-\to\mathcal{H}\otimes W^+. \tag{4.45}$$

Here $\mathcal{H}$ is the Hilbert space realized as a representation space of n oscillators defined by formulas similiar to (4.1) and (4.2), and $W^\pm$ are the semi-spinor spaces introduced above. In matrix realization $\hat{T}$ looks as

$$\hat{T}=\begin{pmatrix} 0 & T \\ 0 & 0 \end{pmatrix}, \tag{4.46}$$

and hence, following the authors of Refs. 40, 63, 62, 50, we will not distinguish T and $\hat{T}$ in the sequel.

It is not difficult to see that

$$T^\dagger T=\mathbb{1}_q \quad \text{and} \quad TT^\dagger=\mathbb{1}_q-\mathcal{P}_0, \tag{4.47}$$

where $\mathcal{P}_0$ is the projector onto the kernel of $T^\dagger$. This state is the tensor product of the oscillator ground state with itself and the lowest weight spinor of $SO(2n)$ (the fermion ground state). Also, by introducing $T_N:=T^N$ with $T_1\equiv T$, we have

$$T_N^\dagger T_N=\mathbb{1}_q \quad \text{and} \quad T_N T_N^\dagger=\mathbb{1}_q-\mathcal{P}_{N-1}, \tag{4.48}$$

where $\mathcal{P}_{N-1}$ is the projector onto the kernel of $T_N^\dagger$, an N-dimensional subspace in $\mathcal{H}\otimes W$. One can show that

$$\dim\ \ker T_N=0 \quad \text{and} \quad \dim\ \operatorname{coker} T_N:=\dim\ \ker T_N^\dagger=N, \tag{4.49}$$

and therefore the index of T_N is given by

$$\operatorname{ind} T_N:=\dim\ \ker T_N-\dim\ \operatorname{coker} T_N=-N. \tag{4.50}$$

The operators T_N and $T_N^\dagger$ are Toeplitz operators.

Now we reduce the equations of motion for the Lagrangian (4.41) to the space $\mathbb{R}^{2n}_\theta\hookrightarrow\mathbb{R}^{p+1}_\theta$ by assuming that all fields depend only on x^α and by taking $A_{\pm\alpha}$ as the only nonvanishing components of the gauge potentials $A_\pm$. To solve the reduced field equations we consider T_N as $q\times q$ matrices with operator entries and introduce the ansatz,

$$A_{+z^a}=-(A_{+\bar{z}^{\bar{a}}})^\dagger=\tau\theta_{a\bar{a}}(T_{N_+}\bar{z}^{\bar{a}}T_{N_+}^\dagger-\bar{z}^{\bar{a}}),\quad A_{-z^a}=0=A_{-\bar{z}^{\bar{a}}}\quad\text{and}\quad\phi=\tau T_{N_+},\tag{4.51}$$

which solves the equation of motion for (4.41).[30,50] More general solutions can also be constructed. For $n=1$ the solution (4.51) describes N_+ vortices on $\mathbb{R}^2_\theta$. In the case $n=2$ it gives a solution for the $U_+(2)\times U_-(2)$ Yang–Mills–Higgs model on $\mathbb{R}^4_\theta$. Some noncommutative SW solutions [e.g., (4.18a), (4.18b) with $N_-=0$] solve the above equations as well but for the gauge group $U_+(1)\times U_-(1)$. These solutions can therefore be regarded as a new kind of tachyon solitons.

3. Noncommutative SW solitons

Note that the SW equations (3.50) with $v_+=v_-=\tau^2=$const coincide with the first order BPS equations for the Lagrangian (4.41), and therefore their solutions also satisfy the equations of motion for (4.41). In particular, the solution given by (4.18) with $N_+\geqslant 1$ and $N_-=0$ is such a solution. Following the general logic of Sen's proposal, it is natural to interpret this solution as a configuration of N_+ stable $D(p-4)$-branes, corresponding to the topologically stable codimension four SW soliton on a $Dp-\overline{Dp}$ brane pair.

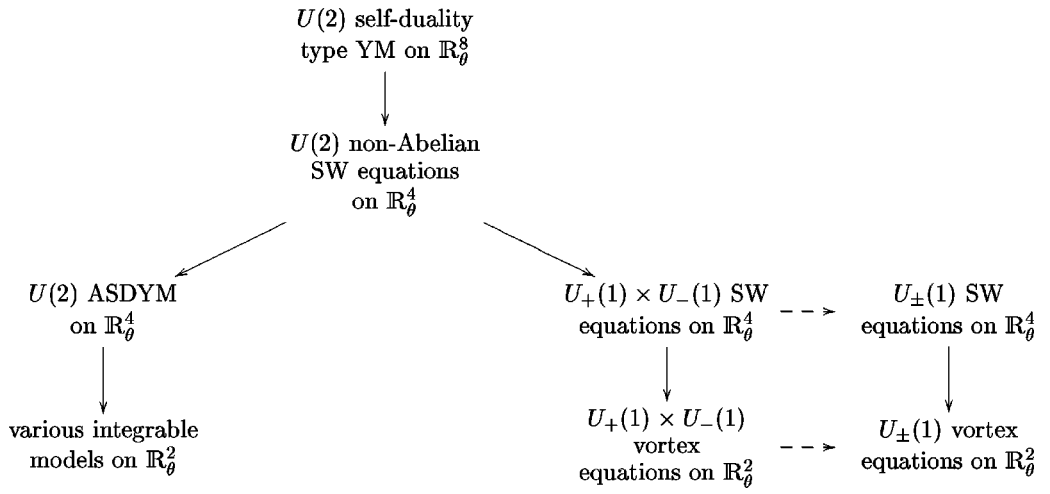
The more general configuration described by (4.18) with $N_\pm\geqslant 1$ can be interpreted in two different ways. First, we may again choose $v_+=v_-=\tau^2=$const. Then one can show that this configuration satisfies the second order equations of motion for the Lagrangian (4.41) but does not satisfy the first order equations (3.50) with constant $v_\pm$. This is natural since this solution corresponds to a system of N_+ $D(p-4)$-branes and N_- $\overline{D(p-4)}$-branes which is not a BPS configuration from the point of view of the Lagrangian (4.41). Second, one may consider the situation where v_+ depends on $\phi\phi^\dagger$ and v_- on $\phi^\dagger\phi$ and take as the low energy effective action the sum of the functional (3.48a) and the Chern–Simons term (3.48b), where the latter contributes to the equations of motion for nonconstant $v_\pm$. Then for proper choices of $v_\pm$ one can obtain configurations which satisfy the noncommutative SW equations. For instance, the choice

$$v_+=\tau^2\quad\text{and}\quad v_-=-\tau^2+2\phi^\dagger\phi\tag{4.52}$$

corresponds to the same tachyon potential $V\sim(\tau^2-\phi\phi^\dagger)^2+(\tau^2-\phi^\dagger\phi)^2$ as in (4.41). However, for the above choice of $v_\pm$ the Chern–Simons term (3.48b) becomes nontrivial and contributes to the equations (3.50) which are the BPS equations for the action $E_\chi+16\pi^2K_\chi$ with E_χ and K_χ determined by (3.48). Therefore, for $v_\pm$ given by (4.52) the configuration (4.18) with $N_\pm\geqslant 1$ is a solution to the SW equations (3.50). So, in both cases the configuration (4.18) may be interpreted as N_+ $D(p-4)$-branes and N_- $\overline{D(p-4)}$-branes. Other solutions to the noncommutative SW equations can be analyzed similarly.

V. CONCLUDING REMARKS

In this paper we have discussed different noncommutative deformations of the (perturbed) SW monopole equations on Euclidean four-dimensional space. Namely, starting from properly deformed $U(2)$ self-duality type YM equations in eight dimensions, we performed a reduction to $U(2)$ noncommutative SW equations on $\mathbb{R}^4_\theta$ with the matter field in the adjoint representation of the gauge group. We then concentrated on the $U_+(1)\times U_-(1)\subset U(2)$ noncommutative SW equations with the matter in the bi-fundamental representation of $U_+(1)\times U_-(1)$. Perturbed versions of these equations have also been discussed. Then, by considering the matter field Φ as an element of a right or left $\mathbb{R}^4_\theta$-module, we have introduced the (perturbed) $U_+(1)$ and $U_-(1)$ SW equations. The commutative limits of all these three Abelian cases are identical to the standard (perturbed) Abelian SW equations on $\mathbb{R}^4$. In summary we may write down the following diagram:



This picture shows the connection between the theories discussed in this paper. Note that the noncommutative vortex equations in two dimensions can easily be obtained via dimensional reduction from the noncommutative SW equations with properly chosen perturbations.

It has been shown that $\mathbb{R}^4_\theta$ supports regular finite-action solutions to the SW equations even if there are no such solutions in the commutative case. This is a well known phenomenon related to the fact that, due to the noncommutativity tensor θ, an additional length scale enters the theory. We have constructed explicit solutions to the $U_+(1)\times U_-(1)$ and $U_\pm(1)$ noncommutative SW equations and interpreted them as D-brane configurations in type II superstring theory. It would be illuminating to generalize the present results to non-Abelian noncommutative SW theory and discuss the latter's relation to superstring theory.

ACKNOWLEDGMENTS

We are grateful to O. Lechtenfeld for useful comments. The work of two of the authors (A.D.P. and A.G.S.) was supported in part by the grants DFG 436 RUS 113/669 and RFBR 02-02-04002. M.W. is grateful to the Studienstiftung des deutschen Volkes for financial support. This work was done within the framework of the DFG priority program in string theory and supported by the grant Le 838/7.

APPENDIX: NONCOMMUTATIVE BOGOMOLNY TRANSFORMATION

In order to derive (3.42) we need the trivial identities

$$(D_\mu\phi)\psi^\dagger=-\phi(D_\mu\psi)^\dagger+\nabla_{+\mu}(\phi\psi^\dagger)\quad\text{and}\quad(D_\mu\phi)^\dagger\psi=-\phi^\dagger(D_\mu\psi)+\nabla_{-\mu}(\phi^\dagger\psi),\tag{A1}$$

where the covariant derivatives $\nabla_{\pm\mu}$ are given by (3.45b). Furthermore, we have

$$[D_\mu,D_\nu]\phi=F_{+\mu\nu}\phi-\phi F_{-\mu\nu}.\tag{A2}$$

Let us consider

$$\begin{aligned}4|F^+_{A_+}+\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2&=-2(F^+_{+\mu\nu}+\chi^+_{+\mu\nu}-\sigma^+_{\mu\nu}(\Phi\otimes\Phi^\dagger)_0)^2\\&=-2(F^+_{+\mu\nu})^2-2\{F^+_{+\mu\nu},\chi^+_{+\mu\nu}\}+2\{F^+_{+\mu\nu},\sigma^+_{\mu\nu}(\Phi\otimes\Phi^\dagger)_0\}\\&\quad-2(\chi^+_{+\mu\nu}-\sigma^+_{\mu\nu}(\Phi\otimes\Phi^\dagger)_0)^2.\end{aligned}\tag{A3}$$

This expression contains

$$(F^+_{+\mu\nu})^2=\tfrac{1}{4}(F_{+\mu\nu}+*F_{+\mu\nu})^2=\tfrac{1}{2}(F_{+\mu\nu})^2+\tfrac{1}{4}\{F_{+\mu\nu},*F_{+\mu\nu}\},\tag{A4a}$$

$$\{F^+_{+\mu\nu},\sigma^+_{\mu\nu}(\Phi\otimes\Phi^\dagger)_0\}=\frac{i}{2}\{F^+_{+12},\phi_1\phi_1^\dagger-\phi_2\phi_2^\dagger\}-\tfrac{1}{2}\{F^+_{+13},\phi_2\phi_1^\dagger-\phi_1\phi_2^\dagger\}$$

$$+\frac{i}{2}\{F^+_{+14},\phi_2\phi_1^\dagger+\phi_1\phi_2^\dagger\}, \tag{A4b}$$

$$-(\chi^+_{+\mu\nu}-\sigma^+_{\mu\nu}(\Phi\otimes\Phi^\dagger)_0)^2=2|\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2. \tag{A4c}$$

Similarly,

$$\begin{aligned}4|F^+_{A_-}+\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2&=-2(F^+_{-\mu\nu}+\chi^+_{-\mu\nu}-\sigma^+_{\mu\nu}(\Phi^*\otimes(\Phi^*)^\dagger)_0)^2\\&=-2(F^+_{-\mu\nu})^2-2\{F^+_{-\mu\nu},\chi^+_{-\mu\nu}\}\\&\quad+2\{F^+_{-\mu\nu},\sigma^+_{\mu\nu}(\Phi^*\otimes(\Phi^*)^\dagger)_0\}\\&\quad-2(\chi^+_{-\mu\nu}-\sigma^+_{\mu\nu}(\Phi^*\otimes(\Phi^*)^\dagger)_0)^2\end{aligned} \tag{A5}$$

with

$$(F^+_{-\mu\nu})^2=\tfrac{1}{2}(F_{-\mu\nu})^2+\tfrac{1}{4}\{F_{-\mu\nu},{}^*F_{-\mu\nu}\}, \tag{A6a}$$

$$\{F^+_{-\mu\nu},\sigma^+_{\mu\nu}(\Phi^*\otimes(\Phi^*)^\dagger)_0\}=-\frac{i}{2}\{F^+_{-12},\phi_1^\dagger\phi_1-\phi_2^\dagger\phi_2\}$$

$$+\tfrac{1}{2}\{F^+_{-13},\phi_1^\dagger\phi_2-\phi_2^\dagger\phi_1\}-\frac{i}{2}\{F^+_{-14},\phi_1^\dagger\phi_2+\phi_2^\dagger\phi_1\}, \tag{A6b}$$

$$-(\chi^+_{-\mu\nu}-\sigma^+_{\mu\nu}(\Phi^*\otimes(\Phi^*)^\dagger)_0)^2=2|\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2. \tag{A6c}$$

A lengthy but straightforward calculation exploiting (A1) and (A2) yields for $\frac{1}{2}|\mathcal{D}_{A_+,A_-}\Phi|^2$ the expression

$$\begin{aligned}\tfrac{1}{2}|\mathcal{D}_{A_+,A_-}\Phi|^2&=\tfrac{1}{2}|iD_3\phi_1-D_4\phi_1+iD_1\phi_2+D_2\phi_2|^2+\tfrac{1}{2}|iD_1\phi_1-D_2\phi_1-iD_3\phi_2-D_4\phi_2|^2\\&=-\frac{i}{2}\{F^+_{+12},\phi_1\phi_1^\dagger-\phi_2\phi_2^\dagger\}+\tfrac{1}{2}\{F^+_{+13},\phi_2\phi_1^\dagger-\phi_1\phi_2^\dagger\}\\&\quad-\frac{i}{2}\{F^+_{+14},\phi_2\phi_1^\dagger+\phi_1\phi_2^\dagger\}+\tfrac{1}{2}|D_{A_+,A_-}\Phi|^2-\nabla_{+\mu}\mathcal{J}_{+\mu}+C_+,\end{aligned} \tag{A7}$$

where

$$\mathcal{J}_{+\mu}=\frac{i}{4}(\epsilon_{\mu\nu12}+\epsilon_{\mu\nu34})\mathcal{J}^{(1)}_{+\nu}+\tfrac{1}{4}(\epsilon_{\mu\nu31}+\epsilon_{\mu\nu24})\mathcal{J}^{(2)}_{+\nu}+\frac{i}{4}(\epsilon_{\mu\nu23}+\epsilon_{\mu\nu14})\mathcal{J}^{(3)}_{+\nu} \tag{A8a}$$

and

$$\mathcal{J}^{(1)}_{+\nu}=\phi_1(D_\nu\phi_1)^\dagger-(D_\nu\phi_1)\phi_1^\dagger-\phi_2(D_\nu\phi_2)^\dagger+(D_\nu\phi_2)\phi_2^\dagger, \tag{A8b}$$

$$\mathcal{J}^{(2)}_{+\nu}=-\phi_1(D_\nu\phi_2)^\dagger+(D_\nu\phi_1)\phi_2^\dagger+\phi_2(D_\nu\phi_1)^\dagger-(D_\nu\phi_2)\phi_1^\dagger, \tag{A8c}$$

$$\mathcal{J}^{(3)}_{+\nu}=\phi_2(D_\nu\phi_1)^\dagger-(D_\nu\phi_2)\phi_1^\dagger+\phi_1(D_\nu\phi_2)^\dagger-(D_\nu\phi_1)\phi_2^\dagger. \tag{A8d}$$

The term C_+ is given by

$$C_+ = -i\phi_2 F^+_{-12}\phi_2^\dagger + i\phi_1 F^+_{-12}\phi_1^\dagger - \phi_2 F^+_{-13}\phi_1^\dagger + i\phi_2 F^+_{-14}\phi_1^\dagger + i\phi_1 F^+_{-14}\phi_2^\dagger + \phi_1 F^+_{-13}\phi_2^\dagger . \tag{A9}$$

In a similar manner, we also have

$$\begin{aligned}\tfrac{1}{2}|(\mathcal{D}_{A_+,A_-}\Phi)^\dagger|^2 = {}& \frac{i}{2}\{F^+_{-12}, \phi_1^\dagger\phi_1 - \phi_2^\dagger\phi_2\} - \tfrac{1}{2}\{F^+_{-13}, \phi_1^\dagger\phi_2 - \phi_2^\dagger\phi_1\} \\ & + \frac{i}{2}\{F^+_{-14}, \phi_1^\dagger\phi_2 + \phi_2^\dagger\phi_1\} + \tfrac{1}{2}|(D_{A_+,A_-}\Phi)^\dagger|^2 - \nabla_{-\mu}\mathcal{J}_{-\mu} + C_- ,\end{aligned} \tag{A10}$$

where

$$\mathcal{J}_{-\mu} = -\frac{i}{4}(\epsilon_{\mu\nu 12} + \epsilon_{\mu\nu 34})\mathcal{J}^{(1)}_{-\nu} - \tfrac{1}{4}(\epsilon_{\mu\nu 31} + \epsilon_{\mu\nu 24})\mathcal{J}^{(2)}_{-\nu} - \frac{i}{4}(\epsilon_{\mu\nu 23} + \epsilon_{\mu\nu 14})\mathcal{J}^{(3)}_{-\nu} \tag{A11a}$$

and

$$\mathcal{J}^{(1)}_{-\nu} = \phi_1^\dagger(D_\mu\phi_1) - (D_\mu\phi_1)^\dagger\phi_1 - \phi_2^\dagger(D_\mu\phi_2) + (D_\mu\phi_2)^\dagger\phi_2 , \tag{A11b}$$

$$\mathcal{J}^{(2)}_{-\nu} = -\phi_2^\dagger(D_\mu\phi_1) + (D_\mu\phi_2)^\dagger\phi_1 + \phi_1^\dagger(D_\mu\phi_2) - (D_\mu\phi_1)^\dagger\phi_2 , \tag{A11c}$$

$$\mathcal{J}^{(3)}_{-\nu} = \phi_1^\dagger(D_\mu\phi_2) - (D_\mu\phi_1)^\dagger\phi_2 + \phi_2^\dagger(D_\mu\phi_1) - (D_\mu\phi_2)^\dagger\phi_1 . \tag{A11d}$$

The term C_- is

$$C_- = i\phi_2^\dagger F^+_{+12}\phi_2 - i\phi_1^\dagger F^+_{+12}\phi_1 - \phi_2^\dagger F^+_{+13}\phi_1 - i\phi_2^\dagger F^+_{+14}\phi_1 - i\phi_1^\dagger F_{+14}\phi_2 + \phi_1^\dagger F_{+13}\phi_2 . \tag{A12}$$

Therefore, we discover that

$$\begin{aligned}&\tfrac{1}{2}|\mathcal{D}_{A_+,A_-}\Phi|^2 + \tfrac{1}{2}|(\mathcal{D}_{A_+,A_-}\Phi)^\dagger|^2 + 4|F^+_{A_+} + \chi^+_+ - \sigma^+(\Phi\otimes\Phi^\dagger)_0|^2 \\ &\quad + 4|F^+_{A_-} + \chi^+_- - \sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2 \\ &\quad = \tfrac{1}{2}|D_{A_+,A_-}\Phi|^2 + \tfrac{1}{2}|(D_{A_+,A_-}\Phi)^\dagger|^2 + 2|F_{A_+}|^2 + 2|F_{A_-}|^2 + 4|\chi^+_+ - \sigma^+(\Phi\otimes\Phi^\dagger)_0|^2 \\ &\quad + 4|\chi^+_- - \sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2 - \tfrac{1}{2}\{F_{+\mu\nu}, {*F_{+\mu\nu}}\} - 2\{F^+_{+\mu\nu}, \chi^+_{+\mu\nu}\} - \nabla_{+\mu}\mathcal{J}_{+\mu} \\ &\quad - \tfrac{1}{2}\{F_{-\mu\nu}, {*F_{-\mu\nu}}\} - 2\{F^+_{-\mu\nu}, \chi^+_{-\mu\nu}\} - \nabla_{-\mu}\mathcal{J}_{-\mu} + \frac{i}{2}\{F^+_{+12}, \phi_1\phi_1^\dagger - \phi_2\phi_2^\dagger\} \\ &\quad - \tfrac{1}{2}\{F^+_{+13}, \phi_2\phi_1^\dagger - \phi_1\phi_2^\dagger\} + \frac{i}{2}\{F^+_{+14}, \phi_2\phi_1^\dagger + \phi_1\phi_2^\dagger\} + C_+ - \frac{i}{2}\{F^+_{-12}, \phi_1^\dagger\phi_1 - \phi_2^\dagger\phi_2\} \\ &\quad + \tfrac{1}{2}\{F^+_{-13}, \phi_1^\dagger\phi_2 - \phi_2^\dagger\phi_1\} - \frac{i}{2}\{F^+_{-14}, \phi_1^\dagger\phi_2 + \phi_2^\dagger\phi_1\} + C_- .\end{aligned}$$

Now suppose that all operators entering this formula are of proper trace-class, e.g., $|\mathrm{Tr}\phi_{1,2}| < \infty$ and $|\mathrm{Tr}F_{\pm\mu\nu}| < \infty$. Then

$$\mathrm{Tr}\Big\{ \frac{i}{2}\{F^+_{+12},\phi_1\phi_1^\dagger-\phi_2\phi_2^\dagger\}-\tfrac{1}{2}\{F^+_{+13},\phi_2\phi_1^\dagger-\phi_1\phi_2^\dagger\}+\frac{i}{2}\{F^+_{+14},\phi_2\phi_1^\dagger+\phi_1\phi_2^\dagger\}+C_+$$
$$-\frac{i}{2}\{F^+_{-12},\phi_1^\dagger\phi_1-\phi_2^\dagger\phi_2\}+\tfrac{1}{2}\{F^+_{-13},\phi_1^\dagger\phi_2-\phi_2^\dagger\phi_1\}-\frac{i}{2}\{F^+_{-14},\phi_1^\dagger\phi_2+\phi_2^\dagger\phi_1\}+C_-\Big\}=0, \tag{A13}$$

since we can use the invariance of the trace under cyclic permutations. In fact, one can easily check that for each term in (A13) there exists a corresponding term having the opposite sign so that the trace is indeed zero.

Finally we obtain

$$\begin{aligned}
&\mathrm{Tr}\{\tfrac{1}{2}|\mathcal{D}_{A_+,A_-}\Phi|^2+\tfrac{1}{2}|(\mathcal{D}_{A_+,A_-}\Phi)^\dagger|^2+4|F^+_{A_+}+\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\\
&\quad+\ 4|F^+_{A_-}+\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2\}\\
&\quad=\mathrm{Tr}\{\tfrac{1}{2}|D_{A_+,A_-}\Phi|^2+\tfrac{1}{2}|(D_{A_+,A_-}\Phi)^\dagger|^2+2|F_{A_+}|^2+2|F_{A_-}|^2+4|\chi^+_+-\sigma^+(\Phi\otimes\Phi^\dagger)_0|^2\\
&\qquad+\ 4|\chi^+_--\sigma^+(\Phi^*\otimes(\Phi^*)^\dagger)_0|^2\}-\mathrm{Tr}\mathcal{T}+\frac{16\pi^2}{|\mathrm{Pf}(2\pi\theta)|}K_\chi,
\end{aligned} \tag{A14}$$

which is the desired result. Note that the choice $\phi_1=\phi$ and $\phi_2=0$ yields the expressions (3.49a) and (3.49b) for the currents $\mathcal{J}_{\pm\mu}$.

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Semiclassical asymptotics for the Maxwell–Dirac system

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(Received 5 May 2003; accepted 22 May 2003)

We study the coupled system of Maxwell and Dirac equations from a semiclassical point of view. A rigorous nonlinear WKB-analysis, locally in time, for solutions of (critical) order $O(\sqrt{\varepsilon})$ is performed, where the small semiclassical parameter $\varepsilon \ll 1$ denotes the microscopic/macroscopic scale ratio. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604455]

I. INTRODUCTION AND SCALING

The *Maxwell–Dirac system* (MD) is fundamental in the relativistic description of spin 1/2 particles. It represents the time-evolution of fast (relativistic) electrons and positrons within external and *self-consistent* generated electromagnetic fields:

$$i\hbar\,\partial_s\Psi=\sum_{k=1}^{3}\alpha^k(-i\hbar c\,\partial_k-e(A_k+A_k^{\mathrm{ext}}))\Psi+e(V+V^{\mathrm{ext}})\Psi+mc^2\beta\Psi,$$
$$\left(\frac{1}{c^2}\partial_s^2-\Delta\right)V=\frac{1}{4\pi\epsilon_0}\rho,\quad \left(\frac{1}{c^2}\partial_s^2-\Delta\right)A=\frac{1}{4\pi c\,\epsilon_0}j, \tag{1.1}$$

where the *particle-* and *current-densities* are defined by

$$\rho:=e|\Psi|^2,\quad j_k:=e\langle\Psi,\alpha^k\Psi\rangle,\quad k=1,2,3. \tag{1.2}$$

Here, $\Psi=\Psi(s,y)\in\mathbb{C}^4$ is the 4-vector of the *spinor field*, normalized s.t.,

$$\int_{\mathbb{R}^3}|\Psi(s,y)|^2\,dy=1, \tag{1.3}$$

with s, $y\equiv(y_1,y_2,y_3)$, denoting the time—resp. spatial coordinates in *Minkowski space*. Further, $V^{(\mathrm{ext})}=V^{(\mathrm{ext})}(s,y)\in\mathbb{R}$ is the *self-consistent* resp. *external electric potential* and $A_k^{(\mathrm{ext})}=A_k^{(\mathrm{ext})}(t,x)\in\mathbb{R}$, the corresponding *magnetic potential*, with $A=(A_1,A_2,A_3)$. In the following, the usual scalar-product for vectors $X,Y\in\mathbb{C}^4$ will be denoted by $\langle X,Y\rangle$ and we shall also write $|X|^2:=\langle X,X\rangle$. The so-called *Dirac matrices* β,α^k, $k=1,2,3$, are explicitly given by

$$\beta:=\begin{pmatrix}\mathbf{1}_2 & 0\\ 0 & -\mathbf{1}_2\end{pmatrix},\quad \alpha^k:=\begin{pmatrix}0 & \sigma^k\\ \sigma^k & 0\end{pmatrix}, \tag{1.4}$$

with $\mathbf{1}_2$, the 2×2 identity matrix and σ^k the 2×2 *Pauli matrices*, i.e.,

$$\sigma^1:=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma^2:=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma^3:=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.5}$$

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Hence, α^k, β are *Hermitian* and moreover one easily checks that the following identities hold for $k,l=1,2,3$:

$$\alpha^k\alpha^l+\alpha^l\alpha^k=2\delta_{kl},$$
$$\alpha^k\beta+\beta\alpha^k=0. \tag{1.6}$$

Finally, the appearing physical constants are the normalized Planck constant $\hbar$, the speed of light c, the permittivity of the vacuum ϵ_0, the particle mass m and the charge e.

Additionally to (1.1), we impose the *Lorentz gauge condition*,

$$\frac{1}{c}\partial_s V(s,y)+\operatorname{div} A(s,y)=0, \tag{1.7}$$

for the initial potentials $V(0,y)$ and $A(0,y)$. The gauge is henceforth conserved during the time-evolution. It ensures that the corresponding *electromagnetic fields* E, B are uniquely determined by

$$E(s,y):=-\frac{1}{c}\partial_s A(s,y)-\nabla V(s,y), \quad B(s,y):=\operatorname{curl} A(s,y). \tag{1.8}$$

The MD equations are the underlying field equations of relativistic *quantum electro-dynamics*, cf. Schwabl (1999), where one considers the system within the formalism of *second quantization*. Nevertheless, in order to obtain a deeper understanding for the interaction of matter and radiation, there is a growing interest in the MD system also for classical fields, since one can expect at least qualitative results; cf. Esteban and Sere (2002). From the mathematical point of view, the strongly nonlinear MD system poses a hard problem in the study of PDE's arising from quantum physics. Well posedness and the existence of solutions on all of $\mathbb{R}^3_y$ but only locally in time, has been proved almost forty years ago in Gross (1996). On the other hand, only partial results (i.e., for small initial data) have been obtained in the quest of global-in-time solutions [Chadam (1973), Georgiev (1991), Flato, Simon, and Tafflin (year)] let alone the study of other qualitative features of this system; cf. [Booth and Radford (1997), Esteban, Georgiev, and Sere (1996), Esteban and Sere (2002), Chadam and Glassey (1976)]. However, there are some recent and quite complete results concerning the *nonrelativistic limit* of the MD equations; cf. Bechouche, Mauser, and Selberg (year) also Masmoudi and Mauser (2001).

In this paper, we shall analyze the MD system in a *semiclassical* regime. To do so, we first rewrite the equations such that there remains only one (positive) *dimensionless* parameter,

$$\delta=\frac{4\pi\hbar c\varepsilon_0}{e^2}, \tag{1.9}$$

which is obtained by replacing $y\to y/\overline{y}$, $s\to s/\overline{s}$ and $\Psi(s,y)\to\overline{y}^{-3/2}\Psi(s/\overline{s},y/\overline{y})$, in order to maintain the normalization condition (1.3), with

$$c\overline{s}=\overline{y} \text{ and } \overline{y}=\frac{e^2}{mc^2\varepsilon_0}. \tag{1.10}$$

Here, we also replaced both, the external and the self-consistent potentials, by $A^{(\mathrm{ext})}(s,y)\to\lambda A^{(\mathrm{ext})}(s/\overline{s},y/\overline{y})$ and $V^{(\mathrm{ext})}(s,y)\to\kappa V^{(\mathrm{ext})}(s/\overline{s},y/\overline{y})$, with $\kappa=c\lambda$ and $\lambda=mc/e$. We assume for the following that $A^{\mathrm{ext}}, V^{\mathrm{ext}}$ are of $O(1)$ in these units. In summary, we obtain the MD system in dimensionless form:

$$i\delta\partial_s\Psi=\sum_{k=1}^{3}\alpha^k(-i\delta\partial_k-(A_k+A_k^{\mathrm{ext}}))\Psi+(V+V^{\mathrm{ext}})\Psi+\beta\Psi,$$
$$\Box V=\rho,\quad \Box A=j, \tag{1.11}$$

where from now on $\Box:=\partial_s^2-\Delta$. In (1.11), s,y represent the *microscopic* time and length scales. Note that in general, δ can*not* be considered as a *small* parameter. For example, in the case of electrons δ is indeed the inverse of the *fine structure constant*, i.e., $\delta\approx 137$. Hence, semiclassical asymptotics in δ, i.e., on (1.11) directly, only make sense for highly charged and consequently heavy particles.

Therefore, we need to rescale the system (1.11) such that the time-evolution can be considered semiclassical, independent of the precise physical properties of the particles. We can suppose that the given external electromagnetic potentials are slowly varying w.r.t. to the microscopic scales, i.e. $V^{\mathrm{ext}}=V^{\mathrm{ext}}(s\varepsilon/\delta,y\varepsilon/\delta)$ and likewise $A^{\mathrm{ext}}=A^{\mathrm{ext}}(s\varepsilon/\delta,y\varepsilon/\delta)$, where from now on ε denotes the small *semiclassical parameter*. Here, the δ is included in the scaling in order to eliminate it from the resulting equation. Hence, observing the evolution on macroscopic scales we are led to

$$y=\frac{\delta}{\varepsilon}x,\quad s=\frac{\delta}{\varepsilon}t. \tag{1.12}$$

Moreover, we want the coefficients of all nonlinearities to be $O(1)$, i.e., they should *not* carry a positive power of ε. It turns out that there exists solutions ψ^ε, which obey this requirement. If we set

$$\frac{\delta}{\varepsilon}\Psi(s,y)=\psi^\varepsilon(t,x), \tag{1.13}$$

then the normalization condition for (1.3) gives

$$\int_{\mathbb{R}^3}|\psi^\varepsilon(t,x)|^2\,dy=\frac{\varepsilon}{\delta}\int_{\mathbb{R}^3}|\Psi(s,y)|^2\,dx=\frac{\varepsilon}{\delta}. \tag{1.14}$$

This implies that we need to look for solutions ψ^ε s.t.,

$$\psi^\varepsilon\sim O(\sqrt{\varepsilon}), \tag{1.15}$$

assuming, as mentioned above, that $\delta\sim O(1)$. We therefore end up with the following *semiclassical scaled* MD system:

$$i\varepsilon\partial_t\psi^\varepsilon=\sum_{k=1}^{3}\alpha^k(-i\varepsilon\partial_k-(A_k^\varepsilon+A^{\mathrm{ext}}))\psi^\varepsilon+\beta\psi^\varepsilon+(V^\varepsilon+V^{\mathrm{ext}})\psi^\varepsilon, \tag{1.16}$$

$$\Box V^\varepsilon=|\psi^\varepsilon|^2, \tag{1.17}$$

$$\Box A_k^\varepsilon=\langle\psi^\varepsilon,\alpha^k\psi^\varepsilon\rangle,\quad k=1,2,3, \tag{1.18}$$

subject to *Cauchy initial data*:

$$\psi^\varepsilon|_{t=0}=\psi_I^\varepsilon(x)\sim O(\sqrt{\varepsilon}),$$
$$V^\varepsilon|_{t=0}=V_I^\varepsilon(x),\quad \partial_tV^\varepsilon|_{t=0}=\tilde{V}_I^\varepsilon(x), \tag{1.19}$$
$$A^\varepsilon|_{t=0}=A_I^\varepsilon(x),\quad \partial_tA^\varepsilon|_{t=0}=\tilde{A}_I^\varepsilon(x).$$

For this nonlinear system, we want to find an asymptotic description of $\psi^\varepsilon \sim O(\sqrt{\varepsilon})$ as $\varepsilon \to 0$, i.e., a semiclassical description. Note that, *equivalently*, one could consider asymptotic solutions of the form

$$\Phi^\varepsilon(t,x) := \frac{1}{\sqrt{\varepsilon}} \psi^\varepsilon(t,x) \sim O(1), \tag{1.20}$$

which do not vanish in the limit $\varepsilon \to 0$ and which again satisfy the semiclassical scaled DM system, modified by the fact that the right hand sides of (1.17), (1.18) are multiplied by an additional factor ε. This illustrates the fact that we are dealing with a *small coupling limit*. We further stress that in our scaling the mass is $O(1)$ and *fixed* as $\varepsilon \to 0$, which is different from the otherwise similar scaling used in Kunze and Spohn, where a classical mechanics analogue of the MD system has been studied. The (rigorous) analysis of semiclassical asymptotics has a long tradition in quantum mechanics, the most common technique being the so called *WKB-method*. Quite recently, a semiclassical approach to the *linear* Dirac equation was taken in Bolte and Keppeler (1999) and also, using *Wigner measures*, in Gérard, Markowich, Mauser, Poupaud (1997) and Spohn (2000). For a broader introduction on linear techniques and results, we refer to Maslov and Feydoriuk (1981), Robert (1998), Sparber, Markowich, and Mauser (2003) and the references given therein. Nonlinear extensions of the WKB-method can be found, for example, in Georgiev (1991) and Grenier (1998), where *scalar-valued* semilinear Schrödinger equations are analyzed. We remark that the case of the nonlinear Dirac 4-system introduces significant new difficulties in the WKB-analysis; some of them are already present in the linear setting.

Mathematically, our approach is inspired by techniques developed in Donat and Rauch (1997), which sometimes go under the name *weakly nonlinear geometrical optics*. Due to the appearance of the small parameter ε in front of each derivative in (1.16) we are in the regime of so-called *dispersive* weakly nonlinear geometrical optics, which differs in several aspects from the nondispersive one. We remark that the latter case is much better studied in the so far existing literature and we refer to Joly, Metivier, and Rauch (1999), for a recent review.

To be more precise, we shall seek a local-in-time solution of (1.16), which asymptotically takes the following form:

$$\begin{aligned} \psi^\varepsilon(t,x) &= \sqrt{\varepsilon}\, u^\varepsilon(t,x,\phi(t,x)/\varepsilon), \\ u^\varepsilon(t,x,\theta) &\sim \sum_{j=0}^{\infty} \varepsilon^{j/2} u_j(t,x,\theta). \end{aligned} \tag{1.21}$$

Here, all the $u_j(t,x,\theta) \in \mathbb{C}^4$ being 2π-periodic w.r.t. $\theta \in \mathbb{R}$. Due to the factor $\varepsilon^{1/2}$, we call them *small semiclassical approximate solutions*, or *small WKB-solutions*. As expected, there are two modes of the phase function $\phi_\pm$, which satisfy the (free) relativistic Hamilton–Jacobi equation, corresponding to positive, resp., negative energies and, of course, convergence of the expansion (1.21) can only hold on a time interval, which corresponds to the existence of smooth solutions $\phi_\pm$. In weakly nonlinear geometrical optics, the homogeneity of the nonlinearity determines the required order of smallness of the asymptotic solution and, as we shall see, the factor $\sqrt{\varepsilon}$ precisely fits with the cubic nonlinearities in (1.16). We will show that for this particular scale we obtain, on the one hand, *independent* propagation of the electronic, resp., positronic phase function $\phi_\pm$ and, the other hand, *nonlinear interaction* of the corresponding principal amplitudes $u_{0,\pm}$.

In other words, we study solutions on the threshold of *adiabatic decoupling*, a phenomena which is already well known in the linear case; cf. Panati, Sohn, and Teufel (19XX). In particular, the importance of the $O(\sqrt{\varepsilon})$-scale for the (linear) Dirac equation is stressed in Fermanian-Kammerer (2003), where one can also find a detailed description of the energy-transfer between electrons and positrons in terms of *two-scale* Wigner measures. These results, together with ours, suggest that if one wants to obtain a semiclassical $O(1)$-approximation in the strongly coupled regime, one needs to take into account simultaneous scales of order ε and $O(\sqrt{\varepsilon})$. These

asymptotic solutions are then appropriate for heavily charged particles. We finally remark, that in the very recent paper [Jeanne (2002)], coupled Gauge-fields are studied from a similar point of view as in our work.

This paper is organized as follows: We collect some preliminaries in Sec. II, then we shall determine the critical exponent and the corresponding eikonal equation of the approximate WKB-type solution in Sec. III. The corresponding ε-oscillations introduced by the nonlinearity are determined in Sec. IV and the nonlinear transport of the approximation along the rays of geometrical optics is obtained in Sec. V. Finally, in Sec. VI we shall prove that there exists a (local-in-time) solution of the MD system which stays close to the approximation and we also collect some further qualitative results.

II. PRELIMINARIES

In the following, we will assume that no external electromagnetic fields are present:

$$V^{\mathrm{ext}}(t,x)\equiv 0, \quad A^{\mathrm{ext}}(t,x)\equiv 0. \tag{2.1}$$

Moreover, we assume that at $t=0$ we have

$$V_I^\varepsilon(x)=\tilde{V}_I^\varepsilon(x)\equiv 0, \quad A_I^\varepsilon(x)=\tilde{A}_I^\varepsilon(x)\equiv 0. \tag{2.2}$$

Neither of these assumptions changes the following analysis significantly. They are only imposed for the sake of simplicity. Further note that the DM system is time-reversible, but w.r.o.g. we shall consider positive times only in the sequel.

Using the fundamental solution of the wave equation in dimension $d=3$ and for times $t>0$, we find the following expression for V, called *the retarded potential*:

$$V^\varepsilon[\psi^\varepsilon](t,x)=\frac{1}{4\pi}\int_{|x-y|\leqslant t}\frac{|\psi^\varepsilon(t-|x-y|,y)|^2}{|x-y|}\,dy=:\ \mathcal{G}_r(t,x)*|\psi^\varepsilon(t,x)|^2, \tag{2.3}$$

where $*$ denotes the convolution w.r.t. (t,x) and

$$\mathcal{G}_r(t,x):=\frac{\Theta(t)}{4\pi|x|}\,\delta(t-|x|). \tag{2.4}$$

Likewise, A^ε can be written as

$$A^\varepsilon[\psi^\varepsilon](t,x)=\mathcal{G}_r(t,x)*\langle\psi^\varepsilon(t,x),\alpha^k\psi^\varepsilon(t,x)\rangle. \tag{2.5}$$

If assumption (2.2) is dropped, we would have to additionally include the homogeneous solution of the wave equation in (2.3), (2.5).

Using these representations, we shall rewrite (1.16)–(1.18) in the form of a *semilinear Dirac equation*:

$$\begin{aligned} i\varepsilon\partial_t\psi^\varepsilon-\mathcal{D}_A^\varepsilon(t,x,\varepsilon D_x)\psi^\varepsilon&=\ 0, x\in\mathbb{R}^3,\ \ t>0,\\ \psi^\varepsilon|_{t=0}&=\ \psi_I^\varepsilon(x), \end{aligned} \tag{2.6}$$

where $\mathcal{D}_A^\varepsilon$ is a *matrix-valued* differential operator ($D_x:=-i\nabla$). The corresponding ε-*dependent* symbol is given by

$$\mathcal{D}_A^\varepsilon(t,x,\xi)=\alpha\cdot(\xi-A^\varepsilon[\psi^\varepsilon](t,x))+\beta+V^\varepsilon[\psi^\varepsilon](t,x), \tag{2.7}$$

where $x,\xi,\in\mathbb{R}^3, t\in\mathbb{R}$. Here and in the following we use the notation

$$\alpha\cdot\xi := \sum_{k=1}^{3} \alpha^k \xi_k . \tag{2.8}$$

Note that in the nonlinear equation (2.6), the potentials $A^\varepsilon[\psi^\varepsilon]$, $V^\varepsilon[\psi^\varepsilon]$ depend *non-locally* on ψ^ε, as indicated by the bracket-notation.

Multiplying (2.6) with ψ^ε and taking imaginary parts, we obtain the usual conservation law for $\|\psi^\varepsilon(t,x)\|_2$, hence the *conservation of charge*:

$$\int_{\mathbb{R}^3} \langle \psi^\varepsilon(t,x), \psi^\varepsilon(t,x)\rangle \, dx = \|\psi^\varepsilon(t,x)\|_2^2 = \text{const.} \tag{2.9}$$

The *free Dirac operator* will be denoted by

$$\mathcal{D}(\varepsilon D_x)\psi^\varepsilon := -i\varepsilon(\alpha\cdot\nabla)\psi^\varepsilon + \beta\psi^\varepsilon, \tag{2.10}$$

with the symbol

$$\mathcal{D}(\xi) = \alpha\cdot\xi + \beta. \tag{2.11}$$

This 4×4 matrix has two different eigenvalues $h_\pm(\xi)$ of multiplicity 2 each:

$$h_\pm(\xi) := \pm\lambda(\xi), \quad \xi\in\mathbb{R}^3, \tag{2.12}$$

where

$$\lambda(\xi) := \sqrt{|\xi|^2+1}, \quad \xi\in\mathbb{R}^3. \tag{2.13}$$

As expected, the eigenvalues $h_\pm(\xi)$ are nothing but the *free Hamiltonian* for a *relativistic* particle. The positive, resp., negative sign in (2.13) corresponds to *electrons*, resp., *positrons*. By straightforward calculations we obtain the following lemma.

Lemma 2.1: The spectral projectors $\Pi_\pm(\xi):\mathbb{C}^4\to\mathbb{C}^4$, *associated to* $h_\pm(\xi)$ *are given by*

$$\Pi_\pm(\xi) := \frac{1}{2}\left(\mathrm{id}_4 \pm \frac{1}{\lambda(\xi)}\mathcal{D}(\xi)\right), \quad \Pi_\pm\Pi_\mp \equiv 0. \tag{2.14}$$

The matrix-valued symbol $\mathcal{D}(\xi)$ can therefore be decomposed into its positive and negative energy part in the following way:

$$\mathcal{D}(\xi) = h_+(\xi)\Pi_+(\xi) + h_-(\xi)\Pi_-(\xi). \tag{2.15}$$

We notice that

$$h_\pm(-\xi) = h_\pm(\xi), \quad \text{whereas} \quad \Pi_\pm(-\xi) = \Pi_\mp(\xi). \tag{2.16}$$

For later purposes, we also define the following definition.

Definition 2.2: The *partial inverse* $\Lambda_\pm(\xi):\mathbb{C}^4\to\mathbb{C}^4$, associated to $\Pi_\pm(\xi)$, is given by

$$\Lambda_\pm(\xi)\Pi_\pm(\xi) = 0, \quad \Lambda_\pm(\xi)\mathcal{D}(\xi)X = (\mathrm{id}_4 - \Pi_\pm(\xi))X, \quad \forall X\in\mathbb{C}^4. \tag{2.17}$$

Finally, we recall the definition of *asymptotic equivalences*.

Definition 2.3: Let $\mathcal{O}\subseteq\mathbb{R}^n$, $n\geqslant 1$, be an open set, $a_j(y)\in C^\infty(\mathbb{R}^n;\mathbb{C}^n)$ and $a^\varepsilon\in C^\infty(]0,\varepsilon_0[\times\mathbb{R}^n;\mathbb{C}^n)$. Then we say that a^ε is asymptotically equivalent to the formal sum $\Sigma_{j=0}^\infty \varepsilon^j a_j$ and write

$$a^\varepsilon(y) \sim \sum_{j=0}^{\infty} \varepsilon^j a_j(y), \tag{2.18}$$

if for every $m>0$, every multiindex σ and every compact subset $\mathcal{K}\subset\mathcal{O}$, there exists a $C_{m,\sigma}>0$, such that

$$\sup_{\mathcal{K}}\left|\partial_y^\sigma\left(a^\varepsilon(y)-\sum_{j=0}^{m}\varepsilon^j a_j(y)\right)\right|\leqslant C_{m,\sigma}\varepsilon^m. \tag{2.19}$$

III. GENERALIZED WKB–ANSATZ AND THE EIKONAL EQUATION

At first we will show that the desired $O(\sqrt{\varepsilon})$-asymptotics for the spinor field fits into the framework of weakly nonlinear (dispersive) geometrical optics, as introduced in Donat and Rauch (1997), for nonlinear hyperbolic systems.

We plug the following *generalized WKB–Ansatz* into Eq. (2.6):

$$\psi^\varepsilon(t,x)=\varepsilon^p\,u^\varepsilon(t,x,\phi(t,x)/\varepsilon),$$

$$u^\varepsilon(t,x,\theta)\sim\sum_{j=0}^{\infty}\varepsilon^{jp}u_j(t,x,\theta), \tag{3.1}$$

where the functions $u_j(t,x,\theta)\in\mathbb{C}^4$ are assumed to be sufficiently smooth and 2π-periodic w.r.t. $\theta\in\mathbb{R}$. This gives

$$\begin{aligned}0=&\ i\varepsilon^{p+1}\partial_t u^\varepsilon-\varepsilon^p\,\mathcal{D}_A^\varepsilon(t,x,\varepsilon D_x)u^\varepsilon\\ =&\ i\varepsilon^{p+1}(\partial_t u^\varepsilon+(\alpha\cdot\nabla)u^\varepsilon)-\varepsilon^p\beta u^\varepsilon+i\varepsilon^p\,(\partial_t\phi+(\alpha\cdot\nabla\phi))\partial_\theta u^\varepsilon+\varepsilon^{3p}\mathcal{N}^\varepsilon[u^\varepsilon],\end{aligned} \tag{3.2}$$

with a *nonlinearity*, $\mathcal{N}^\varepsilon:\mathbb{C}^4\to\mathbb{C}^4$, defined by

$$\mathcal{N}^\varepsilon[u^\varepsilon]:=((\alpha\cdot A^\varepsilon[u^\varepsilon])-V^\varepsilon[u^\varepsilon])u^\varepsilon. \tag{3.3}$$

The strategy is now to expand the right-hand side of (3.2) as

$$\varepsilon^p\sum_{j=0}^{\infty}\varepsilon^{jp}R_j(t,x) \tag{3.4}$$

and choose the coefficients u_j of (3.1) in such a way, that $R_j(t,x)\equiv 0$, $\forall j\in\mathbb{N}$.

It is important to note that the first term on the right hand side of (3.2) is of order ε^{p+1}, whereas the second and the third are $\sim O(\varepsilon^p)$. Since $A^\varepsilon[u^\varepsilon]$, $V^\varepsilon[u^\varepsilon]$ are of order ε^{2p}, by Eqs. (2.3), (2.5), the function $\mathcal{N}^\varepsilon[u^\varepsilon]$ is of order ε^{3p}. This nonlinear term is supposed to be *small*, more precisely, it should not enter into the equation for R_0, describing terms of order $O(\varepsilon^p)$, but rather into expressions of $O(\varepsilon^{p+1})$. Thus we are led to the following *normalization condition:*

$$3p=p+1, \tag{3.5}$$

implying $p=1/2$. With this normalization we have $u^\varepsilon\sim O(\varepsilon^{1/2})$ (just as required by the scaling presented in the introduction), whereas the nonlinear term satisfies $\mathcal{N}^\varepsilon[u^\varepsilon]\sim O(\varepsilon^{3/2})$.

Remark 3.1: The choice $p=1/2$ gives the critical exponent in the sense that for amplitudes $O(\varepsilon^{1/2})$ one can prove simultaneously the existence of the approximate smooth solution for times $t=O(1)$, i.e., on a time-scale *independent* of ε, and nontrivial nonlinear behavior in the principal term of the approximation; cf. Donat and Rauch (1997); and Joly, Metivier, and Rauch (1999).

Setting $R_0(t,x)=0$ yields

$$i(\partial_t\phi+(\alpha\cdot\nabla\phi))\partial_\theta u_0-\beta u_0=0. \tag{3.6}$$

Since $u_j\in C^\infty(\mathbb{R}^4\times\mathbb{S}^1;\mathbb{C}^4)$ it can be *Fourier-expanded* w.r.t. θ,

$$u_0(t,x,\theta)=\sum_{m\in\mathbb{Z}} u_{0,m}(t,x)e^{im\theta}. \tag{3.7}$$

By this procedure, we find the following equation for the coefficients $u_{0,m}$:

$$L(m\,d\phi(t,x))u_{0,m}:=(m\,\partial_t\phi+\mathcal{D}(m\nabla\phi))u_{0,m}=0, \tag{3.8}$$

where $\mathcal{D}(\nabla(m\phi))$ is the 4×4 symbol matrix of the free Dirac operator evaluated at $\xi=(m\phi(t,x))$. In order to have a nontrivial solution $u_{0,m}\neq0$ we impose the condition that there exists an open set $\Omega\subseteq\mathbb{R}^{1+3}$, having a nontrivial intersection with $\{t=0\}$, s.t.,

$$\det L(m\,d\phi(t,x))=0,\quad \forall(t,x)\in\Omega\subseteq\mathbb{R}^{1+3}. \tag{3.9}$$

Using Eqs. (2.12), (2.15), this is equivalent to

$$(m\,\partial_t\phi)^2-|m\nabla\phi|^2=1,\quad \forall(t,x)\in\Omega\subseteq\mathbb{R}^{1+3}. \tag{3.10}$$

Thus, for $m=\pm1$, the phase function ϕ satisfies (in Ω) the *eikonal equation* for the *Klein–Gordon operator,* i.e.,

$$(\partial_t\phi)^2-|\nabla\phi|^2=1,\quad \forall(t,x)\in\Omega\subseteq\mathbb{R}^{1+3}. \tag{3.11}$$

Indeed, it is easy to see that the choices $m=\pm1$ are the only possibilities, since Eq. (3.11) gives

$$(m\partial_t\phi)^2-|m\nabla\phi|^2-1=(m^2-1)((\partial_t\phi)^2-|\nabla\phi|^2)=m^2-1, \tag{3.12}$$

which is different from zero for all $m\neq\pm1$. Hence, in the Fourier-series (3.7), there appear only two nontrivial *harmonics,* which are associated to the eikonal equation (3.11): namely $\exp(i\phi(t,x)/\varepsilon)$, for $m=1$ and $\exp(-i\phi(t,x)/\varepsilon)$, for $m=-1$.

For $m=\pm1$ the equation (3.11) is fulfilled by two possible ϕ's, obtained from

$$\partial_t\phi_\pm(t,x)=h_\pm(\nabla\phi_\pm(t,x))\equiv\pm\sqrt{|\nabla\phi_\pm(t,x)|^2+1}=0. \tag{3.13}$$

This is the *Hamilton–Jacobi equation* for free relativistic particles. The following lemma guarantees the existence and uniqueness of smooth solutions, where from now on, we shall denote by $D^2f(x)$, the Hessian of a given function $f:\mathbb{R}^3\to\mathbb{R}$.

Lemma 3.2: Given $\phi_I\in C^\infty(\mathbb{R}^3;\mathbb{R})$, s.t. $\|D^2\phi_I(x)\|\leqslant C$, there exist $T_\pm>0$ and uniquely determined functions $\phi_\pm\in C^\infty(\Omega_\pm;\mathbb{R})$, where $\Omega_\pm:=[0,T_\pm)\times\mathbb{R}^3$, s.t.

$$\begin{aligned}\partial_t\phi_\pm(t,x)&=h_\pm(\nabla\phi_\pm(t,x)),\quad \forall(t,x)\in\Omega_\pm,\\ \phi|_{t=0}&=\phi_I(x).\end{aligned} \tag{3.14}$$

Proof: We only proof the assertion for ϕ_+, since the other case is completely analogous. The initial value problem is *noncharacteristic* everywhere, since

$$\partial_t\phi_+(0,x)=\sqrt{|\nabla\phi_+(0,x)|^2+1}\ \neq0,\ \forall x\in\mathbb{R}^3. \tag{3.15}$$

Thus, $\partial_t\phi_+(0,x)$ can be obtained from the initial data $\phi_+(0,x)=\phi_I(x)\in C_b^\infty(\mathbb{R}^3)$ at each point $x\in\mathbb{R}^3$. Standard PDE theory then guarantees the existence of a unique smooth solution $\phi_+\in C^\infty(\Omega_+;\mathbb{R})$, as long as

$$1-t\,\|D^2h_+(\nabla\phi_I)\|\,\|D^2\phi_I\|\neq0. \tag{3.16}$$

Since $D^2H(\xi)$ is uniformly bounded, this condition holds by assumption and the assertion is proved. □

Remark 3.3: The assumption in Lemma 3.2 can be relaxed to $\phi_I \in C^\infty(\mathbb{R}^3;\mathbb{R})$. In this case, however, one cannot guarantee the existence of a smooth solution ϕ in a space–time slab, but only in some open set $\mathcal{O}\subset\mathbb{R}^{1+3}$. In the following, this would lead to some technical difficulties, which we want to avoid, though, the whole procedure can be generalized to that case.

By Eq. (3.13), we have

$$-\phi_\pm(t,x)=\phi_\mp(t,x), \tag{3.17}$$

assuming that it holds initially at $\{t=0\}\subset\Omega$. In the following, we therefore consider only the solution to (3.13) with a positive sign in front of the square root and write for it $\phi(t,x)\equiv\phi_+(t,x)$. Also, we henceforth denote by $\Omega:=[0,T_+)\times\mathbb{R}^3$ the slab, in which the existence of a smooth function ϕ is guaranteed. This we can do w.r.o.g., as will become clear in a moment:

Since for $\phi\equiv\phi_+$ it holds that $\partial_t\phi-h_+(\nabla\phi)=0$, Eq. (3.8) implies the following *polarization conditions*, locally for all $(t,x)\in\Omega$:

$$(\Pi_-(\nabla\phi)u_{0,+1})(t,x)=0 \Leftrightarrow (\Pi_+(\nabla\phi)u_{0,+1})(t,x)=u_{0,+1}(t,x). \tag{3.18}$$

Likewise, we get

$$(\Pi_+(\nabla\phi)u_{0,-1})(t,x)=0 \Leftrightarrow (\Pi_-(\nabla\phi)u_{0,-1})(t,x)=u_{0,-1}(t,x). \tag{3.19}$$

One easily checks, using (2.16) and (3.17), that the conditions obtained with the choice $\phi=\phi_-$, are *equivalent* to (3.18), (3.19). Thus, Eq. (3.8) indeed carries two degrees of freedom for the phase, given by $\pm\phi$ (or equivalently ϕ_+, ϕ_-). The amplitudes are then rigidly linked, by (3.18), (3.19).

In summary, we find that the *principal term* $u_0(t,x,\theta)$ in our asymptotic description is given by

$$u_0(t,x,\phi(t,x)/\varepsilon):=u_{0,+1}(t,x)e^{i\phi(t,x)/\varepsilon}+u_{0,-1}(t,x)e^{-i\phi(t,x)/\varepsilon}, \tag{3.20}$$

where the amplitudes are polarized according to (3.18), (3.19). From now on we shall use the simplified notation $u_{0,\pm1}=u_{0,\pm}$.

IV. OSCILLATIONS OF THE NONLINEARITY

Let us determine the response of the wave equations (1.17), (1.18) to r.h.s. source terms induced by functions of the form (3.20):

To this end, we calculate:

$$|u_0(t,x,\phi(t,x)/\varepsilon)|^2=|u_{0,+}(t,x)|^2+|u_{0,-}(t,x)|^2. \tag{4.1}$$

The terms, that mix the electronic and positronic components cancel, since $\Pi_\pm$ is Hermitian and $\Pi_\pm\Pi_\mp\equiv0$. Hence, we get from (2.3) (at least formally), that the scalar potential V generated by the principal term u_0, is simply given by

$$V[u_0]=\mathcal{G}_r(t,x)*(|u_{0,+}(t,x)|^2+|u_{0,-}(t,x)|^2). \tag{4.2}$$

In order to calculate the magnetic potential corresponding to u_0, we first note that, by definition, we have the following identity:

$$\Pi_\pm(\xi)(\alpha\cdot\xi+\beta)=h_\pm(\xi)\ \Pi_\pm(\xi). \tag{4.3}$$

Differentiating w.r.t. ξ_k and multiplying (from the right) with $\Pi_\pm(\xi)$ gives

$$\Pi_\pm(\xi)\alpha^k\Pi_\pm(\xi)=\Pi_\pm(\xi)(\partial_{\xi_k}h_\pm(\xi))\Pi_\pm(\xi)=\pm\frac{\xi_k}{\sqrt{|\xi|^2+1}}\ \Pi_\pm(\xi), \tag{4.4}$$

since $\Pi_{\pm}^2(\xi)=\Pi_{\pm}(\xi)$. The expression

$$\omega_{\pm}(\xi):=\nabla_{\xi}h_{\pm}(\xi)=\pm\frac{\xi}{\lambda(\xi)}, \tag{4.5}$$

is called the electronic, resp., positronic *group velocity*, $\omega_{\pm}\in C^{\infty}(\mathbb{R}^3;\mathbb{R}^3)$. Using this definition, we obtain for $k=1,2,3$:

$$\begin{aligned}\langle u_0(t,x,\phi(t,x)/\varepsilon),\alpha^k u_0(t,x,\phi(t,x)/\varepsilon)\rangle&\\ =\omega_{+,k}(\nabla\phi(t,x))|u_{0,+}(t,x)|^2+\omega_{-,k}(\nabla\phi(t,x))|u_{0,-}(t,x)|^2&\\ +\langle u_{0,+}(t,x),\alpha^k u_{0,-}(t,x)\rangle e^{-i2\phi(t,x)/\varepsilon}+\langle u_{0,-}(t,x),\alpha^k u_{0,+}(t,x)\rangle e^{i2\phi(t,x)/\varepsilon}.&\end{aligned} \tag{4.6}$$

The oscillating terms are usually called the *Zitterbewegung* of the Dirac-current, cf. Schwabl (1999), p. 195. The fact that the current-density corresponding to u_0 carries ε-oscillations is in sharp contrast to the WKB-approach for Schrödinger-type problems; see, e.g., Gérard (1992) and Grenier (1998).

The Zitterbewgung may cause severe problems since *a priori* one cannot exclude the possibility of *resonant interactions* between the principal term u_0 and the magnetic potential $A^{\varepsilon}[u_0]$ obtained from (1.18) with the r.h.s. given by (4.6). If this happens to be the case, our one-phase ansatz (3.1) breaks down and instead one would need to establish a so-called *resonant asymptotic expansion* in the spirit of Joly, Metivier, and Rauch (1993). [We remark that so far, only the case of resonances in one spatial dimension can be treated rigorously; cf. Joly, Metivier, and Rauch (1999).]

We will show that these problems do not appear in our situation. To this end, we need to describe precisely what kind of ε-oscillations are present in $A^{\varepsilon}[u_0]$.

First we note that, by the superposition principle, every term appearing on the r.h.s. of (4.6) generates its own potential field. The nonoscillating terms of (4.6) lead to a standard hyperbolic problem; hence (2.5) gives

$$A_0[u_0](t,x):=\mathcal{G}_r(t,x)*(\omega_+(\nabla\phi)|u_{0,+}|^2+\omega_{-,k}(\nabla\phi)|u_{0,-}|^2)(t,x). \tag{4.7}$$

In order to treat the Zitterbewegung, let us define $Z:=(Z_1,Z_2,Z_3)$ by

$$\begin{aligned}Z_k(t,x,\phi(t,x)/\varepsilon):=\langle u_{0,+}(t,x),\alpha^k u_{0,-}(t,x)\rangle e^{-i2\phi(t,x)/\varepsilon}+\langle u_{0,-}(t,x),\alpha^k u_{0,+}(t,x)\rangle e^{i2\phi(t,x)/\varepsilon},&\\ k=1,2,3.&\end{aligned} \tag{4.8}$$

Using this definition, we can now prove the following lemma.

Lemma 4.1: Let $\Omega\subseteq\mathbb{R}^{1+3}$ be the slab in which existence of a smooth phase $\phi\in C^{\infty}(\Omega;\mathbb{R})$, satisfying (3.14), is guaranteed. Then, given $Z\in C^{\infty}(\Omega\times\mathbb{S}^1;\mathbb{C}^3)$, as in (4.8), there exists a uniquely determined smooth $A^{\varepsilon}\in C^{\infty}(\Omega\times\mathbb{S}^1;\mathbb{C}^3)$, with

$$A^{\varepsilon}(t,x,\theta)\sim\sum_{l=1}^{\infty}\varepsilon^l A_l(t,x,\theta), \tag{4.9}$$

s.t. $A^{\varepsilon}(t,x,\phi(t,x)/\varepsilon)$ satisfies

$$\begin{aligned}&\Box A^{\varepsilon}(t,x)-Z(t,x)\sim 0,\quad \text{in } C^{\infty}(\Omega;\mathbb{C}^3),\\ &A^{\varepsilon}|_{t=0}=\partial_t A^{\varepsilon}|_{t=0}=0.\end{aligned} \tag{4.10}$$

More precisely, $A_l(t,x,\phi(t,x)/\varepsilon)$ can be written in the following form:

$$A_l(t,x,\phi(t,x)/\varepsilon)=A_l^+(t,x)e^{i2\phi(t,x)/\varepsilon}+A_l^-(t,x)e^{-i2\phi(t,x)/\varepsilon}, \tag{4.11}$$

with principal amplitudes $A_1^{\pm} \in C^{\infty}(\Omega;\mathbb{C}^3)$, *given by*

$$A_{1,k}^{\pm}(t,x) = \pm \langle u_0(t,x), \alpha^k u_0(t,x)\rangle. \tag{4.12}$$

Proof: The proof can be done separately for each spatial component of $A^{\varepsilon}(t,x,\theta)$ and for both types of oscillations, corresponding to $\pm 2\phi$. Hence, we are led to the following type of problem:

$$\Box a^{\varepsilon}(t,x) = b(t,x) e^{\pm i2\phi(t,x)/\varepsilon}, \quad (t,x) \in \Omega,$$

$$a^{\varepsilon}|_{t=0} = \partial_t a^{\varepsilon}|_{t=0} = 0, \tag{4.13}$$

for some given $b \in C^{\infty}(\Omega;\mathbb{C})$. Let us define a new variable $f^{\varepsilon}(t,x) \in \mathbb{C}^5$ by

$$f^{\varepsilon}(t,x) := (\partial_1 a^{\varepsilon}, \partial_2 a^{\varepsilon}, \partial_3 a^{\varepsilon}, \partial_t a^{\varepsilon}, a^{\varepsilon})^{\top}(t,x).$$

Further, denoting by

$$\hat{b}(t,x) := (0,0,0,b(t,x),0)^{\top},$$

we can rewrite (4.13) in the form of a symmetric hyperbolic system,

$$(\partial_t + (\lambda \cdot \nabla) + \kappa) f^{\varepsilon}(t,x) = \hat{b}(t,x) e^{\pm i2\phi(t,x)/\varepsilon}, \tag{4.14}$$

with λ^k, κ, denoting realvalued (symmetric) 5×5 matrices. In our case, these matrices are simply given by [see, e.g., Racke (1992), p. 21, for more details]:

$$\lambda^k := -(\delta_{mk}\delta_{n4} + \delta_{m4}\delta_{nk})_{m,n}, \quad \kappa := -(\delta_{5m}\delta_{4n})_{m,n}, \quad m,n = 1,\ldots,5, \tag{4.15}$$

where δ_{ab} denotes the Kronecker symbol and $k = 1,2,3$.

It is now possible to use the existing results on linear geometrical optics, provided the phase $\pm 2\phi$ is *not* characteristic for the system (4.14), i.e.,

$$\det(\pm 2\partial_t\phi(t,x) \pm 2\lambda \cdot \nabla\phi(t,x) + \kappa) \neq 0, \quad \forall (t,x) \in \Omega. \tag{4.16}$$

Computing this determinant, we obtain the condition

$$\pm 32\,(\partial_t\phi)^3((\partial_t\phi)^2 - |\nabla\phi|^2) \neq 0, \quad \forall (t,x) \in \Omega. \tag{4.17}$$

Since, by assumption, ϕ solves the Klein–Gordon eikonal equation (3.11) the second factor on the l.h.s. of (4.17) is equal to one and thus, different from zero in all of Ω. On the other hand we get from (3.11): $(\partial_t\phi)^3 = (|\nabla\phi|^2 + 1)^{3/2} \neq 0$, $\forall (t,x) \in \Omega$. Hence, condition (4.16) is fulfilled and the assertion follows from Theorem 4.4 in Rauch (1992). In particular we get

$$A_{1,k}^{\pm}(t,x) = \frac{\mp 1}{-(\partial_t\phi)^2 + |\nabla\phi|^2} \langle u_0(t,x), \alpha^k u_0(t,x)\rangle = \pm\langle u_0(t,x), \alpha^k u_0(t,x)\rangle, \tag{4.18}$$

which concludes the proof. □

Lemma 4.1 shows that the Zitterbewegung in (4.6) generates a magnetic potential which is small, i.e., at least of order $O(\varepsilon)$. Moreover the ε-oscillations, appearing in A^{ε}, are exactly the *same* as in the (4.6) and hence we can consistently proceed with our one-phase expansion for ψ^{ε}.

Remark 4.2: Although the MD system is hyperbolic, Lemma 4.1 can be considered as an analogu of so-called *elliptic* high frequency asymptotics, the main feature of which is the fact that asymptotic solutions can be obtained by *local* (in t,x) algebraic relations. In other words, the Maxwell system can be considered *transparent* w.r.t. to the oscillations generated by the Dirac equation.

The result of Lemma 4.1 implies that the nonlinearity $\mathcal{N}^\varepsilon[u_0]$, defined in (3.3), admits an asymptotic expansion of the form

$$\mathcal{N}^\varepsilon[u_0](t,x,\theta) \sim \mathcal{N}_0[u_0](t,x,\theta) + \sum_{l=1}^{\infty} \varepsilon^l \mathcal{N}_l(t,x,\theta), \tag{4.19}$$

where, using the expressions (4.2), (4.7), we have

$$\mathcal{N}_0(t,x,\theta) = \left((\alpha \cdot A_0[u_0](t,x)) - V[u_0](t,x)\right) u_0(t,x,\theta), \tag{4.20}$$

and for all $l \geqslant 1$:

$$\mathcal{N}_l(t,x,\theta) := (\alpha \cdot A_l(t,x,\theta))\, u_0(t,x,\theta), \tag{4.21}$$

with A_l given by (4.11).

Note that the expression (4.19) represents two kinds of ε-oscillations: Those described by phase-functions $\pm\phi$ are present in all terms $\mathcal{N}_l$ with $l \geqslant 0$, whereas ε-oscillations with phases $\pm 3\phi$ appear in $\mathcal{N}_l$ with $l > 0$. Also, note that u_0 enters in a *nonlocal* way only in the lowest order term (4.20).

V. NONLINEAR TRANSPORT ALONG RAYS

We need to find an evolution equation, which determines u_0 from the initial data. To this end, let us define an operator $\mathbb{P}$, which projects on the set of harmonics corresponding to solutions of the eikonal equation (3.11).

Definition 5.1: Given some $v \in C^\infty(\mathbb{R}^4 \times \mathbb{S}^1; \mathbb{C}^4)$, which can be represented by

$$v(t,x,\theta) = \sum_{m \in \mathbb{Z}} v_m(t,x) e^{im\theta}, \tag{5.1}$$

we define the action of $\mathbb{P}$ on v, by

$$(\mathbb{P}v)(t,x,\theta) := (\Pi_+(\nabla\phi)v_{+1})(t,x)e^{i\theta} + (\Pi_-(\nabla\phi)v_{-1})(t,x)e^{-i\theta}. \tag{5.2}$$

In words: $\mathbb{P}$ picks modes corresponding to $m = \pm 1$ and multiplies them with the matrices $\Pi_\pm(\nabla\phi)$. Note that, at least in Ω, it holds true that

$$(\mathbb{P}u_0)(t,x,\theta) = u_0(t,x,\theta), \tag{5.3}$$

in view of (3.8) and (3.18), (3.19).

From (3.2), we have that the evolution of u_0 is determined by terms of order $O(\varepsilon^{p+1}) = O(\varepsilon^{3/2})$. Setting the corresponding coefficient in (3.4) equal to zero, i.e., $R_2(t,x) = 0$, yields

$$i(\partial_t\phi + (\alpha\cdot\nabla\phi))\partial_\theta u_2 - \beta u_2 + i(\partial_t u_0 + (\alpha\cdot\nabla)u_0) + \mathcal{N}_0[u_0] = 0, \tag{5.4}$$

with $\mathcal{N}_0[u_0]$ as in (4.20). Equation (5.4) implies

$$i(\partial_t + (\alpha\cdot\nabla))u_0 + \mathcal{N}_0[u_0] \in \mathrm{ran}(i(\partial_t\phi + (\alpha\cdot\nabla\phi))\partial_\theta - \beta). \tag{5.5}$$

Applying $\mathbb{P}$ to (5.4) eliminates the term including u_2, since $\mathbb{P}$ projects on the kernel of $i(\partial_t\phi + (\alpha\cdot\nabla\phi))\partial_\theta - \beta$ and we obtain

$$i\mathbb{P}\partial_t u_0 + i\mathbb{P}(\alpha\cdot\nabla)u_0 + \mathbb{P}\mathcal{N}_0[u_0] = 0. \tag{5.6}$$

Using the fact that $\mathbb{P}u_0 = u_0$, by (5.3), this gives

$$\mathbb{P}\partial_t(\mathbb{P}u_0) + \mathbb{P}(\alpha\cdot\nabla)(\mathbb{P}u_0) = i\mathbb{P}\mathcal{N}_0[\mathbb{P}u_0]. \tag{5.7}$$

This equation is similar to the one appearing in Donat and Rauch (1997), however, in contrast to the quoted work, our nonlinearity constitutes only the first term of an asymptotic expansion of the full $\mathcal{N}^\varepsilon[u_0]$.

We proceed by stating a useful identity:

$$\alpha^k \Pi_\pm(\xi) = \Pi_\mp(\xi)\alpha^k + \omega_{\pm,k}(\xi)\mathbb{I}_4, \tag{5.8}$$

obtained from straightforward calculations. After more lengthy but straightforward calculations, in which we apply the relations (4.3), (4.4), and (5.8), we can express the l.h.s. of (5.7) in the form of a transport operator:

$$\Pi_\pm \partial_t(\Pi_\pm u_0) + \Pi_\pm \alpha\cdot\nabla(\Pi_\pm u_0) = \partial_t u_{0,\pm} + (\omega_\pm(\nabla\phi)\cdot\nabla)u_{0,\pm} + \tfrac{1}{2}\operatorname{div}(\omega_\pm(\nabla\phi))u_{0,\pm}. \tag{5.9}$$

On the other hand, computing the action of the projector $\mathbb{P}$ on the nonlinear term $\mathcal{N}_0[u_0]$, we get

$$\begin{aligned}\mathbb{P}\mathcal{N}_0[\mathbb{P}u_0] = {} & e^{i\phi/\varepsilon}((A_0[u_0]\cdot\omega_+(\nabla\phi)) - V[u_0])\, u_{0,+} \\ & + e^{-i\phi/\varepsilon}((A_0[u_0]\cdot\omega_-(\nabla\phi)) - V[u_0])\, u_{0,-}.\end{aligned} \tag{5.10}$$

Here we have again used (4.4). Thus, we finally conclude, that the time-evolution of the *principal amplitudes* $u_{0,\pm}$ is governed by the following semilinear first-order system:

$$\begin{aligned}(\partial_t + (\omega_+(\nabla\phi)\cdot\nabla))u_{0,+}(t,x) &= \Gamma_+[u_0](t,x)\, u_{0,+}(t,x), \\ (\partial_t + (\omega_-(\nabla\phi)\cdot\nabla))u_{0,-}(t,x) &= \Gamma_-[u_0](t,x)\, u_{0,-}(t,x),\end{aligned} \tag{5.11}$$

where

$$\Gamma_\pm[u_0](t,x) := iA_0[u_0]\cdot\omega_\pm(\nabla\phi) - iV[u_0] - \tfrac{1}{2}\operatorname{div}(\omega_\pm(\nabla\phi)). \tag{5.12}$$

By construction, the polarization of $u_{0,\pm}$ is conserved during the evolution. The system (5.11) determines $(\mathbb{P}u_0)(t,x,\theta)$, from its initial data $(\mathbb{P}u_0)(0,x,\theta)$ and since $(\mathbb{P}u_0) = u_0$, we have completely constructed u_0.

Multiplying (5.11) by $\overline{u_{0,+}}$, resp., $\overline{u_{0,-}}$ and integrating by parts, we obtain the important property of charge-conservation:

$$\int_{\mathbb{R}^3} |u_{0,+}(t,x)|^2 + |u_{0,-}(t,x)|^2 \; dx = \|u_0(t,x)\|_2^2 = \text{const.} \tag{5.13}$$

Given u_0, determined by (5.11), it remains to construct the higher order terms $u_j(t,x,\theta)$, $j \geqslant 1$ of our approximate solution. This can be done by a similar construction as given in Donat and Rauch (1997).

We expand the cubic nonlinearity $\mathcal{N}^\varepsilon[u^\varepsilon]$ in powers of ε:

$$\mathcal{N}^\varepsilon[u_0 + \varepsilon u_1 + \cdots] \sim \mathcal{N}^\varepsilon[u_0] + \varepsilon\mathcal{M}^\varepsilon[u_0,u_1] + \cdots, \tag{5.14}$$

where, using the definitions (4.2), (4.8), we easily compute

$$\begin{aligned}\mathcal{M}^\varepsilon[u_0,u_1] = {} & 2\,(\mathcal{G}_r * \langle u_0,u_1\rangle)u_0 + V[u_0]u_1 + \alpha\cdot(\mathcal{G}_r * Z)\, u_1 \\ & + \left(\sum_{k=1}^3 \alpha^k(\mathcal{G}_r * \langle u_0, \alpha^k u_1\rangle + \mathcal{G}_r * \langle u_1, \alpha^k u_0\rangle)\right) u_0.\end{aligned} \tag{5.15}$$

We need to apply Lemma 4.1 to all terms appearing on the r.h.s of (5.14), which results in a similar expansion as given in (4.19). Hence, after rearranging terms in powers of ε, we can write

$$\mathcal{N}^{\varepsilon}[u_0+\varepsilon u_1+\cdots]\sim\mathcal{N}_0[u_0]+\varepsilon\mathcal{N}_1+\varepsilon\mathcal{M}_0[u_0,u_1]+\cdots. \tag{5.16}$$

Consequently, for $j\geqslant 1$, the $O(\varepsilon^{j/2+1/2})$-coefficient is given by

$$\begin{aligned} R_j(t,x)=&\,i(\partial_t\phi+(\alpha\cdot\nabla\phi))\partial_\theta u_j-\beta u_j+i(\partial_t+(\alpha\cdot\nabla))u_{j-2}\\ &+\mathcal{M}_0[u_0,u_{j-2}]+S(u_0,\ldots,u_{n<j-2}), \end{aligned} \tag{5.17}$$

where, as usual, we impose: $u_n(t,x,\theta)=0$, for all $n<0$. The source term S, only depends on lower order coefficients $u_0,\ldots,u_{n<j-2}$. It is obtained by applying Lemma 4.1 to higher order terms in the expansion (5.14), leading to contributions $\mathcal{N}_l$ and $\mathcal{M}_l$ with: $l+1=j/2$.

We can now decompose

$$u_j(t,x,\theta)=(\mathbb{P}u_j)(t,x,\theta)+(\mathrm{id}_4-\mathbb{P})u_j(t,x,\theta). \tag{5.18}$$

Note that in contrast to u_0, where, in view of (5.3), it holds that

$$(\mathrm{id}_4-\mathbb{P})u_0(t,x,\theta)=0, \tag{5.19}$$

we cannot expect all higher order coefficients u_j to be polarized too. Hence, we need to determine separately $\mathbb{P}u_j$ and $(\mathrm{id}_4-\mathbb{P})u_j$. To this end, we introduce the following definition.

Definition 5.2: Again, let $v(t,x,\theta)$ be given as in Definition 5.1, then we define a partial inverse $\mathbb{Q}$, associated to $\mathbb{P}$, by

$$(\mathbb{Q}v)(t,x,\theta):=(\Lambda_+(\nabla\phi)v_{+1})(t,x)e^{i\theta}+(\Lambda_-(\nabla\phi)v_{-1})(t,x)e^{-i\theta}, \tag{5.20}$$

where $\Lambda_\pm$ is the partial inverse to $\Pi_\pm$, defined by (2.17).

Assume now that we already know u_n, for $n<j$, then $(\mathrm{id}_4-\mathbb{P})u_j$ is determined by setting $(\mathbb{Q}R_j)(t,x,\theta)=0$. This gives

$$(\mathrm{id}_4-\mathbb{P})u_j=-\mathbb{Q}(i(\partial_t+(\alpha\cdot\nabla))u_{j-2}+\mathcal{M}_0[u_0,u_{j-2}]+S(u_0,\ldots,u_{n<j-2})). \tag{5.21}$$

On the other hand, setting $(\mathbb{P}R_{j+2})(t,x,\theta)=0$, we obtain an evolution equation for $\mathbb{P}u_j$:

$$i\mathbb{P}\partial_t(\mathbb{P}u_j)+i\mathbb{P}(\alpha\cdot\nabla\mathbb{P}u_j)=-\mathbb{P}\mathcal{M}_0[u_0,u_j]+r(u_0,\ldots,u_j), \tag{5.22}$$

where

$$r(u_0,\ldots,u_j):=-\mathbb{P}S(u_0,\ldots,u_{n<j})-\mathbb{P}(i\partial_t+i(\alpha\cdot\nabla)-\beta)(\mathrm{id}_4-\mathbb{P})u_j. \tag{5.23}$$

Here, the first term on the r.h.s is already known by the inductive hypothesis and the second one is given by Eq. (5.21). Hence, by induction, one can construct all higher order coefficients $u_j(t,x,\theta)$, $j\geqslant 1$ in this way.

Note, that the left hand side of (5.22) is essentially a transport operator, which can be expressed as shown above. Thus (5.22) constitutes a *linear* first order system, which determines the so-called *propagating part* $\mathbb{P}u_j$ from its initial data.

Remark 5.3: The above construction can be generalized to the case, where, additionally *given* external potentials V^{ext}, A^{ext} are included, and/or nonzero Cauchy initial data for the Maxwell equations (1.17), (1.18) are assumed. In the presence of external fields one checks that, instead of (3.13), the following Hamilton–Jacobi equation, corresponding to $m=1$, holds:

$$\partial_t\phi_\pm\pm\sqrt{|\nabla\phi_\pm-A^{\mathrm{ext}}(t,x)|^2+1}+V^{\mathrm{ext}}(t,x)=0. \tag{5.24}$$

Since no other harmonics with $m\neq 1$ exist, one again ends up with two phases $\phi_\pm(t,x)$, corresponding to the electronic, resp., positronic degrees of freedom. In this case, however, $-\phi_+(t,x)\neq\phi_-(t,x)$, in contrast to (3.17). Also, one obtains an additional matrix-valued *spin-*

transport term, appearing on the left-hand side of (5.11) and which can be found in, for example, Bolte and Keppeler (1999); Fermanian-Kammerer (2003); Panati, Sohn, and Teufel (19XX)

We are now in the position of formulating our first theorem (in which we do not aim to impose the weakest possible assumptions). In the following, $C^\infty_{(0)}$ denotes the space of smooth function, compactly supported in $x \in \mathbb{R}^3$.

Theorem 5.4: *Assume that the initial data $\psi^\varepsilon_I(x)$ admits an asymptotic expansion of the form:*

$$\begin{aligned} \psi^\varepsilon_I(x) &= \sqrt{\varepsilon}\, u^\varepsilon(x, \phi_I(x)/\varepsilon), \\ u^\varepsilon(x,\theta) &\sim \sum_{j=0}^{\infty} \varepsilon^{j/2} \chi_j(x,\theta), \end{aligned} \tag{5.25}$$

where $\phi_I \in C^\infty(\mathbb{R}^3;\mathbb{R})$ satisfies $\|D^2\phi_I\| \leqslant C$. Further, let $\chi_j \in C^\infty_{(0)}(\mathbb{R}^3 \times \mathbb{S}^1;\mathbb{C}^4)$ be s.t.,

$$(\mathbb{P}\chi_j)(x,\theta) = \chi_j(x,\theta), \quad \forall j \in \mathbb{N}. \tag{5.26}$$

Then, there exists a $0 < T^* \leqslant T$, a corresponding domain $\Omega^* := [0,T^*) \cap \Omega$ and a uniquely determined $u^\varepsilon \in C^\infty_{(0)}(\Omega^* \times \mathbb{S}^1;\mathbb{C}^4)$, with

$$u^\varepsilon(t,x,\theta) \sim \sqrt{\varepsilon} \sum_{j=0}^{\infty} \varepsilon^{j/2} u_j(t,x,\theta), \tag{5.27}$$

s.t. $u^\varepsilon(t,x,\phi(t,x)/\varepsilon)$ satisfies:

$$\begin{aligned} i\varepsilon \partial_t u^\varepsilon - \mathcal{D}^\varepsilon_A(t,x,\varepsilon D) u^\varepsilon &\sim 0, \quad \forall (t,x) \in \Omega, \\ u^\varepsilon|_{t=0} &= \psi^\varepsilon_I(x). \end{aligned} \tag{5.28}$$

More precisely we have the following. The principal term u_0 is given by (3.20), satisfies $(\mathbb{P}u_0)(t,x,\theta) = u_0(t,x,\theta)$ and solves (5.7) with initial data $(\mathbb{P}u_0)(0,x,\theta) = \chi_0(x,\theta)$.

For all $j \geqslant 1$, the infinite sequence of equations (5.21), (5.22), uniquely determines $u_j(t,x,\theta)$, with initial data $(\mathbb{P}u_j)(0,x,\theta) = \chi_j(x,\theta)$.

Proof: The existence of a smooth phase $\phi \in C^\infty(\Omega;\mathbb{R})$, on the slab $\Omega \subseteq \mathbb{R}^{1+3}$, is already guaranteed by Lemma 3.2.

Next, consider the case $j=0$: Since $\omega_\pm(\nabla\phi) \in \mathbb{R}^3$, defined by (4.5), satisfies for all multi-indices σ, ν,

$$\sup_{(t,x)\in\Omega} \left| \partial_t^\sigma \partial_x^\nu \omega_{\pm,k}(\nabla\phi(t,x)) \right| < \infty, \quad k = 1,2,3, \tag{5.29}$$

we find that the l.h.s. of (5.11) constitutes a linear symmetric hyperbolic system. From L^2-conservation property (5.13) the usual commutator estimates lead to H^s-regularity, i.e., $u_0 \in C^1(\mathbb{R}^3;H^s)$ for all $s \geqslant 0$. Now, it is a standard result for the linear wave equations in $d=3$ spatial dimensions, that source terms in $H^s(\mathbb{R}^3)$ generate solutions (at least) in $H^s(\mathbb{R}^3)$; cf. Hörmander (1985), Chapter XXIII. This fact and Schauder's lemma imply that the map,

$$u_0(t,\cdot) \mapsto \Gamma_\pm[u_0(t,\cdot)], \tag{5.30}$$

are locally Lipschitz from $H^s((0,t) \times \mathbb{R}^3 \times \mathbb{S}^1)$ to itself, for all $s > 2$, uniformly for $0 \leqslant t < T$. By a standard Picard iteration we therefore obtain a local-in-time existence and uniqueness result in $H^s(\Omega^* \times \mathbb{S}^1)$, for every $s > 2$ and a Sobolev imbedding gives $u_0 \in C^1(\Omega^* \times \mathbb{S}^1;\mathbb{C}^4)$. The proof of the asserted regularity for the t-derivatives follows by using the differential equation to express them in terms of x-derivatives and the finite speed of propagation for the solution of (5.11) implies that u_0 is compactly supported in $\mathbb{R}^3_x$ since χ_0 is also.

Finally, for $j>0$, we have that the amplitudes $u_{j,\pm}$ are determined by the linear symmetric hyperbolic system (5.22), (5.21) and the assertion is proved. □

Once again, we stress the fact that we analyze the MD system in a *weakly coupled regime*. Indeed, the above result implies the following.

Corollary 5.5: Let $u^\varepsilon(t,x,\phi(t,x)/\varepsilon)$ be as in Theorem 5.4; then

$$\begin{aligned} V^\varepsilon[u^\varepsilon](t,x) &\sim \varepsilon V[u_0](t,x)+O(\varepsilon^2),\\ A^\varepsilon[u^\varepsilon](t,x) &\sim \varepsilon A_0[u_0](t,x)+O(\varepsilon^2), \end{aligned} \tag{5.31}$$

where $V[u_0]$, $A_0[u_0]$ are nonoscillating and explicitly given by (4.2), (4.7).

VI. STABILITY AND FURTHER RESULTS

In Theorem 5.4 we obtained a function u^ε, which solves the MD equation up to a residual $R^\varepsilon\sim 0$, compactly supported in $[0,T^*]\times\mathbb{R}^3$. We want to compare u^ε to a true solution ψ^ε and prove that $u^\varepsilon-\psi^\varepsilon\sim 0$ on $\Omega^*=[0,T^*]\times\mathbb{R}^3$.

Theorem 6.1: *Under the assumptions of theorem 5.4, there is an $\varepsilon^*\in(0,1)$, s.t. for $\varepsilon<\varepsilon^*$, there exists a unique smooth $\psi^\varepsilon\in C^\infty_{(0)}(\Omega^*;\mathbb{C}^4)$, satisfying*

$$\begin{aligned} i\varepsilon\partial_t\psi^\varepsilon-\mathcal{D}^\varepsilon_A(t,x,\varepsilon D)\psi^\varepsilon&=0,\quad \forall(t,x)\in\Omega^*,\\ \psi^\varepsilon|_{t=0}&=\psi^\varepsilon_I(x), \end{aligned} \tag{6.1}$$

which is asymptotically equivalent to u^ε, i.e.,

$$\psi^\varepsilon(t,x)\sim u^\varepsilon(t,x,\phi(t,x)/\varepsilon),\quad \text{in } C^\infty_{(0)}(\Omega^*;\mathbb{C}^4). \tag{6.2}$$

Proof: Defining $v^\varepsilon:=u^\varepsilon-\psi^\varepsilon$, we obtain for the following IVP:

$$\begin{aligned} i(\varepsilon\partial_t+\varepsilon(\alpha\cdot\nabla))v^\varepsilon-\beta v^\varepsilon+\mathcal{N}^\varepsilon[u^\varepsilon+v^\varepsilon]-\mathcal{N}^\varepsilon[u^\varepsilon]&=-R^\varepsilon,\quad \text{in } \Omega^*,\\ v^\varepsilon|_{t=0}&=0. \end{aligned} \tag{6.3}$$

The nonlinearity can be handled analogous to the proof of Lemma 6.2, in Donat and Rauch (1997), since for smooth sources the wave equation has smooth solutions, which moreover travel with finite speed. Having this in mind, the rest of the proof is a simple modification of the one of Theorem 6.1 in Donat and Rauch (1997). □

As far as the generation of positronic-modes is concerned, the local-in-time solution $\psi^\varepsilon\sim O(\sqrt{\varepsilon})$ shows the following qualitative behavior:

Corollary 6.2: Let ψ^ε_I be as in Theorem 5.4. If initially $(\Pi_-\psi^\varepsilon_I)(x)=0$, then, for $0\leqslant t<T^*$, it holds: $(\Pi_-\psi^\varepsilon)(t,x)\sim O(\varepsilon^{3/2})$, i.e., no positronic-modes are generated, up to $O(\varepsilon^{3/2})$ and the analogous statement for electrons is valid, too.

Proof: The assertion holds true, since a careful examination of the asymptotic expansion shows that both, u_0 *and* u_1, satisfy $(\mathbb{P}u_j)(t,x,\theta)=u_j(t,x,\theta)$, in Ω^*. □

For completeness, we shall also consider the *matrix-valued Wigner transform* corresponding to ψ^ε, i.e.,

$$w^\varepsilon[\psi^\varepsilon](t,x,\xi):=\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\psi^\varepsilon\left(t,x+\frac{\varepsilon}{2}y\right)\otimes\overline{\psi^\varepsilon}\left(t,x-\frac{\varepsilon}{2}y\right)e^{i\xi\cdot y}\,dy, \tag{6.4}$$

where $\otimes$ denotes the tensor product of vectors. The real-valued 4×4-matrix $w^\varepsilon[\psi^\varepsilon]$ is a *phase-space description* of the quantum state ψ^ε.

Corollary 6.3: Let $\psi^\varepsilon \sim O(\sqrt{\varepsilon})$ be the unique smooth local-time-solution of the MD system, as guaranteed by Theorem (6.1) and let $w^\varepsilon[\psi^\varepsilon] \sim O(\varepsilon)$ be its Wigner transform. Then, up to extraction of subsequences, we have

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}w^\varepsilon[\psi^\varepsilon]=\mu, \quad in \;\; \mathcal{S}'([0,T^*)\times\mathbb{R}^3_x\times\mathbb{R}^3_\xi) weak-\star, \tag{6.5}$$

where the matrix-valued Wigner measure μ is given by $\mu=\mu_+ + \mu_-$, with

$$\mu_\pm(t,x,\xi)=u_{0,\pm}(t,x)\otimes\overline{u}_{0,\pm}(t,x)\;\delta(\xi\mp\nabla\phi(t,x)). \tag{6.6}$$

Proof: Since ϕ has no stationary points within Ω^*, a nonstationary phase argument implies that all Wigner matrix elements, which mix the electronic and positronic components are of order $O(\varepsilon^\infty)$. The assertion then follows from the well known results on Wigner measures; *cf.* Gérard, Markowich, Mauser, and Poupaud (1997) □

We finally remark on the case of the Dirac–Maxwell system where the Dirac particles have vanishing mass. Instead of (3.13) we obtain

$$\partial_t\phi=\pm|\nabla\phi|, \tag{6.7}$$

which is equivalent to the eikonal equation of the wave equation. It follows that in this case Lemma 4.1 cannot hold, since the phases $\pm\phi$ are characteristic for the wave equation. More precisely, they are indeed *everywhere* characteristic, i.e., in all of Ω, which again allows for an asymptotic description of the A^ε, similar to (4.9), (4.11); *cf.* Lax (1957) or Rauch (1999), Chap. 5. In this case, the ε-oscillations are also given by $\exp(\pm 2i\phi/\varepsilon)$, but the corresponding amplitudes $A_l^\pm$ are of course different. The main difference, however, is the fact that in this case the summation index runs from $l=0$ to infinity, i.e., ε-oscillations are present already in the lowest order term. This leads to a more complicated structure of the transport equations for the amplitudes u_j, but apart from that all results remain valid.

ACKNOWLEDGMENTS

This work originated from discussions with P. Gérard (Univ. dé Paris Sud) and N. Mauser (Univ. Vienna). The authors thank J. Rauch and H. Spohn for helpful suggestions and remarks as well as the *TICAM* (Univ. Texas) for its support. This work has also been supported by the Austrian Science Foundation FWF through Grant No. W8, Project No. P14876-No 4, the *START Award* 1999 of Norbert Mauser and the *Wittgenstein Award* 2000 of P.M. Additional financial sponsorship has been given by the EU research network *HYKE*, HPRN-CT-2002-00282.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Algebro–geometric constructions of the discrete Ablowitz–Ladik flows and applications

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(Received 26 November 2002; accepted 7 July 2003)

Resorting to the finite-order expansion of the Lax matrix, the elliptic coordinates are introduced, from which the discrete Ablowitz–Ladik equations and the $(2+1)$-dimensional Toda lattice are decomposed into solvable ordinary differential equations. The straightening out of the continuous flow and the discrete flow is exactly given through the Abel–Jacobi coordinates. As an application, explicit quasiperiodic solutions for the $(2+1)$-dimensional Toda lattice are obtained. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1605820]

I. INTRODUCTION

Since Ablowitz and Ladik introduced the discrete AKNS equations (called also discrete Ablowitz–Ladik equations),[1,2] numbers of researches were conducted in a series of papers.[1–8] For example, there is research conducted for soliton solutions, Bäcklund transformation, Darboux transformation, Hamiltonian structures, conserved quantities, and other properties. The authors of Refs. 9–12 discuss quasiperiodic solutions for the discrete Ablowitz–Ladik equations, which include the discrete nonlinear Schrödinger equation and the discrete mKdV equation. In Ref. 13, the algebraic–geometrical approach was used to study the discrete Ablowitz–Ladik equations, from which the Baker–Akhiezer function and quasiperiodic solutions corresponding to finite-genus Riemann surfaces were obtained.

In this paper, our main aim is to study straightening out of the discrete Ablowitz–Ladik flows, including the continuous flow and discrete flow, based on the ideas in Refs. 14–16. As an application, we obtain quasiperiodic solutions of the $(2+1)$-dimensional Toda lattice. The outline of the present paper is as follows. In Sec. II the discrete Ablowitz–Ladik hierarchy is constructed with the aid of the Lenard gradient sequences. The relation between the $(2+1)$-dimensional Toda lattice and discrete Ablowitz–Ladik equations is discussed. In Sec. III we introduce a Lax matrix, from which a direct relation between the elliptic coordinates and solutions of the discrete Ablowitz–Ladik equations is established. The $(2+1)$-dimensional Toda lattice is separated into solvable ordinary differential equations. In Sec. IV the Abel–Jacobi coordinates are introduced, by which the straightening out of the continuous flow and the discrete flow are studied in detail. In Sec. V the Riemann–Jacobi inversion is discussed, from which the quasiperiodic solutions for the $(2+1)$-dimensional Toda lattice are obtained by using the Riemann theta functions.

II. THE DISCRETE ABLOWITZ–LADIK HIERARCHY

In this section, we shall derive the Ablowitz–Ladik hierarchy. To this end we first introduce the Lenard gradient sequences

$$K_nS_{j-1}(n)=J_nS_j(n),\quad J_nS_{-1}(n)=0,\quad j\geqslant 0, \tag{2.1}$$

$$K_n\hat{S}_{j-1}(n)=J_n\hat{S}_j(n),\quad K_n\hat{S}_0(n)=0,\quad j\leqslant 0, \tag{2.2}$$

and take

$$S_{-1}(n)=\begin{pmatrix}0\\0\\1\end{pmatrix},\quad \hat{S}_0(n)=\begin{pmatrix}-2u_{n-1}\\-2v_n\\1\end{pmatrix} \tag{2.3}$$

as a starting point of Eq. (2.1) or Eq. (2.2), respectively, with two matrix operators

$$K_n=\begin{pmatrix}E & 0 & u_n(E+1)\\ 0 & 1 & v_n(E+1)\\ v_nE & -u_n & \Delta\end{pmatrix},\quad J_n=\begin{pmatrix}1 & 0 & 0\\ 0 & E & 0\\ v_nE & -u_n & \Delta\end{pmatrix}.$$

Here the shift operator E and the difference operator Δ are defined as $Ef(n)=f(n+1)$, $\Delta f(n)=f(n+1)-f(n)$. It is easy to see that

$$\ker K_n=\{c\hat{S}_0(n)|\forall c\},\quad \ker J_n=\{cS_{-1}(n)|\forall c\}. \tag{2.4}$$

Then $S_j(n)$ and $\hat{S}_{-j}(n)$ $(j\geqslant 0)$ are uniquely determined by the recursion relation Eq. (2.1) or Eq. (2.2) up to a term $c_1S_{-1}(n)$ or $c_2\hat{S}_0(n)$, which are always assumed to be zero. The first few members are

$$S_0(n)=2\begin{pmatrix}u_n\\ v_{n-1}\\ -u_nv_{n-1}\end{pmatrix},\quad \hat{S}_{-1}(n)=2\begin{pmatrix}-u_{n-2}+u_{n-1}(u_{n-1}v_n+u_{n-2}v_{n-1})\\ -v_{n+1}+v_n(u_nv_{n+1}+u_{n-1}v_n)\\ -u_{n-1}v_n\end{pmatrix},$$

$$S_1(n)=2\begin{pmatrix}u_{n+1}-u_n(u_{n+1}v_n+u_nv_{n-1})\\ v_{n-2}-v_{n-1}(u_nv_{n-1}+u_{n-1}v_{n-2})\\ -u_{n+1}v_{n-1}-u_nv_{n-2}+u_nv_{n-1}(u_{n+1}v_n+u_nv_{n-1}+u_{n-1}v_{n-2})\end{pmatrix}.$$

Consider the discrete spectral problem[2,17]

$$\chi(n+1)=U_n\chi(n),\quad U_n=\frac{1}{\gamma_n}\begin{pmatrix}\lambda & u_n\\ v_n & \lambda^{-1}\end{pmatrix},\quad \chi(n)=\begin{pmatrix}\chi^{(1)}(n)\\ \chi^{(2)}(n)\end{pmatrix}, \tag{2.5}$$

where u_n and v_n are two potentials, λ is a constant spectral parameter,

$$\gamma_n=\sqrt{1-u_nv_n}.$$

In order to derive the Ablowitz–Ladik hierarchy, we assume that the time dependence of $\chi(n)$ for the spectral problem (2.5) obeys the differential equation

$$\chi(n)_{t_m}=V_n^{(m)}\chi(n),\quad V_n^{(m)}=\begin{pmatrix}A^{(m)}(n) & B^{(m)}(n)\\ C^{(m)}(n) & -A^{(m)}(n)\end{pmatrix}, \tag{2.6}$$

where

$$A^{(m)}(n)=\alpha\sum_{j=0}^{m-1}S_{j-1}^{(3)}(n)\lambda^{2m-2j}+\beta\sum_{j=0}^{-(m-1)}\hat{S}_j^{(3)}(n)\lambda^{-2m-2j}+\frac{1}{2}\alpha S_{m-1}^{(3)}(n)+\frac{1}{2}\beta\hat{S}_{-m}^{(3)}(n),$$

$$B^{(m)}(n)=\alpha\sum_{j=1}^{m} S_{j-1}^{(1)}(n)\lambda^{2m-2j+1}+\beta\sum_{j=-1}^{-m} \hat{S}_{j+1}^{(1)}(n)\lambda^{-2m-2j-1}, \tag{2.7}$$

$$C^{(m)}(n)=\alpha\sum_{j=1}^{m} S_{j-1}^{(2)}(n)\lambda^{2m-2j+1}+\beta\sum_{j=-1}^{-m} \hat{S}_{j+1}^{(2)}(n)\lambda^{-2m-2j-1}.$$

Then the compatibility condition between Eqs. (2.5) and (2.6) yields the zero-curvature equation $U_{nt_m}+U_nV_n^{(m)}-V_{n+1}^{(m)}U_n=0$, which is equivalent to the evolution equation

$$\begin{aligned}
&\gamma_n(\gamma_n^{-1})_{t_m}=\Delta A^{(m)}(n)+\lambda^{-1}v_nEB^{(m)}(n)-\lambda^{-1}u_nC^{(m)}(n),\\
&u_{nt_m}+u_n\gamma_n(\gamma_n^{-1})_{t_m}=\lambda^{-1}EB^{(m)}(n)-\lambda B^{(m)}(n)+u_n(E+1)A^{(m)}(n),\\
&v_{nt_m}+v_n\gamma_n(\gamma_n^{-1})_{t_m}=\lambda EC^{(m)}(n)-\lambda^{-1}C^{(m)}(n)-v_n(E+1)A^{(m)}(n),\\
&\gamma_n(\gamma_n^{-1})_{t_m}=-\Delta A^{(m)}(n)+\lambda u_nEC^{(m)}(n)-\lambda v_nB^{(m)}(n).
\end{aligned} \tag{2.8}$$

From Eqs. (2.1) and (2.2), it is easy to calculate that

$$\begin{aligned}
&\Delta S_{j-1}^{(3)}(n)+v_nES_{j-1}^{(1)}(n)-u_nS_{j-1}^{(2)}(n)=0,\\
&ES_{j-1}^{(1)}(n)-S_j^{(1)}(n)+u_n(E+1)S_{j-1}^{(3)}(n)=0,\\
&S_{j-1}^{(2)}(n)+v_n(E+1)S_{j-1}^{(3)}(n)-ES_j^{(2)}(n)=0,\\
&-\Delta S_{j-1}^{(3)}(n)+u_nES_j^{(2)}(n)-v_nS_j^{(1)}(n)=0,\quad j\geqslant 0,
\end{aligned} \tag{2.9}$$

$$\begin{aligned}
&\Delta \hat{S}_{j-1}^{(3)}(n)+v_nE\hat{S}_{j-1}^{(1)}(n)-u_n\hat{S}_{j-1}^{(2)}(n)=0,\\
&E\hat{S}_{j-1}^{(1)}(n)-\hat{S}_j^{(1)}(n)+u_n(E+1)\hat{S}_{j-1}^{(3)}(n)=0,\\
&\hat{S}_{j-1}^{(2)}(n)+v_n(E+1)\hat{S}_{j-1}^{(3)}(n)-E\hat{S}_j^{(2)}(n)=0,\\
&-\Delta \hat{S}_{j-1}^{(3)}(n)+u_nE\hat{S}_j^{(2)}(n)-v_n\hat{S}_j^{(1)}(n)=0,\quad j\leqslant 0.
\end{aligned} \tag{2.10}$$

Substituting Eq. (2.7) into Eq. (2.8) and using Eqs. (2.9) and (2.10), we obtain

$$\begin{aligned}
&\gamma_n(\gamma_n^{-1})_{t_m}=\tfrac{1}{2}\Delta(\alpha S_{m-1}^{(3)}(n)+\beta\hat{S}_{-m}^{(3)}(n))+\alpha v_nES_{m-1}^{(1)}(n)-\alpha u_nS_{m-1}^{(2)}(n),\\
&u_{nt_m}+u_n\gamma_n(\gamma_n^{-1})_{t_m}=\alpha ES_{m-1}^{(1)}(n)-\beta\hat{S}_{-m+1}^{(1)}(n)+\tfrac{1}{2}u_n(E+1)(\alpha S_{m-1}^{(3)}(n)+\beta\hat{S}_{-m}^{(3)}(n)),\\
&v_{nt_m}+v_n\gamma_n(\gamma_n^{-1})_{t_m}=\beta E\hat{S}_{-m+1}^{(2)}(n)-\alpha S_{m-1}^{(2)}(n)-\tfrac{1}{2}v_n(E+1)(\alpha S_{m-1}^{(3)}(n)+\beta\hat{S}_{-m}^{(3)}(n)),\\
&\gamma_n(\gamma_n^{-1})_{t_m}=-\tfrac{1}{2}\Delta(\alpha S_{m-1}^{(3)}(n)+\beta\hat{S}_{-m}^{(3)}(n))+\beta u_nE\hat{S}_{-m+1}^{(2)}(n)-\beta v_n\hat{S}_{-m+1}^{(1)}(n),
\end{aligned} \tag{2.11}$$

Resorting to the first expression of Eq. (2.9) and the fourth expression of Eq. (2.10), the first and the fourth expressions of Eq. (2.11) can be written as

$$\gamma_n(\gamma_n^{-1})_{t_m}=\tfrac{1}{2}\Delta(\beta\hat{S}_{-m}^{(3)}(n)-\alpha S_{m-1}^{(3)}(n)). \tag{2.12}$$

Substituting Eq. (2.12) into the second and third expressions of Eq. (2.11) and using Eq. (2.10), we obtain the Ablowitz–Ladik hierarchy

$$\begin{aligned} u_{nt_m} &= \alpha E S^{(1)}_{m-1}(n) + \alpha u_n E S^{(3)}_{m-1}(n) - \beta E \hat{S}^{(1)}_{-m}(n) - \beta u_n E \hat{S}^{(3)}_{-m}(n), \\ v_{nt_m} &= -\alpha S^{(2)}_{m-1}(n) - \alpha v_n S^{(3)}_{m-1}(n) + \beta \hat{S}^{(2)}_{-m}(n) + \beta v_n E \hat{S}^{(3)}_{-m}(n), \quad m \geqslant 0. \end{aligned} \tag{2.13}$$

The first two members are

$$u_{t_0} = (\alpha+\beta)u_n, \quad v_{t_0} = -(\alpha+\beta)v_n, \tag{2.14}$$

$$\begin{aligned} u_{nt_1} &= 2(1-u_n v_n)(\alpha u_{n+1} + \beta u_{n-1}), \\ v_{nt_1} &= -2(1-u_n v_n)(\alpha v_{n-1} + \beta v_{n+1}). \end{aligned} \tag{2.15}$$

Equations (2.15) is, respectively, reduced to the coupled discrete nonlinear Schrödinger equation

$$\begin{aligned} u_{nx} &= (1-u_n v_n)(u_{n+1} + u_{n-1}), \\ v_{nx} &= -(1-u_n v_n)(v_{n-1} + v_{n+1}) \end{aligned} \tag{2.16}$$

for $\alpha = \beta = \frac{1}{2}$, $x = t_1$, and the coupled discrete mKdV equation

$$\begin{aligned} u_{nt} &= (1-u_n v_n)(u_{n+1} - u_{n-1}), \\ v_{nt} &= (1-u_n v_n)(v_{n-1} - v_{n+1}) \end{aligned} \tag{2.17}$$

for $\alpha = -\beta = \frac{1}{2}$, $t = t_1$. Since Eqs. (2.16) and (2.17) are compatible, we assume that (u_n, v_n) is a compatible solution of Eqs. (2.16) and (2.17), and introduce a function w_n by

$$w_n = 1 - u_n v_n. \tag{2.18}$$

Then the function w_n satisfies the $(2+1)$-dimensional Toda lattice equation[18,19]

$$\frac{1}{4}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial t^2}\right) \ln w_n = 2w_n - w_{n+1} - w_{n-1}, \tag{2.19}$$

which can be verified through a direct calculation.

III. THE ELLIPTIC COORDINATES

Assume that Eqs. (2.5) and (2.6) have two basic solutions $\psi(n) = (\psi^{(1)}(n), \psi^{(2)}(n))^T$ and $\phi(n) = (\phi^{(1)}(n), \phi^{(2)}(n))^T$. We define a Lax matrix W_n of three functions $f(n), g(n), h(n)$ by

$$W_n = \frac{1}{2}(\phi(n)\psi(n)^T + \psi(n)\phi(n)^T)\sigma = \begin{pmatrix} f(n) & g(n) \\ h(n) & -f(n) \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{3.1}$$

It is easy to verify by (2.5) and (2.6) that

$$W_{n+1}U_n - U_n W_n = 0, \quad W_{nt_m} = [V^{(m)}_n, W_n], \tag{3.2}$$

which imply that the function $\det W_n$ is a constant independent of n and t_m. In fact, we obtain by the first expression of Eq. (3.2) that $W_{n+1} = U_n W_n U_n^{-1}$. Then $\det W_{n+1} = \det W_n$, which means that $\det W_n$ is independent of n. In a way similar to the continuous case, a direct calculation shows that $(\det W_n)_{t_m} = 0$. Equations (3.2) can be written as

$$\begin{aligned}
&\lambda\Delta f(n)+v_nEg(n)-u_nh(n)=0,\\
&\lambda^{-1}Eg(n)-\lambda g(n)+u_n(E+1)f(n)=0,\\
&\lambda Eh(n)-\lambda^{-1}h(n)-v_n(E+1)f(n)=0,\\
&\lambda^{-1}\Delta f(n)-u_nEh(n)+v_ng(n)=0,
\end{aligned}\tag{3.3}$$

and

$$\begin{aligned}
&f(n)_{t_m}=B^{(m)}(n)h(n)-C^{(m)}(n)g(n),\\
&g(n)_{t_m}=2A^{(m)}(n)g(n)-2B^{(m)}(n)f(n),\\
&h(n)_{t_m}=2C^{(m)}(n)f(n)-2A^{(m)}(n)h(n).
\end{aligned}\tag{3.4}$$

Suppose that the functions $f(n)$,$g(n)$, and $h(n)$ are finite-order polynomials in λ,

$$\begin{aligned}
&f(n)=\sum_{j=0}^{N+1}f_{j-1}(n)\lambda^{2(N+1)-2j},\quad g(n)=\sum_{j=1}^{N+1}g_{j-1}(n)\lambda^{2(N+1)-2j+1},\\
&h(n)=\sum_{j=1}^{N+1}h_{j-1}(n)\lambda^{2(N+1)-2j+1}.
\end{aligned}\tag{3.5}$$

Substituting Eq. (3.5) into Eq. (3.3) and comparing the coefficients of the same power of λ yields

$$\begin{aligned}
&K_nG_{j-1}(n)=J_nG_j(n),\quad J_nG_{-1}(n)=0,\\
&K_nG_N(n)=0,
\end{aligned}\tag{3.6}$$

with $G_j(n)=(g_j(n),h_j(n),f_j(n))^T$, $g_{-1}(n)=0$,$h_{-1}(n)=0$. It is easy to see that the equations $J_nG_{-1}(n)=0$ and $K_nG_N(n)=0$ have the general solutions

$$G_{-1}(n)=\alpha_0S_{-1}(n),\tag{3.7}$$

$$G_N(n)=\beta_0\hat{S}_0(n),\tag{3.8}$$

where α_0 and β_0 are constants. Acting with $J_n^{-1}K_n$ and $K_n^{-1}J_n$, respectively, upon Eqs. (3.7) and (3.8) yield

$$\begin{aligned}
&G_0(n)=\alpha_0S_0(n)+\alpha_1S_{-1}(n),\\
&G_{N-1}(n)=\beta_0\hat{S}_{-1}(n)+\beta_1\hat{S}_0(n),
\end{aligned}\tag{3.9}$$

in view of Eqs. (2.1) and (2.2), where α_1 and β_1 are constants. For the sake of convenience, we set $\alpha_0=1$. From Eqs. (3.7)–(3.9), we have

$$\begin{aligned}
&f_{-1}(n)=1,\quad f_0(n)=-2u_nv_{n-1}+\alpha_1,\quad g_0(n)=2u_n,\\
&h_0(n)=2v_{n-1},\quad f_N(n)=\beta_0,\quad g_N(n)=-2\beta_0u_{n-1},\\
&h_N(n)=-2\beta_0v_n,\quad f_{N-1}(n)=-2\beta_0u_{n-1}v_n+\beta_1.
\end{aligned}\tag{3.10}$$

We use $g(n)$ and $h(n)$ as polynomials of λ to define the elliptic coordinates $\{\mu_i(n)\}$ and $\{\nu_i(n)\}$:

$$g(n)=2\lambda u_n\prod_{i=1}^{N}(\zeta-\mu_i(n)),\quad h(n)=2\lambda v_{n-1}\prod_{i=1}^{N}(\zeta-\nu_i(n)) \tag{3.11}$$

with $\zeta=\lambda^2$. By comparing coefficients of the same power for ζ, we get

$$g_1(n)=-g_0(n)\sum_{j=1}^{N}\mu_j(n),\quad h_1(n)=-h_0(n)\sum_{j=1}^{N}\nu_j(n), \tag{3.12}$$

$$\frac{u_{n-1}}{u_n}=(-1)^{N+1}\frac{1}{\beta_0}\prod_{i=1}^{N}\mu_i(n),\quad \frac{v_n}{v_{n-1}}=(-1)^{N+1}\frac{1}{\beta_0}\prod_{i=1}^{N}\nu_i(n). \tag{3.13}$$

As $m=1$ we equating coefficients of λ^{2N+1} from both sides of the second equation of Eq. (3.4),

$$g_0(n)_{t_1}=(\alpha S_0^{(3)}(n)+\beta\hat{S}_{-1}^{(3)}(n))+2\alpha S_{-1}^{(3)}(n)g_1(n)-2\beta f_{-1}(n)\hat{S}_0^{(1)}(n)-2\alpha S_0^{(1)}(n)f_0(n), \tag{3.14}$$

which, together with Eqs. (3.12) and (3.13), implies

$$\begin{aligned}\frac{1}{2}\partial_{t_1}\ln u_n=u_nv_n(-1)^{N+1}&\left[\frac{\alpha\beta_0}{\Pi_{j=1}^{N}\nu_j(n)}-\frac{\beta}{\beta_0}\prod_{j=1}^{N}\mu_j(n)\right]\\&-\alpha\sum_{j=1}^{N}\mu_j(n)+\frac{\beta}{\beta_0}(-1)^{N+1}\prod_{j=1}^{N}\mu_j(n)-\alpha_1\alpha.\end{aligned} \tag{3.15}$$

We now use the original equations (2.15) and (3.13)

$$\frac{1}{2}\partial_{t_1}\ln u_n=(1-u_nv_n)(-1)^{N+1}\left[\frac{\alpha\beta_0}{\Pi_{j=1}^{N}\mu_j(n+1)}+\frac{\beta}{\beta_0}\prod_{j=1}^{N}\mu_j(n)\right]. \tag{3.16}$$

By equating the two expressions of $\frac{1}{2}\partial_{t_1}\ln u_n$, we arrive at

$$w_n=1-u_nv_n=\frac{[\beta_0+(-1)^N\Sigma_{j=1}^{N}\mu_j(n)\Pi_{j=1}^{N}\nu_j(n)+\alpha_1(-1)^N\Pi_{j=1}^{N}\nu_j(n)]\Pi_{j=1}^{N}\mu_j(n+1)}{\beta_0[\Pi_{j=1}^{N}\mu_j(n+1)+\Pi_{j=1}^{N}\nu_j(n)]}. \tag{3.17}$$

Let us consider the function $\det W_n$, which is a $(2N+2)$th-order polynomial in ζ ($\zeta_j=\lambda_j^2$) with constant coefficients of the n flow and t_m flow,

$$-\det W_n=f^2(n)+g(n)h(n)=\prod_{j=1}^{2N+2}(\zeta-\zeta_j)=R(\zeta). \tag{3.18}$$

Substituting Eq. (3.5) into Eq. (3.14) and comparing the coefficients of ζ^{2N+1} and ζ^0 yield

$$\alpha_1=-\frac{1}{2}\sum_{j=1}^{2N+2}\zeta_j,\quad \beta_0=\prod_{j=1}^{2N+2}\lambda_j,\quad 2\beta_0\beta_1=-\sum_{j_1<\cdots<j_{2N+1}}\zeta_{j_1}\cdots\zeta_{j_{2N+1}}. \tag{3.19}$$

Using Eqs. (3.11) and (3.4), we have

$$f(n)|_{\zeta=\mu_k(n)}=\sqrt{R(\mu_k(n))},\quad f(n)|_{\zeta=\nu_k(n)}=\sqrt{R(\nu_k(n))}, \tag{3.20}$$

$$\begin{aligned}
&\frac{\mu_k(n)_{t_1}}{\sqrt{R(\mu_k(n))}}=\frac{u_n^{-1}[\lambda^{-1}B^{(1)}(n)]|_{\zeta=\mu_k(n)}}{\Pi_{i=1,i\neq k}^{N}(\mu_k(n)-\mu_i(n))},\\
&\frac{\nu_k(n)_{t_1}}{\sqrt{R(\nu_k(n))}}=\frac{-v_{n-1}^{-1}[\lambda^{-1}C^{(1)}(n)]|_{\zeta=\nu_k(n)}}{\Pi_{i=1,i\neq k}^{N}(\nu_k(n)-\nu_i(n))},
\end{aligned}\qquad 1\leqslant k\leqslant N, \tag{3.21}$$

with

$$u_n^{-1}[\lambda^{-1}B^{(1)}(n)]|_{\zeta=\mu_k(n)}=2\alpha+\frac{2\beta(-1)^N}{\beta_0\mu_k(n)}\prod_{i=1}^{N}\mu_i(n),$$

$$v_{n-1}^{-1}[\lambda^{-1}C^{(1)}(n)]|_{\zeta=\nu_k(n)}=2\alpha+\frac{2\beta(-1)^N}{\beta_0\nu_k(n)}\prod_{i=1}^{N}\nu_i(n).$$

Then we have

$$\begin{aligned}
&\frac{\mu_k(n)_x}{\sqrt{R(\mu_k(n))}}=\frac{1-\frac{(-1)^N}{\beta_0\mu_k(n)}\Pi_{i=1}^{N}\mu_i(n)}{\Pi_{i=1,i\neq k}^{N}(\mu_k(n)-\mu_i(n))},\\
&\frac{\nu_k(n)_x}{\sqrt{R(\nu_k(n))}}=\frac{-1+\frac{(-1)^N}{\beta_0\nu_k(n)}\Pi_{i=1}^{N}\nu_i(n)}{\Pi_{i=1,i\neq k}^{N}(\nu_k(n)-\nu_i(n))},
\end{aligned}\qquad 1\leqslant k\leqslant N, \tag{3.22}$$

$$\begin{aligned}
&\frac{\mu_k(n)_t}{\sqrt{R(\mu_k(n))}}=\frac{1+\frac{(-1)^N}{\beta_0\mu_k(n)}\Pi_{i=1}^{N}\mu_i(n)}{\Pi_{i=1,i\neq k}^{N}(\mu_k(n)-\mu_i(n))},\\
&\frac{\nu_k(n)_t}{\sqrt{R(\nu_k(n))}}=\frac{-1-\frac{(-1)^N}{\beta_0\nu_k(n)}\Pi_{i=1}^{N}\nu_i(n)}{\Pi_{i=1,i\neq k}^{N}(\nu_k(n)-\nu_i(n))},
\end{aligned}\qquad 1\leqslant k\leqslant N. \tag{3.23}$$

Therefore, if the $(2N+2)$ distinct parameters $\lambda_1,\ldots,\lambda_{2N+2}$ $(|\lambda_k|\neq|\lambda_j|,k\neq j)$ are given, and let $\mu_k(n)$ and $\nu_k(n)$ be solutions of ordinary differential equations (3.22) and (3.23), then (u_n,v_n) determined by Eq. (3.13) solves the coupled discrete nonlinear Schrödinger equation (2.16) and the coupled discrete mKdV equation (2.17). This means that the function w_n by Eq. (2.18) or Eq. (3.17) is a solution of the $(2+1)$-dimensional Toda equation (2.19).

IV. STRAIGHTENING OUT OF THE CONTINUOUS FLOW

In this section, we shall discuss straightening out of the corresponding continuous flow. We first introduce the Riemann surface Γ of the hyperelliptic curve $\xi^2=R(\zeta),R(\zeta)=\Pi_{j=1}^{2N+2}(\zeta-\zeta_j)$, of genus N. On Γ there are two infinite points ∞_1 and ∞_2, which are not branch points of Γ. Equip Γ with the canonical basis of cycles: $a_1,\ldots,a_N$; $b_1,\ldots,b_N$, and the holomorphic differentials

$$\tilde{\omega}_l=\frac{\zeta^{l-1}\,d\zeta}{\sqrt{R(\zeta)}},\quad 1\leqslant l\leqslant N.$$

Then the period matrices A and B defined by

$$A_{ij}=\int_{a_j}\tilde{\omega}_i, \quad B_{ij}=\int_{b_j}\tilde{\omega}_i,$$

are invertible.[20,21] Let $C=A^{-1}$, $\tau=A^{-1}B$. If we normalize $\tilde{\omega}_l$ into the new basis ω_j

$$\omega_j=\sum_{l=1}^{N} C_{jl}\tilde{\omega}_l, \quad 1\leqslant j\leqslant N, \tag{4.1}$$

then we have

$$\int_{a_i}\omega_j=\delta_{ji}, \quad \int_{b_i}\omega_j=\tau_{ji}. \tag{4.2}$$

Now we introduce the Abel map $\mathcal{A}(P)$

$$\mathcal{A}(P)=\int_{P_0}^{P}\omega,$$

which can be extended linearly to the whole divisor group of Γ, $\mathcal{A}$: $\mathrm{Div}(\Gamma)\to\mathcal{J}(\Gamma)=\mathbb{C}^N/\mathcal{T}$, where the lattice $\mathcal{T}$ is spanned by the periodic vectors $\{\delta_k,\tau_k\}$ with components given by Eq. (4.2). The Abel–Jacobi coordinates are defined as

$$\rho^{(1)}(n)=\mathcal{A}\left(\sum_{k=1}^{N} P(\mu_k(n))\right)=\sum_{k=1}^{N}\int_{P_0}^{P(\mu_k(n))}\omega, \tag{4.3}$$

$$\rho^{(2)}(n)=\mathcal{A}\left(\sum_{k=1}^{N} P(\nu_k(n))\right)=\sum_{k=1}^{N}\int_{P_0}^{P(\nu_k(n))}\omega, \tag{4.4}$$

where $P(\mu_k(n))=(\zeta=\mu_k(n),\xi=\sqrt{R(\mu_k(n))})$, $P(\nu_k(n))=(\zeta=\nu_k(n),\xi=\sqrt{R(\nu_k(n))})\in\Gamma$, and P_0 is chosen a base point on Γ. The components of the Abel–Jacobi coordinates in Eqs. (4.3) and (4.4) read

$$\rho_j^{(1)}(n,x,t)=\sum_{k=1}^{N}\int_{P_0}^{P(\mu_k(n,x,t))}\omega_j=\sum_{k=1}^{N}\sum_{l=1}^{N}C_{jl}\int_{\zeta(P_0)}^{\mu_k(n)}\frac{\zeta^{l-1}\,d\zeta}{\sqrt{R(\zeta)}}, \quad 1\leqslant j\leqslant N, \tag{4.5}$$

$$\rho_j^{(2)}(n,x,t)=\sum_{k=1}^{N}\int_{P_0}^{P(\nu_k(n,x,t))}\omega_j=\sum_{k=1}^{N}\sum_{l=1}^{N}C_{jl}\int_{\zeta(P_0)}^{\nu_k(n)}\frac{\zeta^{l-1}\,d\zeta}{\sqrt{R(\zeta)}}, \quad 1\leqslant j\leqslant N, \tag{4.6}$$

where $\lambda(P_0)$ is the local coordinates of P_0. By using Eqs. (4.5) and (3.22), we have

$$\begin{aligned}\partial_x\rho_j^{(1)}(n)&=\sum_{l=1}^{N}\sum_{k=1}^{N}C_{jl}\frac{\mu_k^{l-1}(n)\mu_k(n)_x}{\sqrt{R(\mu_k(n))}}\\&=\sum_{l=1}^{N}\sum_{k=1}^{N}\left[1-\frac{(-1)^N}{\beta_0\mu_k(n)}\prod_{i=1}^{N}\mu_i(n)\right]\frac{\mu_k^{l-1}(n)C_{jl}}{\Pi_{i\neq k}^{N}(\mu_k(n)-\mu_i(n))},\end{aligned}$$

which implies

$$\partial_x\rho_j^{(1)}(n)=C_{jN}+\frac{1}{\beta_0}C_{j1}=\Omega_j^{(1)}, \quad 1\leqslant j\leqslant N \tag{4.7}$$

in view of the equalities

$$\sum_{k=1}^{N}\frac{1}{\mu_k(n)\Pi_{i\neq k}^{N}(\mu_k(n)-\mu_i(n))}=\frac{(-1)^{N+1}}{\Pi_{i=1}^{N}\mu_i(n)},$$
$$\sum_{k=1}^{N}\frac{\mu_k^{l-1}(n)}{\Pi_{i\neq k}^{N}(\mu_k(n)-\mu_i(n))}=\delta_{lN},\quad 1\leqslant l\leqslant N. \tag{4.8}$$

In a similar way, we obtain from Eqs. (4.5), (4.6), (3.22), and (3.23) that

$$\partial_t\rho_j^{(1)}(n)=C_{jN}-\frac{1}{\beta_0}C_{j1}=\Omega_j^{(2)}, \tag{4.9}$$

$$\partial_x\rho_j^{(2)}(n)=-\Omega_j^{(1)},\quad \partial_t\rho_j^{(2)}(n)=-\Omega_j^{(2)},\quad 1\leqslant j\leqslant N. \tag{4.10}$$

V. STRAIGHTENING OUT OF THE DISCRETE FLOW

Let us denote the fundamental solution matrix of Eq. (2.5) by

$$M_n=(\chi_1(n),\chi_2(n))=\begin{pmatrix}p^{(1)}(n) & p^{(2)}(n)\\ q^{(1)}(n) & q^{(2)}(n)\end{pmatrix},\quad M_0=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

which can be expressed explicitly as

$$M_{n+1}=U_nU_{n-1}\cdots U_0. \tag{5.1}$$

By mathematical induction, it is easy to prove that

$$M_1=\frac{1}{\gamma_0}\begin{pmatrix}\lambda & u_0\\ v_0 & \lambda^{-1}\end{pmatrix},$$

$$M_2=\frac{1}{\gamma_0\gamma_1}\begin{pmatrix}\lambda^2+u_1v_0 & \lambda u_0+\lambda^{-1}u_1\\ \lambda v_1+\lambda^{-1}v_0 & u_0v_1+\lambda^{-2}\end{pmatrix},$$

$$M_3=\frac{1}{\gamma_0\gamma_1\gamma_2}\begin{pmatrix}\lambda^3+\lambda(u_1v_0+u_2v_1)+\lambda^{-1}u_2v_0 & \lambda^2u_0+u_0u_2v_1+\lambda^{-2}u_2\\ \lambda^2v_2+u_1v_0v_2+v_1+\lambda^{-2}v_0 & \lambda u_0v_2+\lambda^{-1}(u_0v_1+u_1v_2)+\lambda^{-3}\end{pmatrix}, \tag{5.2}$$

$$p^{(1)}(n)=\frac{1}{\gamma_0\gamma_1\cdots\gamma_{n-1}}\left\{\lambda^n+\lambda^{n-2}\sum_{j=1}^{n-1}u_jv_{j-1}+\cdots+\lambda^{-n+2}u_{n-1}v_0\right\},$$

$$p^{(2)}(n)=\frac{1}{\gamma_0\gamma_1\cdots\gamma_{n-1}}\left\{\lambda^{n-1}u_0+\lambda^{n-3}u_0\sum_{j=1}^{n-2}u_{j+1}v_j+\cdots+\lambda^{-n+1}u_{n-1}\right\},$$

$$q^{(1)}(n)=\frac{1}{\gamma_0\gamma_1\cdots\gamma_{n-1}}\left\{\lambda^{n-1}v_{n-1}+\lambda^{n-3}\left(v_{n-2}+v_{n-1}\sum_{j=1}^{n-2}u_jv_{j-1}\right)+\cdots+\lambda^{-n+1}v_0\right\},$$

$$q^{(2)}(n)=\frac{1}{\gamma_0\gamma_1\cdots\gamma_{n-1}}\times\left\{\lambda^{n-2}u_0v_{n-1}+\lambda^{n-4}\left(u_1v_{n-1}+u_0v_{n-2}+u_0v_{n-1}\sum_{j=1}^{n-3}u_{j+1}v_j\right)+\cdots+\lambda^{-n}\right\}. \tag{5.3}$$

The Lax matrix W_n satisfies the discrete Lax equation (3.2), $W_{n+1}U_n - U_nW_n = 0$, which implies that the solution space of the linear equation $\chi(n+1) = U_n\chi(n)$ is invariant under the action of W_n. Let ϱ be the eigenvalue of W_n in the solution space, and $\chi(n)$ be the associated eigenfunction, which is called the Baker function (after some normalization):

$$\chi(n+1) = U_n\chi(n), \quad W_n\chi(n) = \varrho\chi(n). \tag{5.4}$$

It is easy to see that $\det|\varrho - W_n| = \varrho^2 - f^2(n) - g(n)h(n) = 0$, which yields the algebraic curve Γ. Thus there are two eigenvalues $\varrho^{\pm} = \pm\varrho$, whereby (3.18):

$$\varrho = \sqrt{f^2(n) + g(n)h(n)} = \sqrt{R(\zeta)}. \tag{5.5}$$

An elementary discussion shows that the corresponding Baker functions can be taken as

$$\chi^{\pm}(n) = \chi_1(n) + b^{\pm}\chi_2(n), \tag{5.6}$$

$$\hat{\chi}^{\pm}(n) = c^{\pm}\chi_1(n) + \chi_2(n) \tag{5.7}$$

with

$$b^{\pm} = \frac{\pm\varrho - f(0)}{g(0)}, \quad c^{\pm} = \frac{f(0) \pm \varrho}{h(0)}. \tag{5.8}$$

Theorem 5.1: (Formulas of Dubrovin–Novikov's type): Let $p^{\pm}(n,\lambda)$ and $q^{\pm}(n,\lambda)$ be the first component and the second one, respectively, of the Baker functions $\chi^{\pm}(n,\lambda)$ and $\hat{\chi}^{\pm}(n,\lambda)$. Then

$$p^+(n,\lambda)p^-(n,\lambda) = \frac{g(n)}{g(0)} = \frac{u_n}{u_0}\prod_{j=1}^{N}\frac{\zeta - \mu_j(n)}{\zeta - \mu_j(0)}, \tag{5.9}$$

$$q^+(n,\lambda)q^-(n,\lambda) = \frac{h(n)}{h(0)} = \frac{v_{n-1}}{v_{-1}}\prod_{j=1}^{N}\frac{\zeta - \nu_j(n)}{\zeta - \nu_j(0)}. \tag{5.10}$$

Proof: Resorting to Eq. (5.1) and the first expression of Eq. (3.2), we have

$$W_nM_n = M_nW_0, \tag{5.11}$$

from which a direct calculation derives Eqs. (5.9) and (5.10).

Proposition 5.2: For $\lambda \to \infty$, we have

$$\begin{aligned} p^+(n,\lambda) &= \frac{\lambda^n}{\gamma_0\cdots\gamma_{n-1}}\{1 + O(\lambda^{-2})\}, \\ p^-(n,\lambda) &= \gamma_0\cdots\gamma_{n-1}\frac{u_n\lambda^{-n}}{u_0}\{1 + O(\lambda^{-2})\}, \end{aligned} \tag{5.12}$$

$$\begin{aligned} q^+(n,\lambda) &= \frac{v_{n-1}\lambda^n}{\gamma_0\cdots\gamma_{n-1}v_{-1}}\{1 + O(\lambda^{-2})\}, \\ q^-(n,\lambda) &= \gamma_0\cdots\gamma_{n-1}\lambda^{-n}\{1 + O(\lambda^{-2})\}. \end{aligned} \tag{5.13}$$

Proof: By using Eqs. (5.5) and (3.5), we obtain

$$\varrho = \lambda^{2(N+1)}\{1 + \alpha_1\lambda^{-2} + O(\lambda^{-4})\}, \tag{5.14}$$

which implies

$$b^+=v_{-1}\lambda^{-1}\{1+O(\lambda^{-2})\},\quad b^-=-\frac{\lambda}{u_0}\{1+O(\lambda^{-2})\},$$
$$c^+=\frac{\lambda}{v_{-1}}\{1+O(\lambda^{-2})\},\quad c^-=-u_0\lambda^{-1}\{1+O(\lambda^{-2})\}. \tag{5.15}$$

Set Eq. (5.3) and the first expression of Eq. (5.15) into $p^+(n,\lambda)=p^{(1)}(n,\lambda)+b^+p^{(2)}(n,\lambda)$, we have the first expression of Eq. (5.12). The estimation of the second expression of Eq. (5.12) for $p^-(n,\lambda)$ is obtained from the first one and

$$p^+(n,\lambda)p^-(n,\lambda)=\frac{u_n}{u_0}\{1+O(\lambda^{-2})\}.$$

Similarly, we can prove Eq. (5.13).

According to Eq. (5.8), it is easy to see that λb^+ and λb^-, λc^+ and λc^- are functions of ζ, which can be regarded as the values of the single-valued functions $[\lambda b](P)$ and $[\lambda c](P)$ on the upper and lower sheets of Γ, respectively. Moreover, it is obvious that the following functions are polynomials of $\zeta=\lambda^2$ with degrees as tabled:

$\lambda^{2k-2}p^{(1)}(2k)$	$2k-1$	$\lambda^{2k-1}p^{(1)}(2k+1)$	$2k$
$\lambda^{2k-1}p^{(2)}(2k)$	$2k-1$	$\lambda^{2k}p^{(2)}(2k+1)$	$2k$
$\lambda^{2k-1}q^{(1)}(2k)$	$2k-1$	$\lambda^{2k}q^{(1)}(2k+1)$	$2k$
$\lambda^{2k}q^{(2)}(2k)$	$2k-1$	$\lambda^{2k+1}q^{(2)}(2k+1)$	$2k$

Therefore, the following expressions

$$p^\pm(2k,\lambda)=p^{(1)}(2k,\lambda)+(\lambda b^\pm)\left\{\frac{1}{\lambda}p^{(2)}(2k,\lambda)\right\},$$
$$\lambda p^\pm(2k+1,\lambda)=\lambda p^{(1)}(2k+1,\lambda)+(\lambda b^\pm)p^{(2)}(2k+1,\lambda), \tag{5.16}$$

$$q^\pm(2k,\lambda)=(\lambda c^\pm)\left\{\frac{1}{\lambda}q^{(1)}(2k,\lambda)\right\}+q^{(2)}(2k,\lambda),$$
$$\lambda q^\pm(2k+1,\lambda)=(\lambda c^\pm)q^{(1)}(2k+1,\lambda)+\lambda q^{(2)}(2k+1,\lambda), \tag{5.17}$$

determine four meromorphic functions of ζ on Γ: $p(2k,P)$ and $[\lambda p](2k+1,P)$, $q(2k,P)$ and $[\lambda q](2k+1,P)$.

In the local coordinates $z=\zeta^{-1}$, $\hat{\xi}=\zeta^{-N-1}\xi$, the equation of Γ near infinity is written as

$$\hat{\xi}^2-R_*(z)=0,\quad R_*(z)=\prod_{j=1}^{2N+2}(1-\zeta_j z). \tag{5.18}$$

On Γ there are two infinities and two zeros

$$\infty_s=(z=0,\hat{\xi}=(-1)^s),\quad 0_s=(\zeta=0,\xi=(-1)^s\beta_0),\quad s=1,2,$$

which are located on the upper ($s=2$) and lower ($s=1$) sheets, respectively. By Proposition 5.2, the principal asymptotic terms of the four meromorphic functions near ∞_2 are

$$p^+(2k,P)\sim\frac{\zeta^k}{\gamma_0\cdots\gamma_{2k-1}},\quad \lambda p^+(2k+1,P)\sim\frac{\zeta^{k+1}}{\gamma_0\cdots\gamma_{2k}},$$
$$q^+(2k,P)\sim\frac{v_{2k-1}\zeta^k}{v_{-1}\gamma_0\cdots\gamma_{2k-1}},\quad \lambda q^+(2k+1,P)\sim\frac{v_{2k}\zeta^{k+1}}{v_{-1}\gamma_0\cdots\gamma_{2k}},\tag{5.19}$$

and their principal asymptotic terms near ∞_1 are

$$p^-(2k,P)\sim\frac{u_{2k}}{u_0}\gamma_0\cdots\gamma_{2k-1}\zeta^{-k},\quad \lambda p^-(2k+1,P)\sim\frac{u_{2k+1}}{u_0}\gamma_0\cdots\gamma_{2k}\zeta^{-k},$$
$$q^-(2k,P)\sim\gamma_0\cdots\gamma_{2k-1}\zeta^{-k},\quad \lambda q^-(2k+1,P)\sim\gamma_0\cdots\gamma_{2k}\zeta^{-k}.\tag{5.20}$$

Proposition 5.3: For $\lambda\to 0$, we have

$$p^-(n,\lambda)=\frac{u_{n-1}\lambda^{-n}}{\gamma_0\cdots\gamma_{n-1}u_{-1}}\{1+O(\lambda^2)\},$$
$$p^+(n,\lambda)=\gamma_0\cdots\gamma_{n-1}\lambda^n\{1+O(\lambda^2)\},\tag{5.21}$$

$$q^-(n,\lambda)=\frac{\lambda^{-n}}{\gamma_0\cdots\gamma_{n-1}}\{1+O(\lambda^2)\},$$
$$q^+(n,\lambda)=\frac{v_n}{v_{-1}}\gamma_0\cdots\gamma_{n-1}\lambda^n\{1+O(\lambda^2)\}.\tag{5.22}$$

Proof: It is easy to see that

$$\varrho=\beta_0+\beta_1\lambda^2+O(\lambda^4),$$
$$b^+=-v_0\lambda\{1+O(\lambda^2)\},\quad b^-=\frac{1}{u_{-1}\lambda}\{1+O(\lambda^2)\},\tag{5.23}$$
$$c^+=-\frac{1}{v_0\lambda}\{1+O(\lambda^2)\},\quad c^-=u_{-1}\lambda\{1+O(\lambda^2)\}.$$

Substituting Eq. (5.3) and the third expression of Eq. (5.23) into $p^-(n,\lambda)=p^{(1)}(n,\lambda)+b^-p^{(2)}(n,\lambda)$, we obtain the first expression of Eq. (5.21). The second expression of Eq. (5.21) is given from the first one and

$$p^+(n,\lambda)p^-(n,\lambda)=\frac{u_n}{u_0}\prod_{j=1}^{N}\frac{\mu_j(n)}{\mu_j(0)}\{1+O(\lambda^2)\}=\frac{u_{n-1}}{u_{-1}}\{1+O(\lambda^2)\}.$$

In a similar way, Eq. (5.22) can be proved.

Resorting to Proposition 5.3, the principal asymptotic terms of the four meromorphic functions near 0_2 are

$$p^+(2k,P)\sim\gamma_0\cdots\gamma_{2k-1}\zeta^k,\quad \lambda p^+(2k+1,P)\sim\gamma_0\cdots\gamma_{2k}\zeta^{k+1},$$
$$q^+(2k,P)\sim\frac{v_{2k}}{v_{-1}}\gamma_0\cdots\gamma_{2k-1}\zeta^k,\quad \lambda q^+(2k+1,P)\sim\frac{v_{2k+1}\zeta^{k+1}}{v_{-1}\gamma_0\cdots\gamma_{2k}},\tag{5.24}$$

and their principal asymptotic terms near 0_1 are

$$p^-(2k,P)\sim\frac{u_{2k-1}\zeta^{-k}}{u_{-1}\gamma_0\cdots\gamma_{2k-1}},\quad \lambda p^-(2k+1,P)\sim\frac{u_{2k}\zeta^{-k}}{u_{-1}\gamma_0\cdots\gamma_{2k}},$$
$$q^-(2k,P)\sim\frac{\zeta^{-k}}{\gamma_0\cdots\gamma_{2k-1}},\quad \lambda q^-(2k+1,P)\sim\frac{\zeta^{-k}}{\gamma_0\cdots\gamma_{2k}}. \tag{5.25}$$

Based on the Dubrovin–Novikov's formulas Eqs. (5.9), (5.10) and through an elementary analysis, it is easy to see the following assertions.

Proposition 5.4: The Baker function $p(2k,P)$ is of the properties:

(i) N simple poles at $\mu_1(0),\ldots,\mu_N(0)$ and two poles of kth order at ∞_2 and 0_1;
(ii) N simple zeros at $\mu_1(2k),\ldots,\mu_N(2k)$ and two zeros of kth order at ∞_1 and 0_2.

The Baker function $[\lambda p](2k+1,P)$ has

(i) N simple poles at $\mu_1(0),\ldots,\mu_N(0)$, a pole of $(k+1)$th order at ∞_2 and a pole of kth order at 0_1;
(ii) N simple zeros at $\mu_1(2k+1),\ldots,\mu_N(2k+1)$, a zero of kth order at ∞_1 and a zero of $(k+1)$th order at 0_2.

Proposition 5.5: The Baker function $q(2k,P)$ is of the properties:

(i) N simple poles at $\nu_1(0),\ldots,\nu_N(0)$ and two poles of kth order at ∞_2 and 0_1;
(ii) N simple zeros at $\nu_1(2k),\ldots,\nu_N(2k)$ and two zeros of kth order at ∞_1 and 0_2.

The Baker function $[\lambda q](2k+1,P)$ has

(i) N simple poles at $\nu_1(0),\ldots,\nu_N(0)$, a pole of $(k+1)$th order at ∞_2 and a zero of $(k+1)$th order at 0_2;
(ii) N simple zeros at $\nu_1(2k+1),\ldots,\nu_N(2k+1)$, a zero of kth order at ∞_1 and a pole of kth order at 0_1.

Theorem 5.6: (Straightening out of the discrete flow)

$$\rho^{(s)}(2k)-\rho^{(s)}(0)=2\Omega^{(0)}k\pmod{\mathcal{T}}, \tag{5.26}$$

$$\rho^{(s)}(2k+1)-\rho^{(s)}(0)=2\Omega^{(0)}k+\eta_2\pmod{\mathcal{T}} \tag{5.27}$$

or

$$\rho^{(s)}(n)-\rho^{(s)}(0)=\Omega^{(0)}n+[1-(-1)^n]\eta_0\pmod{\mathcal{T}}, \tag{5.28}$$

where $\mathcal{T}$ is the lattice spanned by the periodic vectors, and

$$\Omega^{(0)}=\tfrac{1}{2}(\eta_2-\eta_1),\quad \eta_0=\tfrac{1}{4}(\eta_1+\eta_2),\quad \eta_s=\int_{0_s}^{\infty_s}\omega,\quad s=1,2.$$

Proof: For $n=2k$, we introduce the meromorphic differential on Γ:

$$\omega(2k)=\left\{\frac{d}{d\zeta}\ln p(2k,P)\right\}d\zeta \tag{5.29}$$

which has poles at $\mu_j(0)$ and $\mu_j(2k)$ with the residues $-1,1$, respectively, and poles at ∞_1, ∞_2, 0_1, 0_2 with the residues k, $-k$, $-k,k$, respectively. Let Ω be the Abel differential of the second kind, and $\omega(P,Q)$ be the normal Abel differential of the third kind with the residue $1,-1$ at P,Q, respectively, and the properties

$$\int_{a_j}\omega(P,Q)=0,\quad \int_{b_j}\omega(P,Q)=2\pi\sqrt{-1}\int_Q^P\omega_j.$$

Here ω_j is the normalized Abel differential of the first kind given by (4.1). Then the differential (2.25) can be expressed as a linear combination of Ω, $\omega(P,Q)$ and ω_j in view of the poles, that is

$$\omega(2k)=\Omega+k\omega[\infty_1,\infty_2]+k\omega[0_2,0_1]+\sum_{j=1}^N\omega[\mu_j(2k),\mu_j(0)]+\sum_{j=1}^N e_j\omega_j, \tag{5.30}$$

where e_j's are some complex numbers. Integrating Eq. (5.30) along a_l and b_l, we obtain that $e_l=2\pi n_l\sqrt{-1}$ and

$$\sum_{j=1}^N\int_{\mu_j(0)}^{\mu_j(2k)}\omega_l=k\left(\int_{0_2}^{\infty_2}-\int_{0_1}^{\infty_1}\right)\omega_l+m_l-\sum_{j=1}^N n_j\tau_{jl}, \tag{5.31}$$

where n_l and m_l are certain integers. This completes the proof of Eq. (5.26) for $s=1$.

For $n=2k+1$, consider the meromorphic differential

$$\begin{aligned}\omega(2k+1)&=\left\{\frac{d}{d\zeta}\ln[\lambda p](2k+1,P)\right\}d\zeta\\&=\Omega+k\omega[\infty_1,\infty_2]+k\omega[0_2,0_1]+\omega[0_2,\infty_2]\\&\quad+\sum_{j=1}^N\omega[\mu_j(2k+1),\mu_j(0)]+\sum_{j=1}^N\hat{e}_j\omega_j,\end{aligned} \tag{5.32}$$

which implies Eq. (5.27) for $s=1$. Similarly, we can prove Eqs. (5.26) and (5.27) for $s=2$.

Note: Now we have a clear evolution picture of the continuous flows and discrete flow through the Abel–Jacobi coordinates: (i) they are straightened out; (ii) they commute each other. Therefore, the compatible solution of various flows are obtained simply by a linear superposition. Specifically, we have

$$\begin{aligned}\rho^{(1)}(n,x)&=\Omega^{(0)}n+\Omega^{(1)}x+[1-(-1)^n]\eta_0+\rho_0^{(1)},\\\rho^{(2)}(n,x)&=\Omega^{(0)}n-\Omega^{(1)}x+[1-(-1)^n]\eta_0+\rho_0^{(2)},\end{aligned} \tag{5.33}$$

for the coupled discrete nonlinear Schrödinger equation (2.16) and

$$\begin{aligned}\rho^{(1)}(n,t)&=\Omega^{(0)}n+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\rho_0^{(1)},\\\rho^{(2)}(n,t)&=\Omega^{(0)}n-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\rho_0^{(2)},\end{aligned} \tag{5.34}$$

for the coupled discrete mKdV equation (2.17), where

$$\Omega^{(1)}=(\Omega_1^{(1)},\ldots,\Omega_N^{(1)})^T,\quad \Omega^{(2)}=(\Omega_1^{(2)},\ldots,\Omega_N^{(2)})^T,$$

$$\rho_0^{(1)}=\sum_{k=1}^N\int_{P_0}^{P(\mu_k(0))}\omega,\quad \rho_0^{(2)}=\sum_{k=1}^N\int_{P_0}^{P(\nu_k(0))}\omega.$$

Further, for the $(2+1)$-dimensional Toda lattice (2.19) we have

$$\begin{aligned}\rho^{(1)}(n,x,t)&=\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\rho_0^{(1)},\\ \rho^{(2)}(n,x,t)&=\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\rho_0^{(2)}.\end{aligned}\tag{5.35}$$

VI. EXPLICIT SOLUTIONS

The expression (5.30) gives the explicit solution of the $(2+1)$-dimensional Toda lattice equation (2.19) in the Abel–Jacobi coordinates $(\rho^{(1)}(n),\rho^{(2)}(n))$. In order to get the solution in the original coordinate w_n, the following steps should be completed:

$$(\rho^{(1)}(n),\rho^{(2)}(n))\to(\mu_j(n),\nu_j(n))\to(u_n,v_n)\to w_n.$$

To this end, we consider the Riemann theorem,[20,21] which asserts that there exist constant vectors $M^{(1)}$ and $M^{(2)}$ (the Riemann constants) such that $\theta(\mathcal{A}(P(\zeta))-\rho^{(l)}(n)-M^{(l)})$ has exactly N zeros at $\mu_1(n),\cdots,\mu_N(n)$ for $l=1$ or $\nu_1(n),\cdots,\nu_N(n)$ for $l=2$. Through a standard treatment,[22–24] we obtain

$$\ln\prod_{j=1}^{N}\mu_j(n)=\ln\frac{\theta(\mathcal{A}(0_1)-\rho^{(1)}(n)-M^{(1)})\,\theta(\mathcal{A}(0_2)-\rho^{(1)}(n)-M^{(1)})}{\theta(\mathcal{A}(\infty_1)-\rho^{(1)}(n)-M^{(1)})\,\theta(\mathcal{A}(\infty_2)-\rho^{(1)}(n)-M^{(1)})}+\sum_{j=1}^{N}\int_{a_j}\ln\lambda\,\omega_j,\tag{6.1}$$

$$\ln\prod_{j=1}^{N}\nu_j(n)=\ln\frac{\theta(\mathcal{A}(0_1)-\rho^{(2)}(n)-M^{(2)})\,\theta(\mathcal{A}(0_2)-\rho^{(2)}(n)-M^{(2)})}{\theta(\mathcal{A}(\infty_1)-\rho^{(2)}(n)-M^{(2)})\,\theta(\mathcal{A}(\infty_2)-\rho^{(2)}(n)-M^{(2)})}+\sum_{j=1}^{N}\int_{a_j}\ln\lambda\,\omega_j,\tag{6.2}$$

$$\sum_{j=1}^{N}\mu_j(n)=\frac{1}{2}(\partial_x+\partial_t)\ln\frac{\theta(\rho^{(1)}(n)+M^{(1)}-\mathcal{A}(\infty_1))}{\theta(\rho^{(1)}(n)+M^{(1)}-\mathcal{A}(\infty_2))}+\sum_{j=1}^{N}\int_{a_j}\lambda\,\omega_j,\tag{6.3}$$

$$\sum_{j=1}^{N}\nu_j(n)=\frac{1}{2}(\partial_x+\partial_t)\ln\frac{\theta(\rho^{(2)}(n)+M^{(2)}-\mathcal{A}(\infty_2))}{\theta(\rho^{(2)}(n)+M^{(2)}-\mathcal{A}(\infty_1))}+\sum_{j=1}^{N}\int_{a_j}\lambda\,\omega_j.\tag{6.4}$$

According to Eqs. (5.35), (6.1)–(6.4) can be written as

$$\begin{aligned}\ln\prod_{j=1}^{N}\mu_j(n)=&\ln\frac{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_1)}{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_2)}\\&+\ln\frac{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_1)}{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_2)}+\varrho_0,\end{aligned}\tag{6.5}$$

$$\begin{aligned}\ln\prod_{j=1}^{N}\nu_j(n)=&\ln\frac{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_3)}{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_4)}\\&+\ln\frac{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_3)}{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_4)}+\varrho_0,\end{aligned}\tag{6.6}$$

$$\sum_{j=1}^{N}\mu_j(n)=\frac{1}{2}(\partial_x+\partial_t)\ln\frac{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_2)}{\theta(\Omega^{(0)}n+\Omega^{(1)}x+\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_2)}+\varrho_1,\tag{6.7}$$

$$\sum_{j=1}^{N}\nu_j(n)=\frac{1}{2}(\partial_x+\partial_t)\ln\frac{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\hat\kappa_4)}{\theta(\Omega^{(0)}n-\Omega^{(1)}x-\Omega^{(2)}t+[1-(-1)^n]\eta_0+\kappa_4)}+\varrho_1,\tag{6.8}$$

where

$$\kappa_1=\rho_0^{(1)}+M^{(1)}-\mathcal{A}(0_1),\quad \hat{\kappa}_1=\rho_0^{(1)}+M^{(1)}-\mathcal{A}(0_2),$$

$$\kappa_2=\rho_0^{(1)}+M^{(1)}-\mathcal{A}(\infty_1),\quad \hat{\kappa}_2=\rho_0^{(1)}+M^{(1)}-\mathcal{A}(\infty_2),$$

$$\kappa_3=\rho_0^{(2)}+M^{(2)}-\mathcal{A}(0_1),\quad \hat{\kappa}_3=\rho_0^{(2)}+M^{(2)}-\mathcal{A}(0_2),$$

$$\kappa_4=\rho_0^{(2)}+M^{(2)}-\mathcal{A}(\infty_1),\quad \hat{\kappa}_4=\rho_0^{(2)}+M^{(2)}-\mathcal{A}(\infty_2),$$

$$\varrho_0=\sum_{j=1}^{N}\int_{a_j}\ln\lambda\,\omega_j,\quad \varrho_1=\sum_{j=1}^{N}\int_{a_j}\lambda\,\omega_j.$$

Substituting Eqs. (6.5)–(6.8) into Eqs. (3.17) yields quasiperiodic solutions of the $(2+1)$-dimensional Toda equation (2.19).

ACKNOWLEDGMENTS

One of the authors (X.G.G.) acknowledges the support by National Natural Science Foundation of China (Project No. 10071075) and the Special Funds for Chinese Major State Basic Research Project ''Nonlinear Science.'' The work described in this paper was supported by a grant from the Research Grants Council of the HKSAR, China (Project No. 9040644).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Unifying scheme for generating discrete integrable systems including inhomogeneous and hybrid models

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(Received 19 May 2003; accepted 20 May 2003)

A unifying scheme based on an ancestor model is proposed for generating a wide range of integrable discrete and continuum as well as inhomogeneous and hybrid models. They include in particular discrete versions of sine-Gordon, Landau–Lifshitz, nonlinear Schrödinger (NLS), derivative NLS equations, Liouville model, (non-)relativistic Toda chain, Ablowitz–Ladik model, etc. Our scheme introduces the possibility of building a novel class of integrable hybrid systems including multicomponent models like massive Thirring, discrete self-trapping, two-mode derivative NLS by combining different descendant models. We also construct inhomogeneous systems like Gaudin model including new ones like variable mass sine-Gordon, variable coefficient NLS, Ablowitz–Ladik, Toda chains, etc. keeping their flows isospectral, as opposed to the standard approach. All our models are generated from the same ancestor Lax operator (or its $q \to 1$ limit) and satisfy the classical Yang–Baxter equation sharing the same r-matrix. This reveals an inherent universality in these diverse systems, which become explicit at their action-angle level. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604456]

I. INTRODUCTION

Though integrable models represent only a special class of nonlinear systems, their numbers and varieties discovered until today have become amazingly large. Therefore it is particularly important now to have well defined schemes, which will be able to generate them in a systematic way, find out their interrelations, detect the fundamental ones and identify their universal properties. Reduction of Lax operators in AKNS spectral problem,[1] classification of soliton bearing equations through self-dual Yang–Mills equation,[2] gauge unification of nonlinear Schrödinger (NLS)-type models[3] are few of such successful approaches. However most of these schemes are designed to deal with the continuous models only, whereas the importance and significance of discrete integrable systems have been well emphasized in recent years.[4] Moreover, the algebraic approach in classical integrable models, though it has a rich and sophisticated formulation through the classical Yang–Baxter equation and the classical r-matrix,[5] as it appears, has not been exploited fully.

Our aim here is therefore to propose an unified algebraic scheme for systematic generation of a large class of integrable discrete models, based on their underlying Poisson bracket (PB) structure. The specialty of this class of models is that they can be easily quantized to yield the corresponding quantum integrable systems and their classification may be done through the associated classical r-matrix with its known trigonometric and rational solutions. We present an integrable discrete ancestor model linked with the trigonometric r-matrix (and its $q \to 1$ form related naturally to the rational solution of r) and containing a set of arbitrary parameters. Various choices of these external parameters define in turn different underlying algebraic structures and the associated Lax operators. This generates through suitable realizations a wide range of diverse integrable systems sharing the same r-matrix with their ancestor model. They are by construction

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integrable discrete models with few of them having also well defined field limits.

Our scheme, the basic idea of which is borrowed from the quantum domain,[6,7] appears to be effective not only in classifying an important class of discrete models as well as their field limits, but also their inhomogeneous extensions. Along with the exactly integrable discrete versions of the well known models like sine-Gordon, Landau–Lifshitz equation, NLS, derivative NLS (DNLS), Liouville model, relativistic and nonrelativistic Toda chain, Ablowitz–Ladik model, we also obtain new inhomogeneous models like variable mass sine-Gordon and more general variable coefficient NLSs, as well as Gaudin model, inhomogeneous Ablowitz–Ladik model and Toda chains. As an important application of our scheme we may construct novel families of integrable hybrid models, by combining different descendant models in different domains of the lattice space (very recently such field models attracted attention[8]), or by fusing copies of a single component model to get its multicomponent generalization. Moreover, the present method of generating integrable inhomogeneous discrete and continuum models reveals the intriguing fact that the conventional approach by considering space–time dependent spectral parameter $\lambda(x,t)$[9–14] is rather restricted and even appears to be misleading, since it would lead in general to a dynamical r-matrix spoiling the underlying algebraic structure and forbidding therefore the possible quantization of the models and their usual action-angle formulation. Moreover, for more general inhomogeneous sine-Gordon and NLS models, as we find here, the conventional treatment of nonisospectral flow would be likely to fail. In our approach on the other hand the necessary isospectrality is kept intact by taking constant λ as in the original homogeneous case and the inhomogeneity is introduced through arbitrary parameters, which act like Casimir operators in the associated Poisson algebra.

Since all these models, in spite of their manifestly diverse forms and nature, are generated from the same ancestor model sharing the same r-matrix (or its $q\to 1$ form), it reveals an intriguing universality among them which is reflected prominently in their description of complete integrability through action-angle variables.

The paper is arranged as follows. In Sec. II we review the theory of integrable systems satisfying classical Yang–Baxter equation associated with classical $r(\lambda-\mu)$ matrix. Section III presents the explicit form of the ancestor model and its $q\to 1$ limit together with the underlying PB algebras. We introduce our generating scheme in Sec. IV and construct concrete models. Section V accounts for the generation of integrable inhomogeneous as well as hybrid models. Section VI focuses on the universal property of all descendant models by explicit construction of their action-angle variables. Section VII is the concluding section.

II. CLASSICAL YANG–BAXTER EQUATION AND INTEGRABLE SYSTEMS

By integrability of a nonlinear discrete system defined on a lattice with sites $j=1,2,\ldots,N$, we mean it in the Liouville sense by requiring the existence of its N number of independent conserved quantities $C_n, n=1,2,\ldots,N$ including the Hamiltonian H of the system with the criteria $\{C_n, C_m\}=0$. Such conserved quantities can be considered as the action variables generated from a spectral parameter λ-dependent transfer matrix as: $\tau(\lambda)=\Sigma_{n=1}^{N} C_n \lambda^n$ and consequently the integrability criteria may be replaced by the single condition

$$\{\tau(\lambda),\tau(\mu)\}=0. \tag{1}$$

For deriving this condition therefore along with the conventional linear spectral problem: $T_{k+1}(\lambda)=L_k(\lambda)T_k(\lambda)$ we define also the PB algebra for its Lax operator $L_k(\lambda)$ in a specific form, which is known as the classical Yang–Baxter equation (CYBE)[5]

$$\{L_k(\lambda)\otimes, L_l(\mu)\}=\delta_{kl}[r(\lambda-\mu), L_k(\lambda)\otimes L_k(\mu)] \tag{2}$$

associated with the classical $r(\lambda-\mu)$-matrix playing the role of structure constants. For the associativity of algebra (2) ensuring its Jacobi identity, the r-matrix in turn must satisfy another form of CYBE,

$$[r_{12}(\lambda-\mu), r_{13}(\lambda-\delta)]+[r_{12}(\lambda-\mu), r_{23}(\mu-\delta)]+[r_{13}(\lambda-\delta), r_{23}(\mu-\delta)]=0. \tag{3}$$

It is crucial to observe that, though there is a variety of Lax operator solutions to (2) with different basic operators and spectral parameter dependence, representing a wide range of integrable systems (for a list see Sec. IV), the associated r-matrix solutions satisfying (3) are only of three types: elliptic, trigonometric, and rational. Moreover most of the known models are linked to the last two cases only, i.e., to the trigonometric r-matrix,

$$r_t(\lambda-\mu)=\frac{1}{i\sin(\lambda-\mu)}\left(\frac{1}{2}\cos(\lambda-\mu)\sigma_3\otimes\sigma_3+\sigma_+\otimes\sigma_-+\sigma_-\otimes\sigma_+\right) \tag{4}$$

or to its $q\to 1$, $\lambda,\ \mu\to 0$ limit given by the rational solution

$$r_r(\lambda-\mu)=\frac{1}{i(\lambda-\mu)}P, \quad \text{where } P=\tfrac{1}{2}(I+\vec{\sigma}\cdot\vec{\sigma}), \tag{5}$$

P being the permutation operator. The above remarkable observation has motivated us to conjecture that all integrable models satisfying the CYBE (2) must be derivable from an ancestor model with their Lax operators obtained as various reductions of this single ancestor Lax operator and this should make the r-matrix, inherited from their ancestor, to be naturally the same for all these descendant models. In the next section we present such an ancestor model in the explicit form associated with the trigonometric r-matrix (4), from which we will be able to generate a rich collection of integrable discrete and continuum models including inhomogeneous as well as hybrid systems, all satisfying the CYBE and sharing the same r-matrix (4) [or its rational limit (5)]. Note that from the CYBE (2) one can go to its global description

$$\{T_N(\lambda)\otimes, T_N(\mu)\}=[r(\lambda-\mu), T_N(\lambda)\otimes T_N(\mu)] \tag{6}$$

for the monodromy matrix

$$T_N(\lambda)=L_N(\lambda)\cdots L_1(\lambda)=\begin{pmatrix} a_N(\lambda) & b_N(\lambda)\\ c_N(\lambda) & d_N(\lambda)\end{pmatrix}. \tag{7}$$

It is important to notice that (6) exhibits exactly the same form as its local relation (2), which reflects a deep underlying Hopf algebra structure, an important characteristic of all such integrable systems.[15] Defining now the transfer matrix as $\tau(\lambda)=\mathrm{tr}T_N(\lambda)=a_N(\lambda)+d_N(\lambda)$ and taking the trace of (6) one can easily derive (since the rhs being the trace of a commutator is zero) the integrability condition (1) for the system. Therefore going backwards in the logical chain we can conclude that the nonlinear systems with its representative Lax operator and the r-matrix satisfying the CYBE (2) must be an integrable system. We shall see below that the relation (6) also carries important information for deriving action-angle variables and reflects an universal property for all integrable systems sharing the same r-matrix and hence belonging to the same class.

Note that in this algebraic approach we are not concerned about the usual Lax pair L,M and do not obtain the dynamical equation from the flatness condition involving them. We on the other hand take the Lax operator $L_k(\lambda)$ satisfying the CYBE as the representative of the integrable model and using it construct the monodromy matrix: $T(\lambda)=\Pi_k L_k(\lambda)$ and then the transfer matrix from its trace $\tau(\lambda)=\mathrm{tr}T(\lambda)$. Expanding further the transfer matrix $\tau(\lambda)$ in spectral parameter λ as described above, we derive the conserved quantities including the Hamiltonian H in the explicit form. The dynamical equation can now be obtained as the Hamilton equation $\psi_t=\{\psi,H\}$, using the fundamental PB relations.

At the lattice constant $\Delta\to 0$ one may recover in some cases the corresponding field model: $L_k(\lambda)\to I+\Delta\mathcal{L}(x,\lambda)+O(\Delta^2)$ with $\mathcal{L}(x,\lambda)$ as the field Lax operator. Though the associated r-matrix remains the same, the CYBE gets deformed and the corresponding monodromy matrix $T(\lambda)$ at the infinite interval limit $l=N\Delta\to\infty$ satisfies also a bit different global CYBE.[5] For continuum models one can extract the conserved quantities more conveniently from the Lax operator using the Ricatti equation derived from the linear spectral problem.

III. ANCESTOR MODELS ASSOCIATED WITH TRIGONOMETRIC AND RATIONAL *r*-MATRIX

As mentioned, our generating scheme for integrable models is based on various reductions of a discrete ancestor Lax operator, which we propose to take in the following form:[7]

$$L_k^{\mathrm{trig(anc)}}(\xi)=\begin{pmatrix} \xi c_1^+ e^{i\alpha S_k^3}+\xi^{-1}c_1^- e^{-i\alpha S_k^3} & 2\sin\alpha S_k^- \\ 2\sin\alpha S_k^+ & \xi c_2^+ e^{-i\alpha S_k^3}+\xi^{-1}c_2^- e^{i\alpha S_k^3} \end{pmatrix}, \quad \xi=e^{i\lambda}, \tag{8}$$

and demand it to satisfy the CYBE (2) with the trigonometric r-matrix (4). $\vec{S}_k$ appearing in (8) are the basic dynamical fields PB algebra of which as specified below is dictated by its integrability and $c_a^{\pm}, a=1,2$ are a set of arbitrary parameters. The structure of the Lax operator (8) becomes clearer if we notice its possible decomposition, after an allowed gauge transformation by $h=e^{i\lambda\sigma_3}$, $L^{t(\mathrm{anc})}(\xi)\to hL^{t(\mathrm{anc})}(\xi)h^{-1}=\xi L_+ +\xi^{-1}L_-$, where $L_\pm$ are spectral parameter ξ-free upper/lower triangular matrices. Note that the r-matrix (4) allows also a similar decomposition (after a similar gauge transformation):

$$r_t\left(\frac{\xi}{\eta}\right)\to\frac{\xi}{\eta}r_+ +\left(\frac{\xi}{\eta}\right)^{-1}r_-, \quad \xi=e^{i\lambda}, \quad \eta=e^{i\mu}$$

with $r_\pm$ being spectral-free upper/lower triangular matrices, which together with $L_\pm$ satisfy the FRT-type[16] PB algebra derivable from the CYBE.[17] The demand of integrability on (8) through the CYBE can be shown to be equivalent to the underlying general algebra

$$\{S_k^3,S_l^\pm\}=\pm i\delta_{kl}S_k^\pm, \quad \{S_k^+,S_l^-\}=i\frac{\delta_{kl}}{\sin\alpha}f(2\alpha S_k^3), \quad \text{with } f(x)=(M^+\sin(x)+M^-\cos(x)), \tag{9}$$

where $M^\pm=\pm\frac{1}{2}\sqrt{\pm 1}(c_1^+c_2^-\pm c_1^-c_2^+)$ are arbitrary parameters acting as central elements with trivial brackets with all others: $\{M^\pm,\cdot\}=0$ and in general may also be site and time dependent. It is important to note that the underlying PB structure (9) is linked with a generalization of the well known quantum group algebra. For generating integrable systems from this ancestor model, we find first a realization of (9) in canonical variables $\{u_k,p_l\}=\delta_{kl}$, in the form

$$S_k^3=u_k, \quad S_k^+=e^{-ip_k}g(u_k), \quad S_k^-=g(u_k)e^{ip_k}, \tag{10}$$

where

$$g(u_k)=[\kappa+\sin\alpha(s-u_k)\{f(\alpha(u_k+s+1))\}]^{1/2}\frac{1}{\sin\alpha}, \tag{11}$$

containing free parameters κ, s and function $f(x)$ as defined in (9). It should be remarked here that realization (10) usually assumes the complex conjugacy $S_k^-=(S_k^+)^*$, which however is not imposed by the integrability condition (9). Note that we have now lots of freedom for generating descendant models from the ancestor Lax operator (8) by using various reductions of (11) under different choices of the arbitrary parameters c's as well as κ and s or its further realization in *bosonic* variables: $\{\psi_k,\psi_l^*\}=i\delta_{kl}$ in (10). Moreover we can multiply these Lax operators from left or right by $\sigma_a, a=1,2,3$, since such transformations are allowed by the CYBE due to a symmetry of (4) and (5) as $[r,\sigma_a\otimes\sigma_a]=0$.

We will demonstrate in the next section that a class of discrete integrable systems with nontrivial deformation parameter q, which may be interpreted as the *relativistic* parameter can be generated in a systematic way from the ancestor Lax operator (8). The nonrelativistic models on the other hand may be constructed in a similar way from the $q\to 1$ limit of (8) given as

$$L_k^{\text{rat.(anc)}}(\lambda)=\begin{pmatrix} c_1^0(\lambda+s_k^3)+c_1^1 & s_k^- \\ s_k^+ & c_2^0(\lambda-s_k^3)-c_2^1 \end{pmatrix}, \tag{12}$$

with $c_a^{0,1}, a=0,1$ being arbitrary parameters. Here due to the corresponding limits of $\vec{S}\to\vec{s}$, $\{c_a^{\pm}\}\to\{c_a^{0,1}\}$, $M^+\to -m^+$, $M^-\to -\alpha m^-$, $\xi\to 1+i\lambda$, the PB algebra (9) reduces to

$$\{s_k^+, s_k^-\}=i\delta_{kl}(2m^+ s_k^3+m^-), \quad \{s_k^3, s_l^{\pm}\}=\pm i\delta_{kl}s_k^{\pm}, \tag{13}$$

where $m^+=c_1^0c_2^0$, $m^-=c_1^1c_2^0+c_1^0c_2^1$ with $\{m^{\pm},\cdot\}=0$. Note that a Casimir operator commuting with all other generators of (13) may be constructed as

$$S^2=s_k^3(m^+s_k^3+m^-)+s_k^+s_k^- \tag{14}$$

and a realization of it (13) given by the generalized *Holstein–Primakov* transformation (HPT)

$$\begin{gathered} s_k^3=s-N_k, \quad s_k^+=g_0(N_k)\psi_k, \quad s_k^-=\psi_k^* g_0(N_k), \\ g_0(N_k)=(m^-+m^+(2s-N_k))^{1/2}, \quad N_k\equiv\psi_k^*\psi_k \end{gathered} \tag{15}$$

in bosonic variables ψ_k, which in fact is the $\alpha\to 0$ limit of (10) and (11). We stress again that since the conjugacy of $s_k^{\pm}$ is not necessarily imposed by the integrability, ψ,ψ^* in (15) in general may not be complex conjugates. Note that the ancestor model (12) represents the undeformed rational class and satisfies the CYBE with the rational r-matrix (5). Equations (8) and (12) serving as the ancestor Lax operators for the discrete integrable models may also yield for some systems the corresponding field models with the Lax operator $\mathcal{L}(x,\lambda)$. The associated r-matrix however would remain the same at the continuum limit, since it is a global nondynamical object independent of site indices. We shall see in Sec. V that parameters c's in general can be space–time dependent and hence could induce inhomogeneity in the model preserving the constancy of the spectral parameter.

IV. UNIFIED GENERATION OF DISCRETE INTEGRABLE MODELS

From the ancestor models proposed we generate here integrable discrete models belonging to both trigonometric and rational class.

A. Relativistic models belonging to trigonometric class

For constructing this class of models we start from the ancestor Lax operator (8) and look into its different realizations by choosing first the arbitrary parameters c's as constants.

(1) *Discrete sine-Gordon model:* Parameter choice $c_1^{\pm}=-c_2^{\pm}=m\Delta$, with m as the constant mass. This gives $M^-=0$, $M^+=-(m\Delta)^2$, and reduces realization (10) correspondingly to yield from (8) (after multiplying it from right by $-i\sigma_1$) the Lax operator

$$L_k(\lambda)=\begin{pmatrix} g(u_k)e^{ip_k\Delta} & m\Delta\sin(\lambda+\alpha u_k) \\ m\Delta\sin(\lambda-\alpha u_k) & e^{-ip_k\Delta}g(u_k) \end{pmatrix}, \quad g^2(u_k)=1-(m\Delta)^2\cos\alpha(2u_k+1). \tag{16}$$

It is important to note that (16) yields exactly the Lax operator of the integrable discrete sine-Gordon model[18] and at the continuum limit $\Delta\to 0$, when $e^{\pm ip_k\Delta}\to 1\pm\Delta ip_k$ and $(u_k,p_k)\to(u(x),p(x))$, recovers clearly the field Lax operator

$$\begin{gathered} L_k(\lambda)=1+\Delta\mathcal{L}(x,\lambda), \quad \mathcal{L}(x,\lambda)=ip(x)\sigma_3+m\sin(\lambda+\alpha u(x))\sigma_+ +m\sin(\lambda-\alpha u(x))\sigma_-, \\ p(x)=\dot{u}(x) \end{gathered} \tag{17}$$

of the well-known sine-Gordon model $u_{tt}-u_{xx}+\sin \alpha u=0$. Remarkably the PB algebra (9) in this case reduces to the classical limit of the celebrated *quantum group*[15] with its familiar relation $\{S^+,S^-\}=-i[2S^3]_q$. We will see in the next section that a more general choice for the parameters would lead to an inhomogeneous extension of this sine-Gordon model.

(2) *Discrete Liouville model:* Parameter choice $c_1^+=c_2^-=\Delta$, $c_1^-=c_2^+=0$. This gives $M^{\pm}=\pm\frac{1}{2}\sqrt{\pm 1}\Delta^2$ and correspondingly reduces (10) to derive from the same ancestor (8) (after multiplying it from right by σ_1) the Lax operator

$$L_k(\xi)=\begin{pmatrix} e^{p_k\Delta}g(u_k) & \Delta\xi e^{\alpha u_k} \\ \dfrac{\Delta}{\xi}e^{\alpha u_k} & g(u_k)e^{-p_k\Delta}\end{pmatrix}, \quad g^2(u_k)=1+\Delta^2 e^{\alpha(2u_k+i)}, \tag{18}$$

which represent the discrete Liouville model[19] and at its field limit ($\Delta\to 0$) the Lax operator $\mathcal{L}=p\sigma_3+e^{\alpha u}[\xi\sigma_+ +(1/\xi)\,\sigma_-]$ of the well known Liouville equation: $u_{tt}-u_{xx}=e^{\alpha u}$. Note that in this case (9) gives a novel PB algebra with exponentially deformed relation like $\{S^+,S^-\}=(1/2\sin\alpha)e^{2i\alpha S^3}$.

It is intriguing to observe here that though the underlying PB structure and hence its realization giving the model are fixed by the choice of $M^{\pm}$, the Lax operator (8) which depends directly on the parameters c's may take different forms for the same model. For example, in the present case with additional choice $c_1^-\neq 0$ would record the same values for $M^{\pm}$, but a different Liouville Lax operator.[20] This opens up therefore a promising possibility for systematically obtaining different useful Lax operators for the same integrable model.

(3) *Relativistic Toda chain:* Different sets of constant choices (i) $c_a^+=1$, $a=1,2$, or (ii) $c_a^-=1$, $a=1,2$, or (iii) $c_1^{\mp}=\pm 1$, or (iv) $c_1^+=1$, with the rest of c's being zero, lead to $M^{\pm}=0$, reducing therefore (9) to the simple PB algebra

$$\{S_k^+,S_l^-\}=0, \quad \{S_k^3,S_l^{\pm}]=\pm i\delta_{kl}S_k^{\pm}, \tag{19}$$

and the realization (10) (after a canonical interchange of variables: $u\to -ip$, $p\to -iu$,) to the form

$$S_k^3=-ip_k, \quad S_k^{\pm}=\alpha e^{\mp u_k}. \tag{20}$$

This generates interestingly from the same ancestor Lax operator (8) different forms of the discrete-time or relativistic Toda chain (RTC). For example, case (iii) yields

$$L_k(\xi)=\begin{pmatrix} \dfrac{1}{\xi}e^{\alpha p_k}-\xi e^{-\alpha p_k} & \alpha e^{u_k} \\ -\alpha e^{-u_k} & 0\end{pmatrix}, \tag{21}$$

recovering the Lax operator found in Ref. 21, while (iv) generates a different Lax operator[22] for the same model. More famous RTC model of Suris[23] however is obtained in this approach after performing a *twisting* transformation with twisting parameter taken as $\pm\alpha$ (of these equivalent cases we consider here only $-\alpha$, for definiteness), which deforms the r_t-matrix (4) by adding a constant matrix Ω to it,[21]

$$r_t\to r_\Omega=r_t-\Omega, \quad \text{where } \Omega=i(\sigma_3\otimes I-I\otimes\sigma_3). \tag{22}$$

As a result the form of the ancestor Lax operator (8) also gets changed with its elements transforming as

$$c_a^{\pm}\to c_a^{\pm}e^{i\alpha S_k^3}, \quad S_k^{\pm}\to\widetilde{S}_k^{\pm}=e^{i1/2\,\alpha S_k^3}S_k^{\pm}e^{i1/2\,\alpha S_k^3}. \tag{23}$$

Implementing the corresponding changes in (21) and using the same realization (20) for the variables (23) we obtain now the explicit form of the Lax operator

$$L_k(\xi)=\begin{pmatrix} \frac{1}{\xi}e^{2\alpha p_k}-\xi & \alpha e^{u_k} \\ -\alpha e^{2\alpha p_k-u_k} & 0 \end{pmatrix}, \tag{24}$$

generating that of the Suris RTC.[23]

(4) *Discrete derivative NLS:* Parameter choice as constants,

$$c_1^+=c_2^+=1, \quad c_1^-=-iq\Delta, \quad c_2^-=\frac{i\Delta}{q}, \text{ giving } M^+=2\Delta\sin\alpha, \quad M^-=2i\Delta\cos\alpha \tag{25}$$

gives (10) a q-bosonic realization as $S_k^+=-Q_k$, $S_k^-=Q_k^*$, $S_k^3=-N_k$, with a PB algebra induced from (9) as

$$\{Q_k,N_l\}=i\delta_{kl}Q, \quad \{Q_k,Q_l^*\}=i\delta_{kl}\frac{\cos(\alpha(2N+1))}{\cos\alpha}, \tag{26}$$

which clearly reduces to the standard bosons ψ_k,ψ_k^* at $\alpha\to 0$. It is worth noting that this new q-bosonic model as realized from the ancestor Lax operator (8) (after introducing Δ) would give

$$L_k(\xi)=\begin{pmatrix} \frac{1}{\xi}q^{-N_k}-i\xi\Delta q^{N_k+1} & Q_k^* \\ Q_k & \frac{1}{\xi}q^{N_k}+i\xi\Delta q^{-(N_k+1)} \end{pmatrix}, \tag{27}$$

which represents an exact lattice version of the DNLS equation.[24] When expressed through bosonic field: $Q=\psi[\Delta([2N]_q/2N\cos\alpha)]^{1/2}$, $N=\Delta|\psi|^2$, Eq. (27) yields at the continuum limit $\Delta\to 0$ the field Lax operator

$$\mathcal{L}(\psi)=-(\tfrac{1}{4}\xi^2-|\psi|^2)\sigma_3+\xi(\psi^*\sigma^+ +\psi\sigma^-) \tag{28}$$

of the well-known Chen–Lee–Liu DNLS equation:[25] $i\psi_t=\psi_{xx}-4i|\psi|^2\psi_x$.

(5) *Ablowitz–Ladik model:* This model involving also another form of q-boson is possible to generate in our scheme, though it needs twisting transformation as in the Suris RTC mentioned above and is associated with the same twisted r_Ω-matrix (22) and the twisted ancestor Lax operator with the change (23). Now the the parameter choice $c_1^+=c_2^-=0$ with $c_1^-=c_2^+=1$ giving $M^\pm=\frac{1}{2}\sqrt{\pm 1}$ (compare with the Liouville case) together with the twisting removes dynamical variables from the diagonal elements of the twisted Lax operator as well as modifies the Poisson algebra of the transformed variables $\tilde{S}_k^\pm$ as derivable from (9). Therefore naming $b_k=2\sin\alpha\tilde{S}_k^+$ we get this modified PB relation as $\{b_k,b_l^*\}=i\delta_{kl}(1-b_k^*b_k)$, confirming the basic variables of the Ablowitz–Ladik model as a type of q-boson with its Lax operator as

$$L_k(\xi)=\begin{pmatrix} \frac{1}{\xi} & b_k^* \\ b_k & \xi \end{pmatrix} \tag{29}$$

related to (22). We will see later how space-time dependent parameters c's give inhomogeneous extensions of this model. Note that another intriguing possibility of generalizing this model arises if we simply consider $c_1^+\neq 0$ in the above construction. It is not dificult to see that, realizing S_k^3

$=-\ln(1-b_k^* b_k)$ this would generate an extra term $\xi c_1^+ (1-b_k^* b_k)^{-2i\alpha}$ in the upper diagonal element of the Ablowitz–Ladik Lax operator (29). Its consequence in the dynamical equation would be an interesting problem to study.

B. Nonrelativistic models belonging to rational class

Deformation parameter $q=e^{i\alpha}$, as we have seen in the above models, serves as the relativistic or the deformed bosonic parameter. We consider now the undeformed limit $q\to 1$ or $\alpha\to 0$, when as explained already, the r-matrix reduces to its rational form (5) and the ancestor Lax operator is converted to (12) with the underlying PB algebra (13).

We find that the integrable models belonging to this rational class are mostly nonrelativistic models, which can be generated in a similar way from the rational ancestor model (12) with different constant choices for parameters $c_a^{0,1}$, $a=1,2$ involved in it.

(6) *Landau–Lifshitz equation (LLE):* Parameter choice $c_a^0=1$, $c_1^1=-c_2^1=-l$ compatible with $m^+=1$, $m^-=0$, reduces (13) to the classical sl_2 spin algebra $\{s_k^\alpha, s_l^\beta\}=i\delta_{kl}\epsilon^{\alpha\beta\gamma}s_l^\gamma$ with spin: $s^2=(s_k^3)^2+s_k^+ s_k^-\equiv \vec{s}_k^2$ as the Casimir operator reduced from (14). The ancestor Lax operator (12) simplifies (ignoring an irrelevant multiplicative factor) to

$$L_k(\lambda)=I+\frac{1}{\lambda-l}\vec{s}_k\cdot\vec{\sigma} \tag{30}$$

representing a discrete version of the LLE. At the continuum limit $\Delta\to 0$ putting $\vec{s}_k\to\Delta\vec{s}(x)$ one gets from the Casimir: $\vec{s}^2(x)=1$ and from the Lax operator $L_k(\lambda)\to I+\Delta\mathcal{L}(\lambda), \mathcal{L}(\lambda)=[1/(\lambda-l)]\vec{s}(x)\cdot\vec{\sigma}$, that for the well known LLE.[26]

(7) *Discrete NLS model:* For the same sl_2 spin algebra transformation (15) yields the standard HPT with $g_0(|\psi_k|)=(2s-\Delta|\psi_k|^2)^{1/2}$ (considering ψ_k,ψ_k^* to be complex conjugates and scaling them by $\sqrt{\Delta}$). This realization by considering parameter $l=0$ leads (12) to the Lax operator of exactly integrable discrete NLS model[18] given by

$$L_k(\lambda)=\begin{pmatrix} \lambda+s-\Delta|\psi_k|^2 & \sqrt{\Delta}\psi^* g_0(|\psi_k|) \\ \sqrt{\Delta}\psi g_0(|\psi_k|) & \lambda-s+\Delta|\psi_k|^2 \end{pmatrix}. \tag{31}$$

At the field limit: $\Delta\to 0$, Eq. (31) yields (after multiplying it from left by $\sigma_3\Delta$ and considering $s=1/\Delta$) the familiar form of the Lax operator

$$\mathcal{L}(\lambda)=\lambda\sigma^3+\sqrt{2}(\psi^*\sigma^+-\psi\sigma^-) \tag{32}$$

for the NLS field equation $i\psi_t=\psi_{xx}+2|\psi|^2\psi$.

(8) *Simple lattice NLS:* On the other hand, a complementary choice $m^+=0$, $m^-=1$, giving $g_0(N_k)=1$ converts (15) directly to the realization $s_k^+=\psi_k$, $s_k^-=\psi_k^*$, $s_k^3=s-\psi_k^*\psi_k$ in bosonic field: $\{\psi_k,\psi_l^*\}=i\delta_{kl}$. Now a compatible choice of parameters: $c_1^0=c_2^1=1$, $c_2^0=c_1^1=0$ together with this bosonic realization generates from the ancestor (12) the Lax operator

$$L_k(\lambda)=\begin{pmatrix} \lambda+s-N_k & \psi_k^* \\ \psi_k & -1 \end{pmatrix}, \quad N_k=\psi_k^*\psi_k, \tag{33}$$

which may be associated with another simple lattice NLS model proposed in Ref. 27 and as noted there ψ,ψ^* may not be complex conjugates at the discrete level. At the continuum limit we recover again the same field Lax operator (32) for the NLS equation and regain also the complex-conjugacy of the fields (see Ref. 27 for details).

(9) *Nonrelativistic Toda chain:* Note that the trivial choice $m^\pm=0$ yields from (13) again the same algebra (19) and therefore we may take the same realization of it as found before. However, the rational form of ancestor model (12) generates now simpler Lax operator

$$L_k(\lambda)=\begin{pmatrix} p_k-\lambda & e^{u_k} \\ -e^{-u_k} & 0 \end{pmatrix} \tag{34}$$

of the nonrelativistic Toda chain associated with the rational r-matrix and described by the Hamiltonian: $H=\Sigma_k \frac{1}{2}p_k^2+e^{(u_k-u_{k+1})}$.

Thus we have demonstrated that discrete and continuum integrable models can be obtained in a unified way from the ancestor Lax operator (8) [or its rational limit (12)] by choosing different sets of constant values for the parameters c's involved in the ancestor model and by using different realizations of the underlying PB algebra. In the next section we find how a more general choice of c's can generate further the inhomogeneous extensions of these integrable models.

We find also a convincing answer to an important question raised above asking why different integrable systems with varied Lax operator solutions should have the same r-matrix, by discovering that all these models are basically obtainable from the same ancestor model (8) associated with the trigonometric r-matrix (4). These descendant models, whose explicit Lax operators we derive here satisfy the CYBE (2) inheriting and sharing the same r-matrix (4). We will see in Sec. VI that this significant fact induces a universality among these seemingly diverse systems by defining their action-angle variables in the same way.

V. INTEGRABLE INHOMOGENEOUS AND HYBRID MODELS WITH ISOSPECTRAL FLOW

We have seen how by fixing the values of certain parameters we could generate a wide spectrum of integrable models belonging to the trigonometric and rational class. We focus here on some promising possibilities to generalize this procedure for constructing novel integrable families of inhomogeneous and hybrid models.

A. Inhomogeneous models

Returning again to the ancestor model (8) we may notice that the parameters $c_a^{\pm}$, $a=1,2$ entering in it [similarly, $c_a^{0,1}$, $a=1,2$ in its rational limit (12)] act like external parameters having trivial PB with all basic variables in their local algebra and therefore, apart from constants as earlier they may be considered in general as site (time) dependent arbitrary functions. As a result $M^{\pm}$ in (10), (11) in turn also become functions $M_k^{\pm}(t), k=1,2,\ldots,N$ [and similarly $m_k^{\pm}(t)$ in (15)] and lead to new integrable descendant models, which are inhomogeneous extensions of the discrete and continuum models constructed above. However this integrable family of inhomogeneous models is obtained in our scheme by keeping the usual isospectral flow. Moreover, such constancy of spectral parameters (except some trivial transformations like shifting, etc.) is essential in this algebraic formalism for satisfying the CYBE (6) with spectral dependent global and nondynamical $r(\lambda-\mu)$-matrix. It is important also to notice that the inhomogeneity is introduced here through a set of different independent parameters: $c_{ak}^{\pm}$ (or $c_{ak}^{0,1}$) with $a=1,2$ and therefore it may not be always possible to absorb them in the single spectral parameter, even by declaring it to be nonisospectral. Therefore we see that, contrary to the standard approach the inhomogeneous models cannot be described in general as nonisospectral flow, at least those that belong to the present family. Moreover isospectrality is a necessary criterion for the CYBE solution, as explained already.

(10) *Variable mass sine-Gordon model:* The construction is parallel to that of the constant mass sine-Gordon model obtained above, where in place of constants we choose now the parameters as four different variable mass: $c_1^{\pm}=m_{1k}^{\pm}(t)\Delta$, $c_2^{\pm}=m_{2k}^{\pm}(t)\Delta$. This would generate from the ancestor Lax operator (8) and realization (10) a general form of a new inhomogeneous sine-Gordon model, which is integrable and satisfies the CYBE associated to the trigonometric r-matrix (4). Particular choices of the inhomogeneities would yield naturally different forms of the variable mass sine-Gordon model, discrete as well as continuum, which seem to have been never considered before.

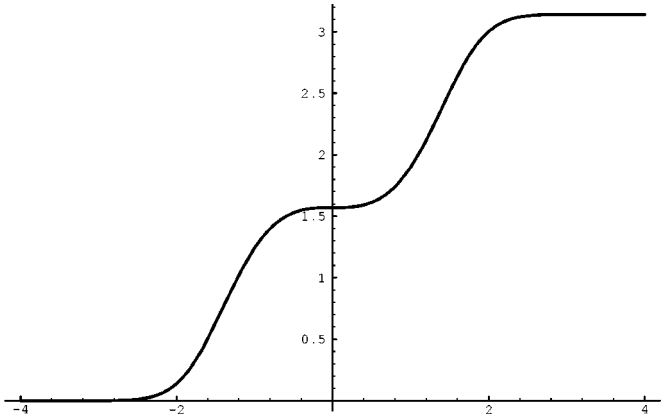

FIG. 1. How the kink solution [for $m_1(x)=1$] deforms in variable mass sine-Gordon model depending on the mass parameter $m_1(x)=x$ and $m_1(x)=x^2$, respectively.

For a demonstration we take up the simplest case when all mass parameters coincide: $m_{ak}^{\pm}(t)=m_k(t)$. This variable mass discrete sine-Gordon model can be described again by the same form (16) by replacing constant m by a variable $m_k(t)$. At the continuum limit this would correspond to a sine-Gordon field model with variable mass $m(x,t)$. If the mass parameter is assumed to be factorized: $m(x,t)\equiv m_0(t)m_1(x)$, by introducing a new coordinate system through nonlinear transformation $(t,x)\rightarrow(T,X)$, $T=\int^t m_0(t')dt'$, $X=\int^x m_1(x)dx'$, the Hamiltonian of the model can be written formally again as the standard sine-Gordon model with unit mass. Nevertheless we notice that even in a further simplified case with $m_0(t)=1$, the soliton solutions in the original system might have quite interesting character depending on the form of the variable mass $m_1(x)$ (see Fig. 1).

(11) *Inhomogeneous NLS model:* Since this model belongs to the rational class, in accordance with our strategy we start with the ancestor Lax operator (12) and consider the parameters involved in it and in realization (15) to be site and time dependent functions: $c_{ak}^{0,1}(t)$, $a=1,2$. With all of them different we naturally get the general inhomogeneous discrete NLS model, which retains its integrability and contrary to the standard approach also its isospectrality, as explained already. For constructing the corresponding field model we take the parameters in the form $c_{1k}^0=g_{1k}$, $c_{2k}^0=-g_{2k}$, $c_{1k}^1=(1/\Delta)+f_{1k}$, $c_{2k}^1=-(1/\Delta)+f_{2k}$, $s=\Delta$ and at the limit $\Delta\rightarrow 0$ obtain the Lax operator

$$\mathcal{L}(\lambda)=\begin{pmatrix}\Lambda_1(x,t) & Q^* \\ -Q & -\Lambda_2(x,t)\end{pmatrix}, \quad \text{where } \Lambda_a(x,t)=\lambda g_a(x,t)+f_a(x,t), \quad a=1,2 \tag{35}$$

and $Q=\psi g_0(x,t)$ with $g_0(x,t)=(g_1(x,t)+g_2(x,t))^{1/2}$, representing an inhomogeneous NLS field model with inhomogeneities introduced by the independent functions $g_a(x,t)$, $f_a(x,t)$, $a=1,2$. It may be stressed again that here the spectral parameter λ is strictly constant and when $\Lambda_1\neq\Lambda_2$, all inhomogeneous parameters apparently cannot be absorbed in this single parameter. It is challenging to derive the explicit form of this integrable variable coefficient general NLS equation, associated with the rational r-matrix (5). For showing that the Lax operator of many known inhomogeneous NLS equations can actually be derived from (35), we consider the particular situation $g_1=g_2\equiv g(x,t)$, $f_1=f_2\equiv f(x,t)$ and rewrite (35) as

$$\mathcal{L}(\lambda)=\Lambda(x,t)\sigma_3+Q^*\sigma_+-Q\sigma_-, \quad \Lambda(x,t)=\lambda g(x,t)+f(x,t). \tag{36}$$

It is remarkable that from this single operator we recover at $g=1$, $f=\alpha t$ the Lax operator of Ref. 9, at $g=1/t$, $f=4x/t$ that of Ref. 10 and similarly at $g=T(t)$, $f=(\alpha/2)xT(t)$ that of Ref. 11. Note however that the actual form of the equations depend also on the time evolution operator M, which is likely to be different in our approach from the known ones, since in our construction the

fundamental canonical PB structure is always preserved. Therefore it would be a challenging problem to derive these new integrable inhomogeneous NLS equations explicitly from their Hamiltonian using the canonical PB.

(12) *Gaudin model:* It is intriguing that just by considering the parameter l in the Lax operator (30) for the discrete LLE to be site dependent: $l \to l_k$, one recovers the Lax operator $L_k(\lambda) = I + [1/(\lambda - l_k)]\vec{s}_k \cdot \vec{\sigma}$ for the celebrated Gaudin model, given by the integrable Hamiltonians $H_k = \sum_{l \neq k}^{N} [1/(l_k - l_l)](\vec{s}_k \cdot \vec{s}_l)$, $k = 1,2,\ldots,N$.[28] This model is associated also with the rational r_r matrix (5).

(13) *Inhomogeneous relativistic and nonrelativistic Toda chains:* It is not difficult to see that by repeating the construction of the Toda chains but taking the parameters to be nonconstants we get integrable inhomogeneous extensions of such models. For example, considering in ancestor Lax operator (12) the parameters to be $c_1^{\pm} = f_k^{\pm}(t)$, $c_2^{\pm} = 0$, but using the same realization as for the original relativistic Toda chain, we get an extension of its Lax operator (21) to include inhomogeneity through arbitrary functions $f_k^{\pm}(t)$:

$$L_k(\xi) = \frac{1}{2}\left(\frac{f_k^-}{\xi} e^{\alpha p_k} - f_k^+ \xi e^{-\alpha p_k} \right)(I + \sigma_3) + \alpha(e^{u_k}\sigma_+ - e^{-u_k}\sigma_-),$$

which therefore would represent a new integrable family of inhomogeneous relativistic Toda chain. We will not present here its explicit form.

At $\alpha \to 0$ this family of relativistic models would go to its nonrelativistic limit represented by the Lax operator

$$L_k(\lambda) = \begin{pmatrix} (p_k - \lambda) + g_{2k} & (c_{1k}^0)^{-1} e^{u_k} \\ -(c_{1k}^0)^{-1} e^{-u_k} & 0 \end{pmatrix}, \tag{37}$$

which is an obvious extension of (34) (by introducing the inhomogeneous parameter $g_{2k} \equiv c_{1k}^1 / c_{1k}^0$ and normalizing it by c_{1k}^0). Without defining any time evolution operator M, we can directly construct from (37) the explicit form of the Hamiltonian through the conserved quantity as $H = C_{N-1}$ and derive the Hamilton equations using the canonical PB between u_k, p_l, yielding $\dot{u}_k = p_k + g_{2k}$ and hence the inhomogeneous Toda chain equation as

$$\frac{\mathrm{d}^2}{\mathrm{dt}^2} u_k = g_1(k) e^{u(k-1) - u(k)} - g_1(k+1) e^{u(k) - u(k+1)} + \dot{g}_2(t) + \text{boundary terms} \tag{38}$$

with arbitrary parameters $g_1(k) = (c_{1k}^0 c_{1k+1}^0)^{-1}$ and $g_2(k)$. Different choices of these parameters would generate from (38) different inhomogeneous Toda chains. For example the particular choices: $g_1(k) = k$, $g_2(k) = \alpha_0 t$ and $g_1(k) = 4k^2 + 1$, $g_2(k) = kt$ derives the Toda chains found in Ref. 12, though in contrast we recover this result in a completely isospectral way.

(14) *Inhomogeneous Ablowitz–Ladik model:* It is easy to notice again that if instead of constants as in the original model, we choose the parameters through arbitrary function $\Gamma(t)$ as $c_1^- = (c_2^+)^{-1} = e^{\Gamma(t)}$, keeping the same trivial choice for $c_1^+ = c_2^- = 0$, we generate from (8) the Lax operator

$$L_k(\xi) = \begin{pmatrix} \dfrac{1}{\xi} e^{\Gamma(t)}, & b_k^* \\ b_k, & \xi e^{-\Gamma(t)} \end{pmatrix}. \tag{39}$$

Remarkably, in spite of our isospectral approach, Eq. (39) recovers exactly the Lax operator of Ref. 13 for arbitrary $\Gamma(t)$ and that of Ref. 14 for $\Gamma(t) = \alpha t$, representing known inhomogeneous Ablowitz–Ladik models.

In a similar way by generalizing the constant parameters to inhomogeneous functions one can generate systematically inhomogeneous extensions of other integrable models constructed here. Note again that all such extensions retain the integrability of the system as well as the isospectrality and the same r-matrix solution.

B. Integrable hybrid models

Our scheme for generating different integrable models from an ancestor model sharing the same r-matrix opens up a possibility of constructing new families of integrable models by *hybridizing* these descended models.

Such constructions can be of two types. The first type of hybrid models may be constructed by using different descendant Lax operators obtained directly from (8) [or alternatively from (12)] as its different but consistent reductions and realizations at different lattice sites. Since all representative Lax operators of these constituent models: $L_k^{d(k)}(\lambda)$, with $d(k)$ denoting different members of the same descendant class inserted at sites k, should share the same r-matrix, the monodromy matrix of this hybrid model: $T^{\{d\}}(\lambda)=\Pi_{d(k),k}L_k^{d(k)}(\lambda)$ must satisfy the global CYBE (6) and represent therefore an integrable system with the set of conserved quantities including the Hamiltonian obtainable as usual through expansion of $\tau^{\rm hyb}(\lambda)=\mathrm{tr}(T^{\{d\}}(\lambda))$ in the spectral parameter. One can generate in this way some exotic hybrid models by combining for example, sine-Gordon and Liouville models, different types of relativistic Toda chain or discrete NLS model, etc., constructed above. These hybrid models presumably would show different dynamics at different domains in the coordinate space. It is encouraging to note that very recently such models have received well deserved attention, though only at the continuum level.[8] We hope that the present idea, based on discrete approach and r-matrix formalism would prove to be promising and fruitful for analyzing such hybrid integrable models.

A second type of hybrid model may be constructed by considering different representation of the Lax operator for different components of the field and inserting their direct product at the same lattice site. As a result one can build new multi-component generalization of a scalar model through the *fused* Lax operator: $L_k^{\{m\}}=\Pi_m L_k^{(m)}$, where each entry in the product would represent individual components. Note that unlike the vector generalization, which needs also enlarged matrix realization for the Lax operator, our multicomponent hybrid models would yield only 2×2 matrix Lax operators. For elaborating this idea we present the detail construction of an integrable hierarchy of two-component DNLS model.

(15) *Integrable hierarchy of two-component DNLS:* Note that in constructing the discrete DNLS model in Sec. IV, the values of $M^{\pm}$ fixed by (25) actually determined the underlying algebra as well as the required realization. It is however crucial to notice now that interchanging the parameters $c_1^{\pm}\leftrightarrow c_2^{\mp}$ would not change the values of $M^{\pm}$ and therefore would lead to the same algebra and its realization, but result to a complementary form for the Lax operator, though representing the same DNLS model. In our construction of the two-component model with fields $\psi_k^{(\beta)}$, $\beta=1,2$ having PB relations $\{\psi_k^{(\beta)},\psi_l^{*(\gamma)}\}=i\delta_{\beta\gamma}\delta_{kl}$, we take $c_a^{\pm}$, $a=1,2$ as in (25) for building the Lax operator $L_k^{(1)}(\psi^{(1)})$ as (27) for the first component. However, for the corresponding construction of $\tilde{L}_k^{(2)}(\psi^{(2)})$ related to the second component we take the complementary choice by considering $c_1^{\pm}\leftrightarrow c_2^{\mp}$. The fused Lax operator taking the form $L_k^{(1,2)}(\psi^{(\beta)})=L_k^{(1)}(\psi^{(1)})\tilde{L}_k^{(2)}(\psi^{(2)})$ represents now a new discrete multicomponent DNLS satisfying the CYBE (2) with the same r-matrix (4). At the continuum limit $\Delta\to 0$, repeating the construction for the scalar DNLS model (28), it is easy to see that the field Lax operator of this two-component model is given simply as a linear superposition $\mathcal{L}(\psi^{(1)},\psi^{(2)})=\mathcal{L}(\psi^{(1)})+\tilde{\mathcal{L}}(\psi^{(2)})$ with the explicit form

$$\mathcal{L}(\psi^{(1)},\psi^{(2)})=\left(\frac{1}{4}\left(\frac{1}{\xi^2}-\xi^2\right)+|\psi|_1^2-|\psi|_2^2\right)\sigma_3+\left(\xi\psi_1^*+\frac{1}{\xi}\psi_2^*\right)\sigma^+ +\left(\xi\psi_1+\frac{1}{\xi}\psi_2\right)\sigma^-,\quad \xi=e^{i\lambda}. \tag{40}$$

It is interesting to show by direct construction that this Lax operator generates an integrable hierarchy of multicomponent DNLS model through the expansion $\ln \tau(\lambda)=\Sigma_{n=0}^{\infty} C_{\pm n}\lambda^{\mp 2n}$ with $H_2=C_2+C_{-2}$ introducing a new two-component generalization of the Chen–Lee–Liu DNLS equation. We are not giving here its explicit form, which can be worked out with little patience. The higher conserved quantities will yield higher order equations. Some similar class of discrete matrix and multicomponent DNLS models was proposed recently.[29]

(16) *Massive Thirring model:* It is remarkable that (40) constructed through a novel hybridization from our ancestor model coincides also with the Lax operator of the bosonic massive Thirring model.[30] Hamiltonian of this relativistic model may be given through the same conserved quantities constructed for the above model in the form $H_1=C_1+C_{-1}$.

(17) *Integrable discrete self-trapping model:* A discrete self-trapping model with two-bosonic modes $\psi^{(a)},\psi^{*(a)},a=1,2$ given by the Hamiltonian

$$H=-\left[\frac{1}{2}\sum_{a}^{2}\ (s_a-N^{(a)})^2+(\psi^{*(1)}\psi^{(2)}+\psi^{*(2)}\psi^{(1)})\right]$$

was studied in Ref. 31. This integrable model is associated with a Lax operator, which may be constructed by fusing two operators as $L(\lambda)=L^{(1)}(\lambda)L^{(2)}(\lambda)$, where $L^{(a)}(\lambda)$ are given by the same Lax operator (33) for each of the modes $a=1,2$.

An interesting line of investigation would be to apply this hybridization method for constructing possible multicomponent extensions of other models like relativistic Toda chain, Ablowitz–Ladik, Liouville model, LLE, Gaudin model, etc. The linear superposition of Lax operators for building new nonlinear integrable systems, as revealed here, seems to be a promising idea worth pursuing.

VI. UNIVERSAL PROPERTIES OF INTEGRABLE DESCENDANT MODELS

We have seen that diverse forms of integrable models: discrete and continuum, homogeneous and inhomogeneous, multicomponent and hybrid models can be generated in a systematic way in our ancestor model scheme. Among this diversity however we find also an unexpected universality. Indeed, as we have found, a wide range of models, namely sine-Gordon, Liouville, DNLS, relativistic Toda chain, etc., including their discrete, inhomogeneous and hybrid variants belong to the trigonometric class, while models like NLS, Toda chain, etc., and their related discrete and inhomogeneous extensions are in the same rational class, which being in fact the undeformed $q\rightarrow 1$ or the nonrelativistic limit of the former class.

The crucial observation is that the diversity of all descendant models belonging to the same class seems to disappear at the global level allowing their description through a universal action-angle variable. The reason for this is very simple. Though these models differ widely at their local level having different forms of the Lax operator, their monodromy matrix $T_N(\lambda)$ (7) satisfies the same global relation (6) with the same r-matrix, which is inherited from their ancestor model and shared by all of them.

As a result, for all models belonging, for example, to the trigonometric class, the PB relations should be given by the same structure constants expressed through the elements of the r_t-matrix (4). For the twisted models, e.g., Suris RTC and Ablowitz–Ladik model the structure constants should similarly be given by the twisted r_Ω-matrix (22). In the same way all models from the rational class should have analogous property expressed through the elements of rational r_r-matrix (5). However, while the action variables are constants in time, the time evolution of angle variables depends on the definition of the Hamiltonians through conserved quantities, which usually differs for different models.

Such differences also bear some additional imprint at the continuum limit, when the monodromy matrix is defined as $T(\lambda)=\lim_{N\rightarrow\infty} L_{\infty}^{-N}(\lambda)T_N(\lambda)L_{\infty}^{-N}(\lambda)$ and the corresponding CYBE is modified as[5] $\{T(\lambda)\otimes,T(\mu)\}=r_+(\lambda-\mu)T(\lambda)\otimes T(\mu)-T(\lambda)\otimes T(\mu)r_-(\lambda-\mu)$, where $r_{\pm}(\lambda-\mu)=\lim_{N\rightarrow\infty} L_{\infty}^{\mp N}(\lambda)\otimes L_{\infty}^{\mp N}(\mu)r(\lambda-\mu)L_{\infty}^{\pm N}(\lambda)\otimes L_{\infty}^{\pm N}(\mu)$. Therefore though the action-angle

description for such models of the same class are again basically the same, the influence of the individual models also enters now due to the appearance of $r_{\pm}$ modified by the asymptotic forms $L_{\infty}(\lambda)$ of the individual Lax operators. Nevertheless it is startling to check that the canonical action-angle variables for widely different field models like DNLS[24] and the sine-Gordon[1] are defined exactly in the same way: $p(\xi)=(1/2\pi c\xi)\ln|a(\xi)|$, $q(\xi)=\arg b(\xi)$ for the continuum modes with PB $\{q(\xi),p(\eta)\}=\delta(\xi-\eta)$, $\xi>0$ and $p_k=(1/2c)\ln\xi_k$, $q_k=\ln b_k$ for the discrete set with $\{q_k,p_l\}=\delta_{kl}$ and similarly for their conjugates $\overline{q_k},\overline{p_l}$.

Therefore we may conclude that all integrable models presented here may be described universally through the ancestor Lax operator (8) and the r_t-matrix (4) (or twisted r_{Ω}) or similarly by the $q\to 1$ limit as the ancestor model (12) and the r_r-matrix (5), where the global relations like action-angle variables are determined by the r-matrix elements alone. The individuality of the models may be reflected only in the definition of their Hamiltonians through conserved quantities and for continuum models, additionally in the limiting forms of their Lax operators.

VII. CONCLUDING REMARKS

We have presented here a unifying scheme based on PB algebra for systematically generating a large class of integrable discrete and continuum models from a single ancestor model. Such models include well known and new integrable systems as well as inhomogeneous models. Based on our construction we conclude that more general and logical approach for inhomogeneous integrable models, at least for models with nondynamical r-matrix, would be to describe them as isospectral flow in inhomogeneous external fields. As another fruitful application of the present scheme we have proposed a simple method for constructing new families of integrable hybrid models by *fusing* different types of descendant models. In spite of the vastly diverse form of these models their common ancestor and common r-matrix reveal an inherent universality in their description through action-angle variables.

We strongly hope that the algebraic approach linked with the quantum group structure formulated here for generating classical integrable discrete as well as field models, though a bit uncommon in the community working in classical integrability, would prove to be much powerful due to its systematic and algorithmic nature. Similarly the novel ideas of construction introduced here, like generating integrable hybrid and multicomponent models and creating integrable inhomogeneity in isospectral flow, are expected to be equally promising.

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General soliton matrices in the Riemann–Hilbert problem for integrable nonlinear equations

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(Received 25 May 2003; accepted 5 June 2003)

We derive the soliton matrices corresponding to an arbitrary number of higher-order normal zeros for the matrix Riemann–Hilbert problem of arbitrary matrix dimension, thus giving the complete solution to the problem of higher-order solitons. Our soliton matrices explicitly give all higher-order multisoliton solutions to the nonlinear partial differential equations integrable through the matrix Riemann–Hilbert problem. We have applied these general results to the three-wave interaction system, and derived new classes of higher-order soliton and two-soliton solutions, in complement to those from our previous publication [Stud. Appl. Math. **110**, 297 (2003)], where only the elementary higher-order zeros were considered. The higher-order solitons corresponding to nonelementary zeros generically describe the simultaneous breakup of a pumping wave (u_3) into the other two components (u_1 and u_2) and merger of u_1 and u_2 waves into the pumping u_3 wave. The two-soliton solutions corresponding to two simple zeros generically describe the breakup of the pumping u_3 wave into the u_1 and u_2 components, and the reverse process. In the nongeneric cases, these two-soliton solutions could describe the elastic interaction of the u_1 and u_2 waves, thus reproducing previous results obtained by Zakharov and Manakov [Zh. Éksp. Teor. Fiz. **69**, 1654 (1975)] and Kaup [Stud. Appl. Math. **55**, 9 (1976)].
[DOI: 10.1063/1.1605821]

I. INTRODUCTION

The importance of integrable nonlinear partial differential equations (PDEs) in $1+1$ dimensions in applications to nonlinear physics can hardly be overestimated. Their importance partially stems from the fact that it is always possible to obtain certain explicit solutions, called solitons, by some algebraic procedure. At present, there is a wide range of literature concerning integrable nonlinear PDEs and their soliton solutions (see, for instance, Refs. 1–4 and the references therein). The reader familiar with the inverse scattering transform method knows that it is zeros of the Riemann–Hilbert problem (or poles of the reflection coefficients in the previous nomenclature) that give rise to the soliton solutions. These solutions are usually derived by using one of the several well-known techniques, such as the dressing method,[1,5,6] the Riemann–Hilbert problem approach,[2,3] and the Hirota method (see Ref. 1). In the first two methods, the pure soliton solution is obtained by considering the asymptotic form of a rational matrix function of the spectral parameter, called the soliton matrix in the following. It is known that the generic case of zeros of the matrix Riemann–Hilbert problem is the case of simple zeros[7–12] (see also Ref. 13). A single simple zero produces a one-soliton solution. Several distinct zeros will produce multisoliton solutions, which describe the interaction (scattering) of individual solitons. As far as the generic case is concerned, there is no problem in the derivation of the corresponding soliton solutions.

However, in the nongeneric cases, when at least one higher-order (i.e., multiple) zero is

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present in the Riemann–Hilbert problem, the situation is not so definite. Higher-order zeros must be considered separately, as, in general, the soliton solutions which correspond to such zeros cannot be derived from the known generic multisoliton solutions by coalescing some of the distinct simple zeros. This is clear from the fact that a higher-order zero generally corresponds to a higher-order pole in the soliton matrix (or its inverse), which cannot be obtained in a regular way by coalescing simple poles in the generic multisoliton matrix. The procedure of coalescing several distinct simple zeros produces only higher-order zeros with equal algebraic and geometric multiplicities (the geometric multiplicity is defined as the dimension of the kernel of the soliton matrix evaluated at the zero), which is just the trivial case of higher-order zeros. For instance, if the algebraic multiplicity is equal to or greater than the matrix dimension, then such coalescing will produce a higher-order zero with the geometric multiplicity no less than the matrix dimension, which could only correspond to the zero solution instead of solitons. Thus the soliton matrices corresponding to higher-order zeros of the Riemann–Hilbert problem require a separate consideration.

Soliton solutions corresponding to higher-order zeros have been investigated in the literature before, mainly for the 2×2-dimensional spectral problem. A soliton solution to the nonlinear Schrödinger (NLS) equation corresponding to a double zero was first given in Ref. 14 but without much analysis. The double- and triple-zero soliton solutions to the KdV equation were examined in Ref. 15 and the general multiple-zero soliton solution to the sine-Gordon equation was extensively studied in Ref. 16 using the associated Gelfand–Levitan–Marchenko equation. In Refs. 17 and 18, higher-order soliton solutions to the NLS equation were studied by employing the dressing method. In Refs. 19–21, higher order solitons in the Kadomtsev–Petviashvili I equation were derived by the direct method and the inverse scattering method. Finally, in our previous publication[22] we have derived soliton matrices corresponding to a single *elementary* higher-order zero—a zero which has the geometric multiplicity equal to 1. Our studies give the general higher-order soliton solutions for the integrable PDEs associated with the 2×2 matrix Riemann–Hilbert problem with a single higher-order zero. Indeed, any zero of the 2×2-dimensional Riemann–Hilbert problem is elementary since a nonzero 2×2 matrix can have only one vector in its kernel.

However, the previous investigations left some of the key questions unanswered. For instance, the general soliton matrix corresponding to a single nonelementary zero remained unknown. Such zeros arise when the matrix dimension of the Riemann–Hilbert problem is greater than 2. Naturally then, the ultimate question—the most general soliton matrices corresponding to an arbitrary number of higher-order zeros in the general $N\times N$ Riemann–Hilbert problem, was not addressed. Because of these unresolved issues, the most general soliton and multisoliton solutions to PDEs integrable through the $N\times N$ Riemann–Hilbert problem (such as the NLS equation,[23] the three-wave interaction system,[2,24–27] and the Manakov equations[28]) have not been derived yet.

In this paper we derive the complete solution to the problem of soliton matrices corresponding to an arbitrary number of higher-order normal zeros for the general $N\times N$ matrix Riemann–Hilbert problem. These normal zeros are defined in Definition 1, and are nonelementary in general. They include almost all physically important integrable PDEs where the involution property [see Eq. (4)] holds. The corresponding soliton solutions can be termed as the higher-order multisolitons, to reflect the fact that these solutions do not belong to the class of the previous generic multisoliton solutions. Our results give a complete classification of all possible soliton solutions in the integrable PDEs associated with the $N\times N$ Riemann–Hilbert problem. In other words, our soliton matrices contain the most general forms of reflection-less (soliton) potentials in the N-dimensional Zakharov–Shabat spectral operator. For these general soliton potentials, the corresponding discrete and continuous eigenfunctions of the N-dimensional Zakharov–Shabat operator naturally follow from our soliton matrices. As an example, we consider the three-wave interaction system, and derive single-soliton solutions corresponding to a nonelementary zero, and higher-order two-soliton solutions. These solutions generate many new processes such as the simultaneous breakup of a pumping wave (u_3) into the other two components (u_1 and u_2) and merger of u_1 and u_2 waves into the pumping u_3 wave, i.e., $u_1+u_2+u_3\leftrightarrow u_1+u_2+u_3$. They also reproduce previous solitons in Refs. 2, 22, 26, 27 as special cases.

The paper is organized as follows. A summary on the Riemann–Hilbert problem is placed in Sec. II. Section III is the central section of the paper. There we present the theory of soliton matrices corresponding to several higher-order zeros under the assumption that these zeros are *normal* (see Definition 1), which include the physically important cases with the involution property [see Eq. (4)]. Applications of these general results to the three-wave interaction system are contained in Sec. IV. Finally, in the Appendix we briefly treat the more general case where the zeros are abnormal.

II. THE RIEMANN–HILBERT PROBLEM APPROACH

The integrable nonlinear PDEs in $1+1$ dimensions are associated with the matrix Riemann–Hilbert problem (consult, for instance, Refs. 1–12, 29–32). The matrix Riemann–Hilbert problem (below we work in the space of $N\times N$ matrices) is the problem of finding the holomorphic factorization, denoted below by $\Phi_+(k)$ and $\Phi_-^{-1}(k)$, in the complex plane of a nondegenerate matrix function $G(k)$ given on an oriented curve γ:

$$\Phi_-^{-1}(k,x,t)\Phi_+(k,x,t)=G(k,x,t)\equiv E(k,x,t)G(k,0,0)E^{-1}(k,x,t), \quad k\in\gamma, \tag{1}$$

where

$$E(k,x,t)\equiv\exp[-\Lambda(k)x-\Omega(k)t].$$

Here the matrix functions $\Phi_+(k)$ and $\Phi_-^{-1}(k)$ are holomorphic in the two complementary domains of the complex k-plane: C_+ to the left and C_- to the right from the curve γ, respectively. The matrices $\Lambda(k)$ and $\Omega(k)$ are called the dispersion laws. Usually the dispersion laws commute with each other, e.g., given by diagonal matrices. We will consider this case [precisely in this case $E(k,x,t)$ is given by the above formula]. The Riemann–Hilbert problem requires an appropriate normalization condition. Usually the curve γ contains the infinite point $k=\infty$ of the complex plane and the normalization condition is formulated as

$$\Phi_\pm(k,x,t)\to I \quad \text{as} \quad k\to\infty. \tag{2}$$

This normalization condition is called the canonical normalization. Setting the normalization condition to an arbitrary nondegenerate matrix function $S(x,t)$ leads to the gauge equivalent integrable nonlinear PDE, e.g., the Landau–Lifshitz equation in the case of the NLS equation.[3] Obviously, the new solution $\hat{\Phi}_\pm(k,x,t)$ to the Riemann–Hilbert problem, normalized to $S(x,t)$, is related to the canonical solution by the following transformation

$$\hat{\Phi}_\pm(k,x,t)=S(x,t)\Phi(k,x,t). \tag{3}$$

Thus, without any loss of generality, we confine ourselves to the Riemann–Hilbert problem under the canonical normalization.

For physically applicable nonlinear PDEs the Riemann–Hilbert problem possesses the involution properties, which reduce the number of the dependent variables (complex fields). The following involution property of the Riemann–Hilbert problem is the most common in applications

$$\Phi_+^\dagger(k)=\Phi_-^{-1}(\overline{k}), \quad \overline{k}=k^*. \tag{4}$$

Here the superscript "†" represents the Hermitian conjugate, and "*" the complex conjugate. Examples include the NLS equation, the Manakov equations, and the N-wave system. The analysis in this article includes this involution (4) as a special case. In this case, the overline of a quantity represents its Hermitian conjugation in the case of vectors and matrices and the complex conjugation in the case of scalar quantities. In other cases, the original and overlined quantities may not be related.

To solve the Cauchy problem for the integrable nonlinear PDE posed on the whole axis x, one usually constructs the associated Riemann–Hilbert problem starting with the linear spectral equation

$$\partial_x \Phi(k,x,t) = \Phi(k,x,t)\Lambda(k) + U(k,x,t)\Phi(k,x,t), \tag{5}$$

whereas the t-dependence is given by a similar equation

$$\partial_t \Phi(k,x,t) = \Phi(k,x,t)\Omega(k) + V(k,x,t)\Phi(k,x,t). \tag{6}$$

The nonlinear integrable PDE corresponds to the compatibility condition of the system (5) and (6):

$$\partial_t U - \partial_x V + [U,V] = 0. \tag{7}$$

The essence of the approach based on the Riemann–Hilbert problem lies in the fact that the evolution governed by the complicated nonlinear PDE (7) is mapped to the evolution of the spectral data given by simpler equations such as (1) and (20a)–(20b). When the spectral data is known, the matrices $U(k,x,t)$ and $V(k,x,t)$ describing the evolution of $\Phi_{\pm}$ can then be retrieved from the Riemann–Hilbert problem. In our case, the potentials $U(k,x,t)$ and $V(k,x,t)$ are completely determined by the (diagonal) dispersion laws $\Lambda(k)$ and $\Omega(k)$ and the Riemann–Hilbert solution $\Phi \equiv \Phi_{\pm}(k,x,t)$. Indeed, let us assume that the dispersion laws are polynomial functions, i.e.,

$$\Lambda(k) = \sum_{j=0}^{J_1} A_j k^j, \quad \Omega(k) = \sum_{j=0}^{J_2} B_j k^j. \tag{8}$$

Then using similar arguments as in Ref. 32 we get

$$U = -\mathcal{P}\{\Phi \Lambda \Phi^{-1}\}, \quad V = -\mathcal{P}\{\Phi \Omega \Phi^{-1}\}. \tag{9}$$

Here the matrix function $\Phi(k)$ is expanded into the asymptotic series,

$$\Phi(k) = I + k^{-1}\Phi^{(1)} + k^{-2}\Phi^{(2)} + \cdots, \quad k \to \infty,$$

and the operator $\mathcal{P}$ cuts out the polynomial asymptotics of its argument as $k \to \infty$. An important property of matrices U and V is that

$$\begin{aligned} \operatorname{Tr} U(k,x,t) &= -\operatorname{Tr} \Lambda(k), \\ \operatorname{Tr} V(k,x,t) &= -\operatorname{Tr} \Omega(k), \end{aligned} \tag{10}$$

which evidently follows from Eq. (9). This property guarantees that the Riemann–Hilbert zeros are (x,t) independent.

Let us consider as an example the physically relevant three-wave interaction system.[2,24,25,27] Set $N=3$,

$$\Lambda(k) = ikA, \quad A = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}, \quad \Omega(k) = ikB, \quad B = \begin{pmatrix} b_1 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & b_3 \end{pmatrix}, \tag{11}$$

where a_j and b_j are real with the elements of A being ordered: $a_1 > a_2 > a_3$. From Eq. (9) we get

$$U = -\Lambda(k) + i[A, \Phi^{(1)}], \quad V = -\Omega(k) + i[B, \Phi^{(1)}]. \tag{12}$$

Setting

$$u_1=\sqrt{a_1-a_2}\Phi_{12}^{(1)},\quad u_2=\sqrt{a_2-a_3}\Phi_{23}^{(1)},\quad u_3=\sqrt{a_1-a_3}\Phi_{13}^{(1)}, \tag{13}$$

assuming the involution (4), and using Eq. (12) in (7) we get the three-wave system:

$$\partial_t u_1+v_1\partial_x u_1+i\varepsilon\overline{u}_2 u_3=0, \tag{14a}$$

$$\partial_t u_2+v_2\partial_x u_2+i\varepsilon\overline{u}_1 u_3=0, \tag{14b}$$

$$\partial_t u_3+v_3\partial_x u_3+i\varepsilon u_1 u_2=0. \tag{14c}$$

Here

$$v_1=\frac{b_2-b_1}{a_1-a_2},\quad v_2=\frac{b_3-b_2}{a_2-a_3},\quad v_3=\frac{b_3-b_1}{a_1-a_3}, \tag{15}$$

$$\varepsilon=\frac{a_1b_2-a_2b_1+a_2b_3-a_3b_2+a_3b_1-a_1b_3}{[(a_1-a_2)(a_2-a_3)(a_1-a_3)]^{1/2}}. \tag{16}$$

The group velocities satisfy the following condition:

$$\frac{v_2-v_3}{v_1-v_3}=-\frac{a_1-a_2}{a_2-a_3}<0. \tag{17}$$

The three-wave system (14) can be interpreted physically. It describes the interaction of three wave packets with complex envelopes u_1, u_2, and u_3 in a medium with quadratic nonlinearity.

In general, the Riemann–Hilbert problem (1)–(2) has multiple solutions. Different solutions are related to each other by the rational matrix functions $\Gamma(k)$ (which also depend on the variables x and t):[2–6,13]

$$\tilde{\Phi}_{\pm}(k,x,t)=\Phi_{\pm}(k,x,t)\Gamma(k,x,t). \tag{18}$$

The rational matrix $\Gamma(k)$ must satisfy the canonical normalization condition: $\Gamma(k)\to I$ for $k\to\infty$ and must have poles only in C_- [the inverse function $\Gamma^{-1}(k)$ then has poles in C_+ only]. Such a rational matrix $\Gamma(k)$ will be called the soliton matrix below, since it gives the soliton part of the solution to the integrable nonlinear PDE.

To specify a unique solution to the Riemann–Hilbert problem the set of the Riemann–Hilbert data must be given. These data are also called the spectral data. The full set of the spectral data comprises the matrix $G(k,x,t)$ on the right-hand side of Eq. (1) and the appropriate discrete data related to the zeros of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$. In the case of involution (4), the zeros of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$ appear in complex conjugate pairs, $\overline{k_j}=k_j^*$. It is known[7–12] (see also Ref. 13) that in the generic case the spectral data include simple (distinct) zeros $k_1,\ldots,k_n$ of $\det\Phi_+(k)$ and $\overline{k_1},\ldots,\overline{k_n}$ of $\det\Phi_-^{-1}(k)$, in their holomorphicity domains, and the null vectors $|v_1\rangle,\ldots,|v_n\rangle$ and $\langle\overline{v_1}|,\ldots,\langle\overline{v_n}|$ from the respective kernels:

$$\Phi_+(k_j)|v_j\rangle=0,\quad \langle\overline{v_j}|\Phi_-^{-1}(\overline{k_j})=0. \tag{19}$$

Using the property (10) one can verify that the zeros do not depend on the variables x and t. The (x,t) dependence of the null vectors can be easily derived by differentiation of (19) and use of the linear spectral equations (5) and (6). This dependence reads

$$|v_j\rangle = \exp\{-\Lambda(k_j)x - \Omega(k_j)t\}|v_{0j}\rangle, \tag{20a}$$

$$\langle\overline{v_j}| = \langle\overline{v}_{0j}|\exp\{\Lambda(\overline{k_j})x + \Omega(\overline{k_j})t\}, \tag{20b}$$

where $|v_{0j}\rangle$ and $\langle\overline{v}_{0j}|$ are constant vectors.

The vectors in Eqs. (20a) and (20b) together with the zeros constitute the full set of the generic discrete data necessary to specify the soliton matrix $\Gamma(k,x,t)$ and, hence, unique solution to the Riemann–Hilbert problem (1)–(2). Indeed, by constructing the soliton matrix $\Gamma(k)$ such that the following matrix functions:

$$\phi_+(k) = \Phi_+(k)\Gamma^{-1}(k), \quad \phi_-^{-1}(k) = \Gamma(k)\Phi_-^{-1}(k) \tag{21}$$

are nondegenerate and holomorphic in the domains C_+ and C_-, respectively, we reduce the Riemann–Hilbert problem with zeros to another one without zeros and hence uniquely solvable (for details see, for instance, Refs. 2–4, 13). Below by matrix $\Gamma(k)$ we will imply the matrix from equation (21) which reduces the Riemann–Hilbert problem (1)–(2) to the one without zeros. The corresponding solution to the integrable PDE (7) is obtained by using the asymptotic expansion of the matrix $\Phi(k)$ as $k\to\infty$ in the linear equation (5). In the N-wave interaction model it is given by formula (12). The pure soliton solutions are obtained by using the rational matrix $\Phi = \Gamma(k)$.

The above set of discrete spectral data (19) holds only for the generic case where zeros of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$ are simple. If these zeros are higher-order rather than simple, what the discrete spectral data should be and how they evolve with x and t is unknown *a priori*. Moreover, we have stressed in Sec. I that the case of higher-order zeros cannot be treated by coalescing simple zeros, thus is highly nontrivial. In the next sections, we give the complete solution to this problem.

III. SOLITON MATRICES FOR GENERAL HIGHER-ORDER ZEROS

In this section we derive the soliton matrices for an arbitrary matrix dimension N and an arbitrary number of higher-order zeros under the assumption that these zeros are normal (see Definition 1). Normal higher-order zeros are most common in practice. In general, they are non-elementary. Our approach is based on a generalization of the idea in our previous paper.[22]

A. Product representation of soliton matrices

Our starting point to tackle this problem is to derive a product representation for soliton matrices. This product representation is not convenient for obtaining soliton solutions, but it will lead to the summation representation of soliton matrices, which is very useful.

In treating the soliton matrix as a product of constituent matrices [called elementary matrices in Ref. 2, see formulas (24) and (27) below] one can consider each zero of the Riemann–Hilbert problem separately. For instance, consider a pair of zeros k_1 and $\overline{k_1}$, respectively, of $\Phi_+(k)$ and $\Phi_-^{-1}(k)$ from Eq. (1), each having order m:

$$\det\Phi_+(k) = (k-k_1)^m\varphi(k), \quad \det\Phi_-^{-1}(k) = (k-\overline{k_1})^m\overline{\varphi}(k), \tag{22}$$

where $\varphi(k_1)\neq 0$ and $\overline{\varphi}(\overline{k_1})\neq 0$. The geometric multiplicity of k_1 $(\overline{k_1})$ is defined as the number of independent vectors in the kernel of $\Phi_+(k_1)$ $(\Phi_-^{-1}(\overline{k_1}))$, see (19). In other words, the geometric multiplicity of k_1 $(\overline{k_1})$ is the dimension of the kernel space of $\Phi_+(k_1)$ $(\Phi_-^{-1}(\overline{k_1}))$. It can be easily shown that the order of a zero is always greater or equal to its geometric multiplicity. It is also obvious that the geometric multiplicity of a zero is less than the matrix dimension. Let us recall how the soliton matrices are usually constructed (see, for instance, Refs. 2 and 13). Starting from the solution $\Phi_\pm(k)$ to the Riemann–Hilbert problem (1)–(2), one looks for the independent vectors in the kernels of the matrices $\Phi_+(k_1)$ and $\Phi_-^{-1}(\overline{k_1})$. Assuming that the geometric multiplicities of k_1 and $\overline{k_1}$ are the same and equal to r_1, then we have

$$\Phi_+(k_1)|v_{i1}\rangle=0, \quad \langle\overline{v}_{i1}|\Phi_-^{-1}(\overline{k}_1)=0, \quad i=1,\ldots,r_1. \tag{23}$$

Next, one constructs the constituent matrix

$$\chi_1(k)=I-\frac{k_1-\overline{k}_1}{k-\overline{k}_1}P_1, \tag{24}$$

where

$$P_1=\sum_{i,j}^{r_1}|v_{i1}\rangle(K^{-1})_{ij}\langle\overline{v}_{j1}|, \quad K_{ij}=\langle\overline{v}_{i1}|v_{j1}\rangle. \tag{25}$$

Here P_1 is a projector matrix, i.e., $P_1^2=P_1$. It can be shown that $\det\chi_1=(k-k_1)^{r_1}/(k-\overline{k}_1)^{r_1}$ (note that the geometric multiplicity r_1 is equal to $\operatorname{rank}P_1$). If $r_1<m$ then one considers the new matrix functions

$$\tilde{\Phi}_+(k)=\Phi_+(k)\chi_1^{-1}(k), \quad \tilde{\Phi}_-^{-1}(k)=\chi_1(k)\Phi_-^{-1}(k).$$

By virtue of Eqs. (23), the matrices $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-^{-1}(k)$ are also holomorphic in the respective half planes of the complex plane (see Lemma 1 in Ref. 22). In addition, k_1 and $\overline{k}_1$ are still zeros of $\det\tilde{\Phi}_+(k)$ and $\det\tilde{\Phi}_-^{-1}(k)$. Assuming that the geometric multiplicities of zeros k_1 and $\overline{k}_1$ in new matrices $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-^{-1}(k)$ are still the same and equal to r_2, then the above steps can be repeated, and we can define matrix $\chi_2(k)$ analogous to Eq. (24). In general, if the geometric multiplicities of zeros k_1 and $\overline{k}_1$ in matrices

$$\tilde{\Phi}_+(k)=\Phi_+(k)\chi_1^{-1}(k)\cdots\chi_{l-1}^{-1}(k), \quad \tilde{\Phi}_-^{-1}(k)=\chi_{l-1}(k)\cdots\chi_1(k)\Phi_-^{-1}(k) \tag{26}$$

are the same and given by r_l $(l=1,2,\ldots)$, then we can define a matrix χ_l similar to Eqs. (24) and (25) but the independent vectors $|v_{il}\rangle$ and $\langle\overline{v}_{il}|$ $(i=1,\ldots,r_l)$ are from the kernels of $\tilde{\Phi}_+(k_1)$ and $\tilde{\Phi}_-^{-1}(\overline{k}_1)$ in Eq. (26). When this process is finished, one would get the constituent matrices $\chi_1(k),\ldots,\chi_r(k)$ such that $r_1+r_2+\cdots+r_n=m$, and the product representation of the soliton matrix $\Gamma(k)$,

$$\Gamma(k)=\chi_n(k)\cdots\chi_2(k)\chi_1(k). \tag{27}$$

This product representation (27) is our starting point of this paper. In arriving at this representation, our assumptions are that the zeros k_1 and $\overline{k}_1$ have the same algebraic multiplicity [see Eq. (22)], and their geometric multiplicities in matrices $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-^{-1}(k)$ of Eq. (26) are also the same for all l's. For convenience, we introduce the following definition.

Definition 1: A pair of zeros k_1 and $\overline{k}_1$ in the matrix Riemann–Hilbert problem is called normal if the zeros have the same algebraic multiplicity, and their geometric multiplicities in matrices $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-^{-1}(k)$ of Eq. (26) are also the same for all l's.

In the text of this paper, we only consider normal zeros of the matrix Riemann–Hilbert problem. The case of abnormal zeros will be briefly discussed in the Appendix.

Remark 1: Under the involution property (4), all zeros are normal. Thus, our results for normal zeros cover almost all the physically important integrable PDEs.

Remark 2: Normal zeros include the elementary zeros of Ref. 22 as special cases, but they are nonelementary in general.

It is an important fact (see Ref. 22, Lemma 2) that the sequence of ranks of the projectors P_l in the matrix $\Gamma(k)$ given by Eq. (27), i.e., built in the described way, is nonincreasing:

$$\text{rank}\, P_n \leqslant \text{rank}\, P_{r-1} \leqslant \cdots \leqslant \text{rank}\, P_1, \tag{28}$$

i.e., $r_n \leqslant r_{n-1} \leqslant \cdots \leqslant r_1$. This result allows one to classify all possible occurrences of a higher-order zero of the Riemann–Hilbert problem for an arbitrary matrix dimension N. In general, for zeros of the same order, different sequences of ranks in Eq. (28) give different classes of higher-order soliton solutions. In Ref. 22 we constructed the soliton matrices for the simplest sequence of ranks, i.e., $1,\ldots,1$. Such zeros are called "elementary." If the matrix dimension $N=2$ (as for the nonlinear Schrödinger equation), then all higher-order zeros are elementary since $\text{rank}\, P_1$ is always equal to 1.

To obtain the product representation for soliton matrices corresponding to several higher-order normal zeros one can multiply the matrices of the type (27) for each zero, i.e., $\Gamma(k) = \Gamma_1(k)\Gamma_2(k)\cdots\Gamma_{N_Z}(k)$, where N_Z is the number of distinct zeros and each $\Gamma_j(k)$ has the form given by formula (27) with n substituted by some n_j.

The product representation (27) of the soliton matrices is difficult to use for actual calculations of the soliton solutions. Indeed, though the representation (27) seems to be simple, derivation of the (x,t) dependence of the involved vectors (except for the vectors in the first projector P_1) requires solving matrix equations with (x,t)-dependent coefficients. One would like to have a more convenient representation, where all the involved vectors have explicit (x,t) dependence. Below we derive such a representation for soliton matrices corresponding to an arbitrary number of higher-order normal zeros.

For the sake of clarity, we consider first the case of a single pair of higher-order zeros, followed by the most general case of several distinct pairs of higher-order zeros.

B. Soliton matrices for a single pair of zeros

Definition 2: For soliton matrices having a single pair of higher-order normal zeros $(k_1,\overline{k_1})$, *suppose* $\Gamma(k)$ *is constructed judiciously as in Eq. (27), with ranks* r_j *of matrices* $P_j(1\leqslant j\leqslant n)$ *satisfying inequality (28), i.e.,*

$$r_n \leqslant r_{n-1} \leqslant \cdots \leqslant r_1.$$

Then a new sequence of positive integers

$$s_1 \geqslant s_2 \geqslant \cdots \geqslant s_{r_1}$$

is defined as follows:

$s_\nu \equiv$ *the index of the last positive integer in the array* $[r_1+1-\nu, r_2+1-\nu, \ldots, r_n+1-\nu]$. *The sequence of integers* $\{r_n, r_{n-1}, \ldots, r_1\}$ *is then the rank sequence associated with the pair of zeros* $(k_1,\overline{k_1})$ *and the new sequence* $\{s_1, s_2, \ldots, s_{r_1}\}$ *is called the block sequence associated with this pair of zeros.*

Remark: It is easy to see that the sum of the block sequence is equal to the sum of all ranks,

$$\sum_{\nu=1}^{r_1} s_\nu = \sum_{l=1}^{n} r_l,$$

with the sum being equal to the algebraic order of the Riemann–Hilbert zeros $(k_1,\overline{k_1})$.

For example, if the rank sequence is {3} [only one constituent matrix in (27)—trivial higher-order zero], then the block sequence is {1,1,1}; if the rank sequence is {1,1,1,1} (an elementary zero), then the block sequence is {4}; if the rank sequence is {2,3,5,7}, then the block sequence is {4,4,3,2,2,1,1}.

With these definitions the most general soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$ for a single pair of higher-order normal zeros $(k_1,\overline{k_1})$ are given as follows. This result is a generalization of our previous result[22] to nonelementary higher-order zeros.

Lemma 1: Consider a single pair of higher-order normal zeros $(k_1,\overline{k_1})$ *in the Riemann–Hilbert problem. Suppose their geometric multiplicity is* r_1, *and their block sequence is* $\{s_1,s_2,\ldots,s_{r_1}\}$. *Then the soliton matrices* $\Gamma(k)$ *and* $\Gamma^{-1}(k)$ *can be written in the following summation forms:*

$$\Gamma(k)=I+\sum_{\nu=1}^{r_1}\overline{\mathcal{S}}_\nu,\quad \Gamma^{-1}(k)=I+\sum_{\nu=1}^{r_1}\mathcal{S}_\nu. \tag{29}$$

Here $\mathcal{S}_\nu$ *and* $\overline{\mathcal{S}}_\nu$ *are the following block matrices,*

$$\overline{\mathcal{S}}_\nu=\sum_{l=1}^{s_\nu}\sum_{j=1}^{l}\frac{|\overline{q}_j^{(\nu)}\rangle\langle\overline{p}_{l+1-j}^{(\nu)}|}{(k-\overline{k}_1)^{s_\nu+1-l}}=(|\overline{q}_{s_\nu}^{(\nu)}\rangle,\ldots,|\overline{q}_1^{(\nu)}\rangle\overline{D}_\nu(k)\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}, \tag{30a}$$

$$\mathcal{S}_\nu=\sum_{l=1}^{s_\nu}\sum_{j=1}^{l}\frac{|p_{l+1-j}^{(\nu)}\rangle\langle q_j^{(\nu)}|}{(k-k_1)^{s_\nu+1-l}}=(|p_1^{(\nu)}\rangle,\ldots,|p_{s_\nu}^{(\nu)}\rangle D_\nu(k)\begin{pmatrix}\langle q_{s_\nu}^{(\nu)}|\\ \vdots\\ \langle q_1^{(\nu)}|\end{pmatrix}, \tag{30b}$$

where $D_\nu(k)$ *and* $\overline{D}_\nu(k)$ *are triangular Toeplitz matrices of the size* $s_\nu\times s_\nu$:

$$\overline{D}_\nu(k)=\begin{pmatrix}\frac{1}{(k-\overline{k}_1)} & 0 & \cdots & 0\\ \frac{1}{(k-\overline{k}_1)^2} & \frac{1}{(k-\overline{k}_1)} & \ddots & \vdots\\ \vdots & \ddots & \ddots & 0\\ \frac{1}{(k-\overline{k}_1)^{s_\nu}} & \cdots & \frac{1}{(k-\overline{k}_1)^2} & \frac{1}{(k-\overline{k}_1)}\end{pmatrix},$$

$$D_\nu(k)=\begin{pmatrix}\frac{1}{(k-k_1)} & \frac{1}{(k-k_1)^2} & \cdots & \frac{1}{(k-k_1)^{s_\nu}}\\ 0 & \ddots & \ddots & \vdots\\ \vdots & \ddots & \frac{1}{(k-k_1)} & \frac{1}{(k-k_1)^2}\\ 0 & \cdots & 0 & \frac{1}{(k-k_1)}\end{pmatrix}. \tag{31}$$

The vectors $|p_i^{(\nu)}\rangle,\langle\overline{p}_i^{(\nu)}|,\langle q_i^{(\nu)}|,|\overline{q}_i^{(\nu)}\rangle$ $(i=1,\ldots,s_\nu)$ *are independent of* k, *and in the two sets* $\{|p_1^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle\}$ *and* $\{\langle\overline{p}_1^{(1)}|,\ldots,\langle\overline{p}_1^{(r_1)}|\}$ *the vectors are linearly independent.*

Remark 1: If $r_1=1$, the zeros k_1 and $\overline{k_1}$ are elementary.[22] In this case, the above soliton matrices reduce to those in Ref. 22.

Remark 2: The total number of all $|p\rangle$ vectors or $\langle\overline{p}|$ vectors from all ν blocks are equal to the algebraic order of the zeros k_1 and $\overline{k_1}$.

Proof: The representation (29) can be proved by induction. Consider, for instance, the formula for $\Gamma(k)$. Obviously, this formula is valid for $n=1$ in Eq. (27), where $\Gamma(k)$ contains only a single

matrix $\chi_1(k)$. Now, suppose that this formula is valid for $n>1$. We need to show that it is valid for $n+1$ as well. Indeed, denote the soliton matrices for n and $n+1$ by $\Gamma(k)$, and $\tilde{\Gamma}(k)$, respectively, the rightmost multiplier in $\tilde{\Gamma}(k)$ being $\tilde{\chi}(k)$. Then we have

$$\tilde{\Gamma}(k)=\Gamma(k)\tilde{\chi}(k)=\left(I+\frac{A_1}{k-\overline{k_1}}+\frac{A_2}{(k-\overline{k_1})^2}+\cdots+\frac{A_n}{(k-\overline{k_1})^n}\right)\left(I+\frac{R}{k-\overline{k_1}}\right)$$

$$=I+\frac{\tilde{A}_1}{k-\overline{k_1}}+\frac{\tilde{A}_2}{(k-\overline{k_1})^2}+\cdots+\frac{\tilde{A}_{n+1}}{(k-\overline{k_1})^{n+1}}, \tag{32}$$

where

$$R\equiv(\overline{k_1}-k_1)\tilde{P}=\sum_{l=1}^{\tilde{r}}|u_l\rangle\langle\overline{u_l}|. \tag{33}$$

Here we have normalized the vectors $|u_l\rangle$ and $\langle\overline{u_l}|$ such that

$$\langle\overline{u_l}|u_i\rangle=(\overline{k_1}-k_1)\,\delta_{l,i}\,, \tag{34}$$

and $\tilde{r}=\operatorname{rank}R$. In view of Eq. (28), we know that $\tilde{r}\geqslant r_1$, where r_1 is the geometric multiplicity of k_1 and $\overline{k_1}$ in the soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$. The coefficients at the poles in $\tilde{\Gamma}(k)$ are given by

$$\tilde{A}_1=A_1+R,\quad \tilde{A}_j=A_j+A_{j-1}R,\quad j=2,\ldots,n,\quad \tilde{A}_{n+1}=A_nR. \tag{35}$$

Consider first the coefficients $\tilde{A}_2$ to $\tilde{A}_{n+1}$. The explicit form of the coefficients A_j can be obtained from Eqs. (29), (30), and (32) as

$$A_j\equiv\sum_{\nu=1}^{r_1}A_j^{(\nu)}=\sum_{\nu=1}^{r_1}\sum_{l=1}^{s_\nu+1-j}|\overline{q}_l^{(\nu)}\rangle\langle\overline{p}_{s_\nu+2-j-l}^{(\nu)}|, \tag{36}$$

where the inner sum is zero if $s_\nu+1-j\leqslant 0$. Substituting this expression into (35) and defining the following new vectors in each block:

$$\langle\tilde{\overline{p}}_1^{(\nu)}|=\langle\overline{p}_1^{(\nu)}|R,\quad \langle\tilde{\overline{p}}_j^{(\nu)}|=\langle\overline{p}_j^{(\nu)}|R+\langle\overline{p}_{j-1}^{(\nu)}|,\quad j=2,\ldots,s_\nu, \tag{37}$$

[for blocks of size 1, $s_\nu=1$, the second formula in (37) is dropped], we then put the coefficients $\tilde{A}_2,\ldots,\tilde{A}_{n+1}$ into the required form

$$\tilde{A}_j=\sum_{\nu=1}^{r_1}\sum_{l=1}^{\tilde{s}_\nu+1-j}|\tilde{\overline{q}}_l^{(\nu)}\rangle\langle\tilde{\overline{p}}_{\tilde{s}_\nu+2-j-l}^{(\nu)}|,\quad j=2,\ldots,n+1,$$

where

$$|\tilde{\overline{q}}_l^{(\nu)}\rangle\equiv|\overline{q}_l^{(\nu)}\rangle,\quad l=1,\ldots,\tilde{s}_\nu-1,$$

and $\tilde{s}_\nu=s_\nu+1$, i.e., the size of each ν-block grows by one as we multiply by $\tilde{\chi}(k)$ in formula (32).

Next, we consider the coefficient $\tilde{A}_1$. Defining the vector $\langle\tilde{\overline{p}}_{\tilde{s}_\nu}^{(\nu)}|\equiv\langle\overline{p}_{s_\nu}^{(\nu)}|$ and utilizing the definition (37), we can rewrite $A_1^{(\nu)}$ as

$$A_1^{(\nu)}=\sum_{l=1}^{\tilde{s}_\nu-1}|\overline{q}_l^{(\nu)}\rangle\langle\tilde{\bar{p}}^{(\nu)}_{\tilde{s}_\nu+1-l}|-\sum_{l=2}^{s_\nu}|\overline{q}_l^{(\nu)}\rangle\langle\overline{p}^{(\nu)}_{s_\nu+2-l}|R. \tag{38}$$

To set $\tilde{A}_1=A_1+R$ into the required form

$$\tilde{A}_1=\sum_{\mu=r_1+1}^{\tilde{r}}|\tilde{\bar{q}}_1^{(\mu)}\rangle\langle\tilde{\bar{p}}_1^{(\mu)}|+\sum_{\nu=1}^{r_1}\sum_{l=1}^{\tilde{s}_\nu}|\tilde{\bar{q}}_l^{(\nu)}\rangle\langle\tilde{\bar{p}}^{(\nu)}_{\tilde{s}_\nu+1-l}|, \tag{39}$$

we must define exactly one new vector $|\tilde{\bar{q}}^{(\nu)}_{\tilde{s}_\nu}\rangle$ for each ν-block [in the second term of Eq. (39)] and $\tilde{r}-r_1$ new blocks of size 1 containing $2(\tilde{r}-r_1)$ new vectors $|\overline{q}_1^{(\mu)}\rangle$ and $\langle\tilde{\bar{p}}_1^{(\mu)}|$. Due to formulas (35) and (38), the new vectors to be defined must satisfy the following equation:

$$\sum_{\mu=r_1+1}^{\tilde{r}}|\tilde{\bar{q}}_1^{(\mu)}\rangle\langle\tilde{\bar{p}}_1^{(\mu)}|+\sum_{\nu=1}^{r_1}|\tilde{\bar{q}}^{(\nu)}_{\tilde{s}_\nu}\rangle\langle\overline{p}_1^{(\nu)}|R=R-\sum_{\nu=1}^{r_1}\sum_{l=2}^{s_\nu}|\overline{q}_l^{(\nu)}\rangle\langle\overline{p}^{(\nu)}_{s_\nu+2-l}|R, \tag{40}$$

where the definition of $\langle\tilde{\bar{p}}_1^{(\nu)}|$ in Eq. (37) has been utilized. Substituting the expression (33) for R into the above equation, we get

$$\sum_{\mu=r_1+1}^{\tilde{r}}|\tilde{\bar{q}}_1^{(\mu)}\rangle\langle\tilde{\bar{p}}_1^{(\mu)}|=\sum_{l=1}^{\tilde{r}}|\xi_l\rangle\langle\overline{u_l}|, \tag{41}$$

where

$$|\xi_l\rangle\equiv\left(I-\sum_{\nu=1}^{r_1}\sum_{l=2}^{s_\nu}|\overline{q}_l^{(\nu)}\rangle\langle\overline{p}^{(\nu)}_{s_\nu+2-l}|\right)|u_l\rangle-\sum_{\nu=1}^{r_1}|\tilde{\bar{q}}^{(\nu)}_{\tilde{s}_\nu}\rangle\langle\overline{p}_1^{(\nu)}|u_l\rangle,\quad l=1,\ldots,\tilde{r}.$$

To show that Eq. (41) is solvable, we need to use an important fact that the matrix

$$\mathcal{M}=(\mathcal{M}_{\nu,l}),\quad \mathcal{M}_{\nu,l}=\langle\overline{p}_1^{(\nu)}|u_l\rangle,\quad \nu=1,\ldots,r_1,\quad l=1,\ldots,\tilde{r}_1,$$

has rank r_1. This fact can be proved by contradiction as follows.

Suppose the matrix $\mathcal{M}$ has rank less than r_1. Then its r_1 rows are linearly dependent. Thus, there are such scalars $C_1,C_2,\ldots,C_{r_1}$, not equal to zero simultaneously, that the vector

$$\langle\eta|\equiv\sum_{\nu=1}^{r_1}C_\nu\langle\overline{p}_1^{(\nu)}|$$

is orthogonal to all $|u_l\rangle$'s, i.e.,

$$\langle\eta|u_l\rangle=0,\quad 1\leqslant l\leqslant\tilde{r}. \tag{42}$$

According to our induction assumption that soliton matrices involving n multipliers in formula (27) have the form (29), we can easily show, by equating the coefficient at the highest pole at $k=\overline{k_1}$ in the left-hand side (lhs) of the identity $\Gamma(k)\Gamma^{-1}(k)=I$ to zero, that $\langle\overline{p}_1^{(\nu)}|\Gamma^{-1}(\overline{k_1})=0$ for all $1\leqslant\nu\leqslant r_1$ (see also Ref. 22). Thus $\langle\eta|\Gamma^{-1}(\overline{k_1})=0$ as well. According to Lemma 1 in Ref. 22, if $\langle\eta|$ is in the kernel of $\Gamma^{-1}(\overline{k_1})$ and is orthogonal to all $|u_l\rangle$'s, then $\langle\eta|$ is in the kernel of $\tilde{\Gamma}^{-1}(\overline{k_1})$ as well, i.e., $\langle\eta|\tilde{\Gamma}^{-1}(\overline{k_1})=0$. But according to our construction of soliton matrices [see Eq. (27)], the vectors $\langle\overline{u_l}|$ $(l=1,\ldots,\tilde{r})$ are all the linearly independent vectors in the kernel of $\tilde{\Gamma}^{-1}(\overline{k_1})$. Thus $\langle\eta|$ must be a linear combination of $\langle\overline{u_l}|$'s. Then in view of Eqs. (34) and (42), we find that $\langle\eta|=0$, which leads to a contradiction.

Now that the matrix $\mathcal{M}$ has rank r_1, then we are able to select vectors $|\tilde{\bar{q}}_{\tilde{s}_\nu}^{(\nu)}\rangle$ ($\nu=1,\ldots,r_1$) such that r_1 of the $\tilde{r}$ vectors $\langle\xi_l|$ are zero. With this choice of $|\tilde{\bar{q}}_{\tilde{s}_\nu}^{(\nu)}\rangle$'s, the rhs of Eq. (41) becomes $\tilde{r}-r_1$ blocks of size 1. Assigning these blocks to the lhs of (41), then Eq. (41) can be solved. Hence we can put the coefficient $\tilde{A}_1$ in the required form (39).

Next we prove that all vectors $\langle\tilde{\bar{p}}_1^{(\nu)}|$ ($1\leqslant\nu\leqslant\tilde{r}$) in the matrix $\tilde{\Gamma}(k)$ are linearly independent. These vectors were defined in the above proof as

$$\langle\tilde{\bar{p}}_1^{(\nu)}|=\langle\overline{p}_1^{(\nu)}|R=\sum_{l=1}^{\tilde{r}}\langle\overline{p}_1^{(\nu)}|u_l\rangle\langle\overline{u_l}|,\quad 1\leqslant\nu\leqslant r_1, \tag{43}$$

and $\langle\tilde{\bar{p}}_1^{(\nu)}|$ for $r_1+1\leqslant\nu\leqslant\tilde{r}$ are simply equal to $\tilde{r}-r_1$ of the vectors $\overline{u_l}$ depending on what $r_1\times r_1$ submatrix of $\mathcal{M}$ has rank r_1. To be definite, let us suppose the first r_1 columns of the matrix $\mathcal{M}$ have rank r_1 (i.e., linearly independent). Then according to the above proof, we can uniquely select vectors $|\tilde{\bar{q}}_{\tilde{s}_\nu}^{(\nu)}\rangle$ ($\nu=1,\ldots,r_1$) such that $|\xi_l\rangle=0$ for $1\leqslant l\leqslant r_1$. Thus,

$$\langle\tilde{\bar{p}}_1^{(\nu)}|=\langle\overline{u_\nu}|,\quad r_1+1\leqslant\nu\leqslant\tilde{r}. \tag{44}$$

Recalling that vectors $\langle\overline{u_\nu}|$ ($1\leqslant\nu\leqslant\tilde{r}$) in the projector R (33) are linearly independent, and the first r_1 columns of matrix $\mathcal{M}$ have rank r_1, we easily see that vectors $\langle\tilde{\bar{p}}_1^{(\nu)}|$ ($1\leqslant\nu\leqslant\tilde{r}$) as defined in Eqs. (43) and (44) are linearly independent.

Last, we prove that the sizes of blocks in representations (29) are given by the block sequence defined in Definition 2. An equivalent statement is that the numbers of matrix blocks with sizes $[1,2,3,\ldots,n]$ are given by the pairwise differences in the sequence of ranks: $[r_1-r_2,r_2-r_3,\ldots,r_{n-1}-r_n,r_n]$, where the last number in the sequence defines the number of blocks of size n. This can be easily proven by the induction argument using the fact that the number of new blocks of size 1 in $\tilde{A}_1$ (35) is given by $\tilde{r}-r_1$, while the sizes of old blocks grow by 1 in each multiplication as in formula (32).

Using similar arguments, we can prove that the representation (29) for $\Gamma^{-1}(k)$ is valid, and vectors $|p_1^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle$ are linearly independent. This concludes the proof of Lemma 1. Q.E.D.

C. Soliton matrices for several pairs of zeros

Next, we extend the above results to the most general case of several pairs of higher-order normal zeros $\{(k_1,\overline{k_1}),\ldots,(k_{N_Z},\overline{k_{N_Z}})\}$. In this general case, the soliton matrix $\Gamma(k)$ can be constructed as a product of soliton matrices (27) for each zero, which are given by the procedure outlined in the beginning of this section [see Eqs. (22) to (27)]. Thus, $\Gamma(k)$ can be represented as

$$\Gamma(k)=\Gamma_1(k)\cdot\Gamma_2(k)\cdots\Gamma_{N_Z}(k). \tag{45}$$

For each pair of zeros $(k_j,\overline{k_j})$, we can define its rank sequence and block sequence by Definition 2 either from $\Gamma(k)$ directly or from the individual matrix $\Gamma_j(k)$ associated with this zero. It is easy to see that using either of $\Gamma(k)$ or $\Gamma_j(k)$ gives the same results. The inverse matrix $\Gamma^{-1}(k)$ can be represented in a similar way.

The product representation (45) for $\Gamma(k)$ and its counterpart for $\Gamma^{-1}(k)$ are not convenient for deriving soliton solutions. Their summation representations such as Eq. (29) are needed. It turns out that $\Gamma(k)$ and $\Gamma^{-1}(k)$ in the general case are given simply by sums of all the blocks from all pairs of zeros plus the unit matrix. Let us formulate this result in the next lemma.

Lemma 2: Consider several pairs of higher-order normal zeros $\{(k_1,\overline{k_1}),\ldots,(k_{N_Z},\overline{k_{N_Z}})\}$ *in the Riemann–Hilbert problem. Denote the geometric multiplicity of zeros* $(k_n,\overline{k_n})$ *as* $r_1^{(n)}$ *and their block sequence as* $\{s_1^{(n)},s_2^{(n)},\ldots,s_{r_1^{(n)}}^{(n)}\}$ ($1\leqslant n\leqslant N_Z$). *Then the soliton matrices* $\Gamma(k)$ *and* $\Gamma^{-1}(k)$ *can be written in the following summation forms:*

$$\Gamma(k)=I+\sum_{n=1}^{N_Z}\sum_{\nu=1}^{r_1^{(n)}}\overline{\mathcal{S}}_\nu^{(n)},\quad \Gamma^{-1}(k)=I+\sum_{n=1}^{N_Z}\sum_{\nu=1}^{r_1^{(n)}}\mathcal{S}_\nu^{(n)}. \tag{46}$$

Here $\mathcal{S}_\nu^{(n)}$ and $\overline{\mathcal{S}}_\nu^{(n)}$ are the following block matrices:

$$\overline{\mathcal{S}}_\nu^{(n)}=(|\overline{q}_{s_\nu^{(n)}}^{(\nu,n)}\rangle,\ldots,|\overline{q}_1^{(\nu,n)}\rangle)\overline{D}_\nu^{(n)}(k)\begin{pmatrix}\langle\overline{p}_1^{(\nu,n)}|\\ \vdots\\ \langle\overline{p}_{s_\nu^{(n)}}^{(\nu,n)}|\end{pmatrix}, \tag{47a}$$

$$\mathcal{S}_\nu^{(n)}=(|p_1^{(\nu,n)}\rangle,\ldots,|p_{s_\nu^{(n)}}^{(\nu,n)}\rangle)D_\nu^{(n)}(k)\begin{pmatrix}\langle q_{s_\nu^{(n)}}^{(\nu,n)}|\\ \vdots\\ \langle q_1^{(\nu,n)}|\end{pmatrix}, \tag{47b}$$

where $D_\nu^{(n)}(k)$ and $\overline{D}_\nu^{(n)}(k)$ are triangular Toeplitz matrices of the size $s_\nu^{(n)}\times s_\nu^{(n)}$:

$$\overline{D}_\nu^{(n)}(k)=\begin{pmatrix}\frac{1}{(k-\overline{k}_n)} & 0 & \cdots & 0\\ \frac{1}{(k-\overline{k}_n)^2} & \frac{1}{(k-\overline{k}_n)} & \ddots & \vdots\\ \vdots & \ddots & \ddots & 0\\ \frac{1}{(k-\overline{k}_n)^{s_\nu^{(n)}}} & \cdots & \frac{1}{(k-\overline{k}_n)^2} & \frac{1}{(k-\overline{k}_n)}\end{pmatrix},$$

$$D_\nu^{(n)}(k)=\begin{pmatrix}\frac{1}{(k-k_n)} & \frac{1}{(k-k_n)^2} & \cdots & \frac{1}{(k-k_n)^{s_\nu^{(n)}}}\\ 0 & \ddots & \ddots & \vdots\\ \vdots & \ddots & \frac{1}{(k-k_n)} & \frac{1}{(k-k_n)^2}\\ 0 & \cdots & 0 & \frac{1}{(k-k_n)}\end{pmatrix}. \tag{48}$$

Vectors $|p_i^{(\nu,n)}\rangle,\langle\overline{p}_i^{(\nu,n)}|,\langle q_i^{(\nu,n)}|,|\overline{q}_i^{(\nu,n)}\rangle$ $(i=1,\ldots,s_\nu^{(n)})$ are independent of k. In addition, for each n, vectors $\{|p_1^{(1,n)}\rangle,\ldots,|p_1^{(r_1^{(n)},n)}\rangle\}$ and $\{\langle\overline{p}_1^{(1,n)}|,\ldots,\langle\overline{p}_1^{(r_1^{(n)},n)}|\}$ are linearly independent, respectively.

Proof: Again we will rely on the induction argument. As it was already mentioned, the general soliton matrix $\Gamma(k)$ corresponding to several distinct zeros can be represented as a product (45) of individual soliton matrices (27) for each zero. For clarity reason and simplicity of the presentation we will give detailed calculations for the simplest case of just one product in (45). Then we will show how to generalize the calculations. Consider soliton matrix $\Gamma(k)$ for two pairs of distinct higher-order zeros $(k_1,\overline{k}_1)$ and $(k_2,\overline{k}_2)$. We have $\Gamma(k)=\Gamma_1(k)\Gamma_2(k)$ and

$$\Gamma(k)=\left(I+\frac{A_1}{k-\overline{k}_1}+\cdots+\frac{A_{n_1}}{(k-\overline{k}_1)^{n_1}}\right)\left(I+\frac{B_1}{k-\overline{k}_2}+\cdots+\frac{B_{n_2}}{(k-\overline{k}_2)^{n_2}}\right). \tag{49}$$

Here n_j $(j=1,2)$ is the number of simple matrices in the product representation (27) for Γ_j. Due to Lemma 1, the coefficients A_j and B_j are given by formulas similar to (36):

$$A_j=\sum_{\nu=1}^{r_1^{(1)}}\sum_{l=1}^{s_\nu^{(1)}+1-j}|\overline{q}_l^{(\nu,1)}\rangle\langle\overline{p}_{s_\nu^{(1)}+2-j-l}^{(\nu,1)}|, \tag{50}$$

$$B_j=\sum_{\nu=1}^{r_1^{(2)}}\sum_{l=1}^{s_\nu^{(2)}+1-j}|\overline{q}_l^{(\nu,2)}\rangle\langle\overline{p}_{s_\nu^{(2)}+2-j-l}^{(\nu,2)}|. \tag{51}$$

On the other hand, by expanding formula (49) into the partial fractions we get

$$\Gamma(k)=I+\frac{\tilde{A}_1}{k-\overline{k}_1}+\cdots+\frac{\tilde{A}_{n_1}}{(k-\overline{k}_1)^{n_1}}+\frac{\tilde{B}_1}{k-\overline{k}_2}+\cdots+\frac{\tilde{B}_n}{(k-\overline{k}_2)^{n_2}}. \tag{52}$$

Consider first the coefficients $\tilde{A}_j$. Multiplication by $(k-\overline{k}_1)^{n_1}$ of both formulas (49) and (52) and taking derivatives at $k=\overline{k}_1$ using the Leibniz rule gives

$$\tilde{A}_{n_1-l}=\frac{1}{l!}\left\{\frac{\mathrm{d}^l}{\mathrm{d}k^l}(k-\overline{k}_1)^{n_1}\Gamma(k)\right\}_{k=\overline{k}_1}=\sum_{j=0}^{l}\frac{A_{n_1-j}}{(l-j)!}\frac{\mathrm{d}^{(l-j)}\Gamma_2}{\mathrm{d}k^{(l-j)}}(\overline{k}_1). \tag{53}$$

In a similar way we get

$$\tilde{B}_{n_2-l}=\sum_{j=0}^{l}\frac{\mathrm{d}^{(l-j)}\Gamma_1}{\mathrm{d}k^{(l-j)}}(\overline{k}_2)\frac{B_{n_2-j}}{(l-j)!}. \tag{54}$$

Now substituting Eqs. (50) and (51) into (53) and (54) and defining new vectors

$$\langle\tilde{\overline{p}}_m^{(\nu,1)}|=\sum_{j=0}^{m-1}\langle\overline{p}_{m-j}^{(\nu,1)}|\frac{1}{j!}\frac{\mathrm{d}^j\Gamma_2}{\mathrm{d}k^j}(\overline{k}_1),\quad m=1,\ldots,s_\nu^{(1)}, \tag{55}$$

and

$$|\tilde{\overline{q}}_m^{(\nu,2)}\rangle=\sum_{j=0}^{m-1}\frac{1}{j!}\frac{\mathrm{d}^j\Gamma_1}{\mathrm{d}k^j}(\overline{k}_2)|\overline{q}_{m-j}^{(\nu,2)}\rangle,\quad m=1,\ldots,s_\nu^{(2)}, \tag{56}$$

we find that

$$\tilde{A}_j=\sum_{\nu=1}^{r_1^{(1)}}\sum_{l=1}^{s_\nu^{(1)}+1-j}|\overline{q}_l^{(\nu,1)}\rangle\langle\tilde{\overline{p}}_{s_\nu^{(1)}+2-j-l}^{(\nu,1)}|, \tag{57}$$

$$\tilde{B}_j=\sum_{\nu=1}^{r_1^{(2)}}\sum_{l=1}^{s_\nu^{(2)}+1-j}|\tilde{\overline{q}}_l^{(\nu,2)}\rangle\langle\overline{p}_{s_\nu^{(2)}+2-j-l}^{(\nu,2)}|, \tag{58}$$

which give precisely the needed representation (46). Note from definitions (55) and (56) that

$$[\langle\tilde{\bar{p}}_1^{(\nu,1)}|,\ldots,\langle\tilde{\bar{p}}_{r_1^{(1)}}^{(\nu,1)}|]=[\langle\bar{p}_1^{(\nu,1)}|,\ldots,\langle\bar{p}_{r_1^{(1)}}^{(\nu,1)}|]\Gamma_2(\bar{k}_1)$$

and

$$[|\tilde{q}_1^{(\nu,2)}\rangle,\ldots,|\tilde{q}_{r_1^{(2)}}^{(\nu,2)}\rangle]=\Gamma_1(\bar{k}_2)[|\bar{q}_1^{(\nu,2)}\rangle,\ldots,|\bar{q}_{r_1^{(2)}}^{(\nu,2)}\rangle].$$

Due to Lemma 1, vectors $\{\langle\bar{p}_1^{(\nu,1)}|,\ldots,\langle\bar{p}_{r_1^{(1)}}^{(\nu,1)}|\}$ and $\{|\bar{q}_1^{(\nu,2)}\rangle,\ldots,|\bar{q}_{r_1^{(2)}}^{(\nu,2)}\rangle\}$ are linearly independent respectively. In addition, matrices $\Gamma_1(\bar{k}_2)$ and $\Gamma_2(\bar{k}_1)$ are nondegenerate. Thus new vectors $\{\langle\tilde{\bar{p}}_1^{(\nu,1)}|,\ldots,\langle\tilde{\bar{p}}_{r_1^{(1)}}^{(\nu,1)}|\}$ and $\{|\tilde{\bar{q}}_1^{(\nu,2)}\rangle,\ldots,|\tilde{\bar{q}}_{r_1^{(2)}}^{(\nu,2)}\rangle\}$ are linearly independent respectively as well. This completes the proof of Lemma 2 for two pairs of higher-order zeros.

It is easy to see that the above procedure of redefining the vectors in the blocks corresponding to different zeros will also work in the general case, when $\Gamma_1(k)$ is replaced by the product $\Gamma_1(k)\cdots\Gamma_n(k)$, and $\Gamma_2(k)$ replaced by $\Gamma_{n+1}(k)$. In this case, the sum over all distinct poles will be present in the left parentheses in formula (49), and consequently there will be more terms in formula (52). Formula (53) will be valid for coefficients $\tilde{A}$ of each zero, and formula (54) remains valid as well. Thus by defining vectors $\langle\tilde{\bar{p}}_m^{(\nu,j)}|$ by formula (55) for each zero k_j $(1\leqslant j\leqslant n)$, and defining vectors $|\tilde{\bar{q}}_m^{(\nu,n+1)}\rangle$ by formula (56) for zero k_{n+1}, we can show that the matrix $\Gamma(k)$ consisting of $n+1$ products of $\Gamma_j(k)$ can be put in the required form (46). This induction argument then completes the proof of Lemma 2. Q.E.D.

The notations in the representation (46) for soliton matrices with several zeros are getting complicated. To facilitate the presentations of results in the remainder of this paper, let us reformulate the representation (46). For this purpose, we define $r_1=r_1^{(1)}+\cdots+r_1^{(N_Z)}$, where $r_1^{(n)}$'s are as given in Lemma 2. Then we replace the double summations in Eq. (46) with single ones,

$$\Gamma(k)=I+\sum_{\nu=1}^{r_1}\bar{\mathcal{S}}_\nu,\quad \Gamma^{-1}(k)=I+\sum_{\nu=1}^{r_1}\mathcal{S}_\nu. \tag{59}$$

Inside these single summations, the first $r_1^{(1)}$ terms are blocks of type (47) for the first pair of zeros $(k_1,\bar{k}_1)$, the next $r_1^{(2)}$ terms are blocks of type (47) for the second pair of zeros $(k_2,\bar{k}_2)$, and so on. Block matrices $\mathcal{S}_\nu$ and $\bar{\mathcal{S}}_\nu$ can be written as

$$\bar{\mathcal{S}}_\nu=\sum_{l=1}^{s_\nu}\sum_{j=1}^{l}\frac{|\bar{q}_j^{(\nu)}\rangle\langle\bar{p}_{l+1-j}^{(\nu)}|}{(k-\bar{\kappa}_\nu)^{s_\nu+1-l}}=(|\bar{q}_{s_\nu}^{(\nu)}\rangle,\ldots,|\bar{q}_1^{(\nu)}\rangle)\bar{D}_\nu(k)\begin{pmatrix}\langle\bar{p}_1^{(\nu)}|\\ \vdots\\ \langle\bar{p}_{s_\nu}^{(\nu)}|\end{pmatrix}, \tag{60a}$$

$$\mathcal{S}_\nu=\sum_{l=1}^{s_\nu}\sum_{j=1}^{l}\frac{|p_{l+1-j}^{(\nu)}\rangle\langle q_j^{(\nu)}|}{(k-\kappa_\nu)^{s_\nu+1-l}}=(|p_1^{(\nu)}\rangle,\ldots,|p_{s_\nu}^{(\nu)}\rangle)D_\nu(k)\begin{pmatrix}\langle q_{s_\nu}^{(\nu)}|\\ \vdots\\ \langle q_1^{(\nu)}|\end{pmatrix}, \tag{60b}$$

where matrices $D_\nu(k)$ and $\bar{D}_\nu(k)$ are triangular Toeplitz matrices of the size $s_\nu\times s_\nu$:

$$\bar{D}_\nu(k)=\begin{pmatrix}\frac{1}{(k-\bar{\kappa}_\nu)} & 0 & \cdots & 0\\ \frac{1}{(k-\bar{\kappa}_\nu)^2} & \frac{1}{(k-\bar{\kappa}_\nu)} & \ddots & \vdots\\ \vdots & \ddots & \ddots & 0\\ \frac{1}{(k-\bar{\kappa}_\nu)^{s_\nu}} & \cdots & \frac{1}{(k-\bar{\kappa}_\nu)^2} & \frac{1}{(k-\bar{\kappa}_\nu)}\end{pmatrix},$$

$$D_\nu(k)=\begin{pmatrix} \frac{1}{(k-\kappa_\nu)} & \frac{1}{(k-\kappa_\nu)^2} & \cdots & \frac{1}{(k-\kappa_\nu)^{s_\nu}} \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \frac{1}{(k-\kappa_\nu)} & \frac{1}{(k-\kappa_\nu)^2} \\ 0 & \cdots & 0 & \frac{1}{(k-\kappa_\nu)} \end{pmatrix}. \tag{61}$$

Here

$$\kappa_\nu=k_j, \quad \text{if} \quad 1+\sum_{l=1}^{j-1} r_1^{(l)}\leqslant\nu\leqslant\sum_{l=1}^{j} r_1^{(l)} \quad (1\leqslant j\leqslant N_Z). \tag{62}$$

In other words, $\kappa_\nu=k_1$ for $1\leqslant\nu\leqslant r_1^{(1)}$, $\kappa_\nu=k_2$ for $r_1^{(1)}+1\leqslant\nu\leqslant r_1^{(1)}+r_1^{(2)}$, etc. In addition, $\{s_\nu, 1+\Sigma_{l=1}^{j-1}r_1^{(l)}\leqslant\nu\leqslant\Sigma_{l=1}^{j}r_1^{(l)}\}$ is the block sequence of the jth pair of zeros $(k_j,\overline{k_j})$. This new representation (59) is equivalent to (46), but it proves to be helpful in the calculations below.

We note that the simplified way of block numeration used in the representation (59) reflects the important property of the solitons matrices: the soliton matrices preserve their form if some of the zeros coalesce (or, vice versa, a zero splits itself into two or more zeros). The only thing that does change is the association of a particular ν-block to the pair of zeros.

The representation (59) [or (46)] is but the first step towards the necessary formulas for the soliton matrices. Indeed, there are twice as many vectors in the expressions (59) for $\Gamma(k)$ and $\Gamma^{-1}(k)$ as compared to the total number of vectors in the constituent matrices in the product of representations of the type (27) for each pair of zeros. As the result, only half of the vector parameters, say $|p_i^{(\nu)}\rangle$ and $\langle\overline{p}_i^{(\nu)}|$, are free. To derive the formulas for the rest of the vector parameters in (59) we can use the identity $\Gamma(k)\Gamma^{-1}(k)=\Gamma^{-1}(k)\Gamma(k)=I$. First of all, let us give the equations for the free vectors themselves.

Lemma 3: The vectors $|p_1^{(\nu)}\rangle,\ldots,|p_{s_\nu}^{(\nu)}\rangle$ *and* $\langle\overline{p}_1^{(\nu)}|,\ldots,\langle\overline{p}_{s_\nu}^{(\nu)}|$ *from each* ν*th block in the representation (59)–(60) satisfy the following linear systems of equations:*

$$\mathbf{\Gamma}_\nu(\kappa_\nu)\begin{pmatrix} |p_1^{(\nu)}\rangle \\ \vdots \\ |p_{s_\nu}^{(\nu)}\rangle \end{pmatrix}=0, \quad \mathbf{\Gamma}_\nu(k)\equiv\begin{pmatrix} \Gamma & 0 & \cdots & 0 \\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Gamma & \Gamma & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Gamma & \cdots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Gamma & \Gamma \end{pmatrix}, \tag{63}$$

$$(\langle\overline{p}_1^{(\nu)}|,\ldots,\langle\overline{p}_{s_\nu}^{(\nu)}|)\overline{\mathbf{\Gamma}}_\nu(\overline{\kappa}_\nu)=0, \quad \overline{\mathbf{\Gamma}}_\nu(k)\equiv\begin{pmatrix} \Gamma^{-1} & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Gamma^{-1} & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Gamma^{-1} \\ 0 & \Gamma^{-1} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Gamma^{-1} \\ 0 & \cdots & 0 & \Gamma^{-1} \end{pmatrix}. \tag{64}$$

Remark: Note that the matrices $\mathbf{\Gamma}_\nu(k)$ and $\mathbf{\Gamma}_\nu^{-1}(k)$ have block-triangular Toeplitz forms, i.e., they have the same (matrix) element along each diagonal.

Proof: The derivation of the systems (63)–(64) exactly reproduces the analogous derivation in Ref. 22 for the case of elementary zeros (as the equations for the νth block resemble analogous

equations for a single block corresponding to a pair of elementary zeros). For instance, the system (63) is derived by considering the poles of $\Gamma(k)\Gamma^{-1}(k)$ at $k=\kappa_\nu$, starting from the highest pole and using the representation (59)–(60) for $\Gamma^{-1}(k)$. The details are trivial and will not be reproduced here. Note that there may be several sets of vectors (from different ν-blocks of the same pair of zeros) which satisfy similar equations if the geometric multiplicity of this pair of zeros is higher than 1. Q.E.D.

Now let us express the $|\overline{q}\rangle$ and $\langle q|$ vectors in the expressions (59)–(60) for $\Gamma(k)$ and $\Gamma^{-1}(k)$ through the $|p\rangle$ and $\langle\overline{p}|$ vectors. This will lead to the needed representation of the soliton matrices given through the $|p\rangle$ and $\langle\overline{p}|$ vectors only. It is convenient to formulate the result in the following lemma.

Lemma 4: The general soliton matrices for several pairs of normal zeros $\{(k_1,\overline{k_1}),\ldots,(k_{N_Z},\overline{k_{N_Z}})\}$ *are given by the following formulas:*

$$\Gamma(k)=I-(|p_1^{(1)}\rangle,\ldots,|p_{s_1}^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle,\ldots,|p_{s_{r_1}}^{(r_1)}\rangle)\overline{\mathcal{K}}^{-1}\overline{\mathcal{D}}(k)\begin{pmatrix}\langle\overline{p}_1^{(1)}|\\ \vdots\\ \langle\overline{p}_{s_1}^{(1)}|\\ \vdots\\ \langle\overline{p}_1^{(r_1)}|\\ \vdots\\ \langle\overline{p}_{s_{r_1}}^{(r_1)}|\end{pmatrix}, \tag{65a}$$

$$\Gamma^{-1}(k)=I-(|p_1^{(1)}\rangle,\ldots,|p_{s_1}^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle,\ldots,|p_{s_{r_1}}^{(r_1)}\rangle)\mathcal{D}(k)\mathcal{K}^{-1}\begin{pmatrix}\langle\overline{p}_1^{(1)}|\\ \vdots\\ \langle\overline{p}_{s_1}^{(1)}|\\ \vdots\\ \langle\overline{p}_1^{(r_1)}|\\ \vdots\\ \langle\overline{p}_{s_{r_1}}^{(r_1)}|\end{pmatrix}, \tag{65b}$$

where s_ν *and* r_1 *are the same as in Lemma 2. The matrices* $\overline{\mathcal{D}}(k)$ *and* $\mathcal{D}(k)$ *are block-diagonal:*

$$\overline{\mathcal{D}}(k)\equiv\begin{pmatrix}\overline{D}_1(k) & & 0\\ & \ddots & \\ 0 & & \overline{D}_{r_1}(k)\end{pmatrix},\quad \mathcal{D}(k)\equiv\begin{pmatrix}D_1(k) & & 0\\ & \ddots & \\ 0 & & D_{r_1}(k)\end{pmatrix}, \tag{66}$$

where the triangular Toeplitz matrices $\overline{D}_\nu(k)$ *and* $D_\nu(k)$ *are defined in formulas (61). The matrices* $\overline{K}$ *and* K *have the following block matrix representation:*

$$\overline{\mathcal{K}}\equiv\begin{pmatrix}\overline{K}^{(1,1)} & \ldots & \overline{K}^{(1,r_1)}\\ \vdots & & \vdots\\ \overline{K}^{(r_1,1)} & \ldots & \overline{K}^{(r_1,r_1)}\end{pmatrix},\quad \mathcal{K}\equiv\begin{pmatrix}K^{(1,1)} & \ldots & K^{(1,r_1)}\\ \vdots & & \vdots\\ K^{(r_1,1)} & \ldots & K^{(r_1,r_1)}\end{pmatrix}, \tag{67}$$

with the matrices $\overline{K}^{(\nu,\mu)}$ *and* $K^{(\nu,\mu)}$ *being given as*

$$\overline{K}^{(\nu,\mu)}=\sum_{j=0}^{s_\nu-1}\sum_{l=0}^{s_\mu-1}\frac{(-1)^l(j+l)!}{j!l!}\frac{H_{-j}^{(\nu)}\overline{Q}_l^{(\nu,\mu)}}{(\kappa_\mu-\overline{\kappa}_\nu)^{j+l+1}},$$

$$K^{(\nu,\mu)}=\sum_{l=0}^{s_\nu-1}\sum_{j=0}^{s_\mu-1}\frac{(-1)^l(l+j)!}{l!j!}\frac{Q_l^{(\nu,\mu)}H_j^{(\mu)}}{(\overline{\kappa}_\nu-\kappa_\mu)^{l+j+1}}. \tag{68}$$

Here $\{H^{(\nu)}_{-s_\nu+1},\ldots,H^{(\nu)}_{s_\nu-1}\}$ *is the basis for the space of* $s_\nu\times s_\nu$*-dimensional Toeplitz matrices, defined as* $(H_j^{(\nu)})_{\alpha,\beta}\equiv\delta_{\alpha,\beta-j}$. *The nonzero elements of matrices* $\overline{Q}_l^{(\nu,\mu)}$ *and* $Q_l^{(\nu,\mu)}$ *are defined as the inner products between the p-vectors from the blocks with indices* ν *and* μ:

$$\overline{Q}_l^{(\nu,\mu)}\equiv\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}(0,\ldots,0,|p_1^{(\mu)}\rangle,\ldots,|p_{s_\mu-l}^{(\mu)}\rangle,\quad Q_l^{(\nu,\mu)}\equiv\begin{pmatrix}0\\ \vdots\\ 0\\ \langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu-l}^{(\nu)}|\end{pmatrix}(|p_1^{(\mu)}\rangle,\ldots,|p_{s_\mu}^{(\mu)}\rangle. \tag{69}$$

Remark 1: In the case of a single pair of zeros $(k_1,\overline{k_1})$ simply replace κ_μ $(\overline{\kappa}_\mu)$ and κ_ν $(\overline{\kappa}_\nu)$ in formula (67) by k_1 $(\overline{k_1})$.

Remark 2: In the case of the involution (4) property, the obvious relations hold:

$$\overline{\kappa}_\nu=\kappa_\nu^*,\quad \langle\overline{p}_j^{(\nu)}|=|p_j^{(\nu)}\rangle^\dagger,\quad \overline{D}_\nu(k)=D_\nu^\dagger(k^*),\quad \overline{K}^{(\nu,\mu)}=(K^{(\mu,\nu)})^\dagger.$$

Proof: We only need to prove that the $|\overline{q}\rangle$ and $\langle q|$ vectors in soliton matrices (59) and (60) are related to the $|p\rangle$ and $\langle\overline{p}|$ vectors by

$$(|\overline{q}_{s_1}^{(1)}\rangle,\ldots,|\overline{q}_1^{(1)}\rangle,\ldots,|\overline{q}_{s_{r_1}}^{(r_1)}\rangle,\ldots,|\overline{q}_1^{(r_1)}\rangle)\overline{\mathcal{K}}=-(|p_1^{(1)}\rangle,\ldots,|p_{s_1}^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle,\ldots,|p_{s_{r_1}}^{(r_1)}\rangle), \tag{70}$$

and

$$\mathcal{K}\begin{pmatrix}\langle q_{s_1}^{(1)}|\\ \vdots\\ \langle q_1^{(1)}|\\ \vdots\\ \langle q_{s_{r_1}}^{(r_1)}|\\ \vdots\\ \langle q_1^{(r_1)}|\end{pmatrix}=-\begin{pmatrix}\langle\overline{p}_1^{(1)}|\\ \vdots\\ \langle\overline{p}_{s_1}^{(1)}|\\ \vdots\\ \langle\overline{p}_1^{(r_1)}|\\ \vdots\\ \overline{p}_{s_{r_1}}^{(r_1)}|\end{pmatrix}, \tag{71}$$

where matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$ are as given in Eq. (67). We will give the proof only for Eq. (70), as the proof for (71) is similar. Note that in the case of involution (4), Eq. (71) follows from (70) by taking the Hermitian conjugate.

To prove Eq. (70), we consider the corresponding expressions (59) and (60) for $\Gamma(k)$,

$$\Gamma(k)=I+\sum_{\nu=1}^{r_1}(|\overline{q}_{s_\nu}^{(\nu)}\rangle,\ldots,|\overline{q}_1^{(\nu)}\rangle)\overline{D}_\nu(k)\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}. \tag{72}$$

We need to determine the $|\overline{q}\rangle$-vectors using Eq. (63). Note that the lth row in the μ-system (63) can be written as

$$\left[\Gamma(\kappa_\mu),\frac{1}{1!}\frac{\mathrm{d}\Gamma}{\mathrm{d}k}(\kappa_\mu),\ldots,\frac{1}{(l-1)!}\frac{\mathrm{d}^{l-1}\Gamma}{\mathrm{d}k^{l-1}}(\kappa_\mu)\right]\begin{pmatrix}|p_l^{(\mu)}\rangle\\ \vdots\\ |p_1^{(\mu)}\rangle\end{pmatrix}=0 \tag{73}$$

for each $1\leqslant\mu\leqslant r_1$. When the expression (72) for $\Gamma(k)$ is substituted into the above equation, we get

$$\sum_{\nu=1}^{r_1}(|\overline{q}_{s_\nu}^{(\nu)}\rangle,\ldots,|\overline{q}_1^{(\nu)}\rangle)\left\{\overline{D}_\nu(\kappa_\mu)\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}|p_l^{(\mu)}\rangle+\frac{1}{1!}\frac{\mathrm{d}\overline{D}_\nu}{\mathrm{d}k}(\kappa_\mu)\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}|p_{l-1}^{(\mu)}\rangle+\cdots\right.$$
$$\left.+\frac{1}{(l-1)!}\frac{\mathrm{d}^{l-1}\overline{D}_\nu}{\mathrm{d}k^{l-1}}(\kappa_\mu)\begin{pmatrix}\langle\overline{p}_1^{(\nu)}|\\ \vdots\\ \langle\overline{p}_{s_\nu}^{(\nu)}|\end{pmatrix}|p_1^{(\mu)}\rangle\right\}=-|p_l^{(\mu)}\rangle. \tag{74}$$

The derivatives of $\overline{D}_\nu(\kappa_\mu)$ can be easily computed as

$$\frac{\mathrm{d}^l\overline{D}_\nu}{\mathrm{d}k^l}(\kappa_\mu)=\sum_{j=0}^{s_\nu-1}\frac{(-1)^l(j+l)!}{j!}\frac{H_{-j}^{(\nu)}}{(\kappa_\mu-\overline{\kappa}_\nu)^{j+l+1}}. \tag{75}$$

Now it is straightforward to verify that all equations of the type (74) can be united in a single matrix equation (70) by padding some columns in the summations of (74) by zeros, precisely as it is done in the definition (69) of $\overline{Q}^{(\nu,\mu)}$. As a result we arrive at the relation (70) between $|\overline{q}\rangle$ and $|p\rangle$ vectors, where the matrix $\overline{\mathcal{K}}$ is precisely as defined in Lemma 4. Q.E.D.

D. Two special cases

Our soliton matrices derived above reproduce all previous results as special cases. The soliton matrices were previously obtained in two special cases: several pairs of Riemann–Hilbert zeros with equal geometric and algebraic multiplicities,[13] and a single pair of elementary higher-order zeros.[22] In the first case, suppose that the geometric and algebraic multiplicities of n pairs of Riemann-Hilbert zeros $\{(k_j,\overline{k}_j),1\leqslant j\leqslant n\}$ are $\{r^{(j)},1\leqslant j\leqslant n\}$, respectively. Then the soliton matrices have been given before[13] (see also Appendix B in Ref. 33) as

$$\Gamma=I-\sum_{i,j=1}^{n}\sum_{m=1}^{r^{(i)}}\sum_{l=1}^{r^{(j)}}\frac{|v_i^{(m)}\rangle(F^{-1})_{im,jl}\langle\overline{v}_j^{(l)}|}{k-\overline{k}_j},\quad \Gamma^{-1}=I+\sum_{i,j=1}^{n}\sum_{m=1}^{r^{(i)}}\sum_{l=1}^{r^{(j)}}\frac{|v_j^{(l)}(F^{-1})_{jl,im}\langle\overline{v}_i^{(m)}|}{k-k_j}, \tag{76}$$

where $r^{(j)}$ vectors $\{|v_j^{(l)}\rangle,1\leqslant l\leqslant r^{(j)}\}$ and $\{\langle\overline{v}_j^{(l)}|,1\leqslant l\leqslant r^{(j)}\}$ are in the kernels of $\Gamma(k_j)$ and $\Gamma^{-1}(\overline{k}_j)$, respectively,

$$\Gamma(k_j)|v_j^{(l)}\rangle=0,\quad \langle\overline{v}_j^{(l)}|\Gamma^{-1}(\overline{k}_j)=0,\quad l=1,\ldots,r^{(j)}, \tag{77}$$

and

$$F_{im,jl}=\frac{\langle\overline{v}_i^{(m)}|v_j^{(l)}\rangle}{k_j-\overline{k}_i}. \tag{78}$$

Moreover,

$$\det \Gamma = \prod_{j=1}^{n} \left(\frac{k-k_j}{k-\overline{k}_j} \right)^{r^{(j)}}.$$

The above special soliton matrices can be easily retrieved from the general soliton matrices (65)–(69) of Lemma 4. Indeed, in this special case, the block sequence of a pair of zeros $(k_j, \overline{k}_j)$ is a row of 1's of length $r^{(j)}$. Thus $s_\nu = 1$ for all ν's. Consequently, matrices D_ν and $\overline{D}_\nu$ in Eq. (66) have dimension 1. In addition, matrices $K^{(\nu,\mu)}$ and $\overline{K}^{(\nu,\mu)}$ in Eq. (68) also have dimension 1, and the summations in their definitions can be dropped since $l=0$ and $j=0$ there. Hence, we get

$$\overline{K}^{(\nu,\mu)} = (K^{(\mu,\nu)})^\dagger = \frac{\langle \overline{p}_1^{(\nu)} | p_1^{(\mu)} \rangle}{\kappa_\mu - \overline{\kappa}_\nu},$$

see (69). Relating $|p\rangle$ vectors $\{|p_1^{(\nu)}\rangle, 1+\Sigma_{l=1}^{j-1} r^{(l)} \leqslant \nu \leqslant \Sigma_{l=1}^{j} r^{(l)}\}$ to $\{|v_j^{(l)}\rangle, 1 \leqslant l \leqslant r^{(j)}\}$ and $\{\langle p_1^{(\nu)}|, 1+\Sigma_{l=1}^{j-1} r^{(l)} \leqslant \nu \leqslant \Sigma_{l=1}^{j} r^{(l)}\}$ to $\{\langle v_j^{(l)}|, 1 \leqslant l \leqslant r^{(j)}\}$ for each $j=1,\ldots,n$, and recalling the definition (62) of κ's, we readily find that our general representation (65) reduces to (76). We note by passing that the soliton matrices (76)–(78) cover the case of simple zeros, where there is just one vector in each kernel in (77).

Our second example is a single pair of elementary higher-order zeros. A higher-order zero is called elementary if its geometric multiplicity is 1.[22] This case has been extensively studied in the literature before (see Refs. 15, 17, 18, 22) for different integrable PDEs. The soliton matrices having similar representation as (65)–(69) for this case were derived in our previous publication.[22] The only difference between that paper's representation and the present one (65)–(69) is the definition of the matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$. However, in this special case, these matrices have just one block each, i.e., $K^{(1,1)}$ and $\overline{K}^{(1,1)}$, since there is just one ν block in the soliton matrices. By comparison of both definitions one can easily establish their equivalence.

E. Invariance properties of soliton matrices

In this section, we discuss the invariance properties of soliton matrices. When the soliton matrix is in the product representation (27) for a single pair of zeros, the invariance property means that one can choose any r_1 linearly independent vectors in the kernels of $\Gamma(k_1)$ and $\Gamma^{-1}(\overline{k}_1)$, or more generally, one can choose any r_l $(1 \leqslant l \leqslant n)$ linearly independent vectors in the kernels of $(\Gamma \chi_1^{-1} \cdots \chi_{l-1}^{-1})(k_1)$ and $(\chi_{l-1} \cdots \chi_1 \Gamma^{-1})(\overline{k}_1)$, and the soliton matrix remains invariant. In other words, given the soliton matrix $\Gamma(k)$, for a fixed set of r_l linearly independent vectors $|v_{il}\rangle$ $(1 \leqslant i \leqslant r_l)$ in the kernels of $(\Gamma \chi_1^{-1} \cdots \chi_{l-1}^{-1})(k_1)$ and another fixed set of r_l linearly independent vectors $\langle \overline{v}_{il}|$ $(1 \leqslant i \leqslant r_l)$ in the kernels of $(\chi_{l-1} \cdots \chi_1 \Gamma^{-1})(\overline{k}_1)$, new sets of vectors

$$[|\tilde{v}_{1l}\rangle, |\tilde{v}_{2l}\rangle, \ldots, |\tilde{v}_{r_l,l}\rangle] = [|v_{1l}\rangle, |v_{2l}\rangle, \ldots, |v_{r_l,l}\rangle] B \tag{79}$$

and

$$\begin{bmatrix} \langle \tilde{\overline{v}}_{1l}| \\ \langle \tilde{\overline{v}}_{2l}| \\ \vdots \\ \langle \tilde{\overline{v}}_{r_l,l}| \end{bmatrix} = \overline{B} \begin{bmatrix} \langle \overline{v}_{1l}| \\ \langle \overline{v}_{2l}| \\ \vdots \\ \langle \overline{v}_{r_l,l}| \end{bmatrix}, \tag{80}$$

where B and $\overline{B}$ are arbitrary k-independent nondegenerate $r_l \times r_l$ matrices, give the same soliton matrix $\Gamma(k)$. This invariance property is obvious from definitions (25) for projector matrices. Note that the invariance transformations (79) and (80) are the most general automorphisms of the respective kernels (i.e., null spaces) of $(\Gamma \chi_1^{-1} \cdots \chi_{l-1}^{-1})(k_1)$ and $(\chi_{l-1} \cdots \chi_1 \Gamma^{-1})(\overline{k}_1)$.

Now let us determine the total number $\mathcal{N}_{\text{free}}$ of free complex parameters characterizing the higher-order soliton solution. For a single pair of the higher-order zeros $(k_1, \overline{k}_1)$ in the case with

no involution, it is given by the total number $\mathcal{N}_{\rm tot}$ $(=2N\Sigma_{l=1}^{n}r_l+2)$ of all complex constants in all the linearly independent vectors in the above null spaces and the pair of zeros $(k_1,\overline{k_1})$, minus the total number $\mathcal{N}_{\rm inv}$ $(=2\Sigma_{l=1}^{n}r_l^2)$ of the free parameters in the invariance matrices (79) and (80). Thus, in the case with no involution, we have

$$\mathcal{N}_{\rm free}\equiv\mathcal{N}_{\rm tot}-\mathcal{N}_{\rm inv}=2N\sum_{l=1}^{n}r_l+2-2\sum_{l=1}^{n}r_l^2. \tag{81}$$

Note that the total number of $|v\rangle$ or $\langle\overline{v}|$ vectors in the product representation (27), given by the sum $\Sigma_{l=1}^{n}r_l$, is equal to the algebraic order of the pair of zeros $(k_1,\overline{k_1})$. In the case of the involution (4), the number $\mathcal{N}_{\rm free}$ is reduced by half. When the soliton matrices have several pairs of zeros as in the product representation (45), the invariance property is similar, and the total number of free soliton parameters is given by the sum of the right-hand side (rhs) of formula (81) for all distinct pairs of zeros.

By analogy, the invariance properties for the summation representation (65) of the soliton matrices are defined as preserving the form of the soliton matrices as well as the equations defining the $|p\rangle$ and $\langle\overline{p}|$ vectors (63) and (64). The equations defining the transformations between different sets of p vectors of the same invariance class must be linear, since all the sets of p vectors in the invariance class satisfy equations (63) and (64) for a *fixed* soliton matrix—i.e., the invariance transformations are a subset of transformations between solutions to a set of *linear* equations. Thus the most general form of the invariance is given by two linear transformations—one for $|p\rangle$ vectors and one for $\langle\overline{p}|$ vectors:

$$(|\tilde{p}_1^{(1)}\rangle,\ldots,|\tilde{p}_{s_1}^{(1)}\rangle,\ldots,|\tilde{p}_1^{(r_1)}\rangle,\ldots,|\tilde{p}_{s_{r_1}}^{(r_1)}\rangle)=(|p_1^{(1)}\rangle,\ldots,|p_{s_1}^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle,\ldots,|p_{s_{r_1}}^{(r_1)}\rangle)B \tag{82}$$

and

$$\begin{pmatrix}\langle\tilde{\bar{p}}_1^{(1)}|\\ \vdots\\ \langle\tilde{\bar{p}}_{s_1}^{(1)}|\\ \vdots\\ \langle\tilde{\bar{p}}_1^{(r_1)}|\\ \vdots\\ \langle\tilde{\bar{p}}_{s_{r_1}}^{(r_1)}|\end{pmatrix}=\overline{B}\begin{pmatrix}\langle\bar{p}_1^{(1)}|\\ \vdots\\ \langle\bar{p}_{s_1}^{(1)}|\\ \vdots\\ \langle\bar{p}_1^{(r_1)}|\\ \vdots\\ \langle\bar{p}_{s_{r_1}}^{(r_1)}|\end{pmatrix}. \tag{83}$$

Different from the product representation of the soliton matrices, the transformation matrices B and $\overline{B}$ in Eqs. (82) and (83) cannot be arbitrary in order to keep the soliton matrices (65) and Eqs. (63) and (64) invariant. Let us call such matrices B and $\overline{B}$ which keep the soliton matrices (65) invariant as the invariance matrices. The form of invariance matrices can be determined most easily by considering the invariance of Eqs. (63) and (64).

Recall from Lemma 3 that all $|p\rangle$ vectors in the soliton matrix (65) satisfy the equation

$$\mathbf{\Gamma_B}\begin{pmatrix}|p_1^{(1)}\rangle\\ \vdots\\ |p_{s_1}^{(1)}\rangle\\ \vdots\\ |p_1^{(r_1)}\rangle\\ \vdots\\ |p_{s_{r_1}}^{(r_1)}\rangle\end{pmatrix}=0,\quad \mathbf{\Gamma_B}\equiv\begin{pmatrix}\mathbf{\Gamma}_1(\kappa_1) & & 0\\ & \ddots & \\ 0 & & \mathbf{\Gamma}_{r_1}(\kappa_{r_1})\end{pmatrix}, \tag{84}$$

where $\mathbf{\Gamma}_\nu(\kappa_\nu)$ is the lower-triangular Toeplitz matrix defined in Eq. (63). The matrix B is an invariance matrix if and only if the above equation is still satisfied when the $|p\rangle$ vectors in Eq. (84) are replaced by the transformed vectors $|\tilde{p}\rangle$ in Eq. (82), and the resulting matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$ are nondegenerate [see Eq. (65)]. Note that the transformation (82) can be rewritten in the following form:

$$\begin{pmatrix} |\tilde{p}_1^{(1)}\rangle \\ \vdots \\ |\tilde{p}_{s_1}^{(1)}\rangle \\ \vdots \\ |\tilde{p}_1^{(r_1)}\rangle \\ \vdots \\ |\tilde{p}_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix} = B^T \begin{pmatrix} |p_1^{(1)}\rangle \\ \vdots \\ |p_{s_1}^{(1)}\rangle \\ \vdots \\ |p_1^{(r_1)}\rangle \\ \vdots \\ |p_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}, \tag{85}$$

where the superscript "T" stands for the matrix transposition. Since the original $|p\rangle$ vectors can be chosen arbitrarily (the matrix $\mathbf{\Gamma_B}$ is determined subsequently from these $|p\rangle$ vectors as well as the $\langle\overline{p}|$ vectors), in order for the above $|\tilde{p}\rangle$ vectors (85) to satisfy Eq. (84) as well, the necessary and sufficient condition is that $\mathbf{\Gamma_B}$ and B^T commute, i.e.,

$$\mathbf{\Gamma_B}\cdot B^T = B^T\cdot\mathbf{\Gamma_B}, \tag{86}$$

and B is nondegenerate. The requirement for the nondegeneracy of B is needed in order for the resulting matrices $\tilde{\mathcal{K}}$ and $\tilde{\bar{\mathcal{K}}}$ to be nondegenerate [see Eq. (96)]. Similarly, we can show that the matrix $\overline{B}$ in Eq. (83) is an invariance matrix if and only if $\overline{\mathbf{\Gamma}}_\mathbf{B}$ and $\overline{B}^T$ commute,

$$\overline{\mathbf{\Gamma}}_\mathbf{B}\cdot\overline{B}^T = \overline{B}^T\cdot\overline{\mathbf{\Gamma}}_\mathbf{B}, \tag{87}$$

and $\overline{B}$ is nondegenerate. Here the block-diagonal matrix $\overline{\mathbf{\Gamma}}_\mathbf{B}$ is

$$\overline{\mathbf{\Gamma}}_\mathbf{B} \equiv \begin{pmatrix} \overline{\mathbf{\Gamma}}_1(\kappa_1) & & 0 \\ & \ddots & \\ 0 & & \overline{\mathbf{\Gamma}}_{r_1}(\kappa_{r_1}) \end{pmatrix}, \tag{88}$$

and upper-triangular Toeplitz matrices $\overline{\mathbf{\Gamma}}_\nu(\kappa_\nu)$ have been defined in Eq. (64). Note that matrices $\mathbf{\Gamma_B}$ and $\overline{\mathbf{\Gamma}}_\mathbf{B}$ have exactly the same forms as $\overline{\mathcal{D}}(k)$ and $\mathcal{D}(k)$, respectively. Thus invariance matrices B^T and $\overline{B}^T$ commute with $\overline{\mathcal{D}}(k)$ and $\mathcal{D}(k)$ as well:

$$\overline{\mathcal{D}}(k)\cdot B^T = B^T\cdot\overline{\mathcal{D}}(k), \quad \mathcal{D}(k)\cdot\overline{B}^T = \overline{B}^T\cdot\mathcal{D}(k). \tag{89}$$

In addition, since $\mathcal{D}^T$ has the same form as $\overline{\mathcal{D}}$, invariance matrices B and $\overline{B}$ also commute with $\mathcal{D}$ and $\overline{\mathcal{D}}$:

$$B\cdot\mathcal{D}(k) = \mathcal{D}(k)\cdot B, \quad \overline{B}\cdot\overline{\mathcal{D}}(k) = \overline{\mathcal{D}}(k)\cdot\overline{B}. \tag{90}$$

The form of these invariance matrices are easy to determine. First of all, the commutability relations (90) demand that the invariance matrix B has a block-diagonal form with each block corresponding to a pair of zeros:

$$B=\begin{pmatrix} B_1 & & & \\ & B_2 & & \\ & & \ddots & \\ & & & B_{N_Z} \end{pmatrix}. \tag{91}$$

Here B_n is a square matrix associated with the nth pair of zeros $(k_n,\overline{k_n})$. The form of each matrix B_n is readily found to be

$$B_n=\begin{pmatrix} B_n^{(1,1)} & \cdots & B_n^{(1,r_1^{(n)})} \\ \vdots & & \vdots \\ B_n^{(r_1^{(n)},1)} & \cdots & B_n^{(r_1^{(n)},r_1^{(n)})} \end{pmatrix}, \tag{92}$$

where $B_n^{(\nu,\mu)}$ is a $s_\nu^{(n)}\times s_\mu^{(n)}$ matrix of the following type:

$$B_n^{(\nu,\mu)}=\begin{pmatrix} 0 & \cdots & 0 & b_1 & b_2 & \cdots & b_{s_\nu^{(n)}-1} & b_{s_\nu^{(n)}} \\ 0 & \ddots & \ddots & 0 & b_1 & b_2 & \ddots & b_{s_\nu^{(n)}-1} \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 & b_1 & b_2 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & b_1 \end{pmatrix}, \quad \nu\geqslant\mu, \tag{93a}$$

$$B_n^{(\nu,\mu)}=\begin{pmatrix} c_1 & c_2 & \cdots & c_{s_\mu^{(n)}-1} & c_{s_\mu^{(n)}} \\ 0 & c_1 & c_2 & \ddots & c_{s_\mu^{(n)}-1} \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & c_2 \\ \vdots & \ddots & \ddots & 0 & c_1 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix}, \quad \nu\leqslant\mu, \tag{93b}$$

$s_1^{(n)}\geqslant s_2^{(n)}\geqslant\ldots\geqslant s_{r_1^{(n)}}^{(n)}$ is the block sequence of zeros $(k_n,\overline{k_n})$ as in Lemma 2 (see Definition 2), and b_j,c_j are arbitrary complex constants which are generally different in different submatrices $B_n^{(\nu,\mu)}$. The invariance matrix $\overline{B}$ has the form of B^T (in general, with arbitrary elements unrelated to those of B).

The above forms (92) and (93) of the invariance matrices B_n and $\overline{B_n}$ follow immediately from the following argument. Consider, for instance, the matrix B_n. The commutability relation with the part of the matrix $\mathcal{D}(k)$ corresponding to the nth pair of zeros, i.e., $\mathcal{D}^{(n)}(k)=\mathrm{diag}[D_1^{(n)}(k),\ldots,D_{r_1^{(n)}}^{(n)}(k)]$ where matrices $D_\nu^{(n)}(k)$ are given by Eq. (48), produces the following set of independent matrix equations:

$$D_\nu^{(n)}(k)B_n^{(\nu,\mu)}=B_n^{(\nu,\mu)}D_\mu^{(n)}(k), \quad \nu,\mu=1,\ldots,r_1^{(n)}. \tag{94}$$

For $\nu=\mu$, the above equations are equivalent to the commutability conditions for the single elementary higher-order zero considered in Ref. 22, thus the form (93) for the diagonal blocks $B_n^{(\nu,\nu)}$ follows accordingly. Consider now the case when $\nu>\mu$ (the other case can be considered similarly). We have then $s_\nu^{(n)}\leqslant s_\mu^{(n)}$, thus the square matrix $D_\mu^{(n)}(k)$ contains the matrix $D_\nu^{(n)}(k)$ in

its lower right corner [consult the definition (48)]. It is easy to conclude, first of all, that the first $\mu-\nu$ columns of the matrix $B_n^{(\nu,\mu)}$ are identically zero, otherwise on the rhs of Eq. (94) we would have higher powers of $(k-k_n)^{-1}$ than the highest power of this quantity on the left-hand side (lhs). Then if we denote the nonzero part of $B_n^{(\nu,\mu)}$ as $\hat{B}_n^{(\nu)}$, the condition (94) becomes

$$D_\nu^{(n)}(k)\hat{B}_n^{(\nu)}=\hat{B}_n^{(\nu)}D_\nu^{(n)}(k),$$

which is equivalent to the one considered above in the case of $\mu=\nu$. Thus the form (93a) for the off-diagonal blocks of the invariance matrix $B_n^{(\nu,\mu)}$ follows as well. Q.E.D.

From the above explicit expressions (91)–(93) for invariance matrices in the summation representation (65), it is easy to see that the total number $\mathcal{N}_{\text{inv}}$ of free complex constants in these invariance matrices coincides with that in the product representation (27) and (45) [see Eq. (81)]. Indeed consider for simplicity just a single pair of zeros. In the case with no involution (4), the total number $\mathcal{N}_{\text{inv}}$ of free complex constants in the invariance matrices (91)–(93) is

$$\begin{aligned}\mathcal{N}_{\text{inv}}&=2\sum_{\nu=1}^{r_1}(2r_1-2\nu+1)s_{r_1-\nu+1}\\&=2\sum_{\mu=1}^{r_1}(2\mu-1)s_\mu\\&=2\left(n\sum_{\mu=1}^{r_n}(2\mu-1)+(n-1)\sum_{\mu=r_n+1}^{r_{n-1}}(2\mu-1)+\cdots+\sum_{\mu=r_2+1}^{r_1}(2\mu-1)\right)=2\sum_{l=1}^{n}r_l^2,\end{aligned}\tag{95}$$

which is exactly the same as that in Eq. (81) for $\mathcal{N}_{\text{inv}}$. Here we have used the fact that the numbers of blocks with sizes $[1,2,3,\ldots,n]$ are given by the differences of the ranks $[r_1-r_2,r_2-r_3,\ldots,r_{n-1}-r_n,r_n]$ (see the end of the proof of Lemma 1 in Sec. III B).

This result is not surprising since the invariance properties of the soliton matrices in the summation representation originate from the invariance properties in the product representation, that is why the respective invariance matrices have the same total number of free parameters. Consequently, the total number of free complex parameters in the summation representation (65) is the same as in the product representation, as expected. In the case with no involution for a single pair of zeros it is given by the same Eq. (81).

Invariance matrices have many important properties. These include (i) the identity matrix I is an invariance matrix; (ii) if B is an invariance matrix, so is cB, where c is any nonzero complex constant; (iii) if B is an invariance matrix, so is B^{-1}; (iv) if B_1 and B_2 are two invariance matrices, so are $B_1\pm B_2$ and $B_1\cdot B_2$. In the former case, $B_1\pm B_2$ should be nondegenerate.

Last, we note that if matrices B and $\overline{B}$ satisfy the commutability relations (90), the transformations (82) and (83) indeed keep the soliton matrices (65) invariant. The proof uses the fact that under the transformation (82) where B is an invariance matrix (the $\langle\overline{p}|$ vectors are held fixed), matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$ are transformed to

$$\tilde{\mathcal{K}}=\mathcal{K}B,\quad \tilde{\overline{\mathcal{K}}}=\overline{\mathcal{K}}B\tag{96}$$

respectively. Similarly, under the transformation (83) while keeping the $|p\rangle$ vectors fixed, matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$ are transformed to

$$\tilde{\mathcal{K}}=\overline{B}\mathcal{K},\quad \tilde{\overline{\mathcal{K}}}=\overline{B}\,\overline{\mathcal{K}}.\tag{97}$$

For a single pair of elementary higher-order zeros these facts have been proved in Ref. 22. The proof for the present general case is given below. Since the proofs for Eqs. (96) and (97) are similar, we only consider Eq. (96).

To prove the transformation (96), we need to recall how matrices $\mathcal{K}$ and $\overline{\mathcal{K}}$ are obtained. The matrix $\overline{\mathcal{K}}$ is derived from Eq. (84). Comparing this equation with (70), we find that

$$(\mathbf{\Gamma_B}-I)\begin{pmatrix} |p_1^{(1)}\rangle \\ \vdots \\ |p_{s_1}^{(1)}\rangle \\ \vdots \\ |p_1^{(r_1)}\rangle \\ \vdots \\ |p_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix} = \overline{\mathcal{K}}^T \begin{pmatrix} |\overline{q}_{s_1}^{(1)}\rangle \\ \vdots \\ |\overline{q}_1^{(1)}\rangle \\ \vdots \\ |\overline{q}_{s_{r_1}}^{(r_1)}\rangle \\ \vdots \\ |\overline{q}_1^{(r_1)}\rangle \end{pmatrix}.$$

Now using the form (85) of the transformation (82) and recalling that B^T and $\mathbf{\Gamma_B}-I$ commute, we readily find that $(\tilde{\overline{\mathcal{K}}})^T = B^T\overline{\mathcal{K}}^T$, thus $\tilde{\overline{\mathcal{K}}} = \overline{\mathcal{K}}B$. As about the matrix $\mathcal{K}$, it is derived from the equation

$$(\langle \overline{p}_1^{(1)}|, \ldots, \langle \overline{p}_{s_1}^{(1)}|, \ldots, \langle \overline{p}_1^{(r_1)}|, \ldots, \langle \overline{p}_{s_{r_1}}^{(r_1)}|)\overline{\mathbf{\Gamma}}_\mathbf{B} = 0,$$

where $\overline{\mathbf{\Gamma}}_\mathbf{B}$ is given by Eqs. (63) and (88). Recall that $\Gamma^{-1}(k)$ is given by Eq. (59), i.e.,

$$\Gamma^{-1}(k) = I + (|p_1^{(1)}\rangle, \ldots, |p_{s_1}^{(1)}\rangle, \ldots, |p_1^{(r_1)}\rangle, \ldots, |p_{s_{r_1}}^{(r_1)}\rangle)\mathcal{D}(k)\begin{pmatrix} \langle q_{s_1}^{(1)}| \\ \vdots \\ \langle q_1^{(1)}| \\ \vdots \\ \langle q_{s_{r_1}}^{(r_1)}| \\ \vdots \\ \langle q_1^{(r_1)}| \end{pmatrix}.$$

Thus, using the transformation (82) and noting that B and $\mathcal{D}$ commute [see Eq. (90)], we readily find that $\tilde{\mathcal{K}} = \mathcal{K}B$, i.e., the equation (96) holds.

Because of Eq. (96) and the commutability relation (90), we see that soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$ in Eq. (65) indeed remain invariant under the transformation (82). Analogously, these soliton matrices are also invariant under the transformation (83) if matrix $\overline{B}$ is an invariance matrix. In the case of involution (4), transformations (82) and (83) need to be performed simultaneously since $|p\rangle$ and $\langle\overline{p}|$ vectors are related by the Hermitian operation. Under these combined transformations, matrix $\mathcal{K}$ transforms to $\tilde{\mathcal{K}} = \overline{B}\mathcal{K}B$, thus soliton matrices (65) remain invariant as well.

The invariance matrices can be used to reduce the number of the free parameters in the soliton solution to the minimum, which is given by the formula (81). They are also used to reduce the (x,t) dependence of the soliton matrices to the simplest possible form (see the next section).

F. Spatial and temporal evolutions of soliton matrices

Finally, we derive the (x,t) dependence of the free vector parameters which enter the soliton matrix (65). The idea is similar to the one used in the derivation of Eqs. (20) in Sec. II. Our starting point is the fact that the soliton matrix $\Gamma(k,x,t)$ satisfies Eqs. (5) and (6) with potentials $U(k,x,t)$ and $V(k,x,t)$:

$$\partial_x \Gamma(k,x,t) = \Gamma(k,x,t)\Lambda(k) + U(k,x,t)\Gamma(k,x,t), \tag{98a}$$

$$\partial_t \Gamma(k,x,t) = \Gamma(k,x,t)\Omega(k) + V(k,x,t)\Gamma(k,x,t). \tag{98b}$$

First we need to find the equations for the triangular block–Toeplitz matrices $\mathbf{\Gamma}_\nu$ and $\overline{\mathbf{\Gamma}}_\nu$. To this goal one needs to differentiate Eqs. (98) with respect to k up to the $(s_\nu - 1)$th order. It is easy to check that the equations for $\mathbf{\Gamma}_\nu$ have the same form as Eqs. (98),

$$\partial_x \mathbf{\Gamma}_\nu(k,x,t) = \mathbf{\Gamma}_\nu(k,x,t)\mathbf{\Lambda}_\nu(k) + \mathbf{U}_\nu(k,x,t)\mathbf{\Gamma}_\nu(k,x,t), \tag{99a}$$

$$\partial_t \mathbf{\Gamma}_\nu(k,x,t) = \mathbf{\Gamma}_\nu(k,x,t)\mathbf{\Omega}_\nu(k) + \mathbf{V}_\nu(k,x,t)\mathbf{\Gamma}_\nu(k,x,t). \tag{99b}$$

Here $\mathbf{\Lambda}_\nu$, $\mathbf{\Omega}_\nu$, $\mathbf{U}_\nu$, and $\mathbf{V}_\nu$ are lower-triangular block–Toeplitz matrices,

$$\mathbf{\Lambda}_\nu \equiv \begin{pmatrix} \Lambda & 0 & \dots & 0 \\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Lambda & \ddots & \ddots & \vdots \\ \vdots & \ddots & \Lambda & 0 \\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Lambda & \dots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Lambda & \Lambda \end{pmatrix},$$

$$\mathbf{\Omega}_\nu \equiv \begin{pmatrix} \Omega & 0 & \dots & 0 \\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Omega & \ddots & \ddots & \vdots \\ \vdots & \ddots & \Omega & 0 \\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Omega & \dots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Omega & \Omega \end{pmatrix}, \tag{100}$$

$$\mathbf{U}_\nu \equiv \begin{pmatrix} U & 0 & \dots & 0 \\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}U & \ddots & \ddots & \vdots \\ \vdots & \ddots & U & 0 \\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}U & \dots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}U & U \end{pmatrix},$$

$$\mathbf{V}_\nu \equiv \begin{pmatrix} V & 0 & \dots & 0 \\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}V & \ddots & \ddots & \vdots \\ \vdots & \ddots & V & 0 \\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}V & \dots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}V & V \end{pmatrix}. \tag{101}$$

Indeed, this is due to the fact that the matrix multiplication in (99) exactly reproduces the Leibniz rule for higher-order derivatives of a product. Similarly, using the equations for Γ^{-1},

$$\partial_x \Gamma^{-1}(k,x,t) = -\Lambda(k)\Gamma^{-1}(k,x,t) - \Gamma^{-1}(k,x,t)U(k,x,t), \tag{102a}$$

$$\partial_t \Gamma^{-1}(k,x,t) = -\Omega(k)\Gamma^{-1}(k,x,t) - \Gamma^{-1}(k,x,t)V(k,x,t), \tag{102b}$$

one finds that

$$\partial_x \overline{\mathbf{\Gamma}}_\nu(k,x,t) = -\overline{\mathbf{\Lambda}}_\nu(k)\overline{\mathbf{\Gamma}}_\nu(k,x,t) - \overline{\mathbf{\Gamma}}_\nu(k,x,t)\overline{\mathbf{U}}_\nu(k,x,t), \tag{103a}$$

$$\partial_t \overline{\mathbf{\Gamma}}_\nu(k,x,t) = -\overline{\mathbf{\Omega}}_\nu(k)\overline{\mathbf{\Gamma}}_\nu(k,x,t) - \overline{\mathbf{\Gamma}}_\nu(k,x,t)\overline{\mathbf{V}}_\nu(k,x,t), \tag{103b}$$

where $\overline{\mathbf{\Lambda}}_\nu$, $\overline{\mathbf{\Omega}}_\nu$, $\overline{\mathbf{U}}_\nu$, and $\overline{\mathbf{V}}_\nu$ are upper-triangular block–Toeplitz matrices:

$$\overline{\mathbf{\Lambda}}_\nu = \begin{pmatrix} \Lambda & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Lambda & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Lambda \\ 0 & \Lambda & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Lambda \\ 0 & \cdots & 0 & \Lambda \end{pmatrix},$$

$$\overline{\mathbf{\Omega}}_\nu = \begin{pmatrix} \Omega & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Omega & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}\Omega \\ 0 & \Omega & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}\Omega \\ 0 & \cdots & 0 & \Omega \end{pmatrix}, \tag{104}$$

$$\overline{\mathbf{U}}_\nu = \begin{pmatrix} U & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}U & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}U \\ 0 & U & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}U \\ 0 & \cdots & 0 & U \end{pmatrix},$$

$$\overline{\mathbf{V}}_\nu = \begin{pmatrix} V & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}V & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}V \\ 0 & V & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}V \\ 0 & \cdots & 0 & V \end{pmatrix}. \tag{105}$$

To obtain the (x,t) dependence of the p vectors, let us differentiate Eqs. (63) and (64). Utilizing Eqs. (100) and (103), we find that

$$\mathbf{\Gamma}_\nu(\kappa_\nu)\left\{ [\partial_x + \mathbf{\Lambda}_\nu(\kappa_\nu)] \begin{pmatrix} |p_1^{(\nu)}\rangle \\ \vdots \\ |p_{s_\nu}^{(\nu)}\rangle \end{pmatrix} \right\} = 0 \tag{106}$$

and

$$\mathbf{\Gamma}_\nu(\kappa_\nu)\left\{[\partial_t+\mathbf{\Omega}_\nu(\kappa_\nu)]\begin{pmatrix}|p_1^{(\nu)}\rangle\\ \vdots\\ |p_{s_\nu}^{(\nu)}\rangle\end{pmatrix}\right\}=0. \tag{107}$$

Due to the invariance properties (the explanation will follow below), we can set the quantities inside the curly brackets of Eqs. (106) and (107) to be zero without any loss of generality:

$$[\partial_x+\mathbf{\Lambda}_\nu(\kappa_\nu)]\begin{pmatrix}|p_1^{(\nu)}\rangle\\ \vdots\\ |p_{s_\nu}^{(\nu)}\rangle\end{pmatrix}=0,\qquad [\partial_t+\mathbf{\Omega}_\nu(\kappa_\nu)]\begin{pmatrix}|p_1^{(\nu)}\rangle\\ \vdots\\ |p_{s_\nu}^{(\nu)}\rangle\end{pmatrix}=0. \tag{108}$$

The reason for it is the uniqueness of solution to the Riemann–Hilbert problem for a given set of the spectral data. Thus, the (x,t) dependence of the $|p\rangle$ vectors is

$$\begin{pmatrix}|p_1^{(\nu)}\rangle\\ \vdots\\ |p_{s_\nu}^{(\nu)}\rangle\end{pmatrix}=\exp\{-\mathbf{\Lambda}_\nu(\kappa_\nu)x-\mathbf{\Omega}_\nu(\kappa_\nu)t\}\begin{pmatrix}|p_{01}^{(\nu)}\rangle\\ \vdots\\ |p_{0s_\nu}^{(\nu)}\rangle\end{pmatrix}. \tag{109}$$

By similar arguments, the (x,t) dependence of the $\langle\overline{p}|$ vectors is given as

$$(\langle\overline{p}_1^{(\nu)}|,\ldots,\langle\overline{p}_{s_\nu}^{(\nu)}|)=(\langle\overline{p}_{01}^{(\nu)}|,\ldots,\langle\overline{p}_{0s_\nu}^{(\nu)}|)\exp\{\overline{\mathbf{\Lambda}}_\nu(\overline{\kappa}_\nu)x+\overline{\mathbf{\Omega}}_\nu(\overline{\kappa}_\nu)t\}. \tag{110}$$

Here the subscript "0" is used to denote constant vectors. The exponential functions in the above two equations can be readily determined. Indeed, by using the property that the operation of raising a diagonal matrix [such as $\Lambda(k)x+\Omega(k)t$ here] to the exponent commutes with the construction of the related triangular block–Toeplitz matrix (see appendix in Ref. 22), we find that

$$\exp\{-\mathbf{\Lambda}_\nu(\kappa_\nu)x-\mathbf{\Omega}_\nu(\kappa_\nu)t\}=\begin{pmatrix}E(k_1) & 0 & \cdots & 0\\ \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}E(k_1) & \ddots & \ddots & \vdots\\ \vdots & \ddots & E(k_1) & 0\\ \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}E(k_1) & \cdots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}E(k_1) & E(k_1)\end{pmatrix} \tag{111a}$$

and

$$\exp\{\overline{\mathbf{\Lambda}}_\nu(\overline{\kappa}_\nu)x+\overline{\mathbf{\Omega}}_\nu(\overline{\kappa}_\nu)t\}=\begin{pmatrix}E^{-1}(\overline{k}_1) & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}E^{-1}(\overline{k}_1) & \cdots & \frac{1}{(s_\nu-1)!}\frac{\mathrm{d}^{s_\nu-1}}{\mathrm{d}k^{s_\nu-1}}E^{-1}(\overline{k}_1)\\ 0 & E^{-1}(\overline{k}_1) & \ddots & \vdots\\ \vdots & \ddots & \ddots & \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}k}E^{-1}(\overline{k}_1)\\ 0 & \cdots & 0 & E^{-1}(\overline{k}_1)\end{pmatrix}, \tag{111b}$$

where $E(k)\equiv\exp\{-\Lambda(k)x-\Omega(k)t\}$.

Given the spatial and temporal evolutions of vectors $|p\rangle$ and $\langle\overline{p}|$, as in Eqs. (109)–(111), the associated soliton matrices (65) can be constructed. Eventually, the soliton solutions are derived from Eq. (5) by taking the limit $k\to\infty$. The soliton solutions for the three-wave interaction model are given by Eqs. (12) and (13). The corresponding eigenfunctions of the N-dimensional

Zakharov–Shabat spectral problem with these soliton (reflectionless) potentials are then simply the column vectors of the soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$ given by (65) with k either equal to one of the zeros $(k_j, \overline{k_j})$ (the eigenfunctions of the discrete spectrum) or taking values on the real axis (the eigenfunctions of the continuous spectrum).

Last, let us show that other solutions to Eqs. (106) and (107), different from those given by Eq. (108), will give the same soliton matrices. Notice that Eqs. (106) for all ν blocks can be written in the following compact form:

$$\mathbf{\Gamma_B}(\partial_x+\mathbf{\Omega_B})\begin{pmatrix} |p_1^{(1)}\rangle \\ \vdots \\ |p_{s_1}^{(1)}\rangle \\ \vdots \\ |p_1^{(r_1)}\rangle \\ \vdots \\ |p_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}=0, \qquad \mathbf{\Omega_B}\equiv\begin{pmatrix} \mathbf{\Omega}_1(\kappa_1) & & 0 \\ & \ddots & \\ 0 & & \mathbf{\Omega}_{r_1}(\kappa_{r_1}) \end{pmatrix}. \tag{112}$$

According to the invariance properties discussed in the Sec. III E, any two vectors in the kernel of matrix $\mathbf{\Gamma_B}$ are linearly dependent. Thus the most general $|p\rangle$ solutions to Eq. (106) are such that

$$(\partial_x+\mathbf{\Omega_B})\begin{pmatrix} |\tilde{p}_1^{(1)}\rangle \\ \vdots \\ |\tilde{p}_{s_1}^{(1)}\rangle \\ \vdots \\ |\tilde{p}_1^{(r_1)}\rangle \\ \vdots \\ |\tilde{p}_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}=B^T(x,t)\begin{pmatrix} |\tilde{p}_1^{(1)}\rangle \\ \vdots \\ |\tilde{p}_{s_1}^{(1)}\rangle \\ \vdots \\ |\tilde{p}_1^{(r_1)}\rangle \\ \vdots \\ |\tilde{p}_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}, \tag{113}$$

where B is an invariance matrix which depends on x and t in general [see Eq. (85)]. To show that these $|\tilde{p}\rangle$ vectors give the same soliton matrices (65) as the $|p\rangle$ vectors from Eq. (108), we define a matrix function $G(x,t)$ which satisfies the following differential equation and initial condition:

$$\partial_x G(x,t)=B^T(x,t)G(x,t), \qquad G|_{x=0}=I.$$

Because the matrix B here is an invariance matrix and $G(x=0)=I$, obviously the function $G(x,t)$ is an invariance matrix as well (note that G is always nondegenerate by construction). In addition, G^{-1} is also an invariance matrix. Now for any solution $|\tilde{p}\rangle$ of Eq. (112), we define new vectors $|p\rangle$ as

$$\begin{pmatrix} |p_1^{(1)}\rangle \\ \vdots \\ |p_{s_1}^{(1)}\rangle \\ \vdots \\ |p_1^{(r_1)}\rangle \\ \vdots \\ |p_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}=G^{-1}\begin{pmatrix} |\tilde{p}_1^{(1)}\rangle \\ \vdots \\ |\tilde{p}_{s_1}^{(1)}\rangle \\ \vdots \\ |\tilde{p}_1^{(r_1)}\rangle \\ \vdots \\ |\tilde{p}_{s_{r_1}}^{(r_1)}\rangle \end{pmatrix}.$$

Then these $|p\rangle$ vectors satisfy the first equation in (108). This can be checked directly by substituting the above equation into (108) and noting that matrices G and $\mathbf{\Omega_B}$ commute by virtue of Eq. (86) and the fact that matrices $\mathbf{\Omega_B}$ and $\mathbf{\Gamma_B}$ have identical form. Since G^{-1} is an invariance matrix,

the $|p\rangle$ and $|\tilde{p}\rangle$ vectors, related as above, naturally give the same soliton matrices (65). Thus there is no loss of generality in picking the particular solutions of Eq. (106) given by Eqs. (108).

IV. APPLICATIONS TO THE THREE-WAVE INTERACTION SYSTEM

To illustrate the above general results, we apply them to the three-wave interaction model (14) and display various higher-order soliton solutions. In this case, the involution property (4) holds, thus all zeros are normal and appear in complex conjugate pairs. The soliton matrix $\Gamma(k)$ is given by Eq. (65a), where $\langle\overline{p}|=|p\rangle^{\dagger}$, and the (x,t) evolution of $|p\rangle$ vectors is given by Eqs. (109) and (111a). The general higher-order soliton solutions of the three-wave system are then given by Eq. (13), where

$$\Phi^{(1)}=\Gamma^{(1)}=-(|p_1^{(1)}\rangle,\ldots,|p_{s_1}^{(1)}\rangle,\ldots,|p_1^{(r_1)}\rangle,\ldots,|p_{s_{r_1}}^{(r_1)}\rangle)\overline{\mathcal{K}}^{-1}\begin{pmatrix}\langle\overline{p}_1^{(1)}|\\ \vdots\\ \langle\overline{p}_{s_1}^{(1)}|\\ \vdots\\ \langle\overline{p}_1^{(r_1)}|\\ \vdots\\ \langle\overline{p}_{s_{r_1}}^{(r_1)}|\end{pmatrix}, \tag{114}$$

and matrix $\overline{\mathcal{K}}$ is given in Eq. (67). In all our solutions, we fix the parameters in the dispersion laws (11) as $(a_1,a_2,a_3)=(1,0.5,-0.5)$ and $(b_1,b_2,b_3)=(1,1.5,0.5)$.

A. Soliton solutions for a single pair of nonelementary zeros

First, we derive soliton solutions corresponding to a single pair of nonelementary zeros. In particular, we consider the rank sequence {1, 2} of a pair of zeros $(k_1,\overline{k_1})$. In this case, $r_1=2$ and $r_2=1$. Using formula (81) (for the case of involution) we get the number of free complex parameters in the soliton solution:

$$\mathcal{N}_{\text{free}}=3(2+1)+1-(4+1)=10-5=5.$$

There are three $|p\rangle$ vectors, $|p_1^{(1)}\rangle$, $|p_2^{(1)}\rangle$, and $|p_1^{(2)}\rangle$ in Eq. (114). When k_1 and the initial values $[|p_{01}^{(1)}\rangle,|p_{02}^{(1)}\rangle,|p_{01}^{(2)}\rangle]$ of these vectors are provided, the soliton solutions (13) will then be completely determined.

In the present case, the block sequence reads $\{s_1,s_2\}=\{2,1\}$, the corresponding invariance matrix B can be readily obtained from the general formula (91) as

$$B=\begin{pmatrix}b_{11} & b_{12} & b_{13}\\ 0 & b_{11} & 0\\ 0 & b_{32} & b_{33}\end{pmatrix},$$

which indeed has five free complex parameters [see Eq. (95)]. The invariance matrix $\overline{B}$ is just the Hermitian conjugate of the B matrix.

To display these soliton solutions, we choose $k_1=1+i$, $|p_{02}^{(1)}\rangle=[-1,i,1-i]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$. When $|p_{01}^{(1)}\rangle=[1,1+i,0.5]^T$ (the generic case), the solutions are plotted in the top row of Fig. 1. In the two nongeneric cases (where some elements of the $|p\rangle$ vectors vanish), $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$ and $|p_{01}^{(1)}\rangle=[1,0,0.5]^T$, the solutions are plotted in the second and third rows of Fig. 1, respectively. We see that in the generic case, three sech waves in the three components interact and then separate into the same sech waves with their positions shifted. In other words, this is a $u_1(\text{sech})+u_2(\text{sech})+u_3(\text{sech})\rightarrow u_1(\text{sech})+u_2(\text{sech})+u_3(\text{sech})$ process. What happens is that the initial pumping (u_3) wave breaks up into two sech waves in the other two components (u_1 and u_2), while simultaneously the two initial u_1 and u_2 waves combine into a pumping sech wave.

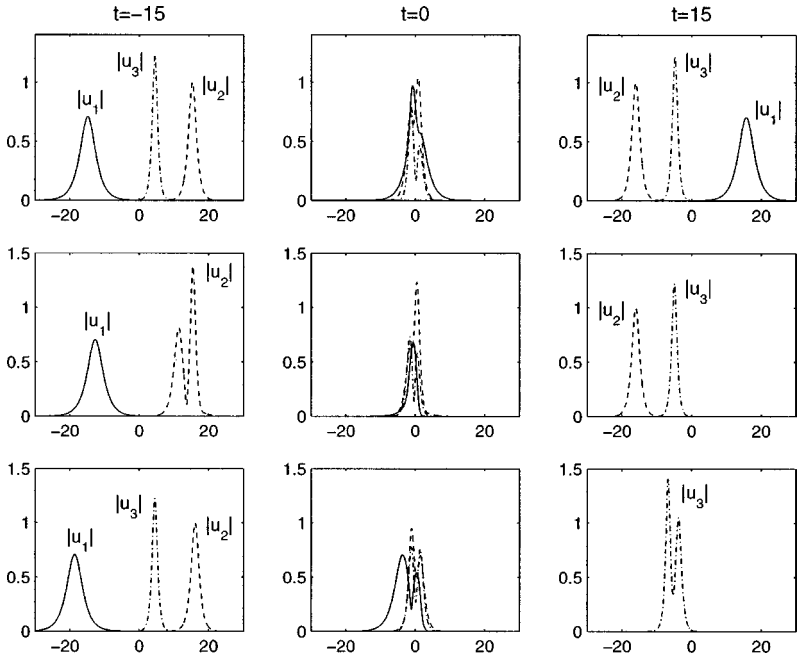

FIG. 1. Soliton solutions in the three-wave system (14) corresponding to a single pair of zeros with rank sequence {1, 2} at time $t=-15$, 0, and 15. Here, $k_1=1+i$, $|p_{02}^{(1)}\rangle=[-1,i,1-i]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$. First row, $|p_{01}^{(1)}\rangle=[1,1+i,0.5]^T$; second row, $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$; third row, $|p_{01}^{(1)}\rangle=[1,0,0.5]^T$.

Thus this process is a combination of two subprocesses: $u_3\to u_1+u_2$ and $u_1+u_2\to u_3$. This phenomenon seems related to the rank sequence {1, 2} of the present solitons and the fact that, the rank sequence {1} itself describes the breakup of a pumping sech wave into two nonpumping sech waves, while the rank sequence {2} itself describes the reserve process. In the nongeneric cases, these solutions can describe the $u_1(\text{sech})+u_2(\text{second order})\to u_2(\text{sech})+u_3(\text{sech})$ process, the $u_1(\text{sech})+u_2(\text{sech})+u_3(\text{sech})\to u_3(\text{second order})$ process (see Fig. 1, second and third rows), and many others. In the solutions of Fig. 1, the a_j and b_j parameters are such that $u_2<u_3<u_1$. If $u_1<u_3<u_2$, the processes will be exactly the opposite (see Ref. 22). Thus our solutions can describe the processes reverse to those of Fig. 1 as well.

B. Soliton solutions for two pairs of simple zeros

Here we derive the soliton solutions corresponding to two pairs of simple zeros in the three-wave system (14). Some solutions belonging to this category have been presented in Refs. 26 and 27. But we will show that those solutions are only special (nongeneric) solutions for two pairs of simple zeros. Below, the more general solutions for this case will be presented.

In this case, $r_1^{(1)}=r_1^{(2)}=1$. By using formula (81), for the case of involution (4), for two pairs of zeros, we readily obtain that the number of free complex parameters in the solution is six:

$$\mathcal{N}_{\text{free}}=2(3\times 1+1-1)=6.$$

Indeed, there are two $|p\rangle$ vectors in Eq. (114). Together with the two zeros k_1 and k_2, there are eight complex parameters in the soliton solutions. However, the 2×2 invariance matrix B in this case is diagonal and has two free (diagonal) complex parameters.

Three solutions, with $k_1=1+i$, $k_2=-1+0.5i$ and three different sets of $|p_{01}^{(1)}\rangle$ and $|p_{01}^{(2)}\rangle$ vectors, are displayed in Fig. 2. In the generic case where $|p_{01}^{(1)}\rangle=[1,1+i,0.5]^T$ and $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$ (see top row of Fig. 2), the solution describes the breakup of a higher-order pumping (u_3) wave into two higher-order u_1 and u_2 waves. This is analogous to solutions for a single pair of elementary zeros with algebraic multiplicity 2 (see Ref. 22). In the nongeneric case

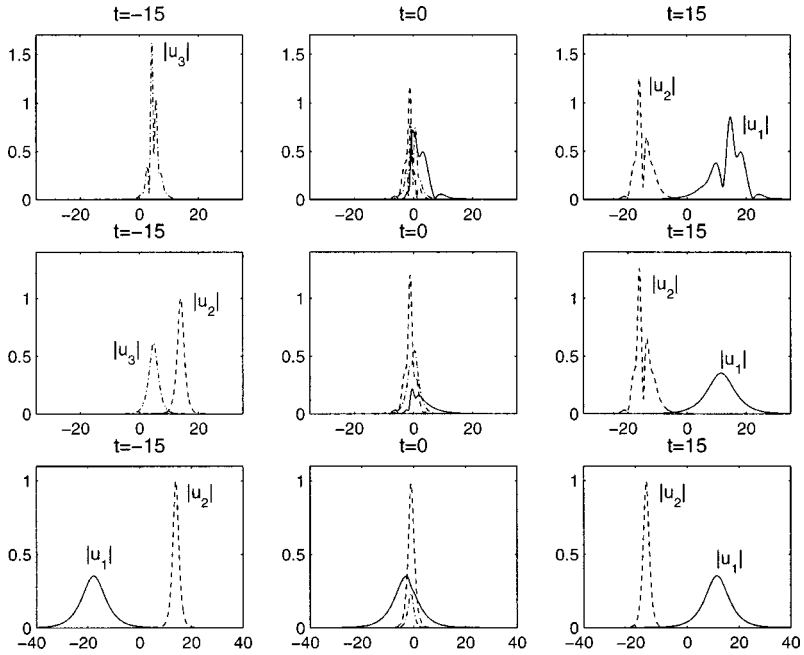

FIG. 2. Soliton solutions in the three-wave system (14) corresponding to two pairs of simple zeros at time $t=-15$, 0, and 15. Here, $k_1=1+i$, $k_2=-1+0.5i$. First row, $|p_{01}^{(1)}\rangle=[1,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$; second row, $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$; third row, $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,0]^T$.

where $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$ and $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$ (second row in Fig. 2), the present solutions can describe the $u_2(\text{sech})+u_3(\text{sech})\rightarrow u_1(\text{sech})+u_2(\text{second order})$ process. This process has been seen in Ref. 22 for elementary zeros as well. More interestingly, in the nongeneric case when $p_{01}^{(1)}[1]=p_{01}^{(2)}[3]=0$, these solutions describe the elastic interaction of a sech u_1 wave with a sech u_2 wave (see bottom row of Fig. 2). These are precisely the soliton solutions presented in Refs. 26 and 27. We see that these solutions are simply nongeneric solutions for two pairs of simple zeros.

C. Soliton solutions for two pairs of higher-order zeros

Last, we consider two pairs of distinct zeros, one simple and the other one elementary with the algebraic multiplicity 2. Let us say k_1 is the elementary zero, and k_2 is the simple zero. Then the rank sequence for k_1 is $\{1, 1\}$, and the rank sequence for k_2 is $\{1\}$. Thus, $r_1^{(1)}=1$, $r_2^{(1)}=1$, and $r_1^{(2)}=1$. By formula (81), we have

$$\mathcal{N}_{\text{free}}=3(1+1)+1-(1+1)+3\times 1+1-1=8.$$

Indeed, in this case $s_1^{(1)}=2$ and $s_1^{(2)}=1$, hence there are 11 complex parameters in the soliton solutions (nine in the three $|p\rangle$ vectors, plus the two zeros k_1 and k_2). The invariance matrix B can be found from the general formula (91) as

$$B=\begin{pmatrix} b_{11} & b_{12} & 0 \\ 0 & b_{11} & 0 \\ 0 & 0 & b_{33} \end{pmatrix},$$

which has three free complex parameters. Thus $\mathcal{N}_{\text{free}}=11-3=8$ as calculated above.

Three solutions, with $k_1=1+i$, $k_2=-1+0.5i$, $|p_{02}^{(1)}\rangle=[-1,i,1-i]^T$, and three different sets of $|p_{01}^{(1)}\rangle$ and $|p_{01}^{(2)}\rangle$ vectors, are displayed in Fig. 3. In the generic case (first row in Fig. 3),

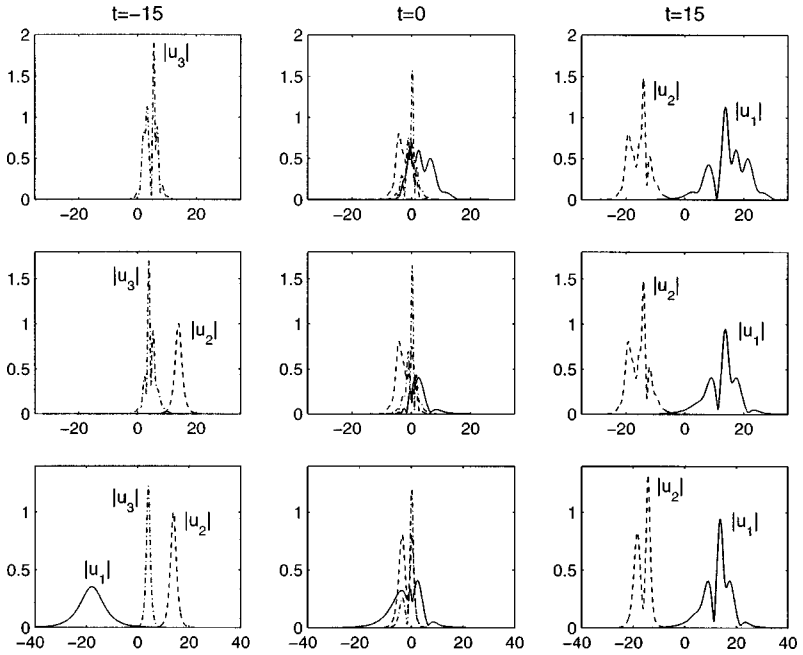

FIG. 3. Soliton solutions in the three-wave system (14) corresponding to two pairs of zeros—one elementary with algebraic multiplicity 2, and the other one simple. Here, $k_1=1+i$ (elementary zero), $k_2=-1+0.5i$ (simple zero), and $|p_{02}^{(1)}\rangle=[-1,i,1-i]^T$. First row, $|p_{01}^{(1)}\rangle=[1,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$; second row, $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,-1]^T$; third row, $|p_{01}^{(1)}\rangle=[0,1+i,0.5]^T$, $|p_{01}^{(2)}\rangle=[1,0.5,0]^T$.

this solution describes the breakup of a higher-order pumping wave (u_3) into the other u_1 and u_2 components (both higher order). In nongeneric cases, it can describe processes such as u_2(sech) $+u_3$(higher order)$\rightarrow u_1$(higher order)$+u_2$(higher order) (second row of Fig. 3), u_1(sech) $+u_2$(sech)$+u_3$(sech)$\rightarrow u_1$(higher order)$+u_2$(higher order) (last row of Fig. 3), and many others. The reverse processes of Fig. 3 can also be described by choosing a_j and b_j values such that $u_1<u_3<u_2$ instead of $u_2<u_3<u_1$ in Fig. 3.

V. CONCLUSION AND DISCUSSION

We have proposed a unified and systematic approach to study the higher-order soliton solutions of nonlinear PDEs integrable by the $N\times N$-dimensional Riemann–Hilbert problem. We have derived the complete solution to the Riemann–Hilbert problem with an arbitrary number of higher-order zeros, and characterized the discrete spectral data. Therefore, we have obtained the most general form of the higher-order multisoliton solutions to nonlinear PDEs integrable through the $N\times N$-dimensional Riemann–Hilbert problem. In other words, the most general reflectionless (soliton) potentials in the N-dimensional Zakharov–Shabat operators have been derived. The eigenfunctions associated with these reflectionless potentials are readily available from our soliton matrices. We have applied these general results to the three-wave interaction system, and new higher-order soliton and two-soliton solutions have been presented. These solutions reveal new processes such as $u_1+u_2+u_3\leftrightarrow u_1+u_2+u_3$. They also reproduce previously known solitons from Refs. 2, 22, 26, and 27 as special cases. Our results can be applied to derive higher-order multisolitons in the NLS equation and the Manakov equations as well, but this is not pursued in this paper.

The results obtained in this paper are significant from both physical and mathematical points of view. Physically, our results completely characterized higher-order solitons and multisolitons in important physical systems such as the three-wave interaction equation, the NLS equation and the Manakov equations. These higher-order solitons can describe new physical processes such as

those displayed in Figs. 1–3. If these integrable equations are perturbed (which is inevitable in a real-world problem), our higher-order solitons then become the starting point for the development of a soliton-perturbation theory which could determine what happens to these higher-order solitons under external or internal perturbations.[34,35] From the mathematical point of view, our results completely characterized the discrete spectral data of higher-order zeros in a general N-dimensional Riemann–Hilbert problem. These results will be useful for many purposes such as proving the completeness of eigenfunctions in a N-dimensional Zakharov–Shabat spectral problem with arbitrary localized potentials. The difficulty of such a proof is caused by higher-order zeros. Hopefully, with our results at hand, this difficulty can be removed.

From a broader perspective, our results are closely related to many other physical and mathematical problems. For instance, the lump solutions in the Kadomtsev–Petviashvili equation are given by the higher-order poles of the time-dependent Schrödinger equation. In Refs. 20 and 21, lump solutions corresponding to certain special higher-order poles were derived, but the most general lump solutions still remain an open question. Note that the time-dependent Schrödinger equation is an infinite-dimensional system compared to our present N-dimensional Riemann–Hilbert system. But the ideas used in this paper might be generalizable to the time-dependent Schrödinger equation as well. This remains to be seen.

ACKNOWLEDGMENTS

This work was supported in part by NASA and AFOSR grants. One of the authors (J.Y.) acknowledges helpful discussions with Jonathan Sands. The first author (V.S.) thanks the University of Vermont for support of his visit during which this work was done. The work by V.S. was also supported by FAPESP of Brazil.

APPENDIX: GENERAL RIEMANN–HILBERT PROBLEM WITH ABNORMAL ZEROS

Here we show that our soliton matrices of Sec. III can be generalized to the case of Riemann–Hilbert problem with abnormal zeros. However, due to the lack of important applications, we will show only a simple example, which corresponds to a pair of zeros with different geometric multiplicities but the same algebraic multiplicity. Then we comment on the general case of several nonpaired zeros.

Let us use the simplest example to show the idea behind generalization of our results to the general Riemann–Hilbert problem with abnormal zeros. Consider one pair of zeros $(k_1,\overline{k_1})$ which have the same algebraic multiplicity 2 but different geometric multiplicities, which here will be 1 and 2, respectively. The corresponding soliton matrices are given as follows:

$$\Gamma(k)=I+\frac{(\overline{k_1}-k_1)(|v_1\rangle\langle\overline{v_1}|+|v_2\rangle\langle\overline{v_2}|)}{k-\overline{k_1}}, \tag{A1}$$

$$\Gamma^{-1}(k)=\left(I+\frac{(k_1-\overline{k_1})|v_1\rangle\langle\overline{v_1}|}{k-k_1}\right)\left(I+\frac{(k_1-\overline{k_1})|v_2\rangle\langle\overline{v_2}|}{k-k_1}\right), \tag{A2}$$

with the conditions that $\langle\overline{v_j}|v_j\rangle=1$, $\langle\overline{v_2}|v_1\rangle=0$, and $\langle\overline{v_1}|v_2\rangle\neq 0$. To verify that the above matrices are indeed inverse to each other it is enough to rewrite the matrix $\Gamma(k)$ in the form

$$\Gamma(k)=\left(I+\frac{(\overline{k_1}-k_1)|v_2\rangle\langle\overline{v_2}|}{k-\overline{k_1}}\right)\left(I+\frac{(\overline{k_1}-k_1)|v_1\rangle\langle\overline{v_1}|}{k-\overline{k_1}}\right) \tag{A3}$$

and take into account that $P_j \equiv |v_j\rangle\langle\overline{v_j}|$ is a projector. Equations (A2) and (A3) are in fact the product representations of the form (27). Now let us show that there are exactly two solutions to $\langle\overline{p}|\Gamma^{-1}(\overline{k_1})=0$. Indeed, the corresponding null vectors are as follows:

$$\langle\overline{p_1}|=\langle\overline{v_1}|, \quad \langle\overline{p_2}|=\langle\overline{v_2}|. \tag{A4}$$

This is due to the fact that $\Gamma^{-1}(\overline{k_1})=(I-P_1)(I-P_2)$. But, on the other hand, there is just one solution to $\Gamma(k_1)|p\rangle=0$: $|p_1\rangle=|v_1\rangle$. Suppose that there is another solution $|p_2\rangle$ to $\Gamma(k_1)|p\rangle=0$ linearly independent from $|p_1\rangle$. We have then using formula (A1) for $\Gamma(k_1)$,

$$|p_2\rangle=|v_1\rangle\langle\overline{v_1}|p_2\rangle+|v_2\rangle\langle\overline{v_2}|p_2\rangle. \tag{A5}$$

Thus $|p_2\rangle=a|v_1\rangle+b|v_2\rangle$. Using this in formula (A5) we get, due to $\langle\overline{v_2}|v_1\rangle=0$ and $\langle\overline{v_1}|v_2\rangle\neq 0$,

$$a|v_1\rangle\langle\overline{v_1}|v_2\rangle=0,$$

which is a contradiction, since $a\neq 0$.

The soliton matrices given by formulas (A1)–(A2) have the following form in the standard notations of Lemma 1 of Sec. III:

$$\Gamma(k)=I+\frac{|\overline{q_1}\rangle\langle\overline{p_2}|+|\overline{q_2}\rangle\langle\overline{p_1}|}{k-\overline{k_1}}, \tag{A6}$$

$$\Gamma^{-1}(k)=I+\frac{|p_1\rangle\langle q_2|+|p_2\rangle\langle q_1|}{k-k_1}+\frac{|p_1\langle q_1|}{(k-k_1)^2}, \tag{A7}$$

where

$$|\overline{q_1}\rangle=(\overline{k_1}-k_1)|v_2\rangle, \quad |\overline{q_2}\rangle=(\overline{k_1}-k_1)|v_1\rangle, \quad \langle q_1|=(k_1-\overline{k_1})^2\langle\overline{v_1}|v_2\rangle\langle\overline{v_2}|,$$

$$\langle q_2|=(k_1-\overline{k_1})\langle\overline{v_1}|, \quad |p_2\rangle=\frac{|v_2\rangle}{(k_1-\overline{k_1})\langle\overline{v_1}|v_2\rangle}.$$

Notice that $\Gamma(k)$ has two blocks of size 1, while $\Gamma^{-1}(k)$ has one block of size 2.

In general, for one pair of zeros with different geometric multiplicities, the soliton matrices have the structure of Lemma 1 but with different numbers of blocks in $\Gamma(k)$ and $\Gamma^{-1}(k)$, while the total number of the $|p\rangle$ and $\langle\overline{p}|$ vectors appearing in these matrices is the same and equals to the order of the pair of zeros. One can proceed to derive the representations similar to those in Lemma 4 for this case. Evidently, due to the way of the derivation, the formulas will be similar with the only difference in the number of blocks and block sizes in $\Gamma(k)$ and $\Gamma^{-1}(k)$.

In the more general case of the Riemann–Hilbert problem with abnormal zeros, the zeros can be nonpaired (for instance, zero of order 2 in C_+ and two simple zeros in C_-). Formally, this case can be obtained by ''splitting'' some of the paired zeros into several distinct zeros in the soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$ discussed above, since this limit is obviously regular [the geometric multiplicity of the zero to be split should be at least equal to the number of the new zeros generated in this way, thus providing for the needed number of blocks; formula (A6), for instance, allows splitting of the zero $k=\overline{k_1}$ of $\Gamma^{-1}(k)$ into two simple zeros]. Thus, the most general case can be handled starting from the case of just one pair of zeros, i.e., the case discussed above. The explicit expressions for the soliton matrices $\Gamma(k)$ and $\Gamma^{-1}(k)$ will involve similar relations between the numbers of zeros, their geometric multiplicities and the numbers and sizes of the ν blocks of vectors as those in Lemma 1, though, obviously, with different particular numbers for each of the two matrices.

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Isomonodromy deformations for the ZS-AKNS system with quadratic spectral variables

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(Received 23 April 2003; accepted 13 May 2003)

We solve the monodromy problem and prove the Painleve property for self-similar ZS-AKNS flows with a quadratic spectral variable in this report. In particular, we obtain meromorphic solutions for the Cauchy problem of the self-similar derivative nonlinear Schrödinger equation. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1603959]

I. INTRODUCTION

The six Painleve transcendents PI-PVI, were introduced by Painleve [Clarkson (1990)] and Gambier (1910) at the beginning of the 20th century from strictly mathematical consideration. They found second order ordinary differential equations of certain general type can either be integrated in terms of known functions or can be reduced to one of the six Painleve equations. Now Painleve transcendents have appeared in a wide range of physical applications [Fokas *et al.* (1988); Ablowitz and Clarkson (1991)].

One of the most important developments in Painleve theory is the discovery that Painleve equations are the compatibility conditions (or isomonodromy conditions) of suitable overdetermined linear systems with regular or irregular singular points [Fuchs (1907), Garnier (1912), Schlesinger (1912), Flaschka and Newell (1980), Jimbo *et al.* (1981a), Jimbo and Miwa (1981, 1982)]. Therefore the Cauchy problem of a given Painleve equation can be formulated as solving the inverse monodromy problem of the associated overdetermined system. Besides, a close connection between Painleve equations and integrable systems was discovered by Ablowitz (1977), Ablowitz *et al.* (1980), Fokas *et al.* (1982,1988,1992), Olver, etc. They found similarity reductions of integrable systems give rise to Painleve transcendents.

In particular, Beals and Sattinger (1993) derived the overdetermined linear systems for the self-similar solutions of the ZS-AKNS (*with linear spectral variables*) and Gelfand–Dikii flows and studied the associated inverse monodromy problems. More precisely, the corresponding overdetermined linear systems concerned are

$$\begin{aligned} \frac{\partial \Psi}{\partial x} &= [zJ + q_1(x)]\Psi, \\ z\frac{\partial \Psi}{\partial z} &= \sum_{j=0}^{n} z^j A_j'(x)\Psi, \end{aligned} \tag{1.1}$$

and

$$\begin{aligned} \frac{\partial \Psi}{\partial x} &= [J_z + q_2(x)]\Psi, \\ z\frac{\partial \Psi}{\partial z} &= A'(x,z)\Psi, \end{aligned} \tag{1.2}$$

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where $x \in \mathbf{R}$, $z \in \mathbf{C}$, J_z and $A(x,z)$ are a matrix and certain polynomial in z^n. (There are recursive formulas between q_1 and A_j', q_2 and A'. See Beals and Sattinger (1993).) They gave a more transparent and simpler treatment for the monodromy problem of some general isomonodromy equations, including Painleve Π, self-similar solutions of Korteweg-de Vries (KdV), modified KdV, nonlinear Schrödinger, and Boussinesq equations.

Under the framework of their results, we solve the monodromy problem for *self-similar ZS-AKNS flows with quadratic spectral variables* in this report. That is, instead of (1.1), we consider the linear system

$$\begin{aligned} \frac{\partial \Psi}{\partial x} &= [z^2 J + z q(x) + p(x)]\Psi, \\ z\frac{\partial \Psi}{\partial z} &= \sum_{j=0}^{2n} z^j A_j(x)\Psi, \end{aligned} \tag{1.3}$$

with $x \in \mathbf{R}$, $z \in \mathbf{C}$. [The constraints satisfied by p, q, and A_j will be explained in (2.1), (2.2) and Theorem 1 of Sec. II.] In particular, meromorphic solutions for the Cauchy problem of the self-similar derivative nonlinear Schrödinger equation (DNLS) are obtained. We also characterize rational solutions of the isomonodromy deformation in our case. More precisely, we prove that generically all rational solutions of (1.3) can be reduced to those of (1.1).

The paper is organized as follows. In Sec. II we introduce the ZS-AKNS flows and self-similar ZS-AKNS flows. Then we derive the overdetermined system for self-similar ZS-AKNS flows. In Sec. III we study the associated direct monodromy problem. We will construct appropriate holomorphic eigenfunctions and study their relations. Our monodromic data are constructed from these relations. We also characterize the monodromic data and justify that self-similar ZS-AKNS flows are isomonodromy deformations. In Sec. IV we study the inverse monodromy problem by solving a Riemann–Hilbert problem and use the analytic and algebraic arguments of the inverse scattering theory in Beals and Caifman (1984) to solve the Cauchy problem of the self-similar ZS-AKNS flow equation. Section V is devoted to the characterization of the rational solutions of the self-similar ZS-AKNS flow equations.

II. ZS-AKNS AND SELF-SIMILAR ZS-AKNS FLOWS

We define the ZS-AKNS-flows according to the work of Lee (1989). First of all, let J be a constant diagonal, traceless matrix with diagonal entries $\lambda_1, \lambda_2, \ldots, \lambda_d$. Let $Q(x,t)$ be off-diagonal, the diagonal part of $P(x,t)$ equal to that of $Q(\mathrm{ad}\, J)^{-1}Q$, and Q, P be smooth. Then a formal eigenfunction $\Phi(x,z) = M(x,z)e^{xz^2J} \overset{\text{def}}{=} \sum_{j=0}^{\infty} f_j(x) z^{-j}\, e^{xz^2J}$ of the first formula in (1.3) exists. That is $f_0 = 1$, $(\partial/\partial x - z^2\, \mathrm{ad}\, J - zQ - P)\sum_{j=0}^{k} f_j z^{-j} = \mathcal{O}(z^{-k+1})$, $k = 1,2,\ldots$. Moreover, let μ be any constant diagonal traceless matrix with diagonal entries $\mu_1, \mu_2, \ldots, \mu_d$, then

$$M\mu M^{-1} \sim \mu + \frac{\mathcal{F}_1}{z} + \frac{\mathcal{F}_2}{z^2} + \cdots. \tag{2.1}$$

It can be shown that the coefficients $\mathcal{F}_j = \mathcal{F}_{j,J,\mu}(x,t)$ are independent of the choice of formal solution M and satisfy

$$\begin{aligned} &\mathcal{F}_0 = \mu, \\ &[J, \mathcal{F}_1] + [Q, \mu] = 0, \\ &\left[\frac{\partial}{\partial x} - P, \mathcal{F}_k\right] - [J, \mathcal{F}_{k+2}] - [Q, \mathcal{F}_{k+1}] = 0, \quad k = 0,1,2,\ldots, \end{aligned} \tag{2.1'}$$

$\mu+\frac{\mathcal{F}_1}{z}+\frac{\mathcal{F}_2}{z^2}+\cdots$ has the same characteristic or minimal polynomial as μ.

Therefore $\mathcal{F}_{2j+1}$ and $\mathcal{F}_{2j+2}$ are traceless polynomials in $\partial^r Q/\partial x^r$, $\partial^s P/\partial x^s$, for $r, s \in \{0,1,...,j\}$.

Definition 1: For $t \in \mathbf{R}$, $x \in \mathbf{R}$, the ZS-AKNS flow is defined by the system of nth order partial differential equations

$$\frac{\partial Q}{\partial t}=[J,\mathcal{F}_{2n+1}],$$

$$\frac{\partial P}{\partial t}=[J,\mathcal{F}_{2n+2}]+[Q,\mathcal{F}_{2n+1}],$$

with $\mathcal{F}_j$ defined by (2.1).

As is well known, the ZS-AKNS flow has the Lax pair:

$$\begin{aligned}\frac{\partial \Phi}{\partial x}(x,z,t)&=[z^2J+zQ+P]\Phi(x,z,t),\\ \frac{\partial \Phi}{\partial t}(x,z,t)&=[\mu z^{2n}+\mathcal{F}_1 z^{2n-1}+\cdots+\mathcal{F}_{2n}]\Phi(x,z,t),\end{aligned} \tag{2.2}$$

where $\mathcal{F}_j$ are defined by (2.1).

Definition 2: The ZS-AKNS flow is self-similar if one of the following equivalent conditions is fulfilled:

(1) There exist constants α, β, such that the eigenfunction Φ of the Lax pair (2.2) *is invariant under $T_{\lambda,\alpha,\beta}$ for $\forall \lambda \in \mathbf{C}$;*

(2) There exist constants α, β, γ such that for $\forall \lambda \in \mathbf{C}$,

$$\lambda^{\gamma} Q(\lambda^{\alpha}x,\lambda^{\beta}t)=Q(x,t),$$

$$\lambda^{2\gamma} P(\lambda^{\alpha}x,\lambda^{\beta}t)=P(x,t),$$

where $T_{\lambda,\alpha,\beta}$ is the scaling operator: $T_{\lambda,\alpha,\beta}f(x,z,t)=f(\lambda^{\alpha}x,\lambda z,\lambda^{\beta}t)$.

Lemma 1: For the scaling operator of self-similar ZS-AKNS flows, the indices $(\alpha,\beta,\gamma)=(-2,-2n,-1)$.

Proof:

$$\frac{\partial}{\partial x}(T_{\lambda,\alpha,\beta}\Phi)=\lambda^{\alpha}T_{\lambda,\alpha,\beta}([z^2J+zQ(x,t)+P(x,t)]\Phi)=\lambda^{\alpha}[\lambda^2 z^2 J+\lambda z Q(\lambda^{\alpha}x,\lambda^{\beta}t)$$

$$+P(\lambda^{\alpha}x,\lambda^{\beta}t)]T_{\lambda,\alpha,\beta}\Phi=[z^2J+zQ(x,t)+P(x,t)]\Phi.$$

Thus $\alpha=-2$ and $\gamma=-1$. Similarly we obtain $\beta=-2n$ by equating

$$\frac{\partial}{\partial t}(T_{\lambda,\alpha,\beta}\Phi)=\lambda^{\beta}T_{\lambda,\alpha,\beta}\frac{\partial \Phi}{\partial t}=\lambda^{\beta}[(\lambda z)^{2n}\mu+(\lambda z)^{2n-1}\mathcal{F}_1(\lambda^{\alpha}x,\lambda^{\beta}t)+\cdots$$

$$+\mathcal{F}_{2n}(\lambda^{\alpha}x,\lambda^{\beta}t)]T_{\lambda,\alpha,\beta}\Phi=[z^{2n}\mu+z^{2n-1}\mathcal{F}_1+\cdots+\mathcal{F}_{2n}]\Phi. \qquad \square$$

Using the scaling operator, we derive the overdetermined system for the self-similar ZS-AKNS flow.

Theorem 1: *The ZS-AKNS flow (2.2) is self-similar if and only if*

$$\frac{\partial \Psi}{\partial x}(x,z)=[z^2J+zq(x)+p(x)]\Psi(x,z), \tag{2.3.1}$$

$$z\frac{\partial \Psi}{\partial z}(x,z)=[2n(z^{2n}\mu+z^{2n-1}F_1(x)+\cdots+F_{2n}(x))+2x(z^2J+zq(x)+p(x))]\Psi(x,z)$$

$$\overset{\text{def}}{=}\sum_{j=0}^{2n}A_j(z)z^j\Psi(x,z)\overset{\text{def}}{=}A(x,z)\Psi(x,z), \tag{2.3.2}$$

with

$$m\mu m^{-1}=\mu+\frac{F_1}{z}+\frac{F_2}{z^2}+\cdots,$$

and me^{xz^2J} *is a formal solution of (2.3.1). Moreover*

$$Q(x,1)=q(x),\quad P(x,1)=p(x),\quad \mathcal{F}_j(x,1)=F_j(x),\quad \Phi(x,z,1)=\Psi(x,z).$$

Proof: Suppose (Q,P) is a self-similar ZS-AKNS flow. Then Definition 2 and Lemma 1 imply that

$$\Phi(x,z,t)=\Phi(\lambda^{-2}x,\lambda z,\lambda^{-2n}t). \tag{2.4}$$

So Φ is a function of x, z only. Set $\lambda^{-2n}t=1$. Let

$$\Phi(x,z,t)=\Phi(t^{-1/n}x,t^{1/2n}z,1)\equiv\Psi(t^{-1/n}x,t^{1/2n}z).$$

Differentiating (2.4) with respect to λ at $\lambda=1$, we get

$$-2x\frac{\partial \Phi}{\partial x}+z\frac{\partial \Phi}{\partial z}-2nt\frac{\partial \Phi}{\partial t}=0. \tag{2.5}$$

Evaluating at $t=1$ and using the Lax pair (2.2), we obtain (2.3.1) and (2.3.2). So the if part is proved. To show the other direction, suppose $\Psi(x,z)$ satisfies (2.3.1) and (2.3.2). Let $\Phi(x,z,t)=\Psi(t^{-1/n}x,t^{1/2n}z)$. Thus $\Phi(x,z,t)=\Phi(\lambda^{-2}x,\lambda z,\lambda^{-2n}t)=\Phi(t^{-1/n}x,t^{1/2n}z,1)$. Therefore we obtain the Euler equation (2.4). Combined with (2.3.1) and (2.3.2) this induces

$$\frac{\partial \Phi}{\partial x}(x,z,t)=[z^2J+zt^{-1/2n}q(t^{-1/n}x)+t^{-1/n}p(t^{-1/n}x)]\Phi(x,z,t)$$

$$\overset{\text{def}}{=}[z^2J+zQ(x,t)+P(x,t)]\Phi(x,z,t),$$

$$\frac{\partial \Phi}{\partial t}(x,z,t)=[z^{2n}\mu+z^{2n-1}t^{-1/2n}F_1(t^{-1/n}x)+\cdots+t^{-1}F_{2n}(t^{-1/n}x)]\Phi(x,z,t)$$

$$\overset{\text{def}}{=}[z^{2n}\mu+z^{2n-1}\mathcal{F}_1(x,t)+\cdots+\mathcal{F}_{2n}(x,t)]\Phi(x,z,t).$$

Note that both $M\mu M^{-1}$ and $\mu+\mathcal{F}_1/z+\mathcal{F}_2/z^2+\cdots$ are invariant under $T_{-2,-2n,-1}$. Here $\Phi(x,z,t)=M(x,z,t)e^{xz^2J}=m(t^{-1/n}x,t^{1/2n}z)e^{xz^2J}$ is a formal solution of $\partial\Phi/\partial x=[z^2J+zQ+P]\Phi$. In addition, $(M\mu M^{-1})(x,1)=m\mu m^{-1}=\mu+F_1/z+F_2/z^2+\cdots=\mu+[\mathcal{F}_1(x,1)]/z$

$+[\mathcal{F}_2(x,1)]/z^2+\cdots$. So $M\mu M^{-1}=\mu+\mathcal{F}_1/z+\mathcal{F}_2/z^2+\cdots$. Therefore (Q,P) is a self-similar ZS-AKNS flow. □

Theorem 2: *The self-similar ZS-AKNS flow satisfies the nonlinear ordinary differential system*

$$\begin{aligned} 2n[J,F_{2n+1}]+(2xq)_x-q=0,\\ 2n[J,F_{2n+2}]+2n[q,F_{2n+1}]+(2xp)_x=0, \end{aligned} \tag{2.6}$$

where F_j are defined as in Theorem 1.

Proof: The theorem can be proved by equating the compatibility condition of (2.3.1) and (2.3.2) and using the recursive formula (2.1′) and $F_j(x)=\mathcal{F}_j(x,1)$. □

Example 1: The derivative nonlinear Schrödinger equation (DNLS),

$$u_t=iu_{xx}\pm(|u|^2u)_x,$$

was first derived by plasma physicists [Mio *et al.* (1976), Mjothus (1976)]. Kaup and Newell obtained the soliton solutions of DNLS in Kaup and Newell (1978), Lee (1989) solved the Cauchy problem of DNLS by studying the associated scattering problem of

$$v_t=\frac{i}{2}v_{xx}\mp\frac{1}{2}v^2\bar{v}_x+\frac{i}{4}v|v|^4. \tag{2.7}$$

Note that (2.7) possesses the Lax Pair

$$\begin{aligned} \frac{\partial\Phi}{\partial x}&=[z^2J+zQ+P]\Phi,\\ \frac{\partial\Phi}{\partial t}&=[z^4\mu+z^3\mathcal{F}_1+\cdots+\mathcal{F}_4]\Phi. \end{aligned} \tag{2.8}$$

with $Q=\left(\begin{smallmatrix}0 & v\\ \pm\bar{v} & 0\end{smallmatrix}\right)$, $P=Q(\mathrm{ad}\,J)^{-1}Q=\pm|v|^2/2i\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$, $J=\mu=\left(\begin{smallmatrix}-i & 0\\ 0 & i\end{smallmatrix}\right)$, $\mathcal{F}_0=\mu$, $\mathcal{F}_1=Q$, $\mathcal{F}_2=P$, $\mathcal{F}_3=1/2i\left(\begin{smallmatrix}0 & v\\ \pm\bar{v}_x & 0\end{smallmatrix}\right)$, and $\mathcal{F}_4=(1/(2i)^3|v|^4\pm1/(2i)^2(v\bar{v}_x-v_x\bar{v}))\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$. Applying Theorems 1 and 2, we then obtain the overdetermined system

$$\begin{aligned} \frac{\partial\Psi}{\partial x}&=[z^2J+zq+p]\Psi,\\ z\frac{\partial\Psi}{\partial z}&=\left[4Jz^4+4qz^3+(4p+2xJ)z^2+\left(2xq-2i\begin{pmatrix}0 & -v_x\\ \pm\bar{v}_x & 0\end{pmatrix}\right)z+2xp\right.\\ &\quad\left.+\left(-\frac{1}{2i}|v|^4\mp(v\bar{v}_x-v_x\bar{v})\right)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right]\Psi. \end{aligned}$$

and nonlinear evolution equation of the self-similar DNLS

$$(2xv)_x-v+2iv_{xx}\mp2v^2\bar{v}_x+iv|v|^4=0. \tag{2.9}$$

III. THE FORWARD MONODROMY PROBLEM

Given an initial value of the self-similar ZS-AKNS flow, we will construct special eigenfunction of the system (2.3.1) and (2.3.2) and extract monodromy data from the relations between these eigenfunctions. We first define the characteristic lines and sectors with respect to (2.3.1) and (2.3.2).

Definition 3: The characteristic lines and sectors are

$$\Sigma(j,k)=\{z\in\mathbf{C}:\quad \mathrm{Re}\, z^{2n}(\mu_j-\mu_k)=0\},$$

$$\Sigma=\cup_{j<k}\Sigma(j,k),$$

$\tilde{\Omega}_\nu$ = *a region bounded by two rays from* Σ, *and its interior contains exactly one ray from each* $\Sigma(j,k)$.

Lemma 2: Suppose that (q,p) *is a self-similar ZS-AKNS flow, i.e., satisfies (2.6). Then for* $\forall x\in\mathbf{R}$, $\forall\tilde{\Omega}_\nu$, *there exists a unique holomorphic solution* Ψ_ν *of (2.3.1) and (2.3.2). Moreover,*

$$\Psi_{\nu+1}(x,z)=\Psi_\nu(x,z)S_\nu,\quad z\in\tilde{\Omega}_\nu\cap\tilde{\Omega}_{\nu+1},$$

$$\Psi_\nu=m_\nu e^{z^2xJ+z^{2n}\mu},\quad m_\nu\sim\sum_{j=0}^{\infty}z^{-j}f_j(x),\quad f_0=1.$$

Here S_ν, *certain constant matrices, are called the Stokes matrices.*

Proof: Our proof follows from a close adaptation of the argument in Beals and Sattinger (1993). First of all, let $f(x,z)=\Sigma_{j=0}^{2n}z^{-j}f_j(x)$, with $f_0=1$, $(\partial/\partial x-z^2\mathrm{ad}\,J-zq-p)\Sigma_{j=0}^{N}z^{-j}f_j(x)=\mathcal{O}(z^{-N+1})$, $N=1,...,2n$. Now we look for a solution of (2.3.2) in the form of $\Psi=f\hat{\Psi}$. Then

$$\frac{\partial\hat{\Psi}}{\partial z}=(2n\mu z^{2n-1}+2xzJ)\hat{\Psi}+r(x,z)\hat{\Psi},\quad r(x,z)=\mathcal{O}\left(\frac{1}{|z|^2}\right).$$

Set $\hat{\Psi}=\hat{m}e^{\Phi}$, $\Phi=z^{2n}\mu+xz^2J$. Then the above differential system is converted into

$$\hat{m}(x,z)=1-\int_{\gamma_z}e^{\Phi(z)-\Phi(\xi)}r(\xi)\hat{m}(x,\xi)e^{-\Phi(z)+\Phi(\xi)}\mathrm{d}\xi. \tag{3.1}$$

Note a proper contour γ_x in

$$\Sigma_{x,z}(j,k)=\{\xi\in\mathbf{C}:\mathrm{Re}\{(z^{2n}-\xi^{2n})(\mu_j-\mu_k)+(z^2-\xi^2)(x\lambda_j-x\lambda_k)\}=0\}$$

can be chosen to show the convergence of the integral representation (3.1). So Ψ_ν exists, is holomorphic in $\tilde{\Omega}_\nu$, and satisfies (2.3.2). The uniqueness of Ψ_ν follows from the asymptotic behavior of m_ν and the property that interior of $\tilde{\Omega}_\nu$ contains exactly one ray from each $\Sigma(j,k)$.

Now we need to justify that Ψ_ν satisfies (2.3.1). Let $\tilde{\Psi}=[\partial/\partial x-(z^2J+zq+p)]\Psi_\nu$. By (2.6), we obtain $\tilde{\Psi}_\nu=\Psi_\nu T(x)$. Hence

$$m_\nu^{-1}\left[\frac{\partial}{\partial x}-(z^2J+zq+p)\right]m_\nu=e^{\Phi}T(x)e^{-\Phi}.$$

Comparing the off-diagonal entries of both sides of the above identity and observing that left-hand side grows polynomially, the right-hand side grows exponentially. So $T(x)$ must be a diagonal matrix. Moreover, the leading term of the left-hand side must be off-diagonal by the properties of J, q, and p. So $T(x)\equiv 0$. □

To analyze the monodromy data at the origin, we first define a generic condition for the potential (q,p).

Definition 4: The potential (q,p) *is proper if (2.3.2) admits a fundamental solution of the form*

$$\Psi(x_0,z)=\omega(x_0,z)z^{A_0(x_0)},\quad \omega(x_0,\cdot)\ \textit{entire},\ \ \omega(x_0,0)=1,$$

where $x_0 \in \mathbf{R}$, *and* $A_0(x_0)=2x_0p(x_0)+2nF_{2n}(x_0)$ *is the leading coefficient of the right-hand side of (2.3.2).*

By (2.6) and the proper condition, we can construct an eigenfunction at the origin.

Lemma 3: Suppose that (q,p) *is a proper self-similar ZS-AKNS flow. Then there is a fundamental solution* $\Psi_0(x,z)$ *of (2.3.1) and (2.3.2) which has the form*

$$\Psi_0(x,z)=f(x,z)z^{A_0(x_0)}, \quad z\in \mathbf{C}\backslash 0,$$

with $f(x,\cdot)$ *entire,* $f(x_0,0)=1$.

So the eigenfunction Ψ_0 has monodromy data $A_0(x_0)$ at the origin. Comparing the eigenfunctions Ψ_ν and Ψ_0 obtained by Lemmas 2 and 3, we obtain the following lemma which describes the relation between the monodromy data at the origin and the Stokes matrices (monodromy data at the infinity).

Lemma 4: Suppose that (q,p) *is a proper self-similar ZS-AKNS flow. Then uniquely there exist constant connection matrices* C_ν *such that* $\Psi_\nu C_\nu^{-1}z^{-A_0(x_0)}$ *is regular and*

$$C_\nu^{-1}e^{-2\pi iA_0(x_0)}C_\nu=S_\nu S_{\nu+1}\cdots S_{\nu-1}.$$

Proof: First we note that from Lemmas 2 and 3, we have that Ψ_ν and Ψ_0 satisfy (2.3.1) and (2.3.2). So there exist connection matrices C_ν, constant matrices, such that

$$\Psi_\nu=\Psi_0C_\nu. \tag{3.2}$$

Hence $\Psi_\nu C_\nu^{-1}z^{-A_0(x_0)}$ is regular. Now by (3.2) and Lemma 3, we have

$$\Psi_\nu(ze^{2\pi i})=\Psi_0(z)e^{2\pi iA_0}C_\nu,$$

and thus

$$\Psi_\nu(ze^{2\pi i})\{S_\nu S_{\nu+1}\cdots S_{\nu-2}S_{\nu-1}\}^{-1}=\Psi_\nu(z)C_\nu^{-1}e^{2\pi iA_0}C_\nu.$$

□

Definition 5: The monodromy transform for a proper self-similar ZS-AKNS flow (q,p) *is defined by:*

$$M(q,p)=\{A_0(x_0),C_\nu,S_\nu,J,\mu\}.$$

Note that through the proofs of Lemmas 2–4 and Coddington and Levinson (1955), this definition depends only on the n-jet of q and p at x_0.

So the nonlinear ordinary differential system (2.6) is an isomonodromy deformation. Note that the monodromic data has the following constraints by Lemmas 2–4.

Theorem 3: *For a proper self-similar ZS-AKNS flow, the monodromic data* $M(q,p)=\{A_0,C_\nu,S_\nu,J,\mu\}$ *satisfies the necessary conditions*

$$\begin{gathered}
(1)\ \ tr\ \ A_0=0,\\
(2)\ \ \det C_\nu=1,\\
(3)\ \ e^{-\Phi}S_\nu e^{\Phi}\ \ \text{is bounded as}\ \ z\to\infty\ \ in\ \ \tilde{\Omega}_\nu\cap\tilde{\Omega}_{\nu+1}, S_{jj}=1,\ \ \Phi=z^{2n}\mu+xz^2J,\\
(4)\ \ C_\nu^{-1}e^{-2\pi iA_0}C_\nu=S_\nu S_{\nu+1}\ldots S_{\nu-1}.
\end{gathered} \tag{3.3}$$

IV. THE INVERSE MONODROMY PROBLEM

We state the main theorem

Theorem 4: *The Cauchy problem of the isomonodromy equation (2.6) can be solved uniquely. Moreover, the solution can be extended meromorphically to* $x \in \mathbf{C}$. *So the self-similar ZS-AKNS flow (2.6) is a Painleve transcendent.*

Proof: Given an initial data $\{q(x_0),(\mathrm{d}/\mathrm{d}x)q(x_0),(\mathrm{d}/\mathrm{d}x)p(x_0),\ldots,(\mathrm{d}^j/\mathrm{d}x^j)q(x_0),(\mathrm{d}^j/\mathrm{d}x^j)p(x_0),\ldots,(\mathrm{d}^{n-1}/\mathrm{d}x^{n-1})q(x_0),(\mathrm{d}^{n-1}/\mathrm{d}x^{n-1})p(x_0)\}$, we get $(\mathrm{d}^n/\mathrm{d}x^n)q(x_0)$, and $(\mathrm{d}^n/\mathrm{d}x^n)p(x_0)$ by solving the isomonodromic equation (2.6) at x_0. Then we can apply Lemmas 2–4 to construct eigenfunction $\Psi(x_0,z)$, $\Psi_0(x_0,z)$ and obtain the monodromic data $\{A_0(x_0),C_\nu,S_\nu,J,\mu\}$ such that the monodromy data satisfy the necessary condition (3.3). [Note that even if (q,p) is not proper, we still can obtain modified versions of Lemmas 3 and 4—Beals and Sattinger (1993).]

Now we formulate the Riemann–Hilbert problem: solving a piecewise holomorphic function $M=\{M_0,M_\nu\}$, such that

$$M_0 \text{ defined in } \{z:|z|\leqslant 1\},$$

$$M_\nu \text{ defined in the region bounded by } S^1,\Gamma_{\nu+1}\cap\{z:|z|\geqslant 1\}, \quad \text{and } \Gamma_\nu\cap\{z:|z|\geqslant 1\},$$

$$M_{\nu+1}=M_\nu e^{\Phi}S_\nu e^{-\Phi}, \text{ on } \Gamma_\nu\cap\{z:|z|>1\}, \quad \Phi=z^{2n}\mu+xz^2J, \tag{4.1}$$

$$M_0=M_\nu C_\nu^{-1}z^{-A_0(x_0)}, \text{ on } S^1$$

$$M(x,\cdot)\text{tends to } 1, \text{ as } |z|\to\infty,$$

where Γ_ν is a ray in the intersection $\tilde{\Omega}_\nu\cap\tilde{\Omega}_{\nu+1}$.

One can justify the cyclic product condition around each intersection point of the contour is fulfilled, since it is as $x=x_0$. Then the Riemann–Hilbert problem can be solved by applying the theory of Beals and Coifman (1984), actually, we first find a piecewise rational function u (rational except on $\Gamma_\nu\cap\{z:|z|>1\}\cup S^1$) such that the jumps of u are close enough to those of (4.1) [Lemma 10.2, Beals and Coifman (1984)]. Then (4.1) is reduced to a solution of a small norm Riemann–Hilbert problem [Lemma 10.18, Beals and Coifman (1984)]. Since the kernel of the integral equation and the jumps of u depend on x holomorphically, so M depends on x meromorphically.

Now let us set $\Psi_\nu(x,z)=M_\nu e^{\Phi}$, for $z\in\Omega_\nu\cap\{z\in\mathbf{C}:|z|\geqslant 1\}$ and extend Ψ_ν to $z\in\Omega_\nu\cap\{z\in\mathbf{C}:|z|\leqslant 1\}$ by setting $\Psi_\nu(x,z)=M_0z^{A_0(x_0)}C_\nu$. Here $\{\Omega_\nu\}$ are the components of $\mathbf{C}\backslash(\cup\Gamma_\nu)$. To prove the solvability, we need to show that $\Psi(x,z)$ satisfies (2.3.1) and (2.3.2).

Define $m_\nu=\Psi_\nu(x,z)e^{-\Phi}$. Therefore $\det m$ is continuous, entire, and tending to 1 at ∞. So m is invertible. Now we can justify that

$$\left\{\left(\frac{\partial}{\partial x}-z^2\mathrm{ad}\,J\right)m\right\}m^{-1}$$

is continuous, piecewise holomorphic, and of order $\mathcal{O}(|z|)$, as $|z|\to\infty$. Similarly

$$\left\{\left(z\frac{\partial}{\partial z}-2nz^{2n}\mathrm{ad}\mu-2xz^2\mathrm{ad}\,J\right)m\right\}m^{-1}$$

is continuous, piecewise holomorphic, and of order $\mathcal{O}(|z^{2n-1}|)$, as $|z|\to\infty$. Therefore we have

$$\frac{\partial\Psi}{\partial x}=[z^2J+zq+p]\Psi,$$

$$z\frac{\partial\Psi}{\partial z}=\sum_{j=0}^{2n}A_j(x)z^j\Psi. \tag{4.2}$$

Finally, note

$$\sum_{j=0}^{2n} A_j(x)z^j = m(x,z)(2nz^{2n}\mu + 2xz^2 J)m(x,z)^{-1} + \mathcal{O}(z^{-1})$$

$$= 2nz^{2n} m(x,z)\mu m(x,z)^{-1} + 2xz^2 J$$

$$+ 2xz(f_1 J - J f_1) + 2x(f_2 J - f_1 J f_1 + J f_1^2 - J f_2) + \mathcal{O}(z^{-1})$$

$$= 2nz^{2n} m(x,z)\mu m(x,z)^{-1} + 2xz^2 J + 2xzq + 2xp + \mathcal{O}(z^{-1}).$$

Here we use the formula $m(\dot{x},z) = 1 + f_1/z + f_2/z^2 + \cdots$,

$$q = -[J,f_1], \quad p = -[J,f_2] - [J,f_1]f_1. \tag{4.3}$$

So Theorems 1 and 2 and (4.2) imply that (q,p) satisfy (2.6) with prescribed initial data.

By (4.3) and the meromorphic property of $M(\cdot,z)$, we prove (q,p) can be extended meromorphically to $x \in \mathbf{C}$. Unique solvability and Painleve property follow from the unique solvability of the Riemann-Hilbert problem (4.1) and the meromorphic property of the extended solution (q,p) constructed above. □

Corollary 5: We can obtain meromorphic solution of the Cauchy problem of the self-similar derivative nonlinear Schrödinger equation.

Proof: This follows from the discussion of Example 1 and Theorem 4. □

V. CHARACTERIZATION OF RATIONALITY

One of the main tools in the inverse scattering methods to construct soliton or rational solutions is setting the continuous data to be trivial and then solving the reduced linear algebraic equations to get them. In this section, we prove that all such proper rational self-similar ZS-AKNS flows satisfying (2.3) are actually self-similar ZS-AKNS flows satisfying (1.1). That is, all such proper rational self-similar ZS-AKNS flows with quadratic spectral variables can actually be reduced to self-similar ZS-AKNS flows with linear spectral variables.

Lemma 6: If (q,p) is a proper self-similar ZS-AKNS flow with monodromy data $S_\nu \equiv 1$, then m, p, and q are rational in x. Here $\Psi = me^{z^{2n}\mu + xz^2 J}$ is the eigenfunction obtained in Lemma 2.

Proof: Since $S_\nu \equiv 1$ and Lemmas 3 and 4 we obtain $m_\nu = m$, and $me^{\Phi} = m_\nu e^{\Phi} = m_\nu e^{xz^2 J + z^{2n}\mu} = \Psi_0 C_\nu = f(x,z)z^A C_\nu$. Thus $C_\nu = C_{\nu'}$ and $e^{2\pi i A} = 1$. This implies that A is diagonizable and has integer-valued eigenvalues. So m is rational in z with a unique pole at the origin. Write m as

$$m = 1 + \frac{f_1}{z} + \cdots + \frac{f_r}{z^r}. \tag{5.1}$$

By (4.3), to prove our lemma, it is sufficient to show $f_1, \ldots, f_r$ are rational in x. By (5.1) and the property that $me^{\Phi} C_\nu^{-1} z^{-A}$ is regular at the origin, we obtain the following linear system for f_j [Beals and Sattinger (1993)]:

$$f_r V_{1-r} = 0,$$

$$(f_r C_1 + f_{r-1})V_{2-r} = 0,$$

$$\vdots$$

$$(f_r C_{r-1} + \cdots + f_1)V_0 = 0,$$

$$(f_r C_r + \cdots + f_1 C_1)V_1 = -V_1, \tag{5.2}$$

$$(f_rC_{r+1}+f_{r-1}C_r+\cdots+f_1C_2)V_2=-C_1V_2,$$

$$\vdots$$

$$(f_rC_{r+s-2}+\cdots+f_1C_{s-1})V_{s-1}=-C_{s-2}V_{s-1},$$

$$(f_rC_{r+s-1}+\cdots+f_1C_s)V_s=-C_{s-1}V_s,$$

where $e^{\Phi}=\Sigma_{j=0}^{\infty}z^jC_j(x)$, and $s=s_1\geqslant s_2\geqslant\cdots\geqslant s_d=-r$ are eigenvalues of $C^{-1}AC$ with corresponding eigenvectors $v_1, v_2,\ldots, v_d$. Finally $V_k=(v_j,v_{j-1},\ldots,v_1)$, the set of eigenvectors with eigenvalues$\geqslant k$. Note that the proper condition implies that $A=A_0=2x_0p(x_0)+2nF_{2n}(x_0)$. So $\operatorname{tr}A=0$. Hence (5.2) is a nonempty system.

Now denote d_j the dimension of the eigenspace corresponding to eigenvalue s_j. We compute the number of linear equations represented by (5.2):

$$\begin{aligned}
&d[(d_{1-r}+d_{2-r}+\cdots)+(d_{2-r}+d_{3-r}+\cdots)+(d_{3-r}+\cdots)+\cdots]\\
&\quad=d[d_{1-r}+2d_{2-r}+3d_{3-r}+\cdots]\\
&\quad=d[(1-r)d_{1-r}+(2-r)d_{2-r}+\cdots]+dr[d_{1-r}+d_{2-r}+\cdots]\\
&\quad=d[\operatorname{tr}\ A+rd_{-r}]+dr[d-d_{-r}]=rd^2. \qquad (5.3)
\end{aligned}$$

Note here we use the proper condition to obtain $\operatorname{tr}A=\operatorname{tr}A_0=0$. So (5.2) is a set of rd^2 equations for rd^2 entries of the f_j. Lemma 6 will be proved by noting that C_j are polynomials in x, and applying Fredholm theorem and the following lemma. □

Lemma 7: There is at most one solution of (5.2).

Proof: Suppose that there are two solution $f=(f_1,f_2,\ldots,f_r)$ and $\tilde{f}=(\tilde{f}_1,\tilde{f}_2,\ldots,\tilde{f}_r)$ of (5.2). Denote

$$m=1+\frac{f_1}{z}+\cdots+\frac{f_r}{z^r},$$

$$\tilde{m}=1+\frac{\tilde{f}_1}{z}+\cdots+\frac{\tilde{f}_r}{z^r}.$$

Hence (5.2) is equivalent to $me^{\Phi}z^{-\hat{A}_0}$ and $\tilde{m}e^{\Phi}z^{-\hat{A}_0}$ are regular at the origin, with $\hat{A}_0=C_\nu^{-1}A_0C_\nu$. Besides, note that $\lim_{z\to\infty}\det(me^{\Phi}z^{-\hat{A}_0})=\lim_{z\to\infty}\det(\tilde{m}e^{\Phi}z^{-\hat{A}_0})=1$. So we derive $\det(me^{\Phi}z^{-\hat{A}_0})=\det(\tilde{m}e^{\Phi}z^{-\hat{A}_0})\equiv 1$. So m and $\tilde{m}$ are invertible. This implies $\tilde{m}m^{-1}$ are entire. Combining the condition that $\lim_{z\to\infty}m=\lim_{z\to\infty}\tilde{m}=1$, we prove $m=\tilde{m}$. □

Lemma 8: Suppose that (q,p) is a proper rational solution of (2.5) with trivial Stokes matrices. Let r be the degree of the pole of m obtained by Lemma 2. Then r is even.

Proof: Since $\Phi=z^2xJ+z^{2n}\mu$, $C_i=0$ for odd i. Hence the system (5.2) can be divided into two independent groups if r is odd. One is a system of

$$\sharp_{\text{odd}}=d(d_{1-r}+2d_{3-r}+3d_{5-r}+4d_{7-r}+\cdots)+d(d_{2-r}+2d_{4-r}+3d_{6-r}+4d_{8-r}+\cdots)$$

number of linear equations for $(r+1)d^2/2$ entries of $f_1, f_3,\ldots, f_r$. The other is a system of

$$\sharp_{\text{even}}=d(d_{3-r}+2d_{5-r}+3d_{7-r}+\cdots)+d(d_{2-r}+2d_{4-r}+3d_{6-r}+4d_{8-r}+\cdots)$$

number of linear equations for $(r-1)d^2/2$ entries of $f_2, f_4,\ldots, f_{r-1}$. Hence by (5.3) and the uniqueness property from Lemma 7, we must have $\sharp_{\text{odd}}-\sharp_{\text{even}}=d(d_{1-r}+d_{3-r}+d_{5-r}+d_{7-r}+\cdots)=(r+1)d^2/2-(r-1)d^2/2=d^2$. That is $d_{1-r}+d_{3-r}+d_{5-r}+d_{7-r}+\cdots=d$. So $d_j=0$ for $\forall_j$ odd. But $d_r\neq 0$ by r is odd. So we get a contradiction. □

Lemma 9: Suppose that (q,p) *is a proper rational solution of (2.6) with trivial Stokes matrices. Then* $q=0$.

Proof: By (4.3), we prove this lemma by showing that $f_1=0$ in (5.1). Again the system (5.2) is divided into two groups by noting that $C_i=0$, for odd i. The group for $f_1, f_3,\ldots, f_{r-1}$ is

$$f_{r-1}V_{2-r}=0,$$

$$(f_{r-1}C_2+f_{r-3})V_{4-r}=0,$$

$$\vdots$$

$$(f_{r-1}C_{r-2}+f_{r-3}C_{r-4}+\cdots+f_1)V_0=0,$$

$$(f_{r-1}C_r+f_{r-3}C_{r-2}+\cdots+f_1C_2)V_2=0,$$

$$\vdots$$

$$(f_{r-1}C_{r+s-2}+\cdots+f_1C_s)V_s=0, \text{ if } s \text{ is even},$$

$$\{\text{or}(f_{r-1}C_{r+s-3}+\cdots+f_1C_{s-1})V_{s-1}=0, \text{ if } s \text{ is odd.}\}$$

Since the constant term in the above system is absent. Lemma 7 implies that all of the odd terms $f_1, f_3,\ldots, f_{r-1}$ vanish. □

Theorem 5: *Proper rational self-similar ZS-AKNS flows satisfying (2.3) with trivial Stokes matrices are self-similar ZS-AKNS flows satisfying (1.1).*

Proof: Suppose (q,p) is a proper rational self-similar ZS-AKNS flow satisfying (2.3), or equivalently, (2.6). By Lemma 9, we get $q=0$. Applying Theorem 1, Lemma 1 and Definition 2, we obtain

$$\frac{\partial\Phi}{\partial x}=[z^2J+P(x,t)]\Phi, \tag{5.4.1}$$

$$\frac{\partial\Phi}{\partial t}=[\mu z^{2n}+\mathcal{F}_1z^{2n-1}+\cdots+\mathcal{F}_{2n}]\Phi, \tag{5.4.2}$$

with

$$P(x,1)=p(x),\ \ \lambda^{-2}P(\lambda^{-2}x,\lambda^{-2n}t)=P(x,t), \tag{5.5}$$

$$M\mu M^{-1}\sim\mu+\frac{\mathcal{F}_1}{z}+\frac{\mathcal{F}_2}{z^2}+\cdots,\ \ M(x,1)=m(x), \tag{5.6}$$

and m is defined by (5.1). The proof of Lemma 9 implies $f_1, f_3,\ldots$ vanish. Hence $\mathcal{F}_{2j-1}\equiv 0$ and (5.4) is reduced to

$$\begin{aligned}\frac{\partial\Upsilon}{\partial x}(x,\zeta,t)&=[\zeta J+P(x,t)]\Upsilon(x,\zeta,t),\\ \frac{\partial\Upsilon}{\partial t}(x,\zeta,t)&=[\zeta^n\mu+\zeta^{n-1}\tilde{\mathcal{F}}_1+\cdots+\tilde{\mathcal{F}}_n]\Upsilon(x,\zeta,t),\end{aligned} \tag{5.7}$$

with $\tilde{M}(x,\zeta,t)e^{x\zeta J}=M(x,z^2,t)e^{xz^2J}$, a formal solution to (5.7), $\tilde{M}\mu\tilde{M}^{-1}(x,\zeta,t)\sim\mu+\tilde{\mathcal{F}}_1/\zeta+\tilde{\mathcal{F}}_2/\zeta^2+\ldots$, and $\mathcal{F}_{2j}(x,t)=\tilde{\mathcal{F}}_j(x,t)$. We then finish the proof by (5.5) and [(8.4),BS]. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Multi-Lagrangians, hereditary operators and Lax pairs for the Korteweg–de Vries positive and negative hierarchies

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(Received 21 June 2002; accepted 23 June 2003)

We present an approach to the construction of action principles (the inverse problem of the calculus of variations), for first order (in time derivatives) differential equations, and generalize it to field theory in order to construct systematically, for integrable equations which are based on the existence of a Nijenhuis (or hereditary) operator, a (multi-Lagrangian) ladder of action principles which is complementary to the well-known multi-Hamiltonian formulation. We work out results for the Korteweg–de Vries (KdV) equation, which is a member of the positive hierarchy related to a hereditary operator. Three negative hierarchies of (negative) evolution equations are defined naturally from the hereditary operator as well, in a concise way, suitable for field theory. The Euler–Lagrange equations arising from the action principles are equivalent to deformations of the original evolution equation, and the deformations are obtained explicitly in terms of the positive and negative evolution vectors. We recognize, after appropriate coordinate transformations, the Liouville, Sinh–Gordon, Hunter–Zheng, and Camassa–Holm equations as negative evolution equations. The multi-Lagrangian ladder for KdV is directly mappable to a ladder for any of these negative equations and other positive evolution equations (e.g., the Harry–Dym and a special case of the Krichever–Novikov equations). For example, several nonequivalent, nonlocal time-reparametrization invariant action principles for KdV are constructed, and a new nonlocal action principle for the deformed system Sinh–Gordon+spatial translation vector is presented. Local and nonlocal Hamiltonian operators are obtained in factorized form as the inverses of all the nonequivalent symplectic two-forms in the ladder. Alternative Lax pairs for all negative evolution vectors are constructed, using the negative vectors and the hereditary operator as only input. This result leads us to conclude that, basically, all positive and negative evolution equations in the hierarchies share the same infinite-dimensional sets of local and nonlocal constants of the motion for KdV, which are explicitly obtained using symmetries and the local and nonlocal action principles for KdV. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1609035]

I. INTRODUCTION

Hereditary or Nijenhuis operators[1–3] play an important role in the description of integrable systems: in terms of these operators, the very definition of the positive and negative hierarchies of

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integrable evolution equations may be given,[4] and they are used to construct, for these equations, symmetries,[4,5] constants of the motion,[5] alternative Lax pairs (Ref. 16), multi-Hamiltonian structures[6] and weakly nonlocal multisymplectic and multi-Hamiltonian structures.[7–9]

The problem of constructing multi-Lagrangian structures (i.e., an infinite ladder of action principles) for the Korteweg–de Vries (KdV) equation has been tackled recently[10,11] in the context of localizable multi-Lagrangian structures, using the bi–Hamiltonian formulation. However, the explicit expression of the action principles associated to each symplectic two-form requires the integration of the respective two-forms, a task which is increasingly difficult as we move to the positive end of the ladder, because of the increasing complexity of the differential terms of the (weakly-nonlocal[9]) two-forms. On the other hand, the symplectic two-forms are increasingly nonlocal as we move to the negative end of the ladder. The known way[11,12] to get rid of the nonlocality problem is to write the action principles in a ''local'' coordinate system (Darboux coordinates) depending on the specific symplectic two-form in the ladder, a process that gets recurrently harder as we move to the negative end. Then, again, the two-form must be integrated by hand in order to get the action principle.

In this work, we make use of the Galilean symmetry[13] and the factorized form of the hereditary operator[14] for the KdV equation, to construct explicitly the action principles for KdV in the positive and negative parts of the ladder. No integration of any two-form is needed, nor is the search for a special coordinate system. The factorized form of the symplectic two-forms allows for the interpretation of the resulting Euler–Lagrange equations (arising from each action principle) as deformed equations, with flows given by KdV+vectors in the positive and negative hierarchies, which are computed explicitly.

Explicit expressions for local and nonlocal constants of the motion for KdV are obtained using symmetries along with the local and nonlocal action principles.

From the action principles obtained for the KdV equation we construct action principles for flows defined by other positive and negative vectors. In particular, a new nonlocal action principle for the Sinh–Gordon (ShG) equation[15] (a negative equation) are constructed.

It is a known result[16] that alternative Lax pairs for the KdV equation and for positive KdV flows may be constructed from the hereditary operator. Here we do the same construction for all the negative KdV flows, and we conclude that the local and nonlocal constants of the motion for KdV, define conserved currents and constants of the motion for all the negative flows as well.

The results here may be mapped to the following equations: a special case of Krichever–Novikov,[17,8] Harry–Dym,[18] Camassa–Holm,[19] Hunter–Zheng,[20] ShG[15] and Liouville, all of which are essentially flows belonging to the KdV positive or negative hierarchies. We stress that the results are quite general and may be extended to other systems related to hereditary operators (e.g., nonlinear Schrödinger equation).

This paper is organized as follows: Section II presents a preview and notation for the method of construction of action principles for given differential evolution equations, and a brief survey of symmetries and constants of the motion in this context. Next, we show the relationship of these principles with Hamiltonian theories, and finally we introduce the hereditary property with the consequent construction of the positive and negative hierarchies of integrable evolution equations. In Sec. III we present and prove theorems on the explicit construction of ladders of action principles and constants of the motion, based on the hereditary operator and the Galilean symmetry (whose definition is quite general and not restricted to KdV), and we show how these action principles give rise to Euler–Lagrange equations which are deformations of the original equations, due to the fact that the symplectic operators have a nonzero kernel.

Section IV is devoted to examples of the above constructions for the KdV equation. We obtain concise expressions for the negative vectors, for the action principles, and for the deformed Euler–Lagrange equations. Symplectic operators are presented in factorized form (this allows for factorized expressions for the Hamiltonian operators). Some known integrable evolution equations are identified within the negative hierarchies. Nonlocal constants of the motion for KdV are concisely obtained using the internal symmetries and the negative action principles. In Sec. V we work out examples of new nonlocal action principles for the ShG equation, which in this context

is identified as a negative vector; we construct Lax pairs for the negative equations, thus showing that the local and nonlocal constants of the motion for KdV also work for negative equations. Finally, some concluding remarks are presented in Sec. VI.

For simplicity, we work in finite-dimensional notation. All assertions and theorems in Secs. II and III are valid in finite dimensions, and they can be extended to the case of field theory in all the instances dealt with in this paper. We have used a Mathematica code of our invention, to confirm the validity of some of the obtained local and nonlocal action principles, symmetries and constants of the motion for KdV and related equations.

II. PREVIEW AND NOTATION

Consider the autonomous equations of motion

$$\dot{q}^a(t)=V^a[q^b(t)], \quad a\in A. \tag{1}$$

A is a given ordered set called ''label set:'' the elements of it label the degrees of freedom of the theory. From now on, we suppress the dependence of the coordinates $\{q^a\}_{a\in A}$ on time when it is obvious.

Example 1: The KdV Equation for the field $u(x,t)$, $x\in[x_-,x_+]$, $t\in\mathbb{R}$, is

$$u_t=-u_{xxx}-12\,u\,u_x \tag{2}$$

(suffixes denote partial differentiation). The label set is $A=[x_-,x_+]$, and $x\in A$ is a continuous index.

We will use standard boundary conditions for the field: $u, u_x, \cdots\to 0$ as $x\to x_\pm$, and we will set $x_\pm=\pm\infty$, although the methods may be extended for the treatment of other boundary conditions as well (in which case the Weiss action principle[21] and the Witten–Zuckerman two-form[22] come into play).

The evolution equation (1) is naturally defined on a vector space spanned by the derivatives $\{\partial/\partial q^a\}_{a\in A}$ (for the infinite-dimensional case, partial derivatives with respect to the coordinates become functional derivatives). We call $V=V^a(\partial/\partial q^a)$ the flow vector or evolution vector for the system (1), where here, and throughout this paper, Einstein summation convention over repeated indices is assumed (for the infinite-dimensional case, the summation is extended to an integration over continuous indices).

A. Action principles

The equations of motion (1) are related to a variational principle with action

$$S[q^a(t),t]=\int_{t_-}^{t_+}\mathrm{d}t\,(P_a(\dot{q}^a-V^a)+K), \tag{3}$$

where the one-form $P[q^b]$ and the zero-form $K[q^b]$ satisfy the following equation:

$$P_{a,b}V^b+P_bV^b_{,a}=K_{,a},$$

with $K_{,a}\equiv\partial K/\partial q^a$.

We rewrite the above equation in terms of invariant structures:

$$\underset{V}{\mathcal{L}}P=\delta K, \tag{4}$$

where $\mathcal{L}_V$ is the Lie derivative along the vector V, and δ is the exterior differential (see Ref. 23 for a definition of these operators).

Definition 2: We call the pair $(P;K)$ a standard Lagrangian pair for V if $K\neq 0$. In the special case $K=0$ we call P a nonstandard Lagrangian (one-form) for V: the latter case allows for the construction of constants of the motion in a direct way[24] (see Theorem 9).

Remark 3: The above objects should not be confused with the usual "Lagrangian density" $L[q,\dot{q},t]=P_a(\dot{q}^a-V^a)+K$, which is the thing that is integrated in time to give the action: $S=\int L\,\mathrm{d}t$. The one-form P is also understood as a momentum map.[11] When P is a nonstandard Lagrangian, it solves the equation for a "conserved covariant."[5]

The general case of objects which depend explicitly on time is easily worked out,[25] but there is no need to do so in the applications of this paper. Nevertheless, for symmetries and constants of the motion the explicit time dependence will be necessarily taken into account. In the sequel, we give the name "time-(in)dependent" to those objects which do (not) depend explicitly on time.

The Euler–Lagrange equations which come from the action (3) are

$$\Sigma_{ab}(\dot{q}^b-V^b)=0,$$

where $\Sigma\equiv\delta P$ is the symplectic two-form or Lagrange bracket whose components are

$$\Sigma_{ab}=P_{b,a}-P_{a,b}.$$

It is worth mentioning that, in Ref. 22, a symplectic two-form is induced by an action principle in essentially the same way we have derived the above symplectic two-form from the action principle (3).

Notice that these Euler–Lagrange equations do not imply the original equations of motion (1); instead they imply deformed or mixed equations, where the deformation is represented by an additive extra term which is an arbitrary linear combination of vectors belonging to the kernel of the symplectic two-form. In the case of KdV, we will obtain the deformations explicitly. See Ref. 24 for examples in the finite-dimensional case.

The symplectic two-form associated to this action principle is easily shown to satisfy

$$\begin{aligned}\delta\Sigma&=0\ (\text{closure}),\\ \underset{V}{\mathcal{L}}\Sigma&=0,\end{aligned}\tag{5}$$

therefore the inverse process could be done: starting from a symplectic two-form Σ for the flow vector V, we construct the standard Lagrangian one-form, from $\delta P=\Sigma$ and the 0-form K is obtained by integration of Eq. (4). This process suffers from technical difficulties, which increase when the objects are infinite dimensional and nonlocal. Fortunately, for the KdV equation there is a constructive way of finding the action principles (see Theorems 6 and 7).

B. Hamiltonian theories are induced from symplectic structures

The relationship of the symplectic two-form with the Hamiltonian formulation is very simple:[26] consider the formal inverse (i.e., except for a finite kernel that the operators may possess) of the above two-form, the time-independent (2,0) tensor J such that $J\cdot\Sigma=\mathbb{I}$. It is possible to show that Σ is closed if and only if J satisfies the Jacobi identity, which we write in the form

$$\underset{J\cdot U}{\mathcal{L}}\,J=J\cdot\delta U\cdot J,\quad\forall\ \text{one-form}\ U.\tag{6}$$

J is known as a Hamiltonian operator or Poisson bracket. Now, Eq. (5) implies $\mathcal{L}_V J=0$. Therefore, according to the Jacobi identity (6), a Hamiltonian theory for the flow V is induced by the symplectic two-form Σ: the equation $V=J\cdot U$ implies $\delta U=0$, thus $V=J\cdot\delta H$, where H is the Hamiltonian, a time-independent 0-form.

C. Symmetries

Symmetries play a crucial role in the construction of the action principles. A symmetry for the system (1) is known as a vector with components η^a that takes solutions into solutions of Eq. (1), in the sense that given any solution $q^a(t)$ such that $\dot{q}^a(t)=V^a[q^b(t)]$, then $\tilde{q}^a \equiv q^a+\epsilon\,\eta^a[q^b,t]$ is also a solution up to order ϵ^2, i.e., $\dot{\tilde{q}}^a(t)=V^a[\tilde{q}^b(t)]+O(\epsilon^2)$.

It is easily seen[27] that this condition leads to the equation $(\partial/\partial t)\,\eta^a+\eta^a_{,b}\,V^b-V^a_{,b}\,\eta^b=0$ or, in a covariant way $[(\partial/\partial t)+\mathcal{L}_V]\,\eta=0$.

Example 4: The Galilean and the dilatation symmetries for the KdV equation are defined, respectively, by

$$\eta_G[u,t]^x=\tfrac{1}{8}-\tfrac{3}{2}t\,u_x,$$
$$\eta_D[u,t]^x=u+\tfrac{1}{2}x\,u_x-t(\tfrac{3}{2}u_{xxx}+18\,u\,u_x). \tag{7}$$

In Ref. 13, there is an open question concerning the role of the Galilean and dilatation symmetries in the construction of constants of the motion for KdV. An answer to this question is given in this work: these symmetries actually lead to action principles for the KdV equation, which are involved in Noetherian and non-Noetherian constructions[27] of constants of the motion (see Theorems 6, 7, and 9).

D. Constants of the motion

A constant of the motion for the system (1) is a functional (0-form) $C[q^a,t]$ which is conserved in time under the evolutionary system: $(D/Dt)\,C[q^b,t]\big|_{\text{on-shell}}\equiv(\partial/\partial t)\,C+C_{,\,a}\,V^a=0$, where the partial time derivative accounts for the explicit time dependence and D/Dt denotes the convective or total derivative along the variable t.

This equation is best written in a covariant way:[27] $[(\partial/\partial t)+\mathcal{L}_V]C=0$.

We will usually work with time-independent constants of the motion: $(\partial/\partial t)\,C=\mathcal{L}_V C=0$.

E. The Hereditary property: Hierarchies of evolution equations

Many integrable systems are related to a Nijenhuis or hereditary operator, which is a time-independent (1,1) tensor R that solves:[26] $\mathcal{L}_{R\cdot\eta}R=R\cdot\mathcal{L}_\eta R$, $\forall$ vector η.

Out of the kernel of this operator, and of its inverse, hierarchies of integrable evolution equations arise which are symmetries of each other[4] (this will be worked out in detail for the KdV case later on).

According to Ref. 4, given a hereditary operator R and a flow vector field (labeled with a number) V_1 such that $\mathcal{L}_{V_1}R=0$, i.e., R is a recursion operator for V_1, then a hierarchy is defined as a semi-infinite collection of evolution vectors: $\{V_j=R^{j-1}\cdot V_1, j=1,\ldots,\infty\}$, which are symmetries of each other: $\mathcal{L}_{V_i}V_j=0$, $i,j\geqslant 1$, and thus every evolution vector in the hierarchy defines an evolution equation which is integrable. In the KdV hierarchy, the KdV equation is the second member (V_2). The first vector (V_1) represents the translation symmetry, and it is shown to generate the kernel of the inverse hereditary operator, R^{-1}. By convention, we refer to the above as a positive hierarchy.

The hereditary property for the operator R may be used to show formally that R^{-1} is also hereditary.[14] Therefore, we could conjecture that new hierarchies (referred to as negative hierarchies) of evolution vectors may be constructed, which first members generate the kernel of the operator R, and successive members are defined by contraction of the first members with powers of the operator R^{-1}. In the KdV case, there are three negative hierarchies. These new negative equations include the ShG, Liouville, Camassa–Holm, and the Hunter–Zheng equations.

F. Notation: The positive and negative hierarchies in terms of the hereditary operators

The analysis is restricted to the KdV hierarchies, but it is easily generalizable to other systems related to hereditary operators.

We will adopt the following notation for evolution vectors in the hierarchies:

$$u_t = V_n^{(k)}[u],$$

where $k=1$ denotes the positive hierarchy; $k=-1,-2,-3$ for the three negative hierarchies, and $n=1,\ldots,\infty$ denotes the place of a vector within the hierarchy, so that we have $n=1$ for the first vector of each hierarchy, i.e., the relevant generator of the kernel of $R^{-\mathrm{sgn}(k)}$:

$$R^{-1}[u]\cdot V_1^{(1)}[u]=0,$$

$$R[u]\cdot V_1^{(-1)}[u]=R[u]\cdot V_1^{(-2)}[u]=R[u]\cdot V_1^{(-3)}[u]=0. \tag{8}$$

Successive members in the hierarchies are defined by recurrence:

$$V_{n+1}^{(k)}[u]=(R[u])^{\mathrm{sgn}(k)}\cdot V_n^{(k)}[u], \quad n\geqslant 1, \quad k=1,-1,-2,-3.$$

In this way, the positive hierarchy begins with the vector $V_1^{(1)}[u]=-u_x$, continues with the KdV vector $V_2^{(1)}[u]=-u_{xxx}-12\,u\,u_x$, and so on (these vectors were called V_1 and V_2 in the preceding subsection).

For the negative hierarchy, as the operator R^{-1} is harder to work with, there is a recurrent way of writing the negative vectors, in terms of R:

$$V_n^{(k)}[u]=R[u]\cdot V_{n+1}^{(k)}[u], \quad n\geqslant 1, \quad k=-1,-2,-3. \tag{9}$$

The explicit expression for negative vectors relies on the factorized form[14,28] of the hereditary operator, and will be realized in Sec. IV in terms of nonlocal fields which, however, are tractable in the same scheme as the local ones.

III. LADDERS OF ACTION PRINCIPLES AND CONSTANTS OF THE MOTION

Complementary to the well-known bi-Hamiltonian formulation,[4] we may find a bi-symplectic or multisymplectic structure starting from the hereditary property. Assume that we have a Nijenhuis operator R along with one closed two-form $\Sigma^{(1)}$ such that $\Sigma^{(2)}\equiv\Sigma^{(1)}\cdot R$ be a closed two-form: then, the two semi-infinite dimensional sets (symplectic ladders) of two-forms

$$\{\Sigma^{(n)}\equiv\Sigma^{(1)}\cdot R^{n-1}, \quad n=1,\ldots,\infty\} \quad (\text{positive symplectic ladder})$$

and

$$\{\Sigma^{(n)}\equiv\Sigma^{(1)}\cdot R^{n-1}, \quad n=0,-1,\ldots,-\infty\} \quad (\text{negative symplectic ladder}),$$

contain only closed two-forms. The distinction between positive and negative ladders is somewhat arbitrary, for it depends on which hereditary operator, R or R^{-1}, is being used, and which symplectic two-form is taken as $\Sigma^{(1)}$.

The proof of the above statement is very simple. In fact, it is equivalent to the proof for the so-called Poisson pencil or set of compatible implectic operators[4] for multi-Hamiltonian theories, after defining the implectic or Hamiltonian operators as the inverses of the two-forms in the ladder.

The above result is independent of any evolution vector. When we consider the vectors in the hierarchies, however, it is easily checked (as it holds in the examples) that $\mathcal{L}_{V_1}\Sigma^{(1)}=0$. Therefore, using Leibnitz rule, all the two-forms in the ladder are symplectic operators for the first evolution vector in the hierarchy.

Using the identity $\mathcal{L}_{R\cdot\eta}\Sigma-\mathcal{L}_{\eta}(\Sigma\cdot R)=i_{R\cdot\eta}\delta\Sigma-i_{\eta}\delta(\Sigma\cdot R)$, which holds for any vector η, (1,1) tensor R and two-form Σ, where i_{η} stands for interior product (contraction of the vector η with the left component of a p-form), we obtain the important result for any hierarchy:

$$\underset{V_j}{\mathcal{L}}\Sigma^{(n)}=0, \quad j=1,2,\ldots,\infty, \quad n=-\infty,\ldots,\infty, \tag{10}$$

which means that a ladder of action principles may be constructed for every evolution vector in the hierarchy (in particular, for the KdV equation).

This fact is used in Ref. 11 to construct action principles, with the only drawback it needs to integrate the two-forms (Poincaré lemma) in order to get the action principles.

Let us assume for the rest of this section that we have a Nijenhuis operator R along with its inverse R^{-1}, a symplectic ladder $\{\Sigma^{(n)},n=-\infty,\ldots,\infty\}$, and a hierarchy $\{V_j,j=1,\ldots,\infty\}$ with the corresponding properties mentioned above.

The purpose of the following section is to construct, for the second evolution vector in the positive hierarchy (though the analysis is easily extended for other positive and negative evolution vectors), the action principles associated to each of the above symplectic two-forms. These action principles are involved in the explicit construction of constants of the motion for the evolution equation.

A. Construction of action principles and constants of the motion out of symmetries and symplectic operators

Heuristically, if we had a symmetry for a given evolution equation we could obtain in a direct way (by contraction of it with any symplectic two-form) a Lagrangian one-form and therefore an action principle for that equation.

We have done this procedure for any equation in the positive hierarchy, using the Galilean symmetry, obtaining as a result a ladder of action principles which are (explicitly) time-dependent (in fact, linear in time). For simplicity, however, we rewrite the actions as time-independent objects, and the discussion will be restricted to the second vector (which corresponds to the KdV equation), which is from now on referred to as the vector V_2.

The following definition will be a key to the construction of the ladder of action principles for the evolution vector V_2, and it permits a generalization to the negative hierarchies as well as to other systems (e.g., nonlinear Schrödinger equation).

Definition 5: The Galilean vector field η_{gal} is a time-independent vector field, defined by three properties,

$$\begin{aligned}
&\underset{\eta_{\mathrm{gal}}}{\mathcal{L}}R=\mathbb{I},\\
&\underset{\eta_{\mathrm{gal}}}{\mathcal{L}}\Sigma^{(1)}=0,\\
&\underset{\eta_{\mathrm{gal}}}{\mathcal{L}}V_2=\alpha V_1,
\end{aligned} \tag{11}$$

where α is a numeric constant.

As a consequence of the definition, it turns out that η_{gal} is a Mastersymmetry[29] for the hierarchy $\{V_j,\ j=1,\ldots,\infty\}$. Explicitly, we have $\mathcal{L}_{V_{j+1}}\eta_{\mathrm{gal}}=(\alpha+j-1)\,V_j$, for $j=1,\ldots,\infty$.

The aim is to construct time-independent standard Lagrangian pairs $(P;K)$, where $\mathcal{L}_{V_2}P=\delta K$. The action principles will read $S[q^a(t)]=\int_{t_-}^{t_+}\mathrm{d}t\,(P_a(\dot{q}^a-V_2^a)+K)$, and the Euler–Lagrange equations will involve the symplectic two-forms in the ladder, i.e., $\delta P=\Sigma$.

Theorem 6: *The one-forms defined by* $P^{(m)}\equiv i_{\eta_{\mathrm{gal}}}\Sigma^{(m+1)}$, *for* $m=-\infty,\ldots,\infty$ *are "integrals" of the symplectic two-forms in the ladder. That is to say,*

$$\delta P^{(m)} = m\,\Sigma^{(m)}, \quad m = -\infty, \ \ldots, \infty. \tag{12}$$

Proof: If we take the exterior derivatives of the one-forms, using the identity

$$\underset{\eta}{\mathcal{L}} = i_\eta\,\delta + \delta\, i_\eta, \tag{13}$$

which holds (for every vector η) when operating on any p-form, we find

$$\delta P^{(m)} = \underset{\eta_{\mathrm{gal}}}{\mathcal{L}}\,\Sigma^{(m+1)} = \underset{\eta_{\mathrm{gal}}}{\mathcal{L}}\,(\Sigma^{(1)}\cdot R^m) = \Sigma^{(1)}\cdot \underset{\eta_{\mathrm{gal}}}{\mathcal{L}}\,(R^m) = m\,\Sigma^{(1)}\cdot R^{m-1} = m\,\Sigma^{(m)}, \quad m \in \mathbb{Z}$$

after using the definition of Galilean vector and Leibnitz rule. □

In order to complete the action principles, there remains to find the second members of the corresponding standard Lagrangian pairs.

Theorem 7: *For each $m \in \mathbb{Z}$, the pair $(P^{(m)};K^{(m)})$ with $K^{(m)} \equiv \alpha/(m+\alpha)\, i_{V_2} P^{(m)}$, is a standard Lagrangian pair for the evolution equation $\dot{q}^a = V_2^a$,* i.e., *$\mathcal{L}_{V_2} P^{(m)} = \delta K^{(m)}$. For $m \neq 0$, the action principle is*

$$S^{(m)}[q^a(t)] = \int_{t_-}^{t_+} P^{(m)}{}_a \left(\dot{q}^a - \frac{m}{m+\alpha} V_2^a \right) \mathrm{d}t. \tag{14}$$

Moreover, the 0-forms $K^{(m)}$ are constants of the motion for the evolution equation, for $m \in \mathbb{Z}$:

$$\underset{V_2}{\mathcal{L}} K^{(m)} = 0.$$

The above is a Noetherian way to construct constants of the motion, for all the action principles in the ladder for KdV are naturally invariant under the KdV flow V_2 itself [see Eq. (10)].

Remark 8: The case $m = 0$ would lead to a trivial action principle from Eq. (14), for the Euler–Lagrange equations are identically zero: it is shown that this case leads to a time-dependent constant of the motion. This does not mean that the symplectic two-form $\Sigma^{(0)}$ defines a trivial action principle. In fact, its associated action principle may be found by hand (see the end of this section), and it is related to the usual action principle for the ShG equation (see Sec. V B).

Proof: Lagrangian pairs. For $m \in \mathbb{Z}$, take Lie derivatives of the one-forms $P^{(m)}$ along the evolution vector V_2, using Leibnitz rule:

$$\underset{V_2}{\mathcal{L}} P^{(m)} = \underset{V_2}{\mathcal{L}}\, i_{\eta_{\mathrm{gal}}} \Sigma^{(m+1)} = -\alpha\, i_{V_1} \Sigma^{(m+1)} = -\alpha\, i_{V_2} \Sigma^{(m)}. \tag{15}$$

But, using the identity (13) and the result (12) we rewrite the last expression to get

$$m \underset{V_2}{\mathcal{L}} P^{(m)} = -\alpha \left(\underset{V_2}{\mathcal{L}} P^{(m)} - \delta\, i_{V_2} P^{(m)} \right),$$

therefore

$$\underset{V_2}{\mathcal{L}} P^{(m)} = \delta \left(\frac{\alpha}{m+\alpha}\, i_{V_2} P^{(m)} \right) \equiv \delta K^{(m)}. \tag{16}$$

Proof: Constants of the motion. We use the above result (16), to find

$$\frac{m+\alpha}{\alpha} \underset{V_2}{\mathcal{L}} K^{(m)} = i_{V_2} \underset{V_2}{\mathcal{L}} P^{(m)} = i_{V_2} \delta K^{(m)} = \underset{V_2}{\mathcal{L}} K^{(m)},$$

which implies $\mathcal{L}_{V_2}K^{(m)}=0,\ m\neq 0$.

For $m=0$ we find a weaker result: Equation (15) implies $\delta\mathcal{L}_{V_2}K^{(0)}=0$. Therefore $\mathcal{L}_{V_2}K^{(0)}=c$, is a number (usually equal to zero) that may be absorbed to define a time-dependent constant of the motion: $\tilde{K}^{(0)}(t)=K^{(0)}-c\,t$. □

For the KdV equation, when $m\geqslant -1$ we get the usual denumerably infinite set of constants of the motion.[30] Notice that this theorem represents also a constructive method to obtain such constants. On the other hand, when $m\leqslant -2$ the constants are numerical or vanishing boundary terms. Amazingly, this fact allows one to construct an infinite number of nonlocal constants of the motion for KdV, using the nonlocal action principles (see Sec. III C).

Proof: Action principles. The action principles (14) arise directly from Eq. (3), using the definition of $K^{(m)}$. □

From the point of view of Theorem 7, the case $m=0$ also leads to a time-dependent constant of the motion. From Eq. (12), it follows that $P^{(0)}=\delta C^{(0)}$, and thus $\mathcal{L}_{V_2}C^{(0)}=K^{(0)}$. But we know that $\mathcal{L}_{V_2}K^{(0)}=c$ is a number. We obtain the following time-dependent constant of the motion for the evolution vector V_2:

$$C[q^a(t),t]=C^{(0)}-t\,K^{(0)}+\frac{c\,t^2}{2}. \tag{17}$$

Finally, for the case $m=0$, a special (''missing'') action principle is constructed by hand from integration of the two-form $\Sigma^{(0)}$, which leads to the one-form $P^{(M)}$, such that $\delta P^{(M)}=\Sigma^{(0)}$. We will have $\mathcal{L}_{V_2}P^{(M)}=\delta K^{(M)}$, and the action is

$$S^{(0)}[q^a(t)]=\int_{t_-}^{t_+}(P_a^{(M)}(\dot{q}^a-V_2^a)+K^{(M)})\,\mathrm{d}t.$$

B. The Euler–Lagrange equations as deformed evolution equations

The Euler–Lagrange equations that arise from variation of each action $S^{(m)}$, $m\in\mathbb{Z}$ are, apart from nonzero numeric factors,

$$\Sigma_{ab}^{(m)}(\dot{q}^b-V_2^b)=0,\quad m\in\mathbb{Z}.$$

The kernel of the symplectic operators, $\mathrm{Ker}\,\Sigma^{(m)}$, is of importance here. For each action principle we obtain an equivalent, deformed, evolution equation

$$\dot{q}^a=V_2^a+\sum_{j=1}^{N_m}\theta_j\,\eta_{j;m}^a,$$

where $N_m=\dim(\mathrm{Ker}\,\Sigma^{(m)})$, the vectors $\{\eta_{j;m}\}_{j=1}^{N_m}$ generate the kernel of $\Sigma^{(m)}$, and $\theta_j=\theta_j(t)$ are arbitrary 0-forms: it can be said that these Euler–Lagrange equations and the action principles acquire extra symmetries (as compared to the symmetries of the original equations).

As the two-forms here are formed by contraction of powers of the hereditary operators R and R^{-1} with $\Sigma^{(1)}$, it is clear that the kernel of the two-forms are computed essentially from vectors in the kernel of the operators R^m and R^{-m}, for $m>0$: as we have mentioned, these are the positive and negative evolution vectors. In Sec. IV, we will find explicitly the deformed equations for the KdV equation in terms of the positive and negative vectors.

C. Construction of nonlocal constants of the motion from symmetries and nonstandard Lagrangian one-forms

Let us assume, as it will be demonstrated in Sec. IV H for the KdV case (under usual boundary conditions), that the constants of the motion from Theorem 7 are $K^{(m)}=0$ or a numeric constant

for $m\leqslant -2$. This implies that $\mathcal{L}_{V_2}P^{(m)}=0$, i.e., $P^{(m)}$ is a nonstandard Lagrangian one-form for the flow V_2. Assume also that the evolution equation defined by the flow V_2 possesses a symmetry η. Then

Theorem 9: *The* 0*-forms defined by* $Q^{(m)}\equiv i_\eta P^{(m)}$, *for* $m\leqslant -2$, *are constants of the motion for the flow* V_2, *i.e.,* $(\partial_t+\mathcal{L}_{V_2})Q^{(m)}=0$ *for* $m\leqslant -2$.

Proof: The proof follows directly from Leibnitz rule. □

The above is a non-Noetherian way[27] to construct constants of the motion, in the sense that the action principles need not be invariant under the relevant symmetry. In Sec. IV J we construct ''generating functions'' for three infinite-dimensional sets of nonlocal constants of the motion for the KdV equation, setting η as a nonlocal internal symmetry for KdV.

IV. EXAMPLE: THE KDV EQUATION

A. Known objects

We begin by presenting the Nijenhuis operator relevant for the KdV hierarchy: as an operator,[4] $R[u]=\mathrm{D}^2+8\,u+4\,u_x\,\mathrm{D}^{-1}$, where D and D^{-1} are, respectively, the derivative and the antiderivative operators: $\mathrm{D}f(x)\equiv \partial f(x)/\partial x$, $\mathrm{D}^{-1}g(x)\equiv\int_{x_-}^{x_+}\epsilon(x-x')\,g(x')\,\mathrm{d}x'$, with $\epsilon(x-x')=1/2\,\mathrm{sign}(x-x')$.

Next, the positive hierarchy begins with the vector $V_1^{(1)}[u]=-u_x$. The second vector in the positive hierarchy is obtained after application of the Nijenhuis operator on the latter vector: $V_2^{(1)}[u]=R[u]\cdot V_1^{(1)}[u]=-u_{xxx}-12\,u\,u_x\equiv V_2[u]$. We see it represents the KdV equation (2).

Next, we write the first symplectic two-form: as an operator,[4] $\Sigma^{(1)}[u]=\mathrm{D}^{-1}$. The second symplectic operator is constructed just by contracting the latter operator with the Nijenhuis operator: $\Sigma^{(2)}[u]=\Sigma^{(1)}[u]\cdot R[u]=\mathrm{D}+4\,u\,\mathrm{D}^{-1}+4\,\mathrm{D}^{-1}u$. These operators are closed under usual boundary conditions for the vector fields: the ladder, then, contains only closed two-forms. Now, it is easy to show that these operators are symplectic for the flow defined by $V_1^{(1)}$, therefore all operators in the ladder are symplectic for the KdV flow $V_2^{(1)}$, as it is stated in Eq. (10).

Finally, the Galilean vector is just the time-independent part of the Galilean symmetry (7): $\eta_{\mathrm{gal}}[u]=\frac{1}{8}$, and the constant in the last of the defining equations (11) is $\alpha=3/2$.

B. Explicit form of the KdV negative hierarchies: Linear generalization and factorization of the hereditary operator

In order to find explicitly the KdV negative hierarchies, we factorize a generalization of the hereditary operator R, which is obtained by addition of a multiple of the identity tensor $\mathbb{I}$:

$$R(\lambda)[u]\equiv R[u]+4\,\lambda\,\mathbb{I}.$$

This is also a hereditary operator, for fixed λ, which is taken as an arbitrary real number.

The idea behind this generalization, is that the kernel of $R(\lambda)[u]$ contains all the negative hierarchies in its Taylor expansion around $\lambda=0$, so we will write the negative hierarchies in a compact way.

Lemma 10: The vectors $V_1^{(-1)}(\lambda)[u]$, $V_1^{(-2)}(\lambda)[u]$, $V_1^{(-3)}(\lambda)[u]$, *defined by*

$$V_1^{(k)}(\lambda)[u]\equiv\sum_{n=0}^{\infty}(-4\,\lambda)^n\,V_{n+1}^{(k)}[u],\quad k=-1,-2\,-3$$

generate the vectorial kernel of $R(\lambda)[u]$.

Conversely, all vectors in the negative hierarchies may be obtained from the vectorial kernel of $R(\lambda)[u]$:

$$V_{n+1}^{(k)}[u]=\frac{1}{n!}(-4)^{-n}\frac{\partial^n}{\partial\lambda^n}V_1^{(k)}(\lambda)[u]\bigg|_{\lambda=0},\quad k=-1,-2\,-3,\ \ n=0,1,\ldots,\infty. \tag{18}$$

Proof: Consider the action of $R[u]$ on the vector $V_1^{(k)}(\lambda)[u]$. Using Eqs. (8) and (9), we get

$$R[u]\cdot V_1^{(k)}(\lambda)[u]=\sum_{n=0}^{\infty}(-4\lambda)^n R[u]\cdot V_{n+1}^{(k)}[u]=\sum_{n=1}^{\infty}(-4\lambda)^n V_n^{(k)}[u]=-4\lambda V_1^{(k)}(\lambda)[u],$$

therefore $R(\lambda)[u]\cdot V_1^{(k)}(\lambda)[u]=(R(\lambda)[u]+4\lambda)\cdot V_1^{(k)}(\lambda)[u]=0$. □

The factorization process[28] implies the definition of auxiliary fields, which are directly related to nonlocal prepotentials found in the literature[14] and to the associated isospectral linear eigenvalue problem:[31]

$$\psi_{xx}+2u\psi=-\lambda\psi, \tag{19}$$

where $\psi=\psi(x,t;\lambda)$. As usual, we assume $\lambda_t=0$, and $u=u(x,t)$ is independent of λ.

Alternatively, we write the above equation as $L(\lambda)\cdot\psi=0$, where $L(\lambda)=\mathrm{D}^2+2u+\lambda$ or, in a factorized way, $L(\lambda)=(1/\psi)\,\mathrm{D}\,\psi^2\,\mathrm{D}\,(1/\psi)$, is the Lax operator. The elements in the kernel of this operator are solutions of the linear problem (19). Two linearly independent solutions are $\psi(\lambda)\equiv\psi(x,t;\lambda)$ and

$$\overline{\psi}(\lambda)\equiv\psi(\lambda)\mathrm{D}^{-1}(1/\psi(\lambda)^2). \tag{20}$$

The above eigenvalue problem may be understood as an extended coordinate system labeled by $\psi(x,t;\lambda)$, with λ as an additional variable (just like x), and which however must solve an extra equation, $L(\lambda)\cdot\psi(\lambda)=0$, which we call constraint. This constraint lets us write derivatives of the field $\psi(\lambda)$ with respect to λ in terms of the field itself, in a nonlocal way. This will be useful in the next section, when we write the negative ladder of action principles. We obtain, apart from integration constants,

$$\begin{aligned}\frac{\partial^n}{\partial\lambda^n}\psi&=(-1)^n n!\,L(\lambda)^{-n}\psi,\\ \frac{\partial^n}{\partial\lambda^n}\overline{\psi}&=(-1)^n n!\,L(\lambda)^{-n}\overline{\psi},\quad n\geqslant 1,\end{aligned} \tag{21}$$

where $L(\lambda)^{-1}=\psi\,\mathrm{D}^{-1}\,(1/\psi^2)\,\mathrm{D}^{-1}\,\psi$, $\psi=\psi(\lambda)$ and $\overline{\psi}=\overline{\psi}(\lambda)$.

Now, the factorization of $R(\lambda)[u]$ is found to be

$$R(\lambda)[u]=\frac{1}{\psi(\lambda)^2}\,\mathrm{D}\,\psi(\lambda)^2\,\mathrm{D}\,\psi(\lambda)^2\,\mathrm{D}\frac{1}{\psi(\lambda)^2}\,\mathrm{D}^{-1}.$$

It is remarkable that the above operator is *linear* in λ, which is a consequence of the constraint (19).

The kernel of the operator $R(\lambda)[u]$ is easily found to be composed by three nonlocal vectors:

$$\begin{aligned}u_t&=V_1^{(-1)}(\lambda)[u]=(\psi(\lambda)^2)_x,\\ u_t&=V_1^{(-2)}(\lambda)[u]=(\psi(\lambda)\,\overline{\psi}(\lambda))_x,\\ u_t&=V_1^{(-3)}(\lambda)[u]=(\overline{\psi}(\lambda)^2)_x,\end{aligned} \tag{22}$$

where $\psi(\lambda)$, $\overline{\psi}(\lambda)$ [see Eq. (20)] are two linearly independent solutions of the constraint (19). These vectors contain the whole negative hierarchies if λ is left arbitrary, as lemma 10 states. A discrete infinite-dimensional representation of these negative vectors, as nonlocal symmetries of the KdV equation, is known.[14] On the other hand, the continuous representation (22) of these

vectors, more suitable for field theory, allows for considering them also as possible evolution equations, which will be recognized as known integrable equations in Sec. V A.

C. Explicit form and Kernel of the inverse hereditary operator R^{-1}

The inverse hereditary operator, $R^{-1}(\lambda)$, is found easily after inverting every factor. Assuming appropriate boundary conditions on the field ψ, we get

$$R^{-1}(\lambda)[u]=\mathrm{D}\,\psi(\lambda)^2\,\mathrm{D}^{-1}\frac{1}{\psi(\lambda)^2}\mathrm{D}^{-1}\frac{1}{\psi(\lambda)^2}\mathrm{D}^{-1}\,\psi(\lambda)^2.$$

It is easy to show that the kernel of this operator is generated by the vector $V_1^{(1)}=-u_x$.

D. Factorization of positive and negative symplectic and Hamiltonian operators

Using the factorized form of the hereditary operators, we get easily the symplectic operators in factorized form. For the positive ones, we have

$$\Sigma^{(2)}[u]=\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}\frac{1}{\psi^2}\mathrm{D}^{-1},$$

$$\Sigma^{(3)}[u]=\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}\frac{1}{\psi^2}\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}\frac{1}{\psi^2}\mathrm{D}^{-1},$$

and so on, where $\psi=\psi(\lambda=0)$. Notice that the inverses of these operators give new nonlocal Hamiltonian operators for KdV.

For the negative ones, on the other hand, we have

$$\begin{aligned}\Sigma^{(0)}[u]&=\psi^2\,\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\,\psi^2,\\ \Sigma^{(-1)}[u]&=\psi^2\,\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\frac{1}{\psi^2}\mathrm{D}^{-1}\,\psi^2,\end{aligned}\tag{23}$$

and so on. By the way, the above expression for $\Sigma^{(0)}[u]$ turns out to solve a puzzle in the recent literature,[10] for it is the inverse of Magri's Hamiltonian operator. As we see, we have got all inverses (in factorized form) of all Hamiltonian operators within the multi-Hamiltonian structure for KdV.

There is another, concise way to write these negative operators, which resembles the way we wrote the negative vectors in terms of the λ-dependent first one. We state the lemma without proof.

Lemma 11: The negative symplectic operators for KdV are written in terms of $\Sigma^{(0)}(\lambda)[u]\equiv\Sigma^{(1)}\cdot R^{-1}(\lambda)[u]$ *in the following way:*

$$\Sigma^{(-n)}[u]=\frac{1}{n!}(-4)^{-n}\frac{\partial^n}{\partial\lambda^n}\Sigma^{(0)}(\lambda)[u]\bigg|_{\lambda=0},\quad n\geqslant 1.$$

A similar formula may be written for the nonlocal Hamiltonian operators.

E. Negative vectors as kernel of positive symplectic operators

The kernel spaces $\mathrm{Ker}\,\Sigma^{(n)}[u]$, for $n=1,\ldots,\infty$, are easily computed in terms of the kernel of positive powers of R, from the fact that $\mathrm{Ker}\,\Sigma^{(1)}[u]$ is null. We get

$$\mathrm{Ker}\,\Sigma^{(n+1)}=\mathrm{span}\{V_m^{(k)}[u],\quad k=-1,-2,-3,\ m=1,\ldots,n\},\quad n\geqslant 0.$$

F. Positive vectors as kernel of negative symplectic operators

Finally we compute the kernel spaces $\mathrm{Ker}\,\Sigma^{(n)}[u]$, for $n=0,-1,\ldots,-\infty$. It is easily seen that the operator $\Sigma^{(0)}[u]$ has a null kernel. This time we have to evaluate the kernel of negative powers of R. We get

$$\mathrm{Ker}\,\Sigma^{(-n)}[u]=\mathrm{span}\{V_m^{(1)}[u],\quad m=1,\ldots,n\},\quad n>0,$$

so that, in particular, the action principle associated to $\Sigma^{(-2)}[u]$ for the KdV equation has the translation vector as well as the KdV vector as generators of its kernel, therefore the action has to be time-reparametrization invariant.[24]

G. Action principles for KdV: Positive Lagrangian ladders

Remark 12: If $P_a\,\delta u^a$ denotes a one-form, where $a\equiv x$ is a continuous index, we will write the component P_a of the one-form as $\mathcal{P}(x,t)$ (which looks more like a density) when dealing with it inside an integral sign.

Following Theorems 6 and 7, we write the action principles from Eq. (14):

$$S^{(m)}[u(x,t)]=\int_{t_-}^{t_+}\int_{x_-}^{x_+}\mathcal{P}^{(m)}[u](x,t)\left(u_t+\frac{m}{m+3/2}(u_{xxx}+12\,u\,u_x)\right)\mathrm{d}x\,\mathrm{d}t,\tag{24}$$

for $m>0$, where

$$\mathcal{P}^{(1)}[u](x,t)=i_{\eta_{\mathrm{gal}}}\Sigma^{(2)}[u]=-(\mathrm{D}+4\,u\,\mathrm{D}^{-1}+4\,\mathrm{D}^{-1}\,u)\,\tfrac{1}{8}=-\,\tfrac{1}{2}(x\,u+\mathrm{D}^{-1}(u)),$$

and successive one-forms are defined by recurrence: $\mathcal{P}^{(m+1)}[u](x,t)=R^{\dagger}[u]\cdot\mathcal{P}^{(m)}[u](x,t)$, where $R^{\dagger}[u]$ is the transpose Nijenhuis operator.

The action principle $S^{(1)}[u(x,t)]$ gives rise to the following Euler–Lagrange equations:

$$\mathrm{D}^{-1}(u_t+u_{xxx}+12\,u\,u_x)=0,$$

which are equivalent to KdV. The associated constant of the motion is

$$H^{(1)}[u]\equiv i_{V_2}P^{(1)}=\frac{1}{2}\int\mathrm{d}x\,(x\,u+\mathrm{D}^{-1}(u))(u_{xxx}+12\,u\,u_x)=\frac{5}{4}\int\mathrm{d}x\,(u_x^2-4\,u^3),$$

which is a member of the known set.

The next action principle is written as Eq. (24), with

$$\mathcal{P}^{(2)}[u](x,t)=R^{\dagger}[u]\cdot\mathcal{P}^{(1)}[u](x,t)=-\,\tfrac{1}{2}(3\,u_x+x\,u_{xx}+6\,x\,u^2+4\,u\,\mathrm{D}^{-1}(u)+6\,\mathrm{D}^{-1}(u^2)).$$

The Euler–Lagrange equations are $2\,(\mathrm{D}+4\,u\,\mathrm{D}^{-1}+4\,\mathrm{D}^{-1}\,u)(u_t+u_{xxx}+12\,u\,u_x)=0$ or, in factorized form, $2\,\mathrm{D}^{-1}\,(1/\psi^2)\,\mathrm{D}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}\,(1/\psi^2)\,\mathrm{D}^{-1}\,(u_t+u_{xxx}+12\,u\,u_x)=0$. These equations are not equivalent to the original equations: instead, they are equivalent to the deformed equations

$$u_t=-u_{xxx}-12\,u\,u_x+\theta_1\,(\psi^2)_x+\theta_2\,(\psi\,\overline{\psi})_x+\theta_3\,(\overline{\psi^2})_x,$$

where θ_j are arbitrary 0-forms that multiply the generators of $\mathrm{Ker}\,\Sigma^{(2)}[u]$, and $\psi=\psi(\lambda=0)$.

We could continue this process constructively, obtaining explicitly the constants of the motion and the action principles as well as the Euler–Lagrange equations: the original KdV equation gets deformed with vectors in the negative hierarchies, as it was mentioned before.

H. Action principles for KdV: Negative Lagrangian ladders

Now we turn to the construction of the negative action principles for KdV, whose action functionals are defined by

$$S^{(m)}[u(x,t)]=\int_{t_-}^{t_+}\int_{x_-}^{x_+}\mathcal{P}^{(m)}[u](x,t)\left(u_t+\frac{m}{m+3/2}(u_{xxx}+12\,u\,u_x)\right)\mathrm{d}x\,\mathrm{d}t,$$

for $m<0$. We only need to evaluate $\mathcal{P}^{(-m)}[u](x,t)=(R^{\dagger}[u])^{-m}\cdot\mathcal{P}^{(0)}[u](x,t)$, for $m<0$. This is done easily after stating the following corollary (from lemma 11).

Corollary 13: The negative one-forms are obtained from the first negative one as follows:

$$\mathcal{P}^{(-n-1)}[u](x,t)=\frac{1}{n!}(-4)^{-n}\frac{\partial^n}{\partial\lambda^n}\mathcal{P}^{(-1)}(\lambda)[u](x,t)\Big|_{\lambda=0},\quad n\geqslant 1,$$

where $\mathcal{P}^{(-1)}(\lambda)[u](x,t)=-\frac{1}{8}\psi^2\,\mathrm{D}^{-1}\,1/\psi^2\,\mathrm{D}^{-1}\,1/\psi^2\,\mathrm{D}^{-1}\psi^2$ *or, using Eq.* (21),

$$\mathcal{P}^{(-1)}(\lambda)[u](x,t)=\tfrac{1}{16}(\psi_\lambda\,\overline{\psi}-\psi\,\overline{\psi}_\lambda).$$

The first negative action principle from Eq. (24) is thus

$$S^{(-1)}[u(x,t)]=\int_{t_-}^{t_+}\int_{x_-}^{x_+}\frac{1}{16}(\psi_\lambda\,\overline{\psi}-\psi\,\overline{\psi}_\lambda)\left(u_t+\frac{-1}{-1+3/2}(u_{xxx}+12\,u\,u_x)\right)\mathrm{d}x\,\mathrm{d}t,$$

or, after some manipulations, $S^{(-1)}[u(x,t)]=\int_{t_-}^{t_+}\int_{x_-}^{x_+}(\frac{1}{16}(\psi_\lambda\,\overline{\psi}-\psi\,\overline{\psi}_\lambda)\,u_t-\frac{1}{4}u)\,dx\,dt$, where we have to evaluate the fields ψ, $\overline{\psi}$ at $\lambda=0$. This action principle is highly nonlocal, even in terms of the auxiliary fields [see Eq. (21)]. However, the Euler–Lagrange equations are obtained as usual, varying the action with respect to the field u, and using the appropriate transformation matrices. We obtain $-\Sigma^{(-1)}[u]\cdot(u_t+u_{xxx}+12\,u\,u_x)=0$, or explicitly, using the fact that the kernel of this operator is generated by $V_1^{(1)}$,

$$u_t=-u_{xxx}-12\,u\,u_x+\theta_1\,u_x,$$

where θ_1 is arbitrary.

We stress there is no need to hesitate about the inclusion of auxiliary fields in the negative action principles, for they are not varied independently. Alternatively, we may map the above action into a mixed action principle, in which the fields ψ, u, and a Lagrange multiplier ρ are varied independently,

$$S^{(-1)}[\psi(x,t),u(x,t),\rho(x,t)]=\int_{t_-}^{t_+}\int_{x_-}^{x_+}\left(\frac{1}{16}\frac{\psi_t}{\psi^3}(\mathrm{D}^{-1}\psi^2)+\frac{1}{8}\frac{\psi_{xx}}{\psi}+\rho\left(u+\frac{\psi_{xx}}{2\,\psi}\right)\right)\mathrm{d}x\,\mathrm{d}t.\tag{25}$$

See Ref. 11 for a general discussion.

The next negative action principles are quite simple. Recall that the evolution vector itself V_2 is in the kernel of the symplectic operators $\Sigma^{(m)}$, for $m=-2,\ldots,-\infty$, so that the action principles should be time-reparametrization invariant.[24] From Eq. (14), the only chance is $K^{(m)}\propto i_{V_2}P^{(m)}=0$ or a numeric constant (which would not change the action principle), for $m\leqslant -2$. This is easily shown, from the fact that the interior product $I(\lambda)=i_{V_1^{(1)}}P^{(-1)}(\lambda)[u]=-\frac{1}{16}\int_{x_-}^{x_+}\mathrm{d}x\,(\psi_\lambda\,\overline{\psi}-\psi\,\overline{\psi}_\lambda)\,u_x$, where $\psi=\psi(\lambda)$, is a numeric constant for all λ: $I(\lambda)=-\frac{1}{32}(x_+-x_-)$. We get, then, manifestly time-reparametrization invariant actions:

$$S^{(-n-1)}[u(x,t)]=\frac{1}{16\,(n!)}(-4)^{-n}\int_{t_-}^{t_+}\int_{x_-}^{x_+}\frac{\partial^n}{\partial\lambda^n}(\psi_\lambda\,\overline{\psi}-\psi\,\overline{\psi}_\lambda)|_{\lambda=0}\,u_t\,\mathrm{d}x\,\mathrm{d}t,\quad n\geqslant 1,$$

and we may use Eq. (21) in order to write the λ-derivatives in terms of nonlocal expressions. For example, the second negative action principle is

$$S^{(-2)}[u(x,t)]=-\frac{1}{64}\int_{t_-}^{t_+}\int_{x_-}^{x_+}(\psi_{\lambda\lambda}\,\overline{\psi}-\psi\,\overline{\psi}_{\lambda\lambda})|_{\lambda=0}\,u_t\,\mathrm{d}x\,\mathrm{d}t,$$

where $\psi_{\lambda\lambda}=2\,\psi\,\mathrm{D}^{-1}\,(1/\psi^2)\,\mathrm{D}^{-1}\,\psi^2\,\mathrm{D}^{-1}\,(1/\psi^2)\,\mathrm{D}^{-1}\,\psi^2$ and $\overline{\psi}=\psi\,\mathrm{D}^{-1}(1/\psi^2)$; the Euler–Lagrange equations are equivalent to

$$u_t=\theta_1\,(u_{xxx}+12\,u\,u_x)+\theta_2\,u_x,$$

where, as usual, θ_j are arbitrary functionals. The invariance $t\to\tau(t)$ is evident.

I. The missing action principle for KdV, a time-dependent constant of the motion and the internal vectors

So far we have obtained two ladders of action principles for the KdV equation: the positive (quasilocal) and the negative ladders (highly nonlocal). However, there is a missing action principle: this is the case $m=0$, which is actually twofold: first, the one-form $P^{(0)}[u]\equiv i_{\eta_{\mathrm{gal}}}\Sigma^{(1)}[u]=-x/8$ is closed: $P^{(0)}[u]=\delta C^{(0)}[u]$, where $C^{(0)}[u]=-\int_{x_-}^{x_+}\mathrm{d}x\,x\,u/8$. From Eq. (17), we obtain a known[30] time-dependent constant of the motion for KdV: $C[u,t]=\frac{1}{8}\int_{x_-}^{x_+}(6\,t\,u^2-x\,u)\,\mathrm{d}x$.

Second, the action principle for the symplectic two-form $\Sigma^{(0)}[u]$ [see Eq. (23)] has to be evaluated by hand. After some hard but straightforward calculations, we find that the one-form $\mathcal{P}^{(M)}[u](x,t)\equiv(\psi^2/4)\mathrm{D}^{-1}[(1/\psi^2)\ln\psi]$ is a solution of $\delta P^{(M)}=\Sigma^{(0)}$.

In this case, we map to the ψ-coordinate system for simplicity. We get the action principle

$$S^{(0)}[\psi,u,\rho]=-\frac{1}{8}\int_{x_-}^{x_+}\left(\frac{\psi_x\,\psi_t}{\psi^2}-\frac{\psi_{xx}^2}{\psi^2}+\rho\left(u+\frac{\psi_{xx}}{2\,\psi}\right)\right)\mathrm{d}x\,\mathrm{d}t.$$

The Euler–Lagrange equations we obtain are as follows: for the field ψ,

$$\frac{1}{\psi}\mathrm{D}\frac{1}{\psi}\left(\psi_t+\psi_{xxx}-3\,\frac{\psi_x\psi_{xx}}{\psi}\right)=0,$$

for the field u, $u=-(\psi_{xx}/2\,\psi)\Rightarrow u_t=-u_{xxx}-12\,u\,u_x$, and for the Lagrange multiplier, $\rho=0$.

Notice that the Euler–Lagrange equations for ψ are equivalent to

$$\psi_t=-\psi_{xxx}+3\,\frac{\psi_x\psi_{xx}}{\psi}+\theta_1\,\psi,$$

where θ_1 is arbitrary. This symmetry is one of the three known[14] internal symmetries (i.e., those which do not affect the field u) of the eigenvalue problem (19). In the ψ-coordinate system we write it as $\psi_t=V_0^{(-2)}[\psi]=-\frac{1}{2}\psi$ (the numeric factor is only for simplicity). In the cited reference it is shown that all negative vectors and the internal symmetries span a loop algebra over $\mathrm{SL}(2,\mathbb{R})$.

J. Nonlocal constants of the motion for KdV

As a final result, we will construct explicitly three new sets of constants of the motion for the KdV equation, starting from the nonlocal objects we have obtained. We denote $\psi=\psi(x,t;\lambda=0)$

for simplicity from here on, unless explicitly stated. Consider the action principle (25): the term which multiplies the velocity ψ_t is the mapping of the Lagrangian one-form $P^{(-1)}[u]$ into ψ-coordinates:

$$\mathcal{P}^{(-1)}[\psi](x,t)=\frac{1}{16\,\psi^3}(\mathrm{D}^{-1}\psi^2).$$

On the other hand, from Theorem 7 we have $\mathcal{L}_{V_2}P^{(-1)}=\delta K^{(-1)}$, where $K^{(-1)}=\frac{3}{16}\int_{x_-}^{x_+}dx\,(\psi_x^2/\psi^2)$. Consider now the 0-form

$$H^{(-2)}[\psi]\equiv -16\,i_{V_0^{(-2)}}P^{(-1)}=-\int_{x_-}^{x_+}dx\,\frac{1}{\psi^2}(\mathrm{D}^{-1}\,\psi^2)$$

or, more concisely, $H^{(-2)}[\psi]=\int_{x_-}^{x_+}dx\,\psi\,\overline{\psi}$.

We use Leibnitz rule to show that this is a constant of motion for the KdV equation, which in ψ coordinates reads $V_2[\psi]=-\psi_{xxx}+3(\psi_x\psi_{xx}/\psi)$: as $\mathcal{L}_{V_2}V_0^{(-2)}[\psi]=0$, we find $\mathcal{L}_{V_2}H^{(-2)}[\psi]=\mathcal{L}_{V_0^{(-2)}}K^{(-1)}[\psi]=0$, where the last equality comes from the fact that $K^{(-1)}[\psi]$ is invariant under scaling of ψ.

Thus $H^{(-2)}[\psi]$ is a nonlocal constant of the motion for the KdV flow. But if we recall that the fields ψ, $\overline{\psi}$ are solutions of the linear problem (19), and that u does not change if these fields are replaced by other arbitrary linear combinations, we get indeed three constants of the motion: $H^{(-1)}[\psi]=\int_{x_-}^{x_+}dx\,\psi^2$, $H^{(-2)}[\psi]=\int_{x_-}^{x_+}dx\,\psi\,\overline{\psi}$, $H^{(-3)}[\psi]=\int_{x_-}^{x_+}dx\,\overline{\psi}^2$.

There is a reference that supports this construction: in Ref. 31, in the context of the eigenvalue ''Schrödinger'' problem (19), the author assumes that the total probability (here denoted by $H^{(-1)}[\psi]$) is equal to 1. But it is indeed a constant of motion of its own. Moreover, these are indeed special cases ($\lambda=0$) of more general constants of motion. Along the same lines, we get three families, parametrized by the eigenvalue λ,

$$H^{(-1)}(\lambda)[\psi]=\int_{x_-}^{x_+}dx\,\psi(\lambda)^2,$$

$$H^{(-2)}(\lambda)[\psi]=\int_{x_-}^{x_+}dx\,\psi(\lambda)\,\overline{\psi}(\lambda),$$

$$H^{(-3)}(\lambda)[\psi]=\int_{x_-}^{x_+}dx\,\overline{\psi}(\lambda)^2. \tag{26}$$

These are real new constants (indeed they contain, in their Taylor series around $\lambda=0$, the constants of the motion from Theorem 9). In order to evaluate them explicitly, take, for example, successive derivatives of the first one with respect to λ, evaluate at $\lambda=0$ and use Eq. (21). We get

$$Q^{(-1;n)}[\psi]\equiv\int_{x_-}^{x_+}dx\,\psi L^{-n}\,\psi,\quad n=0,\ldots,\infty,$$

and we see they are increasingly nonlocal constants of the motion.

It is worth to mention that these nonlocal constants, when mapped to the coordinate system in which the KdV equation maps into the Harry–Dym equation (see Ref. 18), reproduce the results obtained independently in a recent work,[20] and add three more constants to the Harry–Dym equation: the mappings of the nonlocal constants of motion (26) for $\lambda=0$ into the Harry–Dym equation $\omega_t=(\omega^{-1/2})_{sss}$ for the field $\omega(s,t)$, are $H^{(-1)}[\omega]=\int_{s_-}^{s_+}ds\,\omega$, $H^{(-2)}[\omega]=\int_{s_-}^{s_+}ds\,s\,\omega$, $H^{(-3)}[\omega]=\int_{s_-}^{s_+}ds\,s^2\,\omega$.

V. RESULTS FOR OTHER KDV POSITIVE AND NEGATIVE EQUATIONS

A. Some positive, negative and internal vectors as known integrable equations

We write the internal vectors after transformation to Schwartzian coordinates, defined by $\zeta_x(x,t;\lambda)=\psi(x,t;\lambda)^{-2}$. The internal vectors in ζ coordinates are $V_0^{(-1)}[\zeta]=1$, $V_0^{(-2)}[\zeta]=\zeta$, $V_0^{(-3)}[\zeta]=\zeta^2$.

The vectors $V_0^{(-3)}$, $(V_0^{(-3)}-V_1^{(-1)})/2$, and $V_2^{(1)}$ give the evolution equations $\zeta_t=\zeta^2$, $\zeta_t=\frac{1}{2}\zeta^2-\frac{1}{8}(\zeta_{x\lambda}/\zeta_x)$, and $\zeta_t=6\lambda\zeta_x+(3\zeta_{xx}^2/2\zeta_x)-\zeta_{xxx}$, where the fields are evaluated at $\lambda=0$. The last of these equations is a special case of the Krichever–Novikov equation,[8] and the first and the second equations, via the transformation $z=\ln(2\zeta_x)$, may be mapped to the Liouville equation $z_{xt}=\exp z$, and the ShG equation $z_{xt}=\sinh z$. For completeness, we just mention that the associated Camassa–Holm equation[32] and the Hunter–Zheng equation[20] are obtainable from the negative vectors $V_1^{(-2)}$ and $V_1^{(-1)}$, respectively, via suitable coordinate transformations, and that the Harry–Dym equation,[18] just like the above case of the Krichever–Novikov equation, is a mapping of the KdV equation.

B. Action principles for the Sinh–Gordon equation

As a representative of the extension of the results on action principles for equations in the negative hierarchies, we work out some examples for the ShG equation. The results in this section are new up to our knowledge, except when it is explicitly stated. We will work in the z-coordinate system, where the ShG equation is $z_t=V_{\mathrm{ShG}}[z]=\mathrm{D}^{-1}\sinh z$.

1. Pure ShG equation: Symplectic matrix $\Sigma^{(0)}$

We look for a standard Lagrangian pair for the ShG equation of the form $(P^{(M)}[z];K^{(M;\mathrm{ShG})}[z])$, where $\mathcal{P}^{(M)}[z]=-\frac{1}{32}z_x$ is the mapping of $\mathcal{P}^{(M)}[u]$ to z coordinates. The symplectic two-form $\Sigma^{(0)}[z]=\frac{1}{16}\mathrm{D}$ has only one vector in the kernel, namely $V_0^{(-2)}[z]=4$. On the other hand, the standard Lagrangian 0-form solves $(\delta/\delta z)K^{(M;\mathrm{ShG})}[z]=\mathcal{L}_{V_{\mathrm{ShG}}}P^{(M)}[z]=-\frac{1}{32}(\sinh z-z\cosh z)$. We get after integration the usual action principle for the ShG equation,[30]

$$S[z(x,t)]=\frac{1}{32}\int_{t_-}^{t_+}\mathrm{d}t\,\mathrm{d}x\,(-z_x z_t-2\cosh z),$$

and the Euler–Lagrange equations are simply $z_t=\mathrm{D}^{-1}\sinh z+\theta_1$, where θ_1 is arbitrary.

2. ShG equation deformed with first positive vector: Symplectic matrix $\Sigma^{(-1)}$

The next negative one-form, $P^{(-1)}$, reads $\mathcal{P}^{(-1)}[z](x,t)=-\frac{1}{32}e^z(\mathrm{D}^{-1}e^{-z})$. The associated symplectic two-form is $\Sigma^{(-1)}[z]=-\frac{1}{32}(e^z\mathrm{D}^{-1}e^{-z}+e^{-z}\mathrm{D}^{-1}e^z)$, which inherits the kernel (generated from $V_1^{(1)}[z]=-z_x$) from that in the u-coordinate system only for special boundary conditions: defining the boundary terms $\overline{f}\equiv f_+ + f_-$ and $f_\pm=f(x_\pm)$, the expression

$$\Sigma^{(-1)}[z]\cdot V_1^{(1)}[z]=\tfrac{1}{64}(e^z\overline{e^{-z}}-e^{-z}\overline{e^z})$$

is zero only for boundary conditions $z_+=z_-+i\pi(2n+1)$, $n\in\mathbb{Z}$.

For other boundary conditions, however, this Lagrange bracket has no kernel, which will show up in the variational principle for the ShG vector by the fact that the Euler–Lagrange equations get deformed by a factor of the vector $V_1^{(1)}[z]$, which is not arbitrary: it depends on the boundary conditions used for the z coordinates.

In the generic case when $\overline{e^z}\neq 0$ (invertible symplectic two-form $\Sigma^{(-1)}$), the action principle is explicitly

$$S[z(x,t)]=\int_{t_-}^{t_+}\mathrm{d}t\left[-\frac{1}{32}\int_{x_-}^{x_+}\mathrm{d}x\, e^{z}(\mathrm{D}^{-1}e^{-z})(z_t-\mathrm{D}^{-1}\sinh z)+K^{(-1;\mathrm{ShG})}[z]\right],$$

and the Euler–Lagrange equations are

$$\tfrac{1}{32}(e^{z}\,\mathrm{D}^{-1}\,e^{-z}+e^{-z}\,\mathrm{D}^{-1}\,e^{z})(z_t-\mathrm{D}^{-1}\sinh z+\theta[A_+,A_-]\,z_x)=0$$

or, equivalently,

$$z_t-\mathrm{D}^{-1}\sinh z+\theta[A_+,A_-]\,z_x=0,$$

where $K^{(-1;\mathrm{ShG})}[z]=\int_{x_-}^{x_+}\mathrm{d}x\, e^{z}(\mathrm{D}^{-1}e^{-z})^2/128+F[A_+,A_-]$, $A_\pm\equiv\int_{x_-}^{x_+}\mathrm{d}x\, e^{\pm z}$, and θ, F solve the equation:

$$\delta F[A_+,A_-]=-\theta[A_+,A_-]\,(\overline{e^{-z}}\,\delta A_+ +\overline{e^{z}}\,\delta A_-)+\tfrac{1}{8}A_-\,(A_--2\,A_+)\,\delta A_+ . \tag{27}$$

There are many solutions of the above equation for a given set of boundary conditions on the limiting values of $z_\pm$, so we discuss, as examples, only two representative, nonintersecting cases of boundary conditions, for which the symplectic two-form $\Sigma^{(-1)}$ is invertible:

(i) $z_+=-z_-+i\pi(2\,n),\ n\in\mathbb{Z};\ \cosh z_+\neq 0.$
A solution of Eq. (27) is $\theta=-A_+\,A_-/4\,\overline{e^{z}}$, $F=A_+\,A_-^2/512$, which is well defined because of the boundary conditions used.

(ii) $z_+=-z_-+i\pi(2\,n+1),\ n\in\mathbb{Z};\ \sinh z_+\neq 0.$
In this case, a solution of Eq. (27) is

$$\theta=-(A_+^2-A_-^2)/8\,\overline{e^{z}},\quad F=-(A_+^2\,A_--\tfrac{1}{3}(A_+^3+A_-^3))/512.$$

The usual constant of the motion for the ShG equation, $H[z]=\int_{x_-}^{x_+}\mathrm{d}x\cosh z$, works in this case also: under the boundary conditions used, we get

$$\dot{H}[z]=\int_{x_-}^{x_+}\mathrm{d}x\,\sinh z\,(\mathrm{D}^{-1}\sinh z-\theta\,z_x)=\theta\,\overline{\cosh z}=0.$$

C. Alternative Lax pairs and constants of the motion for negative equations

In Ref. 16, the authors find alternative Lax pairs for the KdV equation (as well as for every evolution equation in the KdV positive hierarchy) by making no ansatz: they just use the evolution equation and the hereditary operator.

We present a similar construction, this time for the negative vectors. By so doing we are answering an open question in Ref. 20.

As it is shown in Ref. 16, given an evolution equation $u_t=V[u]$, and a recursion operator R for V (i.e., $\mathcal{L}_V R=0$), it follows that

$$\frac{\mathrm{D}}{\mathrm{D}t}R=[V',R], \tag{28}$$

where V' denotes the Frechet derivative, and the square brackets are the commutators. The above equation defines the alternative Lax pair (R,V').

Now, take R as the hereditary operator $R[u]$, and V as the negative vector $V_1^{(-1)}(\lambda)[u]=(\psi(\lambda)^2)_x$, for arbitrary ν,λ. We need to evaluate the Frechet derivative of this vector with respect to the field u. Using the transformation matrix $\delta\psi/\delta u=-2\,\psi\,\mathrm{D}^{-1}\,(1/\psi^2)\mathrm{D}^{-1}\,\psi^2$, where ψ stands for $\psi(\lambda)$ from here on, we get $V_1^{(-1)}(\lambda)'[u]=-4\,\mathrm{D}\,\psi^2\,\mathrm{D}^{-1}\,(1/\psi^2)\mathrm{D}^{-1}\,\psi^2$. On the other hand, the hereditary operator is

$$R[u]=R(\lambda)[u]-4\,\lambda\,\mathbb{I}=\frac{1}{\psi^2}\mathrm{D}\,\psi^2\,\mathrm{D}\,\psi^2\,\mathrm{D}\frac{1}{\psi^2}\mathrm{D}^{-1}-4\,\lambda\,\mathbb{I},$$

and it is also written as $R[u]=\mathrm{D}^2+8\,u+4\,u_x\,\mathrm{D}^{-1}$. Now we apply the Lax pair equation (28), getting after some rearrangements the operator equation $8\,u_t+4\,u_{xt}\,\mathrm{D}^{-1}=8\,(\psi^2)_x+4\,(\psi^2)_{xx}\,\mathrm{D}^{-1}$, which implies $u_t=(\psi(\lambda)^2)_x$. Recall this equation contains all the negative vectors in the corresponding negative hierarchy, so that the Lax pair we have presented indeed works for all vectors in that hierarchy. Similarly, for the other two negative hierarchies we get the Lax pairs (R, B_2) and (R, B_3), with

$$B_2=V_1^{(-2)}(\lambda)'[u]=-4\,\mathrm{D}\,\psi^2\,\mathrm{D}^{-1}\,\overline{\psi}\,\psi^{-1}\,\mathrm{D}\,\overline{\psi}\,\psi^{-1}\,\mathrm{D}^{-1}\,(\overline{\psi})^{-2}\,\mathrm{D}^{-1}\,\psi\,\overline{\psi},$$

$$B_3=V_1^{(-3)}(\lambda)'[u]=-4\,\mathrm{D}\,\overline{\psi^2}\,\mathrm{D}^{-1}\,(\overline{\psi})^{-2}\,\mathrm{D}^{-1}\,\overline{\psi^2}.$$

In this way, we may construct an infinite number of constants of the motion for the negative vectors, from Adler traces of positive, semi-integer powers of the Nijenhuis operator R: these are just the usual (local) constants of the motion for the KdV equation.[16] A natural conjecture is that Adler traces of positive, semi-integer powers of R^{-1} will give our nonlocal constants for KdV defined in Eq. (26). If that is true, we could infer that the nonlocal constants of the motion for KdV should also work for the negative vectors, which can be explicitly checked. We present the results only for the hierarchy $V_1^{(-1)}(\lambda)$, because Lie derivatives of the results along the internal vector $V_0^{(-3)}$ map the objects into similar ones for the other two negative hierarchies.

(i) Conserved currents: defining the boundary term $f\equiv\tilde{f}(x_+)-f(x_-)$, the integral $H^{(-1)}(\nu)[\psi]=\int_{x_-}^{x_+}\mathrm{d}x\,\psi(\nu)^2$ solves

$$\underset{V_1^{(-1)}(\lambda)}{\mathcal{L}}\;H^{(-1)}(\nu)[\psi]=-\overbrace{E(\nu,\lambda)[\psi]},$$

where $E(\nu,\lambda)[\psi]\equiv[\psi(\lambda)\,\psi_x(\nu)-\psi(\nu)\,\psi_x(\lambda)]/(\lambda-\nu)$.

(ii) Constants of the motion: the expression

$$G^{(-1)}(\nu,\lambda)[\psi,t]=\int_{x_-}^{x_+}\mathrm{d}x\,\psi(\nu)^2+t\,\overbrace{\frac{E(\nu,\lambda)[\psi]^2}{1-t\,E(\lambda,\lambda)[\psi]^2}}$$

is a constant of the motion for the flow $V_1^{(-1)}(\lambda)$. These constants and currents are infinite in number and work for every vector in the respective negative hierarchy, because λ and ν are arbitrary. By considering their Taylor expansion around $\lambda=\nu=0$, the explicit expression for the constants and conserved currents for each negative vector is easily worked out using Eqs. (21) and (18).

VI. CONCLUSION

The Lagrangian point of view determines a unifying scheme for the study of integrable equations belonging to hierarchies related to hereditary operators. For all evolution vectors in these hierarchies, nonlocal symmetries, Lax pairs, constants of the motion, conserved currents and an infinite ladder of action principles all come out in a constructive, explicit way from the same structure. Moreover, new equations, which are mixed or deformed versions of known integrable equations, arise as the Euler–Lagrange equations of the action principles obtained. As an example, we apply this scheme to the KdV equation, and the results are directly mappable to other related equations in the positive KdV hierarchies (e.g., Harry–Dym and a special case of Krichever–Novikov equations) as well as in the negative KdV hierarchies (e.g., Sinh–Gordon, Liouville, Camassa–Holm, and Hunter–Zheng equations): in particular, we obtain a new nonlocal action

principle for the Sinh–Gordon equation which leads to a deformed version of this equation, and an infinite number of nonequivalent, nonlocal action principles for KdV, possessing time-reparametrization invariance, are explicitly found. The construction of alternative Lax pairs for negative equations arises naturally, without any ansatz, from this scheme, and it is shown that negative equations essentially share the constants of the motion (local as well as nonlocal) for the KdV equation.

ACKNOWLEDGMENTS

One of the authors (M.B.) wishes to mention that this work was done in part during a research stay at the Relativity Center, The University of Austin, Texas, U.S.A., where M.B. was invited by Professor L. C. Shepley; M.B. is deeply grateful to him, the professors, and students in the Center for their support and the following people whose comments and suggestions were fundamental for his understanding of the topics involved in the present work: P. J. Morrison, C. deWitt-Morette, C. Valls, J. Zanelli, C. Teitelboim, and R. Troncoso. Finally, M.B. acknowledges the financial support from a Fundación Andes Grant for Doctoral Studies, and a Conicyt Grant for Thesis Completion.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Liénard–Wiechert potentials in even dimensions

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(Received 29 March 2003; accepted 21 July 2003)

The motion of point charged particles is considered in an even dimensional Minkowski space–time. The potential functions corresponding to the massless scalar and the Maxwell fields are derived algorithmically. It is shown that in all even dimensions particles lose energy due to acceleration. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1613040]

I. INTRODUCTION

Recently Gal'tsov[1] and Kazinski *et al.*[2] have considered the Lorentz–Dirac equation for a radiating point charge in a Minkowski space–time of arbitrary dimension. They showed that the mass renormalization is possible only in three and four dimensions. In their discussion, they have also given the retarded Green's functions of the D'Alembert equation in any dimensions which was in fact constructed rigorously a long time ago.[3] Motivated by these works, we are interested in the radiation problem of accelerated point charges in all even dimensions (for the reason why we did not consider odd dimensions, please see Appendix B). Here we find the Liénard–Wiechert potentials corresponding to the massless scalar and the Maxwell fields in all even dimensions. We then use these potentials to relate the radiation from an accelerated point particle to its motion and the geometry of its trajectory. We derive the energy flux for this radiation and show that accelerating point charged particles lose energy in all even dimensions.

In Sec. II, we develop the kinematics of a curve C in a D-dimensional Minkowski manifold $\mathbf{M_D}$. In Sec. III we find the Liénard–Wiechert potentials of massless free scalar fields in an even dimensional Minkowski space. We calculate the energy radiated due to the acceleration. We show that in all even dimensions such particles lose energy, as can be expected. In Sec. IV, we determine the Liénard–Wiechert potentials for the Maxwell theory. We give a recursion relation between the vector potentials of the theory in two consecutive even dimensions. In Sec. IV, we also show that particles carrying electric charges lose energy in all even dimensions. We construct explicit solutions of the electromagnetic vector field due to the acceleration of charged particles in 4,6,8,10 dimensions. We then find the energy fluxes in 4,6,8 dimensions due to acceleration. In Appendix A, we give the Serret–Frenet equations in an arbitrary Minkowski space–time and also some auxiliary tools used in the calculation of the energy flux integrals. In Appendix B, we give a proof of the recursion relation introduced in Sec. IV.

II. CURVES IN *D*-DIMENSIONAL MINKOWSKI SPACE

In our previous works,[4–6] we developed a curve kinematics to be utilized in finding new solutions and in calculating energy fluxes due to the acceleration in the framework of Einstein's general theory of relativity. Here we use the same approach to solve the scalar and Maxwell field

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equations in all even dimensions. For this purpose, we shall now give a summary of the geometry of a regular curve in $\mathbf{M_D}$, Minkowski space–time manifold of dimension D.

Let $z^\mu(\tau)$ describe a smooth curve C in $\mathbf{M_D}$, where τ is the arclength parameter of the curve. From an arbitrary point x^μ outside the curve, there are two null lines intersecting the curve C. These points are called the retarded and the advanced times. Let Φ be the distance (world function) between the points x^μ and $z^\mu(\tau)$, then by definition it is given by

$$\Phi = \tfrac{1}{2}\,\eta_{\mu\nu}\,(x^\mu - z^\mu(\tau))\,(x^\nu - z^\nu(\tau)), \tag{1}$$

where $\eta_{\mu\nu}=\mathrm{diag}(-1,1,\ldots,1)$. Hence Φ vanishes at the retarded, τ_0, and advanced, τ_1, times. In this work we shall focus on the retarded case only. The Green's function for the vector potential chooses this point on the curve C.[7,8] By differentiating Φ with respect to x^μ and letting $\tau=\tau_0$, we get

$$\lambda_\mu \equiv \tau_{,\mu} = \frac{x_\mu - z_\mu(\tau_0)}{R}, \quad R \equiv \dot{z}^\mu(\tau_0)\,(x_\mu - z_\mu(\tau_0)), \tag{2}$$

where R is the retarded distance, λ_μ is a null vector, and a dot over a letter denotes differentiation with respect to τ_0. The derivatives of R and λ_μ, using (2), are given by

$$\lambda_{\mu,\nu} = \frac{1}{R}[\,\eta_{\mu\nu} - \dot{z}_\mu\lambda_\nu - \dot{z}_\nu\lambda_\mu - (A-\epsilon)\,\lambda_\mu\lambda_\nu], \tag{3}$$

$$R_{,\mu} = (A-\epsilon)\,\lambda_\mu + \dot{z}_\mu, \tag{4}$$

where

$$A = \ddot{z}^\mu\,(x_\mu - z_\mu), \quad \dot{z}^\mu\,\dot{z}_\mu = \epsilon = 0, \pm 1. \tag{5}$$

Here $\epsilon = 0, -1$ for null and time-like curves, respectively. Furthermore, we have

$$\lambda_\mu\,\dot{z}^\mu = 1, \quad \lambda^\mu\,R_{,\mu} = 1. \tag{6}$$

Letting $a = A/R$, it is easy to prove that

$$a_{,\mu}\,\lambda^\mu = 0. \tag{7}$$

Similarly, other scalars $(a_1, a_2, \ldots)$, satisfying the same property (7) obeyed by a can be defined

$$a_k \equiv \lambda_\mu \frac{\mathrm{d}^k\,\ddot{z}^\mu}{\mathrm{d}\tau_0^k}, \quad k = 1,2,\ldots,n. \tag{8}$$

Moreover one has

$$a_{k,\alpha}\,\lambda^\alpha = 0, \tag{9}$$

for all k ($k=0$ is also included if we let $a_0 = a$). For a more detailed discussion, please refer to Ref. 4. Here n is a positive integer which depends on the dimension D of the manifold $\mathbf{M_D}$. An analysis using Serret–Frenet frames shows that the scalars (a, a_k) are related to the curvature scalars of the curve C in $\mathbf{M_D}$. The number of such scalars is $D-1$.[9] Hence we let $n = D-1$.

III. MASSLESS SCALAR FIELD

Let ϕ describe a massless scalar field satisfying the free field equation

$$\eta^{\mu\nu}\frac{\partial^2\phi}{\partial x^\mu \partial x^\nu}=0. \tag{10}$$

Let D be a positive even integer, and $\phi^{(D)}$ and $\phi^{(D+2)}$ denote the retarded solutions (Liénard–Wiechert potentials) of the massless scalar field in D and $D+2$ dimensions, respectively. Then

$$\phi^{(D+2)}=\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}\phi^{(D)}. \tag{11}$$

In this recursion relation we emphasize that the expressions on the right-hand side are those of D-dimensions. Take the solution $\phi^{(D)}$ in D-dimensions, take its τ derivative and divide this by the R of D-dimensions. The result is the solution $\phi^{(D+2)}$ of $D+2$-dimensions. For the proof of relation (11) see Appendix B. In the following we explicitly give these solutions for $D=4,6,8,10$:

$$\phi^{(4)}=\frac{c}{R}, \tag{12}$$

$$\phi^{(6)}=\frac{1}{R^2}[\dot{c}-pc], \tag{13}$$

$$\phi^{(8)}=\frac{1}{R^3}[\ddot{c}-3p\dot{c}+(-a_1+3p^2)c], \tag{14}$$

$$\phi^{(10)}=\frac{1}{R^4}\left[\frac{\mathrm{d}^3c}{\mathrm{d}\tau^3}-6p\ddot{c}+(15p^2-4a_1)\dot{c}+\left(-a_2+10pa_1-15p^3+\frac{1}{R}\dot{z}_\alpha\frac{\mathrm{d}^3z^\alpha}{\mathrm{d}\tau^3}\right)c\right], \tag{15}$$

where $c=c(\tau)$ is the (time dependent) scalar charge and $p\equiv a-\epsilon/R$.

The flux of massless scalar field energy is then given by (see Refs. 7 and 11 for this definition and also for the integration surface S)

$$\mathrm{d}E=-\int_S \dot{z}_\mu T^{\mu\nu}_\phi \,\mathrm{d}S_\nu, \tag{16}$$

where $T^{\phi}_{\mu\nu}=\partial_\mu\phi\,\partial_\nu\phi-\frac{1}{4}(\eta^{\alpha\beta}\partial_\alpha\phi\,\partial_\beta\phi)\eta_{\mu\nu}$ is the energy momentum tensor of the massless scalar field ϕ. The surface element $\mathrm{d}S_\mu$ on S is given by

$$\mathrm{d}S_\mu=n_\mu R^{D-3}\mathrm{d}\tau\,\mathrm{d}\Omega, \tag{17}$$

where n_ν is orthogonal to the velocity vector field $\dot{z}_\mu$ which is defined through

$$\lambda_\mu=\epsilon\dot{z}_\mu+\epsilon_1\frac{n_\mu}{R},\qquad n^\mu n_\mu=-\epsilon R^2. \tag{18}$$

Here $\epsilon_1=\pm1$. For the remaining part of this work we shall assume $\epsilon=-1$ (C is a time-like curve). One can consider S in the rest frame as a sphere of radius R. Here $\mathrm{d}\Omega$ is the solid angle. Letting $\mathrm{d}E/\mathrm{d}\tau=N_\phi$, we have

$$N^{(D)}_\phi=-\int_{S^{D-2}}\dot{z}_\mu T^{\mu\nu}_\phi n_\nu R^{D-3}\,\mathrm{d}\Omega, \tag{19}$$

where S^{D-2} is the $(D-2)$-dimensional sphere centered at $\tau=\tau_0$ on the curve C. At very large values of R the energy flux is given by

$$N_\phi^{(D)}=-\int_{S^{D-2}} \mathrm{d}\Omega\, R^{D-3}\,(\dot{z}^\alpha\,\partial_\alpha\,\phi)(n^\beta\,\partial_\beta\,\phi).$$

It turns out that the energy flux expression has a fixed sign for all D. The energy flux of the massless scalar field ϕ as $R\to\infty$ is given by

$$N_\phi^{(D)}=-\epsilon_1\int_{S^{D-2}}[\xi^{(D)}]^2\,\mathrm{d}\Omega,$$

where we obtain R independent functions (for each D) $\xi^{(D)}$ from

$$\xi^{(D)}=\lim_{R\to\infty}[R^{D/2}\,\phi^{(D+2)}].$$

As an example let $D=4$. We take $\phi^{(6)}$ from (13), multiply it by R^2 and let $R\to\infty$ (then $p\to a$), and finally we obtain $\xi^{(4)}$. The explicit expressions of $\xi^{(D)}$ are as follows:

$$\xi^{(4)}=\dot{c}-ac, \tag{20}$$

$$\xi^{(6)}=\ddot{c}-3a\dot{c}+(-a_1+3a^2)c, \tag{21}$$

$$\xi^{(8)}=\frac{\mathrm{d}^3c}{\mathrm{d}\tau^3}-6a\ddot{c}+(15a^2-4a_1)\dot{c}+(-a_2+10aa_1-15a^3)c, \tag{22}$$

$$\xi^{(10)}=\frac{\mathrm{d}^4c}{\mathrm{d}\tau^4}-10a\frac{\mathrm{d}^3c}{\mathrm{d}\tau^3}+(45a^2-10a_1)\ddot{c}-(5a_2-60aa_1+105a^3)\dot{c}$$
$$-(a_3-15aa_2-10a_1^2+105a_1a^2-105a^4)\,c. \tag{23}$$

Hence we have (assuming $c=$constant)

$$N_\phi^{(4)}=-\epsilon_1\left(\frac{4\pi}{3}\right)c^2\,\kappa_1^2, \tag{24}$$

$$N_\phi^{(6)}=-\epsilon_1\left(\frac{8\pi^2}{105}\right)c^2[20\kappa_1^4+7\dot{\kappa}_1^2+7\kappa_1^2\kappa_2^2], \tag{25}$$

$$N_\phi^{(8)}=-\epsilon_1\left(\frac{16\pi^3}{10\,395}\right)c^2\{99[(\ddot{\kappa}_1-4\kappa_1^3-\kappa_1\kappa_2^2)^2+(2\dot{\kappa}_1\kappa_2+\kappa_1\dot{\kappa}_2)^2+\kappa_1^2\kappa_2^2\kappa_3^2]$$
$$+\kappa_1^2[900\kappa_1^4+1100\kappa_1^2\kappa_2^2+3597\dot{\kappa}_1^2]\}. \tag{26}$$

IV. ELECTROMAGNETIC FIELD

In the Lorentz gauge $(\partial_\mu A^\mu=0)$, the Maxwell equations reduce to the wave equation for the vector potential A_μ, $\eta^{\mu\nu}\,\partial_\mu\,\partial_\nu A_\alpha=0$. By using the curve C, we can construct divergence free (Lorentz gauge) vector fields A_α satisfying the wave equation outside the curve C in any even dimension D. Similar to the case of the massless scalar field, such vectors obey the following recursion relation

$$A_\mu^{(D+2)}=\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}A_\mu^{(D)}. \tag{27}$$

In the recursion relation above $A_\mu^{(D)}$ is the electromagnetic vector potential in even D-dimensions, with $\mu=0,1,\ldots,D-1$. On the right-hand side of the recursion relation all operations are done in D-dimensions, just like the scalar case. However the result is to be considered as the electromagnetic vector potential of $D+2$-dimensions, with $\mu=0,1,\ldots,D+1$ on the left-hand side. As an example we have $A_\mu^{(4)}=\dot{z}_\mu/R$ as the electromagnetic vector potential of four dimensions.[8] Here $\dot{z}_\mu$ is the four velocity, R and τ are, respectively, the retarded distance and time in four dimensions. Using the recursion relation (27) the right-hand side becomes

$$\frac{\ddot{z}_\mu - a\dot{z}_\mu}{R^2} + \epsilon\frac{\dot{z}_\mu}{R^3}.$$

We then regard this expression as the solution $A_\mu^{(6)}$ of the Maxwell field equations in six-dimensions. Indeed it satisfies both the Lorentz condition and the field equations of six-dimensions, as can be verified separately. Starting from $D=4$, we can generate all even dimensional vector potentials satisfying the Maxwell equations. For instance, the vector potentials for $D=4,6,8,10$ are explicitly given by

$$A_\mu^{(4)}=\frac{\dot{z}_\mu}{R}, \tag{28}$$

$$A_\mu^{(6)}=\frac{1}{R^2}[\ddot{z}_\mu - p\dot{z}_\mu], \tag{29}$$

$$A_\mu^{(8)}=\frac{1}{R^3}\left[\frac{\mathrm{d}^3 z_\mu}{\mathrm{d}\tau^3} - 3p\ddot{z}_\mu + (-a_1+3p^2)\dot{z}_\mu\right], \tag{30}$$

$$A_\mu^{(10)}=\frac{1}{R^4}\left[\frac{\mathrm{d}^4 z_\mu}{\mathrm{d}\tau^4} - 6p\frac{\mathrm{d}^3 z_\mu}{\mathrm{d}\tau^3} + (15p^2-4a_1)\ddot{z}_\mu + \left(-a_2+10pa_1-15p^3+\frac{1}{R}\dot{z}_\alpha\frac{\mathrm{d}^3 z^\alpha}{\mathrm{d}\tau^3}\right)\dot{z}_\mu\right]. \tag{31}$$

The flux of electromagnetic energy is then given by[7] (the integration surface S is also given in this reference)

$$\mathrm{d}E = -\int_S \dot{z}_\mu T_e^{\mu\nu}\,\mathrm{d}S_\nu, \tag{32}$$

where $T^e_{\mu\nu}=F_{\mu\alpha}F_\nu{}^\alpha - \frac{1}{4}F^2\eta_{\mu\nu}$ is the Maxwell energy momentum tensor, $F_{\mu\nu}=A_{\nu,\mu}-A_{\mu,\nu}$ is the electromagnetic field tensor and $F^2\equiv F^{\alpha\beta}F_{\alpha\beta}$.

Letting $\mathrm{d}E/\mathrm{d}\tau=N_e$,[10] we have

$$N_e^{(D)} = -\int_{S^{D-2}} \dot{z}_\mu T_e^{\mu\nu} n_\nu R^{D-3}\,\mathrm{d}\Omega. \tag{33}$$

At very large values of R, for all even D, we get

$$N_e^{(D)} = -\epsilon_1\int_{S^{D-2}} \xi_\mu^{(D)}\,\xi_\nu^{(D)}\,\eta^{\mu\nu}\,\mathrm{d}\Omega, \tag{34}$$

where

$$\xi_\mu^{(D)} = \lim_{R\to\infty}[A_\mu^{(D+2)}R^{D/2}], \tag{35}$$

so that $\lambda^\mu\,\xi_\mu^{(D)}=0$ for all D.

Here we have two remarks. The first one is on the gauge dependence of (35). The only gauge freedom left in our solutions is $A_\mu \to A_\mu + \partial_\mu \phi$, where ϕ satisfies the scalar wave equation (10). However we have already found the solutions of the scalar wave equation for all even dimensions. It can be shown that the contribution of such scalar functions to the norm of $\xi_\mu^{(D)}$ is zero in the limit $R \to \infty$. Our second remark is on the sign of $N_e^{(D)}$ in (34). The vectors $\xi_\mu^{(D)}$ in all even dimensions are orthogonal to the null vector λ_μ, hence they must be either (i) space-like vectors, (ii) proportional to λ_μ, or (iii) zero vectors.[11] They are zero only when the curve C is a straight line which leads to no radiation. They cannot be proportional to the null vector λ_μ either, because this again leads to the trivial case of zero radiation. In the first three cases (4, 6, 8 dimensions) it can be easily observed that zero radiation implies that $\xi_\mu^{(D)}$ is a zero vector. Hence $\xi_\mu^{(D)}$ is a space-like vector in all even dimensions. Therefore the sign of the right-hand side of (34) is the same in all dimensions. These vectors are explicitly given as follows:

$$\xi_\mu^{(4)} = \ddot{z}_\mu - a\dot{z}_\mu , \tag{36}$$

$$\xi_\mu^{(6)} = \frac{d^3 z_\mu}{d\tau^3} - 3a\ddot{z}_\mu + (-a_1 + 3a^2)\dot{z}_\mu , \tag{37}$$

$$\xi_\mu^{(8)} = \frac{d^4 z_\mu}{d\tau^4} - 6a\frac{d^3 z_\mu}{d\tau^3} + (15a^2 - 4a_1)\ddot{z}_\mu + (-a_2 + 10aa_1 - 15a^3)\dot{z}_\mu , \tag{38}$$

$$\xi_\mu^{(10)} = \frac{d^5 z_\mu}{d\tau^5} - 10a\frac{d^4 z_\mu}{d\tau^4} + (45a^2 - 10a_1)\frac{d^3 z_\mu}{d\tau^3} + (-5a_2 + 60aa_1 - 105a^3)\ddot{z}_\mu + (-a_3 + 15aa_2 + 10a_1^2 - 105a_1 a^2 + 105a^4)\dot{z}_\mu . \tag{39}$$

These lead to the following energy flux expressions:

$$N_e^{(4)} = -\epsilon_1 \frac{8\pi}{3}\kappa_1^2 , \tag{40}$$

$$N_e^{(6)} = -\epsilon_1 \frac{32\pi^2}{15}\left(\dot{\kappa}_1^2 + \kappa_1^2\kappa_2^2 + \frac{9}{7}\kappa_1^4\right), \tag{41}$$

$$N_e^{(8)} = -\epsilon_1 \frac{32\pi^3}{10395}\left\{297\left[\left(\ddot{\kappa}_1 - \frac{4}{3}\kappa_1^3 - \kappa_1\kappa_2^2\right)^2 + (2\dot{\kappa}_1\kappa_2 + \kappa_1\dot{\kappa}_2)^2 + \kappa_1^2\kappa_2^2\kappa_3^2\right] + 4\kappa_1^2[300\kappa_1^4 + 506\kappa_1^2\kappa_2^2 + 825\dot{\kappa}_1^2]\right\}. \tag{42}$$

To be compatible with the classical results,[7,8] one should take $\epsilon_1 = -1$.

V. CONCLUSION

In this work we have considered radiation of scalar and vector fields due to acceleration of point charged particles. We first examined the geometric properties of their paths in an even dimensional Minkowski space $\mathbf{M_D}$. By using the curve kinematics we developed, we have first found the retarded solutions of the scalar field equations in $\mathbf{M_D}$. These solutions describe the potentials of the accelerated scalar charges and we have examined the energy loss due to such a radiation. We have shown that in all even dimensions such scalar point particles lose energy. We have given explicit examples for $D = 4,6,8,10$. We then found the retarded solutions of the Maxwell field equations that describe the point particles carrying electric charges. Again, using the curve kinematics we developed an algorithm to calculate the vector potential A_μ in

$D+2$-dimensions from the one in D-dimensions. We have given explicit examples for $D=4,6,8$. We have calculated the energy flux in each case, and we have shown that particles lose energy due to acceleration in all even dimensions.

ACKNOWLEDGMENTS

This work is partially supported by the Scientific and Technical Research Council of Turkey and by the Turkish Academy of Sciences.

APPENDIX A: SERRET–FRENET FRAMES

In this appendix, we first give the Serret–Frenet frame in D dimensions. Here we shall assume that the curve C described in Sec. II is time-like and has the tangent vector $T^\mu=\dot{z}^\mu$. Starting from this unit tangent vector, by repeated differentiation with respect to the arclength parameter τ_0, one can generate an orthonormal frame $\{T^\mu,N_1^\mu,N_2^\mu,\ldots,N_{D-1}^\mu\}$, the *Serret–Frenet frame*:

$$\dot{T}^\mu=\kappa_1 N_1^\mu, \tag{A1}$$

$$\dot{N}_1^\mu=\kappa_1 T^\mu-\kappa_2 N_2^\mu, \tag{A2}$$

$$\dot{N}_2^\mu=\kappa_2 N_1^\mu-\kappa_3 N_3^\mu, \tag{A3}$$

$$\cdots$$

$$\dot{N}_{D-2}^\mu=\kappa_{D-2} N_{D-3}^\mu-\kappa_{D-1} N_{D-1}^\mu, \tag{A4}$$

$$\dot{N}_{D-1}^\mu=\kappa_{D-1} N_{D-2}^\mu. \tag{A5}$$

Here κ_i $(i=1,2,\ldots,D-1)$ are the curvatures of the curve C at the point $z^\mu(\tau_0)$. The normal vectors N_i $(i=1,2,\ldots,D-1)$ are space-like unit vectors. Hence at the point $z^\mu(\tau_0)$ on the curve we have an orthonormal frame which can be used as a basis of the tangent space (of $\mathbf{M_D}$) at this point. In Sec. II, we have defined some scalars

$$a_k=\frac{\mathrm{d}^k\ddot{z}_\mu}{\mathrm{d}\tau_0^k}\lambda^\mu,$$

where

$$\lambda^\mu=\epsilon T^\mu+\epsilon_1\frac{n^\mu}{R}.$$

Here n^μ is a space-like vector orthogonal to T^μ. It can be expressed as a linear combination of the unit vectors N_i's as

$$n^\mu=\alpha_1 N_1^\mu+\alpha_2 N_2^\mu+\cdots+\alpha_{D-1} N_{D-1}^\mu,$$

where $\alpha_1^2+\alpha_2^2+\cdots+\alpha_{D-1}^2=R^2$. One can choose the spherical angles $\theta,\phi_1,\ldots,\phi_{D-4}\in(0,\pi)$, $\phi_{D-3}\in(0,2\pi)$ such that

$$\alpha_1=R\cos\theta,\quad \alpha_2=R\sin\theta\cos\phi_1,\quad \alpha_3=R\sin\theta\sin\phi_1\cos\phi_2,\ \ldots,$$

$$\alpha_{D-2}=R\sin\theta\sin\phi_1\cdots\sin\phi_{D-4}\cos\phi_{D-3},$$

$$\alpha_{D-1}=R\sin\theta\sin\phi_1\cdots\sin\phi_{D-4}\sin\phi_{D-3}.$$

Hence we can calculate the scalars a_k in terms of the curvatures of the curve C and the angles $(\theta,\phi_1,\ldots,\phi_{D-3})$ at the point $z^\mu(\tau_0)$. We need these expressions in the evaluation of energy flux formulas. As an example we give a and a_1:

$$a=-\epsilon\epsilon_1\kappa_1\cos\theta,\quad a_1=\kappa_1^2-\epsilon\epsilon_1\dot{\kappa}_1\cos\theta+\epsilon\epsilon_1\kappa_1\kappa_2\sin\theta\cos\phi_1. \tag{A6}$$

The rest of the scalars can be determined similarly. It is clear that these scalars, a_k, depend on the curvatures and the spherical angles, for all k.

APPENDIX B: THE PROOF OF THE RECURSION RELATIONS (11) AND (27)

Here we give the proof for the vector potential case. The same type of proof applies also for the scalar case. Using the recursion relation (27) successively we get

$$A_\mu^{(D)}=\left(\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)^{(D/2)-2}\frac{\dot{z}_\mu}{R}. \tag{B1}$$

On the other hand, from Refs. 1 and 2, we have

$$A_\mu^{(D)}=\int G(x-z(\tau))\,\dot{z}_\mu\,\mathrm{d}\tau, \tag{B2}$$

where τ is the parameter of the curve C. The integral here is carried on the range of $\tau\in(-\infty,\infty)$. Here $G(x-z(\tau))$ is the retarded Green function given by

$$G(x-z(\tau))=\theta(x^0-z^0)\,\delta^{(D/2)-2}(\Phi). \tag{B3}$$

Here Φ is the world function given by (1), $\theta(x)$ is the Heaviside step function and $\delta^k(x)\equiv(\mathrm{d}^k/\mathrm{d}x^k)\,\delta(x)$. Here we assume that D is an even integer. [When D is an odd integer, the expression for the Green function in (B3) contains the step function instead of the δ-function. Hence the potentials in all odd dimensions remain nonlocal (integral expressions). This makes our curve kinematics ineffective.] The zeros of Φ denote the advanced and retarded proper times on the curve C, but the step function $\theta(x^0)$ chooses the retarded one. Since the integration is over the curve parameter τ in (B2), it is better to transform the derivative of the delta function with respect to Φ to the derivative with respect to τ. As a simple example consider the $D=6$ case

$$\frac{\mathrm{d}}{\mathrm{d}\Phi}\delta(\Phi)=\left[\frac{1}{\mathrm{d}\Phi/\mathrm{d}\tau}\frac{\mathrm{d}}{\mathrm{d}\tau}\delta(\Phi)\right]_{\Phi=0}. \tag{B4}$$

It is easy to show that $\mathrm{d}\Phi/\mathrm{d}\tau=-R$. The delta function $\delta(\Phi)$ can be expressed as follows:

$$\delta(\Phi)=\frac{\delta(\tau-\tau_0)}{R}+\frac{\delta(\tau-\tau_1)}{R}.$$

The second term will vanish identically due to the step function in (B3). Hence

$$A_\mu^{(6)}=\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}\frac{\dot{z}_\mu}{R},$$

or simply $A^{(6)}=(1/R)(\mathrm{d}/\mathrm{d}\tau)\,A^{(4)}$. This verifies our relation (27). For the general case, we need higher order derivatives of $\delta(\Phi)$ at $\Phi=0$. We find such terms by using (B4) and taking successive derivatives. In the general case, for all $k=0,1,2,\ldots$ we obtain (when $\Phi=0$)

$$\frac{\mathrm{d}^k}{\mathrm{d}\Phi^k}\delta(\Phi)=\left[\left(\frac{-1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)^k\delta(\Phi)\right]. \tag{B5}$$

Using this expression in the Green's function (B3) for $k=D/2-2$, inserting it in the integral equation (B2),

$$A_\mu^{(D)}=\int \theta(x^0-z^0)\,\delta^{D/2-2}(\Phi)\,\dot{z}_\mu\,\mathrm{d}\tau \tag{B6}$$

$$=\int \theta(x^0-z^0)\left(\frac{-1}{R}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)^{D/2-2}\delta(\Phi)\,\dot{z}_\mu\,\mathrm{d}\tau, \tag{B7}$$

and integrating by parts, we obtain (B1).

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The Green–Kubo formula and power spectrum of reversible Markov processes

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(Received 30 May 2003; accepted 30 June 2003)

As is known, the entropy production rate of a stationary Markov process vanishes if and only if the process is reversible. In this paper, we discuss the reversibility of a stationary Markov process from a functional analysis point of view. It is shown that the process is reversible if and only if it has a symmetric Markov semigroup, equivalently, a self-adjoint infinitesimal generator. Applying this fact, we prove that the Green–Kubo formula holds for reversible Markov processes. By demonstrating that the power spectrum of each reversible Markov process is Lorentz-typed, we show that it is impossible for stochastic resonance to occur in systems with zero entropy production. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1610780]

I. INTRODUCTION

The question whether a steady system is in equilibrium, correspondingly, whether a stationary stochastic process is reversible, has attracted much interest from physicists as well as mathematicians.[14,22,35,24–27,9,19,20,34] In nonequilibrium statistical physics, the concept of entropy production was put forward to describe how far a specific state of a system is from its equilibrium state.[14,22,35] In Refs. 26 and 27, a measure-theoretic definition of entropy production rate is given for stochastic processes, unifying different entropy production formulas in various concrete cases. In fact, the entropy production rate of a stationary Markov process can be defined as the specific relative entropy of the probability distribution of the process on the path space with respect to that of its time-reversal. If the state space of the process is a Polish space and its trajectories are right continuous having left limits, then by Theorem 10.4 in Varadhan,[38] it is obvious that the entropy production rate vanishes if and only if the process is reversible. A stochastic process $\xi=\{\xi_t\}_{t\geqslant 0}$ is called *reversible* if for each $t>0$, $\{\xi_s\}_{0\leqslant s\leqslant t}$ has the same distribution with its time-reversal $\{\xi_{t-s}\}_{0\leqslant s\leqslant t}$. For example, suppose that ξ is a stationary, irreducible and positive recurrent continuous-time Markov chain on its canonical orbit space with finite state space X, transition density matrix $Q=(q_{ij})_{i,j\in X}$, and invariant distribution $\Pi=\{\pi_i\}_{i\in X}$. Let $\mathbf{P}$ and $\mathbf{P}^-$ be the distributions of the Markov chain and its time-reversal, respectively, and denote their restrictions on $\mathcal{F}_0^t=\sigma(\xi_s,0\leqslant s<t)$ by $\mathbf{P}_{[0,t)}$ and $\mathbf{P}^-_{[0,t)}$, respectively, then the *entropy production rate* of ξ is defined as

$$e_p := \lim_{t\to+\infty}\frac{1}{t}H(\mathbf{P}_{[0,t)},\mathbf{P}^-_{[0,t)}),$$

where $H(\mathbf{P}_{[0,t)},\mathbf{P}^-_{[0,t)})$ is the relative entropy of $\mathbf{P}_{[0,t)}$ with respect to $\mathbf{P}^-_{[0,t)}$ and is defined by $E^{\mathbf{P}_{[0,t)}}\log(\mathrm{d}\mathbf{P}_{[0,t)}/\mathrm{d}\mathbf{P}^-_{[0,t)})$ in case that $\mathbf{P}_{[0,t)}$ is absolutely continuous with respect to $\mathbf{P}^-_{[0,t)}$, otherwise, by $+\infty$. One sufficient and necessary condition for $\mathbf{P}_{[0,t)}$ and $\mathbf{P}^-_{[0,t)}$ being mutually absolutely continuous is $q_{ij}>0\Leftrightarrow q_{ji}>0$, $\forall i,j\in X$. The formula for e_p is given in Refs. 25–27, in fact,

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$$e_p=\frac{1}{2}\sum_{i,j\in X}(\pi_i q_{ij}-\pi_j q_{ji})\log\frac{\pi_i q_{ij}}{\pi_j q_{ji}}\geqslant 0. \tag{1}$$

Obviously, e_p vanishes if and only if ξ is in *detailed balance* (i.e., $\pi_i q_{ij}=\pi_j q_{ji},\forall i,j\in X$), equivalently, ξ is reversible. We refer the reader to Refs. 26–29, 31, and 33 for detailed discussion about the entropy production and reversibility of diffusion processes (see also Example III.5 below).

For a stationary Markov process, the adjoint semigroup of its Markov semigroup reflects the evolution of the corresponding time-reversed process. In Sec. II we study its Markov semigroup and the relationship with its adjoint semigroup. The following equivalent conditions for the Markov process being reversible are brought out: (1) the semigroup of the process is the same as its adjoint semigroup; (2) the infinitesimal generator of the process is symmetric; and (3) the infinitesimal generator is self-adjoint.

As is known, in the theory of statistical physics, the fluctuation–dissipation theorem holds for systems close to equilibrium in the linear response regime. The Green–Kubo formula is a version of the fluctuation–dissipation theorem. It tells that the transport coefficients (respectively, the susceptibility, i.e., the Fourier transform of the response function) corresponding to the thermodynamic forces in the system can be expressed as the integral of a time-correlation function (respectively, its Fourier transform) of the thermodynamic currents induced by the forces, where the correlation function is evaluated with respect to the equilibrium state of the system.[3,4,7,10–13,15–18,21,36,37] Thus the formula connects the energy dissipation in an irreversible process to the thermal fluctuation in equilibrium. In the case of diffusion processes, the Green–Kubo formula takes its earliest form, the Einstein relation, which says that the integral of the time-correlation function of velocities is equal to the mean value of the diffusion coefficient.[23,6] By means of matrix calculations, Qian *et al.*[30] deduces the Green–Kubo formula for reversible Markov chains with finite states and continuous time parameter. Ruelle shows in Ref. 34 that the Green–Kubo formula holds for some smooth dynamical systems.

In Sec. III, exploiting the results in Sec. II, we verify that the Green–Kubo formula holds for general reversible Markov processes. Concretely, suppose that $\xi=\{\xi_t\}_{t\geqslant 0}$ is a reversible Markov process with initial invariant distribution μ, and f,g are two arbitrary observables in a certain range. Let V^f and $D^{f,g}$ be, respectively, the drift coefficient and the diffusion coefficient of ξ with respect to f and $\{f,g\}$ (see Sec. III below for the definitions), then

$$\frac{1}{2}\int D^{f,g}(x)\mu(\mathrm{d}x)=\int_0^{+\infty}E[V^f(\xi_t)V^g(\xi_0)]\mathrm{d}t.$$

Though our form of the Green–Kubo formula addresses the functions rather than the paths themselves, it holds for plentiful observables and can be widely applied to jump processes and interacting particle systems.

In Sec. IV, we apply the results in Sec. II to discuss the relationship between reversibility and the occurrence of stochastic resonance. Traditionally, *stochastic resonance* means that the response of a nonlinear system to a periodic signal may be enhanced by an optimal strength of noise, and it is marked by the indispensable biased peaky power spectrum. Now stochastic resonance has been extensively studied, ranging from the conventional one with a periodic driving[2,1,8] to the later extended one without any external periodic force.[5,32] We prove that the power spectrum of each reversible Markov process is Lorentz-typed, which means that the spectrum peak is just centered at the origin. Hence it is impossible for stochastic resonance to occur in systems with zero entropy production. Previously, using matrix calculations, Qian *et al.*[30] obtained such a result for reversible continuous-time Markov chains with finite states.

II. EQUIVALENT CONDITIONS FOR A MARKOV PROCESS BEING REVERSIBLE

Let $\xi=\{\xi_t\}_{t\geqslant 0}$ be a stationary Markov process with Polish state space $(X,\mathcal{B})$ and initial distribution μ. Denote by $L^2(X,\mu)$, or simply by L^2, the Hilbert space of real functions on X which are square-integrable with respect to μ. For any $f,g\in L^2$, let

$$\langle f,g\rangle=\int f(x)g(x)\mu(\mathrm{d}x),\quad \|f\|=\sqrt{\langle f,f\rangle}.$$

Denote the transition semigroup of ξ by $\{T(t):t\geqslant 0\}$, i.e.,

$$T(t)f(x)=E[f(\xi_t)|\xi_0=x]=\int f(y)p(t,x,\mathrm{d}y),$$

where $p(t,x,\mathrm{d}y)$ is the transition function of ξ. Notice that

$$E|E(f(\xi_t)|\xi_0)|^2\leqslant E[E(|f(\xi_t)|^2|\xi_0)]=E|f(\xi_t)|^2=\int |f(x)|^2\mu(\mathrm{d}x),$$

since μ is an invariant measure. This implies that $T(t)$ is contractive on $L^2(X,\mu)$, i.e., $\|T(t)\|\leqslant 1$. Assume that $\{T(t)\}$ is strongly continuous, i.e.,

$$\lim_{t\downarrow 0}\|T(t)f-f\|=0,\quad \forall f\in L^2.$$

Then $\{T(t)\}$ is a strongly continuous contraction semigroup on L^2. Denote its infinitesimal generator by $\mathcal{A}$, i.e.,

$$\mathcal{D}(\mathcal{A})=\{f\in L^2:[T(t)f-f]/t \text{ converges in } L^2 \text{ as } t \text{ decreases to } 0\},$$

$$\mathcal{A}f=\lim_{t\downarrow 0}\frac{T(t)f-f}{t},\quad \forall f\in\mathcal{D}(\mathcal{A}).$$

Remark II.1: The strong continuity of $\{T(t)\}$ is weaker than the condition that $\{T(t)\}$ is normal, i.e., $\lim_{t\downarrow 0}\|T(t)f-f\|_\infty=0$ for any $f\in B(X)$, where $B(X)$ is the set of all essentially bounded measurable functions equipped with the supreme norm $\|f\|_\infty=\inf\{M:|f(x)|\leqslant M,\ \mu\text{-a.s.}\}$. The reason is that $\|\cdot\|_\infty$ is stronger than $\|\cdot\|$ and $B(X)$ is dense in $L^2(X,\mu)$ in $\|\cdot\|$.

Now we consider the adjoint semigroup of $\{T(t)\}$ with respect to μ, which is denoted by $\{T^*(t):t\geqslant 0\}$. By the definition of $T(t)$, for any $f,g\in L^2$,

$$\begin{aligned}\langle f,T(t)g\rangle&=\int f(x)T(t)g(x)\mathrm{d}\mu=E[f(\xi_0)T(t)g(\xi_0)]\\&=E[f(\xi_0)E(g(\xi_t)|\xi_0)]=E[f(\xi_0)g(\xi_t)].\end{aligned}\tag{2}$$

Hence

$$\begin{aligned}\langle T^*(t)f,g\rangle&=\langle f,T(t)g\rangle=E[f(\xi_0)g(\xi_t)]\\&=E[E(f(\xi_0)|\xi_t)g(\xi_t)]=\int E(f(\xi_0)|\xi_t=x)g(x)\mu(\mathrm{d}x),\end{aligned}$$

which yields

$$T^*(t)f(x)=E(f(\xi_0)|\xi_t=x).\tag{3}$$

$T(t)$ is contractive, so is $T^*(t)$. $\{T^*(t):t\geqslant 0\}$ can be restricted on its center of strong continuity to become a strongly continuous and contractive semigroup, whose generator is denoted by $\mathcal{A}^-$.

Remark II.2: There are two reasons to denote the generator of $\{T^*(t)\}$ by $\mathcal{A}^-$ rather than $\mathcal{A}^*$. First, in the theory of functional analysis, $\mathcal{A}^*$ is used to denote the adjoint operator of $\mathcal{A}$, i.e.,

$$\mathcal{D}(\mathcal{A}^*)=\{f\in L^2|\ \exists g\in L^2,\ \text{s.t. } \langle f,\mathcal{A}h\rangle=\langle g,h\rangle,\forall h\in\mathcal{D}(\mathcal{A})\},$$

and $\mathcal{A}^*f:=g$. Notice that $\mathcal{A}^-\subset\mathcal{A}^*$, since for any $f\in\mathcal{D}(\mathcal{A}^-)$ and any $h\in\mathcal{D}(\mathcal{A})$, it holds that

$$\langle\mathcal{A}^-f,h\rangle=\lim_{t\downarrow 0}\left\langle\frac{T^*(t)f-f}{t},h\right\rangle=\lim_{t\downarrow 0}\left\langle f,\frac{T(t)h-h}{t}\right\rangle=\langle f,\mathcal{A}h\rangle.$$

Second, by (3), $\{T^*(t)\}$ is actually the semigroup of the time-reversed process of ξ.

Recall that a stationary Markov process ξ being reversible is equivalent to that (ξ_t,ξ_0) has the same joint distribution as (ξ_0,ξ_t) for any $t\geqslant 0$. Therefore, ξ is reversible if and only if $T(t)=T^*(t)$ for any $t\geqslant 0$, which illumines us to study the reversibility by the semigroup theory. Let

$$L^2_{\mathbf{C}}:=\{f+ig:f,g\in L^2\}$$

be the complex Hilbert space, where $i^2=-1$. Denote by $\tilde{T}(t)$ the natural extension of $T(t)$ to $L^2_{\mathbf{C}}$. Then $\{\tilde{T}(t):t\geqslant 0\}$ is also a strongly continuous and contractive semigroup. Its generator $\tilde{\mathcal{A}}$ acts on the domain $\mathcal{D}(\tilde{\mathcal{A}})=\{f+ig:f,g\in\mathcal{D}(\mathcal{A})\}$ as $\tilde{\mathcal{A}}(f+ig)=\mathcal{A}f+i\mathcal{A}g$.

Theorem II.3: *The following statements are equivalent to each other:*

(1) The Markov process ξ is reversible;
(2) $T(t)=T^*(t)$ for any $t\geqslant 0$;
(3) $\{T^*(t)\}$ is a strongly continuous contraction semigroup on $L^2(X,\mu)$, and its infinitesimal generator $\mathcal{A}^-=\mathcal{A}$;
(4) $\mathcal{A}$ is symmetric, i.e., $\langle\mathcal{A}f,g\rangle=\langle f,\mathcal{A}g\rangle$ for any $f,g\in\mathcal{D}(\mathcal{A})$;
(5) $\tilde{\mathcal{A}}$ is self-adjoint.

Proof: (1)$\Leftrightarrow$(2): ξ is reversible if and only if $E[f(\xi_0)g(\xi_t)]=E[f(\xi_t)g(\xi_0)]$ for any $f,g\in L^2$ and $t\geqslant 0$. By (2), it is equivalent to that $\langle f,T(t)g\rangle=\langle T(t)f,g\rangle$, i.e., $T(t)=T^*(t)$ for any $t\geqslant 0$.

(2)$\Rightarrow$(3) is obvious.

(3)$\Rightarrow$(4): Since $\mathcal{A}=\mathcal{A}^-$, $\mathcal{A}\subset\mathcal{A}^*$ by Remark II.2. Therefore, $\mathcal{A}$ is symmetric.

(4)$\Rightarrow$(2): Let $\{R(\lambda):\lambda>0\}$ be the resolvent operators of the semigroup $\{T(t)\}$. For any $f\in L^2$, $R(\lambda)f\in\mathcal{D}(\mathcal{A})$. Since $\mathcal{A}$ is symmetric,

$$\langle\mathcal{A}R(\lambda)f,R(\lambda)g\rangle=\langle R(\lambda)f,\mathcal{A}R(\lambda)g\rangle,\quad\forall f,g\in L^2,\lambda>0.$$

Since $(\lambda I-\mathcal{A})R(\lambda)=id$, $\langle f,R(\lambda)g\rangle=\langle R(\lambda)f,g\rangle$ for any $\lambda>0$. By the inverse Laplace transform, $\langle f,T(t)g\rangle=\langle T(t)f,g\rangle$ for any $t\geqslant 0$. Hence $T(t)=T^*(t)$ for any $t\geqslant 0$.

(4)$\Leftrightarrow$(5): It is not hard to check that $\mathcal{A}$ is symmetric if $\tilde{\mathcal{A}}$ is self-adjoint. Suppose that $\mathcal{A}$ is symmetric. So is $\tilde{\mathcal{A}}$. Denote, respectively, by $\rho(\tilde{\mathcal{A}})$ and $\sigma(\tilde{\mathcal{A}})$ the resolvent set and the spectrum set of $\tilde{\mathcal{A}}$. Since $\tilde{\mathcal{A}}$ is the generator of the strongly continuous and contractive semigroup $\{\tilde{T}(t)\}$, it is closed, and from the Hille–Yosida theorem follows that $(0,+\infty)\subset\rho(\tilde{\mathcal{A}})$. Notice that the spectrum set of a closed symmetric operator can only be one of the following four cases: (1) the closure of the upper half complex plane; (2) the closure of the lower half complex plane; (3) the whole plane and (4) a subset of the real numbers. It follows that $\sigma(\tilde{\mathcal{A}})\subset(-\infty,0]$. Hence $\tilde{\mathcal{A}}$ is self-adjoint. ■

Remark II.4: The equivalence among (2), (3), and (4) in Theorem II.3 is already known. We present the proof here for the convenience of the reader and for the completeness of the discussion.

III. GREEN–KUBO FORMULA FOR REVERSIBLE MARKOV PROCESSES

In this section we use Theorem II.3 to prove that the Green–Kubo formula holds for reversible Markov processes. As before, let $\xi=\{\xi_t\}_{t\geqslant 0}$ be a stationary Markov process. Then $E[f(\xi_{t+u})|\xi_t=x]=T(u)f(x)$ for any $f\in L^2(X,\mu)$ and $t,u\geqslant 0$.

Proposition III.1: For any $f\in\mathcal{D}(\mathcal{A})$,

$$\lim_{u\downarrow 0}\frac{1}{u}E[f(\xi_{t+u})-f(\xi_t)|\xi_t=x]=\mathcal{A}f(x) \quad in\ L^2(X,\mu). \tag{4}$$

For any $f,g\in\mathcal{D}(\mathcal{A})$ *such that* $fg\in\mathcal{D}(\mathcal{A})$,

$$\lim_{u\downarrow 0}\frac{1}{u}E[(f(\xi_{t+u})-f(\xi_t))(g(\xi_{t+u})-g(\xi_t))|\xi_t=x]$$
$$=\mathcal{A}(fg)(x)-(g\mathcal{A}f)(x)-(f\mathcal{A}g)(x) \quad in\ L^1(X,\mu). \tag{5}$$

Proof: Equation (4) is just the definition of the infinitesimal generator. It is sufficient to prove (5) in the case $t=0$ since ξ is stationary. For any functions f,g,

$$(f(\xi_u)-f(\xi_0))(g(\xi_u)-g(\xi_0))=(fg)(\xi_u)-(fg)(\xi_0)-f(\xi_0)(g(\xi_u)-g(\xi_0))$$
$$-(f(\xi_u)-f(\xi_0))g(\xi_0).$$

We then obtain the result since

$$\frac{1}{u}E[f(\xi_0)(g(\xi_u)-g(\xi_0))|\xi_0=x]=\frac{1}{u}f(x)E[g(\xi_u)-g(\xi_0)|\xi_0=x]\to f(x)\mathcal{A}g(x)$$

as u decreases to 0. ■

Definition III.2: For any $f\in\mathcal{D}(\mathcal{A})$, *the drift coefficient of* ξ *at point* x *with respect to* f *is defined as*

$$V^f(x)=\lim_{u\downarrow 0}\frac{1}{u}E[f(\xi_u)-f(\xi_0)|\xi_0=x].$$

Since ξ is stationary and $V^f(x)=\mathcal{A}f(x)$, we have $E[V^f(\xi_t)]=0,\ \forall t\geqslant 0$.

Definition III.3: For any $f,g\in\mathcal{D}(\mathcal{A})$ *such that* $fg\in\mathcal{D}(\mathcal{A})$, *the diffusion coefficient of* ξ *at point* x *with respect to* $\{f,g\}$ *is defined as*

$$D^{f,g}(x)=\lim_{u\downarrow 0}\frac{1}{u}E[(f(\xi_u)-f(\xi_0))(g(\xi_u)-g(\xi_0))|\xi_0=x].$$

Theorem III.4: [*Green–Kubo Formula*] *Assume that the stationary Markov process* ξ *is reversible. Then, for any* $f,g\in\mathcal{D}(\mathcal{A})$ *such that* $fg\in\mathcal{D}(\mathcal{A})$,

$$\frac{1}{2}\int D^{f,g}(x)\mu(\mathrm{d}x)=\int_0^{+\infty}E[V^f(\xi_t)V^g(\xi_0)]\mathrm{d}t.$$

Proof: By Proposition III.1 and (2),

$$E[V^f(\xi_t)V^g(\xi_0)]=E[\mathcal{A}f(\xi_t)\mathcal{A}g(\xi_0)]=\langle T(t)\mathcal{A}f,\mathcal{A}g\rangle. \tag{6}$$

Since ξ is reversible, by Theorem II.3, $\tilde{\mathcal{A}}$ is self-adjoint. Hence $\tilde{\mathcal{A}}$ has a spectral representation

$$\tilde{\mathcal{A}}=\int_{-\infty}^{0}\lambda\,\mathrm{d}E_\lambda\,.$$

It follows that

$$\tilde{T}(t)=\int_{-\infty}^{0}e^{\lambda t}\mathrm{d}E_\lambda\,,\quad \tilde{T}(t)\tilde{\mathcal{A}}=\int_{-\infty}^{0}e^{\lambda t}\lambda\,\mathrm{d}E_\lambda\,.$$

Since $\tilde{\mathcal{A}}\varphi=\mathcal{A}\varphi$ and $\tilde{T}(t)\psi=T(t)\psi$ for any $\varphi\in\mathcal{D}(\mathcal{A})$ and $\psi\in L^2$,

$$\langle T(t)\mathcal{A}f,\mathcal{A}g\rangle=\left\langle\int_{-\infty}^{0}\lambda e^{\lambda t}\mathrm{d}E_\lambda f,\int_{-\infty}^{0}\lambda\,\mathrm{d}E_\lambda g\right\rangle=\int_{-\infty}^{0}\lambda^2e^{\lambda t}\mathrm{d}\langle E_\lambda f,g\rangle. \tag{7}$$

Denote by $|\mathrm{d}\langle E_\lambda f,g\rangle|$ the total variation measure of the sign measure $\mathrm{d}\langle E_\lambda f,g\rangle$, then by the Fubini theorem and the Cauchy–Schwartz inequality,

$$\begin{aligned}\int_0^{+\infty}\int_{-\infty}^{0}\lambda^2e^{\lambda t}|\mathrm{d}\langle E_\lambda f,g\rangle|\mathrm{d}t&=\int_{-\infty}^{0}\int_0^{+\infty}\lambda^2e^{\lambda t}\mathrm{d}t|\mathrm{d}\langle E_\lambda f,g\rangle|\\&=\int_{-\infty}^{0}(-\lambda)|\mathrm{d}\langle E_\lambda f,g\rangle|\\&\leqslant\left[\int_{-\infty}^{0}(-\lambda)\mathrm{d}\|E_\lambda f\|^2\right]^{1/2}\left[\int_{-\infty}^{0}(-\lambda)\mathrm{d}\|E_\lambda g\|^2\right]^{1/2}\\&=\langle-\mathcal{A}f,f\rangle^{1/2}\langle-\mathcal{A}g,g\rangle^{1/2}<+\infty,\end{aligned}$$

therefore, from (6) and (7) it follows that

$$\begin{aligned}\int_0^{+\infty}E[V^f(\xi_t)V^g(\xi_0)]\mathrm{d}t&=\int_0^{+\infty}\int_{-\infty}^{0}\lambda^2e^{\lambda t}\mathrm{d}\langle E_\lambda f,g\rangle\mathrm{d}t\\&=\int_{-\infty}^{0}\int_0^{+\infty}\lambda^2e^{\lambda t}\mathrm{d}t\,d\langle E_\lambda f,g\rangle\\&=\int_{-\infty}^{0}(-\lambda)\mathrm{d}\langle E_\lambda f,g\rangle\\&=\left\langle\int_{-\infty}^{0}(-\lambda)\mathrm{d}E_\lambda f,\int_{-\infty}^{0}\mathrm{d}E_\lambda g\right\rangle=-\langle\mathcal{A}f,g\rangle.\end{aligned}$$

It remains to prove that $\int D^{f,g}(x)\mu(\mathrm{d}x)=-2\langle\mathcal{A}f,g\rangle$. By Proposition III.1,

$$D^{f,g}(x)=\mathcal{A}(fg)(x)-(g\mathcal{A}f)(x)-(f\mathcal{A}g)(x).$$

Since ξ is stationary, $\int\mathcal{A}(fg)(x)\mu(\mathrm{d}x)=0$. Hence

$$\begin{aligned}\int D^{f,g}(x)\mu(\mathrm{d}x)&=\int[\mathcal{A}(fg)(x)-g\mathcal{A}f(x)-f\mathcal{A}g(x)]\mu(\mathrm{d}x)\\&=-\int g\mathcal{A}f(x)\mu(\mathrm{d}x)-\int f\mathcal{A}g(x)\mu(\mathrm{d}x)=-2\langle\mathcal{A}f,g\rangle,\end{aligned}$$

which completes the proof. ■

Example III.5: Suppose that $\xi=\{\xi_t\}_{t\geqslant 0}$ is a stationary diffusion process on $\mathbf{R}^d$ with infinitesimal generator

$$\mathcal{A}=\frac{1}{2}\nabla\cdot(A(x)\nabla)+b(x)\cdot\nabla=\frac{1}{2}\sum_{i,j=1}^{d}\frac{\partial}{\partial x_i}a_{ij}(x)\frac{\partial}{\partial x_j}+\sum_{i=1}^{d}b_i(x)\frac{\partial}{\partial x_i},$$

where $A(x)=(a_{ij}(x))_{1\leqslant i,j\leqslant d}$, $b(x)=(b_1(x),\ \ldots\ ,b_d(x))^T$, the components $a_{ij}(x)$ and $b_i(x)$ are smooth functions on $\mathbf{R}^d$, and the diffusion coefficient $A(x)$ is locally elliptic. By the construction of ξ in Ref. 29, its invariant initial distribution has a strictly positive smooth density ρ, and its transition semigroup is strongly continuous on $L^2(\mathbf{R}^d,\rho)$. As is shown in Refs. 26–29 and 31, the entropy production rate e_p of ξ can be expressed as

$$e_p=\frac{1}{2}\int_{\mathbf{R}^d}(2A^{-1}b-\nabla\log\rho)^TA(2A^{-1}b-\nabla\log\rho)(x)\rho(x)\mathrm{d}x.$$

Moreover, ξ is reversible if and only if e_p vanishes, equivalently, $2A^{-1}b=\nabla\log\rho$. Suppose $x_i,x_j,x_ix_j\in\mathcal{D}(\mathcal{A})$, $\forall i,j$. For each fixed i,j, let $f(x)=x_i$ and $g(x)=x_j$, then direct computation yields that

$$V_i(x):=V^f(x)=b_i(x)+\frac{1}{2}\sum_{k=1}^{d}\frac{\partial a_{ik}}{\partial x_k}(x),\quad V_j(x):=V^g(x)=b_j(x)+\frac{1}{2}\sum_{k=1}^{d}\frac{\partial a_{jk}}{\partial x_k}(x),$$

and $D^{f,g}(x)=a_{ij}(x)$. In fact, they are just the drift coefficients and diffusion coefficients of ξ. In case that ξ is reversible, by Theorem III.4, one can obtain the following Einstein relation:

$$\int_0^{+\infty}E[V_i(\xi_0)V_j(\xi_t)]\mathrm{d}t=\frac{1}{2}\int_{\mathbf{R}^d}a_{ij}(x)\rho(x)\mathrm{d}x,\forall i,j.$$

IV. POWER SPECTRUM OF REVERSIBLE MARKOV PROCESSES

We keep the assumptions and notations as before. By the strong continuity assumption of the transition semigroup $\{T(t):t\geqslant 0\}$, for each observable function $f\in L^2(X,\mu)$, the autocorrelation function $C^f(t)=E[f(\xi_t)f(\xi_0)]-E[f(\xi_t)]E[f(\xi_0)]$ of the stationary process $\{f(\xi_s)\}_{s\geqslant 0}$ is a continuous function of t. Hence the process $\{f(\xi_s)\}$ is L^2-continuous, i.e.,

$$\lim_{t\to 0}E|f(\xi_{s+t})-f(\xi_s)|^2=0,\quad \forall s\geqslant 0.$$

Suppose

$$\int_0^{+\infty}|C^f(t)|\mathrm{d}t<+\infty, \tag{8}$$

then by the Wiener–Khinchin theorem, the spectral distribution function of $\{f(\xi_t)\}$ has a nonnegative density

$$S^f(\phi)=\frac{1}{\pi}\int_0^{+\infty}C^f(t)\cos(\phi t)\mathrm{d}t,\quad \forall\phi\in\mathbf{R}.$$

Theorem IV.1: *Suppose that the stationary Markov process $\xi=\{\xi_t\}_{t\geqslant 0}$ is reversible, then for each observable function $f\in L^2(X,\mu)$ satisfying the condition (8), the spectral density $S^f(\phi)$ is a decreasing function on $[0,+\infty)$, hence it is Lorentz-typed.*

Proof: Let $\hat{f}=f-\int f(x)\mu(\mathrm{d}x)$, then $C^f(t)=\langle\hat{f},T(t)\hat{f}\rangle$. Since ξ is reversible, by Theorem II.3, $\tilde{\mathcal{A}}$ is self-adjoint. Hence $\tilde{\mathcal{A}}$ has a spectral representation

$$\tilde{\mathcal{A}}=\int_{-\infty}^{0}\lambda\,\mathrm{d}E_\lambda\,.$$

By the dominated convergence theorem, one has

$$\lim_{t\to+\infty}T(t)\hat{f}=\lim_{t\to+\infty}\int_{-\infty}^{0}e^{\lambda t}\mathrm{d}E_\lambda\hat{f}=E_{\{0\}}\hat{f},$$

where the convergence is in L^2 sense. Therefore,

$$\lim_{t\to+\infty}C^f(t)=\langle\hat{f},E_{\{0\}}\hat{f}\rangle=\|E_{\{0\}}\hat{f}\|^2,$$

which together with the condition (8) implies $E_{\{0\}}\hat{f}=0$. Then by the Fubini theorem, it follows that

$$\begin{aligned}S^f(\phi)&=\frac{1}{\pi}\int_0^{+\infty}\langle\hat{f},T(t)\hat{f}\rangle\cos(\phi t)\mathrm{d}t=\frac{1}{\pi}\int_0^{+\infty}\cos(\phi t)\mathrm{d}t\int_{(-\infty,0]}e^{\lambda t}\mathrm{d}\langle E_\lambda\hat{f},\hat{f}\rangle\\&=\frac{1}{\pi}\int_0^{+\infty}\cos(\phi t)\mathrm{d}t\int_{(-\infty,0)}e^{\lambda t}\mathrm{d}\langle E_\lambda\hat{f},\hat{f}\rangle=\frac{1}{\pi}\int_{(-\infty,0)}\mathrm{d}\langle E_\lambda\hat{f},\hat{f}\rangle\int_0^{+\infty}e^{\lambda t}\cos(\phi t)\mathrm{d}t\\&=\frac{1}{\pi}\int_{(-\infty,0)}\frac{|\lambda|}{\lambda^2+\phi^2}\mathrm{d}\langle E_\lambda\hat{f},\hat{f}\rangle,\end{aligned}$$

hence the spectral density $S^f(\phi)$ is a decreasing function on $[0,+\infty)$. ■

The Lorentz-typed power spectrum tells that noise could not induce any periodicity of the system modeled by the reversible Markov process ξ since the spectrum peak is just centered at $\phi=0$. Therefore, it is impossible for stochastic resonance to occur in a reversible system, whose entropy production rate vanishes.

Remark IV.2: As is shown above, if the Markov process ξ is reversible, then $C^f(t)$ decreases to $\|E_{\{0\}}\hat{f}\|^2$. Therefore, the condition that $T(t)f$ converges to $\int f(x)\mu(\mathrm{d}x)$ in $L^2(X,\mu)$ is necessary to define the spectral density $S^f(\phi)$. It can be naturally weakened to

$$\lim_{t\to+\infty}\frac{1}{t}\int_0^t T(s)f\,\mathrm{d}s=\int f(x)\mu(\mathrm{d}x).$$

Here we remark that for the stationary Markov process ξ, whether reversible or not, the distribution $\mathbf{P}$ of ξ on its canonical orbit space $(\Omega,\mathcal{F})$ is ergodic with respect to the family of left-shift operators on Ω if and only if its transition semigroup $\{T(t):t\geqslant 0\}$ is ergodic on $L^2(X,\mu)$ in sense that for each $f\in L^2(X,\mu)$,

$$\lim_{t\to+\infty}\frac{1}{t}\int_0^t T(s)f\,\mathrm{d}s=\int f(x)\mu(\mathrm{d}x),$$

where the convergence is in L^2 sense.

ACKNOWLEDGMENTS

This work is supported by the 973 Funds of China for Nonlinear Science, the NSFC 10271008, and the Doctoral Program Foundation of the Ministry of Education.

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Solvable models of Bose–Einstein condensates: A new algebraic Bethe ansatz scheme

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(Received 12 March 2003; accepted 27 May 2003)

A new algebraic Bethe ansatz scheme is proposed to diagonalize classes of integrable models relevant to the description of Bose–Einstein condensation in dilute alkali gases. This is achieved by introducing the notion of $\mathbb{Z}$-graded representations of the Yang–Baxter algebra. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1605495]

I. INTRODUCTION

Theoretical studies into the behavior of Bose–Einstein condensates (BECs) continue at a prolific rate, motivated by the experimental successes of producing condensates of atomic alkali gases[1,2] and superpositions of atomic-molecular alkali gases.[3,4] Many of the theoretical results to date have been obtained through use of the Gross–Pitaevskii mean-field theory and generalizations (see, e.g., Refs. 5–9). However, such mean-field theory approaches have limited applicability in regions of the parameter space where quantum fluctuations dominate. In these cases, only an exact treatment of the model will give a reliable description of the physics.

In our recent work we have shown that one model describing Josephson tunneling between two coupled BECs,[10,11] and another that models coherent superpositions of atomic and molecular BECs,[12] can both in fact be solved exactly in the framework of the algebraic Bethe ansatz. Our intention here is to develop a new mathematical approach which allows us to extend this method to establish that very general classes of Hamiltonians for BECs admit exact solutions. These classes of Hamiltonians cannot be solved in the usual form of the algebraic Bethe ansatz.

In this article, three classes of solvable models relevant to Bose–Einstein condensates of dilute alkali gases are determined. This is achieved by formulating a new scheme for the algebraic Bethe ansatz by introducing the notion of $\mathbb{Z}$-graded representations of the Yang–Baxter algebra. The first model we will present is a six-parameter generalization of the canonical Josephson Hamiltonian[7] (which can also be considered as a two site Bose–Hubbard model) describing a tunnel-coupled pair of trapped Bose–Einstein condensates. The Hamiltonian is also applicable to model solid state Josephson junctions and coupled Cooper pair boxes.[13] The second model we present has six free parameters and the third one has ten parameters. They both describe coherent coupling between atomic and diatomic molecular BECs with additional interactions such as S-wave scattering between the atoms, between the molecules, and between atoms and molecules. Such effects were not included in Refs. 9 and 12 but are important for a quantitative description of experiments.[14] Finally, we formulate the Slavnov formula for the scalar products between a Bethe eigenstate and an arbitrary Bethe vector, which facilitates the exact computation of form factors and correlations functions analogous to the results of Ref. 10.

II. BETHE ANSATZ FOR $\mathbb{Z}$-GRADED REPRESENTATIONS OF THE YANG–BAXTER ALGEBRA

The main ingredient in the study of exactly solvable quantum systems through the algebraic Bethe ansatz,[15,16] is the Yang–Baxter equation

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$$R_{12}(u-v)R_{13}(u)R_{23}(v)=R_{23}(v)R_{13}(u)R_{12}(u-v). \tag{1}$$

Here $R_{jk}(u)$ denotes the matrix in $\mathrm{End}(V\otimes V\otimes V)$ acting nontrivially on the jth and kth spaces and as the identity on the remaining space. The R-matrix solution may be viewed as the structural constants for the Yang–Baxter algebra, denoted $\mathcal{A}$, generated by the monodromy matrix $T(u)$,

$$R_{12}(u-v)T_1(u)T_2(v)=T_2(v)T_1(u)R_{12}(u-v). \tag{2}$$

The simplest case is that for the $sl(2)$ invariant R-matrix, which will be the subject of our study, given by

$$R(u)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(u) & c(u) & 0 \\ 0 & c(u) & b(u) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3}$$

with the rational functions $b(u)=u/(u+\eta)$ and $c(u)=\eta/(u+\eta)$.

Setting

$$T(u)=\begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \tag{4}$$

it follows from the defining relations (2) that

$$\begin{aligned} &[A(u),A(v)]=[D(u),D(v)]=0, \\ &[B(u),B(v)]=[C(u),C(v)]=0, \\ &A(u)C(v)=\frac{u-v+\eta}{u-v}C(v)A(u)-\frac{\eta}{u-v}C(u)A(v), \\ &D(u)C(v)=\frac{u-v-\eta}{u-v}C(v)D(u)+\frac{\eta}{u-v}C(u)D(v). \end{aligned} \tag{5}$$

Note that there are many more relations satisfied by the generators of the Yang–Baxter algebra. However, those given above are the only ones needed for the algebraic Bethe ansatz procedure which we investigate in the following. For convenience, we extend $\mathcal{A}$ by a unit element I which we will represent by the identity matrix in any representation.

We also introduce an auxiliary operator Z, called the *grading operator*, which satisfies the relations

$$[Z,X(u)]=p\{X(u)\}.X(u), \tag{6}$$

where $X=A, B, C,$ or D and $p\{A(u)\}=p\{D(u)\}=0, p\{B(u)\}=1$ and $p\{C(u)\}=-1$. We call $p\{X(u)\}\in\mathbb{Z}$ the *gradation* of $X(u)$ and extend the gradation operation to the entire algebra by the requirement

$$p\{\theta.\phi\}=p\{\theta\}+p\{\phi\} \quad \forall\ \theta,\phi\in\mathcal{A}.$$

This definition for the grading operator is consistent with the defining relations of $\mathcal{A}$ governed by (2).

Let us now define a new class of representations of the Yang–Baxter algebra which we call $\mathbb{Z}$-graded representations. We say that a vector space V, equipped with an endomorphism z, is a $\mathbb{Z}$-graded vector space, denoted (V,z), if it admits a decomposition into subspaces

$$V=\bigoplus_{k=-\infty}^{\infty} V_k$$

such that

$$zV_k=k.V_k, \quad k\in\mathbb{Z}.$$

Note that some of the V_k may be trivial subspaces. Formally, the grading operator can be used to define the following projection operators:

$$P_k=\prod_{\substack{j=-\infty\\ j\neq k}}^{\infty}\frac{(z-jI)}{(k-j)} \tag{7}$$

such that

$$P_kP_l=\delta_{kl}P_l, \quad P_kV_j=\delta_{kj}V_k.$$

We say that a $\mathbb{Z}$-graded vector space

$$V'=\bigoplus_{k=-\infty}^{\infty} V'_k$$

is *equivalent* to V if for some $j\in\mathbb{Z}$ there exists a vector space isomorphism between V'_k and V_{j+k} for all k. This terminology is motivated by the fact that for a given (V,z) one can always generate another $\mathbb{Z}$-graded space (V',z') through the mappings $V'_k\to V_{j+k}$, $z'\to z-jI$ for any $j\in\mathbb{Z}$.

For a given $\mathbb{Z}$-graded V we say that π: $\mathcal{A}\to\mathrm{End}\,V$ provides a $\mathbb{Z}$-graded representation of $\mathcal{A}$ if $\pi(Z)=z$ and the relations (2) and (6) are preserved. In such a case we can write

$$\pi(X(u))=\sum_{j=-\infty}^{\infty}X(u,j),$$

where the matrices $X(u,j)$ satisfy

$$X(u,j)V_k=0 \quad \text{for } j\neq k.$$

More specifically, this means that for $|\psi_k\rangle\in V_k$ we have

$$\pi(X(u)Y(v))|\psi_k\rangle=X(u,k+p\{Y(u)\})Y(v,k)|\psi_k\rangle.$$

In view of the equivalence of the above-defined $\mathbb{Z}$-graded vector spaces, there can also exist equivalent representations. We can define a representation π' equivalent to π by specifying some $k\in\mathbb{Z}$ such that

$$\pi'(Z)=\pi(Z-kI)$$

and for

$$\pi'(X(u))=\sum_{j=-\infty}^{\infty}X'(u,j)$$

the matrices $X'(u,j)$ are defined by

$$X'(u,j)=X(u,j+k), \quad \forall\, j\in\mathbb{Z}.$$

For any $\mathbb{Z}$-graded representation it follows from (5) that the following hold:

$$[A(u,j),A(v,j)]=[D(u,j),D(v,j)]=0,$$

$$B(u,j)B(v,j-1)=B(v,j)B(u,j-1),$$

$$C(u,j)C(v,j+1)=C(v,j)C(u,j+1), \tag{8}$$

$$A(u,j)C(v,j+1)=\frac{u-v+\eta}{u-v}C(v,j+1)A(u,j+1)-\frac{\eta}{u-v}C(u,j+1)A(v,j+1),$$

$$D(u,j)C(v,j+1)=\frac{u-v-\eta}{u-v}C(v,j+1)D(u,j+1)+\frac{\eta}{u-v}C(u,j+1)D(v,j+1),$$

From the defining relations (2) the transfer matrix defined by $\tau(u)=A(u)+D(u)$ commutes for different values of the spectral parameter u; viz.

$$[\tau(u),\tau(v)]=0.$$

Moreover, we may express the representation $\pi(\tau(u))$ of the transfer matrix as

$$\pi(\tau(u))=\sum_{j=-\infty}^{\infty}\tau(u,j)$$

such that

$$\tau(u,j)V_k=0 \quad \text{for } j\neq k$$

and

$$[\tau(u,j),\tau(v,k)]=0, \quad \forall\, j,k.$$

Since $p\{\tau(u)\}=0$, the diagonalization of $\pi(\tau(u))$ is thus reduced to the diagonalization of each of the matrices $\tau(u,j)$ on the $\mathbb{Z}$-graded component V_j, where we have

$$[\tau(u,j),\tau(v,j)]=0.$$

We may restrict our attention to the case of $\tau(u,0)$, as each $\tau(u,j)$ is equivalent to some $\tau'(u,0)$ through the use of equivalent representations as introduced earlier.

In order to formulate the algebraic Bethe ansatz solution for this class of representations, we assume the existence of a pseudovacuum vector $|\chi\rangle\in V_k$ such that

$$A(u,k)|\chi\rangle=\alpha(u,k)|\chi\rangle,$$

$$B(u,k)|\chi\rangle=0,$$

$$C(u,k)|\chi\rangle\neq 0,$$

$$D(u,k)|\chi\rangle=\delta(u,k)|\chi\rangle.$$

The above implies that $|\chi\rangle$ is a maximal weight vector with respect to Z. Without loss of generality we can choose $k=M$, again due to the equivalence of representations discussed earlier, and look for Bethe states defined by

$$\Psi(v_1,\ldots,v_M)\equiv\Psi(\{v_i\})=C(v_1,1)C(v_2,2)\cdots C(v_M,M)|\chi\rangle. \tag{9}$$

It is easy to check that this Bethe state is symmetric with respect to the variables v_i, a feature which plays a crucial role in the following. Acting $A(u,0)$ and $D(u,0)$ on the Bethe state we have

$$A(u,0)\Psi(\{v_i\})=\alpha(u,M)\prod_{i=1}^{M}\frac{u-v_i+\eta}{u-v_i}\Psi(\{v_i\})+\sum_{i=1}^{M}\mathcal{M}_i(u,\{v_j\})\Psi(v_1,\ldots,v_{i-1},u,v_{i+1},\ldots,v_M),$$

$$D(u,0)\Psi(v_1,\ldots,v_M)=\delta(u,M)\prod_{i=1}^{M}\frac{u-v_i-\eta}{u-v_i}\Psi(\{v_i\})+\sum_{i=1}^{M}\mathcal{N}_i(u,\{v_j\})\Psi(v_1,\ldots,v_{i-1},u,v_{i+1},\ldots,v_M), \tag{10}$$

with

$$\mathcal{M}_i(u,\{v_j\})=-\frac{\eta}{u-v_i}\alpha(v_i,M)\prod_{j\neq i}^{M}\frac{v_i-v_j+\eta}{v_i-v_j},$$
$$\mathcal{N}_i(u,\{v_j\})=\frac{\eta}{u-v_i}\delta(v_i,M)\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j}. \tag{11}$$

Requiring

$$\mathcal{M}_i(u,\{v_j\})+\mathcal{N}_i(u,\{v_j\})=0$$

forces $\Psi(v_1,\ldots,v_M)$ to be an eigenstate of $\tau(u,0)$ and leads to the Bethe ansatz equations

$$\frac{\alpha(v_i,M)}{\delta(v_i,M)}=\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j+\eta},\quad i=1,\ldots,M. \tag{12}$$

The corresponding eigenvalue of the matrix $\tau(u,0)$ is

$$\Lambda(u,\{v_i\})=\alpha(u,M)\prod_{i=1}^{M}\frac{u-v_i+\eta}{u-v_i}+\delta(u,M)\prod_{i=1}^{M}\frac{u-v_i-\eta}{u-v_i}.$$

III. EXPLICIT $\mathbb{Z}$-GRADED REALIZATIONS

Next we give two nontrivial $\mathbb{Z}$-graded realizations of the algebra $\mathcal{A}$. One is expressible in terms of two Heisenberg algebras with generators a_i, $a_i^\dagger$, $i=1,2$ and reads $X(u,j)=\tilde{X}(u,j)P_j$ with

$$\tilde{A}(u,j)=u^2+\eta uN+\eta^2N_1N_2-\eta(N_1-N_2)\omega(N+jI)-\omega^2(N+jI)+a_2^\dagger a_1,$$
$$\tilde{B}(u,j)=(u+\omega(N+jI)+\eta N_1)a_2+\eta^{-1}a_1,$$
$$\tilde{C}(u,j)=a_1^\dagger(u-\omega(N+jI)+\eta N_2)+\eta^{-1}a_2^\dagger,$$
$$\tilde{D}(u,j)=a_1^\dagger a_2+\eta^{-2}. \tag{13}$$

Above, P_j are the projections defined by (7), $N_i=a_i^\dagger a_i$, $N=N_1+N_2$ and $\omega(x)$ is an arbitrary polynomial function of x. Note that in the case when $\omega(x)$ is constant, the above-noted realization reduces to that discussed in Refs. 10 and 11 and is factorizable into two local representations of the Yang–Baxter algebra expressible in terms of the two Heisenberg algebras. It is important to note that for generic $\omega(x)$ no such factorization exists.

The representation acts on the infinite dimensional Fock space spanned by the vectors

$$|m,n\rangle=(a_1^\dagger)^m(a_2^\dagger)^n|0\rangle, \quad m,n=0,1,2,\ldots,\infty. \tag{14}$$

For this representation, we choose the pseudovacuum $|\chi\rangle$ as the Fock vacuum $|0\rangle$. The representation of the grading operator Z is chosen to be

$$\pi(Z)=M.I-N.$$

We then have

$$\alpha(u,M)=u^2-\omega^2(M), \quad \delta(u,M)=\eta^{-2} \tag{15}$$

and the Bethe ansatz equations become

$$\eta^2(v_i^2-\omega^2(M))=\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j+\eta} \tag{16}$$

for the diagonalization of the matrix $\tau(u,0)$. The eigenstates (9) in this instance are also eigenstates of the total particle number N with eigenvalue M.

Another $\mathbb{Z}$-graded realization of the Yang–Baxter algebra is $X(u,j)=\tilde{X}(u,j)P_j$ with

$$\begin{aligned}
\tilde{A}(u,j)&=-\eta u^2+u(1-\eta^2(K_z+N_c)-\eta\omega(K_z+N_c+jI))+\eta K_z\\
&\quad-\eta^2K_z\omega(K_z+N_c+jI)-\eta^3N_cK_z+\eta^2cK_+,\\
\tilde{B}(u,j)&=\eta(1-\eta u-\eta\omega(K_z+N_c+jI)-\eta^2N_c)K_--\eta c(u-\eta K_z),\\
\tilde{C}(u,j)&=\eta c^\dagger(u+\eta K_z)-\eta K_+,\\
\tilde{D}(u,j)&=u-\eta K_z+\eta^2c^\dagger K_-.
\end{aligned} \tag{17}$$

Here, the operators $c, c^\dagger$ form a Heisenberg algebra, with $N_c=c^\dagger c$, and the operators K_z, K_+, K_- satisfy the relations of the $su(1,1)$ algebra $[K_z,K_\pm]=\pm K_\pm$, $[K_+,K_-]=-2K_z$. As in the previous example, $\omega(x)$ is an arbitrary polynomial function of x and the above realization is factorizable only in the case when $\omega(x)$ is constant.

For this representation, we choose the pseudovacuum $|\chi\rangle$ as the tensor product of the Fock vacuum $|0\rangle$ with a lowest weight state for the algebra $su(1,1)$ of weight κ. The representation of the grading operator may be chosen as

$$\pi(Z)=M.I-K_z-N_c+\kappa.$$

Then,

$$\alpha(u,M)=(1-\eta u-\eta\omega(M))(u+\eta\kappa), \quad \delta(u,M)=u-\eta\kappa \tag{18}$$

and the Bethe ansatz equations are

$$(1-\eta v_i-\eta\omega(M))\left(\frac{v_i+\eta\kappa}{v_i-\eta\kappa}\right)=\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j+\eta}. \tag{19}$$

IV. THREE MODELS OF BOSE–EINSTEIN CONDENSATES

A. Model 1: Two coupled BECs

Consider the following general Hamiltonian describing Josephson tunneling between two coupled Bose–Einstein condensates

$$H=U_{11}N_1^2+U_{12}N_1N_2+U_{22}N_2^2+\mu_1N_1+\mu_2N_2-\frac{\mathcal{E}_J}{2}(a_1^\dagger a_2+a_2^\dagger a_1). \tag{20}$$

The above-mentioned Hamiltonian generalizes the canonical Josephson Hamiltonian studied in Refs. 10 and 11 in that the couplings U_{11},U_{22} for the S-wave scattering terms can be chosen arbitrarily. It also describes a pair of Cooper pair boxes with capacitive coupling.[13] In the limit $U_{22}\to 0$, then $\langle N_2\rangle \gg \langle N_1\rangle$, which can be considered as a single Cooper pair box coupled to a reservoir.

It is an algebraic exercise to show that the Hamiltonian is related with the matrix $\tilde{\tau}(u,0)=\tilde{A}(u,0)+\tilde{D}(u,0)$ through

$$H=-\frac{\mathcal{E}_J}{2}[\tilde{\tau}(0,0)-\eta^{-2}+(\alpha N+\beta)^2-\eta\sigma N-\eta\delta N^2].$$

Here we have chosen $\omega(N)=\alpha N+\beta$ and the coupling constants are identified as

$$\eta^2=\frac{2(U_{11}+U_{22}-U_{12})}{\mathcal{E}_J},$$

$$\alpha=\frac{U_{11}-U_{22}}{\eta\mathcal{E}_J},$$

$$\beta=\frac{\mu_1-\mu_2}{\eta\mathcal{E}_J},$$

$$\sigma=\frac{\mu_1+\mu_2}{\eta\mathcal{E}_J},$$

$$\delta=\frac{U_{11}+U_{22}}{\eta\mathcal{E}_J}.$$

Noting that

$$N=\eta^{-1}\frac{d\tilde{\tau}}{du}(0,0),$$

the above demonstrates that the Hamiltonian (20) is expressible solely in terms of the matrix $\tilde{\tau}(u,0)$ and its derivative.

Since $[H,N]=0$, the Hamiltonian is block diagonal on the Fock basis (14). Thus on a subspace of the Fock space with fixed particle number N, the diagonalization of $\tilde{\tau}(u,0)$ is equivalent to the diagonalization of $\tau(u,0)$ presented earlier in the Bethe ansatz framework. We then deduce that the solution of (20) for the energy spectrum is

$$E=-\frac{\mathcal{E}_J}{2}\left[\eta^{-2}\prod_{i=1}^{N}\frac{v_i+\eta}{v_i}-(\alpha N+\beta)^2\prod_{i=1}^{N}\frac{v_i-\eta}{v_i}-\eta^{-2}+(\alpha N+\beta)^2-\eta\sigma N-\eta\delta N^2\right], \tag{21}$$

where the parameters $\{v_i\}$ are subject to the Bethe ansatz equations

$$\eta^2(v_i^2-(\alpha N+\beta)^2)=\prod_{j\neq i}^{N}\frac{v_i-v_j-\eta}{v_i-v_j+\eta}.$$

B. Model 2: Homo-atomic-molecular BECs

Next we turn our attention to a two-mode model for an atomic-molecular Bose–Einstein condensate with identical atoms. The Hamiltonian takes the form

$$H=U_{aa}N_a^2+U_{ac}N_aN_c+U_{cc}N_c^2+\mu_aN_a+\mu_cN_c+\Omega(a^\dagger a^\dagger c+c^\dagger aa), \tag{22}$$

which acts on a basis of Fock states analogous to (14). For the case of ^{87}Rb, all of these parameters have been estimated from experiment (see Ref. 8). In the experiment described in Ref. 4, the parameter U_{aa} was varied significantly with a magnetic field.

The Hamiltonian commutes with the total atom number $N=N_a+2N_c$. In terms of a realization of the algebra $su(1,1)$ through

$$K_+=\frac{(a^\dagger)^2}{2},\quad K_-=\frac{a^2}{2},\quad K_z=\frac{2N_a+1}{4}, \tag{23}$$

one may establish the relation between the Hamiltonian and the corresponding transfer matrix $\tilde{\tau}(u,0)=\tilde{A}(u,0)+\tilde{D}(u,0)$ arising from the the realization (17) of the Yang-Baxter algebra is

$$H=\sigma+\delta(N/2+1/4)+\gamma(N/2+1/4)^2+2\eta^{-2}\Omega\tilde{\tau}(0,0),$$

with

$$\frac{d\tilde{\tau}}{du}(0,0)=2-\eta(\eta+\alpha)(N/2+1/4)-\eta\beta.$$

Above we have chosen

$$\omega(K_z+N_c)=\alpha(K_z+N_c)+\beta=\alpha(N/2+1/4)+\beta$$

and the following identification has been made for the coupling constants:

$$\eta=\frac{4U_{aa}+U_{cc}-2U_{ac}}{2\Omega},$$

$$\alpha=\frac{U_{cc}-4U_{aa}}{2\Omega},$$

$$\beta=\frac{2\mu_c-4\mu_a+4U_{aa}-U_{ac}}{4\Omega},$$

$$\sigma=\frac{U_{aa}-2\mu_a}{4},$$

$$\delta=\frac{2\mu_c-U_{ac}}{2},$$

$$\gamma=U_{cc}.$$

By the same argument as before, we conclude that the exact solution for the energy spectrum of (22) is determined by

$$E=\sigma+\delta(M+\kappa)+\gamma(M+\kappa)^2 +2\eta^{-1}\kappa\Omega\left[(1-\eta(\alpha(M+\kappa)+\beta))\prod_{i=1}^{M}\frac{v_i-\eta}{v_i}-\prod_{i=1}^{M}\frac{v_i+\eta}{v_i}\right], \tag{24}$$

where the parameters v_i satisfy the Bethe ansatz equations

$$[1-\eta v_i-\eta(\alpha(M+\kappa)+\beta)]\left(\frac{v_i+\eta\kappa}{v_i-\eta\kappa}\right)=\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j+\eta}. \tag{25}$$

For the representation (23) of the $su(1,1)$ algebra there are two lowest weight vectors; viz. the Fock vacuum $|0\rangle$ and the one particle state $a^\dagger|0\rangle$. It follows that the allowed values for κ in (24) and (25) are $\kappa=1/4, 3/4$. This demonstrates that the solution of the model depends on whether the total particle number $N=2M+2\kappa-1/2$ is even or odd, the effects of which on the energy spectrum can be seen through numerical analysis (cf. Ref. 12).

C. Model 3: Hetero-atomic-molecular BECs

The previous construction can be extended to model an atomic-molecular Bose–Einstein condensate with two distinct species of atoms, denoted a and b. For this case the Hamiltonian takes the form

$$H=U_{aa}N_a^2+U_{bb}N_b^2+U_{cc}N_c^2+U_{ab}N_aN_b+U_{ac}N_aN_c +U_{bc}N_bN_c+\mu_aN_a+\mu_bN_b+\mu_cN_c+\Omega(a^\dagger b^\dagger c+c^\dagger ba), \tag{26}$$

which commutes with the total atom number $N=N_a+N_b+2N_c$ and $\mathcal{I}=N_a-N_b$. Here the model acts on the Fock space spanned by the vectors

$$|l,m,n\rangle=(a^\dagger)^l(b^\dagger)^m(c^\dagger)^n|0\rangle.$$

In order to show the solvability of this model, we adopt the realization of the $su(1,1)$ algebra given by

$$K_+=a^\dagger b^\dagger,\quad K_-=ab,\quad K_z=\frac{N_a+N_b+1}{2}, \tag{27}$$

and observe that the operator $\mathcal{I}$ commutes with the $su(1,1)$ algebra in this representation, hence taking a constant value in any irreducible representation. Due to the symmetry upon interchanging the labels a and b, we can assume without loss of generality that the eigenvalues of $\mathcal{I}$ are non-negative. In particular, note then that the lowest weight states for this realization are of the form

$$|m\rangle=(a^\dagger)^m|0\rangle,\quad m=0,1,2,\ldots$$

and $K_z|m\rangle=(m/2+1/2)|m\rangle$. We conclude that the lowest weight labels κ can be taken from the set $\{1/2, 1, 3/2,\ldots\}$ and the eigenvalue of $\mathcal{I}$ on the irreducible representation labeled by κ is $(2\kappa-1.)$

For this case the relation between the Hamiltonian and the corresponding matrix $\tilde{\tau}(u,0)$ is

$$H=\sigma+\delta(N/2+1/2)+\lambda(N/2+1/2)^2+\rho\mathcal{I}+\nu\mathcal{I}^2+\xi\mathcal{I}(N/2+1/2)+\eta^{-2}\Omega\tilde{\tau}(0,0) \tag{28}$$

with

$$\frac{d\tilde{\tau}}{du}(0,0)=2-\eta(\eta+\alpha)(N/2+1/2)-\eta\beta\mathcal{I}-\eta\gamma.$$

Above we have chosen

$$\omega(K_z+N_b)=\alpha(K_z+N_c)+\beta(2\kappa-1)+\gamma=\alpha(N/2+1/2)+\beta\mathcal{I}+\gamma$$

and the coupling constants are related through the relations

$$\eta=\frac{U_{aa}+U_{bb}+U_{cc}+U_{ab}-U_{ac}-U_{bc}}{\Omega},$$

$$\alpha=\frac{U_{cc}-U_{aa}-U_{bb}-U_{ab}}{\Omega},$$

$$\beta=\frac{2U_{bb}-2U_{aa}+U_{ac}-U_{bc}}{2\Omega},$$

$$\gamma=\frac{2U_{aa}+2U_{bb}+2U_{ab}-U_{ac}-U_{bc}+2\mu_c-2\mu_a-2\mu_b}{2\Omega},$$

$$\sigma=\frac{U_{aa}+U_{bb}+U_{ab}-2\mu_a-2\mu_b}{4},$$

$$\delta=\frac{2\mu_c-U_{ac}-U_{bc}}{2},$$

$$\lambda=U_{cc},$$

$$\rho=\frac{U_{bb}-U_{aa}+\mu_a-\mu_b}{2},$$

$$\nu=\frac{U_{aa}+U_{bb}-U_{ab}}{4},$$

$$\xi=\frac{U_{ac}-U_{bc}}{2}.$$

The exact solution in this instance reads

$$E=\sigma+\delta(M+\kappa)+\lambda(M+\kappa)^2+\rho(2\kappa-1)+\nu(2\kappa-1)^2+\xi(2\kappa-1)(M+\kappa)$$
$$+\eta^{-1}\kappa\Omega\left[(1-\eta(\alpha(M+\kappa)+\beta(2\kappa-1)+\gamma))\prod_{i=1}^{M}\frac{v_i-\eta}{v_i}-\prod_{i=1}^{M}\frac{v_i+\eta}{v_i}\right],$$

where the parameters v_i satisfy the Bethe ansatz equations

$$[1-\eta v_i-\eta(\alpha(M+\kappa)+\beta(2\kappa-1)+\gamma)]\left(\frac{v_i+\eta\kappa}{v_i-\eta\kappa}\right)=\prod_{j\neq i}^{M}\frac{v_i-v_j-\eta}{v_i-v_j+\eta} \tag{29}$$

and the total atom number is given by $N=2M+2\kappa-1$.

V. WAVE FUNCTION SCALAR PRODUCTS

Recall that in the usual algebraic Bethe ansatz for the algebra $\mathcal{A}$ there is a formula originally due to Slavnov[17] (see also Refs. 15 and 18) for the wave function scalar products. The Slavnov formula still applies in the $\mathbb{Z}$-graded case and takes the usual form

$$S_M(\{u_j\},\{v_k\})=\Phi(\{u_j\})\Psi(\{v_k\})=\Phi(\{v_k\})\Psi(\{u_j\})=\frac{\det T(\{u_j\},\{v_k\})}{\det V(\{u_j\},\{v_k\})}, \tag{30}$$

with the entries of the $M\times M$ matrices T and V given by

$$T_{ab}=\frac{\partial}{\partial v_a}\Lambda(u_b,\{v_k\}), \quad V_{ab}=\frac{1}{u_b-v_a}, \quad a,b=1,\ldots,M.$$

$\Phi(\{u_i\})$ is the left vector

$$\Phi(u_1,\ldots,u_M)=\langle\chi|B(u_M,M)\cdots B(u_1,1).$$

Above, we have adopted the usual convention to scale the Yang–Baxter algebra such that $\delta(u,M)=1$. Also, $\{v_k\}$ provide a solution of the Bethe ansatz equation (12) and the parameters $\{u_j\}$ can be chosen arbitrarily.

The Yang–Baxter algebra $\mathcal{A}$ admits a conjugation operation $\dagger:\mathcal{A}\to\mathcal{A}$ defined by

$$A(u)^\dagger=A(u), \quad B(u)^\dagger=C(u), \quad C(u)^\dagger=B(u), \quad D(u)^\dagger=D(u)$$

and extended to all of $\mathcal{A}$ through

$$(\theta.\phi)^\dagger=\phi^\dagger.\theta^\dagger, \quad \forall\ \theta,\phi\in\mathcal{A}$$

such that the defining relations (2) are preserved. Consequently the right vector $\Phi(v_1,\ldots,v_M)^\dagger$ is also an eigenvector of the transfer matrix whenever the Bethe ansatz equations for the parameters $\{v_i\}$ are satisfied. However, it is apparent that the $\mathbb{Z}$-graded representations (13) and (17) we have introduced are not unitary, and generally

$$\Phi(\{v_i\})^\dagger\neq\Psi(\{v_i\}).$$

On the other hand, numerical analysis we have undertaken for the above models indicates that for fixed particle numbers, and generic values of the coupling parameters, the energy spectrum is free of degeneracies. This is presumably due to the fact that the only Lie algebra symmetries for these models are $u(1)$ invariances corresponding to conservation of particle numbers, and the nondegenerate spectra are examples of Hund's noncrossing rule.[19,20] Whenever this is the case, we can conclude that

$$\Phi(\{v_i\})^\dagger=K\Psi(\{v_i\})$$

for some constant K and the Slavnov formula can still be invoked for the computation of form factors and correlation functions (cf. the example of Ref. 10 where it was found $K=\pm1$).

VI. CONCLUSION

In conclusion we have introduced a new scheme for the algebraic Bethe ansatz to diagonalize three classes of integrable models relevant to Bose–Einstein condensates of dilute alkali gases. The extension of this construction to other types of models, such as the Jaynes–Cummings model,[21] and generalized Tavis–Cummings model discussed in Ref. 22, is straightforward.

ACKNOWLEDGMENT

This work is supported by the Australian Research Council.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

On the variational cohomology of *g*-invariant foliations

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(Received 26 March 2003; accepted 25 June 2003)

Let S be an integrable Pfaffian system. If it is invariant under a transversally free infinitesimal action of a finite dimensional real Lie algebra g, we show that the ''vertical'' variational cohomology of S is equal to the Lie algebra cohomology of g with values in the space of the ''horizontal'' cohomology in a maximum dimension. This result, besides giving an effective algorithm for the computation of the variational cohomology of an invariant Pfaffian system, provides a method for detecting obstructions to the existence of infinitesimal actions leaving a given system invariant. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1607513]

I. INTRODUCTION

We study here a problem that arises naturally in connection with the integration of differential systems invariant under finite or infinitesimal group actions, the theory of such systems, as conceived by Sophus Lie and later brought to its full light by Élie Cartan, being discussed in Ref. 7. Let $\mathcal{D}$ be such a differential system (viewed as a sub-manifold of some Jet or Grassmannian bundle) invariant under the action of a finite dimensional real Lie algebra g of infinitesimal contact transformations and let us further assume that $\mathcal{D}$ is integrable and of finite type (otherwise we are led into the realm of infinite Lie pseudogroups) and that the infinitesimal action of g operates transitively in a direction transverse to each solution (Ref. 7, Sec. 13). Then the integration of $\mathcal{D}$ can be reduced to the integration of a finite family of integrable Pfaffian systems that are invariant under the actions of Abelian or simple algebras, these infinitesimal actions being transversally free (Ref. 7, Sec. 4).

The integration of differential equations, in the sense of devising methods that will eventually lead to explicit solutions or at least that will contribute to simplify and reduce the integration problem (e.g., reduce the order of the equations), was a major theme in the second half of the last century, as witnessed by Lie's own writings (Refs. 8, 9, 11, 13). It is therefore not surprising that Lie's ultimate concern should have been precisely the search of such methods. Using the structure of continuous groups, he could easily say which, among the many integration methods known at that time, were the *best* (the sharpest, in the sense that they involved the least number of operations and the lowest orders for these operations) and would claim, with reason, that his were the best (Refs. 8, 10, 11). Inasmuch, he showed in Ref. 12 that ''*la méthode du dernier multiplicateur de Jacobi*'' was the best on the grounds that the infinite continuous group of all volume preserving transformations is simple.

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Élie Cartan abandoned this pursuit, at least as a priority, since, as he claimed, in this endeavor we most often fail rather than succeed. He was the first to point out that we should actually study the *structure* underlying an integration problem and, in understanding this structure, he created integration methods, for invariant differential systems, inconceivable at Lie's time (Refs. 2–5). For such systems, this underlying structure has a very precise meaning and is a direct consequence of the structure of g and of the prescribed invariant infinitesimal action (Refs. 1, 7, Secs. 5–6).

If the differential system $\mathcal{D}$ is invariant under the action of a contact Lie algebra g then its associated Pfaffian system S, obtained by restricting all the contact 1-forms to the underlying manifold $\mathcal{R}$ of $\mathcal{D}$, is integrable and invariant by the restriction of g. Conversely, if S is invariant by the infinitesimal action Φ of a Lie algebra g' then we can extend each vector field $\Phi(v)$, $v \in g'$, to an infinitesimal contact transformation so as to obtain a contact algebra g that leaves $\mathcal{D}$ invariant and such that $\Phi(g') = g|\mathcal{R}$. In general, the actions of g and g' are not transversally free but, as evidenced in Ref. 7, Sec. 5, one can in many cases reach this appropriate setting essentially via restriction and prolongation operations. It therefore becomes relevant, in view of applying the Lie and Cartan theory, to know whether a given integrable Pfaffian system S admits a transversally free invariant infinitesimal action of a given Lie algebra g or, more generally, of some Lie algebra g. Showing the existence of such infinitesimal actions is a rather delicate problem that has to be analyzed in each specific case since there does not seem to exist any general method. On the other hand, showing non-existence can be achieved by displaying some obstructions via cohomological methods and this is actually our main concern in this paper. One last word is due. Whereas the structure of a differential system is a global concept, the integration of such a system can, in a first approach, be viewed as a local problem. Since any integrable Pfaffian system admits locally many automorphisms, in fact, they form an infinite Lie pseudogroup of order one, there exist, in a neighborhood of each point, many transversally free infinitesimal actions leaving the system invariant and the Lie and Cartan theory can always be applied.

The Euler–Lagrange (variational) complex associated to an integrable Pfaffian system S is finite. As is usual, we call *horizontal* that part of the complex preceding the Euler operator E and *vertical* that part subsequent to this operator. The horizontal part is a finite augmentation of E and the vertical part a finite resolution. We show, in Sec. V (Theorem 1), that if S is invariant under a transversally free infinitesimal action of the Lie algebra g then the above finite resolution is equivalent, in positive dimensions, to the Lie algebra complex of g taking values in the horizontal cohomology of maximum dimension. In particular, the resulting cohomology spaces are equal whereupon any discrepancy between the two cohomologies will put in evidence an obstruction to the existence of such an infinitesimal action. The above equivalence also provides an effective method for the computation of the vertical variational cohomology of an invariant Pfaffian system.

Throughout the years, several authors have given distinct though essentially equivalent formulations to the variational complex. We adopt here the approach described in Ref. 6 since it emphasizes the relationship of this complex with the algebra of generalized symmetries. Inasmuch as the usual de Rham complex on a manifold M is the differential complex associated to the algebra of all the vector fields on M, the horizontal part of the variational complex is a de Rham complex associated to the algebra of all trivial symmetries (total derivatives) and the vertical part is a de Rham complex associated to the algebra of all generalized symmetries. Our first task, in this paper, consists in writing down explicitly the complex we shall be dealing with, namely the restriction of the general complex defined in Ref. 6 to an integrable Pfaffian system. This, unfortunately, is a rather long and boring task hence we only state, in Sec. II, a well known lemma that provides all the necessary technical information relevant to the restriction procedure and thereafter construct directly, in Secs. III and IV, the desired complex. It turns out that the trivial symmetries become simply the vector fields annihilated by S and the generalized symmetries become the equivalence classes of the infinitesimal automorphisms of S modulo the trivial symmetries. There is of course nothing new about this restricted complex, just a different make-up. Invariant systems are examined in Sec. V and some examples are discussed in Sec. VI.

For simplicity, we assume that all the data are C^∞ smooth though, in each specific case, C^k

smoothness for some k will suffice. We also assume that all the manifolds are connected and second countable though not necessarily orientable and that all the objects such as functions, vector fields, differential forms, etc. are globally defined on these manifolds unless stated otherwise (e.g., local coordinates, local generators of Pfaffian systems and distributions).

The second named author wishes to thank Piotr Mormul for some very helpful discussions.

II. PFAFFIAN SYSTEMS AND THEIR PROLONGATIONS

Let S be a Pfaffian system, for the time being not necessarily integrable, and $\Sigma = S^{\perp}$ the corresponding distribution, both defined on the manifold M (Ref. 7, Sec. 2). In terms of partial differential equations, it seems preferable to view the distribution Σ (or the Pfaffian system S) as a section of the Grassmannian bundle $\mathbf{G}_1^p M$ of linear contact elements of dimension $p = \operatorname{rank}\Sigma$ or, still better, as the submanifold $\mathcal{R}$ of $\mathbf{G}_1^p M$, an image of this section (Ref. 6, p. 614). Since the dimension p will remain unchanged throughout the present discussion, we abbreviate $\mathbf{G}_k^p M$ by $\mathbf{G}_k$, where k is the order of the contact elements under consideration. Let $\mathcal{R}_1 \subset \mathbf{G}_2$ denote the first prolongation of $\mathcal{R}$.

Lemma 1: The distribution Σ is integrable (involutive) if and only if $\mathcal{R}_1$ projects onto $\mathcal{R}$. A proof of this result can be found in Ref. 7, Sec. 13. This proof tells us, in particular, that a fiber $(\mathcal{R}_1)_X$, $X \in \mathcal{R}$, is either empty or else contains a single element, say Y. The first order linear holonomic contact element $\Sigma_X^{(1)}$ associated to Y is the unique holonomic element tangent to $\mathcal{R}$ at the point X. Since it does not make much sense to define the variational complex for other that *formally integrable* equations (or at least equations that, after prolongation, become formally integrable at large enough orders), we see that in the present situation it becomes natural to assume that Σ is integrable. This does not mean, however, that variational complexes cannot be associated to nonintegrable Pfaffian systems. In this latter context, we ought to specify or determine the dimension $q \leqslant p$ of linear contact elements for which a *sufficient number* of integral contact elements do exist (e.g., Pfaffian systems that are *in involution*, in the sense of Cartan, at dimension q) and consider the variational complex in the realm of the bundles $\mathbf{G}_k^q M$. We shall nevertheless restrict our attention to integrable systems.

When S (or Σ) is integrable, then $\mathcal{R}_1$ is the set of all second order contact elements determined by the p-dimensional integral manifolds of S and the assignement $Y \in \mathcal{R}_1 \mapsto \Sigma_X^{(1)} \subset T_X\mathcal{R}$, $X = \rho_{1,2}(Y)$, is an integrable distribution $\Sigma^{(1)}$, defined on the manifold $\mathcal{R}$, equivalent to Σ via the diffeomorphism $\beta_1 = \rho_{0,1} : \mathcal{R} \to M$. In general, the k-th prolongation $\mathcal{R}_k \subset \mathbf{G}_{k+1}$ is the set of all $(k+1)$-st order contact elements determined by the p-dimensional integral manifolds of S. Furthermore, the assignment $Y \in \mathcal{R}_k \mapsto \Sigma_X^{(k)} \subset T_X\mathcal{R}_{k-1}$, $X = \rho_{k,k+1} Y$, where $\Sigma_X^{(k)}$ is the linear holonomic contact element at order k associated to Y, is an integrable distribution $\Sigma^{(k)}$, defined on the manifold $\mathcal{R}_{k-1}$, equal to the annihilator of the restriction, to $\mathcal{R}_{k-1}$, of the canonical contact structure S_k of $\mathbf{G}_k$ ($[\Sigma^{(k)}]^{\perp} = \iota^* S_k$, $\iota : \mathcal{R}_{k-1} \hookrightarrow \mathbf{G}_k$; cf. Ref. 6, Sec. 2). For any pair of integers $h \leqslant k$, the distributions $\Sigma^{(k)}$ and $\Sigma^{(h)}$ are equivalent via the diffeomorphism $\rho_{h,k} : \mathcal{R}_{k-1} \to \mathcal{R}_{h-1}$ ($\mathcal{R}_0 = \mathcal{R}$, $\Sigma^{(0)} = \Sigma$).

III. THE HORIZONTAL OPERATOR

We now construct directly the so called *horizontal* part of the variational complex associated to an integrable Pfaffian system S, namely that part preceding the Euler operator. We denote by $\mathcal{B}$ the algebra of all the (globally defined) vector fields η tangent to the distribution $\Sigma = S^{\perp}$ ($\eta \in \Gamma(\Sigma)$) and by $\mathcal{F}$ the ring of all the (globally defined) C^{∞} functions on the underlying manifold. The dual space $\mathcal{H} = \mathcal{B}^*$, with respect to the $\mathcal{F}$-module structure, is equal to the set of global sections of the dual bundle $\Sigma^* \simeq T^*M/S$ and, correspondingly, $\wedge \mathcal{H} \simeq \Gamma(\wedge \Sigma^*)$. The differential,

$$d_H : \wedge^s \mathcal{H} \to \wedge^{s+1} \mathcal{H},$$

is defined by the usual formula:

$$d_H\mu(\eta_1,\ldots,\eta_{s+1})=\sum_i(-1)^{i+1}\theta(\eta_i)\,\mu(\eta_1,\ldots,\widehat{\eta_i},\ldots,\eta_{s+1})$$

$$+\sum_{i<j}(-1)^{i+j}\mu([\eta_i,\eta_j],\eta_1,\ldots,\widehat{\eta_i},\ldots,\widehat{\eta_j},\ldots,\eta_{s+1}),\qquad(1)$$

where the η_i are vector fields tangent to Σ, $\theta(\eta_i)$ is the usual Lie derivative and $[\eta_i,\eta_j]$ the usual Lie bracket. Let $(U;x^1,\ldots,x^p,y^1,\ldots,y^q)$ be a foliated chart of Σ for which the integral manifolds, in U, are given by the equations $y^\lambda=c^\lambda$. Then an element of $\wedge\mathcal{H}$ has the local expression

$$\mu=\sum a_{i_1\cdots i_s}dx^{i_1}\wedge\cdots\wedge dx^{i_s},$$

the coefficients $a_{i_1\cdots i_s}$ being C^∞ functions on U, and

$$d_H\mu=\sum(da_{i_1\cdots i_s}|\Sigma)\wedge dx^{i_1}\wedge\cdots\wedge dx^{i_s}=\sum\frac{\partial a_{i_1\cdots i_s}}{\partial x^i}dx^i\wedge dx^{i_1}\wedge\cdots\wedge dx^{i_s},\qquad(2)$$

where $da_{i_1\cdots i_s}|\Sigma$ (resp., dx^i) stands for the restriction of this differential to the integral manifolds of Σ.

We now extend the differential (1) by adding, in the cochains, a term that corresponds in Ref. 6 to the module $\mathcal{C}$ of all the contact 1-forms. Here we consider $\mathcal{C}=\Gamma(S)$ to be the module of all the global sections of S, take the cochain space $\Phi^{r,s}=(\wedge^r\mathcal{C})\otimes(\wedge^s\mathcal{H})$ and consider its elements as horizontal forms with values in $\wedge^r\mathcal{C}$. The extended differential,

$$d_H:(\wedge^r\mathcal{C})\otimes(\wedge^s\mathcal{H})\to(\wedge^r\mathcal{C})\otimes(\wedge^{s+1}\mathcal{H}),$$

is then defined by

$$d_H(\omega\otimes\mu)(\eta_1,\ldots,\eta_{s+1})=\sum_i(-1)^{i+1}\theta(\eta_i)[\mu(\eta_1,\ldots,\widehat{\eta_i},\ldots,\eta_{s+1})\omega]$$

$$+\sum_{i<j}(-1)^{i+j}\mu([\eta_i,\eta_j],\eta_1,\ldots,\widehat{\eta_i},\ldots,\widehat{\eta_j},\ldots,\eta_{s+1})\omega,\qquad(3)$$

where $\eta_i\in\Gamma(\Sigma)$ and $\theta(\eta_i)$ is the Lie derivative. The second term on the right hand side belongs of course to $\wedge^r\mathcal{C}$, the same being true for the first term since S is integrable and consequently $\theta(\eta_i)\,\mathcal{C}\subset\mathcal{C}$. Let

$$(U;x^1,\ldots,x^p,y^1,\ldots,y^q)$$

be a foliated chart for the distribution Σ in which the integral manifolds are given by the slices $y^\lambda=c^\lambda$. Then a typical element of $\Phi^{r,s}$ is locally a sum of terms,

$$\mu=a\,dy^{j_1}\wedge\cdots\wedge dy^{j_r}\otimes dx^{i_1}\wedge\cdots\wedge dx^{i_s}$$

and

$$d_H\mu=\sum_i\frac{\partial a}{\partial x^i}dy^{j_1}\wedge\cdots\wedge dy^{j_r}\otimes dx^i\wedge dx^{i_1}\wedge\cdots\wedge dx^{i_s},\qquad(4)$$

where dx^i stands for the restriction $dx^i|\Sigma$. The last formula as well as the formula (2), though helpful in theoretical considerations, is most often useless in practice since it requires the local integration of Σ. We can nevertheless remedy this situation as follows: We consider any coordinate system $(U;x^i,y^j)$ with the sole requirement that the family $\{dx^i|\Sigma\}$ be free at every point

of U, thus providing a field of coframes for $\Sigma^*|U$. Next, we consider the local basis $\{\eta_i\}$ of Σ defined by $\langle \eta_i, dx^j \rangle = \delta_i^j$. Since Σ is integrable and since each η_i projects onto $\partial/\partial x^i$, it follows that $[\eta_i, \eta_j] = 0$. A typical element of $\Phi^{r,s}$ can now be written locally as a sum of terms,

$$\mu = a\, \omega^{j_1} \wedge \cdots \wedge \omega^{j_r} \otimes dx^{i_1} \wedge \cdots \wedge dx^{i_s},$$

where dx^i stands for $dx^i|\Sigma$ and $\{\omega^\lambda = dy^\lambda - \Sigma_i Y_i^\lambda\, dx^i\}$ is a local basis of S. The formula (3) then reduces to

$$d_H \mu = \sum_i [\theta(\eta_i)(a\, \omega^{j_1} \wedge \cdots \wedge \omega^{j_r})] \otimes dx^i \wedge dx^{i_1} \wedge \cdots \wedge dx^{i_s}, \tag{5}$$

and a similar formula can replace (2), the derivatives $\partial a \ldots / \partial x^i$ being then replaced by $\theta(\eta_i)(a \ldots)$.

Let $\mathcal{I}^r = \mathcal{I}^r(S)$ denote the module of all the (globally defined) invariant forms ω of degree r with respect to the Pfaffian system S, namely those satisfying the following condition (Ref. 7, Sec. 4):

$$\theta(\eta)\omega = 0, \quad \forall\ \eta \in \Gamma(S^\perp).$$

Then, $\mathcal{I}^0 = \mathcal{I}$ is the ring of all the (global) first integrals of S, $\mathcal{I}^r$ is a graded $\mathcal{I}$-sub-algebra of A and the formula (3) shows that the sequence

$$0 \to \mathcal{I}^r \to \Phi^{r,0} \xrightarrow{d_H} \Phi^{r,1} \tag{6}$$

is exact. We next show that the sequence

$$0 \to \mathcal{I} \to \Phi^{0,0} \xrightarrow{d_H} \Phi^{0,1} \xrightarrow{d_H} \cdots \xrightarrow{d_H} \Phi^{0,p} \to 0 \tag{7}$$

is locally exact. In fact, let $(U; x^i, y^\lambda)$ be a foliated chart for Σ. Then the formula (2) defines, for each fixed set of values $y^\lambda = c^\lambda$, the differential of the *de Rham* complex on the corresponding slice, whereupon results the local exactness of (7) since the usual homotopy operators can be written incorporating the parameters y^λ. Let us finally show that

$$\Phi^{r,p-1} \xrightarrow{d_H} \Phi^{r,p} \to 0 \tag{8}$$

is locally exact. A typical element of $\Phi^{r,p}$ is, locally, a sum,

$$\omega = \sum a_{j_1, \ldots, j_r}\, dy^{j_1} \wedge \cdots \wedge dy^{j_r} \otimes dx^1 \wedge \cdots \wedge dx^p,$$

hence, upon integrating for example along x^1, we obtain the element

$$\Omega = \sum A_{j_1, \ldots, j_r}\, dy^{j_1} \wedge \cdots \wedge dy^{j_r} \otimes dx^2 \wedge \cdots \wedge dx^p, \quad \frac{\partial A_{[j]}}{\partial x^1} = a_{[j]},$$

such that $d_H \Omega = \omega$.

IV. THE VERTICAL OPERATOR

Let us next construct the so called *vertical* part of the Euler–Lagrange complex, namely that part subsequent to the Euler operator. We denote by $\mathcal{A}$ the algebra of all the infinitesimal automorphisms of S and by $\mathcal{B}$ the ideal of those vector fields that are tangent to $\Sigma = S^\perp$. The system

S being integrable, any vector field tangent to Σ is an infinitesimal automorphism. Based on the lemma 1, it can be shown that the algebra $\mathcal{S}(\mathcal{R})$ of generalized symmetries of the equation $\mathcal{R}$ associated to S ($\mathcal{S}(D)$ in the notations of Ref. 6, Sec. 9) identifies with $\mathcal{A}/\mathcal{B}$. The following remarks will be used later.

(a) $\mathcal{A}$ is a module over the ring $\mathcal{I}$, $\mathcal{B}$ is a module over $\mathcal{F}$, hence $\mathcal{S}$ is a module over $\mathcal{I}$.

(b) If $\xi\in\mathcal{A}$ is tangent to a leaf of S at a point x_0, then it is also tangent to this leaf at all of its points.

We now define $\Xi^r=\Phi^{r,p}/d_H\Phi^{r,p-1}$ ($p=\dim\Sigma$), denote by $\mathbf{q}_r:\Phi^{r,p}\to\Xi^r$ the quotient map and observe that Ξ^r is an $\mathcal{I}$-module since $d_H\mathcal{I}=0$. An element $\omega\otimes\mu\in(\wedge^r\mathcal{C})\otimes(\wedge^s\mathcal{H})$ can also be considered as an $\mathcal{I}$-multilinear form on $\mathcal{S}(\mathcal{R})$ with values in $\wedge^s\mathcal{H}$ by setting

$$(\omega\otimes\mu)([\xi_1],\ldots,[\xi_r])=\omega(\xi_1,\ldots,\xi_r)\mu,\quad \xi_i\in\mathcal{A},$$

where each $[\xi_i]$ is the class of ξ_i *modulo* $\mathcal{B}$. In fact, when $\eta\in\mathcal{B}$, then $(\omega\otimes\mu)(\ldots,\eta,\ldots)=0$ and consequently $(\omega\otimes\mu)([\xi_1],\ldots,[\xi_r])$ is well defined on $\mathcal{S}(\mathcal{R})$. Furthermore (Ref. 6, Sec. 11), since

$$[d_H(\omega\otimes\mu)](\xi_1,\ldots,\xi_r)=d_H[(\omega\otimes\mu)(\xi_1,\ldots,\xi_r)],$$

the form $d_H(\omega\otimes\mu)$, $\omega\otimes\mu\in(\wedge^r\mathcal{C})\otimes(\wedge^{p-1}\mathcal{H})$, considered as a multilinear form on $\mathcal{S}(\mathcal{R})$, takes values that vanish under the projection $\mathbf{q}_0:\Phi^{0,p}\to\Xi^0$. Hence, to any element $\sigma\in\Xi^r$, we can associate an $\mathcal{I}$-multilinear form $[\sigma]$, defined on $\mathcal{S}(\mathcal{R})$ and taking values in Ξ^0, as follows: We take $\Omega=\Sigma\,\omega_i\otimes\mu_i\in\Phi^{r,p}$ such that $\mathbf{q}_r(\Omega)=\sigma$ and set

$$[\sigma]([\xi_1],\ldots,[\xi_r])=\mathbf{q}_0\,\Omega([\xi_1],\ldots,[\xi_r]).$$

The mapping $\sigma\mapsto[\sigma]$ being injective (Ref. 6, Sec. 11), we are led to consider the formula

$$\begin{aligned}
&d_V(\mathbf{q}_r(\omega\otimes\mu))([\xi_1],\ldots,[\xi_{r+1}])\\
&\quad=\mathbf{q}_0\left\{\sum_i(-1)^{i+1}\theta([\xi_i])[\,\omega([\xi_1],\ldots,\widehat{[\xi_i]},\ldots,[\xi_{r+1}])\mu]\right\}\\
&\qquad+\mathbf{q}_0\left\{\sum_{i<j}(-1)^{i+j}\omega([[\xi_i],[\xi_j]],[\xi_1],\ldots,\widehat{[\xi_i]},\ldots,\widehat{[\xi_j]},\ldots,[\xi_{r+1}])\mu\right\},\qquad(9)
\end{aligned}$$

where $\omega\otimes\mu\in\Phi^{r,p}$ and $\xi_i\in\mathcal{A}$. The second term on the right hand side clearly belongs to Ξ^0. As for the first term, let us write

$$\mu_i=\omega([\xi_1],\ldots,\widehat{[\xi_i]},\ldots,[\xi_{r+1}])\mu\in\Phi^{0,p},$$

and let us assume that some $\xi_j=\eta\in\mathcal{B}$. If $j\neq i$, then $\mu_i=0$ and if $j=i$ then, since $d_H\mu_i=0$,

$$\theta(\eta)\mu_i=i(\eta)d_H\mu_i+d_Hi(\eta)\mu_i=d_Hi(\eta)\mu_i$$

and consequently $\mathbf{q}_0\,\theta(\eta)\mu_i=0$. In any case, (9) provides a well defined multilinear form on $\mathcal{S}(\mathcal{R})$ taking values in Ξ^0 and it can be shown (e.g., in coordinates) that the multilinear form $d_V(\mathbf{q}_r(\omega\otimes\mu))$ is the image of an element $\sigma\in\Xi^{r+1}$.

The Euler–Lagrange (variational) complex associated to the integrable Pfaffian system S is the finite sequence,

$$0\to\mathcal{I}\to\Phi^{0,0}\xrightarrow{d_H}\Phi^{0,1}\xrightarrow{d_H}\cdots\xrightarrow{d_H}\Phi^{0,p-1}\xrightarrow{d_H}\Phi^{0,p}\xrightarrow{E}\Xi^1\xrightarrow{d_V}\cdots\xrightarrow{d_V}\Xi^{q-1}\xrightarrow{d_V}\Xi^q\to0,$$

where E, the *Euler* operator, is the composite,

$$\Phi^{0,p} \xrightarrow{\mathbf{q}_0} \Xi^0 \xrightarrow{d_V} \Xi^1,$$

and $q = \text{rank } S$. This complex is locally exact and reduces, locally, to (7) since Ξ^r vanishes on account of (8).

V. INVARIANT PFAFFIAN SYSTEMS

Let S be an integrable Pfaffian system invariant under the infinitesimal action $\Phi: g \to \chi(M)$ of the finite dimensional real Lie algebra g on the manifold M (Ref. 7, Sec. 3). For every $v \in g$, $\Phi(v) \in \mathcal{A}$, hence the action induces a Lie algebra morphism $\Phi: g \to \mathcal{S}(\mathcal{R})$. If further we assume that the action Φ is transversally free (Ref. 7, Sec. 4), i.e., if

$$(i) \quad \dim g = \dim \Phi(g)_p, \quad \forall\ p \in M,$$

$$(ii) \quad T_p M = \Sigma_p \oplus \Phi(g)_p, \quad \forall\ p \in M,$$

then the above morphism is injective and the following result holds.

Lemma 2: The algebra $\mathcal{S}(\mathcal{R})$ is generated by $\Phi(g)$ over the ring $\mathcal{I}$ of first integrals of S, any $\mathbf{R}$-basis of $\Phi(g)$ is an $\mathcal{I}$-basis of $\mathcal{S}(\mathcal{R})$ and the $\mathcal{I}$-dual $\mathcal{S}(\mathcal{R})^*$ identifies with $\mathcal{I}^1$.

Let us next recall some properties of the invariant forms associated to S. By definition (Ref. 7, Sec. 4), the exterior form ω is an invariant form of S if $\theta(\eta)\,\omega = 0$ for all $\eta \in \Gamma(S^\perp)$. It follows that $\theta(f\,\eta)\,\omega = 0$ for any function f, hence ω is an invariant if and only if $i(\eta)\omega = i(\eta)\,d\omega = 0$, for all $\eta \in \Gamma(S^\perp)$. Consequently, ω is invariant if and only if it can be expressed locally in terms of the first integrals of S and their differentials. When ω is invariant then so are the forms $f\,\omega$, $d\omega$ and $\theta(\xi)\,\omega$, where f is a first integral and ξ an infinitesimal automorphism of S, hence the set of all invariant forms is a differential algebra over the ring $\mathcal{I}$ invariant under the infinitesimal action Φ via the Lie derivative. Let $\{v_i\}$ be a basis of g. The linear forms $\omega^i \in \mathcal{C}$ defined by the conditions $\langle \Phi(v_i), \omega^j \rangle = \delta_i^j$ are a global basis of invariant forms of S, a so-called Cartan basis (Ref. 7, Secs. 6,8), and

$$d\omega^i = \sum_{j<k} c^i_{jk}\, \omega^j \wedge \omega^k,$$

where $\{-c^i_{jk}\}$ is the set of structure constants of g with respect to the above basis. The real subspace $\Omega \subset \Gamma(T^*M)$ generated by forms ω^i only depends on Φ and acts as an $\mathbf{R}$-dual to the space $h = \Phi(g)$. Let us denote by $\mathcal{F}$ be the ring of C^∞ functions on M and by $\wedge\,\Omega$ the exterior algebra of Ω over the field $\mathbf{R}$. Since $\{\omega^i\}$ is a global basis of the Pfaffian system S, it follows that $\mathcal{C} \simeq \Omega \otimes_{\mathbf{R}} \mathcal{F}$ and, more generally, that

$$\Phi^{r,s} = (\wedge^r \mathcal{C}) \otimes_{\mathcal{F}} (\wedge^s \mathcal{H}) \simeq (\wedge^r \Omega) \otimes_{\mathbf{R}} (\wedge^s \mathcal{H}) \simeq (\wedge^r \mathcal{S}(\mathcal{R})^*) \otimes_{\mathcal{I}} (\wedge^s \mathcal{H}). \tag{10}$$

Furthermore, since $d\omega(\xi_1, \xi_2) = -\omega([\,\xi_1, \xi_2\,])$, for any $\omega \in \Omega$ and $\xi_i \in \Phi(g)$, it also follows that the formula (9) reduces, whenever $\omega \in \wedge^r \Omega$ and $\xi_i \in \Phi(g) \subset \mathcal{S}(\mathcal{R})$, to the expression

$$[\, d\omega \otimes \mathbf{q}_0 \mu + (-1)^{\deg \omega}\, \omega \wedge d_V(\mathbf{q}_0 \mu)\,]\,(\xi_1, \ldots, \xi_{r+1}), \tag{11}$$

where $d_V(\mathbf{q}_0 \mu)(\xi)$ is the Lie derivative $\mathbf{q}_0(\theta(\xi)\mu)$. We shall see later that the above formula still holds for any invariant form ω since $d_H \omega = 0$ implies $d_V \omega = d\omega$.

We next consider the elements $\sigma \in \Xi^r$ as i $\mathcal{I}$-multilinear (and skew-symmetric) forms $[\sigma]$ defined on $\mathcal{S}(\mathcal{R})$ and taking values in Ξ^0 (cf. Sec. IV). Each form $[\sigma]$ restricts to an $\mathcal{R}$-multilinear form $\tau = [\sigma]_{\mathbf{R}}$ defined on the real subspace $h \in \mathcal{S}(\mathcal{R})$ and conversely, on account of Lemma 2, each $\mathcal{R}$-multilinear form τ defined on h and taking values in $\sigma \in \Xi^0$ extends, by $\mathcal{I}$-multilinearity, to a form $[\sigma]$ defined on $\mathcal{S}(\mathcal{R})$ and such that $[\sigma]_{\mathbf{R}} = \tau$. Furthermore, since in the realm of real vector spaces the subspace $d_H(\Phi^{0,p-1})$ admits a complement in $\Phi^{0,p}$, the form

τ lifts to a real form $\overline{\tau}$ defined on h and taking values in $\Phi^{0,p}=\wedge^p\mathcal{H}$. Finally, using $\mathcal{F}$-multilinearity on h, $\overline{\tau}$ extends to an $\mathcal{F}$-multilinear form $\tilde{\tau}$ defined on $\chi(M)$ with values in $\wedge^p\mathcal{H}$ by requiring that $i(\eta)\tilde{\tau}=0$, for all $\eta\in\Gamma(\Sigma)$. We thus obtain an element $\tilde{\tau}\in\Phi^{r,p}$ such that $[\tilde{\tau}]_{\mathbf{R}}=\tau$ and consequently the assignment $\sigma\mapsto[\sigma]$ of Sec. IV becomes bijective when S is invariant under a transversally free infinitesimal action. Identifying g with h and thereafter Ω with g^*, the expression (11) or equivalently the formula (9) shows that the cochain complex defining the cohomology of g with values in Ξ^0 and relative to the representation $\rho(v)(\mathbf{q}_0\mu)=\mathbf{q}_0(\theta(\xi)\mu)$, $v\in g$, $\mu\in\Phi^{0,p}$ and $\xi=\Phi(v)$, is equal to

$$\Xi^0\overset{d_V}{\to}\Xi^1\overset{d_V}{\to}\Xi^2\overset{d_V}{\to}\cdots. \tag{12}$$

Since $\mathbf{q}_0$ is surjective, we can rewrite the above complex by

$$\Phi^{0,p}\overset{E}{\to}\Xi^1\overset{d_V}{\to}\Xi^2\overset{d_V}{\to}\cdots, \tag{13}$$

without affecting the cohomology groups in positive dimensions, the latter being the vertical part of the Euler–Lagrange complex associated to S, namely the finite resolution of E.

Theorem 1: *Let S be an integrable Pfaffian system invariant under a transversally free infinitesimal action of the Lie algebra g. Then the finite resolution of the Euler operator E is equal, in positive dimensions, to the cochain complex of the Lie algebra g with values in Ξ^0.*

Since $E=d_V\circ\mathbf{q}_0$, we also infer that the space of cocycles in $\Phi^{0,p}$ (i.e., $\ker E$) is equal to the inverse image, by $\mathbf{q}_0$, of the 0-dimensional cohomology of g, namely the inverse image of the subspace of the g-invariant elements of Ξ^0 ($\rho(v)(\mathbf{q}_0\mu)=0$, $\forall\, v\in g$). Given an integrable Pfaffian system S, we can now confront its variational cohomology with the cohomology of g taking values in Ξ^0 and eventually detect obstructions to the existence of a transversally free infinitesimal action of g leaving S invariant. When $\dim_{\mathbf{R}}\Xi^0<\infty$ (which is very seldom the case), we usually have more information on the cohomology of g. For instance, if g is semi-simple then its cohomology vanishes in dimensions one and two (Whitehead's lemmas) and consequently the same must hold for the variational cohomology.

VI. EXAMPLES

Throughout this section, we replace integrable Pfaffian systems by the corresponding integral foliations. Though all the foliations are naive, the resulting homological calculations are not always so. For the sake of not being too omissive on these calculations, we outline a few in the last example.

A. Example 1: The torus

Let $\mathcal{F}$ be the the foliation on the 2-dimensional torus T whose leaves are the cosets of a 1-dimensional sub-group H. Then $\mathcal{F}$ is invariant under the infinitesimal action generated by any element of the Lie algebra of T ($\equiv\mathbf{R}^2$) this action being transversally free as soon as this element does not belong to the Lie algebra h of H. The variational cohomology at Ξ^1 is equal to $\mathbf{R}$ and, using Green's formula, one shows that the cohomology class of an element $[\omega]\in\Xi^1$ identifies with the real number $\int_T\omega$. When the slope of a generating element of h is rational, the calculations are very simple and both spaces Ξ^0 and Ξ^1 identify with the set of all global first integrals of $\mathcal{F}$. When this slope is irrational, the global first integrals of $\mathcal{F}$ reduce to the constants and it becomes more involved to describe the spaces Ξ^0 and Ξ^1 and to calculate the cohomology. This is an example where the advantage of the Lie algebra cohomology calculations becomes apparent.

B. Example 2: The Möbius strip

Let $\mathcal{F}$ be the foliation on the Möbius strip $\mathcal{M}$ whose leaves are the ''double'' circles, except for the central circle (under the usual identification $(1,y)\equiv(-1,-y)$, $\mathcal{F}$ is the foliation induced by the segments parallel to the x-axis). Both spaces Ξ^0 and Ξ^1 identify again with the set of all global first integrals of $\mathcal{F}$ which in turn identifies with the set of all the even functions defined on the interval $]-1,1[$. The variational cohomology at Ξ^1 vanishes and, whatever the representation $\rho: g=\mathbf{R}\to \mathrm{Der}\ \Xi^0$, the cohomology of g in dimension one is nontrivial (the derivative of an even function usually ceases to be even). This disagreement shows that $\mathcal{F}$ cannot be invariant by any transversally free infinitesimal action, a fact that is geometrically obvious since such an action would provide an orientation to $\mathcal{M}$.

C. Example 3: Foliation with a compact attractor

We consider, on the infinite cylinder $C=\mathbf{R}\times S^1$ with coordinates (t,θ), the foliation $\mathcal{F}$ obtained by integrating the vector field,

$$\eta = t\frac{\partial}{\partial t}+\frac{\partial}{\partial \theta}.$$

The nature of the spaces Ξ^0 and Ξ^1 is rather involved but a straightforward calculation shows that the cohomology at Ξ^1 is null. On the other hand, whatever the representation of the Lie algebra $g=\mathbf{R}$ into $\mathrm{Der}\ \Xi^0$, the Lie algebra cohomology in dimension one cannot vanish. Consequently, the foliation $\mathcal{F}$ does not admit any 1-dimensional transversally free infinitesimal action that leaves it invariant. This fact is also geometrically obvious since the local 1-parameter group (ϕ_u) generated by any such infinitesimal action would be defined, for small u, on a whole neighborhood of the limit circle $\{0\}\times S^1$ and would transform this circle into open compact subsets of the neighboring leaves, this being of course excluded.

An entirely similar situation arises in the double solid torus (two solid tori glued by their boundaries) upon taking the Reeb foliation inside each of the tori. The common boundary torus is the unique compact leaf.

D. Example 4: Spheres and rays

On the space $M=\mathbf{R}^{p+1}-0$, let $\mathcal{F}_1$ be the foliation whose leaves are the spheres centered at the origin and $\mathcal{F}_2$ the foliation whose leaves are the rays issued from the origin. We first consider the *sphere* foliation $\mathcal{F}_1$ and calculate Ξ^0, one possible argument being as follows: Each element $\mu\in\Phi^{0,q}$ identifies canonically with a differentiable 1-parameter family $(\overline{\mu}_\rho)$ of differentiable q-forms defined on the unit sphere S^p and, under this identification, $d_H\mu\in\Phi^{0,q+1}$ also identifies with $(d\overline{\mu}_\rho)$. We next take a differentiable 1-parameter family $(\overline{\mu}_t)$, $t>0$, of p-forms on S^p. Then, upon choosing a fixed volume form Ω on S^p (e.g., the volume form associated to the induced Euclidean metric), we can determine, by integration, a differentiable function $\varphi:\mathbf{R}_+\to\mathbf{R}$ such that $\overline{\mu}_t-\varphi(t)\,\Omega$ is, for each t, a coboundary. Restating the Lemma 4.2 (p. 123) of Ref. 14 in its stronger version (as is proved in the subsequent two pages), we can use it to establish a stronger 1-parameter version of the Lemma 4.2 (p. 126) and prove in the aforementioned context that there exists a differentiable 1-parameter family $(\overline{\eta}_t)$ of $(p-1)$-forms defined on S^p such that $\overline{\mu}_t-\varphi(t)\,\Omega=d\overline{\eta}_t$. Returning to $\Phi^{0,p}$ and taking the form $\tilde{\Omega}=r^*\Omega$, $r:X\mapsto(1/\|X\|)\,X$, defined on M, we conclude that each $\mu\in\Phi^{0,p}$ determines a differentiable function φ such that $\mu-\varphi\,\tilde{\Omega}=d_H\eta$, where $\eta\in\Phi^{0,p-1}$, and consequently that Ξ^0 is equal to the set of all the real-valued differentiable functions defined on $\mathbf{R}_+$ i.e., to the set of all the global first integrals of $\mathcal{F}_1$.

Let us now calculate Ξ^1. Observing that $d\rho$ is a global generator of the Pfaffian system that annihilates $\mathcal{F}_1$, any element $\eta_1\in\Phi^{1,q}$ writes $\eta_1=\eta\wedge d\rho$, with $\eta\in\Phi^{0,q}$, and $d_H\eta_1=(d_H\eta)\wedge d\rho$ since $d_H(d\rho)=0$. Consequently, the element $\mu_1=\mu\wedge d\rho\in\Phi^{1,p}$ is equal to

$d_H\eta_1$, with $\eta_1 \in \Phi^{1,p-1}$, if and only if $\mu = d_H\eta$ hence the present calculation reduces to the previous one and Ξ^1 is again equal to the set of all the global first integrals of $\mathcal{F}_1$.

It now becomes easy to show that the variational cohomology at Ξ^1 is null. The foliation $\mathcal{F}_1$ is of course invariant under many 1-dimensional transversally free infinitesimal actions and the vanishing of the Lie algebra cohomology in dimension one is easily be checked.

We next take the *radial* foliation $\mathcal{F}_2$. Here we can proceed locally, on open sets saturated by rays, and integration along these rays will show that $\Xi^q = 0$, $0 \leqslant q \leqslant p$. The variational as well as the Lie algebra cohomologies vanish, their comparison not revealing the following geometrical facts.

(a) When p is even, there cannot exist a transversally free infinitesimal action leaving the radial foliation $\mathcal{F}_2$ invariant. In fact, since the tangent spaces to $\mathcal{F}_1$ and $\mathcal{F}_2$ are complementary, any such infinitesimal action would project onto the spheres producing an infinitesimal action operating tangentially to the spheres and, in restriction to these spheres, would be free. However, even dimensional spheres do not admit nowhere vanishing vector fields.

(b) When p is odd, such transversally free infinitesimal actions do exist only for $p = 1, 3$. Their nonexistence for $p = 7$ is essentially a consequence of the fact that S^7 is not a Lie group manifold and, for all the other values of p, that the corresponding spheres are not parallelizable.

We can enhance the variational cohomology by adding nontrivial cocycles to the space M. For example, let us take for the manifold M the portion of $\mathbf{R}^{p+1} - 0$ in between the spheres $S^p(1)$ and $S^p(2)$ and identify these two spheres by the radial map. Then $\mathcal{F}_1$ induces a foliation $\overline{\mathcal{F}_1}$ in spheres, $\mathcal{F}_2$ a foliation $\overline{\mathcal{F}_2}$ in circles (in fact, $M \simeq S^p \times S^1$) and one shows, for the foliation $\overline{\mathcal{F}_2}$, that Ξ^0 is equal to the set of all the differentiable functions defined on the sphere $S^p(1)$ or, equivalently, to the set of all the global first integrals of $\overline{\mathcal{F}_2}$. Furthermore, Ξ^r is equal to the product of $\binom{p}{r}$ copies of Ξ^0 and $\Xi^p = \Xi^0$. As for the variational cohomology, we can again apply the 1-parameter version of the Lemmas 4.2 and conclude that it vanishes at Ξ^{r+1} whenever $r+1 < p$ and that it is equal to $\mathbf{R}$ at Ξ^p. Stokes' formula will then show that the cohomology class of an element $[\omega] \in \Xi^p$ identifies with the real number $\int_M \omega$.

Returning to the geometric facts described earlier, we can retrace (a) by looking at the variational cohomology. In fact, since any vector field on an even dimensional sphere has a singularity, whatever the representation ρ of a Lie algebra g into $Der\,\Xi^0 \simeq \chi(S^p)$, the corresponding Lie algebra cohomology cannot vanish in dimension one. As for the property (b), it requires a deeper analysis that seems to be out of reach in the present context. Nevertheless, it can be shown that transversally free Abelian infinitesimal actions leaving $\overline{\mathcal{F}_2}$ invariant cannot exist since the corresponding Lie algebra cohomologies with values in Ξ^0 would vanish in dimension p thus contradicting the variational cohomology.

ACKNOWLEDGMENTS

A.K. thanks Piotr Mormul for some very helpful discussions.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Dirac operators on coset spaces

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(Received 9 April 2003; accepted 16 June 2003)

The Dirac operator for a manifold Q, and its chirality operator when Q is even dimensional, have a central role in noncommutative geometry. We systematically develop the theory of this operator when $Q=G/H$, where G and H are compact connected Lie groups and G is simple. An elementary discussion of the differential geometric and bundle theoretic aspects of G/H, including its projective modules and complex, Kähler and Riemannian structures, is presented for this purpose. An attractive feature of our approach is that it transparently shows obstructions to spin- and spin$_c$-structures. When a manifold is spin$_c$ and not spin, U(1) gauge fields have to be introduced in a particular way to define spinors, as shown by Avis, Isham, Cahen, and Gutt. Likewise, for manifolds like SU(3)/SO(3), which are not even spin$_c$, we show that SU(2) and higher rank gauge fields have to be introduced to define spinors. This result has potential consequences for string theories if such manifolds occur as D-branes. The spectra and eigenstates of the Dirac operator on spheres $S^n=\mathrm{SO}(n+1)/\mathrm{SO}(n)$, invariant under $\mathrm{SO}(n+1)$, are explicitly found. Aspects of our work overlap with the earlier research of Cahen *et al.* © *2003 American Institute of Physics.* [DOI: 10.1063/1.1607514]

I. INTRODUCTION

When a group G acts transitively on a manifold Q with stability group H at a point p, we can identify Q with the coset space G/H. Such spaces are important in the description of Goldstone modes created by the spontaneous breakdown of G to H. Models of spacetime such as the Minkowski spacetime $M^{3,1}$ or its compact Euclidean version S^4 are also of this sort. The group G in these cases is the Poincarè group and SO(5), respectively, while H is the Lorentz group and SO(4), respectively. In addition, coset spaces like $\mathbb{C}P^N$ and S^N have begun to proliferate as D-branes in string and boundary conformal field theories.

The Dirac operator for a manifold Q, and its chirality operator when Q is even-dimensional, have a central role in noncommutative geometry. That is a good motivation for their study. In this work we focus on this enterprise when Q is a coset space. In addition, in a subsequent paper, we shall develop fuzzy versions of certain coset spaces and their Dirac and chirality operators, primarily as a device to regularize quantum field theories thereon, and what we do here is also a preparation for it.

We assume throughout that G is a simple compact connected Lie group and H is a compact connected group. Without loss of generality we assume also that G is simply connected. These

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restrictions on G and H can be relaxed somewhat, G can be semi–simple for instance, and certain noncompact Lie groups G too seem approachable by our methods.

Not all G/H admit a spin-, or even a spin$_c$-structure.[3] One attractive aspect of our approach is that obstructions to spin- and spin$_c$-structure show up transparently and we can also easily see when and how we can overcome them using suitable generalized spin-structures, spin$_K$. The latter in general involve groups K of any dimension, whereas spin$_c$ ($=$spin$_{U(1)}$ in our notation) uses U(1) of dimension 1. The role of K is roughly that of a gauge group, so insisting on the existence of spinors introduces nontrivial gauge symmetry and internal degrees of freedom. In addition, typically, spin$_K$-theories are chiral, left- and right-chiral spinors transforming differently under K. This suggests that there may be a clever way to use fuzzy spaces to get the chiral fermions of the standard model.

There is a simple global appoach to differential geometry on G/H. We introduce this formalism after setting up the preliminaries in Sec. II. We follow this up in Sec. III, introducing spin- and spin$_K$-structures. Their Dirac and chirality operators are formulated in Sec. IV. We call this version of the Dirac operator ''Kähler–Dirac operator,'' as it is similar to the operator with the same name on a complex manifold. There is another equivalent version using projective modules equally useful for fuzzy physics, which we have decided to call the projective Dirac operator. The ''Dirac'' operator then refers to either of these two versions. Section V takes this up and also establishes its equivalence to the Kähler–Dirac operator. Along the way, the differential geometry of Sec. II is also translated to the language of projective modules. The cut-off versions of these expressions have an important role in fuzzy physics. In Sec. V we also explicitly consider the spheres S^n and $\mathbb{C}P^n$. In particular, for spheres, we compute the curvature and Dirac spectrum for the maximally symmetric metric. In Sec. VI we extend the preceding considerations to gravity on G/H.[4] Finally in Sec. VII we discuss the complex and Kähler structures of coset manifolds.

II. DIFFERENTIAL GEOMETRY ON G/H

A. Preliminaries

G is a simple, simply connected, connected, compact Lie group with Lie algebra $\underline{G}$. $\underline{H}$ is a subalgebra of $\underline{G}$ which by exponentiation generates a compact connected Lie group H.

We think of G concretely as $N\times N$ unitary matrices. The Lie algebra $\underline{H}$ then has a basis $\{T(\alpha)\}$ of Hermitian matrices (we follow physics conventions, more correctly $\{iT(\alpha)\}$ span $\underline{H}$), which are trace orthogonal:

$$\mathrm{Tr}T(\alpha)T(\beta)=c\,\delta_{\alpha\beta},\quad c=\mathrm{const}>0. \tag{2.1}$$

Using trace to define scalar product, $\underline{G}$ can be decomposed as the orthogonal direct sum,

$$\underline{G}=\underline{H}\oplus^{\perp}\underline{G/H}. \tag{2.2}$$

Let $\{S(i)\}$ be a basis for $\underline{G/H}$ with

$$\mathrm{Tr}S(i)S(j)=c\,\delta_{ij}. \tag{2.3}$$

We also of course have

$$\mathrm{Tr}S(i)T(\alpha)=0. \tag{2.4}$$

We denote the elements of the basis $\{T(\alpha),S(i)\}$ collectively as Σ_A, $A\in\{\alpha,i\}$.

Let Ad denote the adjoint representation of G. Then $H\subset G$ leaves $\underline{G/H}$ invariant in this representation:

$$h\,S(i)\,h^{-1}=S(j)(\mathrm{Ad}\ \ h)_{ji},\quad h\in H. \tag{2.5}$$

We refer to this representation of H on G/H as $\mathrm{Ad}_{G/H}$, and the corresponding representation of $\underline{H}$ as $\mathrm{ad}_{G/H}$. $\mathrm{Ad}_{G/H}(h)$ are real matrices as the Hermitian conjugation of (2.5) shows. They are also orthogonal as conjugation leaves the relation (2.3) invariant. Thus, if $|G|$, $|H|$ and $|G/H|=|G|-|H|$ denote the dimensions of G, H and G/H, $\{\mathrm{Ad}_{G/H}(h)\}$ is a subgroup of $SO(|G/H|)$:

$$\{\mathrm{Ad}_{G/H}(h)\}\subseteq SO(|G/H|). \tag{2.6}$$

The above discussion implies the following commutation relations:

$$[T(\alpha),T(\beta)]=ic_{\alpha\beta\gamma}T(\gamma),$$

$$[T(\alpha),S(i)]=ic_{\alpha ij}S(j), \tag{2.7}$$

$$[S(i),S(j)]=ic_{ij\alpha}T(\alpha)+ic_{ijk}S(k). \tag{2.8}$$

The structure constants c_{ABC} are real and totally antisymmetric.

We will call c_{ijk} the torsion of the space G/H. Below we will see that it plays exactly the role of the usual torsion for the canonical covariant derivative on G/H.[5] If $c_{ijk}=0$, the homogeneous space G/H is said to be "symmetric."[6] In that case, $\underline{G}$ admits the involutive automorphism:

$$\sigma \;:\; T(\alpha)\to T(\alpha),\quad S(i)\to -S(i), \tag{2.9}$$

leaving $\underline{H}$ fixed. σ lifts to an involutive automorphism Σ of G leaving H fixed, Σ being defined from

$$\Sigma \;:\; e^{i\theta_\alpha T(\alpha)}\to e^{i\theta_\alpha T(\alpha)},\quad e^{i\theta_i S(i)}\to e^{-i\theta_i S(i)}. \tag{2.10}$$

B. Tensor fields on G/H

Let W be a fixed vector space with an orthonormal basis $\{e_i\}$ which carries the representation $\mathrm{Ad}_{G/H}$ of H, $h\;:e_i\to e_j\,\mathrm{Ad}_{G/H}(h)_{ji}$. The vector space $W^{\otimes n}=W\otimes W\otimes\cdots\otimes W$ (n factors) carries the tensor product representation $\mathrm{Ad}_{G/H}^{\otimes n}=\mathrm{Ad}_{G/H}\otimes\mathrm{Ad}_{G/H}\otimes\cdots\otimes\mathrm{Ad}_{G/H}$ (n factors). Let $\mathbb{C}\equiv W^{\otimes 0}$ also denote the one–dimensional complex vector space carrying the trivial representation $\mathrm{Ad}_{G/H}^{\otimes 0}\colon h\to 1$.

Tensor fields of rank n on G/H can be defined to be equivariant functions on G with values in $W^{\otimes n}$. That means the following: for $n=0$ we have scalar fields $f^{(0)}$, complex (or $W^{\otimes 0}$) valued functions on G invariant under the right–action of H on G (equivariance):

$$f^{(0)}=\text{scalar fields:}\quad f^{(0)}(gh)=f^{(0)}(g),\;\;\forall\;\; h\in H. \tag{2.11}$$

A tensor field $f^{(1)}$ of rank 1 has values in W; we can write it as

$$f^{(1)}=f_i^{(1)}e_i,\quad f_i^{(1)}\;:\quad g\to f_i^{(1)}(g)\in\mathbb{C}. \tag{2.12}$$

Equivariance for $n=1$ means the following transformation property under the right action of H on G:

$$f_i^{(1)}(gh)e_i=f_i^{(1)}(g)\mathrm{Ad}_{G/H}(h)_{ij}e_j. \tag{2.13}$$

Therefore

$$f_i^{(1)}(gh)=f_j^{(1)}(g)\mathrm{Ad}_{G/H}(h)_{ji}. \tag{2.14}$$

Let J label the inequivalent irreducible representations of G by unitary matrices $\{D^J(g)\}$; their matrix elements in a convenient orthonormal basis are $D^J_{mn}(g)$. We have that

$$D^J_{mn}(gh)=D^J_{mn'}(g)D^J_{n'n}(h). \tag{2.15}$$

If the representation $h\to D^J(h)$ contains the identity representation of H, we can choose the basis in the representation space so that the index n in (2.15) transforms trivially when $n\in$ an appropriate index set I_0:

$$D^J_{mi_0}(gh)=D^J_{mi_0}(g),\ \forall\ i_0\in I_0. \tag{2.16}$$

From this, (2.11) and Peter–Weyl theorem it follows that we can expand $f^{(0)}$ in the form

$$f^{(0)}(g)=\sum\ \xi^J_{mi_0}D^J_{mi_0}(g),\quad \xi^J_{mi_0}\in\mathbb{C}. \tag{2.17}$$

$\xi^J_{mi_0}$ is zero if $h\to D^J(h)$ fails to contain the trivial representation of H.

Henceforth we assume for notational simplicity that the identity representation occurs only once in the restriction of the irreducible representations J of G to H, and so drop the index i_0 from $\xi^J_{mi_0}$. Otherwise a degeneracy index has to be included here and elsewhere.

In the same way, if the representation $h\to D^J(h)$ contains $\mathrm{Ad}_{G/H}$, we can choose the basis in the representation space so that the index n in (2.15) transforms by $\mathrm{Ad}_{G/H}$ if i,j belong to an appropriate index set I:

$$D^J_{mi}(gh)=D^J_{mj}(g)[\mathrm{Ad}_{G/H}(h)]_{ji},\quad i,j\in I. \tag{2.18}$$

(For notational simplicity we are assuming that $\mathrm{Ad}_{G/H}$ occurs only once in the representation J, otherwise a degeneracy index has to be added here and elsewhere.) Then we can expand $f^{(1)}_i$ in the form

$$f^{(1)}_i(g)=\sum\ \xi^J_m D^J_{mi}(g),\quad \xi^J_m\in\mathbb{C}. \tag{2.19}$$

ξ^J_m now is zero if $h\to D^J(h)$ fails to contain $\mathrm{Ad}_{G/H}$.

Continuing in this vein we see that tensor fields of rank n in component form look like $f^{(n)}_{i_1\cdots i_n}$ and have the expansion

$$f^{(n)}_{i_1\cdots i_n}(g)=\sum\ \xi^J_m D^J_{m,\{i_1\cdots i_n\}}(g),\quad i_k\in I, \tag{2.20}$$

$$D^J_{m,\{i_1\cdots i_n\}}(gh)=D^J_{m,\{j_1\cdots j_n\}}(g)[\mathrm{Ad}_{G/H}(h)]_{j_1i_1}\cdots[\mathrm{Ad}_{G/H}(h)]_{j_ni_n}. \tag{2.21}$$

We have used a convenient multi-index notation for the second index of D^J. The rest should be clear. Tensor fields of diverse permutation symmetries are readily constructed along similar lines.

C. Covariant derivative

Let $\mathcal{T}^{(n)}$ denote the space of tensor fields of rank n, with a typical member $f^{(n)}=\{f^{(n)}_{i_1\cdots i_n}\}$. $\mathcal{T}^{(0)}$ consists of functions, and it is also an algebra under pointwise multiplication. All $\mathcal{T}^{(n)}$ are $\mathcal{T}^{(0)}$-modules. The covariant derivative ∇ is a map,

$$\nabla\ :\quad \mathcal{T}^{(n)}\to\mathcal{T}^{(n+1)},\quad f^{(n)}\to\nabla f^{(n)}, \tag{2.22}$$

where $\nabla f^{(n)}$ has components $(\nabla f^{(n)})_{ii_1\cdots i_n}$. It has in addition to fulfill the following important derivation property. Note that we can take tensor products of $\mathcal{T}^{(n)}$-s (over $\mathcal{T}^{(0)}$, $\mathcal{T}^{(n)}$ being $\mathcal{T}^{(0)}$ modules):

$$\mathcal{T}^{(n)}\otimes\mathcal{T}^{(m)}=\mathcal{T}^{(n+m)},\quad f^{(n)}\otimes f^{(m)}=f^{(n+m)},\tag{2.23}$$

where

$$f^{(n+m)}_{i_1\cdots i_n j_1\cdots j_m}=f^{(n)}_{i_1\cdots i_n}f^{(m)}_{j_1\cdots j_m}.\tag{2.24}$$

Then we require that

$$\nabla(f^{(n)}\otimes f^{(m)})=\nabla f^{(n)}\otimes f^{(m)}+f^{(n)}\otimes\nabla f^{(m)}.\tag{2.25}$$

There is a natural choice for the covariant derivative in our case. We call it hereafter as X. The action of X on functions is

$$[Xf^{(0)}]_i(g)=\frac{d}{dt}\ f^{(0)}(ge^{itS(i)})\Big|_{t=0}.\tag{2.26}$$

$\nabla f^{(0)}$ transforms correctly in view of (2.5). In the same way the action on $f^{(n)}$ is

$$[Xf^{(n)}]_{ii_1\cdots i_n}(g)=\frac{d}{dt}\ f^{(n)}_{i_1\cdots i_n}(ge^{itS(i)})\Big|_{t=0}.\tag{2.27}$$

The right-hand side defines a vector field X_i. Using X_i the covariant derivative in components is $f^{(n)}_{i_1\cdots i_n}\to X_i f^{(n)}_{i_1\cdots i_n}=$rhs of (2.27).

The torsion of the covariant derivative vanishes only if $[X_i,X_j]f^{(0)}=0$. From the definition and (2.7), we have

$$[X_i,X_j]f^{(0)}=-c_{ijk}X_k f^{(0)}\ .\tag{2.28}$$

So there is torsion if $c_{ijk}\neq 0$. But there is an easy way to construct the torsion–free covariant derivative $\overline{X_i}$. Set

$$\begin{aligned}
&\overline{X_i}f^{(0)}=X_i f^{(0)},\\
&\overline{X_i}f^{(1)}_j=X_i f^{(1)}_j+\tfrac{1}{2}c_{ijk}f^{(1)}_k,\\
&\vdots\\
&\overline{X_i}f^{(n)}_{j_1\cdots j_n}=X_i f^{(n)}_{j_1\cdots j_n}+\tfrac{1}{2}c_{ij_1j_1'}f^{(n)}_{j_1'j_2\cdots j_n}+\tfrac{1}{2}c_{ij_2j_2'}f^{(n)}_{j_1j_2'\cdots j_n}+\cdots+\tfrac{1}{2}c_{ij_nj_n'}f^{(n)}_{j_1\cdots j_n'}.
\end{aligned}\tag{2.29}$$

Then

$$[\overline{X_i},\overline{X_j}]f^{(0)}=[X_i,X_j]f^{(0)}+c_{ijk}X_k f^{(0)}=0,\tag{2.30}$$

just as we want.

Gauge fields will certainly have a central role in further developments. So we briefly indicate what they are here. Let us first consider U(1) gauge fields. The general gauge potential is $A_i=\Sigma\xi^J_M D^J_{Mi}$, $\xi^J_M\in\mathbb{C}$. It is subject to the reality condition $\overline{A_i}=-A_i$. Then if $f^{(n)}$ has charge e, its covariant derivative is $(\overline{X_i}+eA_i)f^{(n)}_{i_1\cdots i_n}$, where A_i acts by pointwise multiplication. This definition is compatible with equivariance. We can substitute X_i for $\overline{X_i}$ at the cost of possible torsion.

The gauge covariant derivative for a general gauge group as usual only involves regarding $eA_i(g)$, that is $e\xi^J_M$, to be Lie algebra valued, its action on $f^{(n)}$ in (2.27) is then dictated by the representation content of the latter.

III. SPIN- AND SPIN$_K$-STRUCTURES

Spinorial fields are essential for physics. We can go about constructing them as follows. The orthogonal group SO($|G/H|$) has a double cover Spin($|G/H|$). Associated with SO($|G/H|$), there is also a Clifford algebra $\mathbb{C}\ell(|G/H|)$ with generators $\gamma_1, \gamma_2, \ldots, \gamma_{|G/H|}$:

$$\gamma_i \gamma_j + \gamma_j \gamma_i = 2\delta_{ij}\mathbb{I}. \tag{3.1}$$

Here $\mathbb{I}$ denotes the unit matrix. (Its dimension should be clear from the context.) $\mathbb{C}\ell(|G/H|)$ has one or two inequivalent IRR's of dimension 2^n if $|G/H| = 2n$ or $|G/H| = 2n+1$. In the latter case, the two IRR's are related by a change of sign of all γ_i's. In either case, they generate a unique faithful representation of Spin($|G/H|$) with generators $\Sigma_{ij} = (1/4i)(\gamma_i\gamma_j - \gamma_j\gamma_i)$ which we call Spin$^{\mathbb{C}\ell}(|G/H|)$.

A recursive scheme for constructing anticommuting sets of Hermitian γ-matrices goes as follows. We start with a set of $2^{n-1}\times 2^{n-1}$ matrices γ_i, $i = 1, \ldots, 2n-1$, satisfying Eq. (3.1), and such that $(-i)^{n-1}\gamma_1 \cdots \gamma_{2n-1} = 1$, e.g., for $n=2$, the three Pauli matrices. Then a set of $2^n \times 2^n$ matrices Γ_λ, $\lambda = 1, \ldots, 2n+1$, satisfying Eq. (3.1), and such that $(-i)^n \Gamma_1 \cdots \Gamma_{2n+1} = \mathbb{I}$ is given by

$$\Gamma_i = \begin{pmatrix} 0 & \gamma_i \\ \gamma_i & 0 \end{pmatrix}, \quad i = 1, \ldots, 2n-1, \quad \Gamma_{2n} = \begin{pmatrix} 0 & -i\mathbb{I} \\ i\mathbb{I} & 0 \end{pmatrix}, \quad \Gamma_{2n+1} = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}. \tag{3.2}$$

The matrices $\gamma_1, \ldots, \gamma_{2n-1}$ span $\mathbb{C}\ell(2n-1)$, and the matrices $\Gamma_1, \ldots, \Gamma_{2n}$ span $\mathbb{C}\ell(2n)$, whereas $\Gamma_1, \ldots, \Gamma_{2n+1}$ span $\mathbb{C}\ell(2n+1)$.

A. Spin manifolds

We say that G/H is a spin manifold if the commutative diagram exists, arrows being homomorphisms (which need not be onto):

$$\begin{array}{ccccc} G & \supset & H & \to & \mathrm{Spin}^{\mathbb{C}\ell}(|G/H|) \\ & & \downarrow & & \downarrow^{\mathbb{Z}_2} \\ & & \mathrm{Ad}_{G/H} & \subset & \mathrm{SO}(|G/H|) \end{array} . \tag{3.3}$$

The vertical homomorphisms are there by construction, so what is to be verified is the existence of the horizontal arrow. If it exists, a general spinor can be constructed as follows. We can reduce Spin$^{\mathbb{C}\ell}(|G/H|)$ restricted to H into a direct sum $\oplus\rho$ of unitary irreducible representations of H. Let $g \to D^J(g)$ be the unitary matrix of g in a representation of G which on restriction to H contains $\oplus\rho$. Then we can restrict its second index a to an index set I so that it transforms by $\oplus\rho$ under $g \to gh$:

$$D^J_{\alpha a}(gh) = D^J_{\alpha b}(g) D^J_{ba}(h), \quad a, b \in I\ . \tag{3.4}$$

By construction we know how the Clifford algebra acts on the index $a \in I$. A general spinor ψ then is a function on G with components

$$\psi_a = \sum \xi^J_M D^J_{Ma}. \tag{3.5}$$

Let us look at examples.

Example 1: $\mathbb{C}P^1 = \mathrm{SO}(3)/\mathrm{SO}(2) = [\mathrm{Spin}(3) = \mathrm{SU}(2)]/[\mathrm{Spin}(2) = \mathrm{U}(1)]$. So $G = \mathrm{SU}(2)$, $H = \mathrm{U}(1) = \{e^{i\sigma_3\theta/2}\}$, σ_A the Pauli matrices. Then $S(i) = \sigma_i$, $i = 1,2$, and

$$e^{i\sigma_3\theta/2}\sigma_i e^{-i\sigma_3\theta/2} = \sigma_j R_{ji}(\theta), \quad R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \in \mathrm{SO}(2)\ . \tag{3.6}$$

$\mathrm{Spin}^{\mathbb{C}\ell}(|G/H|)$ is just $H=\{e^{i\sigma_3\theta/2}\}$, the homomorphism $\mathrm{Spin}^{\mathbb{C}\ell}(2)\to\mathrm{SO}(2)$ being $e^{i\sigma_3\theta/2}\to R(\theta)$. Thus (3.3) exists and $\mathrm{SU}(2)/\mathrm{U}(1)=S^2\simeq\mathbb{C}P^1$ is spin.

For a thorough treatment of noncommutative geometry and a Dirac operator on S^2, see Ref. 7.

Example 2: Similar arguments show that all the spheres $S^N=\mathrm{SO}(N+1)/\mathrm{SO}(N)=\mathrm{Spin}(N+1)/\mathrm{Spin}(N)$ are spin. G for S^N is $\mathrm{Spin}(N+1)$ while $H=\mathrm{Spin}(N)$. $\mathrm{Ad}_{G/H}$ is $\mathrm{SO}(N)$, the $\mathbb{Z}_2$-quotient of $\mathrm{Spin}(N)$. Since $\mathrm{Spin}^{\mathbb{C}\ell}(|G/H|)$ is isomorphic to $\mathrm{Spin}(N)$, S^N is spin.

Example 3: $\mathbb{C}P^2=\mathrm{SU}(3)/\mathrm{U}(2)$. So $G=\mathrm{SU}(3)$, $H=\mathrm{U}(2)$. A basis for the 3-dimensional SU(3)-Lie algebra consists of the Gell-Mann matrices λ_A. The U(2) Lie algebra has basis λ_1, λ_2, λ_3, λ_8, the hypercharge Y being $(1/\sqrt{3})\lambda_8$. The $S(i)$ are λ_4, λ_5, λ_6, λ_7. Under U(2), they transform as (K^+,K^0) or $(-\overline{K^0},K^-)$ in particle physics notation. That means that $\mathrm{Ad}_{G/H}=\mathrm{U}(2)$. Regarding U(2) as 2×2 unitary matrices U, we can embed U(2) in SO(4) by the map

$$U\to\frac{1}{2}\begin{pmatrix} U+U^* & i(U-U^*) \\ -i(U-U^*) & U+U^* \end{pmatrix}. \tag{3.7}$$

$\mathrm{Spin}^{\mathbb{C}\ell}(4)$ is the $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$ representation of $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$. It is the double cover of SO(4). Now H is U(2) and $\mathrm{Spin}^{\mathbb{C}\ell}(4)$ has no U(2) subgroup. So $\mathbb{C}P^2$ is not spin.[1]

Example 4: $G=\mathrm{SU}(3)$, $H=\mathrm{SO}(3)$. With G as 3×3 unitary matrices, H consists of all real orthogonal matrices and corresponds to the spin 1 representation of SO(3). G/H is of dimension 5. It carries the spin 2 representation of SO(3), isomorphic (but not equivalent!) to the spin 1 representation. There is no homorphism $\mathrm{SO}(3)\to\mathrm{Spin}^{\mathbb{C}\ell}(5)$ compatible with (3.3), so that SU(3)/SO(3) is not spin.[3]

Let us show this result in more detail. We can show it by establishing that the 2π-rotation in SO(3) becomes a noncontractible loop in SO(5) under the embedding in (3.9). Then the inverse image of SO(3) under the homomorphism $\mathrm{Spin}^{\mathbb{C}\ell}(5)\to\mathrm{SO}(5)$ is SU(2), giving us the result.

Now SO(3) acts on real symmetric traceless 3×3 matrices $T=(T_{ij})$ according to $T\to RTR^T$. This is its spin 2 representation. We can eliminate say T_{33} using $\mathrm{Tr}T=0$, thereby representing it as real transformations on $(T_{11},T_{12},T_{13},T_{22},T_{23})$. SO(5) consists of real transformations on this five-dimensional vector, so we now have the needed explicit embedding of SO(3) in SO(5). Let

$$R(\theta)\ :\ \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

It generates the 2π-rotation loop in SO(3) as θ increases from 0 to 2π. Consider $T'=R(\theta)TR(\theta)^T$. Then as θ increases from 0 to 2π we have a 2π-rotation in the $T_{13}-T_{23}$ plane. But by the time $\theta=\pi$, T_{ab} $(a,b\leqslant2)$ return to T_{ab} so that the rotations in their planes are by 4π or/and 0 [in fact, $\delta_{ab}(T_{11}+T_{22})$ undergoes no change and $T_{ab}-\frac{1}{2}\delta_{ab}(T_{11}+T_{22})$ undergoes 4π-rotation]. The corresponding loop of matrices in SO(5) is the product of an odd number of 2π-rotations and hence cannot be deformed to a point in SO(5). That concludes the proof.

We will now explain the Dirac operators for Spin- and Spin_K-manifolds after discussing Spin_K-structures.

B. Spin_K-manifolds

K and $\mathcal{H}$ are compact connected Lie groups in what follows. *We say that G/H is a Spin_K-manifold if the commutative diagram exists*:

$$\begin{array}{ccccccc} G & \supset & H & \rightarrow & \mathcal{H} & \supset & \mathrm{Spin}^{C\ell}(|G/H|) \\ & & \downarrow & & \downarrow^{K} & \swarrow \mathbb{Z}_2 & \\ & & \mathrm{Ad}_{G/H} & \subset & \mathrm{SO}(|G/H|) & & \end{array} \tag{3.9}$$

K and $\mathbb{Z}_2$ on the arrows are to show that they are the kernels of those homomorphisms.

$\mathrm{Spin}_{U(1)}$ in our language is what mathematicians call Spin_c.

The intersection $\mathrm{Spin}^{C\ell}(|G/H|)\cap K$ clearly contains $\mathbb{Z}_2$. It cannot be larger, for that would mean that the kernel for the slanting arrow exceeds $\mathbb{Z}_2$.

Thus $\mathcal{H}\supset[\mathrm{Spin}^{C\ell}(|G/H|)\times K]/\mathbb{Z}_2$. Its quotient by K being exactly $\mathrm{SO}(|G/H|)$, we conclude that

$$\mathcal{H}=[\mathrm{Spin}^{C\ell}(|G/H|)\times K]/\mathbb{Z}_2, \tag{3.10}$$

giving the following, also a commutative diagram:

$$\begin{array}{ccccccc} G & \supset & H & \rightarrow & \mathcal{H}=[\mathrm{Spin}^{C\ell}(|G/H|)\times K]/\mathbb{Z}_2 & \supset & \mathrm{Spin}^{C\ell}(|G/H|) \\ & & \downarrow & & \downarrow K & \swarrow \mathbb{Z}_2 & \\ & & \mathrm{Ad}_{G/H} & \subset & \mathrm{SO}(|G/H|) & & \end{array} \quad . \tag{3.11}$$

Let us denote the generators of $\mathbb{Z}_2$ in $\mathrm{Spin}^{C\ell}(|G/H|)$ and K by z_{Spin} and z_K, they square to the respective identities. The inclusion of $\mathrm{Spin}^{C\ell}(|G/H|)$ in (3.3) is to be understood as follows. The elements of $\mathcal{H}$ are the equivalence classes,

$$\langle hs,k\rangle=\langle z_{\mathrm{spin}}s,z_K k\rangle, \quad s\in\mathrm{Spin}^{C\ell}(|G/H|), \quad k\in K. \tag{3.12}$$

Then the top inclusion is via the isomorphism

$$s\rightarrow\langle s,e_K\rangle, \quad e_K=\text{ identity of } K. \tag{3.13}$$

As we think of $\mathcal{H}$ as the concrete matrix group obtained by tensoring $\mathrm{Spin}^{C\ell}(|G/H|)$ with a faithful unitary representation of K where z_K is represented by $-\mathbb{I}$,

$$\mathcal{H}=\mathrm{Spin}^{C\ell}(|G/H|)\otimes K, \tag{3.14}$$

we can write -1 for z_{spin} and z_K. The inclusion of $\mathrm{Spin}^{C\ell}(|G/H|)$ is then just $s\rightarrow s\otimes\mathbb{I}$.

Let us motivate the new requirements in (3.9) and (3.11). For a physicist, a spinor changes sign under "2π rotation." $\mathcal{H}$ is the group acting on Spin_K-spinors. We have required it to contain $\mathrm{Spin}^{C\ell}(|G/H|)$, so we can check this requirement by looking at the action of 2π-rotation $\in\mathrm{Spin}^{C\ell}(|G/H|)\subset\mathcal{H}$. As for asking that $H\rightarrow\mathcal{H}$, we can reduce the representation of $\mathcal{H}$ into a direct sum $\oplus\rho$ of irreducible representations ρ of H just as in the discussion of spin structures. The action of the Clifford algebra on $\oplus\rho$ by construction is known. The wave functions of Spin_K-spinors are then given by linear spans of representations of G induced by $\oplus\rho$; see (3.5). Later we shall see how the Dirac operator can be defined on these wave functions.

Example 5: $G=\mathrm{SU}(3)$, $H=\mathrm{U}(2)$, $G/H=\mathbb{C}P^2$. Here we choose $K=\mathrm{U}(1)$. Elements of U(2) can be written as the equivalence classes,

$$\langle s,u\rangle=\langle -s,-u\rangle, \quad s\in\mathrm{SU}(2), \quad u\in\mathrm{U}(1), \tag{3.15}$$

where we identify SU(2) with 2×2 unitary matrices of unit determinant and u with a phase. $\mathrm{Spin}^{C\ell}(4)$ is $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ and $\mathcal{H}$ consists of the equivalence classes

$$\langle s_1,s_2,u\rangle=\langle -s_1,-s_2,-u\rangle. \tag{3.16}$$

With elements of SO(4) represented as $\langle s_1,s_2\rangle=\langle -s_1,-s_2\rangle$, the homomorphism $\mathcal{H}\rightarrow\mathrm{SO}(4)$ is $\langle s_1,s_2,u\rangle\rightarrow(s_1,s_2)$. The homomorphism $H\rightarrow\mathcal{H}$ is also simple:

$$[s,u]\to\langle s,s,u\rangle. \tag{3.17}$$

Thus $\mathbb{C}P^2$ is $\mathrm{Spin}_{U(1)}$ or Spin_c.

Example 6: $G=\mathrm{SU}(3)$, $H=\mathrm{SO}(3)$.

We return to the choices $G=\mathrm{SU}(3)$, $H=\mathrm{SO}(3)$. Choosing $K=\mathrm{U}(1)$ is not helpful now, as we lack a suitable homomorphism $H=\mathrm{SO}(3)\to\mathcal{H}=\mathrm{Spin}^{\mathbb{C}\ell}(5)\otimes_{Z_2}\mathrm{U}(1)$. So SU(3)/SO(3) is not even $\mathrm{Spin}_{\mathrm{U}(1)}$, a result originally due to Landweber and Stong.[3] A better choice is $K=\mathrm{SU}(2)$. Then we can find the homomorphism $H\to\mathcal{H}$ as follows. The image of $\mathrm{Ad}_{G/H}$ in SO(5) is an SO(3) subgroup SO(3)′. Its inverse image in $\mathrm{Spin}^{\mathbb{C}\ell}(5)$ is an SU(2) subgroup SU(2)′. Let $\vec{\Sigma}$ and $\vec{T}$ be the angular momentum generators of SU(2)′ and K. If $\vec{L}$ are the angular momentum generators of H, the map at the level of Lie algebras is just $\vec{L}\to\vec{\Sigma}+\vec{T}$. Hence SU(3)/SO(3) is $\mathrm{Spin}_{\mathrm{SU}(2)}$. More such examples can be found.

C. What is $\overline{X}(i)$ now?

We need the extension of the torsion-free connection with components $\overline{X_i}$ to spinors on general spin_K-manifolds. The first step in this direction is the extension of X_i.

A spinor field $\psi=(\psi_a)$ on a Spin_K-manifold has the expansion

$$\psi_a=\sum\ \xi_M^L D_{Ma}^L, \tag{3.18}$$

where a carries the action of the Clifford algebra. The definition of X_i on ψ is immediate from (2.26):

$$(X_i\psi)(g)=\frac{d}{dt}\sum\ \xi_M^L D_{Ma}^L(ge^{itS(i)})|_{t=0}. \tag{3.19}$$

The definition of $\overline{X_i}$ involves the extension of c_{ijk} to spinors so that it can act on the index a. Now, the generators of the $\mathrm{SO}(|G/H|)$-Lie algebra are M_{ij}, where

$$(M_{ij})_{kl}=-i(\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}). \tag{3.20}$$

Its image in the spinor representation is $(1/4i)[\gamma_i,\gamma_j]$.

Now

$$c_{ij'k'}(M_{j'k'})_{kj}f_k^{(1)}=-2ic_{ikj}f_k^{(1)}. \tag{3.21}$$

Hence

$$\overline{X_i}f_j^{(1)}=X_if_j^{(1)}+\frac{1}{4i}c_{ij'k'}(M_{j'k'})_{kj}f_k^{(1)}. \tag{3.22}$$

From this follows the definition of $\overline{X_i}$ on spinors:

$$\overline{X_i}\psi_a=X_i\psi_a-\tfrac{1}{16}c_{ijk}([\gamma_j,\gamma_k])_{ba}\psi_b. \tag{3.23}$$

A tensor formed of spinors will then transform correctly.

The introduction of gauge fields follows the earlier discussion.

IV. THE DIRAC AND CHIRALITY OPERATORS

The massless Dirac operator for the torsion free connection $\overline{X_i}$ is just

$$D_W = -i\gamma_i^{\mathcal{R}}\overline{X_i}, \tag{4.1}$$

where the superscript $\mathcal{R}$ indicates that the γ's act on spinors on the right. It is self-adjoint. This expression can be gauged, and $\overline{X_i}$ can be substituted by X_i if we can tolerate torsion.

If $|G/H|$ is even, e.g., if G/H is a [co]adjoint orbit, there is also a chirality operator γ anticommuting with D_W:

$$\gamma = (-i)^{1/2|G/H|}\gamma_1\cdots\gamma_{|G/H|} = \gamma^\dagger, \quad \gamma^2 = \mathbb{I}. \tag{4.2}$$

The subscript "W" is to indicate that it is the form of the Dirac operator used by the Watamuras.[8] For even $|G/H|$ there is also the unitarily equivalent Dirac operator,[9]

$$D = e^{i\gamma^{\mathcal{R}}\pi/4}D_W e^{-i\gamma^{\mathcal{R}}\pi/4} = i\gamma^{\mathcal{R}}D_W, \tag{4.3}$$

which is central to fuzzy physics.

V. PROJECTIVE MODULES AND THEIR DIRAC OPERATOR

A. Projective modules

In the algebraic approach to vector bundles, their sections are substituted by elements of projective modules ("of finite type").[10] A projective module is constructed as follows. Let A be an algebra. It can be the commutative algebra $\mathcal{A}$ of C^∞-functions on a manifold M if our interest is in the algebraic description of its vector bundles. But it can also be a noncommutative algebra, in which case there is no evident correspondence with sections of differential geometric vector bundles. Consider $A^N \equiv A \otimes_C \mathbb{C}^N$ with elements $a = (a_1, \ldots, a_N)$, $a_i \in A$. Let P be an $N \times N$ projector with coefficient in A:

$$P_{ij} \in A, \quad P^\dagger = P = P^2. \tag{5.1}$$

Then $A^N P$ (whose elements are vectors α with components $a_j P_{ji}$) is a projective module. The Serre-Swan theorem (Ref. 10) establishes that sections of any vector bundle can be obtained from some N and P.

It is very helpful for subsequent developments to have a projective module description of vector bundles. We can find the appropriate projectors by a known method described nicely by Landi.[11] It goes as follows.

Consider for example a rank 1 tensor field and any particular D^J matrix occurring in its expansion, with elements $D^J_{\rho i}$. We have

$$(D^J)^\dagger_{i\rho}(g)D^J_{\rho j}(g) = \delta_{ij}. \tag{5.2}$$

Let

$$P^J(g)_{\rho\sigma} = D^J_{\rho i}(g)(D^J)^\dagger_{i\sigma}(g). \tag{5.3}$$

Since $P^J(gh) = P^J(g)$ if $h \in H$, $P^J_{\rho\sigma}$ are functions on G/H. In view of (5.2), they are projectors too. If $P^J(g)$ are $|J| \times |J|$ matrices, a projective module describing rank 1 tensor fields is

$$\mathcal{A}^{|J|}P^J = \langle \alpha^J = (\alpha^J_1, \ldots, \alpha^J_{|J|}), \ \ \alpha^J_i = a^J_k P^J_{ki} \rangle. \tag{5.4}$$

There is no unique correspondence between projective modules and vector bundles. Thus for each J, we can find a projector and its module. But all such modules are equivalent, since there are elements $\alpha^J = a^J P^J$ and $\alpha^K = a^K P^K$ which naturally correspond for different J and K:

$$\alpha^J_\rho = \sum \xi^L_M D^L_{Mi} (D^J)^\dagger_{i\rho}, \quad \alpha^K_\sigma = \sum \xi^L_M D^L_{Mi} (D^K)^\dagger_{i\sigma}. \tag{5.5}$$

B. Differential geometry

There is much to be said on the differential geometry on projective modules, but for reasons of brevity we limit ourselves to indicating how to extend the definitions of $X(i)$ and $\overline{X}(i)$.

Let us first focus on the tensorial case. Let

$$P = (P_{\lambda\rho}), \quad P_{\lambda\rho} = D^J_{\lambda i} (D^J)^\dagger_{i\rho} \tag{5.6}$$

be a projector appropriate for rank 1 tensors. Then what substitutes for the torsion-free X_i acting on α^J is ∇_λ, which is defined by

$$\nabla_\lambda \alpha^J_\rho(g) = \sum \xi^L_M \frac{d}{dt} D^L_{Mi}(g e^{itS(j)}) \Big|_{t=0} (D^J)^\dagger_{i\rho}(g) (D^J)^\dagger_{j\lambda}(g). \tag{5.7}$$

It belongs to the projective module for rank 2 tensors with the natural choice $P \otimes P$ of their projectors. A more compact expression for the covariant derivative can be given in terms of the right-invariant vector fields of G, defined by

$$(\mathcal{L}_A f)(g) = -i \frac{d}{dt} f(e^{-it\Sigma_A} g) \Big|_{t=0}, \tag{5.8}$$

so that

$$\mathcal{L}_A (D^J)^\dagger_{\lambda\mu} = (D^J)^\dagger_{\lambda\rho} (\Sigma_A)^J_{\rho\mu}. \tag{5.9}$$

If functions on G/H are regarded as functions on G invariant by the right action of H on G, $\mathcal{L}_A$ on these correspond to ''orbital'' operators of angular momentum.

The vector fields $\mathcal{L}_A$ are related to the left-invariant vector fields X_A by

$$(X_A f)(g) = \frac{d}{dt} f(g e^{it\Sigma_A}) \Big|_{t=0} = -i (\mathcal{L}_B f)(g) (\mathrm{Ad}\, g)_{BA}. \tag{5.10}$$

From this we may derive the following expression for the covariant derivative:

$$\nabla_\lambda = -i\, \mathrm{Ad}\, g_{Ai} (D^J)^\dagger_{i\lambda} \mathcal{J}_A, \quad \mathcal{J}_A = \text{''total angular momentum''} = \mathcal{L}_A - \Sigma^{\mathcal{R}}_A, \tag{5.11}$$

where $\Sigma^{\mathcal{R}}_A$ are the generators appropriate for representation J acting on the right. In fact, applying (5.10) and then (5.9) to the definition (5.7), we find

$$\nabla_\lambda \alpha^J_\rho = -i \Big(\mathcal{L}_A \sum \xi^L_M D^L_{Mi} \Big) D^{J\dagger}_{i\rho} (\mathrm{Ad}\, g)_{Aj} D^{J\dagger}_{j\lambda} = -i (\mathrm{Ad}\, g)_{Aj} D^{J\dagger}_{j\lambda} ((\mathcal{L}_A - \Sigma^{\mathcal{R}}_A) \alpha^J)_\rho. \tag{5.12}$$

∇_λ maps tensors of rank k to $k+1$. It also has the correct derivation property so that it is a covariant differentiation. Also, (5.7) shows that it corresponds to the operator X_i.

We can define the covariant derivative ∇_ρ on spinors corresponding to X_i in the same way, just changing the index i to a in (3.18), and accordingly changing the choice of J as well.

The canonical torsion c_{ijk} generalizes for tensors to

$$\mathcal{C}_{\lambda\rho\sigma} = (D^J)^\dagger_{i\lambda} (D^J)^\dagger_{j\rho} c_{ijk} D^J_{\sigma k}. \tag{5.13}$$

A torsion-free covariant derivative on tensors when $c_{ijk} \neq 0$ is then defined from

$$\overline{\nabla}_\lambda \alpha^J_\rho = \nabla_\lambda \alpha^J_\rho + \tfrac{1}{2}\mathcal{C}_{\lambda\rho\sigma}\alpha^J_\sigma. \tag{5.14}$$

As for spinors, following (3.23), we define a spinorial torsion which is twice the expression

$$-\frac{i}{4}c_{ijk}\frac{1}{2i}(\gamma_j\gamma_k)_{ba} = -\tfrac{1}{8}c_{ijk}(\gamma_j\gamma_k)_{ba}. \tag{5.15}$$

Let J_s be the representation of choice for the projective module of spinors, and J_T for rank 1 tensors. The transform of (5.15) onto spinorial modules is

$$-\tfrac{1}{8}c_{ijk}[D^{J_s}(\gamma_j\gamma_k)(D^{J_s})^\dagger]_{\sigma'\sigma}(D^{J_T})^\dagger_{i\rho}, \tag{5.16}$$

while the torsion-free covariant derivative $\overline{\nabla}_\rho$ acts on a spinor α^{J_s} represented as an element of a projective module as follows:

$$\overline{\nabla}_\rho \alpha^{J_s}_\sigma = \nabla_\rho \alpha^{J_s}_\sigma - \frac{1}{8}\alpha^{J_s}_{\sigma'}c_{ij'k'}(D^{J_s}(\gamma_{j'}\gamma_{k'})(D^{J_s})^\dagger)_{\sigma'\sigma}(D^{J_T})^\dagger_{i\rho}. \tag{5.17}$$

C. The projective Dirac operator for spheres

The equations (5.5) tell us the invertible transformation of a spinor field of Sec. III C to an element of a projective module. So we can transform the Dirac operator D to one acting on this $\mathcal{A}$-module. The result is not illuminating except in special cases like spheres and $\mathbb{C}P^N$, so we take them up first.

1. Even spheres

For $G/H = S^{2n}$, we can choose $G = \mathrm{Spin}^{\mathbb{C}\ell}(2n+1) = \{g\}$, $H = \mathrm{Spin}^{\mathbb{C}\ell}(2n) = \{h\}$, identifying them with the representations given by γ-matrices, $\mathrm{Spin}^{\mathbb{C}\ell}(2n+1)$ and $\mathrm{Spin}^{\mathbb{C}\ell}(2n)$. We denote the γ-matrices of H by γ_i, $i=1,...,2n$, and by $\gamma = (-i)^n\gamma_1\cdots\gamma_{2n}$ the additional gamma matrix of G, and refer to them collectively as $\Gamma_\lambda = (\gamma_i, \gamma)$, $\lambda = 1,...,2n+1$. The generators of H are $\Sigma_{ij} = (1/4i)[\gamma_i, \gamma_j]$, which together with $\Sigma_{2n+1,i} = (1/2i)\,\gamma\gamma_i$ make up the full set of generators $\Sigma_{\mu\nu}$ of G.

The Γ_λ transform as vectors under conjugation by G. That lets us introduce coordinate functions $x = (x_\lambda)$ for S^{2n}, starting from an "origine" $x^0 = (0,\ldots,0,1)$, as follows:

$$\Gamma_\lambda x_\lambda = g\Gamma_{2n+1}g^{-1}, \quad g \in \mathrm{Spin}(2n+1), \quad x_\lambda x_\lambda = 1. \tag{5.18}$$

We let subscript $A = (\mu\nu)$, $\mu > \nu$ stand for either of the multi-indices (ij), (α of Sec. II), or $(2n+1,i)$, (i of Sec. II). For $A = (2n+1,i)$, X_A gives back $X_{2n+1,i} \equiv X_i$ of Sec. II, which is now torsionless, G/H being symmetric.

Since Γ_{2n+1} commutes with Σ_{ij}, D_W can be written as

$$D_W = -i\gamma^{\mathcal{R}}_i X_i = [\Gamma_{2n+1}, \Sigma_A]^{\mathcal{R}} X_A = [\Gamma_\lambda x_\lambda, \Sigma_A]^{\mathcal{R}} X_A, \text{ at } x = x^0, \tag{5.19}$$

while

$$D = i\Gamma^{\mathcal{R}}_{2n+1}D_W = i\Gamma^{\mathcal{R}}_\lambda x_\lambda D_W, \text{ at } x = x^0. \tag{5.20}$$

We choose J to correspond to the preceding Clifford representation to fix the spinorial projective module. We now show that on this module the above Dirac operators have the beautiful forms

$$\mathcal{D}_W = i[\Gamma^{\mathcal{R}}_\lambda x_\lambda, \Sigma^{\mathcal{R}}_A]\mathcal{J}_A, \quad \mathcal{D} = i\Gamma^{\mathcal{R}}_\lambda x_\lambda \mathcal{D}_W, \tag{5.21}$$

$\mathcal{J}_A$ being again the total "orbital" plus "spin" generators $\mathcal{L}_A$ and $-\Sigma_A^{\mathcal{R}}$ of G. The matrices $\Gamma_\lambda^{\mathcal{R}}$, $\Sigma_A^{\mathcal{R}}$ act on the index a of the spinor,

$$\chi_a = \sum \xi_M^K D_{Mb}^K (D^{\mathbb{C}\ell})_{ba}^\dagger , \tag{5.22}$$

on the right as in $(\Gamma_\lambda^{\mathcal{R}}\chi)_a = \chi_b(\Gamma_\lambda)_{ba}$.

In fact, if we apply (5.21), since by (5.9) $\mathcal{J}_A(D^{\mathbb{C}\ell})^\dagger = 0$, we can see that

$$(\mathcal{D}_W\chi)_a = i\sum (\mathcal{L}_A(\xi_M^K D_{Mb}^K))(D^{\mathbb{C}\ell})_{bc}^\dagger [\Sigma_A, \Gamma_\lambda x_\lambda]_{ca}. \tag{5.23}$$

Inserting

$$\begin{aligned}[\Sigma_A, \Gamma_\lambda x_\lambda] &= (\mathrm{Ad}\, g)_{AB} D^{\mathbb{C}\ell}(g)[\Sigma_B, \Gamma_{2n+1}](D^{\mathbb{C}\ell}(g))^\dagger \\ &= i(\mathrm{Ad}\, g)_{A,(2n+1,i)} D^{\mathbb{C}\ell}(g)\gamma_i (D^{\mathbb{C}\ell}(g))^\dagger ,\end{aligned} \tag{5.24}$$

we get

$$(\mathcal{D}_W\chi)_a = -\sum (\mathcal{L}_A \xi_M^K D_{Mb}^K)(\mathrm{Ad}\, g)_{A,(2n+1,i)} (\gamma_i)_{ba'} (D^{\mathbb{C}\ell}(g))_{a'a}^\dagger . \tag{5.25}$$

But the right-invariant vector fields are related to the left-invariant ones by Eq. (5.10), so

$$(\mathcal{D}_W\chi)_a = -i\left(X_i \sum \xi_M^K D_{Mb}^K \right)(\gamma_i)_{bc} (D^{\mathbb{C}\ell}(g))_{ca}^\dagger . \tag{5.26}$$

Writing $\psi_a = \chi_{a'} D_{a'a}^{\mathbb{C}\ell}$, (5.26) shows that under $\mathcal{D}_W$: $\psi_a \to (D_W\psi)_a$, which is the action (5.19). So $\mathcal{D}_W$ is equivalent to D_W. In a similar manner $\mathcal{D}$ is seen to be equivalent to D.

When acting on functions on S^{2n}, we can use our coordinates to express the right-invariant vector fields in the form

$$\mathcal{L}_{\mu\nu} = -i\left(x_\mu \frac{\partial}{\partial x_\nu} - x_\nu \frac{\partial}{\partial x_\mu} \right), \tag{5.27}$$

and therefore the Dirac operators as

$$\mathcal{D}_W = -x_\mu \Gamma_\nu^{\mathcal{R}} (\mathcal{L}_{\mu\nu} - \Sigma_{\mu\nu}^{\mathcal{R}}), \quad \mathcal{D} = -\Sigma_{\mu\nu}^{\mathcal{R}} \mathcal{L}_{\mu\nu} + n. \tag{5.28}$$

To determine the spectrum and eigenspinors of the Dirac operator we need to be more explicit about the group $\mathrm{Spin}(2n+1)$. It has rank n, and IRR's that can be labeled by the components of the highest weight $(m_1, \ldots, m_n)$, with the m_i's all integers or all half integers, and $m_1 \geqslant m_2 \geqslant \cdots \geqslant m_n \geqslant 0$. The Clifford representation $\mathrm{Spin}^{\mathbb{C}\ell}$ has highest weight $(\frac{1}{2}, \ldots, \frac{1}{2})$, dimension 2^n and quadratic Casimir operator $C_2(\mathbb{C}\ell) \equiv C_2(\mathrm{Spin}^{\mathbb{C}\ell}) = \frac{1}{2}\Sigma_{\mu\nu}\Sigma_{\mu\nu} = \frac{1}{4}n(2n+1)$. We indicate by L an IRR associated with the set I_0 of Sec. II B; it has highest weight $(l,0,...,0)$, where l is an integer, and dimension and quadratic Casimir operator,

$$d(L) = \frac{2l+2n-1}{l+2n-1} \frac{(l+2n-1)!}{l!(2n-1)!}, \quad C_2(L) = l(l+2n-1). \tag{5.29}$$

The final piece of required information is

$$L \otimes \mathbb{C}\ell = (l+\tfrac{1}{2}, \tfrac{1}{2}, \ldots, \tfrac{1}{2}) \oplus (l-\tfrac{1}{2}, \tfrac{1}{2}, \ldots, \tfrac{1}{2}), \tag{5.30}$$

with

$$d\left(j,\frac{1}{2},\ldots,\frac{1}{2}\right)=2^n\frac{(j+2n-\frac{3}{2})!}{(j-\frac{1}{2})!(2n-1)!},\quad C_2\left(j,\frac{1}{2},\ldots,\frac{1}{2}\right)=j(j+2n-1)+\frac{1}{2}(n-1)\left(n-\frac{1}{2}\right). \tag{5.31}$$

With this background it is easy to show that the eigenspinors of $\mathcal{D}$ are of the form

$$\chi_a^{JL}=\sum\ \xi_M^{JL}\langle JM|LN,\mathbb{C}\ell a\rangle D^L_{Ni_0},\ \text{with}\ J=\left(l\pm\frac{1}{2},\frac{1}{2},\ldots,\frac{1}{2}\right), \tag{5.32}$$

where M, N and i_0, and a label vectors in the IRR's J, L and $\mathbb{C}\ell$. In fact,

$$(\mathcal{D}\chi)_a=\sum\ \xi_M^{JL}\langle JM|LN',\mathbb{C}\ell a'\rangle(\Sigma_{\mu\nu})_{a'a}(\Sigma^L_{\mu\nu})_{N'N}D^L_{Ni_0}+n\chi_a, \tag{5.33}$$

where $\Sigma^L_{\mu\nu}$ is the representative of $\mathcal{L}_{\mu\nu}$ in the IRR L. "Completing the square" in this equation, one finds

$$\langle JM|LN',\mathbb{C}\ell a'\rangle(\Sigma_{\mu\nu})_{a'a}(\Sigma^L_{\mu\nu})_{N'N}=(C_2(J)-C_2(L)-C_2(\mathbb{C}\ell))\langle JM|LN,\mathbb{C}\ell a\rangle. \tag{5.34}$$

Using the expressions for the various quadratic Casimir operators, the eigenvalues corresponding to the the eigenspinors (5.32) are found to be

$$\rho=\pm(j+n-\tfrac{1}{2}),\ \text{for}\ j=l\pm\tfrac{1}{2}. \tag{5.35}$$

2. Odd spheres

An odd sphere $S^{2n-1}=\mathrm{SO}(2n)/\mathrm{SO}(2n-1)$ differs from an even sphere S^{2n} in important details. The Clifford algebra $\mathbb{C}\ell(2n-1)$ has two inequivalent 2^{n-1}-dimensional representations, with $(-i)^{n-1}\gamma_1\cdots\gamma_{2n-1}=\mathbb{I}$ and $(-i)^{n-1}\tilde{\gamma}_1\cdots\tilde{\gamma}_{2n-1}=-\mathbb{I}$; we may take $\tilde{\gamma}_i=-\gamma_i$, which makes clear that they give a single IRR's of Spin$(2n-1)$, with generators $(1/4i)[\gamma_i,\gamma_j]$. They do give however two inequivalent IRR's of Spin$(2n)$, with generators $((1/4i)[\gamma_i,\gamma_j],-\frac{1}{2}\gamma_i)$ and $((1/4i)[\gamma_i,\gamma_j],\frac{1}{2}\gamma_i)$, let us label them $\mathbb{C}\ell^+$ and $\mathbb{C}\ell^-$.

For covariance it is better to put these two representations together and work with the 2^n-dimensional Γ_μ, $\mu=1,\ldots,2n$, built from the γ_i's as indicated in (3.2); that particular construction gives

$$\Gamma_{2n+1}=(-i)^n\Gamma_1\cdots\Gamma_{2n}=\begin{pmatrix}\mathbb{I}&0\\0&-\mathbb{I}\end{pmatrix},\quad \tilde{\Gamma}_{2n-1}\equiv(-i)^{n-1}\Gamma_1\cdots\Gamma_{2n-1}=\begin{pmatrix}0&\mathbb{I}\\\mathbb{I}&0\end{pmatrix}. \tag{5.36}$$

For $\mathbb{C}\ell(2n-1)$, Γ_μ splits into the two inequivalent IRR's $\frac{1}{2}(\mathbb{I}\pm\tilde{\Gamma}_{2n-1})\Gamma_j\equiv\Gamma_j^{(1,2)}$, $1\leqslant j\leqslant 2n-1$. The corresponding generators of Spin$^{\mathbb{C}\ell}(2n)$ are

$$\Sigma_{\mu\nu}=\frac{1}{4i}[\Gamma_\mu,\Gamma_\nu]=\left\{\ \Sigma_{ij}=\begin{pmatrix}\frac{1}{4i}[\gamma_i,\gamma_j]&0\\0&\frac{1}{4i}[\gamma_i,\gamma_j]\end{pmatrix};\ \Sigma_{2n,i}=\begin{pmatrix}-\frac{1}{2}\gamma_i&0\\0&\frac{1}{2}\gamma_i\end{pmatrix}\right\}, \tag{5.37}$$

and give, as expected, the direct sum $\mathbb{C}\ell^+\oplus\mathbb{C}\ell^-$; for the group elements of Spin$(2n)$ we have

$$g=\begin{pmatrix}D^{\mathbb{C}\ell^+}&0\\0&D^{\mathbb{C}\ell^-}\end{pmatrix},$$

split by the projectors $\frac{1}{2}(\mathbb{I}\pm\Gamma_{2n+1})$.

Spinors carry the direct sum of these two IRR's on their index, and we can use either of the Dirac operators,

$$D_W^{(1,2)}=\frac{1}{2}(\mathbb{I}\pm\tilde{\Gamma}_{2n-1})^{\mathcal{R}}(-i\,\Gamma_i^{\mathcal{R}})X_i, \tag{5.38}$$

or else we can accept fermion doubling and work with $D_W^{(1)}\oplus D_W^{(2)}$.

There is no chirality in odd dimensions, but Γ_{2n} plays a role in space(time)-reflection, and can be used to give Dirac operators equivalent to $D_W^{(1,2)}$:[9]

$$D^{(1,2)}=e^{i\Gamma_{2n}^{\mathcal{R}}\pi/4}D_W^{(1,2)}e^{-i\Gamma_{2n}^{\mathcal{R}}\pi/4}=\tfrac{1}{2}(\mathbb{I}\mp\Gamma_{2n+1}^{\mathcal{R}})\,\Gamma_{2n}^{\mathcal{R}}\,\Gamma_i^{\mathcal{R}}X_i. \tag{5.39}$$

We can introduce coordinates for S^{2n-1}, starting from $x^0=(0,...,1)$, by

$$\Gamma_\lambda x_\lambda=g\Gamma_\lambda x_\lambda^0 g^{-1}=g\Gamma_{2n}g^{-1}\ ,\ \ x_\lambda x_\lambda=1\ . \tag{5.40}$$

Hence at $x=x^0$,

$$\begin{gathered}D_W^{(1,2)}=p(x^0)_{(1,2)}^R[\Gamma_\lambda x_\lambda^0,\Sigma_A]^{\mathcal{R}}X_A,\ \ D^{(1,2)}=\tfrac{1}{2}(\mathbb{I}\mp\Gamma_{2n+1}^{\mathcal{R}})i\Gamma_\lambda^{\mathcal{R}}x_\lambda^0[\Gamma_\lambda x_\lambda^0,\Sigma_A]^{\mathcal{R}}X_A,\\ p(x^0)_{(1,2)}=\frac{1}{2}(\mathbb{I}\pm\tilde{\Gamma}_{2n-1})=\frac{1}{2}\left(\mathbb{I}\pm\frac{(-i)^{n-1}}{(2n-1)!}\epsilon_{\mu_1\cdots\mu_{2n}}\Gamma_{\mu_1}\cdots\Gamma_{\mu_{2n-1}}x^0_{\mu_{2n}}\right).\end{gathered} \tag{5.41}$$

Their covariant forms follow:

$$\begin{gathered}\mathcal{D}_W^{(1,2)}=p(x)_{(1,2)}^{\mathcal{R}}i\,[\Gamma_\lambda^{\mathcal{R}}x_\lambda,\Sigma_A^{\mathcal{R}}]\mathcal{J}_A,\quad \mathcal{D}^{(1,2)}=-\tfrac{1}{2}(\mathbb{I}\mp\Gamma_{2n+1}^{\mathcal{R}})\Gamma_\rho^{\mathcal{R}}x_\rho[\Gamma_\lambda^{\mathcal{R}}x_\lambda,\Sigma_A^{\mathcal{R}}]\mathcal{J}_A,\\ p(x)_{(1,2)}=\frac{1}{2}\left(\mathbb{I}\pm\frac{(-i)^{n-1}}{(2n-1)!}\epsilon_{\mu_1\,\cdots\,\mu_{2n}}\Gamma_{\mu_1}\cdots\Gamma_{\mu_{2n-1}}x_{\mu_{2n}}\right)=g\,p(x^0)\,g^{-1}.\end{gathered} \tag{5.42}$$

$\mathcal{J}_A$ is defined as before.

Proceeding as we did for even spheres, with $\mathcal{L}_{\mu\nu}$ as in Eq. (5.27) the Dirac operators can be rewritten in the form

$$\mathcal{D}_W^{(1,2)}=-p(x)_{(1,2)}^{\mathcal{R}}x_\mu\Gamma_\nu^{\mathcal{R}}(\mathcal{L}_{\mu\nu}-\Sigma_{\mu\nu}^{\mathcal{R}}),\quad \mathcal{D}^{(1,2)}=\tfrac{1}{2}(\mathbb{I}\mp\Gamma_{2n+1}^{\mathcal{R}})(-\Sigma_{\mu\nu}^{\mathcal{R}}\mathcal{L}_{\mu\nu}+n-\tfrac{1}{2}). \tag{5.43}$$

Given their form, it is easy to find one set of eigenvalues and eigenspinors for the Dirac operators $\mathcal{D}^{(1,2)}$, by the same argument that led us to Eq. (5.32). The IRR's of Spin($2n$) are labeled by highest weights $(m_1,\ldots,m_n)$, $m_1\geqslant m_2\cdots\geqslant|m_n|\geqslant 0$ with the m_i all integers or all half integers. The two 2^{n-1}-D spinor representations $\mathbb{C}\ell^{\pm}$ have $(\frac{1}{2},\ldots,\frac{1}{2},\pm\frac{1}{2})$, with quadratic Casimir $C_2(\mathbb{C}\ell^{\pm})=\frac{1}{2}\Sigma_{\mu\nu}\Sigma_{\mu\nu}=\frac{1}{4}n(2n-1)$. The IRR's associated with the set I_0 of Sec. II B are $L=(l,0,...)$, with dimension $d(L)=(l+n-1)\,(l+2n-3)!/(n-1)\,(2n-3)!\,l!$, and quadratic Casimir $C_2(L)=l(l+2n-2)$. Finally,

$$L\otimes\mathbb{C}\ell^{\pm}=(l+\tfrac{1}{2},\tfrac{1}{2},\ldots,\pm\tfrac{1}{2})\oplus(l-\tfrac{1}{2},\tfrac{1}{2},\ldots,\pm\tfrac{1}{2})\ . \tag{5.44}$$

For these last representations we have $C_2(j,\frac{1}{2},\ldots,\pm\frac{1}{2})=(j-\frac{1}{2})(j+2n-\frac{3}{2})+\frac{1}{4}n(2n-1)$.

With all this information, the analog of (5.33), (5.34) give for the eigenvalues

$$\rho_\pm=\pm(j_\pm+n-1),\ \ \text{with}\ j_\pm=l\pm\tfrac{1}{2}. \tag{5.45}$$

There are eigenstates for each of the two inequivalent representations of the Clifford algebra. They are given by

$$\chi^{JL}_{1,a\pm}=\left(\ 0,\ \sum\ \xi^{JL}_M\left\langle\left(j_\pm,\frac{1}{2},\ldots,-\frac{1}{2}\right),M\middle|L,N';\mathbb{C}\ell^-a\right\rangle D^L_{N'i_0}\right),$$
$$\chi^{JL}_{2,a\pm}=\left(\sum\ \xi^{JL}_M\left\langle\left(j_\pm,\frac{1}{2},\ldots,\frac{1}{2}\right),M\middle|L,N';\mathbb{C}\ell^+a\right\rangle D^L_{N'i_0},0\right). \tag{5.46}$$

However, from Eq. (5.39), we have

$$\Gamma^{\mathcal{R}}_\lambda x_\lambda\,\mathcal{D}^{(1,2)}=-\mathcal{D}^{(2,1)}\,\Gamma^{\mathcal{R}}_\lambda x_\lambda, \tag{5.47}$$

and this implies that there is another set of eigenvectors, with the same eigenvalues, given by

$$\tilde\chi^{JL}_{1,a\pm}=\Gamma_\lambda x_\lambda\,\chi^{J,L}_{2,a\mp}=\left(0,\sum\ \xi^{JL}_M\left\langle\left(j_\mp,\frac{1}{2},\ldots,\frac{1}{2}\right),M|D^J|L,i_0;\mathbb{C}\ell^+\alpha\right\rangle D^{\mathbb{C}\ell^-\dagger}_{\alpha a}\right),$$
$$\tilde\chi^{JL}_{2,a\pm}=\Gamma_\lambda x_\lambda\,\chi^{J,L}_{1,a\mp}=\left(\sum\ \xi^{JL}_M\left\langle\left(j_\mp,\frac{1}{2},\ldots,-\frac{1}{2}\right),M|D^J|L,i_0;\mathbb{C}\ell^-\alpha\right\rangle D^{\mathbb{C}\ell^+\dagger}_{\alpha a},0\right). \tag{5.48}$$

D. The projective Dirac operators on $\mathbb{C}P^N$

For reasons of brevity, we focus on $\mathbb{C}P^2$, a case we have already treated in Ref. 12. $\mathbb{C}P^2$ is SU(3)/U(2). If λ_α are the Gell-Mann matrices, it is the orbit of λ_8 under SU(3):

$$\mathbb{C}P^2:\ \{g\lambda_8 g^{-1}\ ,\ g\in \mathrm{SU}(3)\}\ . \tag{5.49}$$

Writing $g\lambda_8 g^{-1}=\lambda_A\xi_A$ analogously to (5.18), we can regard those $\xi\in\mathbb{R}^8$ given by (5.49), as points of $\mathbb{C}P^2$. The stability group at λ_8, or equally well at $\xi^0=(0,\ldots,0,1)$ is U(2). Its generators are $\lambda_1,\lambda_2,\lambda_3,\lambda_8$.

If we can achieve a covariant–looking form for D and D_W looking like (5.19), (5.20), we can find covariant $\mathcal{D}$ and $\mathcal{D}_W$. Towards this end we introduce the Clifford algebra with eight generators γ_A. They can be transformed by the adjoint representation of SU(3) without disturbing their anticommutators:

$$\gamma'_A=\mathrm{Ad}g_{AB}\gamma_B\to\{\gamma'_A,\gamma'_B\}=2\,\delta_{AB}. \tag{5.50}$$

The generators Σ_A in this representation can actually be written using γ_A:

$$\Sigma_A=\frac{1}{4i}f_{ABC}\gamma_B\gamma_C. \tag{5.51}$$

Consider the action $\gamma_A\to[\Sigma_8,\gamma_A]$ of Σ_8 on γ_A. For this action, the eigenvalues of Σ_8 are $\pm\sqrt{3}/2$ and 0. The 0 eigenvalues are for γ_A with $A=1,2,3,8$; thus

$$[\Sigma_8,[\Sigma_8,\gamma_A]]=0,\ \text{if}\ \ A=1,2,3,8,$$
$$=\tfrac{3}{4}\gamma_A,\quad \text{if}\quad A=4,5,6,7. \tag{5.52}$$

This lets us write the Dirac operator in "covariant" form,

$$D_W=-i\frac{4}{3}[\Sigma\cdot\xi^0,[\Sigma\cdot\xi^0,\gamma_A]]^{\mathcal{R}}X_A,\quad (X_Af)(g)=\frac{d}{dt}f(ge^{it\Sigma_A})|_{t=0}. \tag{5.53}$$

The role of Σ_A and γ_A are reversed here for covariantization as compared to spheres.

For the projective module, for the representation D^J, we have the one given by Σ_A. It is $2^{8/2}=16$-dimensional. The transform $\mathcal{D}_W$ of D_W onto this module is immediate:

$$\mathcal{D}_W=-\tfrac{4}{3}[\Sigma\cdot\xi,[\Sigma\cdot\xi,\gamma_A]]^{\mathcal{R}}\mathcal{J}_A. \tag{5.54}$$

In addition to D_W we can also write the Dirac operators,

$$D'=-i\frac{2}{\sqrt{3}}[\Sigma\cdot\xi^0,\gamma_A]X_A,\quad D=i\Gamma(\xi^0)D_W,\ \ \Gamma(\xi^0)=-\gamma_4\gamma_5\gamma_6\gamma_7. \tag{5.55}$$

D' becomes $\mathcal{D}'=-i\,(2/\sqrt{3})\,[\Sigma\cdot\xi,\gamma_A]J_A$ on the projective module. To find $\mathcal{D}$ we need to find the chirality operator $\Gamma(\xi)$ for all ξ. This is in Ref. 12 and is just

$$\Gamma(\xi)=-\frac{1}{4!}\epsilon_{ABCD}(\xi)\gamma_A\gamma_B\gamma_C\gamma_D,\ \ \epsilon_{ABCD}(\xi)=4(\mathrm{ad}\Sigma\cdot\xi)_{[AB}(\mathrm{ad}\ \ \Sigma\cdot\xi)_{CD]} \tag{5.56}$$

([ ]=antisymmetrization). We cannot have an a in χ_a taking values from 1 to 16: that would give 4 spinors. We must have it taking just 4 values and carrying the representation of just γ_A, $A=4,5,6,7$. The explanation of how this is done takes up some space in Ref. 12.

VI. ON RIEMANNIAN STRUCTURE AND GRAVITY

An inverse metric (η^{ij}) is a symmetric nondegenerate field, which defines a map $\mathcal{T}^{(1)}\otimes\mathcal{T}^{(1)}\to\mathcal{T}^{(0)}$ via $f\otimes f'\to\eta^{ij}f_if'_j$. As the f's transform by $\mathrm{Ad}_{G/H}$ under $g\to gh$, (η^{ij}) transform by the product $\mathrm{Ad}^{-1}_{G/H}\otimes\mathrm{Ad}^{-1}_{G/H}$ of its contragradient representation. Or, the metric (η_{ij}) itself transforms by $\mathrm{Ad}_{G/H}\otimes\mathrm{Ad}_{G/H}$.

A particular metric is $(\hat{\delta}_{ij})$, where $\hat{\delta}_{ij}(g)$ is δ_{ij} (δ=Kronecker δ). The torsion-free covariant derivative compatible with $\hat{\delta}$ is $\overline{X}$:

$$\overline{X}\hat{\delta}=0\,. \tag{6.1}$$

The corresponding curvature tensor of G/H can be calculated in terms of the structure constants of G. From their form we have that for any vector field f_i tangent to G/H,

$$[\overline{X}_i,\overline{X}_j]=R_{ijkl}f_l=(c_{ij\alpha}c_{\alpha kl}+\tfrac{1}{4}(2\,c_{ijk'}c_{k'kl}-c_{ikk'}c_{k'jl}-c_{kjk'}c_{k'il}))f_l\,. \tag{6.2}$$

The scalar curvature is then $R=R_{ijij}=c_{ij\alpha}c_{\alpha ij}+\frac{1}{4}c_{ijk'}c_{k'ij}$. For $S^n=\mathrm{Spin}(n+1)/\mathrm{Spin}(n)$, we found in Sec. V C that in a Clifford representation, $[\Sigma_{n+1,i},\Sigma_{n+1,j}]=i\Sigma_{ij}$. So, with the correspondences $i\leftrightarrow(n+1,i)$, $\alpha\leftrightarrow(i,j)$ we have that $c_{ijk}=0$, and the curvature is $R=n(n-1)$.

A more general H-invariant metric η can be defined as follows. Let us decompose G/H into irreducible subspaces under $\mathrm{Ad}_{G/H}$ and let $\{S^{(\sigma)}_m\}$ be a basis for the unitary irreducible representation σ such that

$$\mathrm{Tr}S^{(\sigma)\dagger}_mS^{(\sigma')}_n=c\,\delta_{\sigma\sigma'}\delta_{mn}. \tag{6.3}$$

(Here σ and σ' can be equivalent representations.) Let $X^{(\sigma)}_m$ be the corresponding (in general, complex) vector field, it is a linear combination of X_i. Then a general H-invariant metric η on vector fields $X^{(\sigma)\dagger}_m$ and $X^{(\sigma')}_n$ is the constant function defined by

$$\eta(X^{(\sigma)\dagger}_m,X^{(\sigma')}_n)(g)=\lambda_\sigma\delta_{\sigma\sigma'}\delta_{mn},\ \ \lambda_\sigma\ \text{ a positive constant,} \tag{6.4}$$

independent of g. Such metrics are essential for certain Kähler structures as we shall see in Sec. VII.

The general covariant differential ∇ can be defined in the usual way:

$$\nabla_i \eta_{jk} = \overline{X}_i \eta_{jk} + \Gamma_{ij}^{j'} \eta_{j'k} + \Gamma_{ik}^{k'} \eta_{jk'}. \tag{6.5}$$

The formula shows that Γ transforms by $\mathrm{Ad}_{G/H} \otimes \mathrm{Ad}_{G/H} \otimes \mathrm{Ad}_{G/H}^{-1}$ under the structure group H. As $\overline{X}$ is torsion-free, so is ∇ if as usual $\Gamma_{ij}^k = \Gamma_{ji}^k$. A standard calculation gives the metric-compatible torsion-free ∇, its Γ being given by

$$\Gamma_{ij}^k = -\tfrac{1}{2}\eta^{kk'}(\overline{X}_i \eta_{jk'} + \overline{X}_j \eta_{ik'} - \overline{X}_{k'} \eta_{ij}). \tag{6.6}$$

These Γ_{ij}^k are not Christoffel symbols, for example, they vanish if $c_{ijk} = 0$. Christoffel symbols are defined with respect to some local coordinates x^a on G/H.

Next, introduce $|G/H|$-beins or soldering forms e_i^a such that

$$\eta_{ij} = \eta(X_i, X_j) = e_i^a e_j^b \eta_{ab}. \tag{6.7}$$

The Christoffel symbols are defined from η_{ab} in the usual way.

The spin connection is defined by

$$\nabla_i e_j^a = \overline{X}_i e_j^a + \Gamma_{ij}^k e_k^a + e_j^b (\omega_i)_{ba} = 0, \tag{6.8}$$

where $(\omega_i)_{ba} = -(\omega_i)_{ab}$ and transforms as a tensor field in i under H. The solution for ω_i is standard:

$$(\omega_i)_{ca} = -E_c^j [\overline{X}_i e_j^a + \Gamma_{ij}^k e_k^a], \quad E_c^j e_j^a = \delta_c^a \quad \text{or} \quad E_c^j = \eta^{jk} e_k^a \eta_{ac}. \tag{6.9}$$

The covariant derivative on spinors ψ is given by

$$(\nabla_i \psi)_a = (\overline{X}_i \psi)_a - \tfrac{1}{4}(\omega_i)_{cd} (\gamma_c \gamma_d \psi)_a. \tag{6.10}$$

The Dirac operator in the presence of a gravity field (η_{ij}) is thus

$$D = \eta^{ij} e_j^a \gamma_a \nabla_j. \tag{6.11}$$

All this stuff is very natural. It remains to transport it to projective modules. In the module picture η_{ij} gets transformed to

$$G_{\lambda\rho} = \eta_{ij} (D^J)_{i\lambda}^\dagger (D^J)_{j\rho}^\dagger, \tag{6.12}$$

while η^{ij} becomes

$$G^{\lambda\rho} = \eta^{ij} D_{\lambda i}^J D_{\rho j}^J. \tag{6.13}$$

The projector for the module is

$$P_\sigma^\lambda = G^{\lambda\rho} G_{\rho\sigma} = D_{\lambda i}^J (D^J)_{i\sigma}^\dagger. \tag{6.14}$$

The projective module analogue of $\overline{X}_i$ is the $\overline{\nabla}_\rho$ defined in Sec. V B. Adding the action of

$$\Gamma_{\lambda\mu}^\nu = \Gamma_{ij}^k (D^J)_{i\lambda}^\dagger (D^J)_{j\nu}^\dagger (D^J)_{k\nu}^\dagger \tag{6.15}$$

to $\overline{\nabla}_\rho$ defines the action of ∇_ρ, the metric-compatible torsion-free covariant derivative on tensors ($\nabla_\rho G_{\mu\nu} = 0$).

The action of ∇_ρ on spinorial modules follows from (6.10). We let $\mathcal{J}_\rho$ be the total angular momentum for the representation J_S chosen for spinors, and

$$\mathcal{C}^{(S)}_{\rho\lambda\sigma}=D^{J_S}_{\lambda b}(c_{ijk}\gamma_j\gamma_k)_{ba}(D^{J_S})^\dagger_{a\sigma}(D^{J_T})^\dagger_{i\rho},$$

$$\Omega_{\rho\lambda\sigma}=D^{J_S}_{\lambda b}((\omega_i)_{jk}\gamma_j\gamma_k)_{ba}(D^{J_S})^\dagger_{a\sigma}(D^{J_T})^\dagger_{i\rho}, \tag{6.16}$$

$$\chi_\sigma=\psi_a(D^{J_S})^\dagger_{a\sigma}.$$

Then, as can easily be shown from (5.17) above,

$$(\nabla_\rho\chi)_\sigma=-i(\mathcal{J}_\rho\chi)_\sigma-\chi_\lambda(\tfrac{1}{8}\mathcal{C}^{(S)}+\tfrac{1}{4}\Omega)_{\rho\lambda\sigma}. \tag{6.17}$$

VII. COMPLEX STRUCTURES AND KÄHLER MANIFOLDS

In favorable circumstances, we can push this program ahead and define more refined ideas like complex and Kähler structures on tensors $\mathcal{T}^{(n)}$ and on their projective modules. We indicate how to treat them briefly.

We consider adjoint orbits only for G/H. Thus let $\underline{k}$ be a fixed element of $\underline{G}$ from the Cartan subalgebra $C(\underline{G})$, and H its stability group:

$$H=\langle h\in G: h\underline{k}h^{-1}=\underline{k}\rangle,\ [\underline{k},T(\alpha)]=0\ \forall\ \alpha,\ [\underline{k},S(i)]\neq 0\ \forall\ i\ . \tag{7.1}$$

The Cartan subalgebra of $\underline{H}$, $C(\underline{H})=C(\underline{G})$, since any element of $\underline{G}$ which commutes with $\underline{k}$ is in $\underline{H}$. The manifold G/H, being an adjoint orbit of the simple Lie group G, has even dimension. These observations have the following implications.

Consider the eigenvalue equation

$$[\underline{k},E_a]=\lambda_a E_a\,. \tag{7.2}$$

Then $\lambda_a\neq 0$. The E_a will be of the form $\Sigma_i\xi_{ai}S(i)$, $\xi_{ai}\in\mathbb{C}$, and span the complexification $(\underline{G/H})_c$ of $(\underline{G/H})$.

By (2.7), $(\underline{G/H})_c$ is invariant under the adjoint action of $\underline{k}$. Also, as $\mathrm{Ad}_{G/H}$ is a real, orthogonal representation, the eigenvalues λ_a are real, while of course the $S(i)$ are Hermitian. So the adjoint of (7.2) shows that $E_a^\dagger$ corresponds to the eigenvalue $-\lambda_a$, and that each positive eigenvalue is paired with a negative one. The eigenvalues λ_a may be degenerate.

We choose E_a, $a=1,\ldots,\frac{1}{2}(|G|-|H|)$, to be solutions of (7.2) with $\lambda_a>0$, $E_{-a}=E_a^\dagger$, and the normalization

$$\mathrm{Tr}\,E_a E_b=\delta_{a+b,0}\,. \tag{7.3}$$

So, if $E_a=\xi_{a\,i}S(i)$ (for both signs of a), $\xi_{-a\,i}=\xi^*_{a\,i}$. We choose $c=1$ in (2.1) and (2.3). Then (2.3) and (7.3) show that the matrix $\{\xi_{a\,i}\}$ is unitary as well.

Let $(\underline{G/H})^\pm_c$ denote the span of the eigenvectors $E_{\pm|a|}$ (where we note that $|a|>0$). The subspaces $(\underline{G/H})^\pm_c$ are of precisely the same dimension and

$$(\underline{G/H})_c=(\underline{G/H})^+_c\oplus(\underline{G/H})^-_c\,. \tag{7.4}$$

The elements $E^+=\Sigma_i\xi^iS(i)\in(\underline{G/H})^+_c$ generate vector fields $X^+=\xi^iX_i$ which we define to be holomorphic. Let $\mathcal{H}^+$ denote the space of holomorphic vector fields. Likewise $(\underline{G/H})^-_c$ gives rise to the space $\mathcal{H}^-$ of antiholomorphic vector fields. This splitting of the space of fields $\mathcal{H}$ as the direct sum $\mathcal{H}^+\oplus\mathcal{H}^-$ gives us the complex structure. The (1,1) tensor J of complex analysis is $\pm i$ on $\mathcal{H}^\pm$: for a vector field $X=\xi^iX_i$, $JX=\xi^j\Sigma_{a>0}i(\xi^*_{aj}\xi_{ai}-\xi_{aj}\xi^*_{ai})X_i$.

This complex structure is Kähler. To show it, let us introduce the Maurer–Cartan forms θ^A, defined by $g^{-1}\,dg=i\Sigma_A\theta^A$, or, setting $c=1$ in (2.1), by

$$\theta^A=-i\,\mathrm{Tr}\,\Sigma_A\,g^{-1}\,dg. \tag{7.5}$$

They are dual to the vector fields $X_A=(X_i, X_\alpha)$, so that, for example, $\theta^i(X_j)=\delta_{ij}$, and fulfill

$$d\theta^A=-\frac{i}{2}\mathrm{Tr}(\Sigma_A[\Sigma_B,\Sigma_C])\,\theta^B\wedge\theta^C=\tfrac{1}{2}c_{BCA}\theta^B\wedge\theta^C. \tag{7.6}$$

Consider the particular Maurer–Cartan form,

$$\Theta=-i\mathrm{Tr}\,\underline{k}\,g^{-1}\,dg=\mathrm{Tr}\,(\underline{k}\,\Sigma_A)\,\theta^A=\mathrm{Tr}(\underline{k}\,T(\alpha))\,\theta^\alpha. \tag{7.7}$$

In the last step we used (2.4). For $d\Theta$ we have

$$d\Theta=-\frac{i}{2}\mathrm{Tr}(k\,[\Sigma_B,\Sigma_C])\,\theta^B\wedge\theta^C. \tag{7.8}$$

But using (7.1) we have $\mathrm{Tr}\underline{k}\,[T(\alpha),T(\beta)]=\mathrm{Tr}[\underline{k},T(\alpha)]T(\beta)=0$ and $\mathrm{Tr}\underline{k}\,[T(\alpha),S(i)]=\mathrm{Tr}[\underline{k},T(\alpha)]\,S(i)=0$. Therefore

$$d\Theta=-\frac{i}{2}\mathrm{Tr}(\underline{k}\,[S(i),S(j)])\theta^i\wedge\theta^j\ . \tag{7.9}$$

Remembering that the matrix $\{\xi_{a\,i}\}$ (with a of both signs) is unitary, we may set

$$S(i)\ \theta^i=E_a\,\xi^*_{a\,i}\,\theta^i\equiv E_a\,\theta^a \tag{7.10}$$

(with an implied sum over a of both signs), and rewrite (7.9) as

$$d\Theta=-\frac{i}{2}(\mathrm{Tr}\underline{k}[E_a,E_b])\,\theta^a\wedge\theta^b=-\frac{i}{2}\lambda_a(\mathrm{Tr}\,E_a\,E_b)\,\theta^a\wedge\theta^b=-i\sum_{a>0}\lambda_a\theta^a\wedge\theta^{-a}, \tag{7.11}$$

where we have used (7.2) and (7.3). The vector fields $X_a=\xi_{ai}X_i$ are dual to θ^a: $\theta^a(X_b)=\delta_{a\,b}$. Consequently, the two-form $\Omega=d\Theta$ can be specified by

$$\Omega(X_a,X_b)=d\Theta(X_a,X_b)=-i\lambda_a\delta_{a+b,0}. \tag{7.12}$$

Since all $\lambda_a\neq 0$, it follows from (7.11) that Ω is a symplectic (i.e., closed and nondegenerate) form on G/H. It has been extensively discussed in Ref. 13, where its physical implications are also explained. It fulfills the Kählerian condition

$$\Omega(JX_a,JX_b)=\Omega(X_a,X_b). \tag{7.13}$$

For vector fields $X=\xi^iX_i$, $Y=\eta^iX_i$, we have $\Omega(X,Y)=\Sigma_{a>0}(i\lambda_a)(\xi_{ai}\xi^*_{aj}-\xi_{aj}\xi^*_{ai})\xi^i\eta^j$.

The Kähler metric η on vector fields (X_a, X_b) is given by

$$\eta(X_a,X_b)=\Omega(JX_a,X_b)=|\lambda_a|\,\delta_{a+b,0}. \tag{7.14}$$

The Levi-Civita connection corresponding to this metric is the torsion-less connection compatible with η. Its coefficients are given by the formula (6.6):

$$\frac{1}{2}c_{abc}+\Gamma^c_{ab}=\frac{1}{2}c_{abc}-\frac{|\lambda_a|-|\lambda_b|}{2|\lambda_c|}c_{abc}\,. \tag{7.15}$$

Note from (7.3) and (2.8) that $c_{abc}=\mathrm{Tr}[E_a,E_b]E_{-c}$. So we have the symmetries

$$c_{abc}=c_{b,-c,-a}=c_{-c,a,-b}. \tag{7.16}$$

Also from $\mathrm{Tr}[\underline{k},[E_a,E_b]E_{-c}]=0$ and (7.2) we have that

$$c_{abc} \text{ and } (7.15) = 0 \text{ if } \lambda_a + \lambda_b - \lambda_c \neq 0. \tag{7.17}$$

Finally, we shall show that the Kähler metric on G/H can be derived from a Kähler potential Φ_ζ. It is a function on G/H and depends on a parameter ζ. It has the property

$$X_a X_{-b} \Phi_\zeta = \eta(X_a, X_{-b}), \tag{7.18}$$

for λ_a and λ_b of the same sign and $|\lambda_a| \leqslant |\lambda_b|$. The ordering is needed because of the torsion term in (2.8). It can be discarded when the torsion is zero, that is for symmetric spaces. Note that Φ_ζ can in general be only locally defined on G/H.

The construction of Φ_ζ involves the member of a specific class of unitary representations $\Sigma_K : g \to \Sigma_K(g)$ of G. Let σ_K be the associated representation of $\underline{G}$. Any such representation contains a normalized highest weight vector $|K\rangle$ with eigenvalue K for $\sigma_K(\underline{k})$, which is annihilated by the orthogonal complement of $\underline{k}$ in $\underline{H}$ and the positive roots E_a:

$$\begin{aligned} &\text{(a)} \quad \sigma_K(\underline{k})|K\rangle = K|K\rangle, \quad K > 0, \\ &\text{(b)} \quad \sigma_K(T(\alpha))|K\rangle = 0, \quad \text{if } \mathrm{Tr} T(\alpha)\underline{k} = 0, \\ &\text{(c)} \quad \sigma_K(E_a)|K\rangle = 0, \quad \text{for } \forall \ a > 0. \end{aligned} \tag{7.19}$$

A representation of G fulfilling (a) and (b) always exists: it is induced from the unitary one-dimensional representation of H given by (a) and (b):

$$\Sigma_K(e^{i\xi_\alpha T(\alpha)})|K\rangle = e^{i(K/\mathrm{Tr}\,\underline{k}^2)\mathrm{Tr}(\underline{k}\,\xi_\alpha T(\alpha))}|K\rangle. \tag{7.20}$$

Here we have used

$$\sigma_K(\xi_\alpha T(\alpha))|K\rangle = \frac{K}{\mathrm{Tr}\,\underline{k}^2}\mathrm{Tr}(\underline{k}\,\xi_\alpha T(\alpha))|K\rangle. \tag{7.21}$$

As for (a), (b) and (c) together, it gives the representation of the group G_c generated by $\underline{H}$ and E_a, $a > 0$, induced from the representation $\sigma_K(\underline{H})$, $\sigma_K(E_a)$, $a > 0$.

Let us fix an orthonormal basis $\{e_1, e_2, \ldots, e_M\}$ in the representation space of dimension M (say) of $\Sigma_K(G)$. Choose a vector $|\zeta\rangle = \Sigma_{i=1}^M \zeta_i e_i$, $\zeta_i \in \mathbb{C}$, $\zeta = (\zeta_1, \zeta_2, \ldots, \zeta_M)$, so that $\langle\zeta|\Sigma_K(g)|K\rangle \neq 0$ when g belongs to some open set $\mathcal{O}$. Such a $|\zeta\rangle$ exists since $\langle\zeta|\Sigma_K(g)|K\rangle = 1$ for $|\zeta\rangle = \Sigma_K(g)|K\rangle$. Further, choose $\mathcal{O}$ so that it is invariant under H-action. That is always possible since for $\langle\zeta|\Sigma_K(g)|K\rangle$ changes only by a phase under this action by (7.20).

Now the function ω_ζ, defined by

$$\omega_\zeta(g) = \langle\zeta|\Sigma_K(g)|K\rangle, \quad g \in \mathcal{O}, \tag{7.22}$$

has the properties

$$\begin{aligned} &(X_a \omega_\zeta)(g) = (X_{-a}\overline{\omega_\zeta})(g) = 0, \quad \text{for } \forall a > 0, \\ &\frac{1}{\omega_\zeta(g)}(X_\alpha \omega)_\zeta(g) = -\frac{1}{\overline{\omega_\zeta}(g)}(X_\alpha \overline{\omega_\zeta})(g) = i\frac{K}{\mathrm{Tr}\,\underline{k}^2}\mathrm{Tr}(\underline{k}\,T(\alpha)). \end{aligned} \tag{7.23}$$

Here the overbar denotes complex conjugation. The first line is a direct consequence of the fact that $|K>$ is the highest weight vector, the second line follows from the relation $\omega_\zeta(gh) = \omega_\zeta(g)\Sigma_K(h)$ valid for any $g \in G$, $h \in H$, with the phase factor $\Sigma_K(h)$ given by (7.20).

If $g \in \mathcal{O}$, the Kähler potential is given by the formula

$$\Phi_\zeta = -\frac{\mathrm{Tr}\,\underline{k}^2}{2K}\log\omega_\zeta(g)\,\overline{\omega}_\zeta(g). \tag{7.24}$$

Φ_ζ is a function on $\mathcal{O}/H\subseteq G/H$, since in the product

$$\omega_\zeta(gh)\overline{\omega}_\zeta(gh)=\Sigma_K(h)\omega_\zeta(g)\overline{\Sigma}_K(h)\overline{\omega}_\zeta(g),$$

the phase factors $\Sigma_K(h)$ and $\overline{\Sigma}_K(h)$ cancel. The Kähler potential is closely related to the one-form Θ introduced in (7.7). Thus the exterior derivative d on G can be written as $d=d_+ + d_- + d_0$, where

$$d_\pm f(g)=(X_{\pm|a|}f)(g)\,\theta^{\pm|a|},\quad d_0 f(g)=(X_\alpha f)(g)\,\theta^\alpha\ . \tag{7.25}$$

Now, using (7.23) one obtains

$$\begin{aligned} i(d_+-d_-)\Phi_\zeta &= i(X_{|a|}\Phi_\zeta)\ \theta^{|a|}-i(X_{-|a|}\Phi_\zeta)\ \theta^{-|a|}\\ &= -i\frac{\mathrm{Tr}\,\underline{k}^2}{2K\overline{\omega}_\zeta}(X_{|a|}\overline{\omega}_\zeta)\ \theta^{|a|}+i\frac{\mathrm{Tr}\,\underline{k}^2}{2K\omega_\zeta}(X_{-|a|}\omega_\zeta)\ \theta^{-|a|}\\ &= i\frac{\mathrm{Tr}\,\underline{k}^2}{2K}d\log\frac{\omega_\zeta}{\overline{\omega}_\zeta}+\mathrm{Tr}(\underline{k}\,T(\alpha))\theta^\alpha = i\frac{\mathrm{Tr}\,\underline{k}^2}{2K}d\log\frac{\omega_\zeta}{\overline{\omega}_\zeta}+\Theta. \end{aligned} \tag{7.26}$$

It follows that

$$d\,i(d_+-d_-)\,\Phi_\zeta = d\,\Theta=\Omega. \tag{7.27}$$

The left hand side of (7.27) can be evaluated using the first line of (7.26) and (7.6). Calculating its values on $iX_a\otimes X_{-b}$ for $0<\lambda_a\leqslant\lambda_b$ and $0<-\lambda_a\leqslant-\lambda_b$, we get (7.18). For this calculation, it is also important that $c_{abc}=0$ if $\lambda_a+\lambda_b\neq\lambda_c$.

In another open set $\mathcal{O}'\subset G$, we may have to work with the Kähler potential Φ_η. Then if $\mathcal{O}\cap\mathcal{O}'\neq\varnothing$, the two potentials on $\mathcal{O}\cap\mathcal{O}'$ are related by

$$\Phi_\eta=\Phi_\zeta-\frac{\mathrm{Tr}\,\underline{k}^2}{2K}\log\frac{\omega_\eta}{\omega_\zeta}+\frac{\mathrm{Tr}\,\underline{k}^2}{2K}\log\frac{\overline{\omega}_\eta}{\overline{\omega}_\zeta}. \tag{7.28}$$

The mapping Φ_ζ to Φ_η is often called a gauge transformation.

ACKNOWLEDGMENTS

We are part of a collaboration on fuzzy physics and noncommutative geometry which involves several physicists. The work reported here has benefited greatly by discussions with the members of this collaboration. We thank to Franciscus J. Vanhecke for bringing Ref. 2 to our attention. Our work was supported by the Department of Energy (DOE) and the National Science Foundation (NSF) under Contracts No. DE-FG02-85ER40231 and No. INT-9908763, by I.N.F.N, Italy, and VEGA project 1/7069/20, Slovakia.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Covariant realization of quantum spaces as star products by Drinfeld twists

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(Received 27 February 2003; accepted 7 May 2003)

Covariance of a quantum space with respect to a quantum enveloping algebra ties the deformation of the multiplication of the space algebra to the deformation of the coproduct of the enveloping algebra. Since the deformation of the coproduct is governed by a Drinfeld twist, the same twist naturally defines a covariant star product on the commutative space. However, this product is in general not associative and does not yield the quantum space. It is shown that there are certain Drinfeld twists which realize the associative product of the quantum plane, quantum Euclidean four-space, and quantum Minkowski space. These twists are unique up to a central two-coboundary. The appropriate formal deformation of real structures of the quantum spaces is also expressed by these twists. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1602553]

I. INTRODUCTION

Noncommutative geometries are described by replacing the commutative algebra of functions on an ordinary space with a noncommutative algebra. The noncommutativity is controlled by a perturbation parameter, if it is a small deviation from ordinary geometry. The algebraic aspects of such a perturbation can be detached from questions of convergence and continuity by considering formal power series. A noncommutative geometry is then described as a formal deformation of a commutative algebra[1] or by a star product.[2] Such a description has attracted a lot of attention lately, due to its application to string theory[3] and to the construction of gauge theories on noncommutative spaces.[4]

The description of physical space–time by an algebra alone would not distinguish Minkowski space from, say, Euclidean four-space, which differs by the symmetry that acts on it. Deforming a space algebra which transforms covariantly under a symmetry Lie group will, in general, break the symmetry. But there are deformations, where the symmetry structure can be deformed together with the space, so that covariance is preserved. Quantum spaces[5–7] are such a class of deformations, carrying a covariant representation of the Drinfeld–Jimbo deformation[8,9] of the enveloping symmetry algebra.

The deformation of an enveloping algebra into a Drinfeld–Jimbo algebra is well understood: As algebra over the ring of formal power series the deformed algebra is isomorphic to the undeformed one. In fact, if the Lie algebra is semisimple, it can be shown by cohomological arguments that the enveloping algebra cannot be deformed at all.[1] It is only the Hopf structure which is truly deformed. The deformed and the undeformed coproduct are nonisomorphic but related by inner automorphisms, called Drinfeld twists.[10] Preserving covariance ties the deformation of the enveloping algebra closely to the deformation of the space algebra. Therefore, one ought to be able to use the knowledge about the deformation of the symmetry in order to deform the space algebra accordingly. Such an approach was suggested in Ref. 11, where a Drinfeld twist was used to realize a quantum space as star product on the undeformed space algebra (for a similar approach see Ref. 12). By construction, such a star product is covariant with respect to the action of the

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Drinfeld–Jimbo algebra. However, the star product is in general not associative. The main question of this article is: Is there a Drinfeld twist which implements the associative product of a given quantum space? We will give a positive answer for three particularly interesting cases: the quantum plane, quantum Euclidean four-space, and quantum Minkowski space.

In Sec. II we review quantum spaces as covariant deformations and relate them to star products defined by Drinfeld twists.[11] We recall the definition and properties of Drinfeld twists in the framework of formal algebraic deformations. Real structures of quantum spaces and of the according quantum algebras are taken into account: Gerstenhaber's rigidity theorem for algebras[1] is extended to $*$-algebras (Proposition 1) and the deformation of space algebras is extended to real structures (Proposition 4). In Sec. III we propose a general approach which reduces the algebraic problem of finding a twist which implements the multiplication of a quantum space to a representation theoretic problem. This works well for cases where the representation theory of the symmetry quantum algebra is well understood: We determine the basis which reduces the quantum plane, quantum Euclidean four-space, and quantum Minkowski space as module into its irreducible highest weight subrepresentations, and calculate the multiplication map with respect to this basis. Comparing the multiplication maps with the representations of the twists leads to the main result: There are Drinfeld twists which realize the quantum plane (Proposition 8), quantum Euclidean four-space (Proposition 9), and quantum Minkowski space (Proposition 10) as covariant star products. These twists are unique up to a central two-coboundary.

Throughout this article we assume that $\mathfrak{g}$ is a semisimple Lie algebra, denoting its enveloping algebra by $\mathcal{U}(\mathfrak{g})$. An element $g \in \mathcal{U}(\mathfrak{g})^{\otimes(n+1)}$ is called $\mathfrak{g}$-invariant if it commutes with the n-fold coproduct $\Delta^{(n)}(g) := g\otimes 1^{\otimes n} + 1\otimes g\otimes 1^{\otimes(n-1)} + \cdots + 1^{\otimes n}\otimes g$ of all $g \in \mathfrak{g}$. The formal perturbation parameter is $\hbar$; the completion of a complex vector space or algebra A with respect to the $\hbar$-adic topology is $A[[\hbar]]$. The topological tensor product $\hat{\otimes}$ of two free $\hbar$-adic vector spaces or algebras is avoided by identifying $A[[\hbar]]\hat{\otimes}A'[[\hbar]] \equiv (A\otimes A')[[\hbar]]$. The $\hbar$-adic Drinfeld–Jimbo deformation[8,9] of $\mathcal{U}(\mathfrak{g})$ is denoted by $\mathcal{U}_\hbar(\mathfrak{g})$. The equality of two elements a, $a' \in A[[\hbar]]$ modulo $\hbar^n$ will be written in Landau notation as $a = a' + \mathcal{O}(\hbar^n)$. Recall that if $a = 1 + \mathcal{O}(\hbar)$, then a is invertible and its square root with $\sqrt{a} = 1 + \mathcal{O}(\hbar)$ is defined and unique in $A[[\hbar]]$ (see, e.g., Ref. 13). The symmetric $\hbar$-adic quantum number is defined by $[n] := (e^{\hbar n} - e^{-\hbar n})(e^{\hbar} - e^{-\hbar})^{-1}$ and for natural n the quantum factorial by $[n]! := [1]\cdot[2]\cdots[n]$.

II. QUANTUM SPACES AND DRINFELD TWISTS

A. Quantum spaces

Let $\mathfrak{g}$ be the Lie algebra of the symmetry group of a space and $\mathcal{X}$ be the function algebra of this space. The elements $g \in \mathfrak{g}$ of the Lie algebra act on $\mathcal{X}$ as derivations, $g\triangleright xy = (g\triangleright x)y + x(g\triangleright y)$ for $x, y \in \mathcal{X}$. A generalized way of writing this is

$$g\triangleright xy = (g_{(1)}\triangleright x)(g_{(2)}\triangleright y) \tag{1}$$

for all $g \in \mathcal{U}(\mathfrak{g})$, where we introduce the coproduct of an enveloping algebra by $g_{(1)}\otimes g_{(2)} \equiv \Delta(g) := g\otimes 1 + 1\otimes g$ on the generators $g \in \mathfrak{g}$ and extend it to a homomorphism $\Delta: \mathcal{U}(\mathfrak{g}) \to \mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g})$ on the enveloping algebra.

Using the multiplication map $\mu: \mathcal{X}\otimes\mathcal{X} \to \mathcal{X}$, $\mu(x\otimes y) := xy$ of $\mathcal{X}$ we can write (1) as

$$g\triangleright \mu(x\otimes y) = \mu(\Delta(g)\triangleright[x\otimes y]), \tag{2}$$

the condition for the product μ to be covariant with respect to the action of $\mathcal{U}(\mathfrak{g})$, which is meaningful not only for $\mathcal{U}(\mathfrak{g})$ but for any Hopf algebra. In mathematical terminology, an algebra $\mathcal{X}$ which carries a representation of some Hopf algebra H such that Eq. (1) holds is called an H-module algebra. We will also call it an H-covariant space. The covariant spaces or module algebras of the quantum enveloping algebras $\mathcal{U}_\hbar(\mathfrak{g})$ are called quantum spaces.

As algebra, $\mathcal{U}_\hbar(\mathfrak{g})$ for semisimple $\mathfrak{g}$ is not a true deformation of $\mathcal{U}(\mathfrak{g})$, because $\mathcal{U}_\hbar(\mathfrak{g})$ and $\mathcal{U}(\mathfrak{g})[[\hbar]]$ are isomorphic as algebras (see Sec. II C). This means that every $\hbar$-adic space algebra $\mathcal{X}$

which is a $\mathcal{U}(\mathfrak{g})[[\hbar]]$-module is also a $\mathcal{U}_\hbar(\mathfrak{g})$-module and vice versa. In other words, if we considered only the algebra structure of $\mathcal{U}(\mathfrak{g})$, then there would be no need to replace a commutative space with a noncommutative one when passing from the symmetry algebra to its quantum deformation. It is the Hopf structure which is deformed in an essential way. That is, identifying $\mathcal{U}_\hbar(\mathfrak{g})$ and $\mathcal{U}(\mathfrak{g})[[\hbar]]$ as isomorphic algebras, we can view the quantum deformation as deformation of the Hopf structure of $\mathcal{U}(\mathfrak{g})[[\hbar]]$, $\Delta\to\Delta_\hbar$, $\varepsilon\to\varepsilon_\hbar$, $S\to S_\hbar$. Since the covariance condition (1) ties the algebra structure of a space $\mathcal{X}$ to the coproduct, the multiplication map of the space must be deformed, $\mu\to\mu_\hbar$, along with the deformation of the coproduct, $\Delta\to\Delta_\hbar$, if the covariance is to be preserved. Conversely, deforming the multiplication map of a covariant space, the coproduct of the symmetry algebra must be deformed accordingly,

$$g\triangleright xy=(g_{(1)}\triangleright x)(g_{(2)}\triangleright y)\xrightarrow[\Delta\to\Delta_\hbar]{\mu\to\mu_\hbar} g\triangleright(x\star y)=(g_{(1_\hbar)}\triangleright x)\star(g_{(2_\hbar)}\triangleright y), \tag{3}$$

where $\Delta_\hbar(g)=g_{(1_\hbar)}\otimes g_{(2_\hbar)}$ and $\mu_\hbar(x\otimes y)=x\star y$. While there may be a large class of deformations which are covariant in this sense, we will restrict our attention to quantum spaces.

B. Star products by Drinfeld twists

In the case of quantum spaces, the deformed coproduct belongs to the Drinfeld–Jimbo deformation $\mathcal{U}_\hbar(\mathfrak{g})\cong(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta_\hbar,\varepsilon_\hbar,S_\hbar)$. Drinfeld has observed (Theorem 1) that $\Delta_\hbar$ is related to the undeformed coproduct Δ by an inner automorphism. That is, there is an invertible element $\mathcal{F}\in(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ with $\mathcal{F}=1+\mathcal{O}(\hbar)$, called Drinfeld twist, such that

$$\Delta_\hbar(g):=\mathcal{F}\Delta(g)\mathcal{F}^{-1}. \tag{4}$$

Comparing the covariance condition of the deformed multiplication,

$$g\triangleright\mu_\hbar(x\otimes y)=\mu_\hbar(\Delta_\hbar(g)\triangleright[x\otimes y])=\mu_\hbar(\mathcal{F}\Delta(g)\mathcal{F}^{-1}\triangleright[x\otimes y]) \tag{5}$$

with the covariance property (2) of the undeformed product, we see that Eq. (5) is naturally satisfied if we define the deformed product by[11]

$$\mu_\hbar(x\otimes y):=\mu(\mathcal{F}^{-1}\triangleright[x\otimes y])\ \Leftrightarrow\ x\star y:=(\mathcal{F}^{-1}_{[1]}\triangleright x)(\mathcal{F}^{-1}_{[2]}\triangleright y), \tag{6}$$

where we suppress in a Sweedler-like notation the summation of $\Sigma_i\mathcal{F}_{1i}\otimes\mathcal{F}_{2i}\equiv\mathcal{F}_{[1]}\otimes\mathcal{F}_{[2]}$. Since the elements of the Lie algebra $\mathfrak{g}$ act on the undeformed space algebra $\mathcal{X}$ as derivations, $\mathcal{F}^{-1}$ acts as $\hbar$-adic differential operator on $\mathcal{X}\otimes\mathcal{X}$. Hence, writing out the $\hbar$-adic sum of $\mathcal{F}^{-1}=1+\Sigma_k\hbar^k\mathcal{F}_k^{-1}$ we can define the bidifferential operators

$$B_k(x\otimes y):=\mu(\mathcal{F}_k^{-1}\triangleright[x\otimes y])=(\mathcal{F}^{-1}_{k[1]}\triangleright x)(\mathcal{F}^{-1}_{k[2]}\triangleright y), \tag{7}$$

such that the star product (6) can be written in the more familiar form

$$x\star y:=xy+\hbar B_1(x,y)+\hbar^2B_2(x,y)+\cdots. \tag{8}$$

Even though the twist $\mathcal{F}$ yields by Eq. (4) a coassociative coproduct, Eq. (6) will in general not define an associative product. The associativity condition for $\mu_\hbar$ reads

$$\begin{aligned}(x\star y)\star z&=(\mathcal{F}^{-1}_{[1](1)}\mathcal{F}^{-1}_{[1']}\triangleright x)(\mathcal{F}^{-1}_{[1](2)}\mathcal{F}^{-1}_{[2']}\triangleright y)(\mathcal{F}^{-1}_{[2]}\triangleright z)\\&=(\mathcal{F}^{-1}_{[1]}\triangleright x)(\mathcal{F}^{-1}_{[2](1)}\mathcal{F}^{-1}_{[1']}\triangleright y)(\mathcal{F}^{-1}_{[2](2)}\mathcal{F}^{-1}_{[2']}\triangleright z)=x\star(y\star z),\end{aligned} \tag{9}$$

for all $x, y, z\in\mathcal{X}$. Defining the Drinfeld coassociator

$$\Phi:=(\Delta\otimes\mathrm{id})(\mathcal{F}^{-1})(\mathcal{F}^{-1}\otimes 1)(1\otimes\mathcal{F})(\mathrm{id}\otimes\Delta)(\mathcal{F}), \tag{10}$$

the associativity condition (9) can be written as

$$(\Phi_{[1]}\triangleright x)(\Phi_{[2]}\triangleright y)(\Phi_{[3]}\triangleright z)=xyz. \tag{11}$$

The obvious question to ask is: For a given $\mathcal{U}_\hbar(\mathfrak{g})$-covariant quantum space, is there a Drinfeld twist $\mathcal{F}$ which yields by Eq. (6) the associative product of the quantum space? We do not attempt to answer this question in its generality. Instead, we will consider some prototypical and physically important cases: the quantum plane, quantum Euclidean four-space, and quantum Minkowski space.

C. Drinfeld twists of quantum enveloping algebras

For the reader's convenience we gather in this section some well-known results on formal deformations of algebras and Hopf algebras, essentially due to Gerstenhaber[1] and Drinfeld.[10,14]

An $\hbar$-adic algebra A' is called a deformation of an algebra A if $A'/\hbar A'$ and A are isomorphic as algebras. Analogously, an $\hbar$-adic Hopf algebra H' is called a deformation of a Hopf algebra H if $H'/\hbar H'$ and H are isomorphic as Hopf algebras. Recall that $\mathcal{U}(\mathfrak{g})$ is a Hopf algebra with the canonical Lie Hopf structure defined on the generators $g\in\mathfrak{g}$ as coproduct $\Delta(g)=g\otimes 1+1\otimes g$, counit $\varepsilon(g)=0$, and antipode $S(g)=-g$. The Drinfeld–Jimbo algebra $\mathcal{U}_\hbar(\mathfrak{g})$ is a deformation of this Hopf algebra $\mathcal{U}(\mathfrak{g})$. This can be seen by developing the commutation relations and the Hopf structure of $\mathcal{U}_\hbar(\mathfrak{g})$ as formal power series in $\hbar$ and keeping only the zeroth-order terms, which yields the commutation relations and the Lie Hopf structure of $\mathcal{U}(\mathfrak{g})$.

Gerstenhaber has shown[1] that whenever the second Hochschild cohomology of A with coefficients in A is zero, $H^2(A,A)=0$, then all deformations of A are trivial up to isomorphism. That is, any deformation A' of A is isomorphic to the $\hbar$-adic completion of the undeformed algebra, $A'\cong A[[\hbar]]$. Algebras with this property are called rigid. The second Whitehead lemma states that the second Lie algebra cohomology of a semisimple Lie algebra $\mathfrak{g}$ and, hence, the second Hochschild cohomology of its enveloping algebra is zero. Therefore, the enveloping algebra $\mathcal{U}(\mathfrak{g})$ of a semisimple Lie algebra $\mathfrak{g}$ is rigid. In particular, there is an isomorphism of algebras $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$, by which the Hopf structure Δ', ε', S' of $\mathcal{U}_\hbar(\mathfrak{g})$ can be transfered to $\mathcal{U}(\mathfrak{g})[[\hbar]]$,

$$\Delta_\hbar:=(\alpha\otimes\alpha)\circ\Delta'\circ\alpha^{-1},\quad \varepsilon_\hbar:=\varepsilon'\circ\alpha^{-1},\quad S_\hbar:=\alpha\circ S'\circ\alpha^{-1}, \tag{12}$$

such that α becomes an isomorphism of Hopf algebras from $\mathcal{U}_\hbar(\mathfrak{g})$ to $\mathcal{U}(\mathfrak{g})[[\hbar]]$ with this deformed Hopf structure. Let α' be another such isomorphism and $\Delta'_\hbar$, $\varepsilon'_\hbar$, $S'_\hbar$ be defined as in Eq. (12) with α' instead of α. Then α' is an isomorphism of Hopf algebras from $\mathcal{U}_\hbar(\mathfrak{g})$ to $\mathcal{U}(\mathfrak{g})[[\hbar]]$ with the primed Hopf structure,

$$(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta_\hbar,\varepsilon_\hbar,S_\hbar)\overset{\alpha}{\leftarrow}\mathcal{U}_\hbar(\mathfrak{g})\overset{\alpha'}{\rightarrow}(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta'_\hbar,\varepsilon'_\hbar,S'_\hbar), \tag{13}$$

hence, $\alpha'\circ\alpha^{-1}$ is an isomorphism of Hopf algebras. We conclude that, while the Hopf structure Eq. (12) may depend on the isomorphism α, it is unique up to an isomorphism of Hopf algebras.

As a consequence of the first Whitehead lemma, the first Hochschild cohomology of the enveloping algebra $\mathcal{U}(\mathfrak{g})$ of a semisimple Lie algebra is zero. This implies that the two homomorphisms Δ and $\Delta_\hbar$ from $\mathcal{U}(\mathfrak{g})[[\hbar]]$ to $(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ with $\Delta_\hbar=\Delta+\mathcal{O}(\hbar)$ are related by an inner automorphism, as it was observed by Drinfeld.[10,14]

Theorem 1: *Let $\mathfrak{g}$ be a semisimple Lie algebra, and let $\Delta_\hbar$ be defined as in Eq. (12). Then there is an invertible element $\mathcal{F}\in(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ such that $\Delta_\hbar(g)=\mathcal{F}\Delta(g)\mathcal{F}^{-1}$, which is called a Drinfeld twist from Δ to $\Delta_\hbar$.*

On the first sight Theorem 1 only relates the coproducts. It turns out that the twist of the coproduct relates counit and antipode, as well.

Corollary 1: Let $\mathcal{F}$ be a Drinfeld twist from Δ to $\Delta_\hbar$ as in Theorem 1.

(i) If $\mathcal{F}'$ is another Drinfeld twist, then $\mathcal{F}^{-1}\mathcal{F}'$ is invertible and $\mathfrak{g}$-invariant. Conversely, let $\mathcal{T}\in(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ be invertible and $\mathfrak{g}$-invariant. Then $\mathcal{F}\mathcal{T}$ is a Drinfeld twist.

(ii) $\varepsilon_\hbar = \varepsilon$.

(iii) There is a twist $\mathcal{F}$ *such that* $\varepsilon(\mathcal{F}_{[1]})\mathcal{F}_{[2]} = 1 = \mathcal{F}_{[1]}\varepsilon(\mathcal{F}_{[2]})$, *which implies* $\mathcal{F} = 1 + \mathcal{O}(\hbar)$. *Twists with this property are called counital.*

(iv) The two elements of $\mathcal{U}(\mathfrak{g})[[\hbar]]$ *defined as*

$$\sigma_1^{-1} := S(\mathcal{F}_{[1]}^{-1})\mathcal{F}_{[2]}^{-1}, \quad \sigma_2 := \mathcal{F}_{[1]}S(\mathcal{F}_{[2]}) \tag{14}$$

are invertible, $\sigma_1^{-1}\sigma_2 = \sigma_2\sigma_1^{-1}$ *is central in* $\mathcal{U}(\mathfrak{g})[[\hbar]]$, *and* $\sigma_1 S(g)\sigma_1^{-1} = S_\hbar(g) = \sigma_2 S(g)\sigma_2^{-1}$ *for all* $g \in \mathcal{U}(\mathfrak{g})[[\hbar]]$.

(v) The coassociator Φ *defined as in Eq. (10) is* $\mathfrak{g}$*-invariant.*

(vi) The deformed Hopf structure on $\mathcal{U}(\mathfrak{g})[[\hbar]]$ *is isomorphic to the undeformed one if and only if there is a Drinfeld twist of the form* $\mathcal{F} = (u \otimes u)\Delta u^{-1}$ *for some invertible* $u \in \mathcal{U}(\mathfrak{g})[[\hbar]]$.

A proof can be found in the Appendix. The multiplication of a twist with a $\mathfrak{g}$-invariant element as in (i) is sometimes called a gauge transformation of the twist. Counitality (iii) is often part of the definition of twists. Therefore, we will assume from now on that all Drinfeld twists are counital. It can be shown that there are twists for which the elements σ_1 and σ_2 of (iv) are equal.[15] However, this is not the case for all twists. For example, assume that $\sigma_1 = \sigma_2$ for some twist $\mathcal{F}$, and assume that there is a cubic Casimir $c \in \mathcal{U}(\mathfrak{g})$ with $S(c) = -c$. Then $\mathcal{F}' := \mathcal{F}[1 \otimes (1 + \hbar c)]$ is another Drinfeld twist for which $\sigma_1'^{-1}\sigma_2' = \sigma_1^{-1}\sigma_2(1+\hbar c)^{-1}S(1+\hbar c) = (1+\hbar c)^{-1}(1-\hbar c) \neq 1$. Part (vi) of the corollary applies also to the case where Eq. (12) defines for two different isomorphism α and α' two different coproducts $\Delta_\hbar$ and $\Delta'_\hbar$. Here, the automorphism which relates the two coproducts is $\beta := \alpha'\alpha^{-1}$. Note that elements of the form $(u \otimes u)\Delta u^{-1}$ are two-coboundaries in the sense of Ref. 16. Since Δ is cocommutative, two-coboundaries are symmetric. Hence, the twist (4) of Δ by a coboundary yields a cocommutative coproduct. The coproduct of the Drinfeld–Jimbo deformation is not cocommutative, so it cannot be isomorphic to the undeformed, cocommutative coproduct.

D. Real forms of enveloping algebras

Lie groups are usually viewed as real manifolds, even though they may be naturally defined as complex matrix groups. For example, the universal covering of the Lorentz group $\mathrm{SL}(2,\mathbb{C})$ is viewed as real six-parameter Lie group, the generators being the three rotations and the three boosts. When considering the complexification $\tilde{\mathfrak{g}} := \mathbb{C} \otimes_{\mathbb{R}} \mathfrak{g}$ of a real Lie algebra, we have to keep in mind that nonisomorphic real Lie algebras can have the same complexification. For example, su_2 and $\mathrm{sl}_2(\mathbb{R})$ have the same complexification A_1. A practical method to remember the real Lie algebra which a complexification comes from is to observe that for any real Lie algebra $\mathfrak{g}$ there is an antihomomorphism $*$ defined as $g^* := -g$ for all $g \in \mathfrak{g}$, which can be extended to a conjugate linear antihomomorphism on the complexification by $(\alpha \otimes_{\mathbb{R}} g)^* := \overline{\alpha} \otimes_{\mathbb{R}} g^*$ for all $\alpha \in \mathbb{C}$, $g \in \mathfrak{g}$. This defines a $*$-structure on $\tilde{\mathfrak{g}}$, that is, a conjugate linear antihomomorphism, which is an involution, $*^2 = \mathrm{id}$. Given the $*$-structure we can reconstruct the real Lie algebra as being generated by all elements of the form $(g - g^*) \in \tilde{\mathfrak{g}}$.

The identification of real forms of a complex Lie algebra with $*$-structures can be extended to the enveloping Hopf algebra $\mathcal{U}(\mathfrak{g})$. In general, a $*$-structure on a Hopf algebra is a conjugate linear antihomomorphism $*$, which is an involution and a bialgebra homomorphism, $\Delta(g^*) = (\Delta g)^{*\otimes *}$. Algebras and Hopf algebras with such a $*$-structure are called $*$-algebras and Hopf $*$-algebras, respectively. Finally, if H is a Hopf $*$-algebra and $\mathcal{X}$ an H-module algebra with a $*$-structure, such that in addition to Eq. (1) we have

$$(g \triangleright x)^* = (Sg)^* \triangleright x^* \tag{15}$$

for all $g \in H$, $x \in \mathcal{X}$, then $\mathcal{X}$ is called an H-module $*$-algebra, or a real H-covariant space.

Analogously as for algebras, an $\hbar$-adic $*$-algebra A' is called a deformation of a $*$-algebra A if $A'/\hbar A'$ and A are isomorphic as $*$-algebras. A is called rigid as $*$-algebra if for any deformation A' of A the $\hbar$-adic completion $A[[\hbar]]$ and A' are isomorphic as $*$-algebras.

Proposition 1: Let A be a $*$-algebra with zero first and second Hochschild cohomology, $H^1(A,A)=H^2(A,A)=0$. Then A is rigid as $*$-algebra.

Proof: Let $(A',*')$ be a deformation of $(A,*)$ as $*$-algebra. $H^2(A,A)=0$ implies that A is rigid as algebra, so there is an isomorphism of algebras $\beta:A'\to A[[\hbar]]$. Define $*_\beta:=\beta\circ *'\circ\beta^{-1}$. Because $*'$ is a deformation of $*$, we have $*_\beta=*+\mathcal{O}(\hbar)$, and, thus, as $*^2=\mathrm{id}$, $*_\beta\circ *=\mathrm{id}+\mathcal{O}(\hbar)$. $H^1(A,A)=0$ implies that this algebra automorphism is inner, $(g)^{*_\beta\circ *}=ugu^{-1}$ for some invertible $u\in A[[\hbar]]$. Thus, $g^{*_\beta}=(u^*)^{-1}g^*u^*$ for all $g\in A[[\hbar]]$. Since $*_\beta^2=\mathrm{id}$, we have $(g^{*_\beta})^{*_\beta}=g=(u^*)^{-1}ugu^{-1}u^*$, so $u^{-1}u^*=u^*u^{-1}$ is central. Since $*_\beta$ is a deformation of $*$ we can choose u such that $u=1+\mathcal{O}(\hbar)$ and, thus, $u^{-1}u^*=1+\mathcal{O}(\hbar)$, so the square roots of u^* and $u^{-1}u^*$ are defined and invertible. Define an isomorphism of algebras $\alpha:A'\to A[[\hbar]]$ by

$$\alpha(g):=(u^*)^{1/2}\beta(g)(u^*)^{-1/2}. \tag{16}$$

Using that the square root of a central element is central, we get

$$\begin{aligned} g^{*_\alpha}&:=(\alpha\circ *'\circ\alpha^{-1})(g)\\ &=(u^*)^{1/2}(\beta\circ *'\circ\beta^{-1})[(u^*)^{-1/2}g(u^*)^{1/2}](u^*)^{-1/2}\\ &=(u^*)^{1/2}(u^*)^{-1}(u)^{1/2}g^*(u)^{-1/2}u^*(u^*)^{-1/2}\\ &=(u^{-1}u^*)^{-1/2}g^*(u^{-1}u^*)^{1/2}=g^*, \end{aligned} \tag{17}$$

which shows that $\alpha:(A',*')\to(A[[\hbar]],*)$ is an isomorphism of $*$-algebras. □

This proposition applies in particular to the real forms of enveloping algebras of semisimple Lie algebras. In fact, if $*$ is a $*$-structure on $\mathcal{U}(\mathfrak{g})$ and $*'$ is a $*$-structure on $\mathcal{U}_\hbar(\mathfrak{g})$, such that $(\mathcal{U}_\hbar(\mathfrak{g}),*')$ is a deformation of $(\mathcal{U}(\mathfrak{g}),*)$ as Hopf $*$-algebra, we can (and shall) always use an isomorphism of $*$-algebras $\alpha:(\mathcal{U}_\hbar(\mathfrak{g}),*')\to(\mathcal{U}(\mathfrak{g}),*)$ to transfer the Hopf structure by Eqs. (12). In this case there are twists with particularly interesting properties with respect to the $*$-structure: We will call a twist unitary and real, respectively, if

$$\text{unitary:}\quad (*\otimes *)(\mathcal{F})=\mathcal{F}^{-1}, \tag{18a}$$

$$\text{real:}\quad (*\otimes *)(\mathcal{F})=(S\otimes S)(\mathcal{F}_{21}). \tag{18b}$$

A twist which is both, unitary and real, is called orthogonal.

Proposition 2: There is an orthogonal Drinfeld twist from Δ to $\Delta_\hbar$.

Proof: In Theorem 4.1 of Ref. 17 it was shown that there is always a twist with $(S\otimes S)(\mathcal{F})=\mathcal{F}_{21}^{-1}$. By assumption, the $*$-structure is a homomorphism of coalgebras for both, Δ and $\Delta_\hbar$. Thus, $(*\otimes *)(\mathcal{F}^{-1})\equiv(\mathcal{F}^{-1})^*$ is also a twist, so $\mathcal{T}:=\mathcal{F}^{-1}(\mathcal{F}^{-1})^*=1+\mathcal{O}(\hbar)$ is $\mathfrak{g}$-invariant and $\mathcal{F}':=\mathcal{F}\sqrt{\mathcal{T}}$ is another twist. It is easy to check that $\mathcal{F}'$ is unitary and real. □

E. Real structures on star products

The quantum spaces we want to consider here, the quantum plane and quantum Minkowski space, possess a real structure which is covariant with respect to a real form of the symmetry algebra. That is, $(\mathcal{U}(\mathfrak{g}),*)$ is a Hopf $*$-algebra and $(\mathcal{X},\mu,*)$ is a module $*$-algebra, the action of $\mathcal{U}(\mathfrak{g})$ on $\mathcal{X}$ and the $*$-structures satisfying Eq. (15). For a general twist Eq. (6) will not define a multiplication which is compatible with any real structure. Assume that we deform the product $\mu\to\mu_\hbar$ of the real covariant space $(\mathcal{X},\mu,*)$ but not the $*$-structure. Then

$$
\begin{aligned}
(x\star y)^* &= [(\mathcal{F}^{-1}_{[1]}\triangleright x)(\mathcal{F}^{-1}_{[2]}\triangleright y)]^* \\
&= (\mathcal{F}^{-1}_{[2]}\triangleright y)^*(\mathcal{F}^{-1}_{[1]}\triangleright x)^* \\
&= ([S\mathcal{F}^{-1}_{[2]}]^*\triangleright y^*)([S\mathcal{F}^{-1}_{[1]}]^*\triangleright x^*) \\
&= (\mathcal{F}_{[2]}[S\mathcal{F}^{-1}_{[2]}]^*\triangleright y)^*\star(\mathcal{F}_{[1]}[S\mathcal{F}^{-1}_{[1]}]^*\triangleright x)^*,
\end{aligned}
\tag{19}
$$

which shows that the undeformed $*$-structure is an antihomomorphism with respect to the deformed product, if $\mathcal{F}$ is chosen to be real in the sense of Eq. (18b), which was proved to be possible in Proposition 2. However, the undeformed $*$-structure of $\mathcal{X}$ will in general not satisfy the module $*$-algebra property (15). Thus, while Proposition 1 shows that the undeformed and deformed $*$-structures of the symmetry algebra $\mathcal{U}(\mathfrak{g})[[\hbar]]$ can (and shall) be chosen to coincide, this is not possible for the $*$-structures of the deformed and undeformed space algebras. However, there is a unique element σ of the symmetry algebra which mediates the deformation $*\to *_\hbar$ of the real structure of $\mathcal{X}$ by $x^{*_\hbar}:=\sigma^{-1}\triangleright x^*$. This element is characterized by the following.

Proposition 3: There is a unique element $\sigma\in\mathcal{U}(\mathfrak{g})[[\hbar]]$ such that

$$
\sigma=1+\mathcal{O}(\hbar),\quad S_\hbar(g)=\sigma(Sg)\sigma^{-1},\quad \Delta_\hbar(\sigma)=\sigma\otimes\sigma. \tag{20}
$$

Moreover, $\sigma^*=\sigma$.

Proof: Let $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$ be the isomorphism of algebras which is used to define the deformed Hopf structure by Eqs. (12). Let $\mathcal{R}$ be a universal $\mathcal{R}$-matrix of $\mathcal{U}_\hbar(\mathfrak{g})$ and

$$
\mathcal{R}_\hbar:=(\alpha\otimes\alpha)(\mathcal{R}), \tag{21}
$$

such that $\mathcal{R}_\hbar$ becomes a universal $\mathcal{R}$-matrix with respect to $\Delta_\hbar$. It was shown in Proposition 3.16 of Ref. 10 and Theorem 4.1 of Ref. 17 that there is a Drinfeld twist $\mathcal{F}$ from Δ to $\Delta_\hbar$ such that

$$
\mathcal{R}_\hbar=\mathcal{F}_{21}e^{(\hbar/2)(\Delta(C)-C\otimes 1-1\otimes C)}\mathcal{F}^{-1}\quad\text{and}\quad(S\otimes S)(\mathcal{F})=\mathcal{F}^{-1}_{21}, \tag{22}
$$

with the canonical quadratic Casimir $C:=g_ig_jK^{ij}$, where $\{g_i\}$ is a basis of $\mathfrak{g}$, $K_{ij}:=\mathrm{tr}(\mathrm{ad}g_i\mathrm{ad}g_j)$ is the Killing metric, and K^{ij} its inverse, $K^{ij}K_{jk}=\delta^i_k$.

Let σ_1^{-1} and σ_2 be defined for such a twist as in Eq. (14), and let $\sigma:=\sqrt{\sigma_1\sigma_2}$. Since $\sigma_1^{-1}\sigma_2$ is central, so is its square root. Hence, $S_\hbar(g)=\sigma_1(Sg)\sigma_1^{-1}=\sigma_1\sqrt{\sigma_1^{-1}\sigma_2}(Sg)\sqrt{\sigma_2^{-1}\sigma_1}\sigma_1^{-1}=\sigma(Sg)\sigma^{-1}$.

From the second equation of (22) we deduce $S(\sigma_2)=\sigma_1^{-1}$, so $S(\sigma)=\sigma^{-1}$. From the first equation of (22) we compute $u:=S_\hbar(\mathcal{R}_{\hbar[2]})\mathcal{R}_{\hbar[2]}=\sigma_1S(\sigma_1^{-1})q^{-C}=\sigma_1\sigma_2q^{-C}=\sigma^2q^{-C}$. From the properties of universal $\mathcal{R}$-matrices it follows that $uS_\hbar(u^{-1})=\sigma^4$ is grouplike with respect to $\Delta_\hbar$, $\Delta_\hbar(\sigma_1^4)=\sigma_1^4\otimes\sigma_1^4$. Since σ^4 is grouplike, its fourth root σ is grouplike, as well.

Now let $\sigma'=1+\mathcal{O}(\hbar)$ be another element with $S_\hbar(g)=\sigma'(Sg)\sigma'^{-1}$ which is grouplike with respect to $\Delta_\hbar$. Then $z:=\sigma'\sigma^{-1}$ is central and grouplike, $\Delta_\hbar(z)=z\otimes z=\mathcal{F}^{-1}(z\otimes z)\mathcal{F}=\Delta(z)$, with respect to both coproducts. Since $z=1+\mathcal{O}(\hbar)$ there is an a such that $z=e^{\hbar a}$. Since z is grouplike and central a must be primitive, $\Delta(a)=a\otimes 1+1\otimes a$, and central in every order of $a=\Sigma_i\hbar^ia_i$. Being primitive, the a_i are elements of the Lie algebra, $a_i\in\mathfrak{g}\subset\mathcal{U}(\mathfrak{g})$. Since $\mathfrak{g}$ is semisimple it does not contain nontrivial central elements, so $a_i=0$ for all i, that is, $a=0$. Hence, $z=\sigma'\sigma^{-1}=1$.

Clearly, $\sigma^*=1+\mathcal{O}(\hbar)$. From $S_\hbar=*\circ S_\hbar^{-1}\circ *$ it follows that $S_\hbar(g)=\sigma^*(Sg)(\sigma^*)^{-1}$. Since σ is grouplike with respect to $\Delta_\hbar$, so is σ^*. By uniqueness of an element with properties (20) we conclude that $\sigma^*=\sigma$. □

Now we can show that σ realizes the deformation of the real structure in the promised manner:

Proposition 4: Let $\mathcal{F}$ be a twist from Δ to $\Delta_\hbar$ which is real in the sense of Eq. (18b) and let $(\mathcal{X},\mu,*)$ be an $\hbar$-adic module $*$-algebra of $(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta,\varepsilon,S,*)$. Define $\mu_\hbar$ as in Eq. (6) and $*_\hbar:\mathcal{X}\to\mathcal{X}$ by

$$x^{*_\hbar} := \sigma^{-1} \triangleright x^* \tag{23}$$

for all $x \in \mathcal{X}$, where σ is the unique element of Proposition 3. Then $(\mathcal{X}, \mu_\hbar, *_\hbar)$ is a module $*$-algebra of $(\mathcal{U}(\mathfrak{g})[[\hbar]], \Delta_\hbar, \varepsilon_\hbar, S_\hbar, *)$.

Proof: By construction, $*_\hbar$ is conjugate linear. We have to show that $*_\hbar$ is an algebra antihomomorphism. Writing $\mu_\hbar(x \otimes y) = x \star y$, we get

$$\begin{aligned}
(x \star y)^{*_\hbar} &= \sigma^{-1} \triangleright [(\mathcal{F}^{-1}_{[1]} \triangleright x)(\mathcal{F}^{-1}_{[2]} \triangleright y)]^* \\
&= \sigma^{-1} \triangleright (\mathcal{F}^{-1}_{[2]} \triangleright y)^* (\mathcal{F}^{-1}_{[1]} \triangleright x)^* \\
&= \sigma^{-1} \triangleright ([S\mathcal{F}^{-1}_{[2]}]^* \triangleright y^*)([S\mathcal{F}^{-1}_{[1]}]^* \triangleright x^*) \\
&= \sigma^{-1} \triangleright (\mathcal{F}^{-1}_{[1]} \triangleright y^*)(\mathcal{F}^{-1}_{[2]} \triangleright x^*) \\
&= (\sigma^{-1}_{(1)} \mathcal{F}^{-1}_{[1]} \triangleright y^*)(\sigma^{-1}_{(2)} \mathcal{F}^{-1}_{[2]} \triangleright x^*) \\
&= (\mathcal{F}^{-1}_{[1]} \sigma^{-1}_{(1_\hbar)} \triangleright y^*)(\mathcal{F}^{-1}_{[2]} \sigma^{-1}_{(2_\hbar)} \triangleright x^*) \\
&= (\mathcal{F}^{-1}_{[1]} \sigma^{-1} \triangleright y^*)(\mathcal{F}^{-1}_{[2]} \sigma^{-1} \triangleright x^*) \\
&= (\sigma^{-1} \triangleright y^*) \star (\sigma^{-1} \triangleright x^*) = (y^{*_\hbar}) \star (x^{*_\hbar}),
\end{aligned} \tag{24}$$

where we have used the module $*$-algebra condition (15), the assumed reality (18b) of $\mathcal{F}$, and that σ is grouplike with respect to $\Delta_\hbar$. Since

$$(x^{*_\hbar})^{*_\hbar} = \sigma^{-1} \triangleright (\sigma^{-1} \triangleright x^*)^* = \sigma^{-1} (S\sigma^{-1})^* \triangleright x = \sigma^{-1} \sigma^* \triangleright x = x, \tag{25}$$

$*_\hbar$ is an involution. Finally, the module $*$-algebra condition (15) holds,

$$\begin{aligned}
(g \triangleright x)^{*_\hbar} &= \sigma^{-1} \triangleright (g \triangleright x)^* \\
&= \sigma^{-1} (Sg)^* \triangleright x^* \\
&= (\sigma^{-1})^* (Sg)^* \triangleright x^* \\
&= (S_\hbar g)^* (\sigma^{-1})^* \triangleright x^* \\
&= (S_\hbar g)^* \triangleright (\sigma^{-1} \triangleright x^*) \\
&= (S_\hbar g)^* \triangleright x^{*_\hbar},
\end{aligned} \tag{26}$$

where we have used the properties of σ from Proposition 3. □

F. Representations

The $\hbar$-adic representations of the algebra $\mathcal{U}(\mathfrak{g})[[\hbar]]$ we are most interested in are those which are the $\hbar$-adic completion of the representations of $\mathcal{U}(\mathfrak{g})$. If $D = (V, \rho)$ is a $\mathcal{U}(\mathfrak{g})$-module with complex vector space V and structure homomorphism $\rho: \mathcal{U}(\mathfrak{g}) \to \mathrm{End}_{\mathbb{C}}(V)$, its $\hbar$-adic completion $\overline{D} = (\overline{V}, \overline{\rho})$ is defined on $\overline{V} = V[[\hbar]]$ with an order by order extension of ρ, $\overline{\rho}(\Sigma_k \hbar^k g_k) := \Sigma_k \hbar^k \rho(g_k) \in \mathrm{End}_{\mathbb{C}}(V)[[\hbar]] = \mathrm{End}_{\mathbb{C}[[\hbar]]}(V[[\hbar]])$. In particular, $\overline{V}$ is free over $\mathbb{C}[[\hbar]]$ and $\overline{\rho}$ is $\mathbb{C}[[\hbar]]$-linear. Note that, even if D is an irreducible representation of $\mathcal{U}(\mathfrak{g})$, this is no longer true for $\overline{D}$. For example, $\hbar \overline{V}$ would be an invariant subspace of $\overline{V}$. $\overline{D}$ is irreducible only in the sense that there is no subspace $U \subset V$ such that $\overline{U} := U[[\hbar]]$ is an invariant subspace of $\overline{V}$.

Let $\{E_k, H_k, F_k | k = 1, \ldots, n\}$ be a Cartan–Weyl basis of the semisimple Lie algebra $\mathfrak{g}$, and $\mathfrak{h}$ be the Cartan subalgebra which is generated by $\{H_k\}$. Clearly, $\mathfrak{h}$ is a Lie subalgebra of the enveloping algebra, $\mathfrak{h} \subset \mathcal{U}(\mathfrak{g})[[\hbar]]$. By construction, the $\hbar$-adic Drinfeld–Jimbo deformation of $\mathcal{U}(\mathfrak{g})$ does contain the Cartan subalgebra as a Lie subalgebra, as well, $\mathfrak{h} \subset \mathcal{U}_\hbar(\mathfrak{g})$. Drinfeld has shown that the isomorphism of $\mathcal{U}(\mathfrak{g})[[\hbar]]$ and $\mathcal{U}_\hbar(\mathfrak{g})$ can be chosen to leave the Cartan subalgebra invariant:

Theorem 2 (Drinfeld,[14] Proposition 4.3): *Let* $\mathfrak{g}$ *be a semisimple Lie algebra and* $\mathfrak{h}\subset\mathfrak{g}$ *a Cartan subalgebra. Then there exists an isomorphism of* $\hbar$*-adic algebras* $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$ *such that* $\alpha=\mathrm{id}+\mathcal{O}(\hbar)$ *and* $\alpha|_{\mathfrak{h}}=\mathrm{id}_{\mathfrak{h}}$.

This has important consequences for the representation theory. Recall that every finite-dimensional irreducible representation of $\mathcal{U}(\mathfrak{g})$ is a highest weight representation $D^j=(V^j,\rho^j)$, generated by a highest weight vector $v\in V^j$ with $\rho^j(E_k)v=0$ and $\rho^j(H_k)v=j_k v$ for all k, where $j_k\in(1/2)\mathbb{N}_0$, $j:=(j_1,\ldots,j_n)$ being called the highest weight. Furthermore, there is a basis of V^j which consists of simultaneous eigenvectors of H_k, called the weight basis. The same is true for the finite-dimensional representations of the Drinfeld–Jimbo algebra $\mathcal{U}_q(\mathfrak{g})$ for a fixed value of q,[18,19] the weight-j representation $D_q^j=(V^j,\rho_q^j)$ of $\mathcal{U}_q(\mathfrak{g})$ being defined on the same weight basis as D^j. By the substitution $q\mapsto e^\hbar$, D_q^j can be extended to an $\hbar$-adic representation $D_\hbar^j:=(V^j[[\hbar]],\rho_\hbar^j)$. Since $\mathcal{U}_\hbar(\mathfrak{g})$ and $\mathcal{U}(\mathfrak{g})[[\hbar]]$ are isomorphic as algebras, there is a bijection between their representations. Theorem 2 implies that the isomorphism $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$ can be chosen, such that

$$\rho_\hbar^j=\overline{\rho^j}\circ\alpha. \tag{27}$$

If both $\rho_\hbar^j$ and $\overline{\rho^j}$ are known, this equation can be used to calculate the isomorphism α.

III. CONSTRUCTING COVARIANT STAR PRODUCTS

A. The general approach

As explained in Sec. II B, we are asking if there are Drinfeld twists which implement the product of quantum spaces by Eq. (6). To our knowledge, no Drinfeld twist for the Drinfeld–Jimbo quantum enveloping algebra of a semisimple Lie algebra has ever been computed. This suggests that it will be rather difficult to answer this question on an algebraic level. The representations of Drinfeld twists, however, can be computed as we will demonstrate for $\mathcal{U}_\hbar(\mathrm{su}_2)$ in Proposition 5. Therefore, we propose the following approach, which allows us to tackle the problem on a representation theoretic level:

Consider a $\mathcal{U}_\hbar(\mathfrak{g})$-covariant quantum space algebra $\mathcal{X}_\hbar$ and its undeformed limit, the $\mathcal{U}(\mathfrak{g})$-covariant space algebra $\mathcal{X}$.

(1) Determine the irreducible highest weight representations of all possible Drinfeld twists from Δ to $\Delta_\hbar$.

(2) Determine the basis $\{T_{m,k}^j\}$ of the quantum space $\mathcal{X}_\hbar$ which completely reduces $\mathcal{X}_\hbar$ into irreducible highest weight representations of $\mathcal{U}_\hbar(\mathfrak{g})$,

$$\mathcal{X}_\hbar\cong\bigoplus_{j,k}\mathrm{Span}_{\mathbb{C}[[\hbar]]}\{T_{m,k}^j|m\ \text{ weight of }\ D_\hbar^j\}, \tag{28}$$

such that $g\triangleright T_{m,k}^j=T_{m',k}^j\rho_\hbar^j(g)^{m'}{}_m$ for all $g\in\mathcal{U}_\hbar(\mathfrak{g})$, where m is a weight, j is the highest weight, $\rho_\hbar^j$ is the structure map of the $\hbar$-adic highest weight-j representation $D_\hbar^j$ of $\mathcal{U}_\hbar(\mathfrak{g})$ as explained in Sec. II F, and where k labels the possibly degenerate highest weight-j subrepresentations.

(3) Calculate the multiplication map $\mu_\hbar$ of $\mathcal{X}_\hbar$ with respect to this basis. The undeformed limit $T'^j_{m,k}:=\lim_{\hbar\to 0}T_{m,k}^j$ then yields the basis which completely reduces the undeformed space algebra $\mathcal{X}$. The limit $\mu=\lim_{\hbar\to 0}\mu_\hbar$ is the commutative multiplication map with respect to this basis.

(4) With respect to the basis $\{T'^{j_1}_{m_1,k_1}\otimes T'^{j_2}_{m_2,k_2}\}$ of $(\mathcal{X}\otimes\mathcal{X})[[\hbar]]$ the action of the twist is given by the highest weight representations $(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})$. Now we can check if one of the twists realizes the deformed multiplication map by Eq. (6) as linear operator with respect to this basis.

Since this procedure reduces the algebraic problem to a representation theoretic one, it works well for quantum spaces of $\mathcal{U}_\hbar(\mathrm{su}_2)$, $\mathcal{U}_\hbar(\mathrm{so}_4)$, and $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$ where the representation theory is well understood.

B. The Drinfeld twists of $\mathcal{U}_\hbar(\mathrm{su}_2)$

We now consider the case of $\mathfrak{g}=A_1$, the complex Lie algebra with Cartan–Weyl basis $\{E,H,F\}$ and relations $[H,E]=2E$, $[H,F]=-2F$, $[E,F]=H$. The real form of A_1, which corresponds to the $*$-structure $E^*=F$, $H^*=H$, $F^*=E$, is su_2, the Lie algebra of the group of unitary 2×2-matrices.

Definition 1: The complex $\hbar$-adic algebra generated by E, H, F with commutation relations

$$[H,E]=2E,\quad [H,F]=-2F,\quad [E,F]=\frac{e^{\hbar H}-e^{-\hbar H}}{e^{\hbar}-e^{-\hbar}}, \tag{29}$$

Hopf structure

$$\begin{aligned}
&\Delta'(E)=E\otimes e^{\hbar H}+1\otimes E,\quad S'(E)=-Ee^{-\hbar H},\quad \varepsilon'(E)=0,\\
&\Delta'(F)=F\otimes 1+e^{-\hbar H}\otimes F,\quad S'(F)=-e^{\hbar H}F,\quad \varepsilon'(F)=0,\\
&\Delta'(H)=H\otimes 1+1\otimes H,\quad S'(H)=-H,\quad \varepsilon'(H)=0,
\end{aligned} \tag{30}$$

and involution $E^{*'}=Fe^{\hbar H}$, $F^{*'}=e^{-\hbar H}E$, $H^{*'}=H$ is called $\mathcal{U}_\hbar(\mathrm{su}_2)$, the $\hbar$-deformation of $\mathcal{U}(\mathrm{su}_2)$.[20,21] *It is quasitriangular with universal $\mathcal{R}$-matrix*[22]

$$\mathcal{R}=e^{\hbar(H\otimes H)/2}\sum_{n=0}^{\infty} e^{\hbar n(n-1)/2}\frac{(e^{\hbar}-e^{-\hbar})^n}{[n]!}(E^n\otimes F^n). \tag{31}$$

By construction, the commutation relations and Hopf $*$-structure maps of $\mathcal{U}_\hbar(\mathrm{su}_2)$ coincide in zeroth order of $\hbar$ with those of $\mathcal{U}(\mathrm{su}_2)$. Therefore, $\mathcal{U}_\hbar(\mathrm{su}_2)$ is a deformation of $\mathcal{U}(\mathrm{su}_2)$ as Hopf $*$-algebra. The $\hbar$-adic deformation is obtained from the q-deformation by the substitutions $q=e^{\hbar}$, $K=e^{\hbar H}$, and $K^{-1}=e^{-\hbar H}$. By the same substitution we obtain for each $j\in(1/2)\mathbb{N}_0$ the $\hbar$-adic spin-j $*$-representation

$$\begin{aligned}
&\rho^j_\hbar(E)|j,m\rangle=e^{\hbar(m+1)}\sqrt{[j+m+1][j-m]}\,|j,m+1\rangle,\\
&\rho^j_\hbar(F)|j,m\rangle=e^{-\hbar m}\sqrt{[j+m][j-m+1]}\,|j,m-1\rangle,\\
&\rho^j_\hbar(H)|j,m\rangle=2m|j,m\rangle,
\end{aligned} \tag{32}$$

on the $(2j+1)$-dimensional free $\mathbb{C}[[\hbar]]$-module $V^j[[\hbar]]$ with orthonormal weight basis $\{|j,m\rangle, m=-j,-j+1,...,j\}$, which we denote by $D^j_\hbar:=(V^j[[\hbar]],\rho^j_\hbar)$. Using the coproduct, tensor representations are constructed as

$$D^{j_1}_\hbar\otimes D^{j_2}_\hbar:=(V^{j_1}\otimes V^{j_2},\rho^{j_1\otimes j_2}_\hbar:=(\rho^{j_1}_\hbar\otimes\rho^{j_2}_\hbar)\circ\Delta') \tag{33}$$

and analogously for the undeformed case. The decomposition of such a tensor representation into its irreducible subrepresentations is the Clebsch–Gordan series

$$D^{j_1}_\hbar\otimes D^{j_2}_\hbar\cong D^{|j_1-j_2|}_\hbar\oplus D^{|j_1-j_2|+1}_\hbar\oplus\cdots\oplus D^{j_1+j_2}_\hbar. \tag{34}$$

Let us denote the embedding of the irreducible spin-j component into the tensor representation by $C_q^{j_1j_2j}$ and the projection onto this component by $(C_q^{j_1j_2j})^{-1}$, such that

$$\rho^j_\hbar(g)C_q^{j_1j_2j}=C_q^{j_1j_2j}\rho^{j_1\otimes j_2}_\hbar(g)=C_q^{j_1j_2j}(\rho^{j_1}_\hbar\otimes\rho^{j_2}_\hbar)(\Delta' g) \tag{35}$$

for all $g \in \mathcal{U}_\hbar(\mathrm{su}_2)$. Denoting the basis vectors of $D^{j_1}_\hbar \otimes D^{j_2}_\hbar$ by $|j_1,m_1;j_2,m_2\rangle$ and those of the irreducible spin-j subrepresentation by $|j,m\rangle$, the q–Clebsch–Gordan coefficients are defined as

$$\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)_q := \langle j_1,m_1;j_2,m_2|C_q^{j_1 j_2 j}|j,m\rangle. \tag{36}$$

The q–Clebsch–Gordan coefficients are not unique because the basis vectors $|j,m\rangle$ are only determined up to a phase. We will follow the choice of Ref. 23, where

$$\begin{aligned} \sum_{m_1,m_2} \left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)_q \left(\begin{array}{cc|c} j_1 & j_2 & j' \\ m_1 & m_2 & m' \end{array}\right)_q &= \delta_{mm'}\delta_{jj'}, \\ \sum_{j,m} \left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)_q \left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1' & m_2' & m \end{array}\right)_q &= \delta_{m_1 m_1'}\delta_{m_2 m_2'}. \end{aligned} \tag{37}$$

Clearly, the representation theory of $\mathcal{U}_\hbar(\mathrm{su}_2)$ is a deformation of the one of $\mathcal{U}(\mathrm{su}_2)$. In the limit $\hbar \to 0$ or, equivalently, $q \to 1$ of Eq. (36) we get back the undeformed Clebsch–Gordan coefficients. Since $\mathcal{U}_\hbar(\mathrm{su}_2)$ and $\mathcal{U}(\mathrm{su}_2)[[\hbar]]$ are isomorphic as $*$-algebras their representations are isomorphic, as well. Due to Theorem 2 we can choose the isomorphism $\alpha: \mathcal{U}_\hbar(\mathrm{su}_2) \to \mathcal{U}(\mathrm{su}_2)\times[[\hbar]]$ as in Eq. (27) such that

$$\rho^j_\hbar = \rho^j \circ \alpha, \tag{38}$$

where $\rho^j: \mathcal{U}(\mathrm{su}_2)[[\hbar]] \to \mathrm{End}(V^j)[[\hbar]]$ is the $\hbar$-adically extended structure map of the undeformed enveloping algebra. [We omit the bar which denoted the $\hbar$-adic completion in Eq. (27).] If we set $g = \alpha^{-1}(g')$ in Eq. (35), we thus get

$$\rho^j(g')C_q^{j_1 j_2 j} = C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})(\Delta_\hbar g') \tag{39}$$

for all $g' \in \mathcal{U}(\mathrm{su}_2)$, where $\Delta_\hbar$ is defined as in Eq. (12).

It is rather obvious that the representations of Drinfeld twists should be given by a contraction of the deformed and undeformed Clebsch–Gordan coefficients, as it was already mentioned in Ref. 24.

Proposition 5: Let $\mathcal{F}$ be a counital Drinfeld twist from $\mathcal{U}(\mathrm{su}_2)$ to $\mathcal{U}_\hbar(\mathrm{su}_2)$. The irreducible representations of $\mathcal{F}$ are of the form

$$(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})^{m_1 m_2}{}_{m_1' m_2'} = \sum_{j,m} \eta(j_1,j_2,j) \left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)_q \left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1' & m_2' & m \end{array}\right), \tag{40}$$

where for given values of j_1, j_2, and j the factor $\eta(j_1,j_2,j) \in \mathbb{C}[[\hbar]]$ is a formal power series in $\hbar$ with $\eta(j_1,j_2,j) = 1 + \mathcal{O}(\hbar)$.

Proof: Within a $D^{j_1}\otimes D^{j_2}$ tensor representation we get for all $g \in \mathcal{U}(\mathrm{sl}_2)$

$$\begin{aligned} C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})(C^{j_1 j_2 j'})^{-1}\rho^{j'}(g) &= C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F}\Delta g)(C^{j_1 j_2 j'})^{-1} \\ &= C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})((\Delta_\hbar g)\mathcal{F})(C^{j_1 j_2 j'})^{-1} \\ &= \rho^j(g)C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})(C^{j_1 j_2 j'})^{-1}, \end{aligned} \tag{41}$$

where we have used Eq. (39) and the analogous relation for the undeformed case. Let us develop $\eta := C_q^{j_1 j_2 j}(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})(C^{j_1 j_2 j'})^{-1}$ into an $\hbar$-adic series $\eta = \Sigma_k \hbar^k \eta_k$. Then Eq. (41) implies that

each η_k is a module map from the spin-j' to the spin-j irreducible subrepresentation of the $D^{j_1}\otimes D^{j_2}$ tensor representation. By Schur's lemma each η_k must be zero for $j\neq j'$, while for $j=j'$ the η_k are $\mathbb{C}[[\hbar]]$-scalar multiples of the identity map id_{D^j}. Hence,

$$C_q^{j_1j_2j}(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})(C^{j_1j_2j'})^{-1}=\eta(j_1,j_2,j)\,\delta_{jj'}\mathrm{id}_{D^j}$$

$$\Leftrightarrow(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F})=\sum_j\ \eta(j_1,j_2,j)(C_q^{j_1j_2j})^{-1}C^{j_1j_2j}, \quad (42)$$

where for given j_1, j_2, j, $\eta(j_1,j_2,j)\in\mathbb{C}[[\hbar]]$. Taking matrix elements of the last equation and using the definition (36) of the Clebsch–Gordan coefficients yields Eq. (40). Finally, $\mathcal{F}=1+\mathcal{O}(\hbar)$ implies $\eta(j_1,j_2,j)=1+\mathcal{O}(\hbar)$. □

The Drinfeld twist with the canonically simplest representations would be the one with $\eta(j_1,j_2,j)=1$. Such a twist exists, indeed.

Proposition 6: There is a unique Drinfeld twist $\mathcal{F}_s$, called the standard twist, for which the irreducible representations of Proposition 5 are such that $\eta(j_1,j_2,j)=1$ for all j_1, j_2, j.

Proof: Define a scalar conjugation $u\mapsto\overline{u}$ on $\mathcal{U}(\mathrm{su}_2)$ by extending the identity map on the Cartan–Weyl generators of su_2 to a conjugate linear automorphism of $\mathcal{U}(\mathrm{su}_2)$, e.g., $\overline{\alpha EF}=\overline{\alpha}\overline{E}\overline{F}$ etc. Since both coproducts are real with respect to this conjugation, $\overline{\Delta(g)}=\Delta(\overline{g})$ and $\overline{\Delta_\hbar(g)}=\Delta_\hbar(\overline{g})$, the conjugation of Eq. (4) shows that, if $\mathcal{F}$ is a counital Drinfeld twist, so is $\overline{\mathcal{F}}$ and, hence, $\mathcal{F}':=1/2(\mathcal{F}+\overline{\mathcal{F}})$. In the representation (32) and its undeformed limit the Cartan–Weyl generators are represented by real matrices, thus, $\overline{\rho^j(g)^m{}_{m'}}=\rho^j(g)^m{}_{m'}$. We conclude that if $\eta(j_1,j_2,j)=\eta$ are the factors of the representations of $\mathcal{F}$, $\overline{\eta}$ are those of $\overline{\mathcal{F}}$ and $\eta'=\eta+\overline{\eta}$ those of $\mathcal{F}'$. As in the proof of Proposition 2 the twist $\mathcal{F}'':=\mathcal{F}'(F'^{-1}(F'^*)^{-1})^{1/2}$ is unitary. The factors η'' of the representations of $\mathcal{F}_s$ are real because those of $\mathcal{F}'$ are real, and unitary $\overline{\eta''}=\eta''^{-1}$ because $\mathcal{F}''$ is unitary. Hence, $\eta=\eta(j_1,j_2,j)=1$. Since any two $\mathcal{F}$ with the same representations are equal, $\mathcal{F}''$ is the unique standard twist. □

Proposition 7: The standard twist $\mathcal{F}_s$ is orthogonal.

Proof: It was shown in the proof of Proposition 6 that $\mathcal{F}_s$ is unitary. Moreover,

$$\begin{aligned}(\rho^{j_1}\otimes\rho^{j_2})((S\otimes S)(\mathcal{F}_s))^{m_1m_2}{}_{m_1'm_2'}&=\sum_{j,m}\left(\begin{array}{cc|c}j_1&j_2&j\\-m_1'&-m_2'&m\end{array}\right)_q\left(\begin{array}{cc|c}j_1&j_2&j\\-m_1&-m_2&m\end{array}\right)\\&=\sum_{j,m}\left(\begin{array}{cc|c}j_2&j_1&j\\m_2&m_1&m\end{array}\right)\left(\begin{array}{cc|c}j_2&j_1&j\\m_2'&m_1'&m\end{array}\right)_q\\&=(\rho^{j_1}\otimes\rho^{j_2})(\mathcal{F}_{s21}^{-1})^{m_1m_2}{}_{m_1'm_2'},\end{aligned} \quad (43)$$

where we have used $\rho^j(Sg)^m{}_{m'}=(-1)^{m-m'}\rho^j(g)^{-m'}{}_{-m}$ and that $\left(\begin{smallmatrix}j_1&j_2\\m_1&m_2\end{smallmatrix}\middle|\begin{smallmatrix}j\\m\end{smallmatrix}\right)_q=\left(\begin{smallmatrix}j_2&j_1\\-m_2&-m_1\end{smallmatrix}\middle|\begin{smallmatrix}j\\-m\end{smallmatrix}\right)_q$. We conclude that $(S\otimes S)(\mathcal{F}_s)=\mathcal{F}_{s21}^{-1}=(*\otimes*)(\mathcal{F}_{s21})$. □

C. The quantum plane

The quantum plane[5] is perhaps the simplest nontrivial example of a homogeneous quantum space. In analogy to the undeformed case, the generators x_- and x_+ are defined to carry the fundamental spin-1/2 representation of $\mathcal{U}_\hbar(\mathrm{su}_2)$,

$$g\triangleright x_m:=x_{m'}\rho_\hbar^{1/2}(g)^{m'}{}_m, \quad (44)$$

where the indices run through $\{-,+\}=\{-1/2,+1/2\}$ (summation over repeated upper and lower indices). We also denote the generators by $x\equiv x_-$ and $y\equiv x_+$. Let $\mathbb{C}\langle x_-,x_+\rangle[[\hbar]]$ be the free $\hbar$-adic algebra generated by x_- and x_+. By construction, an algebra which is freely generated by a $\mathcal{U}_\hbar(\mathrm{su}_2)$-module is a $\mathcal{U}_\hbar(\mathrm{su}_2)$-module algebra. The quadratic terms $x_{m_1}x_{m_2}$ thus carry a spin-$(1/2\otimes1/2)$ tensor representation. If we want to divide the free algebra by quadratic relations in

such a way that the quotient algebra is again a $\mathcal{U}_\hbar(\mathrm{su}_2)$-module algebra, we must divide by an ideal which is generated by a submodule of the representation $D^{1/2}_\hbar \otimes D^{1/2}_\hbar \cong D^0_\hbar \oplus D^1_\hbar$ of all quadratic terms. Dividing by $D^1_\hbar$ would yield a deformation of the exterior algebra, whereas dividing by the scalar part $D^0_\hbar$ yields the desired deformation of the commutative algebra of functions on the two-dimensional plane. This amounts to the commutation relations

$$\sum_{m_1,m_2} \left(\begin{matrix} 1/2 & 1/2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} 0 \\ 0 \end{matrix} \right)_q x_{m_1} x_{m_2} = 0 \Leftrightarrow xy = qyx, \tag{45}$$

where $q = e^\hbar$.

Definition 2: The $\hbar$-adic algebra freely generated by $x \equiv x_-$ and $y \equiv x_+$ with commutation relations (45) is called the $\hbar$-adic quantum plane $\mathcal{X}_\hbar(\mathbb{C}^2)$.

We now want to write the product of the quantum plane, $\mu_\hbar(x_1 \otimes x_2) := x_1 x_2$, explicitly as a linear map with respect to a basis. For our purposes, the appropriate choice is the basis which reduces the quantum plane as $\mathcal{U}_\hbar(\mathrm{su}_2)$-module into its irreducible subrepresentations. In order to find such a basis, we recall that, as in the undeformed case, finding the irreducible spin-j subrepresentations is the matter of finding the highest weight-j vectors, that is, the elements of $\mathcal{X}_\hbar(\mathbb{C}^2)$ which transform as $|j,j\rangle$ in Eqs. (32). A simple ansatz shows that, up to scalar multiples, the only element of the quantum plane with this property is x_+^{2j}. Acting on x_+^{2j} with the ladder operator F generates the other basis vectors of the $D^j_\hbar$-subrepresentation. Identifying in Eqs. (32) $|j,m\rangle$ with T^j_m, we have to define

$$T^j_m := q^{(1/2)(j-m)(2m-j+1)} \sqrt{\frac{[j+m]!}{[2j]![j-m]!}} (F^{j-m} \triangleright x_+^{2j}) \tag{46}$$

for $m \in \{-j, -j+1, \ldots, j\}$, such that

$$g \triangleright T^j_m = T^j_{m'} \rho^j_\hbar(g)^{m'}{}_m \tag{47}$$

for all $g \in \mathcal{U}_\hbar(\mathrm{su}_2)$. The basis $\{T^j_m\}$ then reduces the quantum plane into its irreducible subrepresentations, $\mathcal{X}_\hbar(\mathbb{C}^2) = D^0_\hbar \oplus D^{1/2}_\hbar \oplus D^1_\hbar + \cdots$. Calculating Eq. (46) explicitly yields

$$T^j_m = \begin{bmatrix} 2j \\ j+m \end{bmatrix}_{q^{-2}}^{1/2} x_-^{j-m} x_+^{j+m}, \quad \text{where } \begin{bmatrix} n \\ k \end{bmatrix}_{q^{-2}} := q^{k(k-n)} \frac{[n]!}{[n-k]![k]!} \tag{48}$$

is the q-binomial coefficient. By construction, $T^{j_1}_{m_1} T^{j_2}_{m_2}$ carries a spin-$(j_1 \otimes j_2)$ tensor representation which can be reduced using the q–Clebsch–Gordan coefficients. Hence, the elements

$$A^j_m := \sum_{m_1,m_2} \left(\begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} j \\ m \end{matrix} \right)_q T^{j_1}_{m_1} T^{j_2}_{m_2} \tag{49}$$

are either zero or the basis of a spin-j subrepresentation of $\mathcal{X}_\hbar(\mathbb{C}^2)$. Since T^j_m generates the only spin-j subrepresentation. A^j_m must be proportional to T^j_m. Moreover, because of its homogeneous commutation relations the algebra $\mathcal{X}_\hbar(\mathbb{C}^2)$ is graded. That is, the degree of the product of two homogeneous elements $T^{j_1}_{m_1}$ and $T^{j_2}_{m_2}$ is the sum of their degrees, $\deg(T^{j_1}_{m_1} T^{j_2}_{m_2}) = \deg(T^{j_1}_{m_1}) + \deg(T^{j_2}_{m_2}) = 2(j_1 + j_2)$. As A^j_m and T^j_m are proportional, they must have the same degree. Thus, A^j_m has to vanish unless $j = j_1 + j_2$. Looking at the highest weight vectors we find $A^{j_1+j_2}_{j_1+j_2} = x_+^{2(j_1+j_2)} = T^{j_1+j_2}_{j_1+j_2}$. Using the orthogonality relation (37) we can move the q–Clebsch–Gordon coefficients to the left-hand side of Eq. (49). As end result, the multiplication map $\mu_\hbar$ of the quantum plane is given with respect to the basis $\{T^j_m\}$ by

$$\mu_\hbar(T^{j_1}_{m_1}\otimes T^{j_1}_{m_1})=\left(\begin{array}{cc|c} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & m_1+m_2 \end{array}\right)_q T^{j_1+j_2}_{m_1+m_2}. \tag{50}$$

For the undeformed limit of the basis $T'^{j}_{m}:=\lim_{\hbar\to 0} T^{j}_{m}$ and multiplication map $\mu:=\lim_{\hbar\to 0}\mu_\hbar$ one gets

$$T'^{j}_{m}=\left(\begin{array}{c} 2j \\ j+m \end{array}\right)^{1/2} x_-^{j-m}x_+^{j+m}, \quad \mu(T'^{j_1}_{m_1}\otimes T'^{j_1}_{m_1})=\left(\begin{array}{cc|c} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & m_1+m_2 \end{array}\right) T'^{j_1+j_2}_{m_1+m_2}. \tag{51}$$

Comparing Eqs. (50) and (51) with the representations (40) of the Drinfeld twists we obtain the following.

Proposition 8: Let $\mu_\hbar$ be the multiplication map (50) of the $\hbar$-adic quantum plane $\mathcal{X}_\hbar(\mathbb{C}^2)$, $\mu=\lim_{\hbar\to 0}\mu_\hbar$ its undeformed limit, and $\mathcal{F}_s$ the standard twist of Proposition 6. Then $\mu_\hbar$ is the deformation (6) of μ by $\mathcal{F}_s$, $\mu_\hbar(x\otimes y)=\mu(\mathcal{F}_s^{-1}\triangleright[x\otimes y])$.

Finally, let us turn to real structures. Since according to Proposition 3.2 $\mathcal{F}_s$ is real in the sense of Eq. (18b), Proposition 4 applies. Within $\mathcal{U}_\hbar(\mathrm{su}_2)$ we have $S'^2(g)=KgK^{-1}$ with $K=\mathrm{e}^{\hbar H}$ for all $g\in\mathcal{U}_\hbar(\mathrm{su}_2)$. Clearly, K is grouplike, $\Delta'(K)=K\otimes K$. Recall that, in order for the representations of $\mathcal{U}(\mathrm{su}_2)[[\hbar]]$ and $\mathcal{U}_\hbar(\mathrm{su}_2)$ to be related by Eq. (38), we chose the isomorphism $\alpha:\mathcal{U}_\hbar(\mathrm{su}_2)\to\mathcal{U}(\mathrm{su}_2)[[\hbar]]$ according to Theorem 2 such that $\alpha(H)=H$. On the one hand, $S^2_\hbar(g)=(\alpha\circ S'^2\circ\alpha)(g)=KgK^{-1}$. On the other hand, $S^2_\hbar(g)=\sigma^2 g\sigma^{-2}$, for the unique element σ from Proposition 3. Hence, $K\sigma^{-2}=\sigma^{-2}K$ is central, so $S_\hbar(g)=K^{1/2}(Sg)K^{-1/2}$. Since $K^{1/2}=1+\mathcal{O}(\hbar)$ is grouplike the uniqueness of σ implies that $\sigma=K^{1/2}=\mathrm{e}^{\hbar H/2}$. Proposition 4 now tells us that for a given covariant real structure $*$ on the undeformed space algebra $\mathcal{X}\equiv\mathcal{X}(\mathbb{C}^2)=\mathbb{C}[x_-,x_+][[\hbar]]$ of the plane, we have to define the deformed $*$-structure $*_\hbar=*+\mathcal{O}(\hbar)$ by

$$x^{*_\hbar}=\mathrm{e}^{-\hbar H/2}\triangleright x^* \tag{52}$$

such that $(\mathcal{X},\mu_\hbar,*_\hbar)$ becomes a module $*$-algebra of $\mathcal{U}(\mathrm{su}_2)[[\hbar]]$ with respect to the deformed Hopf structure.

D. The quantum Lorentz algebra

We recall the definition of quantum Euclidean algebra in four dimensions and the quantum Lorentz algebra.

Definition 3: The tensor product Hopf $*$-algebra $\mathcal{U}_\hbar(\mathrm{su}_2)\otimes\mathcal{U}_\hbar(\mathrm{su}_2)$ is the $\hbar$-adic quantum enveloping algebra of so_4, $\mathcal{U}_\hbar(\mathrm{so}_4)$. Let $\mathcal{R}$ be the universal $\mathcal{R}$-matrix (31) of $\mathcal{U}_\hbar(\mathrm{su}_2)$. The Hopf algebra obtained by twisting $\mathcal{U}_\hbar(\mathrm{so}_4)$ with $\mathcal{R}_{23}^{-1}=1\otimes\mathcal{R}^{-1}\otimes 1$ together with the $*$-structure

$$(a\otimes b)^*=\mathcal{R}_{21}(b^*\otimes a^*)\mathcal{R}_{21}^{-1} \tag{53}$$

for $a,b\in\mathcal{U}_\hbar(\mathrm{su}_2)$ is the $\hbar$-adic quantum Lorentz algebra $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$.[25]

The tensor Hopf $*$-structure of $\mathcal{U}_\hbar(\mathrm{so}_4)$ is given by $\varepsilon^{\otimes 2}:=\varepsilon\otimes\varepsilon$, $S^{\otimes 2}:=S\otimes S$, $\Delta^{\otimes 2}:=\tau_{23}\circ(\Delta\otimes\Delta)$, where τ is the flip of the tensor factors, $\tau(a\otimes b)=b\otimes a$, and $*^{\otimes 2}:=*\otimes *$. Looking at Corollary 1 (v) for the twist $\mathcal{F}:=\mathcal{R}_{23}^{-1}$ we find that the coassociator is the unit, $\Phi=1$. Twists with unital coassociator are two-cocycles in the sense of Ref. 16. The cocycle property guarantees that the twisted coproduct is coassociative. For the antipode $S(a\otimes b)=\sigma_1(Sa\otimes Sb)\sigma_1^{-1}$ we have to compute $\sigma_1^{-1}=S(\mathcal{F}^{-1}_{[1]})\mathcal{F}^{-1}_{[2]}=(1\otimes S\mathcal{R}_{[1]})(\mathcal{R}_{[2]\otimes 1})=\mathcal{R}_{21}^{-1}$. Whence, the Hopf structure of $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$ reads explicitly

$$\Delta(a\otimes b)=\mathcal{R}_{23}^{-1}\Delta^{\otimes 2}(a\otimes b)\mathcal{R}_{23}, \quad S(a\otimes b)=\mathcal{R}_{21}(Sa\otimes Sb)\mathcal{R}_{21}^{-1}, \tag{54}$$

while according to Corollary 1, (ii) the counit stays undeformed.

In the undeformed case so_4 and $\mathrm{sl}_2(\mathbb{C})$ are real forms of the same complex Lie algebra $A_1\otimes A_1$, that is, $\mathcal{U}(\mathrm{so}_4)$ and $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))$ differ only by their $*$-structure, whereas in the q-deformed

case the Hopf structures differ, as well. The reason for introducing the twist in the Hopf structure of $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$ is that only then the quantum Lorentz algebra contains a Hopf $*$-subalgebra of rotations, embedded by the coproduct $\Delta:\mathcal{U}_\hbar(\mathrm{su}_2)\hookrightarrow\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$, which is an essential feature for its physical interpretation. The $*$-structure of $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))$ is not a twist of the product $*$-structure of $\mathcal{U}_\hbar(\mathrm{so}_4)$, but of the flipped $*$-structure $\tau\circ(*\otimes*)$. While Eq. (53) clearly defines an algebra antihomomorphism, the involution property $*^2=\mathrm{id}$ relies on the additional property $\mathcal{R}^{*\otimes *}=\mathcal{R}_{21}$ of the $\mathcal{R}$-matrix of $\mathcal{U}_\hbar(\mathrm{su}_2)$.

The twisting from $\mathcal{U}_\hbar(\mathrm{so}_4)$ to $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$ can be extended to Drinfeld twists and module algebras.

Corollary 2: Let $\mathcal{F}'$ and $\mathcal{F}''$ be Drinfeld twists from $\mathcal{U}(\mathrm{su}_2)$ to $\mathcal{U}_\hbar(\mathrm{su}_2)$, $\mathcal{R}$ the universal $\mathcal{R}$-matrix of $\mathcal{U}_\hbar(\mathrm{su}_2)$, and $\mathcal{X}$ an $\hbar$-adic $\mathcal{U}_\hbar(\mathrm{su}_2)\otimes\mathcal{U}_\hbar(\mathrm{su}_2)$-module.

(i) $\mathcal{F}'_{13}\mathcal{F}''_{24}$ is a Drinfeld twist of from $\mathcal{U}(\mathrm{so}_4)$ to $\mathcal{U}_\hbar(\mathrm{so}_4)$.

(ii) $\mathcal{R}_{23}^{-1}\mathcal{F}'_{13}\mathcal{F}''_{24}$ is a Drinfeld twist of from $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))$ to $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$.

(iii) If $(\mathcal{X},\mu)$ is a module algebra of $\mathcal{U}_\hbar(\mathrm{so}_4)$ with multiplication map μ, then $(\mathcal{X},\tilde{\mu})$ with the twisted multiplication defined as $\tilde{\mu}(x\otimes y):=\mu(\mathcal{R}_{23}\triangleright[x\otimes y])$ is a module algebra of $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$.

(iv) If $(\mathcal{X},\mu,*)$ is a module $*$-algebra of the Hopf algebra $\mathcal{U}_\hbar(\mathrm{so}_4)$ with flipped $*$-structure $\tau\circ(*\otimes*)$, then $(\mathcal{X},\tilde{\mu},*)$ is a module $*$-algebra of $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))$.

Proof: (i) $\mathcal{F}'_{13}\mathcal{F}''_{24}=\tau_{23}(\mathcal{F}'\otimes\mathcal{F}'')$ is clearly a tensor product twist of the tensor coproduct $\Delta^{\otimes 2}=\tau_{23}\circ(\Delta\otimes\Delta)$

(ii) Twisting in two steps by $\mathcal{F}'_{13}\mathcal{F}''_{24}$ from $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))=\mathcal{U}(\mathrm{so}_4)$ to $\mathcal{U}_\hbar(\mathrm{so}_4)$ and then by $\mathcal{R}_{23}^{-1}$ from $\mathcal{U}_\hbar(\mathrm{so}_4)$ to $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$ is the same as twisting at once by $\mathcal{R}_{23}^{-1}\mathcal{F}'_{13}\mathcal{F}''_{24}$ from $\mathcal{U}(\mathrm{sl}_2(\mathbb{C}))$ to $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$.

(iii) Note that $\tilde{\mu}$ is the twisted multiplication (6) for $\mathcal{F}=\mathcal{R}_{23}^{-1}$. All we have to check is associativity. The defining properties of a universal $\mathcal{R}$-matrix imply that the Drinfeld coassociator (10) is equal to the unit. Hence, Eq. (11) is trivially satisfied.

(iv) Let us denote the flipped $*$ structure by $*_\tau:=\tau\circ(*\otimes*)$. We verify that $\mathcal{F}=\mathcal{R}_{23}^{-1}$ is real in the sense of Eq. (18b),

$$\begin{aligned}(S^{\otimes 2}\otimes S^{\otimes 2})(\mathcal{F})&=1\otimes(S\otimes S)(\mathcal{R}^{-1})\otimes 1\\&=1\otimes(\mathcal{R}_{21}^{-1})^{*\otimes *}\otimes 1\\&=(\mathcal{R}_{[2]}^{-1}\otimes 1)^{*_\tau}\otimes(1\otimes\mathcal{R}_{[1]}^{-1})^{*_\tau}\\&=(*_\tau\otimes *_\tau)(\mathcal{F}_{21}),\end{aligned}\tag{55}$$

where we have used $(S\otimes S)(\mathcal{R})=\mathcal{R}$ and $\mathcal{R}^{*\otimes *}=\mathcal{R}_{21}$. Equation (19) shows that the $*$-structure of $\mathcal{X}$ is an antihomomorphism with respect to both multiplications, μ and $\tilde{\mu}$. Then we have to check Eq. (15). Denoting by $S_{\mathrm{sl}_2(\mathbb{C})}$ and $*_{\mathrm{sl}_2(\mathbb{C})}$ the antipode and $*$-structure of $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$, we get

$$\begin{aligned}[S_{\mathrm{sl}_2(\mathbb{C})}(a\otimes b)]^{*_{\mathrm{sl}_2(\mathbb{C})}}&=[\mathcal{R}_{21}(Sa\otimes Sb)\mathcal{R}_{21}^{-1}]^{*_{\mathrm{sl}_2(\mathbb{C})}}\\&=\mathcal{R}_{21}[(\mathcal{R}_{21}^{-1}((Sb)^*\otimes(Sa)^*)\mathcal{R}_{21})]\mathcal{R}_{21}^{-1}\\&=(Sb)^*\otimes(Sa)^*=[S^{\otimes 2}(a\otimes b)]^{*_\tau},\end{aligned}\tag{56}$$

whence $[(a\otimes b)\triangleright x]^*=[S^{\otimes 2}(a\otimes b)]^{*_\tau}\triangleright x^*=[S_{\mathrm{sl}_2(\mathbb{C})}(a\otimes b)]^{*_{\mathrm{sl}_2(\mathbb{C})}}\triangleright x^*$. □

E. Quantum Minkowski space

Quantum Minkowski space $\mathcal{X}_\hbar(\mathbb{R}^{1,3})$ is a noncommutative deformation of the function algebra on real world 1+3-dimensional space–time.[7] By definition, $\mathcal{X}_\hbar(\mathbb{R}^{1,3})$ is the $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$-module algebra whose generators carry the fundamental representation. It was shown in Corollary 2 that any $\mathcal{U}_\hbar(\mathrm{sl}_2(\mathbb{C}))$-module algebra is the twist of a $\mathcal{U}_\hbar(\mathrm{so}_4)$-module algebra. We will first compute the multiplication map of this $\mathcal{U}_\hbar(\mathrm{so}_4)$-module algebra, quantum Euclidean four-space, and then twist it to obtain the multiplication map of quantum Minkowski space.

Because $\mathcal{U}_\hbar(\mathrm{so}_4)$ is the product Hopf algebra of two $\mathcal{U}_\hbar(\mathrm{su}_2)$, any irreducible representation is the product of two irreducible representations of $\mathcal{U}_\hbar(\mathrm{su}_2)$,

$$D_\hbar^{(j,j')} := (V^j \otimes V^{j'}, \rho_\hbar^j \otimes \rho_\hbar^{j'}). \tag{57}$$

The generators $X_{mm'}$ of the quantum Euclidean four-space are defined to carry the fundamental spin-(1/2,1/2) representation,

$$(g \otimes g') \triangleright X_{mm'} = X_{\tilde{m}\tilde{m}'} \rho_\hbar^{1/2}(g)^{\tilde{m}}{}_m \rho_\hbar^{1/2}(g')^{\tilde{m}'}{}_{m'}, \tag{58}$$

where the indices run through $\{-,+\}=\{-1/2,+1/2\}$. Using Eq. (34), the Clebsch–Gordan decomposition of this representation reads

$$D_\hbar^{(1/2,1/2)} \otimes D_\hbar^{(1/2,1/2)} = D_\hbar^{(0,0)} \oplus D_\hbar^{(1,0)} \oplus D_\hbar^{(0,1)} \oplus D_\hbar^{(1,1)}. \tag{59}$$

The subrepresentation by which we have to divide the free algebra $\mathbb{C}\langle X_{mm'}\rangle[[\hbar]]$ for the right noncommutative limit as $\hbar \to 0$ is $D_\hbar^{(1,0)} \oplus D_\hbar^{(0,1)}$. This corresponds to the quadratic relations

$$\begin{aligned} &\sum_{m_1,m_2,m_1',m_2'} \left(\begin{array}{cc|c} 1/2 & 1/2 & 1 \\ m_1 & m_2 & m \end{array}\right)_q \left(\begin{array}{cc|c} 1/2 & 1/2 & 0 \\ m_1' & m_2' & 0 \end{array}\right)_q X_{m_1 m_1'} X_{m_2 m_2'} = 0, \\ &\sum_{m_1,m_2,m_1',m_2'} \left(\begin{array}{cc|c} 1/2 & 1/2 & 0 \\ m_1 & m_2 & 0 \end{array}\right)_q \left(\begin{array}{cc|c} 1/2 & 1/2 & 1 \\ m_1' & m_2' & m \end{array}\right)_q X_{m_1 m_1'} X_{m_2 m_2'} = 0, \end{aligned} \tag{60}$$

where m runs through $\{-1,0,1\}$. Denoting the generators by $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) := (X_{mm'})$, i.e., $d = X_{++}$ etc., relations (60) read

$$\begin{gathered} ab = qba, \quad ac = qca, \quad bd = qdb, \quad cd = qdc, \\ bc = cb, \quad ad - da = (q - q^{-1})bc, \end{gathered} \tag{61}$$

which are the well-known relations of the algebra of 2×2 quantum matrices.[26] The quantum determinant

$$\det_q := ad - qbc \tag{62}$$

is scalar, $(g \otimes g') \triangleright \det_q = \varepsilon(g \otimes g') \det_q$, and commutes with all generators.

Definition 4: The $\hbar$-adic algebra freely generated by $\{a,b,c,d\}$ with commutation relations (61) is called the $\hbar$-adic quantum Euclidean four-space or the $\hbar$-adic algebra of 2×2 quantum matrices $M_\hbar(2)$.

Quantum Euclidean four-space and $M_q(2)$ are the same algebras, for $\mathrm{SU}_\hbar(2) := M_\hbar(2)/\langle \det_q = 1 \rangle$ is Hopf dual to $\mathcal{U}_\hbar(\mathrm{su}_2)$ in the sense of Ref. 27, which implies that the comodule algebras of $\mathrm{SU}_\hbar(2)$ are the module algebras of $\mathcal{U}_\hbar(\mathrm{su}_2)$. In fact, let Δ be the coproduct of $M_\hbar(2)$, $\Delta(X_{ik}) = \Sigma_j X_{ij} \otimes X_{jk}$, let $T: M_\hbar(2) \to M_\hbar(2)$ be the transposition homomorphism which is defined on the generators by $(X_{ij})^T := X_{ji}$, and let $\pi: M_\hbar(2) \to M_\hbar(2)/\langle \det_q = 1 \rangle$ be the canonical epimorphism, $U^i{}_j := \pi(X_{ij})$ the generators of $\mathrm{SU}_\hbar(2)$, and τ the flip of tensor factors. Then the map $\varphi: M_\hbar(2) \to M_\hbar(2) \otimes \mathrm{SU}_\hbar(2) \otimes \mathrm{SU}_\hbar(2)$ defined as

$$\varphi := [\mathrm{id} \otimes (\pi \circ T) \otimes \pi] \circ \tau_{12} \circ \Delta^{(2)} \Rightarrow \varphi(X_{ij}) = X_{i'j'} \otimes U^{i'}{}_i \otimes U^{j'}{}_j \tag{63}$$

is a homomorphism of algebras because it is a concatenation of homomorphisms, and a corepresentation because $\Delta(U^i{}_k)=U^i{}_j\otimes U^j{}_k$. Hence, $M_\hbar(2)$ together with φ is a comodule algebra of $\mathrm{SO}_\hbar(4):=\mathrm{SU}_\hbar(2)\otimes\mathrm{SU}_\hbar(2)$. The dual of this coaction (63) is the action (58) by which $M_q(2)$ becomes a $\mathcal{U}_\hbar(\mathrm{so}_4)$-module algebra.

A simple ansatz shows that the only homogeneous highest weight vectors of $M_\hbar(2)$ are proportional to $\det_q^k d^l$. In analogy to the quantum plane, we have to define the minimal degree irreducible weight vectors by

$$T^{(j,j)}_{mm'}:=q^{(1/2)[(j-m)(2m-j+1)+(j-m')(2m'-j+1)]}\times\sqrt{\frac{[j+m]![j+m']!}{[2j]!^2[j-m]![j-m']!}}[(F^{j-m}\otimes F^{j-m'})\triangleright d^{2j}], \tag{64}$$

for $j\in 1/2\mathbb{N}_0$, such that they carry a spin-(j,j) representation,

$$(g\otimes g')\triangleright T^{(j,j)}_{mm'}=T'^{(j,j)}_{\tilde m\tilde m'}\rho^j_\hbar(g)^{\tilde m}{}_m\rho^j_\hbar(g')^{\tilde m'}{}_{m'}. \tag{65}$$

The explicit calculation of Eq. (64) leads to

$$T^{(j,j)}_{mm'}=\sum_k q^{k(m'-m-k)}\begin{bmatrix} j-m\\ k\end{bmatrix}_{q^{-2}}\begin{bmatrix} j+m\\ j+m'-k\end{bmatrix}_{q^{-2}}\begin{bmatrix} 2j\\ j+m\end{bmatrix}^{1/2}_{q^{-2}}\begin{bmatrix} 2j\\ j+m'\end{bmatrix}^{-1/2}_{q^{-2}}\times a^{j-m-k}b^kc^{m-m'+k}d^{j+m'-k}, \tag{66}$$

which reduces $M_\hbar(2)$ into irreducible subrepresentations by

$$M_\hbar(2)=\bigoplus_{j\in\mathbb{N}_0/2}\bigoplus_{k\in\mathbb{N}_0}\mathrm{Span}_{\mathbb{C}[[\hbar]]}\{\det_q^k T^{(j,j)}_{mm'}|m,m'=-j,\ldots,j\}. \tag{67}$$

Note that mapping this equation by the canonical epimorphism π onto $\mathrm{SU}_\hbar(2)$ yields the quantum Peter–Weyl decomposition of $\mathrm{SU}_\hbar(2)$ (see Ref. 23, Sec. 4.2.5). As we argued for the quantum plane, the reduction of the product of two irreducible weight vectors with q–Clebsch–Gordan coefficients must again be an irreducible weight vector of the same degree as the product,

$$\sum_{m_1,m_2,m_1',m_2'}\left(\begin{matrix} j_1 & j_2\\ m_1 & m_2\end{matrix}\middle|\begin{matrix} j\\ m\end{matrix}\right)_q\left(\begin{matrix} j_1 & j_2\\ m_1' & m_2'\end{matrix}\middle|\begin{matrix} j'\\ m'\end{matrix}\right)_q T^{(j_1,j_1)}_{m_1m_1'}T^{(j_2,j_2)}_{m_2m_2'}=\delta_{jj'}\beta_{j_1j_2j}\det_q^{j_1+j_2-j}T^{(j,j)}_{mm'}, \tag{68}$$

where the $\beta_{j_1j_2j}\in\mathbb{C}[[\hbar]]$ are $\hbar$-adic scalar coefficients. These coefficients can be easily computed by applying the counit ε of $M_\hbar(2)$, for which we have

$$\varepsilon(T^{(j,j)}_{mm'})=\delta_{mm'},\quad \varepsilon(\det_q)=1, \tag{69}$$

to Eq. (68). This yields $\beta_{j_1j_2j}=1$ for all j_1,j_2,j. Finally, moving the q–Clebsch–Gordan coefficients to the other side of Eq. (68) produces the desired expression for the product $\mu_\hbar$ of $M_\hbar(2)$,

$$\mu_\hbar(T^{(j_1,j_1)}_{m_1m_1'}\otimes T^{(j_2j_z)}_{m_2m_2})=\sum_{m,m',j}\left(\begin{matrix} j_1 & j_2\\ m_1 & m_2\end{matrix}\middle|\begin{matrix} j\\ m\end{matrix}\right)_q\left(\begin{matrix} j_1 & j_2\\ m_1' & m_2'\end{matrix}\middle|\begin{matrix} j\\ m'\end{matrix}\right)_q\det_q^{j_1+j_2-j}T^{(j,j)}_{mm'}. \tag{70}$$

Again, we compare this with the representations (40) and (43) of the Drinfeld twists of $\mathcal{U}_\hbar(\mathrm{su}_2)$ and obtain the following.

Proposition 9: Let $\mu_\hbar$ be the multiplication map (70) of $\hbar$-adic Euclidean four-space $M_\hbar(2)$, $\mu=\lim_{\hbar\to 0}\mu_\hbar$ its undeformed limit, and $\mathcal{F}_s$ the standard twist of Proposition 6. Then $\mu_\hbar$ is the deformation (6) of μ by $\mathcal{F}_{so_4}:=\mathcal{F}_{s13}\mathcal{F}_{s24}$.

Now we can apply Corollary 2 in order to obtain the multiplication map and twist of quantum Minkowski space, twisting once more by $\mathcal{R}_{23}^{-1}$. Of course, the multiplication map of quantum Minkowski space will reproduce the well-known commutation relations of Ref. 7. For the twist we get the following.

Proposition 10: Let $\mu_\hbar$ be the multiplication map of $\hbar$-adic quantum Minkowski space $\mathcal{X}(\mathbb{R}^{1,3})$, $\mu=\lim_{\hbar\to 0}\mu_\hbar$ its undeformed limit, and $\mathcal{F}_s$ the standard twist of Proposition 6. Then $\mu_\hbar$ is the deformation (6) of μ by $\mathcal{F}_{sl_2(\mathbb{C})}:=\mathcal{R}_{23}^{-1}\mathcal{F}_{s13}\mathcal{F}_{s24}$.

Finally, we consider real structures. Since $\mathcal{F}_s$ is real in the sense of Eq. (18b), so is $\mathcal{F}_{so_4}$. Moreover, since $\mathcal{F}_{sl_2(\mathbb{C})}$ is the twist of $\mathcal{F}_{so_4}$ by $\mathcal{R}_{23}^{-1}$, which was shown to be real in the proof of Corollary 2 (iv), $\mathcal{F}_{sl_2(\mathbb{C})}$ is real, as well. Hence, Proposition 4 applies to both, quantum Euclidean four-space and quantum Minkowski space. From a reasoning which is completely analogous to the one that led to Eq. (52) we conclude that the deformation $*_\hbar=*+\mathcal{O}(\hbar)$ of the real structure $*$ of the undeformed Minkowski space–time algebra $\mathcal{X}\equiv\mathcal{X}(\mathbb{R}^{1,3})$ has to be defined by

$$x^{*_\hbar}=(e^{-\hbar H/2}\otimes e^{-\hbar H/2})\triangleright x^* \tag{71}$$

such that $(\mathcal{X},\mu_\hbar,*_\hbar)$ becomes a module $*$-algebra of $\mathcal{U}(sl_2(\mathbb{C}))[[\hbar]]$ with respect to the deformed Hopf structure.

IV. CONCLUSION

It is possible to use Drinfeld twists in order to realize quantum spaces as covariant star products. We have shown this for three important examples, the quantum plane (Proposition 8), quantum Euclidean four-space (Proposition 9), and quantum Minkowski space (Proposition 10). While it was known that the Drinfeld twists control the deformation of enveloping algebras into quantum enveloping algebras, it is now clear that certain twists also control the deformation of spaces into quantum spaces. This is not unexpected, since the covariance condition of the action of a symmetry on a space algebra ties the Hopf structure of the symmetry algebra closely to the multiplicative structure of the space algebra. Our considerations included real structures of quantum enveloping algebras and quantum spaces. In Proposition 4 we have formulated a sufficient condition on the Drinfeld twist, its reality in the sense of Eq. (18b), to be compatible with the real structure of a quantum space, and we have shown that there is a unique element σ of the enveloping algebra which implements the deformation of the real structure.

Star products are often defined by identifying the vector spaces of two space algebras $\mathcal{X}$ and $\mathcal{X}_\hbar$ by an vector space isomorphism, $\varphi:\mathcal{X}\to\mathcal{X}_\hbar$, and transferring the multiplication by $x\star y:=\varphi^{-1}[\varphi(x)\varphi(y)]$. The Moyal–Weyl product is an example of this procedure. The linear isomorphism φ is called an ordering prescription because it defines how an ordered monomial of the commutative algebra $\mathcal{X}$ has to be represented in the noncommutative algebra $\mathcal{X}_\hbar$. For example $\varphi(xy)=\frac{1}{2}[\hat{x}\hat{y}+\hat{y}\hat{x}]$, where $\hat{x}:=\varphi(x)$, $\hat{y}:=\varphi(y)$, for the symmetric ordering. The star product which is obtained by the standard twist of Proposition 8 amounts to the ordering prescription which identifies the basis vectors which completely reduce the space and the quantum space respectively into its irreducible subrepresentations, which is a natural ordering in the context of representation theory. For the quantum plane this is almost the lexicographic (Poincaré–Birkhoff–Witt) ordering,

$$\varphi(x^k y^l)=\begin{bmatrix}k+l\\ k\end{bmatrix}_{q^{-2}}^{1/2}\begin{pmatrix}k+l\\ k\end{pmatrix}^{-1/2}x^k y^l, \tag{72}$$

where we recall that $x\equiv x_-$, $y\equiv x_+$. The basis of the spin-j subrepresentation is unique up to scalar multiples. A rescaling $T^j_m\mapsto\beta(j)T^j_m$ with $\beta(j)=1+\mathcal{O}(\hbar)$ would change the multiplication

map by multiplying the right-hand side of Eq. (50) with $\beta(j)\beta^{-1}(j_1)\beta^{-1}(j_2)$. Identifying the scale factors with the representations $\beta(j)=\rho^j(z)$ of some invertible central element z, the twist which realizes the star product must be redefined by $\mathcal{F}\mapsto\mathcal{F}(z\otimes z)\Delta z^{-1}$. We conclude that the twist of Proposition 8 which realizes the star product of the quantum plane is unique up to a central two-coboundary. The standard twist is the unique twist with the additional property $y^{*n}=y^n$. An analogous statement is true for quantum Euclidean four-space and quantum Minkowski space.

To our knowledge, no Drinfeld twist for the Drinfeld–Jimbo deformation of a semisimple Lie algebra had so far been computed explicitly (see Ref. 15 for the Heisenberg algebra). We have circumvented this problem by reducing the algebraic questions to representation theoretic ones. Although $\mathcal{U}_\hbar(\mathrm{su}_2)$ is the simplest case conceivable, an algebraic order-by-order calculation of the twist runs quickly into overwhelming combinatorial problems.[28] An alternative approach would be the reconstruction of the twist from its representations, which would profit from the computational effort that has gone into the calculation of the q–Clebsch–Gordan coefficients.

APPENDIX: *Proof of Corollary 1*

Let throughout the proof $g\in\mathcal{U}(\mathfrak{g})[[\hbar]]$ be an arbitrary element of the $\hbar$-adic enveloping algebra.

(i) $\mathcal{F}\Delta(g)\mathcal{F}^{-1}=\Delta_\hbar(g)=\mathcal{F}'\Delta(g)\mathcal{F}'^{-1}$ implies that $\mathcal{F}^{-1}\mathcal{F}'$ commutes with $\Delta(g)$ for all g. Conversely, let $\mathcal{T}\Delta(g)\mathcal{T}^{-1}=\Delta(g)$. Then $\mathcal{F}\mathcal{T}\Delta(g)\mathcal{T}^{-1}\mathcal{F}^{-1}=\mathcal{F}\Delta(g)\mathcal{F}^{-1}=\Delta_\hbar(g)$ for all g.

(ii) By the left counit property of $\varepsilon_\hbar$ we get

$$\begin{aligned}\varepsilon(g)&=\varepsilon(\varepsilon_\hbar(g_{(1_\hbar)})g_{(2_\hbar)})\\&=\varepsilon(\varepsilon_\hbar(\mathcal{F}_{[1]})\mathcal{F}_{[2]}\varepsilon_\hbar(g_{(1)})g_{(2)}\varepsilon_\hbar(\mathcal{F}^{-1}_{[1']})\mathcal{F}^{-1}_{[2']})\\&=\varepsilon_\hbar(g_{(1)})\varepsilon(g_{(2)})\varepsilon_\hbar(\mathcal{F}_{[1]})\varepsilon(\mathcal{F}_{[2]})\varepsilon_\hbar(\mathcal{F}^{-1}_{[1']})\varepsilon(\mathcal{F}^{-1}_{[2']})\\&=\varepsilon_\hbar(g_{(1)}\varepsilon(g_{(2)}))=\varepsilon_\hbar(g).\end{aligned}\tag{A1}$$

(iii) Let us define the left and right counit constraints by $l:=\varepsilon(\mathcal{F}_{[1]})\mathcal{F}_{[2]}$ and $r:=\mathcal{F}_{[1]}\varepsilon(\mathcal{F}_{[2]})$. From the left counit property of $\varepsilon_\hbar=\varepsilon$ it follows that $g=\varepsilon(g_{(1_\hbar)})g_{(2_\hbar)}=\varepsilon(\mathcal{F}_{[1]})\mathcal{F}_{[2]}\varepsilon(g_{(1)})g_{(2)}\varepsilon(\mathcal{F}^{-1}_{[1']})\mathcal{F}^{-1}_{[2']}=lgl^{-1}$ and analogously for the right counit property $g=rgr^{-1}$. Hence, $\mathcal{T}:=\varepsilon(l)(r^{-1}\otimes l^{-1})$ is $\mathfrak{g}$-invariant. By (*i*) $\mathcal{F}':=\mathcal{F}\mathcal{T}$ is a twist with $l':=\varepsilon(\mathcal{F}'_{[1]})\mathcal{F}'_{[2]}=\varepsilon(l)\varepsilon(\mathcal{F}_{[1]}r^{-1})\mathcal{F}_{[2]}l^{-1}=\varepsilon(lr^{-1})ll^{-1}=1$, where we have used $\varepsilon(l)=\varepsilon(\mathcal{F}_{[1]}\mathcal{F}_{[2]})=\varepsilon(r)$. Analogously, we find that $r'=1$. Since $\mathcal{F}'$ is invertible, $\mathcal{F}'=\beta 1+\mathcal{O}(\hbar)$ for some complex number $\beta\neq 0$, and $1=l'=\beta+\mathcal{O}(\hbar)$ it follows that $\beta=1$.

(iv) Define $\sigma_1:=S_\hbar(\mathcal{F}_{[1]})\mathcal{F}_{[2]}$. Then

$$\begin{aligned}S_\hbar(g)\sigma_1&=S_\hbar(g_{(1)})\sigma_1 g_{(2)}S(g_{(3)})\\&=S_\hbar(\mathcal{F}_{[1]}g_{(1)(1)})\mathcal{F}_{[2]}g_{(1)(2)}S(g_{(2)})\\&=S_\hbar(g_{(1)(1_\hbar)}\mathcal{F}_{[1]})g_{(1)(2_\hbar)}\mathcal{F}_{[2]}S(g_{(2)})\\&=S_\hbar(\mathcal{F}_{[1]})\varepsilon(g_{(1)})\mathcal{F}_{[2]}S(g_{(2)})=\sigma_1 S(g),\end{aligned}\tag{A2}$$

where we have used the left coinverse property of $S_\hbar$. Analogously, defining $\sigma_2^{-1}:=\mathcal{F}^{-1}_{[1]}S_\hbar(\mathcal{F}^{-1}_{[2]})$ and using the right coinverse property of $S_\hbar$ we get $\sigma_2^{-1}S_\hbar(g)=S(g)\sigma_2^{-1}$. Since $\mathcal{F}$ is invertible, so are σ_1 and σ_2^{-1}. Thus, $S_\hbar$ and S are related by the inner automorphisms $\sigma_1 S(g)\sigma_1^{-1}=S_\hbar(g)=\sigma_2 S(g)\sigma_2^{-1}$. The antipode is surjective, so $\sigma_1^{-1}\sigma_2$ must be central. Moreover, $(\sigma_1^{-1}\sigma_2)(\sigma_1\sigma_2^{-1})=\sigma_1(\sigma_1^{-1}\sigma_2)\sigma_2^{-1}=1$, hence, $\sigma_1^{-1}\sigma_2=\sigma_2\sigma_1^{-1}$. Finally,

$$\sigma_1^{-1}=\sigma_1^{-1}S_\hbar(\mathcal{F}_{[1']}\mathcal{F}^{-1}_{[1]})\mathcal{F}_{[2']}\mathcal{F}^{-1}_{[2]}=\sigma_1^{-1}S_\hbar(\mathcal{F}^{-1}_{[1]})\sigma_1\mathcal{F}^{-1}_{[2]}=S(\mathcal{F}^{-1}_{[1]})\mathcal{F}^{-1}_{[2]},\tag{A3}$$

and, analogously, $\sigma_2=\mathcal{F}_{[1]}S(\mathcal{F}_{[2]})$.

(v) From the coassociativity of $\Delta_\hbar$ we deduce

$$\begin{aligned}[(\Delta_\hbar\otimes\mathrm{id})\circ\Delta_\hbar](g)&=\mathcal{F}_{12}(\Delta\otimes\mathrm{id})(\mathcal{F})(\Delta^{(2)}g)(\Delta\otimes\mathrm{id})(\mathcal{F}^{-1})\mathcal{F}_{12}^{-1}\\&=[(\mathrm{id}\otimes\Delta_\hbar)\circ\Delta_\hbar](g)\\&=\mathcal{F}_{23}(\mathrm{id}\otimes\Delta)(\mathcal{F})(\Delta^{(2)}g)(\mathrm{id}\otimes\Delta)(\mathcal{F}^{-1})\mathcal{F}_{23}^{-1}.\end{aligned}\tag{A4}$$

Hence, the coassociator (10) commutes with all $\Delta^{(2)}g$.

(vi) Since every bialgebra isomorphism is automatically a Hopf algebra isomorphism and since by (ii) the counit stays undeformed, we only have to consider the coproducts. Let Δ and $\Delta_\hbar$ be related by a twist $\mathcal{F}=(u\otimes u)\Delta u^{-1}$. Then $g\mapsto ugu^{-1}$ maps Δ to $\Delta_\hbar$. Conversely, assume that the two Hopf structures are isomorphic, so there is an algebra automorphism β with $\Delta_\hbar=(\beta\otimes\beta)\circ\Delta\circ\beta^{-1}$. Since $\Delta_\hbar=\Delta+\mathcal{O}(\hbar)$ we can choose $\beta=\mathrm{id}+\mathcal{O}(\hbar)$. Since $\mathfrak{g}$ is semisimple we have $H^1(\mathcal{U}(\mathfrak{g}),\mathcal{U}(\mathfrak{g}))=0$, which implies that this automorphism is inner, $\beta(g)=ugu^{-1}$. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Supersymmetric extensions of the Harry Dym hierarchy

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(Received 25 April 2003; accepted 16 June 2003)

We study the supersymmetric extensions of the Harry Dym hierarchy of equations. We obtain the susy-B extension, the doubly susy-B extension as well as the $N=1$ and the $N=2$ supersymmetric extensions for this system. The $N=2$ supersymmetric extension is particularly interesting, since it leads to new classical integrable systems in the bosonic limit. We prove the integrability of these systems through the bi-Hamiltonian formulation of integrable models and through the Lax description. We also discuss the supersymmetric extension of the Hunter–Zheng equation which belongs to the Harry Dym hierarchy of equations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1606527]

I. INTRODUCTION

Supersymmetric extensions of a number of well-known bosonic integrable models have been studied extensively in the past. The supersymmetric Korteweg–de Vries (sKdV) equation,[1] the supersymmetric nonlinear Schrödinger (sNLS) equation[2] and the supersymmetric two-Boson (sTB) equation[3] represent just a few in this category. A simple supersymmetric covariantization of bosonic integrable models, conventionally known as the B supersymmetrization (susy-B), has also attracted a lot of interest because of the appearance of such models in string theories. We have, for instance, the B extensions of the KdV (sKdV-B) equation,[4] the supersymmetric TB (sTB-B) equation[5] and so on. Supersymmetric extensions of integrable models using a number N of Grassmann variables greater than one[6] and supersymmetric construction of dispersionless integrable models[7] have also been studied extensively in the past few years. The extended supersymmetric models are particularly interesting because, in the bosonic limit, they yield new classical integrable systems.

A classic bosonic integrable equation, the so-called Harry Dym (HD) equation,[8] has attracted much interest recently. The proprieties of this equation are discussed in detail in Ref. 9, and we simply emphasize that this equation shares the properties typical of solitonic equations, namely, it can be solved by the inverse scattering transform, it has a bi-Hamiltonian structure and infinitely many symmetries. In fact, the HD equation is one of the most exotic solitonic equations and the hierarchy to which it belongs, has a very rich structure.[10] In this hierarchy we also have nonlocal integrable equations such as the Hunter–Zheng (HZ) equation,[11] which arises in the study of massive nematic liquid crystals as well as in the study of shallow water waves. The HD equation, on the other hand, is relevant in the study of the Saffman–Taylor problem which describes the motion of a two-dimensional interface between a viscous and a nonviscous fluid.[12]

An earlier attempt to supersymmetrize the HD equation is discussed in Ref. 13. However, this study of $N=1$ supersymmetrization introduces a bosonic as well as an independent fermionic superfield, yielding a pair of coupled equations, and, consequently, is not in the conventional spirit of minimal supersymmetrization. In this paper we intend to study the question of supersymmetri-

zation of the HD hierarchy systematically. The paper is organized as follows. In Sec. II we review some of the essential results for the HD equation and its hierarchy. The simpler susy-B extension (sHD-B) and the doubly B extension (sHD-BB) of the HD hierarchy as well their bi-Hamiltonian formulation and Lax pairs are described in Sec. III. In Sec. IV we derive the $N=1$ supersymmetric extensions of the HD (sHD) equation. We find that, in this case, there exist two nontrivial $N=1$ extensions. In the case of one of them, we have a bi-Hamiltonian description (we have not found a Lax representation yet) while in the second case, we have a Lax description (we have not found a Hamiltonian structure yet that satisfies the Jacobi identity). We also describe the supersymmetric extension for the HZ equation. In Sec. V we describe the $N=2$ supersymmetrization of the HD hierarchy which yields four possibilities and we discuss their properties. We end with a brief conclusion in Sec. VI.

II. THE HARRY DYM HIERARCHY

The Harry Dym equation

$$w_t=(w^{-1/2})_{xxx}, \tag{1}$$

appears in many disguised forms, namely,

$$\begin{aligned} v_t&=\tfrac{1}{4}v^3v_{xxx},\\ u_t&=\tfrac{1}{4}u^{3/2}u_{xxx}-\tfrac{3}{8}u^{1/2}u_xu_{xx}+\tfrac{3}{16}u^{-1/2}u_x^3,\\ r_t&=(r_{xx}^{-1/2})_x, \end{aligned} \tag{2}$$

where $v=-2^{1/3}w^{-1/2}$, $u=v^2$, and $r_{xx}=w$, respectively. In this paper, as in Ref. 10, we will confine ourselves, as much as is possible, to the form of the HD equation as given in (1).

The HD equation is a member of the bi-Hamiltonian hierarchy of equations given by

$$w_t^{(n+1)}=\mathcal{D}_1\frac{\delta H_{n+1}}{\delta w}=\mathcal{D}_2\frac{\delta H_n}{\delta w}, \tag{3}$$

for $n=-2$, where the bi-Hamiltonian structures are

$$\begin{aligned} \mathcal{D}_1&=\partial^3,\\ \mathcal{D}_2&=w\partial+\partial w, \end{aligned} \tag{4}$$

and the Hamiltonians for the HD equation are

$$\begin{aligned} H_{-1}&=\int \mathrm{d}x\,(2w^{1/2}),\\ H_{-2}&=\int \mathrm{d}x(\tfrac{1}{8}w^{-5/2}w_x^2). \end{aligned} \tag{5}$$

We note here that the second structure in (4) corresponds to the centerless Virasoro algebra while

$$\mathcal{D}=\mathcal{D}_2+c\mathcal{D}_1 \tag{6}$$

represents the Virasoro algebra with a central charge c. We note also that the recursion operator following from (4), $R=\mathcal{D}_2\mathcal{D}_1^{-1}$, can be explicitly inverted to yield

$$R^{-1}=\tfrac{1}{2}\partial^3w^{-1/2}\partial^{-1}w^{-1/2}. \tag{7}$$

Also, the conserved charges

$$H_0 = -\int dx\, w,$$

$$H_0^{(1)} = \int dx\, (\partial^{-1} w), \tag{8}$$

$$H_0^{(2)} = \int dx\, (\partial^{-2} w),$$

are Casimirs (or distinguished functionals) of the Hamiltonian operator $\mathcal{D}_1$ (namely, they are annihilated by the Hamiltonian structure $\mathcal{D}_1$). As a consequence of this, it is possible to obtain, in an explicit form, equations from (3) for integers n both positive and negative, i.e., $n \in \mathbb{Z}$. As shown in Ref. 10, for $n>0$, we have three classes of nonlocal equations. However, in this paper we will only study the hierarchy associated with the local Casimir H_0 in (8). In this way, for $n=1$, we obtain from (3), with the conserved charges

$$H_1 = \int dx \frac{1}{2} (\partial^{-1} w)^2,$$

$$H_2 = \int dx \frac{1}{2} (\partial^{-2} w)(\partial^{-1} w)^2, \tag{9}$$

the Hunter–Zheng (HZ) equation

$$w_t = -(\partial^{-2} w) w_x - 2(\partial^{-1} w) w, \tag{10}$$

which is also an important equation that belongs to the Harry Dym hierarchy.

The integrability of the HD equation (1) also follows from its nonstandard Lax representation,

$$L = \frac{1}{w} \partial^2,$$

$$\frac{\partial L}{\partial t} = -2[B, L], \tag{11}$$

where

$$B = (L^{3/2})_{\geqslant 2} = w^{-3/2} \partial^3 - \tfrac{3}{4} w^{-5/2} w_x \partial^2. \tag{12}$$

Conserved charges, for $n = 1,2,3,\ldots$, are obtained from

$$H_{-(n+1)} = \operatorname{Tr} L^{(2n-1)/2}. \tag{13}$$

A Lax representation for the HZ equation (10) is also known and is given by (11) with

$$B = \tfrac{1}{4} (\partial^{-2} w) \partial + \tfrac{1}{4} \partial^{-1} (\partial^{-2} w) \partial^2. \tag{14}$$

However, in this case, the operator B is not directly related to L, and, consequently, the Lax equation is not of much direct use (in the construction of conserved charges, etc.).

III. THE susy-B HARRY DYM (sHD-B, sHD-BB) EQUATIONS

The most natural generalization of an equation to a supersymmetric one is achieved simply by working in a superspace. We note, from the HD equation (1), that by a simple dimensional analysis, we can assign the following canonical dimensions to various quantities:

$$[x]=-1, \quad [t]=3, \quad \text{and} \quad [w]=4. \tag{15}$$

The $N=1$ supersymmetric equations are best described in the superspace parametrized by the coordinates $z=(x,\theta)$, where θ represents the Grassmann coordinate ($\theta^2=0$). In this space, we can define

$$D=\frac{\partial}{\partial\theta}+\theta\frac{\partial}{\partial x}, \tag{16}$$

representing the supercovariant derivative. From (16) it follows that

$$D^2=\partial, \tag{17}$$

which determines the dimension of θ to be

$$[\theta]=-\tfrac{1}{2}. \tag{18}$$

Let us introduce the fermionic superfield

$$W=\psi+\theta w, \tag{19}$$

which has the canonical dimension

$$[W]=[\psi]=\tfrac{7}{2}. \tag{20}$$

A simple supersymmetrization of a bosonic system, conventionally known as the B supersymmetric (susy-B) extension,[4] is obtained by simply replacing the bosonic variable w, in the original equation, by

$$(DW)=w+\theta\psi', \tag{21}$$

where W represents a fermionic superfield. This leads to a manifestly supersymmetric equation and following this for the case of the equation (1), we obtain the susy-B HD (sHD-B) equation

$$W_t=\partial^2 D((DW)^{-1/2}), \tag{22}$$

where W is the fermionic superfield (19).

This system is bi-Hamiltonian with the even Hamiltonian operators

$$\begin{aligned}\mathcal{D}_1&=\partial^2,\\ \mathcal{D}_2&=D(DW)D^{-1}+D^{-1}(DW)D,\end{aligned} \tag{23}$$

and the odd Hamiltonians [which follow from (5) under the substitution $w\to(DW)$]

$$\begin{aligned}H_{-1}&=\int \mathrm{d}z\, 2(DW)^{1/2},\\ H_{-2}&=\int \mathrm{d}z\, \tfrac{1}{8}(DW)^{-5/2}(DW_x)^2.\end{aligned} \tag{24}$$

The Casimirs of $\mathcal{D}_1$ can be easily identified with the ones following from (8).

The sHD-B equation (22) has two possible nonstandard Lax representations. Let

$$L=(DW)^{-1}D^4+cW_x(DW)^{-2}D^3. \tag{25}$$

Then, it can be easily checked that the nonstandard Lax equation

$$\frac{\partial L}{\partial t}=[(L^{3/2})_{\geqslant 3},L], \tag{26}$$

leads to the sHD-B equation (22) for $c=0,-1$. Here the projection $(\ )_{\geqslant 3}$ is defined with respect to the powers of the supercovariant derivative D.

For any given integrable bosonic equation, we can also define a doubly susy-B extension as follows. Just as we defined a superspace in the case of $N=1$ supersymmetry, let us define a superspace parametrized by $z=(x,\theta_1,\theta_2)$, where θ_1,θ_2 define two Grassmann coordinates (anticomuting and nilpotent, namely, $\theta_1\theta_2=-\theta_2\theta_1$, $\theta_1^2=\theta_2^2=0$). In this case, we can define two supercovariant derivatives

$$\begin{aligned} D_1&=\frac{\partial}{\partial\theta_1}+\theta_1\frac{\partial}{\partial x},\\ D_2&=\frac{\partial}{\partial\theta_2}+\theta_2\frac{\partial}{\partial x}, \end{aligned} \tag{27}$$

which satisfy

$$D_1^2=D_2^2=\partial, \quad D_1D_2+D_2D_1=0. \tag{28}$$

Such a superspace naturally defines a system with $N=2$ supersymmetry. Let us consider a bosonic superfield, W, in this space which will have the expansion (we denote it by the same symbol as in the case of $N=1$)

$$W=w_0+\theta_1\chi+\theta_2\psi+\theta_2\theta_1w_1. \tag{29}$$

Then, we can simply replace the bosonic variable in the original equation by (D_1D_2W) which leads to the doubly susy-B extension of a given equation. For the HD equation (1), this leads to

$$W_t=\partial D_1D_2((D_1D_2W)^{-1/2}), \tag{30}$$

which defines the sHD-BB equation. This procedure can, of course, be generalized to any N extended supersymmetry and we do not pursue this any further. We simply point out that Eq. (30) is bi-Hamiltonian, as we would expect. For example, it is Hamiltonian with

$$H=\int \mathrm{d}z\,(D_1D_2W_x)^2(D_1D_2W)^{-5/2} \tag{31}$$

and

$$\begin{aligned} \mathcal{D}=&-\partial W\partial^{-2}D_1D_2-D_1D_2\partial^{-2}W\partial+D_1\partial^{-1}WD_2-D_2W\partial^{-1}D_1\\ &+D_1D_2\partial^{-1}W-WD_1D_2\partial^{-1}+D_1W\partial^{-1}D_2-D_2\partial^{-1}WD_1. \end{aligned} \tag{32}$$

The second Hamiltonian structure can also be easily obtained.

IV. THE SUPERSYMMETRIC $N=1$ HARRY DYM (sHD) AND HUNTER–ZHENG (sHZ) EQUATIONS

As we have seen, the susy-B extension of a system is a very simple supersymmetrization. However, to obtain nontrivial supersymmetrizations, we can follow one of the following two approaches. In this section, we will discuss $N=1$ supersymmetrization of the system and correspondingly, it is appropriate to work in the superspace defined in (16)–(19).

With the superfield (19) as our basic variable, the first approach is to write the most general local equation in superspace which is consistent with all canonical dimensions and which reduces to (1) in the bosonic limit. This involves a free parameter and the equation takes the form

$$\begin{aligned} W_t=\tfrac{1}{8}[&-8(5a-2)W_{xxx}(DW)^{-3/2}+2(65a-6)W_x(DW_{xx})(DW)^{-5/2}\\ &+30(5a+2)W_{xx}(DW_x)(DW)^{-5/2}-15(21a+2)W_x(DW_x)^2(DW)^{-7/2}\\ &+W\{8(5a-6)(DW_{xxx})(DW)^{-5/2}+10(a-6)W_{xxx}W_x(DW)^{-7/2}\\ &+35(6-a)W_{xx}W_x(DW_x)(DW)^{-9/2}+40(6-7a)(DW_{xx})(DW_x)(DW)^{-7/2}\\ &+105(3a-2)(DW_x)^3(DW)^{-9/2}\}], \end{aligned} \tag{33}$$

where a is the arbitrary parameter. In the case of the HD equation, it is possible to supersymmetrize the two Hamiltonian structures in (3), which is easily seen from the fact that the second Hamiltonian structure is the centerless Virasoro algebra. Thus, the supersymmetrized Hamiltonian structures follow to be

$$\begin{aligned} \mathcal{D}_1&=D\partial^2,\\ \mathcal{D}_2&=\tfrac{1}{2}[W\partial+2\partial W+(DW)D]. \end{aligned} \tag{34}$$

Requiring Eq. (33) to be bi-Hamiltonian with respect to (34), namely, requiring

$$W_t=\mathcal{D}_1\frac{\delta H_{-1}}{\delta W}=\mathcal{D}_2\frac{\delta H_{-2}}{\delta W}, \tag{35}$$

determines the parameter to be $a=6$. The Hamiltonians in (35), in this case have the forms ($\mathrm{d}z=\mathrm{d}x\,\mathrm{d}\theta$ with $\int \mathrm{d}\theta=0$ and $\int \mathrm{d}\theta\,\theta=1$),

$$\begin{aligned} H_{-1}&=\int \mathrm{d}z\,2W(DW)^{-1/2},\\ H_{-2}&=\int \mathrm{d}z\,\tfrac{1}{8}[W_x(DW_x)(DW)^{-5/2}-15WW_xW_{xx}(DW)^{-7/2}], \end{aligned} \tag{36}$$

and the $N=1$ sHD equation assumes the simple form

$$W_t=D\partial^2(2(DW)^{-1/2}-3WW_x(DW)^{-5/2}). \tag{37}$$

It is worth noting here that this equation differs from the sHD-B equation (22) in the presence of the second term inside the parentheses on the right-hand side, which vanishes in the bosonic limit. [We would like to point out parenthetically that we do not generate the sHD-B equation in this approach because of our requirement that the equation be bi-Hamiltonian with respect to the structures in (34).]

It is easy to check that the Hamiltonian H_{-1} is a Casimir of $\mathcal{D}_2$ and the conserved charge

$$H_0=-\int \mathrm{d}z\,W \tag{38}$$

is a Casimir of $\mathcal{D}_1$. Furthermore, the Hamiltonian structure $\mathcal{D}_2$ can be written in the form

$$\mathcal{D}_2=\tfrac{1}{2}(DW)^{1/2}D(1+X)(DW)^{1/2}, \tag{39}$$

where

$$X\equiv\frac{3}{2}\left(D\frac{W}{(DW)}D^{-1}+D^{-1}\frac{W}{(DW)}D\right)D, \tag{40}$$

and therefore can be formally inverted. Thus, in this case also the associated recursion operator has a formal inverse.

It can be easily checked that the following charges

$$\begin{aligned} H_1&=\int \mathrm{d}z\,\frac{1}{4}(D^{-1}W)(D^{-2}W),\\ H_2&=\int \mathrm{d}z\,\frac{1}{2}(D^{-1}W)(D^{-2}W)(D^{-3}W), \end{aligned} \tag{41}$$

are conserved and reduce to (9) in the bosonic limit. From

$$W_t=\mathcal{D}_1\frac{\delta H_2}{\delta W}=\mathcal{D}_2\frac{\delta H_1}{\delta W}, \tag{42}$$

we obtain the $N=1$ supersymmetric HZ (sHZ) equation

$$W_t=-\tfrac{3}{2}W(D^{-1}W)-W_x(D^{-3}W)-\tfrac{1}{2}(DW)(D^{-2}W). \tag{43}$$

Both the sHD and the sHZ equations are bi-Hamiltonian systems and the infinite set of commuting conserved charges can be constructed recursively. As a result, they decribe supersymmetric integrable systems.

The second approach to finding a nontrivial $N=1$ supersymmetrization of the HD equation is to start with the Lax operator in (11) and generalize it to superspace. Let us start with the most general Lax operator involving non-negative powers of D,

$$L=a_0^2D^4+\alpha_1D^3+a_1D^2+\alpha_2D+a_2, \tag{44}$$

with the identification

$$a_0=(DW)^{-1/2}, \tag{45}$$

where italic coefficients are bosonic and Greek ones are fermionic. It is easy to verify that, in this case, there are only three projections, $(\,)_{\geqslant 0,1,3}$ (with respect to powers of D), that can lead to a consistent Lax equation. Using this ansatz, we have not yet been able to obtain the sHD equation (22) using fractional powers of the Lax operator (44). The Lax pair for this system, therefore, remains an open question.

On the other hand, when

$$\alpha_1=cW_x(DW)^{-2},\quad a_1=a_2=0=\alpha_2, \tag{46}$$

where c is an arbitrary parameter, the nonstandard Lax equation

$$\frac{\partial L}{\partial t}=[(L^{3/2})_{\geqslant 3},L], \tag{47}$$

yields consistent equations only for $c=0,-1,-\frac{1}{2}$. As we have pointed out in the preceding section, for the values of the parameter, $c=0,-1$, we have the sHD-B equation. The third choice of the parameter, therefore, leads to a new nontrivial $N=1$ supersymmetrization of the HD equation. Namely, with

$$L=(DW)^{-1}D^4-\tfrac{1}{2}W_x(DW)^{-2}D^3, \tag{48}$$

the Lax equation

$$\frac{\partial L}{\partial t}=[(L^{3/2})_{\geqslant 3},L], \tag{49}$$

leads to a second $N=1$ supersymmetrization of the HD equation of the form

$$\begin{aligned} W_t=&\tfrac{1}{16}[8D^5((DW)^{-1/2})-3D(W_{xx}W_x(DW)^{-5/2})\\ &+\tfrac{3}{4}(DW_x)^2W_x(DW)^{-7/2}-\tfrac{3}{4}D^{-1}((DW_x)^3(DW)^{-7/2})]. \end{aligned} \tag{50}$$

This is manifestly a nonlocal susy generalization in the variable W which, however, is a completely local equation in the variable (DW).

Since this system of equations has a Lax description, it is integrable and the conserved charges can be calculated in a standard manner and the first few charges take the following forms:

$$\begin{aligned} H_1=&\int \mathrm{d}z\, W_x(DW_x)(DW)^{-5/2},\\ H_2=&\int \mathrm{d}z\, W_x[16(DW_{xxx})(DW)^{-7/2}-84(DW_{xx})(DW_x)(DW)^{-9/2}\\ &+77(DW_x)^3(DW)^{-11/2}], \end{aligned} \tag{51}$$

and so on. However, we have not yet succeeded in finding a Hamiltonian structure which satisfies Jacobi identity (it is clear that the Hamiltonian structure is nonlocal, since the Hamiltonian is local).

V. THE $N=2$ SUPERSYMMETRIC HARRY DYM HIERARCHY

The most natural way to discuss the $N=2$ supersymmetric extension of the HD equation is in the $N=2$ superspace introduced earlier in (27)–(29). Looking at the bosonic superfield W in (29), we note that it has two bosonic components as well as two fermionic components. In the bosonic limit, when we set the fermions to zero, the $N=2$ equation would reduce to two bosonic equations. Since we have only the single HD equation (1) to start with, the construction of such a system is best carried out in the Lax formalism. This also brings out the interest in such extended supersymmetric systems, namely, they lead to new bosonic integrable systems in the bosonic limit.

As in (44), let us consider the most general $N=2$ Lax operator which contains differential operators in this superspace of the following form (taking a more general Lax involving only differential operators does not lead to equations which reduce to the HD equation):

$$\begin{aligned} L=&W^{-1}\partial^2+(D_1W^{-1})(\kappa_1D_1+\kappa_2D_2)\partial+(D_2W^{-1})(\kappa_3D_1+\kappa_4D_2)\partial\\ &+(\kappa_5(D_1D_2W)W^{-2}+\kappa_6(D_1W)(D_2W)W^{-3})D_1D_2, \end{aligned} \tag{52}$$

where $\kappa_i, i=1,2,\ldots,6$ are arbitrary constant parameters. The $N=2$ supersymmetry corresponds to an internal $O(2)$ invariance that rotates $\theta_1\to\theta_2,\theta_2\to-\theta_1$ and correspondingly $D_1\to D_2, D_2\to -D_1$ (thereby rotating the fermion components of the superfield into each other). This invariance, imposed on the Lax operator, identifies

$$\kappa_4=\kappa_1, \quad \kappa_3=-\kappa_2. \tag{53}$$

Using the computer algebra program REDUCE[14] and the special package SUSY2,[15] we are able to study systematically the hierarchy of equations following from the Lax equation

$$\frac{\partial L}{\partial t}=[(L^{3/2})_{\geqslant 2},L]. \tag{54}$$

Here, the projection [which is the highest consistent projection as is also the case with the bosonic HD equation in (12)] is understood as follows. Let us recall that a general pseudodifferential operator in $N=2$ superspace has the form

$$P=\sum_{n=-\infty}^{n=\infty}(P_0^n+P_1^nD_1+P_2^nD_2+P_3^nD_1D_2)\partial^n. \tag{55}$$

For such a pseudodifferential operator, the projection in (54) is defined as

$$P_{\geqslant 2}=P_3^0D_1D_2+(P_1^1D_1+P_2^1D_2+P_3^1D_1D_2)\partial+\sum_{n\geqslant 2}(P_0^n+P_1^nD_1+P_2^nD_2+P_3^nD_1D_2)\partial^n. \tag{56}$$

The consistency of the equation (54) leads to four possible solutions for the values of the arbitrary parameters

(1) $\kappa_1=\kappa_2=\kappa_5=\kappa_6=0$,
(2) $\kappa_2=0,\ \kappa_1=\kappa_5=-\kappa_6/2=1$,
(3) $\kappa_2=\kappa_5=\kappa_6=0,\ \kappa_1=\frac{1}{2}$,
(4) $\kappa_2=0,\ \kappa_1=\kappa_5=\frac{1}{2},\ \kappa_6=\frac{3}{4}$.

We will now discuss the various cases separately in some detail.

The first and the second cases can be discussed together since they lead to the same dynamical equation. Namely, in this case, the two Lax operators take the forms

$$\begin{aligned} L^{(1)}&=W^{-1}\partial^2,\\ L^{(2)}&=W^{-1}\partial^2+(D_1W^{-1})D_1\partial+(D_2W^{-1})D_2\partial-(D_1D_2W^{-1})D_1D_2\\ &=-D_1D_2W^{-1}D_1D_2. \end{aligned} \tag{57}$$

It can be checked that both these Lax operators lead to the same dynamical equation which is nothing other than the sHD-BB equations we have discussed earlier and, therefore, we do not study this any further.

For the third choice of parameters, the Lax operator can be written in the simple form

$$\begin{aligned} L^{(3)}&=W^{-1}\partial^2+\tfrac{1}{2}((D_1W^{-1})D_1+(D_2W^{-1})D_2)\partial\\ &=\tfrac{1}{2}(D_1W^{-1}D_1+D_2W^{-1}D_2)\partial. \end{aligned} \tag{58}$$

The Lax equation (54), in this case, leads to a nontrivial $N=2$ supersymmetric HD equation of the form

$$\begin{aligned} W_t=\tfrac{1}{64}[&2(W^{-1/2})_{xxx}-12(D_1W_{xx})(D_1W)W^{-5/2}-12(D_2W_{xx})(D_2W)W^{-5/2}\\ &+36(D_1W_x)(D_1W)W_xW^{-7/2}+36(D_2W_x)(D_2W)W_xW^{-7/2}\\ &+6(D_1W)(D_2W)(D_1D_2W_x)W^{-7/2}-9(D_1W)(D_2W)(D_1D_2W)W_xW^{-9/2}]. \end{aligned} \tag{59}$$

In the bosonic sector, where we set all the fermions to zero so that [see (29)]

$$W = w_0 + \theta_2\theta_1 w_1, \tag{60}$$

the equation (59) reduces to

$$\begin{aligned} w_{0,t} &= \tfrac{1}{2}(w_0^{-1/2})_{xxx}, \\ w_{1,t} &= \tfrac{1}{64}[-16w_{1,xxx}w_0^{-3/2} + 96w_{1,xx}w_{0,x}w_0^{-5/2} + 72w_{1,x}w_{0,xx}w_0^{-5/2} - 258w_{1,x}w_{0,x}^2w_0^{-7/2} \\ &\quad - 6w_{1,x}w_1^2w_0^{-7/2} + 9w_1^3w_{0,x}w_0^{-9/2} - 108w_1w_{0,xx}w_{0,x}w_0^{-9/2} + 219w_1w_{0,x}^3w_0^{-9/2}]. \end{aligned} \tag{61}$$

The first of the equations in (61) is, of course, the HD equation (1), but is decoupled from the second component. Consequently, even though this set of equations represents a new integrable system, it is not very interesting. Let us note that we can reduce the $N=2$ supersymmetry of this system to $N=1$ supersymmetry in the following way. Let us define

$$W(x,\theta_1,\theta_2) = U(x,\theta_1) + \theta_2 F(x,\theta_1), \tag{62}$$

and set the fermionic superfield $F(x,\theta_1)=0$. This would, therefore, make the superfield W independent of the Grassmann coordinate θ_2 leaving us with $N=1$ supersymmetry. Under such a reduction, it is straightforward to see that the Lax operator (58) and the equation (59) go over to the ones in (48) and (up to multiplicative factors) the corresponding equation (50) with the identification

$$\theta_1 = \theta, \quad U(x,\theta_1) = (DW(x,\theta)). \tag{63}$$

The conserved charges for this system can be obtained from the Lax operator $L^{(3)}$ in a standard manner, but we do not go into the details of this.

The fourth case is probably the most interesting of all. Here, the Lax operator takes the form

$$\begin{aligned} L^{(4)} &= W^{-1}\partial^2 + \tfrac{1}{2}((D_1W^{-1})D_1 + (D_2W^{-1})D_2)\partial - W^{-1/2}(D_1D_2W^{-1/2})D_1D_2 \\ &= -(W^{-1/2}D_1D_2)^2. \end{aligned} \tag{64}$$

Interestingly enough, this Lax operator possesses two nontrivial square roots, namely,

$$\begin{aligned} L_1^{1/2} &= iW^{-1/2}D_1D_2, \\ L_2^{1/2} &= W^{-1/2}\partial + \tfrac{1}{2}[(D_1W^{-1/2})D_1 + (D_2W^{-1/2})D_2 - (W^{-1/2})_x] + \cdots. \end{aligned} \tag{65}$$

We note here that a similar situation also arises in the study of the $N=2$ sKdV hierarchy[16] (for the case of the parameter $a=4$). In such a case, the general hierarchy of equations can be obtained from the Lax equation

$$\frac{\partial L}{\partial t_n} = [(L_1^{n/2}L_2^{1/2})_{\geqslant 2}, L], \tag{66}$$

where $n=0,1,2,\ldots$. For example, the first two flows of the hierarchy take the following forms:

$$\begin{aligned} W_{t_1} &= \tfrac{1}{8}[-4(D_1D_2W_x)W^{-1} + 6(D_1D_2W)W_xW^2 + 6((D_1W)(D_2W_x) - 6(D_2W)(D_1W_x))W^{-2} \\ &\quad - 15(D_1W)(D_2W)W_xW^{-3}], \end{aligned} \tag{67}$$

$$
\begin{aligned}
W_{t_2} = \tfrac{1}{16}[&8(W^{-1/2})_{xxx} - 6(D_1D_2W)(D_1D_2W_x)W^{-5/2} \\
&+ 9(D_1D_2W)^2W_xW^{-7/2} + 3((D_1W)(D_1W_{xx}) + (D_2W)(D_2W_{xx}))W^{-5/2} \\
&- 9((D_1W)(D_1W_x) + (D_2W)(D_2W_x))W_xW^{-7/2} + 9((D_1W)(D_2W)(D_1D_2W))_xW^{-7/2} \\
&- 36(D_1W)(D_2W)(D_1D_2W)W_xW^{-9/2}] .
\end{aligned}
$$

In the bosonic sector, the second equation in (67) gives

$$
\begin{aligned}
w_{0,t_2} &= \tfrac{1}{16}[8(w_0^{-1/2})_{xxx} - 6w_{1,x}w_1w_0^{-5/2} + 9w_1^2w_{0,x}w_0^{-7/2}], \\
w_{1,t_2} &= \tfrac{1}{32}[-8w_{1,xxx}w_0^{-3/2} + 48(w_{1,x}w_{0,x})_xw_0^{-5/2} - 144w_{1,x}w_{0,x}^2w_0^{-7/2} - 6w_{1,x}w_1^2w_0^{-7/2} \\
&\quad + 9w_1^3w_{0,x}w_0^{-9/2} + 12w_1w_{0,xxx}w_0^{-5/2} - 126w_1w_{0,xx}w_{0,x}w_0^{-7/2} + 177w_{0,x}^3w_1w_0^{-9/2}].
\end{aligned}
\tag{68}
$$

This is a new bosonic system of coupled equations, which reduces on setting $w_1 = 0$ to the HD equation and is integrable.

The conserved charges for this last case of $N=2$ supersymmetrization can be constructed as follows:

$$
\begin{aligned}
H_1 &= \int \mathrm{dz}\ \ \mathrm{sRes}\, L_2^{1/2} = \int \mathrm{dz}\,(D_1W)(D_2W)W^{-5/2}, \\
H_2 &= \int \mathrm{dz}\ \mathrm{sRes}(L_1^{1/2}L_2^{1/2}) \\
&= \int \mathrm{dz}[3(D_1D_2W)^2W^{-3} + 3W_x^2W^{-2} + 2((D_1W)(D_1W_x) \\
&\quad + (D_2W)(D_2W_x))W^{-3} + (D_1W)(D_2W)(D_1D_2W)W^{-4}], \\
H_3 &= \int \mathrm{dz}\ \mathrm{sRes}\, L_2^{3/2} = \int \mathrm{dz}[128(D_1D_2W_x)W_xW^{-7/2} - 40(D_1D_2W)^3W^{-9/2} + \cdots],
\end{aligned}
\tag{69}
$$

where $\mathrm{dz} = \mathrm{d}x\,\mathrm{d}\theta_1\,\mathrm{d}\theta_2$ and "sRes" is defined as the coefficient of the $D_1D_2\partial^{-1}$ term in the pseudodifferential operator. We can also perform the $N=1$ reduction of this system. Requiring that the superfield W has no dependence on θ_2, it is clear from the form of the Lax operator in (64) that it reduces to the one involving the second $N=1$ supersymmetrization (just as $L^{(3)}$ does).

VI. CONCLUSIONS

In this paper, we have studied the question of supersymmetrization of the Harry Dym hierarchy systematically. We have used the simpler B supersymmetrization to derive the sHD-B and sHD-BB systems. The analysis of the nontrivial $N=1$ supersymmetrization leads to two such integrable systems. One has a natural bi-Hamiltonian description for which we have not been able to find the Lax description. On the other hand, the second has a natural Lax description for which we have not yet found a Hamiltonian structure that satisfies the Jacobi identity. Both these systems are integrable. The $N=2$ supersymmetrization from the Lax approach yields four possible Lax operators. Two of these describe the sHD-BB system while the other two give nontrivial $N=2$ supersymmetric extensions. In the bosonic limit, one of them leads to the HD equation decoupled from the second component while the other genuinely gives a coupled two component system of equations that is integrable.

ACKNOWLEDGMENTS

One of the authors (Z.P.) thanks the high energy theory group at the University of Rochester for hospitality where this work was done. This work was supported in part by US DOE Grant No. DE-FG-02-91ER40685 as well as by NSF-INT-0089589.

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Positive operator valued measures covariant with respect to an irreducible representation

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(Received 11 February 2003; accepted 18 April 2003)

Given an irreducible representation of a group G, we show that all the covariant positive operator valued measures based on G/Z, where Z is a central subgroup, are described by trace class, trace one positive operators. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598277]

I. INTRODUCTION

Usually, the observables in quantum mechanics are represented by self-adjoint operators that are in one-to-one correspondence with projection valued operator measures. However, in many applications (as, for example, quantum optics, quantum theory of measurement, quantization of classical dynamical systems, and localization observables of relativistic massless particles) this characterization is restrictive and one has to consider a more general description by means of positive operator valued measures (for a review of the applications in physics, see Refs. 3, 6, and 9–11).

In particular, it is of interest both in quantum mechanics and in signal analysis to describe positive operator valued measures that are covariant with respect to a unitary representation of a *symmetry* group G (for a review see Ref. 1 and references therein). In this framework, it is well known[4,13] that, given a square-integrable irreducible representation π of a unimodular group G and a trace class, trace one positive operator T, the family of operators

$$Q(X)=\int_X \pi(g)T\pi(g^{-1})d\mu_G(g)$$

defines a positive operator valued measure (POVM) on G covariant with respect to π (μ_G is a Haar measure on G). In this article, we prove that all the covariant POVMs are of the above form for some T. More precisely, we show this result for non-unimodular groups and for POVMs based on the quotient space G/Z, where Z is a central subgroup.

Let G be a locally compact second countable topological group and Z be a central closed subgroup. We denote by G/Z the quotient group and by $\dot{g}\in G/Z$ the equivalence class of $g\in G$. If $a\in G$ and $\dot{g}\in G/Z$, we let $a[\dot{g}]=\dot{a}\dot{g}$ be the natural action of a on the point $\dot{g}$.

Let $\mathcal{B}(G/Z)$ be the Borel σ-algebra of G/Z. We fix a left Haar measure $\mu_{G/Z}$ on G/Z. Moreover, we denote by Δ the modular function of G and of G/Z.

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By *representation* we mean a strongly continuous unitary representation of G acting on a complex and separable Hilbert space, with scalar product $\langle \cdot,\cdot \rangle$ linear in the first argument.

Let $(\pi,\mathcal{H})$ be a representation of G. A positive operator valued measure Q defined on G/Z and such that

(1) $Q(G/Z)=I$;

(2) for all $X \in \mathcal{B}(G/Z)$,

$$\pi(g)Q(X)\pi(g^{-1})=Q(g[X]) \quad \forall g \in G$$

is called π-*covariant* POVM on G/Z.

Given a representation $(\sigma,\mathcal{K})$ of Z, we denote by $(\lambda^{\sigma},P^{\sigma},\mathcal{H}^{\sigma})$ the imprimitivity system unitarily induced by σ. We recall that $\mathcal{H}^{\sigma}$ is the Hilbert space of (μ_G-equivalence classes of) functions $f:G\to\mathcal{K}$ such that

(1) f is weakly measurable;

(2) for all $z \in Z$,

$$f(gz)=\sigma(z^{-1})f(g) \quad \forall g \in G;$$

(3)

$$\int_{G/Z} \|f(g)\|^2_{\mathcal{K}} \, \mathrm{d}\mu_{G/Z}(\dot{g}) < +\infty$$

with scalar product

$$\langle f_1,f_2 \rangle_{\mathcal{H}^{\sigma}} = \int_{G/Z} \langle f_1(g),f_2(g) \rangle_{\mathcal{K}} \mathrm{d}\mu_{G/Z}(\dot{g}).$$

The representation λ^{σ} acts on $\mathcal{H}^{\sigma}$ as

$$(\lambda^{\sigma}(a)f)(g) := f(a^{-1}g), \quad g \in G,$$

for all $a \in G$. The projection valued measure P^{σ} is given by

$$(P^{\sigma}(X)f)(g) := \chi_X(\dot{g})f(g), \quad g \in G,$$

for all $X \in \mathcal{B}(G/Z)$, where χ_X is the characteristic function of the set X.

We recall some basic properties of square integrable representations modulo a central subgroup. We refer to Ref. 2 for G unimodular and Z arbitrary and to Ref. 7 for G non-unimodular and $Z=\{e\}$. Combining these proofs, one obtains the following result.

Proposition 1: Let $(\pi,\mathcal{H})$ be an irreducible representation of G and γ be the character of Z such that

$$\pi(z)=\gamma(z)I_{\mathcal{H}} \quad \forall z \in Z.$$

The following facts are equivalent:

(1) there exists a vector $u \in \mathcal{H}$ such that

$$0 < \int_{G/Z} |\langle u,\pi(g)u \rangle_{\mathcal{H}}|^2 \mathrm{d}\mu_{G/Z}(\dot{g}) < +\infty; \tag{1}$$

(2) $(\pi,\mathcal{H})$ is a subrepresentation of $(\lambda^{\gamma},\mathcal{H}^{\gamma})$.

If either of the above conditions is satisfied, there exists a self-adjoint injective positive operator C such that

$$\pi(g)C=\Delta(g)^{-1/2}C\pi(g) \quad \forall g \in G,$$

and an isometry $\Sigma:\mathcal{H}\otimes\mathcal{H}^*\to\mathcal{H}^\gamma$ *such that*

(1) for all $u\in\mathcal{H}$ *and* $v\in\mathrm{dom}\ C$

$$\Sigma(u\otimes v^*)(g)=\langle u,\pi(g)Cv\rangle_{\mathcal{H}},\quad g\in G;$$

(2) for all $g\in G$

$$\Sigma(\pi(g)\otimes I_{\mathcal{H}^*})=\lambda(g)\Sigma;$$

(3) the range of Σ *is the isotypic space of* π *in* $\mathcal{H}^\gamma$.

If Eq. (1) is satisfied, $(\pi,\mathcal{H})$ is called *square-integrable modulo Z*. The square of C is called *formal degree* of π (see Ref. 7). In particular, when G is unimodular, C is a multiple of the identity.

II. CHARACTERIZATION OF *Q*

We fix an irreducible representation $(\pi,\mathcal{H})$ of G and let γ be the character such that $\pi|_Z=\gamma I_{\mathcal{H}}$. The following theorem characterizes all the POVM on G/Z covariant with respect to π in terms of positive trace one operators on $\mathcal{H}$.

Theorem 2: *The irreducible representation* π *admits a covariant POVM based on* G/Z *if and only if* π *is square-integrable modulo* Z.

In this case, let C *be the square root of the formal degree of* π. *There exists a one-to-one correspondence between covariant POVMs* Q *on* G/Z *and positive trace one operators* T *on* $\mathcal{H}$ *given by*

$$\langle Q_T(X)v,u\rangle_{\mathcal{H}}=\int_X\langle TC\pi(g^{-1})v,C\pi(g^{-1})u\rangle_{\mathcal{H}}d\mu_{G/Z}(\dot g)\tag{2}$$

for all $u,v\in\mathrm{dom}\ C$ *and* $X\in\mathcal{B}(G/Z)$.

Proof: Let Q be a π-covariant POVM. According to the generalized imprimitivity theorem[5] there exists a representation $(\sigma,\mathcal{K})$ of Z and an isometry $W:\mathcal{H}\to\mathcal{H}^\sigma$ intertwining π with λ^σ such that

$$Q(X)=W^*P^\sigma(X)W$$

for all $X\in\mathcal{B}(G/Z)$.

Define the following closed invariant subspace of $\mathcal{K}$

$$\mathcal{K}_\gamma=\{v\in\mathcal{K}|\sigma(z)v=\gamma(z)v\}.$$

Let σ_1 and σ_2 be the restrictions of σ to $\mathcal{K}_\gamma$ and $\mathcal{K}_\gamma^\perp$, respectively. The induced imprimitivity system $(\lambda^\sigma,P^\sigma,\mathcal{H}^\sigma)$ decomposes into the orthogonal sum

$$\mathcal{H}^\sigma=\mathcal{H}^{\sigma_1}\oplus\mathcal{H}^{\sigma_2}.$$

If $f\in\mathcal{H}^\sigma$ and $z\in Z$, then

$$(\lambda^\sigma(z)f)(g)=f(z^{-1}g)=f(gz^{-1})=\sigma(z)f(g),\quad g\in G.$$

On the other hand, if $u\in\mathcal{H}$ and $z\in Z$, we have

$$(\lambda^\sigma(z)Wu)(g)=(W\pi(z)u)(g)=\gamma(z)(Wu)(g),\quad g\in G.$$

It follows that $(Wu)(g)\in\mathcal{K}_\gamma$ for μ_G—almost every $g\in G$, that is, $Wu\in\mathcal{H}^{\sigma_1}$. So it is not restrictive to assume that

$$\sigma = \gamma I_{\mathcal{K}}$$

for some Hilbert space $\mathcal{K}$. Clearly, we have

$$\mathcal{H}^{\sigma} = \mathcal{H}^{\gamma} \otimes \mathcal{K}, \quad \lambda^{\sigma} = \lambda^{\gamma} \otimes I_{\mathcal{K}}.$$

In particular, π is a subrepresentation of λ^{γ}, hence it is square-integrable modulo Z.

Due to Proposition 1, the operator $W' = (\Sigma^* \otimes I_{\mathcal{K}})W$ is an isometry from $\mathcal{H}$ to $\mathcal{H} \otimes \mathcal{H}^* \otimes \mathcal{K}$ such that

$$W'\pi(g) = (\pi(g) \otimes I_{\mathcal{H}^* \otimes \mathcal{K}})W' \quad \forall g \in G.$$

Since π is irreducible, given Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, a standard result asserts that $\mathcal{C}(\pi \otimes I_{\mathcal{H}_1}, \pi \otimes I_{\mathcal{H}_2}) = I_{\mathcal{H}} \otimes \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. In the present case, this means that

$$W'u = u \otimes B \quad \forall u \in \mathcal{H}$$

for some $B \in \mathcal{H}^* \otimes \mathcal{K}$. Since W' is isometric, B has Hilbert–Schmidt norm 1.

Let $(e_i)_{i \geqslant 1}$ be an orthonormal basis of $\mathcal{H}$ such that $e_i \in \operatorname{dom} C$. Then

$$B = \sum_i e_i^* \otimes k_i,$$

where $k_i \in \mathcal{K}$ and $\Sigma_i \|k_i\|_{\mathcal{K}}^2 = 1$.

If $u \in \operatorname{dom} C$, one has that

$$\begin{aligned}(Wu)(g) &= [(\Sigma \otimes I_{\mathcal{K}})(u \otimes B)](g) \\ &= \sum_i \Sigma(u \otimes e_i^*)(g) \otimes k_i \\ &= \sum_i \langle u, \pi(g) C e_i \rangle_{\mathcal{H}} \otimes k_i \\ &= \sum_i \langle C\pi(g^{-1})u, e_i \rangle_{\mathcal{H}} \otimes k_i \\ &= \sum_i (e_i^* \otimes k_i)(C\pi(g^{-1})u),\end{aligned}$$

where the series converges in $\mathcal{H}^{\sigma}$. On the other hand, for all $g \in G$ the series $\Sigma_i (e_i^* \otimes k_i) \times (C\pi(g^{-1})u)$ converges to $BC\pi(g^{-1})u$, where we identify $\mathcal{H}^* \otimes \mathcal{K}$ with the space of Hilbert–Schmidt operators. By uniqueness of the limit,

$$(Wu)(g) = BC\pi(g^{-1})u, \quad g \in G.$$

If $u, v \in \operatorname{dom} C$, the corresponding covariant POVM is given by

$$\begin{aligned}\langle Q(X)v, u \rangle_{\mathcal{H}} &= \langle P^{\sigma}(X)Wv, Wu \rangle_{\mathcal{H}^{\sigma}} \\ &= \int_{G/Z} \chi_X(\dot{g}) \langle BC\pi(g^{-1})v, BC\pi(g^{-1})u \rangle_{\mathcal{H}} \mathrm{d}\mu_{G/Z}(\dot{g}) \\ &= \int_X \langle TC\pi(g^{-1})v, C\pi(g^{-1})u \rangle_{\mathcal{H}} \mathrm{d}\mu_{G/Z}(\dot{g}),\end{aligned}$$

where

$$T := B^* B$$

is a positive trace class trace one operator on $\mathcal{H}$.

Conversely, assume that π is square integrable and let T be a positive trace class trace one operator on $\mathcal{H}$. Then

$$B := \sqrt{T}$$

is a (positive) operator belonging to $\mathcal{H}^* \otimes \mathcal{H}$ such that $B^* B = T$ and $\|B\|_{\mathcal{H}^* \otimes \mathcal{H}} = 1$. The operator W defined by

$$Wv := (\Sigma \otimes I_{\mathcal{H}})(v \otimes B) \quad \forall v \in \mathcal{H}$$

is an isometry intertwining $(\pi, \mathcal{H})$ with the representation $(\lambda^\sigma, \mathcal{H}^\sigma)$, where

$$\sigma = \gamma I_{\mathcal{H}}.$$

Define Q_T by

$$Q_T(X) = W^* P^\sigma(X) W, \quad X \in \mathcal{B}(G/Z).$$

With the same computation as above, one has that

$$\langle Q_T(X)u, v\rangle_{\mathcal{H}} = \int_X \langle TC\pi(g^{-1})u, C\pi(g^{-1})v\rangle_{\mathcal{H}} \mathrm{d}\mu_{G/Z}(\dot{g})$$

for all $u, v \in \mathrm{dom}\ C$.

Finally, we show that the correspondence $T \mapsto Q_T$ is injective. Let T_1 and T_2 be positive trace one operators on $\mathcal{H}$, with $Q_{T_1} = Q_{T_2}$. Set $T = T_1 - T_2$. Since π is strongly continuous, for all $u, v \in \mathrm{dom}\ C$ the map

$$G/Z \ni \dot{g} \mapsto \langle TC\pi(g^{-1})v, C\pi(g^{-1})u\rangle_{\mathcal{H}} = \Delta(\dot{g})^{-1} \langle T\pi(g^{-1})Cv, \pi(g^{-1})Cu\rangle_{\mathcal{H}} \in \mathbb{C}$$

is continuous. Since

$$\int_X \langle TC\pi(g^{-1})v, C\pi(g^{-1})u\rangle_{\mathcal{H}} \mathrm{d}\mu_{G/Z}(\dot{g}) = \langle [Q_{T_1}(X) - Q_{T_2}(X)]v, u\rangle_{\mathcal{H}} = 0$$

for all $X \in \mathcal{B}(G/Z)$, we have

$$\langle TC\pi(g^{-1})v, C\pi(g^{-1})u\rangle_{\mathcal{H}} = 0 \quad \forall \dot{g} \in G/Z.$$

In particular,

$$\langle TCv, Cu\rangle_{\mathcal{H}} = 0,$$

so that, since C has dense range, $T = 0$. ■

Remark 3: Scutaru shows in Ref. 13 that there exists a one-to-one correspondence between positive trace one operators on $\mathcal{H}$ and covariant POVMs Q based on G/Z with the property

$$\mathrm{tr} Q(K) < +\infty \tag{3}$$

for all compact sets $K \subset G/Z$. Theorem 2 shows that every covariant POVM Q based on G/Z shares property (3).

Remark 4: If G is unimodular, then $C=\lambda I$, with $\lambda>0$, and one can normalize $\mu_{G/Z}$ so that $\lambda=1$. *Hence,*

$$Q_T(X)=\int_X \pi(g)T\pi(g^{-1})\mathrm{d}\mu_{G/Z}(\dot{g}) \quad \forall X\in\mathcal{B}(G/Z),$$

the integral being understood in the weak sense.

Remark 5: If $T=\eta^*\otimes\eta$, with $\eta\in\mathrm{dom}\ C$ and $\|\eta\|_{\mathcal{H}}=1$, we observe that

$$\begin{aligned}\langle Q_T(X)v,u\rangle_{\mathcal{H}}&=\int_X\langle C\pi(g^{-1})v,\eta\rangle_{\mathcal{H}}\langle\eta,C\pi(g^{-1})u\rangle_{\mathcal{H}}d\mu_{G/Z}(\dot{g})\\&=\int_X\langle v,\pi(g)C\eta\rangle_{\mathcal{H}}\langle\pi(g)C\eta,u\rangle_{\mathcal{H}}d\mu_{G/Z}(\dot{g})\\&=\int_X(W_{C\eta}v)(g)\overline{(W_{C\eta}u)(g)}d\mu_{G/Z}(\dot{g})\end{aligned}$$

for all $u,v\in\mathrm{dom}\ C$, where $W_{C\eta}:\mathcal{H}\to\mathcal{H}^\gamma$ is the wavelet operator associated to the vector $C\eta$. In particular,

$$Q_T(X)=W_{C\eta}^*P^\gamma(X)W_{C\eta}.$$

III. TWO EXAMPLES

A. The Heisenberg group

In quantum mechanics, the study of positive operator valued measures covariant with respect to suitable representations of the Heisenberg group is motivated by two problems. They appear as a natural tool in the construction of coherent states associated with the quantum harmonic oscillator (see, for example, Ref. 1). Moreover, they describe the possible localization observables on the phase space of a one dimensional classical particle (for an account, see Ref. 12).

The Heisenberg group H is $\mathbb{R}^3$ with composition law

$$(p,q,t)(p',q',t')=\left(p+p',q+q',t+t'+\frac{pq'-qp'}{2}\right).$$

The center of H is

$$Z=\{(0,0,t)|t\in\mathbb{R}\},$$

and the quotient group G/Z is isomorphic to the Abelian group $\mathbb{R}^2$, with projection

$$q(p,q,t)=(p,q).$$

The Heisenberg group is unimodular with Haar measure

$$\mathrm{d}\mu_{G/Z}(p,q)=\frac{1}{2\pi}\mathrm{d}p\mathrm{d}q.$$

Given an infinite dimensional Hilbert space $\mathcal{H}$ and an orthonormal basis $(e_n)_{n\geqslant 1}$, let a, a^* be the corresponding ladder operators. Define

$$Q = \text{closure of } \frac{1}{\sqrt{2}}(a + a^*),$$

$$P = \text{closure of } \frac{1}{\sqrt{2}i}(a - a^*),$$

It is known[4,8] that the representation

$$\pi(p,q,t) = e^{i(t + pQ + qP)}$$

is square-integrable modulo Z and $C = 1$.

It follows from Theorem 2 that *any* π-covariant POVM Q based on $\mathbb{R}^2$ is of the form

$$Q(X) = \frac{1}{2\pi} \int_X e^{i(pQ+qP)} T e^{-i(pQ+qP)} \mathrm{d}p\, \mathrm{d}q, \quad X \in \mathcal{B}(\mathbb{R}^2),$$

for some positive trace one operator on $\mathcal{H}$. Up to our knowledge, the complete classification of the POVMs on $\mathbb{R}^2$ covariant with respect to the Heisenberg group has been an open problem till now.

B. The $ax+b$ group

The $ax+b$ group is the semidirect product $G = \mathbb{R} \times' \mathbb{R}_+$, where we regard $\mathbb{R}$ as additive group and $\mathbb{R}_+$ as multiplicative group. The composition law is

$$(b,a)(b',a') = (b + ab', aa').$$

The group G is nonunimodular with left Haar measure

$$\mathrm{d}\mu_G(b,a) = a^{-2} \mathrm{d}b\, \mathrm{d}a$$

and modular function

$$\Delta(b,a) = \frac{1}{a}.$$

Let $\mathcal{H} = L^2((0,+\infty), \mathrm{d}x)$ and $(\pi^+, \mathcal{H})$ be the representation of G given by

$$[\pi^+(b,a)f](x) = a^{1/2} e^{2\pi i b x} f(ax), \quad x \in (0,+\infty).$$

It is known[8] that π is square-integrable, and the square root of its formal degree is

$$(Cf)(x) = \Delta(0,x)^{1/2} f(x) = x^{-1/2} f(x), \quad x \in (0,+\infty),$$

acting on its natural domain.

By means of Theorem 2 every POVM based on G and covariant with respect to π^+ is described by a positive trace one operator T according to Eq. (2). Explicitly, let $(e_i)_{i \geqslant 1}$ be an orthonormal basis of eigenvectors of T and $\lambda_i \geqslant 0$ be the corresponding eigenvalues. If $u \in L^2((0,+\infty), \mathrm{d}x)$ is such that $x^{-1/2} u \in L^2((0,+\infty), \mathrm{d}x)$, the π^+-covariant POVM corresponding to T is given by

$$\langle Q_T(X)u,u\rangle_{\mathcal{H}} = \int_X \langle TC\pi^+(g^{-1})u, C\pi^+(g^{-1})u\rangle_{\mathcal{H}} \mathrm{d}\mu_G(g)$$

$$= \int_X \sum_i \lambda_i |\langle C\pi^+(g^{-1})u, e_i\rangle_{\mathcal{H}}|^2 \mathrm{d}\mu_G(g)$$

$$= \sum_i \lambda_i \int_X \left| \int_{\mathbb{R}_+} x^{-1/2} a^{-1/2} e^{-2\pi i b x/a} u\left(\frac{x}{a}\right) \overline{e_i(x)} \mathrm{d}x \right|^2 a^{-2} \mathrm{d}b\,\mathrm{d}a.$$

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Renormalization for the Harper equation for quadratic irrationals

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(Received 29 May 2002; accepted 22 June 2003)

In this paper, we use renormalization methods to study self-similarity in the fluctuations η_i of the Harper equation in the strong-coupling limit for quadratic irrationals of the form $(\sqrt{a^2+4}-a)/2$ for $a\in\mathbb{N}$. Using the decimation method, we obtain a second-order functional recurrence which we prove rigorously has an entire fixed point. This fixed point governs the scaling of the fluctuations η_i in the strong-coupling limit. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1605819]

I. INTRODUCTION

The Harper equation (also known as the almost Mathieu equation),

$$\psi_{i+1}+\psi_{i-1}+2\lambda\cos(2\pi(i\omega+\phi))\psi_i=E\psi_i, \tag{1.1}$$

is an important quantum mechanical model that has been studied extensively in the literature. (For a review we refer the reader to Refs. 10 and 9.) In Eq. (1.1) E is the eigenvalue corresponding to the eigenfunction ψ_i defined on the one-dimensional integer lattice indexed by $i\in\mathbb{Z}$. For $\lambda>1$, Eq. (1.1) has exponentially decaying eigenfunctions ψ_i so that we write $\psi_i=e^{-\gamma|i|}\eta_i$, where $\gamma=\log\lambda$ (the Lyapunov exponent) (see Ref. 1), and η_i is the fluctuation at site i. In terms of η_i, the Harper equation becomes, for $i>0$,

$$\lambda^{-1}\eta_{i+1}+\lambda\eta_{i-1}+2\lambda\cos(2\pi(i\omega+\phi))\eta_i=E\eta_i. \tag{1.2}$$

In this paper we use renormalization methods to study self-similarity in the fluctuations η_i in the strong-coupling limit $\lambda\to\infty$, $E\sim 2\lambda$, for the case of $\omega=(\sqrt{a^2+4}-a)/2$, $a\in\mathbb{N}$, with the phase $\phi=0$. This follows from the work of Ketoja and Satija[3] in which the golden mean case, $\omega=(\sqrt{5}-1)/2)$, is analyzed heuristically. Rigorous results in that case were obtained by Mestel, Osbaldestin, and Winn.[4] General Farey paths were considered by Ketoja and Satija in Ref. 2, although we have not followed this approach here.

Using the so-called *decimation* method of Ketoja and Satija,[2,3] we shall show that the self-similarity in the η_i is determined by a so-called *strong coupling fixed point* of the renormalization operator associated with the recursion

$$t_n(x)=\prod_{i=0}^{a-1} t_{n-1}(-\omega x-i)t_{n-2}(\omega^2 x+a\omega). \tag{1.3}$$

In this paper we shall prove the existence of a fixed point of this recursion and thereby establish the theory on a firm basis. Specifically, we shall prove the following theorem.

Theorem 1: *Let $a\in\mathbb{N}$ and let $\omega=(\sqrt{a^2+4}-a)/2$. Then for each $k\in\mathbb{N}$, there exists a unique, entire function t such that*

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$$t(x)=\left(\prod_{i=0}^{a-1} t(-\omega x-i)\right) t(\omega^2 x+a\omega), \tag{1.4}$$

having a zero of order k at $x=1$ *and satisfying* $t(x)>0$ *on* $(-\omega-(a-1),1)$. *For each k we have* $t(x)=t_*(x)^k$, *where* t_* *is the function corresponding to the case* $k=1$.

The outline of this paper is as follows. In Sec. II we give a brief review of the number-theoretic results, followed by a heuristic derivation of the recurrence (1.3) using the decimation methods of Ketoja and Satija.[2,3] In subsequent sections we give the proof of Theorem 1. The method of proof is an improvement on the techniques employed in Ref. 4.

II. DERIVATION OF THE RENORMALIZATION EQUATIONS

In this section we give a heuristic derivation of the renormalization functional recurrence, based on the decimation method of Ketoja and Satija.

Let us briefly recall some elementary number-theoretic results on which the decimation method is based (see Ref. 8 for further details). Let $a\in\mathbb{N}$ be fixed and let $\omega\in(0,1)$ have continued fraction expansion $[0;a,a,\ldots]$. Then $\omega=(-a+\sqrt{a^2+4})/2$ and satisfies the quadratic equation

$$\omega^2+a\omega=1. \tag{2.1}$$

For these quadratic irrationals the rational convergents p_n/q_n satisfy $p_n=q_{n-1}=G_n$ where $G_{n+1}=aG_n+G_{n-1}$, $G_0=0$, $G_1=1$. An important relation is the following:

$$G_n\omega-G_{n-1}=-(-\omega)^n. \tag{2.2}$$

We now consider (1.2) in the strong-coupling limit $\lambda\to\infty$, at the band edge $E=2\lambda$. Setting $E=2\lambda$, dividing Eq. (1.2) by λ, and letting $\lambda\to\infty$ gives

$$\eta_{i-1}+2(\cos(2\pi(i\omega+\phi))-1)\eta_i=0. \tag{2.3}$$

Following Ketoja and Satija,[3] we define a so-called *decimation* as follows:

$$\eta_{i+G_n}=\hat{t}_n(i)\eta_i. \tag{2.4}$$

Note that this decimation differs from that in Ref. 3, since the coefficient of $\eta_{i+G_{n+1}}$ has been set to zero and we have changed the sign of $\hat{t}_n$. Consequently, (2.4) is only valid in the strong-coupling limit $\lambda\to\infty$.

A general recurrence for t_n may be obtained as follows. Evaluating (2.4) with i set equal to i, $i+G_n$, $i+2G_n,\ldots,i+(a-1)G_n$, gives

$$\eta_{i+G_n}=\hat{t}_n(i)\eta_i$$

$$\eta_{i+2G_n}=\hat{t}_n(i+G_n)\eta_{i+G_n}$$

$$\vdots$$

$$\eta_{i+aG_n}=\hat{t}_n(i+(a-1)G_n)\eta_{i+(a-1)G_n}.$$

Second, evaluating (2.4) at $n-1$ with i set equal to $i+aG_n$ gives

$$\eta_{i+G_{n-1}+aG_n}=\hat{t}_{n-1}(i+aG_n)\eta_{i+aG_n}.$$

Eliminating $\eta_{i+G_n},\ldots,\eta_{i+aG_n}$ between these equations, and using the recurrence for the G_n, we obtain $\eta_{i+G_{n+1}}=\hat{t}_{n+1}(i)\eta_i$, where

$$\hat{t}_{n+1}(i)=\left(\prod_{j=0}^{a-1}\hat{t}_n(i+jG_n)\right)\hat{t}_{n-1}(i+aG_n).$$

We now set the phase $\phi=0$. Evaluating (2.4) at $n=0$ and $n=1$, we obtain $\eta_i=\hat{t}_0(i)\,\eta_i$, $\eta_{i+1}=\hat{t}_1(i)\,\eta_i$, which, on comparing with (2.3) at $i+1$, with $\phi=0$, gives

$$\hat{t}_0(i)=1,\quad \hat{t}_1(i)=\frac{1}{2(1-\cos(2\pi(i+1)\omega))}.$$

Following Ref. 3 we now transform from the discrete variable i to a continuous variable x. We write $x=(-\omega)^{-n}\{i\omega\}$ where $\{\cdot\}$ denotes the fractional part. This transformation must be done carefully since the definition of x depends on the index n of the function. We now write $t_n(x)=\hat{t}_n(i)$, where t_n is a real function of a real variable of period ω^{-n}. Then, we have, for $n>1$,

$$\begin{aligned}
t_{n+1}(x)&=t_{n+1}((-\omega)^{-(n+1)}\{i\omega\})\\
&=\hat{t}_{n+1}(i)\\
&=\left(\prod_{j=0}^{a-1}\hat{t}_n(i+jG_n)\right)\hat{t}_{n-1}(i+aG_n)\\
&=\left(\prod_{j=0}^{a-1}t_n((-\omega)^{-n}\{(i+jG_n)\omega\})\right)t_{n-1}((-\omega)^{-(n-1)}\{(i+aG_n)\omega\})\\
&=\left(\prod_{j=0}^{a-1}t_n((-\omega(-\omega)^{-(n+1)}\{i\omega+j(-(-\omega)^n)\}))\right.\\
&\quad\left.\times t_{n-1}(\omega^2(-\omega)^{-(n+1)}\{(i\omega+a(-(-\omega)^n))\})\right.\\
&=\left(\prod_{j=0}^{a-1}t_n(-\omega x-j)\right)t_{n-1}(\omega^2x+a\omega),
\end{aligned}$$

as required. [In deriving this equation we have implicitly used the periodicity of the function t_n and (2.2).] The initial conditions are now

$$t_0(x)=1,\quad t_1(x)=\frac{1}{2(1-\cos(2\pi(-\omega x+\omega)))},\tag{2.5}$$

since, using $\{i\omega\}=-\omega x$ (for $n=1$) and the periodicity of the cosine function, we have $t_1(x)=t_1((-\omega)^{-1}\{i\omega\})=\hat{t}_1(i)=1/(2(1-\cos(2\pi(i+1)\omega)))=1/(2((1-\cos(2\pi(-\omega x+\omega)))))$. Of particular interest is the singularity/zero structure of these initial conditions. We note that on the interval $[-\omega-(a-1),1]$, the function t_1 has poles of order 2 at the end points $-\omega-(a-1)$ and 1, but no other zeros or singularities. From the recurrence (1.3), we see that $t_2(x)$ has a pole of order 2 at 1, but no other singularities or zeros on the interval $[-\omega-(a-1),1]$. It will then follow that for all $n\geqslant 3$, $t_n(x)$ has a pole of order 2 at 1, but no other zeros or singularities on this interval.

From numerical simulation of the recurrence (1.3), it appears that, starting from the initial conditions (2.5), $t_n(x)$ converges to a solution $t(x)$ of (1.4), with $t(x)$ having a pole of order 2 at 1, and no other singularities or zeros on $[-\omega-(a-1),1]$.

In this paper we prove the existence of this fixed point. It is given by $t(x)=t_*(x)^{-2}$, where t_* is the function given in Theorem 1.

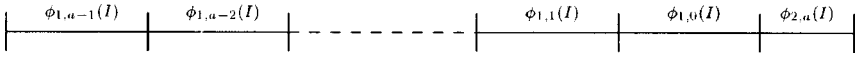

FIG. 1. Diagram to show location of intervals.

III. ITERATED FUNCTION SYSTEM

The analysis of the recurrence (1.3) is based on the iterated function system given by the scaling functions on the right-hand side of (1.3). In this section we define the iterated function system and calculate its fixed point set. The fixed point set is an interval I and the global behavior of the recurrence (1.3) is determined by its behavior close to I.

Define $\phi_{1,i}(x)=-\omega x-i$ for $i=0,...,a-1$ and let $\phi_{2,a}(x)=\omega^2 x+a\omega$. The functions $\{\phi_{1,0},\ldots,\phi_{1,a-1},\phi_{2,a}\}$ are contractions which form an iterated function system (IFS) on $\mathbb{R}$. Let I be the real interval $[-\omega-(a-1),1]$. Then I is the unique compact fixed-point set in $\mathbb{C}$ of the IFS:

Proposition 1: The interval I satisfies $\cup_{i=0}^{a-1}\phi_{1,i}(I)\cup\phi_{2,a}(I)=I$.

Proof: Writing $c=-\omega-(a-1)$, we have $c<0$ and $I=[c,1]$. We calculate $\phi_{1,i}([c,1])=[-\omega-i,-\omega c-i]$, for $i=0,...,a-1$, and $\phi_{2,a}([c,1])=[\omega^2 c+a\omega,1]$. We observe that $\phi_{1,(a-1)}(1)=-\omega-(a-1)=c$, the left-hand end point of I. Moreover, for $k=1,...,a-1$ we have $\phi_{1,k}(c)=\phi_{1,k-1}(1)$, so that the right-hand end point of $\phi_{1,k}(I)$ is the left-hand end point of $\phi_{1,k-1}(I)$. Thus $\cup_{i=0}^{a-1}\phi_{1,i}([c,1])=[c,\phi_{1,0}(c)]=[c,-\omega c]$. Furthermore, we have $\phi_{2,a}(c)=\omega^2(-\omega-(a-1))+a\omega=1-\omega=-\omega c=\phi_{1,0}(c)$, so that $\cup_{i=0}^{a-1}\phi_{1,i}(I)\cup\phi_{2,a}(I)=I$, as required. The locations of the intervals are shown in Fig. 1. □

One further observation which will be useful in what follows is that if V is a nonempty open set in $\mathbb{C}$, containing I, and which is invariant for any one of the affine contractions $\phi_{1,0},\ldots,\phi_{1,a-1}$, $\phi_{2,a}$, then $V=\mathbb{C}$.

IV. THE RENORMALIZATION OPERATORS *R* AND *N*

In terms of the above-mentioned IFS, Eq. (1.4) may be written $t(x)=(\Pi_{i=0}^{a-1}t(\phi_{1,i}(x)))\,t(\phi_{2,a}(x))$. To obtain t_*, we impose the condition $t(x)\sim 1-x$ as $x\to 1$. We also have an associated additive fixed-point equation,

$$T(x)=\left(\sum_{i=0}^{a-1}T(\phi_{1,i}(x))\right)+T(\phi_{2,a}(x)),\quad T(x)\sim\log(1-x)\ \text{ as }\ x\to 1. \tag{4.1}$$

The solution of (1.4) is obtained from a corresponding solution of (4.1), although care must be taken over the logarithmic singularity at $x=1$.

In order to solve (4.1), we introduce the following linear operator R on functions T, given by

$$R(T)(x)=\left(\sum_{i=0}^{a-1}T(\phi_{1,i}(x))\right)+T(\phi_{2,a}(x)). \tag{4.2}$$

A solution of (4.1) corresponds to a fixed point of R, but, unfortunately, the operator R is not a contraction. We may eliminate the unstable direction by introducing the operator N given by $N(T)=R(T)-C(T)$ where $C(T)$ is

$$C(T)=\frac{1}{a}\left(\sum_{i=1}^{a-1}R(T)(\phi_{1,i}(0))+R(T)(\phi_{2,a}(0))\right). \tag{4.3}$$

In Fig. 2 we show of the solution t_* of Eq. (1.4) for the case $a=2$. This figure was obtained as the limit of the iterations of the exponentiated operator $\exp N$ starting from the initial condition $t_0(x)=1-x$.

Our strategy for the proof of Theorem 1 is as follows. We shall describe the functional analytic properties of the operators R and N. In particular, they are compact operators on a suitable space

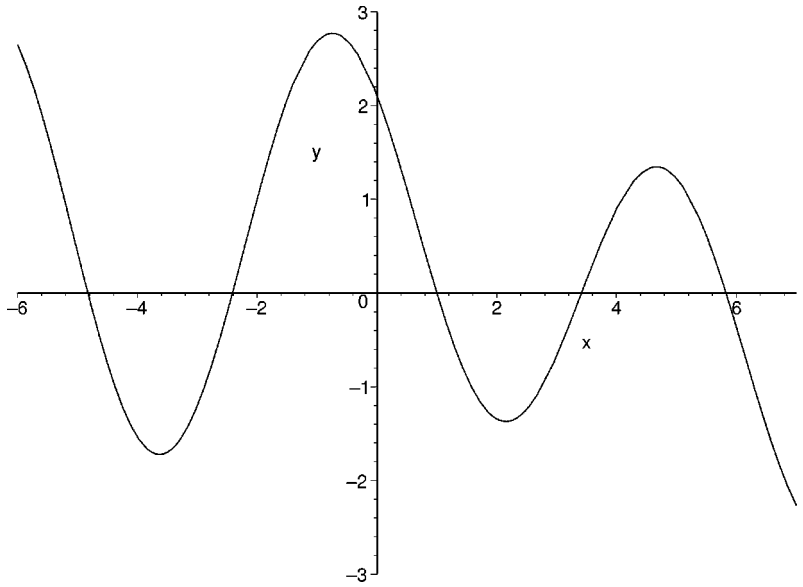

FIG. 2. Graph of the solution t_* of Eq. (1.4) for the case $a=2$.

of analytic functions, and N is spectrally a contraction. Using this fact we prove that there is a fixed point T_* of N with $T_*(x)\sim\log(1-x)$ as $x\to 1$. The operator N has been designed so T_* is also a fixed point of R. We then exponentiate to get an analytic solution of the multiplicative equation (1.4) on a domain in $\mathbb{C}$, which we then extend to the whole complex plane.

A. Function space and properties

In this section we shall define the space of analytic functions in which we shall work. Let r satisfy $\max(1,(a-1)/(1-\omega))<r<1/\omega$. That such an r exists follows from $1/\omega-(a-1)/(1-\omega)=(1-a\omega)/(\omega-\omega^2)>0$, by (2.1). Let $D=D(0,r)=\{z\in\mathbb{C}:|z|<r\}$. We let $\mathcal{F}$ be the space of real analytic functions $f:D\to\mathbb{C}$, $f(z)=\Sigma_{i=0}^{\infty} f_i(z/r)^i$, such that the L^1-norm $\|f\|=\Sigma_{i=0}^{\infty}|f_i|<\infty$. The choice of domain D is motivated by the property

$$\overline{\phi_{1,i}(D)}\subseteq D \quad \text{for } i=0,\ldots,a-1, \quad \overline{\phi_{2,a}(D)}\subseteq D. \tag{4.4}$$

We prove (4.4) as follows. Let $x\in D$ and $0\leqslant i\leqslant a-1$. Then $|\phi_{1,i}(x)|<\omega r+i<\omega r+a-1<\omega r+(1-\omega)r=r$, using $(a-1)/(1-\omega)<r$. Also, $|\phi_{2,a}(x)|<\omega^2 r+a\omega<\omega^2 r+a\omega r=r$, since $r>1$. Thus $\overline{\phi_{1,i}(D)}$, $\overline{\phi_{2,a}(D)}\subseteq D$. From (4.4) we may conclude that the operators R and N are well defined on $\mathcal{F}$.

B. Spectral properties of *R* and *N*

In this section we give a brief account of the spectral properties of the operators N and R and we calculate their spectra explicitly.

Proposition 2: The operators N: $\mathcal{F}\to\mathcal{F}$, R: $\mathcal{F}\to\mathcal{F}$ are compact. The spectrum of R consists of simple eigenvalues $\{\mu_k=a(-\omega)^k+\omega^{2k}:k\geqslant 0\}$, together with 0, while the spectrum of N on $\mathcal{F}$ consists of simple eigenvalues $\{\tilde{\mu}_k=a(-\omega)^k+\omega^{2k}:k\geqslant 1\}$, together with 0, which is also an eigenvalue $\tilde{\mu}_0=0$. The eigenfunctions corresponding to the eigenvalues μ_k and $\tilde{\mu}_k$ are both polynomials of degree k. The spectral radius $r(N)<1$.

Proof: The inclusions (4.4) imply that R and N are analyticity improving and, by standard methods, using the Cauchy estimates to provide uniform bounds on derivatives, one may use Ascoli's theorem to deduce compactness. We obtain the spectrum for N; the corresponding result

for R is proved similarly. We note that all nonzero spectral values of N are eigenvalues since N is compact. Let $\mu \neq 0$ be an eigenvalue of N with eigenfunction $T \in \mathcal{F}$, i.e., $N(T) = \mu T$:

$$\mu T(x) = N(T)(x) = \sum_{i=0}^{a-1} T(-\omega x - i) + T(\omega^2 x + a\omega) - C(T). \tag{4.5}$$

Defining the norm $\|g\|_I = \sup\{|g(x)| : x \in I\}$, and differentiating, we have $\|T^{(j)}\|_I < \infty$ for $j = 0, 1, 2, 3, \ldots$, since I is a compact. Furthermore, we have $|\mu| \|T^{(j)}\|_I = \|N(T)^{(j)}\|_I \leq (a\omega^j + \omega^{2j}) \|T^{(j)}\|_I$. Since $a\omega^j + \omega^{2j} \to 0$ as $j \to \infty$, it follows that $\|T^{(j)}\|_I = 0$ for j sufficiently large, and, since T is analytic, we have $T^{(j)} = 0$. Hence T is a polynomial of degree at most $j-1$. To find the eigenvalues of N, we may therefore assume T is a polynomial, of degree $k \geq 0$, say. Expanding (4.5) and considering the kth-order terms, we have for $k \geq 1$, $\mu = (-\omega)^k a + \omega^{2k}$. For $k = 0$, we have $T(x) = a_0 \neq 0$, and, using (4.3), we find $\mu = 0$. Moreover, it is straightforward to show that for each μ there exists a one-dimensional polynomial eigenspace of N. Finally, we prove that $r(N) < 1$. In fact, for all $a \geq 1$, and for all $k \geq 0$, we have $|\tilde{\mu}_k| \leq a\omega < 1$. The case $k = 0$ is clear, since $\tilde{\mu}_0 = 0$. For $k = 1$, we have $|\tilde{\mu}_1| = a\omega - \omega^2 < a\omega < 1$, as required. For $k \geq 2$, we have $|\tilde{\mu}_k| \leq \omega(\omega^{2k-1} + a\omega^{k-1}) < \omega \leq a\omega$. Hence $|\tilde{\mu}_k| < a\omega < 1$, as before. We deduce that $r(N) < a\omega < 1$.

V. PROOF OF EXISTENCE OF A FIXED POINT OF *R*

We now prove the existence of a fixed point of R. To do this we first of all obtain a fixed point of N and then deduce a fixed point of R. Specifically we prove the following theorem.

Theorem 2: *Let $a \in \mathbb{N}$ and let $\omega = (\sqrt{a^2+4} - a)/2$. Let $r > 0$ satisfy the inequality* $\max(1, (a-1)/(1-\omega)) < r < 1/\omega$. *Then there exists a fixed point T_* of the operator R such that $T_*(x) = \log(1-x) + T_{**}(x)$ where $T_{**} \in \mathcal{F}$.*

From Sec. IV B we know that the spectral radius of N on $\mathcal{F}$ is $r(N) < 1$. We conclude that there exists $\rho \in (r(N), 1)$ and $K > 0$ such that for all $k \geq 1$, $\|N^k(T)\| \leq K\rho^k \|T\|$. Let $T_0(x) = \log(1-x)$, where (here, and in what follows) we take the principal branch of the logarithm. We note that T_0 has a singularity at $1 \in D$, so clearly $T_0 \notin \mathcal{F}$.

We now define a sequence of functions T_n as follows: $T_1 = N(T_0) - T_0$, $T_n = N(T_{n-1})$, $n \geq 2$. We claim that $T_1 \in \mathcal{F}$ so that $T_n \in \mathcal{F}$ for all $n \geq 1$. To prove the claim we observe that

$$\begin{aligned} T_1(x) &= R(T_0)(x) - C(T_0) - T_0(x) \\ &= \sum_{i=1}^{a} \log(i + \omega x) + \log(1 - (\omega^2 x + a\omega)) - C(T_0) - \log(1-x) \\ &= \sum_{i=1}^{a} \log(i + \omega x) + A, \end{aligned}$$

where A is a constant, and we have used (4.2) and $\log(1-(\omega^2 x + a\omega)) - \log(1-x) = \log \omega^2$. It is now clear that the singularities of T_1 are at $x = i/\omega$, for $i = 1, \ldots, a-1$, and, since $r < 1/\omega$, it follows that all the singularities of T_1 lie outside D and so $T_1 \in \mathcal{F}$, and we are done.

We now prove Theorem 2. We have $N^n(T_0) = T_0 + \cdots + T_n$ and it is now immediate that $N^n(T_0)$ converges to a function $T_* = T_0 + T_{**}$ where $T_{**} = \sum_{i=1}^{\infty} T_i \in \mathcal{F}$, since the series $\sum_{i=1}^{\infty} \|T_i\| \leq \sum_{i=1}^{\infty} K\rho^{i-1} \|T_1\| < \infty$. It is clear T_* is a fixed point of N, i.e., $N(T_*) = T_*$, since $N(T_{**}) = T_{**} - T_1$ and $N(T_0) = T_0 + T_1$.

We next show that $R(T_*) = T_*$. Since $N(T_*) = T_*$, we have $R(T_*) = T_* + C(T_*)$. We show that $C(T_*) = 0$. Now $T_*(0) = \sum_{i=0}^{a-1} T_*(\phi_{1,i}(0)) + T_*(\phi_{2,a}(0)) - C(T_*)$, and, hence, $C(T_*) = \sum_{i=1}^{a-1} T_*(\phi_{1,i}(0)) + T_*(\phi_{2,a}(0))$. Recalling (4.3), we now have that

$$C(T_*) = \frac{1}{a}\left(\sum_{i=1}^{a-1} R(T_*)(\phi_{1,i}(0)) + R(T_*)(\phi_{2,a}(0)) \right)$$
$$= \frac{1}{a}\left(\sum_{i=1}^{a-1} T_*(\phi_{1,i}(0)) + T_*(\phi_{2,a}(0)) + aC(T_*) \right)$$
$$= \frac{a+1}{a} C(T_*).$$

We deduce that $C(T_*)=0$, as claimed. This concludes the proof of Theorem 2.

VI. PROOF OF THEOREM 1

We now give the proof of Theorem 1. Let T_* be the fixed point of R given by Theorem 2. Let $t_* = \exp T_*$. Then t_* is analytic on D and we have t_* satisfies Eq. (1.4) there. Moreover, since $T_*(x) \sim \log(1-x)$ as $x \to 1$, we have that t_* has zero of order 1 at $x=1$. This constructs the base solution t_* of Theorem 1. We now extend t_* to the whole of $\mathbb{C}$ by analytic continuation, so that it satisfies (1.4). To do this we use the following lemma:

Lemma 1 (extension lemma): Let t be analytic and satisfy Eq. (1.4) on an open neighborhood U of $[-\omega-(a-1),1]$ *in* $\mathbb{C}$. *Then there exists an analytic extension of t to the whole of* $\mathbb{C}$.

Proof: Consider the set of open, simply connected neighborhoods V of $[-\omega-(a-1),1]$ in $\mathbb{C}$ such that $\phi_{1,i}(V) \subseteq V$, for $i=0,...,a-1$ and $\phi_{2,a}(V) \subseteq V$ and such that there is an analytic extension of t to V. Clearly, since $[-\omega-(a-1),1]$ is the fixed-point set of the iterated function system defined in Sec. III, there exists $V \subseteq U$ satisfying these conditions. Moreover, since the union of two such neighborhoods V is also such a neighborhood, it follows that there is a maximal such neighborhood, V_*, say. Then, by maximality, we have that at least one of $\phi_{1,i}(V_*)=V_*$, for $i=0,...,a-1$ and $\phi_{2,a}(V_*)=V_*$ holds, and, thus, as observed in Sec. III, V_* is the whole of $\mathbb{C}$. □

It is now clear from the lemma that the extension of t_* to $\mathbb{C}$ is possible, since t_* is analytic on $U=D$, which contains $[-\omega-(a-1),1]$. We are therefore able to define for $k \in \mathbb{N}$ the function $t(x) = t_*(x)^k$. Then t is entire, satisfies (1.4), and has a zero of order k at $x=1$.

We next prove that t is unique. Let $k \in \mathbb{N}$. Suppose that t_1 and t_2 are entire functions satisfying Eq. (1.4), with $t_1(x)$, $t_2(x) > 0$ on $[-\omega-(a-1),1)$ and zeros of order k at $x=1$. Let us consider the function $t(x) = t_1(x)/t_2(x)$. Then, on an open neighborhood U of $[-\omega-(a-1),1]$, t is analytic and nonzero and satisfies (1.4). We now extend t to the whole of $\mathbb{C}$ using the extension lemma 1. From the multiplicative property of Eq. (1.4), we have that if $t(x)=0$, for some $x \in \mathbb{C}$, then $t(x')=0$, for some $x' \in U$, a contradiction. Thus t is a nonzero solution of (1.4) on $\mathbb{C}$, and, in particular, on D, with $t(x)>0$ on $[-\omega-(a-1),1]$. We are therefore able to define $\log t$, giving a function T which is a fixed point of R in $\mathcal{F}$, i.e., an eigenfunction with eigenvalue 1. From the spectral analysis of R (Proposition 2), we see that no such eigenfunction exists and thus $T=0$. We conclude that $t=1$ on D and, by extension, on $\mathbb{C}$. It follows that $t_1 = t_2$ on $\mathbb{C}$.

The proof of Theorem 1 is complete.

VII. CONCLUSION

In this paper we have considered the strong coupling fixed point limit of the Harper equation in the case of ω a quadratic irrational of the form $\omega = (\sqrt{a^2+4}-a)/2$, $a \in \mathbb{N}$, and have applied renormalization techniques to study the self-similarity properties of the fluctuations η_i. Although our analysis is only valid in the limit $\lambda \to \infty$, it is believed that it applies for a wider range of λ, and, in particular, large but finite λ.

There are a number of avenues for further research. First, our methods are likely to extend to more general irrational ω with continued fraction $[0;a_1,a_2,\ldots]$. However, it appears that for general ω, the functions t_n will not converge to a fixed point, and, indeed, the fundamental interval I will also vary with n.

Second, the theory for general a presented here can be applied to study problems in which the solutions of the recurrence (1.3) are piecewise constant. Such solutions have application to the study of the correlation function in strange nonchaotic attractors, other quasiperiodcally driven quantum mechanical models, as well as so-called barrier-billiard problems. In particular, the work in Refs. 5 and 6 may be extended from the golden-mean case to general a.

A third direction for future work is the generalization of the so-called Ketoja–Satija orchid, a renormalization strange set for a generalized Harper equation (see Refs. 3 and 7). It is likely that the Ketoja–Satiija orchid and the analysis of its structure can be generalized to irrational numbers other than the golden mean $(\sqrt{5}-1)/2$. Indeed, the goal is to extend the analysis in Ref. 7 to all irrational ω.

ACKNOWLEDGMENTS

The authors would like to thank Andy Osbaldestin for extremely helpful discussions, particularly on the form of the recurrence for $a \geqslant 2$. J.D. wishes to acknowledge the support of the UK Engineering and Physical Sciences Research Council.

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$n=3$ differential calculus and gauge theory on a reduced quantum plane

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(Received 8 March 2003; accepted 1 May 2003)

We discuss the algebra of $N\times N$ matrices as a reduced quantum plane. A $n=3$-nilpotent deformed differential calculus involving a complex parameter q is constructed. The two cases, q 3rd and Nth root of unity are completely treated. As an application, we establish a gauge field theory for the particular cases $n=2$ and $n=3$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1598278]

I. INTRODUCTION

In the literature, there exist different points of view[1–6] to generalize the ordinary differential calculus ($d^2=0$); see, for example, Refs. 7–8, to higher orders. An adequate way leading to such generalizations arises from the graded differential algebra.[1–3] In fact in these references it is seen as a graded q-differential algebra which is the sum of k-graded subspaces, where $k \in\{0,1,2,\ldots,m-1\}$. The relevant differential operator is an endomorphism d satisfying $d^m=0$ and the q-Leibniz rule:

$$d(AB)=(dA)B+qAd(B).$$

The most important property of this calculus is that it involves not only first differentials dx^i, $i=1,\ldots,n$, but also the higher-order differentials $d^jx^i, j=1,\ldots,m-1$.

On the other hand, the differential calculus ($d^2=0$) on noncommutative spaces was also studied by different authors; see Refs. 8–13. These differential calculi are covariant with respect to some symmetry quantum group.

In this paper, we construct a covariant differential calculus $d^3=0$ on the algebra $M_3(C)$ of 3×3 matrices considered as a reduced quantum plane. We will show that our differential calculus is covariant under the algebra of transformations with a quantum group structure. The complex deformation parameter q (3rd-root of unity) will play an important role in constructing gauge field theory on $M_3(C)$.

The paper is organized as follows

We start in Sec. II by defining the algebra of $N\times N$ matrices as a reduced quantum plane, where the deformation parameter q is the Nth root of unity. In Sec. III we construct the covariant differential calculus $d^3=0$ on the two-dimensional reduced quantum plane as in Refs. 1–3. The new objects, d^2x and d^2y, appearing in this construction are seen as the analogous of the differential elements dx and dy in the ordinary differential calculus. In Sec. IV, we generalize this result by considering a complex deformation parameter q Nth root of unity.

In Sec. V, we study the application of this new differential calculus ($d^3=0$) to the gauge field theory on $M_3(C)$. We recall in Sec. VI the differential calculus $d^2=0$,[8,11–13] and we apply it to derive a gauge theory on $M_3(C)$.

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II. PRELIMINARIES ABOUT THE ALGEBRA $M_3(C)$ OF N×N MATRICES AS A REDUCED QUANTUM PLANE

The associative algebra of $N\times N$ matrices is generated by two elements x and y[14] satisfying the relations

$$xy=qyx \tag{1}$$

and

$$x^N=y^N=1, \tag{2}$$

where 1 is the unit matrix and q $(q\neq 1)$ is a complex parameter Nth root of unity.

In the case $N=3$, an explicit matrix realization of generators x and y[11,15] is given by

$$x=\begin{pmatrix} 1 & 0 & 0 \\ 0 & q^{-1} & 0 \\ 0 & 0 & q^{-2} \end{pmatrix}, \tag{3}$$

$$y=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \tag{4}$$

and q satisfies the relation

$$1+q+q^2=0. \tag{5}$$

The associative algebra, noted by $C_q\,[x,y]:=C_q$, of formal power series defined over the two-dimensional quantum plane is generated by x and y with a single quadratic relation $xy=qyx$. It is clear that $C_1\,[x,y]$ coincides with the algebra of polynomials over commuting variables x, y. If the generators x, y do not satisfy any additional relations, the algebra C_q is infinite dimensional.

In the case of the algebra $M_3(C)$ of 3×3 matrices over complex numbers, the generators x, y satisfy the above quadratic relation (1) and the cubic ones $x^3=y^3=1$. Thus the algebra $\tilde{C}_q$ of formal power series over $M_3(C)$ is finite dimensional and generated by $\{1, x, y, x^2, y^2, xy, x^2y, xy^2, x^2y^2\}$. In this case, $\tilde{C}_q=C_q^0/I$ where C_q^0 is the unital extension of C_q and I is the bilateral ideal generated by $x^3-1=0$, $y^3-1=0$. That is, in the sense of Refs. 11, 15, the 3×3 matrices over C are seen as a reduced quantum plane.

We note that the functions of x and y are seen as a finite formal power series with a maximum degree 3; this property will be extremely useful in what follows. In fact, the set of these functions is an associative algebra that is used to introduce a gauge field theory on the reduced quantum plane. This idea will be developed in Secs. V and VII.

III. DIFFERENTIAL CALCULUS WITH NILPOTENCY $n=3$ ON REDUCED QUANTUM PLANE, CASE $q^3=1$

Our aim in this section is to construct a covariant $n=3$ nilpotent differential calculus by mixing two approaches. Namely, we adapt to the reduced quantum plane an idea originally proposed by Kerner,[1–3] and we use Couquereaux's technics[11] to ensure covariance. We denote by Ω the differential algebra generated by x, y, dx, dy, d^2x and d^2y, where the "2-forms" d^2x and d^2y are the second differentials of the basic variables x and y.

Let us introduce the differential operator d that satisfies the following conditions: Nilpotency,

$$d^3=0: \tag{6}$$

and Leibniz rule,

$$d(uv)=d(u)v+q^n u d(v), \tag{7}$$

where u is a form of degree n and q is a 3rd root of unity.

By applying the Leibniz rule on the 1-form we obtain

$$d(f(x)\,dx)=(df(x))\,dx+f(x)\,d^2x; \tag{8}$$

$f(x)$ are the 0-forms in the algebra Ω. The set of transformations leaving covariant our differential calculus is $F\subset \mathrm{Fun}(SL_q(2,C))$ and the covariance is described by the left coaction. We start by explaining this coaction.[16]

The left coaction of the group F on the reduced quantum plane is the linear transformation of coordinates given by

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix}=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\otimes\begin{pmatrix} x \\ y \end{pmatrix}.$$

We also introduce the line vectors with coordinate functions:

$$(x^1,y^1)=(x,y)\otimes\begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

where the matrix elements a, b, c and d do not commute with each other. We require that x_1, y_1, x^1, y^1 satisfy the same relations as x and y. The two constraints $x_1y_1=qy_1x_1$ and $x^1y^1=qy^1x^1$ lead to the relations

$$ac=qca, \quad bd=qdb,$$

$$ab=qba, \quad cd=qdc,$$

$$bc=cb, \quad ad-da=(q-q^{-1})bc.$$

The algebra generated by a, b, c and d is usually denoted $\mathrm{Fun}(GL_q(2,C))$. The q-determinant $D=da-q^{-1}bc$ is in the center of $\mathrm{Fun}(GL_q(2,C))$. If we set it equal to 1, we define the algebra $\mathrm{Fun}(SL_q(2,C))$. Assuming that the supplementary conditions $(x)^3=1$ and $(y)^3=1$ are also verified by the coordinates x_1, y_1, x^1 and y^1 implies $a^3=1$, $b^3=0$, $c^3=0$, $d^3=1$. These new cubic relations on $\mathrm{Fun}(SL_q(2,C))$ yield a new algebra that we denote F. It is also a Hopf algebra. Indeed, it has a coalgebra structure (coproduct) which is compatible with the algebra one (product), this defines a bialgebra structure. An antipode and a co-unit are also defined. For further details on such structures on F, see, for example, Ref. 11.

The mixture of Kerner's idea and Coquereaux's techniques allows us to construct the left covariant differential algebra $\Omega=\{x,y,dx,dy,d^2x,d^2y\}$; see Appendix A. The commutation relations between the generators of Ω are as follows:

$$x\,dx=q^2\,dx\,x, \tag{9}$$

$$x\,dy=q\,dy\,x+(q^2-1)dx\,y, \tag{10}$$

$$y\,dx=q\,dx\,y, \tag{11}$$

$$y\,dy=q^2\,dy\,y, \tag{12}$$

$$dy\,dx=q^2\,dx\,dy, \tag{13}$$

$$x\,d^2x=q^2d^2x\,x, \tag{14}$$

$$y\,d^2x = q\,d^2x\,y, \tag{15}$$

$$y\,d^2y = q^2 d^2y\,y, \tag{16}$$

$$x\,d^2y = q\,d^2y\,x + (q^2-1)d^2x\,y, \tag{17}$$

$$dx\,d^2y = d^2y\,dx + q(1-q)d^2x\,dy, \tag{18}$$

$$dy\,d^2x = d^2x\,dy, \tag{19}$$

$$dx\,d^2x = q\,d^2x\,dx, \tag{20}$$

$$dy\,d^2y = q\,d^2y\,dy, \tag{21}$$

$$d^2y\,d^2x = q^2 d^2x\,d^2y. \tag{22}$$

As in the standard way, we define the partial derivatives in directions x and y through

$$d = \frac{\partial}{\partial x}dx + \frac{\partial}{\partial y}dy = \partial_x dx + \partial_y dy. \tag{23}$$

Consistency conditions as in Ref. 8 yield

$$\partial_x\,\partial_y = q\partial_y\,\partial_x, \tag{24}$$

$$\partial_x\,x = 1 + q^2 x\,\partial_x + (q^2-1)y\,\partial_y, \tag{25}$$

$$\partial_x\,y = qy\,\partial_x, \tag{26}$$

$$\partial_y\,y = 1 + q^2 y\,\partial_y, \tag{27}$$

$$\partial_y\,y = 1 + q^2 y\,\partial_y, \tag{28}$$

$$(dx)^3 = (dy)^3 = 0. \tag{29}$$

The last equality, Eq. (29), can be related to the nilpotency relation encountered in the description of the fractional statistics. More precisely, we recover the description of physical systems that generalize fermions. In a forthcoming paper,[17] we re-introduce these systems using this new differential calculus by establishing an adequate correspondence between our differential calculus and some deformed Heisenberg algebras, as it is done in Ref. 18 for the particular case ($d^2=0$).

Now, we generalize our differential calculus by considering the case $q^N=1$.

IV. DIFFERENTIAL CALCULUS ON A REDUCED QUANTUM PLANE, CASE $q^N=1$

A two-dimensional reduced quantum plane is an associative algebra generated by x and y with relations (1) and (2). One can always define the differential operator "d" satisfying $d^3=0$ ($d^2\neq 0$) and the Leibniz rule

$$d(uv) = d(u)v + (j)^n u d(v), \tag{30}$$

$u\in\Omega^n$ and $v\in\Omega^m$, where Ω^n and Ω^m are the spaces of n and m forms on the reduced quantum plane, respectively.

In contrast to Eq. (7), one has to distinguish between the deformation parameter q and the j parameter, $j^3=1$ ($j\neq 1$) in Eq. (30).

Following the same method of Sec. III, we get the covariant differential calculus:

$$x\,dx = j^2 dx\,x, \tag{31}$$

$$x\,dy = -\frac{jq}{1+q^2} dy\,x + \frac{j^2q^2-1}{1+q^2} dx\,y, \tag{32}$$

$$y\,dx = \frac{j^2-q^2}{1+q^2} dy\,x - \frac{jq}{1+q^2} dx\,y, \tag{33}$$

$$y\,dy = j^2 dy\,y, \tag{34}$$

$$dx\,dy = q\,dy\,dx, \tag{35}$$

$$x\,d^2x = j^2\,d^2x\,x, \tag{36}$$

$$x\,d^2y = -\frac{jq}{1+q^2} d^2y\,x + \frac{j^2q^2-1}{1+q^2} d^2x\,y, \tag{37}$$

$$y\,d^2x = \frac{j^2-q^2}{1+q^2} d^2y\,x - \frac{jq}{1+q^2} d^2x\,y, \tag{38}$$

$$y\,d^2y = j^2 d^2y\,y, \tag{39}$$

$$dx\,d^2x = j\,d^2x\,dx, \tag{40}$$

$$dx\,d^2y = -\frac{q}{1+q^2} d^2y\,dx + \frac{jq^2-j^2}{1+q^2} d^2x\,dy, \tag{41}$$

$$dy\,d^2x = \frac{j-j^2q^2}{1+q^2} d^2y\,dx - \frac{q}{1+q^2} d^2x\,dy, \tag{42}$$

$$dy\,d^2y = j\,d^2y\,dy, \tag{43}$$

$$d^2x\,d^2y = q\,d^2y\,d^2x. \tag{44}$$

If $q=j$, we recover the differential calculus obtained in Sec. III. As an application of this new differential calculus $d^3=0$ on the reduced quantum plane, we construct in the section below a gauge field theory on $M_3(C)$.

V. COVARIANT DERIVATIVE AND CURVATURE ON $M_3(C)$ AS A REDUCED QUANTUM PLANE WITH $d^3=0$

In this section, we use the $n=3$ differential calculus constructed in Sec. III to establish a gauge theory on the reduced quantum plane.

As in the ordinary case, the covariant differential is defined by

$$D\Phi(x,y) = d\Phi(x,y) + A(x,y)\Phi(x,y), \tag{45}$$

where the field $\Phi(x,y)$ is a function on $M_3(C)$ and the gauge field $A(x,y)$ is a 1-form valued in the associative algebra of functions on the reduced quantum plane $M_3(C)$.

We have assumed that the algebra of functions on $M_3(C)$ is a bimodule over the differential algebra Ω.

As usual, the covariant differential D must satisfy

$$DU^{-1}\Phi(x,y) = U^{-1}D\Phi(x,y), \tag{46}$$

where U is an endomorphism defined on Fun$[M_3(C)]$.

This leads to the following gauge field transformation:

$$A(x,y)\to U^{-1}A(x,y)U+U^{-1}dU. \tag{47}$$

In general, the gauge field $A(x,y)$ can be written as

$$A(x,y)=A_x(x,y)dx+A_y(x,y)dy. \tag{48}$$

The differential calculus $n=3$ allows us to define the curvature R as follows:[2,19]

$$D^3\Phi(x,y)=R\Phi(x,y). \tag{49}$$

Direct computations show that R is a ''three-form'' given by

$$R=d^2A(x,y)+dA^2(x,y)+A(x,y)dA(x,y)+A^3(x,y) \tag{50}$$

$$=d^2A(x,y)+(dA(x,y))A(x,y)+(1+q)A(x,y)dA(x,y)+A^3(x,y) \tag{51}$$

$$=d^2A(x,y)+(dA(x,y))A(x,y)-q^2A(x,y)dA(x,y)+A^3(x,y). \tag{52}$$

One has to express the curvature written above in terms of 3-forms constructed from basic generators dx, dy, d^2x and d^2y of the differential algebra Ω. Since we are dealing with a noncommutative space (reduced quantum plane), this task is not straightforward. In fact, the noncommutativity prevents us from rearranging the different terms in Eq. (52) adequately. To overcome this technical difficulty we require that the components of the gauge field $A_x(x,y)$ and $A_y(x,y)$ are expressed as formal power series of the space coordinates x and y.[20–23] The condition, Eq. (2) in Sec. II ($N=3$), is extremely useful, in the sense that it limits the power series to finite ones rather than infinite:

$$A_x(x,y)=a_{mn}x^my^n; \quad m,n=0,1,2, \tag{53}$$

$$A_y(x,y)=b_{kl}x^ky^l; \quad k,l=0,1,2. \tag{54}$$

Using the formulas (1), (31)–(44), (52)–(54), and after technical computations, the desired expression of the curvature arises as

$$\begin{aligned}R=&qF^q_{xy}d^2x\,dy+F^{q^2}_{yx}d^2y\,dx\times[R_{xxy}+qR_{yxx}+q^2R_{xyx}+(1-q)\{\partial_yA_x(x,y)+q\partial_xA_y(x,y)\\&+\partial_yA_Y(x,y)((1-q)f_2(y)-f_1(x,y))+qf_4(x,y)f_0(x,y)-q^2f_6(x,y)+A_y(x,y)(f_5(x,y)\\&+A_y(x,y)A_y(q^2x,y)((1-q)f_2(y)-f_1(x,y))A_y(x,y)A_x(q^2x,y)f_4(x,y)\\&+qA_x(x,y)A_y(qx,q^2y)f_0(x,y)+q^2A_y(x,y)f_4(x,y)A_y(x,y)\\&+A_y(x,y)f_3(x,y)A_y(q^2x,qy)\}]dx\,dx\,dy+[R_{yyx}+qR_{yxy}+q^2R_{xyy}+(1-q)\\&\times\{-q^2\partial_yA_y(x,y)f_0(x,y)-q^2A_y(x,y)f_7(x,y)-A_y(x,y)A_y(q^2x,qy)f_8(x,y)\}]dy\,dy\,dx,\end{aligned} \tag{55}$$

where

$$\begin{aligned}F^q_{xy}&=\partial_xA_y(x,y)-q\partial_yA_x(x,y)+A_x(x,y)A_y(qx,q^2y)-qA_y(x,y)A_x(q^2x,qy),\\F^{q^2}_{yx}&=\partial_yA_x(x,y)-q^2\partial_xA_y(x,y)+A_y(x,y)A_x(q^2x,qy)-q^2A(x,y)A(qx,q^2y),\end{aligned} \tag{56}$$

and the components R_{ijk}, $f_n(x,y)$ $(i,j,k=x,y;\ n=0,1,\ldots,8)$ are given in Appendix B.

The expression of the curvature components, Eq. (80) Appendix B, and the deformed field strength, Eqs. (56), are formally the same as those obtained by Kerner.[2,19] The functions $f_i(x,y)$ $i=0,\ldots,8$ can be interpreted as a direct consequence of the noncommutativity property of the space.

The $n=3$ covariant differential calculus constructed in Secs. III and IV, respectively, for a q 3rd and Nth-root of unity can be seen as a generalization of the case $n=2$. However, one cannot see $d^2=0$ as a certain limit of the $d^3=0$ case. In the next section, we are reminded of the differential calculus $d^2=0$.

VI. DIFFERENTIAL CALCULUS WITH NILPOTENCY $n=2$ ON A REDUCED QUANTUM PLANE

We recall that the exterior differential "d" on the reduced quantum plane obeys the usual properties,[8,11–13] namely i/linearity, ii/nilpotency,

$$d^2=0. \tag{57}$$

iii/Leibniz rule,

$$d(uv)=d(u)v+(-1)^n u d(v), \tag{58}$$

where

$$u\in\Omega^n, v\in\Omega^m \quad \text{and} \quad d(x)=dx, \quad d(y)=dy, \quad d1=0. \tag{59}$$

The q-deformed differential calculus satisfies

$$x\,dx=q^2\,dx\,x, \tag{60}$$

$$x\,dy=q\,dyx+(q^2-1)dx\,y, \tag{61}$$

$$y\,dx=q\,dx\,y, \tag{62}$$

$$y\,dy=q^2\,dy\,y, \tag{63}$$

$$dy\,dx=-q^2\,dx\,dy, \tag{64}$$

$$(dx)^2=(dy)^2=0. \tag{65}$$

So, the differential algebra Ω is generated by x, y, dx and dy, $\Omega=\{x,y,dx,dy\}$.

Using the standard realization of the differential "d:"

$$d=\frac{\partial}{\partial x}dx+\frac{\partial}{\partial y}dy=\partial_x\,dx+\partial_y\,dy, \tag{66}$$

one can prove that

$$\partial_x x=1+q^2x\partial_x+(q^2-1)y\partial_y, \tag{67}$$

$$\partial_y x=qx\partial_x, \tag{68}$$

$$\partial_x y=qy\partial_x, \tag{69}$$

$$\partial_y y=1+q^2y\partial_y. \tag{70}$$

We apply this covariant differential calculus to study the related gauge field theory on $M_3(C)$.

VII. COVARIANT DERIVATIVE AND CURVATURE ON $M_3(C)$ AS A REDUCED QUANTUM PLANE WITH $d^2=0$

The covariant differential is defined as in Sec. VI:

$$D\Phi(x,y)=d\Phi(x,y)+A(x,y)\Phi(x,y). \tag{71}$$

The expression of the curvature is

$$D^2\Phi(x,y)=(dA(x,y)+A(x,y)A(x,y))\Phi(x,y)=R\Phi(x,y). \tag{72}$$

The differential realization of "d," Eqs. (66)–(70), allows to rewrite the expression of the curvature R:

$$R=(\partial_x A_y(x,y)-q\partial_y A_x(x,y))dx\,dy+A_x(x,y)dx\,A_y(x,y)dy. \tag{73}$$

Using the differential calculus, Eqs. (60)–(70), on the reduced quantum plane and the expressions of $A_x(x,y)$, $A_y(x,y)$, Eqs. (53), (54) as a formal power series, it is easy to establish the curvature expression:

$$\begin{aligned}R=&[\partial_x A_y(x,y)-q\partial_y A_x(x,y)+A_x(x,y)A_y(qx,q^2y)-qAy(x,y)A_x(q^2x,qy)\\&+(1-q)A_y(x,y)\{-qb_{12}-b_{10}y+q^2b_{22}x-q^2b_{11}y^2+qb_{20}xy+b_{21}xy^2\}]dx\,dy;\end{aligned} \tag{74}$$

this permits us to identify the q-deformed antisymetric field strength:

$$\begin{aligned}F^q_{xy}&=\partial_x A_y(x,y)-q\partial_y A_x(x,y)+A_x(x,y)A_y(qx,q^2y)-qAy(x,y)A_x(q^2x,qy)\\&=-q\{\partial_y A_x(x,y)-q^2\partial_x A_y(x,y)+A_x(q^2x,qy)A_y(x,y)\\&\quad-q^2A_x(x,y)A_y(q^2x,qy)\}\\&=-qF^{q^2}_{yx},\end{aligned} \tag{75}$$

The comparison of the two expressions of curvature $d^3=0$, Sec. V and $d^2=0$, will be given in the following section.

VIII. DISCUSSIONS AND CONCLUDING REMARKS

In this paper, we have constructed a differential calculus $n=3$ nilpotent on the reduced quantum plane by mixing Kerner's idea and Coquereaux's techniques. The notion of covariance for this differential calculus is also given and we have shown that there is a quantum group structure behind this covariance. As an application, we have constructed a gauge field theory based on this calculus.

In the case $n=3$, the expression of curvature, Eq. (55), contains additional terms, Eqs. (80), (81) (Appendix B) compared with Eq. (74) ($n=2$). These terms can be interpreted as a generic consequence of the extension of the differential calculus $d^2=0$ to the higher order $d^3=0$.

We can also compare our results with those of Kerner *et al.*[2,19] In fact, Eqs. (56), (80) are formally the same as in Refs. 2, 19; they differ only by the appearance of the deformation parameter q. However, there is no analogy of Eq. (81) in Refs. 2, 19. It is a direct consequence of the noncommutativity of the space considered here.

In a forthcoming paper, we shall treat in a mathematical way the correspondence between this calculus and the Heisenberg algebra. This correspondence is based on the bargman Fock representation and will give a new oscillator algebra. To study the minimization of an uncertainty principle, we will try to find the eigenvectors of the annihilation operator in a way to construct the corresponding Klauder's coherent states.[17]

ACKNOWLEDGMENTS

The authors Y. Hassouni and E. H. Zakkari wish to thank the Abdus Salam International Center for Theoretical Physics for financial and scientific support, where a great part of this work has been done. This work was done within the framework of Associateship and Federation Arrangement Schemes of the Abdus Salam ICTP.

APPENDIX A: THE CONSTRUCTION OF A COVARIANT DIFFERENTIAL CALCULUS ON A TWO-DIMENSIONAL QUANTUM PLANE

We start by writing *a priori* $x\,dx$, $x\,dy$, $y\,dx$ and $y\,dy$ in terms of $dx\,x$, $dy\,x$, $dx\,y$ and $dy\,y$, i.e.,

$$x\,dx = a_1\,dx\,x + b_1\,dy\,x + c_1\,dx\,y + d_1\,dy\,y, \tag{A1}$$

$$x\,dy = a_2\,dx\,x + b_2\,dy\,x + c_2\,dx\,y + d_2\,dy\,y, \tag{A2}$$

$$y\,dx = a_3\,dx\,x + b_3\,dy\,x + c_3\,dx\,y + d_3\,dy\,y, \tag{A3}$$

$$y\,dy = a_4\,dx\,x + b_4\,dy\,x + c_4\,dx\,y + d_4\,dy\,y. \tag{A4}$$

Differentiating the commutation relation $xy = qyx$ and replacing $x\,dx$ and $x\,dy$ by their expressions in the formulas above, permits us to fix three unknown coefficients. This leaves us with *nine* independent parameters.

The left coaction of F on a quantum plane is defined by

$$x_1 = a \otimes x + b \otimes y,$$

$$y_1 = c \otimes x + d \otimes y.$$

Hence

$$dx_1 = a \otimes dx + b \otimes dy,$$

$$dy_1 = c \otimes dx + d \otimes dy.$$

We impose that the relations between x_1, y_1 and dx_1, dy_1 be the same as the relations between x, y and dx, dy; these conditions yield to

$$a_2 = a_3 = a_4 = b_1 = b_4 = c_1 = c_4 = d_1 = d_2 = d_3 = 0 \quad \text{and} \quad d_1 = a_4,$$

and the coefficients b_2, b_3, c_2, and c_3 can be expressed in the terms of one unknown coefficient a_1:

$$b_2 = \frac{q(1+a_1)}{1+q^2}, \quad c_2 = \frac{a_1 q^2 - 1}{1+q^2},$$

$$b_3 = \frac{a_1 - q^2}{1+q^2}, \quad c_3 = \frac{q(1+a_1)}{1+q^2}.$$

Differentiating the relations (76)–(79) and noticing that $dx\,dx$, d^2x, $dy\,dy$ and d^2y are independent, we find $a_1 = q^2$. The left covariant differential calculus on a reduced quantum plane is hence constructed, Eqs. (9)–(22).

APPENDIX B: THE CURVATURE COMPONENTS

In this appendix we give the explicit expression of the curvature components appearing in Eq. (55):

$$
\begin{aligned}
R_{xxy} &= \partial_x\partial_x A_y(x,y) + \partial_x A_x(x,y) A_y(q^2x,qy) - q^2 A_x(x,y)\partial_x A_y(qx,q^2y) \\
&\quad + A_x(x,y)A_x(qx,q^2y)A_y(q^2x,qy), \\
R_{yxx} &= \partial_y\partial_x A_x(x,y) + \partial_y A_x(x,y) A_x(x,y) - q^2 A_y(x,y)\partial_x A_x(qx,q^2y) \\
&\quad + A_y(x,y)A_x(q^2x,qy)A_x(x,y), \\
R_{xyx} &= \partial_x\partial_y A_x(x,y) + \partial_x A_y(x,y) A_x(x,y) - q^2 A_x(x,y)\partial_y A(qx,q^2y) \\
&\quad + A_x(x,y)A_y(qx,q^2y)A_x(x,y), \\
R_{yyx} &= \partial_y\partial_y A_x(x,y) + \partial_x A_y(x,y) A(x,y) - q^2 A_x(x,y)\partial_y A_x(qx,q^2y) \\
&\quad + A_y(x,y)A_y(q^2x,qy)A_x(qx,q^2y), \\
R_{yxy} &= \partial_y\partial_x A_y(x,y) + \partial_y A_x(x,y) A_x(x,y) - q^2 A_y(x,y)\partial_x A_y(qx,q^2y) \\
&\quad + A_y(x,y)A_x(q^2x,qy)A_y(x,y), \\
R_{xyy} &= \partial_x\partial_y A_y(x,y) + \partial_x A_y(x,y) A_y(x,y) - q^2 A_x(x,y)\partial_y A_y(qx,q^2y) \\
&\quad + A_x(x,y)A_y(qx,q^2y)A_y(x,y),
\end{aligned}
\tag{B1}
$$

$$
\begin{aligned}
f_0(x,y) &= -b_{11}y^2 - qb_{10}y + q^2b_{22}x + b_{20}xy + qb_{21}xy^2 - b_{21}, \\
f_1(x,y) &= -a_{11}y^2 - a_{10}y + a_{22}x + a_{20}xy + a_{21}xy^2 - a_{12}, \\
f_2(x,y) &= -b_{20}y^2 - q^2b_{21}y - q^2b_{22}y, \\
f_3(x,y) &= -q^2a_{11}y^2 - a_{10}y + q^2a_{22}x + qa_{20}xy + a_{21}xy^2 - qa_{12}, \\
f_4(x,y) &= -q^2b_{11}y^2 - b_{10}y + q^2b_{22}x + qb_{20}xy + b_{21}xy^2 - qb_{12}, \\
f_5(x,y) &= -qb_{21}y^2 - b_{20}y - qb_{22}, \\
f_6(x,y) &= +qa_{12}y^2 + -a_{11}y + qa_{21}xy - qa_{22}xy^2, \\
f_7(x,y) &= +qb_{21}y^2 - b_{11}y + qb_{21}xy^2 - qb_{22}xy^2, \\
f_8(x,y) &= -b_{11}y^2 - b_{10}y + b_{22}x - b_{20}xy + b_{21}xy^2 - b_{12}.
\end{aligned}
\tag{B2}
$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

Imaginary Killing spinors in Lorentzian geometry

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(Received 16 April 2003; accepted 18 June 2003)

We study the geometric structure of Lorentzian spin manifolds, which admit imaginary Killing spinors. The discussion is based on the cone construction and a normal form classification of skew-adjoint operators in signature $(2,n-2)$. Derived geometries include Brinkmann spaces, Lorentzian Einstein–Sasaki spaces and certain warped product structures. Exceptional cases with decomposable holonomy of the cone are possible. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1606524]

I. INTRODUCTION

A classical object of interest in differential geometry are Killing vector fields. These are by definition infinitesimal isometries, which means that the flow of such a vector field preserves the metric. A spinorial analog are the so-called Killing spinor fields φ, which occur on spin manifolds and are defined as solutions of the field equation $\nabla^S_X\varphi=\lambda X\cdot\varphi$ for all vector fields X and some fixed $\lambda\in\mathbb{C}$, where ∇^S denotes the spinor derivative and the center dot denotes the Clifford multiplication.

In Riemannian geometry, it was proved in Ref. 12 that real Killing spinors realize the lower bound of the eigenvalue estimation for the Dirac equation on compact spaces with positive scalar curvature. In the sequel Riemannian spaces admitting Killing spinors were intensively studied (cf. Refs. 11 and 5) and a complete geometric description of such spaces was established. For the case of imaginary Killing spinors this was done by Baum in Ref. 3 and then for real Killing spinors by Ch. Bär using the cone construction and the holonomy classification of Riemannian spaces with parallel spinors (cf. Ref. 1). Both results characterize Riemannian spaces with Killing spinors by the Einstein condition and the existence of certain differential forms, which can be understood as generalized Killing vectors. Real Killing spinors in Lorentzian geometry were first studied in Ref. 9.

In this paper we will treat the Killing spinor equation to an imaginary Killing number λ on a pseudo-Riemannian space with Lorentzian signature. As a technical tool we will use again the cone construction for the investigation. Contrary to the Riemannian case, a holonomy description of the cone cannot be used, since there is no classification of indecomposable holonomy groups for pseudo-Riemannian manifolds. Moreover, the geodesical completeness of a Lorentzian manifold does not imply that a cone with decomposable holonomy is flat. Instead, our geometrical description is mainly based on a normal form classification of skew-adjoint operators in signature $(2,n-2)$, which is more rich than in the Euclidean case (cf. Ref. 10). The derived Lorentzian geometries are then described by the causal properties of the corresponding Dirac current and the existence of parallel spinors or certain Killing forms. Thereby, we will use the knowledge of structure results for Lorentzian manifolds admitting conformal gradient fields (cf. Ref. 13) and twistor spinors with lightlike Dirac current (cf. Ref. 6). Examples of geometries that occur are the Brinkmann spaces with parallel spinors, the Lorentzian Einstein–Sasaki manifolds and certain warped product structures.

The order of the paper is as follows. In the next section we introduce the basic notations and

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definitions appropriate for the study of Killing spinors and state basic curvature conditions for their existence (cf. Proposition 2.1 and 2.2). In Sec. III we recall the cone construction over a Lorentzian base manifold and the correspondence of ''Killing objects'' on the base and parallel objects on its cone (Theorem 3.1). We present the normal form classification of skew-adjoint operators in signature $(2,n-2)$ due to the work of Boubel in Sec. IV. It turns out that there are exactly four generic types of normal forms for skew-adjoint operators coming from a spinor (cf. Corollary 4.7). The cone of a Lorentzian manifold admitting imaginary Killing spinors is furnished with at least one parallel two-form, which corresponds to one of the generic types (Proposition 5.1). According to this type of a parallel two-form on the cone we undertake in three of the four generic cases a discussion of the geometry of Lorentzian manifolds with imaginary Killing spinors. This happens in the last section. The results of the discussion are summerized in Theorem 5.3.

II. BASIC FACTS ON KILLING SPINORS

In this section we recall the definition of Killing spinors on a spin manifold and fix some notations. A basic integrability condition for Killing spinors is stated. For more details we refer to Ref. 5. Moreover, we will come across special Killing forms as they were introduced in Ref. 15.

Let $(M^{n,k},g)$ be a semi-Riemannian spin manifold of dimension $n\geqslant 3$ and signature $(k,n-k)$ (k is the number of timelike vectors in an orthonormal basis at a point). We denote by S the complex spinor bundle and by a center dot the Clifford multiplication on spinors. The Dirac operator $D:\Gamma(S)\to\Gamma(S)$ acting on smooth spinor fields is defined as superposition of spinor derivative ∇^S and Clifford multiplication. A spinor field $\varphi\in\Gamma(S)$ is called *Killing spinor* to the *Killing number* $\lambda\in\mathbb{C}$ if it satisfies the equation

$$\nabla^S_X\varphi=\lambda X\cdot\varphi \quad \text{for all vector fields } X.$$

It follows immediately from this definition that a Killing spinor φ is an eigenspinor of the Dirac operator D to the eigenvalue $-n\lambda$ and φ is obviously a parallel spinor field with respect to the modified spinor derivative $\tilde{\nabla}_\lambda$ defined by

$$\tilde{\nabla}_\lambda:=\nabla^S-\lambda id_{TM}.$$

In particular, this implies that a Killing spinor φ admits no zeros. It holds the following basic integrability condition.

Proposition 2.1 (Ref. 5): Let $\varphi\in\Gamma(S)$ be a Killing spinor to the Killing number $\lambda\in\mathbb{C}$.

(1) It is $\mathcal{W}(\eta)\cdot\varphi=0$ for any two-form η, where $\mathcal{W}$ denotes the Weyl tensor.
(2) $(Ric(X)-4\lambda^2(n-1)X)\cdot\varphi=0$, i.e., the image of the map $Ric-4\lambda^2(n-1)id_{TM}$ is totally lightlike or trivial.
(3) The scalar curvature is constant and given by $\mathrm{scal}=4n(n-1)\lambda^2$. The Killing number λ is real or purely imaginary.

If the Killing number λ is zero ($\mathrm{scal}=0$), φ is a parallel spinor, in case that λ is real and nonzero ($\mathrm{scal}>0$), φ is called real Killing spinor, and in case that λ is purely imaginary ($\mathrm{scal}<0$), φ is called imaginary Killing spinor. We will treat in this paper the Killing spinor equation with imaginary Killing number on a space of Lorentzian signature $(-+\cdots+)$.

So let $(M^{n,1},g)$ be a connected, oriented and time-oriented Lorentzian spin manifold. There exists an indefinite non-degenerate inner product $\langle\cdot,\cdot\rangle$ on the spinor bundle S such that

$$\langle X\cdot\varphi,\psi\rangle=\langle\varphi,X\cdot\psi\rangle,$$

$$X(\langle\varphi,\psi\rangle)=\langle\nabla^S_X\varphi,\psi\rangle+\langle\varphi,\nabla^S_X\psi\rangle$$

for all vector fields X and all spinor fields φ,ψ. Each spinor field $\varphi\in\Gamma(S)$ defines a vector field V_φ on M, the so-called *Dirac current*, by the relation $g(V_\varphi,X):=-\langle X\cdot\varphi,\varphi\rangle$ for all vector fields X. The Dirac current satisfies the following pointwise properties.

Lemma 2.1 (Ref. 14): Let $(M^{n,1},g)$ be a Lorentzian spin manifold and let $\varphi(p)\neq 0$ be a spinor in a point $p\in M^{n,1}$. Then

(1) $V_\varphi(p)\neq 0$ and $V_\varphi(p)$ is causal (i.e., $g_p(V_\varphi,V_\varphi)\leqslant 0$).
(2) If $X\cdot\varphi(p)=\rho\varphi(p)$ for some $0\neq X\in T_pM$ and $\rho\in\mathbb{R}$ then the vector X is parallel to $V_\varphi(p)$.

The lemma makes clear that the Dirac current to a Killing spinor on a Lorentzian manifold is everywhere causal. Moreover, it is now possible to prove a stronger curvature condition for the existence of Killing spinors.

Proposition 2.2: Let $(M^{n,1},g)$ be a Lorentzian spin manifold admitting a Killing spinor φ, whose Dirac current V_φ is timelike. Then (M,g) is an Einstein space.

Proof: Let us assume that $M^{n,1}$ is a non-Einstein space. Then there is an open set U in M, where $H:=\mathrm{Ric}(X)-(\mathrm{scal}/n)X\neq 0$ is lightlike for some vector field X. The Clifford product $H\cdot\varphi$ vanishes and by Lemma 2.1 this implies that H and V_φ are parallel, which is a contradiction to the assumption. □

Especially, for imaginary Killing spinors it holds the following.

Proposition 2.3 (Ref. 5): Let φ be an imaginary Killing spinor on a Lorentzian spin manifold $(M^{n,1},g)$. Then the length $\langle\varphi,\varphi\rangle$ is constant on $M^{n,1}$ and if $\langle\varphi,\varphi\rangle\not\equiv 0$ the space $M^{n,1}$ is Einstein.

Proof: It is $X\langle\varphi,\varphi\rangle=\langle\lambda X\cdot\varphi,\varphi\rangle+\langle\varphi,\lambda X\cdot\varphi\rangle=0$ and with Proposition 2.1 we calculate

$$\frac{1}{4(n-1)}\mathrm{Ric}(X,Y)\langle\varphi,\varphi\rangle=\frac{-1}{4(n-1)}\mathrm{Re}\langle\mathrm{Ric}(X)\cdot\varphi,Y\cdot\varphi\rangle$$
$$=-\mathrm{Re}\langle\lambda^2X\cdot\varphi,Y\cdot\varphi\rangle=\lambda^2g(X,Y)\langle\varphi,\varphi\rangle$$

for all vector fields X and Y, which shows that $\mathrm{Ric}(X)=(\mathrm{scal}/n)X$ in case that $\langle\varphi,\varphi\rangle\neq 0$. □

Propositions 2.2 and 2.3 imply that an imaginary Killing spinor φ on a Lorentzian non-Einstein space $M^{n,1}$ must have vanishing length $\langle\varphi,\varphi\rangle\equiv 0$ and the Dirac current V_φ to φ must be lightlike on an open subset of $M^{n,1}$. We will see later that in this case V_φ is even lightlike everywhere on $M^{n,1}$. Moreover, the Dirac current satisfies

Proposition 2.4: Let φ be an imaginary Killing spinor on a Lorentzian spin manifold $(M^{n,1},g)$. The Dirac current V_φ is a Killing vector field, which in addition satisfies $\nabla_X\,\mathrm{d}V_\varphi^\flat=-4\lambda^2X^\flat\wedge V_\varphi^\flat$.

Proof: It holds

$$g(\nabla_{e_i}V_\varphi,e_j)=-\langle\lambda e_je_i\cdot\varphi,\varphi\rangle-\langle e_j\varphi,\lambda e_i\cdot\varphi\rangle=-g(\nabla_{e_j}V_\varphi,e_i)$$

for all $i,j\in\{1,\ldots,n\}$, where $(e_1,\ldots,e_n)$ is an arbitrary orthonormal basis on $M^{n,1}$. This proves that V_φ is a Killing vector field. Moreover,

$$\mathrm{d}V_\varphi^b=4\lambda\sum_{i<j}\varepsilon_i\varepsilon_j\langle e_ie_j\cdot\varphi,\varphi\rangle e_i^\flat\wedge e_j^\flat,$$

$$\nabla_X\;\mathrm{d}V_\varphi^\flat=4\lambda^2\sum_{i<j}\varepsilon_i\varepsilon_j(\langle e_ie_jX\cdot\varphi,\varphi\rangle-\langle Xe_ie_j\cdot\varphi,\varphi\rangle)e_i^\flat\wedge e_j^\flat=-4\lambda^2X^\flat\wedge V_\varphi^\flat\;.$$

□

In general, a p-form α^p, which solves the equation

$$\nabla_X\,\mathrm{d}\alpha^p=cX^\flat\wedge\alpha^p\quad\text{for all vectors }X$$

and some fixed $c \in \mathbb{R}$, is called a *special Killing p-form* (cf. Ref. 15). Proposition 2.4 states that the dual of the Dirac current to an imaginary Killing spinor is a special Killing one-form. Killing spinors also produce special Killing forms of other degree than 1. For this, we observe that one constructs a p-form α^p_φ to a spinor φ by the rule

$$g(\alpha^p_\varphi, X^p) := -i^{p(p-1)/2}\langle X^p \cdot \varphi, \varphi\rangle \quad \text{for all } p\text{-forms } X^p$$

and, in fact, if p is odd and the Killing number λ of a Killing spinor φ is imaginary (or if p is even and λ is real) then the associated p-form α^p_φ to φ is special Killing.

III. THE CONE $\hat{M}$

In the preceding section we define the Killing spinors and special Killing p-forms on a Lorentzian manifold. In this section we will interpret these as parallel objects on the *cone manifold*. The cone construction was originally applied in order to describe Riemannian geometries admitting real Killing spinors (see Ref. 1) and can be modified here for our requirements. Let $(M^{n,1}, g)$ be a Lorentzian manifold. We consider the cone $\hat{M}$ of signature $(2, n-1)$ on $M^{n,1}$, which is defined as

$$\hat{M} := (M \times \mathbb{R}_+ , \hat{g} := r^2 g - \mathrm{d}r^2) \ .$$

Thereby, let π denote the natural projection of $\hat{M}$ to M. The 1-level $M \times \{1\}$ of the cone $\hat{M}$ is naturally isometric to the base manifold $M^{n,1}$ itself. We denote by $\tilde{X}$ the pullback of an arbitrary base vector field $X \in \Gamma(M)$ to $\hat{M}$ through the projection π. Then we have the following rules for the Levi-Civita connection $\hat{\nabla}$ on the cone:

$$\hat{\nabla}_{\partial_r}\partial_r = 0, \quad \hat{\nabla}_{\partial_r}\tilde{X} = \hat{\nabla}_{\tilde{X}}\partial_r = \frac{1}{r}\tilde{X} \ ,$$

$$\hat{\nabla}_{\tilde{X}}\tilde{Y} = \nabla_X Y - r g(X,Y)\partial_r \, .$$

In case that $M^{n,1}$ is a spin manifold the cone $\hat{M}$ is a spin manifold, too. Then we denote the spinor bundle of the cone with $\hat{S}$. For n even the restriction of $\hat{S}$ to the 1-level $M \times \{1\}$ of the cone is naturally isomorphic to the spinor bundle S on the base manifold $M^{n,1}$ by a map

$$\Phi \ : \ S \ \cong \hat{S}|_{M \times \{1\}}$$

with the property $\Phi(X \cdot \varphi) = X \cdot \Phi(\varphi)$ for all $X \in TM^{n,1}$. Similar, if n is odd, there are isomorphisms $\Phi_\pm : S \cong \hat{S}^\pm|_{M \times \{1\}}$ for the restricted half spinor bundles such that

$$-iX \cdot \Phi_+(\varphi) = \Phi_-(X \cdot \varphi),$$

for all tangent vectors $X \in TM^{n,1}$. With respect to the metric $\hat{g}$ the projection π gives rise to a pullback $\pi^* : \Gamma(\hat{S}|_{M \times \{1\}}) \to \Gamma(\hat{S})$ of spinor fields on the 1-level to the cone. Eventually, we denote by $\mathcal{K}_\lambda(M)$ the space of Killing spinors on $(M^{n,1}, g)$ to the Killing number λ.

Theorem 3.1: *(cf. Refs. 1 and 15) Let $(M^{n,1}, g)$ be a Lorentzian manifold and $\hat{M}$ its cone with signature $(2, n-1)$. The following correspondences exist.*

(1) The special Killing p-forms on $M^{n,1}$ to the positive constant $c = p+1$ are in 1-to-1 *correspondence with the parallel $(p+1)$-forms on the cone $\hat{M}$. The correspondence is given by*

$$\alpha \in \Omega^p(M) \mapsto r^p \, \mathrm{d}r \wedge \alpha - \frac{r^{p+1}}{p+1}\mathrm{d}\alpha \in \Omega^{p+1}(\hat{M}) \ .$$

(2) If $M^{n,1}$ is spin and $\mathrm{scal} = -n(n-1)$ *then there are natural isomorphisms*

$$\begin{aligned} \mathcal{K}_{i/2}(M)\oplus\mathcal{K}_{-i/2}(M) &\cong \mathcal{K}_0(\hat{M}) \\ \varphi &\mapsto \hat{\varphi}:=\pi^*\circ\Phi(\varphi) \end{aligned} \quad \text{for } n \text{ even}$$

$$\begin{aligned} \mathcal{K}_{\pm i/2}(M) &\cong \mathcal{K}_0^{\pm}(\hat{M}) \\ \varphi &\mapsto \hat{\varphi}:=\pi^*\circ\Phi_{\pm}(\varphi) \end{aligned} \quad \text{for } n \text{ odd},$$

where $\mathcal{K}_0^{\pm}(\hat{M})$ is the space of parallel $\pm$-half spinors on the cone.

The Riemannian version of Theorem 3.1 is classical for the application to the case of real Killing spinors. The result for Killing p-forms on Riemannian manifolds was established in Ref. 15. The proof for the correspondence here in case of imaginary Killing spinors φ in Lorentzian geometry is based on the observation that φ is parallel with respect to the modified spinor derivative $\tilde{\nabla}_\lambda$ coming from an affine connection one-form, which takes values in the subset

$$i\mathbb{R}^{1,n-1}\oplus\mathrm{spin}(1,n-1)\cong\mathrm{spin}(2,n-1)$$

of the Clifford algebra $\mathrm{Cliff}^{\mathbb{C}}_{1,n-1}$. We remark for the application of Theorem 3.1 that the metric g on $M^{n,1}$ can be rescaled by a positive constant such that the positive constant c to an arbitrary special Killing p-form equals $p+1$ and the Killing number λ to an arbitrary imaginary Killing spinor satisfies $\lambda^2=-\frac{1}{4}$.

The spinor bundle $S^{n,2}$ on a time-oriented, pseudo-Riemannian spin manifold $(N^{n,2},h)$ of signature $(2,n-2)$ is equipped with an invariant inner product $\langle\cdot,\cdot\rangle_{2,n-2}$ (cf. Ref. 2). Similar to the induced Dirac current of a spinor in Lorentzian geometry, a spinor $\gamma\in\Gamma(S^{n,2})$ induces a two-form α^2_γ on $N^{n,2}$ by the rule

$$h(\alpha^2_\gamma,X^2):=-i\langle X^2\cdot\gamma,\gamma\rangle_{2,n-2} \quad \text{for all two-forms } X^2.$$

In case that $\hat{M}$ is the cone over a Lorentzian spin manifold $M^{n,1}$ the inner product $\langle\cdot,\cdot\rangle_{2,n-1}$ admits the property

$$\langle\varphi,\psi\rangle=-\langle\partial_r\cdot\Phi_-(\varphi),\Phi_+(\psi)\rangle_{2,n-1} \quad \text{for } n \text{ odd},$$

$$\langle\varphi,\psi\rangle=i\langle\partial_r\cdot\Phi(\varphi),\Phi(\psi)\rangle_{2,n-1} \quad \text{for } n \text{ even},$$

on the 1-level of $\hat{M}$, where φ, ψ are spinor fields on $M^{n,1}$. Then the following relation is true.

Lemma 3.2: Let $\varphi\in\Gamma(S)$ be a spinor with Dirac current V_φ on a Lorentzian spin manifold $M^{n,1}$ and let $\hat{\varphi}$ be the corresponding ($\pm$ half) spinor with associated two-form $\alpha^2_{\hat{\varphi}}$ on the cone $\hat{M}$. It holds $V^\flat_\varphi=\partial_r\lrcorner\alpha^2_{\hat{\varphi}}$ on the 1-level $M^{n,1}\subset\hat{M}$.

Proof: With respect to an orthonormal basis $e=(e_0,e_1,\ldots,e_n)$ with $e_0=\partial_r$ in an arbitrary point of the 1-level it holds

$$\begin{aligned} \partial_r\lrcorner\alpha^2_{\hat{\varphi}} &= -i\sum_{i<j}\langle e_ie_j\cdot\hat{\varphi},\hat{\varphi}\rangle_{2,n-1}\cdot\partial_r\lrcorner e_i^*\wedge e_j^* \\ &= -i\sum_{j=1}^{n}\langle\partial_re_j\cdot\hat{\varphi},\hat{\varphi}\rangle_{2,n-1}e_j^* \\ &= -\sum_{j=1}^{n}\langle e_j\varphi,\varphi\rangle e_j^*=V^\flat_\varphi\ . \end{aligned}$$

□

The lemma also shows that $\alpha^2_{\hat{\varphi}}$ is nontrivial for all (half) spinors $\hat{\varphi}\neq 0$ on the cone $\hat{M}$, since the corresponding Dirac current $V^\flat_\varphi$ on $M^{n,1}$ is nontrivial.

IV. NORMAL FORMS FOR SKEW-ADJOINT OPERATORS IN SIGNATURE $(2,n-2)$

In this section we present a complete list of *normal forms* for skew-adjoint endomorphisms acting on the pseudo-Euclidean space $\mathbb{R}^{2,n-2}$ of dimension n and signature $(2,n-2)$. This list was established in Ref. 10. Parallel two-forms on the cone of signature $(2,n-1)$ over a Lorentzian manifold correspond to parallel skew-adjoint operators and are therefore distinguished by the normal forms of the list. This observation will be the crucial point in our description of Lorentzian geometries admitting imaginary Killing spinors in the last section.

Theorem 4.1: (cf. Ref. 10): *Let β be an arbitrary two-form on the pseudo-Euclidean space $\mathbb{R}^{2,n-2}$. Then there exist vector spaces V_i such that $\mathbb{R}^{2,n-2}=\oplus_i V_i$ is an orthogonal direct sum and the skew-adjoint endomorphism b, which corresponds to β, satisfies $b(V_i)\subset V_i$ for all i. Moreover, there is a basis $(e_{i_1},\ldots,e_{i_{r(i)}})$ for every V_i such that the corresponding matrices for the inner product and for b are one pair of blocks as it occurs in the lines of Table I.*

A basis of $\mathbb{R}^{2,n-2}$, in which a skew-adjoint operator takes a normal form, is called an *adapted basis*. There is always an orthogonal decomposition $\mathbb{R}^{2,n-2}=E\oplus P$ to a skew-adjoint operator b such that E is Euclidean and b preserves the decomposition. We call the normal form to b on E an *Euclidean block* and the normal form to b on P a *pseudo-Euclidean block*.

Example 4.2:

(a) Let $\omega_0:=\Sigma_{i=1}^{m} e_{2i-1}^*\wedge e_{2i}^*$ be the standard (pseudo)-Kähler form on $\mathbb{R}^{2,n-2}$, where $(e_1,\ldots,e_{2m})$ is the standard basis. The normal form of the skew-adjoint operator corresponding to a multiple $\omega=\nu\cdot\omega_0$ of the Kähler form with respect to the adapted basis $(e_1,\ldots,e_{2m})$ is built up by one block of the form $B_{II}(\nu)$ (pseudo-Euclidean block) and $(m-1)$ blocks of the form $B(\nu)$ (Euclidean block) (cf. Table I).

(b) A two-form $\omega=l_1^\flat\wedge l_2^\flat$ on $\mathbb{R}^{2,n-2}$, where l_1 and l_2 are lightlike vectors, which span a totally lightlike plane, corresponds as skew-adjoint operator with respect to some adapted basis to a composition of a pseudo-Euclidean block of the form B_{Ia} and an Euclidean 0-block of length $n-4$.

(c) A two-form $\omega=l_1^\flat\wedge t_1^\flat$ on $\mathbb{R}^{2,n-2}$, where l_1 is lightlike, t_1 is timelike and both vectors are orthogonal, corresponds as skew-adjoint operator with respect to some adapted basis to a composition of a block B_{Ib} and a 0-block of length $n-3$.

Let $\hat{\varphi}$ be a spinor on the pseudo-Euclidean space $\mathbb{R}^{2,n-1}$. There corresponds a two-form $\alpha_{\hat{\varphi}}^2$ to $\hat{\varphi}$ on $\mathbb{R}^{2,n-1}$ defined by the rule

$$(\alpha_\varphi^2,x^2):=-i\langle x^2\cdot\varphi,\varphi\rangle_{2,n-2}\quad\text{for all } x^2\in\Lambda^2(\mathbb{R}^{2,n-1^*}),$$

where $(\cdot,\cdot)$ denotes the induced inner product on $\Lambda^2(\mathbb{R}^{2,n-1^*})$ (cf. Sec. III). The following statement is a version of Lemma 3.2 considered in a single point only and the proof for it works the same as before.

Lemma 4.3: Let $\hat{\varphi}$ be a ($\pm$-half) spinor on $\mathbb{R}^{2,n-1}$ and $T\in\mathbb{R}^{2,n-1}$ an arbitrary unit timelike vector. The one-form $\alpha_{T,\hat{\varphi}}:=T\lrcorner\alpha_{\hat{\varphi}}^2$ is dual to the associated vector induced by the spinor φ on the Minkowski space $T^\perp\subset\mathbb{R}^{2,n-1}$, which corresponds naturally to $\hat{\varphi}$.

The lemma imposes a condition on the nature of a two-form induced by a spinor in signature $(2,n-2)$, since the associated vector to a nontrivial spinor on the Minkowski space is not arbitrary, but causal. With some simple calculations we can sort out the normal forms for skew-adjoint operators corresponding to two-forms, which do not satisfy the condition imposed by Lemma 4.3, and therefore cannot be induced by a spinor.

Corollary 4.4: Let ω be a two-form in signature $(2,n-2)$ such that the covector $T\lrcorner\omega$ is causal for every timelike vector $T\in\mathbb{R}^{2,n-2}$.

(1) If there is a timelike T such that $T\lrcorner\omega$ is lightlike then the normal form corresponding to ω is a composition of a pseudo-Euclidean block of the form B_{Ia} or B_{Ib} with an Euclidean 0-block.

TABLE I. These are the building blocks for the normal forms of skew-adjoint operators in signature $(2,n-2)$. The matrices in the first column (denoted by A) indicate an inner product (of index $s\leqslant 2$) with respect to some basis and the matrices in the second column (denoted by B) are skew-adjoint endomorphisms with respect to the inner product in column A and the chosen basis.

Signature (p,q)	$A=$ inner product	$B=$ skew-adjoint operator	
(0,1)	(1)	(0)	
(0,2)	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$B(\mu)=\begin{pmatrix}0&-\mu\\\mu&0\end{pmatrix}$	$\mu\neq 0$
(1,0)	(-1)	(0)	
(1,2)	$\begin{pmatrix}0&0&-1\\0&1&0\\-1&0&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix}$	
(1,1)	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}\lambda&0\\0&-\lambda\end{pmatrix}$	$\lambda\neq 0$
(2,2)	$\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix}$	$B_{Ia}=\begin{pmatrix}0&0&1&0\\0&0&0&1\\0&0&0&0\\0&0&0&0\end{pmatrix}$	
(2,1)	$\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix}$	$B_{Ib}=\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix}$	
(2,4)	$\begin{pmatrix}0&0&-I_2\\0&I_2&0\\-I_2&0&0\end{pmatrix}$	$\begin{pmatrix}0&I_2&0\\0&0&I_2\\0&0&0\end{pmatrix}$	
(2,0)	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$B_{II}(\nu)=\begin{pmatrix}0&-\nu\\\nu&0\end{pmatrix}$	$\nu\neq 0$
(2,2)	$\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix}$	$B_{IIa}=\begin{pmatrix}0&-\nu&1&0\\\nu&0&0&1\\0&0&0&-\nu\\0&0&\nu&0\end{pmatrix}$	$\nu\neq 0$
(2,4)	$\begin{pmatrix}0&0&-I_2\\0&I_2&0\\-I_2&0&0\end{pmatrix}$	$\begin{pmatrix}0&-\nu&I_2&0\\\nu&0&0&I_2\\0&\nu&0&-\nu\\0&0&\nu&0\end{pmatrix}$	$\nu\neq 0$
(2,2)	$\begin{pmatrix}0&I_2\\I_2&0\end{pmatrix}$	$\begin{pmatrix}\lambda I_2&0\\0&-\lambda I_2\end{pmatrix}$	$\lambda\neq 0$
(2,2)	$\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix}$	$\begin{pmatrix}\lambda&0&1&0\\0&-\lambda&0&1\\0&0&\lambda&0\\0&0&0&-\lambda\end{pmatrix}$	$\lambda\neq 0$
(2,2)	$\begin{pmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{pmatrix}$	$B_{IIb}=\begin{pmatrix}\xi&-\nu&0&0\\\nu&\xi&0&0\\0&0&-\xi&\nu\\0&0&-\nu&-\xi\end{pmatrix}$	$\xi,\nu\neq 0$
(2,3)	$\begin{pmatrix}0&0&0&0&1\\0&0&0&-1&0\\0&0&1&0&0\\0&-1&0&0&0\\1&0&0&0&0\end{pmatrix}$	$\begin{pmatrix}0&1&0&0&0\\0&0&1&0&0\\0&0&0&1&0\\0&0&0&0&1\\0&0&0&0&0\end{pmatrix}$	

(2) If $T \lrcorner \omega$ is timelike for all timelike T then the normal form of ω is a composition of B_{II}, B_{IIa} or B_{IIb} ($\nu^2 \geqslant \xi^2$) with an Euclidean block consisting of blocks of the form $B(\mu)$ and/or a 0-block.

With *stabilizer* of a skew-adjoint operator (respectively, two-form) we mean in the following the subgroup of the (pseudo)-orthogonal group, which leaves the operator (respectively, the two-form) invariant under conjugated action. A simple consideration shows the following fact.

Lemma 4.5: The stabilizer of a normal form, which is built from a pseudo-Euclidean block of the form $B_{IIa}(\nu)$ or $B_{IIb}(\nu,\xi)$ and some Euclidean block of length $n-4$ is included in $\mathrm{U}(1,1) \times \mathrm{SO}(n-4)$ *for all eigenvalues ν and $\xi \neq 0$.*

Definition 4.6: Let $\mathbb{R}^{2,n-2}$ be the pseudo-Euclidean space of signature $(2,n-2)$ and $\omega \in \Lambda^2 \mathbb{R}^{2,n-2*}$ be a nontrivial two-form. We say that ω is of

- *Type (I_a) if $\omega = l_1^\flat \wedge l_2^\flat$ for some vectors l_1 and l_2, which span a totally lightlike plane.*
- *Type (I_b) if $\omega = l_1^\flat \wedge t_1^\flat$ for some lightlike vector l_1 and a l_1-orthogonal timelike vector t_1.*
- *Type (II_a) or Kähler type if ω is a nontrivial multiple of the standard Kähler form.*
- *Type (II_b) if there exists a nontrivial Euclidean subspace E in $\mathbb{R}^{2,n-2}$ such that ω restricted to E vanishes and ω is the (pseudo)-Kähler form on the orthogonal complement of E in $\mathbb{R}^{2,n-2}$.*

Lemma 4.5 makes clear, which stabilizers of the normal forms occurring in Corollary 4.4 are maximal.

Corollary 4.7: A two-form ω on $\mathbb{R}^{2,n-2}$, which is of types (I_a), (I_b), (II_a) or (II_b), is exclusively distinguished by its properties that

(1) the covector $T \lrcorner \omega$ is causal for every timelike vector $T \in \mathbb{R}^{2,n-2}$ and
(2) its stabilizer S_ω in $\mathrm{SO}(2,n-2)$ *is maximal, in the sense that there is no nontrivial two-form satisfying the first property, whose stabilizer properly contains S_ω.*

We observe that the stabilizer of a two-form of type (I_a) and type (I_b) acts indecomposable but reducible on $\mathbb{R}^{2,n-2}$, i.e., there exist nontrivial and invariant subspaces of $\mathbb{R}^{2,n-2}$, but the inner product is degenerate on all of them. The stabilizer of a Kähler-type form is $U(1,m-1)$ and acts irreducible on $\mathbb{R}^{2,2m-2}$. The stabilizer of a form of type (II_b) acts decomposable on $\mathbb{R}^{2,n-2}$.

V. IMAGINARY KILLING SPINORS

With the construction of the cone in Sec. III and the normal form classification for skew-adjoint operators in signature $(2,n-2)$ (coming from a spinor) in the preceding section we are now in the position to discuss a geometric description of Lorentzian manifolds admitting imaginary Killing spinors.

In the following, the metric g on the Lorentzian spin manifold $M^{n,1}$ will be scaled such that the Killing number λ to any Killing spinor satisfies $\lambda^2 = -\frac{1}{4}$. We start with a proposition, which characterizes the cone $\hat{M}$ of a Lorentzian manifold $M^{n,1}$ with imaginary Killing spinor and indicates the different cases that are to be considered for the geometry of the base manifold $M^{n,1}$. We remark that the normal form corresponding to a parallel two-form on the cone is in every point the same.

Proposition 5.1: Let $(M^{n,1},g)$ be a Lorentzian spin manifold admitting an imaginary Killing spinor. Then either there exists a parallel two-form ω of type (II_b) on the cone $\hat{M}$ or there exists at least one parallel (half) spinor $\hat{\varphi}$ on $\hat{M}$ such that the induced parallel two-form $\omega = \alpha^2_{\hat{\varphi}}$ is of types (I_a), (I_b) or (II_a).

Proof: Let ψ be an imaginary Killing spinor on $M^{n,1}$. According to Corollary 4.4 the normal form of the skew-adjoint endomorphism corresponding to $\alpha^2_{\hat{\psi}}$ on the cone is a composition with one block of the form B_{Ia}, B_{Ib}, B_{II}, B_{IIa} or B_{IIb}. In case that the normal form is built with a block of the form B_{Ia} or B_{Ib} the parallel two-form $\omega = \alpha^2_{\hat{\psi}}$ is of types (I_a) or (I_b).

In the other cases there exists a biggest number $s>0$ such that the stabilizer of the normal form to $\alpha^2_{\hat{\psi}}$ is included in $\mathrm{U}(1,s-1)\times\mathrm{SO}(n-2s)$. This group includes the holonomy group of the cone $\hat{M}$. In case that $2s=n$ the cone $\hat{M}$ is a Kähler spin manifold. Moreover, since $V^\flat_\psi=\partial_r\lrcorner\alpha^2_{\hat{\psi}}$ is everywhere timelike (Corollary 4.4), the base $M^{n,1}$ is Einstein and hence the cone is Ricci-flat. This implies that there exists a parallel half-spinor $\hat{\varphi}$, which induces a Kähler form on the cone. If $2s<n$ there exists a parallel two-form ω of type (II_b). □

We discuss now a description of the Lorentzian geometries on the base manifold $M^{n,1}$ with imaginary Killing spinor according to the cases (I_a), (I_b), and (II_a) that occur in Proposition 5.1.

A. Type (I_a)

In this case there exists a parallel (half) spinor $\hat{\varphi}$ on the cone $\hat{M}$, which induces a parallel two-form $\omega\neq 0$ that is locally of the form $l_1^\flat\wedge l_2^\flat$ for some lightlike vector fields l_1 and l_2, which span a totally lightlike plane. The dual $V^\flat_\varphi$ of the Dirac current of the imaginary Killing spinor φ, which corresponds to $\hat{\varphi}$ on $\hat{M}$, is equal to $\partial_r\lrcorner\omega$, which shows that the Dirac current V_φ is everywhere lightlike.

There is a known description of Lorentzian metrics admitting *twistor spinors* with lightlike Dirac current. We call a Lorentzian space admitting a lightlike parallel vector field a *Brinkmann space*. Two spinor fields on (pseudo)-Riemannian spaces are said to be *conformally equivalent* if there exists a conformal diffeomorphism, which identifies both spinor fields. In particular, it holds the following.

Proposition 5.2 (see Ref. 6): Let φ be a spinor field, which satisfies the twistor equation $\nabla^S_X\varphi+(1/n)\,X\cdot D\varphi=0$ for all vector fields X, such that the Dirac current V_φ is a lightlike Killing vector field on $M^{n,1}$. If $Ric(V_\varphi,V_\varphi)=0$ then φ is locally conformally equivalent to a parallel spinor on a Brinkmann space.

This gives rise to the following.

Proposition 5.3: Let φ be an imaginary Killing spinor on $M^{n,1}$ such that $\alpha^2_{\hat{\varphi}}$ on $\hat{M}$ is of type (I_a). Then φ is locally conformally equivalent to a parallel spinor on a Brinkmann space.

Proof: From Proposition 2.1 and Lemma 2.1 we know that $\mathrm{Ric}(V_\varphi)=\rho V_\varphi$ for some real function ρ. Then we can apply Proposition 5.2 to prove the result. □

B. Type (I_b)

There exists a parallel (half-) spinor $\hat{\varphi}$ on the cone $\hat{M}$, which induces a parallel two-form ω of type (I_b). In this situation it holds as follows.

Lemma 5.1: The function $f_\varphi:=\sqrt{-g(V_\varphi,V_\varphi)}$ to the imaginary Killing spinor φ on $M^{n,1}$ satisfies the following:

(1) $Hess(f_\varphi)=f_\varphi\cdot g$, i.e., grad f_φ is a conformal gradient field, and $f^2_\varphi=g(\mathrm{grad}\,f,\mathrm{grad}\,f)$,
(2) $\mathrm{grad}\,f_\varphi\neq 0$ and $f_\varphi\neq 0$ on disjoint subspaces, whose complements are dense in $M^{n,1}$.

Proof: The two-form ω can be written as $r\,\mathrm{d}r\wedge V^\flat_\varphi-(r^2/2)\,\mathrm{d}V^\flat_\varphi$ (Theorem 3.1). The two-dimensional parallel sub-bundle $E_\omega\subset TM^{n,1}$, which corresponds to the indecomposable two-form ω is degenerate and there is a unique parallel lightlike direction in E_ω. In particular, there exists a parallel lightlike vector field l_1 on $\hat{M}$. Moreover, we can find locally a timelike vector t_1 of constant length such that $\omega=l_1^\flat\wedge t_1^\flat$. We choose the parallel lightlike field l_1 with the scaling $\hat{g}(t_1,t_1)=-1$. Since l_1 is parallel, there is a unique function f on $M^{n,1}$ such that $l_1^\flat=f\,\mathrm{d}r-r\,\mathrm{d}f$ and $f^2=g(\mathrm{grad}\,f,\mathrm{grad}\,f)$. The function f is a special Killing 0-form on $M^{n,1}$, i.e., grad f is a conformal gradient field. Since neither dr nor the lift of df to the cone are parallel, it is $f\neq 0$ and $\mathrm{grad}\,f\neq 0$ on a dense subset of $M^{n,1}$.

We calculate the function f with respect to φ. The local field $t_1^\flat$ is given by $t_1^\flat=A\,\mathrm{d}r+ru$, where A is a function and u a one-form on $M^{n,1}$. It follows that $V^\flat_\varphi=fu+A\,\mathrm{d}f$ and

$$g(V_\varphi,V_\varphi)=f^2g(u,u)+A^2g(\mathrm{d}f,\mathrm{d}f)+2\,fA\cdot g(u,\mathrm{d}f).$$

Since $g(u,u)=-1+A^2$ and $g(u,\mathrm{d}f)=-Af$, we can conclude $f^2=-g(V_\varphi,V_\varphi)$, which shows that f_φ has the claimed properties. □

The assertions of Lemma 5.1 imply together with Proposition 2.2 that $M^{n,1}$ is Einstein and $\operatorname{grad} f_\varphi$ is a nonhomothetic conformal gradient field. There is a known description of (pseudo)-Riemannian Einstein metrics admitting such conformal fields. In particular, there is the following.

Proposition 5.4 (cf. Ref. 13): Let $(M^{n,1},g)$ be a Lorentzian Einstein space admitting a non-constant solution f of the equation $\mathrm{Hess}(f)=l\cdot g$ for some function l. Then, in a neighborhood of any point with $v:=g(\mathrm{grad}(f),\mathrm{grad}(f))\neq 0$, the metric g is a warped product $\varepsilon\cdot\mathrm{d}t^2+f'^2(t)k$, where $\varepsilon:=\mathrm{sign}(v)$, k is an Einstein metric and f satisfies

$$f''^2+\frac{\varepsilon\,\mathrm{scal}_g}{n(n-1)}f'^2=\frac{\varepsilon\,\mathrm{scal}_k}{(n-1)(n-2)}.$$

This leads to the following.

Proposition 5.5: Let φ be an imaginary Killing spinor on $M^{n,1}$ such that $\alpha^2_{\hat{\varphi}}$ on $\hat{M}$ is of type (I_b). Then, in a neighborhood of any point with V_φ timelike, the metric g is a warped product of the form $\mathrm{d}t^2+f^2k$, where k is a Lorentzian Einstein metric admitting a Killing spinor to the Killing number

(1) $\lambda_k=0$ *and* $f=\exp t$,
(2) $\lambda_k=\frac{1}{2}$ *and* $f=\sinh t$ or
(3) $\lambda_k=(i/2)$ *and* $f=\cosh t$.

Proof: The function $f_\varphi=\sqrt{-g(V_\varphi,V_\varphi)}$ satisfies the assumptions of Proposition 5.4. Since $f_\varphi^2>0$, the warping function $f=f'_\varphi$ must solve the ordinary differential equation $f'^2-n(n-1)f^2=\mathrm{scal}_k$. There are three different solutions $f=\exp t$, $\cosh t$ and $\sinh t$ according to the values $\mathrm{scal}_k=0,\pm(n-1)(n-2)$. In each case the imaginary Killing spinor φ induces a Killing spinor to the Killing number $\mathrm{scal}_k/(n-1)(n-2)$ on the space with Einstein metric k (cf. Ref. 9). □

C. Type (II_a)

Lemma 5.2: Let $(M^{n,1},g)$ be a Lorentzian Einstein manifold with a Killing vector V such that $g(V,V)=-1$ is constant and $V\lrcorner\mathcal{W}=0$ ($\mathcal{W}$ Weyl tensor). Then the operator J defined by $J(X):=\nabla_X V$ on TM satisfies

(1) $J(V)=0$ *and* $J^2(X)=\mathrm{scal}/[n(n-1)]\,(X+g(V,X)V)$,
(2) $(\nabla_X J)(Y)=\mathrm{scal}/n(n-1)\,(g(V,Y)X-g(X,Y)V)$.

Proof: Because V is Killing with constant length, it follows $\nabla_V V=0$ and $g(\nabla_X V,\nabla_Y V)=\mathcal{R}(V,X,Y,V)$, where $\mathcal{R}$ denotes the Riemannian curvature tensor. It is $\mathcal{R}=\mathcal{W}+g\owedge L$, where

$$L=\frac{1}{n-2}\left(\frac{\mathrm{scal}}{2(n-1)}g-\mathrm{Ric}\right)$$

is the Schouten tensor and $\owedge$ denotes the Kulkarni–Nomizu product (cf. Ref. 7). Then from $V\lrcorner\mathcal{W}=0$ we obtain

$$\begin{aligned}g(J^2(X),Y)&=-g(J(X),J(Y))\\&=-g(V,Y)L(X,V)-g(V,X)L(Y,V)\\&\quad-L(X,Y)+g(X,Y)L(V,V)\ .\end{aligned}$$

The relation for J^2 follows immediately, since for $M^{n,1}$ an Einstein space it holds

$$L=-\frac{\mathrm{scal}}{2(n-1)n}g.$$

Moreover, it is $g(\nabla_{e_k}\nabla_{e_i}V,e_j)=\mathcal{R}(e_i,e_j,e_k,V)$ for all $i,j,k\in\{1,\ldots,n\}$ in $p\in M^{n,1}$ arbitrary, where $(e_1,\ldots,e_n)$ is a local parallel frame in p. Then

$$\begin{aligned}g((\nabla_{e_i}J)(e_k),e_l)&=\mathcal{R}(e_k,e_l,e_i,V)\\&=g(e_k,e_i)L(e_l,V)+g(e_l,V)L(e_k,e_i)\\&\quad-g(e_k,V)L(e_l,e_i)-g(e_l,e_i)L(e_k,V)\ ,\end{aligned}$$

which shows the identity for ∇J in an arbitrary point p of $M^{n,1}$. □

A Lorentzian manifold $(M^{n,1},g,V)$ with V a timelike Killing vector of constant length such that the operator $J=\nabla V$ satisfies the both properties of Lemma 5.2, is called a Lorentzian Sasaki manifold. It is well known that a Sasaki structure (V,J) on $M^{n,1}$ corresponds to a Kähler structure on the cone $\hat{M}$ (cf. Refs. 1 and 4).

Proposition 5.6: A Lorentzian spin manifold $(M^{n,1},g)$ with an imaginary Killing spinor φ, whose Dirac current V_φ is timelike and has constant length, is a Lorentzian Einstein–Sasaki manifold. This is exactly the case when the lift $\hat{\varphi}$ induces a Kähler form on the cone $\hat{M}$.

Proof: We have only to show that $V_\varphi\lrcorner\mathcal{W}=0$ on $M^{n,1}$ and then apply Lemma 5.2. With the identity $\mathcal{W}(\eta)\cdot\varphi=0$ (Proposition 2.1) and the relation $X\cdot\eta=-X\lrcorner\eta+X^\flat\wedge\eta$ in the Clifford algebra, where X denotes a vector and η a two-form, we obtain

$$\mathcal{W}(V_\varphi,X,Y,Z)=\langle\varphi,\mathcal{W}(X,Y,Z)\cdot\varphi\rangle=\langle\varphi,Z^\flat\wedge\mathcal{W}(X,Y)\cdot\varphi\rangle\in\mathbb{R}\ \text{ for all }\ X,Y,Z\in TM.$$

But $\langle\varphi,\rho^3\cdot\varphi\rangle\in i\mathbb{R}$ for all three-forms ρ^3, and therefore $V_\varphi\lrcorner\mathcal{W}=0$. □

We summarize the different cases as follows.

Theorem 5.3: *Let $(M^{n,1},g)$ be a Lorentzian spin manifold with imaginary Killing spinor φ.*

(1) If $M^{n,1}$ is not Einstein then $M^{n,1}$ is locally conformally equivalent to a Brinkmann space with parallel spinor.

(2) If $g(V_\varphi,V_\varphi)$ is constant then

- *(i) $g(V_\varphi,V_\varphi)=0$ and $M^{n,1}$ is locally conformally equivalent to a Brinkmann space with parallel spinor or*
- (ii) *$g(V_\varphi,V_\varphi)<0$ and $M^{n,1}$ is a Lorentzian Einstein–Sasaki manifold.*

(3) If the cone $\hat{M}$ is indecomposable and V_φ does not change the causal type then M is either

- *(i) locally conformally equivalent to a Brinkmann space with parallel spinor,*
- (ii) *locally a warped product of the form $\mathrm{d}t^2+f^2k$, where k is a Lorentzian Einstein metric admitting a Killing spinor and $f=\exp t$, $\cosh t$ or $\sinh t$ or*
- *(iii) a Lorentzian Einstein–Sasaki space (and the cone $\hat{M}$ is irreducible).*

(4) If V_φ changes the causal type then the set $Z_\varphi\subset M^{n,1}$, where V_φ is lightlike, is a hypersurface and $M^{n,1}\backslash Z_\varphi$ admits locally a warped product structure as in (3)(ii).

In case that the metric g does not belong to one of those listed in (3), then either V_φ changes the causal type or there is a parallel two-form of type (II_b) on the cone $\hat{M}$.

Remark 5.4:

(1) In fact, there exist examples of imaginary Killing spinors on non-Einstein spaces, which are generated by an appropriate conformal change of certain non-Einstein Brinkmann spaces with parallel spinors (cf. Ref. 9).

(2) *Partial structure results and examples for Lorentzian metrics with parallel or real Killing spinors are known (cf., e.g., Refs. 8 and 9). The warped product structure in case of type* (I_b) *then provides a construction principle for imaginary Killing spinors on Lorentzian spaces. The complete result in Ref. 13 for the description of Einstein spaces with conformal gradient fields does not apply when the field changes the causal type. A characterization in this case is not known and as consequence, Theorem 5.3 does not describe Lorentzian metrics with imaginary Killing spinors when the Dirac current changes the causal type*.

(3) *There is a construction principle for Lorentzian Einstein–Sasaki spin spaces. They appear as* S^1*-fiber bundles over Riemannian Kähler–Einstein spin spaces of negative scalar curvature (cf. Ref. 4).*

(4) *In case that there exists a parallel two-form of type* (II_b) *the cone* $\hat{M}$ *is decomposable. Different from the Riemannian case, this does not imply that the cone is flat, even if the base* $M^{n,1}$ *is geodesically complete. The geometry of the base* $M^{n,1}$ *with imaginary Killing spinor in this case remains to be investigated and is subject of a forthcoming paper*.

Example 5.5: Let $H^{n,1}:=\{x\in\mathbb{R}^{2,n-1}:\|x\|^2=-1\}\subset\mathbb{R}^{2,n-1}$ be the pseudohyperbolic space of signature $(1,n-1)$ with negative scalar curvature $\mathrm{scal}=-n(n-1)$. The space $H^{n,1}$ is geodesically complete, time-orientable and spin. The cone over $H^{n,1}$ is an open subset of $\mathbb{R}^{2,n-1}$. Each parallel (half) spinor on $\mathbb{R}^{2,n-1}$ restricted to $H^{n,1}$ gives rise to an imaginary Killing spinor. It is not difficult to see that every generic type (I_a), (I_b), (II_a), and (II_b) is realized by a two-form, which comes from a parallel (half) spinor on $\mathbb{R}^{2,n-1}$ and thus belongs to an imaginary Killing spinor on $H^{n,1}$. This means that there are examples of imaginary Killing spinors on $H^{n,1}$, $n\geqslant 3$, for each single case when the Dirac current is everywhere lightlike (I_a), changes the causal type (I_b), timelike with constant length (II_a) or everywhere timelike with nonconstant length.

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A matrix model for the β-Jacobi ensemble

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(Received 12 March 2003; accepted 20 May 2003)

This note presents a random matrix model for general ($\beta>0$) β-Jacobi ensembles. This generalizes the well-known MANOVA models for $\beta=1,2,4$ and eliminates the quantization of β (and other parameters) present in the previously known models. This model is a partial answer to an open problem presented by Dumitriu and Edelman, where they also presented models for the β-Laguerre and β-Hermite ensembles. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604184]

I. INTRODUCTION

Classical random matrix theory is concerned with various joint distributions of matrix properties (e.g., eigenvalues and singular values) for matrices given by some distribution. The three classical joint distributions of matrix eigenvalues are the Hermite, Laguerre, and Jacobi distributions, which generalize the single variable Gaussian, Poisson, and beta distributions, respectively (see Ref. 7). These distributions capture the statistical properties of *log-potential* gases (see Refs. 6 and 3) where β is analogous to temperature.

Analytic formulas relating to these distributions were derived by Dyson[2] over real, complex, and quaternion matrix elements. The numerical type of the matrix element was nearly irrelevant, appearing only as a single exponent β which was 1 (real), 2 (complex), or 4 (quaternion). While the formulas remain valid for more general β (real $\beta>0$), it was unknown whether random matrix models existed for such distributions.

Recently, Dumitriu and Edelman[1] have demonstrated that two of the classical distributions, the Laguerre and the Hermite, have random matrix models for general β, thereby removing the artificial ''quantization effect'' of the numerical type from Dyson's formulas. The models were given in the form of real bidiagonal and tridiagonal matrices with independent random entries given by certain (β dependent) χ distributions.

The question of the Jacobi model remained. No matrix model has yet been found which generates eigenvalues under the Jacobi distribution for a more general set of β. This note presents a model of the Jacobi for general β employing a *random rank-1 update* recurrence scheme.

In the following section, I briefly present a review of the β-ensemble results of Dumitriu and Edelman, highlighting two important theorems which I am borrowing from their work. Because the model I present is of a fairly different character than the ones Dumitriu and Edelman presented for the other two ensembles, I present a motivational section, showing how the form of this model came about. Finally, the last section gives a proof of the correctness of this model.

A. Background

Let us denote by N_v a real normally distributed, random variable with zero mean and variance v, and by χ_m a chi distributed, random variable with m degrees of freedom. Note $dens(\chi_m=y)\propto y^{m-1}e^{-(1/2)y^2}$, where m and y may be any positive real. Every single occurrence of a χ or N symbol in the formulas below is independent.

Let us define a *Gaussian* matrix over a field ($\mathbb{R}$ or $\mathbb{C}$) or skew field ($\mathbb{H}$) to be a random matrix whose elements are generated by independent, normally distributed Gaussian random processes G_β (N_1 for real, N_1+iN_1 for complex, and $N_1+iN_1+jN_1+kN_1$ for quaternions). A^* denotes the

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appropriate involution: transpose, Hermitian transpose, or symplectic transpose. Throughout, we will use words like *orthogonal* and *orthonormal* to stand for the appropriate term (e.g., *unitary*) for the appropriate β. Finally, in any equations giving probability densities, we omit the normalizing constants.

Let $\beta=1,2,4$ for $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$, respectively. The m-eigenvalues of a "symmetrized" $m\times m$ Gaussian matrix, $\frac{1}{2}(A+A^*)$, give the β-Hermite ensemble, which has the distribution

$$dens(\lambda_1,\ldots,\lambda_m)=\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_{i=1}^m e^{-(1/2)\lambda_i^2}.$$

The m-eigenvalues of a "squared" $n\times m$ Gaussian matrix, A^*A, give the β-Laguerre ensemble, which has the distribution

$$dens(\lambda_1,\ldots,\lambda_m)=\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_{i=1}^m \lambda_i^a e^{-(1/2)\lambda_i},$$

where $a=\frac{1}{2}\beta(n-m+1)-1, n\geqslant m$ and $\lambda_i>0$.

Finally, there is the β-Jacobi ensemble (also called MANOVA in Ref. 7), which can be modeled as the eigenvalues of the $m\times m$ matrix

$$(A^*A+B^*B)^{-1}A^*A$$

formed from two Gaussian random matrices, A and B, which are $n_1\times m$ and $n_2\times m$ (resp.). These eigenvalues are always real, bounded between 0 and 1, and are distributed according to

$$dens(\lambda_1,\ldots,\lambda_n)=\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_{i=1}^m \lambda_i^a(1-\lambda_i)^b,$$

where $a=\frac{1}{2}\beta(n_1-m+1)-1$, $b=\frac{1}{2}\beta(n_2-m+1)-1$, and $m-1<n_1,n_2$.

These are valid distributions for $\beta>0$ and more general a and b, yet the Gaussian matrix based models above can only be applied when β is 1,2,4 and a,b are in correspondence with the integers. The first models for general β,a,b were found by Edelman and Dumitriu in 2002.[1] They showed that a random tridiagonal matrix,

$$T=\frac{1}{\sqrt{2}}\begin{pmatrix} N_2 & \chi_{(m-1)\beta} & 0 & \cdots & 0 & 0 \\ \chi_{(m-1)\beta} & N_2 & \chi_{(m-2)\beta} & \cdots & 0 & 0 \\ 0 & \chi_{(m-2)\beta} & N_2 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \chi_\beta & N_2 \end{pmatrix},$$

has eigenvalues distributed according to the β-Hermite distribution. They also showed that the eigenvalues of LL^* for a random bidiagonal matrix,

$$L=\begin{pmatrix} \chi_{2a+(m-1)\beta} & 0 & 0 & \cdots & 0 & 0 \\ \chi_{(m-1)\beta} & \chi_{2a+(m-2)\beta} & 0 & \cdots & 0 & 0 \\ 0 & \chi_{(m-2)\beta} & \chi_{2a+(m-3)\beta} & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \chi_\beta & \chi_{2a} \end{pmatrix}, \tag{1}$$

has eigenvalues distributed according to the β-Laguerre distribution.

These results give models for the β-Hermite and β-Laguerre distributions in terms of sparse random matrices, and are thus expected to be computationally more efficient in addition to being more general than the Gaussian matrix models which first motivated them. They have the feature that the corresponding characteristic polynomials can be calculated by a random three term recurrence, generalizing classical three term recurrences satisfied by the Hermite and Laguere polynomials, respectively. From this perspective, the general β-Jacobi ensemble has been constructed (see Ref. 4), but an associated tridiagonal matrix was not found.

B. Motivation and essential result

This section will present and provide the motivation for the matrix model presented for the general β-Jacobi distribution. We will start with the more restricted Gaussian matrix model and reduce it to a model in which the dependence on β,a,b is continuous. This merely gives an alternate model for the β-Jacobi distribution which is guaranteed to be valid for the same set of β,a,b for which the Gaussian matrix model was valid. The proof of its more general validity is in the next section.

We first reformulate the model in a way that avoids the ''squaring'' of the A and B Gaussian matrices. We will assume generic properties of the A and B such as their being full rank. Then

$$(A^*A+B^*B)^{-1}A^*A=(I+(A^*A)^{-1}B^*B)^{-1},$$

allowing us to model the β-Jacobi eigenvalues, λ_i', with the eigenvalues, λ_i, of $(A^*A)^{-1}B^*B$ via the relation $\lambda_i'=1/(1+\lambda_i)$.

Let $A=Q_AR_A^*$ where Q_A is orthogonal and R_A^* $m\times m$ lower triangular, and let $B=Q_BR_B^*$ with Q_B orthogonal and R_B $m\times m$ lower triangular. Then $A^*A=R_AR_A^*$ and $B^*B=R_BR_B^*$, so

$$(A^*A)^{-1}B^*B=(R_AR_A^*)^{-1}R_BR_B^*=(R_A^*)^{-1}R_A^{-1}R_BR_B^*\sim R_A^{-1}R_BR_B^*(R_A^*)^{-1}=(R_A^{-1}R_B)(R_A^{-1}R_B)^*.$$

Thus we see that the eigenvalues of $(A^*A)^{-1}B^*B$ are the squares of the m singular values, σ_i, of $R_A^{-1}R_B$.

We have employed factorizations for A and B into orthogonal and lower triangular matrices. There are a number of ways to carry out such factorizations. The one which we will employ is the QL-decomposition, where one applies a Gramm–Schmidt process starting at the last column and works back to the first. We state without proof an elementary result regarding the distribution of the L factor.

Lemma 1.1 (QL-factorization): Let A be an $n\times m$ Gaussian matrix with $n\geqslant m$. Let $QL=A$ be the QL-factorization. Then L is an $m\times m$ matrix distributed as

$$L=L^{(n,m)}=\begin{pmatrix} \chi_{(n-m+1)\beta} & 0 & 0 & \cdots & 0 \\ G_\beta & \chi_{(n-m+2)\beta} & 0 & \cdots & 0 \\ G_\beta & G_\beta & \chi_{(n-m+3)\beta} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ G_\beta & G_\beta & G_\beta & \cdots & \chi_{n\beta} \end{pmatrix}.$$

It follows that with $Q_AR_A^*$ the QL-factorization of A, R_A is then distributed as $L^{(n_1,m)*}$. Similarly, R_B is distributed as $L^{(n_2,m)*}$. However, it is to our advantage to specify the latter as the equivalent matrix distribution $R^{(n_2,m)}$ specified by

$$R^{(n,m)} = PL^{(n,m)}P = \begin{pmatrix} \chi_{n\beta} & G_\beta & G_\beta & \cdots & G_\beta \\ 0 & \chi_{(n-1)\beta} & G_\beta & \cdots & G_\beta \\ 0 & 0 & \chi_{(n-2)\beta} & \cdots & G_\beta \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \chi_{(n-m+1)\beta} \end{pmatrix},$$

where P denotes the reverse permutation, $P_{i,n-i+1}=1$, $P_{i,j}=0$ otherwise.

Let $Q_A R_A^*$ be the QL-decomposition of A, with R_A then distributed as $L^{(n_1,m)*}$, and $Q_B P R_B P$ be the QL-decomposition of B, with R_B then distributed as $R^{(n_2,m)}$.

We note the following recurrences for R_A and R_B:

$$R_A = \begin{pmatrix} a & \vec{a} \\ 0 & \tilde{R}_A \end{pmatrix},$$

$$R_B = \begin{pmatrix} b & \vec{b} \\ 0 & \tilde{R}_B \end{pmatrix},$$

where $a=\chi_{\beta(n_1-m+1)}$, $\vec{a}=[G_\beta \cdots G_\beta]$, $\tilde{R}_A = L^*_{n_1,m-1}$, $b=\chi_{\beta n_2}$, $\vec{b}=[G_\beta \cdots G_\beta]$, and $\tilde{R}_B = R^{(n_2-1,m-1)}$ (here, use has been made of the fact that G_β and $\overline{G_\beta}$ have the same distribution). Thus,

$$R_A^{-1}R_B = \begin{pmatrix} b/a & \vec{b}/a - \vec{a}\tilde{R}_A^{-1}\tilde{R}_B \\ 0 & \tilde{R}_A^{-1}\tilde{R}_B \end{pmatrix}. \tag{2}$$

At this point we see the basis for a recursive scheme. The lower right block of Eq. (2) is another instance of the same expression with parameters $\tilde{m}=m-1$, $\tilde{n}_1=n_1$ and $\tilde{n}_2=n_2-1$.

Let $\tilde{U}\tilde{\Sigma}\tilde{V}^* = \tilde{R}_A^{-1}\tilde{R}_B$ be the SVD of the lower right block. Then

$$\begin{pmatrix} 1 & 0 \\ 0 & \tilde{U}^* \end{pmatrix} R_A^{-1}R_B \begin{pmatrix} 1 & 0 \\ 0 & \tilde{V} \end{pmatrix} = \begin{pmatrix} b/a & \frac{1}{a}(\vec{b}\tilde{V} - \vec{a}\tilde{U}\tilde{\Sigma}) \\ 0 & \tilde{\Sigma} \end{pmatrix}.$$

The elements of $\tilde{\Sigma}$ are related to a β-Jacobi distribution with parameters $\tilde{n}_1$ and $\tilde{n}_2$. Since the density of Gaussian vectors, $\vec{a}$, $\vec{b}$, is invariant under orthogonal transformations, $\vec{b}\tilde{V} - \vec{a}\tilde{U}\tilde{\Sigma} = [G_\beta \cdots G_\beta](I+\Sigma^2)^{1/2}$. Thus

$$B = \begin{pmatrix} \frac{1}{\chi_{(n_1-m+1)\beta}} & [\chi_{n_2\beta}(1+\sigma_1^2)^{1/2}G_\beta \cdots (1+\sigma_{m-1}^2)^{1/2}G_\beta] \\ 0 & \mathrm{diag}(\sigma_1, \ldots, \sigma_{m-1}) \end{pmatrix} \tag{3}$$

has singular values which are distributed according to the β-Jacobi distribution with parameters n_1, n_2, if $\sigma_1, \ldots, \sigma_{m-1}$ are distributed as the $m-1$ singular values related to another β-Jacobi distribution with parameters n_1, n_2-1.

To remove the last integral dependence of Eq. (3) on β, we can, by a similarity transformation, remove the phases from the G_β, replacing them with real $|G_\beta| = \chi_\beta$ distributions.

II. DETAILS OF THE DUMITRIU AND EDELMAN RESULTS

The proofs of the Hermite and Laguerre results[1] rest on two lemmas about the relation of tridiagonal matrices to their eigenvalues and eigenvectors, which we will now review.

Given a real diagonal matrix Λ with m-eigenvalues, λ_i, and a real unit vector $\hat{v}$, a symmetric tridiagonal matrix can be generated by the familiar recurrence (see Chap. 9 of Ref. 5):

$$T_{k,k}=(\Lambda\hat{v}^{(k)}-T_{k+1,k}\hat{v}^{(k+1)})^t\hat{v}^{(k)},\quad k=m,\ldots,2,$$

$$T_{k,k-1}\hat{v}^{(k-1)}=\Lambda\hat{v}^{(k)}-T_{k+1,k}\hat{v}^{(k+1)}-T_{k,k}\hat{v}^{(k)},\quad k=m,\ldots,2,$$

with

$$T_{m,m}=\hat{v}^t\Lambda\hat{v},$$

$$\hat{v}^{(m)}=\hat{v},$$

giving the tridiagonal elements, $\delta_k=T_{k,k}$ and $\nu_k=T_{k+1,k}$, and a sequence of orthogonal unit vectors, $\hat{v}^{(k)}$, which form the orthogonal eigenvector matrix, $Q=[\hat{v}^{(m)},\hat{v}^{(m-1)},\ldots,\hat{v}^{(1)}]^t$, such that $T=Q^t\Lambda Q$. This mapping, $T:(\lambda_i,\hat{v})\rightarrow(\delta_i,\nu_i)$, is a bijection when the λ_i are distinct and ordered, and the elements of $\hat{v}$ are non-negative. Two lemmas highlight important properties of this mapping.

The first result gives a useful expression for the Jacobian of the tridiagonalization mapping.

Lemma 2.1: Tridiagonal Jacobian. Given m ordered distinct real values, λ_i, and a unit vector, $\hat{v}$, with non-negative elements, the mapping $T:(\lambda_i,\hat{v})\rightarrow(\delta_i,\nu_i)$ is a diffeomorphism with Jacobian given by

$$J=\frac{\partial(\delta_i,\nu_i)}{\partial(\lambda_i,\hat{v}_i)}=\frac{\Pi_{i=1}^{m-1}\nu_i}{\Pi_{i=1}^{m}\hat{v}_i}.$$

The second result expresses the product of differences of the λ_i in terms of $\hat{v}$ and the tridiagonal coefficients.

Lemma 2.2: Vandermonde Identity. Given n eigenvalues λ_i and a unit vector $\hat{v}$, let (δ_i,ν_i) be the coefficients of the associated tridiagonal matrix, $T(\Lambda,\hat{v})$. Then

$$\prod_{i<j}|\lambda_i-\lambda_j|=\frac{\Pi_{i=1}^{m-1}\nu_i^i}{\Pi_{i=1}^{m}\hat{v}_i}.$$

III. PROOF OF THE β-JACOBI RESULT

The starting point for this proof will be the reformulation of the Jacobi model originally supported on $0<\lambda<1$, to be supported on $0\leqslant\lambda<\infty$ with the change of variable, $\lambda'=1/(1+\lambda)$.

Definition 3.1 (modified Jacobi model): The modified Jacobi model *with parameters β,n_1,n_2 is the distribution on m variables λ_i with density:*

$$dens(\lambda_i;n_1,n_2,m,\beta)=\Delta(\lambda_i)^\beta\prod_i\frac{\lambda_i^{(1/2)\beta(n_2-m+1)-1}}{(1+\lambda_i)^{(1/2)\beta(n_1+n_2)}},$$

where $\Delta(\lambda_i)=\Pi_{i<j}|\lambda_i-\lambda_j|$ and $0\leqslant\lambda<\infty$.

Lemma 3.2: The m values λ_i are distributed according to the modified Jacobi model with parameters β,n_1,n_2, iff $\lambda_i'=1/(1+\lambda_i)$ are distributed according to the density

$$dens(\lambda_1',\ldots,\lambda_m')=\prod_{i<j}|\lambda_i'-\lambda_j'|^\beta\prod_i(\lambda_i')^{(1/2)\beta(n_1-m+1)-1}(1-\lambda_i')^{(1/2)\beta(n_2-m+1)-1}.$$

Proof: Let $X=1/2\beta(n_1-m+1)-1$, and $Y=1/2\beta(n_2-m+1)-1$. By change of variables,

$$dens(\lambda_1',\ldots,\lambda_m')\prod_i d\lambda_i'=\prod_{i<j}|\lambda_i'-\lambda_j'|^\beta\prod_i(\lambda_i')^X(1-\lambda_i')^Y\prod_i d\lambda_i',$$

$$dens(\lambda_1,\ldots,\lambda_m)\prod_i\frac{d\lambda_i}{(1+\lambda_i)^2}=\prod_{i<j}\left|\frac{1}{1+\lambda_i}-\frac{1}{1+\lambda_j}\right|^\beta\prod_i\left(\frac{1}{1+\lambda_i}\right)^X\left(\frac{\lambda_i}{1+\lambda_i}\right)^Y\prod_i d\lambda_i,$$

$$\begin{aligned}dens(\lambda_1,\ldots,\lambda_m)\prod_i d\lambda_i&=\prod_{i<j}\left|\frac{\lambda_i-\lambda_j}{(1+\lambda_i)(1+\lambda_j)}\right|^\beta\prod_i\frac{\lambda_i^Y}{(1+\lambda_i)^{X+Y+2}}\prod_i d\lambda_i\\&=\prod_i\left(\frac{1}{1+\lambda_i}\right)^{X+Y+\beta(m-1)+2}\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_i\lambda_i^Y\prod_i d\lambda_i.\end{aligned}$$

□

We now prove a recurrence for the modified Jacobi model.

Theorem 3.3: *Let B be an $m\times m$ random matrix generated as follows:*

$$B=\begin{pmatrix}b/a & \vec{w}/a\\ 0 & \sqrt{\Theta}\end{pmatrix},$$

where $a=\chi_{\beta(n_1-m+1)}$, $b=\chi_{\beta n_2}$, $\vec{w}=(\sqrt{1+\theta_1}\chi_\beta,\ldots,\sqrt{1+\theta_{m-1}}\chi_\beta)$, *and* $\sqrt{\Theta}=\mathrm{diag}(\sqrt{\theta_1},\ldots,\sqrt{\theta_{m-1}})$ *where the $m-1$ values θ_i are distributed according to the modified Jacobi distribution, $dens(\theta_i;n_1,n_2-1,m-1,\beta)$. Then the eigenvalues of B^tB are distributed according to the Jacobi model with parameters (n_1,n_2,m,β).*

Moreover, B^tB is similar to the tridiagonal matrix

$$\begin{pmatrix}\delta & \nu & 0 & \cdots & 0\\ \nu & \delta_{m-1}+\dfrac{\nu^2}{\delta} & \nu_{m-2} & \cdots & 0\\ 0 & \nu_{m-2} & \delta_{m-2} & \cdots & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & 0 & \cdots & \delta_2 & \nu_1\\ 0 & 0 & \cdots & \nu_1 & \delta_1\end{pmatrix},$$

where

$$\delta=(b/a)^2,\quad \nu=(b/a^2)\|\vec{w}\|,$$

and (δ_i,ν_i), $i=1,\ldots,m-1$, are the tridiagonal matrix entries constructed from the $m-1$ positive eigenvalues, θ_i, and the unit vector $\hat{w}$ according to the recurrence given at the beginning of Sec. II.

Proof: We have that the density of B in terms of a,b,w, and θ_i [from the $(m-1)\times(m-1)$ submatrix Θ] is given by

$$dens(a,b,w,\theta_i)=b^{\beta n_2-1}e^{-b^2}a^{\beta(n_1-m+1)-1}e^{-a^2}\left(\prod_i\frac{w_i^{\beta-1}}{(1+\theta_i)^{(1/2)\beta}}\right)e^{-\Sigma_i[w_i^2/(1+\theta_i)]}D(\theta_i),$$

where $D(\theta_i)=dens(\theta_i;n_1-1,n_2,m-1,\beta)$.

Making a change of variables $x=b/a, z_i=w_i/a$ so that

$$B=\begin{pmatrix} x & z \\ 0 & \sqrt{\Theta} \end{pmatrix},$$

we have

$$dens(x,a,z,\theta_i)=(xa)^{\beta n_2-1}e^{-(xa)^2}a^{\beta(n_1-m+1)-1}e^{-a^2}\left(\prod_i \frac{(az_i)^{\beta-1}}{(1+\theta_i)^{(1/2)\beta}}\right)$$
$$\times e^{-\Sigma_i[(az_i)^2/(1+\theta_i)]}D(\theta_i)a^m,$$

which simplifies to

$$dens(x,a,z,\theta_i)=a^{\beta(n_2+n_1)-1}e^{-a^2(1+x^2+\Sigma_i[z_i^2/(1+\theta_i)])}x^{\beta n_2-1}\left(\prod_i \frac{z_i^{\beta-1}}{(1+\theta_i)^{(1/2)\beta}}\right)D(\theta_i).$$

Since a no longer appears explicitly in B it may be integrated out to give the density of B:

$$dens(x,z,\theta_i)=x^{\beta n_2-1}\left(1+x^2+\sum_i \frac{z_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}\left(\prod_i \frac{z_i^{\beta-1}}{(1+\theta_i)^{(1/2)\beta}}\right)D(\theta_i).$$

Given the positivity of x,z_i,θ_i there is a one-to-one mapping from B to B^tB given by

$$B^tB=\begin{pmatrix} x^2 & xz \\ xz^t & \Theta+zz^t \end{pmatrix}=\begin{pmatrix} \delta & v \\ v^t & \Theta+\frac{1}{\delta}vv^t \end{pmatrix},$$

where $\delta=x^2$, $v_i=xz_i$. Making this change of variables, we find that the density for B^tB is given by

$$dens(\delta,v,\theta_i)=\delta^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta+\frac{1}{\delta}\sum_i \frac{v_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}$$
$$\times\prod_i v_i^{\beta-1}\prod_i (1+\theta_i)^{-(1/2)\beta}D(\theta_i).$$

We may express the vector v as a product of a unit vector and its magnitude, $v=\nu\hat{v}$, and make the change of variables,

$$dens(\delta,\nu,\hat{v},\theta_i)=\delta^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta+\frac{\nu^2}{\delta}\sum_i \frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}$$
$$\times\nu^{\beta(m-1)-1}\prod_i \hat{v}_i^{\beta-1}\prod_i (1+\theta_i)^{-(1/2)\beta}D(\theta_i).$$

Substituting the induction,

$$dens(\delta,\nu,\hat{v},\theta_i)=\delta^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta+\frac{\nu^2}{\delta}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}\nu^{\beta(m-1)-1}$$
$$\times\prod_i\hat{v}_i^{\beta-1}\prod_i(1+\theta_i)^{-(1/2)\beta}\Delta(\theta_i)^\beta\frac{(\Pi_i\theta_i)^{(1/2)\beta(n_2-m+1)-1}}{(\Pi_i(1+\theta_i))^{(1/2)\beta(n_2+n_1-1)}}.$$

Since $\theta_i>0$ and $\hat{v}$ is a unit vector with positive entries, the tridiagonal mapping is one-to-one. Let (δ_i,ν_i) be given by

$$T_2=\begin{pmatrix}\delta_{m-1}&\nu_{m-2}&0&\cdots&0\\ \nu_{m-2}&\delta_{m-2}&\nu_{m-3}&\cdots&0\\ 0&\nu_{m-3}&\delta_{m-3}&\cdots&0\\ \cdots&\cdots&\cdots&\cdots&\cdots\\ 0&0&\cdots&\delta_2&\nu_1\\ 0&0&\cdots&\nu_1&\delta_1\end{pmatrix}=T(\theta_i,\hat{v})$$

with, according to Lemma 2.1, the Jacobian given by

$$J=\frac{\partial(\delta_i,\nu_i)}{\partial(\theta_i,\hat{v}_i)}=\frac{\Pi_{i=1}^{m-2}\nu_i}{\Pi_{i=1}^{m-1}\hat{v}_i}.$$

Let Q_2 be the eigenvector matrix of $T(\theta_i,\hat{v})$ with $\hat{v}$ as the first row. Let

$$Q_1=\begin{pmatrix}1&0\\0&Q_2\end{pmatrix}.$$

Then

$$T_1=Q_1B^tBQ_1^t=\begin{pmatrix}\delta&\nu&0&\cdots&0\\ \nu&\delta_{m-1}+\frac{\nu^2}{\delta}&\nu_{m-2}&\cdots&0\\ 0&\nu_{m-2}&\delta_{m-2}&\cdots&0\\ \cdots&\cdots&\cdots&\cdots&\cdots\\ 0&0&\cdots&\delta_2&\nu_1\\ 0&0&\cdots&\nu_1&\delta_1\end{pmatrix}$$

is a tridiagonalization of B^tB. We change variables from $\theta_i,\hat{v}$ to δ_i,ν_i, setting $\delta_m=\delta$ and $\nu_{m-1}=\nu$, obtaining

$$dens(\delta_i,\nu_i)=\delta_m^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta_m+\frac{\nu_{m-1}^2}{\delta_m}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}\nu_{m-1}^{\beta(m-1)}$$
$$\times\prod_i\hat{v}_i^\beta\Delta(\theta_i)^\beta\frac{\det(T_2)^{(1/2)\beta(n_2-m+1)-1}}{\det(I+T_2)^{(1/2)\beta(n_2+n_1)}}\prod_i\frac{1}{\nu_i},$$

where some expressions have been left in terms of θ_i and $\hat{v}$, though as functions of δ_i,ν_i.

Expanding $\Delta(\theta_i)$ with the Vandermonde identity according to Lemma 2.2,

$$\Delta(\theta_i)=\frac{\Pi_i\nu_i^i}{\Pi_i\hat{v}_i},$$

shows

$$dens(\delta_i,\nu_i)=\delta_m^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta_m+\frac{\nu_{m-1}^2}{\delta_m}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}\nu_{m-1}^{\beta(m-1)-1}$$
$$\times\frac{\det(T_2)^{(1/2)\beta(n_2-m+1)-1}}{\det(I+T_2)^{(1/2\beta(n_2+n_1)}}\prod_{i=1}^{m-2}\nu_i^{\beta i-1},$$

which simplifies to

$$dens(\delta_i,\nu_i)=\delta_m^{(1/2)\beta(n_2-m+1)-1}\left(1+\delta_m+\frac{\nu_{m-1}^2}{\delta_m}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}$$
$$\times\frac{\det(T_2)^{1/2\beta(n_2-m+1)-1}}{\det(I+T_2)^{1/2\beta(n_2+n_1)}}\prod_i\nu_i^{\beta i-1}.$$

We observe that $\det(T_2)=\delta_m\det(T_1)$ and obtain

$$dens(\delta_i,\nu_i)=\left(1+\delta_m+\frac{\nu_{m-1}^2}{\delta_m}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right)^{-(1/2)\beta(n_2+n_1)}\frac{\det(T_1)^{(1/2)\beta(n_2-m+1)-1}}{\det(I+T_2)^{(1/2)\beta(n_2+n_1)}}\prod_i\nu_i^{\beta i-1}.$$

Let T_3 be the $(m-3)\times(m-3)$ lower right submatrix of T_2 (and also of T_1). Then

$$\det(I+T_1)=(1+\delta_m)\left(\det(I+T_2)+\frac{\nu_{m-1}^2}{\delta_m}\det(I+T_3)\right)-\nu_{m-1}^2\det(I+T_3)$$
$$=(1+\delta_m)\left(\det(I+T_2)+\frac{\nu_{m-1}^2}{\delta_m(1+\delta_m)}\det(I+T_3)\right)$$
$$=\det(I+T_2)(1+\delta_m)\left(1+\frac{\nu_{m-1}^2}{\delta_m(1+\delta_m)}\frac{\det(I+T_3)}{\det(I+T_2)}\right)$$
$$=\det(I+T_2)\left(1+\delta_m+\frac{\nu_{m-1}^2}{\delta_m}\sum_i\frac{\hat{v}_i^2}{1+\theta_i}\right),$$

where we have observed that

$$\frac{\det(I+T_3)}{\det(I+T_2)}=e_1^t(I+T_2)^{-1}e_1=\sum_i\frac{\hat{v}_i^2}{1+\theta_i}.$$

Thus we have

$$dens(\delta_i,\nu_i)=\frac{\det(T_1)^{(1/2)\beta(n_2-m+1)-1}}{\det(I+T_1)^{(1/2)\beta(n_2+n_1)}}\prod_i\nu_i^{\beta i-1}.$$

At this point, we change variables by $\delta'_{m-1}=\delta_{m-1}+\nu_{m-1}^2/\delta_m$, which has unit Jacobian and express T_1 in the traditional tridiagonal form.

Let $T_1=T(\lambda_i,\hat{q})$ parametrize T_1 by its (non-negative, ordered) eigenvalues λ_i and the (non-negative) unit vector $\hat{q}$. Applying the Vandermonde identity, Lemma 2.2, we have

$$dens(\delta_i,\nu_i)=\frac{\det(T_1)^{(1/2)\beta(n_2-m+1)-1}}{\det(I+T_1)^{(1/2)\beta(n_2+n_1)}}(\Delta(\lambda_i))^\beta\prod_i\hat{q}_i^\beta\prod_i\nu_i^{-1}.$$

Recognizing the Jacobian $\partial(\lambda_i,\hat{q}_i)/\partial(\delta_i,\nu_i)=\Pi_i\hat{q}_i/\Pi_i\nu_i$ we change variables to obtain

$$dens(\lambda_i,\hat{q}_i)=(\Delta(\lambda_i))^{\beta}\frac{\Pi_i\lambda_i^{(1/2)\beta(n_2-m+1)-1}}{\Pi_i(1+\lambda_i)^{(1/2)\beta(n_2+n_1)}}\prod_i \hat{q}_i^{\beta-1},$$

out of which the $\hat{q}_i$ may be integrated to obtain

$$dens(\lambda_i)=(\Delta(\lambda_i))^{\beta}\frac{\Pi_i\lambda_i^{(1/2)\beta(n_2-m+1)-1}}{\Pi_i(1+\lambda_i)^{(1/2)\beta(n_2+n_1)}}.$$

The base case of the induction is trivial. □

IV. DISCUSSION

The style of the model presented here is fairly different from that of the previous models for the Hermite and Laguerre ensembles in that a Jacobi sample in m values is built up from samples on $1,2,\ldots,m-1$ Jacobi values, where at each step a rank-1 update is performed.

It is possible to cast the Hermite and Laguerre models in this form. For example, the L matrix from Eq. (1) can, instead, be written

$$L=L^{(n,m)}=\begin{pmatrix} l & 0 \\ \vec{l} & L^{(n-1,m-1)} \end{pmatrix},$$

where $l=\chi_{n\beta}$ and $\vec{l}=[\chi_\beta,\ldots,\chi_\beta]$. In this case, however, the recursive form is unnecessary, since one can simultaneously bidiagonalize $L^{(n,m)}$ and its $L^{(n-1,m-1)}$ submatrix.

This simultaneous bidiagonalization is possible only because the elements of the $L^{(n-1,m-1)}$ submatrix are not intermingled with the elements of $\vec{l}$ as they are in the Jacobi case. Similar reasoning applies to the Hermite case. This suggests that a wider class of random matrix models is available by using successive rank-1 updates than just sparse forms with independent entries.

ACKNOWLEDGMENTS

The author would like to thank Alan Edelman and Ioanna Dumitriu for posing this problem to him and for laying much of the groundwork in their previous article. The author would also like to thank one of his referees for numerous corrections and suggestions which have greatly increased the clarity of this article.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

How to generate families of spinors

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(Received 27 March 2003; accepted 30 June 2003)

Using a technique [Mankoč Borštnik *et al.*, J. Math. Phys. **43**, 5782 (2002)] to construct a basis for spinors and ''families'' of spinors in terms of Clifford algebra objects, we define other Clifford algebra objects, which transform the state of one ''family'' of spinors into the state of another ''family'' of spinors, changing nothing but the ''family'' number. The proposed transformation works—as does the technique—for all dimensions and any signature and might open a path to understanding families of quarks and leptons [Mankoč Borštnik, Phys. Lett. B **292**, 25 (1992); J. Math. Phys. **34**, 3731 (1993); Int. J. Theor. Phys. **40**, 315 (2001); Borštnik Bračič and Mankoč Borštnik, hep-ph/0301029]. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1610239]

I. INTRODUCTION

In Ref. 1 we presented the technique to construct a spinor basis as products of nilpotents and projections formed from the objects γ^a for which we only need to know that they obey the Clifford algebra. Nilpotents and projections are odd and even objects of γ^a's, respectively, and are chosen to be eigenstates of a Cartan subalgebra of the Lorentz group in the sense that the left multiplication of nilpotents and projectors by the Cartan subalgebra elements multiplies these objects by a number. The technique can be used to construct a spinor basis for any dimension d and any signature in a simple and transparent way. Equipped with graphic representation of basic states, the technique offers an elegant means of seeing all the quantum numbers of states with respect to the Lorentz group, as well as the transformation properties of states under Clifford algebra objects.

Multiplying products of nilpotents and projectors from the left-hand side by any of the Clifford algebra objects, we get a linear combination of these ''basic'' elements back: our basis spans a left ideal, and has $2^{d/2}$ elements for d even and $2^{(d-1)/2}$ elements for d odd.

But there are 2^d products of nilpotents and projectors, all of them linearly independent. Mapping of ideals to spinor representations (treating all as Hilbert space) led accordingly to $2^{d/2}$ replicas of the usual spinor representation for d even and $d^{(d+1)/2}$ for d odd. We called these replicas ''families'' of representations.

The proposed technique was initiated and developed by one of the authors of this paper (N.M.B.), when proposing an approach[2–4] in which all the internal degrees of freedom of either spinors or vectors can be described in the space of d-anticommuting (Grassmann) coordinates, if the dimension of ordinary space is also d.

In the approach of one of us, however, two kinds of γ^a operators—two kinds of Clifford algebra objects—were defined, both fulfilling the same Clifford algebra relations, while one kind anticommutes with the other kind. When one of the two kinds of γ^a's is used to generate nilpotents and projectors, the products of which define when operating in a vacuum state basic vectors

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for the spinor representation of the Lorentz group, it causes another kind of transition among ''families'' of spinors, transforming one state of a ''family'' to a state with the same quantum numbers with respect to the Lorentz group as the starting state but belonging to another ''family.''

We show in this short paper that there are also operators which cause transitions among ''families''[5] within the simple technique presented in Ref. 1. While left multiplication of nilpotents and projectors by Clifford algebra objects generates all the states of one spinor representation (Sec. II), *right multiplication causes transitions among "families"* (Sec. III). (The reader should see also Chevalley's book.[6])

We demonstrate transitions among ''families'' for $d=4$ in Sec. III A.

In this paper, we assume an arbitrary signature of space–time so that our metric tensor η^{ab}, with $a,b \in \{0,1,2,3,5,\ldots\}$ is diagonal with values $\eta^{aa}=\pm 1$, depending on the chosen signature ($+1$ for time-like coordinates and -1 for space-like coordinates).

II. TECHNIQUE TO GENERATE SPINOR REPRESENTATIONS IN TERMS OF CLIFFORD ALGEBRA OBJECTS

We shall briefly repeat the main points of the technique for generating spinor representations from Clifford algebra objects, following Ref. 1. We ask the reader to look for details and proofs in this reference.

We assume the objects γ^a, which fulfill the Clifford algebra

$$\{\gamma^a,\gamma^b\}_+ = I\ 2\eta^{ab} \quad \text{for } a,b \quad \in \{0,1,2,3,5,\ldots,d\}, \tag{1}$$

for any d, even or odd. I is the unit element in the Clifford algebra, while $\{\gamma^a,\gamma^b\}_\pm = \gamma^a\gamma^b \pm \gamma^b\gamma^a$.

We assume the ''Hermiticity'' property for γ^a's,

$$\gamma^{a\dagger} = \eta^{aa}\gamma^a, \tag{2}$$

in order that γ^a are compatible with (1) and formally unitary, i.e., $\gamma^{a\dagger}\gamma^a = I$.

We also define the Clifford algebra objects

$$S^{ab} = \frac{i}{4}[\gamma^a,\gamma^b] := \frac{i}{4}(\gamma^a\gamma^b - \gamma^b\gamma^a) \tag{3}$$

which close the Lie algebra of the Lorentz group $\{S^{ab},S^{cd}\}_- = i(\eta^{ad}S^{bc} + \eta^{bc}S^{ad} - \eta^{ac}S^{bd} - \eta^{bd}S^{ac})$. One finds from Eq. (2) that $(S^{ab})^\dagger = \eta^{aa}\eta^{bb}S^{ab}$ and that $\{S^{ab},S^{ac}\}_+ = \frac{1}{2}\eta^{aa}\eta^{bc}$.

Recognizing from Eq. (3) and the Lorentz algebra relation that two Clifford algebra objects S^{ab},S^{cd} with all indices different commute, we select (out of infinitely many possibilities) the Cartan subalgebra of the algebra of the Lorentz group as follows:

$$\begin{aligned} &S^{0d},S^{12},S^{35},\ldots,S^{d-2\ d-1} \quad \text{if } d=2n, \\ &S^{12},S^{35},\ldots,S^{d-1\ d} \quad \text{if } d=2n+1. \end{aligned} \tag{4}$$

It is useful to define one of the Casimirs of the Lorentz group—the handedness Γ ($\{\Gamma,S^{ab}\}_- = 0$). (For the definition of Γ for any spin in even-dimensional spaces, see Refs. 2–4, 7 and 8.)

$$\begin{aligned} \Gamma &:= (i)^{d/2}\prod_a (\sqrt{\eta^{aa}}\gamma^a) \quad \text{if } d=2n, \\ \Gamma &:= (i)^{(d-1)/2}\prod_a (\sqrt{\eta^{aa}}\gamma^a) \quad \text{if } d=2n+1, \end{aligned} \tag{5}$$

for any integer n. We understand the product of γ^a's in ascending order with respect to index a: $\gamma^0\gamma^1\cdots\gamma^d$. It follows from Eq. (2) for any choice of the signature η^{aa} that $\Gamma^\dagger=\Gamma$, $\Gamma^2=I$.

We also find that for d even, the handedness anticommutes with the Clifford algebra objects γ^a ($\{\gamma^a,\Gamma\}_+=0$), while for d odd it commutes with γ^a ($\{\gamma^a,\Gamma\}_-=0$).

To make the technique simple, we introduce the graphic representation[1] as follows:

$$\begin{aligned}
\overset{ab}{(k)} &:= \frac{1}{2}\left(\gamma^a+\frac{\eta^{aa}}{ik}\gamma^b\right),\\
\overset{ab}{[k]} &:= \frac{1}{2}\left(1+\frac{i}{k}\gamma^a\gamma^b\right),\\
\overset{+}{\bigcirc} &:= \frac{1}{2}(1+\Gamma),\\
\overset{-}{\bullet} &:= \frac{1}{2}(1-\Gamma),
\end{aligned} \tag{6}$$

where $k^2=\eta^{aa}\eta^{bb}$. One can easily check by taking into account the Clifford algebra relation [Eq. (1)] and the definition of S^{ab} [Eq. (3)] that if one multiplies from the left-hand side by S^{ab} the Clifford algebra objects $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$, it follows that

$$\begin{aligned}
S^{ab}\overset{ab}{(k)} &= \frac{1}{2}k\overset{ab}{(k)},\\
S^{ab}\overset{ab}{[k]} &= \frac{1}{2}k\overset{ab}{[k]},
\end{aligned} \tag{7}$$

which means that we get the same objects back multiplied by the constant $\frac{1}{2}k$. This also means that $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$ acting from the left-hand side on anything (on a vacuum state $|\psi_0\rangle$, for example) are eigenvectors of S^{ab}.

We further find

$$\begin{aligned}
\gamma^a\overset{ab}{(k)} &= \eta^{aa}\overset{ab}{[-k]},\\
\gamma^b\overset{ab}{(k)} &= -ik\overset{ab}{[-k]},\\
\gamma^a\overset{ab}{[k]} &= \overset{ab}{(-k)},\\
\gamma^b\overset{ab}{[k]} &= -ik\,\eta^{aa}\overset{ab}{(-k)}.
\end{aligned} \tag{8}$$

It follows that $S^{ac}\overset{ab}{(k)}\overset{cd}{(k)}=-(i/2)\,\eta^{aa}\eta^{cc}\overset{ab}{[-k]}\overset{cd}{[-k]}$, $S^{ac}\overset{ab}{[k]}\overset{cd}{[k]}=(i/2)\overset{ab}{(-k)}\overset{cd}{(-k)}$, $S^{ac}\overset{ab}{(k)}\overset{cd}{[k]}=-(i/2)\,\eta^{aa}\overset{ab}{[-k]}\overset{cd}{(-k)}$, $S^{ac}\overset{ab}{[k]}\overset{cd}{(k)}=(i/2)\,\eta^{cc}\overset{ab}{(-k)}\overset{cd}{[-k]}$. It is useful to deduce the following relations:

$$\overset{ab}{(k)}^{\dagger} = \eta^{aa}\overset{ab}{(-k)}, \quad \overset{ab}{[k]}^{\dagger} = \overset{ab}{[k]}, \tag{9}$$

and

$$\begin{gathered}
\overset{ab}{(k)}\overset{ab}{(k)} = 0, \quad \overset{ab}{(k)}\overset{ab}{(-k)} = \eta^{aa}\overset{ab}{[k]}, \quad \overset{ab}{(-k)}\overset{ab}{(k)} = \eta^{aa}\overset{ab}{[-k]}, \quad \overset{ab}{(-k)}\overset{ab}{(-k)} = 0, \\
\overset{ab}{[k]}\overset{ab}{[k]} = \overset{ab}{[k]}, \quad \overset{ab}{[k]}\overset{ab}{[-k]} = 0, \quad \overset{ab}{[-k]}\overset{ab}{[k]} = 0, \quad \overset{ab}{[-k]}\overset{ab}{[-k]} = \overset{ab}{[-k]}, \\
\overset{ab}{(k)}\overset{ab}{[k]} = 0, \quad \overset{ab}{[k]}\overset{ab}{(k)} = \overset{ab}{(k)}, \quad \overset{ab}{(-k)}\overset{ab}{[k]} = \overset{ab}{(-k)}, \quad \overset{ab}{(-k)}\overset{ab}{[-k]} = 0, \\
\overset{ab}{(k)}\overset{ab}{[-k]} = \overset{ab}{(k)}, \quad \overset{ab}{[k]}\overset{ab}{(-k)} = 0, \quad \overset{ab}{[-k]}\overset{ab}{(k)} = 0, \quad \overset{ab}{[-k]}\overset{ab}{(-k)} = \overset{ab}{(-k)}.
\end{gathered} \tag{10}$$

We recognize in the first equation of the first row and the first equation of the second row the demonstration of the nilpotent and the projector character of the Clifford algebra objects $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$, respectively.

The reader should note that whenever the Clifford algebra objects apply from the left-hand side, they always transform $\overset{ab}{(k)}$ *to* $\overset{ab}{[-k]}$, *never to* $\overset{ab}{[k]}$, *and similarly* $\overset{ab}{[k]}$ *to* $\overset{ab}{(-k)}$, *never to* $\overset{ab}{(k)}$.

According to Ref. 1, we define a vacuum state $|\psi_0\rangle$ so that one finds

$$\begin{gathered}
\langle \overset{ab}{(k)}^{\dagger}\overset{ab}{(k)} \rangle = 1, \\
\langle \overset{ab}{[k]}^{\dagger}\overset{ab}{[k]} \rangle = 1.
\end{gathered} \tag{11}$$

Taking the above-given equations into account it is easy to find a Weyl spinor irreducible representation for d-dimensional space, with d even or odd. (We advise the reader to see Ref. 1.)

For d even, we simply set the starting state as a product of $d/2$, let us say, only nilpotents $\overset{ab}{(k)}$, one for each S^{ab} of the Cartan subalgebra elements [Eq. (4)], applying it on an (unimportant) vacuum state.[1] Then the generators S^{ab}, which do not belong to the Cartan subalgebra, applied to the starting state from the left-hand side, generate all the members of one Weyl spinor,

$$\begin{gathered}
\overset{0d}{(k_{0d})}\overset{12}{(k_{12})}\overset{35}{(k_{35})}\cdots\overset{d-1\ d-2}{(k_{d-1\ d-2})}\psi_0, \\
\overset{0d}{[-k_{0d}]}\overset{12}{[-k_{12}]}\overset{35}{(k_{35})}\cdots\overset{d-1\ d-2}{(k_{d-1\ d-2})}\psi_0, \\
\overset{0d}{[-k_{0d}]}\overset{12}{(k_{12})}\overset{35}{[-k_{35}]}\cdots\overset{d-1\ d-2}{(k_{d-1\ d-2})}\psi_0, \\
\vdots \\
\overset{0d}{[-k_{0d}]}\overset{12}{(k_{12})}\overset{35}{(k_{35})}\cdots\overset{d-1\ d-2}{[-k_{d-1\ d-2}]}\psi_0,
\end{gathered} \tag{12}$$

$$(\overset{od}{k_{0d}})[-\overset{12}{k_{12}}][-\overset{35}{k_{35}}]\cdots(\overset{d-1\ d-2}{k_{d-1\ d-2}})\psi_0,$$

$$\vdots$$

All the states have handedness Γ, since $\{\Gamma,S^{ab}\}_-=0$, which is easily calculated by multiplying from the left-hand side the starting state by Γ of Eq. (5). States belonging to one multiplet with respect to group $SO(q,d-q)$, that is to one irreducible representation of spinors (one Weyl spinor), can have any phase. We chose the simplest one, setting all phases equal to one.

The above graphic representation demonstrated that for d even all the states of one irreducible Weyl representation of a definite handedness follow from the starting state, which is, for example, a product of nilpotents $(\overset{ab}{k})$, by transforming all possible pairs of $(\overset{ab}{k})(\overset{mn}{k})$ into $[-\overset{ab}{k}][-\overset{mn}{k}]$. There are S^{am}, S^{an}, S^{bm}, S^{bn}, which do this. The procedure gives $2^{(d/2-1)}$ states. A Clifford algebra object γ^a applied from the left-hand side transforms a Weyl spinor of one handedness into a Weyl spinor of the opposite handedness. Both Weyl spinors form a Dirac spinor. We call such a set of states a "family."

For d odd a Weyl spinor also has in addition to a product of $(d-1)/2$ nilpotents or projectors either the factor $\overset{+}{\bigcirc}:=\frac{1}{2}(1+\Gamma)$ or the factor $\overset{-}{\bullet}:=\frac{1}{2}(1-\Gamma)$. (See Ref. 1.) As in the case of d even, all the states of one irreducible Weyl representation of a definite handedness follow from a starting state, which is, for example, a product of $\frac{1}{2}(1+\Gamma)$ and $(d-1)/2$ nilpotents $(\overset{ab}{k})$, by transforming all possible pairs of $(\overset{ab}{k})(\overset{mn}{k})$ into $[-\overset{ab}{k}][-\overset{mn}{k}]$. But γ^a's applied from the left-hand side do not change the handedness of the Weyl spinor, since $\{\Gamma,\gamma^a\}_-=0$ for d odd.[1] A Dirac and a Weyl spinor are for d odd identical and a "family" has accordingly $2^{(d-1)/2}$ members of basic states of a definite handedness.

We shall speak about left-handedness when $\Gamma=-1$ and right-handedness when $\Gamma=1$ for either d even or odd.

When the whole Clifford algebra is considered as states in a Hilbert space, then we get "families."

III. "FAMILIES"

When all 2^d states are considered as a Hilbert space, we recognize that for d even there are $2^{d/2}$ "families" and for d odd $2^{(d+1)/2}$ "families" of spinors.

We prove in this section (see also Ref. 5) that there exists an operation which transforms the state of one "family" into the state of another "family," leaving all the properties with respect to the Lorentz group unchanged.

We saw in Sec. II that any Clifford algebra object when multiplying from the left-hand side products of nilpotents and projectors (operating on a vacuum state)—a state of a Dirac spinor—transforms this state into a superposition of states of the same Dirac spinor. We refer to a Dirac spinor as a "family." Since there are 2^d linearly independent states, one finds for d even $2^{d/2}$ "families" and for d odd $2^{(d+1)/2}$ "families" of Dirac spinors. "Families" form left ideals with respect to the multiplication with the Clifford algebra objects.

The question then arises: Which operation transforms the state of one "family" into the state of another "family"?

Statement 1: Right multiplication with the Clifford algebra objects transforms the state of one "family" into the state of another "family."

Proof: The Clifford algebra object $(\overset{ab}{k})$ transforms, when applied from the left-hand side by either γ^a (or by γ^b), into $[-\overset{ab}{k}]$ [Eq. (8)]. One finds this by simply multiplying $(\overset{ab}{k})$ from the

left-hand side by one of these two Clifford algebra objects and taking into account Eq. (1)

$$\gamma^a \overset{ab}{(k)} = \gamma^a \ \frac{1}{2}\left(\gamma^a + \frac{\eta^{aa}}{ik}\gamma^b\right) = \eta^{aa}\frac{1}{2}\left(1 + \frac{i}{-k}\gamma^a\gamma^b\right) = \eta^{aa}\overset{ab}{[-k]}. \tag{13}$$

[And similarly we get $\gamma^b \overset{ab}{(k)} = -ik\overset{ab}{[-k]}$. The product of $\gamma^a\gamma^b$ transforms $\overset{ab}{(k)}$ into itself, multiplying it by $-ik$, since $\overset{ab}{(k)}$ was chosen to be the "eigen vector" of the Cartan subalgebra of the Lorentz algebra in the sense.]

Let us now multiply the same object $\overset{ab}{(k)}$ by γ^a *from the right-hand side*. It follows

$$\overset{ab}{(k)}\gamma^a = \frac{1}{2}\left(\gamma^a + \frac{\eta^{aa}}{ik}\gamma^b\right)\gamma^a = \eta^{aa}\frac{1}{2}\left(1 + \frac{i}{k}\gamma^a\gamma^b\right) = \eta^{aa}\overset{ab}{[k]}. \tag{14}$$

We saw in Eq. (13) that multiplication from the left-hand side by any Clifford algebra object transforms $\overset{ab}{(k)}$ into $\overset{ab}{[-k]}$, never to $\overset{ab}{[k]}$. This means that $\overset{ab}{[k]}$ is going to be a building block of a different "family" than $\overset{ab}{[-k]}$.

Theorem 1: *The two operations—left and right multiplication by* γ^a*—commute.*

Proof: To see this we need to show that the two objects $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$, the second obtained from the first by right multiplication, have all the properties with respect to the Lorentz group (application of the Lorentz algebra objects concerns the left multiplication) equal and that they differ only in the "family" name. Left multiplication by γ^a of the object $\overset{ab}{(k)}$ leads, as we know [Eq. (8)], to $\overset{ab}{[-k]}$, whose $S^{ab}\overset{ab}{[-k]} = -(k/2)\overset{ab}{[-k]}$.

To check the properties of the two Clifford algebra objects $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$ with respect to the Lorentz group, we have to multiply each of the two Clifford algebra objects from the left-hand side by S^{ab}, which is the Cartan subalgebra element. According to Eq. (7) we find $S^{ab}\overset{ab}{(k_{ab})} = (i/2)\frac{1}{2}(\gamma^a\gamma^b\gamma^a + \eta^{aa}/ik\,\gamma^a\gamma^b\gamma^b) = (k/2)\overset{ab}{(k)}$, $S^{ab}\overset{ab}{[k]} = (k/2)\overset{ab}{[k]}$.

Both objects, $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$, have the same eigenvalue for the Cartan subalgebra element S^{ab}, namely $\frac{1}{2}k$. Since right multiplication of the object $\overset{ab}{(k)}$ does not change the properties of the object with respect to the Lorentz group (the properties of which are determined by left multiplication) the two operations—left and right multiplication with γ^a's, both fulfilling the Clifford algebra relation—must commute and the proof is completed.

Since γ^a's are odd Clifford algebra objects, we would like to see the two operations—left and right multiplication with γ^a's—to anticommute rather then commute. With appropriate choice of a phase we can make them commute.

We define[5] *the Clifford algebra objects* $\tilde{\gamma}^a$'s *as operations which operate formally from the left-hand side* (*as* γ^a's *do*) *on objects* $\overset{ab}{(k)}$ *and* $\overset{ab}{[k]}$, *transforming objects to* $\overset{ab}{[k]}$ *and* $\overset{ab}{(k)}$, respectively, *as* γ^a's *would if applied from the right-hand side, up to a phase* i,

$$\tilde{\gamma}^a\overset{ab}{(k)} := -i\overset{ab}{(k)}\gamma^a = -i\,\eta^{aa}\overset{ab}{[k]}, \tag{15}$$

$$\tilde{\gamma}^b(k) := -\overset{ab}{i}(k)\,\gamma^b = -\overset{ab}{k}[k]. \tag{16}$$

One accordingly finds

$$\tilde{\gamma}^a[k] := \overset{ab}{i}[k]\,\gamma^a = \overset{ab}{i}(k), \tag{17}$$

$$\tilde{\gamma}^b[k] := \overset{ab}{i}[k]\,\gamma^b = -k\,\eta^{aa}\overset{ab}{(k)}. \tag{18}$$

We generalize the above definition of $\tilde{\gamma}^a$ to any Clifford algebra object as follows:

$$\tilde{\gamma}^a A = i(-)^{(A)} A\,\gamma^a, \tag{19}$$

with $(-)^{(A)} = -1$, if A is an odd Clifford algebra object and $(-)^{(A)} = 1$, if A is an even Clifford algebra object.

We can prove that $\tilde{\gamma}^a$ obey the same Clifford algebra relation as γ^a,

$$(\tilde{\gamma}^a\tilde{\gamma}^b + \tilde{\gamma}^b\tilde{\gamma}^a)A = -ii((-)^{(A)})^2 A(\gamma^a\gamma^b + \gamma^b\gamma^a) = 2\,\eta^{ab}A \tag{20}$$

and that $\tilde{\gamma}^a$ and γ^a anticommute

$$(\tilde{\gamma}^a\gamma^b + \gamma^b\tilde{\gamma}^a)A = i(-)^{(A)}(-\gamma^b A\,\gamma^a + \gamma^b A\,\gamma^a) = 0. \tag{21}$$

From *Theorem 1* and the above-given calculations, we may write

$$\{\tilde{\gamma}^a, \gamma^b\}_+ = 0, \quad \text{while} \quad \{\tilde{\gamma}^a, \tilde{\gamma}^b\}_+ = 2\,\eta^{ab}. \tag{22}$$

If we define

$$\tilde{S}^{ab} = \frac{i}{4}\ [\tilde{\gamma}^a, \tilde{\gamma}^b] = \frac{1}{4}(\tilde{\gamma}^a\tilde{\gamma}^b - \tilde{\gamma}^b\tilde{\gamma}^a), \tag{23}$$

it follows

$$\tilde{S}^{ab}A = A\,\tfrac{1}{4}(\gamma^b\gamma^a - \gamma^a\gamma^b), \tag{24}$$

manifesting accordingly that $\tilde{S}^{ab}$ fulfill the Lorentz algebra relation as S^{ab} do. Taking into account Eq. (19), we further find

$$\{\tilde{S}^{ab}, S^{ab}\}_- = 0, \quad \{\tilde{S}^{ab}, \gamma^c\}_- = 0, \quad \{S^{ab}, \tilde{\gamma}^c\}_- = 0. \tag{25}$$

One also finds

$$\begin{aligned} &\{\tilde{S}^{ab}, \Gamma\}_- = 0, \quad \{\tilde{\gamma}^a, \Gamma\}_- = 0 \quad \text{for d even,} \\ &\{\tilde{S}^{ab}, \Gamma\}_- = 0, \quad \{\tilde{\gamma}^a, \Gamma\}_+ = 0 \quad \text{for d odd,} \end{aligned} \tag{26}$$

which means that in d even transforming one ''family'' into another with either $\tilde{S}^{ab}$ or $\tilde{\gamma}^a$ leaves handedness Γ unchanged, while the transformation to another ''family'' in d odd with $\tilde{\gamma}^a$ changes the handedness of states, namely the factor $\frac{1}{2}(1 \pm \Gamma)$ changes to $\frac{1}{2}(1 \mp \Gamma)$ in accordance with what we know from before: In spaces with odd d changing the handedness means changing the ''family.''

We advise the reader also to read Refs. 3 and 4 where the two kinds of Clifford algebra objects follow as two different superpositions of a Grassmann coordinate and its conjugate momentum.

We present for $\tilde{S}^{ab}$ some useful relations

$$\tilde{S}^{ab}\overset{ab}{(k)} = \frac{k}{2}\overset{ab}{(k)},$$

$$\tilde{S}^{ab}\overset{ab}{[k]} = -\frac{k}{2}\overset{ab}{[k]},$$

$$\tilde{S}^{ac}\overset{ab\ \ cd}{(k)(k)} = \frac{i}{2}\eta^{aa}\eta^{cc}\overset{ab\ \ cd}{[k][k]},$$

$$\tilde{S}^{ac}\overset{ab\ \ cd}{[k][k]} = -\frac{i}{2}\overset{ab\ \ cd}{(k)(k)}, \tag{27}$$

$$\tilde{S}^{ac}\overset{ab\ \ cd}{(k)[k]} = -\frac{i}{2}\eta^{aa}\overset{ab\ \ cd}{[k](k)},$$

$$\tilde{S}^{ac}\overset{ab\ \ cd}{[k](k)} = \frac{i}{2}\eta^{cc}\overset{ab\ \ cd}{(k)[k]}.$$

According to *Statement 1* we transform the state of one "family" to the state of another "family" by the application of $\tilde{\gamma}^a$ or $\tilde{S}^{ac}$ (formally from the left-hand side) on a state of the first "family" for a chosen a or a,c. To transform all the states of one "family" into states of another "family," we apply $\tilde{\gamma}^a$ or $\tilde{S}^{ac}$ to each state of the starting "family." It is, of course, sufficient to apply $\tilde{\gamma}^a$ or $\tilde{S}^{ac}$ to only one state of a "family" and then use generators of the Lorentz group (S^{ab}), and for d even also γ^a's, to generate all the states of one Dirac spinor.

One must notice that nilpotents $\overset{ab}{(k)}$ and projectors $\overset{ab}{[k]}$ are eigenvectors not only of the Cartan subalgebra S^{ab} but also of $\tilde{S}^{ab}$. Accordingly only $\tilde{S}^{ac}$, which do not carry the Cartan subalgebra indices, cause the transition from one "family" to another "family."

The starting state of Eq. (12) can change, for example, to

$$\overset{0d\quad 12\quad 35\qquad\quad d-1\ d-2}{[k_{0d}][k_{12}](k_{35})\cdots(k_{d-1\ d-2})}, \tag{28}$$

if $\tilde{S}^{01}$ was chosen to transform the Weyl spinor of Eq. (12) to the Weyl spinor of another "family."

In what follows we demonstrate the appearance of "families" for $d=4$ with the Minkowski signature.

"Families" for $d=4$. There are two $(d/2=2)$ operators of the Cartan subalgebra of the Lorentz algebra (which is closed by the operators S^{01}, S^{02}, S^{03}, S^{12}, S^{13}, S^{23}), for which we made a choice, according to Eq. (4) of S^{03} and S^{12}. Following Eq. (5) we find $\Gamma = i\gamma^0\gamma^1\gamma^2\gamma^3$. There are 2^4, that is sixteen basic states, all of them being "eigenstates" of S^{12} and S^{03} in the sense of Eq. (7)

$$\begin{aligned}
&\overset{03}{(\pm i)}\overset{12}{(\pm)} = (\tfrac{1}{2})^2(\gamma^0 \mp \gamma^3)(\gamma^1 \pm i\gamma^2), \quad \overset{03}{(\pm i)}\overset{12}{[\pm]} = (\tfrac{1}{2})^2(\gamma^0 \mp \gamma^3)(1 \pm i\gamma^1\gamma^2),\\
&\overset{03}{[\pm i]}\overset{12}{(\pm)} = (\tfrac{1}{2})^2(1 \pm \gamma^0\gamma^3)(\gamma^1 \pm i\gamma^2), \quad \overset{03}{[\pm i]}\overset{12}{[\pm]} = (\tfrac{1}{2})^2(1 \pm \gamma^0\gamma^3)(1 \pm i\gamma^1\gamma^2),
\end{aligned} \tag{29}$$

TABLE I. Four "families" of the two Weyl spinors of the Lorentz group SO(1,3). Basic vectors are eigenvectors of the two operators of the Cartan subalgebra S^{12} and S^{03}. The eigenvalues of the operator of handedness Γ are also presented. All the basic states are orthonormalized as discussed in Ref. 1. The simplest choice of relative phases is used—all phases are assumed to be equal to $+1$.

a	i	$({}^a\psi_i)_1$	$({}^a\psi_i)_2$	$({}^a\psi_i)_3$	$({}^a\psi_i)_4$	S^{12}	S^{03}	Γ
1	1	$\overset{03}{(+i)}\overset{12}{(+)}$	$\overset{03}{[+i]}\overset{12}{[+]}$	$\overset{03}{[+i]}\overset{12}{(+)}$	$\overset{03}{(+i)}\overset{12}{[+]}$	$\frac{1}{2}$	$\frac{i}{2}$	-1
1	2	$\overset{03}{[-i]}\overset{12}{[-]}$	$\overset{03}{(-i)}\overset{12}{(-)}$	$\overset{03}{(-i)}\overset{12}{[-]}$	$\overset{03}{[-i]}\overset{12}{(-)}$	$-\frac{1}{2}$	$-\frac{i}{2}$	-1
2	1	$\overset{03}{[-i]}\overset{12}{(+)}$	$\overset{03}{(-i)}\overset{12}{[+]}$	$\overset{03}{(-i)}\overset{12}{(+)}$	$\overset{03}{[-i]}\overset{12}{[+]}$	$\frac{1}{2}$	$-\frac{i}{2}$	1
2	2	$\overset{03}{(+i)}\overset{12}{[-]}$	$\overset{03}{[+i]}\overset{12}{(-)}$	$\overset{03}{[+i]}\overset{12}{[-]}$	$\overset{03}{(+i)}\overset{12}{(-)}$	$-\frac{1}{2}$	$\frac{i}{2}$	1

with the "eigenvalues" of the Cartan operator S^{12} equal to $\pm 1/2$ for the $\pm$ sign in the second factor of the graphical presentation and the eigenvalues of the Cartan operator S^{03} equal to $\pm i/2$ for the $\pm i$ sign in the first factor of the graphical representation. All sixteen basic states are orthonormal.[1]

We arrange these sixteen states into four "families" by first choosing the starting state of the first "family" as a product of two nilpotents $\overset{03}{(+i)}\overset{12}{(+)}$. Then we use S^{01}, for example, to find the second state $\overset{03}{[-i]}\overset{12}{[-]}$ of one Weyl spinor. γ^0 generates from the first state of the first Weyl spinor the first state of the second Weyl spinor, namely, $\overset{03}{[-i]}\overset{12}{(+)}$ and S^{01} then the second state of the second spinor $\overset{03}{(+i)}\overset{12}{[-]}$. We set all the phases of the states equal to one.

We transform this first "family" into the second "family" by applying $\tilde{S}^{01}$ (or $\tilde{S}^{02}$, or $\tilde{S}^{31}$, or $\tilde{S}^{32}$) to each of the states of the first "family." By applying $\tilde{\gamma}^a$ to all the states of the first "family" we get the third "family." We also can generate the third "family" from the second by applying $\tilde{\gamma}^1$ (or $\tilde{\gamma}^2$). The fourth "family" can be reached from the first one by the application of $\tilde{\gamma}^1$ (or $\tilde{\gamma}^2$), but it can also be reached from any other with the appropriate choice of operations. For all the "families" the simplest choice of the relative phases, namely, the phase 1, is made.

Each "family" includes two Weyl spinors, one left- and one right-handed. These four "families" are presented in Table I.

We see in Table I that either $\tilde{\gamma}^a$, $a=0,1,2,3$, or $\tilde{S}^{01},\tilde{S}^{02},\tilde{S}^{31},\tilde{S}^{32}$, when applied, change the "family" but do not change either the handedness or the "eigenvalues" of the Cartan subalgebra of the Lorentz algebra.

Any of the four "families" can be used to represent the solution of the Dirac equation for a massive spinor, while massless spinors are either left- or right-handed, so that only half of the space of the massive case is needed to find the solution. The phases chosen for basic states make the matrix representation of γ^a's and S^{ab} equal to the usual ones.

IV. CONCLUSION

In Ref. 1 we constructed the basis for a left ideal out of products of nilpotents and projectors and identified the basis with the spinor space. There are 2^d nilpotents and projectors. Mapping all the ideals to spinor representations, that is treating all as a Hilbert space, leads to "families" of spinors. An irreducible representation of a spinor (a Dirac spinor, which is a Weyl bi-spinor with $2^{d/2}$ members for d even and a Weyl spinor with $2^{(d-1)/2}$ members for d odd) depends on a selection of a "starting" Clifford object. We have for d even $2^{d/2}$ different starting states and for d odd $2^{(d+1)/2}$ different starting states, which can all be made orthogonal with the appropriate

choice of an (unimportant) vacuum state. These are the different bases (that is different spinor spaces, which have all the same properties with respect to the Lorentz group), which we call ''families'' of spinors.

We have shown in this paper that while left multiplication with any Clifford algebra object makes from a ''starting'' state a superposition of basic states of one Dirac spinor, *right multiplication* of a ''starting state'' with any Clifford algebra object makes a superposition of states belonging to different ''families'' but having the same properties with respect to the Lorentz group (defined by left multiplication of Clifford algebra objects) as the starting state. One comes accordingly from one ''family'' to another ''family'' (up to an overall factor) by multiplying the ''starting'' state from the right-hand side by S^{ab}'s for d odd and by S^{ab}'s and γ^a's for d even, if S^{ab} does not belong to the Cartan subalgebra of the Lorentz group.

We have defined in this paper $\tilde{\gamma}^a$'s and $\tilde{S}^{ab}$ with the properties that both transform nilpotents and projectors, when multiplying them from the left-hand side as γ^a's and S^{ab} would if multiplying nilpotents and projectors from the right-hand side. Since neither $\tilde{\gamma}^a$'s nor $\tilde{S}^{ab}$ change properties of nilpotents and projectors (and consequently of a state) with respect to the Lorentz group, and since both—γ^a's and $\tilde{\gamma}^a$'s—are Clifford algebra objects, it follows (with the appropriate choice of phases) that $\{\tilde{\gamma}^a, \gamma^b\}_+ = 0$ and $\{\tilde{\gamma}^a, \tilde{\gamma}^b\}_+ = 2\eta^{ab}$. Consequently, $\tilde{S}^{ab}$ fulfill the same Lorentz algebra relation as S^{ab}. This can be understood since one could construct the spinor basis for a right ideal instead of a left ideal and then use left multiplication to generate ''families.'' (To understand this better, see Refs. 3, 4, 5, and 8.)

We have also demonstrated the application of $\tilde{\gamma}^a$'s and $\tilde{S}^{ab}$ on a basis with the help of the graphic technique introduced in Ref. 1. We demonstrated the procedure for generating ''families'' in the (most familiar) case of $d=1+3$, that is for $d=4$ and one time coordinate, where the number of ''families'' is four.

In conclusion, we must ask ourselves whether the proposed generation of ''families'' can be used to describe the ''families'' of quarks and leptons? This is certainly one of the open problems of the Standard electroweak model. We believe that we have the right way to do this. According to Refs. 4 and 5, one can generate ''families'' of quarks and leptons dynamically if in the covariant derivative $\tilde{S}^{ab}$ appears as charges, accompanied by gauge fields like $\tilde{\omega}_c{}^{ab}$, so that

$$p_o{}^a = p^a - \tfrac{1}{2}\tilde{S}^{ab}\tilde{\omega}_{abc} - \tau^{Ai}A^{Aia}, \tag{30}$$

with τ^{Ai} determining the known charges [U(1),SU(2),SU(3)] and A^{Aia} the corresponding gauge fields. This possibility has been discussed in Ref. 5.

In the presented formalism we worked with the Clifford algebra objects only, using them to express not only the generators of the Lorentz algebra but also the operators transforming one ''family'' into another ''family'' and even the spinor basis for one and several ''families.'' (It is for this reason that we get the ''families'' as explained.) One would accordingly ask oneself if there is possibly any physical reason that the Clifford algebra degrees of freedom are ''more fundamental'' than the spinors.[9]

This is exactly what was taken as the starting point in the works by one of us[2–5] (and which lead to the formalism, presented in this paper) but it is also what is really the case in the Kogut and Susskind lattice fermion formalism.[10] In the latter case the fermion degrees of freedom are interpreted as sitting really on the sites links plaquettes and cubes and hypercubes of a lattice with the double lattice constant. That corresponds to having fields of all the possible antisymmetrized tensor characters, which is just what the Clifford algebra elements have. One therefore has also in the Kogut–Susskind fermions a way of having the Clifford algebra naturally more fundamental than the spinors. Not surprisingly we also get in this case the expected number 4 for families in this lattice model. Also the paper of both of us [8] already introduced ''families'' of spinors with the help of the Clifford algebra objects, but in a slightly different way—the spinor states have two indices.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education, Science and Sport of Slovenia as well as by funds CHRX-CT-94-0621, INTAS 93-3316, INTAS-RFBR 95-0567, SCI-0430-C (TSTS) of Denmark.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 10 OCTOBER 2003

The indefinite anti-self-dual metrics and the Painlevé equations

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(Received 23 April 2003; accepted 20 May 2003)

We classify the SU(2)-invariant anti-self-dual metrics with a signature $(+, +, -, -)$. The metrics are specified by a solution of Painlevé VI, V, III or II. Moreover, we show the geometric meaning of the metrics specified by each type of Painlevé function. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604187]

I. INTRODUCTION

The aim of this article is to classify the anti-self-dual metrics in real dimension four admitting an isometric action of SU(2) with generically three-dimensional orbits. In this article, we study not only the definite metrics, but also the indefinite metrics with a signature $(+, +, -, -)$.

Hitchin[5] shows that the SU(2)-invariant anti-self-dual metric is generically specified by a solution of Painlevé VI with two complex parameters. He used the twistor correspondence[1,13] to associate the anti-self-dual equation and the Painlevé equation. On the twistor space, the lifted action of SU(2) determines a prehomogeneous action of SU(2), and it determines an isomonodromic family of connections on $\mathbb{CP}^1$, and then we obtain the Painlevé equation.

In this framework, Hitchin[5] classified the diagonal anti-self-dual metrics, and Dancer[4] shows that the diagonal scalar-flat Kähler metric is specified by a solution of Painlevé III with a parameter $(0, 4, 4, -4)$, where the *diagonal* metric is the metric in the shape of (1) in Sec. II. Since the anti-self-dual Einstein metrics are diagonal, the classification for diagonal metrics enough serves Hitchin's purpose. However, generically, the SU(2)-invariant metric is in the shape of (4) in Sec. III. In this case, Hitchin shows that the metric is generically specified by a solution of Painlevé VI, but he does not go into detail. We study not only the diagonal metrics but also the nondiagonal metrics. The author[10,11] shows that the SU(2)-invariant anti-self-dual Hermitian metric is specified by a solution of Painlevé III with a parameter $(4\theta, 4(1+\overline{\theta}), 4, -4)$.

The metrics mentioned above are positive definite. In this article we study the indefinite metrics with a signature $(+, +, -, -)$. If the metric is definite, then the anti-self-dual equation reduces to either Painlevé VI or III. On the other hand, we show that, if the metric has a signature $(+, +, -, -)$, then the anti-self-dual equation reduces to not only Painlevé VI or III but also Painlevé V or II. The difference of types of Painlevé is due to the difference of reality on the twistor space.

Painlevé VI is shown to be a deformation equation for a linear problem,

$$\left(\frac{d}{dz}-B_1\right)\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}=0,$$

where B_1 has four simple poles on $\mathbb{CP}^1$.[6] And Painlevé V, IV, III, II are degenerated from Painlevé

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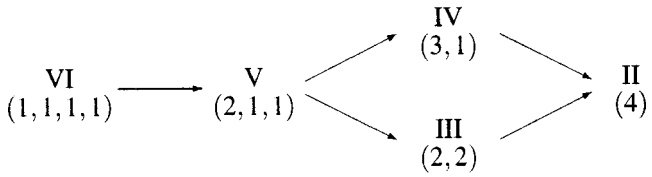
VI:



This is the confluence diagram of poles of B_1, where the Roman numerals represent the types of the Painlevé equation, and the parenthesized numbers represent the orders of poles of B_1. For example, Painlevé V is shown to be a deformation equation for a linear problem with one double and two simple poles.

For the complexified metrics, any type of Painlevé equation from I to VI is derived from the anti-self-dual equation.[8,9] However, it is important to study what types of Painlevé equations are derived from the real anti-self-dual equation.

For the metric with a signature $(+, +, -, -)$, due to the reality of the twistor space, the poles of B_1 make two conjugate pairs. Therefore, the configuration of poles never becomes the type of Painlevé IV.

The multiple pole of B_1 on $\mathbb{CR}$ determines a Hermitian structure, and the multiple pole on $\mathbb{R}$ determines a structure of real twistor surfaces. In each case, we can calculate local exponents at singularities. These local exponents corresponding to the parameter of the Painlevé equation. This is the geometric meaning of the metrics specified by each type of Painlevé function:

(1) Generically, the anti-self-dual metrics are specified by a solution of Painlevé VI with two complex parameters.
(2) If the anti-self-dual metric is specified by a solution of Painlevé III with one complex parameter, then there exists an SU(2)-invariant Hermitian structure.
(3) If the anti-self-dual metric is specified by a solution of Painlevé V with one real and one complex parameter, or Painlevé II with one real parameter, then for any $x \in M$ there exists one real twistor surface passing through x.
(4) If the anti-self-dual metric is specified by a solution of Painlevé III with two real parameters, then for any $x \in M$ there exist two real twistor surfaces passing through x.

II. THE DIAGONAL ANTI-SELF-DUAL EQUATIONS

In this section, we review the anti-self-dual equations on the SU(2)-invariant diagonal metrics. The SU(2)-invariant diagonal metric is represented in the following form:

$$g = w_1 w_2 w_3\, dt^2 + \frac{w_2 w_3}{w_1}\sigma_1^2 + \frac{w_3 w_1}{w_2}\sigma_2^2 + \frac{w_1 w_2}{w_3}\sigma_3^2. \tag{1}$$

w_1, w_2 and w_3 are functions of t, and σ_1, σ_2, σ_3 are left invariant one-forms on each SU(2)-orbit satisfying

$$d\sigma_1 = \sigma_2 \wedge \sigma_3, \quad d\sigma_2 = \sigma_3 \wedge \sigma_1, \quad d\sigma_3 = \sigma_1 \wedge \sigma_2. \tag{2}$$

Tod[14] showed that the (scalar-flat) anti-self-dual equations on the SU(2)-invariant diagonal metric are given by the following system:

$$\begin{aligned}
&\dot{w}_1=-w_2w_3+w_1(\alpha_2+\alpha_3), \quad \dot{w}_2=-w_3w_1+w_2(\alpha_3+\alpha_1),\\
&\dot{w}_3=-w_1w_2+w_3(\alpha_1+\alpha_2), \quad \dot{\alpha}_1=-\alpha_2\,\alpha_3+\alpha_1(\alpha_2+\alpha_3),\\
&\dot{\alpha}_2=-\alpha_3\,\alpha_1+\alpha_2(\alpha_3+\alpha_1), \quad \dot{\alpha}_3=-\alpha_1\,\alpha_2+\alpha_3(\alpha_1+\alpha_2),
\end{aligned} \tag{3}$$

where α_1, α_2, α_3 are auxiliary functions and the dots denote differentiation with respect to t. The anti-self-dual equation (3) has a first integral

$$k=\frac{\alpha_1(w_2^2-w_3^2)+\alpha_2(w_3^2-w_1^2)+\alpha_3(w_1^2-w_2^2)}{8(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_3-\alpha_1)}.$$

Furthermore, if we set

$$x=\frac{\alpha_2-\alpha_1}{\alpha_2-\alpha_3}, \quad q=\frac{w_2(\alpha_1-\alpha_2)(w_2(w_1^2-w_3^2)+2\sqrt{2k}\,w_1w_3(\alpha_1-\alpha_3))}{w_1^2(w_2^2-w_3^2)\alpha_1+w_2^2(w_3^2-w_1^2)\alpha_2+w_3^2(w_1^2-w_2^2)\alpha_3},$$

then the system (3) generically reduces to a family of Painlevé VI with a special parameter

$$(\alpha,\beta,\gamma,\delta)=\left(\frac{(\sqrt{2k}-1)^2}{2},k,-k,\frac{1+2k}{2}\right).$$

We will review the Painlevé equation in the Appendix.

III. THE NONDIAGONAL ANTI-SELF-DUAL EQUATIONS

We can express an SU(2)-invariant metric in the form

$$g=f(\tau)d\tau^2+\sum_{l,m=1}^{3}h_{l\,m}(\tau)\,\sigma_l\sigma_m\,. \tag{4}$$

Using the Killing form, we can diagonalize the metric g on each SU(2)-orbit. Then we can express the metric as follows:

$$g=(abc)^2dt^2+a^2d\hat{\sigma}_1^2+b^2\hat{\sigma}_2^2+c^2\hat{\sigma}_3^2,$$

for some $t=t(\tau)$, $a=a(t)$, $b=b(t)$, $c=c(t)$ and

$$\begin{pmatrix}\hat{\sigma}_1\\ \hat{\sigma}_2\\ \hat{\sigma}_3\end{pmatrix}=R(t)\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{pmatrix},$$

where $R(t)$ is an SO(3)-valued function.

Since $\dot{R}R^{-1}\in\mathfrak{so}(3)$, we obtain

$$d\begin{pmatrix}\hat{\sigma}_1\\ \hat{\sigma}_2\\ \hat{\sigma}_3\end{pmatrix}=R(t)\begin{pmatrix}\sigma_2\wedge\sigma_3\\ \sigma_3\wedge\sigma_1\\ \sigma_2\wedge\sigma_2\end{pmatrix}+\dot{R}\,dt\wedge\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{pmatrix}=\begin{pmatrix}\hat{\sigma}_2\wedge\hat{\sigma}_3\\ \hat{\sigma}_3\wedge\hat{\sigma}_1\\ \hat{\sigma}_1\wedge\hat{\sigma}_2\end{pmatrix}+\begin{pmatrix}0 & \xi_3 & -\xi_2\\ -\xi_3 & 0 & \xi_1\\ \xi_2 & -\xi_1 & 0\end{pmatrix}dt\wedge\begin{pmatrix}\hat{\sigma}_1\\ \hat{\sigma}_2\\ \hat{\sigma}_3\end{pmatrix},$$

for some $\xi_1=\xi_1(t)$, $\xi_2=\xi_2(t)$, $\xi_3=\xi_3(t)$.

If $\xi_1=0$, $\xi_2=0$, $\xi_3=0$, then the matrix $(h_{l\,m})$ can be chosen to be diagonal for all τ, and then we say that g is a diagonal metric.

In the following, we mainly study the nondiagonal case.

We set $w_1=bc$, $w_2=ca$, $w_3=ab$ and determine α_1, α_2, α_3 by

$$\begin{aligned}\dot{w}_1&=-w_2w_3+w_1(\alpha_2+\alpha_3),\\ \dot{w}_2&=-w_3w_1+w_2(\alpha_3+\alpha_1),\\ \dot{w}_3&=-w_1w_2+w_3(\alpha_1+\alpha_2).\end{aligned}\tag{5}$$

Then the scalar curvature s is determined by

$$\begin{aligned}w_1w_2w_3\,s=4(&\dot{\alpha}_1+\dot{\alpha}_2+\dot{\alpha}_3-\alpha_2\alpha_3-\alpha_3\alpha_1-\alpha_1\alpha_2)\\&+\frac{(w_2^2-w_3^2)^2}{w_2^2w_3^2}\xi_1^2+\frac{(w_3^2-w_1^2)^2}{w_3^2w_1^2}\xi_2^2+\frac{(w_1^2-w_2^2)^2}{w_1^2w_2^2}\xi_3^2,\end{aligned}$$

and then the anti-self-dual equations are as follows:[10,11]

$$\begin{aligned}\dot{\alpha}_1=&-\alpha_2\alpha_3+\alpha_1(\alpha_2+\alpha_3)+\frac{1}{4}(w_2^2-w_3^2)^2\left(\frac{\xi_1}{w_2w_3}\right)^2+\frac{1}{4}(w_3^2-w_1^2)(3w_1^2+w_3^2)\left(\frac{\xi_2}{w_3w_1}\right)^2\\&+\frac{1}{4}(w_2^2-w_1^2)(3w_1^2+w_2^2)\left(\frac{\xi_3}{w_1w_2}\right)^2-\frac{w_1w_2w_3\,s}{12},\\ \dot{\alpha}_2=&-\alpha_3\alpha_1+\alpha_2(\alpha_3+\alpha_1)+\frac{1}{4}(w_3^2-w_1^2)^2\left(\frac{\xi_2}{w_3w_1}\right)^2+\frac{1}{4}(w_1^2-w_2^2)(3w_2^2+w_1^2)\left(\frac{\xi_3}{w_1w_2}\right)^2\\&+\frac{1}{4}(w_3^2-w_2^2)(3w_2^2+w_3^2)\left(\frac{\xi_1}{w_2w_3}\right)^2-\frac{w_1w_2w_3\,s}{12},\\ \dot{\alpha}_3=&-\alpha_1\alpha_2+\alpha_3(\alpha_1+\alpha_2)+\frac{1}{4}(w_1^2-w_2^2)^2\left(\frac{\xi_3}{w_1w_2}\right)^2+\frac{1}{4}(w_2^2-w_3^2)(3w_3^2+w_2^2)\left(\frac{\xi_1}{w_2w_3}\right)^2\\&+\frac{1}{4}(w_1^2-w_3^2)(3w_3^2+w_1^2)\left(\frac{\xi_2}{w_3w_1}\right)^2-\frac{w_1w_2w_3\,s}{12},\end{aligned}\tag{6}$$

and

$$\begin{aligned}(w_2^2-w_3^2)\frac{d}{dt}\left(\frac{\xi_1}{w_2w_3}\right)&=\frac{\xi_2}{w_3w_1}\frac{\xi_3}{w_1w_2}(-2w_2^2w_3^2+w_3^2w_1^2+w_1^2w_2^2)\\&\quad+\frac{\xi_1}{w_2w_3}(\alpha_2w_2^2-\alpha_3w_3^2+3\alpha_2w_3^2-3\alpha_3w_2^2),\\ (w_3^2-w_1^2)\frac{d}{dt}\left(\frac{\xi_2}{w_3w_1}\right)&=\frac{\xi_3}{w_1w_2}\frac{\xi_1}{w_2w_3}(-2w_3^2w_1^2+w_1^2w_2^2+w_2^2w_3^2)\\&\quad+\frac{\xi_2}{w_3w_1}(\alpha_3w_3^2-\alpha_1w_1^2+3\alpha_3w_1^2-3\alpha_1w_3^2),\end{aligned}\tag{7}$$

$$(w_1^2-w_2^2)\frac{d}{dt}\left(\frac{\xi_3}{w_1w_2}\right)=\frac{\xi_1}{w_2w_3}\frac{\xi_2}{w_3w_1}(-2w_1^2w_2^2+w_2^2w_3^2+w_3^2w_1^2)$$
$$+\frac{\xi_3}{w_1w_2}(\alpha_1w_1^2-\alpha_2w_2^2+3\alpha_1w_2^2-3\alpha_2w_1^2).$$

Remark 1: If $\xi_1=0$, $\xi_2=0$, $\xi_3=0$ and $s=0$, then the system of equations (5), (6) and (7) reduces to a sixth-order system (3) given by Tod.[14] *Furthermore, if $\alpha_1=w_1$, $\alpha_2=w_2$, $\alpha_3=w_3$, then (5)–(7) reduce to a third-order system which determines the Atiyah–Hitchin family,*[1] *and if $\alpha_1=0$, $\alpha_2=0$, $\alpha_3=0$, then the system reduces to a third-order system which determines the BGPP family.*[3]

Remark 2: If $w_2=w_3$, then we can set $\xi_1=0$, $\xi_2=0$ and $\xi_3=0$ by taking another frame. This is also a diagonal case. Therefore we assume $(w_2-w_3)(w_3-w_1)(w_1-w_2)\neq 0$.

IV. THE ISOMONODROMIC DEFORMATIONS

Let (M,g) be an oriented Riemannian four manifold. We define a manifold Z to be the unit sphere bundle in the bundle of anti-self-dual two-forms, and let π: $Z\to M$ denote the projection. Each point z in the fiber over $\pi(z)$ defines a complex structure on the tangent space $T_{\pi(z)}M$, compatible with the metric and its orientation.

Using the Levi-Civita connection, we can split the tangent space T_zZ into horizontal and vertical spaces, and the projection π identifies the horizontal space with $T_{\pi(z)}M$. This space has a complex structure defined by z and the vertical space is the tangent space of the fiber $S^2\cong\mathbb{CP}^1$ which has its natural complex structure.

The almost complex structure on Z is integrable if and only if the metric is anti-self-dual.[2,13] In this situation Z is called the twistor space of (M,g) and the fibers are called the real twistor lines.

The almost complex structure on Z can be determined by the following (1,0)-forms:

$$\Theta_1=z(e^1+\sqrt{-1}e^2)-(e^0+\sqrt{-1}e^3),$$
$$\Theta_2=z(e^0-\sqrt{-1}e^3)+(e^1-\sqrt{-1}e^2),\tag{8}$$
$$\Theta_3=dz+\tfrac{1}{2}z^2(\omega_1^0-\omega_3^2+\sqrt{-1}(\omega_2^0-\omega_1^3))-\sqrt{-1}z(\omega_3^0-\omega_2^1)+\tfrac{1}{2}(\omega_1^0-\omega_3^2-\sqrt{-1}(\omega_2^0-\omega_1^3)),$$

where $\{e^0,e^1,e^2,e^3\}$ is an orthonormal frame, and ω_j^i are the connection forms determined by $de^i+\omega_j^i\wedge e^j=0$ and $\omega_j^i+\omega_i^j=0$. Then the anti-self-dual condition is

$$d\Theta_1\equiv 0,\ \ d\Theta_2\equiv 0,\ \ d\Theta_3\equiv 0\ \ (\mathrm{mod}\ \Theta_1,\Theta_2,\Theta_3).\tag{9}$$

Theorem 3: *If the metric is positive definite, then the Pfaffian is invariant under conjugate action and $z\mapsto -1/\overline{z}$.*[2] *If the metric has a signature $(+,+,-,-)$, then the Pfaffian is invariant under conjugate action and $z\mapsto\overline{z}$.*

Remark 4: Let $TM^{\mathbb{C}}$ be a complexified tangent space of M. We call the set $\mathcal{C}=\{a\in TM^{\mathbb{C}}\mid g(a,a)=0\}$ a null cone. For $a\in TM^{\mathbb{C}}$, we consider

$$\Theta_1\left(a+\lambda\frac{\partial}{\partial z}\right)=0,\ \ \Theta_2\left(a+\lambda\frac{\partial}{\partial z}\right)=0,\ \ \Theta_3\left(a+\lambda\frac{\partial}{\partial z}\right)=0,\tag{10}$$

as algebraic equations of λ, z. Equations (10) have solutions $\lambda\in\mathbb{C}$, $z\in\mathbb{CP}^1$, if and only if $a\in\mathcal{C}$.

If the metric is SU(2) invariant, we obtain

$$\begin{pmatrix}\Theta_1\\ \Theta_2\\ \Theta_3\end{pmatrix}=\begin{pmatrix}0\\0\\1\end{pmatrix}dz+\begin{pmatrix}v_1\\ v_2\\ v_3\end{pmatrix}dt+A\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{pmatrix}, \tag{11}$$

where $v_1=v_1(z,t)$, $v_2=v_2(z,t)$, $v_3=v_3(z,t)$; $A=(a_{ij}(z,t))_{i,j=1,2,3}$.

If $\det A\equiv 0$, then the metric turns to be diagonal, and the metric is in the BGPP family.[3]

If $\det A\neq 0$, then we obtain

$$\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{pmatrix}\equiv -A^{-1}\left(\begin{pmatrix}0\\0\\1\end{pmatrix}dz+\begin{pmatrix}v_1\\ v_2\\ v_3\end{pmatrix}dt\right), \quad (\mathrm{mod}\ \Theta_1,\ \Theta_2,\ \Theta_3). \tag{12}$$

If we set

$$\begin{pmatrix}s_1\\ s_2\\ s_3\end{pmatrix}:=-A^{-1}\left(\begin{pmatrix}0\\0\\1\end{pmatrix}dz+\begin{pmatrix}v_1\\ v_2\\ v_3\end{pmatrix}dt\right), \tag{13}$$

then

$$d\begin{pmatrix}s_1\\ s_2\\ s_3\end{pmatrix}\equiv\begin{pmatrix}s_2\wedge s_3\\ s_3\wedge s_1\\ s_1\wedge s_2\end{pmatrix}, \quad (\mathrm{mod}\ \Theta_1,\Theta_2,\Theta_3). \tag{14}$$

Since s_1, s_2, s_3 are one-forms on (z,t)-plane, the congruency equation (14) turns to be a plain equation:

$$d\begin{pmatrix}s_1\\ s_2\\ s_3\end{pmatrix}=\begin{pmatrix}s_2\wedge s_3\\ s_3\wedge s_1\\ s_1\wedge s_2\end{pmatrix}. \tag{15}$$

If the metric is positive definite, then s_1, s_2, s_3 are invariant under conjugate action and $z\mapsto -1/\overline{z}$ by Theorem 3. And if the metric has a signature $(+,+,-,-)$, then s_1, s_2, s_3 are invariant under conjugate action and $z\mapsto\overline{z}$.

If we set

$$\Sigma=\frac{1}{\sqrt{2}}\begin{pmatrix}\sqrt{-1}s_2 & -s_1+\sqrt{-1}s_3\\ s_1+\sqrt{-1}s_3 & -\sqrt{-1}s_2\end{pmatrix} \tag{16}$$

$$=:-B_1\,dz-B_2\,dt, \tag{17}$$

then

$$d\Sigma+\Sigma\wedge\Sigma=0. \tag{18}$$

This is the isomonodromy condition for the the following linear problem,[6]

$$\left(\frac{d}{dz}-B_1\right)\begin{pmatrix}y_1\\ y_2\end{pmatrix}=0. \tag{19}$$

B_2 is determined by B_1 from (18).

Lemma 5: The components of B_1 are rational functions of z,

$$B_1=\frac{F(z)}{G(z)},$$

where $F(z)$ *is degree* 2 *and* $G(z)$ *is degree* 4. *If the metric is positive definite, then* $B_1\mapsto -{}^tB_1$ *under conjugate action and* $z\mapsto -1/\overline{z}$. *And if the metric has a signature* $(+,+,-,-)$, *then* $B_1\mapsto -{}^tB_1$ *under conjugate action and* $z\mapsto\overline{z}$.

For this lemma, generically B_1 has four simple poles. In this case, the deformation equation of (19) is Painlevé VI.

Theorem 6: *The anti-self-dual equations on* SU(2)*-invariant metrics generically reduce to Painlevé VI.*

The idea of Hitchin[5] is that the lifted action of SU(2) on the twistor space Z gives a homomorphism of vector bundles $\alpha: Z\times \mathfrak{su}(2)^{\mathbb{C}}\to TZ$, and the inverse of α gives a flat meromorphic SL(2,$\mathbb{C}$)-connection, which determines isomonodromic deformations. Since one-forms Θ_1, Θ_2, Θ_3 on Z can be considered as infinitesimal variations, we can identify Σ with α^{-1}.

First, we review the positive definite metric. By Lemma 5, the poles of B_1 make antipodal pairs $\zeta_0, -1/\overline{\zeta_0}$, and $\zeta_1, -1/\overline{\zeta_1}$ on $\mathbb{CP}^1$.

Therefore, we obtain two types of configuration of poles of B_1:

(a) B_1 has four simple poles ζ_0, $-1/\overline{\zeta_0}$, ζ_1, $-1/\overline{\zeta_1}$ on $\mathbb{CP}^1$,

$$B_1=\frac{A_0}{z-\zeta_0}+\frac{-{}^t\overline{A_0}}{z+1/\overline{\zeta_0}}+\frac{A_1}{z-\zeta_1}+\frac{-{}^t\overline{A_1}}{z+1/\overline{\zeta_1}}.$$

The deformation equation is Painlevé VI with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0-1)^2,\tfrac{1}{2}\overline{\theta_0^2},-\tfrac{1}{2}\theta_1^2,\tfrac{1}{2}(1+\overline{\theta_1^2})),$$

where $\theta_0^2=2\,\mathrm{tr}A_0^2$, $\theta_1^2=2\,\mathrm{tr}A_1^2$.

(b) B_1 has two double poles ζ, $-1/\overline{\zeta}$ on $\mathbb{CP}^1$,

$$B_1=\frac{A_2}{(z-\zeta)^2}+\frac{\sqrt{-1}C}{z-\zeta}+\frac{-\sqrt{-1}C}{z+1/\overline{\zeta}}+\frac{-{}^t\overline{A_2}/\overline{\zeta^2}}{(z+1/\overline{\zeta})^2},$$

where $C=-{}^t\overline{C}$. The deformation equation is Painlevé III with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(4\theta,4(1+\overline{\theta}),4,-4),$$

where $\theta^2=2(\mathrm{tr}(A_2C))^2/\mathrm{tr}A_2^2$.

Theorem 7: *If the metric is positive definite, the anti-self-dual equations reduce to the following Painlevé equations:*

(a) a family of Painlevé VI with two complex parameters,

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0-1)^2,\tfrac{1}{2}\overline{\theta_0^2},-\tfrac{1}{2}\theta_1^2,\tfrac{1}{2}(1+\overline{\theta_1^2})),$$

(b) a family of Painlevé III with one complex parameter,

$$(\alpha,\beta,\gamma,\delta)=(4\theta,4(1+\overline{\theta}),4,-4).$$

Remark 8: It is known that the anti-self-dual equations reduce to Painlevé VI with the parameter as above.[9,5] *Dancer*[4] *shows the diagonal scalar-flat Kähler metric is specified by a solution of Painlevé III with a parameter* $(\alpha,\beta,\gamma,\delta)=(0,4,4,-4)$. *Now, Theorem* 7 (b) *is a generalization of Dancer's result.*

From now on, we will classify the anti-self-dual metrics with a signature $(+,+,-,-)$. By Lemma 5 the poles of B_1 make conjugate pairs $\zeta_0,\overline{\zeta_0}$, and $\zeta_1,\overline{\zeta_1}$ in $\mathbb{CP}^1$. Therefore we obtain five types of metrics corresponding to configuration of poles of B_1.

Theorem 9: *If the metric has a signature* $(+,+,-,-)$, *the anti-self-dual equations reduce to the following five Painlevé equations:*

(a) Painlevé VI with two complex parameters

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0-1)^2,\tfrac{1}{2}\overline{\theta_0^2},-\tfrac{1}{2}\theta_1^2,\tfrac{1}{2}(1+\overline{\theta_1^2})),$$

(b) Painlevé V with one real and one complex parameters

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0+\overline{\theta_0}+\theta_\infty)^2,-\tfrac{1}{2}(\theta_0+\overline{\theta_0}-\theta_\infty)^2,1-\theta_0+\overline{\theta_0},\tfrac{1}{2}),$$

where $\theta_\infty\in\mathbb{R}$.

(c) Painlevé III with one complex parameter

$$(\alpha,\beta,\gamma,\delta)=(4\theta,4(1+\overline{\theta}),4,-4).$$

(d) Painlevé III with with two real parameters

$$(\alpha,\beta,\gamma,\delta)=(4\theta_1,4(1+\theta_2),4,-4).$$

(e) Painlevé II with one real parameter α.

Proof: Since the poles of B_1 make conjugate pairs $\zeta_0,\overline{\zeta_0}$ and $\zeta_1,\overline{\zeta_1}$, we obtain five types of configuration of poles of B_1. In each case, we can calculate local exponents at singularities. These local exponents correspond to the parameter of the Painlevé equation (see Ref. 7).

(a) Generically, B_1 has four simple poles ζ_0, $\overline{\zeta_0}$, ζ_1, $\overline{\zeta_1}$ on $\mathbb{C}\backslash\mathbb{R}$,

$$B_1=\frac{A_0}{z-\zeta_0}+\frac{-{}^t\overline{A_0}}{z-\overline{\zeta_0}}+\frac{A_1}{z-\zeta_1}+\frac{-{}^t\overline{A_1}}{z-\overline{\zeta_1}}.$$

The deformation equation is Painlevé VI with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0-1)^2,\tfrac{1}{2}\overline{\theta_0^2},-\tfrac{1}{2}\theta_1^2,\tfrac{1}{2}(1+\overline{\theta_1^2})),$$

where $\theta_0^2=2\,\mathrm{tr}A_0^2$, $\theta_1^2=2\,\mathrm{tr}A_1^2$.

(b) If $\zeta_0=\overline{\zeta_0}(=\eta)$, then B_1 has one double pole η on $\mathbb{R}$, and two simple poles ζ_1, $\overline{\zeta_1}$ on $\mathbb{C}\backslash\mathbb{R}$,

$$B_1=\frac{C}{(z-\eta)^2}+\frac{-A_2+{}^t\overline{A_2}}{z-\eta}+\frac{A_2}{z-\zeta_1}+\frac{-{}^t\overline{A_2}}{z-\overline{\zeta_1}},$$

where $C=-{}^t\overline{C}$. The deformation equation is Painlevé V with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(\tfrac{1}{2}(\theta_0+\overline{\theta_0}+\theta_\infty)^2,-\tfrac{1}{2}(\theta_0+\overline{\theta_0}-\theta_\infty)^2,1-\theta_0+\overline{\theta_0},\tfrac{1}{2}),$$

where $\theta_0^2=2\,\mathrm{tr}A_2^2$, $\theta_\infty^2=2(\mathrm{tr}(A_2-{}^t\overline{A_2})C)^2/\mathrm{tr}C^2$.

(c) If $\zeta_0=\zeta_1(=\zeta)$, then B_1 has two double poles ζ, $\overline{\zeta}$ on $\mathbb{C}\backslash\mathbb{R}$,

$$B_1=\frac{A_3}{(z-\zeta)^2}+\frac{\sqrt{-1}C}{z-\zeta}+\frac{-\sqrt{-1}C}{z-\overline{\zeta}}+\frac{-{}^t\overline{A_3}}{(z-\overline{\zeta})^2},$$

where $C=-{}^t\overline{C}$. The deformation equation is Painlevé III with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(4\theta,4(1+\overline{\theta}),4,-4),$$

where $\theta^2=2(\mathrm{tr}A_3C)^2/\mathrm{tr}A_2^2$.

(d) If $\zeta_0=\overline{\zeta_0}(=\eta_0)$, $\zeta_1=\overline{\zeta_1}(=\eta_1)$, then B_1 has two double poles η_0, η_1 on $\mathbb{R}$,

$$B_1=\frac{C_1}{(z-\eta_0)^2}+\frac{C_2}{z-\eta_0}+\frac{-C_2}{z-\eta_1}+\frac{C_3}{(z-\eta_1)^2},$$

where $C_i=-{}^t\overline{C_i}$ $(i=1,2,3)$. The deformation equation is Painlevé III with a parameter,

$$(\alpha,\beta,\gamma,\delta)=(4\theta_1,4(1+\theta_2),4,-4),$$

where $\theta_1^2=2(\mathrm{tr}C_1C_2)^2/\mathrm{tr}C_1^2$, $\theta_2^2=2(\mathrm{tr}C_2C_3)^2/\mathrm{tr}C_3^2$.

(e) If $\zeta_0=\overline{\zeta_0}=\zeta_1=\overline{\zeta_1}(=\eta)$, then B_1 has one quadruple pole η on $\mathbb{R}$,

$$B_1=\frac{C_1}{(z-\eta)^4}+\frac{C_2}{(z-\eta)^3}+\frac{C_3}{(z-\eta)^2},$$

where $C_i=-{}^t\overline{C_i}$ $(i=1,2,3)$. If $\det C_1\neq 0$, then the deformation equation is Painlevé II with a parameter,

$$\alpha=\tfrac{1}{2}(1+\mathrm{tr}C_2C_3).$$

If $\det C_1=0$, then the deformation equation is Painlevé I, but since $C_1=-{}^t\overline{C_1}$, this never occurs.

Remark 10: The isomonodromic condition (18) determines the null cone $\mathcal{C}$. B_1 and B_2 determine $\mathcal{C}$ as follows. For

$$a_0\frac{\partial}{\partial t}+a_1\sigma_1^*+a_2\sigma_2^*+a_3\sigma_3^*\in TM^{\mathbb{C}},$$

we consider

$$\frac{a_1}{\sqrt{2}}\begin{pmatrix}0&-1\\1&0\end{pmatrix}+\frac{a_2}{\sqrt{2}}\begin{pmatrix}\sqrt{-1}&0\\0&-\sqrt{-1}\end{pmatrix}+\frac{a_3}{\sqrt{2}}\begin{pmatrix}0&\sqrt{-1}\\\sqrt{-1}&0\end{pmatrix}=-\lambda B_1(z)-a_0B_2(z) \quad (20)$$

as an algebraic equation of λ, z, *which is equivalent with (10). Equation (20) has solutions* $\lambda\in\mathbb{C}$, $z\in\mathbb{CP}^1$, *if and only if* $a_0(\partial/\partial t)+a_1\sigma_1^*+a_2\sigma_2^*+a_3\sigma_3^*\in\mathcal{C}$.

V. HERMITIAN STRUCTURE AND NULL SURFACES

In this section, we will study the geometric meaning of the metrics corresponding with each type of Painlevé function.

Lemma 11: Let g be an anti-self-dual metric. If B_1 has a multiple pole on $z=\zeta(t)$, then the Pfaffian $\Theta_1|_{z=\zeta(t)}$, $\Theta_2|_{z=\zeta(t)}$ is integrable. Conversely, if the Pfaffian $\Theta_1|_{z=\zeta(t)}$, $\Theta_2|_{z=\zeta(t)}$ is integrable for some $\zeta(t)$, then B_1 has a multiple pole on $z=\zeta(t)$.

Proof: If $z=\zeta(t)$ is a multiple zero of $G(z)$, then $G|_{z=\zeta(t)}$ and $dG|_{z=\zeta(t)}$ must be vanish. Furthermore, $\Theta_3\equiv 0(\mathrm{mod}\ \Theta_1,\Theta_2,G,dG)$. Therefore, the Pfaffian $\Theta_1|_{z=\zeta(t)},\Theta_2|_{z=\zeta(t)}$ is integrable.

Conversely, if the Pfaffian $\Theta_1|_{z=\zeta(t)}$, $\Theta_2|_{z=\zeta(t)}$ is integrable for some $z=\zeta(t)$, then $\Theta_3|_{z=\zeta(t)}\equiv 0(\mathrm{mod}\ \Theta_1,\Theta_2)$. Therefore the denominator G of B_1 has zero on $z=\zeta(t)$. Furthermore, $\Theta_3|_{z=\zeta(t)}\equiv 0(\mathrm{mod}\ \Theta_1,\Theta_2,G)$ is equivalent to $dG|_{z=\zeta(t)}=0$, therefore $z=\zeta(t)$ is a double pole of B_1.

In Refs. 10 and 11 we show that if a positive definite SU(2) invariant anti-self-dual metric is specified by a solution of Painlevé III with one complex parameter $(4\theta,4(1+\overline{\theta}),4,-4)$, then the Pfaffian $\Theta_1|_{z=\zeta(t)}$, $\Theta_2|_{z=\zeta(t)}$ ($z=\zeta(t)$ is a double pole of B_1) determines an SU(2) invariant Hermitian structure.

In the same way, we obtain the following theorem for the metric with a signature $(+,+,-,-)$.

Theorem 12: *If the anti-self-dual equations reduce to Painlevé III with one complex parameter* $(4\theta,4(1+\overline{\theta}),4,-4)$, *then there exists an* SU(2)*-invariant Hermitian structure. Conversely, if there exists an* SU(2)*-invariant Hermitian structure, then the anti-self-dual equations reduce to Painlevé III with the parameter above.*

Definition 13: If $g(X,X)=0$, *then* $X\in TM$ *is said to be a null direction.*

The Pfaffian $\Theta_1|_{z=\eta(t)},\Theta_2|_{z=\eta(t)}(\eta(t)\in\mathbb{R})$ determines two dimensional null directions on TM.

Definition 14: Let N be a two dimensional subspace of M. If $g(X,X)=0$ *for any* $X\in TN$, *then N is called a real twistor surface.*

From Lemma 11, if $z=\eta(t)\in\mathbb{R}$ is a multiple pole of B_1, then the Pfaffian $\Theta_1|_{z=\eta(t)},\Theta_2|_{z=\eta(t)}$ is integrable, and then for any $x\in M$ there exists an SU(2)-invariant real twistor surface passing through x. Conversely, for any $x\in M$, if there exists an SU(2)-invariant real twistor surface passing through x, then the real twistor surface is represented by Pfaffian $\Theta_1|_{z=\eta(t)},\Theta_2|_{z=\eta(t)}$ for some $\eta(t)\in\mathbb{R}$, and then $z=\eta(t)$ is a multiple pole of B_1

Theorem 15: *If the anti-self-dual equations reduce to Painlevé V with one real and one complex parameter* $(1/2(\theta_0+\overline{\theta_0}+\theta_\infty)^2,-1/2(\theta_0+\overline{\theta_0}-\theta_\infty)^2,1-\theta_0+\overline{\theta_0},1/2)$, *where* $\theta_\infty\in\mathbb{R}$, *or Painlevé II with one real parameter* α, *then for any* $x\in M$ *there exists one* SU(2)*-invariant real twistor surface passing through x. Conversely, for any* $x\in M$ *there exists one* SU(2)*-invariant real twistor surface passing through x, then the anti-self-dual reduces to Painlevé V or II with the parameter above.*

If the anti-self-dual equations reduce to Painlevé III with two real parameters $(4\theta_1,4(1-\theta_2),4,-4)$, *then for any* $x\in M$ *there exist two* SU(2)*-invariant real twistor surfaces passing through x. Conversely, for any* $x\in M$ *there exist two* SU(2)*-invariant real twistor surfaces passing through x, then the anti-self-dual equation reduces to Painlevé III with the parameter above.*

VI. SUMMARY

We classified the SU(2)-invariant anti-self-dual metric with a signature $(+,+,-,-)$ into the five cases (a)–(e) (Theorem 9). The meaning of the types of the Painlevé equations are as follows:

(1) Generically, the anti-self-dual metric is, specified by a solution of Painlevé VI with two complex parameters.
(2) If the anti-self-dual metric is specified by a solution of Painlevé III with one complex parameter, then there exists an SU(2)-invariant Hermitian structure.
(3) If the anti-self-dual metric is specified by a solution of Painlevé V with one real parameter and one complex parameter, or Painlevé II with one real parameter, then for any $x\in M$ there exists one real twistor surface passing through x.
(4) If the anti-self-dual metric is specified by a solution of Painlevé III with two real parameters, then for any $x\in M$ there exist two real twistor surfaces passing through x.

ACKNOWLEDGMENTS

The author would express his gratitude to Professor Yousuke Ohyama, who introduced him to the subject, for enlightening discussions.

APPENDIX: PAINLEVÉ EQUATIONS

We review the Painlevé second order nonlinear differential equations without moving critical points. We list six equations classified by Painlevé and Gambier, where $\alpha,\beta,\gamma,\delta$ are parameters.[12]

(1) Painlevé I:

$$\frac{d^2q}{dx^2}=6q^2+x.$$

(2) Painlevé II:

$$\frac{d^2q}{dx^2}=2q^3+xq+\alpha.$$

(3) Painlevé III:

$$\frac{d^2q}{dx^2}=\frac{1}{q}\left(\frac{dq}{dx}\right)^2-\frac{1}{x}\frac{dq}{dt}+\frac{1}{x}(\alpha q^2+\beta)+\gamma q^3+\frac{\delta}{q}.$$

(4) Painlevé IV:

$$\frac{d^2q}{dx^2}=\frac{1}{2q}\left(\frac{dq}{dx}\right)^2+\frac{3}{2}q^3+4xq^2+2(x^2-\alpha)q+\frac{\beta}{q}.$$

(5) Painlevé V:

$$\frac{d^2q}{dx^2}=\left(\frac{1}{2q}+\frac{1}{q-1}\right)\left(\frac{dq}{dx}\right)^2-\frac{1}{x}\frac{dq}{dx}+\frac{(q-1)^2}{x^2}\left(\alpha q+\frac{\beta}{q}\right)+\frac{\gamma q}{x}+\frac{\delta q(q+1)}{q-1}.$$

(6) Painlevé VI:

$$\begin{aligned}\frac{d^2q}{dx^2}=&\frac{1}{2}\left(\frac{1}{q}+\frac{1}{q-1}+\frac{1}{q-x}\right)\left(\frac{dq}{dx}\right)^2-\left(\frac{1}{x}+\frac{1}{x-1}+\frac{1}{q-x}\right)\frac{dq}{dx}\\&+\frac{q(q-1)(q-x)}{x^2(x-1)^2}\left\{\alpha+\beta\frac{x}{q^2}+\gamma\frac{x-1}{(q-1)^2}+\delta\frac{x(x-1)}{(q-x)^2}\right\}.\end{aligned}$$

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Double warped space–times

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(Received 8 April 2003; accepted 22 May 2003)

An invariant characterization of double warped space–times is given in terms of Newman–Penrose formalism and a classification scheme is proposed. A detailed study of the conformal algebra of these space–times is also carried out and some remarks are made on certain classes of exact solutions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1605496]

I. INTRODUCTION

Given two metric manifolds (M_1,h_1) and (M_2,h_2) and given two smooth real functions $\theta_1:M_1\to\mathbb{R}$, $\theta_2:M_2\to\mathbb{R}$ (*warping functions*), one can build a new metric manifold (M,g) by setting $M=M_1\times M_2$ and

$$g=e^{2\theta_2}\pi_1^*h_1\otimes e^{2\theta_1}\pi_2^*h_2, \tag{1}$$

where π_1,π_2 above are the canonical projections onto M_1 and M_2, respectively, and will be omitted where there is no risk of confusion (thus writing, from now on: $g=e^{2\theta_2}h_1\otimes e^{2\theta_1}h_2$). One such structure will be called *double warped product manifold*, and gives rise to the so-called *warped product manifold* whenever one of the warping functions is constant, see Refs. 1 and 2.

If $\dim M_1+\dim M_2=4$ and g has Lorentz signature [i.e., one of the manifolds (M_i,h_i) is Lorentz and the other Riemann], then (M,g) will be referred to as a *double warped space–time*, and again, if one of the warping functions is constant, one recovers the definition of *warped space–time* (see Refs. 3 and 4).

In what is to follow and unless otherwise stated, we shall assume that we are dealing with "proper" double warped space–times (i.e., neither of the warping functions is constant); further, and without loss of generality (M_1,h_1) will be assumed Lorentzian and (M_2,h_2) Riemannian.

The considerations in this work will be mainly local, thus we shall assume that for each $p\in M$ there exists a neighborhood U of p such that there is a coordinate system x^a, $a=0,\ldots,3$ on U *adapted* to the product structure in the sense that the line element associated with g can be written as

$$\mathrm{d}s^2=e^{2\theta_2(x^D)}h_{1\ \alpha\beta}(x^\gamma)\mathrm{d}x^\alpha\,\mathrm{d}x^\beta+e^{2\theta_1(x^\gamma)}h_{2\ AB}(x^D)\mathrm{d}x^A\,\mathrm{d}x^B; \tag{2}$$

where $x^{\alpha,\beta,\cdots}$ and $x^{A,B,\cdots}$ will designate the coordinates on the submanifolds M_1 and M_2 of M through p, respectively, while n_1 and n_2 denote their respective dimensions; thus, Greek indices will run from 0 to n_1-1 and capital Latin indices from n_1 to 3. Conversely, if a space–time contains an open neighborhood U on which there exists a coordinate system as the one described above, then it will be referred to as *locally double warped space–time*.

The aim of the present paper is to deal with double warped space–times in much the same way as warped space–times were dealt with previously (see Refs. 3 and 4 and references cited

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therein); thus their geometrical properties will be deducted and studied starting from those of their lower dimensional factors (M_i, h_i) which are, in general, much easier to deal with.

The paper is structured as follows: in Sec. II an invariant characterization of these space–times is given, including their characterization in terms of the Newman–Penrose formalism, and a classification scheme is put forward. Section III contains some results on the curvature structure of such space–times, whereas Secs. IV and V deal with their conformal algebra. Finally, in Sec. VI, a few remarks are made on double warped exact solutions.

II. INVARIANT CHARACTERIZATION AND CLASSIFICATION

Starting with the form (2) of the line element, let us re-write it as follows:

$$ds^2 = e^{2(\theta_1(x^\gamma)+\theta_2(x^D))}[e^{-2\theta_1(x^\gamma)} h_{1\ \alpha\beta}(x^\gamma)\,dx^\alpha\,dx^\beta + e^{-2\theta_2(x^D)} h_{2\ AB}(x^D)\,dx^A\,dx^B], \tag{3}$$

now, the two terms $e^{-2\theta_1(x^\gamma)} h_{1\ \alpha\beta}(x^\gamma)$ and $e^{-2\theta_2(x^D)} h_{2\ AB}(x^D)$ are metrics on the submanifolds M_1 and M_2, say $\hat{h}_1$ and $\hat{h}_2$. The sum of their associated line elements [that is, the expression within the square brackets in (3)], is the line element, say $d\hat{s}^2$ of a decomposable space–time $(M,\hat{g})$ with $M = M_1 \times M_2$ and $\hat{g} = \hat{h}_1 \otimes \hat{h}_2$ (Again, to be correct one should write $\hat{g} = \pi_1^* \hat{h}_1 \otimes \pi_2^* \hat{h}_2$, π_1, π_2 being the canonical projections onto M_1 and M_2, but since there is no risk of confusion, we omit them for the sake of simplicity), thus we have proven:

Lemma 1: A (locally) double warped space–time is always conformally related to a (locally) decomposable space–time, the conformal factor being separable in the coordinates associated with the two factor submanifolds.

In what follows, we shall refer to the factor submanifolds in the decomposable space–time $(M,\hat{g})$ as $(M_1,\hat{h}_1)$ and $(M_2,\hat{h}_2)$, respectively, assuming that $(M_1,\hat{h}_1)$ is Lorentz and $(M_2,\hat{h}_2)$ Riemann; and we shall write the metric of a double warped space–time as $g = \exp(2\theta)\hat{g}$ in the understanding that $\hat{g}$ is the metric of the underlying decomposable space–time and θ separates as the sum of two functions θ_1 and θ_2 on M_1 and M_2, respectively.

Now, the space–time $(M,\hat{g})$ is locally decomposable if its holonomy group is nondegenerately reducible (and globally decomposable if, on top of this, it is simply connected) (see for instance Ref. 5, and references therein), its holonomy type being then R_2, R_3, R_4, R_6, R_7, R_{10}, or R_{13} (see Ref. 6); one then has the following possibilities for $(M,\hat{g})$.[5]

(1) $(M,\hat{g})$ is $1+3$ decomposable if it admits a global, non-null, nowhere zero covariantly constant vector field $\vec{u}$. One then distinguishes between $1+3$ spacelike (holonomy type R_{13}) or $1+3$ timelike (holonomy types R_3, R_6 or R_{10}) depending on the nature of the three-dimensional submanifold orthogonal to the covariantly constant vector field. In a coordinate system adapted to the covariantly constant vector field, say $\vec{u} = \partial_u$, the line element $d\hat{s}^2$ then takes the following forms, respectively:

$$d\hat{s}^2 = -du^2 + \hat{h}_{AB}(x^D)\,dx^A\,dx^B$$

or

$$d\hat{s}^2 = \hat{h}_{\alpha\beta}(x^\gamma)\,dx^\alpha\,dx^\beta + du^2. \tag{4}$$

If another non-null covariantly constant vector field exists in the space–time, then $(M,\hat{g})$ decomposes further and can be referred to as being $1+1+2$ spacelike (type R_4) or $1+1+2$ timelike (type R_2) in an obvious notation.

(2) $(M,\hat{g})$ is $2+2$ decomposable and then two global, linearly independent recurrent null vector fields exist (holonomy type R_7). This is equivalent to saying that in $(M,\hat{g})$ there exist two linearly independent covariantly constant tensor fields of rank 2, say P and Q such that

$$\hat{g}_{ab} = P_{ab} + Q_{ab}$$

with

$$P_{ab/c}=Q_{ab/c}=0; \tag{5}$$

a stroke denoting covariant derivative in $(M,\hat{g})$; the line element reads in this case

$$d\hat{s}^2=\hat{h}_{1\ \alpha\beta}(x^\gamma)dx^\alpha\,dx^\beta+\hat{h}_{2\ AB}(x^D)dx^A\,dx^B, \tag{6}$$

where $\hat{h}_1$ and $\hat{h}_2$ are two two-dimensional metrics on M_1 and M_2, respectively, such that $\pi_1^*\hat{h}_1=P$ and $\pi_2^*\hat{h}_2=Q$.

Going back to the double warped space–time (M,g) conformally related to $(M,\hat{g})$ via (3), it appears natural to consider the following two classes of double warped space–times.

Class A whenever the underlying space–time $(M,\hat{g})$ is $1+3$ decomposable. If necessary, and following the same notation as in the case of warped space–times, we shall distinguish between classes A_1 ($1+3$ spacelike) and A_2 ($1+3$ timelike). Taking into account (3) and (4), we shall write the canonical form of the line element of these space–times as

$$ds^2=e^{2(\theta_1(u)+\theta_2(x^D))}[-du^2+\hat{h}_{AB}(x^D)dx^A\,dx^B], \tag{7}$$

$$ds^2=e^{2(\theta_1(x^\gamma)+\theta_2(u))}[\hat{h}_{\alpha\beta}(x^\gamma)dx^\alpha\,dx^\beta+du^2], \tag{8}$$

respectively.

Class B whenever the underlying space–time $(M,\hat{g})$ is $2+2$ decomposable. The canonical form of the line element will be in this case

$$ds^2=e^{2(\theta_1(x^\gamma)+\theta_2(x^D))}[\hat{h}_{1\ \alpha\beta}(x^\gamma)dx^\alpha\,dx^\beta+\hat{h}_{2\ AB}(x^D)dx^A\,dx^B]. \tag{9}$$

In what is to follow and whenever no confusion may arise, we shall put $\theta\equiv\theta_1(x^\gamma)+\theta_2(x^D)$ and write accordingly

$$g_{ab}=e^{2\theta}\hat{g}_{ab},$$

and also

$$ds^2=e^{2\theta}d\hat{s}^2. \tag{10}$$

Also, we shall denote the covariant derivatives in (M,g) and $(M,\hat{g})$ by ∇ and $\hat{\nabla}$ or a semicolon (;) and a slash (/), respectively. Further, reference will be often made to conformal Killing vectors and their properties, hence it is in order at this point to recall their definition and basic properties; thus, given an n-dimensional manifold V endowed with a metric g of arbitrary signature, a vector field $\vec{X}$ on V is said to be a *conformal Killing vector* (CKV) iff $\mathcal{L}_{\vec{X}}g=2\phi g$ where ϕ is some function of the coordinates (*conformal factor*) and $\mathcal{L}_{\vec{X}}$ stands for the Lie derivative operator with respect to the vector field $\vec{X}$. The former equation can also be written in an arbitrary coordinate chart as

$$X_{a;b}=\phi g_{ab}+F_{ab} \tag{11}$$

and then, from the Bianchi identities, it follows

$$F_{ab;c}=R_{abcd}X^d-\phi_a g_{bc}+\phi_b g_{ac}, \tag{12}$$

$$\mathcal{L}_{\vec{X}}R_{ab}=-(n-2)\phi_{a;b}-\phi^c{}_{;c}g_{ab}, \tag{13}$$

$$\mathcal{L}_{\vec{X}}R=-2\phi R-2(n-1)\phi^c{}_{;c}, \tag{14}$$

$$\mathcal{L}_{\vec{X}} R_{abcd} = 2\phi R_{abcd} - \phi_{a;c} g_{bd} + \phi_{a;d} g_{bc} - \phi_{b;d} g_{ac} + \phi_{b;c} g_{ad}, \tag{15}$$

where $\phi_a \equiv \phi_{,a}$, a semicolon stands for the covariant derivative with respect to the connection associated with the metric, $F_{ab} = -F_{ba}$ is the so-called *conformal bivector*, and R_{abcd}, R_{ab}, and R stand, respectively, for the components in the chosen chart of the Riemann and Ricci tensors and the Ricci scalar. The special cases $\phi =$ constant and $\phi = 0$ correspond, respectively, to $\vec{X}$ being a *homothetic vector* (HV) and a *Killing vector* (KV), the associated bivector is then said to be the *homothetic bivector*, or *Killing bivector*, respectively. A CKV is said to be *proper* whenever it is nonhomothetic (i.e., $\phi \neq$ const); likewise, we shall use "proper homothetic" to designate a HV which is not a KV (i.e., $\phi =$ const$\neq 0$). A proper CKV is said to be a *special CKV* (SCKV) whenever its associated conformal factor ϕ satisfies $\phi_{a;b} = 0$ in any coordinate chart. Further, it is easy to see that the CKV that (V,g) admits form, under the usual Lie bracket operation, a Lie algebra of vector fields which we shall designate as $\mathcal{C}_r(V,g)$, r being its dimension. Similar statements can be made regarding the SCKV, HV, and KV that (V,g) may admit [Lie algebras $\mathcal{S}_r(V,g)$, $\mathcal{H}_r(M,g)$ and $\mathcal{K}_r(V,g)$ respectively (note from the above considerations it follows that in any given space–time $\mathcal{C}_r \supseteq \mathcal{S}_m \supseteq \mathcal{H}_s \supseteq \mathcal{K}_n$, with $r \geqslant m \geqslant s \geqslant n$)]. We refer the reader to Ref. 7 for further details on CKV and their Lie algebra. Going back now to the problem of characterizing class A and B double warped space–times, we see that this can be carried out by "translating" into (M,g) the properties of the preferred vector fields (non-null covariantly constant or null recurrent) that characterize the underlying decomposable space–times $(M,\hat{g})$. Thus we get:

Theorem 1: *The necessary and sufficient condition for* (M,g) *to be a double warped class A space–time is that it admits a non-null, nowhere vanishing CKV* $\vec{X}$ *which is hypersurface orthogonal and such that the gradient of its associated conformal factor* ψ *is parallel to* $\vec{X}$.

Proof: Let (M,g) be a class A double warped space–time, its line element takes then the form (7) and (8) and it is easy to see that $\vec{X} = \partial_u$ is a CKV which satisfies the required properties, in particular, its associated conformal factor ψ is $\psi = \theta_{,u}$ which on account of the form that θ has (separable in u and the rest of the coordinates) is $\psi = \psi(u)$ and therefore $\psi_{,a} \propto X_a$.

The converse also holds for, assume that (M,g) admits a non-null, nowhere vanishing CKV $\vec{X}$ which is hypersurface orthogonal. Since $\vec{X}$ is nonvanishing and hypersurface orthogonal, a coordinate chart exists, say $\{u,x^k\}$, such that

$$\vec{X} = \partial_u, \quad ds^2 = \epsilon e^{2U(u,x^k)} du^2 + h_{ij}(u,x^k) dx^i\, dx^j,$$

where $\epsilon = \pm 1$ (see for example Ref. 8, p. 168). Further, the conformal equations for $\vec{X}$ above are simply $g_{ab,u} = 2\psi g_{ab}$ (with $\psi = \psi(u,x^k)$) which in turn implies

$$\psi(u,x^k) = U_{,u}(u,x^k), \quad h_{ij}(u,x^k) = e^{2U(u,x^k)} \hat{h}_{ij}(x^k)$$

and the above line element can then be written as

$$ds^2 = e^{2U(u,x^k)} [\epsilon du^2 + \hat{h}_{ij}(x^k) dx^i\, dx^j].$$

Finally, imposing that $\psi_{,a} \propto X_a$ yields $\psi = \psi(u)$ and therefore $U(u,x^k) = \theta_1(u) + \theta_2(x^k)$ and the resulting space–time is then class A double warped. □

The characterization of warped space–times can now be easily recovered as the following corollary shows:

Corollary 2: If the CKV $\vec{X}$ *in theorem 1 is a Killing vector (KV) then the space–time is warped of class* A_2 *in the classification given in Ref. 3. If* $\vec{X}$ *is a proper (non-KV) gradient CKV (i.e., if the associated conformal bivector vanishes* $F_{ab} = X_{a;b} - X_{b;a} = 0$*) the space–time is class* A_1 *warped in that classification.*

It is worthwhile noticing that Theorem 1 also provides an invariant characterization of space–times conformal to $1+3$ locally decomposable space–times:

Corollary 3: The necessary and sufficient condition for (M,g) *to be conformally related to a* $1+3$ *decomposable space–time* $(M,\hat{g})$ *is that it admits a non-null, nowhere vanishing conformal Killing vector (CKV)* $\vec{X}$ *which is hypersurface orthogonal.*

Theorem 1 can be conveniently rephrased in terms of Newman–Penrose (NP) formalism[9] through the two following theorems:

Theorem 4: (M,g) *is a class* A_1 *double warped space–time if and only if there exist a function* $U:M\to\mathbb{R}$ *and a canonical complex null tetrad* $\{k_a,l_a,m_a,\overline{m}_a\}$ $(k^a l_a=-m^a\overline{m}_a=-1)$ *in which:*

$$DU=\epsilon+\overline{\epsilon}, \tag{16}$$

$$\triangle U=-(\gamma+\overline{\gamma}), \tag{17}$$

$$\delta U=\kappa+\overline{\pi}=-(\tau+\overline{\nu}), \tag{18}$$

$$\sigma+\overline{\lambda}=0, \tag{19}$$

$$\alpha+\overline{\beta}=0, \tag{20}$$

$$\epsilon+\overline{\epsilon}+\gamma+\overline{\gamma}=\rho+\overline{\mu}, \tag{21}$$

$$D(\rho+\overline{\mu})=-\Phi, \tag{22}$$

$$\triangle(\rho+\overline{\mu})=\Phi, \tag{23}$$

$$\delta(\rho+\overline{\mu})=\overline{\delta}(\rho+\overline{\mu})=0, \tag{24}$$

where $\Phi=\Phi(u)$ *is a real function of the timelike coordinate* u.

Proof: With the notation of Theorem 1 we have that for a class A_1 double warped space–time a coordinate chart $\{u,x^k\}$ exists such that the line element takes the form (7), $\vec{X}=\partial_u$ is then a timelike hypersurface orthogonal CKV with associated conformal factor $\psi(u)=\theta_{1,u}(u)$, and $\vec{u}=\mathbf{e}^{-U}\partial_u$ is a unit timelike vector field parallel to $\vec{X}$ where we put $U(u,x^k)=\theta_1(u)+\theta_2(x^k)$ for convenience, it is then easy to see that, in the above coordinate chart, one has

$$u_{a;b}=(U_{,c}u^c)g_{ab}-U_{,a}u_b \tag{25}$$

and also

$$\psi_{,a}=\Phi\mathbf{e}^{-U}u_a, \tag{26}$$

where $\Phi=\Phi(u)$ is a real function of the timelike coordinate u [to be precise: $\Phi=-\theta_{1,uu}(u)$].

One can define a canonical null tetrad as follows:

$$k_a=\frac{1}{\sqrt{2}}(u_a+x^1_a),\quad l_a=\frac{1}{\sqrt{2}}(u_a-x^1_a),\quad m_a=\frac{1}{\sqrt{2}}(x^2_a+ix^3_a), \tag{27}$$

where x^1_a, x^2_a, x^3_a are spacelike vectors orthogonal to u_a. Expressions (16)–(24) are then obtained by contracting (25) and (26) with the tetrad (27).

On the other hand, contracting (16)–(24) with the dual of (27) one recovers expressions (25) and (26), which, according to Theorem 1, imply that the space–time is class A_1 double warped. □

Theorem 5: (M,g) *is a class* A_2 *double warped space–time if and only if there exist a function* $U:M\to\mathbb{R}$ *and a canonical complex null tetrad* $\{k_a,l_a,m_a,\overline{m}_a\}$ $(k^a l_a=-m^a\overline{m}_a=-1)$ *in which one of the following sets of equations holds:*

$$DU=\epsilon+\overline{\epsilon}, \tag{28}$$

$$\Delta U=-(\gamma+\overline{\gamma}), \tag{29}$$

$$\delta U=-\kappa+\overline{\pi}=\tau+\overline{\nu}, \tag{30}$$

$$\sigma-\overline{\lambda}=0, \tag{31}$$

$$\alpha+\overline{\beta}=0, \tag{32}$$

$$\epsilon+\overline{\epsilon}-(\gamma+\overline{\gamma})=\rho-\overline{\mu}, \tag{33}$$

$$D(\rho-\overline{\mu})=\Phi, \tag{34}$$

$$\Delta(\rho-\overline{\mu})=\Phi, \tag{35}$$

$$\delta(\rho-\overline{\mu})=\overline{\delta}(\rho-\overline{\mu})=0, \tag{36}$$

$$DU=\sigma+\overline{\rho}, \tag{37}$$

$$\Delta U=-(\overline{\lambda}+\mu), \tag{38}$$

$$\delta U=\overline{\alpha}-\beta, \tag{39}$$

$$\delta U+\overline{\delta}U=\pi+\overline{\pi}=-(\tau+\overline{\tau}), \tag{40}$$

$$\kappa+\overline{\kappa}=0, \tag{41}$$

$$\nu+\overline{\nu}=0, \tag{42}$$

$$\epsilon-\overline{\epsilon}=0, \tag{43}$$

$$\gamma-\overline{\gamma}=0, \tag{44}$$

$$\delta(\pi+\overline{\pi})=\overline{\delta}(\pi+\overline{\pi})=\Phi', \tag{45}$$

$$\Delta(\pi+\overline{\pi})=D(\pi+\overline{\pi})=0, \tag{46}$$

$$DU=-\sigma+\overline{\rho}, \tag{47}$$

$$\Delta U=\overline{\lambda}-\mu, \tag{48}$$

$$\delta U=\overline{\alpha}-\beta, \tag{49}$$

$$\delta U-\overline{\delta}U=-\pi+\overline{\pi}=-\tau+\overline{\tau}, \tag{50}$$

$$\kappa-\overline{\kappa}=0, \tag{51}$$

$$\nu-\overline{\nu}=0, \tag{52}$$

$$\epsilon-\overline{\epsilon}=0, \tag{53}$$

$$\gamma-\overline{\gamma}=0, \tag{54}$$

$$-\delta(\pi-\overline{\pi})=\overline{\delta}(\pi-\overline{\pi})=-\Phi'', \tag{55}$$

$$\Delta(\pi-\overline{\pi})=D(\pi-\overline{\pi})=0, \tag{56}$$

where Φ,Φ' *and* Φ'' *are real functions of the spacelike coordinate* u.

Proof: The proof follows along the same lines as that of Theorem 4. If $\vec{X}=\partial_u$ is the hypersurface orthogonal spacelike CKV and $\vec{u}=\mathbf{e}^{-U}\partial_u$ is the unit spacelike vector field parallel to it whose existence are ensured by theorem 1, then a canonical tetrad can be constructed in one of the following ways:

$$k_a=\frac{1}{\sqrt{2}}(u_a+x^3_a),\quad l_a=\frac{1}{\sqrt{2}}(-u_a+x^3_a),\quad m_a=\frac{1}{\sqrt{2}}(x^2_a+\imath x^1_a), \tag{57}$$

$$k_a=\frac{1}{\sqrt{2}}(x^2_a+x^3_a),\quad l_a=\frac{1}{\sqrt{2}}(-x^2_a+x^3_a),\quad m_a=\frac{1}{\sqrt{2}}(u_a+\imath x^1_a), \tag{58}$$

$$k_a=\frac{1}{\sqrt{2}}(x^2_a+x^3_a),\quad l_a=\frac{1}{\sqrt{2}}(-x^2_a+x^3_a),\quad m_a=\frac{1}{\sqrt{2}}(x^1_a+\imath u_a), \tag{59}$$

where u_a,x^1_a,x^2_a are spacelike vectors and x^3_a is a timelike vector.

Equations (28)–(36) are obtained contracting (25) and (26) with tetrad (57), (37)–(46) arise from contracting (25) and (26) with tetrad (58), while contraction of (25) and (26) with tetrad (59) gives rise to (47)–(56). To recover expressions (25) and (26) one must in turn contract those sets of equations with the corresponding dual tetrad. □

Regarding the characterization of class B double warped space–times, we shall first recall the necessary and sufficient condition for a space–time to be conformally related to a $2+2$ decomposable one, as it was given in theorem 3 of Ref. 3, and next give the condition on the conformal factor that makes it separable in the two sets of coordinates adapted to the two two-dimensional factor submanifolds. We do this in the following theorem:

Theorem 6: *The necessary and sufficient condition for* (M,g) *to be conformally related to a* $2+2$ *decomposable space–time* $(M,\hat{g})$ *with* $g=\exp(2\theta)\hat{g}$ *(*θ *being a real function), is that there exist null vectors* $\vec{l}$ *and* $\vec{k}$ $(l^ak_a=-1)$ *satisfying*

$$l_{a;b}=Ae^{-\theta}l_al_b-\theta_{,a}l_b+(\theta_{,c}l^c)g_{ab},\quad k_{a;b}=-Ae^{-\theta}k_al_b-\theta_{,a}k_b+(\theta_{,c}k^c)g_{ab}; \tag{60}$$

for some function A. *Further,* (M,g) *is class B doublewarped if and only if*

$$H^c_a(h^d_b\theta_{,d})_{;c}+2(h^d_b\theta_{,d})(H^c_a\theta_{,c})=0,$$

where

$$h_{ab}\equiv-2k_{(a}l_{b)},\quad H_{ab}\equiv g_{ab}+h_{ab}. \tag{61}$$

Proof: The reader is referred to Theorem 3 of Ref. 3 for a proof of the first part of the theorem. As for the second part, namely that characterizing double warped space–times within the larger class of space–times which are conformal to $2+2$ decomposable ones, notice that Eq. (61) is nothing but the covariant expression of $\partial_\alpha(\partial_A\theta)=0$, where $\{x^\alpha\}$ and $\{x^A\}$ are coordinate charts on the two 2-dimensional submanifolds M_1 and M_2, respectively (see Sec. I). □

As in the former case, Theorem 6 can be expressed in terms of the NP formalism. To do so, a complex null tetrad $\{k_a,l_a,m_a,\overline{m}_a\}\equiv\{z^m_a\}$ is chosen such that $\vec{k}$ and $\vec{l}$ are the vectors in (60); i.e., $k^al_a=-m^a\overline{m}_a=-1$ all other inner products vanishing.
One then has

Theorem 7: *The necessary and sufficient condition for* (M,g) *to be conformally related to a* $2+2$ *decomposable space–time* $(M,\hat{g})$*, with* $g=e^{2\theta}\hat{g}$*, is that there exist a function* $\theta: M\to\mathbb{R}$ *and a canonical complex null tetrad* $\{k_a,l_a,m_a,\overline{m}_a\}$ *as described above such that*

$$\kappa=\sigma=\lambda=\nu=\alpha+\overline{\beta}=\pi+\overline{\tau}=\rho+(\epsilon+\overline{\epsilon})=0,$$

$$Ae^{-\theta}=\mu+(\gamma+\overline{\gamma}), \tag{62}$$

$$\rho=-D\theta, \quad \mu=\Delta\theta, \quad \tau=-\delta\theta,$$

where A *is the real function appearing in (60). Furthermore,* (M,g) *is class B double warped if and only if*

$$\delta\rho=-2\rho\tau, \quad \delta\mu=-2\mu\tau, \quad \rho\mu=0. \tag{63}$$

Proof: Equation (60) for $\vec{l}$ and $\vec{n}=\vec{k}$ becomes in NP formalism

$$\gamma_{1mn}=b\,\eta_{1m}\eta_{1n}-\theta_{,m}\eta_{1n}+\eta_{mn}D\theta, \tag{64}$$

$$\gamma_{2mn}=-b\,\eta_{2m}\eta_{1n}-\theta_{,m}\eta_{2n}+\eta_{mn}\Delta\theta, \tag{65}$$

where $b\equiv Ae^{-\theta}$, $m,n,\ldots$ are tetrad indices and the notation is the same as in Ref. 9. Contracting (64) and (65) with the tetrad vectors, (62) are easily obtained.

On the other hand, the tetrad version of (61), together with the information contained in (62), yields (63).

Conversely, (62) and (63) contracted with the dual tetrad of $\{k_a,l_a,m_a,\overline{m}_a\}$ give Eqs. (60) and (61). □

The characterization of class A and class B double warped space–times given in Theorems 1 and 6, or alternatively 4, 5, and 7 should prove useful in formulating an algorithm for classifying such metrics. This is so because this characterization is coordinate independent although tetrad dependent. In what follows the tetrads described in Theorems 4, 5, and in Theorem 7 will be designated as *dw tetrads of class A and B, respectively*.

Thus, in order to determine whether a given metric g represents a double warped space–time, one can either use Theorems 1, and 6 (coordinate approach), or else their counterparts 4, 5, and 7 through the following scheme:

(1) Determine the Petrov type of the Weyl tensor associated with the metric g and choose a canonical tetrad $\{k_a,l_a,m_a,\overline{m}_a\}$ such that $g_{ab}=2[-l_{(a}k_{b)}+m_{(a}\overline{m}_{b)}]$.
(2) Determine the NP spin coefficients and their NP derivatives in the chosen tetrad (1).
(3) If the scalars determined in step (2) satisfy the relations of Theorem 4 or 5 (respectively, 7) for some function U (respectively, θ), then the space–time is double warped of class A (respectively, B) and the algorithm stops here, otherwise continue the algorithm.
(4) If possible, find the Lorentz transformation of the invariance group that transforms tetrad (1) into a dw tetrad; i.e., such that the corresponding NP spin coefficients and NP derivatives obey the conditions in Theorem 4 or 5 (respectively, 7). If such a transformation exists, the space–time is double warped of class A (respectively, B), otherwise it is not double warped.

The Lorentz transformations considered in step (4) must belong to the invariance group of the Petrov type of the metric since in step (1) one chooses a canonical tetrad. Thus, for instance, if the given metric is of the Petrov type D or N, then in step (4) one looks for spin and boost transformations or for null rotations respectively.

III. CURVATURE STRUCTURE

The purpose of this section is to study the Riemann tensor of double warped space–times in connection with that of the underlying, conformally related, decomposable space–time, with a special emphasis on the algebraic Petrov and Segre types of the associated Weyl and Ricci tensors, respectively.

First of all, notice that since the metric g of the double warped space–time is conformally related to that of the decomposable space–time $\hat{g}$, their respective Weyl conformal tensors and hence their Petrov types, will be equal. The Petrov types of decomposable space–times can be easily calculated and are in most cases related to the holonomy type of the space–time; thus Ref. 5 one has that if the space–time is $1+3$ spacelike (holonomy type R_{13}) the Petrov type can only be I, D, or O, whence it follows that class A_1 double warped space–times can only be of those Petrov types. In the case of $1+3$ timelike decomposable space–times the Petrov type of the Weyl tensor is unrestricted and the same will hold for A_2 double warped space–times. Finally, the Petrov type of $2+2$ decomposable space–times (holonomy type R_7), and hence that of class B double warped ones, can only be D or O. Further, if it is type D the null vectors $\vec{k}$ and $\vec{l}$ in Theorem 6 are principal null directions of the Weyl tensor $C^a{}_{bcd}$, since the corresponding null vectors in the underlying $2+2$ decomposable space–time (that is: the recurrent null vectors $\hat{l}_a = e^{-\theta} l_a$ and $\hat{k}_a = e^{-\theta} k_a$, see Ref. 3 for details) can be easily seen to be principal null directions of the Weyl tensor in $(M,\hat{g})$; i.e., $\hat{C}^a{}_{bcd}$ (which equals $C^a{}_{bcd}$); see Ref. 10.

Regarding the Segre classification of the Ricci tensor, similar comments to those in the case of warped space–times hold; that is: conformal scaling does change the Ricci tensor and therefore the Segre type of double warped space–times is unrestricted in principle. Further, in the case of class A warped space–times we have that the unit vector field $\vec{u}$ (see proof of Theorem 1) is always an eigenvector of the Ricci tensor[3] (and therefore the Segre type of class A_1 warped space–times is {1,111} or one of its degeneracies), while in the case of double warped space–times this is no longer so for, from the Ricci identity specialized to $\vec{u}$ it follows (see Ref. 11):

$$R^a{}_b u_a = -\tfrac{2}{3}\Theta_{,b} + \tfrac{1}{3}(\dot{\Theta} + \Theta^2) u_b ,$$

now, in order for $\vec{u}$ to be an eigenvector of the Ricci tensor, it should be that $\Theta_{,b} \propto u_b$ and then a trivial calculation using the expressions for $\vec{u}$ and the metric that appear in the proof of Theorem 1 shows that either $\Theta = 0$ and then the conformal factor associated with $\vec{X}$ is $\psi = 0$; i.e., $\vec{X}$ is a KV and the space–time is A_2 warped (see Corollary 2) or else $U(u,x^k) = \theta_1(u)$ the space–time thus being type A_1 warped. Since the converse follows trivially, we have shown

Corollary 8: The necessary and sufficient condition for a class A double warped space–time to be a class A warped space–time is that the CKV $\vec{X}$ in Theorem 1 be a Ricci eigenvector (then it is of class A_1 if it is a proper CKV and of class A_2 if it is a KV).

In the case of type B space–times, all Segre types are possible in principle.

To close this section, we next give the expressions of the Ricci tensors and the Ricci scalar. They can be derived easily from Appendix D in Ref. 12. Notice that, in the notation established in the previous section, $\theta_{\alpha,A} = \theta_{\alpha/A} = 0$,

$$\begin{aligned} R_{\alpha\beta} &= \hat{R}_{\alpha\beta} - 2[\theta_{1\ \alpha/\beta} - \theta_{1\ \alpha}\theta_{1\ \beta}] - S\hat{h}_{1\ \alpha\beta}, \\ R_{\alpha B} &= 2\theta_{1\ \alpha}\theta_{2\ B}, \\ R_{AB} &= \hat{R}_{AB} - 2[\theta_{2\ A/B} - \theta_{2\ A}\theta_{2\ B}] - S\hat{h}_{2\ AB}, \end{aligned} \tag{66}$$

where

$$S \equiv \theta^d{}_{/d} + 2\theta^d\theta_d , \tag{67}$$

that is:

$$S=\frac{1}{\sqrt{-\hat{h}_1}}[\sqrt{-\hat{h}_1}\theta_1^{\mu}]_{,\mu}+2\hat{h}_1^{\mu\nu}\theta_{1\,\mu}\theta_{1\,\nu}+\frac{1}{\sqrt{\hat{h}_2}}[\sqrt{\hat{h}_2}\theta_2^{M}]_{,M}+2\hat{h}_2^{MN}\theta_{2\,M}\theta_{2\,N}, \tag{68}$$

where $\hat{h}_1\equiv\det(\hat{h}_1)_{\mu\nu}$, $\hat{h}_2\equiv\det(\hat{h}_2)_{AB}$, and $\theta_{1\,\alpha}\equiv\theta_{1\,,\alpha}$, etc., and $\hat{R}_{ab}$ stands for the components of the Ricci tensor associated with the decomposable metric $\hat{g}$, which turn out to be $\hat{R}_{\alpha\beta}=\hat{R}_{1\,\alpha\beta}$ and $\hat{R}_{AB}=\hat{R}_{2\,AB}$ that is: the Ricci tensors of the metrics $\hat{h}_1$ and $\hat{h}_2$, respectively. Notice that S is separable as a sum in the coordinates x^{α} and x^{A}. For the Ricci scalar one easily gets

$$\begin{aligned}R=e^{-2(\theta_1+\theta_2)}\{\hat{R}-6[&(-\hat{h}_1)^{-1/2}((-\hat{h}_1)^{1/2}\theta_1^{\mu})_{,\mu}+\hat{h}_1^{\mu\nu}\theta_{1\,\mu}\theta_{1\,\nu}\\&+(\hat{h}_2)^{-1/2}((\hat{h}_2)^{1/2}\theta_2^{M})_{,M}+\hat{h}_2^{MN}\theta_{2\,M}\theta_{2\,N}]\},\end{aligned} \tag{69}$$

where $\hat{R}$ denotes the Ricci scalar of the metric $\hat{g}$, which is simply $\hat{R}_1+\hat{R}_2$, i.e., the sum of the Ricci scalars associated with the metrics $\hat{h}_1$ and $\hat{h}_2$.

IV. THE CONFORMAL LIE ALGEBRA OF CLASS B DOUBLE WARPED SPACE–TIMES

The purpose of this section is to make a few remarks on the Lie algebra of CKV, including Killing vectors (KV) and homothetic vectors (HV), of class B double warped space–times.

A double warped space–time (M,g) admits a CKV $\vec{X}$ iff $\mathcal{L}_{\vec{X}}g=2\psi g$ where ψ is some real function. If $\psi=$constant then $\vec{X}$ is a HV and if $\psi=0$ it is a KV.

Now, since a double warped space–time (M,g) is always conformally related to a decomposable one $(M,\hat{g})$, their respective conformal algebras will be equal; and as it turns out, it is relatively simple to deal with the conformal algebra of the decomposable space–time $(M,\hat{g})$. Conformal algebras in locally decomposable space–times have been studied by Coley and Tupper,[13] Capocci and Hall,[14] and (following a different approach) by Tsamparlis.[15] For the sake of completeness, we next summarize the basic results and refer the reader to the above papers for detailed proofs.

Theorem 9: *Let $(M,\hat{g})$ be a 2+2 decomposable space–time; the following results hold regarding its conformal Lie algebra:*

(1) If $(M,\hat{g})$ is conformally flat (CF) its conformal algebra is 15-dimensional, their generators being those of Minkowski's conformal algebra. In this case the two factor submanifolds must each be of constant curvature, say k_1 and k_2, respectively, with $k_1+k_2=0$.

(2) If it is not CF, the only CKV it may admit are KV or HV.

(3) If $(M,\hat{g})$ is not CF its KV are the KV of the submanifolds $(M_i,\hat{h}_i)$, for $i=1,2$; that is: if $\zeta^a=(\zeta^0,\zeta^1)$ is a KV of $(M_1,\hat{h}_1)$, then $\xi^a=(\zeta^0,\zeta^1,0,0)$ is a KV of $(M,\hat{g})$, etc. Also, $(M,\hat{g})$ will admit a HV if and only if each of $(M_i,\hat{h}_i)$ for $i=1,2$ admit a HV, i.e., if $\kappa^a=(\kappa^0,\kappa^1)$ and $\lambda^a=(\lambda^2,\lambda^3)$ are HV of the 2-spaces (adjusted to the same numerical values of the respective homothetic scalars), then $\eta^a=(\kappa^0,\kappa^1,\lambda^2,\lambda^3)$ is an HV of $(M,\hat{g})$ with the same value for its homothetic scalar.

For the case referred to in the above theorem, the reader is also referred to Ref. 16 where a thorough discussion of conformally decomposable $2+2$ space–times is given, along with a classification in terms of their conformal algebra.

V. THE CONFORMAL LIE ALGEBRA OF CLASS A DOUBLE WARPED SPACE–TIMES

We shall dedicate this section to the study of the conformal algebra of class A double warped space–times, which by our previous remarks, will be the same as that of the underlying $1+3$ decomposable space–time in each case. In so doing, we shall give some interesting results on

particular types of CKV (namely: gradient CKV or GCKV for short) in three-dimensional manifolds which, to the best of our knowledge, are new. Most of the results on proper CKV in $1+3$ decomposable space–times can be found in Ref. 13 and also (although no explicit expressions are given) in Ref. 14, we re-derive them here following a different approach which provides interesting information on the geometry of three-dimensional manifolds, and renders along the way useful and interesting results on particular types of CKV (namely: gradient CKV, GCKV for short) also in three-dimensional manifolds which, to the best of our knowledge, do not exist in the literature.

For this section alone, we shall change our notation slightly so as to avoid unnecessary complications, thus, the line element of the decomposable space–time $(M,\hat{g})$ will be written as

$$\mathrm{d}\hat{s}^2=[\epsilon \mathrm{d}u^2+h_{AB}(x^D)\mathrm{d}x^A\,\mathrm{d}x^B],\quad \epsilon=\pm 1. \tag{70}$$

The three-dimensional submanifold coordinated by x^A, $A=1,2,3$ will be noted as V and its metric (of either signature) as h (instead of $\hat{h}$). We shall represent the covariant derivative with respect to the three-dimensional metric h by a slash ("/"), whereas a semicolon ";" will be used to note that with respect to the four-dimensional metric $\hat{g}$. (The reader is reminded that this notation holds only in the present section: notice that, in the rest of the paper, a semicolon stands for the covariant derivative associated with g, the metric of the double warped space–time, whereas a slash stands for that associated with $\hat{g}$, the metric of the decomposable space–time.) The covariantly constant vector is then $\vec{u}=\partial_u$ (i.e., $u_{a;b}=0$ and therefore it is a non-null gradient KV). Finally note that, in the above coordinate system, the covariant derivatives satisfy

$$X_{ab\cdots\ ;u}=X_{ab\cdots\ ,u},\quad X_{ab\cdots\ ;A}=X_{ab\cdots\ /A}$$

for any tensor $X_{ab\cdots}$, and also that

$$R_{ua}=0,\quad R_{AB}=\overset{(3)}{R}_{AB},$$

where $\overset{(3)}{R}_{AB}$ stands for the Ricci tensor associated to the 3-metric h on V.

In order to investigate its conformal algebra, we first make a few trivial remarks in the paragraphs that follow.

First of all, and making an obvious abuse in the notation, we shall represent points in M by their coordinates in the above chart [that is: $p\in M$ with coordinates $x^a(p)=(u,x^A)$ will be represented simply as (u,x^A)]; next we consider the three-dimensional submanifold (hypersurface) consisting of all the points with the same value of the x^0 coordinate, say $x^0=u$, and note it as $V(u)$; i.e., $V(u)=\{(u,x^A)\ :\ u\ \text{fixed}\}$; the induced metric on $V(u)$ is h and, clearly, any two such submanifolds are diffeomorphic amongst themselves [and diffeomorphic to (V,h)] by the one-parameter group of isometries $\{\tau_t\}$ generated by $\vec{u}$ [that is: $\tau_t:V(u)\to V(u+t)$ where $\tau_t(u,x^A)=(u+t,x^A)$ wherever this makes sense].

Note that $\tau_t^*h=h$; that is, the three-dimensional metric h is invariant under the isometries generated by $\vec{u}$. Further, a vector field $\vec{X}$ in M will be invariant under these isometries ($\tau_{t*}\vec{X}=\vec{X}$) iff $[\vec{u},\vec{X}]=0$. In particular, if $\vec{X}$ is tangent to the submanifolds $V(u)$ it follows that it will be invariant under $\{\tau_t\}$ iff its components with respect to the above coordinate basis do not depend on u, i.e., $\vec{X}=X^A(x^D)\partial_A$.

Finally, we shall use the notation $\mathcal{C}_n(V,h)$ ($\mathcal{S}_n(V,h)$, $\mathcal{H}_n(V,h)$ or $\mathcal{K}_n(V,h)$) to designate the n-dimensional conformal (respectively: special conformal, homothetic or Killing) algebra of (V,h). Such an algebra (and therefore all of its subalgebras) is finite dimensional, its dimension being 10 at most (and (V,h) is then conformally flat). If (V,h) is nonconformally flat, then, a remarkable theorem by Hall and Capocci (see Ref. 17) shows that its dimension can be at most 4. In our subsequent developments we will often have to refer to some basis of $\mathcal{C}_n(V,h)$, which we will generically represent by $\{\vec{\zeta}_k\}$, $k=1,\ldots,n$ with associated conformal factors ψ_k; that is

$$\mathcal{L}_{\vec{\zeta}_k} h = 2\psi_k h. \tag{71}$$

Notice that any such basis is invariant under the isometries generated by $\vec{u}$; that is: $[\vec{u},\vec{\zeta}_k]=0$, $k=1,\ldots,n$, hence $\vec{\zeta}_k=\zeta_k^B(x^D)\partial_B$ and therefore also $\psi_k=\psi_k(x^D)$. (Some of the conformal factors ψ_k may be constant if they correspond to homotheties, or zero in the case of Killing vectors.)

We can now consider the problem of finding the CKV of a $1+3$ reducible space–time $(M,\hat{g})$. Let $\vec{Y}\in\mathcal{C}_r(M,\hat{g})$, one then has

$$Y_{a;b}+Y_{b;a}=2\phi\hat{g}_{ab}.$$

In the chosen coordinate chart, $\vec{Y}=Y^u(u,x^B)\partial_u+Y^A(u,x^B)\partial_A$ and the above equation then reads (on account of our previous remarks):

$$Y_{u,u}=\epsilon_1\phi, \tag{72}$$

$$Y_{u,A}+Y_{A,u}=0, \tag{73}$$

$$Y_{A/B}+Y_{B/A}=2\phi h_{AB}. \tag{74}$$

Now, (74) effectively says that for u fixed the vector field $Y^B(u,x^D)\partial_B$ is a CKV in $V(u)$ [equivalently: if a proper CKV is admitted in $(M,\hat{g})$ then, its projection on the submanifolds $V(u)$ is a CKV there], therefore, given $\{\vec{\zeta}_k\}$ a basis for $\mathcal{C}(V,h)$, it follows that it will also be a basis of $\mathcal{C}(V(u),h)$ (u fixed but otherwise arbitrary) whence, on $V(u)$ we shall necessarily have $Y^B(u,x^D)\partial_B=\lambda^k\vec{\zeta}_k$ with $\lambda^k=$constant and summation over $k=1,\ldots,n$ is to be understood; again this will be so for any $V(u)$ (i.e., u fixed but otherwise arbitrary). Finally, since $[\vec{u},\vec{\zeta}_k]=0$, we will have

$$\vec{Y}=Y^u(u,x^B)\partial_u+\lambda^k(u)\vec{\zeta}_k(x^B), \tag{75}$$

where $\lambda^k(u)$, $k=1,\ldots,n$ are n functions of the coordinate u. Substituting this back into (72)–(74) and putting $\phi\equiv\dot{\Sigma}$, where a dot indicates differentiation with respect to u, yields

$$Y_u=\epsilon_1\Sigma, \quad \phi=\dot{\Sigma}=\lambda_k(u)\psi_k(x^B), \tag{76}$$

$$\epsilon_1\Sigma_{,A}+\dot{\lambda}^k\zeta_{k\ A}=0. \tag{77}$$

Further, $\dot{\lambda}^k(u)\vec{\zeta}_k$ is also a CKV in each $V(u)$ [since for u fixed it is a linear combination of the CKV in the basis of $\mathcal{C}(V,h)$] which, on account of (77), is locally a gradient, i.e., $\dot{\lambda}^k\zeta_{k\ A}=-\epsilon_1\Sigma_{,A}$. The question arises as to how many independent GCKV may (V,h) admit, what are they; namely proper CKV, proper HV, or KV, and what does their existence imply on the 3-metric h.

Before proceeding, the following remarks, which follow trivially from the above equations, are in order:

R0: If no GCKV exist in (V,h), then $\dot{\lambda}^k=0$ [i.e., $\lambda^k(u)=$constant] in the above equations and $\phi=\lambda^k\psi_k(x^B)=$constant (since then $\phi=\lambda^k\psi_k(x^D)\equiv\phi(x^D)$, which yields $Y_u=u\phi(x^D)+B(x^D)$, but then $Y_{u,A}+Y_{A,u}=0$ implies $\phi_{,A}=B_{,A}=0$.), that is: $\vec{Y}$ is homothetic in $(M,\hat{g})$ [and $\lambda^k(u)\vec{\zeta}_k$ is also homothetic in (V,h)]. If (V,h) is such that no HV are admitted, then the only CKV that $(M,\hat{g})$ admits are KV.

R1: Let $\vec{\xi}$ be a KV in (V,h), then $\vec{\xi}$ is also a KV of $(M,\hat{g})$.

R2: Let $\vec{Y}$ be a KV in $(M,\hat{g})$. The following situations may then arise:

(a) (V,h) admits no KV, then $\vec{Y}=a\partial_u$ necessarily.

(b) (V,h) admits KV none of which is locally a gradient. Then, if $\{\vec{\xi}_k\}$ is a basis of $\mathcal{K}(V,h)$, one has

$$\vec{Y}=a\partial_u+b^k\vec{\xi}_k \tag{78}$$

with a,b^k arbitrary constants.

(c) (V,h) admits KV some of which are locally gradients (and therefore, by the Killing equation, covariantly constant vectors). Then one can choose a basis for $\mathcal{K}(V,h)$, say $\{\vec{\xi}_1,\ldots,\vec{\xi}_p,\vec{\xi}_{p+1},\ldots,\vec{\xi}_n\}$ (with $p\leqslant 3$) in a way such that $\vec{\xi}_1,\ldots,\vec{\xi}_p$ are covariantly constant. Then

$$\vec{Y}=A(x^B)\partial_u+a^s u\ \ \vec{\xi}_s+b^k\vec{\xi}_k, \tag{79}$$

where a^s,b^k are arbitrary constants, $(s=1,\ldots,p,\ k=1,\ldots,n)$ and $A(x^B)$ satisfies $A_{,B}=a^s\xi_{s\,B}$. Notice that if one of the gradient KV in (V,h) is non-null, the space–time $(M,\hat{g})$ decomposes still further, becoming a $1+1+2$ decomposable space–time. If (V,h) admits two, then a third one is automatically admitted and the space–time $(M,\hat{g})$ is locally flat. We shall return to this later on in the paper.

R3: Let $\vec{\eta}$ be a proper HV in (V,h) with homothetic constant $k(\neq 0)$, then $\vec{Y}=ku\partial_u+\vec{\eta}$ is also a HV of $(M,\hat{g})$ with homothetic constant k. Further, if $\vec{Y}$ is a proper HV of $(M,\hat{g})$ with homothetic constant $k(\neq 0)$, then it is of the form

$$\vec{Y}=ku\partial_u+\vec{\eta}, \tag{80}$$

$\vec{\eta}$ being a (proper) HV in (V,h) scaled so as to have the same value k for its homothetic constant; the above HV is unique up to the addition of KV such as those given by (78) and/or (79) (if GKV exist).

The various possibilities regarding the existence of GCKV in (V,h) can be summarized as follows:

(1) (V,h) admits no GCKV (either proper or homothetic, including Killing). In that case (77) implies $\dot{\lambda}^k=0$ and the rest of the equations imply then that $\vec{Y}$ is a HV, see Eqs. (78) or (80) above. Thus, in this case $(M,\hat{g})$ admits no proper CKV.

(2) The only GCKV that (V,h) admits are gradient KV (GKV). In this case $(M,\hat{g})$ admits a proper CKV (which turns out to be a SCKV) if and only if the GKV is null and (V,h) admits a proper SCKV (i.e., nonhomothetic) such that the gradient of its conformal factor is parallel to the null GKV. Otherwise the only CKV that $(M,\hat{g})$ admits are HV.

(3) (V,h) admits proper gradient HV (GHV); it may also admit GKV, but no proper GCKV exist in (V,h). In this case, $(M,\hat{g})$ does admit a proper CKV which turns out to be special (i.e., SCKV); that is: its associated conformal factor ϕ satisfies $\phi_{a;b}=0$. This SCKV is unique up to the addition of KV and HV which must then take the forms discussed above.

(4) (V,h) admits proper GCKV (GHV and/or GKV can also be admitted in principle). In this case, the space–time admits proper CKV.

Regarding the maximum number of GCKV that a three-dimensional space may admit, one can easily prove the following results:

Proposition 1: Let (V,h) be a three-dimensional Lorentz or Riemann space admitting two independent proper GCKV, say $\vec{\zeta}$ and $\vec{\chi}$, with associated conformal factors ψ and ϕ, respectively, then:

(1) The Lie bracket $[\vec{\zeta},\vec{\chi}]\equiv\vec{\xi}$ is a KV.

(2) The conformal factors are $\psi=k\zeta$ and $\phi=k\chi$, where k is a constant and ζ and χ are the

functions whose gradients are the GCKV $\vec{\eta}$ *and* $\vec{\chi}$*, respectively.*

(3) (V,h) *is of constant curvature and therefore the Cotton–York tensor vanishes, thus being conformally flat.*

Proof: Suppose $\vec{\eta}$ and $\vec{\chi}$ are linearly independent GCKV satisfying

$$\zeta_{A/B}=\psi h_{AB}, \quad \chi_{A/B}=\phi h_{AB},$$

where $\zeta_A=\zeta_{,A}$, $\chi_A=\chi_{,A}$ and also [see comments following Eq. (111)] $\psi=\psi(\zeta)$ and $\phi=\phi(\chi)$. Now, a direct calculation shows that

$$[\vec{\zeta},\vec{\chi}]=\phi\vec{\zeta}-\psi\vec{\chi}\equiv\vec{\xi}$$

that is, $\vec{\eta}$ and $\vec{\chi}$ are surface-forming.

Compute next

$$\mathcal{L}_{[\vec{\zeta},\vec{\chi}]}h_{AB}=\mathcal{L}_{\vec{\zeta}}(\mathcal{L}_{\vec{\chi}}h_{AB})-\mathcal{L}_{\vec{\chi}}(\mathcal{L}_{\vec{\zeta}}h_{AB})=2(\zeta^D\chi_D)(\tilde{\phi}-\tilde{\psi})h_{AB},$$

where $\tilde{\phi}\equiv \mathrm{d}\phi/\mathrm{d}\chi$ and $\tilde{\psi}\equiv \mathrm{d}\psi/\mathrm{d}\zeta$, and also

$$\mathcal{L}_{\vec{\xi}}h_{AB}=\mathcal{L}_{\phi\vec{\zeta}-\psi\vec{\chi}}h_{AB}=(\tilde{\phi}-\tilde{\psi})(\zeta_A\chi_B+\chi_A\zeta_B)$$

therefore

$$(\tilde{\phi}-\tilde{\psi})(\zeta_A\chi_B+\chi_A\zeta_B)=2(\zeta^D\chi_D)(\tilde{\phi}-\tilde{\psi})h_{AB}.$$

An elementary consideration on the ranks of the tensors at both sides of the equation readily shows that

$$\tilde{\phi}-\tilde{\psi}=0;$$

therefore

$$\psi=k\eta, \quad \phi=k\chi$$

and $\vec{\xi}$ is then a KV given by

$$\vec{\xi}=k(\chi\vec{\zeta}-\zeta\vec{\chi}),$$

which is not a gradient: $\xi_{A/B}=k(\zeta_A\chi_B-\chi_A\zeta_B)$.

Now, since both $\vec{\zeta}$ and $\vec{\chi}$ are GCKV their respective conformal bivectors are zero and (12) applied to them yields

$$R_{ABCD}\zeta^D=k(\zeta_A h_{BC}-\zeta_B h_{AC}),$$

$$R_{ABCD}\chi^D=k(\chi_A h_{BC}-\chi_B h_{AC}),$$

which in turn implies, upon contraction with h^{AC},

$$R_{BD}\zeta^D=-2k\zeta_B, \quad R_{BD}\chi^D=-2k\chi_B.$$

Now, in three dimensions one has

$$R_{ABCD}=R_{AC}h_{BD}-R_{AD}h_{BC}+h_{AC}R_{BD}-h_{AD}R_{BC}+(R/2)(h_{AD}h_{BC}-h_{AC}h_{BD})$$

hence, the above equations imply

$$R_{AC}\zeta_B-\zeta_A R_{BC}+(k+R/2)(\zeta_A h_{BC}-\zeta_B h_{AC}=0,$$

$$R_{AC}\chi_B-\chi_A R_{BC}+(k+R/2)(\chi_A h_{BC}-\chi_B h_{AC}=0,$$

contracting the two equations above with ζ^A and χ^A, respectively, we get, since $\zeta^A\zeta_A, \chi^A\chi_A \neq 0$:

$$R_{AC}=(k+R/2)h_{AC}-(3k+R/2)\zeta_A\zeta_C,$$

$$R_{AC}=(k+R/2)h_{AC}-(3k+R/2)\chi_A\chi_C$$

contracting again both equations with, say ζ^C, equating and rearranging terms we get

$$(3k+R/2)\zeta_A=(3k+R/2)(\zeta_C\chi^C)\chi_A$$

but this contradicts our hypothesis of linear independence unless $3k+R/2=0$, i.e., $R=-6k$ $(=\text{constant})$. Then $R_{AB}=-2kh_{AB}$ and $R_{ABCD}=k(h_{AD}h_{BC}-h_{AC}h_{BD})$; that is: (V,h) is of constant curvature and therefore the associated Cotton–York tensor[11] is zero, i.e., h is conformally flat. □

The converse theorem also holds; namely: if (V,h) is a three-dimensional space or space–time of constant curvature (and therefore conformally flat), it admits two linearly independent GCKV whose associated conformal factors are multiples (with the same multiplicative constant) of the functions whose gradients they are.

Furthermore, with the same notation and hypotheses as in the preceding theorem and following a similar procedure to that outlined in its proof, it is easy to prove the following three results:

Lemma 2: Let $\vec{\zeta}$ be a GCKV and $\vec{\xi}$ a GKV (i.e., $\vec{\xi}$ is covariantly constant). Then $\vec{\zeta}$ is necessarily homothetic, that is, it is a GHV.

Proof: Since $\zeta_{A/B}=\psi h_{AB}$ and $\xi_{A/B}=0$ it follows $[\vec{\zeta},\vec{\xi}]=-\psi\vec{\xi}$. Computing next the Lie derivative of h in two different ways, as in the proof of Theorem 1, and then equating yields

$$2(\xi^D\psi_D)h_{AB}=\tilde{\psi}(\zeta_A\xi_B+\xi_A\zeta_B).$$

Again, considerations on the rank of the tensors that appear on both sides of the equation, imply $\psi_A=0$; that is: $\vec{\zeta}$ is a GHV. □

Lemma 3: Let $\vec{\zeta}$ be a GCKV and $\vec{\eta}$ a GHV. Then $\vec{\zeta}$ is necessarily homothetic and therefore it is the linear combination of $\vec{\eta}$ with some GKV.

Proof: Now $\zeta_{A/B}=\psi h_{AB}$ and $\eta_{A/B}=kh_{AB}$, and their Lie bracket is $[\vec{\zeta},\vec{\xi}]=k\vec{\zeta}-\psi\vec{\eta}$. Computing as above the Lie derivative of h in two different ways and then equating implies

$$2(\eta^D\psi_D)h_{AB}=(\eta_A\psi_B+\psi_A\eta_B),$$

which again implies $\psi_A=0$ and the result follows. □

Lemma 4: Let $\vec{\eta}$ and $\vec{\xi}$ be a proper GHV and a GKV, respectively; (V,h) is then flat.

Proof: In this case we have $R_{ABCD}\eta^D=R_{ABCD}\xi^D=0$, hence $R_{AB}\eta^D=R_{AB}\xi^B=0$, and taking into account the expression of the Riemann tensor in terms of the metric and the Ricci tensor (see the proof of Theorem 1 and recall that $\vec{\eta}$ cannot be null), one gets $R_{AB}=(R/2)(h_{AB}-(\eta^D\eta_D)^{-1}\eta_A\eta_B)$; contracting with ξ^B both sides and equating to zero yields immediately $\eta_D\xi^D=R=0$ (since $\vec{\eta}$ and $\vec{\xi}$ are linearly independent), and this in turn implies $R=R_{AB}=0$ and then $R_{ABCD}=0$. □

The same result holds trivially if two linearly independent GKV exist; since in this case two linearly independent constant vector fields in a manifold of dimension three readily imply (constancy of the metric) that a third one must also exist. Thus, we have proven:

Proposition 2: A three-dimensional space or space–time admitting two linearly independent GHV (proper or Killing) is necessarily flat.

Note that from the above Propositions 1 and 2, it follows that if two (or more) independent GCKV exist in the three-space (V,h), then it is of constant curvature (and therefore conformally flat, being flat in several cases) and then it admits 10 CKV (those of flat three-dimensional space). If this is not the case [i.e., (V,h) is not of constant curvature] then it can admit, at most, one GCKV which will then give rise to a proper CKV in $(M,\hat{g})$. If (V,h) admits no GCKV, then no proper CKV exist in $(M,\hat{g})$, just HV (case 1 above).

In the following sections we shall deal with cases 2, 3, and 4 separately, assuming that the GCKV admitted in each case is unique.

A. (V,h) admits a GKV and no proper GHV or GCKV

From the preceding results it follows that unless (V,h) is conformally flat (in which case its conformal algebra is completely known), the GKV, say $\vec{\xi}$, is the unique GCKV it admits. Taking now a basis of $\mathcal{C}_n(V,h)$ as $\{\vec{\xi},\vec{\eta},\vec{\zeta}_k\}$ where $\vec{\zeta}_k$ and $\vec{\eta}$ denote CKV (including KV) and a HV, respectively [in case one exists in (V,h), if not, just set $\vec{\eta}=0$], we can write, from (74)

$$Y_A=\lambda(u)\xi_A+\mu(u)\eta_A+\lambda^k(u)\zeta_A,$$

which substituted into (73) yields

$$-Y_{u,A}=\dot{\lambda}(u)\xi_A+\dot{\mu}(u)\eta_A+\dot{\lambda}^k(u)\zeta_A.$$

Since by hypothesis, $\vec{\xi}$ is the only GCKV in (V,h) and $\vec{\xi}$, $\vec{\eta}$ (if nonzero) and $\vec{\zeta}_k$ are linearly independent vector fields, it follows that $\dot{\mu}(u)=\dot{\lambda}_k(u)=0$ [otherwise the above equation would imply that, for u fixed, $\dot{\mu}(u)\eta_A+\dot{\lambda}^k(u)\zeta_A$ is a GCKV independent of $\vec{\xi}$]; hence $\mu=a_0$ ($=$constant) [and $a_0=0$ if (V,h) admits no proper HV], and $\lambda^k=a^k$ ($=$constant). Therefore

$$Y_A=\lambda(u)\xi_A+a_0\eta_A+a^k\zeta_A$$

and substituting this back into (74), (72), and (73) one has

$$\phi=\dot{\Sigma}=a_0k+a^k\psi_k(x^D), \tag{81}$$

$$Y_u=\epsilon_1(a_0k+a^k\psi_k(x^D))u+B(x^D),\quad \epsilon_1(a_0k+a^k\psi_k(x^D))_{,A}u+B(x^D)_{,A}+\dot{\lambda}(u)\xi_A=0 \tag{82}$$

hence

$$\dot{\lambda}(u)=au+b,$$

i.e.,

$$\lambda(u)=\frac{a}{2}u^2+bu+c$$

and also

$$a^k\psi_k(x^D)=\epsilon_1(-a\xi+m),\quad B(x^D)=-b\xi+n$$

and substituting this into the expressions for the covariant components of $\vec{Y}$, we would get $Y_u=(\epsilon_1a_0k+m)u-(au+b)\xi+n$ and $Y_A=[(a/2)u^2+bu+c]\xi_A+X_A$ where $X_A\equiv a_0\eta_A+a^k\zeta_{kA}$. Notice that the constants n and c can be set equal to zero without loss of generality, as they amount to adding multiples of $\vec{u}=\partial_u$ and $\vec{\xi}$, respectively. On the other hand, X_A are the covariant components of a CKV whose associated conformal factor is $\epsilon_1(-a\xi+m)+a_0k$ [if no HV exists in (V,h) then the CKV has components $X_A=a^k\zeta_{kA}$ and conformal factor $-\epsilon_1(-a\xi+m)$], that is

$$Y_a dx^a = [(\epsilon_1 k a_0 + m)u - (au + b)\xi]du + \left[\left(\frac{a}{2}u^2 + bu\right)\xi_A + X_A\right]dx^A, \tag{83}$$

where

$$X_A = a_0 \eta_A + a^k \zeta_{k\,A}$$

is such that

$$2X_{(A/B)} = 2[\epsilon_1(-a\xi + m) + a_0 k]h_{AB} \tag{84}$$

and the conformal factor associated to $\vec{Y}$ is

$$\phi = \epsilon_1(-a\xi + m) + a_0 k \tag{85}$$

and satisfies $\phi_{a;b} = 0$, that is: $\vec{Y}$ is a SCKV in $(M,\hat{g})$, whereas $\vec{X}$ is also a SCKV in (V,h).

Notice that some of the constants appearing in the above expressions could have been removed by means appropriate redefinitions of the objects (functions and coordinates) in them. However, as it turns out, it is useful to keep them as they appear because this makes the subsequent analysis much more clear. The following possibilities now arise regarding the nature of $\vec{X}$; namely

Case 1: (V,h) admits no proper SCKV nor proper HV, then $a_0 = 0$ and $X_A = a^k \zeta_{k\,A}$ is a KV, that is $a^k \psi_k = \epsilon_1(-a\xi + m) = 0$; i.e., $a = m = 0$ and the conformal factor ϕ above becomes zero, hence, $\vec{Y}$ is a KV which can be seen to be given by

$$Y_a dx^a = -b\xi\, du + b\xi_A\, dx^A + X_A\, dx^A, \quad \vec{X} \in \mathcal{K}(V,h). \tag{86}$$

Case 2: (V,h) admits no proper SCKV but it admits a proper HV (that is: $a_0 \neq 0$). It then follows that $a^k \zeta_{k\,A}$ must be a KV, hence $a^k \psi_k = \epsilon_1(-a\xi + m) = 0$; and then $a = m = 0$ as before. The conformal factor is then constant $\phi = k a_0$, $\vec{Y}$ then being a HV which can be written as

$$Y_a\, dx^a = a_0[\epsilon_1 k u\, du + \eta_A\, dx^A] - b\xi du + b\xi_A\, dx^A + X_A\, dx^A, \tag{87}$$

where the first term within square brackets is a proper HV and the remaining terms are easily recognizable as a KV [see Eq. (86)].

Case 3: (V,h) admits a proper SCKV, $\vec{X}$ such that $2X_{(A/B)} = 2[\epsilon_1(-a\xi)]h_{AB}$; i.e., $a \neq 0$ and the constants $k a_0, m$ (if nonzero) have been absorbed by suitably redefining the function ξ. We then have

$$X_{A/B} = -\epsilon_1 a \xi h_{AB} + F_{AB},$$

where F_{AB} is the conformal bivector. Computing now the Lie bracket of $\vec{\xi}$ and $\vec{X}$ and making use of the above expression together with the fact that $\xi_{A/B} = 0$ we get

$$[\vec{\xi}, \vec{X}] = \vec{\eta}, \quad \eta_A = -\epsilon_1 a \xi \xi_A + F_{AB}\xi^B \tag{88}$$

computing now $\eta_{A/C}$ and making use of Eq. (12) it follows

$$\eta_{A/C} = -\epsilon_1 a(\xi^D \xi_D) h_{AC} \tag{89}$$

that is: $\vec{\eta}$ is either a GHV (whenever $\vec{\xi}$ is non-null, for in that case it can be scaled so that $\xi^D \xi_D = \epsilon_2$, where $\epsilon_2 = \pm 1$), or else $\vec{\eta}$ is a GKV (including $\vec{\eta} = 0$ as a special case). In the former case ($\vec{\eta}$ is a GHV and therefore $\xi^D \xi_D = \epsilon_2$), Proposition 2 above implies that (V,h) is flat. In the latter case ($\vec{\eta}$ is a GKV and $\xi^D \xi_D = 0$), one has from (88) that $\xi^D \eta_D = 0$ and therefore either

$\eta^D \eta_D \neq 0$, in which case again, proposition 2 implies that (V,h) is flat, or else $\vec{\eta}=k\vec{\xi}$ where k is a constant which may be zero (if it is not zero, it can always be chosen equal to 1 by re-scaling $\vec{X}$ appropriately). This is the only nontrivial case [in the sense that (V,h) is not necessarily flat], and it is easy to see that coordinates v,w,y can be chosen so that the three-dimensional line element takes the form:

$$\mathrm{d}\sigma^2 = -2\mathrm{d}v\ \mathrm{d}w + p_{\pm}(w)M^2(y)[q_{\pm}(w)^{-2}\mathrm{d}w^2 + \mathrm{d}y^2], \tag{90}$$

where

$$\begin{gathered} q_{\pm}(w)=n^2w^2\pm 1, \quad p_{+}(w)\equiv q_{+}(w)\exp[\epsilon_1 kn/a\ \cot^{-1} nw] \\ p_{-}(w)\equiv q_{-}(w)\exp[\epsilon_1 kn/a\ \coth^{-1} nw], \quad n=\text{constant}, \end{gathered} \tag{91}$$

the KV $\vec{\xi}$ and SCKV $\vec{X}$ being, respectively,

$$\vec{\xi}=\partial_v, \quad \vec{X}=kv\partial_v+\frac{1}{n^2}q_{\pm}(w)\partial_w. \tag{92}$$

Alternatively, new coordinates can be chosen, which we still call v,w,y, so that Ref. 11 the line element takes the more familiar form

$$\mathrm{d}\sigma^2 = -2\mathrm{d}v\ \mathrm{d}w - 2H(w,y)\mathrm{d}w^2 + \mathrm{d}y^2 \tag{93}$$

and still $\vec{\xi}=\partial_v$ but the function $H(w,y)$ satisfies then a partial differential equation and $\vec{X}$ then takes a form which depends on H. In this case, the Ricci tensor is

$$R_{AB}=H_{,yy}l_A l_B, \tag{94}$$

where $l_A=\xi_A$.

B. (V,h) admits a proper GHV and no proper GCKV

Since a proper HV is unique up to the addition of KV, we can assume that there is just one GHV (in the sense that, if another exists, then their difference must be a gradient KV—in that respect, if any GKV exists in (V,h) we shall consider that has been added to the GHV, therefore, any remaining proper CKV or KV in $\mathcal{C}(V,h)$ will be nongradient), say $\vec{\eta}$ with homothetic constant $k(\neq 0)$; i.e., $\eta_A \equiv \eta_{,A}$ for some function $\eta(x^B)$.

At this point, it is easy to find an expression for the line element associated with h in coordinates adapted to the GHV $\vec{\eta}$. First of all notice that from $\eta_{A/B}=kh_{AB}$ it readily follows that $\vec{\eta}$ cannot be null; next and provided we are not in the vicinity of a fixed point of the HV, we can always choose a coordinate, say $x^1\equiv v$ adapted to $\vec{\eta}$, i.e., $\vec{\eta}=\partial_v$, now the fact that $\vec{\eta}$ is locally a gradient and a HV with homothetic constant k readily implies (by a similar argument to that used previously) that coordinates $x^i\equiv x^2,x^3$ can be chosen so that the line element associated with h reads

$$\mathrm{d}\sigma^2 = e^{2kv}(\epsilon_2\mathrm{d}v^2+\overline{h}_{ij}(x^k)\mathrm{d}x^i\,\mathrm{d}x^j), \quad \epsilon_2=\pm 1 \tag{95}$$

and then $\eta_A\,\mathrm{d}x^A=\epsilon_2\exp(2kv)\mathrm{d}v$, hence $\eta=(\epsilon_2/2k)\exp(2kv)$. Also, since $\overline{h}_{ij}(x^k)$ is a two-dimensional metric, the coordinates x^i can be chosen so that it takes an explicit conformally flat form, i.e.,

$$\mathrm{d}\sigma^2 = e^{2kv}(\epsilon_2\,\mathrm{d}v^2+\Omega^2(x^k)(\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2), \quad \epsilon_2,\epsilon_3=\pm 1, \tag{96}$$

where $\Omega(x^k)$ is some function of its arguments. The line element of $(M,\hat{g})$ then reads

$$d\Sigma^2=\epsilon_1\,\mathrm{d}u^2+e^{2kv}[\,\epsilon_2\,\mathrm{d}v^2+\Omega^2(x^k)(\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2)],\tag{97}$$

where

$$\epsilon_\alpha=\pm 1\quad(\alpha=1,2,3),\quad \epsilon_1\epsilon_2\epsilon_3=-1,\quad \epsilon_1+\epsilon_2+\epsilon_3=+1.$$

Alternatively, the following change of coordinates can be carried out:

$$w\equiv k^{-1}\exp(kv),\quad v=k^{-1}\ln kw,\tag{98}$$

which renders $\vec{\eta}$, η and the line element associated with h in the form

$$\vec{\eta}=kw\partial_w,\quad \eta=\frac{k\epsilon_2}{2}w^2,\quad \mathrm{d}\sigma^2=\epsilon_2\,\mathrm{d}w^2+w^2\Omega^2(x^k)(\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2)\tag{99}$$

hence

$$\mathrm{d}\hat{s}^2=\epsilon_1\,\mathrm{d}u^2+\epsilon_2\,\mathrm{d}w^2+w^2\Omega^2(x^k)(\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2).\tag{100}$$

Now going back to the problem of finding the CKV that $(M,\hat{g})$ admits in this case, let $\{\vec{\eta},\vec{\xi}_k\}$ be a basis for $\mathcal{C}(V,h)$ with $\vec{\eta}$ satisfying

$$\eta_{A/B}=kh_{AB}\tag{101}$$

and $\vec{\xi}_k$ being CKV (including KV) such that no proper CKV (nor any linear combination of them) is a gradient, we then have

$$\zeta_{k\,A/B}+\zeta_{k\,B/A}=2\psi_k h_{AB},$$

where ψ_k is the associated conformal factor.

Equation (74) states that $Y^B(u,x^D)\partial_B$ is a CKV in every $V(u)$ for u fixed, and therefore according to our previous developments, we may write

$$Y^B(u,x^D)\partial_B=\lambda(u)\vec{\eta}+\lambda^k(u)\vec{\xi}_k,\tag{102}$$

which when substituted back again into (72)–(74) yields (recall, the conformal factor ϕ has been renamed as $\dot{\Sigma}$):

$$\dot{\Sigma}(u,x^B)=k\lambda(u)+\lambda^k(u)\psi_k(x^B),\quad Y_u=\epsilon_1[k\mu(u)+\mu^k(u)\psi_k(x^B)+B(x^A)],\tag{103}$$

$$\epsilon_1\mu^k\psi_{k,A}+B_{,A}+\dot{\lambda}\,\eta_A+\dot{\lambda}^k\zeta_{k\ A}=0,\tag{104}$$

where $\mu(u)$ and $\mu^k(u)$ are such that $\dot{\mu}(u)=\lambda(u)$ and $\dot{\mu}^k(u)=\lambda^k(u)$, respectively, and $B(x^A)$ is a function of integration which does not depend on u. Now, (104) above implies that, for u fixed, $\dot{\lambda}^k\zeta_{k\ A}$ must be a GCKV (since η_A is a gradient by assumption), but since, by hypothesis there is none and $\vec{\eta}$, $\vec{\xi}_k$ are independent, it must be $\dot{\lambda}^k=0$, that is $\lambda^k=a^k(=\text{const})$. Plugging this back again into (72) and (73) we get

$$Y_u=\epsilon_1[k\mu(u)+ua^k\psi_k(x^B)+B(x^A)],\quad \epsilon_1 ua^k\psi_{k,A}+B_{,A}+\dot{\lambda}\,\eta_A=0,\tag{105}$$

which, when differentiated with respect to u yields

$$\epsilon_1 a^k\psi_{k,A}+\ddot{\lambda}\,\eta_A=0\tag{106}$$

and two possibilities arise:

case 1: $\ddot{\lambda}=0$, i.e.: $\lambda=au+b$, with a,b constants. Then $a^k\psi_{k,A}=0$, that is: $a^k\psi_k=C$ $(=\text{constant})$.

case 2: $\ddot{\lambda}=a$ (constant), hence $\lambda=a/2u^2+bu+c$ and then $B=-b\eta+m$ and $\epsilon_1 a^k\psi_k=a\eta+C$ where m,C are constants and η is the function such that $\eta_{,A}=\eta_A$.

Case 1: In this case it is straightforward to get from the equations above that $B=-\epsilon a\eta$ and also that $a^k\vec{\zeta}_k$ must satisfy:

$$\mathcal{L}_{a^k\vec{\zeta}_k}h=2Ch$$

that is: $a^k\vec{\zeta}_k$ is a HV, which, on account of the assumed independence of $\vec{\eta}$, $\vec{\zeta}_k$ can be set directly equal to zero. [Alternatively, since homotheties are essentially unique, it would follow $a^k\vec{\zeta}_k=(C/k)\vec{\eta}+\vec{\xi}$, where $\vec{\xi}$ is a KV, which can be absorbed by a suitable redefinition of the constant b in $\lambda=au+b$.] Taking all this into account, redefining nonessential combinations of constants and subtracting any proper KV [i.e., linear combinations of ∂_u and KV in (V,h) such as $\vec{\xi}$ above], we get

$$\vec{Y}=\left[k\left(\frac{a}{2}u^2+pu\right)-\epsilon_1 a\eta\right]\partial_u+(au+p)\vec{\eta},$$

where p is a constant.

It is immediate to check that the above CKV $\vec{Y}$, whose associated conformal factor is $\phi=k(au+p)$, is in fact a SCKV, that is $\phi_{a;b}=0$. Also note that the HV $pu\partial_u+p\vec{\eta}$ can be subtracted from $\vec{Y}$, the resulting vector

$$\vec{Y}'=[k(a/2)u^2-\epsilon_1 a\eta]\partial_u+au\vec{\eta} \tag{107}$$

being, indeed, a SCKV.

Case 2: We now have $\lambda=(a/2)u^2+bu+c$, $B=-b\eta+m$, and also $\epsilon_1 a^k\psi_k=a\eta+C$, where a,b,m and C are constants. This implies that $\vec{X}\equiv a^k\vec{\zeta}_k$ is a CKV in (V,h) whose associated conformal factor is precisely $\epsilon_1(a\eta+C)$. A direct calculation using the forms (96) or (99) readily shows that no such CKV $\vec{X}$ can exist, and therefore this case turns out to be impossible.

C. (V,h) admits a proper GCKV

Let us turn our attention now to the case in which (V,h) admits a proper GCKV. Before analyzing the consequences this has on the conformal algebra of the $1+3$ reducible space–time $(M,\hat{g})$, we shall first explore the situation in a three-space (V,h). To this end, let $\vec{\zeta}$ be a GCKV in (V,h) with associated conformal factor ψ, we then have

$$\zeta_{A/B}=\psi h_{AB},\quad \zeta_A=\zeta_{,A}, \tag{108}$$

where $\zeta=\zeta(x^D)$ is some function. The first equation above readily implies that $\vec{\zeta}$ cannot be null unless it is a KV. Taking a further covariant derivative we have

$$\zeta_{A/BC}=\psi_C h_{AB},\quad \psi_C=\psi_{,C} \tag{109}$$

and the Bianchi identities imply, since $\zeta_{A/B}=\zeta_{B/A}$,

$$R_{ABCD}\zeta^D=\psi_A h_{BC}-\psi_B h_{AC}. \tag{110}$$

Contracting both sides of the above equation with ζ^C yields

$$0=\psi_A\zeta_B-\psi_B\zeta_A \tag{111}$$

and then, unless $\vec{\zeta}$ is a HV (in which case the equation above is satisfied identically) which we are assuming is not, it follows that $\psi=\psi(\zeta)$, hence, from now on we shall write $\psi_A=\tilde{\psi}\zeta_A$, where the tilde stands for the derivative with respect to the function ζ, i.e., $\tilde{\psi}=\mathrm{d}\psi/\mathrm{d}\zeta$. Also, differentiating (111) and using (108) it follows that $\vec{\zeta}$ cannot be a SCKV (unless it is a KV).

Following a procedure similar to the one in Sec. V B, we choose a coordinate v adapted to $\vec{\zeta}$ and two other coordinates x^2,x^3 so that

$$\vec{\zeta}=\partial_v, \quad \zeta_A\,\mathrm{d}x^A=\epsilon_2\exp(2V(v))\mathrm{d}v, \quad \zeta=\epsilon_2\int \mathrm{d}v\,\exp(2V(v)), \tag{112}$$

$$\mathrm{d}\sigma^2=e^{2V(v)}[\,\epsilon_2+\Omega^2(x^k)(\,\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2)] \tag{113}$$

the conformal factor then being $\psi=V'(v)$ where the prime indicates derivative with respect to v. Note that

$$\tilde{\psi}=\frac{\mathrm{d}\psi}{\mathrm{d}\zeta}=\frac{\mathrm{d}\psi}{\mathrm{d}v}\left(\frac{\mathrm{d}\zeta}{\mathrm{d}v}\right)^{-1}=\epsilon_2 V''e^{-2V(v)}. \tag{114}$$

Alternatively, a new coordinate w can be defined such that

$$w\equiv\int dv\,\exp(2V(v)) \tag{115}$$

and then

$$\vec{\zeta}=M(w)\partial_w, \quad M(w)=\exp(V(v(w))), \quad \zeta_A\mathrm{d}x^A=\epsilon_2 M(w)\mathrm{d}w, \quad \text{and } \zeta=\epsilon_2\int \mathrm{d}w\,M(w), \tag{116}$$

$$\mathrm{d}\sigma^2=\epsilon_2\mathrm{d}w^2+M^2(w)\Omega^2(x^k)(\,\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2) \tag{117}$$

the conformal factor is $\psi=M'(w)$ (the prime now meaning derivative with respect to w) and, as before,

$$\tilde{\psi}=\frac{\mathrm{d}\psi}{\mathrm{d}\zeta}=\frac{\mathrm{d}\psi}{\mathrm{d}w}\left(\frac{\mathrm{d}\zeta}{\mathrm{d}w}\right)^{-1}=\epsilon_2\frac{M''}{M}. \tag{118}$$

The above metric describes the situation in which one proper (non-HV) GCKV exists in (V,h), with h being of arbitrary signature.

Let us now go back to the original problem of finding CKV in the $1+3$ reducible space–time whose three-dimensional factor (V,h) we are assuming to admit a GCKV. We next reproduce, for the sake of convenience, the original equations (72)–(74) with the conformal factor ϕ renamed as $\dot{\Sigma}$:

$$Y_{u,u}=\epsilon_1\dot{\Sigma}, \tag{119}$$

$$Y_{u,A}+Y_{A,u}=0, \tag{120}$$

$$Y_{A/B}+Y_{B/A}=2\dot{\Sigma}\,h_{AB}\,. \tag{121}$$

Again, (121) implies that $Y^B(u,x^D)\partial_B$ is a CKV in every $V(u)$ for u fixed.

Now, assume first that only one proper GCKV is admitted in (V,h), say $\vec{\zeta}$ with conformal factor ψ. From our previous developments it follows that no proper GHV or GKV can exist in (V,h); therefore we may consider a basis of $\mathcal{C}(V,h)$ given by $\{\vec{\zeta},\vec{\chi}_k\}$ where, again, $\vec{\chi}_k$ are nongradient CKV (possibly HV and KV) with conformal factors ϕ_k.

From the remark above it follows that

$$Y^B(u,x^D)\partial_B=\lambda(u)\vec{\zeta}+\lambda^k(u)\vec{\chi}_k$$

which, upon substitution into (121), yields

$$\dot{\Sigma}=\lambda(u)\psi(x^D)+\lambda^k(u)\phi_k(x^D)$$

that can be formally integrated to give

$$\Sigma=\psi(x^D)\int \mathrm{d}u\,\lambda(u)+\phi_k(x^D)\int \mathrm{d}u\,\lambda^k(u)+B(x^D),$$

where the terms resulting from the constants of integration arising from $(\int du\lambda(u))$, etc., have been absorbed into the function of integration $B(x^D)$.

Substituting this into (120) and taking into account that $\psi_{,A}=\tilde{\psi}\zeta_A$ we get

$$\left(\int \mathrm{d}u\,\lambda(u)\right)\tilde{\psi}\zeta_A+\left(\int \mathrm{d}u\,\lambda^k(u)\right)\phi_{k,A}+B_{,A}+\dot{\lambda}(u)\zeta_A+\dot{\lambda}^k(u)\chi_{kA}=0 \tag{122}$$

and this implies that, for u fixed, $\dot{\lambda}^k\chi_{kA}$ must be a GCKV independent of ζ_A. Since this is not possible from our assumptions, it follows that $\dot{\lambda}^k=0$, that is $\lambda^k=a^k(=\text{const})$. Therefore the above-given equation reads now

$$\left[\left(\int \mathrm{d}u\,\lambda(u)\right)\tilde{\psi}+\dot{\lambda}(u)\right]\zeta_A+ua^k\phi_{k,A}+B_{,A}=0 \tag{123}$$

and differentiating with respect to u,

$$[\lambda(u)\tilde{\psi}+\ddot{\lambda}(u)]\zeta_A+a^k\phi_{k,A}=0, \tag{124}$$

which readily implies:

$$\tilde{\psi}=k\quad(\text{constant}),\quad k\lambda(u)+\ddot{\lambda}(u)=a\quad(\text{constant}),\quad a^k\phi_k=-a\zeta+c, \tag{125}$$

where c is a constant. Substituting this information back into (123) and taking into account that from $\tilde{\psi}=k$ and $k\lambda(u)+\ddot{\lambda}(u)=a$ it follows $\tilde{\psi}\int \mathrm{d}u\,\lambda(u)+\dot{\lambda}(u)=a\,u$, one easily gets

$$B_{,A}=0,$$

i.e.,

$$B=b\quad(\text{constant}) \tag{126}$$

and then, using $k\int \mathrm{d}u\,\lambda(u)+\dot{\lambda}(u)=a\,u$, Eq. (119) implies

$$Y_u=\epsilon_1(-\zeta\dot{\lambda}+cu+b).$$

Note that b can be set equal to zero without loss of generality, since it simply amounts to adding a constant multiple of the KV $\vec{u}=\partial_u$, and we shall do that in what follows, thus writing

$$Y_u=\epsilon_1(-\zeta\dot{\lambda}+cu). \tag{127}$$

Also, from the above-mentioned developments we get

$$Y_A=\lambda(u)\zeta_A+X_A, \quad X_A\equiv a^k\chi_{kA}, \tag{128}$$

where $\lambda(u)$ satisfies $\ddot{\lambda}+k\lambda=a$, the conformal factor associated with the GCKV $\vec{\zeta}$ is $\psi=k\zeta$, and $\vec{X}$ is a CKV (nongradient by assumption) whose associated conformal $\phi'\equiv a^k\phi_k$ factor is, from Eq. (125) $\phi'=-a\zeta+c$.

Consider next the CKV $\vec{Z}$ defined by $\vec{Z}\equiv(a/k)\vec{\zeta}+\vec{X}$. From the previous paragraph it follows that

$$\mathcal{L}_{\vec{Z}}h_{AB}=2ch_{AB},$$

that is: $\vec{Z}$ is a HV with homothetic constant c, therefore, put $\vec{X}$ above as $\vec{X}=\vec{Z}-(a/k)\vec{\zeta}$ and then

$$Y_A=\left(\lambda(u)-\frac{a}{k}\right)\zeta_A+Z_A, \tag{129}$$

where $\vec{Z}$ is a HV in (V,h) with homothetic constant c. If (V,h) admits no HV, then $c=\vec{Z}=0$ above; thus we finally have

$$\vec{Y}=(-\zeta\dot{\lambda}+cu)\partial_u+\left(\lambda(u)-\frac{a}{k}\right)\vec{\zeta}+\vec{Z}.$$

Since $cu\partial_u+\vec{Z}$ is a HV with homothetic constant c we can subtract it from the above to get

$$\vec{Y}=(-\zeta\dot{\lambda})\partial_u+\left(\lambda(u)-\frac{a}{k}\right)\vec{\zeta} \tag{130}$$

and $\vec{\zeta}$ is now that given by (112) or (99), the corresponding three-dimensional line elements then being (113) or (117), thus we can finally write for the line element of $(M,\hat{g})$ a $1+3$ reducible space–time admitting a CKV under these hypotheses:

$$d\hat{s}^2=\epsilon_1\,du^2+\epsilon_2\,dw^2+M^2(w)\Omega^2(x^k)(\epsilon_3(dx^2)^2+(dx^3)^2), \tag{131}$$

where

$$\epsilon_\alpha=\pm1 \quad (\alpha=1,2,3) \quad \epsilon_1\epsilon_2\epsilon_3=-1, \quad \epsilon_1+\epsilon_2+\epsilon_3=+1.$$

The CKV is then

$$\vec{Y}=(-\zeta\dot{\lambda})\partial_u+\left(\lambda(u)-\frac{a}{k}\right)M(w)\partial_w, \tag{132}$$

where $\lambda(u)$ and $M(w)$ must satisfy [see (118)]

$$\ddot{\lambda}(u)+k\lambda(u)=a, \quad M''(w)=\epsilon_2kM. \tag{133}$$

These equations can be easily integrated for $\epsilon_2k>0,\epsilon_2k<0$ and $\epsilon_2k=0$ obtaining then explicit expressions for both the line element $d\hat{s}^2$ and proper CKV $\vec{Y}$.

In the next theorem, we make an attempt at summarizing the results thus far obtained.

Theorem 10: *Let $(M,\hat{g})$ a 1+3 decomposable space–time; the following results hold regarding its conformal Lie algebra:*

(1) *If* (V,h) *admits no GCKV then the only CKV that* $(M,\hat{g})$ *admits are HV and KV—their forms are those discussed in remarks* $R0$-$R3$ *at the beginning of this section.*

(2) $(M,\hat{g})$ *can admit a proper CKV* $\vec{Y}$ *if and only if* (V,h) *admits a GCKV, which can be either a GKV* $\vec{\xi}$*, or a GHV* $\vec{\eta}$*, or a (proper) GCKV* $\vec{\zeta}$*.*

(3) *If two or more GCKV are admitted by* (V,h)*, then* (V,h) *is of constant curvature and conformally flat (and it is flat if one of the GCKV admitted is a GHV).*

(4) *If only one GCKV is admitted by* (V,h)*, then:*

(a) *If it is a GKV* $\vec{\xi}$*, then* $(M,\hat{g})$ *admits a proper CKV* $\vec{Y}$ *if and only if* $\vec{\xi}$ *is null and a proper SCKV exists also in* (V,h)*,* $\vec{X}$*, such that* $[\vec{\xi},\vec{X}]=k\vec{\xi}$*; the CKV* $\vec{Y}$ *is also a SCKV and the metric is a special type of generalized pp-wave. Otherwise [i.e., if no proper SCKV* $\vec{X}$ *exists in* (V,h) *or it exists but it does not satisfy* $[\vec{\xi},\vec{X}]=k\vec{\xi}$*], then* $\vec{Y}$ *is a HV, possibly KV.*

(b) *If it is a GHV* $\vec{\eta}$ *then* $(M,\hat{g})$ *admits a proper SCKV* $\vec{Y}$ *(unique up to the addition of HV). The line element and* $\vec{Y}$ *are:*

$$\mathrm{d}\hat{s}^2=\epsilon_1\,\mathrm{d}u^2+\epsilon_2\,\mathrm{d}w^2+w^2\Omega^2(x^i)[\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2], \tag{134}$$

$$\epsilon_\alpha=\pm 1\quad(\alpha=1,2,3),\quad \epsilon_1\epsilon_2\epsilon_3=-1,\quad \epsilon_1+\epsilon_2+\epsilon_3=+1$$

$$\vec{Y}=\left(\frac{a}{2}ku^2-\epsilon_1\epsilon_2\frac{a}{2}kw^2\right)\partial_u+au\,\vec{\eta},\quad \vec{\eta}=kw\partial_w\,. \tag{135}$$

(c) *If it is a GCKV* $\vec{\zeta}$ *then* $(M,\hat{g})$ *admits a proper CKV* $\vec{Y}$ *(unique up to the addition of HV). The line element and* $\vec{Y}$ *are:*

$$\mathrm{d}\hat{s}^2=\epsilon_1\,\mathrm{d}u^2+\epsilon_2\,\mathrm{d}w^2+M^2(w)\Omega^2(x^i)[\epsilon_3(\mathrm{d}x^2)^2+(\mathrm{d}x^3)^2], \tag{136}$$

$$\epsilon_\alpha=\pm 1\quad(\alpha=1,2,3),\quad \epsilon_1\epsilon_2\epsilon_3=-1,\quad \epsilon_1+\epsilon_2+\epsilon_3=+1,$$

$$\vec{Y}=-\zeta\dot{\lambda}(u)\,\partial_u+\left(\lambda-\frac{a}{k}\right)\vec{\zeta},\quad \zeta=\epsilon_2\int \mathrm{d}w\,M(w),\quad \vec{\zeta}=M(w)\partial_w \tag{137}$$

and the functions $\lambda(u)$ *and* $M(w)$ *satisfy*

$$\frac{\mathrm{d}^2\lambda}{\mathrm{d}u^2}+k\lambda=a,\quad \frac{\mathrm{d}^2M}{\mathrm{d}w^2}=\epsilon_2 kM. \tag{138}$$

VI. EXAMPLES

In this section we shall briefly discuss instances of double warped space–times. Notice that warped space–times are special cases of double warped ones (i.e., whenever one of the warping functions is constant), and they include relevant classes of space–times such as all the spherically, plane and hyperbolic symmetric space–times, the whole class of Friedmann–Robertson–Walker solutions, the Bertotti–Robertson space–time and many others, see Refs. 3 and 4 for further information.

Fluid space–times. We have not been able to find a proper double warped (i.e., nonwarped) perfect fluid solution due to the complicated form that the field equations take on account of the Ricci tensor (see Sec. III). However, it is indeed possible to find anisotropic fluid solutions satisfying the dominant energy condition (see Ref. 11), as the following two examples show. The energy–momentum tensor is in both cases of the Segre type $\{1,1(11)\}$, and therefore can be written as

$$T_{ab}=\mu u_a u_b+p_1 z_a z_b+p_2[x_a x_b+y_a y_b], \tag{139}$$

where $\{u_a,z_a,x_a,y_a\}$ form an orthogonal tetrad ($-u_a u^a=x^a x_a=y^a y_a=z^a z_a=1$, the rest of the

products being zero), u^a is aligned with the velocity of the fluid, and μ, p_1, p_2 are, respectively, the energy density and two (different) pressures as measured by an observer co-moving with the fluid. The dominant energy condition implies then

$$\mu \geqslant 0, \quad \mu \pm p_1 \geqslant 0, \quad \mu \pm p_2 \geqslant 0. \tag{140}$$

Case 1: Consider the line element given by

$$ds^2 = z(-dt^2 + dx^2) + t(dy^2 + dz^2), \tag{141}$$

where t and z are both non-negative. This space–time can be seen to represent an anisotropic fluid with an energy–momentum tensor given by (139) with

$$u_a = (-z^{1/2}\cosh\Phi, 0, 0, t^{1/2}\sinh\Phi), \qquad z_a = (-z^{1/2}\sinh\Phi, 0, 0, t^{1/2}\cosh\Phi),$$

$$x_a = (0, z^{1/2}, 0, 0), \quad y_a = (0, 0, t^{1/2}, 0),$$

$$\cosh\Phi = \sqrt{\frac{t}{t-z}}, \qquad \sinh\Phi = -\sqrt{\frac{z}{t-z}} \qquad \text{for} \quad t - z > 0$$

$$\cosh\Phi = \sqrt{\frac{z}{z-t}}, \qquad \sinh\Phi = -\sqrt{\frac{t}{z-t}} \qquad \text{for} \quad z - t > 0$$

and also

$$\mu = \frac{|z-t|}{4t^2z^2}, \quad p_1 = \mu, \quad p_2 = \frac{z-t}{4t^2z^2}.$$

This has to be understood as two different open submanifolds; namely, the one defined by $t - z > 0$ and that defined by $z - t > 0$. In both cases the dominant energy condition (140) is satisfied. As a final comment to this example, it can noted that the above metric admits the Killing vectors $\vec{\xi}_1 = \partial_x$, $\vec{\xi}_2 = \partial_y$, and the homothetic vector $\vec{\eta} = t\partial_t + x\partial_x + y\partial_y + z\partial_z$ with homothetic constant $\psi = 3/2$.

Case 2: Consider next the following line element:

$$ds^2 = (m - kz^2)(-dt^2 + dx^2) + (q + kt^2)(dy^2 + dz^2), \tag{142}$$

where m, k, q are constants, $m, q > 0$ and $k \geqslant 0$ in order for the energy conditions and other positivity requirements to be satisfied, and the range of the z coordinate is restricted to $m - kz^2 > 0$. Again, this represents an anisotropic fluid with energy–momentum tensor given by (139) where

$$u_a = (-(m - kz^2)^{1/2}\cosh\Phi, 0, 0, (q + kt^2)^{1/2}\sinh\Phi),$$

$$z_a = (-(m - kz^2)^{1/2}\sinh\Phi, 0, 0, (q + kt^2)^{1/2}\cosh\Phi),$$

$$x_a = (0, (m - kz^2)^{1/2}, 0, 0), \quad y_a = (0, 0, (q + kt^2)^{1/2}, 0),$$

$$\cosh 2\Phi = \frac{qz^2 + mt^2}{|qz^2 - mt^2 + 2kt^2z^2|}.$$

The density μ and the pressures p_1, p_2 are given in this case by

$$\mu = k(m - kz^2)^{-2}(q + kt^2)^{-2}\{k|qz^2 - mt^2 + 2kt^2z^2| + (m - kz^2)(q + kt^2)\},$$

$$p_1 = k(m - kz^2)^{-2}(q + kt^2)^{-2}\{k|qz^2 - mt^2 + 2kt^2z^2| - (m - kz^2)(q + kt^2)\},$$

$$p_2=\frac{(-3\,qm-2\,kt^2m+2\,qkz^2+k^2t^2z^2)k}{(-m+kz^2)^2(q+kt^2)^2}$$

and it can be seen that the dominant energy condition (140) is satisfied.

Vacuum space–times. Notice from the second equation in (66) that any double warped space–time representing a vacuum solution of Einstein's field equations, must in fact be warped (i.e., either $\theta_{1,\alpha}=0$ or $\theta_{2,A}=0$). Examples in this class include Schwarzschild solution and its plane and hyperbolic symmetric equivalents.

The characterization of class A and class B double warped space–times given in Theorems 4, 5, and 7 should prove useful in formulating an algorithm for classifying such metrics. this is so because this characterization is coordinate independent although tetrad dependent. In what follows the tetrads described in Theorems 4, 5, and 7 will be designated as dw tetrads of class A and B, respectively. In order to determine weather g represents a double warped metric we suggest the following classification scheme:

(1) Choose a coordinate system.
(2) Choose a canonical complex null tetrad $\{k_a,l_a,m_a,\overline{m}_a\}$ and write their components in the coordinate system chosen in (1).
(3) Determine the NP spin coefficients and their NP derivatives in tetrad (2).
(4) If the scalars determined in (3) satisfy the relations of Theorems 4 or 5 (Theorem 7) then the metric is a double warped space–time of class A (class B) and the algorithm stops here, otherwise go to step (5).
(5) If possible, find the Lorentz transformations that transform tetrad (2) into a dw tetrad, i.e., such that the corresponding NP spin coefficients and their NP derivatives obey the conditions of Theorems 4 or 5 (Theorem 7). If such transformations exist then the space–time is a double warped space–time of class A (class B), otherwise it is not double warped.

Unfortunately, step (5) of this procedure is not straightforward, since finding the Lorentz transformation which maps tetrad (2) into a dw tetrad can be difficult and such a transformation might not exist in which case the metric is not double warped.

The algorithm described here not only describes a way of determining whether a particular metric is double warped or not but also suggests a method for obtaining such space–times. For example, we suspect that one can obtain type D vacuum warped metrics of class B, for which $\rho=\mu=0$, by following a similar integration procedure to the one performed by Kinnersley.[18] In this paper, Kinnersley chooses coordinates such that $l^\alpha=\delta^\alpha_2$, making $x^2=r$ an affine parameter along l^α. These are the special coordinates given in Ref. 9. The idea would then be to express a dw tetrad in these special coordinates, write the NP equations taking into account (63). In order to determine explicitly the tetrad components in these special coordinates one must integrate the corresponding equations. By following this procedure we hope to obtain such metrics in future work.

ACKNOWLEDGMENTS

This work was partly supported by the Spanish ''Ministerio de Ciencia y Tecnologa'' jointly with FEDER funds through Research Grant No. BFM2001-0988 and by CMAT, University of Minho, Portugal. J.C. gratefully acknowledges the hospitality of the Universidade do Minho (Guimaràes, Portugal), where part of this work was carried out. M.P.M.R. and E.G.L.R.V. wish to thank the Departament de Física, Universitat de les Illes Baleares, for their hospitality during the elaboration of this work.

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The first law of thermodynamics and Dyson–Lieb's perpetuum mobile

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(Received 5 March 2003; accepted 10 June 2003)

Some consequences of Dyson–Lieb's $N^{(7/5)}$ law for the condensation of Bose particles are discussed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1607515]

During the last week of July 2002, Lieb, Yngvason and one of us (HJB) were together in Vienna. Sometimes at lunch we discussed the implications of the problem stability of matter for quantum field theory. Looking more closely at this problem I observed that Dyson–Lieb's $-N^{(7/5)}$ law for the ground-state of bosons leads to problems in particle physics. In this note we shall discuss some of the problems.

The question of the stability of matter was first discussed by Dyson and Lenard.[1] They concluded that matter is stable as a consequence of the Pauli principle. But their calculation contained an estimate of the ground-state energy with errors some ten powers too large. This problem was taken up again by Lieb and Thirring with an estimate close to reality.[2] (These investigations are based on nonrelativistic quantum mechanics with a classical Coulomb field. We shall not discuss the relativistic approach to this problem, which is not in a satisfactory state. For a review see Lieb and Loss.[3]) In order to show that these results hold only for particles obeying the Pauli principle, Dyson and Lieb and co-workers repeated the same investigation for scalar bosons and found that the ground-state energy behaves like $-N^{(7/5)}$. Dyson[4] obtained the upper bound and Lieb with co-workers[5] showed the existence of a lower bound. This is based on the assumption that there exist different kinds of bosons with different electric charges. Moreover, the case considered is that of nonrelativistic quantum mechanics and a classical Coulomb field. If one assumes that a result similar to the above holds also in relativistic quantum field theory with a quantized Coulomb field, then this would have drastic consequences provided scalar bose particles exist as stable or almost stable objects.

Let us denote the two types of particles by A and B. Since they are charged they must appear in pairs A^+,A^- and B^+,B^-. We now construct two machines, one creating pairs A^+,A^- and the other pairs B^+,B^-. With help of magnetic fields the pairs may be separated and A^+,B^- sent to one and A^-,B^+ to another place. For the creation of the pairs we need the energy

$$E_A+E_B\,.$$

Each of the systems formed by one sort of pairs is attractive. If one adds an additional pair to each of the two lumps of $N-1$ pairs one gains the energy

$$(C_A+C_B)\{N^{(7/5)}-(N-1)^{(7/5)}\}\simeq(C'_a+C'_B)N^{(2/5)}.$$

This means if N is sufficiently large,

$$(C'_A+C'_B)N^{(2/5)}>E_A+E_B\,,$$

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holds, i.e., one gains energy. (For C_A and C_B exist only lower and upper bounds, but this does not change the arguments.) This will be called "Dyson–Lieb's perpetuum mobile." Since this is forbidden by the first law of thermodynamics, one has to discuss the possibilities avoiding Dyson–Lieb's perpetuum mobile.

The simplest way would be to postulate that no stable scalar bosons exist. This is in accordance with the experimental experience up to now. But there are theories which include supersymmetries. The GUT and the string theory are only two examples. Depending on the theory, the super-symmetric partner of the electron and the proton will be stable or almost stable particles. This follows from the conservation of charge and nucleon number. Depending on the theory (see, e.g., Ref. 6), the super-symmetric partner will have spin 0 or 1. One knows that the problem of stability of matter in the relativistic situation with a quantized Coulomb field is very delicate. Therefore, it is no danger to guess that also in the spin 1 situation the ground-state energy behaves like $-N^{\alpha}$ with $\alpha>1$. This also leads to Dyson–Lieb's perpetuum mobile and one has to think about possibilities to avoid it.

The first possibility which comes into ones mind is the following. If the pair, say (A^+,B^-), falls into a deep potential cavity, then it might create an electron–positron pair. If this remains at the surface of the lump and combines with particles A^+ and B^-, respectively, then they create neutral particles containing a spin $\frac{1}{2}$ component which do not increase the number N. In this case the perpetuum mobile has stopped. But the surface effect will appear only occasionally. If the lump is large enough, then the particles will form a crystal like an ionic crystal. Although the particles have no extension this could be B1 (NaCl–) or B2 (CsCl structure) in the Strukturbericht designation (see Kleber[7]), which are not close packed. Only at high pressures the system might be forced into a close packed structure, since this gives problems with nearest neighbors of equal charge. This then implies that the electron and positron will be trapped in the conduction band where they can annihilate each other. Therefore, this kind of interaction does not avoid Dyson–Lieb's perpetuum mobile. If one has in mind the super-symmetric partner of the electron and proton, then the formation of an ionic crystal might not be a good picture, but one should think about a system similar to hydrogen. Since condensed hydrogen forms are close packed crystals made out of neutral pairs, the electron–positron pair will destroy such a neutral molecule only occasionally. Therefore, also this is no way out of the perpetuum mobile problem.

The proton is composed of quarks. Therefore, its super-symmetric partner will probably be composed of the super-symmetric partners of the quarks. These will also have entire spin and, therefore, one has to expect that the ground-state energy tends to $-\infty$ with N to infinity.
Our personal conclusion of the discussion is the following:

The first law of thermodynamics forbids the existence of stable super-symmetric partners, i.e. the existence of super-symmetry in the naïve sense.

This argument has some similarity with the conclusion that the second law, together with the existence of the entropy of mixing, implies atomic nature of the matter. However, we think that our conclusion has a more solid base.

ACKNOWLEDGMENTS

This note was inspired by discussions in Vienna. HJB is grateful to the Erwin Schrödinger Institute for the kind hospitality.

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Comment on "Time-dependent solution for a star immersed in a background radiation" [H. Liu and Q. Zhang, J. Math. Phys. 43, 4904 (2002)]

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(Received 4 February 2003; accepted 8 April 2003)

In a recent paper [J. Math. Phys. **43**, 4904 (2002)] Liu and Zhang present a time-dependent solution for a star which is immersed in a background radiation. This solution was obtained by analyzing equations arising from the analysis of a five-dimensional solution that contained their solution. We show that, while their analysis and conclusions are valid, their equations are unnecessarily restrictive when applied to the four-dimensional case. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1610238]

Recently, Liu and Wesson[1] presented a simple class of five-dimensional (5D) solutions. It was further shown that the four-dimensional (4D) part of the 5D metric, together with two restrictions on the metric functions, represents a 4D spherically symmetric solution with heat flux. This form of the solution was further studied by Liu and Zhang[2] in which they showed that the solution could be considered as an exterior of a collapsing star immersed in a homogeneous and isotropic background.

The form of the solution as reported by Liu and Zhang in coordinates $(x^a)=(t,r,\theta,\phi)$ is

$$ds^2=-B(r)dt^2+(1-\lambda t)^2[A(r)dr^2+r^2(d\theta^2+\sin^2\theta\, d\phi^2)], \tag{1}$$

where λ is a constant and the metric functions A and B obey the following equations:

$$\frac{B'}{B}=3\lambda^2 r\frac{A}{B}+\frac{A-1}{r}, \tag{2}$$

$$\frac{A'}{A}=3\lambda^2 r\frac{A}{B}-\frac{A-1}{r}, \tag{3}$$

where primes denote differentiation with respect to r. It was further shown by Liu and Wesson[1] that metric (1) together with the above-given restrictions models a perfect fluid with heat flux in which the energy momentum tensor assumes the following form:

$$T_{ab}=(\rho+p)u_a u_b-pg_{ab}+q_a u_b+u_a q_b, \tag{4}$$

where ρ is the fluid energy density, p is the isotropic pressure, $u_a=(u^0,0,0,0)$ is the fluid four-velocity, and $q_a=(0,q^1,0,0)$ is the radial heat flux vector. The heat flow vector satisfies the condition $q^a u_a=0$ relative to the fluid four-velocity vector. The nontrivial Einstein equations [taking (2) and (3) into account] are given by

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$$\rho = \frac{6\lambda^2}{B(1-\lambda t)^2}, \tag{5}$$

$$p = \frac{2\lambda^2}{B(1-\lambda t)^2}, \tag{6}$$

$$q = \frac{\lambda B'}{A^{1/2}B^{3/2}(1-\lambda t)^2}, \tag{7}$$

where q is a covariant measure of the heat flux ($q^2 = q^a q_a$).

Equations (2) and (3) were obtained by Liu and Wesson[1] from the Ricci tensor for the 5D metric within which (1) was embedded. They assumed that the scalar field was time-like which forced some components of the 4D Ricci tensor to be zero, thus resulting in (2) and (3). An interesting feature of these two equations is that, if $A(r)$ and $B(r)$ satisfy these equations, then the pressure isotropy condition is automatically satisfied and the matter content satisfies the radiation equation of state

$$\rho = 3p. \tag{8}$$

However, if one looks at the metric (1) in isolation, i.e., one does not concern oneself with its origin in the 5D metric, then Eqs. (2) and (3), while simplifying calculations, are unnecessarily restrictive. This is a consequence of the fact that the system consisting of the pressure isotropy equation, viz.

$$\frac{1}{r^2} - \frac{1}{r^2 A} - \frac{A'}{2\,r\,A^2} - \frac{B'}{2\,r\,A\,B} - \frac{A'\,B'}{4\,A^2\,B} - \frac{B'^2}{4\,A\,B^2} + \frac{B''}{2\,A\,B} = 0 \tag{9}$$

and the equation of state

$$\frac{1}{r^2} + \frac{\alpha}{r^2} - \frac{1}{r^2 A} - \frac{\alpha}{r^2 A} + \frac{3\,\lambda^2}{B} + \frac{\alpha\,\lambda^2}{B} + \frac{A'}{r\,A^2} - \frac{\alpha\,B'}{r\,A\,B} = 0 \tag{10}$$

[here we have given the general barotropic equation of state $p = \alpha\rho$—setting $\alpha = 1/3$ regains (8)] is of higher order than the system (2) and (3). Thus a solution of (9) and (10) need not satisfy (2) and (3) while a solution of the latter *must* satisfy the former.

The solutions presented by Liu and Zhang[2] were only approximate. However, exact solutions to (2) and (3) are possible, and indeed have appeared in the literature previously,[3] though in the guise of solutions to (9) and (10). That solution has the form

$$ds^2 = -\beta^2\,Y_o^2\,dt^2 + Y^2(t)\,[2\,Y_o'^2\,dr^2 + Y_o^2\,d\Omega^2] \tag{11}$$

up to the determination of the time-dependence $Y(t)$. In addition to the general solution for $Y(t)$, it was observed in Ref. 3 that a linear form for $Y(t)$ would also suffice.

In order to compare (1) and (11) we need to set

$$\beta^2 = \frac{2\lambda^2(3+\alpha)}{\alpha-1}, \quad Y_o = r, \quad A(r) = 2, \quad B(r) = \beta^2 r^2, \quad Y(t) = (1-\lambda t). \tag{12}$$

Thus the metric

$$ds^2 = -\beta^2 r^2 dt^2 + (1-\lambda t)^2[2dr^2 + r^2\,d\Omega^2] \tag{13}$$

satisfies the pressure isotropy condition as well as the general barotropic equation of state (10). Clearly it will satisfy the radiation equation of state (8) as well.

While our metric (13) does satisfy the general equation of state (10), an attempt to match this metric to the Vaidya solution[4] (which describes the exterior space–time of a radiating star)

$$ds^2 = -\left(1 - \frac{2m(v)}{r}\right)dv^2 - 2\,dv\,dr + r^2(d\theta^2 + \sin^2\theta\, d\phi^2) \tag{14}$$

restricts the value of α to -3 which is unphysical. Thus the solution we present will not satisfy (8) if we match the solution to the Vaidya solution. Indeed, if we match a solution of (2) and (3) to (14), we need to satisfy the condition

$$\lambda = \left.\frac{B'}{2(AB)^{1/2}}\right|_{r=r_\Sigma} \tag{15}$$

at the boundary $r = r_\Sigma$. Thus, given a particular boundary r_Σ, one ought to be able to determine λ. We do not obtain this result in our solution (11) as we have $B \propto \lambda^2$. It would be of interest[5] to find an exact solution to (8) and (9) which can be matched to (14) as the model can be interpreted as a radiating star with an extended atmosphere dissipating energy in the form of radial heat flux.

We observe that the time dependence in the metric (1) is linear. As a result, horizon-free collapse[6] is evident in this model when matching to (14) since m_Σ / r_Σ is independent of time.

We conclude by noting that the solution we present, (13), does not have the same interesting physical properties that the approximate solution of Liu and Zhang[2] does. However, it is an exact solution. It would be useful to examine the full pressure isotropy equation (9) and the general equation of state (10) [or the radiation equation of state (8)] for further exact solutions that may provide similarly interesting physical applications.

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Recovery of a potential from the ratio of reflection and transmission coefficients

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(Received 12 July 2003; accepted 24 July 2003)

For the one-dimensional Schrödinger equation, the analysis is provided to recover the potential from the data consisting of the ratio of a reflection coefficient to the transmission coefficient. It is investigated whether such data uniquely constructs a reflection coefficient, the number of bound states, bound-state energies, bound-state norming constants, and a corresponding potential. In all three cases when there is no knowledge of the support of the potential, the support of the potential is confined to a half-line, and the support is confined to a finite interval, various uniqueness and nonuniqueness results are established, the precise criteria are provided for the uniqueness and the nonuniqueness and the degree of nonuniqueness, and the recovery is illustrated with some explicit examples. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1614871]

I. INTRODUCTION

In this paper we investigate the recovery of the potential of the one-dimensional Schrödinger equation from the data consisting of the ratio of a reflection coefficient to the transmission coefficient. We analyze the cases where the potential has no restriction on its support, half-line support, and compact support. We assume no information about the number of bound states, and in fact we try to recover that number as a part of our inverse problem.

Our work is motivated by the work of Rundell and Sacks[1] where it was shown that a bounded, compactly supported potential with a sufficiently small L^2-norm is uniquely determined by the corresponding ratio of a reflection coefficient to the transmission coefficient. In our paper we show exactly when such a determination is possible.

Consider the Schrödinger equation

$$\psi''(k,x)+k^2\,\psi(k,x)=V(x)\,\psi(k,x), \quad x\in\mathbf{R}, \tag{1.1}$$

where the potential V belongs to the Faddeev class, i.e., it is real valued, measurable, and in $L^1_1(\mathbf{R})$. Here, $L^1_n(J)$ denotes the class of measurable functions on an interval J such that $\int_J dx\,(1+|x|^n)\,|V(x)|$ is finite. The prime is used for the derivative with respect to the spatial coordinate x. The scattering solutions to (1.1) behave like e^{ikx} or e^{-ikx} as $x\to\pm\infty$, and they occur for $k\in\mathbf{R}\backslash\{0\}$. A bound state of (1.1) is a solution that belongs to $L^2(\mathbf{R})$ in the x variable, and it is known[2–7] that the bound states can occur only at certain k values on the positive imaginary axis $\mathbf{I}^+$ in $\mathbf{C}^+$. We use $\mathbf{C}^+$ for the upper-half complex plane and $\mathbf{I}^+:=i(0,+\infty)$; later we will let $\overline{\mathbf{C}^+}:=\mathbf{C}^+\cup\mathbf{R}$ and $\mathbf{I}^-:=i(-\infty,0)$. We will use N to denote the number of bound states, which is known to be finite when V is in the Faddeev class, and suppose that the bound states occur at $k=i\kappa_j$ with the ordering $0<\kappa_1<\cdots<\kappa_N$.

Among the scattering solutions to (1.1) are f_l and f_r, the Jost solutions from the left and right, respectively, satisfying the respective boundary conditions

$$e^{-ikx}f_l(k,x)=1+o(1),\quad e^{-ikx}f_l'(k,x)=ik+o(1),\quad x\to+\infty,$$

$$e^{ikx}f_r(k,x)=1+o(1),\quad e^{ikx}f_r'(k,x)=-ik+o(1),\quad x\to-\infty. \tag{1.2}$$

From the spatial asymptotics

$$f_l(k,x)=\frac{e^{ikx}}{T(k)}+\frac{L(k)\,e^{-ikx}}{T(k)}+o(1),\quad x\to-\infty, \tag{1.3}$$

$$f_r(k,x)=\frac{e^{-ikx}}{T(k)}+\frac{R(k)\,e^{ikx}}{T(k)}+o(1),\quad x\to+\infty,$$

we obtain the transmission coefficient T, and the reflection coefficients L and R from the left and right, respectively. It is known[2–7] that

$$T(-k)=T(k)^*,\quad R(-k)=R(k)^*,\quad L(-k)=L(k)^*,\quad k\in\mathbf{R},$$

$$R(k)=-\frac{L(-k)\,T(k)}{T(-k)},\quad |T(k)|^2+|L(k)|^2=1,\quad k\in\mathbf{R}, \tag{1.4}$$

where the asterisk denotes complex conjugation. In general, R and L are defined only for real k values, but T has a meromorphic extension to $\mathbf{C}^+$. Each bound state corresponds to a (simple) pole of T in $\mathbf{C}^+$ and vice versa. Given $|T(k)|$ for $k\in\mathbf{R}$ and the bound-state poles $k=i\kappa_j$, one can construct T as[2–7]

$$T(k)=\left(\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j}\right)\exp\left(\frac{1}{\pi i}\int_{-\infty}^{\infty}ds\,\frac{\log|T(s)|}{s-k-i0^+}\right),\quad k\in\overline{\mathbf{C}^+}. \tag{1.5}$$

A potential V in the Faddeev class is said to be generic if $T(0)=0$ and exceptional if $T(0)\neq 0$. Generically we have

$$\lim_{k\to 0}\frac{2ik\,L(k)}{T(k)}=(-1)^N|W_0|+o(1),\quad k\to 0\ \text{ in }\mathbf{R}, \tag{1.6}$$

where the Wronskian $W_0:=f_r(0,x)\,f_l'(0,x)-f_r'(0,x)\,f_l(0,x)$ is a nonzero constant. On the other hand, in the exceptional case we have

$$\lim_{k\to 0}\frac{L(k)}{T(k)}=\frac{\gamma_0^2-1}{2\gamma_0}+o(1),\quad k\to 0\ \text{ in }\mathbf{R}, \tag{1.7}$$

where

$$\gamma_0:=\frac{f_l(0,x)}{f_r(0,x)}=(-1)^N\left|\frac{f_l(0,x)}{f_r(0,x)}\right|$$

is a nonzero constant.

A potential in the Faddeev class is uniquely determined from the data $\{L,\{\kappa_j\},\{c_{rj}\}\}$ or $\{L,\{\kappa_j\},\{\gamma_j\}\}$ by using any one of the available methods.[2–7] Here, c_{rj}, for each $j=1,\ldots,N$, represents the bound-state norming constant and γ_j the dependency constant associated with $k=i\kappa_j$, and they are related to the Jost solutions as

$$c_{rj}:=\left[\int_{-\infty}^{\infty}dx\,f_r(i\kappa_j,x)^2\right]^{-1/2},\quad \gamma_j:=\frac{f_l(i\kappa_j,x)}{f_r(i\kappa_j,x)}. \tag{1.8}$$

Given V, we can remove[2–7] all the bound states from the scattering coefficients and construct the resulting potential $V^{[0]}$ corresponding to the transmission coefficient $T^{[0]}$ and the left reflection coefficient $L^{[0]}$, where

$$T(k)=T^{[0]}(k)\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j},\quad L(k)=(-1)^N L^{[0]}(k)\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j}. \tag{1.9}$$

The potential $V^{[0]}$ belongs to the Faddeev class whenever V is in that class.

Without loss of any generality, our main problem can be reduced to the recovery of a potential V in the Faddeev class from the data $\mathcal{D}(k):=L(k)/T(k)$ in the following cases:

(i) V has no restrictions on its support.
(ii) The support of V is confined to a half-line.
(iii) The support of V is confined to a finite interval.

Our paper is organized as follows. In Sec. II we study case (i); we see that our data cannot say anything about the value of N in the exceptional case and hence $N\in\{0,1,2,\dots\}$, and for each such N we have a $2N$-parameter family of potentials corresponding to our data. On the other hand, in the generic case from our data we get $N\in\{0,2,4,\dots\}$ or $N\in\{1,3,5,\dots\}$, as indicated in (1.6); for each allowed N we again have a $2N$-parameter family of potentials corresponding to $\mathcal{D}$. Case (ii) is analyzed in Sec. III, and we show that our data puts a further restriction on the maximum allowable value for N and that $N-1$ cannot exceed the number of zeros of $\mathcal{D}$ on $\mathbf{I}^+$. In particular, in the generic case where $\mathcal{D}$ has no zeros on $\mathbf{I}^+$ and the limit in (1.6) is positive, we conclude that $N=0$ and hence there is a unique potential corresponding to $\mathcal{D}$. We also show that our data restricts the (open) intervals in which the κ_j can occur, depending on the sign of $\mathcal{D}$ on $\mathbf{I}^+$. Then, for each allowed N we obtain an N-parameter family of potentials supported on the positive half-line corresponding to our data. We illustrate the nonuniqueness with some explicit examples. Finally, in Sec. IV, we analyze case (iii) and show that our data further puts severe restrictions on the locations of the κ_j. In this case we show that for each allowed N, there can exist only a discrete number of potentials corresponding to the same $\mathcal{D}$. We provide the exact criteria for the uniqueness as well as the nonuniqueness and the degree of nonuniqueness, and we illustrate the theory with some explicit examples.

II. RECOVERY WITH NO RESTRICTION ON THE SUPPORT

We will analyze the construction of V from the data $\mathcal{D}$ by analyzing the construction of $\{L,\{\kappa_j\},\{c_{rj}\}\}$ from $\mathcal{D}$.

Given $\mathcal{D}(k)$ for $k\in\mathbf{R}$, we can construct $T^{[0]}$. This is because, as seen from (1.9) and the second equation in (1.4), we have

$$\frac{1}{|T^{[0]}(k)|^2}=\frac{1}{|T(k)|^2}=1+|\mathcal{D}(k)|^2,\quad k\in\mathbf{R}, \tag{2.1}$$

and hence, (1.5) and (2.1) imply that

$$T^{[0]}(k)=\exp\left(\frac{1}{2\pi i}\int_{-\infty}^{\infty}ds\,\frac{\log(1/[1+|\mathcal{D}(s)|^2])}{s-k-i0^+}\right),\quad k\in\overline{\mathbf{C}^+}. \tag{2.2}$$

Having found $T^{[0]}$, from (1.9) we get

$$L^{[0]}(k)=(-1)^N\mathcal{D}(k)\,T^{[0]}(k),\quad L(k)=\mathcal{D}(k)\,T^{[0]}(k)\left(\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j}\right). \tag{2.3}$$

Thus, to construct L from $\mathcal{D}$, we must know both the number of bound states and the bound-state energies. In the generic cases, as (1.6) implies, from $\mathcal{D}$ we are only able to determine whether N is even or odd, but in the exceptional case even this is not possible, as implied by (1.7). For $N=0$, as seen from (2.3), $\mathcal{D}$ uniquely determines L and hence also V.

In summary, given the data $\mathcal{D}$, we get, for each value of N, a $2N$-parameter family of corresponding potentials, where $\{\{\kappa_j\},\{c_{rj}\}\}$ represents the parameter set. If $\mathcal{D}(k)$ is bounded at $k=0$ then N can be any non-negative integer; if $\mathcal{D}(k)$ is unbounded at $k=0$, then N is a non-negative integer, which is odd or even depending on the sign of $\lim_{k\to 0}[2ik\,\mathcal{D}(k)]$ as in (1.6).

Example 2.1: Let us demonstrate that we can tell from $\mathcal{D}$ whether N is even or odd in the generic case, but not in the exceptional case. Consider

$$\mathcal{D}(k)=\frac{\alpha}{(k+ic_+)(k+ic_-)},\quad c_\pm:=\sqrt{10\pm\sqrt{\alpha^2+36}},$$

where $\alpha\in[-8,8]$ is a parameter. Note that $\alpha=\pm 8$ corresponds to the generic case and $\alpha\in(-8,8)$ corresponds to the exceptional case. In the generic case from (1.6) we get $2ik\,\mathcal{D}(k)=\alpha/\sqrt{5}+O(k)$ as $k\to 0$, and hence N must be even if $\alpha=8$ and odd if $\alpha=-8$. On the other hand, in the exceptional case, from (1.7) we get $\mathcal{D}(k)=\alpha/\sqrt{64-\alpha^2}+O(k)$ as $k\to 0$, and N can be any non-negative integer. In fact, the corresponding scattering coefficients for $\alpha\in[-8,8]$ are given by

$$L(k)=\frac{(-1)^N\alpha}{(k+2i)(k+4i)}\left(\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j}\right),\quad T(k)=\frac{(k+ic_+)(k+ic_-)}{(k+2i)(k+4i)}\left(\prod_{j=1}^{N}\frac{k+i\kappa_j}{k-i\kappa_j}\right),$$

where $L(0)=-1$ and $T(0)=0$ are assured in the generic case by the choice $N\in\{0,2,4,\dots\}$ if $\alpha=8$ and $N\in\{1,3,5,\dots\}$ if $\alpha=-8$.

III. RECOVERY WITH SUPPORT ON A HALF-LINE

In this section we analyze the construction of V from $\mathcal{D}$ when we further know that the support of V is confined to a half-line. Equivalently, we analyze the construction of $\{L,\{\kappa_j\},\{c_{rj}\}\}$ from our data.

There is no loss of generality in assuming that the support of V is confined to $\mathbf{R}^+$. This can be seen by the following argument. If the support of the potential is known to be confined to the interval $(a,+\infty)$ for some real constant a, then the value of a can be extracted[8] from $\mathcal{D}$; the shift $V(x)\mapsto V(x-a)$ results in $L(k)/T(k)\mapsto L(k)\,e^{2ika}/T(k)$ and hence there is no loss of generality in assuming that $a\equiv 0$. On the other hand, if the support of the potential is known to be confined to $\mathbf{R}^-$, then, because of the first equation in (1.4), our problem can also be formulated as the recovery of V from R/T, which is equivalent to the recovery of V from $\mathcal{D}$.

When the support of V is confined to $\mathbf{R}^+$, it is already known[9–14] that L uniquely determines V. In fact, the meromorphic extension of $L(k)$ from $\mathbf{R}$ to $\mathbf{C}^+$ uniquely determines $\{\{\kappa_j\},\{c_{rj}\}\}$ as indicated in Theorem 3.3 below. Thus, the number of arbitrary parameters appearing in the reflection coefficient L constructed from our data is the same as the number of parameters appearing in the constructed V.

In Sec. II we have seen that $\mathcal{D}$ in the generic case reveals whether N is even or odd. We will next show that knowledge that the support of V is confined to $\mathbf{R}^+$ leads to an upper bound on N both in the generic and exceptional cases.

Proposition 3.1: Assume $V^{[0]}$ is a potential in the Faddeev class, has support in $\mathbf{R}^+$, and has no bound states. Suppose V is the potential obtained by adding N successive bound states to $V^{[0]}$ at $k=i\kappa_j$ with $0<\kappa_1<\cdots<\kappa_N$, and let $L^{[0]}$ denote the left reflection coefficient for $V^{[0]}$ as in (1.9). If the support of V is confined to $\mathbf{R}^+$, then $(-1)^jL^{[0]}(i\kappa_j)>0$ for $j=1,\dots,N$, or equivalently, $(-1)^{N-j}\mathcal{D}(i\kappa_j)>0$.

Proof: If $V\equiv 0$ for $x<0$, from (1.2) and (1.3) we see that

$$f_r(k,x)=e^{-ikx},\quad f_l(k,x)=\frac{e^{ikx}}{T(k)}+\frac{L(k)\,e^{-ikx}}{T(k)},\quad x\leqslant 0. \tag{3.1}$$

Hence, using $1/T(i\kappa_j)=0$, (3.1), and the second equation in (1.8), we reach the conclusion that $\gamma_j=(L/T)(i\kappa_j)$. Then, with the help of (1.9), we get $L^{[0]}(i\kappa_j)=(-1)^N\gamma_j T^{[0]}(i\kappa_j)$. It is already known that $T^{[0]}(k)>0$ on $\mathbf{I}^+$ and $(-1)^{N-j}\gamma_j>0$. Thus, $(-1)^jL^{[0]}(i\kappa_j)>0$ for $j=1,\ldots,N$. With the help of $\mathcal{D}(k)=(-1)^NL^{[0]}(k)/T^{[0]}(k)$, we equivalently claim that $(-1)^{N-j}\mathcal{D}(i\kappa_j)>0$. ■

For $k\in\mathbf{I}^+$ we know that $L^{[0]}(k)$ is real valued and continuous and $1/T^{[0]}(k)>0$; hence, from Proposition 3.1 we obtain the following result.

Corollary 3.2: Assume V belongs to the Faddeev class, has N bound states, and has support in $\mathbf{R}^+$. *Let* $L^{[0]}$ *denote the left reflection coefficient for* $V^{[0]}$, *which is obtained from V by removing all the bound states, as in (1.9). Then,* $L^{[0]}$ *must have at least* $N-1$ *zeros on* $\mathbf{I}^+$, *equivalently,* $\mathcal{D}$ *must have at least* $N-1$ *zeros on* $\mathbf{I}^+$.

Let us note that the zeros of $L^{[0]}$ on $\mathbf{I}^+$, or equivalently those of $\mathcal{D}$, need not be simple, as indicated in Examples 3.8 and 3.9.

The following theorem gives a characterization of the left reflection coefficient corresponding to a potential in the Faddeev class with support confined to $\mathbf{R}^+$. Let

$$\hat{L}(\alpha):=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,L(k)\,e^{ik\alpha},\quad \hat{R}(\alpha)=:-\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,\frac{L(-k)\,T(k)}{T(-k)}e^{ik\alpha}. \tag{3.2}$$

Theorem 3.3: *The left reflection coefficient L corresponds to a unique potential V in the Faddeev class with support in* $\mathbf{R}^+$ *and with N bound states at* $k=i\kappa_j$ $(j=1,\ldots,N)$ *if and only if the following conditions hold:*

(i) *L is continuous on* $\mathbf{R}$, *and* $L(-k)=L(k)^*$ *for* $k\in\mathbf{R}$.
(ii) $|L(k)|\leqslant 1-Ck^2/(1+k^2)$ *on* $\mathbf{R}$ *for some positive constant C*.
(iii) $L(0)\in[-1,1)$.
(iv) *L has a meromorphic extension to* $\mathbf{C}^+$ *with N simple poles occurring at* $k=i\kappa_j$ *and residues* $\mathrm{Res}L(i\kappa_j)=ic_{rj}^2$ *for some positive constants* c_{rj}. *Of course, if* $N=0$ *then the extension of L to* $\mathbf{C}^+$ *is analytic there.*
(v) $L(k)=o(1/k)$ *as* $k\to\infty$ *in* $\overline{\mathbf{C}^+}$.
(vi) *The function* $k/T(k)$, *where* $T(k)$ *is given in (1.5) with* $|T(s)|=\sqrt{1-|L(s)|^2}$, *is continuous in* $\overline{\mathbf{C}^+}$.
(vii) *The functions* $\hat{L}$ *and* $\hat{R}$ *defined in (3.2) are absolutely continuous,* $\hat{L}'\in L_1^1(-\infty,0)$, *and* $\hat{R}'\in L_1^1(a,+\infty)$ *for any* $a<0$.

Proof: The proof is obtained by modifying the characterization conditions on the scattering data[5,7,15] corresponding to a potential in the Faddeev class in order to take into account the vanishing property of the potential on $\mathbf{R}^-$. It is known[9–14] that (iv) is equivalent to vanishing of V on $\mathbf{R}^-$. The slight modification in (vii) is also related to the vanishing of the potential on $\mathbf{R}^-$. ■

In the following we illustrate the recovery of V, or equivalently of L, by presenting some explicit examples.

Example 3.4: Let our data for a potential with support in $\mathbf{R}^+$ be given by

$$\mathcal{D}(k)=\frac{-\sqrt{3}(k-i)(k-3i)}{(k+i)^2(k+\sqrt{5}i)(k+3i)}.$$

Notice that $\mathcal{D}(k)$ is bounded at $k=0$ and hence this corresponds to an exceptional case. Proceeding as in (2.2), or equivalently by solving the Riemann–Hilbert problem [cf. (2.1)]

$$\frac{1}{T^{[0]}(-k)} = (1+|\mathcal{D}(k)|^2)\, T^{[0]}(k), \quad k \in \mathbf{R},$$

we obtain

$$T^{[0]}(k) = \frac{(k+i)(k+\sqrt{5}i)}{(k+\sqrt{2}i)(k+2i)}.$$

From (2.3) we get

$$L^{[0]}(k) = (-1)^N A(k), \quad A(k) := \frac{-\sqrt{3}\,(k-i)(k-3i)}{(k+i)(k+\sqrt{2}i)(k+2i)(k+3i)}.$$

Notice that $\mathcal{D}$ has two zeros on $\mathbf{I}^+$. Hence, the number of bound states of V cannot exceed 3. Since this is the exceptional case, N is allowed to be any of 0, 1, 2, and 3. Recalling the fact that L uniquely determines V because of the support property of V, with the help of the sign restriction indicated in Proposition 3.1, or equivalently, with the help of Theorem 3.3(iv), we obtain all the following possibilities for L and also for V:

(a) For $N=0$, we have $L(k)=A(k)$, and the potential V is uniquely determined.
(b) For $N=1$, we have $L(k)=A(k)\,(k+i\kappa_1)/(k-i\kappa_1)$, where $\kappa_1 \in (0,1)\cup(3,+\infty)$ is the only arbitrary parameter in V.
(c) For $N=2$, we get $L(k)=A(k)\Pi_{j=1}^{2}(k+i\kappa_j)/(k-i\kappa_j)$, with $\kappa_1 \in (1,3)$ and $\kappa_2 \in (3,+\infty)$ being the only two arbitrary parameters in V.
(d) For $N=3$, we have $L(k)=A(k)\Pi_{j=1}^{3}(k+i\kappa_j)/(k-i\kappa_j)$, where $\kappa_1 \in (0,1)$, $\kappa_2 \in (1,3)$, and $\kappa_2 \in (3,+\infty)$ are the only three arbitrary parameters in V.

Example 3.5: Let $\mathcal{D}(k) = 8/k(k+i\sqrt{20})$. This is the generic case because $\mathcal{D}(k)$ is singular at $k=0$. Using (2.1) we obtain $T^{[0]}(k) = k(k+i\sqrt{20})/(k+2i)(k+4i)$. From (1.6) we see that $\lim_{k\to 0}[2ik\,\mathcal{D}(k)] = 8/\sqrt{5}$, which is positive, and therefore $N \in \{0,2,4,\dots\}$. Then, from the first equation in (2.3) we get $L^{[0]}(k) = 8/(k+2i)(k+4i)$. Since $\mathcal{D}$ has no zeros on $\mathbf{I}^+$, Corollary 3.2 implies that the only possibility is $N=0$. Thus, $L(k)=L^{[0]}(k)$, and our data uniquely determines L and V.

Example 3.6: Let $\mathcal{D}(k) = -8/k(k+i\sqrt{20})$. As in Example 3.5, this is the generic case and $T^{[0]}(k) = k(k+i\sqrt{20})/(k+2i)(k+4i)$. From (1.6) we see that $\lim_{k\to 0}[2ik\,\mathcal{D}(k)] = -8/\sqrt{5}$, which is negative, and hence $N \in \{1,3,5,\dots\}$. Then, from the first equation in (2.3) we get $L^{[0]}(k) = 8/(k+2i)(k+4i)$. Since $\mathcal{D}$ has no zeros on $\mathbf{I}^+$, Corollary 3.2 implies that the only possibility is $N=1$. Thus, we get $L(k) = -L^{[0]}(k)\,(k+i\kappa_1)/(k-i\kappa_1)$, where $\kappa_1 \in (0,+\infty)$ is an arbitrary parameter. Because the constructed L contains one arbitrary parameter, there exists a one-parameter family of potentials corresponding to our data.

Example 3.7: Let $\mathcal{D}(k) = -8(k-3i)(k-4i)/k(k+i\sqrt{20})(k+3i)(k+4i)$. As in Example 3.5, this is the generic case and $T^{[0]}(k) = k(k+i\sqrt{20})/(k+2i)(k+4i)$. From (1.6) we see that $\lim_{k\to 0}[2ik\,\mathcal{D}(k)] = -8/\sqrt{5}$, which is negative, and hence $N \in \{1,3,5,\dots\}$. Then, as in Example 3.5 we get $L^{[0]}(k) = 8(k-3i)(k-4i)/(k+2i)(k+3i)(k+4i)^2$. Since $\mathcal{D}$ has two zeros on $\mathbf{I}^+$, N cannot exceed 3. Thus, we must have $N=1$ or $N=3$. In conjunction with Proposition 3.1 or Theorem 3.3(iv), for $N=1$ we get the one-parameter family $L(k) = -L^{[0]}(k)\,(k+i\kappa_1)/(k-i\kappa_1)$ with $\kappa_1 \in (0,3)\cup(4,+\infty)$ and for $N=3$ we get $L(k) = -L^{[0]}(k)\Pi_{j=1}^{3}(k+i\kappa_j)/(k-i\kappa_j)$ with $\kappa_1 \in (0,3)$, $\kappa_2 \in (3,4)$, and $\kappa_3 \in (4,+\infty)$. Thus, our data corresponds to a one-parameter family of potentials when $N=1$, and it corresponds to a three-parameter family of potentials when $N=3$.

Example 3.8: Let $\mathcal{D}(k) = 8(k-i)^2/k(k+i\sqrt{20})(k+i)^2$. We see that $\mathcal{D}$ has exactly one (double) zero on $\mathbf{I}^+$. As in Example 3.5 we get

$$T^{[0]}(k)=\frac{k(k+i\sqrt{20})}{(k+2i)(k+4i)},\quad L^{[0]}(k)=\frac{8(k-i)^2}{(k+2i)(k+4i)(k+i)^2}. \tag{3.3}$$

Note that $\lim_{k\to 0}[2ik\,\mathcal{D}(k)]=8/\sqrt{5}$, which is positive, and hence (1.6) implies that $N\in\{0,2,4,\dots\}$. On the other hand, Corollary 3.2 implies that $N=0$ or $N=2$; however, a sign analysis of $\mathcal{D}$ on $\mathbf{I}^+$ indicates that $\mathcal{D}(i\beta)<0$ for $\beta\in(0,1)\cup(1,+\infty)$ and $\mathcal{D}(i\beta)=0$ for $\beta=1$. Thus, $N=2$ is incompatible with Proposition 3.1. Hence, $N=0$ is the only possibility, and T and L are uniquely determined by our data as equal to $T^{[0]}$ and $L^{[0]}$, respectively, given in (3.3). Therefore, there exists a unique potential corresponding to our data.

Example 3.9: Let $\mathcal{D}(k)=-8(k-i)^2/k(k+i\sqrt{20})(k+i)^2$. The corresponding $T^{[0]}$ and $L^{[0]}$ are the same as in (3.3). From (1.6) we see that $\lim_{k\to 0}[2ik\,\mathcal{D}(k)]=-8/\sqrt{5}$, which is negative, and hence $N\in\{1,3,5,\dots\}$, as implied by (1.6). A sign analysis of $\mathcal{D}$ on $\mathbf{I}^+$ indicates that $\mathcal{D}(i\beta)>0$ for $\beta\in(0,1)\cup(1,+\infty)$ and $\mathcal{D}(i\beta)=0$ for $\beta=1$. Hence, with the help of Corollary 3.2 we conclude that $N=1$ is the only possibility. We thus obtain

$$T(k)=\frac{k(k+i\sqrt{20})(k+i\kappa_1)}{(k+2i)(k+4i)(k-i\kappa_1)},\quad L(k)=\frac{-8(k-i)^2(k+i\kappa_1)}{(k+2i)(k+4i)(k+i)^2(k-i\kappa_1)},$$

with $\kappa_1\in(0,1)\cup(1,+\infty)$. Therefore, our data corresponds to a one-parameter family of potentials, where κ_1 acts as the parameter.

IV. RECOVERY WITH COMPACT SUPPORT

In this section we analyze the recovery of V, or equivalently of L, from $\mathcal{D}$ when it is further known that the support of V is confined to a finite interval. In constructing $\{L,\{\kappa_j\},\{c_{rj}\}\}$ from $\mathcal{D}$, all the results obtained in Secs. II and III are certainly valid in this section as well. We have the following:

(i) In the generic case, we are able to tell via (1.6) whether the non-negative integer N representing the number of bound states of V is even or odd.
(ii) Using (2.2) and the second equation in (2.3), we are able to construct $T^{[0]}$ and determine L except perhaps for the values of $\kappa_1,\dots,\kappa_N$.
(iii) Let us use Z to denote the number of zeros of $\mathcal{D}$ on $\mathbf{I}^+$. From Corollary 3.2 we conclude that $N\leqslant Z+1$. Moreover, Proposition 3.1 imposes a further restriction on N depending on the sign of $\mathcal{D}$ on $\mathbf{I}^+$.
(iv) The quantity $T^{[0]}$, which is uniquely determined by $\mathcal{D}$, has a meromorphic extension to the entire complex plane due to the fact that the support of V is confined to a finite interval. We will show that the set $\{-i\kappa_j\}$ has to be a subset of the set of zeros of $1/T^{[0]}$ on $\mathbf{I}^-$.

The following result is already known,[2] and hence its proof is omitted. By writing the first equation in (1.9) as

$$\frac{k}{T(k)}\prod_{j=1}^{N}\frac{1}{k-i\kappa_j}=\frac{k}{T^{[0]}(k)}\prod_{j=1}^{N}\frac{1}{k+i\kappa_j},$$

which is valid on the entire complex plane, the reader can compare the zeros of $1/T^{[0]}(k)$ and of $1/T(k)$ on the imaginary axis and verify the result stated in (iv) above as well as those in following proposition.

Proposition 4.1: Assume $V^{[0]}$ is real-valued, is integrable, has support confined to a finite interval, and has no bound states. Suppose V is the potential obtained by adding N successive bound states to $V^{[0]}$ at $k=i\kappa_j$ with $0<\kappa_1<\cdots<\kappa_N$, and let $T^{[0]}$ and T denote the transmission coefficients for $V^{[0]}$ and V, respectively. If the support of V is confined to a finite interval, then $k/T^{[0]}(k)$ and $k/T(k)$ are both entire, $1/T^{[0]}$ has a simple zero at $k=-i\kappa_j$ for $j=1,\dots,N$, and any other zero of $1/T^{[0]}$ on $\mathbf{I}^-$ must also be a zero $1/T$ with the same multiplicity.

In the first example below, we show that not every zero of $1/T^{[0]}$ on $\mathbf{I}^-$ necessarily corresponds to a bound state of V. In the second example we illustrate the recovery of L and V from our data.

Example 4.2: Consider the square-well potential supported on the interval $[0, 1]$ with depth equal to $c\alpha^2$ for some $c, \alpha > 0$. The corresponding transmission coefficient satisfies

$$\frac{1}{T(k)} = e^{ik}\left[\cos\gamma + \frac{k^2+\gamma^2}{2ik\gamma}\sin\gamma\right]$$

with $\gamma := \sqrt{k^2 + c\alpha^2}$. It can be easily checked that $1/T(-i\alpha) = 0$ if we choose $\alpha = \ln 8 = 2.079\,44$ and $c = 8/9$, where the overline on a digit indicates a roundoff. With these values, V has exactly one bound state occurring at $k = i\kappa$ with $\kappa = 1.307\,82$. We have $1/T(i\alpha) \neq 0$ and $1/T(i\kappa) = 1/T^{[0]}(-i\kappa) = 0$. In other words, $k = i\alpha$ does not correspond to a bound state of V even though $1/T^{[0]}(-i\alpha) = 0$.

Example 4.3: Let $\mathcal{D}(k) = -\epsilon e^{ik}\sin\sqrt{k^2+\epsilon}/2ik\sqrt{k^2+\epsilon}$, where ϵ is a non-negative parameter. In fact, one corresponding potential is the square well of depth ϵ with support on the interval $[0, 1]$. For each value of ϵ, let us obtain all the potentials corresponding to $\mathcal{D}(k)$ with support confined to a finite interval. We have $\lim_{k\to 0}[2ik\,\mathcal{D}(k)] = -\sqrt{\epsilon}\sin\sqrt{\epsilon}$, and hence the exceptional case occurs when $\sqrt{\epsilon} = p\pi$ for $p = 0,1,\ldots$ and the generic case occurs when $\sqrt{\epsilon} \neq p\pi$. In the generic case we see that the sign of $\lim_{k\to 0}[2ik\,\mathcal{D}(k)]$ is that of $(-1)^{p+1}$ when $p\pi < \sqrt{\epsilon} < (p+1)\pi$, and hence we can tell from ϵ whether p is even or odd. The sign analysis of $\mathcal{D}$ on $\mathbf{I}^+$ shows that Z mentioned in (iii) in the beginning of this section is equal to $\lfloor\sqrt{\epsilon}/\pi\rfloor$, i.e., the greatest integer less than or equal to $\sqrt{\epsilon}/\pi$; in other words, $\mathcal{D}$ has Z zeros on $\mathbf{I}^+$ occurring at $k = iz_j$ with $z_j = \sqrt{\epsilon - (j-1)^2\pi^2}$ for $j = 1,\ldots,Z$. In this particular example, $\mathcal{D}$ happens to have Z zeros on $\mathbf{I}^-$ as well occurring at $k = -iz_j$ symmetrically located with respect to the origin. With the help of (2.1) and (2.2) we obtain

$$\frac{1}{T^{[0]}(k)} = e^{ik}\left[\cos\sqrt{k^2+\epsilon} + \frac{2k^2+\epsilon}{2ik\sqrt{k^2+\epsilon}}\sin\sqrt{k^2+\epsilon}\right]\prod_{j=1}^{Z+1}\frac{k+i\beta_j}{k-i\beta_j}, \tag{4.1}$$

where the $\{\beta_j\}$ is the ordered set with $0 < \beta_1 < \cdots < \beta_{Z+1}$ consisting of those positive β values satisfying $\tan\sqrt{\epsilon-\beta^2} = (2\beta\sqrt{\epsilon-\beta^2})/(\epsilon - 2\beta^2)$. According to (iii) we must have $N \leq Z+1$. Using all these constraints, we can determine all the possibilities for N, the corresponding bound states, reflection coefficient L, and potential V. For example, we have the following:

(a) When $\epsilon = 5$, the above analysis shows that $Z = 0$ and thus $N \leq 1$, we are in the generic case and N must be odd, the quantity $1/T^{[0]}$ given in (4.1) has one simple zero on $\mathbf{I}^-$ at $k = -i\beta_1$, where $\beta_1 = 1.585\overline{7}$, and another one at $k = -i\beta_2$ with $\beta_2 = 1.543\,\overline{34}$. In the former case, we must have $N = 1$ with the bound state occurring at $k = i\beta_1$, and

$$L(k) = \mathcal{D}(k)\,T^{[0]}(k)\frac{k+i\beta_1}{k-i\beta_1} = \frac{-\epsilon\tan\sqrt{k^2+\epsilon}}{2ik\sqrt{k^2+\epsilon} + (2k^2+\epsilon)\tan\sqrt{k^2+\epsilon}}.$$

(b) When $\epsilon = 10$, we find that $Z = 1$ with $z_1 = 0.036\,110\,\overline{2}$, and thus $N \leq 2$, we are in the generic case and N must be even, the quantity $1/T^{[0]}$ given in (4.1) has two simple zeros on $\mathbf{I}^-$ at $k = -i\beta_j$, where $\beta_1 = 0.324\,42\overline{2}$ and $\beta_2 = 2.547\,5\overline{9}$. Thus, we have either of the two cases where $N = 0$ or $N = 2$. For $N = 0$, we get $L(k) = \mathcal{D}(k)\,T^{[0]}(k)$. On the other hand, for $N = 2$ we get

$$L(k) = \mathcal{D}(k)\,T^{[0]}(k)\frac{(k+i\beta_1)(k+i\beta_2)}{(k-i\beta_1)(k-i\beta_2)}.$$

(c) When $\epsilon=50$, we find that we are in the generic case, N must be odd, $Z=2$ with $z_1=3.243\overline{7}$ and $z_2=6.334\,8\overline{6}$, and thus $N\leqslant 3$; moreover, the quantity $1/T^{[0]}$ given in (4.1) has four simple zeros on $\mathbf{I}^-$ at $k=-i\beta_j$, where $\beta_1=1.871\overline{5}$, $\beta_2=5.198\,3\overline{9}$, $\beta_3=5.426\,4\overline{9}$, and $\beta_4=6.637\overline{6}$. Thus, we have either of the two cases where $N=1$ or $N=3$. For the case $N=1$ there is double nonuniqueness with $L(k)=\mathcal{D}(k)\,T^{[0]}(k)\,(k+i\beta_1)/(k-i\beta_1)$ or $L(k)=\mathcal{D}(k)\,T^{[0]}(k)\,(k+i\beta_4)/(k-i\beta_4)$, which is a consequence of $\mathcal{D}(i\beta_1)>0$, $\mathcal{D}(i\beta_2)<0$, $\mathcal{D}(i\beta_3)<0$, and $\mathcal{D}(i\beta_4)>0$. For $N=3$ we again have double nonuniqueness with the three bound states occurring at $k=i\kappa_j$ with the ordered set $\{\kappa_1,\kappa_2,\kappa_3\}$ being equal to either $\{\beta_1,\beta_2,\beta_4\}$ or $\{\beta_1,\beta_3,\beta_4\}$.

(d) When $\epsilon=100$, we find that we are in the generic case, N must be even, $Z=3$ with $z_1=3.342\,6\overline{9}$, $z_2=7.778\overline{7}$, and $z_3=9.493\,7\overline{9}$, and thus $N\leqslant 4$; moreover, the quantity $1/T^{[0]}$ given in (4.1) has six simple zeros on $\mathbf{I}^-$ at $k=-i\beta_j$, where $\beta_1=1.926\,9\overline{3}$, $\beta_2=5.710\,3\overline{8}$, $\beta_3=6.410\,1\overline{4}$, $\beta_4=8.546\,0\overline{7}$, $\beta_5=9.184\,7\overline{6}$, and $\beta_6=9.652\,6\overline{2}$. Thus, we have either of the three cases where $N=0$, $N=2$, or $N=4$. For $N=0$ our data uniquely determines L and V, with $L(k)=\mathcal{D}(k)\,T^{[0]}(k)$. With $L(k)=\mathcal{D}(k)\,T^{[0]}(k)\Pi_{j=1}^{2}(k+i\kappa_j)/(k-i\kappa_j)$ for $N=2$, we have fivefold nonuniqueness where the two bound states occurring at $k=i\kappa_j$ with the ordered set $\{\kappa_1,\kappa_2\}$ being equal to either of $\{\beta_1,\beta_2\}$, $\{\beta_1,\beta_3\}$, $\{\beta_1,\beta_6\}$, $\{\beta_4,\beta_6\}$, and $\{\beta_5,\beta_6\}$. On the other hand, for $N=4$ we have fourfold nonuniqueness where the four bound states occurring at $k=i\kappa_j$ with the ordered set $\{\kappa_1,\kappa_2,\kappa_3,\kappa_4\}$ being equal to either of $\{\beta_1,\beta_2,\beta_4,\beta_6\}$, $\{\beta_1,\beta_2,\beta_5,\beta_6\}$, $\{\beta_1,\beta_3,\beta_4,\beta_6\}$, $\{\beta_1,\beta_3,\beta_5,\beta_6\}$.

ACKNOWLEDGMENTS

The research leading to this paper was supported in part by the National Science Foundation under Grant No. DMS-0204437 and the Department of Energy under Grant No. DE-FG02-01ER45951.

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The Hopf algebra of identical, fermionic particle systems—Fundamental concepts and properties

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(Received 31 March 2003; accepted 1 July 2003)

The Hopf algebra structure of the fermionic Fock space is unravelled. The tools provided by the Hopf algebra formalism are used to rederive in a more straightforward fashion some known theorems and to open the way to natural generalizations of these results. The algebraic concepts of rank, depth and length of a wave function are given. They allow one to cast a wave function into a canonical form that is simpler and more appropriate to a physical interpretation or a numerical treatment. An original algorithm to re-expand a wave function with the least possible number of spin orbitals is described. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1611266]

I. INTRODUCTION

The origin of the Hopf algebra formalism can be traced back[1] to a conjecture regarding a topological invariant by Cartan in 1936.[2] Hopf proved that the conjecture was true,[3] essentially by introducing the Hopf algebra formalism as we use it in the present paper. More precisely, he showed that the cohomology of compact Lie groups and of suitable generalizations of them, all have the structure of an exterior algebra, the very structure of the fermionic Fock space.

Later on, the Hopf algebra formalism was extended to cover more general situations and different problems, e.g., the structure of group algebras, see Ref. 4. For example, in some situations, the definition of an Hopf algebra had to include explicitely the definition of an ''antipode map.'' In the case of Lie groups, this map corresponds to the usual inverse map. However, the antipode exists automatically in the case of the exterior algebra, see Ref. 5, and need not be introduced in the definition of the Hopf algebra structure of the fermionic Fock space.

In the late 1970s, Rota and co-workers put forward the idea of using Hopf algebras to deal with combinatorial aspects of Fock spaces (see, for example, Ref. 6). Seemingly, the physicists community did not echo their investigations. However, quantum groups appeared in physics at about the same period in the completely different context of the quantum inverse scattering method. Raychev[7] reviewed the early uses made of quantum groups and quantum algebras in physics. Since then, Connes and Kreimer have introduced Hopf algebra techniques in the theory of renormalization.[8,9]

The exterior algebra and the algebras coming from algebraic topology (precisely, from the cohomology of topological spaces) are ''fermionic'' in nature. In these algebras, the formal permutation of two elements of the algebra has to take into account a sign factor. This sign factor does not appear when defining the Hopf algebra structure on group algebras and quantum groups.[10] So, the Hopf algebras involved in the theory of group algebras and quantum groups are slightly different from the ones we are interested in here.

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The purpose of this paper is to exploit Hopf algebra techniques as a tool for investigating the physical properties of systems of identical fermionic particles.

Our paper is organized as follows.

First, an elementary presentation of the Hopf algebra structure of the Fock space is given. The properties defining an algebra are not all introduced here, as physicists are usually well acquainted with the exterior algebra structure of the fermionic Fock space. We refer the reader to the appendix of Ref. 7 for a more comprehensive presentation intended for nonspecialists of the properties defining an Hopf algebra. In contrast, the co-algebra structure and the Hopf algebra structure of the Fock space are not so familiar and all the properties defining these structures are provided.

Then, we turn attention to the observables, and more particularly to the density operators, defined on the state space. We show how the Hopf algebra formalism simplifies the derivation of several famous results and how it suggests natural generalizations of the latter. Next, we define some new algebraic concepts to analyze and simplify the expansion of a fermionic wave function. We obtain an original algorithm to re-expand a wave function in a more adapted basis set by using the new tools introduced in the preceding section.

We conclude alluding to the wealth of further studies and possible applications which can attract both physicists and mathematicians.

Notation: Let m be a positive integer, we denote by $\mathcal{S}_m$ the symmetric group of order m and for any permutation $\sigma \in \mathcal{S}_m$, $|\sigma|$ the signature of σ, equal to $+1$ if σ is even and to -1 if σ is odd.

For all non-negative integer $n \leqslant m$, we denote by $\mathcal{P}_{m,n}$ the set of n element subsets of $\{1,\ldots,m\}$, *ordered in increasing order*. The set of ordered subsets of $\{1,\ldots,m\}$ is

$$\mathcal{P}_m := \bigcup_{n=0}^{m} \mathcal{P}_{m,n}.$$

For all $I \in \mathcal{P}_{m,p}$, $I=(i_1,\ldots,i_p)$ we denote by $\overline{I} := (\overline{i}_1,\ldots,\overline{i}_{m-p})$ the element of $\mathcal{P}_{m,m-p}$ such that $I \cup \overline{I} = \{1,\ldots,m\}$. For all $I,J \in \mathcal{P}_m, I=(i_1,\ldots,i_p), J=(j_1,\ldots,j_q)$ we denote by $I//J$ the sequence $(i_1,\ldots,i_p,j_1,\ldots,j_q)$. Note that the latter is not necessarily an element of $\mathcal{P}_m$ since it may not be in increasing order and repeated integers may occur. In contrast, set operators such as $I \cup J$ are assumed to give elements of $\mathcal{P}_m$.

We further define the useful quantities $\rho_{I,J}$ by

$$\begin{aligned} \rho_{I,J} &= 0 \quad \text{if } I \cap J \neq \varnothing, \\ \rho_{I,J} &= (-1)^{|\sigma|} \quad \text{if } I \cap J = \varnothing, \end{aligned} \tag{1}$$

where $\sigma \in \mathcal{S}_{p+q}$ is the permutation that reorders $I//J$ into $I \cup J$. We easily note that,

$$\rho_{I,J} = (-1)^{pq} \rho_{J,I}. \tag{2}$$

For all $I,J,K \in \mathcal{P}_m$, denoting by $I \Delta J$ the symmetrical difference of sets I and J, that is the complement of their intersection $I \cap J$ in their union $I \cup J$, the reader can verify that the following relation is satisfied:

$$\rho_{I,K}\rho_{J,K} = \rho_{I\Delta J,K}\rho^2_{I\cap J,K}, \tag{3}$$

from which we deduce by setting $I=J$,

$$\rho_{\varnothing,K} = 1, \tag{4}$$

II. THE HOPF ALGEBRA STRUCTURE OF THE STATE SPACE

Classical and quantum physics can be described in a unified formalism relying on a duality relationship between an algebra of observables and a vector space of states.[11,12] In this section, the

form embodied by quantum states in the formalism of Hopf algebras is presented, together with other mathematical objects of primary importance to express the quantum mechanics of a system of identical fermionic particles.

We have chosen to use a notation close to the notation currently found in the recent mathematical literature because first, we find it convenient and second, we hope to bridge the gap between quantum physics and this field of mathematics where many ideas and results still have to be exploited by physicists. In that sense, this work is a prolongation of the work accomplished by one of us to introduce exterior algebra techniques into quantum chemistry.[13–16] As it will soon become apparent to the reader, the basic tools of the Hopf algebra formalism are very similar to those of the ''second quantization'' formalism, so they suit naturally the treatment of problems formulated in this framework. However, the Hopf algebra formalism also allows us similar formal manipulations, and much more, within the frame of the ''first quantization.''

A. The graded algebra structure of the Fock space

We denote by $\mathcal{H}$ the one-particle Hilbert space which is the tensor product of an orbital Hilbert space $\mathcal{H}_0$ and a spin Hilbert space $\mathcal{H}_s$,

$$\mathcal{H}=\mathcal{H}_0\otimes\mathcal{H}_s. \tag{5}$$

An element ψ of $\mathcal{H}$ is called a spin orbital and is in general a finite sum of tensor products of orbitals $\theta_i\in\mathcal{H}_0$ with spin functions $\tau_i\in\mathcal{H}_s$,

$$\psi=\sum_i \theta_i\otimes\tau_i. \tag{6}$$

The n-fermion Hilbert space induced by $\mathcal{H}$ is the nth exterior power of $\mathcal{H}$, denoted by $\wedge^n\mathcal{H}$. An element Ψ of $\wedge^n\mathcal{H}$ is an n-fermion wave function. It will be more specifically termed a ''single configuration'' (SC) function if it can be cast in the form of a simple exterior product of n spin orbitals $\psi_1,\ldots,\psi_n$,

$$\Psi=\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_n, \tag{7}$$

which corresponds in the second quantization of a fermionic system formalism to the quantum state

$$\Psi=a_1^\dagger\cdots a_n^\dagger|0\rangle, \tag{8}$$

where $a_i^\dagger$ is the creation operator of a fermion in the spin orbital ψ_i.

The fermionic Fock space of the second quantization $\wedge\mathcal{H}$ is the direct sum of all the $\wedge^n\mathcal{H}$,

$$\wedge\mathcal{H}:=\bigoplus_{n\geqslant 0}\wedge^n\mathcal{H}, \tag{9}$$

where $\mathcal{H}$ is identified to $\wedge^1\mathcal{H}$ and the field of complex or real numbers, denoted by $\mathbb{K}$, is identified to $\wedge^0\mathcal{H}$ through the ''unit map,'' $\mathcal{U}$,

$$\mathcal{U}:\mathbb{K}\mapsto\wedge\mathcal{H}$$

$$\lambda\to\mathcal{U}(\lambda)=\lambda\in\wedge^0\mathcal{H}. \tag{10}$$

Provided with Grassmann's exterior product, $\wedge$, which can be seen as a map from the tensor product $\wedge\mathcal{H}\otimes\wedge\mathcal{H}$ to $\wedge\mathcal{H}$,

$$\mathcal{X}:\wedge\mathcal{H}\otimes\wedge\mathcal{H}\mapsto\wedge\mathcal{H}$$

$$\Phi \otimes \Psi \to \mathcal{X}(\Phi \otimes \Psi) = \Phi \wedge \Psi, \tag{11}$$

it acquires the mathematical structure of an ''exterior algebra.'' Note that when one of its factors is a scalar λ, the exterior product reduces to the multiplication by this scalar,

$$\lambda \wedge \Psi = \Psi \wedge \lambda = \lambda \Psi. \tag{12}$$

The fermionic symmetry which traduces the Pauli exclusion principle is built-in in this exterior algebra because of the following antisymmetry relation between exterior products of one-particle functions:

$$\mathcal{X}(\phi \otimes \psi) = \phi \wedge \psi = -\psi \wedge \phi = -\mathcal{X}(\psi \otimes \phi), \tag{13}$$

which entirely determines the behavior of an n-fermion wave function under the symmetric group $\mathcal{S}_n$. That is to say, for an n-fermion single configuration:

$$\psi_1 \wedge \cdots \wedge \psi_n = (-1)^{|\sigma|} \psi_{\sigma(1)} \wedge \cdots \wedge \psi_{\sigma(n)}. \tag{14}$$

The general case is obtained from Eq. (14) by linearity.

Furthermore, the Fock space is what is termed ''a graded algebra.'' That is to say, Eq. (9) and the following relation hold true:

$$\mathcal{X}(\wedge^p \mathcal{H} \otimes \wedge^q \mathcal{H}) \subseteq \wedge^{p+q} \mathcal{H}. \tag{15}$$

The latter relation simply means that the exterior product of a p-fermion wave function with a q-fermion wave function is a $(p+q)$-fermion wave function. In fact, the graded algebra structure of the Fock space is something physicists are familiar with. In contrast, it has an additional coalgebra structure which has never been exploited, as far as we are aware.

B. The coalgebra structure of the Fock space

Inverting the arrows in Eq. (11), we define an ''exterior coproduct'' or simply ''coproduct'' on single configuration functions by

$$\begin{gathered} \mathcal{Y}: \wedge \mathcal{H} \mapsto \wedge \mathcal{H} \otimes \wedge \mathcal{H}, \\ \psi_1 \wedge \cdots \wedge \psi_n \to \mathcal{Y}(\psi_1 \wedge \cdots \wedge \psi_n) = \sum_{I \in \mathcal{P}_n} \rho_{I,\bar{I}} \psi_{i_1} \wedge \cdots \wedge \psi_{i_p} \otimes \psi_{\bar{i}_1} \wedge \cdots \wedge \psi_{\bar{i}_{n-p}}. \end{gathered} \tag{16}$$

The idea behind the coproduct is to split an n-fermion single configuration function into a p and an $(n-p)$-fermion single configuration functions in all possible ways, where p ranges from 0 to n, the exterior product of the two parts so-obtained giving back the initial function, the sign of the reordering permutation being taken care of. The definition extends by linearity to general wave functions.

As an example, let us write down the formula for $\mathcal{Y}$ acting on a 3-fermion configuration,

$$\begin{aligned} \mathcal{Y}(\psi_a \wedge \psi_b \wedge \psi_c) = {} & \psi_a \wedge \psi_b \wedge \psi_c \otimes 1 + \psi_a \wedge \psi_b \otimes \psi_c - \psi_a \wedge \psi_c \otimes \psi_b + \psi_b \wedge \psi_c \otimes \psi_a + \psi_a \otimes \psi_b \wedge \psi_c \\ & - \psi_b \otimes \psi_a \wedge \psi_c + \psi_c \otimes \psi_a \wedge \psi_b + 1 \otimes \psi_a \wedge \psi_b \wedge \psi_c. \end{aligned} \tag{17}$$

The coproduct is coassociative, i.e.,

$$(\mathcal{Y} \otimes \mathrm{Id}) \circ \mathcal{Y} = (\mathrm{Id} \otimes \mathcal{Y}) \circ \mathcal{Y} \tag{18}$$

(where Id is the identity map acting on the Fock space and $\circ$ the composition of mappings), which expresses the fact that when splitting a single configuration into a tensor product of three subconfigurations by iterating the coproduct twice, the component of the tensor product chosen to apply

the second coproduct does not matter. More generally, iterating the coproduct n times splits a single configuration into a tensor product of $n+1$ subconfigurations and the choice of the components on which the coproduct is successively applied is indifferent.

Another important mapping that is needed to obtain a coalgebra structure is the counit map,

$$\mathcal{V}:\wedge\mathcal{H}\mapsto\mathbb{K}$$

$$\Psi\to\mathcal{V}(\Psi)=0 \quad \text{if } \Psi\in\wedge^n\mathcal{H}, \quad n>0, \tag{19}$$

$$\lambda\to\mathcal{V}(\lambda)=\lambda \quad \text{if } \lambda\in\wedge^0\mathcal{H}.$$

The counit is compatible with the coproduct in the sense that

$$\forall\Psi\in\wedge\mathcal{H}, \quad (\mathcal{V}\otimes\mathrm{Id})\circ\mathcal{Y}(\Psi)=(\mathrm{Id}\otimes\mathcal{V})\circ\mathcal{Y}(\Psi)=\Psi. \tag{20}$$

When the Fock space is endowed with the coproduct and the counit it becomes a coalgebra. In the next section, we show that the algebra and the coalgebra structures are compatible. This makes the Fock space a Hopf algebra.

C. The Hopf algebra structure of the Fock space

The compatibility relationship between the exterior product $\mathcal{X}$ and the exterior coproduct $\mathcal{Y}$ which defines the Hopf algebra structure on the Fock space reads,

Proposition 1 (Hopf algebra fundamental relation):

$$\mathcal{Y}\circ\mathcal{X}=(\mathcal{X}\otimes\mathcal{X})\circ(\mathrm{Id}\otimes T\otimes\mathrm{Id})\circ(\mathcal{Y}\otimes\mathcal{Y}), \tag{21}$$

where T is the twisting map

$$\forall\Phi\in\wedge^p\mathcal{H}, \quad \forall\Psi\in\wedge^q\mathcal{H},$$
$$T(\Psi\otimes\Phi)=(-1)^{pq}\Phi\otimes\Psi. \tag{22}$$

The definition of T extends to more general elements of the Fock space by linearity.

The fundamental Hopf algebra relation expresses the fact that the same decomposition of the product of two single configurations into a tensor product of two subconfigurations is obtained by applying the coproduct to the exterior product of the two single configurations, or alternatively [second member of Eq. (21)], by first splitting each single configuration separately $(\mathcal{Y}\otimes\mathcal{Y})$, then grouping the first tensorial components of each decomposition together and the second components together $(\mathrm{Id}\otimes T\otimes\mathrm{Id})$, and finally by taking the exterior product of the first components on the one hand and the exterior product of the second components on the other hand $(\mathcal{X}\otimes\mathcal{X})$.

More explicitly we have

$$\mathcal{Y}(\psi_1\wedge\cdots\wedge\psi_p\wedge\phi_1\wedge\cdots\wedge\phi_q)=\sum_{I\in\mathcal{P}_p,J\in\mathcal{P}_q}\rho_{I,\bar{I}}\rho_{J,\bar{J}}(-1)^{l(p-k)}\psi_{i_1}\wedge\cdots\wedge\psi_{i_k}\wedge\phi_{j_1}\wedge\cdots\wedge\phi_{j_l}$$
$$\otimes\psi_{\bar{i}_1}\wedge\cdots\wedge\psi_{\bar{i}_{p-k}}\wedge\phi_{\bar{j}_1}\wedge\cdots\wedge\phi_{\bar{j}_{q-l}}. \tag{23}$$

The proof of the formula follows almost immediately from the observation that to extract all the $(k+l)$-element subsequences out of a sequence with $(p+q)$ elements $(1,\ldots,p+q)$ amounts to extracting k elements out of the sequence $(1,\ldots,p)$ and l elements out of the sequence $(p+1,\ldots,p+q)$ in all possible ways, where k runs from 0 to p and l from 0 to q.

D. Hermitian structure of the Fock space

A complex (or Hermitian) Hilbert space is, by definition, endowed with an Hermitian product written $\langle\ |\ \rangle$. (If $\mathbb{K}=\mathbb{R}$, the words "complex" must be replaced by "real," "Hermitian product" by "scalar product," "sesquilinear" by "linear" …, in the present and the following sections.)

If $\mathcal{E}$ and $\mathcal{F}$ are two Hermitian spaces, then their tensor product is also Hermitian, with the Hermitian product defined by

$$\forall e,f\in\mathcal{E},\ \ \forall g,h\in\mathcal{F},\ \ \langle e\otimes g|f\otimes h\rangle := \langle e|f\rangle\cdot\langle g|h\rangle. \tag{24}$$

An illustration of this situation is the one-particle Hilbert space of Eq. (5) whose Hermitian product is formed by multiplication of the orbital Hermitian product ($\langle f|g\rangle=\int f^*\cdot g\ \mathrm{d}\vec{r}$ in $\mathbb{L}^2$) and the spin Hermitian product (the standard Hermitian product in dimension $2S+1$).

Similarly, if $\mathcal{H}$ is an Hermitian space, an Hermitian product is induced on $\wedge^n\mathcal{H}$, by

$$\langle\phi_1\wedge\cdots\wedge\phi_n|\psi_1\wedge\cdots\wedge\psi_n\rangle := \det(\langle\phi_i|\psi_j\rangle)_{i,j\in\{1,\ldots,n\}}, \tag{25}$$

which extends by sesquilinearity to all $\wedge\mathcal{H}$.

Then, making use of Eqs. (14), (24), and (25), the Hopf algebra fundamental formula, rewritten as Eq. (23), immediately yields the Laplace formula to expand a determinant.[17]

Proposition 2 (Laplace formula): For any $\phi_1,\ldots,\phi_n,\psi_1,\ldots,\psi_n\in\mathcal{H}$ and for any $p\leqslant n$, $\forall\sigma\in\mathcal{S}_n$ we have

$$\begin{aligned}\langle\phi_1\wedge\cdots\wedge\phi_n|\psi_1\wedge\cdots\wedge\psi_n\rangle = (-1)^{|\sigma|}\langle\mathcal{Y}(\phi_1\wedge\cdots\wedge\phi_n)|(\psi_{\sigma(1)}\wedge\cdots\wedge\psi_{\sigma(p)})\\ \otimes(\psi_{\sigma(p+1)}\wedge\cdots\wedge\psi_{\sigma(n)})\rangle,\end{aligned} \tag{26}$$

which can be rewritten in a more familiar fashion,

$$\begin{aligned}\det(\langle\phi_i|\psi_j\rangle)_{i,j\in\{1,\ldots,n\}} = \sum_{I\in\mathcal{P}_{n,p}}\rho_{I,\bar{I}}\ (-1)^{|\sigma|}\det(\langle\phi_{i_k}|\psi_{\sigma(j)}\rangle)_{k,j\in\{1,\ldots,p\}}\\ \times\det(\langle\phi_{\bar{i}_k}|\psi_{\sigma(p+j)}\rangle)_{k,j\in\{1,\ldots,n-p\}}.\end{aligned} \tag{27}$$

The Laplace formula extended by sesquilinearity with $\sigma=\mathrm{Id}$, writes,

$$\langle\mathcal{X}(\Theta\otimes\Phi)|\Psi\rangle\equiv\langle\Theta\wedge\Phi|\Psi\rangle=\langle\Theta\otimes\Phi|\mathcal{Y}(\Psi)\rangle, \tag{28}$$

which expresses the duality-like relationship between the exterior product and the coproduct.

III. DENSITY OPERATORS ON THE FOCK SPACE

According to the standard axioms of quantum theory, the outcome of a physical experiment is given by the expectation value of an Hermitian operator acting on the state space, called an observable, over the von Neumann's statistical operator,[18] or "density operator," characterizing the physical state of the system. When the observable contains only p-particle operators ($p\leqslant n$ the total number of particle of the system), its expectation value can be obtained from a more compact mathematical object than the density operator, called the "p-particle reduced density operator." In this section, we present the form assumed by these operators in the Hopf algebra formalism and some of their basic properties.

Remark: In fact, it is transitions between quantum states rather than expectation values which should play the central role in quantum axiomatic, because without transitions there is no physical measurement nor observation possible. However, the importance of observables and density operators in quantum physics remains.

A. Creation, annihilation and density operators

The exterior product map, $\mathcal{X}$, defines in a natural manner, for all $\Psi \in \wedge\mathcal{H}$, the map,

$$\vec{\mathcal{X}}_\Psi : \wedge\mathcal{H} \mapsto \wedge\mathcal{H}$$

$$\Phi \to \vec{\mathcal{X}}_\Psi(\Phi) = \mathcal{X}(\Psi \otimes \Phi) = \Psi \wedge \Phi, \tag{29}$$

called the ''left exterior product by Ψ'' map, or in the second quantization terminology, the ''(left) creation operator of Ψ.'' Similarly we can define a right creation operator by

$$\overleftarrow{\mathcal{X}}_\Psi : \wedge\mathcal{H} \mapsto \wedge\mathcal{H}$$

$$\Phi \to \overleftarrow{\mathcal{X}}_\Psi(\Phi) = \mathcal{X}(\Phi \otimes \Psi) = \Phi \wedge \Psi. \tag{30}$$

The Hermitian product allows us to define the conjugate operator $O^\dagger$ of an operator O acting in $\wedge\mathcal{H}$, by

$$\forall \Phi, \Psi \in \wedge\mathcal{H},\ \langle \Phi | O(\Psi) \rangle = \langle O^\dagger(\Phi) | \Psi \rangle. \tag{31}$$

So a left annihilation operator, $\vec{\mathcal{I}}_\Psi := \vec{\mathcal{X}}_\Psi^\dagger$, also called the ''left interior product by Ψ'' and denoted by $\Psi \hookleftarrow$, is associated to the left creation operator,

$$\vec{\mathcal{I}}_\Psi : \wedge\mathcal{H} \mapsto \wedge\mathcal{H}$$

$$\Phi \to \vec{\mathcal{I}}_\Psi(\Phi) = \Psi \hookleftarrow \Phi. \tag{32}$$

Similarly a right annihilation operator, $\overleftarrow{\mathcal{I}}_\Psi := \overleftarrow{\mathcal{X}}_\Psi^\dagger$, also called ''right interior product by Ψ'' and denoted by $\Psi \hookrightarrow$, is associated to the right creation operator,

$$\overleftarrow{\mathcal{I}}_\Psi : \wedge\mathcal{H} \mapsto \wedge\mathcal{H}$$

$$\Phi \to \overleftarrow{\mathcal{I}}_\Psi(\Phi) = \Phi \hookrightarrow \Psi. \tag{33}$$

The conjugation relationships write, for all $\Theta \in \wedge^{q-p}\mathcal{H}$, $\Psi \in \wedge^p\mathcal{H}$, $\Phi \in \wedge^q\mathcal{H}$,

$$\langle \Theta | \Psi \hookleftarrow \Phi \rangle = \langle \Psi \wedge \Theta | \Phi \rangle, \tag{34}$$

$$\langle \Theta | \Phi \hookrightarrow \Psi \rangle = \langle \Theta \wedge \Psi | \Phi \rangle. \tag{35}$$

Note that the left (respectively, right) interior product by Ψ is an antilinear function of Ψ, so it defines a sesquilinear (respectively, antisesquilinear) map on $\wedge\mathcal{H} \times \wedge\mathcal{H}$, the left (respectively, right) interior product, $\hookleftarrow$ (respectively, $\hookrightarrow$). Then from the exterior product property,

$$\Psi \wedge \Theta = (-1)^{p(q-p)}\ \Theta \wedge \Psi \tag{36}$$

we deduce

$$\Psi \hookleftarrow \Phi = (-1)^{p(q-p)} \Phi \hookrightarrow \Psi, \tag{37}$$

which shows that the left and right interior products differ only by a sign factor. In the following the left interior product will often be referred to more simply as the ''interior product.''

Setting, $\Theta = 1$, in Eqs. (34) and (35) shows that for all p, the restriction of the interior products to $\wedge^p\mathcal{H} \times \wedge^p\mathcal{H}$ reduces to the Hermitian product on $\wedge^p\mathcal{H}$.

The expression of the density operator associated to a wave function $\Psi \in \wedge\mathcal{H}$ translates directly from the second quantization formalism. It corresponds, if Ψ is normalized, $\langle\Psi|\Psi\rangle = 1$, to the annihilation of Ψ followed by its creation:

$$\Gamma_\Psi = \vec{\mathcal{X}}_\Psi \circ \vec{\mathcal{I}}_\Psi . \tag{38}$$

If the wave function is that of a fixed number of particles, $\Psi \in \wedge^n\mathcal{H}$, for all $\Phi \in \wedge^p\mathcal{H}$, $\Gamma_\Psi(\Phi) \in \wedge^p\mathcal{H}$, that is to say, Γ_Ψ preserves the number of particles. We will denote by Γ^p_Ψ its restriction to $\wedge^p\mathcal{H}$. For $p<n$, $\Gamma^p_\Psi = 0$.

The density operators of general quantum states, or "mixed states," or "ensemble states," are linear convex combinations of density operators associated to wave functions, that is, associated to "pure states."

In the next sections we show that the reduced density operators related to Γ_Ψ have a particularly elegant expression in the Hopf algebra formalism, and that the coproduct simplifies greatly the investigation of their properties.

B. Reduced density operators

In this section we consider a fermionic system with a fixed number, n, of particles. A general wave function, $\Psi \in \wedge^n\mathcal{H}$ will have the form,

$$\Psi = \sum_l c_l \psi_{l,1} \wedge \cdots \wedge \psi_{l,n} , \tag{39}$$

with $c_l \in \mathbb{K}$ and $\psi_{l,j} \in \mathcal{H}$ for all l,j. For any $K = (k_1,\ldots,k_p) \in \mathcal{P}_n$, we denote by $\Psi_K \otimes \Psi_{\bar{K}}$ the expression,

$$\Psi_K \otimes \Psi_{\bar{K}} := \rho_{K,\bar{K}} \sum_l c_l \psi_{l,k_1} \wedge \cdots \wedge \psi_{l,k_p} \otimes \psi_{l,\bar{k}_1} \wedge \cdots \wedge \psi_{l,\bar{k}_{n-p}}, \tag{40}$$

so that the coproduct writes,

$$\mathcal{Y}(\Psi) = \sum_{K \in \mathcal{P}_n} \Psi_K \otimes \Psi_{\bar{K}}. \tag{41}$$

Another useful self-explanatory notation is

$$\langle \Phi_1 | \Psi_K \rangle \Psi_{\bar{K}} := \rho_{K,\bar{K}} \sum_l c_l \langle \Phi_1 | \psi_{l,k_1} \wedge \cdots \wedge \psi_{l,k_p} \rangle \psi_{l,\bar{k}_1} \wedge \cdots \wedge \psi_{l,\bar{k}_{n-p}}, \tag{42}$$

$$\langle \Phi_1 | \Psi_K \rangle \langle \Phi_2 | \Psi_{\bar{K}} \rangle := \rho_{K,\bar{K}} \sum_l c_l \langle \Phi_1 | \psi_{l,k_1} \wedge \cdots \wedge \psi_{l,k_p} \rangle \langle \Phi_2 | \psi_{l,\bar{k}_1} \wedge \cdots \wedge \psi_{l,\bar{k}_{n-p}} \rangle. \tag{43}$$

The reduced density operator of a normalized n-fermion wave function, D_Ψ acts on a wave function, $\Phi \in \wedge\mathcal{H}$ in the following way:[16]

$$D_\Psi(\Phi) = \Psi \hookrightarrow \Phi \hookleftarrow \Psi. \tag{44}$$

Here, one does not need to put parentheses indicating whether the left or the right interior product has to be performed first, because the solution obtained is indifferent to the order. Like the density operator, Γ_Ψ, the reduced density operator, D_Ψ, preserves the number of particles. Therefore D_Ψ is the direct sum of its restrictions to the $\wedge^p\mathcal{H}$, the so-called "p-order reduced density operators," D^p_Ψ,

$$D_\Psi = \sum_{p \geqslant 0} D^p_\Psi . \tag{45}$$

Note that D_Ψ coincides with Γ_Ψ on $\wedge^n \mathcal{H}$,

$$D^n_\Psi = \Gamma^n_\Psi , \tag{46}$$

and is null for $p > n$.

One of the difficulties in the study of the reduced density operator seems to have been the lack of a suitable algebraic framework for handling computations. We propose, in the next section, a simple closed formula for these operators by using the coproduct. Owing to this formula and the formal rules governing the Fock space as a Hopf algebra, the solutions of many algebraic problems related to reduced density operators become *natural*. Compare, for example, our proof of Sasaki's formula main corollary (Sec. III G below) with the classical one.[19,20] We begin with exhibiting the relationship between the interior products and the coproduct.

C. Generalization of the Greub formula and application to the reduced density operator

Combining the conjugation relation, Eq. (35) with the generalized Laplace formula Eq. (28) we obtain

$$\langle \Theta | \Psi \hookrightarrow \Phi \rangle = \langle \Theta \otimes \Phi | \mathcal{Y}(\Psi) \rangle, \tag{47}$$

valid for all $\Theta, \Psi, \Phi \in \wedge \mathcal{H}$. If now we restrict ourselves to homogeneous elements of the Fock space (i.e., belonging to a given exterior power of $\mathcal{H}$), $\Theta \in \wedge^{n-q}\mathcal{H}$, $\Psi \in \wedge^n \mathcal{H}$, $\Phi \in \wedge^q \mathcal{H}$, we can write further

$$\begin{aligned}
\langle \Theta \otimes \Phi | \mathcal{Y}(\Psi) \rangle &= \left\langle \Theta \otimes \Phi \middle| \sum_{K \in \mathcal{P}_n} \Psi_K \otimes \Psi_{\bar{K}} \right\rangle, \quad \text{by Eq. (41)} \\
&= \left\langle \Theta \otimes \Phi \middle| \sum_{K \in \mathcal{P}_{n,n-q}} \Psi_K \otimes \Psi_{\bar{K}} \right\rangle, \\
&\quad \text{since } \Theta \text{ is a } (n-q)-\text{fermion function} \\
&= \sum_{K \in \mathcal{P}_{n,n-q}} \langle \Theta | \Psi_K \rangle \cdot \langle \Phi | \Psi_{\bar{K}} \rangle, \text{ by Eq. (24) and Eq. (43)} \\
&= \left\langle \Theta \middle| \sum_{K \in \mathcal{P}_{n,n-q}} \langle \Phi | \Psi_{\bar{K}} \rangle \cdot \Psi_K \right\rangle, \text{ by using Eq.(42).}
\end{aligned}$$

Since this holds for all Θ we obtain through Eq. (47) the following closed formula for the right interior product:

$$\Psi \hookrightarrow \Phi = \sum_{K \in \mathcal{P}_{n,n-q}} \langle \Phi | \Psi_{\bar{K}} \rangle \cdot \Psi_K . \tag{48}$$

Similarly, we have for the left interior product,

$$\Phi \hookleftarrow \Psi = \sum_{K \in \mathcal{P}_{n,q}} \langle \Phi | \Psi_K \rangle \cdot \Psi_{\bar{K}}, \tag{49}$$

which is just a generalization by sesquilinearity of the Greub formula for single configurations,[21]

$$(\phi_1 \wedge \cdots \wedge \phi_q) \hookleftarrow (\psi_1 \wedge \cdots \wedge \psi_n) = \sum_{K \in \mathcal{P}_{n,q}} \rho_{K,\bar{K}} \det(\langle \phi_i | \psi_{k_j} \rangle)_{i,j \leqslant q} \, \psi_{\bar{k}_1} \wedge \cdots \wedge \psi_{\bar{k}_{n-q}}. \tag{50}$$

We are now ready to return to the reduced density operator expression. Rewriting Eq. (44) for $\Phi \in \wedge^q \mathcal{H}$, we have

$$
\begin{aligned}
D^q_\Psi(\Phi) &= \Psi \hookrightarrow \Phi \hookleftarrow \Psi \\
&= \Psi \hookrightarrow \left(\sum_{K \in \mathcal{P}_{n,q}} \langle \Phi | \Psi_K \rangle \cdot \Psi_{\bar{K}} \right), \text{ by Eq. (49)} \\
&= \sum_{K \in \mathcal{P}_{n,q}} \langle \Psi_K | \Phi \rangle \cdot (\Psi \hookrightarrow \Psi_{\bar{K}}), \text{ by antilinearity} \\
&= \sum_{K \in \mathcal{P}_{n,q}} \sum_{L \in \mathcal{P}_{n,q}} \langle \Psi_K | \Phi \rangle \cdot \langle \Psi_{\bar{K}} | \Psi_{\bar{L}} \rangle \Psi_L, \text{ by Eq. (48)} \\
&= \sum_{K \in \mathcal{P}_{n,q}} \sum_{L \in \mathcal{P}_{n,q}} \langle \Psi_{\bar{K}} | \Psi_{\bar{L}} \rangle \vec{\mathcal{X}}_{\Psi_L} \circ \vec{\mathcal{I}}_{\Psi_K}(\Phi).
\end{aligned}
$$

In the last equation, the notation of Eq. (42) has been extended to encompass the case where the functions appear as indices of creation or annihilation operators, that is to say, when we have $\Psi_{\bar{K}} \wedge$, or $\Psi_{\bar{K}} \hookleftarrow$ instead of $\Psi_{\bar{K}}$ in Eq. (42). Also, care must be taken that the coefficients of the expansion, Eq. (42), encapsulated in the pair $\Psi_K, \Psi_{\bar{K}}$ are to be replaced by their complex conjugates, because in fact it is the complex conjugate of Eq. (42) that appears above. Since the above equations hold for all Φ we have the following.

Proposition 3: The reduced density operator of order q associated to Ψ written D^q_Ψ or simply D^q when no ambiguity can arise from the notation, is given by

$$
D^q = \sum_{K,L \in \mathcal{P}_{n,q}} \langle \Psi_{\bar{K}} | \Psi_{\bar{L}} \rangle \ \ \vec{\mathcal{X}}_{\Psi_L} \circ \vec{\mathcal{I}}_{\Psi_K}. \tag{51}
$$

Note that the use of the creation and annihilation operators in Eq. (51) allows us to extend the action of D^q to all $\wedge \mathcal{H}$. Remark also that, in contrast with similar expressions obtained previously, the functions $\Psi_L, \Psi_{\bar{L}}, \Psi_K, \Psi_{\bar{K}}$ in this equation are not single configuration element of an induced basis set, but general multiconfigurational functions.

D. Normalization of reduced density operators

To illustrate further how to manipulate the coproduct, we address the problem of the normalization of reduced density operators. First, we establish some technical identities.

Proposition 4: Let $\Psi \in \wedge^n \mathcal{H}$, $\mathcal{Y}_{p,q}$ denotes the component of the coproduct in $\wedge^p \mathcal{H} \otimes \wedge^q \mathcal{H}$ and $\binom{n}{p}$ the binomial coefficient, then we have

$$
\mathcal{X} \circ \mathcal{Y}_{p,n-p}(\Psi) = \binom{n}{p} \Psi, \tag{52}
$$

$$
\mathcal{X} \circ \mathcal{Y}(\Psi) = 2^n \Psi. \tag{53}
$$

Proof: Since the maps $\mathcal{X} \circ \mathcal{Y}_{p,n-p}$ and $\mathcal{X} \circ \mathcal{Y}$ are linear, we may assume in the proof that Ψ is a single configuration wave function, $\Psi = \psi_1 \wedge \cdots \wedge \psi_n$. Recall then that

$$
\mathcal{Y}_{p,n-p}(\Psi) = \sum_{I \in \mathcal{P}_{n,p}} \rho_{I,\bar{I}} \ \psi_{i_1} \wedge \cdots \wedge \psi_{i_p} \otimes \psi_{\bar{i}_1} \wedge \cdots \wedge \psi_{\bar{i}_{n-p}}.
$$

Therefore

$$\mathcal{X}\circ\mathcal{Y}_{p,n-p}(\Psi)=\sum_{I\in\mathcal{P}_{n,p}}\rho_{I,\bar{I}}\psi_{i_1}\wedge\cdots\wedge\psi_{i_p}\wedge\bar{\psi_{i_1}}\wedge\cdots\wedge\bar{\psi_{i_{n-p}}}.$$

Since we have

$$\psi_{i_1}\wedge\cdots\wedge\psi_{i_p}\wedge\bar{\psi_{i_1}}\wedge\cdots\wedge\bar{\psi_{i_{n-p}}}=\rho_{I,\bar{I}}\psi_1\wedge\cdots\wedge\psi_n,$$

$\rho^2_{I,\bar{I}}=1$, and $\Sigma_{I\in\mathcal{P}_{n,p}}1=\binom{n}{p}$, the proof of the first equation in the proposition follows. The second one is a straightforward corollary of the first.

Proposition 5: In the Hopf algebra (and so in the second quantization) formalism, the trace of the pth-order reduced density operator is equal to the the binomial coefficient, $\binom{n}{p}$*, if the wave function is normalized, since,*

$$\mathrm{Tr}(D^p)=\mathrm{Tr}(D^{n-p})=\binom{n}{p}\|\Psi\|^2\ . \tag{54}$$

(This is not true in certain formalisms where different normalization factors are imposed to the reduced density operators see, e.g., Ref. 22.)

Proof: From Eq. (51) we have

$$\mathrm{Tr}(D^p)=\sum_{K,L\in\mathcal{P}_{n,p}}\langle\Psi_{\bar{K}}|\Psi_{\bar{L}}\rangle\vec{\mathcal{I}}_{\Psi_K}(\Psi_L)$$

and, since $\vec{\mathcal{I}}_{\Psi_K}(\Psi_L)=\langle\Psi_K|\Psi_L\rangle$, the trace is the Hermitian product of two coproducts, so that,

$$\mathrm{Tr}(D^p)=\mathrm{Tr}(D^{n-p})=\langle\mathcal{Y}_{p,n-p}(\Psi)|\mathcal{Y}_{p,n-p}(\Psi)\rangle. \tag{55}$$

From the generalized Laplace formula Eq. (28) we have

$$\mathrm{Tr}(D^p)=\langle\Psi|\mathcal{X}\circ\mathcal{Y}_{p,n-p}(\Psi)\rangle,$$

then we conclude with the previous proposition.

E. Convolution and induction

A p-particle operator, O^p, can be defined as an operator from $\wedge\mathcal{H}$ to $\wedge^p\mathcal{H}$ such that, $O^p(\Psi)=0$, if $\Psi\notin\wedge^p\mathcal{H}$. For example, the Coulomb repulsion, $1/\|\vec{r}_1-\vec{r}_2\|$, between two electrons is a two-electron operator. In this definition, the action of the operator O^p on $\wedge^n\mathcal{H}$, $n\neq p$, is trivial. The actual observable induced by O^p on all $\wedge\mathcal{H}$ is given by

$$O:=O^p*\mathrm{Id}:=\mathcal{X}\circ(O^p\otimes\mathrm{Id})\circ\mathcal{Y}. \tag{56}$$

The operation denoted by $*$ is called the ''convolution'' in the Hopf algebra formalism,

$$A*B:=\mathcal{X}\circ(A\otimes B)\circ\mathcal{Y}. \tag{57}$$

The convolution by the identity is thus a convenient way to induce operators on $\wedge\mathcal{H}$. The restriction of the induced observable, O, to $\wedge^n\mathcal{H}$ for $n\leqslant p$ is O^p, and for $n>p$ it is equivalent to the usual operator used in quantum physics, e.g., $\Sigma_{i<j}1/\|\vec{r}_i-\vec{r}_j\|$ in the case of the Coulomb repulsion operator.

According to quantum physics an n-particle quantum state is determined by its density operator Γ^n. As a matter of fact, the expectation value, $\langle O\rangle$, of any observable, O, is given by

$$\langle O\rangle=\mathrm{Tr}[\Gamma^n\circ O]. \tag{58}$$

The reduced density operator is of paramount importance in applications because if O is the induced operator by a p-particle operator O^p, then, $\forall \Psi \in \wedge^n \mathcal{H}$,

$$\begin{aligned}\langle \Psi | O\Psi \rangle &= \langle \Psi | (\mathcal{X} \circ (O^p \otimes \mathrm{Id}) \circ \mathcal{Y}) \Psi \rangle \\ &= \langle \mathcal{Y}(\Psi) | (O^p \otimes \mathrm{Id}) \circ \mathcal{Y}(\Psi) \rangle \\ &= \sum_{K,L \in \mathcal{P}_n} \langle \Psi_K \otimes \Psi_{\bar{K}} | (O^p \otimes \mathrm{Id})(\Psi_L \otimes \Psi_{\bar{L}}) \rangle \\ &= \sum_{K,L \in \mathcal{P}_{n,p}} \langle \Psi_K | O^p(\Psi_L) \rangle \cdot \langle \Psi_{\bar{K}} | \Psi_{\bar{L}} \rangle \\ &= \mathrm{Tr}\left[\left(\sum_{K,L \in \mathcal{P}_{n,p}} \langle \Psi_{\bar{K}} | \Psi_{\bar{L}} \rangle \vec{\mathcal{X}}_{\Psi_L} \circ \vec{\mathcal{I}}_{\Psi_K} \right) \circ O^p \right] \\ &= \mathrm{Tr}[D^p_\Psi \circ O^p]. \end{aligned} \tag{59}$$

Therefore, only the knowledge of D^p_Ψ, an operator acting on $\wedge^p \mathcal{H}$, and not that of Γ^n_Ψ, an operator acting on $\wedge^n \mathcal{H}$, is required to compute the expectation value of the observable induced on $\wedge^n \mathcal{H}$ by a p-particle operator, with $p < n$. In particular, the energy of a Coulombian system can be expressed exactly in terms of D^2_Ψ since the Coulomb potential involves no more than two-particle interactions.

F. A new proof of Carlson and Keller duality property

The Carlson and Keller duality property for reduced density operators[19] is a useful result which has been used, for example, to prove the generalized Koopmans theorem.[23] We now include a simplified proof of the duality property. Recall that, since reduced density operators are Hermitian, they can be diagonalized in an orthonormal basis and their eigenvalues are real and positive.

Proposition 6: The interior products with Ψ *send any* λ*-eigenvector of* D^p*, with* $\lambda \neq 0$*, to an eigenvector of* D^{n-p} *associated to the same eigenvalue, and the "p-external space," i.e., the* 0*-eigenspace of* D^p *(if* 0 *is an eigenvalue), to the null vector space* $\{\vec{0}\}$.

Proof: Let $\Phi \in \wedge^p \mathcal{H}$ be an eigenvector for D^p with eigenvalue λ. Then, by definition

$$\lambda \cdot \Phi = D^p(\Phi) = \Psi \hookrightarrow \Phi \hookleftarrow \Psi.$$

If $\lambda \neq 0$ this shows that $\Phi \hookleftarrow \Psi \neq 0$ and we have

$$D^{n-p}(\Phi \hookleftarrow \Psi) = \Psi \hookrightarrow (\Phi \hookleftarrow \Psi) \hookleftarrow \Psi = (\Psi \hookrightarrow \Phi \hookleftarrow \Psi) \hookleftarrow \Psi = \lambda \cdot \Phi \hookleftarrow \Psi,$$

so that $\Phi \hookleftarrow \Psi \in \wedge^{n-p} \mathcal{H}$ is an eigenvector for D^{n-p} with the same eigenvalue. The same argument shows that $\Psi \hookrightarrow \Phi \in \wedge^{n-p} \mathcal{H}$ is an eigenvector for D^{n-p}, still with the same eigenvalue. If $\lambda = 0$ then

$$\begin{aligned} 0 &= \langle \Phi | \Psi \hookrightarrow (\Phi \hookleftarrow \Psi) \rangle = \langle \Phi \wedge (\Phi \hookleftarrow \Psi) | \Psi \rangle \quad \text{by Eq. (35)}, \\ &= \langle \Phi \hookleftarrow \Psi | \Phi \hookleftarrow \Psi \rangle \quad \text{by Eq. (34)}, \end{aligned}$$

from which we deduce, $\Phi \hookleftarrow \Psi = \Phi \hookrightarrow \Psi = 0$.

Of course, we can change p in $(n-p)$ in the previous proposition. Thus, we see that the interior products are isomorphisms from the nonzero eigenspaces of D^p to the nonzero eigenspaces of D^{n-p}, which is the Carlson and Keller duality property. We will call the space spanned by the nonzero eigenspaces of D^p, the "p-internal space." Its orthogonal complement is the p-external space already defined. The extension of the interior product isomorphisms to the external space does not seem of physical relevance.

G. A simple derivation of Sasaki's formula main corollary

In the development of the N-representability conditions of reduced density matrices (RDM),[22,24] it was soon considered that the properties of partitioning a system of n particles into two subsystems should be one of the keys to the solution of the problem, and Coleman emphasized in particular the rôle that Sasaki's formula[20,25] should play ["this formula should be extremely useful whenever a system is partitioned into two subsystems" (Ref. 24, pp. 677–678)]. In this section we will not expand on the original Sasaki formula and its interest for the study of reduced density matrices that we prefer calling reduced density operators in this work, unless these operators are represented in some finite basis set. We refer the reader to Chapter 3 of the book by Coleman and Yakulov, Ref. 22, where various applications of the Sasaki formula are given, together with historical references on the subject. Instead, we show here that the main corollary of Sasaki's formula, from the point of view of applications, is obtained easily with the help of the coproduct.

This corollary, also due to Sasaki (Ref. 22, Thm. 3.3), is the following.

Theorem 7: *Assuming $n=p+q$, $p\leqslant q$, if f^p (respectively, f^q) is a complex square integrable function of p (respectively, q) variables, then,*

$$\langle f^p f^q | \mathcal{A}_n f^p f^q \rangle = \sum_{j=0}^{p} (-1)^j \binom{p}{j} \binom{q}{j} \mathrm{Tr}[D^j_{f^p} D^j_{f^q}],$$

where $\mathcal{A}_n$ is the antisymmetrization operator acting on functions of n variables.

One expects that, in the exterior algebra formalism, the technical points of the proof related to the symmetric group actions and the related combinatorial operations should disappear. This is indeed the case. In the exterior algebra formalism, the previous result reads as follows.

Theorem 8: *Let $\Psi \in \wedge^p \mathcal{H}$ and $\Phi \in \wedge^q \mathcal{H}$ and assume, for example, that $q\leqslant p$. Then*

$$\langle \Psi \wedge \Phi | \Psi \wedge \Phi \rangle = \sum_{j \leqslant q} (-1)^j \mathrm{Tr}(D^j_\Psi D^j_\Phi). \tag{60}$$

Proof: We have, according to the generalized Laplace formula Eq. (28),

$$\langle \Psi \wedge \Phi | \Psi \wedge \Phi \rangle = \langle \Psi \otimes \Phi | \mathcal{Y}(\Psi \wedge \Phi) \rangle.$$

According to the Hopf algebra fundamental formula Eq. (23), combined with the notation of Eq. (40) we can write [denoting card (K) the cardinal of set K],

$$\mathcal{Y}(\Psi \wedge \Phi) = \sum_{I \in \mathcal{P}_p, J \in \mathcal{P}_q} (-1)^{\mathrm{card}(J)(p-\mathrm{card}(I))} \Psi_I \wedge \Phi_J \otimes \Psi_{\bar{I}} \wedge \Phi_{\bar{J}},$$

and therefore, making use of Eq. (24),

$$\langle \Psi \otimes \Phi | \mathcal{Y}(\Psi \wedge \Phi) \rangle = \sum_{I \in \mathcal{P}_p, J \in \mathcal{P}_q} (-1)^{\mathrm{card}(J)(p-\mathrm{card}(I))} \langle \Psi | \Psi_I \wedge \Phi_J \rangle \langle \Phi | \Psi_{\bar{I}} \wedge \Phi_{\bar{J}} \rangle.$$

Notice that the terms with $\mathrm{card}(J) \neq (p - \mathrm{card}(I))$ vanish because they contain Hermitian products between functions of different particle numbers. Therefore the computed quantity is equal to

$$\sum_{j \leqslant q} \sum_{I \in \mathcal{P}_{p,(p-j)}, J \in \mathcal{P}_{q,j}} (-1)^j \langle \Psi | \Psi_I \wedge \Phi_J \rangle \langle \Phi | \Psi_{\bar{I}} \wedge \Phi_{\bar{J}} \rangle,$$

and, making use again of Eq. (28), it is equal to

$$\sum_{j\leqslant q}\sum_{I\in\mathcal{P}_{p,(p-j)},J\in\mathcal{P}_{q,j}}(-1)^j\langle\mathcal{Y}(\Psi)|\Psi_I\otimes\Phi_J\rangle\langle\mathcal{Y}(\Phi)|\Psi_{\bar{I}}\otimes\Phi_{\bar{J}}\rangle$$

$$=\sum_{j\leqslant q}\sum_{I,K\in\mathcal{P}_{p,(p-j)},J,L\in\mathcal{P}_{q,j}}(-1)^j\langle\Psi_K|\Psi_I\rangle\langle\Psi_{\bar{K}}|\Phi_J\rangle\langle\Phi_L|\Psi_{\bar{I}}\rangle\langle\Phi_{\bar{L}}|\Phi_{\bar{J}}\rangle$$

which can be recast by renaming the indexes $I\mapsto\bar{I},K\mapsto\bar{K}$ (and noting that $\rho_{K,\bar{K}}\rho_{I,\bar{I}}=\rho_{\bar{K},K}\rho_{\bar{I},I}$), in the form

$$=\sum_{j\leqslant q}(-1)^j\sum_{I,K\in\mathcal{P}_{p,j}}\sum_{J,L\in\mathcal{P}_{q,j}}\langle\Psi_{\bar{K}}|\Psi_{\bar{I}}\rangle\vec{\mathcal{I}}_{\Psi_K}(\Phi_J)\circ\langle\Phi_{\bar{L}}|\Phi_{\bar{J}}\rangle\vec{\mathcal{I}}_{\Phi_L}(\Psi_I)$$

where we recognize inside the sum over j the trace of the operator,

$$\sum_{I,K\in\mathcal{P}_{p,j}}\langle\Psi_{\bar{K}}|\Psi_{\bar{I}}\rangle\vec{\mathcal{X}}_{\Psi_I}\circ\vec{\mathcal{I}}_{\Psi_K}\circ\sum_{J,L\in\mathcal{P}_{q,j}}\langle\Phi_{\bar{L}}|\Phi_{\bar{J}}\rangle\vec{\mathcal{X}}_{\Phi_J}\circ\vec{\mathcal{I}}_{\Phi_L},$$

which is according to Eq. (51), the product $D^j_\Psi D^j_\Phi$, hence the result, Eq. (60).

H. Generalization: partitioning a wave function into several blocks

The part played by the coproduct in the derivation of the previous results suggest some natural generalizations, which are developed in the present section. The idea is now to split the n-fermion wave function in more than two blocks. To this end, we introduce a new notation. We denote by $\mathcal{Y}^{[k]}$ the coproduct iterated k times $(k>0)$,

$$\mathcal{Y}^{[k]}:=(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y})\circ\cdots\circ(\mathrm{Id}\otimes\mathcal{Y})\circ\mathcal{Y}, \tag{61}$$

where in the last iteration factor $(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y})$, the identity appears $k-1$ times. The action of $\mathcal{Y}^{[k]}$ is to split a wave function into $k+1$ blocks and we recall that, because of the coassociativity property, Eq. (18), the result does not depend upon the position of the coproduct in each factor $\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y}$. From its definition we have the recursion formula

$$\mathcal{Y}^{[k]}=(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y})\circ\mathcal{Y}^{[k-1]}. \tag{62}$$

We specify further by $\mathcal{Y}^{[k]}_{i_0,\ldots,i_k}$ the component of the iterated coproduct corresponding to the decomposition of a wave function into the tensor product of $(k+1)$ wave functions of $i_0,\ldots,i_k$-particles.

In a dual manner we define recursively the exterior product iterated k times $(k>0)$, $\mathcal{X}^{[k]}$, by

$$\mathcal{X}^{[k]}:=\mathcal{X}\circ(\mathcal{X}^{[k-1]}\otimes\mathrm{Id}), \tag{63}$$

with $\mathcal{X}^{[0]}:=\mathrm{Id}$.

$\mathcal{X}^{[k]}$ acts on $(k+1)$-component tensor products to form their $(k+1)$-component exterior product counterparts,

$$\mathcal{X}^{[k]}(\Psi_0\otimes\cdots\otimes\Psi_k)=\Psi_0\wedge\cdots\wedge\Psi_k. \tag{64}$$

Endowed with these tools we first generalize Eqs. (52) and (53).

Proposition 9: Let $\Psi\in\wedge^n\mathcal{H}$, and $i_0,\ldots,i_k$ such that $i_0+\cdots+i_k=n$, then we have

$$\mathcal{X}^{[k]}\circ\mathcal{Y}^{[k]}_{i_0,\ldots,i_k}(\Psi)=\binom{n}{i_0,\ldots,i_k}\Psi, \tag{65}$$

$$\mathcal{X}^{[k]}\circ\mathcal{Y}^{[k]}(\Psi)=(k+1)^n\Psi. \tag{66}$$

Proof: The generalized binomial coefficient $\binom{n}{i_0,\ldots,i_k}$ is the number of partitions of a set with n elements into an ordered sequence of k subsets with, respectively, $i_0,\ldots,i_k$ elements. That is,

$$\binom{n}{i_0,\ldots,i_k}=\frac{n!}{i_0!\ldots i_k!}.$$

Since $(k+1)^n$ is the number of partitions of a set with n elements into $k+1$ subsets, the second part of the proposition follows from the first identity. We now prove the first identity by induction on k.

The case $k=1$ corresponds precisely to Eq. (52). Assume then the property true up to $k-1$, and let show that it holds for k.

First we remark that $\mathcal{Y}^{[k]}_{i_0,\ldots,i_k}$ can be constructed on $\wedge^n\mathcal{H}$ from the coproduct in the following manner:

$$\mathcal{Y}^{[k]}_{i_0,\ldots,i_k}=(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y}_{i_{k-1},i_k})\circ\cdots\circ(\mathrm{Id}\otimes\mathcal{Y}_{i_1,n-i_0-i_1})\circ\mathcal{Y}_{i_0,n-i_0}. \tag{67}$$

Remark also that,

$$\mathcal{X}^{[k]}=\mathcal{X}\circ(\mathcal{X}^{[k-2]}\otimes\mathcal{X}). \tag{68}$$

Thus, we have,

$$\begin{aligned}
\mathcal{X}^{[k]}\circ\mathcal{Y}^{[k]}_{i_0,\ldots,i_k}(\Psi)&=\mathcal{X}\circ(\mathcal{X}^{[k-2]}\otimes\mathcal{X})\circ(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y}_{i_{k-1},i_k})\circ(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y}_{i_{k-2},i_{k-1}+i_k})\circ\cdots\\
&\quad\circ(\mathrm{Id}\otimes\mathcal{Y}_{i_1,n-i_0-i_1})\circ\mathcal{Y}_{i_0,n-i_0}(\Psi)\\
&=\mathcal{X}\circ(\mathcal{X}^{[k-2]}\otimes(\mathcal{X}\circ\mathcal{Y}_{i_{k-1},i_k}))\\
&\quad\circ(\mathrm{Id}\otimes\cdots\mathrm{Id}\otimes\mathcal{Y}_{i_{k-2},i_{k-1}+i_k})\circ\cdots\circ(\mathrm{Id}\otimes\mathcal{Y}_{i_1,n-i_0-i_1})\circ\mathcal{Y}_{i_0,n-i_0}(\Psi)\\
&=\mathcal{X}\circ\left(\mathcal{X}^{[k-2]}\otimes\binom{i_{k-1}+i_k}{i_k}\mathrm{Id}\right)\circ\mathcal{Y}^{[k-1]}_{i_0,\ldots,i_{k-2},i_{k-1}+i_k}(\Psi),\ \text{by Eq. (52)}\\
&=\binom{i_{k-1}+i_k}{i_k}\mathcal{X}^{[k-1]}\circ\mathcal{Y}^{[k-1]}_{i_0,\ldots,i_{k-2},i_{k-1}+i_k}(\Psi),\ \text{by Eq. (63)}\\
&=\binom{i_{k-1}+i_k}{i_k}\cdot\binom{n}{i_0,\ldots,i_{k-1}+i_k}\Psi,\ \text{by hypothesis,}
\end{aligned}$$

and the proof follows since

$$\binom{n}{i_0,\ldots,i_k}=\binom{n}{i_0,\ldots,i_{k-1}+i_k}\cdot\binom{i_{k-1}+i_k}{i_k}.$$

Next we generalize Eq. (28).

Proposition 10: For any $\Psi\in\wedge^n\mathcal{H}$ and for any $\Phi_0\in\wedge^{i_0}\mathcal{H},\ldots,\Phi_k\in\wedge^{i_k}\mathcal{H}$ with $i_0+\cdots+i_k=n$, we have

$$\langle\Phi_0\wedge\cdots\wedge\Phi_k|\Psi\rangle=\langle\Phi_0\otimes\cdots\otimes\Phi_k|\mathcal{Y}^{[k]}(\Psi)\rangle. \tag{69}$$

Proof: The proof proceeds by induction. The case $k=1$ is precisely Eq. (28). Let us suppose that the property is true up to $k-1$, then we have by Eq. (62),

$$\begin{aligned}
\langle\Phi_0\otimes\cdots\otimes\Phi_k|\mathcal{Y}^{[k]}(\Psi)\rangle&=\langle\Phi_0\otimes\cdots\otimes\Phi_k|(\mathrm{Id}\otimes\cdots\otimes\mathrm{Id}\otimes\mathcal{Y})\circ\mathcal{Y}^{[k-1]}(\Psi)\rangle\\
&=\langle\Phi_0\otimes\cdots\otimes\Phi_{k-2}\otimes(\Phi_{k-1}\wedge\Phi_k)|\mathcal{Y}^{[k-1]}(\Psi)\rangle\\
&=\langle\Phi_0\wedge\cdots\wedge\Phi_{k-2}\wedge(\Phi_{k-1}\wedge\Phi_k)|\Psi\rangle,\ \text{by hypothesis,}
\end{aligned}$$

where we can drop the parentheses thanks to the associativity of the exterior product.

By combining Eqs. (66) and (69) we immediately deduce the following.

Proposition 11: Let $\Psi,\Phi\in\wedge^n\mathcal{H}$. *Then, for any* k,

$$\langle\Psi|\Phi\rangle=\frac{1}{(k+1)^n}\langle\mathcal{Y}^{[k]}(\Psi)|\mathcal{Y}^{[k]}(\Phi)\rangle. \tag{70}$$

Finally, we generalize Eq. (60), by calculating the square norm of $\Phi=\Phi_0\wedge\cdots\wedge\Phi_k$, where $\forall m\in\{0,\ldots,k\},\Phi_m\in\wedge^{i_m}\mathcal{H}$. The latter can be expressed in the form

$$\Phi_m=\Sigma_l c_{m,l}\ \phi_{l,1+\Sigma_{j=0}^{m-1}i_j}\wedge\cdots\wedge\phi_{l,\Sigma_{j=0}^{m}i_j}$$

with

$$\sum_{j=0}^{-1} i_j=0 \quad\text{and}\quad \sum_{j=0}^{k} i_j=n.$$

That is to say, the indices of the spin orbitals of Φ_m run from $i_0+\cdots+i_{m-1}+1$ to $i_0+\cdots+i_{m-1}+i_m$ so that the indices of the spin orbitals of Φ run from 1 to n.

We extend to more than two subsets the notation of Eqs. (40)–(43), to encapsulate the sums on single configuration functions. However, here we leave out of the notation the sign of the reordering permutation. For example, $\forall m\in\{0,\ldots,k\}$, for any partition of

$$\left\{1+\sum_{j=0}^{m-1} i_j,\ldots,\sum_{j=0}^{m} i_j\right\}$$

into $k+1$ subsets, $I_m^0:=\{j_1^0,\ldots,j_{\mathrm{card}(I_m^0)}^0\},\ldots,I_m^k:=\{j_1^k,\ldots,j_{\mathrm{card}(I_m^k)}^k\}$ we note,

$$\begin{aligned}&\langle\Theta_0|\Phi_{I_m^0}\wedge\Psi_0\rangle\cdots\langle\Theta_k|\Phi_{I_m^k}\wedge\Psi_k\rangle\\&\quad:=\sum_l c_{m,l}\langle\Theta_0|\phi_{j_1^0}\wedge\cdots\wedge\phi_{j_{\mathrm{card}(I_m^0)}^0}\wedge\Psi_0\rangle\cdots\langle\Theta_k|\phi_{j_1^k}\wedge\cdots\wedge\phi_{j_{\mathrm{card}(I_m^k)}^k}\wedge\Psi_k\rangle.\end{aligned} \tag{71}$$

By Eq. (69), we have

$$\begin{aligned}\langle\Phi_0\wedge\cdots\wedge\Phi_k|\Phi_0\wedge\cdots\wedge\Phi_k\rangle&=\langle\Phi_0\otimes\cdots\otimes\Phi_k|\mathcal{Y}^{[k]}(\Phi_0\wedge\cdots\wedge\Phi_k)\rangle\\&=\Sigma_{I_m^l}\ \rho_{I_0^0,\ldots,I_k^0,\ldots,I_0^k,\ldots,I_k^k}\langle\Phi_0|\Phi_{I_0^0}\wedge\cdots\wedge\Phi_{I_k^0}\rangle\cdots\langle\Phi_k|\Phi_{I_0^k}\wedge\cdots\wedge\Phi_{I_k^k}\rangle,\end{aligned}$$

where the sum extends over all partitions

$$\bigsqcup_{l\in\{0,\ldots,k\}} I_m^l=\left\{1+\sum_{j=0}^{m-1} i_j,\ldots,\sum_{j=0}^{m} i_j\right\},$$

for $m=0,\ldots,k$, and where $\rho_{I_0^0,\ldots,I_k^0,\ldots,I_0^k,\ldots,I_k^k}$ is the signature of the permutation reordering the sequence obtained by concatenation $(I_0^0//\cdots//I_k^0//\cdots//I_0^k//\cdots//I_k^k)$, in increasing order.

Now because the scalar product is zero between functions of different number of particles, the nonzero terms of the sum must not only satisfy, $\Sigma_{l=0}^k\mathrm{card}(I_m^l)=i_m$, $\forall m\in\{0,\ldots,k\}$, but also, $\Sigma_{m=0}^k\mathrm{card}(I_m^l)=i_l$, $\forall l\in\{0,\ldots,k\}$. We simply note, $\Sigma'_{I_m^l}$, the previous summation on the I_m^l with this additional restriction. We terminate our calculation by using again Eq. (69) and expanding the iterated coproduct, $\mathcal{Y}^{[k]}$, in terms of another set of partitions, J_m^l, we obtain

$$\begin{aligned}\langle \Phi_0 \wedge \cdots \wedge \Phi_k | \Phi_0 \wedge \cdots \wedge \Phi_k \rangle &= \Sigma'_{I_m^l} \Sigma'_{J_m^l} \rho_{I_0^0,\ldots,I_k^0,\ldots,I_0^k,\ldots,I_k^k} \rho_{J_0^0,\ldots,J_k^0,\ldots,J_0^k,\ldots,J_k^k} \langle \Phi_{J_0^0} | \Phi_{I_0^0} \rangle \cdots \langle \Phi_{J_0^k} | \Phi_{I_k^0} \rangle \cdots \\ &\times \langle \Phi_{J_k^0} | \Phi_{I_0^k} \rangle \cdots \langle \Phi_{J_k^k} | \Phi_{I_k^k} \rangle, \end{aligned} \tag{72}$$

where the complex conjugate of the notation defined in Eq. (71) has been used for the sums over the J_m^l, so that the notation encapsulates the summation,

$$\sum_{\substack{l_0,\ldots,l_k \\ l'_0,\ldots,l'_k}} c^*_{0,l_0} \cdots c^*_{k,l_k} c_{0,l'_0} \cdots c_{k,l'_k}.$$

IV. CANONICAL FORMS OF AN *n*-FERMION WAVE FUNCTION

So far we have dealt with general wave functions of the whole Hilbert space. The expansion Eq. (39) of an n-fermion wave function was completely arbitrary, that is to say, we did not impose any orthogonality condition on the spin orbitals, nor did we exclude linear dependencies from occurring in the expansion.

The physics does not depend upon the choice of the spin orbitals used to expand the wave function, however for practical purposes certain choices are more advantageous than others. In the present section, we propose constraints to reduce the arbitrariness of the expansion Eq. (39). These constraints are based on algebraic concepts which, in general, admit a physical interpretation. The resulting expansions have interesting properties for numerical calculations.

A. Miscellaneous definitions

Definition 12 (rank of a wave function): For any $\Phi \in \wedge\mathcal{H}$ the rank of Φ, $r[\Phi]$, is the least element k of $\mathbb{N} \cup \{+\infty\}$, such that,

$$\exists \mathcal{F} \subseteq \mathcal{H},\ \dim \mathcal{F} = k \ \text{ and } \ \Phi \in \wedge\mathcal{F},$$

where $\dim \mathcal{F}$ *is the dimension of the Hilbert subspace $\mathcal{F}$, and where $\wedge\mathcal{F}$ is identified to a subspace of $\wedge\mathcal{H}$ in a natural way.*

For the sake of simplicity and because we have in view numerical applications, from now on we only consider wave functions of finite rank, however most results could be extended to completely general wave functions.

Definition 13 (depth of a wave function): For any $\Phi \in \wedge^n\mathcal{H}$ the depth of Φ, $d[\Phi]$, is the largest integer k, such that, $\exists \Psi_1 \in \wedge^{p_1}\mathcal{H},\ldots,\exists \Psi_k \in \wedge^{p_k}\mathcal{H}$, with $p_1,\ldots,p_k$ non-negative integers, allowing us to express Φ in the form

$$\Phi = \Psi_1 \wedge \cdots \wedge \Psi_k. \tag{73}$$

Definition 14 (length of a wave function): For any $\Phi \in \wedge^n\mathcal{H}$ the length of Φ, $l[\Phi]$, is the least element k of $\mathbb{N} \cup \{+\infty\}$, such that, $\exists \Psi_1 \in \wedge^n\mathcal{H},\ldots,\exists \Psi_k \in \wedge^n\mathcal{H}$, with $\Psi_1,\ldots,\Psi_k$ SC functions, allowing us to express Φ in the form

$$\Phi = \Psi_1 + \cdots + \Psi_k. \tag{74}$$

In the next sections, we exploit the concepts of rank, depth and length of a wave function to cast a wave function into a simpler and less arbitrary form.

B. Internal spin orbital expansion

By Definition 12, the vector subspace, $\mathcal{F}$, of dimension $r[\Psi]$, associated with a wave function Ψ, is the smallest subspace of $\mathcal{H}$ allowing us to express Ψ. It is precisely the 1-internal space,

denoted by $\mathcal{I}^1[\Psi]$, defined in Sec. III F. Its determination allows the expansion of a given wave function, Ψ, with the least possible number of spin orbitals. The importance of the expansion in terms of internal spinorbitals has already been emphasized and taken advantage of in Refs. 26 and 27. Here we present a new algorithm for reexpanding a wave function in terms of a set of internal spin orbitals suggested by Hopf algebra techniques.

1. Determination of the internal space

An alternative definition of the 1-internal space, or simply the ''internal space,'' is the following.

Definition 15: Let $\Psi \in \wedge^n\mathcal{H}$. The internal space of Ψ is the vector space

$$\mathcal{I}^1[\Psi] := \{\phi \in \wedge^1\mathcal{H}, \exists \Phi \in \wedge^{n-1}\mathcal{H}, \Phi \hookleftarrow \Psi = \phi\}. \tag{75}$$

Notice that the substitution of 1 by p in Eq. (75) gives an alternative definition of the p-internal space, $\mathcal{I}^p[\Psi]$. Potential applications of the p-internal spaces have been proposed in Ref. 16.

The definition, Eq. (75), gives rise to a simple method for computing the internal space: Choose a basis $(\Phi_i)_{i\in B}$ of $\wedge^{n-1}\mathcal{H}$ (possibly adapted to the structure of Ψ, so that in general choosing a suitable subset of the basis will be enough) and compute the set $\{\Phi_i \hookleftarrow \Psi\}_i$. The result is a set of generators of the internal space, from which a basis set can be extracted.

Let us give an example. Consider a system of five spin-$\frac{1}{2}$ fermions whose wave function is expanded in 16 single configuration functions, which are themselves constructed out of 12 orthonormal spin orbitals (six of spin α, $\phi_1^\alpha,\ldots,\phi_6^\alpha$, and six of spin β, $\phi_1^\beta,\ldots,\phi_6^\beta$),

$$\begin{aligned}\Psi = \tfrac{1}{4}\{&\phi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta+\phi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta+\phi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta\\
&+\phi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta+\phi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta\\
&+\phi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta+\phi_2^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta\\
&+\phi_2^\alpha\wedge\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta+\phi_2^\alpha\wedge\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta+\phi_2^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta\\
&+\phi_2^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_2^\alpha\wedge\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta+\phi_2^\alpha\wedge\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta\\
&+\phi_2^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta\}.\end{aligned} \tag{76}$$

Let us compute, for example, the spin orbital ϕ obtained by evaluating $\Phi \hookleftarrow \Psi$, where $\Phi = \phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta$. By definition of the interior product, this amounts to extracting the remaining fifth spin orbital out of the exterior products containing Φ as a factor, and then combining them linearly by using the expansion coefficients of Ψ. Only two SC in the development of Ψ have to be taken into account, namely, $\phi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta$ and $\phi_2^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta$. We get therefore, $\phi = \phi_1^\alpha + \phi_2^\alpha$. For each Φ running over a basis set of 4-fermion SC functions, a similar calculation, gives either zero or an internal spin orbital. In fact, since Ψ contains neither ϕ_5^β nor ϕ_6^β, only the subset of the functions Φ which do not contain these spin orbitals, need to be considered. Standard linear algebra techniques permit one to eliminate the linear dependencies in the set of internal spin orbitals so-obtained, and if needed, to orthonormalize the set. In our pedagogical example, the following set of eight spin orbitals is an orthonormal basis of the internal space, $\{\psi_1^\alpha,\psi_1^\beta,\phi_3^\alpha,\phi_3^\beta,\phi_4^\alpha,\phi_4^\beta,\phi_5^\alpha,\phi_6^\alpha\}$, where we have set

$$\psi_1^\alpha := \frac{1}{\sqrt{2}}(\phi_1^\alpha + \phi_2^\alpha), \quad \psi_1^\beta := \frac{1}{\sqrt{2}}(\phi_1^\beta + \phi_2^\beta). \tag{77}$$

A basis of the external space, its orthocomplement, is $\{\psi_2^\alpha,\psi_2^\beta,\phi_5^\beta,\phi_6^\beta\}$, with

$$\psi_2^\alpha := \frac{1}{\sqrt{2}}(\phi_1^\alpha - \phi_2^\alpha), \quad \psi_2^\beta := \frac{1}{\sqrt{2}}(\phi_1^\beta - \phi_2^\beta). \tag{78}$$

2. Re-expansion of the wave function

In practical applications, the bottleneck of numerical codes expressing a wave function in terms of a, possibly symmetry-adapted, basis set of internal spin orbitals, is not the determination of the internal basis set itself, but the re-expansion of the wave function in the new basis.[27] Here, we describe a simple, original algorithm to express explicitly the wave function in the basis of spin orbitals of the internal space.

One of the main advantages of this algorithm is that it does not require the determination of the whole transformation unlike the re-expansion algorithm of Refs. 28 and 29. One or several re-expansion coefficients can be specifically targeted to take advantage of, for example, the knowledge of the population of the internal basis functions and thereby eliminate the less populated functions as in Ref. 27.

The steps followed by the algorithm are

(1) Compute $\mathcal{Y}_{1,n-1}(\Psi)$.
(2) Obtain a (non-necessarily orthogonal) basis $(\phi_1,\ldots,\phi_k)$ of the internal space, $\mathcal{I}^1[\Psi]$, and target an element $\Phi_I = \phi_{i_1}\wedge\ldots\wedge\phi_{i_n}$ of the basis, $(\Phi_J)_{J\in\mathcal{P}_{k,n}}$, it induces in $\wedge^n\mathcal{I}^1[\Psi]$.
(3) Form the linear combination of the components of $\mathcal{Y}_{1,n-1}(\Psi)$, obtained in the first step, corresponding to the term, $\phi_{i_1}\otimes\Psi_{i_1}$, of the decomposition,
$$\mathcal{Y}_{1,n-1}(\Psi) = \sum_{i=1}^{k} \phi_i\otimes\Psi_i .$$
(4) Compute $\mathcal{Y}_{1,n-2}(\Psi_{i_1})$.
(5) Form the linear combination of the components of $\mathcal{Y}_{1,n-2}(\Psi_{i_1})$, obtained in the previous step, corresponding to the term, $\phi_{i_2}\otimes\Psi_{i_1,i_2}$, of the decomposition,
$$\mathcal{Y}_{1,n-2}(\Psi_{i_1}) = \sum_{i=1}^{k} \phi_i\otimes\Psi_{i_1,i} .$$
(6) Proceed iteratively up to the computation of $\mathcal{Y}_{1,0}(\Psi_{i_1,\ldots,i_{n-1}})$.
(7) Form the linear combination of the components of $\mathcal{Y}_{1,0}(\Psi_{i_1,\ldots,i_{n-1}})$, obtained in the previous step, corresponding to the term, $\phi_{i_n}\otimes\Psi_{i_1,\ldots,i_n}$, of the decomposition,
$$\mathcal{Y}_{1,0}(\Psi_{i_1,\ldots,i_{n-1}}) = \sum_{i=1}^{k} \phi_i\otimes\Psi_{i_1,\ldots,i_{n-1},i} .$$

$\Psi_{i_1,\ldots,i_n}$ is the targeted re-expansion coefficient.

This assertion follows from the following three properties:

(i) Eq. (65), which shows that
$$\Psi = \frac{1}{n!}\mathcal{X}^{[n-1]}\circ\mathcal{Y}^{[n-1]}_{1,\ldots,1}(\Psi). \tag{79}$$

(ii) The fact that by construction,
$$\mathcal{Y}^{[n-1]}_{1,\ldots,1}(\Psi) = \sum_{i_1,\ldots,i_n} \Psi_{i_1,\ldots,i_n}\phi_{i_1}\otimes\cdots\otimes\phi_{i_n}. \tag{80}$$

(iii) The property, $\forall\,\sigma\in\mathcal{S}_n$,
$$\Psi_{\sigma(i_1),\ldots,\sigma(i_n)} = (-1)^{|\sigma|}\Psi_{i_1,\ldots,i_n} \tag{81}$$
allowing one to show that, after taking the iterated exterior product in Eq. (79), a factor $n!$ arises from the summation in the right-hand side of Eq. (80).

The latter property is a direct consequence of the co-commutativity of the coproduct, that is, the fact that the coproduct is invariant under the twisting map,

$$T\circ\mathcal{Y}=\mathcal{Y}. \tag{82}$$

As a remark, we note that the algorithm can easily take advantage of the symmetry of the system, if we demand in the second step that the internal basis set be symmetry-adapted.

Let us illustrate the algorithm on the example of the preceding section and compute the coefficient of, say $\psi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\psi_1^\beta\wedge\phi_3^\beta$. We obtain successively

$$\mathcal{Y}_{1,4}(\Psi)=\psi_1^\alpha\otimes\frac{1}{2\sqrt{2}}(\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta+\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta+\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta+\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta$$
$$+\phi_3^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_3^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta+\phi_4^\alpha\wedge\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_4^\alpha\wedge\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta)+\cdots.$$

Denoting by $\Psi_{1\alpha}$ the 4-fermion function associated to ψ_1^α above,

$$\mathcal{Y}_{1,3}(\Psi_{1\alpha})=\phi_3^\alpha\otimes\frac{1}{2\sqrt{2}}(\phi_5^\alpha\wedge\phi_1^\beta\wedge\phi_3^\beta+\phi_6^\alpha\wedge\phi_1^\beta\wedge\phi_4^\beta+\phi_5^\alpha\wedge\phi_2^\beta\wedge\phi_3^\beta+\phi_6^\alpha\wedge\phi_2^\beta\wedge\phi_4^\beta)+\cdots.$$

Denoting by $\Psi_{1\alpha,3\alpha}$ the 3-fermion function associated to ϕ_3^α above,

$$\mathcal{Y}_{1,2}(\Psi_{1\alpha,3\alpha})=\phi_5^\alpha\otimes\frac{1}{2\sqrt{2}}(\phi_1^\beta\wedge\phi_3^\beta+\phi_2^\beta\wedge\phi_3^\beta)+\cdots.$$

Denoting by $\Psi_{1\alpha,3\alpha,5\alpha}$ the 2-fermion function associated to ϕ_5^α above,

$$\mathcal{Y}_{1,1}(\Psi_{1\alpha,3\alpha,5\alpha})=\psi_1^\beta\otimes\tfrac{1}{2}\phi_3^\beta.$$

We immediately conclude that the targeted coefficient, denoted $\Psi_{1\alpha,3\alpha,5\alpha,1\beta,3\beta}$, is $\frac{1}{2}$ and that all the other expansion coefficients containing the indexes $(1\alpha,3\alpha,5\alpha)$ are zero. Proceeding in the same manner for the other coefficients, we obtain the expansion of Ψ,

$$\Psi=\tfrac{1}{2}\{\psi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_5^\alpha\wedge\psi_1^\beta\wedge\phi_3^\beta+\psi_1^\alpha\wedge\phi_3^\alpha\wedge\phi_6^\alpha\wedge\psi_1^\beta\wedge\phi_4^\beta+\psi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_6^\alpha\wedge\psi_1^\beta\wedge\phi_3^\beta$$
$$+\psi_1^\alpha\wedge\phi_4^\alpha\wedge\phi_5^\alpha\wedge\psi_1^\beta\wedge\phi_4^\beta\}, \tag{83}$$

which is, as expected, much simpler than the initial expansion, Eq. (76).

C. Factorization of a wave function

The interest of an expansion achieving the depth (Definition 13), is to factorize the fermionic wave function into functions of a lesser number of particles. Note that in our definition we do not require the latter functions to be strongly orthogonal, that is to be such that their 1-internal spaces are mutually orthogonal. Therefore there is a difference between the expansion we are investigating and those based on the group functions of McWeeny.[30]

Factorized wave functions arise naturally in quantum mechanics when certain particles are ''frozen'' in a calculation, for example, the core electrons of an atom or a molecule. However, a general wave function may well admit a hidden factorization.

In the present state of the art, little is known about the general problem of finding the depth of a wave function. However, the particular case of the factorization of a wave function by a SC function is fully understood. The solution follows from Ref. 31 [Lemma B, p.234].

Proposition 16: Any linearly independent set of spin orbitals $\psi_1,\ldots,\psi_k$ belonging to the kernel of the creation operator, $\vec{\mathcal{X}}_\Psi$, factorizes Ψ.

That is to say, $\Psi = \psi_1 \wedge \ldots \wedge \psi_k \wedge \Psi'$, where Ψ' can be computed explicitely as

$$\Psi' = \frac{(\psi_1 \wedge \ldots \wedge \psi_k) \leftarrow \Psi}{\langle \psi_1 \wedge \ldots \psi_k | \psi_1 \wedge \ldots \psi_k \rangle}. \tag{84}$$

In particular, the factorization is optimal (that is, k is maximal), if and only if $k = \dim \mathrm{Ker}(\vec{\mathcal{X}}_\Psi)$.

The physical content of the proposition is clear: a spin orbital is fully occupied in the wave function if and only if creating a fermion in this spin orbital gives 0.

For example, if Ψ is the wave function of Eq. (83), let

$$\psi = x_1^\alpha . \psi_1^\alpha + x_1^\beta . \psi_1^\beta + x_3^\alpha . \phi_3^\alpha + x_3^\beta . \phi_3^\beta + x_4^\alpha . \phi_4^\alpha + x_4^\beta . \phi_4^\beta + x_5^\alpha . \phi_5^\alpha + x_6^\alpha . \phi_6^\alpha$$

be an arbitrary internal spin orbital and write

$$\vec{\mathcal{X}}_\Psi(\psi) = \Psi \wedge \psi = 0.$$

The exterior product can be expanded in terms of the 6-fermion SC basis functions of $\wedge^6 \mathcal{I}^1[\Psi]$ induced by the internal basis set. Then, the linear independency of the 6-fermion SC basis functions gives

$$x_3^\alpha = x_3^\beta = x_4^\alpha = x_4^\beta = x_5^\alpha = x_6^\alpha = 0.$$

We deduce that, Ker $(\vec{\mathcal{X}}_\Psi)$ is spanned by $(\psi_1^\alpha, \psi_1^\beta)$, and, in fact,

$$\Psi = \tfrac{1}{2} \psi_1^\alpha \wedge \psi_1^\beta \wedge (\phi_3^\alpha \wedge \phi_5^\alpha \wedge \phi_3^\beta + \phi_3^\alpha \wedge \phi_6^\alpha \wedge \phi_4^\beta + \phi_4^\alpha \wedge \phi_6^\alpha \wedge \phi_3^\beta + \phi_4^\alpha \wedge \phi_5^\alpha \wedge \phi_4^\beta). \tag{85}$$

Note that the method could have been applied before the extraction of the internal spin orbitals, on the expansion, Eq. (76), where the factorization is less obvious. Note also that, with $k = n$, the number of fermions, the proposition provides a necessary and sufficient condition for a wave function to be condensable into a SC function.

D. Decomposition into a direct sum

The potential usefulness of the concept of length of a wave function is obvious. Obtaining the shortest expansion of a given wave function would concentrate the physical information contained in it and facilitate both its retrieval and its interpretation. However, it is still an unsolved mathematical problem, except in very specific cases.[32,33] The only general result is for the case where the wave function admits a direct sum decomposition. Therefore we will only develop this particular case.

An n-fermion wave function Ψ admits a direct sum decomposition if it can be written as a sum of k SC functions Ω_i,

$$\Psi = \sum_{i=1}^{k} \Omega_i, \tag{86}$$

and if the dimension of its internal space, $\mathcal{I}^1[\Psi]$ is $n.k$,

$$\dim \mathcal{I}^1[\Psi] = n.k, \tag{87}$$

or equivalently, if

$$\Omega_1 \wedge \cdots \wedge \Omega_k \neq 0. \tag{88}$$

Note that the definition in Ref. 31 rewritten in Ref. 16 is not correct, because the condition $\forall i \neq j, \Omega_i \wedge \Omega_j \neq 0$ is not sufficient to have Eq. (87).

It is clear that a wave function satisfying Eqs. (86) and (87) is of length k. However, a function of length k does not have to satisfy Eq. (87).

A general method to first diagnose the existence of a direct sum decomposition and then to derive it, has been proposed in Ref. 31. It relies on the observation, that there exists a direct sum decomposition Eq. (86) if and only if there are exactly k groups of n $(n-1)$-fermion functions of the form $\psi \hookleftarrow \Psi$, $\psi \in \mathcal{H}$, such that (i) Each $(n-1)$-fermion functions can be condensed into a SC function. (ii) In each group the internal spaces of the $(n-1)$-fermion functions are included in the same n-dimensional vector space. (iii) The $n.k$ $(n-1)$-fermion functions are linearly independent.

The application of the method to the part of the 3-fermion wave function inside the parentheses in Eq. (85) has been treated in details in Ref. 16. Here, we only give the final result. The 3-fermion wave function does admit a direct sum decomposition after the following change of basis set:

$$\psi_3^\alpha := \frac{1}{\sqrt{2}}(\phi_3^\alpha + \phi_4^\alpha), \quad \psi_3^\beta := \frac{1}{\sqrt{2}}(\phi_3^\beta + \phi_4^\beta), \tag{89}$$

$$\psi_4^\alpha := \frac{1}{\sqrt{2}}(\phi_3^\alpha - \phi_4^\alpha), \quad \psi_4^\beta := \frac{1}{\sqrt{2}}(\phi_3^\beta - \phi_4^\beta), \tag{90}$$

$$\psi_5^\alpha := \frac{1}{\sqrt{2}}(\phi_5^\alpha + \phi_6^\alpha), \quad \psi_5^\beta := \frac{1}{\sqrt{2}}(\phi_5^\beta + \phi_6^\beta), \tag{91}$$

$$\psi_6^\alpha := \frac{1}{\sqrt{2}}(\phi_5^\alpha - \phi_6^\alpha), \quad \psi_6^\beta := \frac{1}{\sqrt{2}}(\phi_5^\beta - \phi_6^\beta). \tag{92}$$

In this new basis, Eq. (85) can be rewritten as

$$\Psi = \tfrac{1}{2}\psi_1^\alpha \wedge \psi_1^\beta \wedge (\psi_3^\alpha \wedge \psi_5^\alpha \wedge \psi_3^\beta + \psi_4^\alpha \wedge \psi_6^\alpha \wedge \psi_4^\beta). \tag{93}$$

Wave functions admitting a direct sum decomposition arise naturally in physics when several resonant structures are needed to describe a quantum system. For example, the Weinbaum wave function for He_2^+,[34] can be cast in the form of the 3-fermion wave function in parentheses in Eq. (93). More general cases where a direct sum factors the wave function, like in Eq. (93) but possibly more complex, have been given in Ref. 26. There are molecules where three electrons share two centers like the nitroxide π-radicals or the HCO_2 σ-radical. Of course, resonant structures involving more than three fermions are common too.

An important remark is that a direct sum decomposition of a n-fermion wave function is unique if $n>2$. So, Eq. (93) is not only much simpler than the initial expansion, Eq. (76) but it is also less arbitrary. In fact, this expansion can be considered as a canonical form for this wave function since the (normalized) spin orbitals have been uniquely determined up to sign factors, if we do not allow the mixing of α- and β-spin orbitals, or up to a linear transformation of the spin orbitals of the SC function factorizing the wave function in the general case.

V. CONCLUSION

In this paper, we have developed the Hopf algebra formalism for the fermionic Fock space. This formalism is immediately applicable to many fields of physics, ranging from solid state physics, quantum chemistry, and atomic physics, where it allows a formulation of all electronic structure problems, to nuclear physics, where it applies to nucleons.

More precisely, we have introduced new algebraic tools which facilitate the investigation of theoretical and numerical problems in quantum physics. The simple proof of the Carlson and

Keller theorem and the derivation of Sasaki's formula main corollary, that we have obtained, illustrate the advantages of our formalism: The tedious action of the symmetric group is eliminated and many numerical and sign factors are encapsulated in the formalism.

Among the new tools, the co-product defined in Sec. II, and its iterated version defined in Sec. III, arguably stand out. They not only pave the way for a natural generalization of many results based on the partitioning of a wave function into blocks, but they also allow a numerical calculation to be broken into successive steps. This has been exploited in an original, parallelizable, algorithm to re-expand a wave function in the least possible number of spin orbitals.

However, if the re-expansion of a wave function in a set of internal spin orbitals is now a well-understood mathematical issue, the problem of extracting the spin orbitals that achieve the (minimal) length of a wave function remains, except in the particular case where the wave function admits a direct sum decomposition. This is a longstanding problem and probably a hard one.

In contrast, the concept of the depth of a wave function is new and the problem of factorizing a wave function by more general functions than SC functions has not received much attention. Progress on this issue could be very important for physical applications because such a factorization allows a reduction in the dimensionality of many calculations and is the basis for geminal or more generally, group function methods. We hope to report new results on this topics in forthcoming studies.

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Scale calculus and the Schrödinger equation

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(Received 7 July 2003; accepted 8 August 2003)

This paper is twofold. In a first part, we extend the classical differential calculus to continuous nondifferentiable functions by developing the notion of scale calculus. The scale calculus is based on a new approach of continuous nondifferentiable functions by constructing a one parameter family of differentiable functions $f(t,\epsilon)$ such that $f(t,\epsilon)\to f(t)$ when ϵ goes to zero. This led to several new notions as representations: fractal functions and ϵ-differentiability. The basic objects of the scale calculus are left and right quantum operators and the scale operator which generalizes the classical derivative. We then discuss some algebraic properties of these operators. We define a natural bialgebra, called quantum bialgebra, associated with them. Finally, we discuss a convenient geometric object associated with our study. In a second part, we define a first quantization procedure of classical mechanics following the scale relativity theory developed by Nottale. We obtain a nonlinear Schrödinger equation via the classical Newton's equation of dynamics using the scale operator. Under special assumptions we recover the classical Schrödinger equation and we discuss the relevance of these assumptions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1618923]

INTRODUCTION

The origin of the fundamental incompatibility between *quantum mechanics* and Einstein's *general relativity* lies in the microscopic geometric structure of space–time. As pointed out by Greene,[27] Feynman,[25] Cohen-Tannoudji and Spiro (Ref. 14, p. 131) and others, space–time is no more a *differentiable* manifold at the *atomic* scale, contrary to the assumption of general relativity.

From this fact, at least two theories have been constructed:

(i) the *string theory*, which implies a dimensional extension of space–time by allowing a closed dimension at the Planck scale;
(ii) the *scale relativity theory* developed by Nottale,[37] which gives up the Einstein's assumption of the differentiability of space–time by considering what he calls a *fractal space–time*, which can be interpreted as a scale dependant nondifferentiable manifold. He then extends Einstein's relativity principle to scale, and develop the *scale relativity principle*.

In this article, we explore this second alternative.

Nottale[37] has studied what are the consequences of the abandon of the differentiability of space–time. This problem is difficult, in particular because the mathematical foundations of such a theory are not yet constructed. For example, Nottale asserts that there exists an ''infinity of geodesics on a fractal space–time.'' This sentence is difficult to understand because we do not know what is a fractal space–time. (We refer to Ref. 20 for a first definition of a fractal manifold and a discussion of the special scale relativity theory.) Even if we identify this set to a nondifferentiable manifold, we do not know what is the sense of ''geodesic.'' As a consequence, we restrict our attention to a far simpler problem, namely the consequences of the loss of differentiability of a given trajectory. A first approach is to consider that only *space* is a nondifferentiable manifold

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and to take the variable t as an absolute variable. As a consequence, trajectories of quantum particles are nondifferentiable curves parametrized by the time variable t. In this case, we have at least the following two consequences.

(i) By Lebesgues theorem,[46] the *length* of a nondifferentiable curve Γ is *infinite*. What does it means from the physical view point ? That given a parameter $\epsilon>0$, which has the sense of a resolution, the lenght L_ϵ of the curve constructed by connecting small arcs of length ϵ on points of Γ, goes to infinity when ϵ goes to zero. As a consequence, the role of ϵ is now fundamental as L_ϵ loses any sense when ϵ is going to zero, contrary to usual differentiable curves where ϵ is only a parameter of precision and L_ϵ goes to a fixed constant L.

Nottale then introduce *fractal functions*, which are resolution (or scale) dependent functions $f(x,\epsilon)$, which converge to nondifferentiable functions, and a (*renormalization like*) differential equation satisfied by L_ϵ, called a *scale law*, which gives the behavior of $f(x,\epsilon)$ when ϵ goes to zero.

(ii) The derivative along the curve has no sense. Nottale introduces a complex operator, which he calls the *scale derivative*. It takes into account the mean-backward and mean-forward derivative along the curve.

Using these tools, he gives an informal derivation of the *Schrödinger equation* from the classical *Newtonian equation of dynamics*, via a quantization procedure which follows from an extension of Einstein's relativity principle called the *scale relativity principle*.

In this paper, we develop a mathematical framework in which we can explicit the quantization procedure, which we call the *scale quantization procedure*.

The plan of the paper is as follows.

In Part I, we define a natural extension of Leibniz differential calculus which can be used on nondifferentiable functions in order to precise points (i) and (ii). We introduce the *Scale calculus*, which formalizes the concept of ϵ-differentiability. In particular, we define an operator called the *scale difference operator*, which is the rigorous mathematical counterpart of Nottale's scale derivative.

In Part II, we define the scale quantization procedure. We give a precise definition of the quantization map, which allows us to associate to the classical Newtonian equation of dynamics a quantized analog. This analog has the form of a generalized nonlinear Schrödinger equation. We then discuss how to obtain the classical Schrödinger equation.

PART I

I. SCALE CALCULUS

A. Introduction

Nondifferentiable functions, and more generally nondifferentiable manifolds, become more and more important in many part of mathematics and physics, like Brownian motion,[24] and quantum mechanical path by Feynman and Hibbs.[26] Despite many works, our understanding of nondifferentiable functions is nonsatisfactory.

A great deal of effort has been devoted to generalize, as long as possible, the classical differential calculus of Leibniz and Newton. This leads to a different kind of fractional calculus (Riemann, Liouville, Weyl,...). All this fractional calculus is based on a pure analytic generalization of the Cauchy formula. As a consequence, and despite their intrinsic interest, they are difficult to interpret (in particular, from the geometrical view point).

The aim of this paper is to introduce a set of ideas, coming from physics, in order to renew our approach to nondifferentiable functions.

In physic, the nondifferentiability is not studied by itself. On the contrary, this is the effect of nondifferentiability with respect to a differentiable model which is being sought. For example, as explained by Greene (Ref. 27, Chap. 5), in *superstring* theory one is led to a new vision of

space–time because the space–time, at the scale of atoms, cannot be considered differentiable at all, as in the general relativity scheme. Here, one focuses on fluctuations with respect to a differentiable character.

Moreover, one usually does not have access via measurement, to the nondifferentiable object (function, manifold), but to an almost everywhere differentiable model of it. This explains also the previous remark: by measure we obtain a differentiable model, and we must see, when the precision of measure increases, if there is no two strong fluctuations with respect to this model. For a differentiable process, the fluctuations decrease. In the case of a nondifferentiable process, one expects larger and larger fluctuations.

This point of view leads to several new concepts: the representation of continuous nondifferentiable functions, fractals functions and ϵ-differentiability. The idea is to associate to each continuous nondifferentiable function $f(t)$, a one parameter family of differentiable function $f(t,\epsilon)$ such that $f(t,\epsilon)\to f(t)$ when ϵ goes to zero. The next step is to give a useful criterion, which says that $f(t,\epsilon)$ is a "good" model for the function f. An important notion is then the minimal resolution which is, more or less, the precision under which, one cannot use a differentiable model without lacking many features of the underlying function f. We then define quantum derivatives and the scale derivative, which reflects the nondifferentiable character of the underlying function f.

We discuss algebraic properties of quantum derivatives, and the scale derivative. These operators act on the set of continuous real valued functions, denoted by C^0. They are first introduced in Ref. 4 in order to discuss the derivation of Schrödinger's equation from the classical Newton's equation of dynamics using Nottale's scale relativity theory.[37]

In this paper, we construct a natural structure of bialgebra, called quantum bialgebra, using specific properties of quantum derivatives. The quantum algebra can be considered as a small deformation of a classical Hopf algebra. Although we are close to a problem related to quantum groups and quasitriangular Hopf algebras introduced by Drinfeld,[22] we stress that quantum bialgebras are new.

There is no natural bialgebra structure associated with the scale derivative. This follows from the lack of a natural composition rule for scale operators that we define in this paper.

We also discuss the natural geometric object associated with a continuous nondifferentiable function. It turns out that this geometric object is, in the simplest case, the product of a differentiable curve Γ by a two points set $A=\{a,b\}$, so $M\times A$. This is a simple example of a noncommutative space studied by Connes,[15] as a preliminary to his noncommutative model of the standard model.

B. About nondifferentiable functions

The aim of this section is to develop a rigorous mathematical understanding of the idea of fluctuation with respect to a differentiable model for continuous nondifferentiable functions.

1. Representation theory and fractals functions

Here, we introduce two dual notions: the representation of nondifferentiable functions and fractal functions. Representations are well suited to develop a mathematical understanding of a nondifferentiable function based on differentiable functions. Fractal functions take their origin in physical problems.

In the following, we denote by C^0 the set of continuous real valued functions, and by C^1 the set of differentiable real valued functions.

Definition 2.1: Let $f\in C^0$; a representation of f is a one parameter family of operator S_ϵ, defined by

$$S_\epsilon:\begin{array}{ccc} C^0 & \to & C^1 \\ f & \mapsto & S_\epsilon(f)=f_\epsilon, \end{array} \tag{I.1}$$

and such that the differentiable functions $f_\epsilon \in C^1$ converge, in C^0-topology, toward f when ϵ goes to zero.

A basic example is obtained by approximating f by mean functions f_ϵ defined by $f_\epsilon(t) = (1/2\epsilon)\int_{t-\epsilon}^{t+\epsilon} f(s)ds$.

More generally, we can consider a *smoothing function* $\Phi(s;t,\epsilon)$ depending on two parameters, t and ϵ, satisfying the normalization

$$\int_{-\infty}^{\infty} \Phi(s;t,\epsilon)ds = 1. \tag{I.2}$$

For any continuous function, we define a representation by

$$f_\epsilon(t) = \int_{-\infty}^{\infty} \Phi(s;t,\epsilon)f(s)ds. \tag{I.3}$$

In practice, we never have access to f. An idea is to define f via a family of functions which are not functionally dependent of f like in (I.1). We are led to the notion of *fractal functions*, first introduced by Nottale[37] (see also Ref. 18).

Definition 2.2: A fractal function is a parametrized function of the form $f(t,\epsilon)$, depending on $\epsilon > 0$, such that the following occurs.

(i) *For all $\epsilon > 0$, the function $f(t,\epsilon) \in C^1$, except at a finite number of points,*
(ii) *There exists an everywhere nondifferentiable function $f(t)$ such that $f(t,\epsilon)$ converges to $f(t)$ when ϵ goes to zero.*

The main difference between Definitions 2.1 and 2.2 is that for fractal functions, one usually does not know an explicit form of the limit function f, we only require an existence result. Moreover, the set of functions $f(t,\epsilon)$ does not refer to the limit f in its definition, which is closest to the *measurement* process in physical experiment.

2.1.1. Examples of fractal functions: Nottale's functions and iteration of affine systems. The basic example of fractal functions is *Nottale's functions* introduced in Ref. 37:

For all $\epsilon > 0$, and for all $0 < \mu < \epsilon$,

$$x(t,\epsilon) = \int \Phi_{\epsilon,\mu}(t,y)x(y,\mu)dy, \tag{I.4}$$

where $\Phi_{\epsilon,\mu}(x,y)$ is a differentiable function such that

$$\int_{-\infty}^{\infty} \Phi_{\epsilon,\mu}(x,y)dy = 1, \ \ \forall\, x \in \mathbf{R}, \tag{I.5}$$

called a smoothing function.

Definition 2.3: Let $\Phi_{\epsilon,\mu}$ be a smoothing function satisfying (I.5). We denote by $\mathcal{N}(\Phi_{\epsilon,\mu})$, and we call Nottale's set associated with $\Phi_{\epsilon,\mu}$, the set of functions defined by (I.4).

We refer to Ref. 18 for basic properties of this set of functions, in particular for a useful equivalence relation.

An interesting example of fractal functions for which the limit function is not explicit is given by the iteration of *affine systems*.[46]

An affine map in $\mathbb{R}^2$, with a coordinates system (x,y), is a map of the form

$$F\begin{pmatrix} x \\ y \end{pmatrix} = M\begin{pmatrix} x \\ y \end{pmatrix} + T, \tag{I.6}$$

where M is a 2×2 matrix and T is a translation vector.

An *affine system* is given by

(i) a positive integer $N \geqslant 2$;

(ii) $N+1$ points of $\mathbb{R}^2$, $A=A_1,\ldots,A_{N+1}=B$. We denote $A_i=(x_i,y_i)$, $x_1=a$, $x_{N+1}=b$. We assume that

$$a=x_1<x_2<\cdots<x_{N+1}=b;$$

(iii) N affine map $F_1,\ldots,F_N$ such that

$$F_i(AB)=A_iA_{i+1}.$$

We denote by F the map defined by

$$F(E)=\bigcup_{i=1}^{N} F_i(E). \tag{I.7}$$

Let z_0 be the affine function on $[a,b]$ whose graph Γ_0 is the segment AB. The image $\Gamma_1=F(\Gamma)$ is the graph of a continuous function, which is affine. For all n, we define the continuous function z_n whose graph is $\Gamma_n=F(\Gamma_{n-1})$. Following Ref. 46, p. 175, the sequence of functions $(z_n)_{n\in\mathbb{N}}$ converge uniformly to a continuous function z_∞ such that $F(\Gamma_\infty)=\Gamma_\infty$.

2. ϵ-differentiability and minimal resolution

a. Minimal resolution: Formal idea. In our point of view, nondifferentiability is always studied via a one parameter familly of differentiable functions f_ϵ. A basic question is the following.

When ϵ goes to zero, can we find a value ϵ_0 such that for $\epsilon>\epsilon_0$, we can assume that the limit function is differentiable and for $\epsilon>\epsilon_0$, we are sure that the limit function is nondifferentiable?

It is equivalent to ask if the nondifferentiable character of a function can be detected via its approximation.

If we can find a quantity $\epsilon(f)$ of this kind, then we call it *minimal resolution*. It is the best order of approximation under which nondifferentiable effects must be taken into account.

In the following we give two ways in order to defined a minimal resolution, by taking two different effects of nondifferentiability.

b. First approach. A basic properties of differentiable functions is that the quantities,

$$\nabla_+^\epsilon f(t)=\frac{f(t+\epsilon)-f(t)}{\epsilon} \quad \text{and} \quad \nabla_-^\epsilon f(t)=\frac{f(t)-f(t-\epsilon)}{\epsilon}, \tag{I.8}$$

keep sense when ϵ goes to zero and are equal.

As a consequence, the following quantity,

$$a_\epsilon f(t)=\left|\frac{f(t+\epsilon)+f(t-\epsilon)-2f(t)}{\epsilon}\right|, \tag{I.9}$$

converges to zero when ϵ goes to zero.

The underlying idea is that the two representations of a function f, given by the forward and backward mean function, defined as

$$f_\epsilon^+(t)=(1/2\epsilon)\int_t^{t+\epsilon} f(s)ds \qquad \text{and} \qquad f_\epsilon^-(t)=(1/2\epsilon)\int_{t-\epsilon}^{t} f(s)ds, \tag{I.10}$$

respectively, must have derivatives which coincide when ϵ goes to zero.

This remark allows us to introduce the following notion of ϵ-h-differentiability.

Definition 2.4: Let $h>0$ be a given real number. A function $f\in C^0$ is said to be ϵ-h-differentiable at point t, if

$$a_\epsilon f(t) < h. \tag{I.11}$$

We can detect the nondifferentiable character of a function by investigating its ϵ-h-differentiability. Precisely, we define the notion of minimal resolution:

Definition 2.5: Let $h>0$ be a given real number and $f \in C^0$. The h-minimal resolution of f at point t, denoted $\epsilon(f,h)(t)$ is defined as $\inf_\epsilon \{a_\epsilon f(t) < h\}$.

Of course, if for a given h, the h-minimal resolution is nonzero, then f is nondifferentiable.

Remark 2.1: The reverse is wrong, as proved by the following example.

Let $f:\mathbb{R}\to\mathbb{R}$ be a function defined by

$$f: \begin{cases} t\cos(1/t), & \text{if } t \neq 0 \\ 0, & \text{if } t = 0. \end{cases} \tag{I.12}$$

This function is derivable for all $t\neq 0$. Then, we have $\epsilon(f,h)(t)=0$ for all $t\neq 0$. This function is not derivable at $t=0$. However, we have $a_\epsilon(f,h)(0)=0$ for all $\epsilon>0$ by parity. As a consequence, $\epsilon(f,h)=0$, even if f is not derivable on $\mathbb{R}$.

For all $\alpha \in]0,1[$, we denote by C^α the set of continuous real valued functions, defined on $[0,1]$ such that the quantity

$$|f|_\alpha = \sup_{0\leqslant x\neq y\leqslant 1} \frac{|f(x)-f(y)|}{|x-y|^\alpha} \tag{I.13}$$

is finite (Hölderian functions of order α). Then, we have the following lemma.

Lemma 2.1: Let $0<\alpha<1$ and $f \in C^\alpha$. For all $t \in]0,1[$, and all $h>0$, the h-minimal resolution of f at point t satisfies

$$\epsilon(f,h)(t) \leqslant \left(\frac{h}{2|f|_\alpha}\right)^{1/\alpha - 1}. \tag{I.14}$$

Remark 2.2: In this example, the minimal resolution depends on $|f|^\alpha$. As a consequence, for a quantum mechanical path, we expect that the minimal resolution depends on the momentum of the particle. This is indeed the case in Nottale's theory,[37] where the minimal resolution is related to the de Broglie length of the particle.

A global order of h-minimal resolution can be defined.

Definition 2.6: Let $h>0$ be given and $f \in C^0$. The h-minimal resolution of f, denoted $\epsilon(f,h)$, is defined by $\epsilon(f,h)=\sup_{t\in \mathcal{D}f}\epsilon(f,h)(t)$, where $\mathcal{D}f$ is the definition domain of f.

In this definition it is important to take the sup of h-minimal resolution of f at point t. As a consequence, if f is differentiable on a small set of point, the h-minimal resolution is however nonzero.

Remark 2.3: We have $\epsilon(f+c,h)=\epsilon(f,h)$ for all $c\in\mathbb{R}$. But, we have $\epsilon(\lambda f,h)\neq\epsilon(f,h)$ for all $\lambda\neq 1$, contrary to the case of Ref. 4. This inequality is related to the fact that a changing momentum induce a change of regularity for the curve. A physical consequence is that the minimal resolution must depend on the momentum.

The connection to representation theory is done through the backward and forward mean functions, f_ϵ^σ, $\sigma=\pm$, introduced before. Indeed, backward and forward mean functions are differentiable functions. They can be used as a classical representation of a given continuous function f. However, if f admits a nonzero h minimal resolution, this means that these functions are not sufficient to capture the complete local behavior of f as long as $\epsilon<\epsilon(f,h)$. Of course, this notion depends on h. In physical problems, the constant h must correspond to a universal constraint, like the Heisenberg constraint in quantum mechanics.

c. Order of divergence. The previous quantity $a_\epsilon f(t)$ gives a criterion distinguishing differentiable and nondifferentiable functions based on the fact that in some case, the left and right

derivative of a nondifferentiable function (when they exist) are different. Of course, the general case is far more complicated. A complete characterization of differentiability is given by the following.

Let f be a continuous real function. We denote

$$D^{\sigma}f(t)=\lim \sup_{\epsilon\to 0^{\sigma}} \frac{f(t+\epsilon)-f(t)}{\epsilon}, \quad \text{and} \quad D_{\sigma}f(t)=\lim \inf_{\epsilon\to 0^{\sigma}} \frac{f(t+\epsilon)-f(t)}{\epsilon}, \quad \sigma=\pm. \tag{I.15}$$

These quantities are always well defined and belong to $\overline{\mathbb{R}}$. By Refs. 45, 31, p. 319, we know that f is differentiable at point t if and only if

$$D^{+}f(t)=D^{-}f(t)=D_{+}f(t)=D_{-}f(t)\in\mathbb{R}. \tag{I.16}$$

By Ref. 45, we know that the set of continuous functions for which the left and right derivative exists and are distinct is of zero measure. By considering the set of nondifferentiable functions, we then deduce that the left and right derivative does not exist on a set of full measure. More precisely, we have two cases: either $D^{\sigma}f(t)$ and $D_{\sigma}f(t)$ exist but are different, or these quantities diverge with ϵ going to zero, for $\sigma=\pm$.

We denote by $\Delta_{\mu}^{\sigma}f(t)$, $\sigma=\pm$ the quantity

$$\Delta_{\mu}^{\sigma}f(t)=\sigma\frac{f(t+\sigma\mu)-f(t)}{\mu}, \quad \sigma=\pm, \tag{I.17}$$

and for $\epsilon>0$, we denote

$$\overline{d}_{\epsilon}^{\sigma}f(t)=\sup_{\mu\leqslant\epsilon}\Delta_{\mu}^{\sigma}f(t), \underline{d}_{\epsilon}^{\sigma}f(t)=\inf_{\mu\leqslant\epsilon}\Delta_{\mu}^{\sigma}f(t). \tag{I.18}$$

A better object to measure the loss of differentiability is the following quantity:

$$A_{\epsilon}f(t)=\begin{matrix}\inf_{\epsilon>0}\{|\overline{d}_{\epsilon}^{+}f(t)-\underline{d}_{\epsilon}^{+}f(t)|<h, |\overline{d}_{\epsilon}^{-}f(t)-\underline{d}_{\epsilon}^{-}f(t)|<h,\\ (1-1_{D^{+}=D_{+}})(1-1_{D^{-}=D_{-}})|\overline{d}_{\epsilon}^{+}f(t)-\overline{d}_{\epsilon}^{-}f(t)|<h,\end{matrix} \tag{I.19}$$

when ϵ goes to zero.

In the Hölderian case, i.e., $f\in C^{\alpha}$, $0<\alpha<1$, this quantity diverges as $\epsilon^{\alpha-1}$. As a consequence, a possible extension of the notion of minimal resolution can be obtained by the following.

Definition 2.7: Let $h>0$; we call minimal resolution the following quantity:

$$\epsilon(f,h)=\inf_{\epsilon>0}\{A_{\epsilon}f(t)<h\}. \tag{I.20}$$

When the left and right derivatives exist, or diverge, the previous quantity reduces to the minimal resolution defined in Sec. I B 6. However, this quantity can distinguish the case where left and right derivatives are not defined but not infinite.

3. Scale law

For an everywhere nondifferentiable function f, the length L_{ϵ} of the graph of the mean function f_{ϵ} goes to infinity when ϵ goes to 0. Of course, this property cannot be used as a definition of an everywhere nondifferentiable function. We can find curves which are rectifiable with infinite length (see Ref. 6). We want to quantify this divergence. A first idea is to find a differential equation which gives the behavior of L_{ϵ} with respect to ϵ like in (Refs. 6, 18). However, this is difficult because L_{ϵ} is not differentiable with respect to ϵ in general. In this section, we define a less rigid definition of scale law and we discuss its properties.

a. Definition: Let f be an everywhere nondifferentiable continuous function on the interval $I=[0,1]$. For $\epsilon>0$, we denote by f_ϵ the mean function associated with f on I, and $\mathcal{L}_\epsilon$ the length of its graph.

Definition 2.8: We say that f satisfies a scale law if there exist functions $l_\epsilon>0$ and $L_\epsilon>0$ such that

$$l_\epsilon \leqslant \mathcal{L}_\epsilon \leqslant L_\epsilon, \tag{I.21}$$

satisfying

$$\mathcal{L}_\epsilon = O(l_\epsilon), \quad \mathcal{L}_\epsilon = O(L_\epsilon), \tag{I.22}$$

and for which there exists a function $E:\mathbb{R}\to\mathbb{R}$, such that

$$\frac{dl_\epsilon}{d\ln\epsilon} = E(l_\epsilon, \ln\epsilon), \frac{dL_\epsilon}{d\ln\epsilon} = E(L_\epsilon, \ln\epsilon). \tag{I.23}$$

The function E is called a scale law.

Of course, when one knows a scale law of f, we deduce a speed of drift for $\mathcal{L}_\epsilon$.

Basic examples of scale laws are given by the following:

(i) For $a>0$, $E(x,t)=a$,

(ii) For $b>0$, $E(x,t)=bx$.

For (i), we obtain graph with logarithmic drift of order $|a|\ln(1/\epsilon)$. For (ii), we obtain the classical power law drift of order $1/\epsilon^b$.

Using this notion, we are led to two different kind of problems.

(i) Let E be a given function. Find the set of function $\mathcal{E}(E)$ such that for all $f\in\mathcal{E}(E)$, a scale law of f is E.

(ii) Let $\mathcal{E}$ be a given set of functions. Find, if it exists, a scale law for each $f\in\mathcal{E}$.

The first problem is equivalent to estimate a given class of functions by the speed of drift of $\mathcal{L}_\epsilon$. This point is difficult and discussed in Ref. 6.

The second one is more natural and discussed in the following.

b. Scale law of Hölderian functions. We first define an important class of continuous functions.

Definition 2.9: We denote by $H^\alpha(c,C)$ the set of real valued continuous functions f such that for all $\epsilon>0$ sufficiently small, and $|t-t'|<\epsilon$, we have

$$c\epsilon^\alpha \leqslant |f(t)-f(t')| \leqslant C\epsilon^\alpha. \tag{I.24}$$

The set H^α corresponds to continuous functions which are Hölder and inverse Hölder of exponent α.

Example: Let $0<\alpha<1$ and $g(t)$ be the function of period 1 defined on $[0,1]$ by

$$g(t)=\begin{cases} 2t, & \text{if } 0\leqslant t\leqslant 1/2 \\ 2-2t, & \text{if } 1/2\leqslant t\leqslant 1. \end{cases} \tag{I.25}$$

The Knopp or Takagi function, defined by

$$K(t)=\sum_{n=0}^{\infty} 2^{-n\alpha} g(2^n t), \tag{I.26}$$

belongs to H^α (see Ref. 46, Sec. 13.1).

We use notations from Definition 2.8.

Theorem 2.1: *Let $0<\alpha<1$ and $f\in H^\alpha(c,C)$ defined on an open interval $U\subset\mathbb{R}$ such that $I=[0,1]\subset U$. For all $\epsilon>0$, we define*

$$l_\epsilon = \epsilon^{\alpha-1}\sqrt{\epsilon^{2(1-\alpha)}+c^2}, L_\epsilon = \epsilon^{\alpha-1}\sqrt{\epsilon^{2(1-\alpha)}+C^2}. \tag{I.27}$$

A scale law for f is then given by

$$E(y,t) = (\alpha-1)(y-1/y). \tag{I.28}$$

Proof: We have

$$\mathcal{L}_\epsilon = \frac{1}{2\epsilon}\int_0^1 \sqrt{4\epsilon^2+(f(x+\epsilon)-f(x-\epsilon))^2}\,dx. \tag{I.29}$$

As $f \in H^\alpha$, we have

$$4c^2\epsilon^{2\alpha} \leqslant (f(x+\epsilon)-f(x-\epsilon))^2 \leqslant 4C^2\epsilon^{2\alpha}. \tag{I.30}$$

As a consequence, we obtain

$$\epsilon^{\alpha-1}\sqrt{\epsilon^{2(1-\alpha)}+c^2} \leqslant \mathcal{L}_\epsilon \leqslant \epsilon^{\alpha-1}\sqrt{\epsilon^{2(1-\alpha)}+C^2}. \tag{I.31}$$

We deduce

$$l_\epsilon \leqslant \mathcal{L}_\epsilon \leqslant L_\epsilon, \tag{I.32}$$

for ϵ sufficiently small.

By differentiating L_ϵ with respect to ϵ, we obtain

$$\frac{dL_\epsilon}{d\epsilon} = \frac{\alpha-1}{\epsilon}\left[L_\epsilon - \frac{1}{L_\epsilon}\right]. \tag{I.33}$$

Using

$$\frac{dL_\epsilon}{d\ln\epsilon} = \epsilon\frac{dL_\epsilon}{d\epsilon}, \tag{I.34}$$

we obtain the scale function $E(y,t) = (\alpha-1)(y-1/y)$. We verify that l_ϵ satisfies the same differential equations. □

The previous result is best analyzed in term of the new variables,

$$x_\epsilon = 1/l_\epsilon, \quad \mathcal{X}_\epsilon = 1/\mathcal{L}_\epsilon, \quad X_\epsilon = 1/L_\epsilon. \tag{I.35}$$

When ϵ goes to 0, we have x_ϵ, X_ϵ and $\mathcal{X}_\epsilon$ which go to 0. Moreover, the scale law for these new functions is

$$\frac{dx}{dt} = (1-\alpha)(x-x^3). \tag{I.36}$$

Indeed, by making the change of variables $x = 1/y$ in the scale law,

$$\frac{dy}{dt} = (\alpha-1)(y-1/y), \tag{I.37}$$

and using the relation

$$\frac{dx}{dt} = -(1/y^2)\frac{dy}{dt}, \tag{I.38}$$

we obtain the result.

The classical linearization theorem of Poincaré (Refs. 2 and 30) allows us to find, in a neighborhood of $x=0$, an analytic change of variables $z=h(x)$, such that the differential equation (I.36) is transformed into

$$\frac{dz}{dt}=(1-\alpha)z. \tag{I.39}$$

The set of Hölderian functions H^{α} induces, up to analytic changes of variables, the linear scale law (I.39).

Remark 2.4: In Galilean scale relativity, the set of functions which admit a linear scale law allows us to define the Djinn variable (see Ref. 18, Sec. 3.2.5 and Sec. 3.3).

c. Nonuniform Hölderian functions. In this section, we consider nonuniform Höderian functions.

Definition 2.10: Let $\alpha(t):\mathbb{R}\to]0,1[$. *We denote by* $H^{\alpha(.)}$ *the set of continuous Hölderian functions satisfying, for all* $h>0$ *sufficiently small,*

$$ch^{\alpha(t)}<|f(t+h)-f(t)|<Ch^{\alpha(t)}, \tag{I.40}$$

where $c>0$, $C>0$ *are constants.*

For $H^{\alpha(.)}$ functions, we have not been able to derive a scale law. We then introduce a weak notion.

Definition 2.11: We say that f *admits weak-scale laws, if there exists* l_{ϵ} *and* L_{ϵ} *such that*

$$l_{\epsilon}\leqslant\mathcal{L}_{\epsilon}\leqslant L_{\epsilon}, \tag{I.41}$$

satisfying

$$\mathcal{L}_{\epsilon}=O(l_{\epsilon}),\quad \mathcal{L}_{\epsilon}=O(L_{\epsilon}), \tag{I.42}$$

and for which we can find two functions: $E_{-}:\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ *and* $E_{+}:\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ *such that*

$$\frac{dl_{\epsilon}}{d\ln\epsilon}=E_{-}(l_{\epsilon},\ln\epsilon),\ \frac{dL_{\epsilon}}{d\ln\epsilon}=E_{+}(L_{\epsilon},\ln\epsilon). \tag{I.43}$$

For all $\epsilon>0$, we define

$$\alpha_i(\epsilon)=\alpha(i/\epsilon i+1/\epsilon), \tag{I.44}$$

with $i=0,\ldots,[1/\epsilon]$, where $[x]$ denotes the integer part of x.

We define

$$\gamma(\epsilon)=\min_{i=0,\ldots,[1/\epsilon]}\alpha_i(\epsilon),\beta(\epsilon)=\max_{i=0,\ldots,[1/\epsilon]}\alpha_i(\epsilon). \tag{I.45}$$

Theorem 2.2: *Let* $f\in H^{\alpha(.)}$. *For all* $\epsilon>0$ *sufficiently small we assume that the exponents (I.45) are differentiable functions with respect to* ϵ. *Then,* f *admits for weak-scale laws,*

$$E_{-}(x,t)=(1-\alpha-t\gamma')(x-x^3),\ E_{+}(x,t)=(1-\alpha-t\beta')(x-x^3). \tag{I.46}$$

C. Scale calculus

In Ref. 4, we introduce the notion of *quantum derivatives*. In this section, we give a less rigid definition, which allows us to discuss more easily algebraic properties of these operators.

1. Left and right quantum difference operators

Let $h>0$ be given. If f possesses a nonzero h-minimal resolution, then for $\epsilon<\epsilon(f,h)$, one must take into account the nondifferentiable character of f with respect to its forward and backward mean representations. A possible way to do it is to say that the backward and forward derivatives of f at ϵ carry different information on the local behavior of f. The idea of quantum derivatives formalize this idea.

Definition 3.1: Let $h>0$, and f be a continuous, real valued function.

If $\epsilon(f,h)>0$, for all $\epsilon(f,h)>\epsilon>0$, we define left and right quantum difference operators of f at point t, the quantities

$$\nabla_+^\epsilon f(t)=\frac{f(t+\epsilon)-f(t)}{\epsilon},\ \nabla_-^\epsilon f(t)=\frac{f(t)-f(t-\epsilon)}{\epsilon}, \tag{I.47}$$

respectively.

If $\epsilon(f,h)=0$, and f is differentiable then

$$\Delta_+^0 f(t)=\Delta_-^0 f(t)=f'(t). \tag{I.48}$$

Remark 3.1: (1) We can give a more rigid definition of quantum derivatives by fixing the ϵ to be the minimal resolution of the function considered for a given $h>0$.

(2) By remark 2.1, we cannot extend the definition of the left and right quantum operators when $\epsilon(f,h)=0$ in order to cover the set of nondifferentiable function with zero minimal resolution.

2. The scale difference operator

The scale difference operator, first introduced in Ref. 4 following Nottale's work,[37] is intended to summarize the information given by a quantum difference operator, needed to perform the local analysis of a given nondifferentiable function.

Definition 3.2: Let $h>0$, and f be a continuous function such that $\epsilon(f,h)\geqslant\epsilon>0$. The ϵ-scale difference operator of f at point t is a complex operator, denoted by $\Box_\epsilon/\Box t$, defined by

$$\frac{\Box_\epsilon f}{\Box t}(t)=\frac{1}{2}(\nabla_+^\epsilon f(t)+\nabla_-^\epsilon f(t))-i\frac{1}{2}(\nabla_+^\epsilon f(t)-\nabla_-^\epsilon f(t)),\ i^2=-1. \tag{I.49}$$

When $\epsilon=0$, and f is differentiable, we have the following useful property.

Lemma 3.1 (Gluing): Let f be a differentiable function. Then, we have

$$\frac{\Box f}{\Box t}=\frac{df}{dt}. \tag{I.50}$$

Moreover, if we denote by $f_\epsilon(t)$ the mean function $f_\epsilon(t)=(1/2\epsilon)\int_{t-\epsilon}^{t+\epsilon}f(s)ds$, we have that

$$\mathrm{Re}\left(\frac{\Box_\epsilon f}{\Box t}(t)\right)=(f_\epsilon)'(t), \tag{I.51}$$

where Re denotes the real part of a complex number. The imaginary part of $\Box_\epsilon f/\Box t$ is the fluctuation of the forward mean function with respect to the backward mean function.

3. Main result

We denote by H^α the set of real valued functions which are Hölder and inverse Hölder of exponent α, which means that for all ϵ sufficiently small, and $|t'-t|\leqslant\epsilon$, there exists $c>0$ and $C>0$, such that

$$c\epsilon^{\alpha} \leqslant |f(t')-f(t)| \leqslant C\epsilon^{\alpha}. \tag{I.52}$$

An important theorem, from the point of view of the scale relativity, is the following.

Theorem 3.1: *Let $h>0$, $f(x,t)$ be a C^n function, $x(t)$ a continuous function such that $\epsilon(x,h)>0$. Then, for $\epsilon(x,h) \geqslant \epsilon > 0$, ϵ sufficiently small, we have*

$$\frac{\Box_{\epsilon} f(x(t),t)}{\Box t} = \frac{\partial f}{\partial t} + \sum_{j=1}^{n} \frac{1}{j!} \frac{\partial^j f}{\partial x^j}(x(t),t)\epsilon^{j-1} a_{\epsilon,j}(t) + o(\epsilon^{1/n}), \tag{I.53}$$

where

$$a_{\epsilon,j}(t) = \tfrac{1}{2}[((\Delta_+^{\epsilon}x)^j - (-1)^j(\Delta_-^{\epsilon}x)^j) - i((\Delta_+^{\epsilon}x)^j + (-1)^j(\Delta_-^{\epsilon}x)^j)]. \tag{I.54}$$

The proof follows from the following lemma.

Lemma 3.2: Let $f(x,t)$ be a real valued function of class C^{n+1}, $n \geqslant 3$, and let $X(t)$ be a continuous real valued function of class $H^{1/n}$. For ϵ sufficiently small, the right and left derivatives of $f(X(t),t)$ are given by

$$\nabla_{\sigma}^{\epsilon} f(X(t),t) = \frac{\partial f}{\partial t}(X(t),t) + \sigma \sum_{i=1}^{n} \frac{1}{i!} \frac{\partial^i f}{\partial x^i}(X(t),t)\epsilon^{-1}(\sigma\epsilon\nabla_{\sigma}^{\epsilon}X(t))^i + o(\epsilon^{1/n}), \tag{I.55}$$

for $\sigma = \pm$.

For $n=2$, we obtain the so-called Itô formula:

$$\nabla_{\sigma}^{\epsilon} f(X(t),t) = \frac{\partial f}{\partial t}(X(t),t) + \frac{\partial f}{\partial x}(X(t),t)\nabla_{\sigma}^{\epsilon}X(t) + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(X(t),t)\epsilon(\nabla_{\sigma}^{\epsilon}X(t))^2 + o(\epsilon^{1/2}). \tag{I.56}$$

Proof: This follows from easy computations. First, we remark that, as $X(t) \in H^{1/n}$, we have $|\epsilon\nabla_{\sigma}^{\epsilon}X(t)| = o(\epsilon^{1/n})$. Moreover,

$$f(X(t+\epsilon),t+\epsilon) = f(X(t)+\epsilon\nabla_{+}^{\epsilon}X(t),t+\epsilon). \tag{I.57}$$

By the previous remark, and the fact that f is of order C^{n+1}, we can make a Taylor expansion up to order n with a controlled remainder:

$$f(X(t+\epsilon),t+\epsilon) = f(X(t),t) + \sum_{k=1}^{n} \frac{1}{k!} \sum_{i+j=k} (\epsilon\nabla_{+}^{\epsilon}X(t))^i \epsilon^j \frac{\partial^k f}{\partial^i x\, \partial^j t}(X(t),t) + o((\epsilon\nabla_{+}^{\epsilon}X(t))^{n+1}). \tag{I.58}$$

As a consequence, we have

$$\epsilon\nabla_{+}^{\epsilon} f(X(t),t) = \sum_{k=1}^{n} \frac{1}{k!} \sum_{i+j=k} (\epsilon\nabla_{+}^{\epsilon}X(t))^i \epsilon^j \frac{\partial^k f}{\partial^i x\, \partial^j t}(X(t),t) + o((\epsilon\nabla_{+}^{\epsilon}X(t))^{n+1}). \tag{I.59}$$

By selecting terms of order less or equal to one in ϵ on the rhs of this equation, we obtain

$$\epsilon\nabla_{+}^{\epsilon} f(X(t),t) = \epsilon\left[\frac{\partial f}{\partial t}(X(t),t) + \sum_{i=1}^{n} \frac{1}{i!} \frac{\partial^i f}{\partial x^i}(X(t),t)\epsilon^{-1}(\epsilon\nabla_{+}^{\epsilon}X(t))^i\right] + o(\epsilon^2\nabla_{+}^{\epsilon}X(t)). \tag{I.60}$$

Dividing by ϵ, we obtain the lemma. □

4. The complex case

In Sec. III, we need to apply the scale operator to *complex valued* functions. We extend the definition of $\square_\epsilon/\square t$ in order to cover this case.

In the following, if $z\in\mathbb{C}$, we denote by Re(z) and Im(z), the real and imaginary part of z.

Definition 3.3: Let $h>0$ and $\mathcal{C}(t)$ be a complex valued function. We denote $\mathcal{C}(t)=\mathcal{C}_r(t)+i\mathcal{C}_m(t)$, where $\mathcal{C}_r(t)=\mathrm{Re}\,\mathcal{C}(t)$ and $\mathcal{C}_m(t)=\mathrm{Im}\,\mathcal{C}(t)$. We define $\square_\epsilon\mathcal{C}/\square t$ by

$$\frac{\square_\epsilon\mathcal{C}}{\square t}=\frac{\square_\epsilon\mathcal{C}_r}{\square t}+i\frac{\square_\epsilon\mathcal{C}_m}{\square t}, \tag{I.61}$$

for $0<\epsilon<\min(\epsilon(\mathcal{C}_r,h),\epsilon(\mathcal{C}_m,h))$.

Remark 3.2: The extension of the scale calculus to complex valued functions is not trivial (as it mixes complex terms in a complex operator).

We then have the following.

Lemma 3.3: Let $h>0$ and $C(x,t):\mathbb{R}\times\mathbb{R}\to\mathbb{C}$ be a C^n complex valued function. Let $x(t)$ be a continuous function such that $\epsilon(x,h)>0$. We denote $\mathcal{C}(t)=C(x(t),t)$. Then, for $0<\epsilon\leqslant\epsilon(x,h)$ sufficiently small, we have

$$\frac{\square_\epsilon\mathcal{C}}{\square t}=\frac{\partial C}{\partial t}+\frac{\square_\epsilon x}{\square t}\frac{\partial C}{\partial x}+\sum_{j=2}^{n}\frac{1}{j!}a_{\epsilon,j}(t)\frac{\partial^j C}{\partial x^j}\epsilon^{j-1}+o(\epsilon^{1/n}), \tag{I.62}$$

where

$$a_{\epsilon,j}(t)=\tfrac{1}{2}[(\Delta_+^\epsilon x)^j-(-1)^j(\Delta_-^\epsilon x)^j]-i\,\tfrac{1}{2}[(\Delta_+^\epsilon x)^j+(-1)^j(\Delta_-^\epsilon x)^j],\quad j=2,\ldots,n. \tag{I.63}$$

D. Algebraic properties of quantum difference operators

In the following, we denote by C^0 the set of continuous real valued functions.

Lemma 4.1: For all $\epsilon>0$, and all $f\in C^0$ and $g\in C^0$, we have

(i) $\nabla_\sigma^\epsilon(f+g)=\nabla_\sigma f+\nabla_\sigma g$, $\sigma=\pm$;
(ii) *For all* $\lambda\in\mathbb{R}$, $\nabla(\lambda f)=\lambda\nabla_\sigma f$, $\sigma=\pm$.

The proof is straightforward and left to the reader.

Our main goal is to compare quantum derivatives to classical derivatives. The main property of classical derivatives is the so called *Leibniz rule*, which says that, $(fg)'=f'g+fg'$. In our case, we have a more complicated formula.

Lemma 4.2: For all $\epsilon>0$, and all $f\in C^0$, $g\in C^0$, we have for $\sigma=\pm$,

$$\nabla_\sigma^\epsilon(fg)(x)=\nabla_\sigma^\epsilon f(x)g(x)+f(x)\nabla_\sigma^\epsilon g(x)+\sigma\epsilon\nabla_\sigma^\epsilon f(x)\nabla_\sigma^\epsilon g(x). \tag{I.64}$$

Proof: Easy computations lead to the following formulas:

$$\nabla_+^\epsilon(fg)(x)=\nabla_+^\epsilon f(x)g(x+\epsilon)+f(x)\nabla_+^\epsilon g(x),$$

$$\nabla_-^\epsilon(fg)(x)=\nabla_-^\epsilon f(x)g(x)+f(x-\epsilon)\nabla_-^\epsilon g(x). \tag{I.65}$$

By definition of the quantum derivatives, we have

$$f(x+\epsilon)=f(x)+\epsilon\nabla_+^\epsilon f(x),\quad g(x-\epsilon)=g(x)-\epsilon\nabla_-^\epsilon g(x). \tag{I.66}$$

By replacing $f(x+\epsilon)$ and $g(x-\epsilon)$ in (I.65), we obtain (I.64). □

Of course, one can derived other formulas. However, Eq. (I.64) is the most symmetric one. Here, we give another expression.

For all ϵ, we denote by $\tau_\epsilon:C^0\to C^0$ the classical translation, defined by

$$\tau_\epsilon(f)(x)=f(x+\epsilon),\ \ \forall x. \tag{I.67}$$

We have the following lemma.

Lemma 4.3: For all ϵ, we have $\nabla^\epsilon_-\circ\tau_\epsilon=\nabla^\epsilon_+$ and $\tau_\epsilon\circ\nabla^\epsilon_\sigma=\nabla^\epsilon_\sigma\circ\tau_\epsilon$.

As a consequence, we obtain the following version of Lemma 4.2.

Lemma 4.4: For all $\epsilon>0$, and all $f\in C^0$, $g\in C^0$, we have

$$\begin{aligned}\nabla^\epsilon_+(fg)(x)&=\nabla^\epsilon_+f(x)h_\epsilon(x)+f(x)\nabla^\epsilon_-h_\epsilon(x),\\ \nabla^\epsilon_-(fg)(x)&=\nabla^\epsilon_-f(x)v_\epsilon(x)+f(x)\nabla^\epsilon_+v_\epsilon(x),\end{aligned} \tag{I.68}$$

where $h_\epsilon=\tau_\epsilon\circ g$ and $v_\epsilon=\tau_{-\epsilon}\circ g$.

In the following, we discuss what are the fundamental differences between quantum derivatives and classical derivations.

1. Derivations

We recall that an operator D on an abstract algebra $(A,.)$, is a derivation if for all $(f,g)\in A^2$, it satisfies the Leibniz relation $D(fg)=Df.g+f.Dg$. We refer to Jacobson (Ref. 32, Chap. 1, Sec. 2, pp. 7–8) for more details.

We denote by $\mathrm{Der}(A)$ the set of derivations on A. $\mathrm{Der}(A)$ is a vector space, but not an algebra. However, by posing $[D_1,D_2]=D_1D_2-D_2D_1$, the usual Lie bracket, the set $(\mathrm{Der}(A),[.,.])$ is a Lie algebra.

We denote by $\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle$ the ring of formal power series on the alphabet $\mathrm{Der}(A)$. We can define a coalgebra structure on $\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle$. We refer to Bourbaki (Ref. 9, Chap. 3) for more details about coalgebras and bialgebras.

Let $u:\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle\to\mathbb{R}$ be the homomorphism associating to each series its constant term.

For each $D\in\mathrm{Der}(A)$ we define a linear map $\Delta:\mathrm{Der}(A)\to\mathrm{Der}(A)\otimes\mathrm{Der}(A)$ by $\Delta(D)=D\otimes 1+1\otimes D$. Then, the following diagram commutes:

$$\begin{array}{ccc} A\otimes A & \overset{\Delta(D)}{\to} & A\otimes A,\\ \nu\downarrow & & \downarrow\nu\\ A & \overset{D}{\to} & A,\end{array} \tag{I.69}$$

where ν is the natural morphism defined by

$$\begin{array}{rcl}\nu: & A\otimes A & \to A,\\ & f\otimes g & \mapsto f.g.\end{array} \tag{I.70}$$

We can extend Δ such that for each $\Delta(D_1D_2)=\Delta(D_1)\Delta(D_2)$, D_1, $D_2\in\mathrm{Der}(A)$, and the usual product on $\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle\otimes\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle$, $(a\otimes b).(c\otimes d)=(ac\otimes bd)$. For each word, $D_1\cdots D_r$, we define $\Delta(D_1\cdots D_r)=\Delta(D_1)\Delta(D_2\cdots D_r)$. We then extend Δ to $\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle$ by linearity. With this definition of Δ, for each $S\in\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle$, the following diagram commutes:

$$\begin{array}{ccc} A\otimes A & \overset{\Delta(S)}{\to} & A\otimes A,\\ \nu\downarrow & & \downarrow\nu\\ A & \overset{S}{\to} & A.\end{array} \tag{I.71}$$

As a consequence, we have the following lemma.

Lemma 4.5: The triple $(\mathbb{R}\langle\langle\mathrm{Der}(A)\rangle\rangle,\Delta,u)$ is a bialgebra.

2. Quantum bialgebra

We follow the previous section on derivations.

Definition 4.1: For all $\epsilon>0$, and $\sigma=\pm$, we denote by ∇_σ^ϵ an operator acting on $C^0\otimes C^0$, where $\otimes$ is the classical tensor product, and defined by

$$\nabla_\sigma^\epsilon:\begin{array}{ccc} C^0\otimes C^0 & \to & C^0\otimes C^0, \\ f\otimes g & \mapsto & \nabla_\sigma^\epsilon f\otimes g+f\otimes\nabla_\sigma^\epsilon g+\sigma\epsilon\nabla_\sigma^\epsilon f\otimes\nabla_\sigma^\epsilon g. \end{array} \tag{I.72}$$

Let $\Omega_\epsilon=\{\nabla_+^\epsilon,\nabla_-^\epsilon\}$ be the alphabet of two letters ∇_+^ϵ and $\nabla_-^\epsilon\}$. We denote by Ω_ϵ^* the set of words $\underline{\omega}=\omega_1\ldots\omega_n$, $\omega_i\in\Omega_\epsilon$ for all $i=1,\ldots,n$, where $\omega_i\omega_j$ denote the natural composition of operators. For example, a possible word is $\nabla_+^\epsilon\nabla_-^\epsilon$.

Remark 4.1: Here we consider the alphabet of quantum operators for a fixed $\epsilon>0$. It is possible that some particular problems of scale relativity require a complete alphabet $\Omega=\{\nabla_\sigma^\epsilon,\sigma=\pm,\epsilon>0\}$.

We denote by $A_\epsilon=\mathbb{R}\langle\langle\Omega_\epsilon\rangle\rangle$ the algebra of formal power series constructed on Ω_ϵ (with its classical algebraic structure).

We can define a linear map from A_ϵ to $A_\epsilon\times_{\mathbb{R}}A_\epsilon$, denoted Δ. First, we define Δ on ∇_σ^ϵ by

$$\begin{array}{c} A_\epsilon\overset{\Delta}{\to}A_\epsilon\otimes A_\epsilon, \\ \nabla_\sigma^\epsilon\mapsto\nabla_\sigma^\epsilon\otimes I+I\otimes\nabla_\sigma^\epsilon+\sigma\epsilon\nabla_\sigma^\epsilon\otimes\nabla_\sigma^\epsilon. \end{array} \tag{I.73}$$

We have the following equality:

$$\nabla_\sigma^\epsilon\circ\nu=\nu\circ\Delta(\nabla_\sigma^\epsilon), \tag{I.74}$$

which is equivalent to the commutativity of the diagram,

$$\begin{array}{ccc} C^0\otimes C^0 & \overset{\Delta(\nabla_{\sigma'}^\epsilon)}{\to} & C^0\otimes C^0, \\ \downarrow\nu & & \downarrow\nu \\ C^0 & \overset{\nabla_\sigma^\epsilon}{\to} & C^0. \end{array} \tag{I.75}$$

We also define $\Delta(I)=I\otimes I$ in order that $I\bigcirc\nu=\nu\bigcirc\Delta(I)$.

We extend Δ to A_ϵ by linearity.

Lemma 4.6: The linear map Δ is an algebra homomorphism.

Proof: The proof is done by induction. Let ∇_σ^ϵ and $\nabla_{\sigma'}^\epsilon$ be two letters of Ω_ϵ. We have

$$\begin{aligned}\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon(fg)=&\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon f.g+f.\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon g+\nabla_\sigma^\epsilon f.\nabla_{\sigma'}^\epsilon g+\nabla_{\sigma'}^\epsilon f.\nabla_\sigma^\epsilon g+\epsilon[\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon f.\nabla_{\sigma'}^\epsilon g+\nabla_{\sigma'}^\epsilon f.\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon g\\&+\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon f.\nabla_\sigma^\epsilon g+\nabla_\sigma^\epsilon f.\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon g]+\epsilon^2\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon f.\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon g.\end{aligned} \tag{I.76}$$

As a consequence, we have

$$\begin{aligned}\Delta(\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon)=&\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon\otimes I+I\otimes\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon+\nabla_\sigma^\epsilon\otimes\nabla_{\sigma'}^\epsilon+\nabla_{\sigma'}^\epsilon\otimes\nabla_\sigma^\epsilon+\epsilon[\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon\otimes\nabla_{\sigma'}^\epsilon+\nabla_{\sigma'}^\epsilon\otimes\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon\\&+\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon\otimes\nabla_\sigma^\epsilon+\nabla_\sigma^\epsilon\otimes\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon]+\epsilon^2\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon\otimes\nabla_\sigma^\epsilon\nabla_{\sigma'}^\epsilon.\end{aligned} \tag{I.77}$$

By definition, the classical product on $A_\epsilon\otimes A_\epsilon$ is defined by the following: for all $a\otimes b$ and $c\otimes d$ in $A_\epsilon\otimes A_\epsilon$, we have

$$(a\otimes b).(c\otimes d)=ac\otimes bd. \tag{I.78}$$

An easy computation proves that

$$\Delta(\nabla_{\sigma}^{\epsilon}\nabla_{\sigma'}^{\epsilon})=\Delta(\nabla_{\sigma}^{\epsilon})\Delta(\nabla_{\sigma'}^{\epsilon}). \tag{I.79}$$

By induction and linearity, we obtain the lemma. □

We define an algebra homomorphism from A_{ϵ} to $\mathbb{R}$, denoted by u, by associating to each formal power series its constant term.

With $u:A_{\epsilon}\to\mathbb{R}$ and $\Delta:A_{\epsilon}\to A_{\epsilon}\otimes A_{\epsilon}$, we define a coalgebra structure on A_{ϵ}.

Lemma 4.7: The triple (A_{ϵ},Δ,u) *is a coalgebra.*

Moreover, as u and Δ are homomorphisms, we obtain the stronger result.

Lemma 4.8: The triple (A_{ϵ},Δ,u) *is a bialgebra.*

We have not found a natural graduation on this bialgebra.

Remark 4.2: (1) It will be interesting to discuss the possible relation to quantum groups introduced by Drinfeld (Refs. 22, 23) and quasi-triangular Hopf algebra. We introduce the natural commutativity involution,

$$\tau:\begin{array}{ccc} A_{\epsilon}\otimes A_{\epsilon} & \to & A_{\epsilon}\otimes A_{\epsilon}, \\ a\otimes b & \mapsto & b\otimes a. \end{array} \tag{I.80}$$

Let $\Delta^{\mathrm{op}}=\tau\circ\Delta$. *The map* τ *is an algebra automorphism of* $A_{\epsilon}\otimes A_{\epsilon}$ *and the following diagram commutes*:

$$\begin{array}{ccc} A_{\epsilon} & \overset{\Delta}{\to} & A_{\epsilon}\otimes A_{\epsilon}, \\ \mathrm{id}_{A_{\epsilon}}\downarrow & & \downarrow\tau \\ A_{\epsilon} & \overset{\Delta^{\mathrm{op}}}{\to} & A_{\epsilon}\otimes A_{\epsilon}. \end{array} \tag{I.81}$$

If (A_{ϵ},Δ,u) *is a quasitriangular algebra, then, following Ref. 43, there exists an invertible element of* $A_{\epsilon}\otimes A_{\epsilon}$ *such that*

$$\Delta^{\mathrm{op}}(a)=R\Delta(a)R^{-1}, \quad \text{for all} \quad a\in A_{\epsilon}. \tag{I.82}$$

In our case, we easily have $\Delta^{\mathrm{op}}=\Delta$ *so that* (A_{ϵ},Δ,u) *so that R is trivial.*

(2) A natural idea is to consider the quantum bialgebra as a "deformation" of the classical Hopf algebra associated with derivations. The word "deformation" must be taken with care, because a notion of deformation for Hopf algebra already exists and it is not clear if this is a good one to consider here.

(3) There is no natural extension of the quantum bialgebra in order to take into account the scale derivative. The basic problem being that the scale derivative is a complex valued operator on real valued functions. Then, we have no natural composition of these operators.

3. A remark on Rieman–Liouville fractional calculus and the local fractional calculus

A basic way to deal with nondifferentiable functions is to use *fractional calculus*. As an example, one can consider the classical (left and right) *Riemann–Liouville derivative*, defined by

$$D_z^{\alpha}f(x)=\frac{\Gamma(\alpha+1)}{2\pi i}\int_0^{z^+} f(t)(t-z)^{-\alpha-1}\,dt, \tag{I.83}$$

for $\alpha\in\mathbb{C}\backslash\{-1,-2,\dots\}$. The Riemann–Liouville derivative is not at all a *derivation* on the algebra of continuous functions. Indeed, one has (see Ref. 40)

$$D_z^{\alpha}(uv)=\sum_{n=0}^{\infty}\left(\begin{array}{c}\alpha\\ n\end{array}\right)D_z^{\alpha-n}uD_z^{n}v. \tag{I.84}$$

Moreover, this operator, which is a direct analytic generalization of the Cauchy formula does not have a clear geometrical interpretation, despite recent advances (see Ref. 3).

In Ref. 5, we have obtain, following a previous work of Kolvankar and Gangal,[29] a derivation, called the (left and right) *local fractional derivative*, by *localizing* the (left and right) Riemann–Liouville derivative.

We have proven that this localization takes a simple form.

Definition 4.2: The right and left local fractional derivative of f at point x_0 of order α is defined by

$$\lim_{x\to x_0^+}\frac{f(x)-f(x_0)}{(x-x_0)^{\alpha}}\quad\text{and}\quad\lim_{x\to x_0^-}\frac{f(x_0)-f(x)}{(x_0-x)^{\alpha}}, \tag{I.85}$$

respectively.

We have introduce the fractional derivative of f at point x_0 by collecting the two quantities $d_+^{\alpha}f(x_0)$ and $d_-^{\alpha}f(x_0)$ in a single quantity, i.e.,

$$d^{\alpha}f(x_0)=\tfrac{1}{2}(d_+^{\alpha}f(x_0)+d_-^{\alpha}f(x_0))+i\,\tfrac{1}{2}(d_+^{\alpha}f(x_0)+d_-^{\alpha}f(x_0)). \tag{I.86}$$

Moreover, we obtain a clear geometrical meaning by connecting the exponent α of differentiation to the local maximal Hölder regularity of the curve.

However, such a derivative has important problems. First, there exists no *integral operator* contrary to the Riemann–Liouville fractional derivative where there exists the Riemann–Liouville integral. Moreover, the set of points on which the local fractional derivative is nonzero is, in most of the cases, trivial, i.e., of zero measure. Precisely, we have the following theorem.

Theorem 4.1: *The fractional differential equations of the form $d^{\alpha}f(x)=a(x)+ib(x)$, $0<\alpha<1$, where $a(x)$ and $b(x)$ are continuous functions such that there exists $x_0\in\mathbb{R}$ such that $|a(x_0)|\neq|b(x_0)|$ have no solutions*.

This theorem solves a conjecture of Ref. 7. It must be pointed out that the condition $|a(x_0)|\neq|b(x_0)|$ is generic.

Proof: We have $d_+^{\alpha}f(x)=c(x)$ and $d_-^{\alpha}f(x)=d(x)$, where $c(x)=a(x)+b(x)$ and $d(x)=a(x)-b(x)$ are continuous functions. By assumption, we have $c(x_0)\neq 0$ and $d(x_0)\neq 0$.

Let us assume that $c(x_0)>0$ [the case where $c(x_0)<0$ is similar]. By continuity, there exits $\epsilon>0$ such that for all x in the open interval $I_{\epsilon}(x_0)=]x_0-\epsilon,x_0+\epsilon[$, we have $d^{\alpha}f(x)>0$. Two cases must be considered: (i) $d_-^{\alpha}f(x_0)>0$ and (ii) $d_-^{\alpha}f(x_0)<0$.

In case (i), we define an open interval $J_{\epsilon}(x_0)$ such that for all $x\in J_{\epsilon}(x_0)$ we have $d^{\alpha}f(x)>0$. As a consequence, the function f is Hölderian of exponent α (see Ref. 4, Theorem 3.9). Moreover, the function f is injective on the interval $x\in K_{\epsilon}(x_0)=J_{\epsilon}(x_0)\cap I_{\epsilon}(x_0)$. Indeed, if there exists $x_1,x_2\in K_{\epsilon}(x_0)$ such that $f(x_1)=f(x_2)$, then by the fractional Rolle's theorem (Ref. 4) there $x\in K_{\epsilon}(x_0)$ such that $d_+^{\alpha}f(x)d_-^{\alpha}f(x)\leqslant 0$, which is impossible by assumption. A continuous function which is injective is strictly monotone (see Ref. 28, Lemma 3.8, p. 207). But a monotone function is almost everywhere differentiable by the Lebesgue theorem (Ref. 31, p. 319), in contradiction with the assumption that $0<\alpha<1$.

In case (ii), we define an open interval $J_{\epsilon}(x_0)$ such that for all $x\in J_{\epsilon}(x_0)$ we have $d^{\alpha}f(x)<0$. Again the function f is a Hölderian function of exponent α. Moreover, by Ref. 4, Theorem 4.9, all points in $K_{\epsilon}(x_0)=J_{\epsilon}(x_0)\cap I_{\epsilon}(x_0)$ are local minima. This is possible if and only if f is a constant function, i.e., a differentiable function in contradiction with the fact that f is Hölderian of exponent $0<\alpha<1$. This concludes the proof of the theorem. □

We can characterize the *spectrum* of f, i.e., the set of values taken by the fractional derivative of a continuous function.

Corollary 4.1: The spectrum of a given α-differentiable function is discontinuous or zero.

Proof: The spectrum cannot be continuous and nonzero by theorem 4.1. As a consequence, the spectrum can be zero or dicontinuous. □

We can be more precise on the nature of this spectrum.

Theorem 4.2: *The set of fractional differential equations* $d^{\alpha}f(x)=a(x)+ib(x)$, *where* $0<\alpha<1$ *and the functions* $c(x)=a(x)+b(x)$, $d(x)=a(x)-b(x)$ *keep a constant sign on a given interval of* $\mathbb{R}$, *has no solutions.*

Proof: This is the same proof as Theorem 4.1. The continuity assumption of Theorem 4.1 being only here to construct an interval where $c(x)$ and $d(x)$ keep a constant sign. □

As a consequence, the spectrum is discontinuous but of very special form, as we cannot find any interval of $\mathbb{R}$ on which we have a constant sign. We define the *Dirichlet function* as follows:

$$\mathcal{D}(x)=\begin{cases}1, & \text{if} \quad x\in\mathbb{Q}\\ -1, & \text{if} \quad x\in\mathbb{R}\backslash\mathbb{Q}.\end{cases} \tag{I.87}$$

Then, the function $a(x)$ and $b(x)$ can be taken such that

$$a(x)=\tfrac{3}{2}\mathcal{D}(x), \quad b(x)=-\tfrac{1}{2}\mathcal{D}(x). \tag{I.88}$$

We can extend all the previous theorems to the case where the order of fractional differentiation is nonconstant, but a function of x.

In Ref. 5, we have derived, in the fractional calulus framework, the Schrödinger equation from Newton's equation of dynamics under the assumption that one-dimensional quantum mechanical trajectories satisfy

$$(d^{\alpha}_{\sigma}f(x))^2=2\overline{h}/2m, \quad \sigma=\pm, \tag{I.89}$$

where $\overline{h}$ is the reduced Planck constant $h/2\pi$ and m is the mass of the particle. Of course, this is impossible by Theorem 4.1, as already proved in Ref. 7. But as the Schrödinger equation is a well established equation of physics, we propose in Ref. 7 to consider a small perturbation of condition (89), like

$$(d^{\alpha}_{\sigma}f(x))^2=2\overline{h}/2m+\epsilon a_{\sigma}(t,f(t)), \quad \sigma=\pm, \tag{I.90}$$

where $0<\epsilon\ll 1$, in order to permit the existence of nontrivial solutions and to obtain a small perturbation of the Schrödinger equation.

However, condition (I.90) lead to a deadlock. Indeed, for ϵ sufficiently small, the quantities $d^{\alpha}_{\sigma}f(x)$ keep a constant sign. As a consequence, by Theorem 4.2 we have no solutions.

All these problems are solved in Part II by using the scale calculus framework.

E. Quantum representation of nondifferentiable functions

We introduce the notion of a quantum geometric representation for a continuous nondifferentiable function. This notion is associated with minimal resolution and the scale derivative. It turns out that a geometric space displaying the basic features of the quantum geometric representation is given by a simplified version of Connes' formulation of the standard model of fundamental interactions within the framework of noncommutative geometry.

1. The quantum representation of a continuous nondifferentiable function

Our previous results allow us to define a natural notion of a scale derivative. The scale derivative, which is a complex valued operator, contains the necessary information in order to perform a local analysis of continuous nondifferentiable functions, and take care of this nondifferentiability.

Let f be a given continuous on a differentiable function. The basic functions associated with f, and from which we can deduce the scale derivative are the forward and backward mean functions defined as $f_\epsilon^+(t)=(1/2\epsilon)\int_t^{t+\epsilon} f(s)ds$ and $f_\epsilon^-(t)=(1/2\epsilon)\int_{t-\epsilon}^t f(s)ds$, respectively.

From a geometrical viewpoint, it means that in order to take into account the nondifferentiable character of f, one must consider the disjoint union $\Gamma_\epsilon^+ \cup \Gamma_\epsilon^-$, where Γ^σ is the graph of f_ϵ^σ, $\sigma = \pm$.

Definition 5.1: Let $h>0$, f be a continuous nondifferentiable function, and $\epsilon(f,h)$ be its minimal resolution. For all $\epsilon>0$, the quantum geometric representation of f, denoted $Q_\epsilon(f)$, is defined by the following:

(i) For all $\epsilon>\epsilon(f,h)$, $Q_\epsilon(f)=\Gamma_\epsilon$;

(ii) for all $0<\epsilon\leqslant\epsilon(f,h)$, $Q_\epsilon(f)=\Gamma_\epsilon^+\cup\Gamma_\epsilon^-$,

where Γ_ϵ, Γ_ϵ^+, Γ_ϵ^-, are the graphs of the mean function f_ϵ, the forward mean function and the backward mean function, respectively.

The nondifferentiability of f induces a change in the geometric structure of the geometric representation of f.

In the following, we consider graphs of real valued functions as a submanifold of $\mathbb{R}^2$. As f_ϵ^+ and f_ϵ^- are differentiable functions, one deals with a disjoint union of differentiable submanifolds Γ_ϵ^+ and Γ_ϵ^-. The basic features of the quantum representation of f, when $0<\epsilon<\epsilon(f,h)$, is that Q_ϵ is composed by two differentiable submanifolds, which are close to each other, their closeness being related to ϵ.

As a consequence, a good understanding of the effects of a nondifferentiable function can be obtained via the following simplified model.

Let M be a one dimensional differentiable submanifold of $\mathbb{R}^2$. Let $A=\{a,b\}$ be a two point space. We consider $Q=M\times A$. Then, Q is the union of two copies of the manifold M: $Q=M_a\cup M_b$.

Remark 5.1: A more accurate model is the following: Let $A_\epsilon=\{a_\epsilon,b_\epsilon\}$ be a two point space, such that for $\epsilon>\epsilon(f,h)$, A_ϵ reduces to a point, i.e., $a_\epsilon=b_\epsilon$. The simplified model is then $Q_\epsilon=M\times A_\epsilon$.

2. Noncommutative geometry

In this paragraph we only sketch a possible connect between our point of view on nondifferentiable functions and noncommutative geometry. The idea is, by the way, to obtain powerful tools to study nondifferentiable functions which will be relevant to physics.

In his book,[15] Connes develops noncommutative geometry. The basic idea is to extend to the noncommutative case the classical result of Gelfand and Naimark relating C^*-algebras and locally compact spaces.

At the end of his book, Connes (Ref. 15, p. 568) discusses a particular example, where his theory already leads to interesting results (this example is viewed as a preliminary step toward a complete noncommutative model for the standard model of quantum particles).

He considers a product of a differentiable manifold (the standard $\mathbb{R}^4$) by a discrete space, $A=\{a,b\}$. Using noncommutative geometry, he can make an analysis on this space. In particular, he defines a ''differential'' operator which contains three terms: the classical derivative on each copy of $\mathbb{R}^4$ and a finite difference.

It will be interesting to discuss the relevance of this construction with respect to our approach to nondifferentiable functions.

PART II

II. SCALE RELATIVITY AND THE SCHRÖDINGER EQUATION

A. Introduction

The Schrödinger equation is one of the basic pieces of quantum mechanics. Many attempts already exist in order to derive it from the expected behaviors of trajectories of quantum particles

or from classical equations of the dynamics. We can cite, for example, the Nelson stochastic approach,[36] the Feynman perturbative approach,[25] and Nottale's approach by the Scale relativity theory.[37]

In the following we discuss the derivation of the Schrödinger equation in the framework of the Scale relativity of Nottale.[37] The main point is that, contrary to the Nelson or Feynman approach, it is based on a *first principle*, namely, the *scale principle of relativity*, which is an extension of the Einstein relativity principle to scales (of time and lengths).

The scale relativity principle introduced by Nottale has a direct consequence on the equations of the dynamics for a given particle. Indeed, they must keep the same form under a scale transform, i.e., going from the classical scale to the atomic scale. Following Feynman and Hibbs, the principal difference between the microscopic and macroscopic scale is that typical paths become nondifferentiable. Then, we must be able to transform the classical differential equations of the dynamics for functions which are not at all differentiable.

This is done using the scale difference operator defined in Part I. The scale relativity principle is then equivalent to changing the classical derivative by the scale difference operator in the Euler–Lagrange equations of the dynamics.

This quantification procedure called the scale quantization can be precisely defined in Sec. II B, by introducing a quantization map, associating with each classical variable and differential operator its quantum counterpart. One of the main problems is then that the scale quantization procedure of the Euler–Lagrange equation is not unique. Indeed, we can first quantify the Lagrangian of the system and then define a quantized Euler–Lagrange equation, or we can quantify directly the classical Euler–Lagrange equation. The main point, proved in the coherence lemma in Sec. II D 2, is that these two procedures coincide.

The scale quantization procedure being precisely defined, we can specialize it to the quantum mechanical case. The principal free parameter in the quantization lies in the order of the regularity of the nondifferentiable curve, i.e., its Hölder exponent. Using the Feynman–Hibbs characterization of quantum paths, as well as the Heisenberg inequalities, we prove in Sec. II C that the Hölder regularity of a quantum path is 1/2. Using this result, we prove in Sec. II D 4 that the quantized analog of the Newtonian equation of dynamics is a generalized nonlinear Schrödinger equation. This is done by introducing a wave-function in Sec. II D 3, which is the direct consequence of the complex nature of the speed, being itself a consequence of the nondifferentiability of the curve. Under special assumptions, which can be interpreted, we recover the classical Schrödinger equation.

B. Scale quantization procedure for classical Lagrangian systems

1. Classical Lagrangian systems and Euler–Lagrange equation

In this article, we only discuss classical Lagrangian systems defined as follows.

Definition 2.1: A Lagrangian $L(x,v,t)$ is called classical if it is of the form kinetic energy +potential, i.e.,

$$L(x,v,t)=K(v)+U(x,t), \tag{II.1}$$

where $K(v)$ is a quadratic form.

The basic example for $K(v)$ is the classical kinetic energy of a particle of mass m given by

$$K(v)=\tfrac{1}{2}mv^2. \tag{II.2}$$

The dynamics associated to a Lagrangian system is determined by the *Euler–Lagrange equations*.

Definition 2.2: Let $L(x,v,t)$ be a classical Lagrangian system. The Euler–Lagrange equation associated with L is the following partial differential equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v}(x(t),v(t),t)\right)=\frac{\partial L}{\partial x}(x(t),v(t),t). \qquad \text{EU}$$

We denote by E the mapping associating to L its Euler–Lagrange equation (EU).

2. The scale quantization procedure

In this section, we define the *scale quantization procedure*, which formalizes Nottale's approach to quantum mechanics. The terminology suggests that the quantization procedure follows ideas coming from the theory of the *scale relativity* developed by Nottale.[37]

a. The scale quantization map We define a map Q which acts on differential operators, variables and functions.

The classical variables x, v, t have quantized analogs which are denoted by $X=Q(x)$, $V=Q(v)$ and $T=Q(t)$.

In Assumption 2.1, we have the following.

Assumption 2.1: We have $Q(t)=t$.

The time variable has then a specific role, being the only variable not affected by the quantization procedure.

We denote also by

$$X(t)=Q(x(t)),\ V(t)=Q(v(t)), \tag{II.3}$$

the quantized version of the position trajectory and speed.

The main point is that we do not know for the moment the regularity of $X(t)$ or $V(t)$.

The first algebraic properties of Q is the following.

Property 2.1 (Quantization of maps): We consider a map $L:(x,v,t)\mapsto L(x,v,t)$. *The quantized map* $Q(L)=\mathcal{L}$ *is defined by*

$$\mathcal{L}:(X,V,t)\mapsto L(X,V,t). \tag{II.4}$$

As a consequence, if L is differentiable with respect to the variable x, v or t then $\mathcal{L}$ is differentiable with respect to X, V or t.

In order to use Q on differential equations, we must precise its behavior with respect to differential operators.

Property 2.2 (Operator): We consider a map of the form $f(t)=L(x(t),v(t),t)$, *where* $x(t)$ *and* $v(t)$ *are differentiable functions. The differential operator* d/dt *acts on operator* f. *By the map* Q, *we define a quantized operator* $Q(d/dt)$ *such that*

$$Q(df/dt)=Q(d/dt).Q(f),$$

where $Q(d/dt)$ *is on operator acting on* $Q(f)$, *depending on the regularity of* $Q(f)$ *with respect to* t:

(*a*) *If* $Q(f)(t)$ *is differentiable with respect to* t, *then* $Q(d/dt)=d/dt$.
(*b*) *If* $Q(f)(t)$ *is nondifferentiable with respect to* t, *then* $Q(d/dt)=\square_\epsilon/\square t$, *where* $\epsilon(X,h)>\epsilon>0$, h *being a constant.*

The constant h must be fixed by physical constraint. In the following, we consider that h has a free parameter.

As $f(t)=L(x(t),v(t),t)$, we have $Q(f)(t)=L(X(t),V(t),t)$. Hence, the regularity of $Q(f)$ with respect to t depends on the regularity of $X(t)$ and $V(t)$ with respect to t.

Moreover, as $v=dx/dt$, we have

$$V(t)=Q\left(\frac{d}{dt}\right)[X(t)]. \tag{II.5}$$

Hence, the regularity of $X(t)$ can induce a change in the form of the speed $V(t)$.

b. Scale quantization of the Euler–Lagrange equation. By the quantization procedure we give the quantized version of the Euler–Lagrange formula (II.7).

Lemma 2.1: The quantized Euler–Lagrange equation $Q(EU)$ is given by

$$Q\left(\frac{d}{dt}\right)\left[\frac{\partial \mathcal{L}}{\partial V}(X(t),V(t),t)\right]=\frac{\partial \mathcal{L}}{\partial X}. \tag{II.6}$$

Proof: The action of Q on the classical Euler–Lagrange equation (EU) gives

$$Q\left(\frac{d}{dt}\right)\left[Q\left(\frac{\partial L}{\partial v}(x(t),v(t),t)\right)\right]=Q\left(\frac{\partial L}{\partial x}\right). \tag{II.7}$$

As L is assumed to be differentiable with respect to the variables v and x, we have, using Property 2.1:

$$Q\left(\frac{d}{dt}\right)\left[\frac{\partial Q(L)}{\partial Q(v)}(Q(x)(t),Q(v)(t),t)\right]=\frac{\partial Q(L)}{\partial Q(x)}. \tag{II.8}$$

With our notations, Eq. (8) gives Eq. (6). This concludes the proof of the lemma. □

As a consequence, in order to precise the quantization procedure, we only have to precise the regularity of $Q(x(t))=X(t)$.

C. Generic trajectories of quantum mechanics

In order to precise the quantization procedure, we investigate the regularity of a quantum-mechanical path.

1. Feynman and Hibbs genericity condition

Feynman and Hibbs have already noted in Ref. 26, pp. 176–177 that the typical path of a quantum mechanical particle is continuous and nondifferentiable. More precisely, there exists a quadratic velocity, i.e., if $X(t)$ denotes the particle trajectory, then

$$\lim_{t\to t'}\frac{(X(t)-X(t'))^2}{t-t'} \text{ exists.} \qquad (FH)$$

As a consequence, we have the following result.

Lemma 3.1: Under Feynman–Hibbs characterization (FH), we have $X(t)\in H^{1/2}$.

We can deduce the following result on the Hausdorff dimension of typical paths of quantum mechanics:

Corollary 3.1: Under Feyman–Hibbs characterization (FH), the Hausdorff dimension of X is 1/2.

Proof: As $X\in H^{1/2}$, this follows from Theorem 20.6, Ref. 46, p. 310. □

On the contrary, the fractal (or Minkowski–Bouligand) dimension Δ is given by

$$\Delta(X)=2-(1/2)=3/2, \tag{II.9}$$

using (Ref. 46, pp. 154–155).

This result has been discussed in great detail by Abbott and Wise.[1]

2. Heisenberg uncertainty principle

The nondifferentiable character of typical paths of quantum mechanics can be seen as a consequence of *Heisenberg uncertainty relations*. We refer to (Ref. 37, pp. 93–95) and Ref. 14, p. 130–131 for details.

Let Δx, Δt, and Δp be the precision of the measurement of the position x, time t and *momentum* p of a given particle. The Heisenberg uncertainty relation on momentum and position is

$$\Delta p \Delta x \geqslant h. \tag{II.10}$$

We have the following relations:

$$x(t \pm \Delta t) = x(t) \pm \Delta x,$$

$$v_\epsilon(t \pm \Delta t) = (x(t+\epsilon) - x(t)/\epsilon) \pm \Delta v, \tag{II.11}$$

where $\epsilon \geqslant \Delta t$ by definition of Δt, and

$$\Delta p = m \Delta v. \tag{II.12}$$

Remark 3.1: The speed of a particle $v(t)$ is defined as the limit of the mean-speed $v_\epsilon(t) = (x(t+\epsilon) - x(t)/\epsilon)$ when ϵ goes to zero. As the time variable t is known only with precision Δt, we must have $\epsilon \geqslant \Delta t$.

What are the relations between Δv, Δx and Δt?

As $\epsilon \geqslant \Delta t$ by assumption, we have by taking the best possible value $\epsilon = \Delta t$,

$$\Delta v \sim 2 \Delta x / \Delta t. \tag{II.13}$$

As a consequence, the Heisenberg uncertainty relation (10) gives

$$m \frac{(\Delta x)^2}{\Delta t} \sim h. \tag{II.14}$$

We deduce that

$$\Delta x \sim \frac{h}{2m} \Delta t^{1/2}. \tag{II.15}$$

Hence, we deduce that the Heisenberg uncertainty relation (10) induces the fact that $X \in H^{1/2}$.

Of course, the previous reasoning can be reversed. If typical paths of quantum mechanics are assumed to be in $H^{1/2}$, then we obtain Heisenberg-like uncertainty relations.

Lemma 3.2: Let $X \in H^{1/2}$, and $0 < \Delta t \ll 1$ be a small parameter. We denote by $\mathcal{X}$ the graph of X, and by $\mathcal{X}(t) = (t, X(t))$ a point belonging to $\mathcal{X} \in \mathbb{R}^2$. We denote by $\Delta x(t) = \|\mathcal{X}(t), \mathcal{X}(t+\Delta t)\|$, where $\|.\|$ is the classical Euclidean norm on $\mathbb{R}^2$. We have

$$\Delta x \sim (\Delta t)^{1/2}, \tag{II.16}$$

for all $t \in \mathbb{R}$.

Proof: This follows from a simple computation. We have

$$\|\mathcal{X}(t), \mathcal{X}(t+\Delta t)\|^2 = (\Delta t)^2 + (X(t+\Delta t) - X(t))^2. \tag{II.17}$$

As $X \in H^{1/2}$, we obtain

$$\|\mathcal{X}(t), \mathcal{X}(t+\Delta t)\|^2 \leqslant (\Delta t)^2 + C^2 \Delta t \sim \Delta t, \tag{II.18}$$

for Δt sufficiently small. □

Of course, this result extends to arbitrary $X \in H^\alpha$, with $0 < \alpha < 1$, for which we obtain

$$\Delta x \sim (\Delta t)^\alpha. \tag{II.19}$$

D. Scale quantization of Newtonian mechanics

1. Quantization of speed

The fact that typical path of quantum mechanics belongs to $H^{1/2}$ has many implications with respect to the quantization procedure. The first one being that the quantized version of the speed v is now complex.

Lemma 4.1 (Quantized speed): Let $Q(x)=X\in H^{1/2}$; then $Q(v)=V\in\mathbb{C}$. Precisely, we have

$$V=\frac{\Box_\epsilon X}{\Box t}. \tag{II.20}$$

Proof: This follows from the quantization procedure. We have

$$v=\frac{dx}{dt}. \tag{II.21}$$

By Q, we obtain

$$V=Q\left(\frac{d}{dt}\right)(X). \tag{II.22}$$

As $X\in H^{1/2}$, we have

$$Q(d/dt)=\Box_\epsilon/\Box t, \tag{II.23}$$

which is a complex number by definition. □

2. Scale relativity and the coherence lemma

a. Scale relativity and Scale Euler–Lagrange equations. The scale-relativity theory developed by Nottale (Refs. 37, 38) extends the Einstein relativity principle to *scale*. A heuristic version of the new relativity principle can be written as follows:

"*The equations of physics keep the same form under any transformation of scale (contractions and dilatations).*"

The mathematical foundation of such a theory is difficult. The main difficulty being that space–time is now a nondifferentiable manifold. We refer to the work of Nottale[37] for more details.

The scale relativity principle has a direct consequence on the form of the equation of motion for a particle.

We first introduce the following "Scale" Euler–Lagrange equation.

Definition 4.1: Let $\mathcal{L}(V,t)$ be a quantized Lagrangian. The Scale Euler–Lagrange equation associated with $\mathcal{L}(X,V,t)$ is the equation

$$\frac{\Box_\epsilon}{\Box t}\left(\frac{\partial\mathcal{L}}{\partial V}(X(t),V(t),t)\right)=\frac{\partial\mathcal{L}}{\partial X}(X(t),V(t),t). \qquad (\mathcal{E}U)$$

We denote by $\mathcal{E}$ the mapping associating equation $(\mathcal{E}U)$ to $\mathcal{L}$.

The scale relativity principle is then equivalent to the following statement.

Statement 4.1 (Scale relativity): *The equation of motion of a quantum-mechanical particle satisfies the Scale Euler–Lagrange equation.*

The main point is that the Scale Euler–Lagrange equation does not follow from the quantization procedure, but from a first principle which fixes the form of the equation of motions.

b. Coherence lemma At this point, we can state the *coherence lemma*, which ensures us that the quantization procedure is well defined. Indeed, the scale relativity principle gives an equation of motion particle in quantum mechanics, i.e., $(\mathcal{E}U)$. But, the quantization procedure can be used

to obtain an equation of motion for the particle as a quantized version of the classical Euler–Lagrange equation, i.e., $Q(\mathrm{EU})$. The main point is that this two constructions are equivalent, i.e., $Q(\mathrm{EU})=\mathcal{E}U$. Precisely, we have the following.

Lemma 4.2 (Coherence): The following diagram commutes,

$$\begin{array}{ccc} L(x,v,t) & \overset{Q}{\rightarrow} & \mathcal{L}(X,V,t) \\ E\downarrow & & \downarrow\mathcal{E} \\ \dfrac{d}{dt}\left[\dfrac{\partial L}{\partial v}(x(t),v(t),t)\right]=\dfrac{\partial U}{\partial x} & \overset{Q}{\rightarrow} & \dfrac{\square_{\epsilon}}{\square t}\left[\dfrac{\partial \mathcal{L}}{\partial V}(X(t),V(t),t)\right]=\dfrac{\partial U}{\partial X}. \end{array} \tag{II.24}$$

Proof: This follows from a direct computation. □

In terms of mapping, the coherence lemma is then equivalent to

$$Q\circ E=\mathcal{E}\circ Q. \tag{II.25}$$

3. Action functional and wave

A basic element of Lagrangian mechanics is the action functional $A(x,t)$ which is related to speed via the equation

$$v=\frac{1}{m}\frac{\partial A}{\partial x}. \tag{II.26}$$

The function $A(x,t)$ is differentiable with respect to x and t. By the quantization procedure, we obtain the analog of the classical action functional for quantum mechanics.

Lemma 4.3 (Quantized action functional): The function $\mathcal{A}=Q(A)$ is a complex valued function $\mathcal{A}(X,t)$ which satisfies

$$V=\frac{1\partial}{m}\frac{\mathcal{A}}{\partial X}. \tag{II.27}$$

Proof: By Q the classical equation (26) gives

$$V=Q(v)=Q\left(\frac{\partial}{\partial x}\right)Q(A). \tag{II.28}$$

As the classical action $A(x,t)$ is differentiable with respect to x, the quantized version $\mathcal{A}(X,t)$ is differentiable with respect to X. As a consequence, we have

$$Q\left(\frac{\partial}{\partial x}\right)=\frac{\partial}{\partial X}. \tag{II.29}$$

This concludes the proof. □

Moreover, the quantization procedure gives us the following relation.

Lemma 4.4 (Action): The quantized action $\mathcal{A}(x,t)$ satisfies

$$\mathcal{L}=\frac{\partial \mathcal{A}}{\partial t}. \tag{II.30}$$

At this point, the main feature of quantum mechanics is to introduce complex speed and action functional. We can discuss the behavior of $\mathcal{A}$ by introducing a complex valued function, which is called the *wave function*.

Definition 4.2 (Wave function): We call wave function associated to X, the complex valued function defined by

$$\psi(X,t)=\exp\left(\frac{i\mathcal{A}(X,t)}{2m\gamma}\right), \tag{II.31}$$

where $\gamma\in\mathbb{R}$ is a constant number.

The constant γ is a normalization constant, which depends on the regularity property of $X(t)$.

The complex nature of V leads naturally to the introduction of the wave function. The wave formalism is then induced by the nondifferentiable character of typical paths of quantum mechanics.

4. The quantized Euler–Lagrange equation

The quantized Euler–Lagrange equation is given by

$$m\frac{\square_\epsilon V(t)}{\square t}=\frac{dU}{dx}(x). \tag{II.32}$$

The complex speed V is related to the wave function, so that Eq. (II.32) can be written in term of ψ.

Theorem 4.1: *Let $X(t)$ be a continuous nondifferentiable function in $H^{1/2}$ and ψ its associated wave function. The quantized Euler–Lagrange equation is of the form*

$$2i\gamma m\left[-\frac{1}{\psi}\left(\frac{\partial\psi}{\partial X}\right)^2\left(i\gamma+\frac{a_\epsilon(t)}{2}\right)+\frac{\partial\psi}{\partial t}+\frac{a_\epsilon(t)}{2}\frac{\partial^2\psi}{\partial X^2}\right]=(U(x)+\alpha(x))\psi+o(\epsilon^{1/2}), \tag{II.33}$$

where $\alpha(x)$ is an arbitrary continuous function, and

$$a_\epsilon(t)=\frac{1}{2}[(\Delta_\epsilon^+X(t))^2-(\Delta_\epsilon^-X(t))^2]-i\frac{1}{2}[(\Delta_\epsilon^+X(t))^2+(\Delta_\epsilon^-X(t))^2]. \tag{II.34}$$

The equation (33) is called the *generalized Schrodinger equation* by Nottale.[37]

Proof: We have

$$V=-i2\gamma\frac{\partial\ln(\psi)}{\partial X}. \tag{II.35}$$

The Euler–Lagrange equation is now given by

$$2i\gamma m\frac{\square_\epsilon}{\square t}\left(\frac{\partial\ln(\psi)}{\partial X}\right)=\frac{dU}{dX}. \tag{II.36}$$

We denote

$$f(X,t)=\frac{\partial\ln(\psi(X,t))}{\partial X}(X,t). \tag{II.37}$$

We apply the main lemma of Sec. I C 4 to compute $\square_\epsilon f(X(t),t)/\square t$ for complex valued functions. We have

$$\frac{\square_\epsilon}{\square t}\left(\frac{\partial \ln(\psi)}{\partial X}(X(t),t)\right)=\frac{\square_\epsilon X}{\square t}\frac{\partial}{\partial X}\left(\frac{\partial \ln(\psi(X,t))}{\partial X}\right)(X(t),t)+\frac{\partial}{\partial t}\left(\frac{\partial \ln(\psi(X,t))}{\partial X}\right)(X(t),t)$$
$$+\frac{1}{2}a_\epsilon(t)\frac{\partial^2}{\partial X^2}\left(\frac{\partial \ln(\psi(X,t))}{\partial X}\right)(X(t),t)+o(\epsilon^{1/2}). \tag{II.38}$$

Elementary calculus gives

$$\frac{\partial \ln(\psi(X,t))}{\partial X}=\frac{1}{\psi}\frac{\partial \psi}{\partial X},\quad \text{and}\quad \frac{\partial}{\partial X}\left(\frac{1}{\psi}\frac{\partial \psi}{\partial X}\right)=\frac{1}{\psi}\frac{\partial^2 \psi}{\partial^2 X}-\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2. \tag{II.39}$$

Moreover, by definition of the wave function ψ and V, we have

$$V=-i2\gamma\frac{\partial \ln \psi(X,t)}{\partial X}. \tag{II.40}$$

Hence, we obtain

$$\frac{\square_\epsilon X}{\square t}=V=-i2\gamma\frac{\partial \ln \psi(X,t)}{\partial X}, \tag{II.41}$$

and

$$\frac{\square_\epsilon X}{\square t}\frac{\partial}{\partial X}\left(\frac{\partial \ln(\psi(X,t))}{\partial X}\right)(X(t),t)=-i2\gamma\frac{\partial \ln(\psi)}{\partial X}\frac{\partial}{\partial X}\left(\frac{\partial \ln(\psi)}{\partial X}\right)(X(t),t),$$
$$=-i\gamma\frac{\partial}{\partial X}\left[\left(\frac{\partial \ln(\psi)}{\partial X}\right)^2\right](X(t),t),$$
$$=-i\gamma\frac{\partial}{\partial X}\left[\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2\right](X(t),t). \tag{II.42}$$

We then have

$$\frac{\square_\epsilon}{\square t}\left(\frac{\partial \ln(\psi(X,t))}{\partial X}(X(t),t)\right)=\frac{\partial}{\partial X}\left[-i\gamma\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2+\frac{\partial \ln(\psi)}{\partial t}+\frac{1}{2}a_\epsilon(t)\left[\frac{1}{\psi}\frac{\partial^2 \psi}{\partial X^2}-\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2\right]\right]$$
$$+o(\epsilon^{1/2}),$$
$$=\frac{\partial}{\partial X}\left[-\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2\left(i\gamma+\frac{a_\epsilon(t)}{2}\right)+\frac{1}{\psi}\frac{\partial \psi}{\partial t}+\frac{a_\epsilon(t)}{2}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial X^2}\right]+o(\epsilon^{1/2}). \tag{II.43}$$

As a consequence, Eq. (38) is equivalent to

$$\frac{\partial}{\partial X}\left[i2\gamma m\left[-\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2\left(i\gamma+\frac{a_\epsilon(t)}{2}\right)+\frac{1}{\psi}\frac{\partial \psi}{\partial t}\right]+\frac{a_\epsilon(t)}{2}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial X^2}\right]=\frac{\partial U}{\partial X}. \tag{II.44}$$

By integrating with respect to X, we obtain

$$i2\gamma m\left[-\frac{1}{\psi^2}\left(\frac{\partial \psi}{\partial X}\right)^2\left(i\gamma+\frac{a_\epsilon(t)}{2}\right)+\frac{1}{\psi}\frac{\partial \psi}{\partial t}\right]+\frac{a_\epsilon(t)}{2}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial X^2}=U(X)+\alpha(X)+o(\epsilon^{1/2}), \tag{II.45}$$

where $\alpha(X)$ is an arbitrary function. This concludes the proof. □

5. Nonlinear Schrödinger equations

Many authors have suggested that the quantum mechanics based on the linear Schrödinger equation is only an approximation of some nonlinear theory with a nonlinear Schrödinger equation. Nonlinear wave mechanics was initiated by De Broglie[11] in order to have a better understanding of the relation between wave and particle (see Ref. 12, p. 227–231).

Many generalizations of the Schrödinger equation exist. We can mention, for example, the *Staruszkievicz*[42] or *Bialynicki–Birula and Mycielsky*[8] modification. All these generalizations are not a consequence of a given principle of physics. For example, the Bialynicki–Birula and Mycielsky modification can be derived, using the hydrodynamical formalism proposed by Madelung,[34] Bohm–Vigier[10] and others, by adding a *pressure term* to the Euler hydrodynamical equation (see Ref. 41, Sec. 2). Of course, one can justify *a posteriori* a given modification by the fact that it solves some relevant problems like the *collapse* of the wave function or the Schrödinger cat paradox (see Ref. 41).

Recently Castro, Mahecha and Rodriguez[13] have proposed a new nonlinear Schrödinger equation based on a generalization of Nottale reasoning.[37] In the one-dimensional case, they obtain

$$i\alpha\frac{\partial\psi}{\partial t}=-\frac{\alpha\,\mathrm{Re}(\alpha)}{2m}\frac{\partial^2\psi}{\partial x^2}+U(x)\psi-i\frac{\alpha\mathrm{Im}(\alpha)}{2m}\left(\frac{\partial\psi}{\partial x}\right)^2\frac{1}{\psi}, \tag{II.46}$$

where $\alpha\in\mathbb{C}$.

If $\mathrm{Im}(\alpha)=0$ and $\alpha=\overline{h}$, then one recovers the classical linear Schrödinger equation.

This generalization is done under two assumptions.

(i) They introduce a complex ''Planck constant'' (i.e., α) by allowing that the normalization constant γ is complex.

(ii) They consider a *complex diffusion coefficient*, which has no counterpart in our case.

The problem is that there is no geometric interpretation of a complex diffusion coefficient, nor of a complex Planck constant. As a consequence, even if Nottale's reasoning is kept in order to derive the new nonlinear Schrödinger equation (II.46), this is an *ad hoc* mathematical generalization.

On the contrary, we have to obtain a nonlinear Schrödinger equation (33) directly from the Scale relativity principle. All our constants have a clear geometrical meaning. Moreover, the nonlinear term is not an *ad hoc* term but is fixed by the theory.

E. Toward the Schrödinger equation

The generalized Schrödinger equation can be simplified in some cases, by assuming that quantum-mechanical paths satisfy special regularity properties.

Theorem 5.1: *Let $X(t)$ be a continuous nondifferentiable function belonging to $H^{1/2}$ such that*

$$a_\epsilon(t)=-i2\gamma. \tag{II.47}$$

Then, the quantized Euler–Lagrange equation takes the form

$$\gamma^2\frac{\partial^2\psi}{\partial X^2}+i\gamma\frac{\partial\psi}{\partial t}=(U(X,t)+\alpha(X))\frac{\psi}{2m}+o(\epsilon^{1/2}). \tag{II.48}$$

We can always choose a solution of Eq. (48) such that

$$\alpha(X)=0. \tag{II.49}$$

In this case, if

$$\gamma = \frac{\overline{h}}{2m}, \qquad (SC)$$

we obtain the classical Schrödinger equation

$$i\overline{h}\frac{\partial \psi}{\partial t} + \frac{\overline{h}^2}{2m}\frac{\partial^2 \psi}{\partial X^2} = U\psi. \tag{II.50}$$

Proof: The only nontrivial, but classical, part concerns the possibility of choosing a phase of the wave function such that $\alpha(X)=0$. The computations follow closely those of Ref. 4, Corollary 1.

Let ψ be a solution of (II.48). The basic idea is that we can always modify the phase of the wave function in order to obtain a solution of (II.48) such that $\alpha(X)=0$. So, let us consider the modified wave function

$$\tilde{\psi}(X,t) = \exp\left(i\frac{\mathcal{A}(X,t)}{2m\gamma} + \theta(X) \right) = \psi(X,t)\Theta(X). \tag{II.51}$$

We have

$$\frac{\partial \tilde{\psi}}{\partial X} = \frac{\partial \psi}{\partial X}\Theta + \psi\Theta',$$

$$\frac{\partial^2 \tilde{\psi}}{\partial X^2} = \frac{\partial^2 \psi}{\partial X^2}\Theta + 2\frac{\partial \psi}{\partial X}\Theta' + \psi\Theta'', \tag{II.52}$$

$$\frac{\partial \tilde{\psi}}{\partial t} = \frac{\partial \psi}{\partial t}\Theta,$$

where $\Theta'(X)$ and $\Theta''(X)$ are the first and second derivative of Θ.

By replacing in (II.48), and assuming that $\alpha(X)=0$, we obtain up to $o(\epsilon^{1/2})$ terms,

$$\Theta\left(i2\gamma m\frac{\partial \psi}{\partial t} + 2\gamma^2 m\frac{\partial^2}{\partial X^2} - U\psi \right) + 4\gamma^2 m\frac{\partial \psi}{\partial X}\Theta' + 2\gamma^2 m\psi\Theta'' = 0. \tag{II.53}$$

As $\psi(X,t)$ is a solution of (II.48) with a given value $\alpha(X)$, we deduce that $\Theta(X)$ must satisfy the following ordinary differential equation:

$$a(X,t)\Theta + b(X,t)\Theta' + c(X,t)\Theta'' = 0, \tag{II.54}$$

where

$$a(X,t) = \alpha(X)\psi, \quad b(X,t) = 4\gamma^2 m\frac{\partial \psi}{\partial X}, \quad c(X,t) = 2\gamma^2 m\psi. \tag{II.55}$$

This is a second order differential equation with nonconstant coefficients. By general theorems on linear differential equations, there always exists a solution. As a consequence, we can always choose $\Theta(X)$ such that $\phi(X,t)\Theta(X)$ satisfies (II.48) with $\alpha(X)=0$. This concludes the proof. □

Difference equations and the Schrödinger condition

The Schrödinger condition (SC) can be precise. We have the following lemma.

Lemma 5.1: The Schrödinger condition (SC) is equivalent to the difference equation

$$\Delta_\epsilon^+ X(t) = \pm\sqrt{\hbar/m}, \tag{II.56}$$

and the following relations:

$$\Delta_\epsilon^+ X(t) = \Delta_\epsilon^- X(t). \qquad (P)$$

Proof: By the definition of $a_\epsilon(t)$ in (II.34), the Schrodinger condition is equivalent to the following system:

$$(\Delta_\epsilon^+ X(t))^2 - (\Delta_\epsilon^- X(t))^2 = 0,$$

$$(\Delta_\epsilon^+ X(t))^2 + (\Delta_\epsilon^- X(t))^2 = 2\hbar/m. \tag{II.57}$$

We deduce that $(\Delta_\epsilon^+ X(t))^2 = (\Delta_\epsilon^- X(t))^2$ and $(\Delta_\epsilon^+ X(t))^2 = \hbar/m$. Hence, we have $\Delta_\epsilon^+ X(t) = \pm\sqrt{\hbar/m}$, a constant independent of t. We obtain

$$\Delta_\epsilon^- X(t) = \Delta_\epsilon^+ (t-\epsilon) = \pm\sqrt{2\hbar/m} = \Delta_\epsilon^+ X(t), \tag{II.58}$$

which concludes the proof. □

As a consequence, we are led to the study of difference equations of the form

$$\Delta_\epsilon^\sigma X(t) = a, \quad \sigma = \pm, \tag{II.59}$$

where $a \in \mathbb{R}$ is a *constant*. This kind of difference equations always have solutions of the form

$$X(t) = X^*(t) + P_\epsilon(t), \tag{II.60}$$

where $X^*(t)$ is a particular solution, and $P_\epsilon(t)$ is an *arbitrary periodic* function of t of period ϵ.

Remark 5.1: Most of the following can be generalized to general difference equations of the form $\Delta_\epsilon^\sigma X(t) = \Phi(t)$, where $\sigma = \pm$ and $\Phi(t)$ is a given function (see Ref. 35, Chap. 8).

Particular solutions always exist. Indeed, if one considers an arbitrary given function $X^*(t)$ defined on $0 \leqslant t < \epsilon$, then the difference equation defines $X^*(t)$ at every point exterior to this interval. Of course, such kinds of solutions are in general not *analytic*. We can define a special particular solution called *the principal solution* following Ref. 35, p. 200.

For (II.59) the principal solution is given by (see Ref. 35, p. 204)

$$X_c^*(t) = a\left(t - c - \frac{\epsilon}{2}\right), \tag{II.61}$$

where c is an arbitrary constant.

Remark 5.2: For $c=0$, $\omega=1$, $a=1$, we obtain the Bernouilli's polynomial $B_1(t)$.

From this section, we deduce the following *structure lemma*.

Lemma 5.2 (structure): The Schrödinger condition is satisfied by continuous functions of the form

$$X_c(t) = \pm\sqrt{\hbar/m}\left(t - c - \frac{\epsilon}{2}\right) + P_\epsilon(t), \tag{II.62}$$

where c is an arbitrary real constant, and $P_\epsilon(t)$ is an arbitrary periodic function belonging to $H^{1/2}$.

We call this set of functions the *principal Schrödinger set*. It gives the structure of typical paths of quantum mechanics in the free case.

Remark 5.3: In Ref. 4, the Schrödinger equation is obtained from a generalized equation under an assumption which is equivalent to a special fractional differential equation. In Ref. 7, we have proved that in the framework of fractional calculus, this fractional equation has no solutions.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

On decoherence

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(Received 31 March 2003; accepted 16 July 2003)

Using a quantum particle in R^3 as a toy model, and following the rules of Schrödinger's quantum mechanics, we discuss to which extent one may be able to use ''decoherence'' to view the quantum particle as a ''classical'' measuring apparatus to measure position. We discuss also very briefly the measurement of momentum and the case of quantum optics. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1616202]

I. INTRODUCTION

While Schrödinger's quantum mechanics has an undisputable extraordinary success as a model of the nonrelativistic behavior of atoms and molecules, the conceptual question ''why most of the macroscopic bodies admit a classical description'' has no satisfactory answer (and not even, perhaps, a clear mathematical formulation).

By ''classical description'' we mean here that the observables can be described as functions on a classical phase space.

On the contrary the superposition principle, which is a distinctive feature of quantum mechanics, allows for the existence of a pure state on which an observable A has no definite value.

It is sometimes stated that for large enough bodies the ''classical behavior'' should arise because the only observable one is able to measure is the mean value of observables defined at a ''microscopic'' level, and our usual perception of the world is a result of an averaging with very small statistical fluctuations, according to some version of the law of large numbers.

But the criterion of how large is the body (i.e., how many atoms it contains), fails. For example, one has manufactured a Bose–Einstein condensate made of several thousands of atoms, and which still shows a quantum mechanical behavior for comparatively large times (of the order of a few milliseconds) whereas the binding of a molecule (composed of a small number of atoms) can fairly well be described using models of rods and strings. It seems that one should make more precise the class of bodies and the class of measurements for which a classical description is legitimate.

For example, one is very far from a proof that, starting with a quantum mechanical description in terms of atoms and molecules, one is able to predict the time evolution of the macroscopic parameters so as to describe the bouncing of two ''physical'' balls. One has a further, related problem: to explain what is the physical mechanism by which some quantum systems can (for all practical purposes) act as classical apparatus. In this regard, let us remark that a solution of this problem would leave essentially untouched the measurement problem of quantum mechanics; if the apparatus can be viewed as a classical statistical Liouville ensemble, the probability of a specific outcome of a measurement is given in terms of classical probability theory.

If an actual measurement of position of a particle is taking place, and the particle is found in the domain D [with probability $p(D)$] the reduction (conditioning) of the probability distribution cannot be traced back to conditioning with respect to the state of the environment, as in classical mechanics, because when one takes into account also the environment one is lead to a theory in a bigger Hilbert space and to entangled states in which the rules of classical probability no longer

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hold. In other words, one cannot attribute to a specific final state of the environment the fact that a specific outcome of the mesurement has occured.

The more difficult (and fascinating) problem of building in the theory something that resembles classical determinism and measurement theory without wave packet reduction, is so far beyond the reach of (linear) Schrödinger quantum mechanics.

In recent years there has been a revival of interest in these issues from the part of research groups interested in the foundations of nonrelativistic quantum mechanics.

Depending on taste and past experience, one has tried a more algebraic approach, making use of the Heisenberg picture and working within the C^*-algebras framework of quantum observables (see, e.g., Refs. 1 and 2), or a more function-analytic approach using Schrödinger's quantum mechanics.

In the first approach one seeks a relevant Abelian subalgebra of operators and a suitable coupling to obtain a macroscopic measurement or otherwise a collection of ''robust'' classical states for an open quantum system to describe the appearance of environment-induced selection rules. In the second approach, one tries to describe possible mechanisms within quantum mechanics through which some specific features (e.g., the superposition principle) are somehow suppressed.

In the authors' opinion, in spite of the very interesting structures that have been constructed, especially in the algebraic context, neither of these approaches has met full success. A major contribution has come from the field of quantum optics, in which one is able to construct ''macroscopic states'' (essentially coherent states of the electromagnetic field in a cavity), to construct (experimentally) a superposition of two such states and to measure the time it takes for the system to exhibit decoherence.[3,4]

Decoherence is attributed to the interaction with the boundaries of the cavity. Although experimentally tested, this mechanism for decoherence, and therefore passage to a classical description, is very difficult to put in mathematical terms. One of the major challenges within mathematical physics is to describe it starting from the rules of quantum mechanics (or rather quantum electrodynamics).

We will come back later to the study of decoherence in quantum optics. In the following, we place ourselves within Schrödinger's quantum mechanics and describe a possible mechanism for generating at least partially some ''classical'' behavior in a quantum system.

We will take as apparatus the simplest quantum system, a particle A of mass M in R^3. This is certainly not a classical system, but we will see that, if its mass M is sufficiently large, and A undergoes scattering with sufficiently many light particles, it behaves, after the interaction has taken place, as a statistical mixture.

We shall analyze the system according to the rules of Schrödinger's approach to quantum mechanics.

In general the quantum mechanical setup will be the following: the system we are considering can be thought of as composed of three subsystems, that conventionally will be referred to as observable $\mathcal{O}$, apparatus $\mathcal{A}$, and environment $\mathcal{E}$. They are described as vectors in a product Hilbert space

$$\mathcal{H}=\mathcal{H}_o\otimes\mathcal{H}_a\otimes\mathcal{H}_e\,. \tag{1}$$

The evolution is described in general by a Hamiltonian

$$H=H_o+H_a+H_e+H^{\text{int}}_{o,a}+H^{\text{int}}_{a,e}+H^{\text{int}}_{o,e}\,, \tag{2}$$

where, for example, H_e is the Hamiltonian that describes the evolution of the environment in absence of the measuring apparatus and of the object to be measured, and $H^{\text{int}}_{a,e}$ describes the interaction between the measuring apparatus and the environment. We assume, as usual, that the interaction between the measuring apparatus and the environment is independent of the presence of the object to be measured.

Our purpose is to find the amount of ''decoherence'' that is induced in the system $\mathcal{A}$ if one neglects the information on the state of the environment (so that one has access only to the outcome of experiments that refer to the system $\mathcal{A}$).

We shall assume that neglecting the information about the system $\mathcal{E}$ can be represented mathematically by taking the trace with respect to $\mathcal{H}_e$.

Notice that if one performs this operation starting with a state which is ''entangled,'' i.e., cannot be represented by a vector $\Psi \in \mathcal{H}$ of the form

$$\phi_o \otimes \phi_a \otimes \phi_e, \quad \phi_q \in \mathcal{H}_q, \quad q = s,a,e,$$

one obtains a state which is represented by a ''density matrix'' (positive trace class operators of trace one) in $\mathcal{H}_o \otimes \mathcal{H}_a$ which is in general not a projection operator, and therefore is not associated to a vector in that space.

In this report, we shall consider first the case where the Hilbert space $\mathcal{H}_o$ is absent; we view this as corresponding to studying the decoherence induced in the (measuring) apparatus due to its interaction with the environment.

We shall be interested in the structure of the resulting density matrix, in order to see which are the ''classical features'' that can emerge.

One such classical feature could be that the resulting density matrix has (almost) diagonal kernel in a specific representation (e.g., in the space representation, or in the momentum representation). We shall comment later on whether this can be considered as an indication that in some sense the measuring apparatus can be treated as a classical ensemble for the measurement of the observable which defines the basis on which the kernel is ''almost'' diagonal.

II. A TOY MODEL OF DECOHERENCE

We will consider the case in which both the apparatus $\mathcal{A}$ and the environment $\mathcal{E}$ are systems composed of N_a, respectively, N_e particle.

The particles in the system $\mathcal{A}$ may be in a bound state (the system $\mathcal{A}$ may be a crystal). The particles in $\mathcal{E}$ are much lighter than those in $\mathcal{A}$ and are scattered by $\mathcal{A}$. Decoherence results from the scattering.

This model has been studied previously making some simplifying physical and mathematical assumptions.[5–11] It has been treated rigorously and in much detail in Ref. 12 in the case of point interactions in one dimension, and in Ref. 13 still in one dimension in the case of a point interaction superimposed to a harmonic potential.

Here we shall study in some detail the case $N_a = N_e = 1$ and $N_a = 1, N_e > 1$ with no interaction between the particles in $\mathcal{E}$ and comment briefly on the other cases.[14]

In the simplest case $N_a = N_e = 1$ one works in the tensor product of the Hilbert spaces

$$\mathcal{H}_a = L^2(R^3, \mathrm{d}x), \quad \mathcal{H}_e = L^2(R^3, \mathrm{d}y),$$

and a generic (pure) state of the system is represented by a function

$$\Psi(x,y) \in L^2(R^6, \mathrm{d}x\, \mathrm{d}y), \quad \|\Psi\| = 1.$$

The quantum mechanical evolution is given by

$$\Psi(t) = \exp\{-iHt\}\Psi(0),$$

where H is the total Hamiltonian.

Without loss of generality (the evolution equations are linear) we shall assume that Ψ has the form

$$\Psi(x,y) = \psi(x)\phi(y), \quad x,y \in R^3$$

and consider first the case

$$H_a = -\frac{1}{2M}\Delta_x, \quad H_e = -\frac{1}{2m}\Delta_y, \quad H^{\rm int}_{a,e} = V(x-y), \tag{3}$$

where Δ is the Laplacean in the indicated variable and the potential V is sufficiently regular so that $H_a + H_e + H_{\rm int}$ is self-adjoint.

We shall then discuss briefly the case $H_a = -(1/2M)\Delta_x + W(x)$. Tracing out the degrees of freedom in H_e corresponds to consider only the expectation values of the observables associated to system $\mathcal{A}$.

We prove first a simple Lemma.

Lemma 2.1: Consider the system described in (3). For any bounded operator in $\mathcal{H}_a$ one has, in the coordinate representation,

$$(e^{-iHt}\Psi, Ae^{-iHt}\Psi) = \int \psi^*(x) A_t(x,x')\psi(x') f_t^{V,\phi}(x,x')\,dx\,dx', \tag{4}$$

where

$$A_t = e^{iH_x^0 t} A e^{-iH_x^0 t}, \quad V_x(y) = V(y-x), \tag{5}$$

$$f_t^V(x,x') = (\exp\{-i(H_e + V_x)t\}\phi, \exp\{-i(H_e + V_{x'})t\}\phi). \tag{6}$$

Remark 2.1: Notice that, by construction one has $f_t^{V,\phi}(x,x) = 1$ and for a generic potential V and a generic vector ψ one has $|f_t^{V,\phi}(x,x')| < 1$ for $x \neq x'$. Moreover it is easy to prove that

$$f_t^0(x,x') = f_0^V(x,x') = 1$$

and that

$$\lim_{t\to\infty} f_t^V(x,x') = (W_+^x \phi, W_+^{x'} \phi),$$

where W_+^x is the wave operator relative to the potential $V_x(y) = V(y-x)$.

If the potential is a function which is periodic on the support of ψ with lattice period Γ one has

$$|f_t^{V,\phi}(x,x')| = 1, \quad x - x' \in \Gamma, \quad x,\ x' \in \mathrm{supp}(\psi)$$

so that if the kernel of ρ is periodic under Γ, the reduced density matrix has also this property.

One should also notice that if $A_t(x,x') = a_t(x)\delta(x-x')$ one has

$$(e^{-iHt}\Psi, Ae^{-iHt}\Psi) = (e^{-iH_x^0 t}\psi, Ae^{-iH_x^0 t}\psi)$$

and if $A = ia\cdot\nabla_x$ one has

$$(e^{-iHt}\Psi, ia\cdot\nabla_x e^{-iHt}\Psi) = (\psi, ia\nabla_x\psi) + \left(\exp\{i(H_e + V_x)t\}\phi, ia_k \frac{\partial V}{\partial x_k} \exp\{i(H_e + V_{x'})t\}\phi\right).$$

■

Proof of Lemma 2.1: Notice first that one has

$$(e^{-iHt}\Phi, Ae^{-iHt}\Phi) = (e^{-iHt}\Phi, UAU^{-1}e^{-iHt}\Phi) \tag{7}$$

for any unitary in $\mathcal{H}_e$, since A commutes with any such operator.

Next, consider the change of variables

$$\xi = x - y, \quad (M+m)\eta = Mx + my$$

with inverse

$$x=\eta-\frac{M}{m+M}\xi,\quad y=\eta-\frac{M}{m+M}\xi.$$

With the notation

$$-\frac{1}{2M}\Delta_x=H_x^0,\quad -\frac{1}{2m}\Delta_y=H_y^0,\quad -\frac{1}{2\mu}\Delta_\xi=H_\xi^0,\quad -\frac{1}{2\nu}\Delta_\eta=H_\eta^0,$$

$$\nu=M+m,\quad \mu^{-1}=m^{-1}+M^{-1},$$

one has

$$H_a^0+H_e^0=H_\xi^0+H_\eta^0.$$

Recalling that

$$H=H_x^0+H_y^0+V(x-y)=H_\xi^0+V(\xi)+H_\eta^0$$

and choosing in (6) $U=e^{-iH_y^0t}$ one has

$$e^{-iH_y^0t}e^{iHt}\Phi=e^{-iH_y^0t}e^{iH_\eta^0t}e^{i(H_\xi^0+V(\xi))t}\Phi=e^{iH_x^0t}e^{-iH_\xi^0t}e^{i(H_\xi^0+V(\xi))t}\Phi.$$

Notice that (4) can be written

$$(e^{-iHt}\Phi,Ae^{-iHt}\Phi)=\int\rho_{\mathrm{red}}(x,x')A(x,x')\,\mathrm{d}x\,\mathrm{d}x',\tag{8}$$

where $A(x,x')$ is the kernel of A in the x-representation, $\rho_{\mathrm{red}}=\rho_0(x,x';t)f(x,x';t)$ and $\rho_0(x,x';t)$ is the kernel (in the x representation) of the free evolution of the initial density matrix.

Therefore one has

$$(e^{-iHt}\Phi,Ae^{-iHt}\Phi)=(\Xi_t,e^{iH_x^0t}Ae^{-iH_x^0t}\Xi_t),\quad \Xi_t(x,y)=e^{iH_\xi^0t}e^{-i(H_\xi^0+V(\xi))t}\psi(x)\,\phi(y).$$

Using the invariance under translations of the Laplacean, changing variables (for fixed x) $\xi\to\xi+x=y$ and performing the integration over y completes the proof of Lemma 1.

□

Remark 2.2: It is easly seen that the same argument can be used in case the environment is composed of N particles which do not interact with each other and interact with the particle in $\mathcal{A}$ through potentials V_k that depend only on $x-y_k$. The analysis follows the same lines as in the previous case, with the same conclusions.

If the particles in $\mathcal{A}$ interact with each other or are acted upon by external potential forces, with smooth enough potentials, Lemma 1 [with the subsitution of $V_x(y)$ with $\Sigma_1^{N_a}V_k(y-x_k)$] holds up to terms of second order in the ratio of the mass of the particles in $\mathcal{E}$ relative to the particles in $\mathcal{A}$.

We give details of this for the case $N_e=N_a=1$ with an ''external'' potential $W(x)$. We remark that one has

$$
\begin{aligned}
&\exp\{it[H_x^0+W(x)+H_y^0+V(y-x)]\}\\
&\quad=\exp\{it[H_\eta^0+W(x)+H_x^0 i+V(\xi)]\}\\
&\quad=\exp\{it[H_\eta^0+W(\eta)+H_\xi^0-V(\xi)]\}\\
&\qquad+\int_0^1 \mathrm{d}s\,\frac{\mathrm{d}}{\mathrm{d}s}\left[\exp\left\{it\left[H_\eta^0+W\left(\eta+\frac{m}{m+M}s\xi\right)+H_\xi^0+V(\xi)\right]\right\}\right.\\
&\quad=\exp\{it[H_x^0+W(x)+H_y^0]\}\cdot\exp\left\{it\left[H_\eta^0+W\left(\eta+\frac{m}{m+M}s\xi\right)+H_\xi^0+V(\xi)\right]\right\}\\
&\qquad-\left.\exp\left\{it\left[H_x^0+W\left(\eta-\frac{m}{m+M}\xi s\right)+H_y^0\right]\right\}\exp\{-iH_\xi^0 t\}\exp\{iH_\xi^0 t+iV(\xi)t\}\right].
\end{aligned}
$$

Setting $\epsilon=m/M$ the derivative with respect to s brings down a factor ϵ and the coefficient vanishes itself at $\epsilon=0$.

Therefore in this case, under suitable regularity assumption on W one has

$$
(e^{-iHt}\Psi,Ae^{-iHt}\Psi)=\int(\psi(x)A_t(x,x')\psi(x')f_t^{V,\phi}(x,x')\psi(x')(1+O(\epsilon^2)),
$$

where

$$
A_t=e^{-i(H_x^0+W(x))t}Ae^{-i(H_x^0+W(x))t},\quad V_x(y)=V(y-x),
$$

$$
f_t^V(x,x')=(\exp\{i(H_e+V_x)t\}\phi,\exp\{i(H_e+V_{x'})t\}\phi).
$$

Repeating the steps of Lemma 2.1 one has the same result. ■

It should be emphasized that for each value of t the map

$$
\rho(x,x')\to\rho_0(x,x';t)f(x,x';t) \tag{9}
$$

is completely positive. This family of maps does not form a semigroup; whether one has a semigroup in the same limit is a very delicate issue, and we will not discuss it.

So far, the formulas we have are exact. To proceed further it is convenient to assume that the particles in $\mathcal{E}$ have a mass much smaller than those in $\mathcal{A}$.

As we shall see, this introduces two different time scales, one for $\mathcal{A}$ and one for $\mathcal{E}$. It is then seen that a partial localization of the system $\mathcal{A}$ with respect to the position variable is obtained in a time short compared with that of the natural spread of the function ψ under free evolution.

In this sense the "decoherence" process considered takes place almost instantaneously for $\mathcal{A}$ and in a very long time for $\mathcal{E}$, so that for $\mathcal{E}$ it can be regarded as a scattering event (and therefore justify the use of the scattering matrix, or rather of the wave operator used in Refs. 6, 8, and 10).

III. VERY LIGHT PARTICLES AS ENVIRONMENT

We shall assume that the particles in $\mathcal{E}$ are much lighter than the particle in $\mathcal{A}$; for concreteness we set $M=1$ for the particles in $\mathcal{A}$ and $m=\epsilon$, $\epsilon\ll 1$ for those in $\mathcal{E}$.

With the introduction of the parameter ϵ one has

$$
f_\epsilon(x,x';t)=(Y_t^x,Y_t^{x'}),\quad Y_t^x=\exp\left\{iH_y^0\frac{t}{\epsilon}\right\}\exp\left\{-i(H_y^0+\epsilon V_x)\frac{t}{\epsilon}\right\}\phi. \tag{10}
$$

It is now clear that we can choose T so small that for $0<t<T$ the effect of the free evolution on ψ is negligeable, and still $T/\epsilon\gg 1$ so that we can approximate f by a scattering regime, as suggested by the presence of t/ϵ in the exponential.

It is also evident from (10) that in the units chosen the interaction is very weak (of order ϵ) and therefore we are in need of having the environment consisting of a large number of particles (of order ϵ^{-1}) to have a decoherence effect of order one.

If the number of light particles interacting with $\mathcal{A}$ in the interval of time $[0,T]$ is still bigger, one may be able to justify the statement that the environment causes "almost instantaneous" reduction to the diagonal of the kernel of the density matrix in the position representation.

Indeed each interaction would provide a factor approximately equal to $(1-\epsilon)^f$, $f>0$ but since there are $0(M\epsilon^{-1})$ such terms their product approaches zero when $\epsilon\to 0$, $M\to\infty$. We shall comment later on the relevance of this to the statement that $\mathcal{A}$ may be used as a classical apparatus for the measurement of position.

Remark 3.1: One should remark that this limit is very singular, in the sense that the sequence of reduced density matrices converge to a state which is not represented by a density matrix for the system $\mathcal{A}$. This is a common feature of limits in which the number of particles involved tends to infinity. ■

Of course, to justify this setting requires that the initial data of the particles in $\mathcal{E}$ satisfy strong hypothesis.

In order to proceed to a more detailed analysis we shall assume that the potential $\epsilon V(y)$ satisfies the assumptions that assure the existence and unitarity of the wave operator W_+. Therefore,

$$s-\lim_{t\to\infty}\left[\exp\left\{-iH_y^0\frac{t}{\epsilon}\right\}\exp\left\{i(H_y^0+\epsilon V_x)\frac{t}{\epsilon}\right\}-W_+^x\right]\phi=0 \tag{11}$$

for any vector vector $\phi\in\mathcal{H}_e$. In (11) $W_{+,\epsilon}^x$ is the outgoing wave operator for the potential ϵV_x, $V_x(y)=V(y-x)$.

It will be convenient to introduce the subset of $\mathcal{H}_e$ consisting of vectors for which the convergence to zero in (11) is "sufficiently fast."

We define for any $\delta\geqslant 0$,

$$K_\delta\equiv\left\{\phi\in\mathcal{H}_e:\ \left\|\left[\exp\left\{-iH_y^0\frac{t}{\epsilon}\right\}\exp\left\{i(H_y^0+\epsilon V_x)\frac{t}{\epsilon}\right\}-W_{+,\epsilon}^x\right]\phi\right\|\leqslant C_\phi\epsilon^{1+\delta}\right\}, \tag{12}$$

where C_ϕ is a positive constant that may depend on ϕ and δ.

From the previous estimates one immediately has the following statement.

Lemma 3.1: If the initial state ϕ of the light particle lies in K_δ, $\delta>0$ one has

$$f\left(x,x';\frac{t}{\epsilon}\right)=(W_{+,\epsilon}^x\phi,W_{+,\epsilon}^{x'}\phi)+O(\epsilon^{1+\delta})=1+\epsilon G_V(x,x')+O(\epsilon^{1+\delta}),\quad 0<t<T, \tag{13}$$

where $G_V(x,x')$ can be computed explicitely from the first order Born expansion of the solution of the Lippmann–Schwinger equation for the potential V. □

To give an explicit expression of $G_V(x,x')$ in (13) we recall that $\phi_{\text{out}}^\epsilon$ is given by the

$$\phi_{\text{out}}^\epsilon(y)=\int \mathrm{d}k\ \phi_{\text{out}}^\epsilon(y,k)\hat{f}(k), \tag{14}$$

where $\phi_{\text{out}}^\epsilon(y,k)$ is the unique solution of the Lippman–Schwinger equation

$$\phi_{\text{out}}^\epsilon(y,k)=e^{iky}-\frac{i}{4\pi}\epsilon\int \mathrm{d}z\,\frac{e^{-i|k||y-z|}}{|y-z|}V(z)\phi_{\text{out}}^\epsilon(z,k),$$

which satisfies the condition $\lim_{|y|\to\infty}(\phi_{\text{out}}^\epsilon(y,k)-e^{i(y,k)})=0$.

Therefore, to order one in ϵ one has

$$W^x_{+,\epsilon}\phi=(\psi^\epsilon_{\rm out}(x))(y)=\phi(y)-\frac{1}{4\pi}\epsilon\int \mathrm{d}k\,\mathrm{d}z\,\frac{e^{-i|k||y-z|}}{|y-z|}V(z+x)e^{i(z,k)}\hat{\phi}(k)+o(\epsilon). \quad (15)$$

From this it is easy to deduce the formula for $G_V(x,x')$.

One can write Eq. (14) in the following form:

$$\phi^\epsilon_{\rm out}(y)=\phi(y)-\frac{\epsilon}{4\pi}\int T^x(y,y')\phi(y')+o(\epsilon)$$

with an explicit form of the kernel $T(y,y')$.

Therefore

$$(\phi^x_{{\rm out},\epsilon},\phi'^x_{{\rm out},\epsilon})=1-\frac{\epsilon}{4}[(\hat{\phi},T^x\hat{\phi})+(T^{x'}\phi,\phi)]+o(\epsilon), \quad (16)$$

where $\hat{\phi}$ is the Fourier transform of ϕ and

$$T^x=\int \mathrm{d}k\int \mathrm{d}z\,\frac{\exp\{-i|k||z-y|\}}{|z-y|}V(x+z)\exp\{i(k.z)\}.$$

Remark 3.2: A more accurate analysis, given in Ref. 12 and in Ref. 13, shows that under more stringent hypotesis on the potential one can obtain, much in the spirit of a Born–Oppenheimer (adiabatic) approximation, an asymptotic expression for the state of the full system which shows quite explicitely that if the initial state is a product state after a time of order ϵ it becomes entangled, and this produces the decoherence if one traces out the degrees of freedom of the light particle. ■

Remark 3.3: Of course, if either N_a or N_e (or both) are greater than 1, one has to deal with for N-body scattering and the expression of the wave operator becomes much more complicated, and consequently a condition analogous to that of belonging to the subspace K_ν is much more difficult to verify, unless the light particles in $\mathcal{E}$ constitute a beam of particles incident on the heavy one with a time delay sufficiently long so that the interaction can be described in terms of a succession of scattering events (in the approximation to order ϵ considered) but sufficiently small so that it is legitimate to neglect the free motion of the particle in $\mathcal{A}$ and therefore to consider that the interaction has led ''instantaneously'' to decoherence. ■

Assume that all the incoming particles in $\mathcal{E}$ belong to K_δ and if one assumes that they arrive at the location of $\mathcal{A}$ at times that are separated by $K\epsilon^{-1}$, $1\ll K<\epsilon^{-\delta}$. One has then an overall effect

$$f^\epsilon_t(x,x')=\Pi_1^N f_{t_k,\phi_k},\quad N=K\epsilon^{-1}$$

and since each of the factors for $x\neq x'$ differs is smaller than one and differs from one for a term of order ϵ one has $\lim_{K\to\infty}\lim_{\epsilon\to 0}f^\epsilon_t(x,x')=0$, $x\neq x'$ (and the convergence to zero is exponentially fast).

We comment now briefly on the conditions on the potential and the state ϕ that imply that ϕ belongs to K^V_ν, so that

$$\left\|\left[\exp\left\{-iH^0_y\frac{t}{\epsilon}\right\}\exp\left\{i(H^0_y+\epsilon V_x)\frac{t}{\epsilon}\right\}-W^x_+\right]\phi\right\|\leqslant C_\phi\epsilon^{1+\delta}.$$

It is convenient to introduce the following class W_α of potentials:

$$V(x)=(1+|x|)^{-\alpha}[V_1(x)+V_2(x)],\quad \alpha>2,\quad x\in R^3,$$

$$V_1\in L^\infty,\quad V_2\in L^2,\quad x\cdot V_1\in L^\infty+L^2,\quad (1+|x|)V_2\in L^\infty+L^2. \quad (17)$$

We also introduce the following set D_ρ of elements $f(x)$ in $L^2(R^3)$,

$$D_\rho:\{f\in L^2,\quad |x|^\rho f(x)\in L^2,\quad \rho>2,\quad f=\xi(H)f\} \tag{18}$$

for some function $\xi\in C_0^\infty(0,+\infty)$ [we have assumed, without loss of generality, that the spectrum of H is absolutely continuous and coincides with $[0,+\infty)$]. The set D_ρ is dense in L^2.

The last condition in the definition of D_ρ means that f has energy bounded away from zero, and equivalently that its asymptotic state has momentum bounded away from zero.
Then we have the following Lemma.

Lemma 3.2: Let $V\in W_\alpha$, $\alpha>2$ *and let* $\phi\in D_\rho$, $\rho>2$. *Then there is a* $\delta>0$ *such that* $f\in K_\delta$ *i.e., for some* $\delta>0$,

$$\|[\exp\{-iH^0t\}\exp\{i(H^0+V)t\}-W_+]\phi\|\leqslant C\|\phi\|t^{-(1+\delta)}. \tag{19}$$

Proof: We shall only give a sketch of the proof. One has, with $U_t^0=e^{iH^0t}$, $U_t=e^{iHt}$,

$$\begin{aligned}
&\|U_t\phi-U_t^0W_+\phi\|\\
&\quad=\|\xi(H)U_t\phi-\xi(H^0)U_t^0W_+\phi\|\|\xi(H)(U_t-U_t^0)W_+\phi+(\xi(H)-\xi(H^0))U_t^0W_+\phi\|\\
&\quad\leqslant\left\|\int_t^\infty \mathrm{d}s\; U_s\xi(H)VU_s^0W_+\phi\right\|+\|(\xi(H)-\xi(H^0))(|Q|)^\alpha\|\|(|Q|)^{-\alpha}U_t^0W_+\phi\|
\end{aligned}$$

for every $\alpha>2$.

The proof is now completed using the following estimates, which follow from geometric scattering theory (for short range potentials, the propagation outside a sufficiently large ball is essentially the same as in the free case, so that $t/|x|$ is of order one on the support of $U_t\phi$ for t very large).

Let V satisfy the hypotheses given above, $\xi\in C_0^\infty((0,+\infty)$. For every real number $\beta\in[0,\alpha]$ and each $\epsilon>0$ there is a constant $c>0$ such that, for all t, $s\in R$ the following estimates hold true:

$$\|(|x|+1)^{-\beta}\xi(H)U_t(|x|+1)^{-\beta}\|\leqslant(I+|t|)^{-\beta+\epsilon},$$

$$\|(|x|+1)^{-\beta}\xi(H)U_{t-s}U_s^0\xi(H^0)(|x|+1)^{-\beta}\|\leqslant(1+|t|)^{-\beta+\epsilon}.$$

We will not give here the proof of these inequalities (see, e.g., Refs. 15–17) but limit ourselves to some comments, that should illustrate the role of the assumptions made on the state ϕ and on the potential V.

First of all, one should remember that integration by parts provides, if $g(y)$ is a function of class C^∞ with support in $(0,\infty)$,

$$\int g(y)e^{ity}\,\mathrm{d}y=\frac{i}{t}\int g'(y)e^{ity}\,\mathrm{d}y.$$

If one uses the spectral decomposition of the free Hamiltonian, and some Sobolev inequalities, one sees that this leads to a fast decrease in time of the sup norm of $e^{iH^0t}\phi$. A convenient way to handle in the same spirit the group e^{iHt} is to introduce the generator D of the dilation group, $D=1/2\,(P\cdot Q+Q\cdot P)$ (Q and P are the vector-valued operators that represent position and momentum).

Notice that

$$[D,\xi(H^0)]=2iH^0\xi'(H^0),\quad [D,V]=\frac{i}{2}(\nabla V\quad P+P\nabla V) \tag{20}$$

for any potential V, and that by Sobolev imbedding $F(H^0+I)^{-1}$ is a bounded operator in $L^2(R^3)$ if $F \in L^2(R^3)$ (this the basis of the commutator method introduced by Mourre and which plays a crucial role in geometric scattering theory).

Therefore for elements ϕ in $L^2(R^3)$ such that $\xi(H^0)\phi=\phi$ for some smooth function ξ with support in $(0,\infty)$ one can "exchange" some decrease at infinity in $|x|$ for a better decrease in time of $(U_t^0\phi)(x)$.

The same strategy can be made to work also for the group U_t but the commutator estimates bring into play the potential V, and the conditions we have stated are required to obtain estimates (24), (25) and therefore (23), upon integration by parts in the relevant variable for the spectral densities of H^0 and of H. □

Remark 3.4: One should remark that, since the particles have mass ϵ a lower bound on the momentum implies a lower bound of order ϵ^{-1} on the velocities wich means that we can have in general $0(\epsilon^{-1})$ independent scattering events in unit time. If $\phi \in K_\delta$ there is still room for $M\epsilon^{-1}$ collisions, with M very large. ■

IV. ON THE RELEVANCE OF "ALMOST DIAGONAL SUPPORT" OF THE REPRESENTATIVE KERNEL

In the preceding section we have seen that scattering by a large number of light particles can lead to "almost total" diagonalization of the reduced density matrix in the coordinate representation. We want to comment now on the relation of this property with the fact that such reduced density matrix may exhibit some features which can be considered analogous to those of a Liouville distribution in configuration space, and therefore may be fit to describe a classical apparatus for the measurement of position.

Let us start with a simple example.

Consider a system defined in C^n by the vector $\phi=\{\phi_k\}$ corresponding to the projection operator

$$\Pi:\Pi_{k,h}=\overline{\phi}_k\phi_h\,.$$

Suppose one modifies Π in Π^ϵ defined by

$$\Pi^\epsilon:\Pi^\epsilon_{k,h}=\exp\left\{-\frac{|k-h|^2}{\epsilon^2}\right\}\Pi_{k,h}\,. \tag{21}$$

It is easy to check that Π^ϵ is a density matrix for every value of the parameter ϵ. For any density matrix ρ define the dispersion with respect to a self-adjoint operator A as

$$\Delta_A(\rho)^2=\mathrm{Tr}(\rho A^2)-(\mathrm{Tr}(\rho A))^2 \tag{22}$$

(in the case ρ is a projection operator this coincides with the usual definition of the dispersion).

Notice that $\Delta_A(\rho)$ is not a linear funcion of ρ.

It is natural to define the effective dispersion of ρ with respect to A as

$$\Delta_A^{\mathrm{eff}}(\rho)=\inf_{c_i,\rho_i}\sum c_i\Delta_A\rho_i\,,\quad \rho=\sum c_i\rho_i\,, \tag{23}$$

where $0<c_i\leqslant 1$, ρ_i are density matrices, and the infimum is taken over all such decompositons.

There is a decomposition of ρ as an orthogonal sum of projection operators which commute with A if and only if $[\rho,A]=0$.

One has then, for any diagonal matrix A for ϵ small enough,

$$\Delta_A^{\mathrm{eff}}(\Pi^\epsilon)\leqslant\epsilon.$$

We may regard the function Δ_A^{eff} as a measure of the possibility of "measuring" A with as little dispersion as possible. One has

$$[A,\rho]=0\Leftrightarrow\Delta_A^{\text{eff}}(\rho)=0.$$

It is easy to prove that for any diagonal matrix A one has

$$\Delta_A^{\text{eff}}(\Pi^\epsilon)\leqslant C\epsilon\|A\|$$

for some positive constant C, which may depend on N.

Define $\Pi^0=\lim_{\epsilon\to 0}\Pi^\epsilon$. One has

$$\Pi^0_{k,h}=|\phi_k|^2\delta_{k,h},$$

so that the density matrix Π^0 represents a statistical mixture of the states $\phi^s=\{\phi^s_{k,h}=\delta_{s,h}\delta_{s,k}\}$ with weight $|\phi_s|^2$.

Consider now a measurement made with the apparatus in the state Π^0 of an observable $\mathcal{O}$ which is represented in the basis chosen by a diagonal matrix $A_{k,h}=a_k\delta_{k,h}$.

According to the statistical interpretation of quantum mechanics, the apparatus is in the state ϕ^k with probability $|\phi_k|^2$. Let us denote by ψ the state of the system $\mathcal{O}$ and by ψ_h the eigenstate of A to the eigenvalue a_k, so that $\psi=\Sigma_i c_i\psi_i$ with $c_i\in C$.

Let us assume that during the measurement the apparatus in the state ψ^k clicks with probability $|c_k|^2$, which is the probability that $\mathcal{O}$ be in the state ϕ_k.

The joint probability will be $\Sigma_k|c_k|^2|\psi_k|^2=\text{Tr}(\Pi^0\Pi_\psi)$ where Π_ψ is the orthogonal projection on the vector ψ and the average result of the measurement of A will be $\text{Tr}\,A\Pi^0$, in accordance with the rules of quantum mechanics.

If the observable A had continuous spectrum (and therefore the corresponding Hilbert space is infinite-dimensional) one expects that a limit procedure would produce the same result.

Returning now to our toy model of decoherence, these considerations lead to the following possible "scenario" (here we follow the established definition of scenario as meaning a rough general picture in which only very few preliminary essential details have been proved or sketched).

Consider the kernel of the reduced density matrix ρ^N_{red} at time T in the coordinate representation

$$\rho^N_{\text{red}}(x,x';T)=\overline{\psi}(x)\quad\psi(x')f^N_T(x,x'),\quad x,x'\in R^3, \tag{24}$$

where the factor $f^N_T(x,x')$ is due to the scattering of N light particles as discussed in Sec. II.

Assuming that the N scattering events take place in time $0=\tau_1<\cdots<\tau_N=T$ such that $\tau_{k+1}-\tau_k=0(\epsilon)$ and that such scattering events may be considered as independent, the function f^N_T has the form

$$f^N_T(x,x')=\Pi_1^N F_{i,\tau_i}(x,x'), \tag{25}$$

where F_{i,τ_i} is a kernel by which one should multiply the reduced density matrix at time τ_i; it contains the kernel due to the decoherence effect due to the interaction with the ith particle and also the kernel which comes from the free propagation of the heavy particle between collisions (recall that in the approximation considered, the effect of each collision is instantaneous).

The explicit form of $f^N_T(x,x')$, even with the approximations we have made, is difficult to find. From the form of each $F_{i,\tau_i}(x,x')$ one can guess that it is a kernel that has value 1 when $x=x'$ and decreases fast away from the diagonal, since each of the factors is less than 1 away from the diagonal.

One may hope therefore that $\rho^N_{\text{red}}(x,x';T)$ is well approximated on S_ψ (the support of ψ) by

$$G(x,x')=C\exp\{-\epsilon^{-2}(x-x')^2\}\overline{\psi}(x)\psi(x'),$$

where C is an appropriate normalization constant [notice that away from S_ψ the "guess" cannot be true, since for each value of the index k one has $\lim_{\inf\{|x|,|x'|\}\to\infty}F_{k,\tau_k}(x,x')=1$] Define $\psi_k(x)=c\psi_k\xi(B_{x_k,\epsilon})$ where $\{x_k\}$ is a regular lattice of points with lattice spacing $\epsilon^{1+\delta}$ and ξ is the characteristic function of the ball centered in x_k and of radius ϵ. Using the explicit form of G one can prove that

$$\lim_{\epsilon\to 0}\Delta_X\rho_{\text{red}}=0$$

so that ρ_{red} is almost dispersion free with respect to the position operator X in R^3 and therefore can be considered, for all practical purposes, as a classical (Liouville) statistical ensemble with Liouville density $\|\psi(x)\|^2$.

Remark 4.1: Notice that if ρ_{red} is almost dispersion-free for the variable that represents position, it must have very large dispersion with respect to the variable that represents momentum, since Heisenberg's uncertainty principle is valid also for density matrices, being a mathematical consequence of the properties of the Fourier transform.

This is easily understood as due to the fact that, by conservation of momentum, each collision changes the momentum of the heavy particle by a finite amount of order ϵ. After $O(K\epsilon^{-1})$ scattering events, with K very large, each component of the momentum of the heavy particle can be changed by an amount which can be of order K. Therefore, if one does not keep track of the momentum of the light particles which have been scattered, the uncertainty in each component of the momentum of the heavy particles is of order K.

■

We should add another remark.

Remark 4.2: According to Heisenberg's uncertainty principle, if the localization in position of ρ_{red} is to order η the localization in momentum can be at most $\hbar/\eta$.

This suggests that one should impose the further condition $\epsilon>\sqrt{\hbar}$ if the resulting ρ_{eff} should have a dispersion of the order of $\sqrt{\hbar}$ as expected from momentum conservation and the fact that the directions of the incoming light particles are random and that each of them has dispersion both in momentum and in position of the order $\sqrt{\hbar}$.

Of course, if the dispersion in position of the incoming light particles is of the order $\hbar^\xi$ with $\xi>\frac{1}{2}$ one can allow a smaller lower bound for ϵ. ■

V. LOCALIZATION IN MOMENTUM

The construction of a reduced density matrix that may be almost diagonal in the momentum representation gives rise to serious mathematical difficulties. It requires models of the interaction of a charged quantum particle with the quantized electromagnetic field, and the construction of such models, even the ones which are only moderately realistic, presents formidable mathematical problems.

In essence, they are also scattering models, in the sense that the field is radiated to infinity in space, and is traced out; in this asymptotic regime the charged particle becomes "dressed" by a cloud of photons, and the "dress" depends on the particle's momentum. This description requires an infrared cutoff, to avoid divergences. When the cutoff is removed, in the momentum representation the kernel of the reduced density matrix becomes "almost" diagonal; this is due to the fact that in the Hilbert space representation of the joint system particle+field as direct integral over the momentum of the particle the states of the field corresponding to different momenta of the particle become "orthogonal" to each other for different values of the momentum.

In fact the representations of the canonical commutation relations assigned to the field for different values of the momentum tend to become inequivalent for different values of the momentum of the charged particle so that in the limit the reduced density matrix that describes the charged particle becomes diagonal in the momentum representation.

We give here only a bare outline of the general scheme; in fact the theory, in spite of the formidable progess made recently, is not yet in its definitive form and the conditions under which the general picture given above is valid would require an analysis which will not be given here.[18–22]

The Nelson model is a prototype for this model of interaction of a charged particle with a quantized electromagnetic field.

This model describes the interaction of a nonrelativistic spinless charged quantum particle linearly coupled to a quantized relativistic scalar Bose field, which is massless and real. The nonrelativistic scalar particles (system $\mathcal{A}$) is described by position and momentum variables x_k, p_l which satisfy the usual Heisenberg relations; the scalar field (system $\mathcal{E}$) is described in Fock space model by creation and annihilation operators $a(k)$, $a^*(k)$ which satisfy the standard commutation relations; $a(k)$ is the annihilation operator for a zero mass particle of momentum k.

Spatial translations are implemented by the total momentum operator

$$P = p + \int k a^*(k) a(k) \mathrm{d}^3 k. \tag{26}$$

The dynamics of the system is generated by the Hamiltonian

$$H = \frac{p^2}{2m} + H^{\mathrm{ph}} + g \int_0^K (a(k) e^{ikx} + a(k)^* e^{-ikx}) \xi(k) |k|^{-1/2} \mathrm{d}^3 k, \tag{27}$$

where

$$H^{\mathrm{ph}} = \int |k| a(k)^* a(k) \mathrm{d}k^3.$$

The function $\xi(k)$ is a cutoff function for low momenta necessary to define in a rigorous way the entire theory (an ultraviolet cutoff K is also needed, but in our context is irrelevant because here we shall be interested only in infrared photons).

The Hamiltonian is invariant under translations in physical space, and therefore admits a decomposition over the spectrum of the total momentum P,

$$H = \int^{\oplus} H(P) \mathrm{d}P, \quad \mathcal{H} = \int^{\oplus} \mathcal{H}_P \, \mathrm{d}P.$$

On each $\mathcal{H}_P$ the Hamiltonian can be written

$$H_P = \frac{|P^{\mathrm{ph}} - p|}{2m} + g \int_0^K (a(k) e^{ikx} + a(k)^* e^{-ikx}) \frac{\xi(k)}{\sqrt{|k|}} \mathrm{d}^3 k \tag{28}$$

and admits a ground state Ω_P.

The dressed one particle wave packets ψ_f, $f \in L^2(R^3)$ defined by

$$\psi_f(P) = f(P) \Omega_P$$

propagate according to

$$\psi_{f(t)} = \exp\{-iHt\} \psi_f, \quad f(t)(P) = f(P) \exp\{-iE(P)t\},$$

where $E(P)$ is the energy of a dressed charged particle of momentum P.

The system admits a wave operator[18,19,21] and has the property that the Hilbert space of the outgoing states [which in this case is $L^2(R^3, \mathrm{d}x) \times \mathcal{F}$, where $\mathcal{F}$ is the Fock space of the field] can be written as the integral over R^3 (momentum space of the particle) of Fock-space states of the field, $\mathcal{H} = \int^{\oplus} \mathcal{H}_p \, \mathrm{d}^3 p$.

One can prove that the asymptotic creation and annihilation operators $a_{\rm as}(k)$, $a^*_{\rm as}(k)$ of the photon field exist, satisfy the usual canonical commutation relations (CCR), and commute with the algebra of position-momentum of the dressed particle (at least in the one-particle sector).

If an infrared cutoff is present, the $a_{\rm as}$, $a^*_{\rm as}$ give a representation of the CCR which is equivalent to the representation given by the a, a^*. Define $W_{\rm as}$ to be the unitary operator that implements this unitary equivalence,

$$a_{\rm as} = W_{\rm as} a W^*_{\rm as}, \quad a^*_{\rm as} = W_{\rm as} a^* W^*_{\rm as}.$$

For the sake of simplicity, we assume that the infrared cutoff function $\xi(k)$ is chosen such that $1-\xi(k)$ is the characteristic function of the interval $|k| \leqslant \epsilon$, so that the unitary operator W depends on ϵ.

Of course, the construction of the dressed states depends on the cutoff, so that for each function f we have a family of dressed states ψ^ϵ_f, and a family of unitary operators $W^\epsilon_{\rm as}$. When the infrared cutoff is removed, i.e., in the limit $\epsilon \to 0$, the two representations become inequivalent and one has[21]

$$\lim_{\epsilon \to 0} (\psi^\epsilon_f, \psi^\epsilon_g) = 0,$$

whenever the support of f in momentum space is disjoint from the support of g.

In this sense, by tracing out the degrees of freedom of the outgoing radiation field and removing the infrared cutoff one has a reduced density matrix of the charged particles in diagonal form in the momentum representation.

This effect can be understood in a qualitative form by remarking that the Hamiltonian of our system is at most quadratic in the creation and annihilation operators of the scalar field, and therefore by a suitable Bogolijubov trasformation it can be written as the sum of a quadratic part in a new set of creation and annihilation operators $b(k), b^*(k)$ and a term which acts as the identity in the Fock space of the $b(k), b^*(k)$.

We denote by W^ϵ the unitary transformation that implements this map in Fock space (due to the presence of the infrared cutoff this unitary operator exists, but of course it depends on the cutoff chosen).

The unitary operator W^ϵ depends on the momentum of charged particle, and can be seen as a dressing trasformation, and is in general different from $W^\epsilon_{\rm as}$ obtained considering the decoupling due to the asymptotic behavior in time.

In order that W^ϵ exists for all values of p it is necessary that the following integral be finite:

$$J = \int_0^\infty |\xi(k)|^2 |k|^{-3} \, {\rm d}^3 k$$

(indeed it can be seen that if it exists for a value of the momentum p then the same is true for all the other values).

Altough the operators $W^\epsilon_{\rm as}$ and W^ϵ are not the same, it is expected that

$$(\psi^\epsilon_f, \psi^\epsilon_g) = 0(CJ^{-1})$$

when the supports of f and g are disjoint.

Therefore the situation is indeed similar to the case of localization in x-space discussed earlier, with J^{-1} playing the role of ϵ.

VI. DECOHERENCE IN QUANTUM OPTICS

We review briefly here the analysis that has been done in quantum optics, in particular in "cavity quantum electrodynamics"[3,4] about decoherence and the appearence of classical proper-

ties. The contributions of quantum optics to a better understanding of the problem are spectacular, mostly due to the fact that its predictions have been tested experimentally.

In quantum optics one defines as ''classical'' (or ''quasiclassical'') the coherent states of the quantized electromagnetic field in a cavity.[23] Since in a cavity the normal modes of the free electromagnetic field are numerable, quantization is done by associating creation and annihilation operators to each degree of freedom in the normal form of the free Hamiltonian (i.e., in the coordinates in which the free Hamiltonian is written as a sum of independent harmonic oscillators), according to the Weyl rules (since the cavity is compact, these rules should be handled with care).

For each degree of freedom, the coherent states are parametrized by a complex number α and are written explicitly as

$$|\alpha\rangle = C \exp\{(\alpha a^{\dagger} - \alpha^* a)\},$$

where $a^{\dagger}$, a are the creation and annihilation operator associated to the degree of freedom considered and C is a normalization constant.

One can verify that the average number of ''photons'' in the state α is $|\alpha|^2$ and under free evolution the coherent state $|\alpha\rangle$ evolves according to the rule $|\alpha\rangle(t) = |\alpha(t)\rangle$ where $\alpha(t) = e^{i\omega t}\alpha(0)$ with ω the frequency of the mode.

In this sense the evolution is ''classical;'' moreover one sees that the dispersion (with respect to the canonical variables) is independent of α and is identical to that of the ''vacuum'' state, defined by $\alpha = 0$.

The ''almost classical'' behavior of the field in a cavity with small value of Q ($Q = \omega\tau$ where τ is the lifetime of the mode and ω its frequency) was demonstrated in Ref. 24.

Cavites with high value of Q keep the coherent state of the electromagnetic field for a time of the order of magnitude of one second (an extremely long time by the standards of modern technology). Coherent states have the further advantage that they can be physically realized by turning on a microwave generator when the field is in the vacuum state.

The atoms are prepared in suitable states and detected after they have interacted with the field. They serve two purposes: to manipulate the field in the cavity and also to measure its state.

The method for generating a quantum superposition of the coherent states, proposed in Ref. 3 and realized in Ref. 4, involves a beam of circular polarized atoms crossing a high-Q cavity C in which a coherent state (a cat) has been previously injected (the use of circular polarized state with high angular momentum is due to their very strong coupling to microwaves and to their very long radiative decay times, due to the fact that their density has main support outside the nucleus).

On either side of the high-Q cavity C there are two cavities R_1 and R_2; these are low-Q cavities (and therefore quasiclassical, see Ref. 24). After having prepared a coherent state inside the cavity by applying a suitable microwave field to the vacuum state (recall that the vacuum state of the quantized electromagnetic field inside the cavity is the lowest energy state, but contains all vacuum fluctuations) one introduces in the system R_1, C, R_2 (in this order) a beam of circular polarized Rydberg atoms (rubidium or cesium). Their velocities are controlled precisely (so that their exit time from the cavity is known with great precision) and they are in very highly excited levels (so that they interact strongly by dipole interaction even with a very weak field).

We shall call e the level of the atoms which are injected, and we assume that there is a slightly lower level, which we shall call g, and that the two level system e, g (e for excited, g for ground) is resonating with the microwave field in R_1 and in R_2. The interaction with a resonant electromagnetic field is analogous to the interaction of a spin with a magnetic field. Denoting by $|e\rangle$ and $|g\rangle$ two representative vectors of the states e, g one can choose the intensity of the field in the cavities R_1 and in R_2 in such a way that one induces a rotation of $\pi/2$ in the ''plane'' $|e\rangle$, $|g\rangle$.

Therefore the first cavity performs the following transformation:

$$|e\rangle \to \frac{1}{\sqrt{2}}(|e\rangle + |g\rangle)$$

(the choice of the initial phases is irrelevant, since only relative phases count).

The cavity C is tuned so that if the atom crosses the cavity in the state e there is an appreciable phase shift of the field, due to a resonance between e and an ''ancilla'' state a of the atom, which resonates with e but not with g.

No appreciable phase shift is induced if the atom is in the state g.

The velocity of the atom can be selected in such a way that this phase shift is (roughly) π. After the beam has crossed the cavities R_1 and C, the entangled state of the combined system atom plus coherent state of the field is therefore

$$\frac{1}{\sqrt{2}}(|e\rangle \otimes |-\alpha\rangle + |g\rangle \otimes |\alpha\rangle).$$

Notice that one can choose for each atom the same representative (i.e., $|e\rangle$ rather then $e^{i\phi}|e\rangle$ for some ϕ that may depend on the atom in the beam) in the Hilbert space description of the state of the atoms and of the coherent state of the field, since only a change in the relative phases is significant.

After having crossed the cavity C, the beam of atoms crosses the low-Q cavity R_2 where, as explained above, there is a further action on the states of the atoms

$$|e\rangle \to \frac{1}{\sqrt{2}}(|e\rangle + |g\rangle), \quad |g\rangle \to \frac{1}{\sqrt{2}}(|g\rangle - |e\rangle).$$

Therefore, after exiting the sequence of cavities R_1, C, R_2 the combined atom-coherent state of the field is as follows:

$$\tfrac{1}{2}[|e\rangle \otimes (|-\alpha\rangle - |\alpha\rangle) + |g\rangle \otimes (|-\alpha\rangle + |\alpha\rangle). \tag{29}$$

If one now makes a measurement of the state of the atom, to find out whether it is in the state e or in the state g, one gets by reduction a quantum superposition of the two coherent states $|\alpha\rangle$ and $|-\alpha\rangle$, and therefore a quantum superposition of two ''classical'' states.

From the point of view of quantum mechanics, this is an obvious statement. The point of the experiment is that now one can determine the time it takes for the quantum superposition to ''become'' (i.e., to behave in successive measurements as) a statistical mixture, namely, a state represented by a density matrix which is not a projector.

This can be done by injecting after a time T in the same sequence of cavities an identical beam of particles.

If the state remains pure (i.e., if there has not been decoherence) one should record a perfect correlation between the measurements on the first and the second atom; if, on the other extreme, decoherence is maximal (the density matrix has eigenvalues $\frac{1}{2}$), the probability of detecting the second atom in the state e is one-half independent of the state that was detected for the first atom.

The experiment was done in 1996 by the group of Haroche in Paris[4] and the result was (in accordance with the theoretical predictions in Ref. 3) that, at least for initial states with $|\alpha| \gg 1$ (very classical from the point of view of coherent states) a sharp decay as a function of T, within an interval of time of the order of 1 millisecond, from the perfectly coherent superposition to a maximal statistical mixture.

The passage from a pure quantum mechanical state to a statistical mixture is, in the present context, attibuted to the interaction with the walls of the cavities. In fact, it is easy to see that the loss of one photon by the coherent state $|\alpha\rangle$ transforms it in the state $\alpha|-\alpha\rangle$ (since the coherent state $|\alpha\rangle$ is an eigenstate of the annihilation operator to the eigenvalue α).

In particular the coherent superposition $|\alpha\rangle+|-\alpha\rangle$ is changed in $|\alpha\rangle-|-\alpha\rangle$ and *vice versa* and therefore detecting an atom in the state e after an interaction with the wall projects the state of the electromagnetic field in a state $|\alpha\rangle+|-\alpha\rangle$ whereas if the interaction had not taken place the projected state would be $|\alpha\rangle-|-\alpha\rangle$.

Since one has no control of the interaction with the boundary, in the analysis of the outcome of the experiment with a beam of particles one ''averages'' over all possible interactions, and after a short time the outcome points to a statistical mixture.

The experiment by the Haroche group is really an impressive ''demonstration'' of the way decoherence sets in for ''macroscopic'' bodies, and points to decoherence times which are too small to be measured for a realistic ''classical'' body.

Still, the theoretical analysis carried out so far is too crude from the point of view of mathematical physics (and in general from the point of view of a clear explanation of the way in which quantum mechanical objects can be regarded as classical) and a more detailed explanation remains a challenge for the future.

VII. CONCLUSIONS

We have described three instances in which the quantum superposition of two (or more) states of a quantum ''macroscopic object'' may be destroyed by the interaction with the environment (decoherence), and thereby may lead, as far as later measurements are performed, to the fact that the state is perceived as a statistical ensemble.

The first instance was the effect of the scattering of a large number of light particles off a heavy quantum particle.

The analysis followed rigorously the lines of traditional Schrödinger's quantum mechanics, with no extra assumptions or shortcuts. The weak point of the analysis is the difficulty of handling properly the scattering by a beam of particles (as compared to the scattering by one particle); a further disturbing point is to consider as ''macroscopic object'' a single heavy quantum particle. This could be remedied by considering a bound state of very many quantum particles, but the mathematical difficulties become prohibitive.

The second instance was the interaction of a charged quantum particle with the quantized electromagnetic field. Here the observable to be measured is momentum. Only a simple model was considered, and the phenomenon of decoherence was due to the presence after the interaction of a cloud of infrared photons accompanying the particle, the cloud being different for different momentum of the asymptotic particle. Admittedly this is the weakest of the examples given, and no comment can be made on the time it takes for the decoherence to be measurable.

The third instance is the only one for which experimental results are available, and therefore to some extent the most convincing one. The ''macroscopic'' systems are the coherent states of the electromagnetic field in a cavity with perfectly conducting walls, the superposition of two coherent states is produced through a beam of atoms and the decoherence is probably due to the interaction of the electromagnetic field with the wall of the cavities. A weak point of this example could be the use of coherent states as an example of macroscopic body, and, from the formal point of view, the unsatisfactory mathematical analysis of the interaction. In view of the major interest of these experiments, a more refined description of the interaction would be welcome.

ACKNOWLEDGMENTS

Thanks are due to R. Figari and A. Teta for numerous discussions about decoherence.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Some results on the eigenfunctions of the quantum trigonometric Calogero–Sutherland model related to the Lie algebra D_4

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(Received 30 July 2003; accepted 2 August 2003)

We express the Hamiltonian of the quantum trigonometric Calogero–Sutherland model related to the Lie algebra D_4 in terms of a set of Weyl-invariant variables, namely, the characters of the fundamental representations of the Lie algebra. This parametrization allows us to solve for the energy eigenfunctions of the theory and to study properties of the system of orthogonal polynomials associated with them such as recurrence relations and generating functions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1618362]

I. INTRODUCTION

Integrable models play a prominent role in theoretical physics. The reason is not only the direct phenomenological interest of some of them, but also the fact that they often provide some deep insights into the mathematical structure of the theories in which they arise and, sometimes, they even reveal unexpected relations among different physical or mathematical theories. In classical mechanics, integrability not only shows up itself in some of the most important and time-honored problems, such as the Keplerian motion or the Lagrange or Kovalevskaya top; it appears also in a plethora of new hypothetical, highly nontrivial sytems discovered mainly during the three last decades of the past century (see Refs. 1 and 2 for comprehensive reviews). Among these, the so-called Calogero–Sutherland models form a distinguished class. The first analysis of a system of this kind was performed by Calogero,[3] who studied, from the quantum standpoint, the dynamics on the infinite line of a set of particles interacting pairwise by rational plus quadratic potentials, and found that the problem was exactly solvable. Soon afterwards, Sutherland[4] arrived at similar results for the quantum problem on the circle, this time with trigonometric interaction, and Moser[5] showed that the classical version of both models enjoyed integrability in the Liouville sense. The identification of the general scope of these discoveries came with the work of Olshanetsky and Perelomov,[6,7] who realized that it was possible to associate models of this kind to all the root sytems of the simple Lie algebras, and that all these models were integrable, both in the classical and in the quantum framework.[8,9] Nowadays, there is a widespread interest in this type of integrable system, and many mathematical and physical applications for them have been found, see, for instance, Ref. 10.

The eigenfunctions of the Calogero–Sutherland Hamiltonian associated with the root system of a simple Lie algebra L are proportional to some polynomials which form a complete orthogonal system in the quantum Hilbert space. For the special values $\kappa_\alpha = 1$, where $g_\alpha = \kappa_\alpha(\kappa_\alpha - 1)$ are the coupling constants, they coincide with the irreducible characters of L. For $L = A_n$, these polynomials provide natural generalizations to n variables of the classical orthogonal polynomials in one indeterminate. In particular, for the case with a trigonometric potential, one obtains a generalized

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system of Gegenbauer polynomials which can be identified with the Jack polynomials.[11] As was shown in Ref. 12 and, following a different approach, in Refs. 13–15, these generalized Gegenbauer polynomials obey a set of recurrence relations which constitute a κ-deformation of the Clebsch–Gordan series of the algebra. The finding of these recurrence relations opened the way to obtain many concrete results on the system of polynomials, such as for example explicit expressions, ladder operators, or generating functions.[16,17] The recurrence relations are also the key ingredient to formulate a perturbative approach to the most general among the Calogero–Sutherland models, that involving the Weierstrass $\wp$-function as potential.[18]

We aim to extend some of the results which have been obtained for A_n to the polynomials related to other simple algebras. For that, we will follow a constructive approach: starting with the Calogero–Sutherland Hamiltonian H, once expressed in a suitable set of independent variables (indeed, the fundamental characters of the underlying algebra), we find that the polynomial part of the solutions of the Schrödinger equation forms an orthogonal family of polynomials diagonalizing a second-order differential operator related to H; these polynomials, indexed by the highest weights of the irreducible representations of the algebra, are defined by means of a recursive formula, and some useful recurrence relations of the type character$\times$polynomial are shown. We think that it is a good idea to begin this program with a concrete case, and we choose to work in this article the problem associated with D_4 because of the triality symmetry exhibited by this algebra, which will helps us in simplifying the treatment.

The organization of the paper is as follows. In Sec. II, we explain how to express the Calogero–Sutherland Hamiltonian in terms of the fundamental characters of the algebra and how to solve the Schrödinger equation. Then, in Sec. III, we obtain the main recurrence relations among the polynomials and use them to give algorithms to calculate some subsets of them. Section IV is devoted to finding the generating functions for some classes of characters and monomials functions of D_4. More recurrence relations and some other relevant results are included in Sec. V, and finally, in Sec. VI, we give some brief conclusions. Also, we offer two appendixes. In Appendix A, for the convenience of the reader, we collect some of the basic facts about D_4 which we use in the main text. In Appendix B we list some polynomials, characters, and monomial functions.

II. THE EIGENVALUE PROBLEM

The Hamiltonian operator for the trigonometric Calogero–Sutherland model related to the root system of a simple Lie algebra of rank r has the form

$$H=\frac{1}{2}(p,p)+\sum_{\alpha\in R^+}\kappa_\alpha(\kappa_\alpha-1)\sin^{-2}(\alpha,q), \tag{1}$$

where $q=(q_1,\ldots,q_r)$, $p=(p_1,\ldots,p_r)$, $(\,,\,)$ is the usual Euclidean inner product in $\mathbf{R}^r$, R^+ is the set of positive roots of the algebra, and κ_α are constants such that $\kappa_\alpha=\kappa_\beta$ if $\|\alpha\|=\|\beta\|$. In particular, for the case of the algebra D_4 (see Appendix A), this leads to the following Schrödinger equation:

$$\begin{gathered} H\Psi^\kappa=E(\kappa)\,\Psi^\kappa,\\ H=-\frac{1}{2}\Delta+\kappa(\kappa-1)\left(\sum_{j<k}^{4}\sin^{-2}(q_j-q_k)+\sum_{j<k}^{4}\sin^{-2}(q_j+q_k)\right),\quad \Delta=\sum_{j=1}^{4}\frac{\partial^2}{\partial q_j^2}. \end{gathered} \tag{2}$$

The q coordinates are assumed to take values in the $[0,\,\pi]$ interval, and therefore the equation can be interpreted as describing the dynamics of a system of four particles moving on the circle. Let us notice, however, that there is not translational invariance. We recapitulate some important facts about this model which follow from the general structure of the quantum Calogero–Sutherland models related to Lie algebras.[9] The ground state energy and (non-normalized) wave function are

$$E_0(\kappa)=2(\rho,\rho)\,\kappa^2=28\,\kappa^2, \tag{3}$$

$$\Psi_0^\kappa(q)=\left\{\prod_{j<k}^{4}\sin(q_j-q_k)\sin(q_j+q_k)\right\}^\kappa,$$

where ρ is the standard Weyl vector, $\rho=\frac{1}{2}\Sigma_{\alpha\in R^+}\alpha$, with the sum extended over all the positive roots of D_4. The excited states depend on a four-tuple of quantum numbers $\mathbf{m}=(m_1,m_2,m_3,m_4)$,

$$H\Psi_{\mathbf{m}}^\kappa=E_{\mathbf{m}}(\kappa)\,\Psi_{\mathbf{m}}^\kappa,$$
$$E_{\mathbf{m}}(\kappa)=2(\lambda+\kappa\rho,\lambda+\kappa\rho), \tag{4}$$

where λ is the highest weight of the irreducible representation of D_4 labeled by $\mathbf{m}$, i.e., $\lambda=\Sigma_{i=1}^4 m_i\lambda_i$, and λ_i are the fundamental weights of D_4. By substitution in (4) of

$$\Psi_{\mathbf{m}}^\kappa(q)=\Psi_0^\kappa(q)\,\Phi_{\mathbf{m}}^\kappa(q), \tag{5}$$

we are led to the eigenvalue problem

$$-\Delta^\kappa\Phi_{\mathbf{m}}^\kappa=\varepsilon_{\mathbf{m}}(\kappa)\,\Phi_{\mathbf{m}}^\kappa \tag{6}$$

with

$$\Delta^\kappa=\frac{1}{2}\Delta+\kappa\sum_{j<k}^{4}\left(\operatorname{ctg}(q_j-q_k)\left(\frac{\partial}{\partial q_j}-\frac{\partial}{\partial q_k}\right)+\operatorname{ctg}(q_j+q_k)\left(\frac{\partial}{\partial q_j}+\frac{\partial}{\partial q_k}\right)\right) \tag{7}$$

and

$$\varepsilon_{\mathbf{m}}(\kappa)=E_{\mathbf{m}}(\kappa)-E_0(\kappa)=2(\lambda,\lambda+2\kappa\rho). \tag{8}$$

Introducing the inverse Cartan matrix $A_{jk}^{-1}=(\lambda_j,\lambda_k)$, we can give a more explicit expression for $\varepsilon_{\mathbf{m}}(\kappa)$:

$$\varepsilon_{\mathbf{m}}(\kappa)=2\sum_{j,k=1}^{4}A_{jk}^{-1}m_jm_k+4\kappa\sum_{j,k=1}^{4}A_{jk}^{-1}m_j=2(m_1^2+m_3^2+m_4^2)+4m_2^2+2(m_1m_3+m_1m_4+m_3m_4)+4m_2(m_1+m_3+m_4)+12\kappa(m_1+m_3+m_4)+20\kappa m_2. \tag{9}$$

The main problem is to solve Eq. (6). As has been shown for the case of the algebra A_n,[13–15] the best way to do that is to use a set of independent variables which are invariant under the Weyl symmetry of the Hamiltonian, namely, the characters of the four fundamental representations of the algebra D_4. Unfortunately, the expression of these characters in terms of the q-variables (which play the role of coordinates on the maximal torus of D_4) is not very simple. Denoting the character of the irreducible representation of maximal weight λ_j as z_j, we find

$$z_1=\sum_{j=1}^{4} x_j+\sum_{j=1}^{4} x_j^{-1},$$

$$z_2=\sum_{i<j}^{4} x_i x_j+\sum_{i<j}^{4} (x_i x_j)^{-1}+\sum_{i,j}^{4} x_i^{-1} x_j,$$

$$z_3=\overline{x}\sum_{i=1}^{4}\frac{1}{x_i}+\frac{1}{\overline{x}}\sum_{i=1}^{4} x_i,$$

$$z_4=\overline{x}+\frac{1}{\overline{x}}+\frac{1}{\overline{x}}\sum_{i<j}^{4} x_i x_j,$$

where $x_j=e^{2iq_j}$, and $\overline{x}=\sqrt{x_1x_2x_3x_4}$. These expressions make the direct change of variables from q_i to z_k quite cumbersome. We refrain from trying that approach, and choose instead an indirect route which has the further advantage of also being applicable to other algebras in which the expressions for the characters are even more involved. We can infer from (7) the structure of Δ^{κ} when written in the z-variables:

$$\Delta^{\kappa}=\sum_{j,k=1}^{4} a_{jk}(z_i)\,\partial_{z_j}\partial_{z_k}+\sum_{j=1}^{4}[b_j^{(0)}(z_i)+\kappa b_j^{(1)}(z_i)]\partial_{z_j}. \tag{10}$$

On the other hand, as is well known,[12] the $\Phi_{\mathbf{m}}^{\kappa}$ are polynomials which, with some precise partial ordering for the monomials to be described later, start as follows:

$$\Phi_{\mathbf{m}}^{\kappa}(z_i)=P_{\mathbf{m}}^{\kappa}(z_i)=z_1^{m_1}z_2^{m_2}z_3^{m_3}z_4^{m_4}+\cdots. \tag{11}$$

Therefore, making use of (9), we conclude that

$$\begin{aligned} a_{jk}(z_i)&=2\,A_{jk}^{-1}\,z_jz_k+\text{lower order terms},\\ b_j^{(r)}(z_i)&=c_j^{(r)}z_j+d_j^{(r)},\quad r=0,1. \end{aligned} \tag{12}$$

Now, to obtain the full expressions for these coefficients, we rely on the fact that, for $\kappa=1$, the $P_{\mathbf{m}}^{\kappa}$ polynomial gives the character of the irreducible representation of D_4 with maximal weight $\Sigma_{i=1}^{4} m_i\lambda_i$, while for $\kappa=0$ the same polynomial is the corresponding symmetric monomial function.[9] Both, characters and monomial functions, can be computed by using the information available in the literature (see, for instance, the ''Reference Chapter'' of Ref. 19). In fact, the following short list of polynomials

$$P_{2,0,0,0}^{(1)}(z)=z_1^2-z_2-1,$$

$$P_{1,1,0,0}^{(1)}(z)=z_1z_2-z_3z_4,$$

$$P_{1,0,1,0}^{(1)}(z)=z_1z_3-z_4,$$

$$P_{0,2,0,0}^{(1)}(z)=z_2^2-z_1z_3z_4+z_2,$$

$$P_{2,0,0,0}^{(0)}(z)=z_1^2-2z_2$$

is all we need to obtain Δ^κ. By substituting these polynomials in (6) and using (9), (10), (12) and the triality symmetry (which here implies that the final expression for Δ^κ should be invariant under permutations of the indices 1,3,4), we get enough simple linear algebraic equations to fix all the coefficients. We give here only the final result:

$$\begin{aligned}\frac{1}{2}\Delta^\kappa=&(z_1^2-2z_2-8)\partial_{z_1}^2+[2z_2^2-4(z_1^2+z_3^2+z_4^2)-2z_1z_3z_4+8z_2]\partial_{z_2}^2+(z_3^2-2z_2-8)\partial_{z_3}^2+(z_4^2\\&-2z_2-8)\partial_{z_4}^2+(2z_1z_2-6z_3z_4-8z_1)\,\partial_{z_1}\partial_{z_2}+(z_1z_3-8z_4)\,\partial_{z_1}\partial_{z_3}+(z_1z_4-8z_3)\,\partial_{z_1}\partial_{z_4}\\&+(2z_2z_3-6z_1z_4-8z_3)\,\partial_{z_2}\partial_{z_3}+(2z_2z_4-6z_1z_3-8z_4)\,\partial_{z_2}\partial_{z_4}+(z_3z_4-8z_1)\,\partial_{z_3}\partial_{z_4}+(6\kappa\\&+1)z_1\partial_{z_1}+[2(5\kappa+1)z_2+8(\kappa-1)]\,\partial_{z_2}+(6\kappa+1)z_3\partial_{z_3}+(6\kappa+1)z_4\partial_{z_4}.\end{aligned}\tag{13}$$

Once the explicit expression for the operator Δ^κ in the z variables is given, the Schrödinger equation can be solved iteratively. By direct application of Δ^κ to $z^{\mathbf{m}}\equiv z_1^{m_1}z_2^{m_2}z_2^{m_3}z_4^{m_4}$, we find

$$\begin{aligned}\Delta^\kappa z^{\mathbf{m}}=&\varepsilon_{\mathbf{m}}(\kappa)\,z^{\mathbf{m}}-\sum_{i=1}^{4}a_{\mathbf{m}}^i z^{\mathbf{m}-\alpha_i}-\sum_{j\in I}b_{\mathbf{m}}^j z^{\mathbf{m}-(\alpha_2+\alpha_j)}-\sum_{ij\in T}c_{\mathbf{m}}^{ij}z^{\mathbf{m}-(\alpha_2+\alpha_i+\alpha_j)}\\&-2a_{\mathbf{m}}^2\sum_{ij\in T}z^{\mathbf{m}-(2\alpha_2+\alpha_i+\alpha_j)}-d_{\mathbf{m}}z^{\mathbf{m}-(\alpha_1+2\alpha_2+\alpha_3+\alpha_4)}-4\sum_{j\in I}a_{\mathbf{m}}^j z^{\mathbf{m}-(\alpha_1+2\alpha_2+\alpha_3+\alpha_4+\alpha_j)},\end{aligned}\tag{14}$$

where the sets of indices are $I=\{1,3,4\}$ and $T=\{13,14,34\}$, and

$$a_{\mathbf{m}}^i=4\,m_i(m_i-1),\quad b_{\mathbf{m}}^j=12m_2m_j,$$

$$c_{\mathbf{m}}^{ij}=16\,m_i\,m_j,\qquad d_{\mathbf{m}}(\kappa)=16\,m_2\left(2-m_2-\kappa+\sum_{j\in I}m_j\right).$$

All monomials in $\Delta^\kappa z^{\mathbf{m}}$ take the form $z^{\mathbf{m}-\mu}$ with μ as a positive root. Thus, the polynomial $P_{\mathbf{m}}^\kappa$ has the form

$$P_{\mathbf{m}}^\kappa(z)=\sum_{\mu\in Q^+(\mathbf{m})}c_\mu z^{\mathbf{m}-\mu},\tag{15}$$

where we choose the normalization $c_0=1$ and, if Q^+ is the cone of positive roots,

$$Q^+(\mathbf{m})=\{\mu\in Q^+|z^{\mathbf{m}-\mu}\ \text{is well defined if}\ z_1z_2z_3z_4=0\}.\tag{16}$$

The above-mentioned partial ordering of monomials is given simply by the height of μ, i.e., $z^{\mathbf{m}-\mu_1}>z^{\mathbf{m}-\mu_2}$ if $ht(\mu_1)<ht(\mu_2)$. From (14), the coefficients c_μ obey the iterative formula

$$c_\mu=\frac{N_\mu}{\varepsilon_{\mathbf{m}-\mu}(\kappa)-\varepsilon_{\mathbf{m}}(\kappa)}\tag{17}$$

with

$$N_\mu=\sum_{i=1}^{4} a^i_{\mathbf{m}-(\mu-\alpha_i)}\, c_{\mu-\alpha_i}+\sum_{j\in I} b^j_{\mathbf{m}-(\mu-\alpha_2-\alpha_j)}\, c_{\mu-(\alpha_2+\alpha_j)}+\sum_{ij\in T} c^{ij}_{\mathbf{m}-(\mu-\alpha_2-\alpha_i-\alpha_j)}\, c_{\mu-(\alpha_2+\alpha_i+\alpha_j)}$$

$$+2\sum_{ij\in T} a^2_{\mathbf{m}-(\mu-2\alpha_2-\alpha_i-\alpha_j)}\, c_{\mu-(2\alpha_2+\alpha_i+\alpha_j)}+d_{\mathbf{m}-(\mu-\alpha_1-2\alpha_2-\alpha_3-\alpha_4)}\, c_{\mu-(\alpha_1+2\alpha_2+\alpha_3+\alpha_4)}$$

$$+4\sum_{j\in I} a^j_{\mathbf{m}-(\mu-\alpha_1-2\alpha_2-\alpha_3-\alpha_4-\alpha_j)}\, c_{\mu-(\alpha_1+2\alpha_2+\alpha_3+\alpha_4+\alpha_j)}\,.$$

Used along with the explicit expressions for the roots given in Appendix A, this formula is suitable for the implementation on a symbolic computer program. A list of polynomials obtained through the use of the formula is offered in Appendix B.

III. THE STRUCTURE OF THE RECURRENCE RELATIONS

As is well known, all the systems of orthogonal polynomials in one indeterminate z, such that $P_m(z)=z^m+\cdots$, satisfy a recursive formula $z\,P_m(z)=a_m\,P_{m+1}(z)+b_m\,P_m(z)+c_m\,P_{m-1}(z)$. In particular, the orthogonal polynomials associated with the trigonometric Calogero–Sutherland model for the case of two particles and Lie algebra A_1 are the classical Gegenbauer polynomials, whose recursive formula is known to be

$$z\,P^\kappa_m(z)=P^\kappa_{m+1}(z)+\frac{m(m-1+2\kappa)}{(m-1+\kappa)(m+\kappa)}\,P^\kappa_{m-1}(z).$$

This formula is reminiscent of the Clebsch–Gordan series for A_1. In fact, for $\kappa=1$ it reduces exactly to this Clebsch–Gordan series: the polynomials are the characters of A_1 and the coefficents are equal to one. Immediately the question arises about the existence of analogous recurrence relations, i.e., with the structure of κ-deformations of the corresponding Clebsch–Gordan series, for the polynomials related to Calogero–Sutherland models associated with other simple Lie algebras. As was shown in Ref. 13, the answer turns out to be in the affirmative for all root systems, but to obtain the expressions for the deformed coefficients it is necessary to proceed through a case-by-case analysis. Once the coefficients are known, many applications are possible. The aim of this section is to fix the structure of the basic recurrence relations for the case of D_4 and to give a simple illustration of their use.

We will study the formulas for $z_i P^\kappa_{\mathbf{m}}(z)$, $i=1,2,3,4$, in full detail. Note, however, that there are different recurrence relations, obtained in a more general context, and sometimes known as (generalized) Pieri formulas.[20] Therefore, as $P^{(1)}_{\mathbf{m}}(z)=z_i$ for $m_j=(\delta_{ji})$, and the recursive formulas are deformations of the Clebsch–Gordan series, we need to know the weights of the irreducible representations whose integral dominant weights are λ_1, λ_2, λ_3, and λ_4. For the case of λ_1, λ_3, and λ_4, these representations have dimension eight. On the other hand, if we act on the highest weight with the Weyl group in the way explained in Appendix A, we obtain eight different weights. Thus, these representations include only one orbit of the Weyl group and we are done. For the case of λ_2, the representation has dimension 28 and the orbit of the Weyl group containing λ_2 has only 24 elements. But $\lambda_2=\alpha^+_{12}$, the highest root, and thus this representation is the adjoint one and includes a second orbit: the Cartan subalgebra, with four elements of weight zero. Thus, we can summarize.

- Weights in z_1: $\pm\lambda_1$, $\pm(\lambda_1-\lambda_2)$, $\pm(\lambda_2-\lambda_3-\lambda_4)$, $\pm(\lambda_3-\lambda_4)$.
- Weights in z_2: $\pm\lambda_2$, $\pm(\lambda_2-2\lambda_j)$, $\pm(2\lambda_2-\lambda_1-\lambda_3-\lambda_4)$, $\pm(\lambda_2+\lambda_i-\lambda_j-\lambda_k)$, $\pm(\lambda_i+\lambda_j-\lambda_k)$, $\pm(\lambda_2-\lambda_1-\lambda_3-\lambda_4)$, 0, with $i,j,k\in I$.
- Weights in z_3: $\pm\lambda_3$, $\pm(\lambda_3-\lambda_2)$, $\pm(\lambda_2-\lambda_1-\lambda_4)$, $\pm(\lambda_1-\lambda_4)$.
- Weights in z_4: $\pm\lambda_4$, $\pm(\lambda_4-\lambda_2)$, $\pm(\lambda_2-\lambda_1-\lambda_3)$, $\pm(\lambda_1-\lambda_3)$.

With these weights, the structure of the recurrence relations results to be as follows:

$$z_1 P^{\kappa}_{m_1,m_2,m_3,m_4}(z) = P^{\kappa}_{m_1+1,m_2,m_3,m_4}(z) + a^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2,m_3,m_4}(z) + b^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1+1,m_2-1,m_3,m_4}(z)$$
$$+ c^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2+1,m_3,m_4}(z) + d^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2+1,m_3-1,m_4-1}(z)$$
$$+ e^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2-1,m_3+1,m_4+1}(z) + f^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2,m_3+1,m_4-1}(z)$$
$$+ g^1_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2,m_3-1,m_4+1}(z),$$

$$z_2 P^{\kappa}_{m_1,m_2,m_3,m_4}(z) = P^{\kappa}_{m_1,m_2+1,m_3,m_4}(z) + A_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2-1,m_3,m_4}(z)$$
$$+ B_{\mathbf{m}}(\kappa)^{1\pm}\, P^{\kappa}_{m_1\pm 2,m_2\mp 1,m_3,m_4}(z) + B_{\mathbf{m}}(\kappa)^{3\pm}\, P^{\kappa}_{m_1,m_2\mp 1,m_3\pm 2,m_4}(z)$$
$$+ B_{\mathbf{m}}(\kappa)^{4\pm}\, P^{\kappa}_{m_1,m_2\mp 1,m_3,m_4\pm 2}(z) + C_{\mathbf{m}}(\kappa)^{\pm}\, P^{\kappa}_{m_1\mp 1,m_2\pm 2,m_3\mp 1,m_4\mp 1}(z)$$
$$+ D_{\mathbf{m}}(\kappa)^{1\pm}\, P^{\kappa}_{m_1\pm 1,m_2\pm 1,m_3\mp 1,m_4\mp 1}(z) + D_{\mathbf{m}}(\kappa)^{3\pm}\, P^{\kappa}_{m_1\mp 1,m_2\pm 1,m_3\pm 1,m_4\mp 1}(z)$$
$$+ D_{\mathbf{m}}(\kappa)^{4\pm}\, P^{\kappa}_{m_1\mp 1,m_2\pm 1,m_3\mp 1,m_4\pm 1}(z) + E_{\mathbf{m}}(\kappa)^{1\pm}\, P^{\kappa}_{m_1\mp 1,m_2,m_3\pm 1,m_4\pm 1}(z)$$
$$+ E_{\mathbf{m}}(\kappa)^{3\pm}\, P^{\kappa}_{m_1\pm 1,m_2,m_3\mp 1,m_4\pm 1}(z) + E_{\mathbf{m}}(\kappa)^{4\pm}\, P^{\kappa}_{m_1\pm 1,m_2,m_3\pm 1,m_4\mp 1}(z)$$
$$+ F_{\mathbf{m}}(\kappa)^{\pm}\, P^{\kappa}_{m_1\pm 1,m_2\mp 1,m_3\pm 1,m_4\pm 1}(z) + G_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2,m_3,m_4}(z),$$

$$z_3 P^{\kappa}_{m_1,m_2,m_3,m_4}(z) = P^{\kappa}_{m_1,m_2,m_3+1,m_4}(z) + a^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2,m_3-1,m_4}(z) + b^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2-1,m_3+1,m_4}(z)$$
$$+ c^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2+1,m_3-1,m_4}(z) + d^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2+1,m_3,m_4-1}(z)$$
$$+ e^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1+1,m_2-1,m_3,m_4+1}(z) + f^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1+1,m_2,m_3,m_4-1}(z)$$
$$+ g^3_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2,m_3,m_4+1}(z),$$

$$z_4 P^{\kappa}_{m_1,m_2,m_3,m_4}(z) = P^{\kappa}_{m_1,m_2,m_3,m_4+1}(z) + a^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2,m_3,m_4-1}(z)$$
$$+ b^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2-1,m_3,m_4+1}(z) + c^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1,m_2+1,m_3,m_4-1}(z)$$
$$+ d^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2+1,m_3-1,m_4}(z) + e^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1+1,m_2-1,m_3+1,m_4}(z)$$
$$+ f^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1-1,m_2,m_3+1,m_4}(z) + g^4_{\mathbf{m}}(\kappa)\, P^{\kappa}_{m_1+1,m_2,m_3-1,m_4}(z),$$

where $B_{\mathbf{m}}(\kappa)^{1\pm}\, P^{\kappa}_{m_1\pm 2,m_2\mp 1,m_3,m_4}(z)$ means $B_{\mathbf{m}}(\kappa)^{1+}\, P^{\kappa}_{m_1+2,m_2-1,m_3,m_4}(z) + B_{\mathbf{m}}(\kappa)^{1-}\, P^{\kappa}_{m_1-2,m_2+1,m_3,m_4}(z)$, etc., and it is understood that all polynomials involving negative quantum numbers are zero. The recurrence relations reflect triality in the fact that not all the coefficients appearing in these formulas are independent. There are coincidences upon permutations of the quantum numbers, for instance

$$a^1_{m_1,m_2,m_3,m_4} = a^3_{m_3,m_2,m_1,m_4} = a^4_{m_4,m_2,m_3,m_1}, \tag{18}$$

and similarly for $b^j_{\mathbf{m}}, c^j_{\mathbf{m}}, d^j_{\mathbf{m}}, e^j_{\mathbf{m}}, f^j_{\mathbf{m}}, g^j_{\mathbf{m}}$. In the same fashion, we have also

$$B^{1\pm}_{m_1,m_2,m_3,m_4} = B^{3\pm}_{m_3,m_2,m_1,m_4} = B^{4\pm}_{m_4,m_2,m_3,m_1} \tag{19}$$

and similarly for $D^{j\pm}_{\mathbf{m}}, E^{j\pm}_{\mathbf{m}}$.

As an example, let us consider a simple case in which only one of the quantum numbers is nonvanishing, namely,

$$z_1 P^{\kappa}_{m,0,0,0}(z) = P^{\kappa}_{m+1,0,0,0}(z) + a_m(\kappa)\, P^{\kappa}_{m-1,0,0,0}(z) + c_m(\kappa)\, P^{\kappa}_{m-1,1,0,0}(z), \tag{20}$$

where we write $a_m(\kappa) = a^1_{m,0,0,0}(\kappa)$ and $c_m(\kappa) = c^1_{m,0,0,0}(\kappa)$. Using formulas

$$P^{\kappa}_{m,0,0,0}(z) = z_1^m - \frac{m(m-1)[4\kappa^2 + 4(m-2)\kappa + (m-1)(m-2)]}{(m-1+\kappa)(m-1+3\kappa)(m-2+\kappa)} z_1^{m-2} - \frac{m(m-1)}{m-1+\kappa} z_1^{m-2} z_2 + \cdots,$$

$$P^{\kappa}_{m,1,0,0}(z) = z_1^m z_2 + \frac{4\,\kappa(\kappa-1)(m-2+2\kappa)}{(m+1+5\kappa)(m+2\kappa)(m-1+\kappa)} z_1^m + \cdots,$$

coming from (17), we obtain the coefficients in (20):

$$a_m(\kappa) = \frac{m(m+2\kappa)(m-1+4\kappa)(m-1+6\kappa)}{(m-1+\kappa)(m-1+3\kappa)(m+3\kappa)(m+5\kappa)},$$

$$c_m(\kappa) = \frac{m(m-1+2\kappa)}{(m+\kappa)(m-1+\kappa)}.$$

As a by-product of triality, we can also write two other recurrence relations with the same coefficients:

$$\begin{aligned} z_3 P^{\kappa}_{0,0,m,0}(z) &= P^{\kappa}_{0,0,m+1,0}(z) + a_m(\kappa)\, P^{\kappa}_{0,0,m-1,0}(z) + c_m(\kappa)\, P^{\kappa}_{0,1,m-1,0}(z), \\ z_4 P^{\kappa}_{0,0,0,m}(z) &= P^{\kappa}_{0,0,0,m+1}(z) + a_m(\kappa)\, P^{\kappa}_{0,0,0,m-1}(z) + c_m(\kappa)\, P^{\kappa}_{0,1,0,m-1}(z). \end{aligned} \tag{21}$$

The first of these recurrence relations can be used to devise an algorithm for the calculation of the polynomials of the form $P^{\kappa}_{m,0,0,0}(z)$ and $P^{\kappa}_{m,1,0,0}(z)$. By multiplying (20) by the differential operator $\Delta^{\kappa} - \varepsilon_{m-1,1,0,0}(\kappa)$, the term involving $P^{\kappa}_{m-1,1,1,0}$ cancels. Using the explicit expressions (9) and (13), we find

$$\begin{aligned} P^{\kappa}_{m+1,0,0,0} = {} & \frac{1}{4(m+\kappa)} [\Delta^{\kappa}, z_1]\, P^{\kappa}_{m,0,0,0}(z) - \frac{1+4\kappa}{2(m+\kappa)} z_1 P^{\kappa}_{m,0,0,0}(z) \\ & + \frac{m(m+2\kappa)(m-1+4\kappa)(m-1+6\kappa)}{(m-1+\kappa)(m-1+3\kappa)(m+\kappa)(m+3\kappa)} P^{\kappa}_{m-1,0,0,0}(z), \end{aligned}$$

where, from (13),

$$\begin{aligned} [\Delta^{\kappa}, z_1] = {} & 4(z_1^2 - 2z_2 - 8)\partial_{z_1} + 2\,(z_1 z_3 - 8z_4)\,\partial_{z_3} + 2\,(z_1 z_4 - 8z_3)\,\partial_{z_4} \\ & + 4\,(z_1 z_2 - 3z_3 z_4 - 4z_1)\,\partial_{z_2} + 2(6\kappa+1)\, z_1. \end{aligned}$$

Once the polynomials $P^{\kappa}_{m,0,0,0}(z)$ are known, the recurrence relation (20) provides a formula for each $P^{\kappa}_{m,1,0,0}(z)$:

$$c_{m+1}(\kappa)\, P^{\kappa}_{m,1,0,0}(z) = z_1\, P^{\kappa}_{m+1,0,0,0}(z) - P^{\kappa}_{m+2,0,0,0}(z) - a_{m+1}(\kappa)\, P^{\kappa}_{m,0,0,0}(z). \tag{22}$$

IV. SOME GENERATING FUNCTIONS

We present in this section the generating functions for some characters and symmetric monomial functions. Let us consider first the case of the monomial functions with only one nonvanishing quantum number in the form $P^{(0)}_{m,0,0,0}(z)$. The generating function for this subset is

$$F_0(t,z)=\sum_{m=0}^{\infty} t^m P^{(0)}_{m,0,0,0}(z). \tag{23}$$

In terms of the x variables, the general expression for these monomial functions is

$$P^{(0)}_{m,0,0,0}(x)=\sum_{j=1}^{4} (x_j^m+x_j^{-m}), \tag{24}$$

and, in particular, we define $P^{(0)}_{0,0,0,0}(z)=8$. In these variables, the computation of $F_0(t,x)$ only requires to sum the geometric series:

$$F_0(t,x)=\sum_{j=1}^{4}\left(\frac{1}{1-tx_j}+\frac{1}{1-\dfrac{t}{x_j}}\right). \tag{25}$$

The change to the original z variables can be done by the inspection of the coefficients of the powers of t in both the numerator and denominator of this rational expression, with the result

$$F_0(t,z)=\frac{N_0(t,z)}{D(t,z)}, \tag{26}$$

where

$$\begin{aligned} N_0(t,z)=&\,8-7z_1\,t+6z_2\,t^2-5(z_3z_4-z_1)\,t^3+4(z_3^2+z_4^2-2z_2-2)\,t^4\\ &-3(z_3z_4-z_1)\,t^5+2z_2\,t^6-z_1\,t^7, \end{aligned} \tag{27}$$

$$D(t,z)=1-z_1\,t+z_2\,t^2-(z_3z_4-z_1)\,t^3+(z_3^2+z_4^2-2z_2-2)\,t^4-(z_3z_4-z_1)\,t^5+z_2\,t^6-z_1\,t^7+t^8.$$

There is an alternative approach. As the monomial functions are eigenfunctions of $\Delta^{(0)}$ with eigenvalues $\varepsilon_{m,0,0,0}(0)=2m^2$, we have

$$\frac{1}{2}\Delta^{(0)}F_0(t,z)=\sum_{m=0}^{\infty} m^2 t^m P^{(0)}_{m,0,0,0}(z),$$

and, therefore, we can write a differential equation for $F_0(t,z)$:

$$[\tfrac{1}{2}\Delta^{(0)}-(t\ \ \partial_t)^2]F_0(t,z)=0, \qquad F_0(0,z)=8. \tag{28}$$

One can verify by substitution that (26) satisfies this equation. When $F_0(t,z)$ is known, we can easily obtain the generating function

$$G_0(t,z)=\sum_{m=0}^{\infty} t^m P^{(0)}_{m,1,0,0}(z) \tag{29}$$

by only recalling (20), which for $\kappa=0$ is simply

$$z_1 P^{(0)}_{m,0,0,0}(z)=P^{(0)}_{m+1,0,0,0}(z)+P^{(0)}_{m-1,0,0,0}(z)+P^{(0)}_{m-1,1,0,0}(z). \tag{30}$$

This gives

$$G_0(t,z)=\frac{M_0(t,z)}{D(t,z)} \tag{31}$$

with

$$M_0(t,z)=z_2-4+(6\,z_1-3\,z_3z_4)\,t+(-8-2\,z_1^2-10\,z_2-z_2^2+4\,z_3^2+2\,z_1z_3z_4+4\,z_4^2)\,t^2$$
$$+(10\,z_1+5\,z_1z_2-3\,z_1z_3^2-4\,z_3z_4+z_2z_3z_4-3\,z_1z_4^2)\,t^3$$
$$+(8\,z_2-4\,z_1^2+2\,z_2^2-z_2z_3^2+4\,z_1z_3z_4-z_2z_4^2)\,t^4+(-6\,z_1-6\,z_1z_2-z_3z_4+z_2z_3z_4)\,t^5$$
$$+(8+6z_1^2+2\,z_2-z_2^2)\,t^6+(-10\,z_1+z_1z_2)\,t^7+(4-z_2)\,t^8.$$

The computation of the generating functions for the characters $P^{(1)}_{m,0,0,0}$ and $P^{(1)}_{m,1,0,0}$ goes through similar arguments. In this case, the eigenvalues are $\varepsilon_{m,0,0,0}(1)=2m^2+12m$. Hence,

$$F_1(t,z)=\sum_{m=0}^{\infty} t^m P^{(1)}_{m,0,0,0}(z)\,, \qquad P^{(1)}_{0,0,0,0}(z)\equiv 1 \tag{32}$$

is the solution of

$$[\tfrac{1}{2}\Delta^{(1)}-(t\,\partial_t)^2-6t\,\partial_t]F_1(t,z)=0, \qquad F_1(0,z)=1. \tag{33}$$

The Weyl character formula implies that the denominator of $F_1(t,z)$ should be the same $D(t,z)$ found before. Thus, we try an ansatz

$$F_1(t,z)=\frac{N_1(t,z)}{D(t,z)} \tag{34}$$

and obtain the simple answer

$$N_1(t,z)=1-t^2. \tag{35}$$

Applying the recurrence relation (20) we obtain the generating function $G_1(t,z)$ for the characters $P^{(1)}_{m,1,0,0}$:

$$G_1(t,z)=\frac{1}{D(t,z)}\{z_2-z_3z_4t+(z_3^2+z_4^2-2z_2-1)\,t^2-(z_3z_4-z_1)\,t^3+z_2\,t^4-z_1\,t^5+t^6\}. \tag{36}$$

V. MORE RECURRENCE RELATIONS AND OTHER RESULTS

In this section, we give the remaining recurrence relations involving the product of a fundamental character times a polynomial with only one nonvanishing quantum number. We also comment on the existence of some peculiar values for κ for which the polynomials associated with some special excited states are proportional to integer powers of the fundamental state wave function.

To obtain the mentioned recurrence relations, it is necessary to compute the coefficients of a limited number of terms of the polynomials involved. Once the form of these terms is known, we can obtain the coefficients in the recurrence relations solving a system of linear algebraic equations. We do not give here the full expressions for the coefficients of the required terms, because some of them are too long, and only list them:

$$P^{\kappa}_{1,0,m,0}(z)=z_1z_3^m+A\,z_3^{m-1}z_4+\cdots,$$

$$P^{\kappa}_{0,m,0,0}(z)=z_2^m+B\,z_2^{m-1}+C\,z_2^{m-2}+D\,z_1z_2^{m-2}z_3z_4+E\,z_1z_2^{m-3}z_3z_4$$
$$+F\,(z_1^2z_2^{m-2}+z_2^{m-2}z_3^2+z_2^{m-2}z_4^2)+\cdots,$$

$$P^{\kappa}_{1,m,0,0}(z)=z_1z_2^m+G\,z_1z_2^{m-1}z_4+H\,z_2^{m-1}z_3z_4+\cdots,$$

$$P^{\kappa}_{0,m,1,1}(z)=z_2^m z_3 z_4+I\,z_1 z_2^m+\cdots,$$

$$P^{\kappa}_{m,0,0,0}(z)=z_1^m+J\,z_1^{m-2}+K\,z_1^{m-2}z_2+\cdots,$$

$$P^{\kappa}_{m,1,0,0}(z)=z_1^m z_2+L\,z_1^{m-2}z_2+N\,z_1^{m-1}z_3 z_4+M\,z_1^m+\cdots,$$

$$P^{\kappa}_{m,0,1,1}(z)=z_1^m z_3 z_4+N\,z_1^{m-1}z_2+O\,z_1^{m+1}+\cdots,$$

$$P^{\kappa}_{1,m,1,1}(z)=z_1 z_2^m z_3 z_4+P\,z_2^m+Q\,z_1 z_2^{m-1}z_3 z_4+R\,(z_1^2 z_2^m+z_2^m z_3^2+z_2^m z_4^2)+S\,z_2^{m+1}+\cdots,$$

$$P^{\kappa}_{2,m,0,0}(z)=z_1^2 z_2^m+T\,z_2^m+U\,z_1 z_2^{m-1}z_3 z_4+W\,z_2^{m+1}+\cdots.$$

The use of the quantities denoted A to W in the previous formulas in the general structure of the recurrence relations give the following results:

• Formulas of type $z_1 P^{\kappa}_{0,0,m,0}(z)$:

$$z_1\,P^{\kappa}_{0,0,m,0}(z)=P^{\kappa}_{1,0,m,0}(z)+b_m(\kappa)P_{0,0,m-1,1}(z),$$

$$z_1\,P^{\kappa}_{0,0,0,m}(z)=P^{\kappa}_{1,0,0,m}(z)+b_m(\kappa)P_{0,0,1,m-1}(z),$$

$$z_3\,P^{\kappa}_{m,0,0,0}(z)=P^{\kappa}_{m,0,1,0}(z)+b_m(\kappa)P_{m-1,0,0,1}(z),$$

$$z_3\,P^{\kappa}_{0,0,0,m}(z)=P^{\kappa}_{0,0,1,m}(z)+b_m(\kappa)P_{1,0,0,m-1}(z),$$

$$z_4\,P^{\kappa}_{m,0,0,0}(z)=P^{\kappa}_{m,0,0,1}(z)+b_m(\kappa)P_{m-1,0,1,0}(z),$$

$$z_4\,P^{\kappa}_{0,0,m,0}(z)=P^{\kappa}_{0,0,m,1}(z)+b_m(\kappa)P_{1,0,m-1,0}(z)$$

with

$$b_m(\kappa)=\frac{m(m-1+4\kappa)}{(m-1+\kappa)(m+3\kappa)}\ .$$

• Formulas of type $z_1\,P^{\kappa}_{0,m,0,0}(z)$:

$$z_1\,P^{\kappa}_{0,m,0,0}(z)=P^{\kappa}_{1,m,0,0}(z)+d_m(\kappa)P_{1,m-1,0,0}(z)+e_m(\kappa)P^{\kappa}_{0,m-1,1,1}(z),$$

$$z_3\,P^{\kappa}_{0,m,0,0}(z)=P^{\kappa}_{0,m,1,0}(z)+d_m(\kappa)P_{0,m-1,1,0}(z)+e_m(\kappa)P^{\kappa}_{1,m-1,0,1}(z),$$

$$z_4\,P^{\kappa}_{0,m,0,0}(z)=P^{\kappa}_{0,m,0,1}(z)+d_m(\kappa)P_{0,m-1,0,1}(z)+e_m(\kappa)P^{\kappa}_{1,m-1,1,0}(z)$$

with

$$d_m(\kappa)=\frac{2m(m+\kappa)(m-1+3\kappa)(m-1+4\kappa)(2m-1+6\kappa)}{(m-1+\kappa)(m-1+2\kappa)(m+3\kappa)(2m-1+5\kappa)(2m+5\kappa)},$$

$$e_m(\kappa)=\frac{m(m-1+3\kappa)}{(m-1+\kappa)(m+2\kappa)}.$$

• Formulas of type $z_2\,P^{\kappa}_{m,0,0,0}(z)$:

$$z_2\,P^{\kappa}_{m,0,0,0}(z)=P^{\kappa}_{m,1,0,0}(z)+f_m(\kappa)\,P_{m-2,1,0,0}(z)+g_m(\kappa)\,P^{\kappa}_{m-1,0,1,1}(z)+h_m(\kappa)\,P^{\kappa}_{m,0,0,0}(z),$$

$$z_2\,P^{\kappa}_{0,0,m,0}(z)=P^{\kappa}_{0,1,m,0}(z)+f_m(\kappa)\,P_{0,1,m-2,0}(z)+g_m(\kappa)P^{\kappa}_{1,0,m-1,1}(z)+h_m(\kappa)\,P^{\kappa}_{0,0,m,0}(z),$$

$$z_2\,P^{\kappa}_{0,0,0,m}(z)=P^{\kappa}_{0,1,0,m}(z)+f_m(\kappa)\,P_{0,1,0,m-2}(z)+g_m(\kappa)\,P^{\kappa}_{1,0,1,m-1}(z)+h_m(\kappa)\,P^{\kappa}_{0,0,0,m}(z)$$

with

$$f_m(\kappa)=\frac{m(m-1)(m-2+2\kappa)(m+2\kappa)(m-1+4\kappa)(m-1+5\kappa)}{(m-2+\kappa)(m-1+\kappa)^2(m-1+3\kappa)(m+3\kappa)(m+4\kappa)},$$

$$g_m(\kappa)=\frac{m(m-1+3\kappa)}{(m-1+\kappa)(m+2\kappa)},$$

$$h_m(\kappa)=\frac{4[-3\kappa^3+5\kappa^2+(6m-1)\kappa+(m^2-1)]}{(m-1+\kappa)(1+3\kappa)(m+1+5\kappa)}.$$

• Formula for $z_2\,P^{\kappa}_{0,m,0,0}(z)$:

$$\begin{aligned}z_2\,P^{\kappa}_{0,m,0,0}(z)=&P^{\kappa}_{0,m+1,0,0}(z)+k_m(\kappa)\,P_{0,m-1,0,0}(z)+p_m(\kappa)\,P^{\kappa}_{1,m-1,1,1}(z)+q_m(\kappa)\,P^{\kappa}_{1,m-2,1,1}(z)\\&+r_m(\kappa)\,[P^{\kappa}_{2,m-1,0,0}(z)+P^{\kappa}_{0,m-1,2,0}(z)+P^{\kappa}_{0,m-1,0,2}(z)]+s_m(\kappa)\,P^{\kappa}_{0,m,0,0}(z)\end{aligned}$$

with

$$\begin{aligned}k_m(\kappa)=&\frac{4m(m+\kappa)^2(m+2\kappa)(m-1+3\kappa)(m-1+4\kappa)^2(2m-1+4\kappa)(m-1+5\kappa)(2m-1+6\kappa)}{(m-1+\kappa)(m-1+2\kappa)^2(m+3\kappa)^2(m+4\kappa)(2m-2+5\kappa)(2m-1+5\kappa)^2(2m+5\kappa)},\end{aligned}$$

$$p_m(\kappa)=\frac{m(m-1+2\kappa)}{(m-1+\kappa)(m+\kappa)},$$

$$q_m(\kappa)=\frac{2m(m-1)(m+\kappa)^2(m-2+2\kappa)(m-1+3\kappa)^3(2m-1+6\kappa)}{(m-2+\kappa)(m-1+\kappa)^2(m-1+2\kappa)^2(m+2\kappa)^2(2m-1+5\kappa)(2m+5\kappa)},$$

$$r_m(\kappa)=\frac{m(m+\kappa)(m-1+3\kappa)(m-1+4\kappa)}{(m-1+\kappa)(m-1+2\kappa)(m+2\kappa)(m+3\kappa)},$$

$$s_m(\kappa)=\frac{-4t_m(\kappa)}{(\kappa+1)(m-1+\kappa)(m+1+4\kappa)(2m-1+5\kappa)(2m+1+5\kappa)},$$

$$\begin{aligned}t_m(\kappa)=&(-1+5m^2-4m^4)+(2+25m-7m^2-40m^3+2m^4)\kappa+(20-35m-123m^2+20m^3)\kappa^2\\&+(-22-115m+63m^2)\kappa^3+(-19+65m)\kappa^4+20\kappa^5.\end{aligned}$$

Finally, we mention that for $\kappa=-\frac{1}{2}(n-1)$, $n\in\mathbf{N}$, the polynomials associated with the dominant weight which is n times the Weyl vector ρ are proportional to a power of the ground state wave function, namely,

$$P^{-(1/2)(n-1)}_{n\rho}=(-1)^n\,2^{12n}\left\{\prod_{j<k}^{4}\sin(q_j-q_k)\sin(q_j+q_k)\right\}^n.$$

This formula can be verified quite easily by direct application of $\Delta^{-(1/2)(n-1)}$ in the form (7) to the right-hand side: one finds that the Schrödinger equation (6) with the appropriate eigenvalue is satisfied. The most convenient way to fix the proportionality constant is by performing an analytic continuation to complex q_i and considering the region $x_i \in \mathbf{R}$ and $x_1 \gg x_2 \gg x_3 \gg x_4 \gg 0$. Then, the polynomials are dominated by the leading order term, $P_{n\rho}^{-(1/2)(n-1)} \simeq z_1^n z_2^n z_3^n z_4^n$, and, on the other hand, using the formulas for the fundamental characters displayed in Sec. II, one finds $z_1 z_2 z_3 z_4 \simeq x_1^3 x_2^2 x_3$ and $\Pi_{j<k}^4 \sin(q_j - q_k)\sin(q_j + q_k) \simeq -2^{-12} x_1^3 x_2^2 x_3$. This gives the proportionality constant written above.

VI. CONCLUSIONS

In this paper, we have shown how to solve the Schrödinger equation for the trigonometric Calogero–Sutherland model related to the Lie algebra D_4 and we have explored some properties of the energy eigenfunctions. The main point is that the use of a Weyl-invariant set of variables, the characters of the fundamental representations, leads to a formulation of the Schrödinger equation by means of a second-order differential operator with polynomial coefficients simple enough to make feasible a recursive method for the treatment of the spectral problem. The eigenfunctions provide a complete system of orthogonal polynomials in four variables, and these polynomials obey recurrence relations which are extensions of the Clebsch–Gordan series of the algebra. The structure of some of these recurrence relations has been fixed and, for particular cases, the coefficients involved have been computed. Also, some generating functions for the polynomials with parameter $\kappa = 1$ and $\kappa = 0$ have been obtained. These generating functions can give some hints about the form of the generating function for general κ, see Ref. 21.

ACKNOWLEDGMENTS

A.M.P. would like to express his gratitude to the Max Planck Institut für Mathematik for hospitality. The work of J.F.N. and W.G.F. has been partially supported by the University of Oviedo, Vicerrectorado de Investigación, Grant MB-03-514-1.

APPENDIX A: SUMMARY OF RESULTS ON THE LIE ALGEBRA D_4

In this appendix, we review some standard facts about the root and weight systems of the Lie algebra D_4 that the reader could find useful to follow the main text. More extensive and sound treatments of these topics can be found in many excellent textbooks, see for instance Refs. 19 and 22.

The most convenient explicit representation of D_4 is

$$D_4 = \left\{ \begin{pmatrix} m & b \\ c & -m^t \end{pmatrix} \;\middle|\; m, b, c \text{ real } 4\times 4 \text{ matrices and } b^t = -b,\ c^t = -c \right\}.$$

This gives dim $D_4 = 28$. One can choose the following linear basis:

$$M_{jk} = E_{j,k} - E_{4+j,4+k}, \quad j,k = 1,2,3,4,$$

$$B_{jk} = E_{j,4+k} - E_{k,4+j}, \quad j,k = 1,2,3,4, \quad j<k,$$

$$C_{jk} = E_{4+j,k} - E_{4+k,j}, \quad j,k = 1,2,3,4, \quad j<k$$

with $(E_{i,j})_{kl} = \delta_{ik}\delta_{jl}$. The Cartan subalgebra is

$$H = \left\{ h = \sum_{i=1}^{4} c_i M_{ii} \;\middle|\; c_i \in \mathbf{R} \right\}$$

and this confirms that the rank of D_4 is four. The matrix commutators

TABLE I. Heights of positive roots.

Height	Positive roots
1	$\alpha_1,\ \alpha_2,\ \alpha_3,\ \alpha_4$
2	$\alpha_{13}=\alpha_1+\alpha_2,\ \alpha_{24}=\alpha_2+\alpha_3,\ \alpha_{24}^{+}=\alpha_2+\alpha_4$
3	$\alpha_{14}=\alpha_1+\alpha_2+\alpha_3,\ \alpha_{14}^{+}=\alpha_1+\alpha_2+\alpha_4,\ \alpha_{23}^{+}=\alpha_2+\alpha_3+\alpha_4$
4	$\alpha_{13}^{+}=\alpha_1+\alpha_2+\alpha_3+\alpha_4$
5	$\alpha_{12}^{+}=\alpha_1+2\alpha_2+\alpha_3+\alpha_4$

$$[h,M_{jk}]=(c_j-c_k)M_{jk},$$

$$[h,B_{jk}]=(c_j+c_k)B_{jk},$$

$$[h,C_{jk}]=-(c_j+c_k)C_{jk}$$

allow us to classify the 24 roots in two groups

$$\alpha_{jk}(h)=c_j-c_k,\quad j\neq k,$$

$$\alpha_{jk}^{\pm}(h)=\pm(c_j+c_k),\quad j<k.$$

One can extract the following basis of simple roots:

$$\alpha_1\equiv(1,\quad -1,\quad 0,\quad 0)=\alpha_{12},\quad \alpha_2\equiv(0,\quad 1,\quad -1,\quad 0)=\alpha_{23},$$

$$\alpha_3\equiv(0,\quad 0,\quad 1,\quad -1)=\alpha_{34},\quad \alpha_4\equiv(0,\quad 0,\quad 1,\quad 1)=\alpha_{34}^{+},$$

where we have given the decomposition of these roots in the basis of H^* dual to diag(M_{ii}), $i=1,2,3,4$. The Euclidean relations among the simple roots are

$$(\alpha_i,\alpha_i)=2,\quad i=1,2,3,4,$$

$$(\alpha_2,\alpha_i)=-1,\quad i=1,3,4,$$

$$(\alpha_i,\alpha_j)=0,\quad i=1,3,4.$$

Thus, the Cartan matrix reads

$$A=\begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & -1 \\ 0 & -1 & 2 & 0 \\ 0 & -1 & 0 & 2 \end{pmatrix}.$$

The positive roots are $\alpha_{ij},\alpha_{ij}^{+},i<j$, and they can be classified by heights as indicated in Table I. The Weyl group is easy to describe. The Weyl reflection on the hyperplane in H^* orthogonal to the root α is

$$s_\alpha(v)=v-2\frac{(\alpha,v)}{(\alpha,\alpha)}\alpha.$$

Applying this formula to $\alpha_{ij},\alpha_{ij}^{\pm}$, one readily finds that the most general Weyl reflection consists in a permutation of the components of v in the e_i basis plus an even number of changes of the signs of these components. This gives $|W|=192$ for the order of the Weyl group. The fundamental weights λ_k can be obtained from the equation $\alpha_i=\Sigma_{j=1}^{4}A_{ji}\lambda_j$. They are

$$\lambda_1=\tfrac{1}{2}(2\alpha_1+2\alpha_2+\alpha_3+\alpha_4)=\tfrac{1}{2}\ (2,\quad 0,\quad 0,\quad 0),$$

$$\lambda_2=\tfrac{1}{2}(2\alpha_1+4\alpha_2+2\alpha_3+2\alpha_4)=\tfrac{1}{2}\ (2,\quad 2,\quad 0,\quad 0),$$

$$\lambda_3=\tfrac{1}{2}(\alpha_1+2\alpha_2+2\alpha_3+\alpha_4)=\tfrac{1}{2}\ (1,\quad 1,\quad 1,\quad -1),$$

$$\lambda_4=\tfrac{1}{2}(\alpha_1+2\alpha_2+\alpha_3+2\alpha_4)=\tfrac{1}{2}\ (1,\quad 1,\quad 1,\quad 1),$$

and the geometry of the weight system is summarized by the relations

$$\|\lambda_1\|=\|\lambda_3\|=\|\lambda_4\|=1,\quad \|\lambda_2\|=\sqrt{2},$$

$$(\lambda_i,\lambda_2)=1,\ \ i=1,3,4,\quad (\lambda_i,\lambda_j)=\tfrac{1}{2},\quad i,j=1,3,4.$$

The Weyl vector is

$$\rho=\frac{1}{2}\sum_{\alpha\in R^+}\alpha=\sum_{j=1}^{4}\lambda_j=3\alpha_1+5\alpha_2+3\alpha_3+3\alpha_4=(3,\quad 2,\quad 1,\quad 0),$$

and the Weyl formula for dimensions applied to the irreducible representation associated to the integral dominant weight $\mathbf{m}=m_1\lambda_1+m_2\lambda_2+m_3\lambda_3+m_4\lambda_4$ gives

$$\dim r(\mathbf{m})=\prod_{\alpha\in R^+}\frac{(\alpha,\mathbf{m}+\rho)}{(\alpha,\rho)}=\frac{P}{1440}$$

with

$$P=\prod_{i=1}^{4}(m_i+1)\ \prod_{j}(m_2+m_j+2)\ \prod_{j<k}(m_2+m_j+m_k+3)$$
$$\times(m_1+m_2+m_3+m_4)(m_1+2m_2+m_3+m_4),$$

where the indices j,k take the values 1, 3, 4. In particular, for the fundamental representations, one finds:

$$\dim r(\lambda_1)=8,\quad \dim r(\lambda_2)=28,$$

$$\dim r(\lambda_3)=8,\quad \dim r(\lambda_4)=8.$$

APPENDIX B: SOME POLYNOMIALS, CHARACTERS, AND MONOMIAL FUNCTIONS

We list here all the polynomials, characters, and monomial functions with total degree lower or equal to three up to triality.

Polynomials:

$$P^{\kappa}_{1,0,0,0}(z)=z_1,$$

$$P^{\kappa}_{0,1,0,0}(z)=z_2+\frac{4(\kappa-1)}{5\kappa+1},$$

$$P^{\kappa}_{2,0,0,0}(z)=z_1^2-\frac{2}{1+\kappa}z_2-\frac{8\kappa}{(1+\kappa)(1+3\kappa)},$$

$$P^{\kappa}_{0,2,0,0}(z)=z_2^2-\frac{2}{1+\kappa}z_1z_3z_4-\frac{2(-1+\kappa)}{(1+\kappa)(1+2\kappa)}(z_1^2+z_3^2+z_4^2)+\frac{4(-3+5\kappa+6\kappa^2+4\kappa^3)}{(1+\kappa)(1+2\kappa)(3+5\kappa)}z_2$$
$$+\frac{16(-1+\kappa)(3+10\kappa+3\kappa^2+2\kappa^3)}{(1+\kappa)(1+2\kappa)(2+5\kappa)(3+5\kappa)},$$

$$P^{\kappa}_{1,1,0,0}(z)=z_1z_2-\frac{3}{1+2\kappa}z_3z_4+\frac{4(-1+\kappa)(-1+2\kappa)}{(1+2\kappa)(2+5\kappa)}z_1,$$

$$P^{\kappa}_{1,0,1,0}(z)=z_1z_3-\frac{4}{1+3\kappa}z_4,$$

$$P^{\kappa}_{3,0,0,0}(z)=z_1^3-\frac{6}{2+\kappa}z_1z_2+\frac{6}{(1+\kappa)(2+\kappa)}z_3z_4-\frac{12(1+2\kappa+2\kappa^2)}{(1+\kappa)(2+\kappa)(2+3\kappa)}z_1,$$

$$P^{\kappa}_{0,3,0,0}(z)=z_2^3-\frac{6}{2+\kappa}z_1z_2z_3z_4+\frac{6}{(1+\kappa)(2+\kappa)}(z_1^2z_3^2+z_1^2z_4^2+z_3^2z_4^2)-\frac{3(2+\kappa+\kappa^2)}{(1+\kappa)^2(2+\kappa)}(z_1^2z_2$$
$$+z_2z_3^2+z_2z_4^2)+\frac{6(10+17\kappa+21\kappa^2+10\kappa^3+2\kappa^4)}{5(1+\kappa)^3(2+\kappa)}z_2^2$$
$$-\frac{3(30+53\kappa+4\kappa^2-15\kappa^3+8\kappa^4)}{5(1+\kappa)^4(2+\kappa)}z_1z_3z_4-\frac{12\kappa(8+10\kappa+\kappa^2+\kappa^3)}{5(1+\kappa)^4(2+\kappa)}(z_1^2+z_3^2+z_4^2)$$
$$+\frac{12(30+119\kappa+159\kappa^2+124\kappa^3+80\kappa^4+24\kappa^5+4\kappa^6)}{5(1+\kappa)^4(2+\kappa)(4+5\kappa)}z_2$$
$$+\frac{16(-30+103\kappa+440\kappa^2+359\kappa^3+98\kappa^4+86\kappa^5+20\kappa^6+4\kappa^7)}{5(1+\kappa)^4(2+\kappa)(3+5\kappa)(4+5\kappa)},$$

$$P^{\kappa}_{2,1,0,0}(z)=z_1^2z_2-\frac{2}{1+\kappa}z_2^2-\frac{1+3\kappa}{(1+\kappa)^2}z_1z_3z_4+\frac{4(-1+\kappa)\kappa^2}{(1+\kappa)^2(3+5\kappa)}z_1^2+\frac{4}{(1+\kappa)^2}(z_3^2+z_4^2)$$
$$-\frac{4(9+27\kappa+28\kappa^2+16\kappa^3)}{(1+\kappa)^2(2+3\kappa)(3+5\kappa)}z_2-\frac{16(3+5\kappa+2\kappa^3)}{(1+\kappa)^2(2+3\kappa)(3+5\kappa)},$$

$$P^{\kappa}_{1,2,0,0}(z)=z_1z_2^2-\frac{2}{1+\kappa}z_1^2z_3z_4-\frac{1+3\kappa}{(1+\kappa)^2}z_2z_3z_4-\frac{2(-1+\kappa)}{(1+\kappa)(1+2\kappa)}z_1^3+\frac{5-\kappa}{(1+\kappa)^2}(z_1z_3^2+z_1z_4^2)$$
$$+\frac{4(-1+\kappa)(9+19\kappa+10\kappa^2+4\kappa^3)}{(1+\kappa)^2(1+2\kappa)(4+5\kappa)}z_1z_2-\frac{4(-1+\kappa)(-5+2\kappa)(1+3\kappa)}{(1+\kappa)^2(1+2\kappa)(4+5\kappa)}z_3z_4$$
$$+\frac{8(-9-57\kappa-72\kappa^2+28\kappa^3-2\kappa^4+4\kappa^5)}{(1+\kappa)^2(1+2\kappa)(3+5\kappa)(4+5\kappa)}z_1,$$

$$P^{\kappa}_{1,1,1,0}(z)=z_1z_2z_3-\frac{3}{1+2\kappa}(z_1^2z_4+z_3^2z_4)-\frac{8(-1+\kappa)}{(1+2\kappa)(2+3\kappa)}z_2z_4$$
$$+\frac{4(12+23\kappa-11\kappa^2+6\kappa^3)}{(1+2\kappa)(2+3\kappa)(3+5\kappa)}z_1z_3-\frac{8(3-22\kappa+4\kappa^2)}{(1+2\kappa)(2+3\kappa)(3+5\kappa)}z_4,$$

$$P^{\kappa}_{1,0,1,1}(z)=z_1z_3z_4-\frac{4}{1+3\kappa}(z_1^2+z_3^2+z_4^2)+\frac{12}{(1+2\kappa)(1+3\kappa)}z_2+\frac{16(1+5\kappa)}{(1+2\kappa)(1+3\kappa)^2}.$$

Characters:

$$P^{(1)}_{1,0,0,0}(z)=z_1,$$

$$P^{(1)}_{0,1,0,0}(z)=z_2,$$

$$P^{(1)}_{2,0,0,0}(z)=z_1^2-z_2-1,$$

$$P^{(1)}_{0,2,0,0}(z)=z_2^2+z_2-z_1z_3z_4,$$

$$P^{(1)}_{1,1,0,0}(z)=z_1z_2-z_3z_4,$$

$$P^{(1)}_{1,0,1,0}(z)=z_1z_3-z_4,$$

$$P^{(1)}_{3,0,0,0}(z)=z_1^3-2z_1z_2+z_3z_4-2z_1,$$

$$P^{(1)}_{0,3,0,0}(z)=z_2^3+3z_2^2+3z_2-2z_1z_2z_3z_4+z_1^2z_3^2+z_1^2z_4^2+z_3^2z_4^2-(z_1^2+z_3^2+z_4^2)z_2 -z_1z_3z_4-z_1^2-z_3^2-z_4^2+1,$$

$$P^{(1)}_{2,1,0,0}(z)=z_1^2z_2-z_2^2-z_1z_3z_4+z_3^2+z_4^2-2z_2-1,$$

$$P^{(1)}_{1,2,0,0}(z)=z_1z_2^2-z_1^2z_3z_4-z_2z_3z_4+z_1(z_3^2+z_4^2)-z_1,$$

$$P^{(1)}_{1,1,1,0}(z)=z_1z_2z_3+z_1z_3-(z_1^2+z_3^2)z_4+z_4,$$

$$P^{(1)}_{1,0,1,1}(z)=z_1z_3z_4-z_1^2-z_3^2-z_4^2+z_2+2.$$

Monomial functions:

$$P^{(0)}_{1,0,0,0}(z)=z_1,$$

$$P^{(0)}_{0,1,0,0}(z)=z_2-4,$$

$$P^{(0)}_{2,0,0,0}(z)=z_1^2-2z_2,$$

$$P^{(0)}_{0,2,0,0}(z)=z_2^2-2\,z_1z_3z_4+2\,z_1^2+2\,z_3^2+2\,z_4^2-4\,z_2-8,$$

$$P^{(0)}_{1,1,0,0}(z)=z_1z_2-3z_3z_4+2z_1,$$

$$P^{(0)}_{1,0,1,0}(z)=z_1z_3-4z_4,$$

$$P^{(0)}_{3,0,0,0}(z)=z_1^3-3z_1z_2+3z_3z_4-3z_1,$$

$$P^{(0)}_{0,3,0,0}(z)=z_2^3+6z_2^2+9z_2-3z_1z_2z_3z_4+3z_1^2z_3^2+3z_1^2z_4^2+3z_3^2z_4^2-3(z_1^2+z_3^2+z_4^2)z_2-9z_1z_3z_4-4,$$

$$P^{(0)}_{2,1,0,0}(z)=z_1^2z_2-2z_2^2-z_1z_3z_4+4z_3^2+4z_4^2-6z_2-8,$$

$$P^{(0)}_{1,2,0,0}(z)=z_1z_2^2-2z_1^2z_3z_4-z_2z_3z_4+2z_1^3+5z_1(z_3^2+z_4^2)-9z_1z_2-5z_3z_4-6z_1,$$

$$P^{(0)}_{1,1,1,0}(z)=z_1z_2z_3+8z_1z_3-3(z_1^2+z_3^2)z_4+4z_2z_4-4z_4,$$

$$P^{(0)}_{1,0,1,1}(z)=z_1z_3z_4-4z_1^2-4z_3^2-4z_4^2+12z_2+16.$$

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A note on Anderson localization for the random hopping model

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(Received 16 March 2003; accepted 6 June 2003)

This short note is devoted to the proof of Lifshitz tails and a Wegner estimate, and thus, band edge localization, for the random hopping model. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1616998]

I. INTRODUCTION

The model we consider in this short note is defined as follows: for $u \in \ell^2(\mathbb{Z}^d)$,

$$(H^\omega u)(x) = \sum_{|x-y|=1} \lambda^\omega((x,y))u(y), \quad x \in \mathbb{Z}^d. \tag{1.1}$$

The coefficients $\lambda^\omega((x,y))$ are real valued, bounded i.i.d. random variables satisfying the minimal symmetry requirement for H^ω to be self-adjoint. Namely, let $\mathcal{E}$ denote the set of edges $\{(x,y) \in \mathbb{Z}^d \times \mathbb{Z}^d;\ |x-y|=1\}$ (here, $|x|=|x_1|+\cdots+|x_d|$ if $x=(x_1, \ldots, x_d)$); define the set of undirected edges to be $\mathcal{E}' := \mathcal{E}/\sim$ [where $(x,y)\sim(x',y')$ if and only if $(x,y)=(x',y')$ or $(x,y)=(y',x')$]. The coefficients $\lambda^\omega(e)$, $e \in \mathcal{E}'$ are supposed to be i.i.d. random variables. Let us note here that (1.1) is a natural discrete analogue of the model studied in Ref. 4.

As H^ω is homogeneous of degree one in the variables $\lambda^\omega(e)$, $e \in \mathcal{E}'$, we may, without restriction, assume that

$$\operatorname*{ess\text{-}sup}_\omega |\lambda^\omega(e)| = 1. \tag{1.2}$$

Under these assumptions, for almost every ω, the operator H^ω is bounded and self-adjoint. Moreover, it is $\mathbb{Z}^d$-ergodic (see, e.g., Refs. 2 and 9); this guarantees that its spectrum is almost surely constant. Call it Σ. Using the classical criterion of Ref. 3, under assumption (1.2), one computes

$$\Sigma = [-2d, 2d].$$

The absolutely continuous, singular continuous and pure point components of the spectrum are also almost surely independent of ω.

The aim of the present note is to show that localization occurs near the edges of Σ.

The $\mathbb{Z}^d$-ergodicity also guarantees the existence of a density of states. In $\mathbb{Z}^d$, consider the cube of size N ($N>1$) and center 0. Denote it by Λ_N. Let Π_N be the projection (cutoff) on this cube. Then, the integrated density of states $k(E)$ of H^ω is defined by

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$$k(E) := \lim_{N \to +\infty} \frac{\#\{\text{eigenvalues of } \Pi_N H^\omega \Pi_N \text{ less than } E\}}{\#\Lambda_N}. \tag{1.3}$$

This limit exists almost surely (see Sec. II for more details); it is a nondecreasing function that takes values in $[0,1]$. Its points of growth are the points of Σ. It thus naturally defines a probability measure supported in Σ; we denote this measure by $\mathrm{d}k$.

It is well known (see, e.g., Refs. 1 and 10) that, in order to prove localization at spectral edges for models of the type (1.1), it is sufficient to prove that the integrated density of states satisfies two conditions:

(1) a regularity condition: e.g., k is Hölder continuous;
(2) a size condition: $\mathrm{d}k$ puts very little weight on the edges of the spectrum; this type of behavior is known as Lifshitz tails.

We prove the following.

Theorem 1.1: *The integrated density of states satisfies*

$$\lim_{\varepsilon \to 0^+} \frac{\log|\log k(-2d+\varepsilon)|}{\log \varepsilon} \leqslant -\frac{d}{2}$$

and

$$\lim_{\varepsilon \to 0^+} \frac{\log|\log(1-k(2d-\varepsilon))|}{\log \varepsilon} \leqslant -\frac{d}{2}. \tag{1.4}$$

To prove the regularity condition mentioned above, we need an additional assumption on the random variables. Let ν be the distribution of $\lambda^\omega(e)$. We assume the following.

$(H1)$: ν admits a locally Lipschitz continuous density, say $g(t)$.

Then, we prove the following.

Theorem 1.2: *The integrated density of states is locally Lipschitz continuous in* $\Sigma \backslash \{0\}$.

As noticed above, using multiscale analysis, Theorem 1.1 and Theorem 1.2 are sufficient to derive that the spectrum is exponentially and dynamically localized in a neighborhood of the points $2d$ and $-2d$ (see, e.g., Refs. 11 and 10).

II. SOME AUXILIARY OPERATORS

We now turn to the proofs of Theorem 1.1 and Theorem 1.2. We introduce some auxiliary periodic operators. For $N \in \mathbb{N}$, define

$$(H_N^\omega u)(x) = \sum_{|x-y|=1} \lambda_N^\omega((x,y))u(y), \quad x \in \mathbb{Z}^d, \tag{2.1}$$

where

$$\lambda_N^\omega((x,y)) = \lambda_N^\omega((x+\gamma, y+\gamma)) \quad \text{for } \gamma \in (2N+1)\mathbb{Z}^d.$$

The operator H_N^ω acting on $\ell^2(\mathbb{Z}^d)$ is $(2N+1)\mathbb{Z}^d$-periodic. Using Floquet theory (see Ref. 6 for details), we know that H_N^ω admits a density of states, say $k_N^\omega(E)$, that satisfies

$$k_N^\omega(E) = \frac{1}{(2\pi)^d} \int_{[-\pi/(2N+1), \pi/(2N+1)]^d} \#\{\text{eigenvalues of } M_N^\omega(\theta) \text{ in } [0,E]\}\mathrm{d}\theta, \tag{2.2}$$

where the $(2N+1)^d \times (2N+1)^d$-matrix $M_N^\omega(\theta)$ only differs from $\Pi_N H^\omega \Pi_N$ by an operator of rank at most CN^{d-1} (for some C independent of N, ω, and θ). Moreover, as a consequence of the $\mathbb{Z}^d$-ergodicity, one obtains, for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R})$,

$$\mathbb{E}[\langle \varphi, \mathrm{d}k_N^\omega(E)\rangle] := \mathbb{E}\left(\int \varphi(\lambda)\mathrm{d}k_N^\omega(\lambda) \right) = \mathbb{E}[\langle \delta_0, \varphi(H_N^\omega)\delta_0\rangle]. \tag{2.3}$$

Equation (2.3) implies $\mathbb{E}[\mathrm{d}k_N^\omega]$ converges when $N \to +\infty$; actually, one can show that the convergence of $\mathbb{E}[\mathrm{d}k_N^\omega]$ is exponentially fast (see, e.g., Refs. 5 and 6). The limit defines a positive measure. Then, (2.2), and the remark following this last equation imply that this measure is the density of states measure of the distribution function which is defined in (1.3).

As a result of this discussion, we see that to prove Theorems 1.1 and 1.2, we only need to prove analogous statements for $\mathbb{E}[k_N^\omega(E)]$ uniformly in N for N large enough.

III. THE PROOF OF THEOREM 1.1

Let us start with the Lifshitz behavior. First, we notice that we only need to deal with the lower edge of the spectrum; indeed, the unitary transform $(Uu)(x) = (-1)^{|x|}u(x)$ conjugates H^ω to $-H^\omega$.

To prove Theorem 1.1, it suffices to prove the following local energy estimate (see, e.g., Refs. 7 and 8).

Lemma 3.1: Fix $a \in (0,1)$. For $u \in \ell^2(\mathbb{Z})$, one has

$$\langle u, H_N^\omega u\rangle \geqslant \langle u, W_N^\omega u\rangle + a\langle |u|, H_0|u|\rangle \tag{3.1}$$

where

(i) *H_0 is the free Laplace operator of $\mathbb{Z}^d$ (i.e., it is equal to $2d + H^\omega$ when $\lambda^\omega(e) = 1$, $\forall e \in \mathcal{E}$); it is non-negative;*

(ii) *the potential W_N^ω is defined by*

$$W_N^\omega(x) = \sum_{\substack{e \in \mathcal{E} \\ x \in e}} \beta(\lambda_N^\omega(e)) \quad \text{where} \quad \beta(t) = \begin{cases} -|t| & \text{if } |t| \geqslant a \\ -a & \text{if } |t| < a. \end{cases} \tag{3.2}$$

(iii) *For $e \in \mathcal{E}$, we say that $x \in e$ if $e = (x,y)$ or $e = (y,x)$ for some y.*

Indeed, we note that the random potential W_N^ω takes values in $[-2d, 2d]$, its minimum is $-2d$. One can then apply the standard argument for operators of the form $H_0 + V^\omega$ (see, e.g., Refs. 5 and 6) to obtain the desired estimate on $\mathbb{E}[k_N^\omega(E)]$ (for N not too large). The exponentially fast convergence of $\mathbb{E}[\mathrm{d}k_N^\omega]$ to $\mathrm{d}k$ then gives (1.4) exactly in the same way as in Refs. 5 and 6.

Proof of Lemma 3.1: To alleviate notations, let us drop the sub- and super-indices ω and N. One start with rewriting

$$\langle u, Hu\rangle = 2\sum_{e \in \mathcal{E}'} \lambda(e)\mathrm{Re}(\overline{u(i(e))}u(t(e))), \tag{3.3}$$

where, for an edge $e = (x,y)$, we have defined $i(e) = x$ and $t(e) = y$.

Note that

$$2\,\mathrm{Re}(\overline{u_1}u_2) = \begin{pmatrix} u_1 & u_2 \end{pmatrix}^* \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{3.4}$$

Consider the spectrum of $\left(\begin{smallmatrix} 0 & \lambda \\ \lambda & 0 \end{smallmatrix}\right)$. Let us first assume that $\lambda = -t < 0$. Then,

$$\sigma\left[\begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}\right] = \{\lambda, -\lambda\} = \{-t, t\}, \tag{3.5}$$

respective eigenvectors being $\vec{e_1} = \binom{1/\sqrt{2}}{1/\sqrt{2}}$ and $\vec{e_2} = \binom{1/\sqrt{2}}{-1/\sqrt{2}}$. Let Π_1 and Π_2, respectively, be the projectors on $\vec{e_1}$ and $\vec{e_2}$; one computes

$$\Pi_1 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \Pi_1 = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \tag{3.6}$$

Using $\beta(\cdot)$ defined in Lemma 3.1, one writes

$$\begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix} = t\Pi_2 - t\Pi_1 \geqslant \beta(t)\Pi_1 + t\Pi_2 = \beta(t) + (t - \beta(t))\Pi_2 \geqslant \beta(t) + a\Pi_2.$$

This with (3.6) and (3.4) implies that, for $\lambda < 0$,

$$2\,\mathrm{Re}(\lambda \overline{u_1} u_2) \geqslant \beta(\lambda)(|u_1|^2 + |u_2|^2) + a\,||u_1| - |u_2||^2. \tag{3.7}$$

This relation is proved in the same way and holds for $\lambda > 0$.

If we now apply (3.7) to each term in the sum (3.3), we obtain

$$\begin{aligned} \langle u, Hu\rangle &= \sum_{e \in \mathcal{E}'} \beta(\lambda)(|u(i(e))|^2 + |u(t(e))|^2) + a \sum_{e \in \mathcal{E}'} ||u(i(e))| - |u(t(e))||^2 \\ &= \langle u, Wu\rangle + a\langle |u|, H_0|u|\rangle, \end{aligned}$$

where the potential W is defined by

$$W(x) = \sum_{\substack{e \in \mathcal{E} \\ x \in e}} \beta(\lambda_N^\omega(e)).$$

This completes the proof of (3.1) and thus of Lemma 3.1.

IV. THE PROOF OF THEOREM 1.2

To prove this lemma, we use the fact that H^ω, hence also $H_N^\omega = \Pi_N H^\omega \Pi_N$, is homogeneous of degree one with respect to the random variables $(\lambda^\omega(e))_{e \in \mathcal{E}'}$; indeed, one has

$$\sum_{e \in \mathcal{E}_N} \lambda^\omega(e) \frac{\partial}{\partial \lambda^\omega(e)} H_N^\omega = H_N^\omega. \tag{4.1}$$

Here, $\mathcal{E}_N$ denotes the set of edges that start and end in Λ_N [i.e., such that $i(e)$ and $t(e)$ belongs to Λ_N]. Note that $\mathcal{E}_N$ is of cardinal bounded by $C\#\Lambda_N$ (for some fixed $C > 0$).

One can use the classical argument of Wegner[12] to derive Theorem 1.2. For the reader's convenience, we detail this proof now.

Pick a compact interval $\Delta \subset (-\infty, 0)$, say, $\Delta \subset (-\infty, -c]$, $c > 0$ fixed. Let $E_N^\omega(\Delta)$ be the spectral projector of H_N^ω on the interval Δ. Then, we need to estimate

$$\#\{\text{eigenvalues of } \Pi_N H^\omega \Pi_N \text{ less than } E\} = \mathrm{tr}(E_N^\omega(\Delta)) = \mathrm{tr}\left(\int_\Delta \partial_E \mathbf{1}_{(-\infty, 0]}(H_N^\omega - E)\,\mathrm{d}E \right). \tag{4.2}$$

Here, $\mathbf{1}_A$ is the characteristic function of the set A. Using (4.1) one computes

$$\mathrm{tr}\left(\sum_{e\in\mathcal{E}_N}\lambda^{\omega}(e)\partial_{\lambda^{\omega}(e)}\mathbf{1}_{(-\infty,0]}(H_N^{\omega}-E)\right)=\mathrm{tr}(-H_N^{\omega}\partial_E\mathbf{1}_{(-\infty,0]}(H_N^{\omega}-E))).$$

For $E\in\Delta$, this gives

$$\mathrm{tr}[\partial_E\mathbf{1}_{(-\infty,0]}(H_N^{\omega}-E)]\leqslant\frac{1}{c}\mathrm{tr}\left(\sum_{e\in\mathcal{E}_N}\lambda^{\omega}(e)\partial_{\lambda^{\omega}(e)}\mathbf{1}_{(-\infty,0]}(H_N^{\omega}-E)\right)$$

hence, by (4.2),

$$c\cdot\mathrm{tr}(E_N^{\omega}(\Delta))\leqslant\int_{\Delta}\sum_{e\in\mathcal{E}_N}\mathrm{tr}(\lambda^{\omega}(e)\partial_{\lambda^{\omega}(e)}\mathbf{1}_{(-\infty,0]}(H_N^{\omega}-E)))\mathrm{d}E.$$

Taking the expectation in both sides of the previous equation, one obtains

$$c\cdot\mathbb{E}[\mathrm{tr}(E_N^{\omega}(\Delta))]\leqslant\sum_{e\in\mathcal{E}_N}\int\prod_{e'\neq e}g(\lambda^{\omega}(e'))\mathrm{d}\lambda^{\omega}(e')\int_{\Delta}\mathrm{d}E\,G_e(E,\omega),\tag{4.3}$$

where

$$G(E,\omega)=G_e(E,\omega)=\int_{-1}^{1}g(\lambda)\lambda\partial_{\lambda}\mathrm{tr}(\mathbf{1}_{(-\infty,0]}(H_N^{\omega}(\lambda,e)-E))\mathrm{d}\lambda.\tag{4.4}$$

Here, $H_N^{\omega}(\lambda,e)$ is the Hamiltonian H_N^{ω} where the random variable $\lambda_{\omega}(e)=\lambda$, and all other random variables are unchanged.

By assumption, g, the common probability density of the random variables $(\lambda^{\omega}(e))_{\gamma}$, is Lipschitz continuous. This enables us to integrate by parts in (4.4) and to obtain

$$G(E,\omega)=[g(\lambda)\lambda F(\lambda,E,\omega)]_{-1}^{1}-\int_{-1}^{1}\partial_{\lambda}(g(\lambda)\lambda)F(\lambda,E,\omega)\mathrm{d}\lambda,\tag{4.5}$$

where we have defined

$$F(\lambda,E,\omega)=\mathrm{tr}[\mathbf{1}_{(-\infty,0]}(H_N^{\omega}(1,e)-E)-\mathbf{1}_{(-\infty,0]}(H_N^{\omega}(-1,e)-E)].$$

As the single-site perturbation $\partial_{\lambda^{\omega}(e)}H^{\omega}$ is of rank 2, the function $|F(\lambda,E,\omega)|$ is bounded by 2. Hence, $|G|$ is bounded by a constant. Plugging this back into (4.3), and using equations (4.2), (4.1) and the fact that Δ is bounded away from 0, one obtains

$$\begin{aligned}&\#\{\text{eigenvalues of }\Pi_N H^{\omega}\Pi_N\text{ less than }E\}\\&=\mathbb{E}(\mathrm{tr}[E_N^{\omega}(\Delta)])\leqslant C\sum_{e\in\mathcal{E}_N}\int_{\omega'}\mathbb{P}(\mathrm{d}\omega')\int_{\Delta}\mathrm{d}E\leqslant C|\Delta||\Lambda|.\end{aligned}$$

In view of the definition of the integrated density of states (1.3), this completes the proof of Theorem 1.2.

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The generalized MIC-Kepler system

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(Received 9 July 2003; accepted 18 August 2003)

This paper deals with the dynamical system that generalizes the MIC-Kepler system. It is shown that the Schrödinger equation for this generalized MIC-Kepler system can be separated in spherical and parabolic coordinates. The spectral problem in spherical and parabolic coordinates is solved. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1619205]

I. INTRODUCTION

The system described by the Hamiltonian

$$\hat{\mathcal{H}}=\frac{1}{2}(-i\nabla-s\mathbf{A})^2+\frac{s^2}{2r^2}-\frac{1}{r}+\frac{c_1}{r(r+z)}+\frac{c_2}{r(r-z)}, \tag{1.1}$$

where c_1 and c_2 are non-negative constants, later on will be called the generalized MIC-Kepler system. (We use the system of units for which $\hbar=m=e=c=1$.)

The MIC-Kepler integrable system was constructed by Zwanziger[1] and rediscovered by McIntosh and Cisneros.[2] This system is described by the Hamiltonian

$$\hat{\mathcal{H}}_0=\frac{1}{2}(-i\nabla-s\mathbf{A})^2+\frac{s^2}{2r^2}-\frac{1}{r}, \tag{1.2}$$

where

$$\mathbf{A}=\frac{1}{r(r-z)}(y,-x,0), \quad \text{and} \quad \operatorname{rot}\mathbf{A}=\frac{\mathbf{r}}{r^3}.$$

Its distinctive peculiarity is the Coulomb hidden symmetry given by the following constants of motion (1.2):

$$\hat{\mathbf{I}}=\frac{1}{2}[(-i\nabla-s\mathbf{A})\times\hat{\mathbf{J}}-\hat{\mathbf{J}}\times(-i\nabla-s\mathbf{A})]+\frac{\mathbf{r}}{r}, \quad \hat{\mathbf{J}}=\mathbf{r}\times(-i\nabla-s\mathbf{A})-s\frac{\mathbf{r}}{r}. \tag{1.3}$$

Here, the operator $\hat{\mathbf{J}}$ defines the angular momentum of the system, while operator $\hat{\mathbf{I}}$ is the analog of the Runge–Lenz vector. These constants of motion, together with the Hamiltonian, form the quadratic symmetry algebra of the Coulomb problem. For fixed negative energy values the motion integrals make up algebra so(4), whereas for positive energy values $-$so(3.1). Due to the hidden symmetry the MIC-Kepler problem is factorized not only in the spherical but parabolic coordinates as well. Hence, the MIC-Kepler system is a natural generalization of the Coulomb problem in the presence of Dirac's monopole. In both cases the monopole number s satisfies the Dirac's rule of charge quantization $s=0,\pm 1/2,\pm 1,\ldots$.

The MIC-Kepler system could be constructed by the reduction of the four-dimensional isotropic oscillator by the use of the so-called Kustaanheimo–Stiefel transformation both on classical and quantum mechanical levels.[3] In the similar way, reducing the two- and eight-dimensional isotropic oscillator, one can obtain the two- (Ref. 4) and five-dimensional[5] analogs of the MIC-

Kepler system. An infinitely thin solenoid providing the system by the spin 1/2, plays the role of monopole in the two-dimensional case, whereas in the five-dimensional case this role is performed by the SU(2) Yang monopole,[6] endowing the system by the isospin. All the above-mentioned systems have Coulomb symmetries and are solved in spherical and parabolic coordinates both in discrete and continuous parts of the energy spectra.[7] There are generalizations of MIC-Kepler systems on the three-dimensional sphere[8] and hyperboloid[9] as well. The MIC-Kepler system has been worked out from different points of view in.[10–14]

For integer values s the MIC-Kepler system describes the relative motion of the two Dirac's dyons (charged magnetic monopoles), where vector $\mathbf{r}$ determines the position of the second dyon with respect to the first one.[1] For half-integer s the presence of the solenoid magnetic field, endowing the system with the spin 1/2, is presupposed (see, e.g., Ref. 4).

The Hamiltonian (1.1) for $s=0$ and $c_i \neq 0$ $(i=1,2)$ reduces to the Hamiltonian

$$\hat{H} = -\frac{1}{2}\Delta - \frac{1}{r} + \frac{c_1}{r(r+z)} + \frac{c_2}{r(r-z)} \tag{1.4}$$

of the generalized Kepler–Coulomb system.[15]

The potential

$$V = -\frac{\alpha}{r} + \frac{c_1}{r(r+z)} + \frac{c_2}{r(r-z)} \tag{1.5}$$

is one of the Smorodinsky–Winternitz-type potentials.[16] The Smorodinsky–Winternitz type potentials where revived and investigated in 1990 by Evans.[17] In the case where $c_1 = c_2$, the potential (1.5) reduces to the Hartmann potential that has been used for describing axially symmetric systems like ring-shaped molecules[18] and investigated from different points of view in Refs. 19–31. In particular, the (quantum mechanical) discrete spectrum for the generalized Kepler–Coulomb system (1.4) is well known,[24,27,29] even for the so-called (q,p)-analog of this system.[29] Furthermore, a path integral treatment of the potential (1.5) has been given in Refs. 23 and 27. Recently, the dynamical symmetry of the generalized Kepler–Coulomb system has been studied in Refs. 29–31, the classical motion of a particle moving in the potential (1.5) has been considered in Ref. 30, and the coefficients connecting the parabolic and spherical bases have been identified in Ref. 31 as Clebsch–Gordan coefficients of the pseudo-unitary group SU(1,1).

The purpose of the present paper is to further study the bound states of the generalized MIC-Kepler system in spherical and parabolic coordinates.

II. SPHERICAL BASIS

The Schrödinger equation with Hamiltonian (1.1) in spherical coordinates (r,θ,φ) may be solved by seeking a wave function ψ of the form

$$\psi(r,\theta,\varphi) = R(r)Z(\theta,\varphi). \tag{2.1}$$

This amounts to finding the eigenfunctions of the set $\{\hat{\mathcal{H}}, \hat{J}_z, \hat{M}\}$ of commuting operators, where the constant of motion $\hat{M}$ reads

$$\hat{M} = \hat{J}^2 + \frac{2c_1}{1+\cos\theta} + \frac{2c_2}{1-\cos\theta}. \tag{2.2}$$

Here $\hat{J}^2$ is the square of the angular momentum, $\hat{J}_z = s - i\partial/\partial\varphi$ its z-component, and $\hat{J}_z\psi = m\psi$.

After substitution the expression (2.1) the variables in the Schrödinger equation are separated and we arrive at the following system of coupled differential equations:

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Z}{\partial\theta}\right)+\frac{1}{4\cos^2\frac{\theta}{2}}\left(\frac{\partial^2}{\partial\varphi^2}-4c_1\right)Z+\frac{1}{4\sin^2\frac{\theta}{2}}\left[\left(\frac{\partial}{\partial\varphi}+2is\right)^2-4c_2\right]Z=-\mathcal{A}Z, \tag{2.3}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{\mathcal{A}}{r^2}R+2\left(E+\frac{1}{r}\right)R=0, \tag{2.4}$$

where $\mathcal{A}$ is a separation constant in spherical coordinates.

The solution of (2.3) is easily found to be

$$Z_{jm}^{(s)}(\theta,\varphi;\delta_1,\delta_2)=N_{jm}(\delta_1,\delta_2)\left(\cos\frac{\theta}{2}\right)^{m_1}\left(\sin\frac{\theta}{2}\right)^{m_2}P_{j-m_+}^{(m_2,m_1)}(\cos\theta)e^{i(m-s)\varphi}, \tag{2.5}$$

where $m_1=|m-s|+\delta_1=\sqrt{(m-s)^2+4c_1}$, $m_2=|m+s|+\delta_2=\sqrt{(m+s)^2+4c_2}$, $m_+=(|m+s|+|m-s|)/2$, and $P_n^{(a,b)}$ denotes a Jacobi polynomial. The quantum numbers m and j run through values: $m=-j,-j+1,\ldots,j-1,j$ and

$$j=\frac{|m+s|+|m-s|}{2},\frac{|m+s|+|m-s|}{2}+1,\ldots\ .$$

The quantum numbers j, m characterize the total momentum of the system and its projection on the axis z. For the (half)integer s j, m are (half)integers.

Furthermore, the separation constant $\mathcal{A}$ is quantized as

$$\mathcal{A}=\left(j+\frac{\delta_1+\delta_2}{2}\right)\left(j+\frac{\delta_1+\delta_2}{2}+1\right). \tag{2.6}$$

The normalization constant $N_{jm}(\delta_1,\delta_2)$ in (2.5) is given (up to a phase factor) by

$$N_{jm}(\delta_1,\delta_2)=\sqrt{\frac{(2j+\delta_1+\delta_2+1)(j-m_+)!\Gamma(j+m_++\delta_1+\delta_2+1)}{4\pi\Gamma(j-m_-+\delta_1+1)\Gamma(j+m_-+\delta_2+1)}}, \tag{2.7}$$

where $m_-=(|m+s|-|m-s|)/2$. The angular wave functions $Z_{jm}^{(s)}$ [see Eq. (2.5)] are convenient to call the ring-shaped monopole harmonics by analogy with the term ''monopole harmonics'' studied by Tamm.[32] These ring-shaped monopole harmonics generalize the functions studied by Hartmann[18] in the case $s=0,\delta_1=\delta_2$. Due to the connecting formula,[33]

$$(\lambda+\tfrac{1}{2})_n\ C_n^{\lambda}(x)=(2\lambda)_nP_n^{(\lambda-(1/2),\lambda-(1/2))}(x) \tag{2.8}$$

between the Jacobi polynomial $P_n^{(a,b)}$ and the Gegenbauer polynomial C_n^{λ}, the case $s=0$, $\delta_1=\delta_2=\delta$ yields

$$Z_{jm}^{(0)}(\theta,\varphi;\delta,\delta)=2^{|m|+\delta}\Gamma\left(|m|+\delta+\frac{1}{2}\right)\sqrt{\frac{(2j+2\delta+1)(j-|m|)!}{4\pi^2\Gamma(j+|m|+2\delta+1)}}$$
$$\times(\sin\theta)^{|m|+\delta}C_{j-|m|}^{|m|+\delta+(1/2)}(\cos\theta)e^{im\varphi}, \tag{2.9}$$

the result already obtained in Ref. 15. [In (2.8), $(a)_n$ stands for a Pochhammer symbol.] The case $\delta=0$ (i.e., $c_1=c_2=0$) can be treated by using the connecting formula

$$P_j^{|m|}(x)=\frac{(-2)^{|m|}}{\sqrt{\pi}}\Gamma\left(|m|+\frac{1}{2}\right)(1-x^2)^{|m|/2}C_{j-|m|}^{|m|+(1/2)}(x) \tag{2.10}$$

between the Gegenbauer polynomial C_n^{λ} and the associated Legandre function.[33] In fact for the $\delta=0$, Eq. (2.9) can be reduced to

$$Z_{jm}^{(0)}(\theta,\varphi;0,0)=\sqrt{\frac{(2j+1)(j-|m|)!}{4\pi(j+|m|)!}}P_j^{|m|}(\cos\theta)e^{im\varphi}, \tag{2.11}$$

an expression (up to a phase factor) that coincides with the usual (surface) spherical harmonics $Y_{lm}(\theta,\varphi)$.

Let us go now to radial equation (2.4). The introduction of (2.6) into the (2.4) leads to

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{1}{r^2}\left(j+\frac{\delta_1+\delta_2}{2}\right)\left(j+\frac{\delta_1+\delta_2}{2}+1\right)R+2\left(E+\frac{1}{r}\right)R=0, \tag{2.12}$$

which is reminiscent of the radial equation for the hydrogen atom except that the orbital quantum number l is replaced here by $j+(\delta_1+\delta_2)/2$. The solution of (2.12) for the discrete spectrum is

$$R_{nj}^{(s)}(r)=C_{nj}(\delta_1,\delta_2)(2\varepsilon r)^{j+[(\delta_1+\delta_2)/2]}e^{-\varepsilon r}F(-n+j+1;2j+\delta_1+\delta_2+2;2\varepsilon r), \tag{2.13}$$

where $n=|s|+1,|s|+2,\ldots$. In (2.13), the normalization factor $C_{nj}(\delta_1,\delta_2)$ reads

$$C_{nj}(\delta_1,\delta_2)=\frac{2\varepsilon^2}{\Gamma(2j+\delta_1+\delta_2+1)}\sqrt{\frac{\Gamma(n+j+\delta_1+\delta_2+1)}{(n-j-1)!}} \tag{2.14}$$

and the parameter ε is defined by

$$\varepsilon=\sqrt{-2E}=\frac{1}{n+\dfrac{\delta_1+\delta_2}{2}}. \tag{2.15}$$

The eigenvalues E are then given by

$$E\equiv E_n^{(s)}=-\frac{1}{2\left(n+\dfrac{\delta_1+\delta_2}{2}\right)^2}. \tag{2.16}$$

In the limiting case $\delta_1=\delta_2=0$, we recover the familiar results for charge-dyon bound system.[1]

III. PARABOLIC BASIS

Let us consider the generalized MIC-Kepler system in the parabolic coordinates. In the parabolic coordinates $\xi,\eta\in[0,\infty),\varphi\in[0,2\pi)$, defined by the formulas

$$x=\sqrt{\xi\eta}\cos\varphi,\quad y=\sqrt{\xi\eta}\sin\varphi,\quad z=\tfrac{1}{2}(\xi-\eta), \tag{3.1}$$

the differential elements of length and volume read

$$dl^2=\frac{\xi+\eta}{4}\left(\frac{d\xi^2}{\xi}+\frac{d\eta^2}{\eta}\right)+\xi\eta d\varphi^2,\quad dV=\tfrac{1}{4}(\xi+\eta)d\xi d\eta d\varphi, \tag{3.2}$$

while the Laplace operator looks like

$$\Delta=\frac{4}{\xi+\eta}\left[\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)+\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right]+\frac{1}{\xi\eta}\frac{\partial^2}{\partial\varphi^2}. \tag{3.3}$$

The substitution

$$\psi(\xi,\eta,\varphi)=\Phi_1(\xi)\Phi_2(\eta)\frac{e^{i(m-s)\varphi}}{\sqrt{2\pi}} \tag{3.4}$$

separates the variables in the Schrödinger equation and we arrive at the following system of equations:

$$\frac{d}{d\xi}\left(\xi\frac{d\Phi_1}{d\xi}\right)+\left[\frac{E}{2}\xi-\frac{m_1^2}{4\xi}+\frac{1}{2}\beta+\frac{1}{2}\right]\Phi_1=0, \tag{3.5}$$

$$\frac{d}{d\eta}\left(\eta\frac{d\Phi_2}{d\eta}\right)+\left[\frac{E}{2}\eta-\frac{m_2^2}{4\eta}-\frac{1}{2}\beta+\frac{1}{2}\right]\Phi_2=0, \tag{3.6}$$

where β is the separation constant.

These equations are analogous with the equations of the hydrogen atom in the parabolic coordinates.[34] Thus, we get

$$\psi^{(s)}_{n_1n_2m}(\xi,\eta,\varphi;\delta_1,\delta_2)=\sqrt{2}\varepsilon^2\Phi_{n_1m_1}(\xi)\Phi_{n_2m_2}(\eta)\frac{e^{i(m-s)\varphi}}{\sqrt{2\pi}}, \tag{3.7}$$

where

$$\Phi_{n_im_i}(x)=\frac{1}{\Gamma(m_i+1)}\sqrt{\frac{\Gamma(n_i+m_i+1)}{(n_i)!}}e^{-(\varepsilon x/2)}(\varepsilon x)^{(m_i/2)}F(-n_i;m_i+1;\varepsilon x). \tag{3.8}$$

Here n_1 and n_2 are non-negative integers

$$n_1=-\frac{|m-s|+\delta_1+1}{2}+\frac{\beta+1}{2\varepsilon},\quad n_2=-\frac{|m+s|+\delta_2+1}{2}-\frac{\beta-1}{2\varepsilon}. \tag{3.9}$$

From the last relations, taking into account (2.16), we get that the parabolic quantum numbers n_1 and n_2 are connected with the principal quantum number n as follows:

$$n=n_1+n_2+\frac{|m-s|+|m+s|}{2}+1. \tag{3.10}$$

Excluding the energy E from Eqs. (3.5) and (3.6), we obtain the additional integral of motion,

$$\hat{X}=\frac{2}{\xi+\eta}\left[\xi\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)-\eta\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)\right]+\frac{\xi-\eta}{2\xi\eta}\frac{\partial^2}{\partial\varphi^2}+is\frac{\xi^2+\eta^2}{\xi\eta(\xi+\eta)}\frac{\partial}{\partial\varphi}-s^2\frac{\xi-\eta}{2\xi\eta}+\frac{2c_1\eta}{\xi(\xi+\eta)}$$
$$-\frac{2c_2\xi}{\eta(\xi+\eta)}+\frac{\xi-\eta}{\xi+\eta} \tag{3.11}$$

with the eigenvalues

$$\beta=\varepsilon\left(n_1-n_2+\frac{|m-s|-|m+s|+\delta_1-\delta_2}{2}\right) \tag{3.12}$$

and eigenfunctions $\psi^{(s)}_{n_1n_2m}(\xi,\eta,\varphi;\delta_1,\delta_2)$.

In Cartesian coordinates, the operator $\hat{X}$ can be rewritten as

$$\hat{X}=z\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-x\frac{\partial^2}{\partial x\partial z}-y\frac{\partial^2}{\partial y\partial z}+is\frac{r+z}{r(r-z)}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)-\frac{\partial}{\partial z}-s^2\frac{r+z}{r(r-z)}+c_1\frac{r-z}{r(r+z)}$$
$$-c_2\frac{r+z}{r(r-z)}+\frac{z}{r}, \tag{3.13}$$

so that it immediately follows that $\hat{X}$ is connected to the z-component $\hat{I}_z$ of the analog of the Runge–Lenz vector (1.3) via

$$\hat{X}=\hat{I}_z+c_1\frac{r-z}{r(r+z)}-c_2\frac{r+z}{r(r-z)} \tag{3.14}$$

and coincides with $\hat{I}_z$ when $c_1=c_2=0$.

Thus we have solved the spectral problem in spherical

$$\hat{\mathcal{H}}\psi=E\psi,\quad \hat{M}\psi=\left(j+\frac{\delta_1+\delta_2}{2}\right)\left(j+\frac{\delta_1+\delta_2}{2}+1\right)\psi,\quad \hat{J}_z\psi=m\psi \tag{3.15}$$

and in parabolic coordinates

$$\hat{\mathcal{H}}\psi=E\psi,\quad \hat{X}\psi=\beta\psi,\quad \hat{J}_z\psi=m\psi, \tag{3.16}$$

where $\hat{\mathcal{H}}$, $\hat{J}_z$, $\hat{M}$, and $\hat{X}$ are defined by the expressions (1.1), (1.3), (2.2), and (3.14).

It is mentioned that all the formulas obtained for $s=0$ yield the corresponding formulas for the generalized Kepler Coulomb system.[15]

ACKNOWLEDGMENTS

The work was carried out with the support of ANSEF No. PS81 grant.

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Random magnetic fields on line graphs

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(Received 7 March 2003; accepted 15 July 2003)

We study the spectral and transport properties of Schrödinger operators on line graphs with random magnetic fields. We show that it has a pure point spectrum with exponentially decaying eigenfunctions on spectral edges, whereas there appears an eigenvalue with infinite multiplicity due to the structure of line graphs. We compute the electrical conductivity which is zero on spectral edges, but is nonzero and finite on the isolated eigenvalue mentioned above. Some related problems are also discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1613377]

I. INTRODUCTION

Recently, the spectral theory of Schrödinger operators on graphs is paid much attention, and various interesting aspects, such as the relationship between the spectrum and the geometrical structure of graphs, are studied. Shirai[17] studied the spectrum of the Laplacian on d-regular infinite graphs, and found a simple formula relating the spectrum of the Laplacian on graphs to that of their line graphs. Ogurisu[15,16] gave a simple proof of results of Shirai[17] by using the notion of supersymmetry and extended them to the case where the magnetic flux is present. The subject of this paper is to consider the Schrödinger operators on line graphs with a certain random magnetic flux, where some unusual spectral properties appear. Mostly we discuss the line graph of $\mathbf{Z}^2$, but our results also apply to other graphs such as that of the triangular or hexagonal lattice discussed in Appendix A.

We first prepare notations and definitions. In this paper, a graph G is defined to be a pair $(V(G),\mathcal{E}(G))$ of a set of vertices $V(G)$ and a set of oriented edges $\mathcal{E}(G)=\{xy:x,y\in V(G)\}$. $\alpha=xy$ stands for the edge with origin x and terminus y and we write $o(\alpha)=x$, $t(\alpha)=y$. For $\alpha=xy\in\mathcal{E}(G)$, we denote the inverse edge by $\overline{\alpha}=yx$. $E(G)$ is the set of unoriented edges where $\alpha,\overline{\alpha}\in\mathcal{E}(G)$ are identified and we denote by $|\alpha|$ the corresponding element in $E(G)$ (i.e., $|\overline{\alpha}|=|\alpha|$). We denote by $l^2(G)$ the Hilbert space of complex-valued square summable functions on $V(G)$ with the inner product

$$\langle f,g\rangle_G=\sum_{x\in V(G)} m_G(x)\overline{f(x)}g(x),$$

where $m_G(x)=\sharp N_x(G)$ $(N_x(G)=\{\alpha\in\mathcal{E}(G):o(\alpha)=x\})$ is the degree of x. The line graph $L(G)$ of a graph G is defined as follows. Its vertex set is the set of edges in G: $V(L(G))=E(G)$ and $|\alpha|,|\beta|\in E(G)$ are connected by an edge $|\alpha||\beta|\in\mathcal{E}(L(G))$ if they have a vertex of G in common.

We naturally regard $\mathbf{Z}^2$ as a graph with $V(\mathbf{Z}^2)=\{x=(x_1,x_2):x_1,x_2\in\mathbf{Z}\}$, $\mathcal{E}(\mathbf{Z}^2)=\{xy:x,y\in V(\mathbf{Z}^2),|x-y|=1\}$ and let H be a bounded self-adjoint operator on $l^2(\mathbf{Z}^2)$,

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$$(Hu)(x)=\sum_{\alpha\in N_x(\mathbf{Z}^2)}(u(x)-e^{iA(\alpha)}u(t(\alpha))),\quad x\in V(\mathbf{Z}^2). \tag{1.1}$$

$A:\mathcal{E}(\mathbf{Z}^2)\to\mathbf{R}$ is a vector potential satisfying $A(\alpha)=-A(\overline{\alpha}),\alpha\in\mathcal{E}(\mathbf{Z}^2)$. For $x=(x_1,x_2)\in\mathbf{Z}^2$, let $f_x=\{x_1,x_1+1\}\times\{x_2,x_2+1\}(\subset V(\mathbf{Z}^2))$ be the plaquette of $\mathbf{Z}^2$ with x as one of its vertices and let

$$\partial f_x=\{x(x+e_1),(x+e_1)(x+e_1+e_2),(x+e_1+e_2)(x+e_2),(x+e_2)x\}$$

$[\subset\mathcal{E}(\mathbf{Z}^2)]$ be the set of edges encircling the plaquette f_x counterclockwise $[e_1=(1,0),e_2=(0,1)]$. The magnetic flux on f_x is then given by

$$\Phi(f_x)=\sum_{\alpha\in\partial f_x}A(\alpha)\in[0,2\pi)\quad(\mathrm{mod}\ 2\pi).$$

The spectral properties of H is determined by $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$ and does not depend on the choice of A with same $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$. Given a vector potential $A:\mathcal{E}(\mathbf{Z}^2)\to\mathbf{R}$, we define the corresponding one on $L(\mathbf{Z}^2)$ by

$$A_L(|\alpha||\beta|)=\frac{A(yx)+A(xz)}{2}, \tag{1.2}$$

for $|\alpha|=|yx|$, $|\beta|=|xz|(x,y,z\in V(\mathbf{Z}^2))$. The Hamiltonian H_L on $l^2(L(\mathbf{Z}^2))$, which is the main subject of this paper, is defined by

$$(H_Lu)(|\alpha|)=\sum_{|\alpha||\beta|\in\mathcal{E}(L(\mathbf{Z}^2))}(u(|\alpha|)-e^{iA_L(|\alpha||\beta|)}u(|\beta|)),\quad|\alpha|\in\mathbf{E}(\mathbf{Z}^2). \tag{1.3}$$

The spectrum of H_L, H satisfy the following relation:[17,15,16]

$$\sigma(H_L)=\sigma(H)\cup\{8\}. \tag{1.4}$$

In this paper, we consider the case where $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$ are random variables. Let

$$A_\omega(xy)=\begin{cases}-B_\omega(2n+1,m) & (x=(2n+1,m),y=(2n+1,m+1)),\\ B_\omega(2n+1,m) & (x=(2n+1,m+1),y=(2n+1,m));\\ 0 & (\text{otherwise})\end{cases}$$

$(n,m\in\mathbf{Z})$, with corresponding magnetic fluxes on each plaquette f_x:

$$\Phi(f_x)=\begin{cases}B_\omega(2n+1,m) & (x=(2n+1,m)),\\ -B_\omega(2n+1,m) & (x=(2n,m)).\end{cases} \tag{1.5}$$

We assume the following conditions on $\{B_\omega(2n+1,m)\}_{n,m\in\mathbf{Z}}$.

Assumption A: $\{B_\omega(2n+1,m)\}_{n,m\in\mathbf{Z}}$ *are real-valued i.i.d. random variables on a probability space* $(\Omega,\mathcal{F},\mathbf{P})$ *and the common distribution of* $\{B_\omega(2n+1,m)\}_{n,m\in\mathbf{Z}}$ *has a density* g *such that supp* $g\subset[-\pi,-c]\cup[c,\pi]$, *on which* g *is Lipshitz continuous, and* $\pm c\in supp\ g$ *for some constant* $0<c<\pi$.

The motivation to study the random flux model on line graphs is the work of Ludwig, Fisher, Shanker, and Grinstein,[10] where similar models are considered to study the transitions in the integer quantum Hall effect. In fact, H_L is one of a few examples which has an isolated eigenvalue with infinite multiplicity as is the Landau level of the Schrödinger operator on $L^2(\mathbf{R}^2)$ with a constant magnetic field. By (1.4) and the fact that[8] $\sigma(H)=[4(1-\cos c/4),4(1+\cos c/4)]$ a.s., we have

$$\sigma(H_L)=\left[4\left(1-\cos\frac{c}{4}\right),4\left(1+\cos\frac{c}{4}\right)\right]\cup\{8\},\quad \text{a.s.}$$

The integrated density of states (IDS) of H,H_L are defined as follows. Let $\mathbf{Z}^2_M=\{x=(x_1,x_2)\in\mathbf{Z}^2:|x_j|\leqslant M,j=1,2\}$ $(M\in\mathbf{N})$ and let $H^M=H|_{\mathbf{Z}^2_M},H^M_L=H_L|_{L(\mathbf{Z}^2_M)}$ be the Hamiltonian H,H_L restricted on $\mathbf{Z}^2_M,L(\mathbf{Z}^2_M)$, respectively [in other words, $\mathbf{Z}^2$ in (1.1), (1.3) is replaced by $\mathbf{Z}^2_M$]. The IDS $k(E),k_L(E)$ of H,H_L is given by

$$k(E)=\lim_{M\to\infty}\frac{1}{\sharp V(\mathbf{Z}^2_M)}\sharp\{\text{eigenvalues of } H^M\leqslant E\},$$

$$k_L(E)=\lim_{M\to\infty}\frac{1}{\sharp V(L(\mathbf{Z}^2_M))}\sharp\{\text{eigenvalues of } H^M_L\leqslant E\}.$$

It is known that $k(E),k_L(E)$ are almost surely deterministic. Our first result concerns the spectrum and the IDS of H_L.

Theorem 1.1: *Under Assumption A, we have the following.*

(1) There exists a constant $R>0$ such that the spectrum of H_L in $I_R:=[4(1-\cos c/4),4(1-\cos c/4)+R]\cup[4(1+\cos c/4)-R,4(1+\cos c/4)]$ is almost surely a pure point with exponentially decaying eigenfunctions (we say Anderson localization holds in such situations);

(2) 8 is an eigenvalue of H_L with infinite multiplicity;

(3) $k_L(E)$ is discontinuous at $E=8$: $k_L(8)-k_L(8-)=1/2$.

It is known that IDS is always continuous for Schrödinger operators on $\mathbf{Z}^d$ with metrically transitive random fields. Theorem 1.1 (1) follows from the result[8] on Anderson localization for H and the ''supersymmetric method'' discussed by Ogurisu.[15,16] The condition that supp $g\subset[-\pi,-c]\cup[c,\pi]$ is required to estimate the derivative of eigenvalues of H^M w.r.t. the magnetic fluxes, which is important to prove the Wegner estimate. To show Anderson localization for H_L, we consider an operator $\psi:l^2(\mathbf{Z}^2)\to l^2(L(\mathbf{Z}^2))_2$ [ψ and $l^2(L(\mathbf{Z}^2))_2$ are defined in Sec. II] with ψ^* its adjoint. Then we have $\sigma(\psi\psi^*)=\sigma(\psi^*\psi)\cup\{0\}$ which is the main ingredient of the proof of (1.4). We show that this relation also ''preserves'' the dense point spectrum which proves Theorem 1.1 (1). Theorem 1.1 (2), (3) is due to the structure of line graphs: there are infinite number of eigenfunctions of finite support, which is used in many areas of mathematical physics. For instance, it is essential to construct an example of the ferromagnetic ground states of the Hubbard model on line graphs.[12] Theorem 1.1 (2) holds for any configuration of magnetic fluxes $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$ (Proposition 2.1), and Theorem 1.1 (3) holds whenever $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$ are metrically transitive random variables on $(\Omega,\mathcal{F},\mathbf{P})$ (Proposition 2.2). On the other hand, in finite graphs, $\dim\ker(H_L-8)$ becomes different when the magnetic field is turned on (Theorem 3.1).

The next topic in this paper is to discuss the transport properties of H_L. Let

$$\sigma(E)=\lim_{\epsilon\downarrow 0}\sigma_\epsilon(E), \tag{1.6}$$

$$\sigma_\epsilon(E)=\epsilon^2\mathbf{E}\sum_{x\in L(\mathbf{Z}^2)}|x|^2|G_L(E+i\epsilon;0,x)|^2,$$

where $\mathbf{E}$ is the expectation w.r.t. $\mathbf{P}$, $G_L(z)=(H_L-z)^{-1},z\in\mathbf{C}\backslash\mathbf{R}$ is the Green's function of H_L, and $G_L(z;x,y)=\langle\delta_x,(H_L-z)^{-1}\delta_y\rangle_{l^2(L(\mathbf{Z}^2))_2}$, $x,y\in L(\mathbf{Z}^2)$ is its matrix element [$\delta_x(y)=1$ $(y=x),=0$ $(y\neq x)$]. $\sigma(E)$ may be regarded as the electrical conductivity of H_L for the Fermi energy $E\in\mathbf{R}$. A formal derivation of Eq. (1.6) is given by McKane-Stone.[11] Moreover, it is possible to derive Eq. (1.6) by the linear response theory under some technical assumptions,[2] or is

also possible to relate $\sigma(E)$ with the charge transport.[14] Our result is that $\sigma(E)$ is equal to zero, where the Anderson localization holds while $\sigma(E)$ takes a finite and nonzero value on the isolated eigenvalue with infinite multiplicity.

Theorem 1.2: *Under Assumption A, we have the following:*

(1) $\sigma(E)=0$ *for* $E\in I_R$, *where* I_R *is the closed interval appearing in Theorem 1.1;*
(2) $0<\sigma(8)<\infty$.

To prove Theorem 1.2 (1), we show two estimates on the IDS $k_L(E)$ (Wegner estimate and Lifshitz tail) by the corresponding ones on H proved by Klopp *et al.*[8] and the supersymmetric argument. Then, $\sigma(E)=0$ is the natural conclusion of the exponential decay estimate of the Green's function given by the multiscale analysis[6] [this also gives an alternative proof of Theorem 1.1 (1)]. Theorem 1.2 (2) comes from the fact that 8 is an isolated eigenvalue of H_L. We remark that σ is zero or infinity in many cases. For instance, in the case of a 1-dimensional Hamiltonian with periodic potential, we have $\sigma_\epsilon(E)\sim\epsilon^{-1}$ if $E\in\sigma(H)^\circ$ and $\sigma_\epsilon(E)\sim\epsilon^2$, if $E\in\rho(H)$.

In Secs. II, IV, we prove Theorems 1.1, 1.2, respectively. In Sec. III, we show other interesting properties of magnetic Schrödinger operators on line graphs. We study $\dim\ker\psi^*$ for finite graphs and show that it becomes different depending on whether magnetic fluxes vanish or not. This is used to show that 8 is an eigenvalue of H_L with infinite multiplicity and to study the IDS of H_L. Moreover, we show, in addition to Eq. (1.4), the nature of the spectrum is also preserved (Theorem 3.3).

In Appendix A, we discuss the extensions of results by Klopp *et al.*[8] to triangular and hexagonal lattices. Then Theorem 1.1, 1.2 also applies to these graphs, telling us the corresponding spectral and transport properties on their line graphs. In Appendix B, we study a model on a ladder which may be called ''the random graph model.'' By using ideas similar to the one for Theorem 1.1, we show that the Anderson localization holds on the whole spectrum. In Appendix C, we discuss an application of the result on $\dim\ker\psi^*$ (Theorem 3.1) to the cycles (defined in Sec. II) and show the converse of the diamagnetic inequality in some cases.

II. PROOF OF THEOREM 1.1

For a graph G, we denote by $l^2(G)_2$ the Hilbert space which is identical to $l^2(G)$ as a set but with an inner product,

$$\langle f,g\rangle_2=2\sum_{x\in V(G)}\overline{f(x)}g(x),\quad \|f\|_2=\sqrt{\langle f,f\rangle_2}.$$

Let $\psi_G: l^2(G)\to l^2(L(G))_2$ and its adjoint $\psi_G^*: l^2(L(G))_2\to l^2(G)$ be

$$(\psi_G f)(|\alpha|)=\frac{1}{2}\sum_{\beta=\alpha,\bar{\alpha}}e^{i[A(\beta)/2]}f(t(\beta)),\quad \alpha\in\mathcal{E}(G),$$

$$(\psi_G^* F)(x)=\frac{1}{m_G(x)}\sum_{\alpha\in N_x(G)}e^{i[A(\alpha)/2]}F(|\alpha|),\quad x\in V(G).$$

We write $\psi=\psi_{\mathbf{Z}^2}, \psi^*=\psi_{\mathbf{Z}^2}^*$ for simplicity. By direct computation, we have

$$\psi^*\psi=-\frac{1}{8}H+1,\quad \psi\psi^*=-\frac{1}{8}H_L+1. \tag{2.1}$$

Equation (1.2) is used here. In what follows, we say that $E\in\mathbf{R}$ is the generalized eigenvalue of H if there exists u which satisfies $Hu=Eu$ and grows at most polynomial order at infinity. In this case, we call u the generalized eigenfunction of H. Then[8] there exists $R>0$, $\Omega_0(\subset\Omega)$ with $\mathbf{P}(\Omega_0)=1$ such that for $\omega\in\Omega_0$, if $E\in I_R:=[4(1-\cos c/4),4(1-\cos c/4)+R]\cup[4(1+\cos c/4)$

$-R,4(1+\cos c/4)]$ is a generalized eigenvalue, then the corresponding generalized eigenfunction u decays exponentially at infinity. Fix $\omega\in\Omega_0$ and let $E\in I_R$, v be generalized eigenvalue of H_L and corresponding generalized eigenfunction, respectively. Then

$$\psi\psi^* v=\left(-\frac{E}{8}+1\right)v, \tag{2.2}$$

and multiplying ψ^* on both sides, we have $H(\psi^* v)=E(\psi^* v)$ with $\psi^* v$ growing at most polynomially at infinity. Therefore since $\omega\in\Omega_0$, $\psi^* v$ and hence $\psi\psi^* v$ decay exponentially. By (2.2), v also decays exponentially which concludes the proof of Theorem 1.1 (1).

To prove Theorem 1.1 (2), it suffices to show dim ker $\psi^*=\infty$ which follows from the lemma given below. We say a subgraph $C(\subset\mathbf{Z}^2)$ is a cycle of length $N(\geqslant 3)$ if there exists $x_1,x_2,\ldots,x_N\in V(\mathbf{Z}^2)$, $x_j\neq x_k$ for $j\neq k$ such that $\alpha_1=x_1x_2,\alpha_2=x_2x_3,\ldots,\alpha_j=x_jx_{j+1},\ldots,\alpha_{N-1}=x_{N-1}x_N,\alpha_N=x_Nx_1\in\mathcal{E}(\mathbf{Z}^2)$. We say C is even (resp., odd) if its length is even (resp., odd). The flux on C is given by

$$\Phi(C)=\sum_{j=1}^{N}A(\alpha_j)(\mathrm{mod}\,2\pi\,).$$

Lemma 2.1: Let $C(\subset\mathbf{Z}^2)$ be a cycle of even length N. If $\Phi(C)=0$, there exists $F\in\ker\psi^*$ which is supported on $E(C)$.

Proof: Set

$$F(|\alpha_1|)=1,\quad F(|\alpha_2|)=(-1)\exp\left[-i\frac{A(\alpha_2)}{2}-i\frac{A(\alpha_1)}{2}\right],$$

$$F(|\alpha_j|)=(-1)^{j-1}\exp\left[-i\frac{A(\alpha_j)}{2}-i(A(\alpha_2)+\cdots+A(\alpha_{j-1}))-i\frac{A(\alpha_1)}{2}\right],$$

for $3\leqslant j\leqslant N$ and $F(|\beta|)=0$ for $|\beta|\notin E(C)$. A direct computation gives $\psi^*F=0$. □

It is possible to take infinite number of even cycles in $\mathbf{Z}^2$, satisfying the assumption of Lemma 2.1. Thus we proved Theorem 1.1(2). Moreover, we have the following.

Proposition 2.1: For any configuration of $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$, we have dim ker $\psi^*=\infty$.

Proof: Let G_x be the subgraph of $\mathbf{Z}^2$ with $V(G_x)=f_x\cup f_{x+e_1}$ and $\mathcal{E}(G_x)=\{yz:y,z\in V(G_x),|y-z|=1\}$. By Theorem 3.1, there exists a function F_x on $E(G_x)$ such that $\psi^*_{G_x}F_x=0$. Let $\tilde{F}_x(|\alpha|)=F_x(|\alpha|)$ for $|\alpha|\in E(G_x)$ and $\tilde{F}_x(|\alpha|)=0$ otherwise. Then $\psi^*\tilde{F}_x=0$. Since $\tilde{F}_x,\tilde{F}_y$ are linearly independent for $|x-y|\geqslant 2$, we have dim ker $\psi^*=\infty$. □

If we have no magnetic flux, i.e., $\Phi(f_x)=0$ for any $x\in\mathbf{Z}^2$, then ker ψ^* contains functions supported on $|\partial f_x|=\{|\alpha|:\alpha\in\partial f_x\}$.[17,15] On the other hand, if $\Phi(f_x)\neq 0$ for any $x\in\mathbf{Z}^2$, the proof of Lemma 2.1 implies that it is impossible and the supports of elements of ker ψ^* must be bigger, while Proposition 2.1 says the edges of two plaquettes $|\partial f_x|\cup|\partial f_{x+e_1}|$ are enough.

Remark 2.1: It is also possible to construct "extended states" for any configuration of magnetic fluxes. To see this, choose the gauge such that the vector potential A vanishes on edges parallel to the x_1-direction: $A(\alpha)=0$ for $\alpha=x(x+e_1)$. Let $|\alpha_{n,m}|\in E(\mathbf{Z}^2)$ be the edge connecting the vertices (n,m) and $(n+1,m)\in V(\mathbf{Z}^2)$. Then $F(|\alpha|)=(-1)^n$ for $|\alpha|=|\alpha_{n,m}|$, and $F(|\alpha|)=0$ otherwise, satisfies the desired properties.

Finally, we study the relationship between IDS of H,H_L.

Proposition 2.2: Suppose $\{\Phi(f_x)\}_{x\in\mathbf{Z}^2}$ are metrically transitive random variables on a probability space $(\Omega,\mathcal{F},\mathbf{P})$. Then IDS of H,H_L satisfy

$$k_L(E)=\begin{cases}\frac{1}{2}k(E) & (E<8),\\ \frac{1}{2}k(E)+\frac{1}{2} & (E\geqslant 8).\end{cases}$$

Proof: Define $\psi_M: l^2(\mathbf{Z}_M^2)\to l^2(L(\mathbf{Z}_M^2))_2$ as ψ restricted on $\mathbf{Z}_M^2$: $\psi_M=\chi_{L(\mathbf{Z}_M^2)}\psi\chi_{\mathbf{Z}_M^2}$ (χ_A is the characteristic function of A) and $\psi_M^*: l^2(L(\mathbf{Z}_M^2))_2\to l^2(\mathbf{Z}_M^2)$ as its adjoint. Let $\tilde{H}^M=8(1-\psi_M^*\psi_M)$, $\tilde{H}_L^M=8(1-\psi_M\psi_M^*)$ be local Hamiltonians of H,H_L, respectively. Since $\dim\ker(\psi_M^*\psi_M-E)=\dim\ker(\psi_M\psi_M^*-E)$ for $E\neq 0$, and since $\sharp V(L(\mathbf{Z}_M^2))-\sharp V(\mathbf{Z}_M^2)\leqslant\dim\ker\psi_M^*\leqslant\sharp V(L(\mathbf{Z}_M^2))-\sharp V(\mathbf{Z}_M^2)+1$ (Theorem 3.1 and Proposition 4.3 in Biggs[4]), we have

$$k_L(E)=\begin{cases}\rho k(E) & (E<8),\\ \rho k(E)+(1-\rho) & (E\geqslant 8),\end{cases}$$

where $\rho=\lim_{M\to\infty}[\sharp V(\mathbf{Z}_M^2)/\sharp V(L(\mathbf{Z}_M^2))=1/2$. □

Proposition 2.2 shows that $k_L(E)$ is discontinuous and thus proves Theorem 1.1 (3). Moreover, it also implies that H_L has an eigenvalue with infinite multiplicity a.s.

Lemma 2.2: Under the assumption of Proposition 2.2, suppose that H_L does not have eigenvalues with infinite multiplicity on an open interval $A(\subset\mathbb{R})$ a.s. Then the IDS of H_L is continuous on A.

Proof: For Borel sets $B(\subset A)$, let

$$I(B):=\lim_{M\to\infty}\frac{1}{\sharp V(L(\mathbf{Z}_M^2))}\sharp\{\text{eigenvalues of }\tilde{H}_L^M\text{ on }B\}.$$

We show $\lim_{\epsilon\to 0}I((a-\epsilon,a+\epsilon))=0$ for $a\in A$. Let $|\alpha|\in E(\mathbf{Z}^2)$. By Birkhoff's ergodic theorem,

$$I(B)=\int_\Omega d\mathbf{P}\int_B\frac{1}{6}\langle dE(\lambda)\delta_{|\alpha|},\delta_{|\alpha|}\rangle_{L(bfZ^2)},\quad\text{a.s.}$$

where $dE(\lambda)$ is the resolution of identity of H_L and

$$\delta_{|\alpha|}(|\beta|)=\begin{cases}1 & (|\beta|=|\alpha|),\\ 0 & (\text{otherwise}),\end{cases}\quad |\beta|\in E(\mathbf{Z}^2).$$

Therefore it suffices to show $I(\{a\})=0$. We consider Lebesgue's decomposition of $dE(\lambda)$ into continuous and singular parts: $dE=dE_c+dE_s$ and let $I(B)=I_c(B)+I_s(B)$ be the corresponding decomposition of $I(B)$. Since dE_c does not have an atom, $I_c(\{a\})=0$. If $a\in\sigma_p(H_L)$, let $\{f_j\}_{j=1}^N$ be the normalized eigenfunctions of H_L corresponding to the eigenvalue a. Then since $\sum_{|\alpha|\in E(\mathbf{Z}_M^2)}6|f_j(|\alpha|)|^2\leqslant 1$,

$$I_s(\{a\})=\lim_{M\to\infty}\frac{1}{\sharp V(L(\mathbf{Z}_M^2))}\sum_{|\alpha|\in E(\mathbf{Z}_M^2)}6\sum_{j=1}^N|f_j(|\alpha|)|^2=0,\quad\text{a.s.}$$

□

III. SOME PROPERTIES ON LINE GRAPHS

In this section, we show some related and interesting properties of magnetic Schrödinger operators on line graphs. First of all, we suppose G is a finite graph and consider the operator $\psi_G^*: l^2(L(G))_2\to l^2(G)$ defined in Sec. II. By definition, $\dim\ker\psi_G^*\geqslant\sharp E(G)-\sharp V(G)$. It is known, if G is bipartite or is an odd cycle and $A(\alpha)=0$ for any $\alpha\in\mathcal{E}(G)$, $\dim\ker\psi_G^*=\sharp E(G)-\sharp V(G)+1$ [Proposition 4.3 in Biggs;[4] a graph G is said to be bipartite if $V(G)$ can be

decomposed into two disjoint subsets: $V(G)=A\cup B, A\cap B=\varnothing$ such that $x,y\in V(G)$ are connected by an edge in $E(G)$ only if $x\in A, y\in B$ or $x\in B, y\in A$]. The following theorem says the situation becomes different when the magnetic flux is turned on.

Theorem 3.1: *Let G be a finite and connected graph without self-loops and multiple edges. Suppose that for some cycle C on G, $\Phi(C)\neq 0$ (resp., π) if C is even (resp., odd). Then* $\dim\ker\psi_G^*=\sharp E(G)-\sharp V(G)$.

When G is a planar graph, $\sharp E(G)-\sharp V(G)=\sharp F(G)-1$ by Euler's formula, where $F(G)$ is the set of faces on G [the faces of a finite planar graph G is the bounded connected components of $\mathbf{R}^2-(V(G)\cup E(G))$ regarding $V(G)\cup E(G)$ as a closed subset of $\mathbf{R}^2$].

Proof: We show $\operatorname{rank}\psi_G^*=\sharp V(G)$. Let $D=\{d_{jk};1\leqslant j\leqslant\sharp V(G),1\leqslant k\leqslant\sharp E(G)\}$ be the $(\sharp V(G))\times(\sharp E(G))$ matrix which is a representation of ψ_G^* on the basis $\{\delta_x\}_{x\in V(G)},\{\delta_{|\alpha|}\}_{|\alpha|\in E(G)}$, where

$$\delta_x(z)=\begin{cases}1 & (z=x),\\ 0 & (\text{otherwise}),\end{cases}\qquad \delta_{|\alpha|}(|\beta|)=\begin{cases}1 & (|\beta|=|\alpha|),\\ 0 & (\text{otherwise}),\end{cases}$$

and let $\{\mathbf{d}_j\}_{j=1}^{\sharp V(G)}(\subset\mathbf{C}^{\sharp E(G)})$ be its row vectors. In what follows, we identify $V(G)$ with the finite set $\{1,\ldots,\sharp V(G)\}$. Suppose that a linear relation is given: $\Sigma_{j=1}^{\sharp V(G)}\beta_j\mathbf{d}_j=\mathbf{0}$, $\beta_j\in\mathbf{C}$. We assume $\beta_h\neq 0$ for some $h\in\{1,\ldots,\sharp V(G)\}$ and show that, for any cycles C on G, $\Phi(C)=0$ (resp., π) if C is even (resp., odd). The supposed linear relation implies that, for $\alpha\in\mathcal{E}(G)$ with $i(\alpha)=k, t(\alpha)=l$ $(k,l\in\{1,\ldots,\sharp V(G)\})$,

$$\beta_l=-\frac{m(l)}{m(k)}e^{iA(\alpha)}\beta_k. \tag{3.1}$$

Therefore, since G is connected, $\beta_h\neq 0$ for some $h\in\{1,\ldots,\sharp V(G)\}$ implies $\beta_k\neq 0$ for any $k\in\{1,\ldots,\sharp V(G)\}$. Let C be a cycle on G of length N. We write $V(C)=\{x_1,\ldots,x_N\}$ and let $\alpha_1=x_1x_2,\ldots,\alpha_j=x_jx_{j+1},\ldots,\alpha_{N-1}=x_{N-1}x_N,\alpha_N=x_Nx_1\in\mathcal{E}(C)$. By (3.1),

$$\beta_{x_{j+1}}=-\frac{m(x_{j+1})}{m(x_j)}e^{iA(\alpha_j)}\beta_{x_j},\quad 1\leqslant j\leqslant N$$

$(x_{N+1}\equiv x_1)$. Since $\beta_k\neq 0$ for any k, we have $(-1)^Ne^{i\Phi(C)}=1$. □

Next, we come back to the case $G=\mathbf{Z}^2$ and we show that, if magnetic fluxes are uniformly away from zero, all elements of $\ker\psi^*$ can be obtained by restricting ψ^* on finite subgraph of $L(\mathbf{Z}^2)$. To be precise, let $\mathbf{Z}_M^2=\{x=(x_1,x_2)\in\mathbf{Z}^2:|x_j|\leqslant M, j=1,2\}$ be the finite box of size $2M+1$ and let

$$N=\cup_{M=1}^{\infty}\ \ker\ \psi_{\mathbf{Z}_M^2}^*$$

be the subspace of $\ker\psi^*$. By Theorem 3.1, $\dim\ker\psi_{\mathbf{Z}_M^2}^*=4M^2-1$. We denote by $\Phi(f)$ the magnetic flux penetrating the face $f\in F(\mathbf{Z}^2)$.

Theorem 3.2: *If $|\Phi(f)|\geqslant c>0$ $(f\in F(\mathbf{Z}^2))$ for some constant $c>0$, then $N=\ker\psi^*$.*

Theorem 3.2 says we can take family of finitely supported elements as a basis of $\ker\psi^*$, whose proof essentially relies on the fact that, because of the magnetic flux, 8 is an isolated point of $\sigma(H_L)$. We prepare the following notations:

$$\chi_M=\chi_{\mathbf{Z}_M^2},\quad \chi_M^L=\chi_{L(\mathbf{Z}_M^2)},$$

$$\psi_M=\chi_M^L\psi\chi_M,\quad \psi_M^*=\chi_M\psi^*\chi_M^L,$$

$$T_M^L=\psi_M\psi_M^*=\chi_M^L\psi\chi_M\psi^*\chi_M^L.$$

We regard ψ_M (resp., ψ_M^*, T_M^L) as an operator on $l^2(\mathbf{Z}_M^2)_2$ (resp. $l^2(L(\mathbf{Z}_M^2))_2$).

Lemma 3.1: For any $M \in \mathbf{N}$, $\psi_M^* \psi_M \geqslant \delta > 0$ *for some* $\delta > 0$.

Proof: By direct computation,

$$(8\psi_M^* \psi_M u)(x) = \sum_{y \in \mathbf{Z}_M^2, |y-x|=1} (u(x) - e^{iA'(x,y)} u(y)), \quad x \in \mathbf{Z}_M^2,$$

where $A'(x,y) = A(x,y) + \pi$. Then ($\mathcal{E}_M = \mathcal{E}(\mathbf{Z}_M^2)$ [resp., $\mathcal{F}_M = F(\mathbf{Z}_M^2)$] is the set of directed edges (resp., faces) on $\mathbf{Z}_M^2$),

$$\begin{aligned}\langle u, 8\psi_M^* \psi_M u \rangle_2 &= \sum_{e \in \mathcal{E}_M} |u(o(e)) - e^{iA'(e)} u(t(e))|^2 \\ &\geqslant \sum_{f \in \mathcal{F}_M} \sum_{e \in \partial f} |u(o(e)) - e^{iA'(e)} u(t(e))|^2 \\ &\geqslant 2 \sum_{f \in \mathcal{F}_M} \left(1 - \cos \frac{\Phi(f)}{4}\right) \sum_{x \in f} |u(x)|^2 = 2 \sum_{x \in \mathbf{Z}_M^2} W_\Phi(x) |u(x)|^2,\end{aligned}$$

where $W_\Phi(x) = \Sigma_{x \in \partial f, f \in \mathcal{F}_M} (1 - \cos[\Phi(f)/4]) > 0$. □

Proof of Theorem 3.2: We suppose that there exists $\varphi \in \ker \psi^*$ such that $\|\varphi\|_2 = 1$, $\varphi \perp N$ and would like to deduce a contradiction. Let

$$\epsilon = \min\left\{\frac{\delta}{2}, \frac{1}{2}\right\}, \quad \varphi_M = \chi_M^L \varphi \in l^2(L(\mathbf{Z}_M^2))_2.$$

Since $\varphi \in \ker \psi^*$ and $T_M^L \varphi_M = \chi_M^L \psi \chi_M \psi^* \chi_M^L \varphi$, $\|T_M^L \varphi_M\|_2 < \epsilon^2$ for some $M \in \mathbf{N}$. We can assume $\|\varphi_M\|_2 > 1 - \epsilon$ by taking $M \in \mathbf{N}$ sufficiently large if necessary. Let $\tilde{T}_M^L = T_M^L|_{(\ker T_M^L)^\perp}$ be the restriction of T_M^L on $(\ker T_M^L)^\perp$. Since $\varphi_M \in (\ker \psi_{\mathbf{Z}_M^2}^*)^\perp \subset (\ker T_M^L)^\perp$, we have $\|\tilde{T}_M^L \varphi_M\|_2 = \|T_M^L \varphi_M\|_2 < \epsilon^2$. Suppose $(-\epsilon, \epsilon) \subset \rho(\tilde{T}_M^L)$. Then

$$1 - \epsilon < \|(\tilde{T}_M^L)^{-1} \tilde{T}_M^L \varphi_M\|_2 \leqslant \frac{1}{\epsilon} \cdot \epsilon^2 = \epsilon,$$

which implies $1 < 2\epsilon$ and contradicts the definition of ϵ. Hence $(-\epsilon, \epsilon) \cap \sigma(\tilde{T}_M^L) \neq \varnothing$ and let $\lambda \in (-\epsilon, \epsilon) \cap \sigma(\tilde{T}_M^L)$ be an eigenvalue of $\tilde{T}_M^L$ with corresponding eigenvector $f \in (\ker T_M^L)^\perp, \|f\|_2 = 1$. We then have

$$T_M^L f = \psi_M \psi_M^* f = \lambda f, \tag{3.2}$$

$$\psi_M^* \psi_M \psi_M^* f = \lambda \psi_M^* f. \tag{3.3}$$

Because $f \in (\ker T_M^L)^\perp$, $\lambda \neq 0$. Then by (3.2), we must have $\psi_M^* f \neq 0$, which, by (3.3), contradicts Lemma 3.1. □

Remark 3.1: Theorem 3.2 can easily be extended to any planar infinite graph G satisfying [$n(f)$ *is the number of vertices in* $f \in F(G)$] *(i)* $\max_{f \in F(G)} n(f) < \infty$; *(ii) for some* $c > 0$, $|\Phi(f)| > c$ [*resp.*, $|\Phi(f) - \pi| > c$] *if* $n(f)$ *is even (resp., odd).*

In the rest of this section, we show that each component of the spectrum and the corresponding spectral subspaces are also related in Eq. (1.4), which holds in general situations. Let $\mathcal{H}^G, \mathcal{H}^L$ be Hilbert spaces and suppose that a bounded operator $\psi: \mathcal{H}^G \to \mathcal{H}^L$ is given with $\psi^*: \mathcal{H}^L \to \mathcal{H}^G$ its adjoint. Let $H_G = \psi^* \psi, H_L = \psi \psi^*$ be bounded self-adjoint operators on $\mathcal{H}^G, \mathcal{H}^L$ and let

$$\mathcal{H}^\sharp = \mathcal{H}^\sharp_{\mathrm{ac}} \oplus \mathcal{H}^\sharp_{\mathrm{sc}} \oplus \mathcal{H}^\sharp_{pp},$$

$$\mathcal{H}^\sharp_c = \mathcal{H}^\sharp_{\mathrm{ac}} \oplus \mathcal{H}^\sharp_{\mathrm{sc}}, \quad \mathcal{H}^\sharp_{\mathrm{sing}} = \mathcal{H}^\sharp_{\mathrm{sc}} \oplus \mathcal{H}^\sharp_{pp}, \quad \sharp = G, L,$$

be the decomposition of $\mathcal{H}^\sharp$ into the spectral subspaces w.r. t. $H^\sharp$ $(\sharp = G, L)$. $\mathcal{H}^\sharp_{\mathrm{ac}}$ (resp., $\mathcal{H}^\sharp_{\mathrm{sc}}, \mathcal{H}^\sharp_{pp}$) stands for the absolutely continuous (resp., singular continuous, pure point) subspace. We assume that

$$\ker\ \psi = \{0\}, \quad \ker\ \psi^* \neq \{0\},$$

which are true if $\mathcal{H}^G = l^2(G), \mathcal{H}^L = l^2(L(G))_2, \psi = \psi_G$ for an infinite graph G which is not a tree. We note that, under this assumption, ψ, ψ^* can be regarded as maps,

$$\psi : \mathcal{H}^G \to (\ker\ \psi^*)^\perp, \quad \psi^* : (\ker\ \psi^*)^\perp \to \mathcal{H}^G,$$

with bounded inverses. Our assertion is that each component of spectrum and spectral subspaces are related as follows.

Theorem 3.3:

$$(1) \quad \sigma_{\mathrm{ac}}(H_G) = \sigma_{\mathrm{ac}}(H_L), \quad \psi \mathcal{H}^G_{\mathrm{ac}} = \mathcal{H}^L_{\mathrm{ac}}, \quad \mathcal{H}^G_{\mathrm{ac}} = \psi^* \mathcal{H}^L_{\mathrm{ac}},$$

$$(2) \quad \sigma_{\mathrm{sc}}(H_G) = \sigma_{\mathrm{sc}}(H_L), \quad \psi \mathcal{H}^G_{\mathrm{sc}} = \mathcal{H}^L_{\mathrm{sc}}, \quad \mathcal{H}^G_{\mathrm{sc}} = \psi^* \mathcal{H}^L_{\mathrm{sc}},$$

$$(3) \quad \sigma_{pp}(H_L) = \sigma_{pp}(H_G) \cup \{0\}, \quad \psi \mathcal{H}^G_{pp} = \mathcal{H}^L_{pp} \cap (\ker\ \psi^*)^\perp,$$

$$\psi^* (\mathcal{H}^L_{pp} \cap (\ker\ \psi^*)^\perp) = \mathcal{H}^G_{pp},$$

where $\sigma_{pp}(H) = \overline{\{\text{eigenvalues of } H\}}$.

As a preliminary of the proof, we note the following.

Lemma 3.2: Let $P^\sharp(\cdot)$ *be the spectral projection of* $H^\sharp$ $(\sharp = G, L)$. *Then for any* $A \in \mathcal{B}$ ($\mathcal{B}$ *is the Borel set in* **R**),

$$\psi P^G(A) = P^L(A)\psi, \quad P^G(A)\psi^* = \psi^* P^L(A).$$

Proof: By definition of H^G, H^L and the boundedness of $\psi, \psi H^n_G = H^n_L \psi$. Then $\psi e^{-tH_G} = e^{-tH_L}\psi$ and by taking the Laplace transform, we have $\psi(H_G - z)^{-1} = (H_L - z)^{-1}\psi$, $z \in \mathbf{C} \setminus \mathbf{R}$. By Stone's formula and regularity of the spectral measure, we have the first assertion. The second one is proved similarly. □

Proof of Theorem 3.3:

(1) We show

$$\psi P^G_{\mathrm{ac}}(A) \mathcal{H}^G = P^L_{\mathrm{ac}}(A) \mathcal{H}^L, \tag{3.4}$$

for any $A \in \mathcal{B}$. $P^\sharp_{\mathrm{ac}}(\cdot)$ is the spectral projection of the absolutely continuous part of $H^\sharp$ [$P^\sharp_{\mathrm{sc}}(\cdot)$ is defined in the same way.] $\sigma_{\mathrm{ac}}(H_G) = \sigma_{\mathrm{ac}}(H_L)$ follows from (3.4). Let $f \in P^G_{\mathrm{ac}}(A)\mathcal{H}^G$. By Lemma 3.2,

$$\langle \psi P^G(A \cap B) f, F \rangle_L = \langle P^L(A \cap B) \psi f, F \rangle_L,$$

for any $F \in \mathcal{H}^L, B \in \mathcal{B}$. $\langle \cdot, \cdot \rangle_\sharp$ is the inner product on $\mathcal{H}^\sharp$ $(\sharp = G, L)$. By the definition of f, we have

$$\langle \psi P^G_{\mathrm{ac}}(B) f, F \rangle_L = \langle P^L(B) P^L(A) \psi f, F \rangle_L.$$

$LHS = 0$ whenever $|B| = 0$ ($|\cdot|$ is the Lebesgue measure on **R**). Letting $F = P^L(A)\psi f$,

$$\langle P^L(B)P^L(A)\psi f, P^L(A)\psi f\rangle_L = 0, \text{ if } |B| = 0.$$

Since $P^L(A)\psi f = \psi P^G(A)f = \psi f$, we have $\psi f \in P^L_{\rm ac}(A)\mathcal{H}^L$.

Conversely, let $G \in P^L_{\rm ac}(A)\mathcal{H}^L (\subset (\ker\psi^*)^\perp)$, $f = \psi^{-1}G$. For any $F \in \mathcal{H}^L, B \in \mathcal{B}$, we have

$$\langle P^L(A\cap B)G, F\rangle_L = \langle \psi P^G(A\cap B)f, F\rangle_L .$$

By the definition of G, we have

$$\langle P^L(B)\psi f, F\rangle_L = \langle P^G(B)P^G(A)f, \psi^* F\rangle_G .$$

$LHS = 0$ if $|B| = 0$. Substituting $F = (\psi^*)^{-1}P^G(A)f$, we have $P^G(A)f \in P^G_{\rm ac}(A)\mathcal{H}^G$. Since $\psi P^G(A)f = G$, we showed $G \in \psi P^G_{\rm ac}(A)\mathcal{H}^G$, proving (3.4). $\mathcal{H}^G_{\rm ac} = \psi^*\mathcal{H}^L_{\rm ac}$ follows similarly.

(2) As in the proof of (1), we show

$$\psi P^G_{\rm sc}(B)\mathcal{H}^G = P^L_{\rm sc}(B)\mathcal{H}^L, \tag{3.5}$$

for any $B \in \mathcal{B}$ which also proves $\sigma_{\rm sc}(H^G) = \sigma_{\rm sc}(H^L)$. To prove $\psi P^G_{\rm sc}(B)\mathcal{H}^G \subset P^L_{\rm sc}(B)\mathcal{H}^L$, let $f \in P^G_{\rm sc}(B)\mathcal{H}^G$. Without loss of generality, we can suppose $f \neq 0$. Let

$$\mu^f_{\rm sc}(\cdot) = \langle P^G(\cdot)f, f\rangle_G = \langle P^G(\cdot\cap B)f, f\rangle_G$$

be a singular continuous measure whose support $B' = \text{supp}\ \mu^f_{\rm sc}$ satisfies $|B'| = 0$. For any $A \in \mathcal{B}, F \in \mathcal{H}^L$,

$$\langle \psi^* P^L(A\backslash B')F, f\rangle_G = \langle P^G(A\backslash B')\psi^* F, f\rangle_G = 0.$$

Substituting $F = \psi f$ in LHS, we have $\langle P^L(A\backslash B')\psi f, \psi f\rangle_L = 0$. Moreover, substituting $G = (\psi^*)^{-1}f$, in the equality $\langle P^L(B')\psi f, G\rangle_L = \langle \psi P^G(B')f, G\rangle_L$, we have $P^L(B')\psi f \neq 0$ implying $\psi f \in \mathcal{H}^L_{\rm sing}$. On the other hand for any $b \in B'$, $P^L(\{b\})\psi f = \psi P^G(\{b\})f = 0$ implying $\psi f \in \mathcal{H}^L_c$. Thus $\psi f \in P^L_{\rm sc}(B)\mathcal{H}^L$.

Conversely, let $F \in P^L_{\rm sc}(B)\mathcal{H}^L (\subset (\ker\psi^*)^\perp)$, $F \neq 0$, $f = \psi^{-1}F$ and let

$$\mu^F_{\rm sc}(\cdot) = \langle P^L(\cdot)F, F\rangle_L = \langle P^L(\cdot\cap B)F, F\rangle_L ,$$

with supp $\mu^F_{\rm sc} = B'$, $|B'| = 0$. For any $A \in \mathcal{B}, G \in \mathcal{H}^L$,

$$\langle P^G(A\backslash B')f, \psi^* G\rangle_G = \langle P^L(A\backslash B')F, G\rangle_L = 0.$$

Substituting $G = (\psi^*)^{-1}f$, we have $\langle P^G(A\backslash B')f, f\rangle_G = 0$. Since $\langle P^G(B')f, \psi^* F\rangle_G = \langle P^L(B')F, F\rangle_L \neq 0$, $P^G(B')f \neq 0$ so that $f \in \mathcal{H}^G_{\rm sing}$. For $b \in B'$, $\psi P^G(\{b\})f = P^L(\{b\})F = 0$ and together with $\ker\psi = \{0\}$, we have $P^G(\{b\})f = 0$ which implies $f \in \mathcal{H}^G_{\rm sc}$. Thus $f \in P^G_{\rm sc}(B)\mathcal{H}^G$ proving (3.5). $\mathcal{H}^G_{\rm sc} = \psi^*\mathcal{H}^L_{\rm sc}$ follows similarly.

(3) Let

$$\sigma_p(H^\sharp) = \{\text{eigenvalues of } H^\sharp\}, \quad \mathcal{H}^\sharp_p = \{\text{eigenfunctions of } H^\sharp\}, \quad \sharp = G, L.$$

Then it is easy to see that

$$\sigma_p(H^L) = \sigma_p(H^G) \cup \{0\},$$

$$\psi\mathcal{H}^G_p = \mathcal{H}^L_p \cap (\ker\ \psi^*)^\perp, \quad \psi^*(\mathcal{H}^L_p \cap (\ker\ \psi^*)^\perp) = \mathcal{H}^G_p .$$

By taking closure, we have the desired relations. □

IV. PROOF OF THEOREM 1.2

To prove Theorem 1.2 (2), we show the Wegner estimate and Lifshitz tail to confirm the assumption of multiscale analysis. By the relation $\sigma(\psi_{\mathbf{Z}_M^2}\psi^*_{\mathbf{Z}_M^2})=\sigma(\psi^*_{\mathbf{Z}_M^2}\psi_{\mathbf{Z}_M^2})\cup\{0\}$ and the Wegner estimate proved by Klopp *et al.*,[8] we have the following: there exists a constant $C>0$ such that

$$\mathbf{P}\{\text{dist}\ (E,\sigma(H_L^M))<\epsilon\}\leqslant C\epsilon M^2, \tag{4.1}$$

for $E\in I_R=[4(1-\cos c/4),4(1-\cos c/4)+R]\cup[4(1+\cos c/4)-R,4(1+\cos c/4)]$ and for any $\epsilon>0$, $M\in\mathbf{N}$. We used the fact that the operator of rank of order M does not affect the inequality (4.1). Similarly, we can show the Lifshitz tail estimate:

$$\limsup_{E\downarrow E_0}\frac{\log(-\log k_L(E))}{\log(E-E_0)}\leqslant -1, \tag{4.2}$$

where $E_0=4(1-\cos c/4)$. Estimates (4.1), (4.2) allow us to use the standard multiscale analysis to conclude that, for $E\in I_R$ and any $p\in\mathbf{N}$,

$$\mathbf{P}\left\{\sup_{\epsilon\neq 0}|G_L^M(E+i\epsilon;0,x)|\leqslant e^{\gamma(M-|x|)}\right\}\geqslant 1-C_pM^{-p}$$

for some $\gamma>0,C_p>0$ and for any sufficiently large $M\in\mathbf{N}$. $G_L^M(z;x,y)=\langle\delta_x,(H_L^M-z)^{-1}\delta_y\rangle_2$. Then $\sigma(E)=0$ follows from Theorem 1.1 in Frölich–Spencer.[6]

To prove Theorem 1.2 (2), let P be the orthogonal projection corresponding to the eigenvalue $E_0=8$. Then (dE_λ is the resolution of the identity)

$$\sigma_\epsilon(E_0)=\epsilon^2\sum_{x\in L(\mathbf{Z}^2)}|x|^2\mathbf{E}\left|\frac{1}{-i\epsilon}\langle 0|P|x\rangle+\int_{\{\lambda\neq E_0\}}\frac{1}{\lambda-(E_0+i\epsilon)}\langle 0|dE_\lambda|x\rangle\right|^2$$

$$=\sum_{x\in L(\mathbf{Z}^2)}|x|^2\mathbf{E}|i\langle 0|P|x\rangle+\epsilon G'(E_0+i\epsilon;0,x)|^2,$$

where $G'(z)=(QH_LQ-z)^{-1},Q=I-P$. Since E_0 is an isolated eigenvalue, the matrix element $P(x,y)$ of P decays exponentially as $|x-y|\to\infty$ and so is Q. Therefore the matrix element of QH_LQ decays exponentially. Then by a version of the Combes–Thomas method[1] and by $E_0\in\rho(QH_LQ)$, $G'(E_0+i\epsilon;0,x)$ decays exponentially as $|x|\to\infty$ uniformly w.r.t. $\epsilon>0$ and $\omega\in\Omega$. Hence

$$\sigma(E_0)=\sum_{x\in L(\mathbf{Z}^2)}|x|^2\mathbf{E}|\langle 0|P|x\rangle|^2<\infty.$$

The rhs of the above equation is called the localization length[3] which is nonzero by the covariance of $P(x,y)$. Thus Theorem 1.2 (2) is proved.

APPENDIX A

In this appendix, we discuss some examples in which the argument by Klopp *et al.*[8] applies. In all cases presented below, we can prove that the Anderson localization holds on spectral edges.

Example 1 [another distribution of random vector potential on $\mathbf{Z}^2$]: In this example, we consider another distribution of the random vector potential on $\mathbf{Z}^2$ as described in Fig. 1. These vector potentials $\{\varphi_n\}$ are assumed to be i.i.d. random variables satisfying Assumption A. We then have

$$\sigma(H)=\left[4\left(1-\cos\frac{c}{4}\right),4\left(1+\cos\frac{c}{4}\right)\right],\quad \text{a.s.}$$

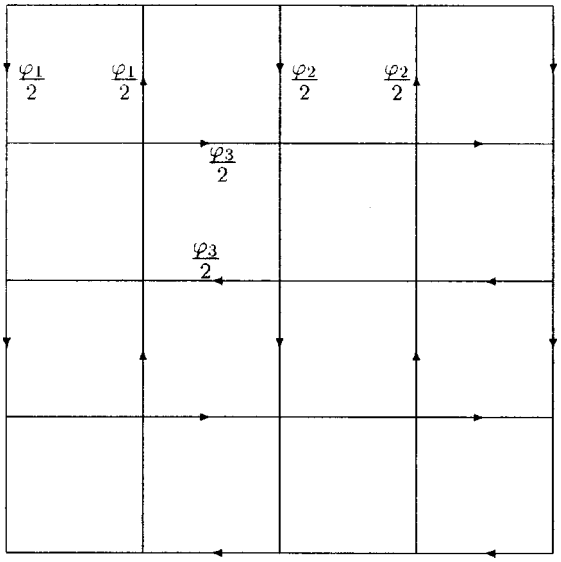

FIG. 1. Square lattice.

Example 2 [triangular lattice]: For the triangular lattice, we put the random vector potential on diagonal edges, as indicated in the Fig. 2. The Hamiltonian H is the same as defined in (1.1). Then we have the ''staggered magnetic flux'' as that on $\mathbf{Z}^2$ discussed in Sec. I. Under Assumption A, the spectrum of H is given by

$$\sigma(H)=\left[6\left(1-\cos\frac{c}{3}\right),6\left(1+\cos\frac{c}{3}\right)\right], \quad \text{a.s.}$$

Example 3 [hexagonal lattice]: To have the ''staggered magnetic flux'' on the hexagonal lattice, we put the random vector potential $\{\varphi_n\}$, as indicated in Fig. 3. Note that there are some faces with no magnetic fluxes (marked as a $\times$ in Fig. 2). Under Assumption A, we have

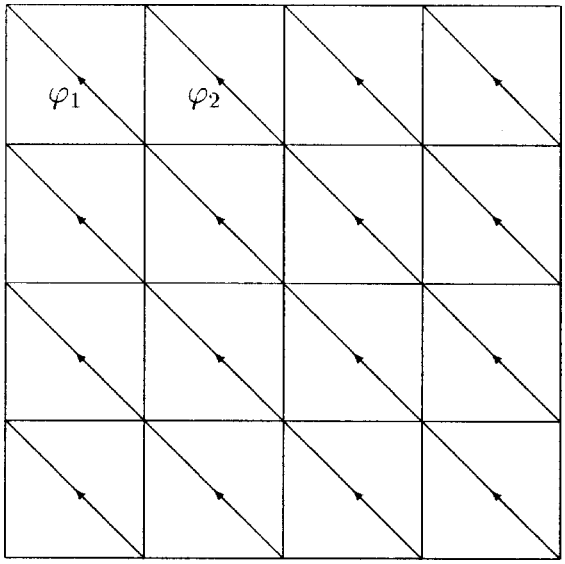

FIG. 2. Triangular lattice.

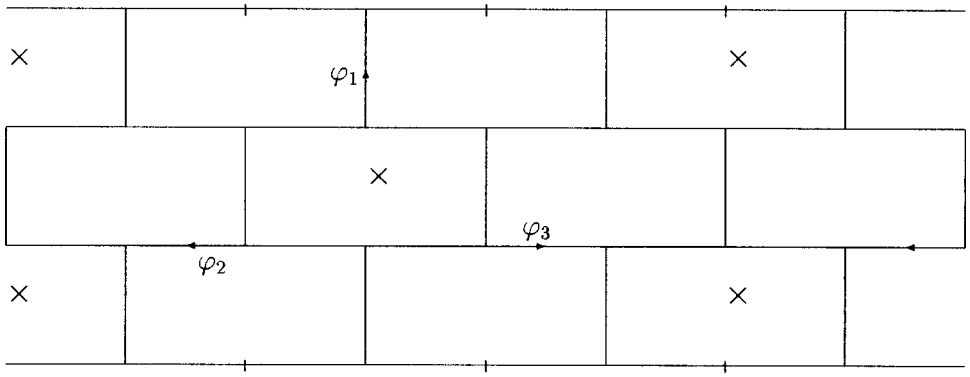

FIG. 3. Hexagonal lattice.

$$\sigma(H)=\left[3-2\sqrt{\frac{5}{4}+\cos\frac{c}{3}},3+2\sqrt{\frac{5}{4}+\cos\frac{c}{3}}\right], \quad \text{a.s.}$$

Furthermore, by using the same argument as in the proof of Theorem 1.1, we have the corresponding results for their line graphs [$d=4$ (resp., $d=6,\ 3$) for the square (resp., triangular, hexagonal) lattice]. That is,

(1) $\sigma(H_L)=\sigma(H)\cup\{2d\}$, a.s., with Anderson localization on spectral edges;
(2) $2d$ is an eigenvalue of H_L with infinite multiplicity;
(3) $k_L(E)$ is discontinuous at $E=2d$: $k_L(2d)-k_L(2d-)=1-2/d$.

APPENDIX B

In this appendix, we study a model which is different from H_L discussed in Theorem 1.1, but for which similar argument works. Let $\Lambda=\{(x_1,x_2):x_1\in\mathbf{Z},x_2=\pm 1\}$ be the ladder and let

$$(H_\Lambda u)(x)=u(x+e_1)+u(x-e_1)+a_\omega(x_1)u(x\pm e_2), \quad u\in l^2(\Lambda),x_2=\mp 1.$$

We suppose $\{a_\omega(x_1)\}_{x_1\in\mathbf{Z}}$ satisfy the following conditions.

Assumption B: $\{a_\omega(x_1)\}_{x_1\in\mathbf{Z}}$ *are real-valued i.i.d. random variables on a probability space* $(\Omega, \mathcal{F}, \mathbf{P})$ *such that the common distribution* ν *is of the Bernoulli type:*

$$\nu=t\delta(p)+(1-t)\delta(q), \quad t\in(0,1), \quad p,q\in\mathbf{R}, \quad p\neq q.$$

$\delta(a)$ is the delta measure supported on $a\in\mathbf{R}$. When $p=1,q=-1$, H_Λ can be regarded as the Bernoulli random flux model while, if $p=0,q=1$, H_Λ can be regarded as a free Hamiltonian on a random graph.

Theorem 6.1: *Under Assumption B, we have the following.*

(1) $\sigma(H_\Lambda)=J\cup(-J)$ *a.s., where* $J=[-2,2]+\{p,q\}$, *which is pure point with exponentially decaying eigenfunctions.*

(2) If $|p|$ *is sufficiently large, then the density of states* (*the Lebesgue–Stieltjes measure corresponding to IDS of* H_Λ) *has a nontrivial singular component.*

Remark 6.1: Although the one-dimensional technique is applicable to H_Λ, *the theory of Lyapunov exponent is complicated in this case.*[7]

The idea of the proof of Theorem 6.1 is to make use of the bipartite structure of Λ which allows us to reduce the problem to that in a one-dimensional Hamiltonian with a Bernoulli-type random potential. Then Theorem 6.1 follows from the result of Anderson localization on such Hamiltonians by Carmona–Klein–Martinelli.[5] It seems that this argument works only for a ladder.

Proof: For $x \in \mathbf{Z}$, we write $x_+ = (x,1), x_- = (x,-1) \in \Lambda$. Let

$$(h(\{a(x)\})f)(x) = f(x-1) + f(x+1) + a(x)f(x), \quad x \in \mathbf{Z}$$

be the Hamiltonian on $l^2(\mathbf{Z})$ with potential $a(x)$. By Theorem 2.1 in Carmona–Klein–Martinelli,[5] there exists $\Omega_0 (\subset \Omega)$ with $\mathbf{P}(\Omega_0) = 1$ such that for $\omega \in \Omega_0$, $h(\{a_\omega(x)\})$ has eigenvalues $\{E_j\}_{j \in \mathbf{N}}$ with $\overline{\{E_j\}}_{j \in \mathbf{N}} = J$ and the set of normalized and exponentially decaying eigenfunctions $\{f_j\}_{j \in \mathbf{N}}$ is a C.O.N.S. on $l^2(\mathbf{Z})$. Fix $\omega \in \Omega_0$ and define functions g_j^1, g_j^2 on Λ,

$$g_j^1(x_\pm) = f_j(x),$$

$$g_j^2(x_+) = (-1)^x f_j(x), \quad g_j^2(x_-) = (-1)^{x-1} f_j(x), \quad j \in \mathbf{N}.$$

It is straightforward to see $H_\Lambda g_j^1 = E_j g_j^1$, $H_\Lambda g_j^2 = -E_j g_j^2$, implying $E_j, -E_j$ are eigenvalues of H_Λ with exponentially decaying eigenfunctions. It suffices to show that $\{g_j^1, g_j^2\}_{j \in \mathbf{N}}$ is C.O.S. on $l^2(\Lambda)$. That they are orthogonal to each other is clear. To see that $\{g_j^1, g_j^2\}_{j \in \mathbf{N}}$ is complete, we decompose $\Lambda = A \cup B$, $A \cap B = \varnothing$ where

$$A = \{x_- : x \text{ is odd}\} \cup \{x_+ : x \text{ is even}\},$$

$$B = \{x_+ : x \text{ is odd}\} \cup \{x_- : x \text{ is even}\}.$$

Then we have

$$g_j^1(y) + g_j^2(y) = \begin{cases} 2 f_j(y_1) & (y \in A), \\ 0 & (y \in B), \end{cases}$$

$$g_j^1(y) - g_j^2(y) = \begin{cases} 0 & (y \in A), \\ 2 f_j(y_1) & (y \in B), \end{cases}$$

and from which the completeness of $\{g_j^1, g_j^2\}_{j \in \mathbf{N}}$ on $l^2(\Lambda)$ follows.

To prove Theorem 6.1 (2), let $\Lambda_M = \{x = (x_1, x_2) \in \Lambda : |x_1| \leqslant M\}$, $\mathbf{Z}_M = \{x \in \mathbf{Z} : |x| \leqslant M\}$ and let $H_{\Lambda_M} = H|_{\Lambda_M} (= \chi_{\Lambda_M} H \chi_{\Lambda_M})$, $h_M = h|_{\mathbf{Z}_M}$ be local Hamiltonians on Λ_M, $\mathbf{Z}_M$, respectively. We define the IDS of H_Λ, h as

$$k_{H_\Lambda}(E) = \lim_{M \to \infty} \frac{1}{\sharp V(\Lambda_M)} \sharp\{\text{eigenvalues of } H_{\Lambda_M} \leqslant E\},$$

$$k_h(E) = \lim_{M \to \infty} \frac{1}{2M+1} \sharp\{\text{eigenvalues of } h_M \leqslant E\}.$$

Since $\lambda \in \sigma(H_{\Lambda_M}) \Leftrightarrow \lambda \in \sigma(h_M)$ or $-\lambda \in \sigma(h_M)$, we have

$$k_{H_\Lambda}(E) = \frac{1}{2} k_h(E) - \frac{1}{2} k_h(-E) + \frac{1}{2}.$$

Theorem 6.1 (2) then follows from Theorem 2.1 in Carmona-Klein–Martinelli.[5] □

APPENDIX C

In this appendix, we consider an application of Theorem 3.1. Let C be the cycle of length N : $V(C) = \{1, \ldots, N\}$, $\mathcal{E}(C) = \{\alpha_j = j(j+1), \ \overline{\alpha_j} = (j+1)j : 1 \leqslant j \leqslant N\}$ $(N+1 \equiv 1)$ and let

$$(H_C f)(x) = t_{|\alpha_{x-1}|} e^{-iA(\alpha_{x-1})} f(x-1) + t_{|\alpha_x|} e^{iA(\alpha_x)} f(x+1) + V(x) f(x),$$

where $t_{|\alpha_x|}>0$, $V(x)\in\mathbf{R}$ $(x=1,\ldots,N,\ \ x+N\equiv x)$. Eigenvalues of H_C are determined by the magnetic flux on C: $\Phi(C)=\Sigma_{x=1}^{N}A(\alpha_x)\ \ (\mathrm{mod}\ 2\pi)$. Let $E(\Phi(C))$ be the lowest eigenvalue of H_C. Then the usual diamagnetic inequality says

$$E(\Phi(C))\geqslant E(\Phi_0),\quad \text{where}\quad \Phi_0=\begin{cases}0 & (N\text{: even}),\\ \pi & (N\text{: odd}).\end{cases}$$

Note that diamagnetic inequality is reversed on the Hubbard model in some cases because of the Fermi statistics (e.g., Lieb–Loss[9] and references therein). However, the converse statement, that is $E(\Phi(C))>E(\Phi_0)$ if $\Phi(C)\neq\Phi_0$ is not known to hold in general except the trivial case where $t_{|\alpha_x|}$ is constant and $V(x)\equiv 0$. Some examples (in the Hubbard model) in which $E(\Phi(C))=E(\Phi_0)$ for some $\Phi(C)\neq\Phi_0$ are discussed in Nakano.[13]

Theorem 7.1: *Suppose the potential V satisfies*

$$V(x)=t_{|\alpha_{x-1}|}+t_{|\alpha_x|},$$

then $E(\Phi_C)>E(\Phi_0)=0$ *if* $\Phi_C\neq\Phi_0$.

In particular, if $\{t_{|\alpha_x|}\}$ is period 2 (i.e., $t_{|\alpha_x|}=t_{|\alpha_{x+2}|}$), V is required to be constant.

Proof: We identify $L(C)$ with C and regard H_C as an operator on $l^2(L(C))_2$. Let $\psi_C^*:l^2(L(C))_2\to l^2(C)$ be

$$(\psi_C^*F)(x)=\sqrt{t_{|\alpha_{x-1}|}}\sum_{\alpha\in N_x(C)}e^{iA(\alpha)/2}F(|\alpha|),\quad F\in l^2(L(C))_2,$$

with ψ_C its adjoint. Then $\psi_C\psi_C^*$ is unitarily equivalent to H_C, for they have the same flux on C. Since $\psi_C\psi_C^*F=0\Leftrightarrow\psi_C^*F=0$, the conclusion follows from Theorem 3.1. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Radon–Nikodym derivatives of quantum operations

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(Received 9 April 2003; accepted 23 July 2003)

Given a completely positive (CP) map T, there is a theorem of the Radon–Nikodym type [W. B. Arveson, Acta Math. **123**, 141 (1969); V. P. Belavkin and P. Staszewski, Rep. Math. Phys. **24**, 49 (1986)] that completely characterizes all CP maps S such that $T-S$ is also a CP map. This theorem is reviewed, and several alternative formulations are given along the way. We then use the Radon–Nikodym formalism to study the structure of order intervals of quantum operations, as well as a certain one-to-one correspondence between CP maps and positive operators, already fruitfully exploited in many quantum information-theoretic treatments. We also comment on how the Radon–Nikodym theorem can be used to derive norm estimates for differences of CP maps in general, and of quantum operations in particular. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1615697]

I. INTRODUCTION

In the mathematical framework of quantum information theory,[1] all admissible devices are modeled by the so-called quantum operations[2,3]—that is, completely positive linear contractions on the algebra of observables of the physical system under consideration. Thus it is of paramount importance to have at one's disposal a good analysis toolkit for completely positive (CP) maps.

There are many useful structure theorems for CP maps. The two best known ones, due to Stinespring[4] and Kraus,[3] are *de rigueur* in virtually all quantum information-theoretic treatments. These theorems are significant because each of them states that a given map is CP if and only if it is expressible in a certain canonical form. However, in many applications we need to consider whole families of CP maps. This necessitates the introduction of comparison tools for CP maps, e.g., when the family of CP maps in question admits some sort of (partial) order.

Mathematically, the set of all CP maps between two algebras of observables is a cone that can be partially ordered in the following natural way. If S and T are two CP maps, we write $S \leqslant T$ if $T-S$ is CP as well. This partial order comes up in, e.g., the problem of distinguishing between two known CP maps with given *a priori* probabilities under the constraint that the average probability of error is minimized.[5] A typical way of dealing with partially ordered cones is to exhibit a correspondence between the cone's order and a partial order of some ''simpler'' objects. This is accomplished by means of theorems of the Radon–Nikodym type, as in the case of, e.g., partial ordering of positive measures or positive linear functionals. There are a number of Radon–Nikodym theorems for CP maps (see, e.g., the work of Arveson,[6] Belavkin and Staszewski,[7] Davies,[2] Holevo,[8] Ozawa,[9] and Parthasarathy[10]) that differ widely in scope and in generality. Thus, the results of Davies, Ozawa, and Holevo have to do with Radon–Nikodym derivatives of CP instruments[9] with respect to scalar measures. On the other hand, ideas common to the Arveson and Belavkin–Staszewski theorems, with further developments by Parthasarathy, are directly applicable to the partial ordering of CP maps described above, and will therefore be the focus of the present article. More specifically, we will demonstrate that certain problems encountered in quantum information-theoretic settings that involve characterization and comparison of CP maps, are best understood in this Radon–Nikodym framework.

The paper is organized as follows. We summarize the salient facts on CP maps and quantum

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operations in Sec. II. In Sec. III we review the Arveson–Belavkin–Staszewski formulation of the Radon–Nikodym theorem for CP maps and state several alternative, but equivalent, versions. The Radon–Nikodym machinery is then applied to the following problems: partial ordering of quantum operations (Sec. IV), characterization of quantum operations by means of positive operators (Sec. V), and estimating norms of differences of CP maps (Sec. VI). Finally some concluding remarks are made in Sec. VII.

II. PRELIMINARIES

A. Completely positive maps

1. Definitions

Let $\mathcal{A}$ and $\mathcal{B}$ be C*-algebras; denote by $\mathcal{A}^+$ the cone of positive elements of $\mathcal{A}$. A linear map $T:\mathcal{A}\to\mathcal{B}$ is called *positive* if $T(\mathcal{A}^+)\subseteq\mathcal{B}^+$. Given some $n\in\mathbb{N}$, let $\mathcal{M}_n$ be the algebra of $n\times n$ complex matrices. The map T is called *n-positive* if the induced map $T\otimes\mathrm{id}_n:\mathcal{A}\otimes\mathcal{M}_n\to\mathcal{B}\otimes\mathcal{M}_n$ is positive, and *completely positive* if it is n-positive for all $n\in\mathbb{N}$.

One typically considers maps $T:\mathcal{A}\to\mathcal{B}(\mathcal{H})$, where $\mathcal{A}$ is a C*-algebra with identity, and $\mathcal{B}(\mathcal{H})$ is the algebra of bounded operators on a complex separable Hilbert space $\mathcal{H}$. Then it can be shown[4] that T is CP if and only if, for each $n\in\mathbb{N}$,

$$\sum_{i,j=1}^{n}\langle\eta_i|T(A_i^*A_j)\eta_j\rangle\geqslant 0\quad\forall\,\eta_i\in\mathcal{H},\quad A_i\in\mathcal{A};\quad i=1,\ldots,n. \tag{1}$$

2. Theorems of Stinespring and Kraus

A fundamental theorem of Stinespring[4] states that, for any normal (i.e., ultraweakly continuous) CP map $T:\mathcal{A}\to\mathcal{B}(\mathcal{H})$, there exist a Hilbert space $\mathcal{K}$, a $*$-homomorphism $\pi:\mathcal{A}\to\mathcal{B}(\mathcal{K})$, and a bounded operator $V:\mathcal{H}\to\mathcal{K}$, such that

$$T(A)=V^*\pi(A)V\quad\forall A\in\mathcal{A}. \tag{2}$$

We will refer to any such triple $(\mathcal{K},V,\pi)$ [or, through a slight abuse of language, to the form (2) of T] as a *Stinespring dilation* of T. Given T, one can construct its Stinespring dilation in such a way that $\mathcal{K}=\pi(\mathcal{A})V\mathcal{H}$, i.e., the set $\{\pi(A)V\psi|A\in\mathcal{A},\psi\in\mathcal{H}\}$ is total in $\mathcal{K}$. With this additional property, the Stinespring dilation is unique up to unitary equivalence,[11] and is called the *minimal Stinespring dilation*.

For the special case of a CP map $T:\mathcal{B}(\mathcal{H}_1)\to\mathcal{B}(\mathcal{H}_2)$, we can always find a Hilbert space $\mathcal{E}$ and a bounded operator $V:\mathcal{H}_2\to\mathcal{H}_1\otimes\mathcal{E}$, such that

$$T(A)=V^*(A\otimes\mathbb{1}_{\mathcal{E}})V\quad\forall A\in\mathcal{A}. \tag{3}$$

This follows from the fact that any normal $*$-representation of the C*-algebra $\mathcal{B}(\mathcal{H})$ is unitarily equivalent to the *amplification map* $A\mapsto A\otimes\mathbb{1}_{\mathcal{E}}$ for some Hilbert space $\mathcal{E}$ (Ref. 12, Sec. 2.7). Any minimal Stinespring dilation of T that has the form (3) will be referred to as its *canonical Stinespring dilation*. The canonical Stinespring dilation is likewise unique up to unitary equivalence.

Another important structure theorem for CP maps is due to Kraus.[3] It says that for any CP map $T:\mathcal{A}\to\mathcal{B}(\mathcal{H})$, with $\mathcal{A}$ being a W*-algebra of operators on some Hilbert space $\mathcal{H}'$, there exists a collection of bounded operators $V_x:\mathcal{H}\to\mathcal{H}'$, such that

$$T(A)=\sum_x V_x^*AV_x, \tag{4}$$

where the series converges in the strong operator topology. If $\dim \mathcal{H}=\infty$, the set $\{V_x\}$ can be chosen in such a way that its cardinality equals the Hilbertian dimension (i.e., the cardinality of any complete orthonormal basis) of $\mathcal{H}$.[11]

The Stinespring dilation (3) and the Kraus form (4) of a CP map $T:\mathcal{B}(\mathcal{H}_1)\to\mathcal{B}(\mathcal{H}_2)$ are related to one another via the correspondence

$$V\psi=\sum_x V_x\psi\otimes e_x \quad \forall\,\psi\in\mathcal{H}_2, \tag{5}$$

where $\{e_x\}$ is an orthonormal system in $\mathcal{E}$. Note that the Kraus operators $\{V_x\}$ depend on the choice of $\{e_x\}$. The adjoint operator $V^*:\mathcal{H}_1\otimes\mathcal{E}\to\mathcal{H}_2$ acts on the elementary tensors $\psi\otimes\chi\in\mathcal{H}_1\otimes\mathcal{E}$ as

$$V^*(\psi\otimes\chi)=\sum_x \langle e_x|\chi\rangle V_x^*\psi.$$

It is not hard to see that when $\mathcal{H}_1$ and $\mathcal{H}_2$ are both finite-dimensional, any canonical Stinespring dilation of T will give rise to at most $\dim\mathcal{H}_1\cdot\dim\mathcal{H}_2$ Kraus operators. This is so because these Kraus operators must be linearly independent elements of the vector space $\mathcal{L}(\mathcal{H}_2,\mathcal{H}_1)$ of all linear operators from $\mathcal{H}_2$ into $\mathcal{H}_1$. Furthermore, the number of terms in such a Kraus decomposition is uniquely determined by T.[13]

3. Partial order of CP maps

The cone $\mathrm{CP}(\mathcal{A};\mathcal{H})$ of all normal CP maps of $\mathcal{A}$ into $\mathcal{B}(\mathcal{H})$ can be partially ordered in the following natural fashion. Given $S,\ T\in\mathrm{CP}(\mathcal{A};\mathcal{H})$, we will write $S\leqslant T$ if $T-S\in\mathrm{CP}(\mathcal{A};\mathcal{H})$. Following Belavkin and Staszewski,[7] we will say that S is *completely dominated by* T. Given a nonnegative real constant c, we will say that S is *completely c-dominated by* T if $S\leqslant cT$. Using the condition (1), we see that $S\leqslant T$ if and only if

$$\sum_{i,j=1}^{n}\langle\eta_i|S(A_i^*A_j)\,\eta_j\rangle\leqslant\sum_{i,j=1}^{n}\langle\eta_i|T(A_i^*A_j)\,\eta_j\rangle \quad \forall\,\eta_i\in\mathcal{H},\ A_i\in\mathcal{A};\ i=1,\ldots,n$$

for each $n\in\mathbb{N}$. We will use the notation $\mathrm{CP}(\mathcal{H}_1,\mathcal{H}_2)$ (note the comma) for the set of all CP maps of $\mathcal{B}(\mathcal{H}_1)$ into $\mathcal{B}(\mathcal{H}_2)$.

B. Quantum operations

Reversible dynamics of a closed quantum-mechanical system with the Hilbert space $\mathcal{H}$ is given, in the Schrödinger picture, by the mapping $\rho\mapsto U\rho U^*$, where ρ is a density operator on $\mathcal{H}$ (i.e., $\mathrm{Tr}\,\rho=1$ and $\rho\geqslant 0$), and $U:\mathcal{H}\to\mathcal{H}$ is a unitary transformation. In the dual Heisenberg picture same dynamics is described by the mapping $A\mapsto U^*AU$ for all $A\in\mathcal{B}(\mathcal{H})$. The two descriptions are equivalent as they yield the same observed statistics, $\mathrm{Tr}(U\rho U^*A)=\mathrm{Tr}(\rho U^*AU)$.

On the other hand, when the system is open because it is either coupled to an environment or is being subjected to a measurement, its most general time evolution is irreversible. This is captured mathematically by means of a *quantum operation*,[3] i.e., a completely positive normal linear map $T:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ with the additional constraint $T(\mathbb{1})\leqslant\mathbb{1}$. In terms of the Kraus form, $T(A)=\Sigma_x V_x^*AV_x$, we have the bound $\Sigma_x V_x^*V_x\leqslant\mathbb{1}$. The corresponding Schrödinger-picture map on density operators, $\rho\mapsto T_*(\rho)$, is defined[14] by

$$\mathrm{Tr}[T_*(\rho)A]=\mathrm{Tr}[\rho T(A)] \quad \forall A\in\mathcal{B}(\mathcal{H}),$$

and can then be extended to the linear span of the density operators, the trace class $\mathcal{T}(\mathcal{H})$. It follows at once that the map T_* is completely positive and trace decreasing in the sense that $\mathrm{Tr}\,T_*(X)\leqslant\mathrm{Tr}\,X$ for any $X\in\mathcal{T}(\mathcal{H})$. In order to retain proper normalization for density operators,

one usually writes the Schrödinger-picture evolution dual to T as $\rho \mapsto T_*(\rho)/\mathrm{Tr}\, T_*(\rho)$. Alternatively, one says that the transformation $\rho \mapsto T_*(\rho)$ *succeeds with probability* $\mathrm{Tr}\, T_*(\rho)$; this probability is equal to unity for all density operators ρ if and only if T is unital, i.e., $T(\mathbb{1})=\mathbb{1}$, so that T_* is trace-preserving. Unital quantum operations are also referred to as *quantum channels*.[1]

The Kraus theorem implies that we can write any quantum operation T as a sum of *pure operations* (Ref. 2, Sec. 2.3), i.e., maps of the form $A \mapsto X^*AX$ with $X^*X \leqslant \mathbb{1}$ (this is equivalent to X being a contraction, $\|X\| \leqslant 1$ where $\|\cdot\|$ is the usual operator norm, $\|X\| = \sup_{\psi \in \mathcal{H}} \|X\psi\|/\|\psi\|$). The qualification ''pure'' is usually interpreted as referring to the fact that, for any pure state $|\psi\rangle\langle\psi|$, the (un-normalized) state $X|\psi\rangle\langle\psi|X^*$ is pure as well.[5] However, as we shall see later, it is a direct consequence of the Radon–Nikodym theorem for CP maps that T is a pure operation if and only if all operations completely dominated by it are its nonnegative multiples. This is analogous to the case of pure states on a C*-algebra $\mathcal{A}$: a state ω on $\mathcal{A}$ is pure if and only if all positive linear functionals φ on $\mathcal{A}$, such that $\omega - \varphi$ is positive are nonnegative multiples of ω (Ref. 15, Sec. 2.3.2).

Given the canonical Stinespring dilation (3) of a quantum channel T (in which case V is an isometry), the Schrödinger-picture operation T_* can be cast in the so-called *ancilla form*

$$T_*(\rho) = \mathrm{Tr}_{\mathcal{E}}\, U(\rho \otimes |\xi\rangle\langle\xi|)U^*, \tag{6}$$

where $\mathrm{Tr}_{\mathcal{E}}(\cdot)$ denotes the partial trace over $\mathcal{E}$, $\xi \in \mathcal{E}$ is a fixed unit vector, and U is the unitary extension of the partial isometry $\hat{U}$ from $\mathcal{H}_2 \otimes [|\xi\rangle\langle\xi|]$ to $\mathcal{H}_1 \otimes \mathcal{E}$ defined by $\hat{U}(\psi \otimes \xi) = V\psi$.[3,16] (We use $[P]$ to denote the closed subspace corresponding to the orthogonal projection P.)

Finally, note that the input and output Hilbert spaces do not have to be the same; in general, quantum operations are completely positive normal linear maps $T: \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$ with $T(\mathbb{1}_{\mathcal{H}_1}) \leqslant \mathbb{1}_{\mathcal{H}_2}$. The corresponding Schrödinger-picture operations are completely positive trace-decreasing maps $T_*: \mathcal{T}(\mathcal{H}_2) \to \mathcal{T}(\mathcal{H}_1)$. Most of the discussion in this section carries over to this case, modulo straightforward modifications; however, one must be careful with the ancilla representation of a general Schrödinger-picture channel T_*. The key caveat here is that the initial ancillary space and the final ''traced-out'' space need not be isomorphic. This yet again underscores the advantages of working in the Heisenberg picture.

C. The norm of complete boundedness

In many information-theoretic studies of noisy quantum channels one needs a quantitative measure of the ''noisiness'' of a channel; this is, in fact, a natural departure point for various definitions of information-carrying capacities of quantum channels.[1,17,18] A good candidate for such a measure is the norm $\|T - \mathrm{id}\|_?$, where the question mark refers to the fact that we have not yet specified a suitable norm.

The choice of the proper norm turns out to be a tricky matter.[1] Let $\mathcal{A}$ and $\mathcal{B}$ be C*-algebras, and consider a linear map Λ: $\mathcal{A} \to \mathcal{B}$. We cannot adopt the operator norm, defined by

$$\|\Lambda\| = \sup\{\|\Lambda(A)\| \,|\, A \in \mathcal{A}, \|A\| \leqslant 1\}, \tag{7}$$

where $\|A\|$ is the (unique) C*-norm on $\mathcal{A}$, because the norm $\|\Lambda \otimes \mathrm{id}_n\|$ of the map $\Lambda \otimes \mathrm{id}_n : \mathcal{A} \otimes \mathcal{M}_n \to \mathcal{B} \otimes \mathcal{M}_n$ can increase with n even if Λ itself is bounded (see Chap. 3 of Ref. 19). What we need is a ''stabilized'' version of (7). A map $\Lambda: \mathcal{A} \to \mathcal{B}$ is called *completely bounded* (CB for short) if there exists some constant $C \geqslant 0$ such that all the maps $\Lambda \otimes \mathrm{id}_n : \mathcal{A} \otimes \mathcal{M}_n \to \mathcal{B} \otimes \mathcal{M}_n$ are uniformly bounded by C, i.e., $\|\Lambda \otimes \mathrm{id}_n\| \leqslant C$. The CB norm $\|\Lambda\|_{\mathrm{cb}}$ is defined to be the smallest constant C for which this holds, i.e.,

$$\|\Lambda\|_{\mathrm{cb}} = \sup_{n \in \mathbb{N}} \|\Lambda \otimes \mathrm{id}_n\|.$$

All CB maps have the property of ''factoring through a Hilbert space,'' as shown in the following key structure theorem (Theorem 3.6 in Ref. 19), given here in a slightly simplified form suitable for our needs.

Theorem II.1: *(Haagerup–Paulsen–Wittstock) Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces, and let $\Lambda:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ be a CB map. Then there exist a Hilbert space $\mathcal{E}$ and operators $V_1,V_2:\mathcal{K}\to\mathcal{H}\otimes\mathcal{E}$ with $\|V_1\|\|V_2\|\leqslant\|\Lambda\|_{\rm cb}$ ($\|\cdot\|$ stands for the operator norm), such that*

$$\Lambda(A)=V_1^*(A\otimes\mathbb{1}_{\mathcal{E}})V_2\,. \tag{8}$$

Conversely, any map Λ of the form (8) satisfies $\|\Lambda\|_{\rm cb}\leqslant\|V_1\|\|V_2\|$.

Note that the Stinespring and the Haagerup–Paulsen–Wittstock theorems together imply that any CP map is automatically CB. In fact, for a CP map T, we have $\|T\|_{\rm cb}=\|T(\mathbb{1})\|$.[20] Also, the difference of two CP maps is always CB.

Theorem II.1 suggests an alternative way to define the CB norm of a map Λ, namely, as

$$\|\Lambda\|_{\rm cb}=\inf\{\|V_1\|\|V_2\|\}, \tag{9}$$

where the infimum is taken over all possible decompositions of Λ in the form (8). Moreover, the theorem guarantees that the infimum in (9) is attained.

In quantum information theory one frequently deals with both the operation $T:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ and its (pre)dual, $T_*:\mathcal{T}(\mathcal{K})\to\mathcal{T}(\mathcal{H})$. As we mentioned in Sec. II B, T and T_* are connected by the relation $\mathrm{Tr}[T(A)B]=\mathrm{Tr}[AT_*(B)]$, $A\in\mathcal{B}(\mathcal{H})$, $B\in\mathcal{T}(\mathcal{K})$. This duality holds also for any normal CB map $\Lambda:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$, so that when Λ is written in the form (8), we have

$$\Lambda_*(A)=\mathrm{Tr}_{\mathcal{E}}V_2AV_1^*\quad\forall A\in\mathcal{T}(\mathcal{K}). \tag{10}$$

This motivates the definition of the dual CB norm,

$$\|\Lambda_*\|_{\rm cb}^*=\inf\{\|V_1\|\|V_2\|\}, \tag{11}$$

where the infimum is taken over all possible decompositions of Λ_* in the form (10). It is now clear that $\|\Lambda\|_{\rm cb}=\|\Lambda_*\|_{\rm cb}^*$ for any normal CB map Λ, so in the future we will always write $\|\Lambda\|_{\rm cb}$, even when working with Λ_*. In fact, the norm (11) was introduced by Kitaev[21] under the name ''diamond norm'' (Kitaev used the notation $\|\Lambda\|_\diamond$). The equivalence of the diamond norm and the CB norm has been alluded to in the literature on quantum information theory[17] but, to the best of our knowledge, no proof of the equivalence was ever presented.

The duality relation between $\Lambda:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ and $\Lambda_*:\mathcal{T}(\mathcal{K})\to\mathcal{T}(\mathcal{H})$ implies that we can also write

$$\|\Lambda\|_{\rm cb}=\sup_{n\in\mathbb{N}}\|\Lambda_*\otimes\mathrm{id}_n\|_1\,,$$

where $\|\Lambda_*\|_1=\sup\{\|\Lambda_*(A)\|_1|A\in\mathcal{T}(\mathcal{K}),\|A\|_1\leqslant1\}$ and $\|A\|_1=\mathrm{Tr}|A|\equiv\mathrm{Tr}\sqrt{A^*A}$ is the trace norm (Sec. VI.6, Ref. 22). For this purpose we can use the well-known variational characterization of the operator norm (Theorem 3.2 in Ref. 23), namely,

$$\|A\|=\sup_{\substack{B\in\mathcal{T}(\mathcal{H})\\ \|B\|_1\leqslant1}}|\mathrm{Tr}(AB)|\quad\forall A\in\mathcal{B}(\mathcal{H}).$$

Then for any normal CB map $\Lambda:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ we have

$$\|\Lambda\| = \sup_{\substack{A\in\mathcal{B}(\mathcal{H})\\ \|A\|\leq 1}} \|\Lambda(A)\| = \sup_{\substack{B\in\mathcal{T}(\mathcal{K})\\ \|B\|_1\leq 1}} \sup_{\substack{A\in\mathcal{B}(\mathcal{H})\\ \|A\|\leq 1}} |\mathrm{Tr}[\Lambda(A)B]| = \sup_{\substack{B\in\mathcal{T}(\mathcal{K})\\ \|B\|_1\leq 1}} \sup_{\substack{A\in\mathcal{B}(\mathcal{H})\\ \|A\|\leq 1}} |\mathrm{Tr}[A\Lambda_*(B)]|$$

$$= \sup_{\substack{B\in\mathcal{T}(\mathcal{K})\\ \|B\|_1\leq 1}} \|\Lambda_*(B)\|_1 = \|\Lambda_*\|_1,$$

which also implies that $\|\Lambda\otimes \mathrm{id}_n\| = \|\Lambda_*\otimes \mathrm{id}_n\|_1$ for all $n\in\mathbb{N}$. Taking the supremum of both sides with respect to n does the job. In a nutshell, the CB norm of a map between algebras of bounded operators on Hilbert spaces can be defined through a variational expression involving the operator norm, whereas the CB norm of the corresponding dual map between the trace classes is determined by a variational expression in the trace norm.

We now summarize the key properties of the CB norm. For any two CB maps $\Lambda:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H}')$ and $\Lambda:\mathcal{B}(\mathcal{H}')\to\mathcal{B}(\mathcal{K}')$, any $A\in\mathcal{B}(\mathcal{H})$, and any $B\in\mathcal{T}(\mathcal{H}')$, we have the following:

(1) $\|\Lambda'\circ\Lambda\|_{\mathrm{cb}}\leq\|\Lambda'\|_{\mathrm{cb}}\|\Lambda\|_{\mathrm{cb}}$,
(2) $\|\Lambda\otimes\Lambda'\|_{\mathrm{cb}} = \|\Lambda\|_{\mathrm{cb}}\|\Lambda'\|_{\mathrm{cb}}$,
(3) $\|\Lambda(A)\|\leq\|\Lambda\|_{\mathrm{cb}}\|A\|$,
(4) $\|\Lambda_*(B)\|_1\leq\|\Lambda\|_{\mathrm{cb}}\|B\|_1$.

For proofs see, e.g., the article of Kitaev[21] or the monographs of Pisier[19] and Paulsen.[20]

III. THE RADON–NIKODYM THEOREM FOR COMPLETELY POSITIVE MAPS

In this section we review a theorem of the Radon–Nikodym type that allows for a complete classification of all CP maps S that are completely dominated by a given CP map T. As we have already mentioned, this theorem can be distilled from the more general results of Arveson[6] and Belavkin and Staszewski.[7] The work of Parthasarathy[10] contains further developments, in particular an analogue of the Lebesgue decomposition for CP maps. The idea is to express all maps S that satisfy $S\leq T$ in the form related to the (minimal) Stinespring dilation of T; this ''Stinespring form'' of the theorem[6,7] is stated in Sec. III A, with the proof included in order to keep the paper self-contained. Then, in Sec. III B, we state and prove two ''Kraus forms'' of the Radon–Nikodym theorem. Finally, some general remarks are given in Sec. III C.

A. The Stinespring form

Before we state and prove the Radon–Nikodym theorem, let us recall a standard piece of notation. Given a C*-algebra $\mathcal{A}$ and a $*$-homomorphism $\pi:\mathcal{A}\to\mathcal{B}(\mathcal{H})$, the set $\{B\in\mathcal{B}(\mathcal{H})\,|\,[A,B]\equiv AB-BA=0, \forall A\in\pi(\mathcal{A})\}$ is called the *commutant* of π and is denoted by $\pi(\mathcal{A})'$.

Theorem III.1: *Consider $S,T\in\mathrm{CP}(\mathcal{A};\mathcal{H})$, and let $(\mathcal{K},V,\pi)$ be the minimal Stinespring dilation of T. Then $S\leq T$ if and only if there exists an operator $\hat{F}\in\pi(\mathcal{A})'$, such that $0\leq\hat{F}\leq\mathbb{1}$ and*

$$S(A) = V^*\pi(A)\hat{F}V = V^*\hat{F}^{1/2}\pi(A)\hat{F}^{1/2}V$$

for all $A\in\mathcal{A}$. The operator $\hat{F}$ is unique in the sense that if $S(A)=V^*\pi(A)YV$ for some $Y\in\pi(\mathcal{A})'$, then $Y=\hat{F}$. We will refer to this operator $\hat{F}$ as the Radon–Nikodym derivative of S with respect to T and denote it by $\mathsf{D}_T S$.

Proof: Suppose $S\leq T$, and let $(\mathcal{K}',V',\pi')$ be the minimal Stinespring dilation of S. Define an operator $\hat{G}:\mathcal{K}\to\mathcal{K}'$ by

$$\hat{G}:\pi(A)V\eta\mapsto\pi'(A)V'\eta \quad \forall A\in\mathcal{A},\eta\in\mathcal{H},$$

and extend it to the linear span of $\pi(\mathcal{A})V\mathcal{H}$. For any finite linear combination $\Psi=\sum_{i=1}^n\pi(A_i)V\eta_i$ we have

$$\begin{aligned}\|\hat{G}\Psi\|^2 &= \sum_{i,j=1}^{n} \langle \eta_i | V'^* \pi'(A_i^* A_j) V' \eta_j \rangle \\ &= \sum_{i,j=1}^{n} \langle \eta_i | S(A_i^* A_j)\, \eta_j \rangle \\ &\leqslant \sum_{i,j=1}^{n} \langle \eta_i | T(A_i^* A_j)\, \eta_j \rangle \\ &= \sum_{i,j=1}^{n} \langle \eta_i | V^* \pi(A_i^* A_j) V \eta_j \rangle = \|\Psi\|^2.\end{aligned}$$

Thus $\hat{G}$ is a densely defined contraction, and therefore extends to a contraction from $\mathcal{K}$ into $\mathcal{K}'$. We will denote this extension also by $\hat{G}$. For the adjoint map $\hat{G}^*$, we have

$$\langle \eta | V^* \hat{G}^* \pi'(A) V' \xi \rangle = \langle \hat{G} V \eta | \pi'(A) V' \xi \rangle = \langle V' \eta | \pi'(A) V' \xi \rangle = \langle \eta | V'^* \pi'(A) V' \xi \rangle \equiv \langle \eta | S(A) \xi \rangle$$

for all $\eta, \xi \in \mathcal{H}$ and $A \in \mathcal{A}$, which implies that $V^* \hat{G}^* \pi'(A) V' \eta = S(A)\, \eta$.

The map $\hat{G}$ intertwines the representations π and π', i.e., $\hat{G}\pi(A) = \pi'(A)\hat{G}$ for any $A \in \mathcal{A}$. Indeed, for all $A, B \in \mathcal{A}$ and $\eta \in \mathcal{H}$ we have

$$\hat{G}\pi(A)\pi(B) V \eta = \hat{G}\pi(AB) V \eta = \pi'(AB) V' \eta = \pi'(A)\pi'(B) V' \eta = \pi'(A)\hat{G}\pi(B) V \eta,$$

and the desired statement follows because of the minimality of the Stinespring dilation $(\mathcal{K}, V, \pi)$. Taking adjoints, we also obtain $\pi(A)\hat{G}^* = \hat{G}^* \pi'(A)$. Letting $\hat{F} = \hat{G}^* \hat{G}$, we see that

$$\hat{F}\pi(A) = \hat{G}^* \hat{G} \pi(A) = \hat{G}^* \pi'(A) \hat{G} = \pi(A) \hat{G}^* \hat{G} = \pi(A) \hat{F},$$

which shows that $\hat{F} \in \pi(\mathcal{A})'$. Finally, for all $A \in \mathcal{A}$ and $\eta \in \mathcal{H}$ we have

$$V^* \hat{F} \pi(A) V \eta = V^* \hat{G}^* \hat{G} \pi(A) V \eta = V^* \hat{G}^* \pi'(A) V' \eta = S(A)\, \eta,$$

thus $S(A) = V^* \hat{F} \pi(A) V = V^* \pi(A) \hat{F} V = V^* \hat{F}^{1/2} \pi(A) \hat{F}^{1/2} V$. The uniqueness of $\hat{F}$ follows from the minimality of $(\mathcal{K}', V', \pi')$.

The converse is clear. ■

For the special case $S, T \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$ we can use the canonical Stinespring dilation (3) and the fact that the commutant of the algebra $\mathcal{B}(\mathcal{H}_1) \otimes \mathbb{C}\mathrm{l}_{\mathcal{E}}$ is isomorphic to $\mathbb{C}\mathrm{l}_{\mathcal{H}_1} \otimes \mathcal{B}(\mathcal{E})$ (Theorem IV.5.9 in Ref. 24), to deduce the following.

Corollary III.2: Let $S, T \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$, and let $T(A) = V^*(A \otimes \mathbb{1}_{\mathcal{E}})V$ be the canonical Stinespring dilation of T. Then $S \leqslant T$ if and only if there exists a positive contraction $F \in \mathcal{B}(\mathcal{E})$, such that $S(A) = V^*(A \otimes F)V$ for all $A \in \mathcal{B}(\mathcal{H}_1)$.

As we already mentioned, the Radon–Nikodym theorem allows one to fully appreciate the term "pure operation." Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces, and consider the map $T(A) = X^* A X$, where $X: \mathcal{H}_2 \to \mathcal{H}_1$ is a contraction. Clearly, $X^* A X$ is the canonical Stinespring dilation of T so, by Theorem III.1, any $S \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$ that satisfies $S \leqslant T$ must be of the form $\lambda X^* A X$ for some $\lambda \in [0,1]$.

Theorem III.1 can also be used to characterize completely all ways to write a given $T \in \mathrm{CP}(\mathcal{A}; \mathcal{H})$ as a finite sum $\Sigma_i T_i$, with $T_i \in \mathrm{CP}(\mathcal{A}; \mathcal{H})$ for all i. It is actually the resulting theorem, stated below, that is referred to as the "Radon–Nikodym theorem for CP maps" in the quantum information literature.[18]

Theorem III.3: *Consider a map $T \in \mathrm{CP}(\mathcal{A}; \mathcal{H})$ with the canonical Stinespring dilation $(\mathcal{K}, V, \pi)$. For any finite decomposition $T = \Sigma_i T_i$ with $T_i \in \mathrm{CP}(\mathcal{A}; \mathcal{H})$ there exist unique positive operators $\hat{F}_i \in \pi(\mathcal{A})'$ that satisfy $\Sigma_i \hat{F}_i = \mathbb{1}_{\mathcal{K}}$, such that $T_i(A) = V^* \pi(A) \hat{F}_i V$.*

Proof: Apply Theorem III.1 separately to each pair (T_i, T), and let $\hat{F}_i = \mathrm{D}_T T_i$. Then $T(A) = \Sigma_i V^* \pi(A) \hat{F}_i V = V^* \pi(A) V$, and $\Sigma_i \hat{F}_i = \mathbb{1}_{\mathcal{K}}$ by the uniqueness part of Theorem III.1. ■

Remark: The decomposition $T = \Sigma_i T_i$ is a particularly simple instance of a CP instrument.[2] As such, it is not difficult to extract Theorem III.3 from more general results of Ozawa.[9] □

B. The Kraus form

Theorem III.1 can be restated in a simple way in terms of the Kraus form of a CP map. In order to do this, we need some additional machinery (Sec. II.15 in Ref. 25).

Let X be a set. Any function $K: X \times X \to \mathbb{C}$ is called a *kernel on X*. The set $\mathcal{K}(X)$ of all kernels on X is a vector space, with the corresponding algebraic operations defined pointwise on $X \times X$. We say that a kernel $K \in \mathcal{K}(X)$ is *positive-definite*, and write $K \geqslant 0$, if for each $n \in \mathbb{N}$ we have

$$\sum_{i,j=1}^{n} \overline{c}_i c_j K(x_i, x_j) \geqslant 0 \quad \forall x_i \in X, c_i \in \mathbb{C}; \;\; i = 1, \ldots, n.$$

Given a pair of kernels $K, K' \in \mathcal{K}(X)$, we will write $K \leqslant K'$ if $K' - K$ is positive-definite. Note that a positive-definite kernel is automatically Hermitian, i.e., $K(x,y) = \overline{K(y,x)}$.

According to the fundamental theorem of Kolmogorov, for any positive-definite kernel $K \in \mathcal{K}(X)$ there exist a Hilbert space $\mathcal{H}_K$ and a map $v_K: X \to \mathcal{H}_K$ such that $\langle v_K(x) | v_K(y) \rangle = K(x,y)$ for all $x, y \in X$, and the set $\{v_K(x) | x \in X\}$ is total in $\mathcal{H}_K$. The pair $(\mathcal{H}_K, v_K)$ is referred to as the *Kolmogorov decomposition* of $\mathcal{K}$ and is unique up to unitary equivalence.

After these preparations, we may state our first result.

Theorem III.4: *Consider two maps $S, T \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$. Let $\{V_x\}_{x \in X}$ be a Kraus decomposition of T induced by the canonical Stinespring dilation $T(A) = V^*(A \otimes \mathbb{1}_{\mathcal{E}})V$, as prescribed in (5). Then $S \leqslant T$ if and only if*

$$S(A) = \sum_{x,y \in X} K(x,y) V_x^* A V_y$$

for some positive-definite kernel $K \in \mathcal{K}(X)$ with $K \leqslant I$, where I is the Kronecker kernel $I(x,y) \equiv \delta_{xy}$.

Proof: Suppose $S \leqslant T$. By Corollary III.2, $S(A) = V^*(A \otimes F)V$ for some positive contraction $F \in \mathcal{B}(\mathcal{E})$. Let $\{e_x\}_{x \in X}$ be the orthonormal system in $\mathcal{E}$, determined by V and $\{V_x\}$ from (5). Then for any $\eta \in \mathcal{H}_2$ we have

$$S(A)\eta = V^*(A \otimes F)V\eta = V^*\left(\sum_{y \in X} AV_y \eta \otimes Fe_y \right) = \sum_{x,y \in X} \langle e_x | Fe_y \rangle V_x^* A V_y \eta.$$

Define the kernel $K \in \mathcal{K}(X)$ by setting $K(x,y) := \langle e_x | Fe_y \rangle$. Then $0 \leqslant F \leqslant \mathbb{1}$ implies that $0 \leqslant K \leqslant I$.

Conversely, suppose we are given

$$T(A) = \sum_{x \in X} V_x^* A V_x$$

and

$$S(A) = \sum_{x,y \in X} K(x,y) V_x^* A V_y$$

for some $K \in \mathcal{K}(X)$ such that $0 \leqslant K \leqslant I$. Let $(\mathcal{H}_K, v_K)$ be the Kolmogorov decomposition of K, and let $\mathrm{fin}(X)$ be the set of all finite subsets of X. Define an operator $G: \mathcal{E} \to \mathcal{H}_K$ by

$$G: \sum_{x \in X_0} c_x e_x \mapsto \sum_{x \in X_0} c_x v_K(x) \quad \forall c_x \in \mathbb{C},\ X_0 \in \mathrm{fin}(X).$$

It is easy to see that, for any $X_0 \in \mathrm{fin}(X)$,

$$\left\| \sum_{x \in X_0} c_x e_x \right\|^2 = \sum_{x \in X_0} |c_x|^2 = 0$$

implies $c_x = 0$ for all $x \in X_0$, and consequently

$$\left\| G\left(\sum_{x \in X_0} c_x e_x \right) \right\|^2 = \sum_{x,y \in X_0} \overline{c_x} c_y K(x,y) \leqslant \sum_{x \in X_0} |c_x|^2 = 0,$$

where the last equality above follows because $K \leqslant I$. Thus G extends to a well-defined linear operator on $\mathcal{E}$, which we will also denote by G. Let $F = G^* G$. Then $\langle e_x | F e_y \rangle = \langle v_K(x) | v_K(y) \rangle = K(x,y)$, and $0 \leqslant K \leqslant I$ implies that $0 \leqslant F \leqslant \mathbb{1}_{\mathcal{E}}$. Thus, for all $A \in \mathcal{B}(\mathcal{H}_1)$ and $\eta \in \mathcal{H}_2$ we have

$$S(A)\eta = \sum_{x,y} K(x,y) V_x^* A V_y = \sum_{x,y \in X} \langle e_x | F e_y \rangle V_x^* A V_y = V^*(A \otimes F) V,$$

so that $S \leqslant T$ by Corollary III.2. ■

Remarks: (1) When the set $\{V_x\}$ is finite, Theorem III.4 says that $S \leqslant T$ for $T(A) = \Sigma_x V_x^* A V_x$ if and only if $S(A) = \Sigma_{x,y} M_{xy} V_x^* A V_y$ for some matrix $M = [M_{xy}]$ with $0 \leqslant M \leqslant \mathbb{1}$.

(2) Since we deal only with separable Hilbert spaces, the index set X is at most countably infinite. □

Another Kraus form of the Radon–Nikodym theorem can be proved directly, without recourse to the theory of positive-definite kernels.

Theorem III.5: *Consider two maps $S,T \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$. Then $S \leqslant T$ if and only if there exist a Kraus decomposition $T(A) = \Sigma_x W_x^* A W_x$, induced by the canonical Stinespring dilation of T, and a set $\{\lambda_x | \lambda_x \in [0,1]\}$, such that $S(A) = \Sigma_x \lambda_x W_x^* A W_x$.*

Proof: Suppose $S \leqslant T$. Let $T(A) = V^*(A \otimes \mathbb{1}_{\mathcal{E}})V$ be the canonical Stinespring dilation of T. Then Corollary III.2 says that $S(A) = V^*(A \otimes F)V$ for some positive contraction $F \in \mathcal{B}(\mathcal{E})$. Write down the spectral decomposition $F = \Sigma_x \lambda_x |\phi_x\rangle\langle\phi_x|$, so that $\lambda_x \in [0,1]$ and $\langle \phi_x | \phi_y \rangle = \delta_{xy}$. Let $\{W_x\}$ be the Kraus decomposition of T determined from (5) by V and $\{\phi_x\}$. Then for any $\eta \in \mathcal{H}_2$ we have

$$S(A)\eta = V^*(A \otimes F)V\eta = V^*\left(\sum_y \lambda_y A W_y \eta \otimes \phi_y \right) = \sum_{x,y} \lambda_y \langle \phi_x | \phi_y \rangle W_x^* A W_y \eta = \sum_x \lambda_x W_x^* A W_x .$$

The converse follows readily from the fact that the map $A \mapsto \Sigma_x (1 - \lambda_x) W_x^* A W_x$ is CP for any choice of $\{W_x\}$ and $\{\lambda_x\}$ with $\lambda_x \in [0,1]$. ■

C. General remarks

Before we go on, we would like to pause and make some general comments about the significance of the Radon–Nikodym theorem for CP maps at large.

The real power of this theorem lies in the fact that it contains the ''traditional'' forms of the Radon–Nikodym theorem as special cases. In order to see this, we will need the following result (see Corollary IV.3.5 and Proposition IV.3.9 in Ref. 24): a positive map T from a C*-algebra $\mathcal{A}$ to another C*-algebra $\mathcal{B}$ is automatically completely positive whenever at least one of $\mathcal{A}$ and $\mathcal{B}$ is Abelian.

With this in mind, let us observe that any positive linear functional φ on a C*-algebra $\mathcal{A}$ is a positive map from $\mathcal{A}$ to $\mathbb{C}$, and therefore is CP. When we apply the Stinespring theorem to φ, we simply recover the GNS representations $(\mathcal{H}, \pi, \Omega)$ of $\mathcal{A}$ induced by φ, where $\mathcal{H}$ is the Hilbert space

of the representation, π is a $*$-isomorphism between $\mathcal{A}$ and a suitable C*-subalgebra of $\mathcal{B}(\mathcal{H})$, and $\Omega \in \mathcal{H}$ is cyclic for π, i.e., $\mathcal{H} = \overline{\pi(\mathcal{A})\Omega}$. Of course, we have then $\varphi(A) = \langle \Omega | \pi(A)\Omega \rangle$ for all $A \in \mathcal{A}$.

Consider first the Abelian case. Let X be a compact Hausdorff space, and let $\mathcal{A}$ be the commutative C*-algebra $\mathcal{C}(X)$ of all complex-valued continuous functions on X. Let φ be a positive linear functional on $\mathcal{C}(X)$. By the Riesz–Markov theorem [see Theorem IV.14 (Ref. 22)], there exists a unique Baire measure μ on X such that $\varphi(f) = \int_X f(x)\mathrm{d}\mu(x)$, $\forall f \in \mathcal{C}(X)$. If φ is a state [i.e., $\varphi(\mathbb{1}_X) = 1$ where $\mathbb{1}_X$ is, of course, the function on X that is identically equal to 1], then μ is a probability measure. The GNS construction yields the cyclic representation $(\mathcal{H}, \pi, \Omega)$, where $\mathcal{H} = \mathcal{L}^2(X, \mathrm{d}\mu)$, $[\pi(f)g](x) = f(x)g(x)$, and $\Omega = \mathbb{1}_X$, such that

$$\varphi(f) = \langle \Omega | \pi(f)\Omega \rangle = \int_X f(x)\mathrm{d}\mu(x).$$

This is the minimal Stinespring dilation of the CP map $\varphi: \mathcal{C}(X) \to \mathbb{C}$; more precisely, we have the isometry $V: \mathbb{C} \to \mathcal{L}^2(X, \mathrm{d}\mu)$ defined by $Vc = c\Omega$, so that $\varphi(f) = V^*\pi(f)V$. Now suppose we are given another positive linear functional η on $\mathcal{C}(X)$ such that $\eta \leqslant \varphi$, i.e., $\eta(f) \leqslant \varphi(f)$ for every non-negative $f \in \mathcal{C}(X)$. Then Theorem III.1 states that there exists a non-negative function $\rho \in \pi(\mathcal{C}(X))' \subseteq \mathcal{L}^\infty(X, \mathrm{d}\mu)$ such that $\eta(f) = V^*\pi(f)\rho V$, i.e.,

$$\eta(f) = \langle \Omega | \rho\pi(f)\Omega \rangle = \int_X \rho(x) f(x)\mathrm{d}\mu(x).$$

Again, by the Riesz–Markov theorem, there exists a unique Baire measure ν on X such that $\eta(f) = \int_X f(x)\mathrm{d}\nu(x)$. It is easy to see that the function ρ is precisely the measure-theoretic Radon–Nikodym derivative $\mathrm{d}\nu/\mathrm{d}\mu$.

The noncommutative case is dealt with in a similar manner. Namely, if φ is a state on a unital C*-algebra $\mathcal{A}$ that admits the cyclic representation $(\mathcal{H}, \pi, \Omega)$, then any positive linear functional η on $\mathcal{A}$ such that $\eta \leqslant \varphi$ has the form $\eta(A) = \langle \Omega | \pi(A)F\Omega \rangle$ for a unique positive contraction $F \in \pi(\mathcal{A})'$. This is, of course, the familiar Radon–Nikodym theorem for states on C*-algebras (see Theorem 2.3.19 in Ref. 15).

IV. PARTIAL ORDERING OF QUANTUM OPERATIONS

The first series of problems we tackle by means of the Radon–Nikodym theorems of Sec. III is connected to the partial ordering of quantum operations with respect to the relation of complete domination, defined in Sec. II.

As mentioned already, all quantum operations $T: \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$ must satisfy $T(\mathbb{1}_{\mathcal{H}_1}) \leqslant \mathbb{1}_{\mathcal{H}_2}$. It turns out that this normalization condition imposes severe restrictions on the structure of their order intervals. In particular, as shown in the following Proposition, no nontrivial difference of quantum channels can be a CP map.

Proposition IV.1: Let $S, T \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$ be quantum channels. Then $T - S \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$ if and only if $S = T$.

Proof: Suppose $T - S \in \mathrm{CP}(\mathcal{H}_1, \mathcal{H}_2)$, or, equivalently, $S \leqslant T$. Then Theorem III.5 implies that there exists a Kraus decomposition $T(A) = \Sigma_x W_x^* A W_x$ such that $S(A) = \Sigma_x \lambda_x W_x^* A W_x$ with $0 \leqslant \lambda_x \leqslant 1$. Because both S and T are channels, $S(\mathbb{1}) = T(\mathbb{1}) = \mathbb{1}$, which implies that $\Sigma_x(1 - \lambda_x)W_x^* W_x = 0$. Since each term in this sum is a positive operator, the only possibility is that $\lambda_x = 1$ for all x, or $S = T$. The converse is obvious. ■

Remark: To obtain an even simpler proof of this proposition, we can use the fact that, for a CP map T, $\|T\|_{\mathrm{cb}} = \|T(\mathbb{1})\|$ (cf. Sec. II C). Indeed, if S and T are channels, then $T(\mathbb{1}) = S(\mathbb{1}) = \mathbb{1}$, and the assumption that $T - S$ is CP yields $\|T - S\|_{\mathrm{cb}} = \|T(\mathbb{1}) - S(\mathbb{1})\| = 0$, or $S = T$. In fact, the same method shows that if S and T are two CP maps with $S(\mathbb{1}) = T(\mathbb{1})$, then $S - T$ cannot be a CP map. □

The only possible order relation between a pair of quantum channels S and T is that, say, T completely c-dominates S for some $c>1$. The latter condition follows from Proposition IV.1 and from the fact that $S\leqslant cT$ implies $\mathbb{1}\leqslant c\mathbb{1}$, which is (trivially) possible only if $c\geqslant 1$. In fact, as pointed out by Parthasarathy,[10] there are pairs of channels T, T' for which there exist constants c, $c'>1$ such that $T'\leqslant cT$ and $T\leqslant c'T'$. To show this, let S_1 and S_2 be arbitrary channels, and define $T=\lambda S_1+(1-\lambda)S_2$ and $T'=\lambda' S_1+(1-\lambda')S_2$, where $0<\lambda$, $\lambda'<1$. Then, setting $c=[\lambda(1-\lambda)]^{-1}$ and $c'=[\lambda'(1-\lambda')]^{-1}$, we see that indeed $T'\leqslant cT$ and $T\leqslant c'T'$. In Parthasarathy's terminology,[10] T and T' are *uniformly equivalent*; this is written $T\equiv_u T'$, and is an equivalence relation.

The next problem we consider has to do with an alternative way to (partially) order quantum operations by means of orthogonal projections on a suitably enlarged Hilbert space. To this end we need to recall some facts about the so-called *positive operator-valued measures* (POVM's for short) (Sec. 3.1 in Ref. 2). Let X be a topological space, Σ_X the σ-algebra of all Borel subsets of X, and $\mathcal{H}$ a Hilbert space. A map $M:\Sigma_X\to\mathcal{B}(\mathcal{H})$ is a POVM on (the Borel subsets of) X if it has the following properties:

(1) (normalization) $M(\varnothing)=0$ and $M(X)=\mathbb{1}$,
(2) (positivity) $M(\Delta)\geqslant 0$ for all $\Delta\in\Sigma_X$,
(3) (σ-additivity) if $\{\Delta_i\}$ is a countable collection of pairwise disjoint Borel sets in X, then $M(\cup_i\Delta_i)=\Sigma_i M(\Delta_i)$, where the sum converges in the weak operator topology.

A POVM that satisfies an additional requirement that each $M(\Delta)$ is an orthogonal projection, i.e., $M(\Delta)^2=M(\Delta)$, is called a *projection-valued measure* (PVM). The resulting resolution of identity is an orthogonal one. The celebrated Naimark dilation theorem (see Theorem 9.3.2 in Ref. 2) says that for every POVM $M:\Sigma_X\to\mathcal{B}(\mathcal{H})$ there exist a Hilbert space $\mathcal{K}$, a unitary $U:\mathcal{H}\to\mathcal{K}$, a Hilbert space $\widetilde{\mathcal{K}}$ containing $\mathcal{K}$ as a closed subspace, and a PVM $E:\Sigma_X\to\mathcal{B}(\widetilde{\mathcal{K}})$, such that, for any $\Delta\in\Sigma_X$, $M(\Delta)=U^*PE(\Delta)PU$, where P is the orthogonal projection from $\widetilde{\mathcal{K}}$ onto $\mathcal{K}$. Furthermore, we can define the partial isometry $V:\mathcal{H}\to\widetilde{\mathcal{K}}$ (with the final projection P) by $V=PU$, so that $M(\Delta)=V^*E(\Delta)V$.[26]

With these lengthy preliminaries out of the way, we can proceed to state and prove our result.

Theorem IV.2: *Consider quantum operations $T_i\in\mathrm{CP}(\mathcal{H}_1,\mathcal{H}_2)$, $i=1,\ldots,n$, that satisfy $T_1\leqslant T_2\leqslant\cdots\leqslant T_n$. Then there exist a Hilbert space $\mathcal{H}$, an isometry $V:\mathcal{H}_2\to\mathcal{H}_1\otimes\mathcal{H}$, and orthogonal projections $\Pi_i\in\mathcal{B}(\mathcal{H})$ such that*

(1) $T_i(A)=V^*(A\otimes\Pi_i)V$, $1\leqslant i\leqslant n$,
(2) $\Pi_1\leqslant\Pi_2\leqslant\cdots\leqslant\Pi_n$.

Conversely, if items 1 and 2 above hold for quantum operations $T_i\in\mathrm{CP}(\mathcal{H}_1,\mathcal{H}_2)$ with some $\mathcal{H}$, V, and $\{\Pi_i\}$, then $T_1\leqslant T_2\leqslant\cdots\leqslant T_n$.

Proof: Suppose that $\{T_i\}$ satisfy the hypothesis of the theorem. Without loss of generality we may take T_n to be a channel, for if not, then we can append to $\{T_i\}_{i=1}^n$ the channel $T_{n+1}(A)=M^*AM+T_n(A)$, where $M:\mathcal{H}_2\to\mathcal{H}_1$ is an operator defined, up to a unitary, through $M^*M=\mathbb{1}-T_n(\mathbb{1})$, so that the resulting collection $\{T_i\}_{i=1}^{n+1}$ still satisfies $T_1\leqslant T_2\leqslant\cdots\leqslant T_{n+1}$.

Define quantum operations S_i, $i=1,\ldots,n$, by $S_1=T_1$ and $S_i=T_i-T_{i-1}$, $1<i\leqslant n$. Then $T_k=\Sigma_{i=1}^k S_i$, $1\leqslant k\leqslant n$. If $T_n(A)=W^*(A\otimes\mathbb{1}_{\mathcal{E}})W$ is the canonical Stinespring dilation of T_n, Theorem III.3 states that there exist positive operators $F_i\in\mathcal{B}(\mathcal{E})$ such that $S_i(A)=W^*(A\otimes F_i)W$, and $\Sigma_i F_i=\mathbb{1}_{\mathcal{E}}$. By the Naimark dilation theorem there exist a Hilbert space $\mathcal{H}$, an isometry $\widetilde{V}:\mathcal{E}\to\mathcal{H}$, and a PVM $\{E_i\}_{i=1}^n$, $E_i\in\mathcal{B}(\mathcal{H})$, such that $F_i=\widetilde{V}^*E_i\widetilde{V}$, $1\leqslant i\leqslant n$. Thus we can write $S_i(A)=V^*(A\otimes E_i)V$, where the isometry $V:\mathcal{H}_2\to\mathcal{H}_1\otimes\mathcal{H}$ is defined by $V=(\mathbb{1}_{\mathcal{H}_1}\otimes\widetilde{V})W$.

For each k, $1\leqslant k\leqslant n$, let $\Pi_k=\Sigma_{i=1}^k E_i$. Since $\{E_i\}$ is an orthogonal resolution of identity, each Π_k is an orthogonal projection, and $\Pi_k\leqslant\Pi_l$ for $k\leqslant l$ by construction. Furthermore,

$$T_k(A)=\sum_{i=1}^k S_i(A)=\sum_{i=1}^k V^*(A\otimes E_i)V=V^*(A\otimes\Pi_k)V,\quad 1\leqslant k\leqslant n,$$

and the forward direction is proved. The proof of the reverse direction is straightforward. ■

It is pertinent to remark that there are situations when the correspondence between POVM's with values in a suitable Hilbert space and decompositions of a given quantum channel T into completely positive summands is not merely a nice mathematical device, but in fact acquires direct physical significance. For instance, Gregoratti and Werner[27] have exploited this correspondence in a scheme for recovery of classical and quantum information from noise by making a generalized quantum measurement (described by a POVM[28]) on the ''environment'' Hilbert space of a noisy quantum channel [the Hilbert space $\mathcal{E}$ in the ''ancilla'' form (6)].

V. CHARACTERIZATION OF QUANTUM OPERATIONS BY POSITIVE OPERATORS

The correspondence between linear maps from a matrix algebra $\mathcal{M}_m$ into a matrix algebra $\mathcal{M}_n$ and linear functionals on $\mathcal{M}_n \otimes \mathcal{M}_m$ (or, by the Riesz lemma, linear operators on $\mathbb{C}_n \otimes \mathbb{C}_m$) has been treated extensively in a variety of forms in the mathematical literature (see, e.g., Refs. 13, 29–32 for a sampling of results related to positive and completely positive maps). More recently, this correspondence has been exploited fruitfully in some quantum information-theoretic contexts, such as optimal cloning maps,[33] optimal teleportation protocols,[34] separability criteria for entangled states,[35] or entanglement generation.[36,37] In this section we will show that the one-to-one correspondence between positive operators on $\mathbb{C}_n \otimes \mathbb{C}_m$ and CP maps $T: \mathcal{M}_m \to \mathcal{M}_n$ (known as the ''Jamiolkowski isomorphism'' in the quantum information community) can be derived using the Radon–Nikodym machinery. We also comment on how this can be accomplished in the infinite-dimensional case with unbounded operators.

A. The Jamiolkowski isomorphism

In this section we consider quantum operations $T: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ in the case of $\dim \mathcal{H} = m < \infty$ and $\dim \mathcal{K} = n < \infty$. Let $\{e_i\}_{i=1}^m$ and $\{f_\mu\}_{\mu=1}^n$ be fixed orthonormal bases of $\mathcal{H}$ and $\mathcal{K}$. (We will use italic indices for the ''input'' Hilbert space, and greek ones for the ''output'' Hilbert space.) Let τ be the tracial state on $\mathcal{M}_m$, $\tau(A) = m^{-1} \operatorname{Tr} A$, and consider the channel $\Phi(A) := \tau(A) \mathbb{1}_{\mathcal{K}}$. It is convenient to write Φ in the Krans form

$$\Phi(A) := \sum_{i=1}^{m} \sum_{\mu=1}^{n} V_{i\mu}^* A V_{i\mu},$$

where $V_{i\mu} = (1/\sqrt{m}) |e_i\rangle\langle f_\mu|$. Note that these mn Kraus operators are linearly independent, which agrees with the minimality requirement. Setting $\mathcal{E} = \mathcal{K} \otimes \mathcal{H}$, we obtain the canonical Stinespring dilation $\Phi(A) = V_\Phi^* (A \otimes \mathbb{1}_{\mathcal{E}}) V_\Phi$, where

$$V_\Phi \psi = \sum_{i=1}^{m} \sum_{\mu=1}^{n} V_{i\mu} \psi \otimes f_\mu \otimes e_i .$$

Whenever we need to specify the dimensions m and n explicitly, we will write $\Phi_{m,n}$ instead of Φ, $V_{m,n}$ instead of V_Φ, etc.

We must emphasize again that the main result of this section, stated as Theorem V.1 below, is not new. Indeed, it has appeared in numerous papers on quantum information theory.[33–37] Our contribution here is to present a new proof of this result that clearly exhibits the Jamiolkowski isomorphism in the Radon–Nikodym framework.

Theorem V.1: *In the notation described above, any CP map $T: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is completely m^2-dominated by Φ. There exists a unique operator $F_T \in \mathcal{B}(\mathcal{E})$ with $0 \leq F_T \leq m^2 \mathbb{1}_{\mathcal{E}}$, such that $\mathsf{D}_\Phi T = \mathbb{1}_{\mathcal{H}} \otimes F_T$, i.e., $T(A) = V_\Phi^* (A \otimes F_T) V_\Phi$. The action of T on any $A \in \mathcal{B}(\mathcal{H})$ can also be expressed in terms of F_T only, namely, as*

$$T(A) = \frac{1}{m} \operatorname{Tr}_{\mathcal{H}} [(\mathbb{1}_{\mathcal{K}} \otimes A^{\mathsf{T}}) F_T], \tag{12}$$

where A^{T} denotes the matrix transpose of A in the basis $\{e_i\}$. Furthermore, T is a quantum operation if and only if $\mathrm{Tr}_{\mathcal{H}} F_T \leqslant m\mathbb{1}_{\mathcal{K}}$.

Proof: Define $\Psi = (1/\sqrt{m})\sum_{i=1}^{m} e_i \otimes e_i$, and let $H_T = T \otimes \mathrm{id}(|\Psi\rangle\langle\Psi|)$. The matrix elements of H_T are given explicitly by

$$\langle f_\mu \otimes e_i | H_T (f_\nu \otimes e_j)\rangle = \frac{1}{m}\langle f_\mu | T(|e_i\rangle\langle e_j|) f_\nu\rangle.$$

For all $A \in \mathcal{B}(\mathcal{H})$ and $\psi \in \mathcal{K}$ we have

$$\begin{aligned} V_\Phi^*(A \otimes H_T)V_\Phi \psi &= \frac{1}{m}\sum_{i,j=1}^{m}\sum_{\mu,\nu=1}^{n} \langle e_i|Ae_j\rangle\langle f_\mu \otimes e_i | H_T(f_\nu \otimes e_j)\rangle |f_\mu\rangle\langle f_\nu|\psi\rangle \\ &= \frac{1}{m^2}\sum_{\mu,\nu=1}^{n} \langle e_i|Ae_j\rangle\langle f_\mu | T(|e_i\rangle\langle e_j|) f_\nu\rangle |f_\mu\rangle\langle f_\nu|\psi\rangle \\ &\equiv \frac{1}{m^2} T(A)\psi, \end{aligned}$$

so that $T \leqslant m^2\Phi$ and $\mathbb{1}_{\mathcal{H}} \otimes m^2 H_T = \mathsf{D}_\Phi T$ by Corollary III.2. Let $F_T = m^2 H_T$. From the uniqueness of the Radon–Nikodym derivative $\mathsf{D}_\Phi T$ it follows that F_T determines T uniquely.

To prove Eq. (12), we need the following useful identity.

Lemma V.2: For all $A \in \mathcal{B}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{E})$, we have

$$V_\Phi^*(A \otimes B)V_\Phi = \frac{1}{m}\mathrm{Tr}_{\mathcal{H}}[(\mathbb{1}_{\mathcal{K}} \otimes A^{\mathsf{T}})B].$$

Proof: Proceed by direct computation; for an arbitrary $\psi \in \mathcal{K}$, we have

$$\begin{aligned} \mathrm{Tr}_{\mathcal{H}}[(\mathbb{1}_{\mathcal{K}} \otimes A^{\mathsf{T}})B]\psi &= \left(\mathrm{Tr}_{\mathcal{H}} \sum_{i,j,k=1}^{m}\sum_{\mu,\nu=1}^{n} \langle e_j|Ae_i\rangle\langle f_\mu \otimes e_j|B(f_\nu \otimes e_k)\rangle |f_\mu\rangle\langle f_\nu| \otimes |e_i\rangle\langle e_k|\right)\psi \\ &= \sum_{i,j=1}^{m}\sum_{\mu,\nu=1}^{n} \langle e_j|Ae_i\rangle\langle f_\mu \otimes e_j|B(f_\nu \otimes e_i)\rangle |f_\mu\rangle\langle f_\nu|\psi\rangle \\ &\equiv m V_\Phi^*(A \otimes B)V_\Phi \psi, \end{aligned}$$

and the lemma is proved. ■

This establishes Eq. (12). Finally, if T is a quantum operation, then $T(\mathbb{1}_{\mathcal{H}}) \leqslant \mathbb{1}_{\mathcal{K}}$. From Lemma V.2 it follows that $T(\mathbb{1}_{\mathcal{K}}) = (1/m)\mathrm{Tr}_{\mathcal{H}} F_T$, that is, $\mathrm{Tr}_{\mathcal{H}} F_T \leqslant m\mathbb{1}$. Conversely, if $T(\mathbb{1}_{\mathcal{H}}) = V_\Phi^*(\mathbb{1}_{\mathcal{K}} \otimes F_T)V_\Phi \leqslant \mathbb{1}_{\mathcal{K}}$, we have $\mathrm{Tr}_{\mathcal{H}} F_T \leqslant m\mathbb{1}_{\mathcal{K}}$ by Lemma V.2. The theorem is proved. ■

Let $T(A) = V^*(A \otimes \mathbb{1}_{\mathcal{F}})V$ be the canonical Stinespring dilation of T. Then it is easily shown that $\dim \mathcal{H} \cdot \dim \mathcal{F} = \mathrm{rank}\, \mathsf{D}_\Phi T$, that is $\dim \mathcal{F} = \mathrm{rank}\, F_T$. Indeed, Theorems III.5 and V.1 together imply that for any CP map $T: \mathcal{M}_m \to \mathcal{M}_n$ there exist operators $\{K_i^T\}_{i=1}^N$ from $\mathcal{M}_n$ into $\mathcal{M}_m$, such that $\Phi_{m,n}(A) = \sum_{i=1}^N (K_i^T)^* A K_i^T$ and $T(A) = \sum_{i=1}^N \lambda_i (K_i^T)^* A K_i^T$, where $\{\lambda_i\}$ are the (non-negative) eigenvalues of F_T. The Kraus operators $\{K_i^T\}_{i=1}^N$ are linearly independent, and are determined by the isometry V_Φ and the eigenvectors $\{\xi_i\}_{i=1}^N$ of F_T through $V_\Phi \psi = \sum_{i=1}^N V_i^T \psi \otimes \xi_i$. Therefore $N \equiv mn$. The number of nonzero terms in the corresponding Kraus decomposition of T is equal to $\mathrm{rank}\, F_T$, so that $\dim \mathcal{F} = \mathrm{rank}\, F_T$.

Last we would like to show how the Radon–Nikodym derivative $\mathsf{D}_\Phi T$ transforms under composition of CP maps. Consider two CP maps $T_1: \mathcal{M}_m \to \mathcal{M}_n$ and $T_2: \mathcal{M}_n \to \mathcal{M}_d$. According to Theorem V.1 we can write

$$T_1(A) = V_{m,n}^*(A \otimes F_1)V_{m,n}, \quad T_2(B) = V_{n,d}^*(B \otimes F_2)V_{n,d}$$

for uniquely determined positive operators $F_1 \in \mathcal{M}_n \otimes \mathcal{M}_m$ and F_2 on $\mathcal{M}_d \otimes \mathcal{M}_n$. For any $A \in \mathcal{M}_m$, we have

$$\begin{aligned} T_2 \circ T_1(A) &= V_{n,d}^*(T_1(A) \otimes F_2)V_{n,d} \\ &= V_{n,d}^*(V_{m,n}^*(A \otimes F_1)V_{m,n} \otimes F_2)V_{n,d} \\ &= V_{n,d}^*(V_{m,n}^* \otimes \mathbb{1}_{d\times n})(A \otimes F_1 \otimes F_2)(V_{m,n} \otimes \mathbb{1}_{d\times n})V_{n,d}, \end{aligned}$$

where $\mathbb{1}_{d\times n}$ denotes the identity operator on the dilation space $\mathbb{C}^d \otimes C^n$ of T_2. Let $\{e_i\}_{i=1}^m$, $\{f_\mu\}_{\mu=1}^n$, and $\{\phi_x\}_{x=1}^d$ be orthonormal bases of $\mathbb{C}^m$, $\mathbb{C}^n$, and $\mathbb{C}^d$, respectively. Then for any $A \in \mathcal{M}_m$ and any $\psi \in \mathbb{C}^d$ we have

$$\begin{aligned} &T_2 \circ T_1(A)\psi \\ &\quad = \frac{1}{mn}\sum_{i,j=1}^{m}\sum_{\mu,\nu=1}^{n}\sum_{x,y=1}^{d} \langle e_i|Ae_j\rangle|\phi_x\rangle\langle\phi_y|\psi\rangle\langle f_\mu \otimes e_i|F_1(f_\nu \otimes e_j)\rangle\langle\phi_x \otimes f_\mu|F_2(\phi_y \otimes f_\nu)\rangle \\ &\quad = \frac{1}{m}\sum_{i,j=1}^{m}\sum_{x,y=1}^{d}\left(\frac{1}{n}\sum_{\mu,\nu=1}^{n}\langle\phi_x \otimes f_\mu|F_2(\phi_y \otimes f_\nu)\rangle\langle f_\mu \otimes e_i|F_1(f_\nu \otimes e_j)\rangle\right)\langle e_i|Ae_j\rangle|\phi_x\rangle\langle\phi_y|\psi\rangle. \end{aligned}$$

Let $\Omega = (1/\sqrt{n})\Sigma_{\mu=1}^n f_\mu \otimes f_\mu$. Define an operator F_{21} on $\mathbb{C}^d \otimes C^m$ by

$$\langle\phi_x \otimes e_i|F_{21}(\phi_y \otimes e_j)\rangle = \langle\phi_x \otimes \Omega \otimes e_i|(F_2 \otimes F_1)(\phi_y \otimes \Omega \otimes e_j)\rangle.$$

Then it is evident from the calculations above that we can write $T_2 \circ T_1(A) = V_{m,d}^*(A \otimes F_{21})V_{m,d}$. By the uniqueness of the Radon–Nikodym derivative, $\mathbb{1}_m \otimes F_{21} = \mathsf{D}_{\Phi_{m,d}}(T_2 \circ T_1)$. Defining the conditional expectation M_Ω from $\mathcal{M}_d \otimes \mathcal{M}_n^{\otimes 2} \otimes \mathcal{M}_m$ onto $\mathcal{M}_d \otimes \mathcal{M}_m$ by

$$M_\Omega(A \otimes B \otimes C) = \langle\Omega|B\Omega\rangle(A \otimes C) \quad \forall A \in \mathcal{M}_d,\ B \in \mathcal{M}_n^{\otimes 2},\ C \in \mathcal{M}_m,$$

we can write more succinctly $F_{21} = M_\Omega(F_2 \otimes F_1)$.

B. Generalization to arbitrary faithful states

The construction described in Sec. V A also goes through if, instead of the tracial state τ, we take an arbitrary *faithful* state ω. As is well-known, for any such state there exist an orthonormal basis $\{e_i\}_{i=1}^m$ and a probability distribution $\{p_i\}_{i=1}^m$ with $p_i > 0$, such that $\omega(A) = \Sigma_{i=1}^m p_i\langle e_i|Ae_i\rangle$ for all $A \in \mathcal{B}(\mathcal{H})$. Furthermore, $\omega(A) = \langle\Omega|(A \otimes \mathbb{1})\Omega\rangle$, where $\Omega = \Sigma_{i=1}^m \sqrt{p_i}e_i \otimes e_i$. (This is, of course, the canonical Stinespring dilation of the CP map ω by means of the GNS construction.) Let $D_\omega \in \mathcal{B}(\mathcal{H})$ denote the density operator corresponding to ω, i.e., $\omega(A) = \mathrm{Tr}(D_\omega A)$. Owing to the faithfulness of ω, D_ω is invertible.

Fix an orthonormal basis $\{f_\mu\}_{\mu=1}^n$ of $\mathcal{K}$, and define the channel $\Phi_\omega : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ through $\Phi_\omega(A) = \omega(A)\mathbb{1}_\mathcal{K}$. The Kraus form of Φ_ω is given by $\Phi_\omega(A) = \Sigma_{i=1}^m\Sigma_{\mu=1}^n V_{i\mu}^* A V_{i\mu}$, where $V_{i\mu} = \sqrt{p_i}|e_i\rangle\langle f_\mu|$, and the canonical Stinespring dilation by $\Phi_\omega(A) = V_\omega^*(A \otimes \mathbb{1}_\mathcal{E})V_\omega$, where again $\mathcal{E} \simeq \mathcal{K} \otimes \mathcal{H}$ and $V_\omega\psi = \Sigma_{i=1}^m\Sigma_{\mu=1}^n V_{i\mu}\psi \otimes f_\mu \otimes e_i$.

Consider the positive operator $F_{T,\omega} = T \otimes \mathrm{id}((D_\omega^{-1} \otimes \mathbb{1})|\Omega\rangle\langle\Omega|(D_\omega^{-1} \otimes \mathbb{1}))$, whose matrix elements are given by $\langle f_\mu \otimes e_i|F_{T,\omega}(f_\nu \otimes e_j)\rangle = (1/\sqrt{p_i p_j})\langle f_\mu|T(|e_i\rangle\langle e_j|)f_\nu\rangle$. For all $A \in \mathcal{B}(\mathcal{H})$ and $\psi \in \mathcal{K}$ we then have

$$V_\omega^*(A\otimes F_{T,\omega})V_\omega\psi=\sum_{i,j=1}^{m}\sum_{\mu,\nu=1}^{n}\sqrt{p_ip_j}\langle e_i|Ae_j\rangle\langle f_\mu\otimes e_i|F_{T,w}(f_\nu\otimes e_j)\rangle|f_\mu\rangle\langle f_\nu|\psi\rangle$$

$$=\sum_{i,j=1}^{m}\sum_{\mu,\nu=1}^{n}\langle e_i|Ae_j\rangle\langle f_\mu|T(|e_i\rangle\langle e_j|)f_\nu\rangle|f_\mu\rangle\langle f_\nu|\psi\rangle\equiv T(A)\psi,$$

so that $T\leqslant\|F_{T,\omega}\|\Phi_\omega$, with $\|F_{T,\omega}\|\leqslant\|D_\omega^{-1}\|^2\|T\|_{\mathrm{cb}}$.

Consequently, for any faithful state ω on $\mathcal{B}(\mathcal{H})$ and any CP map $T:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ there exists a positive constant c such that T is completely c-dominated by Φ_ω; thus T is uniquely determined by the Radon–Nikodym derivative $\mathsf{D}_{\Phi_\omega}T$. Note that in the special case of ω being the tracial state on $\mathcal{M}_m$ we simply recover the results of the preceding section.

C. Generalization to infinite dimensions

In the form stated above, both the Jamiolkowski isomorphism and its generalization to arbitrary faithful states are valid only for CP maps between finite-dimensional algebras. However, in many problems of quantum information theory it is necessary to consider CP maps between algebras of operators on infinite-dimensional Hilbert spaces.

Consider a normal CP map $T:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$, where $\mathcal{H}$ and $\mathcal{K}$ are separable Hilbert spaces. Fix a normal faithful state ω on $\mathcal{B}(\mathcal{H})$; then there exist a complete orthonormal basis $\{e_i\}$ of $\mathcal{H}$ and a probability distribution $\{p_i\}$, $p_i>0$, such that, for any $A\in\mathcal{B}(\mathcal{H})$, $\omega(A)=\langle\Omega|(A\otimes\mathbb{1})\Omega\rangle$ with $\Omega=\Sigma_i\sqrt{p_i}e_i\otimes e_i$. Let D_ω denote the density operator corresponding to ω. Because $\mathcal{H}$ is infinite-dimensional, the inverse of D_ω is an unbounded operator defined on a dense domain, namely the linear span of $\{e_i\}$. Therefore the approach taken in the preceding section will not work; instead, we will characterize T through the Radon–Nikodym derivative of another CP map T_ω (dependent on both T and ω) with respect to the channel $\Phi_\omega=\omega(A)\mathbb{1}_\mathcal{K}$.

Choosing a complete orthonormal basis $\{f_\mu\}$ of $\mathcal{K}$, we can write Φ_ω in the Kraus form $\Phi_\omega(A)=\Sigma_{i,\mu}V_{i\mu}^*AV_{i\mu}$, $V_{i\mu}=\sqrt{p_i}|e_i\rangle\langle f_\mu|$, where the series converges in the strong operator topology. We also have the Stinespring dilation via $\Phi_\omega(A)=V_\omega^*(A\otimes\mathbb{1}_\mathcal{E})V_\omega$, where $\mathcal{E}\simeq\mathcal{K}\otimes\mathcal{H}$ and $V_\omega\psi=\Sigma_{i,\mu}V_{i\mu}\psi\otimes f_\mu\otimes e_i$. To see that this Stinespring dilation is canonical, let $A=(1/\sqrt{p_k})|e_j\rangle\langle e_k|$ and $\psi=f_\nu$. Thus

$$(A\otimes\mathbb{1}_\mathcal{E})V_\omega\psi=e_j\otimes f_\nu\otimes e_k,$$

which shows that the set $\{(A\otimes\mathbb{1}_\mathcal{E})V_\omega\psi|A\in\mathcal{B}(\mathcal{H}),\psi\in\mathcal{K}\}$ is total in $\mathcal{H}\otimes\mathcal{E}$.

Let $F_{T,\omega}=T\otimes\mathrm{id}(|\Omega\rangle\langle\Omega|)$; the matrix elements are

$$\langle f_\mu\otimes e_i|F_{T,\omega}(f_\nu\otimes e_j)\rangle=\sqrt{p_ip_j}\langle f_\mu|T(|e_i\rangle\langle e_j|)f_\nu\rangle.$$

Then for all $A\in\mathcal{B}(\mathcal{H})$ and $\psi\in\mathcal{K}$ we can write

$$V_\omega^*(A\otimes F_{T,\omega})V_\omega\psi=\sum_{i,\mu}\sum_{j,\nu}\sqrt{p_ip_j}\langle f_\mu\otimes e_i|F_{T,\omega}(f_\nu\otimes e_j)\rangle\langle e_i|Ae_j\rangle|f_\mu\rangle\langle f_\nu|\psi\rangle$$

$$=\sum_{i,\mu}\sum_{j,\nu}p_ip_j\langle e_i|Ae_j\rangle\langle f_\mu|T(|e_i\rangle\langle e_j|)f_\nu\rangle|f_\mu\rangle\langle f_\nu|\psi\rangle\equiv T(D_\omega AD_\omega)\psi.$$

We will write $T_\omega(A)$ for $T(D_\omega AD_\omega)$. From the Radon–Nikodym theorem it follows that T_ω is completely dominated by Φ_ω, and that $\mathsf{D}_{\Phi_\omega}T_\omega=\mathbb{1}_\mathcal{H}\otimes F_{T,\omega}$. We can determine the action of T on the "matrix units" $|e_i\rangle\langle e_j|$ via $T(|e_i\rangle\langle e_j|)=(p_ip_j)^{-1}T_\omega(|e_i\rangle\langle e_j|)$.

VI. NORM ESTIMATES FOR DIFFERENCES OF QUANTUM OPERATIONS

In this section we will demonstrate the use of the Radon–Nikodym theorem for CP maps in deriving several useful estimates for CB norms of differences of quantum channels.

Consider two CP maps $T_1, T_2 : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$. Suppose that there exists a CP map $T : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, such that $T_i \leqslant T$, $i = 1, 2$, and let $T(A) = V^*(A \otimes \mathbb{1}_{\mathcal{E}})V$ be the canonical Stinespring dilation of T. By the Radon–Nikodym theorem, there exist positive contractions $F_1, F_2 \in \mathcal{B}(\mathcal{E})$ such that $T_i(A) = V^*(A \otimes F_i)V$, $i = 1, 2$. Then

$$(T_1 - T_2)(A) = T_1(A) - T_2(A) = V^*(A \otimes (F_1 - F_2))V,$$

and the Haagerup–Paulsen–Wittstock theorem immediately implies that

$$\|T_1 - T_2\|_{\mathrm{cb}} \leqslant \|V\| \|(F_1 - F_2)V\| \leqslant \|V\|^2 \|F_1 - F_2\|.$$

If T is a quantum channel, V is an isometry, so that $\|V\| = 1$. Therefore we get

$$\|T_1 - T_2\|_{\mathrm{cb}} \leqslant \|F_1 - F_2\|. \tag{13}$$

In particular, if $S \leqslant T$, then $\|S - T\|_{\mathrm{cb}} \leqslant \|\mathbb{1} - F\|$, where $\mathbb{1} \otimes F$ is the Radon–Nikodym derivative $\mathsf{D}_T S$.

Given two CP maps $T_1, T_2 : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ with (not necessarily minimal) Stinespring dilations $T_i(A) = V_i^*(A \otimes \mathbb{1}_{\mathcal{E}})V_i$, $i = 1,2$, on the common dilation space $\mathcal{E}$, the norm $\|T_1 - T_2\|_{\mathrm{cb}}$ can be bounded from above in terms of V_1 and V_2. Indeed, denoting by π the $*$-homomorphism $\mathcal{B}(\mathcal{H}) \ni A \mapsto A \otimes \mathbb{1}_{\mathcal{E}}$, we can use the Haagerup–Paulsen–Wittstock theorem to obtain

$$\begin{aligned}
\|T_1 - T_2\|_{\mathrm{cb}} &= \|V_1^* \circ \pi \circ V_1 - V_2^* \circ \pi \circ V_2\|_{\mathrm{cb}} \\
&\leqslant \|V_1^* \circ \pi \circ V_1 - V_1^* \circ \pi \circ V_2\|_{\mathrm{cb}} + \|V_1^* \circ \pi \circ V_2 - V_2^* \circ \pi \circ V_2\|_{\mathrm{cb}} \\
&\leqslant (\|V_1\| + \|V_2\|)\|V_1 - V_2\|.
\end{aligned} \tag{14}$$

If T_1 and T_2 are channels, then V_1 and V_2 are isometries. Consequently, $\|V_1\| = \|V_2\| = 1$, and the bound (14) becomes $\|T_1 - T_2\|_{\mathrm{cb}} \leqslant 2\|V_1 - V_2\|$. As the lemma below shows, when the Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$ are finite-dimensional, one can find a common dilation space $\mathcal{E}$ and maps V_1, $V_2 : \mathcal{K} \to \mathcal{H} \otimes \mathcal{E}$, such that $\|T_1 - T_2\|_{\mathrm{cb}}$ can be bounded from below.

Lemma VI.1: For any two CP maps $T_1, T_2 : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ there exist a Hilbert space $\mathcal{E}$ and operators $V_1, V_2 : \mathcal{K} \to \mathcal{H} \otimes \mathcal{E}$ such that $T_i(A) = V_i^*(A \otimes \mathbb{1}_{\mathcal{E}})V_i$, $i = 1, 2$, and

$$\|V_1 - V_2\| \leqslant \dim \mathcal{H} \sqrt{\|T_1 - T_2\|_{\mathrm{cb}}}. \tag{15}$$

Proof: Using Theorem V.1, we can write $\mathcal{E} = \mathcal{K} \otimes \mathcal{H}$ and $V_i = \sqrt{\mathsf{D}_\Phi T_i} V_\Phi = (\mathbb{1}_{\mathcal{H}} \otimes \sqrt{F_{T_i}})V_\Phi$. Then $T_i(A) = V_i^*(A \otimes \mathbb{1}_{\mathcal{E}})V_i$. Next we prove the estimate (15). We have

$$\|V_1 - V_2\| \leqslant \|\mathbb{1}_{\mathcal{H}} \otimes \sqrt{F_{T_1}} - \mathbb{1}_{\mathcal{H}} \otimes \sqrt{F_{T_2}}\| \|V_\Phi\| = \|\sqrt{F_{T_1}} - \sqrt{F_{T_2}}\| \leqslant \sqrt{\|F_{T_1} - F_{T_2}\|}. \tag{16}$$

The last inequality in (16) holds because: (1) $x \mapsto \sqrt{x}$ is an operator monotone function on $[0,\infty)$, i.e., $\sqrt{A} \leqslant \sqrt{B}$ for all operators A, B satisfying $0 \leqslant A \leqslant B$ (Prop. V.1.8 in Ref. 38), (2) for any operator monotone function f with $f(0) = 0$ and any pair of positive operators A, B we have $\|f(A) - f(B)\| \leqslant f(\|A - B\|)$ (Theorem X.1.1 in Ref. 38), and (3) $\|X\| = \|\sqrt{X}\|^2$ for any $X \geqslant 0$ by the spectral mapping theorem. Now $F_{T_i} = (\dim \mathcal{H})^2 T_i \otimes \mathrm{id}(|\Psi\rangle\langle\Psi|)$, where $\Psi = (1/\sqrt{\dim \mathcal{H}}) \Sigma_i e_i \otimes e_i$ for some orthonormal basis $\{e_i\}$ in $\mathcal{H}$. Thus, using the properties of the CB norm, we get

$$\|F_{T_1} - F_{T_2}\| = (\dim \mathcal{H})^2 \|T_1 \otimes \mathrm{id}(|\Psi\rangle\langle\Psi|) - T_2 \otimes \mathrm{id}(|\Psi\rangle\langle\Psi|)\| \leqslant (\dim \mathcal{H})^2 \|T_1 - T_2\|_{\mathrm{cb}}. \tag{17}$$

Combining Eqs. (16) and (17) yields (15). ■

Inequality (15) was also proved by Kitaev,[21] but by quite different means. Here several warnings are in order. In the article of Kitaev[21] the ''canonical representation'' of a CP map $T:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ is defined as $T(A)=\mathrm{Tr}_{\mathcal{F}}WAW^*$ with $\mathcal{F}\simeq\mathcal{K}\otimes\mathcal{H}$. This is not to be confused with the *canonical Stinespring dilation* of T, $T(A)=V^*(A\otimes\mathbb{1}_{\mathcal{E}})V$ [or its dual, $T_*(A)=\mathrm{Tr}_{\mathcal{E}}VAV^*$] which must satisfy the requirement that $\mathcal{H}\otimes\mathcal{E}$ is (the closure of) the linear span of $\{(A\otimes\mathbb{1}_{\mathcal{E}})V\psi|A\in\mathcal{B}(\mathcal{H}),\psi\in\mathcal{K}\}$. Thus $\mathcal{E}$ is, in general, a subspace of $\mathcal{F}=\mathcal{K}\otimes\mathcal{H}$. Furthermore, Kitaev's version of the estimate (15) has $\dim\mathcal{K}$, and not $\dim\mathcal{H}$, multiplying the CB norm on its right-hand side. This is due to the fact that, whereas we cast all CP maps in the Stinespring form $T(A)=W^*(A\otimes\mathbb{1}_{\mathcal{F}})W$, Kitaev prefers to work with the dual representation $T_*(A)=\mathrm{Tr}_{\mathcal{F}}WAW^*$. Since all (bounded) operators on a finite-dimensional Hilbert space are trace-class, T_* trivially extends to a CP map from $\mathcal{B}(\mathcal{K})$ into $\mathcal{B}(\mathcal{H})$.

VII. CONCLUDING REMARKS

In this paper we have shown that the Radon-Nikodym theorem for completely positive maps[6,7,10] is an extremely powerful and versatile tool for problems involving characterization and comparison of quantum operations. The upshot is that if $T(A)=V^*(A\otimes\mathbb{1}_{\mathcal{E}})V$ is the canonical Stinespring dilation of a CP map T, then the set of all CP maps S for which $T-S$ is also CP (we say that S is *completely dominated* by T) is in a one-to-one correspondence with the positive contractions F on $\mathcal{E}$, given explicitly by $S(A)=V^*(A\otimes F)V$. As we have demonstrated, this correspondence brings many seemingly unrelated problems into a common framework.

However, many important questions still remain unanswered. For instance, it is not difficult to convert the above ''Stinespring form'' of the Radon–Nikodym theorem into an equivalent ''Kraus form'' (cf. Sec. III B). The Kraus decomposition of a CP map T involves at most countably many terms, and all maps S completely dominated by T can be characterized in terms of positive-definite kernels on the corresponding indexing set. However, it is not clear how to apply this theorem directly to CP maps given in terms of a ''continual'' Kraus decomposition (as in, e.g., the quantum operational model of Gaussian displacement noise[39]). For example, if U_g is a strongly continuous unitary representation of a compact topological group G on a Hilbert space $\mathcal{H}$, how do we describe all CP maps completely dominated by the channel

$$T(A)=\int_G U_g^*AU_g\,\mathrm{d}\mu(g),$$

where μ is the (normalized) Haar measure on G, in terms of $\{U_g\}$? A partial step in this direction has been taken by Parthasarathy,[10] who constructed a Stinespring dilation of T in terms of $\{U_g\}$ under the assumption that these operators are linearly independent μ-almost everywhere, i.e.,

$$\int_G\varphi(g)U_g\,\mathrm{d}\mu(g)=0\Leftrightarrow\varphi(g)=0\ \ \mu-\text{a.e.}$$

for any $\varphi\in\mathcal{L}^1(G,\mu)$. However, a general solution is still lacking. We hope to address this issue in a future publication.

ACKNOWLEDGMENTS

The author wishes to thank V. P. Belavkin for introducing him to the subject of this paper, and G. M. D'Ariano for stimulating discussions and a careful reading of the paper. This work was supported by the U.S. Army Research Office through MURI Grant No. DAAD19-00-1-0177, and by the Defense Advanced Research Projects Agency through QuIST Grant No. F30602-01-2-0528.

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Perturbation expansions for a class of singular potentials

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(Received 22 November 2002; accepted 8 August 2003)

Harrell's modified perturbation theory [Ann. Phys. (N.Y.) **105**, 379 (1977)] is applied and extended to obtain nonpower perturbation expansions for a class of singular Hamiltonians $H=-(d^2/dx^2)+x^2+(A/x^2)+(\lambda/x^\alpha)$ $(A\geqslant 0,\alpha>2)$, known as generalized spiked harmonic oscillators. The perturbation expansions developed here are valid for small values of the coupling $\lambda>0$, and they extend the results which Harrell obtained for the spiked harmonic oscillator $A=0$. Formulas for the excited states are also developed. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1616996]

I. INTRODUCTION

This is a detailed extension of Harrell's modified perturbation theory[1] for the class of singular potentials

$$H=-\frac{d^2}{dx^2}+x^2+\frac{\lambda}{x^\alpha}\quad(\lambda>0,\alpha>2),\tag{1.1}$$

defined on suitable domains in the Hilbert space $L^2(0,\infty)$ with solutions satisfying Dirichlet boundary conditions. By singular we mean that the familiar Rayleigh–Schrödinger series either do not exist or do not converge. The present work, motivated by Harrell[1] and Greenlee,[2] studies a perturbative and variational analysis of the eigenvalues and eigenfunctions for the family of singular Hamiltonians

$$H=H_0+\lambda V=-\frac{d^2}{dx^2}+x^2+\frac{A}{x^2}+\frac{\lambda}{x^\alpha}\quad(A\geqslant 0)\tag{1.2}$$

known as generalized spiked harmonic oscillator Hamiltonian.[3–10] The extension lies in considering A to range over all non-negative real numbers instead of non-negative integers of the type $l(l+1)$. The main results are the extensions of Harrell's perturbative expansions[1] for the ground-state eigenvalues of the spiked harmonic oscillator Hamiltonian $A=0$. In his elegant investigation, Harrell mentioned briefly the possibility of extending his theory to the case of $A=l(l+1)$, where l is the angular-momentum quantum number; however, his results mostly concern perturbation expansions for ground-state energies of the spiked harmonic oscillator Hamiltonian (1.1). There are two principal reasons for this choice: (1) The interesting Klauder phenomenon[11–13] occurs *only* in the case $A=0$, to the effect that, for sufficiently singular potentials, the perturbation term V cannot be smoothly turned off ($\lambda\to 0$) in the Hamiltonian $H=H_0+\lambda V$ to restore the free Hamiltonian H_0; (2) Rayleigh–Schrödinger perturbation series diverge at some finite order whenever $\alpha>2$.

Klauder's phenomenon does not occur[14–16] if $A>0$. This is the case, for example, in N dimensions with $A=(l+\frac{1}{2}(N-1))(l+\frac{1}{2}(N-3))$ and $l>0$, or with $l=0$ and $N\neq 1$ or 3. In such

cases the domain of the Hamiltonian H *is* stable under the limit $\lambda \to 0$. However, a perturbative analysis for solutions that vanish at the origin is still interesting because of the divergence of the Rayleigh–Schrödinger series at some finite order for any $\alpha > 2$. We are able to conclude in the present paper that the Rayleigh–Schrödinger series will breakdown at the order $n \geqslant 2\nu(\gamma - 1)$ for $\alpha > 2$ where $\nu = 1/(\alpha - 2)$ and $\gamma = 1 + \frac{1}{2}\sqrt{1 + 4A}$. For example, $\alpha \geqslant 2\gamma$ causes the perturbation series to diverge at the first order; for $\alpha \geqslant \gamma + 1$ the second-order perturbation will diverge, etc. These results and some others concerning the convergence of Rayleigh–Schrödinger series which rely heavily of the application of Kato's criterion[17–19] will be the subject of an independent investigation. In the present paper, we concentrate on the development of nonpower perturbation expansions for the Hamiltonian (1.2).

Detwiler and Klander,[20] in their variational study of the spiked harmonic oscillator Hamiltonian (1.1), have shown that for $2 \leqslant \alpha < 3$ the eigenvalues are given by asymptotic series to first order so long as $\lambda > 0$. But for $\alpha > 3$, the ground-state eigenvalues are given by

$$E_0(\lambda) = 3 + k\lambda^{\nu} + o(\lambda^{\nu}),$$

and, for $\alpha = 3$, by

$$E_0(\lambda) = 3 + k'\lambda \log(\lambda) + O(\lambda),$$

where k and k' are to be determined by variational means.[20] Harrell, soon afterwards, modified the Rayleigh–Schrödinger series by utilizing the standard WKB-approximation technique for the lowest few orders. This proved to be quite successful, and he continued to develop a special perturbation theory, now known as singular perturbation theory, and obtained thereby the first few terms of the perturbed λ-expansion for different values of α. This turned out to be a nonpower series expansion and in fact was of exactly the same order as that of Detwiler and Klauder.[20] More specifically, Harrell[1] showed that the asymptotic series for the ground-state eigenvalues of the Hamiltonian (1.1) are explicitly given, for $\nu = 1/(\alpha - 2)$.

For $\alpha \geqslant 4$,

$$E_0(\lambda) = 3 + \frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^{\nu} + O(\lambda^{2\nu}).$$

For $3 < \alpha < 4$,

$$E_0(\lambda) = 3 + \frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^{\nu} - \frac{4\nu\Gamma\left(\dfrac{3-\dfrac{1}{\nu}}{2}\right)}{(1-\nu)\sqrt{\pi}}\lambda + O(\lambda^{2\nu}).$$

For $\alpha = 3$,

$$E_0(\lambda) = 3 - \frac{4}{\sqrt{\pi}}\lambda \log(\lambda) - \frac{10c}{\sqrt{\pi}}\lambda + O(\lambda^2 \log^2(\lambda))$$

$$(c = 0.577\,215\,664\,9 \text{ etc., Euler's constant}).$$

For $\frac{5}{2} < \alpha < 3$,

$$E_0(\lambda) = 3 + \frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^{\nu} + \frac{2\Gamma\left(\dfrac{3-\alpha}{2}\right)}{\sqrt{\pi}}\lambda + O(\lambda^{2\nu}).$$

The paper is organized as follows. In Sec. II, we briefly review the regular perturbation expansions for the Hamiltonian (1.2) and we identify the conditions under which the first- and the second-order corrections of Rayleigh–Schrödinger series exists. In Sec. III, the main theorem used for the development of nonpower perturbation expansions will be introduced and proved. In Sec. IV we introduced a suitable trial wave function. In Secs. V and VI, we extend Harrell's theory to treat the generalized spiked harmonic oscillator Hamiltonians (1.2) for the cases where the Rayleigh–Schrödinger series fails and thereby we show that asymptotic series for the eigenvalues of the Hamiltonian (1.2) are explicitly given by the following.

For $\alpha \geqslant 2(2\gamma-1)$,

$$E_0(\lambda)=2\gamma+\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+O(\lambda^{4\nu(\gamma-1)}).$$

For $2\gamma<\alpha<2(2\gamma-1)$,

$$E_0(\lambda)=2\gamma+\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}-\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(1-2\nu(\gamma-1))\Gamma(\gamma)}\lambda+O(\lambda^{4\nu(\gamma-1)}).$$

For $\alpha=2\gamma$,

$$E_0(\lambda)=2\gamma-\frac{1}{(\gamma-1)\Gamma(\gamma)}\lambda\log(\lambda)+\left[\frac{-c(1+\gamma)+2\log(2(\gamma-1))}{(\gamma-1)\Gamma(\gamma)}\right]\lambda+O(\lambda^2\log^2(\lambda)).$$

For $\gamma+1<\alpha<2\gamma$,

$$E_0(\lambda)=2\gamma+\frac{2\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\nu\Gamma(\gamma)\Gamma(2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(2\nu(\gamma-1)-1)\Gamma(\gamma)}\lambda+O(\lambda^2),$$

where $\nu=1/(\alpha-2)$ and $\gamma=1+\frac{1}{2}\sqrt{1+4A}$. The asymptotic expansions for the case $\alpha\leqslant\gamma+1$ are discussed in Sec. VII, along with some other cases. The connection with the region $0<\alpha<5/2$, overlooked by Harrell, is also investigated. In Sec. VIII, the extension of the perturbation expansions developed in Secs. V–VII to the excited states is discussed and some explicit formulas are derived.

II. ASYMPTOTIC PERTURBATION EXPANSIONS

It is known that although many perturbation expansions diverge, they may actually be asymptotic expansions whose first few terms can yield good approximations. The class of singular Hamiltonian (1.2) affords interesting examples of this phenomenon. Indeed, by regarding the Gol'dman and Krivchenkov Hamiltonian[7] $H_0=-(d^2/dx^2)+x^2+(A/x^2)$, which admits the exact solutions

$$\psi_n(x)=(-1)^n\sqrt{\frac{2(\gamma)_n}{n!\Gamma(\gamma)}}x^{\gamma-1/2}e^{-1/2x^2}\,{}_1F_1(-n,\gamma,x^2) \tag{2.1}$$

with exact eigenenergies

$$E_n=4n+2\gamma,\quad n=0,1,2,\ldots,\quad \gamma=1+\tfrac{1}{2}\sqrt{1+4A}, \tag{2.2}$$

as the unperturbed part, and $V(x)=x^{-\alpha}$ as the perturbation potential, the first-order correction of the Rayleigh–Schrödinger series for the Hamiltonian (1.2) exists only for $\alpha<2\gamma$, while the second-order correction will required $\alpha<\gamma+1$. The first condition $\alpha<2\gamma$ follows from $E_1=(\psi_0,x^{-\alpha}\psi_0)$, while the second condition $\alpha<\gamma+1$ follows[5] from

$$E_2=\sum_{i=1}^{\infty}\frac{|(\psi_0,x^{-\alpha}\psi_i)|^2}{E_i-E_0}.$$

Under these conditions the perturbation expansions for the ground-state eigenvalues up to second-order[5] reads, for small values of λ,

$$\begin{aligned}E(\lambda,\alpha)&=E_0+E_1\lambda+E_2\lambda^2+\cdots\\&=2\gamma+\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}\lambda-\lambda^2\frac{\alpha^2}{16\gamma}{}_4F_3\left(1,1,1+\frac{\alpha}{2},1+\frac{\alpha}{2};2,2,\gamma+1;1\right)+\cdots.\end{aligned}\tag{2.3}$$

In the next sections we develop nonpower perturbation expansions for the cases where the regular Rayleigh–Schrödinger series fails to exist; namely, $\alpha\geqslant 2\gamma$ and $\alpha\geqslant\gamma+1$.

Before we proceed we should note that the functions ${}_1F_1$ and ${}_4F_3$, mentioned above, are special cases of the generalized hypergeometric function[21]

$${}_pF_q(\alpha_1,\alpha_2,\ldots,\alpha_p;\beta_1,\beta_2,\ldots,\beta_q;z)=\sum_{k=0}^{\infty}\frac{\prod_{i=1}^{p}(\alpha_i)_k}{\prod_{j=1}^{q}(\beta_j)_k}\frac{z^k}{k!},\tag{2.4}$$

where p and q are non-negative integers, and none of the β_j $(j=1,2,...,q)$, is equal to zero or to a negative integer. If the series does not terminate (that is to say, none of the α_i, $i=1,2,...,p$, is a negative integer), then the series, in the case $p=q+1$, converges or diverges accordingly as $|z|<1$ or $|z|>1$. For $z=1$, the series is convergent provided $\Sigma_{j=1}^{q}\beta_j-\Sigma_{i=1}^{p}\alpha_i>0$.

Here $(a)_n$, the shifted factorial (or *Pochhammer symbol*), is defined by

$$(a)_0=1,\quad (a)_n=a(a+1)(a+2)\cdots(a+n-1)\ \text{ for }\ n=1,2,\ldots\tag{2.5}$$

and may be expressed in terms of the gamma function by $(a)_k=\Gamma(a+k)/\Gamma(a)$, when a is not a negative integer $-m$, and, in these exceptional cases, $(-m)_k=0$ if $k>m$ and otherwise $(-m)_k=(-1)^k m!/(m-k)!$

III. THE MAIN THEOREM

It is clear that the perturbation approach mentioned in Sec. II cannot apply if $\alpha\geqslant 2\gamma$, since it is clear in this case that the first-order perturbation correction diverges. We construct a modified perturbation series for the operators in this region by considering the perturbation theory of families of self-adjoint operators by an application of the variational method. This is done via Kato's generalization[22,23] of Temple's inequality,[24–26] which can understood from the following discussion. The derivation of bounds on the eigenvalues for self-adjoint operators usually starts from a consideration of the positive definite function given by

$$(\mu,\mu)=([H-\epsilon]\phi,[H-\epsilon]\phi)=(H\phi,H\phi)-(\phi,H\phi)^2+(\epsilon-(\phi,H\phi))^2\geqslant 0,\tag{3.1}$$

where μ is a function of ϕ and ϵ, i.e., $\mu=\mu(\phi,\epsilon)$, H is the operator in question, ϵ is a positive parameter, and ϕ is a suitably chosen normalized trial function. If we expand the normalized function ϕ in terms of the complete set of eigenfunctions $\{\phi_n\}$ of H with eigenvalues $E_n(\lambda)$, $\phi=\Sigma_n a_n\phi_n$, $a_n=(\phi,\phi_n)$, $(\phi,\phi)=1=\Sigma_n|a_n|^2$, we can express the positive definite function in (3.1) as

$$(\mu,\mu)=\sum_n |a_n|^2(E_n(\lambda)-\epsilon)^2\geqslant 0.$$

Let us assume that we have picked the value of ϵ for the closest approach to the ith eigenvalue E_i, i.e.,

$$(\mu,\mu)=\sum_n |a_n|^2(E_n(\lambda)-\epsilon)^2\geqslant (E_i(\lambda)-\epsilon)^2\geqslant 0. \tag{3.2}$$

By combining (3.1) and (3.2), it can be easily seen that

$$\begin{aligned}\epsilon-\sqrt{\|H\phi\|^2-(\phi,H\phi)^2+(\epsilon-(\phi,H\phi))^2}\\ \leqslant E_i(\lambda)\leqslant \epsilon+\sqrt{\|H\phi\|^2-(\phi,H\phi)^2+(\epsilon-(\phi,H\phi))^2}.\end{aligned} \tag{3.3}$$

Now, by setting[26]

$$\epsilon+[(H\phi,H\phi)-(\phi,H\phi)^2+(\epsilon-(\phi,H\phi))^2]^{1/2}=E^L_{i+1}(\lambda), \tag{3.4}$$

where $E^L_{i+1}(\lambda)$ is a lower bound estimate of $E_{i+1}(\lambda)$, we can show that Eq. (3.4) possesses the solution

$$\epsilon=\frac{1}{2}\left[E^L_{i+1}(\lambda)+(\phi,H\phi)-\frac{(H\phi,H\phi)-(\phi,H\phi)^2}{E^L_{i+1}(\lambda)-(\phi,H\phi)}\right] \tag{3.5}$$

provided $(\phi,H\phi)<E^L_{i+1}(\lambda)$. Substituting (3.5) into the lower bound expression in (3.3) yields the Kato–Temple expression for the lower bound:

$$E_i(\lambda)\geqslant(\phi,H\phi)-\frac{(H\phi,H\phi)-(\phi,H\phi)^2}{E^L_{i+1}(\lambda)-(\phi,H\phi)}. \tag{3.6}$$

Similarly, setting

$$\epsilon-[(H\phi,H\phi)-(\phi,H\phi)^2+(\epsilon-(\phi,H\phi))^2]^{1/2}=E^U_{i-1}(\lambda), \tag{3.7}$$

where $E^U_{i-1}(\lambda)$ is an upper bound estimate to the next lowest eigenvalue to $E_i(\lambda)$, yields

$$E_i(\lambda)\leqslant(\phi,H\phi)+\frac{(H\phi,H\phi)-(\phi,H\phi)^2}{(\phi,H\phi)-E^U_{i-1}(\lambda)} \tag{3.8}$$

for $E^U_{i-1}(\lambda)<(\phi,H\phi)$. We let $\eta=(\phi,H\phi)$, and the residual norm $\epsilon=\|(H-\eta)\phi\|$ (hence $\epsilon^2=\|H\phi\|^2-\eta^2$), and $\epsilon^2<(E^L_{i+1}(\lambda)-\eta)(\eta-E^U_{i-1}(\lambda))$, which follows by means of the inequalities $\eta-\epsilon^2/(E^L_{i+1}(\lambda)-\eta)>E^U_{i-1}$ or $\eta+\epsilon^2/(\eta-E^U_{i-1}(\lambda))<E^L_{i+1}(\lambda)$. This indeed ensures that the open interval $(E^U_{i-1}(\lambda),E^L_{i+1}(\lambda))$ contains a single isolated eigenvalue and no other piece of the spectrum. Then it follows from (3.6) and (3.8) that

$$\eta-\frac{\epsilon^2}{E^L_{i+1}(\lambda)-\eta}\leqslant E_i(\lambda)\leqslant\eta+\frac{\epsilon^2}{\eta-E^U_{i-1}(\lambda)}. \tag{3.9}$$

This formula is symmetric with respect to upper and lower bound, as we might expect. It should be noted that (3.9) gives $E_i(\lambda)$ within the error bound of the order ϵ^2: this is very small if ϵ is small, i.e., if ϕ is a good approximate eigenfunction. Indeed, (3.9) implies

$$|E_i(\lambda)-\eta|\leqslant\frac{\epsilon^2}{g}, \tag{3.10}$$

where $g=\min\{\eta-E_{i-1}^U(\lambda),E_{i+1}^L(\lambda)-\eta\}$. Therefore, the error in η depends on the residual norm squared, i.e., on ϵ^2, and on the gap $g>0$ for the eigenvalue is isolated.[1] If (3.9) is applied to the operator $H_0+\lambda V-E_i^\lambda$, where E_i^λ is a variational estimate for the ith eigenvalue of $H_0+\lambda V$, there results[1] the following.

Theorem 1: *If ϕ is normalized trial function for the self-adjoint operator $H=H_0+\lambda V$, where H_0 and V are self-adjoint and E_i^0 is an isolated, nondegenerate stable eigenvalue of H_0, and E_i^λ is a continuous function such that $(\phi,[H_0+\lambda V-E_i^\lambda]\phi)\to 0$ as $\lambda\to 0$, and*

$$\|[H_0+\lambda V-E_i^\lambda]\phi\|=o((\phi,[H_0+\lambda V-E_i^\lambda]\phi)^{1/2}), \tag{3.11}$$

then the eigenvalue of $H_0+\lambda V$ which converges to E_i^0 satisfies

$$E_i(\lambda)=(\phi,[H_0+\lambda V]\phi)+O(\|[H_0+\lambda V-E_i^\lambda]\phi\|^2). \tag{3.12}$$

Proof: To keep the notation simple, let us refer to $E_{i-1}^U(\lambda)$ and $E_{i+1}^L(\lambda)$ in (3.9) by α and β, respectively. Then, from the previous discussion, we have, for $\eta=(\phi,[H_0+\lambda V-E_i^\lambda]\phi)$, that $\alpha<\eta<\beta$, and $\epsilon^2<(\beta-\eta)(\eta-\alpha)$. Further, by applying the Kato–Temple inequality (3.9) to the Hamiltonian $H_0+\lambda V-E_i^\lambda$, we obtain, for normalized ϕ,

$$\eta-\frac{\epsilon^2}{\beta-\eta}\leqslant E_i(\lambda)-E_i^\lambda\leqslant\eta+\frac{\epsilon^2}{\eta-\alpha},$$

where $\epsilon^2=\|[H_0+\lambda V-E_i^\lambda]\phi\|^2-(\phi,[H_0+\lambda V-E_i^\lambda]\phi)^2$. If we divide by η, we obtain after some simplifications

$$-\frac{\left(\frac{\|[H_0+\lambda V-E_i^\lambda]\phi\|}{\eta^{1/2}}\right)^2-\eta}{\beta-\eta}\leqslant\frac{E_i(\lambda)-E_i^\lambda}{\eta}-1\leqslant\frac{\left(\frac{\|[H_0+\lambda V-E_i^\lambda]\phi\|}{\eta^{1/2}}\right)^2-\eta}{\eta-\alpha}. \tag{3.13}$$

However, since ϕ is assumed to be normalized,

$$\frac{E_i(\lambda)-E_i^\lambda}{\eta}-1=\frac{E_i(\lambda)-([H_0+\lambda V]\phi,\phi)}{\eta}=\frac{E_i(\lambda)-([H_0+\lambda V]\phi,\phi)}{\|[H_0+\lambda V-E_i^\lambda]\phi\|^2}\left(\frac{\|[H_0+\lambda V-E_i^\lambda]\phi\|}{\eta^{1/2}}\right)^2.$$

From (3.11), we have for λ sufficiently small,

$$\frac{\|[H_0+\lambda V-E_i^\lambda]\phi\|}{\eta^{1/2}}\leqslant 1.$$

Thus after dividing (3.13) by $(\|[H_0+\lambda V-E_i^\lambda]\phi\|/\eta^{1/2})^2$, we have

$$\left|\frac{E_i(\lambda)-([H_0+\lambda V]\phi,\phi)}{\|[H_0+\lambda V-E_i^\lambda]\phi\|^2}\right|\leqslant\left\{1-\frac{\eta}{\left(\frac{\|[H_0+\lambda V-E_i^\lambda]\phi\|}{\eta^{1/2}}\right)^2}\right\}\max\left\{\frac{1}{\beta-\eta},\frac{1}{\eta-\alpha}\right\}$$

$$\leqslant\max\left\{\frac{1}{\beta-\eta},\frac{1}{\eta-\alpha}\right\}\leqslant C\ \ (\text{constant}),$$

which leads to

$$E_i(\lambda)=([H_0+\lambda V]\phi,\phi)+O(\|[H_0+\lambda V-E_i^{\lambda}]\phi\|^2),$$

as required. □

IV. TRIAL WAVE FUNCTION AND SOLUTION TO A DIFFERENTIAL EQUATION

In this section we shall introduce a suitable trial function in order to obtain eigenvalue perturbation corrections by means of Theorem 1. For singular Hamiltonians of type (1.2), the trial functions are characterized by wave functions with non-integer exponent. This indeed characterizes[27–34] almost all trial functions which have been used previously to study this type of singular Hamiltonian (1.1) and (1.2). Furthermore, the trial functions have to satisfy the physical initial conditions of the problem. In the classical Rayleigh–Schrödinger perturbation theory, the lowest-order trial function for a given eigenvalue is chosen to be the unperturbed eigenfunction, i.e., the exact solutions of the unperturbed Hamiltonian. This is no longer a good choice for the perturbation λV in (1.2) with $\alpha \geqslant 2\gamma$, for

$$\int_{\epsilon}^{\infty} x^{2\gamma-\alpha-1}e^{-x^2}\,dx \approx \epsilon^{-\alpha+2\gamma},$$

which approaches ∞ as ϵ goes to zero. Intuitively, it seems that if the unperturbed eigenfunction was modified slightly near the singular point, so that the expectation value of singular term V was no longer infinite, it would become a reasonable trial function to use to estimate the perturbed eigenvalue. This was the basic idea of the trial wave function used by Detwiler *et al.* to study the Hamiltonian (1.1) and it was employed later by Harrell.[1] Using the notation of Harrell, we start with the (un-normalized) trial wave function

$$\psi(x;\lambda)=W_{\alpha}(x;\lambda)\psi_i(x), \tag{4.1}$$

where $\psi_i(x)$ is given by (2.1) and $W_{\alpha}(x;\lambda)$ is to be determined. It should be noted that far away from the singularity, we expect $\psi(x;\lambda)\sim\psi_i(x)$ for large x, since (1.2) behaves as radial harmonic oscillator Hamiltonian for large x, which, in turn, implies $\lim_{x\to\infty} W_{\alpha}(x;\lambda)=1$. Further, for an arbitrary singular point x_0, not necessarily at the origin, $\psi(x_0;\lambda)=0$, an idea that was borrowed from hard-core problems in quantum mechanics:[20] this forces $W_{\alpha}(x_0;\lambda)=0$; therefore, we must also have $\lim_{x\to 0} W_{\alpha}(x;\lambda)=0$. Using the trial function (4.1), the differential operator (1.2) leads to

$$[H_0+\lambda V-E_i]\psi(x;\lambda)=\left[-\frac{d^2W_{\alpha}(x;\lambda)}{dx^2}-2\frac{dW_{\alpha}(x;\lambda)}{dx}\frac{d}{dx}+\lambda VW_{\alpha}(x;\lambda)\right]\psi_i(x), \tag{4.2}$$

where $E_i\equiv E_i^{\lambda}$ is the variational estimate of H. It is clear from (2.1) that $[d\psi_i(x)/dx]\approx[(\gamma-1/2)/x]\psi_i(x)$ near the origin. Therefore, we may choose $W_{\alpha}(x;\lambda)$ in (4.2) such that

$$\frac{d^2W_{\alpha}(x;\lambda)}{dx^2}+\frac{2(\gamma-\frac{1}{2})}{x}\frac{dW_{\alpha}(x;\lambda)}{dx}-\lambda VW_{\alpha}(x;\lambda)=0 \tag{4.3}$$

and must satisfy the initial conditions

$$\lim_{x\to 0} W_{\alpha}(x;\lambda)=0 \quad \text{and} \quad \lim_{x\to\infty} W_{\alpha}(x;\lambda)=1. \tag{4.4}$$

Equation (4.3) allows us to write Eq. (4.2) as

$$[H_0+\lambda V-E_i]\psi(x;\lambda)=2\frac{dW_{\alpha}(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_i(x). \tag{4.5}$$

To solve (4.3) explicitly, we notice first that the parameter λ can be removed from the equation by a change of variable $z=\lambda^{-\nu}x$ where ν is to be determined shortly. A straightforward calculation shows that Eq. (4.3) becomes

$$\frac{d^2W_\alpha(z)}{dz^2}+\frac{2(\gamma-\frac{1}{2})}{z}\frac{dW_\alpha(z)}{dz}-\frac{\lambda^{(2-\alpha)\nu+1}}{z^\alpha}W_\alpha(z)=0.$$

So, with $\nu=1/(\alpha-2)$, independent of γ, we have

$$\frac{d^2W_\alpha(z)}{dz^2}+\frac{2(\gamma-\frac{1}{2})}{z}\frac{dW_\alpha(z)}{dz}-\frac{W_\alpha(z)}{z^\alpha}=0. \tag{4.6}$$

With another change of variable $Y(z)=z^{\gamma-1}W_\alpha(z)$, (4.6) leads to

$$\frac{d^2Y}{dz^2}+\frac{1}{z}\frac{dY}{dz}-\left[\frac{(\gamma-1)^2}{z^2}+\frac{1}{z^\alpha}\right]Y=0. \tag{4.7}$$

Finally with the further change of variable $\xi=2\nu z^{-(1/2\nu)}$, we have from (4.7),

$$\frac{d^2Y}{d\xi^2}+\frac{1}{\xi}\frac{dY}{d\xi}-\left[1+\frac{[2\nu(\gamma-1)]^2}{\xi^2}\right]Y=0, \tag{4.8}$$

which is the equation of a modified Bessel function[35] of order $2\nu(\gamma-1)$. The solution of Eq. (4.8) is

$$W_\alpha(z)=c_1z^{1-\gamma}I_{2\nu(\gamma-1)}(2\nu z^{-(1/2\nu)})+c_2z^{1-\gamma}K_{2\nu(\gamma-1)}(2\nu z^{-(1/2\nu)}),$$

where I and K denote the modified Bessel functions of the first and second kind, respectively.[35] The initial conditions $\lim_{z\to0}W_\alpha(z)=0$, and $\lim_{z\to\infty}W_\alpha(z)=1$ yields $c_1=0$ and $c_2=[2\nu^{2\nu(\gamma-1)}/\Gamma(2\nu(\gamma-1))]$ by means of

$$K_\nu(z)\approx\frac{1}{2}\Gamma(\nu)\frac{z^\nu}{2} \tag{4.9}$$

as z approach 0. Therefore, we have

$$\begin{aligned}W_\alpha(z)&=\frac{2\nu^{2\nu(\gamma-1)}}{\Gamma(2\nu(\gamma-1))}z^{1-\gamma}K_{2\nu(\gamma-1)}(2\nu z^{-(1/2\nu)}),\quad\text{or more explicitly}\\ W_\alpha(x;\lambda)&=\frac{2\nu^{2\nu(\gamma-1)}}{\Gamma(2\nu(\gamma-1))}\lambda^{\nu(\gamma-1)}x^{1-\gamma}K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)}).\end{aligned} \tag{4.10}$$

Finally, we have for the (un-normalized) wave function (4.1) that

$$\psi(x;\lambda)=\frac{2\nu^{2\nu(\gamma-1)}}{\Gamma(2\nu(\gamma-1))}\lambda^{\nu(\gamma-1)}x^{1-\gamma}K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\psi_i(x). \tag{4.11}$$

It is quite clear by means of Eq. (4.9) that $\lim_{\lambda\to0}\psi(x;\lambda)=\psi_i(x)$ as expected. Consequently, the normalization constant N_λ of $\psi(x;\lambda)$ must satisfy $\lim_{\lambda\to0}N_\lambda=1$. Some properties of the function $K_\nu(z)$ are in order.[35] The physical importance[35] of the function $K_\nu(z)$ lies in the fact that it tends exponentially to zero as $z\to\infty$. The function $K_\nu(z)$ is defined, for unrestricted values of ν, by the equation

$$K_\nu(z)=\frac{\pi}{2\sin(\nu\pi)}[I_{-\nu}(z)-I_\nu(z)], \tag{4.12}$$

where

$$I_\nu(z)=\left(\frac{z}{2}\right)^\nu\sum_{k=0}^{\infty}\frac{(\frac{1}{2}z^2)^k}{k!\Gamma(\nu+k+1)}. \tag{4.13}$$

The apparent discrepancy with (4.12) is resolved by the identity $\Gamma(\nu)\Gamma(1-\nu)=\pi/\sin(\nu\pi)$. For integer values or zero of ν in (4.12), it should be understood that $K_n(z)=\lim_{\nu\to n}K_\nu(z)$, where in this case

$$K_n(z)=\frac{1}{2}\left(\frac{z}{2}\right)^{-n}n^{n-1}\sum_{k=0}^{\infty}\frac{(n-k-1)!}{k!}\left(-\frac{z^2}{4}\right)^k+(-1)^{n+1}\log\left(\frac{z}{2}\right)I_n(z)$$
$$+(-)^n\frac{1}{2}\left(\frac{z}{2}\right)^n\sum_{k=0}^{\infty}\{\psi(k+1)+\psi(n+k+1)\}\frac{\left(\frac{z^2}{4}\right)^k}{k!(n+k)!}, \tag{4.14}$$

while

$$K_0(z)=-\left(c+\log\left(\frac{z}{2}\right)\right)I_0(z)+\sum_{r=1}^{\infty}\frac{\left(\frac{z}{2}\right)^{(2r)}}{(r!)^2}\left\{1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{r}\right\}. \tag{4.15}$$

Here c is Euler's constant $c=0.577\,215\,664\,9$, etc. The following identity will also be used:

$$z\frac{dK_\nu(z)}{dz}=-\nu K_\nu(z)-zK_{\nu+1}(z). \tag{4.16}$$

V. LOWEST-ORDER ASYMPTOTIC PERTURBATION CORRECTIONS FOR $\alpha\geqslant 2\gamma$

In this section, we apply Theorem 1 and the trial function developed in Sec. IV in order to obtain the eigenvalue perturbation expansions for the Hamiltonian (1.2). We consider first the case of $\alpha\geqslant 2\gamma$ which leads to the divergence of the first-order correction of the regular Rayleigh–Schrödinger series. In a purely theoretical approach, Greenlee[2] has shown that the asymptotic perturbation expansion should take the form

$$E_0(\lambda)=E_0+E_1\lambda^{2\nu(\gamma-1)} \tag{5.1}$$

valid for $2\gamma<\alpha$ and $2\nu(\gamma-1)<1$. We note, for consistency, that we have reproduced the expression of Greenlee using our own notation. Equation (5.1) is in complete agreement with our prediction $\alpha>2\gamma$ or $2\nu(\gamma-1)<1$ for $\nu=1/(\alpha-2)$ obtained by means of Theorem 1, as we shall show in this section. In order to apply Theorem 1, we need first the normalization constant N_λ of the trial wave function $\psi(x;\lambda)$, namely Eq. (4.11). This can be found by means of the condition $\|\psi(x;\lambda)\|^2=1$ which leads to expression

$$N_\lambda^{-2}=\frac{4\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)}}{[\Gamma(2\nu(\gamma-1)]^2}\int_0^\infty x^{2(1-\gamma)}[K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})]^2\psi_i(x)^2\,dx. \tag{5.2}$$

Lemma 1: For the ground-state, i.e., $i=0$, we have

$$N_\lambda^2 = 1 + \frac{2\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)} + O(\lambda^{4\nu(\gamma-1)}), \tag{5.3}$$

where $\nu = 1/(\alpha-2)$ *and* $\alpha > 2\gamma$.

Proof: We note, by using (4.9) in (5.2), that $N_\lambda^2 \approx 1$. To find the order of the error term, however, we used the identity (4.12) which leads to $K_\nu(z) = [\Gamma(\nu)/2](z/2)^{-\nu} - [\Gamma(1-\nu)/2\nu] \times (z/2)^{\nu} + \cdots$. Therefore

$$\begin{aligned}[K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})]^2 = {} & \frac{[\Gamma(2\nu(\gamma-1))]^2}{4}(\nu\sqrt{\lambda}x^{-(1/2\nu)})^{-4\nu(\gamma-1)} \\ & - \frac{\Gamma(2\nu(\gamma-1)\Gamma(1-2\nu(\gamma-1))}{4\nu(\gamma-1)} \\ & + \frac{[\Gamma(1-2\nu(\gamma-1))]^2}{4\nu^2}(\nu\sqrt{\lambda}x^{-(1/2\nu)})^{4\nu(\gamma-1)} + \cdots . \end{aligned} \tag{5.4}$$

For the ground state, we have from (2.1) that $\psi_0(x) = \sqrt{2/\Gamma(\gamma)}x^{\gamma-1/2}e^{-x^2/2}$. Thus on substituting (5.4) into (5.2) we have, after some calculations,

$$N_\lambda^2 = \left\{ 1 - \frac{2\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)} + O(\lambda^{4\nu(\gamma-1)}) \right\}^{-1}$$

and the proof of the lemma follows by a very similar argument to that for Taylor's expansion of $1/(1-\delta)$.

The reason of quoting the expansion (5.3) only up to order $\lambda^{4\nu(\gamma-1)}$ was guided by the error term in (3.12), as the following lemma indicates.

Lemma 2: For the ground-state energy of the Hamiltonian (1.2), where $\alpha > 2\gamma$ *[or* $2\nu(\gamma-1) < 1$*], we have*

$$\begin{aligned} E_0(\lambda) = {} & 2\gamma + \frac{16}{\Gamma(\gamma)}\frac{\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1/2}}{[\Gamma(2\nu(\gamma-1)]^2}\int_0^\infty x^{1-(1/2\nu)}e^{-x^2}K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)}) \\ & \times K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})dx + O(\lambda^{4\nu(\gamma-1)}). \end{aligned} \tag{5.5}$$

Proof: Equation (4.10) with (4.16) leads to

$$\frac{dW_\alpha(x;\lambda)}{dx} = \frac{2\nu^{2\nu(\gamma-1)}}{\Gamma(2\nu(\gamma-1))}\lambda^{\nu(\gamma-1)+1/2}x^{-(1/2\nu)-\gamma}K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)}). \tag{5.6}$$

Furthermore, using $\psi_0(x) = \sqrt{2/\Gamma(\gamma)}x^{\gamma-1/2}e^{-x^2/2}$, we find

$$\begin{aligned} \frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x} - \frac{d}{dx}\right]\psi_0(x) = {} & \frac{2\nu^{2\nu(\gamma-1)}\lambda^{\nu(\gamma-1)+1/2}}{\Gamma(2\nu(\gamma-1))}\sqrt{\frac{2}{\Gamma(\gamma)}}x^{1/2-(1/2\nu)}e^{-x^2/2} \\ & \times K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)}), \end{aligned} \tag{5.7}$$

which leads to

$$2\left(W_\alpha(x;\lambda)\psi_0(x), \frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_0(x)\right)$$
$$=\frac{16}{\Gamma(\gamma)}\frac{\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1/2}}{[\Gamma(2\nu(\gamma-1)]^2}\times\int_0^\infty x^{1-(1/2\nu)}e^{-x^2}K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})$$
$$\times K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})dx. \tag{5.8}$$

In order to use theorem 1, however, the trial wave function must be normalized. This is equivalent to multiplying (5.8) by the normalization constant N_λ^2, as given by (5.3). Now, since N_λ^2 is of order $\lambda^{2\nu(\gamma-1)}$, out of the second term in (5.3) the multiplication allows us to have (5.8) as quoted, plus an error term of order $\lambda^{4\nu(\gamma-1)}$ as result of using (4.9). What remains is to show that the expression $\|[H_0+\lambda V-E(\lambda)]\phi_\lambda\|$ in (3.12) is also of order $\lambda^{2\nu(\gamma-1)}$. This follows from (5.7) as follows:

$$\|[H_0+\lambda V-E_0]\psi_0\|=2\left\|\frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_0(x)\right\|$$
$$=2\left[\frac{8\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1}}{\Gamma(\gamma)[\Gamma(2\nu(\gamma-1)]^2}\int_0^\infty x^{1-(1/\nu)}e^{-x^2}\right.$$
$$\left.\times[K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})]^2\,dx\right]^{1/2}$$
$$=O(\lambda^{2\nu(\gamma-1)}),$$

where we have used

$$K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\approx\frac{\Gamma(1-2\nu(\gamma-1))}{2}(\nu\sqrt{\lambda}x^{-(1/2\nu)})^{2\nu(\gamma-1)-1}.$$

The proof of the lemma then follows by use of Theorem 1, Eq. (3.12), and the variational estimate of E_0^λ by means of (2.2). □

Because of the error term in (5.5), it is not necessary to compute the integral in (5.5) exactly but it is sufficient to estimate the integral using the asymptotic series expansions of the modified Bessel functions $K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})$ and $K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})$ by means of (4.12), up to the order cited. Since the order of the error term in (5.5) is $\lambda^{4\nu(\gamma-1)}$ while the integral is of order $\lambda^{2\nu(\gamma-1)}$, we may consider, for fixed α, two regions $0<2\nu(\gamma-1)\leqslant\frac{1}{2}$ and $\frac{1}{2}<2\nu(\gamma-1)<1$, or equivalently $0<4\nu(\gamma-1)\leqslant1$ and $1<4\nu(\gamma-1)<2$. For the first region, we have for the ground-state energy of the Hamiltonian (1.2)

$$E_0(\lambda)=2\gamma+\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+O(\lambda^{4\nu(\gamma-1)}) \tag{5.9}$$

which follows from (5.5) using the asymptotic expansions of $K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})$ and $K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})$ by means of (4.9). In the case $\gamma=3/2$ (i.e., $A=0$ or $\alpha\geqslant4$), Eq. (5.9) yields

$$E_0(\lambda)=3+\frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^\nu+O(\lambda^{2\nu}), \tag{5.10}$$

where $\nu=1/(\alpha-2)$, as shown earlier by Harrell for the spiked harmonic oscillator Hamiltonian (1.1). Important conclusions follow from (5.9). For $\alpha=2(2\gamma-1)$ or $2\nu(\gamma-1)=\frac{1}{2}$, we have

$$E_0(\lambda)=2\gamma+\frac{2}{\Gamma(\gamma)}\sqrt{\lambda}+O(\lambda). \tag{5.11}$$

This provides a single ground-state approximation formula for a wide class of Hamiltonians $H=-(d^2/dx^2)+x^2+(A/x^2)+(\lambda/x^\alpha)$, where α and $\gamma=1+\frac{1}{2}\sqrt{1+4A}$ are related by $\alpha=2(2\gamma-1)$. For example, for $A=0$, i.e., $\gamma=3/2$, which yields $\alpha=4$, we have

$$E_0(\lambda)=3+\frac{4}{\sqrt{\pi}}\sqrt{\lambda}+O(\lambda),$$

as noted by Harrell. If $\alpha=6$, which implies $\gamma=2$ or $A=0.75$, we have

$$E_0(\lambda)=4+2\sqrt{\lambda}+O(\lambda).$$

For the second region $1<4\nu(\gamma-1)<2$, or $2\gamma<\alpha<2(2\gamma-1)$, by using (4.12), we can easily show that

$$\begin{aligned}&K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\\&\quad=\frac{\Gamma(2\nu(\gamma-1))\Gamma(1-2\nu(\gamma-1))}{2\nu\sqrt{\lambda}}x^{(1/2\nu)}\\&\qquad-\frac{[\Gamma(2\nu(\gamma-1))]^2}{4(1-2\nu(\gamma-1))}\nu^{1-4\nu(\gamma-1)}\lambda^{1/2-2\nu(\gamma-1)}x^{-(1/2\nu)+2(\gamma-1)}+\cdots.\end{aligned}$$

Consequently, (5.5) yields, for $\frac{1}{2}<2\nu(\gamma-1)<1$,

$$\begin{aligned}E_0(\lambda)=2\gamma+&\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}-\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(1-2\nu(\gamma-1))\Gamma(\gamma)}\lambda\\&+O(\lambda^{4\nu(\gamma-1)}).\end{aligned} \tag{5.12}$$

Again the result of Harrell for the Hamiltonian (1.1) follows for the case of $\gamma=\frac{3}{2}$, i.e., $A=0$, where, in this case, $3<\alpha<4$ or $\frac{1}{2}<\nu<1$, and

$$E_0(\lambda)=3+\frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^{\nu}-\frac{4\nu\Gamma\left(\frac{3-\frac{1}{\nu}}{2}\right)}{(1-\nu)\sqrt{\pi}}\lambda+O(\lambda^{2\nu}). \tag{5.13}$$

For the rest of this section, we consider the case of $2\nu(\gamma-1)=1$. For this specific value Eqs. (4.10) and (5.6) read, for $z=\lambda^{-\nu}x$,

$$W_\alpha(z)=\frac{z^{1-\gamma}}{\gamma-1}K_1\left(\frac{z^{1-\gamma}}{\gamma-1}\right) \tag{5.14}$$

and

$$\frac{dW_\alpha(z)}{dz}=\frac{z^{1-2\gamma}}{\gamma-1}K_0\left(\frac{z^{1-\gamma}}{\gamma-1}\right), \tag{5.15}$$

respectively. Using the asymptotic expansions

$$K_0(z)=[-c+\log(2)-\log(z)]+O(z^2),\quad K_1(z)=\frac{1}{z}+O(z) \tag{5.16}$$

which follow by means of (4.15) and (4.14), respectively, we obtain the following.

Lemma 3: For the ground state energy of the Hamiltonian (1.2), where $\alpha=2\gamma$ *[or* $2\nu(\gamma-1)=1$*], we have*

$$E_0(\lambda)=2\gamma-\frac{1}{(\gamma-1)\Gamma(\gamma)}\lambda\log(\lambda)+\left[\frac{-c(1+\gamma)+2\log(2(\gamma-1))}{(\gamma-1)\Gamma(\gamma)}\right]\lambda+O(\lambda^2\log^2(\lambda)), \tag{5.17}$$

where $c=0.577\,215\,664\,9$, etc., *is Euler's constant.*

Proof: We should note first, in this case,

$$\|[H_0+\lambda V-E(\lambda)]\psi_0\|^2=O(\lambda^2\log^2(\gamma)),$$

which follows from

$$\|[H_0+\lambda V-E(\lambda)]\psi_0\|^2=\frac{2\lambda^2}{(\gamma-1)^2\Gamma(\gamma)}\int_0^\infty x^{3-2\gamma}e^{-x^2}K_0^2\left(\frac{\sqrt{\lambda}}{\gamma-1}x^{1-\gamma}\right)dx$$

by use of (5.7). Since we are only interested in finding the order in terms of the parameter λ, the problem reduces to a search among the smallest value of $\lambda^2\log^2(\lambda)$, $-\lambda^2\log(\lambda)$, and λ^2, for small values of the parameter λ. Therefore for sufficiently small λ we have $\|[H_0+\lambda V-E(\lambda)]\psi_0\|^2=O(\lambda^2\log^2(\lambda))$ as noted. What remains is to compute

$$2\left(W_\alpha(x;\lambda)\psi_0(x),\frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_0(x)\right)$$
$$=\frac{4\lambda^{3/2}}{(\gamma-1)^2\Gamma(\gamma)}\times\int_0^\infty x^{2-\gamma}e^{-x^2}K_0\left(\frac{\sqrt{\lambda}}{\gamma-1}x^{1-\gamma}\right)K_1\left(\frac{\sqrt{\lambda}}{\gamma-1}x^{1-\gamma}\right)dx$$

by using the asymptotic expansions (5.16) up to the order $\lambda^2\log^2(\lambda)$. The lemma then follows after some straightforward calculations. It is important to note that the normalization constant N_λ, as given by (5.2), yields in this case

$$N_\lambda^{-2}=1+\left\{2\nu^2(-1+2c+2\log(\nu))+\frac{1}{2}\nu c\right\}\frac{\lambda}{\Gamma(\gamma)}+\frac{2\nu^2}{\Gamma(\gamma)}\lambda\log\lambda+\cdots$$

and will contribute to the error term in a similar manner to that mentioned in lemma 2. □

The results of Harrell, the case $\alpha=3$, follows immediately from (5.17) for the case of $A=0$ (or $\gamma=3/2$), i.e., $\nu=1$, namely,

$$E_0(\lambda)=3-\frac{4}{\sqrt{\pi}}\lambda\log(\lambda)-\frac{10c}{\sqrt{\pi}}\lambda+O(\lambda^2\log^2(\lambda)). \tag{5.18}$$

It is clear that these expressions are valid for λ much smaller than unity.

VI. LOWEST-ORDER ASYMPTOTIC PERTURBATION CORRECTIONS FOR $2\gamma>\alpha\geqslant\gamma+1$

In this section, we discuss the case of $2\gamma>\alpha\geqslant\gamma+1$ or equivalently the case of $1<2\nu(\gamma-1)\leqslant 2$. It is clear by now that, for $1<2\nu(\gamma-1)\leqslant 2$, the first-order Rayleigh–Schrödinger corrections exist but the second-order corrections diverge. Thus, the improved perturbation procedure

gives an explicit term between the first and the second order. Let us first consider the case of $1<2\nu(\gamma-1)<2$, here we rely on the asymptotic expansion of the modified Bessel function K as given by (4.12). We note from (4.5) and (5.6) that

$$\|[H_0+\lambda V-E(\lambda)]\psi_0\|^2=\frac{32\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1}}{\Gamma(\gamma)[\Gamma(2\nu(\gamma-1))]^2}\int_0^\infty x^{1-(1/\nu)}e^{-x^2}K^2_{2\nu(\gamma-1)-1}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\mathrm{d}x$$

as a consequence of the known identity $K_\nu(z)=K_{-\nu}(z)$. Using (4.9) we have

$$\|[H_0+\lambda V-E(\lambda)]\psi_0\|^2=O(\lambda^2) \quad (1<2\nu(\gamma-1)<2), \tag{6.1}$$

which leads to the following lemma.

Lemma 4: For the ground-state energy of the Hamiltonian (1.2) where $\alpha>\gamma+1$ [i.e., $1<2\nu(\gamma-1)<2$], we have

$$E_0(\lambda)=2\gamma+\frac{16}{\Gamma(\gamma)}\frac{\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1/2}}{[\Gamma(2\nu(\gamma-1)]^2}\int_0^\infty x^{1-(1/2\nu)}e^{-x^2}$$
$$\times K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})K_{2\nu(\gamma-1)-1}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\mathrm{d}x+O(\lambda^2). \tag{6.2}$$

The proof of this lemma is similar to that of lemma 3, therefore we omit it. The computation of the integral in (6.2) up to the order of λ^2 yields the perturbation expansion

$$E_0(\lambda)=2\gamma+\frac{2\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\nu\Gamma(\gamma)\Gamma(2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(2\nu(\gamma-1)-1)\Gamma(\gamma)}\lambda+O(\lambda^2), \tag{6.3}$$

as the result of

$$K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})=\frac{\Gamma(2\nu(\gamma-1))\Gamma(1-2\nu(\gamma-1))}{2}\Bigg\{(\nu\sqrt{\lambda}x^{-(1/2\nu)})^{-2\nu(\gamma-1)}$$
$$\times\left[\frac{1}{\Gamma(1-2\nu(\gamma-1))}+\frac{(\nu\sqrt{\lambda}x^{-(1/2\nu)})^2}{\Gamma(2-2\nu(\gamma-1)}\right]-(\nu\sqrt{\lambda}x^{(1/2\nu)})^{2\nu(\gamma-1)}$$
$$\times\left[\frac{1}{\Gamma(1+2\nu(\gamma-1))}+\frac{(\nu\sqrt{\lambda}x^{-(1/2\nu)})^2}{\Gamma(2+2\nu(\gamma-1)}\right]\Bigg\}+\cdots.$$

The result of Harrell[1] follows immediately from (6.3) in the special case $A=0$, namely,

$$E_0(\lambda)=3+\frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^\nu+\frac{2\Gamma\left(\frac{3-\alpha}{2}\right)}{\sqrt{\pi}}\lambda+O(\lambda^{2\nu}), \tag{6.4}$$

where $\nu=1/(\alpha-2)$ and $5/2<\alpha<3$.

For the case $2\nu(\gamma-1)=2$, the norm $\|[H_0+\lambda V-E(\lambda)]\psi_0\|$ can be computed easily by means of Eq. (4.5), which yields

$$\|[H_0+\lambda V-E_0]\psi_0\|^2=2\left\|\frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_0(x)\right\|^2$$
$$=\frac{16\lambda^3}{(\gamma-1)^2\Gamma(\gamma)}\int_0^\infty x^{2-\gamma}e^{-x^2}\left[K_1\left(\frac{2\sqrt{\lambda}}{\gamma-1}x^{-(1/2\nu)}\right)\right]^2 dx=O(\lambda^2),$$

as a consequence of

$$K_1(z)=\frac{1}{z}+\left(\frac{1}{4}(-1+2c)+\frac{1}{2}(-\log(2)+\log(z))\right)z+O(z^2).$$

Furthermore, since the trial wave function takes the form

$$\psi(x;\lambda)=2\nu^2\lambda x^{-(1/\nu)}K_2(2\nu\sqrt{\lambda}x^{-(1/2\nu)})\psi_0(x),$$

we may compute the normalization constant Eq. (5.2) as

$$N_\lambda^2=1+\frac{\nu\Gamma\left(\frac{1}{2\nu}\right)}{\Gamma(\gamma)}\lambda+\frac{\nu^4}{\Gamma(\gamma)}\lambda^2\log(\lambda)+O(\lambda^2)$$

in a similar fashion to the proof of lemma 1. Harrell, in his investigation, claims that the ground-state eigenvalue perturbation expansion for the spiked harmonic oscillator Hamiltonian (1.1), $\alpha=5/2$, is given by

$$E_0(\lambda)=3+\frac{2\Gamma(\frac{1}{4})}{\sqrt{\pi}}\lambda+\frac{16}{\sqrt{\pi}}\lambda^2\log(\lambda)+O(\lambda^2). \tag{6.5}$$

The following result does not confirm his claim, but shows that it is slightly different even by means of Harrell's own methodology. As our calculation will show, the ground-state perturbation expansion in the case of $\alpha=5/2$ is actually given by

$$E_0(\lambda)=3+\frac{2\Gamma(\frac{1}{4})}{\sqrt{\pi}}\lambda+\frac{32}{\sqrt{\pi}}\lambda^2\log(\lambda)+O(\lambda^2), \tag{6.6}$$

with a multiple of 2 in the log term in contrast with (6.5). In order to verify (6.6), we adopt two different approaches, first we use Harrell's method then we apply our generalization. We have for $\alpha=5/2$, the asymptotic perturbation expansion according to Harrell reads

$$E_0(\lambda)=3+2\left(W_{5/2}\psi_0,\frac{dW_{5/2}}{dx}\left(\frac{1}{x}-\frac{d}{dx}\right)\psi_0\right)+O(\lambda^2),$$

where $\psi_0(x)=(2/\pi^{1/4})xe^{-x^2/2}$. For $W_{5/2}$, Harrell used the asymptotic approximation of the modified Bessel function

$$K_2(z)=\frac{2}{z^2}-\frac{1}{2}+\left(\frac{1}{16}\left(\frac{3}{2}-2c\right)+\frac{1}{8}(\log(2)-\log(z))\right)z^2+O(z^3)$$

to show that

$$W_{5/2}(z)=1-\frac{4}{\sqrt{z}}+\frac{4\log(z)}{z}-4(4(c+\log(2))-3)z+\cdots \quad \text{for large } z.$$

If we differentiate $W_{5/2}(z)$ with respect to x, keeping in mind $z=\lambda^{-2}x$, we have, after some calculations,

$$2\left(W_{5/2}\psi_0,\frac{dW_{5/2}}{dx}\left(\frac{1}{x}-\frac{d}{dx}\right)\psi_0\right)=\frac{16\lambda}{\sqrt{\pi}}\int_0^\infty x^{3/2}e^{-x^2}\,dx+\frac{64\lambda^2\log\lambda}{\sqrt{\pi}}\int_0^\infty xe^{-x^2}\,dx+\cdots,$$

which yields (6.6), since $\int_0^\infty xe^{-x^2}\,dx=\frac{1}{2}$ and $\int_0^\infty x^{3/2}e^{-x^2}\,dx=\frac{1}{8}\Gamma(\frac{1}{4})$. Numerically, however, Eq. (6.5) is more appealing than (6.6) for a wider range of the parameter λ smaller than unity since (6.6) reduces the applicable range of λ by almost one-half.

Lemma 5: For the ground-state energy of the Hamiltonian (1.2), where $2\nu(\gamma-1)=2$, we have

$$E_0(\lambda)=2\gamma+\frac{\Gamma\left(\frac{1}{2\nu}\right)}{\Gamma(\gamma)}\lambda+\frac{2\nu^3}{\Gamma(\gamma)}\lambda^2\log(\lambda)+O(\lambda^2). \tag{6.7}$$

Proof: For $2\nu(\gamma-1)=2$, we have, using Eq. (6.2), that

$$E_0(\lambda)=2\gamma+\frac{16\nu^4\lambda^{5/2}}{\Gamma(\gamma)}\int_0^\infty x^{1-(1/2\nu)}e^{-x^2}K_2(2\nu\sqrt{\lambda}x^{-(1/2\nu)})K_1(2\nu\sqrt{\lambda}x^{-(1/2\nu)})dx+O(\lambda^2).$$

By means of the asymptotic expansions

$$K_1(z)=\frac{1}{z}+\left(\frac{1}{4}(-1+2c)+\frac{1}{2}\log\left(\frac{1}{2}z\right)\right)z+O(z^2)$$

and

$$K_2(z)=\frac{2}{z^2}-\frac{1}{2}+\left(\frac{1}{16}\left(\frac{3}{2}-2c\right)-\frac{1}{8}\log\left(\frac{1}{2}z\right)\right)z^2+O(z^4),$$

where $z=2\nu\sqrt{\lambda}x^{-(1/2\nu)}$, we have, after some calculations up to order λ^2, that

$$E_0(\lambda)=2\gamma+\frac{4\nu\lambda}{\Gamma(\gamma)}\int_0^\infty x^{1+(1/\nu)}e^{-x^2}\,dx+\frac{4\nu^3}{\Gamma(\gamma)}\lambda^2\log(\lambda)\int_0^\infty xe^{x^2}\,dx+O(\lambda^2).$$

This leads to (6.7), since $\int_0^\infty x^{1+(1/\nu)}e^{-x^2}\,dx=\frac{1}{2}\Gamma(1+(1/2\nu))$.

VII. FURTHER CASES

The expansions developed above can be extended to the case of $2\nu(\gamma-1)>2$ and the region of $\alpha<\frac{5}{2}$ which was not studied by Harrell.[1] For example, in the case of $2<2\nu(\gamma-1)<3$, the second order of the perturbation correction exists but the third order diverges. By using the modified perturbation theory we find

$$E_0(\lambda)=2\gamma+\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(2\nu(\gamma-1)-1)\Gamma(\gamma)}\lambda$$
$$-\frac{2(3-4\nu(\gamma-1))\nu^3\Gamma\left(\gamma-\frac{1}{\nu}\right)}{(2-2\nu(\gamma-1))(1-2\nu(\gamma-1))^2\Gamma(\gamma)}\lambda^2+O(\lambda^3). \tag{7.1}$$

Again in the case of $\gamma=3/2$, Harrell's formula should read, for $7/3<\alpha<5/2$,

$$E_0(\lambda)=3+\frac{4\nu^{2\nu}\Gamma(1-\nu)}{\sqrt{\pi}\Gamma(1+\nu)}\lambda^{\nu}+\frac{4\nu\Gamma\left(\frac{3}{2}-\frac{1}{2\nu}\right)}{(\nu-1)\sqrt{\pi}}\lambda-\frac{4(3-2\nu)\nu^3\Gamma\left(\frac{3}{2}-\frac{1}{\nu}\right)}{(2-\nu)(1-\nu)^2\sqrt{\pi}}\lambda^2+O(\lambda^3), \tag{7.2}$$

where $\nu=1/(\alpha-2)$. Furthermore, for $3<2\nu(\gamma-1)<4$, we have

$$E_0(\lambda)=2\gamma+\frac{4(\gamma-1)\nu^{4\nu(\gamma-1)}\Gamma(1-2\nu(\gamma-1))}{\Gamma(\gamma)\Gamma(1+2\nu(\gamma-1))}\lambda^{2\nu(\gamma-1)}+\frac{2\nu\Gamma\left(\gamma-\frac{1}{2\nu}\right)}{(2\nu(\gamma-1)-1)\Gamma(\gamma)}\lambda$$
$$-\frac{2(3-4\nu(\gamma-1))\nu^3\Gamma\left(\gamma-\frac{1}{\nu}\right)}{(2-2\nu(\gamma-1))(1-2\nu(\gamma-1))^2\Gamma(\gamma)}\lambda^2-\frac{2\nu^5\Gamma\left(\gamma-\frac{3}{2\nu}\right)}{\Gamma(\gamma)(1-2\nu(\gamma-1))^2(2-2\nu(\gamma-1))}\lambda^3$$
$$+O(\lambda^4). \tag{7.3}$$

Similar expressions can be obtained for $n<2\nu(\gamma-1)<n+1$, $n=4,5,...$, as well for $2\nu(\gamma-1)=n$. It is important, however, to note that there are an infinite number of cases as n increases to infinity for $\alpha>2$. For example, if we restrict the value of γ to 3/2, then in this case $2<\alpha<5/2$, and obtain an infinite number of perturbation expansions consisting of analytic parts of degree λ^n in addition to one correction term in each expansion as $2+[1/(1+n)]<\alpha<2+(1/n)$. Similarly, the cases $\alpha=2+[1/(1+n)]$, $n=3,4,...$, need special treatment, as we have mentioned above. It is interesting to note that the λ-term in (7.1) or in (7.3) is identical with the corresponding λ-term in the Rayleigh–Schrödinger series. This can be easily verified by a comparison of the coefficient of λ in (7.1) or in (7.3) with the coefficient of the λ-term in (2.3). However this is clearly not the case for the λ^2-term.

VIII. EXCITED STATES

The perturbation expansions developed so far were restricted to the ground-state energy, however, it is a matter of calculation to extend these results to the excited-state energies. First, it should be noted that the exact solution of the unperturbed part of the Hamiltonian (1.2) has very little to do with the order of the error terms in the perturbation expansions. Therefore it is expected that the order of the error terms remains the same for the excited states, i.e., $i=1,2,...$. Following the discussion in Sec. III, the asymptotic expansions for the eigenvalues for excited states are given by means of Theorem 1 as

$$E_i(\lambda)=2(2i+\gamma)+2\left(W_\alpha(x;\lambda)\psi_i(x),\frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_i(x)\right)$$
$$+O(\|[H_0+\lambda V-E_i^\lambda]W_\alpha(x;\lambda)\psi_i\|^2), \tag{8.1}$$

where $\psi_i(x)$, $i=0,1,2,...$ are given by (2.1) and the energy of the unperturbed Hamiltonian E_i^{λ} is given by (2.2). In order to compute (8.1) explicitly, we notice first that

$$
\begin{aligned}
&2\left(W_\alpha(x;\lambda)\psi_i(x), \frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_i(x)\right) \\
&\quad=\frac{16(\gamma)_i}{i!\Gamma(\gamma)}\,\frac{\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)+1/2}}{[\Gamma(2\nu(\gamma-1)]^2}\times\int_0^\infty x^{1-(1/2\nu)}e^{-x^2} \\
&\quad\times\left[\frac{2(\gamma+i)}{\gamma}\,{}_1F_1(-i;\gamma;x^2)\,{}_1F_1(-i;\gamma+1;x^2)-[{}_1F_1(-i;\gamma;x^2)]^2\right] \\
&\quad\times K_{2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)})K_{1-2\nu(\gamma-1)}(2\nu\sqrt{\lambda}x^{-(1/2\nu)}),dx, \qquad (8.2)
\end{aligned}
$$

where ${}_1F_1$ is the confluent hypergeometric function mentioned earlier Eq. (2.4). In producing (8.2) we have used the following identity:[35]

$$
\frac{d}{dz}\,{}_1F_1(a;b;z)={}_1F_1(a;b;z)-\frac{(b-a)}{b}\,{}_1F_1(a;b+1;z).
$$

For the case of $0<2\nu(\gamma-1)\leqslant\frac{1}{2}$ or $\alpha\geqslant 2(2\gamma-1)$, we find, by means of (4.9), that

$$
\begin{aligned}
&2\left(W_\alpha(x;\lambda)\psi_i(x), \frac{dW_\alpha(x;\lambda)}{dx}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{dx}\right]\psi_i(x)\right) \\
&\quad=\frac{4(\gamma)_i}{i!\Gamma(\gamma)}\,\frac{\Gamma(1-2\nu(\gamma-1))}{\nu\Gamma(2\nu(\gamma-1))}\,\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)} \\
&\quad\times\int_0^\infty xe^{-x^2}\left[\frac{2(\gamma+i)}{\gamma}\,{}_1F_1(-i;\gamma;x^2)\,{}_1F_1(-i;\gamma+1;x^2)-[{}_1F_1(-i;\gamma;x^2)]^2\right]dx.
\end{aligned} \qquad (8.3)
$$

This result required the investigation of some integrals of the type

$$
\int_0^\infty xe^{-x^2}\,{}_1F_1(-i;\gamma;x^2)\,{}_1F_1(-i;\gamma+1;x^2)dx \quad\text{and}\quad \int_0^\infty xe^{-x^2}[{}_1F_1(-i;\gamma;x^2)]^2\,dx.
$$

Lemma 6: For $d>0$ and $s>0$,

$$
\begin{aligned}
&\int_0^\infty t^{d-1}e^{-st}\,{}_1F_1(a;b;kt)\,{}_1F_1(a';b';k't)dt \\
&\qquad=s^{-d}\Gamma(d)\sum_{m=0}^{\infty}\frac{(a)_m(d)_m}{(b)_m}\,\frac{\left(\frac{k}{s}\right)^m}{m!}\,{}_2F_1\left(a',d+m;b';\frac{k'}{s}\right).
\end{aligned}
$$

Proof: From the series representation, Eq. (2.4), of the confluent hypergeometric series ${}_1F_1$, namely,

$$
{}_1F_1(a;b;kt)=\sum_{m=0}^{\infty}\frac{(a)_m}{(b)_m}\,\frac{(kt)^m}{m!}\quad\text{and}\quad {}_1F_1(a';b';k't)=\sum_{n=0}^{\infty}\frac{(a')_n}{(b')_n}\,\frac{(k't)^n}{n!},
$$

we have

$$\int_0^\infty t^{d-1}e^{-st}\,{}_1F_1(a;b;kt)\,{}_1F_1(a';b';k't)\,\mathrm{d}t$$

$$=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(a)_m(a')_n}{(b)_m(b')_n}\frac{k^m k'^n}{m!n!}\int_0^\infty e^{-st}t^{d+n+m-1}\,\mathrm{d}t$$

$$=s^{-d}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(a)_m(a')_n}{(b)_m(b')_n}\frac{k^m k'^n}{m!n!}\left(\frac{1}{s}\right)^n\left(\frac{1}{s}\right)^m(d+m)_n\Gamma(d+m)$$

$$=s^{-d}\sum_{m=0}^{\infty}\left[\sum_{n=0}^{\infty}\frac{(a')_n(d+m)_n}{(b')_n}\frac{\left(\frac{k'}{s}\right)^n}{n!}\right]\frac{(a)_m\left(\frac{k}{s}\right)^m}{(b)_m}\Gamma(d+m)$$

$$=s^{-d}\Gamma(d)\sum_{m=0}^{\infty}\,{}_2F_1\left(a',d+m;b';\frac{k'}{s}\right)\frac{(a)_m(d)_m}{(b)_m}\frac{\left(\frac{k}{s}\right)^m}{m!}$$

with $d>0$ and $s>0$, and where we have used the series representation of ${}_2F_1$ as given by Eq. (2.4) and the Pochhammer's identity $\Gamma(d+m+n)=(d+m)_n\Gamma(d+m)=(d+m)_n(d)_m\Gamma(d)$. □

As a consequence of this lemma, we have

$$\int_0^\infty xe^{-x^2}\,{}_1F_1(-i;\gamma;x^2)\,{}_1F_1(-i;\gamma+1;x^2)\mathrm{d}x=\frac{(\gamma)_i}{2(\gamma+1)_i}\,{}_3F_2(-i,1-\gamma,1;\gamma,1-\gamma-i;1) \tag{8.4}$$

and

$$\int_0^\infty xe^{-x^2}[{}_1F_1(-i;\gamma;x^2)]^2\,\mathrm{d}x=\frac{(\gamma-1)_i}{2(\gamma)_i}\,{}_3F_2(-i,-\gamma,1;\gamma,2-\gamma-i;1), \tag{8.5}$$

where the Chu–Vandermonda identity

$${}_2F_1(-n,a;c;1)=\frac{(c-a)_n}{(c)_n}$$

has been used. Therefore, from (8.3), we have

$$2\left(W_\alpha(x;\lambda)\psi_i(x),\frac{\mathrm{d}W_\alpha(x;\lambda)}{\mathrm{d}x}\left[\frac{(\gamma-\frac{1}{2})}{x}-\frac{d}{\mathrm{d}x}\right]\psi_i(x)\right)$$

$$=\frac{4(\gamma)_i}{i!\Gamma(\gamma)}\frac{\Gamma(1-2\nu(\gamma-1))}{\nu\Gamma(2\nu(\gamma-1))}\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)}$$

$$\times\left[{}_3F_2(-i,1-\gamma,1;\gamma,1-\gamma-i;1)-\frac{(\gamma-1)_i}{2(\gamma)_i}\,{}_3F_2(-i,-\gamma,1;\gamma,2-\gamma-i;1)\right]. \tag{8.6}$$

For $0<2\nu(\gamma-1)\leqslant\frac{1}{2}$ or $\alpha\geqslant 2(2\gamma-1)$, we have

$$E_i(\lambda)=2(2i+\gamma)+\frac{4(\gamma)_i}{i!\Gamma(\gamma)}\frac{\Gamma(1-2\nu(\gamma-1))}{\nu\Gamma(2\nu(\gamma-1))}\nu^{4\nu(\gamma-1)}\lambda^{2\nu(\gamma-1)}$$
$$\times\left[{}_3F_2(-i,1-\gamma,1;\gamma,1-\gamma-i;1)-\frac{(\gamma-1)_i}{2(\gamma)_i}{}_3F_2(-i,-\gamma,1;\gamma,2-\gamma-i;1)\right]$$
$$+O(\lambda^{4\nu(\gamma-1)}),\quad i=0,1,2,\ldots. \tag{8.7}$$

Similar expressions can be obtained for the other cases by means of lemma 6. An immediate extension of Harrell's expansions to excited states $i=1,2,\ldots$ for the Hamiltonian (1.1) can be obtained by setting $\gamma=\frac{3}{2}$ in (8.7).

IX. CONCLUSIONS

In this paper we have applied and extended Harrell's modified perturbation theory to treat a wider class of singular Hamiltonians given by (1.2). Our extensions allow us to recover Harrell's formulas for the spiked harmonic oscillator Hamiltonian (1.1) as special cases. Further, we were able to extend Harrell's results to the exited-state energies, again as special cases of our general treatment. We have also now corrected the perturbation expansion (6.5) for the case $\alpha=\frac{5}{2}$: this formula has been used without correction since the very early work of Harrell. Some interesting questions which remain to be answered are as follows. Is the modified wave function (4.11) sufficient to extend the perturbation expansions presented here to higher orders, or will further modifications need to be introduced? Why can the second-order corrections in (7.1), (7.2), and (7.3) not be recovered from the corresponding terms in the regular Rayleigh–Schrödinger series? Does this fact indicate that the trial wave function indeed requires additional modification? We hope that the present work will encourage further research into this interesting class of singular Hamiltonians.

ACKNOWLEDGMENTS

Partial financial support of this work under Grants Nos. GP3438 and GP249507 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged by two of us (respectively, R.L.H. and N.S.).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

An extension of Fourier analysis for the *n*-torus in the magnetic field and its application to spectral analysis of the magnetic Laplacian

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(Received 9 June 2003; accepted 24 July 2003)

We solved the Schrödinger equation for a particle in a uniform magnetic field in the n-dimensional torus. We obtained a complete set of solutions for a broad class of problems; the torus $T^n=\mathbf{R}^n/\Lambda$ is defined as a quotient of the Euclidean space $\mathbf{R}^n$ by an arbitrary n-dimensional lattice Λ. The lattice is not necessary either cubic or rectangular. The magnetic field is also arbitrary. However, we restrict ourselves within potential-free problems; the Schrödinger operator is assumed to be the Laplace operator defined with the covariant derivative. We defined an algebra that characterizes the symmetry of the Laplacian and named it the magnetic algebra. We proved that the space of functions on which the Laplacian acts is an irreducible representation space of the magnetic algebra. In this sense the magnetic algebra completely characterizes the quantum mechanics in the magnetic torus. We developed a new method for Fourier analysis for the magnetic torus and used it to solve the eigenvalue problem of the Laplacian. All the eigenfunctions are given in explicit forms. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1616203]

I. INTRODUCTION

In this paper we solve the Schrödinger equation for a particle in a uniform magnetic field in an n-dimensional torus. The problem looks plain at first sight but actually it turns out to be a hard problem, which has not been solved before. Hence we begin this paper by a quick explanation of the problem. After that we will describe our strategy to solve it. Subsequently we will briefly mention studies by other people and describe our motivation of this study. At the end of the Introduction we will give guides for quick access to main results of this paper.

An n-dimensional torus, or n-torus, is defined as $T^n=\mathbf{R}^n/\mathbf{Z}^n$. In the coordinate a point $(t^1,\ldots,t^j+1,\ldots,t^n)$ is identified with $(t^1,\ldots,t^j,\ldots,t^n)$ for each $j=1,\ldots,n$. The eigenvalue problem of the ordinary Laplacian in the torus is the equation

$$-\Delta f=-\sum_{j=1}^{n}\left(\frac{\partial}{\partial t^j}\right)^2 f=\varepsilon f \tag{1.1}$$

with the periodic boundary condition

$$f(t^1,\ldots,t^j+1,\ldots,t^n)=f(t^1,\ldots,t^j,\ldots,t^n). \tag{1.2}$$

The eigenvalue problem can be immediately solved by Fourier expansion. A plane-wave function

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$$\chi_k(t^1,\ldots,t^n)=e^{2\pi i\Sigma_{j=1}^n k_j t^j} \tag{1.3}$$

with quantized momenta $k_j\in\mathbf{Z}$ is a solution. The whole set of eigenfunctions $\{\chi_k\,|\,(k_1,\ldots,k_n)\in\mathbf{Z}^n\}$ constitutes a complete orthonormal set of the space of periodic functions over the torus. This is a well-known result.

In this paper we would like to solve an eigenvalue problem of the magnetic Laplacian; the magnetic Laplacian is defined by replacing the partial derivative in the ordinary Laplacian by a covariant derivative as

$$\Delta f=\sum_{j,l=1}^n g^{jl}\left(\frac{\partial}{\partial t^j}-2\pi i A_j\right)\left(\frac{\partial}{\partial t^l}-2\pi i A_l\right)f. \tag{1.4}$$

Here A_l is a component of the $U(1)$ gauge field

$$A_l=\frac{1}{2}\sum_{j=1}^n \phi_{jl}\,t^j+\alpha_l \tag{1.5}$$

with integers $\{\phi_{jl}=-\phi_{lj}\}$ and real numbers $\{\alpha_j\}$. The gauge field $A=\Sigma_{l=1}^n A_l\,\mathrm{d}t^l$ generates a uniform magnetic field $B=\mathrm{d}A=(1/2)\Sigma_{j,l=1}^n\phi_{jl}\,\mathrm{d}t^j\wedge\mathrm{d}t^l$. Moreover, we would like to consider a general oblique torus $T^n=\mathbf{R}^n/\Lambda$; Λ is an n-dimensional lattice. Edges of the unit cell of the lattice do not necessarily cross at a right angle and they do not necessarily have a same length. Hence we introduce a metric g^{jl} in the definition of the magnetic Laplacian (1.4) to take inclined and stretched or shortened unit cells into account. The eigenvalue problem of (1.4) is accompanied by the condition

$$f(t^1,\ldots,t^j+1,\ldots,t^n)=e^{\pi i\Sigma_{k=1}^n\phi_{jk}t^k}f(t^1,\ldots,t^j,\ldots,t^n), \tag{1.6}$$

which we call a twisted periodic condition. Thus the plain problem (1.1) with (1.2) is generalized to the magnetic problem (1.4) with (1.6). At first glance it looks rather straightforward to generalize the problem in this way but it is actually highly nontrivial and difficult to generalize the solution.

Let us see where the difficulty lies. In the case of the ordinary Laplacian, the plane-wave solution (1.3) is a simultaneous eigenfunction of the momentum operators

$$p_j=-i\frac{\partial}{\partial t^j}\quad(j=1,\ldots,n) \tag{1.7}$$

as $p_j\chi_k=2\pi k_j\chi_k$. The Laplacian can be expressed in terms of the momentum operators as $-\Delta=\Sigma_{j=1}^n(p_j)^2$ and, of course, it commutes with the momentum operators. Thus integers $(k_1,\ldots,k_n)$ are good quantum numbers. Then the whole set of simultaneous eigenfunctions $\{\chi_k\}$ forms the complete solutions of the Laplacian problem. This is the way how Fourier analysis works. However, when we turn to the magnetic Laplacian, we may seek for a simultaneous eigenfunction of magnetic momentum operators

$$p_j=-i\left(\frac{\partial}{\partial t^j}-2\pi i A_j\right)\quad(j=1,\ldots,n). \tag{1.8}$$

But such a simultaneous eigenfunction does not exist because magnetic momenta do not commute with each other and instead exhibit commutators

$$[\,p_j,p_l\,]=2\pi i\,\phi_{jl}. \tag{1.9}$$

The magnetic Laplacian can be still expressed in terms of the magnetic momentum operators as $-\Delta=\Sigma_{j=1}^{n}(p_j)^2$ but it does not commute with p_j. Hence, the strategy of ordinary Fourier analysis does not work well for the magnetic Laplacian.

To solve the problem we developed a new method, which we call Fourier analysis for the magnetic torus. This is a main subject of this paper. Let us describe our strategy: First, we will find a group of operators that commute with magnetic momentum operators. We call the group a magnetic translation group. Second, we enlarge a family of operators to define an algebra, which includes magnetic momenta and magnetic translations as its elements. We call the algebra a magnetic algebra and construct its representations. Third, we show that the space of twisted periodic functions over the torus is actually an irreducible representation space of the magnetic algebra. By diagonalizing a maximal commutative subalgebra of the magnetic algebra we obtain a complete orthonormal set of twisted periodic functions. This set of orthogonal functions provides a kind of unitary transformation as the set of plane-wave functions provides the Fourier transformation which bridges between the momentum space and the real space. We note that it is easy to diagonalize the Laplacian in the momentum space. Finally, we get a whole set of eigenfunctions in the real space by applying the unitary transformation. In this procedure the third step is the hardest part and is actually accomplished by lengthy cumbersome calculations. However, the strategy is clear.

We would like to briefly review studies by other people on spectral analysis in magnetic field. Brown[1] first examined the symmetry structure of the Schrödinger equation for an electron in a lattice in a uniform magnetic field and found that the symmetry is described by a noncommutative discrete translation group. At almost the same time Zak[2] also found the same symmetry structure and named the group a magnetic translation group (MTG). Zak[3] immediately built a representation theory of the MTG in the three-dimensional lattice. From the viewpoint of functional analysis, Avron, Herbst, and Simon have been studying spectral problems of the Schrödinger operators in a magnetic field in a series of papers.[4–6] Dubrovin and Novikov[7,8] studied the spectrum of the Pauli operator in a two-dimensional lattice with a periodic magnetic field and intensively analyzed the gap structure above the ground state. Florek[9,10] constructed tensor product representations of the MTG to analyze a three-particle system in a lattice in a magnetic field. Kuwabara[11,12] has been studying quantum-classical correspondence from the viewpoint of spectral geometry. For example, he[11] proved that if the whole set of level spacings of the quantum spectrum is not dense in $\mathbf{R}$, every trajectory of the corresponding classical particle is a closed orbit. Arai[13] found a quantum plane and quantum group structure in the quantum system in a singular magnetic field. Thus we can see that quantum mechanics in a magnetic field has been an active research area. However, we do not find a literature in which the quantum mechanics in an n-torus is solved.

Our study on quantum mechanics in magnetic fields originates from studies of extra-dimension models of the space–time. In extra-dimension models the space–time is assumed to be a base space of a fiber bundle with a compact fiber or a noncompact fiber. The history of extra-dimension models is rather old, but an interest in these models is recently renewed as Arkani-Hamed, Dimopoulos, and Dvali[14] pointed out that the extra-dimension model may solve the hierarchy problem of high energy physics. Inspired with extra-dimension models we[15] built a model which has a circle S^1 as a fiber over an any-dimensional space–times $\mathbf{R}^{D-1}$. Then we found that a twisted boundary condition in the S^1-direction causes spontaneous breaking of the translational symmetry. Based on this observation, we[16] proposed a new mechanism of supersymmetry breaking. Next we[17,18] built a model which has a two-dimensional sphere S^2 as a fiber over the four-dimensional space–times $\mathbf{R}^4$. We solved dynamics in the sphere in a magnetic monopole background and then found that the monopole induces spontaneous breaking of the rotational symmetry and the CP symmetry. We also built a model which has an n-dimensional torus as a fiber and tried to analyze dynamics in the torus in a background magnetic field. However, its analysis was not a straightforward task. Then we studied the symmetry structure of quantum mechanics in the torus in the magnetic field. We[19] constructed the MTG in the n-torus and classified irreducible representations of the MTG.

Armed with these tools we are now ready to solve the spectral problem in the n-torus T^n

$=\mathbf{R}^n/\Lambda$. We decide to solve the problem exhaustively; in our treatment the dimensions of the torus is taken to be arbitrary, lengths and angles of edges of the unit cell of Λ are arbitrary, and an arbitrary constant magnetic field is applied to the torus. Thus we aim to solve the widest class of quantum mechanics in the n-torus in uniform magnetic fields.

For busy readers here we give guides for quick access to main results. In Sec. II we provide a geometric setting to define the problem. The problem to be solved is the eigenvalue problem of the magnetic Laplacian (2.13) with the twist condition (2.5). In Sec. III we find a family of operators that commute with the covariant derivative. Actually they are composition of ordinary displacements and gauge transformations as shown at (3.2). These displacement vectors form a restricted family of vectors as shown at (3.8). These displacement operators generate the magnetic translation group (MTG), which is noncommutative as shown at (3.12). Along (3.16)–(3.28) we construct irreducible representations of the MTG. In Sec. IV we introduce a coordinate system, which will be revealed to be useful later. In Sec. V we define the magnetic algebra by adding differential operators (5.2)–(5.4) and multiplicative operators (5.9) to the MTG. Then we construct and classify irreducible representations of the magnetic algebra. Section VI is devoted to calculation of simultaneous eigenfunctions (6.8) of a maximal commutative subalgebra of the magnetic algebra. Then we obtain a complete orthonormal set of functions over the magnetic torus, which provide an extension of Fourier analysis for the magnetic torus. This is one of the main products of this paper. In Sec. VII by applying this method we solve the original problem, the eigenvalue problem of the magnetic Laplacian. There we obtain a whole set of eigenfunctions (7.11) and eigenvalues (7.12). These are the main results of this paper.

II. GAUGE FIELD IN THE TORUS

Let $\mathbf{t}=(t^1,\ldots,t^n)$ denote a coordinate of an n-dimensional torus $T^n=\mathbf{R}^n/\mathbf{Z}^n$. Namely, a point $(t^1,\ldots,t^j+1,\ldots,t^n)$ is identified with $(t^1,\ldots,t^j,\ldots,t^n)$ in T^n. A uniform magnetic field is generated by the gauge field

$$A=\sum_{k=1}^{n} A_k\,\mathrm{d}t^k=\frac{1}{2}\sum_{j,k=1}^{n}\phi_{jk}\,t^j\,\mathrm{d}t^k+\sum_{k=1}^{n}\alpha_k\,\mathrm{d}t^k. \tag{2.1}$$

Here $\{\phi_{jk}=-\phi_{kj}\}$ and $\{\alpha_j\}$ are real constants. Then the magnetic field is

$$B=\mathrm{d}A=\frac{1}{2}\sum_{j,k=1}^{n}\phi_{jk}\,\mathrm{d}t^j\wedge\mathrm{d}t^k. \tag{2.2}$$

Therefore, the number ϕ_{jk} represents magnetic flux which penetrates the (t^j,t^k)-face of the torus. We call the array of numbers (ϕ_{jk}) a magnetic flux matrix.

Let us introduce a complex scalar field f in the torus. The scalar field couples to the gauge field via the covariant derivative

$$\mathrm{D}f=\mathrm{d}f-2\pi iAf. \tag{2.3}$$

We put the coefficient $2\pi i$ in front of A for later convenience. Topology of the torus imposes a boundary condition on the scalar field. The gauge field itself is not a periodic function on $\mathbf{R}^n$ but it changes its form as

$$A(t^1,\ldots,t^j+1,\ldots,t^n)=A(t^1,\ldots,t^j,\ldots,t^n)+\frac{1}{2}\sum_{k=1}^{n}\phi_{jk}\,\mathrm{d}t^k. \tag{2.4}$$

Therefore, if we make the gauge transformation

$$f(t^1,\ldots,t^j+1,\ldots,t^n)=e^{\pi i\Sigma_{k=1}^n\phi_{jk}t^k}f(t^1,\ldots,t^j,\ldots,t^n), \tag{2.5}$$

the covariant derivative (2.3) remains covariant as

$$\mathrm{D}f(t^1,\ldots,t^j+1,\ldots,t^n)=e^{\pi i\Sigma_{k=1}^n\phi_{jk}t^k}\,\mathrm{D}f(t^1,\ldots,t^j,\ldots,t^n). \tag{2.6}$$

We call the condition (2.5) a twisted periodic condition. There are two ways to bring a point $(t^1,\ldots,t^j+1,\ldots,t^k+1,\ldots,t^n)$ to $(t^1,\ldots,t^j,\ldots,t^k,\ldots,t^n)$. The first way is

$$\begin{aligned}f(t^1,\ldots,t^j+1,\ldots,t^k+1,\ldots,t^n)&=e^{\pi i\{\phi_{jk}+\Sigma_{l=1}^n\phi_{jl}t^l\}}f(t^1,\ldots,t^j,\ldots,t^k+1,\ldots,t^n)\\&=e^{\pi i\{\phi_{jk}+\Sigma_{l=1}^n\phi_{jl}t^l+\Sigma_{l=1}^n\phi_{kl}t^l\}}f(t^1,\ldots,t^j,\ldots,t^k,\ldots,t^n).\end{aligned} \tag{2.7}$$

The other way is

$$\begin{aligned}f(t^1,\ldots,t^j+1,\ldots,t^k+1,\ldots,t^n)&=e^{\pi i\{\phi_{kj}+\Sigma_{l=1}^n\phi_{kl}t^l\}}f(t^1,\ldots,t^j+1,\ldots,t^k,\ldots,t^n)\\&=e^{\pi i\{\phi_{kj}+\Sigma_{l=1}^n\phi_{kl}t^l+\Sigma_{l=1}^n\phi_{jl}t^l\}}f(t^1,\ldots,t^j,\ldots,t^k,\ldots,t^n).\end{aligned} \tag{2.8}$$

To make these two expressions coincide we need to have

$$e^{\pi i\phi_{jk}}=e^{\pi i\phi_{kj}},$$

namely,

$$e^{\pi i(\phi_{jk}-\phi_{kj})}=e^{2\pi i\phi_{jk}}=1. \tag{2.9}$$

Therefore, compatibility of the periodic conditions (2.7) and (2.8) demands that ϕ_{jk} is an integer. Hence, the magnetic flux through each face of the torus is quantized. We call the torus where the magnetic field has been introduced a magnetic torus.

Since two displacements $t^j\mapsto t^j+1$ and $t^k\mapsto t^k+1$ are commutative, we can write the twisted periodic condition (2.5) in a more general form

$$f(\mathbf{t}+\mathbf{m})=e^{\pi i\Sigma_{j,k=1}^n\phi_{jk}m^jt^k}f(\mathbf{t}) \tag{2.10}$$

with an arbitrary $\mathbf{m}=(m^1,\ldots,m^n)\in\mathbf{Z}^n$. An inner product of two twisted periodic functions $f(\mathbf{t})$ and $g(\mathbf{t})$ is defined by

$$\langle f|g\rangle=\int_0^1\mathrm{d}t^1\cdots\int_0^1\mathrm{d}t^n\,f^*(\mathbf{t})g(\mathbf{t}). \tag{2.11}$$

Equipped with this inner product the space of twisted periodic functions becomes a Hilbert space.

To define the Laplacian we need to introduce a metric into the torus. Let Λ be an n-dimensional lattice in the Euclidean space $\mathbf{R}^n$. We equip the torus T^n with a Riemannian structure by identifying T^n with the quotient space $\mathbf{R}^n/\Lambda$. Let $\{\mathbf{u}_1,\ldots,\mathbf{u}_n\}$ be a set of vectors that generates the lattice Λ. Their inner products is denoted by

$$g_{jk}=\langle\mathbf{u}_j,\mathbf{u}_k\rangle \tag{2.12}$$

and its inverse is denoted by g^{jk}. Then the magnetic Laplacian is defined as

$$\Delta f=\sum_{j,k=1}^{n} g^{jk}\left(\frac{\partial}{\partial t^j}-2\pi i A_j\right)\left(\frac{\partial}{\partial t^k}-2\pi i A_k\right)f. \tag{2.13}$$

It is also referred to as the Bochner Laplacian in the literature. The purpose of this paper is to solve the eigenvalue problem of the magnetic Laplacian accompanied by the twisted periodic condition (2.5).

III. MAGNETIC TRANSLATION GROUP

Our goal is to find a complete set of eigenvalues and eigenfunctions of the magnetic Laplacian (2.13) as announced above. A royal road to solving an eigenvalue problem is to detect symmetry. In this section we determine a group of operators that commute with the Laplacian and construct irreducible representations of the group.

The vector space $\mathbf{R}^n$ acts on the torus as isometries. However, the gauge field restricts the admissible class of vectors as seen below. An arbitrary vector $\mathbf{v}\in\mathbf{R}^n$ displaces the gauge field (2.1) as

$$A(\mathbf{t})\mapsto A(\mathbf{t}-\mathbf{v})=A(\mathbf{t})-d\left(\frac{1}{2}\sum_{j,k=1}^{n}\phi_{jk}v^j t^k\right). \tag{3.1}$$

If we perform a gauge transformation of the scalar field simultaneously with the displacement

$$f(\mathbf{t})\mapsto f'(\mathbf{t})=(U(\mathbf{v})f)(\mathbf{t})=e^{\pi i\Sigma_{j,k=1}^{n}\phi_{jk}v^j t^k}f(\mathbf{t}-\mathbf{v}), \tag{3.2}$$

then the covariant derivative is changed covariantly

$$\mathrm{D}f(\mathbf{t})\mapsto \mathrm{D}f'(\mathbf{t})=e^{\pi i\Sigma_{j,k=1}^{n}\phi_{jk}v^j t^k}(\mathrm{D}f)(\mathbf{t}-\mathbf{v}). \tag{3.3}$$

In other words, the transformation $U(\mathbf{v})$ commutes with the covariant derivative as

$$(\mathrm{D}U(\mathbf{v})f)(\mathbf{t})=(U(\mathbf{v})\mathrm{D}f)(\mathbf{t}). \tag{3.4}$$

Hence it commutes with the magnetic Laplacian, which is defined in terms of the covariant derivative. The operator $U(\mathbf{v})$ is unitary with respect to the inner product (2.11).

The displaced function (3.2) also must satisfy the twisted periodic condition. If the original function f satisfies the condition (2.10), the displaced function changes its form as

$$f'(\mathbf{t}+\mathbf{m})=e^{2\pi i\Sigma_{j,k=1}^{n}\phi_{jk}v^j m^k}e^{\pi i\Sigma_{j,k=1}^{n}\phi_{jk}m^j t^k}f'(\mathbf{t}) \tag{3.5}$$

for $\mathbf{m}\in\mathbf{Z}^n$. Thus the displaced function satisfies the condition (2.10) if and only if

$$\sum_{j,k=1}^{n}\phi_{jk}v^j m^k \tag{3.6}$$

is an integer for an arbitrary $\mathbf{m}\in\mathbf{Z}^n$. In other words,

$$\sum_{j=1}^{n}\phi_{jk}v^j \quad (k=1,\ldots,n) \tag{3.7}$$

must be an integer. We call such a restricted vector $\mathbf{v}$ a magnetic shift. The set of magnetic shifts forms an Abelian group

$$\Omega^n=\{\mathbf{v}\in\mathbf{R}^n \mid \phi\mathbf{v}\in\mathbf{Z}^n\}. \tag{3.8}$$

There is a sequence of Abelian subgroups $\mathbf{Z}^n\subset\Omega^n\subset\mathbf{R}^n$. In particular, an integer vector $\mathbf{m}\in\mathbf{Z}^n$ induces a displacement

$$(U(\mathbf{m})f)(\mathbf{t})=e^{\pi i\Sigma_{j,k=1}^n\phi_{jk}m^jt^k}f(\mathbf{t}-\mathbf{m}).$$

However, owing to the twisted periodic condition (2.10), this is reduced to the identity transformation

$$(U(\mathbf{m})f)(\mathbf{t})=f(\mathbf{t}). \tag{3.9}$$

Thus we conclude that the group G of effective transformations is generated by

$$\{U(\mathbf{v}) \mid \mathbf{v}\in\Omega^n/\mathbf{Z}^n\}. \tag{3.10}$$

We call the group G the magnetic translation group. A product of transformations is

$$U(\mathbf{v})U(\mathbf{w})=e^{\pi i\Sigma_{j,k=1}^n\phi_{jk}v^jw^k}U(\mathbf{v}+\mathbf{w}). \tag{3.11}$$

Their commutator is

$$U(\mathbf{v})U(\mathbf{w})U(-\mathbf{v})U(-\mathbf{w})=e^{2\pi i\Sigma_{j,k=1}^n\phi_{jk}v^jw^k}. \tag{3.12}$$

We can say that the MTG is a central extension of the Abelian group $\Omega^n/\mathbf{Z}^n$ by $U(1)$.

We can express the MTG in a standard form. Let $L(n,\mathbf{Z})$ denote a group of the n-dimensional matrices $\{S\}$ of integers such that $\det S=\pm1$. The matrix $S\in L(n,\mathbf{Z})$ acts on $\mathbf{t}\in\mathbf{R}^n$ by $\mathbf{t}\mapsto S\mathbf{t}$ and this action induces an automorphism of the torus $T^n=\mathbf{R}^n/\mathbf{Z}^n$. It also induces a transformation of the magnetic flux matrix as

$$\phi_{jk}\mapsto\phi'_{jk}=\sum_{l,p=1}^n\phi_{lp}S^l{}_jS^p{}_k. \tag{3.13}$$

The Frobenius lemma[20] tells that for any integral antisymmetric matrix there exists a transformation to bring it into a standard form

$$(\phi_{jk})=\begin{pmatrix}
0 & q_1 & & & & & & & & \\
-q_1 & 0 & & & & & & & & \\
 & & 0 & q_2 & & & & & & \\
 & & -q_2 & 0 & & & & & & \\
 & & & & \ddots & & & & & \\
 & & & & & 0 & q_m & & & \\
 & & & & & -q_m & 0 & & & \\
 & & & & & & & 0 & & \\
 & & & & & & & & \ddots & \\
 & & & & & & & & & 0
\end{pmatrix}, \tag{3.14}$$

where $\{q_i\}$ are positive integers and they constitute a sequence $q_1|q_2|\cdots|q_m$, which implies that q_i divides q_{i+1}. For example, we may have a sequence $3|6|12|48$. Of course, $2m\leqslant n$. The vector

subspace of the zero eigenvalue of the matrix ϕ has dimensions $n-2m$ and it is called null directions. In the following we suppose that the flux matrix is in the standard form (3.14).

Now we can write the magnetic shifts (3.8) in a more explicit form. Let $\{\mathbf{e}_1,\ldots,\mathbf{e}_n\}$ be the standard basis of $\mathbf{R}^n$ in the $(t^1,\ldots,t^n)$-coordinate. Then any magnetic shift is uniquely expressed as

$$\mathbf{v}=\sum_{j=1}^{m}\left(\frac{s_{2j-1}}{q_j}\mathbf{e}_{2j-1}+\frac{s_{2j}}{q_j}\mathbf{e}_{2j}\right)+\sum_{k=1}^{n-2m}\theta_{2m+k}\mathbf{e}_{2m+k} \tag{3.15}$$

with integers $\{s_1,\ldots,s_{2m}\}$ and real numbers $\{\theta_{2m+1},\ldots,\theta_n\}$. Namely, the magnetic shifts are generated by $\{(1/q_j)\mathbf{e}_{2j-1},(1/q_j)\mathbf{e}_{2j}\,|\,j=1,\ldots,m\}$ with integral coefficients and $\{\mathbf{e}_{2m+k}\,|\,k=1,\ldots,n-2m\}$ with real coefficients. Hence, if the flux matrix ϕ has null directions $n-2m>0$, the MTG has a continuous component. Otherwise, the MTG is a completely discrete group.

Here we summarize our discussion; the MTG is generated by the unitary operators

$$U_j=U\left(\frac{1}{q_j}\mathbf{e}_{2j-1}\right),\quad V_j=U\left(\frac{1}{q_j}\mathbf{e}_{2j}\right)\quad(j=1,\ldots,m) \tag{3.16}$$

and

$$W_k(\theta)=U(\theta\mathbf{e}_{2m+k})\quad(k=1,\ldots,n-2m). \tag{3.17}$$

According to (3.9), (3.11), (3.12), and (3.14), these generators satisfy the following relations:

$$(U_j)^{q_j}=(V_j)^{q_j}=1, \tag{3.18}$$

$$U_jV_jU_j^{-1}V_j^{-1}=e^{2\pi i/q_j}, \tag{3.19}$$

$$W_k(1)=1, \tag{3.20}$$

$$W_k(\theta)W_k(\theta')=W_k(\theta+\theta'), \tag{3.21}$$

and other trivial commutators.

To solve the eigenvalue problem of the magnetic Laplacian we need to prepare the whole set of irreducible representations of the MTG. Let $\{|r_1,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle\}$ be elements of a representation space that are labeled by

$$r_j\in\mathbf{Z}/\mathbf{Z}_{q_j}\quad(j=1,\ldots,m), \tag{3.22}$$

$$d_k\in\mathbf{Z}\quad(k=1,\ldots,n-2m). \tag{3.23}$$

Then the generators (3.16) and (3.17) are represented by

$$U_j|r_1,\ldots,r_j,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle=|r_1,\ldots,r_j+1,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle, \tag{3.24}$$

$$V_j|r_1,\ldots,r_j,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle=e^{-2\pi ir_j/q_j}|r_1,\ldots,r_j,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle, \tag{3.25}$$

$$W_k(\theta)|r_1,\ldots,r_j,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle=e^{-2\pi id_k\theta}|r_1,\ldots,r_j,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle. \tag{3.26}$$

Thus

$$\mathcal{H}_d = \bigoplus_{r_1=0}^{q_1} \cdots \bigoplus_{r_m=0}^{q_m} \mathbf{C}|r_1,\ldots,r_m;d_1,\ldots,d_{n-2m}\rangle \tag{3.27}$$

provides an irreducible representation space of the MTG. Its dimension is

$$\dim \mathcal{H}_d = q_1 \times q_2 \times \cdots \times q_m . \tag{3.28}$$

The labels r_j and d_k in (3.22) and (3.23) will become good quantum numbers for the Laplacian (2.13). The dimension (3.28) will give the degree of degeneracy of each eigenvalue.

IV. DIAGONALIZATION OF THE MAGNETIC FIELD STRENGTH

To solve the eigenvalue problem of the magnetic Laplacian we need to take the metric (2.12) into account. Remember that the basis $\{\mathbf{u}_1,\ldots,\mathbf{u}_n\}$ generates the lattice Λ in the Euclidean space $\mathbf{R}^n$ and that the torus is isometric to $\mathbf{R}^n/\Lambda$. Let $\mathbf{x}=(x^1,\ldots,x^n)$ be an orthonormal coordinate of $\mathbf{R}^n$. It is related to the normalized coordinate $\mathbf{t}=(t^1,\ldots,t^n)$ via

$$\mathbf{x} = t^1\mathbf{u}_1 + \cdots + t^n\mathbf{u}_n = U\mathbf{t}. \tag{4.1}$$

In these coordinates the magnetic field (2.2) is expressed as

$$B = \frac{1}{2}\sum_{j,k=1}^{n} B_{jk}\,\mathrm{d}x^j\wedge dx^k = \frac{1}{2}\sum_{j,k,l,p=1}^{n} B_{jk}\,u^j{}_l\,u^k{}_p\,\mathrm{d}t^l\wedge\mathrm{d}t^p = \frac{1}{2}\sum_{l,p=1}^{n}\phi_{lp}\,\mathrm{d}t^l\wedge\mathrm{d}t^p. \tag{4.2}$$

The number B_{jk} is areal density of magnetic flux which penetrates the (x^j,x^k)-plane. If we perform a coordinate transformation

$$\mathbf{x} = R\mathbf{y} \tag{4.3}$$

by an orthogonal transformation $R\in O(n,\mathbf{R})$, the components of the field strength is transformed as

$$B = \frac{1}{2}\sum_{j,k=1}^{n} B_{jk}\,\mathrm{d}x^j\wedge\mathrm{d}x^k = \frac{1}{2}\sum_{j,k,l,p=1}^{n} B_{jk}\,R^j{}_l\,R^k{}_p\,\mathrm{d}y^l\wedge\mathrm{d}y^p. \tag{4.4}$$

By a suitable orthogonal transformation the field strength matrix (B_{jk}) can be brought into a standard form

$$\nu = {}^tRB\,R = \begin{pmatrix} 0 & \nu_1 & & & & & & & \\ -\nu_1 & 0 & & & & & & & \\ & & 0 & \nu_2 & & & & & \\ & & -\nu_2 & 0 & & & & & \\ & & & & \ddots & & & & \\ & & & & & 0 & \nu_m & & \\ & & & & & -\nu_m & 0 & & \\ & & & & & & & 0 & \\ & & & & & & & & \ddots \\ & & & & & & & & & 0 \end{pmatrix}, \tag{4.5}$$

where $\{\nu_j\}$ are positive real numbers. The $(t^1,\ldots,t^n)$-coordinate system block-diagonalizes the magnetic flux in the form of (3.14) while $(y^1,\ldots,y^n)$ block-diagonalizes the magnetic field strength in the form of (4.5). The transformations (4.1) and (4.3) are combined into

$$\mathbf{y}={}^tR\mathbf{x}={}^tRU\mathbf{t}=L\mathbf{t}. \tag{4.6}$$

Then we obtain relations among the matrices

$$\phi={}^tUBU={}^tUR\,\nu\,{}^tRU={}^tL\,\nu L. \tag{4.7}$$

The phase factor in (3.2) is rewritten as

$$\begin{aligned}\sum_{j,k=1}^{n} v^j\phi_{jk}t^k&=\sum_{j,k,l,p=1}^{n} v^jL^l{}_j\nu_{lp}L^p{}_kt^k\\&=\sum_{j,l,p=1}^{n} v^jL^l{}_j\nu_{lp}y^p\\&=\sum_{j=1}^{n}\sum_{l=1}^{m} v^j(L^{2l-1}_j\nu_ly^{2l}-L^{2l}_j\nu_ly^{2l-1}).\end{aligned} \tag{4.8}$$

The gauge field (2.1) is expressed in the y-coordinate as

$$A=\frac{1}{2}\sum_{j=1}^{m}\nu_j(y^{2j-1}\,\mathrm{d}y^{2j}-y^{2j}\,\mathrm{d}y^{2j-1})+\sum_{j,k=1}^{n}\alpha_j(L^{-1})^j{}_k\,\mathrm{d}y^k. \tag{4.9}$$

We set

$$\beta_k=\sum_{j=1}^{n}\alpha_j(L^{-1})^j{}_k \tag{4.10}$$

for later use.

Actually, we can choose a transformation matrix L that has zeros in this pattern

$$L=\begin{pmatrix} L^{2i-1}_{2p-1} & L^{2i-1}_{2q} & L^{2i-1}_{2m+r}\\ L^{2j}_{2p-1} & L^{2j}_{2q} & L^{2j}_{2m+r}\\ L^{2m+k}_{2p-1} & L^{2m+k}_{2q} & L^{2m+k}_{2m+r}\end{pmatrix}=\begin{pmatrix} * & 0 & 0\\ * & * & 0\\ * & * & *\end{pmatrix} \tag{4.11}$$

with $i,j,p,q=1,\ldots,m$ and $k,r=1,\ldots,n-2m$. The inverse matrix L^{-1} also has the same pattern of zeros. This distribution of zeros is proved in Appendix A. Then we can rewrite the magnetic shift operators (3.16) and (3.17) with a help of (4.8) in the y-coordinate as

$$U_jf(y^i)=e^{\pi i\Sigma_{l=1}^{m}(1/q_j)(L^{2l-1}_{2j-1}\nu_ly^{2l}-L^{2l}_{2j-1}\nu_ly^{2l-1})}f(y^i-L^i{}_{2j-1}(1/q_j)), \tag{4.12}$$

$$V_jf(y^i)=e^{-\pi i\Sigma_{l=1}^{m}(1/q_j)L^{2l}_{2j}\nu_ly^{2l-1}}f(y^i-L^i{}_{2j}(1/q_j)), \tag{4.13}$$

$$W_k(\theta)f(y^i)=f(y^i-L^i{}_{2m+k}\theta) \tag{4.14}$$

for $j=1,\ldots,m$ and $k=1,\ldots,n-2m$. From (4.11) and (4.7) we get a formula

$$\begin{aligned}\nu_i L^{2i-1}_{2j-1} &= \sum_{l,p=1}^{m} \nu_l L^{2l-1}_{2j-1} L^{2l}_{2p} (L^{-1})^{2p}_{2i} \\ &= \sum_{l,p=1}^{m} (L^{2l-1}_{2j-1} \nu_l L^{2l}_{2p} - L^{2l}_{2j-1} \nu_l L^{2l-1}_{2p})(L^{-1})^{2p}_{2i} \\ &= \sum_{p=1}^{m} q_j \delta_{jp} (L^{-1})^{2p}_{2i} = q_j (L^{-1})^{2j}_{2i}, \end{aligned} \tag{4.15}$$

which will be repeatedly used later.

V. MAGNETIC ALGEBRA

In this section we introduce new operators which act on twisted periodic functions. These new operators and the operators in the MTG generate an algebra, which we call a magnetic algebra. We construct and classify its irreducible representations. In the next section we will prove that the space of twisted periodic functions is actually an irreducible representation of the magnetic algebra. In this sense, the magnetic algebra completely characterizes the quantum mechanics in the magnetic torus.

Now we introduce a family of Hermite operators. Expanding the covariant derivative (2.3) in terms of the y-coordinate

$$Df = i \sum_{l=1}^{n} P_l f \, \mathrm{d}y^l, \tag{5.1}$$

we define differential operators

$$P_{2j-1} = -i\left(\frac{\partial}{\partial y^{2j-1}} + \pi i \nu_j y^{2j} - 2\pi i \beta_{2j-1} \right), \tag{5.2}$$

$$P_{2j} = -i\left(\frac{\partial}{\partial y^{2j}} - \pi i \nu_j y^{2j-1} - 2\pi i \beta_{2j} \right) \quad (j = 1, \ldots, m), \tag{5.3}$$

$$P_{2m+k} = -i\left(\frac{\partial}{\partial y^{2m+k}} - 2\pi i \beta_{2m+k} \right) \quad (k = 1, \ldots, n-2m). \tag{5.4}$$

These are Hermitian with respect to the inner product (2.11). Since $(y^1, \ldots, y^n)$ is an orthonormal coordinate, the Laplacian (2.13) becomes

$$-\Delta f = \sum_{i=1}^{n} (P_i)^2 f. \tag{5.5}$$

Nontrivial commutators among P's are

$$[P_{2j-1}, P_{2j}] = 2\pi i \nu_j \quad (j = 1, \ldots, m). \tag{5.6}$$

The other commutators vanish. We call the operators $\{P_{2j-1}, P_{2j}\}$ transverse momenta while we call the operators $\{P_{2m+k}\}$ longitudinal momenta. Since the covariant derivative commutes with the magnetic shifts as seen at (3.4), the momentum operators $\{P_i\}$ commute with the shift operators $\{U_j, V_j, W_k\}$, which are defined at (3.16) and (3.17).

Next we introduce another family of unitary operators. For this purpose we need an observation; in the t-coordinate that expresses the magnetic flux matrix in the standard form (3.14), t^{2m+k} $(k=1,\ldots,n-2m)$ are genuine cyclic coordinates. That is to say, the twisted periodic function (2.5) is periodic with respect to these coordinates as

$$f(t^1,\ldots,t^{2m+k}+1,\ldots,t^n)=f(t^1,\ldots,t^{2m+k},\ldots,t^n) \quad (k=1,\ldots,n-2m) \tag{5.7}$$

and the magnetic shift (3.2) is reduced to an ordinary continuous shift

$$(W_k(\theta)f)(t^1,\ldots,t^{2m+k},\ldots,t^n)=f(t^1,\ldots,t^{2m+k}-\theta,\ldots,t^n). \tag{5.8}$$

Then we define an operator T^k for each $k=1,\ldots,n-2m$ which acts on f by multiplication

$$(T^k f)(\mathbf{t})=e^{2\pi i\, t^{2m+k}} f(\mathbf{t})=e^{2\pi i \Sigma_{i=1}^n (L^{-1})_i^{2m+k} y^i} f(\mathbf{t}). \tag{5.9}$$

Here we used the inverse L^{-1} of the coordinate transformation (4.6). The operators $\{T^k\}$ are unitary operators with respect to the inner product (2.11). They satisfy

$$W_k(\theta)T^k=e^{-2\pi i\theta}T^k W_k(\theta), \tag{5.10}$$

$$[P_i,T^k]=2\pi(L^{-1})_i^{2m+k}T^k \quad (i=1,\ldots,n;\ k=1,\ldots,n-2m) \tag{5.11}$$

and commute with the other generators of the MTG.

Combining all the operators introduced above we define an algebra $\mathcal{A}$ with the generators $\{P_i,U_j,V_j,W_k(\theta),T^k \mid i=1,\ldots,n;\ j=1,\ldots,m;\ k=1,\ldots,n-2m;\ \theta\in\mathbf{R}\}$ and with the relations (3.18)–(3.21), (5.6), (5.10), (5.11) and other trivial commutators. We call the algebra $\mathcal{A}$ a magnetic algebra. In the following we will construct all the irreducible representations of the algebra $\mathcal{A}$ and classify their unitary equivalence classes.

A subset of generators $\{P_{2j-1},P_{2m+l},V_j,W_l(\theta) \mid j=1,\ldots,m;\ l=1,\ldots,n-2m;\ \theta\in\mathbf{R}\}$ generates a maximal Abelian subalgebra of $\mathcal{A}$. Hence these generators are simultaneously diagonalizable. Their simultaneous eigenstate $|k,r,d\rangle$ is labeled by $r_j\in\mathbf{Z}/\mathbf{Z}_{q_j}$ of (3.22) and $d_l\in\mathbf{Z}$ of (3.23) with new labels

$$k_{2j-1},k_{2m+l}\in\mathbf{R}. \tag{5.12}$$

The generators $\{P_{2j-1},P_{2m+l}\}$ act on these states as

$$P_{2j-1}|k,r,d\rangle=2\pi k_{2j-1}|k,r,d\rangle, \tag{5.13}$$

$$P_{2m+l}|k,r,d\rangle=2\pi k_{2m+l}|k,r,d\rangle, \tag{5.14}$$

and $\{V_j,W_l(\theta)\}$ act as (3.25), (3.26), respectively. The coefficient 2π was set for later convenience. Other generators $\{P_{2j},T^l \mid j=1,\ldots,m;\ l=1,\ldots,n-2m\}$ act on the states as

$$\langle\psi|P_{2j}|k,r,d\rangle=i\nu_j\frac{\partial}{\partial k_{2j-1}}\langle\psi|k,r,d\rangle, \tag{5.15}$$

$$T^l|k_i,r,d_k\rangle=e^{2\pi i\{\Sigma_{j=1}^m(k_{2j-1}+\Delta^l k_{2j-1})\Delta^l k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{lp}d_p\}}|k_i+\Delta^l k_i,r,d_k+\delta_k{}^l\rangle, \tag{5.16}$$

with $\Delta^l k_i=(L^{-1})_i^{2m+l}$. We will determine the $(n-2m)\times(n-2m)$ matrix Z^{lp} later. Here $|\psi\rangle$ represents an arbitrary state. The rests $\{U_j \mid j=1,\ldots,m\}$ act as (3.24). Therefore, in an irreducible representation space the eigenvalues k_{2m+i} are linked to d_l via

$$k_{2m+i}=\sum_{l=1}^{n-2m} d_l(L^{-1})^{2m+l}_{2m+i}-\beta_{2m+i}=\sum_{l=1}^{n-2m}(d_l-\alpha_{2m+l})(L^{-1})^{2m+l}_{2m+i}\quad(i=1,\ldots,n-2m). \tag{5.17}$$

Here the real number β_{2m+i} coincides with the one that appeared in (5.4). We also used the relations (4.10) and (4.11).

The matrix Z^{lp} is determined by the condition $T^{l'}T^{l}=T^{l}T^{l'}$. The action of $T^{l'}T^{l}$ gives

$$\begin{aligned}T^{l'}T^{l}|k_i,r,d_k\rangle=&e^{2\pi i\{\Sigma_{j=1}^{m}(k_{2j-1}+\Delta^{l}k_{2j-1})\Delta^{l}k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{lp}d_p\}}\\&\times e^{2\pi i\{\Sigma_{j=1}^{m}(k_{2j-1}+\Delta^{l}k_{2j-1}+\Delta^{l'}k_{2j-1})\Delta^{l'}k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{l'p}(d_p+\delta_p{}^{l})\}}\\&\times|k_i+\Delta^{l}k_i+\Delta^{l'}k_i,r,d_k+\delta_k{}^{l}+\delta_k{}^{l'}\rangle\end{aligned} \tag{5.18}$$

while the action of $T^{l}T^{l'}$ gives

$$\begin{aligned}T^{l}T^{l'}|k_i,r,d_k\rangle=&e^{2\pi i\{\Sigma_{j=1}^{m}(k_{2j-1}+\Delta^{l'}k_{2j-1})\Delta^{l'}k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{l'p}d_p\}}\\&\times e^{2\pi i\{\Sigma_{j=1}^{m}(k_{2j-1}+\Delta^{l'}k_{2j-1}+\Delta^{l}k_{2j-1})\Delta^{l}k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{lp}(d_p+\delta_p{}^{l'})\}}\\&\times|k_i+\Delta^{l'}k_i+\Delta^{l}k_i,r,d_k+\delta_k{}^{l'}+\delta_k{}^{l}\rangle.\end{aligned} \tag{5.19}$$

To give $T^{l'}T^{l}=T^{l}T^{l'}$ the matrix $Z^{ll'}$ must satisfy

$$\sum_{j=1}^{m}(\Delta^{l}k_{2j-1}\Delta^{l'}k_{2j}/\nu_j)+Z^{l'l}=\sum_{j=1}^{m}(\Delta^{l'}k_{2j-1}\Delta^{l}k_{2j}/\nu_j)+Z^{ll'}. \tag{5.20}$$

A general solution of the above equation is

$$Z^{ll'}=\sum_{j=1}^{m}(\Delta^{l}k_{2j-1}\Delta^{l'}k_{2j}/\nu_j)+S^{ll'}. \tag{5.21}$$

Here we leave an arbitrary symmetric matrix $S^{ll'}=S^{l'l}$ yet undetermined. Actually any choice of $S^{ll'}$ results in an equivalent representation, and therefore we take $S^{ll'}=0$.

A restricted set of vectors $\{|k,r,d\rangle\}$ that are labeled by the mutually independent parameters

$$k_{2j-1}\in\mathbf{R},\quad r_j\in\mathbf{Z}/\mathbf{Z}_{q_j},\quad d_l\in\mathbf{Z}\quad(j=1,\ldots,m;\ l=1,\ldots,n-2m) \tag{5.22}$$

spans a Hilbert space $\mathcal{H}_\alpha$ for each fixed value of $(\alpha_{2m+1},\alpha_{2m+2},\ldots,\alpha_n)$. Thus we conclude that a unitary equivalence class of irreducible representations of the algebra $\mathcal{A}$ has one-to-one correspondence with the parameter $(\alpha_{2m+1},\alpha_{2m+2},\ldots,\alpha_n)\in\mathbf{R}^{n-2m}/\mathbf{Z}^{n-2m}$.

VI. FOURIER ANALYSIS FOR THE MAGNETIC TORUS

Now let us turn to the space of twisted periodic functions. It is a representation space of the magnetic algebra. We will calculate the whole family of eigenfunctions of the maximal Abelian subalgebra of the magnetic algebra. These eigenfunctions $\chi_{k,r,d}(t^1,\ldots,t^n)=\langle t|k,r,d\rangle$ satisfy

$$P_{2j-1}\chi_{k,r,d}=-i\left(\frac{\partial}{\partial y^{2j-1}}+\pi i\nu_j y^{2j}-2\pi i\beta_{2j-1}\right)\chi_{k,r,d}=2\pi k_{2j-1}\chi_{k,r,d}, \tag{6.1}$$

$$P_{2j}\chi_{k,r,d}=-i\left(\frac{\partial}{\partial y^{2j}}-\pi i\nu_j y^{2j-1}-2\pi i\beta_{2j}\right)\chi_{k,r,d}=i\nu_j\frac{\partial}{\partial k_{2j-1}}\chi_{k,r,d}, \tag{6.2}$$

$$P_{2m+l}\,\chi_{k,r,d}=-i\left(\frac{\partial}{\partial y^{2m+l}}-2\pi i\beta_{2m+l}\right)\chi_{k,r,d}=2\pi\left(\sum_{i=1}^{n-2m} d_i(L^{-1})^{2m+i}_{2m+l}-\beta_{2m+l}\right)\chi_{k,r,d}, \tag{6.3}$$

$$U_j\,\chi_{k,r,d}=e^{\pi i t^{2j}}\chi_{k,r,d}\left(t^{2j-1}-\frac{1}{q_j}\right)=\chi_{k,(r+1),d}, \tag{6.4}$$

$$V_j\,\chi_{k,r,d}=e^{-\pi i t^{2j-1}}\chi_{k,r,d}\left(t^{2j}-\frac{1}{q_j}\right)=e^{-2\pi i r_j/q_j}\chi_{k,r,d}, \tag{6.5}$$

$$W_l(\theta)\,\chi_{k,r,d}=\chi_{k,r,d}(t^{2m+l}-\theta)=e^{-2\pi i d_l\theta}\chi_{k,r,d}, \tag{6.6}$$

$$T^l\,\chi_{k,r,d}=e^{2\pi i\, t^{2m+l}}\chi_{k,r,d}=e^{2\pi i\{\Sigma_{j=1}^{m}(k_{2j-1}+\Delta k_{2j-1})\Delta k_{2j}/\nu_j+\Sigma_{p=1}^{n-2m}Z^{lp}d_p\}}\chi_{k+\Delta k,r,(d+1)}, \tag{6.7}$$

for $j=1,\ldots,m$; $l=1,\ldots,n-2m$, and $\theta\in\mathbf{R}$. Here $(r+1)$ is an abbreviation of $(r_i+\delta_{ij})$ and $(d+1)$ is an abbreviation of $(d_p+\delta_p{}^l)$. And $\Delta k_i=(L^{-1})^{2m+l}_{i}$ as given in (5.16). Then $\chi_{k,r,d}$ is a simultaneous eigenfunction of $\{P_{2j-1},P_{2m+l},V_j,W_l(\theta)\}$. In the rest of this section we will solve the set of equations (6.1)–(6.7) to get the solutions

$$\begin{aligned}\chi_{k,r,d}(y^1,\ldots,y^n)=c\,\exp&\left[2\pi i\left\{-\sum_{j=1}^{m}\sum_{l=1}^{n-2m} d_l(L^{-1})^{2m+l}_{2j-1}\beta_{2j}/\nu_j-\frac{1}{2}\sum_{j=1}^{m}\nu_j y^{2j-1}y^{2j}\right\}\right]\\
&\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}\exp\left[2\pi i\left\{\frac{1}{2}\sum_{i,j,l=1}^{m}\nu_l L^{2l-1}_{2i-1}L^{2l}_{2j-1}(q_i\sigma_i+r_i)(q_j\sigma_j\right.\right.\\
&+r_j)/(q_iq_j)+\sum_{j=1}^{m}\beta_{2j-1}\left\{y^{2j-1}-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i)/q_i\right\}\\
&+\sum_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{2l}\left\{y^{2l}-\sum_{i=1}^{m}L^{2l}_{2i-1}(q_i\sigma_i+r_i)/q_i\right\}\\
&+\sum_{k,l=1}^{n-2m}d_k(L^{-1})^{2m+k}_{2m+l}\left\{y^{2m+l}-\sum_{i=1}^{m}L^{2m+l}_{2i-1}(q_i\sigma_i+r_i)/q_i\right\}\\
&\left.\left.+\sum_{j=1}^{m}k_{2j-1}\left\{y^{2j-1}+\beta_{2j}/\nu_j-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i-\gamma_i)/q_i\right\}\right\}\right],\end{aligned} \tag{6.8}$$

where c is a common normalization constant. The coefficients γ_j are given later at (6.13). The fact that the eigenfunctions are uniquely determined up to the common coefficient c implies that the space of twisted periodic function is an irreducible representation space of the magnetic algebra. Consequently, the eigenfunctions (6.8) constitute a complete orthonormal set of the space of twisted periodic functions over the torus. This is one of the main results of this paper. Hence an arbitrary twisted periodic function over the torus can be expanded as

$$f(y^1,\ldots,y^n)=\sum_{k,r,d}\lambda_{k,r,d}\,\chi_{k,r,d}(y^1,\ldots,y^n) \tag{6.9}$$

with unique coefficients $\lambda_{k,r,d}$. Therefore, the complete set $\{\chi_{k,r,d}\}$ provides a new basis for Fourier analysis in the magnetic torus.

In the rest of this section we give detailed lengthy calculations to prove the above statements. The reader may skip them to the next section, where we calculate solutions of the eigenvalue problem of the magnetic Laplacian using the main result (6.8). First, a simultaneous solution of (6.1) and (6.3) is

$$\chi_{k,r,d}(y^1,y^2,\ldots,y^n)=e^{2\pi i\Sigma_{j=1}^{m}\{(k_{2j-1}+\beta_{2j-1})y^{2j-1}-(1/2)\nu_j y^{2j-1}y^{2j}\}}e^{2\pi i\Sigma_{j,l=1}^{n-2m}d_j(L^{-1})_{2m+l}^{2m+j}y^{2m+l}}\times\phi_{k,r,d}(y^2,y^4,\ldots,y^{2m}),\tag{6.10}$$

where $\phi_{k,r,d}(y^2,y^4,\ldots,y^{2m})$ is an arbitrary function to be specified later.

Next let us turn to the other equation (6.5). Using (4.13) we can rewrite (6.5) as

$$e^{-\pi i\Sigma_{l=1}^{m}(1/q_j)L^{2l}_{\ 2j}\nu_l y^{2l-1}}\chi_{k,r,d}(y^i-L^{i}_{\ 2j}/q_j)=e^{-2\pi i r_j/q_j}\chi_{k,r,d}(y^i).\tag{6.11}$$

As discussed at (4.11) we have taken the matrix L such that $L^{2l-1}_{2j}=0$. Therefore, when (6.10) is substituted, the LHS of (6.11) becomes

$$\begin{aligned}&e^{-\pi i\Sigma_{l=1}^{m}(1/q_j)L^{2l}_{\ 2j}\nu_l y^{2l-1}}\chi_{k,r,d}(y^i-L^{i}_{\ 2j}/q_j)\\&\quad=e^{2\pi i\Sigma_{l=1}^{m}\{(k_{2l-1}+\beta_{2l-1})y^{2l-1}-(1/2)\nu_l y^{2l-1}y^{2l}\}}e^{2\pi i\Sigma_{p,l=1}^{n-2m}d_p(L^{-1})_{2m+l}^{2m+p}y^{2m+l}}\\&\qquad\times e^{-2\pi i\Sigma_{p,l=1}^{n-2m}d_p(L^{-1})_{2m+l}^{2m+p}L^{2m+l}_{\ 2j}/q_j}\phi_{k,r,d}(y^{2i}-L^{2i}_{\ 2j}/q_j).\end{aligned}\tag{6.12}$$

Hence, if we set

$$\gamma_j=\sum_{p,l=1}^{n-2m}d_p(L^{-1})_{2m+l}^{2m+p}L^{2m+l}_{\ 2j},\tag{6.13}$$

(6.11) implies that

$$e^{-2\pi i\gamma_j/q_j}\phi_{k,r,d}(y^{2i}-L^{2i}_{\ 2j}/q_j)=e^{-2\pi i r_j/q_j}\phi_{k,r,d}(y^{2i}).\tag{6.14}$$

If we introduce another coordinate system $(z^1,z^2,\ldots,z^m)$ which is related to $(y^2,y^4,\ldots,y^{2m})$ via

$$y^{2i}=\sum_{j=1}^{m}L^{2i}_{\ 2j}(z^j/q_j),\tag{6.15}$$

then (6.14) is rewritten as

$$\phi_{k,r,d}(z^1,\ldots,z^j-1,\ldots,z^m)=e^{2\pi i(\gamma_j-r_j)/q_j}\phi_{k,r,d}(z^1,\ldots,z^j,\ldots,z^m).\tag{6.16}$$

Moreover, if we set

$$\psi_{k,r,d}(z^1,\ldots,z^m)=e^{2\pi i\Sigma_{j=1}^{m}(\gamma_j-r_j)z^j/q_j}\phi_{k,r,d}(z^1,\ldots,z^m),\tag{6.17}$$

then (6.16) implies that

$$\psi_{k,r,d}(z^1,\ldots,z^j-1,\ldots,z^m)=\psi_{k,r,d}(z^1,\ldots,z^j,\ldots,z^m).\tag{6.18}$$

Hence $\psi_{k,r,d}$ is a periodic function with the period 1 and can be expanded in a Fourier series

$$\psi_{k,r,d}(z^1,\ldots,z^j,\ldots,z^m)=\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{k,r,d,\sigma}e^{2\pi i\Sigma_{j=1}^{m}\sigma_j z^j}.\tag{6.19}$$

Note that the inverse transformation of (6.15) is given by

$$(z^j/q_j)=\sum_{i=1}^{m}(L^{-1})^{2j}_{2i}y^{2i}. \tag{6.20}$$

Combining the above equations we can write down the eigenfunction (6.10) in a more specific form as

$$\chi_{k,r,d}(y^1,y^2,\ldots,y^n)=e^{2\pi i\Sigma_{j=1}^{m}\{(k_{2j-1}+\beta_{2j-1})y^{2j-1}-(1/2)\nu_j y^{2j-1}y^{2j}\}}e^{2\pi i\Sigma_{j,l=1}^{n-2m}d_j(L^{-1})^{2m+j}_{2m+l}y^{2m+l}}$$
$$\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{k,r,d,\sigma}\,e^{2\pi i\Sigma_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{2l}y^{2l}}. \tag{6.21}$$

Moreover, referring to (4.11) and (4.14), we can see that (6.21) satisfies (6.6). Thus we have seen that $\chi_{k,r,d}$ is a simultaneous eigenfunction of $\{P_{2j-1},P_{2m+l},V_j,W_l(\theta)\}$ as announced above.

The remaining task is to solve (6.2), (6.4), and (6.7). Let us begin with (6.2). The left-hand side (LHS) of (6.2) is

$$-i\left(\frac{\partial}{\partial y^{2j}}-\pi i\nu_j y^{2j-1}-2\pi i\beta_{2j}\right)\chi_{k,r,d}$$
$$=\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}2\pi\left(-\frac{1}{2}\nu_j y^{2j-1}+\sum_{i=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2j}-\frac{1}{2}\nu_j y^{2j-1}-\beta_{2j}\right)$$
$$\times e^{2\pi i\Sigma_{i=1}^{m}\{(k_{2i-1}+\beta_{2i-1})y^{2i-1}-(1/2)\nu_i y^{2i-1}y^{2i}\}}e^{2\pi i\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{2m+l}y^{2m+l}}c_{k,r,d,\sigma}$$
$$\times e^{2\pi i\Sigma_{i,l=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2l}y^{2l}}.$$

On the other hand, the right-hand side (RHS) of (6.2) is

$$i\nu_j\frac{\partial}{\partial k_{2j-1}}\chi_{k,r,d}=i\nu_j\,e^{2\pi i\Sigma_{i=1}^{m}\{(k_{2i-1}+\beta_{2i-1})y^{2i-1}-(1/2)\nu_i y^{2i-1}y^{2i}\}}e^{2\pi i\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{2m+l}y^{2m+l}}$$
$$\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}\left(\frac{\partial c_{k,r,d,\sigma}}{\partial k_{2j-1}}+2\pi i y^{2j-1}c_{k,r,d,\sigma}\right)$$
$$\times e^{2\pi i\Sigma_{i,l=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2l}y^{2l}}.$$

Therefore, we have an equation

$$i\nu_j\frac{\partial c_{k,r,d,\sigma}}{\partial k_{2j-1}}=2\pi\left(\sum_{i=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2j}-\beta_{2j}\right)c_{k,r,d,\sigma} \tag{6.22}$$

and get its solution

$$c_{k,r,d,\sigma}=c_{0,r,d,\sigma}\,e^{-2\pi i\{\Sigma_{i,j=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2j}\,k_{2j-1}/\nu_j-\Sigma_{j=1}^{m}\beta_{2j}k_{2j-1}/\nu_j\}}. \tag{6.23}$$

Thus (6.21) becomes

$$\chi_{k,r,d}(y^1,y^2,\ldots,y^n)=e^{2\pi i\Sigma_{j=1}^{m}\{(k_{2j-1}+\beta_{2j-1})y^{2j-1}+k_{2j-1}\beta_{2j}/\nu_j-(1/2)\nu_j y^{2j-1}y^{2j}\}}$$
$$\times e^{2\pi i\Sigma_{j,l=1}^{n-2m}d_j(L^{-1})^{2m+j}_{\ 2m+l}y^{2m+l}}$$
$$\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{0,r,d,\sigma}\,e^{2\pi i\Sigma_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{\ 2l}(y^{2l}-k_{2l-1}/\nu_l)}. \tag{6.24}$$

Next we turn to (6.4). With the aid of (4.12) and (4.15) the LHS of (6.4) becomes

$$e^{\pi i\Sigma_{l=1}^{m}(1/q_j)(L^{2l-1}_{\ 2j-1}\nu_l y^{2l}-L^{2l}_{\ 2j-1}\nu_l y^{2l-1})}\chi_{k,r,d}(y^i-L^{i}_{\ 2j-1}/q_j)$$
$$=e^{2\pi i\Sigma_{i=1}^{m}\{-\beta_{2i-1}L^{2i-1}_{\ 2j-1}/q_j-(1/2)(L^{-1})^{2j}_{\ 2i}L^{2i}_{\ 2j-1}/q_j\}}\,e^{-2\pi i\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{\ 2m+l}L^{2m+l}_{\ 2j-1}/q_j}$$
$$\times e^{2\pi i\Sigma_{i=1}^{m}\{(k_{2i-1}+\beta_{2i-1})y^{2i-1}+k_{2i-1}\beta_{2i}/\nu_i-(1/2)\nu_i y^{2i-1}y^{2i}\}}e^{2\pi i\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{\ 2m+l}y^{2m+l}}$$
$$\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{0,r,d,\sigma}\,e^{-2\pi i\Sigma_{i,l=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{\ 2l}L^{2l}_{\ 2j-1}/q_j}$$
$$\times e^{2\pi i\Sigma_{i,l=1}^{m}(q_i\sigma_i+r_i+\delta_{ij}-\gamma_i)(L^{-1})^{2i}_{\ 2l}(y^{2l}-k_{2l-1}/\nu_l)}. \tag{6.25}$$

To make this coincide with the RHS of (6.4) we have a recursive equation

$$e^{2\pi i\Sigma_{i=1}^{m}\{-\beta_{2i-1}L^{2i-1}_{\ 2j-1}/q_j-(1/2)(L^{-1})^{2j}_{\ 2i}L^{2i}_{\ 2j-1}/q_j\}}\,e^{-2\pi i\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{\ 2m+l}L^{2m+l}_{\ 2j-1}/q_j}$$
$$\times e^{-2\pi i\Sigma_{i,l=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{\ 2l}L^{2l}_{\ 2j-1}/q_j}\,c_{0,r,d,\sigma}=c_{0,(r+1),d,\sigma}. \tag{6.26}$$

Here $(r+1)$ means $(r_i+\delta_{ij})$. If we define an $m\times m$ matrix

$$Y_{ij}=\sum_{l=1}^{m}(L^{-1})^{2i}_{\ 2l}L^{2l}_{\ 2j-1}/q_j=\sum_{l=1}^{m}\nu_l L^{2l-1}_{\ 2i-1}L^{2l}_{\ 2j-1}/(q_iq_j), \tag{6.27}$$

it is symmetric as

$$Y_{ij}-Y_{ji}=\sum_{l=1}^{m}(L^{2l-1}_{\ 2i-1}\nu_l L^{2l}_{\ 2j-1}-L^{2l}_{\ 2i-1}\nu_l L^{2l-1}_{\ 2j-1})/(q_iq_j)=\phi_{2i-1,2j-1}/(q_iq_j)=0 \tag{6.28}$$

by virtue of (4.7). Then the solution of (6.26) is

$$c_{0,r,d,\sigma}=c_{0,0,d,\sigma}\,e^{-2\pi i\Sigma_{i,j=1}^{m}\beta_{2i-1}L^{2i-1}_{\ 2j-1}r_j/q_j}e^{-2\pi i\Sigma_{j=1}^{m}\Sigma_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{\ 2m+l}L^{2m+l}_{\ 2j-1}r_j/q_j}$$
$$\times e^{-2\pi i\Sigma_{i,j,l=1}^{m}(q_i\sigma_i+(1/2)r_i-\gamma_i)(L^{-1})^{2i}_{\ 2l}L^{2l}_{\ 2j-1}r_j/q_j}. \tag{6.29}$$

Therefore, (6.24) becomes

$$\chi_{k,r,d}(y^1,y^2,\ldots,y^n)=\exp\Bigg[2\pi i\Bigg\{\sum_{j=1}^{m}\Big\{(k_{2j-1}+\beta_{2j-1})y^{2j-1}+k_{2j-1}\beta_{2j}/\nu_j-\frac{1}{2}\nu_j y^{2j-1}y^{2j}\Big\}$$
$$+\sum_{i,l=1}^{n-2m} d_i(L^{-1})^{2m+i}_{2m+l}\Big(y^{2m+l}-\sum_{j=1}^{m}L^{2m+l}_{2j-1}r_j/q_j\Big)$$
$$-\sum_{i,j=1}^{m}\beta_{2i-1}L^{2i-1}_{2j-1}r_j/q_j+\frac{1}{2}\sum_{i,j=1}^{m}Y_{ij}r_ir_j\Bigg\}\Bigg]$$
$$\times\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{0,0,d,\sigma}\exp\Bigg[2\pi i\sum_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{2l}$$
$$\times\Big(y^{2l}-k_{2l-1}/\nu_l-\sum_{i=1}^{m}L^{2l}_{2i-1}r_i/q_i\Big)\Bigg]. \tag{6.30}$$

Since $(U_j)^{q_j}=1$ by (3.18), the substitution $r_j\mapsto r_j+q_j$ must leave $\chi_{k,r,d}$ invariant. This substitution gives

$$\chi_{k,(r+q),d}(\mathbf{y})=\exp\Bigg[2\pi i\Bigg\{\sum_{i=1}^{m}\Big\{(k_{2i-1}+\beta_{2i-1})y^{2i-1}+k_{2i-1}\beta_{2i}/\nu_i-\frac{1}{2}\nu_i y^{2i-1}y^{2i}\Big\}$$
$$+\sum_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{2m+l}\Big(y^{2m+l}-\sum_{p=1}^{m}L^{2m+l}_{2p-1}r_p/q_p\Big)-\sum_{i,l=1}^{m}\beta_{2i-1}L^{2i-1}_{2l-1}r_l/q_l$$
$$+\frac{1}{2}\sum_{i,p=1}^{m}Y_{ip}r_ir_p-\sum_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{2m+l}L^{2m+l}_{2j-1}-\sum_{i=1}^{m}\beta_{2i-1}L^{2i-1}_{2j-1}+\sum_{i=1}^{m}Y_{ij}r_iq_j$$
$$+\frac{1}{2}Y_{jj}q_jq_j\Big)\Bigg\}\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}c_{0,0,d,(\sigma-1)}\exp\Bigg[2\pi i\Bigg\{-\sum_{i=1}^{m}(q_i\sigma_i+r_i-\gamma_i)Y_{ij}q_j$$
$$+\sum_{i,l=1}^{m}(q_i\sigma_i+r_i-\gamma_i)(L^{-1})^{2i}_{2l}\Big(y^{2l}-k_{2l-1}/\nu_l-\sum_{p=1}^{m}L^{2l}_{2p-1}r_p/q_p\Big)\Bigg\}\Bigg]. \tag{6.31}$$

Here $(\sigma-1)$ is an abbreviation of $(\sigma_i-\delta_{ij})$. We used (4.15). Then we have another recursive equation

$$c_{0,0,d,\sigma}=c_{0,0,d,(\sigma-1)}\exp\Bigg[2\pi i\Bigg\{-\sum_{i,l=1}^{n-2m}d_i(L^{-1})^{2m+i}_{2m+l}L^{2m+l}_{2j-1}-\sum_{i=1}^{m}\beta_{2i-1}L^{2i-1}_{2j-1}$$
$$+\sum_{i=1}^{m}Y_{ij}r_iq_j+\frac{1}{2}Y_{jj}q_jq_j-\sum_{i=1}^{m}(q_i\sigma_i+r_i-\gamma_i)Y_{ij}q_j\Bigg\}\Bigg]. \tag{6.32}$$

Remember that $q_iq_jY_{ij}=\Sigma_{l=1}^{m}\nu_lL^{2l-1}_{2i-1}L^{2l}_{2j-1}=q_jq_iY_{ji}$ is symmetric. The solution of (6.32) is

$$c_{0,0,d,\sigma}=c_{0,0,d,0}\exp\Bigg[2\pi i\Bigg\{-\sum_{i,l=1}^{n-2m}\sum_{j=1}^{m}d_i(L^{-1})^{2m+i}_{2m+l}L^{2m+l}_{2j-1}\sigma_j-\sum_{i,j=1}^{m}\beta_{2i-1}L^{2i-1}_{2j-1}\sigma_j$$
$$+\sum_{i,j=1}^{m}Y_{ij}r_iq_j\sigma_j-\sum_{i,j=1}^{m}((1/2)q_i\sigma_i+r_i-\gamma_i)Y_{ij}q_j\sigma_j\Bigg\}\Bigg]. \tag{6.33}$$

Substituting it into (6.30) and using (4.15), we get

$$\chi_{k,r,d}(\mathbf{y}) = c_{0,0,d,0}\, e^{-\pi i \Sigma_{j=1}^{m} \nu_j y^{2j-1} y^{2j}} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty} \exp\Bigg[2\pi i \Bigg\{ \frac{1}{2} \sum_{i,j=1}^{m} Y_{ij}(q_i\sigma_i + r_i)(q_j\sigma_j + r_j) + \sum_{j=1}^{m} \beta_{2j-1} \Bigg\{ y^{2j-1} - \sum_{i=1}^{m} L^{2j-1}_{2i-1}(q_i\sigma_i + r_i)/q_i \Bigg\} + \sum_{j,l=1}^{m} (q_j\sigma_j + r_j - \gamma_j)(L^{-1})^{2j}_{2l} \Bigg\{ y^{2l} - \sum_{i=1}^{m} L^{2l}_{2i-1}(q_i\sigma_i + r_i)/q_i \Bigg\} + \sum_{i,l=1}^{n-2m} d_i (L^{-1})^{2m+i}_{2m+l} \Bigg\{ y^{2m+l} - \sum_{j=1}^{m} L^{2m+l}_{2j-1}(q_j\sigma_j + r_j)/q_j \Bigg\} + \sum_{j=1}^{m} k_{2j-1} \Bigg\{ y^{2j-1} + \beta_{2j}/\nu_j - \sum_{l=1}^{m} L^{2j-1}_{2l-1}(q_l\sigma_l + r_l - \gamma_l)/q_l \Bigg\} \Bigg\} \Bigg]. \tag{6.34}$$

Finally, we are going to solve (6.7). Its LHS becomes

$$\begin{aligned} & e^{2\pi i\, t^{2m+l}} \chi_{k,r,d} \\ &= c_{0,0,d,0}\, e^{-\pi i \Sigma_{j=1}^{m} \nu_j y^{2j-1} y^{2j}} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty} \exp\Bigg[2\pi i \Bigg\{ \frac{1}{2} \sum_{i,j=1}^{m} Y_{ij}(q_i\sigma_i + r_i)(q_j\sigma_j + r_j) \\ &\quad + \sum_{j=1}^{m} \beta_{2j-1} \Bigg\{ y^{2j-1} - \sum_{i=1}^{m} L^{2j-1}_{2i-1}(q_i\sigma_i + r_i)/q_i \Bigg\} \\ &\quad + \sum_{j,p=1}^{m} \Bigg(q_j\sigma_j + r_j - \gamma_j + \sum_{i=1}^{m} (L^{-1})^{2m+l}_{2i} L^{2i}_{2j} \Bigg) (L^{-1})^{2j}_{2p} \Bigg\{ y^{2p} - \sum_{i=1}^{m} L^{2p}_{2i-1}(q_i\sigma_i + r_i)/q_i \Bigg\} \\ &\quad + \sum_{p,i=1}^{m} (L^{-1})^{2m+l}_{2p} L^{2p}_{2i-1}(q_i\sigma_i + r_i)/q_i \\ &\quad + \sum_{i,p=1}^{n-2m} (d_i + \delta^l_i)(L^{-1})^{2m+i}_{2m+p} \Bigg\{ y^{2m+p} - \sum_{j=1}^{m} L^{2m+p}_{2j-1}(q_j\sigma_j + r_j)/q_j \Bigg\} \\ &\quad + \sum_{p=1}^{n-2m} \sum_{j=1}^{m} (L^{-1})^{2m+l}_{2m+p} L^{2m+p}_{2j-1}(q_j\sigma_j + r_j)/q_j \\ &\quad + \sum_{j=1}^{m} (k_{2j-1} + (L^{-1})^{2m+l}_{2j-1}) \Bigg\{ y^{2j-1} + \beta_{2j}/\nu_j - \sum_{p=1}^{m} L^{2j-1}_{2p-1}(q_p\sigma_p + r_p - \gamma_p)/q_p \Bigg\} \\ &\quad - \sum_{j=1}^{m} (L^{-1})^{2m+l}_{2j-1} \Bigg\{ \beta_{2j}/\nu_j - \sum_{p=1}^{m} L^{2j-1}_{2p-1}(q_p\sigma_p + r_p - \gamma_p)/q_p \Bigg\} \Bigg\} \Bigg]. \end{aligned} \tag{6.35}$$

We set $\Delta^l k_i = (L^{-1})^{2m+l}_{i}$ as before. The change $d_p \mapsto d_p + \delta_p{}^l$ causes a change of γ_j as

$$\begin{aligned}\Delta^l\gamma_j &= \sum_{i=1}^{n-2m} (L^{-1})^{2m+l}_{2m+i} L^{2m+i}_{2j} \\ &= \sum_{i=1}^{n} (L^{-1})^{2m+l}_{i} L^{i}_{2j} - \sum_{i=1}^{m} (L^{-1})^{2m+l}_{2i-1} L^{2i-1}_{2j} - \sum_{i=1}^{m} (L^{-1})^{2m+l}_{2i} L^{2i}_{2j} \\ &= 0 - 0 - \sum_{i=1}^{m} (L^{-1})^{2m+l}_{2i} L^{2i}_{2j} \end{aligned} \tag{6.36}$$

via (6.13) with (4.11). Moreover, we can see that

$$\begin{aligned}\sum_{p=1}^{m} L^{2j-1}_{2p-1}\Delta^l\gamma_p/q_p &= -\sum_{p,i=1}^{m} L^{2j-1}_{2p-1}(L^{-1})^{2m+l}_{2i} L^{2i}_{2p}/q_p \\ &= -\sum_{p,i=1}^{m} (L^{-1})^{2p}_{2j}(L^{-1})^{2m+l}_{2i} L^{2i}_{2p}/\nu_j \\ &= -\sum_{i=1}^{m} (L^{-1})^{2m+l}_{2i}\delta^{2i}_{2j}/\nu_j \\ &= -(L^{-1})^{2m+l}_{2j}/\nu_j \\ &= -\Delta^l k_{2j}/\nu_j . \end{aligned} \tag{6.37}$$

Therefore (6.35) becomes

$$\begin{aligned} & e^{2\pi i\, t^{2m+l}}\chi_{k,r,d} \\ &= c_{0,0,d,0}\, e^{-\pi i\Sigma_{j=1}^{m}\nu_j y^{2j-1}y^{2j}} \exp\Bigg[2\pi i\Bigg\{\sum_{j=1}^{m}(k_{2j-1}+\Delta k_{2j-1})\Delta k_{2j}/\nu_j \\ &\quad -\sum_{j=1}^{m}(L^{-1})^{2m+l}_{2j-1}\Bigg(\beta_{2j}/\nu_j+\sum_{p=1}^{m}L^{2j-1}_{2p-1}\gamma_p/q_p\Bigg)\Bigg\}\Bigg] \\ &\quad \times \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty} \exp\Bigg[2\pi i\Bigg\{\frac{1}{2}\sum_{i,j=1}^{m} Y_{ij}(q_i\sigma_i+r_i)(q_j\sigma_j+r_j) \\ &\quad +\sum_{j=1}^{m}\beta_{2j-1}\Bigg\{y^{2j-1}-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\} \\ &\quad +\sum_{j,p=1}^{m}(q_j\sigma_j+r_j-\gamma_j-\Delta\gamma_j)(L^{-1})^{2j}_{2p}\Bigg\{y^{2p}-\sum_{i=1}^{m}L^{2p}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\} \\ &\quad +\sum_{i,p=1}^{n-2m}(d_i+\delta^l_i)(L^{-1})^{2m+i}_{2m+p}\Bigg\{y^{2m+p}-\sum_{j=1}^{m}L^{2m+p}_{2j-1}(q_j\sigma_j+r_j)/q_j\Bigg\} \\ &\quad +\sum_{j=1}^{m}(k_{2j-1}+\Delta k_{2j-1})\Bigg\{y^{2j-1}+\beta_{2j}/\nu_j-\sum_{p=1}^{m}L^{2j-1}_{2p-1}(q_p\sigma_p+r_p-\gamma_p-\Delta\gamma_p)/q_p\Bigg\}\Bigg\}\Bigg]. \end{aligned} \tag{6.38}$$

In the course of calculation we used the fact $\Sigma_{p=1}^{n}(L^{-1})^{2m+l}_{p}L^{p}_{2i-1}=0$. With the aid of (4.15), (6.36) and the definition (5.21) we can deduce that

$$\sum_{j,p=1}^{m} (L^{-1})^{2m+l}_{2j-1} L^{2j-1}_{2p-1} \gamma_p/q_p = -\sum_{i=1}^{n-2m} Z^{li} d_i . \tag{6.39}$$

Thus we reach

$$\begin{aligned} e^{2\pi i\, t^{2m+l}} \chi_{k,r,d} = {} & e^{-2\pi i \Sigma_{j=1}^{m} (L^{-1})^{2m+l}_{2j-1} \beta_{2j}/\nu_j} c_{0,0,d,0} c^{-1}_{0,0,(d+1),0} \\ & \times e^{2\pi i \{\Sigma_{j=1}^{m} (k_{2j-1}+\Delta k_{2j-1}) \Delta k_{2j}/\nu_j + \Sigma_{i=1}^{n-2m} Z^{li} d_i\}} \chi_{k+\Delta k,r,(d+1)} . \end{aligned} \tag{6.40}$$

To satisfy (6.7) we meet another recursive equation

$$c_{0,0,(d+1),0} = e^{-2\pi i \Sigma_{j=1}^{m} (L^{-1})^{2m+l}_{2j-1} \beta_{2j}/\nu_j} c_{0,0,d,0} \tag{6.41}$$

and we get the solution

$$c_{0,0,d,0} = e^{-2\pi i \Sigma_{j=1}^{m} \Sigma_{l=1}^{n-2m} d_l (L^{-1})^{2m+l}_{2j-1} \beta_{2j}/\nu_j} c_{0,0,0,0} . \tag{6.42}$$

Substituting it into (6.34) we reach the final result

$$\begin{aligned} \chi_{k,r,d}(\mathbf{y}) = {} & c_{0,0,0,0} \exp\left[2\pi i \left\{ -\sum_{j=1}^{m} \sum_{l=1}^{n-2m} d_l (L^{-1})^{2m+l}_{2j-1} \beta_{2j}/\nu_j - \frac{1}{2} \sum_{j=1}^{m} \nu_j y^{2j-1} y^{2j} \right\} \right] \\ & \times \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty} \exp\left[2\pi i \left\{ \frac{1}{2} \sum_{i,j=1}^{m} Y_{ij} (q_i\sigma_i + r_i)(q_j\sigma_j + r_j) \right.\right. \\ & + \sum_{j=1}^{m} \beta_{2j-1} \left\{ y^{2j-1} - \sum_{i=1}^{m} L^{2j-1}_{2i-1} (q_i\sigma_i + r_i)/q_i \right\} \\ & + \sum_{j,l=1}^{m} (q_j\sigma_j + r_j - \gamma_j)(L^{-1})^{2j}_{2l} \left\{ y^{2l} - \sum_{i=1}^{m} L^{2l}_{2i-1} (q_i\sigma_i + r_i)/q_i \right\} \\ & + \sum_{k,l=1}^{n-2m} d_k (L^{-1})^{2m+k}_{2m+l} \left\{ y^{2m+l} - \sum_{i=1}^{m} L^{2m+l}_{2i-1} (q_i\sigma_i + r_i)/q_i \right\} \\ & \left.\left. + \sum_{j=1}^{m} k_{2j-1} \left\{ y^{2j-1} + \beta_{2j}/\nu_j - \sum_{i=1}^{m} L^{2j-1}_{2i-1} (q_i\sigma_i + r_i - \gamma_i)/q_i \right\} \right\} \right] . \end{aligned} \tag{6.43}$$

This is the result (6.8) announced previously. The eigenfunction $\chi_{k,r,d}$ is determined up to a unique normalization constant $c_{0,0,0,0}$. Thus we conclude that the space of twisted periodic functions over the torus is an irreducible representation space of the magnetic algebra $\mathcal{A}$. Finally, we have proved that the set of functions $\{\chi_{k,r,d}\}$ is a complete orthonormal set in the space of twisted periodic functions over the torus as announced at (6.9).

VII. EIGENFUNCTIONS OF THE MAGNETIC LAPLACIAN

In this section we will write down explicitly solutions of the eigenvalue problem of the magnetic Laplacian (2.13) or (5.5), which is expressed in the y-coordinate as

$$\begin{aligned} \Delta f = {} & \sum_{j=1}^{m} \left[\left(\frac{\partial}{\partial y^{2j-1}} + \pi i \nu_j y^{2j} - 2\pi i \beta_{2j-1} \right)^2 f + \left(\frac{\partial}{\partial y^{2j}} - \pi i \nu_j y^{2j-1} - 2\pi i \beta_{2j} \right)^2 f \right] \\ & + \sum_{k=1}^{n-2m} \left(\frac{\partial}{\partial y^{2m+k}} - 2\pi i \beta_{2m+k} \right)^2 f . \end{aligned} \tag{7.1}$$

The function f must satisfy the twisted periodic condition (2.5). We will obtain solutions using the Fourier analysis that is developed in the preceding section.

Here we would like to describe the outline of our method. As mentioned in the preceding section, the Laplacian commutes with the magnetic shift operators, $\{U_j, V_j, W_k\}$. Hence the labels $(r,d)=(r_1,r_2,\ldots,r_m,d_1,d_2,\ldots,d_{n-2m})$, which are defined in (3.22)–(3.26), are good quantum numbers. Moreover, the Laplacian commutes with the longitudinal momentum operators $\{P_{2m+k}\}$. Hence the corresponding momentum eigenvalues $\{k_{2m+k}\}$ are also good quantum numbers and are related to the labels d_l via (5.17). On the other hand, the Laplacian does not commute with the transverse momentum operators $\{P_{2j-1}, P_{2j}\}$. Hence the transverse momentum eigenvalues $\{k_{2j-1}\}$ do not remain good quantum numbers. The Laplacian admits a new set of good quantum numbers $(n_1,n_2,\ldots,n_m)$, which will be introduced later. It will be revealed that eigenfunctions of the Laplacian are actually matrix elements of a unitary transformation,

$$\psi_{n,r,d}(k_1,k_3,\ldots,k_{2m-1})=\langle k,r,d|n,r,d\rangle, \tag{7.2}$$

which relates the quantum numbers n's to k's. In the k-space it is rather easy to get eigenfunctions by the standard method of a harmonic oscillator. On the other hand, the set of eigenfunctions of the momenta and magnetic shifts,

$$\chi_{k,r,d}(y^1,y^2,\ldots,y^n)=\langle y|k,r,d\rangle, \tag{7.3}$$

plays a role a unitary transformation which bridges between the momentum space and the real space like the usual Fourier transformation. Hence the Laplacian eigenfunctions are transformed into the y-coordinate representations by

$$\psi_{n,r,d}(y^1,y^2,\ldots,y^n)=\langle y|n,r,d\rangle=\int_{-\infty}^{\infty} dk_1\, dk_3\cdots dk_{2m-1}\langle y|k,r,d\rangle\,\langle k,r,d|n,r,d\rangle. \tag{7.4}$$

This will give the desired result.

Now let us carry out the program outlined above. We define creation and annihilation operators associated with the transverse momenta as

$$a_j^\dagger=\frac{1}{\sqrt{4\pi\nu_j}}(P_{2j-1}-iP_{2j}),\quad a_j=\frac{1}{\sqrt{4\pi\nu_j}}(P_{2j-1}+iP_{2j})\quad (j=1,\ldots,m). \tag{7.5}$$

It is easily verified that $[a_j,a_k^\dagger]=\delta_{jk}$. Then the Laplacian (5.5) becomes

$$-\Delta=\sum_{j=1}^{m}4\pi\nu_j\left(a_j^\dagger a_j+\frac{1}{2}\right)+\sum_{k=1}^{n-2m}(P_{2m+k})^2. \tag{7.6}$$

The eigenstate $|\Omega\rangle$ for the lowest eigenvalue satisfies

$$0=\langle k|a_j|\Omega\rangle=\frac{1}{\sqrt{4\pi\nu_j}}\langle k|(P_{2j-1}+iP_{2j})|\Omega\rangle=\frac{1}{\sqrt{4\pi\nu_j}}\left(2\pi k_{2j-1}+\nu_j\frac{\partial}{\partial k_{2j-1}}\right)\langle k|\Omega\rangle. \tag{7.7}$$

Here we used (5.13) and (5.15). The solution is

$$\langle k|\Omega\rangle=e^{-\pi\Sigma_{j=1}^{m}(k_{2j-1})^2/\nu_j}. \tag{7.8}$$

States for higher eigenvalues are generated by creation operators as

$$\begin{aligned}\langle k|n\rangle &= \frac{1}{\sqrt{n_1!\cdots n_m!}}\langle k|(a_1^\dagger)^{n_1}\cdots(a_m^\dagger)^{n_m}|\Omega\rangle \\ &= \frac{1}{\sqrt{n_1!\cdots n_m!}}\prod_{j=1}^{m}\left[\frac{1}{\sqrt{4\pi\nu_j}}\left(2\pi k_{2j-1}-\nu_j\frac{\partial}{\partial k_{2j-1}}\right)\right]^{n_j}\langle k|\Omega\rangle \\ &= \frac{1}{\sqrt{n_1!\cdots n_m!}}e^{\pi\Sigma_{j=1}^m(k_{2j-1})^2/\nu_j}\prod_{j=1}^{m}\left[\frac{1}{\sqrt{4\pi\nu_j}}\left(-\nu_j\frac{\partial}{\partial k_{2j-1}}\right)\right]^{n_j}e^{-2\pi\Sigma_{j=1}^m(k_{2j-1})^2/\nu_j} \quad (7.9)\end{aligned}$$

for $n_1,n_2,\ldots,n_m=0,1,2,\ldots$. We are suppressing other labels (r,d). In Appendix B we prove that

$$\begin{aligned}\int_{-\infty}^{\infty}\mathrm{d}k\,e^{2\pi ikz}\cdot e^{\pi k^2/\nu}\left(-\nu\frac{\partial}{\partial k}\right)^n e^{-2\pi k^2/\nu} &= \sqrt{\nu}\,e^{\pi\nu z^2}\left(-i\frac{\partial}{\partial z}\right)^n e^{-2\pi\nu z^2} \\ &= \sqrt{\nu}(i\sqrt{2\pi\nu})^n e^{-\pi\nu z^2}H_n(z\sqrt{2\pi\nu}). \quad (7.10)\end{aligned}$$

In the second line $H_n(\xi)$ is the nth Hermite polynomial. Substituting (6.43) and (7.9) into (7.4) and applying (7.10) we obtain

$$\begin{aligned}\langle y|n,r,d\rangle &= \int_{-\infty}^{\infty}\mathrm{d}k_1\,\mathrm{d}k_3\cdots\mathrm{d}k_{2m-1}\,\langle y|k,r,d\rangle\langle k,r,d|n,r,d\rangle \\ &= c\,\exp\Bigg[2\pi i\Bigg\{-\sum_{j=1}^{m}\sum_{l=1}^{n-2m}d_l(L^{-1})^{2m+l}_{2j-1}\beta_{2j}/\nu_j \\ &\quad -\frac{1}{2}\sum_{j=1}^{m}\nu_j y^{2j-1}y^{2j}\Bigg\}\Bigg]_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}\exp\Bigg[2\pi i\Bigg\{\frac{1}{2}\sum_{i,j=1}^{m}Y_{ij}(q_i\sigma_i+r_i)(q_j\sigma_j+r_j) \\ &\quad +\sum_{j=1}^{m}\beta_{2j-1}\Bigg\{y^{2j-1}-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\} \\ &\quad +\sum_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{2l}\Bigg\{y^{2l}-\sum_{i=1}^{m}L^{2l}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\} \\ &\quad +\sum_{k,l=1}^{n-2m}d_k(L^{-1})^{2m+k}_{2m+l}\Bigg\{y^{2m+l}-\sum_{i=1}^{m}L^{2m+l}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\}\Bigg\}\Bigg] \\ &\quad \times\prod_{j=1}^{m}\Bigg[\sqrt{\frac{\nu_j}{n_j!}}\left(\frac{i}{\sqrt{2}}\right)^{n_j}e^{-\pi\nu_j\{y^{2j-1}+\beta_{2j}/\nu_j-\Sigma_{i=1}^m L^{2j-1}_{2i-1}(q_i\sigma_i+r_i-\gamma_i)/q_i\}^2} \\ &\quad \times H_{n_j}\Bigg(\sqrt{2\pi\nu_j}\Bigg\{y^{2j-1}+\beta_{2j}/\nu_j-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i-\gamma_i)/q_i\Bigg\}\Bigg)\Bigg]. \quad (7.11)\end{aligned}$$

This is the main result of this paper. Using (5.17), we can calculate eigenvalues of the Laplacian (7.6) as

$$-\frac{1}{2}\Delta\psi_{n,r,d}=\Bigg[\sum_{j=1}^{m}2\pi\nu_j\left(n_j+\frac{1}{2}\right)+\frac{1}{2}\sum_{k=1}^{n-2m}\Bigg\{\sum_{l=1}^{n-2m}2\pi(d_l-\alpha_{2m+l})(L^{-1})^{2m+l}_{2m+k}\Bigg\}^2\Bigg]\psi_{n,r,d}. \quad (7.12)$$

Eigenvalues depend on quantum numbers $n_1,n_2,\ldots,n_m=0,1,2,\ldots$ and $d_1,d_2,\ldots,d_{n-2m}=0,\pm1,\pm2,\ldots$ but not on $r=(r_1,r_2,\ldots,r_m)\in\mathbf{Z}_{q_1}\times\mathbf{Z}_{q_2}\times\cdots\times\mathbf{Z}_{q_m}$. Thus each eigenvalue is degenerated by $q_1q_2\cdots q_m$ folds as predicted in (3.28). If a ratio $\nu_i/\nu_j(i\neq j)$ is rational, degeneracy happens more. On the other hand, if $\alpha_{2m+l}=0$, the eigenvalue for $-d_l$ coincides with the one for d_l. If $\alpha_{2m+l}=1/2$, the eigenvalue for $(-d_l+1)$ coincides with the one for d_l. Moreover, for specific values of $\{(L^{-1})^{2m+l}_{2m+k}\}$ we may meet more multifold degeneracy.

Let us discuss physical meanings of the eigenvalue (7.12). It is energy of an electrically charged particle moving in the magnetic field in the torus. In (7.12) we set the coefficient $-1/2$ in front of Δ to adjust the equation to the conventional Schrödinger equation. In the context of classical mechanics, the particle exhibits a cyclic motion with the frequency ν_j in the (y^{2j-1},y^{2j})-plane for each $j=1,2,\ldots,m$. And it exhibits a uniform straight motion along the y^{2m+k}-axis. The whole motion is a superposition of those cyclic and straight motions. When we turn to quantum mechanics, energy of the cyclic motion is quantized and results in the so-called Landau level $2\pi\nu_j(n_j+1/2)$. On the other hand, the longitudinal momentum P_{2m+k} associated with the straight motion is quantized to be $2\pi k_{2m+k}=2\pi\Sigma_{l=1}^{n-2m}(d_l-\alpha_{2m+l})(L^{-1})^{2m+l}_{2m+k}=2\pi\Sigma_{l=1}^{n-2m}d_l(L^{-1})^{2m+l}_{2m+k}-\beta_{2m+k}$ with integers $(d_1,d_2,\ldots,d_{n-2m})$ as explained in (5.17). Along the course of the straight motion the particle flies around the torus and picks up the so-called Aharonov–Bohm effect. Then the momentum is shifted by the Aharonov–Bohm parameters $(\beta_{2m+1},\ldots,\beta_n)$. Accordingly, the kinetic energy of the straight motion is also quantized. The total energy is then given as (7.12).

Moreover, let us examine meanings of other Aharonov–Bohm parameters $(\beta_1,\ldots,\beta_{2m})$. These do not affect the energy (7.12) and hence they have a geometric significance rather than a physical significance. To understand their meaning we rewrite the eigenfunction (6.43) as

$$\begin{aligned}\chi_{k,r,d}(\mathbf{y})=c\exp\Bigg[2\pi i\Bigg\{&\sum_{l=1}^{n-2m}\sum_{j=1}^{m}d_l\{(L^{-1})^{2m+l}_{2j}\beta_{2j-1}-(L^{-1})^{2m+l}_{2j-1}\beta_{2j}\}/\nu_j-\frac{1}{2}\sum_{j=1}^{m}\nu_jy^{2j-1}y^{2j}\\&+\sum_{j=1}^{m}\beta_{2j-1}y^{2j-1}\Bigg\}\Bigg]_{\sum_{\sigma_1,\sigma_2,\ldots,\sigma_m=-\infty}^{\infty}}\exp\Bigg[2\pi i\Bigg\{\frac{1}{2}\sum_{i,j=1}^{m}Y_{ij}(q_i\sigma_i+r_i)(q_j\sigma_j+r_j)\\&+\sum_{j,l=1}^{m}(q_j\sigma_j+r_j-\gamma_j)(L^{-1})^{2j}_{2l}\Bigg\{y^{2l}-\beta_{2l-1}/\nu_l-\sum_{i=1}^{m}L^{2l}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\}\\&+\sum_{k,l=1}^{n-2m}d_k(L^{-1})^{2m+k}_{2m+l}\Bigg\{y^{2m+l}-\sum_{i=1}^{m}L^{2m+l}_{2i-1}(q_i\sigma_i+r_i)/q_i\Bigg\}\\&+\sum_{j=1}^{m}k_{2j-1}\Bigg\{y^{2j-1}+\beta_{2j}/\nu_j-\sum_{i=1}^{m}L^{2j-1}_{2i-1}(q_i\sigma_i+r_i-\gamma_i)/q_i\Bigg\}\Bigg\}\Bigg].\end{aligned}\tag{7.13}$$

To get the above expression we used

$$\sum_{i=1}^{m}L^{2j-1}_{2i-1}\gamma_i/q_i=-\sum_{l=1}^{n-2m}d_l(L^{-1})^{2m+l}_{2j}/\nu_j,\tag{7.14}$$

which is easily derived from (6.36). Thus we can see that the parameters $(\beta_1,\ldots,\beta_{2m})$ induce a displacement

$$(y^{2j-1},y^{2j})\to(y^{2j-1}+\beta_{2j}/\nu_j,y^{2j}-\beta_{2j-1}/\nu_j)\tag{7.15}$$

of the profile $|\chi_{k,r,d}(\mathbf{y})|$. This is the geometric significance of the transverse Aharonov–Bohm parameters.

VIII. CONCLUSION

Here we summarize our discussions. As well-known, a $U(1)$ gauge field replaces the partial derivative by the covariant derivative and generates a magnetic field. As a natural extension of the eigenvalue problem of the ordinary Laplacian in the n-torus, we formulated the eigenvalue problem of the magnetic Laplacian. The ordinary Laplacian admits continuous Abelian symmetry and therefore the usual Fourier analysis is applicable. However, the magnetic Laplacian does not admit continuous Abelian symmetry and therefore the usual Fourier analysis is not applicable to it. Hence, we developed an alternative method, which became an extension of the usual Fourier analysis. We identified symmetry structure of the magnetic Laplacian and defined the magnetic translation group (MTG), which is discrete and non-Abelian in general. Moreover, we defined the magnetic algebra by extending the MTG. We proved that the space of functions on which the magnetic Laplacian acts is an irreducible representation space of the magnetic algebra. By diagonalizing the maximal Abelian subalgebra of the magnetic algebra we obtained a complete orthonormal set of functions $\{\chi_{k,r,d}(\mathbf{y})\}$ over the magnetic torus; those functions are labeled by a set of good quantum numbers (k,r,d). It was rather easy to diagonalize the magnetic Laplacian in the $\mathbf{k}$-space representation. Applying a unitary transformation by $\{\chi_{k,r,d}(\mathbf{y})\}$ to the eigenstate of the magnetic Laplacian, we finally obtained the eigenfunction in the $\mathbf{y}$-space representation. The eigenvalues of the magnetic Laplacian were naturally interpreted as sums of energies of cyclic motions in the transverse directions to the magnetic field and energies of linear motions in the longitudinal direction to it.

New results of this paper are the definition and representations of the magnetic algebra, the proof of irreducibility of the space of twisted periodic functions as a representation space of the magnetic algebra, the complete orthogonal set of functions (6.8) which provides a basis of the extended Fourier analysis, the eigenfunctions (7.11) of the magnetic Laplacian in explicit forms, and the eigenvalues (7.12).

Before closing this paper we would like to discuss briefly possible directions for further development. We treated only the Laplace operator in this paper but for application to physics it is more desirable to treat the Schrödinger operator

$$H = -\tfrac{1}{2}\Delta + V, \tag{8.1}$$

which has a potential energy term V. The potential V is a periodic function; in the t-coordinate it satisfies $V(t^1,\ldots,t^i+1,\ldots,t^n)=V(t^1,\ldots,t^i,\ldots,t^n)$ for each i. It acts on the twisted periodic function $f(\mathbf{t})$ by multiplication. To take the potential term into account we may introduce new operators X^k by

$$(X^j f)(\mathbf{t}) = e^{2\pi i\, t^j} f(\mathbf{t}) \quad (j=1,2,\ldots,2m), \tag{8.2}$$

which belong to the same family of operators T^k of (5.9). Then any periodic potential operator can be expanded as

$$\begin{aligned} V(t^1,\ldots,t^n) &= \sum_{\sigma_1,\sigma_2,\ldots,\sigma_n=-\infty}^{\infty} c_\sigma\, e^{2\pi i(\sigma_1 t^1+\cdots+\sigma_n t^n)} \\ &= \sum_{\sigma_1,\sigma_2,\ldots,\sigma_n=-\infty}^{\infty} c_\sigma\, (X^1)^{\sigma_1}\cdots(X^{2m})^{\sigma_{2m}}(T^1)^{\sigma_{2m+1}}\cdots(T^{n-2m})^{\sigma_n}. \end{aligned} \tag{8.3}$$

We can easily calculate commutators of X's with other operators to get an algebra which is an extension of the magnetic algebra. The resulted algebra is isomorphic to the so-called noncommutative torus[21] although we do not yet examine these relation thoroughly.

Another direction for future development is to solve an eigenvalue problem of the Dirac operator in the n-torus in the background magnetic field. We also construct supersymmetric field theory, which have both scalar and spinor fields as its constituents to pursue a new mechanism of supersymmetry breaking.

ACKNOWLEDGMENTS

One of the authors (S.T.) thanks T. Iwai and I. Tsutsui for their continuous encouragement. The authors thank the Yukawa Institute for Theoretical Physics at Kyoto University. Discussions during the YITP workshop YITP-W-02-18 on ''Quantum Field Theories: Fundamental Problems and Applications'' were useful to complete this work. This work was supported in part by the Grant-in-Aid for Scientific Research of Ministry of Education, Science, and Culture, Grant No. 15540277.

APPENDIX A: DISTRIBUTION OF ZEROS

As shown in (4.11) we prove existence of a transformation matrix L that has zeros in the pattern

$$L=\begin{pmatrix} L^{2i-1}_{2p-1} & L^{2i-1}_{2q} & L^{2i-1}_{2m+r} \\ L^{2j}_{2p-1} & L^{2j}_{2q} & L^{2j}_{2m+r} \\ L^{2m+k}_{2p-1} & L^{2m+k}_{2q} & L^{2m+k}_{2m+r} \end{pmatrix} = \begin{pmatrix} * & 0 & 0 \\ * & * & 0 \\ * & * & * \end{pmatrix} \tag{A1}$$

with $i,j,p,q=1,\ldots,m$ and $k,r=1,\ldots,n-2m$.

In $\mathbf{R}^n$ we have an antisymmetric bilinear form B. We say that a vector $\mathbf{u}$ is longitudinal with respect to B if it satisfies

$$B(\mathbf{u},\mathbf{v})=0 \tag{A2}$$

for arbitrary $\mathbf{v}\in\mathbf{R}^n$. We call

$$M^0=\{\mathbf{u}\in\mathbf{R}^n \mid \forall\mathbf{v}\in\mathbf{R}^n,\ B(\mathbf{u},\mathbf{v})=0\} \tag{A3}$$

a longitudinal vector subspace. Let $(t^1,t^2,\ldots,t^n)$ be the coordinate system that expresses B in the standard form

$$B=\frac{1}{2}\sum_{i,j=1}^{n}\phi_{ij}\,\mathrm{d}t^i\wedge\mathrm{d}t^j=\sum_{j=1}^{m}q_j\,\mathrm{d}t^{2j-1}\wedge\mathrm{d}t^{2j} \tag{A4}$$

as in (3.14). Let $(y^1,y^2,\ldots,y^n)$ be another coordinate system that is related to $(t^1,t^2,\ldots,t^n)$ by a linear transformation $y^i=\Sigma_{j=1}^{n}L^i{}_j\,t^j$. The matrix L is not yet specified. Basis vectors generated by these coordinates are related as

$$\frac{\partial}{\partial t^j}=\sum_{i=1}^{n}\frac{\partial y^i}{\partial t^j}\frac{\partial}{\partial y^i}=\sum_{i=1}^{n}L^i{}_j\frac{\partial}{\partial y^i}, \tag{A5}$$

$$\frac{\partial}{\partial y^j}=\sum_{i=1}^{n}\frac{\partial t^i}{\partial y^j}\frac{\partial}{\partial t^i}=\sum_{i=1}^{n}(L^{-1})^i{}_j\frac{\partial}{\partial t^i}. \tag{A6}$$

Define vector subspaces M^- and M^+ of $\mathbf{R}^n$ as

$$M^-=\mathbf{R}\frac{\partial}{\partial t^1}\oplus\mathbf{R}\frac{\partial}{\partial t^3}\oplus\cdots\oplus\mathbf{R}\frac{\partial}{\partial t^{2m-1}}, \tag{A7}$$

$$M^+ = \mathbf{R}\frac{\partial}{\partial t^2} \oplus \mathbf{R}\frac{\partial}{\partial t^4} \oplus \cdots \oplus \mathbf{R}\frac{\partial}{\partial t^{2m}}. \tag{A8}$$

Then $M^- \oplus M^+ \oplus M^0 = \mathbf{R}^n$. Now let us remember that $\mathbf{R}^n$ is equipped with inner product structure. Then the two-form $B: \mathbf{R}^n \times \mathbf{R}^n \to \mathbf{R}$ can be regarded as an antisymmetric operator $\hat{B}: \mathbf{R}^n \to \mathbf{R}^n$. As a square of a linear operator $\hat{B}^2$ is well-defined and becomes a symmetric operator and therefore is diagonalizable by an orthogonal transformation. $\hat{B}^2$ has nonpositive eigenvalues. The eigenspace W^0 associated with the zero eigenvalue of $\hat{B}^2$ coincides with M^0. Of course,

$$\left\{ \frac{\partial}{\partial t^{2m+1}}, \frac{\partial}{\partial t^{2m+2}}, \ldots, \frac{\partial}{\partial t^n} \right\} \tag{A9}$$

is a basis of $M^0 = W^0$. We take an orthonormal basis

$$\left\{ \frac{\partial}{\partial y^{2m+1}}, \frac{\partial}{\partial y^{2m+2}}, \ldots, \frac{\partial}{\partial y^n} \right\} \tag{A10}$$

of W^0. This implies that

$$L^{2i-1}_{2m+r} = L^{2j}_{2m+r} = (L^{-1})^{2i-1}_{2m+r} = (L^{-1})^{2j}_{2m+r} = 0 \tag{A11}$$

in (A5) and (A6).

Let us step into a difficult part of the proof. Each eigenspace associated with each nonzero eigenvalue of $\hat{B}^2$ can be decomposed into two-dimensional subspaces such that each two-dimensional subspace W_j is irreducible with respect to the action of $\hat{B}$. Thus we get an orthogonal decomposition

$$\mathbf{R}^n = W_1 \perp W_2 \perp \cdots \perp W_m \perp W^0. \tag{A12}$$

Next we define vector subspaces

$$W_j^+ = W_j \cap (M^+ \oplus M^0), \tag{A13}$$

$$W_j^- = W_j \cap (M^+ \oplus M^0)^\perp, \tag{A14}$$

then we can show that both W_j^+ and W_j^- have one dimension. First, note that $\dim W_j^+ + \dim W_j^- = \dim W_j = 2$. If $\dim W_j^+ = 2$, W_j^+ coincides with W_j itself. Since the two-form B is degenerated on $(M^+ \oplus M^0)$, it must be degenerated also on $W_j = W_j^+ \subset (M^+ \oplus M^0)$. This contradicts the fact that W_j is irreducible with respect to $\hat{B}$. On the other hand, if $\dim W_j^- = 2$, W_j^- coincides with W_j itself. Then we can take an arbitrary one-dimensional subspace $M_{-1} \subset W_j = W_j^- \subset (M^+ \oplus M^0)^\perp$. Since W_j is irreducible with respect to $\hat{B}$, B is degenerated on $M_{-1} \oplus M^+ \oplus M^0$. This contradicts the fact that $M^+ \oplus M^0$ is a maximal degenerated subspace of B. Hence we conclude that $\dim W_j^+ = \dim W_j^- = 1$.

We take a normalized vector $\partial/\partial y^{2j}$ of W_j^+. And we take another normalized vector $\partial/\partial y^{2j-1}$ of W_j^- such that $\nu_j = B(\partial/\partial y^{2j-1}, \partial/\partial y^{2j}) > 0$ for each $j = 1, \ldots, m$. Then we obtain a complete orthonormal basis $\{\partial/\partial y^i \mid i = 1,2,\ldots,n\}$ that expresses B in the standard form $B = \Sigma_{j=1}^m \nu_j \, dy^{2j-1} \wedge dy^{2j}$.

Since $\partial/\partial y^{2q} \in W_q^+ \subset M^+ \oplus M^0$, we can say that

$$(L^{-1})^{2i-1}_{2q} = 0 \tag{A15}$$

in (A6). By an elementary argument of linear algebra we can say that

$$L_{2q}^{2i-1}=0. \tag{A16}$$

The proof is over.

APPENDIX B: FOURIER TRANSFORMATION OF THE HERMITE POLYNOMIALS

In our convention the Hermite polynomial is defined as

$$H_n(\xi)=(-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2}. \tag{B1}$$

The formula (7.10) can be deduced by a partial integration and a change of variables as

$$\begin{aligned}\int_{-\infty}^{\infty} dk\, e^{2\pi ikz}\cdot e^{\pi k^2/\nu}\left(-\frac{\partial}{\partial k}\right)^n e^{-2\pi k^2/\nu} &= \int_{-\infty}^{\infty} dk\, e^{-2\pi k^2/\nu}\left(\frac{\partial}{\partial k}\right)^n e^{2\pi ikz}\cdot e^{\pi k^2/\nu}\\ &= e^{\pi\nu z^2}\int_{-\infty}^{\infty} dk\, e^{-2\pi k^2/\nu}\left(\frac{\partial}{\partial k}\right)^n e^{\pi(k+i\nu z)^2/\nu}\\ &= e^{\pi\nu z^2}\int_{-\infty}^{\infty} dk\, e^{-2\pi k^2/\nu}\left(-\frac{i}{\nu}\frac{\partial}{\partial z}\right)^n e^{\pi(k+i\nu z)^2/\nu}\\ &= e^{\pi\nu z^2}\left(-\frac{i}{\nu}\frac{\partial}{\partial z}\right)^n \int_{-\infty}^{\infty} dk\, e^{-\pi(k-i\nu z)^2/\nu-2\pi\nu z^2}\\ &= e^{\pi\nu z^2}\left(-\frac{i}{\nu}\frac{\partial}{\partial z}\right)^n \sqrt{\nu}\, e^{-2\pi\nu z^2}.\end{aligned} \tag{B2}$$

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A class of vector coherent states defined over matrix domains

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(Received 27 May 2003; accepted 31 July 2003)

A general scheme is proposed for constructing vector coherent states, in analogy with the well-known canonical coherent states, and their deformed versions, when these latter are expressed as infinite series in powers of a complex variable z. In the present scheme, the variable z is replaced by matrix valued functions over appropriate domains. As particular examples, we analyze the quaternionic extensions of the canonical coherent states and the Gilmore–Perelomov and Barut–Girardello coherent states arising from representations of SU(1,1). Possible physical applications are indicated. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1617366]

I. INTRODUCTION

One way to define conventional coherent states, over complex domains, is by constructing linear superpositions $|z\rangle$, parametrized by a single complex number z, of vectors $\{\phi_m\}_{m=0}^{\infty}$, which form an orthonormal basis in an infinite dimensional, complex, separable Hilbert space $\mathfrak{H}$:

$$|z\rangle = \mathcal{N}(|z|)^{-1/2} \sum_{m=0}^{\infty} \frac{z^m}{\sqrt{\rho(m)}} \phi_m . \tag{1.1}$$

Here $\{\rho(m)\}_{m=0}^{\infty}$ is a sequence of nonzero, positive numbers, chosen so as to ensure the convergence of the sum in a nonempty open subset $\mathcal{D}$, of the complex plane, and $\mathcal{N}(|z|)$ is a normalization constant, ensuring the condition $\langle z|z\rangle = 1$. The coherent states $|z\rangle$ are also required to satisfy a resolution of the identity condition:

$$\int_{\mathcal{D}} |z\rangle\langle z| d\mu = I \quad , \tag{1.2}$$

where $d\mu$ is an appropriately chosen measure and I is the identity operator on the Hilbert space $\mathfrak{H}$. These coherent states are known to have a large number of interesting properties, linking them to physical applications, orthogonal polynomials, generalized oscillator algebras, etc.[2,8,13,15]

In this article we extend this definition to matrix domains, thereby generating families of vector coherent states. Vector coherent states are well-known mathematical objects, particularly when they are defined as orbits of vectors under the operators of unitary representations of groups (see, for example, Refs. 2, 4, 5, and 17). However, in the present article we take a completely different route for constructing them, although in special cases the link to a group representation will also emerge.

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II. VECTOR COHERENT STATES–THE GENERAL SETUP

Let $\mathcal{R}$ be a measure space, equipped with a measure $d\mathcal{R}$, and $\mathcal{K}$ a second measure space, equipped with a probability measure $d\mathcal{K}$. For $(r,k,\zeta)\in\mathcal{R}\times\mathcal{K}\times[0,2\pi)$, let

$$\mathcal{Z}=A(r)e^{i\zeta\Theta(k)}, \tag{2.1}$$

where $A(r),\Theta(k)$ are two (measurable) $n\times n$ matrix-valued functions with the following properties (assumed to hold for almost all $r\in\mathcal{R}$, with respect to the measure $d\mathcal{R}$ and almost all $k\in\mathcal{K}$, with respect to the measure $d\mathcal{K}$):

$$\Theta(k) \text{ is Hermitian, that is, } \Theta(k)=\Theta(k)^\dagger, \tag{2.2}$$

$$\Theta(k)^2=\mathbb{I}_n=n\times n \quad \text{unit matrix}, \tag{2.3}$$

$$[A(r),\Theta(k)]=A(r)\Theta(k)-\Theta(k)A(r)=0, \tag{2.4}$$

$$A(r)A(r)^\dagger=A(r)^\dagger A(r). \tag{2.5}$$

It is then straightforward to verify (e.g., by direct power series expansion) that

$$\mathcal{Z}=A(r)e^{i\zeta\Theta(k)}=A(r)[\cos\zeta+i\Theta(k)\sin\zeta]. \tag{2.6}$$

Let $\mathcal{D}=\mathcal{R}\times\mathcal{K}\times[0,2\pi)$ and define the measure $d\mu(r,k,\zeta)=d\mathcal{K}(k)d\mathcal{R}(r)d\zeta$ on it.

Let χ^j, $j=1,2,\ldots,n$, be an orthonormal basis in $\mathbb{C}^n$. Then, $\{\chi^j\otimes\phi_m\}$, $j=1,2,\ldots,n$, $m=0,1,2,\ldots,\infty$, is an orthonormal basis in $\hat{\mathfrak{H}}=\mathbb{C}^n\otimes\mathfrak{H}$. For each $\mathcal{Z}$ we define vector coherent states (VCS) as follows:

$$|\mathcal{Z},j\rangle=\mathcal{N}(|\mathcal{Z}|)^{-1/2}\sum_{m=0}^{\infty}\frac{\mathcal{Z}^m}{\sqrt{\rho(m)}}\chi^j\otimes\phi_m, \quad j=1,2,\ldots,n. \tag{2.7}$$

where, once again, $\mathcal{N}(|\mathcal{Z}|)$ is a normalization factor, which depends only on the positive part $|\mathcal{Z}|=[\mathcal{Z}\mathcal{Z}^\dagger]^{1/2}$ of the matrix $\mathcal{Z}$, and $\{\rho(m)\}_{m=0}^{\infty}$ is a sequence of nonzero positive numbers, with $\rho(0)=1$. These have to be chosen in a way such that the following two conditions are satisfied:

$$\text{normalization: } \sum_{j=0}^{n}\langle\mathcal{Z},j|\mathcal{Z},j\rangle=1, \tag{2.8}$$

$$\text{resolution of the identity: } \sum_{j=1}^{n}\int_{\mathcal{D}}W(|\mathcal{Z}|)|\mathcal{Z},j\rangle\langle\mathcal{Z},j|d\mu=\mathbb{I}_n\otimes I, \tag{2.9}$$

where $W(|\mathcal{Z}|)$ is an appropriately chosen positive weight function.

A straightforward computation, using the fact that

$$\mathcal{Z}^m=A(r)^m e^{im\zeta\Theta(k)}=A(r)^m(\cos m\zeta+i\Theta(k)\sin m\zeta),$$

shows that the normalization condition (2.8) implies the finiteness of the sum:

$$\mathcal{N}(|\mathcal{Z}|)=\sum_{m=0}^{\infty}\frac{\mathrm{Tr}|A(r)|^{2m}}{\rho(m)}, \tag{2.10}$$

($|A(r)|=[A(r)A(r)^\dagger]^{1/2}$ denoting the positive part of the matrix $A(r)$).

The resolution of the identity condition (2.9) imposes the following restriction on the weight function $W(|\mathcal{Z}|)$ and the matrices $A(r)$:

$$\int_{\mathcal{R}} \frac{2\pi W(|\mathcal{Z}|)|A(r)|^{2m}}{\mathcal{N}(|\mathcal{Z}|)} d\mathcal{R} = \rho(m)\mathbb{I}_n, \tag{2.11}$$

which can be interpreted as a sort of ''matrix moment condition.''

To see this we note that

$$\begin{aligned}
&\int_{\mathcal{D}} W(|\mathcal{Z}|)\sum_{j=1}^{n} |\mathcal{Z},j\rangle\langle\mathcal{Z},j| d\mu \\
&= \int_{\mathcal{D}} W(|\mathcal{Z}|)\sum_{j=1}^{n} \mathcal{N}(|\mathcal{Z}|)^{-1} \left| \sum_{m=0}^{\infty} \frac{\mathcal{Z}^m}{\sqrt{\rho(m)}} \chi^j \otimes \phi_m \right\rangle \left\langle \sum_{l=0}^{\infty} \frac{\mathcal{Z}^l}{\sqrt{\rho(l)}} \chi^j \otimes \phi_l \right| d\mu \\
&= \sum_{m=0}^{\infty}\sum_{l=0}^{\infty} \int_{\mathcal{D}} \frac{W(|\mathcal{Z}|)}{\mathcal{N}(|\mathcal{Z}|)\sqrt{\rho(m)\rho(l)}} A(r)^m e^{im\zeta\Theta(k)} \\
&\quad \times \left(\sum_{j=1}^{n} |\chi^j\rangle\langle\chi^j| \right) A(r)^{l\dagger} e^{-il\zeta\Theta(k)^\dagger} \otimes |\phi_m\rangle\langle\phi_l| d\mu .
\end{aligned}$$

Using

$$\sum_{j=1}^{n} |\chi^j\rangle\langle\chi^j| = \mathbb{I}_n, \quad \Theta(k)^\dagger = \Theta(k) \quad \text{and}$$

$$\int_0^{2\pi} e^{i(m-\ell)\zeta\Theta(k)} d\zeta = \begin{cases} 0 & \text{if } \ell \neq m \\ 2\pi\mathbb{I}_n & \text{if } \ell = m, \end{cases}$$

we reduce the last line to

$$\begin{aligned}
&\sum_{m=0}^{\infty} \int_{\mathcal{R}}\int_{\mathcal{K}} \frac{2\pi W(|\mathcal{Z}|)}{\mathcal{N}(|\mathcal{Z}|)\rho(m)} A(r)^m A(r)^{m\dagger} \otimes |\phi_m\rangle\langle\phi_m| d\mathcal{R} d\mathcal{K} \\
&= \sum_{m=0}^{\infty} \int_{\mathcal{R}}\int_{\mathcal{K}} \frac{2\pi W(|\mathcal{Z}|)}{\mathcal{N}(|\mathcal{Z}|)\rho(m)} |A(r)|^{2m} \otimes |\phi_m\rangle\langle\phi_m| d\mathcal{R} d\mathcal{K}.
\end{aligned}$$

Since $d\mathcal{K}$ is a probability measure, using the fact that $\Sigma_{m=0}^{\infty}|\phi_m\rangle\langle\phi_m| = I$ and imposing the condition (2.11), we immediately arrive at (2.9).

There is an associated matrix-valued reproducing kernel, $K(\mathcal{Z}^\dagger, \mathcal{Z}')$, with matrix elements,

$$\begin{aligned}
K_{j\ell}(\mathcal{Z}^\dagger, \mathcal{Z}') = \langle \mathcal{Z}, j | \mathcal{Z}', \ell \rangle &= \sum_{m=0}^{\infty} \frac{1}{\rho(m)\sqrt{\mathcal{N}(|\mathcal{Z}|)\mathcal{N}(|\mathcal{Z}'|)}} \\
&\quad \times \langle e^{-im(\zeta'\Theta(k') - \zeta\Theta(k))} A(r')^{m\dagger} A(r)^m \chi^j | \chi^\ell \rangle .
\end{aligned} \tag{2.12}$$

In view of (2.9), this kernel satisfies the reproducing condition,

$$\int_{\mathcal{D}} K(\mathcal{Z}^\dagger, \mathcal{Z}'') K(\mathcal{Z}''^\dagger, \mathcal{Z}') d\mu(k'', r'', \zeta'') = K(\mathcal{Z}^\dagger, \mathcal{Z}') . \tag{2.13}$$

III. GENERALIZED ANNIHILATION, CREATION AND NUMBER OPERATORS

There are a number of operators, associated with the coherent states (1.1), which define the so-called generalized oscillator algebras.[9,10,14,15] Similar operators can also be constructed in the

context of the VCS (2.7). In order to do that, let us first define $x_m=\rho(m)/\rho(m-1)$, for $m=1,2,3,\ldots$. Thus we write $\rho(m)=x_m x_{m-1}\cdots x_1=x_m!$ and define $x_0!=1$. The generalized annihilation or lowering operator, defined on the Hilbert space $\mathfrak{H}$, with respect to the basis $\{\phi_m\}_{m=0}^{\infty}$ is then written as

$$a\phi_m=\sqrt{x_m}\phi_{m-1} \quad \text{with} \quad a\phi_0=0\ . \tag{3.1}$$

In the case where $x_m=m$, we recover from this the standard annihilation operator for a harmonic oscillator. It is also easy to see that this operator acts on the coherent states $|z\rangle$ in the expected manner:

$$a|z\rangle=z|z\rangle\ .$$

Using a, we construct the creation or raising operator $a^\dagger$ and the number operator $N'=a^\dagger a$:

$$a^\dagger\phi_m=\sqrt{x_{m+1}}\phi_{m+1},\quad N'\phi_m=x_m\phi_m\ . \tag{3.2}$$

These three operators generate a Lie algebra (under composition given by the commutator bracket). This is the so-called generalized oscillator algebra, which we denote by $\mathfrak{A}_{\text{osc}}$. In general, the dimension of this algebra is not finite.

On the Hilbert space, $\mathbb{C}^n\otimes\mathfrak{H}$, of the VCS $|\mathcal{Z},j\rangle$, we define the corresponding operators as

$$A=\mathbb{I}_n\otimes a \quad \text{annihilation operator,} \tag{3.3}$$

$$A^\dagger=\mathbb{I}_n\otimes a^\dagger \quad \text{creation operator,} \tag{3.4}$$

$$N=\mathbb{I}_n\otimes N' \quad \text{number operator.} \tag{3.5}$$

They act on the VCS as

$$A|\mathcal{Z},j\rangle=\mathcal{Z}|\mathcal{Z},j\rangle\ , \tag{3.6}$$

$$A^\dagger|\mathcal{Z},j\rangle=\mathcal{N}(\mathcal{Z})^{-1/2}\sum_{m=0}^{\infty}\sqrt{\frac{x_{m+1}}{x_m!}}\ \mathcal{Z}^m\chi^j\otimes\phi_{m+1}\ , \tag{3.7}$$

$$N|\mathcal{Z},j\rangle=\mathcal{N}(\mathcal{Z})^{-1/2}\sum_{m=1}^{\infty}\frac{x_m}{\sqrt{x_m!}}\mathcal{Z}^m\chi^j\otimes\phi_m\ , \tag{3.8}$$

and generate the Lie algebra $\mathbb{I}_n\otimes\mathfrak{A}_{\text{osc}}$, which again is generally not finite dimensional.

Using the operators a and $a^\dagger$, we may also define the (formally) self-adjoint operators,

$$\hat{q}=\frac{a+a^\dagger}{\sqrt{2}} \quad \text{and} \quad \hat{p}=\frac{a-a^\dagger}{\sqrt{2}i}, \tag{3.9}$$

and the related operators

$$Q=\frac{A+A^\dagger}{\sqrt{2}}=\mathbb{I}_n\otimes\hat{q} \quad \text{and} \quad P=\frac{A-A^\dagger}{\sqrt{2}i}=\mathbb{I}_n\otimes\hat{p}\ . \tag{3.10}$$

We shall need these operators later, when constructing minimal uncertainty states.

To end this section, let us note that, as a consequence of the resolution of the identity (2.9), there is a natural isometric embedding of the Hilbert space of the VCS into a space of vector valued functions on the domain $\mathcal{D}$. Indeed, let $\tilde{\mathfrak{H}}=L^2(\mathcal{D},d\mu)$. Then,

$$\mathcal{W}:\mathbb{C}^n\otimes\mathfrak{H}\to\mathbb{C}^n\otimes\tilde{\mathfrak{H}},\quad \text{where}\quad (\mathcal{W}\Psi)^j(\mathcal{Z})=\langle\mathcal{Z},j|\Psi\rangle\,, \tag{3.11}$$

is easily seen to be an isometry.

IV. QUATERNIONIC CANONICAL COHERENT STATES

As a first example of our general construction, we build in this section VCS using the complex representation of quaternions by 2×2 matrices. Using the basis matrices,

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad i\sigma_1=\begin{pmatrix}0&i\\i&0\end{pmatrix},\quad -i\sigma_2=\begin{pmatrix}0&-1\\1&0\end{pmatrix},\quad i\sigma_3=\begin{pmatrix}i&0\\0&-i\end{pmatrix},$$

where σ_1, σ_2, and σ_3 are the usual Pauli matrices, a general quaternion is written as

$$\mathfrak{q}=x_0\sigma_0+i\underline{x}\cdot\underline{\sigma}$$

with $x_0\in\mathbb{R}$, $\underline{x}=(x_1,x_2,x_3)\in\mathbb{R}^3$ and $\underline{\sigma}=(\sigma_1,-\sigma_2,\sigma_3)$. Thus,

$$\mathfrak{q}=\begin{pmatrix}x_0+ix_3&-x_2+ix_1\\x_2+ix_1&x_0-ix_3\end{pmatrix}. \tag{4.1}$$

It is convenient to introduce the polar coordinates:

$$x_0=r\cos\theta,\quad x_1=r\sin\theta\sin\phi\cos\psi,\quad x_2=r\sin\theta\sin\phi\sin\psi,\quad x_3=r\sin\theta\cos\phi\,,$$

where $r\in[0,\infty)$, $\theta,\phi\in[0,\pi]$ and $\psi\in[0,2\pi)$. In terms of these,

$$\mathfrak{q}=A(r)e^{i\theta\sigma(\hat{n})}, \tag{4.2}$$

where

$$A(r)=r\sigma_0\,,\quad \sigma(\hat{n})=\begin{pmatrix}\cos\phi&\sin\phi e^{i\psi}\\\sin\phi e^{-i\psi}&-\cos\phi\end{pmatrix},\quad \text{and}\quad \sigma(\hat{n})^2=\sigma_0\,. \tag{4.3}$$

We denote the field of quaternions by $\mathbb{H}$.

The matrices $A(r)$ and $\sigma(\hat{n})$ satisfy the conditions (2.2)–(2.5). Thus, with $\{\phi_m\}_{m=0}^{\infty}$ an orthonormal basis of an abstract Hilbert space $\mathfrak{H}$ and χ^1,χ^2 an orthonormal basis of $\mathbb{C}^2$, we can define the VCS,

$$|\mathfrak{q},j\rangle=\mathcal{N}(|\mathfrak{q}|)^{-1/2}\sum_{m=0}^{\infty}\frac{\mathfrak{q}^m}{\sqrt{x_m!}}\chi^j\otimes\phi_m\in\mathbb{C}^2\otimes\mathfrak{H}\,,\quad j=1,2, \tag{4.4}$$

where $\mathcal{N}(|\mathfrak{q}|)$ and $x_m!$ have to be chosen appropriately.

In order to determine the normalization constant $\mathcal{N}(|\mathfrak{q}|)$, and the resolution of the identity, first note that in order for the norm of the vector $|\mathfrak{q},j\rangle$ to be finite, we must have

$$\langle\mathfrak{q},j|\mathfrak{q},j\rangle=\mathcal{N}(|\mathfrak{q}|)^{-1}\sum_{m=0}^{\infty}\frac{r^{2m}}{x_m!}<\infty\,.$$

Thus if $\lim_{m\to\infty}x_m=x$, we need to restrict r to $0\leqslant r<L=\sqrt{x}$ for the convergence of the above series. In this case, we define

$$\mathcal{D}=\{(r,\theta,\phi,\psi)|0\leqslant r<L\,,\quad 0\leqslant\phi\leqslant\pi\,,\quad 0\leqslant\theta,\psi<2\pi\}\,,$$

and note that

$$\mathcal{N}(|\mathfrak{q}|)=\mathcal{N}(r)=2\sum_{m=0}^{\infty}\frac{r^{2m}}{x_m!}.$$

[In the special case when $x_m=m$, $\mathcal{N}(|\mathfrak{q}|)=2\exp[r^2]$, and $\mathcal{D}=\mathbb{R}^+\times(0,2\pi]\times S^2$, where S^2 is the surface of the unit two-sphere and (ϕ,ψ) are the angular coordinates of a point on it. Note that in this case, $\mathcal{D}$ can also be identified with TS^2, the tangent bundle of S^2.] On $\mathcal{D}$ we introduce the measure $d\mu(r,\theta,\phi,\psi)=r\ dr\,d\theta\,d\Omega(\phi,\psi)$ with $d\Omega(\phi,\psi)=(1/4\pi)\ \sin\phi\,d\phi\,d\psi$.

To obtain a resolution of the identity, we now have to find a density function $W(|q|)=W(r)$, such that

$$\int_{\mathcal{D}}|\mathfrak{q},j\rangle W(r)\langle\mathfrak{q},j|\,d\mu=\mathbb{I}_2\otimes I\,. \tag{4.5}$$

Since

$$\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi}e^{i(m-l)\theta\sigma(\hat{n})}\sin\phi\,d\phi\,d\theta\,d\psi=\begin{cases}2\pi\ \ \mathbb{I}_2 & \text{if}\ \ m=l\\ 0 & \text{if}\ \ m\neq l,\end{cases}$$

the moment condition (2.11) becomes

$$\int_0^{\infty}\frac{2\pi W(r)r^{2m+1}}{\mathcal{N}(r)}\,dr\,\mathbb{I}_2=x_m!\,\mathbb{I}_2\,.$$

Writing $W(r)=[\mathcal{N}(r)/2\pi]\lambda(r)$, this is equivalent to solving the moment problem

$$\int_0^{L}\lambda(r)r^{2m+1}dr=x_m!\,, \tag{4.6}$$

for determining the auxiliary density $\lambda(r)$. With this choice of λ the resolution of the identity (4.5) will be satisfied. As an example, if $x_m!=m!$ we have $L=\infty$ and then $W(r)=2/\pi$. We shall call the corresponding VCS,

$$|\mathfrak{q},j\rangle=\frac{e^{-r^2/2}}{\sqrt{2}}\sum_{m=0}^{\infty}\frac{\mathfrak{q}^m}{\sqrt{m!}}\chi^j\otimes\phi_m\in\mathbb{C}^2\otimes\mathfrak{H}\,, \tag{4.7}$$

quaternionic canonical coherent states. These are the natural generalizations, to quaternions, of the well known *canonical coherent states*.[2]

$$|z\rangle=e^{-r^2/2}\sum_{m=0}^{\infty}\frac{z^m}{\sqrt{m!}}\phi_m\in\mathfrak{H}\,, \tag{4.8}$$

defined over $\mathbb{C}$. Treating the vectors $|\mathfrak{q},1\rangle$ and $|\mathfrak{q},2\rangle$ as elements of a basis, we shall define a general quaternionic VCS as a linear combination,

$$|\mathfrak{q},\chi\rangle=\sum_{j=1}^{2}c_j|\mathfrak{q},j\rangle,\quad\text{where}\quad c_1,c_2\in\mathbb{C},\quad |c_1|^2+|c_2|^2=1\ ,\quad \chi=\sum_{j=1}^{2}c_j\chi^j\,. \tag{4.9}$$

V. MINIMUM UNCERTAINTY AND ANALYTICITY PROPERTIES

It is well known that the canonical coherent states (4.8) are also states of minimum uncertainty, in the sense that for any one of these states $|z\rangle$,

$$\langle\Delta\hat{q}\rangle_z\langle\Delta\hat{p}\rangle_z=\tfrac{1}{2}\quad(\text{assuming}\quad\hbar=1)\,, \tag{5.1}$$

where, for any operator A on $\mathfrak{H}$ and any vector $\phi \in \mathfrak{H}$,

$$\langle \Delta A \rangle_\phi = [\langle \phi | A^2 \phi \rangle - (\langle \phi | A \phi \rangle)^2]^{1/2}.$$

It is possible to construct quaternionic VCS with similar properties. To see this, first note that the matrix $\mathfrak{q}$ can be diagonalized as

$$\mathfrak{q} = u(\theta,\phi) \begin{pmatrix} z & 0 \\ 0 & \overline{z} \end{pmatrix} u(\theta,\phi)^\dagger, \tag{5.2}$$

where

$$u(\theta,\phi) = \begin{pmatrix} ie^{i\phi/2}\cos\frac{\theta}{2} & -e^{i\phi/2}\sin\frac{\theta}{2} \\ e^{-i\phi/2}\sin\frac{\theta}{2} & -ie^{-i\phi/2}\cos\frac{\theta}{2} \end{pmatrix} \quad \text{and} \quad z = re^{i\psi}.$$

Let $\chi^+(\theta,\phi)$ and $\chi^-(\theta,\phi)$ be the two (normalized) eigenvectors of $\mathfrak{q}$, corresponding to the eigenvalues z and $\overline{z}$, respectively. Define the two quaternionic VCS,

$$|\mathfrak{q},+\rangle = e^{-r^2/2} \sum_{m=0}^{\infty} \frac{\mathfrak{q}^m}{\sqrt{m!}} \chi^+(\theta,\phi) \otimes \phi_m = e^{-r^2/2} \sum_{m=0}^{\infty} \frac{z^m}{\sqrt{m!}} \chi^+(\theta,\phi) \otimes \phi_m, \tag{5.3}$$

$$|\mathfrak{q},-\rangle = e^{-r^2/2} \sum_{m=0}^{\infty} \frac{\mathfrak{q}^m}{\sqrt{m!}} \chi^-(\theta,\phi) \otimes \phi_m = e^{-r^2/2} \sum_{m=0}^{\infty} \frac{\overline{z}^m}{\sqrt{m!}} \chi^-(\theta,\phi) \otimes \phi_m. \tag{5.4}$$

The normalization of these states has been chosen to ensure that $\langle \mathfrak{q},\pm|\mathfrak{q},\pm\rangle = 1$. From the nature of the operators Q and P, defined in (3.10), it is then clear that these states also have minimum uncertainty:

$$\langle \Delta Q \rangle_\pm \langle \Delta P \rangle_\pm = \tfrac{1}{2}. \tag{5.5}$$

Next, let us look a little more closely at the nature of the isometry (3.11), for the quaternionic VCS. Recall that in this case, $\mathcal{D} = \mathbb{R}^+ \times (0,2\pi] \times S^2 \simeq TS^2$. Once again, let $\tilde{\mathfrak{H}} = L^2(\mathcal{D}, d\mu)$. We are interested in the isometry

$$\mathcal{W}: \mathbb{C}^2 \otimes \mathfrak{H} \to \mathbb{C}^2 \otimes \tilde{\mathfrak{H}} \quad \text{with} \quad (\mathcal{W}\mathbf{\Psi})^j(\mathfrak{q}) = \langle \mathbf{\Psi} | \mathfrak{q}, j \rangle. \tag{5.6}$$

A general vector $\mathbf{\Psi} \in \mathbb{C}^2 \otimes \mathfrak{H}$ has the form $\mathbf{\Psi} = \Sigma_{j=1}^2 \chi^j \psi_j$, with $\psi_j \in \mathfrak{H}$. We write $\mathbf{F} = \mathcal{W}\mathbf{\Psi}$ and introduce the functions

$$f_j(z) = \sum_{m=0}^{\infty} \frac{z^m}{\sqrt{m!}} \langle \phi_m | \psi_j \rangle_{\mathfrak{H}}, \quad j = 1,2, \quad \mathbf{f}(z) = \sum_{j=1}^{2} \chi^j f_j(z),$$

$$f_j(\overline{z}) = \sum_{m=0}^{\infty} \frac{\overline{z}^m}{\sqrt{m!}} \langle \phi_m | \psi_j \rangle_{\mathfrak{H}}, \quad j = 1,2, \quad \mathbf{f}(\overline{z}) = \sum_{j=1}^{2} \chi^j f_j(\overline{z}).$$

A straightforward computation then shows that the image of the isometry (5.6) consists of vector valued functions of the type

$$\mathbf{F}(z,\overline{z},\theta,\phi) = \frac{1}{\sqrt{2}} e^{-|z|^2/2} [\mathbb{P}^+(\theta,\phi)\mathbf{f}(\overline{z}) + \mathbb{P}^-(\theta,\phi)\mathbf{f}(z)], \tag{5.7}$$

where $\mathbb{P}^{\pm}(\theta,\phi)$ are eigenprojectors corresponding to the eigenvectors $\chi^{\pm}(\theta,\phi)$, respectively. Thus, for fixed (θ,ϕ), each component function $F^j(z,\overline{z},\theta,\phi)$ is a linear combination of two holomorphic functions $f_1(z), f_2(z)$ and their antiholomorphic counterparts.

VI. RELATION TO THE WEYL–HEISENBERG GROUP

The canonical coherent states (4.8) can be expressed (see, for example, Ref. 2) in the form

$$|z\rangle = e^{za^\dagger - \overline{z}a}\phi_0 = e^{i(p\hat{q}-q\hat{p})}\phi_0, \quad \text{where} \quad z=\frac{q-ip}{\sqrt{2}}. \tag{6.1}$$

We now show that the quaternionic canonical coherent states (4.7) also have the analogous representation:

$$|\mathfrak{q},j\rangle = \frac{1}{\sqrt{2}} e^{\mathfrak{q}\otimes a^\dagger - \mathfrak{q}^\dagger\otimes a}\chi^j\otimes\phi_0. \tag{6.2}$$

To see this, note that

$$[\mathfrak{q}^\dagger\otimes a, \mathfrak{q}\otimes a^\dagger] = r^2\mathbb{I}_2\otimes I.$$

Next, since for two operators A and B, the commutator of which commutes with both A and B, the Baker–Campbell–Hausdorff identity,

$$e^{A+B} = e^{-(1/2)[A,B]}e^A e^B,$$

holds, we may write

$$e^{\mathfrak{q}\otimes a^\dagger - \mathfrak{q}^\dagger\otimes a} = e^{-(1/2)[\mathfrak{q}\otimes a^\dagger, -\mathfrak{q}^\dagger\otimes a]} e^{\mathfrak{q}\otimes a^\dagger} e^{-\mathfrak{q}^\dagger\otimes a}.$$

Since $a^m\phi_0 = 0$ for all $m\geqslant 1$, we have

$$e^{-\mathfrak{q}\otimes a}\chi^j\otimes\phi_0 = \chi^j\otimes\phi_0$$

and

$$e^{\mathfrak{q}\otimes a^\dagger}(\chi^j\otimes\phi_0) = \sum_{m=0}^{\infty}\frac{(\mathfrak{q}\otimes a^\dagger)^m}{m!}\chi^j\otimes\phi_0 = \sum_{m=0}^{\infty}\frac{\mathfrak{q}^m\chi^j\otimes a^{\dagger m}\phi_0}{m!} = \sum_{m=0}^{\infty}\frac{\mathfrak{q}^m}{\sqrt{m!}}\chi^j\otimes\phi_m.$$

Thus,

$$\frac{1}{\sqrt{2}}e^{\mathfrak{q}\otimes a^\dagger - \mathfrak{q}^\dagger\otimes a}\chi^j\otimes\phi_0 = \frac{1}{\sqrt{2}}e^{-r^2/2}\sum_{m=0}^{\infty}\frac{\mathfrak{q}^m}{\sqrt{m!}}\chi^j\otimes\phi_m = |\mathfrak{q},j\rangle.$$

To develop a group theoretical interpretation for the quaternionic canonical coherent states, we go back to the canonical coherent states as written out in (6.1). The operators $\hat{q},\hat{p}$ and I generate an irreducible representation of $\mathfrak{g}_{\mathrm{W-H}}$, the Lie algebra of the Weyl–Heisenberg group $G_{\mathrm{W-H}}$, on the Hilbert space $\mathfrak{H}$. A unitary irreducible representation of $G_{\mathrm{W-H}}$ on $\mathfrak{H}$ is given by the operators $U(\vartheta,q,p) = e^{i(\vartheta I + p\hat{q} - q\hat{p})}$. Thus, $|z\rangle = U(0,q,p)\phi_0$. Turning now to the quaternionic canonical coherent states, as expressed in (6.2), we find, using (5.2),

$$\mathfrak{q}\otimes a^\dagger - \mathfrak{q}^\dagger\otimes a = u(\theta,\phi)\begin{pmatrix} za^\dagger - \overline{z}a & 0 \\ 0 & \overline{z}a^\dagger - za \end{pmatrix} u(\theta,\phi)^\dagger.$$

Thus,

$$e^{\mathfrak{q}\otimes a^\dagger-\mathfrak{q}^\dagger\otimes a}=u(\theta,\phi)\begin{pmatrix}U(0,q,p) & 0\\ 0 & U(0,q,-p)\end{pmatrix}u(\theta,\phi)^\dagger. \tag{6.3}$$

Writing

$$\tilde{U}(\vartheta,\mathfrak{q})=\tilde{U}(\vartheta,q,p,\theta,\phi):=u(\theta,\phi)\begin{pmatrix}U(\vartheta,q,p) & 0\\ 0 & U(\vartheta,q,-p)\end{pmatrix}u(\theta,\phi)^\dagger, \tag{6.4}$$

we observe that for fixed (θ,ϕ) these operators realize a unitary (reducible) representation of $G_{\mathrm{W-H}}$ on $\mathbb{C}^2\otimes\mathfrak{H}$. In terms of these operators,

$$|\mathfrak{q},j\rangle=\frac{1}{\sqrt{2}}\tilde{U}(0,\mathfrak{q})\chi^j\otimes\phi_0=\frac{1}{\sqrt{2}}\tilde{U}(0,q,p,\theta,\phi)\chi^j\otimes\phi_0, \tag{6.5}$$

in complete analogy with the case of the canonical coherent states.

VII. QUATERNIONIC VCS FROM SU(1,1) REPRESENTATIONS

As a second example of the construction of VCS using quaternions, we shall obtain analogs of the Gilmore–Perelomov[12,16] and Barut–Girardello[6] coherent states in this section. Both these families of states arise from the discrete series representations of SU(1,1). Writing $\mathcal{D}_1=\{z\in\mathbb{C}||z|<1\}$, the Gilmore–Perelomov coherent states, labeled by points of $\mathcal{D}_1$, are defined to be

$$|z;\mathrm{G-P}\rangle=(1-r^2)^\kappa\ \sum_{m=0}^{\infty}\left[\frac{(2\kappa)_m}{m!}\right]^{1/2}z^m\phi_m\in\mathfrak{H},\quad r=|z|,\quad \kappa=1,\frac{3}{2},2,\frac{5}{2},\ldots, \tag{7.1}$$

where we have used the Pochhammer symbol,

$$(a)_m=\frac{\Gamma(a+m)}{\Gamma(a)}=a(a+1)(a+2)\cdots(a+m-1),$$

and, as before, the ϕ_m constitute an orthonormal basis of the Hilbert space $\mathfrak{H}$. The index κ labels the unitary irreducible representation of SU(1,1), to which the above coherent states are associated. This representation is carried by the Hilbert space $\mathfrak{H}_{\mathrm{hol}}(\mathcal{D}_1)$, which is the subspace of all holomorphic functions in $L^2(\mathcal{D}_1,(2\kappa-1)d\mu_\kappa)$, where

$$d\mu_\kappa(z,\bar{z})=\frac{(1-r^2)^{2\kappa-2}}{\pi}rdrd\theta,\quad z=re^{i\theta}.$$

An element $g\in\mathrm{SU}(1,1)$ is a complex 2×2 matrix,

$$g=\begin{pmatrix}\alpha & \beta\\ \bar{\beta} & \bar{\alpha}\end{pmatrix},\quad \det g=|\alpha|^2-|\beta|^2=1,$$

and the unitary irreducible representation U^κ, labeled by κ, acts on vectors $f\in\mathfrak{H}_{\mathrm{hol}}(\mathcal{D}_1)$ in the manner

$$(U^\kappa(g)f)(z)=(\alpha-\bar{\beta}z)^{-2\kappa}\ f\left(\frac{\bar{\alpha}z-\beta}{\alpha-\bar{\beta}z}\right).$$

The monomials

$$u_m(z)=\left[\frac{(2\kappa)_m}{m!}\right]^{1/2} z^m$$

form an orthonormal basis in $\mathfrak{H}_{\rm hol}(\mathcal{D}_1)$. Moreover, identifying the abstract Hilbert space $\mathfrak{H}$ with $\mathfrak{H}_{\rm hol}(\mathcal{D}_1)$ and ϕ_m with u_m, it can be shown[2] that the coherent states (7.1) can also be written in the form

$$|z;\mathrm{G-P}\rangle = U^\kappa(\mathcal{Z})\phi_0\,, \quad \text{where} \quad \mathcal{Z}=\frac{1}{\sqrt{1-r^2}}\begin{pmatrix}1 & z\\ \bar z & 1\end{pmatrix}\in \mathrm{SU}(1,1)\,. \tag{7.2}$$

Observe that, in the notation introduced in (1.1), in this case we have

$$\mathcal{N}(|z|)=(1-r^2)^{-2\kappa}, \quad \rho(m)=\left[\frac{(2\kappa)_m}{m!}\right]^{-1}.$$

Thus, $x_m=m/(2\kappa+m-1)$ and since $\lim_{m\to\infty} x_m=1$, this determines the radius of convergence of the infinite series in (7.1) and hence the appearance of the unit disc.

The coherent states (7.1) satisfy the resolution of the identity,

$$\frac{2\kappa-1}{\pi}\int_{\mathcal{D}_1}|z;\mathrm{G-P}\rangle\langle z;\mathrm{G-P}|\,\frac{r\,dr\,d\theta}{(1-r^2)^2}=I\,. \tag{7.3}$$

The representation of the Lie algebra of SU(1,1) on $\mathfrak{H}_{\rm hol}(\mathcal{D}_1)$ is generated by the three operators K_+, K_- and K_3, which satisfy the commutation relations

$$[K_3,K_\pm]=\pm K_\pm\,, \quad [K_-,K_+]=2K_3\,. \tag{7.4}$$

They act on the vectors ϕ_m in the manner

$$K_-\phi_m=\sqrt{m(2\kappa+m-1)}\,\phi_{m-1}\,, \quad K_+=K_-^\dagger\,, \quad K_3\phi_m=(\kappa+m)\phi_m\,. \tag{7.5}$$

Thus $K_-\phi_0=0$ and

$$\phi_m=\frac{1}{\sqrt{m!\,(2\kappa)_m}}K_+^m\phi_0\,.$$

Furthermore, it can be shown[11] that

$$|z;\mathrm{G-P}\rangle=e^{wK_+-\bar wK_-}\phi_0\,, \quad w\in\mathbb{C}, \tag{7.6}$$

where z and w are related by

$$z=\frac{w\tanh(|w|)}{|w|}. \tag{7.7}$$

Equation (7.6) should be compared to (6.1). Note, however, that unlike in that case, the operators K_+ and K_- appearing in (7.6) are not the creation and annihilation operators naturally associated with the expansion in (7.1) [see (3.1)]. Indeed, in the present case the operator a (which we denote $a_{\mathrm{G-P}}$) has the form

$$a_{\mathrm{G-P}}|z;\mathrm{G-P}\rangle=z|z;\mathrm{G-P}\rangle\,, \quad a_{\mathrm{G-P}}\phi_m=\sqrt{\frac{m}{2\kappa+m-1}}\,\phi_{m-1}\,. \tag{7.8}$$

On the other hand, it is possible to define[6] a second set of coherent states $|w;\mathrm{B}-\mathrm{G}\rangle$ for this same representation of SU(1,1), using K_- as the generalized annihilation operator:

$$K_-|w;\mathrm{B}-\mathrm{G}\rangle := a_{\mathrm{B}-\mathrm{G}}|w;\mathrm{B}-\mathrm{G}\rangle = w|w;\mathrm{B}-\mathrm{G}\rangle, \quad w\in\mathbb{C}. \tag{7.9}$$

These states, known as the Barut–Girardello coherent states, are defined for all $w\in\mathbb{C}$ and they are of the form

$$|w;\mathrm{B}-\mathrm{G}\rangle = \frac{|w|^{2\kappa-1}}{\sqrt{I_{2\kappa-1}(2|w|)}}\sum_{m=0}^{\infty}\frac{w^m}{\sqrt{m!(2\kappa+m-1)!}}\phi_m, \tag{7.10}$$

where $I_\nu(x)$ is the order-ν modified Bessel function of the first kind. These coherent states satisfy the resolution of the identity

$$\frac{2}{\pi}\int_{\mathbb{C}}|w;\mathrm{B}-\mathrm{G}\rangle\langle w;\mathrm{B}-\mathrm{G}|K_{2\kappa-1}(2\varrho)I_{2\kappa-1}(2\varrho)\varrho\,d\varrho\,d\vartheta = I, \quad w=\varrho e^{i\vartheta}, \tag{7.11}$$

where, again, $K_\nu(x)$ is the order-ν modified Bessel function of the second kind.

It is now straightforward to write down quaternionic VCS which extend (7.1):

$$|\mathfrak{q},j;\mathrm{G}-\mathrm{P}\rangle = \frac{(1-r^2)^\kappa}{\sqrt{2}}\sum_{m=0}^{\infty}\left[\frac{(2\kappa)_m}{m!}\right]^{1/2}\mathfrak{q}^m\chi^j\otimes\phi_m, \quad r=|\mathfrak{q}|=[\mathfrak{q}\mathfrak{q}^\dagger]^{1/2}, \tag{7.12}$$

where $\mathfrak{q}$ is a quaternionic variable with domain $\mathcal{D}_1\times S^2$, and a similar set of VCS extending (7.10):

$$|\mathfrak{w},j;\mathrm{B}-\mathrm{G}\rangle = \frac{r^{2\kappa-1}}{\sqrt{2I_{2\kappa-1}(2r)}}\sum_{m=0}^{\infty}\frac{\mathfrak{w}^m}{\sqrt{m!(2\kappa+m-1)!}}\chi^j\otimes\phi_m, \quad r=|\mathfrak{w}|, \tag{7.13}$$

the quaternionic variable $\mathfrak{w}$ being defined over the domain TS^2.

In the case of the vectors (7.12), it is also possible, using (7.2), to give a representation theoretic interpretation along the lines of (6.2)–(6.5). Indeed, by virtue of (7.1), (7.2) and the decomposition (5.2) of the quaternion $\mathfrak{q}$, we can immediately rewrite (7.12) as

$$|\mathfrak{q},j;\mathrm{G}-\mathrm{P}\rangle = \frac{1}{\sqrt{2}}u(\theta,\phi)\begin{pmatrix}U^\kappa(\mathcal{Z}) & 0\\ 0 & U^\kappa(\mathcal{Z}^\dagger)\end{pmatrix}u(\theta,\phi)^\dagger\chi^j\otimes\phi_0.$$

Writing

$$\tilde{U}^\kappa(\mathfrak{q}) = u(\theta,\phi)\begin{pmatrix}U^\kappa(\mathcal{Z}) & 0\\ 0 & U^\kappa(\mathcal{Z}^\dagger)\end{pmatrix}u(\theta,\phi)^\dagger,$$

this yields

$$|\mathfrak{q},j;\mathrm{G}-\mathrm{P}\rangle = \frac{1}{\sqrt{2}}\tilde{U}^\kappa(\mathfrak{q})\chi^j\otimes\phi_0, \tag{7.14}$$

which is the analog of (6.5). Moreover, since by (7.6)

$$\tilde{U}^\kappa(\mathfrak{q})\chi^j\otimes\phi_0 = u(\theta,\phi)\begin{pmatrix}e^{wK_+-\bar{w}K_-} & 0\\ 0 & e^{\bar{w}K_+-wK_-}\end{pmatrix}u(\theta,\phi)^\dagger\chi^j\otimes\phi_0$$

with z and w being related by (7.7), we can now transform this to

$$|\mathfrak{q},j;\mathrm{G-P}\rangle=\frac{1}{\sqrt{2}}e^{\mathfrak{w}\otimes K_+-w^\dagger\otimes K_-}\chi^j\otimes\phi_0\,, \tag{7.15}$$

where now the quaternionic variables $\mathfrak{q}$ and $\mathfrak{w}$ are related by

$$\mathfrak{q}=\frac{\mathfrak{w}\tanh(|\mathfrak{w}|)}{|\mathfrak{w}|}. \tag{7.16}$$

Note that while $0\leqslant|\mathfrak{q}|<1$, for the transformed variable $\mathfrak{w}$ we have $0\leqslant|\mathfrak{w}|<\infty$.

Interestingly, there is yet another family of coherent states, again related to the SU(1,1) group, which can be constructed using the two number operators,

$$N_{\mathrm{G-P}}=a^\dagger_{\mathrm{G-P}}a_{\mathrm{G-P}}\quad\text{and}\quad N_{\mathrm{B-G}}=a^\dagger_{\mathrm{B-G}}a_{\mathrm{B-G}}.$$

Indeed, from (7.8) and (7.9),

$$N_{\mathrm{G-P}}\phi_m=\frac{m}{2\kappa+m-1}\phi_m\quad\text{and}\quad N_{\mathrm{B-G}}\phi_m=m(2\kappa+m-1)\phi_m\,. \tag{7.17}$$

Thus we define a third number operator N_{INT}, essentially as one which interpolates between these two:

$$N_{\mathrm{G-P}}N_{\mathrm{INT}}=N_{\mathrm{B-G}}\Rightarrow N_{\mathrm{INT}}\phi_m=(2\kappa+m-1)^2\phi_m\,, \tag{7.18}$$

and the related annihilation operator,

$$a_{\mathrm{INT}}\phi_m=(2\kappa+m-1)\phi_{m-1}\,. \tag{7.19}$$

The corresponding coherent states, defined for all $w\in\mathbb{C}$, are

$$|w;\mathrm{INT}\rangle=\mathcal{N}(r)^{-1/2}\sum_{m=0}^{\infty}\frac{w^m}{(2\kappa+m-1)!}\phi_m\,,\quad r=|w|\,, \tag{7.20}$$

where the normalization constant is given by

$$\mathcal{N}(r)=\frac{{}_1F_2(1;2\kappa,2\kappa;r^2)}{[\Gamma(2\kappa)]^2},$$

in terms of the hypergeometric function

$${}_1F_2(a;b,c;x)=\sum_{m=0}^{\infty}\frac{(a)_m}{(b)_m(c)_m}\cdot\frac{x^m}{m!}.$$

The moment problem for determining the resolution of the identity is now

$$\pi\int_0^\infty r^m\lambda(r)dr=[(2\kappa+m-1)!]^2\,.$$

This can be explicitly solved to yield

$$\lambda(r)=\frac{2}{\pi}r^{2\kappa-1}K_0(2\sqrt{r})\,,$$

where, once again, K_0 is the order-0 modified Bessel function of the second kind. Finally, one obtains

$$\int_{\mathbb{C}} |w;\mathrm{INT}\rangle\langle w;\mathrm{INT}|\, d\mu_{\mathrm{INT}}(w,\overline{w}) = I\,, \tag{7.21}$$

with

$$d\mu_{\mathrm{INT}}(w,\overline{w}) = \frac{2r^{4\kappa-1}}{\pi[\Gamma(2\kappa)]^2} K_0(2r)\ \ {}_1F_2(1;2\kappa,2\kappa;r^2)\, d\theta dr\,. \tag{7.22}$$

The corresponding quaternionic VCS are then

$$|\mathfrak{w},j;\mathrm{INT}\rangle = \frac{1}{\sqrt{2}}\ \frac{\Gamma(2\kappa)}{[{}_1F_2(1;2\kappa,2\kappa;r^2)]^{1/2}} \sum_{m=0}^{\infty} \frac{\mathfrak{w}^m}{(2\kappa+m-1)!}\, \chi^j \otimes \phi_m\,, \tag{7.23}$$

where $r=|\mathfrak{w}|$ and $\mathfrak{w}\in TS^2$.

The fact that the coherent states (7.20) are indeed related to the SU(1,1) group is brought out more clearly by the following observation: computing the commutator $[a_{\mathrm{INT}}, a_{\mathrm{INT}}^\dagger]$ we find

$$[a_{\mathrm{INT}}, a_{\mathrm{INT}}^\dagger]\phi_m = [2(2\kappa+m)-1]\phi_m\,.$$

Let us define a new ''number operator'' $\tilde{N}_{\mathrm{INT}}$ by the action

$$\tilde{N}_{\mathrm{INT}}\phi_m = (2\kappa+m-\tfrac{1}{2})\phi_m \tag{7.24}$$

on the basis vectors ϕ_m. Then we easily establish the commutation relations,

$$[a_{\mathrm{INT}}, a_{\mathrm{INT}}^\dagger] = 2\tilde{N}_{\mathrm{INT}}, \quad [\tilde{N}_{\mathrm{INT}}, a_{\mathrm{INT}}^\dagger] = a_{\mathrm{INT}}^\dagger, \quad [\tilde{N}_{\mathrm{INT}}, a_{\mathrm{INT}}] = -a_{\mathrm{INT}}\,. \tag{7.25}$$

Comparing with (7.4), we find that the three operators $a_{\mathrm{INT}}, a_{\mathrm{INT}}^\dagger$ and $\tilde{N}_{\mathrm{INT}}$ satisfy exactly the same commutation relations as the three generators, K_-, K_+ and K_3 of $\mathfrak{su}(1,1)$, the Lie algebra of SU(1,1). Thus, they also realize a representation of this algebra on $\mathfrak{H}$. The two number operators $\tilde{N}_{\mathrm{INT}}$ and N_{INT} are related as

$$N_{\mathrm{INT}} = \tilde{N}_{\mathrm{INT}}^2 - \tilde{N}_{\mathrm{INT}} + \tfrac{1}{4} = [\tilde{N}_{\mathrm{INT}} - \tfrac{1}{2}]^2\,. \tag{7.26}$$

A similar situation was seen to arise[3] in the case of temporally stable coherent states related to the infinite well and Pöschl–Teller potentials, where the Lie algebra $\mathfrak{su}(1,1)$ appeared as a dynamical algebra. It ought to be pointed out, however, that the representation of $\mathfrak{su}(1,1)$, generated by the operators $K_\pm, K_3$ in (7.4) and (7.5), is different from the one generated by the operators $a_{\mathrm{INT}}^\dagger$, a_{INT} and $\tilde{N}_{\mathrm{INT}}$. Indeed, computing the Casimir operators in the two cases, we find that $1/2(K_-K_+ + K_+K_-) - K_3^2 = \kappa(1-\kappa)$ while $\frac{1}{2}(a_{\mathrm{INT}}a_{\mathrm{INT}}^\dagger + a_{\mathrm{INT}}^\dagger a_{\mathrm{INT}}) - \tilde{N}_{\mathrm{INT}}^2 = \frac{1}{4}$.

VIII. CONCLUSION AND PHYSICAL APPLICATIONS

As amply evident from the above discussion, the method just elaborated for constructing vector coherent states is generic. One could in this manner associate families of VCS to almost any hypergeometric function. More interestingly, the method enables one to associate VCS to certain Clifford algebras and to reducible representations from the principal series of locally compact groups. Some of these results will be presented in a forthcoming publication.[1]

As far as physical applications are concerned, there is a range of possibilities. The quaternionic canonical VCS in (4.7) can be looked upon as amalgams of standard spin-coherent states (as described, for example, in Ref. 16) and the (scalar) canonical coherent states. Thus, $|\mathfrak{q},j\rangle$ can

be considered as a coherent state wave function for a nonrelativistic spinning particle. Suppose that such a particle is placed in a constant external magnetic field $\vec{B}=(B_1,B_2,B_3)$. Its time evolution is then governed by an interaction Hamiltonian of the type $V_I=k\vec{\sigma}\cdot\vec{B}=\omega\Theta(\hat{B})$, where k is a constant, $\vec{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$, $\omega=(\sqrt{3}/2)k\|\vec{B}\|$, $\hat{B}=\vec{B}/\|\vec{B}\|$ and $\Theta(\hat{B})=(2/\sqrt{3})\,\sigma(\hat{B})$. The time evolution generated by this Hamiltonian on a state $\mathbf{\Psi}\in\mathbb{C}^2\otimes\mathfrak{H}$ is given by $\mathbf{\Psi}(t)=e^{i\omega\Theta(\hat{B})t}\mathbf{\Psi}$. Thus, the quaternionic canonical VCS

$$|\mathfrak{q}(t),j\rangle=\frac{e^{-r^2/2}}{\sqrt{2}}\sum_{m=0}^{\infty}\frac{\mathfrak{q}(t)^m}{\sqrt{m!}}\chi^j\otimes\phi_m,\quad \mathfrak{q}(t)=\|\vec{B}\|\;\; e^{i\omega\Theta(\hat{B})t}, \tag{8.1}$$

have immediate interpretation as *coherent* superpositions of time evolved basis states. The discussion in Sec. V now shows that such states have minimum uncertainty whenever the spin is either parallel or anti-parallel to the magnetic field. A second example of the use of quaternionic VCS arises in the study of two-level atoms interacting with a single mode of an electromagnetic field. This leads to coherent states resulting from a Jaynes–Cummings[7] type of Hamiltonian. A fuller description of this construction has been given in Ref. 1. One might state, with justification, that quaternionic VCS could be an extremely useful tool in the study of two-level atomic systems, placed in electromagnetic fields. As a third physical example, the creation and annihilation operators for the VCS (7.23) would generate a dynamical algebra for a spin-$\frac{1}{2}$ particle placed in a Pöschl–Teller potential, in analogy with the discussion in Ref. 3.

ACKNOWLEDGMENTS

We would like to thank M. Bertola for interesting discussions. This work was partly supported by research grants from the NSERC (Canada) and the FCAR (Québec).

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Phase space methods for particles on a circle

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(Received 15 March 2003; accepted 29 July 2003)

The phase space $S\times Z$ for a particle on a circle is considered. Displacement operators in this phase space are introduced and their properties are studied. Wigner and Weyl functions in this context are also considered and their physical interpretation and properties are discussed. All results are compared and contrasted with the corresponding ones for the harmonic oscillator in the $R\times R$ phase space. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1616997]

I. INTRODUCTION

Since the work of Wigner[1] and Moyal,[2] phase space methods have been used extensively in quantum mechanics. A lot of this work is for the harmonic oscillator where both the position and momentum take values in the real line R and the phase space is the plane $R\times R$. There has also been work on finite quantum systems,[3,4] where both the position and momentum take values in Z_N (the integers module N) and the phase space is the lattice $Z_N\times Z_N$. The purpose of this paper is to study phase space methods for quantum particles on a circle. In this case the position takes values on a circle S and the momentum take discrete values in Z (the integers times a factor). In this case the phase space is $S\times Z$. We note that in any area where there is Fourier transform involved (e.g., in signal processing), the phase space can be $R\times R$ or $Z_N\times Z_N$ or $S\times Z$ in the sense that where one of the variables takes values in R or Z_N or S, the dual variable take values in R or Z_N or Z, correspondingly.

Quantum mechanics on a circle is the simplest example of quantum mechanics in a nontrivial topology and has been studied extensively in the literature.[5,6] Physical applications include Aharonov–Bohm phenomena,[7] mesoscopic Aharonov–Bohm rings, Floquet–Bloch wave functions in solid state systems, etc.

In Sec. II we introduce the basic formulism for position and momentum states and operators, taking into account the nontrivial topology of our system (described by the winding number). In Sec. III we introduce displacement operators and study their properties. In Sec. IV we define Wigner and Weyl functions. We show that the properties of the displacement operators lead to analogous properties for the Wigner and Weyl functions. In Sec. V we discuss an example based on a theta wave function (which is the analogue in a circle, of a Gaussian wave function in a real line). Numerical examples for the corresponding Wigner and Weyl functions are discussed. We conclude in Sec. VI with a discussion of our results.

II. POSITION AND MOMENTUM STATES

An electric charge is moving on a circle parametrized by the variable x. The winding number w_x of x is defined as the integer part of the $x/(2\pi r)$ [for negative x it is the integer part of the $x/(2\pi r)$ minus 1]. Let r be the radius of the circle. A magnetostatic flux ϕ is threading the circle in the perpendicular direction. The wave function $R(x)$ obeys the quasiperiodic boundary condition (in units $K_B=\hbar=c=1$),

$$R(x+2\pi r)=R(x)\exp(ie\phi). \tag{1}$$

Similar functions also appear in solid state physics (Bloch functions). They are normalizable within each period,

$$\frac{1}{2\pi r}\int_0^{2\pi r}|R(x)|^2\,\mathrm{d}x=1. \tag{2}$$

Since $R(x)$ is a quasiperiodic function, it can be written as the following Fourier expansion:

$$R(x)=\sum_{N=-\infty}^{\infty}R_N\exp(ip_Nx),\quad p_N=\frac{N+\sigma}{r},\quad \sigma=\frac{e\phi}{2\pi}. \tag{3}$$

The inverse Fourier transform gives

$$R_N=\frac{1}{2\pi r}\int_0^{2\pi r}\exp(-ip_Nx)R(x)\mathrm{d}x. \tag{4}$$

$R(x)$ and R_N can be, respectively, considered as the position and momentum representations of the state $|R\rangle$. So Eq. (3) and Eq. (4) can be written as

$$\langle x|R\rangle=\sum_{N=-\infty}^{\infty}\langle p_N|R\rangle\exp(ip_Nx), \tag{5}$$

$$\langle p_N|R\rangle=\frac{1}{2\pi r}\int_0^{2\pi r}\langle x|R\rangle\exp(-ip_Nx)\mathrm{d}x. \tag{6}$$

Let $|x\rangle$, $|p_N\rangle$ be position and momentum eigenstates, correspondingly. Then

$$|x\rangle=\sum_{N=-\infty}^{\infty}\exp(-ip_Nx)|p_N\rangle,\quad |p_N\rangle=\frac{1}{2\pi r}\int_0^{2\pi r}\mathrm{d}x\exp(ip_Nx)|x\rangle, \tag{7}$$

$$\langle x|y\rangle=(2\pi r)\delta[x-y+2\pi r(w_y-w_x)]\exp[-i2\pi\sigma(w_y-w_x)],\quad \langle p_M|p_N\rangle=\delta_{MN}. \tag{8}$$

It is easily seen that

$$|x+2\pi rw\rangle=\exp(-i2\pi\sigma w)|x\rangle. \tag{9}$$

The completeness can can be expressed as

$$\frac{1}{2\pi r}\int_0^{2\pi r}|x\rangle\langle x|\mathrm{d}x=\sum_{N=-\infty}^{\infty}|p_N\rangle\langle p_N|=\mathbf{1}. \tag{10}$$

Position and momentum operators are defined as

$$\hat{x}=\frac{1}{2\pi r}\int_0^{2\pi r}x|x\rangle\langle x|\mathrm{d}x,\quad \hat{p}=\sum_{N=-\infty}^{\infty}p_N|p_N\rangle\langle p_N|. \tag{11}$$

We note that a different definition of $\hat{x}$ that involves integration from τ to $\tau+2\pi r$ leads to

$$\hat{x}_\tau=\hat{x}+\Pi_\tau,\quad \Pi_\tau=\int_0^{\tau}|x\rangle\langle x|\mathrm{d}x. \tag{12}$$

The $\hat{x}_\tau$ is different from $\hat{x}$ by the projection operator Π_τ. In the special case that $\tau=2\pi rw$ where w is an integer, $\Pi_{2\pi rw}=2\pi rw\mathbf{1}$. It is easily seen that

$$\hat{x}|x\rangle=(x-2\pi rw_x)|x\rangle,\quad \hat{p}|p_N\rangle=p_N|p_N\rangle. \tag{13}$$

III. DISPLACEMENTS AND PARITY

We define displacement operators as

$$D(\alpha,K)\equiv\exp\left(-\frac{i\alpha K}{2r}\right)\exp\left(i\frac{K}{r}\hat{x}\right)\exp(-i\alpha\hat{p}), \tag{14}$$

$$D(\alpha,K)|x\rangle=\exp\left[\frac{iK}{r}\left(x+\frac{\alpha}{2}\right)\right]|x+\alpha\rangle, \tag{15}$$

$$D(\alpha,K)|p_N\rangle=\exp\left(-\frac{i\alpha K}{2r}\right)\exp(-i\alpha p_N)|p_{N+K}\rangle. \tag{16}$$

It is easily seen that

$$D(\alpha,K)D(\beta,M)=D(\alpha+\beta,K+M)\exp\left[i\left(\frac{K\beta}{2r}-\frac{M\alpha}{2r}\right)\right], \tag{17}$$

$$D(\alpha+2\pi rw,K)=(-1)^{Kw}\exp(-i2\pi\sigma w)D(\alpha,K), \tag{18}$$

$$D^{\dagger}(\alpha,K)=D(-\alpha,-K), \tag{19}$$

where w is an integer (the winding number). For later purposes we note that the $D(\alpha,K)\exp(i\alpha\sigma/r)$ is periodic in α. The period is $2\pi r$ if K is even and $4\pi r$ if K is odd number,

$$D(\alpha+2\pi r,K)\exp\left[\frac{i(\alpha+2\pi r)\sigma}{r}\right]=(-1)^{K}\exp\left(\frac{i\alpha\sigma}{r}\right)D(\alpha,K). \tag{20}$$

We also define the parity operator as

$$U_0=\frac{1}{2\pi r}\int_0^{2\pi r}|\alpha\rangle\langle-\alpha|\exp\left(\frac{i2\alpha\sigma}{r}\right)\mathrm{d}\alpha=\sum_{N=-\infty}^{\infty}|p_{-N}\rangle\langle p_N|. \tag{21}$$

The flux factor $\exp(i\alpha\sigma/r)$ has been included in the definition so that the integrand $|\alpha\rangle\langle-\alpha|\exp(i2\alpha\sigma/r)$ is periodic. The parity operator obeys the relations

$$U_0=U_0^{\dagger},\quad U_0^2=I. \tag{22}$$

The flux breaks the parity symmetry. The parity operator acting on the state $|p_{-N}\rangle$ [which has momentum $(-N+\sigma)/r$] gives the state $|p_N\rangle$ [which has momentum $(N+\sigma)/r$]; i.e., it is a parity with momentum origin σ/r. The parity operator acting on the state $|x\rangle$ gives the state $|-x\rangle\exp(-2ix\sigma/r)$. The flux factor $\exp(-2ix\sigma/r)$ corrects the quasiperiodicity caused by the flux into periodicity.

We note here that in the harmonic oscillator case the displacement operators $D(z)=\exp(za^{\dagger}-z^{*}a)$ obey the important relations[8]

$$\int_{-\infty}^{\infty}\mathrm{d}z_R\,D(z)=\sqrt{2}\pi\left|p=\frac{z_I}{\sqrt{2}}\right\rangle\left\langle p=-\frac{z_I}{\sqrt{2}}\right|, \tag{23}$$

$$\int_{-\infty}^{\infty}\mathrm{d}z_I\,D(z)=\sqrt{2}\pi\left|x=\frac{z_R}{\sqrt{2}}\right\rangle\left\langle x=-\frac{z_R}{\sqrt{2}}\right|, \tag{24}$$

$$\int \frac{d^2z}{2\pi} D(z) = U_0, \tag{25}$$

where $z = z_R + iz_I$ and U_0 is here the harmonic oscillator parity operator (defined in Ref. 8). These relations are intimately related with the marginal properties of the Wigner and Weyl functions.

Motivated by this we study here similar relations in our context of quantum mechanics on a circle. We first define the function

$$\Delta(x) = \frac{1}{2\pi}\int_0^{2\pi} \exp(i\beta x)\,d\beta = \exp(-i\pi x)\,\frac{\sin(\pi x)}{\pi x} \equiv \exp(-i\pi x)\,\mathrm{sinc}(x). \tag{26}$$

This is the sinc function (used extensively in areas like digital signal processing) with a phase factor. For integers M,N,

$$\Delta(M-N) = \delta(M,N), \tag{27}$$

where δ is Kronecker's delta. Using Eqs. (15) and (16) can prove that

$$\sum_{K=-\infty}^{\infty} D(\alpha,K) = \left|\frac{\alpha}{2}\right\rangle\left\langle -\frac{\alpha}{2}\right|, \tag{28}$$

$$\frac{1}{2\pi r}\int_0^{2\pi r} D(\alpha,K)\exp\left(\frac{i\alpha\sigma}{r}\right)d\alpha = \begin{cases} |p_{-M}\rangle\langle p_M|, & K=2M, \\ \displaystyle\sum_{N=-\infty}^{\infty} |p_{N+K}\rangle\langle p_N|\,\Delta\left(-\frac{K}{2}-N\right), & K=2M+1. \end{cases} \tag{29}$$

We have explained earlier why the integrations involve the flux factor $\exp(i\alpha\sigma/r)$. It is natural to ask what is the result in Eq. (29) if we do not include the flux factor. We can prove

$$\frac{1}{2\pi r}\int_0^{2\pi r} D(\alpha,K)\,d\alpha = \sum_{N=-\infty}^{\infty} |p_{N+K}\rangle\langle p_N|\,\Delta\left(-\frac{K}{2}-N-\sigma\right). \tag{30}$$

In Eq. (29), integration from $2\pi r$ to $4\pi r$, gives the same result for even K and the same result but with opposite sign for odd K,

$$\frac{1}{2\pi r}\int_{2\pi r}^{4\pi r} D(\alpha,K)\exp\left(\frac{i\alpha\sigma}{r}\right)d\alpha = \begin{cases} |p_{-M}\rangle\langle p_M|, & K=2M, \\ \displaystyle -\sum_{N=-\infty}^{\infty} |p_{N+K}\rangle\langle p_N|\,\Delta\left(-\frac{K}{2}-N\right), & K=2M+1. \end{cases} \tag{31}$$

This is related to the fact [Eq. (20)] that for odd K the $D(\alpha,K)\exp(i\alpha\sigma/r)$ is antiperiodic with period $2\pi r$ (it is periodic with period $4\pi r$). Therefore if we integrate from 0 to $4\pi r$ we get the same result for even K and zero for odd K.

Combining Eqs. (21) and (29) we easily show that

$$\sum_{K=\text{even}} \frac{1}{2\pi r}\int_0^{2\pi r} D(\alpha,K)\exp\left(\frac{i\alpha\sigma}{r}\right)d\alpha = U_0. \tag{32}$$

It is natural to ask what is the result in Eq. (32) if we sum over both even and odd integers. We can prove

$$\sum_{K=-\infty}^{\infty} \frac{1}{2\pi r}\int_0^{2\pi r} D(\alpha,K)\exp\left(\frac{i\alpha\sigma}{r}\right)d\alpha = U_0 + \sum_{M=-\infty}^{\infty}\sum_{N=-\infty}^{\infty} |p_{N+2M-1}\rangle\langle p_N|\,\Delta\left(-M-N+\frac{1}{2}\right). \tag{33}$$

The displaced parity operator is

$$U(\alpha,K)=D(\alpha,K)U_0D^{\dagger}(\alpha,K)=\exp\left(\frac{i\alpha\sigma}{r}\right)D(2\alpha,2K)U_0=\exp\left(-\frac{i\alpha\sigma}{r}\right)U_0D(-2\alpha,-2K). \tag{34}$$

$U(\alpha,K)$ is a periodic function of α with the period πr,

$$U(\alpha+\pi r,K)=U(\alpha,K). \tag{35}$$

We next show that

$$\sum_{K=-\infty}^{\infty}U(\alpha,K)=\tfrac{1}{2}(|\alpha\rangle\langle\alpha|+|\alpha+\pi r\rangle\langle\alpha+\pi r|), \tag{36}$$

$$\frac{1}{2\pi r}\int_0^{2\pi r}U(\alpha,K)\mathrm{d}\alpha=|p_K\rangle\langle p_K|, \tag{37}$$

$$\sum_K\frac{1}{2\pi r}\int_0^{2\pi r}U(\alpha,K)\mathrm{d}\alpha=\mathbf{1}. \tag{38}$$

Equation (36) is proved if we use Eqs. (28) and (34) in conjunction with the fact that

$$\sum_{K=\text{even}}D(\alpha,K)=\frac{1}{2}\left(\left|\frac{\alpha}{2}\right\rangle\left\langle-\frac{\alpha}{2}\right|+\left|\frac{\alpha}{2}+\pi r\right\rangle\left\langle-\frac{\alpha}{2}+\pi r\right|\right). \tag{39}$$

For completeness we also mention that

$$\sum_{K=\text{odd}}D(\alpha,K)=\frac{1}{2}\left(\left|\frac{\alpha}{2}\right\rangle\left\langle-\frac{\alpha}{2}\right|-\left|\frac{\alpha}{2}+\pi r\right\rangle\left\langle-\frac{\alpha}{2}+\pi r\right|\right). \tag{40}$$

Equation (40) can be proved using Eq. (15). We note that in Eq. (36) we have projectors to the diametrically opposite position states $|\alpha\rangle$ and $|\alpha+\pi r\rangle$. This is related to the fact that the displaced parity operator on the left-hand side of Eq. (36), has period πr. Equation (37) can be proved using Eq. (29). Summation over K in Eq. (37) gives Eq. (38).

The displacement operators are related to the displaced parity operators through a two-dimensional Fourier transform. Multiplying the left- and right-hand sides of Eq. (32) with $D(\alpha,K)$ and $[D(\alpha,K)]^{\dagger}$ correspondingly, we can prove

$$\sum_{M=\text{even}}\frac{1}{2\pi r}\int_0^{2\pi r}D(\beta,M)\exp\left(\frac{i\beta\sigma}{r}\right)\exp\left[i\frac{K\beta-M\alpha}{r}\right]\mathrm{d}\beta=U(\alpha,K). \tag{41}$$

IV. WIGNER AND WEYL FUNCTIONS

The Weyl and Wigner functions can be defined in terms of the displacement and parity operator correspondingly, as

$$\tilde{W}(\alpha,K)=\mathrm{Tr}[\hat{\rho}D(\alpha,K)], \tag{42}$$

$$W(x,p_N)=\mathrm{Tr}[\hat{\rho}U(x,N)]. \tag{43}$$

Using the fact that the density matrix is Hermitian, we easily show that the Wigner function is real. The Weyl function is in general complex. We can easily show the following formulas (which can also be used as alternative definitions):

$$\tilde{W}(\alpha,K)=\frac{1}{2\pi r}\int_0^{2\pi r}\left\langle x-\frac{\alpha}{2}\middle|\hat{\rho}\middle|x+\frac{\alpha}{2}\right\rangle \exp\left(i\frac{K}{r}x\right)\mathrm{d}x \tag{44}$$

$$=\sum_{N=-\infty}^{\infty}\langle p_{N-K}|\hat{\rho}|p_N\rangle\exp\left[-i\alpha\left(p_N-\frac{K}{2r}\right)\right]. \tag{45}$$

$$W(x,p_N)=\frac{1}{2\pi r}\int_0^{2\pi r}\langle x-\alpha|\hat{\rho}|x+\alpha\rangle\exp(i2\alpha p_N)\mathrm{d}\alpha \tag{46}$$

$$=\sum_{K=-\infty}^{\infty}\langle p_{N+K}|\hat{\rho}|p_{N-K}\rangle\exp\left(\frac{2ixK}{r}\right). \tag{47}$$

The Wigner function describes the pseudoprobability of finding the particle in phase space, in a way consistent with quantum mechanics and the uncertainty principle. The Weyl function is equal to the overlap of the displaced state with the original state. In this sense, the α,K are position and momentum *increments*. The Weyl function can be understood as a *generalized correlation function*. If we have the wave function $R(x)$ in order to find the correlation we displace it into $R(x+\alpha)$ and take the integral of $R(x)R(x+\alpha)$. In the Weyl function we perform a more general displacement in phase space i.e., a displacement in both position and momentum. Therefore the correlation is a special case of the Weyl function with $\alpha=0$ (or $K=0$). We note that the momentum takes values $(N+\sigma)/r$ and depends on σ. In contrast the momentum increments appearing on the Weyl function take values K/r and do not depend on σ.

The Wigner function is related to the Weyl function through a two-dimensional Fourier transform

$$W(x,p_N)=\frac{1}{2\pi r}\int_0^{2\pi r}\sum_{K=\text{even}}\tilde{W}(\alpha,K)\exp\left(-i\frac{K}{r}x\right)\exp(i\alpha p_N)\mathrm{d}\alpha. \tag{48}$$

This can be proved using Eq. (29) or Eq. (49). This result is intimately connected to the fact that the displacement operator and displaced parity operator are related to each other through a two-dimensional Fourier transform [Eq. (49)].

Using Eqs. (18) and (35) we easily see that the Wigner function is periodic function of x with period πr; and the Weyl function is quasiperiodic with period $2\pi r$:

$$\tilde{W}(\alpha+2\pi rw,K)=(-1)^{Kw}\exp(-i2\pi\sigma w)\tilde{W}(\alpha,K),\quad W(x+\pi r,p_N)=W(x,p_N). \tag{49}$$

The Wigner and Weyl functions depend on the magnetic flux σ although for simplicity in the notation we have not shown this dependence explicitly. They obey the relations

$$\tilde{W}_\sigma(\alpha,K)=\tilde{W}_{\sigma+1}(\alpha,K),\quad W_{\sigma+1}(x,p_N)=W_\sigma(x,p_{N+1}). \tag{50}$$

This is related to the fact that the momentum is $p_N=(N+\sigma)/r$ and as we go from σ to $\sigma+\mathbf{1}$ the momentum p_N is relabeled as p_{N+1}.

The properties of the displacement and parity operator that we proved above can be translated into properties for the Wigner and Weyl functions. Starting with the Weyl function we use Eqs. (28) and (29) to prove that

$$\sum_{K=-\infty}^{\infty}\tilde{W}(\alpha,K)=\left\langle-\frac{\alpha}{2}\middle|\rho\middle|\frac{\alpha}{2}\right\rangle, \tag{51}$$

$$\frac{1}{2\pi r}\int_0^{2\pi r}\widetilde{W}(\alpha,K)\exp\left(\frac{i\alpha\sigma}{r}\right)\mathrm{d}\alpha=\begin{cases}\langle p_M|\rho|p_{-M}\rangle, & K=2M,\\ \sum_{N=-\infty}^{\infty}\langle p_N|\rho|p_{N+K}\rangle\Delta\left(-\frac{K}{2}-N\right), & K=2M+1.\end{cases} \tag{52}$$

We can make here a similar comment to that made for Eq. (29). In Eq. (52), integration from $2\pi r$ to $4\pi r$, gives the same result for even K and the same result but with opposite sign for odd K. Therefore if we integrate from 0 to $4\pi r$ we get the same result for even K and zero for odd K. We can also show that

$$\widetilde{W}(0,0)=1, \quad \widetilde{W}(\alpha,K)=\widetilde{W}^*(-\alpha,-K), \quad |\widetilde{W}(\alpha,K)|\leqslant 1. \tag{53}$$

For the Wigner function we use Eqs. (36), (37), (38) to prove

$$\frac{1}{2\pi r}\int_0^{2\pi r}W(x,p_N)\mathrm{d}x=\langle p_N|\hat{\rho}|p_N\rangle, \tag{54}$$

$$\sum_{N=-\infty}^{\infty}W(x,p_N)=\frac{1}{2}(\langle x|\hat{\rho}|x\rangle+\langle x+\pi r|\hat{\rho}|x+\pi r\rangle), \tag{55}$$

$$\frac{1}{2\pi r}\int_0^{2\pi r}\sum_{N=-\infty}^{\infty}W(x,p_N)\mathrm{d}x=\mathbf{1}. \tag{56}$$

We can also prove that

$$\mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2)=\frac{1}{2\pi r}\int_0^{2\pi r}\sum_{N=-\infty}^{\infty}W_{\rho_1}(x,p_N)W_{\rho_2}(x,p_N)\mathrm{d}x. \tag{57}$$

V. EXAMPLE

As an example, we consider a free particle descibed with the Hamiltonian

$$\hat{H}=\hat{p}^2. \tag{58}$$

We note that the particle feels a vector potential through the quasiperiodic boundary condition.

We assume that at $t=0$ the wave function is a Gaussian on a circle, i.e., a theta function. In order to explain this we introduce the Zak transform[9] on a function $S(y)$ on a real line, defined as

$$R(x,\sigma)=\mathcal{N}\sum_{w=-\infty}^{\infty}S(y=x+2\pi r w)\exp(-i2\pi\sigma w), \tag{59}$$

where $\mathcal{N}$ is used to normalize the function $R(x,\sigma)$ according to Eq. (2). If $S(y;A)$ is a Gaussian wave function

$$S(y;A)=\pi^{-1/4}\exp\left(-\frac{y^2}{2}+\sqrt{2}A\cdot y-AA_R\right), \tag{60}$$

where $A=A_R+iA_I$, then the Zak transform is

$$R(x,\sigma;A)=\mathcal{N}\cdot\pi^{-1/4}\exp\left(-\frac{x^2}{2}+\sqrt{2}Ax-AA_R\right)\Theta_3[-\pi\sigma+i\pi r(x-\sqrt{2}A);i2\pi r^2], \tag{61}$$

where $\Theta_3[u;\tau]$ is theta function,[10] defined as

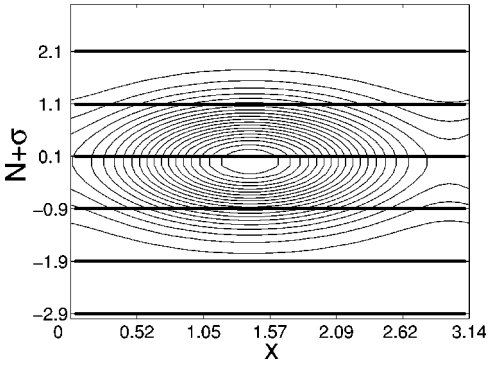

FIG. 1. A contour plot of the Wigner function at $t=0$ as a function of x and for all values of σ. The parallel black lines in the figure show the case $\sigma=0.1$.

$$\Theta_3[u;\tau]=\sum_{n=-\infty}^{\infty}\exp(i\pi\tau n^2+i2nu). \tag{62}$$

We have taken $r=1$, $A=1$ and calculated the Wigner and Weyl functions. Numerical results are shown in Figs. 1–3.

In Fig. 1 we present a contour plot of the Wigner function $W(x,N+\sigma)$ as a function of x and for all values of σ. For a given σ the Wigner function is defined only on the discrete values of the momenta $p_N=(N+\sigma)/r$ and the parallel black lines in the figure show the case $\sigma=0.1$. As expected from Eq. (49), the Wigner function is periodic function of x with period π. Also it has been explained in Eq. (50) that the plotted values of $W(x,p_1)$ for $\sigma=1$ represent the $W(x,p_2)$ for $\sigma=0$.

In Fig. 2 we present the Wigner function as a function of x at a particular momentum $p_0=\sigma$ with $\sigma=0.1$. This is really an appropriate slice of the three-dimensional version of Fig. 1.

In Fig. 3 we present a contour plot of the absolute value of the Weyl function as a function of α for $K=1$ and for all values of σ. The black line in the figure shows the case $\sigma=0.1$.

We calculate the time evolution of this system. This is easily done in the momentum representation as

$$\langle p_N|R(t)\rangle=\exp(it\hat{H})\langle p_N|R(0)\rangle. \tag{63}$$

We need the state of the system at $t=0$ in the momentum representation. If $\tilde{S}(p)$ is the Fourier transform of $S(x)$:

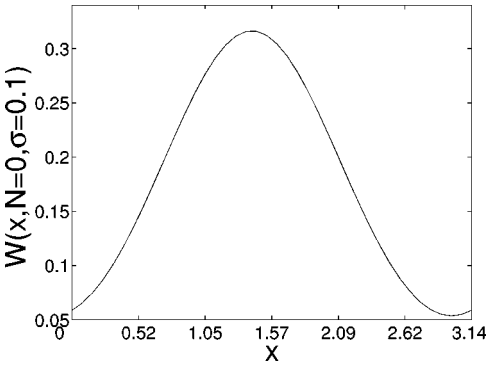

FIG. 2. A slice of the Wigner function of Fig. 1 with $\sigma=0.1$.

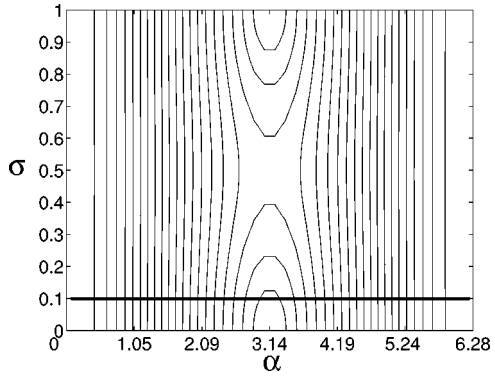

FIG. 3. A contour plot of the absolute value of the Weyl function at $t=0$ for $K=1$, as a function of α and σ. The black line in the figure shows the case $\sigma=0.1$.

$$\tilde{S}(p)=\int_{-\infty}^{+\infty} S(x)\exp(-ipx)\mathrm{d}x, \tag{64}$$

then using Eq. (4), Eq. (59), and Eq. (64) we can prove the relation

$$R_N=\frac{\mathcal{N}}{2\pi r}\tilde{S}(p_N). \tag{65}$$

Since the Fourier transform of Gaussian wave function Eq. (60) is

$$\tilde{S}(p;A)=\sqrt{2}\pi^{1/4}\exp\left(-\frac{p^2}{2}-i\sqrt{2}A\cdot p+AA_I\right), \tag{66}$$

we obtain

$$\langle p_N|R\rangle=\frac{\mathcal{N}\pi^{1/4}}{\sqrt{2}\pi r}\exp\left(-\frac{p_N^2}{2}-i\sqrt{2}A\cdot p_N+AA_I\right). \tag{67}$$

Inserting Eq. (67) into (63) we get

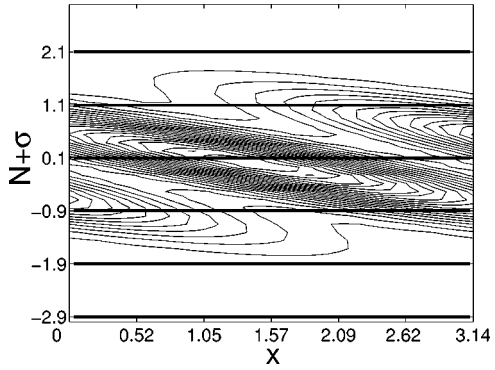

FIG. 4. A contour plot of the Wigner function at $t=1$ as a function of x and for all values of σ. The parallel black lines in the figure show the case $\sigma=0.1$.

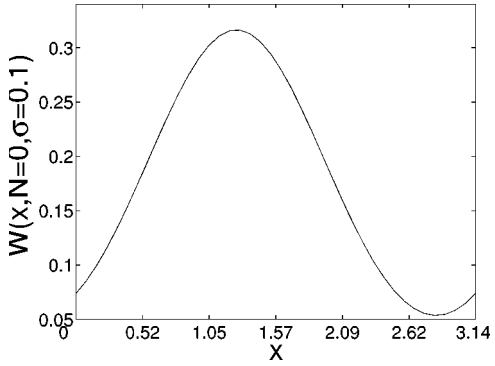

FIG. 5. A slice of the Wigner function of Fig. 4 with $\sigma=0.1$.

$$\langle p_N|R(t)\rangle=\frac{\mathcal{N}\pi^{1/4}}{\sqrt{2}\pi r}\exp\left[-\left(\frac{1}{2}-it\right)p_N^2-i\sqrt{2}A\cdot p_N+AA_I\right]. \tag{68}$$

From that we have calculated for $t=1$ the corresponding Wigner and Weyl functions to the previous ones. Results are shown in Figs. 4–6. The results show the time evolution of the system in the language of Wigner and Weyl functions.

VI. DISCUSSION

Quantum mechanics on a circle has attracted a lot of attention in the literature. It uses topological ideas in the context of quantum mechanics. In this paper we have studied phase space methods in this context. We have introduced displacement operators and studied their properties. There is clearly some analogy with the harmonic oscillator displacement operator properties [given in Eqs. (23), (24), and (25)], but there are also considerable differences. In particular the flux σ plays an important role in the properties of the displacement operators for particles on a circle. Our main results here are Eqs. (28), (29), and (32).

We also introduced Wigner and Weyl functions and discussed their physical interpreration and their properties, which are direct consequence of the displacement operator properties. A numerical example for the theta wave function of Eq. (61) (the analogue on a circle of the Gaussian function on the real line) has been discussed.

The results can be used in the context of Aharonov–Bohm devices, Floquet–Bloch solid state systems, coherent states on a circle,[11] quantum maps and classical and quantum chaos,[12] etc. Fractional Fourier transforms in this context have been discussed in Ref. 13.

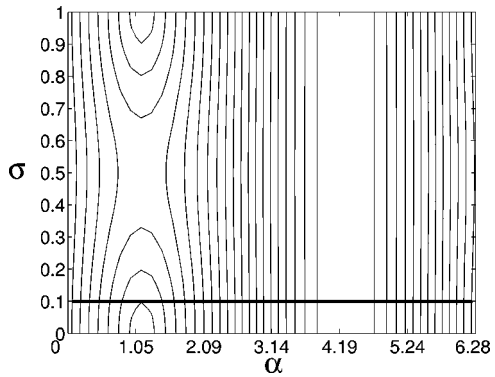

FIG. 6. A contour plot of the absolute value of the Weyl function at $t=1$ for $K=1$, as a function of α and σ. The black line in the figure shows the case $\sigma=0.1$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Mathematical structure of the temporal gauge in quantum electrodynamics

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(Received 13 December 2002; accepted 4 April 2003)

The conflict between Gauss' law constraint and the existence of the propagator of the gauge fields, at the basis of contradictory proposals in the literature, is shown to lead to only two alternatives, both with peculiar features with respect to standard quantum field theory. In the positive (interacting) case, the Gauss' law holds in operator form, but only the correlations of exponentials of gauge fields exist (nonregularity) and the space translations are not strongly continuous, so that their generators do not exist. Alternatively, a Källen–Lehmann representation of the two point function of A_i satisfying locality and invariance under space–time translations, rotations and parity is derived in terms of the two point function of $F_{\mu\nu}$; positivity is violated, the Gauss' law does not hold, the energy spectrum is positive, but the relativistic spectral condition does not hold. In the free case, θ-vacua exist on the observable fields, but they do not have time translationally invariant extensions to the gauge fields; the vacuum is faithful on the longitudinal field algebra and defines a modular structure (even if the energy is positive). Functional integral representations are derived in both cases, with the alternative between ergodic measures on real random fields or complex Gaussian random fields. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1603957]

I. INTRODUCTION

In the treatment of gauge quantum field theories, even if the choice of the gauge, a basic ingredient for the control of the dynamical problem, is irrelevant for the physical conclusions, it crucially affects the mathematical structure of the formulation as well as the way the various mechanisms (mass generation, gauge symmetry breaking, θ-vacua, chiral symmetry breaking, etc.) are effectively realized. In the discussion of the nonperturbative aspects of quantum chromodynamics (QCD)[1] and of the Higgs mechanism,[2] the temporal gauge has been widely used and it is therefore worthwhile to investigate its mathematical structure.

From a technical point of view (the only relevant for the gauge choice), such a gauge has been preferred to others because it is believed to satisfy locality, positivity, and the Gauss' law constraint in operator form, at the only expense of manifest Lorentz covariance. As such, it appears as intermediate between the Coulomb gauge, where locality is lost (besides manifest Lorentz covariance), and the Feynman–Gupta–Bleuler (FGB) gauge,[3,4] where locality holds but positivity and the operator Gauss' law constraint are lost.

The aim of this article is to critically examine the mathematical structure of the temporal gauge and the status of general properties like positivity, operator Gauss' law, positivity of the energy, and relativistic spectrum condition.

The usual formulation of the temporal gauge relies either on canonical quantization as a basis

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of the perturbative expansion or on a functional integral approach to the interacting theory, with a space lattice regularization, which also gives a (lattice regularized) canonical structure. Thus, in both cases one has a CCR algebra at equal times; actually, also in the presence of the interaction, the subalgebra generated by $\mathrm{div}\,A$ and $\mathrm{div}\,E-j_0$ remains canonical, with an interaction independent commutator also at unequal times.

Contrary to the standard case, the CCR structure of the temporal gauge does not uniquely identify its vacuum representation; as a matter of fact, the form of the propagator of the gauge potential has been debated in the literature, but a classification of the possibilities is lacking, especially in connection with basic structural properties, so that also recent textbook presentations of the temporal gauge[5] leave such basic points unsettled. The analysis of such a problem is the main content of this work: we shall classify all time translation invariant states on the CCR algebra in the free case and discuss the implications on the interacting Abelian theory.

The results are the following. Both in the free and the interacting cases positivity and time translation invariance are incompatible with the existence of the correlation functions of the field $\mathrm{div}\,A$, only its exponentials being defined. Positivity also implies that the vacuum satisfies the Gauss' law constraint in operator form and that the space translations are not strongly continuous, so that one cannot define their generators (the momentum) and the relativistic spectrum condition cannot even be defined. In the free case the condition of positivity of the energy spectrum is shown to uniquely select the (nonregular) state considered in Ref. 6 (see also Refs. 7 and 8); other time translational invariant pure states exist, which satisfy the spectral condition only on the observables.

On the other hand, the perturbative expansion and the standard functional integral approach are based on the existence of the propagator of the gauge potential, whose form has been widely discussed in the literaure, with no general sharp conclusion and with proposals often in conflict with basic principles of standard quantum field theory, even in the free case (see Ref. 5). To clarify the problem, we derive a Källen–Lehmann representation of the two point function of the gauge potential in the interacting case under the general conditions of locality and invariance under space–time translations, rotations and parity. The resulting two point function violates positivity and the relativistic spectral condition (but not the positivity of the energy spectrum) and the vacuum cannot be annihilated by the Gauss operator $\mathrm{div}\,E-j_0$ (such features are shared by the FGB gauge, where, however, there is no violation of the relativistic spectral condition). In the free field case, the quasi-free state defined by the two point function gives rise to an indefinite inner product structure which can be discussed as in the FGB gauge in terms of a Hilbert–Krein structure.

The Euclidean functional integral representation is discussed in the positive and in the indefinite case, also with the aim of clarifying the unsatisfactory proposals in the literature (which ignore the violation of Nelson positivity, involve infinite normalizations, formal Faddev–Popov ghosts, improper realization of the Gauss constraint, etc.). In the indefinite case, the representation of the Euclidean fields requires, besides real Gaussian fields $A_i^{tr}(\mathbf{x},\tau)$, $\xi(\mathbf{x},\tau)$, with $\xi(f,\tau)$ the Wiener process, a *complex* Gaussian field $z(\mathbf{x})$. In the positive case, the complex Gaussian field $z(\mathbf{x})$ is replaced by a real random field $\Xi(\mathbf{x})$ with functional measure defined by ergodic means. The correlation functions of the exponentials of the (smeared) fields are therefore represented by integration with the product of the above Gaussian measures and a measure over the spectrum of the Bohr algebra generated by the exponentials of $\Xi(g)$.

II. ALGEBRAIC STRUCTURE

At a formal level the temporal gauge is defined by the gauge condition $A_0=0$, by the canonical commutation relations (CCR)

$$[A_i(\mathbf{x}),\partial_t A_j(\mathbf{y})]=i\,\delta_{ij}\delta(\mathbf{x}-\mathbf{y}), \tag{2.1}$$

and by the CAR relations of the charged fermion fields $\psi(\mathbf{x})$, $\overline{\psi}(\mathbf{y})$. The gauge fields satisfy the following equations of motion:

$$\partial_t^2 A_i - \Delta A_i + \partial_i \operatorname{div} A = j_i, \tag{2.2}$$

where j_μ is the conserved gauge invariant electromagnetic current constructed in terms of the charged fermion fields. We shall denote by $\mathcal{F}_c$ the polynomial algebra generated by the zero time fields $A_i, \dot{A}_i, \psi, \overline{\psi}, j_\mu$, smeared with test functions in $\mathcal{S}(\mathbf{R}^3)$, hereafter called *canonical field algebra*, and by $\mathcal{F}$ the algebra generated by the fields A_i, ψ, $\overline{\psi}$, j_u, smeared with test functions in $\mathcal{S}(\mathbf{R}^4)$.

Equation (2.2) implies that $\operatorname{div} E - j_0$ is time independent so that $\forall g \in \mathcal{S}(\mathbf{R}^3)$

$$(\operatorname{div} E - j_0)(g,t) \equiv (\operatorname{div} E - j_0)(g,h), \quad h \in \mathcal{S}(\mathbf{R}), \quad \int ds\, h(s) = 1,$$

is a well defined time independent operator and therefore its equal time commutators with the fields are well defined operator valued distributions. Such commutators are fixed by the condition that $G \equiv \operatorname{div} E - j_0$ generates time independent gauge transformations; such a property follows from canonical quantization if the gauge invariant point splitting regularization of the current amounts to the addition of terms linear in A_i, $\partial_0 A_i$ to the canonical fermion current. Under such a condition one has

$$[A_i(\mathbf{x},t), G(\mathbf{y},t)] = -i\partial_i \delta(\mathbf{x}-\mathbf{y}). \tag{2.3}$$

As we shall see below, a positive realization of the temporal gauge can only be done in terms of Weyl algebras. We then introduce the algebras:

(1) $\mathcal{A} \equiv$ the polynomial algebra generated by $A(f) \equiv A_i(f_i)$, $\partial_t A(g) = E(g)$, $f_i, g_i \in \mathcal{S}(\mathbf{R}^3)$ (*gauge field algebra*), and $\mathcal{W} \equiv$ the corresponding *gauge Weyl algebra* generated by $\exp i[A(f) + E(g)] \equiv W(f,g)$;

(2) $\mathcal{A}_l \equiv$ the polynomial algebra generated by $A(\partial h) \equiv A_i(\partial_i h)$, $(\operatorname{div} E - j_0)(g)$, $h, g \in \mathcal{S}(\mathbf{R}^3)$, called the *longitudinal field algebra*, and $\mathcal{W}_l$ the corresponding *longitudinal Weyl algebra*, generated by $\exp i[A(\partial h) + (\operatorname{div} E - j_0)(g)] \equiv W_l(h,g)$.

By decomposing test functions into longitudinal and transverse (nonlocal) components and by an analysis in momentum space, it is not difficult to see that in the free case the time evolution of $\mathcal{W}$ is relativistically local, formally,

$$\alpha_t(A(f) + E(g)) = A(f_t) + E(g_t),$$

with $supp\, f_t \cup supp\, g_t$ contained in the causal shadow of $supp\, f \cup supp\, g$. The same analysis shows that Eq. (2.2) has a relativistically causal Green function, so that, in the interacting case, the relativistic locality of the gauge fields in the temporal gauge follows from the relativistic locality of the observable field j_i; this implies local commutativity for the Wightman field algebra $\mathcal{F}$, since the fermion coupling is local. In contrast, in the Coulomb gauge, the fermion coupling is nonlocal and local commutativity is lost.

The free time evolution of the longitudinal Weyl algebra is

$$\alpha_t(W_l(h,k)) = W_l(h, k + t\,h), \tag{2.4}$$

so that the longitudinal fields describe an infinite set of free nonrelativistic particles. In fact, given a complete set $\{f_n\}$ in $L^2(\mathbf{R}^3)$, with $(f_n, -\Delta f_m) = \delta_{n,m}$, the variables

$$q_n \equiv \operatorname{div} A(f_n), \quad p_n \equiv \operatorname{div} E(f_n) \tag{2.5}$$

are canonical and their time evolution is that of free particles

$$\dot{q}_n = p_n, \quad \dot{p}_n = 0.$$

The above algebraic structure follows from canonical quantization at equal times. Its validity is independent of the presence of the interaction, provided an ultraviolet regularization (e.g., by a space lattice cutoff) is introduced, so that the time evolution of the above algebras is well defined. Actually, by Eq. (2.3), $[e^{iA(\partial f,t)}, (\mathrm{div}\, E - j_0)(g,s)]$ is independent of s and therefore such a canonical commutator extends to unequal times and is independent of the interaction

$$[e^{iA_i(\partial_i h)}, (\mathrm{div}\, E - j_0)(g,s)] = -\int d^4x\, \Delta h(x)\, g(\mathbf{x})\; e^{iA_i(\partial_i h)}, \quad h \in \mathcal{S}(\mathbf{R}^4). \tag{2.6}$$

The field algebra $\mathcal{F}$ of the temporal gauge has the following infinite dimensional group of automorphisms [*time independent (small) gauge transformations*]: γ^Λ, $\Lambda(x) \in \mathcal{S}(\mathbf{R}^3)$

$$\gamma^\Lambda(A(f)) = A(f) - \int d^3x\, \Lambda\, \mathrm{div}\, f, \quad \gamma^\Lambda(E(g)) = E(g), \quad \gamma^\Lambda \psi(f) = \psi(e^{i\Lambda} f). \tag{2.7}$$

The γ^Λ commute with the time translations, as a consequence of the gauge invariance of the Lagrangian; they are generated by $G(\Lambda)$ and are unitarily implemented by elements of the longitudinal Weyl algebra.

The automorphisms of Eq. (2.7), with $\Lambda(\mathbf{x}) = \boldsymbol{\alpha}\cdot\mathbf{x}$, are called *large gauge transformations* and are still denoted by γ^Λ. They commute with the time and space translations and are locally generated by the local charges

$$G_R^\Lambda \equiv G(\Lambda f_R), \quad f_R(x) = f(|x|/R), \quad f \in \mathcal{D}(\mathbf{R}),$$

in the sense that the variations of the fields are given by

$$\delta^\Lambda B = \lim_{R\to\infty} -i\,[Q_R^\Lambda, B], \quad \forall B \in \mathcal{F}. \tag{2.8}$$

The *observable subalgebras* $\mathcal{F}_{obs}$, $\mathcal{A}_{obs}$, $\mathcal{W}_{obs}$ are characterized by pointwise invariance under all γ^Λ. $\mathcal{A}_{obs}$ is the algebra generated by $A(f)$, $\mathrm{div}\, f = 0$ and by $E(g)$; $\mathcal{F}_{obs}$ has a nontrivial center which contains the algebra generated by $G(f)$, $f \in \mathcal{S}(\mathbf{R}^3)$. The invariance of the vacuum under large gauge transformations is incompatible with the existence of the correlation functions of the field algebra $\mathcal{F}$ and, as we shall see explicitly in the free case, only holds in the nonregular positive formulation.

The gauge field algebra $\mathcal{A}$, as well as the gauge Weyl algebra $\mathcal{W}$, have the following three parameter group of automorphisms β^θ, $\theta \in \mathbf{R}^3$:

$$\beta^\theta(A(f)) = A(f), \quad \beta^\theta(E(g)) = E(g) + \theta_i \int d^3x\, g_i, \tag{2.9}$$

which generate a background constant (classical) electric field.

The automorphisms β^θ, for simplicity called θ automorphisms, commute with the space translations and have the following commutation relations with the gauge transformations and with the free time evolution

$$\beta^\theta\, \gamma^\Lambda = \gamma^\Lambda\, \beta^\theta, \quad \beta^\theta\, \alpha_t = \alpha_t\, \beta^\theta\, \gamma^{t\,\theta\cdot\mathbf{x}}, \tag{2.10}$$

so that they commute with the free time evolution on the observable algebra. The θ automorphisms are generated on $\mathcal{W}$ (and on $\mathcal{A}$) by the local charges

$$Q_R \equiv A_i(\theta_i f_R). \tag{2.11}$$

Even if the automorphisms β^θ commute with the gauge transformations, the corresponding generators do not. In conclusion, at least in the free case, such transformations have similar properties to those of the chiral transformations in quantum chromodynamics.

III. STATES AND REPRESENTATIONS

In the following we shall adopt the physicist terminology by which a linear normalized functional on a *-algebra $\mathcal{A}$ is briefly called a *state*, even if it is not positive with respect to the *-operation defined on the algebra. A state in the above sense defines a *representation* π_ω of $\mathcal{A}$ with a cyclic vector Ψ_ω and an inner product $(\pi_\omega(A)\,\Psi_\omega,\,\pi_\omega(B)\,\Psi_\omega)=\omega(A^*B)$. A semidefinite representation of a *-algebra $\mathcal{A}$ is called *irreducible* if any bounded operator which commutes with $\mathcal{A}$ is a multiple of the identity.

We shall show that the gauge condition $A_0=0$ does not uniquely fix the vacuum representation of the longitudinal algebra. We shall discuss the general obstructions which arise if, given a positive state on the observable field algebra $\mathcal{F}_{obs}$, one looks for extensions to the field algebra $\mathcal{F}$. Actually, independently of the interaction, we shall show that existence of the correlation functions of the fields requires a nonpositive vacuum state, which cannot be annihilated by the Gauss operator $\operatorname{div}E-j_0$, whereas a positive representation requires a nonregular state on the longitudinal algebra $\mathcal{L}$ generated by $\exp iA_i(\partial_i h)$, $\exp iG(h)$, $h\in\mathcal{S}(\mathbf{R}^4)$. The two alternatives are shown to have very different mathematical features and can in fact be distinguished on the basis of the structural properties that one wants to preserve.

Proposition 3.1: Let ω be a positive vacuum state on $\mathcal{F}_{obs}$, satisfying the cluster property. Then

(i) ω does not have a positive extension to $\mathcal{F}$,

(ii) any positive extension Ω to $\mathcal{L}$ is nonregular and satisfies

$$\Omega(W_l(0,g))=\omega(W_l(0,g))=1,\quad \Omega(W_l(f,g))=0,\quad \text{if}\quad f\neq 0, \tag{3.1}$$

(iii) all positive extensions of ω to an algebra containing $\mathcal{L}$ define a GNS representation π_Ω in which the space translations are not implemented by strongly continuous unitary operators $U(\mathbf{x})$, $\mathbf{x}\in\mathbf{R}^3$, and, therefore, the generator, the momentum, cannot be defined, and

(iv) all positive extensions of ω are invariant under the large (and small) gauge transformations:

$$(\gamma^\Lambda)^*\Omega=\Omega,\quad (\operatorname{div}E(\mathbf{x})-j_0(\mathbf{x}))\,\Psi_\Omega=0. \tag{3.2}$$

Proof: (i) Since $[G(h),\mathcal{F}_{obs}]=0$, by Theorem 4.4 of Ref. 9.

$$G(h)\,\Psi_\omega=c_h\,\Psi_\omega,\quad c_h\in\mathbf{C}, \tag{3.3}$$

and, by Lorentz invariance of ω on $\mathcal{F}_{obs}$, $c_h=0$. By Schwarz' inequality a positive extension Ω satisfies

$$\Omega(G(h)\,B)=0,\quad \forall\ B\in\mathcal{F}. \tag{3.4}$$

This implies

$$\Omega([\operatorname{div}A(f),G(h)])=0,\quad \forall f,h\in\mathcal{S}(\mathbf{R}^4),$$

whereas the algebraic structure, Eq. (2.6), gives

$$\Omega([\operatorname{div}A(f),G(h)])=i\int d^4x\,f(x)\,\Delta h(x).$$

(ii) In fact,

$$|c_h|^2\,\Omega(e^{iA_i(\partial_i f)})=\Omega(W_l(0,-h)\,e^{iA_i(\partial_i f)}W_l(0,h))=e^{i\int d^4x\,f\Delta h}\,\Omega(e^{iA_i(\partial_i f)}),\quad \forall f,h\in\mathcal{S}(\mathbf{R}^4),$$

and, therefore, for $f\neq 0$,

$$\Omega(e^{iA_i(\partial_i f)})=0. \tag{3.5}$$

(iii) In fact, one has

$$\Omega(e^{iA_i(\partial_i h)}\,U(-\mathbf{x})\,e^{-iA_i(\partial_i h)}\,U(\mathbf{x}))=\Omega(e^{iA_i(\partial_i h-\partial_i h_{\mathbf{x}})})$$

and the right hand side vanishes for all $\mathbf{x}\neq 0$ and it is $=1$ for $\mathbf{x}=0$.

(iv) In fact, by Eq. (2.7) one has

$$\frac{d}{d\lambda}\Omega(\gamma^{\lambda\Lambda}(B))=\lim_{R\to\infty} i\,\Omega([\,G_R^{\Lambda},\,\gamma^{\lambda\Lambda}(B)\,])=0$$

as in Eq. (3.3).

The above proposition clarifies the roots of the problems which arise in the quantization of the temporal gauge, by reducing them to very basic structures. The solutions proposed in the literature, relying on an analysis of the free case, involve a non-normalizable vacuum, or the violation of time translation invariance, etc. (for an extensive review, see Ref. 5), so that new problems are somewhat arbitrarily added, hiding the basic issues. The following analysis of the free case makes clear that general properties, like time translation invariance and either positivity or existence of the correlation functions of the fields select exactly two alternatives, yielding solutions in terms of a time translation invariant vacuum over well defined operator algebras.

In particular, the existence of the ground state correlation functions of the fields requires an indefinite inner product space as in the Gupta–Bleuler gauge; alternatively, positivity can be achieved at the price of regularity of the representation of the longitudinal Weyl algebra. A close analog of such a situation appears for free nonrelativistic particles when one asks for the existence of a ground state (see Ref. 10).

In general, given an algebra $\mathcal{A}$, a time translation automorphism α_t and a time traslationally invariant Hermitian linear functional Ω on $\mathcal{A}$, we shall say that the *energy spectral condition* holds if, $\forall A, B\in\mathcal{A}$, the expectations $G_{AB}(t)\equiv\Omega(A\,\alpha_t(B))$ are continuous in t and their Fourier transforms

$$\tilde{G}_{AB}(\omega)=(2\pi)^{-1/2}\int dt\,G_{AB}(t)e^{-i\omega t}$$

are supported in $\mathbf{R}^{+}$.

Proposition 3.2: (1) Let Ω be a state on the gauge field algebra $\mathcal{A}$ invariant under the free time evolution Then

(i) *Ω cannot be positive and*

(ii) *if the restriction ω of Ω to the observable gauge algebra $\mathcal{A}_{obs}$ is semidefinite and satisfies the energy spectral condition, then the GNS representation π_ω of $\mathcal{A}_{obs}$ is irreducible and coincides with the standard vacuum representation of the electromagnetic field algebra.*

(2) Let Ω be a state on the Weyl gauge algebra $\mathcal{W}$ invariant under the free time evolution, satisfying the energy spectral condition, and let its restriction ω to $\mathcal{W}_{obs}$ be semidefinite. Then $\pi_\Omega(\mathrm{div}\,E)=0$, the GNS representation π_ω of $\mathcal{W}_{obs}$ is irreducible and coincides with the standard vacuum representation of the free electromagnetic field (Weyl) algebra.

Proof. (1 i). In fact, by time translation invariance, $\Omega(\partial_t O)=0, \forall O\in\mathcal{A}$, and since, by the equations of motion $\partial_t\,\mathrm{div}\,E=0$, one has

$$\Omega((\mathrm{div}\,E(f))^2)=\Omega(\partial_t(\mathrm{div}\,A(f)\,\mathrm{div}\,E(f)))=0, \tag{3.6}$$

so that positivity implies that the Hilbert space vector Ψ_Ω, which represents Ω (in the GNS representation space), satisfies

$$\operatorname{div} E(f)\,\Psi_\Omega = 0, \quad \forall f \in \mathcal{S}(\mathbf{R}^3).$$

This is incompatible with the CCR since

$$\Omega([A_i(x), \operatorname{div} E(y)]) = -i\,\partial_i\,\delta(\mathbf{x}-\mathbf{y}).$$

(1 ii) By Schwarz' inequality, Eq. (3.7) gives

$$\Omega(O \operatorname{div} E(h)) = 0, \quad \forall O \in \mathcal{A}_{obs}.$$

Thus, the restriction ω of Ω to $\mathcal{A}_{obs}$ yields a representation π_ω such that $\pi_\omega(F_{\mu\nu})$ is a free electromagnetic field with energy spectral condition and the usual argument gives the standard Fock representation; the one-point function $\omega(E) = \omega(\dot{A})$ vanishes by the time translation invariance of Ω.

(2) In fact, time translation invariance implies that for $h \neq 0$, $\Omega(W_l(h,k))$ is independent of k, say $F(h)$. On the other hand, one has

$$\begin{aligned} & e^{i[(\partial h,\, \partial k') - (\partial k,\, \partial h')]/2}\, e^{i\,t\,(\partial h,\, \partial h')/2}\, \Omega(W_l(h,k)\,\alpha_t(W_l(h',k'))) \\ & \quad = F(h+h'), \quad \text{if} \quad h+h' \neq 0, \\ & \quad = \Omega(W_l(0, k+k'+t\,h')) \equiv G(k+k'+t\,h'), \quad \text{if} \quad h+h' = 0. \end{aligned}$$

Thus, the energy spectral condition requires $F(h+h') = 0$, whenever $h+h' \neq 0$, since otherwise, by taking $h = h'$, one would get a negative point of the energy spectrum. It also requires that the distributional Fourier transform $\tilde{G}(\omega)$ of $G(t\,h)$, with respect to the variable t, has support in $\omega = 0$. In fact, putting $h' = -h$, $k = k' = 0$, $d \equiv (\partial h,\, \partial h)/2$, in the above formula we have

$$G_h(\alpha\,t) \equiv G(\alpha h t) = \Omega(W_l(\alpha\,h, 0)\, W_l(-\alpha\,h, \alpha h t))\, e^{it\,\alpha^2\,d} \equiv H(t) e^{i\,t\,\alpha^2 d}.$$

Taking the Fourier transform with respect to t, and using the positive support of the Fourier transform of $H(t)$, we get

$$\operatorname{supp} \tilde{G}_h(\omega) = \operatorname{supp} \tilde{H}((\omega - \alpha^2\,d)/\alpha) \subseteq \mathbf{R}^+,$$

so that

$$\operatorname{supp}_\omega \tilde{G}((\omega + \alpha^2 d)/\alpha) \subseteq \mathbf{R}_+, \quad \operatorname{supp} \tilde{G}(\omega) \subseteq \alpha^{-1}\mathbf{R}_+ - \alpha\,d, \quad \forall \alpha \in \mathbf{R}.$$

Then $\operatorname{supp} \tilde{G} \subseteq [-\alpha\,d, \infty]$ for $\alpha > 0$, and $\operatorname{supp} \tilde{G} \subseteq [-\infty, -\alpha\,d]$ for $\alpha < 0$, which implies $\operatorname{supp} \tilde{G} = \{0\}$. Since, by positivity of Ω, $G(t)$ is bounded, one has $\tilde{G}(\omega) = \delta(\omega)$ and

$$\Omega(W_l(0, t\,k)) = 1, \tag{3.7}$$

so that $\operatorname{div} E$ is a regular variable and all its correlation functions vanish.

The above propositions imply that the representations of the temporal gauge in the free case with positive energy are the following.

A. Positive gauge invariant representation

Proposition 3.3: Invariance under free time evolution and positivity of the energy uniquely determine the positive states Ω on the Weyl field algebra to be of the following form:

$$\Omega(W(f,g)) = 0, \quad \text{if} \quad \operatorname{div}\ f \neq 0, \tag{3.8}$$

$$\Omega(W(f, g+\partial k)) = \Omega(W(f,g)), \tag{3.9}$$

$$\Omega(W(f,g)) = e^{-w(f,g)}, \quad \text{if} \quad \operatorname{div} f = 0, \tag{3.10}$$

where $k \in \mathcal{S}_{\text{real}}(\mathbf{R}^3)$ *and* $w(f,g)$ *is the standard transverse two-point function* $\langle (A(f)+E(g))\,(A(f)+E(g))\rangle_0$, $\operatorname{div} f=0$.

Proof: In fact, by Eqs. (3.7) and (2.1), one has

$$0=\Omega([W(f,g),\operatorname{div} E(k)])=-\int d^3x\, k \operatorname{div} f\, \Omega(W(f,g)),$$

which implies Eq. (3.8). Equation (2.4) and the invariance under time translation implies Eq. (3.9). The last equation follows from Proposition 3.2 which fixes the representation of the observable algebra to be the standard Fock one.

It is not difficult to see that Ω is pure[8] and coincides with the state considered in Ref. 6. Thus, as anticipated, we have a nonregular representation and the ground state correlation functions of the vector potential do not exist. Nonregularity also follows from the requirement of Gauss' law constraint by the results of Refs. 7 and 8. However, the selection of the above representation of $\mathcal{W}$, Eqs. (3.8)–(3.10), crucially depends on the condition of positive energy; in fact, one may find other (nonregular) time translationally invariant pure states which define disjoint representations in which the energy spectral condition is violated.

Proposition 3.4: In the free case, the θ *automorphisms are not unitarily implementable in the GNS representation* π_Ω *given by the state* Ω *defined above, Eqs. (3.8)–(3.10). The states* $\beta^\theta * \Omega$ *are space time translationally invariant and define disjoint nonregular representations of the Weyl field algebra, in which the energy spectral condition is violated.*

Proof: In fact, by using Eqs. (3.8)–(3.10) one has

$$\Omega(e^{i E_j(f_R)/R^3})=e^{-w(0,\, f_R/R^3)} \underset{R\to\infty}{\to} 1,$$

which implies

$$s-\lim_{R\to\infty} e^{i E_j(f_R)/R^3}\,\Psi_\Omega=\Psi_\Omega\,.$$

By the CCR, the same equation holds for any Ψ of the form $A\,\Psi_\Omega$, $A\in\mathcal{W}$, i.e., on a dense set, and therefore on any vector of the representation, since $W(0,R^{-3} f_R)$ is a unitary operator. On the other hand, by Eq. (2.10)

$$\lim_{R\to\infty} \beta^\theta * \Omega(e^{iE_j(f_R)/R^3})=e^{i\theta_j}.$$

Thus, the states $\beta^\theta * \Omega$ define disjoint representations.

Space translation invariance follows from $\beta^\theta \alpha_{\mathbf{x}}=\alpha_{\mathbf{x}}\beta^\theta$ and time translation invariance follows from Eq. (2.9),

$$\begin{aligned}(\beta^\theta * \Omega)(\alpha_t(W(f,g)))&=\Omega(\beta^\theta\,\alpha_t(W(f,g)))=\Omega(\alpha_t\,\gamma^{t\,\theta\cdot\mathbf{x}}\beta^\theta(W(f,g)))\\&=\Omega(\beta^\theta(W(f,g))=(\beta^\theta * \Omega)((W(f,g))).\end{aligned}$$

The energy spectral condition is violated as a consequence of Proposition 3.2.

A characteristic property of the θ-vacua is that they yield a nonvanishing expectation of the electric field, which is the time derivative of the vector potential. This is not incompatible with time translation invariance, because $\beta^\theta * \Omega(E(f))=0$, if $\operatorname{div} f=0$ and, if $\operatorname{div} f\neq 0$, $A(f)$ is nonregularly represented, namely its expectations do not exist, only those of its exponentials do.

Since β^θ commutes with α_t on the observable fields, the energy spectral condition holds for the correlation functions of observables and, in fact, each observable sector $\mathcal{H}_\theta$ has a unique translationally invariant state, which is the lowest energy state.

B. Indefinite regular representations

The perturbative expansion as well as the standard functional integral computations rely on the use of the field variables and therefore implicitly make use of a representation of the field algebra (otherwise the propagator of the vector potential would not exist). However, even in the free case, there is a rich literature on the possible form of the propagator of the gauge field A_i and no general agreement on the conclusion (for a review of the contributions and a detailed bibliography, see Ref. 5).

At the roots of the problem debated in the literature is the identification of gauge invariance with the vacuum being annihilated by the Gauss operator $G=\mathrm{div}\,E-j_0$ and the conflict of this condition with canonical quantization. The solutions proposed, often in conflict with basic features of standard quantum field theory, do not seem to realize that the vanishing of the Gauss operator on the vacuum is only compatible with a nonregular representation, precluding the existence of the propagator of A_i. As a consequence, see Proposition 3.1, a representation of the field algebra requires to abandon positivity, to admit that not all vectors obtained by applying the fields to the vacuum have a physical interpretation and to require the Gauss operator constraint only in expectations on the physical states (a feature common to other nonpositive gauges like the Feynman–Gupta–Bleuler gauge).

Motivated by the lack in the literature of a satisfactory characterization of the two point function of the gauge potential (even in the free case), we shall analyze it under the general condition of space–time translational invariance. In our opinion it is difficult to live without such a condition, as required by a momentum space analysis of the correlation functions or of the Feynman diagrams, according to the general wisdom of quantum field theory (e.g., the positive energy spectral condition needed for the analytic continuation to imaginary times and the functional integral representation of the so obtained Schwinger functions).

In the following, we shall characterize the two point function in the temporal gauge with interaction, under the assumption of locality discussed in Sec. II, in terms of a Källen–Lehmann representation under the additional condition of rotational and parity invariance. The result shows that *(i)* positivity of the energy spectrum is satisfied by the two point function, but not the relativistic spectral condition, *(ii)* the vacuum is a nonpositive functional on the field algebra, and *(iii)* the Gauss' law constraint does not hold as an operator equation on the physical states and can only be required to hold in expectations on such states.

Proposition 3.5: Let Ω be a state on the local field algebra $\mathcal{F}$ invariant under space–time translations, rotations and parity, whose restriction to the observable field algebra satisfies the standard Wightman axioms for vacuum expectation values. Then the two point function of the gauge potential has the following representation ($y\equiv x'-x$):

$$\begin{aligned}\langle A_i(x)\,A_j(x')\rangle &\equiv \Omega(A_i(x)\,A_j(x'))\\ &= \int d^4k\, e^{iky}\int d\rho(m^2)\left(\delta_{ij}-\frac{k_i\,k_j}{\mathbf{k}^2+m^2}\right)\delta(k^2+m^2)\;\theta(k_0)\\ &\quad+\frac{1}{2}iy_0\left[\partial_i\partial_j\,\mathcal{P}(\Delta)\,\delta(\mathbf{y})+\int d^3k\, e^{-i\mathbf{k}\,\mathbf{y}}\int d\rho(m^2)\,k_ik_j(\mathbf{k}^2+m^2)^{-1}\right]\\ &\quad+\partial_i\partial_j a(\mathbf{x}^2),\end{aligned}\tag{3.11}$$

where $\mathcal{P}$ is a polynomial and $d\rho$ is the spectral measure of the two point function of the electromagnetic field

$$\begin{aligned}\langle F_{\mu\rho}F_{\nu\sigma}\rangle(y)&=(g_{\rho\sigma}\,\partial_\mu\partial_\nu+g_{\mu\nu}\partial_\rho\partial_\sigma-g_{\rho\nu}\partial_\mu\partial_\sigma-g_{\mu\sigma}\partial_\nu\partial_\rho)F(y),\\ \widetilde{F}(k)&=\int d\rho(m^2)\;\delta(k^2+m^2)\,\theta(k_0).\end{aligned}\tag{3.12}$$

The condition of a canonical structure at equal times, apart from renormalization constants, requires

$$\mathcal{P}=\text{const}\equiv Z.$$

The arbitrary function $a(\mathbf{x})$ *can be removed by a time independent operator gauge transformation.*

Such a two point function satisfies the positive energy but not the relativistic spectral condition.

In particular, in the free field case, we have

$$\langle A_i A_j\rangle(y)=(\delta_{ij}-\partial_i\partial_j(\Delta)^{-1})D^+(y)+\tfrac{1}{2}i\,y_0\,\partial_i\partial_j(\Delta)^{-1}\delta(\mathbf{y}). \tag{3.13}$$

Proof: Invariance under space–time translation, rotations and parity implies that the two point function can be written in the form

$$\langle A_i A_j\rangle(x)=\delta_{ij}H(x)+\partial_i\partial_j L(x), \tag{3.14}$$

with H, L rotationally invariant distributions; such a decomposition is unique up to a redefinition $H\to H+h(x_0)$, $L\to L-\frac{1}{2}h(x_0)\mathbf{x}^2$, L being defined up to constants. A comparison between the two point function of the electric field given by Eq. (3.12) and that derived from Eq. (3.14) (using $E_i=\partial_0 A_i$) yields

$$\delta_{ij}\partial_0^2(H-F)+\partial_i\partial_j(F+\partial_0^2 L)=0.$$

Such an equation implies

$$H=F+h(t),\quad \partial_i\partial_j\partial_0^2 L=-\partial_i\partial_j F-\delta_{ij}h(t),$$

and one can use the arbitrariness in the definition of H, L to remove $h(t)$. Hence one can write

$$\partial_i\partial_j L=-(\partial_i\partial_j/\partial_0^2)F+a_{ij}(\mathbf{x})+i\,t\,b_{ij}(\mathbf{x}),$$

since the operator $\partial_i\partial_j/\partial_0^2$ is well defined in momentum space, where it corresponds to multiplication of the spectral measure by the bounded function $k_i k_j(\mathbf{k}^2+m^2)^{-1}$; furthermore, by taking the curl one gets $a_{ij}(\mathbf{x})=\partial_i\partial_j a(\mathbf{x}^2)$, $b_{ij}(\mathbf{x})=\partial_i\partial_j b(\mathbf{x}^2)$.

Locality of the commutator $\langle[A_i(x),\partial_0 A_j(y)]\rangle$ requires

$$2\tilde{b}(\mathbf{k})=\int d\rho(m^2)(\mathbf{k}^2+m^2)^{-1}+\mathcal{P}(\mathbf{k}^2),$$

and a canonical structure at equal times requires $\mathcal{P}(\mathbf{k}^2)=Z$. The residual gauge invariance of the equations of motion and of the CCRs under time independent operator gauge transformations

$$A_i(x)\to A_i(x)+\partial_i\varphi(\mathbf{x}),\quad \psi(x)\to :e^{ie\varphi}:(\mathbf{x})\,\psi(x)$$

allows us to eliminate the function $a(\mathbf{x}^2)$.

The Fourier transform of the term linear in time has support on the plane $\omega=0$, $\mathbf{k}$ arbitrary, so that the posivitity of the energy spectrum is satisfied, but not the relativistic spectral condition.

In the free field case both $\operatorname{div} A\Psi_0$ and $\operatorname{div} E\Psi_0$ are vectors of zero indefinite product with themselves, briefly of zero norm or null vectors, which however cannot vanish.

As one should *a priori* expect, whenever a state yields a nontrivial representation of a gauge dependent field algebra,[11] the above indefinite states on the field algebra are not gauge invariant. In fact, one has $\Omega(\gamma^\Lambda(A_i))\neq\Omega(A_i)=0$.

Proposition 3.6: In the free case, the states $\beta^\theta * \Omega$, *with* Ω *any quasi-free (indefinite) state defined by Eq. (3.13) are space translationally invariant on the field algebra, but not time translationally invariant. Only their restrictions to the gauge invariant field algebra are time translationally invariant.*

Proof: In fact, $\forall f \in \mathcal{S}(\mathbf{R}^3)$, one has

$$\beta^\theta * \Omega(\alpha_t(A(f))) = \Omega(A(f)) + t \int d^3x\ \theta_i f_i(\mathbf{x})$$

and, if $\operatorname{div} f = 0$, $\int dx\ \theta_i f_i(\mathbf{x}) = -\int dx\ \boldsymbol{\theta}\cdot\mathbf{x} \operatorname{div} f(\mathbf{x}) = 0$.

In conclusion, the space and time translationally invariant θ-states on the observable field algebra do not have regular time translationally invariant extensions to the field algebra (the time invariant extension are nonregular); in this sense they display a mechanism which is crucial for solving the problem arising in the Ward identities of chiral symmetry breaking in quantum chromodynamics.[11,12]

Since the new structures emerging with respect to the standard case are connected with the longitudinal algebra, it is worthwhile to have a better mathematical control on the properties of its GNS representation given by the state Ω of Proposition 3.5, at least in the free case. As mentioned in Sec. II, Eqs. (2.5), the longitudinal algebra can be discussed in terms of the field variables $\operatorname{div} A_l(f_n)$, $\operatorname{div} \dot{A}_l(f_n)$, $f_n \in \mathcal{S}(\mathbf{R}^3)$. The problem is then reduced to the unique ground state (indefinite) representation of the Heisenberg algebra associated to a countable number of free particles. Such GNS representation has been analyzed in Ref. 10 and the result is the following.

Proposition 3.7: In the free case the quasi-free (indefinite) state Ω *defined by Eq. (3.13) is faithful on the longitudinal algebra* $\mathcal{A}_l$ *generated by* $\operatorname{div} A$, $\operatorname{div} E$, *and the commutant of* $\mathcal{A}_l$ *in the corresponding GNS representation is isomorphic to* $\mathcal{A}_l$.

The GNS representation is given as an infinite tensor product of Fock and anti-Fock representations[13,14] *of the canonical variables*

$$Q_{n,\pm} \equiv (q_n \pm p'_n)/\sqrt{2}, \quad P_{n,\pm} \equiv (\pm p_n + q'_n)/\sqrt{2},$$

with

$$q'_n \equiv i S\, q_n\, S, \quad p'_n \equiv -i\, S\, p_n\, S, \quad \forall n,$$

and S *the antiunitary KMS operator defined by*

$$S\, A\, \Psi_0 = A^* \Psi_0, \quad \forall A \in \mathcal{A}_l.$$

Proof: The proof is the same as for a single free particle.[10]

IV. FUNCTIONAL INTEGRAL REPRESENTATION

We start by discussing the functional integral representation of the temporal gauge in the indefinite case with free time evolution.

By analytic continuation to imaginary time the two point correlation function, Eq. (3.13), gives rise to the following Schwinger function,

$$S_{ij}(x-y) = (\delta_{ij} - \Delta^{-1}\, \partial_i\, \partial_j)\, S(x-y) - \partial_i\, \partial_j\, \Delta^{-1}\, \delta(\mathbf{x}-\mathbf{y})\ |x_0 - y_0|/2, \tag{4.1}$$

where S is the standard Schwinger function of a scalar field. The Schwinger function Eq. (4.1) defines an inner product in $\mathcal{S}^3_{\text{real}}(\mathbf{R}^4)$,

$$\langle f, f\rangle = \langle f, f\rangle_{tr} + \langle f, f\rangle_l,$$

$$\langle f, f\rangle_{tr} \equiv \int d^4x\, d^4y\, f_i(x)(\delta_{ij} - \Delta^{-1}\partial_i\partial_j)\, f_j(y)\, S(x-y), \tag{4.2}$$

$$\langle f, \ f\rangle_l \equiv \int d^4x\, d^4y\, \partial f(x)\, \partial f(y)\, \Delta^{-1}\, \delta(\mathbf{x}-\mathbf{y})\, |x_0 - y_0|/2. \tag{4.3}$$

The transverse inner product $\langle ., .\rangle_{tr}$ is semidefinite and therefore it defines a Gaussian integral with measure $d\mu(A^{tr}(\mathbf{x},\tau))$ and a Euclidean Gaussian field $A_i^{tr}(\mathbf{x},\tau)$.

The longitudinal inner product $\langle ., .\rangle_l$ is indefinite but not degenerate on $\mathcal{S}_l(\mathbf{R}^4) \equiv \{h = \partial_i g_i\,,\ g_i \in \mathcal{S}_{\text{real}}(\mathbf{R}^4)\}$. Therefore, the longitudinal inner product defines the two point Schwinger function of a Gaussian vector field $\partial_i\phi(\mathbf{x},\tau)$ with

$$\langle \phi(\mathbf{x},\tau)\ \phi(\mathbf{y},\sigma)\rangle = \Delta^{-1}\delta(\mathbf{x}-\mathbf{y})\, |\tau-\sigma|/2. \tag{4.4}$$

Thus, $\forall f \in \mathcal{S}(\mathbf{R}^3)$, $\phi(f,\tau)$ is the analog of the variable $q(\tau)$ describing the position of a free particle and Eq. (4.4) corresponds to the ground state Euclidean representation of the Heisenberg algebra with free evolution.[10] Following the results of Ref. 10, a functional integral representation is obtained by introducing the random field

$$A_i(\mathbf{x},\tau) = A_i^{tr}(\mathbf{x},\tau) + \partial_i[\ \xi(\mathbf{x},\tau) + z(\mathbf{x}) - \overline{z}(\mathbf{x})|\tau|], \tag{4.5}$$

where $z(\mathbf{x})$ is a complex Gaussian field with the following expectations

$$\langle z(\mathbf{x})\, z(\mathbf{y})\rangle = 0,\ \langle z(\mathbf{x})\, \overline{z}(\mathbf{y})\rangle = -\tfrac{1}{2}\Delta^{-1}\delta(\mathbf{x}-\mathbf{y}),$$

corresponding to $z = z_1 + iz_2,\ z_1, z_2$ independent real Gaussian fields with

$$\langle z_1^2\rangle = \langle z_2^2\rangle = -\Delta^{-1}\delta(\mathbf{x}-\mathbf{y})/4,$$

and $\xi(\mathbf{x},\tau)$ is a real Gaussian field with

$$\langle \xi(\mathbf{x},\tau)\ \xi(\mathbf{y},\sigma)\rangle = -\tfrac{1}{2}\Delta^{-1}\delta(\mathbf{x}-\mathbf{y})\ (-|\tau-\sigma| + |\tau| + |\sigma|).$$

Clearly, the covariance of ξ is a positive kernel, being the product of the positive kernel $-\Delta^{-1}\,\delta$ and of the Wiener kernel. Hence, the Schwinger functions are represented by

$$\langle A_{i_1}(\mathbf{x}_1,\tau_1)\cdots A_{i_n}(\mathbf{x}_n,\tau_n)\rangle = \int d\mu(A^{tr}(\mathbf{x},\tau))\, dw(\xi(\mathbf{x},\tau))\, d\nu(z(\mathbf{x})) \times \prod_{k=1}^{n}\ (A_i^{tr}(\mathbf{x}_k,\tau_k) + \partial_i(\xi(\mathbf{x}_k,\tau_k) + z(\mathbf{x}_k) - \overline{z}(\mathbf{x}_k)|\tau_k|)), \tag{4.6}$$

where $d\mu, d\nu, dw$ are the functional measures defined by the processes introduced above.

In the positive (nonregular) formulation of Sec. III A the construction of a functional integral representation for the Euclidean correlation functions essentially reduces to the case of the Euclidean correlation functions given by the (nonregular) positive ground state of a nonrelativistic particle, discussed in Ref. 10. In fact, the Euclidean correlation functions of exponentials of fields

$$\Omega(e^{iA(f_1,\tau_1)}\cdots e^{iA(f_n,\tau_n)})$$

obtained from Eqs. (3.8)–(3.10) have the same form as in Ref. 10, Eq. (C.2), with α_k replaced by $\partial_i\phi(f_k)$ and vanish unless

$$\partial_i f_1^i(\mathbf{x}) + \cdots + \partial_i f_n^i(\mathbf{x}) = 0. \tag{4.7}$$

If this condition is satisfied, by Proposition 3.3 and Eqs. (4.2) and (4.3) they coincide with the correlation functions of the indefinite case. Moreover, Eq. (4.7) implies that in the exponential the variable z is smeared with a vanishing test function, and the two point function of $\overline{z}$ vanishes. Therefore, as in Ref. 10, the above correlation functions coincide with those of the exponentials of Gaussian fields

$$A_i^{tr}(f^i,\tau)+\xi(-\partial_i f^i,\tau) \tag{4.8}$$

with the measures $d\mu$, dw introduced above in Eq. (4.6).

As for a free particle, the above correlation functions are therefore given by the ergodic mean over the real variables $\Xi(g)$, $\Xi\in\mathcal{S}'_{\text{real}}(\mathbf{R}^3)$ of the correlation functions of exponentials

$$\exp i\,A_i^{tr}(f^i,\tau)\exp -i\,(\xi(\partial_i f^i,\,\tau)+\Xi(\partial_i f^i)) \tag{4.9}$$

and, therefore, by the Riesz–Markov theorem, they can be represented as integrals over the spectrum Σ of the C^*-algebra generated by $\exp i\,\Xi(g)$, $g\in\mathcal{S}_{\text{real}}(\mathbf{R}^3)$. Σ is the generalization of the spectrum of the Bohr algebra,[15] generated by $\exp i\alpha x$, $x\in\mathbf{R}$, with Ξ corresponding to x and g to α.

In conclusion,

$$\Omega(e^{iA(f_1,\tau_1)}\cdots e^{iA(f_n,\tau_n)})=\int d\mu\,(A^{tr}(\mathbf{x},\tau))\,dw\,(\xi(\mathbf{x},\tau))$$
$$\times\int d\nu_\Sigma(\Xi(g))\prod_{s=1}^{n} e^{i\,A_i^{tr}(f_j^i,\tau_j)}\,e^{-i\,\xi(\partial_i f_j^i,\tau_j)}\,e^{-i\,\Xi(\partial_i f_j^i)}$$

with $d\nu_\Sigma$ the measure on Σ representing the ergodic mean in all the variables $\Xi(g)$;[10] the integral vanishes if Eq. (4.7) does not hold and otherwise coincides with the expectation of a product of exponentials of fields of the form (4.8).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Embeddings in space–times sourced by scalar fields

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(Received 27 November 2001; accepted 21 July 2003)

The extension of the Campbell–Magaard embedding theorem to general relativity with minimally coupled scalar fields is formulated and proven. The result is applied to the case of a self-interacting scalar field for which new embeddings are found, and to Brans–Dicke theory. The relationship between the Campbell–Magaard theorem and the General Relativity Cauchy and initial value problems is outlined. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1610237]

I. INTRODUCTION

There is currently a high level of interest in higher dimensional theories of gravity, motivated in part by recent developments in both string theory and early universe cosmology. There is a growing body of evidence[1] supporting the conjecture that the five perturbative, 10D string theories may correspond to different limiting cases of a more fundamental, nonperturbative, 11D ''M theory,'' which reduces to 11D supergravity in the infrared limit. (For recent reviews, see, e.g., Ref. 2.) Inspired by these advances, the proposal that our observable universe may be regarded as a domain wall or ''brane'' that is embedded in a higher-dimensional space–time has recently become popular in early universe cosmology.[3–6] In the braneworld scenario, the backreaction of the brane results in a higher-dimensional geometry that is nonfactorizable. Consequently this scenario is clearly distinct from the standard Kaluza–Klein compactification scheme. Indeed, in the five-dimensional Randall–Sundrum models, the extra dimension need not be compact.[6]

An important question that arises in such braneworld scenarios is the relationship between the geometry of the apparent, lower-dimensional world and that of the embedding, higher-dimensional space–time. It is therefore important, in view of the above discussion, to develop embedding theorems that enable such questions to be concretely addressed (for an overview and extensive bibliography, see Ref. 7). An important theorem is due to Campbell and Magaard (CM)[8,9] and states that any n-dimensional, (semi-)Riemannian manifold (M^n,g) can be locally and isometrically embedded in an $(n+1)$-dimensional manifold $(N^{n+1},\tilde{g})$, where the Ricci curvature of N^{n+1} vanishes.[8,9] The theorem was suggested by Campbell[8] and a proof was later offered by Magaard.[9] The theorem has been discussed in a number of contexts in the literature.[10–19]

Recently, we showed[16,17] how to extend this theorem to the class of embeddings where $(N^{n+1},\tilde{g})$ is an Einstein space, with a nonzero Ricci tensor that is directly proportional to the metric, $\tilde{g}$. Specific classes of embeddings, such as those of Einstein spaces within Einstein spaces, were established.[16]

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Einstein spaces can be viewed as solutions to General Relativity (GR), where the Ricci curvature is generated by a particular source—the cosmological constant. A natural question to address is whether further extensions of the CM theorem are possible and, in particular, to investigate embeddings in spaces that are sourced by dynamical matter fields. One of the simplest models for matter is a scalar field. In this paper, we extend the CM analysis to include a minimally coupled scalar field with a general potential energy arising through its self-interactions, and for Brans–Dicke theory.[20]

The paper is organized as follows. In Sec. II we extend the CM theorem to spaces sourced by a scalar field, identifying the mathematical conditions that must be satisfied by such a field in order for the embedding of a given manifold to be possible in principle. In Sec. III A, it is shown that minimally coupled, self-interacting scalar fields satisfy these conditions. Examples of such embeddings are given in Sec. III B. The Brans–Dicke field is then considered in Sec. III C. We then outline the clarifying relation between the CM theorem and the GR Cauchy[21–23] and initial value[24–26] problems in Sec. IV. We conclude in Sec. V.

II. CAMPBELL–MAGAARD THEOREM WITH SCALAR FIELD

The proof of the Campbell–Magaard (CM) theorem[8–10] and of its extension to the case when the embedding manifold is an Einstein space[16,17] follows a scheme similar to the methods employed when investigating the GR Cauchy problem, i.e., once the initial conditions for the metric in a three-dimensional hypersurface are given, one would like to know whether the Einstein field equations (EFEs) with a nontrivial source admit a unique solution.

In GR, the space–time metric is determined by the Einstein equations

$$G_{\mu\nu} = -\kappa T_{\mu\nu}, \tag{1}$$

where κ is the Einstein constant and $T_{\mu\nu}$ is the energy–momentum tensor, which is a function of the matter fields and the metric. We consider a scalar field $\overline{\chi}$ defined in a semi-Riemannian manifold $(N^{n+1}, \tilde{g}_{\alpha\beta})$. (In this paper, Latin and Greek indices run from 1 to n and from 1 to $n+1$, respectively.) We assume that the energy–momentum tensor of this field is an analytic function of the field $\overline{\chi}$, its first derivatives, and the metric tensor $\tilde{g}_{\alpha\beta}$:

$$\tilde{T}_{\mu\nu} = \tilde{T}_{\mu\nu}\left(\overline{\chi}, \frac{\partial\overline{\chi}}{\partial x^{\alpha}}, \tilde{g}_{\alpha\beta}\right). \tag{2}$$

Let us choose a coordinate system in which the metric $\tilde{g}_{\alpha\beta}$ has the line element

$$ds^2 = \overline{g}_{ik}\, dx^i\, dx^k + \varepsilon\, \overline{\phi}^2\, dy^2, \tag{3}$$

where $y = x^{n+1}$, $\overline{\phi} = \overline{\phi}(x^1, \ldots, x^n, y)$, $\overline{g}_{ik} = \overline{g}_{ik}(x^1, \ldots, x^n, y)$ and $\varepsilon = \pm 1$.

We suppose that the evolution of $\overline{\chi}$ is governed by a second-order p.d.e. which may be written in the form

$$\frac{\partial^2\overline{\chi}}{\partial y^2} = P\left(\overline{\chi}, \frac{\partial\overline{\chi}}{\partial x^i}, \frac{\partial\overline{\chi}}{\partial y}, \overline{g}_{\alpha\beta}, \frac{\partial\overline{g}_{\alpha\beta}}{\partial x^i}, \frac{\partial\overline{g}_{\alpha\beta}}{\partial y}, \frac{\partial^2\overline{\chi}}{\partial x^i \partial x^k}\right), \tag{4}$$

where P is analytic with respect to each of its arguments. We also make the physically reasonable assumption of energy–momentum conservation:

$$\tilde{\nabla}_{\mu}\tilde{T}^{\mu\nu} = 0, \tag{5}$$

where $\tilde{\nabla}_{\mu}$ is the covariant derivative with respect to $\tilde{g}_{\mu\nu}$.

We now claim that if conditions (2), (4), and (5) hold, it is possible to locally embed any n-dimensional, (semi-)Riemannian manifold (M^n,g) in an $(n+1)$-dimensional space sourced by the scalar field $\overline{\chi}$.

In the coordinates (3), the EFEs take the form

$$\tilde{R}_{ik}=\overline{R}_{ik}+\varepsilon\overline{g}^{jm}(\overline{\Omega}_{ik}\overline{\Omega}_{jm}-2\overline{\Omega}_{jk}\overline{\Omega}_{im})-\frac{\varepsilon}{\overline{\phi}}\frac{\partial\overline{\Omega}_{ik}}{\partial y}+\frac{1}{\overline{\phi}}\overline{\nabla}_i\overline{\nabla}_k\overline{\phi}=-\kappa\left(\tilde{T}_{ik}-\frac{1}{n-1}g_{ik}\tilde{T}\right), \quad (6)$$

$$\tilde{R}^y_i=\frac{\varepsilon}{\overline{\phi}}\overline{g}^{jk}(\overline{\nabla}_j\overline{\Omega}_{ik}-\overline{\nabla}_i\overline{\Omega}_{jk})=-\kappa\tilde{T}^y_i\,, \quad (7)$$

$$\tilde{G}^y_y=-\tfrac{1}{2}\overline{g}^{ik}\overline{g}^{jm}(\overline{R}_{ijkm}+\varepsilon(\overline{\Omega}_{ik}\overline{\Omega}_{jm}-\overline{\Omega}_{jk}\overline{\Omega}_{im}))=-\kappa\tilde{T}^y_y\,, \quad (8)$$

where

$$\overline{\Omega}_{ik}=-\frac{1}{2\overline{\phi}}\frac{\partial\overline{g}_{ik}}{\partial y} \quad (9)$$

and the barred terms are calculated with the metric $\overline{g}_{ik}$ induced on the hypersurface Σ_c of constant $y=c$.

We now state the following lemma:

Lemma 1: Let the functions $\overline{g}_{ik}(x^1,\ldots,x^n,y)$, $\overline{\phi}(x^1,\ldots,x^n,y)$ *and* $\overline{\chi}(x^1,\ldots,x^n,y)$ *be analytic at* $(0,\ldots,0)\in\Sigma_0\subset\Re^{n+1}$. *Assume that the following conditions hold:*

(i) $\overline{g}_{ik}=\overline{g}_{ki}$;

(ii) $\det(\overline{g}_{ik})\neq 0$;

(iii) $\overline{\phi}\neq 0$.

Assume further that $\overline{g}_{ik}$ *and* $\overline{\chi}$ *satisfy Eqs. (4) and (6) in the open set* $U\subset\Re^{n+1}$ *which contains* $0\in\Re^{n+1}$ *and (7) and (8) at* Σ_0. *Then,* $\overline{g}_{ik}$, $\overline{\phi}$, *and* $\overline{\chi}$ *satisfy (7) and (8) in a neighborhood of* $0\in\Re^{n+1}$.

Proof: The key point of the proof is given by (5). First, let us define the tensor $\tilde{F}_{\alpha\beta}=\tilde{G}_{\alpha\beta}+\kappa\tilde{T}_{\alpha\beta}$. By assumption, $\overline{\chi}$ satisfies (4) in a neighborhood $V\subset\Re^{n+1}$ of $0\in\Re^{n+1}$, whence (5) also holds in V. It then follows that $\tilde{F}_{\alpha\beta}$ has vanishing divergence, so

$$\frac{\partial\tilde{F}^y_\beta}{\partial y}=-\frac{\partial\tilde{F}^i_\beta}{\partial x^i}-\tilde{\Gamma}^\mu_{\mu\lambda}\tilde{F}^\lambda_\beta+\tilde{\Gamma}^\mu_{\lambda\beta}\tilde{F}^\lambda_\mu\,.$$

On the other hand, by expressing the Einstein tensor in terms of the Ricci tensor, we can write

$$\tilde{F}^i_k=\tilde{R}^i_k-\delta^i_k(\tilde{R}^j_j+\tilde{G}^y_y)+\kappa\tilde{T}^i_k\,.$$

Again, by assumption,

$$\tilde{R}^i_k=-\kappa\left[\tilde{T}^i_k-\frac{\delta^i_j}{n-1}(\tilde{T}^j_j+\tilde{T}^y_y)\right]$$

holds in $V\subset\Re^{n+1}$ and it then follows that $\tilde{F}^i_k=-\delta^i_k\tilde{F}^y_y$ in V. After some algebra we may then deduce that

$$\frac{\partial\tilde{F}^y_y}{\partial y}=-\varepsilon\overline{\phi}^2\overline{g}^{ij}\frac{\partial\tilde{F}^y_i}{\partial x^j}-2\tilde{\Gamma}^i_{iy}\tilde{F}^y_y+\left(-\varepsilon\frac{\partial(\overline{\phi}^2\overline{g}^{ij})}{\partial y^j}-\varepsilon\overline{\phi}^2\overline{g}^{ij}\tilde{\Gamma}^k_{kj}+\tilde{\Gamma}^i_{yy}\right)\tilde{F}^y_i\,,$$

$$\frac{\partial \tilde{F}^y_i}{\partial y} = \frac{\partial \tilde{F}^y_y}{\partial x^i} + 2\tilde{\Gamma}^y_{yi}\tilde{F}^y_y + (\tilde{\Gamma}^k_{yi} + \varepsilon\overline{\phi}^2\overline{g}^{kj}\tilde{\Gamma}^y_{ij} - \tilde{\Gamma}^\mu_{y\mu}\delta^k_i)\tilde{F}^y_k$$

and since (7) and (8) hold at the hypersurface Σ_0, it follows that $\tilde{F}^y_\beta = 0$ and hence that $\partial\tilde{F}^y_\beta/\partial y|_{y=0} = 0$.

It is not difficult to show by mathematical induction that all the derivatives of $\tilde{F}^y_\beta$ (to any order) vanish at $y=0$. As $\tilde{F}^y_\beta$ is analytic, we may therefore conclude that $\tilde{F}^y_\beta = 0$ in an open set of $\Re^{n+1}$. Thus, (7) and (8) also hold in an open set of $\Re^{n+1}$ which includes the origin and this proves the lemma. □

To proceed, we must now establish that the solutions $\overline{g}_{ik}$, $\overline{\phi}$, and $\overline{\chi}$ do indeed exist. With this in mind, let us now recall the Cauchy–Kowalewski (CK) theorem:[27]

Theorem [Cauchy–Kowalewski]: *Consider the set of partial differential equations*

$$\frac{\partial^2 u^A}{\partial (y^{n+1})^2} = F^A\left(y^\alpha, u^B, \frac{\partial u^B}{\partial y^\alpha}, \frac{\partial^2 u^B}{\partial y^\alpha \partial y^i}, \right), \quad A = 1, \ldots, m, \tag{10}$$

where $u^1, .., u^m$ *are* m *unknown functions of the* $n+1$ *variables* $y^1, \ldots, y^n, y^{n+1}$, $\alpha = 1, \ldots, n+1$, $i = 1, \ldots, n$, $B = 1, \ldots, m$. *Also, let* $\xi^1, \ldots, \xi^m, \eta^1, \ldots, \eta^m$, *be functions of the variables* $y^1, \ldots, y^n$, *and be analytic at* $0 \in \Re^n$. *If the functions* F^A *are analytic with respect to each of their arguments around the values evaluated at the point* $y^1 = \cdots = y^n = 0$, *there exists a unique solution of Eq. (10) which is analytic at* $0 \in \Re^{n+1}$ *and that satisfies the initial conditions*

$$u^A(y^1, \ldots, y^n, 0) = \xi^A(y^1, \ldots, y^n), \tag{11}$$

$$\frac{\partial u^A}{\partial y^{n+1}}(y^1, \ldots, y^n, 0) = \eta^A(y^1, \ldots, y^n), \quad A = 1, \ldots, m. \tag{12}$$

After solving (6) for the second-order derivative of $\overline{g}_{ik}$ with respect to y we find that

$$\frac{\partial^2 \overline{g}_{ik}}{\partial y^2} = -2\varepsilon\kappa\overline{\phi}^2\left(T_{ik} - \frac{1}{n-1}g_{ik}T\right) + \frac{1}{\overline{\phi}}\frac{\partial\overline{\phi}}{\partial y}\frac{\partial\overline{g}_{ik}}{\partial y}$$
$$- \frac{1}{2}\overline{g}^{jm}\left(\frac{\partial\overline{g}_{ik}}{\partial y}\frac{\partial\overline{g}_{jm}}{\partial y} - 2\frac{\partial\overline{g}_{im}}{\partial y}\frac{\partial\overline{g}_{jk}}{\partial y}\right) - 2\varepsilon\overline{\phi}\left(\frac{\partial^2\overline{\phi}}{\partial x^i \partial x^k} - \frac{\partial\overline{\phi}}{\partial x^j}\overline{\Gamma}^j_{ik}\right) - 2\varepsilon\overline{\phi}^2\overline{R}_{ik}. \tag{13}$$

Due to the symmetry of the tensors, $\overline{g}_{ik}$ and T_{ik}, we can rewrite (13) in terms of the components of g_{ik} with $i \leqslant k$. This equation, together with the field equation (4), form a set of $1 + n(n+1)/2$ p.d.e's for the $1 + n(n+1)/2$ unknown functions, $\overline{g}_{ik}$ $(i \leqslant k)$ and $\overline{\chi}$. (Note that $\overline{\phi}$ is a nonzero analytic function that is treated as a known.)

Thus, the p.d.e. system we have just obtained has the canonical form of (10) and, moreover, it satisfies all of the conditions required for the use of the CK theorem. Indeed, by virtue of the properties (2) and (4) imposed on $T_{\alpha\beta}$ and P, the right-hand side of the equations is comprised of functions of the variables

$$x^1, \ldots, x^n, y; \overline{g}_{ik}, \overline{\chi}, \frac{\partial\overline{g}_{ik}}{\partial x^j}, \frac{\partial\overline{g}_{ik}}{\partial y}, \frac{\partial\overline{\chi}}{\partial x^j}, \frac{\partial\overline{\chi}}{\partial y}; \frac{\partial^2\overline{g}_{ik}}{\partial x^j \partial x^m}, \frac{\partial^2\overline{\chi}}{\partial x^j \partial x^m},$$

which are analytic with respect to each of their arguments at

$$x^1 = 0, \ldots, x^n = 0, y = 0; \overline{g}_{ik}|_0, \overline{\chi}|_0, \left.\frac{\partial\overline{g}_{ik}}{\partial x^j}\right|_0, \left.\frac{\partial\overline{g}_{ik}}{\partial y}\right|_0, \left.\frac{\partial\overline{\chi}}{\partial x^j}\right|_0, \left.\frac{\partial\overline{\chi}}{\partial y}\right|_0; \left.\frac{\partial^2\overline{g}_{ik}}{\partial x^j \partial x^m}\right|_0, \left.\frac{\partial^2\overline{\chi}}{\partial x^j \partial x^m}\right|_0,$$

if $|\overline{g}_{ik}|_0 \neq 0$. Therefore, given analytic initial conditions

$$\overline{g}_{ik}(x^1,\ldots,x^n,0)=g_{ik}(x^1,\ldots,x^n), \quad \frac{\partial \overline{g}_{ik}}{\partial y}(x^1,\ldots,x^n,0)=\overline{\phi}(x^1,\ldots,x^n,0)\Omega_{ik}(x^1,\ldots,x^n),$$

$$\overline{\chi}(x^1,\ldots,x^n,0)=\xi(x^1,\ldots,x^n), \quad \frac{\partial \overline{\chi}}{\partial y}(x^1,\ldots,x^n,0)=\eta(x^1,\ldots,x^n), \tag{14}$$

which satisfy $|g_{ik}| \neq 0$, there exists a unique set of functions $\overline{g}_{ik}$ and $\overline{\chi}$ which solve Eqs. (4) and (6) which are analytic at the origin. It should be noted that an important feature of these solutions is the property $|\overline{g}_{ik}| \neq 0$ in some neighborhood of $0 \in \mathfrak{R}^{n+1}$.

If we take the initial conditions g_{ik} as being the metric components of a (semi-)Riemannian space M^n written in some coordinate system, then we can state the following theorem:

Theorem 1: *Let M^n be an n-dimensional, semi-Riemaninan manifold with metric given by $ds^2=g_{ik}dx^i dx^k$, in a coordinate system $\{x^i\}$ of M^n. Let $p \in M^n$ have coordinates $x_p^1=\cdots=x_p^n=0$. Then M^n has a local isometric and analytic embedding (at the point p) in an $(n+1)$-dimensional space sourced by any arbitrary scalar field $\overline{\chi}$ that is characterized by the properties (2), (4), and (5) iff there exist functions $\Omega_{ik}(x^1,\ldots,x^n)$ $(i,k=1,...,n)$, $\xi(x^1,\ldots,x^n)$, $\eta(x^1,\ldots,x^n)$ and $\phi(x^1,\ldots,x^n) \neq 0$ that are analytic at $0 \in \mathfrak{R}^n$ such that*

$$\Omega_{ik}=\Omega_{ki}, \tag{15}$$

$$g^{jk}(\nabla_j \Omega_{ik}-\nabla_i \Omega_{jk})=-\varepsilon \kappa \phi T_i^y(\xi,\eta,g_{ij}), \tag{16}$$

$$g^{ik}g^{jm}(R_{ijkm}+\varepsilon(\Omega_{ik}\Omega_{jm}-\Omega_{jk}\Omega_{im}))=2\kappa T_y^y(\xi,\eta,g_{ij}). \tag{17}$$

Proof: ($\Rightarrow$) If M^n has an embedding in some arbitrary space sourced by a scalar field, then it can be proved[17,28] that there exists a coordinate system in which the metric of the embedding space has the form $ds^2=\overline{g}_{ik}dx^i dx^k+\varepsilon \overline{\phi}^2 dy^2$, where the analytic functions $\overline{g}_{ik}(x^1,\ldots,x^n,y)$ and $\overline{\phi}(x^1,\ldots,x^n,y)$ are such that $\overline{\phi}(x^1,\ldots,x^n,y) \neq 0$ and $\overline{g}_{ik}(x^1,\ldots,x^n,0)=g_{ik}(x^1,\ldots,x^n)$ in an open set of $\mathfrak{R}^n$ which contains the origin. Given that the embedding space is, by assumption, generated by a scalar field $\overline{\chi}$, it follows that $\overline{g}_{ik}$ and $\overline{\phi}$ necessarily satisfy Eqs. (4), (6), and (8) for some field $\overline{\chi}(x^1,\ldots,x^n,y)$ in a neighborhood of $0 \in \mathfrak{R}^{n+1}$. In particular, Eqs. (7) and (8) hold for $y=0$. Therefore, the functions $\Omega_{ik}(x^1,\ldots,x^n)$ $(i,k=1,...,n)$, $\xi(x^1,\ldots,x^n)$, $\eta(x^1,\ldots,x^n)$ and $\phi(x^1,\ldots,x^n)$, as defined by

$$\Omega_{ik}=\overline{\Omega}_{ik}(x^1,\ldots,x^n,0), \quad \xi=\overline{\chi}(x^1,\ldots,x^n,0)\,\eta=\left.\frac{\partial \overline{\chi}}{\partial y}\right|_{y=0}, \quad \phi(x^1,\ldots,x^n)=\overline{\phi}(x^1,\ldots,x^n,0) \tag{18}$$

satisfy Eqs. (15), (16) and (17).

($\Leftarrow$) Suppose that there exist functions $\Omega_{ik}(x^1,\ldots,x^n)$, $\xi(x^1,\ldots,x^n)$, $\eta(x^1,\ldots,x^n)$ and $\phi(x^1,\ldots,x^n) \neq 0$ which satisfy (15), (16), and (17). Choose an analytic function given by $\overline{\phi}(x^1,\ldots,x^n,y) \neq 0$ such that $\overline{\phi}(x^1,\ldots,x^n,0)=\phi(x^1,\ldots,x^n)$. By virtue of the CK theorem, there exists a unique set of analytic functions $\overline{g}_{ik}(x^1,\ldots,x^n,y)$ and $\overline{\chi}(x^1,\ldots,x^n,y)$ that satisfy Eqs. (4) and (6) and the initial conditions (14). Since, by assumption, the initial conditions satisfy Eqs. (15), (16), and (17), Eqs. (7) and (8) are satisfied at $y=0$ by $\overline{g}_{ik}$, $\overline{\phi}$ and $\overline{\chi}$. It follows from Lemma 1 that $\overline{g}_{ik}$, $\overline{\phi}$, and $\overline{\chi}$ also satisfy Eqs. (4), (6), and (8) in an open set of $\mathfrak{R}^{n+1}$ which contains the origin. We conclude, therefore, that the $(n+1)$-dimensional manifold whose line element (3) is expressed in terms of the solutions $\overline{g}_{ik}$ and $\overline{\phi}$ is a space generated by a scalar field. Thus, the (semi-)Riemannian manifold (M^n,g) can indeed be embedded in a space sourced by a scalar field. □

According to Theorem 1, the existence of solutions to Eqs. (15)–(17) is sufficient to ensure that the local, analytic embedding of M^n is possible. The proof that these solutions do in fact exist consists in showing that Eqs. (15)–(17) can be expressed in the canonical form required by the CK theorem (here in its first-derivative version). This can be done by following the method presented in Ref. 10 with no significant modifications, and so we omit the details here. The idea is to use (17) to isolate Ω_{11} which is then substituted into (16) which is to be regarded as a system of p.d.e.'s for n unknown functions: the $n-1$ Ω_{1k} for $k\geqslant 2$ and one other component of Ω, which we call Θ. These p.d.e.'s are in the correct canonical form to employ the CK theorem. Thus, if the analytic functions g_{ik} are given, there exist analytic functions Ω_{ik} which solve Eqs. (15)–(17) and this leads us to the following theorem:

Theorem 2: *Let M^n $(n>1)$ be a piece of a (semi-)Riemannian space with line element $\mathrm{d}s^2=g_{ik}\mathrm{d}x^i\mathrm{d}x^k$, expressed in a coordinate system which covers a neighborhood of a point $p\in M^n$ whose coordinates are $x_p^1=\cdots=x_p^n=0$. If g_{ik} are analytic functions at $0\in\Re^n$, then M^n can be embedded at p in some $(n+1)$-dimensional space sourced by any arbitrary scalar field satisfying conditions (2), (4), and (5). Moreover, the line element of the embedding space is unique if the arbitrary functions to be chosen obey the following conditions:*

(i) *the $[n(n-1)/2]-1$ functions Ω_{ik} $(i\leqslant k, i>1$, and excluding the component $\Theta)$ are analytic at $0\in\Re^n$;*

(ii) *the n functions $\Omega_{1k}(0,x^2,\ldots,x^n)=f_k(x^2,\ldots,x^n)$ $(k>1)$ and $\Theta(0,x^2,\ldots,x^n)=f_1(x^2,\ldots,x^n)$ are analytic at $0\in\Re^{n-1}$, with the coefficient of Ω_{11} in (17) nonzero (to permit the elimination of Ω_{11} in order to set up the p.d.e. system),*

(iii) *a function $\phi(x^1,\ldots,x^{n+1})\neq 0$, analytic at $0\in\Re^{n+1}$, is chosen;*

(iv) *two functions $\xi(x^1,\ldots,x^n)$ and $\eta(x^1,\ldots,x^n)$, analytic at $0\in\Re^n$, are chosen.*

Note that when we refer to a space generated by a scalar field we have in mind a nontrivial solution of the Einstein-scalar system. In other words, we are implicitly considering a solution such that the associated energy–momentum tensor is nonzero. The exclusion of trivial solutions is possible because the initial conditions of the field (the functions ξ and η) are arbitrary and this implies that they can be chosen in such a way that $T_{\alpha\beta}\neq 0$ at Σ_0 (for some α and β). Consequently, continuity requirements imply that the energy–momentum tensor does not vanish in some neighborhood of $0\in\Re^{n+1}$.

We proceed in Sec. III to employ this theorem to establish specific classes of embeddings.

III. APPLICATIONS

A. Self-interacting scalar fields

In this section we consider a real scalar field, χ, minimally coupled to Einstein gravity and self-interacting through a potential, $W(\chi)$. We assume that the potential is a well-behaved, analytic function of the field. The energy–momentum tensor of such a field is given by

$$T_{\alpha\beta}=\nabla_\alpha\chi\nabla_\beta\chi-\tfrac{1}{2}g_{\alpha\beta}(\nabla^\gamma\chi\nabla_\gamma\chi)-g_{\alpha\beta}W(\chi). \tag{19}$$

It easily follows that the energy–momentum tensor (19) has vanishing divergence if χ solves the field equation

$$\nabla^\alpha\nabla_\alpha\chi-\frac{\mathrm{d}W}{\mathrm{d}\chi}=0. \tag{20}$$

In the coordinate system (3) the field equation (20) takes the form of Eq. (4) with

$$P=\varepsilon\phi^2\left(-g^{ik}\frac{\partial^2\chi}{\partial x^i\partial x^k}-g^{\alpha\beta}\Gamma^\gamma_{\alpha\beta}\frac{\partial\chi}{\partial x^\gamma}+\frac{\mathrm{d}W}{\mathrm{d}\chi}\right). \tag{21}$$

Note that the function P, which depends on χ, $\partial\chi/\partial x^i$, $\partial\chi/\partial y$, $g_{\alpha\beta}$, $\partial g_{\alpha\beta}/\partial x^i$, $\partial g_{\alpha\beta}/\partial y$, and $\partial^2\chi/\partial x^i\partial x^k$, is analytic with respect to each of these arguments.

Since conditions (2), (4), and (5) are satisfied by a minimally coupled, self-interacting scalar field, we may conclude the following:

Corollary 1: Let $M^n(n>1)$ *be a piece of a (semi-)Riemannian space with line element* $\mathrm{d}s^2=g_{ik}\mathrm{d}x^i\mathrm{d}x^k$, *expressed in a coordinate system which covers a neighborhood of a point* $p\in M^n$ *whose coordinates are* $x_p^1=\cdots=x_p^n=0$. *If* g_{ik} *are analytic functions at* $0\in\Re^n$, *then* M^n *can be embedded at* p *in some* $(n+1)$*-dimensional space generated by any arbitrary, minimally coupled, self-interacting scalar field.*

Note that M^n is truly Riemannian for $\varepsilon=-1$ and semi-Riemannian for $\varepsilon=+1$.

B. Examples of embeddings with self-interacting scalar fields

We now employ this result to construct embeddings for a class of space–times into higher-dimensional space–times sourced by such a scalar field. We begin with the ansatz

$$\overline{\Omega}_{ij}=C\overline{g}_{ij}, \tag{22}$$

where $C=C(x^\alpha)$ is a scalar function of the coordinates of the embedding metric. We further assume that the scalar field is independent of the embedded metric coordinates, i.e., $\chi=\chi(y)$, and specify $\kappa=1$ and $\varepsilon=1$ for simplicity.

Substituting (22) into (16) implies that $\nabla_i C=0$ and, consequently, that C must be a function of the extra coordinate y alone. Choosing the normal coordinate form for ϕ:

$$\phi=1, \tag{23}$$

then implies that (9) can be integrated to yield the solution

$$\overline{g}_{ij}=a^2(y)g_{ij}, \tag{24}$$

where $C\equiv-\mathrm{d}\ln a/\mathrm{d}y$.

When (22) and (23) are valid, the scalar field equation (20) simplifies to

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}y^2}+\frac{n}{a}\frac{\mathrm{d}a}{\mathrm{d}y}\frac{\mathrm{d}\chi}{\mathrm{d}y}-\frac{\mathrm{d}V}{\mathrm{d}\chi}=0 \tag{25}$$

and by substituting the appropriate components of the energy–momentum tensor (19) into (6) and (8), we find that

$$\overline{R}_{ik}+\overline{\Omega}\overline{\Omega}_{ik}-2\overline{\Omega}_{im}\overline{\Omega}_k^m-\frac{\partial\overline{\Omega}_{ik}}{\partial y}=-\frac{2V}{n-1}\overline{g}_{ik}, \tag{26}$$

$$\overline{R}+\overline{\Omega}^2-\overline{\Omega}_j^i\overline{\Omega}_i^j=\left(\frac{d\chi}{dy}\right)^2-2V. \tag{27}$$

Furthermore, subtracting (27) from the trace of (26) and substituting for the ansatz (22) implies that

$$\frac{n}{a}\frac{\mathrm{d}^2a}{\mathrm{d}y^2}=-\left(\frac{\mathrm{d}\chi}{\mathrm{d}y}\right)^2-\frac{2V}{n-1}. \tag{28}$$

We may solve (28) and (25) for an unknown self-interaction potential, by specifying the functional forms of $a(y)$ and $\chi(y)$:

$$a\equiv(1+\lambda y)^p, \tag{29}$$

$$\chi \equiv q \ln(1+\lambda y), \tag{30}$$

where p, q, and λ are constants. Substituting (29) and (30) into (28) implies that this is consistent if the scalar field potential has an exponential (Liouville) form:

$$V = -\lambda^2\left(\frac{n-1}{2}\right)[np(p-1)+q^2]\exp\left(-\frac{2}{q}\chi\right), \tag{31}$$

and it then follows that the scalar field equation (25) is solved if

$$(p-1)[q^2-p(n-1)]=0. \tag{32}$$

Thus, the embedding is established by solving (26) for the two cases, where $q^2=p(n-1)$ or $p=1$. In the first case, substituting for (29)–(31) implies that the embedding metric, g_{ij}, must have vanishing Ricci tensor. We conclude, therefore, that there is an embedding of n-D Ricci-flat manifolds with metric g_{ij}, in an $(n+1)$-D manifold sourced by a scalar field, with metric given by

$$ds^2=(1+\lambda y)^p g_{ik}dx^i dx^k + dy^2, \tag{33}$$

where the scalar field (30) self-interacts through the exponential potential (31). This generalizes the 4D result of Ref. 29 to arbitrary dimension.

In the second case, where $p=1$, the above-mentioned procedure implies that (26) is solved if

$$R_{ik}=\frac{(q^2-n+1)\lambda^2}{(1+\lambda y)^2}g_{ik} \tag{34}$$

and it follows that the embedded metric is an Einstein space with a nonzero Ricci curvature. The sign and magnitude of the effective cosmological constant of the embedded manifold determine the self-interaction coupling, q, of the scalar field. Indeed, the potential (31) is negative-definite for this embedding. An embedding of this type has been considered within the context of dilatonic braneworld scenarios.[30] It is interesting that the functional form of the potential (31) is the same for the two different classes of embedding. Moreover, potentials of this form arise in compactified supergravity theories.[31]

The above-given embeddings are specific in the sense that for the assumed form of Ω_{ik} given in (22), the embedding is only consistent if the scalar field has an exponential potential. However, Corollary 1 states that an embedding is possible for any analytic potential. This would require some other form for Ω_{ik} to be chosen.

C. Brans–Dicke theory

The Brans–Dicke theory of gravity[20] represents a natural extension of GR, where a nonminimally coupled (''dilatonic'') scalar field parametrizes the space–time dependence of Newton's ''constant.'' Nevertheless, it is well known that this theory is conformally equivalent to GR with a minimally coupled scalar field. Therefore, the following corollary to the above-mentioned theorems is deduced if one is prepared to work within the context of the conformally transformed fields.

Corollary 2: Let $M^n(n>1)$ *be a piece of a (semi-)Riemannian space with line element* $ds^2=g_{ik}dx^i dx^k$, *expressed in a coordinate system which covers a neighborhood of a point* $p\in M^n$ *whose coordinates are* $x_p^1=\cdots=x_p^n=0$. *If* g_{ik} *are analytic functions at* $0\in\Re^n$, *then* M^n *can be embedded at* p *in some* $(n+1)$*-dimensional space which is a solution of the vacuum, Brans–Dicke field equations.*

IV. CAMPBELL–MAGAARD AND THE GR CAUCHY AND INITIAL VALUE PROBLEMS

In Sec. II, we referred to the close relationship between the CM theorem and the GR Cauchy and initial value problems (CP and IVP, respectively). There is a wealth of literature on the latter problems within the context of $(3,0)\rightarrow(3,1)$ embeddings [we denote by (p,q) a manifold with p spacelike and q timelike coordinates], which makes it a valuable source of ideas for embedding theorems. The first idea is to show how the CM theorem follows from a collection of known results. The second idea will be to question whether any of the dimension- or signature-dependent results of the GR CP have useful generalizations. This will lead to possible limitations of the usual methods of constructing higher-dimensional solutions from lower-dimensional ones. We begin by outlining the GR CP and IVP.

By use of the $(3+1)$ split of the space–time line element (here, N is the lapse, N^i is the shift, and h_{ij} is the induced 3-metric)

$$ds^2 = h_{ij}(N\,dx^i + N^i dt)(N\,dx^j + N^j\,dt) - (N\,dt)^2, \tag{35}$$

the ten EFEs may be rewritten as six evolution equations and the four Gauss–Codazzi constraints. The mathematics of this split is the same, up to the signature, as that of splitting the EFEs into Eq. (6) and into Eqs. (7) and (8), if one identifies the lapse to be ϕ and imposes the partial gauge condition that the shift be zero. The GR CP is then the study of the evolution equations given some initial data that obeys the constraints.

It is standard knowledge[21,22] that these evolution equations can be written in the correct form required by the CK theorem, and so we are guaranteed that a solution exists locally and that it is unique. Whereas self-consistency requires the evolution equations to propagate the constraints off the initial hypersurface, it is immediately evident that this follows from the Bianchi identities.

There are additional results about the GR CP having a number of physically desirable features. First, it is Hadamard well-posed[27,21] so that in addition to the existence of a unique solution, the solution depends continuously on the prescribed data. Without this, an arbitrarily small change in the data set could give rise to an arbitrarily large change in the form of the solution which prevents physical predictability. Second, it possesses the ''domain of dependence'' property, i.e., the data can only affect the evolution in regions that are in causal contact with that data, which is a necessary criterion for the good behavior of hyperbolic systems.[21,23] The continuous dependence and domain of dependence properties follow in harmonic coordinates from Leray's theorem,[32,21] which is specific to hyperbolic operators. Finally, it is standard knowledge that the GR CP is well-posed in the presence of scalar fields, electromagnetism, perfect fluids, Brans–Dicke theory, and certain higher-derivative theories.[21]

The IVP or data construction problem (solving the Gauss–Codazzi constraints) is considered to be the most difficult step in the $(3+1)$ formalism of GR.[33] This problem is underdetermined, because there are twelve unknown functions (the components of the 3-metric h_{ik} and the second fundamental form Ω_{ik}), but only four equations. Hawking and Ellis[34] apparently refer to a general result stating that if eight of the unknown functions are specified for a space–time with an arbitrary matter content, the constraint equations may be solved for the remaining four. However, the work they refer to, Ref. 22, considers only two methods (the thin sandwich method and the usual conformal method), neither of which resemble Magaard's method.

We now consider the CM theorem piece by piece. The structure of none of the above-mentioned results is dependent on the dimension. Neither the CK theorem nor the method of expressing the GR evolution equations in the correct form to invoke the CK theorem are affected by the signature. Furthermore the Bianchi identity which guarantees constraint propagation is geometrical and hence equally valid regardless of the signature. Hence, the first part of the proof of the CM theorem (existence, uniqueness, and constraint propagation) follows directly from these results holding for the $(3+1)$-D GR CP.

The second part of the proof, due to Magaard, is a subcase of the result in Hawking and Ellis[34] generalized to arbitrary dimension. However, we emphasize that Magaard's approach differs from that of the usual conformal data construction.[24–26] The former considers the lower-dimensional

metric to be a known function, but the latter considers it to be known only up to a conformal factor. The former is of interest following the new motivation for studying higher-dimensional space–times, whereas the latter has only been employed for three spacelike dimensions using largely signature-dependent (that is, elliptical) methods.

If we are to interpret the CM theorem from a physical point of view, we are well-motivated to demand that the procedure for constructing embeddings is a well-posed problem. The types of embeddings of interest are $(n,1)\rightarrow(n+1,1)$ and $(n,1)\rightarrow(n,2)$, which are forms which are not known to exhibit continuous dependence, respectively. (There is no simple way of investigating whether theorems that hold for one particular signature hold for any other. This is due to significant mathematical differences between elliptic and ''hyperbolic'' operators. From the point of view of the function spaces that underly the analysis, Holder spaces are natural for the study of elliptic operators while Sobolev spaces are natural for the study of hyperbolic operators.) The former is termed the ''sideways problem for a hyperbolic system,'' and arises in a number of nonrelativistic contexts, as summarized by Ames and Straughan.[35] The only general result known for simple examples of such problems is that, given certain bounds, the solution is Holder-stable in some region,[36] but this is not considered to amount to a sufficiently strong theorem to guarantee continuous dependence. The latter is an ultrahyperbolic problem. These remain largely unexplored since they were traditionally considered to be physically irrelevant (see, however, Ref. 37). This implies, for example, that there are problems with the physical interpretation of models based on GR with two timelike dimensions[38] (as also pointed out in $(10+2)$-D supergravity[39]).

If we exclude this second possibility, it may be more promising to approach higher-dimensional embeddings with a two-step procedure of the form $(3,0)\rightarrow(4,0)\rightarrow(4,1)$. The first step could be a boundary problem along the lines considered in Ref. 40, while the second step is a higher-dimensional version of the GR CP. This procedure would allow the bulk to influence the hypersurface in a causal way (in the usual GR sense), which is not possible in a $(3,1)\rightarrow(4,1)$ type of embedding (except perhaps in a perturbative treatment). It is clearly of interest to construct models in which the bulk does play a role that is, in principle, observable and testable. Although the nature of causality in higher-dimensional theories may be substantially different to that of $(3+1)$-D GR,[41] such models would be consistent with a direct extension of GR.

V. CONCLUSION

In this paper, we have proved an extension of the CM embedding theorem,[8,9] where the embedding metric is sourced by one or more scalar fields minimally coupled to GR. We employed this theorem to establish classes of embeddings where the scalar field self-interacts through an exponential potential. The relationship between the CM theorem and the Cauchy and initial value problems of GR was highlighted. This relationship will certainly permit CP and IVP techniques to be adapted to provide further space–time into space–time embeddings.

Embedding theorems are important from both the mathematical and physical points of view. They allow classification schemes for different space–times to be developed as well as providing algorithms for generating new solutions.[42] The primary physical motivation for developing mathematical embedding theorems arises from the resurgence of interest in higher-dimensional theories of gravity and cosmology, most notably the braneworld scenarios.[3–6] In particular, the Randall–Sundrum ''type II'' (RSII) scenario,[6] where a codimension one brane is embedded in five-dimensional anti-de Sitter (AdS_5) space, has attracted considerable attention. Embeddings are also of relevance to the induced ''space–time–matter'' (STM) theory, whereby the 4D universe is viewed as a slice of a 5D universe.[43,44,19] (For reviews, see, e.g., Refs. 14 and 45.) The CM theory was recently employed within the context of both the RSII scenario and STM theory, where the close similarities between the two approaches were highlighted and algorithms for employing the theorem in practice were outlined.[19] The relationship between the two pictures has also been emphasized in Ref. 44.

Although the RSII model was motivated in part by the Horăva–Witten theory for the strongly coupled limit of the $E_8\times E_8$ heterotic string theory,[4] it is an idealized system, in the sense that the higher-dimensional space is assumed to be an Einstein space. It is therefore important to consider

more general settings that are inspired by string theoretic considerations. For example, the supergravity actions contain, in addition to the scalar dilaton field, a number of antisymmetric form-fields. Up on compactification from ten or eleven dimensions, the degrees of freedom associated with these fields can manifest themselves as scalar fields that self-interact through one or more potentials. In particular, scalar fields arise when the form fields have a nontrivial flux over the compactifying dimensions that is able to support a solitonic brane configuration. A specific example is the compactification of the Horăva–Witten theory to five dimensions,[5] where a scalar field arises in the fifth (bulk) dimension with an exponential potential of the form considered in Sec. III B.

In view of the above discussion, it is important to develop the mathematical framework through embedding theorems for studying braneworld models containing scalar fields in the higher dimensions. Unlike almost all current analyses, our treatment in the present work is for the *full* Einstein-scalar field system rather than for some highly symmetric case. This general treatment is appropriate because we are establishing an existence and uniqueness theorem for embeddings into space–times sourced by scalar fields. (This is also the starting point of the perturbative 4D treatment of domain walls presented in Ref. 46.)

It is worth emphasizing that by including scalar fields in our extension of the CM theory, we mean additional, bulk scalar fields, $\overline{\chi}$, and not the higher-dimensional metric component, $\overline{\phi}$, which is an effective scalar field in the Kaluza–Klein and STM approaches. The theorem we have proved therefore provides a starting point for considering a number of open physical questions, such as the possible restrictions that may arise on the energy–momentum tensor of the brane matter fields once the junction conditions are imposed. A related question is whether plausible 4D physics can generically be recovered and whether there are testable corrections to Newton gravity such as those in the RSII scenario.[6] It would be interesting to consider these questions further.

Finally, our generalization in this paper of the CM theorem implies that for a given 4D space–time, there are an infinite number of embedding space–times with one extra dimension, in the sense that there is at least one possible embedding for each functional form of the higher-dimensional energy–momentum tensor, in particular, one per scalar interaction potential of the surrounding 5D space–time. (In the embedding procedure, the energy–momentum tensor is viewed as a function of the coordinates and not as a function of the fields. This implies that the higher-dimensional models are merely encoding solutions rather than specific physical laws. Compare with how Kaluza–Klein theory offered further predictions as a result of the geometrization of the electromagnetic field.) This is arguably an undersirable feature for higher-dimensional theories, since it implies that unique physical predictions cannot be made in the absence of well-founded principles that *select* a particular higher-dimensional space–time. This is similar to the well-known problem in string theory phenomenology, where different particle spectra arise for different Calabi–Yau compactifications.[47] The introduction of discontinuities or branes is unlikely to remove this nonuniqueness property, since there are many possible brane configurations (single, parallel, or intersecting) that could be considered and many possible forms for the higher dimensional bulk space–time, but presently no established way to distinguish between them from a physical point of view. Perhaps, the number of fields and the form of the potential would be restricted in some higher-dimensional theory and by requiring the recovery of (possibly corrected) 4D physics as discussed earlier. Our theorem provides a framework within which these and related questions can be addressed.

ACKNOWLEDGMENTS

E.A. is supported by PPARC. F.D. and C.R. are supported by CNPq. J.E.L. is supported by the Royal Society. We thank M. A. H. MacCallum, N. Ó. Murchadha, and R. Tavakol for helpful discussions and communications.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Parametric phenomena of the particle dynamics in a periodic gravitational wave field

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(Received 9 December 2002; accepted 18 August 2003)

We establish exactly solvable models for the motion of neutral particles, electrically charged point and spin particles [U(1) symmetry], isospin particles [SU(2) symmetry], and particles with color charges [SU(3) symmetry] in a gravitational wave background. Special attention is devoted to parametric effects induced by the gravitational field. In particular, we discuss parametric instabilities of the particle motion and parametric oscillations of the vectors of spin, isospin, and color charge. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1617364]

I. INTRODUCTION

Periodic external fields are known to induce parametric phenomena in physical systems. This includes such effects as parametric oscillations (the oscillation frequency becomes a periodic function of time) and parametric instabilities (exponential growth of certain dynamical quantities).[1–3] Classical examples are the parametric resonance in vibrations of mechanical and electrical systems[1–3] and plasma instabilities in external electromagnetic fields.[4,5] From a mathematical point of view, such phenomena are described by differential equations with periodic coefficients which are subject to Floquet's theory.[2,3,6–9] As we shall demonstrate here, equations of this type naturally appear if one considers the motion of different kinds of particles in a gravitational wave (GW) background. The gravitational wave may play the role of an external periodic pumping field. In fact, most of the attempts for a direct detection of gravitational waves rely on this concept. The mathematical similarity to dynamical equations which are known to describe parametric oscillations and resonances then naturally suggests the possibility of gravitationally induced parametric effects.

The idea of parametric phenomena in GW fields is not new. For a linearized GW field it was discussed in Ref. 10. The first exactly solvable model for the evolution of a kinetic system in a *nonlinear* GW field, demonstrating explicitly the possibility of parametric excitation of a relativistic plasma by a periodic GW, has been established in Ref. 11. At the same time, in the nineties, the problem of parametric resonance during the reheating phase of inflationary models has become an intensely elaborated topic in a cosmological context (see, e.g., Refs. 12–16). More recently, investigations, concerning parametric phenomena in a GW field, have attracted attention again (see, e.g., Refs. 17–19).

The purpose of the present paper is to clarify characteristic features of gravitationally induced parametric effects for simple dynamical configurations. As a first example we consider the motion of an electrically charged point particle which is simultaneously exposed to a constant magnetic field and a gravitational wave with front plane orthogonal to the magnetic field. In the second example we include an additional spin degree of freedom which is described by the Bargmann–

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Michel–Telegdi (BMT) equations.[20] In the third case the electrically charged spin-particle is replaced by a particle with isospin and the magnetic field is replaced by a corresponding Yang–Mills field. The isospin dynamics is governed by Wong's equation[21] for the three-dimensional isospin vector. Finally, we consider the motion of particles with color charge, described by Wong's equation for the eight color degrees of freedom. Using suitably specified Yang–Mills fields, we establish a general scheme which allows a unified treatment of the particle dynamics for all four cases. We show that on a periodic GW background this dynamics is characterized by Hill and Mathieu equations. Well-known stability properties of the latter allow us to classify the particle motion accordingly. This implies parametric oscillations and/or parametric instabilities as generic phenomena. The precession dynamics of the vectors of spin, isospin, and color charge is coupled to the particle motion and parametrically driven as well.

The paper is organized as follows. In Sec. II we establish the basic dynamic equations for the Abelian and non-Abelian subcases to be discussed in the following. In Sec. III the Yang–Mills fields for the latter cases are specified. The (exact) gravitational background is characterized in Sec. IV. Section V is devoted to a compact, general solution for the particle dynamics. A ''sandwich'' GW is considered as a special case. The spin precession for an electrically charged particle is the subject of Sec. VI. Sections VII and VIII discuss the dynamics in the spaces of isospin and color charge, respectively. In Sec. IX we summarize our main results. We use units in which $\hbar = c = 1$.

II. PARTICLE DYNAMICS: BASIC EQUATIONS

Let us consider the evolution of relativistic point particles with either an electric charge and a spin-vector, or an isospin, or a color charge. The concepts of classical particles with isospin [for the SU(2) symmetry] or color charge [for the SU(3) symmetry] are generalizations of the electrically charged particles to the non-Abelian case (see, e.g., Ref. 22). The dynamical equations for the particle momentum p^i, for the spin-vector S^i, and for the charge $Q^{(A)}$, where (A) is a group index, are

$$\frac{Dp^i}{D\tau} = \mathcal{F}^i, \quad \frac{DS^i}{D\tau} = \mathcal{G}^i, \quad \frac{DQ^{(A)}}{D\tau} = \mathcal{G}^{(A)}\ , \tag{1}$$

respectively. Here, D denotes the covariant differential, τ is a parameter along the particle world-line, and $\mathcal{F}^i$ is the force four vector which is orthogonal to the particle momentum $p^i = m\mathrm{d}x^i/\mathrm{d}\tau$, i.e., $p_i\mathcal{F}^i = 0$. The quantity $\mathcal{G}^i$ describes the spin rotation within the BMT theory. The quantity $\mathcal{G}^{(A)}$ is a vector in the group space which determines the non-Abelian charge evolution and plays a similar role for the charge as $\mathcal{F}^i$ plays for the momentum. The limiting case of neutral particles is characterized by $\mathcal{F}^i = \mathcal{G}^i = \mathcal{G}^{(A)} = 0$.

A. Electrically charged point particles

In this case the relevant force is the Lorentz force

$$\mathcal{F}^i = \frac{e}{m} F^i{}_{\cdot k}\, p^k \tag{2}$$

with

$$F_{ik} = \nabla_i A_k - \nabla_k A_i\,, \quad \nabla_k F^{ik} = 0, \tag{3}$$

where F_{ik} is the Maxwell tensor. The particle under consideration is regarded here as a test particle. Moreover, the charge is constant which renders the third equation in (1) irrelevant.

B. Electrically charged spin particles

According to Ref. 20 the evolution of classical relativistic spin particles is governed by

$$\frac{Dp^i}{D\tau}=\frac{e}{m}F^i_{\cdot k}\ p^k \tag{4}$$

and

$$\frac{DS^i}{D\tau}=\frac{e}{2m}\left[gF^i_{\cdot k}S^k+\frac{(g-2)}{m^2}p^iF_{kl}S^kp^l\right]. \tag{5}$$

Here, S^i is the spin four-vector and g is the gyromagnetic ratio. Equation (5) describes the precession of the magnetic moment. It generalizes earlier nonrelativistic equations by Thomas[23] and Bloch,[24] which rely on the circumstance that the ''expectation value of the vector operator representing the 'spin' will necessarily follow the same time dependence as one would obtain from a classical equation of motion'' (cf. Ref. 20). While the particle momentum according to Eq. (4) is independent of the spin vector, the dynamics of the latter is coupled (at least via the covariant derivative) to the particle motion.

C. Isospin particles

Here we have a triplet $I^{(A)}$ of scalar fields representing a vector in the three-dimensional isospin space, i.e., $(A)=(1),(2),(3)$. This space has an Euclidean metric $G_{(A)(B)}$. The relevant force

$$\mathcal{F}^i=\frac{g}{m}F^{(A)i}_{\cdot\ k}\ p^kI^{(B)}G_{(A)(B)}, \tag{6}$$

where g is the interaction constant, has been obtained by Kerner[25] and Wong.[21] The isospin dynamics is determined by Wong's equation[21]

$$\frac{D}{D\tau}I^{(A)}=-\frac{g}{m}\varepsilon^{(A)}_{\cdot(B)(C)}A^{(B)}_ip^iI^{(C)}, \tag{7}$$

where we have used that the structure constants for the SU(2) group coincide with the three-dimensional Levi–Civita symbol $\varepsilon^{(A)}_{\cdot(B)(C)}$. The quantities $A^{(A)}_i$ are the vector potentials in terms of which the Yang–Mills field strength tensor $F^{(B)}_{jk}$ is given by

$$F^{(B)}_{jk}=\nabla_jA^{(B)}_k-\nabla_kA^{(B)}_j+g\varepsilon^{(B)}_{\cdot(K)(L)}A^{(K)}_jA^{(L)}_k. \tag{8}$$

The Yang–Mills field equations are

$$g^{ij}[\nabla_iF^{(A)}_{jk}+g\varepsilon^{(A)}_{\cdot(B)(C)}A^{(B)}_iF^{(C)}_{jk}]=0. \tag{9}$$

Again we consider the particle motion in a given external field. Wong's equation represents a non-Abelian generalization of the equation of motion for electrically charged point particles. It can be obtained as the classical limit from quantum field theory for the case of sufficiently localized quantum states of the matter fields with characteristic length scales much smaller than those associated with the Yang–Mills fields.[26,22]

D. Particles with color charge

For test particles with color charge the force $\mathcal{F}^i$ is given by

$$\mathcal{F}^i=\frac{g}{m}F^{(A)i}_{\cdot k}\ p^k Q^{(B)}G_{(A)(B)}, \tag{10}$$

with the field strength tensor

$$F^{(B)}_{jk}=\nabla_j A^{(B)}_k-\nabla_k A^{(B)}_j+g f^{(B)}_{\cdot\,(K)(L)}A^{(K)}_j A^{(L)}_k, \tag{11}$$

where the $f^{(B)}_{\cdot\,(K)(L)}$ are the structure constants of the SU(3)group. The field equations are

$$g^{ij}[\nabla_i F^{(A)}_{jk}+g f^{(A)}_{\cdot\,(B)(C)}A^{(B)}_i F^{(C)}_{jk}]=0. \tag{12}$$

The quantity $Q^{(A)}$ is the color charge with $(A)=(1)-(8)$. Wong's equation in this case reads

$$\frac{D}{D\tau}Q^{(A)}=-\frac{g}{m}f^{(A)}_{\cdot\,(B)(C)}A^{(B)}_i p^i\ Q^{(C)}. \tag{13}$$

The structure constants $f^{(A)}_{\cdot\,(B)(C)}$ are characterized by the commutator relations

$$[\lambda_{(A)},\lambda_{(B)}]=2i f_{(A)(B)(C)}\lambda^{(C)}, \tag{14}$$

where $\lambda_{(A)}$ are the traceless, Hermitian Gell–Mann matrices (see, e.g., Refs. 27 and 28). In detail we have

$$\begin{gathered} f_{(1)(2)(3)}=1,\quad f_{(4)(5)(8)}=f_{(6)(7)(8)}=\frac{\sqrt{3}}{2},\\ f_{(1)(4)(7)}=f_{(2)(4)(6)}=f_{(2)(5)(7)}=f_{(3)(4)(5)}=-f_{(3)(6)(7)}=-f_{(1)(5)(6)}=\tfrac{1}{2}. \end{gathered} \tag{15}$$

In the following we shall also use the completely symmetric coefficients $d_{(A)(B)(C)}$ of the basic representation which are given by the anti-commutation relations

$$\{\lambda_{(A)},\lambda_{(B)}\}=\tfrac{4}{3}\delta_{(A)(B)}+2d_{(A)(B)(C)}\lambda^{(C)}, \tag{16}$$

where[29,22]

$$\begin{aligned} d_{(1)(4)(6)}&=d_{(1)(5)(7)}=d_{(2)(5)(6)}=d_{(3)(4)(4)}=d_{(3)(5)(5)}=-d_{(2)(4)(7)}=-d_{(3)(6)(6)}\\ &\quad=-d_{(3)(7)(7)}=\tfrac{1}{2},\\ d_{(1)(1)(8)}&=d_{(2)(2)(8)}=d_{(3)(3)(8)}=-d_{(8)(8)(8)}=-2d_{(4)(4)(8)}=-2d_{(5)(5)(8)}\\ &\quad=-2d_{(6)(6)(8)}=-2d_{(7)(7)(8)}=\frac{1}{\sqrt{3}}. \end{aligned} \tag{17}$$

III. YANG–MILLS FIELDS WITH "PARALLEL" POTENTIALS

It is known that for each solution of the general relativistic source free Maxwell equations one can construct a set of solutions of the general relativistic Yang–Mills equations.[30] Following Gal'tsov[31] we will refer to the corresponding Yang–Mills potentials as ''parallel'' potentials. The latter are characterized by

$$A^{(B)}_i=q^{(B)}A_i,\quad F^{(A)}_{ik}=q^{(A)}F_{ik},\quad q^{(B)}q_{(B)}=1,\quad q^{(B)}=\text{const.} \tag{18}$$

Due to the antisymmetry of the structure coefficients the relations (8) and (11) as well as Eqs. (9) and (12) reduce to the linear Maxwell-type forms (3). Nevertheless, compared with Maxwell's theory there exists an additional degree of freedom, namely, the direction of the vector $q^{(A)}$ in the group space.[30] Additionally, the structure coefficients $f^{(B)}_{\cdot\,(K)(L)}$ are different from zero which will result in a qualitatively different dynamics.

A. Isospin particles

In this case the ansatz (18) transforms the first of equations (1) with (6) into

$$\frac{Dp^i}{D\tau}=\frac{gI^{(A)}q_{(A)}}{m}F^i_{\cdot\,k}p^k, \tag{19}$$

which has the structure of the equations of motion of a particle with charge $e\equiv gI^{(A)}q_{(A)}$ under the influence of the Lorentz force (2). Analogously, one can rewrite Eq. (7) for the isospin evolution,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}I^{(A)}=-\Omega\varepsilon^{(A)}_{\cdot\,(B)(C)}q^{(B)}I^{(C)},\quad \Omega\equiv\frac{g}{m}A_ip^i. \tag{20}$$

Because of the antisymmetry of the Levi–Civita symbols, Eq. (20) admits a quadratic integral of motion $I^{(A)}I_{(A)}=\text{const}$, which is a Casimir invariant,[22] normalizable to $I^{(A)}I_{(A)}=1$. In addition, we obtain from (20)

$$q_{(A)}\frac{\mathrm{d}I^{(A)}}{\mathrm{d}\tau}\equiv 0\ ,\ \rightarrow\ \ I^{(A)}q_{(A)}\equiv I=\text{const}. \tag{21}$$

Using the standard definition

$$[\vec{I},\vec{\Omega}]^{(A)}\equiv\varepsilon^{(A)}_{\cdot\,(B)(C)}I^{(B)}\Omega^{(C)},\quad \Omega^{(C)}\equiv\Omega q^{(C)}, \tag{22}$$

of the vector product, Eq. (20) may be written as an equation for the precession of $\vec{I}$,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\vec{I}=[\vec{I},\vec{\Omega}]. \tag{23}$$

The "longitudinal" component $I^{(A)}q_{(A)}$, the projection of the dynamical variable $I^{(A)}$ on the "rotation axis" $q^{(A)}$, remains constant according to (21).

B. Colored particles

Similar to the previous isospin case the color charge evolution equation (13) admits the existence of a quadratic integral of motion $Q^{(A)}Q_{(A)}=\text{const}$ which is the first Casimir invariant.[22] The condition (18) of parallelism in the color space provides a second integral of motion $Q^{(A)}q_{(A)}=\text{const}$, as well. However, the corresponding eight-dimensional evolution equations,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}Q^{(A)}=-\Omega H^{(A)}_{\cdot\,(C)}Q^{(C)},\quad \Omega\equiv\frac{g}{m}A_ip^i\ ,\quad H^{(A)}_{\cdot\,(C)}\equiv f^{(A)}_{\cdot\,(B)(C)}q^{(B)}\ , \tag{24}$$

are more complicated than Eq. (23) for the isospin precession. Different from the SU(2) model there exists a second Casimir invariant

$$\mathcal{Q}=d_{(A)(B)(C)}Q^{(A)}Q^{(B)}Q^{(C)}\,, \tag{25}$$

where $d_{(A)(B)(C)}$ are the totally symmetric group coefficients (17) of the given basic representation of the SU(3) group. In detail it reads

$$\mathcal{Q}=-\frac{1}{\sqrt{3}}(Q^{(8)})^3+\sqrt{3}Q^{(8)}[(Q^{(1)})^2+(Q^{(2)})^2+(Q^{(3)})^2]-\frac{\sqrt{3}}{2}Q^{(8)}[(Q^{(4)})^2+(Q^{(5)})^2+(Q^{(6)})^2$$
$$+(Q^{(7)})^2]+3Q^{(1)}[Q^{(4)}Q^{(6)}+Q^{(5)}Q^{(7)}]+3Q^{(2)}[-Q^{(4)}Q^{(7)}+Q^{(5)}Q^{(6)}]+\tfrac{3}{2}Q^{(3)}[(Q^{(4)})^2$$
$$+(Q^{(5)})^2-(Q^{(6)})^2-(Q^{(7)})^2]. \tag{26}$$

IV. GRAVITATIONAL WAVE BACKGROUND

Our aim in this paper is to study the general dynamics outlined so far in the field of a plane-fronted GW with parallel rays (PP wave). We assume the latter to be an exact solution of Einstein's vacuum field equations with a five-parametric group of isometries G_5, including a covariantly constant null Killing vector (KV).[32] Gravitational waves are usually described either in Fermi coordinates or in the transverse-traceless (TT) gauge. For the merits of each of these choices and for issues of gauge-invariance in the linearized theory see, e.g., Ref. 33. In order to establish a comprehensive picture we start by sketching our basic setting for both cases. For computational ease most of the analysis will then be done in TT coordinates.

A. PP wave in Fermi coordinates

The corresponding line element

$$\mathrm{d}s^2=2\mathrm{d}\bar{u}\,\mathrm{d}\bar{v}-\mathrm{d}y^2-\mathrm{d}z^2-2\mathcal{H}(\bar{u},y,z)\mathrm{d}\bar{u}^2,\quad \bar{u}=\frac{t-x}{\sqrt{2}},\quad \bar{v}=\frac{t+x}{\sqrt{2}}, \tag{27}$$

contains a harmonic function $\mathcal{H}$, obeying

$$\frac{\partial^2\mathcal{H}}{\partial y^2}+\frac{\partial^2\mathcal{H}}{\partial z^2}=0, \tag{28}$$

which is quadratic in y and z for a G_5 symmetry group. Explicitly, we have[32]

$$2\mathcal{H}(\bar{u},y,z)=A(\bar{u})(y^2-z^2)+2B(\bar{u})yz, \tag{29}$$

where $A(\bar{u})$ and $B(\bar{u})$ are arbitrary functions of the retarded time $\bar{u}$. We may define a periodic GW by assuming the variables A and B to be periodic functions of $\bar{u}$. All nonvanishing components of the Riemann tensor, $R_{z\bar{u}z\bar{u}}=-R_{y\bar{u}y\bar{u}}=A(\bar{u})$ and $R_{y\bar{u}z\bar{u}}=-B(\bar{u})$, are periodic for this case. The GW metric in Fermi coordinates is nonsingular for arbitrary retarded times because $\det(g_{ik})\equiv-1\neq0$. However, the weak field approximation $\max|g_{ik}|\ll1$ is correct only close to $y=0$, $z=0$.

B. PP wave in TT gauge

The line element in TT gauge has the form

$$\mathrm{d}s^2=2\mathrm{d}u\,\mathrm{d}v-L^2[\cosh 2\gamma(e^{2\beta}(\mathrm{d}x^2)^2+e^{-2\beta}(\mathrm{d}x^3)^2)+2\sinh 2\gamma\mathrm{d}x^2\,dx^3], \tag{30}$$

where $u=(t-x^1)/\sqrt{2}$ and $v=(t+x^1)/\sqrt{2}$ are the retarded and the advanced times, respectively. For this metric the three KVs which form an Abelian subgroup of G_5 are

$$\xi^i_{(v)}=\delta^i_v,\quad \xi^i_{(2)}=\delta^i_2,\quad \xi^i_{(3)}=\delta^i_3. \tag{31}$$

The KV $\xi^i_{(v)}$ is a covariantly constant null vector, orthogonal to $\xi^i_{(2)}$ and $\xi^i_{(3)}$. The functions $\beta(u)$ and $\gamma(u)$ are arbitrary. We shall focus here on the case of periodic functions $\beta(u)$ and $\gamma(u)$. This definition of periodicity does not, in general, coincide with the definition in Fermi coordinates

given above. However, both concepts of a periodic GW have the same weak-field limit, which in the TT gauge is characterized by $L=1$, $|\beta(u)|\ll 1$ and $|\gamma(u)|\ll 1$. Generally, the function $L(u)$ satisfies the Einstein equation:[33]

$$\ddot{L}+L((\dot{\beta})^2\cosh^2 2\gamma+(\dot{\gamma})^2)=0, \tag{32}$$

where a dot denotes the derivative with respect to the retarded time u. We assume the hypersurface $u=0$ to be the leading front of the GW with

$$\beta(0)=\gamma(0)=0, \quad L(0)=1, \quad \dot{\beta}(0)=\dot{\gamma}(0)=\dot{L}(0)=0. \tag{33}$$

For the special case $\gamma(u)\equiv 0$ [equivalent to $B(\overline{u})\equiv 0$], corresponding to only one polarization direction, the transformation relations between Fermi and TT coordinates are

$$\begin{gathered}\overline{u}=u, \quad \overline{v}=v+\tfrac{1}{4}[(x^2)^2(L^2e^{2\beta})^{\cdot}+(x^3)^2(L^2e^{-2\beta})^{\cdot}], \\ y=Le^{\beta}\cdot x^2, \quad z=Le^{-\beta}\cdot x^3, \quad A(u)=\ddot{\beta}+2\dot{\beta}\frac{\dot{L}}{L}.\end{gathered} \tag{34}$$

The last formula clarifies the relation between the different periodicity definitions given above. For the physically relevant situation where the background factor L changes only slowly compared with the change of the wave factor β (cf. Ref. 33) the last term in the formula for $A(u)$ in Eq. (34) can be neglected. Then we have $A(u)=\ddot{\beta}$ and both periodicity definitions coincide.

V. PARTICLE DYNAMICS: SOLUTIONS

We are interested here in the particle dynamics in given external gravitational and Yang–Mills fields. The restriction (18) to Yang–Mills fields with ''parallel potentials'' simplifies the Kerner–Wong equations since the quantities $I^{(A)}q_{(A)}$ and $Q^{(A)}q_{(A)}$ remain constant. We introduce the cumulative symbol σ for either e, or $gI^{(A)}q_{(A)}$, or $gQ^{(A)}q_{(A)}$, which allows us to write the equation of motion with either (2), or (6), or (10) in the unified form

$$\frac{Dp^i}{D\tau}=\frac{\sigma}{m}F^i{}_{\cdot k}p^k, \quad \frac{\mathrm{d}x^i}{\mathrm{d}\tau}=\frac{p^i}{m}. \tag{35}$$

The orthogonality of the force to the particle momentum corresponds to the quadratic integral

$$g^{ik}p_ip_k=m^2. \tag{36}$$

One may solve this relation for one of the components of the momentum. In Fermi coordinates we have

$$p_{\overline{u}}=\frac{1}{2p_{\overline{v}}}[m^2+p_y^2+p_z^2-2\mathcal{H}(\overline{u},y,z)p_{\overline{v}}^2]. \tag{37}$$

The analogous formula in TT coordinates is

$$p_u=\frac{1}{2p_v}[m^2-g^{\alpha\beta}(u)p_{\alpha}p_{\beta}], \tag{38}$$

where greek indices run from 2 to 3. Both in Fermi and in TT coordinates the covariantly constant null KV has the form $\xi^i_{(\overline{v})}=\delta^i_{\overline{v}}$ and $\xi^i_{(v)}=\delta^i_v$, respectively. In the following we shall restrict ourselves to fields which satisfy

$$\xi^i_{(\bar{v})}F_{ik}=\xi^i_{(v)}F_{ik}=0. \tag{39}$$

This implies that the quantities $\xi^i_{(\bar{v})}p_i$ and $\xi^i_{(v)}p_i$ are integrals of motion (see e.g., Ref. 33),

$$\xi^i_{(\bar{v})}p_i=\xi^i_{(v)}p_i=p_v=C_v=\text{const.} \tag{40}$$

Using the general relationship

$$m\frac{du}{d\tau}=p^u=p^{\bar{u}}=p_v=C_v, \tag{41}$$

one can reparametrize the remaining equations for $C_v\neq 0$, by means of the linear formula (notice that $\bar{u}=u$ [cf. Eq. (34)] holds also in the general case)

$$\tau=\tau_0+\frac{m}{C_v}u. \tag{42}$$

We start our solution procedure by first recalling the reference case of neutral particles.

A. Neutral particles

For a vanishing generalized charge σ the equations of motion in TT coordinates are immediately integrated. The result is

$$p_v(u)=C_v,\quad p_2(u)=C_2,\quad p_3(u)=C_3,\quad p_u=\frac{1}{2C_v}[m^2-g^{\alpha\beta}(u)\;\; C_\alpha C_\beta], \tag{43}$$

where C_2 and C_3 are constants. A particle moving in direction of the GW propagation before the infall of the latter, i.e., $p_2=p_3=0$, will not change its direction. If we additionally have $C_v=mc/\sqrt{2}$, the particle is at rest both before and after the GW infall, since $p_1(u)=p_2(u)=p_3(u)=0$ and $p_0=mc$. An observer at rest, characterized by a four-velocity $V^i=(1/\sqrt{2})(\delta^i_u+\delta^i_v)\equiv\delta^i_0$, would measure the (invariant) particle energy $\mathcal{E}\equiv p^kV_k=(1/\sqrt{2})(p_u+p_v)$. For neutral particles p_v and p_u are given in Eq. (43). Corresponding expressions for charged particles will be obtained in the following.

In Fermi coordinates the situation is as follows. The system (35) reduces to the set of equations

$$\begin{gathered}\dot{y}=-C_v^{-1}p_y,\quad \dot{z}=-C_v^{-1}p_z,\\ C_v^{-1}\dot{p}_y=-A(u)y-B(u)z,\quad C_v^{-1}\dot{p}_z=A(u)z-B(u)y,\end{gathered} \tag{44}$$

for y, z, p_y, and p_z. If the latter set of quantities is known, the component p_u follows via (37). The quantity $\bar{v}(u)$ may be found by solving

$$\dot{\bar{v}}=C_v^{-1}p_u+2\mathcal{H}(u,y,z). \tag{45}$$

The set (44) is a linear, homogeneous first-order system of differential equations. For a GW field with polarization $B(u)\equiv 0$ and with A depending on the retarded time via the dimensionless variable ku, it can be written as

$$y''-\mathcal{A}(ku)y=0,\quad z''+\mathcal{A}(ku)z=0\ . \tag{46}$$

Differentiation with respect to ku is denoted by a prime and $\mathcal{A}(ku)\equiv A(u)/k^2$. For $A(u)\equiv 0$, i.e., in the absence of a gravitational field, $y(u)$ and $z(u)$ are linear functions of the retarded time (and of the affine parameter τ), and the particle has constant momentum. For a periodic function $A(u)$,

Eq. (46) is of the type of Hill's equation.[2,7,8] The solutions are Hill functions. For a dependence $\mathcal{A}(ku)=\delta+\varepsilon\cos(ku)$ where δ and ε are constants, Eq. (46) reduces to Mathieu equations which have solutions of the type[2,3,8]

$$y\propto\exp[\mu ku]\phi(ku)+\exp[-\mu ku]\psi(ku)\,, \tag{47}$$

where ϕ and ψ are periodic functions with the period of $\mathcal{A}(ku)$, i.e., in the present case, $\phi(ku+2\pi)=\phi(ku)$ and $\psi(ku+2\pi)=\psi(ku)$. The solutions consist of products of an exponential function and a periodic function of period 2π. The characteristic exponent μ is a complex constant. For $\mathrm{Re}(\mu)=0$ the solution is stable. In general, it is not periodic again but it is oscillating (Ref. 7, p. 115). For $\mathrm{Re}(\mu)\neq 0$ either the first or the second exponential function in (47) is unbounded and the solution is unstable. The stability properties of Mathieu's equations are well known in the literature and may be visualized by stability regions in an δ–ε diagram [see Ref. 2, Eq. (4.1) and Fig. 5.1]. Let us consider the stability region which is closest to the origin $\delta=\varepsilon=0$. For small positive values of δ and ε the boundary of this region is determined by the line $\delta=\frac{1}{4}-\frac{1}{2}\varepsilon$. Applied to the case $A(u)=A_0\cos(ku)$, i.e., $\delta=0$ and $\varepsilon=A_0/k^2$, this means stable solutions for $\varepsilon=A_0/k^2<1/2$. Since $A_0=\ddot{\beta}(0)=\beta_0 k^2$, we have also $\beta_0<1/2$. Under this condition neutral particles are parametrically oscillating in Fermi coordinates.

While equations of the type of Mathieu's equation and questions of stability will play an essential role in the following investigations of the dynamics of charged particles (see Sec. V B 2), it is obvious that the description for neutral particles is more involved in Fermi coordinates. Therefore, for computational ease and in order to separate charge effects from the neutral particle motion we shall perform the following analysis in TT coordinates.

B. Charged particles

To obtain exactly solvable models for the particle motion we resort to simple field configurations $F^{(A)}_{ik}$. For particles with electric charge we focus on the motion of the latter in a constant homogeneous magnetic field H_0 orthogonal to the GW front plane, which corresponds to a Maxwell tensor

$$F_{jk}=H_0(\delta^2_j\delta^3_k-\delta^3_j\delta^2_k). \tag{48}$$

A corresponding generalization for non-Abelian fields with parallel potentials according to (18) is

$$F^{(A)}_{jk}=q^{(A)}M(\delta^2_j\delta^3_k-\delta^3_j\delta^2_k),\quad M=\mathrm{const}. \tag{49}$$

Both (48) and (49) satisfy (39) with (31). This constitutes a model in which the gravitational wave and the fields (48) or (49) are given, external fields which are independent of each other. It may provide the basis of a perturbative treatment with respect to the GW amplitude within a linearized theory. It is worth mentioning that expressions (48) and (49) are also solutions of the Maxwell- and Yang–Mills equations, respectively, on the background of the exact GW (30) [or (27)]. This allows a study of the corresponding field dynamics on a GW background, which, however, is not the purpose of the present paper.

For the equations of motion in TT coordinates we obtain

$$\frac{\mathrm{d}p_2}{\mathrm{d}\tau}=\frac{M\sigma}{m}(g^{32}p_2+g^{33}p_3),\quad \frac{\mathrm{d}p_3}{\mathrm{d}\tau}=-\frac{M\sigma}{m}(g^{22}p_2+g^{23}p_3). \tag{50}$$

Equivalent second-order equations are

$$\frac{\mathrm{d}^2p_2}{\mathrm{d}u^2}+R_2(u)\frac{\mathrm{d}p_2}{\mathrm{d}u}+W_2(u)p_2=0,\quad p_3=\frac{1}{g^{33}}\left(\frac{1}{\Pi}\dot{p}_2-g^{23}p_2\right), \tag{51}$$

or

$$\frac{d^2p_3}{du^2}+R_3(u)\frac{dp_3}{du}+W_3(u)p_3=0,\quad p_2=\frac{1}{g^{22}}\left(-\frac{1}{\Pi}\dot{p}_3-g^{23}p_3\right), \tag{52}$$

where we have introduced the notations

$$\begin{aligned} R_2(u)&=-\frac{\dot{g}^{33}(u)}{g^{33}(u)}=2\left(\frac{\dot{L}}{L}-\dot{\beta}-\dot{\gamma}\tanh(2\gamma)\right),\\ R_3(u)&=-\frac{\dot{g}^{22}(u)}{g^{22}(u)}=2\left(\frac{\dot{L}}{L}+\dot{\beta}-\dot{\gamma}\tanh(2\gamma)\right), \end{aligned} \tag{53}$$

and

$$\begin{aligned} W_2(u)&=\frac{\Pi^2}{L^4}+\frac{2\Pi}{L^2}\left(\dot{\beta}\sinh(2\gamma)-\frac{\dot{\gamma}}{\cosh(2\gamma)}\right),\\ W_3(u)&=\frac{\Pi^2}{L^4}+\frac{2\Pi}{L^2}\left(\dot{\beta}\sinh(2\gamma)+\frac{\dot{\gamma}}{\cosh(2\gamma)}\right), \end{aligned} \tag{54}$$

with

$$\Pi=\frac{M\sigma}{C_v}=\text{const.} \tag{55}$$

The substitution $\beta\to-\beta$ converts R_3 into R_2 and vice versa, while W_3 is obtained from W_2 by $\beta\to-\beta$ and simultaneously $\Pi\to-\Pi$.

By the substitution

$$p_\alpha=Z_\alpha(u)\exp\left\{-\frac{1}{2}\int_0^u R_\alpha(\zeta)d\zeta\right\} \tag{56}$$

Eqs. (51) and (52) may be transformed into the Hill equations

$$\ddot{Z}_\alpha+F_\alpha(u)Z_\alpha=0, \tag{57}$$

where

$$F_\alpha=W_\alpha-\frac{R_\alpha^2}{4}-\frac{\dot{R}_\alpha}{2}. \tag{58}$$

The detailed form of relations (56) and (58) is

$$p_2=Z_2(u)\sqrt{\cosh(2\gamma)}\frac{e^{\beta}}{L},\quad p_3=Z_3(u)\sqrt{\cosh(2\gamma)}\frac{e^{-\beta}}{L},\quad p_\alpha(0)=Z_\alpha(0)\equiv C_\alpha, \tag{59}$$

and

$$\begin{aligned} F_2(u)=&\frac{\Pi^2}{L^4}+\frac{2\Pi}{L^2}\left(\dot{\beta}\sinh(2\gamma)-\frac{\dot{\gamma}}{\cosh(2\gamma)}\right)+\ddot{\beta}+\ddot{\gamma}\tanh(2\gamma)+\frac{3(\dot{\gamma})^2}{(\cosh(2\gamma))^2}\\ &+(\dot{\beta})^2(\sinh(2\gamma))^2+2\frac{\dot{L}}{L}\dot{\beta}+2\frac{\dot{L}}{L}\dot{\gamma}\tanh(2\gamma)-2\dot{\gamma}\dot{\beta}\tanh(2\gamma), \end{aligned} \tag{60}$$

$$F_3(u)=\frac{\Pi^2}{L^4}+\frac{2\Pi}{L^2}\left(\dot\beta\sinh(2\gamma)+\frac{\dot\gamma}{\cosh(2\gamma)}\right)-\ddot\beta+\ddot\gamma\tanh(2\gamma)+\frac{3(\dot\gamma)^2}{(\cosh(2\gamma))^2}$$
$$+(\dot\beta)^2(\sinh(2\gamma))^2-2\frac{\dot L}{L}\dot\beta+2\frac{\dot L}{L}\dot\gamma\tanh(2\gamma)+2\dot\gamma\dot\beta\tanh(2\gamma), \tag{61}$$

respectively. In a next step we have to solve Hill's equations (57).

1. General solution of Hill's equation

The structure of the solutions of the linear, second-order differential equations (57) is[2,3,7–9]

$$Z_2(u)=C_2H_2(u)-\Pi C_3H_3(u). \tag{62}$$

The functions $H_\alpha(u)$ satisfy the initial conditions

$$H_2(0)=1,\quad \dot H_2(0)=0,\quad H_3(0)=0,\quad \dot H_3(0)=1, \tag{63}$$

and represent the fundamental solutions of Hill's equation (57) with unitary Wronsky determinant. For $Z_3(u)$ we have

$$Z_3(u)=C_3H_3^*+C_2\Pi H_2^*, \tag{64}$$

where

$$H_2^*=-\frac{L^2}{\Pi^2\cosh 2\gamma}\left[\dot H_2+H_2\left(\dot\gamma\tanh 2\gamma+\dot\beta-\frac{\dot L}{L}-\frac{\Pi}{L^2}\sinh 2\gamma\right)\right], \tag{65}$$

$$H_3^*=\frac{L^2}{\cosh 2\gamma}\left[\dot H_3+H_3\left(\dot\gamma\tanh 2\gamma+\dot\beta-\frac{\dot L}{L}-\frac{\Pi}{L^2}\sinh 2\gamma\right)\right], \tag{66}$$

$$H_2^*(0)=\dot H_2(0)=0\,,\quad H_3^*(0)=\dot H_3(0)=1\,. \tag{67}$$

In the absence of gravitational radiation, i.e., for $\beta=\gamma\equiv 0$, $L\equiv 1$, the functions F_α in Eq. (58) reduce to

$$F_2(u)=F_3(u)=\text{const}=\Pi^2\,. \tag{68}$$

Equation (57) then describes harmonic oscillations with

$$H_2=H_3^*\equiv\cos\Pi u,\quad H_3=H_2^*\equiv\frac{1}{\Pi}\sin\Pi u. \tag{69}$$

Since with (42) and (55) we have $\Pi u\to\Omega_H\tau$ where $\Omega_H\equiv eH_0/mc$ is the Larmor frequency, we recover the corresponding particle rotation in flat space–time. Generally, the functions H_2, H_3, H_2^*, and H_3^* cannot be written in terms of elementary functions but are given as series representations. In the following section we shall be interested in expressions for F_2 and F_3 for which the Hill equations (57) specify to Mathieu equations. Then the functions H_α can be expanded in powers of the GW amplitude, where the zeroth order is given by (69).

The analysis so far may be summarized by writing the solution of the equations of motion (51) and (52) in the compact and elegant matrix form

$$\begin{pmatrix}p_2\\p_3\end{pmatrix}=\mathbf{H}(u)\cdot\begin{pmatrix}C_2\\C_3\end{pmatrix}, \tag{70}$$

where

$$\mathbf{H}(u)\equiv\frac{\sqrt{\cosh 2\gamma}}{L}\begin{pmatrix} e^{\beta} & 0 \\ 0 & e^{-\beta}\end{pmatrix}\cdot\begin{pmatrix} H_2(u) & -\Pi H_3(u) \\ \Pi H_2^*(u) & H_3^*(u)\end{pmatrix}. \tag{71}$$

The set of equations (70) and (71) represents the general solution for the momentum of the charged particle in the GW field (30) and the Yang–Mills field (49).

2. A simple model

Now we apply the general formalism to a ''sandwich'' GW (see, e.g., Ref. 33) with polarization $\gamma=0$. Let β be different from zero during a finite retarded time interval T, i.e., $\beta=0$ for $u\leqslant 0$ and $u\geqslant T$. Within the interval $0<u<T$ we assume β to be periodic according to

$$\beta(u)=\beta_0(1-\cos(ku)),\quad (0<u<T). \tag{72}$$

This implies $\beta(0)=\beta(2\pi/k)=0$ and $\dot{\beta}(0)=\dot{\beta}(2\pi/k)=0$. Furthermore, the time scale T is assumed to be small compared with the scale on which the background factor L changes.[33] Under these conditions we may neglect the $\dot{L}/L$ terms in (60) and (61) and use the latter expressions with $L=1$. For this situation the potentials F_2 and F_3 reduce to

$$\begin{aligned} F_2&=\Pi^2+\beta_0k^2\cos(ku)=\Pi^2-R^2_{\cdot u2u},\\ F_3&=\Pi^2-\beta_0k^2\cos(ku)=\Pi^2-R^3_{\cdot u3u}\end{aligned} \tag{73}$$

in the interval $0<u<T$. Replacing now the variable u by ku and denoting the derivative with respect to ku again by a prime, Eq. (57) with (73) specify to

$$\begin{aligned} Z_2''+\left(\frac{\Pi^2}{k^2}+\beta_0\cos(ku)\right)Z_2&=0,\\ Z_3''+\left(\frac{\Pi^2}{k^2}-\beta_0\cos(ku)\right)Z_3&=0.\end{aligned} \tag{74}$$

Both Z_2 and Z_3 obey Mathieu equations. In the absence of the GW, i.e., for $\beta\equiv 0$, we have $F_\alpha(ku)=\Pi^2/k^2=\text{const}$ [here we have used the redefinition $F_\alpha(ku)\equiv F_\alpha(u)/k^2$] and the equations of motion reduce to harmonic oscillator equations with solutions

$$Z_2=p_2=C_2\cos(\Pi u)-C_3\sin(\Pi u), \tag{75}$$

$$Z_3=p_3=C_3\cos(\Pi u)+C_2\sin(\Pi u). \tag{76}$$

Replacing here Π and u according to (55) and (42), we find a particle rotation in the x^20x^3 plane with the angular velocity $\Omega_M\equiv M\sigma/m$, which is, of course, the analogue of the Larmor frequency. Immediately after the wave front, i.e., at $u=0_{+0}$, we have

$$F_2(0)=\frac{\Pi^2}{k^2}+\beta_0,\quad F_3(0)=\frac{\Pi^2}{k^2}-\beta_0. \tag{77}$$

The jump β_0k^2 of the curvature tensor at the front makes the evolutions of the p_2 and p_3 components different. They begin to oscillate with different frequencies and the particle trajectory is no longer circular. Corresponding features hold for the second polarization $\beta\equiv 0$ and $\gamma\neq 0$, for which F_2 and F_3 differ in the term linear in Π [cf. Eqs. (60) and (61)].

The general solutions of Eq. (74) are of the type of "cosine elliptic" and "sine elliptic" functions (see Refs. 7 and 9). As already mentioned, the latter may be expanded in powers of β_0 with the zeroth-order terms (75) and (76).

Equation (74) is of the same type as Eq. (46). With the identifications $\delta \to \Pi^2/k^2$ and $\varepsilon \to \beta_0$, the stability discussion mentioned in Sec. V A may be applied here as well [see Ref. 2, Eq. (4.1) and Fig. 5.1]. Depending on the parameter combinations the solutions may be stable or unstable. Within the stable regions the functions Z_2 and Z_3 are parametrically oscillating which, according to (59), implies a corresponding behavior of the particle momenta. The regions of stable solutions are characterized by stability zones in a $(\Pi/k)^2 \times \beta_0$ plane which are connected together at the points $(\Pi/k)^2 = n^2/4$, $\beta_0 = 0$, where n is an integer.[2]

The analysis of the neutral particle motion in Sec. V A corresponds to the case $\Pi = n = 0$. For $\Pi \neq 0$ the relevant values for the transition points are $n = 1,2,\ldots$. For $n = 1$ we have $\Pi/k = 1/2$. These points on the axis $\beta_0 = 0$ (which corresponds to the absence of the GW) are the only transition points between stable regions which also belong to the stable region. All other boundary points of the stable regions are unstable points. Consequently, any deviation from $\beta_0 = 0$, i.e., even a GW with arbitrary weak amplitude β_0, induces an instability in these critical points. In particular, this is true for the point $\Pi/k = 1/2$ (see Ref. 2, Fig. 5.1). This demonstrates that parametric instabilities are a generic phenomenon for the motion of particles in all the cases considered here. While we have obtained this result in TT coordinates, the transformations (34) allow us to find the corresponding particle momenta in Fermi coordinates as well. The relevant transformations are

$$p_{\bar{v}} = p_v = C_v\,, \quad p_y = p_2(u)\frac{e^{-\beta}}{L} - C_v\left(\frac{\dot{L}}{L} + \dot{\beta}\right) y(u)\,,$$
$$p_z = p_3(u)\frac{e^{\beta}}{L} - C_v\left(\frac{\dot{L}}{L} - \dot{\beta}\right) z(u)\,, \tag{78}$$

where

$$y(u) = L e^{\beta}\left[y(0) - \int_0^u d\zeta\, p_2(\zeta) L^{-2}(\zeta) e^{-2\beta(\zeta)}\right],$$
$$z(u) = L e^{-\beta}\left[z(0) - \int_0^u d\zeta\, p_3(\zeta) L^{-2}(\zeta) e^{2\beta(\zeta)}\right]. \tag{79}$$

It is interesting to realize that there are astrophysical situations for which the existence of such kind of instabilities might be relevant. This can be seen with the help of the following order-of-magnitude estimates. Equation (55) may be written as $\Pi = \Omega_M m/C_v$ with $\Omega_M = M\sigma/m$. For the electromagnetic case one has $\sigma = e$ and $M = H_0$. The interstellar magnetic field is of the order $3-6\times 10^{-6}$ Oe.[34] The integral of motion C_v is equal to $C_v = (\sqrt{m^2 + \vec{p}^2(0)} - p^1(0))/\sqrt{2}$. For nonrelativistic particles $C_v \propto m/\sqrt{2}$ and $\Pi \propto \omega_H \sqrt{2}$. (The coefficient $\sqrt{2}$ disappears if we use the natural parameter τ instead of retarded time u). Using the estimate[34] $\omega_H \propto 10^7 \cdot H_0(\mathrm{Hz})$ we find $\omega_H \approx 10^1 - 10^2$ Hz. This is well within the typical range $1-10^3$ Hz for the frequency k of a GW, generated by rapidly rotating neutron stars (pulsars). Thus, for nonrelativistic particles Π may be of the same order as the GW frequency k. The situation is different for ultrarelativistic particles. Since for particles that move in propagation direction of the GW ($p^1(0) > 0$), we have $C_v \to 0$ for $m \to 0$. Consequently, the quantity Π becomes very large [cf. Eq. (55)], such that $\Pi \gg k$. However, if the particles move in the opposite direction, i.e., $p^1(0) < 0$, any value of C_v is possible. In particular, Π is not excluded to be in the range of about 10^{-3} Hz which is typical for infra-low-frequency GW from relativistic compact binaries.

Since an ensemble of particles will generally not be characterized by a single value of C_v but by a distribution, the quantity C_v may play the role of a tuning parameter in the following sense.

Let us associate a mean value $\langle C_v \rangle$ for the system as a whole and let the system be outside the resonance $\omega_H/k=n/2$ for this $\langle C_v \rangle$, but not very far from it. Since $\Pi=\omega_H m/C_v$, we will very likely find a particular particle with a specific C_v such that for this particle $\Pi/k=n/2$ exactly. Consequently, certain particles of the ensemble might be resonant under these conditions.

VI. EVOLUTION OF THE SPIN FOUR-VECTOR

In this section we focus on the solution of Eq. (5) in external gravitational and magnetic fields. Equations (4) and (5) admit two integrals of motion, namely $p_i S^i=0$ and $S_i S^i=-E_0^2=\text{const}$.[20] In the present context this amounts to

$$p_v S_u+p_u S_v+p_\alpha S^\alpha=0, \quad 2S_u S_v+S_\alpha S^\alpha=-E_0^2, \tag{80}$$

which may be used to eliminate the components S_v and S_u according to

$$S_u=\frac{1}{2p_v}[-p_\alpha S^\alpha \mp \sqrt{(p_\alpha S^\alpha)^2+(m^2-p_\alpha p^\alpha)(E_0^2+S_\alpha S^\alpha)}], \tag{81}$$

and

$$S_v=\frac{1}{2p_u}[-p_\alpha S^\alpha \pm \sqrt{(p_\alpha S^\alpha)^2+(m^2-p_\alpha p^\alpha)(E_0^2+S_\alpha S^\alpha)}], \tag{82}$$

respectively. After the reparametrization (42) the remaining equations are

$$\frac{dS_\alpha}{du}=\frac{1}{2}g^{\sigma\rho}\dot{g}_{\rho\alpha}\left(S_\sigma-p_\sigma\frac{S_v}{C_v}\right)+\frac{e}{2C_v}\left[\ gF_{\alpha k}S^k+\frac{(g-2)}{m^2}p_\alpha F_{kl}S^k p^l\right]. \tag{83}$$

Furthermore, the equation for S_v is

$$\frac{dS_v}{du}=\frac{e(g-2)}{2m^2}F_{kl}S^k p^l. \tag{84}$$

In the following we shall restrict ourselves to the exactly integrable case $g=2$. Under this condition we find from (84) that

$$S_v=\text{const}=E_v. \tag{85}$$

After the substitution

$$S_\alpha=X_\alpha+\frac{E_v}{C_v}p_\alpha, \tag{86}$$

where p_α is assumed to be given by Eq. (70) in terms of Hill (or Mathieu) functions, we obtain a homogeneous equation for the new variable X_α,

$$\frac{\mathrm{d}X_\alpha}{\mathrm{d}u}=\frac{1}{2}g^{\sigma\rho}\dot{g}_{\rho\alpha}X_\sigma+\frac{e}{C_v}F_{\alpha\sigma}g^{\sigma\lambda}X_\lambda. \tag{87}$$

It is convenient to write this equation in the matrix form

$$\frac{\mathrm{d}}{\mathrm{d}u}\mathbf{X}=\left(\mathbf{A}+\frac{\Pi}{L^2}\mathbf{B}\right)\cdot\mathbf{X}, \tag{88}$$

where $\mathbf{X}$ is a column vector with elements X_2 and X_3. The two-dimensional matrices $\mathbf{A}$ and $\mathbf{B}$ have the structures

$$\mathbf{A}=\begin{pmatrix} \dfrac{\dot{L}}{L}+\cosh^2(2\gamma)\dot{\beta} & e^{2\beta}(\dot{\gamma}-\sinh(2\gamma)\cosh(2\gamma)\dot{\beta}) \\ e^{-2\beta}(\dot{\gamma}+\sinh(2\gamma)\cosh(2\gamma)\dot{\beta}) & \dfrac{\dot{L}}{L}-\cosh^2(2\gamma)\dot{\beta} \end{pmatrix}, \tag{89}$$

and

$$\mathbf{B}\equiv\begin{pmatrix} \sinh 2\gamma & -e^{2\beta}\cosh 2\gamma \\ e^{-2\beta}\cosh 2\gamma & -\sinh 2\gamma \end{pmatrix}, \tag{90}$$

respectively. Equation (50) may be written in matrix form as well:

$$\begin{pmatrix} p_2 \\ p_3 \end{pmatrix}^{\cdot}=\frac{\Pi}{L^2}\mathbf{B}\cdot\begin{pmatrix} p_2 \\ p_3 \end{pmatrix}. \tag{91}$$

For the derivative of the combination $p_2^2+p_3^2$ we obtain

$$\frac{\mathrm{d}}{\mathrm{d}u}(p_2^2+p_3^2)=\frac{2\Pi}{L^2}[(p_2^2-p_3^2)\sinh 2\gamma-2p_2p_3\cosh 2\gamma\sinh 2\beta]. \tag{92}$$

In general, the right-hand side of this equation is different from zero, i.e., the particle motion is no longer circular in the GW field.

Equation (88) may be further simplified by changing to a new variable **Y**, defined by

$$\mathbf{X}=\mathbf{T}\cdot\mathbf{Y}, \tag{93}$$

where **T** is supposed to satisfy the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}u}\mathbf{T}=\mathbf{A}\cdot\mathbf{T}. \tag{94}$$

This procedure (cf. Refs. 35 and 36) removes the **A** term in Eq. (88) and gives rise to

$$\frac{\mathrm{d}}{\mathrm{d}u}\mathbf{Y}=\frac{\Pi}{L^2}\hat{\mathbf{B}}\cdot\mathbf{Y} \tag{95}$$

for **Y** with

$$\hat{\mathbf{B}}\equiv\mathbf{T}^{-1}\cdot\mathbf{B}\cdot\mathbf{T}. \tag{96}$$

By direct calculation one checks that the matrix

$$\mathbf{T}=L\cdot\begin{pmatrix} e^{\beta} & 0 \\ 0 & e^{-\beta} \end{pmatrix}\cdot\begin{pmatrix} \cosh\gamma & \sinh\gamma \\ \sinh\gamma & \cosh\gamma \end{pmatrix}\cdot\begin{pmatrix} \cos\psi & -\sin\psi \\ \sin\psi & \cos\psi \end{pmatrix}, \tag{97}$$

where

$$\psi\equiv\int_0^u\dot{\beta}\sinh 2\gamma\,\mathrm{d}u \tag{98}$$

satisfies Eq. (94). The determinants of each of the three two-dimensional matrices in (97) are equal to one. In the absence of the GW field all of them are identical to **I**, i.e.,

$$\mathbf{T}(0)=\mathbf{I}\equiv\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{99}$$

The structure of the third matrix on the right-hand side of Eq. (97) suggests the interpretation as a gravitationally induced rotation with phase $\psi(u)$ and frequency $\dot{\psi}(u)$. For either of the polarizations $\gamma=0$ or $\beta=0$, however, we have $\psi=0$ and the third matrix reduces to $\mathbf{I}$.

Direct calculation of the matrix $\hat{\mathbf{B}}$ in (96) with the help of expressions (90), (97), and (98) yields the surprisingly simple result

$$\hat{\mathbf{B}}\equiv\mathbf{T}^{-1}\cdot\mathbf{B}\cdot\mathbf{T}=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{100}$$

It is remarkable, that the matrix $\hat{\mathbf{B}}$, different from $\mathbf{B}$, does *not* depend on retarded time. This property allows us to find the solution of Eq. (95) in terms of elementary functions as

$$\begin{pmatrix}Y_2(u)\\ Y_3(u)\end{pmatrix}=\mathbf{R}(u)\cdot\begin{pmatrix}Y_2(0)\\ Y_3(0)\end{pmatrix},\quad \mathbf{R}(u)\equiv\begin{pmatrix}\cos\Phi(u) & -\sin\Phi(u)\\ \sin\Phi(u) & \cos\Phi(u)\end{pmatrix}, \tag{101}$$

where

$$\Phi(u)\equiv\Pi\int_0^u\frac{du}{L^2(u)}. \tag{102}$$

The combination

$$Y_2^2(u)+Y_3^2(u)=Y_2^2(0)+Y_3^2(0) \tag{103}$$

is preserved, i.e., the dynamics of $\mathbf{Y}$ represents a rotation in the x^20x^3 plane. The functions $S_2(u)$ and $S_3(u)$ in (86) can now be expressed in terms of the three matrices $\mathbf{H}(u)$, $\mathbf{T}(u)$, and $\mathbf{R}(u)$, given by expressions (71), (97), and (101), respectively:

$$\begin{pmatrix}S_2(u)\\ S_3(u)\end{pmatrix}=\mathbf{T}(u)\cdot\mathbf{R}(u)\cdot\begin{pmatrix}S_2(0)\\ S_3(0)\end{pmatrix}+\frac{E_v}{C_v}[\,\mathbf{H}(u)-\mathbf{T}(u)\cdot\mathbf{R}(u)]\begin{pmatrix}C_2\\ C_3\end{pmatrix}. \tag{104}$$

While the matrices $\mathbf{T}(u)$ and $\mathbf{R}(u)$ are constructed out of elementary functions, the matrix $\mathbf{H}(u)$, according to Eq. (71), consists of Hill functions, which for the special case of Sec. V B 2 reduce to Mathieu functions. The latter, in turn, can be expressed via ''cosine elliptic'' and ''sine elliptic'' functions [see the discussion following Eq. (77)]. All these functions are assumed to be known here. In the absence of the GW,

$$\mathbf{T}(u)\equiv\mathbf{I},\quad \mathbf{H}(u)=\mathbf{R}(u)\equiv\mathbf{R}_0(\tau)=\begin{pmatrix}\cos\Omega_H\tau & -\sin\Omega_H\tau\\ \sin\Omega_H\tau & \cos\Omega_H\tau\end{pmatrix}, \tag{105}$$

and we recover the standard flat space–time rotation of the spin particle,

$$\begin{pmatrix}p_2(\tau)\\ p_3(\tau)\end{pmatrix}=\mathbf{R}_0(\tau)\cdot\begin{pmatrix}C_2\\ C_3\end{pmatrix},\quad \begin{pmatrix}S_2(\tau)\\ S_3(\tau)\end{pmatrix}=\mathbf{R}_0(\tau)\cdot\begin{pmatrix}S_2(0)\\ S_3(0)\end{pmatrix}. \tag{106}$$

Equation (104) represents the general solution for the spin dynamics in the GW field (30) and the magnetic field (48). The structure of the solution (104) allows us to interpret the spin dynamics as composed of three separate contributions, characterized by the matrices $\mathbf{R}(u)$, $\mathbf{T}(u)$, and $\mathbf{H}(u)$. The matrix $\mathbf{R}$ represents a Larmor type precession with the frequency $\Pi/L^2(u)$. As already

mentioned, the matrix **T** describes a gravitationally induced rotation with phase $\psi(u)$ and frequency $\dot{\psi}(u)$, and finally, the matrix **H** accounts for the coupling of the particle motion (70) to the spin dynamics.

VII. ISOSPIN EVOLUTION

In this section as well as in the subsequent one we discuss the dynamics of non-Abelian charges under the influence of external gravitational and Yang–Mills fields. Let us consider Eq. (20) for the SU(2) symmetry group. Since the structure constants for this group coincide with the Levi–Civita symbol, all three directions in the isospin space are equivalent. With the choice $I^{(3)}=I_{(A)}q^{(A)}$ we obtain the following equations for the isospin evolution:

$$\frac{\mathrm{d}I^{(1)}}{\mathrm{d}\tau}=\Omega\cdot I^{(2)},\quad \frac{\mathrm{d}I^{(2)}}{\mathrm{d}\tau}=-\Omega\cdot I^{(1)}. \tag{107}$$

The precession frequency Ω in Eq. (20) is calculated on the particle worldline with p^i from (70) and the potential

$$A_i(u)=\frac{1}{2}M\left[\left(x^2(u)-x^2(0)-\frac{C_2}{\Pi C_v}\right)\delta_i^3-\left(x^3(u)-x^3(0)-\frac{C_3}{\Pi C_v}\right)\delta_i^2\right], \tag{108}$$

corresponding to the constant solution $F_{23}=M$. Differentiating expression (108), we recover the field strength (49). The frequency $\Omega(u)$ in (20) is given by

$$\Omega(u)=\frac{g}{m}(A_2p^2+A_3p^3). \tag{109}$$

Here, the arbitrary constant was chosen such that $\Omega(u=0)=0$. In order to find the terms $x^2(u)-x^2(0)$ and $x^3(u)-x^3(0)$ which are needed in (108), we have to integrate the second equation in (35). The formal solution is

$$x^\alpha(u)-x^\alpha(0)=\frac{1}{C_v}\int_0^u d\xi g^{\alpha\beta}(\xi)p_\beta(\xi), \tag{110}$$

which provides us with

$$\Omega(u)=\frac{gM}{2mC_v}\left\{\int_0^u \mathrm{d}\xi[p^2(\xi)p^3(u)-p^3(\xi)p^2(u)]-\frac{1}{\Pi}[C_2p^3(u)-C_3p^2(u)]\right\}. \tag{111}$$

Again we assume here $p^2(u)$ and $p^3(u)$ to be known, i.e., the particle dynamics is considered to be solved [cf. Eqs. (70) and (71)]. The solution of the system (107) then becomes

$$I^{(1)}=I\cos\Psi(u),\quad I^{(2)}=-I\sin\Psi(u),\quad \Psi(u)=\Psi(0)+\frac{m}{C_v}\int_0^u\Omega(u)\mathrm{d}u. \tag{112}$$

The function $\Psi(u)$ plays the role of the (generally u-dependent) phase of the isospin precession in the external Yang–Mills field.[37] The set of equations (112) with (111) provides a complete description for the isospin dynamics under the influence of the GW (30) and the Yang–Mills field (49).

VIII. COLOR CHARGE EVOLUTION

The SU(3) case may be studied along similar lines although it is technically more extended since more degrees of freedom are involved. As a result, we shall find a richer dynamical structure than in the SU(2) case. With the ansatz (18) and expression (15), Eq. (24) for the color charge dynamics becomes

$$
\begin{aligned}
\frac{dQ^{(1)}}{d\tau} &= -\Omega\left[(q^{(2)}Q^{(3)}-q^{(3)}Q^{(2)})+\frac{1}{2}(q^{(4)}Q^{(7)}-q^{(7)}Q^{(4)})-\frac{1}{2}(q^{(5)}Q^{(6)}-q^{(6)}Q^{(5)})\right],\\
\frac{dQ^{(2)}}{d\tau} &= -\Omega\left[(q^{(3)}Q^{(1)}-q^{(1)}Q^{(3)})+\frac{1}{2}(q^{(4)}Q^{(6)}-q^{(6)}Q^{(4)})+\frac{1}{2}(q^{(5)}Q^{(7)}-q^{(7)}Q^{(5)})\right],\\
\frac{dQ^{(3)}}{d\tau} &= -\Omega\left[(q^{(1)}Q^{(2)}-q^{(2)}Q^{(1)})+\frac{1}{2}(q^{(4)}Q^{(5)}-q^{(5)}Q^{(4)})-\frac{1}{2}(q^{(6)}Q^{(7)}-q^{(7)}Q^{(6)})\right],\\
\frac{dQ^{(4)}}{d\tau} &= -\frac{\Omega}{2}[(q^{(7)}Q^{(1)}-q^{(1)}Q^{(7)})+(q^{(6)}Q^{(2)}-q^{(2)}Q^{(6)})+(q^{(5)}Q^{(3)}-q^{(3)}Q^{(5)})]\\
&\quad -\frac{\sqrt{3}\Omega}{2}[q^{(5)}Q^{(8)}-q^{(8)}Q^{(5)}],\\
\frac{dQ^{(5)}}{d\tau} &= -\frac{\Omega}{2}[(q^{(1)}Q^{(6)}-q^{(6)}Q^{(1)})+(q^{(7)}Q^{(2)}-q^{(2)}Q^{(7)})+(q^{(3)}Q^{(4)}-q^{(4)}Q^{(3)})]\\
&\quad -\frac{\sqrt{3}\Omega}{2}[q^{(8)}Q^{(4)}-q^{(4)}Q^{(8)}],\\
\frac{dQ^{(6)}}{d\tau} &= -\frac{\Omega}{2}[(q^{(5)}Q^{(1)}-q^{(1)}Q^{(5)})+(q^{(2)}Q^{(4)}-q^{(4)}Q^{(2)})+(q^{(3)}Q^{(7)}-q^{(7)}Q^{(3)})]\\
&\quad -\frac{\sqrt{3}\Omega}{2}[q^{(7)}Q^{(8)}-q^{(8)}Q^{(7)}],\\
\frac{dQ^{(7)}}{d\tau} &= -\frac{\Omega}{2}[(q^{(1)}Q^{(4)}-q^{(4)}Q^{(1)})+(q^{(2)}Q^{(5)}-q^{(5)}Q^{(2)})+(q^{(6)}Q^{(3)}-q^{(3)}Q^{(6)})]\\
&\quad -\frac{\sqrt{3}\Omega}{2}[q^{(8)}Q^{(6)}-q^{(6)}Q^{(8)}],\\
\frac{dQ^{(8)}}{d\tau} &= -\frac{\sqrt{3}\Omega}{2}[(q^{(4)}Q^{(5)}-q^{(5)}Q^{(4)})+(q^{(6)}Q^{(7)}-q^{(7)}Q^{(6)})].
\end{aligned}
\tag{113}
$$

The space of color charges may be split into three different subspaces, which correspond to the structures of the SU(2), SU(2)×U(1) and U(1) subgroups of the total group SU(3) (see, e.g., Ref. 38). In the following we consider the vector $q^{(A)}$ to lie in the first, second, and third subspaces, respectively.

A. First special case

Let the vector $q^{(A)}$ have only the three nonzero components $q^{(1)}$, $q^{(2)}$, and $q^{(3)}$. It is then evident that

$$
(Q^{(1)})^2+(Q^{(2)})^2+(Q^{(3)})^2=\text{const}\,, \tag{114}
$$

$$(Q^{(4)})^2+(Q^{(5)})^2+(Q^{(7)})^2+(Q^{(7)})^2=\text{const}, \tag{115}$$

and

$$Q^{(8)}=\text{const}. \tag{116}$$

For the color charges $Q^{(1)}$, $Q^{(2)}$, and $Q^{(3)}$, which correspond to a SU(2) subgroup of the total SU(3) group, the combination (114) is preserved. A similar relation holds for the set $Q^{(4)}$, $Q^{(5)}$, $Q^{(6)}$, and $Q^{(7)}$, while $Q^{(8)}$ is separately conserved. Relations (114)–(116) are also obtained for the case that the only nonvanishing components are $q^{(4)}$, $q^{(5)}$, $q^{(6)}$, and $q^{(7)}$, as well as for the choice $q^{(1)}=q^{(2)}=\cdots=q^{(7)}=0$ and $q^{(8)}\neq 0$. Let us now further specify to the case $q^{(A)}=\delta^{(A)}_{(1)}$. Then the system (113) takes the form

$$\begin{gathered}
\frac{dQ^{(1)}}{d\tau}=0\,,\quad \frac{dQ^{(8)}}{d\tau}=0\,,\\
\frac{dQ^{(2)}}{d\tau}=\Omega Q^{(3)},\quad \frac{dQ^{(3)}}{d\tau}=-\Omega Q^{(2)},\\
\frac{dQ^{(4)}}{d\tau}=\frac{1}{2}\Omega Q^{(7)},\quad \frac{dQ^{(7)}}{d\tau}=-\frac{1}{2}\Omega Q^{(4)},\\
\frac{dQ^{(5)}}{d\tau}=-\frac{1}{2}\Omega Q^{(6)},\quad \frac{dQ^{(6)}}{d\tau}=\frac{1}{2}\Omega Q^{(5)}.
\end{gathered} \tag{117}$$

The color charge $Q^{(1)}$ remains constant because it is the projection $Q^{(A)}q_{(A)}$ of the vector $Q^{(A)}$ on the given preferred direction $q_{(A)}$. The charge $Q^{(8)}$ does not evolve, because for such a $q_{(A)}$ the antisymmetric tensor $H_{(A)(B)}$ in (24) does not contain a nonvanishing component with $(A)=(8)$. The equations for $Q^{(2)},\ldots,Q^{(7)}$ split into *three two-dimensional* subsystems with the pairs $Q^{(2)}$ and $Q^{(3)}$, $Q^{(4)}$ and $Q^{(7)}$, $Q^{(5)}$, and $Q^{(6)}$. The evolution of the first pair ($Q^{(2)}$ and $Q^{(3)}$) corresponds to a precession in the group space with the frequency Ω. It has a solution of the type (112). The dynamics of the pairs $Q^{(4)}$, $Q^{(7)}$ and $Q^{(5)}$, $Q^{(6)}$ is a precession with the frequency $\Omega/2$.

B. Second special case: $q^{(A)}=\delta^{(A)}_{(4)}$

Now we assume $q^{(A)}$ to lie in the second subspace. As an example we consider the case $q^{(A)}=\delta^{(A)}_{(4)}$. For this choice the set of equations (113) can be transformed into

$$\begin{gathered}
\frac{dQ^{(4)}}{d\tau}=0,\quad \frac{d}{d\tau}\left(-\frac{\sqrt{3}}{2}Q^3+\frac{1}{2}Q^8\right)=0\,,\\
\frac{dQ^{(5)}}{d\tau}=\Omega Q^*,\quad \frac{dQ^*}{d\tau}=-\Omega Q^{(5)},\quad Q^*\equiv\frac{1}{2}(Q^{(3)}+\sqrt{3}Q^{(8)}),\\
\frac{dQ^{(1)}}{d\tau}=-\frac{1}{2}\Omega Q^{(7)},\quad \frac{dQ^{(7)}}{d\tau}=\frac{1}{2}\Omega Q^{(1)},\\
\frac{dQ^{(2)}}{d\tau}=-\frac{1}{2}\Omega Q^{(6)},\quad \frac{dQ^{(6)}}{d\tau}=\frac{1}{2}\Omega Q^{(2)}.
\end{gathered} \tag{118}$$

The quantities $Q^{(4)}$ and $-(\sqrt{3}/2)Q^3+\frac{1}{2}Q^8$ remain constant, the projections $Q^{(5)}$ and $Q^*\equiv\frac{1}{2}(Q^{(3)}+\sqrt{3}Q^{(8)})$ precess with the frequency Ω, the pairs $Q^{(1)}$, $Q^{(7)}$ and $Q^{(2)}$, $Q^{(6)}$ precess with $\Omega/2$. Furthermore, one has

$$(Q^{(1)})^2+(Q^{(7)})^2=\text{const}\,,\quad (Q^{(2)})^2+(Q^{(6)})^2=\text{const},$$
$$(Q^{(3)})^2+(Q^{(5)})^2+(Q^{(8)})^2=\text{const}. \tag{119}$$

C. Third special case: $q^{(A)}=\delta^{(A)}_{(8)}$

Finally, let $q^{(A)}$ be parallel to the basis vector in the U(1) subspace, i.e., $q^{(A)}=\delta^{(A)}_{(8)}$. Here we obtain

$$\frac{dQ^{(1)}}{d\tau}=0,\quad \frac{dQ^{(2)}}{d\tau}=0,\quad \frac{dQ^{(3)}}{d\tau}=0,\quad \frac{dQ^{(8)}}{d\tau}=0,$$

as well as

$$\frac{dQ^{(4)}}{d\tau}=\frac{\sqrt{3}}{2}\Omega Q^{(5)},\quad \frac{dQ^{(5)}}{d\tau}=-\frac{\sqrt{3}}{2}\Omega Q^{(4)},$$
$$\frac{dQ^{(6)}}{d\tau}=\frac{\sqrt{3}}{2}\Omega Q^{(7)},\quad \frac{dQ^{(7)}}{d\tau}=-\frac{\sqrt{3}}{2}\Omega Q^{(6)}. \tag{120}$$

The pairs $Q^{(4)}$, $Q^{(5)}$ and $Q^{(6)}$, $Q^{(7)}$ precess with the frequency $(\sqrt{3}/2)\,\Omega$, while $Q^{(1)}$, $Q^{(2)}$, $Q^{(3)}$, and $Q^{(8)}$ are constant.

D. Remarks on the general case

In the general case one expects the color vector $Q^{(A)}$ to rotate in the hypersurface orthogonal to $q^{(A)}$ in the group space. This is illustrated by the following analogy. Let us consider the standard decomposition of the Maxwell tensor with respect to a four-velocity vector V^i of an arbitrary observer,

$$F_{ik}=E_iV_k-E_kV_i-\varepsilon_{ikjl}H^jV^l, \tag{121}$$

where E^i and H^k are the corresponding four-vectors for the electric and magnetic fields, respectively. For $F_{ik}V^k=0$ the comoving observer experiences a magnetic field only which, via the Lorentz force, generates a spatial particle rotation, i.e., a rotation in the hypersurface orthogonal to V^i.

In the present case the vector $q^{(A)}$ plays the role of V^i. Instead of Maxwell's tensor we have to consider [cf. Eq. (24)] the antisymmetric tensor $H_{(A)(C)}=f_{(A)(B)(C)}q^{(B)}$. Since $H_{(A)(C)}q^{(C)}=0$, this represents a group space analogue to the previous case of a pure magnetic field in space–time. Consequently, the color vector rotates in the group space analogously to the momentum vector of a charged particle in a pure magnetic field.

IX. CONCLUSIONS

Charged particles in electromagnetic fields are known to be parametrically influenced by gravitational waves. Typical phenomena are parametric resonances and parametric oscillations. In the present paper we have generalized and extended work in this field to include classical spin particles and particles with non-Abelian charges in specific Yang–Mills fields. Moreover, no weak field approximation was used for the GW. The electrically charged spin particle was described by the Bargmann–Michel–Telegdi equations. For the dynamics of the non-Abelian charges we used Wong's equations for the isospin [SU(2)-symmetry] and for the color charges [SU(3) symmetry]. We derived exact general solutions for the parametric influence of the GW on the particle motion in each of the mentioned cases, including the dynamics of spin, isospin, and color charge. For the case of a special sandwich GW the particle dynamics was reduced to a set of Mathieu equations. Using well-known stability properties of the latter we found that parametric instabilities are a

generic phenomenon for such kind of particle motion. Since spin, isospin, and color charge are coupled to this motion, their dynamics is affected correspondingly. The spin dynamics was shown to be composed of three elements, namely a gravitationally modified Larmor precession, a part due to the coupling to the particle motion, and a pure gravitational part. The vectors of isospin and color charge carry out gravitationally influenced precession motions in their group spaces which we have classified for several cases.

ACKNOWLEDGMENTS

This paper was supported by the Deutsche Forschungsgemeinschaft and NATO Grant No. PST. CLG.977973. The authors thank F.G. Suslikov for useful discussions about the SU(3) symmetry.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Symmetries of the energy–momentum tensor of spherically symmetric Lorentzian manifolds

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(Received 7 May 2003; accepted 27 June 2003)

Matter collineations of spherically symmetric Lorentzian manifolds are considered. These are investigated when the energy–momentum tensor is nondegenerate and also when it is degenerate. We have classified space–times admitting higher symmetries and space–times admitting SO(3) as the maximal isometry group. For the nondegenerate case, we obtain either *four*, *six*, *seven*, or *ten* independent matter collineations in which *four* are isometries and the rest are proper. The results of the previous paper [Sharif and Sehar (Gen. Relativ. Gravit. **35**, 1091 (2003)] are recovered as a special case. It is worth noting that we have also obtained two cases where the energy–momentum tensor is degenerate but the group of matter collineations is finite-dimensional, i.e., *four* or *ten*. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1610779]

I. INTRODUCTION

Since the pioneering work of Katzin, Levine, Davis and their collaborators,[1–5] the study of symmetries has played an important role in the classification of space–times, giving rise to many interesting results with useful applications. The theory of General Relativity (GR), described by Einstein's field equations (EFEs), is highly nonlinear. Due to its nonlinearity, it becomes difficult to find the exact solutions of the EFEs, in particular, if the metric depends on all coordinates.[6] However, this problem can be overcome to some extent if it is assumed that the space–time has some geometric symmetry properties. These symmetry properties are given by Killing vectors (KVs), which then lead to conservation laws.[7–9] A large number of solutions of the EFEs with different symmetry structures have been found[8] and classified according to their properties.[10]

As given by the pioneers, curvature and Ricci tensors play a significant role (in terms of curvature and Ricci collineations) in understanding the geometric structure of metrics. They have provided a detailed study of curvature and Ricci collineations in the context of the related particle and field conservation laws. For a given distribution of matter, the contribution of gravitational potential satisfying EFEs is the principal aim of all investigations in gravitational physics. This has been achieved by imposing symmetries on the geometry compatible with the dynamics of the chosen distribution of matter. In an attempt to study the geometric and physical properties of the electromagnetic fields, different types of collineations have been investigated[11,12] along with many other interesting results. Symmetries of the energy–momentum tensor (also called matter collineations) provide conservation laws on matter fields. These enable us to know how the physical fields, occupying in certain region of space–times, reflect the symmetries of the metric.[13]

There is a large body of recent literature which shows interest in the study of matter collineations (MCs).[14–22] In a recent paper,[14] the study of MCs has been taken for static spherically symmetric space–times (SSS) and some interesting results have been obtained. However, it was incomplete in the sense that (i) only the static case was considered and (ii) some cases were missing, in particular, for finite-dimensional MCs. In this paper, we extend the procedure to

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calculate MCs of SSS both for nondegenerate and also for degenerate cases with special emphasis on the metrics admitting higher symmetries and also SO(3) as the maximal symmetry. We relate them with RCs and isometries. The rest of the paper is organized as follows. Section II contains a brief review of MCs and we write down MC equations for SSS. In Sec. III, we shall solve these MC equations when the energy–momentum tensor is nondegenerate and in Sec. IV MC equations are solved for the degenerate energy–momentum tensor. Section V contains a summary and discussion of the results obtained.

II. MATTER COLLINEATIONS AND ITS EQUATIONS

Let (M,g) be a space–time, where M is a smooth, connected, Hausdorff four-dimensional manifold and g is smooth Lorentzian metric of signature $(+---)$ defined on M. The manifold M and the metric g are assumed smooth (C^{∞}). We shall use the usual component notation in local charts, and a covariant derivative with respect to the symmetric connection Γ associated with the metric g will be denoted by a semicolon and a partial derivative by a comma.

The geometry and matter of a space–time are related through the EFEs given in each coordinate system of M by

$$R_{ab}-\tfrac{1}{2}Rg_{ab}\equiv G_{ab}=\kappa T_{ab} \quad (a,b=0,1,2,3), \tag{1}$$

where κ is the gravitational constant, G_{ab} is the Einstein tensor, R_{ab} is the Ricci and T_{ab} is the matter (energy–momentum) tensor. Also, $R=g^{ab}R_{ab}$ is the Ricci scalar. We have assumed here that the cosmological constant $\Lambda=0$. Using the Bianchi identities, it can easily be shown that

$$G^{ab};b=0 \ (\Leftrightarrow T^{ab};b=0). \tag{2}$$

A smooth vector field ξ is said to preserve a matter symmetry[23] on M if, for each smooth local diffeomorphism ϕ_t associated with ξ, the tensor T and ϕ_t^*T are equal on the domain U of ϕ_t, i.e., $T=\phi_t^*T$. Equivalently, a vector field ξ^a is said to generate a MC if it satisfies

$$\pounds_{\xi}T_{ab}=0 \quad \Leftrightarrow \quad \pounds_{\xi}G_{ab}=0, \tag{3}$$

where £ is the Lie derivative operator, ξ^a is the symmetry or collineation vector. Every KV is a MC but the converse is not true, in general. Collineations can be proper (nontrivial) or improper (trivial). We define a proper MC to be a MC which is not a KV, or a homothetic vector (HV). The MC Eq. (3) can be written in component form as

$$T_{ab,c}\xi^c+T_{ac}\xi^c_{,b}+T_{cb}\xi^c_{,a}=0. \tag{4}$$

The most general form of the metric for a spherically symmetric Lorentzian manifold is given by

$$\mathrm{d}s^2=e^{\nu(t,r)}\mathrm{d}t^2-e^{\mu(t,r)}\mathrm{d}r^2-e^{\lambda(t,r)}\mathrm{d}\Omega^2, \tag{5}$$

where $\mathrm{d}\Omega^2=\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2$. The surviving components of the energy–momentum tensor, given in Appendix A, are T_{00}, T_{01} T_{11}, T_{22}, T_{33}, where $T_{33}=\sin^2\theta T_{22}$.

The MC equations can be written as follows:

$$T_{00,0}\xi^0+T_{00,1}\xi^1+2T_{00}\xi^0_{,0}+2T_{01}\xi^1_{,0}=0, \tag{6}$$

$$T_{01,0}\xi^0+T_{01,1}\xi^1+T_{01}\xi^0_{,0}+T_{11}\xi^1_{,0}+T_{01}\xi^1_{,1}+T_{00}\xi^0_{,1}=0, \tag{7}$$

$$T_{00}\xi^0_{,2}+T_{01}\xi^1_{,2}+T_{22}\xi^2_{,0}=0, \tag{8}$$

$$T_{00}\xi^0_{,3}+T_{01}\xi^1_{,3}+\sin^2\theta T_{22}\xi^3_{,0}=0, \tag{9}$$

$$T_{11,0}\xi^0+T_{11,1}\xi^1+2T_{01}\xi^0_{,1}+2T_{11}\xi^1_{,1}=0, \tag{10}$$

$$T_{01}\xi^0_{,2}+T_{11}\xi^1_{,2}+T_{22}\xi^2_{,1}=0, \tag{11}$$

$$T_{01}\xi^0_{,3}+T_{11}\xi^1_{,3}+\sin^2\theta T_{22}\xi^3_{,1}=0, \tag{12}$$

$$T_{22,0}\xi^0+T_{22,1}\xi^1+2T_{22}\xi^2_{,2}=0, \tag{13}$$

$$T_{22}\xi^2_{,3}+\sin^2\theta T_{22}\xi^3_{,2}=0, \tag{14}$$

$$T_{22,0}\xi^0+T_{22,1}\xi^1+2\cot\theta T_{22}\xi^2+2T_{22}\xi^3_{,3}=0. \tag{15}$$

These are the first-order nonlinear partial differential equations in four variables $\xi^a(x^b)$. We solve these equations for the nondegenerate case, when

$$\det(T_{ab})=T_{22}^2(T_{00}T_{11}-T_{01}^2)\sin^2\theta\neq 0 \tag{16}$$

and for the degenerate case, where $\det(T_{ab})=0$. It is noticed that when $T_{01}=0$ we shall use the notation $T_{aa}=T_a$ for the sake of brevity.

III. MATTER COLLINEATIONS IN THE NONDEGENERATE CASE

In this section, we shall evaluate MCs only for those cases which have nondegenerate energy–momentum tensor, i.e., $\det(T_{ab})\neq 0$. This will be done as two cases; one when M admits higher symmetries and one when SO(3) is the maximal isometry group of M. To this end, we set up the general conditions for the solution of MC equations for the nondegenerate case.

When we solve Eqs. (6)–(15) simultaneously, after some tedious algebra, we get the following solution:

$$\xi^0=\frac{T_{22}}{T_{00}T_{11}-T_{01}^2}[\{(\dot{A}_1T_{11}-A_1'T_{01})\sin\phi-(\dot{A}_2T_{11}-A_2'T_{01})\cos\phi\}\sin\theta + (\dot{A}_3T_{11}-A_3'T_{01})\cos\theta+A_4T_{11}-A_5T_{01}], \tag{17}$$

$$\xi^1=\frac{-T_{22}}{T_{00}T_{11}-T_{01}^2}[\{(\dot{A}_1T_{01}-A_1'T_{00})\sin\phi-(\dot{A}_2T_{01}-A_2'T_{00})\cos\phi\}\sin\theta + (\dot{A}_3T_{01}-A_3'T_{00})\sin\theta+A_4T_{01}-A_5T_{00}], \tag{18}$$

$$\xi^2=-(A_1\sin\phi-A_2\cos\phi)\cos\theta+A_3\sin\theta+c_1\sin\phi-c_2\cos\phi+c_4\ln\left(\tan\frac{\theta}{2}\right)\sin\theta, \tag{19}$$

$$\xi^3=-(A_1\cos\phi+A_2\sin\phi)\csc\theta+(c_1\cos\phi+c_2\sin\phi)\cot\theta+c_4\phi+c_3, \tag{20}$$

where c_1,c_2,c_3,c_4 are arbitrary constants and $A_\nu=A_\nu(t,r)$, $\nu=1,2,3,4,5$. Here dot and prime indicate the differentiation with respect to time and r coordinate, respectively. When we replace these values of ξ^a in MC Eqs. (6)–(15), we obtain the following differential constraints on A_ν with $c_4=0$:

$$2(T_{00}T_{11}-T_{01}^2)(T_{22}\dot{A}_i)^{\cdot}+T_{22}[(2T_{01}\dot{T}_{01}-T_{11}\dot{T}_{00}-T_{01}T_{00}')\dot{A}_i-(2T_{00}\dot{T}_{01}-T_{01}\dot{T}_{00}-T_{00}T_{00}')A_i'] = 0, \quad (i=1,2,3), \tag{21}$$

$$(T_{00}T_{11}-T_{01}^2)[(T_{22}\dot{A}_i)'+(T_{22}A_i')^{\cdot}]+T_{22}[(T_{01}\dot{T}_{11}-T_{11}T_{00}')\dot{A}_i+(T_{01}T_{00}'-T_{00}\dot{T}_{11})A_i']=0, \tag{22}$$

$$2(T_{00}T_{11}-T_{01}^2)(T_{22}A_i')'+T_{22}[(2T_{01}T_{01}'-T_{00}T_{11}'-T_{01}\dot{T}_{11})-(2T_{11}T_{01}'-T_{11}\dot{T}_{11}-T_{01}T_{11}')\dot{A}_i]=0, \tag{23}$$

$$(T_{11}\dot{T}_{22}-T_{01}T_{22}')\dot{A}_i+(T_{00}T_{22}'-T_{01}\dot{T}_{22})A_i'+2A_i=0, \tag{24}$$

$$2(T_{00}T_{11}-T_{01}^2)(T_{22}A_4)^{\cdot}+T_{22}[(2T_{01}\dot{T}_{01}-T_{11}\dot{T}_{00}-T_{01}T_{00}')A_4-(2T_{00}\dot{T}_{01}-T_{01}\dot{T}_{00}-T_{00}T_{00}')A_5]=0, \tag{25}$$

$$(T_{00}T_{11}-T_{01}^2)[(T_{22}A_4)'+(T_{22}A_5)^{\cdot}]+T_{22}[(T_{01}\dot{T}_{11}-T_{11}T_{00}')A_4+(T_{01}T_{00}'-T_{00}\dot{T}_{11})A_5]=0, \tag{26}$$

$$2(T_{00}T_{11}-T_{01}^2)(T_{22}A_5)'+T_{22}[(2T_{01}T_{01}'-T_{00}T_{11}'-T_{01}\dot{T}_{11})A_5-(2T_{11}T_{01}'-T_{11}\dot{T}_{11}-T_{01}T_{11}')A_4]=0, \tag{27}$$

$$(T_{11}\dot{T}_{22}-T_{01}T_{22}')A_4+(T_{00}T_{22}'-T_{01}\dot{T}_{22})A_5=0. \tag{28}$$

Thus the problem of working out MCs for all possibilities of A_i, A_4, A_5 is reduced to solving the set of Eqs. (17)–(20) subject to the above-given constraints. We would solve these to classify MCs of the manifolds admitting higher symmetries than SO(3) and SO(3) as the maximal isometry group.

A. MCs of the space–times admitting higher symmetries

Here we use the constraint equations (21)–(28) to evaluate MCs of the space–times given by Eq. (5) which admit higher symmetries than SO(3). The six cases admitting symmetry groups larger than SO(3) are the following:

(1) $SO(3)\otimes\mathbf{R}$, where $\mathbf{R}=\partial_t$ if and only if
(a) $\nu=\nu(r)$, $\mu=\mu(r)$, $\lambda=2\ln r$ or (b) $\nu=\nu(r)$, $\mu=0$, $\lambda=2\ln a$,
where a is an arbitrary constant,
(2) $SO(3)\otimes\mathbf{R}$, where $\mathbf{R}=\partial_r$ if and only if
(a) $\nu=\nu(t)$, $\mu=\mu(t)$, $\lambda=2\ln t$ or (b) $\nu=0$, $\mu=\mu(t)$, $\lambda=2\ln a$,
(3) $SO(3)\otimes\mathbf{R}$, where $\mathbf{R}=\partial_t+e\partial_r$ if and only if
$\nu=0=\mu$, $\lambda=\lambda(t+er)$ with $e=\pm1$,
(4) SO(4) if and only if $\nu=0$, $\mu=2\ln R(t)$, $\lambda=2\ln R(t)\sin r$ such that
$R\ddot{R}-\dot{R}^2-1\neq0$,
(5) $SO(3)\times\mathbf{R}^3$ if and only if $\nu=0$, $\mu=2\ln R(t)$, $\lambda=2\ln R(t)r$ such that
$R\ddot{R}-\dot{R}^2\neq0$,
(6) SO(1,3) if and only if
(a) $\nu=0$, $\mu=2\ln R(t)$, $\lambda=2\ln R(t)\sinh r$ such that
$R\ddot{R}-\dot{R}^2+1\neq0$, or
(b) $\nu=2\ln Q(r)$, $\mu=0$, $\lambda=2\ln Q(r)\cosh t$ such that
$QQ''-Q'^2+1\neq0$.

Case (1): In this case, we have $T_{01}=0$ and also $\dot{T}_{ab}=0$. Using these values, Eqs. (17)–(28) reduce to

$$\xi^0=\frac{T_2}{T_0}[(\dot{A}_1\sin\phi-\dot{A}_2\cos\phi)\sin\theta+\dot{A}_3\cos\theta+A_4], \tag{29}$$

$$\xi^1=\frac{T_2}{T_1}[(A_1'\sin\phi-A_2'\cos\phi)\sin\theta+A_3'\cos\theta+A_5], \tag{30}$$

$$\xi^2=-(A_1\sin\phi-A_2\cos\phi)\cos\theta+A_3\sin\theta+c_1\sin\phi-c_2\cos\phi, \tag{31}$$

$$\xi^3=-(A_1\cos\phi+A_2\sin\phi)\csc\theta+(c_1\cos\phi+c_2\sin\phi)\cot\theta+c_3, \tag{32}$$

where we have used the notation $T_{aa}=T_a$ for the sake of simplicity. These ξ^a are satisfied subject to the following differential constraints on A_ν:

$$T_1\dot{A}_4+T_0'A_5=0,\quad \left(\frac{T_2}{T_0}A_4\right)'+\frac{T_2}{T_0}\dot{A}_5=0,$$
$$\left(\frac{T_2}{\sqrt{T_1}}A_5\right)'=0,\quad T_2'A_5=0, \tag{33}$$

$$2T_1\ddot{A}_i+T_0'A_i'=0,\quad \left(\sqrt{\frac{T_2}{T_0}}\dot{A}_i\right)'=0,$$
$$\left(\frac{T_2}{\sqrt{T_1}}A_i'\right)'=0,\quad 2T_1A_i+T_2'A_i'=0. \tag{34}$$

It is interesting to note that this case reduces to the nondegenerate case of Ref. 14. However, the possibility of seven MCs is recovered here which was missing there. Now the evaluation of MCs for all possibilities of A_i, A_4, A_5 is reduced to solving the set of Eqs. (29)–(32) subject to the constraints given by Eqs. (33) and (34). A complete solution of these equations is obtained by considering different possibilities of T_2. The last equation of Eq. (33) implies that either

$$\text{(a)}\ \ T_2'=0,\ \ \textit{or}\ \ \text{(b)}\ \ T_2'\neq 0.$$

The first case when $T_2=\beta$, where β is an arbitrary constant, Eq. (34) gives $A_i=0$ and consequently Eqs. (29)–(32) yield

$$\xi^0=A_4(t,r),\ \ \xi^1=A_5(t,r),$$
$$\xi^2=c_1\sin\phi-c_2\cos\phi,\quad \xi^3=(c_1\cos\phi+c_2\sin\phi)\cot\theta+c_3. \tag{35}$$

Further, if we assume that

$$\left[\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\right]'\neq 0,$$

we obtain four MCs identical to the usual KVs of spherical symmetry given by

$$\xi=c_0\frac{T_0}{\beta}\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi. \tag{36}$$

When

$$\left[\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\right]'=0,$$

this implies that

$$\frac{T_0}{\sqrt{T_1}}\left[\frac{T_0'}{2T_0\sqrt{T_1}}\right]'=\alpha,$$

where α is an arbitrary constant which may be positive, zero, or negative. In each case, we have six MCs.

For $\alpha>0$, we obtain

$$\begin{aligned}\xi=&c_0\frac{T_0}{\beta}\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left(-\frac{T_0'}{2\beta\sqrt{\alpha T_1}}\sinh\sqrt{\alpha}t\partial_t+\frac{\sqrt{T_1}}{\beta}\cosh\sqrt{\alpha}t\partial_r\right)\\&+c_5\left(-\frac{T_0'}{2\beta\sqrt{\alpha T_1}}\cosh\sqrt{\alpha}t\partial_t+\frac{\sqrt{T_1}}{\beta}\sinh\sqrt{\alpha}t\partial_r\right).\end{aligned}\tag{37}$$

If $\alpha=0$, we have

$$\begin{aligned}\xi=&c_0\frac{T_0}{\beta}\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left[-\frac{T_0}{\beta}\left(\frac{\gamma}{2}t^2+\frac{1}{\beta}\int\sqrt{T_1}dr\right)\partial_t+\frac{\sqrt{T_1}}{\beta}t\partial_r\right]+c_5\left(\frac{T_0}{\beta}\gamma t\partial_t+\frac{\sqrt{T_1}}{\beta}\partial_r\right),\end{aligned}\tag{38}$$

where

$$\frac{T_0'}{2T_0\sqrt{T_1}}=\gamma,$$

an arbitrary constant. The case $\alpha<0$ yields

$$\begin{aligned}\xi=&c_0\frac{T_0}{\beta}\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)\\&+c_3\partial_\phi+c_4\left(-\frac{T_0'}{2\beta\sqrt{-\alpha T_1}}\sin\sqrt{-\alpha}t\partial_t+\frac{\sqrt{T_1}}{\beta}\cos\sqrt{-\alpha}t\partial_r\right)\\&+c_5\left(\frac{T_0'}{2\beta\sqrt{-\alpha T_1}}\cos\sqrt{-\alpha}t\partial_t+\frac{\sqrt{T_1}}{\beta}\sin\sqrt{-\alpha}t\partial_r\right).\end{aligned}\tag{39}$$

In case (b), when $T_2'\neq0$, it follows from Eqs. (33) and (34) that for

$$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1\neq0,$$

we obtain the same MCs as the usual minimal KVs for spherically symmetry.

If

$$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1=0$$

and

$$\left(\frac{T_2'}{\sqrt{T_0T_1T_2}}\right)'\neq 0,$$

we have seven MCs given by

$$\begin{aligned}\xi=&c_0\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left(-\frac{1}{\sqrt{T_1}}\sin\phi\sin\theta\partial_r-X\sin\phi\cos\theta\partial_\theta-X\cos\phi\csc\theta\partial_\phi\right)\\&+c_5\left(\frac{1}{\sqrt{T_1}}\cos\phi\sin\theta\partial_r+X\cos\phi\cos\theta\partial_\theta-X\sin\phi\csc\theta\partial_\phi\right)\\&+c_6\left(-\frac{1}{\sqrt{T_1}}\cos\theta\partial_r-X\sin\theta\partial_\theta\right),\end{aligned}\tag{40}$$

where $X=T_2'/2T_2\sqrt{T_1}$. If we have $(T_2/\sqrt{T_1})(T_2'/2T_2\sqrt{T_1})'+1=0$, $(T_2'/\sqrt{T_0T_1T_2})'=0$, and $(T_0'/T_2')'\neq 0$, then we get four MCs.

When $(T_2/\sqrt{T_1})(T_2'/2T_2\sqrt{T_1})'+1=0$, $(T_2'/\sqrt{T_0T_1T_2})'=0$, and $T_0'/T_2'=\delta$, an arbitrary constant. For $\delta>0$, we obtain

$$\begin{aligned}\xi=&c_0\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left[\left(\frac{T_2}{T_0}X\sqrt{\delta}\sinh\sqrt{\delta}t\partial_t-\frac{1}{\sqrt{T_1}}\cosh\sqrt{\delta}t\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta\right.\\&\left.+\csc\theta\cos\phi\partial_\phi)X\cosh\sqrt{\delta}t\right]+c_5\left[\left(-\frac{T_2}{T_0}X\sqrt{\delta}\sinh\sqrt{\delta}t\partial_t+\frac{1}{\sqrt{T_1}}\cosh\sqrt{\delta}t\partial_r\right)\sin\theta\cos\phi\right.\\&\left.+(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)X\cosh\sqrt{\delta}t\right]+c_6\left[\left(\frac{T_2}{T_0}X\sqrt{\delta}\sinh\sqrt{\delta}t\partial_t\right.\right.\\&\left.\left.-\frac{1}{\sqrt{T_1}}\cosh\sqrt{\delta}t\partial_r\right)\cos\theta+X\cosh\sqrt{\delta}t\sin\theta\partial_\theta\right]+c_7\left[\left(\frac{T_2}{T_0}X\sqrt{\delta}\cosh\sqrt{\delta}t\partial_t\right.\right.\\&\left.\left.-\frac{1}{\sqrt{T_1}}\sinh\sqrt{\delta}t\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)X\sinh\sqrt{\delta}t\right]\\&+c_8\left[-\left(\frac{T_2}{T_0}X\sqrt{\delta}\cosh\sqrt{\delta}t\partial_t+\frac{1}{\sqrt{T_1}}\sinh\sqrt{\delta}t\partial_r\right)\sin\theta\cos\phi+(\cos\theta\cos\phi\partial_\theta\right.\\&\left.-\csc\theta\sin\phi\partial_\phi)X\sinh\sqrt{\delta}t+c_9\left(\frac{T_2}{T_0}X\sqrt{\delta}\cosh\sqrt{\delta}t\partial_t-\frac{1}{\sqrt{T_1}}X\sinh\sqrt{\delta}t\partial_r\right)\cos\theta\right.\\&\left.+X\sinh\sqrt{\delta}t\sin\theta\partial_\theta\right].\end{aligned}\tag{41}$$

If $\delta=0$, we have

$$\begin{aligned}\xi=&c_0\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left[\left(\frac{T_2}{T_0}X\partial_t-\frac{1}{\sqrt{T_1}}t\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)tX\right]\\&+c_5\left[\left(-\frac{T_2}{T_0}X\partial_t+\frac{1}{\sqrt{T_1}}t\partial_r\right)\sin\theta\cos\phi+(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)tX\right]\\&+c_6\left[\left(\frac{T_2}{T_0}X\partial_t-\frac{1}{\sqrt{T_1}}t\partial_r\right)\cos\theta+tX\sin\theta\right]\\&+c_7\left[\left(-\frac{1}{\sqrt{T_1}}\sin\theta\partial_r-X\cos\theta\partial_\theta\right)\sin\phi-X\csc\theta\cos\phi\partial_\phi\right]\\&+c_8\left[\left(\frac{1}{\sqrt{T_1}}\sin\theta\partial_r+X\cos\theta\partial_\theta\right)\cos\phi-X\csc\theta\sin\phi\partial_\phi\right]\\&+c_9\left(-\frac{1}{\sqrt{T_1}}\cos\theta\partial_r+X\sin\theta\partial_\theta\right).\end{aligned}\tag{42}$$

For $\delta<0$, MCs are given by

$$\begin{aligned}\xi=&c_0\partial_t+c_1(\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi)+c_2(\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi)+c_3\partial_\phi\\&+c_4\left[\left(-\frac{T_2}{T_0}X\sqrt{-\delta}\sin\sqrt{-\delta}t\partial_t-\frac{1}{\sqrt{T_1}}\cos\sqrt{-\delta}t\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta\right.\\&\left.+\csc\theta\cos\phi\partial_\phi)X\cos\sqrt{-\delta}t\right]+c_5\left[\left(\frac{T_2}{T_0}X\sqrt{-\delta}\sin\sqrt{-\delta}t\partial_t+\frac{1}{\sqrt{T_1}}\cos\sqrt{-\delta}t\partial_r\right)\sin\theta\cos\phi\right.\\&\left.+(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)X\cos\sqrt{-\delta}t\right]+c_6\left[\left(-\frac{T_2}{T_0}X\sqrt{-\delta}\sin\sqrt{-\delta}t\partial_t\right.\right.\\&\left.\left.-\frac{1}{\sqrt{T_1}}\cos\sqrt{-\delta}t\partial_r\right)\cos\theta+X\cos\sqrt{-\delta}t\sin\theta\partial_\theta\right]+c_7\left[\left(\frac{T_2}{T_0}X\sqrt{-\delta}\cos\sqrt{-\delta}t\partial_t\right.\right.\\&\left.\left.-\frac{1}{\sqrt{T_1}}\sin\sqrt{-\delta}t\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)X\sin\sqrt{-\delta}t\right]\\&+c_8\left[-\left(\frac{T_2}{T_0}X\sqrt{\delta}\cos\sqrt{-\delta}t\partial_t+\frac{1}{\sqrt{T_1}}\sin\sqrt{-\delta}t\partial_r\right)\sin\theta\cos\phi+(\cos\theta\cos\phi\partial_\theta\right.\\&\left.-\csc\theta\sin\phi\partial_\phi)X\sin\sqrt{-\delta}t+c_9\left(\frac{T_2}{T_0}X\sqrt{-\delta}\cos\sqrt{-\delta}t\partial_t-\frac{1}{\sqrt{T_1}}X\sin\sqrt{-\delta}t\partial_r\right)\cos\theta\right.\\&\left.+X\sin\sqrt{-\delta}t\sin\theta\partial_\theta\right].\end{aligned}\tag{43}$$

From Eqs. (41) to (43), it follows that for each value of δ, we obtain ten independent MCs.

Case (2): In this case, we have $T_{01}=0$ and $T_a'=0$. If we use the transformations $t\leftrightarrow r$, $\xi^0\leftrightarrow\xi^1$, $T_0\leftrightarrow T_1$, the solution of this case can be trivially obtained as in case (1).

Cases (4), (5), (6): The cases (4), (5) and (6a) describe Friedmann Robertson (FRW) space–times whereas case (6b) describes FRW like space–times. For these metrics, the nonvanishing components of Ricci and energy–momentum tensors are given in Appendix B. If any of T_a is zero, we get infinte dimensional MCs. For the nondegenerate case, we have $T_a\neq 0$, which implies the following possibilities:

$$\text{(a)}\quad \frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)-k=0,\quad \text{(b)}\quad \frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)-k\neq 0$$

with

$$\text{(i)}\quad \dot{T}_1=0,\quad \text{(ii)}\quad \dot{T}_1\neq 0,$$

where k has the values $1,0,-1$ for closed, flat, and open FRW space–times, respectively.

In case (ai), we must have $k=0$ and $T_1=a\neq 0$, a is an arbitrary constant. Thus, in addition to the nonproper MCs $\xi_{(1)},\xi_{(2)},\xi_{(3)},\xi_{(4)},\xi_{(5)},\xi_{(6)}$ given in Appendix C, we obtain the following proper MCs:

$$\begin{aligned}
\xi_{(7)}&=\frac{1}{\sqrt{T_0}}\partial_t,\\
\xi_{(8)}&=r\left(\frac{1}{\sqrt{T_0}}\partial_t-Y\partial_r\right)\sin\theta\sin\phi-(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)Y,\\
\xi_{(9)}&=r\left(\frac{1}{\sqrt{T_0}}\partial_t-Y\partial_r\right)\sin\theta\cos\phi-(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)Y,\\
\xi_{(10)}&=r\left(\frac{1}{\sqrt{T_0}}\partial_t-Y\partial_r\right)\cos\theta+Y\sin\theta\partial_\theta,
\end{aligned}\tag{44}$$

where $Y=(1/ar)\int\sqrt{T_0}dt$. This gives ten independent MCs in which six are the usual KVs of of closed FRW metric and the rest are the proper MCs.

Case (aii) also yields ten independent MCs for each value of k. For the value of $k=1$, the proper MCs are given by

$$\begin{aligned}
\xi_{(7)}&=\left(\frac{\sqrt{T_0}}{T_1}\cot r\partial_t-Z\sin^2 r\partial_r\right)\csc r,\\
\xi_{(8)}&=\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t-Z\sin r\cos r\partial_r\right)\sin\theta\sin\phi-Z(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)\csc r\right],\\
\xi_{(9)}&=\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t-Z\sin r\cos r\partial_r\right)\sin\theta\cos\phi-Z(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)\csc r\right],\\
\xi_{(10)}&=\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t-Z\sin r\cos r\partial_r\right)\cos\theta-Z\partial_\theta\right]\csc r,
\end{aligned}\tag{45}$$

where $Z=T_2/2T_1\sqrt{T_0}$. For $k=0$, we have the following proper MCs:

$$\xi_{(7)}=\left(\frac{1}{\sqrt{T_0}}\partial_t-rZ\partial_r\right),$$

$$\begin{aligned}\xi_{(8)}=&\left[\left\{\left(\frac{rT_2}{2T_0}\dot{Z}-\frac{r}{\sqrt{T_0}}\right)\partial_t+\left(\frac{r^2Z}{2}+\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\,\partial_r\right)\right\}\sin\theta\sin\phi\right.\\&\left.-\left(\frac{r}{2}Z-\frac{1}{r}\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\right)(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)\right],\\ \xi_{(9)}=&\left[\left\{\left(\frac{rT_2}{2T_0}\dot{Z}-\frac{r}{\sqrt{T_0}}\right)\partial_t+\left(\frac{r^2Z}{2}+\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\partial_r\right)\right\}\sin\theta\cos\phi\right.\\&\left.-\left(\frac{r}{2}Z-\frac{1}{r}\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\right)(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)\right],\end{aligned}\tag{46}$$

$$\xi_{(10)}=\left[\left\{\left(\frac{rT_2}{2T_0}\dot{Z}-\frac{r}{\sqrt{T_0}}\right)\partial_t+\left(\frac{r^2Z}{2}+\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\,\partial_r\right)\right\}\cos\theta-\left(\frac{r}{2}Z-\frac{1}{r}\int\frac{\sqrt{T_0}}{T_1}\mathrm{d}t\right)\sin\theta\partial_\theta\right].$$

For the value of $k=-1$, the four proper MCs are

$$\xi_{(7)}=\frac{1}{T_1}(\sqrt{T_0}\coth r\partial_t-T_2Z\partial_r)\csc hr,$$

$$\begin{aligned}\xi_{(8)}=&\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t+Z\sinh r\cosh r\partial_r\right)\sin\theta\sin\phi-Z(\cos\theta\sin\phi\partial_\theta+\csc\theta\cos\phi\partial_\phi)\right]\csc hr,\\ \xi_{(9)}=&\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t+Z\sinh r\cosh r\partial_r\right)\sin\theta\cos\phi-Z(\cos\theta\cos\phi\partial_\theta-\csc\theta\sin\phi\partial_\phi)\right]\csc hr,\end{aligned}\tag{47}$$

$$\xi_{(10)}=\left[\left(\frac{T_2}{T_0}\dot{Z}\partial_t+Z\sinh r\cosh r\partial_r\right)\cos\theta-Z\partial_\theta\right]\csc hr.$$

Thus we obtain ten independent MCs for each value of k in which six are the usual isometries of FRW metric and the the remaining four are the proper MCs.

For the case (bi), we must require that $k\neq 0$. When $k=1$, we obtain one proper MC given by

$$\xi_{(7)}=\frac{T_2}{\sqrt{T_0}a}\csc^2 r\partial_t.\tag{48}$$

For $k=-1$, proper MC is

$$\xi_{(7)}=\frac{T_2}{\sqrt{T_0}a}\csc h^2 r\partial_t.\tag{49}$$

This case gives seven independent MCs in which six are nonproper and one is proper MC. It can be checked that the case (bii) gives six independent MCs for each value of k which are usual KVs of FRW space–times. Similarly, case (6b) can be solved to give either six, seven, or ten MCs.

B. MCs of the space–times admitting SO(3) as the maximal isometry group

In this section, we evaluate MCs of the spherically symmetric space–times which admit SO(3) as the maximal isometry group. In these solutions, we take any additional MC (if it exists) to be orthogonal to the SO(3) orbit. For this we must require that $A_i \equiv 0$ and consequently, it follows from Eqs. (17) to (20) that $\xi^0 = \xi^0(t,r)$, $\xi^1 = \xi^1(t,r)$, $\xi^2 = 0$, $\xi^3 = 0$. It is mentioned here that we are considering only diagonal metrics for this case. The nondiagonal metrics can be solved in a similar way. If we make use of the following substitutions

$$\frac{T_2}{T_0}A_4 = C(t,r), \quad \frac{T_2}{T_1}A_5 = D(t,r), \quad \sqrt{T_0} = A(t,r), \quad \sqrt{T_1} = B(t,r)$$

in the constraint Eqs. (21)–(28), then it follows that

$$\dot{C} = -\dot{A}C - A'D, \tag{50}$$

$$A^2C' + B^2\dot{D} = 0, \tag{51}$$

$$D' = -\dot{B}C - B'D, \tag{52}$$

$$\dot{T}_2 C + T_2' D = 0. \tag{53}$$

To solve this system of equations, we have the following possibilities:

$$\text{(i)} \quad \dot{T}_2 = 0, \quad T_2' \neq 0, \quad \text{(ii)} \quad \dot{T}_2 \neq 0, \quad T_2' = 0,$$

$$\text{(iii)} \quad \dot{T}_2 \neq 0, \quad T_2' \neq 0, \quad \text{(iv)} \quad \dot{T}_2 = 0, \quad T_2' = 0.$$

The first possibility does not provide any proper MC if we assume that $\dot{T}_1 \neq 0$. However, the assumption $\dot{T}_1 = 0$, $\dot{T}_0 \neq 0$ gives infinite dimensional MCs.

The second case shows that there does not exist a proper MC with the constraint $T_0' \neq 0$ but the constraints $T_0' = 0$, $T_1' \neq 0$ provide infinite dimensional MCs.

In the third case, when

$$T_0 T_2' \left[\frac{T_1' \dot{T}_2 - \dot{T}_1 T_2'}{2\sqrt{T_1}\dot{T}_2} + \left\{ \ln\left(\frac{\dot{T}_2}{T_2'} \right) \right\}' \right] + T_1 \dot{T}_2 \left[\frac{T_0' \dot{T}_2 - \dot{T}_0 T_2'}{2\sqrt{T_0}T_2'} + \left\{ \ln\left(\frac{\dot{T}_2}{T_2'} \right) \right\}^{\cdot} \right] \neq 0,$$

we do not have a proper MC. However, if

$$T_0 T_2' \left[\frac{T_1' \dot{T}_2 - \dot{T}_1 T_2'}{2\sqrt{T_1}\dot{T}_2} + \left\{ \ln\left(\frac{\dot{T}_2}{T_2'} \right) \right\}' \right] + T_1 \dot{T}_2 \left[\frac{T_0' \dot{T}_2 - \dot{T}_0 T_2'}{2\sqrt{T_0}T_2'} + \left\{ \ln\left(\frac{\dot{T}_2}{T_2'} \right) \right\}^{\cdot} \right] = 0.$$

and

$$\left(\frac{T_0' \dot{T}_2 - \dot{T}_0 T_2'}{2\sqrt{T_0}\dot{T}_2} \right)' = \left[\frac{T_2'}{\dot{T}_2} \left\{ \frac{\dot{T}_1 T_2' - T_1' \dot{T}_2}{2\sqrt{T_1}T_2'} - \left(\frac{\dot{T}_2}{T_2'} \right)' \right\} \right]^{\cdot}$$

then there exists a proper MC given by

$$\exp\left(\int \frac{T_0' \dot{T}_2 - \dot{T}_0 T_2'}{2\sqrt{T_0}\dot{T}_2} \mathrm{d}t \right) \left(\partial_t - \frac{\dot{T}_2}{T_2'} \partial_r \right). \tag{54}$$

If

$$\left(\frac{T_0'\dot{T}_2-\dot{T}_0T_2'}{2\sqrt{T_0}\dot{T}_2}\right)'\neq\left[\frac{T_2'}{\dot{T}_2}\left\{\frac{\dot{T}_1T_2'-T_1'\dot{T}_2}{2\sqrt{T_1}T_2'}-\left(\frac{\dot{T}_2}{T_2'}\right)'\right\}\right]^{\cdot}$$

then this case gives infinite number of MCs.

In the last case, we solve Eqs. (50)–(52), which imply that $\dot{A}B'-A'\dot{B}\equiv\psi(t,r)$. If $\psi=0$, then we must have $\dot{C}=0=D'$ for a nontrivial solution. Thus the constraints $\dot{T}_0T_1'-T_0'\dot{T}_1=0$ together with

$$T_0'\neq 0,\ \left[\frac{T_1}{T_0}\left(\frac{\dot{T}_1}{T_0'}\right)^{\cdot}\right]^{\cdot}=0,$$

yield the following proper MC:

$$\exp\left(\int\frac{T_1}{T_0}\left(\frac{\dot{T}_0}{T_0'}\right)^{\cdot}dr\right)\left(\partial_t-\frac{\dot{T}_0}{T_0'}\partial_r\right). \tag{55}$$

However, for $\dot{T}_0T_1'-T_0'\dot{T}_1=0$ together with

$$T_0'=0,\ T_1'\neq 0,\ \left[\frac{T_1}{T_0}\left(\frac{\dot{T}_1}{T_1'}\right)^{\cdot}\right]^{\cdot}=0,$$

we obtain the proper MC given by

$$\exp\left(\int\frac{T_1}{T_0}\left(\frac{\dot{T}_1}{T_1'}\right)^{\cdot}dr\right)\left(\partial_t-\frac{\dot{T}_1}{T_1'}\partial_r\right). \tag{56}$$

The constraint $\dot{T}_0T_1'-T_0'\dot{T}_1=0$ along with $T_0'=0$, $T_1'=0=\dot{T}_1$, $\dot{T}_0\neq 0$ gives infinite many MCs.

For $\psi\neq 0$, we must have $\dot{C}\neq 0$, $D'\neq 0$ for a nontrivial solution. Let us express $\dot{C}$ and D' as E and F, respectively, so that

$$C=-\frac{B'}{\psi}E(t,r)+\frac{A'}{\psi}F(t,r), \tag{57}$$

$$D=\frac{\dot{B}}{\psi}E(t,r)-\frac{\dot{A}}{\psi}F(t,r). \tag{58}$$

We obtain two linearly independent MCs which are orthogonal to $T_e(\mathrm{SO}(3))$ and are given by

$$X_1=\frac{E}{\psi}(-B'\partial_t+\dot{B}\partial_r), \tag{59}$$

$$X_2=\frac{F}{\psi}(A'\partial_t-\dot{A}\partial_r). \tag{60}$$

The Lie bracket of these vector fields is

$$[X_1,X_2]=\frac{F(\dot{A}E'-A'\dot{E})}{E\psi}X_1+\frac{E(\dot{B}F'-B'\dot{F})}{F\psi}X_2. \tag{61}$$

For its closedness, we must have $F(\dot{A}E'-A'\dot{E})/E\psi=a_1$ and $E(\dot{B}F'-B'\dot{F})/F\psi=a_2$, where a_1 and a_2 are constants. From here we have either (i) $a_1\neq 0$, $a_2=0$, or (ii) $a_1=0$, $a_2\neq 0$ or (iii) $a_1=0=a_2$. The first two possibilities contradict the assumption that $\psi\neq 0$. This shows that the third possibility closes the Lie algebra. Thus we have

$$C'=\frac{B^2}{A^2A'^2+B^2\dot{A}^2}[\{A'(\ddot{A}-\dot{A}^2)-\dot{A}(\dot{A}'-A'\dot{B})\}C+\{A'(\dot{A}'-\dot{A}A')-\dot{A}(A''-A'B')\}D], \tag{62}$$

$$\dot{D}=-\frac{A^2}{A^2A'^2+B^2\dot{A}^2}[\{A'(\ddot{A}-\dot{A}^2)-\dot{A}(\dot{A}'-A'\dot{B})\}C+\{A'(\dot{A}'-\dot{A}A')-\dot{A}(A''-A'B')\}D], \tag{63}$$

along with the compatibility constraint in the components T_0 and T_1 of the energy–momentum tensor given by

$$\left(\ln\frac{A'}{\dot{A}}e^{A-B}\right)'\left(\ln\frac{\dot{B}}{B'}e^{B-A}\right)-\left(\ln\frac{A'}{\dot{A}}e^{A-B}\right)\left(\ln\frac{\dot{B}}{B'}e^{B-A}\right)'=0. \tag{64}$$

IV. MATTER COLLINEATIONS IN THE DEGENERATE CASE

In this section only those cases will be considered for which the energy–momentum tensor is degenerate, i.e., $\det(T_{ab})=0$.

A. MCs of the manifolds admitting higher symmetries

Here we would discuss the MCs of the manifolds admitting higher symmetries than SO(3). For higher symmetries, all metrics have $T_{01}=0$ except the case (3) of the last section. Thus we would discuss the space–times for which $T_{01}=0$ and $\det(T_{ab})=0$, i.e., when at least one of the T_a or their combination is zero. It can be shown that for $T_1=0$, $T_k\neq 0$, $k=0,2$ [case (1) of Sec. III], we obtain infinite dimensional MCs. The solution for $T_0=0$, $T_l\neq 0$, $l=1,2$ [case (2) of Sec. III] also gives infinite dimensional MCs. These have been discussed in detail elsewhere.[14] Here we are interested in exploring the possibilities of finite MCs.

When $T_k'\neq 0$, $(T_0/T_2)'\neq 0$, we obtain four MCs which are the usual KVs of the spherical symmetry. For $T_k'\neq 0$, $(T_0/T_2)'=0$, we obtain ten independent MCs. These are

$$\begin{aligned}\xi^0&=\beta[(\dot{g}_1\sin\phi-\dot{g}_2\cos\phi)\sin\theta+\dot{g}_3\cos\theta]+c_0, \quad \xi^1=0,\\ \xi^2&=-(g_1\sin\phi-g_2\cos\phi)\cos\theta+g_3\sin\theta+c_1\sin\phi-c_2\cos\phi,\\ \xi^3&=-(g_1\cos\phi+g_2\sin\phi)\csc\theta+(c_1\cos\phi+c_2\sin\phi)\cot\theta+c_3,\end{aligned} \tag{65}$$

where $\beta=T_2/T_0\neq 0$ is an arbitrary constant and the function g satisfies the following constraint:

$$\beta\ddot{g}_i(t)-g_i(t)=0. \tag{66}$$

The solution for the nonstatic case can be obtained trivially, which turns out to be the same with different constraints.

B. MCs of the manifolds admitting SO(3) as the maximal isometry group

The metrics which admit SO(3) as the maximal symmetry group yield $\xi^2=0=\xi^3$ and the MC equations reduce to six independent equations which involve

TABLE I. MCs of case (1) for the nondegenerate case admitting higher symmetries. Notice that MCs for the case (2) are the same as for the case (1) which can be obtained trivially by using the transformations given in the Sec. III.

Cases	MCs	Constraints
1ai	4	$\left[\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\right]'\neq 0$
1aii	6	$\left[\frac{T_0}{\sqrt{T_1}}\left(\frac{T_0'}{2T_0\sqrt{T_1}}\right)'\right]'=0$
1bi	4	$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1\neq 0$
1bii	7	$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1=0,\quad \left(\frac{T_2'}{\sqrt{T_0T_1T_2}}\right)'\neq 0$
1biii	4	$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1=0,\quad \left(\frac{T_2'}{\sqrt{T_0T_1T_2}}\right)'=0,\quad \left(\frac{T_0'}{T_2}\right)'\neq 0$
1biv	10	$\frac{T_2}{\sqrt{T_1}}\left(\frac{T_2'}{2T_2\sqrt{T_1}}\right)'+1=0,\quad \left(\frac{T_2'}{\sqrt{T_0T_1T_2}}\right)'=0,\quad \left(\frac{T_0'}{T_2}\right)'=0$

$$\dot{T}_{22}\xi^0+T_{22}'\xi^1=0. \tag{67}$$

This gives rise to the following four cases:

$$\text{(i)}\quad \dot{T}_{22}=0,\ T_{22}'\neq 0,\quad \text{(ii)}\quad \dot{T}_{22}\neq 0,\ T_{22}'=0,$$

$$\text{(iii)}\quad \dot{T}_{22}\neq 0,\ T_{22}'\neq 0,\quad \text{(iv)}\quad \dot{T}_{22}=0,\ T_{22}'=0.$$

If we solve these cases, we may have interesting physical consequences. These will be discussed somewhere else.

V. CONCLUSION

In this paper, we have attempted to classify the most general spherically symmetric space–times according to their MCs. We have found a general solution of the MC equations for the nondegenerate, diagonal, and nondiagonal energy–momentum tensor. Further, we have classified space–times admitting higher symmetries than SO(3) and those which admit SO(3) as the maximal isometry group for both nondegenerate and degenerate cases. It is found that for the nondegenerate and degenerate cases, we recover the earlier known results[14] as a special case. We also obtain some interesting missing results in the earlier work. It is mentioned here that MCs found here coincide with *RCs* but the constraints are entirely different. The summary of the results can be given below in Tables I–IV.

It can be seen from Tables I–IV that each case has different constraints on the energy–momentum tensor. It would be interesting to solve these constraints or at least examples should be constructed to check the dimensions of the MCs. We are able to classify MCs of the space–times with SO(3) as the maximal isometry group only for the nondegenerate case. However, it needs to be completed for the degenerate case. Also, case (3) of Sec. III admitting higher symmetries is kept open. These would be discussed in a separate work.

TABLE II. MCs of cases (4), (5), (6) for the nondegenerate case admitting higher symmetries. It is noted here that the cases (4), (5) and (6a) describe FRW metrics and (6b) FRW-like metrics and have the same MCs in all cases as given below.

Cases	MCs	Constraints
4ai	10	$\frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)^{\cdot}-k=0, \quad \dot{T}_1=0$
4aii	10	$\frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)^{\cdot}-k=0, \quad \dot{T}_1\neq 0$
4bi	7	$\frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)^{\cdot}-k\neq 0, \quad \dot{T}_1\neq 0$
4bii	6	$\frac{T_1}{\sqrt{T_0}}\left(\frac{\dot{T}_2}{2T_1\sqrt{T_0}}\right)^{\cdot}-k\neq 0, \quad \dot{T}_1\neq 0$

TABLE III. MCs for the nondegenerate case admitting SO(3) as the maximal symmetry.

Cases	MCs	Constraints
ia	No proper	$\dot{T}_2=0,\ T_2'\neq 0,\ \dot{T}_1\neq 0$
ib	Infinite No. of MCs	$\dot{T}_2=0,\ T_2'\neq 0,\ \dot{T}_1=0,\ \dot{T}_0\neq 0$
iia	No proper	$\dot{T}_2\neq 0,\ T_2'=0,\ T_0'\neq 0$
iib	Infinite No. of MCs	$\dot{T}_2\neq 0,\ T_2'=0,\ T_0'=0,\ T_1'\neq 0$
iiia	No proper	$\dot{T}_2\neq 0,\ T_2'\neq 0,\ T_0T_2'\left[\frac{T_1'\dot{T}_2-\dot{T}_1T_2'}{2\sqrt{T_1}\dot{T}_2}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}'\right]+T_1\dot{T}_2\left[\frac{T_0'\dot{T}_2-\dot{T}_0T_2'}{2\sqrt{T_0}T_2'}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}^{\cdot}\right]\neq 0$
iiib	One proper	$\dot{T}_2\neq 0,\ T_2'\neq 0,\ T_0T_2'\left[\frac{T_1'\dot{T}_2-\dot{T}_1T_2'}{2\sqrt{T_1}\dot{T}_2}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}'\right]+T_1\dot{T}_2\left[\frac{T_0'\dot{T}_2-\dot{T}_0T_2'}{2\sqrt{T_0}T_2'}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}^{\cdot}\right]=0,$ $\left(\frac{T_0'\dot{T}_2-\dot{T}_0T_2^0}{2\sqrt{T_0}\dot{T}_2}\right)'=\left[\frac{T_2'}{\dot{T}_2}\left\{\frac{\dot{T}_1T_2'-T_1'\dot{T}_2}{2\sqrt{T_1}T_2'}-\left(\frac{\dot{T}_2}{T_2'}\right)'\right\}\right]^{\cdot}$
iiic	Infinite No. of MCs	$\dot{T}_2\neq 0,\ T_2'\neq 0,\ T_0T_2'\left[\frac{T_1'\dot{T}_2-\dot{T}_1T_2'}{2\sqrt{T_1}\dot{T}_2}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}'\right]+T_1\dot{T}_2\left[\frac{T_0'\dot{T}_2-\dot{T}_0T_2'}{2\sqrt{T_0}T_2'}+\left\{\ln\left(\frac{\dot{T}_2}{T_2'}\right)\right\}^{\cdot}\right]=0,$ $\left(\frac{T_0'\dot{T}_2-\dot{T}_0T_2^0}{2\sqrt{T_0}\dot{T}_2}\right)'\neq\left[\frac{T_2'}{\dot{T}_2}\left\{\frac{\dot{T}_1T_2'-T_1'\dot{T}_2}{2\sqrt{T_1}T_2'}-\left(\frac{\dot{T}_2}{T_2'}\right)'\right\}\right]^{\cdot}$
iva	One proper	$\dot{T}_2=0,\ T_2'=0,\ \dot{T}_0T_1'-T_0'\dot{T}_1=0,\ T_0'\neq 0,\ \left[\frac{T_1}{T_0}\left(\frac{\dot{T}_1}{T_0'}\right)^{\cdot}\right]^{\cdot}=0$
ivb	One proper	$\dot{T}_2=0,\ T_2'=0,\ \dot{T}_0T_1'-T_0'\dot{T}_1=0,\ T_0'=0,\ T_1'\neq 0,\ \left[\frac{T_1}{T_0}\left(\frac{\dot{T}_1}{T_0'}\right)^{\cdot}\right]^{\cdot}=0$
ivc	Infinite No. MCs	$\dot{T}_2=0,\ T_2'=0,\ \dot{T}_0T_1'-T_0'\dot{T}_1=0,\ T_0'=0,$ $T_1'=0=\dot{T}_1,\ \dot{T}_0\neq 0$

TABLE IV. MCs of degenerate case admitting higher symmetries.

Cases	MCs	Constraints
*	4	$T_k'\neq 0, \quad \left(\frac{T_0}{T_1}\right)'\neq 0$
**	10	$T_k'\neq 0, \quad \left(\frac{T_0}{T_1}\right)'=0$

ACKNOWLEDGMENTS

I would like to thank the Ministry of Science and Technology (MOST), Pakistan for providing a postdoctoral fellowship at the University of Aberdeen, UK. I also appreciate the comments given by Professor G.S. Hall during its write up.

APPENDIX A

The surviving components of the Ricci tensor are

$$R_{00}=\tfrac{1}{4}e^{\nu-\mu}(2\nu''+\nu'^2-\nu'\mu'+2\nu'\lambda')-\tfrac{1}{4}(2\ddot{\mu}+\dot{\mu}^2-\dot{\nu}\dot{\mu}+4\ddot{\lambda}+2\dot{\lambda}^2-2\dot{\nu}\dot{\lambda}),$$

$$R_{01}=-\tfrac{1}{2}(2\dot{\lambda}'+\dot{\lambda}\lambda'-\nu'\dot{\lambda}-\dot{\mu}\lambda'),$$

$$R_{11}=\tfrac{1}{4}e^{\mu-\nu}(2\ddot{\mu}+\dot{\mu}^2-\dot{\nu}\dot{\mu}+2\dot{\mu}\dot{\lambda})-\tfrac{1}{4}(2\nu''+\nu'^2-\nu'\mu'+4\lambda''+2\lambda'^2-2\mu'\lambda'), \quad \text{(A1)}$$

$$R_{22}=\tfrac{1}{4}e^{\lambda-\nu}(2\ddot{\lambda}+2\dot{\lambda}^2-\dot{\nu}\dot{\lambda}+\dot{\mu}\dot{\lambda})-\tfrac{1}{4}e^{\lambda-\mu}(2\lambda''+2\lambda'^2-\mu'\lambda'+\nu'\lambda')+1,$$

$$R_{33}=R_{22}\sin^2\theta.$$

The Ricci scalar is given by

$$R=\tfrac{1}{2}e^{-\mu}(2\nu''+\nu'^2-\nu'\mu'+2\nu'\lambda'-2\mu'\lambda'+3\lambda'^2+4\lambda'')-2e^{-\lambda}$$
$$-\tfrac{1}{2}e^{-\nu}(2\ddot{\mu}+\dot{\mu}^2-\dot{\nu}\dot{\mu}-2\dot{\nu}\dot{\lambda}+2\dot{\mu}\dot{\lambda}+3\dot{\lambda}^2+4\ddot{\lambda}). \quad \text{(A2)}$$

Using Einstein field equations (1), the nonvanishing components of energy–momentum tensor T_{ab} are

$$T_{00}=\tfrac{1}{4}(\dot{\lambda}^2+2\dot{\mu}\dot{\lambda})-\tfrac{1}{4}e^{\nu-\mu}(4\lambda''+3\lambda'^2-2\mu'\lambda')+e^{\nu-\lambda}, \quad T_{01}=R_{01},$$

$$T_{11}=\tfrac{1}{4}(\lambda'^2+2\nu'\lambda')-\tfrac{1}{4}e^{\mu-\nu}(4\ddot{\lambda}+3\dot{\lambda}^2-2\dot{\nu}\dot{\lambda})-e^{\mu-\lambda},$$
$$T_{22}=\tfrac{1}{4}e^{\lambda-\mu}(2\nu''+\nu'^2-\nu'\mu'+\nu'\lambda'-\mu'\lambda'+\lambda'^2+2\lambda'') \quad \text{(A3)}$$
$$-\tfrac{1}{4}e^{\lambda-\nu}(2\ddot{\mu}+\dot{\mu}^2-\dot{\nu}\dot{\mu}-\dot{\nu}\dot{\lambda}+\dot{\mu}\dot{\lambda}+\dot{\lambda}^2+2\ddot{\lambda}),$$

$$T_{33}=T_{22}\sin^2\theta.$$

APPENDIX B

The nonvanishing components of the Ricci tensor for FRW space–times are given by

$$R_0=-3\frac{\ddot{R}}{R},$$

$$R_1=\frac{(R^3)^{\cdot\cdot}}{3R}-2k,$$

$$R_2=R_1\Sigma^2(k,r), \quad \text{(B1)}$$

$$R_3=R_2\sin^2\theta,$$

where

$$\Sigma(k,r)=\sin r, \quad \text{for } k=1,$$
$$=r, \quad \text{for } k=0,$$
$$=\sinh r, \quad \text{for } k=-1.$$

The Ricci scalar is given by

$$R=-\frac{6}{R^2}(R\ddot{R}+\dot{R}^2-k). \tag{B2}$$

Now, the surviving components of energy–momentum tensor for FRW space–times are given by

$$T_0=\frac{3}{R^2}(\dot{R}^2-k),$$
$$T_1=-(2R\ddot{R}+\dot{R}^2)+k,$$
$$T_2=T_1\Sigma^2(k,r), \tag{B3}$$
$$T_3=T_2\sin^2\theta.$$

APPENDIX C

Linearly independent KVs associated with the FRW space–times are given by Ref. 24 for $k=1$,

$$\xi_{(1)}=\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi,$$
$$\xi_{(2)}=\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi,$$
$$\xi_{(3)}=\partial_\phi,$$
$$\xi_{(4)}=(\sin\theta\partial_r+\cot r\cos\theta\partial_\theta)\sin\phi+\cot r\csc\theta\cos\phi\partial_\phi, \tag{C1}$$
$$\xi_{(5)}=(\sin\theta\partial_r+\cot r\cos\theta\partial_\theta)\cos\phi-\cot r\csc\theta\sin\phi\partial_\phi,$$
$$\xi_{(6)}=\cos\theta\partial_r-\cot r\sin\theta\partial_\theta.$$

For $k=0$, we have

$$\xi_{(1)}=\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi,$$
$$\xi_{(2)}=\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi,$$
$$\xi_{(3)}=\partial_\phi,$$
$$\xi_{(4)}=\left(\sin\theta\partial_r+\frac{1}{r}\cos\theta\partial_\theta\right)\sin\phi+\frac{1}{r}\csc\theta\cos\phi\partial_\phi, \tag{C2}$$
$$\xi_{(5)}=\left(\sin\theta\partial_r+\frac{1}{r}\cos\theta\partial_\theta\right)\cos\phi-\frac{1}{r}\csc\theta\sin\phi\partial_\phi,$$
$$\xi_{(6)}=\left(\cos\theta\partial_r-\frac{1}{r}\sin\theta\partial_\theta\right).$$

For $k=-1$,

$$\xi_{(1)}=\sin\phi\partial_\theta+\cot\theta\cos\phi\partial_\phi,$$

$$\xi_{(2)}=\cos\phi\partial_\theta-\cot\theta\sin\phi\partial_\phi,$$

$$\xi_{(3)}=\partial_\phi,$$

$$\xi_{(4)}=(\sin\theta\partial_r+\coth r\cos\theta\partial_\theta)\sin\phi+\coth r\csc\theta\cos\phi\partial_\phi, \tag{C3}$$

$$\xi_{(5)}=(\sin\theta\partial_r+\coth r\cos\theta\partial_\theta)\cos\phi-\coth r\csc\theta\sin\phi\partial_\phi,$$

$$\xi_{(6)}=\cos\theta\partial_r-\coth r\sin\theta\partial_\theta.$$

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A further solvable three-body problem in the plane

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(Received 11 April 2003; accepted 1 July 2003)

The solution is provided of a three-body problem in the plane, which is the third of a trio recently identified as likely to display a particularly simple time-evolution hence to be amenable to exact treatment. This conjecture, already validated by providing the solution of the first two of these three models, is now completely proven by exhibiting the solution of the third. This finding also demonstrates the conjectured super-Painlevé character of certain nonlinear ordinary differential equations, namely, the fact that their *general* solution is an *entire* function of the independent variable. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1610778]

I. INTRODUCTION

Recently the N-body problem in the plane characterized by the Newtonian equations of motion

$$\ddot{\vec{r}}_n = \omega \hat{k} \wedge \dot{\vec{r}}_n + 2 \sum_{m=1, m \neq n}^{N} r_{nm}^{-2} (\alpha_{nm} + \tilde{\alpha}_{nm} \hat{k} \wedge) \cdot [\dot{\vec{r}}_n (\dot{\vec{r}}_m \cdot \vec{r}_{nm}) + \dot{\vec{r}}_m (\dot{\vec{r}}_n \cdot \vec{r}_{nm}) - \vec{r}_{nm} (\dot{\vec{r}}_m \cdot \dot{\vec{r}}_m)] \quad (1)$$

has been much investigated.[1–7] Here the N two-vectors $\vec{r}_n \equiv \vec{r}_n(t)$ identify the positions, as funtions of the (real) time variable t, of the moving point-particles in a plane which for notational convenience is immersed in three-dimensional space, so that $\vec{r}_n \equiv (x_n, y_n, 0)$; $\hat{k}$ is the unit three-vector orthogonal to that plane, $\hat{k} \equiv (0,0,1)$, so that $\hat{k} \wedge \vec{r}_n \equiv (-y_n, x_n, 0)$; $\vec{r}_{nm} \equiv \vec{r}_n - \vec{r}_m$, hence $r_{nm}^2 \equiv \vec{r}_{nm} \cdot \vec{r}_{nm} \equiv (x_n - x_m)^2 + (y_n - y_m)^2$; superimposed dots denote of course time derivatives; ω is a *positive* constant, which sets the time scale and to which we associate the period

$$T = \frac{2\pi}{\omega}; \quad (2)$$

and the "coupling constants" $\alpha_{nm}, \tilde{\alpha}_{nm}$ are *a priori* arbitrary (of course *real*; a sufficient condition for this system to be Hamiltonian[2] is the requirement that these constants be symmetrical in their two indices, $\alpha_{nm} = \alpha_{mn}, \tilde{\alpha}_{nm} = \tilde{\alpha}_{mn}$, as we hereafter assume). Note that, in the special case without two-body forces ($\alpha_{nm} = \tilde{\alpha}_{nm} = 0$) this N-body problem describes N (equal) charged particles, not interacting among themselves, moving on a plane in the presence of a constant magnetic field

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orthogonal to that plane (''cyclotron''); all solutions are then *completely periodic* with period T, see (2), since each particle moves with such a period on its circular trajectory (the center and radius of which are determined by its initial position and velocity).

To treat the N-body problem (1) it is generally convenient to identify the *real* ''physical'' plane on which the N points $\vec{r}_n \equiv (x_n, y_n, 0)$ move, with the *complex* plane in which the complex numbers $z_n \equiv x_n + i\, y_n$ move. Indeed via this correspondence these equations of motion (1) take the following neater form:

$$\ddot{z}_n - i\,\omega\,\dot{z}_n = 2 \sum_{m=1, m\neq n}^{N} a_{nm} \frac{\dot{z}_n\,\dot{z}_m}{z_n - z_m} \tag{3}$$

with

$$a_{nm} = \alpha_{nm} + i\,\tilde{\alpha}_{nm}\,. \tag{4}$$

Then one notes that, via the change of independent variable

$$z_n(t) = \zeta_n(\tau), \tag{5a}$$

$$\tau \equiv \tau(t) = \frac{\exp(i\omega t) - 1}{i\,\omega}, \tag{5b}$$

the equations of motion (3) become

$$\zeta_n'' = 2 \sum_{m=1, m\neq n}^{N} a_{nm} \frac{\zeta_n'\,\zeta_m'}{\zeta_n - \zeta_m}. \tag{6}$$

Here and generally below primes denote of course differentiations with respect to the (complex) independent variable τ. Note that this change of independent variable (5) implies that the *complex* variable $\tau(t)$ is a periodic function of the *real* variable t (time) with period T [see (2)], and moreover it entails the following very simple relations among the initial data for z_n and ζ_n:

$$z_n(0) = \zeta_n(0), \quad \dot{z}_n(0) = \zeta_n'(0). \tag{7}$$

Hence to obtain the solution of the equations of motion (3), namely of the Newtonian equations of motion (1), one can instead solve, with the *same* initial conditions [see (7)], the equations of motion (6), and then use the change of independent variable (5) to obtain the desired solution of the equations of motion (3). And this clearly implies that, if the solution $\zeta_n(\tau)$ of the equations of motion (6) is *meromorphic* in the complex variable τ, the corresponding solution $z_n(t)$ of the equations of motion (3), namely of the Newtonian equations of motion (1), is *completely periodic* with period T, see (2); unless one of the poles of the meromorphic solution $\zeta_n(\tau)$ of the equations of motion (6) happens to fall exactly on the circle with center at $\tau = i/\omega$ and radius $1/\omega$ in the complex τ-plane, which is traveled counterclockwise by the complex variable τ as the real variable t evolves from the initial condition at $t = 0$, in which case the time evolution hits a singularity: this corresponds to the (special) motions of the N-body problem in the plane characterized by the Newtonian equations of motion (1) in which a singularity occurs in the time evolution, generally corresponding to a particle collision.

It is therefore of interest to identify the particular N-body systems of type (3), characterized by a special choice of the number of particles N and of the coupling constants a_{nm}, see (4), such that the corresponding equations (6) *only* possess solutions $\zeta_n(\tau)$ that are *meromorphic* in τ, or even more remarkably, that *only* possess solutions which are *entire* in τ. In the first case [''*all* solutions $\zeta_n(\tau)$ of (6) are *meromorphic*''] one can then assert that these equations of motion (6) are endowed with the *Painlevé property*; in the second case [''*all* solutions $\zeta_n(\tau)$ of (6) are *entire*''] one can then assert that the equations of motion (6) are endowed with the *super-Painlevé property*.[3]

Note that the corresponding "physical" N-body systems in the plane (1) *only* possess solutions which are *completely periodic* with period T, see (2), except for the special cases of motions that run into singularities (generally due to particle collisions) in the first case, without any exception in the second case. Hence such systems (1) provide examples of *nonlinear harmonic oscillators*.[7]

On the basis of the local analysis of the singularities of the solutions $\zeta_n(\tau)$ of the equations of motion (6) made in Ref. 6, the conjecture has been proffered[3] that, in the context of the three-body problem ($N=3$), and excluding the cases in which two of the three constants a_{nm} vanish (when the three-body problem reduces to a two-body problem), there are altogether 11 cases (corresponding, up to permutations, to 11 different assignments of the triple of coupling constants $a_{12}=a_{21}$, $a_{23}=a_{32}$, $a_{31}=a_{13}$) in which the equations of motion (6) are *Painlevé*, and out of these 11 cases there are three which are *super-Painlevé*. In this paper we focus on the latter three cases, in particular on the one not hitherto solved.

The first *super-Painlevé* case is characterized by equations of motion (6) (with $N=3$) with one vanishing coupling constant and the other two equal to minus one-half, say (of course up to permutations) $a_{12}=a_{21}=0$, $a_{23}=a_{32}=a_{31}=a_{13}=-1/2$. In this case *all* solutions $\zeta_n(\tau)$ of the equations of motion (6) (have been obtained[3] and) are indeed *polynomial* in τ.

The second *super-Painlevé* case is characterized by equations of motion (6) (with $N=3$) with all three coupling constants equal to minus one-half, $a_{12}=a_{21}=a_{23}=a_{32}=a_{31}=a_{13}=-1/2$. In this case *all* solutions $\zeta_n(\tau)$ of the equations of motion (6) (have as well been obtained[4] and) are indeed *exponential* in τ [up to degeneracies, which yield a *polynomial* behavior, and up to the center-of-mass motion, which is of course uniform, see (6)].

The third case is characterized by equations of motion (6) (with $N=3$) with one vanishing coupling constant, one equal to minus one-half and one equal to minus unity, say (of course up to permutations)

$$a_{12}=a_{21}=0, \quad a_{23}=a_{32}=-1/2, \quad a_{31}=a_{13}=-1. \tag{8}$$

This is the case treated in this paper, where we obtain in rather explicit form its *general* solution $\zeta_n(\tau)$, and we prove that it is indeed *entire* in the complex variable τ. These results are detailed in the following Sec. II. The proof of these results is provided in Sec. III, and some final remarks are in Sec. IV.

Let us end this introductory section by recalling that, in the case with all coupling constants equal to unity, $a_{nm}=1$, the N-body problem characterized by the equations of motion (6)—hence as well that characterized by the equations of motion (3) [or equivalently by (1) with $\alpha_{nm}=1$, $\tilde{\alpha}_{nm}=0$, see (4)]—is *completely integrable* indeed *solvable*;[2] in this case the solutions $\zeta_n(\tau)$ of the equations of motion (6) feature however a finite number of square-root branch points, hence this integrable case is not Painlevé. The remarkable characteristics of this *integrable*, indeed *solvable* (see, for instance, Ref. 2), model suggested to call it a "goldfish,"[1] and it was subsequently suggested that this name be attributed to the general model (1) with arbitrary coupling constants, which also displays a very interesting phenomenology.[6]

II. RESULTS

In this section we exhibit the solution of the initial-value problem for the equations of motion (6) with $N=3$ and the assignment (8) of the coupling constants.

Let

$$\zeta_1(\tau)=x(\tau)+Z(\tau), \quad \zeta_2(\tau)=y(\tau)+Z(\tau), \quad \zeta_3(\tau)=-x(\tau)-y(\tau)+Z(\tau), \tag{9}$$

which entails that Z is the center-of-mass coordinate,

$$Z=\tfrac{1}{3}(\zeta_1+\zeta_2+\zeta_3), \tag{10}$$

hence, as clearly implied by the equations of motion (6), it moves uniformly

$$Z''=0, \quad Z(\tau)=Z(0)+Z'(0)\,\tau=Z(0)+V\,\tau. \tag{11}$$

Here and hereafter we indicate with

$$V=\tfrac{1}{3}[\zeta_1'(0)+\zeta_2'(0)+\zeta_3'(0)] \tag{12}$$

the (of course τ-independent) center-of-mass speed.

We now assert (and in the following section we prove) that $x(\tau)$ is given, in terms of $y(\tau)$, by the following formula:

$$x(\tau)=-2\,y(\tau)+[y'(\tau)+V]\,(\tau-\tau_0), \tag{13}$$

with the constant τ_0 (here and below) given in terms of the initial data by the formula

$$\tau_0=\frac{\zeta_3(0)-\zeta_2(0)}{\zeta_2'(0)}. \tag{14}$$

We moreover assert (and in the following section we prove) that $y(\tau)$ is given by the following formulas:

$$y(\tau)=2\,V\,(\tau-\tau_0)+F(\alpha_0,\alpha_1,\alpha_2;K;\tau-\tau_0), \tag{15a}$$

$$F(\alpha_0,\alpha_1,\alpha_2;K;z)=\alpha_0\,F^{(0)}(K;z)+\alpha_1\,F^{(1)}(K;z)+\alpha_2\,F^{(2)}(K;z), \tag{15b}$$

where the three constants $\alpha_0,\alpha_1,\alpha_2$ can be adjusted to fit the initial data, the constant K is given in terms of these data as follows:

$$K=\frac{\zeta_1'(0)\;\zeta_2'(0)\;\zeta_3'(0)}{[\zeta_3(0)-\zeta_2(0)][\zeta_3(0)-\zeta_1(0)]^2}, \tag{16}$$

and the three functions $F^{(j)}(K;z)$ are defined by the following formulas:

$$F^{(j)}(K;z)=z^j\sum_{m=0}^{\infty} c_m^{(j)}\,(2K)^m\,z^{3m}, \tag{17a}$$

$$c_0^{(0)}=1, \quad c_m^{(0)}=-\frac{(6m-6)!}{2\,(3m)!\,(3m-1)!\,(3m-2)!}, \quad m=1,2,3,\ldots, \tag{17b}$$

$$c_0^{(1)}=1, \quad c_m^{(1)}=-\frac{(6m-4)!}{24\,(3m+1)!\,(3m)!\,(3m-1)!}, \quad m=1,2,3,\ldots, \tag{17c}$$

$$c_0^{(2)}=\frac{1}{2}, \quad c_m^{(2)}=\frac{(6m-2)!}{120\,(3m+2)!\,(3m+1)!\,(3m)!}, \quad m=1,2,3,\ldots. \tag{17d}$$

These formulas provide the *general* solution of the equations of motion (6) with $N=3$ and the assignment (8) of the coupling constants, since they contain the six constants $Z(0)$, V, τ_0, α_1, α_2, α_3, which can be adjusted to fit the six initial conditions $\zeta_n(0)$, $\zeta_n'(0)$, $n=1,2,3$. Expressions of the first three of these constants [as well as of the constant K, see (16)] in terms of the initial data are already written above, see (10), (12), (14), while the other three, α_1, α_2, α_3, can be easily obtained from the following system of three linear equations (which is always solvable, since the determinant of the coefficients in its left-hand side is unity, as proven below):

$$\alpha_0 F^{(0)}(K;-\tau_0)+\alpha_1 F^{(1)}(K;-\tau_0)+\alpha_2 F^{(2)}(K;-\tau_0)$$
$$=\frac{1}{3}[-\zeta_1(0)+2\zeta_2(0)-\zeta_3(0)]+\frac{2V[\zeta_3(0)-\zeta_2(0)]}{\zeta_2'(0)}, \tag{18a}$$

$$\alpha_0 F^{(0)\prime}(K;-\tau_0)+\alpha_1 F^{(1)\prime}(K;-\tau_0)+\alpha_2 F^{(2)\prime}(K;-\tau_0)$$
$$=\tfrac{1}{3}[-\zeta_1'(0)+2\zeta_2'(0)-\zeta_3'(0)]-2V, \tag{18b}$$

$$\alpha_0 F^{(0)\prime\prime}(K;-\tau_0)+\alpha_1 F^{(1)\prime\prime}(K;-\tau_0)+\alpha_2 F^{(2)\prime\prime}(K;-\tau_0)=\frac{\zeta_2'(0)\,\zeta_3'(0)}{\zeta_3(0)-\zeta_2(0)}. \tag{18c}$$

This concludes our display of the *general* solution $\zeta_n(\tau)$ of the equations of motion (6) with $N=3$ and the assignment (8) of the coupling constants, and as well of the solution of the corresponding *initial-value* problem. The fact that these solutions $\zeta_n(\tau)$ are *entire* is plain, see (15) and (especially) (17).

These findings provide an explicit solution of the two nonlinear third-order ODEs satisfied by $y(\tau)$ and $x(\tau)$, obtained in Ref. 3 and conjectured there to be *super-Painlevé*. This conjecture is thereby validated; but the fact that the solutions of these nonlinear ODEs also satisfy *linear* (nonautonomous, third order) ODEs (as shown in the following section) presumably decreases the interest of those nonlinear ODEs, at least for the aficionados of Painlevé lore.

III. PROOFS

Let us begin by reformulating, following Ref. 3, the equations of motion (6) with $N=3$ in a more convenient form.

First of all we introduce for notational convenience the three coupling constants a, b, c by setting

$$a_{12}=a_{21}=a, \quad a_{23}=a_{32}=b, \quad a_{31}=a_{13}=c. \tag{19}$$

Next we point out that, as clearly implied by the equations of motion (6), the center of mass, see (10), moves uniformly.

We then introduce the coordinates u_n relative to the center of mass,

$$u_n=\zeta_n-Z, \quad n=1,2,3, \tag{20}$$

which clearly satisfy the restriction

$$u_1+u_2+u_3=0, \tag{21}$$

and we set [for notational convenience, and of course consistently with (21) as well as (9)]

$$u_1=x, \quad u_2=y, \quad u_3=-x-y. \tag{22}$$

It is then a matter of trivial algebra to write the equations of motion (6) (with $N=3$) in terms of the two variables x and y,

$$x''=2\,a\,\frac{(x'+V)\,(y'+V)}{x-y}-2\,c\,\frac{(x'+V)\,(x'+y'-V)}{2x+y}, \tag{23}$$

$$y''=-2\,a\,\frac{(x'+V)\,(y'+V)}{x-y}-2\,b\,\frac{(y'+V)\,(x'+y'-V)}{2y+x}. \tag{24}$$

Let us also note the existence (implied by these equations of motion[6]) of the constant of motion K,

$$K=(x'+V)\,(y'+V)\,(x'+y'-V)\,(x-y)^{2a}\,(2y+x)^{2b}\,(2x+y)^{2c}, \tag{25}$$

where of course $V=Z'(0)$ [see (11)].

We now restrict attention to the coupling constants assignment $a=0$, $b=-1/2$, keeping temporarily still free the option to assign the third coupling constant, c [eventually, to be completely consistent with the assignment (8), we shall set $c=-1$]. Hence the equations of motion now read as follows:

$$x''=-2\,c\,\frac{(x'+V)\,(x'+y'-V)}{2x+y}, \tag{26}$$

$$y''=\frac{(y'+V)\,(x'+y'-V)}{2y+x}, \tag{27}$$

and the associated constant of integration K reads as follows:

$$K=(x'+V)\,(y'+V)\,(x'+y'-V)\,(2y+x)^{-1}\,(2x+y)^{2c}. \tag{28}$$

We now introduce the auxiliary variable

$$\eta(\tau)=\frac{2y(\tau)+x(\tau)}{y'(\tau)+V}, \tag{29}$$

and we note that, as a consequence of (27), there holds the remarkable relation

$$\eta'(\tau)=1, \tag{30}$$

which of course entails

$$\eta(\tau)=\tau-\tau_0 \tag{31}$$

[and note the consistency of the expression (14) of τ_0 with this formula (31), via (29) with (9) and (11)].

We now note that (29) with (31) yield (13), which is therefore now proven, while clearly via (28) and (29) with (31) we can rewrite (26) as follows:

$$x''=-2\,c\,K\,(\tau-\tau_0)\,(2x+y)^{-2c-1}. \tag{32}$$

And the insertion of the expression (13) of x in this equation yields the following third-order ODE for $y(\tau)$:

$$y'''=-2\,c\,K\,[2\,(\tau-\tau_0)\,(y'+V)-3\,y]^{-2c-1}. \tag{33}$$

This ODE becomes particularly simple for two choices of the coupling constant c: for $c=-1/2$, which corresponds to the case treated in Ref. 3; and for $c=-1$, which is the case treated in this paper, to which attention is hereafter restricted. Then this ODE becomes *linear*,

$$y'''=2\,K\,[2\,(\tau-\tau_0)\,(y'+V)-3\,y]. \tag{34}$$

To solve it we now set

$$y(\tau)=2\,V\,(\tau-\tau_0)+F(K;\tau-\tau_0), \tag{35}$$

and we thereby obtain for $F(K;z)$ the neat ODE

$$F'''=2\,K\,[2\,z\,F'-3\,F], \tag{36}$$

where of course the primes denote, here and hereafter, differentiation with respect to the new independent variable $z=\tau-\tau_0$. It is now easy to check that the *general* solution of this linear third-order ODE is provided by (15b) with (17). And it is moreover plain that the three independent solutions $F^{(j)}(K;z)$, $j=1,2,3$, see (17), of this ODE (36) are characterized by the conditions

$$F^{(0)}(K;0)=1, \quad F^{(0)\prime}(K;0)=0, \quad F^{(0)\prime\prime}(K;0)=0, \tag{37a}$$

$$F^{(1)}(K;0)=0, \quad F^{(1)\prime}(K;0)=1, \quad F^{(1)\prime\prime}(K;0)=0, \tag{37b}$$

$$F^{(2)}(K;0)=0, \quad F^{(2)\prime}(K;0)=0, \quad F^{(2)\prime\prime}(K;0)=1, \tag{37c}$$

that clearly guarantee their linear independence, and moreover entail that their Wronskian, which is of course z-independent [thanks to (36)], equals unity,

$$\det\begin{pmatrix} F^{(0)}(K;z) & F^{(1)}(K;z) & F^{(2)}(K;z) \\ F^{(0)\prime}(K;z) & F^{(1)\prime}(K;z) & F^{(2)\prime}(K;z) \\ F^{(0)\prime\prime}(K;z) & F^{(1)\prime\prime}(K;z) & F^{(2)\prime\prime}(K;z) \end{pmatrix}=1. \tag{38}$$

The proof of all the results reported in the preceding section is thereby completed.

It will remain to be seen whether the approach used herein can be exploited to solve other three-body problems of type (6), and in particular some of those singled out in Ref. 3; an obvious candidate is the model characterized by the coupling constants $a_{12}=a_{21}=a=0$, $a_{23}=a_{32}=b=-1/2$, $a_{31}=a_{13}=c=-3/2$, to which the treatment given in this section is still applicable, leading again to the ODE (33), but with a value of c that causes the right-hand side of this ODE to be quadratic [rather than being linear, as is the case, see (34), for the model treated in this paper].

ACKNOWLEDGMENTS

One of us (F.C.) likes to acknowledge with thanks the pleasant hospitality at the Centro Internacional de Ciencias (CIC) in Cuernavaca during the Scientific Gathering on Integrable Systems that took place there in November–December 2002, providing the opportunity for the interaction with another one of us (A.G.) that led eventually to the results reported in this paper.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Gauge principle revisited: Towards a unification of space–time and internal gauge interactions

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(Received 6 November 2002; accepted 27 May 2003)

The minimal coupling principle is revisited under the quantum perspectives of the space–time symmetry. This revision is better realized on a group approach to quantization (GAQ) where group cohomology and extensions of groups play a preponderant role. We first consider the case of the electromagnetic potential; the Galilei and/or Poincaré group is (noncentrally) extended by the ''local'' U(1) group. The resulting group can also be seen as a central extension, parametrized by both the mass and the electric charge, of an infinite-dimensional group, on which GAQ leads to the dynamics of a particle moving in the presence of an electromagnetic field. Then we try the gravitational interaction of a particle by making the space–time translations ''local.'' However, promoting to ''local'' the space–time subgroup of the true symmetry of the quantum free relativistic particle, i.e., the centrally extended by U(1) Poincaré group, results in a new electromagneticlike force of pure gravitational origin. This is a consequence of the space–time translations not being an invariant subgroup of the extended Poincaré group and constitutes a preliminary attempt to a nontrivial mixing of space–time and internal gauge interactions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604183]

I. INTRODUCTION

In the Lagrangian formalism, formulated on the one-jet bundle, $J^1(E)$ of a vector bundle E on Minkowski space–time M,[1,2] promoting a given underlying rigid symmetry to ''local,'' i.e., extending the corresponding Lie algebra by taking the tensor product of it by the algebra of real analytic functions on M, requires the introduction of a derivation law on the module of sections of E, $\Gamma(E)$, which is eventually interpreted as a potential providing the corresponding gauge interaction. This is essentially the formulation of the so-called minimal coupling principle, which culminates in Utiyama's theory.[3] Internal gauge invariance had originally led successfully to electromagnetic interaction associated with U(1), then to Yang–Mills associated with isospin SU(2) (valid only at the ''very strong'' limit), electroweak with $(\mathrm{SU}(2)\otimes\mathrm{U}(1))/Z_2$, and finally to strong interaction associated with color SU(3). The same spirit is shared by later attempts to unify all of these into gauge groups such as SU(5). On the other hand, the ''local'' invariance under external (space–time) symmetries, such as a subgroup of the Poincaré group, has been used to provide a gauge framework for gravity,[4] although fully disconnected from the other (internal) interactions. In fact, a unification of gravity and the other interactions would have supposedly required the nontrivial mixing of the space–time group and some internal symmetry, a task

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explicitly forbidden by the so-called *no-go theorems* by O'Raifeartaigh, Coleman, Mandula, Michel, etc.[5–8] long ago, which stated that there is no finite-dimensional Lie group containing the Poincaré group acting as diffeomorphisms of the base manifold M, the Minkowski space–time, and any internal SU(n) group acting linearly on the fiber of E, except for the direct product. It is worth mentioning that supersymmetry was originally developed in the 1970s, mainly by Salam and Strathdee,[9] in an unsuccessful attempt to invalidate the no-go theorems.

However, the current skill in dealing with Lie group extensions and irreducible representations of (even infinite-dimensional) Lie groups tempts us into revisiting the question of the mixing of symmetries and, accordingly, the unification of interactions in terms of ordinary Lie groups. We propose a simple, yet nontrivial, way of facing the problem of interaction mixing. This consists in identifying one of the U(1) Cartan subgroups in the internal symmetry with the U(1) phase invariance in quantum mechanics. Then, turning the space–time translation subgroup of a centrally extended Poincaré group[10–13] into a ''local'' group automatically promotes the original rigid internal symmetry to the gauge level in a nontrivial way from the physical standpoint. This provides a nontrivial mixing of gravity and the already introduced internal interaction associated with the given unitary symmetry. Here, we seek to demonstrate explicitly the ocurrence of this new phenomenon at least at a given approximation without exhausting all possibilities of the proposed algorithm. This means that our present computational outputs must be understood as being partial, although, at the nonrelativistic limit, they are exact and reveal with precision the mixing effect.[14]

As is well known, the minimal coupling principle can also be formulated on a bundle E of the form $E=\mathbb{R}^3\times\mathbb{R}\to\mathbb{R}$, as corresponding to the case of mechanics, thus making the problem technically easier while keeping the essential point to be discussed here. In this framework, to be followed in the present article, the gauge principle will be revisited by simply substituting the quantum mechanical space–time symmetry for the standard (classical) one. In fact, in a previous letter,[14] we sketched an approach to the problem in this simple and economical way, i.e., in a particle mechanics (versus field theory) framework, and we now undertake a more detailed and formal presentation. A much more involved generalization to quantum field theory is under way.[15]

Since the revision we attempt here lies entirely on symmetry grounds, a (quantum) mechanical formulation tightly attached to a group structure is better suited. There is, in fact, a way of associating physical dynamics with a specific symmetry group. This could be accomplished by means of the rather standard co-adjoint-orbits method of Kirillov,[16] where the Lagrangian is seen as the local potential of the corresponding symplectic form. However, we shall proceed through a group approach to quantization (GAQ),[17,18] which is directly related to the co-homological structure of the symmetry group, and leads directly to the quantum theory, a fact that can be of capital relevance in the near future in passing to the quantum-field-theory level. Co-homology parameters will be directly identified with the physical coupling constants. In this sense, the association of the parameter of the (symplectic) co-homology group of the Galilei group with the particle mass has been emphasized by Souriau.[19]

As an intermediate step between the more standard Lagrangian version of the minimal interaction principle and the one to be presented here, we shall formulate a version ''à la Cartan,'' i.e., in terms of the invariance of the Poincaré–Cartan form[20–23] rather than the Lagrangian, of the part of Utiyama's theory concerning the particle in interaction with the field. Indeed, as mentioned above, the dynamics of the gauge fields themselves will be considerd elsewhere.

The article is organized as follows. Section II is a thorough presentation of basic geometrical aspects of classical and quantum mechanics, mainly those fundamental to the development of the present work. Section III is devoted to the Cartan-like analysis of the minimal coupling principle particularized for the case of electromagnetism and nonrelativistic gravity. In Sec. IV we present explicitly the GAQ with the example of a particle moving in an electromagnetic field. Finally, in Sec. V, we directly present the chief problem of gauging the translation subgroup of the centrally extended Poincaré group giving rise to the new phenomenon of an extra coupling constant mixing nontrivially the geodesic force and the Lorentz one. Some outlooks are included at the end.

II. PHASE INVARIANCE IN QUANTUM MECHANICS

According to the standard approach to quantum mechanics (see, for instance, Ref. 24) a state of the system is characterized by a *ray*, rather than a vector, of a Hilbert space, i.e., normalized wave functions are determined up to a complex number of module 1 or phase. This is a direct consequence of the definition of probability and constitutes a symmetry to be referred to as U(1) or phase invariance in quantum mechanics. Let us approach this symmetry from quite different perspectives to highlight its fundamental features.

A. Behavior of the Schrödinger equation

We shall consider the behavior of the Schrödinger equation corresponding to the free quantum particle

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi, \tag{1}$$

under the Galilei transformations

$$\begin{aligned} t' &= t + b, \\ \vec{x}' &= R\vec{x} + \vec{a} + \vec{V}t, \\ \vec{v}' &= R\vec{v} + \vec{V}. \end{aligned} \tag{2}$$

where R represents rotations, $b \in \mathbb{R}$ and $\vec{a} \in \mathbb{R}^3$ time and space translations, respectively, and $\vec{V} \in \mathbb{R}^3$ Galilean boosts.

Equation (1) acquires an extra term,

$$i\hbar \frac{\partial}{\partial t'}\Psi + i\hbar \vec{V}\cdot \frac{\partial \Psi}{\partial \vec{x}'} = -\frac{\hbar^2}{2m}\nabla'^2\Psi, \tag{3}$$

which can be compensated only by also transforming the wave function. Allowing for a nontrivial phase factor in front of the transformed wave function, of the form

$$\Psi' = e^{(im/\hbar)(\vec{V}\cdot R\vec{x} + (1/2)\vec{V}^2 t)}\Psi, \tag{4}$$

the Schrödinger equation becomes strictly invariant:

$$i\hbar \frac{\partial}{\partial t'}\Psi' = -\frac{\hbar^2}{2m}\nabla'^2\Psi'. \tag{5}$$

The need for a transformation such as (4) accompanying the space–time transformation (2) to accomplish full invariance strongly suggests the adoption of a central extension of the Galilei group as the basic (quantum-mechanical) space–time symmetry for the free particle.[25] The constant $\hbar$ is required to keep the exponent in (4) dimensionless.

The successive composition of two transformations in the extended Galilei group $\tilde{G}$ immediately leads to the group law:

$$\begin{aligned} b'' &= b' + b, \\ \vec{a}'' &= \vec{a}' + R(\vec{\epsilon}')\vec{a} + \vec{V}'b, \\ \vec{V}'' &= \vec{V}' + R(\vec{\epsilon}')\vec{V}, \end{aligned} \tag{6}$$

$$\vec{\epsilon}''=\sqrt{1-\frac{\vec{\epsilon}^{\,2}}{4}}\,\vec{\epsilon}'+\sqrt{1-\frac{\vec{\epsilon}'^{\,2}}{4}}\,\vec{\epsilon}+\frac{1}{2}\,\vec{\epsilon}'\wedge\vec{\epsilon},$$

$$e^{i\phi''}=e^{i\phi'}e^{i\phi}e^{(im/\hbar)[\vec{V}'R'\vec{a}+(1/2)\,b\vec{V}'^{2}]},$$

where $e^{i\phi}\in \mathrm{U}(1)$, and we have made the rotation parameters $\vec{\epsilon}\in\mathbb{R}^3$ explicit, which are restricted to $2\sin(\chi/2)=|\vec{\epsilon}|$, χ being the rotation angle.

B. Semi-invariance in classical mechanics

This phenomenon of extending the space–time symmetry, although conceptually pure quantum mechanical, can also be recast within a (semi-)classical formalism, by requiring the simultaneous extension of the classical phase space by a new variable ϕ, transforming in a nontrivial way under the U(1)-extended symmetry group. The need for such an extension is motivated by the lack of strict invariance of the Poincaré–Cartan form associated with the free particle ($H=p_i\dot{x}^i-L=\vec{p}^{\,2}/2m$),

$$\Theta_{PC}\equiv p_i dx^i-Hdt=\left(\frac{\partial L}{\partial\dot{x}^i}(dx^i-\dot{x}^i dt)+L dt\right)=p_i dx^i-\frac{\vec{p}^{\,2}}{2m}dt \tag{7}$$

under the Galilei group. In fact, it is left only semi-invariant by the infinitesimal transformations associated with (2) in the sense that the Lie derivative of Θ_{PC} with respect to those generators is the differential of a function not necessarily zero:

$$\begin{aligned}
&X_b=\frac{\partial}{\partial t}\Rightarrow L_{X_b}\Theta_{PC}=0,\\
&X_{\vec{a}}=\frac{\partial}{\partial\vec{x}}\Rightarrow L_{X_{\vec{a}}}\Theta_{PC}=0,\\
&X_{\vec{V}}=t\frac{\partial}{\partial\vec{x}}+m\frac{\partial}{\partial\vec{p}}\Rightarrow L_{X_{\vec{V}}}\Theta_{PC}=d(m\vec{x}),\\
&X_{\vec{\epsilon}}=\vec{x}\wedge\frac{\partial}{\partial\vec{x}}+\vec{p}\wedge\frac{\partial}{\partial\vec{p}}\Rightarrow L_{X_{\vec{\epsilon}}}\Theta_{PC}=0.
\end{aligned} \tag{8}$$

The pathology of semi-invariance is parallel to the absence of a clean quotient by the equations of motion. Let us see in some detail the quotient process in going to the solution manifold. In the Cartan formalism the trajectories of a general physical system are the orbits of the kernel of $d\Theta_{PC}$:

$$\begin{aligned}
&\Theta_{PC}\equiv p_i dx^i-Hdt,\\
&\Omega\equiv d\Theta_{PC}=dp_i\wedge dx^i-\frac{\partial H}{\partial x^i}dx^i\wedge dt-\frac{\partial H}{\partial p_i}dp_i\wedge dt.
\end{aligned} \tag{9}$$

Ω has a one-dimensional kernel generated by $X^H\in\mathrm{Ker}\,d\Theta_{PC}$ such that $dt(X^H)=1$,

$$X^H=\frac{\partial}{\partial t}+\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x^i}-\frac{\partial H}{\partial x^i}\frac{\partial}{\partial p_i}, \tag{10}$$

and the associated equations of motion are the Hamilton equations:

$$\frac{dt}{d\tau}=1,$$

$$\frac{dx^i}{d\tau}=\frac{\partial H}{\partial p_i}, \tag{11}$$

$$\frac{dp_i}{d\tau}=-\frac{\partial H}{\partial x^i}.$$

The vector field X^H defines a one-parameter group which divides the *space of movements* $\mathbb{R}\times\mathbb{R}^3\times\mathbb{R}^3$, parametrized by $(t,\vec{x},\vec{p})$, into classes, and $M\equiv\{\mathbb{R}\times\mathbb{R}^3\times\mathbb{R}^3\}/X^H$ constitutes the symplectic *phase space* of the system characterized by the Hamiltonian H; the symplectic form is obtained by the projection of Ω. The change of variables under which the equations of motion on the quotient become trivial is the Hamilton–Jacobi transformation. For the example $H=\vec{p}^2/2m$, corresponding to a free particle, this transformation is

$$\begin{cases} x^i=\dfrac{P^i}{m}\tau+K^i \\ p_i=P_i \\ t=\tau \end{cases} \Leftrightarrow \begin{cases} K^i=x^i-\dfrac{p^i}{m}t, \\ P_i=p_i, \\ \tau=t, \end{cases} \tag{12}$$

where the constants of motion K^i,P_j parametrize the solution manifold M. However, the form Θ_{PC} goes to the quotient except for a total differential:

$$\Theta_{PC}\rightarrow P_i dK^i+d\left(\frac{\vec{P}^2}{2m}\tau\right),$$

$$\omega=dP_i\wedge dK^i. \tag{13}$$

C. Poisson algebra realization

Another equivalent analytical mechanics breakdown claiming a ''generalization'' is the unfair relationship between the Lie brackets of basic symmetries and the corresponding Poisson brackets of the associated Noether invariants. The symplectic form[21–23] is a skew-symmetric ''metric'' and defines an isomorphism $\omega^\flat:\mathcal{X}(M)\leftrightarrow\Lambda^1(M)$ between the vector space of vector fields on M and that of one-forms on M,

$$X\in\mathcal{X}(M)\mapsto\omega(X,\cdot)\equiv i_X\omega\in\Lambda^1(M), \tag{14}$$

associating a bracket $\{,\}$ on $\Lambda^1(M)$ with the Lie bracket of vector fields. In particular, given functions $f,g\in C^\infty(M)$, their differentials are associated with *Hamiltonian vector fields* X_f,X_g.[26] This permits the definition of a Poisson bracket between functions, rather than one-forms, but this time the correspondence $\{,\}\rightarrow[,]$,

$$\{,\}:f,g\mapsto\{f,g\}/d\{f,g\}=-i_{[X_f,X_g]}\omega, \tag{15}$$

is no longer an isomorphism because constant functions have trivial Hamiltonian vector fields. In particular, with regard to the example $H=\vec{p}^2/2m$, and considering K^i,P_j as the basic coordinates for M, we find

$$\{K^i,P_j\}=\delta^i_j\cdot 1\mapsto[X_{K^i},X_{P_j}]=0, \tag{16}$$

that is, a Lie algebra homomorphism whose kernel is the central subalgebra of constant functions, $\mathbb{R}$, generated by 1. It is easy to realize that X_{K^i}, X_{P_j} are nothing other than the generators X_{V^i}, X_{a^j}, respectively, of the action (2) of the unextended Galilei group on the space of movements, written on the solution manifold.[27]

The extension of phase space is required to represent faithfully the (classical) Poisson algebra by means of the generators of the extended symmetry as first-order differential operators, a fact that constitutes the Bohr–Sommerfeld approximation to quantization or prequantization, in the language of geometric quantization.[19,28–30] Let us look at the preliminary steps towards the geometric attempts at quantization.

D. Geometric and group approach to quantization

The existence of a nontrivial kernel in the correspondence between functions and Hamiltonian vector fields is an essential failure of the naive geometric approach to quantization $\hat{}: f \mapsto \hat{f} \equiv X_f$, which would associate the trivial operator to any constant. The simplest way of avoiding this problem consists of enlarging phase space (and/or movements space) with one extra variable providing one extra component to X_f, and generalizing accordingly the equation $i_{X_f} d\Theta_{PC} = -df$ so as to get a nontrivial new component even though f is a constant. On a quantum manifold P, locally isomorphic to $M \times S^1$, with connection form Θ such that the curvature two-form $(d\Theta)$ coincides with $d\Theta_{PC}$, the equation above can be replaced by the set of equations[19]

$$\begin{aligned} i_{\tilde{X}_f} d\Theta &= -df, \\ i_{\tilde{X}_f} \Theta &= f, \end{aligned} \tag{17}$$

generalizing in this way the quantization map which now reads (except perhaps for a minus sign)

$$\hat{}: f \mapsto i\tilde{X}_f. \tag{18}$$

Note that Eq. (17) immediately implies the strict invariance of Θ under $\tilde{X}_f$:

$$L_{\tilde{X}_f} \Theta = d i_{\tilde{X}_f} \Theta + i_{\tilde{X}_f} d\Theta = df - df = 0. \tag{19}$$

Locally, we can write $\Theta = \Theta_{PC} + dz/iz$, $z = e^{i\Phi} \in S^1$, and then $\tilde{X}_f = X_f + [f - \Theta_{PC}(X_f)] \times (iz(\partial/\partial z) - iz^*(\partial/\partial z^*))$, and we immediately see that (17) has a unique solution associating the fundamental (vertical) vector field $\Xi \equiv iz(\partial/\partial z) - iz^*(\partial/\partial z^*) = \partial/\partial\Phi$, dual to dz/iz, with the unity of $\mathbb{R}$.

The quantization map $\hat{}$ is now an isomorphism between the Poisson algebra on M and the Lie subalgebra of vector fields on P that are solutions to (17). For the basic functions, we have

$$\{K^i, P_j\} = \delta^i_j \cdot 1 \leftrightarrow [\tilde{X}_{K^i}, \tilde{X}_{P_j}] = \delta^i_j \cdot \Xi. \tag{20}$$

It is again easy to realize that, in the case of the free particle, the operators $\tilde{X}_{K^i}, \tilde{X}_{P_j}$ are nothing other than the generators $\tilde{X}_{V^i}, \tilde{X}_{a^j}$ of the action (2) and (4) on the extended space of movements (with $\zeta \equiv e^{i\phi} \in S^1$) of the extended Galilei group, that is to say,

$$\begin{aligned} \tilde{X}_b &= X_b, \\ \tilde{X}_{\vec{a}} &= X_{\vec{a}}, \\ \tilde{X}_{\vec{v}} &= X_{\vec{v}} - \frac{1}{\hbar} m\vec{x} \frac{\partial}{\partial \phi}, \end{aligned} \tag{21}$$

$$\tilde{X}_{\vec{\epsilon}} = X_{\vec{\epsilon}},$$

written on the solution manifold.

To pass to the solution manifold, we must take into account the evolution of the new variable $\zeta \in \mathrm{U}(1)$. In fact, the equations of motion in the extended [by U(1)] movement space are given by the vector field $\check{X}$ in the kernel of $d\Theta$ and Θ, simultaneously, satisfying $dt(X)=1$. Locally, and for the choice $\Theta_{PC} = p_i dx^i - H dt$, we find

$$\check{X}^H = X^H + \left\{ H - p_i \frac{\partial H}{\partial p_i} \right\} \Xi. \tag{22}$$

For the free particle, $\check{X}^H$ provides the following new equation, to be added to de Hamilton–Jacobi set (12),

$$\zeta = z e^{-(i/\hbar)(\vec{P}^2/2m)\,t} \Leftrightarrow z = \zeta e^{(i/\hbar)(\vec{p}^2/2m)\,t}. \tag{23}$$

Now the form Θ, originally written in the space of movements as

$$\Theta = p_i dx^i - \frac{\vec{p}^2}{2m} dt + \hbar \frac{d\zeta}{i\zeta}, \tag{24}$$

goes to the quotient, by applying the extended Hamilton–Jacobi transformation (12) and (23), giving

$$\Theta = P_i dK^i + \hbar \frac{dz}{iz}. \tag{25}$$

The space of wave functions Ψ is constituted by the complex functions on P that satisfy the U(1)-equivariance condition, turning Ψ into a section of the principal bundle $P \to M$:[31]

$$\Xi \tilde{\Psi} = i\tilde{\Psi} \leftrightarrow \tilde{\Psi}(K,P,z) = z\Psi(K,P), \tag{26}$$

on which the vector fields $\tilde{X}_f$ act, defining the *prequantum operators*.

Unfortunately, the quantization map $\hat{}$ is faithful but not irreducible as a representation of the Lie algebra of classical functions. At this prequantization level, we are able to reproduce only the Bohr–Sommerfeld–Wilson quantization rules.[30] We know that this representation is reducible because of the existence of nontrivial operators commuting with the basic quantum generators $\hat{K}^i \equiv i\hbar \tilde{X}_{K^i}, \hat{P}_j \equiv -i\hbar \tilde{X}_{P_j}$. In fact, thinking of the simplest case, that of the free particle for example, and adopting for Θ the local expression (25), we get the following basic operators acting on the untilded wave functions Ψ:

$$\hat{K}^i = i\hbar \frac{\partial}{\partial P_i} + K^i, \qquad \hat{P}_j = -i\hbar \frac{\partial}{\partial K^j}, \tag{27}$$

and it is clear that the operators $\check{K}^i \equiv \partial/\partial P_i$ do commute with them.

True quantization requires that all nontrivial operators commuting with basic quantum generators should be trivialized. We must then impose a maximal set of mutually compatible conditions in the form $X\Psi = 0$, for X in some maximal vector space called *polarization*. For instance, in the example above the operator $\partial/\partial P_i$ would be trivial had we imposed the polarization condition $(\partial/\partial P_i)\,\Psi = 0 \to \Psi \neq \Psi(P)$. Finding a polarization, however, is a nontrivial task in general, because two polarization conditions $\hat{a}\Psi = 0$, $\hat{b}\Psi = 0$ are inconsistent if $[\hat{a},\hat{b}] = \hat{1}$ and, once a certain

polarization has been imposed, the set of physical operators that preserve the polarization is severely restricted. Even more, the existence of an invariant polarization, i.e., a polarization preserved by the basic operators, is by no means guaranteed.

A stylish and even practical (at least for fundamental systems) solution to this and other problems comes from the structure itself of the (classical) Poisson algebra seen as a fundamental symmetry of the physical system to be quantized or, more precisely, the (quantum) physical system to be studied. Looking again at the quantum symmetry of the free particle, the extended Galilei group (2), we can adopt its structure as the basic block to provide the whole physical system, including the space and time where the evolution takes place.[17,18] The chief idea is to replace the quantum manifold P with a Lie group $\tilde{G}$ bearing the structure of a principal bundle with structure group U(1) and a connection one-form Θ selected from the canonical invariant forms on the group. The simplest, though sufficiently broad, example of such a class of Lie groups is the case of a central extension of a given group G by U(1).[25] In this situation, the central extensions are parametrized by the second co-homology group of G in U(1), $H^2(G,\mathrm{U}(1))$, and the coordinates in this (vector) space are associated with fundamental constants such as the mass[19] or the electric charge (see Sec. IV). Each co-homology constant is in turn associated with a Lie subalgebra of even dimension (in fact, a symplectic vector space) which will provide a set of canonically conjugate pairs of operators. We shall call them *dynamical* quantities, or the corresponding parameters in the group (classical) dynamical variables.

The virtues of working on a Lie group are multiple, but, for the time being, let us point out that of possessing two sets of natural, mutually commuting operators, that is, the left- and right-invariant vector fields, the latter of which can provide a unitary representation to be reduced by polarization conditions imposed by a subalgebra of the former. With this choice, the connection one-form Θ is the U(1) component of the left-invariant canonical one-form on the group, which is automatically invariant under the right-invariant vector fields. The only apparent drawback of doing so is that the quotient $\tilde{G}/\mathrm{U}(1)$ is not necessarily a symplectic manifold since the curvature two-form $d\Theta$ may have a nontrivial kernel. However, this apparent problem is solved by including in the polarization conditions, formulated in terms of a maximal horizontal subalgebra $\mathcal{P}$ of left-invariant vector fields, the subalgebra of (left-invariant) vector fields $\mathcal{G}_\Theta$ generating the characteristic module of Θ, i.e., $\mathrm{Ker}\Theta \cap \mathrm{Ker}d\Theta$.

It should be stressed that, far from being a drawback, working on the precontact manifold $\tilde{G}$ instead of a proper quantum manifold P allows us to deal with quantum systems without classical limit. In fact, the trajectories of the vector fields in the characteristic subalgebra generalize the classical motion, and the solution of the corresponding equations can be bypassed by including this subalgebra in the polarization as generalized Schrödinger equations.

III. CARTAN-LIKE VERSION OF THE MINIMAL-COUPLING PRINCIPLE: THE ELECTROMAGNETIC AND NONRELATIVISTIC GRAVITATIONAL FORCES

Once the symmetry of the free particle has been posed through the strict invariance of the corresponding extended Poincaré–Cartan (or quantization) form Θ (24) under the action of extended Galilei group, we may postulate the requirement of invariance of a generalized Θ under the Galilei group (noncentrally) extended by the ''local'' group $\mathrm{U}(1)(\vec{x},t)$ (of local phase transformations $e^{i\phi(\vec{x},t)}$). This requirement, along with the minimal substitution in Θ to achieve strict invariance, constitutes the Cartan-like version of the minimal coupling principle for the U(1) rigid symmetry and will lead to the motion of a particle in the presence of an electromagnetic field.

Let us consider the Lie algebra $\tilde{\mathcal{G}}$ of the centrally extended Galilei group $\tilde{G}$ (only nonzero commutators):

$$
\begin{gathered}
[\tilde{X}_{V^i},\tilde{X}_b]=\tilde{X}_{a^i},\quad [\tilde{X}_{V^i},\tilde{X}_{a^j}]=\frac{m}{\hbar}\delta_{ij}\tilde{X}_\phi,\\
[\tilde{X}_{\epsilon^i},\tilde{X}_{\epsilon^j}]=\epsilon_{ij.}{}^k\tilde{X}_{\epsilon^k},\quad [\tilde{X}_{\epsilon^i},\tilde{X}_{V^j}]=\epsilon_{ij.}{}^k\tilde{X}_{V^k},\quad [\tilde{X}_{\epsilon^i},\tilde{X}_{a^j}]=\epsilon_{ij.}{}^k\tilde{X}_{a^k},
\end{gathered}
\tag{28}
$$

which, as mentioned above, leaves strictly invariant the extended Poincaré–Cartan form $\Theta = p_i dx^i - (\vec{p}^2/2m) + \hbar d\phi$, that is, $L_{\tilde{X}_a}\Theta = 0, \forall \tilde{X}_a \in \tilde{\mathcal{G}}$.

Local U(1) transformations generated by $f \otimes X_\phi$, f being a real function $f(\vec{x},t)$, are incorporated into the scheme by adding to (28) the extra commutators:[32]

$$[\tilde{X}_a, f \otimes X_\phi] = (L_{\tilde{X}_a} f) \otimes X_\phi . \tag{29}$$

The Lie derivative of (24) with respect to $f \otimes X_\phi$ gives

$$L_{f \otimes X_\phi}\Theta = d(i_{fX_\phi}\Theta) + i_{fX_\phi} d\Theta = df.$$

Keeping the strict invariance requires modifying Θ by adding a connection term $\Gamma = \Gamma_i dx^i + \Gamma_0 dt$ whose components transform under $\mathrm{U}(1)(\vec{x},t)$ as the space–time gradient of the function f.[33] Additional conditions on Γ will be obtained by requiring strict invariance of $\Theta' \equiv \Theta + \Gamma$ under the complete group. The generators of the action of the whole group on the variables $(t, \vec{x}, \vec{p}, \vec{\Gamma}, \Gamma_0, \phi)$ are

$$\begin{aligned}
\tilde{X}_b &= \frac{\partial}{\partial t}, \\
\tilde{X}_{\vec{a}} &= \frac{\partial}{\partial \vec{x}}, \\
\tilde{X}_{\vec{V}} &= t\frac{\partial}{\partial \vec{x}} + m\frac{\partial}{\partial \vec{p}} + \vec{\Gamma}\frac{\partial}{\partial \Gamma_0} + \frac{m}{\hbar}\vec{x}\frac{\partial}{\partial \phi}, \\
\tilde{X}_{\vec{\epsilon}} &= \vec{x} \wedge \frac{\partial}{\partial \vec{x}} + \vec{p} \wedge \frac{\partial}{\partial \vec{p}} + \vec{\Gamma} \wedge \frac{\partial}{\partial \vec{\Gamma}}, \\
f \otimes X_\phi &= -\vec{\nabla} f \frac{\partial}{\partial \vec{\Gamma}} + \frac{\partial f}{\partial t}\frac{\partial}{\partial \Gamma_0} - \frac{f}{\hbar}\frac{\partial}{\partial \phi}.
\end{aligned} \tag{30}$$

Then, the infinitesimal condition

$$L_X(\Theta') = 0$$

implies the following finite transformation properties of the components of Γ:

$$\begin{aligned}
\vec{\Gamma}' &= R\vec{\Gamma}, \\
\Gamma_0' &= \Gamma_0 + \vec{V} \cdot R\vec{\Gamma},
\end{aligned} \tag{31}$$

under a rotation and a boost, and

$$\begin{aligned}
\vec{\Gamma}' &= \vec{\Gamma} + \vec{\nabla} f, \\
\Gamma_0' &= \Gamma_0 + \frac{\partial f}{\partial t},
\end{aligned} \tag{32}$$

under an element of $\mathrm{U}(1)(\vec{x},t)$.

Let us now compute the simultaneous kernel of Θ' and $d\Theta'$ and write the equations of motion, rewriting the connection Γ as $\Gamma \equiv qA_i dx^i - qA_0 dt$. We then have (omitting the prime over Θ')

$$\Theta = m\vec{v}\cdot d\vec{x} - \tfrac{1}{2}m\vec{v}^2 dt + q\vec{A}\cdot d\vec{x} - qA^0 dt + \hbar\, d\phi, \tag{33}$$

$$\check{X} = \frac{\partial}{\partial t} + \vec{v}\cdot\frac{\partial}{\partial \vec{x}} + \frac{q}{m}\left[\left(\frac{\partial A_j}{\partial x^i} - \frac{\partial A_i}{\partial x^j}\right)v^j - \frac{\partial A^0}{\partial x^i} - \frac{\partial A_i}{\partial t}\right]\frac{\partial}{\partial v_i} - \frac{1}{\hbar}\left[\frac{1}{2}m\vec{v}^2 + q(\vec{v}\cdot\vec{A} - A^0)\right]\frac{\partial}{\partial \phi}. \tag{34}$$

It states the equations of motion of a charged particle of charge q in an electromagnetic field:

$$\frac{d\vec{x}}{dt} = \vec{v},$$

$$m\frac{d\vec{v}}{dt} = q\left[\vec{v}\wedge(\vec{\nabla}\wedge\vec{A}) - \vec{\nabla}A^0 - \frac{\partial\vec{A}}{\partial t}\right], \tag{35}$$

$$\frac{d\phi}{dt} = -\frac{1}{\hbar}\left(\frac{\vec{p}^2}{2m} - \frac{q}{m}\vec{A}\cdot\vec{p}\right).$$

The minimal coupling principle can also be applied to the case of Newtonian gravity by requiring the space and time translation parameters to depend on time. Unlike the electromagnetic gauge principle, which can be directly extended to the relativistic situation, relativistic gravity is much more involved and will be analyzed in Sec. V, mixed with electromagnetism as our central task.

For brevity, let us consider the 1+1-dimensional case. Starting with the unextended Galilei group, we promote the space and time translations to local in the more economical way, that is, turning the corresponding group parameters into functions of time. The gauge algebra is then

$$[f(t)\otimes X_b, X_b] = -\frac{\partial f}{\partial t}\otimes X_b,$$

$$[f(t)\otimes X_b, X_a] = 0, \tag{36}$$

$$[f(t)\otimes X_b, X_V] = f(t)\otimes X_a.$$

According to the minimal prescription, we introduce a connection $\Gamma \equiv h\,dt$ to be added to the free Poincaré–Cartan form, and an extra component in $\partial/\partial h$ to the Galilei generators for nontrivial realization of the current algebra (36). Then the semi-invariance of

$$\Theta'_{PC} = p\,dx - \frac{p^2}{2m}dt + h\,dt \tag{37}$$

under the current algebra (36) fixes the new components in h, so that the complete expression of the Lie algebra of the *unextended* Galilei group with local (depending only on time) space and time translation subgroup becomes

$$f(t)\otimes X_b = f\frac{\partial}{\partial t} + \left(\frac{p^2}{2m} - h\right)\frac{df}{dt}\frac{\partial}{\partial h},$$

$$f(t)\otimes X_a = f\frac{\partial}{\partial x} - p\frac{df}{dt}\frac{\partial}{\partial h},$$

$$X_V = t\frac{\partial}{\partial x} + m\frac{\partial}{\partial p}, \tag{38}$$

$$f(t)\otimes X_h = f\frac{\partial}{\partial h},$$

where we have had to introduce the new local generator $f(t)\otimes X_h$ in order to close the current algebra. The new generator also leaves the form (37) semi-invariant. Strict invariance is now achieved by adding to generators X new components in $\partial/\partial\phi$ with coefficients equal to $-g$, g being such that $i_X d\Theta' = dg$. This results in

$$\begin{aligned}
\widetilde{f(t)\otimes X_b} &= f\frac{\partial}{\partial t} + \left(\frac{p^2}{2m} - h\right)\frac{df}{dt}\frac{\partial}{\partial h} - \frac{f}{\hbar}\left(\frac{p^2}{2m} - h\right)\frac{\partial}{\partial \phi},\\
\widetilde{f(t)\otimes X_a} &= f\frac{\partial}{\partial x} - p\frac{df}{dt}\frac{\partial}{\partial h} + \frac{1}{\hbar}fp\frac{\partial}{\partial \phi},\\
\tilde{X}_V &= t\frac{\partial}{\partial x} + m\frac{\partial}{\partial p} - \frac{m}{\hbar}\left(x - \frac{p}{m}t\right)\frac{\partial}{\partial \phi},\\
\widetilde{f(t)\otimes X_h} &= f\frac{\partial}{\partial h} - \frac{f}{\hbar}\frac{\partial}{\partial \phi}.
\end{aligned} \tag{39}$$

The reason for U(1)-extending after gauging is clear: both processes definitely do not commute. Proceeding the other way round leads, precisely, to the new results of Sec. V.

The Cartan-like equations associated with (37) lead directly to the Newtonian gravity equations if we identify h with the gravitational potential. This potential can be related to the component g_{00} of a metric in the Newtonian limit of general relativity via the expression $g_{00}\approx 1+h$.

IV. GROUP APPROACH TO THE QUANTIZATION OF A PARTICLE MOVING IN AN ELECTROMAGNETIC FIELD

In this and the next section, we shall adopt the GAQ formalism as a generalization of the geometrical approach to quantum mechanics, although we shall be interested, for now, primarily in the classical equations of motion. As mentioned above, we seek to reproduce any dynamical or kinematical quantity or variable out of a Lie group so that notation such as $t,\vec{x},\vec{p}$, etc. will refer to group variables (although directly identifiable with ''physical'' ones once the equations of motion are written).

Let us start by exponentiating the algebra (28)+(29), originally performed on a given movement space, in order to arrive at an abstract Lie group from which to obtain all physical structures. This algebra is infinite dimensional but, for real analytic functions f, the dynamical-variable content of it, in the sense of Sec. II D, is addressed by the (co-homological) structure of the finite-dimensional subalgebra generated by $\tilde{\mathcal{G}}$ along with those generators $f\otimes X_\phi$ with only linear functions, $t\otimes X_\phi$ and $x^i\otimes X_\phi$, to be called X_{A^0} and X_{A^i}, respectively. The rest of the functions contribute only to the characteristic (nondynamical) subalgebra and can be decoupled from the theory. Let us call $\tilde{G}_E$ this finite-dimensional group. It proves to be enough to describe the dynamics of a particle moving in an electromagnetic field if we resort to the trick (see below) of assuming an explicit dependence $A^\mu = A^\mu(\vec{x},t)$ once the one-form Θ will be found. [This procedure is suggested by the possibility of writing an analytic function in the form $f(\vec{x},t)=\phi + A_\mu(\vec{x},t)x^\mu$, where $\phi = f(\vec{0},0)$.] We shall not be involved here with the corresponding quantum field theory.

The group $\tilde{G}_E$ can be given the following group law which extends that of the Galilei group (with parameters $t,\vec{x},\vec{v}\equiv\vec{p}/m$ instead of $b,\vec{a},\vec{V}$, respectively) and agrees with the finite transformation (31) and (32):

$$t'' = t' + t,$$

$$\vec{x}'' = \vec{x}' + R'\vec{x} + \vec{v}'t,$$

$$\vec{v}''=\vec{v}'+R'\vec{v},$$

$$R''=R'R,$$

$$\vec{A}''=\vec{A}'+R'\vec{A}, \tag{40}$$

$$A_0''=A_0'+A_0+\vec{v}'\cdot R'\vec{A},$$

$$\zeta''=\zeta'\zeta e^{i\xi_m(g',g)}e^{i\xi_q(g',g)},$$

$$\xi_m(g',g)\equiv-\frac{m}{\hbar}\left[\vec{v}'\cdot R'\vec{x}+\frac{1}{2}t\vec{v}'^2\right],$$

$$\xi_q(g',g)\equiv-\frac{q}{\hbar}[\vec{A}'\cdot R'\vec{x}+t(\vec{v}'\cdot\vec{A}'-A_0')],$$

where $\xi_m(g',g)$ is a standard Bargmann-like cocycle associated with the Galilei (sub)group, in particular with the symplectic submanifold of coordinates (x^i,v_j), and $\xi_q(g',g)$ is a new cocycle, parametrized by the electric charge, as we shall see, associated with the symplectic submanifold of coordinates (x^i,A_j). Both satisfy the cocycle conditions

$$\xi(g',g)+\xi(g'*g,g'')=\xi(g',g*g'')+\xi(g,g''),$$

$$\xi(0,g)=\xi(g',0)=0$$

intended to maintain the structure of group law after the extension. Since both cocycles are associated with intersecting symplectic submanifold ($\vec{x}$ is in both) we should expect a mixed momentum variable conjugated to $\vec{x}$, to be identified with the minimally coupled momentum. This is the essence of minimal coupling in GAQ.

From (40) we derive left- and right-invariant vector fields and from the former the ζ-component of the left-invariant canonical one-form:

$$\tilde{X}_t^L=\frac{\partial}{\partial t}+\vec{v}\cdot\frac{\partial}{\partial\vec{x}}-\frac{1}{\hbar}\left[\frac{1}{2}m\vec{v}^2+q(\vec{v}\cdot\vec{A}-A_0)\right]\Xi,$$

$$\tilde{X}_{\vec{x}}^L=R\left(\frac{\partial}{\partial\vec{x}}-\frac{1}{\hbar}[m\vec{v}+q\vec{A}]\Xi\right),$$

$$\tilde{X}_{\vec{v}}^L=R\left(\frac{\partial}{\partial\vec{v}}\right),$$

$$\tilde{X}_{\vec{\epsilon}}^L=\sqrt{1-\frac{\vec{\epsilon}^2}{4}}\frac{\partial}{\partial\vec{\epsilon}}-\frac{1}{2}\vec{\epsilon}\wedge\frac{\partial}{\partial\vec{\epsilon}}, \tag{41}$$

$$\tilde{X}_{\vec{A}}^L=R\left(\frac{\partial}{\partial\vec{A}}+\vec{v}\frac{\partial}{\partial\vec{A}_0}\right),$$

$$\tilde{X}_{A_0}^L=\frac{\partial}{\partial A_0},$$

$$\tilde{X}^L_{\zeta}=i\left(\zeta\frac{\partial}{\partial\zeta}-\zeta^*\frac{\partial}{\partial\zeta^*}\right)\equiv\frac{\partial}{\partial\phi}\equiv\Xi,$$

$$\tilde{X}^R_t=\frac{\partial}{\partial t},$$

$$\tilde{X}^R_{\vec{x}}=\frac{\partial}{\partial\vec{x}},$$

$$\tilde{X}^R_{\vec{v}}=\frac{\partial}{\partial\vec{v}}+t\frac{\partial}{\partial\vec{x}},$$

$$\tilde{X}^R_{\vec{\epsilon}}=\sqrt{1-\frac{\vec{\epsilon}^2}{4}}\frac{\partial}{\partial\vec{\epsilon}}+\frac{1}{2}\vec{\epsilon}\wedge\frac{\partial}{\partial\vec{\epsilon}},\tag{42}$$

$$\tilde{X}^R_{\vec{A}}=\frac{\partial}{\partial\vec{A}}-q\vec{x}\Xi,$$

$$\tilde{X}^R_{A_0}=\frac{\partial}{\partial A_0}+qt\Xi,$$

$$\tilde{X}^R_{\zeta}=i\left(\zeta\frac{\partial}{\partial\zeta}-\zeta^*\frac{\partial}{\partial\zeta^*}\right)\equiv\frac{\partial}{\partial\phi}\equiv\Xi,$$

$$\Theta\equiv\hbar\,\theta^{(\zeta)L}=m\vec{v}\cdot d\vec{x}-\frac{1}{2}m\vec{v}^2dt+q\vec{A}\cdot d\vec{x}-qA_0dt+\hbar\frac{d\zeta}{i\zeta}.\tag{43}$$

The commutation relations of (let us say) left generators (omitting rotations, which operate in the standard way) are

$$[\tilde{X}^L_t,\tilde{X}^L_{x^i}]=0,\quad[\tilde{X}^L_t,\tilde{X}^L_{v^i}]=-\tilde{X}^L_{x^i},\quad[\tilde{X}^L_{x^i},\tilde{X}^L_{v^j}]=\frac{m}{\hbar}\delta_{ij}\Xi,$$

$$[\tilde{X}^L_t,\tilde{X}^L_{Ai}]=0,\quad[\tilde{X}^L_t,\tilde{X}^L_{A0}]=-\frac{q}{\hbar}\Xi,\quad[\tilde{X}^L_{x^i},\tilde{X}^L_{Aj}]=\frac{q}{\hbar}\delta_{ij}\Xi,\tag{44}$$

$$[\tilde{X}^L_{x^i},\tilde{X}^L_{A^0}]=0,\quad[\tilde{X}^L_{v^i},\tilde{X}^L_{Aj}]=\delta_{ij}\tilde{X}^L_{A^0},\quad[\tilde{X}^L_{v^i},\tilde{X}^L_{A^0}]=0.$$

If we compute the characteristic module of Θ, i.e., $\mathrm{Ker}d\Theta\cap\mathrm{Ker}\Theta$ for $q=0$, as corresponding to the free particle, we find that it is generated by a left subalgebra

$$\mathcal{G}_\Theta|_{q=0}=\langle\tilde{X}^L_t,\tilde{X}^L_{\vec{\epsilon}},\tilde{X}^L_{\vec{A}},\tilde{X}^L_{A_0}\rangle,\tag{45}$$

leading to the trajectories (12) and (23) for the dynamical (symplectic) variables $\vec{x}$ and $\vec{p}$, and additional ones for the kinematical (nonsymplectic) variables $\vec{\epsilon},\vec{A},A_0$ which decouple from the theory. The quotient of $\tilde{G}_E/\mathrm{U}(1)$ by the generalized equations of motion is a symplectic manifold (the solution manifold) of dimension $3+3$. However, for nonzero q, we have

$$\mathcal{G}_\Theta=\left\langle\tilde{X}^L_{\vec{\epsilon}},\ \tilde{X}^L_{\vec{A}}-\frac{q}{m}\tilde{X}^L_{\vec{v}}\right\rangle,\tag{46}$$

leading to a symplectic manifold of dimension 4+4. We should note that no time evolution appears as an equation of motion. This is because the electromagnetic cocycle lends dynamical character to t as conjugate to A_0. The only characteristic vector field, apart from $\tilde{X}^L_{\vec{\epsilon}}$, which again simply decouples the variables $\vec{\epsilon}$, is the one defining the minimal coupling. In fact, the Noether invariants $i_{\tilde{X}}\Theta$ are

$$i_{\tilde{X}^R_t}\Theta = -\left(\tfrac{1}{2}m\vec{v}^2 + qA_0\right),$$

$$i_{\tilde{X}^R_{\vec{x}}}\Theta = m\vec{v} + q\vec{A} \equiv \vec{P},$$

$$i_{\tilde{X}^R_{\vec{v}}}\Theta = -m(\vec{x} - \vec{v}t) + q\vec{A}t,$$

$$i_{\tilde{X}^R_{\vec{A}}}\Theta = -q\vec{x},$$

$$i_{\tilde{X}^R_{A_0}}\Theta = qt,$$

reproducing, in particular the "canonical momentun" $\vec{P} \equiv m\vec{v} + q\vec{A}$.

Real dynamics appear when we impose the "constraint" $A_{0,i} = A_{0,i}(\vec{x},t)$ on Θ, whose characteristic module turns out now to be generated by $\check{X}$ in (34), thus reproducing the standard equations of motion. The trick of introducing this constraint after the form Θ associated with $\tilde{G}_E$ has been computed can in fact be justified in mathematical terms, although at the price of introducing an explicit infinite parametrization of the field A_μ by means of, for instance, Fourier coefficients $a_\mu(\vec{k})$, $a^*_\nu(\vec{k})$, and, very importantly, an extra space–time translation group associated with this field, let us say χ_μ. That is, the general space–time position on which the field lies conceptually differs from the space–time position of the particle. Under these conditions a cocycle of this infinite-dimensional group can be introduced, contributing the form Θ with the term $q\vec{A}(\vec{x},t) \cdot d\vec{x} - qA_0(\vec{x},t)dt$ where

$$A_\mu(\vec{x},t) = \int \frac{d^3\vec{k}}{2k^o}\{a_\mu(\vec{k})e^{-ik\cdot x} + a^*_\mu(\vec{k})e^{ik\cdot x}\}, \tag{47}$$

that is, the electromagnetic field evaluated on the trajectories of the particle. Now, the above-mentioned constraint proves to be as natural as stating that, on a trajectory, the particle sees the field A_μ evaluated on x_μ rather than on χ_μ. This precise construction, along with the (also infinite-dimensional) cocycle providing dynamical content to the field variables $a_\mu(\vec{k})$, $a^*_\nu(\vec{k})$ themselves, deserves a separate work, which is in progress.

We should say to conclude this section that this study can be repeated with the centrally extended Poincaré group $\tilde{P}$[10,11] (see also Refs. 13 and 14) by promoting to *local* the U(1) transformations and considering the finite-dimensional subgroup $\tilde{P}_E$ analogous to $\tilde{G}_E$.

V. MIXING THE ELECTROMAGNETIC AND GRAVITATIONAL FORCES

Let us now consider the gravitational interaction from our group-theoretical viewpoint (we shall omit $\hbar$ in this section). To this end, we start directly with the centrally extended Poincaré group $\tilde{P}$ and see how the fact that the translation generators produce the central term under commutation with some other generators (boosts) plays a singular role in the relationship between local space–time translations and local U(1) transformations. Symbolically denoting the generators of translations by P, P_0, those of boosts by K and the central one by Ξ, we find

$$[K, f\otimes P] \simeq (L_K f)\otimes P + f\otimes(P_0 + \Xi). \tag{48}$$

This means that turning the translations into *local* symmetry also entails the *local* nature of the U(1) phase. We thus expect a nontrivial mixing of gravity and electromagnetism into an infinite-dimensional electro-gravitational group.

We shall follow steps identical to those given in the former example. In turning the parameters of space–time translations *local*, we replace x^μ with $x^\mu + h^\mu_\nu(\vec{x},x^0)x^\nu$, write a finite-dimensional algebra $\mathcal{P}_{EG}$ keeping only the linear part of local space–time translations ($x^\mu + h^\mu_\nu x^\nu$, with constant $h_{\mu\nu}$), the generators of which will be called $X_{h^{\mu\nu}}$, apply the GAQ formalism and impose the "constraint" $h^{\mu\nu}=h^{\mu\nu}(\vec{x},x^0)$, on the symplectic submanifolds (solution manifolds). However, the co-homological structure of this finite-dimensional electro-gravitational subgroup, $\tilde{P}_{EG}$, is richer than that of $\tilde{P}_E$ and the exponentiation of the Lie algebra $\tilde{\mathcal{P}}_{EG}$ is by far more involved. As mentioned in the Introduction, we attempt only a basic description of the new phenomenology which results from the present revisited gauge principle, although we seek, apart from the exact Lorentz force, an approximate expression for the geodesic force in terms of the metric $g^{\mu\nu} \equiv \eta^{\mu\nu}+h^{\mu\nu}$. Thus, we shall resort only to what seems to be the basic co-homological (fundamental) constants corresponding to the inertial mass m, the electric charge q, the gravitational mass g and the *mixing vertex* coupling constant κ.

Let us write the algebra $\tilde{\mathcal{P}}_{EG}$ in an almost covariant way (the central extensions and induced deformations are necessarily non-covariant). To this end, we parametrize the Lorentz transformations with $\epsilon^{\mu\nu}$ as usual. The proposed explicit algebra is

$$
\begin{aligned}
&[\tilde{X}^L_{x^\mu},\tilde{X}^L_{\epsilon^{\nu\rho}}] = -\eta_{\nu\mu}\tilde{X}^L_{x^\rho}+\eta_{\rho\mu}\tilde{X}^L_{x^\nu}-(m+\kappa q)c(\eta_{\rho\mu}\delta^0_\nu-\eta_{\nu\mu}\delta^0_\rho)\Xi,\\
&[\tilde{X}^L_{x^\mu},\tilde{X}^L_{h^{\nu\rho}}] = -\eta_{\nu\mu}\tilde{X}^L_{x^\rho}-\eta_{\rho\mu}\tilde{X}^L_{x^\nu}+[2(g-mc)\eta_{0\mu}\delta^0_\nu\delta^0_\rho+mc(\eta_{\rho\mu}\delta^0_\nu+\eta_{\nu\mu}\delta^0_\rho)]\Xi,\\
&[\tilde{X}^L_{x^\mu},\tilde{X}^L_{A^\nu}] = -q\,\eta_{\nu\mu}\Xi,\\
&[\tilde{X}^L_{\epsilon^{\mu\nu}},\tilde{X}^L_{\epsilon^{\alpha\beta}}] = -\eta_{\alpha\nu}\tilde{X}^L_{\epsilon^{\mu\beta}}+\eta_{\beta\nu}\tilde{X}^L_{\epsilon^{\mu\alpha}}+\eta_{\alpha\mu}\tilde{X}^L_{\epsilon^{\nu\beta}}-\eta_{\mu\beta}\tilde{X}^L_{\epsilon^{\nu\alpha}},\\
&[\tilde{X}^L_{\epsilon^{\mu\nu}},\tilde{X}^l_{h^{\alpha\beta}}] = -\eta_{\alpha\nu}\tilde{X}^L_{h^{\mu\beta}}-\eta_{\beta\nu}\tilde{X}^L_{h^{\mu\alpha}}+\eta_{\alpha\mu}\tilde{X}^L_{h^{\nu\beta}}+\eta_{\mu\beta}\tilde{X}^L_{h^{\nu\alpha}}+\frac{1}{q}\{\kappa qc(\eta_{\alpha\nu}\delta^\rho_\beta\delta^0_\mu-\eta_{\mu\alpha}\delta^\rho_\beta\delta^0_\nu\\
&\quad+\eta_{\nu\beta}\delta^\rho_\alpha\delta^0_\mu-\eta_{\mu\beta}\delta^\rho_\alpha\delta^0_\nu)-2(g-mc)[(\eta_{\alpha\nu}\delta^\rho_\beta\delta^0_\mu-\eta_{\mu\alpha}\delta^\rho_\beta\delta^0_\nu+\eta_{\nu\beta}\delta^\rho_\alpha\delta^0_\mu\\
&\quad-\eta_{\mu\beta}\delta^\rho_\alpha\delta^0_\nu)\delta^\rho_0+\delta^0_\alpha\delta^0_\beta(\eta_{0\nu}\delta^0_\mu-\eta_{0\mu}\delta^\rho_\nu)]\}\tilde{X}^L_{A^\rho},\\
&[\tilde{X}^L_{\epsilon^{\mu\nu}},\tilde{X}^L_{A^\rho}] = -\eta_{\rho\nu}\tilde{X}^L_{A^\mu}+\eta_{\rho\mu}\tilde{X}^L_{A^\nu},\\
&[\tilde{X}^L_{h^{\mu\nu}},\tilde{X}^L_{h^{\alpha\beta}}] = -\eta_{\alpha\nu}\tilde{X}^L_{\epsilon^{\mu\beta}}-\eta_{\beta\nu}\tilde{X}^L_{\epsilon^{\mu\alpha}}-\eta_{\alpha\mu}\tilde{X}^L_{\epsilon^{\nu\beta}}-\eta_{\mu\beta}\tilde{X}^L_{\epsilon^{\nu\alpha}}\\
&\quad+\frac{1}{q}\{-\kappa qc[\eta_{\alpha\nu}\delta^{0\rho}_{\beta\mu}+\eta_{\beta\nu}\delta^{0\rho}_{\alpha\mu}+\eta_{\alpha\mu}\delta^{0\rho}_{\beta\nu}+\eta_{\beta\mu}\delta^{0\rho}_{\alpha\nu}]\\
&\quad+2(g-mc)[\delta^0_\alpha\delta^0_\beta(\eta_{0\nu}\delta^\rho_\mu+\eta_{0\beta}\delta^\rho_\nu)-\delta^0_\mu\delta^0_\nu(\eta_{0\beta}\delta^\rho_\beta+\eta_{0\alpha}\delta^\rho_\beta)]\}\tilde{X}^L_{A^\rho},\\
&[\tilde{X}^L_{h^{\mu\nu}},\tilde{X}^L_{A^\rho}] = -\eta_{\rho\nu}\tilde{X}^L_{A^\mu}-\eta_{\rho\mu}\tilde{X}^L_{A^\nu},
\end{aligned}
\tag{49}
$$

where $\delta^{0\rho}_{\beta\mu}\equiv\delta^0_\beta\delta^\rho_\mu-\delta^0_\mu\delta^\rho_\beta$ is the Kronecker tensor.

It bears mentioning that one of the central extension parameters, actually g, is really free at the Lie algebra level but must acquire the value $g=mc$ if the present theory is intended to reproduce the standard disconnected electromagnetic and gravitational forces for $\kappa=0$, i.e., when the constant responsible for the mixing of both interactions is switched off. The appearance of

relationships between two co-homology constants, such as $g=mc$, indicates the compatibility of further extensions of the algebra $\mathcal{P}_{EG}$ with the constants already introduced. Such further extensions could generalize the present results.

This algebra must be exponentiated in order to have a group law from which to compute left- and right-invariant vector field and the quantization one-form Θ, just as in the pure electromagnetic example. As stated above, such a process is much more involved and, in principle, a ''perturbative'' algorithm is in order. We shall resort to an approximation formula[34] up to a given order (order 3 in the fully relativistic case and 4 in the nonrelativistic limit given in Ref. 14, although in the latter the expressions obtained prove to be exact already at this order), inspired in the theory of formal groups,[35] which generalizes that of Campbell–Hausdorff in the sense that it allows for expressions which more directly fit actual physical formulas (although the latter is as well valid). In fact, it has been used in a parallel calculation carried out with REDUCE. Here is the approximate group law:

$$x''^{\alpha}=x^{\alpha}+x'^{\alpha}+\eta_{\mu[\nu}\delta_{\rho]}{}^{\alpha}\epsilon'^{\nu\rho}x^{\mu}+\eta_{\mu(\nu}\delta_{\rho)}{}^{\alpha}h'^{\nu\rho}x^{\mu}+\cdots,$$

$$\epsilon''^{\omega\rho}=\epsilon^{\omega\rho}+\epsilon'^{\omega\rho}-\tfrac{1}{4}\eta_{[\alpha[\nu}\delta_{\mu]}{}^{[\omega}\delta^{\rho]}{}_{\beta]}\epsilon'^{\mu\nu}\epsilon^{\alpha\beta}-\tfrac{1}{4}\eta_{(\alpha(\nu}\delta_{\mu)}{}^{[\omega}\delta^{\rho]}{}_{\beta)}h'^{\mu\nu}h^{\alpha\beta}+\cdots,$$

$$h''^{\omega\rho}=h^{\omega\rho}+h'^{\omega\rho}-\tfrac{1}{2}\eta_{(\alpha[\nu}\delta_{\mu]}{}^{(\omega}\delta^{\rho)}{}_{\beta)}\epsilon'^{\mu\nu}h^{\alpha\beta}+\cdots, \tag{50}$$

$$\begin{aligned}A''^{\rho}=&A^{\rho}+A'^{\rho}+(\kappa c\,\eta_{(\alpha[\nu}\delta_{\mu]}{}^{0}\delta_{\beta)}{}^{\rho})\epsilon'^{\mu\nu}h^{\alpha\beta}+\eta_{\rho[\mu}\delta_{\nu]}{}^{\alpha}\epsilon'^{\mu\nu}A^{\rho}\\&+\tfrac{1}{2}(\kappa c\,\eta_{(\alpha(\nu}\delta_{\mu)}{}^{[0}\delta^{\rho]}{}_{\beta)})h'^{\mu\nu}h^{\alpha\beta}-\eta_{\rho(\mu}\delta_{\nu)}{}^{\alpha}h'^{\mu\nu}A^{\rho}+\cdots,\end{aligned}$$

$$\begin{aligned}\varphi''=&\varphi'+\varphi-(m+\kappa q)c\,\eta_{\mu[\nu}\delta_{\rho]}{}^{0}\epsilon'^{\mu\nu}x^{\rho}-mc\,\eta_{\mu(\nu}\delta_{\rho)}{}^{0}h'^{\nu\rho}x^{\mu}+q\,\eta_{\nu\mu}A'^{\nu}x^{\mu}\\&+\tfrac{1}{2}\{(-\tfrac{1}{4}(m+\kappa q)c\,\eta_{\rho[\sigma}\delta_{\gamma]}{}^{0}\eta_{\alpha[\nu}\delta_{\mu]}{}^{[\sigma}\delta^{\gamma]}{}_{\beta]}-(m+\kappa q)c\,\eta_{\sigma[\mu}\delta_{\nu]}{}^{0}\eta_{\rho[\alpha}\delta_{\beta]}{}^{\sigma}))\epsilon'^{\mu\nu}\epsilon'^{\alpha\beta}x^{\rho}\\&-mc\,\eta_{\sigma(\mu}\delta_{\nu)}{}^{\sigma}\eta_{\rho[\alpha}\delta_{\beta]}{}^{\sigma}h'^{\mu\nu}\epsilon'^{\alpha\beta}x^{\rho}+q\,\eta_{\sigma\mu}\eta_{\rho[\alpha}\delta_{\beta]}{}^{\sigma}A'^{\mu}\epsilon'^{\alpha\beta}x^{\rho}\\&+[-\tfrac{1}{4}(m+\kappa q)c\,\eta_{\rho[\sigma}\delta_{\gamma]}{}^{0}\eta_{\alpha(\nu}\delta_{\mu)}{}^{[\sigma}\delta^{\gamma]}{}_{\beta)}-\tfrac{1}{2}\eta_{\rho\sigma}(-\kappa qc\,\eta_{(\alpha(\nu}\delta_{\mu)}{}^{[0}\delta^{\sigma]}{}_{\beta)})]h'^{\mu\nu}h'^{\alpha\beta}x^{\rho}\\&+q\,\eta_{\sigma\mu}\eta_{\rho(\alpha}\delta_{\beta)}{}^{\sigma}A'^{\mu}h'^{\alpha\beta}x^{\rho}\}+\cdots.\end{aligned}$$

From this law we can proceed following identical steps as in the pure electromagnetic case and derive the approximate quantization form Θ, approximate Noether invariants, Poincaré–Cartan form, Lagrangian, etc. Let us write explicitly Θ,

$$\begin{aligned}\Theta=d\varphi+\Big\{&(m+\kappa q)c\,\eta_{\rho[\alpha}\delta_{\beta]}{}^{0}\epsilon^{\alpha\beta}+mc\,\eta_{\rho(\alpha}\delta_{\beta)}{}^{0}h^{\alpha\beta}-q\,\eta_{\alpha\rho}A^{\alpha}\\&+\frac{1}{4}(m+\kappa q)c(\eta_{\sigma[\mu}\delta_{\nu]}{}^{0}\eta_{\rho[\beta}\delta_{\alpha]}{}^{\sigma}+\eta_{\sigma[\alpha}\delta_{\beta]}{}^{0}\eta_{\rho[\nu}\delta_{\mu]}{}^{\sigma})\epsilon^{\mu\nu}\epsilon^{\alpha\beta}-\frac{1}{4}mc(\eta_{\sigma(\mu}\delta_{\nu)}{}^{0}\eta_{\rho(\beta}\delta_{\alpha)}{}^{\sigma}\\&+\eta_{\sigma(\alpha}\delta_{\beta)}{}^{0}\eta_{\rho(\nu}\delta_{\mu)}{}^{\sigma})h^{\mu\nu}h^{\alpha\beta}+\frac{1}{2}[2(m+\kappa q)c\,\eta_{\rho(\mu}\eta_{\nu)[\alpha}\delta_{\beta]}{}^{0}+mc\,\eta_{\rho[\alpha}\eta_{\beta](\mu}\delta_{\nu)}{}^{0}]\\&+\frac{q}{2}\eta_{\nu\rho}\eta_{\omega[\alpha}\delta_{\beta]}{}^{\nu}\epsilon^{\alpha\beta}A^{\omega}-\frac{q}{2}\eta_{\nu\rho}\eta_{\omega(\alpha}\delta_{\beta)}{}^{\nu}h^{\alpha\beta}A^{\omega}\Big\}dx^{\rho}+\cdots,\end{aligned}$$

and, before writing $d\Theta$, perform a change of variables in order to take this presymplectic two-form to almost ''canonical'' (or standard) form:[36]

$$A^{\alpha}\rightarrow A^{\alpha}+\eta_{\sigma\gamma}(\epsilon^{\alpha\sigma}+h^{\alpha\sigma})A^{\gamma}\cdots,$$

$$\begin{aligned}(m+\kappa q)c\,\epsilon^{0i}\rightarrow{}&(m+\kappa q)c\,\epsilon^{0i}+\Sigma_j\{\tfrac{1}{2}(m+\kappa q)c(\epsilon^{ij}-\epsilon^{ji})\epsilon^{0j}+g\,\delta_{ij}h^{00}\epsilon^{0j}-2(m+\kappa q)ch^{ij}\epsilon^{0j}\\&+\cdots\},\\ h^{0j}\rightarrow{}&h^{0j}+\Sigma_i\,\tfrac{1}{2}(\epsilon^{ij}-\epsilon^{ji})h^{0i},\\ h^{00}\rightarrow{}&h^{00}-\tfrac{1}{4}\delta_{ij}h^{0i}\epsilon^{0j}.\end{aligned}\tag{51}$$

After this change $d\Theta$ acquires the expression

$$\begin{aligned}d\Theta={}&d\,\epsilon^{0i}\wedge dx^0(-(m+\kappa q)c(\epsilon^{0i}+h^{0i}))+(m+\kappa q)c\,d\,\epsilon^{0i}\wedge dx^i+d\,h^{00}\wedge dx^0 2mc(1-2\,h^{00})\\&+d\,h^{0i}\wedge dx^0(mch^{0i}-(m+\kappa q)c\,\epsilon^{0i})+d\,h^{00}\wedge dx^i mch^{0i}+d\,h^{0j}\wedge dx^i mc((-1+h^{00})\\&\times\delta_{ij}-h^{ji})-mc\,d\,h^{ij}\wedge dx^i h^{0j}-qdA^0\wedge dx^0+qdA^i\wedge dx^i+\cdots.\end{aligned}$$

The equations of motion can now be obtained à la Cartan by finding the kernel of this Poincaré–Cartan-like form. Then, we have

$$\begin{aligned}(m+\kappa q)c\frac{d^2\vec{x}}{dt^2}={}&q\left[\frac{d\vec{x}}{dt}\wedge\vec{\nabla}\wedge\vec{A}-\partial_0\vec{A}-\vec{\nabla}A^0\right]\\&+mc\Bigg[\partial_0\vec{h}+\vec{\nabla}h^{00}-\frac{d\vec{x}}{dt}\wedge\vec{\nabla}\wedge\vec{h}\\&+\frac{1}{4}\Bigg\{-\partial_0(h^{00}\vec{h})+\frac{d\vec{x}}{dt}\wedge\vec{\nabla}\wedge(h^{00}\vec{h})+\partial_0(\vec{\vec{h}}\cdot\vec{h})-\frac{d\vec{x}}{dt}\wedge\vec{\nabla}\wedge(\vec{\vec{h}}\cdot\vec{h})\\&-2\vec{\nabla}(h^{00^2})+\vec{\nabla}(\vec{h}\cdot\vec{h})\Bigg\}+\cdots\Bigg]\\&+\frac{\kappa qc}{2}\left[\frac{1}{4}\vec{\nabla}(\vec{h}\cdot\vec{h})+\partial_0\vec{h}-\frac{d\vec{x}}{dt}\wedge\vec{\nabla}\wedge\vec{h}+\cdots\right].\end{aligned}\tag{52}$$

The first line in (52) corresponds to the standard (exact) motion of a particle in the presence of an electromagnetic field, except for the value of the inertial mass, which is corrected by κq. The second one reproduces the standard gravito-electromagnetic force,[37] i.e., the approximation in which the gravitational field looks like an electromagnetic one. The third and fourth are the first nonlinear corrections to gravity. The fifth, however, is quite new and represents a force that looks also like the Lorentz force, at the present approximation, but generated by the gravitational potentials, although proportional to q; it should not be confused with the above-mentioned gravito-electromagnetic one. As far as the magnitude of the new Lie algebra co-homology constant κ is concerned, it is limited by experimental clearance for the difference between particle and anti-particle mass, which for the electron is about $10^{-8}m_e$. Even though this is a small value, extremely dense rotating bodies could be able to produce measurable forces. Conversely, a mixing of electromagnetism and gravity predicts a mass difference between charged particles and anti-particles, which could be experimentally tested, by measuring, for instance, the Rydberg constant

$$\left(\sim\frac{M_{\text{antiproton}}\times M_{\text{positron}}}{M_{\text{antiproton}}+M_{\text{positron}}}\right)$$

through the Lamb shift in anti-hydrogen.[38,39]

Let us remark the above-mentioned fact that one of the allowed Lie-algebra co-homology extension parameters, that is g, has been fixed to the particular value $g=mc$ in order to recover

the standard theory for $\kappa=0$. We might say that this requirement, along with another condition of ''analyticity in q'' in the group law, constitutes a group-theoretical setting of the (weak) *equivalence principle*.

Since the present theory has been formulated on the basis of our group approach to quantization, the quantum version of it would proceed in a rather straightforward manner. We shall not insist any more on this particle mechanical study while waiting for a wide generalization allowing for field degrees of freedom. In fact, a natural yet highly nonelementary attempt at an extension of the present theory to quantum field theory is in progress.[15] A further generalization of the present work in which the U(1) subgroup of phase invariance is considered as a Cartan subgroup of a larger internal symmetry group is also in order. Notice that including the phase invariance in, for instance $\mathrm{SU}(2)\otimes\mathrm{U}(1)$, would result in additional phenomenology such as the production of Z_0 particles out of gravity.

ACKNOWLEDGMENT

This work was partially supported by the DGICYT. We desire to thank G. Gibbons for pointing out a relevant misprint in the statement of the ''no-go theorems'' in a preliminary version of this paper. We also thank C. Barceló for valuable comments on the Equivalence Principle and S. Vinitsky for exciting comments on the experimental test for the new constant.

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Existence of suitable weak solutions of complex Ginzburg–Landau equations and properties of the set of singular points

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(Received 25 March 2003; accepted 12 August 2003)

In this paper, we consider the supercritical complex Ginzburg–Landau equation. We discuss the existence of suitable weak solution in Ω, where Ω is a bounded domain in $\mathbb{R}^n$ or the whole space. We also discuss the properties of the set of the singular points of the suitable weak solution in $\mathbb{R}^n$, which means that the possible singular points are located in a bounded ball for any given time and there is no singular point on the whole space after limited time. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1618360]

I. INTRODUCTION AND RESULTS

In this paper we consider the following supercritical complex Ginzburg–Landau (CGL) equations:

$$\begin{aligned} &u_t=(1+i\mu)\Delta u-(1+i\nu)|u|^{2\sigma}u+Ru \quad \text{in } \Omega\times[0,T),\\ &u(x,0)=u_0(x), \quad x\in\Omega,\\ &u(x,t)=0, \quad x\in\partial\Omega, \quad 0<t<T, \end{aligned} \tag{1}$$

where $u(x,t)$ is a complex-valued field, the initial data $u_0\in L^2$, $R>0$, $\mu,\nu\in\mathbb{R}$ and $2/n<\sigma<(n+4)/2n$, Ω is a bounded domain in $\mathbb{R}^n$ or the whole space. When $\Omega=\mathbb{R}^n$, the third line of (1) should be replaced by $u(x,t)\to 0$ as $|x|\to\infty$ for $0<t<T$. This equation, most often considered with a cubic nonlinearity and $n=3$, has a long history in physics as a generic amplitude equation near the onset of instabilities in fluid mechanical systems, as well as in the theory of phase transitions and superconductivity. In this paper, we concentrate on mathematical questions related to the regularity of weak solutions. In the case $\sigma=1$, solutions of (1) have similar scaling properties as solutions of the Navier–Stokes equations. It might be a good model problem in connection with regularity questions regarding the Navier–Stokes equations.

For Eq. (1) in the periodic case, the existence of weak solutions in all cases was obtained in Ref. 1. It is pointed out in Ref. 1 that in the subcritical case ($\sigma n<2$), all weak solutions are regular. When $\sigma n=2$, it is known that singularities cannot develop from sufficiently regular initial data (see Ref. 2 for case $\sigma=2$, $n=2$ and Ref. 1 for the general case). When $\sigma n>2$, regularity results are available only for special values of μ and ν (see Ref. 1).

For Eq. (1), the existence of a weak solution can be obtained by the Galerkin approximation. The full regularity for weak solutions of (1) in the subcritical and critical cases can be obtained by

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the usual bootstrap argument and a refined version of the standard bootstrap argument, respectively. In the supercritical case ($\sigma n>2$) it is not known whether weak solutions are regular for general values of μ and ν.

In Ref. 3, the following version of CGL was considered:

$$u_t=(1+i\mu)\Delta u-i\nu|u|^{2\sigma}u+Ru \quad \text{in } \Omega\times[0,T),$$

$$u(x,0)=u_0(x), \quad x\in\Omega, \tag{2}$$

$$u(x,t)=0, \quad x\in\partial\Omega, \quad 0<t<T.$$

The partial regularity of the suitable weak solution was discussed and the existence of the suitable weak solution was mentioned but without proof in Ref. 3. In this paper we prove the existence of the suitable weak solution of (1). Actually, it also works for (2). For more details on (1) and (2), see Refs. 3, 1, and 2.

Now we give some notations. Let $D=\Omega\times(0,T)$, B_r be the ball in $\mathbb{R}^n$ with radius r, $Q_r=Q_r(x,t)=\{(y,s):|y-x|\leqslant r, t-r^2\leqslant s<t\}$. Let $E_0(u)=\sup_{0<t<T}1/2\int_\Omega|u|^2\mathrm{d}x$, $E_1(u)=\int_0^T\int_\Omega|\nabla u|^2\mathrm{d}x\,\mathrm{d}t$, and $E=E_0+E_1$. Let $H^1(\Omega)=\{u\in L^2(\Omega):\nabla u\in L^2(\Omega)\}$ and $H_0^1(\Omega)$ be the completion of $C_0^\infty(\Omega)$ in $H^1(\Omega)$ and $H^{-1}(\Omega)$ be the dual of $H_0^1(\Omega)$. We omit Ω if there is no confusion.

The definition of suitable weak solution is the following.

Definition 1.1: We say u is a suitable weak solution of (1) on D, if the following conditions are satisfied:

(i) $u\in L^\infty(0,T;L^2(\Omega))\cap L^2(0,T;H^1(\Omega))$.
(ii) u satisfies (1) in the sense of distributions on D.
(iii) (Generalized energy inequality) For each real-valued $\phi\in C_0^\infty(D)$ with $\phi\geqslant 0$, the following inequality holds:

$$2\int\int|\nabla u|^2\phi\,\mathrm{d}x\,\mathrm{d}t+\int\int|u|^{2\sigma+2}\phi\,\mathrm{d}x\,\mathrm{d}t$$
$$\leqslant\int\int|u|^2(\phi'+2\Delta\phi)\mathrm{d}x\,\mathrm{d}t+2\Re\left\{(1+i\mu)\int\int u\nabla\bar{u}\nabla\phi\,\mathrm{d}x\,\mathrm{d}t\right\}+2R\int\int|u|^2\phi\,\mathrm{d}x\,\mathrm{d}t. \tag{3}$$

We have the following existence result.

Theorem 1.1: *Let $u_0\in L^2(\Omega)$. Then there exists a weak solution u of (1) on D satisfying*

$$u\in L^2(0,T;H_0^1)\cap L^\infty(0,T;L^2), \tag{4}$$

$$u(t)\to u_0 \ \text{ weakly in } L^2 \text{ as } t\to 0, \tag{5}$$

and if $\phi\in C^\infty(\overline{D})$, $\phi\geqslant 0$, and $\phi=0$ near $\partial\Omega\times(0,T)$, then for $0<t<T$,

$$\int_{\Omega\times\{t\}}|u|^2\phi+2\int_0^t\int_\Omega|\nabla u|^2\phi+\int_0^t\int_\Omega|u|^{2\sigma+2}\phi$$
$$\leqslant\int_\Omega|u_0|^2\phi(x,0)+\int_0^t\int_\Omega|u|^2(\phi'+2\Delta\phi)+2\Re\left\{(1+i\mu)\int_0^t\int_\Omega u\nabla\bar{u}\nabla\phi\right\}+2R\int_0^t\int_\Omega|u|^2\phi. \tag{6}$$

By the motivation of Ref. 4, we consider the property of the set of singular points of the suitable weak solution with more assumptions on the initial data. We consider (2) for simplicity and have the following theorem.

Theorem 1.2: *Suppose* $u_0 \in L^2(\mathbb{R}^n)$, *and*

$$\frac{1}{2}\int_{\mathbb{R}^n}|u_0|^2|x|\mathrm{d}x = G < \infty. \tag{7}$$

Then there exists a weak solution of the initial value problem of (2) which is regular in the region $\{(x,t):|x|^2 t^{n-2/\sigma} > K_1\}$, *where* $K_1 = K_1(E,G)$ *is a constant depending on* E *and* G.

Remark 1.1: The above theorem means that the set of singular points is restricted in a bounded domain for every time. Actually, there is no singular point in $\mathbb{R}^n$ *after a limited time, see Lemma 3.1.*

The following interpolation inequality is useful in our following proofs.

Lemma 1.1: If $u \in H^1(B_r)$, *then*

$$\int_{B_r}|u|^q \mathrm{d}x \leqslant C\left(\int_{B_r}|\nabla u|^2 \mathrm{d}x\right)^a \left(\int_{B_r}|u|^2\right)^{(q/2)-a} + \frac{C}{r^{2a}}\left(\int_{B_r}|u|^2\right)^{q/2}, \tag{8}$$

where $a = (n/4)(q-2)$, $2 \leqslant q \leqslant 2n/(n-2)$, C *independent of* r. *Moreover, if* u *has mean zero on* B_r *or if* B_r *is replaced by all of* $\mathbb{R}^n$, *then the second term on the right-hand side in (8) may be omitted.*

In the remainder of this paper we prove these two theorems, respectively.

II. PROOF OF THE THEOREM 1.1

We begin with some lemmas concerning the relevant linear systems.

Lemma 2.1: Suppose $f \in L^2(0,T;H^{-1})$, $u \in L^2(0,T;H_0^1)$, *and*

$$u_t = (1+i\mu)\Delta u + f \tag{9}$$

in the sense of distributions on D. *Then* $u_t \in L^2(0,T;H^{-1})$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |u|^2 \mathrm{d}x = 2\Re\int_\Omega u_t \overline{u}\,\mathrm{d}x \tag{10}$$

in the sense of distributions on $(0,T)$, *and* $u \in C([0,T];L^2)$ *after modification on a set of measure zero. Solution of (9) is unique in* $L^2(0,T;H_0^1)$ *for given initial data* $u_0 \in L^2$.

Proof: The proof is standard, see Refs. 4 and 5.

Lemma 2.2: Let $u_0 \in L^2$ *and* $w \in C^\infty(\overline{D};\mathbb{R})$ *with* $w \geqslant 0$. *Then there exists unique function* $u \in C([0,T];L^2) \cap L^2(0,T;H_0^1)$ *such that*

$$u_t = (1+i\mu)\Delta u - (1+i\nu)wu + Ru \tag{11}$$

in the sense of distributions on D *and* $u(0) = u_0$.

Proof: The proof is similar to Ref. 4, and for the proof of uniqueness of solution we need the Grownwall inequality.

Lemma 2.3: Let $u_0 \in L^2$, $w \in C^\infty(\overline{D};\mathbb{R})$ *with* $w \geqslant 0$ *and* u *be a solution of (11). Then for any* $\phi \in C_0^\infty(\overline{D})$ *with* $\phi = 0$ *near* $\partial\Omega \times (0,T)$, *for all* $t \in (0,T)$,

$$\int_{\Omega\times\{t\}}|u|^2\phi+2\int_0^t\int_\Omega|\nabla u|^2\phi+\int_0^t\int_\Omega w|u|^2\phi$$
$$=\int_\Omega|u_0|^2\phi(x,0)+\int_0^t\int_\Omega|u|^2(\phi'+2\Delta\phi)+2\Re\left\{(1+i\mu)\int_0^t\int_\Omega u\nabla\bar{u}\nabla\phi\right\}$$
$$+2R\int_0^t\int_\Omega|u|^2\phi. \tag{12}$$

Proof: Suppose for the moment that ϕ also vanishes near $t=0$; choose Ω_1 so that $\bar{\Omega}_1\subset\Omega$ and supp $\phi\subset\Omega_1\times(0,T)$. Writing $F=-(1+i\nu)wu+Ru\in L^2(D)$, we have

$$u_t=(1+i\mu)\Delta u+F. \tag{13}$$

Mollifying (in $\mathbb{R}^{n+1}$) each term of (13), we obtain sequences of smooth functions $\{u_m\}$ and $\{F_m\}$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}u_m=(1+i\mu)\Delta u_m+F_m, \tag{14}$$

with $u_m\to u$ in $L^2(D)$, $\nabla u_m\to\nabla u$ in $L^2(D)$, and $F_m\to F$ in $L^2(D)$. Multiplying (14) by $\bar{u}_m\phi$, integrating by part on D, and taking the real part, by Lemma 2.1, we have

$$-\int\int|u_m|^2\phi'=2\Re\left\{(1+i\mu)\left[-\int\int|\nabla u_m|^2\phi+\int\int u_m\nabla\bar{u}_m\nabla\phi+\int\int|u_m|^2\Delta\phi\right]\right\}$$
$$+2\Re\int\int F_m\bar{u}_m\phi.$$

We pass to the limit as $m\to\infty$ and obtain

$$-\int\int|u|^2\phi'=-2\int\int|\nabla u|^2\phi+2\Re\left\{(1+i\mu)\int\int u\nabla\bar{u}\nabla\phi\right\}+2\int\int|u|^2\Delta\phi$$
$$+2\Re\int\int F\bar{u}\phi.$$

On the other hand,

$$2\Re\int\int F\bar{u}\phi=2\Re\left(\int\int-(1+i\nu)w|u|^2\phi+R|u|^2\phi\right)=-2\int\int w|u|^2\phi+2R\int\int|u|^2\phi.$$

So we have

$$2\int\int|\nabla u|^2\phi+\int\int w|u|^2\phi=\int\int|u|^2(\phi'+2\Delta\phi)+2R\int\int|u|^2\phi$$
$$+2\Re\left\{(1+i\mu)\int\int u\nabla\bar{u}\nabla\phi\right\}. \tag{15}$$

For the general $\phi\in C^\infty(\bar{D})$, $\phi\geqslant 0$, by the argument in Ref. 4, we obtain (12).

Utilize the "retard mollifier" $\Psi_\delta(u)$ as in Ref. 4, we have the following lemma.

Lemma 2.4: For any $u\in L^\infty(0,T;L^2)\cap L^2(0,T;H_0^1)$,

$$\sup_{0<t<T}\int_\Omega|\Psi_\delta(u)|^2(x,t)\mathrm{d}x\leqslant CE_0(u), \tag{16}$$

$$\int \int_D |\nabla \Psi_\delta(u)|^2 \mathrm{d}x\, \mathrm{d}t \leqslant C E_1(u), \tag{17}$$

where C denotes an universal constant.

Now we are ready to prove Theorem 1.1. For any large integer N, let $\delta = T/N$, and solve

$$\frac{\mathrm{d}}{\mathrm{d}t} u_N = (1+i\mu)\nabla u_N - (1+i\nu)\Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})u_N + R u_N, \tag{18}$$

$$u_N \in L^2(0,T;H_0^1) \cap C([0,T];L^2), \tag{19}$$

$$u_N(0) = u_0. \tag{20}$$

By induction, due to Lemma 2.2, such u_N exist on each $(m\delta,(m+1)\delta)$, $0 \leqslant m \leqslant N-1$. By (10), we have

$$\int_{\Omega\times\{t\}} |u_N|^2 + 2\int_0^t \int_\Omega |\nabla u_N|^2 + 2\int_0^t \int_\Omega \Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})|u_N|^2 = \int_\Omega |u_0|^2 + 2R\int_0^t \int_\Omega |u_N|^2,$$

then

$$\int_{\Omega\times\{t\}} |u_N|^2 \leqslant \int_\Omega |u_0|^2 + 2R\int_0^t \int_\Omega |u_N|^2.$$

By the Grownwall inequality, for $t \in (0,T)$,

$$\int_{\Omega\times\{t\}} |u_N|^2 \mathrm{d}x \leqslant \exp(2RT)\int_\Omega |u_0|^2,$$

then for $t \in (0,T)$,

$$\int_{\Omega\times\{t\}} |u_N|^2 + 2\int_0^t \int_\Omega |\nabla u_N|^2 + 2\int_0^t \int_\Omega \Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})|u_N|^2 \leqslant (1+2RT\exp(2RT))\int_\Omega |u_0|^2,$$

so we have

$$\{u_N\} \text{ is bounded in } L^\infty(0,T;L^2) \cap L^2(0,T;H_0^1). \tag{21}$$

We claim that

$$\frac{\mathrm{d}}{\mathrm{d}t} u_N \in L^p(0,T;H^{-s}), \tag{22}$$

where $s > n/2$ for some $1 < p < \infty$.

By (18) and (21), it is sufficient to check that $\Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})u_N \in L^p(0,T;H^{-s})$. By Lemma 1.1, we have

$$\int_\Omega |u_N|^{2\sigma+1} \leqslant C\left(\int_\Omega |\nabla u_N|^2\right)^a \left(\int_\Omega |u_N|^2\right)^{(2\sigma+1)/2-a} + \frac{C}{r^{2a}}\left(\int_\Omega |u_N|^2\right)^{(2\sigma+1)/2},$$

where

$$a = \frac{n(2\sigma-1)}{4}.$$

For $\sigma<(4+n)/2n$, let $p=4/[n(2\sigma-1)]>1$, we have

$$\int_0^T\left(\int_\Omega |u_N|^{2\sigma+1}\mathrm{d}x\right)^p \mathrm{d}t\leqslant C(E_0^{(2\sigma+1)/2-a})^p E_1+\frac{CT}{r^{2ap}}E_0^{[(2\sigma+1)p]/2}<\infty,$$

so $\Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})u_N\in L^p(0,T;H^{-s})$.

When Ω is bounded in $\mathbb{R}^n$, by (21), (22) and Theorem 2.1 in Chap. III in Ref. 5, $\{u_N\}$ stays in a compact set of $L^2(0,T;L^2)$, then there exists a strongly convergent subsequence of $\{u_N\}$, still denoted by $\{u_N\}$, and u^* with

$$u_N\to u^* \text{ in } L^2(0,T;L^2). \tag{23}$$

By Lemma 1.1, let $r_0=\mathrm{diam}(\Omega)$,

$$\int_\Omega |u_N|^{[2(n+2)]/n}\mathrm{d}x\leqslant C\left(\int_\Omega|\nabla u_N|^2\mathrm{d}x\right)\left(\int_\Omega|u_N|^2\mathrm{d}x\right)^{2/n}+\frac{C}{r_0^2}\left(\int_\Omega|u_N|^2\mathrm{d}x\right)^{(n+2)/n},$$

then integrate from 0 to T,

$$\int_0^T\int_\Omega|u_N|^{[2(n+2)]/n}\mathrm{d}x\mathrm{d}t\leqslant CE_1E_0^{2/n}+\frac{CT}{r_0^2}E_0^{(n+2)/n}<\infty,$$

so $\{u_N\}$ is bounded in $L^{[2(n+2)]/n}(D)$. By (23), for $2\leqslant q<[2(n+2)]/n$,

$$u_N\to u^* \text{ in } L^q(0,T;L^q). \tag{24}$$

When $\Omega=\mathbb{R}^n$, we can only obtain that there exists a subsequence, still denoted by $\{u_N\}$, and u^* satisfying $u_N\to u^*$ strongly in $L^2(0,T;L^2_{\mathrm{loc}})$, $\{u_N\}$ is bounded in $L^{[2(n+2)]/n}(D)$ and then $u_N\to u^*$ strongly in $L^q(0,T;L^q_{\mathrm{loc}})$ for $2\leqslant q<[2(n+2)]/n$, which is enough to get our results.

By (21),

$$u_N\to u^* \text{ weakly in } L^2(0,T;H_0^1), \tag{25}$$

and

$$u_N\to u^* \text{ weak-star in } L^\infty(0,T;L^2). \tag{26}$$

By the definition of Ψ_δ, for some $r<(n+2)/n\sigma$,

$$\Psi_\delta(|\Psi_\delta(u_N)|^{2\sigma})\to|u^*|^{2\sigma} \text{ in } L^r(0,T;L^r), \tag{27}$$

and

$$\Psi_\delta(u_N)\to u^* \textit{ strongly in } L^q(D). \tag{28}$$

So u^* is the solution of (18) in the sense of distributions. From now on, the proof is similar to that in Ref. 4.

III. PROOF OF THE THEOREM 1.2

In this section, we consider the initial value problem of (2) for simplicity. Let $\Omega=\mathbb{R}^n$ and u be a suitable weak solution of (2) on $\mathbb{R}^n\times(0,\infty)$ with initial data $u_0\in L^2$, and for $\phi\in C_0^\infty(\mathbb{R}^n\times\mathbb{R})$ with $\phi\geqslant 0$,

$$\int_{\Omega\times\{t\}}|u|^2\phi+2\int_0^t\int_\Omega|\nabla u|^2\phi\leqslant\int_\Omega|u_0|^2\phi(x,0)+2R\int_0^t\int_\Omega|u|^2\phi+\int_0^t\int_\Omega|u|^2(\phi'+2\Delta\phi)$$
$$+2\Re\left\{(1+i\mu)\int_0^t\int_\Omega u\nabla\bar{u}\nabla\phi\right\}. \tag{29}$$

Here we need a corollary in Ref. 3.

Proposition 3.1: Let $\alpha>2$, $2\sigma+1<\alpha<[2(n+2)]/n$, there exists $\epsilon_0>0$, if u is a suitable weak solution of (2) on Q_r, and moreover,

$$\frac{1}{r^{n+2-\alpha/\sigma}}\int\int_{Q_r}|u|^\alpha\leqslant\epsilon_0, \tag{30}$$

then u is C^{α_0} in $Q_{r/4}$ for some $\alpha_0\in(0,1/2)$.

By the same idea in Ref. 3, we let $v=e^{-Rt}u$, if u is a suitable weak solution of (2), then v is a suitable weak solution of the following problem:

$$v_t=(1+i\mu)\Delta v-i\nu e^{2\sigma Rt}|v|^{2\sigma}v \quad \text{in } \Omega\times(0,T),$$
$$v(x,0)=v_0(x), \quad x\in\Omega, \tag{31}$$
$$v(x,t)=0, \quad x\in\partial\Omega,\ t\in(0,T),$$

and the corresponding generalized energy inequality

$$\int_{\Omega\times\{t\}}|v|^2\phi+2\int_0^t\int_\Omega|\nabla v|^2\phi\leqslant\int_\Omega|v_0|^2\phi(x,0)+\int_0^t\int_\Omega|v|^2(\phi'+2\Delta\phi)$$
$$+2\Re\left\{(1+i\mu)\int_0^t\int_\Omega v\nabla\bar{v}\nabla\phi\right\} \tag{32}$$

holds for any real-valued $\phi\in C^\infty(D)$ with $\phi\geqslant0$ and $\phi(t)\in C_0^\infty(\mathbb{R}^n)$ for each $t\in[0,T]$.

To prove Theorem 1.2, we need the following lemmas.

Lemma 3.1: There exists an absolute constant C such that if $t\geqslant CE^{2\sigma/(n\sigma-2)}$, then u is regular at (x,t).

Proof: By Lemma 1.1,

$$\int_{\mathbb{R}^n}|u|^\alpha dx\leqslant C\left(\int_{\mathbb{R}^n}|u|^2dx\right)^{(\alpha/2)(1-n(1/2-1/\alpha))}\left(\int_{\mathbb{R}^n}|\nabla u|^2dx\right)^{(n\alpha/2)(1/2-1/\alpha)},$$

then

$$\int_0^T\int_{\mathbb{R}^n}|u|^\alpha dx\,dt\leqslant C\left(\sup_t\int_{\mathbb{R}^n}|u|^2dx\right)^{(\alpha/2)(1-n(1/2-1/\alpha))}\int_0^T\left(\int_{\mathbb{R}^n}|\nabla u|^2dx\right)^{(n\alpha/2)(1/2-1/\alpha)}dt$$
$$\leqslant CE_0^{(\alpha/2)(1-n(1/2-1/\alpha))}E_1^{(n\alpha/2)(1/2-1/\alpha)}T^{1-(n\alpha/2)(1/2-1/\alpha)}$$
$$\leqslant CE^{\alpha/2}T^{1-(n\alpha/2)(1/2-1/\alpha)}.$$

When $E\leqslant(\epsilon_0/C)^{2/\alpha}T^{n/2-1/\sigma}$, i.e., $T\geqslant C(\epsilon_0,\alpha)E^{2\sigma/(n\sigma-2)}$,

$$\int_0^T\int_{\mathbb{R}^n}|u|^\alpha dx\,dt\leqslant\epsilon_0T^{(n+2)/2-\alpha/2\sigma}.$$

By Proposition 3.1, if

$$\int \int_{Q_r} |u|^{\alpha} dx\, dt \leqslant \epsilon_0 r^{n+2-\alpha/\sigma},$$

then u is regular in $Q_{r/4}$, so Lemma holds.

Lemma 3.2: Let $\tau = \epsilon + |x|$, $\epsilon \geqslant 0$. *If*

(i) $r \geqslant 2$, $\gamma + n/r > 0$, $\alpha + n/2 > 0$, $\beta + n/2 > 0$, $1/2 \leqslant a \leqslant 1$,

(ii) $\gamma + n/r = a(\alpha + (n-2)/2) + (1-a)(\beta + n/2)$,

(iii) $a(\alpha - 1) + (1-a)\beta \leqslant \gamma \leqslant a\alpha + (1-a)\beta$,

then

$$|\tau^{\gamma} u|_{L^2} \leqslant C |\tau^{\alpha} |\nabla u||_{L^2}^{a} |\tau^{\beta} u|_{L^2}^{1-a}. \tag{33}$$

For $n = 3$, the proof of the lemma has been given in Ref. 4; for the general case, the proof is similar.

Lemma 3.3: Let u *be a suitable weak solution of (2) with (29) holds and* $G < \infty$. *Then for a.e.* $t > 0$,

$$\frac{1}{2} \int_{\mathbb{R}^n} |u|^2 |x| dx + \int_0^t \int_{\mathbb{R}^n} |\nabla u|^2 |x| dx\, dt \leqslant A(t), \tag{34}$$

where $A(t) = G + Ct^{1/2}E$.

Proof: By Lemma 3.2,

$$\int_{\mathbb{R}^n} \frac{|u|^2}{|x|} dx \leqslant C \left(\int_{\mathbb{R}^n} |u|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla u|^2 dx \right)^{1/2},$$

then

$$\int_0^t \int_{\mathbb{R}^n} \frac{|u|^2}{|x|} dx\, dt \leqslant C E_0^{1/2} E_1^{1/2} t^{1/2} \leqslant C E t^{1/2}.$$

Let $\chi(t)$ be C^{∞} on $s \geqslant 0$ with $0 \leqslant \chi \leqslant 1$, $\chi = 1$ for $s \leqslant 1$ and $\chi = 0$ for $s \geqslant 2$. For constants $1 > \lambda \gg \epsilon > 0$, we use the test function $\phi(x) = 1/2\,(\lambda^2 - |x|^2)^{1/2} \chi(\epsilon/\lambda\,|x|)$ in the energy inequality (32). It is easy to verify that $|\nabla \phi| \leqslant C$, $|\Delta \phi| \leqslant C|x|^{-1}$, with C independent of λ and ϵ. Then

$$\int_{\mathbb{R}^n \times \{t\}} |u|^2 \phi\, dx + 2 \int_0^t \int_{\mathbb{R}^n} |\nabla u|^2 \phi dx\, dt \leqslant \int_{\mathbb{R}^n} |u_0|^2 |x| dx + C \int_0^t \int_{\mathbb{R}^n} \left\{ \frac{|u|^2}{|x|} + |u||\nabla u| \right\} dx\, dt.$$

Let $\epsilon \to 0$ and then $\lambda \to 0$,

$$\int_{\mathbb{R}^n \times \{t\}} |u|^2 |x| dx + 2 \int_0^t \int_{\mathbb{R}^n} |\nabla u|^2 |x| dx\, dt \leqslant G + C E t^{1/2}.$$

Now we prove Theorem 1.2. Let S be the set of singular points of u. By Lemma 3.1, if $(x,t) \in S$, then

$$t < C E^{2\sigma/(n\sigma - 2)}. \tag{35}$$

Let $r^2 = 5/4\,t$, $Q = Q_r(x, r^2)$, by Proposition 3.1,

$$\int \int_{Q} |u|^{\alpha} dx\, dt > C \epsilon_0 t^{n+2/2-\alpha/2\sigma}. \tag{36}$$

Let $R=|x|$ and suppose for the moment that $R\geqslant 2r$. Take $\gamma=\alpha=\beta=1/2$, $a=n/(n+2)$, and $p=[2(n+1)]/n$, by Lemma 3.2,

$$||x|^{1/2}|u||_{L^p}^p\leqslant C||x|^{1/2}|\nabla u||_{L^2}^2||x|^{1/2}|u||_{L^2}^{4/n}. \tag{37}$$

Integrate from 0 to t,

$$\int_0^t\int_{\mathbb{R}^n}|x|^{(n+2)/n}|u|^{[2(n+2)]/n}\mathrm{d}x\,\mathrm{d}t\leqslant CA(t)^{2/n}\int_0^t\int_{\mathbb{R}^n}|x||\nabla u|^2\mathrm{d}x\,\mathrm{d}t\leqslant CA(t)^{(2+n)/n}.$$

By (36) and the Hölder inequality,

$$\begin{aligned}C\epsilon_0 t^{n+2/2-\alpha/2\sigma}&\leqslant\int\int_Q|u|^\alpha\mathrm{d}x\,\mathrm{d}t\leqslant r^{n+2-\alpha n/2}\left(\int\int_Q|u|^{[2(n+2)]/n}\mathrm{d}x\,\mathrm{d}t\right)^{\alpha n/[2(n+2)]}\\&\leqslant Cr^{n+2-\alpha n/2}R^{-\alpha/2}A(t)^{\alpha/2}\leqslant K(E,G)t^{n+2/2-\alpha n/4}R^{-\alpha/2},\end{aligned}$$

so

$$R^2t^{n-2/\sigma}\leqslant K_0(E,G,\alpha).$$

For $R\leqslant 2r$,

$$R^2t^{n-2/\sigma}\leqslant 5t^{n+1-2\sigma}\leqslant C(E^{2\sigma/(n\sigma-2)})^{n+1-2/\sigma}.$$

Therefore, Theorem 1.2 holds with $K_1=C\max(K_0,E^{2\sigma/n\sigma-2(n+1-2/\sigma)})$.

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Multiplicative noise: A mechanism leading to nonextensive statistical mechanics

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(Received 10 January 2003; accepted 12 August 2003)

A large variety of microscopic or mesoscopic models lead to generic results that accommodate naturally within Boltzmann–Gibbs statistical mechanics [based on $S_1 \equiv -k\int du\, p(u)\ln p(u)$]. Similarly, other classes of models point toward nonextensive statistical mechanics [based on $S_q \equiv k[1-\int du[p(u)]^q]/[q-1]$, where the value of the entropic index $q \in \Re$ depends on the specific model]. We show here a family of models, with multiplicative noise, which belongs to the nonextensive class. More specifically, we consider Langevin equations of the type $\dot{u} = f(u) + g(u)\xi(t) + \eta(t)$, where $\xi(t)$ and $\eta(t)$ are independent zero-mean Gaussian white noises with respective amplitudes M and A. This leads to the Fokker–Planck equation $\partial_t P(u,t) = -\partial_u[f(u)P(u,t)] + M\partial_u\{g(u)\partial_u[g(u)P(u,t)]\} + A\partial_{uu}P(u,t)$. Whenever the deterministic drift is proportional to the noise induced one, i.e., $f(u) = -\tau g(u)g'(u)$, the stationary solution is shown to be $P(u,\infty) \propto \{1-(1-q)\beta[g(u)]^2\}^{1/(1-q)}$ [with $q \equiv (\tau+3M)/(\tau+M)$ and $\beta = (\tau+M/2A)$]. This distribution is precisely the one optimizing S_q with the constraint $\langle[g(u)]^2\rangle_q \equiv \{\int du\,[g(u)]^2[P(u)]^q\}/\{\int du\,[P(u)]^q\} = \text{const}$. We also introduce and discuss various characterizations of the width of the distributions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1617365]

Ubiquitous systems can be naturally described within Boltzmann–Gibbs (BG) statistical mechanics [based on the entropy $S_1 \equiv -k\int du\, p(u)\ln p(u)$]. These systems have in common the fact that they like *equally* to live everywhere they are allowed to, that is, they are ergodic in the entire phase space. However, there are other systems that, depending on the initial conditions, may prefer a particular subspace. The BG scenario may not be appropriate any longer and an extension of the usual thermostatistical description, taking into account the features of such subspace, would be required. If that subspace has a scale invariant geometry, a hierarchical or multifractal structure, then the model points toward nonextensive statistical mechanics [based on the entropic form $S_q \equiv k\,[1-\int du\,[p(u)]^q]/[q-1]\,,\ \ q \in \Re$][1] (see Ref. 2 for reviews). Among the models which belong to this category, one finds low-dimensional dissipative and conservative maps,[3] fractional and nonlinear Fokker–Planck equations,[4] Langevin dynamics with fluctuating temperature,[5] growth of many-body scale-free networks[6] and long-range many-body classical Hamiltonians.[7] The corresponding value of the entropic index q depends on the specific model, or, more precisely, on the nonextensivity universality class of the model. It is our purpose here to show a large family of models with multiplicative noise which belongs to the nonextensive class.

Microscopic dynamics, containing multiplicative noise, may be encountered in many dynamical processes, such as in stochastic resonance,[8] noise induced phase transitions,[9] granular packings,[10] and others.[11,12] Due to its significance, stochastic processes with multiplicative noise have been the subject of numerous studies in the last decades.[13–15] Here we will consider processes subject to both additive and multiplicative noises and described by the dimensionless stochastic differential equation of the form

$$\dot{u} = f(u) + g(u)\xi(t) + \eta(t), \tag{1}$$

where $u(t)$ is a stochastic variable, f,g are arbitrary functions $[g(0)=0]$, and $\xi(t), \eta(t)$ are uncorrelated and Gaussian-distributed zero-mean white noises, hence satisfying

$$\langle \xi(t)\xi(t')\rangle = 2M\delta(t-t'), \quad \langle \eta(t)\eta(t')\rangle = 2A\delta(t-t'), \tag{2}$$

where $M,A>0$ are the noise amplitudes and stand for "multiplicative" and "additive," respectively. Clearly, some degree of correlation between the two noises can be of physical relevance, however, this remains out of the present scope. The deterministic drift $f(u)$ can be interpreted either as a damping force (whenever u is a velocity-like quantity) or as an external force (when motion is overdamped and u represents a position coordinate). Other interpretations are possible as well, depending on the particular system treated.

It is interesting to note that additive and multiplicative terms in Eq. (1) could be gathered in an effective multiplicative noise term,[16] however we prefer to keep track of both sources independently.

The stochastic differential equation (1) is not completely defined and must be complemented by an additional rule. This is due to the fact that each pulse of the stochastic noise produces a jump in u, then the question arises: which is the value of u to be used in $g(u)$? This is the well-known Itô–Stratonovich controversy.[15,17] In the Itô definition, the value before the pulse must be used, whereas in the Stratonovich definition the values before and after the pulse contribute in a symmetric way. If noise were purely additive, then both definitions agree.

The Fokker–Planck equation for the probability density $P(u,t)$, associated to Eq. (1), can be obtained from the Kramers–Moyal expansion $\partial_t P = \Sigma_{n\geqslant 1}(-\partial_u)^n[D^{(n)}P]$, where the coefficients are given by

$$D^{(n)}(x,t) = \frac{1}{n!}\lim_{\tau\to 0}\frac{[u(t+\tau)-x]^n}{\tau}\bigg|_{u(t)=x}.$$

These coefficients can be readily obtained following the standard lines found for instance in Ref. 15. Using the Stratonovich definition of stochastic integral, one gets

$$D^{(1)}(u,t) = f(u) + Mg(u)g'(u) \equiv J(u), \tag{3}$$

$$D^{(2)}(u,t) = A + M[g(u)]^2 \equiv D(u), \tag{4}$$

while $D^{(n)}(u,t)=0$ for $n\geqslant 3$. Then, one arrives straightforwardly at

$$\partial_t P = -\partial_u j(u), \tag{5}$$

where $j(u)\equiv J(u)P - \partial_u[D(u)P]$ is the current. In the Itô calculation, Eq. (3) becomes $J(u) = f(u)$, that is, the noise-induced (or spurious) drift is missing. In what follows we will adopt the Stratonovich definition. However, this choice will not affect the present discussion excepting for a redefinition of some of the parameters that are involved.

Equation (5) can also be written as

$$\partial_t P = -\partial_u(f(u)P) + M\partial_u(g(u)\partial_u[g(u)P]) + A\partial_{uu}P. \tag{6}$$

In some processes, the deterministic and noise-induced drifts may have the same functional form. Let us set this condition as follows:

$$f(u) = -\tau g(u)g'(u), \tag{7}$$

τ being a proportionality constant. In other words, $f(u)$ is derived from a potential-like function $V(u) = (\tau/2)[g(u)]^2$. Let us note that the particular case $g(u)\propto f(u)\propto u$, which is a natural first choice for a physical system, verifies this condition. However, since no extra calculational difficulties emerge, we will discuss here the more general case (7). Notice that in the absence of deterministic forcing, condition (7) is trivially satisfied for any g by setting $\tau=0$.

In the present paper we will restrict to the stationary solutions for no flux boundary conditions [i.e., such that $j(-\infty)=j(\infty)=j(u)=0$], although more general conditions could in principle also

be considered. If (7) is verified, then, the stationary solution $P_s(u)$ is of the q-exponential form appearing in nonextensive statistical mechanics.[1] More precisely, in that case, one obtains

$$P_s(u) \propto [1+(q-1)\beta[g(u)]^2]^{1/(1-q)}, \tag{8}$$

where $\beta \equiv 1/kT = (\tau+M)/2A$ (where by T we generically mean the amplitude of an effective noise) and

$$q = \frac{\tau+3M}{\tau+M} \quad . \tag{9}$$

As an aside comment let us mention that if we had used the Itô convention we would have obtained $q=(\tau+4M)/(\tau+2M)$. Let us now go back to our Stratonovich choice.

P_s is normalizable if $|g(u)|$ grows with $|u|$ faster than $|u|^{1/(1+\tau/M)}$ $(\tau > -M)$. This probability distribution function (pdf) optimizes

$$S_q \equiv k \frac{1-\int \mathrm{d}u \ \ [P(u)]^q}{q-1}, \tag{10}$$

with the constraint

$$\langle [g(u)]^2 \rangle_q \equiv \frac{\int \mathrm{d}u \ \ [g(u)]^2 [P(u)]^q}{\int \mathrm{d}u [P(u)]^q} = \text{const.} \tag{11}$$

The condition (7) is not necessary for having solutions of the q-exponential form, as it follows along the lines of Refs. 18 and 19, in spite of the fact that the models therein considered are different from the present one.

Let us consider in more detail the case when both the forcing and the multiplicative noise depend on the stochastic variable u as a power law, that is, when the Langevin Eq. (1) becomes

$$\dot{u} = -\gamma u|u|^{r-1} + u|u|^{s-1}\xi(t) + \eta(t), \tag{12}$$

with $r,s \geqslant 0$ and a drift coefficient γ typically positive. In this case, the deterministic drift is derived from a confining potential-like function of the form $V(u)=\gamma|u|^{r+1}/(r+1)$. The corresponding Fokker–Planck equation becomes

$$\partial_t P = -\partial_u(-\gamma u|u|^{r-1}P) + M\partial_u(|u|^s \partial_u[|u|^s P]) + A\partial_{uu}P. \tag{13}$$

Hence, its stationary solution $P_s(u)$ is given by

$$P_s(u) = \frac{P_0 \, \mathrm{e}^{-h(u)}}{\left(1+\dfrac{M}{A}|u|^{2s}\right)^{1/2}} \quad , \tag{14}$$

P_0 being the normalization constant and

$$h(u) \equiv \frac{\gamma|u|^{1+r}}{A[1+r]} \ {}_2F_1\left(\frac{1+r}{2s},1;1+\frac{1+r}{2s};-\frac{M}{A}|u|^{2s}\right), \tag{15}$$

where ${}_2F_1$ is the hypergeometric function.

We shall analyze now some limiting cases.

(A) For vanishing deterministic forcing $(\gamma \to 0)$, Eq. (14) becomes

$$P_s(u) = \frac{P_0}{\left(1+\frac{M}{A}|u|^{2s}\right)^{1/2}}, \tag{16}$$

with

$$P_0 = \frac{(M/A)^{1/(2s)}\ \Gamma\left(\frac{1}{2}\right)}{2\,\Gamma\left(1+\frac{1}{2s}\right)\ \Gamma\left(\frac{1}{2}-\frac{1}{2s}\right)} \quad \text{for } s>1. \tag{17}$$

This pdf is of the q-exponential form (with $q=3$) as expected because, in this case, condition (7) is trivially true since it corresponds to $\tau=0$. Interestingly, in the presence of multiplicative noise, the steady state P_s is normalizable *even in the absence of a confining potential*, as long as $s>1$. The so-called spurious drift which originates from the multiplicative noise term in the Langevin equation is responsible for kicking the system back close to the origin, where fluctuations are smaller. On the other hand, the additive noise plays an essential role, providing fluctuations which avoid the full concentration (at the origin) that would occur otherwise. This type of stabilizing effect of the multiplicative noise is long known.[20]

(B) In the limit $M\to 0$, all other parameters being fixed, i.e., when no multipliciative noise is present, Eq. (14) becomes of the following stretched exponential form:

$$P_s(u) = \frac{\left[\frac{\gamma}{A[1+r]}\right]^{1/(1+r)}}{2\,\Gamma\left(1+\frac{1}{1+r}\right)}\ e^{-(\gamma/A[1+r])|u|^{1+r}}. \tag{18}$$

In particular, for the linear forcing $(r=1)$, the Gaussian pdf is recovered.

(C) In the limit $A\to 0$, i.e., for vanishing strength of the additive noise, the steady state is normalizable for $s<1$ and $p\equiv r+1-2s>0$. The condition $p>0$ implies that the potential of the drift has to be steep enough to confine the system and yield a steady state. Then, we have

$$P_s(u) = \frac{p\ \left[\frac{\gamma}{Mp}\right]^{(1-s)/p}}{2\ \Gamma\left(\frac{1-s}{p}\right)}\ \frac{e^{-(\gamma/Mp)\,|u|^p}}{|u|^s}\ . \tag{19}$$

Vanishing A concentrates the probability at the origin. Again, the Gaussian distribution is recovered for $r=1$ (harmonic forcing) and $s=0$ (additive noise).

The limits analyzed above are not generically interchangeable, that is, convergence is not necessarily uniform.

In the general case where (A,M,γ) are all finite, the same dependence on u as that in Eq. (19) is obtained for sufficiently large $|u|$. In fact, if one defines the dimensionless variable $\overline{u}=u/\lambda$ with $\lambda\equiv(A/M)^{1/2s}$, it is clear that the asymptotic expression of Eq. (14) for $|\overline{u}|\to\infty$ corresponds to both limits $|u|\to\infty$ and $A\to 0$.

For finite (A,M,γ), in the $p=0$ marginal case where the drift and multiplicative-noise exponents are related through $1+r=2s$ [hence condition (7) is verified with $\tau=\gamma/s$], a q-exponential pdf emerges at asymptotically long time. In fact, in that case, the hypergeometric in Eq. (15) becomes ${}_2F_1(1,1;2;-z)=\ln(1+z)/z$ and one gets

$$P_s(u) = \frac{P_0}{(1+|u/\lambda|^{2s})^{1/(q-1)}}\ , \tag{20}$$

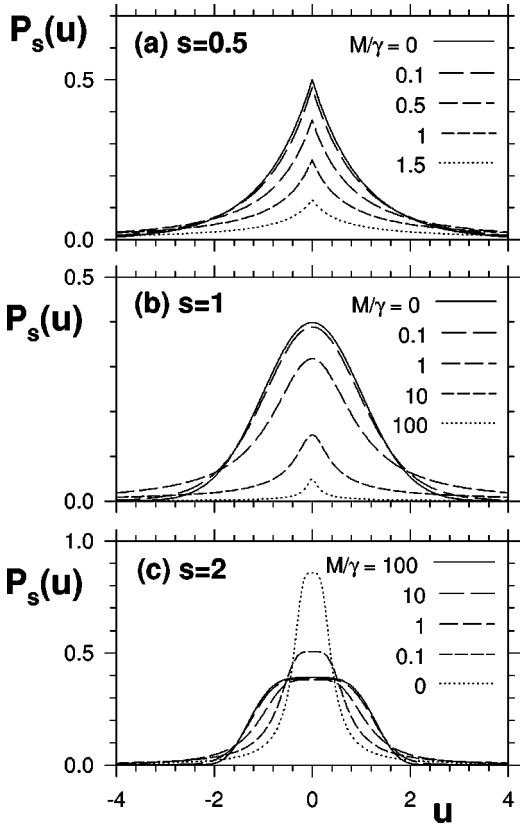

FIG. 1. Steady state pdfs for $s=0.5$ (a), 1 (b), and 2 (c), with $r=2s-1$, $A/\gamma=1$ and different values of M/γ indicated in the figure. Notice that the alternative representation $\lambda\, P_s(u)$ vs u/λ with $\lambda=(A/M)^{1/2s}$ would give profiles independent on the particular choice of A/γ.

with

$$q=\frac{(\gamma/s)+3M}{(\gamma/s)+M} \tag{21}$$

and

$$P_0=\frac{\Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}\right)}{2\lambda\,\Gamma\left(1+\frac{1}{2s}\right)\,\Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}-\frac{1}{2s}\right)} \quad . \tag{22}$$

$P_s(u)$ is normalizable for $s+\gamma/M>1$. Notice that q-exponential pdf's can appear even for negative γ (i.e., for repulsive deterministic forces). The $1+r=2s$ class includes the particular linear case $r=s=1$, that has already been treated in the literature.[11,21] In Fig. 1 we exhibit the steady state pdf (20) for several values of the system parameters.

Assuming that $\langle u\rangle=0$, the width of $P(u,t)$ can be characterized in many ways, such as (i) the inverse of the height at the origin, namely, $1/P(0,t)$; (ii) the width at half height, Δ; (iii) the square root of the mean value of u^2; (iv) the $2s$-root of the mean value of $|u|^{2s}$; (v) the square root of the q-expectation values of u^2; (vi) the $2s$-root of the q-expectation value of $|u|^{2s}$, or even combinations of these, for instance, (vii) $\sqrt{\Delta/P(0,t)}$ (see also Ref. 22). Let us recall that the normalized q-expectation of ψ is defined as

$$\langle \psi \rangle_q(t) \equiv \frac{\int \mathrm{d}u\ \psi(u)[P(u,t)]^q}{\int \mathrm{d}u\ \ [P(u,t)]^q}, \tag{23}$$

hence, $\langle \psi \rangle_1$ equals the usual mean value $\langle \psi \rangle$.

For the usual case where $P(u,t)$ is a Gaussian, all these definitions basically coincide. This is not so in general, as we shall illustrate in what follows for the stationary state of Eq. (20).

(i) The inverse of the height at the origin

$$\frac{1}{P_s(0)} = \lambda\ \frac{2\,\Gamma\left(1+\frac{1}{2s}\right)\ \Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}-\frac{1}{2s}\right)}{\Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}\right)}. \tag{24}$$

(ii) The width at half height

$$\Delta = 2\lambda\ (2^{1/[(\gamma/2sM)\ +\ 1/2]}-1)^{1/2s}. \tag{25}$$

(iii) The square root of the mean value of u^2,

$$\langle u^2 \rangle^{1/2} = \lambda\ \sqrt{\frac{\Gamma\left(\frac{3}{2s}\right)\ \Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}-\frac{3}{2s}\right)}{\Gamma\left(\frac{1}{2s}\right)\ \Gamma\left(\frac{1}{2}+\frac{\gamma}{2sM}-\frac{1}{2s}\right)}}, \tag{26}$$

for $\gamma/M > 3-s$ (otherwise it diverges).

(iv) The $2s$-root of the mean value of $|u|^{2s}$,

$$\langle |u|^{2s} \rangle^{1/2s} = \frac{\lambda}{(\gamma/M-s-1)^{1/2s}} \tag{27}$$

for $\gamma/M > 1+s$ (otherwise it diverges).

(v) The square root of the q-expectation value of u^2,

$$\langle u^2 \rangle_q^{1/2} = \lambda\ \sqrt{\frac{\Gamma\left(\frac{3}{2s}\right)\ \Gamma\left(\frac{3}{2}+\frac{\gamma}{2sM}-\frac{3}{2s}\right)}{\Gamma\left(\frac{1}{2s}\right)\ \Gamma\left(\frac{3}{2}+\frac{\gamma}{2sM}-\frac{1}{2s}\right)}}, \tag{28}$$

for $\gamma/M > 3(1-s)$ (otherwise it diverges).

(vi) The $2s$-root of the q-expectation value of $|u|^{2s}$,

$$\langle |u|^{2s} \rangle_q^{1/2s} = \frac{\lambda}{(\gamma/M+s-1)^{1/2s}}, \tag{29}$$

for $\gamma/M > 1-s$. Notice that this condition has already been encountered. Indeed, it is necessary for normalizability. An important remark is mandatory: of all the above characterizations of width which are based on expectation values (i.e., $\langle u^2 \rangle^{1/2}$, $\langle |u|^{2s} \rangle^{1/2s}$, $\langle u^2 \rangle_q^{1/2}$, and $\langle |u|^{2s} \rangle_q^{1/2s}$), *only the last one does not diverge in any admissible (i.e., normalizable) case*. This is particularly remarkable because this generalized expectation value is, as already seen, precisely the one to be used as constraint in the optimization of S_q. In addition to this, it is worthy noticing that $\langle |u|^{2s} \rangle_q^{1/2s}$ is in all cases comparable to $\sqrt{\Delta/P_s(0)}$, a semiempirical quantity which takes into account the contributions of both body and tails.

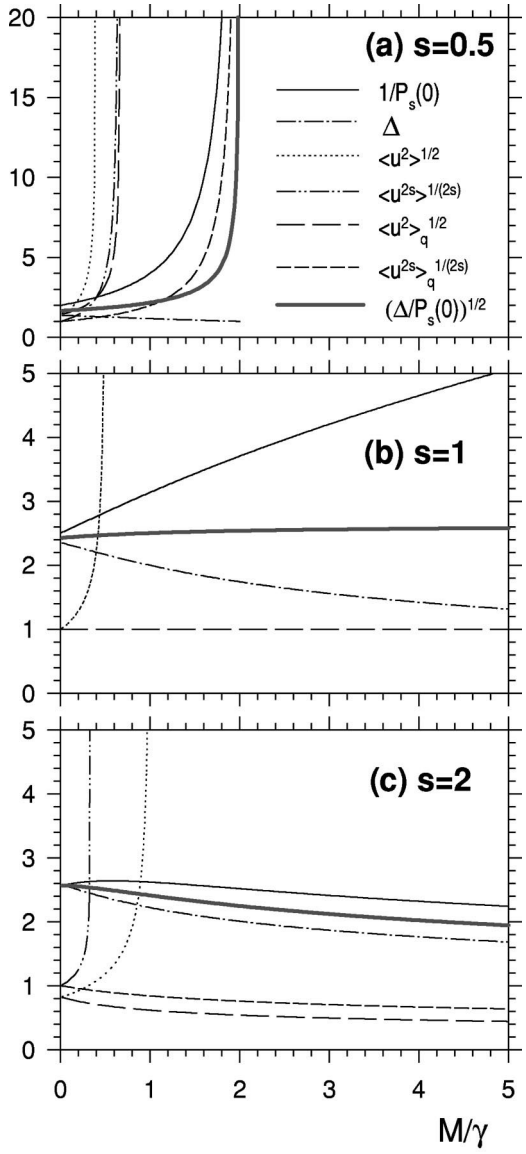

FIG. 2. Different parameters characterizing the ''width'' of the distribution as a function of M/γ for $s=0.5$ (a), 1 (b), and 2 (c), with $r=2s-1$ and $A/\gamma=1$. For $\gamma>0$, normalizability implies $M/\gamma<1/(1-s)$ if $s<1$; for $s\geqslant 1$, the physical region of M/γ extends up to infinity.

In Fig. 2 we exhibit all these quantities as a function of M/γ for typical values of s with $r=2s-1$. As M/γ increases, in all cases, $P_s(u)$ becomes more peaky around the origin (Δ decreases). Moreover, for increasing M/γ and $s=1$, the tail tends to $1/|u|$ [hence $P_s(0)\to 0$]. Also for $s=1/2$, $P_s(0)\to 0$ as the pdf becomes more tailed, but M/γ has the upper bound 2. Contrarily to the previous cases, for $s>1$, as M/γ increases, $P_s(0)$ also increases.

The q-exponential character is not exclusive of the steady state but it also emerges along the time evolution of the pdf, as illustrated in Fig. 3. In this figure we employ the semi-$\ln_q$ representation, where $\ln_q x=(x^{1-q}-1)/(q-1)$. Notice in Figs. 3(b) and 3(c) that the curve for $t\to\infty$ is a straight line. In Fig. 3(c), curves are almost straight lines, thus indicating that the pdf's are very close to q-exponentials along time.

In the presence of multiplicative noise, the system variables directly couple to noise. Therefore, behaviors are observed that can not occur in the presence of additive noise alone. In particu-

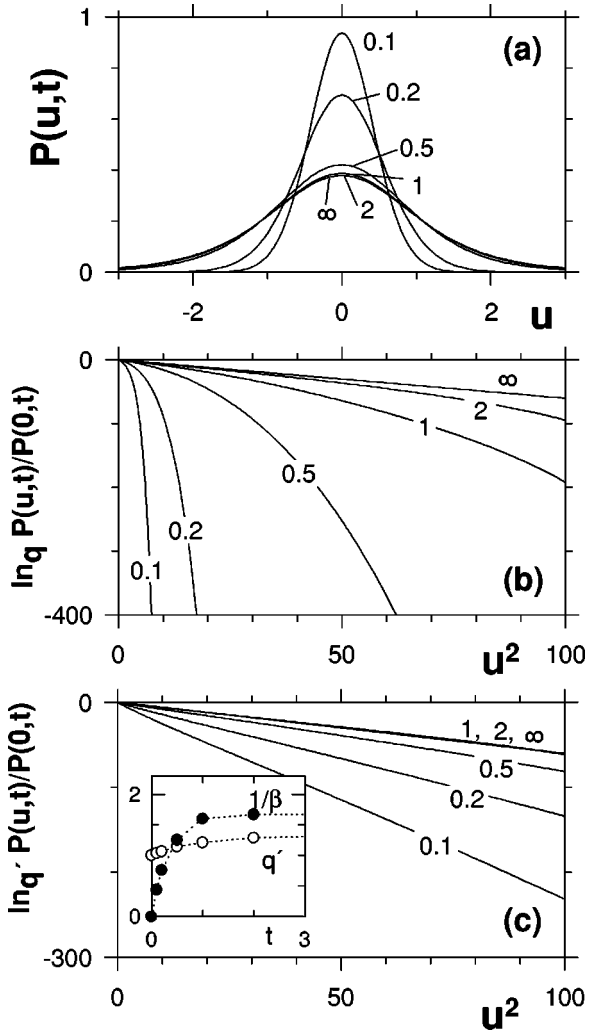

FIG. 3. Time evolution of the pdf for $r=s=1$, $A=\gamma=1$, and $M=0.2$ at different times indicated in the figure, in different representations: linear (a), semi-$\ln_q$ with $q=(\gamma+3M)/(\gamma+M)$ (b), and semi-$\ln_{q'}$, with time dependent q' (c). We used the ansatz $P=P_0(1+(q'-1)\beta u^2)^{1/(1-q')}$, with $P_0=\sqrt{\pi/\beta(q'-1)}\,\Gamma([1/(q'-1)]-\frac{1}{2})/\Gamma(1/(q'-1))$. In the inset we present q' and β vs t. In particular, $q(0)=1$, $1/\beta(0)=0$, $q(\infty)=4/3$, and $1/\beta(\infty)=5/3$.

lar, q-exponential pdf's of the form given by Eq. (8) can arise. For the present processes, q-exponentials do occur either in the absence of forcing ($\gamma=0$) or for drifts verifying Eq. (7), which, for the power-law case, becomes $r=2s-1$. The deterministic forcing does not need to be confining (i.e., $\gamma<0$ is allowed) for the formation of a q-exponential stationary pdf, provided $\gamma/M>1-s$. In any case, if a repulsive effective force prevails for some period of time, the variable u can take large values and power law tails can arise. In particular, a q-exponential occurs when the stochastic forcing is proportional to the deterministic one. Alternatively, during the intervals when the effective force is attractive, the probability tends to concentrate at the origin. Then, at this stage, the additive noise plays a fundamental role allowing the existence of a normalizable steady state by avoiding collapse of the pdf at the origin. When both kinds of noise occur simultaneously, the presence of multiplicative noise can not be formally avoided by a simple transformation of variables. The particular interplay between additive and multiplicative noises as well as that between deterministic and stochastic drifts can lead to the appearance of q-exponentials.

It is worthy to emphasize at this point that the stationary solutions of the present problem have

the general form given by Eq. (14). The q-exponential pdf's represent a special case, which in turn includes the Boltzmann–Gibss pdf as an even more special one, corresponding to the standard thermal equilibrium. Furthermore, the q-exponential pdf's are unique in the sense that they optimize, under appropriate constraints, the entropy functional S_q [Eq. (10)]. This entropic form is in turn unique in the sense that it is the only one which satisfies[23] a set of conditions naturally generalizing both the Shannon and the Kinchin axioms. Also, S_q is consistent with stability (or robustness) of the q-exponential pdf's in the sense described by Abe,[24] whereas Renyi entropy and the normalized version of S_q are not.

Let us conclude by stressing that q-exponentials have also been observed in a variety of similar processes.[5,18,25] The mechanism leading to such distributions is expected to be present in systems with long-range memory, long-range interactions, fractal or hierarchical structures and similar scenarios.

In what concerns the model defined by Eqs. (3)–(5), it is clear that $f(u)$ and $g(u)$ are generically independent functions. However, it does occur that when they are connected through Eq. (7), the q-exponential form emerges naturally. It would no doubt be very interesting if we had a geometrical interpretation of this fact. Hints along this line would be welcome.

As illustrated in Fig. 3 (deterministic drift proportional to the stochastic one), the q-exponential is exact for $t\to\infty$ and it is an excellent approximation $\forall t$.

The best characterizations of the width of the pdf's clearly are those which remain finite under generic circumstances. In our case, this happens for $1/P(0,t)$, Δ, $\langle|u|^{2s}\rangle_q^{1/2s}$ or combinations such as $\sqrt{\Delta/P(0,t)}$. The latter two are preferable since they contain attributes of both body and tails of the pdf. For a mathematically convenient and generic characterization, clearly $\langle|u|^{2s}\rangle_q^{1/2s}$ is the most appropriate.

We are grateful to C.F. Moukarzel for useful remarks and to H. Wio with regard to the comment in Ref. 16. We also acknowledge PRONEX, FAPERJ, and CNPq (Brazilian agencies) for partial financial support.

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On the generalized problem of the Boltzmann equation and the moment method in kinetic theory of gases

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(Received 23 March 2003; accepted 15 July 2003)

In this paper we formulate the generalized problem of the Boltzmann equation based on the kinetic entropy balance equation in conjunction with the maximum entropy principle. First we prove that the solution of this generalized problem is unique. We then prove that the entropy balance equation obtained by Eu in extended irreversible thermodynamics is valid, if, and only if, the one-particle distribution function f_a is the solution of this generalized problem. As a by-product of this result, we also obtain a statistical expression of the thermodynamic entropy balance equation that shares the same formula as the kinetic entropy balance equation. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1615696]

I. INTRODUCTION

In 1949 Grad constructed a formal solution of the Boltzmann equation (BE) by expanding the one-particle distribution function as a generalized Fourier series in terms of a complete orthonormal system of tensor Hermite polynomials.[1] Since then Grad's moment method has been employed as the kinetic foundation of extended irreversible thermodynamics. However the results are satisfactory only in the first order approximation. On the other hand, several different approaches to extended irreversible thermodynamics (EIT) have been proposed in the past, particularly, the theory of EIT by Jou, Casas-Vazquez, and Lebon,[2] the extended thermodynamics (ET) by Müller and Ruggeri,[3] and the modified moment method by Eu.[4] The theories by Jou *et al.*, and by Müller and Ruggeri in particular, are based on the exploitation of the thermodynamic entropy balance equation, where the dynamical equations of the moments are constructed in accordance with the macroscopic entropy principle, while the statistical foundation of the theory is based on the method of maximum entropy principle (MEP).[5] Recently Boillat and Ruggeri[6] further proved the equivalence between the entropy principle and the closure of the moments by the method of MEP. The kinetic foundation of EIT has been a challenging open problem, especially a complete analyis on the relation between kinetic entropy balance equation and thermodynamic entropy balance equation is still lacking in the literature.

The main objective of this paper is to investigate the relationship between the entropy balance equation (EBE) and the moment method from the standpoint of kinetic theory based on the Boltzmann equation. First we formulate the generalized problem of BE in terms of kinetic EBE and the maximum entropy principle. This generalized problem is equivalent to the Boltzmann equation if the entire set of moments are considered. We then prove that the solution of this generalized problem is unique. Next, we apply the solution of the generalized problem to EIT and prove that the thermodynamic EBE obtained by Eu is valid if and only if the one-particle distribution function is the solution of the generalized problem of BE. As a byproduct of this result we show that thermodynamic EBE is equivalent to kinetic EBE. Although there appears to be some overlaps between our work and those in Refs. 2–4 and 6, where MEP is employed to determine the structure of the one-particle distribution function in terms of the moments, however, the ultimate goal of this work is to investigate the relationship between kinetic EBE and thermodynamic EBE in terms of the thermodynamic variables via the Boltzmann equation. This problem has not yet been explored in the literature.

Consider a system of molecules in r components in a region of R^3 with volume V, where no

chemical reactions take place. Let f_a be the one-particle distribution function of species a at space–time $(\vec{r},t)$ with molecular velocity $\vec{v}_a$. The Boltzmann equation of the system can be written as

$$\partial_t f_a + \vec{v}_a \cdot \nabla f_a = \sum_b C(f_a, f_b), \tag{1}$$

where $C(f_a, f_b)$ is the Boltzmann collision integral.

In kinetic theory the entropy density S, the entropy current $\vec{J}_s$ and the entropy production σ, respectively, are defined by

$$\rho S = -\sum_a \int f_a \ [\ell n \ (f_a) - 1] \mathrm{d}\vec{v}_a = -\sum_a \langle f_a, \ \ell n \ (f_a) - 1 \rangle, \tag{2}$$

$$\vec{J}_s = -\sum_a \int f_a \vec{c}_a \ [\ell n \ (f_a) - 1] \mathrm{d}\vec{v}_a = -\sum_a \langle f_a, \vec{c}_a \ [\ell n \ (f_a) - 1] \rangle, \tag{3}$$

$$\sigma = -\sum_{a,b} \int C(f_a, f_b) \ \ell n \ (f_a) \mathrm{d}\vec{v}_a = -\sum_{a,b} \langle C(f_a, f_b), \ell n \ (f_a) \rangle, \tag{4}$$

where we have set the Boltzmann constant $k=1$, and $\vec{c}_a = \vec{v}_a - \vec{v}$ is the peculiar velocity with $\vec{v}$ as the mean velocity. Furthermore, we have adopted the notation $\langle A, B \rangle = \int AB \, \mathrm{d}\vec{v}_a$.

By (1)–(4) we can easily obtain the kinetic EBE,

$$\rho \, \mathrm{d}_t S + \nabla \cdot \vec{J}_s - \sigma = -\sum_a \langle B(f_a), \ell n \ (f_a) \rangle = 0, \tag{5a}$$

$$\sigma \geqslant 0, \tag{5b}$$

where $\mathrm{d}_t = \partial_t + \vec{v} \cdot \nabla$ is the substantial differentation, and $B(f_a) = (\partial_t + \vec{v}_a \cdot \nabla) f_a - \Sigma_b C(f_a, f_b)$. Although (5a) and (5b) are rigorous results of BE; however, they are void of thermodynamic information since S, $\vec{J}_s$, and σ are functions of $(\vec{r},t)$. In order to study irreversible thermodynamics, these quantities must be expressed as functions of the thermodynamic variables. Thus we define the following central moments of the molecular velocity $\vec{v}_a$:

$$\rho_a = \langle f_a, m_a \rangle, \quad c_a = \rho_a \rho^{-1}, \quad \rho = \sum_a \rho_a, \tag{6}$$

$$\rho \vec{v} = \sum_a \langle f_a, m_a \vec{v}_a \rangle, \tag{7}$$

$$\rho e = \sum_a \langle f_a, \tfrac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a \rangle, \tag{8}$$

$$\rho \hat{\phi}^{(m)}_{a,i} = \langle f_a, h^{(m)}_{a,i} \rangle. \tag{9}$$

Here e is the internal energy density, $\{h^{(m)}_{a,i}\}$ is a set of tensor Hermite polynomials constructed by Eu.[4] Notice that $h^{(m)}_{a,i}$, $i=(i_1,\ldots,i_m)$, $1 \leqslant i_k \leqslant 3$, is a tensor of order m as well as a polynomial of degree m. Moreover, $h^{(m)}_{a,i}$ is a linear combination of the tensor Hermite polynomials $H^{(n)}_{a,i}, n \leqslant m$, constructed by Grad.[1] The detailed expressions of $H^{(m)}_{a,i}$ and $h^{(m)}_{a,i}$ can be found in Refs. 1 and 4, respectively. For simplicity, hereafter we drop the tensor index i and denote $h^{(m)}_{a,i} = h^{(m)}_a$, $\hat{\phi}^{(m)}_{a,i} = \hat{\phi}^{(m)}_a$. For future reference we set $\hat{h}^{(0)}_a = m_a$, $\hat{h}^{(m)}_a = m_a \vec{v}_a$, $\hat{h}^{(e)}_a = \frac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a$, $\hat{h}^{(i)}_a$

$=h_a^{(i)}$, $i\geqslant 1$. Thus $\hat{\phi}_a^{(1)}=\vec{J}_a$ is the diffusion flux, $\hat{\phi}_a^{(2)}=\vec{\vec{\pi}}_a$ is the symmetric traceless pressure tensor, $\hat{\phi}_a^{(3)}=\vec{Q}_a$ is the heat flux, etc. We call $\hat{\phi}_a^{(i)}, i\geqslant 1$, the generalized fluxes.

In the classical theory of irreversible thermodynamics,[7] the thermodynamic states are described by the conserved variables $(e,v=\rho^{-1},c_a)$. In order to consider some nonequilibrium phenomena such as ultrasound propagation, light or neutron scattering, etc., it is necessary to include the dissipative fluxes $\hat{\phi}_a^{(i)}$ in addition to the conserved variables e,v,c_a. Let $x=\{e,v,c_a,\hat{\phi}_a^{(i)};\ 1\leqslant a\leqslant r,\ 1\leqslant i\leqslant n\}=(x^1,x^2,\ldots,x^N)$. Depending on the particular problem under consideration, n can be taken as large as necessary. Henceforth we consider x as the set of thermodynamic variables in EIT.

By the definition $B(f_a)=\partial_t f_a+\vec{v}_a\cdot\nabla f_a-\Sigma_b C(f_a,f_b)$, and (6)–(9) we can easily prove the following.

Lemma: The dynamical equations of the thermodynamical variables $x=(e,v,c_a,\hat{\phi}_a^{(k)})$ can be written as

$$\sum_a \langle B(f_a),\hat{h}_a^{(o)}\rangle=\mathrm{d}_t\rho+\rho\nabla\cdot\vec{v}=0, \tag{10}$$

$$\langle B(f_a),\hat{h}_a^{(o)}\rangle=\rho\,\mathrm{d}_t c_a+\nabla\cdot\vec{J}_a=0, \tag{11}$$

$$\sum_a \langle B(f_a),\hat{h}_a^{(m)}\rangle=\rho\,\mathrm{d}_t\vec{v}+\nabla\cdot\vec{\vec{P}}=0, \tag{12}$$

$$\sum_a \langle B(f_a),\hat{h}_a^{(e)}\rangle=\rho\,\mathrm{d}_t e+\nabla\cdot\vec{Q}+\vec{\vec{\pi}}:[\nabla\vec{v}]^{(2)}+p\nabla\cdot\vec{v}=0, \tag{13}$$

$$\langle B(f_a),\hat{h}_a^{(k)}\rangle=\rho\,\mathrm{d}_t\hat{\phi}_a^{(k)}+\nabla\cdot\Psi_a^{(k+1)}-\mathcal{Z}_a^{(k)}-\Lambda_a^{(k)}=0,\quad k\geqslant 1, \tag{14}$$

$$\mathcal{Z}_a^{(k)}=\langle f_a,(\mathrm{d}_t+\vec{c}_a\cdot\nabla)\hat{h}_a^{(k)}\rangle,\quad \Lambda_a^{(k)}=\sum_b \langle C(f_a,f_b),\hat{h}_a^{(k)}\rangle.$$

In (10)–(14), $\vec{\vec{P}}=\vec{\vec{\pi}}+p\hat{I}$ is the pressure tensor, $\hat{I}$ is the unit second order tensor, $[\nabla\vec{v}]^{(2)}$ is the traceless symmetric part of $\nabla\vec{v}$, and "$:$" denotes the scalar product of tensors. Furthermore, $\Psi_a^{(k+1)}=\langle f_a,\vec{c}_a\hat{h}_a^{(k)}\rangle$ is the flux of $\hat{\phi}_a^{(k)}$, $\mathcal{Z}_a^{(k)}$ and $\Lambda_a^{(k)}$ are the kinematic component and the collisional component of the dynamics of $\hat{\phi}_a^{(k)}$.

The proofs of (10)–(14) are cumbersome but straightforward. It should be noted that (10)–(14) do not require $B(f_a)=0$ although $B(f_a)=0$ does emerge as $k\to\infty$. This viewpoint will be further elucidated in the next section. The advantage of adopting $\hat{h}_a^{(0)},\hat{h}_a^{(m)},\hat{h}_a^{(e)}$, and $\hat{h}_a^{(k)}$ is mainly due to the fact that they are directly associated with the thermodynamic variables. Equation (14) is due to Eu, however, similar expressions have also been obtained by Jou *et al.*, and by Müller–Ruggeri.

II. FORMULATION OF THE GENERALIZED PROBLEM OF BE

In this section we formulate the generalized problem of BE. Let $R^+=[0,\infty)$, and G_1,G_2 be open subsets of the velocity space $\mathbb{R}^3$ and the spatial space $\mathbb{R}^3$, respectively. Consider $(\vec{r},t)\in G_2\times\mathbb{R}^+$ as continous parameters. Following the general theory in solving nonlinear problems in PDE's,[8] we first formulate the equivalent problem of BE as follows.

Suppose $f_a,\ \partial_t f_a,\nabla f_a\in L_2(G_1\times G_2\times\mathbb{R}^+)$. If

$$\int_{G_1} B(f_a)u(\vec{v}_a)d\vec{v}_a=\langle B(f_a),u(\vec{v}_a)\rangle=0 \tag{15a}$$

for all $u(\vec{v}_a) \in C^\infty(G_1)$, then $B(f_a)=0$ for every $(\vec{r},t)$ and a.e. for $\vec{v}_a \in G_1$. In particular, let $\{u_n\}$ be a complete orthonormal system of functions in $L_2(G_1)$. Suppose

$$\langle B(f_a), u_n \rangle = 0 \tag{15b}$$

for all n. Then $B(f_a)=0$ for every $(\vec{r},t)$.

Consider $u_n \in \{H_a^{(n)}\}_{n=0}^N$ in (15b), and set

$$f_a^N = f_a^{(0)} \sum_{n=0}^{N} \frac{1}{n!} A_a^n(\vec{r},t)\ H_a^{(n)}(\vec{v}_a),$$

where $f_a^{(0)}$ is the Maxwell Boltzmann distribution. By the orthonormality condition of $H_a^{(i)}$, $A_a^{(n)}$ can be determined by the following procedure:

$$\begin{aligned} \langle B(f_a^N), H_a^{(m)} \rangle &= 0, \quad m \leqslant N, \\ A_a^{(n)} &= 0, \quad n > N, \end{aligned} \tag{16}$$

where $A_a^{(n)}$ are functions of the thermodynamic variables. Thus Grad's moment method can be formulated as a Galerkin scheme given by (16) for any finite N.[8] It is evident that (16) yields a formal solution of BE as $N \to \infty$.

Due to the term $\ell n f_a$ in (2) and (3), it is difficult to obtain simple expressions for S, $\vec{J}_s$, and σ in terms of the thermodynamic variables. In order to overcome this difficulty we resort to the kinetic entropy balance equation (kinetic EBE) (5a) and consider

$$\langle B(f_a), \ell n f_a \rangle = 0. \tag{17}$$

Define

$$\hat{h}_a = (\hat{h}_a^{(0)}, \hat{h}_a^{(m)}, \hat{h}_a^{(e)}, \hat{h}_a^{(k)}), \quad k=1,\ 2,\ldots,n,$$

$$\lambda_a = (\lambda_a^{(0)}, \vec{\lambda}_{(m)}, \lambda_e, \lambda_a^{(k)}), \quad k=1,\ 2,\ldots,n.$$

Here $\lambda_a^{(0)}$ and λ_e are scalar functions, $\vec{\lambda}_{(m)}$ is a vector function, while $\lambda_a^{(k)}$ is a kth order tensor function. These functions are functions of $(\vec{r},t)$. We look for f_a that satisfies (17) under the constraints (6)–(9). In view of (10)–(14) we set

$$\ell n f_a = \lambda_a^{(0)} \hat{h}_a^{(0)} + \vec{\lambda}_{(m)} \cdot \hat{h}_a^{(m)} + \lambda_e \hat{h}_a^{(e)} + \sum_{k=1} \lambda_a^{(k)} : \hat{h}_a^{(k)} = \lambda_a \cdot \hat{h}_a \ \in \ \mathrm{Span}\{\hat{h}_a^{(0)}, \hat{h}_a^{(m)}, \hat{h}_a^{(e)}, \hat{h}_a^{(k)}\}_{k=1}^n. \tag{18}$$

Thus we solve (17) with $\ell n f_a$ given by (18) for appropriate choices of λ_a. Since both λ_a and $\hat{h}_a$ are linearly independent sets, by (17) we have $\langle B(f_a), \hat{h}_a \rangle = 0$. This in turn gives rise to the dynamical equations of the thermodynamic variables (10)–(14). On the other hand, λ_a can be determined by the constraint conditions (6)–(9) that maximize the entropy density function (maximum entropy principle). In analogy with Grad's moment method, we now formulate the generalized problem of BE as follows:

(i) Solve $\langle B(f_a), \ell n f_a \rangle = 0$ with $\ell n f_a$ given by (18).
(ii) Determine λ_a by the constraint conditions (6)–(9) that maximizes the entropy density function.

Notice that step (i) is equivalent to the dynamical equations (10)–(14), while step (ii) determines the structure f_a that satisfies the maximum entropy principle. Since $\{h_a^{(m)}\}$ also forms a

complete orthonormal system of functions in $L_2(G_1)$, by (15b), the solution of this generalized problem also yields a formal solution of BE as $n\to\infty$. The advantage of this method is that EBE is satisfied for any finite n. In the next section we further consider the solution of this generalized problem and its consequences.

III. RELATIONSHIP BETWEEN KINETIC EBE AND THERMODYNAMIC EBE

By (18) f_a can be expressed as

$$f_a(\vec{v}_a,\vec{r},t)=\exp\ [\lambda_a(\vec{r},t)\cdot\hat{h}_a(\vec{c}_a)-\epsilon(\vec{c}_a\cdot\vec{c}_a)^n], \tag{19}$$

where ϵ is an infinitesimal positive real number which is required to ensure that $F_a=\lim_{\epsilon\to0}\int f_a d\vec{v}_a$ is finite. Then $w_a=(F_a)^{-1}f_a$ can be considered as a probability density function. Next we determine the coefficient functions λ_a as follows:

$$\rho_a=\lim_{\epsilon\to0}\langle f_a,\hat{h}_a^{(0)}\rangle=\lim_{\epsilon\to0}\langle f_a^{(0)},\hat{h}_a^{(0)}\rangle,\quad \rho=\sum_a\ \rho_a, \tag{20a}$$

$$\rho\vec{v}=\lim_{\epsilon\to0}\sum_a\ \langle f_a,\hat{h}_a^{(m)}\rangle=\lim_{\epsilon\to0}\sum_a\ \langle f_a^{(0)},\hat{h}_a^{(m)}\rangle, \tag{20b}$$

$$\rho e=\lim_{\epsilon\to0}\sum_a\ \langle f_a,\hat{h}_a^{(e)}\rangle=\lim_{\epsilon\to0}\sum_a\ \langle f_a^{(0)},\hat{h}_a^{(e)}\rangle, \tag{20c}$$

$$\rho\hat{\phi}_a^{(k)}=\lim_{\epsilon\to0}\langle f_a,\hat{h}_a^{(k)}\rangle. \tag{20d}$$

Consequently the solution of the generalized problem of BE can be written as

$$\begin{aligned} f_a^{(M)}&=\exp\left\{(\mu_aT^{-1})\hat{h}_a^{(0)}-T^{-1}\hat{h}_a^{(e)}-\sum_{k=1}^{n}\ (X_a^{(k)}T^{-1}):\hat{h}_a^{(k)}-\epsilon(\vec{c}_a\cdot\vec{c}_a)^n\right\}\\ &=\exp\left\{-T^{-1}\left[-m_a\mu_a+\frac{1}{2}m_a\vec{c}_a\cdot\vec{c}_a+\sum_{k=1}^{n}X_a^{(k)}:\hat{h}_a^{(k)}\right]-\epsilon(\vec{c}_a\cdot\vec{c}_a)^n\right\}, \end{aligned} \tag{21}$$

where T is the local thermodynamics temperature, μ_a the chemical potential of molecular species a,[7] and $X_a^{(k)}=T^{-1}\lambda_a^{(k)}$ determined by (20d) is the generalized potential conjugate to the generalized fluxes $\hat{\phi}_a^{(k)}$. Here T, μ_a and $X_a^{(k)}$ are now functions of the thermodynamic variables that are governed by (10)–(14).

In terms of $f_a^{(M)}$ and the definitions of the entropy density function as well as the entropy current function, we have

$$S_M=T^{-1}\left[e+p\nu-\sum_a\ \mu_ac_a+\sum_k\ X_a^{(k)}:\hat{\phi}_a^{(k)}\right]+0(\epsilon), \tag{22a}$$

$$\vec{J}_M=T^{-1}\left[\vec{Q}-\sum_a\ \mu_a\vec{J}_a+\sum_k\ X_a^{(k)}\cdot\Psi_a^{(k+1)}\right]+0(\epsilon)=T^{-1}\vec{Q}_c+0(\epsilon). \tag{22b}$$

Since the term $0(\epsilon)$ does not contain any physical significance, hereafter we drop this term for simplicity. In general it is rather difficult to find exact solutions for $X_a^{(k)}$ from (22d),[9] however, approximate solutions for $X_a^{(k)}$ can be found in Refs. 2–4. It is well known in probability theory that different probability density functions can have the same set of moments. Thus it is inappropriate to find $X_a^{(k)}$ via $A_a^{(k)}$ in (16).[10]

The exponential form of $f_a^{(M)}$ in (21) has been proposed by Eu. Similar expression of $f_a^{(M)}$ has also been proposed by Müller–Ruggeri. As S_M and $\vec{J}_M$ are functions of the thermodynamic variables, we call S_M and $\vec{J}_M$ the thermodynamic entropy density function and entropy current function, respectively.[11] Now we prove that $f_a^{(M)}$ is the unique solution of the generalized problem of BE. To this end, we assume that f_a is another one-particle distribution function that satisfies (17) and (6)–(9). With the aid of the inequality $\ell n \mathcal{Z} \leqslant \mathcal{Z}-1$, we can easily prove

$$\begin{aligned}\rho S-\rho S_M &= -\sum_a \langle f_a, \ell n f_a - 1\rangle + \lim_{\epsilon\to 0}\sum_a \langle f_a^{(M)}, \ell n f_a^{(M)} - 1\rangle \\ &= \lim_{\epsilon\to 0}\sum_a \left\{ \int f_a \ell n\left(\frac{f_a^{(M)}}{f_a}\right) \mathrm{d}\vec{v}_a + \int (f_a - f_a^{(M)})\mathrm{d}\vec{v}_a \right\} \\ &\leqslant \lim_{\epsilon\to 0}\sum_a \int [(f_a^{(M)} - f_a) + (f_a - f_a^{(M)})]\ \mathrm{d}\vec{v}_a = 0,\end{aligned}$$

where equality holds if and only if $f_a = f_a^{(M)}$. Therfore, among all f_a's that satisfy (17) and the constraint conditions (6)–(9), $f_a^{(M)}$ is the unique one-particle distribution function that maximizes the entropy density function.

Theorem 1: The solution of the generalized problem of the Boltzmann equation is uniquely given by (21).

Next we consider the thermodynamics EBE. By (22b) and the dynamical equations of the thermodynamic variables x in (10)–(14), we can obtain the following equation:[4]

$$\rho T^{-1}\left\{ \mathrm{d}_t e + p\,\mathrm{d}_t \nu - \sum_a \mu_a \mathrm{d}_t c_a + \sum_{a,k} X_a^{(k)} : \mathrm{d}_t \hat{\phi}_a^{(k)} \right\} + \nabla\cdot\vec{J}_M = \Sigma_M, \tag{23a}$$

$$\begin{aligned}\Sigma_M = -T^{-1}\Big\{ &\vec{Q}_c\cdot\nabla \ell n T + \vec{\vec{\pi}} : [\nabla\vec{v}]^{(2)} + \sum_a \vec{J}_a\cdot\nabla\mu_a \\ &- \sum_{a,k} \Psi_a^{(k+1)}\cdot(\nabla X_a^{(k)}) - \sum_{a,k} X_a^{(k)} : (\mathcal{Z}_a^{(k)} + \Lambda_a^{(k)}) \Big\}.\end{aligned} \tag{23b}$$

In order to identify (23a) with thermodynamic EBE and Σ_M with thermodynamic entropy production, we follow the method by Müller–Ruggeri and consider the inequality

$$\rho\,\mathrm{d}_t S_M + \nabla\cdot\vec{J}_M \geqslant 0. \tag{24}$$

The minimization of (24) can be carried out by introducing a function $\Sigma \geqslant 0$ subject to the constraint conditions (10)–(14). Then we have

$$\begin{aligned}\rho\,\mathrm{d}_t S_M + \nabla\cdot\vec{J}_M - \Big\{ \Sigma - \sum_a \alpha_a(\rho\,\mathrm{d}_t c_a + \nabla\cdot\vec{J}_a) - \vec{\alpha}_m\cdot(\rho\,\mathrm{d}_t\vec{v} + \nabla\cdot\vec{\vec{P}}) - \alpha_e(\rho\,\mathrm{d}_t e + \rho p\,\mathrm{d}_t\nu + \nabla\cdot\vec{Q} \\ + \vec{\vec{\pi}} : [\nabla\vec{v}]^{(2)}) - \sum_{a,k} \alpha_a^{(k)} : (\rho\,\mathrm{d}_t\hat{\phi}_a^{(k)} + \nabla\cdot\Psi_a^{(k+1)} - \mathcal{Z}_a^{(k)} - \Lambda_a^{(k)}) \Big\} = 0,\end{aligned} \tag{25a}$$

where α_a, $\vec{\alpha}_m$, α_e, and $\alpha_a^{(k)}$ are Lagrange multipliers. On the other hand, (25a) can be recast as

$$\rho\,\mathrm{d}_t S_M + \nabla\cdot\vec{J}_M - \Sigma = -\sum_a \int B(f_a)\left\{ \alpha_a\hat{h}_a^{(0)} + \vec{\alpha}_m\cdot\ \hat{h}_a^{(m)} + \alpha_e\hat{h}_a^{(e)} + \sum_k \alpha_a^{(k)} :\ \hat{h}_a^{(k)} \right\} \mathrm{d}\vec{v}_a = 0. \tag{25b}$$

But the right-hand side of (25b) is the same as (17) with $\ell n f_a = \hat{\alpha}_a \cdot \hat{h}_a$, $\hat{\alpha}_a = (\alpha_a, \vec{\alpha}_m, \alpha_e, \alpha_a^{(k)})$. By (20a)–(20d) we obtain $\alpha_a = \mu_a T^{-1}$, $\vec{\alpha}_m = 0$, $\alpha_e = -T^{-1}$, and $\alpha_a^{(k)} = -T^{-1} X_a^{(k)}$. Henceforth $\Sigma_M = \Sigma \geqslant 0$, $\vec{J}_M = T^{-1} \vec{Q}_c$, and the evolution of S_M is given by

$$T\, \mathrm{d}_t S_M = \mathrm{d}_t e + p\, \mathrm{d}_t \nu - \sum_a \mu_a \mathrm{d}_t c_a + \sum_{a,k} X_a^{(k)} : \mathrm{d}_t \hat{\phi}_a^{(k)}, \tag{26a}$$

that can be transformed into the well-known Gibbs one-form[2–4]

$$T\, \mathrm{d}S = \mathrm{d}e + p\, \mathrm{d}\nu - \sum_a \mu_a\, \mathrm{d}c_a + \sum_{a,k} X_a^{(k)} : \mathrm{d}\hat{\phi}_a^{(k)}. \tag{26b}$$

Therefore, if $f_a = f_a^{(M)}$, then thermodynamic EBE is given by (23a) and (23b). For the converse, assume (23a) and (23b). Then $f_a = f_a^{(M)}$ follows from (24), (25a), and (25b).

Theorem 2: The thermodynamic entropy balance equation $\rho\, \mathrm{d}_t S_M + \nabla \cdot \vec{J}_M - \Sigma_M = 0$ with $\Sigma_M \geqslant 0$ is given by (23a) and (23b) if and only if f_a is the solution of the generalized problem of the Boltzmann equation.

As a consequence of (25b) and Theorem 2 we have the following.

Corollary: The statistical expression of the thermodynamic entropy balance equation is given by

$$\rho\, \mathrm{d}_t S_M + \nabla \cdot \vec{J}_M - \Sigma_M = -\sum_a \langle B(f_a^M),\ \ell n(f_a^M) \rangle = 0.$$

In other words, thermodynamic EBE and kinetic EBE share the same microscopic formula.

We could have obtained the thermodynamic EBE (23a) from (22a) in conjunction with the dynamical equations of the thermodynamic variables (10)–(14). However this approach relies on finding the integral manifold of the Pfaffian equation $\xi = 0$ under the inaccessibility condition $\xi \Lambda d\xi = 0$,[12] where

$$\xi = \mathrm{d}e + p\, \mathrm{d}\nu - \sum_a \mu_a\, \mathrm{d}c_a + \sum_{a,k} X_a^{(k)} : \mathrm{d}\hat{\phi}_a^{(k)}.$$

Finally we examine the relationship between σ and Σ_M. By (23b) it is evident that Σ_M contains σ as well as other dissipative energies attributable to the dynamics of the moments via the evolution equations (10)–(14). On the other hand, molecular collisions are the only contributor of σ. Therefore Σ_M cannot be obtained from (4) by direct substitution of $f_a = f_a^{(M)}$.

IV. CONCLUSION

Extended irreversible thermodynamics is a phenomenological science. The foundation of EIT constructed by Jou *et al.* and by Müller–Ruggeri is based on the exploitation of the thermodynamic entropy balance equation, while the theory of EIT developed by Eu is based on the modified moment method closely related to the theory of Grad. According to Jou *et al.* and Müller–Ruggeri, the dynamical equations of the moments are constructed such that the thermodynamic EBE is satisified. In the meanwhile, the statistical foundation of the theory is based on the maximum entropy principle that determines the structure of the one-particle distribution function in terms of the moments. Following the general theory in solving nonlinear problems in PDEs, first we formulate the generalized problem of the Boltzmann equation in terms of kinetic EBE in conjunction with the maximum entropy principle. This generalized problem ultimately gives rise to a formal solution of the Boltzmann equation if the entire set of moments are considered. Notice that there are many different f_a's that satisfy the kinetic entropy balance equation (5a). However the maximum entropy principle can be satisfied if and only if $f_a = f_a^{(M)}$. Thus the solution of the generalized problem of BE is uniquely given by (21). We then apply this result to EIT and prove

that thermodynamic EBE given by (23a) and (23b) holds if and only if f_a is the solution of the generalized problem of the Boltzmann equation. As a byproduct of Theorem 2 we obtain a statistical expression of thermodynamic EBE that shares the same formula as the kinetic EBE in (5a). In other words, kinetic EBE is equivalent to thermodynamic EBE if and only if $f_a = f_a^{(M)}$.

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Stochastic dynamics of the scattering amplitude generating *K*-distributed noise

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(Received 18 November 2002; accepted 21 July 2003)

We derive the stochastic dynamics of the complex valued amplitude resulting from coherent scattering from a random population of scatterers when this becomes asymptotically large. Considerations of a random walk model, introduced by Jakeman, are used to derive stochastic differential equations for the amplitude and corresponding intensity and phase stochastic processes. An analysis of the correlation structure in the fluctuations is provided and interpreted geometrically in terms of the gauge invariant properties of the field and the Markov property. A Fokker–Planck description for the evolution of the probability density is given and the equilibrium and detailed balance conditions shown to hold. Expressions for the intensity autocorrelation function and power spectral density are provided in closed form. The practical implications of the stochastic theory are discussed. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1611264]

I. INTRODUCTION

Recent developments in the diffusion based analysis of scattering from random media, reported in Field and Tough (2003), have led to significant results that enable the identification of *K*-distributed noise processes in electromagnetic scattering. The results comprise various stochastic differential equations (SDEs) for the scattered amplitude, intensity, phase and scattering cross section motivated by a combination of theoretical considerations and analysis of empirical data.

The purpose of the present paper is to formulate the stochastic dynamics of the electromagnetic field, scattered from a random medium that consists of a collection of independent component scatterers, whose population size has fluctuations in accordance with the birth–death–immigration (BDI) model (Bartlett, 1966). This is achieved from first principles via considerations of the complex random walk model introduced by Jakeman (Jakeman, 1980). Our results thus provide the theoretical foundation of the anomaly detection technique reported earlier (Field and Tough, 2003), and extend the model to include a detailed description of the intensity autocorrelation function and power spectral density.

The paper is organized as follows. Section II begins with a derivation of the complex amplitude SDE in the case of a constant scattering cross section, i.e., Rayleigh scattering, from considerations of a complex random walk model, and extends this to the *K*-distributed case via the insertion of step number fluctuations. The resulting SDE for the amplitude process is used to derive corresponding SDEs for the intensity and phase processes, and expressions for the squared volatilities of each of these processes are provided. This framework is used to explain the geometrical structure of the correlations in the fluctuations of the complex amplitude.

In Sec. III we provide a Fokker–Planck description for the joint probability density of the scattering cross section and intensity processes and study the asymptotic behavior. It is verified that the model possesses the joint probability appropriate to the *K*-distribution, and that the condition for detailed balance is also satisfied.

Section IV provides a detailed analysis of the finite-time correlation properties of the stochastic model. The Green's functions arising from the Fokker–Planck description are computed and

expressions for the intensity autocorrelation function and power spectral density are provided in closed form. We conclude in Sec. V with an account of the interpretation and practical implications of the theoretical framework proposed.

II. STOCHASTIC DYNAMICS OF AMPLITUDE PROCESS

A. Amplitude

We develop the random walk model with step number fluctuations due to Jakeman (see Jakeman, 1980; Jakeman and Tough, 1988) as a continuous time diffusion process. It is shown in the Rayleigh case of a fixed step number that the amplitude obeys a complex Ornstein–Uhlenbeck equation, and a corresponding SDE in the K-distributed case is derived.

1. Rayleigh scattering

In the Rayleigh case consider the random walk model for the scattered electric field (cf. Jakeman, 1980; Tough, 1987; Jakeman and Tough, 1988),

$$\mathcal{E}_t^{(N)} = \sum_{j=1}^{N} \exp[i\varphi_t^{(j)}] \tag{2.1}$$

for constant population size N. Since Maxwell's equations for the electromagnetic field possess U(1) gauge invariance with respect to duality rotations, i.e., multiplication by $\exp(i\Lambda)$ for constant Λ (cf. Penrose and Rindler, 1984), the assumption of independence of $\{\varphi^{(j)}\}$ implies that these phases are uniformly distributed. Accordingly in (2.1) the phase factors $\{\exp[i\varphi_t^{(j)}]\}$ are independent and uniformly distributed on the unit circle in $\mathbb{C}$. Our (phase) diffusion model therefore takes $\{\varphi_t^{(j)}\}$ as a collection of (displaced) Wiener processes on a suitable time scale, $\varphi_t^{(j)} = \Delta^{(j)} + \mathcal{B}^{1/2} W_t^{(j)}$, with the random initializations $\{\Delta^{(j)}\}$ a set of independent random variables uniformly distributed on the interval $[0,2\pi)$, and thus $\mathrm{d}\varphi_t^{(j)} = \mathcal{B}^{1/2}\,\mathrm{d}W_t^{(j)}$, $\mathrm{d}\varphi_t^{(j)2} = \mathcal{B}\,\mathrm{d}t$. From Ito's formula (e.g., Oksendal, 1998; Karatzas and Shreve, 1988) the Ito differential of (2.1) is

$$\mathrm{d}\mathcal{E}_t^{(N)} = \sum_{j=1}^{N} \left(i\,\mathrm{d}\varphi_t^{(j)} - \frac{1}{2}\,\mathrm{d}\varphi_t^{(j)2} \right) \exp[i\varphi_t^{(j)}]. \tag{2.2}$$

The first term $\Sigma_{j=1}^{N} i\,\mathrm{d}\varphi_t^{(j)} \exp[i\varphi_t^{(j)}]$ on the right-hand side of (2.2) consists of a sum of independent randomly phased Wiener processes, with variance equal to $\mathcal{B}N\,\mathrm{d}t$, while the second term is independent of the scatterer label j. Thus from (2.2) we can write

$$\mathrm{d}\mathcal{E}_t^{(N)} = -\tfrac{1}{2}\mathcal{B}\mathcal{E}_t^{(N)}\,\mathrm{d}t + (\mathcal{B}N)^{1/2}\,\mathrm{d}\xi_t, \tag{2.3}$$

where ξ_t is a complex Wiener process satisfying $|\mathrm{d}\xi_t|^2 = \mathrm{d}t$, $\mathrm{d}\xi_t^2 = 0$. The process ξ_t is adapted to the filtration $\mathcal{F}^{(\varphi)} = \cup_j \mathcal{F}^{(j)}$, where $\mathcal{F}^{(j)}$ is the filtration appropriate to the component scatterer phase $\varphi_t^{(j)}$. The amplitude process Ψ_t is then defined by $\Psi_t = \lim_{N\to\infty}[\mathcal{E}_t^{(N)}/\overline{N}^{1/2}]$ and satisfies the SDE,

$$\mathrm{d}\Psi_t = -\tfrac{1}{2}\mathcal{B}\Psi_t\,\mathrm{d}t + (\mathcal{B}x)^{1/2}\,\mathrm{d}\xi_t, \tag{2.4}$$

where the continuous valued random variable x, the average scattering power, arises from an asymptotically large population via $x = \lim_{N\to\infty}[N/\overline{N}]$.

2. K-distributed noise

In the case of step number fluctuations in the random walk model (2.1), we define the amplitude Ψ_t in a similar manner to the Rayleigh case above, with the modification that we employ a time dependent N_t such that $x_t = \lim_{N_t\to\infty}[N_t/\overline{N}]$. Thus

$$\Psi_t = \lim_{N_t\to\infty}\left\{\frac{1}{\overline{N}^{1/2}}\sum_{j=1}^{N_t}\exp[i\varphi_t^{(j)}]\right\} \tag{2.5}$$

$$= \lim_{N_t\to\infty}\left\{\left(\frac{N_t}{\overline{N}}\right)^{1/2}\frac{1}{N_t^{1/2}}\sum_{j=1}^{N_t}\exp[i\varphi_t^{(j)}]\right\} \tag{2.6}$$

$$= x_t^{1/2}\gamma_t, \tag{2.7}$$

where $\gamma_t = \lim_{N\to\infty}[\mathcal{E}_t^{(N_t)}/N_t^{1/2}]$. According to the arguments given in the Rayleigh case above, γ_t is a complex Ornstein–Uhlenbeck process which obeys the SDE

$$\mathrm{d}\gamma_t = -\tfrac{1}{2}\mathcal{B}\gamma_t\,\mathrm{d}t + \mathcal{B}^{1/2}\,\mathrm{d}\xi_t. \tag{2.8}$$

Observe from (2.4), therefore, that γ_t is a unit power Rayleigh process. The above equation for γ_t can be solved by considering the stochastic differential $\mathrm{d}[\exp(\frac{1}{2}\mathcal{B}t)\gamma_t]$, which leads to the solution

$$\gamma_t = \exp\left(-\frac{1}{2}\mathcal{B}t\right)\left\{\gamma_0 + \mathcal{B}^{1/2}\int_0^t \exp\left(\frac{1}{2}\mathcal{B}s\right)\mathrm{d}\xi_s\right\}. \tag{2.9}$$

We deduce the expectation formulas

$$\mathbb{E}[\gamma_t] = \exp(-\tfrac{1}{2}\mathcal{B}t)\gamma_0, \tag{2.10}$$

$$\mathbb{E}[|\gamma_t|^2] = 1 + \exp(-\mathcal{B}t)(|\gamma_0|^2 - 1). \tag{2.11}$$

From (2.11) it follows that $\lim_{t\to\infty}\mathbb{E}[|\gamma_t|^2] = 1$ and so from (2.7) we find the intensity process, defined by $z_t = |\Psi_t|^2$, satisfies $\mathbb{E}[z_t] = x_t$. The SDE for Ψ_t, as determined by (2.7), can now be derived, via the Ito product formula $\mathrm{d}(X_tY_t) \equiv X_t\,\mathrm{d}Y_t + Y_t\,\mathrm{d}X_t + \mathrm{d}X_t\,\mathrm{d}Y_t$. For this purpose it is convenient to introduce the square-root cross section $r_t = x_t^{1/2}$ and thus, from (2.7), we find $\mathrm{d}\Psi_t = r_t\,\mathrm{d}\gamma_t + \gamma_t\,\mathrm{d}r_t$. Observe that the cross term $\mathrm{d}r_t\,\mathrm{d}\gamma_t$ does not feature in this relation owing to the independence of $W_t^{(x)}$ and $\xi_t^{(\varphi)}$, which originate from the intrinsic scattering population and the scattered electromagnetic field, respectively.

The BDI model (Bartlett, 1966) posits a first order master equation for the population N_t, with respective generation and recombination rates $G = \lambda N + \nu$, $R = \mu N$. For an asymptotically large population, $N\to\infty$, we deduce (Tough, 1987; Jakeman and Tough, 1988; Field and Tough, 2003) that the re-scaled population variate $x \mapsto \alpha x$ satisfies the SDE

$$\mathrm{d}x_t = \mathcal{A}(\alpha - x_t)\mathrm{d}t + (2\mathcal{A}x_t)^{1/2}\,\mathrm{d}W_t^{(x)} \tag{2.12}$$

for an independent Wiener process $W_t^{(x)}$, where $\alpha = \nu/\lambda$. This leads to the asymptotic Γ-distribution for x_t,

$$\Gamma_\alpha(x) = \frac{x^{\alpha-1}\exp(-x)}{\Gamma(\alpha)}, \tag{2.13}$$

so that $\mathrm{Var}[x] = \langle x\rangle = \alpha$. From Ito's formula applied to $r_t = x_t^{1/2}$ we find $\mathrm{d}r_t = \mathrm{d}x_t/2x_t^{1/2} - \mathrm{d}x_t^2/8x_t^{3/2}$, and thus from (2.12),

$$\mathrm{d}r_t = \mathcal{A}\left(\frac{2(\alpha - x_t) - 1}{4r_t}\right)\mathrm{d}t + \left(\frac{\mathcal{A}}{2}\right)^{1/2}\mathrm{d}W_t^{(x)}. \tag{2.14}$$

This leads to the following result.

Proposition 2.1: In the K-distributed case the scattered amplitude is governed by the SDE,

$$\frac{d\Psi_t}{\Psi_t} = -\frac{1}{2}\mathcal{B}\,dt + \frac{\mathcal{B}^{1/2}}{\gamma_t}d\xi_t + \mathcal{A}\left(\frac{2(\alpha - x_t) - 1}{4x_t}\right)dt + \left(\frac{\mathcal{A}}{2x_t}\right)^{1/2} dW_t^{(x)}. \tag{2.15}$$

This evolution is invariant under the U(1) gauge transformation $\Psi_t \mapsto \exp(i\Lambda)\Psi_t$*, for constant* Λ.

In the above expression $\mathcal{A}$ and $\mathcal{B}$ are independent constants with the dimension of frequency. In most situations of interest, however, such as those reported in Field and Tough (2003), the wavelength of the illuminating radiation is such that the two corresponding reciprocal correlation time scales satisfy $\mathcal{A}^{-1} \gg \mathcal{B}^{-1}$. The description of Rayleigh scattering (i.e., constant scattering cross section) is recovered when $\mathcal{A} = 0$. Proposition 2.1 implies the following result.

Corollary 2.2: The squared volatility of the amplitude process Ψ_t *is given by*

$$|d\Psi_t|^2 = \left(\mathcal{B}x_t + \frac{\mathcal{A}z_t}{2x_t}\right)dt. \tag{2.16}$$

It is the *linearity* of the right-hand side above in z_t that enables the anomaly detection mechanism, reported in Field and Tough (2003).

B. Intensity

The stochastic differential of the intensity process z_t can be expressed in terms of the amplitude via the identity

$$dz_t = \Psi_t^*\, d\Psi_t + \Psi_t\, d\Psi_t^* + |d\Psi_t|^2 \tag{2.17}$$

which follows from $z_t = |\Psi_t|^2$. From (2.8) we find

$$\begin{aligned}\Psi_t^*\, d\Psi_t + \Psi_t\, d\Psi_t^* &= x_t(\gamma_t^*\, d\gamma_t + \gamma_t\, d\gamma_t^*) + 2|\gamma_t|^2 r_t\, dr_t \\ &= -\mathcal{B}z_t\, dt + \mathcal{B}^{1/2}x_t(\gamma_t^*\, d\xi_t + \gamma_t\, d\xi_t^*) + \frac{2z_t}{r_t}dr_t.\end{aligned} \tag{2.18}$$

The terms involving $d\xi_t$ above can be combined in terms of a real-valued Wiener process $W_t^{(\varphi)}$ according to

$$\gamma_t^*\, d\xi_t + \gamma_t\, d\xi_t^* \equiv \left(\frac{2z_t}{x_t}\right)^{1/2} dW_t^{(\varphi)}. \tag{2.19}$$

We deduce from (2.16), (2.17), (2.18) that

$$dz_t = -\mathcal{B}z_t\, dt + (2\mathcal{B}z_t x_t)^{1/2}\, dW_t^{(\varphi)} + \frac{2z_t}{r_t}dr_t + \left(\mathcal{B}x_t + \frac{\mathcal{A}z_t}{2x_t}\right)dt. \tag{2.20}$$

In combination with (2.14) this leads to the following result.

Proposition 2.3: The intensity SDE is given by

$$dz_t = \left[\mathcal{B}(x_t - z_t) + \frac{\mathcal{A}z_t(\alpha - x_t)}{x_t}\right]dt + \left(2\mathcal{B}x_t z_t + \frac{2\mathcal{A}z_t^2}{x_t}\right)^{1/2} dW_t^{(z)} \tag{2.21}$$

in which $W_t^{(z)}$ *is correlated with* $W_t^{(x)}$ *of (2.12), and satisfies*

$$\left(\mathcal{B}x_t z_t + \frac{\mathcal{A}z_t^2}{x_t}\right)^{1/2} dW_t^{(z)} = (\mathcal{B}x_t z_t)^{1/2}\, dW_t^{(\varphi)} + \left(\frac{\mathcal{A}}{x_t}\right)^{1/2} z_t\, dW_t^{(x)}. \tag{2.22}$$

The filtration of $W_t^{(\varphi)}$ arises from the constituent phases $\varphi_t^{(j)}$ in the random walk according to (2.19), while that of $W_t^{(x)}$ stems solely from the fluctuations in the endogenously specified population model. Observe that, if $\mathcal{B}=0$, (2.22) implies $W^{(z)}=W^{(x)}$, and from (2.8) γ_t is constant, so $|\gamma_t|^2=\mathbb{E}[|\gamma_t|^2]=1$. Accordingly $z_t=x_t$ is a solution of (2.21), as required by (2.7). From Proposition 2.3 we obtain the following result.

Corollary 2.4: The squared intensity volatility is determined by

$$\mathrm{d}z_t^2=\left(2\mathcal{B}x_tz_t+\frac{2\mathcal{A}z_t^2}{x_t}\right)\mathrm{d}t. \tag{2.23}$$

Alternatively, in terms of the amplitude process Ψ_t, the squared volatility in the intensity z_t can be expressed as

$$\mathrm{d}z_t^2\equiv\Psi_t^2\,\mathrm{d}\Psi_t^{*2}+\Psi_t^{*2}\,\mathrm{d}\Psi_t^2+2z_t|\mathrm{d}\Psi_t|^2 \tag{2.24}$$

which, from (2.15), leads to the above expression for $\mathrm{d}z_t^2$. Observe that for $\mathcal{A}\ll\mathcal{B}$ the dominant contribution to the squared intensity volatility is proportional to the instantaneous value of the intensity. Thus for a Rayleigh time scale $\mathcal{B}^{-1}$, over which x_t remains approximately constant, the time series data for $\mathrm{d}z_t^2$ and z_t should exhibit strong correlation. This feature has been experimentally verified in a case of optical scattering, and is reported in Sec. IV A of Field and Tough (2003).

In terms of the square-root intensity $R_t=\sqrt{z_t}$ an application of Ito's formula to (2.23) yields the following result.

Corollary 2.5: The squared volatility in the modulus amplitude is determined by

$$\mathrm{d}R_t^2=\frac{1}{2}\left(\mathcal{B}x_t+\frac{\mathcal{A}z_t}{x_t}\right)\mathrm{d}t. \tag{2.25}$$

C. Phase

The complex amplitude process can be expressed in polar form $\Psi_t=R_t\exp(i\theta_t)$ and thus, writing $i\,\theta_t=\log(\Psi_t/R_t)$, we deduce from Ito's formula that

$$i\,\mathrm{d}\theta_t=\frac{\mathrm{d}\Psi_t}{\Psi_t}-\frac{1}{2}\left(\frac{\mathrm{d}\Psi_t}{\Psi_t}\right)^2-\frac{\mathrm{d}R_t}{R_t}+\frac{1}{2}\left(\frac{\mathrm{d}R_t}{R_t}\right)^2. \tag{2.26}$$

Since the left-hand side is purely imaginary we can express $\mathrm{d}\theta_t$ in terms of Ψ_t alone as

$$\mathrm{d}\theta_t=\frac{1}{2i}\left[\left(\frac{\mathrm{d}\Psi_t}{\Psi_t}-\frac{1}{2}\left(\frac{\mathrm{d}\Psi_t}{\Psi_t}\right)^2\right)-\left(\frac{\mathrm{d}\Psi_t^*}{\Psi_t^*}-\frac{1}{2}\left(\frac{\mathrm{d}\Psi_t^*}{\Psi_t^*}\right)^2\right)\right]. \tag{2.27}$$

Accordingly, the squared phase volatility is determined by the identity

$$\mathrm{d}\theta_t^2\equiv\frac{|\mathrm{d}\Psi_t|^2}{2z_t}-\frac{\mathrm{d}\Psi_t^2}{4\Psi_t^2}-\frac{\mathrm{d}\Psi_t^{*2}}{4\Psi_t^{*2}}. \tag{2.28}$$

From (2.15) we have

$$\frac{\mathrm{d}\Psi_t}{\Psi_t}-\frac{1}{2}\left(\frac{\mathrm{d}\Psi_t}{\Psi_t}\right)^2=\left(\frac{\mathcal{A}(\alpha-x_t-1)}{2x_t}-\frac{1}{2}\mathcal{B}\right)\mathrm{d}t+\left(\frac{\mathcal{A}}{2x_t}\right)^{1/2}\mathrm{d}W_t^{(x)}+\frac{\mathcal{B}^{1/2}}{\gamma_t}\mathrm{d}\xi_t. \tag{2.29}$$

Hence, from (2.27), θ_t obeys the SDE,

$$\mathrm{d}\theta_t=\frac{\mathcal{B}^{1/2}}{2i|\gamma_t|^2}(\gamma_t^*\,\mathrm{d}\xi_t-\gamma_t\,\mathrm{d}\xi_t^*). \tag{2.30}$$

As in the derivation of the SDE for the intensity, we can express the terms involving ξ_t in (2.30) as a distinct real-valued Wiener process $W_t^{(\theta)}$ according to

$$\frac{1}{2i}(\gamma_t^* \, \mathrm{d}\xi_t - \gamma_t \, \mathrm{d}\xi_t^*) \equiv \left(\frac{z_t}{2x_t}\right)^{1/2} \mathrm{d}W_t^{(\theta)}. \tag{2.31}$$

Thus we obtain the following result.

Proposition 2.6: The total phase θ_t of the complex amplitude process Ψ_t obeys the SDE,

$$\mathrm{d}\theta_t = \left(\frac{\mathcal{B}x_t}{2z_t}\right)^{1/2} \mathrm{d}W_t^{(\theta)}, \tag{2.32}$$

which has vanishing drift.

The result has the following consequence.

Corollary 2.7: The squared total phase volatility is given by

$$\mathrm{d}\theta_t^2 = \frac{\mathcal{B}x_t}{2z_t}\mathrm{d}t. \tag{2.33}$$

Alternatively (2.33) can be derived by applying (2.28) to (2.15). This result accords with the general scaling and symmetry arguments for the behavior of the squared phase volatility put forward in Sec. IV of Field and Tough (2003). The situation should be contrasted with the differentiable model for the process Ψ_t (Jakeman *et al.*, 2001) for which the intensity-weighted phase derivative, instead of its square, has minimal variance.

These relations lead to expressions for the frequency constants $\mathcal{A}$, $\mathcal{B}$ as follows. With respect to an average over the phase fluctuations $\mathrm{d}\varphi_t^{(j)}$ there exists a *residual constant term* in the squared phase volatility, i.e.,

$$\mathbb{E}[\mathrm{d}\theta_t^2/\mathrm{d}t|\mathcal{F}^{(\varphi)}] = \tfrac{1}{2}\mathcal{B}. \tag{2.34}$$

In principle this enables the Rayleigh constant $\mathcal{B}$ to be deduced from scattering data (alternatively an estimate of the Rayleigh correlation time scale $\mathcal{B}^{-1}$ can be found from measuring the time difference between successive peaks in the intensity time series data $\{z_t\}$). Expression (2.33) implies that $x_t = 2\mathcal{B}^{-1} z_t \, \mathrm{d}\theta_t^2/\mathrm{d}t$ and so the instantaneous values of the cross section x_t (and therefore r_t) are observable through the squared phase fluctuations. Consequently, the constant $\mathcal{A}$ can be deduced from the phase fluctuations through the square of (2.14),

$$\frac{\mathrm{d}r_t^2}{\mathrm{d}t} = \frac{1}{2}\mathcal{A}. \tag{2.35}$$

(Cf. Sec. III in Field and Tough, 2003, for an account of the observability of the squared volatilities for discretely sampled time series data.)

D. Correlation of fluctuations

The stochastic dynamics presented in Proposition 2.1 enable one to deduce the correlation structure in the fluctuations of the complex amplitude process Ψ_t.

A geometric insight into these properties can be gained from the symmetry properties of the process Ψ_t. Proposition 2.1 shows that the SDE for Ψ_t is invariant under the U(1) gauge transformation $\Psi_t \mapsto \exp(i\Lambda)\Psi_t$. Since the drift in (2.15) is real valued, the identity (2.27) implies that θ_t has vanishing drift, as seen explicitly from Proposition 2.6. The resulting asymptotic probability distribution is therefore U(1) symmetric.

In respect of time evolution, the SDE (2.15) has the Markov property, that the evolution it determines depends on the instantaneous value of Ψ_t and is independent of the history of the

process $\{\Psi_{t'}|t'<t\}$. This feature yields a preferred symmetry, namely the instantaneous radial direction determined by Ψ_t. The diffusion tensor σ^{ij}, determined by $d\Psi^i\, d\Psi^j=\sigma^{ij}\, dt$ is real and symmetric and therefore diagonalizes over $\mathbb{C}$. In the nondegenerate case its eigenvectors constitute a unique orthogonal pair corresponding to the directions in which the component Wiener increments are independent. On grounds of the above symmetry we anticipate that the space of eigendirections contains the instantaneous radial (and attendant orthogonal θ) direction. This geometrical property can be verified explicitly from (2.19), (2.22), and (2.31), which imply the following.

Proposition 2.8: The cross-correlation between $W_t^{(z)}$, $W_t^{(\theta)}$ vanishes identically, i.e., $dW_t^{(z)}\, dW_t^{(\theta)}=0$. Correspondingly $dR_t\, d\theta_t=0$, i.e., the fluctuations in R_t, θ_t are statistically independent.

In terms of the I,Q component representation the coordinate transformations $I=R\cos\theta$, $Q=R\sin\theta$ and the property $dR_t\, d\theta_t=0$ imply the geometric relation

$$dI_t\, dQ_t=\cos\theta_t\sin\theta_t(dR_t^2-R_t^2\, d\theta_t^2). \tag{2.36}$$

This leads to the following result.

Proposition 2.9: The I_t, Q_t components of Ψ_t are independent if and only if $\sigma_{(R)}=R\sigma_{(\theta)}$, i.e., $\sigma_{(z)}=2z\sigma_{(\theta)}$. A departure from this relation induces a correlation between the Wiener increments in I_t, Q_t.

Alternatively, this result can be derived using the contravariance of the diffusion tensor σ^{ij}, which enables one to translate between its I,Q and R,θ components via the above coordinate transformation (e.g., Risken, 1989). In the general case we find from (2.23), (2.33) that

$$\frac{\sigma_{(z)}^2}{\sigma_{(\theta)}^2}=4z^2+\frac{4\mathcal{A}z^3}{\mathcal{B}x^2}. \tag{2.37}$$

This relation can be used to characterize the geometry of the fluctuations as follows.

Proposition 2.10: In the K-distributed case, $\mathcal{A}\neq 0$, the diffusion tensor is nondegenerate, and the fluctuations δI_t, δQ_t are correlated. The (comoving) error surface S of $\delta\Psi_t$, defined by the quadratic form $\sigma^{II}\delta I_t^2+2\sigma^{IQ}\delta I_t\delta Q_t+\sigma^{QQ}\delta Q_t^2=1$, is an ellipse whose major axis lies in the instantaneous radial direction defined by Ψ_t. Degeneracy occurs only in the Rayleigh case, $\mathcal{A}=0$, for which S is a circle, i.e., the fluctuations in Ψ_t are isotropic.

We remark in general that the random variables I_t, Q_t possess a joint probability distribution that is U(1) symmetric, i.e., given by a surface of revolution about the perpendicular axis to the origin in the I,Q-plane. Nevertheless I_t, Q_t are correlated in general, and become independent only in the Rayleigh case, $\mathcal{A}=0$, for which the surface of revolution is Gaussian. In this case the component I_t, Q_t processes can be described by the pair of (uncoupled) Ornstein–Uhlenbeck processes determined as the real and imaginary parts of (2.4).

III. ASYMPTOTIC BEHAVIOR

A. Equilibrium distribution

We recall the covariant form of the Fokker–Planck equation (FPE) for the asymptotic joint distribution $\mathcal{P}(x,z,t)$ (e.g., Risken, 1989)

$$\frac{\partial\mathcal{P}}{\partial t}=-\sum_i\,\partial_i(b^i\mathcal{P})+\frac{1}{2}\sum_{i,j}\,\partial_i\partial_j(\sigma^{ij}\mathcal{P}). \tag{3.1}$$

From (2.12), (2.21), (2.22) the components of the diffusion tensor in the x,z coordinate representation are given by

$$\sigma^{\mathbf{ij}}=2\begin{pmatrix}\mathcal{A}x & \mathcal{A}z\\ \mathcal{A}z & \mathcal{B}xz+\mathcal{A}z^2/x\end{pmatrix} \tag{3.2}$$

while the drift vector has components

$$b^{\mathbf{i}}=2\begin{pmatrix}\mathcal{A}(\alpha-x)\\ \mathcal{B}(x-z)+\mathcal{A}z(\alpha-x)/x\end{pmatrix}. \tag{3.3}$$

From (3.1), therefore, we deduce the following.

Proposition 3.1: The FPE for the joint distribution of the cross section x_t and intensity z_t is

$$\frac{\partial\mathcal{P}}{\partial t}=\mathcal{B}\{-\partial_z[(x-z)\mathcal{P}]+x\partial_z^2[z\mathcal{P}]\}+\mathcal{A}\left\{-\partial_z\left(\frac{z(\alpha-x)\mathcal{P}}{x}\right)-\partial_x((\alpha-x)\mathcal{P})\right\}$$
$$+\mathcal{A}\left\{\partial_z^2\left(\frac{z^2\mathcal{P}}{x}\right)+2\partial_x\partial_z(z\mathcal{P})+\partial_x^2(x\mathcal{P})\right\}. \tag{3.4}$$

This admits the asymptotic joint distribution

$$\mathcal{P}=\frac{x^{\alpha-2}\exp(-x-z/x)}{\Gamma(\alpha)}. \tag{3.5}$$

Proof: The derivation of (3.4) follows immediately from (3.1), (3.2), and (3.3), while the following identities for the derivatives of the joint distribution:

$$\partial_z\mathcal{P}=-\mathcal{P}/x,$$
$$\partial_z(z\mathcal{P})=(1-z/x)\mathcal{P},$$
$$\partial_z^2(z\mathcal{P})=\left(-\frac{2}{x}+\frac{z}{x^2}\right)\mathcal{P}, \tag{3.6}$$
$$\partial_x\mathcal{P}=\left(\frac{\alpha-1}{x}+\frac{z}{x^2}-1\right)\mathcal{P},$$
$$\partial_x^2\mathcal{P}=\left\{\left(\frac{\alpha-1}{x}+\frac{z}{x^2}-1\right)^2-\frac{\alpha-1}{x^2}-\frac{2z}{x^3}\right\}\mathcal{P},$$

enable one to verify that (3.5) is an asymptotic solution of (3.4). □

Observe from (2.12) and (3.4) that the model behavior of the scattering cross section is *endogenously specified*, i.e., the parameters involved arise from the population alone, independently of the electromagnetic field. Thus (2.12) is independent of z_t. Nevertheless there exists a nonlinear coupling between the x_t, z_t variables, owing to the presence of x_t in (2.21) and the correlation of $W_t^{(x)}$, $W_t^{(z)}$ according to (2.22). Therefore x_t, z_t are statistically dependent random variables, which relation is symmetric. The situation in regard to the endogenous specification of the evolution of the cross section through (2.12) should be contrasted with the previous discussion given in Tough (1987), and its generalizations in Field and Tough (2003) in which it is necessary that the SDE for x_t has an explicit z_t dependence, and in which the Wiener processes $W_t^{(x)}$, $W_t^{(z)}$ are considered to be independent. Although these analyses preserve the joint distribution appropriate to *K*-distributed noise, these models are not so natural from a physical point of view.

B. Detailed balance

The covariant Fokker–Planck equation (3.1) can be re-expressed as the equation of continuity

$$\frac{\partial\mathcal{P}}{\partial t}+\sum_i\partial_i(\mathcal{P}v^i)=0, \tag{3.7}$$

where the *current* v^i is defined by $v^i = b^i - \frac{1}{2}\mathcal{P}^{-1}\Sigma_j \partial_j(\sigma^{ij}\mathcal{P})$. In addition to the the equilibrium condition $\partial\mathcal{P}/\partial t = 0$, the condition for detailed balance states that $v^i = 0$. Explicit calculation using (3.6) shows that v^i vanishes asymptotically. Alternatively, a more intuitive argument for this property is as follows. From (2.7) we have the factorization $z_t = x_t u_t$, where $u_t = |\gamma_t|^2$, in which the factors x_t, u_t are independent random variables. The coordinate transformation $x^{\mathbf{i}} \mapsto x^{\mathbf{i}'}: (x,z) \mapsto (x,u)$ recasts the joint distribution (3.5) and SDEs (2.12), (2.21) such that

$$b^{\mathbf{i}'} = \begin{pmatrix} \mathcal{A}\beta^{\mathbf{1}'}(x) \\ \mathcal{B}\beta^{\mathbf{2}'}(u) \end{pmatrix}, \quad \sigma^{\mathbf{i}'\mathbf{j}'} = \begin{pmatrix} \mathcal{A}\Sigma^{\mathbf{1}'\mathbf{1}'}(x) & 0 \\ 0 & \mathcal{B}\Sigma^{\mathbf{2}'\mathbf{2}'}(u) \end{pmatrix},$$

where the functions $\beta^{\cdot}(\cdot)$, $\Sigma^{\cdot}(\cdot)$ are determined from (2.8), (2.12) and are independent of $\mathcal{A}$, $\mathcal{B}$. The equilibrium condition in the (x,u) representation, obtained by setting the left-hand side of (3.1) equal to zero, implies detailed balance, since this condition holds for arbitrary values of the constants $\mathcal{A}$, $\mathcal{B}$. Consequently, $v^{\mathbf{i}}$ in the (x,z) representation also vanishes, since $v^{\mathbf{i}}$ transforms homogeneously (i.e., tensorially) under coordinate transformations (see, e.g., Risken, 1989).

IV. CORRELATION PROPERTIES

For simplicity we adopt a timescale such that the constant $\mathcal{B}$ of (2.8) is equal to unity. The independent constant $\mathcal{A}$ will then satisfy $\mathcal{A} \ll 1$ in most practical situations of interest (e.g., scattering at radar wavelength), although this condition is not necessary for the validity of the expressions that follow in this section.

A. Intensity autocorrelation

It is convenient to write the intensity process in the product representation $z_t = u_t x_t$. From (2.8) the process $u_t = |\gamma_t|^2$ satisfies the SDE,

$$\mathrm{d}u_t = (1 - u_t)\mathrm{d}t + \sqrt{2u_t}\,\mathrm{d}W_t^{(u)}, \tag{4.1}$$

where $\gamma_t\,\mathrm{d}\xi_t^* + \gamma_t^*\,\mathrm{d}\xi_t = \sqrt{2u_t}\,\mathrm{d}W_t^{(u)}$. The propagator (i.e., Green's function for the corresponding FPE) for the process u_t is given by

$$P(u,t|u_0) = \frac{1}{1-\exp(-t)}\exp\left(-\frac{u + u_0\exp(-t)}{1-\exp(-t)}\right) I_0\left(\frac{2\exp(-t/2)\sqrt{uu_0}}{1-\exp(-t)}\right), \tag{4.2}$$

where I_α denotes the modified Bessel function (e.g., Jeffreys and Jeffreys, 1966). In a similar manner the propagator for (2.12) is given by

$$P(x,t|x_0) = \frac{1}{1-\exp(-\mathcal{A}t)}\left(\frac{x\exp(\mathcal{A}t)}{x_0}\right)^{(\alpha-1)/2} \exp\left(-\frac{(x + x_0\exp(-\mathcal{A}t))}{1-\exp(-\mathcal{A}t)}\right) \times I_{\alpha-1}\left(\frac{2\exp(-\mathcal{A}t/2)\sqrt{xx_0}}{1-\exp(-\mathcal{A}t)}\right). \tag{4.3}$$

This can be re-expressed as a series expansion

$$P(x,t|x_0) = x^{\alpha-1}\exp(-x)\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+\alpha)}\exp(-\mathcal{A}nt)L_n^{\alpha-1}(x)L_n^{\alpha-1}(x_0), \tag{4.4}$$

where the Laguerre polynomials L_n^α are defined by

$$L_n^\alpha(x) = \frac{x^{-\alpha}\exp(x)}{n!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n (x^{\alpha+n}\exp(-x)) \tag{4.5}$$

(cf. Wong, 1963 for corresponding derivations). Combining (4.2), (4.4) leads to the following result.

Proposition 4.1: The propagator for (3.4) is given by

$$P(z,x,t|z_0,x_0)=\frac{1}{x(1-\exp(-t))(1-\exp(-\mathcal{A}t))}\left(\frac{x\exp(\mathcal{A}t)}{x_0}\right)^{(\alpha-1)/2}$$
$$\times\exp\left(-\frac{z/x+z_0\exp(-t)/x_0}{1-\exp(-t)}\right)\exp\left(-\frac{x+x_0\exp(-\mathcal{A}t)}{1-\exp(-\mathcal{A}t)}\right)$$
$$\times I_0\left(\frac{2\exp(-t/2)}{1-\exp(-t)}\sqrt{\frac{zz_0}{xx_0}}\right)I_{\alpha-1}\left(\frac{2\exp(-\mathcal{A}t/2)\sqrt{xx_0}}{1-\exp(-\mathcal{A}t)}\right). \tag{4.6}$$

Thus a general two-point correlation function can be expressed as the integral

$$\langle F_1(x_t,z_t)F_2(x_0,z_0)\rangle=\int_0^\infty \mathrm{d}x\,\mathrm{d}z\,\mathrm{d}x_0\,\mathrm{d}z_0\,F_1(x,z)F_2(x_0,z_0)P(x,z,t|x_0,z_0)$$
$$\times\frac{x_0^{\alpha-2}\exp(-z_0/x_0-x_0)}{\Gamma(\alpha)}. \tag{4.7}$$

As a consequence we have the following result.

Corollary 4.2: The intensity autocorrrelation function is given by

$$\langle z_t z_0\rangle=\langle u_t u_0\rangle\langle x_t x_0\rangle=\alpha(\alpha+\exp(-\mathcal{A}t))(1+\exp(-t)). \tag{4.8}$$

B. Power spectral density

In the additional presence of a Doppler frequency shift ω_0 (the presence of $\omega_0\neq 0$ is important in radar applications; see, e.g., Helmstrom, 1960) the process γ_t of Sec. II is modified to obey the SDE,

$$\mathrm{d}\gamma_t=(-\tfrac{1}{2}+i\omega_0)\gamma_t\,\mathrm{d}t+\mathrm{d}\xi_t. \tag{4.9}$$

The amplitude process Ψ_t determined by (2.15) is *stationary*, since there is no explicit time dependence in (2.15), the phase distribution is uniform, and the modulus amplitude R_t has a stationary distribution in accordance with the stationary K-distribution for the intensity (it is assumed that the distributions of the *initial* values of Ψ and its associated processes are given by their asymptotic stationary distributions). Therefore, we apply the *Wiener–Khintchine theorem* which asserts that the *power spectral density* $S(\omega)$ is equal to the Fourier transform (denoted by a tilde) of the autocorrelation function, i.e., $\langle\tilde{\Psi}(\omega)\tilde{\Psi}(\omega')\rangle=\pi\delta(\omega-\omega')S(\omega)$ where $S(\omega)=\widetilde{\langle\Psi_t\Psi_0^*\rangle}$. The amplitude autocorrelation function satisfies

$$\langle\Psi_t\Psi_0^*\rangle=\langle\sqrt{x_t x_0}\rangle\exp(-|t|/2-i\omega_0 t). \tag{4.10}$$

Using the propagator expansion (4.4), the evaluation of the factor $\langle\sqrt{x_t x_0}\rangle$ proceeds according to

$$\langle \sqrt{x_t x_0}\rangle = \int_0^\infty dx \int_0^\infty dx_0 \frac{x_0^{\alpha-1}\exp(-x_0)}{\Gamma(\alpha)} P(x,t|x_0)\sqrt{x x_0} = \frac{1}{\Gamma(\alpha)}\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+\alpha)}\exp(-\mathcal{A}nt)$$
$$\times\left(\int_0^\infty x^{\alpha-1/2}\exp(-x)L_n^{\alpha-1}(x)dx\right)^2 = \frac{1}{\Gamma(\alpha)}\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+\alpha)}\exp(-\mathcal{A}nt)$$
$$\times\left(\frac{\Gamma(\alpha+\frac{1}{2})\Gamma(n-\frac{1}{2})}{n!\,2\sqrt{\pi}}\right)^2 = \frac{\Gamma(\alpha+\frac{1}{2})^2}{\Gamma(\alpha)^2}\,{}_2F_1(-1/2,-1/2,\alpha,\exp(-\mathcal{A}t)). \tag{4.11}$$

Here the hypergeometric function ${}_2F_1$ is identified from its series expansion. When $t\to\infty$, (4.11) approaches $\langle\sqrt{x}\rangle^2$, as anticipated from the decorrelation of x_t, x_0 over large times. As $t\to 0$ we find, from the identity due to Gauss,

$${}_2F_1(a,b,c,1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, \tag{4.12}$$

that (4.11) reduces to the anticipated form

$$\lim_{t\to 0}\langle\sqrt{x_t x_0}\rangle = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} = \alpha = \langle x\rangle. \tag{4.13}$$

Expressions (4.10), (4.11) lead to the following result.

Proposition 4.3: The autocorrelation function of the complex amplitude process Ψ_t is given by

$$\langle \Psi_t \Psi_0^*\rangle = \frac{\Gamma(\alpha+\frac{1}{2})^2}{\Gamma(\alpha)^2}\,{}_2F_1(-1/2,-1/2,\alpha,\exp(-\mathcal{A}t))\exp(-|t|/2 - i\omega_0 t). \tag{4.14}$$

According to the Wiener–Khintchine theorem, a Fourier transform of this result has the following consequence.

Corollary 4.4: The power spectral density of the K-distributed noise process characterized by (2.15) is given by

$$S(\omega) = 2\,\frac{\Gamma(\alpha+\frac{1}{2})^2}{\Gamma(\alpha)^2}\int_0^\infty {}_2F_1(-1/2,-1/2,\alpha,\exp(-\mathcal{A}t))\exp(-t/2)\cos((\omega-\omega_0)t). \tag{4.15}$$

Expanding the hypergeometric function ${}_2F_1$ as a series and integrating term by term, the resulting series is recognized as a generalized hypergeometric function of unit argument. Thus

$$S(\omega) = 2\Re\left\{\frac{{}_3F_2(-1/2,-1/2,(1/2+i(\omega-\omega_0))/\mathcal{A};\alpha,1+(1/2+i(\omega-\omega_0))/\mathcal{A};1)}{1/2+i(\omega-\omega_0)}\right\}\frac{\Gamma(\alpha+\frac{1}{2})^2}{\Gamma(\alpha)^2}. \tag{4.16}$$

These calculations illustrate how the product representation of the amplitude (2.7) facilitates the analysis of the associated FPE (3.4).

V. INTERPRETATION AND IMPLICATIONS

The study provides the first theoretical account of *K*-distributed noise processes in which the continuous time dynamical features of the electromagnetic scattering process are fully captured. This has been achieved via the formulation of stochastic differential equations for the scattered amplitude, using the primitive assumptions of the complex random walk model.

The results substantiate an earlier proposal for anomaly detection in the context of such processes (Field and Tough, 2003) based on the concept of observability in the fluctuations of the

complex amplitude process over a sample path. In this respect, Corollary 2.2 leads to a correlation between the observed $|d\Psi_t|^2$ and its predicted value of the form $c(|d\Psi_t|^2, z_t)$, which should approximate unity within the domain of validity of the model. This feature enables an anomaly detection mechanism for K-distributed noise processes, which has been successfully tested on experimental data, and is reported in Sec. IV B of Field and Tough (2003). It is of considerable importance that (2.16) can be derived from theoretical considerations alone.

The formulation of the continuous time dynamics is more fundamental than knowledge of certain statistical properties of a model and, moreover, implies the form of all correlation functions and higher order statistics. In this respect we have provided closed form expressions for the intensity autocorrelation function and the power spectral density, which should be applicable in situations of radar and laser physics. The tractability of such expressions is facilitated by the use of computational tools such as *Mathematica* (Wolfram, 1999).

The methodology we have described admits the generalization of the SDE for the scattering cross section (2.12) to more general endogenous models of population processes, such as described in Sec. II of Field and Tough (2003). This could include corresponding descriptions of the electromagnetic scattering processes that lead, e.g., to the Weibull distribution (applied to scatter from land clutter), the intensity compound K-distribution for various radar parameters (e.g., applied to synthetic aperture radar) and other examples (cf. Jakeman and Tough, 1988).

Corollary 2.7 implies that the instantaneous value of the scattering cross section is observable from the scattered amplitude. The cross section is of primary significance in anomaly detection within a random scattering medium (e.g., the sea-surface, heterogeneous media), which had previously been regarded as a hidden physical variable whose instantaneous values were not deducible from the scattering data. The expression (2.25) for the squared volatility in the modulus amplitude should find application to problems in incoherent radar detection where the total scattered phase information is not available.

ACKNOWLEDGMENTS

The authors are grateful to Richard Glendinning, Simon Haykin, Eric Jakeman, Stephen Luttrell, John McWhirter, Andrew Webb, and Christopher Webber for advice and encouragement.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Interacting squares in arbitrary external field

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(Received 16 June 2003; accepted 14 July 2003)

A model of a many-body system composed of squares with contact pair interactions in an arbitrary external field is presented. The formulation uses a mapping of the system onto polydisperse hard core mixtures. On the polydisperse level then, a simplified Hamiltonian function is specified. This assumption together with a further one about the global free energy functional for the pure hard core part of the idealized mixture make the model solvable. It is expected to hold for high temperatures, low densities, or low temperatures. The validity of the method of construction in the latter case is illustrated by a further application to a corresponding lattice system, for which exact results to compare with are readily available when the temperature is sufficiently low. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1613042]

I. INTRODUCTION

In the catalogues of solvable models in statistical mechanics (see, e.g., Refs. 1 and 2), calculations of free energies in the presence of external fields are rarely listed. For example, even the prominent Ising model on $\mathbb{Z}^2$ has only been solved in zero field. As a consequence of the difficulty of the problem, the analysis of many-body systems in external fields developed into a subdiscipline of statistical mechanics, with density functional theory as unifying approach. The basic idea of density functional theory (for a review, see, e.g., Ref. 3) consists in representing thermodynamic potentials in terms of the local particle density ϱ. Besides this well-known transformation to ϱ as new free variable, another profound idea emerged only recently, namely the concept of overcomplete density functional description. This method was introduced by Percus.[4] In such a representation of thermodynamic potentials, use is made of additional variables other than the local particle density to both clarify and better control the structure of the functionals.[3] So far, several overcomplete representations of the statistical mechanics of $D=1$ particle systems with next neighbor interactions in an arbitrary external field have been deduced[5,4,6] (for a historic overview see, e.g., Ref. 6). The purpose of this communication is to initiate the extension of the overcompleteness technique of Cuesta and Tutschka[6] by considering a suitable chosen interacting particle system in $\mathbb{R}^2$ (and on $\mathbb{Z}^2$).

From a physical point of view, their approach is that of introducing the sequence of local densities $\{\varrho_i\}_{i\geqslant 1}$ of blocks (clusters, superparticles,[5] or units) containing i particles connected (bounded or associated[7]) due to the attractive part of the interaction as set of redundant variables. Since then the pair interaction among the blocks is per construction a hard core potential, the resulting free energy functional takes on the polydisperse, additive hard rods mixture form. Consequently, the functional is parameterized by few sums (over the local block densities ϱ_i), which, in turn, can be evaluated (for the $D=1$ next neighbor case) in closed form. Based on this observation, Cuesta and Tutschka[6] show (though indirectly) that the thermodynamic potentials of $D=1$ particle systems with next neighbor interactions in an arbitrary external field are—analogous to the well-known uniform isothermal–isobaric technique (see, e.g., Ruelle[8])—completely characterized by pressure-like quantities $p^{\pm}$, termed effective pressures.[9,10]

From a mathematical viewpoint, they lifted the representation of positive integers n (physically interpreted as number of particles) as sums of other positive integers, known as partitions of n (see, e.g., Andrews[11,12]), to the thermodynamic level. Here, the central observation is that the

number of partitions of n is exponentially bounded (Hardy–Ramanujan formula—see, e.g., Andrews[11,12]).

Cuesta and Tutschka[6] developed these ideas along two examples, the sticky core model, in which the interaction has a 0-range attractive component at the edge of the core, and the prototypical square-well potential. In particular, the full and explicit analysis of the former system was possible because of the contact nature of the adhesive interaction. That is, the particles of a unit are forced to lie, in relative coordinates, on the linear lattice.

While the logic of the overcompleteness scheme of Cuesta and Tutschka,[6] with its resemblance to the isothermal–isobaric method, not only works for the simplified $D=1$ setup, a mathematical analysis of the direct extension of the format to $D>1$ is not within reach. Correspondingly, this communication starts the extension of the overcomplete representation of Cuesta and Tutschka[6] by looking at $D=2$ examples with type of contact pair interactions. This choice of course is based on the very handy properties of the $D=1$ sticky core model. Furthermore, we are going to restrict ourselves to oriented hard square cores.

Our program consists of three steps. First, in Sec. II A, we shall give a reformulation of the sticky rods free energy functional. The topic will be the abstraction from the $D=1$ nature of the solution. Namely, that we are going to work backwards from the elegant and compact effective pressures representation. In particular, we will avoid the closed-form evaluation of the sums over the local block densities (which will most likely not be possible in $D=2$), as well as infer the relation between ϱ and the local block densities $\{\varrho_i\}_{i\geqslant 1}$ directly from the lattice structure of the units (instead from an identity of functional analysis as within the $p^{\pm}$ format)—see formula (2.7). With these preliminary considerations in mind, we shall turn to the crucial part of our program (step two), the extension to $D=2$, pursued in Sec. II B. Following the logic of the Cuesta–Tutschka format, the central theme will be the control of the block configurations. Whereas for the $D=1$ case, the units are completely characterized by the number of connected particles i, in the $D=2$ case, the shape functions of the units are no longer defined by a single integer parameter. This means that while the mapping of our many-body system of squares with contact interactions onto a polydisperse, additive hard core mixture is formally possible, the Hamiltonian function of this mixture will be, foremost due to the geometry of the hard cores (i.e., the units or blocks), hopelessly complicated, and therefore the evaluation of its free energy functional far beyond reach. Hence, in order to set up an analytically tractable scheme, we are forced to specify a sufficiently simple polydisperse hard core mixture type Hamiltonian such that its thermodynamic potentials can be calculated. The idealization we are going to use will restrict the spatial structure of the units to a certain class of compact configurations. Clearly, this simplifying condition means that the model will have a limited domain. In fact it will be easy to guess the thermodynamic region for which the approach is valid. But somewhat more quantitative estimates would certainly be preferable. This question provides the focus of the last step of our program. In Sec. III, the procedure of Sec. II B will be applied to an interacting particle system with next neighbor interactions on $\mathbb{Z}^2$, for which the coexistence curve is well-known (see, e.g., Refs. 1 and 2). This will provide us finally, at least for low temperatures, with an explicit comparison of our idealization with exact results.

II. NONUNIFORM CONTINUOUS SYSTEMS

A. One-dimensional sticky cores

This model is to be interpreted as meaning a system of $D=1$ hard balls with an additional, zero-range attractive interaction at the edge of the core. It can be regarded as a limiting case of a $D=1$ particle system with square-well potential. In the latter system, the pair interaction V between two particles at distance q is (selecting units such that the hard core diameter equals 1)

$$V(q)=\begin{cases} -\mathcal{E} & \text{if } q\in[1,1+d), \\ 0 & \text{if } q\in[1+d,\infty), \\ +\infty & \text{otherwise,} \end{cases} \tag{2.1}$$

where $d \leqslant 1$ is the width of the well and $\mathcal{E} \in \mathbb{R}_+$ the interaction strength. Upon introducing the pair interaction Boltzmann factor

$$e(y,x) = \begin{cases} \exp[-\beta V(y-x)] & \text{if } y \geqslant x, \\ 0 & \text{otherwise,} \end{cases} \tag{2.2}$$

with $x,y \in \mathbb{R}$ as the positions of two neighboring particles and $\beta \in \mathbb{R}_+$ the reciprocal temperature, the pair interaction energy of $D=1$ adhesive systems is characterized through (2.1) as well as (2.2) by the limit

$$\lim_{\substack{\mathcal{E} \to +\infty \\ d \to 0^+}} e(y,x)\big|_{d \exp(\beta\mathcal{E}) \to \lambda} = h_1(y-x) + \lambda\, \delta_1(y-x), \tag{2.3a}$$

where $\delta_a = h_a'$, h_a being the Heaviside function shifted to the right by a, and $\lambda \in \mathbb{R}_+$ the stickiness (coupling or bonding[7]) parameter.

The formulation of the Hamiltonian function is completed via the definition of the local activity

$$z(x) = \exp\{\beta[\mu - U(x)]\}. \tag{2.3b}$$

This term of the Hamiltonian gives the interaction energy between the external field U (and the chemical potential $\mu \in \mathbb{R}$, respectively) and the particle at x.

For the Hamiltonian (2.3), the free energy was first obtained by Percus in 1982 through the inverse operator format.[13] Later on, Cuesta and Tutschka[6] gave an alternative derivation, leading to a physically more transparent representation of the thermodynamic potentials in terms of effective pressures $p^{\pm}$. They also showed the equivalence of the two schemes.

The aim of this section is to infer a reformulation of the sticky rods functional most suitable for the transition to $D=2$. We are going to avoid simplifications specific to the $D=1$ nature of the system. The emphasis will be on the geometric properties of the units. Thus, the functional will be less simple than in the $p^{\pm}$ representation, and therefore, most notably, computationally less efficient, too.

Our reasoning is based on the transformation technique due to Cuesta and Tutschka.[6] This method consists of three stages.

The analysis starts with a decomposition of the $D=1$ sticky core system into units (monomers, dimers, trimers,...) of i, via the attractive part of the pair interaction Boltzmann factor (2.3a), connected particles. By the contact nature of the adhesive interaction, these units have diameter i. Furthermore, the pair interaction among them is per construction a hard core potential. Thus, the original system is mapped onto a polydisperse, additive hard rods mixture with pair interaction Boltzmann factor between component i and j given as [cf. (3.6) of Cuesta and Tutschka[6]]

$$e_{ij}(y,x) = h_{(i+j)/2}(y-x). \tag{2.4a}$$

In the second stage, the composition of the units is incorporated. That is, the partition function of an i-particle unit at x is represented by the local activity $z_i(x)$ of component i of the mixture. The total isothermal measure of a unit of i particles (numbered from left to right, i.e., $x_1 \leqslant x_2 \leqslant x_3 \cdots \leqslant x_i$), centered at x, is via (2.3) given by

$$z(x_i) \int_{\mathbb{R}^{i-1}} \prod_{k=1}^{i-1} \delta_1(x_{k+1} - x_k)\, z(x_k)\, \mathrm{d}(x_1, \ldots, x_{i-1})\big|_{x_i = x + n_i},$$

where $n_i = (i-1)/2$, $i \in \mathbb{N}_+$. Upon using the properties of Dirac's δ-distribution, we therefore have that [cf. (3.5) of Cuesta and Tutschka[6]]

$$z_i(x)=\lambda^{i-1}\prod_{|j|\leqslant n_i} z(x+j),$$

which transcribes via (2.3b) to the completely polydisperse form

$$z_i(x)=C_i(\lambda)\exp\{\beta[\mu_i-U_i(x)]\} \tag{2.4b}$$

with $C_i(\lambda)=\lambda^{i-1}$, the chemical potential μ_i of component i equal to $i\mu$, and the external field given as

$$U_i(x)=\sum_{|j|\leqslant n_i} U(x+j). \tag{2.5}$$

This shows the basic underlying lattice structure of sticky core units most clearly.

On following Percus,[13,4] the local partial (or block) densities $\varrho_i\in L^1(\mathbb{R})$ are now obtainable by

$$\varrho_i(x)=\frac{\delta\ln\Xi}{\delta\ln z_i(x)},$$

where Ξ is the total Gibbs measure of (2.4) with the indices of the blocks determined statistically,[14,4] or, equivalently, of (2.3).

The main property that makes the calculation of the free energy functional $\mathfrak{F}$ of the Hamiltonian function (2.4) rather straightforward is the close resemblance of the latter to the polydisperse additive pure hard rods mixture Hamiltonian, for which the free energy is known.[14,4] Indeed, for $C_i(\lambda)\equiv 1$ the Hamiltonian (2.4) defines a $D=1$ additive mixture of pure hard cores in an external field U_i. Therefore, upon writing $\mathfrak{F}[\{\varrho_i\}_{i\geqslant 1}]=\Sigma_{i\geqslant 1}\int_{\mathbb{R}}\varrho_i(x)U_i(x)\,dx+\bar{\mathfrak{F}}[\{\varrho_i\}_{i\geqslant 1}]$, so that $\bar{\mathfrak{F}}$ denotes the intrinsic free energy functional (see, e.g., Percus[3]), we have due to Vanderlick, Davis, and Percus[14] at once

$$\beta\bar{\mathfrak{F}}[\{\varrho_i\}_{i\geqslant 1}]|_{C_i(\lambda)\equiv 1}=\int_{\mathbb{R}}\left\{\sum_{i\geqslant 1}\varrho_i(x)[\ln\varrho_i(x)-1]-\sigma(x)\ln[1-\tau(x)]\right\}dx$$

with the linear transforms of the densities (cf. Percus[13])

$$\sigma(x)=\sum_{i\geqslant 1}\int_{\mathbb{R}}\sigma^{(i)}(x-x')\varrho_i(x')\,dx',\quad \tau(x)=\sum_{i\geqslant 1}\int_{\mathbb{R}}\tau^{(i)}(x-x')\varrho_i(x')\,dx',$$

and ($h\equiv h_0$)

$$\tau^{(i)}(x)=h\left(\frac{i}{2}-|x|\right),\quad \sigma^{(i)}(x)=\frac{1}{2}|\partial_x\tau^{(i)}(x)|,\quad x\in\mathbb{R}. \tag{2.6}$$

Thus we conclude using definition (2.4b) that

$$\beta\bar{\mathfrak{F}}[\{\varrho_i\}_{i\geqslant 1}]=\int_{\mathbb{R}}\left\{\sum_{i\geqslant 1}\varrho_i(x)\left[\ln\frac{\varrho_i(x)}{C_i(\lambda)}-1\right]-\sigma(x)\ln[1-\tau(x)]\right\}dx.$$

The calculus ends (third stage) by projecting the functional $\mathfrak{F}$ onto the sought free energy F of $D=1$ sticky cores. This transform inverse is accomplished by means of a variational principle. The free energy functional of the original system occurs via an evaluation of the variational formula at the set of minimizing local partial densities.

Again upon using the discrete geometrical nature of the units, we obtain the partition of the local particle density [cf. (3.36) of Cuesta and Tutschka[6]]

$$\varrho(x)=\sum_{i\geqslant 1}\sum_{|j|\leqslant n_i}\varrho_i(x+j). \tag{2.7}$$

This yields

$$\tau(x)=\sum_{i\geqslant 1}\int_{x-\,i/2}^{x+\,i/2}\varrho_i(y)\,\mathrm{d}y=\int_{x-\,1/2}^{x+\,1/2}\varrho(y)\,\mathrm{d}y$$

as well as

$$\sum_{i\geqslant 1}\int_{\mathbb{R}}\varrho_i(x)U_i(x)\,\mathrm{d}x=\int_{\mathbb{R}}\varrho(x)U(x)\,\mathrm{d}x$$

by (2.5). Hence $\mathfrak{F}$ becomes

$$\beta\mathfrak{F}[\varrho,\{\varrho_i\}_{i\geqslant 1}]=\int_{\mathbb{R}}\left\{\varrho(x)\beta U(x)+\sum_{i\geqslant 1}\varrho_i(x)\left[\ln\frac{\varrho_i(x)}{C_i(\lambda)}-1\right]-\sigma(x)\ln[1-\tau(x)]\right\}\mathrm{d}x.$$

From this our overcomplete format free energy F of $D=1$ sticky balls in an external field U is found through the usual minimum principle of classical density functional theory (see, e.g., Refs. 15 and 3). If we evaluate the minimum in two steps, then we infer that

$$\beta F[U]=\min_{\varrho\in D_n}\min\left\{\beta\mathfrak{F}[\varrho,\{\varrho_i\}_{i\geqslant 1}]\colon L^1(\mathbb{R})\ni\varrho_i(x)\geqslant 0\wedge\sum_{i\geqslant 1}\sum_{|j|\leqslant n_i}\varrho_i(x+j)=\varrho(x)\right\} \tag{2.8}$$

with $D_n=\{t\in L^1(\mathbb{R})\colon t(x)\geqslant 0\wedge\int_{\mathbb{R}}t(x)\,\mathrm{d}x=n\}$, n fixed.

Given $\lambda\in\mathbb{R}_+$ and $\varrho\in D_n$, $\mathfrak{F}$ is convex in the local partial densities $\{\varrho_i\}_{i\geqslant 1}$. Thus the minimum in (2.8) with respect to $\{\varrho_i\}_{i\geqslant 1}$ is attained at (setting $m_i=n_i-\frac{1}{2}$)

$$\varrho_i(x)=C_i(\lambda)\frac{\Pi_{|j|\leqslant n_i}\varrho_1(x+j)}{\Pi_{|j|\leqslant m_i}[1-\tau(x+j)]},\quad i>1,$$

and ϱ_1 is found via (2.7). Therefore F simplifies to

$$\beta F[U]=\min_{\varrho\in D_n}\int_{\mathbb{R}}\left\{\varrho(x)[\beta U(x)+\ln\varrho_1(x)]-\sum_{i\geqslant 1}\varrho_i(x)-\frac{1}{2}\left[\varrho\left(x-\frac{1}{2}\right)+\varrho\left(x+\frac{1}{2}\right)\right]\right.$$
$$\left.\times\ln[1-\tau(x)]\right\}\mathrm{d}x, \tag{2.9}$$

which generalizes the findings in Sec. 2.2 of Kierlik and Rosinberg[7] for dimerizing hard rods, controlled by ϱ_1 and ϱ_2, to systems characterized by an arbitrary number of local partial densities. The equivalence of (2.9) and the inverse operator format sticky rods free energy functional[13] can be established through results shown in Sec. 3.2.1 of Cuesta and Tutschka.[6]

B. Plane case

At the outset we have to say what is meant by a many-body system of squares (having only translational degrees of freedom) with ''contact pair interactions.'' Clearly, one would like to go on with a system of sticky squares, in which the attractive part of the pair interaction Boltzmann factor is compressed to a Dirac δ-distribution on the boundary of the hard square core. But this

particle system is not thermodynamically stable. The proof of divergence of the partition function of sticky squares parallels that for sticky discs given by Stell,[16] except that for the quadratic case a particle can interact simultaneously with at most eight neighbors.

As a remedy, we back away from the sticky limit. We look at a system of squares with square-well attraction of well-width $d \in \mathbb{R}_+$ as well as interaction strength $\mathcal{E} \in \mathbb{R}_+$, and let $\mathcal{E}$ depend on d in such a way that $\lambda = d[\exp(\beta\mathcal{E}) - 1]$ remains finite as d tends to zero. Then, for $\lambda \in \mathbb{R}_+$ and sufficiently small $d > 0$ (see below), we define the pair interaction Boltzmann factor of a particle system of squares with ''contact pair interactions'' as given by (selecting units so that the side length of the hard square core equals 1)

$$e(x,y) = h_1(|x-y|_\infty) + \frac{\lambda}{d} h_{1,d}(|x-y|_\infty) \tag{2.10a}$$

with $x,y \in \mathbb{R}^2$ specifying the positions of the particles and $h_{a,b} = h_a - h_{a+b}$. That is, instead of taking the limit $d \to 0$ (the standard sticky limit—see, e.g., Stell[16]), we consider a related pair interaction function with arbitrarily small but fixed $d \neq 0$. The reason for the term ''contact interaction'' is that for sufficiently small $d > 0$ the range of the attraction in (2.10a) is negligible compared to the size of the particles.

The definition of the Hamiltonian function is finished via the local activity z, which generalizes without change to

$$z(x) = \exp\{\beta[\mu - U(x)]\}, \tag{2.10b}$$

where U is again the external field and μ the chemical potential (implicitly including the momentum contributions).

1. Overcompleteness technique

Now we will extend the particular overcomplete form deduced in Sec. II A to $D = 2$. There is no difference at all between the strategy we will use for the planar problem and the logic followed above. There are significant differences in the realizations, however. The central theme of the $D = 1$ analysis is the one-sided nature of the pair interaction Boltzmann factor (2.2). That is, the main properties that make the setup easier in the $D = 1$ context are

(a) the units are defined by a single integer variable, and
(b) the intrinsic free energy functional at $C_i(\lambda) \equiv 1$ is exact.

The $D = 2$ case does not share these properties. Still, there are units in the planar problem that can be characterized by two integer variables, and there is a functional that extrapolates from the polydisperse hard rod mixture functional to that of similar $D = 2$ particle systems. When we want our scheme to be analytically tractable, some suitable assumptions are needed. The guiding principle will be that of simplicity.

We begin again by mapping the given system (2.10) onto an additive polydisperse hard core mixture. This transformation partitions the original system into units of connected particles. Then these units are, in turn, regarded as components of a mixture, in which the interaction among the components is of hard core type. Thus the transformation maps configurations of connected particles of the original system onto components of the mixture. Correspondingly, the Hamiltonian function of this mixture is hopelessly complicated. In order to define a suitable idealization thereof, we restrict ourselves first to configurations of maximal connected particles. That is, via the contact nature of the interaction, we are left with units of square lattice type geometry. But this is not enough. Moreover, in analogy with the characterization of $D = 1$ units by a single integer parameter, we allow only for $D = 2$ units of rectangle-like shapes. Hence we specify units as $D = 2$ arrays of $i_1 \times i_2$ (with $i_1, i_2 \in \mathbb{N}_+$ interpreted as numbers of row and column particles, respectively) maximal connected particles. This extension of (a) to the $D = 2$ level is summarized in the following rule.

Assumption 2.1: The polydisperse representation of a nonuniform system of squares with contact interactions is completely characterized by rectangular arrays of maximal connected particles.

Here some comments are in order.

(1) The cases $(i_1=1)\vee(i_2=1)$ are to be interpreted as essentially one-dimensional, so that we are back to (a) when we specialize Assumption 2.1 to $D=1$. Then, through Assumption 2.1 and the contact nature of the interaction, the units become asymptotically as $d\to 0^+$ rectangles $R_i=\{(x_1,x_2)\in\mathbb{R}^2: |x_k|\leqslant i_k/2,\ k=1,2\}$, where we introduced a double-index $i=(i_1,i_2)$.
(2) Assumption 2.1 cannot possibly be exact. Only a certain class of configurations of connected particles is included.
(3) On the other hand, it is expected to be a good approximation whenever monomers are predominantly present in the system. That is, Assumption 2.1 holds for sufficiently high temperatures and sufficiently dilute states.
(4) At sufficiently low temperatures, there is only a vanishing proportion of units of connected but not maximal connected particles. Furthermore, by the contact nature of the interaction, the dominant units of maximal connected particles tend to minimize their surfaces. Then we may think of the particle system as being composed of compact, quasi close-packed units. Consequently, Assumption 2.1 is expected to be a good approximation for sufficiently low temperatures.
(5) The high density limit has to be treated separately since there will be ''percolation'' of arbitrarily long chains. So that at sufficiently high densities one can expect to enter a regime in which the validity of Assumption 2.1 is very questionable.

Thus, upon combing Assumption 2.1 with (2.10a) we have that the pair interaction Boltzmann factor between components i and j of the mixture is asymptotically as $d\to 0^+$ given by

$$e_{ij}(x,y)\asymp\chi_{\mathbb{R}^2\setminus R_{i+j}}(x-y), \tag{2.11a}$$

where χ_A is the characteristic function of the set A.

In the second stage, the definition of the model Hamiltonian on the polydisperse level is completed. Namely, the local activity $z_i(x)$ is used to encode the partition function of the $i_1\times i_2$ particle unit at x. Again through Assumption 2.1 and the d-range of the attractive part of the pair interaction, the local activity becomes as $d\to 0^+$,

$$z_i(x)\asymp C_i(\lambda,d)\exp\{\beta[\mu_i-U_i(x)]\}. \tag{2.11b}$$

Here, the combinatorial part is given by

$$C_i(\lambda,d)\asymp\frac{\lambda^{q(i)}}{(i_1 i_2)!\, d^{r(i)}}$$

with $q(i)=4i_1i_2-3(i_1+i_2)+2$, as well as $r(i)=0$ if $(i_1=1)\vee(i_2=1)$ and $2i_1i_2-3(i_1+i_2)+4$ otherwise. Moreover, the chemical potential of component i is found as $\mu_i=i_1i_2\,\mu$, and the external field is prescribed by the formula

$$U_i(x)\asymp\sum_{|j_1|\leqslant n_{i_1},|j_2|\leqslant n_{i_2}} U(x_1+j_1,x_2+j_2) \tag{2.12}$$

as $d\to 0^+$.

Accordingly, the local partial density $\varrho_{i_1i_2}$ of the original system is identified with the local particle density of component i of the mixture. Through this interpretation the partial densities can again be used variationally for the original system—see below.

Next we will turn to the calculation of the intrinsic free energy functional of (2.11). In two dimensions, exact solutions are in very short supply, even for pure hard core particle systems. One is therefore forced to evaluate the free energy at $C_i(\lambda,d)\equiv 1$ by means of some extrapolation type of scheme.

Several years ago, Zhang[10] reexamined hard rods in an external field by extending the Reiss–Frisch–Lebowitz (RFL) scaled particle format to the nonuniform case. He showed that the RFL reasoning is exact for nonuniform $D=1$ hard balls and constructed the ''global free energy functional'' which serves as generating functional for all hard rods intrinsic free energy density functionals. The physics of the nonuniform RFL approach is that locally the probability measure of creating a core of diameter a at x, $\mu_a(x)$, characterizes the equilibrium state of the system completely. Hence the excess global free energy functional is equal to the intrinsic ideal gas free energy functional of μ_a. Later on, the scope of global free energy functionals was expanded.[17,18] Cuesta and Martínez-Ratón[17] generalized Zhang's functional to hard rod mixtures. They also observed that for any additive mixture of hard rectangles an intrinsic free energy functional can be extrapolated from the hard rod mixtures global functional and related it to $D=2$ RFL scaled-particle-type arguments. We apply their extrapolation technique in our extension of (b) to $D=2$.

Assumption 2.2: The global free energy functional is the same for additive polydisperse hard rod and hard rectangle mixtures.

We note some properties of the assumption (cf. Cuesta and Martínez-Ratón[17])

(1) Assumption 2.2 is exact for sufficiently rarefied gases.[17]
(2) It is believed that the hard rod mixtures global functional gives the correct order of the thermodynamic potentials for hard rectangle mixtures. Of course this does not mean that the relative errors are small on the whole thermodynamic domain. Assumption 2.2 is expected to be a good approximation up to (at least) intermediate densities. For numerical tests passed by RFL type functionals see, e.g., Ref. 17.

So let us write $\mathfrak{F}[\{\varrho_{i_1i_2}\}]=\Sigma_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\varrho_{i_1i_2}(x)U_{i_1i_2}(x)\,dx+\bar{\mathfrak{F}}[\{\varrho_{i_1i_2}\}]$, such that $\bar{\mathfrak{F}}$ is the intrinsic free energy functional of Hamiltonian (2.11). Then, on using Assumption 2.2, we have due to Zhang[10] (as well as Cuesta and Martínez-Ratón[17]) immediately that

$$\beta\bar{\mathfrak{F}}[\{\varrho_{i_1i_2}\}_{i_1,i_2\geqslant 1}]|_{C_{i_1i_2}(\lambda,d)\equiv 1}$$
$$\asymp\int_{\mathbb{R}^2}\left\{\sum_{i_1,i_2\geqslant 1}\varrho_{i_1i_2}(x)[\ln\varrho_{i_1i_2}(x)-1]-\sigma(x)\ln[1-\tau(x)]+\frac{\nu_1(x)\,\nu_2(x)}{1-\tau(x)}\right\}dx,$$

where

$$\sigma(x)=\sum_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\sigma^{(i_1)}(x_1-x_1')\sigma^{(i_2)}(x_2-x_2')\varrho_{i_1i_2}(x_1',x_2')\,d(x_1',x_2'),$$

$$\nu_1(x)=\sum_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\sigma^{(i_1)}(x_1-x_1')\tau^{(i_2)}(x_2-x_2')\varrho_{i_1i_2}(x_1',x_2')\,d(x_1',x_2'),$$

$$\nu_2(x)=\sum_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\tau^{(i_1)}(x_1-x_1')\sigma^{(i_2)}(x_2-x_2')\varrho_{i_1i_2}(x_1',x_2')\,d(x_1',x_2'),$$

$$\tau(x)=\sum_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\tau^{(i_1)}(x_1-x_1')\tau^{(i_2)}(x_2-x_2')\varrho_{i_1i_2}(x_1',x_2')\,d(x_1',x_2')$$

with $\sigma^{(i)}$ and $\tau^{(i)}$ brought in via (2.6). Correspondingly we find through definition (2.11b) that

$$\beta\bar{\mathfrak{F}}[\{\varrho_{i_1i_2}\}_{i_1,i_2\geqslant 1}]$$
$$\asymp\int_{\mathbb{R}^2}\left\{\sum_{i_1,i_2\geqslant 1}\varrho_{i_1i_2}(x)\left[\ln\frac{\varrho_{i_1i_2}(x)}{C_{i_1i_2}(\lambda,d)}-1\right]-\sigma(x)\ln[1-\tau(x)]+\frac{\nu_1(x)\nu_2(x)}{1-\tau(x)}\right\}\mathrm{d}x.$$

We end (third stage) as in the $D=1$ context by projecting the polydisperse functional $\mathfrak{F}$ onto the desired free energy F of the original system. The transform inverse is obtained via the minimization of $\mathfrak{F}$ with respect to all the $\varrho_{i_1i_2}$ subject to the constraint

$$\varrho(x)\asymp\sum_{i_1,i_2\geqslant 1}\sum_{|j_1|\leqslant n_{i_1},|j_2|\leqslant n_{i_2}}\varrho_{i_1i_2}(x_1+j_1,x_2+j_2),\tag{2.13}$$

which follows from the discrete geometry of the units as $d\to 0^+$. Thus,

$$\tau(x)=\sum_{i_1,i_2\geqslant 1}\int_{x_1-i_1/2}^{x_1+i_1/2}\int_{x_2-i_2/2}^{x_2+i_2/2}\varrho_{i_1i_2}(x_1',x_2')\,\mathrm{d}(x_1',x_2')\asymp\int_{x_1-1/2}^{x_1+1/2}\int_{x_2-1/2}^{x_2+1/2}\varrho(x_1',x_2')\,\mathrm{d}(x_1',x_2'),$$

as well as upon processing (2.12),

$$\sum_{i_1,i_2\geqslant 1}\int_{\mathbb{R}^2}\varrho_{i_1i_2}(x)U_{i_1i_2}(x)\,\mathrm{d}x\asymp\int_{\mathbb{R}^2}\varrho(x)U(x)\,\mathrm{d}x.$$

Therefore $\mathfrak{F}$ takes on the form

$$\beta\mathfrak{F}[\varrho,\{\varrho_{i_1i_2}\}_{i_1,i_2\geqslant 1}]$$
$$\asymp\int_{\mathbb{R}^2}\left\{\varrho(x)\beta U(x)+\sum_{i_1,i_2\geqslant 1}\varrho_{i_1i_2}(x)\left[\ln\frac{\varrho_{i_1i_2}(x)}{C_{i_1i_2}(\lambda,d)}-1\right]-\sigma(x)\ln[1-\tau(x)]\right.$$
$$\left.+\frac{\nu_1(x)\nu_2(x)}{1-\tau(x)}\right\}\mathrm{d}x,$$

so that we finally infer from Assumptions 2.1 and 2.2 for the free energy of a nonuniform system of squares with contact interactions

$$\beta F[U]\asymp\min_{\varrho\in D_n}\min\left\{\beta\mathfrak{F}[\varrho,\{\varrho_{i_1i_2}\}_{i_1,i_2\geqslant 1}]:L^1(\mathbb{R}^2)\ni\varrho_{i_1i_2}(x)\geqslant 0\right.$$
$$\left.\wedge\sum_{i_1,i_2\geqslant 1}\sum_{|j_1|\leqslant n_{i_1},|j_2|\leqslant n_{i_2}}\varrho_{i_1i_2}(x_1+j_1,x_2+j_2)=\varrho(x)\right\}\tag{2.14}$$

with $D_n=\{t\in L^1(\mathbb{R}^2):t(x)\geqslant 0\wedge\int_{\mathbb{R}^2}t(x)\,\mathrm{d}x=n\}$, n fixed.

Given $\lambda\in\mathbb{R}_+$, sufficiently small $d>0$, and $\varrho\in D_n$, the functional appearing on the right-hand side (RHS) of (2.14) is convex in the local partial densities. Hence it attains its minimum with respect to $\{\varrho_{i_1i_2}\}_{i_1,i_2\geqslant 1}$ at

$$\varrho_{i_1 i_2}(x) \asymp C_{i_1 i_2}(\lambda,d)\,\frac{\Pi_{|j_1|\leqslant n_{i_1},|j_2|\leqslant n_{i_2}}\varrho_{11}(x_1+j_1,x_2+j_2)}{\Pi_{|j_1|\leqslant m_{i_1},|j_2|\leqslant m_{i_2}}[1-\tau(x_1+j_1,x_2+j_2)]}$$

$$\times \prod_{|j_1|\leqslant m_{i_1}} \frac{\exp[\mu_2^{(i_2)}(x_1+j_1,x_2)]}{\Pi_{s\in\{-,+\}}\left[1-\tau\left(x_1+j_1,x_2+s\frac{i_2}{2}\right)\right]^{1/2}}$$

$$\times \prod_{|j_2|\leqslant m_{i_2}} \frac{\exp[\mu_1^{(i_1)}(x_1,x_2+j_2)]}{\Pi_{s\in\{-,+\}}\left[1-\tau\left(x_1+s\frac{i_1}{2},x_2+j_2\right)\right]^{1/2}} \quad (i_1\neq 1)\wedge(i_2\neq 1).$$

Here we introduced for $k\in\mathbb{N}$

$$\mu_1^{(k)}(x)=\int_{x_1-(k/2)}^{x_1+(k/2)}\frac{\nu_1(x_1',x_2)}{1-\tau(x_1',x_2)}\,\mathrm{d}x_1', \quad \mu_2^{(k)}(x)=\int_{x_2-(k/2)}^{x_2+(k/2)}\frac{\nu_2(x_1,x_2')}{1-\tau(x_1,x_2')}\,\mathrm{d}x_2',$$

and $m_i=n_i-\frac{1}{2}$, $i\in\mathbb{N}_+$ [remember that we have let $n_i=(i-1)/2$)]. The local monomer density ϱ_{11} is determined through (2.13). Thus F simplifies to

$$\beta F[U]\asymp \min_{\varrho\in D_n}\int_{\mathbb{R}^2}\Bigg\{\varrho(x_1,x_2)[\beta U(x_1,x_2)+\ln\varrho_{11}(x_1,x_2)]-\sum_{i_1,i_2\geqslant 1}\varrho_{i_1 i_2}(x_1,x_2)$$

$$-\frac{1}{4}\sum_{s_1,s_2\in\{-,+\}}\varrho\left(x_1+\frac{s_1}{2},x_2+\frac{s_2}{2}\right)\ln[1-\tau(x_1,x_2)]+\frac{1}{2}\sum_{s\in\{-,+\}}\left[\varrho\left(x_1+\frac{s}{2},x_2\right)\right.$$

$$\left.\times\mu_2^{(1)}(x_1,x_2)+\varrho\left(x_1,x_2+\frac{s}{2}\right)\mu_1^{(1)}(x_1,x_2)\right]-\frac{1}{2}\sum_{i_1,i_2\geqslant 1}\sum_{s\in\{-,+\}}\left[\varrho_{i_1 i_2}\left(x_1+s\frac{i_1}{2},x_2\right)\right.$$

$$\left.\times\mu_2^{(i_2)}(x_1,x_2)+\varrho_{i_1 i_2}\left(x_1,x_2+s\frac{i_2}{2}\right)\mu_1^{(i_1)}(x_1,x_2)\right]+\frac{\nu_1(x_1,x_2)\,\nu_2(x_1,x_2)}{1-\tau(x_1,x_2)}\Bigg\}\,\mathrm{d}(x_1,x_2).$$

2. Uniform limit

Suppose we have a field-free situation with particle density ρ and partial densities $\{\rho_{i_1 i_2}\}_{i_1,i_2\geqslant 1}$. Then it follows from the above that the thermodynamic pressure p and specific free energy f are

$$\beta p(\beta,\rho)\asymp\frac{\xi_0}{1-\rho}+\left(\frac{\xi_1}{1-\rho}\right)^2, \tag{2.15}$$

$$\beta f(\beta,\rho)\asymp\rho\left[\ln\rho_{11}-\ln(1-\rho)+\frac{2\xi_1}{1-\rho}\right]-\xi_0-\frac{\xi_1^2}{1-\rho}, \tag{2.16}$$

where for $(i_1\neq 1)\wedge(i_2\neq 1)$

$$\rho_{i_1 i_2}\asymp C_{i_1 i_2}(\lambda,d)\,\rho_{11}\left(\frac{\rho_{11}}{1-\rho}\right)^{i_1 i_2-1}\left[\exp\left(\frac{\xi_1}{1-\rho}\right)\right]^{2i_1 i_2-(i_1+i_2)}$$

with $\rho=\Sigma_{i_1,i_2\geqslant 1} i_1 i_2\,\rho_{i_1 i_2}$, $\xi_1=\Sigma_{i_1,i_2\geqslant 1} i_2\,\rho_{i_1 i_2}=\Sigma_{i_1,i_2\geqslant 1} i_1\,\rho_{i_1 i_2}$, as well as $\xi_0=\Sigma_{i_1,i_2\geqslant 1}\rho_{i_1 i_2}$.

It is natural to ask whether the model exhibits a phase transition (see, e.g., Ruelle[8]) at sufficiently small d if λ is large enough. Even more so since Lebowitz and Percus[19] showed that

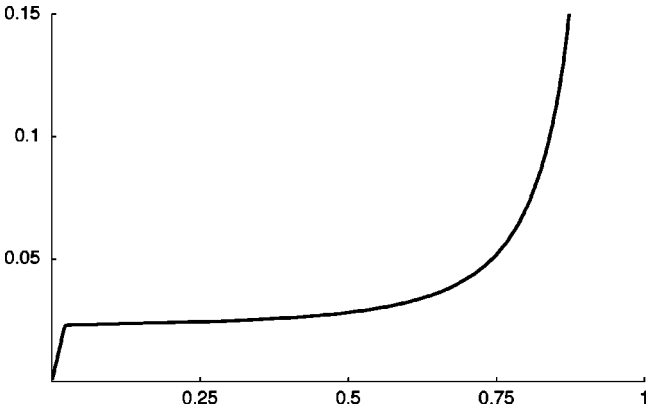

FIG. 1. Finite approximation isotherm for the interacting squares model (2.15): βp as a function of $\rho \in (0,1)$ for $\lambda = 0.15$ and $d = 0.0001$. The upper summation limits of the sums in (2.15) were set equal to 25.

already for a related $D=1$ particle system a first-order phase transition occurs. A curve showing βp as a function of $\rho \in (0,1)$ for $\lambda = 0.15$ and $d = 0.0001$ is depicted in Fig. 1 for which $\rho_{i_1 i_2} = 0$, $(i_1 > n) \vee (i_2 > n)$, $n = 25$. Also from this numerical evaluation one might reasonably expect the existence of a first-order phase transition as n tends to infinity. Up to now we have no proof of this conjecture.

III. LATTICE SYSTEMS

It would also be useful to have the transformation technique for lattice systems since they arise naturally in statistical mechanics. In this section we shall show that the method applies equally well to the prototypical particle system with next neighbor interactions on $\mathbb{Z}^2$. One reason for this choice is that for this system the phase separation line is known (see, e.g., Refs. 1 and 2). This will allow us to compare our polydisperse modeling with exact results. Another notable one is the fact that the restriction of the particle positions to $\mathbb{Z}^2$ makes the system a perfectly reasonable ''toy model'' of squares with contact pair interactions if β is large enough. Namely that the units of maximal connected particles are now by definition of square lattice geometry such that the next neighbor system on $\mathbb{Z}^2$ mimics the continuous one with contact interactions in $\mathbb{R}^2$ modulo the discretized positions of the units.

As a preliminary we are going to start from the $D=1$ case in Sec. III A. The corresponding specific free energy will be calculated by means of elementary combinatorics and through a mapping onto polydisperse hard rod mixtures. In analogy with the above development, the transformation technique will then be lifted to $\mathbb{Z}^2$ in Sec. III B. To see that it indeed gives sensible thermodynamic properties, at least for sufficiently low temperatures, we will finally compare those with exact results.

A. Next neighbor interacting particles on $\mathbb{Z}$

Throughout this subsection we will work in the ''particle'' representation of lattice systems (as opposed to the ''spin'' representation or the ''alloy'' interpretation—see, e.g., Ruelle[8]). Correspondingly, we consider an interval $\Lambda \subset \mathbb{Z}$ of n integers (points or sites), numbered from left to right, and assign to each site i of Λ a variable x_i which takes the value 1 (occupied site) or 0 (empty site). This means that each lattice site can be occupied by at most one particle. The number of particles of a configuration $x = \{x_i : i \in \Lambda\}$ is defined by $N(x) = \#\{i \in \Lambda : x_i = 1\}$. Furthermore, we associate with each configuration x a Hamiltonian or pair interaction energy (cf. Baxter[1])

$$H(x) = -\mathcal{E} \sum_{i=1}^{n-1} x_i x_{i+1},$$

where $\mathcal{E}\in\mathbb{R}_+$ is again the interaction strength. Then the total Gibbs measure for a particle system with next neighbor interactions on Λ is given by (cf. Ruelle[8])

$$Z(\beta,\mu,n)=\sum_{m=0}^{n}\exp(m\beta\mu)\sum_{\substack{x\in\{0,1\}^n\\ N(x)=m}}\exp[-\beta H(x)]$$

and the thermodynamic pressure as

$$\beta p(\beta,\mu)=\lim_{n\to\infty}\frac{1}{n}Z(\beta,\mu,n).$$

1. Partition of the particle density

To evaluate these, we decompose the system into units of i by the negative, i.e., attractive part of the pair interaction connected particles. Consider an arbitrary n-site configuration $x\in\{0,1\}^n$ such that $N(x)=m\geqslant 1$. Denote by k_i the number of times a unit of i connected particles appears in x. Define correspondingly the set

$$A_m=\left\{k=(k_1,\ldots,k_m):\, k_i\in\{0,\ldots,m\}\wedge\sum_{i=1}^{m}k_i i=m\right\}$$

and let for fixed $k\in A_m$

$$C(n,m,k)=\frac{(\Sigma_{i=1}^{m}k_i)!}{k_1!\cdots k_m!}\binom{n-m+1}{\sum_{i=1}^{m}k_i}. \tag{3.1}$$

There are $C(n,m,k)$ (n,m,k)-configurations x with the same energy $H(x)$. Hence the total Gibbs measure becomes

$$Z(\beta,\mu,n)=1+\sum_{m=1}^{n}\exp(m\beta\mu)\sum_{k\in A_m}C(n,m,k)\,\lambda^{\Sigma_{i=1}^{m}(i-1)k_i}, \tag{3.2}$$

where we introduced $\lambda=\exp(\beta\mathcal{E})\geqslant 1$.

We observe that the empty configuration has one partition, the empty partition.

We also observe the close resemblance of (3.1) to the corresponding formula for sticky rods in Sec. 2.1 of Cuesta and Tutschka.[6] The additional binomial coefficient in (3.1) controls the number of empty sites between successive units.

Since there are no more than n terms in the first sum, and since also the number of summands of the second sum is exponentially bounded (cf. the theorem due to Hardy and Ramanujan on the number of partitions of a positive integer—see, e.g., Andrews[11,12]), the leading order asymptotic behavior of Z is determined by the largest summands in (3.2) (see, e.g., Ellis[20]).

A weak form of Stirling's formula, $\ln(n!)=n\ln n-n+O(\ln n)$, gives as n tends to infinity

$$\frac{1}{n}\ln C(n,m,k)=\left(1-\frac{m}{n}\right)\ln\left(1-\frac{m}{n}\right)-\left(1-\frac{m}{n}-\sum_{i=1}^{m}\frac{k_i}{n}\right)\ln\left(1-\frac{m}{n}-\sum_{j=1}^{m}\frac{k_j}{n}\right)$$
$$-\sum_{i=1}^{m}\frac{k_i}{n}\ln\frac{k_i}{n}+O\left(\frac{\ln n}{n}\right).$$

Here the uniform bound of the reminder can be proved via a binary partition of the sum in $\Sigma_{i=1}^{m} O(\ln k_i)$. Therefore, upon introducing the particle density $\rho = m/n$ and the partial densities $\rho_i = k_i/n$ as $n \to \infty$, we infer that

$$\beta p(\beta,\mu) = \max_{\rho \in (0,1)} [\rho\,\beta\mu - \beta f(\beta,\rho)],$$

where the specific free energy is found to be

$$\beta f(\beta,\rho) = \min_{(\rho_1,\ldots)\in A_\rho} \left[\sum_{i\geqslant 1} \rho_i \ln \frac{\rho_i}{\lambda^{i-1}} + \left(1-\rho-\sum_{i\geqslant 1}\rho_i\right) \ln\left(1-\rho-\sum_{i\geqslant 1}\rho_i\right) - (1-\rho)\ln(1-\rho) \right] \tag{3.3}$$

with $A_\rho = \{(r_1,\ldots): r_i \geqslant 0 \wedge \Sigma_{i\geqslant 1} r_i i = \rho\}$.

Fix $\lambda \geqslant 1$ and $\rho \in (0,1)$. Then the function appearing on the RHS of the overcomplete free energy (3.3) is convex in all the ρ_i. Thus it attains its minimum at the unique value

$$\rho_i = \begin{cases} \dfrac{\rho}{[1+\lambda(\theta-1)]^2} & \text{if } i=1, \\ \dfrac{\rho_1}{\left[1+\dfrac{1}{\lambda(\theta-1)}\right]^{i-1}} & \text{otherwise,} \end{cases}$$

where $\theta \equiv \exp[\beta p(\beta,\rho)]$. Through

$$\sum_{i\geqslant 1} \rho_i = \frac{\rho}{1+\lambda(\theta-1)} \tag{3.4}$$

we have that

$$\left(1-\frac{1}{\theta}\right)[1+\lambda(\theta-1)] = \frac{1}{\rho^{-1}-1}, \tag{3.5a}$$

or explicitly

$$\theta = \frac{1}{2\lambda}\left[-1+\frac{1}{\rho^{-1}-1}+2\lambda+\sqrt{\left(1-\frac{1}{\rho^{-1}-1}\right)^2+\frac{4\lambda}{\rho^{-1}-1}}\right], \tag{3.5b}$$

which is the known result (see, e.g., Lavis and Bell[2]). Hence f simplifies to

$$\beta f(\beta,\rho) = \rho\ln(\theta-1) - \rho\ln[1+\lambda(\theta-1)] - (1-\rho)\ln\theta.$$

Note the formal resemblance of these results to those for $D=1$ sticky balls deduced in Sec. 2.1 of Cuesta and Tutschka.[6] This shows that the discrete geometrical nature of the units is the central property linking next neighbor interacting particles on $\mathbb{Z}$ and sticky rods. One could go ahead and convert the treatment of nonuniform $D=1$ sticky cores as presented in Ref. 6 to the discrete case. Then this picture leads to the conjecture that there is a hard rods mixture form free energy functional for $D=1$ next neighbor lattice gases which is completely characterized by effective pressures $p^{\pm}$.[9,10,6] These pressure-like quantities are determined by quadratic equations [cf. (3.47) of Cuesta and Tutschka[6] as well as (3.5)]. The argument may be ended by noting that in the original derivation of the free energy functional for this system by Percus,[21] the solution of the inverse problem is reduced to a quadratic equation, too.

2. Mapping onto a polydisperse mixture

We end this section by adopting the transformation method of Cuesta and Tutschka[6] to the $D=1$ discrete case.

First we observe that an i-particle unit is of "effective" size $a_i=i+1$, $i\in\mathbb{N}_+$, since a unit of i connected particles starts and terminates by definition with an empty site. Again these units interact through hard core potentials, so that a next neighbor lattice gas on $\mathbb{Z}$ can be mapped onto an additive polydisperse hard rods mixture in which the diameter of component i equals $i+1$.

In the second stage, the internal partition function of an i-particle unit, λ^{i-1}, is incorporated. As above, this amounts of encoding λ^{i-1} into the activity of component i. This completes the transformation to a $D=1$ polydisperse hard core mixture. Let us call this mixture for future reference "original" polydisperse mixture. However, in contrast to the continuous case, we cannot directly evaluate the free energy of this mixture at $\lambda=1$. The complication being that the centers of the hard rods do not necessarily lie on $\mathbb{Z}$. To account for this, we go over to a suitable rescaled additive polydisperse hard rods mixture.

So suppose we have a $D=1$ additive polydisperse hard core mixture in an external field. Let the pair interaction Boltzmann factor between component i and j be given by [in the following a bar signifies a quantity of the "rescaled" polydisperse mixture]

$$\overline{e_{ij}}(y,x)=\chi_{\mathbb{N}}(y-x-(i+j+2)) \tag{3.6}$$

with $x,y\in\mathbb{Z}$ denoting the positions of the hard rods. That is, we consider a mixture with even hard core diameters $\overline{a_i}=2(i+1)$. As usual, the influence of the chemical potential $\overline{\mu_i}$ and the external field $\overline{U_i}$ is represented via the local activity $\overline{z_i}$ of component i (see, e.g., Refs. 14 and 18). The setup is ended by introducing all the local partial densities $\overline{\varrho_i}$ accordingly.

For such a polydisperse mixture, the free energy density functional is known exactly.[14,18] Hence, on taking the uniform limit, we would immediately obtain, say, the equation of state for the $D=1$ next neighbor lattice gas if we would be able to project the excess free energy for the rescaled hard rods mixture onto that for the original one at $\lambda=1$.

To do so, we first exclude certain configurations from the configuration space of the rescaled polydisperse system. Let us introduce the predicate $P(i)\Leftrightarrow i$ even. Then the configurations of the original and the rescaled mixture are equivalent by the following rule. The local partial density $\overline{\varrho_i}$ at $x\in\mathbb{Z}$ is equal to 0 whenever

(I) $\neg P(i)\wedge\neg P(x)$ or $P(i)\wedge P(x)$.

In order to have full equivalence between the two systems, we furthermore restrict the domain of the observables for the rescaled mixture to the set

(II) $\{x\in\mathbb{Z}\colon P(x)\}$.

Now let us put everything together. We start from the excess free energy density functional for the rescaled pure hard rods mixture as characterized by the pair interaction Boltzmann factor (3.6). Imposing the boundary conditions (I) and (II), one gets an excess free energy functional which reduces in the uniform limit to the excess free energy for the original $D=1$ polydisperse hard core mixture at $\lambda=1$. From this, upon incorporating the partition functions of the units, λ^{i-1}, the function on the RHS of (3.3) is reproduced, as must be the case.

Finally it may be noted that an alternative form of the equation of state follows most readily from (3.3) through one of the well-known thermodynamic relations (see, e.g., Ruelle[8]). We find that [cf. (2.23) of Lafuente and Cuesta[18]]

$$\beta p(\beta,\rho)=\ln\left[\frac{1-\Sigma_{i\geqslant 1} i\rho_i}{1-\Sigma_{i\geqslant 1}(i+1)\rho_i}\right],$$

which is via $\Sigma_{i\geqslant 1} i\rho_i=\rho$ and (3.4) equivalent to (3.5).

B. Extension to $\mathbb{Z}^2$

We consider the standard example[1] of a system with next neighbor interactions on the square lattice. As before, we use the "particle" representation, so that with every site $i \in \mathbb{Z}^2$ a state variable $x_i \in \{0,1\}$ is associated. Then the lattice energy is[1]

$$H = -\mathcal{E} \sum_{(i,j)} x_i x_j ,$$

where (i,j) signifies an unordered next neighbor pair and $\mathcal{E}$ is as above the interaction strength.

For such a system, several thermodynamic properties are known exactly. Our objective is to transcribe the procedure of Sec. II B to this case, allowing us to study the validity of idealizations such as Assumptions 2.1 and 2.2. The development goes through modulo changes due to the discrete nature of the system. Therefore, there is probably no need to be too detailed in what follows.

1. Restricted overcomplete representation

As in the continuous case, we begin the construction with a decomposition of the system into units of connected particles. Here, two particles are said to be connected if their pair interaction energy equals $-\mathcal{E}$. By applying the transformation technique of Cuesta and Tutschka,[6] this partition of the system can be turned into a mapping onto polydisperse hard core mixtures. However, as was argued in Sec. II B, a mathematical analysis of such a polydisperse mixture is beyond reach. Thus, in order to build a solvable model, we restrict ourselves to a certain class of compact unit configurations. The lattice analogue of Assumption 2.1 reads as follows.

Assumption 3.1: The polydisperse representation of a particle system with next neighbor interactions on $\mathbb{Z}^2$ is completely characterized by rectangular arrays of connected particles.

Recall that this idealization cannot possibly be exact, but that it is expected to be valid at sufficiently high temperatures, low densities, or low temperatures. Again, the high density limit has to be examined separately.

The units interact with each other via hard core potentials. Next the precise nature of these pair interactions will be defined. For $i=(i_1,i_2)$, $i_1,i_2 \in \mathbb{N}_+$, denote by $R_i \subset \mathbb{Z}^2$ a rectangle of side lengths i_1 and i_2, respectively, as well as by $A_i \subset \mathbb{Z}^2$ the "effective" shape of an $i_1 \times i_2$ array of connected particles. Then, in analogy with the $D=1$ case, the interior of the set A_i is given by R_{i-1}; the boundary of A_i represents again the coat of empty sites on the circumference of each unit. Since every site has four next neighbors, A_i is equal to R_{i+1} only modulo the sites on the corners of R_{i+1}. Clearly, we cannot proceed analytically with a polydisperse mixture composed of particles of sorts A_i. So that in contrast to the continuous case, Assumption 3.1 is not strong enough to specify a mathematically tractable polydisperse Hamiltonian. We therefore make the following additional simplification.

Assumption 3.2: An $i_1 \times i_2$ array of connected particles has effective shape R_{i+1}.

The consequences of the assumption may be described as follows. If the system is in a sufficiently dilute state, then the additional excluded volume is negligible compared to the total free volume of the system. Hence Assumption 3.2 holds for sufficiently low densities. On the other hand, Assumption 3.2 should also be a good approximation whenever the predominant units are sufficiently large, since the boundary of A_i is of no consequence in the limit $i_1,i_2 \to \infty$. This means that Assumption 3.2 is expected to be valid for intermediate and high densities if β is sufficiently large, too.

With Assumptions 3.1 and 3.2, the first stage of the transformation can be ended. By now, the next neighbor square lattice gas is mapped onto an additive polydisperse mixture of hard rectangles with side lengths i_1+1 and i_2+1, respectively.

In the second stage, the partition function of an i-unit is appended to the activity of component i of the mixture. Through the next neighbor nature of the interaction, the total isothermal measure of an $i_1 \times i_2$ array of connected particles is found to be $C_{i_1 i_2}(\lambda) = \lambda^{2i_1 i_2 - (i_1 + i_2)}$. This completes the polydisperse setting.

Next we will construct the free energy for this polydisperse mixture at $\lambda = 1$. Once this, say, "level-2" free energy is known, the free energy for the next neighbor interacting particle system on $\mathbb{Z}^2$ (the "level-1" free energy, then) is obtainable via a variational formula (stage three of the transformation technique—see above).

To simplify the computation of the level-2 excess free energy, we can follow the same procedure as in Sec. III A 2. That is, we introduce a nonuniform additive polydisperse mixture of pure hard rectangles with even side lengths $2(i_1+1)$ and $2(i_2+1)$, respectively. This is our "level-3" system. Then the following four disjunctive rules guarantee that all with respect to the level-2 system spurious configurations are excluded from the level-3 configuration space. Depending on the shape of the units, the local partial density of component i of the level-3 system vanishes at $(x_1, x_2) \in \mathbb{Z}^2$ whenever

(I) $(\neg P(i_1) \wedge \neg P(i_2)) \wedge (\neg P(x_1) \vee \neg P(x_2))$,

(II) $(P(i_1) \wedge \neg P(i_2)) \wedge (P(x_1) \vee \neg P(x_2))$,

(III) $(\neg P(i_1) \wedge P(i_2)) \wedge (\neg P(x_1) \vee P(x_2))$, or

(IV) $(P(i_1) \wedge P(i_2)) \wedge (P(x_1) \vee P(x_2))$.

There is a further condition for full equivalence. The domain of the observables is to be restricted to the set

(V) $\{(x_1, x_2) \in \mathbb{Z}^2 : P(x_1) \wedge P(x_2)\}$.

These rules relate the level-3 excess properties and the sought level-2 excess thermodynamic functions at $\lambda = 1$.

Like in the $D = 2$ continuous case, we are forced to evaluate the level-3 excess free energy functional by means of some extrapolation type of scheme. Recently, Lafuente and Cuesta[18] wrote down the discrete version of Zhang's global free energy functional for continuous hard rod mixtures. This RFL scaled-particle-type functional serves as our basic underlying level-3 excess free energy model.

Assumption 3.3: The global free energy functional is the same for additive polydisperse hard rod mixtures on $\mathbb{Z}$ and additive polydisperse hard rectangle mixtures on $\mathbb{Z}^2$.

The same comments as above can be made. Assumption 3.3 is exact for sufficiently low densities, and it is believed to hold up to (at least) intermediate or moderately high densities.[18]

We are now ready to deduce the free energy for next neighbor square lattice gases under Assumptions 3.1–3.3. First take the global free energy functional (Assumption 3.3) and generate the excess free energy density functional for an additive mixture of rectangles with even side lengths $2(i_1+1)$ and $2(i_2+1)$, respectively. Next, introduce a related functional by applying projection (I)–(V). By construction, this functional gives in the uniform limit the excess part of [cf. (3.13) of Lafuente and Cuesta[18]]

$$\beta f^*(\beta, \rho, \{\rho_{i_1 i_2}\}_{i_1, i_2 \geqslant 1})\big|_{C_{i_1 i_2}(\lambda) \equiv 1} = \sum_{i_1, i_2, \geqslant 1} \rho_{i_1 i_2} \ln \rho_{i_1 i_2} + (1-\xi)\ln(1-\xi) - (1-\nu_1)\ln(1-\nu_1) - (1-\nu_2)\ln(1-\nu_2) + (1-\rho)\ln(1-\rho),$$

the specific free energy at $\lambda = 1$ associated with the polydisperse Hamiltonian function specified through Assumption 3.1 and 3.2. Here, the sequence $\{\rho_{i_1 i_2}\}_{i_1, i_2 \geqslant 1}$ represents the partial densities

of the system, $\rho=\Sigma_{i_1,i_2\geqslant 1} i_1 i_2\, \rho_{i_1 i_2}$ is the particle density, $\nu_1=\Sigma_{i_1,i_2\geqslant 1}(i_1+1) i_2\, \rho_{i_1 i_2}$, $\nu_2=\Sigma_{i_1,i_2\geqslant 1} i_1(i_2+1)\, \rho_{i_1 i_2}$, and $\xi=\Sigma_{i_1,i_2\geqslant 1}(i_1+1)(i_2+1)\, \rho_{i_1 i_2}$. Moreover, processing the ideal gas part we conclude that

$$\beta f^*(\beta,\rho,\{\rho_{i_1 i_2}\}_{i_1,i_2\geqslant 1}) = \sum_{i_1,i_2,\geqslant 1} \rho_{i_1 i_2} \ln \frac{\rho_{i_1 i_2}}{C_{i_1 i_2}(\lambda)} + (1-\xi)\ln(1-\xi) - (1-\nu_1)\ln(1-\nu_1) - (1-\nu_2)\ln(1-\nu_2) + (1-\rho)\ln(1-\rho).$$

Finally recall that a variational principle relates the level-1 and level-2 free energy functions (stage three of the transformation technique), so that we infer from Assumptions 3.1–3.3 for the specific free energy of a classical next neighbor square lattice gas

$$\beta f(\beta,\rho) = \min_{(\rho_{11},\ldots)\in A_\rho} \beta f^*(\beta,\rho,\{\rho_{i_1 i_2}\}_{i_1,i_2\geqslant 1})$$

with $A_\rho=\{(r_{11},\ldots): r_{i_1 i_2}\geqslant 0 \wedge \Sigma_{i_1,i_2\geqslant 1} i_1 i_2\, r_{i_1 i_2}=\rho\}$.

Fix $\lambda\geqslant 1$ and suitable $\rho\in(0,1)$ (cf. Assumption 3.2). Then f^* is convex in all the partial densities. Hence the minimum is attained at

$$\rho_{i_1 i_2} = \rho_{11}\left(\frac{\rho_{11}}{1-\xi}\right)^{i_1 i_2 - 1}\left[\frac{\lambda(1-\eta)}{1-\xi}\right]^{2 i_1 i_2 - (i_1+i_2)} \qquad (i_1\neq 1)\wedge(i_2\neq 1),$$

where $\nu_1=\nu_2\equiv\eta$ via spatial symmetry. Therefore f simplifies to

$$\beta f(\beta,\rho) = \rho\ln\rho_{11} + (1-4\rho)\ln(1-\xi) - 2(1-2\rho)\ln(1-\eta) + (1-\rho)\ln(1-\rho).$$

Furthermore, we have for the thermodynamic pressure

$$\beta p(\beta,\rho) = \ln\left[\frac{(1-\eta)^2}{(1-\xi)(1-\rho)}\right]. \tag{3.7}$$

2. Exact coexistence curve

We come now to the final step (step three) in our program. Also for a feeling as to what to expect for the continuous case if β is sufficiently large, we will compare the pressure function (3.7) with the exact equation of state in the two-phase thermodynamic region of the system.

In order to keep things simple, we take $\mathcal{E}=1$, so that the phase separation line can be parametrized by $\lambda=\lambda(\beta)=\exp\beta$ [remember that we have set $\lambda=\exp(\beta\mathcal{E})$]. Then the exact thermodynamic pressure at phase equilibrium for a classical next neighbor square lattice gas is[1,2]

$$\beta p(\beta) = \ln\left(1+\frac{1}{\lambda}\right) + \frac{1}{\pi}\int_0^{\pi/2} \ln\left[\frac{1}{2}(1+\sqrt{1-k_1^2\sin^2\theta})\right] d\theta, \quad \lambda\geqslant\lambda_c, \tag{3.8a}$$

where

$$k_1=\frac{2\sqrt{k}}{1+k}, \quad k=\frac{4\lambda}{(\lambda-1)^2},$$

and λ_c denotes the "critical" value of λ, determined by the quadratic equation $k=1$. This yields via the condition $\lambda\geqslant 1$ the number $\lambda_c=3+2\sqrt{2}$. The exact "conjugate" particle densities at phase equilibrium are found to be[1,2]

$$\rho_\pm(\beta) = \tfrac{1}{2}(1\pm\sqrt[8]{1-k^2}), \quad \lambda\geqslant\lambda_c. \tag{3.8b}$$

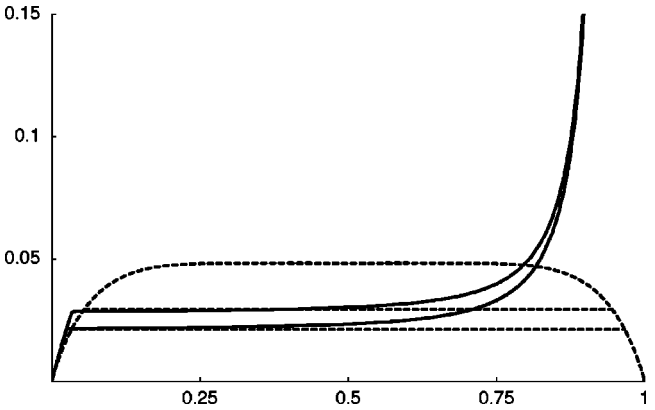

FIG. 2. Finite approximation isotherms (full lines) for the classical next neighbor square lattice gas model (3.7): βp as a function of $\rho \in (0,1)$ for $\lambda = 7$ (upper curve) and $\lambda = 8$ (lower graph). The upper summation limit n of the sums in (3.7) was picked to be 35. The broken lines are the exact phase separation line (3.8) and the corresponding exact pressures at phase equilibrium (3.8a), respectively.

Two $(\beta p, \rho)$ isotherms of (3.7) (full lines) for λ greater than λ_c are shown in Fig. 2. Notice that the upper summation limit n of the sums in (3.7) was set to 35. The broken curve is the exact coexistence curve (3.8) and the broken horizontal lines are the corresponding exact phase equilibrium pressures (3.8a).

While incrementing the summation limit n, the flattish part of the isotherms becomes both flatter and longer. Since the proportion of small units decreases when n increases, the pressure is lower for $n+1$, too. Thus one may conjecture that for sufficiently large n the pressure function (3.7) is a good approximation over a wide range of densities if λ is large enough; according to Fig. 2, an estimate is $\lambda \geqslant 8$. Clearly, what remains to be checked is that the error brought in via Assumption 3.3 will only be felt when ρ is high. It may also be noted that for, say, $\lambda < 8$, at least the ρ_- part of the phase separation line is overestimated. This defect of our model is not uncommon: it affects for example also the well-known mean field square lattice gas (see, e.g., Lavis and Bell[2]).

In summary, the numerical evaluation indicates that the lattice scheme behaves precisely as expected when β is sufficiently large. And this also gives—indirectly—some confidence in the soundness of the continuous $D=2$ extension developed in Sec. II B.

IV. CONCLUDING REMARKS

The construction of the model in $\mathbb{R}^2$ carries over to $\mathbb{R}^D$, where $D \geqslant 3$, essentially without change. But it shall ease the process if from the start we handle the model by symbolic means, since the calculations get a little involved, though, under passage to arbitrary D. While for $D=2$, the characteristic spatial structures are rectangles (cf. Assumption 2.1), for general D, these sets generalize to $(i_1, \ldots, i_D)$ type cuboids in D-dimensional space $\{(x_1, \ldots, x_D) \in \mathbb{R}^D: |x_k| \leqslant i_k/2 \text{ for } k = 1, \ldots, D\}$, where $i_1, \ldots, i_D \in \mathbb{N}_+$. Then, in analogy with Assumption 2.2, the basic underlying free energy model for an additive polydisperse mixture of pure D-cuboids is obtained via the global free energy functional for hard rod mixtures (cf. Cuesta and Martínez-Ratón[17]).

Clearly, to proceed to increasingly complex solvable models, ''less'' compact unit configurations are to be included in a systematic fashion. The point here is not so much that a larger class of unit configurations is introduced, i.e., that of expanding Assumption 2.1, but rather that the new configurations give rise to a polydisperse Hamiltonian function for which Zhang's global free energy functional is no longer applicable (cf. Cuesta and Martínez-Ratón[17]). This means that improvements in the polydisperse representation depend largely on the future development in density functional theory for additive polydisperse pure hard core mixtures.

Yet another obvious question to be considered is whether one can analyze systems with square-well interactions under the milder condition of non-vanishing attraction ranges. The most interesting feature of this class of potentials is that we may now not merely forget the range parameter d of the interactions. Still, the construction proceeds as above when we are willing to start from a $D=1$ particle system with square-well interactions in which the size of connected next neighbor pairs is restricted to finitely many values. Thereafter, the deduction of the free energy for such a ''discretized'' square-well potential follows the method developed in Sec. II A. Like for the asymptotic $d\to 0^+$ case, the extension to $\mathbb{R}^2$ is then carried out by lifting this particular $D=1$ density functional representation to $D=2$ and combining it with suitable idealizations in order to make the model solvable (cf. Assumptions 2.1 and 2.2). Once the discrete version is sufficiently well understood, we get what we really want by taking the continuum limit.

The main theme will be again the incorporation of the unit partition functions into the additive polydisperse hard core mixture format, only that now an asymptotic analysis of these total isothermal measures as $d\to 0^+$ does not suffice. Progress in this direction will be reported in due course.

ACKNOWLEDGMENTS

The author thanks José A. Cuesta, Karl Grill, and Viktor I. Kolyada for valuable discussions. This research was supported by Austrian Science Foundation (FWF) Erwin Schrödinger Grant No. 2218.

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Ring-shaped exact Hopf solitons

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(Received 11 June 2003; accepted 11 July 2003)

The existence of ring-like structures in exact Hopfion solutions is shown. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1612897]

I. INTRODUCTION

Extended solutions are of central importance in different applications of modern field theory, from high energy to condensed matter physics. Their relevance is parallel to the difficulty in the analysis of the nonlinear theories which encode them and the scarce exact results in higher dimensions. To circumvent one of the main problems, the scaling instablity for scalar fields beyond one spatial dimension found by Skyrme[1] and formalized by Derrick,[2] one obvious possibility is nonpolynomial Lagrangians, which are not unfamiliar. Among those attempts the work by Deser, Duff, and Isham,[3] where the simplest choice of just the power required to balance the scaling is analyzed, is of special interest. As the authors discuss, such models have, of course, no free field expansion around a trivial vacuum. But they can have a semiclassical formulation around nontrivial solutions and eventually a small time dependent perturbation of the static solutions. One solution was found and the importance of global transformations was emphasized. This model was further extended by Nicole[4] and put in a more general framework by Kundu.[5] It was rediscovered independently in a series of papers[6] in the context of a new proposal for a generalized integrability,[7] finding infinitely many analytic solutions with general Hopf indices. This was an unsolved problem, which is important for soliton physics and because of the many applications of those maps, combining topology and geometry. In their last paper,[8] a new feature of the Hopfion solutions was discovered, namely, a line singularity in an infinitely thin tube along the z axis from a special current with a nonconserved charge, provided by the geometric method.

In this article we extend the analysis to find that there is in fact another solution of the ring type, which is interesting, as ring structures are typical in higher dimensional soliton analysis, both in numerical[9] and analytical approximations.[10] In fact, these currents and solutions should be relevant for the analytical study of soliton scattering. We also pay special attention to the symmetries, including global aspects of the solution, as many aspects of the model are generic to other local formulations of topological degrees of freedom. Time dependence analysis is also a natural possiblity in the generalized zero curvature approach, as it preserves Lorentz covariance.

II. THE RING-LIKE SOLUTIONS

As shown in Ref. 8, the only models involving the antisymmetric tensor in the complex field u,

$$h_{\mu\nu} = -i\,(\partial_\mu u \partial_\nu u^* - \partial_\nu u \partial_\mu u^*), \tag{1}$$

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which satisfy without constraints the integrability criterion of the geometric approach of Ref. 7 (i.e., infinitely many conserved currents) and which can be derived from an action principle, are those where the Lagrangian is a functional of h^2/f^2, where f is a real function of u and u^*. If one further asks for scaling invariance to allow for stable static solutions, we are lead to the class of models given by the Lagrangian density

$$\mathcal{L}\equiv\left(\frac{h_{\mu\nu}^2}{2\,f^2}\right)^{3/4}, \tag{2}$$

which generalizes and explains choices and solutions found before.[3–6]

We assume from now on that f only depends on uu^*. If $\lim_{|\vec{x}|\to\infty}u(\vec{x})=u_0=\text{const}$ is assumed, then the domain space $\mathbb{R}^3$ has the topology of the three-sphere S^3. If, in addition, the target space may be identified with the two-sphere S^2 via stereographic projection, then u may be interpreted as a map $S^3\to S^2$, which is characterized by an integer winding number (the Hopf index). In this case there exists an infinite number of static, soliton-like solutions to the equations of motion of the model, and these all have integer Hopf index. These solutions were first found in Ref. 6 and they are obtained by inserting into the static equations of motion

$$-h_{ij}\partial^j u\,\partial^i h^2+4h^2\partial^i h_{ij}\partial^j u+i(h^2)^2\partial_{u^*}f=0 \tag{3}$$

(where $h^2\equiv h_{ij}h^{ij}$) the product ansatz

$$u(\eta,\xi,\varphi)\equiv R(\eta)e^{i(m\xi+n\varphi)} \tag{4}$$

in toroidal coordinates

$$\begin{gathered}x=q^{-1}\sinh\eta\cos\varphi,\quad y=q^{-1}\sinh\eta\sin\varphi,\\ z=q^{-1}\sin\xi;\quad q=\cosh\eta-\cos\xi.\end{gathered} \tag{5}$$

As explained elegantly in Ref. 8, the ansatz (4) follows from the conformal symmetry of the equations of motion. If one assumes that f is a function of $T\equiv R^2\equiv uu^*$ only, $\partial_{u^*}f$ simplifies to $\partial_{u^*}f=f_{,T}\,u$. With the ansatz (4), this results in an ordinary differential equation for $R(\eta)$, which may be conveniently expressed in terms of $T\equiv R^2\equiv uu^*$ as

$$\left(\ln\frac{T_{,\eta}}{f}\right)_{,\eta}=\frac{\cosh\eta}{\sinh\eta}\,\frac{n^2-2m^2\sinh^2\eta}{n^2+m^2\sinh^2\eta} \tag{6}$$

and $X_{,\eta}$ denotes derivative of X with respect to η. Further, we assume $m^2>n^2$ in the sequel. A first integral may be found easily,

$$\frac{T_{,\eta}}{f}=k_1\frac{\sinh\eta}{(n^2+m^2\sinh^2\eta)^{3/2}} \tag{7}$$

(here k_1 is a constant of integration), whereas for a further integration the explicit form of the function $f(T)$ is needed.

In the end, we shall choose $f=(1+T)^2$, because we are referring to the solutions of Babelon and Ferreira,[8] but let us briefly mention a class of functions $f(T)$ that leads to a target space with the topology of the two-sphere and, therefore, to genuine Hopf solitons, which can have useful applications. For $f=(1+T)^2$, the expression h_{ij}/f in the Lagrangian density (2) is, in fact, just the pull-back under the map u of the area two-form

$$d\Omega=-i\frac{\mathrm{d}z\,\mathrm{d}z^*}{(1+zz^*)^2} \tag{8}$$

on the two-sphere. A pull-back of this two-form under maps $S^2 \to S^2$ will lead to further acceptable area two-forms (i.e., area two-forms respecting the topology of the target space). If we want to maintain the simple dependence $f=f(T)$, then a class of allowed maps is

$$\phi: \ z \to \sqrt{g(zz^*)}e^{il\ \arg(z)}. \tag{9}$$

These are indeed maps $S^2 \to S^2$ provided that $g(0)=0$ and $g(\infty)=\infty$. Further, l must be an integer. The pullback of the area two-form (8) is

$$\phi_*(d\Omega) = -i\frac{\mathrm{dz}\ \mathrm{dz}^* l g'}{(1+g)^2}, \tag{10}$$

therefore any function f of the type

$$f(T) = \frac{(1+g(T))^2}{l\, g_{,T}} \tag{11}$$

leads to a theory (2) with genuine Hopf solitons.

In the sequel we restrict to the simplest case $f=(1+T)^2$ (the area two-form on the two-sphere). Then the first integral (7) may be easily integrated to yield

$$\frac{1}{1+T} = \frac{k_1}{(m^2-n^2)}\frac{\cosh\eta}{(n^2+m^2\sinh^2\eta)^{1/2}} + k_2, \tag{12}$$

where k_1 and k_2 are two constants of integration. These constants have to be fixed by imposing some boundary conditions on the field u. For this purpose let us introduce the unit vector $\vec{n}$ related to u via stereographic projection

$$\vec{n} = \frac{1}{1+|u|^2}(u+u^*, -i(u-u^*), |u|^2-1) \quad , \quad u = \frac{n_1+in_2}{1-n_3}. \tag{13}$$

If u is supposed to be a true Hopf map, then the number of allowed boundary conditions is, in fact, very restricted. The point is that a true Hopf map should cover the whole target S^2, including the north pole ($\vec{n}=(0,0,1)$, or $T=\infty$) and the south pole ($\vec{n}=(0,0,-1)$, or $T=0$). Therefore, the boundary conditions should be chosen such that T varies between $T=0$ and $T=\infty$. Further, the pre-images of the north pole and the south pole should be one-dimensional lines in $\mathbb{R}^3$. However, the only values of η which define one-dimensional lines (instead of two-dimensional tori, as is the general case), are $\eta=0$, which defines the z axis (together with spatial infinity), and $\eta=\infty$, which defines the circle

$$C = \{\vec{x}\in\mathbb{R}^3: \ z=0 \ \wedge \ r^2=1\}. \tag{14}$$

Therefore, there are two possible choices for the boundary conditions, namely, $T(\eta=0)=0$, $T(\eta=\infty)=\infty$, or $T(\eta=0)=\infty$, $T(\eta=\infty)=0$.

In Ref. 8 the second option was chosen (which we call $T^{(2)}$ for convenience),

$$T^{(2)} = \frac{\cosh\eta - \sqrt{n^2/m^2+\sinh^2\eta}}{\sqrt{1+m^2/n^2\sinh^2\eta}-\cosh\eta}, \quad T^{(2)}(\eta=0)=\infty \quad , \quad T^{(2)}(\eta=\infty)=0. \tag{15}$$

Let us now investigate our first option, for which we get

$$T^{(1)} = (T^{(2)})^{-1}, \quad T^{(1)}(\eta=0)=0 \quad , \quad T^{(1)}(\eta=\infty)=\infty. \tag{16}$$

Now one could simply identify the solitons with the position of their singular value $|u|=\infty$, then the solitons of type $T^{(2)}$ would be identified with the straight line $x=0,y=0$ (the z axis), and the solitons of type $T^{(1)}$ would be ascribed to the circle C. However, this identification is in principle quite arbitrary, and requires a physical motivation.

In Ref. 8 it was shown that the solitions of type $T^{(2)}$ can indeed be identified with the z axis in a well-defined manner. More precisely, there exists a conserved current J_μ which has the property that for solitons of type $T^{(2)}$ it is singular along the z axis. Moreover, a constant flow of this current is emerging from the singular line (the z axis). Here we want to investigate the equivalent problem for solitons of type $T^{(1)}$, which is relevant as rings are common in higher dimensional solitons.[9,10]

So let us briefly review and further develop some results of Ref. 8 on the above-mentioned conserved current, with some more details required for our purposes. There exists (among other symmetries) a symmetry of the action under a transformation which is a combination of a dilatation on three-dimensional domain space plus a specific transformation on target space. The infinitesimal version of this symmetry transformation is given in Ref. 8, but it is, in fact, not difficult to obtain the transformation for finite transformation parameter. Under a dilatation transformation $x\to\Lambda^3 x\equiv e^{3\lambda}x$ (the power three of the dilatation parameter is chosen for later convenience) the action of the theory scales like

$$S\to\Lambda^{-3}S, \tag{17}$$

therefore the theory is invariant if the dilatation is combined with a transformation of the target space variable, $u\to v(u,\overline{u})$, such that

$$\frac{\mathrm{d}u\,\mathrm{d}\overline{u}}{(1+\overline{u}u)^2}\to\frac{\mathrm{d}v\,\mathrm{d}\overline{v}}{(1+\overline{v}v)^2}=\Lambda^2\frac{\mathrm{d}u\,\mathrm{d}\overline{u}}{(1+\overline{u}u)^2}. \tag{18}$$

If we introduce the real coordinates on target space $u=T^{1/2}e^{i\phi}$ (angle and radius squared on the Euclidean plane) and assume that $v=(\tilde{T})^{1/2}(T)e^{i\phi}$ (i.e., u and v have the same argument, and the modulus of v is a function of the modulus T only) then we get

$$\frac{\tilde{T}'(T)\mathrm{d}T\,\mathrm{d}\phi}{(1+\tilde{T})^2}=\Lambda^2\frac{\mathrm{d}T\,\mathrm{d}\phi}{(1+T)^2} \tag{19}$$

or

$$\frac{\tilde{T}'}{(1+\tilde{T})^2}=\frac{\Lambda^2}{(1+T)^2} \tag{20}$$

with the solution

$$\frac{1}{1+\tilde{T}}=\frac{\Lambda^2}{1+T}+c, \tag{21}$$

where c is a constant of integration. If we require the boundary condition $\tilde{T}(0)=0$ then we get

$$\tilde{T}=\frac{\Lambda^2 T}{\Lambda^2+(1+T)(1-\Lambda^2)} \tag{22}$$

or

$$v=\frac{\Lambda u}{[\Lambda^2+(1+\overline{u}u)(1-\Lambda^2)]^{1/2}}. \tag{23}$$

This v indeed fulfills Eq. (18) as may be checked easily. In addition, it reduces to the transformation of Babelon and Ferreira[8] for infinitesimal λ (i.e., $\Lambda=1+\lambda$). Therefore Eq. (23) is the required symmetry transformation on target space. (Observe that this transformation has the funny property that it is well-defined only for $\Lambda^2\leqslant 1$, i.e., for scaling transformations which shrink distances.)

The conserved Noether current related to this symmetry transformation is

$$J_\mu=x^\nu\Theta_{\mu\nu}+j_\mu, \tag{24}$$

where $\Theta_{\mu\nu}$ is the canonical energy–momentum tensor of the theory, and j_μ is

$$j_\mu=-i\left(\frac{h^2}{2(1+T)^4}\right)^{-1/4}\frac{1}{2(1+T)^3}h_{\mu\nu}(u\partial^\nu u^*-u^*\partial^\nu u). \tag{25}$$

Here, the first term of J_μ (containing the energy–momentum tensor) is due to the space dilatation, whereas the second term, j_μ, is due to the specific target space transformation (23). The current obeys the conservation equation $\partial^\mu J_\mu=0$. For static configurations $u(\vec{x})$ this conservation equation may be used to derive the relation

$$E\equiv\partial_t\int d^3xJ^0=\int_\Sigma d\vec{f}\cdot\vec{J}, \tag{26}$$

where E is the static energy of the static configuration,

$$E=4\pi^2\sqrt{|m||n|(|m|+|n|)}, \tag{27}$$

and the integral on the right-hand side of (26) is an integral over surfaces Σ which surround the singularities of the current $\vec{J}$. It turns out that the first term of the current for static fields, $x^j\Theta_{ij}$, is regular everywhere and may, therefore, be ignored in the surface integral of (26) provided that the integration surfaces are chosen such that the enclosed volume is infinitesimal. For the current $\vec{j}$ we find after some calculation

$$\vec{j}=\left(\left|\frac{T_{,\eta}}{(1+T)^2}\right|\right)^{1/2}\frac{T}{1+T}\left(\frac{n^2}{\sinh^2\eta}+m^2\right)^{3/4}(\cosh\eta-\cos\xi)^2\vec{e}_\eta, \tag{28}$$

where $\vec{e}_\eta=(\cosh\eta-\cos\xi)^{-1}\nabla\eta$ is a vector of unit length which is perpendicular to the surfaces of constant η (tori). Observe that $\vec{e}_\eta$ is pointing into the interior of the tori, because η is growing in this direction. We may use the first integral of the equations of motion, (7), for the first factor on the right-hand side containing $T_{,\eta}$, and find

$$\vec{j}=\sqrt{|m||n|(|m|+|n|)}\,\frac{T}{1+T}\,\frac{(\cosh\eta-\cos\xi)^2}{\sinh\eta}\,\vec{e}_\eta. \tag{29}$$

If we ignore the factor $T/(1+T)$ for the moment, then we see that the remaining expression is singular both for $\eta=0$ (along the z axis) and for $\eta=\infty$ (along the circle C). Depending on whether we choose $T^{(1)}$ or $T^{(2)}$ for T, one of the two singularities gets canceled, whereas the other remains. For $T=T^{(2)}$ (the case which was studied in Ref. 8), the singularity along the z axis remains. In this case we choose a very large torus $\eta\ll 1$ as integration surface. For the regular terms the limit $\eta\to 0$ may be performed, such that the integration is extended to the whole space. For the singular $\vec{j}$ the surface integral should be performed for a finite η and the limit $\eta\to 0$ should be taken afterwards. The surface element on the torus surface $\eta=\text{const}$ is

$$\mathrm{d}\vec{f}=\vec{e}_{\eta}\frac{\sinh\eta}{(\cosh\eta-\cos\xi)^2}\mathrm{d}\varphi\,\mathrm{d}\xi, \tag{30}$$

therefore the surface integral is

$$\int_{\eta=\mathrm{const}}\vec{j}\cdot\mathrm{d}\vec{f}=\sqrt{|m||n|(|m|+|n|)}\,\frac{T}{1+T}\int\mathrm{d}\varphi\,\mathrm{d}\xi=4\pi^2\sqrt{|m||n|(|m|+|n|)}\,\frac{T}{1+T}. \tag{31}$$

For $T=T^{(2)}$ this should be evaluated in the limit $\eta\to 0$ for which $T^{(2)}/(1+T^{(2)})$ is equal to one. Therefore the total flux emerging from the singular line (the z axis) is

$$\mathrm{flux}=4\pi^2\sqrt{|m||n|(|m|+|n|)}=E, \tag{32}$$

where E is the static energy (27).

On the other hand, for $T=T^{(1)}$ the singularity is located at the circle C, therefore a tiny torus (large η) should be excluded from the integration region. So we take the limit $\eta\to\infty$ now in the surface integral (31). But $T^{(1)}/(1+T^{(1)})$ is equal to one in this limit, so we find again for the flux the same previous expression (32).

Therefore, for solutions of the type $T^{(1)}$ the singular line is the circle C and a nonzero flux of total amount given in (32) emerges from this singular circle. As a consequence, the solutions of type $T^{(1)}$ are characterized by a ring-like structure, where the ring is located at the position of the circle C, which, as said, is relevant for their physics and especially for the scattering.

III. DISCUSSION

So we indeed found that in addition to the solutions of type $T^{(2)}$ originally obtained by Aratyn, Ferreira, and Zimerman (AFZ) in Ref. 6, which are characterized by a straight line of singular flux according to Babelon and Ferreira, there exist solutions where the singular flux is located along the circle C, forming thereby a ring-like structure. In hindsight, this result is not so surprising, and the ring-like structure is, in fact, the generic case. To see this, let us invoke a further symmetry of the model, namely, constant rotations of the target space S^2. In domain space $\mathbb{R}^3$ such a rotation rotates different level curves (i.e., curves of constant $u=u_0$ for different values of u_0) into each other, because these level curves are the pre-images of points of the target S^2 under the map u. Generically, these level curves are circles, with the only exception of the z axis. Therefore, any rotation on target space which moves the north pole and the south pole will transform a solution of type $T^{(2)}$ into a new solution where the line of singular flux is located along a circle.

On the target space coordinate u such rotations are represented by modular transformations $u\to(a+bu)/(c+du)$, where $ad-bc=1$. A general modular transformation is, however, not compatible with the simple ansatz (4) which was used by AFZ to find solutions. The only nontrivial modular transformation compatible with the ansatz (4) is the inversion map $u\to(1/u)$. And indeed, the composition of the inversion map with the map $(m,n)\to(-m,-n)$ (which again maps a solution to another solution with the same energy) precisely maps the AFZ solutions $T^{(2)}$ to the solutions of type $T^{(1)}$ discussed in this paper.

Besides their interest for the scattering, the results can also be useful—given the generic features of the theory considered—for other higher dimensional models on the sphere and/or using similar scaling arguments, like Skyrme theory and its restriction to the SU(2)/U(1) coset, proposed by Faddeev as an effective theory of QCD at long distances.[11]

ACKNOWLEDGMENTS

C.A. acknowledges support from the Austrian START Award Project No. FWF-Y-137-TEC of N.J. Mauser and J.S.-G. support from the Spanish MCyT and FEDER project Nos. FPA2002-01161 and BFM2002-03881 and discussions with L.A. Ferreira.

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Weak Hopf algebras corresponding to $U_q[sl_n]$

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(Received 16 July 2003; accepted 24 July 2003)

We investigate the weak Hopf algebras of Li based on $U_q[sl_n]$ and Sweedler's finite dimensional example. We give weak Hopf algebra isomorphisms between the weak generalizations of $U_q[sl_n]$ which are ''upgraded'' automorphisms of $U_q[sl_n]$ and hence give a classification of these structures as weak Hopf algebras. We also show how to decompose these examples into a direct sum which leads to unexpected isomorphisms between their algebraic structure. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1616999]

I. INTRODUCTION

Since the introduction of quantum groups,[1] the importance of Hopf algebras has been widely recognized in both mathematics and physics. Generalizations of Hopf algebras have been considered, usually motivated by some application in mathematical physics. The most well-known example of the generalizations may be quasi-Hopf algebras where the coassociativity of a Hopf algebra is relaxed,[2] but at the same time keeping the category of modules monoidal. A similar type of relaxation of coassociativity is also found in truncated quasi-Hopf algebras[3] and rational Hopf algebras.[4] This is where the notion of a weak coproduct was introduced, such that $\Delta(1) \neq 1 \otimes 1$, and was motivated by the study of symmetries in low dimensional quantum field theory. One problem that arose was the fact that the dual of these structures was not associative, which led to further problems in defining crossed products and a double construction.[5] Although these issues have already been addressed in Refs. 6 and 7, the question still arose as to the possibility of defining a structure which could still provide nonintegral dimensions for the quantum field theories in a similar way to the weak quasi-Hopf algebras,[3] but at the same time be coassociative. This was the motivation behind defining the weak Hopf algebras of Refs. 5, 8, and 9. Since these are not bialgebras, but *almost* bialgebras,[10] there were also axioms required to define a weak antipode, differing slightly from the usual ones of a Hopf algebra such that the category of finite dimensional modules was still monoidal, and also with a rigidity structure defined through a generalized antipode.[9] Another question then arose as to the possibility of defining a weak antipode on bialgebras. Li has introduced the notion of a weak Hopf algebra to mean a bialgebra on which is defined such a weak antipode.[10,11] In this paper, we investigate these weak Hopf algebras as defined by Li.

The concept of a weak Hopf algebra is rather new. There are not many examples known, though several have appeared in the literature. One example is given by the semigroup algebra of any regular monoid which gives a generalization of the well-known group algebra.[11] The other known examples were given in Ref. 12 where the authors presented two weak Hopf generalizations of the quantized enveloping algebra $U_q[sl_2]$.

The purpose of this paper is twofold. First, we wish to propose some minor adjustments to the examples given in Ref. 12. Second, we extend the construction to the case of other known Hopf algebras such as $U_q[sl_n]$[13] and Sweedler's Hopf algebra.[14,15] It is also evident that we can define weak extensions of quantum superalgebras in a similar way. As a consequence, we shall have a lot of new nontrivial examples of weak Hopf algebras. We believe that for a deeper understanding

of weak Hopf algebras as well having some insight into their applications, it is important to have various examples.

The paper is organized as follows. In Sec. II we give a brief summary of the definition of weak Hopf algebra. Following that, Sec. III has a closer look at the examples given in Ref. 12 and we propose slightly modified versions of these examples. We then realize in Sec. IV that for $U_q[sl_n]$ there is a plethora of examples which leads us to finding isomorphisms between structures, thus giving a classification in some sense of weak Hopf algebras corresponding to $U_q[sl_n]$. The following section looks at weak extensions of Sweedler's famous finite dimensional Hopf algebra, where we also show that with our construction, in general we can decompose the weak Hopf algebra into a direct sum of the original bialgebra with some other subalgebra. This leads to ''unexpected'' algebra isomorphisms between structures in some cases.

II. WEAK HOPF ALGEBRAS

For the reader's convenience we recall the definition of a weak Hopf algebra in the sense of Li and Duplij.[10,12] Let $(H,\Delta,\varepsilon,m,u)$ be a bialgebra over a field K, where $\Delta:H\to H\otimes H$ is the coproduct, $\varepsilon:H\to K$ is the counit, $m:H\otimes H\to H$ the product and $u:K\to H$ the unit of H. The following properties define H:

$$m(m\otimes \mathrm{id})=m(\mathrm{id}\otimes m),$$

$$m(u\otimes \mathrm{id})=\mathrm{id}=m(\mathrm{id}\otimes u),$$

$$(\mathrm{id}\otimes\Delta)\Delta=(\Delta\otimes\mathrm{id})\Delta,$$

$$(\varepsilon\otimes\mathrm{id})\Delta=\mathrm{id}=(\mathrm{id}\otimes\varepsilon)\Delta,$$

$$(m\otimes m)(\mathrm{id}\otimes\sigma\otimes\mathrm{id})(\Delta\otimes\Delta)=\Delta\circ m,$$

$$\varepsilon\otimes\varepsilon=\varepsilon\circ m.$$

Here $\sigma:H\otimes H\to H\otimes H$ is the flip operator $\sigma(h_1\otimes h_2)=h_2\otimes h_1$ for all $h_1,h_2\in H$.

H is a weak Hopf algebra if there is a weak antipode $T:H\to H$ which is an algebra homomorphism satisfying the two conditions

$$T*\mathrm{id}*T=T, \tag{2.1}$$

$$\mathrm{id}*T*\mathrm{id}=\mathrm{id}, \tag{2.2}$$

with the convolution product $*$ defined over maps on H by

$$a*b\equiv m(a\otimes b)\Delta:H\to H.$$

Note that the antipode of a Hopf algebra is a weak antipode due to the fact that $u\circ\varepsilon:H\to H$ is the identity of the convolution product $*$. Recall that $S:H\to H$ is an antipode if it satisfies

$$S*\mathrm{id}=u\circ\varepsilon, \tag{2.3}$$

$$\mathrm{id}*S=u\circ\varepsilon. \tag{2.4}$$

For example, we see that

$$S*\mathrm{id}=u\circ\varepsilon$$

$$\Rightarrow \mathrm{id}*S*\mathrm{id}=\mathrm{id}*u\circ\varepsilon$$

$$\Rightarrow \mathrm{id}*S*\mathrm{id}=\mathrm{id}.$$

In fact S needs only be a left or right antipode, meaning it satisfies only one of the two equalities (2.3) or (2.4), in order for it to be a weak antipode.

III. WEAK $U_q[sl_2]$

In this section we give a summary of the examples of weak $U_q[sl_2]$ presented in Ref. 12. It is notable that the defining relations of the "J-weak" quantum algebra $v\mathfrak{sl}_q(2)$ given in that paper can be simplified, and we give a minor adjustment to this example and show that it is in fact a weak Hopf algebra. We also give one other example generalizing $U_q[sl_2]$ which uses a mixture of the two examples from Ref. 12.

We remind the reader that the usual $U_q[sl_2]$ relations to which we refer, in terms of the four generators E,F,K,K^{-1}, are as follows:

$$K^{-1}K=KK^{-1}=1, \tag{3.1}$$

$$KEK^{-1}=q^2E, \tag{3.2}$$

$$KFK^{-1}=q^{-2}F, \tag{3.3}$$

$$EF-FE=\frac{K-K^{-1}}{q-q^{-1}}. \tag{3.4}$$

The coalgebra structure (coproduct Δ, counit ε) is given by

$$\Delta(K^{\pm 1})=K^{\pm 1}\otimes K^{\pm 1},$$

$$\Delta(E)=E\otimes K+1\otimes E,$$

$$\Delta(F)=F\otimes 1+K^{-1}\otimes F,$$

$$\varepsilon(E)=\varepsilon(F)=0,$$

$$\varepsilon(K^{\pm 1})=1.$$

It is clear that when we wish to determine the explicit action of the antipode, we apply the definition (2.3) and (2.4) to an arbitrary element in the algebra and solve. In all cases we can solve explicitly due to the existence of the invertible group-like elements $1,K,K^{-1}$. The obvious first step in generalization to the weak Hopf case would be to attempt to remove the invertibility of these elements. This was the main idea in Ref. 12 when generalizing the above definition.

First, all weak extensions of $U_q[sl_2]$ have generators $E,F,K,\overline{K}$ satisfying

$$K\overline{K}=\overline{K}K\equiv J, \tag{3.5}$$

$$K\overline{K}K=K, \quad \overline{K}K\overline{K}=\overline{K}, \tag{3.6}$$

$$EF-FE=\frac{K-\overline{K}}{q-q^{-1}}. \tag{3.7}$$

In what follows we usually write the generators with subscripts (following Ref. 12) to differentiate the definitions.

Definition 1 (from Ref. 12): $w\mathfrak{sl}_q(2)$ is the algebra generated by the four elements E_w, F_w, K_w, $\overline{K}_w$ satisfying (3.5), (3.6), (3.7) along with the relations

$$K_w E_w = q^2 E_w K_w, \tag{3.8}$$

$$\overline{K}_w E_w = q^{-2} E_w \overline{K}_w, \tag{3.9}$$

$$K_w F_w = q^{-2} F_w K_w, \tag{3.10}$$

$$\overline{K}_w F_w = q^2 F_w \overline{K}_w. \tag{3.11}$$

Here the invertibility of K and $\overline{K}$ has been relaxed, and instead of the identity, the element J_w has been introduced. It can be seen that this element J_w satisfies

$$aJ_w = J_w a, \quad \forall a \in w\mathfrak{sl}_q(2).$$

To demonstrate this we check

$$E_w J_w \overset{(3.5)}{=} E_w K_w \overline{K}_w \overset{(3.8)}{=} q^{-2} K_w E_w \overline{K}_w \overset{(3.9)}{=} K_w \overline{K}_w E_w \overset{(3.5)}{=} J_w E_w. \tag{3.12}$$

A similar calculation is performed for F_w and the calculations for K_w and $\overline{K}_w$ are trivial.

Also note that due to the relations (3.6), J_w is an idempotent. Namely,

$$J_w^2 = J_w.$$

The coalgebra structure is defined as follows. The coproduct and counit are, respectively, given by

$$\Delta_w(E_w) = 1 \otimes E_w + E_w \otimes K_w,$$

$$\Delta_w(F_w) = F_w \otimes 1 + \overline{K}_w \otimes F_w,$$

$$\Delta_w(K_w) = K_w \otimes K_w,$$

$$\Delta_w(\overline{K}_w) = \overline{K}_w \otimes \overline{K}_w,$$

$$\varepsilon_w(E_w) = \varepsilon_w(F_w) = 0,$$

$$\varepsilon_w(K_w) = \varepsilon_w(\overline{K}_w) = 1.$$

It can be verified that they are both algebra homomorphisms so that

$$\Delta_w(xy) = \Delta_w(x)\Delta_w(y)$$

and

$$\varepsilon_w(xy) = \varepsilon_w(x)\varepsilon_w(y)$$

for all $x,y \in w\mathfrak{sl}_q(2)$, thus preserving the defining relations. With this coproduct a corresponding weak antipode can be determined by solving equations (2.1) and (2.2) with the above coproduct. The only possible weak antipode in this case is

$$T_w(1) = 1,$$

$$T_w(K_w) = \overline{K}_w,$$

$$T_w(\overline{K}_w) = K_w, \tag{3.13}$$

$$T_w(E_w) = -E_w\overline{K}_w,$$

$$T_w(F_w) = -K_wF_w.$$

It can be shown that T_w is an algebra antihomomorphism, that is, $T(ab)=T(b)T(a)$. Note that with the above bialgebra structure it is not possible to determine an antipode in the usual sense. As we mentioned previously, this was the motivation for relaxing (3.1) to (3.5) in order to provide weak antipodes which are not antipodes. For example, to solve the equation

$$S*\mathrm{id}(K)=\varepsilon(K)1 \Rightarrow S(K)K=1,$$

we would need an inverse of the element K.

Another possible definition given in Ref. 12 is the following.

Definition 2 (from Ref. 12): $v\mathfrak{sl}_q(2)$ is the algebra generated by the four elements E_v, F_v, K_v, $\overline{K}_v$ satisfying (3.5), (3.6), (3.7) along with the relations

$$K_vE_v\overline{K}_v = q^2E_v, \tag{3.14}$$

$$K_vF_v\overline{K}_v = q^{-2}F_v. \tag{3.15}$$

In this case, $J_v=K_v\overline{K}_v$ satisfies the relation

$$J_va = aJ_v = a, \tag{3.16}$$

for $a=E_v$, F_v, K_v, $\overline{K}_v$ (and hence J_v). To demonstrate, we have

$$E_vJ_v \overset{(3.5)}{=} E_vK_v\overline{K}_v \overset{(3.14)}{=} q^{-2}K_vE_v\overline{K}_vK_v\overline{K}_v \overset{(3.6)}{=} q^{-2}K_vE_v\overline{K}_v \overset{(3.14)}{(=E_v)} \overset{(3.6)}{=} q^{-2}K_v\overline{K}_vK_vE_v\overline{K}_v$$
$$\overset{(3.14)}{=} K_v\overline{K}_vE_v \overset{(3.5)}{=} J_vE_v.$$

For the generator F_v, a similar calculation can be done. For the cases K_v and $\overline{K}_v$, the calculation is trivial. The most remarkable consequence of this property is that the analogue of defining relation (3.7) presented in Ref. 12 which was in the form

$$E_vJ_vF_v - F_vJ_vE_v = \frac{K_v-\overline{K}_v}{q-q^{-1}},$$

reduces to (3.7) by the above argument. Therefore in what follows we shall always use relation (3.7) and not the relation above.

The coalgebra structure for this second definition is as follows:

$$\begin{aligned}\Delta_v(E_v) &= J_v\otimes E_v + E_v\otimes K_v,\\ \Delta_v(F_v) &= F_v\otimes J_v + \overline{K}_v\otimes F_v,\end{aligned} \tag{3.17}$$

with the remaining actions coinciding precisely with the case of definition 1.

Moreover, relations (3.14) and (3.15) can be manipulated to those of definition 1. We demonstrate that

$$K_vE_v \overset{(3.6)}{=} K_v\overline{K}_vK_vE_v \overset{(3.5),(3.16)}{=} K_vE_v\overline{K}_vK_v \overset{(3.14)}{=} q^2E_vK_v.$$

The other relations can be verified in a similar way. Although the coproduct is different to that of definition 1, there exists a weak antipode which is the same as (3.13) in the case of definition 1.

This indicates that much of the discussion in Ref. 12 relating to $v\mathfrak{sl}_q(2)$ is redundant. However, we would like to make it clear that we consider the paper[12] rich in ideas and an inspiration to our current investigations.

There are other possibilities for defining weak extensions of $U_q[sl_2]$. These involve mixtures of definition 1 and definition 2 over the generators E,F. For example, we can say that one case is where E satisfies the relations (3.8), (3.9) and F satisfies (3.15), along with all the other relations common to both definition 1 and definition 2. The coproduct would then have the action

$$\Delta(E)=1\otimes E+E\otimes K,$$

$$\Delta(F)=F\otimes J+\overline{K}\otimes F,$$

along with the usual group-like coproduct for K and $\overline{K}$. The weak antipode would still be the same as in definitions 1 and 2.

We can also swap this mixture of definitions and say that E satisfies those relations of definition 2, but F satisfies the relations of definition 1. This case is actually isomorphic to the first mixture, as we shall see later. In the section on weak $U_q[sl_n]$ we give a more formal way of notating such mixtures.

So we now have some clues as to how we may approach the problem of defining weak extensions of $U_q[sl_n]$. It is clear that there will be many possible combinations of generators satisfying either of the two definitions in the general case. This then begs the question: how would we know which mixtures of the two definitions lead to isomorphic algebras? To this end we have an important observation regarding some of the automorphisms of the original quantum algebra $U_q[sl_n]$ which "lift up" to isomorphisms between weak Hopf structures. We shall look at these isomorphisms in more detail in the next section.

In general, we say that a generator satisfying the relations of definition 1 is of type 1, and is type 2 if it satisfies the relations of definition 2.

IV. WEAK $U_q[sl_n]$

A. Mixing definitions

For the case of $w\mathfrak{sl}_q(n)$, which has simple generators E_i, F_i, K_i and $\overline{K_i}$ $(i=1,\ldots,n-1)$, we can choose either definition 1 or 2 to describe the relations between any E_i and the $K_j/\overline{K_j}$ and similarly for any F_i. This is what is meant by the word "mixture." The relations satisfied by the generators are as follows, for all i,j unless specified otherwise:

$$\begin{gathered}
K_iK_j=K_jK_i,\ \ \overline{K_i}\,\overline{K_j}=\overline{K_j}\,\overline{K_i},\ \ K_i\overline{K_j}=\overline{K_j}K_i,\quad K_i\overline{K_i}=J,\\
JK_j=K_jJ=K_j,\ \ J\overline{K_j}=\overline{K_j}J=\overline{K_j},\\
E_iF_j-F_jE_i=\delta_{ij}\frac{K_i-\overline{K_i}}{q-q^{-1}},\\
E_i^2E_{i\pm1}-(q+q^{-1})E_iE_{i\pm1}E_i+E_{i\pm1}E_i^2=0,\\
F_i^2F_{i\pm1}-(q+q^{-1})F_iF_{i\pm1}F_i+F_{i\pm1}F_i^2=0,\\
E_iE_j=E_jE_i,\ \ F_iF_j=F_jF_i,\ \ |i-j|\geqslant 2.
\end{gathered}\tag{4.1}$$

We also need to specify the relations between the E_i and the K_j, for example. Let a_{ij} denote the Cartan matrix for $sl(n)$, $a_{ii}=2$, $a_{i,i\pm1}=-1$ and zero otherwise. If E_i satisfies

$$K_jE_i=q^{a_{ij}}E_iK_j,\quad E_i\overline{K_j}=q^{a_{ij}}\overline{K_j}E_i,\quad \forall j,\tag{4.2}$$

we say E_i satisfies definition 1, or simply E_i is type 1. However, if E_i satisfies

$$K_j E_i \overline{K}_j = q^{a_{ij}} E_i, \quad \forall j, \tag{4.3}$$

we say E_i satisfies definition 2, or simply E_i is type 2. The same convention holds for F_i by replacing E_i with F_i and a_{ij} with $-a_{ij}$ in the above relation. Notice also that J is defined for all i, so, for example,

$$J = K_i \overline{K}_i = K_j \overline{K}_j, \quad i \neq j.$$

The coproduct has the following action:

$$\begin{aligned}
\Delta(K_i) &= K_i \otimes K_i, \\
\Delta(\overline{K}_i) &= \overline{K}_i \otimes \overline{K}_i, \\
\Delta(E_i) &= \begin{cases} 1 \otimes E_i + E_i \otimes K_i, & E_i \text{ is type } 1 \\ J \otimes E_i + E_i \otimes K_i, & E_i \text{ is type } 2, \end{cases} \\
\Delta(F_i) &= \begin{cases} F_i \otimes 1 + \overline{K}_i \otimes F_i, & F_i \text{ is type } 1 \\ F_i \otimes J + \overline{K}_i \otimes F_i, & F_i \text{ is type } 2, \end{cases}
\end{aligned} \tag{4.4}$$

while the action of the counit is

$$\varepsilon(1) = \varepsilon(K_i) = \varepsilon(\overline{K}_i) = 1, \quad \varepsilon(E_i) = \varepsilon(F_i) = 0.$$

The weak antipode T will always have the form

$$\begin{aligned}
T(1) &= 1, \\
T(K_i) &= \overline{K}_i, \\
T(\overline{K}_i) &= K_i, \\
T(E_i) &= -E_i \overline{K}_i, \\
T(F_i) &= -K_i F_i,
\end{aligned}$$

regardless of the type of the generators E_i and F_i.

In order to notate these mixtures for $w\mathfrak{sl}_q(n)$ we use a binary notation, where a 1 indicates the use of a type 1 generator and a 0 indicates the use of a type 2 generator. We list the $2(n-1)$ simple generators E_i and F_i, starting with the E_i followed by the F_i. We then write down a list of 0's and 1's in the order corresponding to the generators determined by their type. This then gives an integer from 0 to $2^{2(n-1)}-1$ in binary representation which contains all the information as to which particular mixture of definition we are using for the relations between the generators E_i and F_i and all the $K_j/\overline{K}_j$. We denote this integer d and the algebra is expressed as $w\mathfrak{sl}_q^d(n)$. In total there are $2^{2(n-1)}$ possible mixtures for $w\mathfrak{sl}_q^d(n)$.

Note that we cannot have different definitions for the relations between the same generator with different K_i's because the coproduct could not possibly be consistent with those defining relations.

For example, in the case of $w\mathfrak{sl}_q(4)$ we have the simple generators (not including the K_i), $E_1, E_2, E_3, F_1, F_2, F_3$. Hence there are $2^6 = 64$ different possibilities for relations with the K_i. The notation $w\mathfrak{sl}_q^{43}(4)$ has the following meaning. Since the number 43 has the binary represen-

tation 101011, this is interpreted to mean that the simple generators E_1, E_3, F_2, F_3 are type 1 with the remaining ones E_2, F_1 being type 2. This information is determined by superimposing the list of binary digits $\{1,0,1,0,1,1\}$ with the list of simple generators in the order $\{E_1, E_2, E_3, F_1, F_2, F_3\}$.

It should also be noted that the algebra $w\mathfrak{sl}_q^3(2)$ coincides with $w\mathfrak{sl}_q(2)$ given in Ref. 12 (and in section III above) and the example $v\mathfrak{sl}_q(2)$ of Ref. 12 is precisely $w\mathfrak{sl}_q^0(2)$ in our notation.

B. Isomorphic structures

Now we look in more detail at the weak Hopf algebras of type $U_q[sl_n]$ using mixtures of the two types of generators. In some cases where $d_1 \neq d_2$, there exists a weak Hopf algebra isomorphism $w\mathfrak{sl}_q^{d_1}(n) \simeq w\mathfrak{sl}_q^{d_2}(n)$. It is therefore worth investigating all possible isomorphisms in order to classify the weak extensions based on our criteria. As we shall see in this section, the isomorphisms are derived from a subset of the set of automorphisms on the algebra $U_q[sl_n]$. In other words, a subset of the automorphisms on $U_q[sl_n]$ "lift up" to isomorphisms between the weak Hopf extensions. The reason only a subset can be considered, as we shall see later, is because some of the automorphisms of $U_q[sl_n]$ lose their invertibility when upgraded to act on the weak $w\mathfrak{sl}_q^d(n)$, so therefore cannot be isomorphisms.

If $(A, \Delta, \varepsilon, T)$ and $(B, \Delta', \varepsilon', T')$ are weak Hopf algebras, then a weak Hopf algebra isomorphism $\psi: A \to B$ is an invertible algebra homomorphism satisfying

$$(\psi \otimes \psi) \circ \Delta = \Delta' \circ \psi, \tag{4.5}$$

$$\varepsilon = \varepsilon' \circ \psi, \tag{4.6}$$

$$\psi \circ T = T' \circ \psi. \tag{4.7}$$

For example, consider the algebra $w\mathfrak{sl}_q^1(2)$. This has generators $E^{(1)}, F^{(1)}, K^{(1)}, \overline{K}^{(1)}$ (and $1^{(1)}$) satisfying

$$K^{(1)}\overline{K}^{(1)} = \overline{K}^{(1)}K^{(1)} \equiv J^{(1)},$$

$$K^{(1)}\overline{K}^{(1)}K^{(1)} = K^{(1)}, \quad \overline{K}^{(1)}K^{(1)}\overline{K}^{(1)} = \overline{K}^{(1)},$$

$$K^{(1)}F^{(1)} = q^{-2}F^{(1)}K^{(1)}, \quad \overline{K}^{(1)}F^{(1)} = q^2F^{(1)}\overline{K}^{(1)},$$

$$K^{(1)}E^{(1)}\overline{K}^{(1)} = q^2E^{(1)},$$

$$E^{(1)}F^{(1)} - F^{(1)}E^{(1)} = \frac{K^{(1)} - \overline{K}^{(1)}}{q - q^{-1}},$$

since the binary representation of $1 = \{0,1\}$ is superimposed with the list of generators $\{E^{(1)}, F^{(1)}\}$ and so $E^{(1)}$ is type 2 and $F^{(1)}$ is type 1. Let us now consider the coalgebra structure of this algebra. The coproduct Δ and counit ε are, respectively, given by

$$\Delta(K^{(1)}) = K^{(1)} \otimes K^{(1)},$$

$$\Delta(\overline{K}^{(1)}) = \overline{K}^{(1)} \otimes \overline{K}^{(1)},$$

$$\Delta(E^{(1)}) = J^{(1)} \otimes E^{(1)} + E^{(1)} \otimes K^{(1)},$$

$$\Delta(F^{(1)}) = F^{(1)} \otimes 1^{(1)} + \overline{K}^{(1)} \otimes F^{(1)},$$

$$\varepsilon(E^{(1)})=\varepsilon(F^{(1)})=0,$$

$$\varepsilon(K^{(1)})=\varepsilon(\overline{K}^{(1)})=1.$$

Now consider the map $\psi: w\mathfrak{sl}_q^1(2)\to w\mathfrak{sl}_q^2(2)$ defined by the action

$$\psi(E^{(1)})=F^{(2)},$$

$$\psi(F^{(1)})=E^{(2)},$$

$$\psi(K^{(1)})=\overline{K}^{(2)},$$

$$\psi(\overline{K}^{(1)})=K^{(2)},$$

where we have employed an obvious notation with superscripts. This map derives from the so-called Cartan involution on $U_q[sl_2]$. In the weak case it can be seen to be a weak Hopf algebra isomorphism since it preserves the generator type (that is, it is consistent with the defining relations) and is also consistent with Eqs. (4.5)–(4.7).

In general the rule is that such an isomorphism must map a type 1 generator into a type 1 generator and similarly for type 2. We demonstrate the sort of calculation required to show consistency with the relations. Take, for example,

$$\begin{aligned}\text{lhs}&=\psi(K^{(1)})\psi(E^{(1)})\psi(\overline{K}^{(1)})=\overline{K}^{(2)}F^{(2)}K^{(2)}=q^2\overline{K}^{(2)}(K^{(2)}F^{(2)}\overline{K}^{(2)})K^{(2)}\\&=q^2F^{(2)}=q^2\psi(E^{(1)})=\text{rhs}.\end{aligned}$$

The other relations can be realized in a similar fashion. To demonstrate consistency with the coproduct, we can use Eq. (4.5) to determine Δ' in this case. For example, applying both sides of (4.5) to $E^{(1)}$ gives

$$(\psi\otimes\psi)\Delta(E^{(1)})=(\psi\otimes\psi)(J^{(1)}\otimes E^{(1)}+E^{(1)}\otimes K^{(1)})=J^{(2)}\otimes F^{(2)}+F^{(2)}\otimes\overline{K}^{(2)},$$

$$\Delta'(\psi(E^{(1)}))=\Delta'(F^{(2)}).$$

This then gives the action of Δ' on $F^{(2)}$. The remaining actions are

$$\Delta'(E^{(2)})=E^{(2)}\otimes 1^{(2)}+K^{(2)}\otimes E^{(2)},$$

$$\Delta'(K^{(2)})=K^{(2)}\otimes K^{(2)},$$

$$\Delta'(\overline{K}^{(2)})=\overline{K}^{(2)}\otimes\overline{K}^{(2)}.$$

Note that this is not the coproduct given in Eqs. (4.4), but it is in fact the opposite coproduct, $\Delta^{\sigma}=\sigma\circ\Delta$ (σ being the flip operator), which we know from the theory of bialgebras is a perfectly acceptable one. It is also straightforward to verify (4.6) holds. Because the action of the weak antipode is dependent on the coproduct, T' will be different to the one presented earlier. It is straightforward to verify that it does indeed exist, and that Eq. (4.7) is satisfied.

Although there are undoubtedly many other possibilities to extend $U_q[sl_2]$ to a weak structure, the extensions presented in this paper based on that of Ref. 12 total three, namely, $w\mathfrak{sl}_q^0(2)$, $w\mathfrak{sl}_q^1(2)\simeq w\mathfrak{sl}_q^2(2)$, and $w\mathfrak{sl}_q^3(2)$. In each case the weak antipode has the same action, that of (3.13).

C. Number of unique structures

We now address the question of the number of possible weak Hopf algebra isomorphisms $\psi: w\mathfrak{sl}_q^d(n) \to w\mathfrak{sl}_q^{d'}(n),\ d \neq d'$.

It is well known that for $U_q[sl_n]$ there are several types of automorphisms.[16] The most relevant to this paper are the Dynkin diagram automorphisms and the Cartan involution, since they give rise to Hopf algebra automorphisms and antiautomorphisms, respectively. We consider maps ρ_d and ω_d which have the same actions as the Dynkin diagram automorphism and the Cartan involution, respectively, but applied to the weak Hopf algebra $w\mathfrak{sl}_q^d(n)$. These maps then become isomorphisms between weak Hopf structures. Their actions are given by

$$\rho_d(E_i^{(d)}) = E_{n-i}^{(d')}, \quad \rho_d(F_i^{(d)}) = F_{n-i}^{(d')}, \quad \rho_d(K_i^{(d)}) = K_{n-i}^{(d')}, \quad \rho_d(\overline{K}_i^{(d)}) = \overline{K}_{n-i}^{(d')},$$

$$\omega_d(E_i^{(d)}) = F_i^{(d'')}, \quad \omega_d(F_i^{(d)}) = E_i^{(d'')}, \quad \omega_d(K_i^{(d)}) = \overline{K}_i^{(d'')}, \quad \omega_d(\overline{K}_i^{(d)}) = K_i^{(d'')},$$

where the indices d (corresponding to the source), d' and d'' (corresponding to the targets) are used to differentiate between the structures. Note that ρ_d and ω_d map into different spaces which justifies the use of the different indices d' and d''. With these actions, it can be easily verified that

$$\rho_{d'} \circ \rho_d = \mathrm{id}, \quad \omega_{d''} \circ \omega_d = \mathrm{id}.$$

Lusztig[17] has also given a set of algebra automorphisms defined on the quantized enveloping algebras. However, when applied to our weak generalizations, they are found to be noninvertible and therefore are not isomorphisms between weak Hopf algebras.

Although we know of the existence of other algebra isomorphisms which exist between structures, the only known weak Hopf algebra isomorphisms are ρ_d and ω_d. We will comment more on these algebra isomorphisms in Sec. V.

One important point is that ρ_d and ω_d both preserve the generator type, so for example if $E_i^{(d)}$ is a type 1 generator, so are $E_{n-i}^{(d')}$ and $F_i^{(d'')}$. Therefore ρ_d and ω_d must correspond to maps (say r_d and w_d, respectively) defined on the non-negative integers such that

$$\rho_d : w\mathfrak{sl}_q^d(n) \to w\mathfrak{sl}_q^{r_d(d)}(n),$$

$$\omega_d : w\mathfrak{sl}_q^d(n) \to w\mathfrak{sl}_q^{w_d(d)}(n).$$

Once we know the action of the maps r_d and w_d, this should allow us to be able to determine which structures are isomorphic and hence lead to a classification.

To this end, we write d in terms of its binary expansion

$$d = (d_0, d_1, \ldots, d_{n-2} | d_{n-1}, \ldots, d_{2n-3}),$$

where the bar separates the values representing the E_i and F_i, and where the d_i have values of either 0 or 1. Then $r_d(d)$ and $w_d(d)$ have the expansions

$$w_d(d) = (d_{n-1}, \ldots, d_{2n-3} | d_0, \ldots, d_{n-2}),$$

$$r_d(d) = (d_{n-2}, \ldots, d_0 | d_{2n-3}, \ldots, d_{n-1}).$$

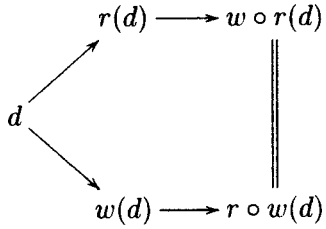
In terms of the components of the binary expansion we have

$$w_d(d_k) = d'_{3n-4-k \bmod 2(n-1)},$$

$$r_d(d_k) = d''_{n-1+k \bmod 2(n-1)}.$$

This simplifies the problem of determining isomorphic structures and allows us to explicitly count the number of unique structures for each n.

It is worth noting that $\rho\circ\omega=\omega\circ\rho$, so the only isomorphisms we need to consider are ρ, ω and $\rho\circ\omega$ (we have dropped the subscripts for convenience). According to this prescription, there can only be at most four structures which are isomorphic. In some cases there could be two and in others there could be no isomorphisms. These cases are referred to below as degenerate. The situation can be summarized in the following diagram



where in some cases the arrows could be equalities, in which case there would be one of the aforementioned degeneracies. In order to count the number of unique (nonisomorphic) weak extensions of $ws\mathfrak{l}_q^d(n)$, we list all the possible degenerate cases;

(1) $w(d)=d$,
(2) $r(d)=d$,
(3) $r(d)=w(d)$,

and consider their intersection $(1)\cap(2)\cap(3)$, union $(1)\cup(2)\cup(3)$ and their union's complement $\overline{(1)\cup(2)\cup(3)}$ in order to count the total number of unique cases. We note that some of these cases will lead to exactly two isomorphic structures, and combinations of the above cases will lead to no isomorphic structures. We aim to separate each of these situations and then add the number of structures relating to each.

Case (1): The only d satisfying $w(d)=d$ is of the form

$$d=(d_0,d_1,\ldots,d_{n-2}|d_0,d_1,\ldots,d_{n-2}).$$

Therefore the total number of cases satisfying case (1) is 2^{n-1}.

Case (2): We separate this case into two cases corresponding to n being odd and even. For $n=2m+1$ the only d satisfying case (2) is of the form

$$d=(d_0,d_1,\ldots,d_{m-1},d_{m-1},\ldots,d_0|d_{2m},d_{2m+1},\ldots,d_{3m-1},d_{3m-1},\ldots,d_{2m}),$$

so there are $2^{2m}=2^{n-1}$ possibilities. For $n=2m$ the only d satisfying case (2) has the form

$$d=(d_0,\ldots,d_{m-2},d_{m-1},d_{m-2},\ldots,d_0|d_{2m-1},\ldots,d_{3m-3},d_{3m-2},d_{3m-3},\ldots,d_{2m-1}),$$

so there are $2^{2(m-1)+2}=2^{2m}=2^n$ possibilities.

Case (3): The only d satisfying this case is of the form

$$d=(d_0,d_1,\ldots,d_{n-2}|d_{n-2},\ldots,d_0),$$

so there are 2^{n-1} possibilities.

$(1)\cap(2)\cap(3)$: Once again we treat the case for n is even and odd separately. For $n=2m+1$, d is of the form

$$d=(d_0,d_1,\ldots,d_{m-1},d_{m-1},\ldots,d_0|d_0,d_1,\ldots,d_{m-1},d_{m-1},\ldots,d_0),$$

so there are $2^m=2^{(n-1)/2}$ possibilities. For $n=2m$, d is of the form

$$d=(d_0,\ldots,d_{m-2},d_{m-1},d_{m-2},\ldots,d_0|d_0,\ldots,d_{m-2},d_{m-1},d_{m-2},\ldots,d_0),$$

giving $2^m=2^{n/2}$ possibilities.

$(1)\cup(2)\cup(3)$: Combining the above three cases and subtracting twice their intersection gives the union, for which there are $3.2^{2m}-2^{m+1}$ possibilities for $n=2m+1$ and $2^{2m+1}-2^{m+1}$ possibilities for $n=2m$. The compliment of the union then has $2^{4m}-3.2^{2m}+2^{m+1}$ possibilities for $n=2m+1$ and $2^{4m-2}-2^{2m+1}+2^{m+1}$ possibilities for $n=2m$.

To calculate the exact number of unique structures we consider the fact that case (1) without cases (2) or (3) (and permutations) will have precisely two structures which are isomorphic, or put another way, isomorphic structures in these cases come in pairs. Therefore we need to half the number obtained above when counting the total number of structures. Similarly for the structures which do not fall into these degenerate cases. There will be exactly four isomorphic structures so we need to divide the number corresponding to $(1)\cup(2)\cup(3)$ by 4.

Therefore the number of nonisomorphic structures, say Z_n, is

$$Z_{2m+1}=\frac{2^{2m}-2^m}{2}+\frac{2^{2m}-2^m}{2}+\frac{2^{2m}-2^m}{2}+2^m+\frac{2^{4m}-3.2^{2m}+2^{m+1}}{4}=2^{4m-2}+\frac{3}{4}.2^{2m},$$

$$Z_{2m}=\frac{2^{2m-1}-2^m}{2}+\frac{2^{2m}-2^m}{2}+\frac{2^{2m-1}-2^m}{2}+2^m+\frac{2^{4m-2}-2^{2m+1}+2^{m+1}}{4}=2^{4m-4}+2^{2m-1}.$$

Putting these two cases together gives

$$Z_n=2^{n-4}(7+(-1)^n+2^n),$$

which is the number of unique weak Hopf structures corresponding to $w\mathfrak{sl}_q^d(n)$.

This formula for Z_n has been verified up to $n=10$ by directly applying the maps ρ, ω and $\rho\circ\omega$ and then counting the number of unique structures. To give the reader an idea of the number of structures, we have the table below.

n	2	3	4	5	6	7	8	9	10
Z_n	3	7	24	76	288	1072	4224	16 576	66 048

We also list for $n\leqslant 4$ all the values of d, putting isomorphic values in brackets $\{,\}$. For $n=2$ we have already determined that the values

$$d=0,\{1,2\},3$$

give the three unique structures. For $n=3$ the values of d for the seven structures are

$$d=0,\{1,2,4,8\},\{3,12\},\{5,10\},\{6,9\},\{7,11,13,14\},15.$$

For $n=4$ the 24 values of d are

$$d=0,\{1,4,8,32\},\{2,16\},\{3,6,24,48\},\{5,40\},\{7,56\},\{9,36\},\{10,17,20,34\},\{11,25,38,52\},\{12,33\},$$
$$\{13,37,41,44\},\{14,28,35,49\},\{15,39,57,60\},18,\{19,22,26,50\},\{21,42\},\{23,58\},\{27,54\},$$
$$\{29,43,46,53\},\{30,51\},\{31,55,59,62\},45,\{47,61\},63.$$

All cases up to $n=10$ have been calculated, but are obviously too unwieldy to include in the article.

V. DIRECT SUM DECOMPOSITION AND SWEEDLER'S EXAMPLE

We now look in more detail at the algebraic structure and show that the upgraded quantized enveloping algebra automorphisms are not the only algebra isomorphisms between the various $w\mathfrak{sl}_q^d(n)$.

First recall Sweedler's example[14] of a finite dimensional Hopf algebra, denoted H. H is generated by elements I,G,X (where I is the identity element) satisfying the relations

$$G^2=I,$$

$$GX=-XG,$$

$$X^2=0.$$

The coproduct is given by

$$\Delta(G)=G\otimes G,$$

$$\Delta(X)=X\otimes G+I\otimes X,$$

and the counit given by

$$\varepsilon(G)=1=\varepsilon(I), \quad \varepsilon(X)=0.$$

The antipode S is given by the action

$$S(G)=G, \quad S(I)=I, \quad S(X)=GX.$$

Clearly H is four dimensional with basis $\{I,G,GX,X\}$.

In order to give an example of a weak Hopf algebra based on this structure with generators $\{1,g,x\}$ (we now use lower case symbols), instead of using the relation $g^2=1$, we impose the relation $g^3=g$. Moreover, we can choose either the relation $gx=-xg$, in which case we refer to x as a type 1 generator (analagous to the notion discussed at the end of Sec. III), or we can choose the relation $gxg=-x$, in which case we call x a type 2 generator. A type 2 generator is also a type 1 generator, but not conversely, since $g^2\neq 1$.

For the first case, we choose x to be type 1. Denote the algebra by H_1. The following relations are satisfied:

$$g^3=g,$$

$$gx=-xg,$$

$$x^2=0,$$

along with the same coproduct and counit as in the usual Hopf case (given above). Solving Eqs. (2.1) and (2.2) gives the weak antipode

$$T(1)=1,$$

$$T(g)=g,$$

$$T(x)=gx,$$

which has the same action as the antipode from the Hopf case but nevertheless is not an antipode. The defining relations imply that H_1 is six dimensional with basis

$$\{1,g,g^2,x,gx,g^2x\}.$$

Note that the element g^2 is a central idempotent. This is easily verified with the defining relations.

It is with this example that we demonstrate explicitly how to obtain a direct sum decomposition for an algebra with a central idempotent. This procedure will then be extended to the case of $w\mathfrak{sl}_q^d(n)$.

H_1 has a direct sum decomposition

$$H_1 = H_1^0 \oplus H_1^1,$$

where H_1^0 is the subalgebra with basis $\{(1-g^2)x, 1-g^2\}$, on which multiplication by g^2 is zero (indicated in the superscript), and H_1^1 is the subalgebra with basis $\{g, g^2, gx, g^2x\}$ on which multiplication by g^2 is the identity (also indicated in the superscript). In fact, these two subalgebras are determined by setting

$$\begin{aligned} H_1^0 &= (1-g^2)H_1, \\ H_1^1 &= g^2 H_1. \end{aligned} \tag{5.1}$$

It is straightforward to verify that the map $\psi: H_1^1 \to H$ with the action

$$\psi(g) = G,$$

$$\psi(g^2) = I,$$

$$\psi(gx) = GX,$$

$$\psi(g^2x) = X,$$

defines a weak Hopf algebra isomorphism, where I, G, X are the generators of the original Sweedler Hopf algebra H. Since H appears as a subalgebra of H_1, we can simply apply $\psi^{-1} \otimes \psi^{-1}$ to the R-matrix of H (see Ref. 15) to obtain an R-matrix $\mathcal{R}$ of H_1 satisfying

$$\mathcal{R}\Delta(a) = \sigma \circ \Delta(a)\mathcal{R}, \quad \forall a \in H_1,$$

$$\mathcal{R}_{13}\mathcal{R}_{23} = (\Delta \otimes \mathrm{id})(\mathcal{R}),$$

$$\mathcal{R}_{13}\mathcal{R}_{12} = (\mathrm{id} \otimes \Delta)(\mathcal{R}).$$

Such an R-matrix is then given by

$$\mathcal{R} = g^2 \otimes g^2 - 2p \otimes p + \alpha(g^2x \otimes g^2x - 2g^2x \otimes px + 2px \otimes px),$$

where $p = (g^2 - g)/2$ and α is an arbitrary parameter. This $\mathcal{R}$ is not invertible, but it satisfies the regularity condition[12]

$$\mathcal{R}\hat{\mathcal{R}}\mathcal{R} = \mathcal{R}, \tag{5.2}$$

$$\hat{\mathcal{R}}\mathcal{R}\hat{\mathcal{R}} = \hat{\mathcal{R}}, \tag{5.3}$$

where

$$\hat{\mathcal{R}} = g^2 \otimes g^2 - 2p \otimes p + \alpha(g^2x \otimes g^2x - 2px \otimes g^2x + 2px \otimes px).$$

It should also be noted that the Sweedler Hopf algebra H also appears as a subalgebra of H_1 with its generators defined by

$$I = 1,$$

$$G=1+g-g^2,$$

$$X=(1+\alpha g)gx,$$

where α is an an arbitrary constant. However, this is just an observation and has no consequence to the results of our paper, since this subalgebra is only isomorphic to H as an algebra, not a bialgebra.

Now we look at the algebra H_2, which corresponds to the choice of the generator x to be of type 2. This implies the following relations:

$$g^3=g,$$

$$gxg=-x,$$

$$x^2=0.$$

The only difference with the coproduct in this case is with the action defined on the generator x, which is now given by

$$\Delta(x)=x\otimes g+g^2\otimes x,$$

and the counit is the same as usual. The algebra H_2 is five dimensional with basis $\{1,g,x,gx,g^2\}$. Note that g^2 is a central idempotent. Defining

$$H_2^0=(1-g^2)H_2,$$

$$H_2^1=g^2H_2,$$

the decomposition

$$H_2=H_2^0\oplus H_2^1$$

still holds, where the superscripts still refer to the action of g^2, but now H_2^0 has basis $\{1-g^2\}$ and H_2^1 has basis $\{g^2,g,x,gx\}$.

Once again it is possible to verify that there exists a weak Hopf algebra isomorphism $\varphi:H_2^1\rightarrow H$ with the following action:

$$\varphi(g^2)=I,$$

$$\varphi(g)=G,$$

$$\varphi(x)=X,$$

$$\varphi(gx)=GX.$$

In a similar way to both of the examples above, for a quantized enveloping algebra $U\equiv U_q[sl_n]$, its weak extension U_w and some other algebraic structure U_0, a decomposition of the form

$$U_w=U_0\oplus U=(1-J)U_w\oplus JU_w$$

exists due to there being a central idempotent J whose existence derives from the relaxation of the invertibility of group-like elements in the algebra. In fact it is straightforward to prove the fact that for any d,

$$U_q[sl_n]\simeq J.w\mathfrak{sl}_q^d(n).$$

This result is another way of stating Proposition 1 from the paper.[12]

From another point of view, we could say that a weak extension is nothing but the original Hopf algebra plus some other algebra in which is contained all the information regarding the weak structure. In this case, it would help to know what conditions U_0 would have to satisfy in order that U_w has a weak Hopf structure. This has not been the approach of this paper as we saw in the last section. Since there are no other weak Hopf algebra isomorphisms on the weak $w\mathfrak{sl}_q^d(n)$, the classification *as weak Hopf algebras* is complete. However, if we were to consider all possible algebra isomorphisms, this direct sum decomposition is important since it leads to discovering several ''unexpected'' isomorphisms which do not arise from the action of the automorphisms in the quantised enveloping algebra case.

Since we only need the presence of a central idempotent to achieve this direct sum decomposition, we can apply this idea to the weak extensions of $U_q[sl_n]$ from the previous section, since the element J is always a central idempotent. However, it does not affect our classification of the weak Hopf algebra structure from the previous section. To demonstrate, we show that, rather unexpectedly, there is an algebra isomorphism $\psi: w\mathfrak{sl}_q^{10}(3)\rightarrow w\mathfrak{sl}_q^{9}(3)$.

We first apply the direct sum decomposition to $U=w\mathfrak{sl}_q^{10}(3)$ and $V=w\mathfrak{sl}_q^{9}(3)$ such that

$$U=(1-J)U\oplus JU\equiv U_0\oplus U_1$$

and similarly

$$V=(1-J')V\oplus J'V\equiv V_0\oplus V_1.$$

Explicitly we have U_0 generated by $\langle(1-J)E_1,(1-J)F_1,1-J\rangle$ and U_1 generated by $\langle J,JE_1,JF_1,E_2,F_2,K_1,K_2,\overline{K}_1,\overline{K}_2\rangle$. For V, denoting its generators by a prime, we have V_0 generated by $\langle(1-J')E_1',(1-J')F_2',1-J'\rangle$ and V_1 generated by $\langle J',J'E_1',E_2',F_1',J'F_2',K_1',K_2',\overline{K}_1',\overline{K}_2'\rangle$. It is straightforward to show that both U_1 and V_1 are isomorphic as (weak) Hopf algebras to $U_q[sl(3)]$. It is also easy to verify that U_0 and V_0 are both Abelian with the same number of generators and are therefore isomorphic as algebras. Combining these two facts leads to the isomorphism $\psi: U\rightarrow V$, the action of which is given by

$$\psi(1)=1,$$

$$\psi(E_1)=(1-J')F_2'+F_1',$$

$$\psi(E_2)=J'F_2',$$

$$\psi(F_1)=E_1',$$

$$\psi(F_2)=E_2',$$

$$\psi(K_i)=\overline{K}_i',$$

$$\psi(\overline{K}_i)=K_i'.$$

The map ψ is consistent with all the defining relations so is therefore an algebra homomorphism and it can be shown to have inverse

$$\psi^{-1}(E_1')=F_1,$$

$$\psi^{-1}(E_2')=F_2,$$

$$\psi^{-1}(F_1')=JE_1,$$

$$\psi^{-1}(F_2')=(1-J)E_1+E_2,$$

$$\psi^{-1}(K_i')=\overline{K}_i,$$

$$\psi^{-1}(\overline{K}_i')=K_i.$$

Therefore ψ is an isomorphism.

If we set the action of the coproduct Δ for U and allow the freedom to choose the coproduct Δ' of V consistently with ψ, then we end up having to compare the action of $(\psi\otimes\psi)\circ\Delta$ with $\Delta'\circ\psi$. Applying both of these maps to the generators will clearly give a noncoassociative Δ'. Therefore the ψ only can be considered as an algebra isomorphism. However, it is uncertain whether or not this coproduct Δ' would define a quasibialgebra.[2] This certainly raises some interesting questions relating to whether or not these isomorphisms could correspond to some kind of Drinfeld twist. If so, then perhaps our classification is only a much smaller classification of the structures as quasibialgebras. This idea may warrant further investigation.

VI. CONCLUDING REMARKS

We have seen that it is possible to define weak extensions of $U_q[sl_n]$ by only relaxing some of the relations in the original algebra. As we saw in the work of Li and Duplij,[12] one nice way of doing this is to relax invertibility of the group-like elements to a more general regularity condition and also to impose one of two relations on the other generators. This allows us to define many examples.

One observation is that it is also possible to extend the definition of a quantized superalgebra[18] to the weak case by using the same idea of relaxing the invertibility of the generators K and $\overline{K}$. We demonstrate with the algebra $w\mathfrak{osp}_q^d(2|1)$ which has generators $\{K,\overline{K},V_+,V_-\}$. We define the parity of these generators to be $p(K)=p(\overline{K})=0$, $p(V_\pm)=1$.

The following relations are satisfied:

$$K\overline{K}=\overline{K}K,\quad K\overline{K}K=K,\quad \overline{K}K\overline{K}=\overline{K},$$

$$KV_\pm=q^{\pm1}V_\pm K,\quad \overline{K}V_\pm=q^{\mp1}V_\pm\overline{K}, \tag{6.1}$$

$$\{V_+,V_-\}=-\frac{1}{4}\frac{K-\overline{K}}{q-q^{-1}}.$$

Keeping in theme with the preceding sections, if in addition the following relations are satisfied:

$$KX\overline{K}=q^{\pm1}X,$$

where $X=V_+$ or V_-, then we call X a type 2 generator. Otherwise we call X a type 1 generator. This example is almost exactly like the case of $w\mathfrak{sl}_q^d(2)$ in that we have the same notion of generators of type 1 and 2. The coalgebra structure is of the same form, and the only real difference is that the weak antipode is a graded algebra antihomomorphism, so it satisfies $T(ab)=(-1)^{p(a)p(b)}T(b)T(a)$.

All the weak Hopf algebras given in this paper have noncocommutative coproducts. This implies existence of universal R-matrices that could give new solutions of quantum Yang–Baxter equations as mentioned in Refs. 10 and 12. One direction for future work is to investigate the form of such R-matrices. We expect the expressions would not be that different to those of the original Hopf algebra due to the direct sum decomposition of Sec. V. In fact, in Sec. V we gave one possible R-matrix for the finite dimensional weak Hopf generalization of Sweedler's well-known example using these facts.

Section V also demonstrates the fact that there are many algebra isomorphisms between structures. In this paper we did not investigate all possible isomorphisms, but instead gave a small existence proof that such isomorphisms do indeed exist. It would be interesting to classify these structures as algebras using this observation.

A question that arose during our investigation is one related to automorphisms and twisting, especially in the usual quantized enveloping algebra case. As we have already mentioned, the algebra automorphisms are well known for the quantized enveloping algebras, some of which are also bialgebra automorphisms. We are currently unaware of whether or not, corresponding to every algebra automorphism $\psi: A \rightarrow A$, there exists a twist element $F \in A \otimes A$ such that

$$(\psi \otimes \psi)\Delta(a) = F.\Delta(\psi(a)).F^{-1}, \quad \forall a \in A.$$

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Givental formula in terms of Virasoro operators

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(Received 26 February 2003; accepted 22 May 2003)

We present a conjecture that the universal enveloping algebra of differential operators $\partial/\partial t_k$ over $\mathbb{C}$ coincides in the origin with the universal enveloping algebra of the (Borel subalgebra of) Virasoro generators from the Kontsevich model. Thus, we can decompose any (pseudo)differential operator to a combination of the Virasoro operators. Using this decomposition we present the right-hand side of the Givental formula [math.AG/0008067] as a constant part of the differential operator we introduce. In the case of $\mathbb{CP}^1$ studied in the paper by Song and Song [hep-th/0103254], the left-hand side of the Givental formula is a unit, which imposes certain constraints on this differential operator. We explicitly check that these constraints are correct up to $O(q^4)$. We also propose a conjecture of factorization modulo Hirota equation of the differential operator introduced and check this conjecture with the same accuracy. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1615695]

I. INTRODUCTION

It is well known that $\mathcal{N}=2$ supersymmetric sigma-model with target space M, defined on the genus g Riemann surface, through twisting, leads to the topological field theory.[1] For $D=2$ sigma-model, the correlation functions of such topological field theory are known to be some intersection numbers on the target space, and the fields of this theory, which we call primary fields, are in one-to-one correspondence with the elements of $H^*(M)$ (see, for example, Ref. 2). Thus, for any genus g, the free energy $F_M^g(s)$ of the theory, as a function of couplings s to primary fields (the space of such couplings is called small phase space) is a generating function for such intersection numbers on the target space. The genus zero free energy $F_M^0(s)$ is described by associativity—WDVV equations.[2,3]

Coupling of the topological field theory to the topological gravity leads to the so-called topological string theory. The genus g free energy $\mathcal{F}_M^g(t)$ of this theory, which depends on infinitely many coupling constants t (couplings to gravitational descendants), describes intersection theory on the compactified moduli spaces of genus g punctured Riemann surfaces. We will denote coordinates on the big phase space as t, while on the small phase space, subspace of the big one, as s. Combining $\mathcal{F}_M^g(t)$ for all g into the sum and exponentiating $\tau_M(t)=\exp\Sigma_{g=0}\hbar^{g-1}\mathcal{F}_M^g(t)$, one gets a general object which depends on the manifold and is the function of infinitely many coupling constants. We call it τ-function.[4] This function can be considered from many different points of view, which lead to different conditions on $\tau_M(t)$ (Refs. 2, 5–7) (Virasoro constraints, dilaton and divisor equations). However, in general, they do not seem to be restrictive enough to determine $\tau_M(t)$ completely.

In fact, there are at least two examples of the manifold M when the function τ_M for topological field theory with the target space M turns out to be the τ-function of integrable hierarchy. The first example is the point. Its function $\tau_\bullet$, which corresponds to the pure topological gravity,[2] is the τ-function for the KdV hierarchy.[8,9] It can be realized as the matrix integral (famous Kontsevich model[10])

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$$\tau_\bullet(T)=\frac{\int \mathrm{d}H\, e^{-1/3\mathrm{Tr}\,H^3+\mathrm{Tr}\,M^2H}}{\int \mathrm{d}H\, e^{-\mathrm{Tr}MH^2}}, \tag{1}$$

over $N\times N$ Hermitian matrix, the coupling constants, i.e., the times from the integrable point of view, are defined as follows:

$$T_k=-\frac{1}{k}\mathrm{Tr}\,M^{-k}. \tag{2}$$

Invariance of this matrix integral with respect to the change of variables,[11] namely,

$$H\to H+\epsilon_p\,, \tag{3}$$

with $\epsilon_p=M^{2p}$ leads to the Virasoro constraints $L_n\tau_\bullet(T_k)=0$, $n\geqslant -1$ (see, for instance, Refs. 12–14 with Ref. 15),

$$L_n=\frac{1}{2}\sum_{k\ odd} kT_k\frac{\partial}{\partial T_{k+2n}}+\frac{1}{4}\sum_{\substack{a+b=2n\\ a,b\ \ odd\ \ and>0}}\frac{\partial^2}{\partial T_a\partial T_b}+\frac{T_1^2}{4}\delta_{n,-1}+\frac{1}{16}\delta_{n,0}-\frac{\partial}{\partial T_{3+2n}},\quad n\geqslant -1. \tag{4}$$

These Virasoro operators form the Borel subalgebra of the Virasoro algebra,

$$[L_n\,,L_m]=(n-m)L_{n+m}\,. \tag{5}$$

The second example, $M=\mathbb{CP}^1$, conjectured to correspond to the Toda hierarchy,[6,16] has been proved in the interesting paper.[17] The τ-function for it can also be represented as some matrix integral. By analogous consideration, this representation leads to the Borel subalgebra of some other Virasoro algebra which annihilates the τ-function. Therefore, one could expect that the function τ_M associated with any manifold, is the τ-function for some integrable hierarchy. This is one of the reasons why we generally call it τ-function.

For several particular manifolds there exist some explicit formulas for F_M^g. The example, of $M=\mathbb{CP}^1$ is, in a sense, the only foreseeable: its whole free energy vanishes on the small phase space, except genus zero and genus one, which are, correspondingly,[18]

$$F^0_{\mathbb{CP}^1}=\tfrac{1}{2}(s_P)^2s_Q+e^{s_Q} \tag{6}$$

and

$$F^1_{\mathbb{CP}^1}=-s_Q/24. \tag{7}$$

For $\mathbb{CP}^2$ the genus zero free energy is of the form

$$F^0_{\mathbb{CP}^2}=\frac{1}{2}s_P(s_Q)^2+\frac{1}{2}(s_P)^2s_R+\sum_{d=1}N_d^{(0)}\frac{(s_R)^{3d-1}}{(3d-1)!}\exp(s_Qd), \tag{8}$$

and for the expansion coefficients $N_d^{(0)}$ there is the recursive relation[5]

$$N_d^{(0)}=(3d-4)!\sum_{l+k=d}\frac{N_l^{(0)}N_k^{(0)}}{(3l-1)!(3k-1)!}k^2l[3kl+l-2k]. \tag{9}$$

Here the numbers $N_d^{(0)}$ and $N_d^{(1)}$ are numbers of degree d rational (elliptic) curves passing through $3d-1$ (respectively, $3d$) points.

For the genus one free energy

$$F^1_{\mathbb{CP}^2}=\frac{-s_Q}{8}+\sum_{d=1} N^{(1)}_d \frac{(s_R)^{3d}}{(3d)!}\exp(ds_Q), \tag{10}$$

analogous recursion relation was derived in Ref. 19, using Virasoro constraints for $\mathbb{CP}^n$ and the topological recursion relations (see also Ref. 20)

$$N^{(1)}_n=N^{(0)}_n\frac{1}{72}n(n-1)(n-2)+\sum_{k+l=n}(3n-1)!\,\frac{N^{(0)}_k}{(3k-1)!}\,\frac{N^{(1)}_l}{(3l)!}\,\frac{l}{9}(3k^2-2k). \tag{11}$$

However, in general, there are no expressions for higher genera similar to (9), (11), and only a few first terms in the series like (8), (10) are found.

The problem is to construct a regular procedure for finding $F^M_g(s)$. In this paper, we make a modest contribution to solving this problem. It is based on the remarkable formula which was proposed in Ref. 21 with the help of the localization technique, and connects the Kontsevich τ-function ($\tau_\bullet$, function for the point on the big phase space) with the τ-function for some (for instance, projective) manifold M on the small phase space, with the genus zero and one contributions omitted[22]

$$e^{\Sigma_{g>1}\hbar^{g-1}F^g_M(s)}=\left[e^{D_M(s)}\prod_j \tau_\bullet(\hbar\Delta_j;t^{(j)}_0,t^{(j)}_1,\ldots)\right]_{t^{(i)}_k=T^i_k(s)}. \tag{12}$$

Here s_i are coordinates on the small phase space for the manifold M, indices i,j run from 1 to $K=\dim(H^*(M))$, and $D_M(s)$ is the bilinear pseudodifferential[23] operator acting on $t^{(i)}_k$,

$$D_M(s)=\frac{\hbar}{2}\sum_{k,l=0}^{\infty}\sum_{i,j} V^{ij}_{kl}(s)\Delta^{1/2}_i(s)\Delta^{1/2}_j(s)\partial_{t^{(i)}_k}\partial_{t^{(j)}_l}, \tag{13}$$

$V^{ij}_{kl}(s)$, $\Delta_i(s)$, and $T^i_k(s)$ being some functions which can be presented in terms of the genus zero potential $F^0_M(s)$, more precisely on its third derivatives (Refs. 21 and 24).

Formula (12) was studied in Ref. 24 for the first nontrivial example of the manifold M, $\mathbb{CP}^1$.

Since, as we know from the explicit form of the free energy on the small phase space for $\mathbb{CP}^1$ the lhs of (12) is unity, formula (12) can be considered as an equation imposed on the Kontsevich τ-function. We call it the Song equation.[25]

In Ref. 24 all the necessary coefficients Δ,V, and T were calculated, and (12) was checked extensively using the expansion in $\hbar$ with the accuracy of $O(\hbar^4)$. This calculation involves the explicit form of $\tau_\bullet(t)$ as a series in times.

In our paper, we reformulate the problem of calculation on the right-hand side (rhs) of (12) for given V and T realizing some particular differential operator D'_M easily connected with D_M [see (15)] via Virasoro operators.

Namely, the shift operator

$$\exp\sum_{i=1}^{K}\sum_{k=2}^{\infty} T^i_k(s)\partial_{t^{(i)}_k} \tag{14}$$

obviously commutes with $D_M(s)$, and for the operator

$$D'_M(s)=D_M(s)+\sum_{i=1}^{K}\sum_{k=2}^{\infty} T^i_k(s)\partial_{t^{(i)}_k} \tag{15}$$

we have the equality

$$\left[e^{D_M(s)}\prod_j \tau_\bullet(\hbar\Delta_j;t_0^{(j)},t_1^{(j)},\ldots)\right]_{t_k^{(i)}=T_k^i(s)}=\left[e^{D'_M(s)}\prod_j \tau_\bullet(\hbar\Delta_j;t_0^{(j)},t_1^{(j)},\ldots)\right]_{t_k^{(i)}=0}. \quad (16)$$

The general idea of the paper is to present the operator $e^{D'_M}$ in the origin of the space of times $t_k^{(i)}$ in terms of the Virasoro operators (this means, that we consider rhs modulo term, proportional to the positive powers of the times t) (4),

$$e^{D'_M}\Big|_{t=0}=\sum_{[l_1],[l_2],\ldots,[l_K]}^{\infty} P^M_{[l_1],[l_2],\ldots,[l_K]}(s)L_{[l_1]}\otimes L_{[l_2]}\otimes\cdots\otimes L_{[l_K]}\Big|_{t=0}. \quad (17)$$

Here $L_{[l]}$ are products of the Virasoro operators with the non-negative multiplicities m_i, given by multi-indices $[l]$: for $[l]=(m_{-1},m_0,\ldots,m_r)$ we define

$$L_{[l]}:=L_r^{m_r}\cdots L_0^{m_0}L_{-1}^{m_{-1}}, \quad (18)$$

and, if all multiplicities m_i vanish,

$$L_{[0]}=1, \quad (19)$$

where we denote $[0]:=(0,0,\ldots,0)$. Since all the Virasoro operators of the Borel subalgebra annihilate the Kontsevich τ-function, the action of the operator presented in this way on the $\tau_\bullet$'s at the point $t=0$ is trivial, that is, the only nonvanishing contribution to the left-hand side (lhs) of (12) is given by the constant term proportional to (19):

$$e^{\Sigma_{g>1}\hbar^{g-1}F^g_M(s)}=P^M_{[0],[0],\ldots,[0]}(s). \quad (20)$$

In particular, the Song equation in terms of D' is

$$\exp[D'_{\mathbb{CP}^1}]\tau(\hbar,x)\tau(\hbar,y)|_{x_n=y_n=0}=1. \quad (21)$$

In the case of $\mathbb{CP}^1$, one can expand the operator $D'_{\mathbb{CP}^1}$ in the series in $q:=\exp(-s_Q/2)$,

$$e^{D'_{\mathbb{CP}^1}}=1+\sum_{n=1}^{\infty} q^n\sum_{[l_1],[l_2]} P^{\mathbb{CP}^1(n)}_{[l_1],[l_2]}(\hbar)L_{[l_1]}\otimes L_{[l_2]}\Big|_{t=0}. \quad (22)$$

Since for $\mathbb{CP}^1$ the lhs of (12) is equal to 1, the Song equation is equivalent to the condition

$$P^{\mathbb{CP}^1(n)}_{[0],[0]}=0, \quad n\geqslant 1. \quad (23)$$

In this paper, we check this condition with the accuracy of $O(q^4)$.

The paper contains two conjectures. The first conjecture which states that any differential operator in times t with constant coefficients can be presented as a combination of the Virasoro operators with some multiplicities at the origin helps to deal with the Givental formula. The second conjecture, whose general structure is still unknown, in particular the case of $M=\mathbb{CP}^1$ claims that the operator $D'_{\mathbb{CP}^1}$ (22) can be factorized into the sum of two parts, which are tensor squares of differential operators, modulo Hirota equations. Both of these conjectures are checked perturbatively in the example of $\mathbb{CP}^1$ with the accuracy of $O(q^4)$.

The paper is organized as follows: in Sec. II we represent the main results of Ref. 24 and explicitly present the Virasoro and Hirota constraints which we use in our calculations. Sections III and IV are devoted to our two conjectures, while Sec. V contains some concluding remarks.

II. MAIN INGREDIENTS

In Ref. 24 it was shown that, denoting $t_n^{(+)}=x_n$ and $t_n^{(-)}=y_n$, one has the following differential operator:

$$D_{\mathbb{CP}^1}:=\frac{\hbar}{2}\sum_{k,l\geqslant 0}\left(V_{kl}^{++}(\partial_{x_k}\partial_{x_l}+\partial_{y_k}\partial_{y_l})+2i(-1)^{l-1}V_{kl}^{+-}\partial_{x_k}\partial_{y_l}\right), \tag{24}$$

and introducing α being c-numbers

$$\alpha_{m+1}=-\frac{(2m+1)^2}{8(m+1)}\alpha_m, \quad \alpha_0=1, \tag{25}$$

we can represent times[26] T^+

$$T_n^+=\begin{cases}0, & n=0,1\\ -\dfrac{\alpha_{n-1}}{2^{n-1}}\exp\left[\dfrac{-(n-1)s_Q}{2}\right], & n\geqslant 2.\end{cases} \tag{26}$$

In the case of $\mathbb{CP}$ we have two times on the small phase space but third derivatives of the free energy depend only on one coordinate, s_Q. This means that all components of our construction depend on this one coordinate. α being c-numbers,

$$\alpha_{m+1}=-\frac{(2m+1)^2}{8(m+1)}\alpha_m, \quad \alpha_0=1. \tag{27}$$

Coefficients V^{++} and V^{+-} in (24) can be presented as bilinear combinations of T_k^+ similar to those in the paper (the proper formula has a slight mistake therein):[24]

$$V_{kl}^{++}=\sum_{n=0}^{k-1}\frac{(-1)^n(4(l+n+1)(k-n)-1)}{(2l+2n+1)(2k-2n-1)}T_{l+n+2}^+T_{k-n+1}^++(-1)^{k+1}\frac{T_{l+k+2}^+}{2l+2k+1},$$

$$V_{kl}^{+-}=i(-1)^l\left[\sum_{n=0}^{k-1}\frac{2(l+2n+1-k)}{(2l+2n+1)(2k-2n-1)}T_{l+n+2}^+T_{k-n+1}^++2(l+k+1)\frac{T_{l+k+2}^+}{2l+2k+1}\right]. \tag{28}$$

Taking into account that, in (26) $T_0^+=T_1^+=0$, one can explicitly substitute the Kontsevich τ-function to (12) in the case $M=\mathbb{CP}^1$, and check the equality, expanding the operator and τ-functions in the $\hbar$-series,

$$\exp[D_{\mathbb{CP}^1}]\tau_\bullet(\hbar,x)\tau_\bullet(\hbar,y)|_{x_n=y_n=T_n^+}=:1+\sum_{n=1}^{\infty}a_n\hbar^n. \tag{29}$$

In this way, one gets an infinite family of equations on the coefficients of the decomposition of $\tau_\bullet(\hbar,t)$,

$$a_n=0, \quad \forall n>0. \tag{30}$$

In Ref. 24, the first three equations were explicitly checked.

The Virasoro operators corresponding to our normalization of times, are (see, for example, Ref. 27)

$$L_n=\begin{cases}\displaystyle\sum_{m=1}^{\infty}\tilde{t}_m\partial_{m-1}+\frac{1}{2\hbar}t_0^2, & n=-1\\ \displaystyle\sum_{m=0}^{\infty}\left(m+\frac{1}{2}\right)\tilde{t}_m\partial_m+\frac{1}{16}, & n=0\\ \displaystyle\sum_{m=0}^{\infty}\frac{\Gamma(n+m+\frac{3}{2})}{\Gamma(m+\frac{1}{2})}\tilde{t}_m\partial_{m+n}+\frac{\hbar}{2}\sum_{m=0}^{n-1}(-1)^{m+1}\frac{\Gamma(n-m+\frac{1}{2})}{\Gamma(-m-\frac{1}{2})}\partial_m\partial_{n-m-1}, & n>0,\end{cases} \tag{31}$$

with $\tilde{t}_m:=t_m-\delta_{m,1}$, $\partial_m=\partial/\partial t_m$. They annihilate the Kontsevich τ-function,

$$L_n\tau_*(\hbar,t)=0,\ \ n\geqslant -1. \tag{32}$$

It is also known that any KdV τ-function, in particular, the Kontsevich one, solves the Hirota bilinear equations, the first three of which being (see, for instance, Ref. 28)

$$\begin{aligned}&(\hbar D_0^4-12D_0D_1)\tau(t)\cdot\tau(t)=0,\\ &\left(-24D_1^2+\hbar D_0^3D_1+\frac{\hbar^2}{12}D_0^6\right)\tau(t)\cdot\tau(t)=0,\\ &\left(-D_1^2+\frac{\hbar^2}{360}D_0^6+D_0D_2\right)\tau(t)\cdot\tau(t)=0,\end{aligned} \tag{33}$$

which we denote for the sake of brevity as

$$\mathbf{H}_i=0,\ \ i=1,2,3. \tag{34}$$

III. CONNECTION BETWEEN SONG AND VIRASORO EQUATIONS

Consider an arbitrary operator of the form

$$B:=\partial_1^{n_1}\partial_2^{n_2}\cdots\partial_k^{n_k},\quad n_i\geqslant 0,\quad \sum_{i=1}^{k}n_k>0, \tag{35}$$

for some finite k. We experimentally check for small k and n that this operator can be presented as a combination of the Virasoro operators (31) at the origin of the space of times t,

$$B=\sum_{m_{-1},\ldots,m_r=0}^{\infty}c_{m_r,\ldots,m_0,m_{-1}}L_r^{m_r}\cdots L_0^{m_0}L_{-1}^{m_{-1}}\Big|_{t=0}=:\sum_{[l]}c_{[l]}L_{[l]}\Big|_{t=0}, \tag{36}$$

for some finite r, dependent on n and k, where we introduced multi-index $[l]=(m_{-1},m_0,\ldots,m_r)$. Some of the multiplicities m_i, and even all of them, can vanish. Namely, we expressed 27 derivatives, which are necessary for our perturbative calculation (see below), in terms of the Virasoro operators. Using explicit form of the Virasoro operators we can get some answers for actions of the differetial operators on the tau-function, not representing them as a combination of Virasoro operators, for example,

$$\frac{\partial}{\partial T_1}^{n_0}\frac{\partial}{\partial T_3}^{n_1}\tau_*(T_1,T_3,\ldots)\Big|_{T_1=T_3=\cdots=0}=\frac{1}{3}\left(\frac{3}{2}\right)^{n_1}\left(\frac{1}{6\hbar}\right)^{n_0/3}\frac{\Gamma\left(-\frac{n_0}{3}\right)}{\Gamma(-n_0)}\frac{\Gamma(n_1+\frac{1}{3}n_0+\frac{1}{24})}{\Gamma(\frac{1}{3}n_0+\frac{1}{24})}. \tag{37}$$

For example,

$$\begin{aligned}\partial_0 &= -L_{-1}|_{t=0},\\ \partial_0^2 &= L_{-1}^2|_{t=0},\\ \partial_0^3 &= -L_{-1}^3|_{t=0}+\frac{1}{\hbar},\\ \partial_2 &= \frac{1}{30}\hbar L_{-1}^2\Big|_{t=0}-\frac{4}{15}L_1\Big|_{t=0}.\end{aligned} \tag{38}$$

If this is correct for arbitrary B, one can present any pseudodifferential operator as a combination of the Virasoro operators at the origin of the space of times t. Thus, one can present any tensor product of N differential operators as a sum of tensor products of combinations of the Virasoro operators

$$\sum_{[l_1],[l_2],\ldots,[l_N]}^{\infty} P_{[l_1],[l_2],\ldots,[l_N]} L_{[l_1]}\otimes L_{[l_2]}\otimes\cdots\otimes L_{[l_N]}\Big|_{t=0}, \tag{39}$$

with P being some coefficients.

This representation can be appropriate for our consideration. In particular, one has

$$e^{D'_M}=\sum_{[l_1],[l_2],\ldots,[l_K]}^{\infty} P^M_{[l_1],[l_2],\ldots,[l_K]}(s) L_{[l_1]}\otimes L_{[l_2]}\otimes\cdots\otimes L_{[l_K]}\Big|_{t=0}. \tag{40}$$

Here the operator

$$D'_M(s)=D_M(s)+\sum_{i=1}^{K}\sum_{k=2}^{\infty} T^i_k(s)\partial_{t^{(i)}_k} \tag{41}$$

is the combination of the D_M and the operator, which shifts the times $t^{(i)}_k=T^i_k$ to zero.

Since all the Virasoro operators of the Borel subalgebra annihilate $\tau_\bullet$, calculation of the action of the operator on the product of $\tau_\bullet$'s in the origin is equivalent to calculating $P_{[0],[0],\ldots,[0]}$. One observes that the lhs of (12) is equal to the identity component of the decomposition of operator $e^{D'_M}$ in terms of Virasoro operators

$$e^{\Sigma_{g>1}\hbar^{g-1}F^g_M(s)}=P^M_{[0],[0],\ldots,[0]}(s). \tag{42}$$

In our particular case, moving our times to the origin is equivalent to changing the operator D: for the operator

$$D'_{\mathbb{CP}^1}=D_{\mathbb{CP}^1}+\sum_{n=2}^{\infty} T^+_n\left(\frac{\partial}{\partial x_n}+\frac{\partial}{\partial y_n}\right), \tag{43}$$

the Song equation is

$$\exp[D']\tau_\bullet(\hbar,x)\tau_\bullet(\hbar,y)|_{x=y=0}=1. \tag{44}$$

Now we can check the Song equation perturbatively, not specifying the explicit form of $\tau_\bullet$. This is the advantage of our approach, since the approach of Ref. 24 required the explicit form of $\tau_\bullet$. To study this equation perturbatively, we can expand the operator in the series in q,

$$\exp[D'_{\mathbb{CP}^1}]=:1+\sum_{n=1}^{\infty} q^n \sum_{[l_1],[l_2]} P^{\mathbb{CP}^1(n)}_{[l_1],[l_2]}(\hbar) L_{[l_1]}\otimes L_{[l_2]}\Big|_{t=0}, \tag{45}$$

and all we must check is that

$$P^{\mathbb{CP}^1(m)}_{[0][0]}=0 \quad \forall m>0. \tag{46}$$

We check this up to $n=3$.

The explicit expression for the operator $e^{D'_{\mathbb{CP}^1}}|_{x=y=0}$ acting on $\tau_\bullet$'s looks like

$$\begin{aligned}
e^{D'_{\mathbb{CP}^1}}\tau\otimes\tau|_{x=y=0}=1+([&-\tfrac{1}{30}L_1\tau+(-\tfrac{7}{120}L_{-1}^2\tau+\tfrac{1}{8}(L_{-1}\tau)^2)\hbar]q+[(\tfrac{1}{3600}(L_1\tau)^2+\tfrac{1}{3600}L_1^2\tau\\
&+\tfrac{1}{504}L_2\tau)+(\tfrac{109}{50\,400}L_{-1}\tau+\tfrac{53}{8400}L_{-1}L_0\tau-\tfrac{1}{240}L_{-1}\tau L_{-1}L_1\tau+\tfrac{7}{7200}L_{-1}^2L_1\tau\\
&-\tfrac{7}{240}L_{-1}\tau L_0\tau+\tfrac{7}{7200}L_{-1}^2\tau L_1\tau)\hbar+(\tfrac{49}{57\,600}L_{-1}^4\tau-\tfrac{7}{960}L_{-1}\tau L_{-1}^3\tau\\
&+\tfrac{499}{57\,600}(L_{-1}^2\tau)^2)\hbar^2]q^2+[(-\tfrac{97}{453\,600}L_3\tau-\tfrac{1}{648\,000}L_1^3\tau-\tfrac{1}{30\,240}L_1L_2\tau\\
&-\tfrac{1}{216\,000}L_1^2\tau L_1\tau-\tfrac{1}{30\,240}L_2\tau L_1\tau)+(\tfrac{31}{7200}(L_0\tau)^2+\tfrac{14\,951}{3\,024\,000}L_{-1}\tau L_1\tau\\
&-\tfrac{53}{504\,000}L_{-1}L_0\tau L_1\tau-\tfrac{53}{504\,000}L_{-1}L_0L_1\tau+\tfrac{1}{4032}L_{-1}\tau L_{-1}L_2\tau-\tfrac{7}{864\,000}L_1^2\tau L_{-1}^2\tau\\
&+\tfrac{1}{28\,800}L_{-1}\tau L_{-1}L_1^2\tau+\tfrac{1}{28\,800}(L_{-1}L_1\tau)^2-\tfrac{1}{17\,280}L_{-1}^2L_2\tau-\tfrac{1}{17\,280}L_2\tau L_{-1}^2\tau\\
&-\tfrac{61}{252\,000}L_0^2\tau-\tfrac{1319}{1\,814\,400}L_{-1}L_1\tau+\tfrac{7}{14\,400}L_{-1}\tau L_0L_1\tau-\tfrac{7}{864\,000}L_{-1}^2L_1^2\tau\\
&-\tfrac{151}{324\,000}L_0\tau-\tfrac{7}{432\,000}L_{-1}^2L_1\tau L_1\tau+\tfrac{7}{14\,400}L_{-1}L_1\tau L_0\tau)\hbar+(\tfrac{7}{57\,600}L_{-1}L_1\tau L_{-1}^3\tau\\
&+\tfrac{1121}{1\,728\,000}L_{-1}\tau L_{-1}^2\tau-\tfrac{53}{288\,000}L_{-1}^3L_0\tau+\tfrac{49}{57\,600}L_{-1}^3\tau L_0\tau-\tfrac{4567}{12\,0960\,000}L_{-1}^3\tau\\
&-\tfrac{1103}{288\,000}L_{-1}L_0\tau L_{-1}^2\tau+\tfrac{7}{57\,600}L_{-1}\tau L_{-1}^3L_1\tau+\tfrac{661}{403\,200}L_{-1}\tau L_{-1}^2L_0\tau\\
&-\tfrac{499}{1\,728\,000}L_{-1}^2L_1\tau L_{-1}^2\tau-\tfrac{49}{3\,456\,000}L_{-1}^4L_1\tau-\tfrac{49}{3\,456\,000}L_{-1}^4\tau L_1\tau)\hbar^2\\
&+(-\tfrac{6643}{13\,824\,000}L_{-1}^4\tau L_{-1}^2\tau+\tfrac{199}{460\,800}(L_{-1}^3\tau)^2+\tfrac{49}{460\,800}L_{-1}\tau L_{-1}^5\tau\\
&-\tfrac{343}{41\,472\,000}L_{-1}^6\tau)\hbar^3]q^3)|_{t=0}+O(q^4).
\end{aligned} \tag{47}$$

This form seems to be convenient, since the operator $D'_{\mathbb{CP}^1}$ is symmetric in x and y. Now, if one uses the explicit expression for the τ-function $\tau_\bullet$, conditions (46) for $m=3n$ reproduce the conditions $a_n=0$ from (30). They are only those conditions that restrict the coefficients V^{++}, V^{+-}, and T^+.

IV. LINEAR EQUATION FROM THE BILINEAR ONE

The Song equation is quadratic in $\tau_\bullet$. Thus, if one manages to presents the operator $e^{D'_{\mathbb{CP}^1}}$ as

$$e^{D'_{\mathbb{CP}^1}}=f(\hbar,q,L)^{\otimes 2}+2\hbar q g(\hbar,q,L)^{\otimes 2}, \tag{48}$$

the Song equation is equivalent to the system of two linear equations

$$\begin{aligned}
f(\hbar,q,L)\tau_\bullet|_{t=0}&=1,\\
g(\hbar,q,L)\tau_\bullet|_{t=0}&=0.
\end{aligned} \tag{49}$$

Here f and g are some operators expressed in terms of the Virasoro operators at the origin.

It turns out that the conjecture (48) is slightly incorrect, instead, with the accuracy of $O(q^4)$, one gets

$$[e^{D'_{\mathbb{CP}^1}} - f(\hbar,q,L)^{\otimes 2} - 2\hbar q g(\hbar,q,L)^{\otimes 2}]\tau\otimes\tau|_{t=0} = \left[\frac{\hbar}{768}q^2\mathbf{H}_1 - \left(\frac{11}{12\,288}\mathbf{H}_2 + \frac{21}{1024}\mathbf{H}_3 + \frac{17}{737\,280}\hbar^2 L_{-1}^2\mathbf{H}_1 - \frac{1}{46\,080}\hbar L_1\mathbf{H}_1\right)q^3\right]\Big|_{t=0}, \tag{50}$$

where $\mathbf{H}$'s are combinations bilinear in τ which correspond to the Hirota equations

$$\mathbf{H}_1(t=0) = ((2L_{-1}^4\tau - 8L_{-1}\tau L_{-1}^3\tau + 6(L_{-1}^2\tau)^2)\hbar + 8L_{-1}\tau - 16L_{-1}L_0\tau + 16L_{-1}\tau L_0\tau)|_{t=0},$$

$$\begin{aligned}\mathbf{H}_2(t=0) = (&32L_0\tau - \tfrac{64}{3}L_0^2\tau + \tfrac{64}{3}(L_0\tau)^2 + (-2L_{-1}^3\tau + \tfrac{4}{3}L_{-1}^3L_0\tau + 2L_{-1}\tau L_{-1}^2\tau - 4L_{-1}\tau L_{-1}^2L_0\tau \\ &+ 4L_{-1}L_0\tau L_{-1}^2\tau - \tfrac{4}{3}L_{-1}^3\tau L_0\tau)\hbar + (-L_{-1}\tau L_{-1}^5\tau + \tfrac{1}{6}L_{-1}^6\tau + \tfrac{5}{2}L_{-1}^4\tau L_{-1}^2\tau \\ &- \tfrac{5}{3}(L_{-1}^3\tau)^2)\hbar^2)|_{t=0},\end{aligned}$$

$$\begin{aligned}\mathbf{H}_3(t=0) = ((&\tfrac{16}{15}L_0\tau + \tfrac{8}{15}L_{-1}L_1\tau - \tfrac{8}{15}L_{-1}\tau L_1\tau - \tfrac{8}{9}L_0^2\tau + \tfrac{8}{9}(L_0\tau)^2) \\ &+ (-\tfrac{1}{15}L_{-1}^3\tau + \tfrac{1}{15}L_{-1}\tau L_{-1}^2\tau)\hbar + (\tfrac{1}{180}L_{-1}^6\tau - \tfrac{1}{30}L_{-1}\tau L_{-1}^5\tau \\ &+ \tfrac{1}{12}L_{-1}^4\tau L_{-1}^2\tau - \tfrac{1}{18}(L_{-1}^3\tau)^2)\hbar^2)|_{t=0}.\end{aligned} \tag{51}$$

The operators f and g are, respectively,

$$\begin{aligned}f(\hbar,q,L) = 1 + (&-\tfrac{1}{60}L_1 - \tfrac{7}{240}\hbar L_{-1}^2)q + (-\tfrac{13}{3150}\hbar L_{-1} + \tfrac{19}{1400}\hbar L_{-1}L_0 + \tfrac{1}{1008}L_2 + \tfrac{7}{14\,400}\hbar L_{-1}^2L_1 \\ &+ \tfrac{1}{7200}L_1^2 - \tfrac{101}{57\,600}\hbar^2L_{-1}^4)q^2 + \tfrac{1}{2}((-\tfrac{97}{453\,600}L_3 - \tfrac{1}{648\,000}L_1^3 - \tfrac{1}{30\,240}L_1L_2) \\ &+ (-\tfrac{19}{42\,000}L_{-1}L_0L_1 - \tfrac{59}{63\,000}L_0^2 - \tfrac{7}{864\,000}L_{-1}^2L_1^2 - \tfrac{1}{17\,280}L_{-1}^2L_2 + \tfrac{937}{162\,000}L_0 \\ &- \tfrac{311}{28\,350}L_{-1}L_1)\hbar + (\tfrac{101}{3\,456\,000}L_{-1}^4L_1 - \tfrac{187}{756\,000}L_{-1}^3 + \tfrac{31}{24\,000}L_{-1}^3L_0)\hbar^2 \\ &- \tfrac{793}{41\,472\,000}L_{-1}^6\hbar^3)q^3 + O(q^4),\end{aligned} \tag{52}$$

$$\begin{aligned}g(\hbar,q,L) = \tfrac{1}{4}L_{-1} + (&-\tfrac{1}{240}L_{-1}L_1 + \tfrac{1}{320}\hbar L_{-1}^3 - \tfrac{1}{20}L_0)q + ((\tfrac{97}{6300}L_1 + \tfrac{1}{1200}L_0L_1 \\ &+ \tfrac{1}{4032}L_{-1}L_2 + \tfrac{1}{28\,800}L_{-1}L_1^2) + (-\tfrac{1}{2400}L_{-1}^2 - \tfrac{47}{33\,600}L_{-1}^2L_0 - \tfrac{1}{19\,200}L_{-1}^3L_1)\hbar \\ &- \tfrac{1}{460\,800}L_{-1}^5\hbar^2)q^2 + O(q^3).\end{aligned} \tag{53}$$

V. CONCLUSION

In this paper, we presented two conjectures, which could help in the ''experimental'' work with the Givental formula (12), and perturbatively checked them for the simplest example of the manifold $\mathbb{CP}^1$. In spite of the lack of the complete proof for these conjectures, and even clear formulation of the second one, they could be of some use. One way to use them is to present the differential operator corresponding to the manifold M, completely in terms of the Virasoro operators with the constant coefficients $P^M_{[l_1],[l_2],\ldots,[l_N]}$ [we should mention, that this is not equivalent to present $D'_M(s)$ in such form],

$$e^{D'_M(s)}=\left[\exp\sum_{[l_1],[l_2],\ldots[l_N]}^{\infty}P^M_{[l_1],[l_2],\ldots,[l_N]}L_{[l_1]}\otimes L_{[l_2]}\otimes\cdots\otimes L_{[l_N]}\right]\Bigg|_{t=0}. \tag{54}$$

This is equivalent to finding the τ-function of the manifold M on the small phase space, if one additionally knows the genus 1 free energy (the genus zero free energy explicitly enters the coefficients on the rhs). We do not know how to do this nonperturbatively, even for $M=\mathbb{CP}^1$. The other way is to proceed with perturbative calculations of free energies, for example, in the case of $M=\mathbb{CP}^2$, using formula (12) and ideas of this paper.

Another interesting way to go is to study the formula analogous to (12) such that its lhs contains the free energy (with genus 0 and 1 contributions subtracted) on the big phase space.[1] It gives almost τ_M, modulo genus zero and genus one contributions. However, the structure of the rhs is far less transparent in this case.

One also can approach to the Givental formula (12) from another side. Namely, one can take some known τ-function, insert it on the lhs and study the structure of the differential operator on the rhs. The interesting example to deal with is provided by the τ-function for the generalized Kontsevich model.[14]

ACKNOWLEDGMENTS

The author is grateful to A. Mironov for careful reading of the paper and useful discussions, to A. Chervov and V. Poberezhny for discussions, and especially to A. Morozov for initiating this work and careful support during the work. The author also acknowledges the kind hospitality of the Les Houches summer school and ICTP spring school on superstrings and related matters. This work was partly supported by the RFBR Grant No. 00-02-16477, grant for support of young scientists No. 02-02-06504, Russian President's Grant No. 00-15-99296 and Grant No. INTAS-00-334.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Geometric phase and modulus relations for probability amplitudes as functions on complex parameter spaces

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(Received 28 May 2002; accepted 29 July 2003)

We investigate general differential relations connecting the respective behaviors of the phase and modulus of probability amplitudes of the form $\langle \psi_f | \psi \rangle$, where $|\psi_f\rangle$ is a fixed state in Hilbert space and $|\psi\rangle$ is a variable state, treated as a section of a U(1) bundle over a complex subspace of the corresponding ray space $\mathcal{R}=\mathbb{C}P^n$. Amplitude functions on such holomorphic line bundles, while not strictly holomorphic, nevertheless satisfy generalized Cauchy–Riemann conditions involving the U(1) Berry–Simon connection on the parameter space. These conditions entail invertible relations between the gradients of the phase and modulus, therefore allowing for the reconstruction of the phase from the modulus (or vice versa) and other conditions on the behavior of either polar component of the amplitude. As a special case, we consider amplitude functions valued on the space of pure states, the ray space $\mathcal{R}=\mathbb{C}P^n$, where transition probabilities have a geometric interpretation in terms of geodesic distances as measured with the Fubini–Study metric. In conjunction with the generalized Cauchy–Riemann conditions, this geodesic interpretation leads to additional relations, in particular, a novel connection between the modulus of the amplitude and the phase gradient, somewhat reminiscent of the WKB formula. Finally, a connection with geometric phases is established. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1612895]

I. INTRODUCTION

The study of correlations between the behavior of the phase and modulus of complex probability amplitudes is a relevant topic in a number of physical problems such as the ''phase problem'' in diffraction theory,[1] the study of phase singularities[2] and the semiclassical or WKB approximation[3] to name a few. In the phase problem, for instance, the aim is to infer phase information in the diffracted wave from the observed cross section, which only involves the magnitude of the wave. In the study of phase dislocations, it is known that regions of vanishing amplitude are characterized by surrounding regions of generally nonuniform vortex-type phase singularities. Finally, in the semiclassical approximation, the phase gradient is in correspondence with the classical momentum and the behavior of the magnitude of the amplitude is correlated to the phase gradient by Liouville's theorem.

From a different standpoint, significant insight into the geometrical meaning of both the modulus and the phase of probability amplitudes has emerged from the study of the ray space $\mathcal{R}$ (also known as projective Hilbert space), particularly in connection with geometric phases,[4–7] quantum information theory,[8,9] and other topics falling under the general category of geometric quantum mechanics.[10,11] From the work of Berry,[4] Simon,[5] and Aharonov and Anandan[6] amongst others, it is known that under cyclic evolution a geometric phase factor is acquired by the ampli-

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tude, which is interpreted as the holonomy associated with a natural connection (the so-called Berry–Simon connection) on the U(1) bundle over $\mathcal{R}$, and which is proportional to the symplectic area enclosed by the circuit in $\mathcal{R}$. Samuel and Bhandari[7] have also shown that the so-called Pancharatnam phase difference between any two states can be expressed as a line integral of the Berry–Simon connection along the geodesic connecting the two states, as measured with the Fubini–Study metric, the natural metric on $\mathcal{R}$. Finally, there exists a natural geometric interpretation to transition probabilities in the ray space as the cosine of the geodesic distance with respect to the Fubini–Study metric,[10] a measure that is intimately related to information-theoretic measures of statistical distance between two probability distributions.[8,9]

In the present paper, the aim is to shed additional insight into the correlation between the phase and magnitude of transition probability amplitudes from the point of view of geometric quantum mechanics. Specifically, we study amplitudes of the form $\langle \psi_f|\psi\rangle$, where $|\psi_f\rangle$ is any fixed state in Hilbert space and $|\psi\rangle$ is parametrized on a complex parameter subspace $\mathcal{M}$ of the ray space $\mathcal{R}$, or, in particular, the ray space itself. We then obtain general geometric relations between the two polar components of the amplitude arising from holomorphicity and metric constraints natural to such complex parameter spaces. We note that a number of state families of broad physical interest are valued on complex parameter spaces, including the family of coherent and more generally squeezed states, the Bloch sphere of spin-1/2 states, as well as complex extensions of real parameter families.

A brief summary of the main results and the structure of the paper is in order. In Sec. II we spell out in greater detail the geometric setting involved, which is more precisely that of *holomorphic line bundles* over the complex parameter space $\mathcal{M}$. Such bundles share with the more general line bundles over arbitrary parameter spaces (arising, for instance, in connection with Berry phases) two important geometric objects, namely, the Berry–Simon connection $\mathbf{A}=-i\langle\psi|\mathbf{d}\psi\rangle$ and the quantum geometric tensor $\mathbf{H}\propto\langle\mathbf{d}\psi|\otimes|\mathbf{d}\psi\rangle-\langle\psi|\mathbf{d}\psi\rangle\otimes\langle\mathbf{d}\psi|\psi\rangle$. The symmetric part of $\mathbf{H}$ gives rise to a ''quantum'' metric on $\mathcal{M}$ (the Fubini–Study metric when $\mathcal{M}=\mathcal{R}$), while the antisymmetric part, here denoted by Ω, is proportional to the field-strength tensor associated with the connection. There are, however, additional constraints that follow from the fact that $\mathcal{M}$ is a complex submanifold of $\mathcal{R}$. In particular, state sections of the corresponding line bundle satisfy generalized holomorphicity conditions and the base manifold inherits from the ray space its Kähler structure. These constraints are then used in Sec. III to show that the polar components of $\langle\psi_f|\psi\rangle=\sqrt{p}\,e^{i\eta}$ satisfy a generalized version of Cauchy–Riemann conditions on the logarithm of $\langle\psi_f|\psi\rangle$, the relations

$$\nabla\log\sqrt{p}=\mathbf{\Omega}\cdot(\nabla\eta-\mathbf{A}),$$

$$(\nabla\eta-\mathbf{A})=-\mathbf{\Omega}\cdot\nabla\log\sqrt{p},$$

where the inner product is with respect to the quantum metric on $\mathcal{M}$. With the aid of these conditions, it is then possible to reconstruct either polar component of the amplitude from the parametric dependence of the other, as well as to obtain additional constraints on the behavior of p and η. A brief illustration of the the generalized Cauchy–Riemann conditions on the Bloch sphere is given in Sec. IV. In Sec. V we turn to the case when $\mathcal{M}=\mathcal{R}$, where we explore the consequences of previously obtained results in conjunction with an additional geometric relation that exists between the transition probability p and geodesic distances as measured by the Fubini–Study metric. In particular, we give a generalization of the Samuel and Bhandari result for the Pancharatnam phase for nongeodesic paths. More importantly, it is shown that the transition amplitude can be parametrized entirely in terms of its phase according to the formula

$$\langle\psi_f|\psi\rangle=\frac{e^{i\eta}}{\sqrt{1+q\|\nabla\eta-\mathbf{A}\|^2}},\tag{1.1}$$

where q is an arbitrary parameter in the definition of the metric. Prompted by a certain resemblance to the WKB formula $\psi_{\mathrm{WKB}}(x)=e^{i\eta(x)}/\sqrt{|\nabla\eta|}$, a trajectory interpretation to the phase gradient on $\mathcal{R}$ is obtained. Finally, in Sec. VI, we establish a connection between our results and the geometric phase acquired during cyclic and noncyclic evolutions.

II. GEOMETRY OF HOLOMORPHIC LINE BUNDLES

We devote some time to introduce the relevant geometric aspects that are involved. Let the map $\tilde{\psi}:\mathcal{M}\to\mathcal{H}$ define a family of unnormalized state vectors $|\,\tilde{\psi}(z)\,\rangle\in\mathcal{H}$, which only depend on a set of local holomorphic coordinates z^a on $\mathcal{M}$. The family $|\psi\rangle$ is then obtained by projecting $|\tilde{\psi}\rangle$ onto the set of pure normalized state vectors according to

$$|\psi(z,\overline{z})\rangle=\frac{e^{i\gamma(z,\overline{z})}}{\sqrt{\langle\tilde{\psi}(\overline{z})|\tilde{\psi}(z)\rangle}}|\tilde{\psi}(z)\rangle\,, \tag{2.1}$$

where γ is some (real) phase factor that for the moment will be assumed to be an arbitrary function of z and $\overline{z}$.

It will also be convenient to keep in mind alternative parametrizations of $|\psi\rangle$ in terms of the set of real coordinates (x^a,y^a) related to z^a $(\overline{z}^a)$ as usual by $z^a=x^a+iy^a$ $(\overline{z}^a=x^a-iy^a)$, and more generally in terms of arbitrary real coordinates on $\mathcal{M}$ which will be denoted by ξ^μ with the index μ ranging from 1 to $2k$ [throughout the section we use italic indices $a,b,\ldots$ (ranging from 1 to k) to denote complex coordinates or their real and imaginary components and greek indices to denote general coordinates].

Neglecting for the moment the fact that $\mathcal{M}$ is a complex manifold, we see that there is a correspondence between a point in $\mathcal{M}$ and a pure-state density matrix $|\psi\rangle\langle\psi|$, and therefore a point in the ray space $\mathcal{R}$, the equivalence class of states under the equivalence relation $|\psi\rangle\sim e^{i\phi}|\psi\rangle$. The geometric setting is therefore that of the U(1) or line bundle $P(\mathcal{M},\mathrm{U}(1))$ over the parameter space $\mathcal{M}$,[5,12,13] on which a choice of $|\psi\rangle$ with a given phase factor γ corresponds to a particular choice of local section.

Now, as is well known in the context of geometric phases,[14] there is a natural geometric connection that can be defined on the line bundle over a parameter space $\mathcal{M}$, which is expressed locally by the so-called Berry–Simon (BS) connection one-form $\mathbf{A}=A_\mu\mathrm{d}\xi^\mu$, with components

$$A_\mu=-i\langle\psi|\partial_\mu\psi\rangle\,, \tag{2.2}$$

where $\partial_\mu=\partial/\partial\xi^\mu$ in arbitrary coordinates. This connection is naturally induced by the Dirac inner product on Hilbert space $\langle\phi|\psi\rangle$ in the sense that the horizontal motion defined by this connection corresponds to infinitesimal variations orthogonal to $|\psi\rangle$, i.e., $\langle\psi|\,\delta_{\mathrm{Horiz}}\psi\rangle=0$. The resulting covariant derivative of a section $|\psi\rangle$,

$$D_\mu|\psi\rangle\equiv[\partial_\mu-iA_\mu]|\psi\rangle\,, \tag{2.3}$$

therefore satisfies $\langle\psi|D_\mu\psi\rangle=0$. By virtue of Eq. (2.1), it is clear that under a U(1) gauge transformation $|\psi\rangle\to e^{i\delta\gamma}|\psi\rangle$, A_μ transforms as $A_\mu\to A_\mu+\partial_\mu\delta\gamma$, in such a way that $D_\mu|\psi\rangle$ transforms homogeneously as $D_\mu|\psi\rangle\to e^{i\delta\gamma}D_\mu|\psi\rangle$. Furthermore, a U(1) gauge transformation may always be introduced so that the connection form is set to zero at least at one point in $\mathcal{M}$. As usual, the failure of the covariant derivative to commute in different directions is measured by the curl of $\mathbf{A}$.

When $\mathcal{M}$ is a complex manifold as is the case in question, there is added richness brought about by the complex nature of the base space. In particular, it is possible to construct a more refined notion of the line bundle over $\mathcal{M}$, namely a *Holomorphic line bundle*.[12,13,15,16] The notion of such bundles rests on a generalization of the concept of a holomorphic function, in the sense that by a suitable gauge transformation it is possible to have a section satisfy, *at a given point*, the

standard holomorphic condition $(\partial/\partial\overline{z^a})\,|\psi\rangle = 0$. Let us see how this comes about with the parametrization in Eq. (2.1). By construction we have that the un-normalized vector $|\tilde{\psi}\rangle$ satisfies the holomorphic condition,

$$\frac{\partial}{\partial\overline{z^a}}|\,\tilde{\psi}(z)\,\rangle = 0\,, \tag{2.4}$$

with $\overline{z^\alpha} = x^a - iy^a$. It is clear however, that $|\psi\rangle$ is not strictly holomorphic, as the antiholomorphic coordinates $\overline{z^a}$ appear not only in the phase factor γ, but more importantly in the normalization factor which involves the antiholomorphic map $\langle\tilde{\psi}(\overline{z})|$. Thus we have in general that

$$\frac{\partial}{\partial\overline{z^a}}|\,\psi\rangle = \left[\frac{\partial}{\partial\overline{z^a}}\log\frac{e^{i\gamma}}{\sqrt{\langle\tilde{\psi}|\tilde{\psi}\rangle}}\right]|\,\psi\rangle\,. \tag{2.5}$$

Now, taking the inner product of this expression with $|\psi\rangle$ itself, we find that

$$\langle\,\psi|\,\frac{\partial}{\partial\overline{z^a}}|\,\psi\rangle = \left[\frac{\partial}{\partial\overline{z^a}}\log\frac{e^{i\gamma}}{\sqrt{\langle\tilde{\psi}|\tilde{\psi}\rangle}}\right]. \tag{2.6}$$

Expressing the BS one-form in the complex basis as $\mathbf{A} = A_a\mathbf{d}z^a + A_{\overline{a}}\mathbf{d}\overline{z}^a$, with

$$A_a = -i\langle\,\psi|\partial_a\psi\rangle\,,\quad A_{\overline{a}} = -i\langle\,\psi|\partial_{\overline{a}}\psi\rangle \tag{2.7}$$

[where $\partial_a = (\partial/\partial z^a)$, $\partial_{\overline{a}} = (\partial/\partial\overline{z^a})$], and finally splitting the covariant derivative D into holomorphic and antiholomorphic components, we have

$$D_a = \frac{\partial}{\partial z^a} - iA_a\,,\quad D_{\overline{a}} = \frac{\partial}{\partial\overline{z^a}} - iA_{\overline{a}}.$$

Thus, we find from Eqs. (2.5) and (2.6) that the section $|\psi\rangle$ satisfies a generalized ''gauge covariant'' holomorphic condition

$$D_{\overline{a}}|\,\psi\rangle = 0. \tag{2.8}$$

However, it is always possible to ''gauge away'' the BS connection at least at one point. At that point then, the section satisfies the usual holomorphic condition $\partial_{\overline{a}}|\,\psi\rangle = 0$. Thus, modulo a U(1) gauge transformation, $|\psi\rangle$ is a locally holomorphic section. For future reference, we shall also need the dual, now antiholomorphic condition, on the bra $\langle\psi|$. This is given by

$$\langle D_a\psi| = [\,\partial_a + iA_a]\langle\psi| = 0\,. \tag{2.9}$$

We now consider geometric aspects of the base space $\mathcal{M}$ and introduce additional objects that will be of use later. The horizontal motion associated with the BS connection on the line bundle over $\mathcal{M}$ induces naturally on the base space $\mathcal{M}$ a gauge-invariant rank-2 Hermitian tensor

$$H_{\mu\nu} = q\,\langle D_\mu\psi|D_\nu\psi\rangle\,, \tag{2.10}$$

which Berry[17] has named the *quantum geometric tensor*. Here, q is any strictly positive real number to be adjusted for convenience. The real part of $H_{\mu\nu}$ is positive definite and symmetric, and thus defines a metric $g_{\mu\nu}$ on $\mathcal{M}$, the *quantum metric*, with line element

$$\mathrm{d}s^2 = g_{\mu\nu}\,\mathrm{d}\xi^\mu\,\mathrm{d}\xi^\nu = q[\,\langle\mathrm{d}\psi|\mathrm{d}\psi\rangle - \langle\mathrm{d}\psi|\,\psi\rangle\langle\,\psi|\mathrm{d}\psi\rangle\,]\,. \tag{2.11}$$

In turn, the imaginary part of H is antisymmetric and is closely related to the curl of the BS connection one-form $\mathbf{A}$:

$$\mathbf{\Omega} = \mathrm{Im}\, H = \frac{q}{2}\langle \mathbf{d}\psi| \wedge |\mathbf{d}\psi\rangle = \frac{q}{2}\mathbf{dA}\,. \tag{2.12}$$

Since $\mathbf{d}^2 = 0$ it follows that $\mathbf{\Omega}$ is automatically closed.

When $\mathcal{M}$ is the base space for the Hermitian line bundle, considerable simplifications follow. First of all, from the generalized holomorphic condition $|D_{\bar{a}}\psi\rangle = 0$ and its dual, we have that in complex coordinates the quantum geometric tensor takes as components

$$H_{\bar{a}b} = \langle D_{\bar{a}}\psi | D_b \psi\rangle\,, \quad H_{ab} = 0\,. \tag{2.13}$$

This implies that the metric, as well as the two-form $\mathbf{\Omega}$ may be written out as

$$\begin{aligned} \mathbf{g} &= g_{a\bar{b}}\,\mathbf{dz}^a \otimes \mathbf{d\bar{z}}^b + g_{\bar{a}b}\,\mathbf{d\bar{z}}^a \otimes \mathbf{dz}^b\,, \\ \mathbf{\Omega} &= i g_{a\bar{b}}\,\mathbf{dz}^a \wedge \mathbf{d\bar{z}}^b\,, \end{aligned} \tag{2.14}$$

where $g_{a\bar{b}} = g_{\bar{b}a} = \frac{1}{2}H_{a\bar{b}}$. Note that if the metric is nondegenerate (as we shall assume henceforth), it then follows, on the one hand, that the U(1) connection $\mathbf{A}$ is nontrivial, and on the other, that both $\mathbf{g}$ and $\mathbf{\Omega}$ admit inverses. In particular, the inverse metric takes the form

$$\mathbf{g}^{-1} = g^{a\bar{b}}\partial_a \otimes \partial_{\bar{b}} + g^{\bar{a}b}\partial_{\bar{a}} \otimes \partial_b\,, \tag{2.15}$$

where $g^{\bar{a}b} = g^{b\bar{a}}$ satisfies $g_{a\bar{b}}g^{\bar{b}c} = \delta_a^c$.

To understand the significance of Eq. (2.14), we now introduce the so-called complex structure, the defining tensorial object for a complex manifold. In complex coordinates, the complex structure tensor J takes the canonical form

$$J^a{}_b = i\,\delta^a{}_b\,, \quad J^{\bar{a}}{}_{\bar{b}} = -i\,\delta^{\bar{a}}{}_{\bar{b}} \tag{2.16}$$

with the remaining components vanishing. The complex structure satisfies $J^\mu{}_\lambda J^\lambda{}_\nu = -\delta^\mu{}_\nu$ (i.e., $J^2 = -1$) and implements the multiplication by i $(-i)$ on vector fields with holomorphic (antiholomorphic) indices. In terms of J, it is readily verified that the metric satisfies

$$g_{\mu\nu} = J^\gamma{}_\mu J^\lambda{}_\nu g_{\gamma\lambda}\,. \tag{2.17}$$

In this case one says that the metric is *Hermitian*. In turn, the two-form $\mathbf{\Omega}$ is what is known as the *Kähler form* of the metric, defined by

$$\Omega_{\mu\nu} = g_{\lambda\nu}J^\lambda{}_\mu\,, \tag{2.18}$$

i.e., $\Omega_{\mu\nu} = -J_{\mu\nu}$. The expressions for $\mathbf{g}$ and $\mathbf{\Omega}$ in Eq. (2.14), where $g_{ab} = g_{\bar{a}\bar{b}} = \Omega_{ab} = \Omega_{\bar{a}\bar{b}} = 0$, are the canonical forms that a Hermitian metric and its Kähler form take in complex coordinates.

When the Kähler form $\mathbf{\Omega}$ is closed, as in our case, $\mathcal{M}$ is known as a Kähler manifold and the metric a Kähler metric. The offshoot of this is a compatibility between the Hemitian and Riemannian structures of the manifold, embodied by the fact that

$$\mathbf{d}\Omega = 0 \Leftrightarrow \nabla_\mu J^\nu{}_\lambda = 0\,, \tag{2.19}$$

where ∇_μ denotes covariant differentiation of ordinary tensor fields on $\mathcal{M}$ with respect to the affine connection associated with the metric g. The condition $d\mathbf{\Omega} = 0$ entails that the Hermitian components $g_{a\bar{b}}$ of the metric and the Kähler form satisfy in complex coordinates the symmetry conditions

$$\partial_c g_{a\bar{b}} = \partial_a g_{c\bar{b}}, \quad \partial_{\bar{c}} g_{\bar{a}b} = \partial z^{\bar{a}} \partial g_{\bar{c}b}. \tag{2.20}$$

From the definition of the affine connection in arbitrary coordinates, $\Gamma^{\mu}_{\nu\lambda} = \frac{1}{2} g^{\mu\gamma}(\partial_\mu g_{\nu\gamma} + \partial_\nu g_{\mu\gamma} - \partial_\gamma g_{\mu\nu})$, it is then straightforward to verify that in complex coordinates the affine connection takes the form

$$\Gamma^{a}{}_{bc} = g^{\bar{d}a} \partial_b g_{c\bar{d}}, \quad \Gamma^{\bar{a}}{}_{\bar{b}\bar{c}} = g^{\bar{a}d} \partial_{\bar{b}} g_{d\bar{c}}, \tag{2.21}$$

with the symbols mixing holomorphic and antiholomorphic indices vanishing. Covariant differentiation with respect to a holomorphic (antiholomorphic) coordinate therefore acts like regular differentiation on antiholomorphic (holomorphic) indices. Another way of saying this is that the *affine* connection preserves the separation between holomorphic and antiholomorphic tensor fields. We remark that in complex manifolds that are not Kähler, it is still possible to define a Hermitian connection taking the form of Eq. (2.21) and satisfying $\nabla J = 0$, but this connection will not coincide with the affine connection.

A second consequence of the symmetry conditions in Eq. (2.20) is that the Kähler metric may be derived locally from a scalar potential function, the so-called *Kähler potential*, according to $g_{a\bar{b}} = \partial_a \partial_{\bar{b}} K(z,\bar{z})$. This can be seen by noting from Eq. (2.6) that

$$\mathbf{A} = \mathbf{d}\gamma + \frac{1}{2i} \partial_a \log\langle\tilde{\psi}|\tilde{\psi}\rangle \, \mathbf{d}z^a - \frac{1}{2i} \partial_{\bar{a}} \log\langle\tilde{\psi}|\tilde{\psi}\rangle \mathbf{d}\bar{z}^a, \tag{2.22}$$

from which we see that

$$\mathbf{\Omega} = \frac{q}{2} \mathbf{dA} = \frac{iq}{2} \partial_a \partial_{\bar{b}} \log\langle\tilde{\psi}|\tilde{\psi}\rangle \mathbf{d}z^a \wedge \mathbf{d}\bar{z}^b. \tag{2.23}$$

Consequently, from Eq. (2.14), we have that

$$g_{a\bar{b}} = \frac{q}{2} \partial_a \partial_{\bar{b}} \log\langle\tilde{\psi}|\tilde{\psi}\rangle, \tag{2.24}$$

so that an appropriate *Kähler* potential is given by

$$\tilde{K} = (q/2) \log\langle\tilde{\psi}|\tilde{\psi}\rangle. \tag{2.25}$$

Note however that this potential is not uniquely defined, since one is free to add to $K(z,\bar{z})$ any function of the form $f_1(z) + f_2(\bar{z})$ without changing $g_{a\bar{b}}$. Note finally that a choice of gauge in which $\gamma(z,\bar{z}) = \mathrm{Re}[f(z)] = \frac{1}{2}[f(z) + f^*(\bar{z})]$ for some arbitrary holomorphic function $f(z)$, is equivalent to a reparametrization of $|\psi\rangle$ in which in Eq. (2.1), the phase γ is set to zero and the un-normalized vector $|\tilde{\psi}\rangle$ gets replaced by $|\tilde{\psi}'\rangle = e^{f(z)}|\tilde{\psi}\rangle$. In such case, all geometric objects of interest for us, namely, the Berry–Simon connection and the second-rank tensors obtained from the quantum geometric tensor, can be derived from the Kähler potential $\tilde{K}' = (q/2)\log\langle\tilde{\psi}'|\tilde{\psi}'\rangle$.[18] The freedom that remains in the choice of f corresponds to the freedom in the definition of the Kähler potential.

III. GENERALIZED CAUCHY–RIEMANN CONDITIONS

We now explore the consequences on the behavior of the polar components of any transition amplitude

$$\langle\psi_f|\psi(\xi)\rangle = \sqrt{p(\xi)}\, e^{i\eta(\xi)},$$

where $|\psi(\xi)\rangle$ is a section of a holomorphic line bundle over a complex submanifold $\mathcal{M}\in\mathcal{R}$, i.e., of the form of Eq. (2.1), as described in the preceding section, and ξ are arbitrary real coordinates on $\mathcal{M}$.

The first thing to note is that due to the arbitrariness in the definition of the phase γ in Eq. (2.5), the notion of phase $\langle\psi_f|\psi\rangle$ is tied to the choice of gauge. Specifically, the phase $\eta\equiv\arg\langle\psi_f|\psi\rangle$, transforms under the U(1) gauge transformations $|\psi\rangle\rightarrow e^{i\delta\gamma}|\psi\rangle$ as

$$\eta\rightarrow\eta+\delta\gamma.$$

It then becomes convenient to introduce a gauge-invariant notion of phase variation by means of the *BS*-connection This is done by defining a *gauge invariant phase gradient*

$$V_\mu\equiv\partial_\mu\eta-A_\mu\,. \tag{3.1}$$

Clearly, the one-form $\mathbf{V}=V_\mu\mathbf{d}\xi^\mu$ is not closed but rather satisfies $\mathbf{dV}=-\mathbf{dA}=-(2/q)\mathbf{\Omega}$. The modulus of $\langle\psi_f|\psi\rangle$, $\sqrt{p}\equiv|\langle\psi_f|\psi\rangle|$, is of course gauge invariant.

Now, since $|\psi_f\rangle$ is assumed to be a constant vector, it follows from Eq. (2.8) that the amplitude $\langle\psi_f|\psi\rangle$ is as well subject to the generalized holomorphic (antiholomorphic) conditions when expressed in local complex coordinates

$$\left[\frac{\partial}{\partial\bar{z}^a}-iA_{\bar{a}}\right]\langle\psi_f|\psi\rangle=0\,, \tag{3.2}$$

$$\left[\frac{\partial}{\partial z^a}+iA_a\right]\langle\psi|\psi_f\rangle=0\,. \tag{3.3}$$

Assuming then that $\langle\psi_f|\psi\rangle\neq0$, the logarithm of the amplitude can be defined analytically, and we find that

$$\begin{aligned} i[\partial_{\bar{a}}\eta-A_{\bar{a}}]+\partial_{\bar{a}}\log\sqrt{p}=0,\\ -i[\partial_a\eta-A_a]+\partial_a\log\sqrt{p}=0\,. \end{aligned} \tag{3.4}$$

As mentioned earlier, by a suitable choice of gauge it is possible to have the section $|\psi\rangle$ satsify ordinary Cauchy–Riemann conditions at a specified point. Correspondingly, the above conditions can be brought locally to the form of ordinary Cauchy–Riemann conditions.

For our purposes, it will be more convenient to cast the above expression in terms of the Kähler form $\mathbf{\Omega}$ which has a more immediate interpretation in terms of the Berry–Simon connection $\mathbf{A}$ (recall that $\mathbf{\Omega}=(q/2)\mathbf{dA}$). Using the facts that $J^\nu{}_\mu V_\nu=J_{\nu\mu}V^\nu=\Omega_{\mu\nu}V^\nu=\Omega_\mu{}^\nu V_\nu$ and that in mixed-rank form $J^2=\Omega^2=-1$, we then have the following alternative expressions:

$$\partial_\mu\log\sqrt{p}=\Omega_\mu{}^\nu[\,\partial_\nu\eta-A_\nu]\,, \tag{3.5a}$$

$$\partial_\mu\eta=A_\mu-\Omega_\mu{}^\nu\partial_\nu\log\sqrt{p}\,. \tag{3.5b}$$

We shall refer to these as the *generalized Cauchy Riemann conditions* satisfied by the polar components of the amplitude $\langle\psi_f|\psi\rangle$. These conditions constitute the first important result of the paper, and will serve as a starting point for a number of additional relations that will be derived in the forthcoming.

The most important consequence of Eq. (3.5) is the existence of the reconstruction formulas on $\mathcal{M}$,

$$\eta(\xi)-\eta(\xi_0)=\int_{\xi_0}^{\xi}\mathrm{d}\xi^\mu[A_\mu-\Omega_\mu{}^\nu\partial_\nu\log\sqrt{p}\,] \tag{3.6}$$

and

$$\sqrt{\frac{p(\xi)}{p(\xi_0)}}=\exp\left[\int_{\xi_0}^{\xi} d\xi^{\mu}\,\Omega_{\mu}{}^{\nu}[\,\partial_{\nu}\eta-A_{\nu}]\right], \tag{3.7}$$

by means of which one polar component of the amplitude $\langle\psi_f|\psi\rangle$ can be obtained from the other by line integration once the connection is specified. Since both formulas arise from exact differentials, the choice of integration path can be left arbitrary as long as any two paths may be deformed continuously into one another within a simply connected region excluding singularities. However, since the individual terms in the integrands are not generally exact, all terms must be evaluated along the same path. This path independence must reflect itself, therefore, in ancillary relations that both p and η have to satisfy in order to guarantee that the left-hand sides of Eqs. (3.5a) and (3.5b) are exact differentials, conditions that will be examined in more detail shortly.

Before doing so, we use the fact that the quantum metric in Eq. (2.11) on $\mathcal{M}$ is a Hermitian metric to establish relations on the magnitude and angle between the gauge invariant gradients $\nabla\eta-\mathbf{A}$ and $\nabla\log\sqrt{p}$ on $\mathcal{M}$. The Hermitian condition on the metric is that the complex structure should preserve the inner product, i.e., $\mathbf{X}\cdot\mathbf{Y}=(J\mathbf{X})\cdot(J\mathbf{Y})$. This implies from the generalized Cauchy–Riemann conditions that the gauge invariant gradients have the same magnitude as defined in terms of the quantum metric,

$$|\nabla\log\sqrt{p}\,|=|\nabla\eta-\mathbf{A}|\,. \tag{3.8}$$

A second property of a Hermitian metric is that $\mathbf{X}\cdot\mathbf{J}\mathbf{X}=0$, a property that in a Kähler manifold follows automatically from the antisymmetry of the Kähler form $\mathbf{\Omega}$. It follows therefore from Eq. (3.5) that

$$\nabla p\cdot(\nabla\eta-\mathbf{A})=0\,. \tag{3.9}$$

A particular consequence is therefore that lines of constant phase and constant transition probability necessarily meet at right angles wherever $\mathbf{A}$ is made to to vanish by a choice of gauge.

Next, we turn to the previously mentioned integrability conditions. The most evident one comes from rearranging Eq. (3.5b) to read $\Omega_{\mu}{}^{\nu}\partial_{\nu}\log\sqrt{p}=A_{\mu}-\partial_{\mu}\eta$, in which case we see that the one-form $\mathbf{\Omega}\cdot\mathbf{d}\log\sqrt{p}$ is equivalent to the BS connection up to the gauge term $\mathbf{d}\eta$. Correspondingly, the curl of $\Omega_{\mu}{}^{\nu}\partial_{\nu}\log\sqrt{p}$ must lead to the same curl of A_{μ}, which, up to a constant, is nothing more than the Kähler form. Using the fact that the Kähler form is covariantly constant, we then have

$$\Omega_{\nu}{}^{\gamma}\nabla_{\mu}\nabla_{\gamma}\log\sqrt{p}-\Omega_{\mu}{}^{\gamma}\nabla_{\nu}\nabla_{\gamma}\log\sqrt{p}=\frac{2}{q}\Omega_{\mu\nu}\,.$$

Multiplying on both sides by the Kähler form and using $\Omega^2=-1$, the equation can then be transformed to

$$[\nabla_{\mu}\nabla_{\nu}+\Omega_{\mu}{}^{\alpha}\Omega_{\nu}{}^{\beta}\nabla_{\alpha}\nabla_{\beta}]\log\sqrt{p}=-\frac{2}{q}g_{\mu\nu}\,. \tag{3.10}$$

The interpretation of this equation becomes more straightforward in complex coordinates, in which case it reads

$$q\nabla_{a}\nabla_{\bar{b}}\log\sqrt{p}=-g_{a\bar{b}}\,. \tag{3.11}$$

Since $\nabla_{a}\nabla_{\bar{b}}\log\sqrt{p}=\partial_{a}\partial_{\bar{b}}\log\sqrt{p}$, we further see that the condition *is that* $-q\log\sqrt{p}$ *is a Kähler potential for the quantum metric on* $\mathcal{M}$. This can be seen more clearly by noting from Eq. (2.1) that

$$q \log \sqrt{p} = \frac{q}{2} \log[\langle \psi_f | \psi \rangle \langle \psi | \psi_f \rangle] = -\frac{q}{2} \log \langle \tilde{\psi} | \tilde{\psi} \rangle + q \log \langle \psi_f | \tilde{\psi} \rangle + q \log \langle \tilde{\psi} | \psi_f \rangle .$$

Apart from the purely holomorphic and antiholomorphic functions $\log\langle\psi_f|\tilde{\psi}\rangle$ and $\log\langle\tilde{\psi}|\psi_f\rangle$, respectively, this is nothing more than minus the Kähler potential $\tilde{K} = (q/2) \log\langle\tilde{\psi}|\tilde{\psi}\rangle$ mentioned in Sec. II.

Concerning the second integrability condition, we can use the fact that $\partial_\mu \log \sqrt{p}$ is a gradient to obtain from (3.5a) that

$$[\nabla_\mu \delta^\beta_\nu + \Omega_\mu{}^\alpha \Omega_\nu{}^\beta \nabla_\alpha](\nabla_\beta \eta - A_\beta) = 0 , \tag{3.12}$$

a condition that in complex coordinates takes the form

$$\nabla_a(\nabla_{\bar{b}} \eta - A_{\bar{b}}) + \nabla_{\bar{b}}(\nabla_a \eta - A_a) = 0 . \tag{3.13}$$

Further insight into this condition is obtained from Eq. (2.22) in which case we see that $\nabla_a A_{\bar{b}} + \nabla_{\bar{b}} A_a$ is nothing more than $2\partial_a \partial_{\bar{b}} \gamma$. Therefore, under the restricted choice of $\gamma = \frac{1}{2}[f(z) + \overline{f(z)}]$ mentioned previously as the condition in which all geometric quantities can be derived from the Kähler potential, we have that $\partial_a \partial_{\bar{b}} \gamma = 0$ and therefore that

$$\nabla_a \nabla_{\bar{b}} \eta = 0 .$$

In other words, the second condition expresses the fact that modulo a gauge term mixing holomorphic and antiholomorphic coordinates, the phase η is a linear combination of a purely holomorphic and a purely antiholomorphic function. This can be seen most clearly by noting from Eq. (2.1) that

$$\eta = \gamma + \frac{1}{2i} \log\langle \psi_f | \tilde{\psi} \rangle - \frac{1}{2i} \log\langle \tilde{\psi} | \psi_f \rangle .$$

We see therefore that the integrability conditions, Eqs. (3.10) and (3.12), ensuring the consistency of the generalized Cauchy–Riemann conditions in Eq. (3.5) are rather trivial consequences of the parametrization of state sections on a holomorphic line bundle. Still, they lead to nontrivial constraints on the behavior of the phase and modulus of the amplitude when the parameter space is viewed as a general Riemannian manifold.

In particular, by contracting indices in Eqs. (3.10) and (3.12) we determine that the phase and modulus of $\langle \psi_f | \psi \rangle$ satisfy locally the scalar conditions

$$\nabla \cdot (\nabla \eta - \mathbf{A}) = 0, \tag{3.14a}$$

$$\nabla^2 \log \sqrt{p} = -\frac{2k}{q}, \tag{3.14b}$$

where k is the complex dimension of $\mathcal{M}$ and $\nabla\cdot$ and ∇^2 are the divergence and Laplacian operators on $\mathcal{M}$ associated with the quantum metric. Note that since it is always possible to choose $\nabla \cdot \mathbf{A} = 0$ (for instance, with the restricted choice of gauge mentioned previously), the first condition can always be brought to the form $\nabla^2 \eta = 0$.

Finally, it is interesting to note that from the scalar conditions [Eq. (3.14)] and Eqs. (3.8) and (3.9), one obtains

$$\nabla \cdot [p\,(\nabla \eta - \mathbf{A})] = 0, \tag{3.15}$$

$$\frac{1}{2} |\nabla \eta - \mathbf{A}|^2 - \frac{1}{2} \frac{\nabla^2 \sqrt{p}}{\sqrt{p}} = \frac{k}{q}, \tag{3.16}$$

a set of equations analogous to the generalized Hamilton–Jacobi equation and the probability conservation equation arising from the time-independent Schrödinger equation a free particle in a magnetic field. That the probability amplitude $\langle \psi_f | \psi \rangle$ therefore satisfies on $\mathcal{M}$ the corresponding Schödinger equation

$$-\frac{1}{2}(\nabla - i\mathbf{A}) \cdot (\nabla - i\mathbf{A}) \langle \psi_f | \psi \rangle = \frac{k}{q} \langle \psi_f | \psi \rangle$$

can be verified by noting that in complex coordinates $g^{a\bar{b}} D_a D_{\bar{b}} \langle \psi_f | \psi \rangle = 0$ and using the commutation relation

$$[D_a, D_{\bar{b}}] = -\frac{2i}{q} \Omega_{a\bar{b}} = \frac{2}{q} g_{a\bar{b}}.$$

The analogy between $(\nabla \eta - \mathbf{A})$ and a velocity field suggests that it may be possible to establish a trajectory interpretation for the invariant phase gradient. We shall see in Sec. V that such an interpretation is indeed possible on the ray space.

IV. PHASE/MODULUS RELATIONS ON THE BLOCH SPHERE

Let us for the moment flesh out the preceding results with a simple concrete illustration. Consider the family of spin-1/2 states $|\hat{n}\rangle$ represented by points on the Bloch sphere labeled by the usual polar angles θ, ϕ,

$$|\hat{n}\rangle = \begin{pmatrix} \cos\dfrac{\theta}{2} \\ \sin\dfrac{\theta}{2} e^{i\phi} \end{pmatrix}, \tag{4.1}$$

where the basis used is the standard $|\pm\rangle$ eigenbasis of σ_3. As is well known, the two-sphere is in fact a complex manifold, namely the complex projective space $\mathbb{C}P^1$. To see this, note that the parametrization of the unnormalized state $|\tilde{\psi}\rangle$,

$$|\tilde{\psi}(z)\rangle = \begin{pmatrix} 1 \\ z \end{pmatrix}, \tag{4.2}$$

maps, according to Eq. (2.1), to the quantum state section [Eq. (4.1)] after the identification

$$z = \tan\frac{\theta}{2} e^{i\phi}, \quad \gamma = 0. \tag{4.3}$$

The map corresponds to a stereographic projection of the sphere to the complex plane, mapping the south pole into $z = \infty$.

We proceed by calculating the geometric objects of interest. From the Kähler potential, $\tilde{K} = (q/2) \log\langle\tilde{\psi}|\tilde{\psi}\rangle = (q/2) \log(1 + z\bar{z})$, it is straightforward to compute the metric element, i.e.,

$$\mathrm{ds}^2 = q \frac{\mathrm{dz}\, \mathrm{d}\bar{z}}{(1+|z|^2)^2} = \frac{q}{4}[\mathrm{d}\theta^2 + \sin^2\theta\, \mathrm{d}\phi^2]. \tag{4.4}$$

Choosing $q = 4$ for this example, the quantum metric reduces to the usual metric on the unit sphere, with nonvanishing components

$$g_{\theta\theta} = 1, \quad g_{\phi\phi} = \sin^2\theta.$$

The BS connection form is more straightforward to calculate from Eq. (4.1) and we find that

$$\mathbf{A}=\sin^2\frac{\theta}{2}\,\mathbf{d}\phi=\frac{1}{2}(1-\cos\theta)\,\mathbf{d}\phi\,. \tag{4.5}$$

The BS connection leads therefore to the Kähler form

$$\mathbf{\Omega}=\frac{q}{2}\,\mathbf{dA}=\sin\theta\,\mathbf{d}\theta\wedge\mathbf{d}\phi\,, \tag{4.6}$$

which is immediately recognized as the volume form for the unit two-sphere.

With this, it is then possible to express the generalized Cauchy–Riemann conditions for the polar components of some amplitude $\langle\psi_f|\hat{n}\rangle$ in a more conventional form by embedding them in three-dimensional space. Letting $\hat{n}$ now stand for $\vec{r}/r$ and using standard vector notation, the connection becomes

$$\vec{A}=\frac{1}{2r}\left[\frac{1-\cos\theta}{\sin\theta}\right]\hat{\phi}\,, \tag{4.7}$$

which is the usual ''Dirac string'' vector potential for a magnetic charge 1/2 located at the origin and with the string singularity along the south pole. Equations (3.5a) and (3.5b) now read

$$\vec{\nabla}\log\sqrt{p}=-\hat{n}\times(\vec{\nabla}\eta-\vec{A}),$$

$$\vec{\nabla}\eta=\vec{A}+\hat{n}\times\vec{\nabla}\log\sqrt{p}\,, \tag{4.8}$$

where p and η are assumed to depend only on the polar angles. We verify this in a simple example. Take

$$\langle-|\hat{n}\rangle=\sin\frac{\theta}{2}e^{i\phi}\,, \tag{4.9}$$

where from we see that $\sqrt{p}=\sin(\theta/2)$ and $\eta=\phi$ so that

$$\vec{\nabla}\log\sqrt{p}=\frac{1}{2r}\cot\frac{\theta}{2},\hat{\theta}$$

and $\vec{\nabla}\eta=(1/r\sin\theta)\hat{\phi}$. The gauge invariant phase gradient is therefore

$$\vec{\nabla}\eta-\vec{A}=\frac{1}{2r\sin\theta}\left[1-\frac{1}{2}(1-\cos\theta)\right]\hat{\phi}=\frac{1}{2r}\cot\frac{\theta}{2}\,\hat{\phi}$$

and thus we verify that $\vec{\nabla}\log\sqrt{p}=-\hat{n}\times(\vec{\nabla}\eta-\vec{A})$.

More generally, we obtain a coordinate-independent geometric interpretation of the phase gradient for a transition amplitude $\langle\hat{m}|\hat{n}\rangle$ for fixed $|\hat{m}\rangle$ not necessarily on the same section as $|\hat{n}\rangle$. Since the transition probability is

$$p=|\langle\hat{m}|\hat{n}\rangle|^2=\tfrac{1}{2}(1+\hat{n}\cdot\hat{m})\,, \tag{4.10}$$

using $\vec{\nabla}(\hat{n}\cdot\hat{m})=(\hat{m}-(\hat{m}\cdot\hat{n})\hat{n})/r$ we obtain

$$\hat{n}\times\vec{\nabla}\log\sqrt{p}=\left(\frac{1}{2r}\right)\frac{\hat{n}\times\hat{m}}{1+\hat{n}\cdot\hat{m}}\,. \tag{4.11}$$

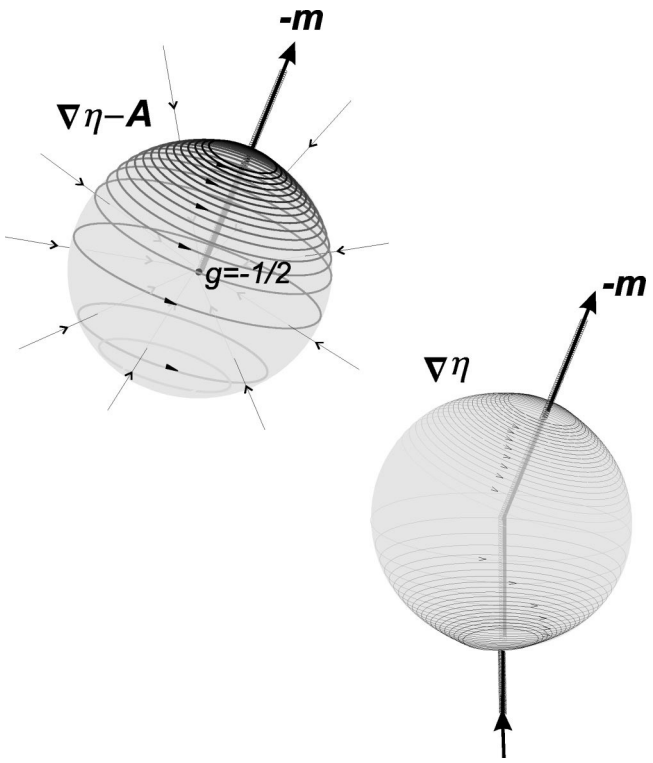

FIG. 1. Interpretation of the gauge invariant phase gradient as the vector potential on the unit sphere for a magnetic charge $-1/2$, and the phase gradient as the vector potential on the sphere for a trapped flux line of flux 2π.

But noting that the vector potential may also be expressed as $\vec{A}=(1/2r)\,[\hat{z}\times\hat{n}/(1+\hat{n}\cdot\hat{z})]$, we see by comparison that $\hat{n}\times\vec{\nabla}\log\sqrt{p}$, and hence the invariant phase gradient $\vec{\nabla}\eta-\vec{A}$, is the vector potential in a *fixed* gauge [specified by Eq. (4.11)] for a magnetic monopole of charge $-1/2$ centered at the origin with the string singularity running along the $-\hat{m}$ axis. Thus, the phase gradient $\vec{\nabla}\eta$ is nothing more than the sum of two vector potentials for two magnetic charges of opposite sign at the origin, with the respective Dirac flux strings running along the directions $-\hat{z}$ and $-\hat{m}$. Equivalently, we can say that the phase gradient $\vec{\nabla}\eta$ is the local vector potential at the exterior of single trapped-flux-line running along $-\hat{z}$ axis into the origin and exiting along the $-\hat{m}$ axis (Fig. 1), with the flux enclosed being $1/2\times 4\pi=2\pi$.

Some global properties of the phase dependence now become evident. First, the invariant phase gradient has only one vortex-like singularity at $\hat{n}=-\hat{m}$, where the amplitude $\langle\hat{m}|\hat{n}\rangle$ vanishes, with a circulation $\oint(\vec{\nabla}\eta-\vec{A})\cdot d\vec{l}=2\pi$. On the other hand, the actual phase gradient has, generically, two such singularities with circulation $\oint\vec{\nabla}\eta\cdot\mathrm{d}\vec{l}=\pm 2\pi$ at the two points on the unit sphere where the flux line crosses. One of these points is fixed to be $\hat{n}=-\hat{m}$ corresponding to the actual singularity at $\langle\hat{m}|\hat{n}\rangle=0$; the other point reflects the string singularity in the connection and is therefore dependent on the choice of section $|\hat{n}\rangle$. Note that while additional singularities may be created by means of singular gauge transformations, the string singularity associated with the connection cannot be removed. The exception is when the string singularity happens to be precisely at $\hat{n}=-\hat{m}$, in which case both singular points disappear and the phase is essentially a constant up to nonsingular gauge transformations.

V. ADDITIONAL PHASE/MODULUS RELATIONS ON THE RAY SPACE

So far, we have considered phase/modulus relations for transition amplitudes of the form $\langle\psi_f|\psi\rangle$ where $|\psi\rangle$ is a section of the holomorphic bundle over an arbitrary complex pure quantum

state manifold. Any such space is itself a complex submanifold of the so-called ray space $\mathcal{R}$, the entire space of pure quantum states modulo a phase transformation. If $n+1$ is the dimensionality of the Hilbert space of the quantum system, then the ray space is the complex projective space $\mathbb{C}P^{n-1}$. A state section $|\psi\rangle$ over $\mathcal{R}$ is therefore a section over a holomorphic line bundle as well, and hence the results of the preceding section hold without change. However, on the ray space, it is possible to establish an additional geometric relation between the transition probability $p=|\langle\psi_f|\psi\rangle|^2$ and geodesic distances on $\mathcal{R}$ as measured with the quantum metric. By virtue of the generalized Cauchy–Riemann conditions (3.5), this new relation has far-reaching consequences, as we now show.

On the ray space, the quantum metric $ds^2=q[\,\langle d\psi|d\psi\rangle-\langle d\psi|\psi\rangle\langle\psi|d\psi\rangle\,]$ is known as the *Fubini–Study* metric, and is the most natural Riemannian metric on the ray space as it the only one invariant under unitary transformations. Geometrically, the metric arises quite naturally by defining for two arbitrary rays in Hilbert space $[\,|\phi\rangle\,]$ and $[\,|\psi\rangle\,]$ (represented by the normalized states $|\phi\rangle$ and $|\psi\rangle$), the distance function[10]

$$s(\phi,\psi)=\sqrt{q}\cos^{-1}|\langle\psi|\phi\rangle|\,. \tag{5.1}$$

The Fubini–Study metric is then obtained by choosing $|\phi\rangle$ and $|\psi\rangle$ on the same section and taking the limit when $|\phi\rangle$ goes to $|\psi\rangle$, in which case

$$|\phi\rangle\simeq|\psi\rangle+|d\psi\rangle+\tfrac{1}{2}|d^2\psi\rangle\,,$$

thus yielding the infinitesimal distance function $ds(\phi,\psi)=\sqrt{q}\sqrt{\langle d\psi|d\psi\rangle-\langle d\psi|\psi\rangle\langle\psi|d\psi\rangle}$.

From the above considerations it holds, therefore, that the modulus of the amplitude $\langle\psi_f|\psi(\xi)\rangle$ can be expressed as a function of the Fubini–Study geodesic distance $s(\xi)$ between the rays $[\,|\psi\rangle\,]$ and the fixed state $[\,|\psi_f\rangle\,]$, according to

$$\sqrt{p(\xi)}=\cos\left(\frac{s(\xi)}{\sqrt{q}}\right). \tag{5.2}$$

From this, we deduce that the gradient of $\log\sqrt{p}$ is given by

$$\nabla\log\sqrt{p}=-\frac{1}{\sqrt{q}}\tan\left(\frac{s}{\sqrt{q}}\right)\nabla s\,.$$

Now, since the modulus of the gradient measures the rate of change with respect to the metric length, it is clear that

$$|\nabla s|^2=1\,. \tag{5.3}$$

Translated in terms of $\sqrt{p}$, we then have that

$$q|\nabla\log\sqrt{p}\,|^2=\tan^2\left(\frac{s}{\sqrt{q}}\right)=\frac{1}{p}-1\,. \tag{5.4}$$

A brief comment on the statistical interpretation of this expression is in order. On the ray space, we may define for any observable $\hat{A}$, the corresponding expectation value function $A(\xi)=\langle\psi|\hat{A}|\psi\rangle$. It is then possible to show (see, e.g., Ref. 11) that the uncertainty $\langle\Delta A^2\rangle=\langle\psi|\hat{A}^2|\psi\rangle-A(\xi)^2$ is related to the gradient of $A(\xi)$ by

$$\frac{4}{q}\langle\Delta A^2\rangle=g^{\mu\nu}(\nabla_\mu A)(\nabla_\nu A)=|\nabla A|^2\,,$$

where $g^{\mu\nu}$ is the inverse to the Fubini–Study metric. Taking $\hat{A}$ to be the projection operator $\hat{\Pi} = |\psi_f\rangle\langle\psi_f|$, we obtain $\langle\Pi\rangle = p$ and $\langle\Delta\Pi^2\rangle = p(1-p)$. Thus,

$$|\nabla p\,|^2 = \frac{4}{q}\langle\Delta\Pi^2\rangle = \frac{4}{q}p(1-p)\,, \tag{5.5}$$

which can be seen to follow directly from Eq. (5.4). Therefore, the connection between the transition probability and the Fubini–Study metric is such that the variation of p with respect to the geodesic distance is, up to a proportionality constant, the variance in the frequency with which $|\psi_f\rangle$ is obtained given $|\psi\rangle$.[8]

Let us then proceed to explore a number of consequences that follow from this connection in conjunction with previously obtained results stemming from the generalized Cauchy–Riemann conditions in Eq. (3.5). Thus far we have seen that from the phase of $\langle\psi_f|\psi\rangle$ it is possible to recover the functional dependence of its modulus by means of line integration. It is now easy to show that in the ray space, the modulus of the amplitude can also be obtained by *differentiation* of the phase. For this we note, as shown earlier, that from the generalized Cauchy–Riemann conditions and the definition of the quantum metric it follows that $|\nabla \log\sqrt{p}|^2 = |\nabla\eta - \mathbf{A}|^2$. Using Eq. (5.4) we see therefore that

$$|\nabla\eta - \mathbf{A}|^2 = 1/p - 1\,,$$

and hence that the transition probability can also be expressed as

$$p = \frac{1}{1+q\,|\nabla\eta - \mathbf{A}|^2}\,. \tag{5.6}$$

With this, the following expression for the amplitude emerges:

$$\langle\psi_f|\psi\rangle = \frac{e^{i\eta}}{\sqrt{1+q\,|\nabla\eta - \mathbf{A}|^2}}\,, \tag{5.7}$$

signifying that, in a sense, all the information in the amplitude $\langle\psi_f|\psi\rangle$ is already contained in its phase factor.

It is also interesting to note that if the invariant phase gradient is treated as some velocity field as in semiclassical physics, then Eq. (5.7) for the amplitude bears a slight resemblance to the WKB formula $\psi(x) \propto e^{i\eta}/\sqrt{|\eta'|}$ in one dimension (note however the different powers of η' in the radical). The resemblance is sufficiently intriguing to motivate an interpretation of the invariant phase gradient as a sort of velocity field of certain trajectories on the ray space. This can be done as follows. From the generalized Cauchy–Riemann condition, Eq. (3.5), we have that

$$\nabla_\mu \log\sqrt{p} = \Omega_{\mu\nu}V^\nu\,. \tag{5.8}$$

Using Eq. (5.6), we substitute $p = (1+qV_\lambda V^\lambda)^{-1}$ to obtain

$$-\frac{q}{2}\frac{\nabla_\mu(V_\nu V^\nu)}{1+qV_\lambda V^\lambda} = \Omega_{\mu\nu}V^\nu. \tag{5.9}$$

We now use the fact that

$$\frac{1}{2}\nabla_\mu(V_\nu V^\nu) = V^\nu\nabla_\mu V_\nu = V^\nu\nabla_\nu V_\mu + V^\nu(\nabla_\mu V_\nu - \nabla_\nu V_\mu) = V^\nu\nabla_\nu V_\mu - \frac{2}{q}V^\nu\Omega_{\mu\nu}\,, \tag{5.10}$$

where we have used the fact that $\mathbf{dV} = \mathbf{d}(\mathbf{d}\eta - \mathbf{A}) = -\mathbf{dA} = -(2/q)\boldsymbol{\Omega}$. Hence we have that

$$\nabla_{\mathbf{V}} V^{\mu} = \frac{1}{q}(1 - q|\mathbf{V}|^2)\, \Omega^{\mu}{}_{\nu} V^{\nu}, \tag{5.11}$$

where $\nabla_{\mathbf{V}} = V^{\nu}\nabla_{\nu}$ is the covariant derivative along the vector field V^{μ}. Now note that because of the antisymmetry of $\mathbf{\Omega}$, the magnitude of $\mathbf{V}$ is preserved along its integral lines, i.e., $\nabla_{\mathbf{V}}|\mathbf{V}|^2 = 0$, in consistency with the the fact that the transition probability is constant in the direction of $\mathbf{V}$. Parametrizing the integral curves of $\mathbf{V}$ in terms of the geodesic distance along the curve as $V^{\mu} = |\mathbf{V}|\,(d\xi^{\mu}/ds)$, we obtain the equation

$$\frac{\mathrm{d}^2\xi^{\mu}}{\mathrm{d}s^2} + \Gamma^{\mu}_{\nu\lambda}\frac{\mathrm{d}\xi^{\nu}}{\mathrm{d}s}\frac{\mathrm{d}\xi^{\lambda}}{\mathrm{d}s} = e_{|\mathbf{V}|}F^{\mu}{}_{\nu}\frac{\mathrm{d}\xi^{\mu}}{\mathrm{d}s}, \tag{5.12}$$

where $e_{|\mathbf{V}|}$ is a specific constant to each curve given by

$$e_{|\mathbf{V}|} = \frac{1 - q|\mathbf{V}|^2}{2|\mathbf{V}|},$$

and $F^{\mu}{}_{\nu}$ is the field strength associated with the Berry–Simon connection ($\mathbf{F} = \mathbf{dA}$). From this we see that integral curves of the invariant phase gradient vector field V^{μ} are in correspondence with trajectories on the ray space of charged particles subject to the magnetic field associated with the Berry–Simon connection. The significance of these trajectories will not be explored in the present paper. Still, these results in conjunction with Eq. (5.7) suggest a procedure by which the whole transition amplitude may be obtained from the solution to a corresponding mechanical problem on the ray space.

To conclude this section, it is worth noting a simplification on the ray space of the scalar integrability condition, Eq. (3.14b), that follows from Eq. (5.4), namely,

$$\nabla^2 p = -\frac{4(k+1)}{q}\left[p - \frac{1}{k+1}\right]. \tag{5.13}$$

Since the ray space is compact, $\int_{\mathcal{R}} \mathrm{d}\mu\, \nabla^2 p = 0$, and therefore a volume integration over the entire space of this equation entails that

$$\langle p \rangle_{\mathcal{R}} = \frac{\int_{\mathcal{R}} \mathrm{d}\mu\, p}{\int_{\mathcal{R}} \mathrm{d}\mu} = \frac{1}{k+1},$$

in consistency with the fact that the average of $|\psi\rangle\langle\psi|$ over the entire ray space should be the completely mixed density matrix of a $k+1$ dimensional Hilbert space. Equation (5.13) then tells us that the deviation of the transition probability from its average value on the ray space is an eigenfunction of the Laplacian operator with eigenvalue $-(4/q)(k+1)$. This is easily verified for the Bloch sphere ($k=1$ and choosing $q=4$), in which case $p - \frac{1}{2} = \frac{1}{2}\hat{n}\cdot\hat{m}$ is made up of spherical harmonics of order $l=1$.

VI. GEOMETRIC PHASES

To conclude, we connect the present results with known results on geometric phases. As a first application we make a connection with a result of Samuel and Bhandari on the Pancharatnam phase. Pancharatnam[19] suggested that an operational definition of what it meant for two quantum states to be ''in'' or ''out of'' phase was naturally provided by the inner product between the two states. The phase $\eta = \arg\langle\psi_f|\psi\rangle$ is therefore also called the *Pancharatnam phase difference*. Samuel and Bhandari[7] have shown that this phase has an intrinsic geometric meaning as it can be obtained from the Berry–Simon connection using the geodesic rule, i.e.,

$$\eta = \int \mathrm{d}\xi'^{\mu} A_{\mu}, \tag{6.1}$$

where the integral is evaluated along the geodesic connecting the ray $[|\psi_f\rangle]$ with $[|\psi\rangle]$ and where it is assumed that $|\psi_f\rangle$ is an element of the same state section as $|\psi\rangle$. With the aid of the Cauchy–Riemann and the relationship between p and the geodesic distance, it is now seen that for an arbitrary integration path between the two rays Eq. (6.1) generalizes to

$$\eta = \eta_o + \int \mathrm{d}\xi^{\mu} A_{\mu} + \frac{1}{\sqrt{q}} \int \mathrm{d}\xi^{\mu} \Omega_{\mu}{}^{\nu} \partial_{\nu} s \tan \frac{s}{\sqrt{q}}, \tag{6.2}$$

where s denotes the geodesic distance from the initial ray to point of integration. If the path of integration is chosen along the geodesic, then from the antisymmetry of the Kähler form, the differential $\mathrm{d}\xi^{\mu} \Omega_{\mu}^{\nu} \partial_{\nu} s$ vanishes and equation is obtained up to the phase relating $|\psi_f\rangle$ with the element of the section $|\psi\rangle$ at $[\,|\psi_f\rangle\,]$.

Next, we turn to geometric phases under time evolution. As is well known, in the course of time evolution the amplitude between the instantaneous state of a system $|\psi;t\rangle$, and the initial state $|\psi;0\rangle$ acquires a total phase that can be decomposed into dynamical and geometric parts. It has been shown by Aharonov and Anandan[6] that when the system undergoes a cyclic evolution so that the state returns to the initial ray, the geometric contribution to the phase difference acquired is given by $-\oint \mathbf{A}$. The result generalizes a previous result by Berry,[4] in which the same geometric phase difference is acquired in the course of adiabatic evolution if the initial state is initially an eigenstate of an adiabatically varying Hamiltonian.

We now wish to generalize the above results by showing that the phase difference between the exact state $|\psi;t\rangle$ and any arbitrary state $|\psi_f\rangle$ can also be separated into dynamic and geometric contributions and give explicit formulas for the geometric component. The idea then is to consider the phase of an amplitude $\langle \psi_f|\psi;t\rangle$,

$$\beta = \arg\langle \psi_f|\psi;t\rangle,$$

where the state $|\psi;t\rangle$ satisfies the evolution equation

$$i\partial_t|\psi;t\rangle = \hat{H}(t)|\psi;t\rangle\,.$$

We consider, as an intermediate step, some arbitrary state section $|\psi(\xi)\rangle$ on the U(1) bundle over the ray space, so that at any given time the time evolved state may be written as

$$|\psi;t\rangle = e^{i\phi(t)}|\psi(\xi(t))\rangle\,.$$

Substituting into the Schrödinger equation and taking the inner product with $|\psi;t\rangle$, we then find that the phase factor $\phi(t)$ satisfies

$$\dot{\phi} = -\langle \psi|\hat{H}(t)|\psi\rangle + i\langle \psi(\xi)|\partial_t|\psi(\xi)\rangle = -\langle \hat{H}(t)\rangle - A_{\mu}\dot{\xi}^{\mu}\,.$$

Now, letting $\eta = \arg\langle\psi_f|\psi\rangle$, we then have

$$\dot{\beta} = \dot{\phi} + \dot{\eta} \tag{6.3}$$

$$= -\langle \hat{H}(t)\rangle - A_{\mu}\dot{\xi}^{\mu} + \eta_{,\mu}\dot{\xi}^{\mu}\,. \tag{6.4}$$

Thus we recognize the term $\eta_{,\mu} - A_{\mu}$ as the invariant phase gradient for the transition amplitude corresponding to the state section in question. We can then apply the generalized Cauchy–Riemann conditions to deduce finally that

$$\dot{\beta} = -\langle \hat{H}(t) \rangle - \dot{\xi}^{\mu} \Omega_{\mu}{}^{\nu} \partial_{\nu} \log \sqrt{p(\xi)} \ . \tag{6.5}$$

The result shows that in the course of time evolution, the amplitude $\arg\langle \psi_f | \psi; t \rangle$ acquires aside from the dynamical phase, a geometric component

$$\beta_g = -\int \mathrm{d}\xi^{\mu} \Omega_{\mu}{}^{\nu} \partial_{\nu} \log \sqrt{p(\xi)} \, . \tag{6.6}$$

To see the connection between this result and the cyclic geometric phase we recall that the curl of $\Omega_{\mu}{}^{\nu} \partial_{\nu} \log \sqrt{p(\xi)} \mathbf{d}\xi^{\mu}$ is the same curl as the curl of $\mathbf{A}$. Thus, when the evolution on the ray space is cyclic, we obtain the usual geometric phase $-\oint \mathbf{A}$. Note also that the present results can be extended to any complex submanifold of $\mathcal{R}$ if under time evolution the state remains on the manifold, for instance by virtue of adiabatic time evolution.

ACKNOWLEDGMENTS

This paper is dedicated to the memory of Jeeva Anandan from whom the author benefited in many stimulating discussions of the ideas presented herein. The author would also like to thank Y. Aharonov, P. Mazur, and E.C.G. Sudarshan for helpful discussions. This work was supported in part by the Office of Naval Research under Grant No. N00014-00-1-0383. Support from Colciencias-BID II is kindly acknowledged.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Plethysms and interacting boson models

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(Received 25 February 2003; accepted 2 July 2003)

A short review of the plethysm technique aiming to its application in finding branching rules for the reduction of an irreducible representation of a group under the restriction to one of its subgroups is given. The algebraic structure of the interacting boson model and some of its extensions is given together with the branching rules needed to classify their basis states, obtained by the use of plethysms. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1611265]

I. INTRODUCTION

In the study of irreducible representations (irreps) of the full linear group GL(n) in n dimensions an important role is played by the so called Schur functions.[1–3] In a given irrep $\{\lambda\}$ of GL(n) the character of each of its elements A is the Schur function $\{\lambda\}$ evaluated with the eigenvalues of A.

A Schur function is expressed in terms of *fundamental symmetrical quantities* a_i, h_i, and s_i,[4] polynomials in n unknowns that are left invariant under permutations of these unknowns. The plethysm of Schur functions turned out a powerful tool to determine branching rules for the reduction of irreps of GL(n) subgroups under restriction to some of their subgroups.[4,5] The plethysm operation of Schur functions was discovered by Littlewood[6] as a third way of combining two Schur function to obtain a linear combination of Schur functions of a same degree. With few exceptions,[4,7,8] it remainded almost unknown to physicists due to the great difficulties involved in its calculation. With the appearence of powerful computers the tedious labor of computing plethysms was no more a problem and new efforts were made in order to find algorithms for computing them.[5,9–13]

In most applications to physical problems such as in nuclear structure[5,7] and in the present work only a particular class of plethysm is needed, namely that in which the left factor is a symmetric Schur function and in the expansion only those Schur functions with no more than a given number of rows are considered. In that case, using an induction formula for computing plethysms with both factors being symmetric Schur functions given in Ref. 13, we developed an algorithm[5] to compute plethysms with a symmetric Schur function in the left and all Schur functions of a given degree at right.

A field in which the plethysm technique can show all its power is the interacting boson model (IBM) and its generalizations.

The IBM when originally introduced by Arima and Iachello[14] is 1975 takes the nucleons outside a core of an even–even nucleus couple then into pairs to form bosons with angular momentum 2(d-bosons) and 0(s-bosons), no other degree of freedom, besides their z-component being taken into account. To work in the second quantization formalism they introduce 5 (for d-bosons) $+1$(for s-bosons)$=6$ creation and annihilation boson operators. The space of states is taken as polynomials of degree N (number of boson pairs) in creation operators acting on a vacuum realizing in this way the basis states of irreducible symmetric representations of U(6).

These bosons interact among themselves by interactions that preserve angular momentum and number of boson pairs so that their Hamiltonian can be written in terms of Casimir invariants of U(6) subgroups.

This original verson is nowadays referred to as IBM-1. Some extensions of the model appeared[15] in order to account for other degrees of freedom and the inclusion of bosons with other angular momenta. The unitary group is enlarged and a very rich algebraic structure arises. The basis states of the irreps of these unitary groups are labeled by labels of irreps of their subgroups in chains ending with $O^+(3)$, the rotation group in three dimensions. To this end one needs to know how an irrep of a group branches into irreps of some of its subgroups. We will show in this paper how plethysms can be used to find these branching rules. Besides, the cases here studied can serve as examples for applications in other areas.

II. SUMMARY OF PLETHYSMS

A partition $(\lambda)\equiv(\lambda_1,\lambda_2,\ldots,\lambda_n)$ is a set of nonnegative integers (parts) λ_i such that $\lambda_1+\lambda_2+\cdots+\lambda_n=n$. If, in addition, they satisfy $\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_n$, the partition is called *standard*. Since we will deal only with standard partitions we will omit the word standard. Usually in a partition the null parts are omitted and the repeated ones are exponentiated. We will use greek letters to denote a partition and italic letters to denote a single part of a partition. To each partition one associates a Young diagram, an array of n boxes with λ_1 boxes in the first row, λ_2 in the second and so on. Due to that the nonzero parts of a partition are referred to as *rows* and the conjugate partition of a given partition $(\lambda_1,\lambda_2,\ldots,\lambda_p,0,\ldots,0)$ is defined as the partition whose Young diagram is obtained from that of (λ) by interchange of rows and columns, i.e.,

$$(\tilde{\lambda})=(p^{\lambda_p},(p-1)^{\lambda_{p-1}-\lambda_p},\ldots,2^{\lambda_2-\lambda_3},1^{\lambda_1-\lambda_2}). \tag{1}$$

Given a set of n variables $x_1,x_2,\ldots,x_n$ and a partition (λ) of r, the Schur function $\{\lambda\}$ associated to (λ) is defined as[4,6]

$$\{\lambda\}=\frac{1}{r!}|Z_r|^{[\lambda]}, \tag{2}$$

where Z is the matrix

$$Z_r=\begin{pmatrix} s_1 & 1 & 0 & 0 & \ldots & \ldots & \ldots & 0 \\ s_2 & s_1 & 2 & 0 & \ldots & \ldots & \ldots & 0 \\ s_3 & s_2 & s_1 & 3 & 0 & \ldots & \ldots & 0 \\ \ldots & \ldots & \ldots & .. & \ldots & \ldots & \ldots & 0 \\ s_{r-1} & s_{r-2} & \ldots & \ldots & \ldots & \ldots & s_1 & r-1 \\ s_r & s_{r-1} & \ldots & \ldots & \ldots & \ldots & s_2 & s_1 \end{pmatrix} \tag{3}$$

and $s_i\equiv s_i(x_1,x_2,\ldots,x_n)$ is the sum of ith powers of each variable $x_1,x_2,\ldots,x_n$. In this notation of Schur function the variables and their number n are implied while r, called its *degree*, is obtained by $r=\lambda_1+\lambda_2+\cdots+\lambda_r$.

In (2), $|Z|^{(\lambda)}$ is the immanant of Z, an extension of the concept of determinant, given by

$$|Z|^{(\lambda)}=\sum_P \chi^{[\lambda]}(P)z_{1p_1}z_{2p_2}\cdots z_{rp_r}, \tag{4}$$

where the sum is over all permutations $P=(p_1,p_2,\ldots,p_r)$ of the integers $1,2,\ldots,r$ and $\chi^{[\lambda]}(P)$ is the character of permutation P in the irrep $[\lambda]$ of the symmetric group $S(r)$.

As a consequence of definition (2) a Schur function is an homogeneous polynomial of degree r in the variables $x_1, x_2, \ldots, x_n$, being identically null for partitions (λ) of r into more than n nonzero parts.

Expression (2) can be worked out to produce an alternative definition[6,9] of the Schur function

$$\{\lambda\} = \frac{|(x_i)^{\lambda_j + n - j}|}{|(x_i)^{n-j}|}, \tag{5}$$

where $|f_j(x_i)|$ denotes the determinant of a matrix M with elements $M_{i,j} = f_j(x_i)$.

A pair of Schur functions $\{\lambda'\}$, $\{\lambda''\}$ of degrees r' and r'' can be combined into three different ways to produce linear combination of Schur functions $\{\lambda'''\}$ of degree r''': inner (or direct) product, outer product and plethysm. These three operations will be denoted, respectively, as

$$\begin{aligned}
\{\lambda'\} \times \{\lambda''\} &= \sum_{\lambda'''} \alpha(\{\lambda'\} \times \{\lambda''\} \to \{\lambda'''\})\{\lambda'''\}, \\
\{\lambda'\}\{\lambda''\} &= \sum_{\lambda'''} \alpha(\{\lambda'\}\{\lambda''\} \to \{\lambda'''\})\{\lambda'''\}, \\
\{\lambda'\} \otimes \{\lambda''\} &= \sum_{\lambda'''} \alpha(\{\lambda\} \otimes \{\lambda''\} \to \{\lambda'''\})\{\lambda'''\},
\end{aligned} \tag{6}$$

where $\alpha(\cdots)$ is a non-negative integer denoting the multiplicity of $\{\lambda'''\}$ in the expansion. For clarity we attach to it an argument denoting the kind of operation that produced it.

In the inner product the degrees of the Schur functions involved are all equal, i.e., $r''' = r' = r'' = n$, and the expansion coefficients α are the coefficients of reduction of the Kronecker product of $S(n)$ irreps $[\lambda']$ and $[\lambda'']$.

In the outer product one has $r''' = r' + r''$ and the coefficients α are obtained by making the product of a Schur function in variables $(x_1, x_2, \ldots, x_{n'})$ by another in variables $(y_1, y_2, \ldots, y_{n''})$ and expressing it as a linear combination of Schur functions in variables $(z_1, z_2, \ldots, z_{n'''})$ with $z_i = x_i$ for $1 \leqslant i \leqslant n'$ and $z_{n'+i} = y_i$ for $1 \leqslant i \leqslant n''$. Littlewood obtained a procedure to find the coefficients of the outer product known in the literature as ''Littlewood's rules.''

To define plethysm one needs first to introduce the concept of *invariant matrix*.

Let $T(A)$ be an $m \times m$ matrix whose elements t_{ij} are given homogeneous polynomials of degree r in the elements of A. Let $T(B)$ be a matrix built with the *same* polynomials t_{ij} now in the elements of B. If

$$T(A)T(B) = T(AB) \tag{7}$$

for any nonsingular $m \times m$ matrices A, B then the matrix $T(A)$ is called an invariant matrix(of degree r) of A.

It follows from (7) that, once the set of polynomial t_{ij} is fixed, the set of matrices $\mathcal{D}^T(A) \equiv T(A)$ is a representation of $\mathrm{GL}(n)$.

As the Kronecker product of two representations of a group is also a representation of this group, the Kronecker product of invariant matrices is also an invariant matrix, in general reducible. Schur[1] demonstrated that *if A is an $n \times n$ matrix, there are as many irreducible invariant matrices of A of degree r as are the partitions of r with no more than n nonzero parts and the trace of them are the Schur functions of degree r in the eigenvalues of A*. These irreducible invariant matrices are then labeled by those partitions and denoted by $A^{[\mu]}$. The details of construction of irreducible invariant matrices can be found in Refs. 16 and 17.

Since an invariant matrix of an invariant matrix is also an invariant matrix of the original matrix, it can be decomposed into irreducible components

$$[A^{[\mu]}]^{[\nu]}=\sum_{\lambda}\ \kappa_{\lambda\mu\nu}A^{[\lambda]}. \tag{8}$$

Let us denote by r_μ, r_ν, and r_λ, the degrees of $\{\mu\}$, $\{\nu\}$, and $\{\lambda\}$, respectively. Since the elements of $A^{[\mu]}$ are polynomials of degree r_μ in the elements of A and those of $[A^{[\mu]}]^{[\nu]}$ are polynomials of degree r_ν in the components of $A^{[\mu]}$, it follows that $r_\lambda=r_\mu r_\nu$.

Equation (8) led Littlewood[6] to define a third composition rule of Schur functions denoted by the symbol $\otimes$ and defined as

$$\{\mu\}\otimes\{\nu\}=\sum_{\lambda}\ \kappa_{\lambda\mu\nu}\{\lambda\}, \tag{9}$$

where the Schur functions $\{\lambda\}$ and the numerical coefficients $\kappa_{\lambda\mu\nu}$ are those given in (8). This operation was later on named *plethysm*.

The plethysm operation has the following properties:[4,6,8]

$$\{\lambda\}\otimes(\{\mu\}\otimes\{\nu\})=(\{\lambda\}\otimes\{\mu\})\otimes\{\nu\}, \tag{10}$$

$$\{\lambda\}\otimes(\{\mu\}\pm\{\nu\})=\{\lambda\}\otimes\{\mu\}\pm\{\lambda\}\otimes\{\nu\}, \tag{11}$$

$$(\{\lambda\}+\{\mu\})\otimes\{\nu\}=\sum_{\lambda'\lambda''}\ \alpha(\{\lambda'\}\{\lambda''\}\rightarrow\{\nu\})(\{\lambda\}\otimes\{\lambda'\})(\{\mu\}\otimes\{\lambda''\}), \tag{12}$$

$$(\{\lambda\}-\{\mu\})\otimes\{\nu\}=\sum_{\lambda'\lambda''}\ (-)^{r''}\alpha(\{\lambda'\}\{\lambda''\}\rightarrow\{\nu\})(\{\lambda\}\otimes\{\lambda'\})(\{\mu\}\otimes\{\tilde{\lambda}''\}), \tag{13}$$

$$\{\lambda\}\otimes(\{\mu\}\{\nu\})=(\{\lambda\}\otimes\{\mu\})(\{\lambda\}\otimes\{\nu\}), \tag{14}$$

$$(\{\lambda\}\{\mu\})\otimes\{\nu\}=\sum_{\lambda'\lambda''}\ \alpha(\{\lambda'\}\times\{\lambda''\}\rightarrow\{\nu\})(\{\lambda\}\otimes\{\lambda'\})(\{\mu\}\otimes\{\lambda''\}), \tag{15}$$

$$[\{\lambda\}\otimes\{\mu\}]^T=\begin{cases}\{\tilde{\lambda}\}\otimes\{\mu\} & \text{for } r_\lambda \text{ even},\\ \{\tilde{\lambda}\}\otimes\{\tilde{\mu}\} & \text{for } r_\lambda \text{ odd}.\end{cases} \tag{16}$$

The sum in Eqs. (12), (13), and (15) includes the cases $\{\lambda'\}=\{0\}\equiv 1$, $\{\lambda''\}=\{\nu\}$ and $\{\lambda'\}=\{\nu\}$, $\{\lambda''\}=\{0\}\equiv 1$. Also, r'' and r_λ are the degrees of $\{\lambda''\}$ and $\{\lambda\}$.

In Eq. (16) we used the notation

$$\left[\sum_i\ a_i\{\lambda\}^{(i)}\right]^T=\sum_i\ a_i\widetilde{\{\lambda\}^{(i)}}, \tag{17}$$

where a_i are numerical factors, $\{\lambda\}^{(i)}$ Schur functions and $\widetilde{\{\lambda\}^{(i)}}$ their conjugate.

A. Special plethysms

The plethysm calculation is, in general, a hard and tedious task. Nevertheless there are special cases with closed and simple expressions

$$\{\lambda\}\otimes\{1\}=\{1\}\otimes\{\lambda\}=\{\lambda\}, \tag{18}$$

$$\{\lambda\}\otimes\{0\}=\{0\},\quad \{0\}\otimes\{\lambda\}=\delta_{\{\lambda\},\{r_\lambda\}}\{0\}, \tag{19}$$

$$\{r\}\otimes\{2\}=\sum_{i=0}^{[r/2]}\{2r-2i,2i\}, \tag{20}$$

$$\{r\}\otimes\{1^2\}=\sum_{i=1}^{[(r+1)/2]}\{2r-(2i-1),(2i-1)\}, \tag{21}$$

$$\{2\}\otimes\{r\}=\sum_{\lambda}\{\lambda\}_{\text{even}}, \tag{22}$$

$$\{1^2\}\otimes\{r\}=\sum_{\lambda}\widetilde{\{\lambda\}_{\text{even}}}, \tag{23}$$

$$\{1^r\}\otimes\{2\}=\{1^{2r}\}+\sum_{i=1}^{[r/2]}\{2^{2i},1^{2r-4i}\},\quad r \text{ even}, \tag{24}$$

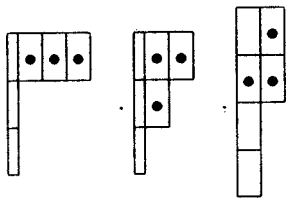
$$\{1^r\}\otimes\{1^2\}=\{1^{2r}\}+\sum_{i=1}^{[r/2]}\{2^{2i},1^{2r-4i}\},\quad r \text{ odd}, \tag{25}$$

$$\{1^r\}\otimes\{1^2\}=\sum_{i=1}^{[(r+1)/2]}\{2^{2i-1},1^{2r-2(2i-1)}\},\quad r \text{ even}, \tag{26}$$

$$\{1^r\}\otimes\{2\}=\sum_{i=1}^{[(r+1)/2]}\{2^{2i-1},1^{2r-2(2i-1)}\},\quad r \text{ odd}. \tag{27}$$

Equation (18) follows from plethysms definition while Eq. (19) is set for consistency. In Eq. (22) $\{\lambda\}_{\text{even}}$ means partition of $2r$ with all parts even. Equations (23)–(27) follow from conjugation of Eqs. (22), (20), and (21). In Ref. 13 there are formulas for the calculation of plethysms $\{\lambda\}\otimes\{\mu\}$ when both Schur functions are symmetric or/and antisymmetric. To explain them we need the following definition: a *k-border strip* of a Young diagram associated to a given partition (λ) is a sequence of k squares in which the first of them is the last one of the first line of (λ) and the next square to a given one is the one below it, if it exists, or the one to its left, otherwise.

For example, the three-border strips of (41^2), (321), and (2^21^2) are the squares with the symbol $\cdot$ in the figures below, respectively,



When $\{\lambda\}$ and $\{\mu\}$ are both symmetric, one has

$$\{n\}\otimes\{m\}=\frac{1}{m}\sum_{k=1}^{m}\{n\}(x^k)(\{n\}\otimes\{m-k\}),\quad m\geqslant 1, \tag{28}$$

with

$$\{n\}(x^k)=\sum_{\nu}C_{n,k,\nu}\{\nu\}. \tag{29}$$

In (29) the $\{\nu\}$'s are all Schur functions of degree nk. The coefficients $C_{n,k,\nu}$ are obtained from the Young diagram associated to (ν) removing, in sequence, n k-border strips. If in all steps the resulting diagram represents a standard partition then

$$C_{n,k,\nu}=(-)^l \tag{30}$$

with $l=$(number of lines in the k-border strips)$-n$. If in some step the resulting diagram does not represent a standard partition, then $C_{n,k,\nu}=0$. As example, from the figures above one has

$$C_{2,3,\{41^2\}}=(-)^{4-2}=1, \quad C_{2,3,\{321\}}=(-)^{5-2}=-1, \quad C_{2,3,\{2^21^2\}}=0.$$

Equation (28) allows one to relate the plethysm of two symmetric Schur functions with the plethysms of symmetric Schur functions of smaller degrees. In this way, using $\{n\}\otimes\{1\}\equiv\{n\}$ as starting point one computes all the plethysms of type $\{n\}\otimes\{m\}$. This equation, together with

$$\{n\}\otimes\{1^m\}=(-)^{m+1}\{n\}\otimes\{m\}+\sum_{k=1}^{m-1}(-)^{k+1}(\{n\}\otimes\{k\})(\{n\}\otimes\{1^{m-k}\}), \tag{31}$$

$$\{1^n\}\otimes\{1^m\}=(-)^{m+1}\{1^n\}\otimes\{m\}+\sum_{k=1}^{m-1}(-)^{k+1}(\{1^n\}\otimes\{k\})(\{1^n\}\otimes\{1^{m-k}\}), \tag{32}$$

$$\{1^n\}\otimes\{m\}=\begin{cases}[\{n\}\otimes\{m\}]^T & \text{for } n \text{ even},\\ [\{n\}\otimes\{1^m\}]^T & \text{for } n \text{ odd}\end{cases} \tag{33}$$

allows us to compute plethysms with both Schur functions symmetric and/or antisymmetric.

A very common situation which arises in applications is when one needs to compute plethysms of a same Schur function by many (sometimes all) Schur functions of a given degree to the right. (This is the case of the applications that we will make in Secs. III–VII.) For such cases we proposed in Ref. 5 the following algorithm that allows to compute, in a build up way, all plethysms $\{\lambda\}\otimes\{\mu\}_r$ with $\{\lambda\}$ a fixed Schur function and $\{\mu\}_r$ all Schur functions of degree r, once the plethysms $\{\lambda\}\otimes\{r\}$ and $\{\lambda\}\otimes\{\mu\}_{r'}$, with $r'<r$ have already been computed.

(1) Find all partitions of r and order them in descending order of all their parts read from left to right.

(2) For each partition $\{\mu\}=\{\mu_1,\mu_2,\ldots,\mu_t,0,\ldots,0\}$ perform the outer product $\{\mu_1,\mu_2,\ldots,\mu_{t-1}\}\{\mu_t\}$, order the irreps in the reduction as in item (1), then use Eqs. (11) to obtain the equation

$$\{\lambda\}\otimes\{\mu\}=(\{\lambda\}\otimes\{\mu_1,\mu_2,\ldots,\mu_{t-1}\})(\{\lambda\}\otimes\{\mu_t\})-\sum_{\{\mu'\}<\{\mu\}}\alpha(\{\mu_1,\mu_2,\ldots,\mu_{t-1}\}\{\mu_t\}\rightarrow\{\mu'\})\{\lambda\}\otimes\{\mu'\}, \tag{34}$$

where the symbol $\prec$ means preceding, following the ordering in item (1).

Since $\{\mu_1,\mu_2,\ldots,\mu_{t-1}\}$ and $\{\mu_t\}$ have smaller degree than $\{\mu\}$, the plethysms $\{\lambda\}\otimes\{\mu_1,\mu_2,\ldots,\mu_{t-1}\}$ and $\{\lambda\}\otimes\{\mu_t\}$ have already been computed in the induction process. On the other hand, the plethysms $\{\lambda\}\otimes\{\mu'\}$ also have been computed since $\{\mu'\}$ precedes $\{\mu\}$.

The formulas here given and the above algorithm suffice for calculating all plethysms needed in this work.

B. Special branching rules

The use of plethysms to compute branching rules is based in the theorem.[4]

If under the restriction $G\rightarrow H$ the character $\dagger 1\ddagger$ of group G decomposes as

$$\{\!|1|\!\} = (\alpha) + (\beta) + \cdots + (\omega), \tag{35}$$

then the character $\{\!|\lambda|\!\}$ *of* G *decomposes into the characters* (ρ) *of* H *according to the characters contained in the plethysm*

$$[(\alpha) + (\beta) + \cdots + (\omega)] \otimes \{\!|\lambda|\!\}. \tag{36}$$

This plethysm can be obtained expressing the characters of G and H in terms of characters of GL(n), computing the resulting plethysms of GL(n) characters and re-expressing the result in terms of characters of H in order to obtain the final result.

Using the association irrep $\leftrightarrow$ character this theorem gives us the coefficients of the reduction of the irrep $\{\!|\lambda|\!\}$ of G in the direct sum of irreps (ρ) of H.

To illustrate the use of this theorem, let us consider some general cases that will be used later on. The first step toward the use of Eq. (36) is to find the decomposition (35). One way of finding it is by constructing a realization of basis states of irreps and generators of groups G and H.

One such realization is provided by the *boson calculus*[18] in which a set of boson operators $b_i^\dagger$ (creation) and b_i (annihilation) is introduced and the generators and basis states of irreps are written in terms of them.

The boson operators satisfy the usual commutation relations

$$[b_i, b_j^\dagger] = \delta_{ij}, \quad [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0, \quad i,j = 1,2,\ldots,n, \tag{37}$$

and the b_i's annihilate the vacuum state $|0\rangle$.

For U(n) the generators are realized by

$$\mathcal{C}_i^j = b_i^\dagger b_j, \quad i,j = 1,2,\ldots,n, \tag{38}$$

while the maximum weight basis states of symmetric irreps $\{N,0,\ldots,0\} \equiv \{N\}$ are realized by

$$|\{N\}\text{m.w.}\rangle = \frac{1}{\sqrt{N!}} (b_1^\dagger)^N |0\rangle, \tag{39}$$

from which it follows that the basis states of irrep $\{1\}$ of U(n) are realized by

$$|\{1\}i\rangle = b_i^\dagger |0\rangle, \quad i = 1,2,\ldots,n. \tag{40}$$

The generators of U($n-1$) are the $\mathcal{C}_i^j$ given in Eq. (38) for $i,j = 1,2,\ldots,n-1$. Acting then in (40) one sees that the U(n) irrep $\{1\}$ splits into two U($n-1$) irreps $\{1\}$ and $\{0\}$ with basis states

$$|\{1\}i\rangle = b_i^\dagger |0\rangle, \quad i = 1,2,\ldots,n-1 \quad \text{and} \quad |\{0\}\rangle = b_n^\dagger |0\rangle. \tag{41}$$

Therefore one obtains

$$\{1\} = \{1\} + \{0\} \quad \text{for U}(n) \supset \text{U}(n-1). \tag{42}$$

For O(n) the generators are $\mathcal{L}_i^j = \mathcal{C}_i^j - \mathcal{C}_j^i$ and reduction (35) read as

$$\{1\} = (1). \tag{43}$$

[We denote the irreps of unitary (U) and orthogonal (O) groups as quantities inside braces and parentheses, respectively.]

Consider the case in which U(n) acts on a vector space $\mathcal{E} = \mathcal{E}' + \mathcal{E}''$ with dimensions n' and n'' such that $n = n' + n''$. We then split n into two terms n' and n'' and consider U(n') as the group with generators $\mathcal{C}_{i'}^{j'}$ for $i',j' = 1,2,\ldots,n'$ and U(n'') that with generators $\mathcal{C}_{i''}^{j''}$ with $i'',j'' = n' + 1, n'+2, \ldots, n'+n'' = n$. The basis (40) splits into two

$$|\{1\}i'\rangle = b^\dagger_{i'}|0\rangle, \quad i' = 1,2,\ldots,n',$$

$$|\{1\}i''\rangle = b^\dagger_{i''}|0\rangle, \quad i'' = n'+1, n'+2,\ldots,n'+n'' = n, \tag{44}$$

realizing the basis states of irreps $\{1\}'\{0\}''$ and $\{0\}'\{1\}''$ of $U(n')\oslash U(n'')$, respectively. We then have

$$\{1\} = \{1\}'\{0\}'' + \{0\}'\{1\}'' \quad \text{for } U(n'+n'') \supset U(n')\oslash U(n''). \tag{45}$$

For the case in which $U(n)$ acts on a vector space $\mathcal{E} = \mathcal{E}' \otimes \mathcal{E}''$ with dimensions n' and n'' one uses boson operators with two indices, each one associated to transformations in each subspace,

$$[b_{is}, b^\dagger_{jt}] = \delta_{ij}\delta_{st}, \quad [b_{is}, b_{jt}] = [b^\dagger_{is}, b^\dagger_{jt}] = 0, \quad i,j = 1,2,\ldots,n', \quad s,t = 1,2,\ldots,n''. \tag{46}$$

The basis states of irrep $\{1\}$ are realized by

$$|\{1\}is\rangle = b^\dagger_{is}|0\rangle, \quad i = 1,2,\ldots,n', \quad s = 1,2,\ldots,n''. \tag{47}$$

Since the $U(n')$ generators $\mathcal{C}^j_i = \Sigma_s b^\dagger_{is} b_{js}$ act on the first index and those $C^t_s = \Sigma_i b^\dagger_{is} b_{it}$ of $U(n'')$ on the second, one concludes that

$$\{1\} = \{1\}'\{1\}'' \quad \text{for } U(n'n'') \supset U(n') \times U(n''). \tag{48}$$

Using Eq. (42) in Eq. (36), the branching rule for the reduction $U(n) \supset U(n-1)$ is given by computing the plethysm

$$(\{1\}+\{0\})\otimes\{\lambda\} = \sum_{\lambda'\lambda''} \alpha(\{\lambda'\}\{\lambda''\} \to \{\lambda\})(\{1\}\otimes\{\lambda'\})(\{0\}\otimes\{\lambda''\})$$

$$= \sum_{\lambda' n''} \alpha(\{\lambda'\}\{n''\} \to \{\lambda\})\{\lambda'\}, \tag{49}$$

where use was made of (12), (18), and (19). By Littlewood rules, one sees that the Schur functions that contain $\{\lambda\}$ in the expansion of its outer product by a symmetric Schur function are those $\{\lambda'\}$ satisfying

$$\lambda_i \geqslant \lambda'_i \geqslant \lambda_{i+1}, \quad i = 1,2,\ldots,i-1. \tag{50}$$

Then one concludes that under restriction $U(n) \supset U(n-1)$ the $U(n)$ irrep $\{\lambda\}$ reduces as

$$\{\lambda\} = \sum_{\lambda'} \{\lambda'\}, \tag{51}$$

where $\{\lambda'\}$ are the $U(n-1)$ irreps satisfying Eq. (50). These are the well known *in-betweeness* conditions introduced by Gelfand[19] in the labeling of basis states of $U(n)$ irreps.

To compute the branching of irrep $\{\lambda\}$ of $U(n'+n'')$ into irreps of $U(n')\oslash U(n'')$, according to Eqs. (36) and (45) we need to compute the plethysm

$$(\{1\}'\{0\}'' + \{0\}'\{1\}'')\otimes\{\lambda\} = \sum_{\mu\nu} \alpha(\{\mu\}\{\nu\} \to \{\lambda\})((\{1\}'\{0\}'')\otimes\{\mu\})(\{0\}'\{1\}''\otimes\{\nu\}), \tag{52}$$

where use was made of Eq. (12). Using Eq. (15) one has

$$(\{1\}'\{0\}'')\otimes\{\mu\})=\sum_{\gamma\rho}\alpha(\{\gamma\}\times\{\rho\}\to\{\mu\})(\{1\}'\otimes\{\gamma\})(\{0\}''\otimes\{\rho\})=\{\mu\}\{0\}=\{\mu\} \quad (53)$$

using Eqs. (18) and (19) and the result $\{\mu\}\times\{n\}=\{\mu\}$ on inner product of Schur functions. Analogously $(\{0\}'\{1\}'')\otimes\{\nu\}$ gives $\{\nu\}$ and one concludes that

$$\{\lambda\}=\sum_{\mu\nu}\alpha(\{\mu\}\{\nu\}\to\{\lambda\})\{\mu\}'\{\nu\}'' \quad \text{for } U(n'+n'')\supset U(n')\oslash U(n''), \quad (54)$$

$\{\mu\}',\{\nu\}''$ being irreps of $U(n')$ and $U(n'')$, respectively.

To compute the branching of irrep $\{\lambda\}$ of $U(n'n'')$ into irreps of $U(n')\times U(n'')$, according to Eqs. (36) and (48) we need to compute the plethysm,

$$(\{1\}'\{1\}'')\otimes\{\lambda\}=\sum_{\mu\nu}\alpha(\{\mu\}\times\{\nu\}\to\{\lambda\})(\{1\}'\otimes\{\mu\})(\{1\}''\otimes\{\nu\}), \quad (55)$$

where use was made of Eq. (15). Using Eq. (18) one concludes that

$$\{\lambda\}=\sum_{\mu,\nu}\alpha(\{\mu\}\times\{\nu\}\to\{\lambda\})\{\mu\}'\{\nu\}'' \quad \text{for } U(n')\times U(n''), \quad (56)$$

$\{\mu\}',\{\nu\}''$ being irreps of $U(n')$ and $U(n'')$, respectively.

When $\{\lambda\}$ is a symmetric representation the inner product in Eq. (56) requires that the irreps of $U(n')$ and $U(n'')$ be the same.

Equation (43) is of no use for producing branching rules since it gives a trivial result. For this case one uses the known result.[4,6]

The character $\{\lambda\}$ *of* $U(n)$ *decomposes into* $O(n)$ *characters* (λ'') *by the relation*

$$\{\lambda\}=\sum_{\lambda''}\left[\sum_{\lambda'}\alpha(\{\lambda'\}\{\lambda''\}\to\{\lambda\})\right](\lambda''), \quad (57)$$

where the sum is made in the irreps $\{\lambda'\}$ *with even parts*.

When $\{\lambda\}$ is a symmetric representation both Schur functions $\{\lambda'\}$ and $\{\lambda''\}$ are symmetric and Eq. (57) gives

$$\{N\}=(N)+(N-2)+\cdots+(0) \text{ or } (1) \quad \text{for } U(n)\supset O(n). \quad (58)$$

We give in Table I the branching rules in the reduction $U(n)\supset O(n)$ for the lowest degree $U(n)$ irreps with no more than three rows.

For small values of n some $O(n)$ characters in Eq. (57) may have more than the allowed number $[n/2]$ of rows. In this case, they are worked out using *modified rules*.[20] For $U(3)\supset O^+(3)$, Eq. (57) and the corresponding modification rules are equivalent to the *Elliott rules*[7] for the branching of U(3) irrep $\{f_1,f_2,f_3\}$ into $O^+(3)$ irreps (L).

(1) Define

$$\lambda=f_1-f_2, \quad \mu=f_2-f_3, \quad \overline{\lambda}=\max(\lambda,\mu), \quad \overline{\mu}=\min(\lambda,\mu). \quad (59)$$

(2) Introduce an extra label K that can assume the values

$$K=\overline{\mu},\overline{\mu}-2,\ldots,0 \text{ or } 1. \quad (60)$$

(3) To each K corresponds a set of L values

$$L=K,K+1,\ldots,K+\overline{\lambda}, \quad \text{for } K\neq 0,$$

TABLE I. $U(n)\supset O(n)$ branching rules for $U(n)$ irreps with no more than three rows and the lowest degrees.

$\{0\}=(0)$
$\{1\}=(1)$
$\{2\}=(2)+(0)$
$\{1^2\}=(1^2)$
$\{3\}=(3)+(1)$
$\{21\}=(21)+(1)$
$\{1^3\}=(1^3)$
$\{4\}=(4)+(2)+(0)$
$\{31\}=(31)+(2)+(1^2)$
$\{2^2\}=(2^2)+(2)+(0)$
$\{21^2\}=(21^2)+(1^2)$
$\{5\}=(5)+(3)+(1)$
$\{41\}=(41)+(3)+(21)+(1)$
$\{32\}=(32)+(3)+(21)+(1)$
$\{31^2\}=(31^2)+(21)+(1^3)$
$\{2^21\}=(2^21)+(21)+(1)$
$\{6\}=(6)+(4)+(2)+(0)$
$\{51\}=(51)+(4)+(31)+(2)+(1^2)$
$\{42\}=(42)+(4)+(31)+(2^2)+2(2)+(0)$
$\{3^2\}=(3^2)+(31)+(1^2)$
$\{41^2\}=(41^2)+(31)+(21^2)+(1^2)$
$\{321\}=(321)+(31)+(2^2)+(21^2)+(2)+(1^2)$
$\{2^3\}=(2^3)+(2^2)+(2)+(0)$
$\{7\}=(7)+(5)+(3)+(1)$
$\{61\}=(61)+(5)+(41)+(3)+(21)+(1)$
$\{52\}=(52)+(5)+(41)+(32)+2(3)+(21)+(1)$
$\{43\}=(43)+(41)+(32)+(3)+(21)+(1)$
$\{51^2\}=(51^2)+(41)+(31^2)+(21)+(1^3)$
$\{421\}=(421)+(41)+(32)+(31^2)+(2^21)+(3)+2(21)+(1)$
$\{3^21\}=(3^21)+(32)+(31^2)+(21)+(1^3)$
$\{32^2\}=(32^2)+(32)+(2^21)+(3)+(21)+(1)$
$\{8\}=(8)+(6)+(4)+(2)+(0)$
$\{71\}=(71)+(6)+(51)+(4)+(31)+(2)+(1^2)$
$\{62\}=(62)+(6)+(51)+(42)+2(4)+(31)+(2^2)+2(2)+(0)$

$$L=\overline{\lambda},\overline{\lambda}-2,\ldots,0 \quad \text{or} \quad 1 \quad \text{for } K=0. \tag{61}$$

The inverse result, that is, the expression of $O(n)$ characters in terms of those of $U(n)$ is also needed. It can be obtained by subtractions using tables of $U(n)\supset O(n)$ reductions or by use of the result[4,21]

$$(\lambda)=\{\lambda\}+\sum_{\eta}\left[\sum_{\gamma}(-)^{r/2}\alpha(\{\gamma\}\{\eta\}\rightarrow\{\lambda\}\right]\{\eta\}, \tag{62}$$

where r is the degree of $\{\gamma\}$ and these are taken among the set of Schur functions that in Frobenius' notation[4] assume the form

$$\begin{pmatrix} a+1 \\ a \end{pmatrix}, \quad \begin{pmatrix} a+1 & b+1 \\ a & b \end{pmatrix}, \quad \begin{pmatrix} a+1 & b+1 & c+1 \\ a & b & c \end{pmatrix}, \ldots . \tag{63}$$

When (λ) is symmetric one obtains from Eq. (58) and also from Eq. (62),

$$(N)=\{N\}-\{N-2\} \quad \text{for } N\geqslant 2. \tag{64}$$

Table B-4 in Ref. 4 gives a list of reductions (62) for irreps $\{\lambda\}$ of degree up to 16 and parts not greater than 4.

III. IBM-1

In the original IBM, now named IBM-1, the valence nucleons of even–even nuclei are joined in pairs to form a s- or d-boson, without distinguishing protons from neutrons. Then the building blocks are creation $(s^\dagger, d_\mu^\dagger)$ and annihilation (s, d_μ) boson operators satisfying the commutation relations

$$[s, s^\dagger] = 1, \quad [d_\mu, d_{\mu'}^\dagger] = \delta_{\mu\mu'}, \quad \mu, \mu' = 0, \pm 1, \pm 2, \tag{65}$$

all other commutators vanishing. In a compact notation one can define, say,

$$b_\rho^\dagger \text{ with } b_\rho^\dagger = d_{\rho-3}^\dagger \quad \text{for } \rho = 1,2,3,4,5 \quad \text{and} \quad b_6^\dagger = s^\dagger \tag{66}$$

and analogously for b_ρ, recovering Eq. (37). Using linear combinations of creation and annihilation operators that preserve the number of bosons, it is possible to construct $\mathrm{O}^+(3)$ Racah tensors of ranks $\ell = 0,1,2,3,4$. Linear combinations of these tensors realize[15,22] the infinitesimal generators of U(6) subgroups in the three chains ending with $\mathrm{O}^+(3) \supset \mathrm{O}^+(2)$,

$$\begin{array}{cccccccccc} & \nearrow & \mathrm{U}(5) & \supset & \mathrm{O}^+(5) & \supset & \mathrm{O}^+(3) & \supset & \mathrm{O}^+(2) & \text{(I)}, \\ \mathrm{U}(6) & \rightarrow & \mathrm{SU}(3) & \supset & \mathrm{O}^+(3) & \supset & \mathrm{O}^+(2) & & & \text{(II)}, \\ & \searrow & \mathrm{O}^+(6) & \supset & \mathrm{O}^+(5) & \supset & \mathrm{O}^+(3) & \supset & \mathrm{O}^+(2) & \text{(III)}. \end{array} \tag{67}$$

With one-index boson operators only symmetrical irreps can be realized. Then the U(6) irrep is $\{N\}$ where N denotes the number of bosons.

Let us examine the branching rules in chain (I) of Eq. (67). The U(5) labels are given by the general result (51). Then the U(5) irrep is symmetrical $\{N_d\}$, where N_d is the number of d-bosons and can assume the values

$$N_d = N, N-1, \ldots, 0. \tag{68}$$

Each U(5) irrep $\{N_d\}$, being symmetric, branches as (58) into $\mathrm{O}^+(5)$ irreps

$$\{N_d\} = (N_d) + (N_d - 2) + \cdots + (0) \text{ or } (1). \tag{69}$$

To find the branching in $\mathrm{O}^+(5) \supset \mathrm{O}^+(3)$ one observes that the generators of U(5) were constructed only with operators $d_\mu^\dagger$ and d_μ so one has

$$(1) = (2) \quad \text{for } \mathrm{O}^+(5) \supset \mathrm{O}^+(3). \tag{70}$$

According to Eq. (36) the branching of a *general* $\mathrm{O}^+(5)$ irrep $\{\lambda\}$ into $\mathrm{O}^+(3)$ irreps is found computing the plethysm $(2) \otimes (\lambda)$. The character (2) of $\mathrm{O}^+(3)$ is given by $(2) = \{2\} - \{0\}$. Since (λ) is an $\mathrm{O}^+(5)$ irrep it has at most two lines, then we expand it using Eq. (62) in terms of Schur functions with up to two rows:

$$(\lambda) = \sum_k \alpha_k \{k\} + \sum_{\mu_1, \mu_2} \alpha_{\mu_1, \mu_2} \{\mu_1, \mu_2\}. \tag{71}$$

The plethysm $(2) \otimes (\lambda)$ is then

$$\begin{aligned} (2) \otimes (\lambda) &= (\{2\} - \{0\}) \otimes \left[\sum_k \alpha_k \{k\} + \sum_{\mu_1, \mu_2} \{\mu_1, \mu_2\} \right] \\ &= \sum_k \alpha_k [\{2\} \otimes \{k\} - \{2\} \otimes \{k-1\}] + \sum_{\mu_1 \mu_2} \alpha_{\mu_1 \mu_2} [\{2\} \otimes \{\mu_1, \mu_2\} - \{2\} \otimes \{\mu_1 - 1, \mu_2\} \\ &\quad - \{2\} \otimes \{\mu_1, \mu_2 - 1\} + \{2\} \otimes \{\mu_1 - 1, \mu_2 - 1\}], \end{aligned} \tag{72}$$

TABLE II. $O^+(5)\supset O^+(3)$ branching rules for $O^+(5)$ irreps of degrees up to 8.

$(0)=(0)$
$(1)=(2)$
$(2)=(2)+(4)$
$(1^2)=(1)+(3)$
$(3)=(0)+(3)+(4)+(6)$
$(21)=(1)+(2)+(3)+(4)+(5)$
$(4)=(2)+(4)+(5)+(6)+(8)$
$(31)=(1)+(2)+2(3)+(4)+2(5)+(6)+(7)$
$(2^2)=(0)+(2)+(3)+(4)+(6)$
$(5)=(2)+(4)+(5)+(6)+(7)+(8)+(10)$
$(41)=(1)+(2)+2(3)+2(4)+2(5)+2(6)+2(7)+(8)+(9)$
$(32)=(1)+2(2)+(3)+2(4)+2(5)+(6)+(7)+(8)$
$(6)=(0)+(3)+(4)+2(6)+(7)+(8)+(9)+(10)+(12)$
$(51)=(1)+(2)+2(3)+2(4)+3(5)+2(6)+3(7)+2(8)+2(9)+(10)+(11)$
$(42)=(0)+(1)+2(2)+2(3)+3(4)+2(5)+3(6)+2(7)+2(8)+(9)+(10)$
$(3^2)=(1)+2(3)+(4)+(5)+(6)+(7)+(9)$
$(7)=(2)+(4)+(5)+(6)+(7)+2(8)+(9)+(10)+(11)+(12)+(14)$
$(61)=(1)+(2)+2(3)+2(4)+3(5)+3(6)+3(7)+3(8)+3(9)+2(10)+2(11)+(12)+(13)$
$(52)=(0)+(1)+2(2)+3(3)+3(4)+3(5)+4(6)+3(7)+3(8)+3(9)+2(10)++(11)+(12)$
$(43)=(1)+2(2)+2(3)+2(4)+3(5)+2(6)+2(7)+2(8)+(9)+(10)+(11)$
$(8)=(2)+(4)+(5)+(6)+(7)+2(8)+(9)+2(10)+(11)+(12)+(13)+(14)+(16)$
$(71)=(1)+(2)+2(3)+2(4)+3(5)+3(6)+4(7)+3(8)+4(9)+3(10)+3(11)+2(12)+2(13)+(14)$
$+(15)$
$(62)=(1)+3(2)+2(3)+4(4)+4(5)+4(6)+4(7)+5(8)+3(9)+4(10)+3(11)+2(12)+(13)+(14)$
$(53)=2(1)+2(2)+3(3)+3(4)+4(5)+3(6)+4(7)+3(8)+3(9)+2(10)+2(11)+(12)+(13)$
$(4^2)=(0)+(2)+(3)+2(4)+(5)+2(6)+(7)+(8)+(9)+(10)+(12)$

where plethysms with Schur functions associated to nonstandard partitions are disregarded. The final result is obtained by expressing the Schur functions resulting from plethysms in terms of $O^+(3)$ irreps (L) using Eqs. (59)–(61).

In IBM-1 the $O^+(5)$ irrep (λ) is symmetric, then one uses Eqs. (71) and (72) with $\alpha_{\mu_1,\mu_2}=0$. The terms with $\alpha_{\mu_1,\mu_2}\neq 0$ will be used in IBM-2 and 3. In Table II the $O^+(5)\supset O^+(3)$ branching rules for $O^+(5)$ irreps with the lowest degrees are given.

Now let us find the branching rules in chain (II) of Eq. (67). To find the decomposition (35) for $U(6)\supset SU(3)$ in chain (II) one observes that the U(3) irreps must have the (L) multiplets (2) and (0) contained in irrep $\{1\}$ of U(6) [the reduction $U(3)\supset SU(3)$ has only one SU(3) irrep with labels given by Eq. (59)]. Using Elliott's rules (59)–(61) one sees that the U(3) irrep must be $\{2\}$. We then have

$$\{1\}=\{2\}\equiv(2,0) \quad \text{for } U(6)\supset U(3)\ [\text{or} \quad SU(3)]. \tag{73}$$

Using Eq. (73) and Eq. (36) one has that the U(3)[SU(3)] irreps contained in the irrep $\{\lambda\}$ of U(6) are

$$\{\lambda\}=\sum_{\mu}\ \alpha(\{2\}\otimes\{\lambda\}\rightarrow\{\mu\})\{\mu\}, \tag{74}$$

where in the plethysms only irreps with no more than three rows are considered and these produce SU(3) irreps $(\mu_1-\mu_2,\mu_2-\mu_3)$ in Elliott's notation. Table III presents the branching $U(6)\supset SU(3)$ for U(6) irreps with no more than three rows and the lowest degrees.

The branching rule in $SU(3)\supset O^+(3)\supset O^+(2)$ is given by Elliott's rules (59)–(61).

Since in IBM-1 the U(6) irrep $\{\lambda\}$ is a symmetric irrep $\{N\}$, the plethysm in Eq. (74) is given by Eq. (22) and one obtains

TABLE III. Branching rules for $U(6)\supset SU(3)$ for U(6) irreps with no more than three rows and lowest degrees.

$\{0\}=(0,0)$
$\{1\}=(2,0)$
$\{2\}=(4,0)+(0,2)$
$\{1^2\}=(2,1)$
$\{3\}=(6,0)+(2,2)+(0,0)$
$\{21\}=(4,1)+(2,2)+(1,1)$
$\{1^3\}=(3,0)+(0,3)$
$\{4\}=(8,0)+(4,2)+(0,4)+(2,0)$
$\{31\}=(6,1)+(4,2)+(2,3)+(1,2)+(2,0)+(3,1)$
$\{2^2\}=(4,2)+(0,4)+(2,0)+(3,1)$
$\{21^2\}=(5,0)+(2,3)+(1,2)+(0,1)+(3,1)$
$\{5\}=(10,0)+(6,2)+(2,4)+(4,0)+(0,2)$
$\{41\}=(8,1)+(6,2)+(4,3)+(5,1)+(2,4)+(3,2)+(4,0)+(1,3)+(2,1)+(0,2)$
$\{32\}=(6,2)+(4,3)+(5,1)+(2,4)+(3,2)+2(4,0)+(1,3)+(2,1)+(0,2)$
$\{31^2\}=(7,0)+(4,3)+(5,1)+2(3,2)+(0,5)+(1,3)+2(2,1)+(1,0)$
$\{2^21\}=(5,1)+(2,4)+(3,2)+(4,0)+(1,3)+(2,1)+(0,2)$
$\{6\}=(12,0)+(8,2)+(4,4)+(6,0)+(0,6)+(2,2)+(0,0)$
$\{51\}=(10,1)+(8,2)+(6,3)+(7,1)+(4,4)+(5,2)+(6,0)+(2,5)+(3,3)+(4,1)+(1,4)+2(2,2)+(1,1)$
$\{42\}=(8,2)+(6,3)+(7,1)+2(4,4)+(5,2)+2(6,0)+2(3,3)+2(4,1)+(0,6)+(1,4)+3(2,2)+(1,1)+(0,0)$
$\{41^2\}=(9,0)+(6,3)+(7,1)+2(5,2)+(2,5)+2(3,3)+2(4,1)+(1,4)+(2,2)+2(3,0)+2(0,3)+(1,1)$
$\{3^2\}=(6,3)+(5,2)+(6,0)+(2,5)+(3,3)+(4,1)+(2,2)+(3,0)+(0,3)$
$\{321\}=(7,1)+(4,4)+2(5,2)+(6,0)+(2,5)+2(3,3)+3(4,1)+2(1,4)+3(2,2)+(3,0)+(0,3)+2(1,1)$
$\{2^3\}=(6,0)+(3,3)+(0,6)+2(2,2)+(0,0)$
$\{7\}=(14,0)+(10,2)+(6,4)+(8,0)+(2,6)+(4,2)+(0,4)+(2,0)$
$\{61\}=(12,1)+(10,2)+(8,3)+(9,1)+(6,4)+(7,2)+(8,0)+(4,5)+(5,3)+(6,1)+(2,6)+(3,4)+2(4,2)$
$+(1,5)+(2,3)+(3,1)+(0,4)+(1,2)+(2,0)$
$\{52\}=(10,2)+(8,3)+(9,1)+2(6,4)+(7,2)+2(8,0)+(4,5)+2(5,3)+2(6,1)+(2,6)+2(3,4)+4(4,2)+(1,5)$
$+2(2,3)+2(3,1)+2(0,4)+(1,2)+2(2,0)$
$\{51^2\}=(11,0)+(8,3)+(9,1)+2(7,2)+(4,5)+2(5,3)+2(6,1)+2(3,4)+(4,2)+2(5,0)+(0,7)+(1,5)$
$+3(2,3)+2(3,1)+2(1,2)+(0,1)$

$$\{N\}=\sum_{\mu_1,\mu_2,\mu_3}\{2\mu_1,2\mu_2,2\mu_3\}\equiv\sum_{\mu_1\mu_2\mu_3}(2(\mu_1-\mu_2),2(\mu_2-\mu_3)), \tag{75}$$

where (μ_1,μ_2,μ_3) are (standard)partitions of N into three parts.

The branching for the first link $U(6)\supset O^+(6)$ in chain (III) is found using Eq. (57). Note that in (57) the branching is for $U(n)\supset O(n)$ and we need a further reduction $O(n)\supset O^+(n)$. For the cases treated here the O(6) and $O^+(6)$ irreps are the same.

In IBM-1 the U(6) irrep $\{\lambda\}$ being symmetric implies that Eq. (57) has a simple expression:

$$\{N\}=(N)+(N-2)+\cdots+(0)\quad\text{or}\quad(1)\quad\text{for } U(6)\supset O^+(6). \tag{76}$$

To find the branching rule in the link $O^+(6)\supset O^+(5)$ one first observes that Eq. (42) gives

$$(1)=(1)+(0)\quad\text{for } O^+(6)\supset O^+(5). \tag{77}$$

Next one writes the $O^+(6)$ irrep (λ) in terms of U(6) irreps $\{\mu\}$:

$$(\lambda)=\sum_{\mu}\ \alpha_{\mu}\{\mu\} \tag{78}$$

and computes the plethysm

$$((1)+(0))\otimes(\lambda)=\sum_{\mu}\ \alpha_{\mu}((1)+(0))\otimes\{\mu\}=\sum_{\mu}\ \alpha_{\mu}\left[\sum_{\nu',k}\ \alpha(\{\nu'\}\{k\}\rightarrow\{\mu\})\{\nu'\}\right]. \tag{79}$$

The resulting U(5) irreps are then converted into $O^+(5)$ irreps by use of Eq. (57).

In IBM-1 the $O^+(6)$ irrep is symmetric and, in this case, Eq. (78) becomes

$$(0)=\{0\},\quad (1)=\{1\}\quad \text{and}\ (k)=\{k\}-\{k-2\}\quad \text{for}\ k\geqslant 2 \tag{80}$$

and Eq. (79) gives

$$((1)+(0))\otimes(k)=\sum_{p,q}\ [\alpha(\{p\}\{q\}\rightarrow\{k\})-\alpha(\{p\}\{q\}\rightarrow\{k-2\})]\{p\}. \tag{81}$$

Expressing $\{p\}$ in terms of $O^+(5)$ irreps by means of Eq. (58) one has the final result

$$(k)=(k)+(k-1)+\cdots+(0)\quad \text{for}\ O^+(6)\supset O^+(5). \tag{82}$$

For general $O^+(6)$ irreps $(\sigma)=(\sigma_1,\sigma_2,\sigma_3)$, computer calculations using Eq. (79) shows the branching rule

$$(\sigma)=\sum_{\rho_1=\sigma_2}^{\sigma_1}\ \sum_{\rho_2=\sigma_3}^{\sigma_2}\ (\rho_1,\rho_2)\quad \text{for}\ O^+(6)\supset O^+(5), \tag{83}$$

the usual inbetweeness conditions for Gelfand labels.

IV. IBM-2

In IBM-2 two kinds of bosons are considered, one formed by proton pairs and other by neutron pairs, denoted by

$$s^{\dagger}_{\pi},\ d^{\dagger}_{\pi,\mu},\quad s^{\dagger}_{\nu},\ d^{\dagger}_{\nu,\mu},\quad \mu=0,\pm 1,\pm 2,\quad \pi\quad \text{for protons},\quad \nu\quad \text{for neutrons} \tag{84}$$

and similarly for annihilation operators. The commutation relations are the same as Eq. (65) concerning angular momentum labels and neutron operators commute with proton operators.

Using the compact notation

$$b^{\dagger}_{\rho,\alpha},\ b_{\rho,\alpha},\quad \rho=\pi,\nu,\quad \alpha=1,2,\ldots,6, \tag{85}$$

the commutation relations become

$$[b_{\rho\alpha},b^{\dagger}_{\rho'\alpha'}]=\delta_{\rho\rho'}\delta_{\alpha\alpha'},\ \ [b_{\rho\alpha},b_{\rho'\alpha'}]=[b^{\dagger}_{\rho\alpha},b^{\dagger}_{\rho'\alpha'}]=0. \tag{86}$$

With these operators one constructs operators

$$\mathcal{C}^{\rho'\alpha'}_{\rho\alpha}=b^{\dagger}_{\rho\alpha}b_{\rho'\alpha'} \tag{87}$$

that under commutation close the Lie algebra of U(12). The operators $C_{\alpha}^{\alpha'}=\mathcal{C}_{\pi\alpha}^{\pi\alpha'}$ and $\mathcal{C}_{\alpha}^{\alpha'}=\mathcal{C}_{\nu\alpha}^{\nu\alpha'}$ generate the Lie algebras of $U_{\pi}(6)$ and $U_{\nu}(6)$, respectively. We have then a particular case of the reduction $U(n_1+n_2)\supset U(n_1)\oslash U(n_2)$ studied in Sec. II B. Using the results there obtained one has the branching rule

$$\{\lambda\}=\sum_{\lambda',\lambda''}\alpha(\{\lambda'\}\{\lambda''\}\rightarrow\{\lambda\})\{\lambda'\}_{\pi}\{\lambda''\}_{\nu} \quad \text{for } U(12)\supset U_{\pi}(6)\oslash U_{\nu}(6). \tag{88}$$

With operators (84) [or (85)] one can construct only symmetrical irreps $\{N\}$ of U(12) and Eq. (88) reduces to

$$\{N\}=\sum_{k=0}^{N}\{N-k\}_{\pi}\{k\}_{\nu} \quad \text{for } U(12)\supset U_{\pi}(6)\oslash U_{\nu}(6). \tag{89}$$

The basis states of irrep $\{N\}$ must be also basis states for an irrep of $O_{\pi+\nu}^{+}(3)$, the group of simultaneous rotations of protons and neutrons. This can be achieved by use of *lattice of algebras*, in contrast with *chains of algebras* in IBM-1.

The simplest lattice is obtained when we use chains (I), (II), and (III) separately for protons and for neutrons and only in the last step one couples $O_{\pi}^{+}(3)$ with $O_{\nu}^{+}(3)$ to obtain $O_{\pi+\nu}^{+}(3)$:

$$\begin{array}{ccccccccc}
 & & & \nearrow U_{\pi}(5)\supset & O_{\pi}^{+}(5)\searrow & & & & \\
 & & U_{\pi}(6) & \rightarrow SU_{\pi}(3) & \rightarrow & O_{\pi}^{+}(3) & & & \\
 & \nearrow & & \searrow O_{\pi}^{+}(6)\supset & O_{\pi}^{+}(5)\nearrow & & \searrow & & \\
U(12) & & & & & & & O_{\pi+\nu}^{+}(3)\supset & O_{\pi+\nu}^{+}(2). \\
 & \searrow & & \nearrow U_{\nu}(5)\supset & O_{\nu}^{+}(5)\searrow & & \nearrow & & \\
 & & U_{\nu}(6) & \rightarrow SU_{\nu}(3) & \rightarrow & O_{\nu}^{+}(3) & & & \\
 & & & \searrow O_{\nu}^{+}(6)\supset & O_{\nu}^{+}(5)\nearrow & & & &
\end{array} \tag{90}$$

This is a trivial extension of IBM-1 and L_{π} and L_{ν} are coupled to give

$$L_{\pi+\nu}=L_{\pi}+L_{\nu}, \quad L_{\pi}+L_{\nu}-1,\ldots,|L_{\pi}-L_{\nu}|. \tag{91}$$

Another lattice is

$$\begin{array}{ccccccc}
U_{\pi}(6) & & & U_{\pi+\nu}(5)\supset O_{\pi+\nu}^{+}(5) & & & (I_1) \\
 & \searrow & \nearrow & & \searrow & & \\
 & U_{\pi+\nu}(6) & \rightarrow SU_{\pi+\nu}(3) & & \rightarrow & O_{\pi+\nu}^{+}(3)\supset O_{\pi+\nu}^{+}(2) & (II_1) \\
 & \nearrow & \searrow & & \nearrow & & \\
U_{\nu}(6) & & & O_{\pi+\nu}^{+}(6)\supset O_{\pi+\nu}^{+}(5) & & & (III_1)
\end{array} \tag{92}$$

in which the algebras of $U_{\pi}(6)$ and $U_{\nu}(6)$ are joined in the first step. In the first link one has $U_{\pi}(6)\times U_{\nu}(6)\rightarrow U_{\pi+\nu}(6)$ and the branching rules are given by the Kronecker product of U(6) irreps. In this case, the irreps of $U_{\pi}(6)$ and $U_{\nu}(6)$ are both symmetric by Eq. (89) and the irreps of $U_{\pi+\nu}(6)$ can have one or two rows. Chains (I_1), (II_1), and (III_1) are the same as (I), (II), and (III) but now the U(6), U(5), $O^{+}(6)$, and $O^{+}(6)$ irreps can be two-rowed.

Another type of lattice of algebras is obtained by joining the neutron and proton algebras at the second step:

$$
\begin{array}{lll}
\mathrm{U}_\pi(6)\supset\mathrm{U}_\pi(5) & & \\
\qquad\searrow & & \\
\qquad\quad \mathrm{U}_{\pi+\nu}(5)\supset\mathrm{O}^+_{\pi+\nu}(5)\supset\mathrm{O}^+_{\pi+\nu}(3)\supset\mathrm{O}^+_{\pi+\nu}(2) & (\mathrm{I}_2), & \\
\qquad\nearrow & & \\
\mathrm{U}_\nu(6)\supset\mathrm{U}_\nu(5) & & \\
\mathrm{U}_\pi(6)\supset\mathrm{SU}_\pi(3) & & \\
\qquad\searrow & & \\
\qquad\quad \mathrm{SU}_{\pi+\nu}(3)\supset\mathrm{O}^+_{\pi+\nu}(3\supset\mathrm{O}^+_{\pi+\nu}(2), & (\mathrm{II}_2), & (93)\\
\qquad\nearrow & & \\
\mathrm{U}_\nu(6)\supset\mathrm{SU}_\nu(3) & & \\
\mathrm{U}_\pi(6)\supset\mathrm{O}^+_\pi(6) & & \\
\qquad\searrow & & \\
\qquad\quad \mathrm{O}^+_{\pi+\nu}(6)\supset\mathrm{O}^+_{\pi+\nu}(5)\supset\mathrm{O}^+_{\pi+\nu}(3)\supset\mathrm{O}^+_{\pi+\nu}(2) & (\mathrm{III}_2). & \\
\qquad\nearrow & & \\
\mathrm{U}_\nu(6)\supset\mathrm{O}^+_\nu(6) & &
\end{array}
$$

The branching rules for the irreps of the joined algebras are obtained by Kronecker products and the resulting irreps can be one- and two-rowed. The Kronecker product expansion of irreps of unitary groups are given by the outer product of Schur functions:

$$\{\lambda\}_\pi\{\mu\}_\nu=\sum_\rho\ \alpha(\{\lambda\}\{\mu\}\to\{\rho\})\{\rho\}_{\pi+\nu}. \tag{94}$$

The Kronecker product of O(6) irreps is done by expressing the O(6) characters in terms of Schur functions, making the outer products and re-expressing the result in terms of O(6) irreps. In Table IV we give the Kronecker product of O(6) irreps with the lowest product degrees.

V. IBM-3

This model was proposed by Elliott and White[23] in order to take into account the isospin degree of freedom. It differs from IBM-2 by the inclusion of a third kind of boson, the δ-boson, formed by a proton–neutron pair. There are 18 creation operators

$$s^\dagger_\pi,\ d^\dagger_{\pi,\mu},\ s^\dagger_\nu,\ d^\dagger_{\nu,\mu},\ s^\dagger_\delta,\ d^\dagger_{\delta,\mu}\quad(\mu=0,\pm1,\pm2) \tag{95}$$

and the corresponding annihilation operators. Operators of different pairs of bosons commute among themselves while each set π, ν and δ satisfies bose commutation relations.

One has again lattices of algebras now starting with

$$\mathrm{U}(18)\supset\mathrm{U}_\pi(6)\oslash\mathrm{U}_\nu(6)\oslash\mathrm{U}_\delta(6) \tag{96}$$

and ending with $\mathrm{O}^+_{\pi+\nu+\delta}(3)\supset\mathrm{O}^+_{\pi+\nu+\delta}(2)$.

By an extension of the calculation done to obtain Eq. (54) one obtains

$$\{\lambda\}=\sum_{\mu,\sigma,\rho}\ \alpha(\{\mu\}\{\sigma\}\{\rho\}\to\{\lambda\})\{\mu\}_\pi\{\sigma\}_\nu\{\rho\}_\delta\quad\text{for }\mathrm{U}_\pi(6)\oslash\mathrm{U}_\nu(6)\oslash\mathrm{U}_\delta(6). \tag{97}$$

Since in IBM-3 the U(18) irrep is symmetric, Eq. (97) reduces to

TABLE IV. Kronecker product of O(6) irreps with lowest total degrees.

$(1)(1)=(0)+(1^2)+(2)$
$(2)(1)=(1)+(21)+(3)$
$(1^2)(1)=(1)+(1^3)+(21)$
$(3)(1)=(2)+(31)+(4)$
$(21)(1)=(1^2)+(2)+(21^2)+(2^2)+(31)$
$(1^3)(1)=(1^2)+(21^2)$
$(2)(2)=(0)+(1^2)+(2)+(2^2)+(31)+(4)$
$(1^2)(2)=(1^2)+(2)+(21^2)+(31)$
$(1^2)(1^2)=(0)+(1^2)+(2)+(21^2)+(2^2)$
$(4)(1)=(3)+(41)+(5)$
$(31)(1)=(21)+(3)+(31^2)+(32)+(41)$
$(2^2)(1)=(21)+(2^21)+(32)$
$(21^2)(1)=(1^3)+(21)+(2^21)+(31^2)$
$(3)(2)=(1)+(21)+(3)+(32)+(41)+(5)$
$(21)(2)=(1)+(1^3)+2(21)+(2^21)+(3)+(31^2)+(32)+(41)$
$(1^3)(2)=(1^3)+(21)+(31^2)$
$(3)(1^2)=(21)+(3)+(31^2)+(41)$
$(21)(1^2)=(1)+(1^3)+2(21)+(2^21)+(3)+(31^2)+(32)$
$(1^3)(1^2)=(1)+(1^3)+(21)+(2^21)$
$(5)(1)=(4)+(51)+(6)$
$(41)(1)=(31)+(4)+(41^2)+(42)+(51)$
$(32)(1)=(2^2)+(31)+(321)+(3^2)+(42)$
$(31^2)(1)=(21^2)+(31)+(321)+(41^2)$
$(2^21)(1)=(21^2)+(2^2)+(2^3)+(321)$
$(4)(2)=(2)+(31)+(4)+(42)+(51)+(6)$
$(31)(2)=(1^2)+(2)+(21^2)+(2^2)+2(31)+(321)+(3^2)+(4)+(41^2)+(42)+(51)$
$(2^2)(2)=(2)+(21^2)+(2^2)+(2^3)+(31)+(321)+(42)$
$(21^2)(2)=(1^2)+2(21^2)+(2^2)+(31)+(321)+(41^2)$
$(4)(1^2)=(31)+(4)+(41^2)+(51)$
$(31)(1^2)=(2)+(21^2)+(2^2)+2(31)+(321)+(4)+(41^2)+(42)$
$(2^2)(1^2)=(1^2)+(21^2)+(2^2)+(31)+(321)+(3^2)$
$(21^2)(1^2)=(1^2)+(2)+2(21^2)+(2^2)+(2^3)+(31)+(321)$
$(3)(3)=(0)+(1^2)+(2)+(2^2)+(31)+(3^2)+(4)+(42)+(51)+(6)$

$$\{N\}=\sum_{p=0}^{N}\sum_{q=0}^{N-p}\{p\}_\pi\{q\}_\nu\{N-p-q\}_\delta \quad \text{for } \mathrm{U}_\pi(6)\oslash\mathrm{U}_\nu(6)\oslash\mathrm{U}_\delta(6). \tag{98}$$

As in IBM-2, a trivial lattice is obtained joining the three algebras in the first step by the link

$$\mathrm{U}_\pi(6)\oslash\mathrm{U}_\nu(6)\oslash\mathrm{U}_\delta(6)\supset\mathrm{U}_{\pi+\nu+\delta}(6). \tag{99}$$

In this case we will have a triple Kronecker product of U(6) irreps and the resulting $\mathrm{U}_{\pi+\nu+\delta}(6)$ irreps can be three-rowed. From this point on one follows chains (I), (II), and (III) in which the irreps of U(5) and O(6) can be three-rowed and those of O(5) two-rowed.

A more interesting lattice, from the physical point of view, is the one that works separately with space and isospin degrees of freedom and joins then at the end. To this end let us denote creation and annihilation operators by

$$b^\dagger_{\rho\ell m},\quad b_{\rho\ell m}\quad (\rho=\pi,\nu,\delta,\quad m=-\ell,-\ell+1,\ldots,\ell),$$

or

$$b^{\dagger}_{\rho\alpha}, \quad b_{\rho\alpha} \quad (\rho=\pi,\nu,\delta, \quad \alpha=1,2,\ldots,6) \tag{100}$$

so that the commutation relations read as

$$[b_{\rho\alpha},b^{\dagger}_{\rho'\alpha'}]=\delta_{\rho\rho'}\delta_{\alpha\alpha'}, \quad [b_{\rho\alpha},b_{\rho'\alpha'}]=[b^{\dagger}_{\rho\alpha},b^{\dagger}_{\rho'\alpha'}]=0. \tag{101}$$

The U(18) infinitesimal generators will then be realized by

$$\mathcal{C}^{\rho'\alpha'}_{\rho\alpha}=b^{\dagger}_{\rho\alpha}b_{\rho'\alpha'}, \tag{102}$$

while

$$C^{\rho'}_{\rho}=\sum_{\alpha=1}^{6}\mathcal{C}^{\rho'\alpha}_{\rho\alpha} \quad \text{and} \quad \mathcal{C}^{\alpha'}_{\alpha}=\sum_{\rho=1}^{3}\mathcal{C}^{\rho\alpha'}_{\rho\alpha} \tag{103}$$

are generator of the Lie algebras of $U_S(6)$ (space) and $U_T(3)$ (isospin), respectively.

We then have as first link in this lattice,

$$U(18)\supset U_S(6)\times U_T(3). \tag{104}$$

The U(18) irrep will be symmetric and, according to Eq. (56), the branching law in Eq. (104) will be

$$\{N\}=\sum_{n_1,n_2,n_3}\{n_1,n_2,n_3\}_S\{n_1,n_2,n_3\}_T, \tag{105}$$

where (n_1,n_2,n_3) is a (standard) partition of N into three parts.

For $U_T(3)$ one uses the chain $U_T(3)\supset O^+_T(3)\supset O^+_T(2)$ and the branching rule is given by Elliott's rules, Eqs. (59)–(61).

From $U_S(6)$ one can follow each of chains (I), (II), and (III) and use the results of Sec. III for three-rowed U(6) irreps.

For $U_S(6)\supset U_S(5)$, Eqs. (50) and (51) give

$$\{f_1,f_2,f_3\}=\sum_{f'_1=f_2}^{f_1}\sum_{f'_2=f_3}^{f_2}\sum_{f'_3=0}^{f_3}\{f'_1,f'_2,f'_3\}. \tag{106}$$

For $U(5)\supset O(5)$ one uses Eq. (57) and Table I. The three-rowed $O^+(5)$ irreps $(\omega_1,\omega_2,\omega_3)$ in Eq. (57) must be interpreted using the modification rules

$$(\omega_1,\omega_2,1)\equiv(\omega_1,\omega_2), \quad (\omega_1,\omega_2,\omega_3>1) \ \text{disregarded.} \tag{107}$$

For $O^+(6)\supset O^+(5)$ one uses Eq. (83).

For $U_S(6)\supset SU_S(3)$ one uses Eq. (74) where now Schur functions $\{\mu\}$ with up to three rows must be considered.

VI. IBM-4

In IBM-4, proposed by Elliott and Evans,[24] the bosonic pairs, besides the spatial degree of freedom, have also spin–isospin degrees of freedom in the combination $S=0$, $T=1$ and $S=1$, $T=0$. The model has thus $6\times6=36$ bosonic creation operators

$$b^{\dagger}_{(\ell m_\ell)(Sm_S)(Tm_T)} \quad \text{with} \quad \ell=0,2,\ -\ell\leqslant m_\ell\leqslant\ell,$$

$$S=m_S=0,\ T=1,\ m_T=0,\pm1,$$

$$S=1,\ m_S=0,\pm1,\ T=m_T=0 \tag{108}$$

and corresponding annihilation operators. The operators

$$\mathcal{C}^{(\ell' m'_\ell)(S' m'_S)(T' m'_T)}_{(\ell m_\ell)(Sm_S)(Tm_T)}=b^{\dagger}_{(\ell m_\ell)(Sm_S)(Tm_T)}b_{(\ell' m'_\ell)(S' m'_S)(T' m'_T)} \tag{109}$$

generate the Lie algebra of U(36) while

$$C^{(S' m'_S)(T' m'_T)}_{(Sm_S)(Tm_T)}=\sum_{\ell m_\ell}\mathcal{C}^{(\ell m_\ell)(S' m'_S)(T' m_T)'}_{(\ell m_\ell)(Sm_S)(Tm_T)} \quad \text{and} \quad \mathcal{C}^{\ell' m'_\ell}_{\ell m_\ell}=\sum_{Sm_STm_T}\mathcal{C}^{(\ell' m'_\ell)(Sm_S)(Tm_T)}_{(\ell m_\ell)(Sm_S)(Tm_T)} \tag{110}$$

generate the Lie algebras of $\mathrm{U}_{ST}(6)$ and $\mathrm{U}_L(6)$ in the chain

$$\mathrm{U}(36)\supset\mathrm{U}_L(6)\times\mathrm{U}_{ST}(6). \tag{111}$$

An arbitrary irrep of U(36) branches into irreps of $\mathrm{U}_L(6)\times\mathrm{U}_{ST}(6)$ according to Eq. (56). Since the U(36) irreps that one can realize with (108) and (109) are only symmetric ones, Eq. (56) gives

$$\{N\}=\sum_{\mu}\{\mu\}_L\{\mu\}_{ST}, \tag{112}$$

where (μ) are (standard) partitions of N into six parts. For $\mathrm{U}_L(6)$ one follows chains (I), (II), and (III), now with all irreps in their greatest generality.

To treat $\mathrm{U}_{ST}(6)$ one observes that

$$C^{(00)(1m')}_{(00)(1m)} \quad \text{and} \quad C^{(1m)(00)}_{(1m)(00)}$$

generate the Lie algebras of $\mathrm{U}_S(6)$ and $\mathrm{U}_T(3)$ in the link

$$\mathrm{U}_{ST}(6)\supset\mathrm{U}_S(3)\oslash\mathrm{U}_T(3), \tag{113}$$

which allows us to treat spin and isospin separately. The branching rules in this link are given by Eq. (54):

$$\{\lambda\}=\sum_{\mu\nu}\alpha(\{\mu\}\{\nu\}\to\{\lambda\})\{\mu\}_S\{\nu\}_T \quad \text{for } \mathrm{U}_{ST}(6)\supset\mathrm{U}_S(3)\oslash\mathrm{U}_T(3). \tag{114}$$

The simplest case is when $\{\lambda\}$ is symmetric,

$$\{N\}_{ST}=\sum_{k=0}^{N}\{N-k\}_S\{k\}_T. \tag{115}$$

The next one is

$$\{N-1,1\}=\sum_{k=1}^{N-1}\{k\}_S\{N-k\}_T+\sum_{k=2}^{N}[\{N-k\}_S\{k-1,1\}_T+\{k-1,1\}_S\{N-k\}_T]. \tag{116}$$

Another chain of interest is

$$U_{ST}(6)\supset SU_{ST}(4)\supset SU_S(2)\times SU_T(2). \tag{117}$$

To find the reduction (35) for this chain one observes that the basis states for irrep $\{1\}$ of $U_{ST}(6)$ are

$$\sum_{\ell m_\ell} b^\dagger_{(\ell m_\ell)(Sm_S)(Tm_T)}|0\rangle \quad \text{with } S=M_S=0, \quad T=1, \quad M_T=0,\pm 1,$$

$$S=1, \quad m_S=0,\pm 1, \quad T=m_T=0. \tag{118}$$

The states with the first and second sets of labels are basis states for irreps $\{0\}_S\{1\}_T$ and $\{1\}_S\{0\}_T$ of $SU_S(2)\times SU_T(2)$, respectively. The U(4) irrep $\{11\}$ has exactly this $SU_S(2)\times SU_T(2)$ reduction, so one has

$$\{1\}=\{11\} \text{ for } U_{ST}(6)\supset U_{ST}(4)[SU_{ST}(4)] \tag{119}$$

and according to Eq. (36) one has the branching rule

$$\{\lambda\}=\sum_\mu \alpha(\{11\}\otimes\{\mu\}\to\{\lambda\})\{\mu\}, \quad \text{for} \quad U_{ST}(6)\supset U_{ST}(4)[SU_{ST}(4)], \tag{120}$$

where only the Schur functions with up to four rows are considered in the plethysm. This plethysm can be computed by use of Eq. (23) as input in the algorithm given in Sec. II A. In Table V one gives the branching rules for the reduction $U_{ST}(6)\supset U_{ST}(4)$ for $U_{ST}(6)$ irreps with the lowest degrees.

The branching rules for the reduction $U(4)\supset SU(2)\times SU(2)$ are given by Eq. (56). Table 11-18 in Ref. 25 gives the branching rules for this reduction for U(3) irreps of degrees up to 10.

VII. IBM-1 G AND F

IBM-1 can be extended by introducing bosons with angular momenta 3,4,.... In order to deal with states of positive parity only bosons with even angular momenta are introduced. Bosons with odd angular momenta are used to deal with spectra with even and odd parity levels.

The inclusion of boson pairs of angular momenta $\ell=4$ in IBM-1 gave birth to IBM-1G. In this model one has the boson creation operators

$$b_{\ell m} \quad \text{with} \quad \ell=0,2,4, \quad -\ell\leqslant m\leqslant \ell \tag{121}$$

and the corresponding annihilation operators and the group involved will be U(15). One then has to search for chains ending with $O^+(3)\supset O^+(2)$. One of such chains,

$$U(15)\supset SU(3)\supset O^+(3)\supset O^+(2) \tag{122}$$

was studied in Ref. 26. There, the generators of the Lie algebra of SU(3) in chain (122) are realized as

$$\begin{aligned} X^{(1)}_\mu &= \sqrt{1/7}\ [d^\dagger\times\tilde{d}]^{(1)}_\mu+\sqrt{6/7}\ [g^\dagger\times\tilde{g}]^{(1)}_\mu, \\ X^{(2)}_\mu &= \sqrt{1/70}\ \{4\sqrt{7/15}\ [d^\dagger\times\tilde{s}+s^\dagger\times\tilde{d}\ ]^{(2)}_\mu-11\sqrt{2/21}\ [d^\dagger\times\tilde{d}]^{(2)}_\mu \\ &\quad +36\sqrt{1/105}\ [d^\dagger\times\tilde{g}+g^\dagger\times\tilde{d}]^{(2)}_\mu-2\sqrt{33/7}\ [g^\dagger\times\tilde{g}]^{(2)}_\mu]\}, \end{aligned} \tag{123}$$

where $[T^{(k_1)}\times T^{(k_2)}]^{(k)}_m$ denotes coupling of $O^+(3)$ Racah tensors via Clebsch–Gordan coefficients to produce m components of $O^+(3)$ tensors of rank k and $\tilde{b}$, as in Ref. 15, is defined by $\tilde{b}_{\ell m}=(-)^{\ell-m}b_{\ell-m}$.

TABLE V. $U_{ST}(6)\supset U_{ST}(4)$ branching rules for $U_{ST}(6)$ irreps with no more than 4 rows and lowest degrees.

$\{1\}=\{1^2\}$
$\{2\}=\{1^4\}+\{2^2\}$
$\{1^2\}=\{21^2\}$
$\{3\}=\{3^2\}+\{2^21^2\}$
$\{21\}=\{321\}+\{2^21^2\}$
$\{1^3\}=\{31^3\}+\{2^3\}$
$\{4\}=\{4^2\}+\{3^21^2\}+\{2^4\}$
$\{31\}=\{431\}+\{3^21^2\}+\{32^21\}$
$\{2^2\}=\{42^2\}+\{3^21^2\}+\{2^4\}$
$\{21^2\}=\{421^2\}+\{3^22\}+\{32^21\}$
$\{1^4\}=\{32^21\}$
$\{5\}=\{3^22^2\}+\{4^21^2\}+\{5^2\}$
$\{41\}=\{541\}+\{4^21^2\}+\{4321\}+\{3^22^2\}$
$\{32\}=\{532\}+\{4^21^2\}+\{4321\}+\{3^22^2\}$
$\{31^2\}=\{531^2\}+\{4^22\}+\{4321\}+\{42^3\}+\{3^31\}$
$\{2^21\}=\{52^21\}+\{43^2\}+\{4321\}+\{3^22^2\}$
$\{21^3\}=\{4321\}+\{42^3\}+\{3^31\}$
$\{6\}=\{3^4\}+\{4^22^2\}+\{5^21^2\}+\{6^2\}$
$\{51\}=\{651\}+\{5^21^2\}+\{5421\}+\{4^22^2\}+\{43^22\}$
$\{42\}=\{642\}+\{5^21^2\}+\{5421\}+\{53^21\}+2\{4^22^2\}+\{3^4\}$
$\{41^2\}=\{641^2\}+\{5^22\}+\{5421\}+\{532^2\}+\{4^231\}+\{43^22\}$
$\{3^2\}=\{63^2\}+\{5421\}+\{43^22\}$
$\{321\}=\{6321\}+\{543\}+\{5421\}+\{53^21\}+\{532^2\}$
$+\{4^231\}+\{4^22^2\}+\{43^22\}$
$\{31^3\}=\{5421\}+\{532^2\}+\{4^231\}+\{43^22\}$
$\{2^3\}=\{62^3\}+\{53^21\}+\{4^3\}+\{4^22^2\}+\{3^4\}$
$\{2^21^2\}=\{53^21\}+\{532^2\}+\{4^231\}+\{43^22\}$
$\{7\}=\{4^23^2\}+\{5^22^2\}+\{6^21^2\}+\{7^2\}$
$\{61\}=\{761\}+\{6^21^2\}+\{6521\}+\{5^22^2\}+\{5432\}+\{4^23^2\}$
$\{52\}=\{752\}+\{6^21^2\}+\{6521\}+\{6431\}+2\{5^22^2\}$
$+\{5432\}+\{4^23^2\}$
$\{51^2\}=\{751^2\}+\{6^22\}+\{6521\}+\{642^2\}+\{5^231\}+\{5432\}$
$+\{53^3\}+\{4^32\}$
$\{43\}=\{743\}+\{6521\}+\{6431\}+\{5^22^2\}+\{5432\}+\{4^23^2\}$

To find how the U(15) irrep $\{1\}$ branches into irreps of chain (122) one observes that this irrep has three sub-bases with basis vectors $s^+|0\rangle, d^+_\mu|0\rangle$, and $g^+_\mu|0\rangle$ that are left invariant by the action of generators $X^{(1)}_\mu$, showing that $\{1\}$ contains $L=0,2,4$ multiplets. On the other hand, the generators $X^{(2)}_\mu$ mix these sub-bases showing that the SU(3) irrep contained in $\{1\}$ is irreducible. Examining the L-content of SU(3) irreps of dimension 15 one finds that the irrep $\{4\}$ has these L multiplets. Therefore one has

$$\{1\}=\{4\} \quad \text{for} \quad U(15)\supset U(3)[SU(3)] \tag{124}$$

in chain (122).

From Eq. (36) one then obtains

$$\{\lambda\}=\sum_\mu \alpha(\{4\}\otimes\{\lambda\}\to\{\mu\})\{\mu\} \quad \text{for} \quad U(15)\supset U(3), \tag{125}$$

where in the plethysm only the Schur functions $\{\mu\}$ with no more than three rows are considered. As before, only U(15) symmetric irreps are realized, so the only *reduced* plethysms needed are $\{4\}\otimes\{m\}$. Table VI lists the $U(15)\supset SU(3)$ branching rules for U(15) symmetric irreps with lowest degrees

TABLE VI. $U(15)\supset SU(3)$ branching rules for symmetric U(15) irreps of lowest degrees.

$\{0\}=\{0\}$
$\{1\}=(4,0)$
$\{2\}=(0,4)+(8,0)+(4,2)$
$\{3\}=(0,0)+(0,6)+(2,2)+(3,3)+(4,4)+(6,3)+(8,2)+(6,0)+(12,0)$
$\{4\}=2(4,0)+(0,2)+(1,3)+2(2,4)+(3,5)+2(4,6)+(12,2)+2(8,4)+(5,1)+(4,3)+2(6,2)+(8,1)$
$+(10,0)+(5,4)+(7,3)+(0,8)+(16,0)+(10,3)$
$\{5\}=2(0,4)+(2,3)+4(4,2)+(6,1)+3(8,0)+2(2,0)+(3,1)+2(8,3)+(16,2)+2(3,4)+3(5,3)+(1,5)$
$+3(2,6)+2(4,5)+4(6,4)+(14,3)+(1,8)+(3,7)+(5,6)+2(7,5)+(0,10)+(20,0)+2(4,8)+(6,7)$
$+2(8,6)+3(10,2)+(9,4)+(12,1)+(11,3)+(10,5)+(14,0)+2(9,1)+2(12,4)+(7,2)$
$\{6\}=2(0,0)+2(9,6)+4(2,2)+4(3,3)+7(4,4)+(6,9)+2(5,8)+2(1,4)+2(4,1)+2(2,5)+2(5,2)+5(6,3)$
$+4(0,6)+5(6,0)+3(7,1)+7(8,2)+2(4,10)+2(10,1)+4(12,0)+5(5,5)+3(4,7)+4(7,4)+6(6,6)$
$+5(9,3)+4(8,5)+2(11,2)+5(10,4)+3(12,3)+3(14,2)+(13,4)+3(12,6)+(16,1)+(15,3)+(14,5)$
$+(18,0)+(24,0)+2(16,4)+3(8,8)+(18,3)+(20,2)+2(1,7)+4(3,6)+4(2,8)+2(7,7)+2(13,1)$
$+2(11,5)+(10,7)+2(0,12)+2(3,9)$
$\{7\}=5(4,0)+5(9,2)+13(8,4)+8(7,6)+8(6,8)+2(5,10)+8(10,3)+8(9,5)+6(8,7)+3(7,9)+6(11,4)$
$+8(10,6)+3(9,8)+5(12,5)+3(11,7)+2(13,6)+3(0,2)+(2,1)+3(1,3)+3(3,2)+9(2,4)+4(5,1)$
$+7(4,3)+11(6,2)+(28,0)+3(1,6)+8(3,5)+8(5,4)+9(7,3)+5(0,8)+4(2,7)+12(4,6)+9(6,5)$
$+8(5,7)+4(4,9)+2(3,11)+(19,3)+3(4,12)+(6,11)+3(8,10)+2(10,9)+5(3,8)+5(2,10)+(1,12)$
$+(24,2)+(22,3)+6(8,1)+7(10,0)+5(11,1)+9(12,2)+(0,14)+2(20,4)+3(14,1)+4(16,0)+4(1,9)$
$+(22,0)+6(13,3)+2(15,2)+6(14,4)+3(16,3)+2(17,1)+3(18,2)+2(15,5)+(17,4)+3(12,8)$
$+2(14,7)+3(16,6)+(18,5)+(20,1)$

In IBM-1F one considers boson pairs with angular momenta 0, 2, and 3 and the resulting group is U(13). For physical reasons it is interesting to single out the bosons with odd angular momentum and then one will have lattices of groups like

$$\begin{array}{ccccccc} & & \nearrow & \mathrm{U}(5)\supset \mathrm{O}^+(5) & \searrow & & \\ & \mathrm{U}_{sd}(6) & \to & \mathrm{SU}(3) & \to & \mathrm{O}^+_{sd}(3) & \\ \nearrow & & \searrow & \mathrm{O}^+(6)\supset \mathrm{O}^+(5) & \nearrow & & \searrow \\ \mathrm{U}(13) & & & & & & \mathrm{O}^+(3)\supset \mathrm{O}^+(2). \\ \searrow & & & & & & \nearrow \\ & \mathrm{U}_f(7)\supset \mathrm{O}^+(7) & & & \supset & \mathrm{O}^+_f(3) & \end{array} \tag{126}$$

The branching rules for the reduction $\mathrm{U}(13)\supset \mathrm{U}_{sd}(6)\oslash \mathrm{U}_f(7)$ are given by Eq. (54) that, in IBM-1F, reduces to

$$\{N\}=\sum_{N_f}\{N-N_f\}\{N_f\} \quad \text{for} \quad \mathrm{U}(13)\supset \mathrm{U}_{sd}(6)\oslash \mathrm{U}_f(7). \tag{127}$$

Since, by Eq. (128), the $\mathrm{U}_{sd}(6)$ irrep is symmetric, the sd branch in (127) is exactly equal to IBM-1 up to $\mathrm{O}^+_{sd}(3)$.

The $\mathrm{U}_f(7)$ irrep, being symmetric, produces the branch

$$\{N_f\}=(N_f)+(N_f-2)+\cdots+(0) \quad \text{or} \quad (1) \quad \text{for} \quad \mathrm{U}_f(7)\supset \mathrm{O}^+(7). \tag{128}$$

For the link $\mathrm{O}^+(7)\supset \mathrm{O}^+(3)$ one has obviously $(1)=(3)$ and the branching rule is obtained by calculating the plethysm

$$\begin{aligned}(3)\otimes(N_f)&=(\{3\}-\{1\})\otimes(\{N_f\}-\{N_f-2\})\\ &=\{3\}\otimes\{N_f\}-(\{3\}\otimes\{N_f-1\})\{1\}+(\{3\}\otimes\{N_f-2\})(\{1^2\}-\{0\})\\ &\quad+(\{3\}\otimes\{N_f-3\})(\{1\}-\{1^3\})\\ &\quad-(\{3\}\otimes\{N_f-4\})\{1^2\}+(\{3\}\otimes\{N_f-5\})\{1^3\},\end{aligned} \tag{129}$$

TABLE VII. $O^+(7)\supset O^+(3)$ branching rules for $O^+(7)$ symmetric irreps of degrees up to 10.

$(0)=(0)$
$(1)=(3)$
$(2)=(2)+(4)+(6)$
$(3)=(1)+(3)+(4)+(5)+(6)+(7)+(9)$
$(4)=(0)+(2)+(3)+2(4)+(5)+2(6)+(7)+2(8)+(9)+(10)+(12)$
$(5)=(1)+(2)+2(3)+(4)+3(5)+2(6)+3(7)+2(8)+2(9)+2(10)+2(11)+(12)+(13)+(15)$
$(6)=(0)+2(2)+2(3)+3(4)+2(5)+4(6)+3(7)+4(8)+3(9)+4(10)+2(11)+3(12)+2(13)+2(14)$
$+(15)+(16)+(18)$
$(7)=2(1)+(2)+3(3)+3(4)+4(5)+4(6)+5(7)+4(8)+6(9)+4(10)+5(11)+4(12)+4(13)+3(14)$
$+3(15)+2(16)+2(17)+(18)+(19)+(21)$
$(8)=(0)+(1)+3(2)+2(3)+5(4)+4(5)+6(6)+5(7)+7(8)+6(9)+7(10)+6(11)+7(12)+5(13)$
$+6(14)+4(15)+5(16)+3(17)+3(18)+2(19)+2(20)+(21)+(22)+(24)$
$(9)=2(1)+2(2)+5(3)+4(4)+6(5)+6(6)+8(7)+7(8)+9(9)+8(10)+9(11)+8(12)+9(13)+7(14)$
$+8(15)+6(16)+6(17)+5(18)+5(19)+3(20)+3(21)+2(22)+2(23)+(24)+(25)+(27)$
$(10)=2(0)+(1)+4(2)+4(3)+6(4)+6(5)+9(6)+8(7)+10(8)+9(9)+12(10)+10(11)+12(12)$
$+10(13)+11(14)+10(15)+10(16)+8(17)+9(18)+6(19)+7(20)+5(21)+5(22)+3(23)+3(24)$
$+2(25)+2(26)+(27)+(28)+(30)$

where the plethysms $\{3\}\otimes\{m\}$ with negative m's are taken as null. After computing the plethysms and the outer products one uses Elliott's rules (59)–(61) to obtain the final L_f values. Branching rules for $O^+(7)\supset O^+(3)$ resulting from Eq. (129) are given in Table VII for $N=1,2,\ldots,10$.

One could obtain the L_f values using the reduction $U(7)\supset O^+(3)$ without the intermediate group $O^+(7)$. In this case, Eq. (35) will be $\{1\}=(3)$ and the result for U(7) symmetric irreps is

$$\{N_f\}=\sum_{k=0}^{3}\sum_{\mu}\alpha(\{3\}\otimes\{N_f-k\}\rightarrow\{\mu\})\{\mu\}\{1^k\}, \tag{130}$$

where in the plethysms only Schur functions with up to three rows are considered. The U(3) irreps resulting from the Kronecker products must be converted to $O^+(3)$ using Elliott's rules. Obviously the L_f values obtained using Eqs. (128) and (129) and Eq. (130) are the same.

VIII. FINAL COMMENTS

The branching rules for IBM-1 are known in the literature, each one being obtained by a different method. By the plethysm approach here presented all of them are obtained in a single unified way and the results obtained are used to other extensions of IBM. For some of these extensions the branching rules found in the literature are given only for simple cases without an explanation of how they were obtained, preventing the reader from extending tables when needed. The material presented in this paper provides to the reader all the material to check our tables and extend them as long as he needs. Besides, the approach here used can be applied, *mutatis mutandis* on other situations that need the knowledge of branching rules of subgroups of $GL(n)$.

The tables here presented were obtained by computer programs which, by control, perform dimension tests. To avoid misprints, the output of these programs are read by another program that produces the latex source files of the tables.

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Canonical factorization and diagonalization of Baxterized braid matrices: Explicit constructions and applications[a)]

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(Received 9 May 2003; accepted 23 July 2003)

Braid matrices $\hat{R}(\theta)$, corresponding to vector representations, are spectrally decomposed obtaining a ratio $f_i(\theta)/f_i(-\theta)$ for the coefficient of each projector P_i appearing in the decomposition. This directly yields a factorization $(F \times(-\theta))^{-1}F(\theta)$ for the braid matrix, implying also the relation $\hat{R}(-\theta)\hat{R}(\theta) = I$. This is achieved for $\mathrm{GL}_q(n)$, $\mathrm{SO}_q(2n+1)$, $\mathrm{SO}_q(2n)$, $\mathrm{Sp}_q(2n)$ for all n and also for various other interesting cases including the eight-vertex matrix. We explain how the limits $\theta \to \pm\infty$ can be interpreted to provide factorizations of the standard (non-Baxterized) braid matrices. A systematic approach to diagonalization of projectors and hence of braid matrices is presented with explicit constructions for $\mathrm{GL}_q(2)$, $\mathrm{GL}_q(3)$, $\mathrm{SO}_q(3)$, $\mathrm{SO}_q(4)$, $\mathrm{Sp}_q(4)$ and various other cases such as the eight-vertex one. For a specific nested sequence of projectors diagonalization is obtained for all dimensions. The canonical property implemented in the diagonalizers is mutual orthogonality of the rows. In each factor $F(\theta)$ our diagonalizer again factors out all dependence on the spectral parameter θ as a diagonal matrix. Applications of our formalism to the construction of L-operators and transfer matrices are indicated. In an Appendix our type of factorization is compared to another one proposed by other authors. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1613378]

I. INTRODUCTION

Let $\hat{R}(\theta)$ be a braid matrix Baxterized with a spectral parameter θ and satisfying, in standard notations,

$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\acute{\theta})\hat{R}_{12}(\acute{\theta}) = \hat{R}_{23}(\acute{\theta})\hat{R}_{12}(\theta+\acute{\theta})\hat{R}_{23}(\theta). \tag{1.1}$$

The term Baxterization refers to the inclusion of a spectral parameter θ which has to be suitably altered for each factor precisely as shown in (1.1). In presence of such a parameter the matrix $\hat{R}(\theta)$ will be called Baxterized. In absence of such a spectral parameter we will simply use the term braid matrix. The latter will be systematically extracted from the Baxterized ones as limiting cases where the spectral parameters tend to infinity. This extraction will be performed explicitly for each case in the following sections. In Secs. 2 and 3 of Ref. 1 we have shown in full detail how one solves a set of functional equations to obtain the θ-dependence of the coefficients of the projectors in spectral decompositions for unitary, orthogonal and symplectic cases for arbitray dimensions. Such derivations give the essential content of the term ''Baxterization.'' Here, apart from θ, $\hat{R}(\theta)$ can depend on other parameters such as q, which will not always be denoted explicitly. Vector representations with $N^2 \times N^2$ braid matrices are implied in all cases. The corresponding YB (Yang-Baxter) martix is

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$$R(\theta)=P\hat{R}(\theta), \tag{1.2}$$

where the permutation matrix P is defined to be [with $i=(1,2,\ldots,N)$]

$$P=\sum_{ij} E_{ij}\otimes E_{ji}. \tag{1.3}$$

The matrix E_{ij} has zero elements except for a single unit one at (ij).

We assume that the polynomial equation of minimal degree satisfied by $\hat{R}(\theta)$ has distinct roots. When this holds $\hat{R}(\theta)$ can be spectrally decomposed on a basis of projectors P_i, satisfying

$$P_iP_j=\delta_{ij}P_i, \quad \sum_i P_i=I_{N^2\times N^2}. \tag{1.4}$$

Suppressing arguments for the time being, if (with $k_i\neq k_j$ for $i\neq j$)

$$\prod_{i=1}^{p}(\hat{R}-k_iI)=0, \tag{1.5}$$

then defining

$$P_i=\prod_{j\neq i}\frac{(\hat{R}-k_jI)}{(k_i-k_j)} \quad (i=1,2,\ldots p), \tag{1.6}$$

the set P_i can be shown to satisfy (1.4) and one obtains

$$\hat{R}=\sum_i^p k_iP_i. \tag{1.7}$$

On the other hand, given (1.7) one obtains (1.5). The P's on the right can, in general, depend on parameters such as q. *But in all cases they will be independent of the spectral parameter* θ. In $R(\theta)$ all θ-dependence is to be found in the coefficients k_i. This is consistent with (1.6) and (1.7) and is fundamental for the considerations below.

In all cases to be considered, not only will we obtain explicit spectral decomposition of $\hat{R}(\theta)$, but also *a specific factorized form* of each k_i,

$$k_i(\theta)=\frac{f_i(\theta)}{f_i(-\theta)} \tag{1.8}$$

when

$$\hat{R}(\theta)=\sum_i k_i(\theta)P_i=\sum_i\frac{f_i(\theta)}{f_i(-\theta)}P_i. \tag{1.9}$$

This will be our first major step.

The number of projectors and their matrix elements are specific to the case considered. But they always satisfy (1.4). In Ref. 1, (1.9) has been obtained explicitly for $\mathrm{GL}_q(n)$, $\mathrm{SO}_q(2n+1)$, $\mathrm{SO}_q(2n)$ and $\mathrm{Sp}_q(2n)$ for all n. The results are recapitulated in Secs. II and III. In Secs. IV–VII we obtain (1.9) for various interesting cases, including the eight-vertex matrix.

An evident, but for us crucial, consequence of (1.4) is that for well-defined and mutually commuting but otherwise *arbitrary* coefficients (a_i,b_i),

$$\left(\sum_i a_i P_i\right)\left(\sum_i b_i P_i\right)=\left(\sum_i a_i b_i P_i\right)=\left(\sum_i b_i P_i\right)\left(\sum_i a_i P_i\right). \tag{1.10}$$

Hence, once a spectral decomposition (1.7) has been obtained $\hat{R}$ can be expressed as a product of arbitrary number of factors

$$\hat{R}=\prod_n \left(\sum_i k_i^{(n)} P_i\right), \quad \left(\prod_n k_i^{(n)}=k_i\right). \tag{1.11}$$

Of particular interest to us is the factorization

$$\hat{R}(\theta)=\sum_i \frac{f_i(\theta)}{f_i(-\theta)} P_i=\left(\sum_i f_i^{-1}(-\theta)P_i\right)\left(\sum_i f_i(\theta)P_i\right)=(F(-\theta))^{-1}F(\theta), \tag{1.12}$$

where

$$F(\theta)=\sum_i f_i(\theta)P_i\,. \tag{1.13}$$

This implies the so-called ''unitarity''

$$\hat{R}(-\theta)\hat{R}(\theta)=I_{N^2\times N^2}. \tag{1.14}$$

One obtains from (1.2), since $P^2=I$,

$$R(\theta)=(P(F(-\theta))^{-1}P)PF(\theta)=(F_{21}(-\theta))^{-1}PF_{12}(\theta). \tag{1.15}$$

In (1.12) and (1.15) the key feature is the change of sign of θ in F^{-1}.

Other interesting choices are possible. Thus, for example, defining

$$\acute{F}(\theta)=\sum_i \left(\frac{f_i(\theta)}{f_i(-\theta)}\right)^{1/2} P_i=(\acute{F}(-\theta))^{-1}, \tag{1.16}$$

one obtains

$$\hat{R}(\theta)=(\acute{F}(-\theta))^{-1}\acute{F}(\theta)=(\acute{F}(\theta))^2 \tag{1.17}$$

and

$$R(\theta)=(\acute{F}_{21}(-\theta))^{-1}P\acute{F}_{12}(\theta)=(\acute{F}_{21}(\theta))P\acute{F}_{12}(\theta). \tag{1.18}$$

Here, even for real $\hat{R}(\theta)$, for certain domains of θ the factor $\acute{F}(\theta)$ can be complex.

Compare (1.15) and (1.18) to a Drinfeld twist[2–4] of P:

$$R''(\theta)=(F''_{21}(\theta))^{-1}PF''_{12}(\theta). \tag{1.19}$$

[This is presented for direct comparison with (1.15). In this particular case such a twist is trivial. It is well known that in other contexts Drinfeld twists can play major roles.]

In (1.15) there is $(-\theta)$ on the left and in (1.18) there is no inversion of $\acute{F}_{21}(\theta)$. P satisfies the YB equation with the trivial $\hat{R}=P^2=I$ for the braid matrix. (P also satisfies the braid equation with $R=P^2=I$.) The properties of $R''(\theta)$ will depend on those of $F''(\theta)$ (such as cocycle conditions). In our case, since one *starts* from solutions of (1.1) one does not have to verify if $F(\theta)$ and $\acute{F}(\theta)$ satisfy suitable constraints, so far as the braid equation is concerned.

The present situation may also be compared to "contraction" of YB matrices to nonstandard, Jordanian forms. Without even trying to explain the terminology we refer to two[5,6] of our series of relevant papers (where original sources are cited). We mention this only to point out that, as compared to (1.15), (1.18), and (1.19), the role of P is, so to say, reversed. For the nonstandard case R is a Drinfeld twist of I,

$$R=(F_{21})^{-1}F, \quad \hat{R}=F^{-1}PF. \tag{1.20}$$

The nontrivial matrix $\hat{R}$ is now "triangular" since from (1.20)

$$(\hat{R})^2=I. \tag{1.21}$$

The ambiguities arising in factorizing [compare (1.13) and (1.16)], or in defining $f_i(\theta)$ for a given $k_i(\theta)$ in (1.8), become particularly relevant in considering the limits $\theta\to\pm\infty$. From (1.9) one has evidently

$$\hat{R}(0)=\sum_i P_i=I. \tag{1.22}$$

It will be seen in the following sections that in each case for $\theta\to\pm\infty$ one obtains the standard (non-Baxterized) braid matrices ($\hat{R}$ and the inverse) satisfying

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12}=\hat{R}_{23}\hat{R}_{12}\hat{R}_{23}. \tag{1.23}$$

This equation can be considered, consistently with (1.1) as the limiting form (with arguments suppressed) as both $(\theta,\acute{\theta})\to+\infty$, say. If one denotes

$$\lim_{\theta\to+\infty}\hat{R}(\theta)=\hat{R}, \tag{1.24}$$

then consistently with (1.14)

$$\lim_{\theta\to-\infty}\hat{R}(\theta)=\hat{R}^{-1}. \tag{1.25}$$

In these limits special features arise concerning factorizations. It is helpful to consider a simple but frequently encountered example. Suppose that for some $f_i(\theta)$ one has (dropping the index i and setting $q=e^h$)

$$\frac{f(\theta)}{f(-\theta)}=\frac{\sinh(h-\theta)}{\sinh(h+\theta)}. \tag{1.26}$$

The evident singularity at $\theta=-h$ can be excluded by definition from the domain of θ. Now, as $\theta\to\pm\infty$,

$$\frac{f(\theta)}{f(-\theta)}\to-q^{\mp 2}. \tag{1.27}$$

But what about the factor $f(\theta)$? How does it behave when separated in the factor $F(\theta)$ or $\acute{F}(\theta)$ exhibited before?

(1) For the choice

$$f(\pm\theta)=\sinh(h\mp\theta), \tag{1.28}$$

separately both $f(\theta)$ and $f(-\theta)$ both diverge.

(2) The choice

$$f(\theta)=\left(\frac{\sinh(h-\theta)}{\sinh(h+\theta)}\right)^{1/2}=\frac{\sinh(h-\theta)}{(\sinh(h-\theta)\sinh(h+\theta))^{1/2}} \tag{1.29}$$

gives consistently with (1.27) finite but imaginary limits

$$f(\theta)\to\pm iq^{\mp 1},\quad f(-\theta)\to\mp iq^{\pm 1}. \tag{1.30}$$

(3) But more generally than in (1.29) one may choose for any well-defined $y(\theta)$,

$$f(\theta)=\frac{\sinh(h-\theta)}{(y(\theta)y(-\theta))^{1/2}}. \tag{1.31}$$

Setting, for example,

$$f(\theta)=\frac{\sinh(h-\theta)}{(\cosh(h-\theta)\cosh(h+\theta))^{1/2}}, \tag{1.32}$$

one obtains real, finite limits consistent with (1.28),

$$\theta\to+\infty,\quad f(\pm\theta)\to\mp q^{\mp 1}, \tag{1.33}$$

with an evident analogous result for $\theta\to-\infty$.

We will assume that each $f_i(\theta)$ in $F(\theta)$ has thus been suitably defined [choosing an appropriate $y(\theta)$]. Then even $\hat{R}$ satisfying (1.23) can be considered to be factorized as in (1.12), the implicit spectral parameter not being exhibited in the limits $\theta\to\pm\infty$. In this sense, the unitarity (1.14) can still be considered to be implicit. Note that even if each $f_i(\theta)$ has limits analogous to (1.33) with different powers of q, one *cannot* express the factorization as $(F(-q))^{-1}F(q))$ since the projectors, in general, are q-dependent (though always independent of θ). It is essential to think in terms of θ even when it is, in the limits above, implicit. The implementation of a spectral parameter, the passage from (1.23) to (1.1), renders many aspects more complex. But it also provides an extra margin of maneuver, making possible the canonical factorization (1.12) whose interest will be studied later on.

Our factorizations are directly based on the resolution (1.9). Other classes of factorizations can also be envisaged. One such class with upper and lower triangular factors for the YB matrix $R(\theta)$, leading to interesting properties, has been studied by Maillet *et al.* in a series of papers.[7–9] This formalism is compared with ours in Appendix A.

Since all braid matrices studied (Secs. II–VII) are systematically found to lead to spectral decompositions with each coefficient of the form (1.8) and (1.9) a more general study of such forms should be of interest. Here we will limit our observations to the following feature. Let

$$\hat{R}'(\theta)=\sum_i\frac{g_i(\theta)}{g_i(-\theta)}P_i, \tag{1.34}$$

where, apart from being well-defined, the g's are as yet arbitrary. In general, $\hat{R}'(\theta)$ does *not* satisfy (1.1). But defining

$$H(\theta)=\sum_i\frac{g_i(\theta)}{f_i(\theta)}P_i\equiv\sum_i h_i(\theta)P_i, \tag{1.35}$$

where $f_i(\theta)$ corresponds to (1.9), a solution $\hat{R}(\theta)$ of (1.1) on the *same* basis of projectors is

$$\hat{R}'(\theta)=(H(-\theta))^{-1}\hat{R}(\theta)H(\theta). \tag{1.36}$$

Any two matrices decomposable on the same spectral basis [satisfying (1.4)] are always related as above.

Substituing in (1.1)

$$\hat{R}(\theta)=H(-\theta)\hat{R}'(\theta)H(\theta)^{-1}, \tag{1.37}$$

one can rephrase (1.1) in terms of $\hat{R}'$ and H. One obtains

$$\hat{R}'_{12}(\theta)X_1\hat{R}'_{23}(\theta+\hat{\theta})X_2\hat{R}'_{12}(\hat{\theta})X_3=X_4\hat{R}'_{23}(\hat{\theta})X_5\hat{R}'_{12}(\theta+\hat{\theta})X_6\hat{R}'_{23}(\theta), \tag{1.38}$$

where

$$X_1=(H_{12}(\theta))^{-1}H_{23}(-\theta-\hat{\theta})$$

and so on.

Now, along with the properties of $f_i(\theta)$, those of $g_i(\theta)$ will determine the content of this equation for $\hat{R}'$. Further study in this direction is beyond the scope of this work.

Our first basic step is the systematic expression of the solutions of (1.1) in the form (1.9). The next major one is the simultaneous diagonalization of each projector P_i in (1.9) and hence of $\hat{R}(\theta)$. Our approach is presented step by step in Sec. IX. Explicit examples of diagonalizations of lower dimensional cases of Secs. II and III [$\mathrm{Gl}_q(2),\mathrm{Gl}_q(3),\mathrm{SO}_q(3),\mathrm{SO}_q(4),\mathrm{Sp}_q(4)$] are collected together in Appendix B. At the end of Secs. IV–VII the diagonalizations are presented explicitly for each case. Our Sec. VIII is an exception, where a nested sequence of projectors with simple, attactive features is presented for arbitrary dimensions without constructing explicit solutions of the braid equation. On the contrary, here the diagonalizer is obtained quite simply for arbitrary dimensions.

A *canonical* feature sought for in our formalism is the *mutual orthogonality of the rows* of the matrix diagonalizing $\hat{R}(\theta)$. The elegant and useful consequences of such a feature are pointed out. In the factorized form, our diagonalizer factors out again in each factor all θ-dependence as a diagonal matrix.

Applications of our spectral decompositions and diagonalizations to the construction of L-operators and to transfer matrices are discussed respectively in Secs. X and XI.

II. FACTORIZATION OF BRAID MATRICES OF $\mathrm{GL}_q(N)$, $\mathrm{SO}_q(N)$ AND $\mathrm{Sp}_q(N)$

We recapitulate below the relevant essential results of Ref. 1. The standard q-dependent $N^2\times N^2$ projectors[10] are assumed to be known. For Sp_q always $N=2n$.

The same notations will be used for projectors in different cases though they are different. The overall normalizing factor for $\hat{R}(\theta)$ is chosen to obtain 1 for the element (11) at top left. (See, however, Sec. VII.)

For $\mathrm{GL}_q(N)$ one has two projectors (P_+,P_-) satisfying (1.4). For $\hat{R}(\theta)$ satisfying (1.1), setting $h=\ln q$, one obtains

$$\begin{aligned}\hat{R}(\theta)&=P_+ +\frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_-\\&=(P_+ +(\sinh(h+\theta))^{-1}P_-)(P_+ +\sinh(h-\theta)P_-)\\&\equiv(F(-\theta))^{-1}F(\theta).\end{aligned} \tag{2.1}$$

To illustrate (1.12) we have implemented one simple possible choice for $F(\theta)$. Ambiguities discussed in Sec. I [from (1.28) to (1.32)] *are always present in this and other examples to follow*. This statement will not be repeated in successive sections.

For $SO_q(N)$, for $N=(2n+1)$ and also for $N=2n$, one has a basis of three projectors (P_+, P_-, P_0) and two possibilities:

$$\hat{R}(\theta)=P_+ + \frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_- + \frac{\cosh((N/2)h-\theta)}{\cosh((N/2)h+\theta)}P_0 \tag{2.2}$$

or

$$\hat{R}(\theta)=P_+ + \frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_- + \frac{\sinh((N/2-1)h-\theta)\sinh(h-\theta)}{\sinh((N/2-1)h+\theta)\sinh(h+\theta)}P_0 . \tag{2.3}$$

For $Sp_q(2n)$ one obtains

$$\hat{R}(\theta)=P_+ + \frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_- + \frac{\sinh((n+1)h-\theta)}{\sinh((n+1)h+\theta)}P_0 \tag{2.4}$$

or

$$\hat{R}(\theta)=P_+ + \frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_- + \frac{\cosh(nh-\theta)\sinh(h-\theta)}{\cosh(nh+\theta)\sinh(h+\theta)}P_0 . \tag{2.5}$$

The expressions for $F(\theta)$ and $(F(-\theta))^{-1}$ are evident in each case. See, however, the remarks below (2.1). For each case

$$\hat{R}(0)=I. \tag{2.6}$$

For $\theta \to \pm\infty$, carefully taking limits, one respectively obtains for $GL_q(N)$

$$\hat{R}=P_+ - q^{\mp 2}P_- , \tag{2.7}$$

for $SO_q(N)$

$$\hat{R}=P_+ - q^{\mp 2}P_- + q^{\mp N}P_0 , \tag{2.8}$$

and for $Sp_q(N)$

$$\hat{R}=P_+ - q^{\mp 2}P_- - q^{\mp(N+2)}P_0 . \tag{2.9}$$

These are the standard (non-Baxterized) braid matrices[10] satisfying (1.23). Concerning factorization see the relevant discussion in Sec. I [from (1.23) to (1.33)].

For $q=1$ $(h=0)$ all these matrices become trivial. This situation is to be contrasted with the corresponding one in Sec. III.

III. A NEW CLASS OF BRAID MATRICES FOR $SO_q(N)$ AND $Sp_q(N)$

This was presented in Sec. 4 of Ref. 1. The solution for $SO_q(3)$ appeared already in Ref. 11. The structure (1.9) is again present and hence also the factorization (1.12).

We recapitulate:

Define

$$d=(1+\epsilon[N-\epsilon])^{-1}=\left(1+\epsilon\frac{q^{N-\epsilon}-q^{-N+\epsilon}}{q-q^{-1}}\right)^{-1}, \tag{3.1}$$

where for $SO_q(N)$

$$\epsilon=1, \quad N=3,4,\ldots,$$

and for $\mathrm{Sp}_q(N)$

$$\epsilon=-1, \quad N=4,6,\ldots.$$

Define also

$$\tanh \eta=\sqrt{1-4d^2}. \tag{3.2}$$

The reality of η is implied by (3.1) since $4d^2<1$. Now with such an η,

$$\hat{R}(\theta)=P_+ + P_- + \frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}P_0 \tag{3.3}$$

$$=I+\left(\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}-1\right)P_0 \tag{3.4}$$

can be shown[1] to satisfy (1.1). The promised srtucture is explicit in (3.3).

One has as usual

$$\hat{R}(0)=I \tag{3.5}$$

and for $\theta\rightarrow\pm\infty$

$$\hat{R}(\pm\infty)=P_+ + P_- - e^{\mp 2\eta}P_0 \tag{3.6}$$

$$=I-(1+e^{\mp 2\eta})P_0, \tag{3.7}$$

where

$$e^{\mp 2\eta}=\frac{1\mp\sqrt{1-4d^2}}{1\pm\sqrt{1-4d^2}}. \tag{3.8}$$

These provide a new class of (non-Baxterized) braid matrices $\hat{R}^{\pm 1}$ satisfying (1.23). The $R^{\pm 1}=P\hat{R}^{\pm 1}$ are new solutions of the YB equation for SO_q and Sp_q with ϵ and N as given below (3.1).

Moreover, from (3.1), for $q=1$,

$$d=\frac{\epsilon}{N}, \tag{3.9}$$

and from (3.2), for $q=1$,

$$(\tanh \eta)_{(q=1)}=\sqrt{1-\frac{4}{N^2}}\equiv\tanh \hat{\eta}. \tag{3.10}$$

Denoting

$$(P_0)_{(q=1)}=\hat{P}_0 \tag{3.11}$$

and so on, one obtains from (3.3) and (3.7), respectively,

$$(\hat{R}(\theta))_{(q=1)}=\hat{P}_+ + \hat{P}_- + \frac{\sinh(\hat{\eta}-\theta)}{\sinh(\hat{\eta}+\theta)}\hat{P}_0 \tag{3.12}$$

and

$$(\hat{R}^{(\pm 1)})_{(q=1)}=\hat{P}_{+}+\hat{P}_{-}-e^{\mp 2\hat{\eta}}\hat{P}_{0}. \tag{3.13}$$

The braid matrix (3.13) satisfies a nontrivial Hecke condition

$$(\hat{R}-I)(\hat{R}+e^{-2\hat{\eta}}I)=0 \tag{3.14}$$

and cannot be twisted back to I. This situation should be compared to the corresponding one in Sec. II.

Note that we are *not* expanding in powers of $h(=lnq)$ to extract the so-called "classical" r-matrix. We are directly setting $q=1$ and yet getting quite nontrivial results.

IV. TWO EXOTIC CASES ($S03$, $S14$)

Two special braid matrices arising in the classification of 4×4 YB matrices of Ref. 12 were Baxterized in Ref. 13. Other aspects were already studied in previous papers of the series.[14] Some "exotic" features are briefly recapitulated below in the present context:

(i) complex projectors for $S03$ (for real $\hat{R}$), and
(ii) extended freedom of parametrization for $S14$.

Our solutions presented in Sec. III can be considered to be an exotic class in arbitrary dimensions ($N^2\times N^2, N\geqslant 3$). For even N one has two types, exotic orthogonal and exotic symplectic.

$S03$: The braid matrix

$$\hat{R}=\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \tag{4.1}$$

satisfies

$$(\hat{R}-(1+i)I)(\hat{R}-(1-i)I)=0. \tag{4.2}$$

The corresponding projectors

$$P_{(\pm)}=\tfrac{1}{2}(I\pm i(\hat{R}-I)) \tag{4.3}$$

provide the spectral decomposition

$$\hat{R}=(1-i)P_{(+)}+(1+i)P_{(-)}. \tag{4.4}$$

Altering suitably the normalization of Ref. 13 gives the Baxterization (with $z=e^{\theta}$)

$$\hat{R}(z)=\left(\frac{f(z)}{f(z^{-1})}\right)^{1/2}P_{(+)}+\left(\frac{f(z^{-1})}{f(z)}\right)^{1/2}P_{(-)}, \tag{4.5}$$

where

$$f(z)=(z+z^{-1})+i(z-z^{-1}). \tag{4.6}$$

Thus we obtain the form (1.9) and (1.12) follows.

One can rewrite (4.5) in the explicitly real form

$$\hat{R}(z)=(z^2+z^{-2})^{-1/2}((\sqrt{2}z)^{-1}\hat{R}+\sqrt{2}z\hat{R}^{-1}) \tag{4.7}$$

and verify again

$$\hat{R}(z^{-1})\hat{R}(z)=I. \tag{4.8}$$

The unitary matrix M, where

$$\sqrt{2}M=\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ i & 0 & 0 & 1 \end{pmatrix}, \tag{4.9}$$

diagonalizes $P_{(\pm)}$ giving

$$M\hat{R}M^{-1}=\mathrm{diag}(1-i,1-i,1+i,1+i)\,, \tag{4.10}$$

$$(z^2+z^{-2})^{1/2}M\hat{R}(z)M^{-1}=\frac{1}{\sqrt{2}z}\mathrm{diag}(1-i,1-i,1+i,1+i)+\frac{z}{\sqrt{2}}\mathrm{diag}(1+i,1+i,1-i,1-i). \tag{4.11}$$

The diagonal elements are complex with real trace.

*S*14: Here

$$\hat{R}=\begin{pmatrix} 0 & 0 & 0 & q \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ q & 0 & 0 & 0 \end{pmatrix}. \tag{4.12}$$

The projectors (*three* even for a 4×4 $\hat{R}$)

$$P_{(0)}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad 2P_{(\pm)}=\begin{pmatrix} 1 & 0 & 0 & \pm1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \pm1 & 0 & 0 & 1 \end{pmatrix} \tag{4.13}$$

give

$$\hat{R}=P_{(0)}+q(P_{(+)}-P_{(-)}). \tag{4.14}$$

Baxterization gives

$$\hat{R}(z)=P_{(0)}+v(z)(P_{(+)}-P_{(-)})\,, \tag{4.15}$$

where $v(z)$ is *arbitrary*. (See Ref. 13 for details.)

One can indeed set (with $z=e^{\theta}$, say)

$$v(z)=\frac{f(z)}{f(z^{-1})}, \quad -v(z)=\frac{(z-z^{-1})}{(z^{-1}-z)}\frac{f(z)}{f(z^{-1})} \tag{4.16}$$

and factorize. But more freedom is present, as compared to (1.1) and all previous examples. Denoting $\hat{R}(v(z))$ by $\hat{R}(v)$ one obtains

$$\hat{R}_{12}(v)\hat{R}_{23}(v')\hat{R}_{12}(v'')=\hat{R}_{23}(v'')\hat{R}_{12}(v')\hat{R}_{23}(v), \tag{4.17}$$

where (v,v',v'') are mutually independent.

Amusingly, $\hat{R}$ of $S14$ is diagonalized by (4.1), the $\hat{R}$ of $S03$ giving

$$\mathrm{diag}(q,1,1,-q). \tag{4.18}$$

V. AFFINE $\mathcal{U}_q(\widehat{sl}_2)$

We start below directly with the matrix $\overline{R}_{VV}(z)$ [Eqs. (3.13) and (3.14)] of Sec. 3.2 of Ref. 15. We obtain the spectral resolution and factorization [finding back the Baxterization of $\mathrm{GL}_q(2)$ of Sec. II]. Thus, apart from a possible overall factor, the braid matrix of $\mathcal{U}_q(\widehat{sl}_2)$ is

$$\hat{R}(z)=P\overline{R}_{VV}(z)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & zc & b & 0 \\ 0 & b & c & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{5.1}$$

where

$$b=\frac{(1-z)q}{(1-q^2z)}, \quad c=\frac{(1-q^2)}{(1-q^2z)}. \tag{5.2}$$

Define the following basis satisfying (1.4),

$$P_{(0)}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (q+q^{-1})P_{(\pm)}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & q^{\pm 1} & \pm 1 & 0 \\ 0 & \pm 1 & q^{\mp 1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5.3}$$

Note the specific q-dependence of $P_{(\pm)}$. Relabeling $(P_{(0)}+P_{(+)})$ as $P_{(+)}$ makes the relation to $\mathrm{GL}_q(2)$ clearer. On the other hand, (5.3) with $q=1$ corresponds to the basis for the six-vertex model (Sec. VI).

Setting $q=e^h$, $z=e^\theta$ one can write (5.1) as

$$\hat{R}(\theta)=P_{(0)}+P_{(+)}+\frac{\sinh(h-\theta/2)}{\sinh(h+\theta/2)}P_{(-)}, \tag{5.4}$$

where

$$\frac{\sinh(h-\theta/2)}{\sinh(h+\theta/2)}=\frac{(q^2-z)}{(q^2z-1)}=\frac{z^{-1/2}q-z^{1/2}q^{-1}}{z^{1/2}q-z^{-1/2}q^{-1}}. \tag{5.5}$$

Factorizations of the type (1.12) are now evident. Also evidently from (5.4)

$$\hat{R}(z^{-1})\hat{R}(z)=\hat{R}(-\theta)\hat{R}(\theta)=I. \tag{5.6}$$

Any supplementary overall factor, unless of the form

$$\frac{\rho(z)}{\rho(z^{-1})}, \tag{5.7}$$

will be incompatible with (5.6). The results for $\theta\to\pm\infty$ are displayed below for comparison with the corresponding results for the six-vertex (Sec. VI) and the eight-vertex (Sec. VII) to follow.

For $\theta \to \infty$

$$\hat{R}(\theta) \to \hat{R} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-q^{-2}) & q^{-1} & 0 \\ 0 & q^{-1} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.8}$$

For $\theta \to -\infty$

$$\hat{R}(\theta) \to \hat{R}^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & q & (1-q^{2}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.9}$$

For $R = P\hat{R}$ one recognizes the familiar lower and upper triangular YB matrices of $\mathrm{GL}_q(2)$. Thus (5.1) is, indeed, a Baxterized form of (5.8) and (5.9) for a particular choice of basis and parametrization.

The matrix

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & q & 1 & 0 \\ 0 & -q^{-1} & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5.10}$$

diagonalizes each projector, giving

$$M\hat{R}(\theta)M^{-1} = \mathrm{diag}\left(1,1,\frac{\sinh(h-\theta/2)}{\sinh(h+\theta/2)},1\right). \tag{5.11}$$

We have factorized the basic matrix (5.1). After supplementary quasi-Hopf twists[15] one can seek again a spectral resolution to study analogous possibilities provided that (5.6) is conserved.

VI. THE SIX-VERTEX MODEL

The more general eight-vertex case is treated in Sec. VII. But we introduce already at this stage a basis of projectors, satisfying (1.4), adequate for the eight-vertex matrix.

Define

$$2P_{1(\pm)} = \begin{pmatrix} 1 & 0 & 0 & \pm 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \pm 1 & 0 & 0 & 1 \end{pmatrix}, \quad 2P_{2(\pm)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \pm 1 & 0 \\ 0 & \pm 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.1}$$

For the six-vertex we need only the subset

$$P_{(0)} = P_{1(+)} + P_{1(-)}, \quad P_{(\pm)} = P_{2(\pm)}. \tag{6.2}$$

Leaving aside all well-known relations, via reparametrizations and limiting processes, to rational affine cases, we illustrate our approach using the trigonometric parametrization and, in

particular, the ''ferroelectric'' regime. Extensive discussions and references can be found in the review.[16] [N.B. Our $\hat{R}$ corresponds to R in the notation of Ref. 16. See, for example, (2.19) of Ref. 16.]

With our standard normalization (Sec. II) in view we define (with $\gamma>0$, $\theta>0$)

$$x=\frac{\sinh\gamma}{\sinh(\gamma+\theta)},\quad y=\frac{\sinh\theta}{\sinh(\gamma+\theta)}. \tag{6.3}$$

(Though $\theta>0$ for this regime, we will consider later the limits $\theta\to\pm\infty$.) The braid matrix is

$$\hat{R}(\theta)=\begin{pmatrix}1&0&0&0\\0&x&y&0\\0&y&x&0\\0&0&0&1\end{pmatrix}. \tag{6.4}$$

Implementing (6.1) and (6.2),

$$\hat{R}(\theta)=P_{(0)}+(x+y)P_{(+)}+(x-y)P_{(-)}=P_{(0)}+\frac{\cosh\frac{1}{2}(\gamma-\theta)}{\cosh\frac{1}{2}(\gamma+\theta)}P_{(+)}+\frac{\sinh\frac{1}{2}(\gamma-\theta)}{\sinh\frac{1}{2}(\gamma+\theta)}P_{(-)}. \tag{6.5}$$

We have thus the structure (1.9) and hence the factorization (1.12). From (6.3) as

$$\theta\to\pm\infty,\quad x\to 0,\ y\to e^{\mp\gamma}. \tag{6.6}$$

Hence the corresponding limits of $\hat{R}(\theta)$ give respectively [see the discussion starting with (1.23)] for the non-Baxterized YB matrix

$$R^{\pm 1}=(P\hat{R})^{\pm 1}=\mathrm{diag}(1,e^{\mp\gamma},e^{\mp\gamma},1). \tag{6.7}$$

This is a special class of even the simplest and the first solution $H_{3.1}$ in the classification of 4×4 YB matrices,[12] namely,

$$R=\mathrm{diag}(p,q,r,s). \tag{6.8}$$

In view of the eight-vertex case to follow it is convenient to choose the diagonalizer ($M=M^{-1}$) as

$$\sqrt{2}M=\begin{pmatrix}1&0&0&1\\0&1&1&0\\0&1&-1&0\\1&0&0&-1\end{pmatrix}. \tag{6.9}$$

Now

$$M\hat{R}(\theta)M^{-1}=\mathrm{diag}(1,\ x+y,\ x-y,\ 1). \tag{6.10}$$

The crucial difference, for the parametrizations adopted, between (5.1) and (6.4) is the extra factor z in the second diagonal element of (5.1). This leads to the q-dependent projectors in (5.3) as compared to the elements $\pm\frac{1}{2}$ only in (6.1). Finally one is led (for $\theta\to\pm\infty$) to triangular and to diagonal YB matrices in Secs. V and VI, respectively.

VII. THE EIGHT-VERTEX BRAID MATRIX

The braid matrix of the quantum affine algebra $\mathcal{A}_{q,p}(\widehat{sl}_2)$ corresponds to the eight-vertex model. Some references relatively directly relevant to our purpose are Refs. 15 and 17–19. These cite other basic sources.

Here the symmetrical structure of (6.4) is generalized (with $z=e^{\theta}$) to

$$\hat{R}(z)=\begin{pmatrix} a(z) & 0 & 0 & d(z) \\ 0 & c(z) & b(z) & 0 \\ 0 & b(z) & c(z) & 0 \\ d(z) & 0 & 0 & a(z) \end{pmatrix}. \tag{7.1}$$

There are well-known expressions for the elements in different equivalent forms in terms of elliptic functions. The role of a specific class of overall factors for specific realizations of (a,b,c,d) will be commented upon later on. Implementing now the full set (6.1) with $a(z)=a$ and so on,

$$\hat{R}(z)=(a+d)P_{1(+)}+(a-d)P_{1(-)}+(c+b)P_{2(+)}+(c-b)P_{2(-)}. \tag{7.2}$$

We have thus a spectral decomposition in terms of the simple basis (6.1) with *constant* coefficients $\pm\frac{1}{2}$. The next steps [in order to implement (1.9) and hence (1.12] consist in explicit constructions of functions $f_{1(\pm)}(z)$ and $f_{2(\pm)}(z)$ such that (7.2) satisfies (1.1) for

$$(a\pm d)=\frac{f_{1(\pm)}(z)}{f_{1(\pm)}(z^{-1})}, \quad (c\pm b)=\frac{f_{2(\pm)}(z)}{f_{2(\pm)}(z^{-1})}. \tag{7.3}$$

These solutions are *directly* obtained from Eqs. (3.28) and (3.29) of Ref. 15 in terms of infinite products

$$(x;a)_{\infty}=\prod_{n\geqslant 0}(1-xa^{n}). \tag{7.4}$$

Noting that

$$q\,\frac{1\pm q^{-1}z}{1\pm qz}=\pm\frac{q^{1/2}z^{-1/2}\pm q^{-1/2}z^{1/2}}{q^{1/2}z^{1/2}\pm q^{-1/2}z^{-1/2}}, \tag{7.5}$$

one obtains from the results cited above (writing z for ζ and slightly reordering the factors)

$$a\pm d=\frac{(\mp p^{1/2}q^{-1}z;p)_{\infty}(\mp p^{1/2}qz^{-1};p)_{\infty}}{(\mp p^{1/2}q^{-1}z^{-1};p)_{\infty}(\mp p^{1/2}qz;p)_{\infty}}, \tag{7.6}$$

$$c\pm b=\frac{(q^{1/2}z^{-1/2}\pm q^{-1/2}z^{1/2})}{(q^{1/2}z^{1/2}\pm q^{-1/2}z^{-1/2})}\,\frac{(\mp pq^{-1}z;p)_{\infty}(\mp pqz^{-1};p)_{\infty}}{(\mp pq^{-1}z^{-1};p)_{\infty}(\mp pqz;p)_{\infty}}. \tag{7.7}$$

Our objectives are attained. We have arrived at (1.9) and (1.12). In view of the factored structures of (7.6) and (7.7) the comments (Sec. I) concerning varied possibilities in selecting $f(\theta)$ are now particularly relevant. Several factors lead to more alternatives.

As $\theta=lnz\to\pm\infty$, $z\to\infty$ and $z\to 0$, respectively. The extra factor in $(c\pm b)$ contributes

$$\left(\frac{q^{1/2}z^{-1/2}\pm q^{-1/2}z^{1/2}}{q^{1/2}z^{1/2}\pm q^{-1/2}z^{-1/2}}\right)_{z\to\pm\infty}=\pm q^{\mp 1}. \tag{7.8}$$

The ratios of the infinite products [considering the leading term in (7.4) for $n \leqslant k$] give (for $\theta \to \pm\infty$, respectively) for both (7.6) and (7.7) a factor

$$\lim_{k\to\infty} q^{\mp 2k}. \tag{7.9}$$

However, we are still free to choose an overall normalizing factor. One can choose, for example, a factor $(a+d)^{-1}$. Such a factor absorbs the limiting factor (7.9). From (7.8) and (7.9), for

$$(a',b',c',d') = (a+d)^{-1}(a,b,c,d), \tag{7.10}$$

$$\lim_{\theta\to\pm\infty} (a',b',c',d') = (1,q^{\mp 1},0,0). \tag{7.11}$$

Note that since $(a(z)+d(z))$ i.e., $(a(\theta)+d(\theta))$ is itself of the form $x(\theta)(x(-\theta))^{-1}$, such a normalization conserves the unitarity (1.14) already satisfied by $(a,b,\ c,d)$.

However, if one prefers to maintain the simpler symmetry of the parametrization (7.6) and (7.7) one may choose to absorb the factors (7.9) by a normalizing factor, say

$$\frac{(q^2z;1)_\infty}{(q^2z^{-1};1)_\infty}. \tag{7.12}$$

This conserves (1.14) and *again* gives the right hand side of (7.11) as limits [for (a,b,c,d) normalized by (7.12)]. This is a particularly simple choice albeit, evidently, not unique. We do not propose to examine here normalizations adopted in the cited sources.

After such a normalization one obtains

$$\lim_{\theta\to\pm\infty} (P\hat{R}(\theta)) = \mathrm{diag}(1,q^{\mp 1},q^{\mp 1},1). \tag{7.13}$$

Thus indeed one finds again a diagonal YB matrix. Compare (6.7) and the comments preceding (5.8).

The diagonalizer M of (6.9) gives now with any normalization factor N and (7.2)

$$M\hat{R}(\theta)M^{-1} = N\ \mathrm{diag}(a+d,c+b,c-b,a-d). \tag{7.14}$$

VIII. A NESTED SEQUENCE OF PROJECTORS FOR HIGHER DIMENSIONS

The eight-vertex matrix has complex features due to the presence of four functions (a,b,c,d) and their realizations in terms of elliptic functions. On the other hand, its symmetry permits a spectral resolution on a basis of particularly simple symmetrical projectors with *constant* elements $(\approx \pm 1)$. For $N^2\times N^2$ matrices with $N>2$ one can construct different types of generalization of such a basis with constant elements. One example can be easily extracted from the multistate model presented in Sec. 4 of Ref. 16 (where original sources are cited). Let us consider the simplest such case $(N=3)$.

Let E_{ij} be the matrices defined below (1.3). A set of projectors satisfying (1.4) and suitable for the specral decomposition of a particular class of 9×9 $\hat{R}(\theta)$ is

$$\begin{gathered} 2P_{1(\pm)} = (E_{11}+E_{99}\pm E_{19}\pm E_{91}), \quad 2P_{2(\pm)} = (E_{22}+E_{44}\pm E_{24}\pm E_{42}), \\ 2P_{3(\pm)} = (E_{33}+E_{77}\pm E_{37}\pm E_{73}), \quad 2P_{4(\pm)} = (E_{66}+E_{88}\pm E_{68}\pm E_{86}), \quad P_{55} = E_{55}. \end{gathered} \tag{8.1}$$

Generalizations for $N>3$ are not difficult to write down.

Additional simplifications arise in (4.1) of Ref. 16 since the functions of (γ,θ) implemented are of the six-vertex type. One feature should be noted. The action of P for $N=3$ interchanges the

rows (2,4), (3,7) and (6,8). Hence when the basis (8.1) is implemented $\hat{R}$ and $R(=P\hat{R})$ have fairly analogous structures (as for the 4×4 six- and eight-vertex matrices). Such a feature, though worth noting, is not essential and is indeed not present in the standard cases of Sec. II. Instead of presenting full details concerning the above-mentioned possibility, we briefly present another one. For $N=2$ this coincides with (6.1). This basis does *not* have (for $N>2$) the simple property of (8.1) and its generalizations for $N>3$ under the action of P. But it exhibits a particularly simple canonical nested structure. The prescription for diagonalization is also particularly simple.

For $n=N^2=2l$ define

$$2P_{i(\pm)}=(E_{ii}+E_{n-i+1,n-i+1}\pm E_{i,n-i+1}\pm E_{n-i+1,i}),\quad (i=1,2,\ldots,l). \tag{8.2}$$

For $n=2l+1$ one has in addition

$$P_{l+1}=E_{l+1,l+1}. \tag{8.3}$$

To diagonalize this set satisfying (1.4) now define

$$\sqrt{2}M=\sqrt{2}M^{-1}=\sum_{i=1}^{l}(E_{ii}+E_{i,n-i+1}+E_{n-i+1,i}-E_{n-i+1,n-i+1})+E_{l+1,l+1}. \tag{8.4}$$

For $n=2l$, the last term is absent.

One obtains

$$MP_{i(+)}M^{-1}=E_{i,i},\quad MP_{i(-)}M^{-1}=E_{n-i+1,n-i+1}\quad (i=1,2,..l). \tag{8.5}$$

When it is present, P_{l+1} is already diagonal and commutes with M. Hence, if (with the last term present only for odd n and with $\varepsilon=\pm$)

$$\hat{R}(z)=\sum_{i=1}^{l}\sum_{\varepsilon}\left(\frac{f_{i(\varepsilon)}(z)}{f_{i(\varepsilon)}(z^{-1})}P_{i(\varepsilon)}\right)+\frac{f_{l+1}(z)}{f_{l+1}(z^{-1})}P_{l+1}, \tag{8.6}$$

$$M\hat{R}(z)M^{-1}=\sum_{i=1}^{l}\left(\frac{f_{i(+)}(z)}{f_{i(+)}(z^{-1})}E_{ii}+\frac{f_{i(-)}(z)}{f_{i(-)}(z^{-1})}E_{n-i+1,n-i+1}\right)+\frac{f_{l+1}(z)}{f_{l+1}(z^{-1})}E_{l+1,l+1}. \tag{8.7}$$

The two sets [the one generalizing (8.1) for all n and the one given by (8.2) and (8.3)] can be shown to be related through a similarity transformation. But the matrix of conjugation does not possess a tensored structure $G\otimes G$ (and hence the tensored components of the base space are not transformed individually). The question of existence and construction of solutions of (1.1) for the parametrization (8.6) is beyond the scope of this article.

Let us conclude with a closer look at the simplest nontrivial case. For $N=3$, with a maximum number of functions in the coefficients and suppressing arguments [$x(\theta)=x$ and so on],

$$\hat{R}(\theta)=\sum_{\varepsilon}((x+\varepsilon y)P_{1(\varepsilon)}+(u+\varepsilon v)P_{2(\varepsilon)}+(a+\varepsilon d)P_{3(\varepsilon)}+(c+\varepsilon b)P_{4(\varepsilon)})+wP_5. \tag{8.8}$$

The diagonalizer is

$$\sqrt{2}M=\sqrt{2}M^{-1}=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}. \tag{8.9}$$

This generalizes (6.9) as one moves up from the 4×4 to the 9×9 case in our sequence. Note the central element [at (55)] appearing for odd $n(=9)$:

$$M\hat{R}(\theta)M^{-1}=\mathrm{diag}((x+y),(u+v),(a+d),(c+b),w,(c-b),(a-d),(u-v),(x-y)). \tag{8.10}$$

If, say, $y=0$ one can redefine $(P_{1(+)}+P_{1(-)})$ as a single projector $P_{(1)}$ and so on [continuing to satisfy (1.4)]. The number of functions available increases with the number of projectors, but so does the number of constraints due to the braid equation (1.1). Let us note, however, that for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ after fixing the normalization one has only two functions to satisfy four complicated functional equations.[1] Yet one emerges with *three* independent solutions in both the cases (Secs. II and III). A close study of particular cases in the present context might also lead to interesting possibilities. One recognizes (7.2) and (7.14) as subcases of (8.8) and (8.10), respectively.

IX. DIAGONALIZATION AND FACTORIZATION

Diagonalization of braid matrices was studied in Ref. 1. It was used to elucidate certain aspects of associated noncommutative spaces. Here it will be studied in the context of factorization.

For the 4×4 matrices (Secs. IV–VII) the diagonalizer M has been presented for each case explicitly. In Sec. VIII M has been obtained for the nested sequence explicitly for arbitray dimensions. The results for the lower dimensional cases of $(A,B,C,D)_q$ type algebras are collected in Appendix B. We will see how the diagonalizer leads to a striking structure for each factor in (1.12). But to start with it is worthwhile to recapitulate some basic features noted in Ref. 1.

(i) From (1.6) and (1.7) it is evident that if there exists an invertible matrix M diagonalizing $\hat{R}(\theta)$ it must diagonalize each projector P_i *separately*.

(ii) A projector, when diagonalized, can have only $+1$ or 0 as diagonal elements.

(iii) The number of unit elements on the diagonal is equal to the trace of the projector, obligatorily a positive integer. For different P_i in (1.4) these elements can never coincide due to orthogonality. In standard notations[10] one has for $\mathrm{GL}_q(N)$

$$P_{(+)}+P_{(-)}=I_{N^2\times N^2} \tag{9.1}$$

with

$$2TrP_{(\pm)}=N(N\pm1). \tag{9.2}$$

For $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N=2n)$ one has

$$P_{(+)}+P_{(-)}+P_0=I_{N^2\times N^2}, \tag{9.3}$$

and with $\epsilon=\pm 1$ respectively [as below (3.1)]

$$2TrP_{(\pm)}=N(N\pm 1)\mp(\epsilon\pm 1),\quad TrP_0=1. \tag{9.4}$$

(iv) If necessary, implementing a simple supplementary conjugation the elements on the diagonal can be reordered. Exploiting this possibility we introduce the following conventions:

For $GL_q(N)$ the unit elements of $P_{(-)}$ are grouped at the top, followed by those of $P_{(+)}$. Thus for $GL_q(3)$ and

$$\hat{R}(\theta)=P_{(+)}+vP_{(-)}, \tag{9.5}$$

once M is constructed we obtain

$$M\hat{R}(\theta)M^{-1}=\mathrm{diag}(v,v,v,1,1,1,1,1,1,). \tag{9.6}$$

For SO_q and Sp_q the chosen ordering is $(P_0,P_{(-)},P_{(+)})$. Thus for $SO_q(3)$ and

$$\hat{R}(\theta)=P_{(+)}+vP_{(-)}+wP_{(0)}, \tag{9.7}$$

$$M\hat{R}(\theta)M^{-1}=\mathrm{diag}(w,v,v,v,1,1,1,1,1). \tag{9.8}$$

Generalizations are evident.

(v) Since each diagonalized P_i (denoted below by D_i) is thus *completely* fixed beforehand one can (assuming the invertibility of M to be confirmed *a posteriori*) write separately for each P_i with the same M,

$$MP_i=D_iM. \tag{9.9}$$

Here both P_i and D_i are known giving explicit *linear* constraints on the elements of M. One avoids the construction of M^{-1} to start with.

(vi) The block structures in (9.6) and (9.8) and their evident generalizations reveal the extent to which M is arbitrary:

Let M_i denote a matrix of dimension $(TrP_i\times TrP_i)$, with a nonzero determinant but with otherwise *arbitrary* elements. Then, in obvious notations, a supplementary conjugation of (9.6) by a block-diagonal (bd) matrix

$$(M_{(-)},M_{(+)})_{(bd)} \tag{9.10}$$

and one of (9.8) by

$$(M_{(0)},M_{(-)},M_{(+)})_{(bd)} \tag{9.11}$$

leaves the diagonal forms invariant.

(vii) The arbitrariness thus exhibited, instead of being a source of embarrassment, provides a wide margin of maneuver exploitable to select an M with particularly attractive properties. We choose the following canonical feature:

mutual orthogonality of the rows of M.

[Except for the complex, unitary M of (4.9) for the exotic $S03$ such an orthogonality holds for all the cases we study.]

Agreeable consequences are the following.

(1) The inverse of M is obtained effortlessly. The prescription is: Take the transpose M^T of M. Normalize each element of the column j of M^T by the *same* factor c_j such that for each j

$$\left(\sum_i M_{ij}^2\right) c_j = 1. \tag{9.12}$$

Thus one obtains M^{-1}. Examples can be found in Ref. 1.

(2) Each row of M, transposed to a column, provides an eigenvector of M and all together a complete set.

A. Consequences for factorization

For

$$\hat{R}(\theta) = \sum_i \frac{f_i(\theta)}{f_i(-\theta)} P_i, \tag{9.13}$$

$$M\hat{R}(\theta)M^{-1} = \mathrm{diag}\left(\frac{f_1(\theta)}{f_1(-\theta)}, \ldots; \frac{f_2(\theta)}{f_2(-\theta)}, \ldots; \ldots\right). \tag{9.14}$$

Here the multiplicity of $f_i(\theta)$ is equal to TrP_i. Note that M is *independent* of θ. It diagonalizes each P_i (independent of θ) and hence also $\hat{R}$.

Define

$$D(\theta) = \mathrm{diag}(f_1(\theta), \ldots; f_2(\theta), \ldots; \ldots), \quad M(\theta) = D(\theta)M. \tag{9.15}$$

Now, starting with (1.13),

$$\hat{R}(\theta) = (F(-\theta))^{-1}F(\theta) = (M^{-1}D(-\theta)M)^{-1}(M^{-1}D(\theta)M) = (M(-\theta))^{-1}M(\theta). \tag{9.16}$$

In each factor all θ-dependence is thus again factorized in a diagonal matrix $D(\theta)$. Some consequences will be studied in the following sections.

X. *L*-OPERATORS

Here we indicate the general features that arise as one implements our formalism in the construction of L-operators. It is well known that the FRT definitions[10] [with their $R^{(+)} = (PRP)$ and with $L_2^{\varepsilon} = PL_1^{\varepsilon}P$]

$$(PRP)L_1^{\pm}L_2^{\pm} = L_2^{\pm}L_1^{\pm}(PRP), \quad (PRP)L_1^{+}L_2^{-} = L_2^{-}L_1^{+}(PRP) \tag{10.1}$$

give in terms of $\hat{R} = PR$

$$\hat{R}L_2^{\pm}L_1^{\pm} = L_2^{\pm}L_1^{\pm}\hat{R}, \quad \hat{R}L_2^{+}L_1^{-} = L_2^{-}L_1^{+}\hat{R}. \tag{10.2}$$

Taking one more step we define (with $\varepsilon = \pm$ below)

$$L_2^{\varepsilon}P = PL_1^{\varepsilon} \equiv \hat{L}_{\varepsilon} \tag{10.3}$$

when

$$L_2^{\varepsilon}L_1^{\varepsilon'} = L_2^{\varepsilon}PPL_1^{\varepsilon'} = \hat{L}_{\varepsilon}\hat{L}_{\varepsilon'}$$

and

$$\hat{R}\hat{L}_{\varepsilon}\hat{L}_{\varepsilon} = \hat{L}_{\varepsilon}\hat{L}_{\varepsilon}\hat{R}, \quad \hat{R}\hat{L}_{+}\hat{L}_{-} = \hat{L}_{-}\hat{L}_{+}\hat{R}. \tag{10.4}$$

All this is before Baxterization. When the spectral parameter is introduced a more general formulation is

$$\hat{R}(\theta-\theta')\hat{L}_{\varepsilon}(\theta)\hat{L}_{\varepsilon}(\theta')=\hat{L}_{\varepsilon}(\theta')\hat{L}_{\varepsilon}(\theta)\hat{R}(\theta-\theta'),$$

$$\hat{R}(\theta-\theta')\hat{L}_{+}(\theta)\hat{L}_{-}(\theta')=\hat{L}_{-}(\theta')\hat{L}_{+}(\theta)\hat{R}(\theta-\theta'). \tag{10.5}$$

(For affine cases extra factors $q^{\pm c}$ can appear in the argument of $\hat{R}$ in the last equation. But the above formulation suffices to illustrate our approach.)

One can introduce a development such as

$$\hat{L}_{\varepsilon}(\theta)=\frac{1}{\rho(\theta)}\sum_{n\geqslant 0}(\hat{L}_{(\varepsilon,n)}e^{n\theta}+\hat{L}_{(\varepsilon,-n)}e^{-n\theta}). \tag{10.6}$$

But for clarity in our illustrative approach let us concentrate on a particularly simple case.[20] When the spectral basis on the right of (1.9) has only two projectors, $\hat{R}(\theta)$ can be expressed quite simply in terms of $\hat{R}^{\pm 1}$. [A more general result is obtained (3.49) of Ref. 1.] Thus for $\mathrm{GL}_q(N)$ from (2.1) one obtains

$$\hat{R}(\theta)=\frac{e^{h+\theta}\hat{R}-e^{-h-\theta}\hat{R}^{-1}}{e^{h+\theta}-e^{-h-\theta}}. \tag{10.7}$$

From (3.3) [redefining $(P_{+}+P_{-})$ as P_1, say] one obtains for this new class of solutions

$$\hat{R}(\theta)=P_1+\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}P_0=\frac{e^{(\eta+\theta)}\hat{R}-e^{(-\eta-\theta)}\hat{R}^{-1}}{e^{(\eta+\theta)}-e^{(-\eta-\theta)}}. \tag{10.8}$$

Here η is defined for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ as in (3.1) and (3.2). [Setting $\hat{R}(0)=I$ one obtains the linear relation between $\hat{R}$ and $\hat{R}^{-1}$.] For such cases, defining [analogously to (3.5.9) of Ref. 20, but in terms of our $\hat{L}$]

$$\hat{L}(\theta)\equiv(e^{\theta}\hat{L}_{+}-e^{-\theta}\hat{L}_{-}), \tag{10.9}$$

all the three relations (10.4) can be encapsulated in the *single* one

$$\hat{R}(\theta-\theta')\hat{L}(\theta)\hat{L}(\theta')=\hat{L}(\theta')\hat{L}(\theta)\hat{R}(\theta-\theta'). \tag{10.10}$$

[As (10.10) is developed, inserting (10.8) and (10.9), the terms $\hat{L}_{\pm}\hat{L}_{\mp}$ appear in "wrong order," $\hat{R}\hat{L}_{-}\hat{L}_{+}$ and so on. Now, expressing $\hat{R}$ in terms of $\hat{R}^{-1}$ and vice versa, one can extract the relations (10.4) with different factors depending on arbitrary (θ,θ').]

We will use this compact formulation adapted to our special class of braid matrices (Sec. III) to illustrate the consequences of our formalism. For more general cases [see (10.5) and (10.6)] the basic features will be analogous along with more elaborate sets of equations. Some indications will be given of such generalizations. Let us, however, come back to our special case:

Implementing (10.8) in (10.10) one obtains

$$\begin{aligned}
&P_0(\hat{L}(\theta)\hat{L}(\theta')-\hat{L}(\theta')\hat{L}(\theta))P_0=0,\\
&P_1(\hat{L}(\theta)\hat{L}(\theta')-\hat{L}(\theta')\hat{L}(\theta))P_1=0,\\
&P_0((e^{\eta-\theta+\theta'}-e^{-\eta+\theta-\theta'})\hat{L}(\theta)\hat{L}(\theta')-(e^{\eta+\theta-\theta'}-e^{-\eta-\theta+\theta'})\hat{L}(\theta')\hat{L}(\theta))P_1=0,\\
&P_1((e^{\eta+\theta-\theta'}-e^{-\eta-\theta+\theta'})\hat{L}(\theta)\hat{L}(\theta')-(e^{\eta-\theta+\theta'}-e^{-\eta+\theta-\theta'})\hat{L}(\theta')\hat{L}(\theta))P_0=0.
\end{aligned} \tag{10.11}$$

Here, as in the general case (10.21) below, the constraints are exhaustive due to the resolution of the identity provided by $\Sigma P_i = I$. This aspect is evident in the equivalent form obtained below [(10.17)–(10.19)] via diagonalization.

Here the P_i do not depend on θ but only on q. So now implementing (10.9) dependence on (θ, θ') becomes entirely explicit. The coefficients of $e^{(n\theta + n'\theta')}$ for different (n, n') must vanish separately. Only the factors $e^{\pm\eta}$, given by (3.1) and (3.2) as

$$\tanh \eta = \sqrt{(1 - 4([N - \epsilon] + \epsilon)^{-2})} \tag{10.12}$$

and q-dependent through $[N - \epsilon]$, characterize the L-algebra for this specific class of solutions.

As emphasized in Sec. III, this class remains nontrivial even for $q = 1$. Now for both cases $(\epsilon = \pm 1)$, denoting η as $\hat{\eta}$ for $q = 1$,

$$\tanh \hat{\eta} = \pm N^{-1}\sqrt{N^2 - 4}. \tag{10.13}$$

But the projectors $(\hat{P}_0, \hat{P}_1)$ are still different for the two cases $(\mathrm{SO}_q, \mathrm{Sp}_q)$.

We now present the consequences of diagonalization (Sec. IX). Both for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ (remembering that $P_1 = P_+ + P_-$) one obtains

$$MP_0M^{-1} = \mathrm{diag}(1,0,\ldots,0), \quad MP_1M^{-1} = \mathrm{diag}(0,1,\ldots,1) \tag{10.14}$$

with

$$TrP_0 = 1, \quad TrP_1 = N^2 - 1. \tag{10.15}$$

[Explicit expression for M are given, in Appendix B, only for $\mathrm{SO}_q(3), \mathrm{SO}_q(4)$ and $\mathrm{Sp}_q(4)$.]

Define

$$K(\theta) = M\hat{L}(\theta)M^{-1} = e^{\theta}(M\hat{L}_+M^{-1}) - e^{-\theta}(M\hat{L}_-M^{-1}). \tag{10.16}$$

Here M is different for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$. See Sec. IX and our particularly simple prescription for M^{-1} when the rows of M are mutually orthogonal. Our diagonalization leads to

$$(K(\theta)K(\theta') - K(\theta')K(\theta))_{ij} = 0, \quad (i,j) = (1,1) \quad (i > 1,\ j > 1), \tag{10.17}$$

and for $j > 1$ to

$$((e^{\eta - \theta + \theta'} - e^{-\eta + \theta - \theta'})K(\theta)K(\theta') - (e^{\eta + \theta - \theta'} - e^{-\eta - \theta + \theta'})K(\theta')K(\theta))_{1j} = 0, \tag{10.18}$$

$$((e^{\eta + \theta - \theta'} - e^{-\eta - \theta + \theta'})K(\theta)K(\theta') - (e^{\eta - \theta + \theta'} - e^{-\eta + \theta - \theta'})K(\theta')K(\theta))_{j1} = 0. \tag{10.19}$$

This is the most compact form of the constraints on the L-operators. Those on the elements of $\hat{L}(\theta)$ are now obtained from

$$\hat{L}(\theta) = M^{-1}\hat{K}(\theta)M.$$

Then one can implement Gauss decomposition, if so desired, for the elements of $L^{\pm}$ to obtain results more directly comparable to those for standard cases. But *all information* is encapsulated in (10.17)–(10.19). All θ-dependence can be extracted as exponential factors giving the final constraints as coefficients. For $\mathrm{SO}_q(3)$, for example, our equations furnish the 16 (for $j = 2,\ldots,9$) constraints which involve η.

For the more general case [(10.5)–(10.7)], where

$$\hat{R}(\theta) = \sum_i^p \frac{f_i(\theta)}{f_i(-\theta)} P_i, \tag{10.20}$$

the set (10.11) is generalized to the following p^2 constraints:

$$P_i(f_i(\theta-\theta')f_j(-\theta+\theta')\hat{L}_\varepsilon(\theta)\hat{L}_{\varepsilon'}(\theta')-f_i(-\theta+\theta')f_j(\theta-\theta')\hat{L}_{\varepsilon'}(\theta')\hat{L}_\varepsilon(\theta))P_j=0, \tag{10.21}$$

where

$$(\varepsilon,\varepsilon')=((++),(--),(+-)) \quad (i,j=1,\ldots,p).$$

Diagonalization and the definition

$$K_\varepsilon(\theta)=M\hat{L}_\varepsilon(\theta)M^{-1}=\frac{1}{\rho(\theta)}\sum_n (M\hat{L}_{\varepsilon,n}M^{-1}e^{n\theta}+M\hat{L}_{\varepsilon,-n}M^{-1}e^{-n\theta}) \tag{10.22}$$

reduce (10.21) to

$$f_i(\theta-\theta')f_j(-\theta+\theta')(K_\varepsilon(\theta)K_{\varepsilon'}(\theta'))_{i',j'}-f_i(-\theta+\theta')f_j(\theta-\theta')(K_{\varepsilon'}(\theta')K_\varepsilon(\theta))_{i',j'}=0. \tag{10.23}$$

Here, for a given (i,j), the ranges of (i',j') are fixed by TrP_i, TrP_j and the order chosen (Sec. IX and Appendix B) for the elements unity in diagonalizing the projectors. A simple example is provided by (10.18) and (10.19). If the expansion (10.22) is a finite series [(10.9) being an extreme example], one can extract the limits for θ and $(\theta-\theta')\to\pm\infty$, since the dependence on these parameters can be made explicit as factored coefficients. But for a correct extraction the functions $f_i(\theta)$ have to be properly defined [as noted below (1.33)].

XI. TRANSFER MATRICES AND DIAGONALIZATION

A. General formulation

We start by introducing notations analogous to those of Sec. X for the row-to-row transfer matrix $T^{(L)}(\theta)$, satisfying

$$\hat{R}(\theta-\theta')(T^{(L)}(\theta)\otimes T^{(L)}(\theta'))=(T^{(L)}(\theta)'\otimes T^{(L)}(\theta))\hat{R}(\theta-\theta'). \tag{11.1}$$

Here, apart from evident analogies (since we have again a class of L-functions), specific features arise concerning the component blocks of $T^{(L)}$. The dimensions of the blocks increase with the length of the row according to standard prescriptions.

Matrix multiplication for a $N^2\times N^2$ matrix $\hat{R}(\theta)$ is defined by labeling $T^{(L)}$ for any L by N^2 blocks. If I be the $N\times N$ unit matrix,

$$\begin{aligned}T^{(L)}(\theta)\otimes T^{(L)}(\theta')&=(T^{(L)}(\theta)\otimes I)(I\otimes T^{(L)}(\theta'))=(P(I\otimes T^{(L)}(\theta)P)(P(T^{(L)}(\theta')\otimes I)P)\\&=(P(I\otimes T^{(L)}(\theta))((T^{(L)}(\theta')\otimes I)P)=(PT_2^{(L)}(\theta))(T_1^L(\theta')P)\\&=\hat{T}^{(L)}(\theta)\hat{T}^{(L)}(\theta'),\end{aligned} \tag{11.2}$$

where

$$\hat{T}^{(L)}\equiv PT_2^{(L)}=T_1^{(L)}P$$

are $N^2\times N^2$ matrices in terms of blocks of $T^{(L)}$.

Thus,

$$\hat{R}(\theta-\theta')(\hat{T}^{(L)}(\theta)\hat{T}^{(L)}(\theta'))=(\hat{T}^{(L)}(\theta)'\hat{T}^{(L)}(\theta))\hat{R}(\theta-\theta'). \tag{11.3}$$

Thus the mixture of matrix multiplication and tensor product in (11.1) has been rephrased as matrix multiplications of $\hat{R}$ and $\hat{T}$. Instead of (T_1, T_2), the same $\hat{T}$ now appears throughout.

For (1.9), namely,

$$\hat{R}(\theta) = \sum_{i=1}^{p} \frac{f_i(\theta)}{f_i(-\theta)} P_i, \tag{11.4}$$

one obtains, as in Sec. X, a complete set of p^2 constraints

$$P_i(f_i(\theta-\theta')f_j(-\theta+\theta')\hat{T}^{(L)}(\theta)\hat{T}^{(L)}(\theta') - f_i(-\theta+\theta')f_j(\theta-\theta')\hat{T}^{(L)}(\theta')\hat{T}^{(L)}(\theta))P_j = 0. \tag{11.5}$$

Using the diagonalizer M of the braid matrix (Sec. IX and Appendix B) define

$$\hat{R}_d(\theta) = M\hat{R}(\theta)M^{-1}, \quad \hat{K}^{(L)}(\theta) = M\hat{T}^{(L)}(\theta)M^{-1}. \tag{11.6}$$

One obtains from (11.3), in terms of the *diagonal* matrix $\hat{R}_d$,

$$\hat{R}_d(\theta-\theta')(\hat{K}^{(L)}(\theta)\hat{K}^{(L)}(\theta')) = (\hat{K}^{(L)}(\theta)'\hat{K}^{(L)}(\theta))\hat{R}_d(\theta-\theta'). \tag{11.7}$$

This corresponds to

$$f_i(\theta-\theta')f_j(-\theta+\theta')(\hat{K}^{(L)}(\theta)\hat{K}(L)(\theta'))_{i'j'} - f_i(-\theta+\theta')f_j(\theta-\theta')(\hat{K}^{(L)}(\theta')\hat{K}^{(L)}(\theta))_{i'j'} = 0. \tag{11.8}$$

We have explained below (10.23) of Sec. X how the domain of $(i'j')$ depends on the conventions adopted for the diagonalizations of the projectors P_i and P_j. It was also pointed out before that such a set of constraints is exhaustive.

The elements of $\hat{K}^{(L)}(\theta)$ are linear combinations of those of $T^{(L)}(\theta)$, the coefficients being independent of θ (since M is so). The bilinear algebraic relations due to (11.1) between $T_{ij}^{(L)}(\theta)$ attain their simplest form in (11.8) in terms of these linear combinations. Construction of a "$\hat{K}$-basis" (a complete set of states specifically adapted to the action of the blocks of $\hat{K}$) would permit a full exploitation of (11.8).

B. Particular cases

We now consider two particular cases. The first one is chosen because it is familiar and extensively studied. The content of (11.8) for the six-vertex case can be compared to well-known results. (See Refs. 7–9 and 16 and basic sources cited in these references.) The second one is chosen as a relatively simple but new example of a multi-state model. It corresponds to our special class of solutions (Sec. III) for $SO_q(3)$. This can be compared to a different class of multistate models.[16]

1. The six-vertex case

Inserting in (11.6) the results of Sec. VI with M given by (6.9),

$$\hat{R}_d(\theta-\theta') = \mathrm{diag}(1, u, v, 1) \tag{11.9}$$

where

$$u = \frac{\cosh\frac{1}{2}(\gamma-\theta+\theta')}{\cosh\frac{1}{2}(\gamma+\theta-\theta')}, \quad v = \frac{\sinh\frac{1}{2}(\gamma-\theta+\theta')}{\sinh\frac{1}{2}(\gamma+\theta-\theta')}. \tag{11.10}$$

[Other interesting choices of M are possible. But (6.9) is adequate for our present purposes.] Now let

$$\hat{T}^{(L)}(\theta)=\begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{11.11}$$

where each entry is a $2^L\times 2^L$ block obtained according to standard prescriptions (e.g., Secs. 2 and 3 of Ref. 16). From (6.9), (11.2) and (11.6) one obtains

$$2\hat{K}^{(L)}(\theta)=\begin{pmatrix} A+D & B+C & B-C & A-D \\ B+C & A+D & D-A & C-B \\ B-C & A-D & -A-D & -B-C \\ A-D & B-C & B+C & A+D \end{pmatrix} \tag{11.12}$$

$$=(A+D)\begin{pmatrix} s_0 & 0 \\ 0 & -s_3 \end{pmatrix}+(A-D)\begin{pmatrix} 0 & -s_2 \\ s_1 & 0 \end{pmatrix}+(B+C)\begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix}+(B-C)\begin{pmatrix} 0 & s_3 \\ s_0 & 0 \end{pmatrix}, \tag{11.13}$$

where

$$s_0=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad s_3=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad s_1=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_2=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Note that

$$Tr\hat{K}^{(L)}(\theta)=Tr(A+D)=TrT^{(L)}(\theta),$$

and if V is an eigenvector of $\hat{K}(\theta)$, then $M^{-1}V$ is one of $\hat{T}^{(L)}(\theta)$.

Now (11.8) reduces to

$$(\hat{K}^{(L)}(\theta)\hat{K}(L)(\theta')-x\hat{K}^{(L)}(\theta')\hat{K}^{(L)}(\theta))_{ij}=0, \tag{11.14}$$

where, (u,v) being given by (11.10), one obtains x as follows for values of (i,j) indicated at right:

$$\begin{gathered} x=1, \quad (i,j)=(1,1),(2,2),(3,3),(4,4),(1,4),(4,1); \\ x=u, \quad (i,j)=(1,2),(4,2); \quad x=u^{-1}, \quad (i,j)=(2,1),(2,4); \\ x=v, \quad (i,j)=(1,3),(4,3); \quad x=v^{-1}, \quad (i,j)=(3,1),(3,4); \\ x=\frac{u}{v}, \quad (i,j)=(3,2); \quad x=\frac{v}{u}, \quad (i,j)=(2,3). \end{gathered} \tag{11.15}$$

Thus we obtain the simplest form of the constraints implied by (11.1) or (11.3).

2. A special class of multistate models [$SO_q(3)$ example]

We consider now the class of braid matrices presented in Sec. III and explicitly diagonalized for $SO_q(3)$, as well as for $SO_q(4)$, in Appendix B. [We consider only $SO_q(N)$. For $Sp_q(N)$ certain states have negative weights.] The precise way in which the model is "nonminimal," with more than two possible states per link, will be explained at the end by comparing it with another class of models studied in Sec. IV of Ref. 16 (where original sources are cited).

We start with (B8)–(B10). Using the notations of (10.8) the braid matrix is (with η defined in Sec. III)

$$\hat{R}(\theta)=P_1+\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}P_0=I+\left(\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}-1\right)P_0. \tag{11.16}$$

For $N=3$ (see Sec. 4 of Ref. 1),

$$(q+q^{-1}+1)P_0=q^{-1}E_{11}\otimes E_{33}+q^{-1/2}E_{12}\otimes E_{32}+E_{13}\otimes E_{31}+q^{-1/2}E_{21}\otimes E_{23}+E_{22}\otimes E_{22}+q^{1/2}E_{23}\otimes E_{21}+E_{31}\otimes E_{13}+q^{1/2}E_{32}\otimes E_{12}+qE_{33}\otimes E_{11}. \tag{11.17}$$

Setting $\epsilon=1$ and $N=3$ in (3.1) and (3.2),

$$2\cosh\eta=(q+q^{-1}+1), \tag{11.18}$$

and for M given by (B10)

$$M\hat{R}(\theta)M^{-1}=\mathrm{diag}\left(\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)},1,1,1,1,1,1,1,1\right). \tag{11.19}$$

Hence (11.8) reduces to

$$(\hat{K}^{(L)}(\theta)\hat{K}(L)(\theta')-K^{(L)}(\theta')\hat{K}^{(L)}(\theta))_{ij}=0 \tag{11.20}$$

for $(i,j)=(1,1)$ and for $i>1$, $j>1$. For $j=(2,3,\ldots,9)$ one obtains

$$(\sinh(\eta-\theta+\theta')\hat{K}^{(L)}(\theta)\hat{K}^{(L)}(\theta')-\sinh(\eta+\theta-\theta')\hat{K}^{(L)}(\theta')\hat{K}^{(L)}(\theta))_{1j}=0, \tag{11.21}$$

$$(\sinh(\eta+\theta-\theta')\hat{K}^{(L)}(\theta)\hat{K}^{(L)}(\theta')-\sinh(\eta-\theta+\theta')\hat{K}^{(L)}(\theta')\hat{K}^{(L)}(\theta))_{j1}=0. \tag{11.22}$$

Thus we obtain the complete set of constraints in the simplest and the most compact form. The foregoing structure is directly generalizable to all N. But for $N>4$ one has either to construct the corresponding M or to use (11.5) with (11.16). A study of the $\hat{K}$-basis adapted to the foregoing set of constraints is beyond the scope of this article. We conclude with some comments and comparisons.

In six- or eight-vertex models two states are possible for each link. But nonzero Boltzmann weights are associated to a subset of the 2^4 elements of the braid matrix. When three states are possible per link (of a plane lattice) one can implement a 9×9 matrix (with 3^4 elements) attributing again nonzero weights to a subset of the possible states, corresponding to the nonzero elements of the matrix.

The number of nonzero elements in (11.16) is $15(=3(2.3-1))$. For $\mathrm{SO}_q(N)$ this number, for our class of solution of Sec. III, is $N(2N-1)$. In Sec. 4 of Ref. 16 a class of models is studied where one has precisely the same number of nonzero weights out of N^4 elements (with the symbol q for our N). Apart from this feature, the block structure in (4.12) of Ref. 16 [namely, $(11),(1j),(j1),(ij)$ with $(i>1,\ j>1)$] corresponds also to the structure of our set of constraints [(11.20)–(11.22)] for $\hat{K}(\theta)$. We will not study here the different possibilities concerning block structures but emphasize that in spite of the foregoing features the two classes are basically different. For $N=2$ that of Ref. 16 reduces to the six-vertex case, whereras our special class does not exist. Ours is obtained for $\mathrm{SO}_q(N)$ and for all $N\geqslant3$ can be diagonalized to the form (11.19) with (N^2-1) unit elements.

Finally let us note the situation for $q=1$. As pointed out at the end of Sec. III, this class of $\hat{R}(\theta)$ remains nontrivial, even quite interesting, for $q=1$. There is, of course, additional simplicity. Thus denoting (P_0,η) for $q=1$ by $(\hat{P}_0,\hat{\eta})$ one obtains for SO(3), for example,

$$3\hat{P}_0 = E_{11}\otimes E_{33} + E_{12}\otimes E_{32} + E_{13}\otimes E_{31} + E_{21}\otimes E_{23} + E_{22}\otimes E_{22} + E_{23}\otimes E_{21} + E_{31}\otimes E_{13} + E_{32}\otimes E_{12} + E_{33}\otimes E_{11} \tag{11.23}$$

and

$$\cosh\hat{\eta} = \frac{3}{2}, \quad \sinh\hat{\eta} = \frac{\sqrt{5}}{2}. \tag{11.24}$$

It is amusing to note the relation of $\sinh\hat{\eta}$ with the Golden Mean.

XII. REMARKS

The first essential step in our approach has been the spectral decomposition of the braid matrices $\hat{R}(\theta)$, obtaining the coefficient of the projector P_i in the form of a ratio $f_i(\theta)/f_i(-\theta)$.

The next major step was diagonalization. But here again the projectors play a basic role. The fact that the same matrix M must diagonalize each projector appearing in the decomposition permits a systematic extraction of the necessary constraints on M and also the exploitation of the remaining freedom in an efficient fashion. This is explained in detail in Sec. IX. Along with diagonalization a remarkable new feature arises in the factorization. In each factor the dependence on the spectral parameter θ can again be factorized out as a diagonal matrix by implementing the diagonalizer.

Various directions opened up deserve further exploration. The present work, despite its length, stops short at various points. Applications of our formalism to L-operators and to transfer matrices have merely been adumbrated. Thus the introduction of basis states specifically adapted to the form of the constraints obtained (''$\hat{K}$-basis'') can be particularly helpful. For the braid matrices of Sec. II the diagonalizers have been constructed explicitly (Appendix B) only for lower dimensions. While for $\mathrm{GL}_q(N)$ the general prescription should not be difficult to obtain, for $\mathrm{SO}_q(2n+1)$, $\mathrm{SO}_q(2n)$ and $\mathrm{Sp}_q(2n)$ one has, among other things, to obtain the mutually orthogonal $(2n+1)$-plets and $2n$-plets (Appendix B). The problem of solving the braid equation (1.1) implementing the nested sequence of projectors of Sec. VIII has not been addressed.

We hope to study elsewhere some of the aspects mentioned above. But let us take finally a look back at the factorization phenomenon. We have exhibited our type of factorization essentially for all interesting cases. One may ask why it is present systematically? The answer at a general level has already been noted below (1.10) and in (1.11). This involves also (1.5) and (1.6). For braid matrices with simple roots, for (1.5), one has always a spectral decomposition. And this directly implies the possibility of factorizing such matrices in an unlimited number of ways. We have indeed studied braid matrices with multiple roots[14] without straightforward spectral decompositions. But they constitute a very restricted set of special cases. Even among the ''exotics'' there are other spectrally decomposable cases.[15] This is one reason for displaying the latter ones in Sec. IV. But one may yet ask why in spectral decompositions the form (1.8), namely, $f_i(\theta)/f_i(-\theta)$, of the coefficients, leading to (1.12), is ubiquitous? In this context one should remember that if $\hat{R}$ is a solution of the braid equation (1.1), then $\hat{R}^{-1}$ is also one. Hence if the general solution of the functional constraints of Baxterization is obtained (as in Ref. 1, for example) in terms of a single parameter, θ then one must be able to invert $\hat{R}$ by suitably changing θ. The simplest and most elegantly symmetrical form is obtained in a parametrization where *such an inversion corresponds simply to a change of sign of* θ. This is precisely what is achieved by (1.9). This in turn immediately gives (1.12). The non-Baxterized standard braid matrices (each one with its inverse) are then obtained (as shown always explicitly in the preceding sections) for the two limiting values $\theta\to\pm\infty$. The very naturalness of the factorization thus obtained should incite one to search for applications revealing its full significance. Our diagonalizations, directly related to spectral decomposition and hence inevitably to the factorization, increase the scope significantly. Concerning such applications we have made a beginning in Secs. X and XI.

APPENDIX A: COMPARISON WITH TRIANGULAR FACTORIZATION

We compare here our factorization scheme with that proposed by Maillet *et al.*[7,8] We start with notations and general features.

For our $R_q(\theta)$, where $q=e^h$, define

$$z_1=e^{(h-\theta)}, \quad z_2=e^{(h+\theta)}. \tag{A1}$$

Then as

$$\theta\to-\theta, \quad (z_1,z_2)\to(z_2,z_1). \tag{A2}$$

The unitarity (1.14) is now (in terms of $R=P\hat{R}$)

$$R_{21}(z_2,z_1)R_{12}(z_1,z_2)=I. \tag{A3}$$

In Refs. 7 and 8 the proposed factorization is

$$R_{12}(z_1,z_2)=(F_{21}(z_2,z_1))^{-1}F_{12}(z_1,z_2), \tag{A4}$$

where the aim is to obtain lower triangular F_{12}. Our (1.12) corresponds (implicitly with a *different* F) to

$$R_{12}(z_1,z_2)=(F_{21}(z_2,z_1))^{-1}PF_{12}(z_1,z_2). \tag{A5}$$

Note the presence of P in (A5). In a complementary fashion, for the braid matrix (A4) leads to

$$\hat{R}_{12}(z_1,z_2)=(F_{12}(z_2,z_1))^{-1}PF_{12}(z_1,z_2) \tag{A6}$$

as compared to our (1.12)

$$\hat{R}_{12}(z_1,z_2)=(F_{12}(z_2,z_1))^{-1}F_{12}(z_1,z_2). \tag{A7}$$

This last form permits us to fully exploit the spectral decomposition.

Let us note the following features:

(i) Given a $R(z_1,z_2)$ one has to extract $F(z_1,z_2)$ from (A4). For higher dimensions this (and in particular the explicit construction of F^{-1}) is difficult. So, assuming invertibility, the authors start from

$$(F_{21}(z_2,z_1))R_{12}(z_1,z_2)=F_{12}(z_1,z_2). \tag{A8}$$

For the 4×4 matrix of the six-vertex model (see our Sec. VI) explicit triangular factors in (A4) are obtained. For constructing transfer matrices ''partial'' F-matrices are defined.

Given our Baxterization, *our type of factorization is obtained effortlessly as a byproduct*. In Ref. 1 the forms (1.9) (reproduced here in Secs. II and III) were obtained in a quest for elegance. Factorization was not a goal.

(ii) The limiting cases $\theta\to\pm\infty$ corresponds to $(z_1,z_2)\to(0,\infty),(\infty,0)$, respectively. We have systematically extracted the standard (non-Baxterized) braid matrices as the corresponding limits of the θ-dependent braid matrices (Secs. II–VII) and explained in what sense precisely (Sec. I) the factorization can still be considered to be conserved.

(iii) It is instructive to compare different types of factorization explicitly for the simple example of the six-vertex matrix.

Setting $\theta=(\lambda-\mu)$ in (69) of Ref. 7 one obtains from (89) and (90) of Ref. 7, using a block-diagonal notation,

$$F_{12}(\theta)=(1,B,1)_{bd}, \tag{A9}$$

where the 2×2 block B is

$$B=\begin{pmatrix} 1 & 0 \\ \dfrac{\sinh\eta}{\sinh(\eta+\theta)} & \dfrac{\sinh\theta}{\sinh(\eta+\theta)} \end{pmatrix}. \tag{A10}$$

Using the results of Sec. VI one obtains for our F,

$$F(\theta)=(1,C,1)_{bd}, \tag{A11}$$

where

$$C=\begin{pmatrix} e^{1/2(\gamma-\theta)} & e^{-1/2(\gamma-\theta)} \\ e^{-1/2(\gamma-\theta)} & e^{1/2(\gamma-\theta)} \end{pmatrix}. \tag{A12}$$

(iv) Define the diagonal matrices

$$D(\theta)=\mathrm{diag}(1,\cosh\tfrac{1}{2}(\gamma-\theta),\sinh\tfrac{1}{2}(\gamma-\theta),1), \tag{A13}$$

$$(D(-\theta))^{-1}=\mathrm{diag}(1,(\cosh\tfrac{1}{2}(\gamma+\theta))^{-1},(\sinh\tfrac{1}{2}(\gamma+\theta))^{-1},1). \tag{A14}$$

Now, using the M of (6.9), $\hat{R}(\theta)$ of (6.5) and using (6.10), one can write (with an M independent of θ)

$$\hat{R}(\theta)=(M^{-1}(D(-\theta))^{-1})(D(\theta)M)\equiv(M(-\theta))^{-1}M(\theta). \tag{A15}$$

Now in each factor $M(\theta)$ all θ-dependence is again factorized as a diagonal matrix. This is a general feature of this approach.

We have compared different types of factorization. One can hope to implement fruitfully in different contexts their complementary features such as those indicated above.

APPENDIX B: EXPLICIT DIAGONALIZATIONS

In Sec. IX general aspects of diagonalization of braid matrices have been presented. Here we give explicit expressions for matrices M diagonalizing $\hat{R}(\theta)$ for $\mathrm{GL}_q(2)$, $\mathrm{GL}_q(3)$, $\mathrm{SO}_q(3)$, $\mathrm{SO}_q(4)$ and $\mathrm{Sp}_q(4)$.

The result for $\mathrm{GL}_q(2)$ effectively appears in Sec. V in a form suited to the context. Here we give an equivalent form consistent with the canonical convention of Sec. IX [see (9.5) and (9.6)]. Though we stop with $\mathrm{GL}_q(3)$, one can see the general structure of M for $\mathrm{GL}_q(n)$ emerging. For the orthogonal and the symplectic cases the situation will be discussed at the end.

In each case below the rows of M will be mutually orthogonal.

Hence M^{-1}, always given by the prescription (9.12), will not be displayed explicitly.

For $\mathrm{GL}_q(n)$ we adopt [with the matrices E_{ij} defined below (1.3)] the normalization

$$R_q=\sum_i E_{ii}\otimes E_{ii}+q^{-1}\sum_{i\neq j} E_{ii}\otimes E_{jj}+(1-q^{-2})\sum_{j>i} E_{ij}\otimes E_{ji}. \tag{B1}$$

The braid matrix is

$$\hat{R}_q=PR_q=P_{(+)}-q^{-2}P_{(-)}. \tag{B2}$$

With the notations of Sec. II,

$$\hat{R}_q(\theta)=P_{(+)}+\frac{\sinh(h-\theta)}{\sinh(h+\theta)}P_{(-)}\equiv P_{(+)}+v(\theta)P_{(-)}. \tag{B3}$$

The projectors depend on $q(=e^h)$ but not on θ.

For $n=2$ and

$$M=(E_{12}-q^{-1}E_{13})+(E_{22}+qE_{23})+E_{31}+E_{44}, \tag{B4}$$

$$M\hat{R}_q(\theta)M^{-1}=\mathrm{diag}(v(\theta),1,1,1). \tag{B5}$$

For $n=3$ and

$$\begin{aligned}M=&(E_{12}-q^{-1}E_{14})+(E_{23}-q^{-1}E_{27})+(E_{36}-q^{-1}E_{38})\\&+(E_{42}+qE_{44})+(E_{53}+qE_{57})+(E_{66}+qE_{68})+E_{71}+E_{85}+E_{99},\end{aligned} \tag{B6}$$

$$M\hat{R}_q(\theta)M^{-1}=\mathrm{diag}(v(\theta),v(\theta),v(\theta),1,1,1,1,1,1). \tag{B7}$$

The emerging general structure of M for $\mathrm{GL}_q(n)$ is as follows:

There are $\frac{1}{2}n(n-1)$ rows with two nonzero elements $(1,-q^{-1})$, suitably shifted horizontally in successive rows to assure mutual orthogonality. Then there are $\frac{1}{2}n(n-1)$ rows with two nonzero elements $(1,q)$ in the corresponding columns [as in (B6)]. Then there are n rows with a single nonzero element 1 in otherwise empty columns.

For $\mathrm{SO}_q(3)$, $\mathrm{SO}_q(4)$, and $\mathrm{Sp}_q(4)$

$$\hat{R}_q(\theta)=P_{(+)}+v(\theta)P_{(-)}+w(\theta)P_{(0)}. \tag{B8}$$

For the orthogonal case the three possibilities for $v(\theta)$ and $w(\theta)$ are given (with $n=3$ and $n=4$, respectively) by (2.2), (2.3), and also (3.3) with $\epsilon=1$. For the symplectic case the relevant equations are (2.4), (2.5) (N.B. with $n=2$ there) and (3.3) with $\epsilon=-1$.

For $\mathrm{SO}_q(3)$ define

$$s=-q^{-1/2}(1-q),\quad t=-q^{-3/2}(1+q). \tag{B9}$$

Now,

$$\begin{aligned}M=&(E_{13}+q^{1/2}E_{15}+qE_{17})+(E_{22}-qE_{24})+(E_{36}-qE_{38})+(E_{43}+sE_{45}-E_{47})\\&+E_{51}+(E_{62}+q^{-1}E_{64})+(E_{73}+tE_{75}+q^{-2}E_{77})+(E_{86}+q^{-1}E_{88})+E_{99}\end{aligned} \tag{B10}$$

gives

$$M\hat{R}_q(\theta)M^{-1}=\mathrm{diag}(w(\theta),v(\theta),v(\theta),v(\theta),1,1,1,1,1). \tag{B11}$$

For $\mathrm{SO}_q(4)$

$$\begin{aligned}M=&(E_{14}+qE_{17}+qE_{1,10}+q^2E_{1,13})+(E_{24}+qE_{27}-q^{-1}E_{2,10}-E_{2,13})+(E_{32}-qE_{35})+(E_{43}-qE_{49})\\&+(E_{58}-qE_{5,14})+(E_{6,12}-qE_{6,15})+(E_{74}-q^{-1}E_{77}+qE_{7,10}-E_{7,13})+E_{81}+(E_{92}+q^{-1}E_{95})\\&+(E_{10,3}+q^{-1}E_{10,9})+(E_{11,4}-q^{-1}E_{11,7}-q^{-1}E_{11,10}+q^{-2}E_{11,13})+(E_{12,8}+q^{-1}E_{12,14})\\&+(E_{13,12}+q^{-1}E_{13,15})+E_{14,11}+E_{15,6}+E_{16,16}\end{aligned} \tag{B12}$$

gives

$$M\hat{R}_q(\theta)M^{-1}=\mathrm{diag}(w(\theta),v(\theta),v(\theta),v(\theta),v(\theta),v(\theta),1,1,1,1,1,1,1,1). \tag{B13}$$

For $\mathrm{Sp}_q(4)$

$$M=(E_{14}+qE_{17}-q^3E_{1,10}-q^4E_{1,13})+(E_{24}-q^{-1}E_{27}+qE_{2,10}-E_{2,13})+(E_{32}-qE_{35})$$
$$+(E_{43}-qE_{49})+(E_{58}-qE_{5,14})+(E_{6,12}-qE_{6,15})+(E_{74}+qE_{77}+q^{-3}E_{7,10}+q^{-2}E_{7,13})$$
$$+(E_{84}-q^{-1}E_{87}-q^{-1}E_{8,10}+q^{-2}E_{8,13})+(qE_{92}+E_{95})+(qE_{10,3}+E_{10,9})$$
$$+(qE_{11,8}+E_{11,14})+(qE_{12,12}+E_{12,15})+E_{13,1}+E_{14,6}+E_{15,11}+E_{16,16} \tag{B14}$$

gives

$$M\hat{R}_q(\theta)M^{-1}=\mathrm{diag}(w(\theta),v(\theta),v(\theta),v(\theta),v(\theta),v(\theta),1,1,1,1,1,1,1,1,1,1). \tag{B15}$$

Note that the multiplicity of $v(\theta)$ is 6 in (B13) and 5 in (B15).

Other examples of M can be found near the ends of Secs. IV–VII. In Sec. VIII M is obtained for arbitrary dimensions.

For $\mathrm{GL}_q(n)$ one encounters as elements of different rows, apart from singlets (unity), only the mutually orthogonal doublets

$$(1,-q^{-1}),\quad (1,\,q).$$

But for $\mathrm{SO}_Q(3)$ one has [implementing (B9)] also the mutually orthogonal triplets

$$(1,\,q^{1/2},\,q),\quad (1,\,s,-1),\quad (1,\,t,\,q^{-2}).$$

For $\mathrm{SO}_q(4)$ and $\mathrm{Sp}_q(4)$, respectively, one similarly encounters the mutually orthogonal quadruplets

$$(1,\,q,\,q,\,q^2),\ (1,\,q,\,-q^{-1},\,-1),\ (1,\,-q^{-1},\,q,\,-1),\ (1,\,-q^{-1},\,-q^{-1},\,q^{-2}),$$
$$(1,\,q,\,-q^3,\,-q^4),\ (1,\,-q^{-1},\,q,\,-1),\ (1,\,q,\,q^{-3},\,q^{-2}),\ (1,\,-q^{-1},\,-q^{-1},\,q^{-2}).$$

In Sec. VII of Ref. 1 the relations of such multiplets with particular types of q-deformed surfaces (spheres, hyperboloids) have been pointed out. In constructing M for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ for higher dimensions a key feature would be the general structure of the corresponding N mutually orthogonal N-plets.

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The fourth Painlevé equation and associated special polynomials

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(Received 27 February 2003; accepted 14 May 2003)

In this article rational solutions and associated polynomials for the fourth Painlevé equation are studied. These rational solutions of the fourth Painlevé equation are expressible as the logarithmic derivative of special polynomials, the Okamoto polynomials. The structure of the roots of these Okamoto polynomials is studied and it is shown that these have a highly regular structure. The properties of the Okamoto polynomials are compared and contrasted with those of classical orthogonal polynomials. Further representations are given of the associated rational solutions in the form of determinants through Schur functions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1603958]

I. INTRODUCTION

In this article we are concerned with rational solutions and associated special polynomials for the fourth Painlevé equation (P_{IV})

$$w''=\frac{(w')^2}{2w}+\frac{3}{2}w^3+4zw^2+2(z^2-\alpha)w+\frac{\beta}{w}, \tag{1.1}$$

where $'\equiv \mathrm{d}/\mathrm{d}z$ and α and β are arbitrary constants.

The six Painlevé equations (P_I-P_{VI}), discovered by Painlevé, Gambier and their colleagues while studying second order ordinary differential equations of the form

$$w''=F(z,w,w'), \tag{1.2}$$

where F is rational in w' and w and analytic in z, have the property that the solutions have no movable branch points, i.e., the locations of multi-valued singularities of any of the solutions are independent of the particular solution chosen and so are dependent only on the equation; this is now known as the *Painlevé property* (cf. Ref. 50). For P_{IV}, all local solutions can be analytically continued to single-valued meromorphic functions in the complex plane[95] (see also Refs. 47 and 79). Although first discovered from strictly mathematical considerations, the Painlevé equations have arisen in a variety of important physical applications including statistical mechanics, plasma physics, nonlinear waves, quantum gravity, quantum field theory, general relativity, nonlinear optics and fiber optics. For example, P_{IV} has relevance within the fields of fluid mechanics,[111] nonlinear optics[30] and quantum gravity.[32,33] Further, the Painlevé equations have attracted much interest since they arise in many physical situations and as reductions of the soliton equations which are solvable by inverse scattering (cf. Refs. 1, 4, and 51, and references therein, for further details).

The Painlevé equations can be thought of as nonlinear analogs of the classical special functions. Indeed Iwasaki, Kimura, Shimomura, and Yoshida[52] characterize the six Painlevé equations as ''the most important nonlinear ordinary differential equations'' and state that ''many specialists believe that during the twenty-first century the Painlevé functions will become new members of

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the community of special functions.'' The general solutions of the Painlevé equations are transcendental in the sense that they cannot be expressed in terms of known elementary functions and so require the introduction of a new transcendental function to describe their solution. However it is well-known that $P_{II}-P_{VI}$ possess hierarchies of rational solutions for special values of the parameters (see, for example, Refs. 8, 10, 13, 31, 37, 46, 47, 62, 68, 74–77, 85–88, 105, 106, 109, 110, 113, and 115, and the references therein). These hierarchies are usually generated from ''seed solutions'' using the associated Bäcklund transformations and frequently can be expressed in the form of determinants through ''τ-functions.''

Vorob'ev[109] and Yablonskii[113] expressed the rational solutions of the second Painlevé equation (P_{II})

$$w''=2w^3+zw+\alpha, \tag{1.3}$$

where α is an arbitrary constant, in terms of the logarithmic derivative of certain polynomials which are now known as the *Yablonskii-Vorob'ev polynomials*. Okamoto[87] obtained analogous polynomials related to some of the rational solutions of P_{IV}; these polynomials are now known as the *Okamoto polynomials*. Further, Okamoto noted that they arise from special points in parameter space from the point of view of symmetry, which is associated to the affine Weyl group of type $A_2^{(2)}$. Umemura[104] associated analogous special polynomials with certain rational and algebraic solutions of P_{III}, P_V and P_{VI} which have similar properties to the Yablonskii-Vorob'ev polynomials and the Okamoto polynomials; see also Refs. 11, 78, 102, 103, and 114. Subsequently, there have been several studies of special polynomials associated with the rational solutions of P_{II},[37,54,56,98] the rational and algebraic solutions of P_{III},[55,84] the rational solutions of P_{IV},[37,57,82] the rational solutions of P_V,[73,81] and the algebraic solutions of P_{VI}.[60,61,72,99,100] However the majority of these papers are concerned with the combinatorial structure and determinant representation of the polynomials, often related to the Hamiltonian structure and affine Weyl symmetries of the Painlevé equations. Typically these polynomials arise as the ''τ-functions'' for special solutions of the Painlevé equations and are generated through nonlinear, three-term recurrence relations which are Toda equations that arise from the associated Bäcklund transformations of the Painlevé equations. The coefficients of these special polynomials have some interesting, indeed somewhat mysterious, combinatorial properties (see Refs. 78 and 102–104). Additionally, these polynomials have been expressed as special cases of *Schur polynomials*, which are irreducible polynomial representations of the general linear group $\mathrm{GL}(n)$ and arise as τ-functions of the Kadomtsev–Petviashvili (KP) hierarchy.[53] The Yablonskii–Vorob'ev polynomials associated with P_{II} are expressible in terms of two-reduced Schur functions,[54,56] and are related to the τ-function for the rational solution of the modified Korteweg–de Vries (mKdV) equation since P_{II} arises as a similarity reduction of the mKdV equation. The Okamoto polynomials associated with P_{IV} are expressible in terms of three-reduced Schur functions[57,82] since P_{IV} arises as a similarity reduction of the Boussinesq equation (cf. Ref. 23), which belongs to the so-called three-reduction of the KP hierarchy.[53]

It is also well-known that $P_{II}-P_{VI}$ possess solutions which are expressible in terms of the classical special functions; these are often referred to as ''one-parameter families of solutions.'' For P_{II} these special function solutions are expressed in terms of Airy functions $\mathrm{Ai}(z)$,[8,29,40,87] for P_{III} they are expressed in terms of Bessel functions $J_\nu(z)$,[65,75,77,88] for P_{IV} they are expressed in terms of Weber–Hermite (parabolic cylinder) functions $D_\nu(z)$,[13,36,45,64,76,87] for P_V they are expressed in terms of Whittaker functions $M_{\kappa,\mu}(z)$, or equivalently confluent hypergeometric functions ${}_1F_1(a;c;z)$,[43,66,86,110] and for P_{VI} they are expressed in terms of hypergeometric functions ${}_2F_1(a,b;c;z)$;[35,67,85] see also Refs. 1, 44, 46, 48, and 97. Some classical orthogonal polynomials arise as particular cases of these special function solutions and thus yield rational solutions of the associated Painlevé equations, especially in the representation of rational solutions through determinants. For P_{III} and P_V these are in terms of associated Laguerre polynomials $L_n^{(k)}(z)$,[17,55,73,81] for P_{IV} in terms of Hermite polynomials $H_n(z)$,[13,57,76,87] and for P_{VI} in terms of Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$.[72,100] In fact, all rational solutions of P_{VI} arise as particular cases of the special solutions given in terms of hypergeometric functions.[74]

This article is organized as follows. The Okamoto polynomials, which were introduced by Okamoto,[87] and associated rational solutions for P_{IV} are studied in Sec. II. We relate these special polynomials to the determinantal form of rational solutions of P_{IV}, and compare the properties of these special polynomials with properties of classical orthogonal polynomials. In Secs. III and IV, the generalized Hermite polynomials and generalized Okamoto polynomials, which were introduced by Noumo and Yamada[82] and are generalizations of the Okamoto polynomials, and associated rational solutions for P_{IV} are studied, respectively. In Sec. V we discuss the determinantal form of rational solutions of P_{IV}. Finally in Sec. VI we discuss our results and pose some open questions.

II. FOURTH PAINLEVÉ EQUATION AND THE OKAMOTO POLYNOMIALS

A. Rational solutions of P_{IV}

Lukashevich,[64] Gromak,[45] and Murata[76] (see also Refs. 13, 47, and 105) have proved the following theorem.

Theorem 2.1: P_{IV} *has rational solutions if and only if*

$$\alpha=m, \quad \beta=-2(1+2n-m)^2, \tag{2.1}$$

or

$$\alpha=m, \quad \beta=-\tfrac{2}{9}(1+6n-3m)^2, \tag{2.2}$$

with $m, n\in\mathbb{Z}$. *Further, the rational solutions for these parameter values are unique.*

Three simple rational solutions of P_{IV} are

$$w_1(z;\pm 2,-2)=\pm 1/z, \quad w_2(z;0,-2)=-2z, \quad w_3(z;0,-\tfrac{2}{9})=-\tfrac{2}{3}z. \tag{2.3}$$

It is known that there are three families of unique rational solutions of P_{IV}, which have the solutions (2.3) as the simplest members. These are summarized in the following theorem (see Refs. 13, 76, and 105 for further details).

Theorem 2.2: *There are three families of rational solutions of* P_{IV}, *which have the forms*

$$w_1(z;\alpha_1,\beta_1)=P_{1,n-1}(z)/Q_{1,n}(z), \tag{2.4a}$$

$$w_2(z;\alpha_2,\beta_2)=-2z+P_{2,n-1}(z)/Q_{2,n}(z), \tag{2.4b}$$

$$w_3(z;\alpha_3,\beta_3)=-\tfrac{2}{3}z+P_{3,n-1}(z)/Q_{3,n}(z), \tag{2.4c}$$

where $P_{j,n}(z)$ *and* $Q_{j,n}(z)$, $j=1, 2, 3$, *are polynomials of degree n, and*

$$(\alpha_1,\beta_1)=(\pm m,-2(1+2n+m)^2), \quad m,n\in\mathbb{Z}, \ n\leqslant -1, \ m\geqslant -2n, \tag{2.5a}$$

$$(\alpha_2,\beta_2)=(m,-2(1+2n+m)^2), \quad m,n\in\mathbb{Z}, \ n\geqslant 0, \ m\geqslant -n, \tag{2.5b}$$

$$(\alpha_3,\beta_3)=(m,\tfrac{2}{9}(1+6n-3m)^2), \quad m,n\in\mathbb{Z}. \tag{2.5c}$$

The three hierarchies given in this theorem are known as the "$-1/z$ hierarchy," the "$-2z$ hierarchy" and the "$-\frac{2}{3}z$ hierarchy," respectively (see Ref. 13 where the terminology was introduced). The "$-1/z$ hierarchy" and the "$-2z$ hierarchy" form the set of rational solutions of P_{IV} with parameter values given by (2.1) and the "$-2/3z$ hierarchy" forms the set with parameter values given by (2.2). The rational solutions of P_{IV} with parameter values given by (2.1) lie at the vertexes of the "Weyl chambers" and those with parameter values given by (2.2) lie at the vertexes of the "Weyl chamber."[105] These are summarized in Fig. 1, which depicts the

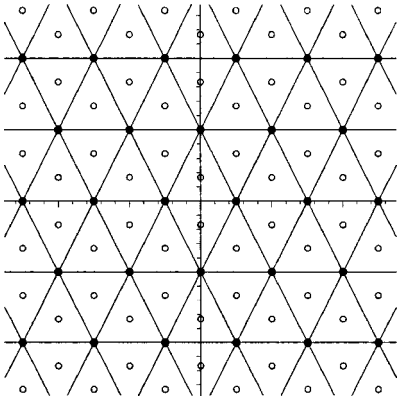

FIG. 1. Special solutions of PIV.

$(\alpha, \sqrt{-2\beta})$ plane, where α and β are the parameters in P_{IV}. The dots denote the rational solutions of P_{IV} with parameter values given by (2.1) and the circles denote the rational solutions with parameter values given by (2.2). On the horizontal and diagonal lines, P_{IV} possesses special function solutions, often called one-parameter families of solutions, which are expressible in terms of Whittaker functions $M_{\kappa,\mu}(\xi)$ and $W_{\kappa,\mu}(\xi)$, or equivalently parabolic cylinder functions $D_\nu(\xi)$ (see Sec. V A).

B. Okamoto polynomials

In a comprehensive study of the fourth Painlevé equation P_{IV}, Okamoto[87] (see also Refs. 37, 57, 82, and 102) defined two sets of polynomials analogous to the Yablonskii–Vorob'ev polynomials associated with P_{II}. These polynomials are defined in Theorems 2.3 and 2.5 below, where they have been scaled compared to Okamoto's original definition, where the polynomials were monic, so that they are for the standard version of P_{IV}.

Theorem 2.3: *Suppose that $Q_n(z)$ satisfies the recursion relation*

$$Q_{n+1}Q_{n-1}=\frac{9}{2}\left[Q_n\frac{\mathrm{d}^2Q_n}{\mathrm{d}z^2}-\left(\frac{\mathrm{d}Q_n}{\mathrm{d}z}\right)^2\right]+[2z^2+3(2n-1)](Q_n)^2 \tag{2.6}$$

or equivalently

$$Q_{n+1}Q_{n-1}=[9\mathrm{D}_z^2+2z^2+3(2n-1)]Q_n\cdot Q_n, \tag{2.7}$$

where D_z is the Hirota operator defined by

$$\mathrm{D}_zF(z)\cdot G(z)=\left[\left(\frac{\mathrm{d}}{\mathrm{d}z_1}-\frac{\mathrm{d}}{\mathrm{d}z_1}\right)F(z_1)G(z_2)\right]_{z_1=z_2=z} \tag{2.8}$$

with $Q_0(z)=Q_1(z)=1$. Then

$$w_n=w(z;\alpha_n,\beta_n)=-\frac{2}{3}z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{Q_{n+1}(z)}{Q_n(z)}\right]\right\} \tag{2.9}$$

satisfies P_{IV} with $(\alpha_n,\beta_n)=(2n,-\frac{2}{9})$.

Remarks 2.4:

(1) The first few polynomials $Q_n(z)$, which are referred to as the *Okamoto polynomials*, are given in Table I.

TABLE I. Okamoto polynomials I defined by (2.6).

$$
\begin{aligned}
Q_2 &= 2z^2+3\\
Q_3 &= 8z^6+60z^4+90z^2+135\\
Q_4 &= 64z^{12}+1344z^{10}+9360z^8+30\,240z^6+56\,700z^4+170\,100z^2+127\,575\\
Q_5 &= 1024z^{20}+46\,080z^{18}+817\,920z^{16}+7\,603\,200z^{14}+41\,731\,200z^{12}+155\,675\,520z^{10}+493\,970\,400z^8\\
&\quad +1\,886\,068\,800z^6+5\,304\,568\,500z^4+5\,304\,568\,500z^2+3\,978\,426\,375\\
Q_6 &= 32\,768z^{30}+2\,703\,360z^{28}+95\,477\,760z^{26}+1\,916\,006\,400z^{24}+24\,472\,627\,200z^{22}+212\,580\,910\,080z^{20}\\
&\quad +1\,332\,821\,952\,000z^{18}+6\,627\,106\,886\,400z^{16}+30\,481\,566\,192\,000z^{14}+148\,952\,283\,480\,000z^{12}\\
&\quad +702\,723\,772\,951\,200z^{10}+2\,375\,788\,921\,506\,000z^8+4\,874\,463\,476\,883\,000z^6\\
&\quad +6\,451\,495\,778\,227\,500z^4+9\,677\,243\,667\,341\,250z^2+4\,838\,621\,833\,670\,625
\end{aligned}
$$

(2) The polynomials $Q_n(z)$ are polynomials of degree $n(n-1)$; in fact they are monic polynomials in $\zeta=\sqrt{2}z$ with integer coefficients, which is the form in which Okamoto[87] originally defined these polynomials. Further, the polynomials $Q_n(z)$ are even polynomials, i.e., monic polynomials in $\zeta^2=2z^2$ of degree $\frac{1}{2}n(n-1)$.

(3) Making the transformation

$$Q_n(z)=c^{n^2}\tau_n(z)\exp\left\{-\frac{z^4}{27}+\frac{1}{3}(1-2n)z^2\right\},$$

with $c^2=\frac{9}{2}$ in (2.6), yields the Toda equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\zeta^2}(\ln\tau_n)=\frac{\tau_{n+1}\tau_{n-1}}{\tau_n^2}.$$

(4) The hierarchy of rational solutions of $\mathrm{P_{IV}}$ defined by (2.9) can be derived using the following Bäcklund transformation of $\mathrm{P_{IV}}$

$$\tilde{w}(z;\tilde{\alpha},\tilde{\beta})=\frac{(w'-w^2-2zw)^2+2\beta}{2w[w'-w^2-2zw+2(\alpha+1)]},\quad \tilde{\alpha}=\alpha+2,\quad \tilde{\beta}=\beta, \tag{2.10}$$

where $w\equiv w(z;\alpha,\beta)$, which is the Bäcklund transformation $\mathcal{T}_+$ derived by Murata[76] and the Schlesinger transformation $\mathcal{R}^{[5]}$ derived by Fokas, Mugan, and Ablowitz[34] (see also Ref. 14). Specifically

$$w_{n+1}=\frac{9[w_n'-w_n^2-2zw_n]^2-4}{18w_n[w_n'-w_n^2-2zw_n+4n+2]}, \tag{2.11}$$

where $w_n=w(z;2n,-\frac{2}{9})$, with "seed solution" $w_0=w(z;0,-\frac{2}{9})=-\frac{2}{3}z$.

(5) The solutions w_n are members of the so-called "$-\frac{2}{3}z$" hierarchy of rational solutions of $\mathrm{P_{IV}}$, recall Theorem 2.2, which is one of three hierarchies of rational solutions of $\mathrm{P_{IV}}$ (see, for example, Refs. 13 and 76 for further details).

The second set of polynomials introduced by Okamoto[87] is defined in the following theorem.

Theorem 2.5: *Suppose that $R_n(z)$ satisfies the recursion relation*

$$R_{n+1}R_{n-1}=\frac{9}{2}\left[R_n\frac{\mathrm{d}^2R_n}{\mathrm{d}z^2}-\left(\frac{\mathrm{d}R_n}{\mathrm{d}z}\right)^2\right]+2(z^2+3n)(R_n)^2 \tag{2.12}$$

or equivalently

$$R_{n+1}R_{n-1}=[9\mathrm{D}_z^2+2(z^2+3n)]R_n\cdot R_n, \tag{2.13}$$

where D_z is the Hirota operator (2.8), with $R_0(z)=1$ and $R_1(z)=\sqrt{2}z$. Then

TABLE II. Okamoto polynomials II defined by (2.12).

$$
\begin{aligned}
R_2 &= 4z^4+12z^2-9\\
R_3 &= \sqrt{2}z(16z^8+192z^6+504z^4-2835)\\
R_4 &= 256z^{16}+7680z^{14}+80\,640z^{12}+362\,880z^{10}+453\,600z^8-1\,905\,120z^6-14\,288\,400z^4\\
&\quad -21\,432\,600z^2+8\,037\,225\\
R_5 &= \sqrt{2}z(4096z^{24}+245\,760z^{22}+5\,990\,400z^{20}+77\,414\,400z^{18}+569\,721\,600z^{16}+2\,246\,952\,960z^{14}\\
&\quad +1\,600\,300\,800z^{12}-35\,663\,846\,400z^{10}-275\,837\,562\,000z^8-1\,103\,350\,248\,000z^6\\
&\quad -1\,737\,776\,640\,600z^4+3\,258\,331\,201\,125)\\
R_6 &= 262\,144z^{36}+27\,525\,120z^{34}+1\,259\,274\,240z^{32}+33\,195\,294\,720z^{30}+560\,170\,598\,400z^{28}\\
&\quad +6\,324\,632\,616\,960z^{26}+47\,742\,002\,880\,800z^{24}+219\,281\,707\,008\,000z^{22}+228\,319\,944\,652\,800z^{20}\\
&\quad -5\,825\,689\,309\,440\,000z^{18}-63\,304\,058\,468\,851\,200z^{16}-412\,776\,567\,979\,776\,000z^{14}\\
&\quad -1\,810\,902\,281\,636\,448\,000z^{12}-4\,651\,958\,555\,820\,576\,000z^{10}-4\,025\,733\,365\,613\,960\,000z^8\\
&\quad +11\,272\,053\,423\,719\,088\,000z^6+47\,553\,975\,381\,314\,902\,500z^4+47\,553\,975\,381\,314\,902\,500z^2\\
&\quad -11\,888\,493\,845\,328\,725\,625
\end{aligned}
$$

$$w(z;\alpha_n,\beta_n)=-\frac{2}{3}z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{R_{n+1}(z)}{R_n(z)}\right]\right\}, \tag{2.14}$$

for $n\geqslant 0$, *satisfies* $\mathrm{P_{IV}}$ *with* $(\alpha_n,\beta_n)=(2n+1,-8/9)$.

Remarks 2.6:

(1) The first few polynomials $R_n(z)$ are given in Table II.

(2) The polynomials $R_n(z)$ are polynomials of degree n^2, in fact they are monic polynomials in $\zeta=2z$ with integer coefficients, which is the form in which Okamoto[87] originally defined these polynomials.

(3) Making the transformation

$$R_n(z)=c^{n^2}\tau_n(z)\exp\left\{-\frac{z^4}{27}-\frac{2}{3}nz^2\right\},$$

with $c^2=\frac{9}{2}$ in (2.12), yields the Toda equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\zeta^2}(\ln\tau_n)=\frac{\tau_{n+1}\tau_{n-1}}{\tau_n^2}.$$

(4) The hierarchy of rational solutions of $\mathrm{P_{IV}}$ defined by (2.14) can be derived using the Bäcklund transformation (2.10) of $\mathrm{P_{IV}}$, derived by Murata[76] and Fokas, Mugan, and Ablowitz.[34] Hence

$$\hat{w}_{n+1}=\frac{9[\hat{w}_n'-\hat{w}_n^2-2z\hat{w}_n]^2-16}{18\hat{w}_n[\hat{w}_n'-\hat{w}_n^2-2z\hat{w}_n+4n+4]}, \tag{2.15}$$

where $\hat{w}_n=w(z;2n+1,2n-\frac{8}{9})$, with "seed solution"

$$\hat{w}_0=w(z;1,-\tfrac{8}{9})=-\tfrac{2}{3}z+1/z. \tag{2.16}$$

(5) The solutions $\hat{w}_n$ are also members of the so-called "$-\frac{2}{3}z$" hierarchy of rational solutions of $\mathrm{P_{IV}}$, recall Theorem 2.2.

(6) The two hierarchies of rational solutions of $\mathrm{P_{IV}}$ given by (2.9) and (2.14) are linked by the Schlesinger transformations $\mathcal{R}^{[1]}$ and $\mathcal{R}^{[3]}$ for $\mathrm{P_{IV}}$ given by Fokas, Mugan, and Ablowitz:[34]

$$\mathcal{R}^{[1]}: \quad w^{[1]}=\frac{(w'+\sqrt{-2\beta})^2-w^2[2\sqrt{-2\beta}-4\alpha-4+(w+2z)^2]}{2w(w^2+2zw-w'-\sqrt{-2\beta})},$$
$$\alpha^{[1]}=\alpha+1, \quad \beta^{[1]}-\tfrac{2}{3}(-2+\sqrt{-2\beta})^2, \tag{2.17}$$

$$\mathcal{R}^{[3]}: \quad w^{[3]}=\frac{(w'-\sqrt{-2\beta})^2+w^2[2\sqrt{-2\beta}+4\alpha+4-(w+2z)^2]}{2w(w^2+2zw-w'+\sqrt{-2\beta})},$$
$$\alpha^{[3]}=\alpha+1, \quad \beta^{[3]}=-\tfrac{2}{3}(2+\sqrt{-2\beta})^2, \tag{2.18}$$

where $w\equiv w(z;\alpha,\beta)$, $w^{[j]}\equiv w(z;\alpha^{[j]},\beta^{[j]})$. Specifically, for $n\geqslant 0$

$$\hat{w}_n=\frac{(w_n'+\frac{2}{3})^2-w_n^2[8n+\frac{8}{3}-(w_n+2z)^2]}{2w_n(w_n^2+2zw_n-w_n'-\frac{2}{3})}, \tag{2.19}$$

$$w_{n+1}=\frac{(\hat{w}_n'+\frac{4}{3})^2+\hat{w}_n^2[8n+\frac{16}{3}-(\hat{w}_n+2z)^2]}{2\hat{w}_n(\hat{w}_n^2+2z\hat{w}_n-\hat{w}_n'-\frac{4}{3})}. \tag{2.20}$$

(7) The Schlesinger transformations $\mathcal{R}^{[1]}$, $\mathcal{R}^{[3]}$, and $\mathcal{R}^{[5]}$ are related by

$$\mathcal{R}^{[1]}\mathcal{R}^{[3]}=\mathcal{R}^{[3]}\mathcal{R}^{[1]}=\mathcal{R}^{[5]} \tag{2.21}$$

from the definition given by Fokas, Mugan, and Ablowitz.[34]

Fukutani, Okamoto and Umemura[37] and Kametaka[58] have proved the following Theorem concerning the roots of the Okamoto polynomials. Further Fukutani, Okamoto, and Umemura[37] also give a purely algebraic proof of Theorems 2.3 and 2.5.

Theorem 2.7:

(1) For every positive integer n, the polynomials $Q_n(z)$ and $R_n(z)$ have simple roots.
(2) Each pair of polynomials $\{Q_n(z),Q_{n+1}(z)\}$, $\{R_n(z),R_{n+1}(z)\}$, $\{Q_n(z),R_n(z)\}$ does not have a common root.

Kametaka[58] also proved the following theorem.

Theorem 2.8: *The polynomials $Q_n(z)$ and $R_n(z)$ have the form*

$$Q_n(z)=\prod_{j=1}^{n(n-1)}(\zeta-a_{n,j}), \quad R_n(z)=\prod_{j=1}^{n^2}(\zeta-b_{n,j}), \quad \zeta=\sqrt{2}z. \tag{2.22}$$

If

$$A_n=\max_{1\leqslant j\leqslant n(n-1)}\{|a_{n,j}|\}, \quad B_n=\max_{1\leqslant j\leqslant n^2}\{|b_{n,j}|\}, \tag{2.23}$$

then for $n\geqslant 1$

$$\tfrac{1}{3}(2n+3)\leqslant A_n^2\leqslant\tfrac{9}{2}(2n+1), \quad \tfrac{2}{3}(n^2-1)/n\leqslant B_n^2\leqslant 9(n-1). \tag{2.24}$$

In Figs. 2 and 3 plots of the locations of the roots for the Okamoto polynomials $Q_n(z)=0$, defined by (2.6), and $R_n(z)=0$, defined by (2.12), for $n=3,4,...,8$, respectively, are given. These both take the form of two ''triangles'' with the polynomials $R_n(z)$ having an additional row of roots on a straight line between the two ''triangles.''

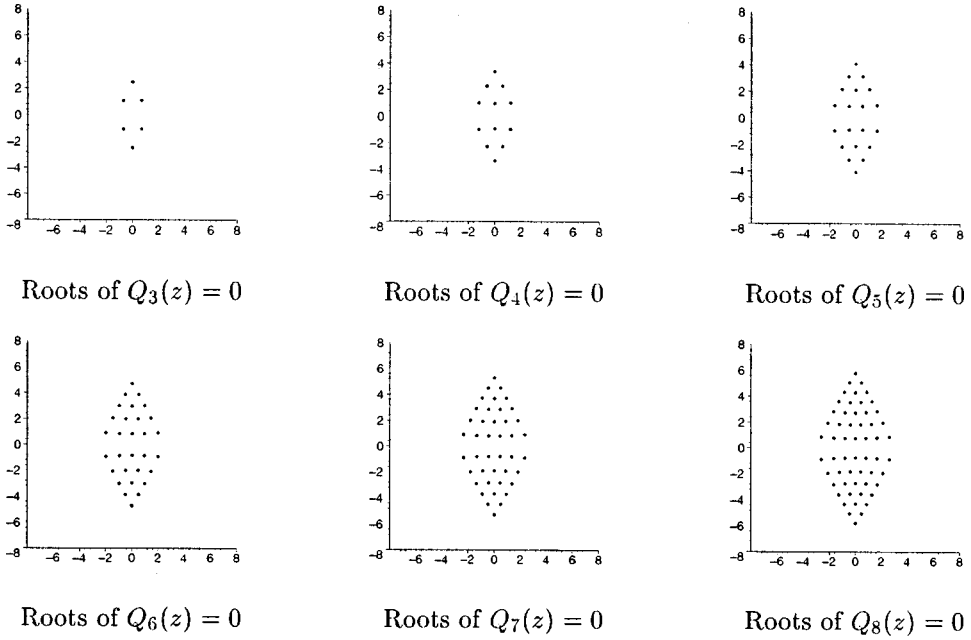

FIG. 2. Locations of roots of some Okamoto polynomials I defined by (2.6).

III. GENERALIZED HERMITE POLYNOMIALS

Noumi and Yamada[82] generalized the results of Okamoto[87] and introduced the *generalized Hermite polynomials* $H_{m,n}(z)$, which are defined in Theorem 3.1 and discussed below in this section, and *generalized Okamoto polynomials* $Q_{m,n}(z)$, which are defined in Theorem 4.1 and discussed in Sec. IV. Noumi and Yamada[82] expressed both the generalized Hermite polynomials and the generalized Okamoto polynomials in terms of Schur functions related to the so-called

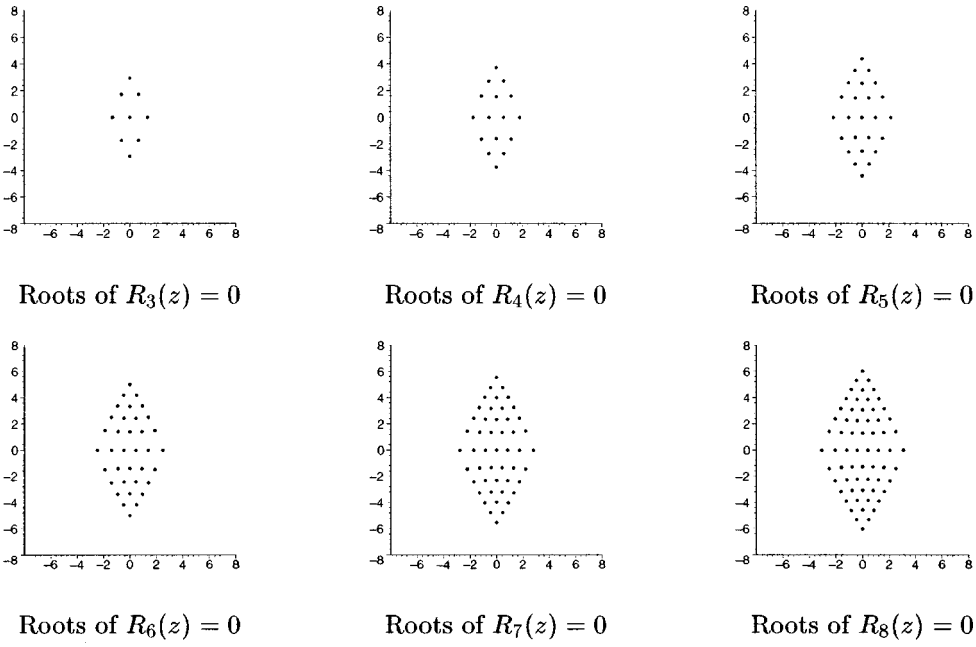

FIG. 3. Locations of roots of some Okamoto polynomials II defined by (2.12).

modified Kadomtsev–Petviashvili (mKP) hierarchy. Kajiwara and Ohta[57] also expressed rational solutions of P_{IV} in terms of Schur functions by expressing the solutions in the form of determinants. Further, Noumi and Yamada[82] obtained their results on rational solutions of P_{IV} by considering the symmetric representation of P_{IV} given by the system

$$\begin{aligned} &\varphi_1'+\varphi_1(\varphi_2-\varphi_3)+2\mu_1=0,\\ &\varphi_2'+\varphi_2(\varphi_3-\varphi_1)+2\mu_2=0,\\ &\varphi_3'+\varphi_3(\varphi_1-\varphi_2)+2\mu_3=0, \end{aligned} \tag{3.1}$$

where μ_1, μ_2, and μ_3 are arbitrary constants, with $\mu_1+\mu_2+\mu_3=1$, and the constraint $\varphi_1+\varphi_2+\varphi_3=-2z$. Then eliminating $\varphi_2(z)$ and $\varphi_3(z)$, $w(z)=\varphi_1(z)$ satisfies P_{IV} with $(\alpha,\beta)=(\mu_3-\mu_2,-2\mu_1^2)$, which was derived by Bureau[15]—see also Refs. 7, 80, 83, 93, and 108.

First we discuss the generalized Hermite polynomials $H_{m,n}(z)$.

Theorem 3.1: *Suppose that $H_{m,n}(z)$ satisfies the recurrence relations*

$$2mH_{m+1,n}H_{m-1,n}=H_{m,n}H_{m,n}^n-(H_{m,n}')^2+2mH_{m,n}^2, \tag{3.2a}$$

$$2nH_{m,n+1}H_{m,n-1}=-H_{m,n}H_{m,n}^n+(H_{m,n}')^2+2nH_{m,n}^2, \tag{3.2b}$$

or equivalently

$$4mH_{m+1,n}H_{m-1,n}=(\mathrm{D}_z^2+4m)H_{m,n}\cdot H_{m,n}, \tag{3.3a}$$

$$4nH_{m,n+1}H_{m,n-1}=-(\mathrm{D}_z^2-4n)H_{m,n}\cdot H_{m,n}, \tag{3.3b}$$

where D_z is the Hirota operator (2.8), with

$$H_{0,0}=H_{1,0}=H_{0,1}=1,\quad H_{1,1}=2z, \tag{3.4}$$

and $m,n\geqslant 0$. Then

$$w_{m,n}^{(\mathrm{I})}=w(z;\alpha_{m,n}^{(\mathrm{I})},\beta_{m,n}^{(\mathrm{I})})=-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{H_{m,n+1}}{H_{m,n}}\right)\right\}\equiv-2m\,\frac{H_{m+1,n}H_{m-1,n+1}}{H_{m,n+1}H_{m,n}}, \tag{3.5}$$

$$w_{m,n}^{(\mathrm{II})}=w(z;\alpha_{m,n}^{(\mathrm{II})},\beta_{m,n}^{(\mathrm{II})})=\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{H_{m+1,n}}{H_{m,n}}\right)\right\}\equiv2n\,\frac{H_{m,n+1}H_{m+1,n-1}}{H_{m+1,n}H_{m,n}}, \tag{3.6}$$

is a solution of P_{IV}, respectively, for the parameters

$$\alpha_{m,n}^{(\mathrm{I})}=-(m+2n+1),\quad \beta_{m,n}^{(\mathrm{I})}=-2m^2, \tag{3.7}$$

$$\alpha_{m,n}^{(\mathrm{II})}=2m+n+1,\quad \beta_{m,n}^{(\mathrm{II})}=-2n^2. \tag{3.8}$$

Remarks 3.2:

(1) The rational solutions of P_{IV} defined by (3.5) and (3.6) include all the solutions in the "$-1/z$" and "$-2z$" hierarchies, as is easily verified by comparing the parameters in (3.7) and (3.8) with those in (2.5a) and (2.5b). Further, they are the set of rational solutions of P_{IV} with parameter values given by (2.1).

(2) Some generalized Hermite polynomials $H_{m,n}(z)$ are given in Appendix A.

(3) Each generalized Hermite polynomial $H_{m,n}(z)$ is a polynomial of degree mn with integer coefficients.[82] In fact, $H_{m,n}(\frac{1}{2}x)$ is a monic polynomial in x of degree mn with integer coefficients.

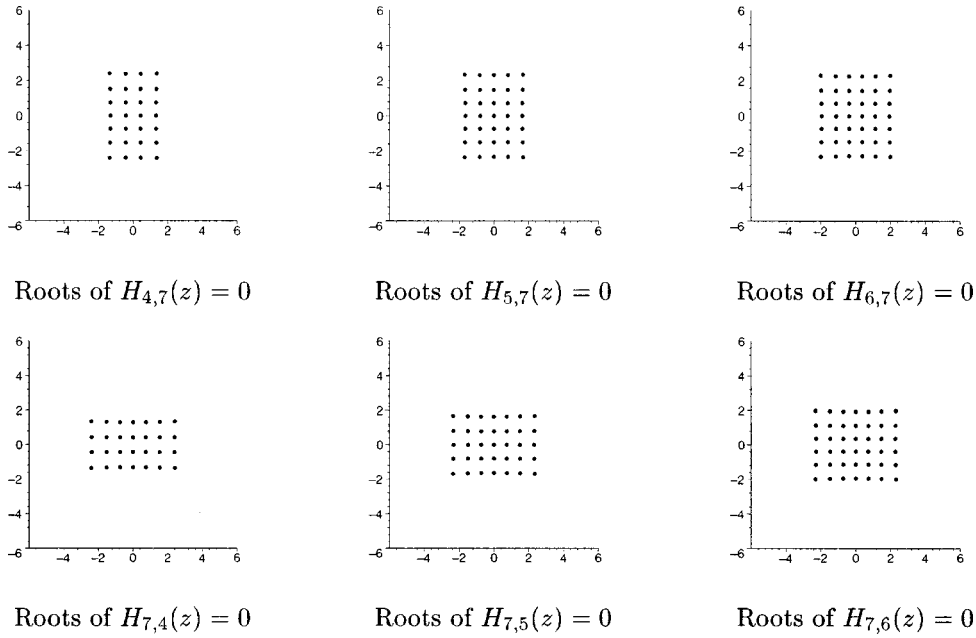

FIG. 4. Locations of roots of some generalized Hermite polynomials defined by (3.2).

(4) The polynomial $H_{m,n}(z)$ has only even powers of z if mn is even and odd powers of z if mn is odd.

(5) The polynomial $H_{2n,2n}(z)$ is of the form $p_n(z^4)$ where $p_n(\xi)$ is a polynomial of degree n^2 and the polynomial $H_{2n+1,2n+1}(z)$ is of the form $z\hat{p}_n(z^4)$ where $\hat{p}_n(\xi)$ is a polynomial of degree n^2+n.

(6) The polynomials $H_{m,n}(z)$ possess the symmetry

$$H_{m,n}(\mathrm{i}z)=\mathrm{i}^{mn}H_{n,m}(z) \tag{3.9}$$

(note that mn is the degree of $H_{m,n}$).

(7) $H_{n,1}(z)=H_n(z)$ and $H_{1,n}(z)=\mathrm{i}^{-n}H_n(\mathrm{i}z)$, where $H_n(z)$ is the usual Hermite polynomial defined by

$$H_n(z)=(-1)^n\exp(z^2)\frac{\mathrm{d}^n}{\mathrm{d}z^n}\{\exp(-z^2)\} \tag{3.10}$$

or alternatively through the generating function

$$\sum_{n=0}^{\infty}\frac{H_n(z)x^n}{n!}=\exp(2xz-x^2). \tag{3.11}$$

(8) Plots of the locations of the roots of the polynomials $H_{m,7}(z)$, $H_{7,n}(z)$ for $4\leqslant m\leqslant 6$ and $4\leqslant n\leqslant 6$ are given in Fig. 4. These plots, which are invariant under reflections in the real and imaginary z-axes, take the form of $m\times n$ "rectangles," though these are only approximate rectangles as can be seen by looking at the actual values of the roots.

IV. GENERALIZED OKAMOTO POLYNOMIALS

In this section we discuss the *generalized Okamoto polynomials* $Q_{m,n}(z)$ which were introduced by Noumi and Yamada[82] and are defined in Theorem 4.1 below. We have reindexed these polynomials by setting $Q^{[\mathrm{NY}]}_{m,n}(z)=Q_{m-n,n}(z)$, i.e., $Q^{[\mathrm{NY}]}_{m+n,n}(z)=Q_{m,n}(z)$, where $Q^{[\mathrm{NY}]}_{m+n,n}(z)$ is the

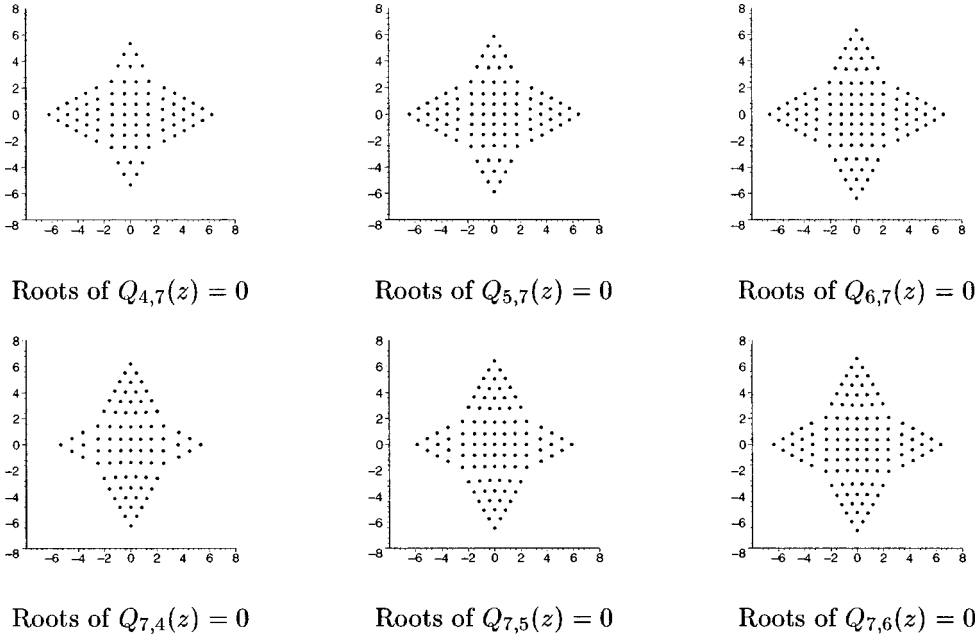

FIG. 5. Locations of roots of some generalized Okamoto polynomials defined by (4.1).

polynomial defined Noumi and Yamada,[82] since we feel that $Q_{m,n}(z)$ is more natural, especially when one studies the plots of the locations of the roots for various generalized Okamoto polynomials in Fig. 5.

Theorem 4.1: *Suppose that* $Q_{m,n}(z)$ *satisfies the recurrence relations*

$$Q_{m+1,n}Q_{m-1,n}=\tfrac{9}{2}[Q_{m,n}Q''_{m,n}-(Q'_{m,n})^2]+[2z^2+3(2m+n-1)]Q^2_{m,n}, \tag{4.1a}$$

$$Q_{m,n+1}Q_{m,n-1}=\tfrac{9}{2}[Q_{m,n}Q''_{m,n}-(Q'_{m,n})^2]+[2z^2+3(1-m-2n)]Q^2_{m,n}, \tag{4.1b}$$

or equivalently

$$Q_{m+1,n}Q_{m-1,n}=[9\mathrm{D}_z^2+2z^2+3(2m+n-1)]Q_{m,n}\cdot Q_{m,n}, \tag{4.2a}$$

$$Q_{m,n+1}Q_{m,n-1}=[9\mathrm{D}_z^2+2z^2+3(1-m-2n)]Q_{m,n}\cdot Q_{m,n}, \tag{4.2b}$$

where D_z *is the Hirota operator (2.8), with*

$$Q_{0,0}=Q_{1,0}=Q_{0,1}=1, \quad Q_{1,1}=\sqrt{2}z. \tag{4.3}$$

Then

$$w^{(\mathrm{I})}_{m,n}=w(z;\alpha^{(\mathrm{I})}_{m,n},\beta^{(\mathrm{I})}_{m,n})=-\frac{2}{3}z-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{Q_{m,n+1}}{Q_{m,n}}\right)\right\}, \tag{4.4}$$

$$w^{(\mathrm{II})}_{m,n}=w(z;\alpha^{(\mathrm{II})}_{m,n},\beta^{(\mathrm{II})}_{m,n})=-\frac{2}{3}z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{Q_{m+1,n}}{Q_{m,n}}\right)\right\} \tag{4.5}$$

are solutions of $\mathrm{P_{IV}}$, *respectively, for the parameters*

$$\alpha^{(\mathrm{I})}_{m,n}=-2n-m, \quad \beta^{(\mathrm{I})}_{m,n}=-\tfrac{2}{9}(3m-1)^2, \tag{4.6}$$

$$\alpha_{m,n}^{(\mathrm{II})}=2m+n, \quad \beta_{m,n}^{(\mathrm{II})}=-\tfrac{2}{9}(3n-1)^2. \tag{4.7}$$

Remarks 4.2:

(1) The rational solutions of P_{IV} defined by (4.4) and (4.5) include all the solutions in the "$-\frac{2}{3}z$" hierarchy, as is easily verified by comparing the parameters in (4.6) and (4.7) with those in (2.5c). Further, they are the set of rational solutions of P_{IV} with parameter values given by (2.2).

(2) Some generalized Okamoto polynomials $Q_{m,n}(z)$ are given in Appendix B.

(3) Each polynomial $Q_{m,n}(z)$ is a polynomial of degree $d_{m,n}=m^2+n^2+mn-m-n$ with integer coefficients.[82] Further, $Q_{m,n}(z)$ is a monic polynomial in $\zeta=\sqrt{2}z$ of degree $d_{m,n}$ with integer coefficients.

(4) The polynomials $Q_{2m+1,2n+1}(z)$ have only odd powers of z while the other generalized Okamoto polynomials have only even powers of z.

(5) The polynomial $Q_{2n,2n}(z)$ is of the form $q_n(z^4)$ where $q_n(\xi)$ is a polynomial of degree $n(3n-1)$ and the polynomial $Q_{2n+1,2n+1}(z)$ is of the form $z\hat{q}_n(z^4)$ where $\hat{q}_n(\xi)$ is a polynomial of degree $n(3n+2)$.

(6) The original Okamoto polynomials defined in Theorems 2.3 and 2.5 are, respectively, given by

$$Q_m(z)=Q_{m,0}(z), \quad R_m(z)=Q_{m,1}(z). \tag{4.8}$$

(7) The polynomials $Q_{m,n}(z)$ possess the symmetry

$$Q_{m,n}(\mathrm{i}z)=\exp(\tfrac{1}{2}\pi\mathrm{i}d_{m,n})Q_{n,m}(z), \tag{4.9}$$

where $d_{m,n}=m^2+n^2+mn-m-n$ is the degree of $Q_{m,n}$.

(8) The hierarchies of rational solutions of P_{IV} generated from the generalized Hermite polynomials $H_{m,n}(z)$ defined in Theorem 3.1 and the generalized Okamoto polynomials $Q_{m,n}(z)$ defined in Theorem 4.1 are linked by the Schlesinger transformations $\mathcal{R}^{[2]}$ (or $\mathcal{R}^{[4]}$) and $\mathcal{R}^{[5]}\equiv\mathcal{R}^{[1]}\mathcal{R}^{[3]}$ given by Fokas, Mugan, and Ablowitz.[34]

(9) Plots of the locations of the roots of the polynomials $Q_{m,7}(z)$, $Q_{7,n}(z)$ for $4\leqslant m\leqslant 6$ and $4\leqslant n\leqslant 6$ are given in Fig. 5. The roots of the polynomial $Q_{m,n}(z)$ take the form of $m\times n$ "rectangles" with an "equilateral triangle," which have either $m-1$ or $n-1$ roots on each of its sides. These are only approximate rectangles and equilateral triangles as can be seen by looking at the actual values of the roots. We remark that as for the generalized Hermite polynomials above, the plots are invariant under reflections in the real and imaginary z-axes.

V. DETERMINANTAL FORM OF RATIONAL SOLUTIONS OF P_{IV}

A. $-1/z$ and $-2z$ hierarchies

Kajiwara and Ohta[57] and Noumi and Yamada[82] derived representations of the "$-1/z$" and "$-2z$" hierarchies of rational solutions for P_{IV} in the form of determinants, which are described in the following theorem.

Theorem 5.1: *Suppose that $\tau_{m,n}(z)$ and $\hat{\tau}_{m,n}(z)$ are the $n\times n$ determinants of Hankel type defined by*

$$\tau_{m,n}(z)=\begin{vmatrix} H_m(z) & H_{m+1}(z) & \cdots & H_{m+n-1}(z) \\ H_{m+1}(z) & H_{m+2}(z) & \cdots & H_{m+n}(z) \\ \vdots & \vdots & \ddots & \vdots \\ H_{m+n-1}(z) & H_{m+n}(z) & \cdots & H_{m+2n-2}(z) \end{vmatrix}, \tag{5.1}$$

$$\hat{\tau}_{m,n}(z)=\begin{vmatrix} \hat{H}_m(z) & \hat{H}_{m+1}(z) & \cdots & \hat{H}_{m+n-1}(z) \\ \hat{H}_{m+1}(z) & \hat{H}_{m+2}(z) & \cdots & \hat{H}_{m+n}(z) \\ \vdots & \vdots & \ddots & \vdots \\ \hat{H}_{m+n-1}(z) & \hat{H}_{m+n}(z) & \cdots & \hat{H}_{m+2n-2}(z) \end{vmatrix}, \tag{5.2}$$

respectfully, with $\tau_{m,0}(z)=1$ *and* $\hat{\tau}_{m,0}(z)=1$, *where* $H_m(z)$, $m=0,1,2,...$, *are the Hermite polynomials and* $\hat{H}_m(z)=\mathrm{i}^{-m}H_m(\mathrm{i}z)$. *Then*

$$w_{m,n}^{(\mathrm{I})}=w(z;\alpha_{m,n}^{(\mathrm{I})},\beta_{m,n}^{(\mathrm{I})})=-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\tau_{m,n}(z)}{\tau_{m,n+1}(z)}\right]\right\}, \tag{5.3}$$

$$\hat{w}_{m,n}^{(\mathrm{I})}=w(z;\hat{\alpha}_{m,n}^{(\mathrm{I})},\hat{\beta}_{m,n}^{(\mathrm{I})})=\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\hat{\tau}_{m,n+1}(z)}{\hat{\tau}_{m,n}(z)}\right]\right\} \tag{5.4}$$

are solutions of $\mathrm{P_{IV}}$ *for the respective parameters*

$$\alpha_{m,n}^{(\mathrm{I})}=-(m+2n+1),\quad \beta_{m,n}^{(\mathrm{I})}=-2m^2,\quad m,n\in\mathbb{Z},\quad m\geqslant 0,\quad n\geqslant 0, \tag{5.5}$$

$$\hat{\alpha}_{m,n}^{(\mathrm{I})}=m+2n+1,\quad \hat{\beta}_{m,n}^{(\mathrm{I})}=-2m^2,\quad m,n\in\mathbb{Z},\quad m\geqslant 0,\quad n\geqslant 0, \tag{5.6}$$

and

$$w_{m,n}^{(\mathrm{II})}=w(z;\alpha_{m,n}^{(\mathrm{II})},\beta_{m,n}^{(\mathrm{II})})=-2z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\tau_{m,n+1}(z)}{\tau_{m+1,n}(z)}\right]\right\}, \tag{5.7}$$

$$\hat{w}_{m,n}^{(\mathrm{II})}=w(z;\hat{\alpha}_{m,n}^{(\mathrm{II})},\hat{\beta}_{m,n}^{(\mathrm{II})})=-2z-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\hat{\tau}_{m,n+1}(z)}{\hat{\tau}_{m+1,n}(z)}\right]\right\} \tag{5.8}$$

are solutions of $\mathrm{P_{IV}}$, *respectively, for the parameters*

$$\alpha_{m,n}^{(\mathrm{II})}=n-m,\quad \beta_{m,n}^{(\mathrm{II})}=-2(m+n+1)^2,\quad m,n\in\mathbb{Z},\quad m\geqslant 0,\quad n\geqslant 0, \tag{5.9}$$

$$\hat{\alpha}_{m,n}^{(\mathrm{II})}=m-n,\quad \hat{\beta}_{m,n}^{(\mathrm{II})}=-2(m+n+1)^2,\quad m,n\in\mathbb{Z},\quad m\geqslant 0,\quad n\geqslant 0. \tag{5.10}$$

Remarks 5.2:

(1) The τ-function $\tau_{m,n}(z)$ is related to the generalized Hermite polynomial $H_{m,n}(z)$ through

$$\tau_{m,n}(z)=c_{m,n}H_{m,n}(z), \tag{5.11}$$

for some constant $c_{m,n}$.

(2) The τ-function $\tau_{m,n}(z)$ can also be written as determinant of Hankel type

$$\tau_{m,n}(z)=2^{(n-1)n/2}\prod_{k=1}^{n-1}(m+k)^k\begin{vmatrix} H_{m+n-1}(z) & H'_{m+n-1}(z) & \cdots & H^{(n-1)}_{m+n-1}(z) \\ H'_{m+n-1}(z) & H''_{m+n-1}(z) & \cdots & H^{(n)}_{m+n-1}(z) \\ \vdots & \vdots & \ddots & \vdots \\ H^{(n-1)}_{m+n-1}(z) & H^{(n)}_{m+n-1}(z) & \cdots & H^{(2n-2)}_{m+n-1}(z) \end{vmatrix}, \tag{5.12}$$

where $H_n(z)$ is the Hermite polynomial, and $H_m^{(n)}(z)=\mathrm{d}^nH_m/\mathrm{d}z^n$ since $H_n(z)$ satisfies the recurrence relations

$$H_{n+1}-2zH_n+2nH_{n-1}=0,\quad H_{n+1}=2zH_n-H'_n,\quad H'_n=2nH_{n-1}.$$

Therefore the rational solutions of P_{IV} expressed in terms of the generalized Hermite polynomials $H_{m,n}(z)$ are actually just special cases of the solutions of P_{IV} which are expressible in terms of classical special functions. To show this we use the following theorem.

Theorem 5.3: *If $\sigma_{\nu,n}(z)$ is the $n\times n$ determinant of Hankel type defined by*

$$\sigma_{\nu,n}(z)=\begin{vmatrix} \varphi_\nu(z) & \varphi_\nu'(z) & \cdots & \varphi_\nu^{(n-1)}(z) \\ \varphi_\nu'(z) & \varphi_\nu''(z) & \cdots & \varphi_\nu^{(n)}(z) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_\nu^{(n-1)}(z) & \varphi_\nu^{(n)}(z) & \cdots & \varphi_\nu^{(2n-2)}(z) \end{vmatrix}, \tag{5.13}$$

where $\varphi_\nu(z)$ satisfies

$$\varphi_\nu''-2z\varphi_\nu'+2\nu\varphi_\nu=0, \tag{5.14}$$

then

$$w(z;\alpha_{\nu,n}^{(\mathrm{I})},\beta_{\nu,n}^{(\mathrm{I})})=-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\sigma_{\nu,n+1}(z)}{\sigma_{\nu,n}(z)}\right]\right\}, \tag{5.15}$$

$$w(z;\alpha_{\nu,n}^{(\mathrm{II})},\beta_{\nu,n}^{(\mathrm{II})})=-2z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\sigma_{\nu,n+1}(z)}{\sigma_{m+1,n}(z)}\right]\right\} \tag{5.16}$$

are solutions of P_{IV}, respectively, for the parameters

$$\alpha_{\nu,n}^{(\mathrm{I})}=-(\nu+n+2),\quad \beta_{\nu,n}^{(\mathrm{I})}=-2(\nu-n+1)^2,$$

$$\alpha_{\nu,n}^{(\mathrm{II})}=2n-\nu-1,\quad \beta_{\nu,n}^{(\mathrm{II})}=-2(\nu+2)^2.$$

Proof: See Ref. 87.

The general solution of Eq. (5.14) is

$$\varphi_\nu(z)=z^{-1/2}\{AM_{(1/2)\nu+1/4,1/4}(z^2)+BW_{(1/2)\nu+1/4,1/4}(z^2)\}\exp(\tfrac{1}{2}z^2), \tag{5.17}$$

or equivalently

$$\varphi_\nu(z)=\{AD_\nu(\sqrt{2}z)+BD_{-\nu}(\sqrt{2}z)\}\exp(\tfrac{2}{3}z^2), \tag{5.18}$$

where A and B are arbitrary constants, $M_{\kappa,\mu}(\xi)$ and $W_{\kappa,\mu}(\xi)$ are *Whittaker functions* which satisfy

$$\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2}=\left(\frac{\mu^2-\frac{1}{4}}{\xi^2}-\frac{\kappa}{\xi}+\frac{1}{4}\right)u, \tag{5.19}$$

and $D_\nu(\xi)$ is the *parabolic cylinder function* which satisfies

$$\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2}=\left(\frac{1}{4}\xi^2-\nu-\frac{1}{2}\right)u \tag{5.20}$$

(see Refs. 5 and 112 for further information on Whittaker and parabolic cylinder functions). Thus the rational solutions of P_{IV} generated by the generalized Hermite polynomials $H_{m,n}(z)$ are special cases of the special function solutions, often called *one-parameter families of solutions*, which are expressible in terms of Whittaker functions $M_{\kappa,\mu}(\xi)$ and $W_{\kappa,\mu}(\xi)$, or equivalently parabolic cylinder functions $D_\nu(\xi)$.

B. $-\frac{2}{3}z$ hierarchy

Kajiwara and Ohta[57] and Noumi and Yamada[82] also derived representations of the "$-\frac{2}{3}z$" hierarchy of rational solutions for P_{IV} in the form of determinants. First we consider the representations in the form of determinants of the rational solutions for P_{IV} arising from the Okamoto polynomials $Q_n(z)$ and $R_n(z)$ defined by Theorems 2.3 and 2.5, respectively, which are described in the following theorem.

Theorem 5.4: *Let $p_k(z)$ be the polynomial defined by*

$$\sum_{k=0}^{\infty} p_k(z)\lambda^k = \exp(2\sqrt{2}z\lambda + 6\lambda^2) \tag{5.21}$$

with $p_k(z)=0$ for $k<0$, and $\tau_{N,n}(z)$ be the $n\times n$ determinant

$$\tau_{N,n}(z) = \begin{vmatrix} p_N(z) & p_{N+1}(z) & \cdots & p_{N+n-1}(z) \\ p_{N-3}(z) & p_{N-2}(z) & \cdots & p_{N+n-4}(z) \\ \vdots & \vdots & \cdots & \vdots \\ p_{N-3n+3}(z) & p_{N-3n+4}(z) & \cdots & p_{N-2n+2}(z) \end{vmatrix} \tag{5.22}$$

for $N\geqslant 2n-2$ and $n\geqslant 1$. Then the Okamoto polynomials are given by

$$Q_n(z) = c_n\tau_{2n,n}(z), \quad R_n(z) = d_n\tau_{2n-1,n}(z), \tag{5.23}$$

where c_n and d_n are positive integers, and so

$$w_n^{[1]}(z) = w(z;\alpha_n^{[1]},\beta_n^{[1]}) = -\frac{2}{3}z + \frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\tau_{2n+2,n+1}(z)}{\tau_{2n,n}(z)}\right]\right\}, \tag{5.24}$$

$$w_n^{[2]}(z) = w(z;\alpha_n^{[2]},\beta_n^{[2]}) = -\frac{2}{3}z + \frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[\frac{\tau_{2n+1,n+1}(z)}{\tau_{2n-1,n}(z)}\right]\right\} \tag{5.25}$$

satisfy P_{IV} *with* $(\alpha_n^{[1]},\beta_n^{[1]}) = (2n,-\frac{2}{9})$ *and* $(\alpha_n^{[2]},\beta_n^{[2]}) = (2n+1,-\frac{8}{9})$, *respectively*.

Proof: See Refs. 57 and 82.

The Okamoto polynomials $Q_n(z)$ and $R_n(z)$ can be expressed in terms of Schur polynomials

$$Q_n(z) = c_n S_{(2n,2n-2,\ldots,2)}(x), \quad R_n(z) = d_n S_{(2n-1,2n-3,\ldots,1)}(x), \tag{5.26}$$

where c_n and d_n are positive integers, $(x)=(x_1,x_2,x_3,\ldots)=(2\sqrt{2}z,6,0,\ldots)$ and

$$S_{(i_1,i_2,\ldots,i_m)}(x) = \begin{vmatrix} p_{i_1}(z) & p_{i_1+1}(z) & \cdots & p_{i_1+m-1}(z) \\ p_{i_2-1}(z) & p_{i_2}(z) & \cdots & p_{i_2+m-2}(z) \\ \vdots & \vdots & \cdots & \vdots \\ p_{i_m-m+1}(z) & p_{i_m-m+2}(z) & \cdots & p_{i_m}(z) \end{vmatrix} \tag{5.27}$$

with the polynomials $p_k(z)$ defined by (5.21).

Theorem 5.5: *Let $\tau_{N,M}$ be the $n\times n$ determinant, with $n=\max(M,N)$, given in terms of Schur polynomials*

$$\tau_{N,M} = \begin{cases} S_{(M+2n,M+2n-2,\ldots,M+2,M^2,(M-1)^2,\ldots,1^2)}(x), & \text{for } M<N=M+n \\ S_{(N+2n-1,N+2n-3,\ldots,N+1,N^2,(N-1)^2,\ldots,1^2)}(x), & \text{for } N<M=N+n, \end{cases} \tag{5.28}$$

where $M \geqslant 0$, $N \geqslant 0$, $n \geqslant 1$, $(x)=(x_1,x_2,x_3,\ldots)=(2\sqrt{2}z,6,0,\ldots)$ *and* $S_{(i_1,i_2,\ldots,i_m)}(x)$ *is defined by (5.27), with the polynomials* $p_k(z)$ *defined by (5.21). Then*

$$w_{M,N}^{(\mathrm{I})}=w(z;\alpha_{M,N}^{(\mathrm{I})},\beta_{M,N}^{(\mathrm{I})})=-\frac{2}{3}z-\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{\tau_{M,N+1}}{\tau_{M,N}}\right)\right\}, \tag{5.29}$$

$$w_{M,N}^{(\mathrm{II})}=w(z;\alpha_{M,N}^{(\mathrm{II})},\beta_{M,N}^{(\mathrm{II})})=-\frac{2}{3}z+\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left(\frac{\tau_{M+1,N}}{\tau_{M,N}}\right)\right\} \tag{5.30}$$

are solutions of $\mathrm{P_{IV}}$, *respectively, for the parameters*

$$\alpha_{M,N}^{(\mathrm{I})}=2N-M+2,\quad \beta_{M,N}^{(\mathrm{I})}=-\tfrac{2}{9}(3M+1)^2,$$

$$\alpha_{M,N}^{(\mathrm{II})}=2M-N+1,\quad \beta_{M,N}^{(\mathrm{II})}=-\tfrac{2}{9}(3N+2)^2.$$

Proof: See Refs. 57 and 82.

VI. CONCLUSIONS

In this article we have studied properties of special polynomials associated with rational solutions of $\mathrm{P_{IV}}$. In particular we have demonstrated that the roots of these polynomials have a very symmetric, regular structure. These are analogous to the results in Refs. 20 and 25, where it is shown that the roots of the special polynomials associated with rational solutions of $\mathrm{P_{II}}$ and the $\mathrm{P_{II}}$ hierarchy and rational and algebraic solutions of $\mathrm{P_{III}}$ have a very symmetric, regular structure. For $\mathrm{P_{II}}$ and $\mathrm{P_{III}}$ the roots of the special polynomials associated with rational and algebraic solutions have an approximate ''triangular'' structure, while for $\mathrm{P_{IV}}$ the poles also have approximate ''rectangular'' and combinations of rectangular and triangular structures. This seems to be yet another remarkable property of the Painlevé equations, indeed more generally of ''integrable'' differential equations.

Ablowitz and Segur[3] demonstrated a close connection between completely integrable partial differential equations solvable by inverse scattering, so-called the soliton equations, and the Painlevé equations. For example, $\mathrm{P_{IV}}$ arises as a symmetry reduction of a variety of significant partial differential equations including the Boussinesq and modified Boussinesq equations;[18,19,23,45,90] the classical Boussinesq equation;[24,59,92] the dispersive long wave equations;[89] the Kadomtsev–Petviashvili equation;[27,28,96] the cubic nonlinear Schrödinger equation;[14,16,49] the quintic nonlinear Schrödinger equation;[38,39] the derivative nonlinear Schrödinger equation;[21,26,30] the Davey–Stewartson equations;[22] the potential and modified nonlinear Schrödinger equations and the potential anisotropic Heisenberg Spin Chain;[91] the *N*-wave interaction equations;[63,71] and the self-dual Yang–Mills field equations.[1,68] Thus the rational solutions of $\mathrm{P_{IV}}$ described here generate rational solutions of these partial differential equations and so one can study the motion of poles of these rational solutions. There has been considerable interest in the motion of poles of rational solutions of completely integrable nonlinear partial differential equations, which is governed by Calogero–Moser type systems; for example, for the Korteweg–de Vries equation,[2,6,9] the Boussinesq equation,[41] the classical Boussinesq system[92] and the nonlinear Schrödinger equation.[49] However, we shall not pursue this further here.

An application of rational solutions of the Painlevé equations is given by Marikhin[69] (see also Ref. 70) who discusses their Coulomb gas representation. It is shown that any rational solution of $\mathrm{P_{IV}}$ determines some steady-state distribution of electric charges for the two-dimensional Coulomb gas in a parabolic potential. The Coulomb gas representation of a rational solution of $\mathrm{P_{IV}}$ has the form

$$w(z)=Bz+\sum_{j=1}^{N}\frac{\sigma_j}{z-z_j}, \tag{6.1}$$

where $\sigma_j = \pm 1$, $B = 0, -2, -\frac{2}{3}$ and z_j, $j = 1,2,...,N$ are the locations of the poles. Further, the locations of the poles z_j satisfy

$$\sum_{j=1,j\neq k}^{N} \frac{\sigma_j}{z_k - z_j} = -(1+B)z_k, \quad k = 1,2,...,N. \tag{6.2}$$

The results described in this article show that for the rational solutions of $\mathrm{P_{IV}}$, then either

(1) $B = 0$ or $B = -2$ and $N = mn$, with m and n positive integers, when the rational solutions are expressible in terms of generalized Hermite polynomials $H_{m,n}(z)$; or
(2) $B = -\frac{2}{3}$ and $N = m^2 + n^2 + mn - m - n$, with m and n positive integers, when the rational solutions are expressible in terms of generalized Okamoto polynomials $Q_{m,n}(z)$.

The special case of (6.2) with $B = 0$ and $\sigma_j = 1$ for $j = 1,2,...,N$ is called the *Stieltjes relations*;[94] see also Ref. 107 for a discussion on the relationship between the Stieltjes relations and rational solutions of $\mathrm{P_{IV}}$ expressed in terms of Hermite polynomials.

An important, well-known property of classical orthogonal polynomials, such as the Hermite, Laguerre and Legendre polynomials whose roots all lie on the real line (cf. Refs. 5, 12, and 101), is that the roots of successive polynomials interlace. Thus for a set of orthogonal polynomials $\varphi_n(z)$, for $n = 0,1,2,...$, if $z_{n,m}$ and $z_{n,m+1}$ are two successive roots of $\varphi_n(z)$, i.e., $\varphi_n(z_{n,m}) = 0$ and $\varphi_n(z_{n,m+1}) = 0$, then $\varphi_{n-1}(\zeta_{n-1}) = 0$ and $\varphi_{n+1}(\zeta_{n+1}) = 0$ for some ζ_{n-1} and ζ_{n+1} such that $z_{n,m} < \zeta_{n-1}$, $\zeta_{n+1} < z_{n,m+1}$. Further, the derivatives $\varphi_n'(z)$ and $\varphi_{n+1}'(z)$ also have roots in the interval $(z_{n,m}, z_{n,m+1})$, that is $\varphi_n'(\xi_n) = 0$ and $\varphi_{n+1}'(\xi_{n+1}) = 0$ for some ξ_n and ξ_{n+1} such that $z_{n,m} < \xi_n$, $\xi_{n+1} < z_{n,m+1}$. An interesting open question is whether there are analogous results for the generalized Hermite polynomials $H_{m,n}(z)$ and the generalized Okamoto polynomials $Q_{m,n}(z)$. Clearly there are notable differences since the generalized Hermite and generalized Okamoto polynomials are polynomials with complex roots whereas classical orthogonal polynomials $\varphi_n(z)$ have real roots. The pattern of the roots of $H_{m,n}(z)$ and $Q_{m,n}(z)$ are highly symmetric and structured, suggesting that they have interesting properties. A particularly interesting question is whether there is any ''interlacing of roots'' analogous to that for classical orthogonal polynomials. Clearly this warrants further analytical study as does an investigation of the relative locations of the roots for $H_{m,n}(z)$ and $Q_{m,n}(z)$ and their derivatives. Again, we shall not pursue these questions further here.

Some other interesting open questions for the generalized Hermite polynomials $H_{m,n}(z)$ and the generalized Okamoto polynomials $Q_{m,n}(z)$ include the following:

(1) Are there generating functions $\Phi(x,y,z)$ and $\Psi(x,y,z)$ for the generalized Hermite polynomials $H_{m,n}(z)$ and the generalized Okamoto polynomials $Q_{m,n}(z)$ such that

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} H_{m,n}(z)x^m y^n = \Phi(x,y,z), \quad \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} Q_{m,n}(z)x^m y^n = \Psi(x,y,z)?$$

(2) Do the generalized Hermite polynomials $H_{m,n}(z)$ and the generalized Okamoto polynomials $Q_{m,n}(z)$ satisfy ordinary differential equations or pure difference equations, rather than differential-difference equations (3.2) and (4.1), respectively?

ACKNOWLEDGMENTS

I wish to thank Mark Ablowitz, Frédérick Cheyzak, Chris Cosgrove, Andy Hone, Nalini Joshi, Arieh Iserles, Alexander Its, Elizabeth Mansfield and Marta Mazzocco for their helpful comments and illuminating discussions. I also thank the Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, for their hospitality where this research was commenced; in particular I thank Willard Miller and Peter Olver. This research arose while involved with the ''Digital Library of Mathematical Functions'' project (see http://dlmf.nist.gov); in particular I

thank Frank Olver and Dan Lozier for the opportunity to participate in this project. I also thank Colin and Janet Mansfield for their kind hospitality at "Morning View," Gulgong, Australia, while much of this paper was written.

APPENDIX A: THE GENERALIZED HERMITE POLYNOMIALS

$$H_{n,0}=H_{0,n}=1, \quad n\geqslant 0,$$

$$H_{1,1}=2z,$$

$$H_{1,2}=4z^2+2,$$

$$H_{1,3}=8z^3+12z,$$

$$H_{1,4}=16z^4+48z^2+12,$$

$$H_{1,5}=32z^5+160z^3+120z,$$

$$H_{2,1}=4z^2-2,$$

$$H_{2,2}=16z^4+12,$$

$$H_{2,3}=64z^6+96z^4+144z^2-72,$$

$$H_{2,4}=256z^8+1024z^6+1920z^4+720,$$

$$H_{2,5}=1024z^{10}+7680z^8+23\,040z^6+19\,200z^4+14\,400z^2-7200,$$

$$H_{3,1}=8z^3-12z,$$

$$H_{3,2}=64z^6-96z^4+144z^2+72,$$

$$H_{3,3}=512z^9+2304z^5-4320z,$$

$$H_{3,4}=4096z^{12}+12\,288z^{10}+46\,080z^8+30\,720z^6-57\,600z^4+172\,800z^2+43\,200,$$

$$H_{3,5}=32\,768z^{15}+245\,760z^{13}+1\,105\,920z^{11}+2\,150\,400z^9+1\,382\,400z^7+4\,838\,400z^5 -4\,032\,000z^3-6\,048\,000z,$$

$$H_{4,1}=16z^4-48z^2+12,$$

$$H_{4,2}=256z^8-1024z^6+1920z^4+720,$$

$$H_{4,3}=4096z^{12}-12\,288z^{10}+46\,080z^8-30\,720z^6-57\,600z^4-172\,800z^2+43\,200,$$

$$H_{4,4}=65\,536z^{16}+983\,040z^{12}-1\,843\,200z^8+32\,256\,000z^4+6\,048\,000,$$

$$H_{4,5}=1\,048\,576z^{20}+5\,242\,880z^{18}+35\,389\,440z^{16}+78\,643\,200z^{14}+68\,812\,800z^{12} +206\,438\,400z^{10}+1\,290\,240\,000z^8-3\,612\,672\,000z^6-3\,386\,880\,000z^4-3\,386\,880\,000z^2 +846\,720\,000,$$

$$H_{5,1}=32z^5-160z^3+120z,$$

$$H_{5,2}=1024z^{10}-7680z^{8}+23\,040z^{6}-19\,200z^{4}+14\,400z^{2}+7200+1024z,$$

$$H_{5,3}=32\,768z^{15}-245\,760z^{13}+1\,105\,920z^{11}-2\,150\,400z^{9}+1\,382\,400z^{7}-4\,838\,400z^{5}$$
$$-4\,032\,000z^{3}+6\,048\,000z,$$

$$H_{5,4}=1\,048\,576z^{20}-5\,242\,880z^{18}+35\,389\,440z^{16}-78\,643\,200z^{14}+68\,812\,800z^{12}$$
$$-206\,438\,400z^{10}+1\,290\,240\,000z^{8}+3\,612\,672\,000z^{6}-3\,386\,880\,000z^{4}+3\,386\,880\,000z^{2}$$
$$+846\,720\,000.$$

APPENDIX B: THE GENERALIZED OKAMOTO POLYNOMIALS

$$Q_{0,0}=Q_{0,1}=1,$$

$$Q_{0,2}=2z^{2}-3,$$

$$Q_{0,3}=8z^{6}-60z^{4}+90z^{2}-135,$$

$$Q_{0,4}=64z^{12}-1344z^{10}+9360z^{8}-30\,240z^{6}+56\,700z^{4}-170\,100z^{2}+127\,575,$$

$$Q_{0,5}=1024z^{20}-46\,080z^{18}+817\,920z^{16}-7\,603\,200z^{14}+41\,731\,200z^{12}-155\,675\,520z^{10}$$
$$+493\,970\,400z^{8}-1\,886\,068\,800z^{6}+5\,304\,568\,500z^{4}-5\,304\,568\,500z^{2}+397\,8426\,375,$$

$$Q_{1,0}=1,$$

$$Q_{1,1}=\sqrt{2}z,$$

$$Q_{1,2}=4z^{4}-12z^{2}-9,$$

$$Q_{1,3}=\sqrt{2}z(16z^{8}-192z^{6}+504z^{4}-2835),$$

$$Q_{1,4}=256z^{16}-7680z^{14}+80\,640z^{12}-362\,880z^{10}+453\,600z^{8}+1\,905\,120z^{6}-14\,288\,400z^{4}$$
$$+21\,432\,600z^{2}+8\,037\,225,$$

$$Q_{1,5}=\sqrt{2}z(4096z^{24}-245\,760z^{22}+5\,990\,400z^{20}-77\,414\,100z^{18}+569\,721\,600z^{16}$$
$$-2\,246\,952\,960z^{14}+1\,600\,300\,800z^{12}+35\,663\,846\,400z^{10}-275\,837\,562\,000z^{8}$$
$$+1\,103\,350\,248\,000z^{6}-1\,737\,776\,640\,600z^{4}+3\,258\,331\,201\,125),$$

$$Q_{2,0}=2z^{2}+3,$$

$$Q_{2,1}=4z^{4}+12z^{2}-9,$$

$$Q_{2,2}=16z^{8}-504z^{4}-567,$$

$$Q_{2,3}=128z^{14}-1344z^{12}-6048z^{10}+75\,600z^{8}-158\,760z^{6}-238\,140z^{4}-1\,071\,630z^{2}+535\,815,$$

$$Q_{2,4}=2048z^{22}-64\,512z^{20}+483\,840z^{18}+3\,144\,960z^{16}-61\,689\,600z^{14}+297\,198\,720z^{12}$$
$$-445\,798\,080z^{10}-1\,114\,495\,200z^{8}-5\,851\,099\,800z^{6}+43\,883\,248\,500z^{4}$$
$$-13\,164\,974\,550z^{2}+19\,747\,461\,825,$$

$$Q_{2,5}=65\,536z^{32}-4\,325\,376z^{30}+106\,168\,320z^{28}-1\,021\,870\,080z^{26}-3\,019\,161\,600z^{24}$$
$$+169\,374\,965\,760z^{22}-1\,749\,906\,063\,360z^{20}+8\,630\,650\,828\,800z^{18}$$
$$-16\,958\,158\,963\,200z^{16}-26\,480\,405\,952\,000z^{14}-87\,626\,070\,604\,800z^{12}$$
$$+3\,976\,032\,953\,692\,800z^{10}-18\,976\,520\,915\,352\,000z^{8}+28\,464\,781\,373\,028\,000z^{6}$$
$$+64\,045\,758\,089\,313\,000z^{2}-24\,017\,159\,283\,492\,375,$$

$$Q_{3,0}=8z^{6}+60z^{4}+90z^{2}+135,$$

$$Q_{3,1}=\sqrt{2}z(16z^{8}+192z^{6}+504z^{4}-2835),$$

$$Q_{3,2}=128z^{14}+1344z^{12}-6048z^{10}-75\,600z^{8}-158\,760z^{6}+238\,140z^{4}-1\,071\,630z^{2}-535\,815,$$

$$Q_{3,3}=\sqrt{2}z(1024z^{20}-241\,920z^{16}+12\,700\,800z^{12}-371\,498\,400z^{8}-2\,925\,549\,900z^{4}$$
$$+6\,582\,487\,275),$$

$$Q_{3,4}=32\,768z^{30}-737\,280z^{28}-7\,741\,440z^{26}+251\,596\,800z^{24}-377\,395\,200z^{22}$$
$$-21\,398\,307\,840z^{20}+89\,159\,616\,000z^{18}+740\,024\,812\,800z^{16}-6\,753\,840\,912\,000z^{14}$$
$$+9\,127\,715\,688\,000z^{12}-35\,598\,091\,183\,200z^{10}+390\,209\,845\,662\,000z^{8}$$
$$+646\,926\,849\,387\,000z^{6}-1\,617\,317\,123\,467\,500z^{4},$$

$$Q_{4,0}=64z^{12}+1344z^{10}+9360z^{8}+30\,240z^{6}+56\,700z^{4}+170\,100z^{2}+127\,575,$$

$$Q_{4,1}=256z^{16}+7680z^{14}+80\,640z^{12}+362\,880z^{10}+453\,600z^{8}-1\,905\,120z^{6}-14\,288\,400z^{4}$$
$$+-21\,432\,600z^{2}+8\,037\,225,$$

$$Q_{4,2}=2048z^{22}+64512z^{20}+483\,840z^{18}-3\,144\,960z^{16}-61\,689\,600z^{14}-297\,198\,720z^{12}$$
$$-445\,798\,080z^{10}+1\,114\,495\,200z^{8}-5\,851\,099\,800z^{6}-43\,883\,248\,500z^{4}$$
$$-13\,164\,974\,550z^{2}-19\,747\,461\,825,$$

$$Q_{4,3}=32\,768z^{30}+737\,280z^{28}-7\,741\,440z^{26}-251\,596\,800z^{24}-377\,395\,200z^{22}$$
$$+21\,398\,307\,840z^{20}+89\,159\,616\,000z^{18}-740\,024\,812\,800z^{16}-6\,753\,840\,912\,000z^{14}$$
$$-9\,127\,715\,688\,000z^{12}-35\,598\,091\,183\,200z^{10}-390\,209\,845\,662\,000z^{8}$$
$$+646\,926\,849\,387\,000z^{6}+1\,617\,317\,123\,467\,500z^{4}+2\,425\,975\,685\,201\,250z^{2}$$
$$-727\,792\,705\,560\,375,$$

$$Q_{4,4}=1\,048\,576z^{40}-920\,125\,440z^{36}+277\,762\,867\,200z^{32}-40\,649\,991\,782\,400z^{28}$$
$$+2\,948\,686\,820\,352\,000z^{24}-167\,891\,551\,278\,796\,800z^{20}+2\,734\,590\,598\,399\,296\,000z^{16}$$
$$+153\,399\,294\,526\,645\,440\,000z^{12}-560\,866\,170\,613\,047\,390\,000z^{8}$$
$$+6\,795\,109\,374\,734\,997\,225\,000z^{4}+1\,528\,899\,609\,315\,374\,375\,625,$$

$$
\begin{aligned}
Q_{4,5} = {} & 67\,108\,864\,z^{52} - 2\,617\,245\,696z^{50} - 49\,073\,356\,800z^{48} + 2\,944\,401\,408\,000z^{46} \\
& - 1\,987\,470\,950\,400z^{44} - 1\,149\,685\,695\,774\,720z^{42} + 8\,060\,089\,065\,799\,680z^{40} \\
& + 206\,994\,105\,748\,684\,800z^{38} - 2\,405\,543\,476\,808\,908\,800z^{36} \\
& - 15\,932\,255\,610\,765\,312\,000z^{34} + 295\,715\,856\,449\,367\,244\,800z^{32} \\
& + 468\,712\,752\,961\,801\,420\,800z^{30} - 24\,709\,482\,371\,771\,817\,984\,000z^{28} \\
& + 77\,864\,358\,097\,369\,718\,784\,000z^{26} + 795\,923\,196\,743\,966\,054\,400\,000z^{24} \\
& - 4\,243\,708\,209\,176\,903\,061\,504\,000z^{22} + 21\,619\,544\,333\,125\,112\,390\,016\,000z^{20} \\
& - 299\,508\,747\,778\,795\,635\,400\,320\,000z^{18} + 647\,925\,715\,931\,874\,373\,113\,120\,000z^{16} \\
& + 4\,908\,134\,681\,808\,587\,435\,606\,400\,000z^{14} - 531\,714\,590\,529\,263\,638\,857\,360\,000z^{12} \\
& - 27\,117\,444\,116\,992\,445\,581\,725\,360\,000z^{10} + 221\,326\,198\,307\,805\,989\,674\,376\,100\,000z^{8} \\
& - 251\,235\,144\,025\,077\,069\,360\,102\,600\,000z^{6} - 235\,532\,947\,523\,509\,752\,525\,096\,187\,500z^{4} \\
& - 423\,959\,305\,542\,317\,554\,545\,173\,137\,500z^{2} + 105\,989\,826\,385\,579\,388\,636\,293\,284\,375,
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,0} = {} & 1024z^{20} + 46\,080z^{18} + 817\,920z^{16} + 7\,603\,200z^{14} + 41\,731\,200z^{12} + 155\,675\,520z^{10} \\
& + 493\,970\,400z^{8} + 1\,886\,068\,800z^{6} + 5\,304\,568\,500z^{4} + 5\,304\,568\,500z^{2} + 3\,978\,426\,375,
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,1} = {} & \sqrt{2}z(4096z^{24} + 245\,760z^{22} + 5\,990\,400z^{20} + 77\,414\,400z^{18} + 569\,721\,600z^{16} \\
& + 2\,246\,952\,960z^{14} + 1\,600\,300\,800z^{12} - 35\,663\,846\,400z^{10} - 275\,837\,562\,000z^{8} \\
& - 1\,103\,350\,248\,000z^{6} - 1\,737\,776\,640\,600z^{4} + 3\,258\,331\,201\,125),
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,2} = {} & 65\,536z^{32} + 4\,325\,376z^{30} + 106\,168\,320z^{28} + 1\,021\,870\,080z^{26} - 3\,019\,161\,600z^{24} \\
& - 169\,374\,965\,760z^{22} - 1\,749\,906\,063\,360z^{20} - 8\,630\,650\,828\,800z^{18} \\
& - 16\,958\,158\,963\,200z^{16} + 26\,480\,405\,952\,000z^{14} - 87\,626\,070\,604\,800z^{12} \\
& - 3\,976\,032\,953\,692\,800z^{10} - 18\,976\,520\,915\,352\,000z^{8} - 28\,464\,781\,373\,028\,000z^{6} \\
& - 64\,045\,758\,089\,313\,000z^{2} - 24\,017\,159\,283\,492\,375,
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,3} = {} & \sqrt{2}z(1\,048\,576z^{40} + 62\,914\,560z^{38} + 920\,125\,440z^{36} - 14\,722\,007\,040z^{34} \\
& - 543\,449\,088\,000z^{32} - 3\,594\,009\,968\,640z^{30} + 44\,997\,584\,486\,400z^{28} \\
& + 748\,655\,463\,628\,800z^{26} + 1\,257\,364\,568\,678\,400z^{24} - 46\,066\,277\,117\,952\,000z^{22} \\
& - 433\,373\,509\,191\,168\,000z^{20} - 1\,556\,239\,013\,941\,248\,000z^{18} \\
& - 2\,809\,510\,888\,766\,400\,000z^{16} - 3\,686\,0782\,860\,615\,168\,000z^{14} \\
& - 200\,599\,077\,457\,920\,960\,000z^{12} + 368\,158\,306\,863\,949\,056\,000z^{10} \\
& + 4\,271\,211\,606\,976\,283\,970\,000z^{8} + 5\,694\,948\,809\,301\,711\,960\,000z^{6} \\
& + 14\,949\,240\,624\,416\,993\,895\,000z^{4} - 16\,817\,895\,702\,469\,118\,131\,875),
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,4} = {} & 67\,108\,864 z^{52} + 2\,617\,245\,696 z^{50} - 49\,073\,356\,800 z^{48} - 2\,944\,401\,408\,000 z^{46} \\
& - 1\,987\,470\,950\,400 z^{44} + 1\,149\,685\,695\,774\,720 z^{42} + 8\,060\,089\,065\,799\,680 z^{40} \\
& - 206\,994\,105\,748\,684\,800 z^{38} - 2\,405\,543\,476\,808\,908\,800 z^{36} \\
& + 15\,932\,255\,610\,765\,312\,000 z^{34} + 295\,715\,856\,449\,367\,244\,800 z^{32} \\
& - 468\,712\,752\,961\,801\,420\,800 z^{30} - 24\,709\,482\,371\,771\,817\,984\,000 z^{28} \\
& - 77\,864\,358\,097\,369\,718\,784\,000 z^{26} + 795\,923\,196\,743\,966\,054\,400\,000 z^{24} \\
& + 4\,243\,708\,209\,176\,903\,061\,504\,000 z^{22} + 21\,619\,544\,333\,125\,112\,390\,016\,000 z^{20} \\
& + 299\,508\,747\,778\,795\,635\,400\,320\,000 z^{18} + 647\,925\,715\,931\,874\,373\,113\,120\,000 z^{16} \\
& - 4\,908\,134\,681\,808\,587\,435\,606\,400\,000 z^{14} - 531\,714\,590\,529\,263\,638\,857\,360\,000 z^{12} \\
& + 27\,117\,444\,116\,992\,445\,581\,725\,360\,000 z^{10} + 221\,326\,198\,307\,805\,989\,674\,376\,100\,000 z^{8} \\
& + 251\,235\,144\,025\,077\,069\,360\,102\,600\,000 z^{6} - 235\,532\,947\,523\,509\,752\,525\,096\,187\,500 z^{4} \\
& + 423\,959\,305\,542\,317\,554\,545\,173\,137\,500 z^{2} + 105\,989\,826\,385\,579\,388\,636\,293\,284\,375,
\end{aligned}
$$

$$
\begin{aligned}
Q_{5,5} = {} & \sqrt{2} z (4\,294\,967\,296 z^{64} - 10\,050\,223\,472\,640 z^{60} + 9\,440\,928\,674\,611\,200 z^{56} \\
& - 4\,799\,694\,645\,913\,190\,400 z^{52} + 1\,479\,019\,198\,616\,174\,592\,000 z^{48} \\
& - 298\,074\,520\,339\,239\,193\,804\,800 z^{44} + 40\,130\,199\,529\,452\,261\,605\,376\,000 z^{40} \\
& - 3\,950\,308\,378\,552\,575\,299\,420\,160\,000 z^{36} + 314\,495\,232\,283\,673\,308\,338\,831\,360\,000 z^{32} \\
& - 9\,746\,999\,000\,216\,774\,308\,402\,790\,400\,000 z^{28} \\
& - 505\,448\,497\,430\,935\,762\,827\,679\,395\,840\,000 z^{24} \\
& + 48\,584\,980\,146\,093\,597\,896\,433\,359\,616\,000\,000 z^{20} \\
& - 153\,023\,737\,152\,188\,370\,417\,676\,206\,480\,000\,000 z^{16} \\
& + 10\,774\,671\,374\,774\,675\,258\,232\,848\,185\,680\,000\,000 z^{12} \\
& - 124\,404\,922\,781\,115\,493\,935\,517\,424\,775\,450\,000\,000 z^{8} \\
& - 261\,250\,337\,840\,342\,537\,264\,586\,592\,028\,445\,000\,000 z^{4} \\
& + 183\,691\,643\,793\,990\,846\,514\,162\,447\,520\,000\,390\,625.
\end{aligned}
$$

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On effective constraints for the Riemann–Lanczos system of equations

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(Received 18 February 2003; accepted 21 August 2003)

There have been conflicting points of view concerning the Riemann–Lanczos problem in three and four dimensions. Using direct differentiation on the defining partial differential equations, Massa and Pagani (in four dimensions) and Edgar (in dimensions $n \geqslant 3$) have argued that there are effective constraints so that not all Riemann tensors can have Lanczos potentials; using Cartan's criteria of integrability of ideals of differential forms Bampi and Caviglia have argued that there are no such constraints in dimensions $n \leqslant 4$, and that, in these dimensions, all Riemann tensors can have Lanczos potentials. In this article we give a simple direct derivation of a constraint equation, confirm explicitly that known exact solutions of the Riemann–Lanczos problem satisfy it, and argue that the Bampi and Caviglia conclusion must therefore be flawed. In support of this, we refer to the recent work of Dolan and Gerber on the three-dimensional problem; by a method closely related to that of Bampi and Caviglia, they have found an ''internal identity'' which we demonstrate is precisely the three-dimensional version of the effective constraint originally found by Massa and Pagani, and Edgar. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1619203]

I. INTRODUCTION

In two recent papers Dolan and Gerber[1,2] have revisited the Riemann–Lanczos problem,[3] i.e., whether a Riemann tensor R_{abcd} can be generated from a three-index tensor potential H_{abc},

$$R_{abcd} = 2H_{ab[c;d]} + 2H_{cd[a;b]}, \tag{1}$$

where the potential H_{abc} satisfies

$$H_{abc} = H_{[ab]c} \quad H_{[abc]} = 0. \tag{2}$$

We follow the conventions of Ref. 4. Since there will be expressions which involve sums of terms with, respectively, the Ricci tensor and the square of the Ricci tensor, a consistent convention is essential. In particular it should be noted that in Refs. 5–7 a different convention was used for the Ricci tensor and so there are some sign differences between some equations in this paper and their counterparts in Refs. 5–7.

In the literature there are two apparently conflicting answers to the Riemann–Lanczos problem in four dimensions: Massa and Pagani[5] have argued that

> *"... for the class of spacetime metrics satisfying $R_{ab} = \lambda g_{ab}$ one of the integrability conditions of the system (1) takes the form $R^2 - 2R_{abcd}R^{abcd} = 0$, i.e., it imposes a restriction on the geometry itself,"*

whereas Bampi and Caviglia[8] have argued that

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> *"..., in the four-dimensional case no integrability condition is required. In other words, looking at the class of singular solutions allows a potential to exist without any restriction ... on the geometric structure of the underlying Riemann manifold."*

These two papers were written at the same time, and neither refers to the other. Of course this uncertainty would be dispelled if there were explicit examples of Lanczos potentials in reasonably general spaces; however, the only known examples are a few in flat[3,9] and conformally flat spaces[9] and a few very special space–times in Ref. 1.

Dolan and Gerber[1,2] rely on the results and to some extent on the method from Ref. 8, and state in Ref. 1 that the paper of Massa and Pagani in Ref. 5, and the subsequent work by Edgar in Refs. 6 and 7,

> *"... used a different approach ... and is not applicable here."*

We agree with Massa and Pagani[5] that if the representation (1) exists for arbitrary Riemann tensors, then it would have very significant implications for both the mathematical viewpoint and physical applications of general relativity. Therefore it is important to determine whether the representation (1) exists for all spaces (as argued in Refs. 8, 1, and 2), or whether it only exists for a restricted number of spaces (as argued in Refs. 5–7). If the latter case, it would be interesting to know whether there exist other effective constraints. Moreover, we believe that the work in Refs. 5–7 is very applicable to the work in Refs. 8 and 9 and Refs. 1 and 2, and a fuller understanding of the links between these two lines of investigation should clarify the apparent contradiction.

So, in this article, we shall first look at the analogous flat space problem which illustrates very simply some of the important points. Then we demonstrate in a very simple unambiguous manner that (1) implies an integrability condition which is an effective constraint for dimensions $n>2$ and therefore limits the class of spaces which can permit a Lanczos potential with properties (2) via (1). Moreover, we will show explicitly, that the Lanczos potentials of those very special spaces found in Refs. 1, 3, and 9 satisfy this restriction. Furthermore, we demonstrate that the nontrivial ''internal identity'' found recently by Dolan and Gerber in the three-dimensional problem[1] is precisely the effective constraint found in Refs. 5–7, and we argue that the Bampi–Caviglia analysis[8] is therefore flawed. We propose that the Janet–Riquier approach used in Ref. 1 should be applied to other dimensions.

II. EFFECTIVE CONSTRAINTS ON RIEMANN–LANCZOS SYSTEM

We consider first the more general problem in n-dimensional spaces of whether any *Riemann-candidate tensor*, $\hat{R}_{abcd}$—a tensor having the algebraic index symmetries of the Riemann tensor—can be generated from a potential H_{abc} by

$$\hat{R}_{abcd} = 2H_{ab[c;d]} + 2H_{cd[a;b]}, \tag{3}$$

where the potential H_{abc} satisfies (2).

A. Riemann-candidate–Lanczos problem in *n*-dimensional flat spaces

It is trivial to show that in flat space, although at the first derivative level we can only eliminate one of the potential terms,

$$\hat{R}^{ab}_{[cd;e]} = 2H_{[cd}{}^{[a;b]}{}_{;e]}, \tag{4}$$

by taking another derivative we can obtain

$$\hat{R}^{[ab}{}_{[de;f]}{}^{c]} = 0. \tag{5}$$

It is important to check whether (5) is an *effective* constraint for arbitrary $\hat{R}_{abcd}$—in the sense that not all Riemann-candidates $\hat{R}_{abcd}$ satisfy (5)—or whether there are situations when the left-hand

side is identically zero; it is obvious that the left-hand side is identically zero for dimensions $n=2$, but in all other dimensions it is an effective constraint. This is an important point, and the effectiveness of the constraint should not be taken for granted. (In the Weyl-candidate–Lanczos problem[9–13] a similar calculation gives an analogous equation which turns out to be trivially satisfied in four and five dimensions;[14,15] this was because any trace-free tensor $A^{[abc]}{}_{[def]}$ is identically zero in dimensions $n\leqslant 5$.[16,17]) To prove the effectiveness of this constraint we can simply choose a local Cartesian coordinate system $x^i, i=1,\ldots,n$, for $n>2$ and construct a simple counterexample, e.g., $R_{1312}=R_{1213}=\sin x^3 \sin x^2$, all other Riemann tensor components zero.

Therefore the representation (3), in flat space $(n>2)$, is valid only for a subset of Riemann candidates which satisfy (5), and possibly other additional constraints, i.e., (5) is obviously a necessary condition for a potential to satisfy (3), but whether it is a sufficient condition is an open question. This is an important example which illustrates two principles: it shows that a particular constraint on the geometry of the space, i.e., putting the curvature tensor $R_{abcd}=0$, can imply a specific constraint on the Riemann candidate $\hat{R}_{abcd}$; on the other hand, although the constraint is quite restrictive, yet it does permit a significant class of exceptions, for instance, a set of Riemann candidates which satisfy the "flat space Bianchi equations," $\hat{R}_{ab[cd;e]}=0$; in this case $H_{abc}=(h_{bc;a}-h_{ac;b})$ and $\hat{R}_{abcd}$ has the form of the Riemann tensor in the linearized theory.[3,9]

Of course, the analysis in this subsection does not say anything directly about the Riemann–Lanczos problem in curved spaces, since in flat space the constraint is trivially satisfied. However, we believe that the curved space analog of this constraint (5) is the crucial equation in the Riemann-candidate–Lanczos problem and the Riemann–Lanczos problem.

B. Riemann-candidate–Lanczos problem in *n*-dimensional flat spaces

In general curved spaces we can carry out on (3) the same differentiation steps as led to (5), but this time the right-hand side of Eq. (5) becomes complicated. However, by taking traces, we can easily find a much simpler subset, with significant properties. Noting that

$$\hat{R}_{ab}\equiv\hat{R}^{i}{}_{aib}=2H^{i}{}_{a[i:b]}+2H^{i}{}_{b[i:a]} \quad \text{and} \quad \hat{R}\equiv\hat{R}^{i}{}_{i}=4H^{ij}{}_{i:j}, \tag{6}$$

we find that, after some rearranging of (3),

$$\begin{aligned}\hat{R}^{;a}{}_{a}-2\hat{R}^{ab}{}_{;ab}&=4H^{ij}{}_{i;j}{}^{a}{}_{a}-4(H^{i}{}_{a[i;b]}+H^{i}{}_{b[i;a]})^{;ab}\\&=2R_{,a}H^{aj}{}_{j}+4R^{ab}H_{a}{}^{j}{}_{j;b}-4R^{ab;c}H_{cab}+2R^{abcd}H_{abc;d}.\end{aligned} \tag{7}$$

In flat space this equation (7) is the triple trace of (5). [The left-hand side of (7) is equivalent to $3\hat{R}^{[ab}{}_{[ab;c]}{}^{c]}$ for $n>2$; we begin instead with $\hat{R}^{;a}{}_{a}-2\hat{R}^{ab}{}_{;ab}$ which means that our analysis also includes the case $n=2$.] The next step is the important one: by substituting $\hat{R}_{abcd}$ in the last term on the right-hand side we eliminate some of the remaining ackward potential terms as well as introducing the Riemann candidate explicitly also on the right-hand side,

$$\hat{R}^{;a}{}_{a}-2\hat{R}^{ab}{}_{;ab}=2R_{,a}H^{aj}{}_{j}+4R^{ab}H_{a}{}^{j}{}_{j;b}-4R_{ab;c}H^{cab}+\tfrac{1}{2}R^{aijk}\hat{R}_{aijk}. \tag{8}$$

By decomposing R_{abcd} and $\hat{R}_{abcd}$ into their trace-free parts with $R_{ab}=S_{ab}+Rg_{ab}/n$, $\hat{R}_{ab}=\hat{S}_{ab}+\hat{R}g_{ab}/n$, we obtain the alternative form

$$\begin{aligned}2\hat{S}^{ab}{}_{;ab}+\frac{2-n}{n}\hat{R}^{;a}{}_{a}=&\left(\frac{4}{n}-2\right)R_{,a}H^{aj}{}_{j}-4S^{ab}H_{a}{}^{j}{}_{j;b}+4S_{ab;c}H^{cab}\\&-\frac{1}{2}C^{abcd}\hat{C}_{abcd}+\frac{2}{n-2}S^{ab}\hat{S}_{ab}+\frac{n-2}{n}R\hat{R}.\end{aligned} \tag{9}$$

1. n=2

Equation (9) is not valid for $n=2$, but the previous equation (8) is. However, when we substitute $n=2$ with $R_{abcd}=Rg_{a[c}g_{d]b}$ and $\hat{R}_{abcd}=\hat{R}g_{a[c}g_{d]b}$ into (8) the constraint collapses to a trivial identity, and so in two dimensions this particular constraint is not effective.

2. n>2

We cannot conclude that (9) is an *effective* constraint on all geometries, and on all Riemann candidates, because of the existence of the potential H_{abc} and its derivatives alongside the Riemann candidate $\hat{R}_{abcd}$ and the Riemann tensor R_{abcd}. However, for Einstein spaces ($S_{ab}=0=R_{,a}$), we obtain an expression with no explicit terms in the potential H_{abc},

$$2\hat{S}^{ab}{}_{;ab}+\frac{2-n}{n}\hat{R}^{;a}{}_{a}=-\frac{1}{2}C^{abcd}\hat{C}_{abcd}+\frac{n-2}{n}R\hat{R}, \tag{10}$$

and, in particular, for spaces of constant curvature, we obtain

$$2\hat{S}^{ab}{}_{;ab}+\frac{2-n}{n}\hat{R}^{;a}{}_{a}=\frac{n-2}{n}R\hat{R}. \tag{11}$$

Therefore, for Einstein spaces, we find that the existence of a potential H_{abc} in (3) leads to an *effective* constraint because those terms which are explicit in the potential all disappear, and we get a condition (10) which directly links the background space geometry via the Riemann tensor R_{abcd} with the Riemann-candidate $\hat{R}_{abcd}$.

There are some very special situations where this restriction (10) is satisfied trivially; e.g., if the Riemann candidate $\hat{R}_{abcd}$ satisfied a Bianchi-type equation, $\hat{R}_{ab[cd:e]}=0$ and also has its Weyl and Ricci scalar parts zero, $\hat{C}_{abcd}=0=\hat{R}$. Of course we cannot conclude that in such situations a Lanczos potential will exist; we must also remember that there could be additional constraints at this order, or at higher orders of differentiation.

Turning to spaces other than Einstein space, important questions arise: e.g., with respect to a particular non-Einstein space, do there exist more constraints? Can all Riemann candidates or some Riemann candidates or no Riemann candidates be generated by a potential from (3)? It is easy to see that there must always be some Riemann candidates, since in a particular space, if we choose a particular tensor H_{abc} with the symmetries (2), we can then define a subclass of Riemann candidates via (3) which will automatically satisfy the constraint (9). However, our analysis is unable to tell us whether, in all non-Einstein spaces, for arbitrary Riemann candidates there exists a potential H_{abc} with the symmetries (2) such that both the system (3) and the constraint (9) are satisfied.

Therefore what we are able to conclude for the Riemann-candidate–Lanczos problem is that

(i) for $n=2$ the constraint (9) linking the Riemann-candidate tensor and the geometry is trivially satisfied;
(ii) for $n>2$ the constraint (9) linking the Riemann-candidate tensor and the geometry is effective in some spaces, e.g., (10), and so not all Riemann-candidates can admit Lanczos potentials in all spaces via the representation (3); and
(iii) for $n>2$, we know that there are some spaces and Riemann-candidate tensors which can admit Lanczos potentials via the representation (3) with (9) also satisfied identically. We do not know if there are more situations where Riemann-candidate tensors can admit Lanczos potentials via the representation (3), but if there are, then (9) will be satisfied identically. We also do not know if there are more constraints.

C. Riemann–Lanczos problem in *n*-dimensional curved spaces

When we specialize to the Riemann–Lanczos problem, i.e., $\hat{R}_{abcd} \equiv R_{abcd}$, we find that, as a consequence of (1), the left-hand side of (9) is identically zero via the contracted Bianchi identity, giving

$$0 = \left(\frac{4}{n} - 2 \right) R_{,a} H^{aj}{}_{j} - 4 S^{ab} H_{a}{}^{j}{}_{j;b} + 4 S_{ab;c} H^{cab} - \frac{1}{2} C^{abcd} C_{abcd} + \frac{2}{n-2} S^{ab} S_{ab} + \frac{n-2}{n} R^2. \tag{12}$$

We can then conclude that for $n > 2$ we cannot have a Lanczos potential H_{abc} for a space of (nonzero) constant curvature, and for $n \geqslant 4$ the only Einstein spaces which can have a Lanczos potential are those subjected to the restriction

$$C^{aijk} C_{aijk} = 2 \frac{n-2}{n} R^2. \tag{13}$$

This restriction is *effective* since there are no explicit terms involving the potential, and what we have is a direct condition on the geometry, which clearly not all Einstein spaces satisfy; in fact (13) is an additional invariant condition linking two Riemann scalar invariants in Einstein spaces.

This restriction (12) is only one scalar equation and so in general it, in itself, would not appear to be a very strong restriction on the class of Riemann tensors. For instance, in four dimensions we know that there exist 14 Riemann scalar invariants—in general; however, when we specialize to vacuum four-dimensional space–times we note that this constraint (13) excludes all Petrov types of the Weyl tensor except the very specialized Petrov types N and III. So, in vacuum in four-dimensional space–times, (13) is a very strong restriction. Although Petrov type N and III spaces are not restricted by (13), we cannot immediately conclude that they admit Lanczos potentials via (1); we must again remember that there could be additional constraints at this order, or at higher orders of differentiation.

As regards spaces other than Einstein spaces, we know that there are a few explicit special examples of Riemann tensors with Lanczos potentials, e.g., some conformally flat spaces given in Ref. 9, and three four-dimensional spacetimes and one three-dimensional space given in Ref. 1.

To confirm the significance of the integrability condition (12) for the Riemann–Lanczos problem we have shown that all of these special examples (with the exception of the Kasner space–time in Ref. 1 where the calculations were too complicated) are non-Einstein spaces and we have demonstrated explicitly that they satisfy (12). [In Ref. 8, three examples of conformally flat four-dimensional spacetimes are given and it is simple to confirm that the respective Lanczos potentials satisfy (12). In Ref. 1, Lanczos potentials are given for an example of Debever and Godel four-dimensional spacetimes, and also a Lanczos potential is given for an example of a Godel three-dimensional space; in these spaces it is straightforward, with the help of *GRTensorII*,[18] to confirm that (12) is satisfied.] Whether potentials can be found for the Riemann tensors of all non-Einstein spaces cannot be decided from the above analysis.

Therefore what we are able to conclude for the Riemann–Lanczos problem is that

(i) for $n = 2$ the constraint (12) on the Riemann tensor is trivially satisfied;
(ii) for $n > 2$ the constraint (12) on the Riemann tensor is effective in some spaces, e.g., (13), and so not all Riemann tensors can admit Lanczos potentials via the representation (1);
(iii) for $n > 2$, we do know that there are some special examples of Riemann tensors which can admit Lanczos potentials via the representation (1), and they also satisfy (12). We do not know if there are any others, but if there are, then the constraint (12) must be satisfied. We do not know if there are any more constraints.

The existence of this constraint for the Riemann–Lanczos problem was originally demonstrated in four dimensions by Massa and Pagani,[5] who set up the problem in ordinary tensor notation, but carried out the actual derivation of the crucial constraint equation in tensor-valued

differential forms. This calculation was quite involved, and strictly four-dimensional. (In Ref. 5 a different sign convention was used for the Ricci tensor from that used in this paper, and this convention was also used in Refs. 6 and 7; so there are some sign differences between this version of the equation and that in Refs. 5–7.) The tensor-valued differential form part of the derivation of the integrability condition was rederived by Edgar in Ref. 6 in ordinary tensor notation, but the argument was still strictly four-dimensional. Subsequently, a more direct and complete derivation of the constraint equation—with no explicit dimension imposed—was given in Ref. 7, and an even simpler variation by Höglund.[19] The derivation given above for the Riemann-candidate–Lanczos problem is based on the version in Ref. 19.

III. EFFECTIVE CONSTRAINTS FOR THE PARALLEL PROBLEM

In their investigations Bampi and Caviglia[8,9] did not in fact deal with $\hat{R}_{abcd}$ and H_{abc} directly but rather with their respective counterparts N_{abcd} and T_{abc} which satisfied

$$N_{abcd} = 2T_{ab[c;d]} + 2T_{cd[a;b]}, \tag{14}$$

where N_{abcd} and T_{abc} have only the respective symmetries,

$$T_{abc} = T_{[ab]c} \quad \text{and} \quad N_{abcd} = N_{[ab][cd]} = N_{cdab}. \tag{15}$$

Their motivation for studying this parallel problem was that they were able to show that this problem and the Riemann-candidate–Lanczos problem were mathematically equivalent—*in four dimensions*. For other dimensions, any positive results for the existence of potentials for all N_{abcd} would also apply to the narrower Riemann-candidate–Lanczos problem, and hence to the even narrower Riemann–Lanczos problem; but negative results for the parallel problem would, in general, be irrelevant to the narrower Riemann-candidate–Lanczos and Riemann–Lanczos problems.

A. $n>4$

We can immediately find the integrability condition

$$N_{[abcd;e]} = 0 \tag{16}$$

and confirm that this is always an *effective* constraint. So we can conclude that in this parallel problem not all tensors N_{abcd} can be written in terms of a potential; this result does not permit us to draw any conclusion about the associated Riemann-candidate–Lanczos problem.

B. $n>2$

If we carry out again the antisymmetrization over five indices as in (16), we just obtain the trivial identity in dimensions 3 and 4. So, instead, to find effective constraints for $5>n>2$, we have to carry out the same procedure as in Sec. II involving two differentiations; but since we already know that there are restrictive integrability conditions for the Riemann-candidate–Lanczos problem, there is no purpose in investigating further the parallel problem as a means of investigating the narrower Riemann-candidate–Lanczos problem. However, for completeness we point out that in the calculations leading to the constraint (8), the only index symmetries used were those of the type (15), and so we can deduce that the parallel problem is subject to the constraint

$$N^{;a}{}_{a} - 2N^{ab}{}_{;ab} = 2R_{,a}T^{aj}{}_{j} + 4R^{ab}T_{a}{}^{j}{}_{j;b} - 4R_{ab;c}T^{cab} + \tfrac{1}{2}R^{aijk}N_{aijk}, \tag{17}$$

which in flat space simplifies to

$$N^{;a}{}_{a} - 2N^{ab}{}_{;ab} = 0. \tag{18}$$

As argued in the last section, these constraints are effective.

In summary, we can conclude that, since our investigation found the existence of effective constraints in the parallel problem, we cannot draw any conclusions about the original Riemann-candidate–Lanczos problem, since in all cases the constraints in the parallel problem may or may not be present in the narrower Riemann-candidate–Lanczos problem. However, the occurence of the integrability conditions (16)–(18) and the role played by dimension will be of interest in the next section.

IV. "GENERIC," "ORDINARY," AND "SINGULAR" SOLUTIONS

From the type of investigaton in Secs, II and III on the constraints due to integrability conditions, we are only able to directly draw limited conclusions. For more complete conclusions we need a procedure which will distinguish between the respective situations where there are indeed effective constraints (even if we cannot find them explicitly), and where there are no effective constraints and the existence of a potential is always guaranteed. This is clearly the role of Cartan's local criteria of integrability of ideals of exterior forms,[20–22] as set out in Refs. 8 and 9. Furthermore, if the system is not in involution and we do find some effective constraints, we can prolong the original system to take account of these constraints, and then also use Cauchy's criteria to analyze the prolonged system. If the prolonged system is not in involution, then the process can be repeated until either an involutive system is obtained, or we encounter inconsistencies.

As noted in the last section, Bampi and Caviglia[8] considered the parallel problem (14) for the tensors N_{abcd} and T_{abc} as a means of studying the Riemann-candidate–Lanczos problem (3). We shall now discuss their results, and compare with our results in the previous two sections.

A. $n>4$

In Ref. 8 it is stated that in higher dimensions there will be nontrivial restrictions on the data. In fact we have obtained this result very easily in (16). This result has no direct relevance to the narrower Riemann-candidate–Lanczos problem.

B. $n=4$

In their first paper, Bampi and Caviglia[9] showed that the equation (14) does not always admit a solution for a given N_{abcd}. More precisely, they showed the nonexistence of solutions under certain generic conditions on N_{abcd}, or, as Massa and Pagani[5] pointed out, Bampi and Caviglia[9] showed that the representation (3) does not exhaust the totality of the set of tensors N_{abcd} (which in four dimensions is equivalent to the set of Riemann candidates $\hat{R}_{abcd}$), and, hence, since the Riemann tensors themselves are only a proper subset of this larger class of Riemann candidates, this result says nothing about the validity of (3) for Riemann tensors.

This generic result for the Riemann-candidate–Lanczos problem given by Bampi and Caviglia[9] was strengthened in their second paper[8] where it was stated in Theorem 1 that there never exist "regular" ("ordinary") solutions to (14) for any tensor N_{abcd} in four dimensions, so this result now includes the Riemann–Lanczos problem, i.e., there never exist "regular" ("ordinary") solutions to (1) for any Riemann tensor R_{abcd} in four dimensions. If we interpret "regular" solutions to mean the existence of the most general solutions with no constraints on the class of tensors N_{abcd} and the underlying space, then the conclusion in Theorem 1 does not contradict the results in Sec. III of this article.

The difficulty is with Theorem 2 in Ref. 8. The original system (14) is not in involution and so is prolonged, and as a result of the analysis of the prolonged system, Bampi and Caviglia find no constraints, and conclude in Theorem 2[8] that in four dimensions, although the representation (14) never permits "regular" ("ordinary") solutions to (14), it always admits "singular" ("non-ordinary") solutions for all tensors N_{abcd} (equivalently for all Riemann candidates $\hat{R}_{abcd}$). Therefore, in Ref. 8 the "singular" solutions are argued to have what appears to be exactly the same general properties as "regular" solutions, with no constraints on the data N_{abcd} or on the background space.[23]

Normally we expect that such ''singular'' solutions would involve some restrictions on the set of tensors N_{abcd} and/or on the underlying space. However, Bampi and Caviglia[8] claim that these ''singular'' solutions are, to their own surprise, not subject to any integrability conditions, and they state that

> *"... the class of "singular" solutions allows a potential to exist without any restriction on N_{abcd} and on the geometric structure of the underlying Riemann manifold ...."*

This conclusion in Theorem 2[8] contradicts the results in Sec. III of this article, in particular the very simple obvious effective constraint (17) for flat space (flat space is not excluded in the analysis in Ref. 8). We suspect that this claim of no constraints on these ''singular'' solutions is not due simply to a misinterpretation of the properties of ''singular'' solutions but, more fundamentally, to a fault in the calculations in Ref. 8. We would point out that the only constraint—the ''internal identity'' $A_{[abcde]}=0$ in the notation of Ref. 8—discovered in the calculations for Theorem 2 in Ref. 8 is precisely the very obvious integrability condition (18) which we found directly in Sec. III, and which is of course trivially satisfied in four dimensions. What is most surprising about the method of application of Cauchy's criteria in Refs. 8 and 9 is that the possibility of constraints existing after two differentiations—involving linear combination of components of B_{abcdef} in the notation of Refs. 8 and 9—does not arise; whereas, from our work in Sec. III, and in particular the simple effective constraint equation (18), it is clear that this is precisely where we expect constraints. Unfortunately, it is not easy to check the accuracy of the argument in Ref. 8 at this level, since no explicit details were given leading to the conclusion that $s_3'=s_3$, for the Cartan characters.

C. $n=3$

For the parallel problem, it is stated in Ref. 8 that, under ''generic'' conditions, there does not exist any ''regular'' solution because of the existence of an ''internal identity''; however, in their second paper,[8] Bampi and Caviglia conclude, by the same argument as in four dimensions, that there always exist ''singular'' solutions independently of the choice of $\hat{R}_{abcd}$ and the geometry of the space. So we have here the same situation as in four dimensions, involving a contradiction with the effective constraint found in Sec. III. Of course, we should remember that the parallel problem is not equivalent to the Riemann-candidate–Lanczos problem in three dimensions, and a negative result in the former has no direct relevance to the latter.

Significantly, in the next section, we will find that Dolan and Gerber,[1] using an alternative but related method to Ref. 8 for the direct Riemann–Lanczos problem, have found an explicit constraint which is effective, and this constraint is precisely the three-dimensional version of the effective constraint which we discussed in Sec. II.

D. $n=2$

In Ref. 9 it is stated that there will always be ''regular'' solutions, and there is no contradiction with the integrability condition (9) in Sec. II since with the substitution $n=2$ the constraint is trivially satisfied. Finally, we turn to the results on the differential gauge. It is stated in Ref. 8 that even when an arbitrary differential gauge condition on $H_{ab}{}^{c}{}_{;c}$ (e.g., $H_{ab}{}^{c}{}_{;c}=0$) is put alongside the condition (3), there will always be ''singular'' solutions in four dimensions. As we have discussed above, we believe that the result that there are always ''singular'' solutions is flawed. But the question arises, in those special cases where there are ''singular'' solutions (with a restriction on the Riemann candidates and/or the geometry), whether the differential gauge can be chosen arbitrarily. We believe that this question of gauge is still, in general, open.

V. THE RIEMANN–LANCZOS PROBLEM BY THE JANET–RIQUIER APPROACH

Dolan and Gerber[1,2] have considered the direct Riemann–Lanczos problem (1) with the symmetries (2) for some very special spaces from the exterior derivative viewpoint along the same

lines as in Refs. 8 and 9, but also they have considered the problem directly as a system of partial differential equations in two and three dimensions[1] using the related Janet–Riquier[24,25] approach. In fact, their analysis is valid also for the more general Riemann-candidate–Lanczos problem (3).

A. $n=2$

This problem has been shown by the Janet–Riquier approach always to have solutions; in fact it is a very simple problem which has also been integrated directly in Ref. 1. There is no contradiction with the integrability condition (9) in Sec. II, since we have already noted for $n=2$ that the constraint is not effective.

B. $n=3$

Using the Janet–Riquier approach, Dolan and Gerber[1] have found that the original Riemann–Lanczos problem is not in involution and so there are no ''regular'' solutions. After one prolongation, obtained by adding one ''internal identity,'' they found that the prolonged system was involutive. They point out that their ''internal identity'' is not trivial, and they give it in invariant form as

$$f^{(R)}{}_{12[12;3]3}+f^{(R)}{}_{23[12;3]1}+f^{(R)}{}_{31[12;3]2}=0, \tag{19}$$

where

$$f^{(R)}{}_{abcd}\equiv R_{abcd}-2H_{ab[c;d]}-2H_{cd[a;b]}. \tag{20}$$

This is precisely the constraint

$$f^{(R)}{}_{[ab|[de;f]|c]}=0 \tag{21}$$

since there is only one component of (21) in three dimensions; and since in three dimensions there is no trace-free part to $f^{(R)}{}_{abcd}$, the constraint (21) can be rewritten more compactly as

$$2\,f^{(R)aib}{}_{i;ab}-f^{(R)ij}{}_{ij}{}^{;a}{}_{a}=0 \quad . \tag{22}$$

When the substitution (20) is made into this last equation, we obtain

$$R^{;a}{}_{a}-2R^{ab}{}_{;ab}=4H^{ij}{}_{i;j}{}^{a}{}_{a}-4(H^{i}{}_{a[i;b]}+H^{i}{}_{b[i;a]})^{ab} \quad , \tag{23}$$

which is precisely (the Riemann tensor version of) Eq. (7), and leads to an effective constraint (8) as shown. Of course, for a Riemann tensor, the left-hand side will be indentically zero due to the Bianchi identity, but we can see that the analysis also gives the constraint for the more general Riemann-candidate–Lanczos problem.

Therefore, the "internal identity" above (19) is precisely the three-dimensional version of the effective constraint (12) for the Riemann–Lanczos problem found in Sec. II. Furthermore, since the prolonged system, created by adding this constraint has been shown to be involutive in Ref. 1, this must be the only constraint. Also in Ref. 1 there is an explicit example in three dimensions of a Lanczos potential, which can be interpreted as a singular solution for the unprolonged problem, or as a regular solution for the prolonged problem. We have confirmed directly that it satisfies the constraint (9) in Sec. II [equivalently the ''internal identity'' (19) which was found in Ref. 1].

VI. CONCLUSION

We have confirmed that two successive differentiations of the defining equations (3) of the Riemann-candidate–Lanczos problem leads to an effective constraint in $n>2$ dimensions, and known solutions of the problem have been shown explicitly to satisfy this constraint. Furthermore, we have shown that the results in Refs. 5–7 are directly relevant to the work of Dolan and Gerber;[1,2] in particular the ''internal identity'' found in Refs. 1 and 2 for the three-dimensional

Riemann–Lanczos problem is precisely the effective constraint found in Refs. 5–7. The existence of this effective constraint contradicts the results in Ref. 8 for three and four dimensions.

It is significant that, using a method similar to the approach in Refs. 8 and 9, in three dimensions, Dolan and Gerber have found in Ref. 2 exactly the three-dimensional version of the effective constraint originally found by Refs. 5–7. This reinforces our suspicion that the approach in Refs. 8 and 9 is flawed, and an attempt should be made to reinvestigate the prolonged system at the level of the second derivatives of the Riemann tensor for all dimensions from the exterior differential system viewpoint. (Dolan and Gerber[2] have only briefly mentioned the problem in some other dimensions from the exterior differential system viewpoint as used in Refs. 8 and 9, but have not developed it further.) However, it seems that the Janet–Riquier method for partial differential equations is shorter and perhaps more transparent, and so it would be preferable to first apply this approach, as used in two and three dimensions in Ref. 1, to other dimensions; then this could be compared with the exterior differential system approach.

We also note the significant role that the dimension of the space has played at a number of crucial places in our arguments; whether a constraint is effective or not can depend on the dimension. The constraint (8) is effective for $n>2$, but trivial for $n=2$; in the parallel problem as well as the constraint (17) for $n>2$, an additional constraint (16) occurs for $n>4$. The role of dimension is even more subtle for the Weyl–Lanczos problem where complicated constraints involving the second derivatives of the Weyl tensor are valid only for dimensions $n\geqslant 6$, while constraints involving the third derivatives of the Weyl tensor are valid only for dimensions $n\geqslant 5$; there are no constraints for $n=4$.[10–15]

In summary, we note that not all Riemann candidates and Riemann tensors have potentials in dimensions $n>2$, because of the existence of an effective constraint, although there are special cases where such potentials do exist. From Refs. 1 and 2 it is known that prolongation with this one constraint gives an involutive system, in three dimensions and it is still an open question whether prolongation with this one constraint can lead to involution in higher dimensions; a preliminary investigation of the flat space case by the Janet–Riquier approach would suggest that all the equations corresponding to (5) may be needed.

ACKNOWLEDGMENTS

The continuing financial support of Vetenskapsrådet (the Swedish Research Council) is acknowledged. Thanks to Anders Hoglund and Fredrik Andersson for many helpful discussions.

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analogy is given. It would seem that Bampi and Caviglia (Ref. 8) view the distinction as simply a technical matter: solutions involving the maximal Cartan characters are ''regular'' solutions, while solutions from a prolonged system with less than the maximal Cartan characters are ''singular'' solutions.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 11 NOVEMBER 2003

Hierarchy of random chaotic maps with an invariant measure

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(Received 17 June 2003; accepted 24 June 2003)

Hierarchy of one and many-parameter families of random chaotic maps and one-parameter random elliptic maps of **cn** type with an invariant measure have been introduced. Using the invariant measure (Sinai–Ruelle–Bowen measure), the Kolmogorov–Sinai entropy of the random chaotic maps have been calculated analytically, where the numerical simulations support the results. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1610240]

I. INTRODUCTION

The problem of the transition to chaos in deterministic systems has been the subject of much interest, and, for low-dimensional dynamics, it has been found that this transition most often occurs via a small number of often observed routes (e.g., period doubling and intermittency). Usually the analytic calculation of invariant measure of dynamical systems is a nontrivial task, hence there are limited number of maps with invariant measure like, Ulam–von Neumann map,[1] Chebyshev maps,[2] Katsura–Fukuda map,[3] piecewise parabolic map,[4] Tent map,[5] Elliptic map,[6] and finally hierarchy of one and many-parameter families of trigonometric chaotic and one-parameter elliptic chaotic maps of **cn** type with their couplings.[7–10]

Here in this article we present a new hierarchy of random chaotic maps with an invariant measure, where using the invariant measure we discuss analytically the transition to chaos in these random dynamical systems. Random chaotic maps have attracted the attention of physicists in the realm of theoretical biology, disordered systems, and cellular automata for its possible application to studies of DNA replication, cell differentiation, and evolution theory.[11,12] Additionally, random chaotic maps are of interest as models of convection by temporarily irregular fluid flows.[13]

In this paper we consider random chaotic maps where, on each iteration, the map function $\Phi(x,\alpha)$ is chosen randomly from a hierarchy of maps with an invariant measure which is introduced in our previous papers.[7,8,10]

There are two noticeable advantages of random chaotic maps that are presented through this article. First they are measurable dynamical systems so they can be studied analytically. Second, they have the property of being either chaotic or having stable period one fixed point.

The paper is organized as follows. Section II is devoted to the introduction of the random chaotic map models. Then, in Sec. III, we introduce the Sinai–Ruelle–Bowen (SRB) measure of random chaotic maps. The calculation of Kolmogorov–Sinai (KS) entropy of random chaotic maps via their SRB measure is presented in Sec. IV. Section V is devoted to the Lyapunov characteristic exponent and the paper ends with a brief conclusion in Sec. VI.

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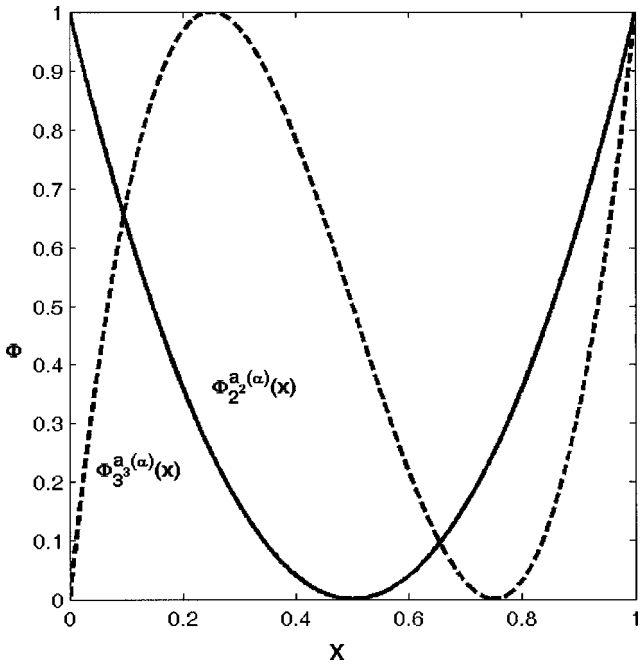

FIG. 1. Plot of $\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_3^{a_3(\alpha)}(x)$ map for $\alpha=0.15$. The location of maxima and minima and their values (0 or 1) are independent of parameter α, as shown.

II. HIERARCHY OF ONE- AND MANY-PARAMETER RANDOM CHAOTIC MAPS

The random chaotic map can be obtained via random choice from an ensemble of maps according to some probability distribution. Therefore, for a given ensemble of maps Φ_i, $i=1,2,...$ with probability $p_i \geqslant 0$ with $\Sigma p_i = 1$, the corresponding random chaotic map can be defined as

$$\Phi(x,p)=\Phi_i(x) \quad \text{with probability } p_i\,. \tag{2.1}$$

Here in this paper we try to construct the hierarchy of random chaotic maps with an invariant measure by choosing the ensemble of one and many parameters of maps of trigonometric and elliptic types of Refs. 7, 8, and 10 as follows.

A. One-parameter random chaotic maps

The families of one-parameter maps of the interval $[0,1]$ with an invariant measure are defined as the ratio of polynomials of degree N:[7]

$$\Phi_N^{\alpha}(x)=\frac{\alpha^2\left(1+(-1)^N{}_2F_1\left(-N,N,\frac{1}{2},x\right)\right)}{(\alpha^2+1)+(\alpha^2-1)(-1)^N{}_2F_1\left(-N,N,\frac{1}{2},x\right)}=\frac{\alpha^2(T_N(\sqrt{x}))^2}{1+(\alpha^2-1)(T_N(\sqrt{x})^2)}, \tag{2.2}$$

where N is an integer greater than one. Also

$${}_2F_1(-N,N,\tfrac{1}{2},x)=(-1)^N T_{2N}(\sqrt{x})$$

is a hypergeometric polynomial of degree N and $T_N(x)$ is a Chebyshev polynomial of type I; obviously these map the unit interval $[0,1]$ into itself, respectively. $\Phi_N^{\alpha}(x)$ is an $(N-1)$-nodal map, that is, it has $(N-1)$ critical points in unit interval $[0,1]$ (see Fig. 1), since its derivative is

proportional to the derivative of the hypergeometric polynomial ${}_2F_1(-N,N,\frac{1}{2},x)$, which is itself a hypergeometric polynomial of degree $(N-1)$, hence it has $(N-1)$ real roots in unit interval [0,1]. Defining the Shwarzian derivative[14] $S(\Phi_N^\alpha(x))$ as

$$S(\Phi_N^\alpha(x))=\frac{\Phi_N^{\alpha\,\prime\prime\prime}(x)}{\Phi_N^{\alpha\,\prime}(x)}-\frac{3}{2}\left(\frac{\Phi_N^{\alpha\,\prime\prime}(x)}{\Phi_N^{\alpha\,\prime}(x)}\right)^2=\left(\frac{\Phi_N^{\alpha\,\prime\prime}(x)}{\Phi_N^{\alpha\,\prime}(x)}\right)'-\frac{1}{2}\left(\frac{\Phi_N^{\alpha\,\prime\prime}(x)}{\Phi_N^{\alpha\,\prime}(x)}\right)^2,$$

with a prime denoting differentiation with respect to variable x, one can show that

$$S(\Phi_N^\alpha(x))=S({}_2F_1(-N,N,\tfrac{1}{2},x))\leqslant 0.$$

Therefore, the maps $\Phi_N^\alpha(x)$ have at most $N+1$ attracting periodic orbits,[14] also from the definition of these maps, we see that for odd N, both $x=0$ and $x=1$ belong to one of the n cycles, while for even N, only $x=1$ belongs to one of the n cycles. In the following we give $\Phi_2^\alpha(x)$ and $\Phi_3^\alpha(x)$ as examples:

$$\Phi_2^\alpha(x)=\frac{\alpha^2(2x-1)^2}{4x(1-x)+\alpha^2(2x-1)^2},\quad \Phi_3^\alpha(x)=\frac{\alpha^2x(4x-3)^2}{\alpha^2x(4x-3)^2+(1-x)(4x-1)^2}.$$

Using the hierarchy of families of one-parameter maps (2.2), we can generate a new hierarchy of random chaotic maps with an invariant measure, denoted by $\Phi_{N_i}^\alpha(x,p_i)$, which can be written as

$$\Phi_{N_i}^\alpha(x,p_i)=\Phi_{N_i}^{a_{N_i}(\alpha)}(x)\quad \text{with probability } p_i, \tag{2.3}$$

where $\Sigma_{i=1}^m p_i=1$ and the parameter $a_N(\alpha)$ is defined as

$$a_N(\alpha)=\frac{\Sigma_{k=0}^{[(N-1)/2]}C_{2k+1}^N\left(\frac{\alpha}{1-\alpha}\right)^{-k}}{\Sigma_{k=0}^{[N/2]}C_{2k}^N\left(\frac{\alpha}{1-\alpha}\right)^{-k}}, \tag{2.4}$$

with the symbol [ ] as the greatest integer part, and

$$C_k^n=\frac{n!}{k!(n-k)!}.$$

As examples in the following we give $\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_3^{a_3(\alpha)}(x)$:

$$\Phi_2^{a_2(\alpha)}(x)=\frac{\alpha^2(2x-1)^2}{x(1-x)+\alpha^2(2x-1)^2},$$

$$\Phi_3^{a_3(\alpha)}(x)=\frac{x(4x-3)^2(2\alpha+1)^2}{x(4x-3)^2(2\alpha+1)^2+(1-x)(4x-1)^2(3-2\alpha)^2}.$$

B. Many-parameter random chaotic maps

Even though one can define many-parameter random chaotic maps with an invariant measure, for simplicity we restrict ourselves here in this paper to two-parameter ones.[8] Random two-parameter maps are defined as

$$\Phi_{N_i,N_j}^{\alpha_i,\alpha_j}(x,p_{ij})=\Phi_{N_i,N_j}^{\alpha_i,\alpha_j}(x)\quad \text{with probability } p_{ij}, \tag{2.5}$$

where $\Sigma_{i,j} P_{ij}=1$ and $\Phi^{\alpha_i,\alpha_j}_{N_i,N_j}(x)=\Phi^{\alpha_i}_{N_i}(\Phi^{\alpha_j}_{N_j}(x))$ with

$$\alpha_i^{-1}=\alpha_j\times\frac{A_{N_j}(\alpha)}{B_{N_j}(\alpha)}\times\frac{A_{N_i}\left(\frac{1}{\eta^{\alpha_j}_{N_j}(\alpha)}\right)}{B_{N_i}\left(\frac{1}{\eta^{\alpha_j}_{N_j}(\alpha)}\right)},\quad \eta^{\alpha_j}_{N_j}(\alpha)=\alpha_j\times\left(\frac{\alpha}{1-\alpha}\right)\times\left(\frac{A_{N_j}(\alpha)}{B_{N_j}(\alpha)}\right)^2, \tag{2.6}$$

where the polynomials $A(x)$, $B(x)$ are defined as

$$A(x)=\sum_{k=0}^{[N/2]} C^N_{2k}\left(\frac{x}{1-x}\right)^k,\quad B(x)=\sum_{k=0}^{[(N-1)/2]} C^N_{2k+1}\left(\frac{x}{1-x}\right)^k. \tag{2.7}$$

$\Phi^{\alpha_i,\alpha_j}_{N_i,N_j}(x)$ consist of composition of maps with negative Shwarzian derivative, therefore these maps have at N_iN_j+1 attracting periodic orbits.[14] As it was shown,[8] these maps have only single period one stable fixed points.

C. One-parameter random elliptic maps

The families of one-parameter elliptic maps of **cn**[15] at the interval [0,1] are defined as the ratio of Jacobian elliptic functions of **cn** types in the following form:[10]

$$\Phi^{\alpha}_N(x)=\frac{\alpha^2(cn(Ncn^{-1}(\sqrt{x})))^2}{1+(\alpha^2-1)(cn(Ncn^{-1}(\sqrt{x})))^2}. \tag{2.8}$$

Obviously, these map the unit interval [0,1] into itself. One can show that

$$S(\Phi^{\alpha}_N(x))=S(cn(Ncn^{-1}(\sqrt{x})^2)))\leqslant 0,$$

since $(\mathrm{d}/\mathrm{d}x)\,(cn(Ncn^{-1}(\sqrt{x})^2)))$ can be written as

$$\frac{\mathrm{d}}{\mathrm{d}x}(cn(Ncn^{-1}(\sqrt{x})^2)))=A\prod_{i=1}^{N-1}(x-x_i),$$

with $0\leqslant x_1<x_2<x_3<\cdots<x_{N-1}\leqslant 1$, then we have

$$S(cn(Ncn^{-1}(\sqrt{x})^2)))=\frac{-1}{2}\sum_{J=1}^{N-1}\frac{1}{(x-x_j)^2}-\left(\sum_{j=1}^{N-1}\frac{1}{(x-x_j)}\right)^2<0.$$

Therefore, the maps $\Phi^{\alpha}_N(x)$, are $(N-1)$-nodal maps, that is, they have $(N-1)$ critical points in unit interval [0,1][14] and they have only a single period one stable fixed point or they are ergodic. As an example, we give in the following $\Phi^{\alpha}_2(x)$:

$$\Phi^{\alpha}_2(x)=\frac{\alpha^2((1-k^2)(2x-1)+k^2x^2)^2}{(1-k^2+2k^2x-k^2x^2)^2+(\alpha^2-1)((1-k^2)(2x-1)+k^2x^2)^2}.$$

Now, with the hierarchy of families of one-parameter elliptic maps (2.9), we can generate a new hierarchy of one-parameter random elliptic maps with an invariant measure denoted by $\Phi^{\alpha}_{N_i}(x,p_i)$, which can be written as

$$\Phi^{\alpha}_{N_i}(x,p_i)=\Phi^{a_{N_i}(\alpha)}_{N_i}(x)\quad \text{with probability } p_i, \tag{2.9}$$

where $\Sigma_{i=1}^m p_i=1$ and $a_{N_i}(\alpha)$ is the same as given in (2.12).

III. INVARIANT MEASURE OF RANDOM CHAOTIC MAPS

Characterizing invariant measure for a given nonlinear dynamical system is a fundamental problem which connects dynamical theory to statistics and statistical mechanics. A well-known example is the Ulam and von Neumann map which has an invariant measure $\mu = 1/\sqrt{x(1-x)}$.[1]

Let us recall that for a deterministic map $\Phi(x)$, the invariant probability measure $\mu(x)$ is the eigenfunction of the Perron–Frobenius(PF) operator $\mathbf{L}$ related to maximum eigenvalue 1,[16,17]

$$L\mu(x) = \mu(x), \tag{3.1}$$

where the operator L is defined as

$$Lf(x) = \int \delta(y - \Phi(x)) f(y)\mathrm{d}y = \sum_{z=\Phi^{-1}(x)} \frac{f(z)}{|\Phi'(z)|}. \tag{3.2}$$

In the case of random chaotic map, the average probability density can be found by the straightforward generalization of (3.1) as shown in the following:

$$\overline{L}\mu_{\mathrm{av}}(x) = \mu_{\mathrm{av}}(x), \tag{3.3}$$

where

$$\overline{L} = \sum_{i=1}^{m} p_i L_i . \tag{3.4}$$

In the above-mentioned equation L_i is the Perron–Frobenius operator associated with map $\Phi_i(x)$. It should be mentioned that for trigonometric maps,[7] their composition[8] and their coupling[9] the eigenstate of PF operator $\mathbf{L}$ corresponding to largest eigenvalues has already been obtained in our previous papers. Now, we choose the hierarchy of trigonometric maps $\Phi_{N_i}^{a_N(\alpha)}(x)$, as the ensemble of maps. Then $\Phi_{N_i}^{a_N(\alpha)}(x, p_i)$-invariance of average density $\mu_{\mathrm{av}}(x,\alpha)$ implies that the average density should satisfy the following formal (PF) integral equation:

$$\mu_{\mathrm{av}}(y,\alpha,p) = \sum_{i=1}^{m} p_i \int_0^1 \delta(y - \Phi_{N_i}^{a_{N_i}(\alpha)}(x))\mu_i(x,\alpha)\mathrm{d}x. \tag{3.5}$$

Obviously, Eq. (3.5) is the generalization of Eq. (3.2) for random trigonometric maps. As shown in Ref. 7, each integral appearing on the right-hand side of (3.5) can be written as

$$\mu_i(y,\alpha) = \sum_{x_{ij}\varepsilon\Phi^{-1}(y)} \mu_i(x_{ij},\alpha)\frac{\mathrm{d}x_{ij}}{\mathrm{d}y}. \tag{3.6}$$

Using the prescription of Ref. 7 one can show that $\mu_i(x,\alpha)$, the invariant measure associated with trigonometric maps $\Phi_{N_i}^{a_{N_i}(\alpha)}(x)$, has the following form (for details refer to Appendix A):

$$\mu_i(x,\alpha) = \mu(x,\alpha) = \frac{1}{\pi}\frac{\sqrt{\alpha(1-\alpha)}}{\sqrt{x(1-x)}(\alpha + (1-2\alpha)x)}, \tag{3.7}$$

that is, the invariant measure $\mu_i(x,\alpha)$ given in (3.7) satisfies Eq. (3.6). Now, multiplying both sides of Eq. (3.6) by p_i and summing over i, we get

$$\mu_{\mathrm{av}}(x,\alpha,p) = \sum_{i=1}^{m} p_i\mu_i(x,\alpha) = \mu(x,\alpha) = \sum_{i=1}^{m} p_i \times \sum_{x_{ij}\varepsilon\Phi^{-1}(y,p_i)} \mu_i(x,\alpha)\mathrm{d}x_{ij}. \tag{3.8}$$

Therefore, the density $\mu(x,\alpha)$ given in (3.7) is the average invariant measure for ensemble of trigonometric chaotic maps $\Phi_{N_i}^{\alpha_i}(x)$ and it satisfies PF-equation (3.5), hence $\mu_{\mathrm{av}}(x,\alpha)$ is the invariant or SRB measure[17,18] of random trigonometric maps given in (2.4) defined on the interval [0,1]. Also, as relation (3.7) shows $\mu_{\mathrm{av}}(x,\alpha)=\mu_i(x,\alpha)$, hence the average invariant measure for random trigonometric maps is equal to the invariant measure of each map of the ensemble.

Also, one can show that the average density $\mu_{\mathrm{av}}(x,\alpha)$ given in (3.7) has the following asymptotic form of delta function as α goes to zero and one, respectively, that is, we have

$$\mu_{\mathrm{av}}(x,\alpha)_{\alpha\to 0}=\delta(x), \tag{3.9}$$

$$\mu_{\mathrm{av}}(x,\alpha)_{\alpha\to 1}=\delta(x-1), \tag{3.10}$$

where the first one corresponds to invariant measure associated with fixed point $x=0$ and the latter one corresponds to the fixed point $x=1$. It is straightforward to show that the random trigonometric maps are well defined for $\alpha>1$, where they have fix point $(x=1)$,[7] therefore, they possess Dirac delta function invariant measure for $\alpha>1$, too.

Similarly one can show that the average density of two-parameter (many-parameter) random trigonometric maps is the same as the average invariant measure $\mu_{\mathrm{av}}(x,\alpha)$ given in (3.7) (for details refer to Appendix A).

Finally, in the case of elliptic random chaotic maps, as shown in Ref. 10, for small values of elliptic parameter **k**, elliptic maps are topologically conjugated with trigonometric maps. Hence, for small **k** the average invariant measure of one-parameter random elliptic maps of **cn** type is also the same as the average invariant measure $\mu_{\mathrm{av}}(x,\alpha)$ given in (3.7).

IV. KOLMOGOROV–SINAI ENTROPY OF RANDOM CHAOTIC MAPS

KS entropy or metric entropy[17] measures how chaotic a dynamical system is and it is proportional to the rate at which information about the state of dynamical system is lost in the course of time or iteration. Therefore, it can also be defined as the average rate of loss of information for a discrete measurable dynamical system $(\Phi(x,p),\mu_{\mathrm{av}})$. By introducing a partition $\alpha=A_c(n_1,\ldots,n_\gamma)$ of the interval [0,1] into individual laps A_i, one can define the usual entropy associated with the partition by

$$H(\mu_{\mathrm{av}},\gamma)=-\sum_{i=1}^{n(\gamma)} m(A_c)\ln m(A_c),$$

where $m(A_c)=\int_{n\in A_i}\mu_{\mathrm{av}}(x,\alpha)\mathrm{d}x$ is the invariant measure of A_i. Defining an nth refining $\gamma(n)$ of γ:

$$\gamma^n=\bigcup_{k=0}^{n-1}(\Phi(x,p))^{-(k)}(\gamma),$$

then an entropy per unit step of refining is defined by

$$h(\mu_{\mathrm{av}},\Phi(x,p),\gamma)=\lim_{n\to\infty}\left(\frac{1}{n}H(\mu_{\mathrm{av}},\gamma)\right),$$

now, if the size of individual laps of $\gamma(N)$ tends to zero as n increases, the above-mentioned entropy is reduced to the well-known KS entropy, that is,

$$h(\mu_{\mathrm{av}},\Phi(x,p))=h(\mu_{\mathrm{av}},\Phi(x,p),\gamma).$$

KS entropy is actually a quantitative measure of the rate of information lost with the refining and it can be written as[16]

$$h(\mu_{\rm av},\Phi(x,p))=\sum_{i=1}^{m} p_i\int \mu_{\rm av}(x,\alpha)\ln\left|\frac{d\Phi_i(x)}{dx}\right|dx, \tag{4.1}$$

which is also a statistical mechanical expression of the Lyapunov Characteristic exponent, which is the mean divergence rate of two nearby orbits. The measurable random dynamical system $(\Phi(p,x),\mu_{\rm av})$ is chaotic for $h(\mu_{\rm av},\Phi(x,p))>0$ and predictive for $h(\mu_{\rm av},\Phi(x,p))=0$. Using the fact that the invariant measure for these random chaotic maps is equal to invariant measure of each map of ensemble of maps, one can show that KS entropy of these random chaotic maps is the average KS entropy of maps of ensemble, that is we have

$$h(\mu_{\rm av},\Phi(x,p))=\sum_{i=1}^{m} p_i\times h(\mu_i,\Phi_i(x)). \tag{4.2}$$

A. KS-entropy of one-parameter random trigonometric maps

With a description similar to the one that we presented in Ref. 7, one can calculate the KS entropy of hierarchy of trigonometric maps $\Phi_{N_i}^{a_{N_i}(\alpha)}(x)$, where we quote only the result as follows (for details refer to Appendix B):

$$h(\mu_i,\Phi_{N_i}^{a_{N_i}(\alpha)}(x))=\ln\left(\frac{N_i\left(\frac{1}{1-\alpha}+2\sqrt{\frac{\alpha}{1-\alpha}}\right)^{N_i-1}}{\left(\Sigma_{k=0}^{[N_i/2]}C_{2k}^{N_i}\left(\frac{\alpha}{1-\alpha}\right)^k\right)\left(\Sigma_{k=0}^{[(N_i-1)/2]}C_{2k+1}^{N_i}\left(\frac{\alpha}{1-\alpha}\right)^k\right)}\right). \tag{4.3}$$

Therefore, substituting for KS entropy of one-parameter trigonometric map in Eq. (4.1), we get the following expression for KS entropy of one-parameter random trigonometric maps $h(\mu_{\rm av},\Phi_{N_i}^{\alpha}(x,p_i))$:

$$h(\mu_{\rm av},\Phi_{N_i}^{\alpha}(x,p_i))=\sum_{i=1}^{m} p_i\ln\left(\frac{N_i\left(\frac{1}{1-\alpha}+2\sqrt{\frac{\alpha}{1-\alpha}}\right)^{N_i-1}}{\left(\Sigma_{k=0}^{[N_i/2]}C_{2k}^{N_i}\left(\frac{\alpha}{1-\alpha}\right)^k\right)\left(\Sigma_{k=0}^{[(N_i-1)/2]}C_{2k+1}^{N_i}\left(\frac{\alpha}{1-\alpha}\right)^k\right)}\right). \tag{4.4}$$

Using the asymptotic Dirac delta function form of the average density $\mu_{\rm av}(x,\alpha)$ for limiting values of $\alpha=0$, and 1 given in (3.9) and (3.10), respectively, one can show that KS entropy of one-parameter random trigonometric maps takes the following form:

$$h(\mu_{\rm av},\Phi_{N_i}^{\alpha}(x,p_i))=\sum_{i=1}^{m} p_i\ln\left|\left.\frac{d\Phi_{N_i}^{a_{N_i}(\alpha)}(x)}{dx}\right|_{x=0}\right|=\sum_{i=1}^{m} p_i\ln\left|\frac{N_i}{a_{N_i}^2(\alpha)}\right|=0 \tag{4.5}$$

as $\alpha\to 0$, and

$$h(\mu_{\rm av},\Phi_{N_i}^{\alpha}(x,p_i))=\sum_{i=1}^{m} p_i\ln\left|\left.\frac{d\Phi_{N_i}^{a_{N_i}(\alpha)}(x)}{dx}\right|_{x=1}\right|=\sum_{i=1}^{m} p_i\ln|N_i a_{N_i}^2(\alpha)| \tag{4.6}$$

as $\alpha\to 1$ and for $\alpha>1$, respectively.

It is straightforward to see that each sum on the right-hand side of (4.4) has the asymptotic form $(1-\alpha)^{1/2}$ as $\alpha\to 1_-$. Thus $h(\mu_{\rm av},\Phi_{N_i}^{\alpha}(x,p_i))$ has the following asymptotic form as ($\alpha\to 1_-$)

$$\begin{cases} h(\mu_{\rm av},\Phi_{N_i}^{\alpha\to 1^-}(x,p_i))\sim(1-\alpha)^{1/2}, \\ h(\mu_{\rm av},\Phi_{N_i}^{\alpha\to 0^+}(x,p_i))\sim(\alpha)^{1/2}, \end{cases} \tag{4.7}$$

respectively. The above asymptotic form indicates that the maps $\Phi_{N_i}^{\alpha}(x,p_i)$ belong to the same universality class which are different from the universality class of pitch fork bifurcating maps but their asymptotic behavior is similar to class of intermittent maps,[19] even though intermittency cannot occur in these maps for any values of parameter $a_N(\alpha)$, since the maps $\Phi_{N_i}^{\alpha}(x,p_i)$ and their n-composition $\Phi^{(n)}$ do not have minimum values other than zero and maximum values other than one in the interval [0,1].

B. KS entropy of many-parameter random trigonometric maps

Similarly, one can calculate KS entropy of many-parameter random chaotic maps by referring to the method described in Ref. 8 (for details refer to Appendix B):

$$h(\mu_{\rm av},\Phi_{N_i,N_j}^{\alpha_i\alpha_j}(x,p_{ij}))=\sum_{i,j} p_{ij}\times\ln\left(\frac{N_iN_j\left(1+\sqrt{\frac{1-\alpha}{\alpha}}\right)^{2(N_j-1)}(1+\sqrt{\eta_{N_j}^{\alpha_j}(\alpha)})^{2(N_i-1)}}{A_{N_j}(\alpha)B_{N_j}(\alpha)A_{N_i}(\eta_{N_j}^{\alpha_j}(\alpha))B_{N_i}(\eta_{N_j}^{\alpha_j}(\alpha))}\right). \tag{4.8}$$

With respect to the one-parameter random trigonometric chaotic maps, the numerical and theoretical calculations predict different asymptotic behavior for many-parameter random trigonometric maps, as an example of asymptotic of the composed maps ($\phi_{2,3}^{\alpha_1\alpha_2}(x)$ and $\phi_{3,2}^{\alpha_1,\acute{\alpha}_2}(x)$), the KS entropy $h(\mu_{\rm av},\Phi)$ is presented in the following:

$$\begin{aligned} h(\mu_{\rm av},\Phi)=&p\ln\left(\frac{3((1-\alpha)+\sqrt{\alpha(1-\alpha)})^4((2\alpha+1)(1-\alpha)+\alpha_2^2(3-2\alpha)\sqrt{\alpha(1-\alpha)})^2}{(1-\alpha)^3(1+2\alpha)(3-2\alpha)((1-\alpha)(1+2\alpha)^2+\alpha_2^2\alpha(3-2\alpha)^2)}\right)\\ &+(1-p)\ln\left(\frac{3((1-\alpha)+\sqrt{\alpha(1-\alpha)})^4((2\alpha+1)(1-\alpha)+\acute{\alpha}_2^2(3-2\alpha)\sqrt{\alpha(1-\alpha)})^2}{(1-\alpha)^3(1+2\alpha)(3-2\alpha)((1-\alpha)(1+2\alpha)^2+\acute{\alpha}_2^2\alpha(3-2\alpha)^2)}\right) \end{aligned} \tag{4.9}$$

with the following relation among the parameters:

$$\alpha_2^{-1}=\frac{\alpha_1(1-\alpha)(1+2\alpha)^3}{2(3-2\alpha)((1-\alpha)(1+2\alpha)-\alpha_1\alpha(3-2\alpha)^2)},$$

$$\acute{\alpha}_2^{-1}=\frac{\alpha_1(1-\alpha)(1+2\alpha)^3}{2(3-2\alpha)((1-\alpha)(1+2\alpha)-\alpha_1\alpha(3-2\alpha)^2)},$$

which is obtained from relation (2.8). Now choosing $\alpha_2=\acute{\alpha}_2$ and $\alpha=\alpha_2^{\nu}/(1+\alpha_2^{\nu})$, $0<\nu<2$, the entropy given by (4.9) reads:

$$\begin{aligned} h=&p\ln\left(\frac{3(1+\sqrt{\alpha_2^{\nu}})^4(1+3\alpha_2^{\nu})(1+\alpha_2^{\nu+2}\sqrt{\alpha_2^{\nu}})}{(3+\alpha_2^{\nu})(1+3\alpha_2^{\nu})((3\alpha_2^{\nu}+1)+\alpha_2^{\nu+2}(3+\alpha_2^{\nu})^2)}\right)\\ &+(1-p)\ln\left(\frac{3(1+\sqrt{\alpha_2^{\nu}})^4(1+3\alpha_2^{\nu})(1+\alpha_2^{\nu+2}\sqrt{\alpha_2^{\nu}})}{(3+\alpha_2^{\nu})(1+3\alpha_2^{\nu})((3\alpha_2^{\nu}+1)+\alpha_2^{\nu+2}(3+\alpha_2^{\nu})^2)}\right), \end{aligned} \tag{4.10}$$

which has the following asymptotic behavior:

$$\begin{cases} h(\mu_{\rm av},\Phi)\sim\alpha_2^{\nu/2} & \text{as} \quad \alpha_2\to 0\,(\alpha\to 0), \\ h(\mu_{\rm av},\Phi)\sim\left(\dfrac{1}{\alpha_2}\right)^{\nu/2} & \text{as} \quad \alpha_2\to\infty\,(\alpha\to 1). \end{cases}$$

The above asymptotic behaviors indicate that for an arbitrary value of $0<\nu<2$ the maps $\Phi_{2,3}^{\alpha_1,\alpha_2}(x,p_{ij})$ belong to the universality class which is different from the universality class of one-parameter trigonometric maps of $\Phi_{N_i}^{\alpha}(x,p_i)$ (2.2) or the universality class of pitch fork bifurcating maps.

C. KS entropy of one-parameter random elliptic maps

For random one-parameter elliptic maps of **cn** type, KS entropy, for small values of elliptic parameter would be equal to KS entropy of one-parameter random trigonometric chaotic maps presented in (4.3) (considering the fact that random elliptic maps are topologically conjugated with random trigonometric maps[10]).

V. LYAPUNOV EXPONENT OF RANDOM CHAOTIC MAPS

The Lyapunov exponent λ provides the simplest information about chaoticity and can be computed considering the separation of two nearby trajectories evolving in the same realization of the random process, and for random chaotic maps given in (2.3) and (5.1), it can be defined as[20]

$$\lambda(x_0)=\lim_{n\to\infty}\frac{1}{n}\sum_{k=0}^{n-1}\ln\left|\frac{d\Phi(x_k,p)}{dx}\right|, \tag{5.1}$$

where

$$x_k=\overbrace{\Phi_N\circ\Phi_N\circ\ldots\circ\Phi_N^k(x_0)}.$$

It is obvious that its negative values indicate that the system is in fix point (attractor) regime, while its positive values indicate that the system is measurable (the Invariant measure given in (3.9, 12)).[20] Also, the Lyapunov number is independent of initial point, provided that the motion inside the invariant manifold is ergodic, thus $\lambda(x_0)$ characterizes the invariant manifold of random map as a whole. Birkhof ergodic[21] theorem implies the equality of KS entropy and Lyapunov number, of the measurable map like $\Phi(x,p)$,

$$h(\mu_{\rm av},\Phi(x,p))=\lambda(x_0).$$

Also, comparing KS entropy of these maps with their Lyapunov exponent confirms this prediction [see Figs. 2(a), 2(b), and 3]. In chaotic region, random chaotic maps are ergodic as Birkhof ergodic theorem predicts. In the nonchaotic region of the parameter, the Lyapunov characteristic exponent is negative definite, since in this region, we have only single period fixed points without bifurcation.

VI. CONCLUSION

In this paper we have discussed the dynamical characterization of systems whose evolution is described by random chaotic maps. We have studied the application of Perron–Frobenius operator to the analysis of the dynamical behavior of random dynamical systems in order to derive the invariant measure of the system. Again, this interesting property is due to the existence of invariant measure for a region of the parameter space of these maps.

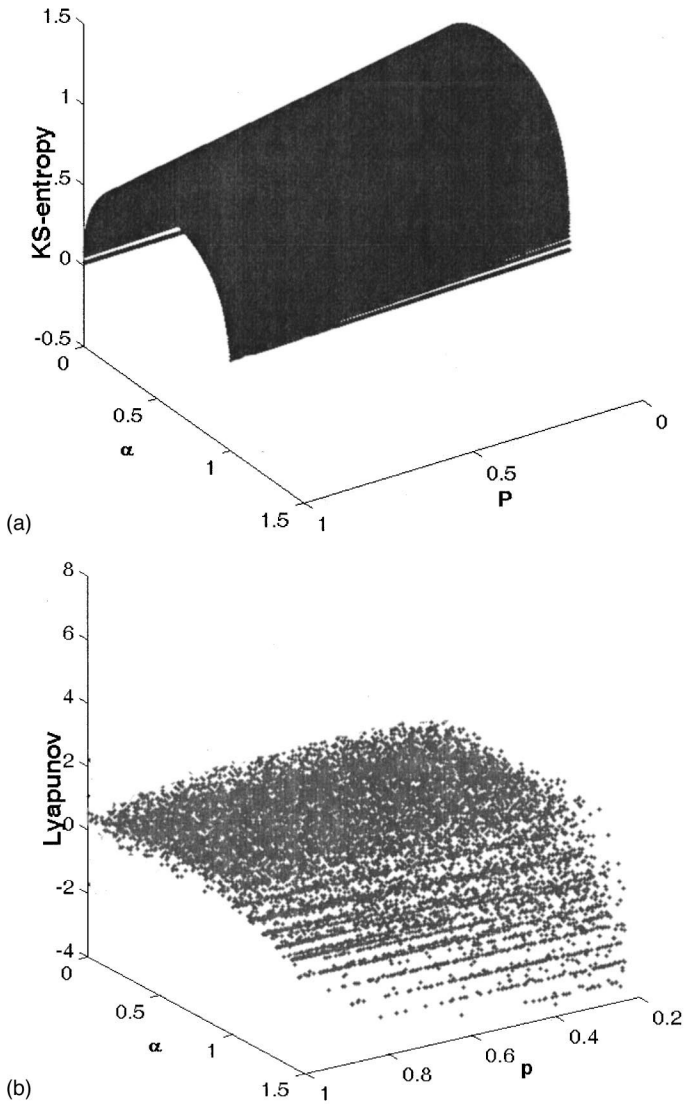

FIG. 2. (a) The variation of KS entropy of one-parameter random trigonometric map for ensemble of ($\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_3^{a_3(\alpha)}(x)$) in terms of parameters α and p. (b) The variation of Lyapunov characteristic exponent of one-parameter random trigonometric map for ensemble of ($\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_3^{a_3(\alpha)}(x)$) in term of parameters α and p.

APPENDIX A: DETAIL OF DERIVATION OF INVARIANT MEASURE

In this appendix we try to obtain the invariant measure of maps $\Phi_3^{a_3(\alpha)}(x)$ and $\Phi_{2,2}^{\alpha_1,\alpha_2}(x)$.
(a) First denoting $\Phi_3^{a_3(\alpha)}(x)$ by y, we can write

$$16(a_3^2(\alpha)(y-1)-y)x^3-24(a_3^2(\alpha)(y-1)-y)x^2+9(a_3^2(\alpha)(y-1)-y)x+y=0,$$

where

$$a_3(\alpha)=\frac{2\alpha+1}{3-2\alpha}$$

and solving it for x, we get

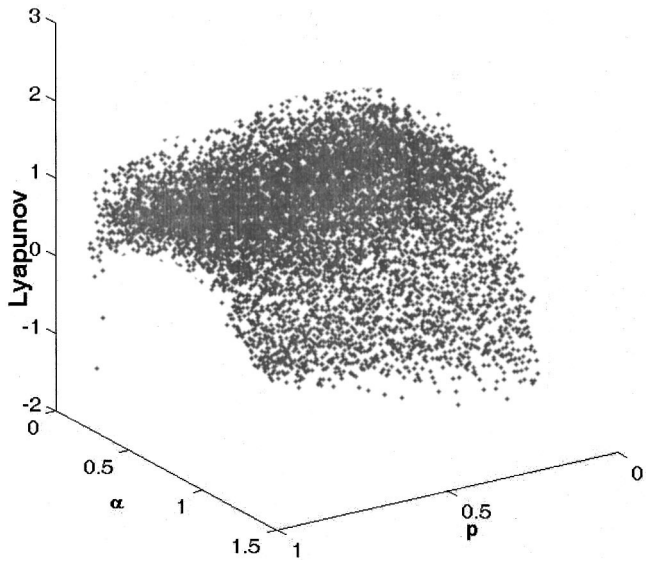

FIG. 3. The variation of KS entropy of one-parameter random elliptic maps for ensemble of ($\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_3^{a_3(\alpha)}(x)$) in terms of parameters α and p.

$$\begin{cases} x_k=\dfrac{1}{2}\left(1+\cos\left(\dfrac{\arcsin(2z-1)+2k\pi}{3}-\dfrac{3\pi}{2}\right)\right), \quad k=1,2,3, \\ z=\dfrac{y}{a_3^2(\alpha)+(1+a_3^2(\alpha))y}. \end{cases}$$

Then, taking the derivative of x_k with respect to y, we obtain

$$\left|\frac{dx_k}{dy}\right|=\frac{\sqrt{x_k(1-x_k)}}{3a_3(\alpha)\sqrt{y(1-y)}}(a_3^2(\alpha)+(1-a_3^2(\alpha))y), \quad k=1,2,3,$$

therefore, FP equation reads (3.6)

$$\mu(y,\alpha)=\frac{(a_3^2(\alpha)+(1-a_3^2(\alpha))y)}{3a_3^2(\alpha)\sqrt{y(1-y)}}\sum_{k=1}^{3}\sqrt{x_k(1-x_k)}\mu(x_k,\alpha). \tag{A1}$$

Now, by suggesting the following form for $\mu_{\Phi_3^{a_3(\alpha)}}(x)$,

$$\mu(x,\alpha)=\frac{1}{\sqrt{x(1-x)}(a+bx)}, \tag{A2}$$

the last term in (A1) can be written as

$$\sum_{k=0}^{3}\sqrt{x_x(1-x_k)}\mu(x_k,\alpha)=\frac{(3a^2+2ab(x_1+x_2+x_3)+b^2(x_1x_2+x_1x_2+x_2x_3))}{(a^3+a^2b(x_1+x2+x_3)+ab^2(x_1x_2+x_1x_3+x_2x_3)+b^3x_1x_2x_3)}.$$

Using relation (A1), we can write Shure's invariant polynomials of roots x_k, $k=1,2,3$ in terms of y:

$$\begin{cases} x_1+x_2+x_3=\frac{3}{2}, \\ x_1x_2+x_1x_3+x_2x_3=\frac{9}{16}, \\ x_1x_2x_3=\dfrac{z}{16}. \end{cases}$$

Then subsisting the results that obtained in (A1) we get

$$a+b=1, \quad a=\frac{\alpha}{1-\alpha}, \quad b=\frac{1-2\alpha}{1-\alpha}, \tag{A3}$$

which leads to the invariant measure (3.7).

(b) Also denoting $\Phi_2^{a_2(\alpha_2)}(x)$ by y and $\Phi_2^{a_2(\alpha_1)}(y)$ by z, respectively, we can write

$$\begin{cases} y=\Phi_2^{a_2(\alpha_2)}(x), \\ z=\Phi_2^{a_2(\alpha_1)}(y)=\Phi_{2,2}^{\alpha_1,\alpha_2}(x), \end{cases}$$

now, inverting the above-given equations, we get

$$x_{\pm,\pm}=\frac{1}{2}\left(1\pm\sqrt{\frac{a_2^2(\alpha_2)(1-y_\pm)}{a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_\pm}}\right), \quad y_\pm=\frac{1}{2}\left(1\pm\sqrt{\frac{a_2^2(\alpha_1)(1-z)}{a_2^2(\alpha_1)+(1-a_2^2(\alpha_1))z}}\right).$$

Then, taking the derivative of $x_{\pm,\pm}$ with respect to z, we obtain

$$\frac{\mathrm{d}x_{\pm,\pm}}{\mathrm{d}z}=\frac{\mathrm{d}x_{\pm,\pm}}{\mathrm{d}y_\pm}\frac{\mathrm{d}y_\pm}{\mathrm{d}z}=\frac{a_2(\alpha_1)}{4}\frac{a_2(\alpha_2)}{4}\frac{1}{\sqrt{(1-y_\pm)(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2)y_\pm)^3}}$$

$$\times\frac{1}{\sqrt{(1-z)(a_2^2(\alpha_1)+(1-a_2^2(\alpha_1)z)^3}}$$

and subsisting it in (3.6), we get

$$\mu(z,\alpha)=\sum_{\pm,\pm}\frac{\mathrm{d}x_{\pm,\pm}}{\mathrm{d}z}\mu(x_{\pm,\pm},\alpha).$$

Again using the anzatz (A2) for invariant measure $\mu(x_{\pm,\pm},\alpha)$, we get

$$\mu(z,\alpha)=\sum_{\pm}\frac{a_2(\alpha_1)}{4}\frac{a_2(\alpha_2)}{4}$$

$$\times\frac{1}{\sqrt{(1-z)(a_2^2(\alpha_1)+(1-a_2^2(\alpha_1))z)^3}}\frac{1}{\sqrt{(1-y_\pm)(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_\pm)^3}}$$

$$\times\sum_{\pm}\frac{1}{\sqrt{x_{\pm,\pm}(1-x_{\pm,\pm})}(a+bx_{\pm,\pm})}. \tag{A4}$$

Now, the last expression in (A4) can be written as

$$\sum_{\pm}\frac{1}{\sqrt{x_{\pm,\pm}(1-x_{\pm,\pm})}(a+bx_{\pm,\pm})}$$

$$=\frac{1}{\sqrt{(1-y_{\pm})}}\frac{2a+b(x_{\pm,-}+x_{\pm,+})}{(a^2+ab(x_{\pm,-}+x_{\pm,+})+b^2x_{\pm,-}x_{\pm,+})}$$

$$=\frac{1}{y_{\pm}(1-y_{\pm})}\frac{4(2a+b)}{4(a^2+ab)(a_2^2(\alpha_2)+(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_{\pm})+b^2y_{\pm})},$$

where we have used the following identity for roots $x_{\pm,+}$ and $x_{\pm,-}$:

$$\begin{cases} x_{\pm,-}+x_{\pm,+}=1, \\ x_{\pm,-}\times x_{\pm,+}=\dfrac{y_{\pm}}{4(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_{\pm})}. \end{cases}$$

Therefore, we have

$$\mu(z,\alpha)=\sum_{\pm}\frac{a_2(\alpha_1)}{4}\frac{a_2(\alpha_2)}{4}\frac{1}{\sqrt{(1-z)(a_2^2(\alpha_1)+(1-a_2^2(\alpha_1))z)^3}}$$
$$\times\frac{1}{y_{\pm}(1-y_{\pm})}\frac{1}{a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_{\pm}}$$
$$\times\frac{4(2a+b)}{4(a^2+ab)(a_2^2(\alpha_2)+(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y_{\pm})+b^2y_{\pm})}$$

and substituting for sum and product of root $y_{\pm}$, we get

$$a+b=1,\quad a=\frac{\alpha}{1-\alpha},\quad b=\frac{1-2\alpha}{1-\alpha}.$$

APPENDIX B: CALCULATION OF ENTROPY OF THE MAPS $\Phi_2^{a_2(\alpha)}(x)$ AND $\Phi_{2,2}^{\alpha_1,\alpha_2}(x)$

In this appendix we calculate the entropy of the maps $\Phi_2^{a_2(\alpha)}(x)$ and $\Phi_{2,2}^{\alpha_1,\alpha_2}(x)$.

(a) Using expression (4.1), we have

$$h(\mu,\Phi_2^{a_2(\alpha)}(x))=\frac{1}{\pi}\int_0^{\infty}\mathrm{d}x\frac{\sqrt{\alpha(1-\alpha)}}{\sqrt{x(1-x)}(\alpha+(1-2\alpha)x)}\ln\left|\frac{1}{a_2^2(\alpha)}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{4a_2^2(\alpha)x(1-x)}{1+4a_2^2(\alpha)x(1-x)}\right)\right|$$

or

$$=\frac{1}{\pi}\int_0^{\infty}\mathrm{d}x\frac{\sqrt{\alpha(1-\alpha)}}{\sqrt{x(1-x)}(\alpha+(1-2\alpha)x)}$$
$$\times[\ln|4a_2^2(\alpha)(1-2x)|-2\ln|4x(x-1)(a_2^2(\alpha)-1)-1|].$$

Now, making the following change of variable

$$x=\frac{\alpha(1+\cos\theta)}{(1+(2\alpha-1)\cos\theta)},$$

we get

$$h(\mu,\Phi_2^{a_2(\alpha)}(x))=\ln(1+2\sqrt{\alpha(1-\alpha)}), \tag{B1}$$

where in the evaluation of above integral we have used the following integral:

$$\frac{1}{\pi}\int_0^{2\pi} d\theta \ln(A+B\cos\theta+C\cos 2\theta)=2\ln\Delta,$$

$$\Delta=\frac{1}{\pi}\left(\frac{\sqrt{A-3C+\sqrt{(A+C)^2-B^2}}}{2}+\frac{\sqrt{A+B+C}-\sqrt{A-B+C}}{2}\right).$$

The above integral has been evaluated by using the well-known mean values theorem of analytic function

$$\frac{1}{\pi}\int_0^{2\pi} d\theta \ln|f(z_0+R\exp i\theta)|=|f(z_0)|$$

by choosing $f(z)=\alpha+\beta\exp i\theta+\gamma\exp 2i\theta$.

(b) Similarly using (4.1), we obtain the following expression for the entropy of the map $\Phi_{2,2}^{\alpha_1,\alpha_2}(x)$:

$$h(\mu,\Phi_{2,2}^{\alpha_1,\alpha_2}(x))=\frac{1}{\pi}\int_0^{\infty} dx\,\mu(x,\alpha)\ln\left|\frac{d}{dx}\Phi_{2,2}^{\alpha_1,\alpha_2}(x)\right|$$

or

$$h(\mu,\Phi_{2,2}^{\alpha_1,\alpha_2}(x))=\frac{1}{\pi}\int_0^{\infty} dx\,\mu(x,\alpha)\left[\ln\left|\frac{d}{dx}\Phi_2^{a_2(\alpha_2)}(x)\right|+\ln\left|\frac{d}{dy}\Phi_2^{a_2(\alpha_1)}(y)\right|\right]. \tag{B2}$$

In order to calculate the last integral in (B2), first we make the following change of variable by inverting $\Phi_2^{a_2(\alpha_2)}(x)$,

$$x_{\pm}=\frac{1}{2}\left(1\pm\sqrt{\frac{a_2^2(\alpha_2)(1-y)}{a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y}}\right), \tag{B3}$$

then the last term in (B2) reduces to

$$=\frac{1}{\pi}\sum_{k=\pm}\int_{x_k^i}^{x_k^f} dx_k\frac{\alpha\sqrt{1-\alpha}}{\sqrt{x_k(1-x_k)}(\alpha+(1-2\alpha)x_k)}\ln\left|\frac{d}{dy}\Phi_2^{a_2(\alpha_1)}(y)\right|, \tag{B4}$$

where x_k^i and x_k^f denote the initial and end point of kth branch of the inversion function ($k=+$ and $k=-$). Then, taking the derivative of $x_{\pm}$ with respect to y, we obtain

$$\frac{dx_{\pm}}{dy}=\frac{a_2(\alpha_2)}{4}\cdot\frac{1}{\sqrt{(1-y)(a_2^2(\alpha_2)+(1-a_2^2(\alpha_2))y)^3}}.$$

Now, inserting the derivative of $x_{\pm}$ with respect to y in relation (B4) and changing the order of sum and integrating, we get

$$=\frac{1}{4\pi}\int_0^\infty dy\,\frac{a_2(\alpha_1)}{\sqrt{(1-y)(a_2^2(\alpha_2)+(1+a_2^2(\alpha_2)y))^3}}$$

$$\times\ln\left|\frac{d}{dy}\Phi_2^{a_2(\alpha_1)}(y)\right|\sum_{k=\pm}\frac{\sqrt{\alpha(1-\alpha)}}{\sqrt{x_k(1-x_k)}(\alpha+(1-2\alpha)x_k)}.$$

Using relation (A5), we can write

$$\sum_{k=\pm}\frac{\sqrt{\alpha(1-\alpha)}}{\sqrt{x_k(1-x_k)}(\alpha+(1-2\alpha)x_k)}=\frac{\sqrt{a_2^2(\alpha_1)+(1-a_2^2(\alpha_1))y}}{\sqrt{y}\sqrt{\alpha(1-\alpha)}}$$

$$\cdot\frac{a_2^2(a_2(\alpha_1))+(1-a_2^2(\alpha_1))y}{a_2^2(\alpha_1)+(1-a_2^2(\alpha_1))y+\dfrac{(1-2\alpha)}{(1-\alpha)^2}y},$$

therefore, (B4) reduces to

$$=\frac{1}{\pi}\int_0^\infty dy\,\frac{a_2(\alpha_1)}{\sqrt{y(1-y)}}\,\frac{\sqrt{\alpha(1-\alpha)}}{(4\alpha(1-\alpha)(a_2^2(\alpha_2)+(1-\alpha_2^2y)+y(1-2\alpha)^2)}\ln\left|\frac{d}{dy}\Phi_2^{a_2(\alpha_1)}(y)\right|$$

$$=\ln\left(\frac{2\sqrt{\alpha(1-\alpha)}+a_2(\alpha_2)}{4\alpha(1-\alpha)+a_2^2(\alpha_2)}\right).$$

Finally, we get

$$h(\mu,\phi_{2,2}^{\alpha_1,\alpha_2}(x))=\ln\left(\frac{(1+2\sqrt{\alpha(1-\alpha)})(a_2(\alpha_2)+2\sqrt{\alpha(1-\alpha)})}{a_2(\alpha_1)+4\alpha(1-\alpha)}\right). \tag{B5}$$

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Tau functions and residues

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(Received 13 May 2003; accepted 20 August 2003)

We consider the residues of Laurent series of several variables as well as the residues of pseudodifferential operators of several variables and establish relations between such residues and tau functions associated to pseudodifferential operators of several variables. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1621055]

I. INTRODUCTION

Integrable nonlinear partial differential equations have been studied in numerous papers during the past few decades, and they include many well-known equations in mathematical physics such as the Korteweg–de Vries (KdV) equation, Kadomtsev–Petviashvili (KP) equation, and nonlinear Schrödinger equation. Such equations are also known as soliton equations because they possess solitary waves, or solitons, as solutions.

One way of systematically producing a large number of soliton equations is by using Lax equations, which describe certain compatibility conditions for pairs of differential or pseudodifferential operators. Indeed, a collection of soliton equations called the KP-hierarchy is determined by a system of Lax equations. Thus, solutions of Lax equations determine solutions of the associated soliton equations. One of the important contributions of the Japanese school was the interpretation of solutions of Lax equations in terms of tau functions.[1] Tau functions are closely related to Baker functions, which can be written as quotients of values of tau functions. Lax equations can also be interpreted as certain bilinear identities involving residues and Baker functions.

Pseudodifferential operators of one variable are formal Laurent series in the formal inverse ∂^{-1} of the differentiation operator $\partial = d/dx$ with respect to the single variable x, and they are essential components in the construction of Lax equations. For this reason pseudodifferential operators have played a major role in the theory of soliton equations. In a recent paper, Parshin[2] studied pseudodifferential operators of several variables by considering formal Laurent series in the formal inverses of $\partial_1,\ldots,\partial_n$ with $\partial_i = d/dx_i$ for $1 \leqslant i \leqslant n$. Among other things, he introduced a generalization of the KP-hierarchy. More specifically, he constructed Lax equations, zero curvature (or Zakharov–Shabat) equations, and Sato–Wilson equations by using pseudodifferential operators of several variables. He also discussed a relation between this generalized KP-hierarchy and some natural Poisson structure on the space of pseudodifferential operators of several variables. Some of Parshin's results were extended further in Refs. 3 and 4. For example, in Ref. 3 Baker functions associated to the Lax equations of Parshin were introduced and were shown to satisfy some of the well-known properties of the usual Baker functions. Tau functions associated to pseudodifferential operators of several variables and their connections with Baker functions were studied in Ref. 4.

In this article we consider the residues of Laurent series of several variables as well as the residues of pseudodifferential operators of several variables. We establish relations between such residues and tau functions associated to pseudodifferential operators of several variables.

II. PSEUDODIFFERENTIAL OPERATORS

Throughout this article we fix a positive integer n, and consider the variables $x_1,\ldots,x_n$ as well as the corresponding differentiation operators

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$$\partial_1=\frac{\partial}{\partial x_1},\quad \ldots,\quad \partial_n=\frac{\partial}{\partial x_n}.$$

In this section we review pseudodifferential operators expressed in terms of $\partial_1,\ldots,\partial_n$ and the associated Lax equations following Parshin.[2]

We first describe the usual multi-index notation, which will be used often in this article. Given $\alpha=(\alpha_1,\ldots,\alpha_n)\in\mathbb{Z}^n$, we have

$$\partial^\alpha=\partial_1^{\alpha_1}\cdots\partial_n^{\alpha_n},\quad |\alpha|=\alpha_1+\cdots+\alpha_n,$$

with $\partial=(\partial_1,\ldots,\partial_n)$. We also write $\alpha\geqslant\beta$ for $\beta=(\beta_1,\ldots,\beta_n)\in\mathbb{Z}^n$ if $\alpha_i\geqslant\beta_i$ for each i, and use $\mathbf{0}$ and $\mathbf{1}$ to denote the elements (0,...,0) and (1,...,1) in $\mathbb{Z}^n$, respectively.

Let $\mathbb{C}((x_1))\cdots((x_n))$ be the field of iterated Laurent series with respect to the variables $x_1,\ldots,x_n$ over $\mathbb{C}$, and denote by P the space of iterated formal Laurent series

$$P=\mathbb{C}((x_1))\cdots((x_n))((\partial_1^{-1}))\cdots((\partial_n^{-1}))$$

in the formal inverses of $\partial_1,\ldots,\partial_n$ over the field $\mathbb{C}((x_1))\cdots((x_n))$. Thus, for example, an element $\psi\in P$ can be written in the form

$$\psi=\sum_{\alpha\leqslant\nu} f_\alpha(x)\partial^\alpha \tag{1}$$

for some $\nu\in\mathbb{Z}^n$, where $x=(x_1,\ldots,x_n)$. The Leibniz rule determines a multiplication operation on P given by

$$\left(\sum_\alpha f_\alpha(x)\partial^\alpha\right)\left(\sum_\beta h_\beta(x)\partial^\beta\right)=\sum_{\alpha,\beta}\sum_{\gamma\geqslant\mathbf{0}}\binom{\alpha}{\gamma}f_\alpha(x)(\partial^\gamma h_\beta(x))\partial^{\alpha+\beta-\gamma}, \tag{2}$$

where $\binom{\alpha}{\gamma}=\binom{\alpha_1}{\gamma_1}\cdots\binom{\alpha_n}{\gamma_n}$ for elements $\alpha=(\alpha_1,\ldots,\alpha_n)$ and $\gamma=(\gamma_1,\ldots,\gamma_n)$ of $\mathbb{Z}^n$ with $\gamma\geqslant\mathbf{0}$.

We now set

$$\mathbb{Z}_+^n=\{\alpha\in\mathbb{Z}^n\,|\,\alpha\geqslant\mathbf{0},\,|\alpha|\geqslant 1\},$$

and assume that each coefficient $f_\alpha(x)$ in (1) is a function of the infinitely many variables $\{t_\alpha|\,\alpha\in\mathbb{Z}_+^n\}$. We allow this set to include the variables $x_1,\ldots,x_n$ by using the identities

$$t_{\mathbf{e_1}}=x_1,\ldots,t_{\mathbf{e_n}}=x_n, \tag{3}$$

where $\mathbf{e_1}=(1,0,\ldots,0),\ldots,\ \mathbf{e_n}=(0,\ldots,0,1)$ are the standard basis elements for the $\mathbb{Z}$-module $\mathbb{Z}^n$. Thus we may write the element $\psi\in P$ in (1) in the form

$$\psi=\sum_{\alpha\leqslant\nu} f_\alpha(t)\partial^\alpha$$

with $t=(t_\alpha)_{\alpha\in\mathbb{Z}_+^n}$. If the same element ψ can be written in the form

$$\psi=\sum_{i=-\infty}^{\nu_n} a_i\partial_n^i=\sum_{i=-\infty}^{\nu_n} a_i(t;\partial_1,\ldots,\partial_{n-1})\partial_n^i$$

with $\nu_n\geqslant 0$, we set

$$\psi_+ = \sum_{i=0}^{\nu_n} a_i \partial_n^i, \quad \psi_- = \psi - \psi_+ = \sum_{i=-\infty}^{-1} a_i \partial_n^i;$$

if $\nu_n < 0$, we set $\psi_+ = 0$ and $\psi_- = \psi$. Thus we have $\psi = \psi_+ + \psi_-$ for all $\psi \in P$, and therefore P has a decomposition of the form

$$P = P_+ + P_-, \tag{4}$$

where P_+ is the set of elements of P of the form $\Sigma_{i=0}^{m} a_i \partial_n^i$ for some non-negative integer m, and P_- is the set of elements of the form $\Sigma_{j=-\infty}^{k} b_j \partial_n^j$ with $k < 0$.

Let P^n be the Cartesian product of n copies of P, and consider an element $L = (L_1, \ldots, L_n) \in P^n$. Given $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{Z}_+^n$, we set

$$[L_+^\alpha, L] = L_+^\alpha L - L L_+^\alpha = (L_+^\alpha L_1 - L_1 L_+^\alpha, \ldots, L_+^\alpha L_n - L_n L_+^\alpha) = ([L_+^\alpha, L_1], \ldots, [L_+^\alpha, L_n]) \in P^n \tag{5}$$

and $\partial_\alpha = \partial_{t_\alpha} = \partial / \partial t_\alpha$, so that

$$\partial_\alpha L = (\partial_\alpha L_1, \ldots, \partial_\alpha L_n). \tag{6}$$

Then the generalized Lax equation is given by

$$\partial_\alpha L = [L_+^\alpha, L] \tag{7}$$

for all $\alpha \in \mathbb{Z}_+^n$. By (5) and (6) we see that (7) is equivalent to the system of equations

$$\frac{\partial L_i}{\partial t_\alpha} = [L_+^\alpha, L_i] \tag{8}$$

for $1 \leqslant i \leqslant n$. We now consider the subset P_0^n of P^n defined by

$$P_0^n = \{(L_1, \ldots, L_n) \in P^n \mid [L_i, L_j] = 0,\ 1 \leqslant i, j \leqslant n\}, \tag{9}$$

where $[L_i, L_j] = L_i L_j - L_j L_i$.

Proposition II.1: (i) Let $L_i \in \partial_i + P_-$ for each i with $1 \leqslant i \leqslant n$. Then the operator $L = (L_1, \ldots, L_n) \in P^n$ belongs to P_0^n if and only if there is an element $\phi \in 1 + P_-$ such that

$$L_i = \phi \partial_i \phi^{-1}$$

for each $i \in \{1, \ldots, n\}$, that is, $L = \phi \partial \phi^{-1}$.

(ii) Let ϕ be an element of $1 + P_-$ satisfying the condition

$$\partial_\alpha \phi = -(\phi \partial^\alpha \phi^{-1})_- \phi \tag{10}$$

for $\alpha \in \mathbb{Z}_+^n$. Then the operator

$$L = \phi \partial \phi^{-1} = (\phi \partial_1 \phi^{-1}, \ldots, \phi \partial_n \phi^{-1}) \in P^n \tag{11}$$

satisfies the Lax equation (7).

(iii) If L is an element of P_0^n satisfying the Lax equation (7) for all $\alpha \in \mathbb{Z}_+^n$, then we have

$$\frac{\partial L_+^\beta}{\partial t_\alpha} - \frac{\partial L_+^\alpha}{\partial t_\beta} = [L_+^\alpha, L_+^\beta] \tag{12}$$

for all $\alpha, \beta \in \mathbb{Z}_+^n$.

Proof: See Theorem 1 and Proposition 4 in Ref. 2. □

Example II.2: We consider an element $L=(L_1,L_2)\in P_0^2$ *satisfying (12) for* $\alpha=(1,1)$ *and* $\beta=(1,2)$, *where the pseudodifferential operators* L_1,L_2 *are given by*

$$\begin{aligned} L_1&=\partial_1+a\partial_2^{-1}+b\partial_2^{-2}+O(\partial_2^{-3}),\\ L_2&=\partial_2+c\partial_1\partial_2^{-1}+d\partial_2^{-1}+e\partial_2^{-2}+O(\partial_2^{-3}) \end{aligned} \tag{13}$$

for some functions a, b, c, d, *and* e. *We shall determine a system of partial differential equations satisfied by* a, b, c, d, *and* e. *If* f *is a function, we shall write* f_x *and* f_y *for* $\partial_1 f$ *and* $\partial_2 f$, *respectively. Using the multiplication rule (2), we have*

$$\begin{aligned} L_1L_2&=\partial_1\partial_2+a+c\partial_1^2\partial_2^{-1}+(c_x+d)\partial_1\partial_2^{-1}+(b+d_x)\partial_2^{-1}\\ &\quad+(ac+e)\partial_1\partial_2^{-2}+(ad+e_x)\partial_2^{-2}+O(\partial_2^{-3}),\\ L_2L_1&=\partial_1\partial_2+a+a_y\partial_2^{-1}+b\partial_2^{-1}+b_y\partial_2^{-2}+c\partial_1(\partial_1\partial_2^{-1}+a\partial_2^{-2})\\ &\quad+d(\partial_1\partial_2^{-1}+a\partial_2^{-2})+e\partial_1\partial_2^{-2}+O(\partial_2^{-3})\\ &=\partial_1\partial_2+a+c\partial_1^2\partial_2^{-1}+d\partial_1\partial_2^{-1}+(a_y+b)\partial_2^{-1}\\ &\quad+(ac+e)\partial_1\partial_2^{-2}+(ad+a_xc+b_y)\partial_2^{-2}+O(\partial_2^{-3}). \end{aligned} \tag{14}$$

From these relations and the condition $[L_1,L_2]=L_1L_2-L_2L_1=0$ *in (9) we obtain*

$$c_x=0,\quad a_y=d_x,\quad a_xc+b_y=e_x. \tag{15}$$

From (14) we have

$$L_+^\alpha=(L_1L_2)_+=\partial_1\partial_2+a. \tag{16}$$

On the other hand, using (13) and (14), we obtain

$$L_+^\beta=(L_1L_2^2)_+=((L_1L_2)L_2)_+=\partial_1\partial_2^2+a\partial_2+2c\partial_1^2+2d\partial_1+b+2d_x. \tag{17}$$

Keeping in mind the condition $c_x=0$ *in (15), we have*

$$\begin{aligned} L_+^\alpha L_+^\beta&=\partial_1^2\partial_2^3+\partial_1(a\partial_2^2+a_y\partial_2)+2\partial_1(c\partial_1^2\partial_2+c_y\partial_1^2)+2\partial_1(d\partial_1\partial_2+d_y\partial_1)+\partial_1(b\partial_2+b_y)\\ &\quad+2\partial_1(d_x\partial_2+d_{xy})+a(\partial_1\partial_2^2+a\partial_2+2c\partial_1^2+2d\partial_1+b+2d_x)\\ &=\partial_1^2\partial_2^3+2a\partial_1\partial_2^2+a_x\partial_2^2+2c\partial_1^3\partial_2+2d\partial_1^2\partial_2+(a_y+b+4d_x)\partial_1\partial_2\\ &\quad+(a^2+a_{yx}+b_x+2d_{xx})\partial_2+2c_y\partial_1^3+(2d_y+2ac)\partial_1^2\\ &\quad+(2ad+b_y+4d_{yx})\partial_1+b_{yx}+2d_{xyx}+ab+2ad_x. \end{aligned}$$

Similarly, we have

$$\begin{aligned} L_+^\beta L_+^\alpha&=\partial_1^2\partial_2^3+\partial_1(a\partial_2^2+2a_y\partial_2+a_{yy})+a\partial_1\partial_2^2+a^2\partial_2+aa_y+2c\partial_1^3\partial_2+2c(a\partial_1^2+2a_x\partial_1+a_{xx})\\ &\quad+2d\partial_1^2\partial_2+2ad\partial_1+2a_xd+(b+2d_x)\partial_1\partial_2+ab+2ad_x\\ &=\partial_1^2\partial_2^3+2a\partial_1\partial_2^2+a_x\partial_2^2+2c\partial_1^3\partial_2+2d\partial_1^2\partial_2+(2a_y+b+2d_x)\partial_1\partial_2+(a^2+2a_{yx})\partial_2\\ &\quad+2ac\partial_1^2+(2ad+4a_xc+a_{yy})\partial_1+aa_y+2a_{xx}c+2a_xd+ab+2ad_x+a_{yyx}. \end{aligned}$$

Thus we obtain

$$\begin{aligned} L_+^\alpha L_+^\beta-L_+^\beta L_+^\alpha&=(2d_x-a_y)\partial_1\partial_2+(b_x+2d_{xx}-a_{yx})\partial_2+2c_y\partial_1^3-2d_y\partial_1^2\\ &\quad+(4d_{yx}+b_y-4a_xc-a_{yy})\partial_1+b_{yx}+2d_{xyx}-aa_y-2a_{xx}c-2a_xd-a_{yyx}. \end{aligned} \tag{18}$$

On the other hand, if we let $t_\alpha = s$ *and* $t_\beta = t$, *by (16) and (17) the left hand side of (12) can be written as*

$$\frac{\partial L_+^\beta}{\partial s} - \frac{\partial L_+^\alpha}{\partial t} = a_s\partial_2 + 2c_s\partial_1^2 + 2d_s\partial_1 + b_s + 2d_{xs} - a_t. \tag{19}$$

Thus by comparing (18) and (19) we obtain

$$\begin{gathered} a_y = 2d_x, \quad a_s + a_{yx} = b_x + 2d_{xx}, \quad c_y = 0, \\ c_s + d_y = 0, \quad a_{yy} + 2d_s + 4a_x c = b_y + 4d_{yx}, \\ a_t + b_{yx} + 2d_{xyx} = aa_y + 2a_{xx}c + 2a_x d + a_{yyx} + b_s + 2d_{xs}. \end{gathered} \tag{20}$$

Thus we see that the functions a, b, c *and* d *satisfy the system of partial differential equations (15) and (20).*

III. BAKER AND TAU FUNCTIONS

In this section we review Baker functions and tau functions associated to pseudodifferential operators of several variables discussed in Sec. II. More details can be found in Refs. 3 and 4.

First, in addition to the infinite set $\{t_\alpha | \alpha \in \mathbb{Z}_+^n\}$ of variables considered in Sec. II, we need to introduce an additional set of complex variables $z_1, \ldots, z_n$. We then consider the formal series $\xi(t,z)$ defined by

$$\xi(t,z) = \sum_{\alpha \in \mathbb{Z}_+^n} t_\alpha z^\alpha, \tag{21}$$

where $z = (z_1, \ldots, z_n)$ and $z^\alpha = z_1^{\alpha_1} \cdots z_n^{\alpha_n}$ for $\alpha = (\alpha_1, \ldots, \alpha_n)$. If $\phi \in 1 + P_-$ is as in Sec. II satisfying (10), we define the associated *Baker function* $w(t,z)$ by

$$w(t,z) = \phi e^{\xi(t,z)}. \tag{22}$$

Since $x_i = t_{\mathbf{e_i}}$ for $1 \leqslant i \leqslant n$ by (3), we see that

$$\partial_i e^{\xi(t,z)} = \frac{\partial}{\partial x_i} e^{\xi(t,z)} = \frac{\partial}{\partial t_{\mathbf{e_i}}} e^{\xi(t,z)} = z^{\mathbf{e_i}} e^{\xi(t,z)} = z_i e^{\xi(t,z)}.$$

Thus, if $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{Z}_+^n$, we have

$$\partial^\alpha e^{\xi(t,z)} = \partial_1^{\alpha_1} \cdots \partial_n^{\alpha_n} e^{\xi(t,z)} = \partial_{\mathbf{e_1}}^{\alpha_1} \cdots \partial_{\mathbf{e_n}}^{\alpha_n} e^{\xi(t,z)} = z_1^{\alpha_1} \cdots z_n^{\alpha_n} e^{\xi(t,z)} = z^\alpha e^{\xi(t,z)}.$$

Hence, if $\phi = 1 + \Sigma_\alpha a_\alpha(t)\partial^\alpha \in 1 + P_-$, then the Baker function in (22) can be written in the form

$$w(t,z) = \hat{w}(t,z) e^{\xi(t,z)}, \tag{23}$$

where $\hat{w}(t,z)$ is a formal power series in $z_1, \ldots, z_n$ given by

$$\hat{w}(t,z) = 1 + \sum_\alpha a_\alpha(t) z^\alpha. \tag{24}$$

If $L = (L_1, \ldots, L_n) = \phi\partial\phi^{-1} \in P^n$ is an element associated to $\phi \in 1 + P_-$ satisfying (10) as in (11), then the Baker function $w = w(t,z)$ given by (22) satisfies $Lw = zw$, that is, $L_i w = z_i w$ for each $i \in \{1, \ldots, n\}$ (see Lemma 3.1 in Ref. 3). In addition, it can also be shown that

$$\partial_\alpha w = L_+^\alpha w \tag{25}$$

for all $\alpha \in \mathbb{Z}_+^n$ (see Lemma 3.2 in Ref. 3).

In order to discuss tau functions, for each vector $s=(s_1,\ldots,s_n)\in\mathbb{C}^n$, we define the operator $G(s)$ on the space of functions of the form $f(t,z)=f((t_\alpha)_{\alpha\in\mathbb{Z}_+^n},(z_1,\ldots,z_n))$ by

$$G(s)f(t,z)=f((t_\alpha-\alpha^{-\mathbf{1}}s^{-\alpha})_{\alpha\in\mathbb{Z}_+^n},z), \tag{26}$$

where $\alpha^{-\mathbf{1}}s^{-\alpha}=\alpha_1^{-1}\cdots\alpha_n^{-1}s_1^{-\alpha_1}\cdots s_n^{-\alpha_n}$ according to the multi-index notation. For each $k\in\{1,\ldots,n\}$ we also define the differential operator $\mathcal{D}_k(z)$ by

$$\mathcal{D}_k(z)=\sum_{\alpha\in\mathbb{Z}_+^n}\alpha_k\alpha^{-1}z^{-\alpha-\mathbf{e_k}}\partial_\alpha-\frac{\partial}{\partial z_k}. \tag{27}$$

If $h(z)=h(z_1,\ldots,z_n)$ is a Laurent series in $z_1,\ldots,z_n$ written in the form $h(z)=\Sigma_\alpha b_\alpha z^\alpha$, then we define its residue with respect to z by

$$\mathrm{Res}_z h(z)=b_{-\mathbf{1}}=b_{(-1,\ldots,-1)}. \tag{28}$$

We consider a subset $\hat{P}_-$ of P_- given by

$$\hat{P}_-=\left\{\sum_\alpha f_\alpha(x)\partial^\alpha \,\middle|\, \alpha\leqslant-\mathbf{1} \text{ whenever } f_\alpha(x)\neq 0\right\}. \tag{29}$$

Assuming that $\hat{w}(t,z)$ is the formal power series in (24) associated to the Baker function in (22) with $\phi\in 1+\hat{P}_-$, then the corresponding tau function $\tau(t)$ is a function of $t=(t_\alpha)_{\alpha\in\mathbb{Z}_+^n}$ satisfying the relation

$$\mathrm{Res}_z z^\alpha\mathcal{D}_k(z)\ln\hat{w}(t,z)=-\alpha_k(\alpha+\mathbf{1}-\mathbf{e_k})^{-1}\partial_{\alpha+\mathbf{1}-\mathbf{e_k}}\ln\tau(t). \tag{30}$$

It can be shown that the Baker function in (22) can be expressed in terms of this tau function by

$$w(t,z)=(G(z)\tau(t)/\tau(t))e^{\xi(t,z)},$$

where $G(z)$ is the operator in (26) (see Ref. 4 for details).

IV. TAU FUNCTIONS AND RESIDUES

Let P be the space of iterated Laurent series considered in Sec. II. In this section we describe residues of elements of P as well as those of formal Laurent series in n variables. We then establish relations between tau functions and such residues. These relations generalize corresponding results in the one variable case (see Sec. 7.7 in Ref. 5).

In addition to the residue with respect to z in (28), we consider the one with respect to ∂ as follows. Given an element $\psi=\Sigma_{\alpha\leqslant\nu}f_\alpha(t)\partial^\alpha\in P$, we define its residue with respect to ∂ by

$$\mathrm{Res}_\partial\psi=f_{-\mathbf{1}}(t)=f_{(-1,\ldots,-1)}(t).$$

If $1\leqslant i\leqslant n$ and $\nu=(\nu_1,\ldots,\nu_n)$, then the same element $\psi\in P$ can be written in the form

$$\psi=\sum_{k\leqslant\nu_i}F_{k,i}\partial_i^k,$$

where

$$F_{k,i}=\sum_{\alpha\leqslant\nu,\alpha_i=k} f_\alpha(t)\partial_1^{\alpha_1}\cdots\partial_{i-1}^{\alpha_{i-1}}\partial_{i+1}^{\alpha_{i+1}}\cdots\partial_n^{\alpha_n}.$$

Then the residue of ψ with respect to ∂_i is defined by

$$\mathrm{Res}_{\partial_i}\psi=F_{-1,i}.$$

The next theorem provides a relation between the tau function and the residue of $\hat{w}(t,z)$ with respect to z.

Theorem IV.1: *Let $\hat{w}(t,z)$ be the formal power series in (24) associated to the Baker function as in (22) with $\phi\in 1+\hat{P}_-$. Then the corresponding tau function $\tau(t)$ satisfies*

$$\partial_{\mathbf{1}}\partial_\alpha\ln\tau(t)=-\partial_\alpha\mathrm{Res}_z\hat{w}(t,z) \tag{31}$$

for all $\alpha\in\mathbb{Z}_+^n$.

Proof: If $\alpha=\mathbf{e_k}$ with $1\leqslant k\leqslant n$, then we have

$$\alpha_k=1,\quad \alpha+\mathbf{1}-\mathbf{e_k}=\mathbf{1},\quad z^\alpha=z^{\mathbf{e_k}}=z_k;$$

hence in this case the relation (30) can be written as

$$\mathrm{Res}_z z_k\left(\sum_{\alpha\in\mathbb{Z}_+^n}\alpha_k\alpha^{-1}z^{-\alpha-\mathbf{e_k}}\partial_\alpha-\frac{\partial}{\partial z_k}\right)\ln\hat{w}(t,z)=-\partial_{\mathbf{1}}\ln\tau(t), \tag{32}$$

where we used (27). Given $\alpha\in\mathbb{Z}_+^n$, we have

$$\partial_\alpha\ln\hat{w}(t,z)=\frac{\partial_\alpha\hat{w}(t,z)}{\hat{w}(t,z)}=\frac{\partial_\alpha(w(t,z)e^{-\xi(t,z)})}{\hat{w}(t,z)}=\frac{(\partial_\alpha w(t,z))e^{-\xi(t,z)}}{\hat{w}(t,z)}+\frac{w(t,z)\partial_\alpha e^{-\xi(t,z)}}{\hat{w}(t,z)}.$$

However, we see that $\partial_\alpha w=L_+^\alpha w$ by (25) and

$$\partial_\alpha e^{-\xi(t,z)}=-z^\alpha e^{-\xi(t,z)}.$$

Hence it follows that

$$\partial_\alpha\ln\hat{w}(t,z)=\frac{L_+^\alpha w}{w}-z^\alpha=\mathrm{O}(z^{\alpha-\mathbf{e_n}}).$$

Thus (32) reduces to

$$\partial_{\mathbf{1}}\ln\tau(t)=\mathrm{Res}_z z_k\left(\frac{\partial}{\partial z_k}\ln\hat{w}(t,z)\right)=\mathrm{Res}_z z_k\left(\frac{\Sigma_\alpha\alpha_k a_\alpha(t)z^{\alpha-\mathbf{e_k}}}{1+\Sigma_\alpha a_\alpha(t)z^\alpha}\right)$$

$$=\mathrm{Res}_z z_k\left(\frac{\Sigma_\alpha\alpha_k a_\alpha(t)z^\alpha}{1+\Sigma_\alpha a_\alpha(t)z^\alpha}\right)=-a_{-\mathbf{1}}(t);$$

hence we obtain (31). □

We now state the relation between the tau function and the residue of L^α with $L=\phi\partial\phi^{-1}\in P^n$ and $\alpha\in\mathbb{Z}_+^n$ with respect to ∂ assuming that the dressing operator ϕ belongs to $1+\hat{P}_-$.

Theorem IV.2: *Let ϕ be an element of $1+\hat{P}_-$ satisfying (10), and let $L=\phi\partial\phi^{-1}\in P^n$ be as in (11). Then the tau function corresponding to the Baker function $w(t,z)=\phi e^{\xi(t,z)}$ satisfies the relation*

$$\partial_{\mathbf{1}}\partial_\alpha\ln\tau(t)=\mathrm{Res}_\partial L^\alpha \tag{33}$$

for all $\alpha\in\mathbb{Z}_+^n$.

Proof: If $L=(L_1,\dots,L_n)$ and $\partial=(\partial_1,\dots,\partial_n)$, from the relation $L=\phi\partial\phi^{-1}$ we obtain

$$\phi\partial_i=L_i\phi \tag{34}$$

for $1\leqslant i\leqslant n$. Since $\phi\in 1+\hat{P}_-$, the operators ϕ and L_i can be written in the form

$$\phi=1+\sum_{j\leqslant -1} b_j\partial^j, \quad L_i=\partial_i+u_0\partial_i^{-1}+u_1\partial_i^{-1}+\cdots,$$

where the b_j and u_k are expressions involving $\partial_1,\dots,\partial_{i-1},\partial_{i+1},\dots,\partial_n$ as well as $t=\{t_\alpha|\alpha\in\mathbb{Z}_+^n\}$. Thus we have

$$\phi\partial_i=\partial_i+b_{-1}+b_{-2}\partial_i^{-1}+\cdots,$$

$$L_i\phi=\partial_i+b_{-1}+(\partial_i b_{-1}+b_{-2}+u_0)\partial_i^{-1}+\mathrm{O}(\partial_i^{-2}).$$

From these relations and (34) we obtain

$$u_0=-\partial_i b_{-1},$$

which implies that

$$\mathrm{Res}_{\partial_i}L_i=-\partial_i\mathrm{Res}_{\partial_i}\phi \tag{35}$$

for each $i\in\{1,\dots,n\}$. By (8) each operator L_i satisfies

$$\partial_\alpha L_i=[L_+^\alpha,L_i]=[L^\alpha-L_-^\alpha,L_i]=[L^\alpha,L_i]+[L_i,L_-^\alpha]. \tag{36}$$

However, by Proposition II.1 the operator L belongs to P_0^n in (9); hence L_i commutes with L_j for all $i,j\in\{1,\dots,n\}$, and therefore we have

$$[L^\alpha,L_i]=[L_1^{\alpha_1}\cdots L_n^{\alpha_n},L_i]=0.$$

Thus (36) reduces to

$$\partial_\alpha L_i=[L_i,L_-^\alpha]. \tag{37}$$

If $\mathrm{Res}_{\partial_i}L_-^\alpha=r$, then we have

$$\begin{aligned}[L_i,L_-^\alpha]&=(\partial_i+u_0\partial_i^{-1}+\cdots)(r\partial_i^{-1}+\mathrm{O}(\partial_i^{-2}))-(r\partial_i^{-1}+\mathrm{O}(\partial_i^{-2}))(\partial_i+u_0\partial_i^{-1}+\cdots)\\&=(\partial_i r)\partial_i^{-1}+\mathrm{O}(\partial_i^{-2});\end{aligned}$$

hence we see that

$$\mathrm{Res}_{\partial_i}[L_i,L_-^\alpha]=\partial_i r=\partial_i\mathrm{Res}_{\partial_i}L_-^\alpha.$$

Using this, (35) and (37), we have

$$\partial_i\partial_\alpha\mathrm{Res}_{\partial_i}(\phi)=-\mathrm{Res}_{\partial_i}(\partial_\alpha L_i)=-\mathrm{Res}_{\partial_i}[L_i,L_-^\alpha]=-\partial_i\mathrm{Res}_{\partial_i}L_-^\alpha=-\partial_i\mathrm{Res}_{\partial_i}L^\alpha.$$

From this and the fact that the operators ∂_i and $\mathrm{Res}_{\partial_i}$ commute, we obtain

$$\partial_i\partial_\alpha\mathrm{Res}_\partial\phi=\partial_i\partial_\alpha\mathrm{Res}_{\partial_1}\cdots\mathrm{Res}_{\partial_n}\phi=-\mathrm{Res}_{\partial_1}\cdots\widehat{\mathrm{Res}}_{\partial_i}\cdots\mathrm{Res}_{\partial_n}\partial_i\partial_\alpha\mathrm{Res}_{\partial_i}\phi=-\partial_i\mathrm{Res}_\partial L^\alpha$$

for each $i \in \{1,\ldots,n\}$, where $\widehat{(\cdot)}$ means suppressing $(\cdot)$. Since ϕ is determined only up to multiplication by an element of $1+\hat{P}_-$ with constant coefficients, we may conclude that

$$\partial_\alpha \mathrm{Res}_\partial \phi = -\mathrm{Res}_\partial L^\alpha.$$

On the other hand, using (31), we have

$$\partial_\alpha \mathrm{Res}_\partial \phi = \partial_\alpha \mathrm{Res}_z \hat{w}(t,z) = -\partial_{\mathbf{1}} \partial_\alpha \ln \tau(t).$$

Hence we obtain (33), and the proof of the theorem is complete. □

V. CONCLUDING REMARKS

When the number of variables n is equal to one, the sets P_- and $\hat{P}_-$ in (4) and (29), respectively, coincide. The set P_0^n is also the same as P^n for $n=1$, and in this case the results in Sec. IV are well known.[5] Thus Theorems IV.1 and IV.2 extend the known results in the one variable case to the case of several variables.

ACKNOWLEDGMENTS

This research was partially supported by a PDA award from the University of Northern Iowa. The author would like to thank the referee for various helpful comments.

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Tiling spaces are inverse limits

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(Received 8 May 2003; accepted 17 July 2003)

Let M be an arbitrary Riemannian homogeneous space, and let Ω be a space of tilings of M, with finite local complexity (relative to some symmetry group Γ) and closed in the natural topology. Then Ω is the inverse limit of a sequence of compact finite-dimensional branched manifolds. The branched manifolds are (finite) unions of cells, constructed from the tiles themselves and the group Γ. This result extends previous results of Anderson and Putnam, of Ormes, Radin, and Sadun, of Bellissard, Benedetti, and Gambaudo, and of Gähler. In particular, the construction in this paper is a natural generalization of Gähler's. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1613041]

I. BACKGROUND

In the last few years, it has become clear that many spaces of tilings of $\mathbb{R}^d$ can be viewed as inverse limit spaces. Anderson and Putnam[1] began this program for substitution tilings. Given a substitution, they showed that the corresponding space of tilings of $\mathbb{R}^d$ is the inverse limit of a branched d-manifold K under an expansive map from K to itself. If the substitution has a property called "forcing the border,"[8] then the manifold K is constructed by stitching all the tile types together along possible common boundaries. If the substitution does not force the border, then the construction is similar, only using collared tiles. (A collared tile is a tile that is labeled by the pattern of tiles that touch it.) For this construction to work, the tilings must involve only a finite number of tile types (up to translation), meeting full-face to full-face. In particular, the construction does not apply to tilings like the pinwheel,[11] where tiles appear in an infinite number of orientations.

Ormes, Radin, and Sadun[9] extended the Anderson–Putnam construction to substitution tilings of $\mathbb{R}^d$ on which the entire Euclidean group acts continuously. Tiles may appear in arbitrary orientations, but there can only be a finite number of tile types *up to Euclidean motion*, and tiles must meet full-face to full-face. The branched manifold has dimension $d(d+1)/2$, which is the dimension of the Euclidean group.

In this construction, a cell in the branched manifold K is not a tile. Rather, a cell is the product of a (possibly collared) tile with $SO(d)$, modulo any (finite!) rotational symmetry that the tile might have. This gives a description of all the ways a tile containing the origin may be placed. The substitution (call it σ) replaces each oriented tile with a union of oriented tiles, giving a map from K to itself. Such a union of tiles is called a *supertile* of order 1. The substitution applied to a supertile of order 1 gives a supertile of order 2, and so on.

A point $(x_0,x_1,\ldots)$ in the inverse limit $\leftarrow_\sigma K$ is a consistent description of a tiling, with x_0 telling how the origin sits inside a tile, x_1 telling how the origin sits inside a supertile of order 1, and x_n telling how the origin sits inside a supertile of order n. If the substitution forces its border (or if we are using collared tiles), the sequence $(x_0,x_1,\ldots)$ gives a consistent description of a unique tiling of $\mathbb{R}^d$.

More recently, Gähler[5] and Bellissard, Benedetti, and Gambaudo[3] have each applied inverse limit methods to tilings that need not be generated by a substitution. If x is a tiling of $\mathbb{R}^d$ that has finitely many tile types *up to translation*, meeting full-face to full-face, then the continu-

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ous hull of x (i.e., the closure of the translational orbit of x) is the inverse limit of a sequence of compact branched manifolds K_0, K_1, K_2, ..., under a sequence of maps $\sigma_n : K_n \to K_{n-1}$, where each branched manifold K_n is the union of (marked) tiles from the original tiling. Of the two constructions, Gähler's is conceptually simpler, but that of Bellissard, Benedetti, and Gambaudo appears to be calculationally stronger, leading to results such as gap-labeling theorems.[2]

This paper is an extension of Gähler's construction to tilings of arbitrary Riemannian homogeneous spaces, with general symmetry group. The generalization of the Bellissard–Benedetti–Gambaudo approach to arbitrary spaces is being done independently by Benedetti and Gambaudo.[3]

II. THEOREM AND PROOF

Before stating and proving the result, we must establish some notation. Let M be a Riemannian homogeneous space (such as $\mathbb{Z}^d$, $\mathbb{R}^d$, $\mathbf{H}^2$, $\mathbf{H}^2 \times \mathbb{R}^3$, etc.), and pick a point to be the origin. Let G be the group of isometries of M, let Γ be a closed subgroup of G, and let Γ_0 be the subgroup of Γ that fixes the origin. Let Ω be a collection of tilings of M. We give Ω the topology that two tilings are ϵ-close if they agree on a ball of size $1/\epsilon$ around the origin, up to the action of an ϵ-small element of Γ. We assume that Ω is closed under the action of Γ (i.e., Ω is a union of Γ-orbits), and that Ω is compact. This implies that Ω has finite local complexity, up to the action of Γ.

Theorem: *Ω is the inverse limit of a sequence of compact branched manifolds $K_1, K_2, \ldots$, and continuous maps $\sigma_n : K_n \to K_{n-1}$. The dimension of the branched manifold is the dimension of Γ.*

The idea of the proof is quite simple. A point in the n-th approximant K_n is a description of a tile containing the origin, its nearest neighbors (sometimes called the "first corona"), its second nearest neighbors (the "second corona") and so on out to the n-th nearest neighbors. (For these purposes, tiles that meet at a point are considered nearest neighbors.) The map $\sigma_n : K_n \to K_{n-1}$ simply forgets the n-th corona. A point in the inverse limit is then a consistent prescription for constructing a tiling out to infinity. In other words, it is a tiling.

What remains is to actually construct K_n out of geometric pieces and show that K_n is a branched manifold.

First suppose that the tiles are polytopes that meet full-face to full-face. We consider two tiles t_1, t_2 in (possibly different) tilings of M to be equivalent if a patch of the first tiling, containing t_1 and its first n coronas, is identical, up to the action of Γ, to a similar patch around t_2. Since Ω has finite local complexity, there are only finitely many equivalence classes, each of which is called an n-collared tile.

For each n-collared tile t_i, we consider how such a tile can be placed around the origin. Let $s_i \subset t_i$ be the set of points where the origin may sit. By finite local complexity, there can only be a finite number of connected components to s_i, and each component is a submanifold of t_i with the same dimension as Γ/Γ_0.

If t_i does not admit any symmetry, then for each point $p \in s_i$, Γ_0 acts simply transitively on the ways to place t_i down with the spot p landing at the origin. The set of ways to place t_i is therefore a principal Γ_0 bundle over s_i, which we denote E_i. The cell $C_i \subset K_n$ associated with t_i is then exactly E_i.

If there are no topological obstructions to trivializing this bundle, we make the identification

$$C_i = E_i = s_i \times \Gamma_0 . \tag{1}$$

If M is flat, then there is a *canonical* trivialization of the frame bundle, and this descends to a canonical product (1). If Γ acts transitively on M, then $s_i = t_i$ is contractible, and the decomposition (1), while not canonical, is guaranteed to exist. Although there do exist tilings where neither of these conditions are met, the author knows of no examples where C_i fails to be trivializable.

If t_i admits a discrete symmetry (e.g., is a regular n-gon in a tiling of $\mathbb{R}^2$ or $\mathbf{H}^2$), then more than one point in $s_i \times \Gamma_0$ may describe the same placement of a tile containing the origin. In that case, the cell associated to t_i is the quotient of the Γ_0 bundle E_i by the symmetry. That is,

$$C_i = E_i/\Gamma_{t_i} \quad (= s_i \times_{\Gamma_{t_i}} \Gamma_0, \text{ if } E_i \text{ is trivializable}), \tag{2}$$

where $\Gamma_{t_i} \subset \Gamma_0$ is the group of symmetries of t_i. Since t_i is a collared tile, Γ_{t_i} must be a discrete subgroup of Γ_0. (Even if a tile had a continuous symmetry, its first corona could not.) By construction, Γ_{t_i} acts without fixed points on E_i, so the interior of C_i is indeed a manifold. (For instance, if $M = \mathbb{R}^2$ and Γ is the Euclidean group, then C_i is a Seifert fibered space. There may be multiple fibers over points of symmetry, but the total space is smooth.)

A patch of a tiling in which the origin is on the boundary of two or more tiles is described by points on the boundary of two or more cells, and these points must be identified. The branched manifold K_n is the disjoint union of the cells C_i, modulo this identification. Since we are using n-collared tiles with $n \geqslant 1$, each of the points being identified carries complete information about the placement of all the tiles that meet the origin, together with their first $n-1$ coronas.

We must show that a neighborhood of such a branch point is the union of topological disks whose tangent spaces may be identified. Each such disk is obtained by taking a patch of a tiling in which the above data is actually realized, and considering its orbit under the action of a neighborhood of the identity in Γ. This shows that the dimension of K_n is the dimension of Γ.

Finally, we remove the assumption that the tiles are polytopes that meet full-face to full-face. To a tiling by other shapes we may associate a pattern of marked points, where a special point is chosen from each tile and labeled by the type of that tile. The Voronoi cells of those points are then polytopes whose faces, properly subdivided, meet full-face to full-face. The original tiling and the tiling by Voronoi cells are mutually locally derivable,[4] and so are described by the same topological space, and hence by the same inverse limit structure. ■

In this construction, the group Γ_0 acts naturally on each space K_n, and the maps σ_n are equivariant, from which we have the following:

Corollary: The space Ω/Γ_0 of tilings modulo rotation is the inverse limit of a sequence of compact branched orbifolds K_n/Γ_0.

III. EXAMPLES

(1) If $M = \Gamma = \mathbb{Z}^d$, then we have a $\mathbb{Z}^d$ subshift. The total space Ω is a Cantor set. The n-th approximant K_n is a finite collection of points, corresponding to a decomposition of the Cantor set into a finite number of clopen sets. This decomposition becomes finer as $n \to \infty$, and the Cantor set is recovered as the inverse limit.

(2) If $M = \mathbb{R}^d$ and $\Gamma = \mathbb{Z}^d$, then (up to a fixed translation) Ω is a space of tilings of $\mathbb{R}^d$ by square tiles centered at the lattice points. This is a different description of the previous example. In these examples, note that Ω does not have to be the hull of a single tiling, and that the $\mathbb{Z}^d$ action need not be minimal. The $\mathbb{Z}$ subshift on two letters, in which one of the letters appears at most twice, is neither minimal nor the closure of a single orbit, but is an inverse limit space.

(3) The (d-fold) suspension of a $\mathbb{Z}^d$ subshift has $M = \Gamma = \mathbb{R}^d$. This is a space of tilings of $\mathbb{R}^d$ by unit cubes oriented parallel to the coordinate axes.

(4) A $\mathbb{Z}^d$ subshift may be suspended in some directions but not in others. For instance, the suspension of a $\mathbb{Z}^2$ subshift in the x direction is a space of tilings of $\mathbb{R}^2$ by square tiles, meeting full-face to full-face, whose centers have an integral y coordinate. In this case $M = \mathbb{R}^2$ and $\Gamma = \mathbb{R} \times \mathbb{Z}$.

(5) The Penrose tiling space, or any other tiling of $\mathbb{R}^d$ with a finite set of prototiles up to translation, has $M = \Gamma = \mathbb{R}^d$. Since Γ_0 is trivial and Γ is the full translation group, the cells C_i can be identified with the collared tiles t_i themselves. This is precisely Gähler's construction. Such a space is homeomorphic to the suspension of a $\mathbb{Z}^d$ subshift.[12]

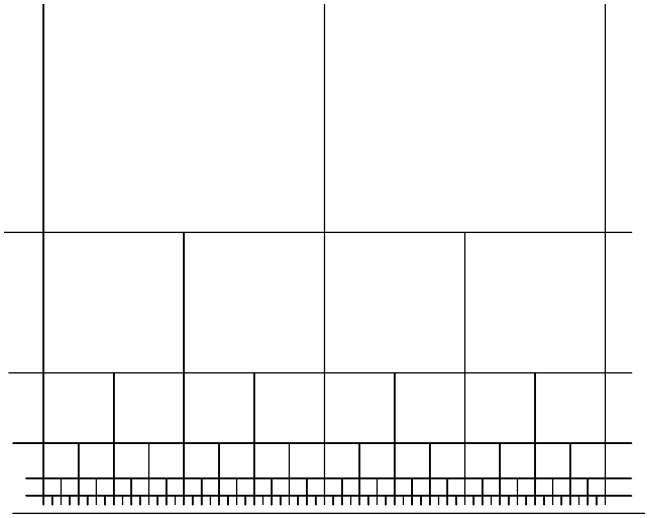

FIG. 1. Penrose's dyadic tiling of hyperbolic space.

(6) The pinwheel tiling space[11] has $M=\mathbb{R}^2$ and Γ the 2-dimensional Euclidean group.[9]

(7) In tiling hyperbolic space, there are a number of interesting choices for Γ. If Γ is a discrete group, then we have the analog of a subshift, associating letters to a discrete set of points in the space being tiled. At the other extreme, one can take Γ to be the entire group of isometries of $\mathbf{H}^n$.

(8) One-dimensional orientable hyperbolic attractors are either solenoids or one-dimensional tiling spaces.[13,1] However, the dyadic solonoid *can* be viewed as a tiling space, of $\mathbf{H}^2$ rather than $\mathbb{R}^1$, following a construction of Penrose.[10] See Fig. 1. In the upper-half-plane model, the basic tile looks like a rectangle, with the sides of the rectangle geodesics, with the top and bottom edges horocyclic, and with the size chosen such that the bottom edge has twice the length of the top edge. Here the group is $\Gamma=\mathbb{Z}\ltimes\mathbb{R}$, acting on $\mathbf{H}^2$ by $(n,t)(x,y)=(t+2^n x,2^n y)$.

(9) More generally, any geometric substitution in $\mathbb{R}^d$ gives rise to a space of tilings of $\mathbf{H}^{d+1}$, with group $\Gamma=\mathbb{Z}\ltimes\mathbb{R}^d$. As with the dyadic solenoid, it does not matter whether the substitution is invertible, since the $\mathbb{Z}$ action enforces the hierarchy. Goodman-Strauss has adapted this construction to produce a strongly aperiodic set of prototiles for $\mathbf{H}^2$ (Ref. 7) and to develop a general formalism for describing tilings of hyperbolic space.[6]

IV. CONCLUSIONS AND OPEN PROBLEMS

The inverse limit structure of Ω implies that the Čech cohomology $H^*(\Omega)$ is the direct limit of $H^*(K_n)$ under the pullback maps σ_n^*. Every element of $H^*(\Omega)$ is the pullback, under the natural projection $\pi_n:\Omega\to K_n$, of a cohomology class in K_n, for n sufficiently large. If (and only if) $H^*(\Omega)$ is finitely generated, then for n large enough the entire cohomology of Ω is the quotient of $H^*(K_n)$ by the kernel of π_n^*.

To make effective use of this principle, however, requires specific knowledge of the tiling space in question. For substitution tilings, it is easiest to work with the Anderson–Putnam inverse limit construction, rather than that constructed here, although in fact the two are shift equivalent. For cut-and-project tilings with sufficiently nice ''windows,'' Gähler[5] has shown that π_n^* is actually an isomorphism in cohomology for n sufficiently large, with the required size of n computable from the geometry of the window.

The inverse limit structure of tiling spaces is related to a possible fiber bundle structure. Locally, Ω looks like a piece of Γ times a Cantor set. Can these neighborhoods be stitched together to yield a fiber bundle (with a Cantor set fiber) over a compact manifold? Is that manifold the quotient of the identity component of Γ by a co-compact subgroup? When $M=\Gamma=\mathbb{R}^d$, the answer to both questions is yes,[12] but the general case is not known.

ACKNOWLEDGMENTS

Many thanks to the organizers and participants in the August 2002 conference on Aperiodic Order, Dynamical Systems, Operator Algebras and Topology at the University of Victoria, British Columbia. The results of this paper are a direct consequence of the talks at that conference (especially those of Franz Gähler and Jean-Marc Gambaudo) and the discussions that ensued. Additional thanks to Charles Radin and Michael Baake for assistance with the manuscript. This work was partially supported by the Texas Advanced Research Program.

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A Grassmann integral equation

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(Received 15 May 2003; accepted 21 June 2003)

The present study introduces and investigates a new type of equation which is called *Grassmann integral equation* in analogy to integral equations studied in real analysis. A Grassmann integral equation is an equation which involves Grassmann (Berezin) integrations and which is to be obeyed by an unknown function over a (finite-dimensional) Grassmann algebra $\mathcal{G}_m$ (i.e., a sought after element of the Grassmann algebra $\mathcal{G}_m$). A particular type of Grassmann integral equations is explicitly studied for certain low-dimensional Grassmann algebras. The choice of the equation under investigation is motivated by the effective action formalism of (lattice) quantum field theory. In a very general setting, for the Grassmann algebras $\mathcal{G}_{2n}$, $n=2,3,4$, the finite-dimensional analogues of the generating functionals of the Green functions are worked out explicitly by solving a coupled system of nonlinear matrix equations. Finally, by imposing the condition $G[\{\bar{\Psi}\},\{\Psi\}] = G_0[\{\lambda\bar{\Psi}\},\{\lambda\Psi\}]+\text{const}$, $0<\lambda\in\mathbf{R}$ ($\bar{\Psi}_k$, Ψ_k, $k=1,\ldots,n$, are the generators of the Grassmann algebra $\mathcal{G}_{2n}$), between the finite-dimensional analogues G_0 and G of the (''classical'') action and effective action functionals, respectively, a special Grassmann integral equation is being established and solved which also is equivalent to a coupled system of nonlinear matrix equations. If $\lambda\neq 1$, solutions to this Grassmann integral equation exist for $n=2$ (and consequently, also for any even value of n, specifically, for $n=4$) but not for $n=3$. If $\lambda=1$, the considered Grassmann integral equation (of course) has always a solution which corresponds to a Gaussian integral, but remarkably in the case $n=4$ a further solution is found which corresponds to a non-Gaussian integral. The investigation sheds light on the structures to be met for Grassmann algebras $\mathcal{G}_{2n}$ with arbitrarily chosen n. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1612896]

I. INTRODUCTION

The problem to be studied in the present paper is a purely mathematical one and one might arrive at it within various research programmes in mathematics and its applications. Our starting point will be (lattice) quantum field theory[1–4] and for convenience we will mainly use its terminology throughout the study (incidentally, for a finite-dimensional problem). However, one could equally well rely on the terminology of statistical mechanics or probability theory throughout. We will be interested in certain aspects of differential calculus in Grassmann (Graßmann) algebras[5] and in particular in Grassmann analogues to integral equations studied in real analysis which we will call *Grassmann integral equations*. A Grassmann integral equation is an equation which involves Grassmann (Berezin) integrations and which is to be obeyed by an unknown function over a (finite-dimensional) Grassmann algebra $\mathcal{G}_m$ (i.e., a sought after element of the Grassmann algebra $\mathcal{G}_m$). To the best of our knowledge this problem is considered for the first time in this paper. Of course, the following comment is due. Bearing in mind that in a Grassmann algebra taking a (Grassmann) derivative and an integral are equivalent operations we could equally well

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denote any Grassmann integral equation as a Grassmann differential equation. There is an extensive literature on supersymmetric extensions of differential equations. Corresponding research has been performed in areas such as supersymmetric field theory (see, e.g., Ref. 6, Vol. 3), superconformal field theory, the study of supersymmetric integrable models (see, e.g., Refs. 7, 8), and superanalysis (for a review of the latter see the recent book by Khrennikov,[9] in particular Chap. 2, and references therein). Only few mathematical references exist which treat pure Grassmann differential equations (understood in the narrow sense, i.e., in a nonsupersymmetric setting).[10–12] In the physics literature, specifically in the quantum field theoretic literature, such equations (in general, for infinite-dimensional Grassmann algebras) can be found in studies of purely fermionic models by means of the Schwinger–Dyson equations[13–20] or the Schrödinger representation (Refs. 21, 22 and follow-up references citing these). Within the framework of supersymmetric generalizations of conventional analysis, it is customary to consider all structures in strict analogy to real (complex) analysis. Consequently, as we will be lead to the problem of Grassmann integral equations from the corresponding problem in real analysis the choice of this term should not lead to any objection. Incidentally, it might be interesting to note that Khrennikov[9] mentions [at the end of Chap. 2, p. 102 (p. 106 of the English translation)] integral equations (item 9) among the subjects which have not yet been studied in superanalysis.

Having characterized in general the subject of the present study we will now explain in somewhat greater detail the problem we are interested in and where it arises from. Our motivation for the present investigation derives from quantum field theory. Quantum field theory is a rich subject with many facets and is being studied on the basis of a number of approaches and methods. For the present purpose, we rely on the functional integral approach to Lagrangian quantum field theory (see, e.g., Ref. 14, Ref. 15, Chap. 9, p. 425, Ref. 16, Ref. 6, Vol. I, Chap. 9, p. 376). To begin with, consider the theory of a scalar field ϕ in k-dimensional Minkowski space–time. By the following equations one defines generating functionals for various types of Green functions of this field (see, e.g., Ref. 14, Ref. 15, *loc. cit.*, Ref. 16, Ref. 17, Chap. 6, Ref. 6, Vol. II, Chap. 16, p. 63),

$$Z[J]=C\int D\phi e^{i\Gamma_0[\phi]+i\int \mathrm{d}^k x\, J(x)\phi(x)}, \tag{1}$$

$$W[J]=-i\ln Z[J], \tag{2}$$

$$\Gamma[\bar{\phi}]=W[J]-\int \mathrm{d}^k x\, J(x)\bar{\phi}(x), \tag{3}$$

$$\bar{\phi}(x)=\frac{\delta W[J]}{\delta J(x)}. \tag{4}$$

From Eq. (3) one finds the relation

$$\frac{\delta\Gamma[\bar{\phi}]}{\delta\bar{\phi}(x)}=-J(x). \tag{5}$$

In Eq. (1), $\int D\phi$ denotes the (infinite-dimensional) functional integration over the scalar field ϕ. $Z[J]$ is the generating functional of the Green functions,[23,24] $W[J]$ is the generating functional of the connected Green functions while the (first) Legendre transform $\Gamma[\bar{\phi}]$ of $W[J]$ is the generating functional of the one-particle-irreducible (1PI) Green functions. $\Gamma_0[\phi]$ is the so-called classical action of the theory and C some fixed normalization constant. $\Gamma[\bar{\phi}]$ is also called the effective action of the theory and, in principle, any information one might ever be interested in can be derived from it.

Equation (1) defines a map, $g_1:\Gamma_0[\phi]\to Z[J]$, from the class of functionals called classical actions to the class of functionals Z. Furthermore, we have mappings, $g_2:Z[J]\to W[J]$, [Eq. (2)],

and $g_3: W[J] \to \Gamma[\bar{\phi}]$ [Eq. (3)]. These three maps together define a map $g_3 \circ g_2 \circ g_1 = f: \Gamma_0[\phi] \to \Gamma[\bar{\phi}]$ from the set of so-called classical actions to the set of effective actions (we will call f the "action map"). In general, the action map is mathematically not well-defined in quantum field theory due to the occurrence of ultraviolet divergencies and one has to apply a regularization procedure for making proper mathematical sense of the above equations. A widely applied approach which is very natural from a mathematical point of view consists in studying quantum field theory not on a space–time continuum but on a space–time lattice (see, e.g., Refs. 1–4). The map f can be represented by the following single equation which can be derived from the Eqs. (1)–(3):

$$e^{i\Gamma[\bar{\phi}]} = C \int D\phi e^{i\Gamma_0[\phi+\bar{\phi}] + i\int d^k x\, J(x)\phi(x)}. \tag{6}$$

$J(x)$ is given here by Eq. (5), consequently, Eq. (6) is only an implicit representation of the map f. For any quantum field theory, the properties of the action map f are of considerable interest but are hard if not impossible to study in general. In the simplest case, Γ_0 is a quadratic functional of the field ϕ (reasonably chosen to ensure that the functional integral is well defined). Then, the functional integral is Gaussian and one immediately finds (free field theory; const is some constant depending on the choice of C)

$$\Gamma[\phi] = \Gamma_0[\phi] + \text{const.} \tag{7}$$

There are very few other cases in which the formalism can explicitly be studied beyond perturbation theory. A number of exact results exist in quantum mechanics (which can be understood as quantum field theory in $0+1$-dimensional space-time; see, e.g., Refs. 25, 26). For some quantum field theoretic results see, e.g., Ref. 27.

It is common and successful practice in mathematics and physics to approach difficult infinite-dimensional problems from their finite-dimensional analogues. For example, in numerical studies within the framework of lattice quantum field theory the infinite-dimensional functional integral as present in Eq. (6) is replaced by a multidimensional multiple integral. The simplest finite-dimensional analogue of Eq. (6) is being obtained by replacing the infinite-dimensional functional integral by an one-dimensional integral over the real line. [More precisely, we obtain it from the Euclidean field theory version of Eq. (6) where the imaginary unit i in the exponent is replaced by $(-)1$. g' denotes here the first derivative of the function g.]

$$e^{g(y)} = C \int_{-\infty}^{+\infty} dx\, e^{g_0(x+y) - g'(y)x}. \tag{8}$$

Still, even the study of Eq. (8) represents a formidable task. The consideration of the (one-dimensional) analogues of the Eqs. (1)–(6) is often pursued under the name of zero-dimensional field theory [Refs. 28–42, Ref. 15, Subsec. 9-4-1, p. 463, Refs. 43–46, Refs. 18, 47–58, Ref. 59, Chap. 9, p. 211, Refs. 60–64; we have included into the list of reference also articles on the static ultralocal single-component scalar model but left aside papers on the corresponding $O(N)$ symmetric model].

For simplicity, the above discussion has been based on the consideration of a bosonic quantum field. However, fermionic (Grassmann valued) quantum fields are also of considerable physical interest (for a general discussion of Grassmann variables see Ref. 5). The analogue of Eq. (6) for a purely fermionic field theory of the Grassmann field Ψ, $\bar{\Psi}$ reads as follows:

$$e^{i\Gamma[\bar{\Psi},\Psi]} = C \int D(\chi,\bar{\chi})\ \ e^{i\Gamma_0[\bar{\chi}+\bar{\Psi},\chi+\Psi] + i\int d^k x\ (\bar{\eta}(x)\chi(x) + \bar{\chi}(x)\eta(x))}, \tag{9}$$

$$\bar{\eta}(x) = \frac{\delta\Gamma[\bar{\Psi},\Psi]}{\delta\Psi(x)}, \quad \eta(x) = -\frac{\delta\Gamma[\bar{\Psi},\Psi]}{\delta\bar{\Psi}(x)}. \tag{10}$$

Here, $D(\chi,\overline{\chi})$ denotes the infinite-dimensional Grassmann integration and the functional derivatives used in (10) are left Grassmann derivatives. The finite-dimensional (fermionic) analogues of the Eqs. (1)–(5) and (9), (10) consequently read[65–69]

$$Z[\{\overline{\eta}\},\{\eta\}]=C\int\prod_{l=1}^{n}(\mathrm{d}\chi_l\,\mathrm{d}\overline{\chi_l})e^{\,G_0[\{\overline{\chi}\},\{\chi\}]+\Sigma_{l=1}^{n}\,(\overline{\eta}_l\chi_l+\overline{\chi}_l\eta_l)}, \tag{11}$$

$$W[\{\overline{\eta}\},\{\eta\}]=\ln Z[\{\overline{\eta}\},\{\eta\}], \tag{12}$$

$$G[\{\overline{\Psi}\},\{\Psi\}]=W[\{\overline{\eta}\},\{\eta\}]-\sum_{l=1}^{n}\,(\overline{\eta}_l\Psi_l+\overline{\Psi}_l\eta_l), \tag{13}$$

$$\overline{\Psi}_l=-\frac{\partial W[\{\overline{\eta}\},\{\eta\}]}{\partial\eta_l},\quad \Psi_l=\frac{\partial W[\{\overline{\eta}\},\{\eta\}]}{\partial\overline{\eta}_l}, \tag{14}$$

and

$$e^{\,G[\{\overline{\Psi}\},\{\Psi\}]}=C\int\prod_{l=1}^{n}(\mathrm{d}\chi_l\,\mathrm{d}\overline{\chi_l})e^{\,G_0[\{\overline{\chi}+\overline{\Psi}\},\{\chi+\Psi\}]+\Sigma_{l=1}^{n}\,(\overline{\eta}_l\chi_l+\overline{\chi}_l\eta_l)}, \tag{15}$$

$$\overline{\eta}_l=\frac{\partial G[\{\overline{\Psi}\},\{\Psi\}]}{\partial\Psi_l},\quad \eta_l=-\frac{\partial G[\{\overline{\Psi}\},\{\Psi\}]}{\partial\overline{\Psi}_l}, \tag{16}$$

respectively. $\{\overline{\Psi}\}$, $\{\Psi\}$ denote the sets of Grassmann variables $\overline{\Psi}_l$, $l=1,\ldots,n$ and Ψ_l, $l=1,\ldots,n$, respectively, which are the generators of the Grassmann algebra $\mathcal{G}_{2n}$ [more precisely, we are considering a Grassmann algebra $\mathcal{G}_{4n}$ as the χ_l, $\overline{\chi_l}$ in Eq. (15) are also Grassmann variables, but we will ignore this mathematical subtlety in the following]. These generators obey the standard relations

$$\Psi_l\Psi_m+\Psi_m\Psi_l=\overline{\Psi}_l\Psi_m+\Psi_m\overline{\Psi}_l=\overline{\Psi}_l\overline{\Psi}_m+\overline{\Psi}_m\overline{\Psi}_l=0. \tag{17}$$

In this paper, we will concentrate on the explicit study of the Eqs. (15), (16) for small values of n ($n=2,3,4$) (some of the calculations have been performed by means of a purpose designed Mathematica program[70]). The Eqs. (15), (16) define (implicitly) a map f between the elements G_0 and G of the Grassmann algebra $\mathcal{G}_{2n}$ (in analogy to the infinite-dimensional case, we call the map f the action map). As we will see, the Eqs. (15), (16) are equivalent to a coupled system of nonlinear matrix equations which however can successively be solved completely (for a general exposition of matrix equations see, e.g., Refs. 71 and 72). This way, we will explicitly work out the action map f for the following fairly general ansatz for G_0:

$$\begin{aligned}G_0[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)}&+\sum_{l,m=1}^{n}A^{(2)}_{l,m}\overline{\Psi}_l\Psi_m+\left(\frac{1}{2!}\right)^2\sum_{l_1,l_2,m_1,m_2=1}^{n}A^{(4)}_{l_1l_2,m_1m_2}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\Psi_{m_1}\Psi_{m_2}\\&+\left(\frac{1}{3!}\right)^2\sum_{l_1,l_2,l_3,m_1,m_2,m_3=1}^{n}A^{(6)}_{l_1l_2l_3,m_1m_2m_3}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\overline{\Psi}_{l_3}\Psi_{m_1}\Psi_{m_2}\Psi_{m_3}+\cdots\\&+\left(\frac{1}{n!}\right)^2\sum_{l_1,\ldots,l_n,m_1,\ldots,m_n=1}^{n}A^{(2n)}_{l_1\cdots l_n,m_1\cdots m_n}\overline{\Psi}_{l_1}\cdots\overline{\Psi}_{l_n}\Psi_{m_1}\cdots\Psi_{m_n}.\end{aligned} \tag{18}$$

Here, $A^{(0)}$ is some constant and the coefficients $A^{(2k)}_{\ldots}$, $k>1$, are chosen to be completely antisymmetric in the first and in the second half of their indices, respectively.

Although the explicit determination of the action map f between G_0 and G for low-dimensional Grassmann algebras represents previously unknown information, it may seem that the study of the map f for low-dimensional Grassmann algebras is a mathematical exercise of purely academic nature as quantum field theory and statistical mechanics are concerned with infinitely many degrees of freedom. To some extent this view may be justified for the time being but one should also take note of the fact that results for the Grassmann algebras $\mathcal{G}_{2n}$ and $\mathcal{G}_{2(n-1)}$ are closely related. To see this observe the following. Put in Eq. (18) considered in the case of the Grassmann algebra $\mathcal{G}_{2n}$ the coefficient $A^{(2)}_{n,n}$ equal to one but all other coefficients $A^{(2k)}_{\ldots}$, $k>1$, equal to zero whose index set $\{\ldots\}$ contains at least one index with value n.

$$A^{(2)}_{n,n}=1, \tag{19}$$

$$A^{(2k)}_{\ldots n\ldots}=0, \quad k>1. \tag{20}$$

Then, perform in Eq. (15) the Grassmann integrations with respect to χ_n, $\overline{\chi_n}$. Up to the factor $(\exp \overline{\Psi}_n\Psi_n)$ present on both sides (no summation with respect to n here) Eq. (18) then coincides with Eq. (18) considered in the case of the Grassmann algebra $\mathcal{G}_{2(n-1)}$. Consequently, results obtained for low-dimensional Grassmann algebras tightly constrain structures to be found for Grassmann algebras $\mathcal{G}_{2n}$ with arbitrarily chosen n. In fact, we will use this observation in two ways. On the one hand, we will rely on it in order to check the explicit results obtained for $n=4$ and $n=3$ for compatibility with those obtained for $n=3$ and $n=2$, respectively. On the other hand, on the basis of the above observation we will extrapolate some results obtained for $n=2,3,4$ to arbitrary n which can be used later in the future as working hypothesis for further studies.

Having explicitly worked out the action map f between G_0 and G for low-dimensional Grassmann algebras, we will not stop our investigation at this point but pursue our study still one step further. In the Refs. 28, 73, and 74 it has been argued (in a quantum field theoretic context), that it might be physically sensible and interesting to look for actions $\Gamma_0[\phi]$ which are not quadratic functionals of the field ϕ (i.e., which do not describe free fields) but for which Eq. (7) also applies. For the purpose of the present investigation we will slightly extend our search. We will look for solutions to the equation $(0<\lambda\in\mathbf{R})$

$$G[\{\overline{\Psi}\},\{\Psi\}]=G_0[\{\lambda\overline{\Psi}\},\{\lambda\Psi\}]+\Delta_f(\lambda). \tag{21}$$

λ can be considered here as a finite-dimensional analogue of a wave function renormalization constant in continuous space–time quantum field theory. $\Delta_f(\lambda)$ is some constant which is allowed to depend on λ. Equation (21) turns the implicit representation of the map f given by the Eqs. (15), (16) into a Grassmann integral equation for $G_0[\{\overline{\Psi}\},\{\Psi\}]$ (more precisely, into a nonlinear Grassmann integro-differential equation). As we will see, this Grassmann integral equation is equivalent to a coupled system of nonlinear matrix equations whose solution in turn is equivalent to the solution of the considered Grassmann integral equation. In the present study, to us Eq. (21) is just a mathematical problem to be studied. The possible relevance of any solution of Eq. (21) to physical problems will remain beyond the scope of the present paper. Some comments in this respect can be found in Refs. 28 and 73.

The plan of the paper is as follows. In Sec. II we work out explicitly the action map f between G_0 and G. Section II A contains some mathematical preliminaries while the following three sections are devoted to the cases $n=2,3,4$, respectively. Section II E finally studies the extrapolation of some of the results obtained to Grassmann algebras $\mathcal{G}_{2n}$ with arbitrarily chosen n. Section III is concerned with the study of the Grassmann integral equation (21). On the basis of the results obtained in Sec. II, in Secs. III A–III C it is solved for $n=2,3,4$, respectively. Then, Sec. III D contains an analysis of certain aspects of the solutions of the Grassmann integral equation found for $n=4$. In Sec. IV the discussion of the results and conclusions can be found. The paper is supplemented by three Appendixes.

II. THE ACTION MAP FOR LOW-DIMENSIONAL GRASSMANN ALGEBRAS

A. Some definitions

To simplify the further considerations we introduce a set of $\binom{n}{k}\times\binom{n}{k}$ matrices $\mathsf{A}^{(2k)}$ $(k=1,\ldots,n)$ by writing (choose $l_1<l_2<\cdots<l_k$, $m_1<m_2<\cdots<m_k$),

$$\mathsf{A}^{(2k)}_{LM}=A^{(2k)}_{l_1\cdots l_k,m_1\cdots m_k} \tag{22}$$

(we identify the indices L, M with the ordered strings $l_1\cdots l_k$, $m_1\cdots m_k$) or, more generally (not requesting $l_1<l_2<\cdots<l_k$, $m_1<m_2<\cdots<m_k$)

$$\mathsf{A}^{(2k)}_{LM} = \mathrm{sgn}[\sigma_a(l_1,\ldots,l_k)]\mathrm{sgn}[\sigma_b(m_1,\ldots,m_k)]A^{(2k)}_{l_1\cdots l_k,m_1\cdots m_k}. \tag{23}$$

The indices L,M label the equivalence classes of all permutations of the indices $l_1,\ldots,l_k$ and $m_1,\ldots,m_k$, respectively, and σ_a, σ_b are the permutations which bring the indices l_i,m_i $(i=1,\ldots,k)$ into order with respect to the $<$ relation [i.e., $\sigma_a(l_1)<\sigma_a(l_2)<\cdots<\sigma_a(l_k)$, $\sigma_b(m_1)<\sigma_b(m_2)<\cdots<\sigma_b(m_k)$]. The matrix elements of the matrix $\mathsf{A}^{(2k)}$ are arranged according to the lexicographical order of the row and column indices L, M. [We identify the indices L, M with the ordered strings $\sigma_a(l_1)\cdots\sigma_a(l_k)$, $\sigma_b(m_1)\cdots\sigma_b(m_k)$, respectively.]

We also define a set of (dual) $\binom{n}{k}\times\binom{n}{k}$ matrices $\mathsf{A}^{(2k)\star}$ $(k=1,\ldots,n)$ by writing

$$\mathsf{A}^{(2k)\star}=\mathcal{E}^{(k)}\mathsf{A}^{(2k)T}\mathcal{E}^{(k)T}, \tag{24}$$

where the $\binom{n}{k}\times\binom{n}{k}$ matrix $\mathcal{E}^{(k)}$ is defined by

$$\mathcal{E}^{(k)}_{LM}=\epsilon_{l_1\cdots l_{n-k}m_1\cdots m_k}, \tag{25}$$

consequently,

$$\mathcal{E}^{(k)T}=(-1)^{(n-k)k}\mathcal{E}^{(n-k)}. \tag{26}$$

[Quite generally, for any $\binom{n}{k}\times\binom{n}{k}$ matrix B we define $\mathsf{B}^\star$ by $\mathsf{B}^\star=\mathcal{E}^{(k)}\mathsf{B}^T\mathcal{E}^{(k)T}$.] It holds ($\mathbf{1}_r$ is the $r\times r$ unit matrix)

$$\mathcal{E}^{(k)}\mathcal{E}^{(k)T}=\mathbf{1}_{\binom{n}{k}}, \tag{27}$$

$$\mathcal{E}^{(k)T}\mathcal{E}^{(k)}=\mathbf{1}_{\binom{n}{k}}. \tag{28}$$

The transition from a matrix B to the matrix $\mathsf{B}^\star$ corresponds to applying the Hodge star operation to the two subspaces of the Grassmann algebra $\mathcal{G}_{2n}$ generated by the two sets of Grassmann variables $\{\overline{\Psi}\}$ and $\{\Psi\}$ and interchanging them (cf., e.g., Ref. 75, Part II, Chap. 4, p. 50). This operation on the matrix B is an involution as $(\mathsf{B}^\star)^\star=\mathsf{B}$.

Furthermore, it turns out to be convenient to define arrays of partition functions (i.e., their finite-dimensional analogues). First, we choose

$$C=e^{-G_0[\{0\},\{0\}]} = e^{-A^{(0)}}. \tag{29}$$

This choice in effect cancels any constant term in Eq. (18) (in this respect also see Ref. 73, p. 288). Now, we define[76] (we apply the convention $\int \mathrm{d}\chi_i\,\chi_j=\delta_{ij}$)

$$P=\mathsf{P}^{(2n)\star}=C\int\prod_{l=1}^{n}(\mathrm{d}\chi_l\,\mathrm{d}\overline{\chi_l})\,e^{G_0[\{\overline{\chi}\},\{\chi\}]}. \tag{30}$$

We then define arrays of partition functions $\mathsf{P}^{(2n-2k)\star}$ [these are $\binom{n}{k}\times\binom{n}{k}$ matrices] for subsystems of Grassmann variables where k degrees of freedom have been omitted (in slight misuse of physics terminology we denote a pair of Grassmann variables $\overline{\Psi}_l$, Ψ_m by the term degree of freedom; $l_1<l_2<\cdots<l_k$, $m_1<m_2<\cdots<m_k$ in the following):

$$\mathsf{P}^{(2n-2k)\star}_{LM}=\frac{\partial}{\partial A^{(2)}_{l_1,m_1}}\cdots\frac{\partial}{\partial A^{(2)}_{l_k,m_k}}P \tag{31}$$

$$=(-1)^k\frac{\partial}{\partial\eta_{l_1}}\frac{\partial}{\partial\overline{\eta}_{m_1}}\cdots\frac{\partial}{\partial\eta_{l_k}}\frac{\partial}{\partial\overline{\eta}_{m_k}}Z[\{\overline{\eta}\},\{\eta\}]\Big|_{\overline{\eta}=\eta=0}. \tag{32}$$

Recursively, Eq. (31) can be written as follows [$l_k>l_{k-1}$, $m_k>m_{k-1}$; note the different meaning of the indices L, M on the left-hand side (lhs) and on the right-hand side (rhs) of the equation]:

$$\mathsf{P}^{(2n-2k)\star}_{LM}=\frac{\partial\,\mathsf{P}^{(2n-2k+2)\star}_{LM}}{\partial A^{(2)}_{l_k,m_k}}. \tag{33}$$

Let us illustrate the above definitions by means of a simple example. Choose

$$G_0[\{\overline{\chi}\},\{\chi\}]=\sum_{l,m=1}^{n}A^{(2)}_{l,m}\overline{\chi}_l\chi_m. \tag{34}$$

Then

$$Z[\{\overline{\eta}\},\{\eta\}]=\det\mathsf{A}^{(2)}e^{-\overline{\eta}[\mathsf{A}^{(2)}]^{-1}\eta} \tag{35}$$

and

$$\mathsf{P}^{(2n-2k)\star}=C^{\,n-k}(\mathsf{A}^{(2)}) \tag{36}$$

[cf. the references cited in relation to Eq. (A2) of Appendix A and Ref. 77, Sec. 2, Ref. 78, also see Ref. 17, Chap. 1, Sec. 1.9]. Here, $C^{n-k}(\mathsf{A}^{(2)})$ is the $(n-k)$th supplementary compound matrix of the matrix $\mathsf{A}^{(2)}$ (for a definition and some properties of compound matrices see Appendix A). By virtue of Eq. (A6) (see Appendix A) it holds

$$\mathsf{P}^{(2n-2k)\star}\mathsf{P}^{(2k)}=\mathsf{P}^{(2k)}\mathsf{P}^{(2n-2k)\star}=\det\mathsf{A}^{(2)}\mathbf{1}_{\binom{n}{k}}. \tag{37}$$

B. Explicit calculation: $n=2$

The case of the Grassmann algebra $\mathcal{G}_4$ ($n=2$) to be treated in the present section is still algebraically fairly simple but already exhibits many of the features which we will meet in considering the larger Grassmann algebras $\mathcal{G}_6$, $\mathcal{G}_8$. Therefore, to some extent this section serves a didactical purpose in order to give the reader a precise idea of the calculations to be performed in the following two sections. These calculations will proceed exactly by the same steps as in this section but the algebraic complexity of the expressions will grow considerably. Also from a practical, calculational point of view it is advisable to choose an approach which proceeds stepwise from the most simple case ($n=2$) to the more involved ones ($n=3,4$) in order to accumulate experience in dealing with this growing complexity. On the other hand, the case $n=2$ is special in some respect and deserves attention in its own right.

According to our general ansatz (18) we put

$$G_0[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)}+\sum_{l,m=1}^{2}A^{(2)}_{l,m}\overline{\Psi}_l\Psi_m+A^{(4)}_{12,12}\overline{\Psi}_1\overline{\Psi}_2\Psi_1\Psi_2 \tag{38}$$

and $G[\{\overline{\Psi}\},\{\Psi\}]$ can be written in the same way

$$G[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)\prime}+\sum_{l,m=1}^{2} A^{(2)\prime}_{l,m}\overline{\Psi}_l\Psi_m+A^{(4)\prime}_{12,12}\overline{\Psi}_1\overline{\Psi}_2\Psi_1\Psi_2. \tag{39}$$

No other terms will occur for symmetry reasons. One quickly finds for the partition function [cf. Eq. (30)]

$$P=e^{A^{(0)\prime}}=\mathsf{P}^{(4)\star}=\det \mathsf{A}^{(2)}-\mathsf{A}^{(4)\star}. \tag{40}$$

Of course, here $\mathsf{A}^{(4)\star}=A^{(4)}_{12,12}$ applies—again ignoring the fact that (very formally) these constants live in different spaces, cf. Eq. (24). The notation $\mathsf{P}^{(4)\star}$ is introduced in order to indicate how in larger Grassmann algebras this partition function transforms under linear (unitary) transformations of the two subsets $\{\overline{\Psi}\}$, $\{\Psi\}$ of the generators of the Grassmann algebra. Clearly, $\mathsf{P}^{(4)\star}$ then transforms exactly the same way as $\mathsf{A}^{(4)\star}$ does and this fact suggests the chosen notation. (The same will apply to any other partition function $\mathsf{P}^{(2n)\star}$ for larger Grassmann algebras $\mathcal{G}_{2n}$.) The result of the map $g_2\circ g_1$ reads (adj B denotes here the adjoint matrix of the matrix B)

$$W[\{\overline{\eta}\},\{\eta\}]=\ln \mathsf{P}^{(4)\star}-\sum_{l,m=1}^{2}\frac{(\mathrm{adj}\mathsf{A}^{(2)})_{lm}}{\mathsf{P}^{(4)\star}}\overline{\eta}_l\eta_m+\frac{A^{(4)}_{12,12}}{(\mathsf{P}^{(4)\star})^2}\overline{\eta}_1\overline{\eta}_2\eta_1\eta_2. \tag{41}$$

The only assumption made to arrive at this result is that $\mathsf{P}^{(4)\star}\neq 0$. We can now proceed on the basis of the general Eq. (13) specified to $n=2$,

$$G[\{\overline{\Psi}\},\{\Psi\}]=W[\{\overline{\eta}\},\{\eta\}]-\sum_{l=1}^{2}(\overline{\eta}_l\Psi_l+\overline{\Psi}_l\eta_l). \tag{42}$$

We insert Eq. (39) onto the lhs of Eq. (42) and the explicit expressions for $\overline{\eta}$, η found from Eq. (39) according to Eq. (16) on its rhs. Comparing coefficients on both sides we find the following two coupled equations:

$$\mathsf{A}^{(2)\prime}=2\mathsf{A}^{(2)\prime}-\mathsf{A}^{(2)\prime}\frac{\mathrm{adj}\mathsf{A}^{(2)}}{\mathsf{P}^{(4)\star}}\mathsf{A}^{(2)\prime}, \tag{43}$$

$$A^{(4)\prime}_{12,12}=4A^{(4)\prime}_{12,12}-2\frac{\mathrm{tr}[\mathsf{A}^{(2)\prime}\ \mathrm{adj}\mathsf{A}^{(2)}]}{\mathsf{P}^{(4)\star}}A^{(4)\prime}_{12,12}+\left(\frac{\det \mathsf{A}^{(2)\prime}}{\mathsf{P}^{(4)\star}}\right)^2 A^{(4)}_{12,12}. \tag{44}$$

Equation (43) can immediately be simplified to read

$$\mathsf{A}^{(2)\prime}=\mathsf{A}^{(2)\prime}\frac{\mathrm{adj}\,\mathsf{A}^{(2)}}{\mathsf{P}^{(4)\star}}\mathsf{A}^{(2)\prime}. \tag{45}$$

From Eq. (45) one recognizes that the matrix $\mathsf{A}^{(2)\prime}$ is the generalized {2}-inverse of the matrix $\mathrm{adj}\,\mathsf{A}^{(2)}/\mathsf{P}^{(4)\star}$ (cf., e.g., Ref. 79, Chap. 1, p. 7).

We can now successively solve the Eqs. (43), (44). Choosing $\det \mathsf{A}^{(2)\prime}\neq 0$ [By virtue of Eq. (45) this entails $\det \mathsf{A}^{(2)}\neq 0$.], we immediately find from Eq. (45)

$$\mathsf{A}^{(2)\prime}=\left(\frac{\mathsf{P}^{(4)\star}}{\det \mathsf{A}^{(2)}}\right)\mathsf{A}^{(2)}. \tag{46}$$

Inserting this expression for $\mathsf{A}^{(2)\prime}$ into Eq. (44) yields the following solution:

$$A^{(4)\prime}_{12,12}=\left(\frac{\mathsf{P}^{(4)\star}}{\det \mathsf{A}^{(2)}}\right)^2 A^{(4)}_{12,12}\,. \tag{47}$$

In analogy to Eq. (40), we can now define a quantity

$$\mathsf{P}^{(4)\star\prime}=\det \mathsf{A}^{(2)\prime}-\mathsf{A}^{(4)\star\prime} \tag{48}$$

and from Eqs. (46), (47) we find [taking into account Eq. (40)]

$$\mathsf{P}^{(4)\star\prime}=\frac{(\mathsf{P}^{(4)\star})^3}{(\det \mathsf{A}^{(2)})^2}=\left(\frac{\mathsf{P}^{(4)\star}}{\det \mathsf{A}^{(2)}}\right)^2 \mathsf{P}^{(4)\star}. \tag{49}$$

Taking the determinant on both sides of Eq. (46) provides us with the following useful relation:

$$\det \mathsf{A}^{(2)\prime}=\frac{(\mathsf{P}^{(4)\star})^2}{\det \mathsf{A}^{(2)}}. \tag{50}$$

Up to this point, very little is special to the case $n=2$ and we will meet the analogous equations in the next sections.

We turn now to some features which are closely related to the algebraic simplicity of the case $n=2$ and which cannot easily be identified in larger Grassmann algebras. The Eqs. (49) and (50) can now be combined to yield the equation

$$\mathsf{P}^{(4)\star\prime}=\frac{\det \mathsf{A}^{(2)\prime}}{\det \mathsf{A}^{(2)}}\,\mathsf{P}^{(4)\star}, \tag{51}$$

which is converted ($\mathsf{P}^{(4)\star}, \det \mathsf{A}^{(2)\prime}\neq 0$ entail $\mathsf{P}^{(4)\star\prime}\neq 0$) into

$$\frac{\det \mathsf{A}^{(2)\prime}}{\mathsf{P}^{(4)\star\prime}}=\frac{\det \mathsf{A}^{(2)}}{\mathsf{P}^{(4)\star}}\,. \tag{52}$$

An equivalent form of Eq. (52) is

$$\frac{A^{(4)\prime}_{12,12}}{\det \mathsf{A}^{(2)\prime}}=\frac{A^{(4)}_{12,12}}{\det \mathsf{A}^{(2)}}. \tag{53}$$

From Eqs. (52) and (53) we recognize that for $n=2$ the action map f has an invariant which can be calculated from the left- or right-hand sides of these equations.

We are now going to invert the action map f.[80] From Eqs. (49) and (52) we easily find

$$\mathsf{P}^{(4)\star}=\frac{(\det \mathsf{A}^{(2)\prime})^2}{\mathsf{P}^{(4)\star\prime}}=\left(\frac{\det \mathsf{A}^{(2)\prime}}{\mathsf{P}^{(4)\star\prime}}\right)^2 \mathsf{P}^{(4)\star\prime}. \tag{54}$$

Equation (52) also allows us to find the following inversion formulas for the map f from Eqs. (46), (47):

$$\mathsf{A}^{(2)}=\left(\frac{\det \mathsf{A}^{(2)\prime}}{\mathsf{P}^{(4)\star\prime}}\right)\mathsf{A}^{(2)\prime}, \tag{55}$$

$$A^{(4)}_{12,12}=\left(\frac{\det \mathsf{A}^{(2)\prime}}{\mathsf{P}^{(4)\star\prime}}\right)^2 A^{(4)\prime}_{12,12}\,. \tag{56}$$

From the above equations we see that for $n=2$ the action map f can easily be inverted (once one assumes $\mathsf{P}^{(4)\star}\neq 0$, $\det \mathsf{A}^{(2)}\neq 0$, $\mathsf{P}^{(4)\star\prime}\neq 0$, $\det \mathsf{A}^{(2)\prime}\neq 0$).

C. Explicit calculation: $n=3$

The case $n=3$ is already considerably more involved in comparison with the case $n=2$ treated in the preceding section. In the present and the next sections, as far as possible and appropriate we will apply the same wording as in Sec. II B in order to emphasize their close relation.

We start by parametrizing G_0 and G according to our general ansatz [cf. Eq. (18) and Eqs. (38), (39)].

$$G_0[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)}+\sum_{l,m=1}^{3}A^{(2)}_{l,m}\overline{\Psi}_l\Psi_m+\frac{1}{4}\sum_{l_1,l_2,m_1,m_2=1}^{3}A^{(4)}_{l_1l_2,m_1m_2}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\Psi_{m_1}\Psi_{m_2}$$
$$+A^{(6)}_{123,123}\overline{\Psi}_1\overline{\Psi}_2\overline{\Psi}_3\Psi_1\Psi_2\Psi_3, \tag{57}$$

$$G[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)\prime}+\sum_{l,m=1}^{3}A^{(2)\prime}_{l,m}\overline{\Psi}_l\Psi_m+\frac{1}{4}\sum_{l_1,l_2,m_1,m_2=1}^{3}A^{(4)\prime}_{l_1l_2,m_1m_2}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\Psi_{m_1}\Psi_{m_2}$$
$$+A^{(6)\prime}_{123,123}\overline{\Psi}_1\overline{\Psi}_2\overline{\Psi}_3\Psi_1\Psi_2\Psi_3. \tag{58}$$

For the partition function we find [cf. Eq. (30)]

$$P=e^{A^{(0)\prime}}=\mathsf{P}^{(6)\star}=\det\mathsf{A}^{(2)}-\mathrm{tr}(\mathsf{A}^{(4)\star}\mathsf{A}^{(2)})-\mathsf{A}^{(6)\star} \tag{59}$$
$$=-2\det\mathsf{A}^{(2)}+\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})-\mathsf{A}^{(6)\star}. \tag{60}$$

In analogy to Eq. (40), here $\mathsf{A}^{(6)\star}=A^{(6)}_{123,123}$ applies. In the lower line [Eq. (60)], we use the notation [cf. Eqs. (31) and (40)]

$$\mathsf{P}^{(4)}=C_2(\mathsf{A}^{(2)})-\mathsf{A}^{(4)},\quad \mathsf{P}^{(4)\star}=\mathrm{adj}\,\mathsf{A}^{(2)}-\mathsf{A}^{(4)\star} \tag{61}$$

[$\mathrm{adj}\,\mathsf{A}^{(2)}=C_2(\mathsf{A}^{(2)})^\star$].

After some calculation we obtain the following expression for $W[\{\overline{\eta}\},\{\eta\}]$ (to arrive at it we only assume $\mathsf{P}^{(6)\star}\neq 0$):

$$W[\{\overline{\eta}\},\{\eta\}]=\ln\mathsf{P}^{(6)\star}-\frac{\mathsf{P}^{(4)\star}_{lm}}{\mathsf{P}^{(6)\star}}\overline{\eta}_l\eta_m-\frac{\mathsf{A}^{(2)\star}_{ML}}{\mathsf{P}^{(6)\star}}\overline{\eta}_{l_1}\overline{\eta}_{l_2}\eta_{m_1}\eta_{m_2}-\frac{1}{2}\left(\frac{\mathsf{P}^{(4)\star}_{lm}}{\mathsf{P}^{(6)\star}}\overline{\eta}_l\eta_m\right)^2$$
$$+\frac{1}{\mathsf{P}^{(6)\star}}\left[1-\frac{\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})}{\mathsf{P}^{(6)\star}}+\frac{2\det\mathsf{P}^{(4)\star}}{(\mathsf{P}^{(6)\star})^2}\right]\overline{\eta}_1\overline{\eta}_2\overline{\eta}_3\eta_1\eta_2\eta_3. \tag{62}$$

Here and in the following we use the notation $B_{ML}\overline{\eta}_{l_1}\overline{\eta}_{l_2}\eta_{m_1}\eta_{m_2}$ for a multiple sum over l_1, l_2, m_1, m_2 with the restrictions $l_1<l_2$, $m_1<m_2$ applied; $L=\{l_1,l_2\}$, $M=\{m_1,m_2\}$. The analogous convention is also applied to multiple sums over more indices. To arrive at the further results it is useful to take note of the equation

$$(\mathsf{P}^{(4)\star}_{lm}\overline{\eta}_l\eta_m)^2=-2\,C_2(\mathsf{P}^{(4)\star})_{LM}\,\overline{\eta}_{l_1}\overline{\eta}_{l_2}\eta_{m_1}\eta_{m_2}\,. \tag{63}$$

We proceed now exactly the same way as in Sec. II B. We insert Eq. (58) onto the lhs of Eq. (13) and the explicit expressions for $\overline{\eta}$, η found from Eq. (58) according to Eq. (16) on its rhs. Again, comparing coefficients on both sides we find the following three coupled nonlinear matrix equations:

$$\mathsf{A}^{(2)\prime}=2\mathsf{A}^{(2)\prime}-\mathsf{A}^{(2)\prime}\frac{\mathsf{P}^{(4)\star}}{\mathsf{P}^{(6)\star}}\mathsf{A}^{(2)\prime}, \tag{64}$$

$$\mathsf{A}^{(4)\star\prime}=4\mathsf{A}^{(4)\star\prime}+\mathsf{A}^{(4)\star\prime}\frac{\mathsf{A}^{(2)\prime}\mathsf{P}^{(4)\star}-\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(4)\star})\mathbf{1}_3}{\mathsf{P}^{(6)\star}}$$
$$+\frac{\mathsf{P}^{(4)\star}\mathsf{A}^{(2)\prime}-\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)\prime})\mathbf{1}_3}{\mathsf{P}^{(6)\star}}\mathsf{A}^{(4)\star\prime}-\mathrm{adj}\,\mathsf{A}^{(2)\prime}\frac{\mathsf{P}^{(6)\star}\mathsf{A}^{(2)}-\mathrm{adj}\,\mathsf{P}^{(4)\star}}{(\mathsf{P}^{(6)\star})^2}\mathrm{adj}\,\mathsf{A}^{(2)\prime}, \tag{65}$$

$$A^{(6)\prime}_{123,123}=6A^{(6)\prime}_{123,123}+\frac{2}{\mathsf{P}^{(6)\star}}\Big\{-A^{(6)\prime}_{123,123}\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)\prime})+\mathrm{tr}(\mathsf{P}^{(4)\star}\mathrm{adj}\mathsf{A}^{(4)\star\prime})$$
$$+\mathrm{tr}(\mathsf{A}^{(2)}\mathrm{adj}\mathsf{A}^{(2)\prime})\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{A}^{(4)\star\prime})-\det\mathsf{A}^{(2)\prime}\mathrm{tr}(\mathsf{A}^{(2)}\mathsf{A}^{(4)\star\prime})+\frac{(\det\mathsf{A}^{(2)\prime})^2}{2}\Big\}$$
$$+\frac{2}{(\mathsf{P}^{(6)\star})^2}\Big\{\det\mathsf{A}^{(2)\prime}\mathrm{tr}(\mathsf{A}^{(4)\star\prime}\mathrm{adj}\ \mathsf{P}^{(4)\star})-\mathrm{tr}[\mathrm{adj}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(4)\star})]\,\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{A}^{(4)\star\prime})$$
$$-\frac{1}{2}(\det\mathsf{A}^{(2)\prime})^2\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})\Big\}+\frac{2}{(\mathsf{P}^{(6)\star})^3}(\det\mathsf{A}^{(2)\prime})^2\det\mathsf{P}^{(4)\star}. \tag{66}$$

Equation (64) is equivalent to the equation

$$\mathsf{A}^{(2)\prime}=\mathsf{A}^{(2)\prime}\frac{\mathsf{P}^{(4)\star}}{\mathsf{P}^{(6)\star}}\mathsf{A}^{(2)\prime}. \tag{67}$$

The matrix $\mathsf{A}^{(2)\prime}$ is the generalized {2}-inverse of the matrix $\mathsf{P}^{(4)\star}/\mathsf{P}^{(6)\star}$ (cf., e.g., Ref. 79, Chap. 1, p. 7).

In analogy to the procedure applied in Sec. II B, we can now successively solve the Eqs. (64)–(66). Choosing $\det\mathsf{A}^{(2)\prime}\neq 0$ [by virtue of Eq. (67) this entails $\det\mathsf{P}^{(4)\star}\neq 0$], we immediately find from Eq. (67) an explicit expression for $\mathsf{A}^{(2)\prime}$. This can be inserted into Eq. (65) to also find an explicit expression for $\mathsf{A}^{(4)\star\prime}$. Finally, both these explicit expressions for $\mathsf{A}^{(2)\prime}$ and $\mathsf{A}^{(4)\star\prime}$ can now be inserted into Eq. (66) to solve it for $A^{(6)\prime}_{123,123}$. The results obtained read as follows:

$$\mathsf{A}^{(2)\prime}=\mathsf{P}^{(6)\star}[\mathsf{P}^{(4)\star}]^{-1}=\frac{\mathsf{P}^{(6)\star}}{\det\mathsf{P}^{(4)\star}}\mathrm{adj}\,\mathsf{P}^{(4)\star}, \tag{68}$$

$$\mathsf{A}^{(4)\star\prime}=-\frac{(\mathsf{P}^{(6)\star})^2}{\det\mathsf{P}^{(4)\star}}\left[\frac{\mathsf{P}^{(6)\star}}{\det\mathsf{P}^{(4)\star}}\mathsf{P}^{(4)\star}\mathsf{A}^{(2)}\mathsf{P}^{(4)\star}-\mathsf{P}^{(4)\star}\right], \tag{69}$$

$$A^{(6)\prime}_{123,123}=\frac{(\mathsf{P}^{(6)\star})^5}{(\det\mathsf{P}^{(4)\star})^2}\left\{1-\frac{2}{\det\mathsf{P}^{(4)\star}}\mathrm{tr}[\mathrm{adj}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})]\right\}+\frac{3(\mathsf{P}^{(6)\star})^4}{(\det\mathsf{P}^{(4)\star})^2}\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})-\frac{4(\mathsf{P}^{(6)\star})^3}{\det\mathsf{P}^{(4)\star}}. \tag{70}$$

In deriving Eq. (70) we have made use of the identity (B2) given in Appendix B. In analogy to the Eqs. (61) and (59), we can now define

$$\mathsf{P}^{(4)\star\prime}=\mathrm{adj}\,\mathsf{A}^{(2)\prime}-\mathsf{A}^{(4)\star\prime}, \tag{71}$$

$$\mathsf{P}^{(6)\star\prime}=\det\mathsf{A}^{(2)\prime}-\mathrm{tr}(\mathsf{A}^{(4)\star\prime}\mathsf{A}^{(2)\prime})-\mathsf{A}^{(6)\star\prime}, \tag{72}$$

and from the Eqs. (68)–(70) we find

$$\mathsf{P}^{(4)\star\prime}=\frac{(\mathsf{P}^{(6)\star})^3}{(\det\mathsf{P}^{(4)\star})^2}\mathsf{P}^{(4)\star}\mathsf{A}^{(2)}\mathsf{P}^{(4)\star}, \tag{73}$$

$$\mathsf{P}^{(6)\star\prime}=-\frac{(\mathsf{P}^{(6)\star})^5}{(\det \mathsf{P}^{(4)\star})^2}\left\{1-\frac{2}{\det \mathsf{P}^{(4)\star}}\,\mathrm{tr}[\,\mathrm{adj}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})]\right\}-\frac{2(\mathsf{P}^{(6)\star})^4}{(\det \mathsf{P}^{(4)\star})^2}\,\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{A}^{(2)})+\frac{2(\mathsf{P}^{(6)\star})^3}{\det \mathsf{P}^{(4)\star}}. \tag{74}$$

Taking the determinant on both sides of the Eqs. (68) and (73) provides us with the following useful relations:

$$\det \mathsf{A}^{(2)\prime}=\frac{(\mathsf{P}^{(6)\star})^3}{\det \mathsf{P}^{(4)\star}}, \tag{75}$$

$$\det \mathsf{P}^{(4)\star\prime}=\frac{(\mathsf{P}^{(6)\star})^9}{(\det \mathsf{P}^{(4)\star})^4}\det \mathsf{A}^{(2)}. \tag{76}$$

Finally, also for the case $n=3$ we derive equations which describe the inverse of the action map f (the comment made in Ref. 80 of Sec. II B also applies here). From Eqs. (68), (69), (73), we find

$$\mathsf{P}^{(4)\star}=\mathsf{P}^{(6)\star}[\mathsf{A}^{(2)\prime}]^{-1}=\frac{\mathsf{P}^{(6)\star}}{\det \mathsf{A}^{(2)\prime}}\,\mathrm{adj}\,\mathsf{A}^{(2)\prime}, \tag{77}$$

$$\mathsf{A}^{(4)\star}=\frac{\mathsf{P}^{(6)\star}}{\det \mathsf{A}^{(2)\prime}}\left\{\frac{\mathsf{P}^{(6)\star}}{(\det \mathsf{A}^{(2)\prime})^3}\,\mathrm{adj}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(4)\star\prime}\mathsf{A}^{(2)\prime})-\mathrm{adj}\,\mathsf{A}^{(2)\prime}\right\}, \tag{78}$$

$$\mathsf{A}^{(2)}=\frac{\mathsf{P}^{(6)\star}}{(\det \mathsf{A}^{(2)\prime})^2}\,\mathsf{A}^{(2)\prime}\mathsf{P}^{(4)\star\prime}\mathsf{A}^{(2)\prime}, \tag{79}$$

where now $\mathsf{P}^{(6)\star}$ is being understood as a function of the primed quantities whose explicit shape remains to be determined. Inserting Eqs. (77), (78) into Eq. (74) allows us to derive the following explicit representation of the partition function $\mathsf{P}^{(6)\star}$ in terms of the primed quantities:

$$\mathsf{P}^{(6)\star}=(\det \mathsf{A}^{(2)\prime})^2\left\{2\det \mathsf{A}^{(2)\prime}-2\,\mathrm{tr}(\mathsf{P}^{(4)\star\prime}\mathsf{A}^{(2)\prime})+\frac{2}{\det \mathsf{A}^{(2)\prime}}\,\mathrm{tr}[\,\mathrm{adj}(\mathsf{P}^{(4)\star\prime}\mathsf{A}^{(2)\prime})]-\mathsf{P}^{(6)\star\prime}\right\}^{-1}. \tag{80}$$

In principle, on the basis of this result also an explicit representation of $A^{(6)}_{123,123}$ in terms of the primed quantities can be established [relying on Eq. (59)] but we refrain from also writing it down here. As one recognizes from Eq. (80), in the case $n=3$ the description of the inverse of the action map f already involves fairly complicated expressions and we will not attempt to generalize these in the next section to the case $n=4$.

The results obtained in the present section can be checked for consistency in two ways. First, based on the procedure described in the Introduction in the context of Eqs. (19) and (20) one can convince oneself that the results—wherever appropriate—are consistent with the results obtained in Sec. II B for the case of the Grassmann algebra $\mathcal{G}_4$ $(n=2)$. Second, choosing for $G_0[\{\overline{\Psi}\},\{\Psi\}]$ the form (34) one can also convince oneself that then $\mathsf{A}^{(2)\prime}=\mathsf{A}^{(2)}$ and $\mathsf{A}^{(4)\star\prime}$, $A^{(6)\prime}_{123,123}$ vanish as expected.

D. Explicit calculation: $n=4$

We are now prepared to study the algebraically most involved case to be treated in the present paper—the case of the Grassmann algebra $\mathcal{G}_8$ $(n=4)$. The calculational experience collected in the last two sections allows us to manage the fairly involved expressions.

We start again by parametrizing G_0 and G according to our general ansatz [cf. Eq. (18)],

$$G_0[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)}+\sum_{l,m=1}^{4}A^{(2)}_{l,m}\overline{\Psi}_l\Psi_m+\frac{1}{4}\sum_{l_1,l_2,m_1,m_2=1}^{4}A^{(4)}_{l_1l_2,m_1m_2}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\Psi_{m_1}\Psi_{m_2}$$
$$+\frac{1}{36}\sum_{l_1,l_2,l_3,m_1,m_2,m_3=1}^{4}A^{(6)}_{l_1l_2l_3,m_1m_2m_3}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\overline{\Psi}_{l_3}\Psi_{m_1}\Psi_{m_2}\Psi_{m_3}$$
$$+A^{(8)}_{1234,1234}\overline{\Psi}_1\overline{\Psi}_2\overline{\Psi}_3\overline{\Psi}_4\Psi_1\Psi_2\Psi_3\Psi_4. \tag{81}$$

For G the analogous representation can be used,

$$G[\{\overline{\Psi}\},\{\Psi\}]=A^{(0)\prime}+\sum_{l,m=1}^{4}A^{(2)\prime}_{l,m}\overline{\Psi}_l\Psi_m+\frac{1}{4}\sum_{l_1,l_2,m_1,m_2=1}^{4}A^{(4)\prime}_{l_1l_2,m_1m_2}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\Psi_{m_1}\Psi_{m_2}$$
$$+\frac{1}{36}\sum_{l_1,l_2,l_3,m_1,m_2,m_3=1}^{4}A^{(6)\prime}_{l_1l_2l_3,m_1m_2m_3}\overline{\Psi}_{l_1}\overline{\Psi}_{l_2}\overline{\Psi}_{l_3}\Psi_{m_1}\Psi_{m_2}\Psi_{m_3}$$
$$+A^{(8)\prime}_{1234,1234}\overline{\Psi}_1\overline{\Psi}_2\overline{\Psi}_3\overline{\Psi}_4\Psi_1\Psi_2\Psi_3\Psi_4. \tag{82}$$

The partition function reads [cf. Eq. (30)]

$$P=e^{A^{(0)\prime}}=\mathsf{P}^{(8)\star}=\det\mathsf{A}^{(2)}-\mathrm{tr}[\mathsf{A}^{(4)\star}C_2(\mathsf{A}^{(2)})]+\tfrac{1}{2}\mathrm{tr}(\mathsf{A}^{(4)\star}\mathsf{A}^{(4)})-\mathrm{tr}(\mathsf{A}^{(6)\star}\mathsf{A}^{(2)})+\mathsf{A}^{(8)\star} \tag{83}$$
$$=6\det\mathsf{A}^{(2)}-2\,\mathrm{tr}[\mathsf{P}^{(4)\star}C_2(\mathsf{A}^{(2)})]+\tfrac{1}{2}\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{P}^{(4)})+\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)})+\mathsf{A}^{(8)\star}. \tag{84}$$

In analogy to Eq. (40), here $\mathsf{A}^{(8)\star}=A^{(8)}_{1234,1234}$ applies. In the lower line [Eq. (84)], we have made use of the expressions [cf. Eqs. (61), (59)]

$$\mathsf{P}^{(4)\star}=C_2(\mathsf{A}^{(2)})^{\star}-\mathsf{A}^{(4)\star}, \tag{85}$$

$$\mathsf{P}^{(6)\star}=\mathrm{adj}\,\mathsf{A}^{(2)}-\mathsf{F}_a(\mathsf{A}^{(2)},\mathsf{A}^{(4)})-\mathsf{A}^{(6)\star} \tag{86}$$

($\mathrm{adj}\,\mathsf{A}^{(2)}=C_3(\mathsf{A}^{(2)})^{\star}$). The form F_a is defined as follows:

$$\mathsf{F}_a(\mathsf{A}^{(2)},\mathsf{A}^{(4)})_{lm}=\epsilon_{lrK}\epsilon_{msN}\mathsf{A}^{(2)}_{sr}\mathsf{A}^{(4)}_{NK}. \tag{87}$$

In making the transition from Eq. (83) to Eq. (84) we have used the relations

$$2\,\mathrm{tr}[C_2(\mathsf{A}^{(2)})\mathsf{A}^{(4)\star}]=\mathrm{tr}[\mathsf{F}_a(\mathsf{A}^{(2)},\mathsf{A}^{(4)})\mathsf{A}^{(2)}], \tag{88}$$

$$C_2(\mathsf{A}^{(2)})C_2(\mathsf{A}^{(2)})^{\star}=C_2(\mathsf{A}^{(2)})^{\star}C_2(\mathsf{A}^{(2)})=\det\mathsf{A}^{(2)}\mathbf{1}_6 \tag{89}$$

[Eq. (89) is a special case of Eq. (A6), see Appendix A]. As next step, we can calculate $W[\{\overline{\eta}\},\{\eta\}]$ which reads (to arrive at it we only assume $\mathsf{P}^{(8)\star}\neq 0$)

$$W[\{\overline{\eta}\},\{\eta\}]=\ln\mathsf{P}^{(8)\star}-\frac{\mathsf{P}^{(6)\star}_{lm}}{\mathsf{P}^{(8)\star}}\overline{\eta}_l\eta_m-\frac{\mathsf{P}^{(4)\star}_{LM}}{\mathsf{P}^{(8)\star}}\overline{\eta}_{l_1}\overline{\eta}_{l_2}\eta_{m_1}\eta_{m_2}-\frac{1}{2}\left(\frac{\mathsf{P}^{(6)\star}_{lm}}{\mathsf{P}^{(8)\star}}\overline{\eta}_l\eta_m\right)^2$$
$$+\frac{1}{\mathsf{P}^{(8)\star}}\left[\mathsf{A}^{(2)\star}-\frac{\mathsf{F}_a(\mathsf{P}^{(6)\star},\mathsf{P}^{(4)\star})^{\star}}{\mathsf{P}^{(8)\star}}+\frac{2\,C_3(\mathsf{P}^{(6)\star})}{(\mathsf{P}^{(8)\star})^2}\right]_{LM}\overline{\eta}_{l_1}\overline{\eta}_{l_2}\overline{\eta}_{l_3}\eta_{m_1}\eta_{m_2}\eta_{m_3}$$
$$+\frac{1}{\mathsf{P}^{(8)\star}}\left\{1-\frac{\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)})}{\mathsf{P}^{(8)\star}}-\frac{\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{P}^{(4)})}{2\,\mathsf{P}^{(8)\star}}+\frac{2\,\mathrm{tr}[\mathsf{P}^{(4)}C_2(\mathsf{P}^{(6)\star})]}{(\mathsf{P}^{(8)\star})^2}\right.$$
$$\left.-\frac{6\det\mathsf{P}^{(6)\star}}{(\mathsf{P}^{(8)\star})^3}\right\}\overline{\eta}_1\overline{\eta}_2\overline{\eta}_3\overline{\eta}_4\eta_1\eta_2\eta_3\eta_4. \tag{90}$$

In the following, we need a number of forms which we list here for further reference. The index convention applied here requires some explanation. For example, $(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{ltur}$ up to the sign denotes elements of the 6×6 matrix $\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)}$. If $l<t$, $u<r$, it denotes the matrix element $(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{\{l,t\}\{u,r\}}$. If $l>t$, $u<r$, it denotes the matrix element $(-\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{\{t,l\}\{u,r\}}$ and if $l<t$, $u>r$, it denotes the matrix element $(-\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{\{l,t\}\{r,u\}}$. And finally, if $l>t$, $u>r$, it denotes the matrix element $(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{\{t,l\}\{r,u\}}$. Of course, $(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{\{l,t\}\{u,r\}}=0$ if $l=t$ or $u=r$. In the following, summation is understood over repeated indices:

$$\mathsf{F}_b(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})_{LM}=\epsilon_{Lrk}\,(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})_{sr}\,\epsilon_{skM}\,, \tag{91}$$

$$\mathsf{F}_c(\mathsf{A}^{(4)\star\prime},\mathsf{P}^{(6)\star},\mathsf{A}^{(4)\star\prime})_{lm}=(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{ltur}\mathsf{P}^{(6)\star}_{sr}(\mathcal{E}^{(2)}\mathsf{A}^{(4)\star\prime})_{stum}\,, \tag{92}$$

$$\mathsf{F}_{d1}(\mathsf{A}^{(4)\star\prime},\mathsf{A}^{(2)\prime},\mathsf{P}^{(4)}C_2(\mathsf{A}^{(2)\prime})^\star)_{lm}=(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{lrtu}\mathsf{A}^{(2)\prime}_{sr}[\mathcal{E}^{(2)}\mathsf{P}^{(4)}C_2(\mathsf{A}^{(2)\prime})^\star]_{tsum}\,, \tag{93}$$

$$\mathsf{F}_{d2}(C_2(\mathsf{A}^{(2)\prime})^\star\mathsf{P}^{(4)},\mathsf{A}^{(2)\prime},\mathsf{A}^{(4)\star\prime})_{lm}=[C_2(\mathsf{A}^{(2)\prime})^\star\mathsf{P}^{(4)}\mathcal{E}^{(2)}]_{lutr}\mathsf{A}^{(2)\prime}_{sr}(\mathcal{E}^{(2)}\mathsf{A}^{(4)\star\prime})_{tusm}\,, \tag{94}$$

$$\mathsf{F}_e(\mathsf{A}^{(2)\prime},\mathsf{A}^{(4)\prime},\mathsf{A}^{(4)\prime},\mathsf{A}^{(2)\prime})_{LM}=\mathcal{E}^{(2)}_{Lab}\mathsf{A}^{(2)\prime}_{ra}(\mathcal{E}^{(2)}\mathsf{A}^{(4)\prime})_{rtbu}(\mathsf{A}^{(4)\prime}\mathcal{E}^{(2)})_{dtsu}\mathsf{A}^{(2)\prime}_{cs}\mathcal{E}^{(2)}_{cdM}\,, \tag{95}$$

$$\mathsf{F}_f(\mathsf{A}^{(4)\star\prime},\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star},\mathsf{A}^{(4)\prime})_{lm}=(\mathsf{A}^{(4)\star\prime}\mathcal{E}^{(2)})_{lcda}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})_{ba}(\mathcal{E}^{(2)}\mathsf{A}^{(4)\prime})_{bdcm}\,, \tag{96}$$

$$\begin{aligned}\mathsf{F}_g(&C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)},\mathsf{P}^{(6)\star},\mathsf{P}^{(6)\star},\mathsf{P}^{(4)}C_2(\mathsf{P}^{(6)\star}))_{LM}\\&=\mathcal{E}^{(2)}_{Lab}[\mathcal{E}^{(2)}C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}]_{arbt}\mathsf{P}^{(6)\star}_{rs}\mathsf{P}^{(6)\star}_{tu}[\mathsf{P}^{(4)}C_2(\mathsf{P}^{(6)\star})\mathcal{E}^{(2)}]_{csdu}\mathcal{E}^{(2)}_{cdM}\,.\end{aligned} \tag{97}$$

To arrive at the further results it is useful to take note of the equation

$$(\mathsf{P}^{(6)\star}_{lm}\overline{\eta}_l\eta_m)^2=-2C_2(\mathsf{P}^{(6)\star})_{LM}\overline{\eta}_{l_1}\overline{\eta}_{l_2}\eta_{m_1}\eta_{m_2}. \tag{98}$$

We now apply exactly the same procedure as in Secs. II B, II C. We insert Eq. (82) onto the lhs of Eq. (13) and the explicit expressions for $\overline{\eta}$, η found from Eq. (82) according to Eq. (16) on its rhs. Again, comparing coefficients on both sides we find the following four coupled nonlinear matrix equations:

$$\mathsf{A}^{(2)\prime}=2\mathsf{A}^{(2)\prime}-\mathsf{A}^{(2)\prime}\frac{\mathsf{P}^{(6)\star}}{\mathsf{P}^{(8)\star}}\mathsf{A}^{(2)\prime}, \tag{99}$$

$$\begin{aligned}\mathsf{A}^{(4)\star\prime}=&4\mathsf{A}^{(4)\star\prime}-\frac{\mathsf{F}_b(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})}{\mathsf{P}^{(8)\star}}\mathsf{A}^{(4)\star\prime}-\mathsf{A}^{(4)\star\prime}\frac{\mathsf{F}_b(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime})}{\mathsf{P}^{(8)\star}}\\&-C_2(\mathsf{A}^{(2)\prime})^\star\frac{\mathsf{P}^{(8)\star}\mathsf{P}^{(4)}-C_2(\mathsf{P}^{(6)\star})^\star}{(\mathsf{P}^{(8)\star})^2}C_2(\mathsf{A}^{(2)\prime})^\star,\end{aligned} \tag{100}$$

$$\begin{aligned}\mathsf{A}^{(6)\star\prime}=&6\mathsf{A}^{(6)\star\prime}+\frac{1}{\mathsf{P}^{(8)\star}}\{\mathsf{A}^{(6)\star\prime}[\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}-\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})\mathbf{1}_4]\\&+[\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}-\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime})\mathbf{1}_4]\mathsf{A}^{(6)\star\prime}-\mathsf{F}_c(\mathsf{A}^{(4)\star\prime},\mathsf{P}^{(6)\star},\mathsf{A}^{(4)\star\prime})\\&+\mathsf{F}_{d1}(\mathsf{A}^{(4)\star\prime},\mathsf{A}^{(2)\prime},\mathsf{P}^{(4)}C_2(\mathsf{A}^{(2)\prime})^\star)+\mathsf{F}_{d2}(C_2(\mathsf{A}^{(2)\prime})^\star\mathsf{P}^{(4)},\mathsf{A}^{(2)\prime},\mathsf{A}^{(4)\star\prime})\\&+\mathrm{adj}(\mathsf{A}^{(2)\prime})\mathsf{A}^{(2)}\,\mathrm{adj}(\mathsf{A}^{(2)\prime})\}-\frac{1}{(\mathsf{P}^{(8)\star})^2}\{\mathsf{F}_{d1}(\mathsf{A}^{(4)\star\prime},\mathsf{A}^{(2)\prime},C_2(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})^\star)\\&+\mathsf{F}_{d2}(C_2(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime})^\star,\mathsf{A}^{(2)\prime},\mathsf{A}^{(4)\star\prime})+\mathrm{adj}(\mathsf{A}^{(2)\prime})\mathsf{F}_a(\mathsf{P}^{(6)\star},\mathsf{P}^{(4)\star})\mathrm{adj}(\mathsf{A}^{(2)\prime})\}\\&+\frac{2}{(\mathsf{P}^{(8)\star})^3}\mathrm{adj}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}),\end{aligned} \tag{101}$$

$$
\begin{aligned}
A^{(8)\prime}_{1234,1234} = 8A^{(8)\prime}_{1234,1234} + \frac{1}{\mathsf{P}^{(8)\star}}\{ & -2A^{(8)\prime}_{1234,1234}\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}) - 2\,\mathrm{tr}[\mathsf{P}^{(6)\star}\mathsf{F}_a(\mathsf{A}^{(6)\star\prime},\mathsf{A}^{(4)\star\prime})] \\
& - 2\,\mathrm{tr}[\mathsf{A}^{(2)\prime}\mathsf{A}^{(6)\star\prime}\mathsf{A}^{(2)\prime}\mathsf{F}_a(\mathsf{A}^{(2)\prime},\mathsf{P}^{(4)})] - \mathrm{tr}[\mathsf{P}^{(4)}\mathsf{F}_e(\mathsf{A}^{(2)\prime},\mathsf{A}^{(4)\prime},\mathsf{A}^{(4)\prime},\mathsf{A}^{(2)\prime})] \\
& - \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(\mathsf{P}^{(4)\star}C_2(\mathsf{A}^{(2)\prime}),\mathbf{1}_4,\mathsf{A}^{(4)\star\prime}\mathsf{A}^{(4)\prime})] - \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(\mathsf{A}^{(4)\prime}\mathsf{A}^{(4)\star\prime},\mathbf{1}_4,C_2(\mathsf{A}^{(2)\prime})\mathsf{P}^{(4)\star})] \\
& + \mathrm{tr}[\mathsf{A}^{(4)\star\prime}C_2(\mathsf{A}^{(2)\prime})\mathsf{F}_b((\mathrm{adj}\,\mathsf{A}^{(2)\prime})\mathsf{A}^{(2)})] + \mathrm{tr}[C_2(\mathsf{A}^{(2)\prime})\mathsf{A}^{(4)\star\prime}\mathsf{F}_b(\mathsf{A}^{(2)}\,\mathrm{adj}\,\mathsf{A}^{(2)\prime})] \\
& + (\det\mathsf{A}^{(2)\prime})^2\} + \frac{1}{(\mathsf{P}^{(8)\star})^2}\{2\,\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{A}^{(6)\star\prime}\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star})\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}) \\
& - 2\,\mathrm{tr}(\mathsf{A}^{(2)\prime}\mathsf{A}^{(6)\star\prime}\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}) + \mathrm{tr}[\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}\mathsf{F}_c(\mathsf{A}^{(4)\star\prime},\mathsf{P}^{(6)\star},\mathsf{A}^{(4)\star\prime})] \\
& - \mathrm{tr}[\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}\mathsf{F}_f(\mathsf{A}^{(4)\star\prime},\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star},\mathsf{A}^{(4)\prime})] + \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}),\mathbf{1}_4,\mathsf{A}^{(4)\star\prime}\mathsf{A}^{(4)\prime})] \\
& + \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(\mathsf{A}^{(4)\prime}\mathsf{A}^{(4)\star\prime},\mathbf{1}_4,C_2(\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}))] \\
& - \mathrm{tr}[\mathsf{F}_a(\mathsf{P}^{(6)\star},\mathsf{P}^{(4)\star})\mathsf{F}_a(\mathbf{1}_4,\mathsf{A}^{(4)\star\prime}C_2(\mathsf{A}^{(2)\prime}))\mathrm{adj}\,\mathsf{A}^{(2)\prime}] \\
& - \mathrm{tr}[\mathsf{F}_a(\mathbf{1}_4,C_2(\mathsf{A}^{(2)\prime})\mathsf{A}^{(4)\star\prime})\mathsf{F}_a(\mathsf{P}^{(6)\star},\mathsf{P}^{(4)\star})\mathrm{adj}\,\mathsf{A}^{(2)\prime}] \\
& - (\det\mathsf{A}^{(2)\prime})^2[\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)}) + \tfrac{1}{2}\mathrm{tr}(\mathsf{P}^{(4)\star}\mathsf{P}^{(4)})]\} \\
& + \frac{2}{(\mathsf{P}^{(8)\star})^3}\{\mathrm{tr}[\mathsf{A}^{(4)\star\prime}C_2(\mathsf{A}^{(2)\prime})\mathsf{F}_b(\mathrm{adj}\ (\mathsf{P}^{(6)\star}\mathsf{A}^{(2)\prime}))] \\
& + \mathrm{tr}[C_2(\mathsf{A}^{(2)\prime})\mathsf{A}^{(4)\star\prime}\mathsf{F}_b(\mathrm{adj}\ (\mathsf{A}^{(2)\prime}\mathsf{P}^{(6)\star}))] \\
& + (\det\mathsf{A}^{(2)\prime})^2\mathrm{tr}[\mathsf{P}^{(4)}C_2(\mathsf{P}^{(6)\star})]\} - \frac{6}{(\mathsf{P}^{(8)\star})^4}(\det\mathsf{A}^{(2)\prime})^2\det\mathsf{P}^{(6)\star}. \qquad (102)
\end{aligned}
$$

Equation (99) is equivalent to the equation

$$
\mathsf{A}^{(2)\prime} = \mathsf{A}^{(2)\prime}\frac{\mathsf{P}^{(6)\star}}{\mathsf{P}^{(8)\star}}\mathsf{A}^{(2)\prime}. \qquad (103)
$$

The matrix $\mathsf{A}^{(2)\prime}$ is the generalized {2}-inverse of the matrix $\mathsf{P}^{(6)\star}/\mathsf{P}^{(8)\star}$ (cf., e.g., Ref. 79, Chap. 1, p. 7).

For solving the Eqs. (99)–(102) we apply again the same method as in Secs. II B and II C. Choosing $\det\mathsf{A}^{(2)\prime} \neq 0$ [by virtue of Eq. (103) this entails $\det\mathsf{P}^{(6)\star} \neq 0$], we immediately find from Eq. (103) an explicit expression for $\mathsf{A}^{(2)\prime}$. This can be inserted into Eq. (100) to also find an explicit expression for $\mathsf{A}^{(4)\star\prime}$.

$$
\mathsf{A}^{(2)\prime} = \mathsf{P}^{(8)\star}\,[\mathsf{P}^{(6)\star}]^{-1} = \frac{\mathsf{P}^{(8)\star}}{\det\mathsf{P}^{(6)\star}}\mathrm{adj}\,\mathsf{P}^{(6)\star}, \qquad (104)
$$

$$
\mathsf{A}^{(4)\star\prime} = -\frac{(\mathsf{P}^{(8)\star})^2}{\det\,\mathsf{P}^{(6)\star}}\left[\frac{\mathsf{P}^{(8)\star}}{\det\mathsf{P}^{(6)\star}}C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}C_2(\mathsf{P}^{(6)\star}) - C_2(\mathsf{P}^{(6)\star})\right]. \qquad (105)
$$

To arrive at Eq. (105) we have relied on the following calculation [cf. Appendix A, Eqs. (A6), (A5)]:

$$C_2(\mathsf{A}^{(2)\prime})^\star = (\mathsf{P}^{(8)\star})^2 C_2([\mathsf{P}^{(6)\star}]^{-1})^\star = \frac{(\mathsf{P}^{(8)\star})^2}{\det \mathsf{P}^{(6)\star}} C_2([\mathsf{P}^{(6)\star}]^{-1})^{-1} = \frac{(\mathsf{P}^{(8)\star})^2}{\det \mathsf{P}^{(6)\star}} C_2(\mathsf{P}^{(6)\star}). \tag{106}$$

Having obtained explicit expressions for $\mathsf{A}^{(2)\prime}$ and $\mathsf{A}^{(4)\star\prime}$ we can now insert them into Eq. (101) to solve it. We find

$$\begin{aligned}\mathsf{A}^{(6)\star\prime} = {} & \frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2} \mathsf{P}^{(6)\star} \Big\{ \mathsf{A}^{(2)} - \frac{1}{2 \det \mathsf{P}^{(6)\star}} \mathsf{F}_{d1}(\mathsf{P}^{(4)}, \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}) \\ & - \frac{1}{2 \det \mathsf{P}^{(6)\star}} \mathsf{F}_{d2}(\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, \mathsf{P}^{(4)}) \Big\} \mathsf{P}^{(6)\star} \\ & + \frac{3(\mathsf{P}^{(8)\star})^4}{(\det \mathsf{P}^{(6)\star})^2} \mathsf{P}^{(6)\star} \mathsf{F}_a(\mathsf{P}^{(6)\star}, \mathsf{P}^{(4)\star}) \mathsf{P}^{(6)\star} - \frac{4(\mathsf{P}^{(8)\star})^3}{\det \mathsf{P}^{(6)\star}} \mathsf{P}^{(6)\star} \end{aligned} \tag{107}$$

$$\begin{aligned} = {} & \frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2} \mathsf{P}^{(6)\star} \mathsf{A}^{(2)} \mathsf{P}^{(6)\star} \\ & + \frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^4} \mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star})) \\ & + \frac{3(\mathsf{P}^{(8)\star})^4}{(\det \mathsf{P}^{(6)\star})^2} \mathsf{P}^{(6)\star} \mathsf{F}_a(\mathsf{P}^{(6)\star}, \mathsf{P}^{(4)\star}) \mathsf{P}^{(6)\star} - \frac{4(\mathsf{P}^{(8)\star})^3}{\det \mathsf{P}^{(6)\star}} \mathsf{P}^{(6)\star}. \end{aligned} \tag{108}$$

The equivalence of Eqs. (107) and (108) is based on the relation

$$\begin{aligned} & (\det \mathsf{P}^{(6)\star}) \mathsf{P}^{(6)\star} \mathsf{F}_{d1}(\mathsf{P}^{(4)}, \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}) \mathsf{P}^{(6)\star} \\ & \quad = (\det \mathsf{P}^{(6)\star}) \mathsf{P}^{(6)\star} \mathsf{F}_{d2}(\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, \mathsf{P}^{(4)}) \mathsf{P}^{(6)\star} \\ & \quad = -\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star})). \end{aligned} \tag{109}$$

Finally, inserting Eqs. (104), (105), (108) into (102) allows us to find the following explicit solution for $A^{(8)\prime}_{1234,1234}$:

$$\begin{aligned} A^{(8)\prime}_{1234,1234} = {} & \frac{(\mathsf{P}^{(8)\star})^7}{(\det \mathsf{P}^{(6)\star})^2} \{1 - 2\,\mathrm{tr}[\mathsf{A}^{(2)} \mathsf{F}_a((\mathsf{P}^{(6)\star})^{-1}, \mathsf{P}^{(4)})]\} \\ & + \frac{(\mathsf{P}^{(8)\star})^7}{(\det \mathsf{P}^{(6)\star})^4} \{\mathrm{tr}[\mathsf{P}^{(4)} \mathsf{F}_g(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}, \mathsf{P}^{(6)\star}, \mathsf{P}^{(6)\star}, \mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}))] \\ & - \tfrac{1}{2}\,\mathrm{tr}[\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}\mathsf{P}^{(4)\star} C_2(\mathsf{P}^{(6)\star})^\star, \mathbf{1}_4, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)})] \\ & - \tfrac{1}{2}\,\mathrm{tr}[\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})^\star \mathsf{P}^{(4)\star}\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathbf{1}_4, \mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}))]\} \\ & + \frac{(\mathsf{P}^{(8)\star})^6}{(\det \mathsf{P}^{(6)\star})^2} \Big\{ \frac{11}{2} \mathrm{tr}(\mathsf{P}^{(4)}\mathsf{P}^{(4)\star}) + 5\,\mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)}) \\ & - \frac{5}{\det \mathsf{P}^{(6)\star}} \mathrm{tr}[\mathsf{F}_a(\mathbf{1}_4, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}) \mathsf{F}_a(\mathbf{1}_4, \mathsf{P}^{(4)\star} C_2(\mathsf{P}^{(6)\star})^\star)] \Big\} \\ & + 18 \frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2} \mathrm{tr}[\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star})] - 30 \frac{(\mathsf{P}^{(8)\star})^4}{\det \mathsf{P}^{(6)\star}}. \end{aligned} \tag{110}$$

In analogy to the Eqs. (85), (86) and (83), we can now define

$$\mathsf{P}^{(4)\star\prime} = C_2(\mathsf{A}^{(2)\prime})^\star - \mathsf{A}^{(4)\star\prime}, \tag{111}$$

$$\mathsf{P}^{(6)\star\prime} = \mathrm{adj}\,\mathsf{A}^{(2)\prime} - \mathsf{F}_a(\mathsf{A}^{(2)\prime}, \mathsf{A}^{(4)\prime}) - \mathsf{A}^{(6)\star\prime}, \tag{112}$$

$$\mathsf{P}^{(8)\star\prime} = \det \mathsf{A}^{(2)\prime} - \mathrm{tr}[\mathsf{A}^{(4)\star\prime} C_2(\mathsf{A}^{(2)\prime})] + \tfrac{1}{2}\mathrm{tr}(\mathsf{A}^{(4)\star\prime}\mathsf{A}^{(4)\prime}) - \mathrm{tr}(\mathsf{A}^{(6)\star\prime}\mathsf{A}^{(2)\prime}) + \mathsf{A}^{(8)\star\prime}, \tag{113}$$

and from Eqs. (104), (105), (108), (110), we find

$$\mathsf{P}^{(4)\star\prime} = \frac{(\mathsf{P}^{(8)\star})^3}{(\det \mathsf{P}^{(6)\star})^2} C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \tag{114}$$

$$\begin{aligned}
\mathsf{P}^{(6)\star\prime} = &-\frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2}\mathsf{P}^{(6)\star}\Bigg\{\mathsf{A}^{(2)} - \frac{1}{2\det \mathsf{P}^{(6)\star}}\mathsf{F}_{d1}(\mathsf{P}^{(4)}, \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}) \\
&- \frac{1}{2\det \mathsf{P}^{(6)\star}}\mathsf{F}_{d2}(\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, \mathsf{P}^{(4)})\Bigg\}\mathsf{P}^{(6)\star} \\
&- \frac{2(\mathsf{P}^{(8)\star})^4}{(\det \mathsf{P}^{(6)\star})^2}\mathsf{P}^{(6)\star}\mathsf{F}_a(\mathsf{P}^{(6)\star}, \mathsf{P}^{(4)\star})\mathsf{P}^{(6)\star} + \frac{2(\mathsf{P}^{(8)\star})^3}{\det \mathsf{P}^{(6)\star}}\mathsf{P}^{(6)\star}
\end{aligned} \tag{115}$$

$$\begin{aligned}
= &-\frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2}\mathsf{P}^{(6)\star}\mathsf{A}^{(2)}\mathsf{P}^{(6)\star} \\
&- \frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^4}\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathsf{P}^{(6)\star}, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star})) \\
&- \frac{2(\mathsf{P}^{(8)\star})^4}{(\det \mathsf{P}^{(6)\star})^2}\mathsf{P}^{(6)\star}\mathsf{F}_a(\mathsf{P}^{(6)\star}, \mathsf{P}^{(4)\star})\mathsf{P}^{(6)\star} + \frac{2(\mathsf{P}^{(8)\star})^3}{\det \mathsf{P}^{(6)\star}}\mathsf{P}^{(6)\star},
\end{aligned} \tag{116}$$

$$\begin{aligned}
\mathsf{P}^{(8)\star\prime} = &\frac{(\mathsf{P}^{(8)\star})^7}{(\det \mathsf{P}^{(6)\star})^2}\{1 - 2\mathrm{tr}[\mathsf{A}^{(2)}\mathsf{F}_a((\mathsf{P}^{(6)\star})^{-1}, \mathsf{P}^{(4)})]\} \\
&+ \frac{(\mathsf{P}^{(8)\star})^7}{(\det \mathsf{P}^{(6)\star})^4}\{\mathrm{tr}[\mathsf{P}^{(4)}\mathsf{F}_g(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}, \mathsf{P}^{(6)\star}, \mathsf{P}^{(6)\star}, \mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}))] \\
&- \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)}\mathsf{P}^{(4)\star} C_2(\mathsf{P}^{(6)\star})^\star, \mathbf{1}_4, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)})] \\
&- \tfrac{1}{2}\mathrm{tr}[\mathsf{F}_c(C_2(\mathsf{P}^{(6)\star})^\star\mathsf{P}^{(4)\star}\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}), \mathbf{1}_4, \mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star}))]\} \\
&+ 4\frac{(\mathsf{P}^{(8)\star})^6}{(\det \mathsf{P}^{(6)\star})^2}\Bigg\{\mathrm{tr}(\mathsf{P}^{(4)}\mathsf{P}^{(4)\star}) + \mathrm{tr}(\mathsf{P}^{(6)\star}\mathsf{A}^{(2)}) \\
&- \frac{1}{\det \mathsf{P}^{(6)\star}}\mathrm{tr}[\mathsf{F}_a(\mathbf{1}_4, C_2(\mathsf{P}^{(6)\star})\mathsf{P}^{(4)})\mathsf{F}_a(\mathbf{1}_4, \mathsf{P}^{(4)\star} C_2(\mathsf{P}^{(6)\star})^\star)]\Bigg\} \\
&+ 12\frac{(\mathsf{P}^{(8)\star})^5}{(\det \mathsf{P}^{(6)\star})^2}\mathrm{tr}[\mathsf{P}^{(4)} C_2(\mathsf{P}^{(6)\star})] - 16\frac{(\mathsf{P}^{(8)\star})^4}{\det \mathsf{P}^{(6)\star}}.
\end{aligned} \tag{117}$$

Taking the determinant on both sides of the Eqs. (104) and (114) provides us with the following useful relations:

$$\det \mathsf{A}^{(2)\prime} = \frac{(\mathsf{P}^{(8)\star})^4}{\det \mathsf{P}^{(6)\star}}, \tag{118}$$

$$\det \mathsf{P}^{(4)\star\prime} = \frac{(\mathsf{P}^{(8)\star})^{18}}{(\det \mathsf{P}^{(6)\star})^{6}} \det \mathsf{P}^{(4)\star}. \tag{119}$$

In deriving Eq. (119) we have relied on the following (Sylvester–Franke) identity [cf. Appendix A, Eq. (A8)].

$$\det C_2(\mathsf{P}^{(6)\star}) = (\det \mathsf{P}^{(6)\star})^3. \tag{120}$$

We can finally check the obtained results for consistency in the same way as done at the end of the preceding section for $n=3$. First, based on the procedure described in the Introduction in the context of Eqs. (19), (20) one can convince oneself again that the results—wherever appropriate—are consistent with the results obtained in Sec. II C for the case of the Grassmann algebra $\mathcal{G}_6$ ($n=3$). Second, choosing for $G_0[\{\bar{\Psi}\},\{\Psi\}]$ the form (34) one can also convince oneself that then $\mathsf{A}^{(2)\prime} = \mathsf{A}^{(2)}$ and $\mathsf{A}^{(4)\star\prime}$, $\mathsf{A}^{(6)\star\prime}$, $A^{(8)\prime}_{1234,1234}$ vanish as expected. Given the combinatorial factors involved, this represents a fairly sensitive check of the present results.

E. Some heuristics for arbitrary *n*

Having gained a fairly broad calculational and structural experience in the preceding sections in considering the present formalism for the case of the Grassmann algebras $\mathcal{G}_{2n}$, $n=2,3,4$, we are going to generalize now some of the obtained results to arbitrary values of n. This analytic extrapolation is a heuristic procedure with heuristic purposes. No proof is being attempted here which would need to be the subject of a separate study.

From Eqs. (46), (68), (104) and (47), (69), (105) we infer the following general (for arbitrary values of n) form of the matrices $\mathsf{A}^{(2)\prime}$, $\mathsf{A}^{(4)\prime}$ (of course, the result for $\mathsf{A}^{(2)\prime}$ is elementary),

$$\mathsf{A}^{(2)\prime} = \mathsf{P}^{(2n)\star}[\mathsf{P}^{(2n-2)\star}]^{-1} = \frac{\mathsf{P}^{(2n)\star}}{\det \mathsf{P}^{(2n-2)\star}} \operatorname{adj} \mathsf{P}^{(2n-2)\star}, \tag{121}$$

$$\mathsf{A}^{(4)\prime} = -\frac{(\mathsf{P}^{(2n)\star})^2}{\det \mathsf{P}^{(2n-2)\star}} \left[\frac{\mathsf{P}^{(2n)\star}}{\det \mathsf{P}^{(2n-2)\star}} C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star} \mathsf{P}^{(2n-4)\star} C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star} - C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star} \right]. \tag{122}$$

Emphasizing the role of the effective propagator $\mathsf{P}^{(2n-2)\star}/\mathsf{P}^{(2n)\star}$ [cf. Eq. (121)] we can rewrite Eq. (122) in the following form:

$$\mathsf{A}^{(4)\prime} = -\frac{C_{n-2}\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)^{\star}}{\det\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)} \frac{\mathsf{P}^{(2n-4)\star}}{\mathsf{P}^{(2n)\star}} \frac{C_{n-2}\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)^{\star}}{\det\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)} + \frac{C_{n-2}\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)^{\star}}{\det\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)}. \tag{123}$$

Unfortunately, the results obtained in the preceding sections do not yet admit any reliable analytical (heuristic) extrapolation to arbitrary values of n for further quantities beyond $\mathsf{A}^{(2)\prime}$, $\mathsf{A}^{(4)\prime}$. For example, to heuristically derive an analogous expression for $\mathsf{A}^{(6)\prime}$ one would have to perform a calculation for $n=5$ first in order to approach this task. However, in analogy to the preceding sections it is still possible to derive one further result for arbitrary n. Again, writing [cf. Eqs. (48), (71), (111)]

$$\mathsf{P}^{(4)\star\prime} = C_2(\mathsf{A}^{(2)\prime})^{\star} - \mathsf{A}^{(4)\star\prime} \tag{124}$$

we find from Eqs. (121), (122) [cf. Eqs. (49), (73), (114)]

$$\mathsf{P}^{(4)\prime}=\frac{(\mathsf{P}^{(2n)\star})^3}{(\det \mathsf{P}^{(2n-2)\star})^2}C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star}\mathsf{P}^{(2n-4)\star}C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star}. \tag{125}$$

In analogy to Eq. (123), this can equivalently be written as

$$\mathsf{P}^{(4)\prime}=\frac{C_{n-2}\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)^{\star}}{\det\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)}\frac{\mathsf{P}^{(2n-4)\star}}{\mathsf{P}^{(2n)\star}}\frac{C_{n-2}\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)^{\star}}{\det\left(\dfrac{\mathsf{P}^{(2n-2)\star}}{\mathsf{P}^{(2n)\star}}\right)}. \tag{126}$$

To arrive at Eq. (125) we have relied on the following calculation [cf. Appendix A, Eqs. (A6), (A5)]:

$$\begin{aligned}C_2(\mathsf{A}^{(2)\prime})&=(\mathsf{P}^{(2n)\star})^2C_2([\mathsf{P}^{(2n-2)\star}]^{-1})\\&=(\mathsf{P}^{(2n)\star})^2C_2(\mathsf{P}^{(2n-2)\star})^{-1}\\&=\frac{(\mathsf{P}^{(2n)\star})^2}{\det \mathsf{P}^{(2n-2)\star}}C_{n-2}(\mathsf{P}^{(2n-2)\star})^{\star}.\end{aligned} \tag{127}$$

Taking the determinant on both sides of the Eqs. (121) and (126) yields the relations [cf. Eqs. (50), (75), (118) and (76), (119)]

$$\det \mathsf{A}^{(2)\prime}=\frac{(\mathsf{P}^{(2n)\star})^n}{\det \mathsf{P}^{(2n-2)\star}}, \tag{128}$$

$$\det \mathsf{P}^{(4)\star\prime}=\frac{(\mathsf{P}^{(2n)\star})^{3\binom{n}{2}}}{(\det \mathsf{P}^{(2n-2)\star})^{2(n-1)}}\det \mathsf{P}^{(2n-4)}. \tag{129}$$

In deriving Eq. (129) we have relied on the (Sylvester–Franke) identity [cf. Appendix A, Eq. (A8)]

$$\det C_{n-2}(\mathsf{P}^{(2n-2)\star})=(\det \mathsf{P}^{(2n-2)\star})^{\binom{n-1}{n-3}}. \tag{130}$$

III. THE GRASSMANN INTEGRAL EQUATION

Having obtained in the preceding section explicit formulas for the action map f for the case of the Grassmann algebras $\mathcal{G}_{2n}$, $n=2,3,4$, we can now concentrate on the study of certain particular relations between $G_0[\{\overline{\Psi}\},\{\Psi\}]$ and $G[\{\overline{\Psi}\},\{\Psi\}]$. As explained in the Introduction we are interested in the equation $(0<\lambda\in\mathbf{R})$

$$G[\{\overline{\Psi}\},\{\Psi\}]=G_0[\{\lambda\overline{\Psi}\},\{\lambda\Psi\}]+\Delta_f(\lambda). \tag{131}$$

$\Delta_f(\lambda)$ is some constant which is allowed to depend on λ and which we choose to obey [in view of Eq. (29), we have the freedom to do so]

$$\Delta_f(1)=0. \tag{132}$$

For $\lambda=1$, Eq. (131) is the fixed point equation for the action map f (cf. Ref. 73, p. 288). Equation (131) applied to Eq. (15), the latter reads $(\widetilde{C}=\exp[-A^{(0)}-\Delta_f(\lambda)])$

$$e^{\,G_0[\{\lambda\overline{\Psi}\},\{\lambda\Psi\}]}=\widetilde{C}\int\prod_{l=1}^{n}(\mathrm{d}\chi_l\,\mathrm{d}\overline{\chi}_l)\,e^{\,G_0[\{\overline{\chi}+\overline{\Psi}\},\{\chi+\Psi\}]+\Sigma_{l=1}^{n}(\overline{\eta}_l\chi_l+\overline{\chi}_l\eta_l)}, \tag{133}$$

$$\overline{\eta}_l = \frac{\partial G_0[\{\lambda\overline{\Psi}\},\{\lambda\Psi\}]}{\partial\Psi_l}, \quad \eta_l = -\frac{\partial G_0[\{\lambda\overline{\Psi}\},\{\lambda\Psi\}]}{\partial\overline{\Psi}_l}. \tag{134}$$

Clearly, this a Grassmann integral equation for $G_0[\{\overline{\Psi}\},\{\Psi\}]$ (more precisely, a nonlinear Grassmann integro-differential equation). In view of Eq. (18), Eq. (131) is equivalent to

$$A^{(0)\prime} = A^{(0)} + \Delta_f(\lambda), \tag{135}$$

$$\mathsf{A}^{(2k)\prime} = \lambda^{2k}\mathsf{A}^{(2k)}, \quad k>0. \tag{136}$$

Equation (136) represents a coupled system of nonlinear matrix equations. We are now going to solve Eq. (133) [i.e., Eq. (131)] for $n=2,3,4$ by solving Eq. (136).

A. The case $n=2$

Applying Eq. (136) for $k=1$ to Eq. (46), we find

$$\mathsf{P}^{(4)\star} = \lambda^2 \det \mathsf{A}^{(2)}. \tag{137}$$

Equation (40) then immediately yields

$$A^{(4)}_{12,12} = (1-\lambda^2)\det \mathsf{A}^{(2)}. \tag{138}$$

$\mathsf{A}^{(2)}$ remains an arbitrary matrix with $\det \mathsf{A}^{(2)} \neq 0$. To determine $A^{(0)}$ imagine that the action $G_0[\{\overline{\Psi}\},\{\Psi\}]$ specified by Eq. (138) would have been induced by some action $G_{-1}[\{\overline{\Psi}\},\{\Psi\}] = G_0[\{\lambda^{-1}\overline{\Psi}\},\{\lambda^{-1}\Psi\}]$ [by means of Eq. (15)—replacing G by G_0 and G_0 by G_{-1}, respectively] with the partition function $P(G_{-1}) = \lambda^{-2}\det \mathsf{A}^{(2)}$ [cf. Eq. (40)]. Then (cf. Ref. 80 of Sec. II B)

$$A^{(0)} = \ln P(G_{-1}) = \ln\det \mathsf{A}^{(2)} - 2\ln\lambda \tag{139}$$

and, consequently,

$$\Delta_f(\lambda) = 4\ln\lambda. \tag{140}$$

From the above considerations we see that for $n=2$, Eq. (131) has always a solution for any value of λ $(0<\lambda\in\mathbf{R})$. For $\lambda=1$ the solution corresponds to a Gaussian integral while for $\lambda\neq 1$ it corresponds to some non-Gaussian integral [cf. Eq. (133)]. Consequently, for any even value of n Eq. (131) has always a solution for any value of λ $(0<\lambda\in\mathbf{R})$. This follows from the fact that these solutions can be constructed as a sum of $n=2$ solutions with a common value of λ.

B. The case $n=3$

Applying Eq. (136) for $k=1$ to Eq. (68), we find

$$\mathsf{P}^{(6)\star}\mathbf{1}_3 = \lambda^2\mathsf{P}^{(4)\star}\mathsf{A}^{(2)} = \lambda^2\mathsf{A}^{(2)}\mathsf{P}^{(4)\star} \tag{141}$$

$$= \lambda^2[\det \mathsf{A}^{(2)}\mathbf{1}_3 - \mathsf{A}^{(4)\star}\mathsf{A}^{(2)}] = \lambda^2[\det \mathsf{A}^{(2)}\mathbf{1}_3 - \mathsf{A}^{(2)}\mathsf{A}^{(4)\star}]. \tag{142}$$

Furthermore, combining Eqs. (75), (76), (71), (136) we obtain the relations

$$\lambda^6 \det \mathsf{P}^{(4)\star} \det \mathsf{A}^{(2)} = (\mathsf{P}^{(6)\star})^3, \tag{143}$$

$$\lambda^{12}\frac{(\det \mathsf{P}^{(4)\star})^5}{\det \mathsf{A}^{(2)}} = (\mathsf{P}^{(6)\star})^9. \tag{144}$$

From these two equations we can conclude that

$$\det \mathsf{P}^{(4)\star} = \pm \lambda^3 (\det \mathsf{A}^{(2)})^2, \tag{145}$$

$$\mathsf{P}^{(6)\star} = \pm \lambda^3 \det \mathsf{A}^{(2)}. \tag{146}$$

Taking into account the above equations, from Eq. (69) we find then

$$\mathsf{A}^{(4)\star} = -\left(1 \mp \frac{1}{\lambda}\right) \mathsf{P}^{(4)\star}. \tag{147}$$

By virtue of Eq. (61) this entails

$$\mathsf{A}^{(4)\star} = (1 \mp \lambda)\,\mathrm{adj}\,\mathsf{A}^{(2)}, \tag{148}$$

$$\mathsf{P}^{(4)\star} = \pm \lambda\ \mathrm{adj}\,\mathsf{A}^{(2)}. \tag{149}$$

One easily sees that Eq. (149) is in line with the result (145). Finally, applying Eqs. (136), (141), (145), (146) to Eq. (70) we calculate $A^{(6)}_{123,123}$. It reads

$$A^{(6)}_{123,123} = (\lambda \mp 1)^2 (\pm \lambda - 4) \det \mathsf{A}^{(2)}. \tag{150}$$

Applying the same procedure to Eq. (74), we find the consistency equation

$$(\lambda \mp 1)^3 = 0, \tag{151}$$

which has only one solution, namely $\lambda = 1$ (choose the upper sign). This solution is just the elementary one which corresponds to a Gaussian integral [cf. Eq. (133)].

C. The case $n=4$

Applying Eq. (136) for $k=1$ to Eq. (104), we find

$$\mathsf{P}^{(8)\star} \mathbf{1}_4 = \lambda^2 \mathsf{P}^{(6)\star} \mathsf{A}^{(2)} = \lambda^2 \mathsf{A}^{(2)} \mathsf{P}^{(6)\star} \tag{152}$$

$$= \lambda^2 [\det \mathsf{A}^{(2)} \mathbf{1}_4 - \mathsf{F}_a(\mathbf{1}_4, C_2(\mathsf{A}^{(2)})^\star \mathsf{A}^{(4)\star}) - \mathsf{A}^{(6)\star} \mathsf{A}^{(2)}]$$

$$= \lambda^2 [\det \mathsf{A}^{(2)} \mathbf{1}_4 - \mathsf{F}_a(\mathbf{1}_4, \mathsf{A}^{(4)\star} C_2(\mathsf{A}^{(2)})^\star) - \mathsf{A}^{(2)} \mathsf{A}^{(6)\star}]. \tag{153}$$

Furthermore, combining Eqs. (118), (119), (111), (136) we obtain the relations

$$\lambda^8 \det \mathsf{P}^{(6)\star} \det \mathsf{A}^{(2)} = (\mathsf{P}^{(8)\star})^4, \tag{154}$$

$$\lambda^{24} (\det \mathsf{P}^{(6)\star})^6 = (\mathsf{P}^{(8)\star})^{18}. \tag{155}$$

From these two equations we can conclude that

$$\det \mathsf{P}^{(6)\star} = \lambda^8 (\det \mathsf{A}^{(2)})^3, \tag{156}$$

$$\mathsf{P}^{(8)\star} = \pm \lambda^4 \det \mathsf{A}^{(2)}. \tag{157}$$

We can now apply Eq. (136) to the Eqs. (105) and (114). Taking into account Eqs. (85), (111), we can derive from these two equations the following compound matrix equation:

$$C_2(\mathsf{P}^{(6)\star} \mathsf{A}^{(2)}) = (\lambda^2 \det \mathsf{A}^{(2)})^2 \mathbf{1}_6. \tag{158}$$

Its solution reads [cf. Ref. 81, Sec. 3, p. 149, Eq. (11)]

$$\mathsf{P}^{(6)\star} = \pm\lambda^2 \,\mathrm{adj}\,\mathsf{A}^{(2)}. \tag{159}$$

Equation (159) is in line with Eq. (156) [the signs on the rhs are fixed by making reference to Eqs. (152), (157)]. We can now take into account Eq. (159) in considering Eq. (114) further. Eq. (114) then yields the following matrix equation:

$$\mathsf{P}^{(4)} C_2(\mathsf{A}^{(2)})^\star = \pm C_2(\mathsf{A}^{(2)})\mathsf{P}^{(4)\star}. \tag{160}$$

By virtue of Eq. (85), Eq. (160) can equivalently be written as

$$\mathsf{A}^{(4)} C_2(\mathsf{A}^{(2)})^\star = \pm C_2(\mathsf{A}^{(2)})\mathsf{A}^{(4)\star}. \tag{161}$$

We will not study here the complete set of solutions of Eq. (161). This would need to be the subject of a study in its own. Here, it suffices to mention that for the ansatz (α is some arbitrary constant, B some 4×4 matrix)

$$\mathsf{A}^{(4)} = \alpha C_2(\mathsf{B})^\star. \tag{162}$$

Equation (161) reads

$$C_2(\mathsf{A}^{(2)}\mathsf{B})^\star = \pm C_2(\mathsf{A}^{(2)}\mathsf{B}). \tag{163}$$

For the upper sign, this is exactly the type of compound matrix equation studied in Ref. 81. Of course, Eq. (161) has solutions which correspond to two $n=2$ solutions (with a common value of λ) discussed at the end of Sec. III A.[82] Here, we want to go beyond these solutions.

For the present purpose, we consider in Eq. (161) only the upper sign on the rhs and study the ansatz ($\kappa \in \mathbf{R}$)

$$\mathsf{P}^{(4)} = \kappa C_2(\mathsf{A}^{(2)}), \tag{164}$$

$$\mathsf{A}^{(4)} = (1-\kappa) C_2(\mathsf{A}^{(2)}), \tag{165}$$

which is a special version of Eq. (162). Inserting this ansatz into Eq. (107) and taking into account Eqs. (136), (157), (159), we find

$$\mathsf{A}^{(6)\star} = (\lambda^2 - 6\kappa^2 + 9\kappa - 4)\,\mathrm{adj}\,\mathsf{A}^{(2)}. \tag{166}$$

Applying the same procedure to Eq. (115), we obtain the following consistency condition:

$$\lambda^2 - 3\kappa^2 + 3\kappa - 1 = \lambda^2 - 3\kappa(\kappa-1) - 1 = 0. \tag{167}$$

Furthermore, applying the ansatz (164) to Eq. (110) and taking into account Eqs. (136), (157), (159) yields

$$A^{(8)}_{1234,1234} = (\lambda^4 + 20\lambda^2 - 24\lambda^2\kappa + 72\kappa^3 - 147\kappa^2 + 108\kappa - 30)\det \mathsf{A}^{(2)}. \tag{168}$$

Again, subjecting Eq. (117) to the same procedure we obtain yet another consistency condition,

$$2\lambda^2 - 3\lambda^2\kappa + 9\kappa^3 - 15\kappa^2 + 9\kappa - 2 = (2-3\kappa)[\lambda^2 - 3\kappa(\kappa-1) - 1] = 0. \tag{169}$$

Obviously, this equation is fulfilled if λ, κ obey Eq. (167). Consequently, we can restrict our attention to solutions of Eq. (167).

From Eq. (167) we conclude that the ansatz (164) provides us with solutions of Eq. (131) for any value of $\lambda \geqslant 1/2$ (if κ assumes real values only). Of particular interest to us are solutions of Eq. (167) for $\lambda = 1$ (see Refs. 28 and 73). In this case, Eq. (167) reads

$$\kappa(\kappa - 1) = 0. \tag{170}$$

Clearly, this equation has two solutions,

$$\kappa_{\mathrm{I}}=1, \tag{171}$$

$$\kappa_{\mathrm{II}}=0. \tag{172}$$

The corresponding expressions for the action $G_0=G$ then read as follows:

$$G_{0\mathrm{I}}[\{\overline{\Psi}\},\{\Psi\}]=G_{0\mathrm{I}}(G_q)=\ln\det \mathsf{A}^{(2)}+G_q, \tag{173}$$

$$G_{0\mathrm{II}}[\{\overline{\Psi}\},\{\Psi\}]=G_{0\mathrm{II}}(G_q)=\ln\det \mathsf{A}^{(2)}+G_q-\tfrac{1}{2}G_q^2+\tfrac{1}{2}G_q^3-\tfrac{3}{8}G_q^4, \tag{174}$$

$$G_q=G_q[\{\overline{\Psi}\},\{\Psi\}]=\sum_{l,m=1}^{4} A^{(2)}_{l,m}\overline{\Psi}_l\Psi_m=\overline{\Psi}\mathsf{A}^{(2)}\Psi. \tag{175}$$

As one can see from Eq. (133) $G_{0\mathrm{I}}$ corresponds to a Gaussian integral while $G_{0\mathrm{II}}$ corresponds to some non-Gaussian integral. While it is well known that for the action $G_0=G_{0\mathrm{I}}$ the equation $G=G_0$ applies it is indeed a remarkable fact that the same is true for $G_0=G_{0\mathrm{II}}$. However, this is not yet the end of remarkable features of these actions. It is also instructive to work out for $\kappa_{\mathrm{I}}=1$ and $\kappa_{\mathrm{II}}=0$ the corresponding expressions for $W[\{\overline{\eta}\},\{\eta\}]$ on the basis of Eq. (90).

$$W_{\mathrm{I}}[\{\overline{\eta}\},\{\eta\}]=W_{\mathrm{I}}(W_q)=G_{0\mathrm{I}}(W_q)=\ln\det \mathsf{A}^{(2)}+W_q, \tag{176}$$

$$W_{\mathrm{II}}[\{\overline{\eta}\},\{\eta\}]=W_{\mathrm{II}}(W_q)=G_{0\mathrm{II}}(W_q)=\ln\det \mathsf{A}^{(2)}+W_q-\tfrac{1}{2}W_q^2+\tfrac{1}{2}W_q^3-\tfrac{3}{8}W_q^4, \tag{177}$$

$$W_q=W_q[\{\overline{\eta}\},\{\eta\}]=-\overline{\eta}[\mathsf{A}^{(2)}]^{-1}\eta. \tag{178}$$

Again, while the relation $W_{\mathrm{I}}=G_{0\mathrm{I}}$ is well known in the present context the equality $W_{\mathrm{II}}=G_{0\mathrm{II}}$ comes as a complete surprise and one can only wonder which general principle is manifesting here itself. We will explore this issue in the next section.

D. Further analysis

We can characterize the solutions $G_{0\mathrm{I}}$, $G_{0\mathrm{II}}$ of the equation (131) found for $n=4$, $\lambda=1$, in the preceding section by two properties which may be of general significance. The first one is related to the identity $W=G_0$ [Eqs. (176) and (177)]. One immediately recognizes that for

$$[\mathsf{A}^{(2)}]^2=-\mathbf{1}_4, \tag{179}$$

$\exp G_0=\exp G_{0\mathrm{I}}(=\exp G=Z)$ and $\exp G_0=\exp G_{0\mathrm{II}}$ are *self-reciprocal* Grassmann functions (of course, this is a well-known property of $\exp G_{0\mathrm{I}}$):

$$\int \prod_{l=1}^{4}(\mathrm{d}\chi_l\,\mathrm{d}\overline{\chi}_l)\;\; e^{\,G_0[\{\overline{\chi}\},\{\chi\}]\,+\,\overline{\eta}\chi\,+\,\overline{\chi}\eta}=e^{\,G_0[\{\overline{\eta}\},\{\eta\}]} \tag{180}$$

[$\det \mathsf{A}^{(2)}=1$, cf. Eq. (179)],[83] i.e., they are eigenfunctions to the Fourier–Laplace transformation[84] to the eigenvalue 1. The term self-reciprocal function is taken from real (complex) analysis where it also denotes eigenfunctions of some integral transformation, in particular, the Fourier transformation.[85–91]

The second property of the solutions $G_{0\mathrm{I}}$, $G_{0\mathrm{II}}$ is related to the identity $G=W$ [apply the fixed point condition $G=G_0$ to the Eqs. (176), (177)]. Taking into account Eqs. (173)–(178), Eqs. (13), (16) tell us that

$$G(G_q)=G(W_q)-\sum_{l=1}^{4}(\overline{\eta}_l\Psi_l+\overline{\Psi}_l\eta_l), \tag{181}$$

$$\overline{\eta}_l=\frac{\partial G(G_q)}{\partial\Psi_l}=-G'(G_q)(\overline{\Psi}\mathsf{A}^{(2)})_l, \tag{182}$$

$$\eta_l=-\frac{\partial G(G_q)}{\partial\overline{\Psi}_l}=-G'(G_q)(\mathsf{A}^{(2)}\Psi)_l. \tag{183}$$

Here,

$$G'(G_q)=\frac{\partial G(G_q)}{\partial G_q}, \tag{184}$$

where G_q is treated as a formal parameter for the moment. In view of Eqs. (182), (183) it holds

$$W_q=-G_q[G'(G_q)]^2. \tag{185}$$

Taking into account the Eqs. (182), (183), (185), Eq. (181) can be written as

$$G(s)=G(-s[G'(s)]^2)+2sG'(s),\quad s=G_q. \tag{186}$$

Equation (186) is of a very general nature. Its shape does not depend on the value of n. Its derivation depends on the fact only that G, W are functions of G_q, W_q, respectively, and that the identity $G=W$ holds. As we demonstrate in Appendix C, Eq. (186) can also be derived under analogous conditions starting from a (Euclidean space–time) version of Eqs. (1)–(5) for a scalar field on a finite lattice. Consequently, until further notice we disregard the fact that s is a bilinear in the Grassmann algebra generators and simply understand Eq. (186) as an equation for a function $G=G(s)$. We will now analyze Eq. (186) further.

Equation (186) appears to be somewhat involved but it can be simplified the following way. We can differentiate both sides of Eq. (186) with respect to s. The resulting equation can be transformed to read

$$\{2s\ G''(s)+G'(s)\}\{1-G'(s)G'(-s[G'(s)]^2)\}=0\,. \tag{187}$$

Equation (187) is being obeyed if either one of the two following equations of very different mathematical nature is respected:

$$2sG''(s)+G'(s)=0, \tag{188}$$

$$G'(s)G'(-s[G'(s)]^2)=1. \tag{189}$$

The solution of the linear differential equation (188) reads

$$G'(s)\sim e^{-\sqrt{s}} \tag{190}$$

entailing

$$G(s)\sim(1+\sqrt{s})e^{-\sqrt{s}}. \tag{191}$$

As $G(s)$ depends on $\sqrt{s}$ this solution is of no relevance in the context of Grassmann algebras. To see this note that the function $G(s)$ contains odd powers of $\sqrt{s}$ in its (Taylor) expansion (in terms of $t=\sqrt{s}$) around $s=0$. If s is being interpreted as a bilinear form in the generators of the

Grassmann algebra these terms have no interpretation within the Grassmann algebra framework.[92] Consequently, in the following we can concentrate our attention onto the nonlinear functional equation (189).

To gain further insight it turns out to be convenient now to define the following functions [the definition in Eq. (193) could equally well read $d(t)=-i\ b(t)$]:

$$b(t)=t\ G'(t^2)\ =\ \frac{1}{2}\frac{\partial}{\partial t}G(t^2), \tag{192}$$

$$d(t)=ib(t). \tag{193}$$

Then, having multiplied both sides by $-\sqrt{s}$ Eq. (189) can be written as ($t=\sqrt{s}$)

$$d^2(t)=d(d(t))=-t. \tag{194}$$

This is an iterative functional equation: the function $d(t)$ is the (second) iterative root of $-\mathbf{1}$ (for a review of iterative functional equations see Ref. 93, in particular Chap. 11, p. 421, Ref. 94, in particular Chap. XV, p. 288, also see Ref. 95, Chap. 2, p. 36). The functional equation (194) has been studied by Massera and Petracca[96] who have pointed out its relation to the equivalent functional equation

$$h(h(x))=\frac{1}{x}. \tag{195}$$

[Define the involution $q(x)=(1-x)/(1+x)$. If $h(x)$ is a solution of Eq. (195) the function $q\circ h\circ q$ is a solution of Eq. (194).] This functional equation characterizes functions h for which $h^{-1}=1/h$ (note in this context Refs. 97–101, in particular Ref. 101, p. 712). Equation (194) has also been studied for real functions in Ref. 102, Chap. II, Sec. 5, p. 54, and in Refs. 103–106. Of course, in view of Eq. (193) in general we are concerned with complex solutions of Eq. (194).

If the function $G'(s)$ has a definite symmetry under $s\rightarrow -s$ Eq. (194) can be simplified to some extent [getting rid of the imaginary unit i present in Eq. (193)]. If $G'(s)$ is an even function [i.e., up to some constant $G(s)$ is odd] Eq. (194) can be written as

$$b^2(t)=b(b(t))=t. \tag{196}$$

This iterative functional equation is a special case of the functional equation $b^k(t)=t$ which is being called the *Babbage equation* (it has been studied first by Charles Babbage.[107–110] See Ref. 94, Chap. XV, Sec. 1, p. 288, Ref. 93, Sec. 11.6, p. 450, for more information and references, recent references not referred to in Refs. 94, 93 are Refs. 111, 112). Solutions $b(t)$ of Eq. (196) (i.e., solutions of the Babbage equation for $k=2$) are called *involutory functions* [*(second) iterative roots of unity/identity, periodic functions/maps*]. If, for example, the function $G(s)$ stands in correspondence to a Gaussian integral [cf. Eq. (133)], $G(s)=s$ and, consequently,

$$b(t)=t. \tag{197}$$

This is the most elementary involutory function one can think of. Note, that the set of solutions of Eq. (196) is very large as this set is equivalent to the set of even function (see, e.g., Refs. 113, 114, Ref. 93, p. 451). If $G'(s)$ is an odd function [i.e., $G(s)$ is even] Eq. (194) can be written as

$$b^2(t)=b(b(t))=-t. \tag{198}$$

However, this case is not very interesting as real functions solving Eq. (198) are necessarily discontinuous (Ref. 94, Chap. XV, §4, p. 299, Refs. 103, 97–101, 104, Ref. 93, Subsec. 11.2B, p. 425).

The above consideration can be applied to the solutions of the Grassmann integral equation found in Sec. III C. Equation (173) is of course being described by Eq. (197) [$b_{\mathrm{I}}(t)=t$]. From Eq. (174) we recognize that the function $G_{\mathrm{II}}(s)$ does not have a definite symmetry under $s\rightarrow -s$. We find

$$b_{\mathrm{II}}(t)=t\ (1-t^2+\tfrac{3}{2}\,t^4-\tfrac{3}{2}\,t^6). \tag{199}$$

and one can check that the corresponding function $d_{\mathrm{II}}(t)=ib_{\mathrm{II}}(t)$ indeed fulfills Eq. (194) at order t^7. [Going through the above arguments one can convince oneself that this is the appropriate order in t one has to take into account for the Grassmann algebra $\mathcal{G}_8$. Order t^7 corresponds to order s^3 in Eq. (189).]

IV. DISCUSSION AND CONCLUSIONS

While most of the explicit expressions obtained in the present paper for the Grassmann algebras $\mathcal{G}_{2n}$, $n=2,3,4$, have been obtained here for the first time, some of them can be compared to results derived earlier by other authors. The point is that partition functions for specific (finite-dimensional) fermionic systems have been obtained by a number of authors and some of these results can be used for direct comparison with the present results. For example, our expressions (40), (60), (84), can be seen to agree with Eq. (8), p. 694, of Ref. 115. Furthermore, our Eq. (40) is in line with Eq. (13), p. 1298, of Ref. 116, the same applies to our Eq. (60) and its counterpart, Eq. (14), p. 1298, Ref. 116. Also Eq. (16), p. 1298, Ref. 116 (for $n=3$, $l=3$ and $n=4$, $l=2,3,4$) gives the same results as our Eqs. (60), (84). And finally, our Eq. (84) agrees with Eq. (10), p. 1083, of Ref. 117 (for $N=4$).

Our consideration of the action map f in the present paper has been motivated by the formalism of (lattice) quantum field theory. However, the consideration of certain modifications of the map f might also be of some interest from various points of view. Let us consider a special set of modifications which can be described by replacing the Eqs. (16) by the equations

$$\overline{\eta}_l=\frac{\partial\widetilde{G}[\{\overline{\Psi}\},\{\Psi\}]}{\partial\Psi_l},\quad \eta_l\ =\ -\frac{\partial\widetilde{G}[\{\overline{\Psi}\},\{\Psi\}]}{\partial\overline{\Psi}_l} \tag{200}$$

(G is replaced by $\widetilde{G}$). For example, if one is just interested in the fixed point condition for the action map f [i.e., in the Eq. (131) for $\lambda=1$] it might make sense to consider instead of the action map f a different map $\tilde{f}$ [described by the Eqs. (16), (200), respectively] having the same set of fixed points but which is algebraically or numerically easier to study. One such modification consists in choosing $\widetilde{G}=G_0$ [cf. Ref. 73, p. 291, Eq. (2.9)]. The implicit representation of the map f given in Eqs. (15), (16) would then turn into an explicit representation of the map $\tilde{f}$ which might be easier to handle in some respect. As an aside in this context, we mention that for this map $\tilde{f}$ the equations (43), (64), (99) (replace $\mathsf{A}^{(2)\prime}$ on the rhs by $\mathsf{A}^{(2)}$) exhibit a *formal* similarity to the main equation for the Schulz iteration scheme for the calculation of the inverse of a matrix [see Eq. (7), p. 58, in Ref. 118].[119–123] The similarity, however, is only formal as in general the matrix $\mathsf{P}^{(2n-2)\star}/\mathsf{P}^{(2n)\star}$ is not invariant under the map $\tilde{f}$ [for the simplest case, $n=2$, for example, one can convince oneself of this fact starting from Eqs. (43), (44) where one has to omit in this case the primes on the rhs].

As already mentioned the investigation performed in the present study within the framework of Grassmann algebras has been inspired by a problem in quantum field theory which in its simplest version (within zero-dimensional field theory) is a problem in real/complex analysis. The standard analysis analogue of the Grassmann integral equation studied in Chap. 3 (for $\lambda=1$) reads [cf. Eq. (8)]

$$e^{g(y)} = C \int_{-\infty}^{+\infty} \mathrm{d}x \, e^{g(x+y) - g'(y)x}. \tag{201}$$

This is a nonlinear integro-differential equation for the real function $g(x)$. Clearly, the elementary function $g(x) = -ax^2/2,\ 0 < a \in \mathbf{R}\ [C = \sqrt{a/(2\pi)}]$ solves this equation. However, the interesting question is if this equation has any other (nonelementary) solution which stands in correspondence to a non-Gaussian integral. No qualitative information seems to be available in the mathematical literature in this respect. As pointed out in Ref. 28, Sec. 4, p. 859 (p. 475 of the English transl.), Eq. (201) is a very complicated equation. The main difficulty in explicitly finding any nonelementary solution to it (if it exists at all—we just assume this for the time being) consists in the fact that it is very difficult if not impossible to calculate for an arbitrary function $\exp g(x)$ its Fourier (or Laplace) transform explicitly. The question now arises if the analysis in Sec. III D of the solutions of the Grassmann integral equation found for $n = 4$, $\lambda = 1$, might help in overcoming this problem. We do not have any final answer on this but in our view it makes sense to say: perhaps. The solutions of the Grassmann integral equation found for $n = 4$, $\lambda = 1$, are characterized by two properties which are not related to the anticommuting character of Grassmann variables. The solutions were related, first, to eigenfunctions of the Fourier–Laplace transformation to the eigenvalue 1 (i.e., to self-reciprocal functions) and, second, to some iterative functional equation. Now, it seems to be reasonable to assume that also (some) solutions of Eq. (201) might be characterized by these two properties. The two sets of functions obeying one of these two principles are very large and one might think that the intersection of these two sets contains also other functions than just the functions given by $g(x) = -ax^2/2$. The task of solving Eq. (201) then is equivalent to studying eigenfunctions of the Fourier transformation to the eigenvalue 1, i.e., self-reciprocal functions $\exp g(x)$.[124–126] They obey the equation

$$e^{g(y)} = \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}} e^{iyx} e^{g(x)}. \tag{202}$$

The consideration of eigenfunctions of the Fourier transformation solves the above mentioned problem of finding their Fourier transforms at once.[127] There is a vast mathematical literature on self-reciprocal functions (in particular for the Fourier transformation) but in our context it makes sense to concentrate on a certain subclass of self-reciprocal functions. Klauder (Ref. 128, p. 375, Ref. 59, Subsec. 10.4, p. 246) has pointed out the relevance of infinitely divisible characteristic functions in a quantum field theoretic context. This entails in our context that the self-reciprocal functions $\exp g(x)$ should be self-reciprocal probability densities (positive definite ones, in addition: without zeros—this follows from infinite divisibility). The subject of self-reciprocal (positive definite) probability densities has been studied for some time in probability theory (Refs. 129–135, Ref. 136, Subsec. 7.5, p. 122, Refs. 137, 138, Ref. 139, Chap. 6, p. 148, Ref. 140; see Refs. 137, 139 for some further references). Of most relevance to the present problem is the work by Teugels[130] who describes explicit methods to construct solutions of Eq. (202) (also note Ref. 140 in this respect). From the solutions $\exp g(x)$ of (202) (which are even functions) we define the function $G = G(-x^2/2) = g(x)$.[141,142] The function $d(t)$ [Eq. (193)] associated with it then has to obey the functional equation (194) in order to ensure that the function $g(x)$ solves Eq. (201). In the case under discussion, the equations (192)–(194) can be reformulated the following way. Define the functions

$$\tilde{b}(x) = -\frac{\partial g(x)}{\partial x} = -\frac{\partial}{\partial x} G\left(-\frac{x^2}{2}\right) = xG'\left(-\frac{x^2}{2}\right), \tag{203}$$

$$\tilde{d}(x) = i\tilde{b}(x). \tag{204}$$

Then, from Eq. (194) one can derive the following iterative functional equation which has to be fulfilled:

$$\tilde{d}^2(x)=\tilde{d}(\tilde{d}(x))=-x. \tag{205}$$

As in Sec. III D, one can now assume a certain behavior of the function $g(x)$. Assuming again that the function $G'(s)$ is an even function [i.e., up to some constant $G(s)$ is odd] Eq. (205) can be written as

$$\tilde{b}^2(x)=\tilde{b}(\tilde{b}(x))=x. \tag{206}$$

However, this case is not very interesting as it does not lead to any non-Gaussian function $\exp g(x)$ [Ref. 143, Theorem 3, p. 117 (Teor. Veroyatn. Prim.), p. 119 (Theor. Prob. Appl.); note that Lukacs uses the term self-reciprocal in this article in a different sense than we do in the present paper]. Assuming that $G'(s)$ is an odd function [i.e., $G(s)$ is even] Eq. (205) can be written as

$$\tilde{b}^2(x)=\tilde{b}(\tilde{b}(x))=-x. \tag{207}$$

However, this case is also not very interesting as real functions solving Eq. (207) are necessarily discontinuous (Ref. 94, Chap. XV, Sec. 4, p. 299, Refs. 103, 97–101, 104, Ref. 93, Subsec. 11.2B, p. 425). Consequently, Eq. (205) cannot sensibly be simplified by the above considerations. However, the sketched program still faces another challenge. At first glance, it is not obvious how to combine the existent theory of self-reciprocal probability densities with the theory of iterative functional equations in an operationally effective way in order to find nonelementary solutions of Eq. (201) (or its multidimensional generalizations) which correspond to non-Gaussian integrals. This will have to be the subject of further research.

This discussion has brought us to the end of the present study. What are its main results? From a mathematical point of view, the paper introduces a new type of equation which has not been studied before—a Grassmann integral equation. The concrete equation studied has been shown to be equivalent to a coupled system of nonlinear matrix equations which can be solved (Sec. III). From the point of view of standard quantum field theory, the main results of the present article are as follows. For low-dimensional Grassmann algebras the present paper derives explicit expressions for the finite-dimensional analogue of the effective action functional in terms of the data specifying a fairly general ansatz for the corresponding analogue of the so-called ''classical'' action functional (Sec. II). This is a model study which in some way can be understood as the fermionic (Grassmann) analogue of zero-dimensional field theory and which may turn out to be useful in several respect. Moreover, for an arbitrary Grassmann algebra (related to an arbitrary purely fermionic ''lattice quantum field theory''—on a finite lattice) on the basis of the explicit results obtained for low-dimensional Grassmann algebras an exact expression for the four-fermion term of the finite lattice analogue of the effective action functional is derived in a heuristic manner [Sec. II E, Eq. (123)]. From the point of view of the conceptual foundations of quantum field theory, the present study demonstrates on the basis of a finite-dimensional example that the (Grassmann) integral equation proposed in Refs. 28, 73 can have solutions which are equivalent to non-Gaussian integrals (Sec. III). This certainly will be of interest in various respect. To illustrate this point let us repeat in compact form some of the results found for the Grassmann algebra $\mathcal{G}_8$ in Sec. III C (these results are specific for this Grassmann algebra). Define for an arbitrary invertible 4×4 matrix B $(\det \mathsf{B}\neq 0)$ the Grassmann bilinears

$$G_q=\sum_{l,m=1}^{4} \mathsf{B}_{lm}\overline{\chi}_l\chi_m=\overline{\chi}\mathsf{B}\chi, \tag{208}$$

$$W_q=-\sum_{l,m=1}^{4} [\mathsf{B}^{-1}]_{lm}\overline{\eta}_l\eta_m=-\overline{\eta}[\mathsf{B}]^{-1}\eta. \tag{209}$$

Then, the following equation applies:

$$\int \prod_{l=1}^{4} (\mathrm{d}\chi_l\, \mathrm{d}\overline{\chi_l})\, e^{(\overline{\eta}\chi+\overline{\chi}\eta)} \exp[G_q - \tfrac{1}{2} G_q^2 + \tfrac{1}{2} G_q^3 - \tfrac{3}{8} G_q^4] = \det \mathsf{B} \exp[W_q - \tfrac{1}{2} W_q^2 + \tfrac{1}{2} W_q^3 - \tfrac{3}{8} W_q^4]. \tag{210}$$

This should be compared to the well-known, corresponding result for a Gaussian integral

$$\int \prod_{l=1}^{4} (\mathrm{d}\chi_l\, \mathrm{d}\overline{\chi_l})\, e^{(\overline{\eta}\chi+\overline{\chi}\eta)} \exp[G_q] = \det \mathsf{B} \exp[W_q]. \tag{211}$$

Moreover, in Sec. III C it has been found that the (Grassmann) function $G_q - \frac{1}{2} G_q^2 + \frac{1}{2} G_q^3 - \frac{3}{8} G_q^4$ is the (first) Legendre transform of the function $W_q - \frac{1}{2} W_q^2 + \frac{1}{2} W_q^3 - \frac{3}{8} W_q^4$ [cf. Eqs. (181)–(183)]. This entails that these functions behave exactly the same way as the functions G_q and W_q. It is clear that any Grassmann algebra $\mathcal{G}_{8k}$, $1 \leqslant k \in \mathbf{N}$, supports equations of the type (210) [simply by multiplying k copies of Eq. (210)]. Given the role that Gaussian integrals and their properties play in quantum field theory, statistical physics and probability theory it will be interesting to explore the implications and applications of the above results in the future.

ACKNOWLEDGMENTS

I am grateful to K. J. Falconer for sending me a reprint of Ref. 103 and to U. Prells for providing me with an advance copy of Ref. 155.

APPENDIX A

Here we collect some formulas for compound matrices.[144] Let B, D be $n \times n$ matrices. The *compound matrix* $C_k(\mathsf{B})$, $0 \leqslant k \leqslant n$, is a $\binom{n}{k} \times \binom{n}{k}$ matrix of all order k minors of the matrix B. The indices of the compound matrix entries are given by ordered strings of length k. These strings are composed from the row and column indices of the matrix elements of the matrix B the given minor of the matrix B is composed of. Typically, the entries of a compound matrix are ordered lexicographically with respect to the compound matrix indices. (We also apply this convention.) The *supplementary (or adjugate) compound matrix* $C^{n-k}(\mathsf{B})$ (sometimes also referred to as the *matrix of the* kth *cofactors*) of the matrix B is defined by the equation [cf. Eq. (24)]

$$C^{n-k}(\mathsf{B}) = C_{n-k}(\mathsf{B})^{\star}. \tag{A1}$$

The components of the supplementary compound matrix $C^{n-k}(\mathsf{B})$ can also be defined by means of the following formula [here, $l_1 < l_2 < \cdots < l_k$, $m_1 < m_2 < \cdots < m_k$; Ref. 145, Chap. IV, Sec. 89, p. 75, Ref. 146, Chap. 3, p. 18; also see our Eqs. (31)–(36)]

$$C^{n-k}(\mathsf{B})_{LM} = \frac{\partial}{\partial \mathsf{B}_{l_1 m_1}} \cdots \frac{\partial}{\partial \mathsf{B}_{l_k m_k}} \det \mathsf{B}. \tag{A2}$$

This comparatively little known definition of (matrices of) cofactors (supplementary compound matrices) is essentially due to Jacobi (Ref. 147, Sec. 10, p. 301, p. 273 of the 'Gesammelte Werke,' p. 25 of the German transl.; also see the corresponding comment by Muir in Ref. 148, Part I, Chap. IX, pp. 253–272, in particular pp. 262/263).

For compound matrices holds ($\mathbf{1}_r$ is the $r \times r$ unit matrix, α some constant)

$$C_k(\alpha \mathbf{1}_n) = \alpha^k \mathbf{1}_{\binom{n}{k}}. \tag{A3}$$

Important relations are given by the *Binet–Cauchy formula*

$$C_k(\mathsf{B}) C_k(\mathsf{D}) = C_k(\mathsf{BD}) \tag{A4}$$

from which immediately follows

$$C_k(\mathsf{B}^{-1}) = C_k(\mathsf{B})^{-1}, \tag{A5}$$

the *Laplace expansion*

$$C_k(\mathsf{B})C^{\ n-k}(\mathsf{B}) = C^{\ n-k}(\mathsf{B})C_k(\mathsf{B}) = C_k(\mathsf{B})C_{n-k}(\mathsf{B})^\star = C_{n-k}(\mathsf{B})^\star C_k(\mathsf{B}) = \det \mathsf{B}\ \ \mathbf{1}_{\binom{n}{k}}, \tag{A6}$$

Jacobi's theorem [a consequence of the Eqs. (A6) and (A5)]

$$C_k(\mathsf{B}^{-1}) = \frac{1}{\det \mathsf{B}} C^{\ n-k}(\mathsf{B}) = \frac{1}{\det \mathsf{B}} C_{n-k}(\mathsf{B})^\star, \tag{A7}$$

and the *Sylvester–Franke theorem*

$$\det C_k(\mathsf{B}) = (\det \mathsf{B})^{\binom{n-1}{k-1}}. \tag{A8}$$

Compound matrices are treated in a number of references. A comprehensive discussion of compound matrices can be found in Ref. 149, Chap. V, pp. 63–87, Ref. 150, Chap. V, pp. 90–110, and, in a modern treatment, in Ref. 151, Chap. 6, pp. 142–155. More algebraically oriented modern treatments can be found in Ref. 75, Part I, Chap. 2, Sec. 2.4, pp. 116–159, Part II, Chap. 4, pp. 1–164 (very thorough), Ref. 152, Chap. 7, Sec. 7.2, pp. 411–420, and Ref. 153, Vol. 3, Chap. 2, Sec. 2.4, pp. 58–68. Concise reviews of the properties of compound matrices are given in Refs. 154, 155. Also note Refs. 156 and 157.

APPENDIX B

Let B be a 3×3 matrix. Then, the following identities apply:

$$\mathrm{adj}\, \mathsf{B} = \mathsf{B}^2 - \mathsf{B}\ \ \mathrm{tr}\mathsf{B} + \tfrac{1}{2}(\mathrm{tr}\, \mathsf{B})^2 \mathbf{1}_3 - \tfrac{1}{2}\mathrm{tr}(\mathsf{B}^2)\mathbf{1}_3, \tag{B1}$$

$$\mathrm{tr}(\mathrm{adj}\, \mathsf{B}) = \tfrac{1}{2}(\mathrm{tr}\, \mathsf{B})^2 - \tfrac{1}{2}\mathrm{tr}(\mathsf{B}^2). \tag{B2}$$

Equation (B1) can be derived by means of the Cayley–Hamilton theorem [cf. e.g., Ref. 158, Subsec. 2.4, p. 264, Eq. (2.4.7), Ref. 159, Sec. 7, p. 154, Eq. (29)].

APPENDIX C

In this appendix we want to rederive Eq. (186) starting from a (Euclidean space–time) version of the Eqs. (1)–(5) on a finite lattice with k sites. The equations (3), (5) then read

$$G[\phi] = W[J] - \sum_{l=1}^{k} J_l \phi_l, \tag{C1}$$

$$J_l = -\frac{\partial G}{\partial \phi_l}. \tag{C2}$$

In analogy to the Eqs. (175), (178) we define (B is a symmetric $k\times k$ matrix)

$$G_q = G_q[\phi] = -\frac{1}{2}\sum_{l,m=1}^{k} \mathsf{B}_{lm}\phi_l\phi_m = -\frac{1}{2}\phi \mathsf{B} \phi, \tag{C3}$$

$$W_q = W_q[J] = \frac{1}{2}\sum_{l,m=1}^{k} (\mathsf{B}^{-1})_{lm} J_l J_m = \frac{1}{2} J \mathsf{B}^{-1} J. \tag{C4}$$

Now we assume that G, W depend on ϕ, J only as functions of $G_q[\phi]$, $W_q[J]$, respectively, and, in addition, that the identity $G=W$ holds. Then, in analogy to the Eqs. (181)–(183) the Eqs. (C1), (C2) read

$$G(G_q)=G(W_q)-\sum_{l=1}^{k} J_l\phi_l, \tag{C5}$$

$$J_l=-\frac{\partial G(G_q)}{\partial \phi_l}=-G'(G_q)(\phi \mathsf{B})_l. \tag{C6}$$

Here, again

$$G'(G_q)=\frac{\partial G(G_q)}{\partial G_q}. \tag{C7}$$

In view of Eq. (C6) it holds

$$W_q=-G_q[G'(G_q)]^2. \tag{C8}$$

Taking into account the Eqs. (C6), (C8), Eq. (C5) can be written as

$$G(s)=G(-s[G'(s)]^2)+2sG'(s), \quad s=G_q, \tag{C9}$$

and this equation completely agrees with Eq. (186).

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A central extension of $U_q\,\mathrm{sl}(2|2)^{(1)}$ and R-matrices with a new parameter

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(Received 14 July 2003; accepted 21 July 2003)

In this paper, using a quantum superalgebra associated with the universal central extension of $\mathrm{sl}(2|2)^{(1)}$, we introduce new R-matrices having an extra parameter x. As $x\to 0$, they become those associated with the symmetric and antisymmetric tensor products of the copies of the vector representation of $U_q\,\mathrm{sl}(2|2)^{(1)}$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1616251]

I. INTRODUCTION

The Yang–Baxter equation (YBE for short) has played important roles in study of statistical mechanics, knot theory, conformal field theory, etc.,[1] and many of its solutions are associated with finite dimensional irreducible representations of quantum affine algebras[2,3] and superalgebras.[4] We call the solutions of the YBE the *R-matrices*.

If a finite dimensional simple Lie superalgebra is $A(m,n)$, $B(m,n)$, $C(n)$, $D(m,n)$, $F(4)$, $G(3)$, or $D(2,1;\alpha)$ $(\alpha\neq 0,-1)$, it is called a *basic classical Lie superalgebra*[5,6] (BCLS for short). We first recall that $A(m,n)$ coincides with $\mathrm{sl}(m+1|n+1)$ if and only if $m\neq n$, and that $\mathrm{sl}(m+1|m+1)$ is a one-dimensional central extension of $A(m,m)$. Let $\mathfrak{g}$ be a BCLS and $\overline{\mathfrak{g}}$ the universal central extension (UCE for short) of $\mathfrak{g}$. We also recall that $\overline{\mathfrak{g}}=\mathfrak{g}$ if $\mathfrak{g}\neq A(m,m)$ for any m, and that $\overline{A(m,m)}=\mathrm{sl}(m+1|m+1)$ $(m\geqslant 2)$ and $\overline{A(1,1)}=\mathfrak{d}$. Here $\mathfrak{d}$ is the Lie superalgebra called $D(2,1;-1)$.[7] The $\mathfrak{d}$ is a two- (respectively, three-) dimensional central extension of $\mathrm{sl}(2|2)$ [respectively, $A(1,1)$]. The UCE of $\mathfrak{g}\otimes\mathbb{C}[t,t^{-1}]$ is given by the affine version $\overline{\mathfrak{g}}^{(1)}=\overline{\mathfrak{g}}\otimes\mathbb{C}[t,t^{-1}]\oplus\mathbb{C}c$ of $\overline{\mathfrak{g}}$.[7] Motivated by this fact, we direct our attention to the quantum superalgebra $U_q\mathfrak{d}^{(1)}$ (strictly speaking, $\widetilde{U}=\widetilde{U}_q\mathfrak{d}^{(1)}$) in order to give new R-matrices $\check{R}(u,v;x)$ satisfying the (twisted) YBE:

$$\begin{aligned}&(\check{R}(v,w;x)\otimes I)(I\otimes\check{R}(u,w;q^n x))(\check{R}(u,v;x)\otimes I)\\&\quad=(I\otimes\check{R}(u,v;q^n x))(\check{R}(u,w;x)\otimes I))(I\otimes\check{R}(v,w;q^n x))\end{aligned}\tag{1}$$

for some integer n, where u, v, $x\in\mathbb{C}$ are continuous parameters. This can be viewed as a quantum dynamical YBE (see the Appendix). The R-matrices we will give are such that as $x\to 0$, they become the $U_q\,\mathrm{sl}(2|2)^{(1)}$ R-matrices[4,8–10] associated with the symmetric and antisymmetric tensor products of the copies of the vector representation φ of $U_q\,\mathrm{sl}(2|2)^{(1)}$. One of our tools is a four-dimensional irreducible representation ρ_x of $\widetilde{U}$ with the parameter x such that $\rho_0=\varphi\circ p$, where $p:\widetilde{U}\to U_q\,\mathrm{sl}(2|2)^{(1)}$ is the natural epimorphism.

The paper is organized as follows. In Sec. II, we introduce $\widetilde{U}$ and ρ_x. In Sec. III, we give $\check{R}(u,v;x)$ associated with ρ_x. In Sec. IV, we give all the $\check{R}(u,v;x)$'s mentioned above using the fusion process.

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II. A CENTRAL EXTENSION OF $U_q\,\mathrm{sl}(2|2)^{(1)}$

Let $\mathcal{E}=\oplus_{i=0}^{4}\mathbb{C}\varepsilon_i$ be the five-dimensional vector space. Define the symmetric bilinear form $(\,,\,)$ on $\mathcal{E}$ by $(\varepsilon_0,\varepsilon_0)=0$, $(\varepsilon_1,\varepsilon_1)=(\varepsilon_2,\varepsilon_2)=1$, $(\varepsilon_3,\varepsilon_3)=(\varepsilon_4,\varepsilon_4)=-1$, and $(\varepsilon_i,\varepsilon_j)=0$ $(i\neq j)$. Let $\alpha_0:=\varepsilon_0-\varepsilon_1+\varepsilon_4$ and $\alpha_i:=\varepsilon_i-\varepsilon_{i+1}$ $(1\leqslant i\leqslant 3)$. Define the parity $p(\alpha_i)$ to be $(4-(\alpha_i,\alpha_i)^2)/4$. Then the Cartan matrix of $A(1,1)^{(1)}$ is given by the 4×4 matrix (a_{ij}), where $a_{ij}=2(\alpha_i,\alpha_j)/((\alpha_i,\alpha_i)+2p(\alpha_i))$.

Throughout this paper, we assume $q\in\mathbb{C}$ to be such that $q\neq 0$ and $q^r\neq 1$ for every positive integer r. Let $\tilde{U}=\tilde{U}_q\mathfrak{d}^{(1)}$ be the associative $\mathbb{C}$-algebra presented by the generators s, $K_i^{\pm}$, E_i, F_i $(0\leqslant i\leqslant 3)$ and the defining relations:

$$s^2=1,\quad sK_is=K_i,\quad sE_is=(-1)^{p(\alpha_i)}E_i,\quad sF_is=(-1)^{p(\alpha_i)}F_i,$$

$$K_iK_i^{-1}=1,\quad K_iK_j=K_jK_i,$$

$$K_iE_jK_i^{-1}=q^{(\alpha_i,\alpha_j)}E_j,\quad K_iF_jK_i^{-1}=q^{-(\alpha_i,\alpha_j)}F_j,$$

$$[E_i,F_j]=\delta_{ij}\frac{K_i-K_i^{-1}}{q-q^{-1}}\quad \text{if } (i,j) \text{ is neither } (2,0) \text{ nor } (0,2),$$

$$K_2[E_2,F_0]\in Z(\tilde{U}),\quad K_2^{-1}[E_0,F_2]\in Z(\tilde{U}),$$

where $[E_i,F_j]:=E_iF_j-(-1)^{p(\alpha_i)p(\alpha_j)}F_jE_i$ and $Z(\tilde{U})$ is the center of $\tilde{U}$. We view $\tilde{U}$ as the (non-$\mathbb{Z}_2$-graded) Hopf algebra with the comultiplication $\Delta:\tilde{U}\to\tilde{U}\otimes\tilde{U}$ satisfying

$$\Delta(s)=s\otimes s,\quad \Delta(K_i)=K_i\otimes K_i,$$

$$\Delta(E_i)=E_i\otimes 1+K_is^{p(\alpha_i)}\otimes E_i+\delta_{i0}(q-q^{-1})s[E_0,F_2]\otimes E_2,$$

$$\Delta(F_i)=F_i\otimes K_i^{-1}+s^{p(\alpha_i)}\otimes F_i-\delta_{i0}(q-q^{-1})F_2\otimes[E_2,F_0].$$

We do not give the antipode and the counit; we do not need them. We define $\Delta^{(n-1)}:\tilde{U}\to\tilde{U}^{\otimes n}$ by letting $\Delta^{(1)}=\Delta$ and $\Delta^{(m)}=(\mathrm{id}_{\tilde{U}}\otimes\Delta^{(m-1)})\circ\Delta$ $(m\geqslant 2)$.

Remark: (1) The above comultiplication is not standard. Taking the twisting[11] for the $\tilde{U}$, we get the standard comultiplication of a quantum superalgebra defined for a Dynkin diagram other than the one associated with the Cartan matrix (a_{ij}) (see above); the $A(1,1)^{(1)}$ has the two Dynkin diagrams.

(2) Let $\tilde{U}'$ be the subalgebra of $\tilde{U}$ generated by $K_i^{\pm}$, E_i, F_i. Then $\tilde{U}=\tilde{U}'\oplus\tilde{U}'s$. There exists a nonzero ideal J of $\tilde{U}'$ such that $\tilde{U}'/J$ can be regarded as $U_q\mathfrak{d}^{(1)}$. We can get generators of J in the same way as in Ref. 12. By the same argument as in the proof of Theorem 8.4.3 of Ref. 12, we can get the natural epimorphism from $U_q\mathfrak{d}^{(1)}$ to $U_q\,\mathrm{sl}(2|2)^{(1)}$.

Let $V_x=\mathbb{C}^4$ be the four-dimensional vector space, where $x\in\mathbb{C}$ is a parameter. Set $\theta(i):=(1-(\varepsilon_i,\varepsilon_i))/2$. Define the irreducible representation $\rho_x:\tilde{U}\to\mathrm{End}(V_x)$ by

$$\rho_x(s)=\sum_{j=1}^{4}(-1)^{\theta(j)}E_{jj},\quad \rho_x(K_i)=\sum_{j=1}^{4}q^{(\alpha_i,\varepsilon_j)}E_{jj},$$

$$\rho_x(E_0)=E_{41},\quad \rho_x(E_1)=E_{12},$$

$$\rho_x(E_2)=E_{23}+xE_{41},\quad \rho_x(E_3)=E_{34},$$

$$\rho_x(F_0)=-E_{14}-xq^{-1}E_{32},\quad \rho_x(F_1)=E_{21},$$

$$\rho_x(F_2)=E_{32},\quad \rho_x(F_3)=-E_{43}.$$

Let $\tilde{U}^0=\tilde{U}_q\mathfrak{d}$ be the subalgebra of $\tilde{U}$ generated by s, $K_i^{\pm}$, E_i, F_i $(1\leqslant i\leqslant 3)$. Define the vector subspaces $V_x^{(i)}=V_{x,y}^{(i)}$ $(i=1,2)$ of $V_x\otimes V_y$ by

$$V_x^{(1)}:=\mathbb{C}(e_3\otimes e_3)\oplus\mathbb{C}(e_4\otimes e_4)\oplus\bigoplus_{i<j}\mathbb{C}(e_i\otimes e_j-(-1)^{\theta(i)\theta(j)}qe_j\otimes e_i$$
$$+\delta_{i1}\delta_{j2}(q^2ye_3\otimes e_4+xe_4\otimes e_3))$$

and

$$V_x^{(2)}:=\mathbb{C}(e_1\otimes e_1)\oplus\mathbb{C}(e_2\otimes e_2)\oplus\bigoplus_{i<j}\mathbb{C}(e_i\otimes e_j+(-1)^{\theta(i)\theta(j)}q^{-1}e_j\otimes e_i).$$

Lemma 1: $V_x^{(1)}$ is an irreducible $\tilde{U}^0$-module. Moreover $V_x\otimes V_y$ is a completely reducible $\tilde{U}^0$-module if and only if $y=qx$. If this is the case, $V_x^{(2)}$ is an irreducible $\tilde{U}^0$-module which is not isomorphic to $V_x^{(1)}$; in particular, $V_x\otimes V_{qx}$ has an irreducible $\tilde{U}^0$-submodule decomposition $V_x^{(1)}\oplus V_x^{(2)}$.

Proof: For each $1\leqslant i\leqslant 4$, the weight space including $e_i\otimes e_i$ is one dimensional. Hence, if $V_x\otimes V_y$ is a completely reducible $\tilde{U}^0$-module, there exists an irreducible $\tilde{U}^0$-module including $e_i\otimes e_i$. Using this fact, we can check the lemma directly. □

III. *R*-MATRIX FOR THE VECTOR REPRESENTATION

Define $P_x^{(i)}\in\mathrm{End}(V_x\otimes V_{qx})$ $(i=1,2)$ by $P_x^{(i)}(v)=\delta_{ij}v$ $(v\in V_x^{(j)})$. Set

$$\check{R}^{\square}(u,v;x):=(q^2u-v)P_x^{(1)}+(q^2v-u)P_x^{(2)},\tag{2}$$

where $u,v\in\mathbb{C}$. Then

$$\check{R}^{\square}(u,v;x)=(q^2v-u)\sum_{i=1}^{2}E_{ii}\otimes E_{ii}+(q^2u-v)\sum_{i=3}^{4}E_{ii}\otimes E_{ii}+(q^2-1)\sum_{i<j}(vE_{ii}\otimes E_{jj}+uE_{jj}\otimes E_{ii})$$
$$-q(u-v)\sum_{i\neq j}(-1)^{\theta(i)\theta(j)}E_{ij}\otimes E_{ji}+x(q^2-1)(u-v)(qE_{31}\otimes E_{42}-q^2E_{32}\otimes E_{41}$$
$$-E_{41}\otimes E_{32}+qE_{42}\otimes E_{31}).\tag{3}$$

For $u\in\mathbb{C}^{\times}$, define $\chi_u\in\mathrm{Aut}(\tilde{U})$ by $\chi_u(s)=s$, $\chi_u(K_i)=K_i$, $\chi_u(E_i)=u^{-\delta_{i0}}E_i$ and $\chi_u(F_i)=u^{\delta_{i0}}F_i$. Set $\rho_{u,v,x}:=(\rho_x\otimes\rho_{qx})\circ(\chi_u\otimes\chi_v)\circ\Delta$. Using (2) and Lemma 1, we can directly check that

$$\check{R}^{\square}(u,v;x)\rho_{u,v,x}(X)=\rho_{v,u,x}(X)\check{R}^{\square}(u,v;x)\tag{4}$$

for $X\in\tilde{U}$.

Theorem 1: *The $\check{R}^{\square}(u,v;x)$ satisfies the YBE in the form of (1) with $n=1$.*

Proof: Let E_i', F_i', H_i' $(0\leqslant i\leqslant 3)$ be the Chevalley generators of $\mathrm{sl}(2|2)^{(1)}$. Then there exists a representation $\hat{\psi}_u:\mathrm{sl}(2|2)^{(1)}\to\mathrm{End}(\mathbb{C}^4)$ sending E_i', F_i', H_i' to the limits of $\rho_x\circ\chi_u(E_i)$, $\rho_x\circ\chi_u(F_i)$, $(q-q^{-1})^{-1}\rho_x\circ\chi_u(K_i-K_i^{-1})$ as $(q,x)\to(1,0)$, respectively. Notice that $\psi:=\hat{\psi}_{1|\mathrm{sl}(2|2)}$ is an irreducible representation of $\mathrm{sl}(2|2)$ and that there exist a highest root vector $E'_{\alpha_1+\alpha_2+\alpha_3}$ and a lowest root vector $E'_{-(\alpha_1+\alpha_2+\alpha_3)}$ of $\mathrm{sl}(2|2)$ such that

$$u\psi(E'_{\alpha_1+\alpha_2+\alpha_3})=\hat{\psi}_u(F_0),\quad u^{-1}\psi(E'_{-(\alpha_1+\alpha_2+\alpha_3)})=\hat{\psi}_u(E_0).\tag{5}$$

Then, using (4), together with the same argument used in the proof of Proposition 3 in Ref. 3, we get the theorem. □

IV. *R*-MATRIX FOR THE (ANTI-)SYMMETRIC TENSORS

Here we use a similar process to the fusion process.[13–15] To begin with, we recall some facts[16,17] about the Hecke algebra $H_n(q^2)$ associated with the symmetric group S_n; the $H_n(q^2)$ is the associative $\mathbb{C}$-algebra presented by the generators h_i $(1\leqslant i\leqslant n-1)$ and the defining relations: $(h_i-q^2)(h_i+1)=0$, $h_ih_{i+1}h_i=h_{i+1}h_ih_{i+1}$ and $h_ih_j=h_jh_i$ $(|i-j|\geqslant 2)$. We abbreviate $H_n(q^2)$ to H. We know that there exists a $\mathbb{C}$-basis $\{h(\sigma)|\sigma\in S_n\}$ of H such that $h(1)=1$, $h(\sigma_i)=h_i$ and $h(\sigma'\sigma)=h(\sigma')h(\sigma)$ if $\ell(\sigma'\sigma)=\ell(\sigma')+\ell(\sigma)$. Here σ_i is the simple transposition $(i,i+1)$ and $\ell(\sigma)$ is the length of σ with respect to σ_i's.

Set

$$e_+ := \sum_{\sigma\in S_n} h(\sigma), \quad e_- := \sum_{\sigma\in S_n} (-q^{-2})^{\ell(\sigma)} h(\sigma).$$

Then $h_ie_+=q^2e_+$, $h_ie_-=-e_-$, and

$$e_\pm^2 = \left(\sum_{\sigma\in S_n} q^{\pm 2\ell(\sigma)}\right) e_\pm. \tag{6}$$

Now we treat *R*-matrices. Let $W_x^{(n)} := V_x\otimes V_{qx}\otimes\cdots\otimes V_{q^{n-1}x}$. Set

$$\check{R}_i(u,v;x) := I^{\otimes i-1}\otimes\check{R}^{\square}(u,v;q^{i-1}x)\otimes I^{\otimes n-i+1}\in \mathrm{End}(W_x^{(n)}).$$

By Theorem 1, we can define $\check{R}(a;x|\sigma)\in\mathrm{End}(W_x^{(n)})$, $a\in(\mathbb{C}^\times)^n$, and $\sigma\in S_n$, inductively by

$$\check{R}(a;x|1)=I^{\otimes n}, \quad \check{R}(a;x|\sigma_i)=\check{R}_i(a_i,a_{i+1};x)$$

and

$$\check{R}(a;x|\sigma'\sigma)=\check{R}(\sigma[a];x|\sigma')\check{R}(a;x|\sigma) \quad \text{if } \ell(\sigma'\sigma)=\ell(\sigma')+\ell(\sigma),$$

where $\sigma[a] := (a_{\sigma^{-1}(1)},\ldots,a_{\sigma^{-1}(n)})$. By Theorem 1 and (2), there exists a unique representation $\pi_x^{(n)}: H\to\mathrm{End}(W_x^{(n)})$ such that $\check{R}_i(u,v;x)=\pi_x^{(n)}(uh_i-vq^2h_i^{-1})$.

Let $p_\pm := (1,q^{\mp 2},\ldots,q^{\mp 2(n-1)})\in\mathbb{C}^n$. Let $\gamma_n\in S_n$ be such that $\gamma_n(i)=n-i+1$.

Lemma 2: Let $u\in\mathbb{C}$. Then

$$\check{R}(up_\pm;x|\gamma_n)=u^{\ell(\gamma_n)}a_\pm(q)\pi_x^{(n)}(e_\pm)$$

for some $a_\pm(q)\in\mathbb{C}^\times$.

This can be checked directly; a similar formula has been given in Sec. 5 in Ref. 14.

Let $V_{\pm,x} := \pi_x^{(n)}(e_\pm)W_x^{(n)}$. By (6), $d_\pm(n) := \dim V_{\pm,x}$ does not depend on q or x. For $a\in(\mathbb{C}^\times)^n$, define the representation $\rho_{a,x}:\widetilde{U}\to\mathrm{End}(W_x^{(n)})$ by

$$\rho_{a,x} := (\rho_x\otimes\cdots\otimes\rho_{q^{n-1}x})\circ(\chi_{a_1}\otimes\cdots\otimes\chi_{a_n})\circ\Delta^{(n-1)}.$$

By (4), we have

$$\check{R}(a;x|\sigma)\rho_{a,x}(X)=\rho_{\sigma[a],x}(X)\check{R}(a;x|\sigma) \tag{7}$$

for $X\in\widetilde{U}$. By Lemma 2 and (7), we may define the representation $\rho_{u,x}^{\pm,(n)}:\widetilde{U}\to\mathrm{End}(V_{\pm,x})$ by $\rho_{u,x}^{\pm,(n)}(X)=\rho_{\gamma_n[up_\pm],x}(X)_{|V_{\pm,x}}$. Notice that

$$\rho_{u,x}^{\pm,(n)} = \rho_{1,x}^{\pm,(n)} \circ \chi_u . \tag{8}$$

We have a representation $\hat{\psi}_u^{\pm,(n)} : \mathrm{sl}(2|2)^{(1)} \to \mathrm{End}(\mathbb{C}^{d_\pm(n)})$ sending E_i', F_i', H_i' to the limits of $\rho_{u,x}^{\pm,(n)}(E_i)$, $\rho_{u,x}^{\pm,(n)}(F_i)$, $(q-q^{-1})^{-1}\rho_{u,x}^{\pm,(n)}(K_i - K_i^{-1})$ as $(q,x) \to (1,0)$. Define the representation $\psi^{\pm,(n)}$ of $\mathrm{sl}(2|2)$ to be $(\hat{\psi}_1^{\pm,(n)})_{|\mathrm{sl}(2|2)}$. Then $\psi^{+,(n)}$ (respectively, $\psi^{-,(n)}$) is the n-fold symmetric (respectively, antisymmetric) tensor product of the vector representation ψ of $\mathrm{sl}(2|2)$. By Ref. 18, we have the following.

Lemma 3: The $\psi^{\pm,(n)}$ is irreducible. Moreover $d_\pm(n) \neq 0$.

Define $\tau \in S_{2n}$ by $\tau(i) = i+n$, $\tau(n+i) = i \ (1 \leqslant i \leqslant n)$. For $g, h \in \mathbb{C}^n$, let $g \cup h := (g_1, \ldots, g_n, h_1, \ldots, h_n) \in \mathbb{C}^{2n}$. Let S_n be embedded into S_{2n} in the natural way. By Lemma 2, we have

$$\begin{aligned}
&\check{R}(\gamma_n[up_\pm] \cup \gamma_n[vp_\pm]; x|\tau)(\pi_x^{(n)}(e_\pm) \otimes \pi_{q^n x}^{(n)}(e_\pm)) \\
&= \frac{(uv)^{-\ell(\gamma_n)}}{a_\pm(q)^2} \check{R}(\gamma_n[up_\pm] \cup \gamma_n[vp_\pm]; x|\tau)\check{R}(up_\pm; x|\gamma_n)\check{R}(vp_\pm; x|\tau\gamma_n\tau) \\
&= \frac{(uv)^{-\ell(\gamma_n)}}{a_\pm(q)^2} \check{R}(up_\pm \cup vp_\pm; x|\gamma_n\tau\gamma_n) \\
&= \frac{(uv)^{-\ell(\gamma_n)}}{a_\pm(q)^2} \check{R}(vp_\pm; x|\gamma_n)\check{R}(up_\pm; x|\tau\gamma_n\tau)\check{R}(up_\pm \cup vp_\pm; x|\tau) \\
&= (\pi_x^{(n)}(e_\pm) \otimes \pi_{q^n x}^{(n)}(e_\pm))\check{R}(up_\pm \cup vp_\pm; x|\tau).
\end{aligned}$$

Hence we may set

$$\check{R}^{\pm,(n)}(u,v;x) := \check{R}(\gamma_n[up_\pm] \cup \gamma_n[vp_\pm]; x|\tau)_{|V_{\pm,x} \otimes V_{\pm,q^n x}}$$

$\in \mathrm{End}(V_{\pm,x} \otimes V_{\pm,q^n x})$.

Let $\rho_{u,v}^{\pm,(n)} := (\rho_{u,x}^{\pm,(n)} \otimes \rho_{v,q^n x}^{\pm,(n)})\Delta$. Notice that

$$\rho_{u,v}^{\pm,(n)}(X) = (\rho_{\gamma_n[up_\pm] \cup \gamma_n[vp_\pm],x}(X))_{|V_{\pm,x} \otimes V_{\pm,q^n x}}. \tag{9}$$

By (7) and (9), we have

$$\check{R}^{\pm,(n)}(u,v;x)\rho_{u,v}^{\pm,(n)}(X) = \rho_{v,u}^{\pm,(n)}(X)\check{R}^{\pm,(n)}(u,v;x) \tag{10}$$

for $X \in \widetilde{U}$.

Theorem 2: *The $\check{R}^{\pm,(n)}(u,v;x)$ satisfies the YBE in the form of (1).*

Proof: By (5), we have $u\psi^{\pm,(n)}(E'_{\alpha_1+\alpha_2+\alpha_3}) = \hat{\psi}_u^{\pm,(n)}(F_0)$ and $u^{-1}\psi^{\pm,(n)}(E'_{-(\alpha_1+\alpha_2+\alpha_3)}) = \hat{\psi}_u^{\pm,(n)}(E_0)$. Noting this fact and using (8), (10) and Lemma 3, together with the same argument as in the proof of Proposition 3 in Ref. 3, we have the theorem. □

ACKNOWLEDGMENTS

The author thanks E. Date, M. Okado, and Y. Koga for valuable comments. The author also thanks Y.Z. Zhang for telling him about face-type dynamical R-matrices.

APPENDIX: QUANTUM DYNAMICAL *R*-MATRIX

Here we show that the $\check{R}^{\pm,(n)}(u,v;x)$ can be viewed as a dynamical R-matrix. Let $\mathfrak{h}$ be a finite dimensional commutative Lie algebra. Let V be a finite dimensional diagonalizable $\mathfrak{h}$-module, i.e.,

$V=\oplus_{\mu\in\mathfrak{h}^*}V_\mu$, where $V_\mu:=\{v|h.v=\mu(h)v\}$. We say that a (meromorphic) function $\check{R}':\mathbb{C}^2\times\mathfrak{h}^*\to\mathrm{End}(V\otimes V)$ is a *quantum dynamical R-matrix* if it satisfies the quantum dynamical YBE (see Ref. 19, for example):

$$(\check{R}'(v,w,\lambda)\otimes I)\check{R}'_{23}(u,w,\lambda-h^{(1)})(\check{R}'(u,v,\lambda)\otimes I)=\check{R}'_{23}(u,v,\lambda-h^{(1)})(\check{R}'(u,w,\lambda)\otimes I)\times\check{R}'_{23}(v,w,\lambda-h^{(1)}),$$

where $\check{R}'_{23}(u,v,\lambda-h^{(1)})\in\mathrm{End}(V^{\otimes 3})$ is defined by

$$\check{R}'_{23}(u,v,\lambda-h^{(1)})_{|V_\mu\otimes V\otimes V}=(I\otimes\check{R}'(u,v,\lambda-\mu))_{|V_\mu\otimes V\otimes V}.$$

Let $\mathfrak{h}''=\mathbb{C}$ and let $\mathfrak{h}''$ act on $\mathbb{C}^{d_\pm(n)}$ by $z.v=-nzv$. Let $a\in\mathbb{C}$ be such that $e^a=q$. Define $\check{R}'':\mathbb{C}^2\times(\mathfrak{h}'')^*\to\mathrm{End}(\mathbb{C}^{d_\pm(n)}\otimes\mathbb{C}^{d_\pm(n)})$ by $\check{R}''(u,v,\lambda)=\check{R}^{\pm,(n)}(u,v;e^{a\lambda(1)})$. By Theorem 2, $\check{R}''$ is a quantum dynamical *R*-matrix.

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ERRATUM

Erratum: Canonical coherent states for the relativistic harmonic oscillator [J. Math. Phys. 36, 3191 (1995)]

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 [DOI: 10.1063/1.1615698]

In the mentioned paper[1] we introduced higher-order (nonpolynomial), relativistic creation and annihilation operators, $\hat{a},\hat{a}^\dagger$, with canonical commutation relation $[\hat{a},\hat{a}^\dagger]=1$ rather than the covariant one $[\hat{z},\hat{z}^\dagger]\approx$energy and naturally associated with the $SL(2,R)$ group. The canonical (relativistic) coherent states were then defined as eigenstates of $\hat{a}$. Also, a canonical, minimal representation was constructed in configuration space by means of eigenstates of a canonical position operator.

Unfortunately, the expression of the operator $\hat{\kappa}$ (closely related to the energy operator) just after formula (18), then after formula (34), was miswritten. In fact, we printed the classical function of κ in terms of the functions z and z^* [see Eq. (2)], whereas the correct, quantum expression is

$$\hat{\kappa}=\frac{1}{2N}+\sqrt{\left(1-\frac{1}{2N}\right)^2+\frac{2}{N}\hat{z}^\dagger\hat{z}}.$$

This misprint had not been detected because we always used the power series expansion [formula (17)], which features a full independence on the (energy eigenstate) basis $\{|n\rangle\}$. However, very recently, Kastrup dealing with an analogous construction[2] has detected the above-mentioned misprint.[3] We are very grateful to him for pointing it out.

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Sharp reconstruction of unsharp quantum observables

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(Received 28 May 2003; accepted 7 August 2003)

A well defined procedure exists which allows us to ''reconstruct'' a sharp, i.e., standard, quantum observable A starting from a given commutative unsharp observable F. In this work we prove that the outcomes of measurements of F can be consistently interpreted as the result of a stochastic diffusion of outcomes of its sharp reconstruction A. Furthermore, for every sharp observable B, such that F is unsharp realization of B, we explicitly construct a real mapping g such that $A=g(B)$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623615]

I. INTRODUCTION

In order to describe general physical magnitudes of a quantum system described in a Hilbert space $\mathcal{H}$, the notion of *unsharp observable* has been introduced and investigated by several authors:[1–4]

Definition 1: An unsharp observable is a mapping

$$F:\mathcal{B}(\mathbf{R})\rightarrow\mathcal{F}(\mathcal{H})$$

so that

$(u1)$ $F(\mathbf{R})=\mathbf{1}$,

$(u2)$ $F(\cup\Delta_j)=\Sigma F(\Delta_j)$ *if* $\Delta_j\cap\Delta_k=\varnothing$ *when* $j\neq k$,

where $\mathcal{F}(\mathcal{H})=\{\Phi:\mathcal{H}\rightarrow\mathcal{H}$, *linear, and* $\mathbf{0}\leqslant\Phi\leqslant\mathbf{1}\}$ *is the set of effects, and the series converges in the weak operator topology.* [$\mathcal{B}(\mathbf{R})$ *denotes the Borel* σ*-algebra on the set* $\mathbf{R}$ *of real numbers.*]

In other terms, an unsharp observable is a positive operator valued (POV) measure, where $p(F;\Delta)=\langle\psi|F(\Delta)\psi\rangle$ is interpreted as the probability that the outcome of a measurement of the observable represented by F belongs to Δ. *Sharp* observables, describing the observables of standard quantum theory,[5] are projection valued (PV) measures $E:\mathcal{B}(\mathbf{R})\rightarrow\mathcal{E}(\mathcal{H})$, where $\mathcal{E}(\mathcal{H})$ denotes the set of all projection operators of Hilbert space $\mathcal{H}$. Hence they form a particular subset of the larger set of unsharp observables.

If F is a *commutative* unsharp observable, i.e., if

$$[F(\Delta_1),F(\Delta_2)]=\mathbf{0},\quad\forall\Delta_1,\Delta_2\in\mathcal{B}(\mathbf{R}),$$

a sharp observable E can be explicitly constructed,[6] together with a family $\{w_\Delta\}_{\Delta\in\mathcal{B}(\mathbf{R})}$ of real functions on $\mathbf{R}$ such that

$$F(\Delta)=\int w_\Delta(\lambda)dE_\lambda,$$

where $E_\lambda=E(-\infty,\lambda]$ is the resolution of the identity of self-adjoint operator $A=\int\lambda dE_\lambda$ (Sec. II).

Since $p(F;\Delta)=\int_\Delta w_\Delta(\lambda)d\|E_\lambda\psi\|^2$ and $d\|E_\lambda\psi\|^2=p(E;(\lambda,\lambda+d\lambda])$, these results suggest that the outcomes of measurements of F can be interpreted as the result of a stochastic diffusion of the outcomes of E, *by interpreting* $w_\Delta(\lambda)$ *as the probability that outcome* λ *of* E *turns into an*

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outcome in Δ *for* F. In short, we can say that F *is an unsharp realization of* E. The physical cause of such a diffusion could be the imprecision of the measuring apparatus, or some other albeit unknown cause. The main aim of the present work is to check the consistency of this interpretation for commutative unsharp observables. A first mathematical condition to be required is that for every possible value λ of sharp reconstructed observable E, mapping $\Delta \to w_\Delta(\lambda)$ must behave as a probability measure. In Sec. III we prove that this is true for a ring $\mathcal{R}(\mathcal{S})=\{\Delta\}$ of sets which generates the σ-algebra of Borel.

Furthermore, since a given commutative unsharp observable F is simultaneously the unsharp realization of many different sharp observables E^B, E^C, etc., as well as of our own reconstruction E, a more fundamental problem of consistency arises: the intepretation of F as an unsharp realization of sharp reconstruction E must be consistent with the inteprepretation of F as an unsharp realization of E^B, E^C, etc. This second kind of consistency would fail, for instance, if $[E,E^B]\neq \mathbf{0}$. In Sec. IV we show that, whenever F is an unsharp realization of some sharp observable E^B, we can concretely construct a real function g so that every outcome λ of the sharp reconstruction E satisfies

$$\lambda = g(\mu),$$

where μ is the outcome of E^B. The existence of such a function is a condition, denoted by (C) in Sec. IV, which ensures consistency. The fact that we have a way to construct mapping g allows us to investigate concrete examples; for instance, in Sec. IV C we find that the sharp reconstruction of the general 1-0 observable generated by an effect ϕ is the sharp observable represented by just self-adjoint operator ϕ itself.

Section V is devoted to interpret these results and to locate the present work within the literature about the subject.

II. SHARP RECONSTRUCTION OF UNSHARP OBSERVABLES

Let E be a sharp observable corresponding to the self-adjoint operator A. Often it happens that the real apparatus used to measure this observable does not have an infinite precision. Let us suppose that this imprecision can be described by means of a family $\{w_\Delta\}_{\Delta\in\mathcal{B}(\mathbf{R})}$ of non-negative functions, defined on the spectrum $\sigma(A)$, with the following interpretation: $w_\Delta(\lambda)$ is the probability that, when the outcome of A is λ, the measuring apparatus yields an outcome $\mu\in\Delta$. This implies that

$$\text{(PM)}\quad \textit{mapping}\quad w_{(\cdot)}(\lambda):\mathcal{B}(\mathbf{R})\to[0,1],\quad \Delta\to w_\Delta(\lambda)$$

is a probability measure for every number λ *in the spectrum of* A.

The probability that the actually measured value belongs to $\Delta\in\mathcal{B}(\mathbf{R})$ is $p(\Delta)=\langle\psi|w_\Delta(A)\psi\rangle$, where operator $w_\Delta(A)=\int w_\Delta(\lambda)dE_\lambda$ is an effect. The outcoming mapping $F:\mathcal{B}(\mathbf{R})\to\mathcal{F}(\mathcal{H})$, $\Delta\to f(\Delta)$ may be seen to be an unsharp observable. The outcomes of F can be considered as the result of the stochastic diffusion, described by $w_\Delta(\lambda)$, of the outcomes of E. Hence, for every sharp observable E and every family of functions w_Δ satisfying (PM), a correspondence

$$E\to F,\quad F(\Delta)=\int w_\Delta(\lambda)dE_\lambda, \tag{1}$$

can be established, which associates an unsharp observable F to E. We call F in (1) an *unsharp realization* of E. In this section we show how correspondence (1) can be reversed.

The problem of reversing correspondence (1) consists in starting from a given unsharp observable F and then in looking for a sharp observable E so that (1) holds. It has been found that the reversing correspondence is successful if F is a *commutative* unsharp observable.[7,6] In such a case an explicit procedure has been established which allows us to obtain

(i) a sharp observable E, called *the sharp reconstruction of* F;
(ii) a family of functions $\{w_\Delta\}$ so that $F(\Delta)=w_\Delta(A)$,

where $A=\int\lambda dE_\lambda$ and $E_\lambda=E((-\infty,\lambda])$. In the present section we outline such a reconstruction procedure.

We can assume, without losing generality, that the *physical spectrum* $\tilde{\sigma}(F)=\{\lambda\in\mathbf{R}|\forall\,\delta>0, F(\lambda-\delta,\lambda+\delta)>\mathbf{0}\}$ of unsharp observable F we start from is bounded and $\tilde{\sigma}(F)\subseteq[0,1]$ (Ref. 6) [($\tilde{\sigma}(F)$ is the support of POV measure F and represents the set of possible outcomes of F; for a sharp observable E, $\tilde{\sigma}(E)$ coincides just with the mathematical spectrum $\sigma(A)$ of the corresponding self-adjoint operator A].

Let us consider the countable family $\mathcal{S}=\{\Delta_j\}$, where

$$\Delta_j=\begin{cases}\left[0,\dfrac{1}{2^p}\right] & \text{if } j=2^p,\ p\in\mathbf{N},\\ \left(\dfrac{j-2^p}{2^p},\dfrac{j-2^p+1}{2^p}\right] & \text{if } 2^p<j<2^{p+1},\ p\in\mathbf{N}.\end{cases}\tag{2}$$

Family $\mathcal{S}$ is a semi-ring of intervals which generates whole σ-algebra $\mathcal{B}([0,1])$. We take into account also the family of effects corresponding to these intervals:

$$\{F_j\},\quad \text{where}\quad F_j=F(\Delta_j).\tag{3}$$

The procedure consists of a sequence of steps, which allows us to determine sharp reconstruction E and functions w_{Δ_j} up to an arbitrary degree of approximation.

A. Step *n*

At step n, a n-dimensional hypercube $Q^{(n)}=[0,1]^n$ is considered, whose edges lying on the axes are denoted by $C_1,C_2,\ldots,C_n$. Effect $F_j=F(\Delta_j)$ is assigned to edge $C_j\equiv[0,1]$ which is decomposed into the following 2^{n-1} subintervals:

$$\begin{aligned}C_{j,1}^{(n)}&=\left[0,\frac{1}{2^{n-1}}\right],C_{j,2}^{(n)}=\left(\frac{1}{2^{n-1}},\frac{2}{2^{n-1}}\right],\ldots,\\ C_{j,k}^{(n)}&=\left(\frac{k-1}{2^{n-1}},\frac{k}{2^{n-1}}\right],\ldots,C_{j,2^{n-1}}^{(n)}=\left(\frac{2^{n-1}-1}{2^{n-1}},1\right].\end{aligned}\tag{4}$$

These decompositions give rise to the decomposition of hypercube $Q^{(n)}$ into $2^{n(n-1)}$ sub-hypercubes of the kind

$$Q^{(n)}(\mathbf{k})=C_{1,k_1}^{(n)}\times C_{2,k_2}^{(n)}\times\cdots\times C_{n,k_n}^{(n)};$$

here $(k_1,k_2,\ldots,k_n)\equiv\mathbf{k}\in\{1,2,\ldots,2^{n-1}\}^n$ picks out sub-hypercube $Q^{(n)}(\mathbf{k})$ [$\mathbf{k}/2^{n-1}$ is the vertex of $Q^{(n)}(\mathbf{k})$ with the greatest distance from $(0,0,\ldots,0)$].

We will locate the spectrum of desired self-adjoint operator A within real interval $[0,1]$. To determine the resolution of the identity of A we decompose such an interval $[0,1]$ into $N(n)=2^{n(n-1)}$ intervals

$$\begin{aligned}I_1^{(n)}&=[0,\lambda_1^{(n)}],I_2^{(n)}=(\lambda_1^{(n)},\lambda_2^{(N)}],\ldots,\\ I_k^{(n)}&=(\lambda_{k-1}^{(n)},\lambda_k^{(n)}],\ldots,I_{N(n)}^{(n)}=(\lambda_{N(n)-1}^{(n)},1],\end{aligned}\tag{5}$$

where

$$\lambda_1^{(n)}=\frac{1}{N(n)},\quad \lambda_2^{(n)}=\frac{2}{N(n)},\ldots,\lambda_k^{(n)}=\frac{k}{N(n)},\ldots,\lambda_{N(n)-1}^{(n)}=\frac{N(n)-1}{N(n)},\quad \lambda_{N(n)}^{(n)}=1. \tag{6}$$

Then, the resolution of the identity E_λ of A is defined on points $\lambda_k^{(n)}$. To obtain this result, a suitable projection operator $E(I_k^{(n)})$ is assigned to each subinterval $I_k^{(n)}$ in such a way that $E(I_j^{(n)})\perp E(I_k^{(n)})$ if $j\neq k$, and then we put $E_{\lambda_k^{(n)}}=\Sigma_{j=1}^{k}E(I_j^{(n)})$.

Projection operator $E(I_k^{(n)})$ is assigned in the following way. Since the number of sub-hypercubes and that of intervals $I_k^{(n)}$ is the same, a bijection

$$I:\{Q^{(n)}(\mathbf{k})\}\rightarrow\{I_k^{(n)}\}$$

exists. Then, given $I_k^{(n)}$, we denote the projection onto C_j of sub-hypercube $Q^{(n)}(\mathbf{k})=I^{-1}(I_k^{(n)})$ by $C_{j,k_j}^{(n)}$. For every $j=1,2,\ldots,n$, let $E_\lambda^{(j)}$ be the resolution of the identity of self-adjoint operator $F_j\equiv F(\Delta_j)$ defined in (3). Then we put

$$E(I_k^{(n)})=E^{(1)}(C_{1,k_1}^{(n)})\cdot E^{(2)}(C_{2,k_2}^{(n)})\cdots E^{(n)}(C_{n,k_n}^{(n)}), \tag{7}$$

where $E^j(C_{j,k_j}^{(n)})=\int_{C_{j,k_j}^{(n)}}dE_\lambda^{(j)}$.

At the same step n we define, for every $j=1,2,\ldots,n$, a step function $\sigma_j^{(n)}$ on $[0,1]$, continuous on the left, in the following way. Given interval $I_k^{(n)}=(\lambda_{k-1}^{(n)},\lambda_k^{(n)}]$, we define $\sigma_j^{(n)}(\lambda)$, for all $\lambda\in I_k^{(n)}$, as the projection on edge C_j of the vertex of sub-hypercube $I^{-1}(I_k^{(n)})$ with the greatest distance from $(0,0,\ldots,0)$. For each fixed j, these step functions are continuous on the left, and they can be used to form a sequence $\{\sigma_j^{(n)}\}_{n\in\mathbf{N}}$.

B. Main theorem

The following theorem collects the main results proved in Ref. 6.

Theorem 1: *If bijection* $I:\{Q^{(n)}(\mathbf{k})\}\rightarrow\{I_k^{(n)}\}$ *satisfies the following conditions,*

(i) $Q^{(n+1)}(l_1,\ldots,l_{n+1})\subseteq Q^{(n)}(k_1,\ldots,k_n)\times C_{n+1}$ *then* $I(Q^{(n+1)}(l_1,\ldots,l_{n+1}))\subseteq I(Q^{(n)}(k_1,\ldots,k_n))$;

(ii) $\sigma_j^{(n+1)}(\lambda)=\sigma_j^{(n)}(\lambda)$ *for all* $\lambda\in\Lambda(n+1)$, *where* $\Lambda(n)=\{\lambda_0^{(n)}=0,\lambda_k^{(n)},\ k=1,2,\ldots,2^{n(n-1)}\}$,

then the following statements hold:

(1) Family $\{E_\lambda\}_{\lambda\in\mathbf{R}}\subseteq\mathcal{E}(\mathcal{H})$, *where* $E_\lambda\psi=\lim_{\lambda_k^{(n)}\rightarrow\lambda^+}E_{\lambda_k^{(n)}}\psi$, *may be seen to be a resolution of the identity.*

(2) Once defined

$$A^{(n)}=\sum_{k=1}^{N(n)}\lambda_k^{(n)}[E_{\lambda_k^{(n)}}-E_{\lambda_{k-1}^{(n)}}]\quad \textit{where}\quad E_{\lambda_0^{(n)}}^{(n)}=\mathbf{0}, \tag{8}$$

we can see that $A=\int\lambda dE_\lambda=\lim_{n\rightarrow\infty}A^{(n)}$ *is a bounded self-adjoint operator and the limit converges with respect to the operator norm.*

(3) For every $j\in\mathbf{N}$, *sequence* $\{\sigma_j^{(n)}\}_n$ *uniformly converges to a function* w_{Δ_j} *which is continuous on the left on* $[0,1]$, *whereas we put* $w_{\Delta_j}(\lambda)=0$ *if* $\lambda\notin[0,1]$.

(4) $F(\Delta_j)=\int w_{\Delta_j}(\lambda)dE_\lambda=w_{\Delta_j}(A)$.

In Ref. 6 it is shown that bijection I can be always explicitly defined in such a way that (i) and (ii) in Theorem 1 hold. Thus, we have an explicit well defined procedure allowing us to approach, up to an arbitrary degree of approximation, the sharp reconstruction

$$E:\mathcal{B}([0,1])\rightarrow\mathcal{E}(\mathcal{H}),\quad E(\Delta)=\int_\Delta dE_\lambda$$

of a given commutative unsharp observable F, and also functions w_{Δ_j}, for $\Delta_j \in \mathcal{S}$. In Sec. III C we show how to find w_Δ for every $\Delta \in \mathcal{B}([0,1])$.

III. PROBLEM OF CONSISTENCY

The results shown in Sec. II prompt us to interpret a commutative unsharp observable F as an *unsharp realization of its sharp reconstruction* E in the following precise sense:

($\mathcal{J}$) *The outcomes of unsharp observable* F *are interpreted as the result of a stochastic diffusion of the outcomes of sharp reconstruction* E *of* F, $w_\Delta(\lambda)$ *being the probability that the outcome of* F *belongs to* Δ *when the outcome of* E *is* λ.

This interpretation allows us to establish and understand the physical relationships between sharp and commutative unsharp observables. However, before adopting this interpretation it is necessary to verify its consistency. Interpretation ($\mathcal{J}$) should imply that the probability that an outcome of F belongs to an interval $\Delta_j \in \mathcal{S}$ [see (2)] is

$$\langle \psi | F(\Delta_j)\psi \rangle = \int w_{\Delta_j}(\lambda) d\|E_\lambda \psi\|^2.$$

Therefore the consistency of the interpretation requires the following conditions:

(i) All functions w_{Δ_j} must have the Lebesgue–Stieltjes integral with respect to $\alpha(\lambda) = \|E_\lambda \psi\|^2$.

(ii) Mapping $\mathcal{S} \to [0,1]$, $\Delta \to w_\Delta(\lambda)$ must behave as a probability measure.

The following Secs. III A and B are devoted to showing that these conditions are really satisfied. In particular we prove that for every $\lambda \in \sigma(A)$, mapping $\Delta \to w_\Delta(\lambda)$ is a probability measure on $\mathcal{R}(\mathcal{S})$, the ring generated by $\mathcal{S}$, which in its turn generates $\mathcal{B}([0,1])$. As a consequence of such an additivity and of the σ-additivity of POV measure F, in Sec. III C we show that for every $\Delta \in \mathcal{B}([0,1])$ a function w_Δ can be defined such that $F(\Delta) = w_\Delta(A)$. In Sec. IV we shall introduce and solve a more fundamental problem of consistency.

A. Integrability

We recall[8] that a function $f:[0,1] \to \mathbf{R}$ has the Lebesgue–Stieltjes integral with respect to a nondecreasing function $\alpha:[0,1] \to [0,1]$ (hence, of bounded variation) if and only if $f(\lambda(\alpha))$ has the Lebesgue integral (with respect to variable α) on the interval $[0,1]$, where $\lambda(\alpha)$ is the solution, possibly many-valued, of equation

$$\alpha(\lambda(\alpha)) = \alpha.$$

In this case the Lebesgue–Stieltjes integral of f is

$$\int f(\lambda) d\alpha(\lambda) = \int f(\lambda(\alpha)) d\alpha.$$

Every step function $\sigma_j^{(n)}$ defined in Sec. II A has the Lebesgue–Stieltjes integral with respect to $\alpha(\lambda) = \langle E_\lambda \psi | \psi \rangle$. Indeed, function $\phi_j^{(n)}(\alpha) = \sigma_j^{(n)}(\lambda(\alpha))$ always has the Lebesgue integral, and

$$\int \sigma_j^{(n)}(\lambda(\alpha)) d\alpha = \sum_k \sigma_j^{(n)}(\lambda_k^{(n)})[\alpha(\lambda_k^{(n)}) - \alpha(\lambda_{k-1}^{(n)})] = \int \sigma_j^{(n)}(\lambda) d\alpha(\lambda).$$

Therefore, function $|\sigma_j^{(n)}(\lambda(\alpha)) - \sigma_j^{(n+1)}(\lambda(\alpha))|$ has the Lebesgue integral, too, and

$$\int |\sigma_j^{(n)}(\lambda(\alpha)) - \sigma_j^{(n+1)}(\lambda(\alpha))| d\alpha$$

$$= \int |\sigma_j^{(n)}(\lambda) - \sigma_j^{(n+1)}(\lambda)| d\alpha(\lambda) \leq Sup_\lambda\{|\sigma_j^{(n)}(\lambda) - \sigma_j^{(n+1)}(\lambda)|\}[\alpha(1) - \alpha(0^-)]$$

$$= \frac{1}{2^{n-1}}.$$

This means that sequence $\{\sigma_j^{(n)}(\lambda(\alpha))\}_{n\in\mathbf{N}}$ is Cauchy in the mean. Then its limit $w_{\Delta_j}(\lambda(\alpha))$ is integrable and

$$\int w_{\Delta_j}(\lambda(\alpha)) d\alpha = \int w_{\Delta_j}(\lambda) d\alpha(\lambda).$$

This shows that all functions $w_{\Delta_j}(\lambda)$ have their own Lebesgue–Stieltjes integrals.

B. Additivity

In this subsection we prove that if $\Delta, \Delta_{j_1}, \Delta_{j_2}, \ldots, \Delta_{j_r} \in \mathcal{S}$, with $\Delta_{j_i} \cap \Delta_{j_k} = \varnothing$ when $i \neq k$, and $\Delta = \cup_k \Delta_{j_k}$, then $w_\Delta(\lambda) = \Sigma_k w_{\Delta_{j_k}}(\lambda)$, for all $\lambda \in \sigma(A)$.

First we consider the case that λ is just an eigenvalue of A, i.e., $\lambda \in \sigma_p(A)$; in this case there is an eigenvector ψ so that $A\psi = \lambda\psi$. This, according to a standard result of spectral theory (see, for instance, theorem VII.2 in Ref. 9), implies that $w_\Delta(A)\psi = w_\Delta(\lambda)\psi$ and $w_{\Delta_{j_k}}(A)\psi = w_{\Delta_{j_k}}(\lambda)\psi$. Since $F(\Delta) = \Sigma_k F(\Delta_{j_k})$ follows from $\Delta = \cup_k \Delta_{j_k}$, we have $w_\Delta(A)\psi = w_\Delta(\lambda)\psi = F(\Delta)\psi = \Sigma_k F(\Delta_{j_k})\psi = \Sigma_k w_{\Delta_{j_k}}(A)\psi = \Sigma_k w_{\Delta_{j_k}}(\lambda)\psi$, i.e.,

$$w_\Delta(\lambda) = \sum_k w_{\Delta_{j_k}}(\lambda).$$

Now we consider the case that λ is an *interior* point of continuous spectrum $\sigma_c(A) = \sigma(A) \backslash \sigma_p(A)$, so that there is an open interval $(\lambda - \delta, \lambda + \delta) \subseteq \sigma(A)$.

We recall the following result of standard spectral theory:

real number μ belongs to spectrum $\sigma(C)$ of a bounded self-adjoint operator C iff $h > 0$ implies $E(\lambda - h, \lambda + h) \neq \mathbf{0}$ iff a sequence $\{\varphi_n\} \subseteq \mathcal{H}$ exists so that $\|\varphi_n\| = 1$ and $\lim_n (C - \mu)\varphi_n = 0$ (see VII.3 in Ref. 9).

For every n there is a vector ψ_n, $\|\psi_n\| = 1$, so that $E(\lambda - \delta/n, \lambda]\psi_n = \psi_n$, otherwise interval $(\lambda - \delta/n, \lambda]$ would be not in the spectrum $\sigma(A)$, against the hypothesis. We have $\|[w_\Delta(A) - w_\Delta(\lambda)]\psi_n\| = \|\int [w_\Delta(\mu) - w_\Delta(\lambda)] dE_\mu \psi_n\| = \|\int_{\lambda - \delta/n}^{\lambda} [w_\Delta(\mu) - w_\Delta(\lambda)] dE_\mu \psi_n\| \leq \max_{\mu \in (\lambda - \delta/n, \lambda]} \times \{|w_\Delta(\mu) - w_\Delta(\lambda)| \to 0$ as $n \to \infty$ because w_{Δ_j} is continuous on the left in λ [see (3) of Theorem 1 in Sec. II B]. Similarly, $\|[w_{\Delta_{j_k}}(A) - w_{\Delta_{j_k}}(\lambda)]\psi_n\| \to 0$ as $n \to \infty$.

Then, by Definition 1,

$$|w_{\cup_k \Delta_{j_k}}(\lambda) - \sum_k w_{\Delta_{j_k}}(\lambda)| = \left\| \left[F(\cup_k \Delta_{j_k}) - \sum_k F(\Delta_{j_k}) \right] \psi_n - \left[w_{\cup_k \Delta_{j_k}}(\lambda) - \sum_k w_{\Delta_{j_k}}(\lambda) \right] \psi_n \right\|$$

$$= \left\| [F(\cup_k \Delta_{j_k}) - w_{\cup_k \Delta_{j_k}}(\lambda)]\psi_n - \sum_k (F(\Delta_{j_k}) - w_{\Delta_{j_k}}(\lambda))\psi_n \right\| \to 0,$$

as $n \to \infty$.

Therefore, $w_{\cup_k \Delta_{j_k}}(\lambda) = \Sigma_k w_{\Delta_{j_k}}(\lambda)$.

The only case still to be considered is that of a number λ which is on the boundary of $\sigma(A)$ but λ is not an eigenvalue of A, so that E_μ is continuous in λ. We redefine all functions $w_{\Delta_i}(\lambda) = \int_{\Delta_i} d\mu$ for these λ, where μ is the Lebesgue measure, so that $w_{\cup_k \Delta_{j_k}}(\lambda) = \Sigma_k w_{\Delta_{j_k}}(\lambda)$

obviously holds. This redefinition does not affect relations $F(\Delta_i)=w_{\Delta_i}(A)=\int w_{\Delta_i}(\lambda)dE_\lambda$ because these points are at most a countable family, and E_μ is continuous in all such points.

The additivity of $w_{(\cdot)}(\lambda)$ on semi-ring $\mathcal{S}$ allows us to additively extend $w_{(\cdot)}(\lambda)$ on ring $\mathcal{R}(\mathcal{S})$ generated by $\mathcal{S}$.

C. Functions w_Δ for $\Delta\in\mathcal{B}([0,1])$

If Δ is an open set in $[0, 1]$, then there is a disjoint, at most countable, sequence $\{\Delta_{j_k}\}\subseteq\mathcal{R}(\mathcal{S})$ such that $\Delta=\cup_k\Delta_{j_k}$. By (u2) in Definition 1, we have

$$F(\Delta)=\sum_k F(\Delta_{j_k})=\sum_k \int w_{\Delta_{j_k}}(\lambda)dE_\lambda .$$

For every $m\in\mathbf{N}$, we have $[0,1]=(\cup_{k=1}^m\Delta_{j_k})\cup\tilde{\Delta}$, for a suitable set $\tilde{\Delta}\in\mathcal{R}(\mathcal{S})$ disjoint from $(\cup_{k=1}^m\Delta_{j_k})$. Then $1=w_{[0,1]}(\lambda)=\Sigma_{k=1}^m w_{\Delta_{j_k}}(\lambda)+w_{\tilde{\Delta}}(\lambda)$, since $\Delta\to w_\Delta(\lambda)$ is additive on $\mathcal{R}(\mathcal{S})$. Therefore sequence $\Sigma_{k=1}^m w_{\Delta_{j_k}}(\lambda)$, increasing with respect to m, is bounded by 1, and it must converge for every λ. Thus

$$F(\Delta)=\sum_k \int w_{\Delta_{j_k}}(\lambda)dE_\lambda=\int \sum_k w_{\Delta_{j_k}}(\lambda)dE_\lambda$$

follows, for instance, from theorem VII.2.d in Ref. 9.

Therefore, for every open set $\Delta\in[0,1]$, by using functions $w_{\Delta_{j_k}}$ we can construct a function $w_\Delta=\Sigma_k w_{\Delta_{j_k}}$ such that $F(\Delta)=\int w_\Delta(\lambda)dE_\lambda$. This result is a consequence of the σ-additivity of POV measure F we start from. Similarly, a function w_Δ such that $F(\Delta)=w_\Delta(A)$ can be constructed for all $\Delta\in\mathcal{B}([0,1])$, as done in Ref. 6.

However, on the basis of these results, we cannot state that $\Delta\to w_\Delta(\lambda)$ is σ-additive, but only that it is additive on ring $\mathcal{R}(\mathcal{S})$. The σ-additivity would imply that $\Delta\to w_\Delta(\lambda)$ can be extended to a (σ-additive) probability measure on $\mathcal{B}([0,1])$. The problem of the σ-additivity of $\Delta\to w_\Delta(\lambda)$ is an open question we are facing for a further development of the present work.

IV. A MORE FUNDAMENTAL PROBLEM OF CONSISTENCY

Let F be a commutative unsharp observable, and let E be the sharp reconstruction of F, corresponding to self-adjoint operator A, obtained by reversing correspondence (1) by means of the procedure described in Sec. II. Let us suppose that F is *actually* the unsharp realization of a given, but unknown, sharp observable E^B, with $B=\int\mu dE^B_\mu$, different from the sharp reconstruction E. Our proposed interpretation ($\mathcal{J}$) of F as the unsharp realization of E could be inconsistent with the simultaneous, inevitable, interpretation of F as an unsharp realization of E^B. For instance, the consistency would fail if $[A,B]\neq\mathbf{0}$. In such a case there would be a fundamental problem in interpreting F as an unsharp realization of E, because $[A,B]\neq\mathbf{0}$ forbids assigning, even hypothetically, simultaneous values to observables E and E^B.

However, such a problem of consistency does not occur if the following condition holds.

(C) *If E^B and $\{w^B_\Delta\}$ are respectively a sharp observable and a family of functions satisfying condition (PM) in Sec. II, so that*

$$F(\Delta)=w^B_\Delta(B),$$

then a real function g exists so that $A=g(B)$.

If condition (C) holds, then the above described problem of consistency cannot arise because every outcome λ of E can be interpreted, according to standard quantum theory, as the result of the transformation of the outcome μ of E^B by means of mapping g, i.e., $\lambda=g(\mu)$ (for instance, see Ref. 5, assertion **F**, Chap. III). In this case $[A,B]=\mathbf{0}$, of course.

In this section we show that for every self-adjoint operator B, with $\sigma(B)\subseteq[0,1]$ and resolution of the identity E^B_μ, such that $E^B\to F$ in the sense of (1), it is possible to concretely construct, by an explicit procedure, a real function g (which is Lebesgue–Stieltjes integrable with respect to $\beta(\mu)=\langle\psi|E^B_\mu\psi\rangle$ for all $\psi\in\mathcal{H}$) so that $A=g(B)$. As a consequence, condition (C) is satisfied and thus the problem of consistency pointed out above does not arise; in so doing we have the further advantage of having a well defined mathematical procedure to find g.

A. Basic proposition

Our result is based on Proposition 1 proven in this subsection.

By $\{w^B_\Delta\}_{\Delta\in\mathcal{B}([0,1])}$ we denote the family of functions defined on $\sigma(B)$ and Lebesgue–Stieltjes integrable with respect to $\beta(\lambda)=\langle E^B_\lambda\psi|\psi\rangle$ so that $F(\Delta)=w^B_\Delta(B)=\int w^B(\mu)dE^B_\mu$. Let $C^{(n)}_{j,k}\subseteq[0,1]$ be one of the subintervals of edge C_j defined in (4) at step n of the procedure outlined in Sec. II, and let $E^{(j)}_\lambda$ be the resolution of the identity of $F_j=F(\Delta_j)$. Then

$$E^{(j)}(C^{(n)}_{j,k})=E^{(j)}_{k/2^{n-1}}-E^{(j)}_{k-1/2^{n-1}}=\int\chi_{C^{(n)}_{j,k}}(\lambda)dE^{(j)}_\lambda=\chi_{C^{(n)}_{j,k}}(F(\Delta_j)). \tag{9}$$

For every j,

$$F(\Delta_j)=\int w^B_{\Delta_j}(\mu)dE^B_\mu. \tag{10}$$

From (9) we have

$$E^{(j)}(C^{(n)}_{j,k})=\chi_{C^{(n)}_{j,k}}(F(\Delta_j))=\chi_{C^{(n)}_{j,k}}(w^B_{\Delta_j}(B))=\int\chi_{C^{(n)}_{j,k}}(w^B_{\Delta_j}(\mu))dE^B_\mu.$$

The above expression follows from the rules of operator functional calculus (e.g., Ref. 8, pp. 342–347).

Therefore,

$$E^{(j)}(C^{(n)}_{j,k})=\int\chi_{[w^B_{\Delta_j}]^{-1}(C^{(n)}_{j,k})}(\mu)dE^B_\mu=E^B([w^B_{\Delta_j}]^{-1}(C^{(n)}_{j,k})). \tag{11}$$

Let us consider an interval of the kind $I^{(n)}_k=(\lambda^{(n)}_{k-1},\lambda_k]$ in (5). Then

$$E(I^{(n)}_k)=E_{\lambda^{(n)}_k}-E_{\lambda^{(n)}_{k-1}}=\prod_{j=1}^n E^{(j)}(C^{(n)}_{j,l(j,k)})\quad\text{by (7)}$$

$$=\prod_{j=1}^n E^B([w^B_{\Delta j}]^{-1}(C^{(n)}_{j,l(j,k)}))\quad\text{by (11)}$$

where $C^{(n)}_{j,l(j,k)}$ is the projection on jth edge C_j of sub-hypercube $I^{-1}(I^{(n)}_k)$. We have $E^B(\Delta_1\cap\Delta_2)=E^B(\Delta_1)\cdot E^B(\Delta_2)$, $\forall\Delta_1,\Delta_2\in\mathcal{B}([0,1])$, and then

$$E(I^{(n)}_k)=E^B(\cap^n_{j=1}[w^B_{\Delta j}]^{-1}(C^{(n)}_{j,l(j,k)})). \tag{12}$$

For every subinterval $I^{(n)}_k$ in (5) we define the Borel set

$$c(I^{(n)}_k)=\{\cap^n_{j=1}[w^B_{\Delta j}]^{-1}(C^{(n)}_{j,l(j,k)})\}. \tag{13}$$

Now we shall prove the following proposition.

Proposition 1: Borel's sets $c(I^{(n)}_k)$ defined by (13) satisfy the following conditions:

(i) $E(I^{(n)}_k)=E^B(c(I^{(n)}_k))$.

(ii) *If* $I_k^{(n+1)} \subseteq I_{j(k)}^{(n)}$, *then* $c(I_k^{(n+1)}) \subseteq c(I_{j(k)}^{(n)})$.
(iii) $I_k^{(n)} \cap I_i^{(n)} = \varnothing$ *implies* $c(I_k^{(n)}) \cap c(I_i^{(n)}) = \varnothing$.
(iv) $\cup_k c(I_k^{(n)}) = \sigma(B)$.

Proof: Condition (i) follows from (12).

(ii) If $I_k^{(n+1)} \subseteq I_{j(k)}^{(n)}$, then, by (i) in Theorem 1, we obtain $I^{-1}(I_k^{(n+1)}) \subseteq I^{-1}(I_{j(k)}^{(n)}) \times C_{n+1}$.

Therefore, subintervals $C_{j,k_j}^{(n+1)}$ and $C_{j,k_j'}^{(n)}$ which are the respective projections of sub-hypercubes $I^{-1}(I_k^{(n+1)})$, $I^{-1}(I_{j(k)}^{(n)})$ on jth edge C_j are such that $C_{j,k_j}^{(n+1)} \subseteq C_{j,k_j'}^{(n)}$. Then, by (13),

$$c(I_k^{(n+1)}) \subseteq c(I_{j(k)}^{(n)}). \tag{14}$$

(iii) If $I^{-1}(I_k^{(n)}) = \Pi_{j=1}^n C_{j,l(j,k)}^{(n)}$ and $I^{-1}(I_i^{(n)}) = \Pi_{j=1}^n C_{j,l(j,i)}^{(n)}$, then we can see that $I_k^{(n)} \cap I_i^{(n)} = \varnothing$ implies $I^{-1}(I_k^{(n)}) \cap I^{-1}(I_i^{(n)}) = \varnothing$, because I is bijective.

Therefore, there exists j_0 so that $C_{j_0,l(j_0,k)}^{(n)} \cap C_{j_0,l(j_0,i)}^{(n)} = \varnothing$; hence we have $\varnothing = \{[w_{\Delta_{j_0}}^B]^{-1}(C_{j_0,l(j_0,k))}^{(n)}\} \cap \{[w_{\Delta_{j_0}}^B]^{-1}(C_{j_0,l(j_0,i)}^{(n)})\}$ [recall that $X \cap Y = \varnothing \Rightarrow f^{-1}(X) \cap f^{-1}(Y) = \varnothing$ holds for any function f]. Thus, from (13), $c(I_k^{(n)}) \cap c(I_i^{(n)}) = \varnothing$ follows.

(iv) For every j, $\cup_k C_{j,l(j,k)}^{(n)} = [0,1]$ and $[w_{\Delta_j}^B]^{-1}([0,1]) = \sigma(B)$. Then

$$\begin{aligned}
\cup_k c(I_k^{(n)}) &= \cap_{j=1}^n \{\cup_k [w_{\Delta_j}^B]^{-1}(C_{j,l(j,k)}^{(n)})\} \\
&= \cap_{j=1}^n [w_{\Delta_j}^B]^{-1}(\cup_k C_{j,l(j,k)}^{(n)}) \\
&= \cap_{j=1}^n [w_{\Delta_j}^B]^{-1}([0,1]) = \cap_{j=1}^n \sigma(B) = \sigma(B).
\end{aligned}$$

B. Construction of function *g*

Now we define a sequence of functions $\{g^{(n)}\}$ which converges to a function $g = \lim_{n\to\infty} g^{(n)}$ with respect to the uniform topology of bounded functions. We shall prove that $A = g(B)$.

To construct sequence $\{g^{(n)}\}$ we make use of Proposition 1.

Let us consider the countable family $\mathcal{I} = \{I_k^{(n)}\}_{k,n}$ of all intervals defined in (5). By means of (13), we define mapping

$$c: \mathcal{I} \to \mathcal{B}(\mathbf{R}), \quad I_j^{(n)} \to c(I_j^{(n)}) \subseteq \sigma(B).$$

Fixed n, by (iii) and (iv) in Proposition 1, for every $\mu \in \sigma(B)$ a unique k exists so that $\mu \in c(I_k^{(n)})$. Then, it is possible to define the function

$$g^{(n)}: \sigma(B) \to \cup_n \Lambda(n), \quad \mu \in c(I_k^{(n)}) \to g^{(n)}(\mu) = \lambda_k^{(n)}. \tag{15}$$

Therefore, we can write

$$\lambda_k^{(n)} E(I_k^{(n)}) = \lambda_k^{(n)} E^B(c(I_k^{(n)})) = \lambda_k^{(n)} \int \chi_{c(I_k^{(n)})}(\mu) dE_\mu^B. \tag{16}$$

Thus we have $g^{(n)}(\mu) = \Sigma_k \lambda_k^{(n)} \chi_{c(I_k^{(n)})}(\mu)$.

By replacing (16) in (8) we obtain

$$\begin{aligned}
A^{(n)} &= \sum_k \lambda_k^{(n)} E^A(I_k^{(n)}) = \sum_k \int \lambda_k^{(n)} \chi_{c(I_k^{(n)})}(\mu) dE_\mu^B \\
&= \int_{\sigma(B)} \sum_k \lambda_k^{(n)} \chi_{c(I_k^{(n)})}(\mu) dE_\mu^B \\
&= \int_{\sigma(B)} g^{(n)}(\mu) dE_\mu^B,
\end{aligned} \tag{17}$$

having used Proposition 1.

Now we can prove that functions $g^{(n)}$ converge as $n\to\infty$ to a function $g:\sigma(B)\to[0,1]$ with respect to the uniform topology.

Let $\mu\in\sigma(B)$ be so that $\mu\in c(I_k^{(n+1)})$; then a unique index $j(k)$ exists, so that

$$I_k^{(n+1)}\subseteq I_{j(k)}^{(n)}. \tag{18}$$

From Proposition 1 (ii) it follows that

$$c(I_k^{(n+1)})\subseteq c(I_{j(k)}^{(n)}), \tag{19}$$

hence $\mu\in c(I_{j(k)}^{(n)})$. By (15) and (18) we obtain

$$g^{(n+1)}(\mu)=\lambda_k^{(n+1)}\in(\lambda_{j(k)-1)}^{(n)},\lambda_{j(k)}^{(n)}] \text{ and } g^{(n)}(\mu)=\lambda_{j(k)}^{(n)}.$$

Therefore, $|g^{(n)}(\mu)-g^{(n+1)}(\mu)|\leqslant 1/2^{n(n-1)}$ for every $\mu\in\sigma(B)$. Thus sequence $\{g^{(n)}\}$ uniformly converges to a function $g:\sigma(B)\to[0.1]$.

Finally, we can prove that function g, so defined, is Lebesgue–Stieltjes integrable with respect to $\beta(\mu)=\langle E_\mu^B\psi|\psi\rangle$, for every ψ, and that $A=g(B)$. From (17) it follows that every function defined in (15) is Lebesgue–Stieltjes integrable with respect to $\beta(\mu)=\langle E_\mu^B\psi|\psi\rangle$, $\forall\ \psi$.

Therefore, $|g^{(n+1)}(\mu)-g^{(n)}(\mu)|$ is Lebesgue–Stieltjes integrable, too. This implies that $|g^{(n+1)}(\mu(\beta))-g^{(n)}(\mu(\beta))|$ is Lebesgue integrable and

$$\int |g^{(n+1)}(\mu(\beta))-g^{(n)}(\mu(\beta))|d\beta=\int |g^{(n+1)}(\mu)-g^{(n)}(\mu)|d\beta(\mu)\leqslant\frac{1}{2^{n(n-1)}}. \tag{20}$$

Then sequence $\{g^{(n)}(\mu(\beta))\}$ is Cauchy in the mean, and therefore its limit $g(\mu(\beta))$ is Lebesgue integrable and $g(\mu)$ is Lebesgue–Stieltjes integrable. According to (17) we have

$$g(B)=\int g(\mu)dE_\mu^B=\lim_n\int g^{(n)}(\mu)dE_\mu^B=\lim_n A^{(n)}=A,$$

that is to say $A=g(B)$.

C. The general 1-0 observable

Now we shall concentrate on a particular kind of unsharp observable. Given any nontrivial effect ϕ, the *1-0 unsharp observable* Φ generated by ϕ is

$$\Phi(\Delta)=\begin{cases}\phi & \text{if } 1\in\Delta \text{ and } 0\notin\Delta,\\ \mathbf{1}-\phi & \text{if } 0\in\Delta \text{ and } 1\notin\Delta,\\ \mathbf{1} & \text{if } 1,0\in\Delta,\\ 0 & \text{if } 1\notin\Delta \text{ and } 0\notin\Delta.\end{cases} \tag{21}$$

Unsharp observable Φ is nothing but the observable which takes value 1 when ϕ occurs and value 0 when ϕ does not occur. It is the most elementary kind of unsharp observable. We shall prove that in this simple case the self-adjoint operator A representing the sharp reconstruction of Φ coincides, modulo a bijection, with ϕ itself. The family $\{\Phi(\Delta)\}_{\Delta\in\mathcal{B}(\mathbf{R})}$ contains only two nontrivial effects ϕ and $\mathbf{1}-\phi$. Since ϕ itself is a self-adjoint operator, it has a resolution of the identity E_λ^ϕ so that $\phi=\int\lambda dE_\lambda^\phi$. If we put $B=\phi$, then we can immediately find the family $\{w^\phi(\Delta)\}_\Delta$ so that $\Phi(\Delta)=w_\Delta^\phi(\phi)$:

$$w_{\Delta}^{\phi}(\mu)=\begin{cases}\mu & \text{if } 1\in\Delta \text{ and } 0\notin\Delta,\\ 1-\mu & \text{if } 0\in\Delta \text{ and } 1\notin\Delta,\\ 1 & \text{if } 1,0\in\Delta,\\ 0 & \text{if } 1\notin\Delta \text{ and } 0\notin\Delta.\end{cases} \tag{22}$$

Therefore, we can explicitly construct function g so that $A=g(\phi)$, according to Sec. IV B, where A is the sharp reconstruction of Φ. We prove that this function g is invertible. The injectivity of g means that the sharp observable represented by $B=\phi$ differs from the sharp reconstruction only for the scale used to measure their respective values, therefore they are essentially the same.

Having fixed $n\geqslant 5$, given any $\mu\in\sigma(\phi)$, let $I_{k(n,\mu)}^{(n)}=(\lambda_{k(n,\mu)-1}^{(n)},\lambda_{k(n,\mu)}^{(n)}]$ be the unique interval among (5) so that $\mu\in c(I_{k(n,\mu)}^{(n)})$, according to (iii) and (iv) of Proposition 1. Then, according to (15),

$$g^{(n)}(\mu)=\lambda_{k(n,\mu)}^{(n)}.$$

Lemma 1: If $\mu\in\sigma(B)$, then $\mu=\lim_n \sigma_3^{(n)}(g^{(n)}(\mu))$.

Proof: Given $\mu\in\sigma(B)$, for every fixed n, a unique index $k(n,\mu)$ exists so that $\mu\in c(I_{k(n,\mu)}^{(n)})$. Since by (13) $c(I_{k(n,\mu)}^{(n)})=\cap_{j=1}^{n}[w_{\Delta_j}^{\phi}]^{-1}(C_{j,l(j,k)}^{(n)})$, μ must belong to all sets $[w_{\Delta_j}^{\phi}]^{-1}(C_{j,l(j,k)}^{(n)})$, $j=1,2,\ldots,n$. In particular, by (22) we have $w_{\Delta_3}^{\phi}(\mu)=\mu$, which implies

$$\mu\in[w_{\Delta_3}^{\phi}]^{-1}(C_{3,l(3,k)}^{(n)})=C_{3,l(3,k)}^{(n)})=\left(\sigma_3^{(n)}(\lambda_{k(n,\mu)}^{(n)})-\frac{1}{2^{(n-1)}},\sigma_3^{(n)}(\lambda_{k(n,\mu)}^{(n)})\right].$$

Since the length of $C_{3,l(3,k)}^{(n)}$ vanishes when $n\to\infty$, we have

$$\lim_{n\to\infty}\sigma_3^{(n)}(\lambda_{k(n,\mu)}^{(n)})=\mu.$$

Lemma 2: Sequence $\{g^{(n)}(\mu)\}_n$ is strictly decreasing.

Proof: By (18) in Sec. IV B, we see that $g^{(n+1)}(\mu)=\lambda_{k(n+1,\mu)}^{(n+1)}\leqslant\lambda_{k(n,\mu)}^{(n)}$ therefore $\{\lambda_{k(n,\mu)}^{(n)}\}$ is not increasing.

On the other hand, using an argument similar to that of Lemma 1 we get

$$\mu\in[w_{\Delta_5}^{\phi}]^{-1}(C_{5,l(5,k)}^{(n)}),\quad \forall n.$$

Since $w_{\Delta_5}^{\phi}(\eta)=0$, then $0\in C_{5,l(5,k)}^{(n)}$, which implies $C_{5,l(5,k)}^{(n)}=[0,1/2^{(n-1)}]$. Therefore,

$$\sigma_5^{(n)}(\lambda_{k(n,\mu)}^{(n)})=\frac{1}{2^{(n-1)}}. \tag{23}$$

Then if $\lambda_{k(n,\mu)}^{(n)}=\lambda_{k(n+1,\mu)}^{(n+1)}$, according to (ii) in Theorem 1 we would have

$$\sigma_5^{(n)}(\lambda_{k(n,\mu)}^{(n)})=\sigma_5^{(n+1)}(\lambda_{k(n+1,\mu)}^{(n+1)}),$$

which contradicts (23).

Proposition 2: Function $g:\sigma(\phi)\to[0,1]$, $g(\mu)=\lim_n g^{(n)}(\mu)$ is injective.

Proof: Given $\mu_1,\mu_2\in[0,1]$, we consider sequences $\{g^{(n)}(\mu_i)=\lambda_{k(n,\mu_i)}^{(n)}\}_n$, $i=1,2$. If $g(\mu_1)=g(\mu_2)$, then

$$\lim_{n\to\infty}\lambda_{k(n,\mu_1)}^{(n)}=\lim_{n\to\infty}\lambda_{k(n,\mu_2)}^{(n)}=\lambda.$$

The terms of sequences $\{\lambda^{(n)}_{k(n,\mu_i)}\}_n$ are the right bounds of intervals $I^{(n)}_{k(n,\mu_i)}$, which satisfy $I^{(n+1)}_{k(,n+1,\mu_i)} \subset I^{(n)}_{k(n,\mu_i)}, \forall n$. Therefore $\lambda = \lim_{n\to\infty} \lambda^{(n)}_{k(n,\mu_i)}$ is such that either $\lambda \in I^{(n)}_{k(n,\mu_i)}$ or $\lambda = \lambda^{(n)}_{k(n,\mu_i)-1}, \forall n$. In the second case the sequence is constant and equal to λ. But, by Lemma 2, sequence $\{\lambda^{(n)}_{k(n,\mu)}\}_n$ can never be constant. Thus we have to conclude that $\lambda \in I^{(n)}_{k(n,\mu_i)}$, for both $i=1,2$ and $\forall n$. Then, $I^{(n)}_{k(n,\mu_1)} = I^{(n)}_{k(n,\mu_2)}$ for all n; hence

$$\lambda^{(n)}_{k(n,\mu_1)} = \lambda^{(n)}_{k(n,\mu_2)}, \quad \forall n.$$

According to Lemma 1,

$$\mu_1 = \lim_{n\to\infty} \sigma_3^{(n)}(\lambda^{(n)}_{k(n,\mu_1)}) = \lim_{n\to\infty} \sigma_3^{(n)}(\lambda^{(n)}_{k(n,\mu_2)}) = \mu_2.$$

Thus, the proposition is proved.

V. INTERPRETATION OF RESULTS

The results proven in this work show that it is possible to assign a sharp observable E to each commutative unsharp observable F, in such a way that F can be consistently interpreted as an unsharp realization of E, according to $(\mathcal{J})$ in Sec. IV. The consistency of such an assignment is not a trivial problem, because correspondence (1) allows us to obtain the same F starting from several, different sharp observables E^B, E^C etc. Every one of these sharp observables could be the sharp observable actually turned into F because of a stochastic diffusion of its outcomes.

But every one of them could not. Indeed, the stochastic diffusion leading from a sharp observable E^D to a commutative unsharp observable F by means of correspondence (1) destroys a certain amount of information, which is no longer recoverable. The loss of information intrinsic in this process impedes the determination of the starting sharp observable E^D from the outcoming unsharp observable F. However, our results of Sec. IV B say that whatever sharp observable E^B is actually turned into F, its outcomes μ must be related to the outcomes λ of our reconstruction E by a mapping g so that $\lambda = g(\mu)$.

Therefore, our reconstruction E is the unique sharp observable, *modulo* a bijection, which is related in such a way to all sharp observables which have the possibility of being turned into F via (1).

From the point of view of information theory, our result entails that the reconstruction E is the unique sharp version of unsharp observable F which contains the same information carried by F. All other sharp versions of F have an information content which is redundant with respect to that of F.

In the literature we find[10,11] successful attempts to relate an unsharp observable with a sharp one, which are based on the following theorem of Neumark.[8,10,11]

Neumark's Theorem: *Let $F:\mathcal{B}(\mathbf{R})\to\mathcal{F}(\mathcal{H})$ be a POV measure which acts on Hilbert space $\mathcal{H}$. Then there exists a Hilbert space $\widetilde{\mathcal{H}}$ in which $\mathcal{H}$ is embedded as a subspace, and a PV measure $\widetilde{E}:\mathcal{B}(\mathbf{R})\to\mathcal{E}(\widetilde{\mathcal{H}})$, which acts on $\widetilde{\mathcal{H}}$, such that $F(\Delta)=P\widetilde{E}(\Delta)P$, where P is the projection operator of $\widetilde{\mathcal{H}}$ which projects onto $\mathcal{H}$.*

Our approach is basically different from the ones based on Neumark's theorem. Indeed, the latter introduces *dilations* $\widetilde{H},\widetilde{E}$, which have not a direct physical interpretation. In our approach, on the contrary, to every commutative unsharp observable F we associate the sharp reconstruction E which pertains to the *same system* and to the same Hilbert space $\mathcal{H}$ of the original unsharp observable; therefore, the problem of intepreting dilations does not arise.

It is also known that for every commutative unsharp observable F there is a unique PV measure $P:\mathcal{B}(\mathcal{D})\to\mathcal{E})(\mathcal{H})$, where $\mathcal{D}$ is the space of probabilty measures on $\mathbf{R}$, such that $F(\Delta) = \int_{\mathcal{D}} \mu(\Delta) P(d\mu)$. This mathematical characterization[10–15] found several interesting applications. For instance, Twareque Ali[16] used it for extending Mackey's imprimitivity theorem[17] to covariance

systems based on commutative unsharp observables rather than on sharp ones. The characterization we deal with in the present work has a more physical nature, though we cannot exclude the existence of a link between these two characterization.

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Lüders theorem for coherent-state POVMs

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(Received 6 August 2003; accepted 27 August 2003)

Lüders' theorem states that two observables commute if measuring one of them does not disturb the measurement outcomes of the other. We study measurements which are described by continuous positive operator-valued measurements (or POVMs) associated with coherent states on Lie groups. In general, operators turn out to be invariant under the *Lüders* map if their P- and Q-symbols coincide. For a spin corresponding to SU(2), the identity is shown to be the only operator with this property. For a particle, a countable family of linearly independent operators is identified which are invariant under the *Lüders* map generated by the coherent states of the Heisenberg–Weyl group, H_3. The *Lüders* map is also shown to implement the anti-normal ordering of creation and annihilation operators of a particle. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623001]

I. INTRODUCTION

In this article we determine operators B which are invariant under a generalized *Lüders* map

$$B \mapsto \Lambda(B) = \int_{\mathbb{X}} d\mu(\Omega)\, E(\Omega) B E(\Omega)\,, \tag{1}$$

where each $E(\Omega)$ is a projection operator labeled by a point Ω of a manifold $\mathbb{X}$. These operators constitute a continuous positive operator-valued measure, or POVM, with a resolution of unity:

$$\int_{\mathbb{X}} d\mu(\Omega)\, E(\Omega) = I\,. \tag{2}$$

Any operator B, bounded or not, will be called *Lüders* if it is invariant under *Lüders*' map,

$$\Lambda(B) = B\,. \tag{3}$$

The operator B acts on a complex separable Hilbert space $\mathcal{H}$, and the operator $E(\Omega)$ is a member of a (over-) complete family of projectors on coherent states $|\Omega\rangle$ associated with an irreducible, unitary representation of a Lie group G in the space $\mathcal{H}$.

This setting generalizes the traditional approach to minimally disturbing (or *ideal*) *Lüders* measurements. Given a self-adjoint operator with spectral decomposition $A = \Sigma_i^N a_i E_i$, $N \leqslant \infty$, the projectors E_i are complete and orthogonal,

$$\sum_{i=1}^{N} E_i = I\,, \quad E_i E_j = E_i \delta_{ij}\,, \quad i,j = 1,\ldots,N \leqslant \infty\,. \tag{4}$$

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If a nonselective, ideal measurement of A is performed on a quantum system with density operator ρ, its state undergoes a *Lüders* transformation:

$$\rho \mapsto \Lambda(\rho) = \sum_{i=1}^{N} E_i \rho E_i \,, \tag{5}$$

which extends to a linear, completely positive map. If, for some operator B, one has

$$\mathrm{Tr}\,[\rho B] = \mathrm{Tr}\,[\Lambda(\rho) B] \,, \quad \text{for all } \rho \,, \tag{6}$$

then the *Lüders* measurement of A does not disturb the measurement of B. In other words, the expectation value of B with respect to *any* density operator ρ is not affected by measuring A. Introduce the *dual Lüders* map Λ^D, acting on operators defined on $\mathcal{H}$, by

$$\mathrm{Tr}\,[\Lambda(\rho) B] = \mathrm{Tr}\,[\rho \Lambda^D(B)] \,. \tag{7}$$

Since Eq. (6) is supposed to hold for any ρ, one must have

$$\Lambda^D(B) = B \,, \tag{8}$$

which, after dropping the superscript, is the discrete counterpart of Eq. (3). Now we can state *Lüders*' theorem:

$$\Lambda(B) = B \quad \Leftrightarrow \quad [B, E_i] = 0 \,, \quad \text{for all } i = 1,2,\ldots \,, \tag{9}$$

i.e., it is necessary and sufficient for $A = \Sigma_i^N a_i E_i$ to commute with a (bounded) operator B if the measurement of A should not disturb any measurement of B.

Originally, this theorem has been shown to hold for orthogonal projections;[1] after generalizations to some discrete POVMs had been obtained,[2] the theorem was expected to hold under very general conditions. However, the existence of a nonintuitive counterexample has been proved nonconstructively in Ref. 3. It is our purpose to extend the validity of *Lüders*' theorem to *continuous* POVMs which are associated with coherent states on Lie groups.

A. Outline and summary

In the following, we will consider POVMs which consist of continuous families of one-dimensional projections onto coherent states, or CS-POVMs, for short. The CS-POVMs for a spin and for a particle provide well-known examples, being associated with the group SU(2) and the Heisenberg–Weyl group H_3, respectively. However, coherent states can be defined for general Lie groups G while retaining many of their properties. We will begin to discuss the *Lüders* map in general terms and specialize to particular groups only later.

When considering *Lüders*' map generated by coherent states of an arbitrary (simple and simple connected) Lie group G, a first general observation is that

- the P- and the Q-symbol of a *Lüders* operator coincide for the CS-POVM associated with a Lie group G.

Subsequently, we will derive a simple form of this constraint by expanding the symbol of the operator in terms of harmonic functions associated with the group G. The resulting condition on the expansion coefficients will be shown to imply that

- for the CS-POVM of a *spin* only multiples of the identity operator are *Lüders*;
- for the CS-POVM of a *particle* a countable family of linearly independent, unbounded *Lüders* operators exists, none of which commutes with the elements of the POVM.

Thus, for both the groups SU(2) and H_3, multiples of the identity are found to be the only *bounded Lüders* operator, and they commute with the elements of the corresponding CS-POVM: consequently, *Lüders*' theorem also applies to these CS-POVMs.

Finally, it will be shown that the *Lüders* map implements antinormal ordering for operators which can be written as power series of particle annihilation and creation operators.

II. *LÜDERS* THEOREM FOR POVMS OF COHERENT STATES

A. Coherent states on Lie groups and harmonic functions

Given any finite-dimensional (simple and simply connected) Lie group G, there is a canonical way to introduce coherent states $|\Omega\rangle$ labeled by the points Ω of a well-defined manifold $\mathbb{X}$. To do so, consider a unitary irreducible representation $T(g)$ on a Hilbert space $\mathcal{H}$ of the elements $g \in G$. Following closely the presentation given in Ref. 4, we choose a reference (or fiducial) state $|\psi_0\rangle$ and define the set of coherent states by

$$|\psi_g\rangle = T(g)|\psi_0\rangle, \quad g \in G. \tag{10}$$

Up to a phase, the reference state is left invariant by the elements h of the isotropy subgroup $H \subset G$,

$$T(h)|\psi_0\rangle = e^{i\phi(h)}|\psi_0\rangle, \quad h \in H \subset G. \tag{11}$$

Therefore, each group element can be written as as product

$$g = \Omega h, \quad \Omega \in \mathbb{X} = G/H, \quad h \in H, \tag{12}$$

where $\mathbb{X}$ is the coset space obtained from dividing G by its subgroup H. As the phase of a state has no physical relevance, the set of coherent states is in a one-to-one correspondence with the points $\Omega(g)$ of the manifold $\mathbb{X}$. This suggests to denote coherent states by $|\Omega\rangle \equiv |\psi_\Omega\rangle$. A fundamental property of the coherent states $|\Omega\rangle$ is their completeness in Hilbert space $\mathcal{H}$,

$$\int_{\mathbb{X}} d\mu(\Omega)\, |\Omega\rangle\langle\Omega| = I, \tag{13}$$

where integration is over the coset space $\mathbb{X}$ with (approximately normalized) invariant measure $d\mu(\Omega)$, and I is the identity in $\mathcal{H}$.

Coherent states $|\Omega\rangle$ can be used to define symbolic representations of operators, i.e., c-number valued functions on the manifold $\mathbb{X}$ which can be understood as the phase space of a classical system associated with the Lie group G.[5] The Q-symbol of an operator B acting in Hilbert space $\mathcal{H}$ is given by its expectation value in coherent states,

$$Q_B(\Omega) = \langle\Omega|B|\Omega\rangle, \quad \Omega \in \mathbb{X}; \tag{14}$$

due to analyticity properties of $Q_B(\Omega)$, these "diagonal" matrix elements are sufficient to uniquely determine the operator B. The P-symbol of B (Refs. 6 and 7) arises if one expresses B as a linear combination of projection operators $|\Omega\rangle\langle\Omega|$:

$$B = \int_{\mathbb{X}} d\mu(\Omega)\, P_B(\Omega)\, |\Omega\rangle\langle\Omega|. \tag{15}$$

The existence of the symbols $Q_B(\Omega)$ and $P_B(\Omega)$ depends in a subtle way on the properties of the operator B (Ref. 5) but they are unique whenever they exist. Furthermore, one can think of the symbols $Q_A(\Omega)$ and $P_A(\Omega)$ as being dual to each other (cf. Ref. 5), and, at least for particle coherent-states, they are related to normal and anti-normal ordering of creation and annihilation operators.[5,8]

It is useful to introduce the harmonic functions $Y_\nu(\Omega)$ associated with the manifold $\mathbb{X}$ and, hence, with the group G. Consider the Hilbert space $L^2(\mathbb{X},\mu)$ of square integrable functions $u(\Omega)$ on the manifold $\mathbb{X}$, with integration measure $d\mu(\Omega)$. The eigenfunctions $Y_\nu(\Omega)$ of the Laplace–Beltrami operator on $\mathbb{X}$ (Ref. 9) constitute a complete orthonormal set of functions in $L^2(\mathbb{X},\mu)$ since they satisfy

$$\sum_\nu Y_\nu^*(\Omega)Y_\nu(\Omega')=\delta(\Omega-\Omega'), \tag{16}$$

the right-hand side being a delta function with respect to the measure $\mu(\Omega)$, as well as

$$\int_{\mathbb{X}} d\mu(\Omega)\, Y_\nu^*(\Omega)Y_{\nu'}(\Omega)=\delta_{\nu\nu'}. \tag{17}$$

Depending on the manifold $\mathbb{X}$ being compact or not, the right-hand side of (17) must be understood as a Kronecker-delta or a Dirac-delta function (or suitable combinations thereof). There is a simple expression for the (modulus of) the overlap of two coherent states in terms of harmonic functions:

$$|\langle\Omega'|\Omega\rangle|^2=\sum_\nu \tau_\nu Y_\nu(\Omega')Y_\nu^*(\Omega), \quad \tau_\nu\in\mathbf{R}, \tag{18}$$

where the numbers or functions τ_ν depend on the actual group.

B. *Lüders* map for CS-POVMs

It is straightforward to generalize the *Lüders* map (1) to POVMs which can be written in terms of integrals of an operator valued density with respect to a positive measure μ as follows. Let (Ω_0,Σ,μ) be a measure space. Assume that, for the Hilbert space $\mathcal{H}=L^2(\Omega_0,\mu)$, there is a family of positive linear operators $E_\omega\in L(\mathcal{H})$, $\omega\in\Omega_0$, which provide a resolution of unity,

$$\int_{\Omega_0} d\mu(\omega)\, E_\omega = I. \tag{19}$$

Then the operators

$$E(\sigma)=\int_\sigma d\mu(\omega)\, E_\omega, \quad \sigma\in\Sigma, \tag{20}$$

define a POVM which is of the required form.

It is natural to associate with the POVM in (20) a *Lüders* map $\Lambda(B)$ of an operator B by defining

$$\Lambda(B)=\int_\Omega d\mu(\omega)\, E_\omega^{1/2} B\, E_\omega^{1/2}, \tag{21}$$

which is a unital, completely positive linear map on $L(\mathcal{H})$. Due to the completeness relation (13), the self-adjoint coherent-state projectors

$$E_\Omega\equiv|\Omega\rangle\langle\Omega|=E_\Omega^{1/2}, \quad \Omega\in\mathbb{X}, \tag{22}$$

are seen to define a POVM in the sense just described.

Any operator B defined on $L^2(\mathbb{X},\mu)$ is *Lüders* with respect to the CS-POVM $E_\Omega, \Omega\in\mathbb{X}$, if it satisfies the relation $B=\Lambda(B)$ with E_ω in (21) replaced by E_Ω,

$$B=\int_{\mathbb{X}} d\mu(\Omega)\,|\Omega\rangle\langle\Omega|B|\Omega\rangle\langle\Omega| = \int_{\mathbb{X}} d\mu(\Omega)\,Q_B(\Omega)|\Omega\rangle\langle\Omega|\,. \tag{23}$$

Upon comparing this equation with (15), we observe that the *Lüders* property has, for any CS-POVM, the following general interpretation: an operator B is *Lüders* if and only if its P- and Q-symbols coincide,

$$P_B(\Omega)=Q_B(\Omega)\,. \tag{24}$$

To the best of our knowledge, this set of operators—which we will call *well-ordered*—has not been introduced before.

The constraint (23) takes a particularly simple form upon expanding the Q-symbol of B in harmonic functions,

$$Q_B(\Omega)=\sum_{\nu} B_\nu Y_\nu(\Omega)\,, \tag{25}$$

which is possible according to (16). The expansion coefficients are given by

$$B_\nu=\int_{\mathbb{X}} d\mu(\Omega)\,Q_B(\Omega)Y_\nu^*(\Omega)\,. \tag{26}$$

Take the expectation value of (23) in the coherent state $|\Omega'\rangle$ and use the relation (18) for the overlap $|\langle\Omega'|\Omega\rangle|^2$. This leads to

$$Q_B(\Omega')=\sum_{\nu} \tau_\nu\left[\int_{\mathbb{X}} d\mu(\Omega)Q_B(\Omega)Y_\nu^*(\Omega)\right]Y_\nu(\Omega')=\sum_{\nu} \tau_\nu B_\nu Y_\nu(\Omega')\,, \tag{27}$$

where (26) has been used. Uniqueness of the expansion (25) implies that the coefficients of a *Lüders* operator must satisfy the condition

$$B_\nu=\tau_\nu B_\nu\,, \quad \text{for all } \nu\,. \tag{28}$$

As mentioned above, the actual form of the quantities τ_ν depend on the group G under consideration. To proceed, we therefore need to specify the system of coherent states we work with, that is, the group G. Explicit conclusions about *Lüders* operators for CS-POVMs will be derived now for the groups SU(2) and H_3.

III. *LÜDERS* OPERATORS FOR THE CS-POVM OF A SPIN

Consider a Hilbert space $\mathcal{H}_s$ of dimension $(2s+1)$, carrying an irreducible representation of the group $G=\mathrm{SU}(2)$. Each space $\mathcal{H}_s$ is associated with a spin of length $s\in\{\frac{1}{2},1,\frac{3}{2},\ldots\}$. To introduce spin-coherent states, it is convenient to select states of highest (lowest) weight $|\pm s\rangle$ as reference states (cf. Refs. 5 and 10). These states are invariant under a change of phase, hence the isotropy group is given by $H=\mathrm{U}(1)$. Therefore, the coset space is the surface of a sphere: $\mathbb{X}=\mathrm{SU}(2)/\mathrm{U}(1)=\mathcal{S}^2$, which corresponds to the phase space of a classical spin.

The resolution of unity I in $\mathcal{H}_s$ using spin-coherent states $|\mathbf{n}\rangle$ reads

$$I=\int_{\mathcal{S}^2} d\mu(\mathbf{n})\,|\mathbf{n}\rangle\langle\mathbf{n}|\,, \quad d\mu(\mathbf{n})=\frac{2s+1}{4\pi}\sin\vartheta d\vartheta\, d\varphi\,, \tag{29}$$

where each unit vector $\mathbf{n}\in\mathbb{R}^3$ denotes a point with spherical coordinates (ϑ,φ), located on the unit sphere $\mathcal{S}^2$. The continuous family of operators

$$E_{\mathbf{n}}=|\mathbf{n}\rangle\langle\mathbf{n}|\,,\quad\text{with}\quad I=\int_{\mathcal{S}^2}d\mu(\mathbf{n})\,E_{\mathbf{n}}\,,\tag{30}$$

defines the CS-POVM of SU(2). Being a projector, the positive square root of each operator $E_{\mathbf{n}}$ is equal to itself: $E_{\mathbf{n}}^{1/2}=|\mathbf{n}\rangle\langle\mathbf{n}|$. Therefore, a self-adjoint operator $B\in L(\mathcal{H}_s)$ is *Lüders* with respect to the POVM (30) if

$$B=\int_{\mathcal{S}^2}d\mu(\mathbf{n})|\mathbf{n}\rangle\langle\mathbf{n}|B|\mathbf{n}\rangle\langle\mathbf{n}|\equiv\int_{\mathcal{S}^2}d\mu(\mathbf{n})Q_B(\mathbf{n})|\mathbf{n}\rangle\langle\mathbf{n}|\,.\tag{31}$$

Following the strategy outlined earlier, we will show now that any operator B satisfying (31) must be a real multiple of unity: $B=\lambda I$, so that B commutes with all elements of the CS-POVM for a spin,

$$[B,E_{\mathbf{n}}]=0\,,\quad\mathbf{n}\in\mathcal{S}^2\,.\tag{32}$$

Consider the expectation value of Eq. (31) in the coherent state $|\mathbf{n}'\rangle$,

$$Q_B(\mathbf{n}')=\int_{\mathcal{S}^2}d\mu(\mathbf{n})\,Q_B(\mathbf{n})|\langle\mathbf{n}|\mathbf{n}'\rangle|^2\,.\tag{33}$$

The function $Q_B(\mathbf{n})$, the Q-symbol of the operator B, is smooth on the sphere $\mathcal{S}^2$, and it can be written as a linear combination of $(2s+1)^2$ spherical harmonics $Y_{lm}(\mathbf{n})$,

$$Q_B(\mathbf{n})=\sqrt{\frac{4\pi}{2s+1}}\sum_{l=0}^{2s}\sum_{m=-l}^{l}B_{lm}Y_{lm}(\mathbf{n})\,,\tag{34}$$

with expansion coefficients

$$B_{lm}=\sqrt{\frac{4\pi}{2s+1}}\int_{\mathcal{S}^2}d\mu(\mathbf{n})\,Q_B(\mathbf{n})\,Y_{lm}^*(\mathbf{n})\,.\tag{35}$$

Note that these expressions are connected to the general formulas through identifying $Y_\nu(\Omega)\leftrightarrow\sqrt{4\pi/(2s+1)}Y_{lm}(\mathbf{n})$. Rewrite the scalar product (33) by means of the addition theorem for spherical harmonics,

$$\begin{aligned}|\langle\mathbf{n}|\mathbf{n}'\rangle|^2&=\left(\frac{1+\mathbf{n}\cdot\mathbf{n}'}{2}\right)^{2s}\\&=\sum_{l=0}^{2s}\frac{2l+1}{2s+1}\left\langle\begin{matrix}s&l\\s&0\end{matrix}\middle|\begin{matrix}s\\s\end{matrix}\right\rangle^2P_l(\mathbf{n}\cdot\mathbf{n}')\\&=\frac{4\pi}{2s+1}\sum_{l=0}^{2s}\sum_{m=-l}^{l}\left\langle\begin{matrix}s&l\\s&0\end{matrix}\middle|\begin{matrix}s\\s\end{matrix}\right\rangle^2Y_{lm}^*(\mathbf{n})Y_{lm}(\mathbf{n}')\,,\end{aligned}\tag{36}$$

where the functions $P_l(x)$ are the Legendre polynomials. Upon inserting (34) and (36), integration of the right-hand side of Eq. (33) gives (after replacing $\mathbf{n}'$ by $\mathbf{n}$)

$$Q_B(\mathbf{n})=\sqrt{\frac{4\pi}{2s+1}}\sum_{l=0}^{2s}\sum_{m=-l}^{l}\left\langle\begin{matrix}s&l\\s&0\end{matrix}\middle|\begin{matrix}s\\s\end{matrix}\right\rangle^2B_{lm}Y_{lm}(\mathbf{n})\,.\tag{37}$$

This expansion and Eq. (34) can only hold simultaneously if the coefficients of the harmonics satisfy

$$B_{lm}=\left\langle\begin{matrix}s&l\\s&0\end{matrix}\middle|\begin{matrix}s\\s\end{matrix}\right\rangle^2B_{lm}\,,\tag{38}$$

which is (28) for the group SU(2). The m-independent Clebsch–Gordan coefficients correspond to the numbers τ_ν introduced in (18), and they take values

$$\left\langle \begin{matrix} s & l \\ s & 0 \end{matrix} \middle| \begin{matrix} s \\ s \end{matrix} \right\rangle^2 = \frac{(2s)!(2s+1)!}{(2s-l)!(2s+1+l)!}. \tag{39}$$

Since

$$\left\langle \begin{matrix} s & 0 \\ s & 0 \end{matrix} \middle| \begin{matrix} s \\ s \end{matrix} \right\rangle = 1\,, \quad 0 < \left\langle \begin{matrix} s & l \\ s & 0 \end{matrix} \middle| \begin{matrix} s \\ s \end{matrix} \right\rangle < 1\,, \quad l = 1,2,\ldots,2s, \tag{40}$$

the coefficients B_{lm} with $l \neq 0$ in (38) must vanish; thus, the expansion (34) of a *Lüders* operator satisfying (31) contains only one nonzero term, B_{00}, and B is proportional to $Y_{00}(\mathbf{n})$, i.e., the identity. Hence, it commutes with any operator, including the set $E_{\mathbf{n}}$, so that Eq. (32) follows. At the same time we have shown that the identity is the only operator in $\mathcal{H}_s$ such that its Q- and P-symbols coincide.

IV. *LÜDERS* OPERATORS FOR THE CS-POVM OF A PARTICLE

The kinematics of a quantum particle on the real line $\mathbb{R}$ is described by the creation and annihilation operators a and its adjoint $a^\dagger$ which satisfy $[a,a^\dagger]=I$. The operators a, $a^\dagger$, and the identity I generate the Heisenberg–Weyl algebra h_3; finite transformations, that is, elements of the *group* H_3, are given by the phase-space displacement or shift operators

$$D(\alpha) = \exp[\alpha a^\dagger - \alpha^* a]\,, \quad \alpha \in \mathbb{C}\,. \tag{41}$$

In fact, they provide an irreducible projective representation of the group H_3 in $L_2(\mathbb{R})$,

$$D(\alpha)D(\alpha') = \exp\left[\frac{i}{2}(\alpha\alpha'^* - \alpha^*\alpha')I\right] D(\alpha+\alpha')\,. \tag{42}$$

The (overcomplete) family of coherent states $|\alpha\rangle$ in the Hilbert space $L_2(\mathbb{R})$ is obtained by displacing the fiducial state $|0\rangle$, say, with $a|0\rangle = 0$, by arbitrary amounts $\alpha \in \mathbb{C}$:

$$|\alpha\rangle = D(\alpha)|0\rangle\,. \tag{43}$$

The isotropy subgroup of H_3 is again isomorphic to $\mathrm{U}(1) \sim \exp[i\gamma I], \gamma \in [0,2\pi)$, so that the manifold labeling coherent states is given by the complex plane $\mathbb{X} = H_3/\mathrm{U}(1) = \mathbb{C}$, corresponding indeed to the phase space of a classical particle on the real line.

The completeness relation for the particle-coherent states reads

$$I = \int_{\mathbb{C}} d\mu(\alpha)\, |\alpha\rangle\langle\alpha|\,, \quad d\mu(\alpha) = \frac{1}{\pi} d^2\alpha\,, \tag{44}$$

and it can be understood as defining a POVM for the continuous family of projection operators

$$E_\alpha = |\alpha\rangle\langle\alpha| = E_\alpha^{1/2}\,, \quad \alpha \in \mathbb{C}\,. \tag{45}$$

The operator B on $L_2(\mathbb{R})$ is *Lüders* with respect to the POVM $E_\alpha, \alpha \in \mathbb{C}$, if it is invariant under the *Lüders* map $B \mapsto \Lambda(B)$, i.e.,

$$B = \int_{\mathbb{C}} d\mu(\alpha)\, |\alpha\rangle\langle\alpha|B|\alpha\rangle\langle\alpha| = \int_{\mathbb{C}} d\mu(\alpha)\, Q_B(\alpha) |\alpha\rangle\langle\alpha|\,, \tag{46}$$

where $\langle\alpha|B|\alpha\rangle = Q_B(\alpha)$ is the Q-symbol of the operator B. As shown earlier, this relation forces the Q-symbol of a *Lüders* operator to coincide with its P-symbol,

$$B = \frac{1}{\pi}\int_{\mathbb{C}} d\mu(\alpha) P(\alpha) |\alpha\rangle\langle\alpha| , \tag{47}$$

if it exists.

We will now search for *bounded Lüders* operators B which commute the members E_α of the CS-POVM (44) for a particle. We begin to look at simple examples of *Lüders* operators, followed by a systematic construction of all well-ordered *Lüders* operators. In addition to the identity, a countable family of *unbounded*, linearly independent *Lüders* operators will emerge, none of which commutes with the elements of the CS-POVM. Finally, an unexpected relation of the *Lüders* map to operator orderings is established for particle coherent states.

A. Examples of unbounded *Lüders* operators

It is straightforward to apply the map Λ to unbounded operators such as position $Q=(a+a^\dagger)/2$ and momentum $P=(a-a^\dagger)/2i$. Using the equation $a|\alpha\rangle = \alpha|\alpha\rangle$ and its adjoint implies that

$$\begin{aligned}\Lambda(Q) &= \int_{\mathbb{C}} d\mu(\alpha)\, |\alpha\rangle\langle\alpha|Q|\alpha\rangle\langle\alpha| = \int_{\mathbb{C}} d\mu(\alpha)\, \frac{1}{2}(\alpha+\alpha^*)|\alpha\rangle\langle\alpha| \\ &= \frac{1}{2}\int_{\mathbb{C}} d\mu(\alpha)\, a|\alpha\rangle\langle\alpha| + \frac{1}{2}\int_{\mathbb{C}} d\mu(\alpha)\, |\alpha\rangle\langle\alpha|a^\dagger = Q ,\end{aligned} \tag{48}$$

and similarly

$$\Lambda(P) = P . \tag{49}$$

While being invariant under Λ, the operators Q and P are neither positive nor bounded, and they do not commute with the projectors E_α since the expectation value of the commutator in the coherent state $|\beta\rangle$ is, in general, different from zero:

$$\langle\beta|[Q,E_\alpha]|\beta\rangle = \tfrac{1}{2}((\alpha-\alpha^*)-(\beta-\beta^*))|\langle\alpha|\beta\rangle|^2 . \tag{50}$$

Using the relation $D^\dagger(\alpha) a D(\alpha) = a-\alpha$, its adjoint, and the commutation relations of a and $a^\dagger$, one shows that *Lüders*' map acts on the operators Q^2 and P^2 according to

$$\begin{aligned}\Lambda(Q^2) &= Q^2 + 2\langle 0|Q^2|0\rangle I = Q^2 + \tfrac{1}{2} I , \\ \Lambda(P^2) &= P^2 + 2\langle 0|P^2|0\rangle I = P^2 + \tfrac{1}{2} I .\end{aligned} \tag{51}$$

Consequently, appropriate quadratic combinations of position and momentum turn out to be *Lüders*,

$$\Lambda_\Gamma(Q^2 - P^2) = Q^2 - P^2 . \tag{52}$$

However, this indefinite, unbounded operator does not commute with all projections E_α as follows from $\langle 0|[Q^2-P^2,E_\alpha]|0\rangle = (\alpha^2-\alpha^{*2})|\langle 0|\alpha\rangle|^2$, for example. In the next section a family of similar *Lüders* operators will be constructed.

B. Construction of *Lüders* operators

Let us turn now to the problem of finding all operators which are *Lüders* with respect to the CS-POVM E_α of a particle, i.e, all well-ordered operators. The argument will resemble the one given in the case of a spin.

Expand the Q-symbol of an operator B as

$$Q_B(\alpha)=\int_{\mathbb{C}} d\mu(\xi)\, B_\xi \exp[\alpha\xi^*-\alpha^*\xi]\,, \tag{53}$$

where the coefficients B_ξ are given by

$$B_\xi=\int_{\mathbb{C}} d\mu(\alpha)\, Q_B(\alpha)\exp[-(\alpha\xi^*-\alpha^*\xi)]\,. \tag{54}$$

Here, the functions $\exp[\alpha\xi^*-\alpha^*\xi]$ are the complete orthonormal set of harmonic functions in the complex plane, corresponding to $Y_\nu(\Omega)$. Since the Q-symbol of a Hermitian operator is real, $Q_B(\alpha)=\langle\alpha|B|\alpha\rangle^*=Q_B^*(\alpha)$, the coefficients must satisfy the relation

$$\begin{aligned} B_\xi^* &= \int_{\mathbb{C}} d\mu(\alpha)\, Q_B^*(\alpha)\exp[-(\alpha^*\xi-\alpha\xi^*)] \\ &= \int_{\mathbb{C}} d\mu(\alpha)\, Q_B(\alpha)\exp[-(\alpha(-\xi)^*-\alpha^*(-\xi))]=B_{-\xi}\,. \end{aligned} \tag{55}$$

We will turn (46) into a condition for the expansion coefficients B_ξ of a *Lüders* operator which can be solved explicitly. Take the expectation value of the operator B in (46) in the coherent state $|\beta\rangle$, and use the identity

$$|\langle\alpha|\beta\rangle|^2=\exp[-|\alpha-\beta|^2]=\int_{\mathbb{C}} d\mu(\xi)\, e^{-\xi\xi^*}\exp[\beta\xi^*-\beta^*\xi]\exp[-\alpha\xi^*+\alpha^*\xi]\,, \tag{56}$$

leading to

$$\begin{aligned} Q_B(\beta) &= \int_{\mathbb{C}} d\mu(\xi)\, e^{-\xi\xi^*}\left[\int_{\mathbb{C}} d\mu(\alpha)\, Q_B(\alpha)\exp[-(\alpha\xi^*-\alpha^*\xi)]\right]\exp[\beta\xi^*-\beta^*\xi]\,, \\ &= \int_{\mathbb{C}} d\mu(\xi)\, e^{-\xi\xi^*}B_\xi\exp[\beta\xi^*-\beta^*\xi]\,, \end{aligned} \tag{57}$$

where (54) has been used. Due to the uniqueness of the expansion (53), the expansion coefficients of any *Lüders* operators must satisfy

$$B_\xi=e^{-\xi\xi^*}B_\xi\,, \tag{58}$$

which is the equivalent of (38) for continuous variables. Consequently, the coefficients B_ξ are necessarily zero for all values of ξ except $\xi=0$, and there are no solutions in terms of ordinary functions. If allowing for generalized functions, B_ξ is necessarily a distribution of finite order,[11] that is, a linear combination of a δ-distribution and finite derivatives of it,

$$B_\xi=\sum_{n+m=0}^{N} b_{nm}\partial_\xi^n\partial_{\xi^*}^m\delta(\xi)\,,\quad b_{nm}\in\mathbb{C},\quad n,m=0,1,2,\ldots,\quad N=0,1,2,\ldots\,. \tag{59}$$

The function B_ξ must satisfy (55) leading to

$$b_{nm}=(-)^{m+n}b_{mn}^*\,,\quad n,m=0,1,2,\ldots\,, \tag{60}$$

and the $\delta(\xi)$-function is real,

$$\delta(\xi)=\int_{\mathbb{C}} d\mu(\alpha)\exp[\alpha\xi^*-\alpha^*\xi]=\delta(-\xi)=\delta^*(\xi)\,. \tag{61}$$

Only some of the distributions (59) will satisfy (58) since one must have

$$Q_B(\alpha)=\int_{\mathbb{C}} d\mu(\xi)[D_N\delta(\xi)]e^{-\xi\xi^*}e^{\alpha\xi^*-\alpha^*\xi}=\int_{\mathbb{C}} d\mu(\xi)[D_N\delta(\xi)]e^{\alpha\xi^*-\alpha^*\xi}\,, \tag{62}$$

where

$$D_N=\sum_{n+m=0}^{N} b_{nm}\partial_\xi^n\partial_{\xi^*}^m\,. \tag{63}$$

Partial integrations in (62) lead to the requirement

$$[D_N^\dagger e^{-\xi\xi^*}e^{\alpha\xi^*-\alpha^*\xi}]_{\xi=\xi^*=0}=[D_N^\dagger e^{\alpha\xi^*-\alpha^*\xi}]_{\xi=\xi^*=0}\,, \tag{64}$$

where the adjoint $D_N^\dagger$ of D_N is obtained from replacing b_{nm} by $(-)^{n+m}b_{nm}$ in (63). It is shown in the Appendix that this condition is satisfied if and only if

$$b_{nm}=0\,,\quad 1\leqslant m,n\leqslant N\,, \tag{65}$$

i.e., only terms b_{nm} with at least one index (that is, m or n or both) equal to zero will contribute to the symbol of a well-ordered operator. Therefore, only coefficients of the form

$$B_\xi=\sum_{n=0}^{N}(b_{n0}\partial_\xi^n+(-)^n b_{n0}^*\partial_{\xi^*}^n)\delta(\xi) \tag{66}$$

occur which, upon partial integration in (53), give rise to Q-symbols of *Lüders* operators,

$$Q_B(\alpha)=\sum_{n=0}^{N}(b_{n0}\alpha^{*n}+b_{n0}^*\alpha^n)\,. \tag{67}$$

The operators corresponding to these symbols are given by

$$B=b_0 I+\sum_{n=1}^{N}(b_n^q B_n^q+b_n^p B_n^p)\,, \tag{68}$$

i.e., a linear combination of the identity and $2N$ Hermitian operators

$$B_n^q=\frac{1}{2}(a^n+a^{\dagger n})\quad\text{and}\quad B_n^p=\frac{1}{2i}(a^n-a^{\dagger n})\,,\quad n=1,2,\ldots,N\,, \tag{69}$$

which satisfy (46), and $(2N+1)$ real coefficients

$$b_0=2b_{00}\,,\quad b_n^q=b_{n0}+b_{n0}^*\,,\quad b_n^p=\frac{1}{i}(b_{n0}-b_{n0}^*)\,,\quad n=1,2,\ldots,N\,. \tag{70}$$

If $N=2$, for example, it follows that not only the operators Q,P, and Q^2-P^2 are *Lüders* but also

$$B_2^p=\frac{1}{2i}(a^2-a^{\dagger\,2})\propto QP+PQ\,. \tag{71}$$

Every *bounded Lüders* operator is necessarily a multiple of the identity.

C. *Lüders* map and operator ordering

It is easy to understand why the operators $B_n, n=1,2,\ldots,N$, in (70) are *Lüders*. Consider any Hermitian operator B given as a finite polynomial in a and $a^\dagger$. Using their commutation relation, one can bring the annihilation operators either to the right or to the left,

$$B(a,a^\dagger)=\sum_{m,n}\beta^{\mathcal{N}}_{nm}a^{\dagger\,m}a^n=\sum_{m,n}\beta^{\mathcal{A}}_{nm}a^m a^{\dagger\,n}\,, \tag{72}$$

corresponding to normal and antinormal ordering of B, respectively.[12] It is straightforward to calculate the *Lüders* transform of B if it is written in normal order:

$$\Lambda(B(a,a^\dagger))=\sum_{m,n}\beta^{\mathcal{N}}_{nm}\,\Lambda(a^{\dagger\,m}a^n)=\sum_{m,n}\beta^{\mathcal{N}}_{nm}a^n a^{\dagger\,m}\,, \tag{73}$$

since

$$\Lambda(a^{\dagger\,m}a^n)=\int_{\mathbb{C}}d\mu(\alpha)\,|\alpha\rangle\langle\alpha|a^{\dagger\,m}a^n|\alpha\rangle\langle\alpha|=\int_{\mathbb{C}}d\mu(\alpha)\,\alpha^n|\alpha\rangle\langle\alpha|\alpha^{*\,m}$$

$$=a^n\left(\int_{\mathbb{C}}d\mu(\alpha)\,|\alpha\rangle\langle\alpha|\right)a^{\dagger\,m}=a^n a^{\dagger\,m}\,. \tag{74}$$

Thus, the effect of Λ is to push each creation operator $a^\dagger$ to the right as if it would commute with the annihilation operator a. In other words, the map Λ provides an explicit form of the operator $\mathcal{A}$ which generates antinormal order of an operator.[8] This operator and its twin $\mathcal{N}$, which brings a given operator into normal order, are useful tools to evaluate expectation values or Baker–Campbell–Hausdorff relations, for example.[8]

To conclude: if an operator B is to be invariant under Λ, the normally and antinormally ordered forms of an operator B must coincide,

$$\sum_{m,n}\beta^{\mathcal{N}}_{nm}a^n a^{\dagger\,m}=\sum_{m,n}\beta^{\mathcal{A}}_{nm}a^m a^{\dagger\,n}\,, \tag{75}$$

that is, $\beta^{\mathcal{N}}_{nm}=\beta^{\mathcal{A}}_{nm}$. This is obviously true for the linear combinations of powers of a and $a^\dagger$ given in (70), defining the family of well-ordered operators.

V. DISCUSSION

We have shown that there is only one *Lüders* operator, the identity (and its multiples), for the CS-POVM of SU(2) while a countable family of linearly independent, unbounded, and well-ordered operators exists in the case of H_3. Due to the linearity of map Λ, all their linear combinations are well-ordered as well. It is plausible that our study exhausts all possibilities which may arise for CS-POVMs of general (simple and simply connected) Lie groups: we expect only the identity as a *Lüders* operator for *compact* Lie groups such as SU(N), and a countable family for a CS-POVM associated with noncompact groups such as $\mathrm{SU}(N-n,n), 1\leqslant n<N$. If we restrict our attention to bounded operators, we conjecture *Lüders*' theorem to hold with respect to the CS-POVM of any Lie group G.

APPENDIX: CONSTRUCTION OF WELL-ORDERED OPERATORS

We will show here that any operator compatible with (46) must have a Q-symbol with expansion coefficients of the following form:

$$B_\xi = \sum_{n=0}^{N} \left(b_{n0}\partial_\xi^n + (-)^n b_{n0}^* \partial_{\xi^*}^n\right)\delta(\xi)\,, \quad N<\infty; \tag{A1}$$

this means, in particular, that most of the coefficients b_{nm} are equal to zero:

$$b_{nm}=0\,, \quad \text{for } 1\leqslant m,n\leqslant N\,. \tag{A2}$$

In a first step, evaluate the right-hand-side of (64):

$$\left[\sum_{n+m=0}^{N} (-)^{n+m} b_{nm}\partial_\xi^n \partial_{\xi^*}^m e^{\alpha\xi^* - \alpha^*\xi}\right]_{\xi=0} = \sum_{n+m=0}^{N} (-)^m b_{nm}\alpha^m \alpha^{*\,n}\,. \tag{A3}$$

To evaluate the left-hand side, use the relation

$$\partial_\xi(e^{-\xi\xi^*} f(\xi)) = e^{-\xi\xi^*}(-\xi^* + \partial_\xi) f(\xi) \tag{A4}$$

and its complex conjugate for any smooth function f. This leads to

$$\partial_\xi^n \partial_{\xi^*}^m e^{-\xi\xi^*} = e^{-\xi\xi^*}(-\xi^* + \partial_\xi)^n(-\xi + \partial_{\xi^*})^m = e^{-\xi\xi^*}\sum_{\nu=0}^{n}\sum_{\mu=0}^{m}\binom{n}{\nu}\binom{m}{\mu}(-\xi^*)^{n-\nu}\partial_\xi^\nu(-\xi)^\mu\partial_{\xi^*}^{m-\mu}\,. \tag{A5}$$

According to Eq. (64), these operators must be applied to the function $e^{\alpha\xi^* - \alpha^*\xi}$. Each derivative ∂_{ξ^*} produces a factor α, while the action of the derivatives ∂_ξ is more complicated:

$$\begin{aligned}\partial_\xi^\nu((-\xi)^\mu e^{\alpha\xi^* - \alpha^*\xi}) &= \sum_{s=0}^{\nu}\binom{\nu}{s}\frac{\partial(-\xi)^\mu}{\partial\xi^s}\frac{\partial^{\nu-s}e^{\alpha\xi^*-\alpha^*\xi}}{\partial\xi^{\nu-s}} \\ &= \sum_{s=0}^{\nu}\binom{\nu}{s}\frac{\mu!(-)^s}{(\mu-s)!}(-\xi)^{\mu-s}(-\alpha^*)^{\nu-s}e^{\alpha\xi^*-\alpha^*\xi}\,;\end{aligned} \tag{A6}$$

due to $1/\Gamma(-k)=0, k=0,1,2,\ldots$, there are no contributions to the sum if s exceeds μ. Now that the derivatives have been evaluated, one can set $\xi=\xi^*=0$ in the resulting expression: the terms with nonzero powers of ξ or ξ^* vanish, and the sums simplify according to

$$(-\xi)^{\mu-s}\to\delta_{\mu s} \quad \text{and} \quad (-\xi^*)^{n-\nu}\to\delta_{n\nu}\,. \tag{A7}$$

The left-hand-side of (64) becomes

$$\sum_{n+m=0}^{N}(-)^m b_{nm}\sum_{s=0}^{s_0} s!\binom{m}{s}\binom{n}{s}\alpha^{m-s}\alpha^{*\,n-s}\,, \tag{A8}$$

where $s_0=\min(m,n)$. Note that the term with $s=0$ in this expression is identical to the right-hand side of (A3) which implies that the equality (62) is satisfied if

$$\sum_{n+m=0}^{N}(-)^m b_{nm}\sum_{s=1}^{s_0} s!\binom{m}{s}\binom{n}{s}\alpha^{m-s}\alpha^{*\,n-s}=0 \tag{A9}$$

holds for all complex numbers α. This equation does not restrict the coefficients $b_{n0}, 0\leqslant n\leqslant N$, and $b_{0m}, 0\leqslant m\leqslant N$: if either m or n are equal to zero, the sum over s is empty since $s_0=0$. However, *all* other coefficients must vanish as can be seen in the following way. Writing $\alpha = r\exp[i\varphi]$, Eq. (A9) turns into a sum of terms multiplying phase factors $\exp[i(m-n)\varphi] \equiv \exp[ik\varphi]$, $k=0,1,2,\ldots,N-1$. Each of these terms must vanish individually due to the linear independence of the exponentials. Their coefficients, in turn, are power series in r which can be

shown to vanish identically only if $b_{1N}=0$ for $\exp[i(N-1)\varphi]$, $b_{2N}=0$, which implies that $b_{1\,N-2}=0$ for $\exp[i(N-2)\varphi]$, etc. Taking into account that $b_{nm}=(-)^{m+n}b_{nm}^{*}$, the coefficients B_{ξ} of *Lüders* operators finally read

$$B_{\xi}=\left(\sum_{n=0}^{N} b_{n0}\partial_{\xi}^{n}+\sum_{m=0}^{N} b_{0m}\partial_{\xi*}^{m}\right)\delta(\xi)=\sum_{n=0}^{N}\left(b_{n0}\partial_{\xi}^{n}+(-)^{n}b_{n0}^{*}\partial_{\xi*}^{n}\right)\delta(\xi). \tag{A10}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Casimir force between surfaces close to each other

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(Received 27 June 2003; accepted 8 September 2003)

Casimir interactions (due to the massless scalar field fluctuations) of two surfaces which are close to each other are studied. After a brief general presentation of the technique, explicit calculations are performed for specific geometries. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1624471]

I. INTRODUCTION

Experiments to observe and measure Casimir forces have so far been performed with the geometrical setups involving two (actually disconnected) surfaces.[1] The original parallel plate Casimir interaction is exact for infinite plane surfaces,[2] which in practice means that valid for planes very close to each other. Effect for the parallel plane geometry were first verified in 1958.[3] Recently the experiment for this geometry was improved to a higher precision of 15%.[4] The Casimir experiments other than the above mentioned ones have been performed for a sphere close to a plane configuration:[5] which do not give rise the precise alignment problem of the parallel planes. Note that the calculation for the sphere-plane geometry gets closed to be exact if the radius of the sphere is small compared to the distance to the plane.[6] Sphere–sphere geometry has also been studied subject to the similar approximation as the sphere–plane problem.[7]

Single cavity experiments so far have not been realized,[8] which we think would be very interesting: For example, inserting the data from quantum dots (i.e., radius $\simeq 10^{-7}$ cm) into the theoretical expression for the vacuum energy of a spherical cavity capable of confining electromagnetic field,[1] one gets (in $\hbar = c = 1$ units) 0.5×10^{6} cm$^{-1} = 10$ eV for the Casimir energy which is of appreciable magnitude.[9] This is comparable to the total energy between the parallel plates of the latest experiment,[4] i.e., $E = (\pi^2/720d^3)(\text{area of plates}) \simeq [\pi^2/720(5\times 10^{-3})^3]\cdot(2\times 2)$ cm$^{-1} \simeq 10^{6}$ cm^{-1}. With the advances in nanotechnology, quantum dots can be constructed with variety of materials. If one can measure Casimir forces in cavities of different materials, then we may learn more about the effect, i.e., whether it is purely geometrical, or it is dependent on the microstructure of the confining walls.

Our purpose in the present work is to study some nontrivial two-boundary geometries which give simple, explicit formulas for the Casimir energies. The systems we deal with are made of surfaces close to each other. We employ an approximation based essentially on assigning an average constant value to the coordinates normal to the surfaces. In principle it is possible to write exact Casimir energy expressions for two boundary geometries with finite separations. There are indeed such formulations for coaxial cylinders of infinite height;[10,11] and for cocentric spheres.[8,11,12] These formulations however involve integrations over the ratios of the product of Bessel functions; thus the explicit energy expressions seem available only in the limiting cases of small (or perhaps large) separations. This is the case, for example, for the coaxial cylinders where the explicit result is given for the close boundaries;[10] and, for the cocentric spheres in ''narrow slit'' limit.[8]

We perform our calculations for the vacuum fluctuations of massless scalar fields between surfaces close to each other. For massive fields, for any realistic experimental setups the Casimir energies are extremely small. The expressions always involve a factor $e^{-\mu\triangle}$, where μ is the mass

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and $\triangle$ is the separation; which for electron and for nanometer distances is $e^{-2,5\times10^{10}\times10^{-7}} \simeq e^{-2500}$; thus it is practically zero.

In Sec. II we give brief outline of our approach. We then proceed with specific examples: Coaxial infinite cylinders (for which our result agrees quite well with the recent calculations[10]), cocentric tori, coaxial cylindrical boxes of finite height, cocentric spheres (the result we get agrees with the one given in Ref. 8) and coaxial conical surfaces. We hope that, considering the recent advances in the stable nanotubes[13] some of these geometries may be realized to offer experimental tests.

II. CASIMIR ENERGY FOR THE REGION BETWEEN TWO BOUNDARIES WHICH ARE CLOSE TO EACH OTHER

We first choose the suitable spatial curvilinear coordinates η^j, $j=1,2,3$ for the geometry we deal with. The corresponding Minkowski metric and the Klein–Gordon operator are then

$$ds^2 = dt^2 - g_{ij}\, d\eta^i\, d\eta^j \tag{1}$$

and $[g \equiv \det(g_{ij})]$

$$\Delta^{\mathrm{KG}} = \frac{\partial^2}{\partial t^2} - \frac{1}{\sqrt{g}}\frac{\partial}{\partial \eta^i} g^{ij}\sqrt{g}\frac{\partial}{\partial \eta^j}. \tag{2}$$

The Green function is (overbar stands for complex conjugation)

$$G = \sum_{\lambda_1,\lambda_2,\lambda_3} \frac{e^{i\omega(\lambda)(t-t')}}{2\omega(\lambda)} \Phi_{\omega(\lambda)}(\eta)\overline{\Phi_{\omega(\lambda)}(\eta')}, \tag{3}$$

where $\Phi_{\omega(\lambda)}(\eta)$ and $\omega^2(\lambda)$ are the eigenfunctions and eigenvalues of the equation for the massless scalar field

$$-\frac{1}{\sqrt{g}}\frac{\partial}{\partial \eta^i} g^{ij}\sqrt{g}\frac{\partial}{\partial \eta^j}\Phi_{\omega(\lambda)}(\eta) = \omega^2(\lambda)\Phi_{\omega(\lambda)}(\eta). \tag{4}$$

(For massive scalar field one only changes ω^2 by $\omega^2+\mu^2$; with μ being the mass.) We assume that the above equation is separable in the spatial coordinates η^j. Here η and λ stand for the collection of the coordinates η^j and the corresponding quantum numbers λ_j (which are specified by the boundary conditions), respectively. The functions $\Phi_{\omega(\lambda)}(\eta)$ are normalized with respect to the norm

$$\|\Phi\|^2 = \int_A d^3\eta\sqrt{g}|\Phi(\eta)|^2, \tag{5}$$

where A is the domain of the coordinates η^j. The vacuum energy density can then be obtained by calculating the coincidence limit derivatives as

$$T = \mathrm{Reg}\left[\lim_{t,\eta^j\to t',\eta'^j}\left(\frac{\partial^2}{\partial t\partial t'} + g^{ij}\frac{\partial^2}{\partial\eta^i\partial\eta'^j}\right)G(\eta,\eta')\right]. \tag{6}$$

''Reg'' stands for regularization. In the specific examples it means that we have to subtract the terms (in the Plana sum formulas to be employed over the modes) corresponding to the vacuum energy of the free space, the boundary energy, etc. To calculate the Casimir energy one needs the eigenvalues of the problem. The eigenvalues $\omega^2(\lambda)$ depend on three quantum numbers λ_j corresponding to the degrees of freedom in directions η^j in which we assume that Eq. (4) can be

separated. We further assume that after the separation of variables the eigenvalue equations in coordinates η^1, η^2 can be trivially solved, and the corresponding quantum numbers λ_1, λ_2 are easily obtained. This assumption does not introduce a strong restriction. In fact many problems in the literature are of that type. For example, when one studies the Casimir energy inside a spherical cavity, only the nontrivial problem is the radial equation in which one has to deal with the roots of the Bessel functions to impose the boundary condition.[1]

In this work we employ an approximation method to calculate the nontrivial spectral parameter λ_3, which is valid if the problem involves two boundaries in direction η^3, which are close to each other.

After the separation, the problem in hand in η_3 can be converted into the Schrödinger form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}(\eta^3)^2} + W_{\lambda_1\lambda_2}(\eta_3) \right] \Phi_{\lambda_3}(\eta^3) = E(\lambda)\Phi_{\lambda_3}(\eta^3). \tag{7}$$

The form of the potential $W_{\lambda_1\lambda_2}(\eta_3)$ and the relation between $\omega^2(\lambda)$ and $E(\lambda)$ depend on the choice of coordinate systems. The explicit examples are given in the following sections. The boundary conditions we wish to impose for the type of geometries under investigation are

$$\Phi_{\lambda_3}(\eta_0^3) = 0, \quad \Phi_{\lambda_3}(\eta_1^3) = 0, \tag{8}$$

where $\eta_0^3 < \eta_1^3$. In practice these boundary conditions require dealing with the roots of special functions which are quite involved. However, if the boundaries are close to each other, instead of (7) we can employ the simpler Schrödinger equation,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}(\eta^3)^2} + V^0_{\lambda_1\lambda_2}(\eta^3) \right] \Phi^0_{\lambda_3}(\eta^3) = E^0(\lambda)\Phi^0_{\lambda_3}(\eta^3), \tag{9}$$

where the constant potential in the region is given by

$$V^0_{\lambda_1\lambda_2}(\eta_3) = \begin{cases} \infty, & \eta^3 = \eta_0^3, \quad \eta^3 = \eta_1^3, \\ W_{\lambda_1\lambda_2}(\sqrt{\eta_0^3\eta_1^3}), & \eta^3 \in (\eta_0^3, \eta_1^3). \end{cases} \tag{10}$$

The eigenvalue equation (9) has the following solutions:

$$E^0(\lambda) = \left(\frac{\pi\lambda_3}{\Delta} \right)^2 + W_{\lambda_1\lambda_2}(\sqrt{\eta_0^3\eta_1^3}) \tag{11}$$

and

$$\Phi^0_{\lambda_3}(\eta^3) = \sqrt{\frac{2}{\Delta}} \sin\left(\frac{\pi\lambda_3}{\Delta}\eta^3 \right), \tag{12}$$

where $\Delta = \eta_1^3 - \eta_0^3$ and $\lambda_3 = 1,2,\ldots$. The system given by (9) is a good approximation if the condition

$$\max_{\eta^3 \in (\eta_0^3, \eta_1^3)} |W_{\lambda_1\lambda_2}(\eta_3) - W^0_{\lambda_1\lambda_2}| \ll \min_{\lambda_3} |E^0(\lambda)| \tag{13}$$

is satisfied.

In the following sections we apply this approximation method to the specific geometries.

III. CASIMIR ENERGY IN THE REGION BETWEEN TWO CLOSE COAXIAL CYLINDERS

In the cylindrical coordinates, i.e., with the metric

$$ds^2 = dt^2 - dz^2 - dr^2 - r^2\, d\phi^2, \tag{14}$$

the eigenvalue problem we must solve is

$$-\left[\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}\right]\Phi = \omega^2 \Phi. \tag{15}$$

After solving for the trivial coordinates z and ϕ we have

$$\Phi = \frac{e^{ipz+im\phi}}{2\pi\sqrt{r}} v_{nm}(r). \tag{16}$$

Here $v_{nm}(r)$ are the normalized wave functions corresponding to the radial equation

$$\left[-\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2}\right] v_{nm} = \mu_{nm}^2 v_{nm}, \tag{17}$$

with

$$\omega_{pnm} = \sqrt{p^2 + \mu_{nm}^2}. \tag{18}$$

The quantum number n should be determined from the boundary conditions on the coaxial cylinders with the radii $r_0 < r_1$,

$$v_{nm}(r_0) = 0, \quad v_{nm}(r_1) = 0. \tag{19}$$

The solution of (17) satisfying the boundary condition at r_0 is given in terms of the Bessel functions as

$$v_{nm}(r) = \sqrt{\mu_{nm} r}\, \frac{J_m(\mu_{nm} r_0) N_m(\mu_{nm} r) - J_m(\mu_{nm} r) N_m(\mu_{nm} r_0)}{\Omega_{nm}}, \tag{20}$$

where Ω_{nm} is obtained from the normalization

$$\int_{r_0}^{r_1} dr |v_{nm}(r)|^2 = 1. \tag{21}$$

In practice however the above integral is very difficult to calculate for arbitrary values of r_0 and r_1. The spectrum μ_{nm} should be determined from the boundary condition at r_1 which is a quite involved equation. However, if the cylindrical surfaces are close to each other we can rely on the approximation method summarized in the preceding section. Instead of the eigenvalue problem (17) we consider the following:

$$\left[-\frac{d^2}{dr^2} + V(r)\right] v_{nm}^0 = (\mu_{nm}^0)^2 v_{nm}^0 \tag{22}$$

with the constant potential

$$V(r)=\begin{cases}\infty, & r=r_0, \quad r=r_1,\\ \dfrac{m^2-\frac{1}{4}}{r_0 r_1}, & r\in(r_0,r_1).\end{cases} \tag{23}$$

The above equation is then trivially solved as

$$v^0_{nm}=\sqrt{\frac{2}{\Delta}}\sin(\mu^0_{nm}(r-r_0)), \quad \Delta\equiv r_1-r_0 \tag{24}$$

with the spectrum

$$\mu^0_{nm}=\sqrt{\frac{\pi^2 n^2}{\Delta^2}+\frac{m^2-\frac{1}{4}}{r_0 r_1}}; \quad n=1,2,3,\ldots. \tag{25}$$

For the present specific case the condition (13) is valid for $\Delta\ll r_0$. The Green function of the system is then easy to deal with,

$$G=\frac{1}{\sqrt{rr'}}\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}p\,\frac{e^{i\omega^0_{pnm}(t-t')+ip(z-z')+im(\phi-\phi')}}{8\pi^2\omega^0_{pnm}}v^0_{nm}(r)v^0_{nm}(r'), \tag{26}$$

where

$$\omega^0_{pnm}=\sqrt{p^2+(\mu^0_{nm})^2}. \tag{27}$$

To obtain the vacuum energy density we insert the above Green function into the coincidence limit formula

$$T=\ \mathrm{Reg}\left[\frac{1}{2}\lim_{t,r,z,\phi\to t',r',z',\phi'}\left(\partial_t\partial_{t'}+\partial_r\partial_{r'}+\partial_z\partial_{z'}+\frac{1}{r^2}\partial_\phi\partial_{\phi'}\right)G\right], \tag{28}$$

where "Reg" stands for regularization which will be defined explicitly. The total vacuum energy per unit height is

$$E_{\mathrm{cyl}}=\int_0^{2\pi}\mathrm{d}\phi\int_{r_0}^{r_1}r\,\mathrm{d}r\,T=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi}\sum_{m=-\infty}^{\infty}\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega^0_{pnm}\right]. \tag{29}$$

In the above equation the regularization is required in n summation for we have boundary in the radial direction. The regularized sum is given by

$$\mathrm{Reg}\left[\sum_{n=1}^{\infty}F(n)\right]=i\int_0^{\infty}\mathrm{d}t\,\frac{F(it)-F(-it)}{e^{2\pi t}-1}, \tag{30}$$

which is the part of the well-known Plana formula

$$\sum_{n=0}^{\infty}F(n)=\frac{F(0)}{2}+\int_0^{\infty}\mathrm{d}n\,F(n)+\mathrm{Reg}\left[\sum_{n=1}^{\infty}F(n)\right]. \tag{31}$$

The integration over dn (the second term) corresponding to the free space energy (the volume singularity) and, $n=0$ term (the surface singularity) are substracted for regularization.[1]

We first apply (31) to the index m in (29) and arrive at

$$E_{\mathrm{cyl}}=E_0+E_1, \tag{32}$$

where

$$E_0=\int_0^\infty\int_0^\infty\frac{\mathrm{d}p\,\mathrm{d}m}{\pi}\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega_{pnm}^0\right] \tag{33}$$

and

$$E_1=\int_0^\infty\frac{\mathrm{d}p}{\pi}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\left[\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega_{pnm}^0\right]\right]\right]. \tag{34}$$

At this point we like to stress that the $\mathrm{Reg}\,\Sigma_m$ in the above formula does not mean that there is an actual regularization in m summation. It is only a part of the Plana formula. Applying the Plana formula to the index n we may represent E_1 in the following form:

$$E_1=E_{11}+E_{12}+E_{13}, \tag{35}$$

where

$$E_{11}=\int_0^\infty\frac{\mathrm{d}p}{\pi}\sum_{n=1}^{\infty}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{pnm}^0\right], \tag{36}$$

$$E_{12}=\int_0^\infty\frac{\mathrm{d}p}{2\pi}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{p0m}^0\right], \tag{37}$$

and

$$E_{13}=-\int_0^\infty\int_0^\infty\frac{\mathrm{d}p\,\mathrm{d}n}{\pi}\sum_{n=1}^{\infty}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{pnm}^0\right]. \tag{38}$$

We see that contributions E_0 and E_{13} have similar integral representation. Making suitable change of variables they can be represented as

$$E_0=\frac{1}{2R^2}T\left(\frac{\pi R}{\Delta}\right),\quad E_{13}=-\frac{\Delta}{2\pi R^3}T(1), \tag{39}$$

where $R=\sqrt{r_0r_1}$ and

$$T(b)=\int_0^\infty z\,\mathrm{d}z\,\mathrm{Reg}\left[\sum_{n=1}^{\infty}\sqrt{\left|z^2-\frac{1}{4}+b^2n^2\right|}\right]. \tag{40}$$

For $z\geqslant\frac{1}{2}$ the relation

$$\sqrt{(ix)^2+c^2}=i\sqrt{x^2-c^2},\quad x\geqslant c \tag{41}$$

implies

$$\mathrm{Reg}\left[\sum_{n=1}^{\infty}\sqrt{\left|z^2-\frac{1}{4}+b^2n^2\right|}\right]=-2\int_{(1/b)\sqrt{z^2-\frac{1}{4}}}^\infty\mathrm{d}n\,\frac{\sqrt{b^2n^2-z^2+\frac{1}{4}}}{e^{2\pi n}-1}. \tag{42}$$

In a similar fashion for $z<\frac{1}{2}$ we have

$$\mathrm{Reg}\left[\sum_{n=1}^{\infty}\sqrt{\left|z^2-\frac{1}{4}+b^2n^2\right|}\right]=-2\int_{(1/b)\sqrt{\frac{1}{4}-z^2}}^{\infty}\mathrm{d}n\,\frac{\sqrt{b^2n^2-z^2+\frac{1}{4}}}{e^{2\pi n}-1}. \tag{43}$$

Therefore

$$T(b)=-2\int_0^{\infty}z\,\mathrm{d}z\int_{(1/b)\sqrt{|z^2-\frac{1}{4}|}}^{\infty}\mathrm{d}n\,\frac{\sqrt{b^2n^2-z^2+\frac{1}{4}}}{e^{2\pi n}-1} \tag{44}$$

or

$$T(b)=-\frac{b^3}{360}-\frac{b^3}{8\pi^4}\int_0^{(\pi/b)}\mathrm{d}y\,f(y), \tag{45}$$

where

$$f(y)=y^3\int_1^{\infty}\mathrm{d}x\,\frac{\sqrt{1+x^2}}{e^{yx}-1}. \tag{46}$$

To calculate E_0, let $b=\pi R/\Delta$ (that is $b\gg 1$) in (44) and (45). Since $f(0)=0$ and $f(y)$ behaves as a linear function in the neighborhood of $y=0$ the integration over y can be estimated as

$$\int_0^{\pi/b}\mathrm{d}y\,f(y)\simeq\frac{1}{2}f\left(\frac{\pi}{b}\right)\frac{\pi}{b} \tag{47}$$

or

$$\int_0^{\pi/b}\mathrm{d}y\,f(y)\simeq\frac{1}{2}\left(\frac{\pi}{b}\right)^2\int_{\pi/b}^{\infty}\mathrm{d}s\,\frac{\sqrt{s^2+(\pi/b)^2}}{e^{yx}-1}\simeq\frac{\pi^2}{12}\left(\frac{\pi}{b}\right)^2. \tag{48}$$

Combining (48) and (39) we obtain

$$E_0\simeq-\frac{\pi^3R}{720\Delta^3}-\frac{\pi}{192R\Delta}. \tag{49}$$

It is easy to observe that $T(1)$ is negligibly small in comparision with $T(\pi R/\Delta)$; thus, contribution E_{13} is dropped.

The contributions E_{11} and E_{12} appear to be of the higher order in small parameter Δ/R. Indeed we have

$$E_{12}=-\frac{1}{8\pi^2R^2}\left(\int_0^{\infty}\frac{x^3\,\mathrm{d}x}{\sqrt{1+x^2}}\int_1^{\infty}\mathrm{d}y\,\frac{\sqrt{y^2-1}}{e^{\pi xy}-1}+\int_0^1\frac{x^3\,\mathrm{d}x}{\sqrt{1-x^2}}\int_1^{\infty}\mathrm{d}y\,\frac{\sqrt{y^2+1}}{e^{\pi xy}-1}\right). \tag{50}$$

We can easily estimate the upper limit of the above integrals. The first one is smaller than $\frac{1}{7200}$, while the second is smaller than $\frac{1}{6}$. Thus

$$|E_{12}|<\frac{1}{48\pi^2R^2}. \tag{51}$$

Finally we evaluate the term E_{11} (see the Appendix) which is exponentially small,

$$E_{11}\simeq-\frac{1}{4\pi R\Delta}e^{-2\pi^2(R/\Delta)}. \tag{52}$$

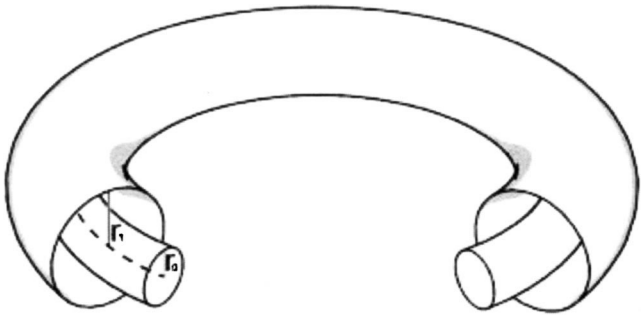

FIG. 1. Casimir energy in the region between two tori.

The final result for the Casimir energy between the close cylinders is then equal to E_0, that is we have

$$E_{\mathrm{cyl}}=-\frac{\pi^3 R}{720\Delta^3}\left(1+\frac{15}{2\pi^2}\frac{\Delta^2}{R^2}\right). \tag{53}$$

Note that the inclusion of the second term in the above expression does not contradict our approximation of (23), for the contribution of the first term after this approximation in the potential would be of the order Δ^3/R^3. It is easy to check that in the $R/\Delta\to\infty$ limit the above result becomes the same as the parallel plate energy.

Finally we like to remark that, for one-boundary geometries, for example, for D-dimensional ball there are satisfactory techniques to deal with the problem involving the roots of Bessel functions.[14] We hope that these techniques may also be adopted for geometries with two boundaries. For boundaries close to each other however, we can rely on the result of (53), for it gives the correct limit of parallel plates in the $R/\Delta\to\infty$ limit.

IV. CASIMIR ENERGY IN THE REGION BETWEEN TWO TORI

The problem (see Fig. 1) differs from the previous one by the boundary condition. Instead of (19), the solution of the e-value equation (15) should satisfy

$$\Phi|_{r=r_0}=\Phi|_{r=r_1}=0,\quad \Phi|_{z=0}=\Phi|_{z=L}, \tag{54}$$

where L is the circumference of the tori. For $\Delta\ll r_0$ we have

$$\Phi=\frac{e^{i(2\pi kz/h)+im\phi}}{2\pi\sqrt{r}}\sqrt{\frac{2}{\Delta}}\sin\left(\frac{\pi n}{\Delta}(r-r_0)\right) \tag{55}$$

and

$$\omega_{knm}=\sqrt{\left(\frac{2\pi k}{L}\right)^2+\left(\frac{m}{R}\right)^2+\left(\frac{\pi n}{\Delta}\right)^2-\frac{1}{4R^2}}, \tag{56}$$

where k, $m\in Z$ and $n=1,2,3,\ldots$; and $R^2=r_0r_1$ as in the preceding section. The total energy between the close tori is

$$E_{\mathrm{tor}}=\frac{1}{2}\sum_{m=-\infty}^{\infty}\mathrm{Reg}\left[\sum_{k=-\infty}^{\infty}\sum_{n=1}^{\infty}\omega_{knm}\right]. \tag{57}$$

Note that unlike the previous case, since the degree of freedom along the tori (i.e., along the z coordinate) is also restricted, we have to perform regularization for the k-summation too. Applying the Plana formula to the double sum over n and k we get

$$\sum_{m=-\infty}^{\infty}\int_0^{\infty}\mathrm{d}k\sum_{n=1}^{\infty}\omega_{knm}=\int_0^{\infty}\int_0^{\infty}\mathrm{d}k\,\mathrm{d}n\,\omega_{knm}+2\int_0^{\infty}\mathrm{d}k\,\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega_{knm}\right]$$
$$-\int_0^{\infty}\mathrm{d}k\,\omega_{k0m}+2\sum_{n=1}^{\infty}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{knm}\right]. \tag{58}$$

Dropping the first and the third terms in the above expression we arrive at the regularized double sum

$$\mathrm{Reg}\left[\sum_{k=-\infty}^{\infty}\sum_{n=1}^{\infty}\omega_{knm}\right]=2\int_0^{\infty}\mathrm{d}k\,\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega_{knm}\right]+2\sum_{n=1}^{\infty}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{knm}\right]. \tag{59}$$

Thus,

$$E_{\mathrm{tor}}=E_{\mathrm{tor}}^0+E_{\mathrm{tor}}^1, \tag{60}$$

where

$$E_{\mathrm{tor}}^0=\sum_{m=-\infty}^{\infty}\int_0^{\infty}\mathrm{d}k\,\mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega_{knm}\right] \tag{61}$$

and

$$E_{\mathrm{tor}}^1=\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty}\mathrm{Reg}\left[\sum_{m=1}^{\infty}\omega_{knm}\right]. \tag{62}$$

We first observe that E_{tor}^0 is proportional to the Casimir energy for the coaxial cylinders considered in the preceding section. Namely, we have

$$E_{\mathrm{tor}}^0=LE_{\mathrm{cyl}}. \tag{63}$$

In the Appendix we show that

$$E_{\mathrm{tor}}^1\simeq-\frac{3}{32\Delta}e^{-2\pi(L/\Delta)}, \tag{64}$$

which is negligible small. The total energy in the region between two tori is then equal to one given by (63),

$$E_{\mathrm{tor}}=-\frac{\pi^3RL}{720\Delta^3}\left(1+\frac{15}{2\pi^2}\frac{\Delta^2}{R^2}\right). \tag{65}$$

V. COAXIAL CYLINDRICAL BOXES OF FINITE HEIGHT

Instead of (54), the solution of the e-value equation (15) should satisfy

$$\Phi|_{r=r_0}=\Phi|_{r=r_1}=0,\quad \Phi|_{z=0}=\Phi|_{z=L}=0 \tag{66}$$

with L being the height of the cylinders. For $\Delta\ll r_0$ we have

$$\Phi=\frac{\sin\left(\frac{\pi k}{L}z\right)e^{im\phi}}{\pi\sqrt{r\pi}}\sqrt{\frac{2}{L\Delta}}\sin\left(\frac{\pi n}{\Delta}(r-r_0)\right) \tag{67}$$

and

$$\omega_{knm}=\sqrt{\left(\frac{\pi k}{L}\right)^2+\left(\frac{m}{R}\right)^2+\left(\frac{\pi n}{\Delta}\right)^2-\frac{1}{4R^2}}, \tag{68}$$

where $m\in Z$ and $n,k=1,2,3,\ldots$; and $R^2=r_0r_1$ as in the preceding section. The total energy between the close cylinders is then

$$E_{\text{box}}=\frac{1}{2}\sum_{m=-\infty}^{\infty}\text{Reg}\left[\sum_{k=1}^{\infty}\sum_{n=1}^{\infty}\omega_{knm}\right] \tag{69}$$

or

$$E_{\text{box}}=\frac{1}{2}\sum_{m=-\infty}^{\infty}\int_0^{\infty}dk\,\text{Reg}\left[\sum_{n=1}^{\infty}\omega_{knm}\right]+\frac{1}{4}\sum_{m=-\infty}^{\infty}\text{Reg}\left[\sum_{n=1}^{\infty}\omega_{0nm}\right]+\frac{1}{2}\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty}\text{Reg}\left[\sum_{k=1}^{\infty}\omega_{knm}\right]. \tag{70}$$

The first term on the right-hand side of the above formula is equal to LE_{cyl}. The third term is similar to E^1_{tor}. Namely, we have to multiply E^1_{tor} by $\frac{1}{2}$ and make a change $L\to 2L$. For $L\gg\Delta$ it is exponentially small

$$\frac{1}{2}\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty}\text{Reg}\left[\sum_{k=1}^{\infty}\omega_{knm}\right]\simeq\frac{\pi R}{32L\Delta}e^{-4\pi(L/\Delta)}. \tag{71}$$

Coming to the second term applying the Plana formula to the summation over m we get

$$\frac{1}{4}\sum_{m=-\infty}^{\infty}\text{Reg}\left[\sum_{n=1}^{\infty}\omega_{0nm}\right]=\frac{\zeta(3)R}{16\Delta^2}+O\left(\frac{1}{R}\right). \tag{72}$$

The final form is then summation of the LE_{cyl} and the above term,

$$E_{\text{box}}\simeq-\frac{\pi^3RL}{720\Delta^3}+\frac{R\zeta(3)}{16\Delta^2}. \tag{73}$$

Inspecting the above result we observe that the energy is positive around $L\leqslant\frac{3}{2}\Delta$ (within our approximation). Around this value of the height, the radial force $F_{\text{rad}}=-\partial E/\partial\Delta$ is repulsive. The force on the axial direction $F_{\text{axial}}=-\partial E/\partial L$ however, is repulsive for all values of L, which forces the cylinders to become of infinite length. When L becomes longer than $\frac{3}{2}\Delta$, the radial force also becomes attractive.

VI. CASIMIR ENERGY BETWEEN TWO CLOSE COCENTRIC SPHERES

We employ the spherical coordinates

$$ds^2=dt^2-dr^2-r^2(d\theta^2+\sin^2\theta\,d\phi^2) \tag{74}$$

and insert the solution in terms of the spherical harmonics

$$\Phi=Y^l_m(\theta,\phi)\frac{v_{ln}(r)}{r},\quad l=0,1,2,\ldots,\quad -l\leqslant m\leqslant l \tag{75}$$

into the Klein–Gordon equation (4). The resulting radial eigenvalue problem we have to deal with is

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{(l+\frac{1}{2})^2}{r^2}\right]v_{ln}(r)=(\omega_{ln})^2 v_{ln}(r) \tag{76}$$

subject to the boundary conditions

$$v_{ln}(r_0)=0, \quad v_{ln}(r_1)=0. \tag{77}$$

Here $r_0<r_1$ are the radii of the spheres and n is the radial quantum number to be determined by the boundary conditions. To satisfy the boundary conditions one has to deal with the roots of the radial wave function $v_{nl}(r)$ which as in the preceding section are the Bessel functions (with m replaced by $l+1/2$). However, since we are interested in $\Delta\equiv r_1-r_0\ll r_0$ limit, we can proceed as we have done in the preceding section. For the radial wave functions and the eigenvalues we obtain

$$v^0_{ln}(r)=\sqrt{\frac{2}{\Delta r}}\sin(\omega^0_{ln}(r-r_0)), \tag{78}$$

$$(\omega^0_{ln})^2=\frac{\pi^2 n^2}{\Delta^2}+\frac{\left(l+\frac{1}{2}\right)^2}{R^2}, \quad n=1,2,\ldots. \tag{79}$$

With the above approximated radial eigenfunctions and eigenvalues we can write the Green function as

$$G=\sum_{n=1}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{e^{i\omega_{ln}(t-t')}}{2\omega^0_{ln}}v^0_{ln}(r)v^0_{ln}(r')Y^l_m(\theta,\phi)\overline{Y^l_m(\theta',\phi')}. \tag{80}$$

Integrating the vacuum energy density

$$T=\ \mathrm{Reg}\left[\frac{1}{2}\lim_{t,r,\theta,\phi\to t',r',\theta',\phi'}\left[\partial_t\partial_{t'}+\partial_r\partial_{r'}+\frac{1}{r^2}\partial_\theta\partial_{\theta'}+\frac{1}{r^2\sin^2\theta}\partial_\phi\partial_{\phi'}\right]G\right] \tag{81}$$

over the volume between two cocentric spheres we get the total energy

$$E=\sum_{l=0}^{\infty}(l+\tfrac{1}{2})\ \ \mathrm{Reg}\left[\sum_{n=1}^{\infty}\omega^0_{ln}\right]. \tag{82}$$

Applying the Plana formula to the n summation and dropping the $n=0$ term and the integration over n we get

$$E=-\frac{2\Delta}{\pi R^2}\int_1^{\infty}\mathrm{d}n\,F(n), \tag{83}$$

where

$$F(n)=\sum_{s=1/2}^{\infty}\frac{s^3}{e^{2(\Delta/R)sn}-1}. \tag{84}$$

To use the Plana formula[1]

$$\sum_{k=0}^{\infty} f(k+\tfrac{1}{2}) = \int_0^{\infty} dy\, f(y) - i\int_0^{\infty} dy \frac{f(iy)-f(-iy)}{1+e^{2\pi y}} \tag{85}$$

we have to get rid of the poles of the function $F(n)$ at the imaginary axis $2(\Delta/R)ns = 2i\pi m$. Thus we work with the function

$$F_\beta = \sum_{s=1/2}^{\infty} \frac{s^3}{e^{2(\Delta/R)x(s+\beta)}-1} \tag{86}$$

with $\beta > 0$. Then (83) becomes

$$E = -\frac{\pi^3 R}{360\Delta^3} + E', \tag{87}$$

where

$$E' = \frac{1}{2\pi\Delta}\lim_{\beta\to 0}\int_0^{\infty}\frac{ds\, s^3}{e^{2\pi s}+1}\int_{2\Delta/R} dx \sqrt{x^2-\left(\frac{2\Delta}{R}\right)^2}\left(\frac{1}{e^{x(\beta+is)}-1}+\frac{1}{e^{x(\beta-is)}-1}\right). \tag{88}$$

Using $2\Delta/R \ll 1$ we get

$$E' \simeq -\frac{\pi}{288\Delta}. \tag{89}$$

Thus the total energy in the region between the spheres is

$$E = -\frac{\pi^3 R^2}{360\Delta^3}\left(1+\frac{5\Delta^2}{4\pi^2 R^2}\right). \tag{90}$$

In $R/\Delta \to \infty$ it is obvious that the above energy approaches the parallel plate formula.

VII. CASIMIR INTERACTIONS OF TWO CLOSE COAXIAL CONES

The geometry we like to present in this section is two cones with common axis at positive z-direction and appeces at the origin (see Fig. 2). By close cones we mean the appex angles θ_1 and θ_1 are close to each other, that is

$$\Delta \equiv \theta_1 - \theta_0 \ll \sqrt{\sin\theta_0 \sin\theta_1} \equiv \Theta. \tag{91}$$

In the above approximation the solutions we employ (in spherical coordinates) which vanishes at the surfaces $\theta = \theta_0$ and $\theta = \theta_1$ are

$$\Phi^{\omega}_{nm} = \sqrt{\frac{\omega}{r}} J_{\mu_{nm}}(\omega r)\frac{e^{im\phi}}{\sqrt{\pi\Delta}}\sin\left(\frac{\pi n}{\Delta}(\theta-\theta_0)\right), \tag{92}$$

where

$$\mu_{nm} = \sqrt{\left(\frac{\pi n}{\Delta}\right)^2+\left(\frac{m}{\Theta}\right)^2}. \tag{93}$$

The energy ω in (92) is continuous. The Green function is (with the cutoff factor β)

$$G = \sum_{n=1}^{\infty}\sum_{m=0}^{\infty}\sum_{m=-l}^{l}\frac{e^{-\beta\omega+i\omega(t-t')}}{2\omega}\Phi^{\omega}_{nm}(r,\theta,\phi)\overline{\Phi^{\omega}_{nm}(r',\theta',\phi')}. \tag{94}$$

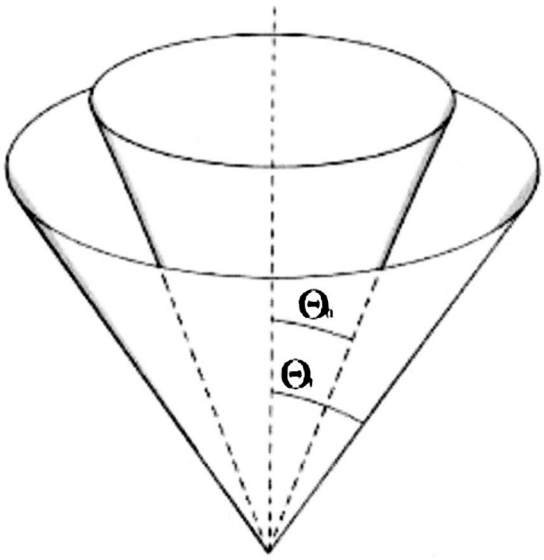

FIG. 2. Geometry of two cones with common axis at the positive z-direction and appeces at the origin.

Note that in this section we employ a different regularization method than in the previous ones. The cutoff method is more suitable for the continuous energy spectra. Inserting the Green function of (94) into the coincidence limit formula and then integrating over θ and ϕ, we arrive at the vacuum energy density at r,

$$E=\frac{1}{4\pi r}\,\mathrm{Reg}_{\beta}\left[\left(\frac{\partial^2}{\partial r^2}+2\,\frac{\partial^2}{\partial\beta^2}\right)\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty}\frac{Q_{-1/2+\mu_{nm}}\left(1+\frac{\beta^2}{2r^2}\right)}{r}\right]. \tag{95}$$

Reg_{β} stands for the cutoff regularization, that is, we pick the finite part of the expression in $\beta\to 0$ limit. In deriving (95) we used the formula[15]

$$\int_0^{\infty}\mathrm{d}\omega\, e^{-\beta\omega}(J_{\nu}(\omega r))^2=\frac{1}{\pi r}\,Q_{\nu-1/2}\left(1+\frac{\beta^2}{2r^2}\right), \tag{96}$$

where $Q_{\nu}(x)$ is Legendre function of the second kind. We rewrite the expression (95) as

$$E=n\,\frac{1}{2\pi r^4}\;\mathrm{Reg}_{y}\left[\hat{O}\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty}Q_{-1/2+\mu_{nm}}(1+y^2)\right] \tag{97}$$

with

$$y\equiv\frac{\beta}{\sqrt{2}r},\quad \hat{O}\equiv 1+2y\,\frac{\partial}{\partial y}+\frac{y^2+1}{2}\,\frac{\partial^2}{\partial y^2}. \tag{98}$$

Applying the Plana formula to the summation over m we arrive at

$$E=E_0+E_1, \tag{99}$$

where

$$E_0=\frac{1}{\pi r^4}\ \mathrm{Reg}_y\left[\hat{O}\sum_{n=1}^{\infty}\int_0^{\infty}\mathrm{d}m\,Q_{-1/2+\mu_{nm}}(1+y^2)\right] \tag{100}$$

and

$$E_1=\frac{1}{r^4}\ \mathrm{Reg}_y\left[\hat{O}\sum_{n=1}^{\infty}\int_{\pi\Theta n/\Delta}^{\infty}\frac{\mathrm{d}m\tanh\sqrt{\left(\frac{m}{\Theta}\right)^2-\left(\frac{\pi n}{\Delta}\right)^2}}{e^{2\pi m}-1}P_{-\frac{1}{2}+i\sqrt{(m/\Theta)^2-(\pi n/\Delta)^2}}(1+y^2)\right]. \tag{101}$$

Making use of $\pi\Theta n/\Delta\gg 1$, $\tanh x\leqslant 1$, and

$$\mathrm{Reg}_y[\hat{O}P_{-1/2+is}(1+y^2)]=\frac{7}{8}-\frac{s^2}{2} \tag{102}$$

we get

$$|E_1|\leqslant\frac{1}{r^4}\left|\sum_{n=1}^{\infty}\int_{(\pi\Theta n/\Delta}^{\infty}\mathrm{d}m\,e^{-2\pi m}\left(\frac{7}{8}-\frac{\left(\frac{m}{\Theta}\right)^2-\left(\frac{\pi n}{\Delta}\right)^2}{2}\right)\right|. \tag{103}$$

That is,

$$|E_1|\leqslant\frac{\Theta}{4\pi\Delta r^4}e^{-2\pi^2(\Theta/\Delta)}. \tag{104}$$

Thus E_1 is negligible small. To evaluate E_0, we apply the Plana formula to the summation over n in (100). The formula we obtain is

$$E_0=\mathcal{E}+\frac{\Theta\Delta}{2\pi r^4}A-\frac{\Theta}{2\pi r^4}B, \tag{105}$$

where

$$\mathcal{E}=\frac{\Theta\Delta}{2\pi r^4}\int_0^{\infty}\mathrm{d}x\int_x^{\infty}\mathrm{d}y\,\frac{\tanh\sqrt{y^2-x^2}}{e^{2\Delta y}-1}\left(\frac{7}{4}+x^2-y^2\right), \tag{106}$$

$$A=\mathrm{Reg}_y\left[\hat{O}\int_0^{\infty}\mathrm{d}s\,sQ_{-1/2+s}(1+y^2)\right], \tag{107}$$

$$B=\mathrm{Reg}_y\left[\hat{O}\int_0^{\infty}\mathrm{d}s\,Q_{-1/2+s}(1+y^2)\right]. \tag{108}$$

Changing the variables $y=t$, $x^2=t^2-k^2$ (106) can be rewritten as

$$\mathcal{E}=\frac{\Theta\Delta}{2\pi r^4}\int_0^{\infty}\frac{\mathrm{d}t\,t}{e^{2\Delta t}-1}\int_0^1\frac{\mathrm{d}k\,k}{\sqrt{1-k^2}}\tanh(kt)\left(\frac{7}{4}-k^2t^2\right). \tag{109}$$

Inspecting the integrals over k, that is, the terms

$$f_1(t)=\int_0^1\frac{\mathrm{d}k\,k}{\sqrt{1-k^2}}\tanh(kt) \tag{110}$$

and

$$f_2(t)=\int_0^1 \frac{\mathrm{d}k\,k^3}{\sqrt{1-k^2}}\tanh(kt), \tag{111}$$

we see that both approach very fast from the value $f_1(0)=f_2(0)=0$ to their respective asymptotic values $f_1(t\to\infty)=1$ and $f_2(t\to\infty)=0.66=\frac{2}{3}$.

Let us treat the second term in (109) in detail. We approximate $f_2(t)$ as

$$f_2(t)\simeq\begin{cases} at, & t\in[0,b], \\ \frac{3}{2}, & t\in[b,\infty), \end{cases} \tag{112}$$

where a and b are both of order 1. The second term in (109) then becomes

$$\mathcal{E}_2=-\frac{\Theta\Delta}{2\pi r^4}\left(a\int_0^b \frac{\mathrm{d}t\,t^4}{e^{2\Delta t}-1}+\int_b^\infty \frac{\mathrm{d}t\,t^3}{e^{2\Delta t}-1}\right). \tag{113}$$

Since $\Delta\ll 1$, we can approximate the denominator of the first integrand as $e^{2\Delta t}-1\simeq 2\Delta t$. In the second integral making the change of variables $2\Delta t=s$, we can replace the lower boundary as $2b\Delta\simeq 0$. Thus (113) becomes

$$\mathcal{E}_2\simeq-\frac{\Theta\Delta}{2\pi r^4}\left(\frac{ab^4}{8\Delta}+\frac{1}{16\Delta^4}\int_0^\infty \frac{\mathrm{d}s\,s^3}{e^s-1}\right)=-\frac{\Theta ab^4}{16\pi r^4}-\frac{\Theta\pi^3}{720r^4\Delta^3}. \tag{114}$$

It is obvious that the first term is negligible compared to the second. Similar treatment shows that the first term in (109) gives contributions of orders $O(\Delta)$ and $O(1/\Delta)$ both are small. Inspecting (100) we see that the second and third terms in E_0 are also negligible. Thus the final result for our Casimir energy is

$$E\simeq\mathcal{E}_2\simeq-\frac{\Theta\pi^3}{720r^4\Delta^3}. \tag{115}$$

Note that the above ''density'' is an expression obtained after integrating over Θ and ϕ. If we divide (115) to the angular integral

$$\int_{\theta_0}^{\theta_1}\sin\theta\int_0^{2\pi}\mathrm{d}\phi\simeq 2\pi\Theta\Delta \tag{116}$$

we obtain the energy density averaged over the angular variables:

$$E\simeq\mathcal{E}_2=-\frac{\pi^2}{1440r^4\Delta^4}+O(\Delta^{-3}). \tag{117}$$

In small Δ limit the above result is in perfect agreement with the energy density in the region between two infinite planes with angle Δ between them (i.e., the wedge problem),[16]

$$E=-\frac{1}{1440r^4\Delta^2}\left(\frac{\pi^2}{\Delta^2}-\frac{\Delta^2}{\pi^2}\right). \tag{118}$$

VIII. SUMMARY AND CONCLUSIONS

We have calculated the Casimir energies for the massless scalar field for regions between surfaces close to each other. In suitable limits, the results we obtained approach the expected

parallel plate formula for the infinite coaxial cylinders and cocentric spheres. Formulas for the infinite coaxial cylinders and cocentric spheres are in good agreement with the close distance limits of the recent results in the literature.[10,8]

For the geometry of coaxial cones the formula we obtained approaches the wedge problem with small angle, as expected.

In all the geometries considered the surfaces are attracted to each others. However, we have repulsive in the axial direction of the coaxial cylindrical boxes with finite height; and, centrifugal force in the radial direction for cocentric tori.

We hope that some geometries, for example, the coaxial cylinders and cocentric tori, may be materialized by virtue of the metallic nanostructures.

ACKNOWLEDGMENTS

The authors thank Alikram Aliev for useful theoretical discussions; and R. O. Onofrio for bringing some of the experiments including theirs to our attention. The authors thank Turkish Academy of Sciences (TUBA) for its support.

APPENDIX (REF. 15)

Estimation of E_{11}

We drop the factor $1/4R^2$ in the spectra ω^0_{pnm}. In Sec. II we have seen that this factor leads to the terms of the order $(\Delta/R)^2$ in comparision with the spectra $\sqrt{p^2+(\pi^2n^2/\Delta^2)+(m^2/R^2)}$. We have

$$E_{11}\simeq-\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{\pi}\sum_{n=1}^{\infty}\int_{R\sqrt{p^2+(\pi^2n^2/\Delta^2)}}^{\infty}\mathrm{d}m\,\frac{\sqrt{\frac{m^2}{R^2}-p^2-\frac{\pi^2n^2}{\Delta^2}}}{e^{2\pi m}-1}. \tag{A1}$$

Since for $n=1,2,\ldots$ the integration variable m is greater than $R\sqrt{p^2+(\pi^2n^2/\Delta^2)}\gg 1$ one can make the approximation

$$E_{11}\simeq-\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{\pi}\sum_{n=1}^{\infty}\int_{R\sqrt{p^2+(\pi^2n^2/\Delta^2)}}^{\infty}\mathrm{d}m\,e^{-2\pi m}\sqrt{\frac{m^2}{R^2}-p^2-\frac{\pi^2n^2}{\Delta^2}}. \tag{A2}$$

Using the integral representation for the modified Bessel functions we get

$$E_{11}\simeq=-\frac{1}{2\pi^2}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi}\sum_{n=1}^{\infty}\frac{\partial K_0(2\pi Rs\sqrt{p^2+(\pi n/\Delta)^2})}{\partial R}. \tag{A3}$$

We first use the integral

$$\int_0^{\infty}\mathrm{d}\lambda\,K_0(x\sqrt{\lambda^2+b^2})=\frac{\pi}{2x}e^{-xb} \tag{A4}$$

and then take summation over n and arrive at

$$E_{11}\simeq-\frac{1}{4\pi R\Delta}e^{-2\pi^2(R/\Delta)}. \tag{A5}$$

Estimation of E^1_{tor}

In a fashion parallel to the evaluation of E_{11} making the advantage of $R\gg\Delta$ we can bring E^1_{tor} into the following form:

$$E^1_{\rm tor} \simeq \frac{1}{8\pi}\frac{\partial}{\partial L}\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty} K_0\left(2L\sqrt{\frac{m^2}{R^2}+\frac{\pi^2 n^2}{\Delta^2}}\right). \tag{A6}$$

From

$$\sum_{m=-\infty}^{\infty} K_0\left(2L\sqrt{\frac{m^2}{R^2}+\frac{\pi^2 n^2}{\Delta^2}}\right) = 2\int_0^{\infty} dm\, K_0\left(2L\sqrt{\frac{m^2}{R^2}+\frac{\pi^2 n^2}{\Delta^2}}\right) + 2\pi\int_{\pi Rn/\Delta}^{\infty}\frac{dm\, J_0\left(2L\sqrt{\frac{m^2}{R^2}+\frac{\pi^2 n^2}{\Delta^2}}\right)}{e^{2\pi m}-1}, \tag{A7}$$

using the approximation $1/e^{2\pi m}-1 \simeq e^{-2\pi m}$ for $m \geqslant \pi Rn/\Delta$ we arrive at

$$\sum_{m=-\infty}^{\infty} K_0\left(2L\sqrt{\frac{m^2}{R^2}+\frac{\pi^2 n^2}{\Delta^2}}\right) = \pi R\left(\frac{e^{-2\pi(L/\Delta)n}}{2L}+\frac{e^{-2\pi n(\sqrt{\pi^2R^2+L^2}/\Delta)}}{\sqrt{\pi^2R^2+L^2}}\right). \tag{A8}$$

Thus we have

$$E^1_{\rm tor} \simeq -\frac{R}{8}\frac{\partial}{\partial L}\left(\frac{1}{2L}\frac{1}{e^{2\pi(L/\Delta)}-1}+\frac{1}{\sqrt{\pi^2R^2+L^2}}\frac{1}{e^{2\pi(\sqrt{\pi^2R^2+L^2}/\Delta)}-1}\right). \tag{A9}$$

Since $L=2\pi R$ the dominant term in the above expression is

$$E^1_{\rm tor} \simeq -\frac{3}{32\Delta}e^{-2\pi(L/\Delta)}. \tag{A10}$$

[1] For a list of reviews and monographs including the history of experiments see V. M. Mostepanenko and N. N. Trunov, *The Casimir Effects and its Applications* (Oxford University Press, New York, 1997); M. P. Roberts, hep-th/0012062.
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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

On the nonrelativistic Lee model

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(Received 11 July 2003; accepted 5 September 2003)

In this work we present two rigorous results on the nonrelativistic Lee model following a method proposed by Rajeev in an unpublished article (S. G. Rajeev, hep-th 9902025). Thus this short paper should be considered as a commentary on Rajeev. In the unpublished paper of Rajeev, the renormalization of the Hamiltonian is accomplished at the level of resolvents. We first establish that the renormalized resolvent of the interacting Hamiltonian indeed defines a unique closed densely defined operator acting on the free Fock space of bosons. Next we give a justification in the mean field approximation that the ground state energy is bounded from below and the system has a good thermodynamic limit by elaborating along the original arguments of Rajeev. Our arguments in two dimensions do not yield better bounds, but this could be due to the inadequacy of the method used. In both cases though the ground state energy is not significantly altered to give a nontrivial ground state energy per particle. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1624093]

I. INTRODUCTION

Originally the Lee model is introduced in Ref. 2 as a soluble simple relativistic model. This model was not meant to be realistic, but one wants to capture some nonperturbative aspects of field theories which require a renormalization. Its nonrelativistic simplification also has some of these merits and it is even simpler. A detailed discussion of this model from the point of view of the scattering matrix is given in the book by Henley and Thirring.[3] They find the solution to the quantum equations of motion and thus give an exact solution of the scattering matrix of the system. This is a model of a heavy particle which can be taken at rest at the origin and a field of nonrelativistic bosons which can form a compound with the heavy particle due to an attractive interaction. The bosons should not be excited too high levels since then the nonrelativitic approximation will break down. There are some attempts to understand this model in depth,[4] but a proper analysis of any number of bosons was not given prior to Ref. 1. In a truly remarkable work Rajeev took a fresh look at nonrelativistic models which require renormalization. The most interesting example in this article is the study of bosons which have an attractive local interaction in two and three dimensions. Rajeev also looks at the nonrelativistic Lee model as a simpler application of his method. He gives the complete solution of the bound state energies of this model for all boson numbers as an operator equation. This equation can be written as an integral equation for the wave functions and the energy levels. There are two questions left incomplete in his work: Rajeev's approach can be thought of as an extension of the ideas of Krein on the singular differential operators to the interacting field theory models (see for the modern point of view on these problems the valuable book by Albeverio and Kurasov[5]). In fact, the interactions one talks about in these models are essentially singular ones when written as ordinary quantum mechanical models. Rajeev's method renormalizes the resolvent of the interacting Hamiltonian directly and his

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point is that an attempt to write the renormalized Hamiltonian is futile because there is no simple way to write it; the interaction is at a point. One can say that the Hamiltonian looks like the free one but the boundary conditions of the wave functions will be different and this is what defines a different Hamiltonian (recall that in infinite dimensions and unbounded operator is defined by its action and its domain). However in the field theoretical approach one must prove that the resulting family of renormalized resolvents actually defines the resolvent family of a unique closed densely defined operator. This is essential since the time evolution of the interacting quantum system must be given by a unitary operator family parametrized by time. Its infinitesimal generator is the Hamiltonian of the system by Stone's theorem. We will show that this is indeed the case.

Using the mean field approximation Rajeev attempts to show that the ground state is bounded from below when the number of bosons go to infinity. Our contribution here is an attempt to fill a gap in his arguments. We are not completely successful since we could not really prove the original claim in the paper in its full generality but with a condition on the coupling constant. We also give an argument in two dimensions and show that the Hamiltonian is bounded from below but in this case again we could not show that the minimum energy state is when all the bosons are in zero momentum state and there is a composite with energy μ. However we can prove that the ground state energy per particle is still m, the rest energy of a free boson. In this sense the interaction is not stong enough.

The plan of the paper is the following: we first review the approach to nonrelativistic Lee model from Ref. 1 (the reader should consult this work to understand the discussion here) then prove that the resolvent family indeed defines a unique Hamiltonian. Next, we prove that the ground state is bounded from below in three dimensions. We extend this discussion to the two dimensional case as well. The paper is rather technical, yet we relegated some of the longer computations to an Appendix.

II. RAJEEV'S APPROACH TO THE NONRELATIVISTIC BOSONIC LEE MODEL

To facilitate the reading of the paper, we will review some of the aspects of the nonrelativistic Lee model as it is presented in Rajeev's work. We add some details as well. If the reader is already familiar with the original work he or she can skim through this part. Let us write down the Hamiltonian of the nonrelativistic Lee model with a cut-off,

$$H = H_0 + H_{1\Lambda}, \tag{1}$$

where

$$H_0 = \int [dp]\phi^\dagger(p)\phi(p)\omega(p), \quad \omega(p) = m + \frac{p^2}{2m}, \tag{2}$$

$$H_{1\Lambda} = \mu_\Lambda \frac{1-\sigma_3}{2} + g\int [dp]\rho_\Lambda(p)[\phi(p)\sigma_- + \phi^\dagger(p)\sigma_+], \tag{3}$$

where μ_Λ is a bare parameter to be adjusted (see below) and $\sigma_\pm, \sigma_3$ are the Pauli spin matrices acting on $\mathbf{C}^2$. There is a conserved quantity,

$$Q = \frac{1-\sigma_3}{2} + \int [dp]\phi^\dagger(p)\phi(p), \tag{4}$$

which means that we have an up state and $n+1$ bosons or down state and n bosons. We can think of the down state as a bound state of the system. By rewriting the resolvent of this operator, Rajeev shows that the normal ordering and by the following choice of bare mass difference:

$$\mu_\Lambda = \mu + g^2 \int [dp]\rho_\Lambda(p)^2 \frac{1}{\omega(p)-\mu}, \tag{5}$$

the renormalized resolvent thus obtained remains well-defined as $\Lambda \to \infty$. Here one should think of μ as the energy of the composite state which consists of a boson and the attractive heavy particle at the center.

In this limit the resolvent becomes

$$R(E)=\begin{pmatrix} \alpha(E) & \beta^{\dagger}(E) \\ \beta(E) & \Phi^{-1}(E) \end{pmatrix}, \tag{6}$$

$$\alpha(E)=\frac{1}{H_0-E}+\frac{1}{H_0-E}\int [dq]\phi^{\dagger}(q)\Phi^{-1}(E)\int [dp]\phi(p)\frac{1}{H_0-E},$$

$$\beta(E)=-\Phi^{-1}(E)\int [dp]\phi(p)\frac{1}{H_0-E},$$

and we have Rajeev's principal operator

$$\Phi(E)=H_0-E+\mu+4\pi^2 g^2(2m)^{3/2}[\sqrt{H_0+m-E}-\sqrt{m-\mu}]$$
$$-g^2\int [dp\,dq]\phi^{\dagger}(p)\frac{1}{H_0+\omega(p)+\omega(q)-E}\phi(q).$$

The advantage of this approach now is clear, the scattering states of this Hamiltonian should be the same as the free Hamiltonian but the bound states can only come from the zero eigenvalues of $\Phi(E)$. In fact there is a normalizable solution to this condition given by the state

$$\begin{pmatrix} \dfrac{g}{H_0-\mu}\displaystyle\int [dp]\phi^{\dagger}(p)|0\rangle \\ |0\rangle \end{pmatrix}. \tag{7}$$

This will be a bound state if we take $\mu<m$ which is physically meaningful if we want this model to describe the attractive interaction of such a two state system with bosons.

As indicated in Ref. 1 the last term has a negative sign and we will prove below that it is a negative operator, and this complicates matters. The analysis given by Rajeev shows that the spectrum of the principal operator is bounded from below. The drawback of the method is that the estimate produces a bound which depends on the number of bosons and in three dimensions this bound does not have a good thermodynamic limit. We will show later on by modifying an argument due to Rajeev that if we use the mean field approximation this bound on the ground state energy can be drastically improved. In fact, our method will show that if the coupling constant is below a certain value the energy of the ground state is given by the naive expectation, $\mu+nm$, where n is the number of bosons.

Let us recall the key steps in deriving a lower bound on the spectrum, first note the difficulty that the principal operator is the difference of two positive definite operators, assuming $E<(n+1)m$, by rewriting it as

$$\Phi(E)=H_0-E+\mu+4\pi^2 g^2(2m)^{3/2}[\sqrt{H_0+m-E}-\sqrt{m-\mu}]$$
$$-g^2\int_0^{\infty} ds\left[\int [dp]e^{-sp^2/2m}\phi(p)\right]^{\dagger} e^{-s[H_0+2m-E]}\left[\int [dq]e^{-sq^2/2m}\phi(q)\right].$$

To find a simple estimate we can write the Principal operator as

$$\Phi(E)=K(E)^{1/2}(1-\tilde{U}(E))K(E)^{1/2}, \tag{8}$$

where

$$K(E)=H_0-E+\mu+4\pi^2g^2(2m)^{3/2}[\sqrt{H_0+m-E}-\sqrt{m-\mu}], \tag{9}$$

and

$$\tilde{U}(E)=g^2\int [dp\,dq]\phi^\dagger(p)\frac{1}{K^{1/2}(E-\omega(p))(H_0+\omega(p)+\omega(q)-E)K^{1/2}(E-\omega(q))}\phi(q). \tag{10}$$

Here clearly

$$K(E)\geqslant nm+(\mu-E), \tag{11}$$

and we can give an estimate on the norm of $\tilde{U}(E)$, by using the arguments given in Ref. 1:

$$\|\tilde{U}(E)\|^2\leqslant g^4n^2\frac{(2m)^3}{[nm+\mu-E]}C, \tag{12}$$

where C is a constant given explicitly as an integral in Ref. 1. Assuming we can choose E such that the norm is less than one and knowing that the $\tilde{U}(E)$ is a positive operator we can find the estimate

$$\Phi(E)\geqslant\|K(E)\|(1-\|\tilde{U}(E)\|); \tag{13}$$

if this is a strictly positive operator we have an invertible operator $\Phi(E)$, which gives us the estimate for the lowest possible choice of E for which the resolvent is well-defined as

$$E<nm+\mu-g^4n^2(2m)^3C^2, \quad \text{or} \quad E_{\text{gr}}\geqslant nm+\mu-g^4n^2(2m)^3C^2. \tag{14}$$

Here notice that E is chosen outside of the spectrum lying on the real axis. This is why when we talk about the ground state energy the inequality should be reversed since now we are talking about the lowest value we can assign inside the spectrum. The use of the same symbol E for both cases hopefully will not cause too much confusion. One can check that this choice indeed gives us $\|U(E)\|<1$. This result unfortunately implies that the system does not have a good thermodynamic limit. If we assume that the mean field theory gives a good estimate of the ground state when $n\to\infty$, Rajeev shows that this result is not true and there is no difficulty in the thermodynamic limit. In two dimensions the same argument leads to

$$E_{\text{gr}}\geqslant nm+\mu-ng^2 2mC, \tag{15}$$

which implies that there is a good thermodynamic limit yet the ground state energy is modified enough to cause the energy per particle to be different than that of the free theory. We will see that in fact the situation in two dimensions is not as good as in three dimensions when we use the same mean field theory estimates, but the interaction is not strong enough to validate the above conclusions based on rough estimates. It is an interesting open question to prove the same estimates without using mean field theory, directly at the operator level.

III. DISCUSSION OF THE RENORMALIZED RESOLVENT

Since Rajeev derives the formula above for the resolvent by using a renormalization process the resulting one parameter family of bounded operators does not necessarily define an operator. That is, it may not be the resolvent family of a densely defined closed self-adjoint operator. For a quantum system, the evolution of the system is always defined by a unitary operator and its infinitesimal form (by Stone's theorem) defines a closed densely defined self-adjoint operator which corresponds to the Hamiltonian. We can show by a brute force computation that the operator family indeed satisfies the resolvent equation below,

$$R(E)-R(E')=(E-E')R(E)R(E'). \tag{16}$$

This is a necessary condition but it is not sufficient; the following theorem giving a sufficient condition is taken from Ref. 6.

Theorem: Let us assume that we have a set of bounded operators $R(z)$ on $\Delta\subset\mathbf{C}$, where Δ is an unbounded subset of the complex plane. We assume that this family satisfies the resolvent equation. If there is a sequence $\lambda_n\in\Delta$, such that $|\lambda_n|\to\infty$ as $n\to\infty$, and

$$\lim_{n\to\infty} -\lambda_n R(\lambda_n)x=x, \quad \text{for all } x\in\tilde{\mathcal{H}}, \tag{17}$$

where $\tilde{\mathcal{H}}$ refers to the underlying Hilbert space in general, then $R(z)$ is the resolvent family of a unique densely defined closed operator.

The resolvent acts on a subspace of the Fock space which has n or $n+1$ particles. Above we have seen that the operator family is bounded if we choose $E<-(\cos t)n^2$, and this makes $\|\tilde{U}(E)\|<1$. Thus we may choose a sequence of integers l, and define $\lambda_l=-ml^2$ and start $l>(\cos t)'n$. This is not the only sequence we could use, but it is a simple choice and it satisfies the hypothesis. Recall that the resolvent is given by

$$R(E)=\begin{pmatrix} \alpha(E) & \beta^\dagger(E) \\ \beta(E) & \Phi(E)^{-1} \end{pmatrix}, \tag{18}$$

which acts on vectors of the type $\binom{f_n}{f_{n+1}}\subset\mathcal{F}(\mathcal{H})\otimes\mathbf{C}^2$.

The limit condition in the theorem becomes the following three conditions:

$$\left\|\left[\frac{ml^2}{H_0+ml^2}-1\right]f+\left[\frac{ml^2}{H_0+ml^2}b^\dagger\Phi(-ml^2)^{-1}b\,\frac{1}{H_0+ml^2}\right]f\right\|\to 0,$$

$$\left\|\frac{ml^2}{H_0+ml^2}b\Phi(-ml^2)^{-1}f\right\|\to 0,$$

$$\|[ml^2\Phi(-ml^2)^{-1}-1]f\|\to 0, \quad \text{as} \quad l\to\infty,$$

for all vectors f with a fixed number of bosons in the Fock space. We will show how these can be proved by using some operator estimates, which are given in the Appendix. The first term already has a piece which is the resolvent of the free Hamiltonian, therefore it is enough to prove that the second part converges strongly to zero. In fact we have a better result,

$$\left\|\frac{1}{H_0+ml^2}b^\dagger\right\|\leqslant\frac{C_1}{l^{1/2}}, \tag{19}$$

for some number C_1. Thus we have now

$$\left\|\frac{ml^2}{H_0+ml^2}b^\dagger\Phi(-ml^2)^{-1}b\,\frac{1}{H_0+ml^2}f\right\|\leqslant ml^2\left\|\frac{1}{H_0+ml^2}b^\dagger\right\|\,\|\Phi(-ml^2)^{-1}\|\left\|b\,\frac{1}{H_0+ml^2}\right\|$$
$$\leqslant l^2\frac{C_1}{l^{1/2}}\frac{C_2}{l^2(1-C_3/l^2)}\frac{C_1}{l^{1/2}}\|f\|\leqslant\frac{C}{l}\|f\|.$$

This implies that the last term in fact goes uniformly to zero (in a sector with a finite number of bosons). In the middle part we already used the estimate on the norm of $\Phi(E)$, and our choice of l is such that $\|\Phi(-ml^2)\|<1$. Next we have

$$\left\| \frac{ml^2}{H_0+ml^2} b\Phi(-ml^2)^{-1} f \right\| \leqslant nC_4(l)\|f\|, \tag{20}$$

and $C_4(l)\mapsto 0$ as $l\to\infty$. To show this one we will use the following inequality:

$$bK^{-1/2}(E)(1-\tilde{U}(E))^{-1}K^{-1/2}(E) = bK^{-1}(E) + (bK^{-1/2}(E)\tilde{U}(E))(1-\tilde{U}(E))^{-1}K^{-1/2}(E). \tag{21}$$

We use now the norm estimates

$$\begin{aligned}
&\left\| \frac{ml^2}{H_0+ml^2} bK^{-1/2}(-ml^2)(1-\tilde{U}(-ml^2))^{-1}K^{-1/2}(-ml^2) \right\| \\
&\quad \leqslant \left\| \frac{ml^2}{H_0+ml^2} \right\| \ \|bK^{-1}(-ml^2)\| + \left\| \frac{ml^2}{H_0+ml^2} \right\| \ \|bK^{-1/2}(-ml^2)\tilde{U}(-ml^2)\| \\
&\qquad \times \|(1-\tilde{U}(-ml^2))^{-1}K^{-1/2}(-ml^2)\|.
\end{aligned}$$

We can divide these terms in the manner shown because each one is actually bounded. In fact the first term will be shown to go to zero as l goes to infinity and the middle term in the second part also goes to zero. More precisely we have the following inequalities:

$$\|bK^{-1}(-ml^2)\| \leqslant \frac{C_5}{l^{1/2}},$$

$$\|bK^{-1/2}(-ml^2)\tilde{U}(-l^2)\| \leqslant \frac{C_6}{l^{1/4}},$$

where the derivations of these estimates are given in the Appendix. To justify our approach, let us note that the operator family

$$\frac{ml^2}{H_0+ml^2} \tag{22}$$

is uniformly bounded since it is the resolvent of H_0, which means it converges strongly to the identity operator. This implies that the operator family is bounded acting on any vector in the Hilbert space, and now we can invoke the principle of uniform boundedness to conclude that this family is uniformly bounded. The last norm is also finite as can be verified easily. For the last condition we again use

$$K^{-1/2}(E)(1-\tilde{U}(E))^{-1}K^{-1/2}(E) = K^{-1}(E) + (K^{-1/2}(E)\tilde{U}(E))(1-\tilde{U}(E))^{-1}K^{-1/2}(E), \tag{23}$$

to write the upper bound,

$$\|[ml^2K^{-1}(-ml^2)-1]f\| + \|l^2K^{-1}(-ml^2)\| \ \|\tilde{U}(-ml^2)\| \ \|(1-\tilde{U}(-ml^2))^{-1}\|\|f\|. \tag{24}$$

Now the first term goes to zero which can be justified in a simple way, and the other one has $\|l^2K^{-1}(-ml^2)\|$ bounded and the norm $\|\tilde{U}(-ml^2)\|$ goes to zero as $l\to\infty$, which shows that the last claim is satisfied. This concludes that the desired conditions hold and the above family of operators indeed is the resolvent family of a unique closed densely defined operator acting on $\mathcal{F}(\mathcal{H})\otimes\mathbf{C}^2$.

IV. BOSONIC LEE MODEL IN THE LARGE *n*

In this section we will go over the details of the mean field approximation as presented in the paper of Rajeev. We modify some of the original arguments and we believe we reach a rigorous lower bound for the ground state energy. We follow exactly the same lines of reasoning up to the equation (122) in Rajeev's work:[1] Let us assume that as the number of particles in the system increases the mean field approximation becomes valid. All the bosons occupy the same state $u(p)$; we normalize it to the boson number,

$$\|u\|^2 = \int |u(p)|[dp] = n. \tag{25}$$

The energy levels of the system can be estimated as $E = E_{\text{mean}}(u) + O(n^{-\beta})$. Rajeev's principal operator becomes a principal function,

$$\Phi(E,u) = h_0(u) - E + \mu + 4\pi^2 g^2 (2m)^{3/2}[\sqrt{h_0(u)+m-E} - \sqrt{m-\mu}] - g^2 \int [dp\, dq] \frac{u^*(p)u(q)}{h_0(u)+\omega(p)+\omega(q)-E},$$

and here

$$h_0(u) = \int [dp]\omega(p)|u(p)|^2. \tag{26}$$

We must solve the equation $\Phi(E,u)=0$ to get E as a function of u and we must find the u that gives the smallest possible value of E subject to the constraint $\|u\|^2 = n$. Since the functional form of Φ is complicated a direct application of the variational calculus seems out of reach. Rajeev shows that the energy can indeed be solved as a function of u,

$$E = nm + \mu + (2m-\mu)nK(v) + f_1(nU)[nK(v) - 1], \tag{27}$$

where f_1 is the inverse function for

$$[\lambda + 2m]^{-1/2}(\lambda + \mu + (2\pi g)^2 (2m)^{2/3}[\sqrt{\lambda+m} - \sqrt{m-\mu}]) = nU, \tag{28}$$

and U is given as

$$U = g^2 (2m)^{3/2} V = g^2 (2m)^{3/2} \int [dp\, dq] \frac{v^*(p)v(q)}{p^2+q^2+1}, \tag{29}$$

and here

$$u(p) = \sqrt{n}[2m(2m+\lambda)]^{3/4} v(\sqrt{[2m(2m+\lambda)]}p), \tag{30}$$

with

$$\lambda = h_0(u) - E. \tag{31}$$

This is allowed since n is large but finite everywhere. We will first show that $U \geqslant 0$. To accomplish this we rewrite V as follows:

$$V=\int [dp\,dq]\frac{v^*(p)v(q)}{p^2+q^2+1}=\int_0^\infty ds\int [dp\,dq]v^*(p)e^{-(p^2+q^2+1)s}v(p)$$
$$=\int_0^\infty ds\,e^{-s}\left|\int [dp]v(p)e^{-p^2s}\right|^2\geqslant 0.$$

Thus its minimum value is zero. f_1 is an increasing function of its argument. We would like to find the minimum by choosing appropriate functions. Let us first note that to reduce the energy we should make the factor multiplying f_1 negative. We can do this by scaling the kinetic energy functional $K(v_a)=a^2K(v)$ if $v_a(p)=a^{-3/2}v(a^{-1}p)$. If we choose $a=1/n$,

$$E=nm+\mu+(2m-\mu)\frac{K(v)}{n}-f_1(nU_a)\left[1-\frac{K(v)}{n}\right]. \tag{32}$$

If we set $K(v)<n$, the last term is negative, thus increasing the argument of f_1 gives a lower bound for the energy. We note now that

$$\int [dp\,dq]\frac{v_a^*(p)v_a(q)}{p^2+q^2+1}\leqslant a^2K(v)\left[\int \frac{[dp\,dq]}{(1+p^2+q^2)^2p^2q^2}\right]^{1/2}=a^2K(v)4\pi^{3/2}. \tag{33}$$

Using $a=1/n$, and replacing the argument with this bigger value we get a lower bound for the energy,

$$E\geqslant nm+\mu+(2m-\mu)\frac{K(v)}{n}-f_1\left(4\pi^{3/2}(2m)^{3/2}g^2\frac{K(v)}{n}\right)\left[1-\frac{K(v)}{n}\right]. \tag{34}$$

We will now replace this with even a lower estimate. Notice that the original function that we inverted to find f_1 satisfies the following inequality:

$$\frac{\sigma}{\sqrt{\sigma+2m-\mu}}<f_1^{-1}(\sigma). \tag{35}$$

Now we use the following fact:

$$\text{if}\quad f_2^{-1}(\sigma)<f_1^{-1}(\sigma)\quad\text{then}\quad f_1(x)<f_2(x). \tag{36}$$

The inverse of function on the previous inequality is easy to find and if we replace the function f_1 with this upper bound we keep the lower bound. If we call the constants in front of $y=K(v)/n$ as c_1, we find that

$$E\geqslant nm+\mu(2m-\mu)y-f_2(c_1y)[1-y], \tag{37}$$

where $0\leqslant y<1$ and

$$f_2(c_1y)=\frac{1}{2}(c_1^2y^2+\sqrt{c_1^4y^4+4(2m-\mu)c_1^2y^2}), \tag{38}$$

we can use another estimate since $0\leqslant y<1, y^4<y^2$,

$$f_2(c_1y)<\frac{1}{2}\sqrt{c_1^4+4(2m-\mu)c_1^2}\left(\frac{c_1^2}{\sqrt{c_1^4+4(2m-\mu)c_1^2}}y^2+y\right). \tag{39}$$

We note that now we have an inequality of the form $f_1(y)<A^2(B^2y^2+y)$ with the obvious identifications of A,B. If we place this back into the energy estimate,

$$E \geqslant nm + \mu + [(2m-\mu) - A^2(B^2 y + 1)(1-y)]y. \tag{40}$$

Since $B^2 < 1$ the function $A^2(B^2 y+1)(1-y)$ is a decreasing function for $0 \leqslant y \leqslant 1$. We can set $y=0$ to make it maximum, and we have

$$E \geqslant nm + \mu[(2m-\mu) - A^2]y. \tag{41}$$

Clearly when $(2m-\mu) > A^2$, the minimum of this function on the right is achieved if $y=0$. This gives us a lower bound,

$$E \geqslant nm + \mu. \tag{42}$$

We can show that for arbitrarily small ϵ we can choose wave functions which will give the opposite inequality,

$$nm + \mu + \epsilon > E. \tag{43}$$

So we found a sufficient condition, which we can rewrite for the coupling constant,

$$g^2 < \frac{1}{8\pi^{3/2} m} \sqrt{\left(2 - \frac{\mu}{m}\right)(\sqrt{2}-1)}. \tag{44}$$

If we want to get a dimensionless ratio, we may compare the coupling constant to the bound state energy, this means we should write the above inequality as

$$g^2 \mu < \frac{1}{8\pi^{3/2}} \sqrt{\left(2 - \frac{\mu}{m}\right)(\sqrt{2}-1)} \frac{\mu}{m}, \tag{45}$$

here $g^2\mu$ is dimensionless.

It is interesting that the same analysis in $2+1$ dimensions is harder. We follow the same reasoning. The equation for λ then becomes

$$\lambda + \mu + \frac{1}{2} g^2 m \pi \ln\left[1 + \frac{\lambda + \mu}{m - \mu}\right] = n(2m) g^2 \int [dp\, dq] \frac{v^*(p) v(q)}{p^2 + q^2 + 1}. \tag{46}$$

Clearly we can now invert the function of λ on the right, to find

$$E = nm + \mu + (2m-\mu) n K(v) - h_1(nU)[1 - nK(v)], \tag{47}$$

where h_1 represents this inverse function. We see that the inverse function h_1 is actually dominated by the linear function nU; thus we may change the equality to

$$E \geqslant nm + \mu + (2m-\mu) n K(v) - nU[1 - nK(v)]. \tag{48}$$

Again we assume that by a scaling argument $nK(v) < 1$ is chosen (otherwise the energy has a bigger value). Let us estimate the function U in terms of $K(v)$. Here we face a problem, the integral diverges. Instead we choose a small parameter ϵ, which at the end will be taken to zero in a specific way. We can now show that

$$I(\epsilon) = \int \frac{[dp\, dq]}{p^{2-2\epsilon} q^{2-2\epsilon} (p^2 + q^2 + 1)} = \frac{1}{\epsilon^2} C_1 + O\left(\frac{1}{\epsilon}\right), \tag{49}$$

where C_1 is a constant which can be found. Then,

$$U \leqslant \left[\int [dp] p^{2-2\epsilon} |v(p)|^2\right] I(\epsilon)^{1/2}. \tag{50}$$

We will now estimate the integral in parantheses by using an inequality,

$$x^{2-2\epsilon} \leqslant \delta + \left[\frac{\epsilon}{\delta}\right]^{\epsilon/1-\epsilon} x^2, \tag{51}$$

where $0<\delta<1$ and $0<\epsilon<1$. This gives us

$$\int [dp] p^{2-2\epsilon} |v(p)|^2 \leqslant \delta + \left[\frac{\epsilon}{\delta}\right]^{\epsilon/1-\epsilon} \int [dp] p^2 |v(p)|^2. \tag{52}$$

If we insert this back into our estimate for the energy we have the same inequality,

$$E \geqslant nm + \mu + (2m-\mu)y - (2m)g^2 \left[n\delta + \left(\frac{\delta}{\epsilon}\right) y \right] I(\epsilon)^{1/2} (1-y), \tag{53}$$

where $0 \leqslant y < 1$ is chosen. In our problem the interesting question is the behavior of the ground state energy in the thermodynamic limit, that is, as $n \to \infty$. Also physically one expects that the mean field approximation is good if $n \gg 1$. In what follows we assume that $n \to \infty$ but of course this in reality represents the situation with a very large number of particles. To control the lower bound as $n \to \infty$ we assume that $\epsilon = \tau(n)$ where τ is an increasing function of n which tends to ∞ as $n \to \infty$. If we put the ϵ behavior of $I(\epsilon)$ into our estimate,

$$E \geqslant nm + \mu + (2m-\mu)y - (2m)g^2 C_1^{1/2} [n\delta\tau(n) + [\tau(n)\delta]^{1/1-\tau(n)} \tau(n) y](1-y). \tag{54}$$

If we want the large n behavior of the ground state energy to be least influenced by the number of particles we can choose $\delta(n) = 1/n\tau(n)^2$ and we see that in this limit

$$E \geqslant nm + \mu + (2m-\mu)y - (2m)g^2 C_1^{1/2} [n\tau(n)]^{1/\tau(n)-1} \tau(n) y(1-y). \tag{55}$$

If we look at now the logarithm of the exponential we find

$$z = \ln[n\tau(n)]^{1/\tau(n)-1} = \frac{1}{\tau(n)} \ln[n\tau(n)], \tag{56}$$

this will have a finite limit as $n \to \infty$ if, $\tau(n) = \ln(n)$. Then we can replace the exponential (for sufficiently large n) by e^2,

$$E \geqslant nm + \mu + (2m-\mu)y - (2m)g^2 e^2 C_1^{1/2} \ln(n) y(1-y). \tag{57}$$

This shows that the energy of the ground state may decrease by a logarithm of the number of particles in the system. Of course there is a linear piece proportional to mass, and this determines the leading behavior of the system. If we define the average energy per particle E/n this will be m the mass of each particle as $n \to \infty$, which implies that the interaction becomes unimportant as we increase the number of particles.

An interesting possiblity appears if we assume that the coupling constant in each sector could be adjusted. Then if we set $g^2(n)\ln(n) \leqslant (2m-\mu)/2me^2 C_1^{1/2}$ this will imply that the minimum energy solution occurs when $y=0$, which gives us $E_{gr} = nm + \mu$, that is when there is a composite particle and all the other particles sit at the $p=0$ state. Our analysis gives only a sufficient condition and a more careful analysis may remove this condition and give a weaker one.

ACKNOWLEDGMENTS

Above all we would like to thank S. G. Rajeev for discussions and for his valuable insights. We thank E. Langmann for a careful reading and suggestions. We also thank the members of our group at Bogazici University and also members of the Gursey Institute for discussions. O.T.T.'s

research was supported by the Turkish Academy of Sciences, in the framework of the Young Scientist Award Program (OTT-TUBA-GEBIP/2002-1-18) and also by Bogazici University Research Grant No. 03B301.

APPENDIX: VARIOUS NORM ESTIMATES

We give an estimate of the norm of $(H_0+ml^2)^{-1}b^\dagger$, by using the action of creation–annihilation operators on normalizable Fock states. First let us find the action of this operator on such a state $|f\rangle$ given by

$$|f\rangle=\int \Pi_i[dp_i]f(p_1,\ldots,p_n)|p_1,\ldots,p_n\rangle, \tag{A1}$$

$$\frac{1}{H_0+ml^2}b^\dagger|f\rangle=\int \Pi_i[dp_i][dq]\frac{1}{\Sigma_i p_i^2/2m+q^2/2m+(n+1)m+ml^2} \times f(p_1,\ldots,p_n)|p_1,\ldots,p_n,q\rangle. \tag{A2}$$

The norm of this state satisfies the inequality

$$\left\|\frac{1}{H_0+ml^2}b^\dagger|f\rangle\right\|^2\leqslant\int \Pi[dp_i][dq]\left(\frac{1}{q^2/2m+ml^2}\right)^2|f(p_1,\ldots,p_n)|^2 \leqslant\int[dq]\frac{1}{(q^2/2m+ml^2)^2}\int\Pi[dp_i]|f|^2\leqslant\frac{C_1}{l}\|f\|^2.$$

Let us compute the same for $bK^{-1}(-l^2)|f>$; this gives us

$$\int \Pi_{k>1}[dp_k] \times\left(\int[dp_1]\frac{gnf(p_1,p_2,\ldots,p_n)}{(\Sigma_j p_j^2+nm+\mu+ml^2+4\pi^2g^2(2m)^{3/2}[\sqrt{\Sigma_j p_j^2/2m+nm+ml^2}-\sqrt{m-\mu}])}\right) \times|p_2,\ldots,p_n\rangle.$$

The square of the norm of such a state can be estimated, by noting that we can ignore various positive contributions in the denominator, to be smaller than

$$\int \Pi_{k>1}[dp_k]\left(\int[dp_1]\frac{gn|f(p_1,\ldots,p_n)|}{\Sigma_{j>1}p_j^2/2m+(n-1)m+ml^2}\frac{1}{p_1^2/2m+ml^2}\right)^2 \leqslant\int\Pi_{k>1}[dp_k]g^2n^2\left(\int[dp_1]|f(p_1,\ldots,p_n)|^2\int[dp]\frac{1}{(p^2/2m+ml^2)^2}\right)\leqslant C_2n^2\|f\|^2\frac{1}{l}.$$

Before we start the estimate on $bK^{-1/2}(-ml^2)\tilde{U}(-ml^2)$ we will reorganize it at the operator level as

$$bK^{-1/2}(-ml^2)\tilde{U}(-ml^2)=g\int[dq\,dp]K^{-1}(-ml^2-\omega(q))[H_0+p^2/2m+q^2/2m+2m +ml^2]^{-1}K^{-1/2}(-ml^2-\omega(p))\phi(p) \;+\int[dp\,dr\,dq]\phi^\dagger(q) \times K^{-1}(-ml^2-\omega(q)-\omega(r))[H_0+p^2/2m+q^2/2m+r^2/2m+3m +ml^2]^{-1}K^{-1/2}(-ml^2-\omega(p)-\omega(r))\phi(p)\phi(r).$$

This implies that we can estimate each operator separately: for the first, it is better to express its effect on a state $|f\rangle$, in terms of the defining function f,

$$f(p_1,\ldots,p_n)\mapsto \int [dpdq]f(p,p_2,\ldots,p_n)K^{-1}(-ml^2-\omega(q))[H_0+\omega(p)+\omega(q) +ml^2]^{-1}K^{-1/2}(-ml^2-\omega(p)). \tag{A3}$$

Let us call this map $(Af)(p_2,\ldots,p_n)$. The L^2 norm of this resulting $n-1$ particle wave function can be estimated, by neglecting various positive terms in the denominator, to be less than

$$\begin{aligned}
\|Af\|^2 &< g^2n^2\int \Pi_{j>1}[dp_j] \\
&\quad\times\left[\int [dpdq]\frac{|f(p,p_2,\ldots,p_n)|}{[q^2/2m+nm+ml^2][p^2/2m+q^2/2m+nm+ml^2][p^2/2m+nm+ml^2]^{1/2}}\right]^2 \\
&< g^2n^2\|f\|^2\int [dp]\left[\int \frac{[dq]}{[q^2/2m+ml^2][p^2/2m+q^2/2m+nm+ml^2]}\right]^2\frac{1}{p^2/2m+nm+ml^2} \\
&< C_2g^2n^2\|f\|^2\int \frac{dp}{[p^2/2m+nm+ml^2]^{1+3/4}}\left[\int \frac{[dq]}{[q^2/2m+nm+ml^2]^{1+5/8}}\right]^2 \\
&< C_2'g^2n^2\frac{1}{(nm+ml^2)^{1/2}}.
\end{aligned}$$

The second term has a symmetrization and this gives various interference terms as well, all of these terms as well as the noninterfering terms can be shown to be smaller than the following expression (the details of this computation are long but relatively straigthforward):

$$\int \Pi_{i\geqslant 3}[dp_i][dq]\left[\int \frac{[dp\,dr]|f(p,r,p_3,\ldots,p_n)|}{(q^2/2m+r^2/2m+nm+ml^2)(p^2/2m+r^2/2m+nm+ml^2)^{1/2}} \times\frac{1}{(p^2/2m+q^2/2m+r^2/2m+nm+ml^2)}\right]^2;$$

now we can further estimate this by repeated application of the Cauchy–Schwartz inequality,

$$\begin{aligned}
&\leqslant \|f\|^2\int \frac{[dr\,dq]}{(q^2/2m+r^2/2m+nm+ml^2)^2} \\
&\quad\times\left[\int \frac{[dp]}{(p^2/2m+r^2/2m+q^2/2m+nm+ml^2)^4}\right]^{1/2}\left[\int \frac{[dp']}{(p'^2/2m+nm+ml^2)^2}\right]^{1/2} \\
&\leqslant \|f\|^2\int \frac{[dq\,dr]}{(r^2/2m+q^2/2m+nm+ml^2)^{13/4}}\frac{C_5}{(nm+ml^2)^{1/4}} \leqslant \|f\|^2\frac{C_6}{(nm+ml^2)^{1/2}};
\end{aligned}$$

thus the norm of this part of the operator is bounded by $C_7/l^{1/2}$ which goes to zero as $l\to\infty$. Thus the combination of these two types of terms indeed go to zero. In a simple way we can check that $\|[l^2K(-ml^2)-1]|f>\|\to 0$, as $l\to\infty$:

$$
\begin{aligned}
&\|[l^2K(-ml^2)-1]|f\rangle\|^2 \\
&\quad=\int \Pi_j[dp_j]|f(p_1,\ldots,p_n)|^2 \\
&\qquad\times\frac{[\Sigma_j p_j^2/2m+nm+\mu+4\pi^2(2m)^{3/2}(\sqrt{\Sigma_j p_j^2/2m+nm+m+ml^2}-\sqrt{m-\mu})]^2}{[\Sigma_j p_j^2/2m+nm+\mu+ml^2+4\pi^2(2m)^{3/2}(\sqrt{\Sigma_j p_j^2/2m+(n+1)m+ml^2}-\sqrt{m-\mu})]^2} \\
&\quad\leqslant\int_{|p_j|\leqslant m\sqrt{l}}\Pi_j[dp_j]|f(p_1,\ldots,p_n)|^2 \\
&\qquad\times\frac{[nm^2l/2m+nm+\mu+4\pi^2(2m)^{3/2}(\sqrt{nlm^2/2m+nm+m+ml^2}-\sqrt{m-\mu})]^2}{m^2l^4} \\
&\qquad+\int_{|p_j|>m\sqrt{l}}\Pi_j[dp_j]|f(p_1,\ldots,p_n)|^2<\frac{C_8}{l^2}\|f\|^2+\int_{|p_j|>m\sqrt{l}}\Pi_j[dp_j]|f(p_1,\ldots,p_n)|^2.
\end{aligned}
$$

Note that the second term can be made smaller than any $\epsilon>0$, by choosing l sufficiently large, since $\|f\|$ is finite; thus the result follows.

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Boundary conformal fields and Tomita–Takesaki theory

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(Received 20 June 2003; accepted 9 September 2003)

Motivated by formal similarities between the continuum limit of the Ising model and the Unruh effect, this paper connects the notion of an Ishibashi state in boundary conformal field theory with the Tomita–Takesaki theory for operator algebras. A geometrical approach to the definition of Ishibashi states is presented, and it is shown that, when normalizable, the Ishibashi states are cyclic separating states, justifying the operator state corespondence. When the states are not normalizable Tomita–Takesaki theory offers an alternative approach based on left Hilbert algebras, making possible extensions of our construction and the state-operator correspondence. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1625872]

I. INTRODUCTION

Since their introduction and exploitation, particularly by Cardy, there has been a strong interest in boundary states in conformal field theory.[3–6,14] However, there are many other interesting examples of quantum field theories with boundary. For example, the Unruh effect,[25] in which an observer accelerating through a vacuum detects a thermal spectrum of particles, can be linked to the splitting of two-dimensional Minkowski space into two Rindler-type space–times, and the horizon or boundary between them (see particularly Refs. 22, 25, and 2). An even more obvious example of a boundary, though in momentum rather than configuration space, is the Fermi energy level. Although physically very different, these share mathematical features which we shall study in this paper, placing boundary conformal field theory within the broader context of operator algebras associated with quantum field theories with boundaries. We shall concentrate on the boundary states, where the broader context suggests an alternative mathematical description of Ishibashi states, which avoids the normalizability problem. The key mathematical tool, suggested already by the Unruh effect, is Tomita–Takesaki theory, whose primary physical use is usually to study thermal states and the KMS condition (see Sec. IV and Ref. 24).

To see how this comes about we first consider the treatment of the Ishibashi boundary states in conformal field theory. In the physics literature conformal symmetry is usually expressed in terms of a Lie algebra which is the direct sum of two (commuting) copies of the Virasoro algebra, a central extension of the vector fields vect(S^1) on a circle. The Virasoro algebra is generated by elements L_n (or by $\tilde{L}_n$ for the other copy) for $n \in \mathbf{Z}$, with the Lie brackets given in terms of the central charge $c \in \mathbf{R}$ by

$$[L_m, L_n] = (m-n)L_{m+n} + \frac{cn(n^2-1)}{12}\delta_{m+n,0},$$

$$[\tilde{L}_m, \tilde{L}_n] = (m-n)\tilde{L}_{m+n} + \frac{cn(n^2-1)}{12}\delta_{m+n,0}.$$

Introducing $L_n = -L(z^{n+1}\partial/\partial z)$ and $\tilde{L}_n = -\tilde{L}(\overline{z}^{n+1}\partial/\partial\overline{z})$, these commutation relations define pro-

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jective representations L and $\tilde{L}$ of vect(S^1) with essentially the same multiplier σ. We shall often write $L(X)$ for the representation of a general holomorphic vector field X, and $\tilde{L}(Y)$ for an antiholomorphic vector field Y.

The Ishibashi states Ω are supposed to satisfy $L_n^*\Omega=\tilde{L}_n\Omega$, for all $n\in\mathbf{Z}$ (where $L_n^*=L_{-n}$). This condition can be regarded as a replacement for the highest weight condition that $L_n\Omega=0=\tilde{L}_n\Omega$ for $n>0$. Unfortunately, the vectors Ω which occur in the physics literature are almost always unnormalizable, that is, they are not really vectors in the representation space at all.

Another useful feature of conformal field theories is the operator-state correspondence in which an algebra element a is identified with the vector $a\Omega$. In fact, this identification map is surjective just when the vector Ω is a cyclic vector, and is one-to-one when Ω is separating (that is, $a\Omega$ vanishes only when $a=0$). The operator-state correspondence also means that the algebra can also be regarded as an inner product space, and so should in fact be some sort of Hilbert algebra (a $*$-algebra which is also a pre-Hilbert space with certain properties linking the multiplication and inner product). Now left Hilbert algebras and cyclic separating vectors are united in Tomita–Takesaki theory.[24,7,8,22] Moreover, that theory can cope with the situation when there is only the Hilbert algebra, but no cyclic separating vector Ω, as happens when the Ishibashi states are not normalizable.

In this setting other features of conformal field theory find a natural place. For example, left and right multiplication in the Hilbert algebra generate two commuting von Neumann algebras of operators, which Tomita theory shows to be anti-isomorphic. This is just the sort of structure exhibited by the two algebras generated by the L_n and the $\tilde{L}_n$. In fact, we shall often find it convenient to forget the detailed structure of the Virasoro algebra and simply work with two commuting (or graded commuting) algebras $\mathcal{A}_+$ and $\mathcal{A}_-$ which are related by some conjugate linear homomorphism $a\mapsto\tilde{a}$, such that $\tilde{\tilde{a}}=a$. We associate to the boundary a left Hilbert algebra, $\mathcal{A}_0$, having the given commuting anti-isomorphic algebras as its left and right von Neumann algebras. In some cases this Hilbert algebra can be generated by a generalized Ishibashi vector Ω satisfying $a^*\Omega=\tilde{a}\Omega$, for all $a\in\mathcal{A}_+$.

In this paper we shall show how this viewpoint enables us to reconstruct various results from the physics literature. Section II explains how the geometrical link between boundaries and involutions provides an easy characterization of a subgroup of the conformal group respecting the boundary, and of the Ishibashi states. This is extended in Sec. III to $*$-algebras having an antilinear involutory automorphism. In Sec. IV it is shown that these definitions pick out cyclic separating vectors, bringing the ideas into the framework of Tomita–Takesaki theory. Section V looks at properties of symmetries of such a system. The ideas are brought together in Sec. VI to show how Tomita–Takesaki theory provides a replacement for Ishibashi states when, as usually happens, these are not normalizable. Finally we discuss the situation when a region has several disconnected boundaries. The two appendices review the Unruh effect from the perspective of conformal field theory and the fermion field theory arising as the continuum limit of the Ising model.

While working on this topic we became aware of work by Wassermann,[27] which also investigates boundary conformal field theory using operator algebras, but with somewhat different objectives. The monograph by Evans and Kawahigashi[9] explains the links between operator algebras and ordinary conformal field theory.

II. THE CONFORMAL GROUP

The vector fields are the Lie algebra of the orientation preserving diffeomorphisms of the circle $H=\mathrm{Diff}^+(S^1)$. In practice, however, the Lie algebra action of vector fields does not always exponentiate to a well-defined action of H, and, as Isham has remarked,[13] it really makes more sense to consider a pseudogroup of locally defined transformations. Alternatively, one might allow for groups or Lie algebras by working in the context of a Hopf algebra, but, for simplicity, having signaled the technical obstacle, we shall proceed as though the group actions existed, leaving the reader to reinterpret results in those few cases where necessary.

The key to the study of boundaries in quantum conformal theory, as in its classical analog, is the method of images. The boundary separates two regions, the physically interior region and its reflection outside the curve. The reflection, which reverses the holomorphic structure, fixes the boundary. For example, in two dimensions the unit circle C is the fixed point set of the antiholomorphic involution $\kappa_C: z \mapsto 1/\overline{z}$ which interchanges the unit disc and the exterior, while the real axis is the set fixed by conjugation $\kappa_{\mathbf{R}}: z \mapsto \overline{z}$. By the Riemann mapping theorem the interior of any Jordan curve in $\mathbf{C}$ can be mapped to the unit disc by a map Φ, so for any such curve there is an antiholomorphic involution $\kappa = \Phi^{-1}\kappa_C\Phi$ which interchanges the inside and outside of the curve, though one has to be careful about behavior on the curve itself. (In practice, it is more convenient to use the map F taking the interior to the upper half plane, and $\kappa = F^{-1}\kappa_{\mathbf{R}}F$, so that $\kappa(z) = F^{-1}\overline{F(z)}$, where $\overline{F}(z) = \overline{F(\overline{z})}$.) The product of two antiholomorphic involutions is holomorphic (for example, $\kappa\kappa_{\mathbf{R}}(z) = F^{-1}\overline{F}(z)$), and so products of even numbers of such involutions generate a subgroup of the conformal group, which is clearly normal as the conjugate of a product of involutions is the product of their conjugates. Using the fact that the conformal group is the product of two copies of the diffeomorphism group of the circle, together with Cartan's result that diffeomorphism groups have simple Lie algebras,[12] we see that a group with the Lie algebra of the whole conformal group is generated in this way.

The boundary involutions induce antilinear automorphisms of any algebras associated with the surface, and we shall argue that these provide a dense subalgebra with the structure of a Tomita or modular Hilbert algebra, which encodes the information about the boundary normally described using Ishibashi states.

A conformal transformation of S can be reflected to give a conformal transformation in the subgroup G_κ commuting with the involution κ.

Lemma 2.1: The restriction of the multiplier to G_κ is trivial.

Proof: We start by considering the case of the upper half plane and involution $\kappa = \kappa_{\mathbf{R}}: z \mapsto \overline{z}$ defining the real axis. A conformal transformation $F: z \mapsto F(z)$ commutes with $\kappa_{\mathbf{R}}$ if and only if $F(\overline{z}) = \overline{F(z)}$, or equivalently $F = \overline{F}$. To find the effect on the multiplier we need to work at the Lie algebra level, where a typical vector field has the form

$$X + Y = \sum_n X_n z^{n+1}\frac{\partial}{\partial z} + \sum_n Y_n \overline{z}^{n+1}\frac{\partial}{\partial \overline{z}}.$$

We easily calculate that

$$\kappa(X+Y)\kappa = \sum_n \overline{Y}_n z^{n+1}\frac{\partial}{\partial z} + \sum_n \overline{X}_n \overline{z}^{n+1}\frac{\partial}{\partial \overline{z}},$$

so that $X+Y$ commutes with κ if and only if $Y_n = \overline{X}_n$ for all n (or equivalently $Y = \kappa X \kappa$). In the real Lie algebra of G we also have $X_n = -\overline{X}_{-n}$. Thus in the real Lie algebra of G_κ one has $X_n = -Y_{-n}$, so that it is generated by elements of the form $z^{-n+1}\partial/\partial z - \overline{z}^{n+1}\partial/\partial \overline{z}$. (In more abstract form the elements of this subalgebra have the form $X + X^\kappa$, where $X^\kappa = \kappa X \kappa$.)

The representations are thus generated by $L_{-n} - \tilde{L}_n$. Now, since the L_m and $\tilde{L}_n$ commute,

$$[L_{-m} - \tilde{L}_m, L_{-n} - \tilde{L}_n] + (m-n)(L_{-m-n} - \tilde{L}_{m+n}) = [L_{-m}, L_{-n}] + (m-n)L_{-m-n} + [\tilde{L}_m, \tilde{L}_n] - (m-n)\tilde{L}_{m+n}.$$

The first two terms give $-\delta_{m+n,0}cn(n^2-1)/12$, while the last pair gives the same with n replaced by $-n$, so that there is cancellation, and the multiplier vanishes on this subalgebra.

Although we have only proved the result for $\kappa_{\mathbf{R}}$, any other involution is conjugate to this and conjugation does not affect the triviality of the multiplier. □

Note: The characterization of the elements of the Lie subalgebra as having the form $X+X^\kappa$ works more generally, and these are represented by $L(X)+\tilde{L}(X^\kappa)$. For unitary representations of the real algebra $L(X)=-L(X)^*$, so that the subalgebra is represented by elements of the form $-L(X)^*+\tilde{L}(X^\kappa)$. One then checks that, for any holomorphic vector fields X and Y,

$$\begin{aligned}&[-L(X)^*+\tilde{L}(X^\kappa),-L(Y)^*+\tilde{L}(Y^\kappa)]+L([X,Y])^*-\tilde{L}([X,Y]^\kappa])\\&\quad=[L(X)^*,L(Y)^*]+L([X,Y])^*+[\tilde{L}(X^\kappa),\tilde{L}(Y^\kappa)]-\tilde{L}([X^\kappa,Y^\kappa])\\&\quad=-([L(X),L(Y)]-L([X,Y]))^*+([\tilde{L}(X^\kappa),\tilde{L}(Y^\kappa)]-\tilde{L}([X^\kappa,Y^\kappa])),\end{aligned}$$

which cancels to give 0.

The corresponding condition for the conformal group $G=H\times H$ is obtained by taking the tensor product $\mathcal{V}$ of the σ-representations V and $\tilde{V}$ obtained by exponentiating L and $\tilde{L}$: $V(\exp(X))=\exp(L(X))$ and $\tilde{V}(\exp(X))=\exp(\tilde{L}(X))$. As we readily see, the subgroup commuting with the involution is

$$G_\kappa=\{(x,x^\kappa)\in H\times H: x\in H\}.$$

We may look for a vector Ω_κ in the representation space which is an eigenvector for all elements $g\in G_\kappa$:

$$\mathcal{V}(g)\Omega_\kappa=\lambda(g)\Omega_\kappa.$$

This is a quantum mechanical analog of the curve itself for a conformal field theory based in the interior of the fixed point set of κ. (For consistency the multiplier on the subgroup G_κ must be trivial, but that is assured by the Lemma.)

The eigenvector Ω_κ must also be an eigenvector for the Lie algebra of G_κ and, when the boundary is the real axis, we know that this is generated by $L_{-n}-\tilde{L}_n=L_n^*-\tilde{L}_n$. The simplest case is when the eigenvalues vanish (or Ω_κ is actually fixed by the subgroup G_κ), giving $(L_n^*-\tilde{L}_n)\Omega_\kappa=0$, for all $n\in\mathbf{N}$, which is the Ishibashi condition. This condition can also be expressed in the form $L(X)^*\Omega_\kappa=\tilde{L}(X^\kappa)\Omega_\kappa$, valid for any boundary curve. (When the eigenvalue is non-vanishing one may subtract half of it from each L and $\tilde{L}$, to obtain new operators satisfying the same commutation relations whose kernel contains Ω_κ, so that the condition that the vector be fixed by G_κ is less special than appears at first sight.) We deduce the following result.

Lemma 2.2: The Ishibashi condition on a vector Ω_κ is equivalent to Ω_κ being a vector fixed by the representation of G_κ, or annihilated by its Lie algebra.

Note: It follows from the definition of the Ishibashi boundary state Ω that

$$\langle\Omega,\tilde{V}(\tilde{x}_j)V(x_k)\Omega\rangle=\langle\tilde{V}(\tilde{x}_j^{-1})\Omega,V(x_k)\Omega\rangle=\langle V(x_j^{-1})^*\Omega,V(x_k)\Omega\rangle=\langle V(x_j)\Omega,V(x_k)\Omega\rangle$$

defines a positive matrix. In Euclidean algebraic field theory this is the reflection positivity condition.[18,11]

The advantage of this more abstract characterization is that similar constructions could be made for any group G with a multiplier σ with subgroups H, on which the multiplier is totally nondegenerate, and K on which σ is trivial, such that $H\cap K=\{1\}$ and $G=HK$. In some ways the special feature of conformal field theory is that all boundaries are (more or less) equivalent. The mass m bosons in the positive z half of $\mathbf{R}^3$ with Dirichlet boundary conditions, for example, still have an obvious Green's function

$$G_{\mathbf{R}}(\mathbf{r},\mathbf{a})=\frac{e^{-m|\mathbf{r}-\mathbf{a}|}}{4\pi|\mathbf{r}-\mathbf{a}|}-\frac{e^{-m|\mathbf{r}-\tilde{\mathbf{a}}|}}{4\pi|\mathbf{r}-\tilde{\mathbf{a}}|},$$

where $\tilde{\mathbf{a}}$ is the reflection of $\mathbf{a}$ in the plane $z=0$. However, the same Dirichlet problem in the unit sphere has Green's function

$$G_C(\mathbf{r},\mathbf{a})=\frac{e^{-m|\mathbf{r}-\mathbf{a}|}}{4\pi|\mathbf{r}-\mathbf{a}|}-\frac{e^{-m\lambda|\mathbf{r}-\tilde{\mathbf{a}}|}}{4\pi\lambda|\mathbf{r}-\tilde{\mathbf{a}}|},$$

where $\tilde{\mathbf{a}}$ is now the inverse of $\mathbf{a}$ with respect to the sphere, and $\lambda=|\mathbf{a}|$, so that this nonconformally invariant system has rather different forms of Green's function for the two boundaries.

III. BOUNDARY STATES FOR ALGEBRAS

We may encode the effect of the boundary on the conformal Lie algebra by defining the map

$$\alpha_\kappa[L(X)+\tilde{L}(Y)]=L(X^\kappa)+\tilde{L}(Y^\kappa).$$

From the properties of κ it is clear that α_κ is an antilinear involution, and, using the same argument as in the alternative proof of Lemma 2.1, α_κ is an additive and multiplicative $*$-homomorphism. It is therefore an antilinear automorphism.

Returning to the general situation, we write $\mathcal{A}_+$ for the algebra of fields in S, $\mathcal{A}_-$ for those on $\tilde{S}$, and Ω for the boundary state in a space on which both algebras operate. We assume that an involutory antilinear $*$-isomorphism $\alpha_\kappa:\mathcal{A}_+\to\mathcal{A}_-$ can be associated with the geometric involution κ. We shall sometimes write $\alpha_\kappa(a)=\tilde{a}$. This can be extended to an involution α_κ of the algebras generated by $\mathcal{A}_+$ and $\mathcal{A}_-$ by defining $\alpha_\kappa|_{\mathcal{A}_-}=\alpha_\kappa^{-1}|_{\mathcal{A}_-}$. A boundary state Ω_κ is required to satisfy

$$a^*\Omega_\kappa=\alpha_\kappa(a)\Omega_\kappa,$$

for all $a\in\mathcal{A}_+$, and since α_κ is an involution, the same applies to the whole algebra generated by $\mathcal{A}_+$, and $\mathcal{A}_-$.

We have seen that these relations hold when $\mathcal{A}_+$ is the enveloping algebra of one copy of the Virasoro algebra and $\mathcal{A}_-$ the other, or when $\mathcal{A}_+$ and $\mathcal{A}_-$ are suitable group algebras for the corresponding groups. However, there are other examples such as the massless free fermion theory which is the continuum limit of the Ising model[10,16] (see Appendix B). Fermion theories are described by canonical anticommutation relation algebras CAR(W) over a complex inner product space W, and are generated by creation operators $c(w)$, depending linearly on $w\in W$, and their adjoint annihilation operators, satisfying the canonical anticommutation relations

$$[c(w)^*,c(z)]_+=\langle w,z\rangle 1,\quad [c(w),c(z)]_+=0.$$

References 10 and 16 describe the boundary states in terms of a Bogoliubov transformation K. This would normally be given in terms of Bogoliubov operators A (linear) and B (antilinear) on W, which would be thought of as defining an automorphism of the CAR algebra:

$$c_{(A,B)}(w)=c(Aw)-c(Bw)^*.$$

The conditions for this to be an automorphism ($c_{(A,B)}$ and c satisfy the same anticommutation relations) can be written as

$$A^*A+B^*B=1,\quad A^*B+B^*A=0.$$

When A is invertible we may introduce the antilinear operator $Z=BA^{-1}$ and rewrite the second condition as $Z+Z^*=0$. The connection with the Ishibashi states comes from the observation that the condition $c_{(A,B)}(w)^*\Omega=0$ (for all $w\in W$) defining a Fock vacuum Ω, can be rewritten as

$$c(w)^*\Omega=c(Zw)\Omega,$$

which looks like an Ishibashi condition with $\alpha_\kappa(c(w))=c(Zw)$.

The problem with this approach is that in the case of the Ising model Z is not a Hilbert–Schmidt operator, and so (by the Shale–Stinespring criterion[20]) the Bogoliubov transformation is not implementable, as the papers acknowledge, so that Ω does not lie in the same representation space as the Fock vacuum for c. However, in this case the space W decomposes into $W_+ \oplus W_-$, the orthogonal direct sum of two subspaces, corresponding to the two sides of the boundary and the Ishibashi criterion is needed not for all $w\in W$, but only for w in the subspace W_+. This provides an alternative interpretation of the condition on Ω.

Suppose that (as happens in the example) A maps each of $W_\pm$ to itself, while B sends $W_\pm$ to $W_\mp$. The condition that A^*B+B^*A should vanish is now automatically satisfied on the subspace W_+, though the condition $A^*A+B^*B=1$ is still needed. We shall write $c_\pm$ for the restriction of c to $W_\pm$, and then we have $c_{(A,B)}(w)=c_+(Aw)-c_-(Bw)^*$, for $w\in W_+$. This formula is essentially the Araki–Powers–Størmer purification map,[1,19] which realizes a quasi-free state of W_+ as the restriction of a Fock state for the ''doubled'' space $W=W_+\oplus W_-$. (Quasi-free states have all their n-point correlation functions given in terms of the two-point correlation functions by the same formulas as for Fock states, for example in the fermion case by Wick's determinant formula.) Purification is generally used when Z is invertible (so that W really is a double), and Z need no longer satisfy a Hilbert–Schmidt condition. In the example of the Ising model Z is indeed invertible, and this provides a better interpretation of the Ishibashi condition.

Before stating the key result we note that this example shares with the conformal algebra the property that there are simple commutation relations between $\mathcal{A}_+$ and $\mathcal{A}_-$ (which intersect only in $\mathbf{C}1$). For the Ising model $\mathcal{A}_+=\mathrm{CAR}(W_+)$, and $\mathcal{A}_-=\mathrm{CAR}(W_-)$. We shall assume that in general we have a relation of the sort

$$a\,\alpha_\kappa(b)=\epsilon(b,a^*)\,\alpha_\kappa(b)\,a,$$

with $\epsilon(b,a^*)\in\mathbf{C}$, for all $a,b\in\mathcal{A}_+$. [In the case of the Virasoro algebra $\epsilon(a,b)$ is identically 1, and for homogeneous elements of the CAR algebra of degrees $d(a)$ and $d(b)$ it is $(-1)^{d(a)d(b)}$.] For consistency we now require

$$\alpha_\kappa(ab)\Omega_\kappa=b^*a^*\Omega_\kappa=b^*\alpha_\kappa(a)\Omega_\kappa=\epsilon(a,b)\alpha_\kappa(a)b^*\Omega_\kappa=\epsilon(a,b)\alpha_\kappa(a)\alpha_\kappa(b)\Omega_\kappa,$$

suggesting that κ should satisfy $\alpha_\kappa(ab)=\epsilon(a,b)\alpha_\kappa(a)\alpha_\kappa(b)$. In practice algebras such as the Virasoro and CAR algebras are graded and we can use this formula as a way of generating the whole algebra from its degree one subspace, which is where the condition on Ω_κ is initially given.

When the algebra and its image enjoy a commutation relation of this sort they generate the algebra $\mathcal{A}=\mathcal{A}_+\alpha_\kappa(\mathcal{A}_+)$. One can, if so desired, generalize the notion of crossed product to this setting and work with the crossed product $\langle\kappa\rangle\bowtie\mathcal{A}$ of the algebra $\mathcal{A}_+\alpha_\kappa(\mathcal{A}_+)$ by the group $\langle\kappa\rangle\cong\mathbf{Z}_2$ generated by κ.

IV. TOMITA–TAKESAKI THEORY

We now turn to a very important property of Ω_κ, which does not seem to have been given much prominence. In the presence of a boundary the algebras are doubled due to reflection, and we have seen how this doubling can be interpreted as a version of the Araki–Powers–Størmer (APS) purification construction. (This already links it to numerous quite different physical situations where quasi-free states appear naturally, as, for example, for systems at nonzero temperatures.)

The cyclic vector of the quasi-free states constructed by nontrivial doubling is usually also separating, that is $a\Omega=0$ for $a\in\mathcal{A}_+$ only if $a=0$. In fact this is easy to prove directly.

Theorem 4.1: Suppose that $\mathcal{A}_+$, α_κ, ϵ are as above, and that $\mathcal{H}$ is a module for $\mathcal{A}_+\alpha_\kappa(\mathcal{A}_+)$. If there exists a cyclic vector Ω_κ satisfying $\alpha_\kappa(a)\Omega_\kappa=a^*\Omega_\kappa$ for all $a\in\mathcal{A}_+$, then it is cyclic and separating for $\mathcal{A}_+$.

Proof: The commutation property for $\mathcal{A}_+$ and $\alpha_\kappa(\mathcal{A}_+)$ permits us to order any product of elements of $\mathcal{A}_+$ and $\mathcal{A}_-$ with the elements of $\mathcal{A}_+$ to the left, and those of $\mathcal{A}_-$ to the right. If Ω_κ is a cyclic vector for the double algebra then the space is the closure of the span of products acting on Ω_κ. Now, any element of $\mathcal{A}_-$ has the form $\alpha_\kappa(a)$ for $a\in\mathcal{A}_+$, and, if $\alpha_\kappa(a)\Omega_\kappa = a^*\Omega_\kappa$ for all $a\in\mathcal{A}_+$, then this can be replaced by $a^*\Omega_\kappa$. Using the commutation property a^* can be taken to the left of the other elements of $\mathcal{A}_-$ acting on Ω_κ, and the process repeated until we have only elements of $\mathcal{A}_+$ acting on Ω_κ, showing that $\mathcal{A}_+$ also generates the whole space from Ω_κ. We could have argued similarly that Ω_κ is also cyclic for $\mathcal{A}_-$, which is equivalent to its being separating for $\mathcal{A}_+$. (For if $a\Omega_\kappa=0$ for $a\in\mathcal{A}_+$, then for any $b\in\mathcal{A}_+$ we have

$$a\alpha_\kappa(b)\Omega_\kappa = \epsilon(b,a^*)\alpha_\kappa(b)a\Omega_\kappa = 0,$$

and, since Ω_κ is also cyclic for $\mathcal{A}_-$, this shows that a annihilates the whole space, so that $a=0$.) □

We may now define the Tomita operator $S_\kappa : a\Omega_\kappa \mapsto a^*\Omega_\kappa$, for $a\in\mathcal{A}_+$. By definition S_κ is an involution and fixes Ω_κ, but also

$$S_\kappa a S_\kappa b\Omega_\kappa = S_\kappa a b^*\Omega_\kappa = b a^*\Omega_\kappa = b\alpha_\kappa(a)\Omega_\kappa = \alpha_\kappa(a)b\Omega_\kappa,$$

showing that $\alpha_\kappa(a)=S_\kappa a S_\kappa$. Thus we may obtain an action of the crossed product by sending κ to S_κ.

We have already noted that a cyclic separating vector is precisely what is needed to justify the state-operator correspondence, since there is a one-to-one correspondence between algebra elements $a\in\mathcal{A}_+$ and the vectors $a\Omega_\kappa$. (This has long been known in quantum field theory in the context of the Reeh–Schlieder theorem. A similar connection between cyclic separating vectors and reflection properties has been used purely as a mathematical tool in Ref. 15.) In Tomita–Takesaki theory this correspondence is used to give the algebra an inner product $\langle a,b\rangle = \langle a\Omega_\kappa, b\Omega_\kappa\rangle$ with respect to which it is a left Hilbert $*$-algebra.[24,7,8,23] (This is a $*$-algebra, which is also an inner product space, such that the map $a\mapsto a^*$ is closable, the left multiplication action of the algebra on itself defines a bounded nondegenerate $*$-representation.) In conformal field theory one tends to work with the much smaller algebra of primary fields. This has the advantage of giving a much smaller Frobenius algebra, but loses other structure such as the adjoint.

Tomita–Takesaki theory gives us far more than this. The operator S_κ, defined earlier, has a polar decomposition with positive part given by the positive linear operator $\Delta_\kappa = S_\kappa^* S_\kappa$, and antiunitary part $J_\kappa = S_\kappa \Delta_\kappa^{-1/2}$, which is also an involution. (The association of boundary states to antiunitary operators has been noted in a somewhat different form by Watts. One can construct a representation of the cross product by mapping κ to S_κ, but when $\Delta_\kappa\neq 1$ this is not antiunitary, and so one does not obtain a $*$-representation.) It is then known that the state defined by Ω satisfies the KMS condition at inverse temperature 1, with respect to the one-parameter unitary automorphism group $a\mapsto a_t = \Delta^{it} a \Delta^{-it}$ that is

$$\langle \Omega, ab\Omega\rangle = \langle \Omega, b\Delta a\Delta^{-1}\Omega\rangle.$$

It is also known that J defines a spatial anti-isomorphism between $\mathcal{A}_+$ and its commutant $\mathcal{A}_+'$ (the operators on the space $\mathcal{A}_+\Omega$ which commute with $\mathcal{A}_+$), that is $\mathcal{A}_+' = J\mathcal{A}_+ J^{-1}$. [In the Ising model the commutant is a modified version of CAR(W_-).] In fact J is also an involution. In conformal theories it can be considered as representing κ in a unitary–antiunitary representation of the conformal group extended by κ.

V. SYMMETRIES OF THE SYSTEM

Usually the physical algebra will also have symmetries, acting as automorphisms, as, for example, the conformal group acts as automorphisms of the CAR algebra. We can then form the crossed product of the symmetry group and algebra. For boundary theories it makes sense to

consider a group G which contains the symmetry group G_0 as a normal subgroup of index 2, where we think of G as the extension of G_0 by the addition of the boundary involution κ. The group G_0 acts by automorphisms α_g of $\mathcal{A}_+$ and elements of the nontrivial coset in G/G_0 by antilinear automorphisms. For consistency the map $g \mapsto \alpha_g$ is a homomorphism, which means that $\alpha_\kappa \alpha_g \alpha_\kappa = \alpha_{\kappa g \kappa}$.

The $*$-representations of the crossed product algebra correspond naturally to covariant representations (V, π) consisting of a projective representation V of the group and a $*$-representation π of the algebra, which satisfy $V(g)\pi(a) = \pi(\alpha_g(a))V(g)$.

Lemma 5.1: Let (V, π) be a covariant representation of $(G, \mathcal{A}_+)$, with consistency between the involutions in the sense that $\alpha_\kappa \alpha_g \alpha_\kappa = \alpha_{\kappa g \kappa}$, and suppose that there is a unique generalized Ishibashi vector Ω_κ for $\mathcal{A}_+$. Then Ω_κ is also an eigenvector for G.

Proof: Using the covariance condition in the form $V(g)\pi(a)^* = \pi(\alpha_g(a))^* V(g)$, we therefore have

$$\pi(\alpha_g(a))^* V(g)\Omega_\kappa = V(g)\pi(a)^*\Omega_\kappa = V(g)\pi(\alpha_\kappa(a))\Omega_\kappa = \pi(\alpha_g\alpha_\kappa(a))V(g)\Omega_\kappa.$$

When $g \in G_\kappa$ this can be written as $\pi(\alpha_\kappa\alpha_g(a))V(g)\Omega_\kappa$. Replacing $\alpha_g(a)$ by a gives

$$\pi(a)^* V(g)\Omega_\kappa = \pi(\alpha_\kappa(a))V(g)\Omega_\kappa,$$

so that by uniqueness $V(g)\Omega_\kappa$ is a multiple of Ω_κ, showing that Ω_κ also defines a boundary state for G. □

VI. LEFT HILBERT ALGEBRAS

Unfortunately, although our reinterpretation of the boundary states avoids the infinities caused by nonimplementable Bogoliubov transformations, it still does not banish non-normalizable vectors completely. (There are other ways of circumventing this problem, for example using Connes' composition of correspondences.[27])

In diagonalizable minimal conformal field theories the representation space for the conformal group $G = H \times H$ decomposes into a finite number of copies of spaces equivalent to $\mathcal{H}_V \otimes \mathcal{H}_V^*$, where V is an irreducible σ-representation of H on $\mathcal{H}_V$, and V^* denotes the dual representation on the dual space $\mathcal{H}_V^*$, defined by $V^*(x)f = f \circ V(x)^{-1} = f \circ V(x)^*$. We may identify $\mathcal{H}_V \otimes \mathcal{H}_V^*$ with the Hilbert–Schmidt operators $\mathcal{L}_{\mathrm{HS}}(\mathcal{H}_V)$ on $\mathcal{H}_V$, and the projective representations V and $\tilde{V}$ as the natural left and right actions on operators. Identifying the boundary state Ω_κ with a linear operator it must satisfy

$$\Omega_\kappa = V(g)\tilde{V}(g^\kappa)\Omega_\kappa = V(g)\Omega_\kappa V(g)^{-1},$$

so that, by irreducibility, Ω_κ is a multiple of the identity, which (for infinite-dimensional V) is not Hilbert–Schmidt, so that Ω_κ is not normalizable.

The situation is somewhat analogous to the Peter–Weyl theory for compact groups, where the $H \times H$ representation space $L^2(H)$ decomposes into a direct sum of $\mathcal{L}_{\mathrm{HS}}(\mathcal{H}_V)$ for irreducible V, and the Plancherel theorem tells us that the δ function at the identity of H is the sum of multiples of the identity in each component, except that in this case the V are finite-dimensional. In fact, the similarity can be taken much further, if we recall that the conformal group is a direct product group $H \times H$, with $H = \mathrm{Diff}^+(S^1)$, and the subgroup $G_\kappa = \{(x, x^\kappa) : x \in H\}$ is almost a diagonal subgroup. Were we dealing with a square-integrable representation, the fact that Ω_κ is fixed by G_κ would tell us that the projective representation of G is contained in that induced by the trivial representation of G_κ. [A vector ψ in the representation space defines a function $g \in G \mapsto \psi'(g) = \langle g \cdot \Omega, \psi \rangle$. Since Ω is fixed by $h \in G_\kappa$, we have $\psi'(gh) = \sigma(g,h)\psi'(g)$, showing that ψ' satisfies the equivariance condition for the induced representation space, and for square-integrable representations the map $\psi \mapsto \psi'$ is unitary up to a scalar factor.] In practice this does not make sense because $G/G_\kappa \cong H$ is not locally compact so we lack a quasi-invariant measure needed for

the usual inducing construction. However, it formally resembles the construction of the projective representation of $H\times H$ induced from the diagonal subgroup. This would act on $L^2(G/G_\kappa)\cong L^2(H)$, and is the product of the left regular σ and right regular $\overline{\sigma}$-representations of H, giving a very clear analogy with the Peter–Weyl theory.

Fortunately Tomita theory was devised precisely to provide a remedy for the absence of a cyclic separating vector by using only a left Hilbert algebra. One can still define the antilinear map S as the closure of $S(a)=a^*$, and $\Delta=S^*S$, $J=S\Delta^{-1/2}$. Then $\langle b^*,a^*\rangle=\langle Sb,Sa\rangle=\langle a,\Delta b\rangle$ for a positive operator Δ. As well as the obvious relation $(ab)^*=b^*a^*$ we may set $(ab)^*=\tilde{a}b^*$. It follows that

$$\widetilde{(ab)}c^*=[(ab)c]^*=[a(bc)]^*=\tilde{a}(bc)^*=\tilde{a}\tilde{b}c^*$$

and $\widetilde{ab}=\tilde{a}\tilde{b}$, so that we have an antilinear homomoprhism $a\mapsto\tilde{a}$ as before. Moreover,

$$\tilde{a}c^*b^*=\tilde{a}(bc)^*=(abc)^*=c^*(ab)^*=c^*\tilde{a}b^*,$$

where $\tilde{a}$ commutes with $\mathcal{A}_+$. When the algebra has an identity $1=1^*$ then

$$a^*1=a^*=\tilde{a}1,$$

showing that $\Omega=1$ is a generalized Ishibashi vector, and we may think of the algebra as consisting of the $a\Omega$.

This is the situation in which we find ourselves in the case of the Hilbert–Schmidt operators. In our case with our non-normalizable state being a multiple of the identity it is clear that we should just take the Hilbert–Schmidt operators as the left Hilbert algebra.

In this case, since

$$\langle b^*,a^*\rangle=\mathrm{tr}(b^{**}a^*)=\mathrm{tr}(a^*b)=\langle a,b\rangle,$$

we see that the modular operator is in this case $\Delta_V=1$. This means that S_V is itself antiunitary, providing a slightly different perspective on Watts' identification of boundary states with antiunitary maps.[6] This contrasts with the case of the free fermion model discussed earlier, where Δ is certainly not 1. At first sight this contradicts the fact that this is also a conformal model. However, those fermions were on $\mathbf{R}$ not the circle as in the minimal conformal model.

One immediate consequence of the fact that S_κ is antiunitary is that we can extend our projective representation U of the conformal group to a unitary–antiunitary representation of the group which includes κ, by setting $U(\kappa)=J_\kappa=S_\kappa$. The standard Tomita–Takesaki theory tells us that $\mathcal{A}'_+=J_\kappa\mathcal{A}_+J_\kappa$, and since $\mathcal{A}'_+=\mathcal{A}_-$, this shows explicitly that the quantum action of κ interchanges the quantum algebras of observables inside and outside the boundary.

VII. MULTIPLE BOUNDARIES

Similar methods can be applied when a region has several boundaries. For example, when there are two boundaries associated with involutions κ_1 and κ_2, one has to look for a state Ω which is an eigenvector for the elements of $G_{\kappa_1,\kappa_2}=G_{\kappa_1}\cap G_{\kappa_2}$. This subgroup can also be thought of as $G_{\kappa_1}\cap G_{\kappa_1\kappa_2}$, that is the subgroup of G_{κ_1} which commutes with the holomorphic transformation $\kappa_1\kappa_2$. In classical conformal problems there are two common approaches to problems in a wedge with angle π/N. One is to calculate the Green's function using the images of the various products of reflections in its two boundaries. The other is to carry out the conformal transformation $z\mapsto z^N$ which maps the wedge to the half-plane where the Green's function is already known (using a single image). The approach we have been using shows a simple connection between these, by producing the transformation which simplifies the problem. In fact, the holomorphic functions invariant under $\kappa_1\kappa_2$ form a ring of holomorphic functions of a new variable which is the transform of z.

As examples we consider regions bounded by two straight lines. There are two cases to consider, the case when the lines meet in a point, which we take to be 0, and the case when they are parallel in the finite plane. In the first case we denote by κ_θ the reflection in the half-line of complex numbers with argument θ. This takes z to $e^{2i\theta}\overline{z}$, and so the product $\kappa_\theta\kappa_0$ associated with the wedge where the argument lies in $(0,\theta)$ is the rotation which takes z to $e^{2i\theta}z$. When $\theta=\pi/N$ this rotation has finite order N. By considering the Laurent expansion, any holomorphic function which is invariant under such rotations must be a function of z^N. The map $z\mapsto z^N$ is precisely the map from the wedge to the half-plane.

The other possibility for a region bounded by two straight lines is the strip between two parallel lines. For definiteness let us take the strip where the imaginary part of z lies in $(0,1/2\,\beta)$. Reflection in the upper line takes z to $\overline{z}+i\beta$, and the product of the two reflections maps z to $z+i\beta$. Again we see that the holomorphic functions invariant under this transformation are holomorphic functions of $\exp(2\pi z/\beta)$, so that this time we have recovered the transformation $z\mapsto\exp(2\pi z/\beta)$ which maps the strip to the half plane.

In a region with multiple boundaries one has involutions J_{κ_i} representing the different involutions and the map $\kappa_i\kappa_j$ is represented by the linear operator $J_{\kappa_i}J_{\kappa_j}$. In the example of the strip, double reflection of the upper half-plane maps it to a subset of itself, and accordingly $J_{\kappa_i}J_{\kappa_j}$ gives an endomorphism of the algebra $\mathcal{A}_+$. This is very similar in form to the Longo canonical endomorphism of $\mathcal{A}_+$ defined by its image subalgebra.[17] (That is in some ways more like the case when $\beta=0$, but with two different algebras sharing the same boundary.)

ACKNOWLEDGMENTS

M.S. is grateful to INDAM and to EPSRC, which funded parts of this work.

APPENDIX A: THE UNRUH EFFECT IN CONFORMAL FIELD THEORY

Sewell showed how to understand the Unruh effect in terms of KMS states.[22,26] This also shows the role of the Rindler horizon in providing a boundary between two space–time algebras. There is also a direct conformal field theory argument for the effect, modeled on an argument in Ref. 4.

The world line of an observer with uniform acceleration a in a fixed direction is given in terms of the proper time τ by

$$(ct,x)=\frac{c^2}{a}(\sinh(a\tau/c),\cosh(a\tau/c)),$$

and this motivates the use of Rindler coordinates

$$(ct,x)=\frac{c^2}{a}e^{a\xi/c^2}(\sinh(a\tau/c),\cosh(a\tau/c)).$$

We may rewrite the transformation as

$$x\pm ct=\frac{c^2}{a}\exp(a(\xi\pm c\tau)/c^2).$$

This suggests, on performing a Wick rotation $t\mapsto it$, the conformal transformation $z=c^2/a\,\exp(a\zeta/c^2)$, from $\zeta=\xi+ic\tau$ to $z=x+ict$. We calculate that $dz/d\zeta=\exp(a\zeta/c^2)$.

Suppose now that the field $\phi(z)$ has typical Fock correlation functions

$$\langle\phi(z_1)^*\phi(z_2)\rangle=|z_1-z_2|^{-2h},$$

and conformal weight (h,h), so that on transforming to the new coordinates

$$\langle \phi(\zeta_1)^* \phi(\zeta_2) \rangle = ac^{-2} |e^{ha\zeta_1/c^2} e^{ha\zeta_2/c^2}| |e^{a\zeta_1/c^2} - e^{a\zeta_2/c^2}|^{-2h}$$
$$= ac^{-2} |e^{a(\zeta_1-\zeta_2)/c^2} - e^{-a(\zeta_1-\zeta_2)/c^2}|^{-2h}.$$

Now the last expression is unchanged by the translation $\zeta_1 \mapsto \zeta_1 + i2\pi c^2/a$, which in terms of the original problem involves adding $i\pi c/a$ to τ_1. Such a periodicity in imaginary time is the KMS condition at inverse temperature $\beta = 2\pi c/a$, thus giving the Unruh effect.

APPENDIX B: THE CONTINUUM ISING MODEL

It is known that the Ising model has a continuum limit (as the lattice spacing goes to 0), which is described by a canonical anticommutation relation algebra over the complex inner product space $W = \mathcal{S}(\mathbf{R})$ (the Schwartz functions), and one has the smeared creation and annihilation operators

$$c(w) = \int w(x) a^*(x)\, dx, \quad c(w)^* = \int \overline{w(x)} a(x)\, dx.$$

In the case studied in Refs. 10 and 16 the boundary at $x = 0$ separates the positive real axis, which is the physically interesting part of the space, from its mirror image. Denoting by $c(w_+)$ the operator which creates the fermion state w_+ on the physically interesting side of the boundary, it turns out that the boundary state Ω_κ satisfies $c(w_+)^* \Omega_\kappa = c(Kw_+)\Omega_\kappa$, for a certain operator K, mostly simply expressed in terms of the Fourier transform $\mathcal{F}W_+(p)$ by $(\mathcal{F}Kw_+)(p) = K(p)(\mathcal{F}w_+)(-p)$, where $K(p) = -ip/(E_p \pm m)$, $E_p = \sqrt{p^2+m^2}$ and the sign depends on the type of boundary condition. (Reference 10 expresses K in terms of the rapidity θ rather than $p = m \tanh \theta$.) This fits our previous framework with $\alpha_\kappa(c(w_+)) = c(Kw_+)$.

Subtleties arise because the algebra is represented on the standard Fock–Dirac space generated by a vacuum killed by creators of negative energy states and by annihilators of positive energy states, so that there is a second boundary in momentum space, the Fermi level of the free Dirac theory. Here the boundary separates positive from negative energies, and, as above, the Dirac vacuum state Ω is killed by creators of negative energy states and by annihilators of positive energy states. The annihilators of negative energy states $c(w_-)^*$ are then reinterpreted as creators of a positron $\tilde{c}(\mathcal{C}w_-)$ ($\mathcal{C}$ being charge conjugation), and the defining identity $c(w_-)^*\Omega = \tilde{c}(\mathcal{C}w_-)\Omega$ can be interpreted as another example of the same class.

As mentioned in Sec. III,[10,16] try to interpret K in terms of a Bogoliubov transformation with $K = Z = BA^{-1}$. However, the operator K^*K can be considered as the integral operator with the distributional kernel $k(p,q) = |K(p)|^2 \delta(p-q)$, from which it is obvious that the Hilbert–Schmidt norm

$$\mathrm{tr}(K^*K) = \int_{\mathbf{R}} k(p,p)\, dp$$

diverges, and so the Bogoliubov transformation is not implementable.

Since K is normal, the condition $A^*A + B^*B = 1$ reduces to $(AA^*)^{-1} = 1 + K^*K$, so we take

$$A = (1+K^*K)^{-1/2} : W_+ \to W_+, \quad B = KA : W_+ \to W_-.$$

The adjoint antilinear map $K^* : W_- \to W_+$ can be similarly used to extend the operators A and B to W_- by defining

$$A = (1+K^*K)^{-1/2} : W_- \to W_-, \quad B = -K^*A : W_- \to W_+.$$

(It can be shown that this choice is essentially unique.[21]) Then for $w \in W$ we set $c_K(w) = c(Aw) - c(Bw)^*$.

The Fock vacuum vector Ω_κ, killed by the annhilation operators $c_K(w)^*$, therefore satisfies

$$0=c_K(A^{-1}w_+)^*\Omega_\kappa=c(w_+)^*\Omega_\kappa-c(Kw_+)\Omega_\kappa,$$

giving the required image condition on Ω_κ. [There is a second condition that

$$0=c_K(A^{-1}w_-)^*\Omega_\kappa=c(w_-)^*\Omega_\kappa+c(K^*w_-)\Omega_\kappa,$$

from which we deduce that $c(w_-)^*\Omega_\kappa=-c(K^*w_-)\Omega_\kappa$ for all $w_-\in W_-$.]

As mentioned in Sec. III, the restriction to CAR(W_+) of the state defined by Ω_κ is quasi-free. The injection of W_+ into the double W is given by $I_Kw_+=Aw_++Bw_-$.

It is now easy to compute S at the one particle level, since we have

$$Sc(w_+)\Omega_\kappa=c(w_+)^*\Omega_\kappa=c(Kw_+)\Omega_\kappa$$

and, since S is an involution,

$$Sc(w_-)^*\Omega_\kappa=c(K^{-1}w_-)\Omega_\kappa.$$

Similarly, we have

$$Sc(w_-)\Omega_\kappa=-c(K^*w_+)\Omega_\kappa,\quad Sc(w_+)^*\Omega_\kappa=-c(K^{*-1}w_+)\Omega_\kappa.$$

Thus on the one-particle space S has the matrix form

$$S\sim\begin{pmatrix}0&K^{-1}&0&0\\K&0&0&0\\0&0&0&-K^{*-1}\\0&0&-K^*&0\end{pmatrix},$$

giving

$$\Delta\sim S^*S=\begin{pmatrix}K^*K&0&0&0\\0&(KK^*)^{-1}&0&0\\0&0&KK^*&0\\0&0&0&(K^*K)^{-1}\end{pmatrix}.$$

Thus in this case there is a nontrivial modular operator, and S is not antiunitary.

It is well known that the KMS condition facilitates the calculation of correlation functions. For example, we have

$$\begin{aligned}\langle c(w_+)^*c(z_+)\rangle&=\langle c(z_+)\Delta c(w_+)^*\Delta\rangle\\&=\langle c(z_+)c(K^*Kw_+)^*\rangle=\langle K^*Kw_+,z_+\rangle-\langle c(K^*Kw_+)^*c(z_+)\rangle,\end{aligned}$$

so that $\langle c((1+K^*K)w_+)^*c(z_+)\rangle=\langle K^*Kw_+,z_+\rangle$, and

$$\langle c(w_+)^*c(z_+)\rangle=\langle(1+K^*K)^{-1}K^*Kw_+,z_+\rangle.$$

This illustrates the fact that this interpretation of the boundary states also provides a useful tool for calculation.

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Stochastic Wess–Zumino–Novikov–Witten model on the torus

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(Received 24 April 2003; accepted 30 June 2003)

We define the Brownian motion on a torus group. We define the stochastic integral of a one-form over each canonical cycle of the torus and the stochastic integral on a two-form over the torus. We cannot apply martingale theory in order to define these stochastic integrals. We define a stochastic cohomology in the Chen–Souriau sense of the torus group, which allows us to define the stochastic Wess–Zumino term on the torus group. We show that it is related to the stochastic holonomy over a stochastic line bundle on the loop group. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1614870]

I. INTRODUCTION

Let us recall Segal's axioms of conformal field theory. Consider the set of possibly disconnected Riemann surfaces Σ with analytic parametrization p_i, $i \in I$ of the boundary loops, negative (positive) for $i \in I_-$ (I_+) and with a Riemannian surface agreeing with the conformal structure of Σ, trivial around the boundary. Let us fix an Hilbert space H with an antiunitary involution P.

Segal's axioms: A real conformal field theory is an assignment

$$(\Sigma, p_i, g) \to A(\Sigma, p_i, g), \tag{1.1}$$

where

$$A(\Sigma, p_i, g): \otimes_{i \in I_-} H \to \otimes_{i \in I_+} H \tag{1.2}$$

are trace-class operators (empty tensor are equal to C) satisfying to the following properties.

Property 1: If (Σ, p_i, g) is the disjoint union of $(\Sigma^\alpha, p^\alpha_{i_\alpha}, g^\alpha)$, then

$$A(\Sigma, p_i, g) = \otimes_\alpha A(\Sigma^\alpha, p^\alpha_{i_\alpha}, g^\alpha). \tag{1.3}$$

Property 2: If we reverse the sense of the time in p_{i_0}, we get another loop called $\tilde{p}_{i_0}$ and if $i_0 \in I_+$, then

$$(A(\Sigma, \tilde{p}_{i_0}, p_{i'}, g) x_{i_0} \otimes x, y) = (A(\Sigma, p_i, g) x, P x_{i_0} \otimes y) \tag{1.4}$$

with $i' \neq i_0$, $x \in \otimes_{i \in I_-} H$, $y \in \otimes_{i \in I_+ - i_0} H$.

Property 3: If F is a conformal diffeomorphism from Σ^1 into Σ^2, then

$$A(\Sigma^1, p^1_i, F^* g^2) = A(\Sigma^2, F \circ p^1_i, g^2). \tag{1.5}$$

Property 4: If Σ' is obtained from Σ by identifying the boundary loops $i_1 \in I_-$ and $i_2 \in I_+$, then

$$A(\Sigma', p'_i, g) = \mathrm{Tr}_{i_1, i_2} A(\Sigma, p_i, g), \tag{1.6}$$

where i' is different from i_1 and i_2 and Tr_{i_1, i_2} is the trace between factors i_1 and i_2 in the tensor product of H.

Property 5: If $\tilde{\Sigma}$ is the complex conjugate of Σ, then

$$A(\tilde{\Sigma},p_i,g)=A(\Sigma,p_i,g)^*. \tag{1.7}$$

Property 6: If σ is a real smooth function on Σ vanishing in a neighborhood of $\partial\Sigma$, then

$$A(\Sigma,p_i,\exp[\sigma]g)=\exp\left[\frac{ci}{24\pi}\int_\Sigma(1/2\partial\sigma\wedge\bar{\partial}\sigma+R_g\sigma)\right]A(\Sigma,p_I,g), \tag{1.8}$$

where R_g is the curvature form of g and c is a positive constant.

These axioms as it is noticed by Gawedzki (Ref. 24, pp. 106–107) may be deduced from the physicists intuitive representation of the amplitudes A by formal functional integrals. H is a space of functions over the loop space LM of a finite dimensional space M. P consists on the time reversing on LM combined with the complex conjugation. The amplitudes A are represented as formal integrals over maps $\psi:\Sigma\to M$ fixed on $\partial\Sigma$ (we refer to Refs. 9, 24, 25, 19, and 63 for surveys):

$$\int_{\psi\circ p_i=f_i}\mathrm{d}\mu(\psi)=\int_{\psi\circ p_i=f_i}\exp[-I(\psi)]\mathrm{d}D(\psi)=A(\Sigma,p_i,g)(f_i), \tag{1.9}$$

where $\mathrm{d}D(\psi)$ is the formal Lebesgue measure over the sets of maps ψ and $I(\psi)$ the energy of the map ψ.

Felder–Gawedzki–Kupiainen[23] have introduced a line bundle over the loop space of the compact manifold M and have said that the Hilbert space of the theory is the Hilbert space of section of this line bundle over the loop space. A particularly interesting case is when the surface Σ is a torus. In such case, we consider the double loop space, and by property 4, the theory should be related to the trace of the semi-group associated to the amplitude when we consider cylinders.

Moreover, if we consider a finite dimensional spin manifold M, the index of the Dirac operator D over M is equal to an integral over the loop space of M. There are several approaches of it. One can use probability, and we refer to the survey of Léandre[33] for various proofs of the Index theorem by using probability, including Bismut's proof. The second approach uses physicists supersymmetric paths integrals, and we refer to the works of Rogers[58,59] for a rigorous approach to supersymmetric proofs of physicists of the Index theorem.

Over the loop space, the index of the Dirac–Ramond operator should be an integral over the loop space of the loop space,[68,60] that is an integral over random tori. This integral should be the partition function of the supersymmetric nonlinear σ-model. We refer to the two surveys of Léandre[41,42] for a beginning of Index theory over the loop space.

In the case where the manifold is the linear space R^n, (1.9) is a Gaussian measure, which corresponds to the free field measure. Since in two dimensions, the Green kernel associated to the diagonal has a singularity on the diagonal, the random field associated to (1.9) is in fact a random distribution (see Refs. 51, 64, and 26): the random field is very irregular. It is difficult to state what is a distribution with values in a curved manifold, because the notion of distribution is linear.

If $\Sigma=[0,1]\times[0,1]$, there is another process indexed by Σ with values in R, which is the Brownian sheet and which is continuous (as a matter of fact, the Brownian sheet is only Hoelder). $(\partial^2/\partial s\partial t)\psi$ is the white noise over $[0,1]\times[0,1]$. On Σ, there is a natural order, and it is possible after the works of Cairoli[14] to study the stochastic differential equation in Itô meaning:

$$\delta_{s,t}x_{s,t}=A(x_{s,t})\,\delta_{s,t}\psi \tag{1.10}$$

by using martingale theory, where A is a vector field over R. This gives an example of a non-Gaussian random field parametrized by the square. In the Gaussian case, this gives the Brownian motion over the flat path space. Doss and Dozzi[20] have studied the formal action which is associated to (1.10), that is they have studied the large deviation theory. Léandre and Russo[46] studied

the behavior of the density of the solution $x_{s,t}$ of (1.10) when $(s,t)\to(0,0)$ by using the Malliavin calculus over the Brownian sheet.[54] Norris[52] has succeeded to give a geometrical meaning to (1.10) and has constrained $x_{s,t}$ to live over a curved manifold.

But it is difficult to generalize (1.10) to the case where the world sheet is not the square $[0,1]\times[0,1]$, because (1.10) uses the multiparameter martingale theory.

Airault–Malliavin in a series of papers (some of them are published, for instance, in Ref. 1) have constructed the Brownian motion over a loop group. For that, they use the Brownian motion in a Sobolev space with values in the Lie algebra of the Lie group G. This gives a random field indexed by the cylinder $[0,1]\times S^1$ into G. Various works were done later (see Ref. 18, for instance). Fang and Zhang[22] have studied the formal action which is associated to the Brownian motion over a loop group, that is they have performed the large deviations theory. The action is hyperbolic with contrast of (1.9). In the case of the flat Brownian sheet on $[0,1]\times[0,1]$, the Gaussian measure is given formally by

$$\mathrm{d}\nu(\psi)=\frac{1}{Z}\exp\left[-\int_{[0,1]\times[0,1]}\left|\frac{\partial^2}{\partial s\,\partial t}\psi(s,t)\right|^2\mathrm{d}s\,\mathrm{d}t\right]\mathrm{d}D(\psi), \tag{1.11}$$

where $\mathrm{d}D(\Psi)$ is the formal Lebesgue measure over the fields. Airault–Malliavin equation gives the Brownian motion over the loop group unlike the construction of the Ornstein–Uhlenbeck process over a loop space constructed by using the theory of Dirichlet forms, which gives another process (see Refs. 2, 21, 41, and 45).

Infinite-dimensional diffusion processes over infinite-dimensional manifolds have a long history initiated by Kuo[32] in 1972. The Russian school has studied infinite dimensional processes over infinite dimensional manifolds (see Refs. 4, 18, and 5). We refer to Ref. 3 too for a theory of stochastic processes over Hilbert manifolds.

Brzezniak–Elworthy[11] have done a general theory of infinite dimensional manifolds over M-type-2 Banach spaces. The interest of M-type-2 Banach spaces is that there is a Doob inequality for martingales over them. They apply their theory to the case of the free loop space of a manifold. This produces random cylinders with values in a compact Riemannian manifold, or the Brownian motion with values in the loop space of a Riemannian manifold. The cylinders are only Hoelder.

Brzezniak–Léandre[13] have extended the construction of Ref. 11 to the case where we consider Brownian pants. The world sheet has two output circle boundaries and one input circle boundary. This gives an application from $E_c\otimes E_c$ into E_c, where E_c is the Banach space of bounded continuous functions over the loop space. This means that the Brownian pants are Feller. This gives an approach to one of Segal's axiom of conformal field theory,[61] the Hilbert space of the loop space being replaced by the Banach space of continuous functionals over it.

Felder–Gawedzki–Kupiainen[23] have introduced a line bundle over the loop space in order to understand the Hilbert space associated to the loop space, by using Deligne cohomology. This Hilbert space should be the Hilbert space of sections of this line bundle.

Léandre[44] has considered random pants. The exit loops are random and Hoelder. The starting loop is a point. This defines a measure over the product of exit loop spaces, instead of a formal measure as in Ref. 23 or in Ref. 25. Reference 44 applies the apparatus of Ref. 35 to define a line bundle over the product of exit loop spaces, with fiber almost surely defined. Therefore, Ref. 44 defines the random parallel transport of an element of this line bundle. This leads to the definition of two parameters stochastic integrals over a pant. Reference 33 gives a stochastic analogous of the considerations of Ref. 23 with Hilbert spaces, instead of Banach spaces as in Ref. 13.

Reference 44 gives a generalization of Ref. 12, where the authors were considering a diffusion over C^1 loop space endowed with a true line bundle. The parallel transport of an element of this line bundle over the random diffusion paths was studied in Ref. 12 and leads to two parameters integrals, the internal time integral of the loop being a ordinary integral and the propagation time integral of the loop being stochastic.

The construction of Felder–Gawedzki–Kupiainen was done in order to understand the so-called Wess–Zumino–Novikov–Witten model. In (1.10), we replace $\mathrm{d}\mu(\psi)$ by

$$d\mu_k(\psi) = \exp\left[-I(\psi) + 2i\pi k \int_V \omega \right] dD(\psi), \tag{1.12}$$

where V is a volume with boundary ψ, ω is the canonical three-form over M which is supposed to be a compact simple simply connected Lie group and k is an integer.

In this work, we are motivated by the case where Σ has no boundary, and is a torus T^2 in order to simplify the exposition. This means, we try to consider a trace in infinite dimension instead of considering the semigroup as it is motivated by Segal's axiom.

First of all, we construct a measure over the torus group $T^2(G)$, where G is a Lie group. For that, we consider the Brownian motion over the torus group, by considering Brzezniak–Elworthy equation,[11] where we consider the Brownian motion with values in a convenient Sobolev space of functions from T^2 into Lie(G). This increases the number of parameters: there are two parameters which come from the torus and one parameter which comes from the propagation of an element of the Torus group. We get the heat kernel measure over the torus group. This measure is invariant under the natural action of T^2 over $T^2(G)$.

The stochastic Wess–Zumino–Novikov–Witten model on the torus requires that one understand the topological Wess–Zumino term $\int_V \omega$. This requires that one understand what are the set of Z-valued one-form over the space of random tori. It is the purpose of Sec. V of this work. We give a definition of a stochastic differential calculus for the space of random tori in the manner of Chen–Souriau, and we show that the stochastic cohomology groups in the Chen–Souriau sense of the space of random tori are equal to the determinsitic de Rham cohomology groups of the space of Hoelder maps $g(\bullet): T^2 \to G$ [we suppose that $T^2(G)$ is connected]. This gives a two-dimensional analogous to the stochastic Chen–Souriau calculus over the loop space of Léandre.[34,36–40,47] This allows us to define a general stochastic Wess–Zumino term over the torus group.

Moreover, over T^2, there are two natural parameters s and t, which leads to a family of circles $S_t: s \to (s,t)$. We suppose that the free loop group $L(G)$ is simply connected. Since there are line stochastic integrals over the circle S_t, we can define a family of stochastic line bundles ξ_t over the loop group. We define the stochastic parallel transport $\tau_{0,t}$ from ξ_0 to ξ_t along the path in the loop group $t \to \{s \to g(s,t)\}$ where $g(\bullet,\bullet)$ is an element of $T^2(G)$. This leads to a two-dimensional stochastic integral over the torus (we refer to the works of Pipiras–Taqqu[56] for an analogous approach of stochastic integrals for the fractional Brownian motion. (See Refs. 27, 43, and 44 for analogous approaches.) The main theorem of this paper is the following.

Theorem I.1: We find

$$\exp\left[2i\pi k \int_V \omega \right] = \mathrm{Tr}\, \tau_{0,1}. \tag{1.13}$$

This corresponds to a stochastic extension to the works of Konno[30] in the classical case, i.e., the case where we consider the smooth torus group instead of strong Hoelder torus group. In the classical case, Konno constructed a line bundle ξ_t over the loop group of loop $s \to g(s,t)$, and considered the parallel transport $\tau_{0,t}$ (surely defined unlike in our case, where the stochastic parallel transport is almost surely defined) along the path $t \to \{s \to g(s,t)\}$ and showed that $\mathrm{Tr}\, \tau_{0,1} = \exp[2i\pi \int_V \omega]$ surely. In the classical case, (1.13) is true surely, instead to be true only almost surely as in Theorem I.1.

This paper presents another point of view to construct random surfaces. It corresponds to a query of P. Lévy to construct nonlinear random surfaces.

We refer to the two surveys of Léandre[41,42] about analysis over loop space and mathematical physics.

We thank B. Julia and C. Schweigert for valuable comments.

We thank the Centre Emile Borel, Institut Henry Poincaré, where this work was done at the occasion of an activity about string theory.

II. BROWNIAN TORI IN A LIE GROUP

We consider a compact Lie group G of dimension d, equipped of its bi-invariant Riemannian metric. The scalar product over Lie G is denoted by $\langle,\rangle$. We can imbed it isometrically in a special orthogonal group.

Let $T^2=S^1\times S^1$ be the two-dimensional torus. $(s,t)=S$ denotes one of its elements. We consider the Hilbert space of maps $\gamma(S)$ from T^2 into Lie(G) endowed with the following metric:

$$\|\gamma\|^2_{T^2}=\int_{T^2}|\gamma(S)|^2\,dS+\int_{T^2}\left\langle\frac{\partial}{\partial s}\gamma(S),\frac{\partial}{\partial s}\gamma(S)\right\rangle dS+\int_{T^2}\left\langle\frac{\partial}{\partial t}\gamma(S),\frac{\partial}{\partial t}\gamma(S)\right\rangle dS$$
$$+\int_{T^2}\left\langle\frac{\partial^2}{\partial s\,\partial t}\gamma(S),\frac{\partial^2}{\partial s\,\partial t}\gamma(S)\right\rangle dS<\infty. \tag{2.1}$$

By using an integration by parts formula, we can show that

$$\|\gamma\|^2_{T^2}=\int_{T^2}\langle\gamma(S),(-\partial^2/\partial s^2+1)(-\partial^2/\partial t^2+1)\,\gamma(S)\rangle dS$$

such that the operator of the theory is $L=(-\partial^2/\partial s^2+1)(-\partial^2/\partial t^2+1)$ instead to be the Laplacian over T^2 as it would be the case in quantum field theory.

We consider the Brownian motion with values in the maps from the torus into Lie G, with reproducing kernel given by (2.1). Let us denote by $t\to B_t(\bullet)$ this infinite-dimensional Brownian motion. We choose the Hilbert space structure (2.1) in order to simplify the exposition.

Namely, let us consider the free loop space of Lie G endowed with the Hilbert structure

$$\|\gamma\|^2_{S^1}=\int_0^1|\gamma(s)|^2\,ds+\int_0^1|\gamma'(s)|^2\,ds. \tag{2.2}$$

We can find an element $e(s)$ of this Hilbert space such that

$$\gamma(0)=\langle\gamma,e\rangle_{S^1}, \tag{2.3}$$

where $e(s)=\lambda\exp[-s]+\mu\exp[s]$ for $0\leqslant s\leqslant 1$ such that $e(0)=e(1)$ but $e'(0)\neq e'(1)$. Since this Hilbert structure is invariant under the natural rotation of a loop, we have

$$\gamma(t)=\langle\gamma,e(\bullet-t)\rangle_{S^1}. \tag{2.4}$$

Let us consider the map $E(S)=e(s)e(t)$. From the Hilbert structure chosen in (2.1), we get if γ is a map from the torus in Lie(G) that

$$\gamma(0)=\langle\gamma,E\rangle_{T^2} \tag{2.5}$$

and since the metric (2.1) is invariant by translation

$$\gamma(S)=\langle\gamma,E(\bullet-S)\rangle_{T^2}. \tag{2.6}$$

[We worked as if we were in R instead of Lie(G) in order to simplify the exposition.]

$t\to B_t(S)$ is a finite-dimensional Brownian motion with covariance $\|E(\bullet-S)\|^2_{T^2}$. The correlation between $B_\bullet(S)$ and $B_\bullet(S')$ is given by $\langle E(\bullet-S),E(\bullet-S')\rangle_{T^2}=E(S'-S)$. (If we suppose we work in R. In the other case, we look coordinates by coordinates.)

Let us write $S=(s,t)$ and $S'=(s+\Delta s,t+\Delta t)$. We have

$$B_\bullet(S')-B_\bullet(S)=B_\bullet(s+\Delta s,t+\Delta t)-B_\bullet(s,t+\Delta t)+B_\bullet(s,t+\Delta t)-B_\bullet(s,t). \tag{2.7}$$

We deduce, since the random field $(u,S)\to B_u(S)$ is Gaussian, that

$$\|B_u(S')-B_u(S)\|_{L^p}^p \leqslant C\sqrt{|\Delta s|}^p + C\sqrt{|\Delta t|}^p. \tag{2.8}$$

We deduce by the Kolmogorov lemma (see Ref. 49) that the three-dimensional random field $(u,S)\to B_u(S)$ has an Hoelder modification.

We will construct the Brownian motion over the torus group, following the idea of Ref. 11. We consider a family of stochastic differential equations in the Stratonovitch sense:

$$\begin{aligned} \mathrm{d}_u g_u(S) &= g_u(S)\mathrm{d}_u B_u(S), \\ g_0(S) &= e. \end{aligned} \tag{2.9}$$

Theorem I.1: $(u,S)\to g_u(S)$ has almost surely a modification which is Hoelder in (u,S) for $u\leqslant 1$.

Proof: We convert the equation in Itô meaning. We find another linear equation. We write in order to simplify the notations:

$$\begin{aligned} \delta_u g_u(S) &= g_u(S)\,\delta_u B_u(S) + C g_u(S)\mathrm{d}u, \\ g_0(S) &= e, \end{aligned} \tag{2.10}$$

where δ denotes the Itô integral.

We get

$$\begin{aligned} \delta_u(g_u(S)-g_u(S')) = (g_u(S)-g_u(S'))\,\delta_u B_u(S) + g_u(S')(\delta_u B_u(S)-\delta_u B_u(S')) + C(g_u(S) \\ - g_u(S'))\mathrm{d}u. \end{aligned} \tag{2.11}$$

By using (2.8) and the Burkholder–Davies–Gundy inequality, we deduce that for $u\leqslant 1$,

$$E[|g_u(S)-g_u(S')|^p] \leqslant C\int_0^u E[|g_v(S)-g_v(S')|^p]\mathrm{d}v + C\mathrm{d}(S,S')^{p/2}, \tag{2.12}$$

where d is the Riemannian distance on the torus.

By using Gronwall lemma, we deduce that

$$E[|g_u(S)-g_u(S')|^p] \leqslant C\mathrm{d}(S,S')^{p/2} \tag{2.13}$$

fou $u\leqslant 1$. Moreover, clearly,

$$E[|g_u(S)-g_{u'}(S)|^p] \leqslant |u-u'|^{p/2}. \tag{2.14}$$

We deduce the theorem by using Kolmogorov lemma (Ref. 49). □

We can consider the law μ of the random map $S\to g_1(S)$ over the torus group $T^2(G)$. We can consider the torus group $T^2_{\epsilon,*}(G)$ (see Sec. V for details) of maps $g(\bullet)$ from the torus T^2 into G such that

$$\lim_{S\to S'} \frac{\mathrm{d}(g(S),g(S'))}{\mathrm{d}(S,S')^{\epsilon}} = 0 \tag{2.15}$$

uniformly over the torus when $S\to S'$. We can find a ϵ such that by the previous theorem, μ is a measure over $T^2_{\epsilon,*}(G)$.

Moreover, since the Hilbert structure (2.1) is invariant under translation in the torus T^2, the law μ is invariant under translation for T^2.

III. LINE INTEGRALS

We get two families of random loops in the group deduced from the random field $g(S)$. The first family is the family of loops given by $s \to g(s,t)$ where we fix t and the second one is given by $t \to g(s,t)$ when we fix s. Let ω be a one form over G. We would like to define the Stratonovitch line integral,

$$A_t^1 = \int_0^1 \langle \omega(g(s,t)), \mathrm{d}_s g(s,t) \rangle \tag{3.1}$$

and the Stratonovitch line integral

$$A_s^2 = \int_0^1 \langle \omega(g(s,t)), \mathrm{d}_t g(s,t) \rangle, \tag{3.2a}$$

where ω is a one-form over G conveniently extended in a one form over R^N, if G is imbedded in R^N.

Since the computations in all the cases are similar, we will consider only the case of A_0^1.

Let $\mathrm{d}B_u$ be a Brownian motion with values in the Lie algebra of G. We consider the solution of the stochastic differential equation which gives the Brownian motion starting from e in the Lie group G:

$$\mathrm{d}_u g_u = g_u \, \mathrm{d}_u B_u \, . \tag{3.2b}$$

The equation of the differential of the stochastic flow associated to (3.2b) is given by (see Refs. 29, 31, and 6):

$$\mathrm{d}_u \phi_u = \phi_u \, \mathrm{d}_u B_u \tag{3.3}$$

and the inverse of the differential of the flow is given by an analogous equation.

Let us consider a finite-dimensional family $B_u(\alpha)$ of Brownian motions in the Lie algebra of G, depending smoothly of a finite-dimensional parameter α where $B_u(\alpha)$ lives in a finite-dimensional family of Brownian motions. We consider the stochastic differential equation depending on a parameter

$$\mathrm{d}g_u(\alpha) = g_u(\alpha) \mathrm{d}B_u(\alpha). \tag{3.4}$$

The solution of Eq. (3.4) has a smooth version in the finite-dimensional parameter α. $(\partial/\partial\alpha) g_u(\alpha)$ is for instance the solution of the linear differential equation with second member

$$\frac{\partial}{\partial \alpha} g_u(\alpha) = \frac{\partial}{\partial \alpha} g_u(\alpha) \mathrm{d}B_u(\alpha) + g_u(\alpha) \mathrm{d}_u \frac{\partial}{\partial \alpha} B_u(\alpha). \tag{3.5}$$

This equation can be solved by the method of variation of constant. We get

$$\frac{\partial}{\partial \alpha} g_u(\alpha) = \phi_u(\alpha) \int_0^u \phi_v^{-1}(\alpha) \mathrm{d}_v \frac{\partial}{\partial \alpha} B_v(\alpha). \tag{3.6}$$

We will write $s \to B_\bullet(s,0) = B_\bullet(s)$, and in order to define stochastic line integrals, we will follow the method of Refs. 43 and 44, but in this case, it is much more simpler, because there is no conditioning. By using the properties of the Hilbert structure (2.1), the covariance between $B_\bullet(s)$ and $B_\bullet(s')$ is given by $e(s-s')$. Let us suppose that $0 \leqslant s \leqslant s+\Delta s \leqslant t \leqslant t+\Delta t \leqslant 1$, and let us compute the covariance of $B_\bullet(s+\Delta s) - B_\bullet(s)$ and of $B_\bullet(t+\Delta t) - B_\bullet(t)$. It is given by

$$e(s+\Delta s-t-\Delta t)-e(s-t-\Delta t)-e(s-t+\Delta s)+e(s-t)=Ce''(s-t)\Delta t\Delta s+O(\Delta t+\Delta s)^3 \tag{3.7}$$

because e is smooth over $[-1,0]\sim[0,1]$. [We use the periodicity assumption over $e(\bullet)$. The only singularity in $e(\bullet)$ comes from 0 identified to 1 in the circle.]

This shows us that we can diagonalize the four nonindependent Brownian motions $B_\bullet(s)$, $B_\bullet(s+\Delta s)$, $B_\bullet(t)$, $B_\bullet(t+\Delta t)$. We find two couples of independent Brownian motions $(w_\bullet(1),w_\bullet(2))$ and $(w_\bullet(3),w_\bullet(4))$ such that

$$\begin{aligned} B_\bullet(s)&=w_\bullet(1),\\ B_\bullet(s+\Delta s)&=\alpha(s,\Delta s)w_\bullet(1)+\beta(s,\Delta s)w_\bullet(2),\\ B_\bullet(t)&=w_\bullet(3),\\ B_\bullet(t+\Delta t)&=\alpha(t,\Delta t)w_\bullet(3)+\beta(t,\Delta t)w_\bullet(4). \end{aligned} \tag{3.8}$$

Moreover t does not belong to $[s,s+\Delta s]$, such that the covariance of $B_\bullet(s+\Delta s)-B_\bullet(s)$ and $B_\bullet(t)$ behaves as Δs because $e(s+\Delta s-t)-e(s-t)_\bullet=e'(s-t)\Delta s+O(\Delta s)^2$.

Moreover,

$$\alpha(s,\Delta s)=C+C\Delta s+O(\Delta s)^{3/2}, \tag{3.9}$$

$$\beta(s,\Delta s)=C\sqrt{\Delta s}+C\Delta s+O(\Delta s)^{3/2}, \tag{3.10}$$

because $e(s+\Delta s-s)-e(0)=e'_+(0)\Delta s=+O(\Delta s)^2$ because e has semiderivatives in 0 and $\Delta s>0$ and $B_\bullet(s+\Delta s)$ has a constant variance. From (3.7), we deduce that $\langle w_\bullet(1),w_\bullet(4)\rangle=O(\sqrt{\Delta t})$, $\langle w_\bullet(3),w_\bullet(2)\rangle=O(\sqrt{\Delta s})$ and that the correlator $\langle w_\bullet(2),w_\bullet(4)\rangle=O(\sqrt{\Delta s\Delta t})$. We remark that $(\partial/\partial\sqrt{\Delta s})\alpha(s,\Delta s)_{\Delta s=0}=0$.

We imbed G isometrically in a space of linear matrices. It follows from the previous considerations that in law

$$g_\bullet(s+\Delta s)=g_\bullet(s)+\sqrt{\Delta s}g^1_\bullet(s)+\Delta s g^2_\bullet(s)+o(\Delta s)^{3/2}, \tag{3.11}$$

where $g^1_\bullet(s)=\phi_\bullet(w_\bullet(1))\int_0^\bullet\phi_u(w_\bullet(1))^{-1}(\partial/\partial\sqrt{\Delta s})\beta(s,0)\mathrm{d}w_u(2)$. We do not write the analogous expression for $g^2_\bullet(s)$. There is a double integral in $\mathrm{d}w_\bullet(2)$ where the simple derivative of $\beta(s,\Delta)$ in $\sqrt{\Delta s}$ appear and a simple integral where the second derivative in $\sqrt{\Delta s}$ of $\alpha(s,\Delta s)$ and $\beta(s,\Delta s)$ appear. $(\bullet)$ is the time of the differential equation (2.9). Moreover, in law

$$g_\bullet(t+\Delta t)=g_\bullet(t)+\sqrt{\Delta t}g^1_\bullet(t)+\Delta t g^2_\bullet(t)+O(\Delta t)^{3/2}. \tag{3.12}$$

Let f and h be two smooth functions over the matrix space. We suppose they are bounded as well as their derivatives of all orders. We have the estimate which follows from the properties listed after (3.8), (3.9), and (3.10):

$$E[f(g_u(s))g^1_u(s)h(g_v(t))g^1_v(t)]=C(s,t)\sqrt{\Delta s\Delta t}+O(\sqrt{\Delta s}+\sqrt{\Delta t})^{3/2}, \tag{3.13}$$

where $C(s,t)$ is continuous. Namely, we conditionate by $w_\bullet(2)$ and $w_\bullet(4)$. There are terms which are $w_\bullet(1)$ and $w_\bullet(3)$ measurables in the expression we want to estimate. When we conditionate by $w_\bullet(2)$ and $w_\bullet(4)$, the expressions belong to all the Sobolev spaces of Malliavin calculus in $w_\bullet(2)$ and $w_\bullet(4)$. We can apply Clark–Ocone formula (Ref. 53) to these expressions. We deduce since $\langle w_\bullet(3),w_\bullet(2)\rangle=O(\sqrt{\Delta s})$ and $\langle w_\bullet(1),w_\bullet(4)\rangle=O(\sqrt{\Delta t})$ that the Itô integral which appears in the Clark–Ocone formula are in $O(\sqrt{\Delta s})\mathrm{d}w_\bullet(2)$ and in $O(\sqrt{\Delta t})\mathrm{d}w_\bullet(4)$. These lead to expressions of the type

$$O(\sqrt{\Delta s})\int_{[0,1]^3}\alpha(s_1,s_2,s_3)\mathrm{d}w_{s_1}(2)\mathrm{d}w_{s_2}(2)\mathrm{d}w_{s_3}(4), \tag{3.14}$$

where we used either Itô integral or Stratonovitch integral. We convert it in Skorokhod integral (whose expectation is 0) and we find a counterterm in $O(\Delta s)$ (we can suppose that $\Delta s=\Delta t$ as we will do in the sequel). For that we used the following result: let f be a smooth functional with bounded derivatives of all orders in a finite number of $g_u(s)$ or in $g_u(t)$. Let F be the associated Wiener cylindrical functional. Let $\widetilde{F}=E[F|w_\bullet(2),w_\bullet(4)]$. It is a smooth functional in the sense of Malliavin calculus in $w_\bullet(2)$, $w_\bullet(4)$ and its derivatives $D^k\widetilde{F}(t_1\ldots,t_k)$ have an estimate in $O(\sqrt{\Delta s})^k$.

We consider a smooth one-form ω_v in the spaces of matrices with bounded derivatives of all orders which depends smoothly from a finite dimensional parameter v. We suppose that the derivatives in the parameter v are bounded.

We consider 2^N, N being a big integer, and the dyadic subdivision of $[0,1]$ associated to 2^N. We call it s_i with $s_i<s_{i+1}$ such that $s_{i+1}-s_i=2^{-N}$. If $s\in[s_i,s_{i+1}]$, we call

$$g_u^N(s)=g_u(s_i)+\frac{s-s_i}{s_{i+1}-s_i}(g_u(s_{i+1})-g_u(s_i)), \tag{3.15}$$

$s\to g_1^N(s)$ is piecewise differentiable. We consider the random variable

$$A_v^N=\int_0^1\langle\omega(g_1^N(s),\mathrm{d}_s g_1^N(s)\rangle. \tag{3.16}$$

Let us give the following decomposition of A_v^N:

$$\begin{aligned}A_v^N&=\sum\int_{s_i}^{s_{i+1}}\langle\omega(g_1^N(s))-\omega(g_1^N(s_i)),\mathrm{d}_s g_s^N(s)\rangle+\sum\int_{s_i}^{s_{i+1}}\langle\omega(g_1^N(s_i),\mathrm{d}_s g_s^N(s)\rangle\\&=A_v^N(\langle,\rangle)+A_v^N(\delta).\end{aligned} \tag{3.17}$$

The Itô term is $A_v^N(\delta)$ and the Stratonovitch counterterm is $A_v^N(\langle,\rangle)$. The Itô term can be divided into two pieces: the first one is when in (3.11) we take the term in $g_\bullet^1(s)$ and the second one is when we take in (3.12) the term in $g_\bullet^2(s)$. We get the decomposition, of the Itô term in $A_v^N(\delta_1)+A_V^N(\delta_2)$. The term which diverges *a priori* is $A_v^N(\delta_1)$. But we can use (3.12), and show that when $N\to\infty$,

$$E[A_v^N(\delta_1)^2]\to\int_{S_1\times S_1}C(s,t)\mathrm{d}s\,\mathrm{d}t+\int_{S_1}C(s)\mathrm{d}s, \tag{3.18}$$

where $C(s,t)$ is continuous.

Moreover, the second part in the Itô term checks clearly

$$E[A_v^N(\delta_2)^2]\to\int_{S_1\times S_1}C_1(s,t)\mathrm{d}s\,\mathrm{d}t+\int_{S_1}C_1(s)\mathrm{d}s. \tag{3.19}$$

Since the counterterm which is due to the Stratonovitch correction is a *a priori* less diverging, we can see in an analogous way that

$$E[A_v^N(\langle,\rangle)^2]\to\int_{S_1\times S_1}C_2(s,t)\mathrm{d}s\,\mathrm{d}t+\int_{S_1}C_2(s)\mathrm{d}s. \tag{3.20}$$

These remarks justify but do not prove the following proposition.

Proposition III.1: When $N\to\infty$, the sequence of random variables A_v^N tends in L^2 to a limit random variable called $\int_{S^1}\langle\omega_v(g_1(s)),\mathrm{d}_s g_1(s)\rangle=A_v$. Moreover, there exists a smooth version of the line integral A_v in v.

Proof: Let us forget for the moment the parameter v. Let us write

$$A^N=\sum_i \int_{[s_i,s_{i+1}]}\langle\omega(g_1^N(s)),\mathrm{d}_s g_1^N(s)\rangle=\sum (B_i^N+C_i^N), \tag{3.21}$$

where B_i^N is the bracket term

$$B_i^N=\int_{[s_i,s_{i+1}]}\langle\omega(g_1^N(s))-\omega(g_1^N(s_i)),\mathrm{d}_s g_1^N(s)\rangle \tag{3.22}$$

and C_i^N is the Itô term,

$$C_i^N=\langle\omega(g_1(s_i)),\Delta_s g_1(s_i)\rangle. \tag{3.23}$$

We write

$$C_i^N=D_i^N+E_i^N+O(2^{-3N/2}), \tag{3.24}$$

where

$$D_i^N=\sqrt{s_{i+1}-s_i}\langle\omega(g_1(s_i)),g_1^1(s_i)\rangle \tag{3.25}$$

and

$$E_i^N=(s_{i+1}-s_i)\langle\omega(g_1(s_i)),g_1^2(s_i)\rangle. \tag{3.26}$$

First step: convergence of ΣE_i^N.

In $g_1^2(s_i)$ whose writing is derived from (3.5) by taking another derivative, there is a linear integral which comes from the second derivative of $\alpha(s_i+\Delta s_i)$, from a second derivative in $\beta(s,\Delta s)$ in $\sqrt{\Delta s}$ and a double integral which comes from taking only one derivative in $\beta(s,\Delta s)$. The term in the linear integral can be treated in the following way: we get $\Sigma E_{i,1}^N$. If $M>N$,

$$\left(\sum E_{i,1}^N-\sum E_{j,1}^M\right)^2=\left(\sum_i\left(\sum_{[s-j,s_{j+1}]\subseteq[s_i,s_{i+1}]}E_{i,1}^N-E_{j,1}^M\right)\right)^2. \tag{3.27}$$

In order to compute $\Sigma_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]}E_{i,1}^N-E_{j,1}^M$, we write $s_{i+1}-s_i=\Sigma\, s_{j+1}-s_j$ such that we can write the sum to estimate

$$\sum\sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]}(s_{j+1}-s_j)(\langle\omega(g_1(s_i),\tilde{g}_1(s_i)\rangle-\langle\omega(g_1(s_j)),\tilde{g}_1(s_j)\rangle), \tag{3.28}$$

$\tilde{g}_1(s_i)$ is the term in the simple integral where we take the second derivatives in $\sqrt{\Delta s}$ of $\alpha(s,\Delta s)$ and $\beta(s,\Delta s)$. The terms which are integrated depend continuously from s. Therefore the contribution where we take two derivatives of $\alpha(s,\Delta s)$ vanish. It remains to consider the contribution where we take two derivatives of $\beta(s,\Delta s)$. We can replace the terms considered by

$$\sum_i\sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]}\langle\omega(g_1(s_i)),\overline{g}_1(s_i)\rangle-\langle\omega(g_1(s_j)),\overline{g}_1(s_j)\rangle, \tag{3.29}$$

where we have replaced the term in two derivatives by $\sqrt{\Delta s_j} B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j)$. We write $B_\bullet(s+\Delta s_i)-B_\bullet(s_i)=\Sigma\, B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j)$ and we see that $\langle B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j), B_\bullet(s_{j'}+\Delta s_{j'})-B_\bullet(s_{j'})\rangle = O(\Delta s_j \Delta s_{j'})$ if $j\neq j'$ and equal to $O(\Delta s_j)$ if $j=j'$. This shows that the L^2 norm of

$$\sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} (\langle \omega(g_1(s_i)), \overline{g_1}(s_i)\rangle - \langle \omega(g_1(s_j)), \overline{g_1}(s_j)\rangle) \tag{3.30}$$

behaves as $O(1/N)\Delta s_j$ because $\omega(g_1(s))$ depends continuously of s and after using the disintegration argument used after (3.13).

The problem arises when we take the double integral. In order to study the behavior of its sum, we can replace $w_\bullet(2)$ in (3.8) by $B_\bullet(s_i+\Delta s_i)-B_\bullet(s_i)$ and take the double stochastic integral which is associated by taking the derivative of the flow $\phi_u(s_i)$ associated to the equation $\mathrm{d}g_u(s_i)=g_u(s_i)\mathrm{d}B_u(s_i)$. Namely, we consider a double integral of the type

$$\int_{0<u<v<1} \sqrt{\Delta s_i}\phi_u^{-1}\, \mathrm{d}w_u(2)\sqrt{\Delta s_i}\phi_v^{-1}\, \mathrm{d}w_v(2), \tag{3.31}$$

which behaves modulo an error term in $O(\Delta s_i)^{3/2}$ as

$$\int_{0<u<v<1} \phi_u^{-1}\Delta_{s_i} B_u(s_i)\,\phi_v^{-1}\Delta_{s_i} B_v(s_i). \tag{3.32}$$

For the convergence of E_i^N, we can assimilate $(s_{i+1}-s_i)g_u^2(s_i)$ with the double integral $\alpha_u(s_i)$ after performing these replacements. Let $N'>N$ and s_j be the dyadic subdivision which is associated. We sum over $[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]$. We get

$$\begin{aligned}&\langle \omega(g_t(s_i)), \alpha_t(s_i))\rangle - \sum_j \langle \omega(g_t(s_j)), \alpha_t(s_j)\rangle \\ &\quad = \sum_j \left(\langle \omega(g_t(s_i))-\omega(g_t(s_j)), \alpha_t(s_j)\rangle + \left\langle \omega(g_t(s_i)), \alpha_t(s_i)-\sum_j \alpha_t(s_j)\right\rangle\right) = \delta_i^N+\epsilon_i^N.\end{aligned} \tag{3.33}$$

The sum of the first term tends to 0 in L^2. The difficult term to estimate is the term in ϵ_i^N. In the double integral which compose $\alpha_t(s_i)$, we write

$$B_\bullet(s_i+\Delta s_i)-B_\bullet(s_i)=\sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j). \tag{3.34}$$

We distribute the integrands. Over each $\mathrm{d}B_\bullet(s_i+\Delta s_i)-\mathrm{d}B_\bullet(s_i)$, there is in the double integral a term which $B_\bullet(s_i)$ is measureable, which is adapted and depends on a continuous way of s_i. Since it depends on a continuous way from s_i, we can replace it when we distribute by the corresponding term in s_j in $\alpha_t(s_i)$. After distributing in $\alpha_t(s_i)-\Sigma\alpha_t(s_j)$, the diagonal terms are substracted, and it remains to study the process

$$\delta_t^N=\sum_i \left\langle \omega(g_t(s_i)) \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}],[s_{j'},s_{j'+1}]\subseteq[s_i,s_{i+1}]j\neq j'} \int_{0<u<v<t} r_u(s_j)\mathrm{d}_u\Delta_{s_j}B_u(s_j) \right.$$
$$\left. \times r_v(s_{j'})\mathrm{d}_v\Delta_{s_{j'}}B_v(s_{j'}) \right\rangle. \tag{3.35}$$

We decompose the semimartingale δ_t^N into a finite variational part which converges by using (3.7) to 0 and a martingale part M_t^N. Namely, we can convert the double Stratonovitch integral which appears in (3.35) in an Itô integral. The boring term arises when we replace the double Stratonovitch integral by an Itô integral in (3.35). We would like to show that this martingale tends to 0. For that, we compute its quadratic variation. We get a sum over all quadruple $[s_{j_1},s_{j_1+1}]$, $[s_{j_2},s_{j_2+1}]$, $[s_{j_3},s_{j_3+1}]$, and $[s_{j_4},s_{j_4+1}]$.

First case: Let us suppose that all the elements of the quadruple are different. The contribution of each quadruple is in $2^{-4N'}$ by the properties listed after (3.8), (3.9), (3.10) which express that the covariance of $B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j)$ and of $B_\bullet(s_{j'+1})-B_\bullet(s_{j'})$ in term of $\Delta s_j\Delta s_{j'}$ and the covariance of $(B_\bullet(s_j+\Delta s_j)-B_\bullet(s_j))$ and of $B_\bullet(t)$ in Δs_j if t does not belong to $[s_j,s_{j+1}]$. Namely, if the intervals $[s_{j_1},s_{j_1+1}]$, $[s_{j_2},s_{j_2+1}]$ do not intersect and if s_{j_3} and s_{j_4} do not belong to these intervals, we have only to show by using the Itô formula that

$$E\left[\int_{0<u<v} r_u(s_{j_1})\mathrm{d}_u\Delta_{s_{j_1}}B_u(s_{j_1})\int_{0<u<v} r_u(s_{s_{j_2}})\mathrm{d}_u\Delta_{s_{j_2}}B_u(s_{j_2})r_v(s_{J_3})r_v(s_{j_4})\right]=O(\Delta s_{j_1}\Delta s_{j_2}), \tag{3.36}$$

because the right bracket between $\Delta_{s_{j_3}}B(s_{j_3})$ and $\Delta_{s_{j_4}}B(s_{j_4})$ is in $O(\Delta s_{j_3}\Delta s_{j_4})$. We take the conditional expectation of $r_v(s_{j_3})$ and $r_v(s_{j_4})$ along the Gaussian space spanned by $B_\bullet(s_{j_1})$, $B_\bullet(s_{j_2})$, $\Delta_{s_{j_1}}B(s_{j_1})$, and $\Delta_{s_{j_2}}B_\bullet(s_{j_2})$. We can suppose that $r_v(s_{j_3})$ and $r_v(s_{j_4})$ are measurable over this Gaussian space. But r_v is solution of the stochastic differential equation giving the flow of the Brownian motion over the Lie group, and is therefore a stochastic integral. We use the following rules for calculating different conditional expectation for the solution of this flow. We consider the solution of the stochastic differential equation starting from the identity

$$\mathrm{d}A_t=A_t(\mathrm{d}B_t+\mathrm{d}\tilde{B}_t), \tag{3.37}$$

where B_t and $\tilde{B}_t$ are two independent Brownian motions. We can write $A_t=W_tV_t$ where $\mathrm{d}V_t=V_t\,\mathrm{d}B_t$ and $\mathrm{d}W_t=W_tV_t\,\mathrm{d}\tilde{B}_t\,V_t^{-1}$. After using this remark in order to calculate the conditional expectation, we disintegrate along $\Delta_{s_{j_1}}B_\bullet(s_{j_1})$ and $\Delta_{s_{j_2}}B_\bullet(s_{j_2})$ as in (3.13), and we conclude by using the consideration following (3.8), (3.9), (3.10).

They are at most $2^{2N}2^{4(N'-N)}$ such possibilities. The total contribution is 2^{-2N} which tends to 0 when $N\to\infty$.

Second case: There are three different intervals $[s_j,s_{j+1}]$. This can come from a concatenation of two times d_v for $u<v$ in the stochastic integral (3.28) after converting it in a double Itô integral or a concatenation of the same term d_u in the stochastic integral (3.28). The contribution of each term is $2^{-3N'}$ by doing as in the first case. They are at most $2^N2^{(N'-N)}2^{2(N'-N)}=2^{3N'}2^{-2N}$ such possibilities. The total contribution behaves in 2^{-2N} which tends to 0 when $N\to\infty$.

Third case: There are two different intervals $[s_j,s_{j+1}]$. The contribution of each element which appears is in $2^{-2N'}$ by doing as in the first case. There are at most $2^N2^{2(N'-N)}$ such terms. The total contribution is in 2^{-N} which converges to 0 when $N\to\infty$.

This shows us that ΣE_i^N is a Cauchy sequence in L^2.

Second step: Convergence of the ltô term ΣD_i^N.

We write

$$\alpha_i^N = D_i^N - \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} D_j^{N'} \tag{3.38}$$

and we would like to show that $\Sigma \alpha_i^N \to 0$ in L^2.

There are two terms to study.

(i) The contribution of $E[\alpha_i^N \alpha_{i'}^N]$ for $i \neq i'$. By (3.13),

$$\sum_{i\neq i'} E[\alpha_i^N \alpha_{i'}^N] \to 2\int_{S^1\times S^1} C_2(s,t)\,\mathrm{d}s\,\mathrm{d}t - 2\int_{S^1\times S^1} C_2(s,t)\,\mathrm{d}s\,\mathrm{d}t = 0. \tag{3.39}$$

(ii) The contribution of $\Sigma_i E[(\alpha_i^N)^2]$. By using the consideration of the first step, we can write modulo a term which vanishes

$$\begin{aligned}\alpha_i^N &= \langle \omega(g_1(s_i)), \Delta_{s_i} g_i(s_i)\rangle - \sum_{[s_j,s_{j+1}]} \langle \omega(g_1(s_j)), \Delta_{s_j} g_1(s_j)\rangle \\ &= \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} \langle \omega(g_1(s_i)) - \omega(g_1(s_j)), \Delta_{s_j} g_1(s_j)\rangle = \sum_j \beta_j^N .\end{aligned} \tag{3.40}$$

To study its convergence, we write

$$\begin{aligned} B_\cdot(s_i) &= w_\cdot(1), \\ B_\cdot(s_j) &= \alpha(s_i,s_j) w_\cdot(1) + \beta(s_i,s_j) w_\cdot(2), \\ B_\cdot(s_j = \Delta s_j) &= \alpha(s_i,s_j,\Delta s_j) w_\cdot(1) + \beta(s_i,s_j,\Delta s_j) w_\cdot(2) + \gamma(s_i,s_j,\Delta s_j) w_\cdot(3), \\ B_\cdot(s_{j'}) &= \alpha(s_i,s_{j'}) w_\cdot(1) + \beta(s_i,s_{j'}) w_\cdot(4), \\ B_\cdot(s_{j'} + \Delta s_{j'}) &= \alpha(s_i,s_j,\Delta s_{j'}) w_\cdot(1) + \beta(s_i,s_{j'},\Delta s_{j'}) w_\cdot(4) + \gamma(s_i,s_{j'},\Delta s_{j'}) w_\cdot(5). \end{aligned} \tag{3.41}$$

We have $\gamma(s,t,\Delta t) = C(s,t)\sqrt{\Delta t} + O(\Delta t)$, $\beta(s,t,\Delta t) - \beta(s,t) = C(s,t)\Delta t + O(\Delta t)^{3/2}$, and $\alpha(s,t,\Delta t) - \alpha(s,t) = C'(s,t)\Delta t + O(\Delta t)^{3/2}$. We deduce that $\langle w_\cdot(5), w_\cdot(3)\rangle = o(\Delta s_j)$, $\langle w_\cdot(5), w_\cdot(2)\rangle = O(\sqrt{\Delta s_j})$, and $\langle w_\cdot(5), w_\cdot(1)\rangle = O(\sqrt{\Delta s_j})$. In a similar way, we have $\langle w_\cdot(3), w_\cdot(1)\rangle = O(\sqrt{\Delta s_j})$, $\langle w_\cdot(3), w_\cdot(4)\rangle = O(\Delta s_j)$ (we used the fact that $\Delta s_j = \Delta s_{j'}$). With this decomposition, we write the analogous of (3.11) and (3.12) for $g_\cdot(s_j + \Delta s_j)$ by doing the conditional expectation along the Gaussian processes $w_\cdot(5), w_\cdot(4), w_\cdot(2), w_\cdot(3)$ and for $g_\cdot(s_{j'} + \Delta s_{j'})$. We find if $j \neq j' E[\beta_j^N \beta_{j'}^N] = o(I/N) 2^{-2N'}$ and in the other cases $E[|\beta_j^N|^2] = o(1/N) 2^{-N'}$. Therefore, $E[|C_i^N|^2] = o(1/N) 2^{-N}$ and $\Sigma_i E[|C_i^N|^2] \to 0$.

Third step: Study of the convergence of ΣB_i^N.

We write

$$\omega(g_1^N(s)) - \omega(g_1(s_i)) = \frac{s - s_i}{\sqrt{s_{i+1} - s_i}} g_1^1(s_i)\alpha(g_1(s_i)) + O(s - s_i) \tag{3.42}$$

and

$$\mathrm{d}_s g_1^N(s) = \frac{\mathrm{d}s}{\sqrt{s_{i+1} - s_i}} g_1^1(s_i) + \mathrm{d}s\, g_1^2(s_i) + \mathrm{d}s\, O(s_{i+1} - s_i). \tag{3.43}$$

The more singular term in B_i^N is

$$\alpha_i^N=\int_{s_i}^{s_{i+1}}\frac{s-s_i}{s_{i+1}-s-i}\langle g_1^1(s_i),\alpha(g_1(s_i),g_1^1(s_i))\rangle \mathrm{ds}=(s_{i+1}-s_i)\langle g_1^1(s_i)\alpha(g_1(s_i)),g_1^1(s_i)\rangle. \tag{3.44}$$

There is in the previous contribution a quadratic expression in $g_1^1(s_i)$. These expressions can be treated exactly as in the first step of the convergence of ΣE_i^N, by writing $\langle g_1^1(s_i),g_1^1(s_i)\rangle$ as a double integral and replacing $(s_{i+1}-s_i)\langle g_1^1(s_i),g_1^1(s_i)\rangle$ by a double stochastic integral where we have removed $\sqrt{\Delta s_i}w_\bullet(1)$ by $\Delta_{s_i}B_\bullet(s_i)$. The sum of the others terms tends clearly to 0.

In order to show that $\int_{S^1}\langle \omega_v(g_1(s)),\mathrm{d}_s g_1(s)\rangle$ has a smooth version, we show that the system of derivatives of A_v^N in v converges in L^2. We conclude by using the embedding Sobolev theorem as in Ref. 29. □

We consider a more intrinsic approximation of the line integral. We use if $g_1(s_i,t),g_1(s_{i+1},t)$ are close,

$$F_N(s,g_1(s_i,t),g_1(s_{i+1},t))=\exp\left[\frac{s-s_i}{s_{i+1}-s_i}\log(g_1(s_{i+1},t)g_1(s_i,t)^{-1})\right]g(s_i,t) \tag{3.45}$$

conveniently extended over the set of all matrices. We set

$$\tilde{g}_1^N(s,t)=F_N(s,g_1(s_i,t),g_1(s_{i+1},t)). \tag{3.46}$$

We consider $\tilde{A}_v^N$ as in (3.15) with this new approximation. If we look at the asymptotic expansion of F_N, we see that the more singular term in $\mathrm{d}_s\tilde{g}_1^N(s,t)$ and $\mathrm{d}_s g_1^N(s,t)$ coincides. This justifies the following theorem.

Theorem III.2: $\tilde{A}_v^N$ tends in L^2 for the C^k topology over each compact of the parameter set to the Stratonovitch integral $\int_{S^1}\langle \omega_v(g(s,t)),\mathrm{d}_s g(s,t)\rangle$ which has a smooth version in v.

Remark: We do not know if the Stratonovitch integrals of Theorem III.2 and of Proposition III.1 coincide. In the sequel, we will use the version of Theorem III.1, because it is a geometrical version.

Remark: Instead of integrating over a circle, we can integrate over a segment.

IV. INTEGRAL OF A TWO FORM

We imbed G into a matrix algebra isometrically. Let $g(s,t)$ be the random field parametrized by the torus with values in G. Let 2^N be an integer, and s_i be the associated dyadic subdivision of S^1 and t_j be the associated dyadic subdivision of a copy of S^1. We consider the polygonal approximation of $g(s,t)$, if $(s,t)\in[s_i,s_{i+1}]\times[t_j,t_{j+1}]=T_{i,j}$.

$$\begin{aligned}g^N(s,t)&=g(s_i,t_j)+\frac{s-s_i}{s_{i+1}-s_i}(g(s_{i+1},t_j)-g(s_i,t_j))+\frac{t-t_j}{t_{j+1}-t_j}(g(s_i,t_{j+1})-g(s_i,t_j))\\&\quad+\frac{t-t_j}{t_{j+1}-t_j}\frac{s-s_i}{s_{i+1}-s_i}(g(s_{i+1},t_{j+1})-g(s_i,t_{j+1})-g(s_{i+1},t_j)+g(s_i,t_j))\\&=g(s_i,t_j)+\alpha_1^N(s)+\alpha_2^N(t)+\alpha_3^N(s,t).\end{aligned} \tag{4.1}$$

Let us consider a two-form ω over G, conveniently extended in a two-form ω over the matrix algebra bounded with bounded derivatives of all orders. We suppose that the two-form depends on a finite-dimensional parameter v. We consider

$$A_v^N=\int_{T^2}(g^N)^*\omega_v=\int_{S^1\times S^1}\langle \omega_v(g^N(s,t)),\mathrm{d}_s g^N(s,t),\mathrm{d}_t g^N(s,t)\rangle. \tag{4.2}$$

Let us denote by $\Delta_{t_j} g(s_i,t_j)$ the quantity $g(s_i,t_{j+1})-g(s_i,t_j)$, by $\Delta_{s_i} g(s_i,t_j)$ the quantity $g(s_{i+1},t_j)-g(s_i,t_j)$ where we have imbedded the group G in a linear space. If $i\neq i'$, $j\neq j'$, we will see later that

$$E[\Delta_{s_i} g(s_i,t_j)\Delta_{t_j} g(s_i,t_j)\Delta_{s_{i'}} g(s_{i'},t_{j'})\Delta_{t_{j'}} g(s_{i'},t_{j'})]+O(\Delta s_i \Delta t_j \Delta s_{i'}\Delta t_{j'}), \tag{4.3}$$

where we take a quadratic expression homogeneous in each term in each increment. The most diverging term in the quantity A_v^N is

$$\sum_{i,j} \langle \omega_v(g(s_i,t_j)),\Delta_{s_i} g(s_i,t_j),\Delta_{t_j} g(s_i,t_j)\rangle. \tag{4.4}$$

When the length of the subdivision tends to zero, the L^2-norm of this expression tends to

$$\int_{T^2\times T^2} C(s,t,s',t')\mathrm{d}s\,\mathrm{d}s'\,\mathrm{d}t\,\mathrm{d}t' + \int_{S^1\times T^2} C(s,t,t')\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}t'$$
$$+ \int_{T^2\times S^1} C(s,s',t)\mathrm{d}s\,\mathrm{d}s'\,\mathrm{d}t + \int_{S^1\times S^1} C(s,t)\mathrm{d}s\,\mathrm{d}t. \tag{4.5}$$

This justifies without to prove the following proposition.

Proposition IV.1: When $N\to\infty$, the traditional integral A_v^N tends for the C^k topology over each compact of the parameter space in L^2 to the stochastic integral in the Stratonovich sense:

$$\int_{T^2} g^*\omega_v = \int_{S^1\times S^1} \langle \omega(g(s,t)),\mathrm{d}_s g(s,t),\mathrm{d}_t g(s,t)\rangle, \tag{4.6}$$

where the stochastic integral $\int_{T^2} g^*\omega_v$ has a smooth version in v.

Proof: We suppose first that there is no auxiliary parameter. We can write

$$A^N = \int_{T^2} \langle \omega(g^N(s,t)),\mathrm{d}_s\alpha_1^N(s),\mathrm{d}_t\alpha_2^N(t)\rangle + \int_{T^2} \langle \omega(g^N(s,t)),\mathrm{d}_s\alpha_1^N(s),\mathrm{d}_t\alpha_3^N(s,t)\rangle$$
$$+ \int_{T^2} \langle \omega(g^N(s,t)),\mathrm{d}_s\alpha_3^N(s,t),\mathrm{d}_t\alpha_2^N(t)\rangle + \int_{T^2} \langle \omega(g^N(s,t)),\mathrm{d}_s\alpha_3^N(s,t),\mathrm{d}_t\alpha_3^N(s,t)\rangle$$
$$= A_1^N + A_2^N + A_3^N + A_4^N. \tag{4.7}$$

Step I: Convergence of A_1^N. We repeat the considerations of Sec. III for $s\to B_\bullet(s,t_j)$ and $t\to B_\bullet(s_i,t)$. If we fix t_j, we get by (3.11) an asymptotic expansion in order 3. We get expressions in the asymptotic expansion in $g_\bullet^{1;\bullet}(s_i,t_j)$, $g_\bullet^{2;\bullet}(s_i;t_j)$, and $g^{3;\bullet}(s_i,t_j)$. If we fix s_i, we go in (3.11) to an asymptotic expansion at order 3. We get derivatives in law $g_\bullet^{\bullet;1}(s_i,t_j)$, $g^{\bullet;2}(s_i,t_j)$, and $g_\bullet^{\bullet;3}(s_i,t_j)$.

We get

$$A_1^N = \sum_{i,j} \langle \omega(g(s_i,t_j)),g(s_{i+1},t_j)-g(s_i,t_j),g(s_i,t_{j+1})-g(s_i,t_j)\rangle$$
$$+ \sum_{i,j} \int_{T_{i,j}} \langle \omega(g^N(s,t))-\omega(g(s_i,t_j)),\mathrm{d}_s\alpha_1^N(s),\mathrm{d}_t\alpha_2^N(t)\rangle$$
$$= B_1^N + B_2^N, \tag{4.8}$$

B_1^N is the Itô term, which is apparently the most diverging when $N\to\infty$. B_2^N is the Stratonovitch counterterm.

Step I.1: Convergence of the Itô term B_1^N.

We write as in (3.11),

$$g(s_{i+1},t_j)-g(s_i,t_j)=\sqrt{s_{i+1}-s_i}g^{1;\bullet}(s_i,t_j)+(s_{i+1}-s_i)g^{2;\bullet}(s_i,t_j)+(s_{i+1}-s_i)^{3/2}g^{3;\bullet}(s_i,t_j)+O(s_{i+1}-s_i)^2 \tag{4.9}$$

and we write as in (3.11),

$$g(s_i,t_{j+1})-g(s_i,t_j)=\sqrt{t_{j+1}-t_j}g^{\bullet;1}(s_i,t_j)+(t_{j+1}-t_j)g^{\bullet;2}(s_i,t_j)+(t_{j+1}-t_j)^{3/2}g^{\bullet;3}(s_i,t_j)+O(s_{i+1}-s_i)^2. \tag{4.10}$$

This will lead to stochastic integrals in $\sqrt{s_{i+1}-s_i}g^{1;\bullet}(s_i,t_j)$ and in $\sqrt{t_{j+1}-t_j}g^{\bullet;1}(s_i,t_j)$ which apparently do not converge and to integrals in $(s_{i+1}-s_i)g^{2;\bullet}(s_i,t_j)$ as in $(t_{j+1}-t_j)g^{\bullet;2}(s_i,t_j)$ which will lead to classical integrals. We deduce the following decomposition of the Itô term B_1^N:

$$B_1^N=C_1^N+C_2^N+C_3^N+C_4^N+C_5^N+\text{error}. \tag{4.11}$$

(i) C_1^N is the double stochastic integral in the time direction s and in the time direction t,

$$C_1^N=\sum_{i,j}\sqrt{\Delta s_i}\sqrt{\Delta t_j}\langle\omega(g(s_i,t_j)),g^{1;\bullet}(s_i,t_j),g^{\bullet;1}(s_i,t_j)\rangle. \tag{4.12}$$

(ii) C_2^N is a stochastic integral in the direction s and a classical integral in the direction t,

$$C_2^N=\sum_{i,j}\sqrt{\Delta s_i}\Delta t_j\langle\omega(g(s_i,t_j)),g^{1\bullet}(s_i;t_j),g^{\bullet;2}(s_i;t_j)\rangle. \tag{4.13}$$

(iii) C_3^N is a vanishing term,

$$C_3^N=\sum_{i,j}\sqrt{\Delta s_i}\Delta t_j^{3/2}\langle\omega(g(s_i,t_j)),g^{1;\bullet}(s_i,t_j),g^{\bullet;3}(s_i,t_j)\rangle+\sum_{i,j}(\Delta s_i)^{3/2}\sqrt{\Delta t_j}\langle\omega(g(s_i,t_j)),g^{3;\bullet}(s_i,t_j),g^{\bullet;1}(s_i,t_j)\rangle. \tag{4.14}$$

(iv) C_4^N is a classical integral in the time direction s and a stochastic integral in the time direction t,

$$C_4^N=\sum_{i,j}\Delta s_i\sqrt{\Delta t_j}\langle\omega(g(s_i,t_j)),g^{2;\bullet}(s_i,t_j),g^{\bullet;1}(s_i,t_j)\rangle. \tag{4.15}$$

(v) C_5^N is a classical integral in the time direction s and in the time direction t,

$$C_5^N=\sum_{i,j}\Delta s_i\Delta t_j\langle\omega(g(s_i,t_j)),g^{2;\bullet}(s_i,t_j),g^{\bullet;2}(s_i,t_j)\rangle. \tag{4.16}$$

C_1^N is the more *a priori* divergent term when N tends to ∞ and C_5^N will lead to a double classical integral on the torus.

Step I.1.1: For integers N, N' such that $N'>N$, we consider $C_1^N=\Sigma_{i,j}C_{i,j,1}^N$.

We consider a bigger integer N' than N and we consider

$$D_{i,j,1}^{N'}=C_{i,j,1}^N-\sum_{T_{i',j'}\subseteq T_{i,j}}C_{i',j',1}^{N'}. \tag{4.17}$$

Let us consider first the case where $0\leqslant s+\Delta s\leqslant s'\leqslant s'+\Delta s'\leqslant 1$ and $0\leqslant t+\Delta t\leqslant t'\leqslant t'+\Delta t'\leqslant 1$. We get if f and g are smooth functions with bounded derivatives of all orders

$$E[f(g(s,t))h(g(s',t'))g^{1;\bullet}(s,t)g^{\bullet;1}(s,t)g^{1;\bullet}(s',t')g^{\bullet;1}(s',t')]$$
$$= C(s,t,s',t')\sqrt{\Delta s}\sqrt{\Delta t}\sqrt{\Delta s}\sqrt{\Delta t'} + \text{error}. \tag{4.18}$$

In order to see that, we begin by diagonalizing $B_\bullet(s,t)$ and $B_\bullet(s',t')$.

$$B_\bullet(s,t) = w_\bullet(1). \tag{4.19}$$

We write

$$\begin{aligned} B_\bullet(s+\Delta s,t) &= \alpha(s,t,\Delta s)w_\bullet(1) + \beta(s,t,\Delta s)w_\bullet(3), \\ B_\bullet(s,t+\Delta t) &= \alpha(s,t,\Delta t)w_\bullet(1) + \beta(s,t,\Delta t)w_\bullet(4), \end{aligned} \tag{4.20}$$

and the analogous formulas for $B_\bullet(s'+\Delta s',t')$ and $B_\bullet(s',t'+\Delta t')$ with some other new auxiliary Brownian motions $w_\bullet(5)$ and $w_\bullet(6)$. Moreover

$$\alpha(s,t,\Delta s) = C + C\sqrt{\Delta s} + C\Delta s^{3/2} + O(\Delta s)^2 \tag{4.21}$$

and

$$\beta(s,t,\Delta s) = C\sqrt{\Delta s} + C\Delta s + C(\Delta s)^{3/2} + O(\Delta s)^2 \tag{4.22}$$

the same asymptotic results being true when we reverse the role of *s, t.*

The main result is the following:

$$\langle B_\bullet(s+\Delta s,t) - B_\bullet(s,t), B_\bullet(u,v)\rangle = O(\Delta s) \tag{4.23}$$

if u does not belong to $]s,s+\Delta s[$, the same equality being true if we reverse the role of s and t. We use the fact that the Green kernel associated to the two-dimensional problem is the product of the Green kernels associated to the one-dimensional problem by the remark following (2.5).

Moreover,

$$\langle B_\bullet(s+\Delta s,t) - B_\bullet(s,t), B_\bullet(u,v+\Delta v) - B_\bullet(u,v)\rangle = O(\Delta s \Delta v). \tag{4.24}$$

It is equal, namely, to

$$\begin{aligned} &e(s+\Delta s-u)e(t-v-\Delta v) - e(s-u)(t-v-\Delta v) + e(s+\Delta s-u)e(t-v) - e(s_u)e(t-v) \\ &\quad = (e(s+\Delta s-u) - e(s-u))(e(t-v-\Delta v) - e(t-v)), \end{aligned} \tag{4.25}$$

if u does not belong to $]s,s+\Delta s[$ and t does not belong to $]v,v+\Delta v[$. Moreover,

$$\langle B_\bullet(s+\Delta s,t) - B_\bullet(s,t), B_\bullet(s'+\Delta s',u) - B_\bullet(s',u)\rangle = O(\Delta s \Delta s') \tag{4.26}$$

if $]s',s'+\Delta s'[\cap]s,s+\Delta s[= 0$ by analogous reasons, and using the fact that the Green kernel associated to $B_\bullet(s,t)$ is the products of the one-dimensional Green kernels.

In order to simplify the exposure, we write $\Delta t = \Delta t' = \Delta s = \Delta s'$. We conditionate $B_\bullet(s,t)$ and $B_\bullet(s',t')$ by $w_\bullet(3)$, $w_\bullet(4)$, $w_\bullet(5)$, $w_\bullet(6)$. We use the formula (3.38) in order to compute this conditionating for $g(s,t)$ and $g(s',t')$, and after the Clark–Ocone formula (see Ref. 53) in order to compute the conditional of $h(g(s,t))$ as an Itô integral in $w_\bullet(3)$, $w_\bullet(4)$, $w_\bullet(5)$, and $w_\bullet(5)$ with term bounded by $\sqrt{\Delta s}$ by (4.23). We get to take the expectation of the product of four Itô integrals or five or six. We can estimate its expectation by using the Itô formula and (4.24), (4.25) by applying iteratively the Itô formula and the Clark–Ocone formula. We reduce iteratively the length of the iterated integral we have to compute. The same result holds by the same arguments for

$$E[f(g(s,t'))h(g(s',t))g^{1;\bullet}(s,t')g^{\bullet;1}(s,t')g^{1;\bullet}(s',t)g^{\bullet;1}(s',t)]$$
$$= C(s,t,s',t')\sqrt{\Delta s}\sqrt{\Delta t}\sqrt{\Delta s'}\sqrt{\Delta t'} + \text{error} \tag{4.27}$$

if we suppose that $\Delta s = \Delta s' = \Delta t = \Delta t'$.

We deduce from the previous considerations that

$$E\left[\sum_{i\neq:i';j\neq j'} D^{N'}_{i,j,1}D^{N'}_{i',j',1}\right] \to 2\int_{T^4} C(s,t,s',t')\,ds\,dt\,ds'\,dt' - 2\int_{T^4} C(s,t,s',t')\,ds\,dt\,ds'\,dt' = 0. \tag{4.28}$$

Let us now study the behavior of

$$E\left[\sum_{i,j\neq j'} D^{N'}_{i,j,1}D^{N'}_{i,j',1}\right] \tag{4.29}$$

when $N' \to \infty$.

By the previous considerations, the contributions of the $T_{k,l}$ strictly interior to $T_{i,j}$ and of the $T_{k',l'}$ strictly interior to $T_{i,j'}$ vanish. Therefore, it is enough to study the contribution of

$$C^{1,N'}_{i,j,1} = \sqrt{\Delta s_i}\sqrt{\Delta t_j}\langle \omega(g(s_i,t_j)), g^{1;\bullet}(s_i,t_j), g^{\bullet;1}(s_i;t_j)\rangle$$
$$- \sum_{i'} \sqrt{\Delta s_{i'}}\sqrt{\Delta t_j}\langle \omega(g(s_{i'},t_j)), g^{1;\bullet}(s_{i'},t_j), g^{\bullet;1}(s_{i'},t_j)\rangle \tag{4.30}$$

for $[s_{i'}, s_{i'+1}] \subseteq [s_i, s_{i+1}]$. We would like to show that $E[\Sigma_{i,j\neq j'} C^{1,N'}_{i,j,1} C^{1,N'}_{i,j',1}]$ tends to 0 when $N' \to \infty$. We will see later (see step I.1.2, step I.1.3, and step I.1.4) that we can replace $\sqrt{\Delta s_i} g^{1;\bullet}(s_i,t_j)$ by $\Delta_{s_i} g(s_i,t_j)$ and $\sqrt{\Delta t_j} g(s_i,t_j)$ by $\Delta_{t_j} g(s_i,t_j)$. It is enough therefore to consider the behavior of

$$C^{2,N'}_{i,j,1} = \langle \omega(g(s_i,t_j)), \Delta_{s_i} g(s_i,t_j), \Delta_{t_j} g(s_i,t_j)\rangle - \sum_{i'} \langle \omega(g(s_{i'},t_j)), \Delta_{s_{i'}} g(s_{i'},t_j), \Delta_{t_j} g(s_{i'},t_j)\rangle \tag{4.31}$$

and to show that $E[\Sigma_{i,j\neq j'} C^{2,N'}_{i,j,1} C^{2,N'}_{i,j',1}]$ tends to 0.

But

$$\sum \Delta_{s_{i'}} g(s_{i'},t_j) = \Delta_{s_i} g(s_i,t_j). \tag{4.32}$$

Therefore

$$C^{2,N'}_{i,j,1} = \sum \langle \omega(g(s_i,t_j)) - \omega(g(s_{i'},t_j)), \Delta_{s_{i'}} g(s_{i'},t_j), \Delta_{t_j} g(s_i,t_j)\rangle$$
$$+ \sum \langle \omega(g(s_{i'},t_j)), \Delta_{s_{i'}} g(s_{i'},t_j), \Delta_{t_j} g(s_i,t_j) - \Delta_{t_j} g(s_{i'},t_j)\rangle = C^{3,N'}_{i,j,1} + C^{4,N'}_{i,j,1}. \tag{4.33}$$

By using the techniques of the next steps, we can replace $\Delta_{s_{i'}} g(s_{i'},t_j)$ by $\sqrt{\Delta s_{i'}} g^{1;\bullet}(s_{i'},t_j)$ and $\Delta_{t_j} g(s_{i'},t_j)$ by $\sqrt{\Delta t_j} g^{\bullet;1}(s_{i'},t_j)$ and $\Delta_{t_j} g(s_{i'},t_j)$ by $\sqrt{\Delta t_j} g^{\bullet;1}(s_{i'},t_j)$ and $\Delta_{t_j} g(s_i,t_j)$ by $\sqrt{\Delta t_j} g^{\bullet;1}(s_i,t_j)$. We get two quantities $C^{5,N'}_{i,j,1}$ and $C^{6,N'}_{i,j,1}$.

We compute $\Sigma_{i,j\neq j'}E[(C^{5,N'}_{i,j,1}C^{5,N'}_{i,j',1})]$. There are two contributions. The first one is when we consider twice the same $s_{i'}$. There are four types of increments which appear (s_i,t_j), $(s_{i'},t_j)$, $(s_i,t_{j'})$, and (s'_i,t_jj'). We take the conditional expectation along $\Delta_{s_{i'}}B_\bullet(s_{i'},t_j)$, $\Delta_{t_j}B_\bullet(s_i,t_j)$, $\Delta_{s_{i'}}B(s_{i'},t_{j'})$, and $\Delta_{t_{j'}}B_\bullet(s_i,t_{j'})$ or more precisely along the Brownian motion which arise from the diagonalization (4.20) of the Brownian motions $B_\bullet(s_i,t_j)$, $B_\bullet(s_{i'},t_j)$, $B_\bullet(s_i,t_{j'})$, and $B_\bullet(s_{i'},t_{j'})$. The Stratonovitch integrals $g^{1;\bullet}(s,t)$ and $g^{\bullet;1}(s,t)$ are in fact Itô integrals. Moreover we can compute the conditional law of $g(s_i,t_j)$, $g(s_{i'},t_j)$, $g(s_i,t_{j'})$, $g(s_{i'},t_{j'})$ by using (3.38) and the Clark–Ocone formula to express the quantities which appear in this way as stochastic integral which are martingales and whose bracket with the others terms can be estimated by (4.20). There is a product of Martingale Itô integrals, whose expectation can be estimated by using successivly the Itô formula and the Clark–Ocone formula. We conclude by using (4.23), (4.24), and (4.26). We get that the contribution when there is one coincidence leads to a term in $O(1/N)\Delta s_{i'}\Delta t_j\Delta t_{j'}$. When there is no coincidence, we condition by $\Delta_{s_{i'}}B_\bullet(s_{i'},t_j)$, $\Delta_{t_j}B_\bullet(s_i,t_j)$, $\Delta_{s_{i''}}B_\bullet(s_{i''},t_j)$, and $\Delta_{t_j}B_\bullet(s_i,t_{j'})$, or more precisely by the Brownian motions arising from the diagonalization (4.20). We proceed as before, and we get a contribution in $o(1/N)\Delta_{s_{i'}}\Delta_{s_{i''}}\Delta_{t_j}\Delta_{t_{j'}}$ Therefore $E[\Sigma_{i,j\neq j'}C^{5,N'}_{i,j,1}C^{5,N'}_{i,j',1}]\to 0$.

By the same type of trick and performing the conditional expectation along the increment $\Delta_sB_\bullet(s,t)$ and $\Delta_tB_\bullet(s,t)$ or more precisley by conditioning along the Brownian motions which appears in the diagonalization (4.20) in $C^{6,N'}_{i,j,1}C^{6+,N'}_{i,j',1}$ and after using the Clark–Ocone formula, we see that $\Sigma_{i,j\neq j'}E[C^{6,N'}_{i,j,1}C^{6,N'}_{i,j',1}]\to 0$. The same holds for $E[\Sigma_{i,j\neq j'}C^{5,N'}_{i,j,1}C^{6,N'}_{i,j',1}]$.

Let us study the behavior of $E[\Sigma_{i,j}(D^{N'}_{i,j,1})^2]$. By the considerations which will follow in the next step, it is enough to study the behavior of

$$\begin{aligned}
&\left\langle \omega(g(s_i,t_j)),\sum \Delta_{s_{i'}}g(s_{i'},t_j),\sum \Delta_{t_{j'}}g(s_i,t_{j'})\right\rangle\\
&\quad-\sum \langle\omega(g(s_{i'},t_{j'})),\Delta_{s_{i'}}g(s_{i'},t_{j'}),\Delta_{t_{j'}}g(s_{i'},t_{j'})\rangle\\
&\quad=\Bigg\{\sum_{i',j'}\langle\omega(g(s_i,t_j)),\Delta_{s_{i'}}g(s_{i'},t_{j'}),\Delta_{t_{j'}}g(s_i,t_{j'})\rangle\\
&\qquad-\sum_{i',j'}\langle\omega(g(s_i,t_j)),\Delta_{s_{i'}}g(s_{i'},t_{j'}),\Delta_{t_{j'}}g(s_{i'},t_{j'})\rangle\Bigg\}+\sum\langle\omega(g(s_{i'},t_{j'}))\\
&\qquad-\omega(g(s_i,t_j)),\Delta_{s_{i'}}g(s_{i'},t_{j'}),\Delta_{t_{j'}}g(s_{i'},t_{j'})\rangle=\widetilde{G}^{N'}_{i,j,1}+G^{3,N'}_{i,j,1},
\end{aligned}\tag{4.34}$$

where we do the summation over $[s_{i'},s_{i'+1}]\subseteq[s_i,s_{i+1}]$ and $[t_{j'},t_{j'+1}]\subseteq[t_j,t_{j+1}]$. In $\widetilde{G}^{N'}_{i,j,1}$, we write

$$\begin{aligned}
&\Delta_{s_{i'}}g(s_{i'},t_j)\Delta_{t_{j'}}(g(s_i,t_{j'})-\Delta_{s_{i'}}g(s_{i'},t_{j'})\Delta_{t_{j'}}g(s_{i'},t_{j'})\\
&\quad=(\Delta_{s_i}g(s_i,t_j)-\Delta_{s_i}g(s_i,t_{j'}))\Delta_{t_{j'}}g(s_i,t_{j'})+\Delta_{s_{i'}}g(s_{i'},t_{j'})(\Delta_{t_{j'}}g(s_i,t_{j'})-\Delta_{t_{j'}}g(s_{i'},t_{j'})),
\end{aligned}\tag{4.35}$$

and we deduce a decomposition of $\widetilde{G}^{N'}_{i,j,1}$ into $G^{1,N'}_{i,j,1}+G^{2,N'}_{i,j,1}$. In $G^{1,N'}_{i,j,1}$, $G^{2,N'}_{i,j,1}$, and $G^{2,N'}_{i,j,1}$, we can replace $\Delta_{s_{i'}}g(_{i'},t_j)$, $\Delta_{t_{j'}}g(s_i,t_{j'})$ by $\sqrt{\Delta s_{i'}}g^{1;\bullet}(s_{i'},t_j)$ and $\sqrt{\Delta t_{j'}}g^{\bullet;1}g(s_i,t_{j'})$ and $\Delta_{s_{i'}}g(s_{i'},t_{j'})$ by $\sqrt{\Delta s_{i'}}g^{1;\bullet}(s_{i'},t_{j'})$ and $\Delta_{t_{j'}}g(s_{i'},t_{j'})$ by $\sqrt{\Delta t_{j'}}g^{\bullet;1}(s_{i'},t_{j'})$ by $\sqrt{\Delta t_{j'}}g^{\bullet;1}(s_{i'},t_{j'})$. We get $G^{3,N'}_{i,j,1}$ and $G^{4,N'}_{i,j,1}$.

We have six terms to estimate: $E[\Sigma_{i,j}(G^{1,N'}_{i,j,1})^2]$, $E[\Sigma_{i,j}(G^{2,N'}_{i,j,1})^2]$, $E[\Sigma_{i,j}(G^{3,N'}_{i,j,1})^2]$, $E[\Sigma_{i,j}G^{1,N'}_{i,j}G^{2,N'}_{i,j}]$, $E[\Sigma_{i,j}G^{1,N'}_{i,j,1}G^{3,N'}_{i,j,1}]$, $E[\Sigma\, G^{2,N'}_{i,j,1}G^{3,N'}_{i,j,1}]$. We can do the multiplication term by

term in each product that appears. In each term, we distribute another time. There are four terms where two expressions in $g^{1;\bullet}$ and $g^{\bullet;1}$ appear. We condition by the set of increments in the leading Brownian motion which appears in these expressions, or more precisely of the terms which appear after the diagonalization (4.20) in $\Delta_s B(s,t)$ and $\Delta_t B(s,t)$. We use (3.38) and the Clark–Ocone formula (see Ref. 53). We use (4.23), (4.24), and (4.26). When we develop, there is the possibility that we get exactly 4 times $s_{i'}$, $s_{i''}$, $t_{j'}$, and $t_{j''}$, which lead to a contribution in $O(1/N)\Sigma_{i'\neq i'',j'\neq j''}\Delta s_{i'}\Delta s_{i''}\Delta t_{j'}\Delta t_{j''}$. There is a contribution when there are three different s_i, $t_{j'}$, $t_{j''}$ or $s_{i'}$, $s_{i''}$, t_j which lead to a contribution in $\Sigma_{i,j'\neq j''}O(1/N)\Delta s_i\Delta t_{j'}\Delta t_{j''}$ or $\Sigma_{i'\neq i'',j}O(1/N)\Delta s_{i'}\Delta s_{i''}\Delta t_j$ and a contribution where we get only two times s_i and t_j which leads to a contribution in $\Sigma_{i,j}O(1/N)\Delta s_i\Delta t_j$. Therefore, $\Sigma_{i,j}G^{3,N'}_{i,j,1}$ tends to 0 in L^2.

By the same argument, $\Sigma_{i,j}G^{1,N'}_{i,j,1}$ and $\Sigma^{2,N'}_{i,j}$ tend to 0 in L^2. By using this type of argument, we can get the requested limits.

Step I.1.2: Study of the convergence of the terms C_2^N and C_4^N where we mix stochastic integral and classical integral.

This term is simpler to treat than the double stochastic integral, which is most diverging, which appears. But it leads to some complications, because in $g^{\bullet;2}(s,t)$, there are some double stochastic integral in the dynamical time u which appears. We write

$$C_2^N=\sum_{i,j} C^N_{i,j,2}. \tag{4.36}$$

We consider a bigger integer N' and we write

$$D^{N'}_{i,j,2}=C^N_{i,j,2}-\sum_{T_{i',j'}\subseteq T_{i,j}} C^{N'}_{i',j',2}. \tag{4.37}$$

We have the following behavior:

$$\begin{aligned}&E[f(g(s,t))h(g(s',t'))g^{1;\bullet}(s,t)g^{\bullet;2}(s,t)g^{1;\bullet}(s',t')g^{\bullet;2}(s',t')]\\&\quad=C(s,t,s',t')\sqrt{\Delta s}\sqrt{\Delta s'}+\text{error}.\end{aligned} \tag{4.38}$$

If $\Delta s=\Delta t$ and if $0\leqslant s\leqslant s+\Delta s\leqslant s'\leqslant s'+\Delta s'\leqslant 1$ and $0\leqslant t\leqslant t+\Delta t\leqslant t'\leqslant t'+\Delta t'\leqslant 1$. $C(s,t,s',t')$ is continuous. Namely, $g^{\bullet;2}(s,t)$ and $g^{\bullet;2}(s',t')$ are given by double stochastic integrals in the term $w_\bullet(3)$ or $w_\bullet(4)$ which appear in (4.20). It is the far most complicated term, the terms in simple stochastic integrals can be treated as before. We condition after by the increments $\Delta_t B_\bullet(s,t)$, $\Delta_{t'}B_\bullet(s',t')$, $\Delta_s B_\bullet(s,t)$, and $\Delta_{s'}B_\bullet(s',t')$ or more precisely by the terms which arise from the diagonalization in (4.20). We write the double Stratonovitch integral which appears in $g^{\bullet;2}(s,t)$ or $g^{\bullet;2}(s',t')$ as double Itô integral and a simple integral. After using the Clark–Ocone formula, the expectation of the product of at most eight terms and at least two Itô integrals must be computed. We use Itô formula successively and Clark–Ocone formula successively in order to get our estimate.

We have analogous formulas we do not write. Therefore,

$$E\left[\sum_{i\neq i';j\neq j'} D^{N'}_{i,j,2}D^{N'}_{i',j',2}\right]\to 2\int_{T^4}C(s,t,s',t')\mathrm{d}s\,\mathrm{d}s'\,\mathrm{d}t\,\mathrm{d}t'-2\int_{T^4}C(s,t,s',t')\mathrm{d}s\,\mathrm{d}s'\,\mathrm{d}t\,\mathrm{d}t'=0. \tag{4.39}$$

Let us study now the behavior of

$$E\left[\sum_{i,j\neq j'} D^{N'}_{i,j,2}D^{N'}_{i,j',2}\right]. \tag{4.40}$$

By the considerations which will follow, it is enough to study

$$C^{N'}_{i,j,2}=\Delta t_j\langle\omega(g(s_i,t_j)),\Delta_{s_i}g(s_i,t_j),g^{\bullet,2}(s_i,t_j)\rangle$$
$$-\sum_{i',j'}\Delta t_{j'}\langle\omega(g(s_{i'},t_{j'})),\Delta_{s_{i'}}g(s_{i'},t_{j'}),g^{\bullet,2}(s_{i'},t_{j'})\rangle. \tag{4.41}$$

But we can write

$$\Delta_{s_i}g(s_i,t_j)=\sum\Delta_{s_{i'}}g(s_{i'},t_j) \tag{4.42}$$

such that

$$C^{N'}_{i,j,2}=\Delta t_j\left\langle\omega(g(s_i,t_j)),\sum\Delta_{s_{i'}}g(s_{i'},t_j),g^{\bullet,2}(s_i,t_j)\right\rangle$$
$$-\sum\Delta t_{j'}\langle\omega(g(s_{i'},t_{j'})),\Delta_{s_{i'}}g(s_{i'},t_{j'}),g^{\bullet,2}(s_{i'},t_{j'})\rangle$$
$$=\left\{\sum_{i',j'}\Delta t_{j'}\langle\omega(g(s_i,t_j)),\Delta_{s_{i'}}g(s_{i'},t_j),g^{\bullet,2}(s_i,t_j)\rangle\right.$$
$$-\Delta t_{j'}\langle\omega(g(s_i,t_j),\Delta_{s_{i'}}g(s_{i'},t_{j'}),g^{\bullet,2}(s_{i'},t_{j'}))\rangle\}+\sum_{i',j'}\Delta t_{j'}\{\langle\omega(g(s_i,t_j))$$
$$\left.-\omega(g(s_{i'},t_{j'}),\Delta_{s_i}g(s_{i'},t_{j'}),g^{\bullet,2}(s_{i'},t_{j'}))\rangle\right\}=C^{1,N'}_{i,j,2}+C^{2,N'}_{i,j,2}. \tag{4.43}$$

In $C^{1,N'}_{i,j,2}$ and $C^{2,N'}_{i,j,2}$, we can replace, by the considerations which will follow, $\Delta_{s_{i'}}(g(s_{i'},t_{j'}))$ by $\sqrt{\Delta s_{i'}}g^{1,\bullet}(s_{i'},t_{j'})$ and $\Delta_{s_{i'}}(g(s_{i'},t_j))$ by $\sqrt{\Delta s_{i'}}g^{1,\bullet}(s_{i'},t_j)$. We get expressions $C^{3,N'}_{i,j,2}$ and $C^{4,N'}_{i,j,2}$. We distribute the term which appears in $\Sigma(C^{4,N'}_{i,j,2}C^{4,N'}_{i,j',2})$, there are four terms with increments $\sqrt{\Delta s_{i'}}g^{1;\bullet}(s_{i'},t_{j'})$, $\sqrt{\Delta s_{i''}}g^{1;\bullet}(s_{i''},t_{j''})$ and $\Delta t_{j'}g^{\bullet;2}(s_{i'},t_{j'})$, $\Delta t_{j''}g^{\bullet;2}(s_{i''},t_{j''})$ which appear. We condition by the Brownian motions which are obtained after diagonalizing the increments of the leading Brownian motions which appear in these formulas and we get as before a norm in L^2 which tends to 0.

We have to study three terms: $E[\Sigma-i,j\neq j'C^{3,N'}_{i,j,2}C^{3,N'}_{i,j',2}]$, $E[\Sigma_{i,j\neq j'}C^{4,N'}_{i,j,2}C^{4,N'}_{i,j',2}]$, and $E[\Sigma_{i,j\neq j'}C^{3,N'}_{i,j,2}C^{4,N'}_{i,j',2}]$. The behavior of $E[\Sigma_{i,j\neq j'}C^{3,N'}_{i,j,2}C^{3,N'}_{i,j',2}]$ is the most complicated to treat.

We write

$$C^{3,N'}_{i,j,2}=\left\{\sum_{i',j'}\sqrt{\Delta s_{i'}}\Delta t_{j'}\langle\omega(g(s_i,t_j)),g^{1,\bullet}(s_{i'},t_j),g^{\bullet,2}(s_i,t_j)\rangle\right.$$
$$\left.-\sum_{i',j'}\sqrt{\Delta s_{i'}}\Delta t_{j'}\langle\omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_{j'}),g^{\bullet,2}(s_i,t_j)\rangle\right\}$$
$$+\left\{\sum_{i',j'}\sqrt{\Delta s_i}\Delta t_{j'}\langle\omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_{j'}),g^{\bullet;2}(s_i,t_j)-g^{\bullet;2}(s_{i'},t_j)\rangle\right\}$$
$$+\left\{\sum_{i',j'}\sqrt{\Delta s_{i'}}\Delta t_{j'}\langle\omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_{j'}),g^{\bullet,2}(s_{i'},t_j)-g^{\bullet;2}(s_{i'},t_{j'})\rangle\right\}$$
$$=C^{5,N'}_{i,j,2}+C^{6,N'}_{i,j,2}+C^{7,N'}_{i,j,2}. \tag{4.44}$$

By the previous considerations, we have only to estimate $E[\Sigma_{i,j\neq j'}C^{5,N'}_{i,j,2}C^{5,N'}_{i,j',2}]$, $E[\Sigma_{i,j\neq j'}C^{6,N'}_{i,j,2}C^{6,N'}_{i,j',2}]$, and $E[\Sigma_{i,j\neq j'}C^{7,N'}_{i,j,2}C^{7,N'}_{i,j',2}]$ as well as the sum where there exist other coincidences of indices i, i', j, j'. We must estimate the analogous quantities where we mix $C^{5,N'}_{i,j,2}$ and $C^{6,N'}_{i,j',2}$, the term where we mix $C^{5,N'}_{i,j,2}$ and $C^{6,N'}_{i,j',2}$ and $C^{7,N'}_{i,j',2}$, and the term where we mix $C^{6,N'}_{i,j,2}$ and $C^{7,N'}_{i,j',2}$. We will omit to write the details of the convergence of these mixed terms to 0. Clearly,

$$E\left[\sum_{i,jj'} C^{5,N'}_{i,j,2}C^{5,N'}_{i,j',2}\right]\to 0. \tag{4.45}$$

Namely, if we do the multiplication of each term in the sum, there are six increments which appear $\Delta_{s_{i'_1}}B(s_{i'_1},t_{j_1})$, $\Delta_{s_{i'_1}}B(s_{i'_1},t_{j'_1})$, $\Delta_{t_{j_1}}B(s_{i_1},t_{j_1})$, $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j_2})$, $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j'_2})$, and $\Delta_{t_{j_2}}B(s_{i_2},t_{j_2})$. Their mutual covariances satisfy to (4.23), (4.24), and (4.26) because $j_1\neq j_2$ and because we do not have to consider when we do the multiplication term by term the interaction between $\Delta_{s_{i'_1}}(s_{i'_1},t_{j_1})$ and $\Delta_{s_{i'_1}}B(s_{i'_1},t_{j'_1})$ and the interaction between $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j'_2})$ and $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j_2})$. We conclude after conditioning along these increments, or more precisely the Brownian motions which appear when we use the diagonalization (4.20). This allows us to show (4.45).

Moreover,

$$E\left[\sum_{i,j\neq j'} C^{6,N'}_{i,j,2}C^{6,N'}_{i,j',2}\right]\to 0. \tag{4.46}$$

Namely, when we do the product term by term in (4.46), there are six increments which appear $\Delta_{s_{i'_1}}B(s_{i'_1},t_{j'_1})$, $\Delta_{t_{j_1}}B(s_{i_1},t_{j_1})$, $\Delta_{t_{j_1}}B(s_{i'_1},t_{j_1})$, $\Delta_{t_{j_1}}B(s_{i_1},t_{j_1})$, $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j'_2})$, and the terms $\Delta_{t_{j_2}}B(s_{i_2},t_{j_2})$, $\Delta_{t_{j_2}}B(s_{i'_2},t_{j_2})$. We can apply (4.23), (4.24), and (4.26) to these increments because we do not have to take the covariance between $\Delta_{t_{j_1}}B(s_{i_1},t_{j_1})$ and $\Delta_{t_{j_1}}B(s_{i'_1},t_{j_1})$ and the covariance between $\Delta_{t_{j_2}}B(s_{i_2},t_{j_2})$ and $\Delta_{t_{j_2}}(s_{i'_2},t_{j_2})$.

Let us consider the most complicated term $C^{7,N'}_{i,j,2}$ because in $g^{\bullet;2}(s_{i'},t_j)$ and in $g^{\bullet;2}(s_{i'},t_{j'})$ in (4.45), it is not the same subdivision in t_j. But since we consider

$$E\left[\sum_{i,j\neq j'} C^{7,N'}_{i,j,2}C^{7,N'}_{i,j',2}\right], \tag{4.47}$$

there are six increments to consider. They are $\Delta_{s_{i'_1}}B(s_{i'_1},t_{j'_1})$, $\Delta_{t_{j_1}}B(s_{i'_1},t_{j_1})$, $\Delta_{t_{j'_1}}B(s_{i'_1},t_{j'_1})$, $\Delta_{s_{i'_2}}B(s_{i'_2},t_{j'_2})$, $\Delta_{t_{j_2}}B(s_{i'_2},t_{j_2})$, and $\Delta_{t_{j'_2}}B(s_{i'_2},t_{j'_2})$, and we do not have to consider the correlation between $\Delta_{t_{j_1}}B(s_{i'_1},t_{j_1})$ and $\Delta_{t_{j'_1}}B(s_{i'_1},t_{j'_1})$ and the correlation $\Delta_{t_{j_2}}B(s_{i'_2},t_{j_2})$ and $\Delta_{t_{j'_2}}(s_{i'_2},t_{j'_2})$. We can apply (4.23), (4.24), (4.26) for the correlations we consider, and we can conclude as previously.

By the same reason

$$\sum_{i\neq i',j} E[C^{5,N'}_{i,j,2}C^{5,N'}_{i',j,2}]\to 0, \tag{4.48}$$

$$\sum_{i\neq i',j} E[C^{6,N'}_{i,j,2}C^{6,N'}_{i',j,2}]\to 0. \tag{4.49}$$

The same arguments arise when we consider

$$\sum_{i\neq i',j} E[C^{7,N'}_{i,j,2}C^{7,N'}_{i',j,2}]. \tag{4.50}$$

It remains to treat the case where there are two coincidences, that is to treat the case of $\Sigma E[(C^{5,N'}_{i,j,2})^2]$, $\Sigma E[(C^{6,N'}_{i,j,2})^2]$, and $\Sigma E[(C^{7,N'}_{i,j,2})^2]$, after doing the same restriction about the mixed terms. But as a matter of fact, we can show simply that

$$\sum_{i,j} E[(C^{5,N'}_{i,j,2})^2]\to 0. \tag{4.51}$$

We have, namely, the correlators between the following increments to consider: $\Delta_{s_{i'_1}}B(s_{i'_1},t_j)$, $\Delta_{s'i_1}B(s_{i'_1},t_{j'_1})$, $\Delta_{t_j}B(s_i,t_j)$, $\Delta_{s_{i'_2}}(s_{i'_2},t_j)$, and $\Delta_{s'_{i_2}}B(s_{i'_2},t_{j'_1})$. But we have $t_{j'_1}\geqslant t_j$ and $t_{j'_2}\geqslant t_j$. Therefore

$$\langle \Delta_{s_{i'_1}}B(s_{i'_1},t_{j'_1}),\Delta_{s'_1}B(s_{i'_1},t_j)\rangle = e(t_{j'_1}-t_j)(e(-\Delta s_{i'_1})+e(\Delta s_{i'_1})-2e(0)) = C\Delta s_{i'_1}e(t_{j'_1}-t_j), \tag{4.52}$$

because $t_{j'_1}\geqslant t_j$ and because e has half derivatives in 0. This remark allows us to repeat the previous considerations as well as to use (4.23), (4.24), and (4.26).

Moreover

$$\sum E[(C^{6,N'}_{i,j,2})^2]\to 0. \tag{4.53}$$

We have no difficulty to show that because we do not have to consider the covariance of a $g^{1;0}(s_{i'},t_j)$ and a $g^{1;0}(s_{i'},t_{j'})$ and because $\langle g^{1;\bullet}(s_{i'},t_j),\ g^{1;\bullet}(s_{i''},t_j)\rangle = CO(\sqrt{\Delta s_{i'}\Delta_{s_{i''}}})$.

The difficult part is to show that $\Sigma E[(C^{7,N'}_{i,j,2})^2]\to 0$, because two different subdivisions $[t_{j'},t_{j'+1}]$ and $[t_j,t_{j+1}]$ appear and because $t_{j'}\in[t_j,t_{j+1}]$. We write the details of this limit, because it is the most complicated, the other limits are simpler. We write

$$\begin{aligned} C^{7,N'}_{i,j,2} &= \sum \sqrt{\delta s_{i'}}\Delta t_{j'}\langle \omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_j),g^{\bullet;2}(s_{i'},t_j)-g^{\bullet;2}(s_{i'},t_{j'})\rangle \\ &+\sum \sqrt{\Delta s_{i'}}\Delta t_{j'}\langle \omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_{j'})-g^{1;\bullet}(s_{i'},t_j),g^{\bullet;2}(s_{i'},t_j)\rangle \\ &-\sum <\sqrt{\Delta s_{i'}}\Delta t_{j'}\langle \omega(g(s_i,t_j)),g^{1;\bullet}(s_{i'},t_{j'})-g^{1;\bullet}(s_{i'},t_j),g^{\bullet;2}(s_{i'},t_{j'})\rangle \\ &= C^{8,N'}_{i,j,2}+C^{9,N'}_{i,j,2}+C^{10,N'}_{i,j,2}\ . \end{aligned} \tag{4.54}$$

By the previous considerations, the terms $E[\Sigma(C^{9,N'}_{i,j,2})^2]$ and $E[\Sigma(C^{10,N'}_{i,j,2})^2]$ tend to 0. The main difficulty is to show that

$$E\left[\sum_{i,j}(C^{8,N'}_{i,j,2})^2\right]\to 0. \tag{4.55}$$

If these results are true, the term where we mix $C^{8,N'}_{i,j,2}$, $C^{9,N'}_{i,j,2}$, and $C^{10,N'}_{i,j,2}$ can be treated by Cauchy–Schwartz inequality. We proceed for that as it was done in the previous part. We remark, by the same considerations as in the first part, that it is enough to replace $\Delta t_j g^{\bullet;2}(s_{i'},t_j)$ by a double stochastic iterated integral $\int_{0<u<v<1}\alpha_u(s_{i'},t_j)(\mathrm{d}B_u(s_{i'},t_{j+1})-\mathrm{d}B_u(s_{i'},t_j))\alpha_v(s_{i'})$ $\times(\mathrm{d}B_v(s_{i'},t_{j+1})-\mathrm{d}B_v(s_{i'},t_j))$ where α_u and α_v are $B(s_{i'},t_j)$ measurable. By the same argument, we replace $\Delta t_{j'}g^{\bullet;2}(s_{i'},t_{j'})$ by a double stochastic integral $\int_{0<u<v<1}\alpha_u(s_{i'},t_{j'})$ $\times(\mathrm{d}B_u(s_{i'},t_{j'+1})-\mathrm{d}B_u(s_{i'},t_{j'}))\alpha_v(s_{i'},t_{j'})(\mathrm{d}B_v(s_{i'},t_{j'+1})-\mathrm{d}B_v(s_{i'},t_{j'}))$, where $\alpha_u(s_{i'},t_{j'})$

and $\alpha_v(s_{i'},t_{j'})$ are $B_\bullet(s_{i'},t_{j'})$ measurable. To study the behavior when $N'\to\infty$, we can replace without difficulty in this last expression $\alpha_u(s_{i'},t_{j'})$ by $\alpha_u(s_{i'},t_j)$. We write

$$\mathrm{d}B_\bullet(s_{i'},t_{j+1})-\mathrm{d}B_\bullet(s_{i'},t_j)=\sum \mathrm{d}B_\bullet(s_{i'},t_{j'+1})-\mathrm{d}B_\bullet(s_{i'},t_{j'}) \tag{4.56}$$

and we distribute in the first term of (4.55). The diagonal terms cancel, and we have to estimate when $N\to\infty$ the behavior of

$$C_{i,j,2}^{11,N'}=\sum \sqrt{\Delta s_{i'}}\langle\omega(g(s_i,t_j)),g^{1,\bullet}(s_{i'},t_j)\rangle\sum_{t_k\neq t_{k'}}\int_{0<u<v<1}\langle\alpha(u)(\mathrm{d}B_u(s_{i'},t_{k+1})$$
$$-\mathrm{d}B_u(s_{i'},t_k))\alpha(v)(\mathrm{d}B_v(s_{i'},t_{k'+1})-\mathrm{d}B_v(s_{i'},t_{k'})\rangle, \tag{4.57}$$

where we sum over $[t_k,t_{k+1}]\subseteq[t_j,t_{j+\beta 1}]$ and $[t_{k'},t_{k'+1}]\subseteq[t_j,t_{j+1}]$ for the sharper dyadic subdivision associated to $2^{N'}$. Instead of taking the following expression in time 1, let us take it in time r. We get a process $\Sigma\, C_{i,j,2,r}^{11,N'}$ [we replace $g(s_i,t_j)$ by $g_r(s_i,t_j)$, $g^{1,\bullet}(s_{i'},t_j)$ by $g_r^{1,\bullet}(s_{i'},t_j)$, and the double integral between 0 and 1 by a double integral between 0 and r]. Let us consider the finite variational part $V_r^{N'}=\Sigma\, V_{i,j,2,r}^{N'}$ and the martingale part $M_r^{N'}=\Sigma\, M_{i,j,2,r}^{N'}$ associated to this process.

Let us begin to study the finite variational part of this process $V_r^{N'}$. This can come from a contraction between $\omega(g(s_i,t_j))$ and $g^{1,\bullet}(s_i',t_j)$ which leads to a term in $\sqrt{\Delta s_i'}$, which is multiplied by a term in $\sqrt{\Delta s_i'}$. But the L^2 norm of the sum $\Sigma_{t_k\neq t_{k'}}$ can be estimated. We decompose first $\Sigma_{t_k\neq t_k}$ in a martingale term and a finite variational term. There is first a contraction between α_v and $\mathrm{d}B_v(s_i',t_{k'+1})-\mathrm{d}B_v(s_i',t_{k'})$ which leads to a term in $t_{k'+1}-t_{k'}$ The stochastic integral in u can be estimated. We see the martingale term. By Itô formula $\|\Sigma_{t_k\neq t_{k'}}\int_0^v\alpha_u(\delta B_u(s_i',t_{k+1})-\delta B_u(s_i',t_k)\|_{L^2}^2$ can be estimated in $\Sigma(t_{k'+1}-t_{k'})(t_{k''+1}-t_{k''})+\Sigma(t_{k+1}-t_k)=(t_{j+1}-t_j)^2+(t_{j+1}-t_j)$. Therefore the L^2 norm of this term behaves in $\sqrt{t_{j+1}-t_j}$. But since there is $(t_{k'+1}-t_{k'})$ in time u, we have a behavior of this contribution in $\Delta s_i(t_{j+1}-t_j)^{3/2}$ whose sum vanish when $N\to\infty$. The second term comes from a contraction between $\mathrm{d}B_u(s_i',t_{k+1})-\mathrm{d}B_u(s_i',t_k)$ and $\mathrm{d}B_v(s_i',t_{k'+1})-\mathrm{d}B_v(s_i',t_{k'})$ which leads to a term in $(t_{k+1}-t_k)(t_{k'+1}-t_{k'})$ and therefore to a contribution in $(t_{j+1}-t_j)^2$. Therefore the total contribution is in $\Delta s_i(t_{j+1}-t_j)^2$, whose sum vanish when $N\to\infty$, because $\langle g^{1,\bullet}(s'i',t_j),g^{1,\bullet}(s_{i''},t_j)\rangle=O\sqrt{\Delta s_{i'}\Delta s_{i''}}$.

There is a contraction between $\omega(g(s_i,t_j))$ and $\mathrm{d}B_v(s_i',t_{k'+1})-\mathrm{d}B_v(s_i',t_{k'})$ which is in $(t_{k'+1}-t_{k'})$. This term cancels, because when we take the square of the L^2 norm of the sum, it behaves in $\Sigma_{i',i''}\Delta_{s_{i'}}\Delta_{s-i''}I_{i',i''}$, where $I_{i',i''}$ is a sum of quadruple $t_{k'}$, $t_{k''}$, t_{k^3}, t_{k^4} which behaves in $O(t_{j+1}-t_j)^3$ and a sum $\Sigma_{i'}\Delta s_{i'}I_{i'}$ where $I_{i'}$ has a bound in $(t_{j+1}-t_j)^{3/2}$. The sum of these terms vanish, when $N\to\infty$ (see Sec. III for analogous considerations).

Let us estimate the martingale term $M_{i,j,2,r}^{N'}$. Let us estimate the L^2 norm of $M_r^{N'}$. We use Itô formula. It behaves as $\Sigma_{i',i''}\Delta s_{i''}\Delta s_{i'}I_{i,i'}+\Sigma_{i'}\Delta s_{i'}I_{i'}$ where $I_{i',i''}$ has a bound in $(t_{j+1}-t_j)^{3/2}$ and $I_{i'}$ the same. Therefore the L^2 norm of $M_r^{N'}$ vanish when $N\to\infty$.

Step I.1.3: Study of the behavior of the double classical integral C_5^N.

We write

$$C_5^N=\sum C_{i,j,5}^N=\sum \Delta s_i\Delta t_j\langle\omega(g(s_i,t_j)),g^{2,\bullet}(s_i,t_j),g^{\bullet,2}(s_i,t_j)\rangle. \tag{4.58}$$

We consider $N'>N$ and study

$$D_{i,j,5}^{N'}=C_{i,j,5}^N-\sum_{T_{i',j'}\subseteq T_{i,j}} C_{i',j',5}^{N'}. \tag{4.59}$$

We write

$$D^{N'}_{i,j,5}=C^{2,N'}_{i,j,5}+C^{3,N'}_{i,j,5} \tag{4.60}$$

with

$$C^{2,N'}_{i,j,5}=\sum_{T_{i',j'}\subseteq T_{i,j}} \Delta s_{i'}\Delta t_{j'}\langle \omega(g(s_i,t_j))-\omega(g(s_{i'},t_{j'})),g^{2;\bullet}(s_i,t_j)\bullet,g^{\bullet;2}(s_i,t_j)\rangle \tag{4.61}$$

and

$$\begin{aligned} C^{3,N'}_{i,j,5}=&\sum_{T_{i',j'}\subseteq T_{i,j}} \Delta s_{i'}\Delta t_{j'}\langle \omega(g(s_{i'},t_{j'})),g^{2;\bullet}(s_i,t_j),g^{\bullet;2}(s_i,t_j)\rangle \\ &-\langle \omega(g(s_{i'},t_{j'})),g^{2;\bullet}(s'_i,t'_j),g^{\bullet;2}(s_{i'},t_{j'})\rangle. \end{aligned} \tag{4.62}$$

It is clear that $\Sigma\, C^{2,N'}_{i,j,5}\to 0$ in L^2 because $g^{2;2}(s_i,t_j)$ is bounded in L^2.

In order to estimate $C^{3,N'}_{i,j,5}$, we can replace $\omega(g(s_{i'},t_{j'}))$ by $\omega(g(s_i,t_j))$. We can replace $\Delta s_{i'}g^{2;\bullet}(s_{i'},t_{j'})$ by a double stochastic integral in the dynamical time $uI^{2;\bullet}(s_{i'},t_{j'})$ as it was done in (4.57) and do the same transformation for the other $g^{2;\bullet}$ and $g^{\bullet;2}$ which appear in $C^{3,N'}_{i,j,5}$ such that we have only to show that $\Sigma^{4,N'}_{i,j,5}\to 0$ in L^2 where

$$C^{4,N'}_{i,j,5}=\langle \omega(g(s_i,t_j)),I^{2;\bullet}(s_i,t_j),I^{\bullet;2}(s_i,t_j)\rangle-\sum_{T_{i',j'}\subseteq T_{i,j}} \langle \omega(g(s_i,t_j)),I^{2;\bullet}(s_{i'},t_{j'}),I^{\bullet;2}(s_{i'},t_{j'})\rangle. \tag{4.63}$$

We write

$$d\Delta_{s_i} B\bullet(s_i,t_j)=\sum_{s_{i'}} d\Delta_{s_{i'}} B\bullet(s_{i'},t_j) \tag{4.64}$$

and

$$d\Delta_{t_j} B\bullet(s_i,t_j)=\sum_{t'_j} d\Delta_{t_{j'}} B\bullet(s_i,t_{j'}) \tag{4.65}$$

and we distribute in $I^{2;\bullet}(s_i,t_j)$ and $I^{\bullet;2}(s_i,t_j)$. We get that the expression $I^{2;\bullet}(s_i,t_j)$ is equal to $\Sigma_{s^1_{i'},s^2_{i'}\in[s_i,s_{i+1}]}I^{2;\bullet}(s^1_{i'},s^2_{i'},t_j)$ and that $I^{\bullet;2}=\Sigma_{t^1_{j'},t^2_{j'}\in[t_j,t_{j+1}]}I^{\bullet;2}(s_i,t^1_{j'},t^2_{j'})$ after distributing in these stochastic integrals. Only the contribution where $s^1_{i'}=s^2_{i'}$ and $t^1_{j'}=t^2_{j'}$ do not vanish when $N'\to\infty$, by the same considerations as in (3.36). These terms are nothing else, modulo some small error terms of $I^{2;\bullet}(s_{i'},t_j)$ and $I^{\bullet;2}(s_i,t_{j'})$. We have only to show that $\Sigma_{i,j}C^{5,N'}_{i,j,5}\to 0$ in L^2 where

$$C^{5,N'}_{i,j,5}=\sum_{T_{i',j'}\subseteq T_{i,j}} \langle \omega(g(s_i,t_j)),I^{2;\bullet}(s_{i'},t_{j'}),I^{\bullet;2}(s_{i'},t_{j'})\rangle-\langle \omega(g(s_i,t_j)),I^{2;\bullet}(s_{i'},t_j),I^{\bullet;2}(s_i,t_{j'})\rangle. \tag{4.66}$$

But we can show that the L^2 norm of $I^{2;\bullet}(s_{i'},t_j)-I^{2;\bullet}(s_{i'},t'_j)$ is $O(4/N')\Delta s_{i'}$ because the right-hand bracket of $B\bullet(s_{i'+1},t_j)-B\bullet(s_{i'},t_j)-B\bullet(s_{i'+1},t_{j'})+B(s_{i'},t_{j'})$ is in $O((s_{i'+1}-s_{i'})\times(t_j-t_{j'}))$.

Step I.1.4: Study of the vanishing term C^N_3.

We write $C^N_3=\Sigma^N_{i,j,3}$ where the L^2 norm of $C^N_{i,j,3}$ is in $O(\Delta s_i\Delta t_j^{3/2})$. But we have if $s_i\neq s_{i'}$, by using the previous techniques

$$E[\langle \omega(g(s_i,t_j)),g^{1;\bullet}(s_i,t_j),g^{\bullet;3}(s_i,t_j)\rangle\langle \omega(g(s_{i'},t_{j'})),g^{1,\bullet}(s_{i'},t_{j'}),g^{\bullet,3}(s_{i'},t_{j'})\rangle]$$
$$=O(\sqrt{\Delta s_i}\sqrt{\Delta s_{i'}}). \tag{4.67}$$

Therefore $E[(C_3^N)^2]\to 0$.

Step I.2: Convergence of B_2^N.

We write in probability

$$\omega(g^N(s,t))-\omega(g(s_i,t_j))=\nabla\omega(g(s_i,t_j))(g^N(s,t))-g(s_i,t_j)+\nabla^2\omega(g(s_i,t_j))(g^N(s,t)$$
$$-g(s_i,t_j))^2+O(\Delta t_j^{3/2})+O(\Delta s_i^{3/2}). \tag{4.68}$$

The residual term converges to 0 by the previous arguments. It remains to treat the main term. We recall

$$g^N(s,t)-g(s_i,t_j)=\frac{s-s_i}{s_{i+1}-s_i}(g(s_{i+1},t_j)-g(s_i,t_j))+\frac{t-t_j}{t_{j+1}-t_j}(g(s_i,t_{j+1})-g(s_i,t_j))$$
$$+\frac{t-t_j}{t_{j+1}-t_j}\frac{s-s_i}{s_{i+1}-s_i}(g(s_{i+1},t_{j+1})-g(s_i,t_{j+1})-g(s_{i+1},t_j)+g(s_i,t_j)). \tag{4.69}$$

Moreover

$$\int_{s_i}^{s_{i+1}}\frac{s-s_i}{s_{i+1}-s_i}\mathrm{d}s=s_{i+1}-s_i. \tag{4.70}$$

The integral of the first term of (4.69) leads to the convergence of the sum of random quantities of a type analogous to already considered quantities, which contains some ''brackets'' of the type $\langle\nabla\omega(g(s_i,t_j))\cdot\Delta_{s_i}g(s_i,t_j),\Delta_{s_i}g(s_i,t_j),\Delta_{t_j}g(s_i,t_j)\rangle$ which converges by the methods used before. We can treat by the same method the convergence of $\langle\nabla\omega(g(s_i,t_j))(g(s_i,t_{j+1})-g(s_i,t_j)),\Delta_{s_i}g(s_i,t_j),\Delta_{t_j}g(s_j,t_j)\rangle$ which converge by the same methods as before. The term in $(t-t_j)(s-s_i)/(\Delta t_j\Delta s_i)$ leads to analogous terms. If we consider the term where the square of $g^N(s,t)-g(s_i,t_j)$ appears, there is a term in $\langle\nabla^2\omega(g(s_i,t_j));\Delta_{s_i}g(s_i,t_j)^2,\Delta_{s_i}g(s_i,t_j),\Delta_{t_j}g\times(s_i,t_j)\rangle$ whose sum vanishes in L^2 by the same considerations as in step I.1.4. The only problem comes when we take sum of the type $\Sigma_{i,j}\langle\nabla^2\omega(g(s_i,t_j))\cdot\Delta_{s_i}g(s_i,t_j)\cdot\Delta_{t_i}g(s_i,t_j),\Delta_{s_i}g(s_i,t_j),\Delta_{t_i}g(s_i,t_j)\rangle$ whose treatment is similar to step I.1.3 by expanding a product of integrals into iterated integrals of length 2.

Step II: Convergence of A_2^N and A_3^N.

The treatment for A_2^N and A_3^N are similar. So we will treat only the case of A_2^N.

We write

$$A_2^N=\sum_{i,j}\langle\omega(g(s_i,t_j)),\mathrm{d}_s\alpha_3^N(s,t),\mathrm{d}_t\alpha_2^N(t)\rangle$$
$$=\sum_{i,j}\int_{T_{i,j}}\langle\omega(g^N(s,t))-\omega(g(s_i,t_j)),\mathrm{d}_s\alpha_3^N(s,t),\mathrm{d}_t\alpha_2^N(t)\rangle=B_1^N+B_2^N. \tag{4.71}$$

Step II.1: Convergence of B_1^N.

$$\int_{T_{i,j}} \langle \omega(g(s_i,t_j)), \mathrm{d}_s\, \alpha_3^N(s,t), \mathrm{d}_t \alpha_2^N(t), \rangle$$

$$= \int_{T_{i,j}} \frac{\mathrm{d}s}{s_{i+1}-s_i} \frac{(t-t_j)\mathrm{d}t}{(t_{j+1}-t_j)^2} \langle \omega(g(s_i,t_j)), g(s_{i+1},t_{j+1})$$

$$- g(s_i,t_{j+1}) - g(s_i+1,t_j) + g(s_i,t_j), g(s_i,t_{j+1}) - g(s_i,t_j)\rangle. \tag{4.72}$$

The integral over $T_{i,j}$ is constant.

We write

$$g(s_{i+1},t_{j+1}) - g(s_i,t_{j+1}) - g(s_{i+1},t_j) + g(s_i,t_j)$$

$$= \{g(s_{i+1},t_{j+1}) - g(s_i,t_{j+1})\} - \{g(s_{i+1},t_j) - g(s_i,t_j)\} = \gamma_{i,j}^1 - \gamma_{i,j}^2. \tag{4.73}$$

The term in $\gamma_{i,j}^2$ can be treated as in step I.1. The term in $\gamma_{i,j}^1$ can be treated as in step I.1, because the increments between $\Delta_{s_i} B(s_i,t_j)$ and $\langle \Delta_{s_i} B(s_i,t_{j+1})\rangle$ satisfy to (4.52), and we can do as in the treatment of (4.52).

Step II.2: Convergence of B_2^N.

We use (4.68) and we conclude as in step I.2.

Step III: Convergence of A_4^N.

We write

$$A_4^N = \sum_{i,j} \int_{T_{i,j}} \langle \omega(g(s_i,t_j)), \mathrm{d}_s \alpha_3^N(s,t), \mathrm{d}_t \alpha_3^N(s,t)\rangle$$

$$+ \sum_{i,j} \int_{T_{i,j}} \langle \omega(g^N(s,t)) - \omega(g(s_i,t_j)), \mathrm{d}_s \alpha_3^N(s,t), \mathrm{d}_t \alpha_3^N(s,t)\rangle$$

$$= B_1^N + B_2^N. \tag{4.74}$$

Step III.1: Convergence of B_1^N.

We write with the notations of (4.73):

$$\int_{T_{i,j}} \langle \omega(g(s_i,t_j)), \mathrm{d}_s \alpha_s^N(s,t), \mathrm{d}_t \alpha_3^N(s,t))\rangle$$

$$= 2 \int_{T_{i,j}} \frac{(t-t_j)\mathrm{d}t}{t_{j+1}-t_j} \frac{\mathrm{d}s}{s_{i+1}-s_i} \langle \omega(g(s_i,t_j)), \gamma_{i,j}^1 + \gamma_{i,j}^2, \gamma_{i,j}^1 + \gamma_{i,j}^2\rangle. \tag{4.75}$$

The integral over $T_{i,j}$ is constant. In order to treat the sum, we write the second $\gamma_{i,j}^1 + \gamma_{i,j}^2$ as $\delta_{i,j}^1 + \delta_{i,j}^2$ where

$$\delta_{i,j}^1 = g(s_{i+1},t_{j+1}) - g(s_{i+1},t_j) \tag{4.76}$$

and

$$\delta_{i,j}^2 = -g(s_i,t_{j+1}) + g(s_i,t_j) \tag{4.77}$$

and we perform the limit as in the previous considerations.

Step III.2: Convergence of B_2^N.

We write

$$\int_{T_{i,j}} \alpha^N(s,t) \langle \omega(g^N(s,t)) - \omega(g(s,t)), \gamma_{i,j}^1 + \gamma_{i,j}^2, \delta_{i,j}^1 + \delta_{i,j}^2\rangle \mathrm{d}s\, \mathrm{d}t \tag{4.78}$$

and we use (4.68) for $\alpha^N(s,t)$ a suitable function of (s,t).

When the form depends on a finite-dimensional parameter, we show that the approximation of the stochastic integrals converge for all the derivatives of ω and we conclude by using the Sobolev imbedding theorem as in Ref. 29. That is we consider the integrals

$$\int_{T^2}\langle \nabla_u^{\alpha}\omega(g^N(s,t)),\mathrm{d}_s g^N(s,t),\mathrm{d}_t g^N(s,t)\rangle, \tag{4.79}$$

which converge in L^2 for all multiindices α. □

We would like to get the same theorem with a more intrinsic approximation $\tilde{g}^N(s,t)$ of the random field $g(s,t)$. As in the Sec. III, the finite-dimensional approximations of the integral $\int_{T^2}\tilde{g}^{N,*}\omega$ will converge in L^2, but we do not know if they will converge to the same limit integral of $\int_{T^2} g^{N,*}\omega$.

For that if $g(s,t_j)$ and $g(s,t_{j+1})$ are close, we use the functions

$$F^N(t,g(s,t_j),g(s,t_{j+1}))=\exp\left[\frac{t-t_j}{t_{j+1}-t_j}\log(g(s,t_{j+1})g^{-1}(s,t_j))\right]g(s,t_j) \tag{4.80}$$

conveniently extended to the whole sets of matrices.

We approximate $g(s,t_{j+1})$, $g(s,t_j)$ as follows:

$$F_N(s,g(s_i,t_{j+1}),g(s_{i+1},t_{j+1}))=\exp\left[\frac{s-s_i}{s_{i+1}-s_i}\log(g(s_{i+1},t_{j+1})g^{-1}(s_i,t_{j+1}))\right]g(s_i,t_{j+1}) \tag{4.81}$$

conveniently extended over the whole matrix algebras as well as its inverse. Moreover,

$$F^N(s,g(s_i,t_j),g(s_{i+1},t_j)]=\exp\left[\frac{s-s_i}{s_{i+1}-s_i}\log(g(s_{i+1},t_j)g^{-1}(s_i,t_j))\right]g(s_i,t_j) \tag{4.82}$$

conveniently extended as well as its inverse to the set of all matrices.

We take as approximation

$$\begin{aligned}\tilde{g}^N(s,t)=\exp\Bigg[&\frac{t-t_j}{t_{j+1}-t_j}\log(F^N(s,g(s_i,t_{j+1},g(s_{i+1},t_{j+1})))\\&\times(F^N)^{-1}(s,g(s_i,t_j),g(s_{i+1},t_j)))\Bigg]F^N(s,g(s_i,t_j),g(s_{i+1},t_j)).\end{aligned} \tag{4.83}$$

We have the asymptotic expansion

$$\begin{aligned}F^N(t,g(s,t_j),g(s,t_{j+1}))=&g(s,t_j)+\frac{t-t_j}{t_{j+1}-t_j}(g(s,t_{j+1})-g(s,t_j))\\&+O\left(\left(\frac{t-t_j}{t_{j+1}-t_j}\right)^2(g(s,t_{j+1}-g(s,t_j))^2)\right).\end{aligned} \tag{4.84}$$

We imbed in this expression the approximation of $g(s,t_{j+1})$ and of $g(s,t_j)$. This shows that, in the expansion of $\tilde{g}^N(s,t)$, the more singular term is the same in (4.1), modulo some more regular terms which converge. The main Itô integral is the same, but we do not know if the correcting terms are the same.

We get the main result of this part.

Theorem IV.2: When $N\to\infty$, the traditional integral $\tilde{A}_v^N=\int_{T^2}(\tilde{g}^N)^*\omega_v$ converges in L^2 to the stochastic Stratonovitch integral,

$$\int_{T^2} g^* \omega_v = \int_{S^1 \times S^1} \langle \omega(g(s,t)), \mathrm{d}_s g(s,t), \mathrm{d}_t g(s,t) \rangle. \tag{4.85}$$

Moreover, $\int_{T^2} g^* \omega_v$ has a smooth version in v.

Remark: We ignore if the stochastic integral of Theorem IV.2 is equal to the stochastic integral of Proposition IV.1. In the rest of this paper, we will use the version of Theorem IV.2.

Remark: We can consider in the previous theorem a 2-tensor which is not necessarily a two-form.

V. STOCHASTIC COHOMOLOGY OF THE SPACE OF RANDOM TORI

Let us suppose that G is compact of dimension d and let us consider the torus T^2. We introduce the quantity ϵ of proposition II.3. We consider the space $T^2_{\epsilon,*}(G)$ of strong Hoelder map $\eta(\bullet)$ with parameter ϵ from T^2 into G. Strong Hoelder with parameter ϵ means that uniformly

$$\lim_{S \to S'} \frac{\mathrm{d}(\eta(S), \eta(S'))}{\mathrm{d}(S,S')^\epsilon} = 0, \tag{5.1}$$

where $\mathrm{d}(\eta(S), \eta(S'))$ denotes the Riemannian distance over the group between $\eta(S)$ and $\eta(S')$ and $\mathrm{d}(S,S')$ denotes the Riemannian distance on the torus.

We can consider the set $T^2_{\epsilon,*}(G)$ of strong Hoelder maps with parameter ϵ from T^2 into G. It is by general theory (Refs. 7 and 8) an infinite Banach dimensional manifold. By general theory,[7,8] there is a smooth partition of unity associated to a cover of $T^2_{\epsilon,*}(G)$ by open subsets V_i which is locally finite.

Moreover the topology of $T^2_{\epsilon,*}(G)$ coincides with the trace topology of $T^2_{\epsilon,*}(R^N)$ if we imbed isometrically G into R^N: in others words, we can consider strong Hoelder maps from T^2 into R^N and constrain them to belong to G. Over $T^2_{\epsilon,*}(R^N)$, we have to add some conditions in order to define its topology. As a matter of fact, we choose as Banach norm over $T^2_{\epsilon,*}(R^N)$ the following:

$$\sup_{S,S' \in T^2} \frac{|\eta(S) - \eta(S')|}{\mathrm{d}(S,S')^\epsilon} + \sup |\eta(S)|. \tag{5.2}$$

We can define a basis of contractible open sets of $T^2_{\epsilon,*}(G)$ as follows: let $g_{sm}(\bullet)$ be a smooth element of $T^2_{\epsilon,*}(G)$. Let us suppose that the following condition over $g(\bullet)$ holds:

$$\sup \mathrm{d}(e, \eta^{-1}(S)\, \eta_{sm}(S)) < r$$

such that we can define $\psi(S) = \log[\eta(S) \eta_{sm}^{-1}(S)]$ if r in * is small enough. Moreover, let us suppose that the following condition holds:

$$\sup_{S,S'} \frac{|\psi(S) - \psi(S')|}{\mathrm{d}(S,S')^\epsilon} < r'.$$

We get an open subset $V(\eta_{sm}(\bullet), r, r')$ of $T^2_{\epsilon,*}(G)$ which constitutes a basis of the topology of $T^2_{\epsilon,*}(G)$ when r and r' are small enough and $\eta_{sm}(\bullet)$ describes the set of smooth elements of $T^2_{\epsilon,*}(G)$. By similar considerations, we can produce an atlas of the infinite-dimensional manifold $T^2_{\epsilon,*}(G)$ without using the general considerations of Refs. 7 and 8. Moreover if r and r' are small enough, $V(\eta_{sm}(\bullet), r, r')$ is contractible. The retraction map $\Psi(t, g(\bullet))$ (t belonging in $[0,1]$) from $V(\eta_{sm}(\bullet), r, r')$ to $\{\eta_{sm}(\bullet)\}$ is constituted by

$$\eta(\bullet) \to \{S \to \exp[t \log[\eta(S)\, \eta_{sm}^{-1}(S)]]\, \eta_{sm}(S)\}. \tag{5.3}$$

In order to show the continuity and the differentiability of the map $\Psi(t,\bullet)$, we see that in the previous trivialization the map $\Psi(t,\bullet)$ is nothing else than the map $\psi(\bullet)\to t\psi(\bullet)$ which is clearly smooth in t and $\psi(\bullet)$ for the strong Hoelder topology. It can be proved too by using the following theorem.

Theorem V.1: Let F be a map from $T^2\times R^N$ into R^N which is bounded with bounded derivatives of all orders. Let Ψ be the Nemytski map from $T^2_{\epsilon,*}(R^N)$ into $T^2_{\epsilon,*}(R^N)$:

$$\eta(\bullet)\to\{S\to F(S,\eta(S)\}. \tag{5.4}$$

Then Ψ is smooth for the strong Hoelder topology.

Proof: Let us first check that $\Psi(g(\bullet))$ belongs to $T^2_{\epsilon,*}(R^N)$. Since F is bounded, $\Psi(g(\bullet))$ is bounded. Moreover,

$$|F(S,\eta(S))-F(S',\eta(S'))|\leqslant C(\mathrm{d}(S,S')+|\eta(S)-\eta(S')|). \tag{5.5}$$

This shows clearly that (5.1) is checked as well as (5.2) for $\Psi(g(\bullet))$.

Let us show the continuity of Ψ. Let $\eta(\bullet)$ and $\eta^1(\bullet)$ in $T^2_{\epsilon,*}(R^N)$. We have to estimate

$$F(S,\eta(S))-F(S,\eta^1(S))-F(S',\eta(S'))+F(S',\eta^1(S'))=A_1-A_2, \tag{5.6}$$

where

$$A_1=\int_0^1\langle \mathrm{d}F(S,\eta(S)+u(\eta^1(S)-\eta(S))),\eta^1(S)-\eta(S)\rangle \mathrm{d}u \tag{5.7}$$

and

$$A_2=\int_0^1\langle \mathrm{d}F(S',\eta(S')+u(\eta^1(S')-\eta(S'))),\eta^1(S')-\eta(S')\rangle \mathrm{d}u. \tag{5.8}$$

We have $A_1-A_2=B_1+B_2$ with

$$B_1=\int_0^1\langle \mathrm{d}F(S,\eta(S)+u(\eta^1(S)-\eta(S))),\eta^1(S)-\eta(S)+\eta(S')-\eta^1(S')\rangle \mathrm{d}u \tag{5.9}$$

and

$$B_2=\int_0^1\langle \mathrm{d}F(S,\eta(S)+u(\eta^1(S)-\eta(S)))-\mathrm{d}F(S',\eta(S')+u(\eta^1(S')-\eta(S'))),\eta(S')-\eta^1(S')\rangle \mathrm{d}u. \tag{5.10}$$

Since $\mathrm{d}F$ is bounded, we can estimate $|B_1|\mathrm{d}(S,S')^{-\epsilon}$ in $C|\eta(S)-\eta^1(S)-\eta(S')+\eta^1(S')|\mathrm{d}(S,S')^{-\epsilon}$. Moreover, we can estimate $|B_2|\mathrm{d}(S,S')^{-\epsilon}$ by

$$C\frac{\mathrm{d}(S,S')}{\mathrm{d}(S,S')^{\epsilon}}|\eta(S')-\eta^1(S')|+C\frac{|\eta(S)-\eta(S')|}{\mathrm{d}(S,S')^{\epsilon}}|(\eta(S')-\eta^1(S')|$$
$$+C|\eta^1(S)-\eta^1(S')-\eta(S)+\eta(S')|\mathrm{d}(S,S')^{-\epsilon}|\eta(S')-\eta^1(S')|. \tag{5.11}$$

This shows us the continuity of Ψ. In order to see that, notice that the supremum norm of $S\to\eta(S)$ in term of the Hoelder norm of this map and that $\sup \mathrm{d}(S,S')/\mathrm{d}(S,S')^{\epsilon}<\infty$ as well as $\sup|\eta(S)-\eta(S')|/\mathrm{d}(S,S')^{\epsilon}<\infty$.

Let us show the differentiability. Let us consider $\eta(S)+h(S)$, h being small.

$\Psi(\eta(\bullet)+h(\bullet))-\Psi(\eta(\bullet))$ is the function defined by

$$F(S,\eta(S)+h(S))-F(S,\eta(S))=\langle F'(S,\eta(S)),h(S)\rangle + \int_0^1 \langle F''(S,\eta(S)+uh(S)),h(S)h(S)\rangle \mathrm{d}u, \quad (5.12)$$

$D\Psi: h(\bullet)\to\{S\to\langle F'(S,\eta(S)),h(S)\rangle\}$ is continuous. Namely,

$$\langle F'(S,\eta(S)),h(S)\rangle-\langle F'(S',\eta(S'))h(S')\rangle=\langle F'(S,\eta(S))-F'(S',\eta(S')),h(S)\rangle + \langle F'(S',\eta(S')),h(S)-h(S')\rangle. \quad (5.13)$$

But F' is bounded with bounded derivatives and $h(S)-h(S')$ can be estimated in terms of the Hoelder norm of h as well as $h(S)$. Moreover, $S\to F'(S,\eta(S))$ is strong Hoelder. This shows that $D\Psi$ is a continuous linear application. Let us estimate

$$\langle F''(S,\eta(S)+u(h(S)),h(S)h(S)\rangle-\langle F''(S',\eta(S')+uh(S')),h(S')h(S')\rangle=A_1+A_2 \quad (5.14)$$

with

$$A_1=\langle F''(S,\eta(S)+uh(S)),h(S)h(S)-h(S')h(S')\rangle \quad (5.15)$$

and

$$A_2=\langle F''(S,\eta(S)+u(h(S)))-F''(S',(\eta(S')+u(h(S'))),h(S')h(S')\rangle. \quad (5.16)$$

We have

$$|A_2 \mathrm{d}(S,S')^{-\epsilon}|\leqslant C\frac{|h(S')|^2}{\mathrm{d}(S,S')^{\epsilon}}(\mathrm{d}(S,S')+|\eta(S)-\eta(S')|+|h(S)-h(S')|). \quad (5.17)$$

This gives an estimate in terms of the square of the norm of h for the norm defining the topology of $T^2_{\epsilon,*}(R^N)$, because the uniform norm of $S\to h(S)$ can be estimated in term of the Hoelder norm of $h(\bullet)$ and because $|\eta(S)-\eta(S')|/\mathrm{d}(S,S')^{\epsilon}$ is bounded.

For A_1, we write

$$\langle F''(C),h(S)h(S)-h(S')h(S')\rangle=\langle F''(C),h(S)\cdot(h(S)-h(S'))\rangle + \langle F''(C),h(S')(h(S)-h(S'))\rangle \quad (5.18)$$

[we used the symmetry of F'' in order to establish the previous formula, that is $\langle F''(C),h(S)h(S')\rangle=\langle F''(C),h(S')h(S)\rangle$], in order to conclude.

We omit to write the proofs for higher order differentiability of Ψ. □

Remark: we can consider a family Ψ_u parametrized by u belonging to an open subset O of R^n:

$$\Psi_u(\eta(\bullet))=\{S\to F(u,S,\eta(S))\}, \quad (5.19)$$

where F is bounded with bounded derivatives of all orders and show that $\Psi_u(\eta(\bullet))$ is jointly smooth in u and $\eta(\bullet)$, for the strong Hoelder topology.

Let us recall briefly the machinery of sheaf cohomology. We refer to Ref. 67 for more precisions. Let M be a topological space. It will be later $T^2_{\epsilon,*}(G)$.

Definition V.2: A presheaf $P=\{\Gamma(U;P);\rho(U,V)\}$ of R-vector spaces is a collection of vector spaces $\Gamma(U;P)$ indexed by the open subsets U of M and a restriction map $\rho(V;U):\Gamma(V;P)\to\Gamma(U;P)$ for $u\subseteq V$ such that if $U\subseteq V\subseteq W$ we have

$$\rho(U;W)=\rho(U;V)\circ\rho(V;W) \quad (5.20)$$

and such that $\rho(U;U)=Id$.

Definition V.3: A sheaf $\tilde{S}=\{\Gamma(U;\tilde{S});\rho(U;V)\}$ of R vector spaces is a presheaf such that for any cover U_i by open sublets of M, the following two properties are checked.

(i) If the restriction to $U\cap U_i$ of a section f belonging to $\Gamma(U;\tilde{S})$ equal the restriction to $U\cap U_i$ of another section g of $\Gamma(U;\tilde{S})$, then $f=g$.

(ii) Let us give a system of section f_i of $\Gamma(U_i;\tilde{S})$ such that the restriction to $U_i\cap U_j$ of f_i is equal to the restriction to $U_i\cap U_j$ of f_i. Then there exists a unique $f\in\Gamma(U;\tilde{S})$ such that its restriction to $U_i\cap U$ are equal to the restriction of f_i. to $U\cap U_i$.

Definition V.4: A morphism of sheaf $\mathrm{d}:\tilde{S}\to\tilde{S}'$ is a collection of linear mappings d_U from $\Gamma(U;\tilde{S})$ into $\Gamma(U;\tilde{S}')$ which are compatible with the operations of restrictions.

Definition V.5: A morphism of sheaf $\mathrm{d}:\tilde{S}\to\tilde{S}'\to\tilde{S}''$ is exact if $\mathrm{d}^2=0$ and if for every open subset V, there exists an open subset U included in V such that $\mathrm{Im}(\mathrm{d}_U)=\mathrm{Ker}(d_U)$.

This means that we have a kind of Poincaré lemma.

Definition V.6: Let $\tilde{S}=\tilde{S}^{-1}$ be a sheaf. The sequence $\tilde{S}=\tilde{S}^{-1}\to\tilde{S}^0\to\cdots\to\tilde{S}^k\to\tilde{S}^{k+1}\to\cdots$ is called a resolution of the sheaf $\tilde{S}$ if all the maps $\tilde{S}^{i-1}\to\tilde{S}^i\to\tilde{S}^{i+1}$ are exacts.

Definition V.7: A sheaf over M is said to be fine if for each locally finite cover U_i by open subsets, there exists for each i an endomorphism l_i of the sheaf $\tilde{S}$ such that

(i) $\mathrm{Suppl}\, l_i\subseteq U_i$,
(ii) $\Sigma\, l_i=1$.

The first condition means that if $U\cap U_i=\varnothing$, $l_i f=0$ if $f\in\Gamma(U;\tilde{S})$. $\{l_i\}$ is called a partition of unity, respectively, to the cover (U_i).

The main theorem-definition in sheaf cohomology is the following (see Ref. 67):

Theorem-Definition V.8: Let $\tilde{S}=\tilde{S}^{-1}$ be a sheaf in real vector spaces. Let $\tilde{S}=\tilde{S}^{-1}\to\tilde{S}^0\to\cdots\to\tilde{S}^k\to\tilde{S}^{k+1}\to\cdots$ be a resolution of $\tilde{S}$ by fine sheafs $\tilde{S}^k$. Then $\mathrm{Ker}_{\Gamma(M;\tilde{S}^k)}\mathrm{d}/\mathrm{Im}_{\Gamma(M;\tilde{S}^{k-1})}\mathrm{d}$ is independent of the resolution of the sheaf $\tilde{S}$ by fine sheaves and is called the kth cohomology group of $\tilde{S}$.

As particular case of this theorem, we can consider the constant sheaf over $T^2_{\epsilon,*}(G)$: over an open set U we consider the set of constant maps over U. There is a natural restriction map. Λ^k_{det} is constituted from the sheaf of k-forms. $\Gamma(U;\Lambda^k_{\mathrm{det}})$ is the space of smooth k-form over the open subset U of $T^2_{\epsilon,*}(G)$ for the strong-Hoelder topology. The (deterministic) exterior derivative realizes an exact morphism of sheaves $\Lambda^k_{\mathrm{det}}\to\Lambda^{k+1}_{\mathrm{det}}\to\Lambda^{k+2}_{\mathrm{det}}$, because we have, as we have seen, a basis of the topology of $T^2_{\epsilon,*}(G)$ constituted of contractible sets, because the Nemytski maps are smooth for the strong Hoelder topology, which implies that we have a kind of Poincaré lemma. Moreover, there are partition of unity in $T^2_{\epsilon,*}(G)$. We have exhibited a resolution of the constant sheaf of $T^2_{\epsilon,*}(G)$ in fine sheaves.

We deduce.

Theorem V.9: The sheaf cohomology groups of $T^2_{\epsilon,*}(G)$ are equal to the de Rham cohomology groups of $T^2_{\epsilon,*}(G)$.

We would like to generalize this theorem for stochastic form, which are almost surely defined, containing stochastic integrals as we will see for instance in the next part.

Let Ω be the probability space underlying the construction of the Brownian motion $t\to B_t(\bullet)$ of the first part.

Definition V.10: A stochastic plot of dimension m of $T^2_{\epsilon,*}(G)$ is given by a countable family (O,ϕ_i,Ω_i) where O is an open subset of R^m such that:

(i) The Ω_i constitute a measurable partition of Ω.

(ii) $\phi_i(u)(\bullet)=(S\to F(u,S,\eta(S)))$ where F is a smooth function over $O\times T^2\times R^N$ with bounded derivatives of all orders.

(iii) Over Ω_i, for all $u\in O$, $\phi_i(u)(\bullet)\in T^2_{\epsilon,*}(G)$.

We identify two stochastic plots (O,ϕ^1_i,Ω^1_i) and (O,ϕ^2_j,Ω^2_j) if $\phi^1_i=\phi^2_j$ almost surely as applications defined over O over $\Omega^1_i\cap\Omega^2_j$.

Definition V.11: Let V be an open subset of $T^2_{\epsilon,*}(G)$. An element $\Gamma^k(V,st)\sigma_{V,st}$ is given by

the following data: let (O,ϕ_i,Ω_i) be a stochastic plot with values in $T^2_{e,\epsilon,*}(G)$. Let O_i be the reciprocal image over Ω_i of V by ϕ_i. Over O_i, we associate a random smooth k-form $\sigma_{O_i}=\phi^*\sigma_{V,st}$. Moreover, this system of random forms satisfies the following conditions.

(i) Let j a smooth deterministic map from O^1 into O^2 be given, and $\phi_2=(O^2,\phi_i^2,\Omega_i)$ be a stochastic plot. We associate the composite plot $\phi_1=\phi_2\circ j=(O^1,\phi_i^1,\Omega_i)$ defined by $\phi_i^1(u_1)=\phi_i^2(j(u_1))$. We have clearly $O_i^1=j^{-1}O_i^2$ and we suppose that $(\phi^1)^*\sigma_{V,st}=j^*(\phi^2)^*\sigma_{V;st}$ almost surely, or in other words, that over Ω_i we have almost surely

$$\sigma_{O_i^1}=j^*\sigma_{O_i^2}. \tag{5.21}$$

(ii) If (O,ϕ_i^1,Ω_i^1) and (O,ϕ_i^2,Ω_i^2) are two stochastic plots such that $\phi_i^1=\phi_j^2\circ\psi$ on a set of probability different of 0 for a given transformation of some Ω_i^1 into some Ω_j^2, then as finite-dimensional differential forms, we have almost surely:

$$\sigma_{O_i^1}=\sigma_{O_j^{2\circ}}\psi. \tag{5.22}$$

The following theorem is clear.

Theorem V.12: The system of R-vector spaces $\Gamma^k(V;st)$ determines a sheaf over $T^2_{\epsilon,*}(G)$, denoted $\Lambda^k(st)$.

We have the following lemma.

Lemma V.13: The sheaf $\Lambda^k(st)$ is fine.

Proof: Let V_α be a locally finite open cover of $T^2_{\epsilon,*}(G)$ and let $f_\alpha(\eta(\bullet))$ be an associated partition of unity. Let $\sigma_{V,st}$ be a form in $\Gamma^k(V,st)$. We associate $l_\alpha\sigma_{V,st}$ as follows: if we consider a stochastic plot (O,ϕ_i,Ω_i) and the associated finite-dimensional random forms σ_{O_i} over $\phi_i^{-1}(V)=O_i$ over Ω_i, we consider for $l_\alpha\sigma_{V,st}$ the form $f_\alpha(\phi_i)\sigma_{O_i}$.

Definition V.14: We define the stochastic exterior derivative as a morphism of the sheaf $\Lambda^k(st)$ into the sheaf $\Lambda^{k+1}(st)$ as follows: we consider $\sigma_{V,st}\in\Gamma^k(V,st)$ and a stochastic plot (O,ϕ_i,Ω_i). It corresponds to a finite-dimensional random form σ_{O_i} over $O_i=\phi_i^{-1}U$ over Ω. The form corresponding to $\mathrm{d}\sigma_{V,st}$ by using this stochastic plot is $\mathrm{d}\sigma_{O_i}$. By the naturality of the finite-dimensional exterior derivative, the set of $\mathrm{d}\sigma_{O_i}$ satisfy clearly to the properties of Definition V.11.

Lemma V.15: Let $\tilde{S}^{-1}$ be the constant real sheaf over $T^2_{\epsilon,*}(G)$. $\tilde{S}^{-1}\to\Lambda^0(st)\to\cdots\Lambda^k(st)\to\Lambda^{k+1}(st)\cdots$ constitutes a resolution of the constant sheaf S^{-1}.

Proof: The proof is exactly the same proof of Lemma 4.3. of Ref. 40. We use a contractible neighborhood $U\subseteq V$ where V is an open subset of $T^2_{e,\epsilon,*}(G)$ for the strong Hoelder topology as it was defined in the beginning of this part, and the retraction map defined in (5.3) $g(\bullet)\to\Psi(t,\eta(\bullet))$ after extending the logarithm of the Lie group into a smooth bounded functional with bounded derivatives over the whole space R^N. If (O,ϕ_i,Ω_i) is a plot, we use the extended plot $\phi_i^{\mathrm{ext}}(t,u)=\Psi(t,\phi_i(u))$ defined over $O\times[0,1]$. If $O_i=\phi_i^{-1}(U)$ over Ω_i, the main remark is that $(\phi_i^{\mathrm{ext}})^{-1}(U)$ contains $O_i\times[0,1]$ almost surely over Ω_i. We conclude by using the Cartan formula which gives the Lie derivative of a form in terms of its exterior derivative as in Ref. 36 and in Ref. 40. Let g_λ be the retraction $(u,\epsilon)\to(u,\lambda_\epsilon)$. We get if $\sigma_{U,st}$ is a closed stochastic form over U:

$$\sigma^{\mathrm{ext}}_{O_i\times[0,1]}=g_0^*\sigma^{\mathrm{ext}}_{O_i\times[0,1]}+\mathrm{d}\int_0^1 g_\lambda^* i_{(\partial g_\lambda/\partial\lambda)}\sigma^{\mathrm{ext}}_{O_i\times[0,1]}\,\mathrm{d}\lambda. \tag{5.23}$$

If the degree of $\sigma_{U,st}$ is strictly positive, $g_0^*\sigma^{\mathrm{ext}}_{O_i\times[0,1]}=0$ and

$$\sigma^{\mathrm{ext}}_{O_i\times[0,1]}=\mathrm{d}\int_0^1 g_\lambda^* i_{(\partial g_\lambda/\partial\lambda)}\sigma^{\mathrm{ext}}_{O_i\times[0,1]}\,\mathrm{d}\lambda. \tag{5.24}$$

Therefore

$$\sigma^{\text{ext}}_{O_i\times\{1\}}=\sigma_{O_i}=\mathrm{d}_u\int_0^1 g_\lambda^* i_{(\partial g_\lambda/\partial\lambda)}\sigma^{\text{ext}}_{O_i\times[0,1]}\,\mathrm{d}\lambda \tag{5.25}$$

and $\int_0^1 g_\lambda^* i_{(\partial g_\lambda/\partial\lambda)}\sigma^{\text{ext}}_{O_i\times[0,1]}\,\mathrm{d}\lambda$ defines a form $\overline{\sigma}_{U,st}$ over U.

If the degree of the stochastic form is equal to 0, we have

$$\sigma_{O_i}=\sigma^{\text{ext}}_{O_i\times\{0\}}=\sigma^{\text{ext}}_{O_i\times\{1\}}=C, \tag{5.26}$$

where C is almost surely constant and does not depend of the plot by property (ii) of Definition V.11. □

We deduce from the previous two lemmas:

Theorem V.16: the stochastic de Rham cohomology of degree k of $T^2_{\epsilon,*}(G)$ is equal to the sheaf cohomology of degree k of $T^2_{\epsilon,*}(G)$.

Corollary V.17: The stochastic de Rham cohomology groups of $T^2_{\epsilon,*}(G)$ are equal to the deterministic de Rham cohomology groups of $T^2_{\epsilon,*}(G)$.

We could give the definition of a general stochastic Z-valued form on $T^2_{\epsilon,*}(G)$ and the definition of the boundary of a random simplex as it was done in Ref. 34. We could do the definition of a random cycle as it was done in Ref. 34. But for the sequel, we need only to do this for a one-form and for stochastic curves: let $[a,b]$ be an interval and a random plot associated to this interval l (we skip the technicalities coming up when we consider the closed interval $[a,b]$ and not an open interval $]a,b[$). We write $l=([a,b],\phi_i,\Omega_i)$. Let σ_{st} be a stochastic one form. We consider $l^*\sigma_{st}$ defined over Ω_i by σ_i and over Ω_i we define

$$\int_l\sigma_{st}=\int_a^b\sigma_i\,. \tag{5.27}$$

We can consider a sum or a difference l of oriented random plots l^k with oriented boundaries and we say they constitute a one-dimensional cycle l if their random boundaries (which are constituted by random points in $T^2_{\epsilon,*}(G)$) cancel. We set

$$\int_l\sigma_{st}=\sum\int_{l^k}\sigma_{st}\,. \tag{5.28}$$

In the following, we will do the following hypothesis.

Hypothesis H.1: $T^2_{\epsilon,*}(G)$ is connected.

This allows us to define a stochastic curve joining $e(\bullet)$ to $\eta(\bullet)$. We work over $V(\eta(\bullet),r,r')$. If $\eta(\bullet)$ belongs to this contractible set, we choose by using (5.3) a distinguished curve joining $\eta_{sm}(\bullet)$ to $\tilde{g}(\bullet)$, and we choose a deterministic curve joining $e(\bullet)$ to $\eta_{sm}(\bullet)$. We find a countable cover of $T^2_{\epsilon,*}(G)$ by such contractible open sets, and we deduce a measurable countable partition of Ω into Ω_i such that over each Ω_i, $\eta(\bullet)$ belongs to only one of the selected contractible set of $T^2_{\epsilon,*}(G)$. This allows to give an example of stochastic curve joining $e(\bullet)$ to $\tilde{g}(\bullet)$. It is a sum of oriented stochastic intervals l_k ($0\leqslant k\leqslant n$, n deterministic) such that the end of l_j coincides with the beginning of l_{j+1} over each measurable set Ω_i defining this plot and such that the end of l_n is $\eta(\bullet)$.

Let $\mathrm{d}\mu$ the image law of $\eta(\bullet)=g_1(\bullet)$ over $T^2_{\epsilon,*}(G)$.

Definition V.18: Let σ_{st} be a closed Z-valued one-form. Let k be an integer. The generalized Wess–Zumino–Novikov–Witten model of level k associated to the stochastic form on the torus is given by the measure over $T^2_{\epsilon,*}(G)$:

$$\mathrm{d}\mu_k=\exp\left[i2\pi k\int_l\sigma_{st}\right]\mathrm{d}\mu, \tag{5.29}$$

where l is a stochastic curve joining $e(\bullet)$ to $\eta(\bullet)$.

We remark, since the form σ_{st} is Z-valued, that the expression $\exp[i2\pi k\int_l \sigma_{st}]$ does not depend almost surely of the stochastic curve joining $e(\bullet)$ to $\eta(\bullet)$. Namely, if l and l' are two stochastic curves joining $e(\bullet)$ to $\eta(\bullet)$, $\int_l \sigma_{st}$ and $\int_{l'} \sigma_{st}$ differ by a random integer.

VI. STOCHASTIC WESS–ZUMINO TERM AND LINE BUNDLE

Let us consider the three-form closed ω on the simple Lie group G Z-valued ω and which, at the level of the Lie algebra, is equal to

$$\omega(X,Y,Z)=\frac{1}{8\pi^2}\langle [X,Y],Z\rangle. \tag{6.1}$$

We extend ω in a three-form over R^N. Let us introduce the stochastic one-form

$$\sigma_{st}=\int_{T^2}\omega=\int_{T^2}\langle \omega(\eta(s,t)),\mathrm{d}_s\eta(s,t),\mathrm{d}_t(\eta(s,t))\rangle, \tag{6.2}$$

σ_{st} is a stochastic one-form in the sense of Sec. V. Let $u\in O\subseteq R^m\to\{S\to F_i(u,S,\eta(S))\}$ be a stochastic plot where $S\to F_i(u,S,\eta(S))$ belongs to $T^2_{\epsilon,*}(G)$ over Ω_i where the Ω_i constitute a measurable partition of Ω. We write

$$\sigma_O(X)=\int_{T^2}\langle \omega(F_i(u,S,\eta(S))),\mathrm{d}_sF_i(u,S,\eta(S)),\mathrm{d}_tF_i(u,S,\eta(S)),\partial_X F_i(u,S,\eta(S))\rangle, \tag{6.3}$$

where X is a vector field on O. It realizes by theorem IV.2 a random one form over $O\subseteq R^m$, which checks by the approximation procedures of the double stochastic integral, the condition of compatibility of definition V.11.

If we consider the polygonal approximation $\eta^N(S)$ of $\eta(S)$ and if we replace in $\sigma_{st}\eta(S)$ by $\eta^N(s)$, we get a random form σ_O^N over the finite-dimensional set O which tends in L^2 for the C^k topology over each compact of O to σ_O.

Theorem VI.1: Let us suppose G simple, such that ω is closed and Z-valued. Then σ_{st} is a stochastic form which is closed Z-valued.

Proof: σ_{st} defines a true form σ over the space of piecewise differentiable maps from T^2 into G, which is closed Z-valued because ω is closed Z-valued (see Refs. 50 and 23). Let us show that it is Z-valued. We consider a loop in $T^2_{sm}(G)$ where $T^2_{sm}(G)$ denotes the set of piecewise differentiable maps from T^2 into G. This gives since T^2 has no boundary a three-dimensional cycle V in G. But $\int_l\sigma=\int_V\omega\in Z$, because ω is Z-valued.

σ is closed, because it corresponds to a Chen form over the loop space of the loop space. The associated two-form over the loop space is $\alpha=\int_{S^1}\langle\omega(\eta_s),\mathrm{d}_s\eta_s,\bullet,\bullet\rangle$, which is closed over the loop space. Therefore, $\mathrm{d}\sigma_O^N=0$ which tends in L^2 for the C^k topology to $\mathrm{d}\sigma_O$. Therefore $\mathrm{d}\sigma_O=0$ almost surely.

Let l be a one-dimensional stochastic cycle in the space $T^2_{\epsilon,*}(G)$ defined as in Sec. V. We can approach it by stochastic cycles l^N but with values in the set of piecewise differentiable maps from T^2 into G. Moreover, by the rule of approximations of stochastic integrals, $\int_{l^N}\sigma\to\sigma_{st}$ in L^2. But $\int_{l^N}\sigma$ belongs to Z almost surely. This shows that $\int_l\sigma_{st}$ belongs to Z almost surely. □

Definition VI.2: The Wess–Zumino term is $\exp[2i\pi k\int_l\sigma_{st}]$ for l a random curve in the sense of Sec. V, joining the constant torus to $g(\bullet)$. The Wess–Zumino–Novikov–Witten measure is

$$\mathrm{d}\mu_k=\exp\left[2i\pi k\int_l\sigma_{st}\right]\mathrm{d}\mu. \tag{6.4}$$

Remark: There is a curve l_{st} in some sense canonical with the definition of the measure which joins $e(\bullet)$ to $\eta(\bullet)=g_1(\bullet)$. It is the curve $u\to g_u(\bullet)$. We could define the three-dimensional stochastic integral

$$\int_V \omega = \int_{[0,1]\times T^2} \langle \omega(g_u(S)), \mathrm{d}_s g_u(S), \mathrm{d}_t g_u(S), \mathrm{d}_u g_u(S)\rangle = \int_{l_{st}} \sigma_{st} \tag{6.5}$$

such that the stochastic Wess–Zumino term satisfies almost surely to

$$\exp\left[2i\pi k \int_l \sigma_{st}\right] = \exp\left[2i\pi k \int_{l_{st}} \sigma_{st}\right]. \tag{6.6}$$

We can introduce a stochastic two-form $\tau(\omega)$ (see Ref. 10)

$$\tau_{st}(\omega) = \int_{S^1} \langle \omega(\eta(S)), d_s \eta(S), \bullet, \bullet\rangle \tag{6.7}$$

and show it defines a Z-valued two-form over the loop space $L_t(G) s \to \eta(s,t)$ by repeating the considerations of Refs. 36, 37, 38, 34, 39, and 40 by considering the following poor diffeology.

Definition VI.3: A stochastic plot of dimension m of $L_t(G)$ is given by a countable family (O, ϕ_i, Ω_i) where O is an open subset of R^m such that

(i) The Ω_i constitute a measurable partition of Ω.
(ii) $\phi_i(u)(\bullet) = \{s \to F_i(u,s,\eta(s,t))\}$ where F_i is a smooth function over $O \times S^1 \times R^N$ with bounded derivatives of all orders.
(iii) On Ω_i, for all $u \in O$, $\phi_i(u)(\bullet)$ belongs to the loop group $L(G)$.

We identify two stochastics plots $(O, \phi_i^1, \Omega_i^1)$ and $(O, \phi_j^2, \Omega_j^2)$ if $\phi_i^1 = \phi_j^2$ almost surely over $\Omega_i^1 \cap \Omega_j^2$.

If $\phi_i(u)$ is a stochastic plot,

$$\phi_i^* \tau_{st}(\omega)(X,Y) = \int_{S^1} \langle \omega(F_i(u,s,\eta(s,t))), \mathrm{d}_s F_i(u,s,\eta(s,t)), \partial_X F_i(u,s,\eta(s,t)), \partial_Y F_i(u,s,\eta(s,t))\rangle \tag{6.8}$$

if (X,Y) are two vector fields on O. We consider the stochastic one-form

$$\beta_{st} = 1/2 \int_{S^1} \langle g(s,t)^{-1}\, \mathrm{d}_s \eta(s,t), \eta(s,t)_\bullet^{-1}\rangle \mathrm{d}s. \tag{6.9}$$

Let us consider a stochastic plot (O, ϕ_i, Ω_i):

$$\beta_O(X) = 1/2 \int_{S^1} \langle F_i(u,s,\eta(s,t))^{-1}\, \mathrm{d}_s F_i(u,s,\eta(s,t)), F_i(u,s,\eta(s,t))^{-1} \partial_X F_i(u,s,\eta(s,t))\rangle \tag{6.10}$$

if u belongs to the finite-dimensional open set O of R^m and X is a vector field over O. It defines by the rules of line integrals of Sec. III a stochastic one-form over $L_t(G)$ if we extend $g \to g^{-1}$ into a smooth functional from R^N into R^N with bounded derivatives of all orders.

We consider the canonical two-form over $L_t(G)$ (see Ref. 57),

$$\sigma_{st} = \int_{S^1} \langle \eta(s,t)^{-1} \bullet, \mathrm{d}_s(\eta(s,t)^{-1} \bullet)\rangle. \tag{6.11}$$

The pullback of this form through a plot is

$$\sigma_O(X,Y)=\int_{S^1}\langle F(u,s,\eta(s,t))^{-1}\partial_X F(u,s,\eta(s,t)),\mathrm{d}_s(F(u,s,\eta(s,t))^{-1}\partial_Y F(u,s,\eta(s,t))\rangle + \text{antisymmetry}, \tag{6.12}$$

where X and Y are two vector fields over the parameter space O which defines the plot.

By using the approximations of the line integrals given in Sec. III, we get (see Ref. 57, p. 49)

$$\mathrm{d}\beta_{st}=\tau_{st}(2\pi\omega)-\sigma_{st}. \tag{6.13}$$

We can look the apparatus of Refs. 35, 34, 36, and of Ref. 44 to define a stochastic line bundle ξ_t over $L_t(G)$, whose curvature is $2\pi k\tau_{st}(\omega)$ for k an integer. Let us recall how to do that (see Ref. 35, pp. 463–464): let ζ_i be a countable system of finite energy loops in the group such that the balls O_i of radius δ for the uniform norm centered in ζ_i determine an open cover of $L(M)$. We can suppose that δ is small. The loop ζ_i constitutes a distinguished point in O_i. We construct if ζ belongs to O_i a distinguished curve joining ζ to ζ_i called $l(\zeta_i,\zeta)$ since δ is small $\zeta_i(s)$ and $\zeta(s)$ are joined by a unique geodesic for the Lie group structure. $l_u(\zeta_i,\zeta)$ is the loop $s\to\exp_{\zeta_i(s)}\times[u(\zeta(s)-\zeta_i(s))]$ where $\zeta(s)-\zeta_i(s)$ is the vector of the unique geodesic joining $\zeta_i(s)$ to $\zeta(s)$ and exp the exponential of Lie group associated to the canonical Riemannian structure over the Lie group. This allows us to define over O_i a distinguished path joining $\zeta(\bullet)$ to $\zeta_i(\bullet)$. We get a distinguished path joining $e(\bullet)$ to $\zeta_i(\bullet)$, $l_i(e(\bullet),\zeta_i(\bullet))$ and, by concataining these two paths, we get a distinguished path joining $\zeta(\bullet)$ to $e(\bullet)l_i(\zeta(\bullet),\zeta_i(\bullet))$ over O_i.

The second step is to specify a distinguished surface bounded by $l_i(e(\bullet),\zeta(\bullet))$ and $l_j(e(\bullet),\zeta(\bullet))$, where $\zeta(\bullet)\in O_i\cap O_j$. We suppose $O_i\cap O_j$ nonempty. Since δ is small, there is a path $u\to\exp_{\zeta_i(\bullet)}[u(\zeta_j(\bullet)-\zeta_i(\bullet))]$ joining $\zeta_i(\bullet)$ to $\zeta_j(\bullet)$. Because $L(G)$ is supposed simply connected, we can fill in by a surface the deterministic triangle constituted by the path joining $e(\bullet)$ to ζ_i, the path joining ζ_i to ζ_j and the path joining ζ_j to $e(\bullet)$. We can moreover fill in the small stochastic triangle constituted by $l_\bullet(\zeta_i,\zeta)$, $l_\bullet(\zeta_j,\zeta)$ and the path $u\to\exp_{\zeta_i(\bullet)}[u(\zeta_j(\bullet)-\zeta_i(\bullet))]$ by a surface which uses exponential maps joining $l_t(\zeta_i,\zeta)(s)$ and $l_t(\zeta_j,\zeta)$. We can glue the small stochastic surface and the big deterministic surface which are obtained by this procedure. We get a surface $B^t_{i,j}(g(\bullet))$ which satisfies to our requirement. We can integrate $\tau_{st}(2\pi\omega)$ over this surface $B^t_{i,j}(\zeta(\bullet))$ by using the techniques of Sec. III. We set

$$\rho^t_{i,j}(\zeta(\bullet))=\exp\left[-\sqrt{-1}k\int_{B^t_{i,j}(\zeta(\bullet))}\tau_{st}(2\pi\omega)\right] \tag{6.14}$$

[see Ref. 35 (2.28)].

Definition VI. 4: A measurable section ϕ of the line bundle ξ^t associated to the stochastic transgression $\tau_{st}(2\pi\omega)$ over $L_t(G)$ is a collection of random variables $\alpha^t_i L_t(G)$ measurable over O_i with values in C submitted to the rules

$$\alpha^t_j=\alpha^t_i\rho^t_{i,j} \tag{6.15}$$

almost surely over $O_i\cap O_j$. The Hilbert space of sections Ξ^t of the line bundle ξ^t is the space of measurable sections of ξ^t such that

$$E[\|\alpha^t\|^2]<\infty, \tag{6.16}$$

where $\|\alpha^t\|=\|\alpha^t_j\|$ over O_j, definition which is consistent because $\rho^t_{i,j}$ is of modulus one in (6.15).

In the sequel we consider $L^2(\Xi^t)\otimes L^2(\mu)$.

We have a process which applies $L_0(G)$ to $L_t(G)$ by using $t\to(s\to\eta(s,t))$. Let us recall that the parallel transport over a loop l in a simply connected manifold M with curvature R is equal to $\exp[i2\pi\int_\Sigma R]$ where Σ is a two-dimensional surface with boundary l. In the present context, the surface is obtained as follows: we consider the path $t\to\{s\to\eta(s,t)\}$, which defines if we consider the two indices together a torus, and the distinguished path joining this path to $e(\bullet)$ in $T^2_{\epsilon,*}(G)$.

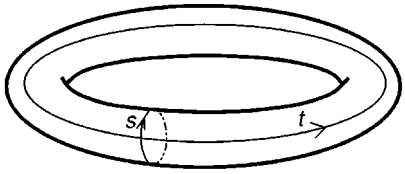

FIG. 1. Torus endowed with the two canonical cycles. The oriented vertical cycle is endowed with the time *s*. The canonical horizontal cycle is endowed with time *t*.

This produces a distinguished stochastic surface Σ in $L(G)$, and therefore a volume V in G whose boundary is $\eta(\bullet)$. $\exp[2\pi\sqrt{-1}k\int_\Sigma \tau^{st}(\omega)]=\exp[2\pi\sqrt{-1}k\int_V \omega]$. The theory of Ref. 44, but in a simpler case, because we do not have to use Deligne cohomology allows us to exhibit a stochastic parallel transport $\tau_{0,1}$ from $L^0(G)$ into $L^0(G)$ which realizes a map from $L^2(\Xi^0)\otimes L^2(\mu)$ into itself. (See Fig. 1.) (Also see Refs. 15–17, 28, 48, 55, 62, 63, 65, and 66.)

Theorem VI.5: We find

$$\int \mathrm{d}\mu_k = E_\mu[\mathrm{Tr}(\tau_{0,1})], \tag{6.17}$$

where $\tau_{0,1}$ is the stochastic parallel transport over the loop in the loop group $t\to\{s\to\eta(s,t)\}$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Charge density and electric charge in quantum electrodynamics

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(Received 17 March 2003; accepted 8 July 2003)

The convergence of integrals over charge densities is discussed in relation with the problem of electric charge and (nonlocal) charged states in quantum electrodynamics. Delicate points like the domain dependence of local charges as quadratic forms and the class of time smearing ensuring strong convergence of integrals of charge densities are analyzed and shown to be crucial in QED, also for the control of vacuum polarization effects leading to time dependence of the charge (Swieca phenomenon). The possibility of constructing physical charged states in the Feynman–Gupta–Bleuler gauge as limits of local state vectors is discussed, compatibly with the vanishing of the Gauss charge on local states. A modification of the Dirac exponential factor which yields the physical Coulomb fields from the Feynman–Gupta–Bleuler fields is shown to remove the infrared divergence of scalar products of local and physical charged states, allowing for a construction of physical charged fields with well-defined correlation functions with local fields. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623928]

I. INTRODUCTION

The simple relation between charge density and electric charge in classical electrodynamics does not extend trivially to the quantum case, because of problems due to vacuum polarization and infinite volume integration.

Quite generally, the relation between local charges and global conserved charges has been extensively discussed in the seventies, in relation with the proof of the Goldstone theorem[1–4] and it has become standard wisdom in the quantum field theory (QFT) framework in which all the relevant information are carried by the local states.

The problem changes substantially if the relevant charged states are nonlocal, as it is the case of quantum electrodynamics (QED).[5] As a consequence, one cannot rely on the standard strategy of controlling the convergence of local charges on the domain of local states, and in fact the limit of local charges, as quadratic forms, crucially depends on the domain which is considered. Moreover, as discussed by Swieca,[6] on the charged states obtained by applying Coulomb fields to the vacuum, the local charge given by the integral of the density with the standard smearing in space and time does not converge to the electric charge and its limit is even time dependent.

This difficulty requires an analysis of the convergence of suitably time-smeared integrals of the charge density; as we shall see, not only the standard time smearing does not work, but also Requardt's space–time smearing prescription[4] requires a modification in order to obtain the correct result for the renormalized charge. Actually, the basic point is the control of the construction of charged states, which is related to the infrared problem and is a deep nonperturbative problem, both in the general algebraic approach and in the approach which uses fields operators.[7]

Even in perturbation theory a rigorous control on the construction of charged states is far from trivial. In the (positive) Coulomb gauge the (nonlocal) charged fields are difficult to handle[8] and the standard strategy is to use a local formulation at the expense of positivity, as in the Feynman–Gupta–Bleuler gauge. In this case, the charged states should be the obtained by an appropriate

construction in terms of local (unphysical) states. Such a possibility has been advocated by Dirac and Symanzik[9,8] who proposed explicit formulas for nonlocal charged (Coulomb) fields in terms of the local Feynman–Gupta–Bleuler fields. Such a construction, which involves nontrivial ultraviolet and infrared problems has recently been refined by Steinmann (DSS construction, Refs. 10 and 13) on the basis of a perturbative expansion.

An important issue is whether the above states can be constructed only in terms of expectations of the observables or they exist as vectors in a space in which local states are dense. In the latter case, the control of limits of local states requires a topology and the topology defined by the Wightman functions of the local fields is too weak to give a unique space; thus, the possibility of reaching the physical charged states, characterized by a Coulomb delocalization, depends on the choice of a topology. For example, the implicit use of the standard (Krein) metric on the asymptotic fields A_μ^{as} excludes the presence of charged states in the corresponding physical space, as pointed out by Zwanziger in his investigations on the infrared problem in QED.[11] A possible nonperturbative construction of physical charged states as limits of local states was discussed in Ref. 12, with the use of a Hilbert–Krein topology which takes into account the effects of the infrared problem. In our opinion, the non uniqueness of such Hilbert–Krein majorant topologies, which are associated to the Wightman functions of the local fields in order to obtain weakly complete inner product spaces of states, should not be regarded as a mathematical oddness, being related to the allowed large distance behavior or ''boundary conditions'' at infinity.

The possibility of constructing physical charged states as limits of local state vectors in a weak topology has been recently denied[13] on the basis of an argument by which the local Gauss charge, corresponding to the integral of $\operatorname{div} E$, vanishes on the local states and therefore on any weak closure of them; thus no weak closure of the local states could contain physical charged states. A main conclusion of our analysis is that the assumptions involved in the argument underestimate the delicate role of such topologies for the convergence of local charges in QED.

In view of the problems which arise in QED, in Sec. II we discuss in general charges defined as limits of quadratic forms, their crucial dependence on the domain and their relation to global charge operators; in particular, attention is paid to the case in which the relevant domains arise by applying nonlocal field operators to the vacuum.

In Sec. III we consider the problem of weak convergence of local charges, which is shown to be very relevant for the Steinmann argument. Strong convergence on the vacuum is shown to be a general consequence of a stronger version of Requardt's theorem, which also allows for an improved time smearing procedure, necessary for obtaining the correct value of the charge on Coulomb charged states. Such a time smearing procedure avoids the time dependence effects due to vacuum polarization while preserving the correct value of the charge.

In Sec. IV, we discuss convergence of Gauss local charges on physical charged states, on the basis of the standard local formulations of QED, the Feynman–Gupta–Bleuler gauge. Quite generally, independently of the use of a Hilbert–Krein topology, it is shown that the construction of physical charged state vectors as limits of local states in a weak topology is incompatible with convergence, in the same weak topology, of the Gauss local charges, even with a time smearing a la Requardt, on local states. A simple model is discussed which mimics the relation between charge density and charge in QED and displays the compatibility between the vanishing of the Gauss charge on a dense domain of local states and its strong convergence to a nonzero electric charge on the physical space. In Sec. V we compare the construction of physical charged states of Ref. 12 with the DSS construction analyzed by Steinmann.[10,13] We show that the infrared divergence in the matrix elements of physical charged states with local states is avoided by the modified DSS exponential used in Ref. 12, which only differs from the standard factor by a gauge term. In this way one removes the obstruction pointed out by Steinmann[13] as an argument for the impossibility of constructing physical charged fields with well-defined correlation functions with local fields.

II. CHARGES AS LIMITS OF QUADRATIC FORMS

The analysis of the charge operator in QED presents subtle features arising from the Coulomb delocalization of charged states.[5,12] It is therefore convenient to start by an analysis of charges as integrals over a local density on general (not necessarily local) domains.

In this section we shall show that (i) charges defined as limits of quadratic forms Q_R on dense domains $\mathcal{D}\times\mathcal{D}$ in general (including the quantum field theory case) crucially depend on the domain; e.g., Q_R may converge to zero on $\mathcal{D}\times\mathcal{D}$ and have a nonzero limit on $\mathcal{D}_1\times\mathcal{D}_1$, if $\mathcal{D}\cap\mathcal{D}_1$ is not dense, (ii) such a phenomenon cannot occur if Q_R converges weakly on $\mathcal{D}$ and on $\mathcal{D}_1$.

Quite generally, in quantum field theory the problem of associating an (unbroken) charge Q to the integral over a local density

$$Q_R=\int_{|x|\leqslant R} \mathrm{d}x\, j_0(x,0), \quad \partial_\mu j^\mu=0,$$

is delicate and deserves special attention. Intuitively, one thinks of defining a state of charge q, as satisfying

$$Q\,\Psi=\lim_{R\to\infty} Q_R\Psi=q\Psi,$$

but as emphasized by Schoer and Stichel,[14] the limit does not exist as a weak limit, even if some smearing in time is made with $\alpha(x_0)$, $\alpha\in\mathcal{D}(\mathbf{R})$ and even if Ψ is a local state, briefly $\Psi\in\mathcal{D}_0$. In the latter case, the limit exists[3] as a sesquilinear form on $\mathcal{D}_0\times\mathcal{D}_0$,

$$\lim_{R\to\infty}(\Phi, Q_R\Psi)=Q(\Phi,\Psi), \quad \Phi,\Psi\in\mathcal{D}_0.$$

Furthermore, if Q_R defines an unbroken symmetry on the local fields the limit sesquilinear form defines an (Hermitian) operator Q on $\mathcal{D}_0$.

A. Domains and limits of quadratic forms

In general, the limit of Hermitian operators Q_R as forms on domains $\mathcal{D}\times\mathcal{D}$, crucially depends on the domain $\mathcal{D}$, in particular, the limit on $\mathcal{D}\times\mathcal{D}$ does not constrain the limit on $\mathcal{D}_1\times\mathcal{D}_1$, $\mathcal{D}_1\neq\mathcal{D}$.

Such a domain dependence in general persists, as shown by the example below, even if Q_R converges to an Hermitian sesquilinear form Q on $\mathcal{D}\times\mathcal{D}$ satisfying the boundedness condition

$$|Q(\Phi,\Psi)|\leqslant C_\Psi\|\Phi\|, \quad \forall\Phi,\Psi\in\mathcal{D}, \tag{2.1}$$

and therefore identifies an (Hermitian) operator Q with domain $\mathcal{D}$. Furthermore, even if Eq. (2,1) holds, it is not at all guaranteed that, $\forall\,\chi$,

$$(\chi, Q\Psi)=\lim_{R\to\infty}(\chi, Q_R\Psi), \quad \forall\Psi\in\mathcal{D}. \tag{2.2}$$

In fact, such an equation means that $Q_R\mathcal{D}$ converge weakly. By the convergence of Q_R on $\mathcal{D}\times\mathcal{D}$, weak convergence of $Q_R\,\mathcal{D}$ is equivalent to the boundedness of the norms $||Q_R\,\Psi||$, for each fixed $\Psi\in\mathcal{D}$.

In particular, as shown by the example below, even if $(\Phi, Q_R\,\Psi)$ converges to zero $\forall\Phi,\Psi\in\mathcal{D}$, one cannot conclude that $\forall\chi$, $\lim_{R\to\infty}(\chi,Q_R\Psi)=0$. [This also shows that the failure of Eq. (2.2) does not depend on Q_R converging to an unbounded or a bounded operator.]

The general phenomenon is that, if Q_R converge to an operator Q_0 on $\mathcal{D}_0\times\mathcal{D}_0$ and to an operator Q_1 on $\mathcal{D}_1\times\mathcal{D}_1$, the two operators Q_0 and Q_1 are in general not related, in the sense of the following:

Definition 2.1: Two densely defined Hermitian operators Q_0, Q_1 are said to be related *if there is an Hermitian operator Q of which Q_0 and Q_1 are restrictions. They will be said to be* weakly related *if there is a densely defined Hermitian operator Q_2 to which both Q_0 and Q_1 are related.*

The above relations are symmetric and the second notion is strictly weaker, since, e.g., different self-adjoint extensions of an Hermitian operator are not restrictions of the same Hermitian operator. An example of limits of quadratic forms which define not weakly related operators is given below.

Example: Let us consider $L^2([0,\pi],\mathrm{d}x)$, $\mathcal{D}_0 \equiv$ the space of C^∞ functions vanishing at the origin, $\mathcal{D}_1 \equiv$ the linear span of $f_1(x) \equiv 1$ and $f_n(x) \equiv \sin nx - \alpha_n \sin x$, $n \geqslant 2$, $\alpha_n \equiv 1/2\int_0^\pi \sin nx$, so that $(f_1, f_n) = 0$.

Clearly, both $\mathcal{D}_0$ and $\mathcal{D}_1$ are dense domains; in fact, if f is orthogonal to $\mathcal{D}_1$ one has

$$c_n \equiv (f, \sin nx) = \alpha_n (f, \sin x) = \alpha_n c_1, \quad n \geqslant 2.$$

Furthermore

$$0 = (\pi/2) \int_0^\pi \mathrm{d}x\, f(x) = \sum_{n \geqslant 1} c_n \int_0^\pi \mathrm{d}x \sin nx = 2\left(\sum_{n \geqslant 2} \alpha_n^2 c_1 + c_1 \right)$$

implies $c_1 = 0$, i.e., $f = 0$. Now, let Q_R be the multiplication operator by a regular function $q_R(x)$ converging to $\delta(x)$ as a distribution; then

$$(\mathcal{D}_0, Q_R \mathcal{D}_0) \to 0, \quad (\mathcal{D}_1, Q_R \mathcal{D}_1) \to (\mathcal{D}_1, P_1 \mathcal{D}_1) \neq 0,$$

with P_1 the projection on f_1. Thus, the limits of the Hermitian operators Q_R define two bounded operators which are not even weakly related.

Convergence of Q_R on $\mathcal{D}_0 \times \mathcal{D}_0$ to an operator Q_0 constrains convergence to an operator on any domain $\mathcal{D} \times \mathcal{D}$, such that $\mathcal{D} \cap \mathcal{D}_0$ is dense.

Proposition 2.1: Let the Hermitian operators Q_R converge to an operator Q_0 on $\mathcal{D}_0 \times \mathcal{D}_0$ and to an operator Q_1 on $\mathcal{D}_1 \times \mathcal{D}_1$;

(i) *if $\mathcal{D}_1 \cap \mathcal{D}_0$ is dense, then Q_0 and Q_1 are weakly related;*
(ii) *if $\mathcal{D}_1 \supset \mathcal{D}_0$, then Q_0 and Q_1 are related;*
(iii) *in both cases, if Q_0 is essentially self-adjoint on $\mathcal{D}_1 \cap \mathcal{D}_0$, then Q_1 is contained in the closure of Q_0;*
(iv) *if Q_0 and Q_1 are not related, then Q_R does not converge to an operator Q on $\mathcal{D} \times \mathcal{D}$, $\mathcal{D} = \mathcal{D}_0 + \mathcal{D}_1$.*

Proof: The Hermiticity of Q_R implies that both Q_i, $i = 0, 1$ are densely defined Hermitian operators and so is their restriction Q to $\mathcal{D}_1 \cap \mathcal{D}_0$. In case (ii) Q_1 extends Q_0, in case (i) Q_1 and Q_0 extend Q. If Q_R converge to Q on $\mathcal{D} \times \mathcal{D}$, both Q_0 and Q_1 are restrictions of Q, so that Q_0 and Q_1 are related.

Proposition 2.2: If both $Q_R \mathcal{D}_0$ and $Q_R \mathcal{D}_1$ converge weakly, then the two limits define Hermitian operators Q_0 and Q_1 which are related.

Proof: Hermiticity of the limit forms follows from that of Q_R and the existence of weak limits implies that the limit forms define operators Q_0 on $\mathcal{D}_0$ and Q_1 on $\mathcal{D}_1$. The weak limit of Q_R exists also on $\mathcal{D}_0 + \mathcal{D}_1$ and by the same argument defines an Hermitian operator Q which extends Q_0 and Q_1.

As a result, if Q_0 is essentially self-adjoint, Q_1 is contained in its closure and in particular if $Q_0 = 0$, also $Q_1 = 0$, in other terms if $Q_R \mathcal{D}_0$ converges to zero weakly and $Q_R \mathcal{D}_1$ converges weakly, then $Q_1 = 0$.

B. Convergence of local charges in quantum field theory

A general situation which occurs in quantum field theory is described in terms of translational invariant (field) algebras $\mathcal{A}_0$, $\mathcal{A}_1$, a (unique translationally invariant) cyclic vector Ψ_0, domains

$$\mathcal{D}_0=\mathcal{A}_0\Psi_0, \quad \mathcal{D}_1=\mathcal{A}_1\Psi_0,$$

and local Hermitian charges Q_R, with domains containing $\mathcal{D}_0$ and $\mathcal{D}_1$ and with $(\Psi_0, Q_R\Psi_0)=0$. In general, Q_R is the integral of the zero component of a local conserved (operator valued tempered distribution) current j_μ with suitable smearing:

$$Q_R=\int \mathrm{d}^4x\, j_0(\mathbf{x},x_0)\, f_R(\mathbf{x})\, \alpha(x_0)=j_0(f_R\,\alpha), \tag{2.3}$$

$$f_R(x)=f(|x|/R)\in\mathcal{D}(\mathbf{R}^3), \quad f(x)=1, \text{ if } |x|\leqslant 1, \ f(x)=0, \text{ if } |x|\geqslant 2,$$

$$\alpha\in\mathcal{D}(\mathbf{R}), \quad \text{supp } \alpha\subset[-a,a],\ a<1, \ \int \mathrm{d}t\, \alpha(t)=1.$$

If $\mathcal{A}_0$ is a local (field) algebra and $(\mathcal{D}_0, Q_R\mathcal{D}_0)$ converges as $R\to\infty$, the limit defines an operator Q_0, iff

$$\lim_{R\to\infty}(\Psi_0, [Q_R, \mathcal{A}_0]\Psi_0)=0, \tag{2.4}$$

equivalently[3] iff

$$\lim_{R\to\infty}(\mathcal{D}_0, Q_R\Psi_0)=0. \tag{2.5}$$

Nonlocal algebras may be relevant in the discussion of nonlocal states, e.g., asymptotic states, or charged states in the Coulomb gauge; a local and a nonlocal field algebra, $\mathcal{A}_0$ and $\mathcal{A}_1$, occur in the construction of charged states in QED.

Proposition 2.3: Let $\mathcal{D}=\mathcal{A}\Psi_0$, $\mathcal{A}$ an algebra invariant under translations; if on $\mathcal{D}\times\mathcal{D}$, Q_R converge to an operator Q, then

$$\lim_{R\to\infty}(\mathcal{D}, Q_R\Psi_0)=0. \tag{2.6}$$

Proof: The spectral representations of the space translations gives

$$((U(\mathbf{a})-1)^4A\Psi_0, Q_R\Psi_0)=\int \mathrm{d}J_A(\mathbf{k})(e^{i\mathbf{k}\cdot\mathbf{a}}-1)^4R^3\tilde{f}(R\mathbf{k}), \quad \forall A\in\mathcal{A}, \tag{2.7}$$

where $\mathrm{d}J_A(\mathbf{k})=\int \mathrm{d}J_A(\mathbf{k},k_0)\,\tilde{\alpha}(k_0)$ is a complex measure of polynomial growth. Now, since for any polynomial $P(\mathbf{k})$,

$$|(e^{i\mathbf{k}\cdot\mathbf{a}}-1)^4\,R^3\tilde{f}(R\mathbf{k})\,P(\mathbf{k})|\leqslant\frac{|R\mathbf{k}\cdot\mathbf{a}|^4}{R}|\tilde{f}(R\mathbf{k})P(R\mathbf{k})|\left|\frac{P(\mathbf{k})}{P(R\mathbf{k})}\right|\leqslant\frac{C}{R}\to 0,$$

in the limit $R\to\infty$, the right-hand side (rhs) of Eq. (2.6) converges to zero and therefore, by the density of $\mathcal{D}$, one has

$$(U(\mathbf{a})-1)^4\,Q\,\Psi_0=0, \quad \forall\,\mathbf{a}.$$

Then, since $U(\mathbf{a})-1$ is a normal operator, it follows that $(U(\mathbf{a})-1)\,Q\,\Psi_0=0$, and by the uniqueness of the translationally invariant state $Q\Psi_0=\lambda\Psi_0$; actually $Q\,\Psi_0=0$, because $(\Psi_0, j_0\Psi_0)=0$.

Thus, under the same assumptions, one has that the charge Q' defined in terms of the limit of the commutator,[15] coincides with Q, i.e.,

$$(\mathcal{D}, Q'\,A\Psi_0)\equiv \lim_{R\to\infty}(\mathcal{D}, [Q_R, A]\,\Psi_0)=\lim_{R\to\infty}(\mathcal{D}, Q_R A\Psi_0). \tag{2.8}$$

The domain dependence of charge operators obtained as limits of quadratic forms appears also in the above quantum field theory framework. In particular, as a result of Proposition 2.1, if Q_R converges to zero on $\mathcal{D}_0\times\mathcal{D}_0$, the convergence to a nonzero operator on $\mathcal{D}_1\times\mathcal{D}_1$ is excluded if $\mathcal{D}_1\cap\mathcal{D}_0$ is dense, but may be allowed if $\mathcal{D}_1\cap\mathcal{D}_0$ is not dense, even if $\Psi_0\in\mathcal{D}_1\cap\mathcal{D}_0$.

Such features are illustrated and displayed by the following example.

Example. Let ϕ be a massless scalar field, ψ a free Dirac field, $\mathcal{A}_0$ the algebra generated by $\partial_i\phi$, $i=1,2,3$ and by ψ and $\mathcal{A}$ the algebra generated by $\partial_i\phi$ and by ψ_d, with

$$\psi_d(x)=\psi(x)\,U(x),\quad U(x)=e^{i\phi(f_x)},$$

$$\phi(f_x)=\int \mathrm{d}y\;\phi(y)f(y-x),\quad f\in\mathcal{D}(\mathbf{R}^4),\quad \int \mathrm{d}x\;f(x)=1.$$

Then we consider the local charges

$$Q_R{}^{\phi}\equiv \partial_0\phi(f_R\,\alpha,),\quad Q_R{}^{\psi}\equiv j_0(f_R\,\alpha),\quad j_\mu(x)=:\bar{\psi}\gamma_\mu\psi:,$$

$$Q_R=Q_R{}^{\psi}+Q_R{}^{\phi}$$

and the Fock representation of ψ,ϕ, with Fock vacuum Ψ_0. Since by locality

$$\lim_{R\to\infty}[Q_R{}^{\phi}, \mathcal{A}_0]=0,\quad \lim_{R\to\infty}(\mathcal{D}_0, Q_R\,\Psi_0)=0,$$

we have

$$\lim_{R\to\infty}(\mathcal{D}_0, Q_R\,\mathcal{D}_0)=(\mathcal{D}_0, Q^{\psi}\,\mathcal{D}_0),$$

where Q^{ψ} is the unbroken fermionic charge. On the other hand, since $\lim_R[Q_R, \psi_d(g)]=0$ we have

$$\lim_{R\to\infty}(\mathcal{D}, Q_R\,\mathcal{D})=0.$$

In conclusion Q_R converge to the unbroken fermionic charge on $\mathcal{D}_0\times\mathcal{D}_0$ and to the zero charge on $\mathcal{D}\times\mathcal{D}$.

It is worthwhile to note that the limit of the operators Q_R does not define an operator on $\mathcal{D}_{\text{ext}}\times\mathcal{D}_{\text{ext}}$, where $\mathcal{D}_{\text{ext}}=\mathcal{D}_0+\mathcal{D}$ (since the corresponding bilinear form is discontinuous on the left). Moreover, one has a symmetry breaking condition on the algebra $\mathcal{A}_{\text{ext}}$ generated by $\mathcal{A}_0$ and $\mathcal{A}_1$: $[Q_R, \mathcal{A}_{\text{ext}}]\,\Psi_0$ converges weakly (actually strongly) and

$$\lim_{R\to\infty}(\Psi_0, [Q_R, \psi^{\dagger}\psi_d]\,\Psi_0)\neq 0.$$

This fact is actually a consequence of Q_0 and Q_1 being not related. In general if Q_R converges on $\mathcal{D}_i\times\mathcal{D}_i$, $i=0,1$ to operators Q_i which are not related, then, for the algebra $\mathcal{A}$ generated by $\mathcal{A}_0$ and $\mathcal{A}_1$, one cannot have both weak convergence of $[Q_R, \mathcal{A}]\,\Psi_0$ and

$$\lim_{R\to\infty}(\Psi_0,[\,Q_R,\mathcal{A}]\,\Psi_0)=0. \tag{2.9}$$

In fact, by Eq. (2.6),

$$(\mathcal{D}_i,Q_iA\Psi_0)\equiv\lim_{R\to\infty}(\mathcal{D}_i,[Q_R,A\,]\Psi_0),\quad \forall A\in\mathcal{A}_i.$$

Now, if Eq. (2.9) holds, by a standard argument[15] one gets an Hermitian operator Q on $\mathcal{D}\equiv\mathcal{A}\Psi_0$, which extends Q_0 and Q_1, in contrast with their being not related.

III. CONVERGENCE OF TIME SMEARED INTEGRAL OF CHARGE DENSITY. THE VACUUM SECTOR OF QED

In this section we discuss weak and strong convergence of local charges, in particular in the vacuum sector of QED.

As found by Requardt,[2] the weak limit of Q_R on local states can be obtained under general conditions by a suitable time smearing of the charge density, namely, by considering, with f_R, α as in Eq. (2.3),

$$Q_R\equiv j_0(f_R\,\alpha_R),\quad \alpha_R(x_0)\equiv\alpha(|x_0|/R)/R. \tag{3.1}$$

Actually, one can strengthen Requardt's theorem and obtain strong convergence (Proposition 3.1), also with a more general time smearing $\alpha_{T(R)}$, which will prove necessary in the charged sectors of QED.

We recall that if j_μ is a Lorentz covariant conserved tempered current, the two point function of the charge density is of the form

$$\langle j_0(x)\,j_0(y)\rangle=-\Delta\,J(x-y),$$

with J a Lorentz invariant tempered distribution of positive type; we denote by $\mathrm{d}\nu(k^2)$ the spectral measure defined by J.

Proposition 3.1: If the spectral measure $\mathrm{d}\nu$ *satisfies the (infrared) regularity condition*

$$\mathrm{d}\nu(k^2)=k^2\,\mathrm{d}\sigma(k^2),\quad \mathrm{d}\sigma\ \ a\ \ measure,$$

then, setting $Q_{R,T(R)}\equiv j(f_R\alpha_{T(R)})$ *one has*

(i) $s-\lim_{R\to\infty}Q_{R,R}\,\Psi_0=0$*;*

(ii) $s-\lim_{R\to\infty}Q_{R,T(R)}\,\Psi_0=0$ *for all functions* $T(R)$*, with* $T(R)/R\to 0$*, satisfying* $T(R)>R^{1/3}$ *and* $R\int_0^\varepsilon \mathrm{d}\sigma(s)\,s/(1+T(R)^2s^2)^2\to 0$*,* $\varepsilon>0$ *(such T(R) exist for all* $\mathrm{d}\sigma$*);*

(iii) if, for $k^2\in[0,\varepsilon)$*,* $\varepsilon>0$*,* $\mathrm{d}\sigma(k^2)/\mathrm{d}\,k^2\leqslant C$*, the above strong convergence to zero is obtained by choosing* $T=R^{1/3+\delta}$*,* $\delta>0$*.*

Proof: In fact, one has

$$\|Q_{R,T}\,\Psi_0\|^2=\int \mathrm{d}\nu(k^2)\,\mathrm{d}^3q\,\frac{|\mathbf{q}\tilde{f}(\mathbf{q})|^2}{2\sqrt{(|\mathbf{q}|/R)^2+k^2)}}\,R\,|\tilde{\alpha}(T\sqrt{(|\mathbf{q}|/R)^2+k^2})|^2.$$

Since α is of fast decrease, $\forall\, N\in\mathbf{N}$,

$$|\tilde{\alpha}(T\sqrt{(|\mathbf{q}|/R)^2+k^2})|^2\leqslant\frac{C_N}{1+((T|\mathbf{q}|/R)^2+T^2k^2)^N}\leqslant\frac{C_N}{1+(T^2k^2)^N},$$

and since $\mathrm{d}\nu$ is tempered there is an $M\in\mathbf{N}$ such that $(1+k^2)^{-M}\,\mathrm{d}\sigma(k^2)\equiv\mathrm{d}\sigma'(k^2)$ is a finite measure. Then, by taking $N=M+2$, one has

$$\|Q_{R,T}\Psi_0\|^2 \leqslant C'\frac{R}{T}\int \mathrm{d}\sigma'(s^2)\,\frac{Ts}{(1+T^2s^2)^2} \equiv \frac{R}{T}G(T).$$

The integrand function is bounded and converges to zero pointwise, when $T\to\infty$, so that by the dominated convergence theorem $G(T)\to 0$. Thus (i) is proved; moreover strong convergence to zero holds if one chooses $R=TG(T)^{-1+\delta}$, $\delta>0$ and (ii) follows since $\forall\,\varepsilon>0$,

$$\int_\varepsilon^\infty \mathrm{d}\sigma'(k^2)\,T\sqrt{k^2}/(1+T^2k^2)^2 = O(1/T^3).$$

If the hypothesis of (iii) holds one can bound the integral from 0 to ε by

$$C\int_0^\varepsilon \mathrm{d}s^2\frac{Ts}{(1+T^2s^2)^2} \leqslant \frac{C}{T^2}\int_0^\infty \mathrm{d}u^2\,\frac{u}{(1+u^2)^2} = O(1/T^2).$$

Thus, the strong convergence to zero is obtained if $T(R)=R^{1/3+\delta}$, $\delta>0$.

In the physical vacuum sector $\mathcal{H}_0$ of QED the assumptions of Proposition 3.1 for the spectral measure of the electric current are satisfied since

$$\langle \partial F_0(x)\,\partial F_0(y)\rangle = \int k^2\,\mathrm{d}\rho(k^2)\,\mathrm{d}^3k\,|2\sqrt{\mathbf{k}^2+k^2}|^{-1}\,\mathbf{k}^2 e^{ik(x-y)},\ \partial F_\mu \equiv \partial^\nu F_{\mu\nu},$$

with $\mathrm{d}\rho(k^2)$ the spectral measure of the two point function of $F_{\mu\nu}$. Hence, for $T(R)$ as in (ii) of Proposition 3.1,

$$\lim_{R\to\infty}\|\partial F_0(f_R,\alpha_{T(R)})\,\Psi_0\|^2 = 0 \tag{3.2}$$

and therefore $Q_{R,T(R)}=j_0(f_R\,\alpha_{T(R)})$ converges strongly to zero on the dense domain $\mathcal{D}_0^{ph}$ obtained by applying local bounded observable operators to the vacuum. Equation (3.2) with $T=R$ was also obtained by D'Emilio.[16]

The situation is completely different if one adopts the standard smearing,[1,2] with a fixed $\alpha(x_0)$,

$$\tilde{Q}_R = j_0(f_R\,\alpha).$$

Proposition 3.2: The operators $\tilde{Q}_R$ have the following properties:

(i) *they converge to zero on $\mathcal{D}_0^{ph}\times\mathcal{D}_0^{ph}$;*

(ii) *$\tilde{Q}_R\Psi_0$ does not converge weakly in $\mathcal{H}_0$, nor does $\tilde{Q}_R\Psi$, $\forall\Psi=U\Psi_0$, U a bounded local operator;*

(iii) *there are vectors $\Psi\in\mathcal{H}_0$ such that*

$$\lim_{R\to\infty}\langle\Psi,\tilde{Q}_R\Psi_0\rangle$$

depends on the time smearing test function α (time dependence of the charge)

(iv) *there are operators F such that,*

$$\lim_{R\to\infty}\langle\Psi_0,[\tilde{Q}_R,F]\Psi_0\rangle \neq 0$$

(*Swieca phenomenon*[6]).

Proof: Since in the physical vacuum sector $\tilde{Q}_R=((\partial F))(f_R\,\alpha)$, (i) follows by locality and Maison theorem.[3]

For (ii), the same calculation done above for Q_R now gives

$$\|\tilde{Q}_R \Psi_0\|^2 = R \int k^2 \, \mathrm{d}\rho(k^2) \, \mathrm{d}^3 q \, \frac{|\mathbf{q}\tilde{f}(\mathbf{q})|^2}{2\sqrt{(|\mathbf{q}|/R)^2 + k^2)}} R \, |\tilde{\alpha}(\sqrt{(|\mathbf{q}|/R)^2 + k^2})|^2,$$

so that $\tilde{Q}_R \Psi_0$ cannot converge weakly. Furthermore, $\forall \Psi = U\Psi_0$,

$$\tilde{Q}_R U \Psi_0 = [\tilde{Q}_R, U]\Psi_0 + U\tilde{Q}_R \Psi_0$$

and the first term on the rhs converges by locality; since the second term does not converge weakly, neither does the lhs.

In order to construct the vector Ψ of (iii) we consider

$$\Psi_R \equiv F_{0\,i}((\partial_i \Delta^{-1} g) f_R \, h) \, \Psi_0, \quad g \in \mathcal{D}(\mathbf{R}^3), \quad h \in \mathcal{D}(\mathbf{R}).$$

Such vectors converge strongly to a vector $\Psi \in \mathcal{H}_0$, for $R \to \infty$, since the Fourier transform of $(\Delta^{-1} g)(\mathbf{x}) \, h(x_0)$ is square integrable with respect to the measure $\mathrm{d}\rho(k^2) \, \mathrm{d}^3 k \, |k_0|^{-1} |\mathbf{k}|^2 \, k^2$ defined by the Fourier transform of $<(\partial F)_0(x) \, (\partial F)_0(y)>_0$. Then, we have

$$\lim_{R\to\infty} \langle \Psi, \tilde{Q}_R \Psi_0 \rangle = \lim_{R\to\infty} \int \mathrm{d}\rho(k^2) \, \mathrm{d}^3 k \, |2k_0|^{-1} \, k^2 \tilde{f}_R(\mathbf{k}) \, \tilde{\alpha}(k_0) \, \bar{\tilde{g}}(\mathbf{k}) \, \bar{\tilde{h}}(k_0)$$

$$\to \bar{\tilde{g}}(0) \int \mathrm{d}\rho(m^2) \, m \, \tilde{\alpha}(m) \, \bar{\tilde{h}}(m),$$

which displays the dependence on α.

The operators $F_R \equiv F_{0\,i}((\partial_i \Delta^{-1} g) f_R \, h)$ converge strongly to an operator F on the dense domain $\mathcal{A}_L \Psi_0$, $\mathcal{A}_L$ = the algebra of strictly localized (bounded) observables, since they converge strongly on Ψ_0 and $[F_R, A]$, $A \in \mathcal{A}_L$, becomes independent of R, for R sufficiently large by locality. Then, we have

$$\lim_{R\to\infty} \langle \Psi_0, [\tilde{Q}_R, F] \Psi_0 \rangle = \bar{\tilde{g}}(0) \int \mathrm{d}\rho(m^2) \, m \, (\tilde{\alpha}(m) \, \bar{\tilde{h}}(m) - \tilde{\alpha}(-m) \, \bar{\tilde{h}}(-m))$$

which does not vanish in general.

The vector Ψ reflects the infrared behavior of "dipole states" of the form $\psi_c^\dagger(f) \, \psi_c(g) \, \Psi_0$, where $\psi_c(g)$ is the electron field in the Coulomb gauge, constructed, e.g., according to the Dirac–Symanzik–Steinmann[8,10] prescription. Thus, in QED, even in the vacuum sector, the naive idea of the charge as the integral of the charge density gives rise to substantial problems because of vacuum polarization effects which disappear only with a suitable time smearing. The same problems arise in the charged sectors of the Coulomb gauge, as stressed by Swieca;[6] they are a general consequence of the nonlocality of the charged Coulomb fields.

In general, the standard procedure, Eq. (2.3), corresponds to taking, in the corresponding correlation functions in momentum space, the limit $\mathbf{k} \to 0$ and gives a δ function in ω only in expectations on local states. On the other hand, Requardt time smearing corresponds to taking a limit $\mathbf{k}, \omega \to 0$ on the light cone; in expectations on local states, it coincides with that of the standard smearing and it is α independent. As discussed in the Appendix, α independence does not hold on the (nonlocal) charged states of QED and therefore a modification of Requardt's prescription is required for QED.

IV. CHARGE DENSITY AND CHARGE IN LOCAL FORMULATIONS OF QED

The discussion of charge integrals in the charged sectors is not covered by the standard analysis because, as a consequence of the local Gauss' law, charged states cannot be obtained from the vacuum by local fields. In this section we discuss the limit of the Gauss charges

$$Q_R^G = (\partial F)_0(f_R\, \alpha_R)$$

in the Feynman–Gupta–Bleuler formulation of QED and the implications on the possibility of constructing physical state vectors as weak limits of local states.

A direct discussion in the Coulomb gauge would involve the limit of local charges as quadratic forms on domains obtained from the vacuum by the nonlocal Coulomb fields, with the problems discussed in Sec. II.

Even in perturbation theory the control of the Coulomb gauge is difficult and the standard strategy is to use a local formulation at the expense of positivity; this is the case of the Feynman or Gupta–Bleuler gauge. In this case, the charged fields and the vector potential A_μ are local but their vacuum expectation values cannot satisfy positivity; the corresponding Wightman functions define an indefinite inner product space $\mathcal{D}_0 = \mathcal{F}\Psi_0$ (with $\mathcal{F}$ the local field algebra), with inner product denoted by $\langle .,. \rangle$, which does not contain physical charged states.[5,12]

As suggested by perturbation theory, nonlocal physical charged states may be obtained as suitable limits of local unphysical charged state vectors. A possible nonperturbative construction of physical charged state vectors along these lines was discussed in Ref. 12.

Quite generally, a crucial issue is that the definition and the control of the limit of local charged state vectors requires a topology; even in the positive case the weak topology on $\mathcal{D}_0$ defined by the seminorms $p_y(x) = |\langle x, y \rangle|$, i.e., by the Wightman functions is too weak; on the other hand, the inner product space $\mathcal{D}_0$ does not identify a unique Hilbert–Krein majorant topology τ (Ref. 12) and one has different closures $\mathcal{K}_\tau = \overline{\mathcal{D}_0}^\tau$. For the physical interpretation, the relevant space is the physical subspace $\mathcal{K}'_\tau \subset \mathcal{K}_\tau$, identified by a subsidiary condition (which in QED selects gauge invariant states) and different topologies may give rise to isomorphic physical spaces.

In general, Ref. 12 the dependence of the space $\mathcal{K}'_\tau$ on the topology τ should not be regarded as a mathematical oddness, since different closures of $\mathcal{D}_0$ reflect different "boundary conditions" at infinity. Even in the standard theory of unbounded Hermitian operators the local domain of C^∞ functions of compact support may allow different self-adjoint extensions, corresponding to different boundary conditions; in the physical applications the choice of one instead of the other is dictated by physical considerations.[12,17] In the QED case the lack of nonuniqueness reflects the physical fact that different Hilbert–Krein topologies, defined by majorant inner products $(.,.)$, correspond to different large distance behaviors of the limit states, classified in particular by the velocity parameter of their Lienard–Wiechert electromagnetic fields at large distances.[12] Thus, the choice of the Hilbert–Krein topology is governed by physical considerations since it determines the class of vector states which one can constructively associate to the Wightman functions, i.e., the corresponding closure $\mathcal{K}$ of the vector space $\mathcal{D}_0$. For these reasons it should not be a surprise that $\mathcal{D}_0$ may allow different extensions. Even in the algebraic approach the construction of the charged states, which correspond to nonlocal morphisms of the algebra of observables, is not under sharp control and in any case does not resolve the multiplicity associated to the large distance behavior.[18]

The choice of the Hilbert–Krein topology in local formulations of QED was discussed at length in Ref. 12 also in connection with the Zwanziger unsuccessful attempt to construct physical charged states, as a result of a too restrictive Hilbert–Krein topology.

It has been argued[13] that the Gauss charge converges weakly to zero on the local states as a consequence of the vanishing of the Gauss charge commutators with local fields, and that this prevents the construction of physical state with nonzero Gauss charge as limits of local states. We shall examine the weak points of this argument in order.

First, the vanishing of the Gauss charge commutators with local fields implies the vanishing of the Gauss charge as a quadratic form on $\mathcal{D}_0 \times \mathcal{D}_0$ [see Eq. (2.8) and the Appendix]. The vanishing of the Gauss charge on a closure of $\mathcal{D}_0$ would follow (see Proposition 4.2 below) if one had weak convergence of $Q_R^G \mathcal{D}_0$ in the topology which defines such a closure of $\mathcal{D}_0$.

As we shall see the validity of such a property is not constrained by the correlation functions of the local fields and does not hold in general. Actually (see the Example below and the follow-

ing section) one may find a Hilbert–Krein topology τ which avoids the weak convergence of Q_R^G and allows for the construction of physical charged state vectors.

The failure of the τ-weak convergence of $Q_R^G\mathcal{D}_0$ should not appear strange, since it involves a topology whose role is merely that of linking the physical nonlocal charged states to the unphysical local states. It should be stressed that the Gauss charge Q_R^G may well converge weakly or even strongly on a dense domain $\mathcal{D}^{ph}$ of physical states, with respect to the intrinsic Hilbert topology of the physical space. This means that $\forall\Phi\in\mathcal{H}^{ph}$, $\Psi\in\mathcal{D}^{ph}$ (equivalently $\forall\Phi\in\mathcal{H}'$, $\Psi\in\mathcal{D}'$, where $\mathcal{H}'$ denotes the distinguished subspace of $\mathcal{K}$ satisfying the subsidiary condition and $\mathcal{D}'$ a dense subspace of $\mathcal{H}'$), one has that

$$\lim_{R\to\infty}\langle\Phi,Q_R\Psi\rangle=\lim_{R\to\infty}\langle\Phi,Q_R^G\Psi\rangle,\quad Q_R\equiv j_0(f_R\alpha_R)$$

exists, equivalently

$$\langle Q_R^G\Psi,Q_R^G\Psi\rangle=\|Q_R^G\Psi\|^2 \tag{4.1}$$

are bounded. This, however, does not mean that $Q_R\mathcal{D}'$ or $Q_R^G\mathcal{D}'$ converge weakly with respect to the Hilbert–Krein closure $\mathcal{K}$, since weak convergence in $\mathcal{K}$ amounts to the boundedness of

$$\|Q_R^G\Psi\|_{\mathrm{HK}}^2\equiv(Q_R^G\Psi,Q_R^G\Psi),$$

where $(.,.)$ is the majorant inner product which defines the Hilbert–Krein topology and the corresponding closure $\mathcal{K}$ of the local states $\mathcal{D}_0$.

Actually, independently of any Hilbert–Krein majorant, there is a conflict between the construction of the physical charged states in terms of the Wightman functions of the local field algebra $\mathcal{F}$ and the weak convergence of Q_R^G in the corresponding extension $\mathcal{D}$ of $\mathcal{D}_0$. This difficulty is an intrinsic one, since it only involves the Wightman functions of $\mathcal{F}$ and the existence of the physical charged states in an extension $\mathcal{D}$ of $\mathcal{D}_0$ compatible with the inner product $\langle,\rangle$ defined by the Wightman functions, namely, such that the sequences of elements of $\mathcal{D}_0$ which define the extension, have convergent inner products $\langle,\rangle$.[19] No reference is needed to a Hilbert–Krein majorant topology, even if, clearly, any Hilbert–Krein majorant defines a weak extension. To clarify this point we introduce the following.

Definition 4.1: *Given two vector spaces D_0 and D_1, with inner products $\langle,\rangle^{(0)}$ and $\langle,\rangle^{(1)}$, we say that D_1 can be realized in a weak extension of D_0 if there exists an inner product vector space $\mathcal{V}$ containing a weakly dense inner product subspaces isomorphic to D_0 and a subspace isomorphic to D_1.*

If D_0 and D_1 are defined by the vacuum correlation functions of two field algebras $\mathcal{A}_0$, $\mathcal{A}_1$, the property of D_1 being realized in a extension of D_0 is implied by the existence of joint vacuum correlation functions of $\mathcal{A}_0$ and $\mathcal{A}_1$. In the case of local formulations of QED, if the correlation functions of the physical field algebra $\mathcal{F}_1$, e.g., of the field algebra of the Coulomb gauge, can be constructed in terms of the correlation functions of the local field algebra $\mathcal{F}$, one has an extended field algebra $\mathcal{F}_{\mathrm{ext}}$ generated by $\mathcal{F}$ and $\mathcal{F}_1$, and $\mathcal{D}_1=\mathcal{F}_1\Psi_0$ is realized in an extension of $\mathcal{D}_0=\mathcal{F}\Psi_0$.

Proposition 4.1: *Let D be a nondegenerate vector space with inner product $\langle,\rangle$, D_0 a weakly dense subspace and $D_1\subset D$; let Q_R be Hermitian charges and*

$$\lim_{R\to\infty}\langle D_0,Q_R D_0\rangle=0, \tag{4.2}$$

$$\lim_{R\to\infty}\langle D_1,Q_R D_1\rangle\neq 0. \tag{4.3}$$

Then, $Q_R D$ cannot converge in the weak topology defined by $\langle,\rangle$.

In concrete, if physical charged states Ψ may be obtained as limits of the local states of $\mathcal{D}_0$ in a Hilbert–Krein topology τ, i.e., they belong to a (Hilbert–Krein) extension $\mathcal{D}$ of $\mathcal{D}_0$ and

$$\lim_{R\to\infty}\langle\mathcal{D}_0, Q_R^G\Psi\rangle=\langle\mathcal{D}_0, Q\Psi\rangle\neq 0, \quad \lim_{R\to\infty}\langle\mathcal{D}_0, Q_R^G\Psi_0\rangle=0, \tag{4.4}$$

then $Q_R^G\mathcal{D}_0$ cannot converge weakly with respect to τ.

Proof: Since D_0 is dense and D is nondegenerate, Eq. (4.2) and weak convergence imply that $Q_R D_0$ converges weakly to zero. Thus

$$\langle w-\lim_{R\to\infty} Q_R D, D_0\rangle=\lim_{R\to\infty}\langle D, Q_R D_0\rangle=0$$

and, again by the density of D_0, $Q_R D$ converges weakly to zero, which is incompatible with Eq. (4.3).

By Eqs. (4.4) and locality $\langle\mathcal{D}_0, Q_R^G\mathcal{D}_0\rangle\to 0$ and therefore, by the density of $\mathcal{D}_0$, weak convergence implies $Q_R^G\mathcal{D}_0\to 0$ and

$$\langle\mathcal{D}_0, Q\Psi\rangle=\lim_{R\to\infty}\langle\mathcal{D}_0, Q_R^G\Psi\rangle=\lim_{R\to\infty}\langle Q_R^G\mathcal{D}_0, \Psi\rangle=0.$$

Thus, the construction of physical charged states in a Hilbert–Krein extension of $\mathcal{D}_0$ is incompatible with weak convergence of the Gauss charge ${Q_R}^G$ on $\mathcal{D}_0$.

The failure of weak convergence of ${Q_R}^G\Psi_0$ gives rise to the same problems and features discussed in Sec. II; in particular the domain dependence of the limits of ${Q_R}^G$ allows the vanishing of such a limit on $\mathcal{D}_0\times\mathcal{D}_0$ compatibly with its being nonzero on a domain containing nonlocal states (as are the physical charged states).

A Hilbert–Krein topology which allows the construction of physical charged states, avoiding the weak convergence of ${Q_R}^G\mathcal{D}_0$, was discussed in Ref. 12 in terms of the properties of the asymptotic fields $\mathcal{A}_\mu^{as}$. The mechanism is clearly displayed by the following.

Example: Let ψ_0 be a (canonical) free massive Dirac field and ϕ_1, ϕ_2 two massless scalar fields satisfying the following (equal times) commutation relations:

$$[\,\phi_1, \phi_2\,]=0, \quad [\,\pi_1, \pi_2\,]=0, \quad [\,\phi_i, \pi_i\,]=0, \quad \pi_i\equiv\partial_0\phi_i, \quad i=1,2,$$

$$[\,\pi_1(\mathbf{x}), \phi_2(\mathbf{y})\,]=[\,\pi_2(\mathbf{x}), \phi_1(\mathbf{y})\,]=-i\,\delta(\mathbf{x}-\mathbf{y}).$$

Then, the fields

$$\begin{gathered}\phi_\pm\equiv(\phi_1\pm\phi_2)/\sqrt{2}, \quad \pi_\pm\equiv(\pi_1\pm\pi_2)/\sqrt{2},\\ \psi(x)\equiv U(x)\psi_0(x), \quad U(x)\equiv:e^{i\phi_2}:(x)\end{gathered} \tag{4.5}$$

satisfy the following commutators and anticommutators:

$$\begin{gathered}[\,\phi_\pm(x), \phi_\pm(y)\,]=\pm i\,D(x-y), \quad [\,\phi_\pm(x), \phi_\mp(y)\,]=0,\\ [\,\phi_\pm(x), \psi(y)\,]=\pm iD(x-y)\psi(y), \quad \{\,\psi(x), \overline{\psi}(y)\,\}=iS(x-y),\end{gathered} \tag{4.6}$$

where D, S are the standard commutator functions for massless scalar and Dirac fields. Thus, $\phi_\pm$ and ψ are local fields.

Our field theory model is defined by the vacuum correlation functions of the field algebra $\mathcal{F}$ generated by ψ, ϕ_1 and $\partial_\mu\phi_2$, $\mu=0,1,\ldots,3$ and their Wick products; such correlation functions do not satisfy positivity.

Now, we consider the following local charges:

$$Q_R{}^{\phi} \equiv \partial_0 \phi_1(f_R \alpha_R), \quad Q_R \equiv j_0(f_R \alpha_R), \quad Q_R{}^{G} \equiv Q_R - Q_R{}^{\phi}, \tag{4.7}$$

where

$$j_\mu(x) = :\overline{\psi}\, \gamma_\mu\, \psi: (x) = :\overline{\psi_0}\, \gamma_\mu\, \psi_0: (x).$$

The factorization of the correlation functions of ψ_0 and $\phi_\pm$ implies that Q_R converges to an unbroken (nonzero) ''electron'' charge in sense of quadratic forms on $\mathcal{F}\Psi_0$ and in fact the correlation functions with unequal numbers of ψ and $\overline{\psi}$ vanish. Actually, $Q_R \mathcal{F}\Psi_0$ converges strongly with respect to any Hilbert–Krein topology chosen to turn $\mathcal{F}\Psi_0$ into a pre-Hilbert space, provided it is a product over fermion and boson Fock spaces since, by positivity of the correlation functions of ψ_0,

$$\| Q_R \Psi_0 \|^2_{\mathrm{HK}} = \langle Q_R \Psi_0, Q_R \Psi_0 \rangle \to 0. \tag{4.8}$$

The charge $Q_R{}^{G}$ requires a quite different discussion. The field algebra $\mathcal{F}$ is neutral under $Q_R{}^{G}$,

$$\lim_{R \to \infty} [\, Q_R{}^{G}, \mathcal{F}\,] = 0. \tag{4.9}$$

Therefore, setting $\mathcal{D}_0 \equiv \mathcal{F}\Psi_0$, by the argument at the beginning of Sec. II B, one has

$$\lim_{R \to \infty} \langle \mathcal{D}_0, Q_R{}^{G}\, \mathcal{D}_0 \rangle = \lim_{R \to \infty} \langle \mathcal{D}_0, Q_R{}^{G} \Psi_0 \rangle = 0.$$

In the analogy with the local formulation of QED, the local charge $Q_R{}^{G}$ plays the role of the Gauss charge, Q_R plays the role of the electron charge $j_0(f_R\, \alpha_R)$ and $Q_R{}^{\phi}$ plays the role of the longitudinal charge $\partial_0 \partial A(f_R\, \alpha_R)$, all smeared in time a la Requardt. As in the QED case the correlation functions of $Q_R{}^{\phi}$ vanish.

The relevant question is whether by taking suitable limits of the local states of $\mathcal{D}_0$ one can construct the analog of the physical charged states, i.e., states Ψ satisfying the following condition:

(i) positivity, i.e.,
$$\langle \Psi, \Psi \rangle \geqslant 0;$$
(ii) relativistic spectral condition;
(iii) vanishing expectation of the ''longitudinal'' field $\partial_0 \phi_1$,
$$\langle \Psi, \partial_0 \phi_1 \Psi \rangle = 0;$$
(iv) nonzero Gauss charge, i.e.,
$$\lim_{R \to \infty} \langle \Psi, Q_R{}^{G} \Psi \rangle = \lim_{R} \langle \Psi, Q_R \Psi \rangle \neq 0.$$

In the following, such states will be briefly referred to as ''physical'' charged states.

Similarly to the QED case, the selection of states of $\mathcal{D}_0$ satisfying (i)–(iii) is obtained by means of a supplementary condition

$$\partial_0 \phi_1^{-} \Psi = 0, \tag{4.10}$$

which amounts to the exclusion of ϕ_2 components.

As in the QED case, the subspace $\mathcal{D}_0' \subset \mathcal{D}_0$ satisfying the subsidiary condition has zero electric charge; in fact one has $\mathcal{D}_0' = \mathcal{F}_0' \Psi_0$, where $\mathcal{F}_0'$ is the field algebra generated by ϕ_1 and by the Wick products

$$:\overline{\psi} \Gamma\, \psi: = :\overline{\psi_0 \Gamma}\, \psi_0:,$$

with Γ any element of the algebra generated by the gamma matrices. The problem is whether physical charged states may lie in some completion of $\mathcal{D}_0$; as one can easily guess the candidates for the physical states are the free fermion states $\mathcal{A}_f\Psi_0$, $\mathcal{A}_f$=the algebra generated by ψ_0.

If one looks for a Hilbert–Krein completion $\mathcal{K}$ of $\mathcal{D}_0$ given by a Krein topology on the boson space, a sufficient condition for $\mathcal{A}_f\Psi_0$ belonging to $\mathcal{K}$ is that the Hilbert–Krein majorant $(\,,\,)$ has a Fock structure and, at the level of the two point function $\langle\phi_i\,\phi_j\rangle$, $i,j=1,2$, is given by a measure (in k space) of the form

$$\begin{pmatrix} |\mathbf{k}|^2\,\beta(|\mathbf{k}|) & 0 \\ 0 & |\mathbf{k}|^{-2}\,\beta(|\mathbf{k}|)^{-1} \end{pmatrix}\frac{\mathrm{d}^3k}{|\mathbf{k}|},$$

with

$$\beta(|\mathbf{k}|)\sim_{|\mathbf{k}|\to 0}|\mathbf{k}|^{-2\delta},\quad \beta(|\mathbf{k}|)\sim_{|\mathbf{k}|\to\infty}|\mathbf{k}|^{2\delta},\quad \delta>0.$$

This is in fact the condition which allows the construction of the field ϕ_2 and therefore of $U(x)$ from the derivatives $\partial_\mu\phi_2$, so that ψ_0 can be recovered from ψ. More generally, the metric leading to a majorization may be chosen independently for each charged sector, i.e., β may depend on the charge q.

It is instructive to discuss the relation between the existence of charged states and the convergence properties of ${Q_R}^G$, which play a crucial role in Steinmann argument. First

$$\|{Q_R}^G\Psi_0\|^2\equiv\langle {Q_R}^G\Psi_0,\,{Q_R}^G\Psi_0\rangle\to 0,$$

i.e., $s-\lim {Q_R}^G\Psi_0=0$ in the Hilbert topology defined by the semidefinite Wightman two point function of $j_0-\partial_0\phi_1$, exactly as in the QED case [Sec. III, Eq. (3.2)].

However, the weak convergence of ${Q_R}^G\Psi_0$ in $\mathcal{K}$, i.e., with respect to the Hilbert–Krein space to which the physical charged states belong, requires the boundedness of the norm

$$\begin{aligned}\|{Q_R}^G\Psi_0\|^2_{\mathrm{HK}}&=({Q_R}^G\Psi_0,\,{Q_R}^G\Psi_0)\\ &=\int \mathrm{d}^3k|\mathbf{k}|^{-1}|\mathbf{k}|^2\,\beta(|\mathbf{k}|)\tilde{\alpha}(Rk_0)|^2\,|R^3\tilde{f}(R\mathbf{k})|^2\\ &=\int \mathrm{d}^3q\,|\mathbf{q}|\,\beta(|\mathbf{q}|/R)|\tilde{\alpha}(|\mathbf{q}|)|^2\,|\tilde{f}(\mathbf{q})|^2\sim R^{2\delta},\end{aligned}$$

which requires $\delta\leqslant 0$. A similar calculation for the weak convergence of ${Q_R}^G\psi\Psi_0$ in $\mathcal{K}$ involves the choice of the majorization of the boson field correlations in the $q=1$ sector and requires $\delta_{q=1}\leqslant 0$, whereas the existence of physical states with charge $q=1$ requires $\delta_{q=1}>0$.

In conclusion, in the space $\mathcal{K}$ defined by the above metric with $\delta>0$, there are two dense domains $\mathcal{D}_0=\mathcal{F}\Psi_0$ and $\mathcal{D}_1=\mathcal{F}_1\Psi_0$, with $\mathcal{F}_1$ the field algebra generated by ψ_0 and by ϕ_1, $\partial_\mu\phi_2$, with the properties

(1) ${Q_R}^G$ converges to the zero operator on $\mathcal{D}_0\times\mathcal{D}_0$.
(2) ${Q_R}^G\Psi_0$ converges to zero strongly in the Wightman (semidefinite) scalar product, but it does not converge (even) weakly in the extended space $\mathcal{K}$; moreover ${Q_R}^G$ on local charged states does not converge weakly in $\mathcal{K}$.
(3) ${Q_R}^G$ converges to the nonzero "electron" charge on $\mathcal{D}_1\times\mathcal{D}_1$.
(4) ${Q_R}^G$ converges strongly on any vector of $\mathcal{D}_1$ satisfying the supplementary condition [Eq. (4.10)], in the intrinsic Hilbert topology defined by the Wightman functions.

The model also displays the intrinsic conflict between the construction of the physical charged states and the weak convergence of ${Q_R}^G$ in the extended space which contains them; in fact, in the model divergences appear in the limit of matrix elements $\langle e^{i\phi_2}\Psi_0,\,{Q_R}^G\Psi_0\rangle$. The model also

indicates that in QED the Gauss charge *converges strongly* to the electric charge on a dense domain of physical states (in the intrinsic Hilbert topology of the physical space), a property which is not shared in general by local charges in quantum field theories.

V. COMMENTS ON THE CONSTRUCTION OF PHYSICAL CHARGED STATES

The construction of physical charged states in local formulations of QED, like the Feynman–Gupta–Bleuler gauge, is a relevant issue because it is strictly related to a nonperturbative solution of the infrared problem and provides theoretical support and clarification of the standard perturbative calculations. In Ref. 13, it is argued that physical charged states cannot be obtained as weak limits of the local states, which are at the basis of the perturbative expansion, and that they can only be defined as limits of morphisms of the algebra of observables. The arguments for such a conclusion are on one side the convergence to zero of the Gauss charge in any weak closure of the local states (the weakness of such an argument was discussed in the preceding section) and on the other side the divergence of the matrix elements between local states and the physical charged states constructed according to the Dirac–Symanzik–Steinmann (DSS) prescription. In this section we shall critically examine the latter argument and show that a modification of the DSS prescription along the lines discussed in Ref. 12, leads to convergent results for the construction of physical charged state vectors as weak limits of local states.

For this purpose, we adopt the general framework of Ref. 12 and in particular we shall base the discussion on the following assumptions.

(i) (*existence of asymptotic limits of the vector potential*) the asymptotic limits A_μ^{as}, $as=in/out$, of A_μ exist as (covariant) free fields with the local states in their domains.

(ii) (*infrared coherence of "essentially local" states*) there are states Ψ, in a weak extension of $\mathcal{D}_0$, with $\langle\Psi,\Psi\rangle>0$ having a decomposition into (improper) states χ^α, with $\langle\chi^\alpha,\chi^\alpha\rangle=1$, which are coherent states for A_μ^{in} (or for A_μ^{out})

$$(A_\mu^{\text{in}})^-(k)\,\chi^\alpha=-\delta(k^2)\,F_\mu^{\alpha,-}(k)\,\chi^\alpha,\qquad k^\mu F_\mu^{\alpha,-}(k)=-e\,G(k),\quad G(0)=1, \tag{5.1}$$

with $G(k)$ a real symmetric rotationally invariant regular function.

For concreteness, the index α, which labels the improper states, can be thought of as arising in the direct integral decomposition with respect to the spectrum of the electron momentum P_μ^{ch}. For nonperturbative and perturbative arguments, which support (I) and (II), we refer to Ref. 12.

We then introduce a function $F_\mu^\alpha(k)$, with $kF^\alpha(k)=e\,\text{sign}\,k_0\,G(k)$, determined by its restriction $F_\mu^{\alpha,-}(k)$ to $C^-=\{\mathbf{k},-|\mathbf{k}|\}$ and by the reality condition $F_\mu^\alpha(k)=\overline{F_\mu^\alpha(-k)}$, and an operator valued distribution $F_\mu(k)$, with

$$[\,F_\mu(k),A^{\text{in}}\,]=0,\quad F_\mu^-(k)\,\chi^\alpha=F_\mu^{\alpha,-}(k)\,\chi^\alpha.$$

Then, the field

$$B_\mu^{\text{in}}(k)\equiv A_\mu^{\text{in}}(k)-\delta(k^2)\,F_\mu(k), \tag{5.2}$$

defined on $\mathcal{D}_\Psi\equiv\mathcal{A}^{\text{in}}\Psi$, $\mathcal{A}^{\text{in}}$ the field *-algebra generated by A_μ^{in}, satisfies

$$B_\mu^{\text{in},-}(x)\,\Psi=0. \tag{5.3}$$

A physical charged state Ψ_{ph} is then obtained by setting

$$\Psi_{ph}=e^{ie\,B_\mu^{\text{in}}(f^\mu)}\,\Psi, \tag{5.4}$$

provided that the (real) function f^μ satisfies

$$\delta(k^2)k^\mu \tilde{f}_\mu(k) = i\,\delta(k^2)\,G(k). \tag{5.5}$$

This equation corresponds to the Fourier transform of the Dirac condition $\partial^\mu f_\mu(x) = \delta^4(x)$ restricted to the light cone, since B^{in} is a free massless field, with ultraviolet regularization provided by $G(k)$. Clearly, all solutions of the Dirac condition $k^\mu \tilde{f}_\mu(k) = iG(k)$ are also solutions of Eq. (5.5).

Equation (5.5) implies a singularity for $\tilde{f}_\mu$ of order at least $1/k_0$ on the light cone and therefore the construction of Ψ_{ph}, through Eq. (5.4), involves the introduction of an infrared cutoff in f_μ. The point is whether its removal can be done in the correlation functions of $e^{ie\,B^{\text{in}}_\mu(f^\mu)}$ and local fields (i.e., Coulomb electron fields exist in the closure of the Gupta–Bleuler space) or only in the expectation of observables on Ψ_{ph}.

Since by Eq. (5.3) Ψ provides a Fock representation of B^{as}, the existence of Ψ_{ph} in a Hilbert–Krein closure of $\mathcal{D}_\Psi$ can be reduced to the finiteness of the two point function

$$\langle B^{\text{in}}_\mu(f_\mu)\Psi,\ \eta\, B^{\text{in}}_\nu(f^\nu)\,\Psi\rangle = (B^{\text{in}}_\mu(f_\mu)\Psi,\, B^{\text{in}}_\nu(f^\nu)\,\Psi) = \int \mathrm{d}^4k\, H^{\mu\,\nu}(k)\,\delta(k^2)\,\bar{\tilde{f}}_\mu(k)\,\tilde{f}_\nu(k) \equiv \|\tilde{f}\|^2_{\text{HK}}, \tag{5.6}$$

where η is the operator which defines the corresponding Fock Hilbert–Krein majorant topology. Such a majorization property implies that

$$\|\tilde{f}\|^2_{\text{HK}} \geqslant |\langle B^{\text{in}}_\mu(f_\mu)\Psi,\, B^{\text{in}}_\nu(f^\nu)\,\Psi\rangle| = \left| \int \mathrm{d}^4k\, g^{\mu\,\nu}\,\delta(k^2)\,\bar{\tilde{f}}_\mu(k)\,\tilde{f}_\nu(k) \right| = |\langle f, f\rangle| \tag{5.7}$$

and therefore, in particular, f_μ should be chosen so that the indefinite product $\langle f, f\rangle$ is finite.

The DSS solution of $k^\mu \tilde{r}_\mu(k) = i\,G(k)$, namely, $\tilde{r}_i(k) = -i\,k_i G(k)\,|\mathbf{k}|^{-2}$, $\tilde{r}_0(k) = 0$, does not work, since one obtains

$$\langle r, r\rangle = \int \mathrm{d}^3k\,|\mathbf{k}|^{-5} k_i\,k_j\,g^{i\,j}\,G(k)^2/2,$$

which is logarithmically divergent for $\mathbf{k}\to 0$ and therefore, by Eq. (5.7), it excludes the convergence of $\|\tilde{f}\|_{\text{HK}}$ for any choice of a majorant Hilbert–Krein topology. This corresponds to the divergence of the two point function $\langle \Psi_0,\, \psi(x)\,\bar{\Psi}_p(y)\,\Psi_0\rangle$ pointed out by Steinmann (Ref. 13, Chap. 12, p. 190).

However, as discussed in Ref. 12, a suitable choice of f_μ avoids the divergence of $\langle f, f\rangle$ and allows for a finite Hilbert–Krein norm.

In fact, all functions of the form $\tilde{f}_\mu(k) = \tilde{r}_\mu(k) - ik_\mu \tilde{g}(\mathbf{k})$ are solutions of Eq. (5.5). Since they differ from the DSS solution by a pure gauge, they lead to the same expectations for all observables, but they have different indefinite inner products:

$$\langle f, f\rangle = \int \mathrm{d}^3k\, G(\mathbf{k})\,(G(\mathbf{k}) + 2|\mathbf{k}|^2\,\tilde{g})\,|\mathbf{k}|^{-3}/2,$$

which vanishes with the choice $\tilde{g}(\mathbf{k}) = -|\mathbf{k}|^{-2} G(\mathbf{k})/2$. Such a choice gives

$$\tilde{f}_\mu = -i\overline{k}_\mu\,|\mathbf{k}|^{-2}\,G(\mathbf{k})/2, \quad \overline{k} \equiv (k_0, -\mathbf{k}); \tag{5.8}$$

the corresponding operator $A^{\text{in}}_\mu(f^\mu)$ describes "zero norm" (unphysical) in photons and their control depends on the choice of the metric.

The above construction of charged states, based on Eqs. (5.4)–(5.8), coincides with that of Ref. 12, apart from an infrared convergent gauge term, since in Eq. (91) of Ref. 12 for the "infrared dressing" U,

$$c_\mu(k)=(\sqrt{2}\,|\mathbf{k}|)^{-1}(ak_\mu+b\overline{k}_\mu),\quad a\,b=1,$$

$$\eta\mathrm{d}^+(f)\,\eta+\mathrm{d}^+(f)=(2|\mathbf{k}|)^{-1/2}a_\mu^+(k^\mu h+\tfrac{1}{2}\overline{k^\mu}|\mathbf{k}|^{-2}G(\mathbf{k})),$$

with $h(\mathbf{k})=O(|\mathbf{k}|^{-2+\delta})$, $\delta>0$.

It remains to characterize the conditions on the Hilbert–Krein topology which give $\|\tilde{f}\|_{\mathrm{HK}}<\infty$. For this purpose, in the photon k-space we introduce four orthogonal four vectors $\varepsilon^1_\mu(k)$, $\varepsilon^2_\mu(k)$, k_μ, $\overline{k}_\mu$, where $\varepsilon^1_\mu(k)$, $\varepsilon^2_\mu(k)$ are (transverse) polarization vectors. Thus, the most general rotation covariant form of $H^{\mu\,\nu}(k)$ is

$$H^{\mu\,\nu}(k)=\beta(|\mathbf{k}|)\,k^\mu k^\nu/2|\mathbf{k}|^2+\gamma(|\mathbf{k}|)\,\overline{k}^\mu\overline{k}^\nu/2|\mathbf{k}|^2+P^{\mu\,\nu}(k),$$

where $P^{\mu\,\nu}$ denotes the projection on the transverse polarization. Then, since

$$\sum_\nu k^\nu k^\nu=2|\mathbf{k}|^2,\quad \sum_\nu H^{\mu\,\nu}(k)\,k^\nu=\beta(|\mathbf{k}|)\,k^\mu,\quad \sum_\nu H^{\mu\,\nu}(k)\,\overline{k}^\nu=\gamma(|\mathbf{k}|)\overline{k}^\mu$$

positivity of the matrix $H^{\mu\,\nu}$ requires $\beta,\ \gamma>0$. Furthermore, since the metric $\eta(k)$ is given by

$$(\eta^{-1}(k))^{\mu\,\nu}=\sum_\sigma g^{\mu\,\sigma}H^{\sigma\,\nu}(k),$$

the condition $\eta^2=1$ requires $\beta\,\gamma=1$. Thus, one gets

$$\|\tilde{f}\|^2_{\mathrm{HK}}=\int \mathrm{d}^3k\,G(\mathbf{k})^2(4\,|\mathbf{k}|^3\,\beta(|\mathbf{k}|))^{-1},$$

which is finite if $\beta(|\mathbf{k}|)\geqslant|\mathbf{k}|^{-\delta}$, $\delta>0$, for $\mathbf{k}\to0$. This corresponds to the choice of the metric discussed in the Erice lectures Ref. 12, especially pp. 323 and 324, where one can also find a characterization of the metric on the asymptotic fields A^{in}_μ under general condition on the Fock structure of the representation of A^{in} given by Ψ_{ph}. Weak convergence of the gauge term $\partial_0\,\partial A(f_R\,\alpha_R)\,\Psi$, which is expected to govern the weak convergence of $Q_R{}^G\,\Psi$ (Ψ the "essentially local" states at the basis of the construction), would require $\delta\leqslant0$, as in the Example of Sec. IV. In fact, one has

$$\|\partial_0\,\partial A(f_R\,\alpha_R)\,\Psi\|^2_{\mathrm{HK}}=\|(B_R+C_R)\,\Psi\|^2_{\mathrm{HK}},\quad B_R\equiv\partial_0\,\partial B(f_R\,\alpha_R),$$

$$C_R\equiv-e/2\int \mathrm{d}^3q\,G(\mathbf{q}/R)\,\tilde{f}(\mathbf{q})\,[\tilde{\alpha}(|\mathbf{q}|)+\tilde{\alpha}(-|\mathbf{q}|)].$$

Now, $\|C_R\,\Psi\|^2_{\mathrm{HK}}$ remains bounded in R and

$$\|B_R\,\Psi\|^2_{\mathrm{HK}}=\int \mathrm{d}^4k\,\theta(k_0)\,\delta(k^2)\,k_0^2\,H^{\mu\,\nu}(k)k^\mu k^\nu\,|\tilde{f}_R(\mathbf{k})\,\tilde{\alpha}_R(k_0)|^2$$

$$=\int \mathrm{d}^3q\,|\mathbf{q}|^3\,|\tilde{f}(\mathbf{q})\,\tilde{\alpha}(|\mathbf{q}|)|^2\,\beta(|\mathbf{q}|/R)$$

diverges if $\delta>0$.

A similar discussion of the choice of the solution of the Dirac condition, can be done for the DSS construction of the physical fields in terms of the local Gupta–Bleuler fields. Again the solution given by Eq. (5.8) yields states which differ from the DSS states by a gauge transformation $\exp(ie\partial A(g))$ and by the exponential $\exp(ie[\,\partial A(g),A(r)\,])$ of an infrared divergent phase, so that all the expectations of observables coincide with those of the DSS solution. However, it is

easy to see that the above phase removes the divergence to order e^2 of the scalar product $\langle \Psi_0, \psi(x)\Psi(y)\,\Psi_0\rangle$, pointed out by Steinmann (Ref. 13, p. 190) as evidence of the claimed impossibility of constructing physical charged state vectors as weak limits of local states.

APPENDIX

In the standard case, locality and unitarity of space–time translations imply[3] that, for expectation on local states Ψ, Eq. (2.8) applies and one has

$$\lim_{R\to\infty} (\Psi, j_0(f_R,\alpha)\,\Psi) = \lim_{R\to\infty} (\Psi, j_0(f_R,\alpha_R)\,\Psi) = \lim_{T\to\infty}\lim_{R\to\infty} (\Psi, j_0(f_R,\alpha_T)\,\Psi). \tag{A1}$$

Actually, the argument for the vanishing of $\lim_{R\to\infty}\langle A\, j_0(f_R,\alpha)\rangle$ only uses locality and the property that the Fourier transforms of $\langle A\, j_0(x)\rangle$, A local, are measures. Perturbation theory indicates that this holds in the Feynman–Gupta–Bleuler formulation of QED, where the vanishing of $\lim_{R\to\infty}\langle A\ \partial^i F_{i0}(f_R,\alpha)\rangle$ also follows from the cluster property of the local fields in perturbation theory. For charged states in QED, obtained through a DSS-like construction, one may obtain sufficient localization properties so that the matrix elements $\langle \Psi_{ph}, j_0(\mathbf{x},x_0)\,\Psi_{ph}\rangle$ differ by the corresponding elements on local states, in the spacelike complement of a double cone, by corrections of order $|\mathbf{x}|^{-6}$, uniformly in $|x_0|\langle T_0, T_0\rangle 0$.[20] However, the matrix elements of j_i on such states decrease as $|\mathbf{x}|^{-2}$:[20]

$$\langle \Psi_{ph}, j_i(\mathbf{x}, x_0)\,\Psi_{ph}\rangle = (e/4\pi)\int \mathrm{d}^3z\ \partial_i^{\mathbf{x}}|\mathbf{x}-\mathbf{z}|^{-1}\partial_0^2 K(\mathbf{z}, x_0) + O(|\mathbf{x}|^{-4}),$$

where K is the commutator function of the electromagnetic field and Eq. (A1) does not hold for the Gauss charge. In fact, one has

$$\lim_R \langle \Psi_{ph}, \partial_0\partial^i F_{i0}(f_R,t)\Psi_{ph}\rangle = \lim_R \langle \Psi_{ph}, -\partial_i j_i(f_R,t)\Psi_{ph}\rangle$$
$$= e\int \mathrm{d}^3z\ \partial_0^2 K(\mathbf{z},t) = -\,e\int \omega\,\mathrm{d}\omega\,(\omega\widetilde{K})(0,\omega)\,e^{i\omega t}.$$

The vanishing of the last expression for all t would imply

$$\omega\widetilde{K}(0,\omega) = \lambda\ \delta(\omega)$$

and therefore, by Lorentz covariance,

$$\widetilde{K}(k) = \lambda\ \varepsilon(k_0)\ \delta(k^2),$$

i.e., a free theory. Thus, the expectation value of the electric charge, i.e., the electric flux at space infinity, in a charged state defined by Coulomb charged fields is time dependent, even if its time derivative vanishes at $t=0$ (by antisymmetry in ω). A current j_i with nonzero flux at infinity is therefore present, "induced" by vacuum polarization effects.

The renormalized charge is given by the limit of the matrix elements of the electric flux, with a suitable smearing in time [f_R, $\alpha_T(R)$ as before]

$$\lim_{R\to\infty} \langle \Psi_{ph}, \partial_i F_{i0}(f_R\,\alpha_{T(R)})\,\Psi_{ph}\rangle.$$

In fact, by putting

$$\widetilde{K}(k) = \int \mathrm{d}\rho(m^2)\ \varepsilon(k_0)\ \delta(k^2-m^2),$$

it follows

$$\lim_{R\to\infty}\langle \Psi_{ph}, \partial_i F_{i0}(f_R \alpha_{T(R)})\,\Psi_{ph}\rangle = e \lim_{R\to\infty}\int \mathrm{d}\rho(m^2)\,\mathrm{d}^3k\,R^3\tilde{f}(R\mathbf{k})\,\tilde{\alpha}(T(R)\sqrt{\mathbf{k}^2+m^2})$$

$$= e\int \mathrm{d}\rho(m^2)\,\mathrm{d}^3q\,\tilde{f}(\mathbf{q})\,\tilde{\alpha}((T(R)/R)\sqrt{\mathbf{q}^2+R^2m^2}).$$

Now, for $m^2>0$, $(T(R)/R)\sqrt{\mathbf{q}^2+R^2m^2}>T(R)m$ and $(1+m^2)^M\tilde{\alpha}(Tm)$ is bounded uniformly in T by a function of fast decrease and converges pointwise to zero. For $m^2=0$, the argument of $\tilde{\alpha}$ converges to zero if $T(R)/R\to 0$ and is equal to $|\mathbf{q}|$ if $T=R$. Then, by the dominated convergence theorem, if $T(R)/R\to 0$ one gets λe, with λ the ρ measure of the point $m^2=0$, which is one by the renormalization condition of the asymptotic electromagnetic field. On the other hand, for $T(R)=R$ one gets

$$e\lim_{R\to\infty}\int \mathrm{d}^3q\,\mathrm{d}\rho(m^2)\,\tilde{f}(\mathbf{q})\,\tilde{\alpha}(\sqrt{\mathbf{q}^2+R^2m^2}) = \lambda e \int \mathrm{d}^3k\,\tilde{\alpha}(|\mathbf{k}|)\,\tilde{f}(\mathbf{k}) \equiv \lambda e\, C(\alpha,f), \quad \text{(A2)}$$

again by the Lebesgue dominated convergence theorem. Thus, Requardt's prescription gives the renormalized charge up to a factor $C(\alpha,f)$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

A geometric renormalization group in discrete quantum space–time

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(Received 18 June 2003; accepted 11 August 2003)

We model quantum space–time on the Planck scale as dynamical networks of elementary relations or time dependent random graphs, the time dependence being an effect of the underlying dynamical network laws. We formulate a kind of geometric renormalization group on these (random) networks leading to a hierarchy of increasingly coarse-grained networks of overlapping lumps. We provide arguments that this process may generate a fixed limit phase, representing our continuous space–time on a mesoscopic or macroscopic scale, provided that the underlying discrete geometry is critical in a specific sense (geometric long range order). Our point of view is corroborated by a series of analytic and numerical results, which allow us to keep track of the geometric changes, taking place on the various scales of the resolution of space–time. Of particular conceptual importance are the notions of dimension of such random systems on the various scales and the notion of geometric criticality. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1619579]

I. INTRODUCTION

Among the various approaches to *quantum gravity* [or (quantum) space–time physics] there exists one which assumes that physics and, in particular, space–time itself are basically discrete on the presumed fundamental Planck level. This working philosophy is shared by a variety of more or less related research programs which, however, employ different technical concepts and follow different lines of reasoning when it comes to the concrete realization of such a program (for a small and incomplete list of papers of other groups see, e.g., Refs. 1–22; for further references see below).

Our own approach has been developed in Refs. 23–29. It generalizes the concept of *cellular automata* to so-called *cellular networks* which live on, in general, very large irregular and dynamical *graphs*. That is, both the nodes *and* the bonds are assumed to be dynamical degrees of freedom and interact with each other. An important ingredient of the *dynamical laws* is the possibility that bonds are switched on and off in the course of network evolution so that also the overall wiring or the geometry of the global network is a dynamically changing structure.

If one starts from such discrete model theories, two important points are the following: first, the definition of a (class of) primordial dynamics, which, in one way or the other, have the potential to lead to our well-known effective (causal) dynamical evolution laws on an emergent continuum space–time, and second (and closely related to the first problem), the control of this continum limit as a limit of a sequence of increasingly coarse grained intermediate theories. That is, one of the central issues is it, to reconstruct and recover the ordinary continuum physics and mathematics, starting from the remote Planck level. Some steps in this direction have been made in the above mentioned papers. They depend of course crucially on the kind of model theory being adopted and the general working philosophy.

In the following we will develop a kind of *geometric renormalization process* leading, as we

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hope, in the end to a fixed point (or rather, phase), representing some continuum theory. Our renormalization scheme carries the flavor of our particular framework, that is, the global structure and large scale patterns, existing in large networks and graphs. In some qualitative sense it is inspired by the *real-space block variable* approach to renormalization in the critical regime of statistical mechanics. One should note, however, that the implementation of such a program on the Planck scale is necessarily much more involved and ambitious as compared to the typical scales of standard physics. The reason is that both the patterns, living *in* the ambient network *and* this ambient space itself, have to be renormalized, and it turns out to be a complicated enterprise to keep track of the relevant geometric changes and characteristics on the various scales of resolution of space–time. In particular, among other things, also the dimension of the underlying spaces will change in general during the renormalization process.

Remark: We want to emphasize that, in the absence of a fixed and independent background space, the clue consists of performing the renormalization steps in an *intrinsic* way, without referring to some embedding space or other external geometric concepts. On the other hand, the technical methods being developed are expected to be useful also in other areas of modern physics and can be employed in other coarse-graining schemes, for example in the field of *dynamical triangulation* and *simplicial complexes*.

Before we begin with the discussion of the technical details of our program, we want to add some remarks about the wider physical context to which such ideas do belong. Illuminating ideas about discreteness on a fundamental level have already been entertained by Wheeler *et al.* (see e.g. the last pages in Ref. 30 or Refs. 31 and 32, respectively, another early source is Ref. 33). There even exist earlier sources which are, however, fueled by a slightly different complex of ideas, namely, extending the quantum mechanical concept of nonvanishing commutation relations down to the Planck scale. That is, one assumes Heisenberg-like commutation relations for the space–time coordinates of events. Our point of view is a little bit different in so far as we try to derive such relations and quantum mechanics in general as an emergent phenomenon appearing on a mesoscopic scale compared to the Planck scale. But, nevertheless, we think that there exist a number of cross relations (see, for example, Refs. 34–36).

Discrete structures like partial orders have, for example, been treated by Isham and co-workers.[17] A broad and general approach towards discrete physics in general has been developed by T. D. Lee and his group (for a collection see Vol. 3 of his selected papers[37]). Last but not least, there is the huge body of work subsumed under the catchword *random geometry* or *dynamical triangulation* (Ref. 38 or 39) which is, however, mostly concerned with the discretization of a preexisting continuous initial manifold. There may be interesting connections between our framework and these other approaches, but, for the time being, we refrain from commenting on them in this article to keep our work within reasonable length.

As a last point we want to mention some interesting cross-fertilization. In the papers mentioned above we based our analysis on a class of dynamical network laws which incorporate a mutual interaction between the local states defined on the nodes of the underlying graph and the nearby bonds. This allows us to treat both the dynamics of the ordinary degrees of freedom *on* the graph and the dynamical change of the geometry of the network on the same footing.

We recently observed that similar ideas have been entertained within the framework of cellular automata (see, e.g., Refs. 40 and 41), the models being called *structurally dynamic cellular automata* or SDCA. As far as we can see at the moment, the adopted technical framework is not exactly the same, but we think a comparison of both approaches should turn out to be profitable. We conclude this introduction with a brief description of what we are going to do in the following.

In the following, one of our central goals is to study characteristics of large graphs and networks with the help of statistical methods. Quite unexpectedly, we found that similar methods and techniques are developed at the moment in areas which, at first glance, seem to be quite far from foundational space–time physics. In our view this shows that there may be a certain meta trend towards the creation of a science of the behavior of large and intricatedly connected networks (see Refs. 42 and 43).

In the next section we explain the basics of the framework we are employing. In Sec. III we

briefly introduce the concept of a *random graph*. To establish some contact to other existing approaches, we show in Sec. IV that our network naturally carries also the structure of *causal sets*. The concrete construction of the renormalization steps towards an envisaged continuum theory begins with Sec. V, which contains also a series of rigorous analytical and numerical results which are of technical relevance in the subsequent reasoning. In Sec. VI we study some simple toy models which (despite their simplicity) show that there indeed do exist fixed points in the category of infinite graphs under our geometric renormalization process. In Sec. VII we study the behavior of the particularly important geometric concept of *graph* or *network dimension* and its behavior under renormalization and, in Sec. VIII, which is kind of a conclusion, we analyze the kind of *geometric criticality* which is in our view essential in order to arrive at nontrivial macroscopic limit space–times.

We recently came upon a beautiful discussion of some work of Gromov,[44] which shows that there may be some deep and interesting connections between our framework, developed in the following, and ideas of coarse graining in, for example, geometric group theory by Gromov (see also Refs. 45–47 cited in Sec. VII).

II. PROTOGEOMETRY AND PROTODYNAMICS

In a first step we want to motivate why we choose exactly the kind of model theory we are discussing in the following. On the one side, we have a working philosophy which is similar to the one expounded by 't Hooft in, e.g., Refs. 20–22. That is, we entertain the idea that, for example, quantum theory may well emerge as an *effective (continuum) theory* on the mesoscopic scale of an underlying discrete more microscopic theory. As we want our underlying *(pre)geometry* to *co-evolve* with the patterns living in this substratum, we developed the above mentioned generalization of the more regular cellular automata.

Another essential property of such *discrete dynamical systems* is, while the basic ingredients and elementary building blocks are reasonably simple, their potential for the emergence of very complex behavior on the more macroscopic scales, thus supporting the speculation that such systems may be capable of generating viable continuum theories.

We now begin to introduce the necessary technical ingredients. We start with the definition of some notions of graph theory.

Definition 2.1: A simple, countable, labeled, undirected graph, G, consists of a countable set of nodes or vertices, V, and a set of edges or bonds, E, each connecting two of the nodes. There exist no multiple edges (i.e., edges, connecting the same pair of nodes) or elementary loops (a bond, starting and ending at the same node). In this situation the bonds can be described by giving the corresponding set of unordered pairs of nodes. The members of V are denoted by x_i, the bonds by e_{ij}, connecting the nodes x_i and x_j.

Remarks: We could also admit a noncountable vertex set. The above restriction is only made for technical convenience. From a physical point of view one may argue that the *continuum* or uncountable sets are idealizations, anyhow. The notions *vertex, node* or *edge, bond* are used synonymously. Furthermore, the labelling of the nodes is only made for technical convenience (to make some discussions easier) and does not carry a physical meaning. As in general relativity, all models being invariant under *graph isomorphisms* (i.e., relabeling of the nodes and corresponding bonds) are considered to be physically equivalent.

In the above definition the bonds are not directed (but oriented; see below). In certain cases it is also useful to deal with directed graphs.

Definition 2.2: A directed graph is a graph as above, with E consisting now of directed bonds or ordered pairs of nodes. In this case we denote the edge, pointing from x_i to x_j, by d_{ij}. There may also exist the opposite edge, denoted by d_{ji}.

Observation 2.3: An undirected graph, as in Definition 2.1, can be considered as a particular directed graph with e_{ij} corresponding to the pair of directed edges, d_{ij}, d_{ji}.

Remark 2.4: We introduced and studied algebraic and functional analytic structures like, e.g., Hilbert spaces and Dirac operators on such graphs in Refs. 25 and 27. In such situations, the bonds, e_{ij}, d_{ij}, can be given a concrete algebraic meaning with

$$e_{ij} := d_{ij} - d_{ji} = -e_{ji}. \tag{1}$$

It is now suggestive to regard the edges between pairs of points as describing their (direct) interaction. This becomes more apparent if we impose dynamical network laws on these graph structures so that they become a particular class of discrete dynamical systems. Henceforth, we denote such a dynamical network, which is supposed to underly our continuous space–time manifold, by QX ("*quantum space*"). We want to make the general remark that the *cellular networks*, introduced in the following, can either be regarded as mere models of a perhaps more hypothetical character, encoding, or rather simulating, some of the expected features of a surmised *quantum space–time* or, on the other hand, as a faithful realization of the primordial substratum, underlying our macroscopic space–time picture. Up to now, this is a matter of taste.

For technical convenience and to keep matters reasonably simple, we choose a discrete overall clock-time (not to be confused with the *physical time* which is rather supposed to be an emergent and intrinsic characteristic, related to the evolution of quasi-macroscopic patterns in such large and intricately wired networks). In principle the clock-time can also be made into a local dynamical variable. Furthermore, we assume the node set of our initial network to be fixed and independent of clock-time (in contrast to the bonds). We will see in the following sections that this property will change under the renormalization steps, i.e., on the highler levels, the class of *lumps* or *meta-nodes* may become dependent on time.

We assume that each node, x_i, or bond, e_{ik}, carries an internal (for simplicity) discrete *state space*, the internal states being denoted by s_i or J_{ik}. In simple examples we chose, for instance,

$$s_i \in q \cdot \mathbb{Z}, \quad J_{ik} \in \{-1,0,+1\}, \tag{2}$$

with q an elementary quantum of information and

$$e_{ki} = -e_{ik} \Rightarrow J_{ki} = -J_{ik}. \tag{3}$$

In most of the studied cellular automata systems even simpler internal state spaces are chosen like, e.g., $s_i \in \{0,1\}$. This is at the moment not considered to be a crucial point. The above choice is only an example.

In our approach the bond states are dynamical degrees of freedom which, *a fortiori*, can be switched off or on (see below). Therefore, the *wiring*, that is, the pure *geometry* (of relations), of the network is a clock-time dependent, dynamical property and is *not* given in advance. Consequently, the nodes and bonds are typically not arranged in a more or less regular array, a regular lattice say, with a fixed near-/far-order. This implies that *geometry* will become to some degree a *relational* (Machian) concept and is no longer a static background.

As in cellular automata, the node and bond states are updated (for convenience) in discrete clock-time steps, $t = z \cdot \tau$, $z \in \mathbb{Z}$, with τ being an elementary clock-time interval. This updating is given by some *local* dynamical law (examples are given below). In this context *local* means that the node/bond states are changed at each clock-time step according to a prescription with input the overall state of a certain neighborhood (in some topology) of the node/bond under discussion.

A simple example of such a local dynamical law we have in mind is given in the following definition (first introduced in Ref. 25).

Definition 2.5 (example of a local law): At each clock-time step a certain quantum q is exchanged between, say, the nodes x_i, x_k, connected by the bond e_{ik} such that

$$s_i(t+\tau) - s_i(t) = q \cdot \sum_k J_{ki}(t) \tag{4}$$

(i.e., if $J_{ki} = +1$ a quantum q flows from x_k to x_i etc.).

The second part of the law describes the back reaction *on the bonds (and is, typically, more subtle). We assume the existence of two critical parameters $0 \leqslant \lambda_1 \leqslant \lambda_2$ with*

$$J_{ik}(t+\tau)=0 \quad \text{if} \quad |s_i(t)-s_k(t)|=:|s_{ik}(t)|>\lambda_2, \tag{5}$$

$$J_{ik}(t+\tau)=\pm 1 \quad \text{if} \quad 0<\pm s_{ik}(t)<\lambda_1, \tag{6}$$

with the special proviso that

$$J_{ik}(t+\tau)=J_{ik}(t) \quad \text{if} \quad s_{ik}(t)=0. \tag{7}$$

On the other side,

$$J_{ik}(t+\tau)=\begin{cases} \pm 1, & J_{ik}(t)\neq 0, \\ 0, & J_{ik}(t)=0, \end{cases} \quad \text{if} \quad \lambda_1 \leqslant \pm s_{ik}(t) \leqslant \lambda_2. \tag{8}$$

In other words, bonds are switched off if local spatial charge fluctuations are too large or switched on again if they are too small, their orientation following the sign of local charge differences, or remain inactive.

Another interesting law arises if one exchanges the roles of λ_1 *and* λ_2 *in the above law, that is, bonds are switched off if the local node fluctuations are too small and are switched on again if they exceed* λ_2.

We make the following observation:

Observation 2.6 (gauge invariance): The above dynamical law depends nowhere on the absolute values of the node "charges" but only on their relative differences. By the same token, charge is nowhere created or destroyed. We have

$$\Delta\left(\sum_{QX} s(x)\right)=0 \tag{9}$$

(Δ *denoting the change in total charge of the network between two consecutive clock-time steps). To avoid artificial ambiguities we can, e.g., choose a fixed reference level, taking as initial condition at* $t=0$ *the following constraint,*

$$\sum_{QX} s(x)=0. \tag{10}$$

We resume what we consider to be the crucial ingredients of network laws. We are interested in the following.

(1) As in gauge theory or general relativity, our evolution law should implement the mutual interaction of two fundamental substructures, put a little bit vaguely: "*geometry*" acting on "*matter*" and vice versa, where in our context "*geometry*" is assumed to correspond in a loose sense to the local and/or global array of bond states and "*matter*" to the structure of the node states.
(2) By the same token the alluded *self-referential* dynamical circuitry of mutual interactions is expected to favor a kind of *undulating behavior* or *self-excitation* above a return to some uninteresting *equilibrium state* (being devoid of stable structural details), as is frequently the case in systems consisting of a single component which directly acts back on itself. This propensity for the *autonomous* generation of undulation patterns is in our view an essential prerequisite for some form of "*protoquantum behavior*" we hope to recover on some coarse grained and less primordial level of the network dynamics.
(3) In the same sense we expect the large scale pattern of switching-on and -off of bonds to generate a kind of "*protogravity*."

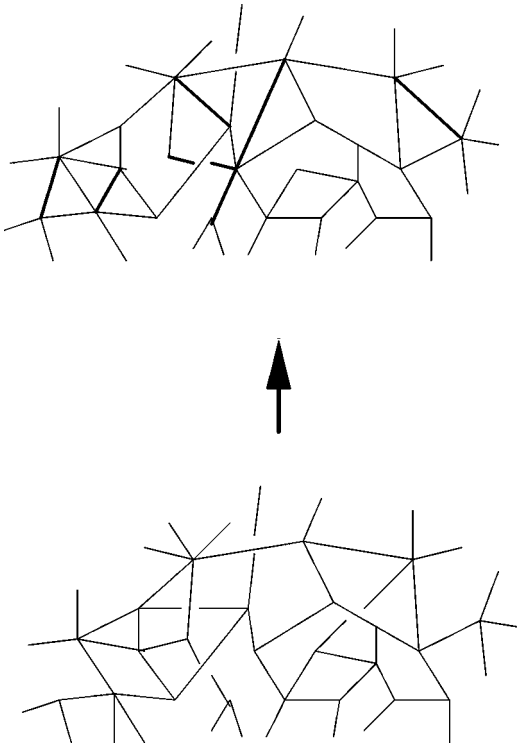

FIG. 1. Dynamic graph.

Remark: The above dynamical law shows that bonds with $J_{ik}=0$ at clock-time t do not participate in the dynamics in the next time step. We hence may consider them as being temporally inactive. The shape of the network, neglecting all the internal states on the nodes and bond together with the inactive bonds, we call the *wiring diagram*.

If one concentrates solely on this *wiring diagram*, Fig. 1 describes one clock-time step in the life of a *dynamic graph*. In the picture only a small subgraph is shown and the deletion and creation of edges (that is, elementary interactions among nodes or possible information channels). The new bonds are represented as bold lines. It should be emphasized that the graph is *not* assumed to be a triangulation of some preexisting smooth manifold. This is emphasized by the existence of edges, connecting nodes which are not necessarily close with respect to, e.g., the Euclidean distance.

We have pictured our proto space–time on the Planck scale as a fluctuating network of dynamic relations or exchange of pieces of information between a given set of nodes. At each fixed clock-time step there exist in this network certain subclusters of nodes which are particularly densely entangled and the whole graph can be covered by this uniquely given set of subclusters of nodes and the respective induced subgraphs. We dealt with these distinguished clusters of nodes (called cliques or lumps) in quite some detail in, e.g., Ref. 26 or 28. We emphasize the interesting relations to earlier ideas of Menger and Rosen *et al.*, which have been discussed in Ref. 28.

One of our core ideas is that the seemingly structureless (mathematical) points, making up our ordinary continuous manifolds, would display a rich nested internal structure if looked at under a magnification or resolution so that the lumpy structure of space–time became visible. We think this hidden substructure will become particularly relevant when it comes to the interpretation of *quantum phenomena* (Ref. 29, where possible relations to some interesting ideas of Connes have been set up).

From a more technical or practical point of view we need a general principle which allows us to lump together subsets of nodes, living on a certain level of resolution of space–time, to get the

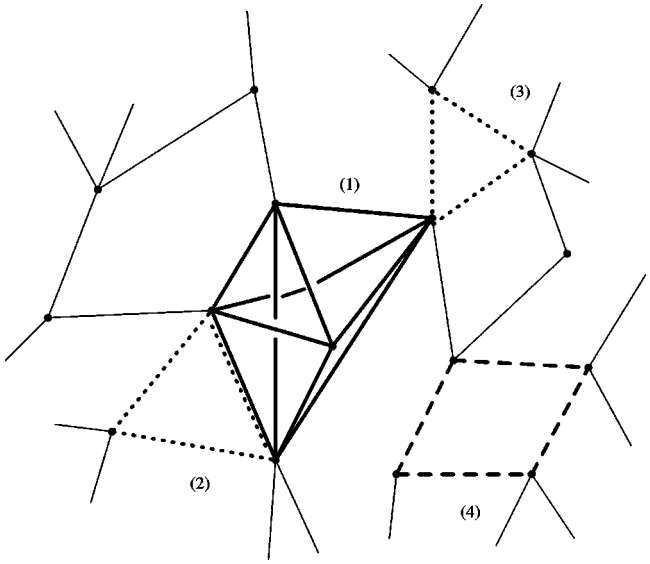

FIG. 2. Cliques.

building blocks of the next level of coarse graining (see below). After a series of such coarse graining steps we will wind up with a nested structure of lumps, containing smaller lumps and so forth, which, after appropriate *rescaling*, may yield in the end some quasi-continuous but nested structure. This principle is provided by the following mathematical concept.

Definition 2.7 (subsimplices and cliques): With G a given fixed graph and V_i *a subset of its vertex set V, the corresponding* induced subgraph *over* V_i *(that is, its edges being the corresponding edges, occurring in G) is called a subsimplex, if all its pairs of nodes are connected by a bond. In this class, which is in fact partially ordered, the order being given by graph inclusion, there exist certain* maximal subsimplices, *that is, subsimplices so that every addition of another node of the underlying graph(together with the respective bonds existing in G pointing to other nodes of the chosen subset) destroys this property. These maximal simplices are usually called* cliques *in combinatorics (we call them also lumps) and are the candidates for our construction of* physical points. *Henceforth we denote them by* C_i.

It has been described in detail in, e.g., Sec. 4 of Ref. 26 how these cliques can be constructed in an algorithmic way, starting from an arbitrary node. Note in particular that a given node will, in general, belong to many different (overlapping) cliques or lumps. The situation is illustrated in Fig. 2. In this figure we have drawn a subgraph of a larger graph. (1) denotes a clique, i.e., a maximal subsimplex. Subsets of nodes of such a clique support subsimplices (called faces in algebraic topology), the clique being the maximal element in this partial ordered set. (2) and (3) are other, smaller cliques which overlap with (1) in a common bond or node. (4) is an example of a subgraph which is not a clique or subsimplex. Evidently, each node or bond lies in at least one clique. The smallest possible cliques which can occur in a connected graph consist of two nodes and the corresponding edge.

III. DYNAMICAL NETWORKS AS RANDOM GRAPHS

A. The statistical hypothesis

As we are dealing with very large graphs, which are, *a fortiori*, constantly changing their shape, that is, their distribution of (active) bonds, we expect the dynamics to be sufficiently stochastic so that a point of view may be appropriate, which reminds us of the working philosophy of *statistical mechanics*. This does, however, not imply that our evolving network is nothing but a

simple *random graph* as introduced below (cf. the remarks at the end of this section). It rather means that some of its geometric characteristics can, or should, be studied within this well-developed context.

Visualizing the characteristics and patterns being prevalent in large and ''typical'' graphs was already a notorious problem in *combinatorial graph theory* and led to the invention of the *random graph* framework (see the more complete discussion in Ref. 26). The guiding idea is to deal with graphs of a certain type in a probabilistic sense. This turns out to be particularly fruitful as many graph characteristics (or their absence) tend to occur with almost certainty in a probabilistic sense (as has been first observed by Erdös and Rényi). The standard source is Ref. 48 (for further references see Ref. 26).

Another strand of ideas stems from the theory of dynamical systems and cellular automata, where corresponding statistical and ensemble concepts are regularly employed. Typically, we are looking for *attractors* in phase space, which are assumed to correspond to large scale, that is, after *coarse graining* and *rescaling*, quasi continuous or macroscopic patterns of the system. Experience shows that such a structure or the approach towards attractors is in many cases relatively robust to the choice of initial configurations or microscopic details and, hence, suggests an ensemble picture.

Furthermore, since the early days of statistical mechanics, the ensemble point of view (see, for example, Ref. 49) is, at least partly, corroborated by the philosophy that time averages can be translated (under favorable conditions) into ensemble averages. In our context this means the following. Denoting the typical length/time scale of ordinary quantum theory by $[l_{qm}]$, $[t_{qm}]$, we have

$$[l_{qm}] \gg [l_{pl}], \quad [t_{qm}] \gg [t_{pl}], \tag{11}$$

the latter symbols denoting the Planck scale. Under renormalization the mesoscopic scales comprise a huge number of microscopic clock-time intervals and degrees of fredom of the network under discussion.

A fortiori, the networks, we are interested in, correspond to graphs, having typically a huge *vertex degree*, i.e., number of independent channels being connected with a given typical node of the graph. That is, we expect large local fluctuations in microscopic grains of space or time. Put differently, the network locally traverses a large number of different microscopic states in a typical mesoscopic time interval, $[t_{qm}]$. This observation suggests that, on a mesoscopic or macroscopic scale, microscopic patterns will be washed out or averaged over.

B. The random graph framework

One kind of probability space is constructed as follows. Take all possible labeled graphs over n nodes as probability space $\mathcal{G}$ (i.e., each graph represents an elementary event). The maximal possible number of bonds is $N := \binom{n}{2}$, which corresponds to the unique *simplex graph* (denoted usually by K_n). Give each bond the *independent probability* $0 \leqslant p \leqslant 1$ (more precisely, p is the probability that there is a bond between the two nodes under discussion). Let G_m be a graph over the above vertex set, V, having m bonds. Its probability is then

$$pr(G_m) = p^m \cdot q^{N-m}, \tag{12}$$

where $q := 1-p$. There exist $\binom{N}{m}$ different labeled graphs G_m, having m bonds, and the above probability is correctly normalized, i.e.,

$$pr(\mathcal{G}) = \sum_{m=0}^{N} \binom{N}{m} p^m q^{N-m} = (p+q)^N = 1. \tag{13}$$

This probability space is sometimes called the space of *binomially random graphs* and denoted by $\mathcal{G}(n,p)$. Note that the number of edges is binomially distributed, i.e.,

$$pr(m)=\binom{N}{m}p^m q^{N-m} \tag{14}$$

and

$$\langle m\rangle=\sum\ m\cdot pr(m)=N\cdot p. \tag{15}$$

The really fundamental observation made already by Erdös and Rényi (a rigorous proof of this deep result can, e.g., be found in Ref. 50) is that there are what physicists would call *phase transitions* in these *random graphs*. To go a little bit more into the details we have to introduce some more graph concepts.

Definition 3.1 (graph properties): Graph properties *are certain particular* random variables *(indicator functions of so-called events) on the above probability space* $\mathcal{G}$*, i.e., a graph property,* Q*, is represented by the subset of graphs of the sample space having the property under discussion.*

Some examples are (i) connectedness of the graph, (ii) existence and number of certain particular subgraphs (such as subsimplices, etc.), (iii) other geometric or topological graph properties, etc.

In this context Erdös and Rényi made the following important observation.

Observation 3.2 (threshold function): A large class of graph properties *(e.g., the* monotone increasing ones*, cf. Ref. 48 or 50) have a so-called* threshold function*,* $m^*(n)$*, with* $m^*(n):=N\cdot p^*(n)$*, so that for* $n\to\infty$ *the graphs under discussion have* property Q almost surely *for* $m(n)>m^*(n)$ *and* almost surely not *for* $m(n)<m^*(n)$ *or vice versa [more precisely: for* $m(n)/m^*(n)\to\infty$ *or* 0*; for the details see the above cited literature]. That is, by turning on the probability* p*, one can drive the graph one is interested in beyond the phase transition threshold belonging to the graph property under study. Note that, by definition, threshold functions are only unique up to "factorization," i.e.,* $m_2^*(n)=O(m_1^*(n))$ *is also a threshold function.*

Calculating these graph properties is both a fascinating and quite intricate enterprise. In Ref. 26 we mainly concentrated on properties of *cliques*, their distribution (with respect to their order, r, i.e., number of vertices), frequency of occurence of cliques of order r, degree of mutual overlap, etc. We then related these properties to the various assumed stages and phases of our space–time manifold.

We can introduce various *random function* on the above probability space. For each subset $V_i\subset V$ of order r we define the following random variable:

$$X_i(G):=\begin{cases}1 & \text{if } G_i \text{ is an } r\text{-simplex},\\ 0 & \text{else},\end{cases} \tag{16}$$

where G_i is the corresponding induced subgraph over V_i in $G\in\mathcal{G}$ (the probability space). Another random variable is then the *number of* r*-simplices in* G, denoted by $Y_r(G)$, and we have

$$Y_r=\sum_{i=1}^{\binom{n}{r}} X_i \tag{17}$$

with $\binom{n}{r}$ the number of r-subsets $V_i\subset V$. With respect to the probability measure introduced above we have for the *expectation values*

$$\langle Y_r\rangle=\sum_i\ \langle X_i\rangle \tag{18}$$

and

$$\langle X_i\rangle = \sum_{G\in\mathcal{G}} X_i(G)\cdot pr(G_i = r\text{-simplex in } G). \tag{19}$$

These expectation values were calculated in Ref. 26. We have, for example,

$$\langle X_i\rangle = p^{\binom{r}{2}}. \tag{20}$$

The probability that such a subsimplex is maximal, i.e., is a clique, is then

$$pr(G_r \text{ is a clique}) = (1-p^r)^{n-r}\cdot p^{\binom{r}{2}}. \tag{21}$$

As there exist exactly $\binom{n}{r}$ possible different r-sets in the node set V, we arrive at the following conclusion:

Conclusion 3.3 (distribution of subsimplices and cliques): The expectation value of the random variable "number of r-subsimplices" *is*

$$\langle Y_r\rangle = \binom{n}{r}\cdot p^{\binom{r}{2}}. \tag{22}$$

For Z_r, the number of r-cliques *(i.e., maximal! r-simplices) in the random graph, we have then the following relation*:

$$\langle Z_r\rangle = \binom{n}{r}\cdot (1-p^r)^{n-r}\cdot p^{\binom{r}{2}}. \tag{23}$$

These quantities, as functions of r (the *order* of the subsimplices) have quite a peculiar numerical behavior. We are interested in the typical *order of cliques* occurring in a generic random graph (where typical is understood in a probabilistic sense).

Definition 3.4 (clique number): The maximal order of occurring cliques contained in G is called its clique number, $cl(G)$. *It is another random variable on the probability space $\mathcal{G}(n,p)$.*

It is remarkable that this value is very sharply defined in a typical random graph. Using the above formula for $\langle Z_r\rangle$, we can give an approximative value, r_0, for this expectation value and get

$$r_0 \approx 2\,\log(n)/\log(p^{-1}) + O(\log\log(n)) \tag{24}$$

(cf. Chap. XI.1 of Ref. 48). It holds that practically all the occurring cliques fall in the interval $(r_0/2, r_0)$. We illustrate this with the following tables. Our choice for n, the number of vertices, is 10^{100}. The reason for this seemingly very large number is that we want to deal with systems ultimately simulating our whole universe or continuous space–time manifolds (see the more detailed discussion in Ref. 26). We first calculate r_0.

p	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
r_0	4370	2063	1291	901	664	502	382	286	200

(25)

(for reasons we do not understand we made some numerical errors in the original Table 1 in Ref. 26, p. 2043).

It is more complicated to give numerical estimates of the distribution of cliques, that is $\langle Z_r\rangle$. After some manipulations and approximations we arrived (Ref. 26, p. 2051f) at the following approximative formula and numerical table (the numerical values are given for $p=0.7$; note that for this parameter the maximal order of occurring cliques, r_0, was approximately 1291)

$$\log(\langle Z_r\rangle) \approx r\cdot\log(n) + n\cdot\log(1-p^r) + r^2/2\cdot\log(p) \tag{26}$$

(with $r^2/2$ an approximation of $r(r-1)/2$) for r sufficiently large).

r	600	650	800	1000	1200	1300	1400
$\log(\langle Z_r \rangle)$	$-5.7\cdot 10^6$	$3.2\cdot 10^4$	$3.2\cdot 10^4$	$2.5\cdot 10^4$	$8.4\cdot 10^3$	$-0.75\cdot 10^2$	$-1.1\cdot 10^4$

(27)

[In the original Table 2 of Ref. 26 the numerical values for small and large r's, lying outside the interval $(r_0/2, r_0)$, were wrong as we neglected numerical contributions which are only vanishingly small in the above interval.] The above table nicely illustrates how fast the frequency of cliques of order r drops to zero outside the above interval.

As to the interpretation of these findings, one should remind the reader that the above results apply to the generic situation, that is, do hold for typical graphs (in very much the same sense as in corresponding discussions in the foundations of statistical mechanics). An evaluation of the combinatorial expressions in this and the following sections shows that frequently the same kind of extreme probabilistic concentration around, for example, *most probable values* occurs as in ordinary statistical mechanics.

What is not entirely clear is how far the random graph approach can be applied to our complex dynamical networks. Our working philosophy is that these results serve to show, what we hope, is the qualitative behavior of such systems. As our systems follow deterministic dynamical laws, starting from certain initial conditions, the behavior cannot be entirely random in the strict sense. This holds more so since we expect the systems to evolve towards *attracting sets* in phase space and/or generate some large scale patterns. On the other hand, due to the constant reorientation of the bonds, being incident with an arbitrary but fixed node and the generically large vertex degrees of the nodes, one may assume that the system is sufficiently random on small scales, so that the random graph picture reproduces at least the qualitative behavior of such extremely complex systems.

To make this picture more quantitative, the general strategy is the following. We count the typical number of active bonds in our evolving network at a given clock-time t, calculate from this the corresponding bond probability, $p(t)$, and relate this snapshot of our network to a random graph with the same! bond probability. This should yield at least some qualitative clues. That is, we expect that qualitative characteristics of our evolving network can, at each given clock-time, be related to the characteristics of a corresponding random graph. In this specific sense, one may regard the *bond probability*, $p(t)$, as the crucial *order parameter* of our network, regarded as a statistical system. (We note that we implemented such networks on a computer and made detailed studies of their dynamical behavior and stochastic properties, see Ref. 51. Our investigations showed that at least qualitatively the expected phenomena came out correctly.)

IV. CELLULAR NETWORKS AS CAUSAL SETS

In this section we want to make contact with an approach to quantum gravity, being based on the concept of *causal sets*. We again emphasize that, for reasons of technical simplicity, we treat *time* as a global nondynamical quantity, being well aware that this may be a severe restriction. On the other hand, the notorious so-called *problem of time* has not yet been settled anyhow in quantum gravity and needs an extra and careful treatment. Under this proviso we want to show that our *cellular networks* and *lump-spaces* automatically have the structure of causal sets, with this extra structure being induced by our local dynamical laws. On the most elementary level we start from our above initial network.

We argued above that we want to neglect the details of the (time dependent) internal states of nodes and bonds and only keep track of the bonds which are in operation at a given clock-time, t, that is, the bonds with $J_{ik} \neq 0$. Doing this, we arrive at the concept of *time dependent graphs*, $G(t)$.

Definition 4.1: $G(t)$ is a graph with a fixed (time independent) node set, V, but a time dependent set of active bonds, $E(t)$. In principle we could also make the node set time dependent, the above assumption is mainly made for convenience.

The local dynamical laws can as well be viewed as a prescription, by which local pieces (quanta) of information are transported between the active bonds of the network. The nodes, which

can be reached from a given node in a single clock-time step, are called its *nearest neighbors*, nn, the *next-nearest neighbors*, nnn, are correspondingly defined and so on.

What we have defined up to now corresponds to the *foliation* of space–time into an aggregate of spacelike slices. We now form the union of these slices and define

$$G := \bigcup_t G(t). \tag{28}$$

In our above mentioned papers (see, in particular, Ref. 23) we exploited the fact that graphs carry a natural metric structure

$$d(x_i, x_j) := \inf\{\text{length of paths, connecting } x_i \text{ and } x_j\}, \tag{29}$$

where path length is the discrete number of edges of the path. This defines a neighborhood structure on a graph

$$U_l(x_0) := \{\text{nodes } x_i \text{ with } \ d(x_0, x_i) \leqslant l\}. \tag{30}$$

We now will transform G into a *partial ordered set* (*poset*) by introducing additional (*causal*) bonds and relabeling the nodes. From now on we denote the nodes in $G(t)$ by $x_i(t)$, that is, one and the same node x_i carries an additional time label $t \in \mathbb{Z} \cdot \tau$, depending on the time slice $G(t)$ under discussion and is denoted by $x_i(t)$. For each node, $x_i(t)$ we draw new edges to the nodes $x_j(t+1)$ lying in $G(t+1)$, provided that $x_j(t)$ is a nn of $x_i(t)$ in $G(t)$ [including the node $x_i(t+1)$ itself!]. For convenience we usually drop the extra time element τ.

Definition 4.2: We call the edges lying in $G(t)$, that is the original edges of the (time dependent!) graph, the spatial edges *(at time t), the edges which connect the neighbors in consecutive slices, $G(t)$, $G(t+1)$, are dubbed* causal edges. *That is, an elementary* causal neighborhood *of, say, $x_i(t)$ consists of all the nodes, $x_j(t+1)$, in $G(t+1)$, with $x_j(t)$, having spatial distance, $d(x_i(t), x_j(t)) \leqslant 1$, in $G(t)$ [that is, the node, $x_i(t+1)$ itself plus the nodes having distance one].*

(It may be helpful to envisage the spatial edges as carrying a red color and the causal edges a green one.)

We can now proceed by introducing the *forward-* or *future cone* and *backward-* or *past cone*, respectively.

Definition 4.3: To the forward cone of $x(t)$ belong those nodes, $y(t')$, $t' \geqslant t$, which can be connected by a causal edge sequence, γ, starting in $x(t)$. Such an admissible sequence consists of $(t'-t)$ elementary steps. An analogous definition holds for the members of the past cone. Given two nodes, $x(t)$, $y(t')$ with $t' \geqslant t$, we can intersect the forward cone of $x(t)$ with the backward cone of $y(t')$ and get the corresponding double cone.

Remark: Note that the causal and metric relations are relatively subtle as compared to, for instance, ordinary *special relativity*, where we deal with one and the same topological space structure for all times. In our space–time graph, G, the spatial wiring is constantly changing on a microscopic scale, due to the imposed local dynamical law. That is, two nodes may become nearest neighbors in $G(t)$ while being far apart for earlier or later times and vice versa. This can happen since bonds are permanently annihilated and created.

Conclusion 4.4: The above causal distance concept has already some of the crucial ingredients of the metric properties, known from general relativity. Furthermore, it is of a markedly stochastic character.

What we have said above creates in a natural way some *partial order* on the set of nodes. We do not want to reproduce all the technical notions, which are presumably well known or can be found in, e.g., the papers of Sorkin *et al.*, mentioned above, or in, say, Ref. 52 or 53. In the definition of the partial ordered set (poset), only the causal (green) bonds enter [with their (non)existence being a consequence of the respective (non)existence of the spatial (red) bonds].

Definition 4.5: We have $x_j(t') \geq x_i(t)$, $t' \geq t$, if the nodes can be connected by a causal path, lying in the forward cone. The nodes, lying on a causal edge sequence, we call chains; sets of mutually spacelike nodes are called antichains.

This order relation is clearly reflexive, antisymmetric and transitive. We remark the following point.

It trivially holds (by assumption) that $x_i(t') \geq x_i(t)$, that is, for the same node at different times. This implies that for two nodes, x_i, x_j, it follows

$$x_j(t') \geq x_i(t) \;\Rightarrow\; x_j(t'') \geq x_i(t) \tag{31}$$

for all times, $t'' \geq t'$, as we can continue the causal path from $x_i(t)$ to $x_j(t')$ by the trivial path, $x_j(t') - x_j(t'')$.

V. THE GEOMETRIC COARSE-GRAINING OR RENORMALIZATION PROCESS

A. The general picture

One of our central hypotheses is to regard the ordinary space or space–time as a medium having a complicated internal dynamical fine structure, which is largely hidden on the ordinary macroscopic scales due to the low level of (only mesoscopic) resolution of space–time processes as compared to, e.g., the Planck scale. The corresponding process of *coarse graining*, described in the following, may be also called a *geometric renormalization*, in which the resolution of the details of space–time is steadily scaled down to the level of ordinary continuum physics. Some preliminary ideas of this renormalization process have already been been decribed in Refs. 26 and 28.

In the following we deal with a generic large network or graph, G, as a typical representative of the members of the class $\{G(t)\}$, described above. The individual renormalization steps consist of the following constructions.

(i) Starting from a given fixed graph, G, pick the (generic) *cliques*, C_i, in G, i.e., the subgraphs, forming maximal subsimplices or cliques in G with their order lying in the above mentioned interval, $(r^0/2, r^0)$.

(ii) These cliques form the new nodes of the *clique-graph*, G_{cl} of G. The corresponding new bonds are drawn between cliques, having a (sufficient degree of) overlap. Size, overlap and distribution of cliques in a generic (*random*) graph have been analyzed in Ref. 26; for more details see the following subsection.

(iii) That is, both *marginal* cliques (if they do exist at all) and *marginal* overlaps are deleted. In this respect a coarse-graining step includes also a certain *purification* of the graph structure.

Remark 5.1: What is considered to be a "sufficient overlap" depends of course on the physical context and the general working philosophy. As we noted above, a particular node will in general belong to several, and in the case of densely entangled graphs to many, cliques. The minimal possible overlap is given by a single common node. If, on the other hand, the cliques on a certain level of coarse graining are comparatively large, comprising, say, typically several hundred nodes, it may be reasonable to neglect marginal, *i.e., to small, overlaps as physically irrelevant and define a sufficient degree of overlap to consist of an appreciable fraction of the typical clique order. Correspondingly, too small cliques, not lying in the above introduced interval, $(r_0/2, r_0)$, are deleted (if they do exist at all!, see the estimates in Sec. III). The numerical effect of such choices will be studied in the following.*

Definition 5.2: We call the graph, defined above, the (purified) clique graph, G_{cl}, constructed from the initial graph, G.

It is an important question whether graphs and networks are connected, that is, if there exists a path or edge sequence, connecting each pair of vertices. This question becomes, *a fortiori*, relevant in the following (sub)sections if the coarse-graining or renormalization steps are performed on a given fixed graph. The following lemma is useful.

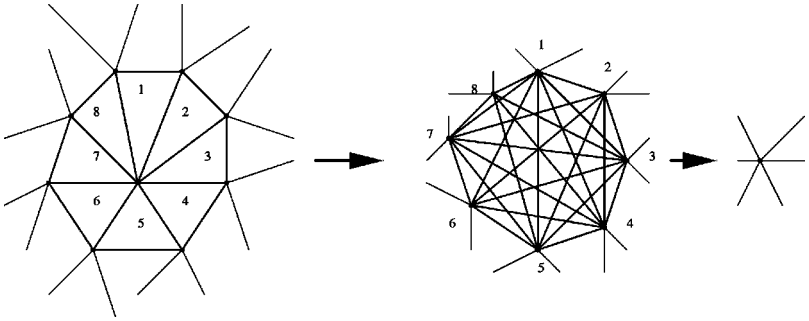

FIG. 3. Coarse graining.

Lemma 5.3: If G is a connected graph, that is, each pair of vertices, x,y can be connected by a finite path or edge sequence, depicted as $x=x_0-x_1-\cdots-x_n=y$, then the ordinary (unpurified) clique graph, G_{cl}, is again connected.

Proof: Let x_0 lie in a certain clique, C_0 and y in a clique C_{n+1}. By algorithmic construction (cf. Ref. 26), the vertices $x_0-x_1, x_1-x_2, \ldots, x_{n-1}-x_n$ are lying in certain cliques $C_1,\ldots,C_n$ with

$$C_0\cap C_1\neq\emptyset,\quad C_1\cap C_2\neq\emptyset,\ldots,\quad C_n\cap C_{n+1}\neq\emptyset \tag{32}$$

by construction ($x_i\in C_i\cap C_{i+1}$). Hence, each pair of cliques, C,C', can be connected by a finite sequence of pairwise overlapping cliques. In other words, the ordinary clique graph is again connected. □

This result is, for example, useful in cases where graphs are so sparsely connected that, viewed in the random graph picture, there is a nonzero probability that they are disconnected. The above construction shows that at least the consecutive sequence of unpurified clique graphs $G_0\rightarrow G_1\rightarrow G_2\rightarrow\cdots$ consists of connected graphs, provided the initial graph, G_0, is connected, with G_{i+1} being the clique graph of G_i. On the other hand, if we take instead the purified clique graph, in which only overlaps of a certain degree are taken into account which are greater than some prescribed value, it may happen that the clique graph is no longer connected.

We want to repeat the above described coarse-graining process several or perhaps many times (if necessary) without the necessity of introducing new principles at each step of the construction. The transition from a graph to its clique graph represents such a *universal principle*, which works on each level of the renormalization process. In the end we hope to arrive at a (quasi-)continuous manifold, displaying, under appropriate magnification, an intricate internal fine structure. This should (or rather, can only be expected to) happen if the original network has been in a (quasi-)*critical* state as will be described in the following (see in particular Sec. VIII).

On each level of coarse-graining, that is, after each renormalization step, labeled by $l\in\mathbb{Z}$, we get, as in the block spin approach to critical phenomena, a new level set of cliques or lumps, C_i^l (i labeling the cliques on renormalization level l), consisting on their sides of $(l-1)$-cliques which are the l-nodes of level l, starting from the level $l=0$ with $G=:G_0$. That is, we have

$$C_j^l=\bigcup_{i\in j} C_i^{(l-1)},\quad C_i^{(l-1)}=\bigcup_{k\in i} C_k^{(l-2)},\ \text{ etc.} \tag{33}$$

[$i\in j$ denoting the $(l-1)$-cliques, belonging, as meta nodes, to the l-clique, C_j]. These cliques form the meta nodes in the next step.

Definition 5.4: The cliques, C_i^0, of $G=:G_0$ are called zero-cliques. They become the one-nodes, x_i^1, of level one, i.e., of G_1. The one-cliques, C_i^1, are the cliques in G_1. They become the two-nodes, x_i^2, of G_2, etc. Correspondingly, we label the other structural elements, for example, one-edges, two-edges or the distance functions, $d_l(x_i^l,x_j^l)$. These higher-level nodes and edges are also called meta-nodes and -edges, respectively.

Figure 3 shows how the (meta) nodes and bonds form in two consecutive steps. In this

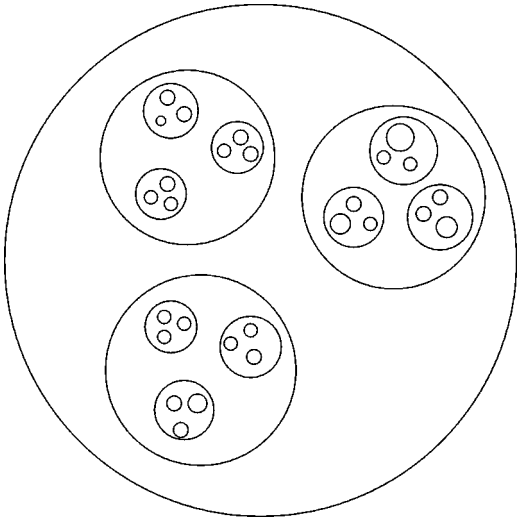

FIG. 4. Lumps.

example and in the selected subgraph under discussion the cliques on level 0 are triangles. Some of them have a common bond but all of them are hanging together via a common (central) node. In this example we draw a bond on level 1 if the cliques of level 0 have at least one node in common.

Remark 5.5: The picture may lead to the wrong impression that the network becomes sparser after each step. Quite to the contrary, the number of cliques in G_{cl} may be much larger than the number of nodes in the original graph, G [cf. the table in Eq. (27)]. This happens if there is an appreciable overlap among the occurring cliques, that is, a given node may belong to many different cliques. On the other hand, after several renormalization steps, the picture becomes stable in the generic case (see the following subsection).

The above illustration can be understood in two different ways. On the one hand, read from left to right, the resolution of space appears to be reduced. The cluster of cliques on the left happens to be contracted to a single node of the next level. On the other hand, according to our working philosophy, we can regard the node on the right as still containing the structure on the left, which could, in principle, be recovered when increasing the resolving power of our space–time microscope, i.e., by increasing, e.g., the energy. This is expressed in Fig. 4 (where for the sake of graphical clarity, the mutual overlaps of the occurring cliques of the same level is not represented!). Understood in this latter sense we call these space–time points also *lumps*, that is, we regard them as objects, having an inner structure. Different aspects of this structure emerge on the respective scale of resolution or magnification. We provided arguments in Ref. 29 that in our view even quantum theory is just such an emergent aspect which shows up at the typical quantum scale.

We want to briefly mention the possibly far-reaching interplay on the higher levels of coarse-graining between these deleted, too marginal, overlaps and the more *local* wiring stemming from the nonmarginal overlaps. We discussed this point at length in Ref. 29. We argued there that these deleted meta bonds are responsible for the translocal behavior of quantum theory. In the following we are, however, chiefly concerned with the emergence of smooth and local behavior, leading, hopefully, to (quasi)classical space–time structures).

B. The analytic and numerical results

We begin this subsection with a general remark concerning the character of our approximations.

Remark 5.6: As the individual terms in our combinatorial expressions are typically either extremely large or small and are frequently, as in statistical mechanics, very sensitive to the given range of parameters, it is a quite delicate matter to make safe estimates. Among other things we usually have to take logarithms and compare them. That is, if for example $\log(a) \gg \log(b)$, *we sometimes choose to neglect* $\log(b)$ *in a contribution like* $\log(a)+\log(b)$ *in the further calculations. For the original expression this may have the effect that we replace* $b \cdot a$ *by* a. *To give an example, we sometimes approximate* $10^2 \cdot 10^{100}$ *by* 10^{100}. *Otherwise we had to take into account a lot of only marginal contributions which would make the calculations rather cumbersome. On the other hand, this is of course only justified, if we are only interested in qualitative results and provided that the final result is insensitive to such an approximation.*

We made more detailed remarks in Ref. 26, formulas (62) ff., where we discussed the approximation of, e.g., binomial coefficients and their logarithms.

We have seen that the cliques in a large generic random graph of *order n* and *bond probability p* are with high probability concentrated in the interval $(r_0/2, r_0)$ with respect to their order, r, with

$$r_0 \approx 2\log(n)/\log(p^{-1}) + O(\log\log(n)) \tag{34}$$

and with the expectation of r-cliques

$$\langle Z_r \rangle = \binom{n}{r} \cdot (1-p^r)^{n-r} \cdot p^{\binom{r}{2}}. \tag{35}$$

We can test our general working philosophy concerning the effects of coarse graining and renormalization by analytically and numerically calculating various properties of the *clique graph* of a generic random graph. These calculations become increasingly intricate with increasing complexity of the asked questions. Some of the analysis has already been done in, e.g., Sec. 4.2 of Ref. 26 (called "*The Unfolded Epoch*") to which we refer the reader for more technical details.

The meta-nodes of the clique graph, G_{cl}, are the cliques of G. The meta-bonds in G_{cl} are given by the overlap of cliques in G. As we want, on physical grounds, to ignore marginal, that is, too small overlaps, it is important to calculate the expected number of r'-cliques, $\langle N(C_0; r', l) \rangle$, having an overlap of order l with a given fixed r-clique, C_0, with both r and r' lying in the above interval of generic cliques.

In Ref. 26, Sec. 4.2 we derived the following formula for this stochastic quantity (C_0 being a fixed r-clique):

$$\langle N(C_0; r', l) \rangle = \frac{\binom{r}{l} \cdot \binom{n-r}{r'-l} \cdot p^{\binom{r'}{2}-\binom{l}{2}}}{(1-p^r)^{n-r}.} \cdot P_{r',l} \tag{36}$$

with $P_{r',l}$ a lengthy combinatorial expression [formula (69) in Ref. 26] which we can neglect for the parameters n, r, r', chosen by us, that is,

$$n \ggg r, r' \gg l.$$

That is, in this regime we approximated $P_{r',l}$ by one. It can not, however, be neglected if this assumption is violated!

After some manipulations we arrive at the following approximative formula [Ref. 26, formula (74)], where we choose, for convenience, $r' = r$, as we are at the moment only interested in qualitative or generic results:

$$\begin{aligned} \log\langle N(C_0; r', l) \rangle &\approx (r'-l) \cdot (\log(n) - \log(r'-l)) + \tfrac{1}{2} \cdot (r')^2 \cdot \log(p) \\ &\approx \log\langle Z_{r'} \rangle - l \cdot \log(n) - r' \log(r') \end{aligned} \tag{37}$$

with

$$\log\langle Z_r \rangle \approx r\log(n) + \tfrac{1}{2} \cdot r^2 \cdot \log(p). \tag{38}$$

for this range of parameters [cf. also Ref. 26, formula (60) ff.].

The total expected number of r'-cliques having an overlap $l \geqslant l_0$ with a given r-clique is

$$\sum_{l \geqslant l_0} \langle N(C_0; r', l) \rangle \tag{39}$$

(the admissible l's being bounded by the minimum of r and r'). For $l=0$ we get the expected number of r'-cliques, having zero overlap with the given fixed r-clique, C_0, that is we have approximately (remember our simplifying assumption $r=r'$)

$$\log\langle N(C_0; r', l=0) \rangle \approx \log\langle Z_{r'} \rangle - r' \cdot \log(r'). \tag{40}$$

As n is so large, the total number of r'-cliques, having overlap $l \geqslant l_0$ with C_0, can be approximated by the number of cliques fullfilling the lower bound l_0. On the other hand, the total number of expected generic cliques, N_{cl}, in the random graph, G, that is, the cliques with order lying in the respective interval $(r_0/2, r_0)$, is roughly

$$N_{cl} \approx r_0/2 \cdot \langle Z_{\overline{r}} \rangle \tag{41}$$

with $\overline{r}$ an appropriate value in the above interval (this replacement can be made as the numerical values in this interval behave relatively uniformly). We define the *local group* of a generic clique as the set of generic cliques, having nonmarginal overlap with the fixed given clique. From the above reasoning we can now infer the following important conclusion.

Conclusion 5.7:

$$\langle N_{loc.gr.} \rangle \approx N_{cl}/(n^{l_0} \cdot \overline{r}^{\overline{r}}) \tag{42}$$

with n the number of nodes in the graph, G, N_{cl} the number of generic cliques in the corresponding clique graph, l_0 the degree of overlap of the generic cliques, and $\overline{r}$ some appropriate value in the interval $[r_0/2, r_0]$, $n \gg r, r' \gg l_0$ being assumed (where the second $\gg$ is not so pronounced as the first one; n is usually gigantic compared to the clique size r!).

Such estimates are central in the following as they provide information about the local structure of the clique graph.

From the above formulas and numerical results we can now infer interesting properties of the clique graph of a typical graph of order, n, and bond probability, p. The expected order of the *local group* in the clique graph is, by the same token, the *average vertex degree* in the clique graph, that is,

$$\langle v_{cl} \rangle \approx N_{cl}/(n^{l_0} \cdot \overline{r}^{\overline{r}}). \tag{43}$$

From this we can immediately infer the bond probability of the clique graph,

$$p_{cl} = \langle v_{cl} \rangle/(N_{cl}-1) \approx \langle N_{loc.gr.} \rangle / N_{cl} \approx n^{-l_0} \cdot \overline{r}^{-\overline{r}}, \tag{44}$$

and see that it is already considerably smaller than the bond probability of the underlying microscopic graph we started from which, in our numerical example, was assumed to be of order one.

We take our above numerical example, $n=10^{100}$, $p=0.7$, which implies $r_0=1291$, and assume that an appreciable overlap for generic cliques should be of the order of, say, 50 nodes. As typical clique size we take $\overline{r}=r_0/2$ (remember that we are at the moment only interested in qualitative results). The clique graph has roughly $N_{cl} \approx 10^{10^4}$ generic cliques, that is, meta-nodes of the first level. With the bond probability in the clique graph, $p_{cl} \approx 10^{-7 \cdot 10^3}$, we now can calculate the distribution and order of cliques of the first level, that is, cliques of cliques. This provides important information about the near order of the clique graph and the effects of the renormalization steps.

As the order of these cliques of the first level turns out to be already quite small, it is reasonable to avoid our approximative formulas and determine the respective clique number, r_0, by explicitly calculating the number where $\langle Z_r \rangle$ drops from a very large number to effectively zero. The result shows that for $overlap = 50$ of the original cliques (of the zero level), the cliques of the next higher level comprise only very few cliques of the zero level. That is, the near order of $G_1 := G_{cl}$ is already much coarser or less erratic as compared to the near order in the original graph. The results are described in the following observation.

Observation 5.8: For the above numerical parameters we get a typical clique size on the first coarse grained level of order r=2 or 3 and an expected number of cliques of the first level of the order of $\log(N_{cl}) = 10^4$ (*which is comparable to the number of cliques of the zero level*!).

We can control the sensitivity of our results to the chosen degree of overlap. We see below that the results do not depend critically on the numerical details as long as the parameters are roughly of the same order. For example, for $overlap = 30$ we get, performing the corresponding calculations, the following result.

Observation 5.9: For clique-overlap=30 *the clique size on the first level increases slightly to a value of* $r_0 = 4$.

In the following we present some more characteristics of the clique graph with overlap 50:

(i) average vertex degree $\approx 10^{(10^4 - 7 \cdot 10^3 + 3)}$,

(ii) expected number of bonds $= \langle v_{cl} \rangle \cdot 0.5 \cdot \langle n_{cl} \rangle \approx 0.5 \cdot 10^{5 \cdot 10^3 + 10^4 + 6}$.

An important question is whether the (purified) clique graph, G_1, is still connected. In Ref. 26 we gave the threshold value for the corresponding $p^*(n)$, which is

$$p^*(N_{cl}) = \log(N_{cl})/N_{cl} \approx 10^4/10^{10^4} = 10^{-(10^4 - 4)} \ll p_{cl} \approx 10^{-7 \cdot 10^3}, \tag{45}$$

that is,

$$p_{cl}/p^*(n) \approx 10^{3 \cdot 10^3}. \tag{46}$$

Conclusion 5.10: For the numerical data we employed the web of lumps is almost surely *connected. On the other hand, after one renormalization step, the purified net of cliques is more sparsely connected than the initial microscopic net.*

Summing up what we have accomplished so far in this subsection, we have the following row of graph characteristics for the particular set of numerical parameters we employed:

(i) $l = 0$: number of nodes $n_0 = 10^{100}$, bond probability $p_0 = 0.7$, clique number $r_0 = 1291$.

(ii) $l = 1$: $n_1 \approx 10^{10^4}$, $p_1 \approx 10^{-7 \cdot 10^3}$, $r_1 = 3$, $\langle vertex \ \ degree \rangle \approx 10^{0.3 \cdot 10^4}$.

The respective values were calculated by using the following approximative formulas:

$$p_1 = n_0^{-l_0 \cdot \overline{r}^{-\overline{r}}}, \ l_0 = 50 \ , \ n_1 \approx r_0/2 \cdot \langle Z_r^{(0)} \rangle \tag{47}$$

($\langle Z_r^{(0)} \rangle$ is the distribution function of cliques in the initial graph, G_0 and $\overline{r}$ is some average or typical value).

The expected order of cliques on level 1 is only 2 or 3. That is, taking the next step from level 1 to level 2 we may assume an overlap $l_1 = 1$, i.e., we may take the ordinary clique graph. With this value we can calculate the corresponding characteristics of G_2, the graph having as nodes cliques, consisting of nodes of level 1. Before we proceed with the numerical estimates we first have to check whether the approximations we have made above are still valid for this new regime of parameters!

Now, r, r', l are very small and of comparable size. That is, our above approximative formulas are no longer valid. On the other hand, for r, r', l near one, it becomes possible to evaluate the combinatorial expressions directly. For the expected number of nodes on level 2, that is, expected

number of cliques on level 1, we insert our parameters into the formula for $\langle Z_r^{(1)}$ [cf. formula (35)] and get an approximate value, $n_2 \approx 10^{10^4}$ (which is of the same order as $n_1!$).

The calculation of the vertex degree, that is, $\langle N^{(1)}(C_0,r',l)\rangle$ with, e.g., $r'=2, l=1$, is numerically more delicate since now we have to take into account also the term $P_{r',l}$ in formula (36); up to now we approximated by one. Furthermore, we now face the problem of having to deal with small differences of extremely large numbers in the various occurring expressions and/or factors which are extremely small or large and tend to cancel each other.

Fortunately, there is a more direct way to get sufficiently precise results in this regime. We saw that typical cliques in G_1 are of order two or three. The assumed overlap is $l=1$. We can hence infer that the expected number of cliques, overlapping with a fixed given clique, C_0, is roughly the same as the number of nodes, being connected with one of the nodes of C_0. We conclude that

$$p_2 = \langle N^{(1)}(C_0,r',l)\rangle \approx p_1 \approx 10^{-7\cdot 10^3}. \tag{48}$$

With these values for n_2, p_2, we can calculate r_2 and again get $r_2=3$. We hence have for $l=2$

(i) $n_2 \approx 10^{10^4}$ (number of cliques of level 1) and
(ii) $p_2 \approx p_1 \approx 10^{-7\cdot 10^3}$, $r_2=3$.

For the following levels the parameters are now stable and the same as for level two.

Conclusion 5.11: We see that after only two steps we have arrived at a coarse-grained graph with a large number of nodes, a very small bond probability and small cliques, which shows that the geometric near- and far-order has unfolded. We further conclude that the following renormalization steps would no longer alter appreciably the graph characteristics calculated above for the levels G_1, G_2. That is, at least as far as these particular graph properties are concerned, we have already reached a quasi-stable regime, so that the assumption of the existence of fixed phases or attractors does not seem too far-fetched. We can also infer that all the graphs are almost surely connected.

On the other hand, we do not expect that a smooth limit manifold, having, e.g., a fixed integer dimension, does emerge quasi automatically in the pure random graph framework. A further important ingredient will be the action of some appropriately chosen local law as we have introduced it above. (See the corresponding discussions in our mentioned prior work.)

IV. FIXED POINT BEHAVIOR

Starting from a sufficiently large network or graph, $G=G_0$, and performing the consecutive steps, described above, denoting the transition from G_l to G_{l+1}, i.e., from a graph to its (purified) clique graph, by R (standing for *renormalization*), we have

$$R: G_l \to G_{l+1}, \quad G_l = R^l G_0, \quad R^l = R\cdots R \quad (l\text{-times}). \tag{49}$$

The philosophy of the renormalization group is that initial systems, lying on the *critical submanifold*, approach a *fixed point* under R^l for $l\to\infty$. In statistical mechanics the limit systems represent rather a *limit phase*, i.e., a statistical system with the finer details still fluctuating. In the same sense we can at best hope that our presumed limit network of lumps represents a similar limit phase, that is, a network which is only invariant and homogeneous on a larger scale of resolution, while the fine structure is still constantly changing.

The geometric concepts, which have to be further clarified, are the notions of *geometric (fixed) phase* and *critical network state*. We want to emphasize that we cannot expect that these characterizations will be a simple task. Quite to the contrary, both concepts represent subtle and delicate properties. In general, the emerging array of lumps will not fit automatically into something which does resemble a smooth macroscopic manifold, having for example a well-defined and integer (macroscopic) dimension (among other things). Possible obstacles are already well-known on the

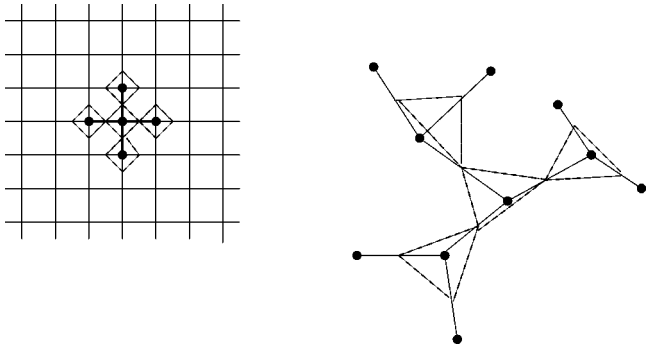

FIG. 5. Fixed point behavior.

much simpler level of simplicial complexes. In order that such a complex has the chance to approximate a manifold, a variety of subtle incident relations between the occurring individual simplices have to be fulfilled (see, e.g., Ref. 54).

In our context these relations on the more coarse-grained scales will depend on the appropriate choice of the microscopic local dynamical laws on the Planck scale we started from. Experience with complex systems in general and cellular automata in particular tells us that the class of appropriate laws will be a very small and peculiar set in the space of possible interaction laws. See the corresponding findings in the regime of *selforganized criticality*,[55] the catchword being *complexity at the edge of chaos*.

In other words, as the whole approach appears to be relatively new and the task formidable, we will make what are perhaps only some first steps towards a solution of these problems. In a first step we will convince ourselves that the renormalization procedure described by us does not lead to nonsensical results (we have already previously seen that some gross characteristics of the network seem to become stable after only a few renormalization steps). We show that there do exist examples of graphs which display fixed point or fixed phase behavior in a more microscopic sense. These graphs are, however, simple and very regular and are not meant to represent possible examples of networks, underlying our continuum space–time. They rather serve at best as illustrative toy models.

In the following section we then introduce a geometrical core concept designed to classify such irregular network structures, i.e., the notion of *graph dimension*. We show how it behaves under our renormalization process. The corresponding analytic results indicate what kind of *critical behavior* is presumably needed to have a physically reasonable limit behavior.

We illustrate our framework with the help of some simple examples (see also Fig. 5). Note that in the following examples the minimal admissible clique overlap is assumed to be one common node!

(1) *The graph* $\mathbb{Z}^2$*: The set of nodes are parametrized as* $V=\{(i,j),\, i,j\in\mathbb{Z}\}$*. Edges are drawn between the following nodes:*

$$(i,j),(i',j') \quad \text{with} \quad |i'-i|+|j'-j|=1. \tag{50}$$

We determine the cliques at the various levels, given by G_l (see also the following figure).

(G_0) A node, (i,j), belongs to the following zero-cliques:

$$\{(i+1,j),(i,j)\} \quad \{(i,j+1),(i,j)\} \tag{51}$$

and $+$ replaced by $-$, that is, the order of the zero-cliques is 2, the diameter (that is, the maximal distance between two nodes) is 1, and the maximal mutual overlap is 1.

(G_1) A zero-node, (i,j) belongs to the following one-cliques,

$$\{(i,j),(i\pm 1,j)(i,j\pm 1)\}, \tag{52}$$

and the cliques formed around the nn-nodes of (i,j). The order relative to G_0 is 5, the diameter is 2, and maximal overlap is 2.

(G_2) The order of two-cliques relative to G_0 is 13, diameter is 3, and maximal overlap is 8.

Remark: Note that the above values of order and diameter refer to the start graph G_0.

With increasing l, the maximal overlap becomes large, due to the particular structure of the graph, $\mathbb{Z}^2$. One sees that for large l the hierarchical structure of the corresponding tower of graphs, G_l, becomes very dense and entangled, a feature one would also expect from something like a *continuum*.

On the other side, it is instructive to perform also the above mentioned rescaling and compare the various levels at the same scale, viz., inspect the pure graph structure. This will make explicit the fixed point behavior we are particularly interested in.

($G_0 \to G_1$) The one-nodes of G_1 (i.e., the zero-cliques) we represent by the midpoints of the edges of the start graph, $G_0 := \mathbb{Z}^2$. Four of these zero-cliques meet at a common node, (i,j), say. We represent the one-edges as the line segments, connecting these midpoints. This yields a new, rotated lattice (plus two extra diagonal edges).

($G_1 \to G_2$) These four one-nodes (the one-cliques) form now the two-nodes. They form a simplex having six one-edges. We inscribe these two-nodes in G_0 by placing them in the centers of the one-cliques, that is the original lattice points of G_0. We draw a two-edge if two of these one-cliques have a common one-node (that is, a zero-clique!). We can convince ourselves that the emerging graph, G_2, is isomorphic to the start graph, G_0. We hence make the interesting observation:

Observation 6.1: Starting from $G_0 = \mathbb{Z}^2$, we see that G_2 is combinatorially isomorphic to G_0, meaning that there exists an invertible map, $\Phi: G_0 \to G_2$, mapping nodes on nodes and bonds on bonds and preserving the combinatorial structure in the following way (with e_{ij} an edge of G_0):

$$e_{ij} \in E(G_0) \leftrightarrow \Phi(e_{ij}) \quad connects \quad \Phi(x_i), \Phi(x_j). \tag{53}$$

The same holds for G_1, G_3, etc.

Conclusion 6.2: The sequence of graphs, $G_0, G_1, G_2, \ldots$, decomposes in exactly two sets of isomorphic graphs,

$$\{G_0, G_2, \ldots\} \quad , \quad \{G_1, G_3, \ldots\} \tag{54}$$

under the renormalization group

$$\mathcal{R} := \{R^i\}, \quad R^i: G_0 \to G_i, \quad R^2: G_i \to G_{i+2}. \tag{55}$$

Corollary 6.3: A corresponding observation can be made for a general lattice, $\mathbb{Z}^n$.

(2) *The trivalent infinite tree:* In order to get a better feeling for what can happen, we study some more elementary examples. Let us take an infinite trivalent tree. The zero-cliques are again two-sets of vertices or line segments, connecting nn. The graph, G_1, is again represented by connecting the midpoints of these line segments. The resulting one-cliques are three-sets or triangles. Taking them as the two-nodes of G_2, we see that G_2 is again isomorphic to G_0 as in the $\mathbb{Z}^2$-case.

Observation 6.4: For a trivalent infinite tree, the sequence of graphs, $G_0, G_1, G_2, \ldots$, decomposes into two subsets. The situation is the same as for the preceding example.

(3) *The triangulated* $\mathbb{R}^2$: We introduce another simple example. We triangulate $\mathbb{R}^2$ by using the above lattice, $\mathbb{Z}^2$, and complement it by drawing the diagonals, pointing from (i,j) to $(i+1, j+1)$. The zero-cliques are these triangles. Without a purification, bonds in the graph, G_1, are drawn if two zero-cliques meet at a common node or zero-edge. The emerging one-cliques have the shape of hexagons, i.e., they are six-simplices. Repeating this process, one sees that G_2 is isomorphic to G_1.

Observation 6.5: In the case of the above triangulation of $\mathbb{R}^2$, *we have a start graph,* G_0, *while all the graphs,* $G_1, G_2, \ldots$, *are isomorphic. In other words, we now have a fixed point of the renormalization group.*

Conclusion 6.6: We have seen that there exist examples in the category of graphs which display phenomena like invariant sets or fixed points under our geometric renormalization group.

These observations open up interesting vistas. While we have not yet shown that the above invariant sets or fixed points have the character of *attracting sets*, that is, whether there exist large *basins of attraction* in the category of graphs under the repeated application of the map, R, we strongly surmise that this is true. Furthermore, the concept of *self-similarity* suggests itself (see also the next section) a notion we have already introduced and studied in Ref. 23, to construct graphs with *fractal dimension*.

VII. GRAPH DIMENSION UNDER THE RENORMALIZATION GROUP

We repeatedly mentioned the possibility of *geometric* or *topological phase transitions* in evolving networks of the kind we are having in mind. In Ref. 23 we developed and studied the concept of *graph dimension* in quite some detail. We concluded that, from the physical point of view, the number of nodes which can be reached by, say, l steps starting from a given node is an important characteristic as is its limiting and scaling behavior as a function of l. This is the crucial and *intrinsic* property, which underlies implicitly most of the calculations in the physics of phase transitions and many other phenomena, which are triggered by the collective interaction of many constituents. Its true significance is, however, frequently hidden as the reasoning is usually performed by using the properties of the embedding space (viz., its ordinary dimension).

Remark: We learned recently that such growth properties are also important characteristics in geometric group theory and related subjects in pure mathematics (see, e.g., Refs. 45, 46, or 47).

We will investigate the behavior of this quantity under the application of our renormalization group. In Ref. 23 we introduced the two variants, defined below. They are not strictly equivalent but coincide in the more regular situations. In the following, for the sake of brevity, we only use the first notion.

Definition 7.1 (internal scaling dimension): Let x *be an arbitrary node of* G. *Let* $\#(U_n(x))$ *denote the number of nodes in* $U_n(x)$. *We consider the sequence of real numbers* $\underline{D}_n(x) := \ln(\#(U_n(x))/\ln(n)$. *We say* $\underline{D}_S(x) := \liminf_{n\to\infty} D_n(x)$ *is the* lower *and* $\overline{D}_S(x) := \limsup_{n\to\infty} D_n(x)$ *the* upper internal scaling dimension *of* G *starting from* x. *If* $\underline{D}_S(x) = \overline{D}_S(x) =: D_S(x)$, *we say* G *has internal scaling dimension* $D_S(x)$ *starting from* x. *Finally, if* $D_S(x) = D_S \forall x$, *we simply say* G *has* internal scaling dimension D_S.

Definition 7.2 (connectivity dimension): Let x *again be an arbitrary node of* G. *Let* $\#(\partial U_n(x))$ *denote the number of nodes in the boundary of* $U_n(x)$. *We set* $\tilde{D}_n(x) := \ln(\#(\partial U_n(x))/\ln(n) + 1$ *and define* $\underline{D}_C(x) := \liminf_{n\to\infty} \tilde{D}_n(x)$ *as the* lower *and* $\overline{D}_C(x) := \limsup_{n\to\infty} \tilde{D}_n(x)$ *as the* upper connectivity dimension. *If lower and upper dimension coincide, we say* G *has* connectivity dimension $D_C(x) := \overline{D}_C(x) = \underline{D}_C(x)$ starting from x. *If* $D_C(x) = D_C$ *for all* x *we call* D_C *simply the* connectivity dimension *of* G.

Remark: The above does not imply that this notion is the only relevant topological characteristic of large networks. It clearly is not sufficient to describe *all* of the mesoscopic or macroscopic properties, but we think it is, as in the continuum, a very important concept.

We already proved in Ref. 23 that this kind of dimension is stable under a variety of transformations, in particular under *local* ones. In Sec. 5.2.5 of Ref. 23 we showed that, in order to change the dimension of a graph, we have to introduce long-range effects or interactions. This reminds one of the behavior of *critical systems*.

We now compare the dimension of a graph, G, with the dimension of its clique graph, G_{cl}, where, for the time being, we take the clique graph in its original meaning. That is, we draw a bond if two cliques have a nonvoid overlap of arbitrary size.

Let us assume, for convenience, that G has the scaling dimension, D, that is, for every node, x_0, we have

$$\lim_{l} \ln(\#(U_l))/\ln l = D. \tag{56}$$

Furthermore, we assume for simplicity that the node degree of G is globally bounded, i.e.,

$$v_i \leqslant v < \infty \quad \text{for all} \quad x_i. \tag{57}$$

We choose a fixed node, x_0, lying in a fixed clique, C_0. We have to calculate the number of one-nodes, that is, the number of zero-cliques, $\#(U_l^{cl}(C_0))$, lying in $U_l^{cl}(C_0)$ with the distance, d_1, now measured in the clique graph, G_{cl}. That is, a clique, C_l, lies in $U_l^{cl}(C_0)$ if C_0 and C_l can be connected by a sequence of l' cliques with $l' \leqslant l$ so that two consecutive cliques have a nonzero overlap. For each zero-node, x_l', lying in some $C_{l'}$ with $d_1(C_0, C_{l'}) \leqslant l$, we can estimate the distance to the node x_0 in C_0. There exists, by definition, a sequence of overlapping cliques,

$$C_o, C_1, \ldots, C_{l'}, \quad l' \leqslant l. \tag{58}$$

For two neighboring cliques, C_i, C_j, we have

$$d_0(x_i, x_j) \leqslant 2, \; x_i \in C_i, x_j \in C_j. \tag{59}$$

For each intermediate consecutive pair of cliques we need one step (a bond from a node in the overlap $C_{i-1} \cap C_i$ to a node in $C_i \cap C_{i+1}$), for the initial and final pair we need at most two steps. We hence get

$$d_0(x_0, x_{l'}) \leqslant l' + 2. \tag{60}$$

Lemma 7.3: For two arbitrary nodes

$$x_0 \in C_0, x_{l'} \in C_{l'} \quad \text{with} \quad d_1(C_0, C_{l'}) \leqslant l \tag{61}$$

we have

$$d_0(x_0, x_{l'}) \leqslant l' + 2 \tag{62}$$

and hence

$$|U_l^{cl}(C_0)| \subset U_{l+2}(x_0) \tag{63}$$

with $|U_l^{cl}(C_0)|$ *the set of zero-nodes, lying in* $U_l^{cl}(C_0)$ (*the latter set now understood as the set of its zero-nodes). This implies*

$$\#(|U_l^{cl}(C_0)|) \leqslant \#(U_{l+2}(x_0)). \tag{64}$$

From observation 4.2 of Ref. 26 we know that each node, x_i, can lie in at most 2^{v_i} different cliques, with $v_i \leqslant v$. This yields the crude, but *a priori*, estimate

$$\#(U_l^{cl}(C_0)) \leqslant \#(U_{l+2}(x_0)) \cdot 2^v, \tag{65}$$

which is the desired upper bound on the number of cliques, lying in $U_l^{cl}(C_0)$. We conclude that, for an infinite graph with $v_i \leqslant v < \infty$, we have for the dimension of its clique graph

$$\overline{D}_{cl} \leqslant D \tag{66}$$

since

$$\ln(\#(U_l^{cl}(C_0)))/\ln(l) \leqslant \ln(\#(U_{l+2}(n_0)))/\ln(l) + v \cdot \ln(2)/\ln(l). \tag{67}$$

For $l\to\infty$ we get the above result.

We want to prove a corresponding lower bound. Take an arbitrary node, $x_{l'}$, in $U_l(x_0)$. By definition, there exists a node- (edge-)sequence

$$x_0-x_1-\cdots-x_{l'} \quad \text{with} \quad l'\leqslant l. \tag{68}$$

On the other side, there exists a sequence of cliques, C_i, with each consecutive pair of nodes, $(x_{i-1},x_i)\in C_i$. These cliques do exist because, starting from the connected pair, (x_{i-1},x_i), we get such a clique by extending this germ in one of (possibly) several ways to a clique (cf. Sec. 4 of Ref. 26). We can conclude that for each node, $x_{l'}\in U_l(x_0)$, and $x_0\in C_0$, we have

$$x_{l'}\in\left|U^{cl}_{l+1}(C_0)\right|. \tag{69}$$

(Note that the clique, containing both x_0 and x_1, may be different from the start clique, C_0!)

We then have

$$U_l(x_0)\subset\left|U^{cl}_{l+1}(C_0)\right| \quad \text{and} \quad \#(U_l(x_0))\leqslant\#(\left|U^{cl}_{l+1}(C_0)\right|). \tag{70}$$

With $v_i\leqslant v$ for all x_i, the maximal order of a clique is bounded from above by $(v+1)$. This implies

$$\#(\left|U^{cl}_{l+1}(C_0)\right|)\leqslant(v+1)\cdot\#(U^{cl}_{l+1}(C_0)) \tag{71}$$

and

$$\#(U^{cl}_{l+1}(C_0))\geqslant\#(U_l(x_0))/(v+1). \tag{72}$$

We hence get

$$\ln(\#(U^{cl}_{l+1}(C_0)))/\ln(l+1)\geqslant\ln(\#(U_l(x_0)))/\ln(l+1)-\ln(v+1)/\ln(l+1). \tag{73}$$

With

$$\ln(l+1)=\ln(l\cdot(1+l^{-1}))=\ln(l)+\ln(1+l^{-1}) \tag{74}$$

and $l\to\infty$, we see that

$$\underline{D}_{cl}\geqslant D \tag{75}$$

and get the important theorem:

Theorem 7.4: *Assuming that G has dimension D and globally bounded node degree, $v_i\leqslant v<\infty$, we have that D_{cl} also exists and it holds*

$$D_{cl}=D. \tag{76}$$

Note that this result does hold for the ordinary clique graph, viz. arbitrary overlap, viz., no purification. In other words, under these assumptions, the renormalization steps do not change the graph dimension.

This result is reminiscent of a similar observation in statistical mechanics where the non-coarse-grained Gibbsian entropy happens to be a *constant of motion*. The same happens here. In the ordinary clique graph each original bond occurs in at least one clique, i.e., there is no real (or, more precisely, not enough) coarse graining.

VIII. CRITICAL NETWORK STATES

In Sec. V B we derived formulas for the size of the so-called local group of a clique in a random graph, that is the set of cliques with which a given clique has a (sufficient) common

overlap. If one is in the parameter regime in which the cliques are still densely and complicately entangled (typically the first renormalization steps) and compares the number of bonds in the *purified* clique graph, that is, bonds being defined by a sufficient! overlap, with the number of bonds in the corresponding (unpurified) clique graph, the latter number exceeds the former one by many orders. Put differently, in this situation the number of *marginal* overlaps of cliques is much bigger. All these marginal overlaps are deleted in the purification or renormalization process.

The last theorem in the preceding section shows that we will not get a dimensional reduction without sufficient purification. If we go through the proof, we see that the first part does hold unaltered for the purified clique graph. In the second part, however, we used an argument which does only hold for ordinary clique graphs [see the remarks following formula (68)]. The existence of the row of overlapping cliques, employed there, can only be guaranteed if the degrees of overlap are left arbitrary. We hence can infer the following.

Corollary 8.1: For the purified clique graph, with overlaps exceeding a certain fixed number, l_0, *we can only prove*

$$D_{cl} \leqslant D. \tag{77}$$

Having for example the picture in mind, frequently invoked by Wheeler and others, of a space–time foam, with a concept of dimension depending on the scale of resolution (see, e.g., Box 44.4 on p. 1205 in Ref. 30), we infer from our above observations that this may turn out to be both an interesting and not entirely trivial topic. We have to analyze under what specific conditions the dimension can actually shrink under coarse-graining, so that we may start from a very erratic network on, say, the Planck scale, and arrive in the end at a smooth macroscopic space–time having perhaps an integer dimension of, preferably, value 4 or so.

We remarked already in the introduction that geometric change or geometric phase transitions are supposed to be related to some sort of *critical state* of the network. Our previous observations about the possibility of dimensional change under coarse graining together with an interesting observation already made in Ref. 23, lemma 4.10, allows us to *almost rigorously* prove what kind of criticality is in fact necessary to achieve this goal.

We showed there that it is not so easy to modify the dimension of a graph by *local* alterations.

Proposition 8.2: Additional insertions of bonds between arbitrarily many nodes, y,z, *having original graph distance,* $d(y,z) \leqslant k \quad , \quad k \in \mathbb{N}$ *arbitrary but fixed, do not change* $\underline{D}(x)$ *or* $\overline{D}(x)$.

From this we learn the following. Phase transitions in graphs, changing the dimension, have to be intrinsically *nonlocal*. That is, they necessarily involve nodes having an arbitrarily large distance in the original graph. We think this is a crucial observation from the physical point of view. On the one side, it shows that systems have to be *critical* in a peculiar way, that is, having a lot of distant correlations or, rather, correlations on all scales (cf. also Smolins's discussion in e.g., Ref. 4 and elsewhere). On the other side, it fits exactly with our working philosphy that quantum theory is a *residual* and *coarse-grained* effect of such largely hidden long range correlations.[29]

If we apply these findings to our renormalization steps, that is, passing from a graph to its associated (purified) clique graph, this implies the following. We saw that assuming a network or graph, G, having a dimension, D, the unpurified clique graph still has

$$D_{cl} = D. \tag{78}$$

On the other hand, denoting the purified clique graph by $\hat{G}_{cl}$, we have the estimate

$$\hat{D}_{cl} \leqslant D_{cl} = D. \tag{79}$$

The transition from G_{cl} to $\hat{G}_{cl}$ consists of the deletion of marginal overlaps among cliques (with the necessary criteria provided by the physical context). That is, $\hat{G}_{cl}$ lives on the same node set (the set of cliques) but has fewer (meta)bonds. The above proposition shows that this does *not* automatically guarantee that we really have

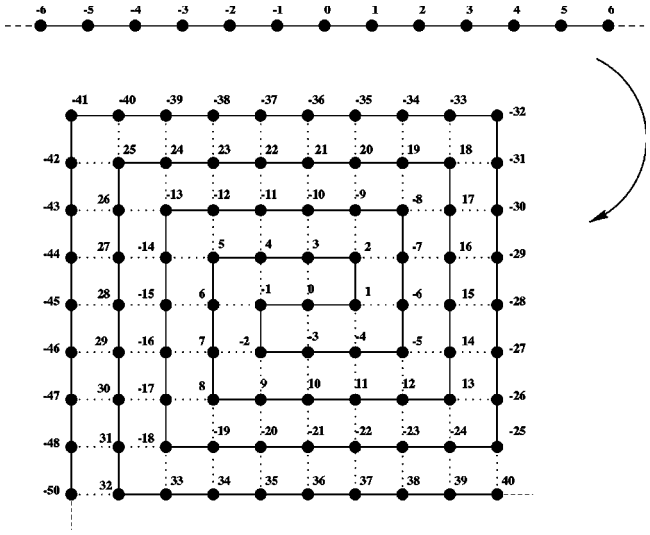

FIG. 6. Change of dimension.

$$\hat{D}_{cl} < D_{cl}\,. \tag{80}$$

Quite to the contrary, we learned that this can only be achieved if the bond deletions happen in a very specific way.

On G_{cl} we have, as on any graph, a natural distance or neighborhood structure, given by the canonical graph metric, $d_{cl}(C_i, C_j)$. Note that the above proposition holds as well for bond deletions instead of insertions. We thus infer that bond deletions in G_{cl} between cliques which are not very far apart in the final purified graph $\hat{G}_{cl}$ cannot alter the final dimension of $\hat{G}_{cl}$. More precisely, only bond deletions between cliques having distances in $\hat{G}_{cl}$ which approach infinity in a specific way can have an effect.

Conclusion 8.3: We conclude that only the bond deletions between very distant cliques (with respect to $\hat{G}_{cl}$), with this distance being unbounded, can decrease the dimension of $\hat{G}_{cl}$ as compared to G_{cl}. More precisely, there has to be a substantial bond deletion on all scales up to infinity.

The above observation reminds one of the *scale invariance* of *critical systems* in other contexts. We exemplify this by a simple but instructive example (see Fig. 6).

This [inhomogeneous; it slightly depends on the reference point (0,0)] construction has already been given in Sec. 5.2.5 of Ref. 23. One takes the lattice, $\mathbb{Z}_2$, inscribes in it, starting from the point (0,0), two nonintersecting outwardly spiraling edge sequences:

$$(0,0)\to(1,0)\to(1,1)\to(0,1)\to(-1,+1)\to(-2,+1)\to(-2,0)\to\cdots \tag{81}$$

and

$$(0,0)\to(-1,0)\to(-1,-1)\to(0,-1)\to(+1,-1)\to(+2,-1)\to(+2,0)\to\cdots. \tag{82}$$

We consider this inscribed graph as a representation of the one-dimensional lattice, $\mathbb{Z}_1$, with the node labeling running from $-\infty$ to $+\infty$.

$$0\to1\to2\to3\to4\to5\to\cdots \tag{83}$$

and

$$0\to-1\to-2\to-3\to-4\to-5\to\cdots. \tag{84}$$

Remark 8.4: The embedded graph, being isomorphic to $\mathbb{Z}_1$, *is in fact a* spanning tree *relative to the ambient graph,* $\mathbb{Z}_2$.

One can now see that the extra bonds, occurring in $\mathbb{Z}_2$, not belonging to the representation of $\mathbb{Z}_1$, connect nodes of a larger and larger distance with respect to the labeling of $\mathbb{Z}_1$. We have for example bonds in $\mathbb{Z}_2$ between pairs of nodes with the $\mathbb{Z}_1$-labels,

$$0,3\,;\,3,-10\,;\,-10,21\,;\,21,-36\ldots \tag{85}$$

and correspondingly for other sequences of nodes. That is, the embedded graph is one-dimensional, lying in a two-dimensional graph, while the node sets are identical. The preceding discussion and the figure illustrate and confirm what we have said above about the type of necessary criticality and long-range correlations.

To employ this example for our renormalization group approach, we can replace the original nodes (with the $\mathbb{Z}_1$-labeling) by certain cliques of arbitrary order and choose the overlaps appropriately, so that the above representation of $\mathbb{Z}_1$ becomes the *purified* clique graph of the total graph. We arrive at a coarse-grained graph of dimension one, starting from an unpurified graph of dimension two or a larger dimension.

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Existence of the self-graviting Chern–Simons vortices

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(Received 7 June 2003; accepted 4 September 2003)

We prove existence of multivortex solutions of the self-dual Einstein–Chern–Simons–Higgs system, proposed by Clément [Phys. Rev. D **54**, 1844–1847 (1996)]. We consider both the topological and the nontopological boundary conditions for open, conformally flat manifolds. For nontopological boundary conditions we use perturbation argument from a solution of the Liouville equation combined with the implicit function theorem. Using this argument we have existence for arbitrary positive number for the gravitational constant. For topological boundary condition we construct solutions for small gravitational constant by using the super/subsolution method. For sufficiently large gravitational constant we have a nonexistence result for the radially symmetric topological solutions. We also obtain the decay estimates near infinity for both of the topological and the nontopological solutions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625871]

I. THE EINSTEIN–CHERN–SIMONS–HIGGS MODEL

The well-known Abelian Chern–Simons–Higgs (CSH) model[9,11] can be generalized to the Einstein–Chern–Simons–Higgs (ECSH) model if we couple the CSH model to gravity.

The Abelian ECSH model is defined by the action:[6]

$$I=\int \mathrm{d}^3x\left\{-\frac{1}{16\pi G}\sqrt{|g|}R-\frac{\kappa}{4}\varepsilon^{\mu\nu\rho}F_{\mu\nu}A_\rho+\sqrt{|g|}\,[g^{\mu\nu}D_\mu\phi(D_\nu\phi)^*-V(|\phi|)]\right\}, \qquad (1.1)$$

where $g_{\mu\nu}$ is the $(2+1)$ dimensional Lorentzian metric with the signature $(+,-,-)$, R is a scalar curvature, $G>0$ is a gravitational constant, A_μ $(\mu=0,1,2)$ is the gauge field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, ϕ is a complex scalar field, $D_\mu\phi=(\partial_\mu+iqA_\mu)\phi$ with q representing the charge of the electron, $\varepsilon^{\mu\nu\rho}$ is the skew symmetric tensor with $\varepsilon^{012}=1$, and κ is the Chern–Simons coupling constant. The Higgs potential $V(|\phi|)$ shall be specified later on.

It has been shown by Valtancoli[20] that the ECSH model admits the self-dual stationary multivortex solutions provided that a suitable eighth-order potential is chosen. Cangemi–Lee[2] considered the Einstein–Maxwell–Chern–Simons–Higgs model, and obtained a set of self-dual equations by imposing some additional conditions on A_μ, ϕ and the real field $\mathcal{N}$. When a certain limit is taken, this model[2] reduces to the ECSH model, and we can obtain self-dual equations for the ECSH model. The ECSH model was also studied by Clément,[6] who obtained self-dual ECSH system by imposing a weaker condition $g_{00}=1$ and by decomposing Ricci tensor $R_{\mu\nu}$. In this paper we follow[6] and establish existence results for our model equations. These models are actually generalizations of the Einstein–Abelian–Higgs (EAH) model considered in Refs. 7, 12, and 23 which models the cosmic strings with the matter as the Abelian–Higgs fields. For the EAH model, only topological solutions are admissible for the finiteness of the total energy. See Refs. 18 and 21 for the rigorous mathematical studies of the EAH model.

Unlike the Einstein–Abelian–Higgs model, ECSH model admits both topological and nontopological boundary conditions to give finite total energy. The purpose of this paper is to con-

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struct multivortex solutions of the ECSH model with the topological and the nontopological boundary conditions, respectively.

The Euler–Lagrange equation for the action (1.1) is the Einstein equation

$$R_{\mu\nu}-\tfrac{1}{2}g_{\mu\nu}R=8\pi G T_{\mu\nu} \tag{1.2}$$

coupled with the matter field equations for (A_μ,ϕ)

$$(\kappa/2\sqrt{|g|})\varepsilon^{\mu\lambda\nu}F_{\mu\lambda}=iqg^{\nu\rho}(\phi^*(D_\rho\phi)-\phi(D_\rho\phi)^*), \tag{1.3}$$

$$(1/\sqrt{|g|})D_\mu(\sqrt{|g|}g^{\mu\nu}D_\nu\phi)=-\partial V/\partial\phi^*, \tag{1.4}$$

where the energy-momentum tensor $T_{\mu\nu}$ is given by

$$T_{\mu\nu}=((D_\mu\phi)^*(D_\nu\phi)+(D_\mu\phi)(D_\nu\phi)^*)-g_{\mu\nu}(g^{\alpha\beta}(D_\alpha\phi)^*(D_\beta\phi)-V).$$

We make the ansatz for stationary solutions

$$\begin{aligned} ds^2&=N_*^2(dt+\omega_j\,dx^j)^2+\gamma_{jk}\,dx^j\,dx^k,\\ A_\mu\,dx^\mu&=A_0(dt+\omega_j\,dx^j)+\overline{A}_j\,dx^j. \end{aligned} \tag{1.5}$$

Here $N_*\geqslant 0$; N_*, A_0, ω_j, $\overline{A}_j$ and γ_{jk} are functions of (x^1,x^2) only.

With the help of the Euler–Lagrange equations (1.2)–(1.4) and the decomposition of Ricci tensor $R_{\mu\nu}$, Clément has derived the self-duality condition

$$\overline{D}_j\phi=\mp(i/\sqrt{\gamma})\gamma_{jk}\varepsilon^{kl}\overline{D}_l\phi, \tag{1.6}$$

by imposing the condition $N_*=\sqrt{g_{00}}\equiv 1$. (See Ref. 6 for the details.) Moreover, it was shown in Ref. 6 that if the Higgs potential V takes the specific form

$$V=\frac{q^4}{\kappa^2}|\phi|^2(|\phi|^2-\varepsilon^2)^2-2\pi G\kappa^2\left[\frac{q^2}{\kappa^2}(|\phi|^2-\varepsilon^2)^2+C\right]^2,$$

then the self-dual equations for the stationary solutions of (1.2)–(1.4) are given as follows:

$$A_0=\pm(q/\kappa)(|\phi|^2-\varepsilon^2), \tag{1.7}$$

$$\overline{B}=-A_0[(2q^2/\kappa)|\phi|^2-8\pi G\kappa(A_0^2+C)], \tag{1.8}$$

$$R_\gamma=(8\pi G\kappa(A_0^2+C))^2+16\pi G[\gamma^{jk}(\overline{D}_j\phi)(\overline{D}_k\phi)^*-2V], \tag{1.9}$$

$$b=-8\pi G\kappa(A_0^2+C), \tag{1.10}$$

where ε^2, C are integration constants, $\overline{D}_j\phi=\partial_j\phi+iq\overline{A}_j\phi$ with $\overline{A}_j=A_j-\omega_jA_0$, ε^{kl} is the skew symmetric 2-tensor with $\varepsilon^{12}=1$, $\gamma=\det(\gamma_{jk})$ and

$$\overline{B}=(1/\sqrt{\gamma})(\partial_1\overline{A}_2-\partial_2\overline{A}_1),\quad b=(1/\sqrt{\gamma})(\partial_1\omega_2-\partial_2\omega_1).$$

We may also choose a time gauge in which $\partial^j\omega_j=0$ in conformal coordinates, so that ω_j is the curl of a real potential ω, which leads $\Delta\omega=-\sqrt{\gamma}\,b$.

We note that a solution of (1.7)–(1.10) is also a stationary solution of (1.2)–(1.4).

It is well-known that the Gauss–Codazzi equation coupled with (1.2) implies the constraint equation (see, e.g., Ref. 7) $R_\gamma=-16\pi G T_{00}$. The total stationary energy E is given by

$$E=-\frac{1}{16\pi G}\int_{\mathbb{R}^2}R_\gamma\sqrt{\gamma}\,dx.$$

The integration constant C in (1.8)–(1.10) is subject to a physical constraint to give the finite energy: at the spatial infinity, we assume $|\phi|$ approaches uniformly to some constant value ϕ_∞ and $\overline{B}(\infty)=0$. We consider the two cases

$$\text{(i)}\quad \phi_\infty=0,\quad C=-q^2\varepsilon^4/\kappa^2\quad (\textbf{nontopological boundary condition}) \tag{1.11}$$

and

$$\text{(ii)}\quad \phi_\infty=\varepsilon,\quad C=0\quad (\textbf{topological boundary condition}). \tag{1.12}$$

We note that if $G=0$ and the metric (1.5) is set to be a $(2+1)$-dimensional Minkowski metric (i.e., $N_*=1$, $\omega_j\equiv 0$, and $\gamma_{jk}=-\delta_{jk}$), the ECSH model reduces to the CSH model proposed by Hong–Kim–Pac[9] and Jackiw–Weinberg.[11] There are now some existence results available for vortices with the topological boundary condition,[17,22] the nontopological boundary condition[4,16] and the periodic boundary condition[1,19] to the CSH model. In particular double vortex condensates, including some blow-up analysis, have been studied in relation to the existence of extremal functions for a Sobolev inequality of the Moser–Trudinger's type.[15]

In this paper, we study the self-dual equations (1.7)–(1.10) of the ECSH model and construct multivortex solutions with the topological and the nontopological boundary conditions respectively. More precisely, we have

Theorem 1.1 (Existence of nontopological solutions): *Let $N>0$ and finite points $p_1,\dots,p_N\in\mathbb{R}^2$ be given. Then, there is a constant $\delta_0=\delta_0(G\varepsilon^2,N)$ such that for all $\delta\in(0,\delta_0)$ the system (1.7)–(1.10) has a smooth solution (g,A,ϕ) with the following properties:*

(i) $(M,\gamma_{jk})=(\mathbb{R}^2,-e^\eta\delta_{jk})$, *i.e.,* (M,γ_{jk}) *is conformally flat.*

(ii) ϕ *vanishes at* $p_1,\dots,p_N$, *and satisfies the boundary condition (1.11).*

(iii) *The conformal factor* e^η *satisfies the decay estimate*

$$e^{\eta}(x)=O(|x|^{-(32\pi G\varepsilon^2(N+1))/(16\pi G\varepsilon^2+1)-8\pi G\varepsilon^2\beta_1(\delta)})\quad \text{as } |x|\to\infty \tag{1.13}$$

for some $\beta_1(\delta)$ *with* $\beta_1(\delta)=O(\delta^2)$ *as* $\delta\to 0$, *and* $|\phi|^2$, $\overline{B}$, $|\overline{D}\phi|^2$ *satisfy*

$$|\phi|^2+\overline{B}+|\overline{D}\phi|^2=O(|x|^{-(2N+4+32\pi G\varepsilon^2)/(16\pi G\varepsilon^2+1)-\beta_2(\delta)})\quad as\ \ |x|\to\infty$$

for some $\beta_2(\delta)$ *with* $\beta_2(\delta)=O(\delta^2)$ *as* $\delta\to 0$.

(iv) *The energy* E *has the value*

$$E=\pi\varepsilon^2\left(\frac{4N+4}{16\pi G\varepsilon^2+1}+\beta_1(\delta)\right), \tag{1.14}$$

which is obviously nonquantized.

In the above if $G\varepsilon^2$ *is sufficiently small, then* $\beta_1(\delta)>0$. *If* $8\pi G\varepsilon^2 N<8\pi G\varepsilon^2+1$, *then* $\beta_2(\delta)>0$.

Theorem 1.2 (Existence and nonexistence of topological solutions): *Let $N>0$ and $p_1,\dots,p_N\in\mathbb{R}^2$ be given.*

Case 1: If $G\varepsilon^2$ *is sufficiently small, then the system (1.7)–(1.10) has a smooth solution* (g,A,ϕ) *with the following properties:*

(i) $(M,\gamma_{jk})=(\mathbb{R}^2,-e^\eta\delta_{jk})$.

(ii) ϕ *vanishes at* $p_1,\dots,p_N$ *and satisfies the boundary condition (1.12).*

(iii) *The total energy* E *is given by*

$$E=2\pi\varepsilon^2 N,$$

and obviously quantized.

(iv) *The conformal factor* e^η *satisfies the decay estimate*

$$e^{\eta(x)}=O(|x|^{-16\pi G\varepsilon^2 N})\quad as\quad |x|\to\infty, \tag{1.15}$$

and the terms $\varepsilon^2-|\phi|^2$, $\overline{B}$, $|\overline{D}\phi|^2$ *satisfy the decay estimates*

$$|\overline{B}|+|\overline{D}\phi|^2+|\varepsilon^2-|\phi|^2|=O(\exp(-(1-\delta)m|x|^{1-8\pi G\varepsilon^2 N})) \quad as \quad |x|\to\infty$$

for any $\delta>0$, *where*

$$m=\frac{2q^2\varepsilon^2}{\kappa}\frac{\exp(-4\pi G\varepsilon^2)}{1-8\pi G\varepsilon^2 N}.$$

Case 2: If $G\varepsilon^2\geqslant 1/8\pi N$, *then every radially symmetric solution* (g,A,ϕ) *satisfies* $\lim_{|x|\to\infty}|\phi(x)|=+\infty$.

Theorem 1.1 and Theorem 1.2 will be proved with the reduction of (1.7)–(1.10) to a system of elliptic equations. If we transform conformally from (M,γ_{jk}) into $(\mathbb{R}^2,\delta_{jk})$ by $\gamma_{jk}=-e^{\eta}\delta_{jk}$, then the equation (1.6) becomes

$$\overline{D}_1\phi\mp i\overline{D}_2\phi=0. \tag{1.16}$$

We choose the ''plus'' sign. Following the argument of Jaffe–Taubes (Ref. 10, Chap. 3) we can deduce from (1.16) that the zeros of ϕ are finite, and we have the representation $\phi(z)=(z-p_j)^{n_j}f(z)$ in a neighborhood of a zero p_j of ϕ with the multiplicity n_j for a smooth nonvanishing function f.

Introducing a new variable u by

$$\phi=\exp\left(\frac{1}{2}u+\sum_{j=1}^{N} i\arg(z-p_j)\right), \quad z=x_1+ix_2\in\mathbb{C}=\mathbb{R}^2, \tag{1.17}$$

where we allow the overlapping of zeros, p_j's, we can deduce from (1.16) and (1.17) that

$$e^{\eta}\overline{B}=\frac{1}{2q}\left(\Delta u-4\pi\sum_{j=1}^{N}\delta_{p_j}\right). \tag{1.18}$$

From (1.8) and (1.18) we obtain

$$\Delta u=-\frac{2q^4}{\kappa^2}e^{\eta}(e^u-\varepsilon^2)\left(8\pi Ge^{2u}-(16\pi G\varepsilon^2+2)e^u+8\pi G\frac{\kappa^2}{q^2}\left(C+\frac{q^2\varepsilon^4}{\kappa^2}\right)\right)+4\pi\sum_{j=1}^{N}\delta_{p_j}. \tag{1.19}$$

Moreover, it follows from (1.8) and (1.16) that

$$\begin{aligned}\gamma^{jk}(\overline{D}_j\phi)^*(\overline{D}_k\phi)&=\frac{i}{2}e^{-\eta}\varepsilon^{jk}\partial_j(\phi^*\overline{D}_k\phi-\phi(\overline{D}_k\phi)^*)+q|\phi|^2\overline{B}\\&=q|\phi|^2\overline{B}-\tfrac{1}{2}e^{-\eta}\Delta|\phi|^2=2V+q\varepsilon^2\overline{B}-4\pi G\kappa^2(A_0^2+C)^2\\&\quad+8\pi G\kappa^2C(A_0^2+C)-\tfrac{1}{2}e^{-\eta}\Delta|\phi|^2.\end{aligned}$$

Then we obtain from (1.9) that

$$R_{\gamma}=16\pi G(q\varepsilon^2\overline{B}+8\pi G\kappa^2C(A_0^2+C))-8\pi Ge^{-\eta}\Delta|\phi|^2.$$

Since $\Delta\eta=R_{\gamma}e^{\eta}$, we obtain from (1.7) and (1.8) that

$$\Delta(\eta+8\pi G e^u)=16\pi G e^{\eta}\left[-8\pi G\frac{q^4\varepsilon^2}{\kappa^2}e^{3u}+\left(24\pi G\frac{q^4\varepsilon^4}{\kappa^2}+\frac{2q^4\varepsilon^2}{\kappa^2}+8\pi G q^2 C\right)e^{2u}\right.$$
$$\left.-\left(24\pi G\frac{q^4\varepsilon^6}{\kappa^2}+\frac{2q^4\varepsilon^4}{\kappa^2}+24\pi G q^2\varepsilon^2 C\right)e^u+8\pi G\kappa^2\left(\frac{q^2\varepsilon^4}{\kappa^2}+C\right)^2\right]. \tag{1.20}$$

If (η,u) is a solution of the elliptic equations (1.19)–(1.20), then the solution (A,ϕ,ω_j) can be recovered by (1.17), (1.7) and the formula

$$\overline{A}_1=\frac{1}{q}\mathrm{Re}((i\partial_1-\partial_2)\ln\phi),\quad \overline{A}_2=\frac{1}{q}\mathrm{Im}((i\partial_1-\partial_2)\ln\phi),$$

$$\omega_j=-\frac{1}{2\pi}\int_{\mathbb{R}^2}\frac{\varepsilon^{jk}(x_k-y_k)}{|x-y|^2}b(y)e^{\eta}(y)\,dy$$

with b given by (1.10). Therefore, we have shown that the self-dual equations (1.7)–(1.10) can be reduced to the elliptic equations (1.19)–(1.20).

II. EXISTENCE OF NONTOPOLOGICAL SOLUTIONS

In this section, we study the system of equations (1.19)–(1.20) with the nontopological boundary condition, i.e., $C=-q^2\varepsilon^4/\kappa^2$.

Set $a=8\pi G\varepsilon^2$ and $\lambda=2q^4\varepsilon^4/\kappa^2$. Under the scaling $u\mapsto u+\ln\varepsilon^2$, we obtain the following system of equations:

$$\begin{aligned}\Delta(\eta+ae^u)&=-\lambda a e^{\eta+u}(ae^{2u}-2(a+1)e^u+2),\\ \Delta u&=-\lambda e^{\eta+u}(ae^{2u}-(3a+2)e^u+2(a+1))+4\pi\sum_{j=1}^{N}\delta_{p_j}.\end{aligned} \tag{2.1}$$

The system (2.1) is our main equation to study in this section.

Let us introduce some auxiliary functions

$$f(z)=(N+1)\prod_{i=1}^{N}(z-p_i),\quad F(z)=\int_0^z f(\zeta)d\zeta,\quad z=x_1+ix_2,$$

$$h_{\epsilon,\sigma}(z)=\frac{4}{\lambda(2a+1)(1+|\epsilon^{N+1}F(z)+\sigma|^2)^2},$$

$$\rho_{\epsilon,\sigma}(z)=\epsilon^{2N+2}|f(z)|^2h_{\epsilon,\sigma}(z),\quad \rho(r)=\frac{4(N+1)^2r^{2N}}{\lambda(2a+1)(1+r^{2N+2})^2},$$

where $\sigma=\sigma_1+i\sigma_2\in\mathbb{C}=\mathbb{R}^2$. Notice that

$$\Delta\ln h_{\epsilon,\sigma}=-2\lambda(2a+1)\rho_{\epsilon,\sigma}.$$

It is easily seen that

$$(v_1,v_2)=\left(\frac{a}{2a+1}\ln h_{\epsilon,\sigma},\frac{a+1}{2a+1}\ln h_{\epsilon,\sigma}\right)$$

is a solution of

$$\Delta v_1 = -2\lambda a \epsilon^{2N+2} |f(z)|^2 e^{v_1+v_2},$$

$$\Delta v_2 = -2\lambda (a+1) \epsilon^{2N+2} |f(z)|^2 e^{v_1+v_2}.$$

The main idea of the proof is that the solution of (2.1) can be considered as a perturbation of

$$\left(\frac{a}{2a+1} \ln h_{\epsilon,\sigma}, \ln|e^{N+1} f(z)|^2 + \frac{a+1}{2a+1} \ln h_{\epsilon,\sigma} \right).$$

Let $\alpha \in (0,1)$ be given. Following Ref. 4, we introduce the Banach spaces X_α and Y_α as

$$X_\alpha = \left\{ u \in L^2_{\mathrm{loc}}(\mathbb{R}^2) \,\middle|\, \int_{\mathbb{R}^2} (1+|x|^{2+\alpha}) |u(x)|^2 \, dx < \infty \right\}$$

equipped with the norm $\|u\|^2_{X_\alpha} = \int_{\mathbb{R}^2} (1+|x|^{2+\alpha}) |u(x)|^2 \, dx$, and

$$Y_\alpha = \left\{ u \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^2) \,\middle|\, \|\Delta u\|^2_{X_\alpha} + \left\| \frac{u(x)}{1+|x|^{1+\alpha/2}} \right\|^2_{L^2(\mathbb{R}^2)} < \infty \right\}$$

equipped with the norm

$$\|u\|^2_{Y_\alpha} = \|\Delta u\|^2_{X_\alpha} + \left\| \frac{u(x)}{1+|x|^{1+\alpha/2}} \right\|_{L^2(\mathbb{R}^2)}.$$

Proposition 2.1 [Chae–Imanuvilov (Ref. 4)]: Let $\alpha \in (0,1)$.

(1) If $v \in Y_\alpha$ *is a harmonic function, then* $v \equiv$ const.
(2) There are constants $C_1 > 0$ *such that for all* $v \in Y_\alpha$

$$|v(x)| \leqslant C_1 \|v\|_{Y_\alpha} (\ln^+|x| + 1), \quad \forall x \in \mathbb{R}^2,$$

where $\ln^+|x| = \max\{\ln|x|, 0\}$.

We recall some results about weighted space $M^2_{s,\delta}$ which is the closure of $C^\infty_0(\mathbb{R}^2)$ with respect to the norm

$$\|\phi\|_{M^2_{s,\delta}} = \sum_{|\alpha| \leqslant s} \|\sigma_*^{(\delta+|\alpha|)} \partial^\alpha_x \phi\|_{L^2},$$

where $\sigma_*(x) = (1+|x|^2)^{1/2}$, s is a non-negative integer, $\delta \in \mathbb{R}$ and $\phi \in C^\infty_0(\mathbb{R}^2)$. It is well known that $M^2_{s,\delta}$ has the following properties.

Lemma 2.1 (McOwen (Refs. 13 and 14)):

(1) $M^2_{s',\delta'} \subset M^2_{s,\delta}$ *if* $s' \geqslant s$ *and* $\delta' \geqslant \delta$. *If* $s' > s$ *and* $\delta' > \delta$, *the inclusion is compact.*
(2) If $-1 < \delta < 0$ *then the Laplacian* Δ, $\Delta: M^2_{2,\delta} \to M^2_{0,\delta+2}$ *is an injection with closed range* $\{f \in M^2_{0,\delta+2} | \int_{\mathbb{R}^2} f = 0\}$, *and* $\|u\|_{M^2_{2,\delta}} \leqslant C \|\Delta u\|_{M^2_{0,\delta+2}}$ *with* C *independent of* u [*Cantor (Ref. 3)*].
(3) For any $\delta, l \in \mathbb{R}$, *the map* $f \mapsto f\sigma_*^l$ *is a continuous map from* $M^2_{2,\delta}$ *into* $M^2_{2,\delta-l}$.
(4) Let $s > 1$ *and* $\delta < 1$. *There is a constant* $C > 0$ *such that* $\|f\sigma_*^\delta\|_{L^\infty} \leqslant C \|f\|_{M^2_{s,0}}$ *for all* $f \in C^\infty_0$. *Therefore, if* $\delta > -1$ *and* $f \in M^2_{2,\delta}$ *then* $\|f\sigma_*^\beta\|_{L^\infty} \leqslant C \|f\|_{M^2_{2,\delta}}$ *for* $\beta < 1 + \delta$.

We note that for $\alpha \in (0,1)$,

$$X_\alpha = M^2_{0,1+(\alpha/2)} \hookrightarrow L^1(\mathbb{R}^2), \quad M^2_{2,-1+(\alpha/2)} \hookrightarrow Y_\alpha.$$

With the help of Lemma 2.1, we can also prove the following lemma (see, e.g., Ref. 14).

Lemma 2.2: Given $v \in Y_\alpha$, *there exists a function* $v_* \in Y_\alpha$ *such that*

$$v(x)=\frac{1}{2\pi}\left(\int_{\mathbb{R}^2}\Delta v(y)\,dy\right)\ln(1+|x|^2)^{1/2}+v_*(x),\quad \forall x\in\mathbb{R}^2$$

with $|v_*(x)|\leqslant C\|v\|_{Y_\alpha}$ *for some constant* C. *Moreover,* $v_*(x)=v_\infty+o(|x|^\gamma)$ *as* $|x|\to\infty$ *for* $-\alpha/2<\gamma<0$ *and some constant* v_∞.

Setting

$$\zeta(z)=\frac{1}{a}\,\eta(z)-\frac{1}{2a+1}\ln h_{\epsilon,\sigma}(z),$$

and

$$v(z)=u(z)-\ln|\epsilon^{N+1}f(z)|^2-\frac{a+1}{2a+1}\ln h_{\epsilon,\sigma}(z),$$

we can rewrite (2.1) as

$$\begin{aligned}&\Delta(\zeta+|\epsilon^{N+1}f(z)|^2h_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^v)\\&\quad=-\lambda\rho_{\epsilon,\sigma}e^{a\zeta+v}[a|\epsilon^{N+1}f(z)|^4h_{\epsilon,\sigma}^{(2a+2)/(2a+1)}e^{2v}-2(a+1)|\epsilon^{N+1}f(z)|^2h_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^v+2]\\&\qquad+2\lambda\rho_{\epsilon,\sigma},\end{aligned}\tag{2.2}$$

$$\begin{aligned}\Delta v=&-\lambda\rho_{\epsilon,\sigma}e^{a\zeta+v}[a|\epsilon^{N+1}f(z)|^4h_{\epsilon,\sigma}^{(2a+2)/(2a+1)}e^{2v}-(3a+2)|\epsilon^{N+1}f(z)|^2h_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^v\\&+2(a+1)]+2\lambda(a+1)\rho_{\epsilon,\sigma}.\end{aligned}\tag{2.3}$$

We denote

$$g_{\epsilon,\sigma}(z)=\epsilon^{-2}\rho_{\epsilon,\sigma}(z/\epsilon).$$

Note that $\lim_{(\epsilon,\sigma)\to 0}g_{\epsilon,\sigma}(z)=\rho(|z|)$.

Making change of variables $z\to z/\epsilon$, and denoting $\tilde{h}_{\epsilon,\sigma}(z)=h_{\epsilon,\sigma}(z/\epsilon)$, $\tilde{\zeta}(z)=\zeta(z/\epsilon)$ and $\tilde{v}(z)=v(z/\epsilon)$, we can rewrite (2.2)–(2.3) as

$$\begin{aligned}&\Delta(\tilde{\zeta}+|\epsilon^Nf(z/\epsilon)|^2\tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^{\tilde{v}})\\&\quad=-\lambda g_{\epsilon,\sigma}e^{a\tilde{\zeta}+\tilde{v}}[a|\epsilon^{N+1}f(z/\epsilon)|^4\tilde{h}_{\epsilon,\sigma}^{(2a+2)/(2a+1)}e^{2\tilde{v}}-2(a+1)\\&\qquad\times|\epsilon^{N+1}f(z/\epsilon)|^2\tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^{\tilde{v}}+2]+2\lambda g_{\epsilon,\sigma},\end{aligned}\tag{2.4}$$

$$\begin{aligned}\Delta\tilde{v}=&-\lambda g_{\epsilon,\sigma}e^{a\tilde{\zeta}+\tilde{v}}[a|\epsilon^{N+1}f(z/\epsilon)|^4\tilde{h}_{\epsilon,\sigma}^{(2a+2)/(2a+1)}e^{2\tilde{v}}-(3a+2)\\&\times|\epsilon^{N+1}f(z/\epsilon)|^2\tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)}e^{\tilde{v}}+2(a+1)]+2\lambda(a+1)g_{\epsilon,\sigma}.\end{aligned}\tag{2.5}$$

To transform (2.4)–(2.5) further we consider the ordinary differential equation

$$L_1w=\frac{\partial^2w}{\partial r^2}+\frac{1}{r}\frac{\partial w}{\partial r}+2\lambda(2a+1)\rho w=f\quad\text{in }\mathbb{R}_+.\tag{2.6}$$

The function $\varphi_0\in Y_\alpha$ defined by $\varphi_0(r)=(1-r^{2N+2})/(1+r^{2N+2})$ belongs to $\ker L_1$.

Lemma 2.3 [Chae–Imanuvilov (Ref. 4)]. Given $\alpha\in(0,1/2)$, $f=f(r)$ *with* $f\in X_\alpha\cap C^1(\mathbb{R}_+)$, *the ordinary differential equation (2.6) has a solution* $w\in Y_\alpha$ *given by the formula*

$$w(r)=\varphi_0(r)\left\{\int_0^r\frac{\phi_f(s)-\phi_f(1)}{(1-s)^2}ds+\frac{\phi_f(1)r}{1-r}\right\}\tag{2.7}$$

with

$$\phi_f(r)=\left(\frac{1+r^{2N+2}}{1-r^{2N+2}}\right)^2\frac{(1-r)^2}{r}\int_0^r\varphi_0(t)tf(t)\mathrm{d}t,$$

where $\phi_f(1)$ *and* $w(1)$ *are defined as limits of* $\phi_f(r)$ *and* $w(r)$ *as* $r\to 1$.

Lemma 2.4: Let

$$\phi_0(r)=\left(\frac{4}{\lambda(2a+1)}\right)^{(a+1)/(2a+1)}\frac{(N+1)^2r^{2N}}{(1+r^{2N+2})^{(2a+2)/(2a+1)}},$$

and w_0 *be a solution of the equation*

$$L_1w_0=-a\Delta\phi_0+\lambda(2a+1)(a+2)\rho\phi_0 \quad in\ \ \mathbb{R}_+,$$

obtained by substituting $f=-a\Delta\phi_0+\lambda(2a+1)(a+2)\rho\phi_0$ *in the solution formula (2.7). Then there holds the pointwise estimate*

$$|w_0(r)|\leqslant C\lambda^{-(a+1)/(2a+1)}\ln(r+1),\quad \forall r>0$$

and the asymptotic formula

$$w_0(r)=-\tilde{C}\lambda^{-(a+1)/(2a+1)}\ln r+w_\infty+o(1)\quad as\ \ r\to\infty,$$

where w_∞, C, $\tilde{C}$ *are the constants independent of* r *and* λ.

Proof: We observe from formula (2.7) that

$$w_0(r)=\varphi_0(r)\int_2^r\left(\frac{1+s^{2N+2}}{1-s^{2N+2}}\right)^2\frac{I(s)}{s}\mathrm{d}s+(\text{bounded function of } r)$$

as $r\to\infty$, where

$$I(s)=\int_0^s\varphi_0(\tau)\tau(-a\Delta\phi_0+\lambda(2a+1)(a+2)\rho\phi_0)(\tau)\mathrm{d}\tau.$$

Since $\Delta\varphi_0=-2\lambda(2a+1)\rho\varphi_0$,

$$-\int_0^\infty a\varphi_0\Delta\phi_0(\tau)\tau\,\mathrm{d}\tau=-\int_0^\infty a\phi_0\Delta\varphi_0(\tau)\tau\,\mathrm{d}\tau=2\lambda a(2a+1)\int_0^\infty\rho\phi_0\varphi_0(\tau)\tau\,\mathrm{d}\tau.$$

Substituting $\tau^2=t$ in the integrand of $I(\infty)$, then

$$\begin{aligned}I(\infty)&=C_0\int_0^\infty\frac{t^{2N}(1-t^{N+1})}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\mathrm{d}t\\&=C_0\int_0^1\frac{t^{2N}(1-t^{N+1})}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\mathrm{d}t+C_0\int_1^\infty\frac{t^{2N}(1-t^{N+1})}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\mathrm{d}t\\&=C_0\int_0^1\frac{t^{2N}(1-t^{N+1})}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\mathrm{d}t+C_0\int_1^0\frac{s^{[2(a+1)(N+1)]/(2a+1)}(1-s^{N+1})}{(1+s^{N+1})^{(8a+5)/(2a+1)}}\\&\quad\mathrm{d}s\ \ (\text{with substitution } s=1/t)\\&=C_0\int_0^1\frac{t^{2N}(1-t^{N+1})(1-t^{[2(-aN+a+1)]/(2a+1)})}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\mathrm{d}t,\end{aligned}$$

where $C_0=2(3a+2)(N+1)^4(4/\lambda(2a+1))^{(a+1)/(2a+1)}$. Then it is easily seen that $I(\infty)$ is positive (*respectively*, negative) if and only if $aN<a+1$ (*respectively*, $aN>a+1$).

In view of Proposition 2.1 and Lemma 2.2, we obtain

$$w_0(x) = -I(\infty)\ln|x| + w_\infty + o(1) \quad \text{as } |x| \to \infty$$

for some constant w_∞. □

Let ϕ_0, w_0 be the functions given in Lemma 2.4. We define ζ_0 and v_0 as

$$\begin{aligned} \zeta_0(r) &= \left(-\frac{a+1}{2a+1}\phi_0 + \frac{1}{2a+1} w_0 + \lambda a \int_0^r \frac{1}{s} \int_0^s \rho\phi_0(t) t \, dt \, ds \right), \\ v_0(r) &= \left(\frac{a(a+1)}{2a+1}\phi_0 + \frac{a+1}{2a+1} w_0 - \lambda a^2 \int_0^r \frac{1}{s} \int_0^s \rho\phi_0(t) t \, dt \, ds \right). \end{aligned} \tag{2.8}$$

Then ζ_0 and v_0 satisfy the asymptotic behaviors

$$\begin{aligned} \zeta_0(r) &= \left(-\frac{1}{2a+1} I(\infty) + \lambda a \int_0^\infty \rho\phi_0(t) t \, dt \right) \ln r + \zeta_\infty + o(1), \\ v_0(r) &= \left(-\frac{a+1}{2a+1} I(\infty) - \lambda a^2 \int_0^\infty \rho\phi_0(t) t \, dt \right) \ln r + v_\infty + o(1) \quad \text{as } r \to \infty, \end{aligned} \tag{2.9}$$

for some constants ζ_∞, v_∞. Here, $I(\infty)$ is given in the proof of Lemma 2.4.

Proposition 2.1 implies that given a and N, we can choose a neighborhood V_α of the origin in $Y_\alpha \times Y_\alpha$ and a constant $\epsilon_1 = \epsilon_1(a,N) > 0$ such that the mappings $P_1, P_2 : V_\alpha \times \mathbb{R}^2 \times (-\epsilon_1, \epsilon_1) \to X_\alpha$ given by

$$\begin{aligned} P_1(\zeta, v, \sigma, \epsilon) &= \Delta(\zeta + \zeta_0 + |\epsilon^N f(z/\epsilon)|^2 \tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)} e^{\epsilon^2(v+v_0)}) \\ &\quad + \lambda \epsilon^{-2} g_{\epsilon,\sigma} e^{\epsilon^2(a\zeta + v + a\zeta_0 + v_0)} [a|\epsilon^{N+1} f(z/\epsilon)|^4 \tilde{h}_{\epsilon,\sigma}^{(2a+2)/(2a+1)} e^{2\epsilon^2(v+v_0)} \\ &\quad - 2(a+1)|\epsilon^{N+1} f(z/\epsilon)|^2 \tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)} e^{\epsilon^2(v+v_0)} + 2] - 2\lambda\epsilon^{-2} g_{\epsilon,\sigma}, \end{aligned}$$

$$\begin{aligned} P_2(\zeta, v, \sigma, \epsilon) &= \Delta(v + v_0) + \lambda \epsilon^{-2} g_{\epsilon,\sigma} e^{\epsilon^2(a\zeta + v + a\zeta_0 + v_0)} [a|\epsilon^{N+1} f(z/\epsilon)|^4 \tilde{h}_{\epsilon,\sigma}^{(2a+2)/(2a+1)} e^{2\epsilon^2(v+v_0)} \\ &\quad - (3a+2)|\epsilon^{N+1} f(z/\epsilon)|^2 \tilde{h}_{\epsilon,\sigma}^{(a+1)/(2a+1)} e^{\epsilon^2(v+v_0)} + 2(a+1)] - 2\lambda(a+1)\epsilon^{-2} g_{\epsilon,\sigma} \end{aligned}$$

are well defined.

Define $P(\zeta, v, \sigma, \epsilon) = (P_1(\zeta, v, \sigma, \epsilon), P_2(\zeta, v, \sigma, \epsilon))$. Then the problem of solving equation (2.4)–(2.5) is reduced to that of finding a mapping $\epsilon \mapsto (\zeta_\epsilon^*, v_\epsilon^*, \sigma_\epsilon^*)$ from $(-\epsilon_1, \epsilon_1)$ into $Y_\alpha \times Y_\alpha \times \mathbb{R}^2$, satisfying the functional equation

$$P(\zeta_\epsilon^*, v_\epsilon^*, \sigma_\epsilon^*, \epsilon) = (0,0). \tag{2.10}$$

We note that once a solution $(\zeta_\epsilon^*, v_\epsilon^*, \sigma_\epsilon^*, \epsilon)$ of (2.10) is found, then our solution pair is recovered by the formula

$$\begin{aligned} \eta(x) &= \frac{a}{2a+1} \ln h_{\epsilon,\sigma_\epsilon^*}(x) + a\epsilon^2 \zeta_0(\epsilon x) + a\epsilon^2 \zeta_\epsilon^*(\epsilon x), \\ u(x) &= \ln|\epsilon^{N+1} f(z)|^2 + \frac{a+1}{2a+1} \ln h_{\epsilon,\sigma_\epsilon^*}(x) + \epsilon^2 v_0(\epsilon x) + \epsilon^2 v_\epsilon^*(\epsilon x). \end{aligned} \tag{2.11}$$

It follows from Lemma 2.4 and (2.8) that ζ_0 and v_0 satisfy

$$\Delta\zeta_0+2\lambda\rho(a\zeta_0+v_0)=-\Delta\phi_0+2\lambda(a+1)\rho\phi_0,$$

$$\Delta v_0+2\lambda(a+1)\rho(a\zeta_0+v_0)=\lambda(3a+2)\rho\phi_0,$$

which imply that $P(0,0,0,0)=(0,0)$.

Let us introduce a linear operator $A: Y_\alpha\times Y_\alpha\times\mathbb{R}^2\to X_\alpha\times X_\alpha$ defined by

$$\begin{aligned}A(\zeta,v,\sigma_1,\sigma_2)=&\left(\Delta\zeta-\frac{4(a+1)}{2a+1}\Delta(\sigma_1\phi_0\varphi_+ +\sigma_2\phi_0\varphi_-)+2\lambda\rho(a\zeta+v)\right.\\&-8\lambda\rho\left(a\zeta_0+v_0-\frac{(a+1)(3a+2)}{2a+1}\phi_0\right)(\sigma_1\varphi_+ +\sigma_2\varphi_-),\\&\Delta v+2\lambda(a+1)\rho(a\zeta+v)-4\lambda\rho\left(2(a+1)(a\zeta_0+v_0)\right.\\&\left.\left.-\frac{(3a+2)^2}{2a+1}\phi_0\right)(\sigma_1\varphi_+ +\sigma_2\varphi_-)\right)\end{aligned}$$

with the functions $\varphi_+(r,\theta)$, $\varphi_-(r,\theta)\in Y_\alpha$ given by

$$\varphi_+(r,\theta)=\frac{r^{N+1}\cos(N+1)\theta}{1+r^{2N+2}},\quad \varphi_-(r,\theta)=\frac{r^{N+1}\sin(N+1)\theta}{1+r^{2N+2}}.$$

We note that $P: V_\alpha\times\mathbb{R}^2\times(-\epsilon_1,\epsilon_1)\to X_\alpha\times X_\alpha$ is C^1 with respect to (ζ,v,σ), and is C^0 with respect to ϵ. A straightforward calculation shows that $P'_{(\zeta,v,\sigma)}(0,0,0,0)=A$.

Lemma 2.5: Let $N>0$. Then

$$\int_{\mathbb{R}^2}\left(\lambda[2(2a+1)(a\zeta_0+v_0)-(a+2)(3a+2)\phi_0]\rho\varphi_\pm^2+\frac{a(a+1)}{2a+1}\phi_0\varphi_\pm\Delta\varphi_\pm\right)dx<0. \tag{2.12}$$

Proof: Note that $L_1(a\zeta_0+v_0)=-a\Delta\phi_0+\lambda(2a+1)(a+2)\rho\phi_0$, and

$$L_1\left(\frac{1}{16(1+r^{2N+2})^2}\right)=\frac{(N+1)^2r^{4N+2}}{(1+r^{2N+2})^4}.$$

Since $\Delta\varphi_\pm=-2\lambda(2a+1)\rho\varphi_\pm$, the left-hand side of (2.12) is computed as

$$\begin{aligned}(\text{lhs})&=\int_{\mathbb{R}^2}(2\lambda(2a+1)(a\zeta_0+v_0)\rho\varphi_\pm^2-\lambda(5a^2+10a+4)\rho\phi_0\varphi_\pm^2)dx\\&=\pi\int_0^\infty\frac{8(N+1)^2r^{4N+2}}{(1+r^{2N+2})^4}(a\zeta_0+v_0)r\,dr-\pi\lambda(5a^2+10a+4)\int_0^\infty\rho\phi_0\frac{r^{2N+2}}{(1+r^{2N+2})^2}r\,dr\\&=I_1+I_2.\end{aligned}$$

Integrating by parts, we obtain

$$\begin{aligned}I_1&=\pi\int_0^\infty\frac{1}{2(1+r^{2N+2})^2}L_1(a\zeta_0+v_0)r\,dr\\&=\pi\int_0^\infty\frac{1}{2(1+r^{2N+2})^2}(-a\Delta\phi_0+\lambda(2a+1)(a+2)\rho\phi_0)r\,dr.\end{aligned}$$

Therefore,

$$
\begin{aligned}
(\text{lhs}) &= \pi \int_0^\infty \left\{ \frac{-a\Delta\phi_0}{2(1+r^{2N+2})^2} + (12a^2+25a+10)\frac{\lambda\rho\phi_0}{2(1+r^{2N+2})^2} \right. \\
&\quad \left. -(5a^2+10a+4)\frac{\lambda\rho\phi_0}{(1+r^{2N+2})} \right\} r\,\mathrm{d}r \\
&= \frac{\pi(N+1)^2}{2}\left(\frac{4}{\lambda(2a+1)}\right)^{(a+1)/(2a+1)} \int_0^\infty \left\{ \frac{-ar^{2N}}{(1+r^{2N+2})^{(2a+2)/(2a+1)}} \Delta\left(\frac{1}{(1+r^{2N+2})^2}\right) \right. \\
&\quad + \frac{4(12a^2+25a+10)}{2a+1}\frac{(N+1)^2 r^{4N}}{(1+r^{2N+2})^{(10a+6)/(2a+1)}} \\
&\quad \left. - \frac{8(5a^2+10a+4)}{2a+1}\frac{(N+1)^2 r^{4N}}{(1+r^{2N+2})^{(8a+5)/(2a+1)}} \right\} r\,\mathrm{d}r.
\end{aligned}
$$

Since

$$
\Delta\left(\frac{1}{(1+r^{2N+2})^2}\right) = -8(N+1)^2\left(\frac{3r^{2N}}{(1+r^{2N+2})^4} - \frac{2r^{2N}}{(1+r^{2N+2})^3}\right),
$$

we have by substituting $r^2=t$

$$
\begin{aligned}
(\text{lhs}) &= C_1(8a+5)\int_0^\infty \frac{t^{2N}}{(1+t^{N+1})^{(10a+6)/(2a+1)}}\,\mathrm{d}t - C_1(6a+4)\int_0^\infty \frac{t^{2N}}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\,\mathrm{d}t \\
&= C_1(2a+1)\frac{N}{N+1}\int_0^\infty \left\{ \frac{t^{N-1}}{(1+t^{N+1})^{(8a+5)/(2a+1)}} - \frac{t^{N-1}}{(1+t^{N+1})^{(6a+4)/(2a+1)}} \right\}\mathrm{d}t \\
&= -C_1(2a+1)\frac{N}{N+1}\int_0^\infty \frac{t^{2N}}{(1+t^{N+1})^{(8a+5)/(2a+1)}}\,\mathrm{d}t < 0,
\end{aligned}
$$

where we set

$$
C_1 = \frac{\pi(N+1)^4(3a+2)}{2a+1}\left(\frac{4}{\lambda(2a+1)}\right)^{(a+1)/(2a+1)}.
$$

□

We define an operator $L: Y_\alpha \to X_\alpha$ by

$$
Lv = \Delta v + 2\lambda(2a+1)\rho v.
$$

Lemma 2.6 [Chae-Imanuvilov (Ref. 4)]: The operator L satisfies

$$
\ker L = \operatorname{span}\{\varphi_0, \varphi_+, \varphi_-\}, \quad \operatorname{Im} L = \left\{ f \in X_\alpha \,\middle|\, \int_{\mathbb{R}^2} f\varphi_\pm\,\mathrm{d}x = 0 \right\}.
$$

Proposition 2.2: Let $\alpha \in (0,1/2)$ *and* $N>0$. *The operator* $A: Y_\alpha \times Y_\alpha \times \mathbb{R}^2 \to X_\alpha \times X_\alpha$ *is onto and* $\ker A$ *is four-dimensional. More precisely, we have*

$$
\ker A = \operatorname{span}\{(\varphi_0,(a+1)\varphi_0),(\varphi_+,(a+1)\varphi_+),(\varphi_-,(a+1)\varphi_-),(1,-a)\}\times\{(0,0)\}. \tag{2.13}
$$

Proof: Given $f_1, f_2 \in X_\alpha$, we show that the following system of equations:

$$\Delta\zeta-\frac{4(a+1)}{2a+1}\Delta(\sigma_1\phi_0\varphi_+ +\sigma_2\phi_0\varphi_-)+2\lambda\rho(a\zeta+v)$$

$$-8\lambda\rho\left(a\zeta_0+v_0-\frac{(a+1)(3a+2)}{2a+1}\phi_0\right)(\sigma_1\varphi_+ +\sigma_2\varphi_-)=f_1, \tag{2.14}$$

$$\Delta v+2\lambda(a+1)\rho(a\zeta+v)-4\lambda\rho\left(2(a+1)(a\zeta_0+v_0)-\frac{(3a+2)^2}{2a+1}\phi_0\right)(\sigma_1\varphi_+ +\sigma_2\varphi_-)=f_2 \tag{2.15}$$

has a solution in $Y_\alpha\times Y_\alpha\times\mathbb{R}^2$.

Define

$$C_0=-4\lambda\int_{\mathbb{R}^2}(2(2a+1)(a\zeta_0+v_0)-(a+2)(3a+2)\phi_0)\rho\varphi_\pm^2\,dx-\frac{4a(a+1)}{2a+1}\int_{\mathbb{R}^2}\phi_0\varphi_\pm\Delta\varphi_\pm\,dx,$$

and let $C_\pm=\int_{\mathbb{R}^2}(af_1+f_2)\varphi_\pm dx$. Lemma 2.5 shows that $C_0\neq 0$. Since $\mathrm{Im}\,L=\{f\in X_\alpha|\int_{\mathbb{R}^2}f\varphi_\pm dx=0\}$, there exists $w_1\in Y_\alpha$ such that

$$Lw_1=af_1+f_2+\frac{4a(a+1)}{2a+1}\Delta\left(\frac{C_+}{C_0}\phi_0\varphi_+ +\frac{C_-}{C_0}\phi_0\varphi_-\right)+4\lambda\rho[2(2a+1)(a\zeta_0+v_0)$$

$$-(a+2)(3a+2)\phi_0]\left(\frac{C_+}{C_0}\varphi_+ +\frac{C_-}{C_0}\varphi_-\right).$$

Let $w_2\in Y_\alpha$ be the Newtonian potential of h, where

$$h=(a+1)f_1-f_2+\frac{4(a+1)^2}{2a+1}\Delta\left(\frac{C_+}{C_0}\phi_0\varphi_+ +\frac{C_-}{C_0}\phi_0\varphi_-\right)$$

$$-4\lambda a(3a+2)\rho\left(\frac{C_+}{C_0}\phi_0\varphi_+ +\frac{C_-}{C_0}\phi_0\varphi_-\right)\in X_\alpha.$$

Then

$$(\zeta,v,\sigma)=\left(\frac{w_1+w_2}{2a+1},\frac{(a+1)w_1-aw_2}{2a+1},\frac{C_+}{C_0},\frac{C_-}{C_0}\right)$$

is a solution of the system (2.14)–(2.15), which implies that $A:Y_\alpha\times Y_\alpha\times\mathbb{R}^2\to X_\alpha\times X_\alpha$ is onto.

On the other hand, suppose that $(\zeta,v,\sigma_1,\sigma_2)\in\ker A$. Since

$$\int_{\mathbb{R}^2}\varphi_\pm(aP'_{1(\zeta,v,\sigma)}(0,0,0,0)+P'_{2(\zeta,v,\sigma)}(0,0,0,0))(\zeta,v,\sigma)dx=0,$$

it follows from Lemma 2.5 and Lemma 2.6 that $\sigma_1=\sigma_2=0$. Then $a\zeta+v\in\ker L$ and $(a+1)\zeta-v=\mathrm{const}$. Lemma 2.6 implies that $\ker A$ is four-dimensional and given by (2.13). □

We are now ready to prove Theorem 1.1.

Proof of Theorem 1.1: Let

$$Y^*=\mathrm{span}\{(\varphi_0,(a+1)\varphi_0),(\varphi_+,(a+1)\varphi_+),(\varphi_-,(a+1)\varphi_-),(1,-a)\}.$$

We decompose $Y_\alpha\times Y_\alpha=Y^*\oplus(Y^*)^\perp$ and set $U_\alpha=(Y^*)^\perp\times\mathbb{R}^2$. Proposition 2.2 shows that $P'_{(\zeta,v,\sigma)}(0,0,0,0):U_\alpha\to X_\alpha\times X_\alpha$ is a bijection for $\alpha\in(0,1/2)$.

Then the implicit function theorem, applied to the functional $P:[(Y^*)^\perp\cap V_\alpha]\times\mathbb{R}^2\times(-\epsilon_1,\epsilon_1)\to X_\alpha\times X_\alpha$, implies that for $\alpha\in(0,1/2)$ there exist a constant $\epsilon_0\in(0,\epsilon_1)$ and a continuous function $\epsilon\mapsto(\zeta_\epsilon^*,v_\epsilon^*,\sigma_\epsilon^*)$ from $(0,\epsilon_0)$ into a neighborhood of 0 in U_α such that

$$P(\zeta_\epsilon^*, v_\epsilon^*, \sigma_\epsilon^*, \epsilon) = (0,0), \quad \text{for all } \epsilon \in (0, \epsilon_0).$$

Let (η, u) be the functions recovered by the formula (2.11). Then $\gamma_{jk} = -e^{\eta}\delta_{jk}$ and

$$\phi(x) = \varepsilon \exp\left(\frac{1}{2} u(x) + \sum_{j=1}^{N} i \arg(z - p_j) \right),$$

$$\overline{A_1} = \frac{1}{q} \mathrm{Re}(2i\partial^* \ln \phi), \quad \overline{A_2} = \frac{1}{q} \mathrm{Im}(2i\partial^* \ln \phi),$$

$$A_0 = -\frac{q}{\kappa} \varepsilon^2 (e^{u(x)} - 1), \quad \omega_j = \varepsilon^{jk} \partial_k \omega,$$

where $\partial^* = (\partial_1 + i\partial_2)/2$ and

$$\omega(x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \ln|x-y| e^{\eta(y)} b(y)\, dy,$$

where $b(x) = -8\pi G (q^2 \varepsilon^4 / \kappa) e^{u(x)} (e^{u(x)} - 2)$, give rise to a smooth solution (g, A, ϕ) of the system (1.7)–(1.10). Indeed, the functions ζ, v defined as

$$\zeta(z) = \frac{1}{a} \eta(z) - \frac{1}{2a+1} \ln h_{\epsilon,\sigma}(z), \quad v(z) = u(z) - \ln|\epsilon^{N+1} f(z)|^2 - \frac{a+1}{2a+1} \ln h_{\epsilon,\sigma}(z)$$

are solutions of (2.2)–(2.3). Elliptic regularity estimates imply that ζ and v are smooth. On the other hand, a straightforward calculation shows that $\overline{A_1}$ and $\overline{A_2}$ are computed as

$$\overline{A_1} = -\frac{1}{2q} \left(\partial_2 v + \frac{a+1}{2a+1} \partial_2 \ln h_{\epsilon,\sigma} \right), \quad \overline{A_2} = \frac{1}{2q} \left(\partial_1 v + \frac{a+1}{2a+1} \partial_1 \ln h_{\epsilon,\sigma} \right)$$

and hence $\overline{A_1}, \overline{A_2}$ are smooth. Following Jaffe–Taubes (Ref. 10, Chap. 3), we deduce from (1.16) that there exists a smooth function $\alpha = \alpha(z, \overline{A})$ such that we have the representation $\phi(z) = (z - z_j)^{n_j} e^{\alpha}$ near each z_j, and thus ϕ is smooth near each z_j. (ϕ is smooth on $\mathbb{R}^2 \setminus \cup_{j=1}^N \{z_j\}$ obviously by the standard elliptic regularity.)

Now we check the asymptotic behavior of the solution (η, u) recovered by the formula (2.11). Let us define a norm $\|\cdot\|_{V_\alpha}$ by $\|(\zeta, v)\|_{V_\alpha} = (\|\zeta\|_{Y_\alpha}^2 + \|v\|_{Y_\alpha}^2)^{1/2}$. Then

$$\begin{aligned} \zeta_\epsilon^*(\epsilon x) &= \frac{1}{2\pi} \left(\int_{\mathbb{R}^2} \Delta \zeta_\epsilon^*(y) dy \right) \ln|x| + O(1) \epsilon^2 \ln \frac{1}{\epsilon}, \\ v_\epsilon^*(\epsilon x) &= \frac{1}{2\pi} \left(\int_{\mathbb{R}^2} \Delta v_\epsilon^*(y) dy \right) \ln|x| + O(1) \epsilon^2 \ln \frac{1}{\epsilon} \quad \text{as } |x| \to \infty, \end{aligned} \tag{2.16}$$

where $O(1)$ is uniformly bounded with respect to $|x|$ as well as ϵ ($\epsilon \leqslant r_0 < 1$). From the continuity of the function $\epsilon \mapsto (\zeta_\epsilon^*, v_\epsilon^*)$ from $(0, \epsilon_0)$ into V_α, we have $\|(\zeta_\epsilon^*, v_\epsilon^*)\|_{V_\alpha} \to 0$ as $\epsilon \to 0$. Thus there exist $\epsilon_2 \in (0, \epsilon_0)$, $\beta_1 = \beta_1(\epsilon)$, and $\beta_2 = \beta_2(\epsilon)$ such that $\beta_i(\epsilon) = O(\epsilon^2)$ $(i = 1,2)$ as $\epsilon \to 0$ and

$$\eta(x) = -\left(\frac{4a(N+1)}{2a+1} + a\beta_1(\epsilon) \right) \ln|x| + O(1) \epsilon^2 \ln \frac{1}{\epsilon},$$

$$u(x) = -\left(\frac{2N+4+4a}{2a+1} + \beta_2 \right) \ln|x| + O(1) \epsilon^2 \ln \frac{1}{\epsilon} \quad \text{as } |x| \to \infty$$

for all $\epsilon \in (0,\epsilon_2)$. Here, $O(1)$ is uniformly bounded with respect to $|x|$ as well as ϵ ($\epsilon \leqslant r_0 < 1$). Indeed, it follows from (2.9) that

$$\beta_1 = \frac{\epsilon^2}{2a+1} I(\infty) - \lambda a \epsilon^2 \int_0^\infty \rho \phi_0(t) t \, dt - \frac{\epsilon^2}{2\pi} \int_{\mathbb{R}^2} \Delta \zeta_\epsilon^*(y) \, dy,$$

$$\beta_2 = \frac{(a+1)\epsilon^2}{2a+1} I(\infty) + \lambda a^2 \epsilon^2 \int_0^\infty \rho \phi_0(t) t \, dt - \frac{\epsilon^2}{2\pi} \int_{\mathbb{R}^2} \Delta v_\epsilon^*(y) \, dy.$$

We notice that

$$\int_{\mathbb{R}^2} |\Delta \zeta_\epsilon^*(y)| + |\Delta v_\epsilon^*(y)| \, dy \leqslant C \| (\zeta_\epsilon^*, v_\epsilon^*) \|_{Y_\alpha} \to 0 \quad \text{as} \quad \epsilon \to 0.$$

Then e^η satisfies (1.13) and

$$|\phi|^2 = e^u = O(|x|^{-(2N+4+4a)/(2a+1) - \beta_2}) \quad \text{as} \quad |x| \to \infty.$$

Recall that

$$|x||\nabla u(x)| \leqslant C \left(\sup_\Omega |u| + \sup_\Omega |x|^2 |\Delta u| \right),$$

where $\Omega = \{ y \in \mathbb{R}^2 \, | \, |x|/2 \leqslant |y| \leqslant |x| \}$ with $|x|$ sufficiently large (see, e.g., Ref. 8). Since (1.16) implies that $\overline{D}_1 \phi = \phi \partial u$ and $\overline{D}_2 \phi = i \phi \partial u$,

$$|\overline{D}_1 \phi|^2 + |\overline{D}_2 \phi|^2 = \tfrac{1}{2} e^u |\nabla u|^2 = O(|x|^{-(2N+4+4a)/(2a+1) - \beta_2}) \quad \text{as} \quad |x| \to \infty.$$

The decay estimate of $\overline{B}$ can be obtained from (1.8).

We now compute the energy E.

$$E = -\frac{1}{16\pi G} \int_{\mathbb{R}^2} R_\gamma \sqrt{\gamma} \, dx = -\frac{\varepsilon^2}{2a} \int_{\mathbb{R}^2} \Delta \eta \, dx.$$

We can rewrite $h_{\epsilon,\sigma_\epsilon^*}$ as

$$h_{\epsilon,\sigma_\epsilon^*}(r,\theta) = \frac{4}{\lambda(2a+1)} \frac{1}{(\epsilon^{2N+2} r^{2N+2} + p(r,\theta))^2},$$

where $p(r,\theta) = \Sigma_{k=0}^{2N+1} q_k(\theta) r^k$. Then

$$\begin{aligned} \int_{|x|=R} \frac{a}{2a+1} \frac{\partial}{\partial \nu} \ln h_{\epsilon,\sigma_\epsilon^*}(z) \, d\sigma &= -\frac{4a(N+1)}{2a+1} \int_0^{2\pi} \frac{\epsilon^{2N+2} R^{2N+2} + R \dfrac{\partial}{\partial r} p(R,\theta)}{\epsilon^{2N+2} R^{2N+2} + p(R,\theta)} \, d\theta \\ &= -\frac{8\pi a(N+1)}{2a+1} + O(R^{-1}), \end{aligned}$$

where $\partial/\partial \nu$ is the outward normal derivative on the circle $\{|x| = R\}$. Also,

$$r\frac{\partial \zeta_0}{\partial r} = -\frac{(a+1)}{2a+1} r\frac{\partial \phi_0}{\partial r} + \frac{1}{2a+1} r\frac{\partial w_0}{\partial r} + \lambda a \int_0^r \rho\phi_0(t) t\, dt$$

$$= o(1) + \frac{1}{2a+1}\varphi_0(r)\int_0^r \varphi_0(t) t f(t) dt + \lambda a \int_0^r \rho\phi_0(t) t\, dt.$$

(with $f = -a\Delta\phi_0 + \lambda(2a+1)(a+2)\phi_0) = o(1) - \frac{1}{2a+1} I(\infty) + \lambda a \int_0^\infty \rho\phi_0(t) t\, dt \quad$ as $\quad r \to \infty,$

where $I(\infty)$ was given in the proof of Lemma 2.4. Finally,

$$\lim_{R\to\infty} \int_{|x|=R} \epsilon \frac{\partial \zeta_\epsilon^*}{\partial r}(\epsilon x) d\sigma = \lim_{R\to\infty} \int_{|x|=\epsilon R} \frac{\partial \zeta_\epsilon^*}{\partial r}(x) d\sigma = \lim_{R\to\infty} \int_{|x|<\epsilon R} \Delta \zeta_\epsilon^*(x) dx = \int_{\mathbb{R}^2} \Delta \zeta_\epsilon^*\, dx,$$

and

$$\left| \int_{\mathbb{R}^2} \Delta \zeta_\epsilon^* dx \right| \le C \| (\zeta_\epsilon^*, v_\epsilon^*) \|_{V_\alpha} = o(1) \quad \text{as } \epsilon \to 0.$$

Therefore we obtain

$$\int_{\mathbb{R}^2} \Delta\eta = \lim_{R\to\infty} \int_{|x|=R} \frac{\partial \eta}{\partial \nu} d\sigma$$

$$= -\frac{8\pi a(N+1)}{2a+1} + 2\pi\epsilon^2 \left(-\frac{a}{2a+1} I(\infty) + \lambda a^2 \int_0^\infty \rho\phi_0(t) t\, dt \right) + a\epsilon^2 \int_{\mathbb{R}^2} \Delta\zeta_\epsilon^*(x) dx$$

$$= -\frac{8\pi a(N+1)}{2a+1} - 2\pi a \beta_1.$$

In view of (2.11), we can prove (1.14).

The proof of Theorem 1.1 is complete. □

III. EXISTENCE AND NONEXISTENCE OF TOPOLOGICAL SOLUTIONS

In this section, we study the system of equations (1.19)–(1.20) with the topological boundary condition, i.e., $C=0$. In this case, we can derive a single elliptic equation contrary to the nontopological case. As in the previous section, we consider the scaling $u \to u + \ln \varepsilon^2$ and let $a = 8\pi G \varepsilon^2$. The equations for the unknown (η, u) are given by

$$\Delta u = \frac{2q^4}{\kappa^2} \varepsilon^4 e^\eta (2e^u(e^u-1) - a(e^u-1)^3) + 4\pi \sum_{j=1}^N \delta_{p_j} \tag{3.1}$$

and

$$\Delta(\eta + a e^u) = \frac{2q^4}{\kappa^2} a\varepsilon^4 e^\eta (2e^u(e^u-1) - a(e^u-1)^3). \tag{3.2}$$

Then the function

$$\eta - a\left(u - e^u - \sum_{j=1}^N \ln|x-p_j|^2 \right)$$

is harmonic, and we assume it to be a constant. Then the metric is given by

$$e^{\eta}=C_0e^{a(u-e^u)}\prod_{j=1}^{N}\frac{1}{|x-p_j|^{2a}}, \tag{3.3}$$

where we assume $C_0\geqslant 1$. The metric (3.3) is everywhere regular, and is geodesically complete if and only if $aN\leqslant 1$.

Define the background functions

$$u_0=\sum_{j=1}^{N}\ln\left(\frac{|x-p_j|^2}{1+|x-p_j|^2}\right),\quad w_0=\sum_{j=1}^{N}\ln(1+|x-p_j|^2).$$

Let $u=u_0+v$. Then the system (3.1)–(3.3) reduces to the single nonlinear elliptic equation

$$\Delta v=\lambda e^{av-aw_0-ae^{u_0+v}}(2e^{u_0+v}(e^{u_0+v}-1)-a(e^{u_0+v}-1)^3)+g, \tag{3.4}$$

where $\lambda=(2q^4/\kappa^2)\,C_0\varepsilon^4$ and

$$g=\Delta w_0=\sum_{j=1}^{N}\frac{4}{(1+|x-p_j|^2)^2}.$$

Equation (3.4) is our main equation to study in this section. Proof of Theorem 1.2, case 1 consists of Lemma 3.7-Lemma 3.9 below. We first construct a subsolution of the equation (3.4). Define $B_r(x)=\{y\in\mathbb{R}^2||x-y|<r\}$. For $p_1,\ldots,p_N\in\mathbb{R}^2$, choose $\alpha>0$ so that $B_\alpha(p_i)\cap B_\alpha(p_j)=\varnothing$ if $i\neq j$, and fix a constant β so that $\beta>(N+1/4)\alpha^4\exp(1/\alpha^2)$.

For each $j=1,\ldots,N$, define

$$w_j(x)=\begin{cases}-\beta\exp\left(\dfrac{1}{|x-p_j|^2-\alpha^2}\right) & \text{if } |x-p_j|<\alpha,\\ 0 \quad \text{if } |x-p_j|\geqslant\alpha,\end{cases}$$

and define $w=w_1+\cdots+w_N\in C_0^\infty$.

Lemma 3.7: There exist constants λ_0, $a_0>0$ such that if $\lambda\geqslant\lambda_0$, $a\leqslant a_0$ and $\lambda a\leqslant 1$, then w is a subsolution of (3.4).

Proof: We may assume that $a\leqslant 1/N$. If $|x|$ is sufficiently large, then $2e^{u_0}(e^{u_0}-1)-(1/N)\times(e^{u_0}-1)^3<0$ and hence

$$\begin{aligned}&|x|^4e^{-aw_0-ae^{u_0}}(2e^{u_0}(e^{u_0}-1)-a(e^{u_0}-1)^3)\\ &\quad\leqslant|x|^4e^{-(1/N)(1+w_0)}\left(2e^{u_0}(e^{u_0}-1)-\frac{1}{N}(e^{u_0}-1)^3\right)\to-2e^{-1/N}N\leqslant-2/e \quad \text{as} \quad |x|\to\infty.\end{aligned}$$

Since $\lim_{|x|\to\infty}|x|^4\,g(x)=4N$, there exist two constants $R>\alpha+\sup_{1\leqslant i\leqslant N}|p_i|$ and $\lambda_1>0$ depending only on N such that if $|x|\geqslant R$ and $\lambda\geqslant\lambda_1$,

$$\Delta w>\lambda e^{aw-aw_0-ae^{u_0+w}}(2e^{u_0+w}(e^{u_0+w}-1)-a(e^{u_0+w}-1)^3)+g. \tag{3.5}$$

Since $\Delta w(p_j)=4\beta(1/\alpha^4)\exp(-1/\alpha^2)>4N+1$,

$$\Delta w>g+1 \quad \text{in} \quad \cup_{j=1}^{N}B_{r_0}(p_j)$$

for some constant $r_0>0$. Therefore if $\lambda a\leqslant 1$

$$\Delta w\geqslant\lambda e^{aw-aw_0-ae^{u_0+w}}(2e^{u_0+w}(e^{u_0+w}-1)-a(e^{u_0+w}-1)^3)+g \tag{3.6}$$

in $\cup_{j=1}^{N}B_{r_0}(p_j)$.

Define two constants m_1, m_2 by

$$m_1 = \inf\{e^{u_0(x)+w(x)} | x \in B_R(0) \setminus \cup_{j=1}^N B_{r_0}(p_j)\},$$

$$m_2 = \sup\{e^{u_0(x)+w(x)} | x \in B_R(0) \setminus \cup_{j=1}^N B_{r_0}(p_j)\}.$$

There exist constants $a_0, C_0 > 0$ such that if $a \leqslant a_0$,

$$2m_i(m_i-1) - a(m_i-1)^3 \leqslant -C_0 < 0 \quad (i=1,2).$$

Then if $a \leqslant a_0$,

$$2e^{u_0+w}(e^{u_0+w}-1) - a(e^{u_0+w}-1)^3 \leqslant -C_0$$

in $B_R(0) \setminus \cup_{j=1}^N B_{r_0}(p_j)$.

Let $M_0 = \inf\{w(x) - w_0(x) - e^{u_0(x)+w(x)} | x \in B_R(0) \setminus \cup_{j=1}^N B_{r_0}(p_j)\}$. Then there exists a constant $\lambda_0 \geqslant \lambda_1$ such that if $\lambda \geqslant \lambda_0$,

$$-\lambda\, C_0 e^{a_1 M_0} + \|g\|_\infty < -\|\Delta w\|_\infty .$$

Therefore if $\lambda \geqslant \lambda_0$ and $a \leqslant a_0$, then

$$\begin{aligned} &\lambda e^{aw - aw_0 - ae^{u_0+w}}(2e^{u_0+w}(e^{u_0+w}-1) - a(e^{u_0+w}-1)^3) \\ &\quad \leqslant -\lambda C_0 e^{a(w-w_0-e^{u_0+w})} \leqslant -\lambda C_0 e^{a_0 M_0} < \Delta w - g \end{aligned} \tag{3.7}$$

in $B_R(0) \setminus \cup_{j=1}^N B_{r_0}(p_j)$.

It follows from (3.5)–(3.7) that if $\lambda \geqslant \lambda_0$, $a \leqslant a_0$ and $\lambda a \leqslant 1$, then w is a subsolution of the equation (3.4). □

Hereafter we will assume that $\lambda \geqslant \lambda_0$, $a \leqslant a_0$ and $\lambda a \leqslant 1$. Consider the maximal solution v_A of

$$\Delta v = 2\lambda e^{av - aw_0 - ae^{u_0+v}}(e^{u_0+v}-1) + g.$$

Since v_A satisfies $0 < v_A < -u_0$ (Ref. 21), we can use v_A as a supersolution of (3.4).

Define

$$F(x,y) = \lambda e^{ay - aw_0(x) - ae^{u_0(x)+y}}(2e^{u_0(x)+y}(e^{u_0(x)+y}-1) - a(e^{u_0(x)+y}-1)^3),$$

and

$$K = 1 + \sup_{y \leqslant v_A(x)} \left| \frac{\partial F}{\partial y} \right| .$$

We apply the following iterative scheme:

$$(\Delta - K)v_{n+1} = F(x, v_n) - Kv_n + g, \tag{3.8}$$

$$v_{n+1}(x) \to 0 \quad \text{as } |x| \to \infty, \quad n = 0,1,\ldots, \tag{3.9}$$

$$v_0 = v_A .$$

Lemma 3.8: There holds the inequality

$$v_n > v_{n+1} > w \quad in \ \mathbb{R}^2, \quad n = 0,1,2,\ldots .$$

Proof: Since $v_A, g \in L^2(\mathbb{R}^2)$ and $|F(x,v_0)| \leqslant C|u_0+v_A|$, there exists a unique smooth solution $v_1 \in H^2(\mathbb{R}^2)$ of (3.8)–(3.9) with $n=0$. Then

$$(\Delta - K)(v_0 - v_1) < 0 \quad \text{in } \mathbb{R}^2,$$

$$(\Delta - K)(v_1 - w) < (F(x,v_0) - F(x,w)) - K(v_0 - w) = \left(\frac{\partial F}{\partial y}(x,\zeta_0) - K \right)(v_0 - w)$$

$$< 0 \quad (w < \zeta_0 < v_0).$$

Since $\lim_{|x|\to\infty}(v_0 - v_1) = \lim_{|x|\to\infty}(v_1 - w) = 0$, maximum principle implies that $v_0 > v_1 > w$.

Suppose that $v_{n-1} > v_n > w$ for $n \geqslant 1$. Since $|F(x,v_n)| \leqslant C|u_0+v_n| \in L^2(\mathbb{R}^2)$, then there exists a unique smooth solution $v_{n+1} \in H^2(\mathbb{R}^2)$ of (3.8)–(3.9). Then

$$(\Delta - K)(v_n - v_{n+1}) = (F(x,v_{n-1}) - F(x,v_n)) - K(v_{n-1} - v_n) < 0$$

and

$$(\Delta - K)(v_{n+1} - w) < (F(x,v_n) - F(x,w)) - K(v_n - w) < 0$$

by the mean value theorem. Since $\lim_{|x|\to\infty}(v_{n+1} - w) = \lim_{|x|\to\infty}(v_n - v_{n+1}) = 0$, maximum principle implies that $v_n > v_{n+1} > w$. □

By the standard bootstrap argument, we see that $v \equiv \lim_{n\to\infty} v_n$ is a smooth solution of the equation (3.4).

Decay estimates: We investigate the decay estimate of a solution v of the equation (3.4) satisfying $w \leqslant v \leqslant -u_0$. Let $u = u_0 + v$. Then u is a solution of

$$\Delta u = \lambda \prod_{j=1}^{N} \frac{1}{|x-p_j|^{2a}} e^{au - ae^u}(2e^u(e^u-1) - a(e^u-1)^3) \quad \text{in } \mathbb{R}^2 \backslash \{p_1, \ldots, p_N\}.$$

It is easily seen that the metric (3.3) satisfies the decay estimate (1.15).

Lemma 3.9: Suppose that $aN < 1$. Given $\epsilon > 0$, there are positive constants $R(\epsilon)$, $M(\epsilon)$ such that

$$u(x) > -M(\epsilon) e^{-(1-\epsilon)m|x|^{1-aN}}, \quad m = \frac{\sqrt{2\lambda}\, e^{-a/2}}{1-aN} \tag{3.10}$$

for $|x| > R(\epsilon)$.

Proof: Given $\epsilon > 0$, let $w(x) = M e^{-(1-\epsilon)m|x|^{1-aN}}$. Then

$$\Delta w = 2\lambda e^{-a}(1-\epsilon)^2 |x|^{-2aN} \left(1 - \frac{1}{(1-\epsilon)m} |x|^{-1+aN} \right) w, \quad |x| > 0.$$

There exists $R(\epsilon) > 0$ such that

$$\lambda \prod_{j=1}^{N} \frac{1}{|x-p_j|^{2a}} e^{au - ae^u}(2e^u - a(e^u-1)^2)(e^u-1) < 2\lambda e^{-a}(1-\epsilon)^2 |x|^{-2aN} u$$

for $|x| > R(\epsilon)$. Then

$$\Delta(u+w) < 2\lambda e^{-a}(1-\epsilon)^2 |x|^{-2aN}(u+w)$$

for $|x|>R(\epsilon)$. Choose $M(\epsilon)$ sufficiently large so that $(u+w)|_{|x|=R(\epsilon)}>0$. Then maximum principle implies (3.10). □

Let u be the solution of (3.1) and η be given in (3.3). Then $\gamma_{jk}=-e^{\eta}\delta_{jk}$, and

$$\phi(x)=\varepsilon\exp\left(\frac{1}{2}u(x)+\sum_{j=1}^{N} i\arg(z-p_j)\right),$$

$$\overline{A}_1=\frac{1}{q}\mathrm{Re}(2i\partial^*\ln\phi),\quad \overline{A}_2=\frac{1}{q}\mathrm{Im}(2i\partial^*\ln\phi),$$

$$A_0=-\frac{q}{\kappa}\varepsilon^2(e^{u(x)}-1),\quad \omega_j=\varepsilon^{jk}\partial_k\omega,$$

where $\partial^*=(\partial_1+i\partial_2)/2$, and

$$\omega(x)=-\frac{1}{2\pi}\int_{\mathbb{R}^2}\ln|x-y|e^{\eta(y)}b(y)\,dy,$$

where $b(x)=-8\pi G(q^2\varepsilon^4/\kappa)(e^{u(x)}-1)^2$, give rise to a smooth solution (g,A,ϕ) of the system (1.7)–(1.10) as in the preceding section.

From Lemma 3.9 we can show that

$$|\varepsilon^2-|\phi|^2|+|\overline{B}|=O(e^{-(1-\delta)m|x|^{1-8\pi G\varepsilon^2 N}})\quad \text{as}\quad |x|\to\infty \tag{3.11}$$

for each $\delta>0$.

Since (1.16) implies that $\overline{D}_1\phi=\phi\partial u$ and $\overline{D}_2\phi=i\phi\partial u$, and hence $|\overline{D}_1\phi|^2+|\overline{D}_2\phi|^2=\frac{1}{2}e^u|\nabla u|^2$. Recall that

$$|x||\nabla u(x)|\leqslant C_1(\sup_{\Omega}|u|+|x|^2\sup_{\Omega}|\Delta u|),$$

where $\Omega=\{y\in\mathbb{R}^2||x|/2\leqslant|y|\leqslant 3|x|/2\}$ (see, e.g., Ref. 8). Then, $|\overline{D}_j\phi|$ satisfies the decay estimate (3.11).

The energy, as is computed in the previous section, is given by

$$E=-\int_{\mathbb{R}^2}q\varepsilon^2\overline{B}\sqrt{|\gamma|}\,dx=-\frac{\varepsilon^2}{2}\int_{\mathbb{R}^2}\lambda e^{\eta}(2e^u(e^u-1)-a(e^u-1)^3)\,dx=\frac{\varepsilon^2}{2}\int_{\mathbb{R}^2}\Delta w_0\,dx=2\pi\varepsilon^2 N.$$

This completes the proof of Theorem 1.2 in the case 1.

Case 2 of Theorem 1.2: In case that the field configuration is radially symmetric, (3.1) and (3.2) imply that $H\equiv\eta+ae^u-au+2aN\ln|x|$ is harmonic and hence H must be a constant. Therefore, we obtain a single equation

$$\Delta u=\lambda|x|^{-2aN}e^{au-ae^u}(2e^u(e^u-1)-a(e^u-1)^3)+4\pi N\delta_0, \tag{3.12}$$

where λ is a constant. When $u=u(r)$, (3.12) is equivalent to[5]

$$u_{rr}+\frac{1}{r}u_r=\lambda r^{-2aN}e^{au-ae^u}(2e^u(e^u-1)-a(e^u-1)^3),\quad r>0 \tag{3.13}$$

$$\lim_{r\to 0}\frac{u(r)}{\ln r}=2N,\quad \lim_{r\to 0}ru_r(r)=2N.$$

Under the new variables

$$t=\ln r, \quad U(t)=u(e^t),$$

the equation (3.13) becomes

$$\begin{aligned} U''(t)&=\lambda e^{2(1-aN)t}e^{aU(t)-ae^{U(t)}}(2e^{U(t)}(e^{U(t)}-1)-a(e^{U(t)}-1)^3) \\ &=\lambda e^{2(1-aN)t}\frac{\mathrm{d}}{\mathrm{d}U}(e^{aU-ae^U}(e^U-1)^2), \quad -\infty<t<\infty \end{aligned} \tag{3.14}$$

with $\lim_{t\to-\infty} U(t)/t=\lim_{t\to-\infty} U'(t)=2N$.

In case that $aN\geqslant 1$, it can be shown that (3.13) has a solution via shooting method. Let $u=u(r)$ be a solution of (3.13) and $U(t)=u(e^t)$. We multiply both sides of (3.14) by $U'(t)$ and integrate over $(-\infty,s)$. Then we obtain

$$\begin{aligned} (U'(s))^2&=4N^2+2\lambda e^{2(1-aN)s}e^{aU(s)-ae^{U(s)}}(e^{U(s)}-1)^2 \\ &\quad+4\lambda(aN-1)\int_{-\infty}^{s} e^{2(1-aN)t}e^{aU(t)-ae^{U(t)}}(e^{U(t)}-1)^2\,\mathrm{d}t. \end{aligned} \tag{3.15}$$

Then (3.15) implies that $ru_r(r)=U'(t)\geqslant 2N$ for all $r>0$. Then

$$u(r)-u(1)\geqslant\int_1^r\frac{2N}{\tau}\mathrm{d}\tau=2N\ln r.$$

Thus the range of u fills $\mathbb{R}$.

The proof of Theorem 1.2 case 2 is now complete. □

ACKNOWLEDGMENTS

This work was supported by Korea Research Foundation Grant No. KRF-2002-015-CS0003.

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General solutions of Einstein's spherically symmetric gravitational equations with junction conditions

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(Received 8 July 2003; accepted 18 August 2003)

Einstein's spherically symmetric interior gravitational equations are investigated. Following Synge's procedure, the most general solution of the equations is furnished in case T_1^1 and T_4^4 are prescribed. The existence of a total mass function, $M(r,t)$, is rigorously proved. Under suitable restrictions on the total mass function, the Schwarzschild mass $M(r,t)=m$, implicitly defines the boundary of the spherical body as $r=B(t)$. Both Synge's junction conditions as well as the continuity of the second fundamental form are examined and solved in a general manner. The weak energy conditions for an *arbitrary boost* are also considered. The most general solution of the spherically symmetric anisotropic fluid model satisfying both junction conditions is furnished. In the final section, various exotic solutions are explored using the developed scheme including gravitational instantons, interior T-domains, and D-dimensional generalizations. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1621056]

I. INTRODUCTION

As motivation, let us consider various solutions of a toy model of the partial differential equation

$$\frac{\partial^2 W(x,t)}{\partial x^2} - \frac{\partial^2 W(x,t)}{\partial t^2} = T_0 . \tag{1}$$

Here, T_0 is a prescribed constant. (i) A particular solution is provided by $W(x,t)=x-t+(T_0/4)(x^2-t^2)$ which satisfies the initial value problem $W(x,0)=x+T_0x^2/4$ and $[\partial W(x,t)/\partial t]_{|t=0}=-1$. (ii) A class of general solutions of the same equation is given by $W(x,t)=h(x+t)+T_0/4(x^2-t^2)$, where h is of class C^2 but otherwise arbitrary. This class contains infinitely many solutions but excludes infinitely many other solutions including the solution in (i). (iii) The most general solution of this partial differential equation is furnished by $W(x,t)=f(x-t)+g(x+t)+T_0/4(x^2-t^2)$. Here both f and g are of class C^2 and otherwise arbitrary. This class contains *all* possible (smooth) solutions of the equation.

Einstein's gravitational field equations, $G^i_j+8\pi(G/c^2)T^i_j=0$, inside matter are a system of second order, quasilinear, coupled partial differential equations in four space–time variables. It is

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almost impossible to obtain the most general solution for such a system in case the T^i_j's are prescribed. However, if the space–time admits a group of motions or symmetry, then the equations simplify considerably. In fact, in the arena of spherical symmetry, using the curvature coordinates, Synge[1] obtained the most general solutions where T^1_1 and T^4_4 are prescribed (the most logical prescription from a physical perspective). The interior was continuously patched to the exterior Schwarzschild metric across the junction of the spherical material in the local sense. However, the mathematical conditions assuring the existence of a boundary were not derived. Moreover, satisfaction of Synge's own junction conditions, $T^i_j n^j|_{\partial D}$ was not completed.

In Sec. II we write the spherically symmetric interior equations in curvature coordinates. Then, we exhibit the most general solution following Synge's prescriptions.

In Sec. III we prove the mathematical existence of a function, $M(r,t)$. Physically, this is the ''total mass'' of the spherical body with coordinate radius r at coordinate time t. Under some reasonable assumptions, the implicit function theorem[2] guarantees the existence of a solution to $r=B(t)$ for the equation $M(r,t)=m$, the Schwarzschild mass. The curve $r=B(t)$ yields, in a natural way, the desired boundary for the spherical body. It is important to note that this patching is general and is therefore valid for junctions between various interior layers (as in, for example, multilayered stars) as well as interior-vacuum patching.

In Sec. IV we obtain necessary and sufficient conditions for the satisfaction of Synge's junction conditions[1] across the junction. Moreover, we also investigate the Israel–Sen–Lanczos–Darmois (ISLD) junction conditions[3] across the junction and obtain general solutions of the problem.

In Sec. V we examine the weak energy conditions[4] thoroughly for the spherically symmetric scenario. We obtain the general solution of the inequalities in terms of four arbitrary slack functions.

In Sec. VI the class of spherically symmetric $[T^i_j]$ with real eigenvalues is critically studied. As a particular application, the anisotropic fluid model (which contains the perfect fluid as a special case) is explored exhaustively. Theorems are proved on the most general solution of the corresponding field equations with *both* junction conditions of Synge and those of ISLD. Other special examples (black holes, etc.) are also treated.

In the last section, exotic spherically symmetric solutions and their relation to the proposed scheme are explored. Signature changing metrics as well as the Euclidean gravitational instantons[5] are furnished. Next, T-domain[6] equations and general solutions are provided. A special class of T-domain solutions yields the so-called eternal black holes. Another special class of T-domain solutions involve complex eigenvalues of the stress-energy tensor. Such examples were already found in exotic black holes.[7] Finally, we give motivation for, and briefly investigate, spherically symmetric interior equations in arbitrary dimension $D\geqslant 3$. The corresponding general solution is provided.[8]

II. SOLUTION OF THE SPHERICALLY SYMMETRIC FIELD EQUATIONS

We adopt notations and conventions from Synge's book,[1] except that covariant derivatives are denoted by ∇_k. Physical units are chosen so that $c=1$ and $\kappa:=8\pi G$.

Einstein's gravitational equations are furnished by

$$\mathcal{E}_{ij}:=G_{ij}+\kappa T_{ij}=0, \tag{2a}$$

$$\mathcal{T}^i:=\nabla_j T^{ij}=0, \tag{2b}$$

$$\nabla_j \mathcal{E}^{ij}-\kappa \mathcal{T}^i\equiv 0. \tag{2c}$$

It is assumed that the metric functions, $g_{ij}(x)$, are of class C^3 and the functions $T_{ij}(x)$ are of class C^1.

A spherically symmetric metric, in the curvature coordinate chart, and the natural orthonormal tetrad are characterized by

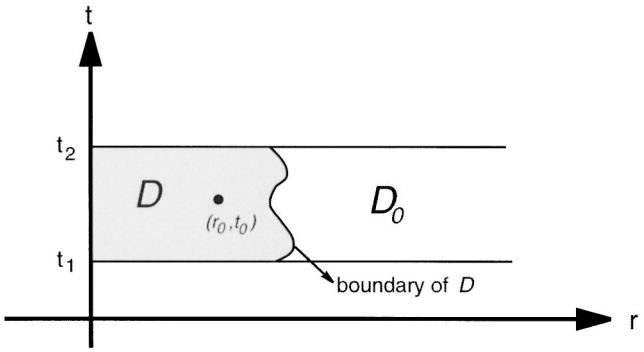

FIG. 1. The considered domain with boundary, ∂D, which separates the interior domain D and the vacuum domain D_0.

$$\begin{gathered} ds^2 = e^{\alpha(r,t)}\,dr^2 + r^2[d\theta^2 + \sin^2\theta\, d\phi^2] - e^{\gamma(r,t)}\,dt^2, \\ e^i_{(1)} = e^{-\alpha(r,t)/2}\delta^i_{(1)}, \quad e^i_{(2)} = r^{-1}\delta^i_{(2)}, \quad e^i_{(3)} = (r\sin\theta)^{-1}\delta^i_{(3)}, \quad e^i_{(4)} = e^{-\gamma(r,t)/2}\delta^i_{(4)}. \end{gathered} \tag{3}$$

Nontrivial equations and identities from (2a)–(3) are provided by

$$\mathcal{E}^1_1 = r^{-2}[1 - e^{-\alpha}(1 + r\gamma_{,1})] + \kappa T^1_1 = 0, \tag{4a}$$

$$\mathcal{E}^2_2 \equiv \mathcal{E}^3_3 = \frac{1}{2}e^{-\alpha}\left[-\gamma_{,11} + \frac{1}{2r}(r\gamma_{,1}+2)(\alpha-\gamma)_{,1}\right] + \frac{1}{2}e^{-\gamma}\left[\alpha_{,44} + \frac{1}{2}\alpha_{,4}(\alpha-\gamma)_{,4}\right] + \kappa T^{\,2}_{\,2} = 0, \tag{4b}$$

$$\mathcal{E}^1_4 = \frac{1}{r}(e^{-\alpha})_{,4} + \kappa T^1_4 = 0, \tag{4c}$$

$$\mathcal{E}^4_4 = \frac{1}{r^2}[1 - (re^{-\alpha})_{,1}] + \kappa T^4_4 = 0, \tag{4d}$$

$$\mathcal{T}_1 = T^1_{1,1} + T^4_{1,4} + \frac{2}{r}\left[1 + \frac{r}{4}\gamma_{,1}\right]T^1_1 + \frac{1}{2}(\alpha+\gamma)_{,4}T^4_1 - \frac{1}{2}\gamma_{,1}T^4_4 - \frac{2}{r}T^2_2 = 0, \tag{4e}$$

$$\mathcal{T}_4 = T^1_{4,1} + T^4_{4,4} + \frac{2}{r}\left[1 + \frac{r}{4}(\alpha+\gamma)_{,1}\right]T^1_4 + \frac{1}{2}\alpha_{,4}(T^4_4 - T^1_1) = 0, \tag{4f}$$

$$\mathcal{E}^1_{1,1} + \mathcal{E}^4_{1,4} + \frac{2}{r}\left[1 + \frac{r}{4}\gamma_{,1}\right]\mathcal{E}^1_1 + \frac{1}{2}(\alpha+\gamma)_{,4}\mathcal{E}^4_1 - \frac{1}{2}\gamma_{,1}\mathcal{E}^4_4 - \frac{2}{r}\mathcal{E}^2_2 - \kappa\mathcal{T}_1 \equiv 0, \tag{4g}$$

$$\mathcal{E}^1_{4,1} + \mathcal{E}^4_{4,4} + \frac{2}{r}\left[1 + \frac{r}{4}(\alpha+\gamma)_{,1}\right]\mathcal{E}^1_4 + \frac{1}{2}\alpha_{,4}(\mathcal{E}^4_4 - \mathcal{E}^1_1) - \kappa\mathcal{T}_4 \equiv 0. \tag{4h}$$

We study and solve these equations in a two-dimensional domain given by

$$D := \{(r,t):\ 0 < r < B(t),\ \ t_1 < t < t_2\}. \tag{5}$$

Note that one may relax the restriction to the domain $r_0 < r < B(t)$ in which case radial integrals in the following should possess the lower limit of r_0. In such a case, an inner boundary will exist at r_0 and the junction conditions discussed later should be applied to the inner boundary as well. The outer boundary curve, $r = B(t)$, will be explicitly determined later (see Fig. 1).

Synge's strategy of solving the field equations is the following:

(i) Prescribe $T_4^4 \equiv T_{(4)}^{(4)}$ from desirable physical properties and solve $\mathcal{E}_4^4 = 0$ to obtain $e^{-\alpha} = g^{11}$.
(ii) Prescribe $T_1^1 \equiv T_{(1)}^{(1)}$ or relate it to T_4^4 by an equation of state and solve $\mathcal{E}_1^1 - \mathcal{E}_4^4 = 0$ to obtain $e^{\gamma} = -g_{44}$.
(iii) Define T_4^1 by the equation $\mathcal{E}_4^1 = 0$.
(iv) Define $T_2^2 \equiv T_{(2)}^{(2)}$ by the conservation equation $\mathcal{T}_1 = 0$.
(v) By the preceding step, the identity (4g) implies that $\mathcal{E}_2^2 = 0$.
(vi) By the identity (4h), the conservation equation $\mathcal{T}_4 = 0$ is satisfied.

At this stage, *all the field equations, conservation laws and identities are satisfied*. One may impose further restrictions to the above scheme. For example, in the case of the perfect fluid, the conservation equation (4e) becomes a differential equation for the pressure (or the energy density, if an equation of state exists), which must be solved. As well, one may require that further equations, such as matter field equations, need to be satisfied.

Regardless of the variants on the above scheme, all solutions must satisfy the following most general solution yielded by

$$e^{-\alpha(r,t)} = 1 - \frac{\kappa}{r}\left[f^2(t) - \int_{0_+}^{r} T_4^4(x,t)\, x^2\, \mathrm{d}x \right], \tag{6a}$$

$$e^{\gamma(r,t)} = e^{-\alpha(r,t)} \left\{ \exp\left[h(t) + \kappa \int_{0_+}^{r} [T_1^1(x,t) - T_4^4(x,t)] e^{\alpha(x,t)} x\, \mathrm{d}x \right] \right\}, \tag{6b}$$

$$T_4^1(r,t) := \frac{1}{r^2}\left[2\, f(t)\dot{f}(t) - \int_{0_+}^{r} T_{4,4}^4 x^2\, \mathrm{d}x \right], \tag{6c}$$

$$T_2^2 \equiv T_3^3 := \frac{r}{2}[T_{1,1}^1 + T_{1,4}^4] + \left[1 + \frac{r}{4}\gamma_{,1} \right] T_1^1 + \frac{r}{4}(\alpha+\gamma)_{,4} T_1^4 - \frac{r}{4}\gamma_{,1} T_4^4, \tag{6d}$$

with $\dot{f}(t) := \mathrm{d}f(t)/\mathrm{d}t$. Here, $f(t)$ and $h(t)$ are *two arbitrary functions of integration* which are of class C^3. Synge[1] set $f^2(t) \equiv 0$ to avoid a singularity at the center. However, this function may be important in certain cases such as the study of wormholes. The function $h(t)$ was absorbed by a transformation of the time coordinate though this is not always possible.[8,9] We retain these functions for generality and to satisfy junction conditions later.

III. CONSERVATION EQUATIONS, THE TOTAL MASS FUNCTION AND THE BOUNDARY

We notice from the equations (4c) and (4d) the existence of two *additional* differential identities:

$$(r^2 G_4^1)_{,1} + (r^2 G_4^4)_{,4} \equiv 0, \tag{7a}$$

$$(\alpha+\gamma)_{,1} G_4^1 + \alpha_{,4}(G_4^4 - G_1^1) \equiv 0. \tag{7b}$$

However, because of $\nabla_k G_4^k \equiv 0$, only one of the above additional identities is independent. Therefore, there must exist additional conservation equations

$$\mathcal{T}_{4a} := (r^2 T_4^1)_{,1} + (r^2 T_4^4)_{,4} = 0, \tag{8a}$$

$$\mathcal{T}_{4b} := (\alpha+\gamma)_{,1} T_4^1 + \alpha_{,4}(T_4^4 - T_1^1) = 0, \tag{8b}$$

$$\mathrm{d}\left[\frac{\kappa}{2} r^2 T_4^1(r,t)\, \mathrm{d}t - \frac{\kappa}{2} r^2 T_4^4(r,t)\, \mathrm{d}r \right] = 0, \tag{8c}$$

$$\mathcal{T}_4 \equiv \frac{1}{r^2}[\mathcal{T}_{4a}+\mathcal{T}_{4b}]. \tag{8d}$$

The first of these equations has a simple physical interpretation. Integrating over a sphere, the equation relates the rate of change of energy in a sphere of radius r to the total energy flux entering or leaving the boundary of the sphere. The equation (8a) in the star-shaped domain D guarantees, by the converse Poincaré lemma[10] the existence of a function $M(r,t)$ of class at least C^2 such that

$$\mathrm{d}M(r,t)=\frac{\kappa r^2}{2}[T_4^1(r,t)\,\mathrm{d}t-T_4^4(r,t)\,\mathrm{d}r], \tag{9a}$$

$$M_{,1}=-\frac{\kappa}{2}r^2T_4^4(r,t), \tag{9b}$$

$$M_{,4}=\frac{\kappa}{2}r^2T_4^1(r,t). \tag{9c}$$

From the equations (4d), (6a), and (6c), we conclude that

$$2M(r,t)=\kappa f^2(t)-\kappa\int_{0_+}^{r}T_4^4(x,t)x^2\,\mathrm{d}x, \tag{10a}$$

$$\lim_{r\to 0^+}M(r,t)=\frac{\kappa}{2}f^2(t), \tag{10b}$$

$$e^{-\alpha(r,t)}=1-\frac{2M(r,t)}{r}, \tag{10c}$$

$$e^{\gamma(r,t)}=\left[1-\frac{2M(r,t)}{r}\right]\exp[h(t)+\chi(r,t)], \tag{10d}$$

$$\chi(r,t):=\kappa\int_0^r\left[\frac{T^1{}_1(x,t)-T_4^4(x,t)}{x-2M(x,t)}\right]x^2\,\mathrm{d}x. \tag{10e}$$

We tacitly assume that $r-2M(r,t)\neq 0$ in D. The physical interpretation of $M(r,t)$ is the "total mass" contained in the spherical volume of "radius" r and at "time" t.

Next we wish to study the level curves of the function $M(r,t)$. For the existence of such curves we state the following version of the implicit function theorem.[2]

Theorem 1: *Let $M(r,t)$ be a function of at least class C^1 in D such that for a point (r_0,t_0) in D, the function $M(r_0,t_0)=c$, a constant. Suppose that $M_{,1|(r_0,t_0)}\neq 0$. Then there exists a function $B(t;c)$ of class at least C^1 in the neighborhood of (r_0,t_0) such that $r=B(t;c)$ is a solution of $M(r,t)=c$ in that neighborhood with $r_0=B(t_0;c)$.*

The boundary curve $r=B(t)$ of the spherical body in the definition (5) is defined by the following:

$$B(t):=\lim_{c\to m_-}B(t;c),$$

$$\partial D:=\{(r,t):r=B(t),\quad t_1<t<t_2\}, \tag{11}$$

(see Fig. 1). Here, $m>0$ physically represents the total Schwarzschild mass of the body. It is assumed that $M>0$, $M_{,1}>0$ or $T_4^4<0$ in D.

It is clear from the implicit definition of the boundary curve, ∂D: $r=B(t)$ that

$$M(B(t),t)\equiv m,$$
$$\dot{B}(t)=-\left[\frac{M_{,4}}{M_{,1}}\right]_{|\partial D}=\left[\frac{T_4^1}{T_4^4}\right]_{|\partial D}. \tag{12}$$

The spherical body collapses in case $M_{,4}(r,t)>0$ and expands in case $M_{,4}(r,t)<0$.

In case the measurable speed of the boundary is less than the speed of light, we must have

$$e^{\alpha-\gamma}_{|\partial D}[\dot{B}(t)]^2<1,$$
$$[e^{-\alpha}(M_{,1})^2-e^{-\gamma}(M_{,4})^2]_{|\partial D}>0,$$
$$\left[\frac{T_4^1}{T_4^4}\right]^2_{|\partial D}<\left[1-\frac{2m}{B(t)}\right]^2\exp[h(t)+\chi(B(t),t)], \tag{13}$$
$$B(t)\neq 2m.$$

The interior domain D, the boundary ∂D, and the exterior (vacuum) domain D_0 are explained in the equations (6a), (6b), and (11) and in Fig. 1. Following Synge, we shall now match continuously the interior metric to the exterior metric (transformable to the Schwarzschild chart). We must use the equations (10d), (10e), and (11) to arrive at

$$g^{11}(r,t)=e^{-\alpha(r,t)}=\begin{cases}1-\dfrac{2M(r,t)}{r} & \text{for } 0<r<B(t),\quad t_1<t<t_2,\\ 1-\dfrac{2m}{B(t)} & \text{for } r=B(t),\quad t_1<t<t_2,\\ 1-\dfrac{2m}{r} & \text{for } B(t)<r<\infty,\quad t_1<t<t_2,\end{cases} \tag{14}$$

$$-g_{44}(r,t)=e^{\gamma(r,t)}=\begin{cases}\left[1-\dfrac{2M(r,t)}{r}\right]\exp[h(t)+\chi(r,t)] & \text{for } 0<r<B(t),\quad t_1<t<t_2,\\ \left[1-\dfrac{2m}{B(t)}\right]\exp[h(t)+\chi(B(t),t)] & \text{for } r=B(t),\quad t_1<t<t_2,\\ \left[1-\dfrac{2m}{r}\right]\exp[h(t)+\chi(B(t),t)] & \text{for } B(t)<r<\infty,\quad t_1<t<t_2.\end{cases} \tag{15}$$

The exterior metric can be easily transformed to the Schwarzschild coordinates. We shall next investigate both Synge's[1] and ISLD's[3] junction conditions.

IV. JUNCTION CONDITIONS

A. Synge's junction condition

Synge's junction conditions read

$$T^i_j n_{i|\partial D}=0,$$
$$n_i n^i=1, \tag{16}$$

with n^i a unit normal at the boundary. In the present case, with the help of (13) we can write for the relevant normal components

$$n_{,1}=\left.\frac{M_{,1}}{\sqrt{e^{-\alpha}M^2_{,1}-e^{-\gamma}M^2_{,4}}}\right|_{\partial D},$$
$$n_{,4}=\left.\frac{M_{,4}}{\sqrt{e^{-\alpha}M^2_{,1}-e^{-\gamma}M^2_{,4}}}\right|_{\partial D}. \tag{17}$$

The equations (16) reduce to

$$[T^1_1 M_{,1}+T^4_1 M_{,4}]_{|\partial D}=0, \tag{18a}$$

$$[T^1_4 M_{,1}+T^4_4 M_{,4}]_{|\partial D}=0. \tag{18b}$$

By the equations (9b) and (9c), the junction condition (18b) is *identically satisfied*. Moreover, the other junction condition (18a) yields

$$\left.\begin{vmatrix} T^1_1 & T^1_4 \\ T^4_1 & T^4_4 \end{vmatrix}\right|_{\partial D}=0$$

or

$$[e^{\gamma-\alpha}T^1_1 M_{,1}-T^1_4 M_{,4}]_{|\partial D}=0. \tag{19}$$

There exist two possible cases here. In case the boundary is static, we must have from (12) and (19),

$$\dot{B}(t)\equiv 0,$$
$$T^1_1 T^4_{4|\partial D}\equiv 0, \tag{20}$$
$$h(t) \quad \text{is an arbitrary function.} \tag{21}$$

This case does *not* imply that the interior metric is necessarily static.

In case the boundary is nonstatic, we obtain from (9b), (9c), (12), and (19),

$$\dot{B}(t)\neq 0,$$
$$T^1_1 T^4_{4|\partial D}<0,$$
$$e^{h(t)}=\left[1-\frac{2m}{B(t)}\right]^{-2}\exp[-\chi(B(t),t)][\dot{B}(t)]^2\left|\frac{T^4_4}{T^1_1}\right|_{|\partial D}>0. \tag{22}$$

Thus, the function $h(t)$, which originated as an arbitrary function of integration, can be utilized to satisfy the junction conditions.

B. Israel–Sen–Lanczos–Darmois junction condition

Next we consider the ISLD junction conditions. Namely, we consider the continuity of the second fundamental form at the junction. For this purpose, the three-dimensional metric for the hypersurface corresponding to $\partial D \times S^2$ is obtained from (15) as

$$d\sigma^2 := ds^2_{|r=B(t)} = B^2(t)[d\theta^2 + \sin^2\theta\, d\phi^2] - \left\{\left[1 - \frac{2m}{B(t)}\right]\exp[h(t) + \chi(B(t),t)] - [\dot{B}(t)]^2\right\} dt^2. \tag{23}$$

The extrinsic curvature components[11] calculated from the interior and exterior metrics are the following:

$$K^{\pm}_{\theta\theta} = \lim_{\delta \to 0_+}\left\{ - \frac{re^{-\alpha}}{\sqrt{e^{-\alpha} - e^{-\gamma}[\dot{B}(t)]^2}}\right\}_{|r=B(t)\pm\delta},$$

$$K^{\pm}_{\phi\phi} = \sin^2\theta\, K^{\pm}_{\theta\theta}, \tag{24}$$

$$2K^{\pm}_{tt} = \lim_{\delta \to 0_+}\left\{ \frac{1}{\sqrt{e^{-\alpha} - e^{-\gamma}[\dot{B}(t)]^2}}[2\ddot{B}(t) + e^{\gamma-\alpha}\gamma_{,1} + \dot{B}(t)(2\alpha - \gamma)_{,4} + [\dot{B}(t)]^2(\alpha - 2\gamma)_{,1} - [\dot{B}(t)]^3 e^{\alpha-\gamma}\alpha_{,4}]\right\}_{|r=B(t)\pm\delta}.$$

It is clear from (14), (15), and (23) that

$$K^{-}_{\theta\theta} - K^{+}_{\theta\theta} \equiv 0, \tag{25}$$

$$K^{-}_{\phi\phi} - K^{+}_{\phi\phi} \equiv 0. \tag{26}$$

To show the continuity of K_{tt} across ∂D, we consider the function

$$2L^{\pm} := \lim_{\delta \to 0_+}\{e^{\gamma-\alpha}\gamma_{,1} + \dot{B}(t)(2\alpha - \gamma)_{,4} + [\dot{B}(t)]^2(\alpha - 2\gamma)_{,1} - [\dot{B}(t)]^3 e^{\alpha-\gamma}\alpha_{,4}\}_{r=B(t)\pm\delta}. \tag{27}$$

The continuity of L across ∂D implies, from (15) and (4a)–(4f) (after a long calculation), the following algebraic equation:

$$0 \equiv 2\kappa^{-1}\left[1 - \frac{2m}{B(t)}\right]e^{h(t)+\chi(B(t),t)}[L^{-} - L^{+}] = U(t)e^{2h(t)} + V(t)e^{h(t)} + W(t). \tag{28}$$

Here,

$$U(t) := B(t)\left[1 - \frac{2m}{B(t)}\right]^2 e^{2\chi(B(t),t)}T^1_{1|r=B(t)},$$

$$V(t) := -B(t)\dot{B}^2(t)\{e^{\chi(B(t),t)}(T^1_1 - T^4_4)\}_{|r=B(t)}, \tag{29}$$

$$W(t) := -B(t)[\dot{B}(t)]^4\left[1-\frac{2m}{B(t)}\right]^{-2} T^4_{4|r=B(t)}.$$

Analyzing the above quadratic (or possibly linear) equation for $e^{h(t)}$, we obtain the following solutions:

$$\text{Case I:}\quad T^1_{1|\partial D}=\dot{B}(t)\,T^4_{4|\partial D}\equiv 0 \quad \text{and} \quad h(t) \quad \text{is arbitrary;} \tag{30a}$$

$$\text{Case II:}\quad e^{h(t)}=[\dot{B}(t)]^2 e^{-\chi(B(t),t)}\left[1-\frac{2m}{B(t)}\right]^{-2} \quad \text{for} \quad \begin{cases} (i)\ \ T^1_{1|\partial D}\equiv 0,\ \ \dot{B}(t)T^4_{4|\partial D}\neq 0, \\ (ii)\ \ (T^1_1-T^4_4)_{\partial D}=0, \\ (iii)\ \ T^1_{1|\partial D}\neq 0,\ \ T^4_{4|\partial D}=0; \end{cases} \tag{30b}$$

$$\text{Case III:}\quad T^1_{1|\partial D}>0, \quad T^4_{4|\partial D}<0, \quad \dot{B}(t)\neq 0,$$

$$\text{and}\quad e^{h(t)}=-[\dot{B}(t)]^2 e^{-\chi(B(t),t)}\left[1-\frac{2m}{B(t)}\right]^{-2}\left|\frac{T^4_4}{T^1_1}\right|_{|\partial D}. \tag{30c}$$

It is clear that Synge's conditions (21) and (22) satisfy the ISLD conditions (30a) and (30c). Case II represents a possible mathematical extension of the ISLD junction conditions to a nontimelike boundary.

V. WEAK ENERGY CONDITIONS

Next the weak energy conditions in spherical symmetry are studied. We consider an observer with an *arbitrary boost* which, to our knowledge, has not been calculated before.

In terms of the orthonormal components (denoted by indices in parentheses), the weak energy conditions[4] can be stated as

$$T_{(a)(b)}u^{(a)}u^{(b)}\geqslant 0 \tag{31}$$

for every timelike vector $u^{(a)}$ satisfying

$$[u^{(1)}]^2+[u^{(2)}]^2+[u^{(3)}]^2-[u^{(4)}]^2=-1, \tag{32}$$

with $u^{(4)}>0$ as dictated by reasonable physics.

The general solution of the above nonlinear algebraic equation (32) is given by

$$u^{(1)}=\sinh\beta\cos\theta,\ \ u^{(2)}=\sinh\beta\sin\theta\cos\phi,\ \ u^{(3)}=\sinh\beta\sin\theta\sin\phi,\ \ u^{(4)}=\cosh\beta,$$

$$\beta\in\mathbb{R},\quad \theta\in(0,\pi),\quad \phi\in(-\pi,\pi). \tag{33}$$

For spherical symmetry, choosing the orthonormal basis of (3), the inequality (31) together with equations (33) yield

$$[T_{(1)(1)}-T_{(2)(2)}]x^2y^2+T_{(2)(2)}x^2+2T_{(1)(4)}xy+T_{(4)(4)}\geqslant 0, \tag{34}$$

$$x:=\tanh\beta,\quad y:=\cos\theta.$$

Analyzing the inequality (34) for all $(x,y)\in[-1,1]\times[-1,1]$, we conclude, after much calculation, that either

$$\text{(i)}\quad T_{(1)(1)}\equiv T_{(2)(2)},\quad T_{(1)(4)}\equiv 0,\quad T_{(4)(4)}\geqslant 0,\quad T_{(4)(4)}+T_{(1)(1)}\geqslant 0, \tag{35a}$$

or else

$$\text{(ii)} \quad T_{(1)(1)} > T_{(2)(2)}, \quad (T_{(1)(4)})^2 \leqslant T_{(4)(4)}[T_{(1)(1)} - T_{(2)(2)}],$$

$$(T_{(1)(4)})^2 \leqslant [T_{(1)(1)} - T_{(2)(2)}][T_{(4)(4)} + T_{(2)(2)}]. \tag{35b}$$

We can solve the inequalities (35a) and (35b) by utilizing slack functions

$$T^4_4 = T^{(4)}_{(4)} = -E^2(r,t), \tag{36a}$$

$$T^2_2 = T^{(2)}_{(2)} = P^2(r,t) - [E(r,t)\sin Q(r,t)]^2, \tag{36b}$$

$$T^1_1 = T^{(1)}_{(1)} = P^2(r,t) - [E(r,t)\sin Q(r,t)]^2 + H^2(r,t), \tag{36c}$$

$$e^{(\alpha-\gamma)/2} T^1_4 = T_{(1)(4)} = -H(r,t)E(r,t)\cos Q(r,t). \tag{36d}$$

Here, the slack functions $E(r,t)$, $P(r,t)$, $Q(r,t)$, $H(r,t)$ are of class C^1 but otherwise arbitrary.

VI. REAL EIGENVALUES OF $[T^i_j]$ AND ANISOTROPIC FLUID MODELS

First, we analyze and solve the problem of a spherically symmetric T^i_j possessing real eigenvalues. Recall that the eigenvalue problem for T^i_j is given by

$$T^i_j E^j_{(a)} = \lambda_{(a)} E^i_{(a)} \quad . \tag{37}$$

In the spherically symmetric case, $T^1_2 = T^1_3 = T^2_4 = T^3_4 \equiv 0$, $T^2_2 \equiv T^3_3$. Therefore, the eigenvalues of T^i_j are given by

$$\begin{aligned} \lambda_{(2)} &\equiv \lambda_{(3)} = T^2_2, \\ 2\lambda_{(1)} &= T^1_1 + T^4_4 + \sqrt{\Delta}, \\ 2\lambda_{(4)} &= T^1_1 + T^4_4 - \sqrt{\Delta}, \\ \Delta &:= (T^1_1 - T^4_4)^2 - e^{\alpha-\gamma}(T^1_4)^2. \end{aligned} \tag{38}$$

It is clear that $\Delta < 0$ will imply complex eigenvalues. We restrict ourselves in this section to the case where the stress-energy tensor possesses real eigenvalues ($\Delta \geqslant 0$).

In a static model, $T^1_4 \equiv 0$ and $\Delta \geqslant 0$ is automatically valid. In case of the weak energy conditions in (35a), (35b) and the corresponding solutions in (36a)–(36d),

$$\Delta = P^4 + 2P^2(H^2 + E^2\cos^2 Q) + (H - E^2\cos^2 Q)^2 \geqslant 0, \tag{39}$$

and thus real eigenvalues are guaranteed. (However, $\Delta \geqslant 0$ may *not* imply the weak energy conditions.)

Assuming the existence of real eigenvalues, the corresponding natural orthonormal eigenvectors are furnished by

$$\begin{aligned} &E^i_{(2)} = r^{-1}\delta^i_{(2)}, E^i_{(3)} = (r\sin\theta)^{-1}\delta^i_{(3)}, \quad E^1_{(1)} = \tfrac{1}{2}\nu_{(1)}[T^4_4 - T^1_1 - \sqrt{\Delta}], \\ &E^2_{(1)} = E^3_{(1)} \equiv 0, \quad E^4_{(1)} = -\nu_{(1)}T^4_1, \quad E^1_{(4)} = -\nu_{(4)}T^1_4, \quad E^2_{(4)} = E^3_{(4)} \equiv 0, \\ &E^4_{(4)} = \tfrac{1}{2}\nu_{(4)}(T^1_1 - T^4_4 + \sqrt{\Delta}), \end{aligned} \tag{40}$$

$$[\nu_{(1)}]^2 := \frac{2e^{-\alpha}}{\sqrt{\Delta}[T^1_1 - T^4_4 + \sqrt{\Delta}]},$$

$$[\nu_{(4)}]^2 := \frac{2e^{-\gamma}}{\sqrt{\Delta}[T^1_1 - T^4_4 + \sqrt{\Delta}]}.$$

The decomposition of the spherically symmetric T^{ij} in terms of the real eigenvalues and eigenvectors is accomplished by

$$T^{ij} = [\lambda_{(1)} - \lambda_{(2)}]E^i_{(1)}E^j_{(1)} + \lambda_{(2)}g^{ij} + [\lambda_{(2)} - \lambda_{(4)}]E^i_{(4)}E^j_{(4)}. \tag{41}$$

It is worth noting that the above algebraic structure of the stress-energy tensor is common to *many* different physical arenas. For example, the anisotropic fluid is specified by

$$p_\parallel := \lambda_{(1)}, \quad p_\perp := \lambda_{(2)} \equiv \lambda_{(3)} = T^2_2, \quad \mu := -\lambda_{(4)},$$

$$u^i := E^i_{(4)}, \quad s^i := E^i_{(1)},$$

$$T^{ij} = (\mu + p_\perp)u^i u^j + p_\perp g^{ij} + (p_\parallel - p_\perp)s^i s^j. \tag{42}$$

The physical quantities are the energy density (μ) the radial pressure ($p_\parallel$) and the angular or transverse pressures ($p_\perp$). Anisotropic fluid models have received much attention mainly in the arenas of stellar structure theory, black holes, and cosmology.[12–14] Note that the nomenclature ''anisotropic fluid'' is misleading. The stress-energy tensor in (42) actually represents a fluid which is *not necessarily* isotropic.

In case $\lambda_{(1)} \equiv \lambda_{(2)} \equiv \lambda_{(3)}$ (or $p_\parallel = p_\perp =: p$), the equation (42) yields the well-known perfect fluid stress-energy tensor,

$$T^{ij} = (\mu + p)u^i u^j + pg^{ij}. \tag{43}$$

This equation implies, by Eqs. (6d) and (38), the *isotropy equation*

$$\sqrt{(T^1_1 - T^4_4)^2 - e^{2\alpha - h - \chi}(T^1_4)^2} = rT^1_{1,1} + \left[1 - \frac{r}{2}\alpha_{,1} + \frac{\kappa r^2}{2}e^{\alpha}(T^1_1 - T^4_4)\right](T^1_1 - T^4_4) - e^{-(h+\chi)/2}[e^{2\alpha - (h+\chi)/2}T^1_4]_{,4}. \tag{44}$$

It is a formidable equation to solve in general (see Ref. 15 for detailed considerations of the static case).

In case the spatial eigenvalues are identically zero, the stress-energy tensor in (42) reduces to that of an incoherent dust.

In case we identify $p = \lambda_{(2)} \equiv \lambda_{(3)}$, $\mu = -\lambda_{(4)}$, $\alpha := \lambda_{(1)} - \lambda_{(2)}$, the stress-energy tensor is

$$T^{ij} = (\mu + p)u^i u^j + pg^{ij} + \alpha s^i s^j. \tag{45}$$

The above T^{ij} is due to a perfect fluid plus a tachyonic (spacelike) dust. Such a stress-energy tensor has been considered in a cosmological model[13] where the dust contributes to the dark matter or dark energy component of the universe.

Now we are in a position to state and prove the main theorems of this section involving anisotropic fluids.

Theorem 2: *Let the spherically symmetric interior equations (4a)–(4d) and the conservation equations (4e), (4f) hold in the coordinate convex domain D defined by (5). Moreover, let the*

stress-energy tensor T^i_j be that of an anisotropic fluid given by (42). Also, let the physical conditions $T^4_4 \leqslant 0$ and $T^1_1 - T^4_4 \geqslant 0$ be satisfied in D. Then, the most general solutions of all the equations and inequalities are furnished by the following:

$$0<q_1<1, \quad 0<q_2<1, \tag{46}$$

$$2M(r,t) := \kappa q_1 \left\{ F^2(q_2 t) + \int_{0^+}^{r} E^2(x,q_2 t) x^2 \, dx \right\} > 0,$$

$$e^{-\alpha(r,t)} = 1 - \frac{2M(r,t)}{r},$$

$$e^{\gamma(r,t)} = e^{-\alpha(r,t)} \exp[h(t) + \chi(r,t)],$$

$$\chi(r,t) := \kappa q_1 \int_{0^+} e^{\alpha(x,t)} [E^2(x,q_2 t)\cos^2 Q(x,q_2 t) + P^2(x,q_2 t)] x \, dx,$$

$$\Delta(r,t) = (q_1)^2 [E^2 \cos^2 Q + P^2]^2 - \frac{4}{\kappa^2 r^4} e^{\alpha-\gamma} (M_{,4})^2 \geqslant 0,$$

$$\frac{2}{q_1}\mu(r,t) = (q_1)^{-1}\sqrt{\Delta} + E^2[1+\sin^2 Q] - P^2 \geqslant 0,$$

$$\frac{2}{q_1} p_{\|}(r,t) = (q_1)^{-1}\sqrt{\Delta} - E^2[1+\sin^2 Q] + P^2 \geqslant 0,$$

$$\frac{p_{\perp}(r,t)}{q_1} = \frac{1}{2r}[r^2(P^2 - E^2 \sin^2 Q)]_{,1} + r\left\{ \frac{1}{4}(E^2\cos^2 Q + P^2)\gamma_{,1} - (kq_1)^{-1} e^{-(\alpha+\gamma)/2} [e^{(3\alpha-\gamma)/2} M_{,4}]_{,4} \right\},$$

$$u^1 = -\frac{2\sqrt{2}}{\kappa e^{\gamma/2} r^2 \Delta^{1/4}} \frac{M_{,4}}{\sqrt{q_1(E^2\cos^2 Q + P^2) + \sqrt{\Delta}}}, \quad u^2 = u^3 \equiv 0,$$

$$u^4 = \frac{1}{\sqrt{2} e^{\gamma/2} \Delta^{1/4}} \sqrt{q_1(E^2\cos^2 Q + P^2) + \sqrt{\Delta}} > 0,$$

$$s^1 = \mp \frac{1}{\sqrt{2} e^{\alpha/2} \Delta^{1/4}} \sqrt{q_1(E^2\cos^2 Q + P^2) + \sqrt{\Delta}}, \quad s^2 = s^3 \equiv 0,$$

$$s^4 = \mp \frac{2\sqrt{2} e^{\alpha/2-\gamma} M_{,4}}{\kappa r^2 \Delta^{1/4} \sqrt{q_1(E^2\cos^2 Q + P^2) + \sqrt{\Delta}}}. \tag{47}$$

Here, the functions $F(q_2 t)$, $h(t)$, $E(r,q_2 t)$ (not identically zero) are of at least class C^3 in D. Aside from these restrictions, the functions are arbitrary.

For proof of the above theorem we used the equations (6a)–(6d), (10a)–(10e), (36a)–(36d), (38), (40), (41), and (42). The two parameters in (46) may appear to be superfluous. However, note that in the limit $q_1 \to 0_+$, the solutions in (46) yield the flat space metric. Moreover, for $0<q_1$

<1 and $\lim q_2 \to 0_+$, the metric goes over to a static one. Furthermore, sufficiently small positive values of q_1 and q_2 facilitate satisfaction of the complicated inequalities $1-(2M/r)>0$ and $\Delta>0$.

We consider here a specific example of an exotic black hole. Consider the following:

$$F(q_2 t)\equiv 0, \quad E^2(r,q_2 t) := \frac{j r^{j-3}}{(1-q_2 t)^j}, \quad 3 \leqslant j,$$

$$2M(r,t)=\kappa q_1 \left[\frac{r}{1-q_2 t}\right]^j, \quad r=B(t):=\left(\frac{2m}{\kappa q_1}\right)^{1/j}(1-q_2 t),$$

$$e^{-\alpha(r,t)}=\left[1-\frac{\kappa q_1 r^{j-1}}{(1-q_2 t)^j}\right],$$

$$T_1^1(r,q_2 t) := k^{-2} q_1 E^2(r,q_2 t), \quad \sqrt{3} \leqslant k,$$

$$\chi(r,q_2 t)=-(1+k^{-2})\ln\left[1-\frac{\kappa q_1 r^{j-1}}{(1-q_2 t)^j}\right],$$

$$e^{\gamma(r,t)}=\left[1-\frac{\kappa q_1 r^{j-1}}{(1-q_2 t)^j}\right]^{-1/k^2} e^{h(t)}. \tag{48}$$

The above describes a mathematically rigorous collapse model for an anisotropic fluid black hole.[7]

Now we shall consider the junction conditions for the solutions given in (48). We state and prove the following corollary to the preceding theorem.

Corollary: Let the conditions stated in the previous theorem be valid in D with $E(r,q_2 t) \neq 0$. *Moreover, let both Synge's junction conditions* $T^{ij}M_{,j|\partial D}\equiv 0$ *and the ISLD junctions conditions* $[K_{ij}]_{\partial D}=0$ *hold on* ∂D. *Then, either,*

$$\sin^2 Q(r,q_2 t)\, E^2(r,q_2 t)=P^2(r,q_2 t)+[B(t)-r]^{\nu^2} N(r,q_2 t) \geqslant 0, \quad \nu^2 \in \{1,2\} \cup [3,\infty)$$

and

$$F^2(q_2 t)=(c_0)^2+\int_t^{t_2} d\tau \left\{ \int_{0_+}^{B(t)} x^2 \frac{\partial}{\partial \tau}[E^2(x,q_2 \tau)]\, dx \right\} \geqslant 0, \tag{49a}$$

or else

$$F^2(q_2 t)=f^2(q_2 t)+\int_t^{t_2} d\tau \left\{ \int_{0_+}^{B(t)} x^2 \frac{\partial}{\partial \tau}[E^2(x,q_2 \tau)]\, dx \right\}, \tag{49b}$$

$$E^2(r,q_2 t)=\frac{P^2}{\operatorname{sech}^2[R(r,q_2 t)]+\sin^2 Q} > 0, \quad \dot{f}(q_2 t) \neq 0,$$

and

$$e^{h(t)}=4\left\{\left(1-\frac{2m}{r}\right)^{-2} e^{-\chi(r,t)}\left[\frac{M_{,4}\cosh(R(r,q_2 t))}{\kappa q_1 r^2 E^2(r,q_2 t)}\right]^2\right\}_{|r=B(t)} > 0.$$

Here, $N(r,q_2 t)$, $R(r,q_2 t)$, *and* $f(q_2 t)$ *are functions of at least class* C^3 *in D but otherwise arbitrary.*

Proof: By the equations (36c) and (49a) it follows that

$$(q_1)^{-1}T^1_1=-[B(t)-r]^{\nu^2}N(r,q_2t),\quad T^1_{1|r=B(t)}\equiv 0.$$

Furthermore,

$$\left[\frac{2M_{,4}}{\kappa q_1}\right]_{|r=B(t)}=\frac{\mathrm{d}F^2(q_2t)}{\mathrm{d}t}+\int_{0^+}^{B(t)}x^2\frac{\partial}{\partial t}E^2(x,q_2t)\,\mathrm{d}x\equiv 0.$$

Therefore, by (21) and (30a), both Synge's condition and the ISLD conditions are satisfied.

In the second case, by the equations in (36c) and (49b) it is deduced that

$$\kappa^{-1}T^1_1(r,q_2t)=P^2-E^2(r,q_2t)\sin^2 Q=E^2(r,q_2t)\operatorname{sech}^2[R(r,q_2t)]>0. \tag{50}$$

Moreover, $M_{,4}\neq 0$ and

$$e^{h(t)}=\left(1-\frac{2m}{r}\right)^{-2}e^{-\chi(r,t)}\left[\frac{(T^1_4)^2}{-T^4_4T^1_1}\right]_{|r=B(t)}.$$

Thus, both equations (22) and (30c) are satisfied. ■

We have previously proved[8] that under the two conditions $T^1_4\equiv 0$ and $T^1_{1,4}\equiv 0$, the solutions of the equations (4a)–(4f) can be transformed into a static solution. This is the interior version Birkhoff's theorem. We can investigate directly the static limit of equations (4a)–(4f). Under suitable assumptions, including $[\mathrm{d}M(r)/\mathrm{d}r]>0$, the boundary, ∂D, of the spherical body is given by $r=b$, a positive constant. Now, the general solution will be furnished in the following statement.

Theorem 3: *Let the static version of the spherically symmetric field equations and one conservation law (4a)–(4f) hold in the domain* $D:=\{(r,t):0<r<b,\ t_1<t<t_2\}$. *Moreover, let the stress-energy tensor be given by (42), satisfying* $\mu(r)>0$, $\mu(r)+p_\parallel>0$. *If, in addition, both Synge's and the ISLD junction conditions hold at* $r=b$, *then the general solutions of the static equations are furnished by*

$$0<q_1<1,\quad b>0,\quad c_0\in\mathbb{R},\quad \nu^2\in\{1,2\}\cup[3,\infty),$$

$$2M(r)=\kappa\left[(c_0)^2+\int_0^r x^2\mu(x)\,\mathrm{d}x\right]>0,$$

$$e^{-\alpha(r)}=1-\frac{2M(r)}{r},$$

$$\chi(r):=\kappa\int_{0^+}^r e^{\alpha(x)}[\mu(x)+p_\parallel(x)]x\,\mathrm{d}x,$$

$$e^{\gamma(r)}=e^{\chi(r)-\alpha(r)},$$

$$\Delta(r)=[\mu(r)+p_\parallel(r)]^2>0,$$

$$\mu(r)=q_1E^2(r)>0,\ p_\parallel=q_1[P^2(r)-(\sin^2 Q(r))E^2(r)],$$

$$p_\perp=\frac{1}{2r}\left\{r^2p_{\parallel,1}+\frac{r}{4}p_\parallel\gamma_{,1}\right\},$$

$$u^i=e^{-\gamma(r)/2}\delta^i_{(4)},\quad s^i=\pm e^{\alpha(r)/2}\delta^i_{(1)},$$

$$(\sin^2 Q(r))E^2(r):=P^2(r)+(b-r)^{\nu^2}N(r)>0. \tag{51}$$

Here, $E(r)$, $P(r)$, $Q(r)$, and $N(r)$ are functions of at least class C^3. Moreover, these functions and the parameters c_0 and ν are arbitrary save for the restrictions imposed above. Proof follows from (46) and (49a). Note that to avoid a singularity at $r=0$ (if this is included in the domain), the constant c_0 should be set equal to zero so that $\lim_{r\to 0} M(r)=0$.

An illustrative example will be provided in the following:

$$0<q_1<1, \quad b>0, \; c_0=0,$$

$$E^2(r):=3, \quad 2M(r)=\kappa q_1 r^3,$$

$$3\sin^2 Q(r):=P^2(r)-3\kappa q_1(b-r)\left\{\frac{b+r}{[3\sqrt{1-\kappa q_1 b^2}-\sqrt{1-\kappa q_1 r^2}][\sqrt{1-\kappa q_1 r^2}+\sqrt{1-\kappa q_1 b^2}]}\right\}$$

$$>0,$$

$$e^{\alpha(r)}=1-\kappa q_1 r^2,$$

$$e^{\gamma(r)}=\left[\frac{3\sqrt{1-\kappa q_1 b^2}-\sqrt{1-\kappa q_1 r^2}}{3\sqrt{1-\kappa q_1 b^2}-1}\right]^2,$$

$$\mu(r)=3q_1, \quad p_\parallel \equiv p_\perp =: p(r)=3q_1\left[\frac{\sqrt{1-\kappa q_1 r^2}-\sqrt{1-\kappa q_1 b^2}}{3\sqrt{1-\kappa q_1 b^2}-\sqrt{1-\kappa q_1 r^2}}\right],$$

$$p(b)=0. \tag{52}$$

The above obviously yields the well-known interior Schwarzschild constant density solution.

One final example which illustrates the use of this scheme is that of the inner layers of a static neutron star.[16] In this case, the energy density, $\mu=T_{(4)(4)}=-T_4^4$ is known from the quantum mechanics of degenerate Fermions. As well, there is the ultrarelativistic fluid equation of state, which should be valid in the inner layers of the star. We summarize as follows:

$$\mu(k_F)=\frac{8\pi^2}{h^3}\int_0^{k_F} k^2(k^2+m_n^2)^{1/2}\,\mathrm{d}k.$$

Here h is Planck's constant, k_F is the Fermi momentum and m_n is the neutron mass. Since the extreme relativistic limit is employed, the mass terms may be neglected compared to the Fermi momentum so that a pressure calculation gives

$$p_\parallel \equiv p_\perp = \tfrac{1}{3}\mu. \tag{53}$$

Also, $\mu(r)$ is obtained by utilizing (53) along with the linear combination $G_1^1-G_4^4=\frac{2}{3}\kappa\mu(r)$. Now the isotropy equation (44) of the general solution reads, in terms of $\mu(r)$,

$$\mu(r)_{,r}=-\frac{4}{r^2}\mu(r)\left[1-\frac{2M(r)}{r}\right]^{-1}\left[\frac{\kappa\mu(r)r^3}{6}+M(r)\right]. \tag{54}$$

Noting relation (9b) and assuming a series solution in r we arrive at the following:

$$M(r)=\frac{3}{14}r, \quad \mu(r)=\frac{3}{7\kappa r^2},$$

which, from (6a) and (6b) yields

$$e^{\gamma}=\frac{4}{7}\frac{r}{r_0},\quad e^{\alpha}=\frac{7}{4} \tag{55}$$

with r_0 a constant. The neighborhood about $r=0$ is excised as the singularity at this point is due to the ultrarelativistic approximation. Also, this solution is not valid for outer layers of the star where deviations from the ultrarelativistic case are significant.

VII. EXOTIC SPHERICALLY SYMMETRIC SOLUTIONS

The exact solutions in (10a)–(10e) can be generalized by abandoning the weak energy conditions to express

$$2\kappa^{-1}M(r,t)=f^2(t)-\int_{0^+}^{r}T_4^4(x,t)x^2\,\mathrm{d}x, \tag{56a}$$

$$e^{-\alpha(r,t)}=1-\frac{2M(r,t)}{r}>0, \tag{56b}$$

$$e^{\gamma(r,t)}=\left[1-\frac{2M(r,t)}{r}\right]e^{\chi(r,t)}H(t), \tag{56c}$$

$$\chi(r,t):=\kappa\int_{0^+}^{r}e^{\alpha(x,t)}[T_1^1(x,t)-T_4^4(x,t)]x\,\mathrm{d}x, \tag{56d}$$

$$H(t)\neq 0. \tag{56e}$$

There are many situations when the solutions to these equations may prove to be ''exotic'' in some sense. For example, the equations (56b)–(56e) reveal that the condition signature$[g_{ij}]=+2$ may *not* be preserved everywhere. A simple example may be considered in the exact vacuum metric given by

$$\mathrm{d}s^2=\left(1-\frac{2m}{r}\right)^{-1}\mathrm{d}r^2+r^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2)+\left(1-\frac{2m}{r}\right)t^3\,\mathrm{d}t^2. \tag{57}$$

In case $t<0$, the metric is obviously transformable to the Schwarzschild solution. However, for $t>0$ the line element (57) yields the spherically symmetric vacuum gravitational instanton solution. In (57), $\lim_{t\to 0}g_{44}(r,t)=0$, indicating the existence of a horizon. All the null rays from the Schwarzschild universe suddenly halt on such a horizon. It may be called the *instanton horizon*. Signature changing metrics in general relativity have been studied in Refs. 7 and 17. The most general spherically symmetric instanton solution in curvature coordinates is furnished by the equations (56a)–(56e) with the choice $H(t)=-e^{h(t)}<0$.

Next, consider spherically symmetric T-domain solutions (Ref. 6 and references therein). The metric is locally expressible as

$$\begin{gathered}\mathrm{d}s^2=e^{\lambda(T,R)}\,\mathrm{d}R^2+T^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2)-e^{\nu(T,R)}\,\mathrm{d}T^2,\\ D_T:=\{(T,R):\ T_1<T<T_2,\ R_1<R<R_2\}.\end{gathered} \tag{58}$$

Einstein's field equations $G_j^i+\kappa\Theta_j^i=0$ can be solved with the metric (58). The general solution [''dual'' to the solutions in (6a)–(6d)], is furnished by

$$e^{-\nu(T,R)}=\frac{1}{T}\left[\sigma(R)-\kappa\int_{T_0}^{T}(T')^2\Theta_1^1(T',R)\mathrm{d}T'\right]-1=:\frac{2\Xi(T,R)}{T}-1>0\,, \tag{59a}$$

$$e^{\lambda(T,R)}=\left[\frac{2\Xi(T,R)}{T}-1\right]\exp\left\{\beta(R)+\kappa\int_{T_0}^{T}e^{\nu(T',R)}[\Theta_4^4(T',R)-\Theta_1^1(T',R)]T'\,\mathrm{d}T'\right\}, \quad (59b)$$

$$\Theta_1^4(T,R):=\frac{2}{\kappa T^2}[\Xi(T,R)]_{,1}, \quad (59c)$$

$$\Theta_2^2\equiv\Theta_3^3=\frac{T}{2}[\Theta_{4,4}^4+\Theta_{4,1}^1]+\left[1+\frac{T}{4}\lambda_{,4}\right]\Theta_4^4+\frac{T}{4}(\lambda+\nu)_{,1}\Theta_1^4-\frac{T}{2}\alpha_{,4}\Theta_1^1, \quad (59d)$$

all other Θ_j^i's$\equiv 0$.

Here, the functions $\sigma(R)$ and $\beta(R)$ are of class C^3 but otherwise arbitrary. The "total tension" function, $\Xi(T,R)$ is generated by the tension density since, in the T domain, it is Θ_1^1 which appears in (59a). This class of solutions includes eternal black hole solutions.

Another special case of T-domain solutions occurs whenever the stress-energy tensor matrix $[\Theta_j^i]$ admits complex eigenvalues. The algebraic criterion of such occurrence is provided by the strict inequality

$$\Delta^\sharp:=(\Theta_4^4-\Theta_1^1)^2+4\Theta_4^1\Theta_1^4<0. \quad (60)$$

As an example, the following Θ_j^i has appeared in the late stages of gravitational collapse studies:[7]

$$0<q_1<1,\quad 0<q_2<1,\quad 3\leqslant j,\quad \sqrt{3}\leqslant k,$$

$$\Theta_1^1(T,R)=-\frac{jq_1T^{j-3}}{(1-q_2R)^j}<0,$$

$$\Theta_4^4(T,R)=k^{-2}jq_1\frac{T^{j-3}}{(1-q_2R)^j}>0,$$

$$\Theta_1^4(T,R)=\frac{jq_1q_2T^{j-2}}{(1-q_2R)^j}>0. \quad (61)$$

Finally, we shall consider the spherically symmetric field equations in an arbitrary D-dimensional manifold (with $D\geqslant 3$).[8] There has been much study on the possibility of extra dimensions in light of superstring theories. In the low energy sector, many of these theories reproduce a higher dimensional general relativity in which, above some energy scale, all dimensions may be considered noncompact. These higher dimensional field equations may therefore have relevance in these theories.

The metric in curvature coordinates is provided by

$$\mathrm{d}s^2=e^{\alpha(r,t)}\,\mathrm{d}r^2+r^2\,\mathrm{d}\Omega_{(D-2)}^2-e^{\gamma(r,t)}\,\mathrm{d}t^2\quad , \quad (62)$$

with

$$\mathrm{d}\Omega_{(D-2)}^2=\left[\mathrm{d}\theta_{(0)}^2+\sum_{n=1}^{D-3}\mathrm{d}\theta_{(n)}^2\left(\prod_{m=1}^{n}\sin^2\theta_{(m-1)}\right)\right],$$

$$\tilde{D}:=\{(r,\theta_{(0)},\ldots,\theta_{(D-3)},t)\in\mathbb{R}^D:\quad t_1<t<t_2,\ \ 0<r_1<r<r_2,$$

$$0<\theta_{(0)},\ldots,\theta_{(D-4)}<\pi,\ \ 0\leqslant\theta_{(D-3)}<2\pi\}. \quad (63)$$

The D-dimensional field equations and conservation laws read

$$\mathcal{E}^1_1=\frac{D-2}{2r^2}[(D-3)(1-e^{-\alpha})-re^{-\alpha}\gamma_{,1}]+\kappa T^1_1=0\ , \tag{64a}$$

$$\mathcal{E}^2_2=-\frac{e^{-\gamma}}{4}[\gamma_{,4}\alpha_{,4}-(\alpha_{,4})^2-2\alpha_{,44}]-\frac{e^{-\alpha}}{4}\Bigg[2\gamma_{,11}+(\gamma_{,1})^2+\frac{2(D-3)}{r}(\gamma-\alpha)_{,1}-\gamma_{,1}\alpha_{,1}$$
$$+\frac{2}{r^2}(D-3)(D-4)\Bigg]+\frac{2(D-3)(D-4)}{r^2}+\kappa T^2_2=0, \tag{64b}$$

$$\mathcal{E}^4_1=\frac{D-2}{2r}e^{-\gamma}\alpha_{,4}+\kappa T^4{}_1=0\ ,\quad \mathcal{E}^{\theta_n}_{\theta_n}\equiv\mathcal{E}^2_2, \tag{64c}$$

$$\mathcal{E}^4_4=\frac{D-2}{2r^2}[(D-3)(1-e^{-\alpha})+re^{-\alpha}\alpha_{,1}]+\kappa T^4_4=0\ , \tag{64d}$$

$$\mathcal{T}^1=T^1_{1,1}+T^4_{1,4}+\left[\frac{1}{2}\gamma_{,1}+\frac{D-2}{r}\right]T^1_1+\frac{1}{2}(\gamma+\alpha)_{,4}T^4_1-\left[\frac{1}{2}\gamma_{,1}T^4_4+\frac{D-2}{r}T^2_2\right]=0, \tag{64e}$$

$$\mathcal{T}^4=T^4_{4,4}+T^1_{4,1}+\frac{1}{2}\alpha_{,4}(T^4_4-T^1_1)+\frac{1}{2}T^1_4\left[(\alpha+\gamma)_{,1}+\frac{2(D-2)}{r}\right]=0. \tag{64f}$$

The general solution of the Einstein field equations and conservation equations furnished utilizing the scheme in this paper is

$$e^{-\alpha(r,t)}=1+\frac{2\kappa}{(D-2)r^{D-3}}\int_{r_1}^{r}T^4_4(x,t)x^{D-2}\,dx-\frac{\kappa f^2(t)}{r^{D-3}}=:1-\frac{2M(r,t)}{r^{D-3}}, \tag{65a}$$

$$e^{\gamma(r,t)}=e^{-\alpha(r,t)}\exp\left\{h(t)+\frac{2\kappa}{D-2}\int_{r_1}^{r}\left[\frac{T^1_1(x,t)-T^4_4(x,t)}{x^{D-3}-2M(x,t)}\right]x^{D-2}\,dx\right\}. \tag{65b}$$

Again, the functions $f(t)$ and $h(t)$ are of class C^3 but otherwise arbitrary.

VIII. CONCLUDING REMARKS

In summary, the general solution to the spherically symmetric Einstein field equations was provided in the case when the energy density and parallel pressure are known. Both Synge's junction conditions and the Israel–Sen–Lancsoz–Darmois junction conditions have been studied and solved in general. The junction or boundary is defined by the existence of a total interior mass which has been rigorously proved in Sec. III. The weak energy conditions in spherical symmetry for arbitrary boost were presented and solved utilizing slack function methods. Specific matter models have also been considered including the anisotropic fluid satisfying both junction conditions, which includes the perfect fluid as a special case. Finally, exotic extensions were considered.

ACKNOWLEDGMENT

We would like to thank Tegai Sergei of the Department of Theoretical Physics at Krasnoyarsk State University for bringing to our attention the fact that case II of the ISLD junction conditions corresponds to a nontimelike boundary.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Double structures and double symmetries for the general symplectic gravity models

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(Received 10 July 2003; accepted 3 September 2003)

By using the so-called double-complex function method, a doubleness symmetry for each member of the class of stationary axisymmetric general symplectic gravity models is found and exploited so that some double-complex $(n+1)\times(n+1)$ matrix Ernst-like potential for any non-negative integer n can be constructed and the associated motion equations can be extended into a double-complex matrix Ernst-like form. Then double symmetry symplectic groups $Sp(2(n+1),\mathcal{R}(J))$ of the theories are given and verified that their actions can be realized concisely by double-complex matrix form generalizations of the fractional linear transformation on the Ernst potential. These results demonstrate that the theories under consideration possess more and richer symmetry structures. The special cases $n=0$ and $n=1$ correspond, respectively, to the pure Einstein gravity and the Einstein–Maxwell-dilaton–axion theories. Moreover, as an application, for each $n=0,1,2,\ldots$, an infinite chain of double-solutions of the general symplectic gravity model is obtained, which shows that the double-complex method is more effective. Some of the results in this paper cannot be obtained by the usual (nondouble) scheme. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1624092]

I. INTRODUCTION

The double-complex function method (DCFM),[1] which organically combines the ordinary complex with the so-called hyperbolic complex[2] function theories, has been effectively used to some mathematical physics problems (see, e.g., Refs. 1,3–9). In these studies, the DCFM and its extended version[8,9] have been extensively used to the dimensionally reduced Einstein gravity theories and the self-dual gauge field theories as powerful tools for finding new symmetries and generating new solutions of the associated field equations. These results are important for understanding the related theories.

More recently, on the other hand, much attention had been paid to the study of symmetries for the dimensionally reduced low energy effective (super)string theories (see, e.g., Refs. 10–22). Such theories describe various interacting ''matter'' fields coupled to gravity. The 2-dimensionally reduced Einstein–maxwell-dilaton–axion (EMDA) theory[14,15,19–22] is a typical and important example of these models. In Ref. 23, Kechkin and Yurova developed a series of symplectic gravity models, each of them is a generalization of the EMDA theory so that it describes a coupled system of n Abelian vector fields and the symmetric $n\times n$ matrix extensions of the dilaton and the Kalb–Ramond fields for $n=1,2,\ldots$. We shall call these general symplectic gravity models ''SGM-n'' theories for brevity. Thus the EMDA theory corresponds to the case of SGM-1.

For the EMDA theory and its generalizations, the SGM-n theories, some symmetries and solution generating techniques have been given,[14,15,19–24] moreover, some of their properties similar to the reduced vacuum Einstein theory have been noted.[19–21,23] However, only the ordinary complex functions are used in these schemes. In the present paper, we shall show that, by using the DCFM, a doubleness symmetry of the SGM-n theories can be found and exploited fully, then

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more and richer symmetries and solution generating methods can be obtained, some of these results cannot be obtained by using only the ordinary (nondouble) schemes.

In a previous paper,[25] we have given a double formulation of the 2-dimensionally reduced Einstein-dilaton–axion theory[26,27] and obtained some new results. Now we generalize the study further to the stationary axisymmetric (SAS) SGM-*n* theories. Since the Ernst-like potentials involved here are matrices (rather than scalar functions), the generalization is not trivial.

In the *Preliminaries* below, for use later, some related concepts and notations of the double-complex numbers[1] are briefly recalled. In Sec. II, motion equations of the SAS SGM-*n* theories are extended into a double-complex matrix Ernst-like form. Section III gives double symmetry groups of the SGM-*n* theories, which are double-real $2(n+1)$-dimensional symplectic groups. Then the actions of these symmetry groups are explicitly written as convenient and concise double-complex matrix fractional linear transformation forms. In Sec. IV, the doubleness symmetry property of the SGM-*n* theories is further used and some double dual transformations are introduced. By using these dual transformations together with the double symmetry groups given in Sec. III, for each $n=0,1,2,\ldots$, we obtain an infinite chain of double-solutions of the SGM-*n* theories considered. Finally, Sec. V gives some summary and discussions.

Preliminaries:[1] Let J denote the double-imaginary unit, i.e., $J=i$ ($i^2=-1$), or $J=\varepsilon$ ($\varepsilon^2=+1$, $\varepsilon\neq\pm 1$). If a series $\Sigma_{n=0}^{\infty}|a_n|$, $a_n\in\mathcal{R}$ (real number field), is convergent, then

$$a(J)=\sum_{n=0}^{\infty} a_n J^{2n} \tag{1.1}$$

is called a double-real number, which corresponds to a pair (a_C,a_H) of ordinary real numbers, where $a_C:=a(J=i)$, $a_H:=a(J=\varepsilon)$. All of the double-real number with ordinary addition and multiplication constitute a field, we call it double-real number field and denote it by $\mathcal{R}(J)$. When $a(J)$ and $b(J)$ both are double-real numbers, then

$$c(J)=a(J)+Jb(J) \tag{1.2}$$

is called a double-complex number; it corresponds to a pair (c_C, c_H), where $c_C:=c(J=i)=a_C+ib_C$ is an ordinary complex number, $c_H:=c(J=\varepsilon)=a_H+\varepsilon b_H$ is called a hyperbolic complex number. From the above definitions, we see that the double-imaginary unit J takes the role of an analysis link between c_C and c_H. All double-complex numbers with usual addition and multiplication constitute a commutative ring, which is denoted by $\mathcal{C}(J)$. The double-complex conjugation of a double-complex number $c(J)$ is defined by $\overline{c(J)}:=a(J)-Jb(J)$; this implies that $\overline{J}=-J$.

In this paper, we also use the double-imaginary unit commutation operator "$\circ$," that is defined as

$$\circ: J\to \mathring{J}, \quad \mathring{i}=\epsilon, \quad \mathring{\epsilon}=i. \tag{1.3}$$

Obviously, $\mathring{J}$ is the double-imaginary unit, too.

II. DOUBLE-COMPLEX MATRIX ERNST FORMULATION FOR THE SGM-*n* THEORIES

Following Ref. 23, we consider a class of gravity models with action

$$S=\int\left\{-R+\mathrm{Tr}\left[\frac{1}{2}(\partial p\, p)^2-pFF^T+\frac{1}{3}(pH)^2\right]\right\}\sqrt{-g}d^4x, \tag{2.1}$$

where $g_{\mu\nu}$ is the metric (signature $+---$, $\mu,\nu=0,1,2,3$), $R=R^{\mu\nu}{}_{\mu\nu}$ is the Ricci scalar of $g_{\mu\nu}$, $g=\det(g_{\mu\nu})$, p is a symmetric $n\times n$ matrix with scalar field components (for the EMDA case, $p=e^{-2\phi}$, ϕ is the dilaton field), and

$$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu, \tag{2.2}$$

$$H_{\mu\nu\lambda}=\partial_\mu B_{\nu\lambda}-\tfrac{1}{2}(A_\mu F^T_{\nu\lambda}+F_{\nu\lambda}A^T_\mu)+\text{cyclic},$$

in which $B_{\mu\nu}$ is a symmetric $n\times n$ matrix containing the antisymmetric Kalb–Ramond tensor fields (i.e., $B^T_{\mu\nu}=B_{\mu\nu}$, $B_{\mu\nu}=-B_{\nu\mu}$) and A_μ is a $n\times 1$ column of Abelian vector fields. The SGM-n action (2.1) gives the pure Einstein and the EMDA theories, respectively, when $n=0$ and $n=1$ and provides their generalization for an arbitrary non-negative integer n. These special models arise in the low energy limit of the heterotic string theory after the compactification of extra dimensions on a torus.

Now we consider the 2-dimensional reduction of the above SGM-n theories. For definiteness, we consider the stationary axisymmetric (SAS) case, in which the 4-dimensional space–time line element is chosen as the Lewis–Papapetrou form (the space–time coordinates are explicitly written as $x^0=t$, $x^1=\varphi$, $x^2=\rho$, $x^3=z$):

$$ds^2=f(dt-\omega\,d\varphi)^2-f^{-1}[e^{2\gamma}(dz^2+d\rho^2)+\rho^2\,d\varphi^2], \tag{2.3}$$

where f, ω, and γ are real functions of ρ and z only.

After reduction to the SAS case, in addition to the above metric variables, the set of SGM-n dynamical quantities contains two Lorentzian components A_0, A_1 of the $n\times 1$ column 4-potential A_μ, one nontrivial Lorentzian component B_{01} of the $n\times n$ symmetric matrix Kalb–Ramond field $B_{\mu\nu}$ and the $n\times n$ symmetric matrix p of the Lorentzian scalar fields. Also, all of these fields are dependent only on the coordinates ρ and z. In terms of these, the dynamical motion equations of the SAS SGM-n theory can be divided into two groups. The first group can be written as[23]

$$\nabla(\rho^{-1}P\nabla\Omega P)=0, \tag{2.4a}$$

$$\nabla(\rho\nabla P P^{-1}+\rho^{-1}P\nabla\Omega P\Omega)=0, \tag{2.4b}$$

where the gradient operator $\nabla:=(\partial_\rho,\partial_z)$ and the two $(n+1)\times(n+1)$ symmetric real matrices P and Ω are defined by the so-called original (nondualized) field variables as

$$P=\begin{pmatrix} f-2A_0^T pA_0 & -\sqrt{2}A_0^T p \\ -\sqrt{2}pA_0 & p \end{pmatrix},$$
$$\Omega=\begin{pmatrix} \omega & -\sqrt{2}(A_1+\omega A_0)^T \\ -\sqrt{2}(A_1+\omega A_0) & (A_1+\omega A_0)A_0^T+A_0(A_1+\omega A_0)^T-2B_{01} \end{pmatrix}. \tag{2.5}$$

Thus, if P and Ω are known by solving the motion equations (2.4), we can directly obtain the original fields f, ω, A_0, A_1, B_{01} and p.

The second group of the motion equations, namely the corresponding Einstein equations, can be written as

$$\partial_\rho\gamma=\tfrac{1}{4}\mathrm{Tr}[\rho((J^P_\rho)^2-(J^P_z)^2)+\rho^{-1}((J^\Omega_\rho)^2-(J^\Omega_z)^2)],$$
$$\partial_z\gamma=\tfrac{1}{2}\mathrm{Tr}[\rho J^P_\rho J^P_z-\rho^{-1}J^\Omega_\rho J^\Omega_z], \tag{2.6}$$

where we have introduced two matrix currents:

$$J^P:=P^{-1}\nabla P,\quad J^\Omega:=P^{-1}\nabla\Omega,$$

and the components of these currents are defined as $J^P_\rho:=P^{-1}\partial_\rho P$, $J^P_z:=P^{-1}\partial_z P$, etc. Subsequently, the function γ can be obtained by a simple integration of the equations (2.6) provided that

the solution (P,Ω) of (2.4) is known. The existence of γ is assured by Eqs. (2.4). Since γ is completely determined by P and Ω, we shall focus our attention on Eqs. (2.4) in the following.

To find the double symmetric structures of the SGM-n theories, we note that the equations (2.4) imply that we can introduce the transformations of the matrix functions P,Ω as follows:

$$\begin{aligned} &T\colon P\to T(P)=\rho P^{-1},\\ &V\colon T(P),\ \Omega\to V_{T(P)}(\Omega)=\int \rho^{-1}P\partial_z\Omega\ P\,d\rho-\rho^{-1}P\,\partial_\rho\Omega\ P\,dz\\ &\qquad\qquad=\int \rho(T(P))^{-1}\partial_z\Omega(T(P))^{-1}\,d\rho-\rho(T(P))^{-1}\,\partial_\rho\Omega(T(P))^{-1}\,dz. \end{aligned} \tag{2.7}$$

It can be directly shown that the above transformations T and V both are invertible. In fact, by a suitable choice of the integration constants, we have

$$T^2(P)=P,\qquad V_PV_{T(P)}(\Omega)=-\Omega. \tag{2.8}$$

Now, by the transformation $(P,\Omega)\to(P_H,\Omega_H):=(T(P),\Omega)$, the equations (2.4) are written as

$$\begin{aligned} \nabla^2\Omega_H&=(\nabla P_H)P_H^{-1}(\nabla\Omega_H)+(\nabla\Omega_H)P_H^{-1}(\nabla P_H),\\ \nabla^2P_H&=(\nabla P_H)P_H^{-1}(\nabla P_H)+(\nabla\Omega_H)P_H^{-1}(\nabla\Omega_H), \end{aligned} \tag{2.9a}$$

where the Laplace operator $\nabla^2\equiv\partial_\rho^2+\rho^{-1}\partial_\rho+\partial_z^2$; and by the transformation $(P,\Omega)\to(P_C,\Omega_C):=(P,V_{T(P)}(\Omega))$, the field equations (2.4) can be written as

$$\begin{aligned} \nabla^2\Omega_C&=(\nabla P_C)P_C^{-1}(\nabla\Omega_C)+(\nabla\Omega_C)P_C^{-1}(\nabla P_C),\\ \nabla^2P_C&=(\nabla P_C)P_C^{-1}(\nabla P_C)-(\nabla\Omega_C)P_C^{-1}(\nabla\Omega_C). \end{aligned} \tag{2.9b}$$

Therefore, now we can introduce a double-complex $(n+1)\times(n+1)$ matrix potential,

$$E(J)=P(J)+J\Omega(J), \tag{2.10}$$

and naturally obtain a double-complex SGM-n field equation,

$$\nabla^2E(J)=\nabla E(J)P^{-1}(J)\nabla E(J), \tag{2.11}$$

by combining Eq. (2.9a) with (2.9b), where $P(J)$ and $\Omega(J)$ both are double-real $(n+1)\times(n+1)$ symmetric matrix functions of ρ and z. The equation (2.11) is a matrix-form generalization of the double-complex Ernst equation in SAS vacuum Einstein theory.[1,28] Thus the dynamical motion equations of the SAS SGM-n theories have been written out in a double-complex matrix Ernst-like form. When taking $J=i$, then $E_C=P_C+i\Omega_C$ and Eq. (2.11) gives the equations (2.9b). The ordinary complex matrix potential E_C has been introduced essentially in Ref. 23. On the other hand, when taking $J=\varepsilon$, then $E_H=P_H+\varepsilon\Omega_H$ and Eq. (2.11) gives (2.9a). The fact that the SAS SGM-n field equations can be written into a single double-complex matrix Ernst-like equation reflects that the theories under consideration for any $n\geqslant 0$ possess some so-called doubleness symmetry.

According to the discussions above and noticing that if (P,Ω) is a solution of Eqs. (2.4), so is $(P,-\Omega)$, it can be readily verified that if a double-complex solution $E(J)$ of Eq. (2.11) is known, then we can obtain a pair of real solutions of SAS SGM-n field equations (2.4) as follows:

$$\begin{aligned} (P,\Omega)&=(P_C,V_{P_C}(\Omega_C)),\\ (\hat P,\hat\Omega)&=(T(P_H),\Omega_H), \end{aligned} \tag{2.12}$$

and the existence of $V_{P_C}(\Omega_C)$ is ensured by Eq. (2.11). Noted that the double-imaginary unit J takes a role of an analytical link in the DCFM,[1] we call the two solutions in (2.12) to be dual to each other. Similar to the discussions given in Ref. 1, we see that the double-complex method presented above essentially implies an analytically continuation of the Neugebauer–Kramer-like transformation for the SGM-n theories.[23,29] It is this analytically continuation that make us able to obtain two real solutions of SGM-n theory directly from a double-complex matrix Ernst-like potential $E(J)$. In the following sections, we give some applications of this doubleness method.

III. DOUBLE SYMMETRY GROUPS OF THE SAS SGM-*n* THEORIES

Based on the results in Sec. II, if we introduce the $2(n+1)\times 2(n+1)$ double-real matrix function,

$$M(J)=\begin{pmatrix} \Omega(J)P^{-1}(J)\Omega(J)-J^2P(J) & \Omega(J)P^{-1}(J) \\ P^{-1}(J)\Omega(J) & P^{-1}(J) \end{pmatrix}, \tag{3.1}$$

then the double-complex matrix Ernst-like equation (2.11) can be written as

$$\nabla[\rho M^{-1}(J)\nabla M(J)]=0. \tag{3.2}$$

It is obvious that the double-real matrix function $M(J)$ in (3.1) satisfies the conditions

$$M^T(J)=M(J), \quad M(J)\,\eta M(J)=-J^2\,\eta, \tag{3.3}$$

where

$$\eta:=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad I \text{ is the } (n+1)\text{-dimensional unit matrix.} \tag{3.4}$$

Conversely, if $M(J)$ is a double solution of (3.2), (3.3), we can obtain a double-complex solution of (2.11) by

$$E(J)=M_{22}^{-1}(J)+JM_{12}(J)M_{22}^{-1}(J), \tag{3.5}$$

where we have expressed the $2(n+1)\times 2(n+1)$ matrix $M(J)$ in terms of $(n+1)\times(n+1)$ blocks $\{M_{AB}(J), A,B=1,2\}$ as

$$M(J)=\begin{pmatrix} M_{11}(J) & M_{12}(J) \\ M_{21}(J) & M_{22}(J) \end{pmatrix},$$

and the conditions (3.3) assure that the double-real $(n+1)\times(n+1)$ matrices $M_{22}^{-1}(J)$ and $M_{12}(J)M_{22}^{-1}(J)$ both are symmetric. It is clear that the equations (3.2), (3.3) are invariant under a double transformation as

$$M(J)\to M_G(J):=G(J)\,M(J)\,G^T(J), \tag{3.6}$$

where $G(J)$ is a $2(n+1)\times 2(n+1)$ double-real matrix satisfying

$$G^T(J)\,\eta G(J)=\eta. \tag{3.7}$$

Therefore, the SAS SGM-n field equations possess a double-real symplectic symmetry group $Sp(2(n+1),\mathcal{R}(J))$. The symmetry transformation (3.6) includes the double gauge, double scale and double Ehlers-like transformations, etc. of the SGM-n theories.

The double symmetry transformation (3.6) can also be more concisely expressed in terms of the double-complex matrix Ernst-like potential $E(J)=P(J)+J\Omega(J)$. To this end, it is convenient to write the element $G(J)$ of $Sp(2(n+1),\mathcal{R}(J))$ as

$$G(J)=\begin{pmatrix} a(J) & b(J) \\ c(J) & d(J) \end{pmatrix}, \tag{3.8}$$

where $a(J)$, $b(J)$, $c(J)$ and $d(J)$ are double-real $(n+1)\times(n+1)$ matrices satisfying

$$\begin{gathered} a^T(J)c(J)=c^T(J)a(J), \quad b^T(J)d(J)=d^T(J)b(J), \\ a^T(J)d(J)=c^T(J)b(J)+I. \end{gathered} \tag{3.9}$$

Now for a $(n+1)\times(n+1)$ matrix F, we define the action of $G(J)$ on F by the following double-complex matrix fractional linear transformation:

$$G(J)[F]:=[a(J)F+Jb(J)][J^3c(J)F+d(J)]^{-1}. \tag{3.10}$$

Then, associated with a double-complex potential $E(J)$ in (2.10), we consider an element $G_E(J)$ of $Sp(2(n+1),\mathcal{R}(J))$ as

$$G_E(J):=\begin{pmatrix} e(J) & \Omega(J)(e^T(J))^{-1} \\ 0 & (e^T(J))^{-1} \end{pmatrix}, \tag{3.11}$$

where the double-real vielbein $e(J)$ is defined such that $P(J)=e(J)e^T(J)$, and by (3.10) we have

$$G_E(J)[I]=E(J)=P(J)+J\Omega(J). \tag{3.12}$$

Moreover, we find that the $2(n+1)\times 2(n+1)$ double-real matrix $M(J)$ in (3.1) can be written, in terms of the above $G_E(J)$, as

$$M(J)=G_E(J)K(J)G_E^T(J), \tag{3.13}$$

where

$$K(J):=\begin{pmatrix} -J^2I & 0 \\ 0 & I \end{pmatrix}. \tag{3.14}$$

From Eqs. (3.6), (3.10), (3.12) and (3.13), it follows that

$$M(E'(J)):=M_G(J)=G(J)M(J)G^T(J)=G(J)G_E(J)K(J)G_E^T(J)G^T(J)=G_{E'}(J)K(J)G_{E'}^T(J); \tag{3.15}$$

here

$$G_{E'}(J)=G(J)G_E(J). \tag{3.16}$$

Besides, it can be verified that the double-complex matrix fractional linear transformation (3.10) is consistent with the group property:

$$G(J)[G'(J)[F]]=(G(J)G'(J))[F]. \tag{3.17}$$

Therefore, from (3.16) and (3.12) we have

$$E'(J):=G_{E'}(J)[I]=G(J)G_E(J)[I]=G(J)[E(J)], \tag{3.18}$$

and finally we obtain the $Sp(2(n+1),\mathcal{R}(J))$ symmetry transformation (3.6) expressed by the action on the double-complex matrix potential $E(J)$ as

$$E'(J)=G(J)[E(J)]=[a(J)E(J)+Jb(J)][J^3c(J)E(J)+d(J)]^{-1}. \tag{3.19}$$

This is a matrix form generalization of the double-complex fractional linear transformation of the double-complex Ernst potential in the case of vacuum gravity.[1,30]

IV. INFINITE CHAINS OF DOUBLE-SOLUTIONS OF THE SGM-*n* THEORIES

Noted the conditions (3.9), the matrix generalized double-complex fractional linear transformation (3.19) evidently contains the double matrix Ehlers-like transformation provided $c(J) \neq 0$. We denote the transformations of this type by $\alpha(J)$.

On the other hand, Eq. (2.11) [or equivalently, Eqs. (3.2)–(3.4)] allows us to introduce a double duality mapping $\beta(J)$ which is defined by

$$\beta(J): E(J) \to \hat{E}(J) = \hat{P}(J) + J\hat{\Omega}(J), \tag{4.1}$$

where

$$\hat{P}(J) = T(P(\mathring{J})), \quad \hat{\Omega}(J) = \mathring{J}^2 V_{P(\mathring{J})}(\Omega(\mathring{J})), \tag{4.2}$$

and the commutated double-imaginary unit $\mathring{J}$ is defined by (1.3). It can be verified that if $E(J)$ is a double-complex solution of Eq. (2.11), then so is $\hat{E}(J)$.

It should be pointed out that $E(J)$ and $\hat{E}(J)$ are equivalent in view of solving Eq. (2.4), i.e., they give the essentially same SAS SGM-*n* solutions. However, it is important that under the double transformation $\alpha(J)$, $E(J)$ and $\hat{E}(J)$ give different solutions, i.e., in general we have $\beta(J)\alpha(J) \neq = \alpha(J)\beta(J)$. Moreover, $\alpha(J)$, $\beta(J)$ both are invertible in the sense of transformations acting on the solution spaces of the SGM-*n* theories. Thus, from a known double solution $E_0(J)$, we can obtain an infinite chain of double-complex solutions of Eq. (2.11) by using $\alpha(J)$, $\beta(J)$ successively and alternately:

$$\cdots \hat{E}_{-2}(J) \overset{\alpha(J)}{---} \hat{E}_{-1}(J) \overset{\beta(J)}{=\!=} E_{-1}(J) \overset{\alpha(J)}{---} E_0(J) \overset{\beta(J)}{=\!=} \hat{E}_0(J) \overset{\alpha(J)}{---} \hat{E}_1(J) \overset{\beta(J)}{=\!=} E_1(J) \overset{\alpha(J)}{---} E_2(J) \cdots . \tag{4.3}$$

This gives a type of double solution generating techniques of the SGM-*n* theories and from each obtained $E_k(J)$ [or equivalently $\hat{E}_k(J)$] for $k = 0, \pm 1, \pm 2, \ldots$, and a fixed n, we can get a pair of dual *real* solutions of the SGM-*n* theory by using the formula (2.12). This shows that the double-complex method is more effective. The double-solution chain (4.3) is a matrix form generalization of the analogous results for pure gravity theory.[1,31]

V. SUMMARY AND DISCUSSIONS

The series of the symplectic gravity models developed in Ref. 23 is further studied by using the double-complex function method and then the doubleness symmetry of the SAS SGM-*n* theories for any non-negative integer n is found. In virtue of the double formulation, the doubleness symmetry is exploited more fully so that the dynamical motion equations of the theories under consideration can be written into double-complex Ernst-like forms; these are matrix form generalizations of the double-complex Ernst equation in the SAS vacuum Einstein gravity[1,28] and make us be able to obtain more symmetries and solutions of the SGM-*n* theories. We give the double symmetry groups $Sp(2(n+1), \mathcal{R}(J))$ of the studied theories and verify that the actions of these symmetry groups on the SGM-*n* solution spaces can be realized concisely by double-complex matrix form generalizations of the fractional linear transformation on the Ernst potential. Moreover, by introducing a double duality mapping $\beta(J)$, an infinite chain of double-solutions of the SGM-*n* theory (for each n) can be generated from a known solution $E_0(J)$; thus we obtain a double-solution generating method. These results show that the considered SGM-*n* theories possess more and richer symmetry structures than previously expected.

There are some formal analogies between the SGM-*n* theories and the vacuum Einstein theory. However, because the potentials in the SGM-*n* ($n \geqslant 1$) theories are noncommuting matri-

ces rather than ordinary scalar functions (as in the case of vacuum Einstein gravity), the related studies for the former are essentially complicated. Explicit representations of the Geroch-like group actions and concrete soliton solution construction methods of the SGM-*n* theories and their double forms need more investigations and will be considered in forthcoming works.

ACKNOWLEDGMENT

This work was supported by Science Foundition from the Education Department of Liaoning Province, China.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Universes encircling five-dimensional black holes

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(Received 25 June 2003; accepted 2 September 2003)

We clarify the status of two known solutions to the five-dimensional vacuum Einstein field equations derived by Liu, Mashhoon, and Wesson (LMW) and Fukui, Seahra, and Wesson (FSW), respectively. Both 5-metrics explicitly embed four-dimensional Friedman–Lemaître–Robertson–Walker cosmologies with a wide range of characteristics. We show that both metrics are also equivalent to five-dimensional topological black hole (TBH) solutions, which is demonstrated by finding explicit coordinate transformations from the TBH to LMW and FSW line elements. We argue that the equivalence is a direct consequence of Birkhoff's theorem generalized to five dimensions. Finally, for a special choice of parameters we plot constant coordinate surfaces of the LMW patch in a Penrose–Carter diagram. This shows that the LMW coordinates are regular across the black and/or white hole horizons. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1623617]

I. INTRODUCTION

Over the past few years, there has been a marked resurgence of interest in models with noncompact or large extra-dimensions. Three examples of such scenarios immediately come to mind—namely, the braneworld models of Randall & Sundrum[1,2] [henceforth RS] and Arkani–Hamed, Dimopoulos and Dvali[3,4] [henceforth ADD], as well as the older space–time–matter (STM) theory.[5] The RS model is motivated from certain ideas in string theory, which suggest that the particles and fields of the standard model are naturally confined to a lower-dimensional hypersurface living in a noncompact, higher-dimensional bulk manifold. The driving goal behind the ADD picture is to explain the discrepancy in scale between the observed strength of the gravitational interaction and the other fundamental forces. This is accomplished by noting that in generic higher-dimensional models with compact extra dimensions, the bulk Newton's constant is related to the effective four-dimensional constant by factors depending on the size and number of the extra dimensions. Finally, STM or induced matter theory proposes that our universe is an embedded 4-surface in a vacuum 5-manifold. In this picture, what we perceive to be the source in the four-dimensional Einstein field equations is really just an artifact of the embedding; or in other words, conventional matter is induced from higher-dimensional geometry.

Regardless of the motivation, if extra dimensions are to be taken seriously then it is useful to have as many solutions of the higher-dimensional Einstein equations at our disposal as possible. These metrics serve as both arenas in which to test the feasibility of extra dimensions, as well as guides as to where four-dimensional general relativity may break down. This simplest type of higher-dimensional field equations that one might consider is the five-dimensional vacuum field equations $\hat{R}_{AB}=0$. (In this paper, uppercase italic indices run $0\cdots4$ while lowercase greek indices run $0\cdots3$, and five-dimensional curvature tensors are distinguished from the four-dimensional counterparts by hats. Also, commas in subscripts indicate partial differentiation.) This condition is most relevant to the STM scenario, but can also be applied to the RS or ADD pictures. There are a fair number of known solutions that embed 4-manifolds of cosmological or spherically symmet-

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ric character; one can consult the book by Wesson[5] for an accounting of these metrics.

However, when searching for new solutions to vacuum field equations, one must keep in mind a known peril from four-dimensional work; i.e., any new solution could be a previously discovered metric written down in terms of strange coordinates. Our purpose in this paper is to demonstrate that two five-dimensional vacuum solutions in the literature are actually isometric to a generalized five-dimensional Schwarzschild manifold. Both of these solutions have been previously analyzed in the context of four-dimensional cosmology because they both embed submanifolds with line elements matching that of standard Friedman–Lemaître–Robertson–Walker (FLRW) models with flat, spherical, or hyperbolic spatial sections. In Sec. II A, we discuss the first of these 5-metrics, which was originally written down by Liu and Mashhoon[6] and later rediscovered in a different form by Liu and Wesson.[7] We will see that this metric naturally embeds FLRW models with fairly general, but not unrestricted, scale factor behavior. Several different authors have considered this metric in a number of different contexts,[8–11] including the RS braneworld scenario. The second 5-metric—which was discovered by Fukui, Seahra, and Wesson[12] and is the subject of Sec. II B—also embeds FLRW models with all types of spatial curvature, but the scale factor is much more constrained. We will pay special attention to the characteristics of the embedded cosmologies in each solution, as well as the coordinate invariant geometric properties of the associated bulk manifolds.

The latter discussion will reveal that not only do the Liu–Mashhoon–Wesson (LMW) and Fukui–Seahra–Wesson (FSW) metrics have a lot in common with one another, they also exhibit many properties similar to that of the topological black hole (TBH) solution of the five-dimensional vacuum field equations, which we introduce in Sec. III. This prompts us to suspect that the LMW and FSW solutions are actually isometric to topological black hole manifolds. We confirm this explicitly by finding transformations from standard black hole to LMW and FSW coordinates in Secs. IV A and IV B, respectively. We argue that the equivalence of the three metrics is actually a consequence of a higher-dimensional version of Birkhoff's theorem in Sec. IV C. In Sec. V, we discuss which portion of the extended five-dimensional Kruskal manifold is covered by the LMW coordinate patch and obtain Penrose–Carter embedding diagrams for a particular case. Section VI summarizes and discusses our results.

II. TWO 5-METRICS WITH FLRW SUBMANIFOLDS

In this section, we introduce two 5-metrics that embed four-dimensional FLRW models. Both of these are solutions of the five-dimensional vacuum field equations, and are hence suitable manifolds for STM theory. Our goals are to illustrate what subset of all possible FLRW models can be realized as hypersurfaces contained within these manifolds, and to find out about any five-dimensional curvature singularities or geometric features that may be present.

A. The Liu–Mashhoon–Wesson metric

Consider a five-dimensional manifold $(M_{\mathrm{LMW}}, g_{AB})$. We define the LMW metric *Ansatz* as

$$\mathrm{d}s^2_{\mathrm{LMW}} = \frac{a_{,t}^2(t,\ell)}{\mu^2(t)}\mathrm{d}t^2 - a^2(t,\ell)\,\mathrm{d}\sigma^2_{(k,3)} - \mathrm{d}\ell^2. \tag{1}$$

Here, $a(t,\ell)$ and $\mu(t)$ are undetermined functions, and $d\sigma^2_{(k,3)}$ is the line element on maximally symmetric 3-spaces $\mathbb{S}_3^{(k)}$ with curvature index $k=+1,0,-1$:

$$\mathrm{d}\sigma^2_{(k,3)} = \mathrm{d}\psi^2 + S_k^2(\psi)(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2), \tag{2}$$

where

$$S_k(\psi) \equiv \begin{cases} \sin\psi, & k=+1, \\ \psi, & k=0, \\ \sinh\psi, & k=-1. \end{cases} \tag{3}$$

It is immediately obvious that the $\ell=$constant hypersurfaces Σ_ℓ associated with (1) have the structure of FLRW models: $\mathbb{R}\times\mathbb{S}_3^{(k)}$. We should note that the original papers (Refs. 6 and 7) did not really begin with a metric *Ansatz* like (1); rather, the g_{tt} component of the metric was initially taken to be some general function of t and ℓ. But one rapidly closes in on the above line element by direct integration of one component of the vacuum field equations $\hat{R}_{AB}=0$; namely, $\hat{R}_{t\ell}=0$. The other components are satisfied if

$$a^2(t,\ell)=[\mu^2(t)+k]\ell^2+2\nu(t)\ell+\frac{\nu^2(t)+\mathcal{K}}{\mu^2(t)+k}, \tag{4}$$

where $\mathcal{K}$ is an integration constant. As far as the field equations are concerned, $\mu(t)$ and $\nu(t)$ are *completely arbitrary* functions of time. However, we should constrain them by appending the condition

$$a(t,\ell)\in\mathbb{R}^+\Rightarrow a^2(t,\ell)>0 \tag{5}$$

to the system. This restriction ensures that the metric signature is $(+----)$ and t is the only timelike coordinate. Now, if a is taken to be real, then it follows that ν must be real as well. Regarding (4) as a quadratic equation in ν, we find that there are real solutions only if the quadratic discriminant is non-negative. This condition translates into

$$\mathcal{K}\leqslant a^2(t,\ell)[\mu^2(t)+k]. \tag{6}$$

If $\mathcal{K}$ is positive this inequality implies that we must choose $\mu(t)$ such that $\mu^2+k>0$. This relation will be important shortly.

The reason that this solution is of interest is that the induced metric on $\ell=$constant hypersurfaces is isometric to the standard FLRW line element. To see this explicitly, consider the line element on the $\ell=\ell_0$ 4-surface:

$$\mathrm{d}s^2_{(\Sigma_\ell)}=\frac{a^2_{,t}(t,\ell_0)}{\mu^2(t)}\mathrm{d}t^2-a^2(t,\ell_0)\,\mathrm{d}\sigma^2_{(k,3)}\,. \tag{7}$$

Let us perform the four-dimensional coordinate transformation

$$\Theta(t)=\int_t\frac{a_{,u}(u,\ell_0)}{\mu(u)}\mathrm{d}u\Rightarrow\mu(t(\Theta))=\mathcal{A}'(\Theta), \tag{8}$$

where

$$\mathcal{A}(\Theta)=a(t(\Theta),\ell_0), \tag{9}$$

and we use a prime to denote the derivative of functions of a single argument. This puts the induced metric in the FLRW form

$$\mathrm{d}s^2_{(\Sigma_\ell)}=\mathrm{d}\Theta^2-\mathcal{A}^2(\Theta)\,\mathrm{d}\sigma^2_{(k,3)}\,, \tag{10}$$

where Θ is the cosmic time and $\mathcal{A}(\Theta)$ is the scale factor.

So, the geometry of each of the Σ_ℓ hypersurfaces is indeed of the FLRW type. But what kind of cosmologies can be thus embedded? Well, if we rewrite the inequality (6) in terms of $\mathcal{A}$ and $\mathcal{A}'$ we obtain

$$\mathcal{K}\leqslant\mathcal{A}^2(\mathcal{A}'^2+k). \tag{11}$$

Since $\mathcal{A}$ is to be interpreted as the scale factor of some cosmological model, it satisfies the Friedman equation:

$$\mathcal{A}'^2 - \tfrac{1}{3}\kappa_4^2 \rho \mathcal{A}^2 = -k. \tag{12}$$

Here, ρ is the total density of the matter energy in the cosmological model characterized by $\mathcal{A}(\Theta)$ and $\kappa_4^2 = 8\pi G$ is the usual coupling constant in the four-dimensional Einstein equations. This implies a relation between the density of the embedded cosmologies and the choice of μ,

$$\mu^2 + k = \tfrac{1}{3}\kappa_4^2 \rho \mathcal{A}^2. \tag{13}$$

This into the inequality (11) yields

$$\mathcal{K} \leqslant \tfrac{1}{3}\kappa_4^2 \rho \mathcal{A}^4. \tag{14}$$

Therefore, we can successfully embed a given FLRW model on a Σ_ℓ 4-surface in the LMW solution if the total density of the model's cosmological fluid and scale factor satisfy (14) for all Θ. An obvious corollary of this is that we can embed any FLRW model with $\rho > 0$ if $\mathcal{K} < 0$.

There is one other point about the intrinsic geometry of the Σ_ℓ hypersurfaces that needs to be made. Notice that our four-dimension coordinate transformation (8) has

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = \frac{a_{,t}}{\mu}, \tag{15}$$

which means that the associated Jacobian vanishes whenever $a_{,t} = 0$. Therefore, the transformation is really only valid in between the turning points of a. Also notice that the original 4-metric (7) is badly behaved when $a_{,t} = 0$, but the transformed one (10) is not when $\mathcal{A}' = 0$. We can confirm via direct calculation that the Ricci scalar for (7) is

$${}^{(4)}R = -\frac{6\mu}{a}\frac{\mathrm{d}\mu}{\mathrm{d}t}\left(\frac{\partial a}{\partial t}\right)^{-1} - \frac{6}{a^2}(\mu^2 + k). \tag{16}$$

We see that ${}^{(4)}R$ diverges when $a_{,t} = 0$, provided that $\mu\mu_{,t}/a \neq 0$. Therefore, there can be genuine curvature singularities in the intrinsic 4-geometry at the turning points of a. These features are hidden in the altered line element (10) because the coordinate transformation (8) is not valid in the immediate vicinity of any singularities, hence the Θ-patch cannot cover those regions (if they exist). We mention that this four-dimensional singularity in the LMW metric has been recently investigated by Xu, Liu, and Wang,[13] who have interpreted it as a four-dimensional event horizon.

Now, let us turn our attention to some of the five-dimensional geometric properties of M_{LMW}. We can test for curvature singularities in this 5-manifold by calculating the Kretschmann scalar

$$\mathfrak{R}_{\mathrm{LMW}} \equiv \hat{R}^{ABCD}\hat{R}_{ABCD} = \frac{72\mathcal{K}^2}{a^8(t,\ell)}. \tag{17}$$

We see there is a singularity in the 5-geometry along the hypersurface $a(t,\ell) = 0$. [Of course, whether or not $a(t,\ell) = 0$ for any $(t,\ell) \in \mathbb{R}^2$ depends on the choice of μ and ν.] This singularity is essentially a linelike object because the radius a of the three-dimensional $\mathbb{S}_3^{(k)}$ subspace vanishes there. Other tools for probing the 5-geometry are Killing vector fields on M_{LMW}. Now, there are by definition six Killing vectors associated with symmetry operations on $\mathbb{S}_3^{(k)}$, but there is also at least one Killing vector that is orthogonal to that submanifold. This vector field is given by

$$\xi_A^{\mathrm{LMW}}\,\mathrm{d}x^A = \frac{a_{,t}}{\mu}\sqrt{h(a) + \mu^2(t)}\,\mathrm{d}t + \sqrt{a_{,\ell}^2 - h(a)}\,\mathrm{d}\ell. \tag{18}$$

Here, we have defined

$$h(x) \equiv k - \frac{\mathcal{K}}{x^2}. \tag{19}$$

Using the explicit form of $a(t,\ell)$ from Eq. (4), we can verify that ξ satisfies Killing's equation

$$\nabla_B \xi^{\mathrm{LMW}}_A + \nabla_A \xi^{\mathrm{LMW}}_B = 0, \tag{20}$$

via computer. Also using (4), we can calculate the norm of ξ^{LMW}, which is given by

$$\xi^{\mathrm{LMW}} \cdot \xi^{\mathrm{LMW}} = h(a). \tag{21}$$

This vanishes at $ka^2 = \mathcal{K}$. So, if $k\mathcal{K} > 0$ the 5-manifold contains a Killing horizon. If the horizon exists then ξ^{LMW} will be timelike for $|a| > \sqrt{|\mathcal{K}|}$ and spacelike for $|a| < \sqrt{|\mathcal{K}|}$.

To summarize, we have seen that FLRW models satisfying (14) can be embedded on a Σ_ℓ 4-surface within the LMW metric, but that there are four-dimensional curvature singularities wherever $a_{,t} = 0$. The LMW 5-geometry also possesses a linelike singularity where $a(t,\ell) = 0$, as well as a Killing horizon across which the norm of ξ^{LMW} changes sign.

B. The Fukui–Seahra–Wesson metric

For the time being, let us set aside the LMW metric and concentrate on the FSW solution. On a certain 5-manifold $(M_{\mathrm{FSW}}, g_{AB})$, this is given by the line element

$$\mathrm{d}s^2_{\mathrm{FSW}} = \mathrm{d}\tau^2 - b^2(\tau,w)\,\mathrm{d}\sigma^2_{(k,3)} - \frac{b^2_{,w}(\tau,w)}{\zeta^2(w)}\mathrm{d}w^2, \tag{22a}$$

$$b^2(\tau,w) = [\zeta^2(w) - k]\tau^2 + 2\chi(w)\tau + \frac{\chi^2(w) - \mathcal{K}}{\zeta^2(w) - k}. \tag{22b}$$

This metric (22a) is a solution of the five-dimensional vacuum field equations $\hat{R}_{AB} = 0$ with $\zeta(w)$ and $\chi(w)$ as arbitrary functions. Just as before, we call Eq. (22a) the FSW metric *Ansatz*, even though it was not the technical starting point of the original paper.[12] We have written (22) in a form somewhat different from that of Ref. 12; to make contact with their notation we need to make the correspondences

$$[F(w)]_{\mathrm{FSW}} \equiv k - \zeta^2(w), \tag{23a}$$

$$[h(w)]_{\mathrm{FSW}} \equiv [\chi^2(w) + \mathcal{K}]/[\zeta^2(w) - k], \tag{23b}$$

$$[g(w)]_{\mathrm{FSW}} \equiv 2\chi(w), \tag{23c}$$

$$[\mathcal{K}]_{\mathrm{FSW}} \equiv -4\mathcal{K}, \tag{23d}$$

where $[\cdots]_{\mathrm{FSW}}$ indicates a quantity from the original FSW work. A cursory comparison between the LMW and FSW vacuum solutions reveals that both metrics have a similar structure, which prompts us to wonder about any sort of fundamental connection between them. We defer this issue to the next section, and presently concern ourselves with the properties of the FSW solution in its own right.

Just as for the LMW metric, we can identify hypersurfaces in the FSW solution with FLRW models. Specifically, the induced metric on $w = w_0$ hypersurfaces Σ_w is

$$\mathrm{d}s^2_{(\Sigma_w)} = \mathrm{d}\tau^2 - b^2(\tau,w_0)\,\mathrm{d}\sigma^2_{(k,3)}. \tag{24}$$

We see that for the universes on Σ_w, τ is the cosmic time and $b(\tau,w_0)$ is the scale factor. It is useful to perform the following linear transformation on τ:

TABLE I. Characteristics of the four-dimensional cosmologies embedded on the Σ_w hypersurfaces in the FSW metric.

	$\zeta_0^2-k>0$	$\zeta_0^2-k<0$
$\mathcal{K}>0$	Big bang	Big bang and big crunch
$\mathcal{K}=0$	Big bang	$\mathcal{B}\in\mathbb{C}$ for all $\Theta\in\mathbb{R}$
$\mathcal{K}<0$	No big bang/crunch	$\mathcal{B}\in\mathbb{C}$ for all $\Theta\in\mathbb{R}$

$$\tau(\Theta)=\Theta-\frac{\chi_0}{\zeta_0^2-k}, \tag{25}$$

where we have defined $\zeta_0\equiv\zeta(w_0)$ and $\chi_0\equiv\chi(w_0)$. This puts the induced metric into the form

$$\mathrm{d}s^2_{(\Sigma_w)}=\mathrm{d}\Theta^2-\mathcal{B}^2(\Theta)\,\mathrm{d}\sigma^2_{(k,3)}, \tag{26a}$$

$$\mathcal{B}(\Theta)=\sqrt{\frac{(\zeta_0^2-k)^2\Theta^2-\mathcal{K}}{\zeta_0^2-k}}. \tag{26b}$$

Unlike the LMW case, the cosmology on the Σ_w hypersurfaces has restrictive properties. If $\zeta_0^2-k>0$, the scale factor $\mathcal{B}(\Theta)$ has the shape of one arm of a hyperbola with a semimajor axis of length $\sqrt{-\mathcal{K}/(\zeta_0^2-k)}$. Note that this length may be complex depending on the values of ζ_0, k, and $\mathcal{K}$. That is, the scale factor may not be defined for all $\Theta\in\mathbb{R}$. When this is the case, the embedded cosmologies involve a big bang and/or a big crunch. Conversely, it is not hard to see if $\zeta_0^2-k<0$ and $\mathcal{K}>0$ then the cosmology is re-collapsing; i.e., there is a big bang and a big crunch. However, if $\zeta_0^2-k<0$ and $\mathcal{K}\leqslant 0$, then there is no Θ interval where the scale factor is real. We have summarized the basic properties of the embedded cosmologies in Table I. Finally, we note that if $\zeta_0^2-k>0$ then

$$\lim_{\Theta\to\infty}\mathcal{B}(\Theta)=(\zeta_0^2-k)^{1/2}\Theta. \tag{27}$$

Hence, the late time behavior of such models approaches that of the empty Milne universe.

Lake[14] has calculated the Kretschmann scalar for vacuum 5-metrics of the FSW type. When his formula is applied to (22), we obtain

$$\mathfrak{R}_{\mathrm{FSW}}\equiv\hat{R}^{ABCD}\hat{R}_{ABCD}=\frac{72\mathcal{K}^2}{b^8(\tau,w)}. \tag{28}$$

As for the LMW manifold, this implies the existence of a linelike singularity in the 5-geometry at $b(\tau,w)=0$. We also find that there is a Killing vector on M_{FSW}, which is given by

$$\xi_A^{\mathrm{FSW}}\,\mathrm{d}x^A=\sqrt{b_{,\tau}+h(b)}\,\mathrm{d}\tau+\frac{b_{,w}}{\zeta}\sqrt{\zeta^2-h(b)}\,\mathrm{d}w, \tag{29a}$$

$$0=\nabla_A\xi_B^{\mathrm{FSW}}+\nabla_B\xi_A^{\mathrm{FSW}}. \tag{29b}$$

The norm of this Killing vector is relatively easily found by computer,

$$\xi^{\mathrm{FSW}}\cdot\xi^{\mathrm{FSW}}=h(b). \tag{30}$$

Hence, there is a Killing horizon in M_{FSW} where $h(b)=0$. Obviously, the ξ^{FSW} Killing vector changes from timelike to spacelike—or *vice versa*—as the horizon is traversed.

In summary, we have seen how FLRW models with scale factors of the type (22b) are embedded in the FSW solution. We found that there is a linelike curvature singularity in $M_{\rm FSW}$ at $b(\tau,w)=0$ and the bulk manifold has a Killing horizon where the magnitude of $\xi^{\rm FSW}$ vanishes.

III. CONNECTION TO THE FIVE-DIMENSIONAL TOPOLOGICAL BLACK HOLE MANIFOLD

When comparing equations (17) and (28), or (21) and (30), it is hard not to believe that there is some sort of fundamental connection between the LMW and FSW metrics. We see that

$$\mathfrak{R}_{\rm LMW}=\mathfrak{R}_{\rm FSW}, \quad \xi^{\rm LMW}\cdot\xi^{\rm LMW}=\xi^{\rm FSW}\cdot\xi^{\rm FSW}, \tag{31}$$

if we identify $a(t,\ell)=b(\tau,w)$. Also, we notice that the LMW solution can be converted into the FSW metric by the following set of transformations/Wick rotations:[15]

$$\begin{gathered}\psi\to i\psi, \quad t\to w,\\ \ell\to\tau, \quad k\to -k,\\ \mathcal{K}\to-\mathcal{K}, \quad {\rm d}s_{\rm LMW}\to i\,{\rm d}s_{\rm FSW}.\end{gathered} \tag{32}$$

These facts lead us to the strong suspicion that the LMW and FSW metrics actually describe the same 5-manifold.

But which 5-manifold might this be? We established in the previous section that both the LMW and FSW metrics involve a five-dimensional linelike curvature singularity and Killing horizon if $k\mathcal{K}>0$. This reminds us of another familiar manifold: that of a black hole. Consider the metric of a ''topological'' black hole (TBH) on a 5-manifold $(M_{\rm TBH},g_{AB})$:

$${\rm d}s^2_{\rm TBH}=h(R)\,{\rm d}T^2-h^{-1}(R)\,{\rm d}R^2-R^2\,{\rm d}\sigma^2_{(k,3)}. \tag{33}$$

The adjective ''topological'' comes from the fact that the manifold has the structure $\mathbb{R}^2\times\mathbb{S}_3^{(k)}$, as opposed to the familiar $\mathbb{R}^2\times S_3$ structure commonly associated with spherical symmetry in five dimensions. That is, the surfaces $T=$constant and $R=$constant are not necessarily 3-spheres for the topological black hole; it is possible that they have flat or hyperbolic geometry. One can confirm by direct calculation that (33) is a solution of $\hat{R}_{AB}=0$ for any value of k, and that the constant $\mathcal{K}$ that appears in $h(R)$ is related to the mass of the central object. The Kretschmann scalar on $M_{\rm TBH}$ is

$$\mathfrak{R}_{\rm TBH}=\hat{R}^{ABCD}\hat{R}_{ABCD}=\frac{72\mathcal{K}^2}{R^8}, \tag{34}$$

implying a linelike curvature singularity at $R=0$. There is an obvious Killing vector in this manifold, given by

$$\xi^{\rm TBH}_A\,{\rm d}x^A=h(R)\,{\rm d}T. \tag{35}$$

The norm of this vector is trivially

$$\xi^{\rm TBH}\cdot\xi^{\rm TBH}=h(R). \tag{36}$$

There is therefore a Killing horizon in this space located at $kR^2=\mathcal{K}$.

Now, Eqs. (34) and (36) closely match their counterparts for the LMW and FSW metrics, which inspires the hypothesis that not only are the LMW and FSW isometric to one another, they are also isometric to the metric describing topological black holes. However, while these coincidences provide fairly compelling circumstantial evidence that the LMW, FSW, and TBH metrics are equivalent, we do not have conclusive proof—that will come in the next section.

IV. COORDINATE TRANSFORMATIONS

In this section, our goal is to prove the conjecture that the LMW, FSW, and TBH solutions and the five-dimensional vacuum field equations are isometric to one another. We will do so by finding two explicit coordinate transformations that convert the TBH metric to the LMW and FSW metrics, respectively. This is sufficient to prove the equality of all three solutions, since it implies that one can transform from the LMW to the FSW metric—or vice versa—via a two-stage procedure.

A. Transformation from Schwarzschild to Liu–Mashhoon–Wesson coordinates

We first search for a coordinate transformation that takes the TBH line element (33) to the LMW line element (1). We take this transformation to be

$$R=\mathcal{R}(t,\ell), \quad T=\mathcal{T}(t,\ell). \tag{37}$$

Notice that we have *not* assumed $R=a(t,\ell)$—as may have been expected from the discussion of the preceding section—in order to stress that we are starting with a general coordinate transformation. We will soon see that by demanding that this transformation forces the TBH metric into the form of the LMW metric *Ansatz*, we can recover $R=a(t,\ell)$ with $a(t,\ell)$ given explicitly by (4). In other words, the coordinate transformation specified in this section will fix the functional form of $a(t,\ell)$ in a manner independent of the direct attack on the vacuum field equations found in Refs. 6 and 7.

When (37) is substituted into (33), we get

$$\begin{aligned} ds^2_{\mathrm{TBH}}=&\left[h(\mathcal{R})\mathcal{T}^2_{,t}-\frac{\mathcal{R}^2_{,t}}{h(\mathcal{R})}\right]dt^2+2\left[h(\mathcal{R})\mathcal{T}_{,t}\mathcal{T}_{,\ell}-\frac{\mathcal{R}_{,t}\mathcal{R}_{,\ell}}{h(\mathcal{R})}\right]dt\,d\ell \\ &+\left[h(\mathcal{R})\mathcal{T}^2_{,\ell}-\frac{\mathcal{R}^2_{,\ell}}{h(\mathcal{R})}\right]d\ell^2-\mathcal{R}^2(t,\ell)\,d\sigma^2_{(k,3)}. \end{aligned} \tag{38}$$

For this to match equation (1) with $\mathcal{R}(t,\ell)$ instead of $a(t,\ell)$ we must have

$$\frac{\mathcal{R}^2_{,t}}{\mu^2(t)}=h(\mathcal{R})\mathcal{T}^2_{,t}-\frac{\mathcal{R}^2_{,t}}{h(\mathcal{R})}, \tag{39a}$$

$$0=h(\mathcal{R})\mathcal{T}_{,t}\mathcal{T}_{,\ell}-\frac{\mathcal{R}_{,t}\mathcal{R}_{,\ell}}{h(\mathcal{R})}, \tag{39b}$$

$$-1=h(\mathcal{R})\mathcal{T}^2_{,\ell}-\frac{\mathcal{R}^2_{,\ell}}{h(\mathcal{R})}, \tag{39c}$$

with $\mu(t)$ arbitrary. Under these conditions, we find

$$ds^2_{\mathrm{TBH}}=\frac{\mathcal{R}^2_{,t}(t,\ell)}{\mu^2(t)}dt^2-\mathcal{R}^2(t,\ell)\,d\sigma^2_{(k,3)}-dy^2, \tag{40}$$

which is obviously the same as the LMW metric *Ansatz* (1). However, the precise functional form of $\mathcal{R}(t,\ell)$ has yet to be specified.

To solve for $\mathcal{R}(t,\ell)$, we note Eqs. (39a) and (39c) can be rearranged to give

$$\mathcal{T}_{,t}=\epsilon_t\frac{\mathcal{R}_{,t}}{h(\mathcal{R})}\sqrt{1+\frac{h(\mathcal{R})}{\mu^2(t)}}, \tag{41a}$$

$$\mathcal{T}_{,\ell}=\epsilon_\ell\frac{1}{h(\mathcal{R})}\sqrt{\mathcal{R}^2_{,\ell}-h(\mathcal{R})}, \tag{41b}$$

where $\epsilon_t = \pm 1$ and $\epsilon_\ell = \pm 1$. Using these in (39b) yields

$$\mathcal{R}_{,\ell} = \pm \sqrt{h(\mathcal{R}) + \mu^2(t)}. \tag{42}$$

Our task is to solve the system of PDEs formed by Eqs. (41) and (42) for $\mathcal{T}(t,\ell)$ and $\mathcal{R}(t,\ell)$. Once we have accomplished this, the coordinate transformation from (1) to (33) is found.

Using the definition of $h(\mathcal{R})$, we can expand Eq. (42) to get

$$\pm 1 = \frac{\mathcal{R}}{\sqrt{(\mu^2+k)\mathcal{R}^2 - \mathcal{K}}} \frac{\partial \mathcal{R}}{\partial \ell}. \tag{43}$$

Integrating both sides with respect to ℓ yields

$$\sqrt{(\mu^2+k)\mathcal{R}^2 - \mathcal{K}} = (\mu^2+k)(\pm \ell + \gamma), \tag{44}$$

where $\gamma = \gamma(t)$ is an arbitrary function of time. Solving for $\mathcal{R}$ gives

$$R^2 = \mathcal{R}^2(t,\ell) = [\mu^2(t)+k]\ell^2 + 2\nu(t)\ell + \frac{\nu^2(t)+\mathcal{K}}{\mu^2(t)+k}, \tag{45}$$

where we have defined

$$\nu(t) = \pm \gamma(t)[\mu^2(t)+k], \tag{46}$$

which can be thought of as just another arbitrary function of time. We have hence seen that the functional form of $\mathcal{R}(t,\ell)$ matches exactly the functional form of $a(t,\ell)$ in Eq. (4). This is despite the fact that the two expressions were derived by different means: (45) from conditions placed on a coordinate transformation, and (4) from the direct solution of the five-dimensional vacuum field equations.

When our solution for $\mathcal{R}(t,\ell)$ is set into Eqs. (41), we obtain a pair of PDEs that expresses the gradient of $\mathcal{T}$ in the (t,ℓ) plane as known functions of the coordinates. This is analogous to a problem where one is presented with the components of a two-dimensional force and is asked to find the associated potential. The condition for integrablity of the system is that the curl of the force vanishes, which in our case reads

$$0 \overset{?}{=} \epsilon_t \frac{\partial}{\partial \ell}\left(\frac{\mathcal{R}_{,t}}{h(\mathcal{R})} \sqrt{1 + \frac{h(\mathcal{R})}{\mu^2(t)}} \right) - \epsilon_\ell \frac{\partial}{\partial t}\left(\frac{1}{h(\mathcal{R})} \sqrt{\mathcal{R}_{,\ell}^2 - h(\mathcal{R})} \right). \tag{47}$$

We have confirmed via computer that this condition holds when $\mathcal{R}(t,\ell)$ is given by Eq. (45), provided we choose $\epsilon_t = \epsilon_\ell = \pm 1$. Without loss of generality, we can set $\epsilon_t = \epsilon_\ell = 1$. Hence, Eqs. (41) are indeed solvable for $\mathcal{T}(t,\ell)$ and a *coordinate transformation from (33) to (1) exists*.

The only thing left is the tedious task of determining the explicit form of $\mathcal{T}(t,\ell)$. We spare the reader the details and just quote the solution, which can be checked by explicit substitution into (41). For $k = \pm 1$, we get

$$\mathcal{T}(t,\ell) = \frac{1}{k}\int_t \left\{ \frac{1}{\mu(u)} \frac{\mathrm{d}}{\mathrm{d}u}\nu(u) - \left[\frac{\nu(u)}{\mu^2(u)+k} \right] \frac{\mathrm{d}}{\mathrm{d}u}\mu(u) \right\} \mathrm{d}u + \frac{1}{k}\left(\mu(t)\ell - \frac{\mathcal{K}}{2\sqrt{k\mathcal{K}}} \ln \frac{1+\mathcal{X}(t,\ell)}{1-\mathcal{X}(t,\ell)} \right), \tag{48a}$$

$$\mathcal{X}(t,\ell) \equiv \frac{k}{\sqrt{k\mathcal{K}}} \frac{[\mu^2(t)+k]\ell + \nu(t)}{\mu(t)}. \tag{48b}$$

For $k = 0$, we obtain

$$\mathcal{T}(t,\ell)=\frac{1}{\mathcal{K}}\int_t\left\{\frac{\nu^2(u)}{\mu^3(u)}\frac{\mathrm{d}}{\mathrm{d}u}\nu(u)-\frac{\nu(u)[\nu^2(u)+\mathcal{K}]}{\mu^4(u)}\frac{\mathrm{d}}{\mathrm{d}u}\mu(u)\right\}\mathrm{d}u$$
$$+\frac{1}{\mathcal{K}}\left\{\frac{1}{3}\mu^3(t)\ell^3+\mu(t)\nu(t)\ell^2+\left[\frac{\nu^2(t)+\mathcal{K}}{\mu(t)}\right]\ell\right\}. \tag{49}$$

Recall that in these expression, μ and ν can be regarded as free functions. Taken with (45), these equations give the transformation from TBH to LMW coordinates explicitly.

Before moving on, there is one special case that we want to highlight. This is defined by $k\mathcal{K}<0$, which implies that there is no Killing horizon in the bulk for real values of R and we have a naked singularity. If we have a spherical 3-geometry, then this is the case of a negative mass black hole. We have that $\sqrt{k\mathcal{K}}=i\sqrt{-k\mathcal{K}}$, which allows us to rewrite Eq. (48) as

$$\mathcal{T}(t,\ell)=\frac{1}{k}\left\{\mu(t)\ell+\frac{\mathcal{K}}{\sqrt{-k\mathcal{K}}}\arctan\left(\frac{k}{\sqrt{-k\mathcal{K}}}\frac{[\mu^2(t)+k]\ell+\nu(t)}{\mu(t)}\right)\right\}$$
$$+\frac{1}{k}\int_t\left\{\frac{1}{\mu(u)}\frac{\mathrm{d}}{\mathrm{d}u}\nu(u)-\left[\frac{\nu(u)}{\mu^2(u)+k}\right]\frac{\mathrm{d}}{\mathrm{d}u}\mu(u)\right\}\mathrm{d}u. \tag{50}$$

In obtaining this, we have made use of the identity

$$\arctan z=\frac{1}{2i}\ln\frac{1+iz}{1-iz},\quad z\in\mathbb{C}. \tag{51}$$

To summarize this section, we have successfully found a coordinate transformation between the TBH to LMW coordinates. This establishes that those two solutions are indeed isometric, and are hence equivalent.

B. Transformation from Schwarzschild to Fukui–Seahra–Wesson coordinates

We now turn our attention to finding a transformation between the TBH and FSW line elements. The procedure is very similar to the one presented in the preceding section. We begin by applying the following general coordinate transformation to the TBH solution (33):

$$T=\mathsf{T}(\tau,w),\quad R=\mathsf{R}(\tau,w). \tag{52}$$

Again, instead of identifying $\mathsf{R}(\tau,w)=b(\tau,w)$ as given by (22b), we regard it as a function to be solved for. To match the metric resulting from this transformation with (22a) we demand

$$+1=h(\mathsf{R})\mathsf{T}_{,\tau}^2-\frac{\mathsf{R}_{,t}^2}{h(\mathsf{R})}, \tag{53a}$$

$$0=h(\mathsf{R})\mathsf{T}_{,\tau}\mathsf{T}_{,w}-\frac{\mathsf{R}_{,\tau}\mathsf{R}_{,w}}{h(\mathsf{R})}, \tag{53b}$$

$$-\frac{\mathsf{R}_{,w}^2}{\zeta^2(w)}=h(\mathsf{R})\mathsf{T}_{,w}^2-\frac{\mathsf{R}_{,w}^2}{h(\mathsf{R})}. \tag{53c}$$

Here, $\zeta(w)$ is an arbitrary function. Compare this to the previous system of PDEs (39). We have essentially swapped and changed the signs of the left-hand sides of (39a) and (39c), as well as replaced $\mathcal{R}_{,t}$ with $\mathsf{R}_{,w}$ and $\mu(t)$ with $\zeta(w)$. This constitutes a sort of identity exchange $t\to w$ and $\ell\to\tau$. The explicit form of the TBH metric after this transformation is applied is

$$\mathrm{d}s^2_{\mathrm{TBH}} = \mathrm{d}\tau^2 - \mathsf{R}^2(\tau,w)\,\mathrm{d}\sigma^2_{(k,3)} - \left[\frac{\mathsf{R}_{,w}(t,w)}{\zeta(w)}\right]^2 \mathrm{d}w^2. \tag{54}$$

This matches the FSW metric *Ansatz* (22a), but the functional form of $\mathsf{R}(\tau,w)$ is yet to be determined by the coordinate transformation (53).

Let us now determine it by repeating the manipulations of the preceding section. We find that R satisfies the PDE,

$$\mathsf{R}_{,\tau} = \pm\sqrt{\zeta^2(w) - h(\mathsf{R})}, \tag{55}$$

which is solved by

$$\mathsf{R}^2(\tau,w) = [\zeta^2(w) - k]\tau^2 + 2\chi(w)\tau + \frac{\chi^2(w) - \mathcal{K}}{\zeta^2(w) - k}. \tag{56}$$

Here, χ is an arbitrary function. In a manner similar to before, we see that the coordinate transformation fixes the solution for $\mathsf{R}(\tau,w)$, and that it matches the solution for $b(\tau,w)$ obtained directly from the five-dimensional vacuum field equations (22b).

The solution for T is obtained without difficultly as before. For $k = \pm 1$, we get

$$\mathsf{T}(\tau,w) = \frac{1}{k}\int_w \left\{\frac{1}{\zeta(u)}\frac{\mathrm{d}}{\mathrm{d}u}\chi(u) - \left[\frac{\chi(u)}{\zeta^2(u) - k}\right]\frac{\mathrm{d}}{\mathrm{d}u}\zeta(u)\right\}\mathrm{d}u + \frac{1}{k}\left\{\zeta(w)\tau - \frac{\mathcal{K}}{2\sqrt{k\mathcal{K}}}\ln\frac{1+\mathsf{X}(\tau,w)}{1-\mathsf{X}(\tau,w)}\right\}, \tag{57a}$$

$$\mathsf{X}(\tau,w) \equiv \frac{k}{\sqrt{k\mathcal{K}}}\,\frac{[\zeta^2(w) - k]\tau + \chi(w)}{\zeta(w)}. \tag{57b}$$

For $k = 0$, we obtain

$$\mathsf{T}(\tau,w) = \frac{1}{\mathcal{K}}\int_w \left\{\frac{\chi^2(u)}{\zeta^3(u)}\frac{\mathrm{d}}{\mathrm{d}u}\chi(u) - \frac{\chi(u)[\chi^2(u) - \mathcal{K}]}{\zeta^4(u)}\frac{\mathrm{d}}{\mathrm{d}u}\zeta(u)\right\}\mathrm{d}u + \frac{1}{\mathcal{K}}\left\{\frac{1}{3}\zeta^3(w)\tau^3 + \zeta(w)\chi(w)\tau^2 + \left[\frac{\chi^2(w) - \mathcal{K}}{\zeta(w)}\right]\tau\right\}. \tag{58}$$

These transformations [Eqs. (56)–(58)] are extremely similar to the ones derived in the preceding section. Just as before, there are special issues with the $k\mathcal{K} < 0$ case that can be dealt with using the identity (51); but we defer such a discussion as it does not add much to what we have established.

In conclusion, we have succeeded in finding a coordinate transformation from the TBH to FSW metrics. Since we have already found a transformation from TBH to LMW, this allows us to also conclude that a coordinate transformation between the FSW and LMW metrics exists as well.

C. Comment: the generalized Birkhoff theorem

Before moving on, we would like to make a comment about how the equivalence of the LMW, FSW, and TBH metrics relates to the issue of a generalized version of the Birkhoff theorem. Both the LMW and FSW *Ansätze* are of the general form

$$\mathrm{d}s^2 = A^2(t,\ell)\,\mathrm{d}t^2 - B^2(t,\ell)\,\mathrm{d}\sigma^2_{(k,3)} - C^2(t,\ell)\,\mathrm{d}\ell^2. \tag{59}$$

To this line element, we can apply the coordinate transformation

$$R = B(t,\ell) \tag{60}$$

to obtain

$$ds^2 = P^2(t,R)\,dt^2 - R^2\,d\sigma^2_{(k,3)} - 2N(t,R)\,dt\,dR - Q^2(t,R)\,dR^2. \tag{61}$$

Here, P, Q, and N are related to the original metric functions A, B, and C, but their precise form is irrelevant. Then, we apply the diffeomorphism

$$dt = M(T,R)\,dT + \frac{N(t,R)}{P^2(t,R)}\,dR, \tag{62}$$

where $M(T,R)$ is an integrating factor that should satisfy

$$\frac{1}{M}\frac{\partial M}{\partial R} = \frac{\partial}{\partial t}\frac{N}{P^2}, \tag{63}$$

in order to ensure that dt is a perfect differential. In these coordinates, the line element is

$$ds^2 = f(T,R)\,dT^2 - g(T,R)\,dR^2 - R^2\,d\sigma^2_{(k,3)}. \tag{64}$$

Again, f and g are determined by the original metric functions and the integrating factor. This structure is strongly reminiscent of the general spherically symmetric metric from four-dimensional relativity. The only difference is that the line element on a unit 2-sphere $d\Omega^2$ has been replaced by $d\sigma^2_{(k,3)}$. In the four-dimensional case, Birkhoff's theorem tells us that the only solution to the vacuum field equations with the general spherically symmetric line element is the Schwarzschild metric. The theorem has been extended to the multidimensional case by Bronnikov and Melnikov,[16] who showed that the five-dimensional vacuum solution with line element (64) is unique and given by the TBH metric. So, in retrospect it is perhaps apparent that the LMW, FSW, and TBH solutions are equivalent—any five-dimensional vacuum solution that can be cast in the form of (59) must be isometric to the TBH metric. We conclude by noting that this type of argument extends to the case of five-dimensional Einstein spaces as well, because another variation of Birkhoff's theorem derived by Bronnikov and Melnikov is applicable. That is, if there is a cosmological constant in the bulk—as in the popular Randall and Sundrum braneworld models—a metric solution of the form (59) will be equivalent to a deSitter or anti-deSitter TBH manifold. For example, the "wavelike" solutions sourced by a cosmological constant found by Ponce de Leon[17] should be isometric to five-dimensional Schwarzschild–AdS black holes.

V. PENROSE–CARTER DIAGRAMS OF FLRW MODELS EMBEDDED IN THE LIU–MASHHOON–WESSON METRIC

We have now established that the LMW, FSW, and TBH solutions of the vacuum field equations are mutually isometric. This means that they each correspond to coordinate patches on the same five-dimensional manifold. Now, it is well known that the familiar Schwarzschild solution in four dimensions only covers a portion of what is known as the extended Schwarzschild manifold.[18] It stands to reason that if there is a Killing horizon in the TBH metric, then the (T,R) coordinates will also only cover part of some extended manifold M. This raises the question: what portion of the extended manifold M is covered by the (t,ℓ) or (τ,w) coordinates? This is interesting because it is directly related to the issue of what portion of M is spanned by the universes embedded on the Σ_ℓ and Σ_w hypersurfaces.

We do not propose to answer these questions for all possible situations because there are a wide variety of choices of free parameters. We will instead concentrate on one particular problem: namely, the manner in which the Liu–Mashhoon–Wesson coordinates cover the extended manifold M when $k=+1$, $\mathcal{K}>0$, and for specific choices of μ and ν. The restriction to spherical S_3 submanifolds means that the maximal extension of the (T,R) coordinate patch proceeds analogously to the four-dimensional Kruskal construction. The calculation can be straightforwardly generalized to the Fukui–Seahra–Wesson coordinates if desired.

We first need to find the five-dimensional generalization of Kruskal–Szekeres coordinates for the $k=+1$ TBH metric. (See Ref. 19 for background information about the four-dimensional formalism.) Let us apply the following transformations to the metric (33):

$$R_*=R+\frac{1}{2}m\ln\left|\frac{R-m}{R+m}\right|,\quad u=T-R_*,\quad v=T+R_*, \tag{65}$$

where we have defined $\mathcal{K}\equiv m^2$ such that the event horizon is at $R=m$. We then obtain

$$\mathrm{d}s^2_{\mathrm{BH}}=\operatorname{sgn}h(R)\,\frac{(R^2+m^2)e^{-2R/m}}{R^2}e^{-u/m}e^{v/m}\,\mathrm{d}u\,\mathrm{d}v-R^2\,\mathrm{d}\Omega_3^2. \tag{66}$$

Here, we have changed the ''TBH'' label to ''BH'' to stress that we are dealing with an ordinary black hole with spherical symmetry. This metric is singularity free at $R=m$. The next transformation is given by

$$\tilde{U}=\mp\operatorname{sgn}h(R)\,e^{-u/m},\quad \tilde{V}=\pm e^{v/m}, \tag{67}$$

which puts the metric in the form

$$\mathrm{d}s^2_{\mathrm{BH}}=m^2\left(1+\frac{m^2}{R^2}\right)e^{-2R/m}\,\mathrm{d}\tilde{U}\,\mathrm{d}\tilde{V}-R^2\,\mathrm{d}\Omega_3^2. \tag{68}$$

This is very similar to the four-dimensional Kruskal–Szekeres coordinate patch on the Schwarzschild manifold. The aggregate coordinate transformation from (T,R) to $(\tilde{U},\tilde{V})$ is given by

$$\tilde{U}=\mp\operatorname{sgn}h(R)\,e^{-T/m}e^{R/m}\sqrt{\left|\frac{R-m}{R+m}\right|}, \tag{69a}$$

$$\tilde{V}=\pm e^{T/m}e^{R/m}\sqrt{\left|\frac{R-m}{R+m}\right|}. \tag{69b}$$

From these, it is easy to see that the horizon corresponds to $\tilde{U}\tilde{V}=0$. Now, what are we to make of the sign ambiguity in these coordinate transformations? Recall that in four dimensions, the extended Schwarzschild manifold involves two copies of the ordinary Schwarzschild space–time interior and exterior to the horizon. It is clear that something analogous is happening here: the mapping $(T,R)\to(\tilde{U},\tilde{V})$ is double valued because the original (T,R) coordinates can correspond to one of two different parts of the extended manifold. This is best illustrated with a Penrose–Carter diagram, which is given in Fig. 1. As is the usual practice, to obtain such a diagram we ''compactify'' the $(\tilde{U},\tilde{V})$ coordinates by introducing

$$U=\frac{2}{\pi}\arctan\tilde{U},\quad V=\frac{2}{\pi}\arctan\tilde{V}. \tag{70}$$

Figure 1 has all of the usual properties: null geodesics travel on 45° lines, the horizons appear at $U=0$ or $V=0$, the singularities show up as horizontal features at the top and bottom, and each point in the two-dimensional plot represents a 3-sphere. Also, in quadrant I the T coordinate increases from bottom to top, while the reverse is true in quadrant II. We see that the top sign in the coordinate transformation (69) maps (T,R) into regions I or III of the extended manifold where $V>0$, while the lower sign defines a mapping into II or IV where $V<0$.

Having obtained the transformation to Kruskal–Szekeres coordinates, we can now plot the trajectory of the Σ_ℓ hypersurfaces through the extended manifold by using (45) and (48) in (69) to find $U(t,\ell)$ and $V(t,\ell)$. But there is one wrinkle: we need to flip the sign of the (T,R)

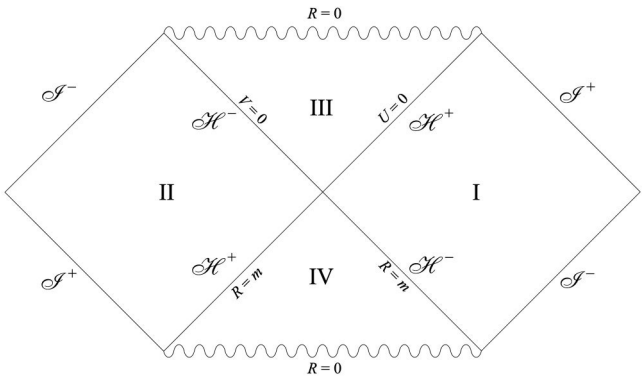

FIG. 1. Penrose–Carter diagram of a five-dimensional black hole manifold.

$\rightarrow(U,V)$ transformation whenever the path crosses the $V=0$ line, which is not hard to accomplish numerically. In Fig. 2 we present Penrose–Carter embedding diagrams of Σ_ℓ and Σ_t hypersurfaces associated with the LMW metric for the following choices of parameters and free functions:

$$m=\tfrac{1}{2}, \quad \mu(t)=\cot t, \quad \nu(t)=\frac{\sqrt{3}}{2}. \tag{71}$$

This gives

$$a(t,\ell)=\sqrt{\left(\ell\,\csc t+\frac{\sqrt{3}}{2}\sin t\right)^2+\tfrac{1}{4}\,\sin^2 t}. \tag{72}$$

Our choices imply that it is sensible to restrict $t\in(0,\pi)$. For $\ell\neq 0$, the cosmologies embedded on Σ_ℓ do *not* undergo a big bang or big crunch and $a\rightarrow\infty$ as $t\rightarrow 0$ or π. The $\ell=0$ cosmology simply has $a(t,0)=\sin t$. That is, we have a recollapsing model. The induced metric for that hypersurface is

$$\mathrm{d}s^2_{(\Sigma_0)}=\sin^2 t\,(\mathrm{d}t^2-\mathrm{d}\Omega_3^2), \tag{73}$$

that of a closed radiation-dominated universe.

In Fig. 2(a) we show the Σ_ℓ hypersurfaces of this model in a Penrose–Carter diagram. In this plot it is easy to visually determine where each trajectory begins when $t=0$, but because of the scale it is difficult to note precisely where they end up at when $t=\pi$. By careful analysis of the numeric results, we have determined the following facts: The $\ell=0$ trajectory emanates from the middle of the singularity in the white hole region IV at $t=0$ and terminates on the future singularity in region III at $t=\pi$. The surfaces with $\ell>0$ begin at $\mathcal{I}^+$ in I and terminate on $\mathcal{I}^-$ in the same region. The models with $\ell<0$ all begin on $\mathcal{I}^-$ and terminate on $\mathcal{I}^+$ in region II. We mention in passing that this plot bears some qualitative resemblance to the figures of Mukohyama *et al.*,[20] who showed the equivalence of a known solution of the five-dimensional field equations with a cosmological constant and the topological Schwarzschild–AdS black hole in the context of brane-world scenarios; but many details are significantly different.

One of the most striking features of this plot is the cusps present in the majority of the Σ_ℓ curves. These sharp corners suggest some sort of singularity in the embedding at their location. We can search for the singularity by examining scalars formed from the extrinsic curvature of the Σ_ℓ 4-surfaces. Let us consider

$$h^{\alpha\beta}K_{\alpha\beta}=\frac{a_{,t\ell}}{a_{,t}}+3\,\frac{a_{,\ell}}{a}. \tag{74}$$

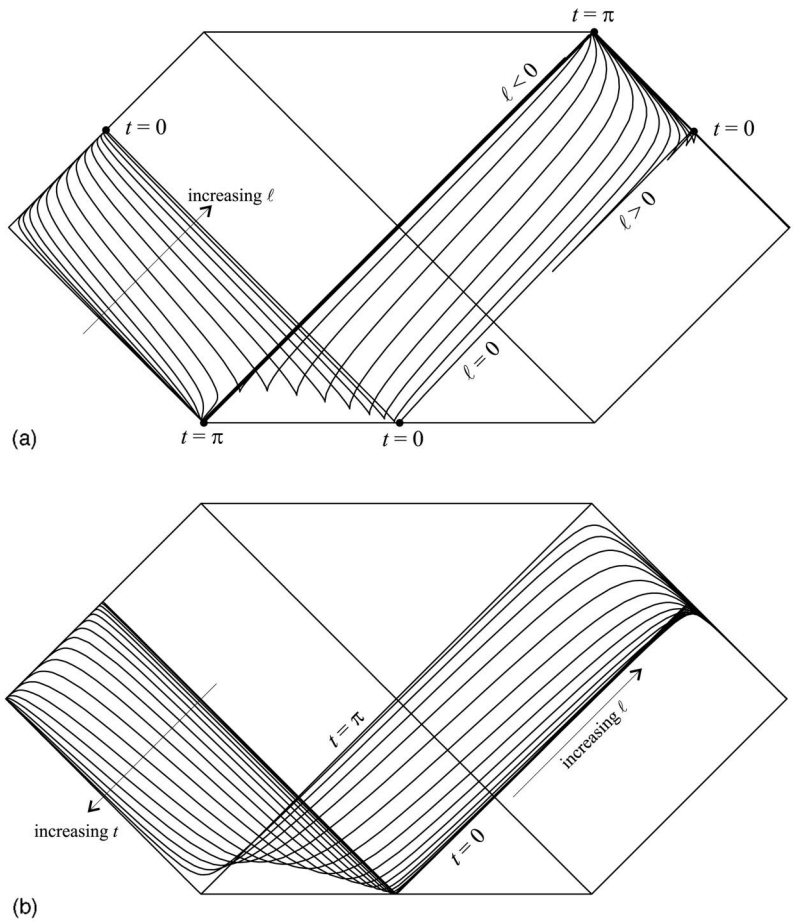

FIG. 2. (a) Σ_ℓ hypersurfaces of the LMW metric for the special choices (71). Each point in the Penrose–Carter diagram represents a 3-sphere. We restrict $t\in(0,\pi)$. The corresponding values of ℓ range from ~ -2.2 to 0.3 in equal logarithmic intervals. Note that even though the two points marked $t=\pi$ appear to be on the $U=0$ line, they are actually located on $\mathcal{I}^+$ in region II and $R=0$ in region III. This can be explicitly confirmed by greatly enlarging the scale of the plot. (b) Isochrones of the LMW metric for the special choices (71). We restrict $\ell\in(-5,5)$. The corresponding values of t range from 0 to $\sim\pi/2$ in equal logarithmic intervals. A portion of the $t=\pi$ surface is also shown, which appears to be coincident with $\mathcal{H}^+$. However, in reality it is only parallel to $U=0$, but the finite separation between the two surfaces is impossible to discern without greatly enlarging the scale of the plot.

One can confirm directly that this diverges whenever $a_{,t}=0$ and $a_{,t\ell}\neq 0$. At such positions, we find sharp corners in the Σ_ℓ hypersurfaces. This makes it clear that if we wanted to use the LMW coordinates as a patch on the extended five-dimensional black hole manifold, we would have to restrict t to lie in an interval bounded by times defined by the turning points of a. This is in total concurrence with the analysis of singularities in the intrinsic 4-geometry performed in Sec. II A—the cusps correspond to singularities in the induced metric on Σ_ℓ. Actually we have confirmed that the curves with cusps generally have two curvature anomalies, but those additional features tend to get compressed into a region too small to resolve in Fig. 2(a). What is also interesting about these plots is how the LMW metric occupies a fair bit of territory in M (some of the Σ_ℓ hypersurfaces span regions I, II, and IV). Like the Kruskal–Szekeres coordinates, the LMW patch is regular across the horizon(s).

The exact portion of the extended manifold spanned by our model is a little clearer in Fig. 2(b). In this plot, we show the Σ_t spacelike hypersurfaces—or isochrones—of the LMW metric. These stretch from spacelike infinity in region II to a point on $\mathcal{I}^+$ in region I. The LMW time t is

seen to run from bottom to top in I and *vice versa* in II. We also see clearly that there is a portion of the white hole region IV that is not covered by the LMW metric with $t \in (0,\pi)$. The $t=\pi$ line appears to coincide with $U=0$, but is in actuality displaced slightly to the left. Notice that the area bounded by the $t=\pi/2$ and $t=\pi$ curves is relatively small, from which it follows that the portions of the Σ_ℓ surfaces with $\pi/2 \lesssim t \lesssim \pi$ tend to occupy an extremely compressed portion of the embedding diagram.

In summary, we have presented embedding diagrams for the Σ_ℓ and Σ_t hypersurfaces associated with the LMW metric in the Penrose–Carter graphical representation of the extended five-dimensional black hole manifold. This partially answers the question of which portion of M is occupied by the LMW metric. However, the calculation was for specific choices of μ, ν, and $\mathcal{K}$. We have no doubt that more general conclusions are attainable, but that is a subject for a different venue.

VI. SUMMARY AND DISCUSSION

In this paper, we introduced two solutions of the five-dimensional vacuum field equations, the Liu–Mashhoon–Wesson and Fukui–Seahra–Wesson metrics, in Secs. II A and II B, respectively. We showed how both of these embed certain types of FLRW models and studied the coordinate invariant properties of the associated 5-manifolds. We found that both solutions had linelike curvature singularities and Killing horizons, and that their Kretschmann scalars were virtually identical. These coincidences prompted us to suspect that the LMW and FSW metrics are actually equivalent, and that they are also isometric to the five-dimensional topological black hole metric introduced in Sec. III. This was confirmed explicitly in Sec. IV, where transformations from Schwarzschild-type to LMW and FSW coordinates were derived. The strategy employed in that section was to transform the TBH line element into the form of the LMW and FSW metric *Ansätze*, which resulted in two sets of solvable PDEs. Therefore, those calculations comprise independent derivations of the LMW and FSW metrics. In Sec. IV C, we showed how the relationship between the LMW, FSW, and TBH metrics was a consequence of a generalized version of Birkhoff's theorem. Finally, in Sec. V we performed a Kruskal extension of the five-dimensional black hole manifold and plotted the Σ_ℓ and Σ_t hypersurfaces of the LMW metric in a Penrose–Carter diagram for certain choices of μ, ν, and $\mathcal{K}$.

Obviously, our main result is that the LMW and FSW metrics are nontrivial coordinate patches on five-dimensional black hole manifolds. We saw explicitly that the LMW coordinates could cover multiple quadrants of the maximally symmetric manifold, and that they were regular across the event horizon. This puts them in the same category as the Eddington–Finkelstein (EF) or Painlevé–Gullstrand (PG) coordinates associated with four-dimensional Schwarzschild black holes,[21] which are also horizon piercing patches that do not involve implicit functions, such as $R=R(U,V)$ in the Kruskal–Szekeres covering. The LMW coordinates differ from the EF or PG patches in that they are five dimensional and orthogonal. All of these features make them an attractive tool for the study of black hole physics in five dimensions. In particular, they provide ''rest-frame'' coordinates for embedded four-dimensional universes. That is, in both the LMW and FSW coordinates, universes are defined simply as 4-surfaces comoving in ℓ or w. And unlike standard Schwarzschild-type coordinates, the LMW or FSW 5-metrics are regular as the universe crosses the black hole horizon(s). Such coordinates may have some utility in the study of quantized braneworld models, where the bad behavior of coordinates across horizons apparently results in a complicated canonical phase-space description of the brane's dynamics.[22]

Finally, we discuss the temptation to generalize these coordinates to other types of black holes and different dimensions. One could easily imagine repeating the manipulations of Sec. IV for different choices of $h(R)$, which could be selected to correspond to any spherically symmetric black hole in any dimension. However, a difficulty arises when one tries to integrate equations like

$$\mathcal{R}_{,\ell} = \pm \sqrt{h(\mathcal{R}) + \mu^2(t)} \tag{75}$$

to obtain $\mathcal{R}=\mathcal{R}(t,\ell)$ explicitly. It turns out that this in not necessarily easy to do if $h(\mathcal{R})\neq k-\mathcal{K}/\mathcal{R}^2$. For example, if h corresponds to an N-dimensional topological black hole [i.e., $h(\mathcal{R})=k-\mathcal{K}/\mathcal{R}^{N-3}$] we obtain complicated implicit definitions of $\mathcal{R}$ involving generalized hypergeometric functions. For even $N=4$, it is unclear how to invert such an equation to find $\mathcal{R}=\mathcal{R}(t,\ell)$ explicitly. So it seems that the five-dimensional case is somewhat special. However, we do not preclude the possibility that there are other special cases out there, that our procedure could be improved upon, or that one could find suitable coordinates by direct assault on the N-dimensional field equations. Such issues are best addressed by future work.

ACKNOWLEDGMENTS

We would like to thank T. Liko for useful discussions, and NSERC and OGS for financial support.

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The second variation of a null geodesic

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(Received 13 July 2003; accepted 2 September 2003)

Confined to the second derivative of the variation of a null geodesic, the proper acceleration of the timelike curves obtained from the variation goes infinity as they approach the null geodesic except that the variation vector is a generalized Jacobi field on the null geodesic and the second variation β_2 is constant on the null geodesic. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623931]

It is well-known that an observer in ''hyperbolic'' motion in Minkowski space–time has a constant proper acceleration (the magnitude of the four-acceleration). The proper acceleration of the observers in the family approaches infinity as we consider those observers in the family whose world lines approach the null curve.[1] This is a well-known fact first written by Rindler in his book.[1] The main purpose of an earlier paper[2] is to generalize this result to curved space–times to a future-complete null geodesic, that is, given a null geodesic $\gamma_0(\lambda)$, up to the first derivative of the variation, the variation of $\gamma_0(\lambda)$ will give a smooth one-parameter family of timelike curves whose acceleration approaches infinity as the timelike curves go to the null geodesic. There are many cases such that only the second variation is not zero (with the first variation zero), for example, with end points fixed, the variation of a null geodesic with a pair of conjugate point between the end points. This article mainly extends the result to similar cases and gives the condition that the acceleration of the timelike curves in the family goes to infinity as they approach the null geodesic.

We therefore suppose that $\gamma_0(\lambda)$ is a null geodesic. Precisely, we have the following definition of the variation of $\gamma_0(\lambda)$:

Let (M,g_{ab}) be a four-dimensional curved space–time and $\gamma_0: [0,\lambda_q]\to M$ be a null geodesic, which will later be denoted by $\gamma_0(\lambda)$ with λ its affine parameter, and with $p,\ q\in\gamma_0(\lambda)$. We define a variation of γ_0 to be a C^1 map[3] $\sigma:(-\varepsilon,\varepsilon)\times[0,\lambda_q]\to M$ such that the following hold.

(1) $\sigma(0,\lambda)=\gamma_0(\lambda)$.
(2) There is a subdivision $0=\lambda_1<\lambda_2<\cdots<\lambda_n=\lambda_q$ of $[0,\lambda_q]$ such that σ is C^3 on each $[0,\varepsilon)\times[\lambda_i,\lambda_{i+1}]$.
(3) For each constant $u\in(-\varepsilon,\varepsilon)$ and $u\neq 0$, $\sigma(u,\lambda)$ is a timelike curve and is represented by $\gamma_u(\lambda)$.
(4) The first derivative of the variation is zero. (Later, we will explain what is meant by the first derivative of the variation is zero.)

Denote by $(\partial/\partial\lambda)^a_u\equiv v^a_u$ the tangent vector to the curve $\gamma_u(\lambda)$. Then $(\partial/\partial\lambda)^a_0\equiv v^a_0$ satisfies the null geodesic equation:

$$v^b_0\nabla_b v^a_0=0, \tag{1}$$

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where ∇_a is the unique derivative operator associated with g_{ab}, i.e., $\nabla_a g_{bc}=0$. Let $(\partial/\partial u)^a$ be the tangent vector to the curve $\sigma(u,\lambda)$ with $\lambda=\text{const}$, and define the variation vector field Z^a on $\gamma_0(\lambda)$ by

$$Z^a=\left(\frac{\partial}{\partial u}\right)^a\Bigg|_{u=0}. \tag{2}$$

Then it is not difficult to see that the Lie derivative of $(\partial/\partial u)^a$ with respect to $(\partial/\partial\lambda)^a$ vanishes,[3] i.e.,

$$L_{\partial/\partial\lambda}\left(\frac{\partial}{\partial u}\right)^a=0,$$

that is,

$$v_u^b\nabla_b\left(\frac{\partial}{\partial u}\right)^a=\left(\frac{\partial}{\partial u}\right)^b\nabla_b v_u^a. \tag{3}$$

If we denote $g_{ab}v_u^a v_u^b$ by $-\alpha_u^2$, that is,

$$-\alpha_u^2=g_{ab}v_u^a v_u^b, \tag{4}$$

and decompose $-\alpha_u^2$ into Taylor series,

$$-\alpha_u^2=g_{ab}v_u^a v_u^b=-\alpha_0^2+\beta_1 u+\beta_2 u^2+O(u^3), \tag{5}$$

where

$$\alpha_0^2=g_{ab}v_0^a v_0^b=0. \tag{6}$$

From the requirement (4) of the variation, the first derivative of the variation is zero, that is

$$\beta_1=\frac{\partial(-\alpha^2)}{\partial u}\Bigg|_{u=0}=0. \tag{7}$$

There are many cases with $\beta_1=\partial(-\alpha^2)/\partial u\,|_{u=0}=0$: (1) the variation of a null geodesic with end points p,q fixed when there is a point $r\in(p,q)$ conjugate to p along the null geodesic. (2) When a null geodesic γ_0, orthogonal to a spacelike two-surface φ, is from φ to q with a point $r\in(\varphi,q)$ conjugate to φ along $\gamma_0(\lambda)$, there is a variation of the null geodesic from φ to q. These variations belong to the case.

From Eqs. (7) and (3), it is easy to see

$$\begin{aligned}\frac{\partial(-\alpha_u^2)}{\partial u}&=\left(\frac{\partial}{\partial u}\right)^c\nabla_c[g_{ab}v_u^a v_u^b]=2g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^c\nabla_c v_u^b=2g_{ab}v_u^a v_u^c\nabla_c\left(\frac{\partial}{\partial u}\right)^b\\&=2v_u^c\nabla_c\left[g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right]-2g_{ab}\left(\frac{\partial}{\partial u}\right)^b v_u^c\nabla_c v_u^a\\&=2\frac{\partial}{\partial\lambda}\left[g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right]-2g_{ab}\left(\frac{\partial}{\partial u}\right)^b v_u^c\nabla_c v_u^a,\end{aligned} \tag{8}$$

therefore, with Eq. (1), one gets

$$\beta_1=\left.\frac{\partial(-\alpha_u^2)}{\partial u}\right|_{u=0}=2\frac{\partial}{\partial\lambda}[g_{ab}v_0^aZ^b]=2\frac{dh}{d\lambda}. \tag{9}$$

$\beta_1=0$ induces that

$$h=g_{ab}v_0^aZ^b \tag{10}$$

is constant along the null geodesic $\gamma_0(\lambda)$.

Therefore, one gets

$$-\alpha_u^2=g_{ab}v_u^av_u^b=\beta_2u^2+O(u^3). \tag{11}$$

$\beta_2=\frac{1}{2}\partial^2(-\alpha_u^2)/\partial u^2|_{u=0}$ follows from Eq. (8) (see detail in Ref. 3):

$$\begin{aligned}\frac{1}{2}\frac{\partial^2(-\alpha_u^2)}{\partial u^2}&=\frac{\partial^2}{\partial\lambda\,\partial u}\left[g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right]-\left(\frac{\partial}{\partial u}\right)^d\nabla_d\left[g_{ab}\left(\frac{\partial}{\partial u}\right)^bv_u^c\nabla_cv_u^a\right]\\&=\frac{\partial^2}{\partial\lambda\,\partial u}\left[g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right]-\left[g_{ab}v_u^c\nabla_cv_u^a\left(\frac{\partial}{\partial u}\right)^d\nabla_d\left(\frac{\partial}{\partial u}\right)^b\right]\\&\quad-\left[\left(\frac{\partial}{\partial u}\right)^a\left(\frac{\partial}{\partial u}\right)^d\nabla_d(v_u^c\nabla_cv_{ua})\right].\end{aligned}$$

The term $(\partial/\partial u)^d\nabla_d(v_u^c\nabla_cv_{ua})$ in the third part of the above equation is simplified:

$$\begin{aligned}\left(\frac{\partial}{\partial u}\right)^d\nabla_d(v_u^c\nabla_cv_{ua})&=\left(\left(\frac{\partial}{\partial u}\right)^d\nabla_dv_u^c\right)\nabla_cv_{ua}+v_u^c\left(\frac{\partial}{\partial u}\right)^d\nabla_d\nabla_cv_{ua}\\&=\left(\left(\frac{\partial}{\partial u}\right)^d\nabla_dv_u^c\right)\nabla_cv_{ua}+v_u^c\left(\frac{\partial}{\partial u}\right)^d\nabla_c\nabla_dv_{ua}+R_{dcae}v_u^cv_u^e\left(\frac{\partial}{\partial u}\right)^d\\&=\left(\left(\frac{\partial}{\partial u}\right)^d\nabla_dv_u^c\right)\nabla_cv_{ua}+v_u^c\nabla_c\left[\left(\frac{\partial}{\partial u}\right)^d\nabla_dv_{ua}\right]-\left(v_u^c\nabla_c\left(\frac{\partial}{\partial u}\right)^d\right)\nabla_dv_{ua}\\&\quad+R_{dcae}v_u^cv_u^e\left(\frac{\partial}{\partial u}\right)^d\\&=v_u^d\nabla_d\left(v_u^c\nabla_c\left(\frac{\partial}{\partial u}\right)_a\right)+R_{dcae}v_u^cv_u^e\left(\frac{\partial}{\partial u}\right)^d,\end{aligned}$$

that is

$$\left(\frac{\partial}{\partial u}\right)^d\nabla_d\tilde{A}_{ua}=\left(\frac{\partial}{\partial u}\right)^d\nabla_d(v_u^c\nabla_cv_{ua})=v_u^d\nabla_d\left(v_u^c\nabla_c\left(\frac{\partial}{\partial u}\right)_a\right)+R_{dcae}v_u^cv_u^e\left(\frac{\partial}{\partial u}\right)^d, \tag{12}$$

where the relation $\nabla_c\nabla_dv_{ua}-\nabla_d\nabla_cv_{ua}=-R_{dcae}v_u^e$ in the second step and Eq. (3) in the fourth step have been used, and $\tilde{A}_{ua}$ is defined by $\tilde{A}_{ua}=v_u^c\nabla_cv_{ua}$, and is different from the proper acceleration of the timelike curve $\gamma_u(\lambda)$ [see the following for the definition of the proper acceleration of $\gamma_u(\lambda)$]. The equation (12) is very important in the later argument. Finally, one gets

$$\begin{aligned}\frac{1}{2}\frac{\partial^2(-\alpha_u^2)}{\partial u^2}&=\frac{\partial^2}{\partial\lambda\,\partial u}\left[g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right]-\left[g_{ab}(v_u^c\nabla_cv_u^a)\left(\frac{\partial}{\partial u}\right)^d\nabla_d\left(\frac{\partial}{\partial u}\right)^b\right]\\&\quad-\left[\left(\frac{\partial}{\partial u}\right)^av_u^d\nabla_d\left(v_u^c\nabla_c\left(\frac{\partial}{\partial u}\right)_a\right)+R_{dcae}v_u^cv_u^e\left(\frac{\partial}{\partial u}\right)^a\left(\frac{\partial}{\partial u}\right)^d\right],\end{aligned} \tag{13}$$

so

$$\beta_2=\left[\frac{1}{2}\frac{\partial^2(-\alpha_u^2)}{\partial u^2}\right]_{u=0}=\left[\frac{\partial^2}{\partial\lambda\,\partial u}\left(g_{ab}v_u^a\left(\frac{\partial}{\partial u}\right)^b\right)\right]_{u=0}-[Z^a v_0^d\nabla_d(v_0^c\nabla_c Z_a)+R_{dcae}v_0^c v_0^e Z^d Z^a], \tag{14}$$

where Eq. (1) has been used.

The parameter λ of the timelike curve, $\gamma_u(\lambda)$, defined above is not, in general, the proper time of the curve. If one reparametrizes the curve $\gamma_u(\lambda)$ by its proper time τ, i.e., the parameter satisfying

$$g_{ab}\left(\frac{\partial}{\partial\tau}\right)_u^a\left(\frac{\partial}{\partial\tau}\right)_u^b=-1,$$

then

$$\left(\frac{\partial}{\partial\tau}\right)^a=\left(\frac{d\lambda}{d\tau}\right)\left(\frac{\partial}{\partial\lambda}\right)_u^a=\left(\frac{d\lambda}{d\tau}\right)v_u^a.$$

With Eq. (4), one has

$$\left(\frac{d\lambda}{d\tau}\right)^2=\frac{1}{\alpha_u^2}. \tag{15}$$

The four-acceleration of the timelike curve γ_u is defined as

$$A^a=\left(\frac{\partial}{\partial\tau}\right)^b\nabla_b\left(\frac{\partial}{\partial\tau}\right)^a=\frac{d\lambda}{d\tau}v_u^b\nabla_b\left(\frac{d\lambda}{d\tau}v_u^a\right)=\left(\frac{1}{\alpha_u^2}\right)\tilde{A}_u^a-\frac{1}{2\alpha_u^4}v_u^a v_u^b\nabla_b\alpha_u^2, \tag{16}$$

or one writes the above equation as

$$\tilde{A}_u^a=\alpha_u^2A^a+\frac{1}{2\alpha_u^2}v_u^a v_u^b\nabla_b\alpha_u^2. \tag{17}$$

Select the pseudo-orthogonal basis E_1^a, E_2^a, E_3^a, E_4^a that is parallelly transported along the null geodesic $\gamma_0(\lambda)$ with

$$\begin{gathered}E_4^a=v_0^a,\ \ g_{ab}E_i^aE_i^b=1,\ \ i=1,2;\ \ g_{ab}E_i^aE_i^b=0,\ \ i=3,4;\\ g_{ab}E_i^aE_j^b=0,\ \ i=1,2,j=3,4\ \ g_{ab}E_3^aE_4^b=-1,\ \ g_{ab}E_1^aE_2^b=0.\end{gathered} \tag{18}$$

With Eq. (10), then it is easy to see

$$Z^a=Z^1E_1^a+Z^2E_2^a+hE_3^a+Z^4E_4^a. \tag{19}$$

For constant λ, the above basis is constant vectors, they can be equally parallelly transported along the curve $\sigma(u,\lambda)$, $\lambda=$const, which are denoted by $E_i^a(u,\lambda)$, $i=1,2,3,4$, and at $u=0$, $E_i^a(0,\lambda)=E_i^a$. One can rewrite the vector $\tilde{A}_u^a$ as

$$\tilde{A}_u^a=\sum_{i=1}^4\tilde{A}_u^iE_i^a(u,\lambda),$$

and

$$\left[\left(\frac{\partial}{\partial u}\right)^d \nabla_d \tilde{A}_u^a\right]_{u=0} = \sum_{i=1}^4 \left[E_i^a(u,\lambda)\left(\frac{d\tilde{A}_u^i}{du}\right)\right]_{u=0} = \sum_{i=1}^4 E_i^a\left(\frac{d\tilde{A}_u^i}{du}\right)_{u=0},$$

with Eq. (12), and taking the limit $u\to 0$, then

$$\sum_{i=1}^4 E_i^a\left(\frac{d\tilde{A}_u^i}{du}\right)_{u=0} = v_0^d \nabla_d (v_0^c \nabla_c Z^a) + g^{ab} R_{dcbe} v_0^c v_0^e Z^d. \tag{20}$$

Denote by $\overline{C}^a$ the term $v_0^d \nabla_d (v_0^c \nabla_c Z^a) + g_{ab} R_{dcbe} v_0^c v_0^e Z^d$, which is $\overline{C}^a = \Sigma_{i=1}^4 \overline{C}^i E_i^a$. Using Eqs. (10) and (19), and the the antisymmetry property of the Riemann tensor R_{abcd}, that is, the second term on the left side of Eq. (20) is contracted to zero by the vector v_{0a}, it is not difficult to see that Eq. (20) implies $(d\tilde{A}_u^3/du)_{u=0} = \overline{C}^3 = 0$, that is,

$$\left[\left(\frac{\partial}{\partial u}\right)^d \nabla_d \tilde{A}_u^a\right]_{u=0} = \left(\frac{d\tilde{A}_u^1}{du}\right)_{u=0} E_1^a + \left(\frac{d\tilde{A}_u^2}{du}\right)_{u=0} E_2^a + \left(\frac{d\tilde{A}_u^4}{du}\right)_{u=0} E_4^a \tag{21}$$

$$= \overline{C}^1 E_1^a + \overline{C}^2 E_2^a + \overline{C}^4 E_4^a. \tag{22}$$

The detailed form of $(d\tilde{A}_u^i/du)_{u=0} = \overline{C}^i$, $i = 1,2,4$, is determined by Eq. (20).

First one assumes $\overline{C}^1\overline{C}^1 + \overline{C}^2\overline{C}^2 > 0$, which means

$$\tilde{A}_u^1 = u\overline{C}^1 + 0(u^2),\ \ \tilde{A}_u^2 = u\overline{C}^2 + 0(u^2),\ \ \tilde{A}_u^4 = u\overline{C}^4 + O(u^2), \tag{23}$$

$$g_{ab}\tilde{A}_u^a \tilde{A}_u^b = u^2(\overline{C}^1\overline{C}^1 + \overline{C}^2\overline{C}^2) + 0(u^3),\ \ \overline{C}^1\overline{C}^1 + \overline{C}^2\overline{C}^2 > 0. \tag{24}$$

Now, by Eqs. (17) and (11), calculate

$$g_{ab}\tilde{A}_u^a \tilde{A}_u^b = \alpha_u^4 A^a A_a - \frac{1}{4}\alpha_u^2\left[\frac{1}{\alpha_u^2}\frac{\partial \alpha_u^2}{\partial \lambda}\right]^2 \tag{25}$$

$$= \beta_2^2 A^a A_a u^4 + \frac{1}{8\beta_2}\left[\frac{d\beta_2}{d\lambda}\right]^2 u^2 + O(u^3). \tag{26}$$

From Eq. (11), one gets $\beta_2 < 0$. Unless $A^2 = A^a A_a$ approaches infinity, the equations (24) and (26) are not compatible. Therefore, one gets that under the condition $\overline{C}^1\overline{C}^1 + \overline{C}^2\overline{C}^2 > 0$, the magnitude of the proper acceleration of the timelike curves in the family goes to infinity as $u\to 0$.

Second, one supposes that $\overline{C}^1\overline{C}^1 + \overline{C}^2\overline{C}^2 = 0$ and $\overline{C}^4 \neq 0$ is retained generally on the range $[0,\lambda]$. The assumption induces

$$\begin{gathered}\tilde{A}_u^1 = 0(u^2),\\ \tilde{A}_u^2 = 0(u^2),\\ \tilde{A}_u^4 = u\overline{C}^4 + 0(u^2),\\ g_{ab}\tilde{A}_u^a \tilde{A}_u^b = 0 + 0(u^4).\end{gathered} \tag{27}$$

Equation (27) means vector $\tilde{A}_u^a$ is null up to u^3. By Eq. (26), there are only two possibilities: one is

$$\frac{d\beta_2}{d\lambda} \neq 0, \tag{28}$$

the other is

$$\frac{d\beta_2}{d\lambda} = 0. \tag{29}$$

When the first possibility (28) is selected, it is easy to see

$$\lim_{u\to 0} A \to \infty; \tag{30}$$

while the second possibility (29) is satisfied, Eq. (30) may not be met.

Third, one supposes that $\overline{C^1}=\overline{C^2}=\overline{C^4}=0$ is retained on the range $[0,\lambda]$, which means the variation vector field Z^a is a Jacobi field on the null geodesic $\gamma_0(\lambda)$. The equation (27) is satisfied; the result is the same as in the case $\overline{C^1}=\overline{C^2}=0$ and $\overline{C^4}\neq 0$.

In the second and the third cases, the variation vector Z^a is really the generalized or strict Jacobi field on the null geodesic $\gamma_0(\lambda)$. According to Ref. 3, the generalized Jacobi field J^a on the null geodesic $\gamma_0(\lambda)$ satisfies

$$\frac{d^2J^i}{d\lambda^2} + R^i_{4j4}J^j = 0, \quad i=1,2; \tag{31}$$

where the pseudo-orthogonal basis (18) has been used to write the above equation. The equation (31) only concerns the spacelike components of the vector J^a, and is used to define the conjugate points on the null geodesic.[3] The strict Jacobi field on the null geodesic $\gamma_0(\lambda)$ is defined as[3,4]

$$v_0^d\nabla_d(v_0^c\nabla_c Z^a) + g^{ab}R_{dcbe}v_0^c v_0^e Z^d = 0. \tag{32}$$

In conclusion, when the variation vector field Z^a is not the generalized Jacobi field on the null geodesic γ_0, the timelike curves $\gamma_u(\lambda)$, which come from the variation, have acceleration approaching infinity as $u\to 0$. When the variation vector field Z^a is the generalized Jacobi field on the null geodesic γ_0, there are two possibilities: one is $d\beta_2/d\lambda \neq 0$, which again induces the infinity of the acceleration of the timelike curves $\gamma_u(\lambda)$ as $u\to 0$; the other is $d\beta_2/d\lambda = 0$, only this case makes the acceleration of the timelike curves $\gamma_u(\lambda)$ finite possibly as $u\to 0$.[5]

The following are two applications of the above results:

(1) The null geodesic $\gamma_0(\lambda)$ with a point r in (p,q) conjugate to p along $\gamma_0(\lambda)$. The variation $\sigma(u,\lambda)$ of $\gamma_0(\lambda)$ satisfies the following conditions: $\sigma(u,0)=p$ and $\sigma(u,\lambda_q)=q$, which means the end-points of the variation are fixed, that is, $\gamma_u(\lambda)$, $u\neq 0$ is a timelike curve from p to q. The first variation is zero.[3] In this case, because $\overline{C^1}=\overline{C^2}=0$ in the range $[0,\lambda]$ means that the end-point q is conjugate to the end-point p, which induces that the curves $\gamma_u(\lambda)$, $u\neq 0$ are null geodesics and contradict the assumption of their being timelike. So, $\overline{C^1}=\overline{C^2}=0$ in the range $[0,\lambda]$ can not be retained. The only selection is $\overline{C^1}\,\overline{C^1}+\overline{C^2}\,\overline{C^2}>0$, therefore the acceleration of the curves $\gamma_u(\lambda)$, $u\neq 0$, approaches infinity as $u\to 0$.

In Ref. 3, it is shown in detail that the timelike curves $\gamma_u(\lambda)$, $u\neq 0$, satisfy the requirement $-\alpha_u^2 = g_{ab}v_u^a v_u^b < 0$ at every point on $\gamma_u(\lambda)$, $u\neq 0$, in the range $\lambda\in[0,\lambda_q]$. In the example of Ref. 3 the variation vector Z^a is not the generalized Jacobi field on the null geodesic γ_0, that is, using the above language, $\overline{C^1}\,\overline{C^1}+\overline{C^2}\,\overline{C^2}>0$, so, the acceleration of the time-like curves in the example in the reference[3] goes to infinity as $u\to 0$.

(2) When the null geodesic γ_0, orthogonal to a spacelike two-surface φ, is from φ to q with a point $r\in(\varphi,q)$ conjugate to φ along $\gamma_0(\lambda)$, there will be a variation of $\gamma_0(\lambda)$ which will give a timelike curve from φ to q. The first variation is also zero.[3] Similarly, if the variation field

Z^a is not the generalized Jacobi field, then the acceleration of the curves $\gamma_u(\lambda)$, $u \neq 0$, approaches infinity as $u \to 0$; on the contrary, when Z^a is the generalized Jacobi field, the variation may be the variation of the geodesics $\gamma_u(\lambda)$,[6] which means the curves $\gamma_u(\lambda)$, $u \neq 0$, must be timelike geodesics whose acceleration is zero.

We reinforce the main points again. Under the second derivative of the variation of a null geodesic, there are two results concerning the proper acceleration of the timelike curves obtained from the second variation of the null geodesic:

(1) When the variation field Z^a is not the generalized Jacobi field on the null geodesic, the proper acceleration of the observers in the family approaches infinity as we consider whose world lines approach the null geodesic.
(2) When the variation field Z^a is the generalized Jacobi field on the null geodesic, their proper acceleration approaches infinity as their world lines approach the null geodesic under the condition of the second derivative variation $\beta_2 \neq \text{const}$ in the range $[0,\lambda_q]$; otherwise, their proper acceleration may be finite as their world lines approach the null geodesic.

ACKNOWLEDGMENTS

We are supported by the National Science Foundation of China under Grant No. 10073002.

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Hamiltonian equations in $\mathbb{R}^3$

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(Received 8 April 2003; accepted 18 August 2003)

The Hamiltonian formulation of $N=3$ systems is considered in general. The most general solution of the Jacobi equation in $\mathbb{R}^3$ is proposed. The form of the solution is shown to be valid also in the neighborhood of some irregular points. Compatible Poisson structures and corresponding bi-Hamiltonian systems are also discussed. Hamiltonian structures, the classification of irregular points and the corresponding reduced first order differential equations of several examples are given. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1619204]

I. INTRODUCTION

The Hamiltonian formulation of a system of dynamical equations is important not only in mathematics but also in physics and other branches of natural sciences. They in general describe conserved systems. Among all possible odd dimensional cases, the three dimensional dynamical systems have a unique position. The Jacobi equation in this case reduces to a single scalar equation for three components of the Poisson structure J. Due to this property $N=3$ dynamical systems attracted much research to derive new Hamiltonian systems.[6–12] More recently[1,2] a large class of solutions of the Jacobi equation in $\mathbb{R}^3$ was given. Poisson structures, in all dimensions, were also considered in Ref. 3. In this work, we consider a general solution of the Jacobi equation in $\mathbb{R}^3$. We find the compatible Poisson structures and give the corresponding bi-Hamiltonian systems. We give all explicit examples in a special section and Table I at the end.

Let us give necessary information about the Poisson structures in $\mathbb{R}^3$. A matrix $J=(J_{ij})$, $i,j=1,2,3$, defines a Poisson structure in $\mathbb{R}^3$ if it is skew-symmetric, $J_{ij}=-J_{ji}$, and its entries satisfy the Jacobi equation

$$J^{li}\partial_l J^{jk}+J^{lj}\partial_l J^{ki}+J^{lk}\partial_l J^{ij}=0, \tag{1}$$

where $i,j,k=1,2,3$. Here we use the summation convention, meaning that repeated indices are summed up. Let us introduce the following notations. For matrix J put $J_{12}=u$, $J_{31}=v$, $J_{23}=w$. Then the Jacobi equation (1) takes the form

$$u\partial_1 v-v\partial_1 u+w\partial_2 u-u\partial_2 w+v\partial_3 w-w\partial_3 v=0. \tag{2}$$

It can also be rewritten as

$$u^2\partial_1\frac{v}{u}+w^2\partial_2\frac{u}{w}+v^2\partial_3\frac{w}{v}=0. \tag{3}$$

[We assume that none of the functions u, v and w vanish. If any one of these functions vanishes then Eq. (2) becomes trivial for the remaining two variables; see Remark 1.]

We consider the general solution of the Jacobi equation (3) and show that it has the following form:

$$J^{ij}=\mu\epsilon^{ijk}\partial_k\Psi, \tag{4}$$

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where μ and Ψ are arbitrary differentiable functions of x_i, $i=1,2,3$ and ϵ^{ijk} is the Levi–Civita symbol. We also consider special solutions given by

$$u\partial_1 v - v\partial_1 u = 0,\ w\partial_2 u - u\partial_2 w = 0, \quad \text{which implies} \quad v\partial_3 w - w\partial_3 v = 0. \tag{5}$$

Such Poisson structures appear in many examples. We show that this special class of solutions belongs to the general form (4). We introduce these special solutions to study the irregular points of the Poisson structures. All the irregular points of the Poisson structure matrix J given in the examples,[1] we know so far, come from this special form. Hence they are also irregular points of the form (4) we give.

II. THE GENERAL SOLUTION

Assuming that $u\neq 0$, let $\rho = v/u$ and $\chi = w/u$; then Eq. (2) can be written as

$$\partial_1\rho - \partial_2\chi + \rho\partial_3\chi - \chi\partial_3\rho = 0. \tag{6}$$

This equation can be put in a more suitable form by writing it as

$$(\partial_1 - \chi\partial_3)\rho - (\partial_2 - \rho\partial_3)\chi = 0. \tag{7}$$

Introducing differential operators D_1 and D_2 defined by

$$D_1 = \partial_1 - \chi\partial_3, \quad D_2 = \partial_2 - \rho\partial_3, \tag{8}$$

one can write Eq. (7) as

$$D_1\rho - D_2\chi = 0. \tag{9}$$

Lemma 1: Let Eq. (9) be satisfied. Then there are new coordinates $\overline{x_1},\overline{x_2},\overline{x_3}$ such that

$$D_1 = \partial_{\overline{x_1}} \quad \text{and} \quad D_2 = \partial_{\overline{x_2}}. \tag{10}$$

Proof: If Eq. (9) is satisfied, it is easy to show that the operators D_1 and D_2 commute, i.e.,

$$D_1\circ D_2 - D_2\circ D_1 = 0.$$

Hence, by the Frobenius theorem (see Ref. 4, p. 40) there exist coordinates $\overline{x_1},\overline{x_2},\overline{x_3}$ such that the equalities (10) hold. □

The coordinates $\overline{x_1},\overline{x_2},\overline{x_3}$ are described by the following lemma.

Lemma 2: Let ζ be a common invariant function of D_1 and D_2, i.e.,

$$D_1\zeta = D_2\zeta = 0, \tag{11}$$

then the coordinates $\overline{x_1},\overline{x_2},\overline{x_3}$ of Lemma 1 are given by

$$\overline{x_1} = x_1, \quad \overline{x_2} = x_2, \quad \overline{x_3} = \zeta. \tag{12}$$

Moreover from (11) we get

$$\chi = \frac{\partial_1\zeta}{\partial_3\zeta}, \quad \rho = \frac{\partial_2\zeta}{\partial_3\zeta}. \tag{13}$$

Theorem 1: *All Poisson structures in $\mathbb{R}^3$, except at some irregular points, take the form (4), i.e., $J_{ij} = \mu\,\epsilon_{ijk}\,\partial_k\,\zeta$. Here μ and ζ are some differentiable functions in $\mathbb{R}^3$*

Proof: Using (13), the entries of matrix J, in the coordinates $\overline{x_1},\overline{x_2},\overline{x_3}$, can be written as

$$u=\mu\partial_3\zeta,$$

$$v=\mu\partial_2\zeta, \tag{14}$$

$$w=\mu\partial_1\zeta.$$

Thus matrix J has the form (4) ($\Psi=\zeta$). □

Remark 1: So far we assumed that $u\neq 0$. If $u=0$ then the Jacobi equation becomes quite simpler, $v\partial_3 w-w\partial_3 v=0$, which has the simple solution $w=v\,\xi(x_1,x_2)$, where ξ is an arbitrary differentiable of x_1 and x_2. This class is also covered by the general solution (4) by letting Ψ independent of x_3.

A well known example of a dynamical system with a Poisson structure of the form (4) is the Euler equations.

Example 1: Consider the Euler equations (Ref. 4, pp. 397–398),

$$\dot{x}_1=\frac{I_2-I_3}{I_2I_3}x_2x_3,$$

$$\dot{x}_2=\frac{I_3-I_1}{I_3I_1}x_3x_1, \tag{15}$$

$$\dot{x}_3=\frac{I_1-I_2}{I_1I_2}x_1x_2,$$

where $I_1,I_2,I_3\in\mathbb{R}$ are some (nonvanishing) real constants. This system admits a Hamiltonian representation of the form (4). The matrix J can be defined in terms of function $\Psi=-\frac{1}{2}(x_1^2+x_2^2+x_3^2)$ and $\mu=1$, so

$$u=-x_3,$$

$$v=-x_2, \tag{16}$$

$$w=-x_1,$$

and $H=x_1^2/2I_1+x_2^2/2I_2+x_3^2/2I_3$.

Recently, a large set of solutions of the Jacobi equation (3) satisfying (5) was given in Ref. 1. For all such solutions the Darboux transformation and Casimir functionals were obtained; see Ref. 1.

Definition 1: For every domain $\Omega\in\mathbb{R}^3$ let $\mathbf{I}_a(\Omega)$ be the set of all solutions of (5) defined in Ω with $u(x)$, $v(x)$, and $w(x)$ being $C^1(\Omega)$.

Following Ref. 1 we have as follows.

Proposition 1: Let $\eta(x_1,x_2,x_3),\psi_i(x_i),\phi_i(x_i)$, $i=1,2,3$, be arbitrary differentiable functions defined in Ω. Then the functions

$$u(x)=\eta(x_1,x_2,x_3)\psi_1(x_1)\psi_2(x_2)\phi_3(x_3),$$

$$v(x)=\eta(x_1,x_2,x_3)\psi_1(x_1)\phi_2(x_2)\psi_3(x_3), \tag{17}$$

$$w(x)=\eta(x_1,x_2,x_3)\phi_1(x_1)\psi_2(x_2)\psi_3(x_3),$$

define a solution of Eq. (5) belonging to $\mathbf{I}_a(\Omega)$.

Definition 2: For every domain $\Omega\in\mathbb{R}^3$, let $\mathbf{I}_b(\Omega)$ be the set of all solutions of (5) defined in Ω where one of the functions $u(x)$, $v(x)$, and $w(x)$ is zero and the others are not identically zero in Ω.

Following Ref. 1 we have Proposition 2.

Proposition 2: Let $\eta(x_1,x_2,x_3),\xi_i(x_i)$, $i=1,2,3$, *be arbitrary differentiable functions defined in* Ω. *Then the functions*

$$u(x)=0,\quad v(x)=\eta(x_1,x_2,x_3)\xi_2(x_2),\quad w(x)=\eta(x_1,x_2,x_3)\xi_1(x_1) \tag{18}$$

define a solution of Eq. (1) belonging to $\mathbf{I}_b(\Omega)$, $u=0$. *Similar solutions can be given in the case* $v=0$ *and the case* $w=0$.

Remark 2: All of the Poisson structures described in Ref. 1 have the form (4). For the Poisson structure J, given by (17), assume ψ_1, ψ_2, and ψ_3 to be nonvanishing and define $\mu=\eta(x_1,x_2,x_3)\psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$ and

$$\Psi=\int^{x_1}\frac{\phi_1}{\psi_1}dx_1+\int^{x_2}\frac{\phi_2}{\psi_2}dx_2+\int^{x_3}\frac{\phi_3}{\psi_3}dx_3;$$

then J has form (4). For the Poisson structure J, given by (18), define $\mu=\eta(x_1,x_2,x_3)$ and $\Psi=\int^{x_1}\xi_1(x_1)+\int^{x_3}\xi_2(x_2)$; then J has form (4).

Let us give two examples of systems that admit a Hamiltonian representation described by the Proposition 1 and Proposition 2.

Example 2: Consider the Lotka–Voltera system,[8,9]

$$\begin{aligned}\dot{x}_1&=-abcx_1x_3-bc\mu_0x_1+cx_1x_2+c\nu x_1,\\ \dot{x}_2&=-a^2bcx_2x_3-abc\mu_0x_2+x_1x_2,\\ \dot{x}_3&=-abcx_2x_3-abc\nu_0x_3+bx_1x_3,\end{aligned} \tag{19}$$

where $a,b,c,\mu_0,\nu_0\in\mathbb{R}$ are constants.

The matrix J is given by

$$\begin{aligned}u&=cx_1x_2,\\ v&=-bcx_1x_3,\\ w&=-x_2x_3,\end{aligned} \tag{20}$$

and $H=abx_1+x_2-ax_3+\nu_0\ln x_2-\mu_0\ln x_3$.

Example 3: Consider the Lorenz system[8]

$$\begin{aligned}\dot{x}_1&=\frac{1}{2}x_2,\\ \dot{x}_2&=-x_1x_3,\\ \dot{x}_3&=x_1x_2.\end{aligned} \tag{21}$$

The matrix J is given by

$$\begin{aligned}u&=\tfrac{1}{4},\\ v&=0,\\ w&=-\tfrac{1}{2}x_1,\end{aligned} \tag{22}$$

and $H=x_2^2+x_3^2$. Many other examples are given in Sec. III.

In the derivation of the general solution, Theorem 1, we assumed that one of the components of matrix J is different from zero. In addition our derivation is valid only in a neighborhood of a regular point of J (matrix $J\neq 0$ at this point). If $p\in\mathbb{R}^3$ is an irregular point where $u(p)=v(p)=w(p)=0$ it is not clear whether our solution is valid in a neighborhood of such a point. Here we shall show that the Poisson structures given by (4) preserve their form in the neighborhood of the following irregular points.

Lemma 3: The solution of the equation (1) defined in Proposition 1 and Proposition 2 and written in the form (4) preserve their form in the neighborhood of the irregular points, lines and planes in $\mathbb{R}^3$ *defined below*

(a) Irregular points. Let $p=(p_1,p_2,p_3)$ *be such that* $\phi_1(p_1)=\phi_2(p_2)=\phi_3(p_3)=0$ *and* $\psi_i(p_i)\neq 0$, $i=1,2,3$; *then p is an irregular point where the general form (4) is preserved.*

(b) Irregular lines or irregular planes. Let $p=(p_1,p_2,p_3)\in\mathbb{R}^3$ *be such that* $\eta(p_1,x_2,x_3)=0$ $[\eta(x_1,p_2,x_3)=0$ *or* $\eta(x_1,x_2,p_3)=0]$ *and* $\psi_i(p_i)\neq 0$, $i=1,2,3$; *then* $x_1=p_1$ $(x_2=p_2$ *or* $x_3=p_3)$ *is an irregular plane, where the general form (4) is preserved. Let* $x_1=p_1$, $x_2=p_2$ *be such that* $\eta(p_1,p_2,x_3)=0$ $[\eta(p_1,x_2,p_3)=0$ *or* $\eta(x_1,p_2,p_3)=0]$ *and* $\psi_i(p_i)\neq 0$, $i=1,2,3$ *then* $x_1=p_1$, $x_2=p_2$ $(x_1=p_1,x_3=p_3$ *or* $x_2=p_2,x_3=p_3)$ *is an irregular line, where the general form (4) is preserved.*

Proof: The solution given in Proposition 1 and Proposition 2 solves the following equations (without any division):

$$u\partial_1 v-v\partial_1 u=0,$$
$$-u\partial_2 w+w\partial_2 u=0, \tag{23}$$
$$v\partial_3 w-w\partial_3 v=0.$$

The general form (4), given in Remark 2, is also preserved at such points since we can define $\mu=\eta(x_1,x_2,x_3)\psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$ and

$$\Psi=\int^{x_1}\frac{\phi_1}{\psi_1}dx_1+\int^{x_2}\frac{\phi_2}{\psi_2}dx_2+\int^{x_3}\frac{\phi_3}{\psi_3}dx_3,$$

or if one of the components of J is zero, assume $u=0$, we define $\mu=\eta(x_1,x_2,x_3)$ and $\Psi=\int^{x_1}\xi_1(x_1)+\int^{x_3}\xi_2(x_2)$. □

Example 4: For the Euler system considered in Example 1 the Poisson structure, given by (16), has irregular point $p=(0,0,0)$. The irregular point $p=(0,0,0)$ satisfies the conditions of Lemma 3, the functions $\Psi=-\frac{1}{2}(x_1^2+x_2^2+x_3^2)$, $\mu=1$ in terms of which the Poisson structure is given, are well defined in a neighborhood of $p=(0,0,0)$.

III. BI-HAMILTONIAN SYSTEM

In general the Darboux theorem states that (see Ref. 4), locally, all Poisson structures can be reduced to the standard one (a Poisson structure with constant entries). The above theorem, Theorem 1, resembles the Darboux theorem for $N=3$. All Poisson structures, at least locally, can be cast into the form (4). This result is important because the Darboux theorem is not suitable for obtaining multi-Hamiltonian systems in $\mathbb{R}^3$, but we will show that our theorem is effective for this purpose. Writing the Poisson structure in the form (4) allows us to construct bi-Hamiltonian representations of a given Hamiltonian system.

Definition 3: Two Hamiltonian matrices J and $\tilde{J}$ *are compatible, if the sum* $J+\tilde{J}$ *defines also a Poisson structure.*

The compatible Poisson structures can be used to construct bi-Hamiltonian equations.

Definition 4: A Hamiltonian equation is said to be bi-Hamiltonian if it admits two Hamiltonian representations with compatible Poisson structures,

$$\frac{dx}{dt} = J\nabla H = \tilde{J}\nabla \tilde{H}, \tag{24}$$

where J and $\tilde{J}$ are compatible.

Lemma 4: Let Poisson structures J and $\tilde{J}$ have the form (4), so $J^{ij} = \mu \epsilon^{ijk}\partial_k \Psi$ and *$\tilde{J}^{ij} = \tilde{\mu}\epsilon^{ijk}\partial_k \tilde{\Psi}$. Then J and $\tilde{J}$ are compatible if and only if there exists a differentiable function $\Phi(\Psi, \tilde{\Psi})$ such that*

$$\tilde{\mu} = \mu \frac{\partial_{\tilde{\Psi}} \Phi}{\partial_{\Psi} \Phi}, \tag{25}$$

provided that $\partial_{\Psi} \Phi \equiv \partial\Phi/\partial\Psi \neq 0$ and $\partial_{\tilde{\Psi}} \Phi \equiv \partial\Phi/\partial\tilde{\Psi} \neq 0$.

This suggests that all Poisson structures in $\mathbb{R}^3$ have compatible pairs, because the condition (25) is not so restrictive on the Poisson matrices J and $\tilde{J}$. Such compatible Poisson structures can be used to construct bi-Hamiltonian systems.

Lemma 5: Let J be given by (4) and $H(x_1, x_2, x_3)$ is any differentiable function; then the Hamiltonian equation,

$$\frac{dx}{dt} = J\nabla H = -\mu\, \nabla\Psi \times \nabla H, \tag{26}$$

is bi-Hamiltonian with the second structure given by $\tilde{J}$ with entries

$$\begin{aligned} \tilde{u}(x) &= \tilde{\mu}\, \partial_3 g(\Psi(x_1 x_2 x_3), H(x_1, x_2, x_3)), \\ \tilde{v}(x) &= -\tilde{\mu}\, \partial_2 g(\Psi(x_1 x_2 x_3), H(x_1, x_2, x_3)), \\ \tilde{w}(x) &= \tilde{\mu}\, \partial_1 g(\Psi(x_1 x_2 x_3), H(x_1, x_2, x_3)), \end{aligned} \tag{27}$$

and $\tilde{H} = h(\Psi(x_1 x_2 x_3), H(x_1, x_2, x_3))$, $\tilde{\Psi} = g(\Psi(x_1, x_2, x_3), H(x_1, x_2, x_3))$, $\tilde{\mu} = \mu\,(\partial_{\tilde{\Psi}}\Phi/\partial_{\Psi}\Phi)$. Provided that there exist differentiable functions $\Phi(\Psi, \tilde{\Psi})$, $h(\Psi, H)$, and $g(\Psi, H)$ satisfying the following equation:

$$\frac{\partial g}{\partial \Psi}\frac{\partial h}{\partial H} - \frac{\partial g}{\partial H}\frac{\partial h}{\partial \Psi} = \frac{\Phi_1(\Psi, g)}{\Phi_2(\Psi, g)}, \tag{28}$$

where $\Phi_1 = \partial_{\Psi}\Phi|_{(\Psi, g)}$, $\Phi_2 = \partial_{\tilde{\Psi}}\Phi|_{(\Psi, g)}$.

Proof: By Lemma 4, J and $\tilde{J}$ are compatible and it can be shown by a straightforward calculation that the equality (being a bi-Hamiltonian system),

$$\tilde{J}\nabla\tilde{H} = J\nabla H, \tag{29}$$

or

$$\tilde{\mu}\, \nabla\, \tilde{\Psi} \times \nabla \tilde{H} = \mu\, \nabla\, \Psi \times \nabla\, H \tag{30}$$

is guaranteed by (28). Hence the system

$$\frac{dx_1}{dt} = \mu \partial_3 \Psi\, \partial_2 H - \partial_2 \Psi\, \partial_3 H,$$

$$\frac{dx_2}{dt} = -\mu\partial_3\Psi\partial_1 H + \partial_1\Psi\partial_3 H,$$

$$\frac{dx_3}{dt} = \mu\partial_2\Psi\partial_1 H - \partial_1\Psi\partial_2 H, \tag{31}$$

is bi-Hamiltonian. □

Remark 3: The Hamiltonian function H is a conserved quantity of the system. It is clear from the expression (31) that the function Ψ is another conserved quantity of the system. Hence for a given Hamiltonian system there is a duality between H and Ψ. Such a duality arises naturally because a simple solution of the equation (28) is $\tilde{\Psi}=H$, $\tilde{H}=\Psi$ and $\tilde{\mu}=-\mu$. Thus we have a hierarchy of Hamiltonians that start with a Casimir of the second structure and terminates with a Casimir of the first structure. Such systems are equivalent to the quasi-bi-Hamiltonian systems of lower dimension with nondegenerate Poisson structures (see Ref. 5, pp. 185–220).

Remark 4: Using Lemma 5 we can construct infinitely many compatible Hamiltonian representations by choosing functions Φ, g, h satisfying (28). If we fix functions Φ and g, then Eq. (28) became linear first order partial differential equations for h. For instance, taking $g=\Psi H$ and $\tilde{\mu}=-\mu$, which fixes Φ, we obtain $h=\ln H$. Thus we a obtain second Hamiltonian representation with $\tilde{J}$ given by $\tilde{\Psi}=\Psi H$ and $\tilde{H}=\ln H$.

IV. EXAMPLES

Let us give examples of Hamiltonian systems. For each Hamiltonian system we give the Hamiltonian H and functions Ψ and μ in terms of which the corresponding Poisson structure may be written, using (4). Functions H and Ψ are first integrals of the system so one can use them to reduce the system to a first order ordinary differential equation. We give the reduced equation for the examples. We also give irregular points for the Poisson structures. For all examples except Example 7 the form of the Poisson structure (4) is preserved in a neighborhood of irregular points (function Ψ and μ are well defined). For Example 7 the form of the Poisson structure (4) is not preserved; the function Ψ is not defined in a neighborhood of irregular points but the Hamiltonian function is also not defined at the irregular points. Hence this system does not have a Hamiltonian formulation in the neighborhood of such points. Examples 6–12 satisfy the special case given in Proposition 1 and Proposition 2. Please see Ref. 1 for the examples and related references.

Example 6: For the Euler system considered in Example 1 we gave a Poisson structure in terms of functions Ψ,μ and the Hamiltonian. The reduced equations are

$$x_1 = \left(C_1 + \frac{I_1(I_3-I_2)}{I_3(I_2-I_1)}x_3^2\right)^{1/2},$$

$$x_2 = \left(C_2 + \frac{I_2(I_3-I_1)}{I_3(I_1-I_2)}x_3^2\right)^{1/2}, \tag{32}$$

$$\dot{x}_3 = \left(C_1 + \frac{I_1(I_3-I_2)}{I_3(I_2-I_1)}x_3^2\right)^{1/2}\left(C_2 + \frac{I_2(I_3-I_1)}{I_3(I_1-I_2)}x_3^2\right)^{1/2}.$$

The Poisson structure is given by (16). It has an irregular point $p=(0,0,0)$ (the origin).

Example 7: The Lotka–Voltera system considered in Example 2 has the matrix J given by $\Psi=-\ln x_1 - b\ln x_2 + c\ln x_3$, $\mu=x_1x_2x_3$ and the Hamiltonian $H=abx_1+x_2-ax_3+\nu_0\ln x_2 - \mu_0\ln x_3$.

The reduced equations can be obtained using equalities

$$-\ln x_1 - b\ln x_2 + c\ln x_3 = C_1,$$

$$abx_1+x_2-ax_3+\nu_0\ln x_2-\mu_0\ln x_3=C_2. \tag{33}$$

The Poisson structure is given by (20). It has irregular lines given by $x_i=0$ and $x_j=0$, $i,j=1,2,3$, $j\neq i$ (coordinate lines). Both Ψ and H are not defined at these points. So, the system does not have a Hamiltonian formulation at these points.

Example 8: The Lorentz system considered in Example 3 has the matrix J given by $\Psi=\frac{1}{4}(x_3-x_1^2)$, $\mu=1$ and the Hamiltonian $H=x_1^2+x_3^2$.

The reduced equations are

$$\begin{aligned} x_1&=(C_1-x_3)^{1/2},\\ x_2&=(C_2-x_3^2)^{1/2},\\ \dot{x}_3&=(C_1-x_3)^{1/2}(C_2-x_3^2)^{1/2}. \end{aligned} \tag{34}$$

The Poisson structure is given by (22). It has no irregular points.

Example 9: Consider Kermac–Mackendric system,[8,10]

$$\begin{aligned} \dot{x}_1&=-rx_1x_2,\\ \dot{x}_2&=rx_1x_2-ax_2,\\ \dot{x}_3&=ax_2, \end{aligned} \tag{35}$$

where $r,a\in\mathbb{R}$ are constants.

The matrix J is given by $\Psi=x_1+x_2+x_3$, $\mu=x_1x_2$ and the Hamiltonian is $H=rx_3+a\ln x_1$.

The reduced equations are

$$\begin{aligned} x_2&=C_1+\frac{a}{r}\ln x_1-x_1,\\ x_3&=C_2-\frac{a}{r}\ln x_1,\\ \dot{x}_1&=-rx_1\left(C_1+\frac{a}{r}\ln x_1-x_1\right). \end{aligned} \tag{36}$$

The Poisson structure is given by

$$\begin{aligned} u&=x_1x_2,\\ v&=x_1x_2,\\ w&=x_1x_2. \end{aligned} \tag{37}$$

It has irregular planes $x_1=0$ and $x_2=0$ (coordinate planes).

Example 10: Consider the May–Leonard system,[8]

$$\begin{aligned} \dot{x}_1&=-x_2^{-\alpha}x_3^{-\alpha},\\ \dot{x}_2&=-x_1^{-\alpha}x_3^{-\alpha},\\ \dot{x}_3&=-x_1^{-\alpha}x_2^{-\alpha}. \end{aligned} \tag{38}$$

The matrix J is given by $\Psi=[1/(1-\alpha)^2](x_2^{1-\alpha}-x_1^{1-\alpha})$, $\mu=1$ and the Hamiltonian is $H=x_1^{1-\alpha}-x_3^{1-\alpha}$, $\alpha<0$.

The reduced equations are

$$x_2=(C_1+x_1^{1-\alpha})^{1/(1-\alpha)},$$

$$x_3=(C_2+x_1^{1-\alpha})^{1/(1-\alpha)}, \tag{39}$$

$$\dot{x}_1=-(C_1+x_1^{1-\alpha})^{\alpha/(1-\alpha)}(C_2+x_1^{1-\alpha})^{\alpha/(1-\alpha)}.$$

The Poisson structure J is given by

$$u=0,$$

$$v=\frac{x_2^{-\alpha}}{\alpha-1}, \tag{40}$$

$$w=\frac{x_1^{-\alpha}}{\alpha-1}.$$

It has an irregular line $x_1=0$, $x_2=0$ (coordinate line).

Example 11: Consider the Maxvel–Bloch system,[8]

$$\dot{x}_1=x_2,$$

$$\dot{x}_2=x_1x_3, \tag{41}$$

$$\dot{x}_3=-x_1x_2.$$

The matrix J is given by $\Psi=-(1/2v)(x_2^2+x_3^2)$, $\mu=1$ and the Hamiltonian is $H=\frac{1}{2}\alpha(x_2^2+x_3^2)-(1/v)(x_3+x_1^2)$, $v\neq 0$.

The reduced equations are

$$x_1=\left(C_1+\frac{\alpha v}{2}C_2-x_3\right)^{1/2},$$

$$x_2=(C_2-x_3^2)^{1/2}, \tag{42}$$

$$\dot{x}_3=-\left(C_1+\frac{\alpha v}{2}C_2-x_3\right)^{1/2}(C_2-x_3^2)^{1/2}.$$

The Poisson structure is given by

$$u=\frac{-1}{v}x_3,$$

$$v=\frac{-1}{v}x_2, \tag{43}$$

$$w=0.$$

It has an irregular line $x_2=0$, $x_3=0$ (coordinate line).

Example 12: Consider systems that are obtained from the Lorenz system,[13]

$$\begin{aligned}\dot{x}&=\sigma(x-y),\\ \dot{y}&=-y+rx-xz,\\ \dot{z}&=-bz+xy.\end{aligned}\tag{44}$$

Following Ref. 12, for an appropriate subset of parameters by recalling we have the following.

(i) **Lorentz(1) system:**

$$\begin{aligned}\dot{x}_1&=\sigma x_2 e^{(\sigma-1)t},\\ \dot{x}_2&=x_1 e^{(1-\sigma)t}(r-x_3 e^{-2\sigma t}),\\ \dot{x}_3&=x_1 x_2 e^{(\sigma-1)t}.\end{aligned}\tag{45}$$

The matrix J is given by $\Psi=-(r/4\sigma)\,x_1^2 e^{(1-\sigma)t}-\frac{1}{4}x_2^2 e^{(\sigma-1)t}-\frac{1}{4}x_3^2 e^{(1-3\sigma)t}$, $\mu=1$ and the Hamiltonian is $H=x_1^2-2\sigma x_3$.

The reduced equations are

$$\begin{aligned}x_1&=(C_1+2\sigma x_3)^{1/2},\\ x_2&=\left(C_2-\frac{r}{\sigma}(C_1+2\sigma x_3)e^{2(1-\sigma)t}-x_3^2 e^{2(1-2\sigma)t}\right)^{1/2},\\ \dot{x}_3&=(C_1+2\sigma x_3)^{1/2}\left(C_2-\frac{r}{\sigma}(C_1+2\sigma x_3)e^{2(1-\sigma)t}-x_3^2 e^{2(1-2\sigma)t}\right)^{1/2}e^{(1-\sigma)t}.\end{aligned}\tag{46}$$

The Poisson structure is given by

$$\begin{aligned}u&=\tfrac{1}{2}x_3 e^{(1-3\sigma)t},\\ v&=\tfrac{1}{2}x_2 e^{(\sigma-1)t},\\ w&=-\frac{r}{2\sigma}x_1 e^{(1-\sigma)t}.\end{aligned}\tag{47}$$

It has an irregular point $x_1=0$, $x_2=0$, $x_3=0$ (the origin).

(ii) **Lorentz(3) system:**

$$\begin{aligned}\dot{x}_1&=\sigma x_2 e^{(\sigma-1)t},\\ \dot{x}_2&=-x_1 x_3 e^{-\sigma t},\\ \dot{x}_3&=x_1 x_2 e^{-\sigma t}.\end{aligned}\tag{48}$$

The matrix J is given by $\Psi=-\frac{1}{4}x_1^2 e^{-\sigma t}+(\sigma/2)\,x_3 e^{(\sigma-1)t}$, $\mu=1$ and the Hamiltonian is $H=x_2^2+x_3^2$.

The reduced equations are

$$\begin{aligned}x_1&=(C_1 e^{\sigma t}+2\sigma x_3 e^{(2\sigma-1)t})^{1/2},\\ x_2&=(C_2-x_3^2)^{1/2},\\ \dot{x}_3&=(C_1 e^{\sigma t}+2\sigma x_3 e^{(2\sigma-1)t})^{1/2}(C_2-x_3^2)^{1/2}e^{-\sigma t}.\end{aligned}\tag{49}$$

The Poisson structure is given by

$$u=\tfrac{1}{2}\sigma e^{(\sigma-1)t},$$
$$v=0, \tag{50}$$
$$w=-\tfrac{1}{2}x_1e^{-\sigma t}.$$

It has no irregular points.

(iii) **Lorentz(5) system:**

$$\dot{x}_1=x_2,$$
$$\dot{x}_2=rx_1-x_1x_3e^{-t}, \tag{51}$$
$$\dot{x}_3=x_1x_2e^{-t}.$$

The matrix J is given by $\Psi=\frac{1}{4}x_1^2e^{-t}-\frac{1}{2}x_3$, $\mu=1$ and the Hamiltonian is $H=-rx_1^2+x_2^2+x_3^2$.

The reduced equations are

$$x_1=(C_1e^t+2x_3e^t)^{1/2},$$
$$x_2=(C_2+rC_1e^t+2rx_3e^t-x_3^2)^{1/2}, \tag{52}$$
$$\dot{x}_3=(C_1e^t+2x_3e^t)^{1/2}(C_2+rC_1e^t+2rx_3e^t-x_3^2)^{1/2}e^{-t}.$$

The Poisson structure is given by

$$u=\tfrac{1}{2},$$
$$v=0, \tag{53}$$
$$w=-\tfrac{1}{2}x_1e^{-t}0.$$

It has no irregular points.

Example 13: Consider systems that are obtained from the Rabinovich system,[14]

$$\dot{x}=-\nu_1x+hy+yz,$$
$$\dot{y}=hx-\nu_2y-xz, \tag{54}$$
$$\dot{z}=-\nu_3z+xy.$$

Following Ref. 12, for an appropriate subset of parameters by recalling we have the following.

(i) **Rabinovich (1) system:**

$$\dot{x}_1=hx_2+x_2x_3e^{-2\nu t},$$
$$\dot{x}_2=hx_1-x_1x_3e^{-2\nu t}, \tag{55}$$
$$\dot{x}_3=x_1x_2.$$

The matrix J is given by $\Psi=\frac{1}{8}x_1^2-\frac{1}{8}x_2^2-\frac{1}{4}x_3^2e^{-2\nu t}$, $\mu=1$ and the Hamiltonian is $H=x_1^2+x_2^2-4hx_3$.

The reduced equations are

$$x_1=(C_1+x_3^2e^{-2\nu t}+2hx_3)^{1/2},$$
$$x_2=(C_2-x_3^2e^{-2\nu t}+2hx_3)^{1/2}, \tag{56}$$
$$\dot{x}_3=(C_1+x_3^2e^{-2\nu t}+2hx_3)^{1/2}(C_2-x_3^2e^{-2\nu t}+2hx_3)^{1/2}.$$

The Poisson structure is given by

$$u=\tfrac{1}{2}x_3e^{-2\nu t},$$
$$v=\tfrac{1}{4}x_2, \tag{57}$$
$$w=-\tfrac{1}{4}x_1.$$

It has an irregular point $x_1=0$, $x_2=0$, $x_3=0$ (the origin).

(ii) **Rabinovich (2) system:**

$$\dot{x}_1=hx_2+x_2x_3e^{-\nu t},$$
$$\dot{x}_2=hx_1-x_1x_3e^{-\nu t}, \tag{58}$$
$$\dot{x}_3=x_1x_2e^{-\nu t}.$$

The matrix J is given by $\Psi=\frac{1}{8}x_1^2e^{-\nu t}+\frac{1}{8}x_2^2e^{-\nu t}-\frac{1}{2}hx_3$, $\mu=1$ and the Hamiltonian is $H=x_1^2-x_2^2-2x_3^2$.

The reduced equations are

$$x_1=(C_1e^{\nu t}+C_2+x_3^2+2hx_3e^{\nu t})^{1/2},$$
$$x_2=(C_1e^{\nu t}-C_2-x_3^2+2hx_3e^{\nu t})^{1/2}, \tag{59}$$
$$\dot{x}_3=(C_1e^{\nu t}+C_2+x_3^2+2hx_3e^{\nu t})^{1/2}(C_1e^{\nu t}-C_2-x_3^2+2hx_3e^{\nu t})^{1/2}e^{-\nu t}.$$

The Poisson structure is given by

$$u=-\tfrac{1}{2}h,$$
$$v=\tfrac{1}{4}x_2e^{-\nu t}, \tag{60}$$
$$w=\tfrac{1}{4}x_1e^{-\nu t}.$$

It has no irregular points.

(iii) **Rabinovich (3) system:**

$$\dot{x}_1=x_2x_3e^{\nu_3 t},$$
$$\dot{x}_2=-x_1x_3e^{-\nu_3 t}, \tag{61}$$
$$\dot{x}_3=x_1x_2e^{(\nu_3-2\nu)t}.$$

The matrix J is given by $\Psi=\frac{1}{4}x_2^2e^{(\nu_3-2\nu)t}+\frac{1}{4}x_3^2e^{-\nu_3 t}$, $\mu=1$ and the Hamiltonian is $H=x_1^2+x_2^2$.

The reduced equations are

$$x_1=(C_1-x_2^2)^{1/2},$$
$$x_3=(C_2e^{-\nu_3 t}-x_3^2e^{-2(\nu-\nu_3)t})^{1/2}, \tag{62}$$
$$\dot{x}_2=(C_1-x_2^2)^{1/2}(C_2e^{-\nu_3 t}-x_3^2e^{-2(\nu-\nu_3)t})^{1/2}e^{(\nu_3-2\nu)t}.$$

The Poisson structure is given by

$$u=\tfrac{1}{2}x_3e^{-\nu_3 t},$$
$$v=\tfrac{1}{2}x_2e^{(\nu_3-2\nu)t}, \tag{63}$$
$$w=0.$$

It has an irregular line $x_2=0$, $x_3=0$ (coordinate line).

(iv) **Rabinovich (4) system:**

$$\dot{x}_1 = hx_2 e^{\nu_1 t} + x_2 x_3 e^{\nu_1 t},$$
$$\dot{x}_2 = hx_1 e^{-\nu_1 t} - x_1 x_3 e^{-\nu_1 t}, \tag{64}$$
$$\dot{x}_3 = x_1 x_2 e^{-\nu_1 t}.$$

The matrix J is given by $\Psi = -\frac{1}{4}x_1^2 e^{-\nu t} - \frac{1}{4}x_2^2 e^{\nu_1 t} + hx_3 e^{\nu_1 t}$, $\mu = 1$ and the Hamiltonian is $H = x_2^2 + (h - x_3)^2$.

The reduced equations are

$$x_1 = (C_1 e^{\nu t} - (C_2 - (h + x_3))e^{(\nu_1 + \nu)t})^{1/2},$$
$$x_2 = (C_2 - (h - x_3)^2)^{1/2}, \tag{65}$$
$$\dot{x}_3 = (C_1 e^{\nu t} - (C_2 - (h + x_3))e^{(\nu_1 + \nu)t})^{1/2}(C_2 - (h - x_3)^2)^{1/2} e^{-\nu_1 t}.$$

The Poisson structure is given by

$$u = he^{\nu_1 t},$$
$$v = -\tfrac{1}{2}x_2 e^{\nu_1 t}, \tag{66}$$
$$w = -\tfrac{1}{2}x_1 e^{-\nu t}.$$

It has no irregular points.

(v) **Rabinovich (5) system:**

$$\dot{x}_1 = hx_2 e^{-\nu_2 t} + x_2 x_3 e^{-\nu_2 t},$$
$$\dot{x}_2 = hx_1 e^{\nu_2 t} - x_1 x_3 e^{\nu_2 t}, \tag{67}$$
$$\dot{x}_3 = x_1 x_2 e^{-\nu_2 t}.$$

The matrix J is given by $\Psi = \frac{1}{4}x_1^2 e^{\nu_2 t} + \frac{1}{4}x_2^2 e^{-\nu_2 t} - hx_3 e^{\nu_2 t}$, $\mu = 1$ and the Hamiltonian is $H = x_1^2 - (h + x_3)^2$.

The reduced equations are

$$x_1 = (C_1 + (h + x_3)^2)^{1/2},$$
$$x_2 = (C_2 e^{\nu_2 t} - (C_1 + (h - x_3))e^{2\nu_2 t})^{1/2}, \tag{68}$$
$$\dot{x}_3 = (C_1 + (h + x_3)^2)^{1/2}(C_2 - (C_1 + (h - x_3))e^{2\nu_2 t})^{1/2} e^{-\nu_2 t}.$$

The Poisson structure is given by

$$u = -he^{\nu_2 t},$$
$$v = \tfrac{1}{2}x_2 e^{-\nu_2 t}, \tag{69}$$
$$w = \tfrac{1}{2}x_1 e^{\nu_2 t}.$$

It has no irregular points.

(vi) **Rabinovich (6) system:**

$$\dot{x}_1 = x_2 x_3 e^{(\nu_1 - 2\nu_3)t},$$
$$\dot{x}_2 = -x_1 x_3 e^{-\nu_1 t}, \tag{70}$$
$$\dot{x}_3 = x_1 x_2 e^{-\nu_1 t}.$$

The matrix J is given by $\Psi = -\frac{1}{4}x_1^2 e^{-\nu_1 t} - \frac{1}{4}x_2^2 e^{(\nu_1 - 2\nu_2)t}$, $\mu = 1$ and the Hamiltonian is $H = x_2^2 + x_3^2$.

The reduced equations are

$$x_1=(C_1e^{\nu_1 t}+x_2^2e^{2(\nu_1-\nu_2)t})^{1/2},$$
$$x_3=(C_2-x_2^2)^{1/2}, \tag{71}$$
$$\dot{x}_2=-(C_1e^{\nu_1 t}+x_2^2e^{2(\nu_1-\nu_2)t})^{1/2}(C_2-x_2^2)^{1/2}e^{-\nu_1 t}.$$

The Poisson structure is given by

$$u=0,$$
$$v=-\tfrac{1}{2}x_2e^{(\nu_1-2\nu_2)t}, \tag{72}$$
$$w=-\tfrac{1}{2}x_1e^{-\nu_1 t}.$$

It has an irregular line $x_1=0$, $x_2=0$ (coordinate line).

(vii) **Rabinovich (7) system:**

$$\dot{x}_1=x_2x_3e^{-\nu_2 t},$$
$$\dot{x}_2=-x_1x_3e^{(\nu_2-2\nu_3)t}, \tag{73}$$
$$\dot{x}_3=x_1x_2e^{-\nu_2 t}.$$

The matrix J is given by $\Psi=\frac{1}{4}x_1^2e^{(\nu_2-2\nu_3)t}+\frac{1}{4}x_2^2e^{-\nu_2 t}$, $\mu=1$ and the Hamiltonian is $H=x_1^2-x_3^2$.

The reduced equations are

$$x_2=(C_1e^{\nu_2 t}-x_1^2e^{2(\nu_2-\nu_3)t})^{1/2},$$
$$x_3=(C_2+x_1^2)^{1/2}, \tag{74}$$
$$\dot{x}_1=(C_1e^{\nu_2 t}-x_1^2e^{2(\nu_2-\nu_3)t})^{1/2}(C_2+x_1^2)^{1/2}e^{-\nu_2 t}.$$

The Poisson structure is given by

$$u=0,$$
$$v=\tfrac{1}{2}x_2e^{\nu_2 t}, \tag{75}$$
$$w=\tfrac{1}{2}x_1e^{\nu_2-2\nu_3 t}.$$

It has an irregular line $x_2=0$, $x_3=0$ (coordinate line).

Example 14: Consider systems that are obtained from the RTW system,[14]

$$\dot{x}=\gamma x+\delta y+z-2y^2,$$
$$\dot{y}=\gamma y-\delta x+2xy, \tag{76}$$
$$\dot{z}=-2z(x+1),$$

for an appropriate subset of parameters by recalling. Following Ref 12 we have the following.

(i) **RTW(1) system:**

$$\dot{x}_1=\delta x_2+x_3e^{-2t}-2x_2^2,$$
$$\dot{x}_2=-\delta x_1+2x_1x_2, \tag{77}$$
$$\dot{x}_3=-x_1x_3,$$

where δ is an arbitrary constant. The matrix J is given by $\Psi=\frac{1}{2}(x_1^2-x_2^2+x_3e^{-t})$, $\mu=1$ and the Hamiltonian is $H=x_3(2x_2-\delta)$.

The reduced equations are

$$x_1=\left(C_1-x_3e^{-t}+\left(\frac{C_2+\delta x_3}{2x_3}\right)^2\right)^{1/2},$$
$$x_2=\frac{C_2+\delta x_3}{2x_3},$$
$$\dot{x}_3=-\left(C_1-x_3e^{-t}+\left(\frac{C_2+\delta x_3}{2x_3}\right)^2\right)^{1/2}x_3. \tag{78}$$

The Poisson structure is given by

$$u=\frac{1}{2}e^{-2t},$$
$$v=x_2, \tag{79}$$
$$w=x_1.$$

It has no irregular points.

(ii) **RTW(2) system:**

$$\dot{x}_1=\delta x_2+x_3e^{-t}-2x_2^2e^{-t},$$
$$\dot{x}_2=-\delta x_1+2x_1x_2e^{-t}, \tag{80}$$
$$\dot{x}_3=-x_1x_3e^{-t},$$

where δ is an arbitrary constant. The matrix J is given by $\Psi=-(\delta/2)(x_1^2+x_2^2)-x_3x_2e^{-t}$, $\mu=1$ and the Hamiltonian is $H=x_1^2+x_2^2+x_3$.

The reduced equations are

$$x_1=\left(C_2-x_3-\left(C_1e^t-\frac{\delta}{2}C_2+\frac{\delta}{2}x_3\right)^2\right)^{1/2},$$
$$x_2=C_1e^t-\frac{\delta}{2}C_2+\frac{\delta}{2}x_3, \tag{81}$$
$$\dot{x}_3=\left(C_2-x_3-\left(C_1e^t-\frac{\delta}{2}C_2+\frac{\delta}{2}x_3\right)^2\right)^{1/2}x_3e^{-t}.$$

The Poisson structure is given by

$$u=-x_2e^{-t},$$
$$v=-\delta x_2-x_3e^{-t}, \tag{82}$$
$$w=-\delta x_1.$$

It has an irregular point $x_1=0$, $x_2=0$, $x_3=0$ (the origin).

(iii) **RTW(3) system:**

$$\dot{x}_1=(x_3-2x_2)e^{-t},$$
$$\dot{x}_2=2x_1x_2e^{-t}, \tag{83}$$
$$\dot{x}_3=-2x_1x_3e^{-t}.$$

The matrix J is given by $\Psi=(x_1^2-x_2^2+x_3)e^{-t}$, $\mu=1$ and the Hamiltonian is $H=x_2x_3$.

The reduced equations are

$$x_1=\left(C_1e^t-x_3-\frac{C_2^2}{x_3^2}\right)^{1/2},$$
$$x_2=\frac{C_2}{x_3}, \tag{84}$$
$$\dot{x}_3=-2\left(C_1e^t-x_3-\frac{C_2^2}{x_3^2}\right)^{1/2}x_3e^{-t}.$$

The Poisson structure is given by

$$u=e^{-t},\quad v=2x_2e^{-t},\quad w=2x_1e^{-t}. \tag{85}$$

It has no irregular points.

(iv) **RTW(4) system:**

$$\dot{x}_1=x_3e^{-(\gamma+2)t}-2x_2^2e^{\gamma t},\quad \dot{x}_2=2x_1x_2e^{\gamma t},\quad \dot{x}_3=-2x_1x_3e^{\gamma t}, \tag{86}$$

where γ is an arbitrary constant. The matrix J is given by $\Psi=(x_1^2-x_2^2)e^{\gamma t}+x_3e^{-(\gamma+2)t}$, $\mu=1$ and the Hamiltonian is $H=x_2x_3$.

The reduced equations are

$$x_1=\left(C_1e^{-\gamma t}-x_3e^{-2(\gamma+1)t}+\frac{C_2^2}{x_3^2}\right)^{1/2},\quad x_2=\frac{C_2}{x_3},\quad \dot{x}_3=-2\left(C_1e^{-\gamma t}-x_3e^{-2(\gamma+1)t}+\frac{C_2^2}{x_3^2}\right)^{1/2}x_3e^{\gamma t}. \tag{87}$$

The Poisson structure is given by

$$u=e^{-(2+\gamma)t},\quad v=2x_2e^{\gamma t},\quad w=2x_1e^{\gamma t}. \tag{88}$$

It has no irregular points.

(v) **RTW(5) system:**

$$\dot{x}_1=\delta x_2+x_3-2x_2^2e^{-2t},\quad \dot{x}_2=-\delta x_1+2x_1x_2e^{-2t},\quad \dot{x}_3=-2x_1x_3e^{-2t}, \tag{89}$$

where δ is a nonvanishing constant. The matrix J is given by $\Psi=(\delta e^{-2t}/2)(x_1^2-x_2^2)+(\delta/2)x_3$, $\mu=1$ and the Hamiltonian is $H=x_1^2+x_2^2+(2/\delta)x_2x_3$.

The reduced equations are

$$x_1=\left(C_1e^{2t}+x_2^2+e^{2t}\frac{C_2-C_1e^{2t}-2x_2^2}{\frac{\delta}{2}x_2+e^{2t}}\right)^{1/2},\quad x_3=\frac{C_2-C_1e^{2t}-2x_2^2}{\frac{\delta}{2}x_2+e^{2t}}, \tag{90}$$

$$\dot{x}_2=-\delta\left(C_1e^{2t}+x_2^2+e^{2t}\frac{C_2-C_1e^{2t}-2x_2^2}{\frac{\delta}{2}x_2+e^{2t}}\right)^{1/2}+2\left(C_1e^{2t}+x_2^2+e^{2t}\frac{C_2-C_1e^{2t}-2x_2^2}{\frac{\delta}{2}x_2+e^{2t}}\right)^{1/2}x_2e^{-2t}.$$

TABLE I. Examples of Hamiltonian systems given in the text. In each example we give a Hamiltonian H and a Poisson structure J [J is given in terms of μ, Ψ by Eq. (4)].

	Poisson matrix		Hamiltonian
System	Ψ	μ	
Euler	$-\frac{1}{2}(x_1^2+x_2^2+x_3^2)$	1	$\frac{x_1^2}{2I_1}+\frac{x_2^2}{2I_2}+\frac{x_3^2}{2I_3}$
Lotka–Voltera	$\ln\frac{x_3^c x_2^{bc}}{x_1}$	$x_1x_2x_3$	$a(bx_1-x_3)+x_2+\ln\frac{x_2^\nu}{x_3^\mu}$
Lorenz	$\frac{1}{4}(x_3-x_1^2)$	1	$x_2^2+x_3^2$
Kermac–Mackendric	$x_1+x_2+x_3$	x_1x_2	$a\ln x_1+rx_3$
May–Leonard	$\frac{1}{(1-\alpha)^2}(x_2^{1-\alpha}-x_1^{1-\alpha})$	1	$x_1^{1-\alpha}-x_3^{1-\alpha}$
Maxvel–Bloch	$-\frac{1}{2v}(x_2^2+x_3^2)$	1	$\frac{1}{2}\alpha(x_2^2+x_3^2)-\frac{1}{v}(x_3+x_1^2)$
Lor.(1)	$-\left(\frac{r}{\sigma}x_1^2+x_2^2\right)\frac{e^{(\sigma-1)t}}{4}-x_3^2\frac{e^{(1-3\sigma)t}}{4}$	1	$x_1^2-2\sigma x_3$
Lor.(3)	$-\frac{1}{4}x_1^2e^{-\sigma t}+\frac{\sigma}{2}x_3e^{(\sigma-1)t}$	1	$x_2^2+x_3^2$
Lor.(5)	$\frac{1}{4}x_1^2e^{-t}-\frac{1}{2}x_3$	1	$-rx_1^2+x_2^2+x_3^2$
Rab.(1)	$\frac{1}{8}x_1^2-\frac{1}{8}x_2^2-\frac{1}{4}x_3^2e^{-2\nu t}$	1	$x_1^2+x_2^2-4hx_3$
Rab.(2)	$\frac{1}{8}x_1^2e^{-\nu t}+\frac{1}{8}x_2^2e^{-\nu t}-\frac{1}{2}hx_3$	1	$x_1^2-x_2^2-2x_3^2$
Rab.(3)	$\frac{1}{4}x_2^2e^{(\nu_3-2\nu)t}+\frac{1}{4}x_3^2e^{-\nu_3 t}$	1	$x_1^2+x_2^2$
Rab.(4)	$-\frac{1}{4}x_1^2e^{-\nu t}-\frac{1}{4}x_2^2e^{\nu_1 t}+hx_3e^{\nu_1 t}$	1	$x_2^2+(h-x_3)^2$
Rab.(5)	$\frac{1}{4}x_1^2e^{\nu_2 t}+\frac{1}{4}x_2^2e^{-\nu_2 t}-hx_3e^{\nu_2 t}$	1	$x_1^2-(h+x_3)^2$
Rab.(6)	$-\frac{1}{4}x_1^2e^{-\nu_1 t}-\frac{1}{4}x_2^2e^{(\nu_1-2\nu_2)t}$	1	$x_2^2+x_3^2$
Rab.(7)	$\frac{1}{4}x_1^2e^{(\nu_2-2\nu_3)t}+\frac{1}{4}x_2^2e^{-\nu_2 t}$	1	$x_1^2-x_3^2$
RTW.(1)	$\frac{1}{2}(x_1^2-x_2^2+x_3e^{-t})$	1	$x_3(2x_2-\delta)$
RTW.(2)	$-\frac{\delta}{2}x_1^2-\left(\frac{\delta}{2}x_2^2+x_3x_2\right)e^{-t}$	1	$x_1^2+x_2^2+x_3$
RTW.(3)	$(x_1^2-x_2^2+x_3)e^{-t}$	1	x_2x_3
RTW.(4)	$(x_1^2-x_2^2)e^{\gamma t}+x_3e^{-(\gamma+2)t}$	1	x_2x_3
RTW.(5)	$\frac{\delta e^{-2t}}{2}(x_1^2-x_2^2)+\frac{\delta}{2}x_3$	1	$x_1^2+x_2^2+\frac{2}{\delta}x_2x_3$

The Poisson structure is given by

$$u=e^{-(2+\gamma)t},\qquad v=2x_2e^{\gamma t},\qquad w=2x_1e^{\gamma t}. \tag{91}$$

It has no irregular points.

V. CONCLUSION

We considered the Jacobi equation for the case $N=3$. We have found the most general Poisson structure J in the neighborhood of regular points. This form is quite suitable for the study of the multi-Hamiltonian structure of the system. We found all possible compatible Poisson structures and corresponding bi-Hamiltonian systems. We studied our solution in the neighborhood of the irregular points of the Poisson structure and showed that it keeps its form. As an application of our results we gave several examples which were reported earlier[8–15] as bi-Hamiltonian systems. In these examples we give the Casimirs, components of the Poisson matrix, the reduced equations and irregular points. Among all examples that we observed, only the Lotka–Voltera system has a special position. Our solution is not valid in the neighborhood of irregular points for this system. On the other hand the Hamiltonian function is not defined at such points as well. Hence the Lotka–Voltera equation does not have the Hamiltonian formulation in the neighborhood of such points.

ACKNOWLEDGMENTS

We would like to thank Dr. J. Grabowski and Dr. G. Marmo for drawing our attention to their work.[3] We thank to Dr. P. Olver for his constructive criticisms. We also thank the referee for several suggestions. This work was partially supported by the Scientific and Technical Research Council of Turkey and by the Turkish Academy of Sciences.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Lax pair and super-Yangian symmetry of the nonlinear super-Schrödinger equation

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(Received 10 June 2003; accepted 4 September 2003)

We consider a version of the nonlinear Schrödinger equation with M bosons and N fermions. We first solve the classical and quantum versions of this equation, using a super-Zamolodchikov–Faddeev (ZF) algebra. Then we prove that the hierarchy associated to this model admits a super-Yangian $Y(gl(M|N))$ symmetry. We exhibit the corresponding (classical and quantum) Lax pairs. Finally, we construct explicitly the super-Yangian generators, in terms of the canonical fields on the one hand, and in terms of the ZF algebra generators on the other hand. The latter construction uses the well-bred operators introduced recently. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625078]

I. INTRODUCTION

The nonlinear Schrödinger (NLS) equation is one of the most studied systems in quantum integrable systems (for a review, see, e.g., Ref. 1), and its simplest (scalar) version played an important role in the development of the (quantum) inverse scattering method.[2] As usual in quantum integrable systems, its integrability relies on the existence of an infinite-dimensional symmetry algebra. In integrable systems, natural candidates for such algebras are the celebrated quantum groups associated to (affine) Lie algebras, or the Yangians. Indeed, it is known[3] that the quantum NLS model with spin 1/2 fermions and repulsive interaction on the line has a Yangian symmetry $Y(sl(2))$. More generally, its vectorial version, based on N-component bosons or on N-component fermions, was shown to possess a $Y(gl(N))$ symmetry.[4] The integrability can also be grounded on the existence of an infinite series of mutually commuting Hamiltonians, which thus generates a whole hierarchy of equations. In the case of scalar NLS equation, the hierarchy contains well-known models, such as the modified KdV equation.

It was natural to seek a supersymmetric version (including both bosons and fermions) of these models which admits the super-Yangian based on superalgebras $gl(M|N)$ as symmetry algebra. Different versions of such a generalization were already proposed, from the simple boson-fermion systems related to NLS,[5,6] or superfields formulation[7,8] of NLS, up to more algebraic studies of these models.[9,10] The difficulty with such generalizations is to keep the fundamental notion of integrability while allowing for the existence of supersymmetry. Even when some of the suggested supersymmetric systems were shown to pass some integrability conditions,[11] the status of such models remained not clearly established, and one is still looking for, e.g., their Lax presentation or their underlying infinite-dimensional symmetry algebra.

Another $\mathbb{Z}_2$-graded version of NLS was introduced by Kulish,[12] the fields being super-matrix valued and thus associated to both fermions and bosons. However, only the finite interval was studied, using the thermodynamical Bethe ansatz (see also Ref. 13), and the explicit quantum solutions are not known. The symmetry (super) algebra is also lacking in this presentation.

The aim of this article is to present a ''super-vectorial'' version (close to the matricial version introduced by Kulish) of the NLS model on the infinite line which includes M bosons **and** N

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fermions fields. The advantage of this version relies on its manifest integrability and the existence of quantum canonical solutions, which we will explicitly construct using a super-ZF algebra (Sec. II). Indeed, these solutions can be associated to a whole hierarchy of mutually commuting Hamiltonians, as it should be for an integrable model. It also admits, as we will show (Sec. III), a Lax presentation both at classical and quantum level (without using a superfield formalism). As usual, the Lax pair presentation allows us to recover the hierarchy of our super-NLS equation. Finally, this super-NLS hierarchy possesses a super-Yangian symmetry and we will construct it, both using the quantum canonical solutions or the super-ZF generators (Sec. IV).

II. NONLINEAR SUPER-SCHRÖDINGER EQUATION

A. The usual nonlinear Schrödinger equation

The NLS equation reads

$$(i\partial_t+\partial_x^2)\phi_i(x,t)=2g\phi^{\dagger j}(x,t)\phi_j(x,t)\phi_i(x,t),\quad i=1,...,N,\quad \text{with } g>0, \tag{2.1}$$

where summation over repeated indices is understood. It is obtained from the (time-independent) Hamiltonian

$$H(\phi_i,\phi_j^\dagger)=\int_{-\infty}^{\infty}dx(\partial_x\phi^{\dagger j}(x)\partial_x\phi_j(x)+g\phi^{\dagger i}(x)\phi^{\dagger j}(x)\phi_j(x)\phi_i(x)) \tag{2.2}$$

using the Hamiltonian equation of motion $\partial_t F=\{H,F\}$, valid for any functional $F(\phi_i,\phi_j^\dagger)$, where the Poisson bracket (PB) is canonically associated to ϕ and $\phi^\dagger$.

A solution *à la Rosales*[14] can be written as follows:

$$\phi_i(x,t)=\sum_{n=0}^{\infty}(-g)^n\phi_i^{(n)}(x,t),\quad g>0, \tag{2.3}$$

with

$$\begin{aligned}
\phi_i^{(n)}(x,t)&=\int_{\mathbb{R}^{2n+1}}d^n\mathbf{p}d^{n+1}\mathbf{q}\lambda^{k_1}(p_1)\cdots\lambda^{k_n}(p_n)\lambda_{k_n}(q_n)\cdots\lambda_{k_1}(q_1)\lambda_i(q_0)\frac{e^{i\Omega_n(x,t;\mathbf{p},\mathbf{q})}}{Q_n(\mathbf{p},\mathbf{q},0)},\\
\Omega_n(x,t;\mathbf{p},\mathbf{q})&=\sum_{j=0}^{n}(q_jx-q_j^2t)-\sum_{i=1}^{n}(p_ix-p_i^2t),\\
Q_n(\mathbf{p},\mathbf{q},\varepsilon)&=\prod_{i=1}^{n}(p_i-q_{i-1}+i\varepsilon)(p_i-q_i+i\varepsilon),\\
d^n\mathbf{p}d^{n+1}\mathbf{q}&=\prod_{\substack{i=1\\j=0}}^{n}\frac{dp_i}{2\pi}\frac{dq_j}{2\pi},
\end{aligned} \tag{2.4}$$

where we have denoted $\mathbf{p}=(p_1,\ldots,p_n)$, $\mathbf{q}=(q_0,\ldots,q_n)$.

The Rosales solution is fundamental since its structure is preserved upon quantization[15] and we shall see below that this result survives when one includes fermions. The NLS equation and its hierarchy admit the Yangian $Y(gl(N))$ as symmetry, and the explicit construction of its generators was given in Ref. 3 [for $sl(2)$, in terms of canonical fields] and Ref. 4 [for $sl(N)$, in terms of the ZF generators]. A Lax pair formulation can be found in Refs. 16 and 17 (for NLS equation) and in Refs. 18 and 19 (for its vectorial generalization).

B. Classical nonlinear super-Schrödinger equation

We consider a generalized version of the NLS equation which includes both bosons and fermions. Due to the use of auxiliary spaces (see the Appendix), the corresponding equation will formally look like the original one, but let us insist that the present version is a ''supersymmetric'' version of it. While the similarities allow us to build the solution of the nonlinear super-Schrödinger equation, the differences will appear, for instance, in the nature of the symmetry algebra (see below).

We define $\Phi(x)=\sum_{j=1}^{M+N}\phi_j(x)e_j$, where e_j is an $(M+N)$-column vector in the auxiliary space and summation is understood for repeated indices. Here ϕ_j, $j=1,...,M$, and ϕ_j, $j=M+1,...,M+N$, are the bosonic and fermionic components, respectively. By fermionic functions, we mean Grassmann-valued functions depending on the real variable x, the integrations throughout the article being always in real (or complex) variables. For convenience, we set $K=M+N$. We shall also need adjoints of the fields

$$\Phi^\dagger(x)=\phi_i^\dagger(x)e_i^\dagger, \quad x\in\mathbb{R}. \tag{2.5}$$

The Hamiltonian reads

$$H(\Phi,\Phi^\dagger)=\int_{-\infty}^{\infty}dx(\partial_x\Phi^\dagger(x)\partial_x\Phi(x)+g(|\Phi(x)|^2)^2), \tag{2.6}$$

or, in components,

$$H(\Phi,\Phi^\dagger)=\int_{-\infty}^{\infty}dx(\partial_x\phi^{\dagger j}(x)\partial_x\phi_j(x)+g\phi^{\dagger j}(x)\phi^{\dagger k}(x)\phi_k(x)\phi_j(x)). \tag{2.7}$$

The canonical Poisson brackets for the basic fields $\Phi(x)$, $\Phi^\dagger(y)$ with corresponding components $\phi_i(x)$, $\phi_j^\dagger(y)$ take the following form:

$$\{\Phi_1(x),\Phi_2^\dagger(y)\}=i\delta_{12}\delta(x-y)=-\{\Phi_2^\dagger(y),\Phi_1(x)\} \quad \text{(globally)}, \tag{2.8}$$

$$\{\phi_j(x),\phi_k^\dagger(y)\}=i\delta_{jk}\delta(x-y)=-(-1)^{[j][k]}\{\phi_k^\dagger(y),\phi_j(x)\} \quad \text{(in components)}. \tag{2.9}$$

The field $\Phi(x,t)$ of components $\phi_i(x,t)$ satisfies the following Hamiltonian equation of motion which we call the classical nonlinear super-Schrödinger (NLSS) equation:

$$i\partial_t\Phi(x,t)=-\partial_x^2\Phi(x,t)+2g|\Phi(x,t)|^2\Phi(x,t) \quad \text{(globally)}, \tag{2.10}$$

$$i\partial_t\phi_j(x,t)=-\partial_x^2\phi_j(x,t)+2g(\phi_k^\dagger(x,t)\phi_k(x,t))\phi_j(x,t) \quad \text{(in components)}. \tag{2.11}$$

These equations are simply derived from the Hamiltonian equations of motion $\partial_t\Phi(x,t)=\{H,\Phi(x,t)\}$ and $\partial_t\phi_i(x,t)=\{H,\phi_i(x,t)\}$. The equations of motion are (formally) the same as the usual ones and the solution *à la Rosales* (2.3) and (2.4) is still valid in our case:

Theorem 2.1: *The solution of the classical NLSS equation (2.11) is given by*

$$\phi_j(x,t)=\sum_{n=0}^{\infty}(-g)^n\phi_j^{(n)}(x,t) \quad where \tag{2.12}$$

$$\phi_j^{(n)}(x,t)=\int_{\mathbb{R}^{2n+1}}d^n\mathbf{p}d^{n+1}\mathbf{q}\sum_{k_1,\ldots,k_n=1}^{K}\lambda_{k_1}^\dagger(p_1)\cdots\lambda_{k_n}^\dagger(p_n)\lambda_{k_n}(q_n)\cdots\lambda_{k_1}(q_1)\lambda_j(q_0)\frac{e^{i\Omega_n(x,t;\mathbf{p},\mathbf{q})}}{Q_n(\mathbf{p},\mathbf{q},0)}, \tag{2.13}$$

using the same notations as in (2.4).

Proof: Substituting into the NLSS equation, it amounts to the following identity being satisfied,

$$\sum_{j=0}^{n} q_j^2 - \sum_{i=1}^{n} p_i^2 - \left(\sum_{j=0}^{n} q_j - \sum_{i=1}^{n} p_i \right)^2 = -2 \sum_{c=1}^{n-1} \sum_{a=1}^{c} (p_{a+1} - q_a)(p_{c+1} - q_{c+1}),$$

which is readily seen to hold. ■

Note that, due to the $\mathbb{Z}_2$-graded tensor product, the ordering of the $\lambda^\dagger$'s and of the λ's, respectively, matters.

C. Quantizing NLSS

1. Graded ZF algebra

We write a graded version of the ZF algebra,[20,21] using auxiliary spaces and entities containing bosonic and fermionic components (see the Appendix):

$$\mathbf{A}(k) = a_i(k) e_i \quad \text{and} \quad \mathbf{A}^\dagger(k) = a_i^\dagger(k) e_i^\dagger, \quad k \in \mathbb{R}. \tag{2.14}$$

Definition 2.2: The graded ZF algebra reads

$$\mathbf{A}_1(k_1)\mathbf{A}_2(k_2) = R_{21}(k_2 - k_1)\mathbf{A}_2(k_2)\mathbf{A}_1(k_1), \tag{2.15}$$

$$\mathbf{A}_1^\dagger(k_1)\mathbf{A}_2^\dagger(k_2) = \mathbf{A}_2^\dagger(k_2)\mathbf{A}_1^\dagger(k_1)R_{21}(k_2 - k_1), \tag{2.16}$$

$$\mathbf{A}_1(k_1)\mathbf{A}_2^\dagger(k_2) = \mathbf{A}_2^\dagger(k_2)R_{12}(k_1 - k_2)\mathbf{A}_1(k_1) + \boldsymbol{\delta}_{12}\delta(k_1 - k_2), \tag{2.17}$$

where

$$R_{12}(k) = \frac{k\mathbb{1}\otimes\mathbb{1} - igP_{12}}{k + ig} \tag{2.18}$$

is the R-matrix for the super-Yangian $Y(gl(M|N)) \equiv Y(M|N)$, *and* P_{12} *is the super-permutation operator:*

$$P_{12} = \sum_{i,j=1}^{K} (-1)^{[j]} E_{ij} \otimes E_{ji}. \tag{2.19}$$

Note that for even vectors u, v and even matrices B, C (as defined in the Appendix), one has $P_{12}(u \otimes v) = v \otimes u$ and $P_{12}(B \otimes C)P_{12} = C \otimes B$.

The R-matrix has the following useful properties:

$$R_{21}(k) = R_{12}(k), \tag{2.20}$$

$$R_{12}(k_1 - k_2)R_{21}(k_2 - k_1) = \mathbb{1}\otimes\mathbb{1}, \tag{2.21}$$

$$R_{12}^\dagger(k_1 - k_2) = R_{21}(k_2 - k_1). \tag{2.22}$$

For quantities of definite $\mathbb{Z}_2$-grade, we define their super-commutator by

$$[\![B, C]\!] = BC - (-1)^{[B][C]}CB. \tag{2.23}$$

Then, after some calculations, one shows that the component version of the ZF algebra reads $(j, k = 1, \ldots, K)$

$$[\![a_j(k_1),a_k(k_2)]\!]=\frac{-ig}{k_2-k_1+ig}(a_j(k_2)a_k(k_1)+(-1)^{[j][k]}a_k(k_2)a_j(k_1)), \tag{2.24}$$

$$[\![a_j^\dagger(k_1),a_k^\dagger(k_2)]\!]=\frac{-ig}{k_2-k_1+ig}(a_j^\dagger(k_2)a_k^\dagger(k_1)+(-1)^{[j][k]}a_k^\dagger(k_2)a_j^\dagger(k_1)), \tag{2.25}$$

$$[\![a_j(k_1),a_k^\dagger(k_2)]\!]=\frac{-ig}{k_1-k_2+ig}\left((-1)^{[j][k]}a_k^\dagger(k_2)a_j(k_1)+\delta_{jk}\sum_{\ell=1}^{K}a_\ell^\dagger(k_2)a_\ell(k_1)\right)+\delta_{jk}\delta(k_1-k_2). \tag{2.26}$$

Note that these relations ensure the existence of a PBW basis, generated by the monomials having $a^\dagger$'s on the left of the a's, the a's on one hand, and the $a^\dagger$'s on the other hand, being ordered according to the magnitude of the "impulsions" k_j.

2. Fock representation

The previous algebra can be represented on a Fock space, which is most useful for our quantization of NLSS, and we follow the basic ideas of Ref. 15 (further developed in, e.g. Refs. 22 and 23). A detailed presentation of the graded version when $M=N=1$ has been given in Ref. 24. The general case follows the same lines, so that we just sketch the results, referring to Ref. 24 for more details about the $\mathbb{Z}_2$-graded case.

We introduce $\mathcal{F}_R=\oplus_{n=0}^{\infty}\mathcal{H}_R^n$ where $\mathcal{H}_R^0=\mathbb{C}$,

$$\mathcal{H}_R^1=\left\{\boldsymbol{\varphi}(p)=\sum_{j=1}^{K}\varphi_j(p)e_j \ \text{ s.t. } \ \varphi_j\in L^2(\mathbb{R}),j=1,...,K\right\}\equiv KL^2(\mathbb{R}),$$

and for $n\geqslant 2$

$$\begin{aligned}\mathcal{H}_R^n=\Bigg\{&\boldsymbol{\varphi}_{1\ldots n}(p_1,\ldots,p_n)\\ &=\sum_{i_1,\ldots,i_n=1}^{K}\varphi_{i_1,\ldots,i_n}(p_1,\ldots,p_n)(e_{i_1}\otimes\cdots\otimes e_{i_n}) \ \text{ s.t. } \ \varphi_{i_1,\ldots,i_n}\in L^2(\mathbb{R}^n),\\ &i_1,\ldots,i_n=1,...,K, \quad \text{and } \boldsymbol{\varphi}_{1\ldots i,i+1\ldots n}(p_1,\ldots,p_i,p_{i+1},\ldots,p_n)\\ &\qquad=R_{i,i+1}(p_i-p_{i+1})\boldsymbol{\varphi}_{1\ldots i+1,i\ldots n}(p_1,\ldots,p_{i+1},p_i,\ldots,p_n).\end{aligned}$$

There exists a (vacuum) vector $\Omega\in\mathcal{D}$ which is cyclic with respect to $\mathbf{A}^\dagger(k)$ and annihilated by $\mathbf{A}(k)$.

The scalar product which we define below on $\mathcal{H}_R^n$ provides the usual L^2 topology and $\mathcal{F}_R$ is the completed vector space over $\mathbb{C}$ for this topology.

The sesquilinear form $\langle,\rangle$ defined on $\mathcal{H}_R^n\times\mathcal{H}_R^n$, $n\geqslant 1$, by

$$\langle\boldsymbol{\varphi},\boldsymbol{\psi}\rangle=\int_{\mathbb{R}^n}d^np\ \boldsymbol{\varphi}_{1\ldots n}^\dagger(p_1,\ldots,p_n)\boldsymbol{\psi}_{1\ldots n}(p_1,\ldots,p_n), \tag{2.27}$$

$$\boldsymbol{\varphi}_{1\ldots n}^\dagger(p_1,\ldots,p_n)=(-1)^{\sum_{k=1}^{n-1}([i_1]+\cdots+[i_k])[i_{k+1}]}\overline{\varphi^{i_1\cdots i_n}}(e_{i_1}^\dagger\otimes e_{i_2}^\dagger\otimes\cdots\otimes e_{i_n}^\dagger) \tag{2.28}$$

is a (Hermitian) scalar product.

We introduce the finite particle space $\mathcal{F}_R^0\subset\mathcal{F}_R$, spanned by the sequences $(\varphi,\boldsymbol{\varphi}_1,\ldots,\boldsymbol{\varphi}_{1\cdots n},\ldots)$ with $\boldsymbol{\varphi}_{1\cdots n}\in\mathcal{H}_R^n$ and $\boldsymbol{\varphi}_{1\cdots n}=0$ for n large enough. As (2.27) is defined for all n, it extends naturally to $\mathcal{F}_R^0$. In this context, the vacuum state is $\Omega=(1,0,...,0,...)$, so that it is normalized to 1.

We are now able to define the (smeared) creation and annihilation operators $A(\mathbf{f})$ and $A^\dagger(\mathbf{f})$ on $\mathcal{F}_R^0$ through their action: $A(\mathbf{f})\Omega=0$ and for $\boldsymbol{\varphi}_{0\cdots n}\in\mathcal{H}_R^{n+1}$,

$$[A(\mathbf{f})\boldsymbol{\varphi}]_{1\cdots n}(p_1,\ldots,p_n)=\sqrt{n+1}\int_{\mathbb{R}}dp_0\,\mathbf{f}_0^{\dagger}(p_0)\boldsymbol{\varphi}_{0\cdots n}(p_0,p_1,\ldots,p_n). \tag{2.29}$$

Similarly, for $\boldsymbol{\varphi}_{1\ldots n}\in\mathcal{H}_R^n$:

$$[A^{\dagger}(\mathbf{f})\boldsymbol{\varphi}]_{0\cdots n}(p_0,\ldots,p_n)=\frac{1}{\sqrt{n+1}}\boldsymbol{\varphi}_{1\cdots n}(p_1,\ldots p_n)f_0(p_0)+\frac{1}{\sqrt{n+1}}\sum_{k=1}^{n}R_{k-1,k}(p_{k-1}-p_k)\cdots R_{0k}(p_0-p_k)\boldsymbol{\varphi}_{0\cdots\hat{k}\cdots n}(p_0,\ldots,\widehat{p_k},\ldots,p_n)\mathbf{f}_k(p_k), \tag{2.30}$$

where the hatted symbols are omitted.

It is easily checked that (2.29) and (2.30) are indeed elements of $\mathcal{H}_R^n$ and $\mathcal{H}_R^{n+1}$, respectively. Therefore, we have operators acting on $\mathcal{F}_R^0$ (linearity in $\boldsymbol{\varphi}$ obvious) with the additional property that they are bounded (i.e., continuous) on each finite particle sector $\mathcal{H}_R^n$. Another essential feature is the adjointness of these operators with respect to $\langle,\rangle$:

$$\forall\boldsymbol{\varphi}\in\mathcal{H}_R^n,\ \ \forall\boldsymbol{\psi}\in\mathcal{H}_R^{n+1},\quad \forall\mathbf{f}\in\mathcal{H}_R^1,\quad \langle\boldsymbol{\varphi},A(\mathbf{f})\boldsymbol{\psi}\rangle=\langle A^{\dagger}(\mathbf{f})\boldsymbol{\varphi},\boldsymbol{\psi}\rangle. \tag{2.31}$$

At this stage, the Fock representations $\mathbf{A}(p)$, $\mathbf{A}^{\dagger}(p)$ of the generators of the ZF algebra appear as operator-valued distributions through the definition

$$A(\mathbf{f})=\int_{\mathbb{R}}dp\,\mathbf{f}^{\dagger}(p)\mathbf{A}(p),\quad A^{\dagger}(\mathbf{f})=\int_{\mathbb{R}}dp\,\mathbf{A}^{\dagger}(p)\mathbf{f}(p). \tag{2.32}$$

It is readily shown from these definitions that $\mathbf{A}(p)$ and $\mathbf{A}^{\dagger}(p)$ satisfy the exchange relations (2.15)–(2.17), thus providing the desired representation.

We now have all the ingredients to deduce results for the whole Fock space $\mathcal{F}_R$ while working on smaller and more intuitive spaces dense in $\mathcal{F}_R$, using the continuity of the operators. In our case, one has to define such a "state space" $\mathcal{D}\subset\mathcal{F}_R$ in the sense of distributions as follows: $\mathcal{D}^0=\mathbb{C}$ and

$$\mathcal{D}^n=\left\{\int_{\mathbb{R}^n}d^np\,\mathbf{A}_1^{\dagger}(p_1)\cdots\mathbf{A}_n^{\dagger}(p_n)\Omega\mathbf{f}(p_1,\ldots,p_n);\ \ \mathbf{f}\in K^nL^2(\mathbb{R}^n)\right\},\quad n\geqslant 1.$$

Then, $\mathcal{D}$ is spanned by the sequences $\boldsymbol{\chi}=(\chi,\boldsymbol{\chi}_1,\ldots,\boldsymbol{\chi}_{1\cdots n},\ldots)$, where $\boldsymbol{\chi}_{1\cdots n}\in\mathcal{D}^n$ and $\boldsymbol{\chi}_{1\cdots n}=0$ for n large enough. We also define

$$\mathcal{D}_0^0=\mathbb{C},\quad \mathcal{D}_0^n=\{\tilde{A}_1^{\dagger}(\mathbf{f}_1,t)\cdots\tilde{A}_n^{\dagger}(\mathbf{f}_n,t)\Omega,\mathbf{f}_1>\cdots>\mathbf{f}_n\}\subset\mathcal{H}_R^n,\quad n\geqslant 1, \tag{2.33}$$

where

$$\begin{aligned}\tilde{A}^{\dagger}(\mathbf{f},t)&=\int_{\mathbb{R}}dx\tilde{\mathbf{A}}^{\dagger}(x,t)\mathbf{f}(x),\\ \tilde{\mathbf{A}}^{\dagger}(x,t)&=\int_{\mathbb{R}}dp\mathbf{A}^{\dagger}(p)e^{iqx-iq^2t},\end{aligned}\qquad x,t\in\mathbb{R}, \tag{2.34}$$

and the space $\mathcal{D}_0$ is the linear span of sequences $\boldsymbol{\chi}=(\chi,\boldsymbol{\chi}_1,\ldots,\boldsymbol{\chi}_{1\cdots n},\ldots)$, where $\boldsymbol{\chi}_{1\cdots n}\in\mathcal{D}_0^n$ and $\boldsymbol{\chi}_{1\cdots n}=0$ for n large enough. We also introduce the following partial ordering relation:

$$\mathbf{f}>\mathbf{g}\Leftrightarrow\forall i,j=1,\ldots,K,\quad \forall x\in\mathrm{supp}(\mathbf{f}_i),\quad \forall y\in\mathrm{supp}(g_j),\quad x>y,$$

which is just the extension of the ordering of the momenta k_i in the definition of a state space basis $|k_1,\ldots,k_n\rangle$. Then, one shows that $\mathcal{D}$ and $\mathcal{D}_0$ are dense in $\mathcal{F}_R$.

Summarizing, we have constructed a graded ZF algebra and its Fock representation $\mathcal{F}_R$ and, inspired by earlier works,[15,16,25–27] we shall see that this allows us to construct the quantum version of NLSS and its solution.

3. Quantization of the fields

Following Refs. 15 and 27, we simply write the quantum version of $\phi_j^{(n)}(x,t)$ as

$$\phi_j^{(n)}(x,t)=\int_{\mathbb{R}^{2n+1}} d^n\mathbf{p}\, d^{n+1}\mathbf{q} \sum_{k_1,\dots,k_n=1}^{K} a_{k_1}^\dagger(p_1)\cdots a_{k_n}^\dagger(p_n)a_{k_n}(q_n)\cdots a_{k_1}(q_1)a_j(q_0)\frac{e^{i\Omega_n(x,t;\mathbf{p},\mathbf{q})}}{Q_n(\mathbf{p},\mathbf{q},\varepsilon)} \tag{2.35}$$

using the same notations as in (2.4) and an $i\epsilon$ contour prescription. The global field reads

$$\Phi(x,t)=\sum_{n=0}^{\infty}(-g)^n\Phi^{(n)}(x,t) \quad \text{with} \quad \Phi^{(n)}(x,t)=\phi_j^{(n)}(x,t)e_j\,. \tag{2.36}$$

From (2.31), we deduce

$$\Phi^\dagger(x,t)=\sum_{n=0}^{\infty}(-g)^n\Phi^{\dagger(n)}(x,t) \tag{2.37}$$

with

$$\Phi^{\dagger(n)}(x,t)=\int_{\mathbb{R}^{2n+1}} d^n\mathbf{p}\, d^{n+1}\mathbf{q}\mathbf{A}^\dagger(q_0)\mathbf{A}_1^\dagger(q_1)\cdots\mathbf{A}_n^\dagger(q_n)\mathbf{A}_n(p_n)\cdots\mathbf{A}_1(p_1)\frac{e^{-i\Omega_n(x,t;\mathbf{p},\mathbf{q})}}{Q_n(\mathbf{p},\mathbf{q},-\varepsilon)}. \tag{2.38}$$

Just like we dealt with $A(\mathbf{f})$ and $A^\dagger(\mathbf{f})$, we are naturally led to introduce

$$\Phi(\mathbf{f},t)=\int_{\mathbb{R}}\mathbf{f}^\dagger(x)\Phi(x,t), \quad \Phi^\dagger(\mathbf{f},t)=\int_{\mathbb{R}}\Phi^\dagger(x,t)\mathbf{f}(x). \tag{2.39}$$

And just like we did in Ref. 24, one shows that $\Phi(\mathbf{f},t)$ and $\Phi^\dagger(\mathbf{f},t)$ are indeed well-defined operators on a common invariant domain which turns out to be $\mathcal{D}_0$. These fields also satisfy the following fundamental requirement.

Theorem 2.3: *The quantum fields* $\Phi(\mathbf{f},t)$, $\Phi^\dagger(\mathbf{g},t)$ *satisfy the equal time canonical commutation relations as operators on* $\mathcal{F}_R^0$

$$[\Phi(\mathbf{f},t),\Phi(\mathbf{g},t)]=[\Phi^\dagger(\mathbf{f},t),\Phi^\dagger(\mathbf{g},t)]=0, \tag{2.40}$$

$$[\Phi(\mathbf{f},t),\Phi^\dagger(\mathbf{g},t)]=\langle\mathbf{f},\mathbf{g}\rangle. \tag{2.41}$$

Proof: The proof is the same as in the ordinary NLS equation, see Ref. 15 or 23 for details. ■

One then deduces the equal time CCR in components for the operator-valued distributions $\phi_j(x,t)$, $\phi_k^\dagger(y,t)$:

$$[\![\phi_j(x,t),\phi_k(y,t)]\!]=[\![\phi_j^\dagger(x,t),\phi_k^\dagger(y,t)]\!]=0, \tag{2.42}$$

$$[\![\phi_j(x,t),\phi_k^\dagger(y,t)]\!]=\delta_{jk}\delta(x-y). \tag{2.43}$$

Let us remind that for $j,k=M+1,\dots K$, the above CCR correspond to anticommutator, consistent with the fermionic nature of these fields.

4. Time evolution

We first wish to emphasize that the form of the Hamiltonian (2.7) cannot be reproduced here owing to the nature of the fields (products of distributions are not defined). Fortunately, the power of the ZF algebra and the quantum inverse method [leading to (2.35) and (2.36)] rescues us by delivering a simple, freelike Hamiltonian in terms of oscillators. Indeed, one easily checks that the Hamiltonian defined by

$$H=\int_{\mathbb{R}} dp\, p^2 \mathbf{A}^\dagger(p)\mathbf{A}(p) \tag{2.44}$$

is self-adjoint, i.e., $H^\dagger=H$. Moreover,

$$\forall \boldsymbol{\varphi}\in\mathcal{D},\quad [H\boldsymbol{\varphi}]_{1\cdots n}(p_1,\ldots,p_n)=(p_1^2+\cdots+p_n^2)\boldsymbol{\varphi}_{1\cdots n}(p_1,\ldots,p_n), \tag{2.45}$$

which shows that $\mathcal{D}$ is also an invariant domain for H and that this operator has the correct eigenvalues. Finally, H generates the time evolution of the field:

$$\Phi(f,t)=e^{iHt}\Phi(f,0)e^{-iHt}. \tag{2.46}$$

Therefore, H, so defined, is the Hamiltonian of our quantum system.

Note that (2.45) and (2.46) have to be understood as operator equalities and must be evaluated on $\mathcal{D}$.

The freelike expression for H in terms of creation and annihilation oscillators may be surprising at first glance, but it is actually a mere consequence of the rather complicated exchange relations (2.15)–(2.17). One can say that the effect of the nonlinear term has been encoded directly in the oscillators instead of the Hamiltonian (or equivalently the Lagrangian) of the field theory, yielding a (possibly misleading) simple expression for H. One may finally wonder about the coupling constant which seems to disappear. Once again, it is actually present through the R-matrix in the exchange relations.

Besides, the quantum nonlinear super-Schrödinger equation holds in the following form:

$$\forall \boldsymbol{\varphi},\boldsymbol{\psi}\in\mathcal{D},\quad (i\partial_t+\partial_x^2)\langle\boldsymbol{\varphi},\Phi(x,t)\boldsymbol{\psi}\rangle=2g\langle\boldsymbol{\varphi},{:}\Phi\Phi^\dagger\Phi{:}(x,t)\boldsymbol{\psi}\rangle. \tag{2.47}$$

5. Correlation functions

Again following the case of NLS, one shows that for $\boldsymbol{\varphi},\boldsymbol{\psi}\in\mathcal{D}$, one has

$$\mathbf{f}>\mathbf{g},\quad \langle\boldsymbol{\varphi},\Phi^\dagger(\mathbf{g},t)\tilde{A}^\dagger(\mathbf{f},t)\boldsymbol{\psi}\rangle=\langle\boldsymbol{\varphi},\tilde{A}^\dagger(\mathbf{f},t)\Phi^\dagger(\mathbf{g},t)\boldsymbol{\psi}\rangle, \tag{2.48}$$

for $\mathbf{g}>\mathbf{f}_i$, $i=1,\ldots,n$,

$$\langle\boldsymbol{\varphi},\Phi^\dagger(\mathbf{g},t)\tilde{A}^\dagger(\mathbf{f}_1,t)\cdots\tilde{A}^\dagger(\mathbf{f}_n,t)\Omega\rangle=\langle\boldsymbol{\varphi},\tilde{A}^\dagger(\mathbf{g},t)\tilde{A}^\dagger(\mathbf{f}_1,t)\cdots\tilde{A}^\dagger(\mathbf{f}_n,t)\Omega\rangle \tag{2.49}$$

and for any $\mathbf{f}_1>\mathbf{f}_2>\cdots>\mathbf{f}_n$,

$$\langle\boldsymbol{\varphi},\Phi(\mathbf{g},t)\tilde{A}^\dagger(\mathbf{f}_1,t)\cdots\tilde{A}^\dagger(\mathbf{f}_n,t)\Omega\rangle=\sum_{j=1}^{n}\langle\mathbf{g},\mathbf{f}_j\rangle\langle\boldsymbol{\varphi},\tilde{A}^\dagger(f_1,t)\cdots\widehat{\tilde{A}^\dagger}(\mathbf{f}_j,t)\cdots\tilde{A}^\dagger(\mathbf{f}_n,t)\Omega\rangle. \tag{2.50}$$

This proves that the correlation functions of the NLSS model are completely determined, e.g.,

$$\langle \Omega, \Phi(\mathbf{g}_1,t)\cdots\Phi(\mathbf{g}_m,t)\Phi^\dagger(\mathbf{f}_1,t)\cdots\Phi^\dagger(\mathbf{f}_n,t)\Omega\rangle = \delta_{m,n}\sum_{\sigma\in S_n}\prod_{i=1}^{n}\langle \mathbf{g}_{\sigma(i)},\mathbf{f}_i\rangle,$$

$$\langle \boldsymbol{\varphi}_{1\cdots p}, \Phi(\mathbf{g}_1,t)\cdots\Phi(\mathbf{g}_n,t)\Phi^\dagger(\mathbf{f}_1,t)\cdots\Phi^\dagger(\mathbf{f}_m,t)\Omega\rangle$$
$$= \delta_{m,n+p}\sum_{\sigma\in S_{n+p}}\left(\prod_{i=1}^{n}\langle \mathbf{g}_{\sigma(i)},\mathbf{f}_i\rangle\right)\langle \boldsymbol{\varphi}_{1\cdots p}, \mathbf{g}_{\sigma(n+1)}\cdots\mathbf{g}_{\sigma(n+p)}\rangle.$$

Similar expressions can be obtained when dealing with the fields $\Phi(x,t)$ and $\Phi^\dagger(x,t)$.

III. LAX PAIR AND SUPER-YANGIAN SYMMETRY FOR NLSS

Let us stress once again that we aim at generalizing known results of integrability and symmetry for the nonlinear Schrödinger equation to the case of an arbitrary number of bosons **and** fermions. This physical motivation can be carried out by using appropriately the graded formalism presented in the Appendix. Furthermore, we also want to transport our results to the quantum case, which leads us to adopt the convenient Hamiltonian form of our model.

A. Classical Lax pairs

We define the Lax even super-matrix in $gl(M+1|N)$

$$L(\lambda;x) = \frac{i\lambda}{2}\Sigma + \Omega(x) \quad \text{with } \Sigma = \mathbb{I}_{K+1,K+1} - 2E_{K+1,K+1} \tag{3.1}$$

and

$$\Omega(x) = i\sqrt{g}\sum_{j=1}^{K}(\phi_j(x)E_{j,K+1} - \phi_j^\dagger(x)E_{K+1,j}). \tag{3.2}$$

Let us stress that, as above, the elementary matrices E_{jk} (with 1 at position j, k) are $\mathbb{Z}_2$-graded, with $[E_{jk}]=[j]+[k]$, $[j]=[K+1]=0$ for $1\leqslant j\leqslant M$ and $[j]=1$ for $M<j\leqslant K$. With this convention, the $gl(M+1|N)$ superalgebra has the unusual matrix form

$$\begin{pmatrix} M\times M & & M\times 1 \\ & N\times N & \\ 1\times M & & 1\times 1 \end{pmatrix},$$

where the size of the submatrices corresponding to bosonic generators have been explicitly written.

Using the PB of the ϕ's, it is easy to compute that

$$\{L_1(\lambda;x), L_2(\mu;y)\} = i\delta(x-y)[r(\lambda-\mu), L_1(\lambda;x) + L_2(\mu;y)] \tag{3.3}$$

with

$$r(\lambda-\mu) = \frac{g}{\lambda-\mu}\Pi_{12}, \tag{3.4}$$

where we have introduced the $(K+1)\times(K+1)$ super-permutation

$$\Pi_{12} = \sum_{i,j=1}^{K+1}(-1)^{[j]}E_{ij}\otimes E_{ji}.$$

Definition 3.1: We define the transition matrix by

$$\partial_x T(\lambda;x,y)=L(\lambda;x)T(\lambda;x,y), \quad x>y, \tag{3.5}$$

with the "initial condition" $T(\lambda;x,x)=\mathbb{I}$.

$T(\lambda;x,y)$ obeys the iterative equation

$$T(\lambda;x,y)=E(\lambda;x-y)+E(\lambda;x)\int_y^x dz\,\Omega(z)E(\lambda;z)T(\lambda;z,y), \tag{3.6}$$

where we have introduced

$$E(\lambda;x)=\exp\left(\frac{ix\lambda}{2}\Sigma\right)=e^{ix\lambda/2}\mathbb{I}_{K+1}+(e^{-ix\lambda/2}-e^{ix\lambda/2})E_{K+1,K+1}. \tag{3.7}$$

Property 3.2:

$$\{T_1(\lambda;x,y),T_2(\mu;x,y)\}=[r(\lambda-\mu),T(\lambda;x,y)\otimes T(\mu;x,y)]. \tag{3.8}$$

Proof: The equation (3.6) implies that

$$T(\lambda;x,y)=\sum_{n=0}^{\infty} T^{(n)}(\lambda;x,y), \tag{3.9}$$

$$T^{(n)}(\lambda;x,y)=\int_{\mathbb{R}^n} d^n z\,\theta(x>z_1>z_2>\cdots>z_n>y)E(\lambda;x-z_1)\Omega(z_1)$$
$$\times E(\lambda;z_1-z_2)\Omega(z_2)\cdots\Omega(z_n)E(\lambda;z_n-y). \tag{3.10}$$

It is then simple to show that

$$\{\Phi_1(w),T_2(\lambda;x,y)\}=\sqrt{g}\,\theta(x>w>y)T_2(\lambda;x,w)\sigma_{12}^- T_2(\lambda;w,y), \tag{3.11}$$

$$\{\Phi_2(w),T_1(\lambda;x,y)\}=\sqrt{g}\,\theta(x>w>y)T_1(\lambda;x,w)\sigma_{21}^- T_1(\lambda;w,y), \tag{3.12}$$

$$\{\Phi_1^\dagger(w),T_2(\lambda;x,y)\}=\sqrt{g}\,\theta(x>w>y)T_2(\lambda;x,w)\sigma_{12}^+ T_2(\lambda;w,y), \tag{3.13}$$

$$\{\Phi_2^\dagger(w),T_1(\lambda;x,y)\}=\sqrt{g}\,\theta(x>w>y)T_1(\lambda;x,w)\sigma_{21}^+ T_1(\lambda;w,y), \tag{3.14}$$

where we have defined

$$\sigma_{12}^-=\sum_{j=1}^{K} e_j\otimes E_{K+1,j}; \quad \sigma_{12}^+=\sum_{j=1}^{K}(-1)^{[j]}e_j^\dagger\otimes E_{j,K+1}. \tag{3.15}$$

From the form (A5) one also computes

$$\{\Phi_1(w),T_2(\lambda;x,y)\}=i(e_j\otimes\mathbb{I})\frac{\delta T_2(\lambda;x,y)}{\delta\phi_j^\dagger(w)}, \tag{3.16}$$

$$\{\Phi_2(w),T_1(\lambda;x,y)\}=i(\mathbb{I}\otimes e_j)\frac{\delta T_1(\lambda;x,y)}{\delta\phi_j^\dagger(w)}, \tag{3.17}$$

$$\{\Phi_1^\dagger(w),T_2(\lambda;x,y)\}=-i(-1)^{[j]}(e_j^\dagger\otimes\mathbb{I})\frac{\delta T_2(\lambda;x,y)}{\delta\phi_j(w)}, \tag{3.18}$$

$$\{\Phi_2^\dagger(w),T_1(\lambda;x,y)\}=-i(-1)^{[j]}(\mathbb{I}\otimes e_j^\dagger)\frac{\delta T_1(\lambda;x,y)}{\delta\phi_j(w)}. \tag{3.19}$$

This shows that the PB can be rewritten as

$$\{T_1(\lambda,x,y),T_3(\mu,x,y)\}=i\int_{\mathbb{R}}dw(\{\Phi_2^\dagger(w),T_1(\lambda;x,y)\}\{\Phi_2(w),T_3(\mu;x,y)\}$$
$$-\{\Phi_2^\dagger(w),T_3(\mu;x,y)\}\{\Phi_2(w),T_1(\lambda;x,y)\}). \tag{3.20}$$

Inserting (3.11) and (3.13) in this expression, one gets

$$\{T_1(\lambda;x,y),T_2(\mu;x,y)\}=ig\int_y^x dw\,T_1(\lambda;x,w)T_2(\mu;x,w)(\pi_{12}-\pi_{21})T_1(\lambda;w,y)T_2(\mu;w,y),$$
$$\text{where}\quad \pi_{12}=\sum_{j=1}^{K}E_{j,K+1}\otimes E_{K+1,j}. \tag{3.21}$$

Finally, a direct calculation shows that

$$\frac{\partial}{\partial w}(T_1(\lambda;x,w)T_2(\mu;x,w)\Pi_{12}T_1(\mu;w,y)T_2(\lambda;w,y))$$
$$=i\frac{\lambda-\mu}{2}T_1(\lambda;x,w)T_2(\mu;x,w)(\pi_{12}-\pi_{21})T_1(\lambda;w,y)T_2(\mu;w,y), \tag{3.22}$$

so that we get (3.8). ■

Property 3.3: The following limits are well defined:

$$T^-(\lambda;x)=\lim_{y\to-\infty}T(\lambda;x,y)E(\lambda;y), \tag{3.23}$$

$$T^+(\lambda;y)=\lim_{x\to\infty}E(\lambda;-x)T(\lambda;x,y), \tag{3.24}$$

$$T(\lambda)=T^+(\lambda;z)T^-(\lambda;z)=\lim_{\substack{x\to\infty\\ y\to-\infty}}E(\lambda;-x)T(\lambda;x,y)E(\lambda;y). \tag{3.25}$$

$T(\lambda)$ *is called the monodromy matrix.*

Proof: Using the equality $E(\lambda;x)\Omega(z)=\Omega(z)E(\lambda;-x)$, valid for any x, z, $T^{(n)}(\lambda;x,y)$ can be conveniently rewritten as

$$T^{(n)}(\lambda;x,y)=E(\lambda;x)\int_{\mathbb{R}^n}d^nz\,\theta(x>z_1>\cdots>z_n>y)$$
$$\times E\left(\lambda;2\sum_{j=1}^{n}(-1)^jz_j\right)\left(\prod_{k=1}^{n}\Omega(z_k)\right)E(\lambda;-y), \tag{3.26}$$

which shows that the limits are well defined. ■

Property 3.4:

$$\{T_1(\lambda),T_2(\mu)\}=r_+(\lambda-\mu)T(\lambda)\otimes T(\mu)-T(\lambda)\otimes T(\mu)r_-(\lambda-\mu) \tag{3.27}$$

with

$$r_+(\lambda-\mu)=\frac{g}{\lambda-\mu}(P_{12}+E_{K+1,K+1}\otimes E_{K+1,K+1})+i\pi g\,\delta(\lambda-\mu)(\pi_{12}-\pi_{21}), \tag{3.28}$$

$$r_-(\lambda-\mu)=\frac{g}{\lambda-\mu}(P_{12}+E_{K+1,K+1}\otimes E_{K+1,K+1})-i\pi g\,\delta(\lambda-\mu)(\pi_{12}-\pi_{21}), \tag{3.29}$$

where P_{12} is the super-permutation in the space of $K\times K$ matrices.

Proof: Direct calculation, plugging (3.25) into (3.8), and using the Cauchy principal value $\lim_{\lambda\to\infty} p.v.(e^{\pm i\lambda x}/x)=\pm i\pi\delta(x)$. ■

Introducing $t(\lambda)$, the $K\times K$ submatrix of $T(\lambda)$ with the last row and column removed, and $D(\lambda)=T_{K+1,K+1}(\lambda)$, one finally computes:

$$\{t_1(\lambda),t_2(\mu)\}=\frac{g}{\lambda-\mu}[P_{12},t(\lambda)\otimes t(\mu)], \tag{3.30}$$

$$\{D(\lambda),t(\mu)\}=0, \tag{3.31}$$

$$\{D(\lambda),D(\mu)\}=0. \tag{3.32}$$

Equation (3.30) shows that $t(\lambda)$ defines a classical version of the super-Yangian $Y(gl(M|N))$. Equation (3.32) shows that $D(\lambda)$ can be taken as a generating function for a hierarchy, and (3.31) proves that the super-Yangian is a symmetry of this hierarchy. It remains to identify this hierarchy.

Lemma 3.5: Only $T^{(2n)}(\lambda)$, $n\in\mathbb{Z}_+$, contribute to the super-Yangian generators $t(\lambda)$ and to the Hamiltonian generating function $D(\lambda)$.

Expanding $t(\lambda)$ and $D(\lambda)$ as series in λ^{-1}, one has $T^{(2n)}(\lambda)=o(\lambda^{-n})$.

Proof: It is clear that $T^{(n)}(\lambda)$ contains the product of exactly n matrices Ω, the other matrices entering in its definition being diagonal. Due to the form of Ω, only products of an even number of such matrices will contribute to $t(\lambda)$ and $D(\lambda)$.

To show the λ dependence, we consider the integration on z_{2j} and z_{2j+1}, and perform an integration by part, assuming that the fields Φ and $\Phi^\dagger$ are vanishing at infinity:

$$\begin{aligned}&\int_{-\infty}^{z_{2j-1}}dz_{2j}\int_{-\infty}^{z_{2j}}dz_{2j+1}\,E(\lambda;2z_{2j}-2z_{2j+1})\Omega(z_{2j})\Omega(z_{2j+1})I_{j,n}(z_{2j+1},\ldots,z_{2n})\\&=\frac{i}{\lambda}\Sigma\int_{-\infty}^{z_{2j-1}}dz_{2j}\Bigg[\Omega(z_{2i})^2I_{j,n}(z_{2j+1},\ldots,z_{2n})-\int_{-\infty}^{z_{2j}}dz_{2j+1}\,E(\lambda;2z_{2j}-2z_{2j+1})\\&\quad\times\Omega(z_{2j})\partial_{2j+1}(\Omega(z_{2j+1})I_{j,n}(z_{2j+1},z_{2j+2},\ldots,z_{2n}))\Bigg].\end{aligned}$$

Above, ∂_k stands for $\partial/\partial z_k$, and $I_{j,n}(z_{2j+1},z_{2j+2},\ldots,z_{2n})$ denotes the other integrals (depending on z_k, $k\geqslant 2j$) which enters into the definition of $T^{(n)}(\lambda)$.

It is clear that one can do this integration for all z_{2j}, $j=1,\ldots,n$, and any number of times, so that the lowest power of λ^{-1} is n. ■

Property 3.6: The first Hamiltonians generated by $D(\lambda)$ read

$$D^{(1)}=igN \quad \text{with} \quad N=\int_{-\infty}^{\infty}dx\,\Phi^\dagger(x)\Phi(x), \tag{3.33}$$

$$D^{(2)}=-\frac{1}{2}g^2N^2+gP \quad \text{with} \quad P=\int_{-\infty}^{\infty}dx\,\Phi^\dagger(x)\partial\Phi(x), \tag{3.34}$$

$$D^{(3)}=-\frac{ig^3}{6}N^3+ig^2NP+igH, \tag{3.35}$$

$$H=\int_{-\infty}^{\infty}dx\,\partial\Phi^\dagger(x)\partial\Phi(x)+g\int_{-\infty}^{\infty}dx(\Phi^\dagger(x)\Phi(x))^2. \tag{3.36}$$

This shows that $D(\lambda)$ generates the Hamiltonians of the NLSS hierarchy, so that (3.31) proves that $Y(gl(M|N))$ is a symmetry of this hierarchy.

Proof: We use the techniques given in the above proof, focusing on the $(K+1,K+1)$ matrix element. The bounds in the integrals are simplified using the property

$$(\Omega(x_1)\partial^k\Omega(x_2)\Omega(x_3)\partial^l\Omega(x_4))_{K+1,K+1}=(\Omega(x_1)\partial^k\Omega(x_2))_{K+1,K+1}(\Omega(x_3)\partial^l\Omega(x_4))_{K+1,K+1}. \tag{3.37}$$

■

B. Time evolution

Strictly speaking, we have, up to now, constructed only the linear operator $L(\lambda;x)$ introduced in the Zakharov–Shabbat scheme.[2] This operator is only the first element of the Lax pair (L,M). It is sufficient to solve the problem, but for completeness, we now introduce M, the second element of the Lax pair.

The Lax pair is a reformulation of the equations of motion as the commutativity of two differential operators:

$$\left[\frac{\partial}{\partial x}-L(\lambda;x,t),\frac{\partial}{\partial t}-M(\lambda;x,t)\right]=0, \tag{3.38}$$

which amounts to the compatibility condition of the auxiliary system

$$\begin{aligned}\partial_x u&=L(\lambda;x,t)u,\\ \partial_t u&=M(\lambda;x,t)u.\end{aligned} \tag{3.39}$$

Starting from the definitions (3.1) and (3.2), it is a straightforward calculation to show that for

$$M(\lambda;x,t)=-\frac{i\lambda^2}{2}\Sigma+ig\Omega(x,t)\Sigma\Omega(x,t)-\sqrt{g}(\Sigma\partial_x+i\lambda)\Omega(x,t) \tag{3.40}$$

the condition (3.38) is equivalent to

$$(i\Sigma\partial_t+\partial_x^2)\Omega(x,t)=2g|\Phi(x,t)|^2\Omega(x,t), \tag{3.41}$$

which just reproduces the equations of motion (2.10) and their counterpart for $\Phi^\dagger(x,t)$.

As it should be clear from the system (3.39), $M(\lambda;x,t)$ is associated to time evolution in the same way $L(\lambda;x,t)$ is associated to spacial translation. This is confirmed by the following:

Property 3.7: The time evolution of the transfer and monodromy matrices is given by

$$\partial_t T(\lambda;x,y,t)=M(\lambda;x,t)T(\lambda;x,y,t)-T(\lambda;x,y,t)M(\lambda;y,t), \tag{3.42}$$

$$\partial_t T_+(\lambda;y,t)=-\frac{i\lambda^2}{2}\Sigma T(\lambda;y,t)-T(\lambda;y,t)M(\lambda;y,t), \tag{3.43}$$

$$\partial_t T_-(\lambda;x,t)=M(\lambda;x,t)T(\lambda;x,t)+\frac{i\lambda^2}{2}T(\lambda;x,t)\Sigma, \tag{3.44}$$

$$\partial_t T(\lambda;t) = -\frac{i\lambda^2}{2}[\Sigma, T(\lambda;t)]. \tag{3.45}$$

Proof: The first equation is proven showing that

$$Z(\lambda;x,y,t) = \partial_t T(\lambda;x,y,t) - M(\lambda;x,t)T(\lambda;x,y,t) + T(\lambda;x,y,t)M(\lambda;y,t)$$

obeys the differential equations ($x>y$):

$$\partial_x Z(\lambda;x,y) = L(\lambda;x)Z(\lambda;x,y),$$

$$\partial_y Z(\lambda;x,y) = -Z(\lambda;x,y)L(\lambda;y),$$

together with the initial condition $Z(\lambda;x,x,t)=0$.

The other equations are proved through the limits $x\to\infty$, $y\to-\infty$ using $\lim_{|x|\to\infty} M(\lambda;x,t) = -(i\lambda^2/2)\Sigma$. ■

To conclude this section, let us remark that the time-evolution (3.45) shows that we have

$$T(\lambda;x,y,t) = e^{it\lambda^2\Sigma/2}T(\lambda;x,y,0)e^{-it\lambda^2\Sigma/2} \tag{3.46}$$

in accordance with the ZF formulation of the Hamiltonian.

C. Quantum Lax pair

Following Sklyanin,[28] we define the following.

Definition 3.8: The quantum transition matrix $\mathcal{T}(\lambda;x,y)$ is the Wick (normal)-ordered classical transition matrix $T(\lambda;x,y)$ regarded as a functional of the quantum canonical fields $\Phi(x)$, $\Phi^\dagger(x)$:

$$\mathcal{T}(\lambda;x,y) = :T(\lambda;x,y):. \tag{3.47}$$

Here and below the normal ordering is defined as

$$:\phi_j(x)\phi_k^\dagger(y):=(-1)^{[j][k]}\phi_k^\dagger(y)\phi_j(x), \quad \forall x,y,$$

and extended to monomials in ϕ, $\phi^\dagger$ in the usual way, i.e., with all the ϕ's on the right of the $\phi^\dagger$'s, keeping the original order between the ϕ's and between the $\phi^\dagger$'s.

For convenience, we also define a symbol ‡‡ which acts on operators and is not to be confused with the symbol : :. It simply guarantees the ordering of Φ, $\Phi^\dagger$ in an expression containing $L(\lambda;x)$ and other (normal-ordered) functionals of the quantum fields without changing the internal ordering of the functionals. For example, if $A=:a:$ and $B=:b:$, then

$$\ddagger AL(\lambda;x)B\ddagger = \frac{i\lambda}{2}A\Sigma B + i\sqrt{g}\sum_{j=1}^{K}((-1)^{[j][A]}\phi_j(x)AE_{K+1,j}B - (-1)^{[j][B]}AE_{j,K+1}B\phi_j^\dagger(x)).$$

The previous definition gives rise to many questions dealing with operator theory and functional analysis which were answered for the bosonic case in the very detailed review[1] by Gutkin. But for the sake of brevity, we mimic the compact, albeit more formal, approach of Sklyanin since it contains all the fundamental and physical ideas, bearing in mind that everything is well defined.

In this sense, the quantum transition matrix is the fundamental solution of the quantum auxiliary problem

$$\partial_x \mathcal{T}(\lambda;x,y) = \ddagger L(\lambda;x)\mathcal{T}(\lambda;x,y)\ddagger \quad \text{with} \quad \mathcal{T}(\lambda;x,x)=\mathbb{1} \tag{3.48}$$

and satisfies

$$\partial_y \mathcal{T}(\lambda;x,y) = -\ddagger \mathcal{T}(\lambda;x,y) L(\lambda;y) \ddagger,$$

$$\mathcal{T}(\lambda;x,y)\mathcal{T}(\lambda;y,z) = \mathcal{T}(\lambda;x,z) \quad \text{for } x<y<z \text{ or } x>y>z,$$

where $L(\lambda;x)$ is the Lax even super-matrix defined in (3.1) and (3.2).

This system of first-order differential equations together with the given initial condition is equivalent to the following Volterra integral representations:

$$\mathcal{T}(\lambda;x,y) = \mathbb{1} + \int_y^x d\omega \ddagger L(\lambda;\omega)\mathcal{T}(\lambda;\omega,y)\ddagger, \tag{3.49}$$

$$\mathcal{T}(\lambda;x,y) = \mathbb{1} + \int_y^x d\omega \ddagger \mathcal{T}(\lambda;x,\omega)L(\lambda;\omega)\ddagger. \tag{3.50}$$

In order to reach our final goal there are several steps which all rely on one simple idea extensively used in the inverse problem literature, that is two quantities are equal if and only if they satisfy the same first-order differential equation with the same initial condition. This is what is called ''the differential equation approach'' by Gutkin in Ref. 1. He criticized this approach but showed that it gives the correct answer using the ''discrete approximation approach'' which amounts to the same line of argument but deals with finite differences on subintervals of $[x,y]$ instead of a true derivative.

The first step is to obtain the commutation relations of matrix elements of the transition matrix and we need two preliminary lemmas.

Lemma 3.9: $\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)$ *satisfies the following differential system:*

$$\partial_x\{\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\} = \ddagger \mathcal{L}_{12}(\lambda,\mu;x)\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\ddagger, \tag{3.51}$$

$$\mathcal{T}_1(\lambda;x,x)\mathcal{T}_2(\mu;x,x) = \mathcal{T}_2(\mu;x,x)\mathcal{T}_1(\lambda;x,x) = \mathbb{1}\otimes\mathbb{1}, \tag{3.52}$$

where

$$\mathcal{L}_{12}(\lambda,\mu;x) = L_1(\lambda;x) + L_2(\mu;x) + g\pi_{12}. \tag{3.53}$$

Proof: The idea is once again to use the equivalence between the differential problem and the Volterra integral representation of the solution. Indeed, taking care of the ordering of the fields when using (3.49) and (3.50), one gets

$$\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y) = \mathbb{1}\otimes\mathbb{1} + \int_y^x d\omega \ddagger \mathcal{L}_{12}(\lambda,\mu;\omega)\mathcal{T}_1(\lambda;\omega,y)\mathcal{T}_2(\mu;\omega,y)\ddagger.$$

■

Lemma 3.10: The operator $\mathcal{L}_{12}(\lambda,\mu;x)$ *satisfies the following relation:*

$$\mathcal{R}_{12}(\lambda-\mu)\mathcal{L}_{12}(\lambda,\mu;x) = \mathcal{L}_{21}(\mu,\lambda;x)\mathcal{R}_{12}(\lambda-\mu), \tag{3.54}$$

where $\mathcal{R}_{12}(\lambda-\mu) = \mathbb{1} - ir(\lambda-\mu)$*, and* $r(\lambda-\mu)$ *is given by (3.4).*

Proof: Direct calculation using

$$[\Pi_{12}, L_1(\lambda;x) + L_2(\mu;x)] = i(\lambda-\mu)(\pi_{12} - \pi_{21}),$$

where π_{12} has been defined in (3.21). ■

We can now formulate the basic result of this paragraph.

Theorem 3.11: *The quantum transition matrix* $\mathcal{T}(\lambda;x,y)$ *satisfies the following finite volume commutation relations:*

$$\mathcal{R}_{12}(\lambda-\mu)\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)=\mathcal{T}_2(\mu;x,y)\mathcal{T}_1(\lambda;x,y)\mathcal{R}_{12}(\lambda-\mu). \tag{3.55}$$

Proof: Using the fact that $\mathcal{R}_{12}(\lambda)$ is a numerical, invertible (for λ real and nonzero) matrix, Lemmas 3.9 and 3.10 imply that the quantities $\mathcal{T}_2(\mu;x,y)\mathcal{T}_1(\lambda;x,y)$ and $\mathcal{R}_{12}(\lambda-\mu)\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\mathcal{R}_{12}^{-1}(\lambda-\mu)$ satisfy the same first-order differential equation with the same initial condition. ■

Let us remark that if we restore the Planck constant in the canonical commutation relations, then $\mathcal{R}_{12}(\lambda-\mu)=\mathbb{1}-i\hbar r(\lambda-\mu)$ and we recover the relation (3.8) for the classical transition matrix, given that as $\hbar\to 0$, $\mathcal{T}(\lambda;x,y)\to T(\lambda;x,y)$ and $[,]\to i\hbar\{,\}$ and keeping the terms of order $\hbar$.

We are now in position to define the quantum monodromy matrix as an appropriate limit of the quantum transition matrix to obtain the infinite volume commutation relations corresponding to (3.55). The crucial difference with respect to the classical case comes from the nontrivial commutation relations of the quantum fields, which produces the term proportional to g in $\mathcal{L}_{12}(\lambda,\mu;x)$.

Therefore, one cannot define the limit as in (3.25) and insert it directly in the finite volume commutation relations. Instead, we are led to compare the asymptotic behavior of $\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)$, for which we have information with that of $\mathcal{T}_1(\lambda;x,y)$, $\mathcal{T}_2(\mu;x,y)$ separately, whose commutation relations in the infinite interval limit we are looking for.

Definition 3.12: The quantum equivalents of (3.23)–(3.25) are defined by

$$\mathcal{T}^-(\lambda;x)=:T^-(\lambda;x):,\quad \mathcal{T}^+(\lambda;y)=:T^+(\lambda;y):,\quad \mathcal{T}(\lambda)=:T(\lambda):, \tag{3.56}$$

and $\mathcal{T}(\lambda)=\mathcal{T}^+(\lambda;z)\mathcal{T}^-(\lambda;z)$ *is the quantum monodromy matrix.*

$E(\lambda;x)$ being a numerical matrix, one immediately deduces

$$\partial_x\mathcal{T}^-(\lambda;x)=\ddagger L(\lambda;x)\mathcal{T}^-(\lambda;x)\ddagger, \tag{3.57}$$

$$\partial_x\mathcal{T}^+(\lambda;x)=-\ddagger\mathcal{T}^+(\lambda;x)L(\lambda;x)\ddagger. \tag{3.58}$$

As a first step, we look for information on $\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^-(\mu;x)$ from what we know of $\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)$. This is gathered in the following lemma.

Lemma 3.13:

$$\lim_{y\to-\infty}\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\xi_{12}(\lambda,\mu;y)=\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^-(\mu;x)C_{12}(\lambda,\mu), \tag{3.59}$$

where, π_{12} *being defined as in (3.21), we have introduced*

$$\xi_{12}(\lambda,\mu;y)=\exp\left[\left(\frac{i\lambda}{2}\Sigma_1+\frac{i\mu}{2}\Sigma_2+g\pi_{12}\right)y\right], \tag{3.60}$$

$$C_{12}(\lambda,\mu)=\mathbb{1}\otimes\mathbb{1}-\frac{ig}{\lambda-\mu+i\varepsilon}\pi_{12}. \tag{3.61}$$

Proof: Let

$$\Lambda(\lambda,\mu;x)=\lim_{y\to-\infty}\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\xi_{12}(\lambda,\mu;y), \tag{3.62}$$

$$\Lambda^-(\lambda,\mu;x)=\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^-(\mu;x). \tag{3.63}$$

Rewriting $\mathcal{L}_{12}(\lambda,\mu;x)=\mathcal{L}_0(\lambda,\mu)+\Omega_1(x)+\Omega_2(x)$ with $\mathcal{L}_0(\lambda,\mu)=(i\lambda/2)\Sigma_1+(i\mu/2)\Sigma_2+g\pi_{12}$, one easily gets from (3.51) the integral representation

$$\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)=\xi_{12}(\lambda,\mu;x-y)+\int_y^x d\omega\,\ddagger\mathcal{T}_1(\lambda;x,\omega)\mathcal{T}_2(\mu;x,\omega)(\Omega_1(\omega)+\Omega_2(\omega))\ddagger\xi_{12}(\lambda,\mu;\omega-y), \tag{3.64}$$

which shows that $\Lambda(\lambda,\mu;x)$ is well defined and also satisfies

$$\partial_x\Lambda(\lambda,\mu;x)=\ddagger\mathcal{L}_{12}(\lambda,\mu;x)\Lambda(\lambda,\mu;x)\ddagger.$$

Now following the same line of argument as in Lemma 3.9, we get

$$\partial_x\Lambda^-(\lambda,\mu;x)=\ddagger\mathcal{L}_{12}(\lambda,\mu;x)\Lambda^-(\lambda,\mu;x)\ddagger.$$

Consequently,

$$\Lambda(\lambda,\mu;x)=\Lambda^-(\lambda,\mu;x)C_{12}(\lambda,\mu),\quad \forall x, \tag{3.65}$$

and we can determine $C_{12}(\lambda,\mu)$ from the asymptotic behavior as $x\to-\infty$. From the physical requirement that

$$\lim_{x\to\pm\infty}|\Phi(x)|=0$$

and Eq. (3.64), we see that

$$\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\underset{\substack{y\to-\infty\\ x\to y}}{\sim}\xi_{12}(\lambda,\mu;x-y),$$

implying

$$\Lambda(\lambda,\mu;x)\underset{x\to-\infty}{\sim}\xi_{12}(\lambda,\mu;x). \tag{3.66}$$

On the other hand, from (3.57), $\Lambda^-(\lambda,\mu;x)$ can be represented as

$$\Lambda^-(\lambda,\mu;x)=E_1(\lambda;x)E_2(\mu;x)+\int_{-\infty}^x d\omega\,\ddagger\mathcal{T}_1(\lambda;x,\omega)\mathcal{T}_2(\mu;x,\omega)\times(\Omega_1(\omega)+\Omega_2(\omega)+g\pi_{12})\ddagger E_1(\lambda;\omega)E_2(\mu;\omega),$$

so that

$$\Lambda^-(\lambda,\mu;x)\underset{x\to-\infty}{\sim}E_1(\lambda;x)E_2(\mu;x)+I(\lambda,\mu;x),$$

where

$$I(\lambda,\mu;x)=g\int_{-\infty}^x d\omega\,\xi_{12}(\lambda,\mu;x-\omega)\pi_{12}E_1(\lambda;\omega)E_2(\mu;\omega)$$

can be evaluated from the knowledge of

$$\xi_{12}(\lambda,\mu;x)=E_1(\lambda;x)E_2(\mu;x)+2g\frac{\sin([(\lambda-\mu)/2]x)}{\lambda-\mu}\pi_{12}$$

and an $i\varepsilon$ prescription to get

$$I(\lambda,\mu;x)=\frac{ig}{\lambda-\mu+i\varepsilon}e^{-i[(\lambda-\mu)/2]x}\pi_{12}.$$

Now, adopting the regularization

$$2g\,\frac{\sin([(\lambda-\mu)/2]x)}{\lambda-\mu}=\frac{-ig}{\lambda-\mu+i\varepsilon}[e^{i[(\lambda-\mu)/2]x}-e^{-i[(\lambda-\mu)/2]x}],$$

we see that (3.65) holds for $C_{12}(\lambda,\mu)$ given in (3.61). ■

Theorem 3.14: *The commutation relations for the quantum matrices* $\mathcal{T}^{\pm}(\lambda;x)$ *and* $\mathcal{T}(\lambda)$ *for real* λ *and* μ *take the following form:*

$$\begin{aligned}&\mathcal{R}_{12}(\lambda-\mu)\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^-(\mu;x)C_{12}(\lambda,\mu)=\mathcal{T}_2^-(\mu;x)\mathcal{T}_1^-(\lambda;x)C_{21}(\mu,\lambda)\mathcal{R}_{12}(\lambda-\mu),\\&\mathcal{R}_{12}(\lambda-\mu)C_{12}(\mu,\lambda)\mathcal{T}_1^+(\lambda;x)\mathcal{T}_2^+(\mu;x)=C_{21}(\lambda,\mu)\mathcal{T}_2^+(\mu;x)\mathcal{T}_1^+(\lambda;x)\mathcal{R}_{12}(\lambda-\mu),\end{aligned}\tag{3.67}$$

$$\mathcal{R}_{12}^+(\lambda-\mu)\mathcal{T}_1(\lambda)\mathcal{T}_2(\mu)=\mathcal{T}_1(\mu)\mathcal{T}_2(\lambda)\mathcal{R}_{12}^-(\lambda-\mu),$$

where, defining $\mathbb{1}_K=\Sigma_{i=1}^K E_{ii}$,

$$\begin{aligned}\mathcal{R}_{12}^{\pm}(\lambda-\mu)=&\frac{-ig}{(\lambda-\mu)}\mathbb{1}_K\otimes\mathbb{1}_K+P_{12}+\pi_{21}+\frac{(\lambda-\mu)^2+g^2}{(\lambda-\mu+i\varepsilon)^2}\pi_{12}+\frac{\lambda-\mu-ig}{\lambda-\mu}E_{K+1,K+1}\otimes E_{K+1,K+1}\\&\pm\pi g\,\delta(\lambda-\mu)(\mathbb{1}_K\otimes E_{K+1,K+1}-E_{K+1,K+1}\otimes\mathbb{1}_K).\end{aligned}$$

Proof: We start with the proof of the first equality. Lemma 3.13 gives

$$\lim_{y\to-\infty}\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\xi_{12}(\lambda,\mu;y)=\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^-(\mu;x)C_{12}(\lambda,\mu),$$

which in turn yields

$$\lim_{y\to-\infty}\mathcal{T}_2(\mu;x,y)\mathcal{T}_1(\lambda;x,y)\xi_{21}(\mu,\lambda;y)=\mathcal{T}_2^-(\mu;x)\mathcal{T}_1^-(\lambda;x)C_{21}(\mu,\lambda).$$

Multiplying (3.55) on the right by $\xi_{12}(\lambda,\mu;y)$ and using the property

$$\mathcal{R}_{12}(\lambda-\mu)\xi_{12}(\lambda,\mu;y)=\xi_{21}(\mu,\lambda;y)\mathcal{R}_{12}(\lambda-\mu)$$

we get

$$\mathcal{R}_{12}(\lambda-\mu)\mathcal{T}_1(\lambda;x,y)\mathcal{T}_2(\mu;x,y)\xi_{12}(\lambda,\mu;y)=\mathcal{T}_2(\mu;x,y)\mathcal{T}_1(\lambda;x,y)\xi_{21}(\mu,\lambda;y)\mathcal{R}_{12}(\lambda-\mu),$$

which gives the first equality in the limit $y\to-\infty$. The second equality is proved along the same line of argument. Now, combining the two equations and using the properties

$$\mathcal{T}(\lambda)=\mathcal{T}^+(\lambda;x)\mathcal{T}^-(\lambda;x)\quad\text{and}\quad\mathcal{T}_2^+(\mu;x)\mathcal{T}_1^-(\lambda;x)=\mathcal{T}_1^-(\lambda;x)\mathcal{T}_2^+(\mu;x),$$

we get

$$\mathcal{R}_{12}(\lambda-\mu)C_{12}(\mu,\lambda)\mathcal{T}_1(\lambda)\mathcal{T}_2(\mu)C_{12}(\lambda,\mu)=C_{21}(\lambda,\mu)\mathcal{T}_2(\mu)\mathcal{T}_1(\lambda)C_{21}(\mu,\lambda)\mathcal{R}_{12}(\lambda-\mu),$$

which take the form (3.67) if we define

$$\mathcal{R}_{12}^+(\lambda-\mu)=C_{12}^{-1}(\lambda,\mu)\Pi_{12}\mathcal{R}_{12}(\lambda-\mu)C_{12}(\mu,\lambda),\tag{3.68}$$

$$\mathcal{R}^{-}_{12}(\lambda-\mu)=C_{12}(\mu,\lambda)\Pi_{12}\mathcal{R}_{12}(\lambda-\mu)C^{-1}_{12}(\lambda,\mu), \tag{3.69}$$

whose explicit calculation we leave to the reader. ■

Let us extract the information contained in (3.67). We start by particularizing some entries of the quantum monodromy matrix $(i,j=1,...,K)$:

$$t_{ij}(\lambda)=(\mathcal{T}(\lambda))_{ij}, \tag{3.70}$$

$$b_j(\lambda)=(\mathcal{T}(\lambda))_{j,K+1}, \tag{3.71}$$

$$D(\lambda)=(\mathcal{T}(\lambda))_{K+1,K+1}. \tag{3.72}$$

Theorem 3.15: *The exchange relations of the entries of the quantum monodromy matrix read as follows:*

$$[\![t_{ij}(\lambda),t_{kl}(\mu)]\!]=ig(-1)^{[j][k]+[i]([j]+[k])}\frac{t_{kj}(\lambda)t_{il}(\mu)-t_{kj}(\mu)t_{il}(\lambda)}{\lambda-\mu}, \tag{3.73}$$

$$t_{ij}(\lambda)D(\mu)=D(\mu)t_{ij}(\lambda), \tag{3.74}$$

$$D(\lambda)D(\mu)=D(\mu)D(\lambda), \tag{3.75}$$

$$b_j(\lambda)b_k(\mu)=\frac{\mu-\lambda}{\mu-\lambda-ig}(-1)^{jk}b_k(\mu)b_j(\lambda)-\frac{ig}{\mu-\lambda-ig}b_j(\mu)b_k(\lambda), \tag{3.76}$$

$$b_j(\lambda)D(\mu)=\frac{\lambda-\mu-ig}{\lambda-\mu-i\varepsilon}D(\mu)b_j(\lambda). \tag{3.77}$$

Proof: By direct calculation. ■

Relations (3.73)–(3.75) are the quantum counterparts of Eqs. (3.30)–(3.32) and the same interpretation holds but for the quantum hierarchy here. As such, the super-Yangian $Y(gl(M|N))$ is a quantum symmetry of the hierarchy generated by $D(\lambda)$, which is just the quantum analog of Property 3.6 as can be seen from

$$D(\lambda)=1+\frac{ig}{\lambda}N+\frac{g}{\lambda^2}\left(P-\frac{g}{2}N(N-1)\right)+\frac{ig}{\lambda^3}\left(H+g(N-1)P-\frac{g^2}{6}N(N-1)(N-2)\right)+O\left(\frac{1}{\lambda^4}\right).$$

D. ZF algebra from Lax pair

The two relations (3.76) and (3.77) will allow us to recover the ZF algebra. Indeed, all the quantities of Theorem 3.15 are functionals of Φ, $\Phi^{\dagger}$, themselves involving the ZF generators [cf. (2.35)], and one can get the ZF algebra out of them as follows.

Property 3.16: Defining $a_j(\lambda)=(1/\sqrt{\pi g})b_j(\lambda)D(\lambda)^{-1}$, *Eqs. (3.76) and (3.77) give*

$$a_j(\lambda)a_k(\mu)=\frac{\mu-\lambda}{\mu-\lambda+ig}(-1)^{jk}a_k(\mu)a_j(\lambda)-\frac{ig}{\mu-\lambda+ig}a_j(\mu)a_k(\lambda). \tag{3.78}$$

Proof: Direct calculation from Theorem 3.15. ■

To complete our algebra, we need the exchange relations between $a_j(\lambda)$ and $a^{\dagger}_k(\mu)$. Contrary to the original one (bosonic) component case, this is not directly obtained from what we already have since there is no simple conjugate relationship for the entries of the monodromy matrix. We are naturally led to introduce a conjugate Lax super-matrix defined by

$$\overline{L}(\lambda;x)=-\frac{i\lambda}{2}\Sigma-i\sqrt{g}\phi_j^\dagger(x)E_{K+1,j}+i\sqrt{g}\phi_j(x)E_{j,K+1} \tag{3.79}$$

and the associated transition matrix

$$\partial_x\overline{\mathcal{T}}(\lambda;x,y)=\ddagger\overline{\mathcal{T}}(\lambda;x,y)\overline{L}(\lambda;x)\ddagger. \tag{3.80}$$

Now, to obtain information between the entries of $\mathcal{T}(\lambda;x,y)$ and $\overline{\mathcal{T}}(\mu;x,y)$ following the same steps as in Lemmas 3.9 and 3.10 and Theorem 3.11, one sees that we actually need to work with the super-transposed Lax matrix. The corresponding operation on an even super-matrix $A=\Sigma_{i,j=1}^{K+1}A_{ij}E_{ij}$ reads

$$A^t=\sum_{i,j=1}^{K+1}A_{ij}E_{ij}^t=\sum_{i,j=1}^{K+1}(-1)^{[i]([i]+[j])}A_{ji}E_{ij}. \tag{3.81}$$

It satisfies $(A^t)^t=A$ and $(AB)^t=B^tA^t$ for any even super-matrices A and B. We get

$$L^t(\lambda;x)=\frac{i\lambda}{2}\Sigma+i\sqrt{g}(-1)^{[j]}\phi_j(x)E_{K+1,j}-i\sqrt{g}\phi_j^\dagger(x)E_{j,K+1} \tag{3.82}$$

and the associated transition matrix

$$\partial_x\mathcal{T}^t(\lambda;x,y)=\ddagger\mathcal{T}^t(\lambda;x,y)L^t(\lambda;x)\ddagger. \tag{3.83}$$

Therefore, instead of (3.51) we get

$$\partial_x\{\overline{\mathcal{T}_1}(\lambda;x,y)\mathcal{T}_2^t(\mu;x,y)\}=\ddagger\overline{\mathcal{T}_1}(\lambda;x,y)\mathcal{T}_2^t(\mu;x,y)\Gamma_{12}(\lambda,\mu;x)\ddagger, \tag{3.84}$$

$$\partial_x\{\mathcal{T}_1^t(\mu;x,y)\overline{\mathcal{T}_2}(\lambda;x,y)\}=\ddagger\mathcal{T}_1^t(\mu;x,y)\overline{\mathcal{T}_2}(\lambda;x,y)\Gamma'_{12}(\lambda,\mu;x)\ddagger, \tag{3.85}$$

with

$$\Gamma_{12}(\lambda,\mu;x)=\overline{L_1}(\lambda;x)+L_2^t(\mu;x)+g\pi_{12}^{t_2},$$

$$\Gamma'_{12}(\lambda,\mu;x)=L_1^t(\mu;x)+\overline{L_2}(\lambda;x)+g\pi_{12}^{t_1}.$$

Now the key point is to find an invertible numerical matrix $\mathcal{R}'_{12}(\lambda)$ solution of the new Yang–Baxter equation

$$\mathcal{R}'_{12}(\lambda,\mu)\Gamma_{12}(\lambda,\mu;x)=\Gamma_{21}(\lambda,\mu;x)\mathcal{R}'_{12}(\lambda,\mu).$$

It is given by

$$\mathcal{R}'_{12}(\lambda,\mu)=\frac{ig}{\lambda-\mu}\Pi_{12}^{t_1}+\frac{\lambda-\mu-ig(M-N)}{\lambda-\mu}\Pi_{12}. \tag{3.86}$$

Following the same procedure as above, we finally deduce the infinite volume commutation relations under the form

$$\mathcal{R}'^{+}_{12}(\lambda-\mu)\overline{\mathcal{T}_1}(\lambda)\mathcal{T}_2^t(\mu)=\mathcal{T}_1^t(\mu)\overline{\mathcal{T}_2}(\lambda)\mathcal{R}'^{-}_{12}(\lambda-\mu) \tag{3.87}$$

with

$$\mathcal{R}'^{\pm}_{12}(\lambda-\mu)=\frac{ig}{\lambda-\mu}P^{t_1}_{12}+\frac{\lambda-\mu-ig(M-N)}{\lambda-\mu}(P_{12}+\pi_{12}+\pi_{21})$$
$$+\frac{(\lambda-\mu-ig)(\lambda-\mu-ig(M-N))}{(\lambda-\mu+i\varepsilon)^2}E_{K+1,K+1}\otimes E_{K+1,K+1}$$
$$\mp\pi g\,\delta(\lambda-\mu)(\pi^{t_1}_{21}-\pi^{t_2}_{21}).$$

All these results are the generalization to the graded case of Ref. 19 (K, the total number of bosonic or fermionic particles is replaced in our case by $M-N$, the difference of bosonic and fermionic particles). Accordingly, we get the same conclusions collected in the following proposition.

Property 3.17: Let $a^\dagger_i(\lambda)=(1/\sqrt{\pi g})(D^{-1})^\dagger(\lambda)b^\dagger_j(\lambda)$. *Then*

$$a_i(\lambda)a^\dagger_j(\mu)=\frac{\lambda-\mu}{\lambda-\mu+ig}(-1)^{[i][j]}a^\dagger_j(\mu)a_i(\lambda)-\delta_{ij}\frac{ig}{\lambda-\mu+ig}\sum_{\ell=1}^{K}a^\dagger_\ell(\mu)a_\ell(\lambda)+\delta_{ij}\delta(\lambda-\mu),\tag{3.88}$$

$$a^\dagger_i(\lambda)a^\dagger_j(\mu)=\frac{\mu-\lambda}{\mu-\lambda+ig}(-1)^{[i][j]}a^\dagger_j(\mu)a^\dagger_i(\lambda)-\frac{ig}{\mu-\lambda+ig}a^\dagger_i(\mu)a^\dagger_j(\lambda).\tag{3.89}$$

Proof: Noting that

$$b_j(\lambda)=\mathcal{T}^t(\lambda)_{K+1,j},\quad D(\lambda)=\mathcal{T}^t(\lambda)_{K+1,K+1},$$
$$b^\dagger_j(\lambda)=\overline{\mathcal{T}}(\lambda)_{K+1,j},\quad D^\dagger(\lambda)=\overline{\mathcal{T}}(\lambda)_{K+1,K+1},$$

(3.87) gives

$$D^\dagger(\lambda)D(\mu)=D(\mu)D^\dagger(\lambda),$$

$$D(\mu)b^\dagger_i(\lambda)=\frac{\lambda-\mu-ig}{\lambda-\mu+i\varepsilon}b^\dagger_i(\lambda)D(\mu),\quad b_j(\mu)D^\dagger(\lambda)=\frac{\lambda-\mu-ig}{\lambda-\mu+i\varepsilon}D^\dagger(\lambda)b_j(\mu),$$

$$b_i(\lambda)b^\dagger_j(\mu)=\frac{\mu-\lambda-ig}{\mu-\lambda+i\varepsilon}(-1)^{[i][j]}b^\dagger_j(\mu)b_i(\lambda)+\delta_{ij}\frac{ig(\mu-\lambda-ig)}{(\mu-\lambda+i\varepsilon)^2}\sum_{\ell=1}^{K}b^\dagger_\ell(\mu)b_\ell(\lambda)$$
$$+\delta_{ij}\pi g\,\delta(\lambda-\mu)D^\dagger(\mu)D(\lambda),$$

which in turn yields (3.88). The proof of (3.89) is similar. ■

IV. EXPLICIT CONSTRUCTION OF THE SUPER-YANGIAN GENERATORS

A. Super-Yangian generators in terms of canonical fields

We consider the classical case. The quantum case can be done in a similar way, with correction terms due to the noncommutativity of the fields Φ, $\Phi^\dagger$.

For any $K\times K$-matrix $\sigma\in gl(M|N)$, we introduce

$$Q^{(0)}_\sigma=\int dx\,\Phi^\dagger(x)\sigma\Phi(x)=\int dx\sum_{j,k=1}^{K}\phi^\dagger_j(x)\sigma^{jk}\phi_k(x),\tag{4.1}$$

$$Q^{(1)}_\sigma=\int dx\,\Phi^\dagger(x)\sigma\partial\Phi(x)-\frac{g}{2}\int dxdy\,sg(x-y)\Phi^\dagger(x)\sigma\Phi(y)\cdot\Phi^\dagger(y)\Phi(x),\tag{4.2}$$

$$Q_\sigma^{(2)}=\int dx\,\Phi^\dagger(x)\sigma\partial^2\Phi(x)-\frac{g}{2}\int dxdy\,sg(x-y)(\Phi^\dagger(x)\sigma\partial\Phi(y)-\partial\Phi^\dagger(x)\sigma\Phi(y))\Phi^\dagger(y)\Phi(x)$$
$$+\frac{g^2}{4}\int dxdydz\,sg(x-y)sg(y-z)\Phi^\dagger(y)\Phi(x)\cdot\Phi^\dagger(x)\sigma\Phi(z)\cdot\Phi^\dagger(z)\Phi(y). \tag{4.3}$$

The coefficients in (4.2) and (4.3) are fixed in such a way that

$$\{H,Q_\sigma^{(n)}\}=0,\quad n=0,1,2, \tag{4.4}$$

so that $Q_\sigma^{(n)}$ are indeed symmetry generators of the NLSS equation. With these definitions, it is a simple calculation to show

$$\{Q_\sigma^{(0)},Q_\omega^{(n)}\}=iQ_{[\![\sigma,\omega]\!]}^{(n)},\quad n=0,1,2, \tag{4.5}$$

$$\begin{aligned}\{Q_\sigma^{(1)},Q_\omega^{(1)}\}=iQ_{[\![\sigma,\omega]\!]}^{(2)}-i\left(-\frac{g}{2}\right)^2\int dxdydt\,S(x,y,t)(\Phi^\dagger(x)\sigma\Phi(y)\cdot\Phi^\dagger(y)\omega\Phi(t)\\ -\Phi^\dagger(x)\omega\Phi(y)\cdot\Phi^\dagger(y)\sigma\Phi(t))\Phi^\dagger(t)\Phi(x),\\ S(x,y,t)=sg(t-x)sg(x-y)+sg(x-y)sg(y-t)+sg(y-t)sg(t-x).\end{aligned} \tag{4.6}$$

Equation (4.5) shows that $Q_\sigma^{(0)}$, $\sigma\in gl(M|N)$, generates a $gl(M|N)$ superalgebra, and that $Q_\sigma^{(n)}$ (n fixed) form a representation of it. The second term in (4.6) reflects the nonlinear commutation relation of the super-Yangian.

Note that we have

$$Q_{\mathbb{I}}^{(0)}=N\quad\text{and}\quad Q_{\mathbb{I}}^{(1)}=P, \tag{4.7}$$

so that Eq. (4.5) shows that $Q_\sigma^{(n)}$ commutes with N and P. Moreover, we have the supersymmetrylike relations:

$$\begin{aligned}&\{Q_\sigma^{(0)},Q_\sigma^{(0)}\}=2iN,\\ &\{Q_\sigma^{(0)},Q_\sigma^{(1)}\}=2iP,\end{aligned}\quad\text{as soon as}\quad\sigma^2=\mathbb{I}\quad\text{and}\quad[\sigma]=1. \tag{4.8}$$

However, let us remark that $Q_{\mathbb{I}}^{(2)}$ is not the NLSS Hamiltonian:

$$Q_{\mathbb{I}}^{(2)}=H+\frac{g^2}{4}\int dxdydz\,sg(x-y)sg(y-z)\Phi^\dagger(y)\Phi(x)\cdot\Phi^\dagger(x)\sigma\Phi(z)\cdot\Phi^\dagger(z)\Phi(y).$$

$Q_{\mathbb{I}}^{(2)}$ corresponds to a central generator which, if it were the Hamiltonian, would lead to nonlocal equation of motion for Φ. On the contrary, H commutes with the generators $Q_\sigma^{(n)}$ and provides local equation of motion.

B. Super-Yangian generators in terms of ZF generators

We have obtained the ZF-algebra (2.15) and (2.17) from the commutation relations of the quantum monodromy matrix. This shows the central importance of this algebra and one is naturally led to take it as a starting point. This is the very idea developed in Ref. 29 and we use it to construct a realization of the generators of the super-Yangian symmetry in terms of the ZF oscillators.

First of all, we need to generalize all the basic results of Ref. 29 to our graded formalism. It is actually readily obtained since the fundamental idea of the properties given in Refs. 29 and 4 is the possibility of relabelling the auxiliary spaces which holds for our global formalism as the reader can check. Thus, we are in position to apply any result from Ref. 29 in our context. Here

is our strategy: we start from the ZF algebra (corresponding to the algebra $\mathcal{A}_R$ in Ref. 29), introduce the associated well-bred vertex operator $T(\lambda)$ and use the explicit expression of our R-matrix to derive the first two terms of the expansion of $T(\lambda)$ in power series of λ^{-1}. Then we show that this approach actually coincides with the previous Lax pair formulation so that we have a realization of the generators of the super-Yangian symmetry for the hierarchy associated to the nonlinear super-Schrödinger equation in terms of the ZF oscillators. This completes and confirms the deep relationships between the quantum canonical field description (cf. Sec. IV A) and the ZF algebra approach.

Definition 4.1: The vertex operators $T_{ij}(\lambda)$ $(i,j=1,...,K)$ associated to the ZF algebra $\mathcal{A}_R$ are defined by $T(\lambda)=T^{ij}(\lambda)E_{ij}\in\mathcal{A}_R\otimes\mathbb{C}^{K^2}$ with

$$T_\infty(\lambda)=\mathbb{1}+\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n!}a^\dagger_{n\cdots 1}T^{(n)}_{\infty 1\cdots n}a_{1\cdots n}, \tag{4.9}$$

where

$$a^\dagger_{n\ldots 1}=(a_{1\cdots n})^\dagger=a^\dagger_n(k_n)\cdots a^\dagger_1(k_1),$$

$$T^{(n)}_{\infty 1\cdots n}=T^{(n)}_{\infty 1\cdots n}(\lambda,k_1,\ldots,k_n)\in(\mathbb{C}^{\otimes K^2})^{\otimes(n+1)}(\lambda,k_1,\ldots,k_n),$$

and integration is implied over the spectral parameters $k_1,\ldots,k_n$ (the summation over the auxiliary spaces being understood as in the Appendix).

$T_\infty(\lambda)$ is said to be well-bred (on $\mathcal{A}_R$) if

$$T_\infty(\lambda)a_1(\mu)=R_{1\infty}(\mu-\lambda)a_1(\mu)T_\infty(\lambda)\quad\text{and}\quad T_\infty(\lambda)a^\dagger_1(\mu)=a^\dagger_1(\mu)R_{\infty 1}(\lambda-\mu)T_\infty(\lambda) \tag{4.10}$$

with R given by (2.18).

Then, from Ref. 29 we can directly assert the following.

Property 4.2: The well-bred vertex operators $T_\infty(\lambda)$ obey Faddeev–Reshetikhin–Takhtajan (FRT) relations

$$R_{\infty\infty'}(\lambda-\mu)T_\infty(\lambda)T_{\infty'}(\mu)=T_{\infty'}(\mu)T_\infty(\lambda)R_{\infty\infty'}(\lambda-\mu), \tag{4.11}$$

so that they generate the super-Yangian algebra $Y(gl(M|N))$. In addition, they form a symmetry super-algebra for the hierarchy $H^{(n)}$ defined by

$$H^{(n)}=\int_{-\infty}^{\infty}dk\,k^n a^\dagger(k)a(k),\quad n\in\mathbb{Z}_+, \tag{4.12}$$

forming an Abelian algebra of Hermitian operators and governing the flows of the scattering operators a, $a^\dagger$ as follows:

$$e^{iH^{(n)}t}a(k)e^{-iH^{(n)}t}=e^{-ik^nt}a(k),$$

$$e^{iH^{(n)}t}a^\dagger(k)e^{-iH^{(n)}t}=e^{ik^nt}a^\dagger(k).$$

Now, recalling the results obtained in Sec. II C 4, Property 3.6 and Eqs. (3.73)–(3.75), we see that both descriptions of our integrable system (in terms of canonical fields or ZF scattering operators) are equivalent. But in this operation, we have gained an explicit realization of the super-Yangian generators.

To do this, we use the inductive relations obtained in Theorem 3.3 of Ref. 29 order by order in the spectral parameter λ. Let us rewrite

$$T_\infty(\lambda)=\mathbb{1}+\frac{ig}{\lambda}\sum_{p=0}^{\infty}T_\infty^{\{p\}}\lambda^{-p}, \tag{4.13}$$

where, accordingly,

$$T_\infty^{\{p\}}=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n!}a^\dagger_{n\cdots 1}T^{(n)\{p\}}_{\infty 1\cdots n}a_{1\cdots n}$$

for some $T^{(n)\{p\}}_{\infty 1\cdots n}\in(\mathbb{C}^{\otimes K^2})^{\otimes(n)}(k_1,\ldots,k_n)$.

Our goal is to determine $T_\infty^{\{0\}}$ and $T_\infty^{\{1\}}$, that is the first two "levels" of the super-Yangian generators. To do this we note that the inductive relations of Theorem 3.3 in Ref. 29 at first order in λ take the form

$$T^{(n+1)}_{\infty 0\cdots n}=T^{(n)}_{\infty 1\cdots n}-T^{(n)}_{\infty 0\cdots n-1}+O(\lambda^{-2}), \tag{4.14}$$

which, under the knowledge of

$$T^{(1)\{0\}}_{\infty 0}=\mathbb{1}+P_{\infty 0},$$

yields

$$T^{(n+1)\{0\}}_{\infty 0\cdots n}=(-1)^n\sum_{k=0}^{n}(-1)^k\binom{n}{k}P_{\infty k},$$

where P_{ij} is the super-permutation of auxiliary spaces i and j, so that

$$T_\infty^{\{0\}}=\sum_{n=0}^{\infty}\frac{(-1)^{n+1}}{n!}\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}a^\dagger_{n\cdots 0}P_{\infty k}a_{0\cdots n}. \tag{4.15}$$

Now that we have the explicit form of $T_\infty^{\{0\}}$ we can use it to evaluate the commutator $[T_{\infty'}^{\{1\}},T_\infty^{\{0\}}]$ directly and compare the result to that obtained from the FRT relations (4.11) at order λ^{-2}. The latter calculation yields

$$[T_{\infty'}^{\{1\}},T_\infty^{\{0\}}]=[P_{\infty'\infty},T_\infty^{\{1\}}]. \tag{4.16}$$

As for the former, the well-bred relations (4.10) at order λ^{-2} read

$$[T_\infty^{\{0\}},a_0(\mu)]=(\mathbb{1}+P_{0\infty})a_0(\mu),$$

$$[T_\infty^{\{1\}},a_0(\mu)]=\mu(\mathbb{1}+P_{0\infty})a_0(\mu)+ig(\mathbb{1}+P_{0\infty})a_0(\mu)(\mathbb{1}+T_\infty^{\{0\}}),$$

$$[T_\infty^{\{0\}},a_0^\dagger(\mu)]=-a_0^\dagger(\mu)(\mathbb{1}+P_{\infty 0}),$$

$$[T_\infty^{\{1\}},a_0^\dagger(\mu)]=-\mu a_0^\dagger(\mu)(\mathbb{1}+P_{\infty 0})+iga_0^\dagger(\mu)(\mathbb{1}+P_{\infty 0})(\mathbb{1}-T_\infty^{\{0\}}),$$

which will be useful in calculating

$$[T_{\infty'}^{\{1\}},T_\infty^{\{0\}}]=\sum_{n=0}^{\infty}\frac{(-1)^{n+1}}{n!}\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}[T_{\infty'}^{\{1\}},a^\dagger_{n\cdots 0}P_{\infty k}a_{0\cdots n}].$$

Note that this procedure can be iterated to evaluate $T_{\infty'}^{\{n\}}$ for an arbitrary n through $[T_{\infty'}^{\{n\}},T_\infty^{\{0\}}]$. Now,

$$[T^{\{1\}}_{\infty'},a^\dagger_{n\cdots 0}P_{\infty k}a_{0\cdots n}]=\sum_{i=0}^{n}a^\dagger_{n\cdots 0}P_{\infty k}a_0\cdots[T^{\{1\}}_{\infty'},a_i]\cdots a_n+\sum_{i=0}^{n}a^\dagger_n\cdots[T^{\{1\}}_{\infty'},a^\dagger_i]\cdots a^\dagger_0P_{\infty k}a_{0\cdots n}$$

$$=[P_{\infty\infty'},(\mu_k-n-1)a^\dagger_{n\cdots 0}P_{\infty k}a_{0\cdots n}]+a^\dagger_{n\cdots 0}[P_{\infty\infty'},P_{\infty k}]T^{\{0\}}_{\infty'}a_{0\cdots n}$$

$$+\sum_{i=0}^{k-1}a^\dagger_{n\cdots 0}[P_{\infty k},P_{\infty\infty'}]P_{\infty' i}a_{0\cdots n}+\sum_{i=k+1}^{n}a^\dagger_{n\cdots 0}P_{\infty' i}[P_{\infty k},P_{\infty\infty'}]a_{0\cdots n}.$$

This expression can be considerably simplified in $[T^{\{1\}}_{\infty'},T^{\{0\}}_{\infty}]$ using the properties of the binomial coefficients to combine the last three terms. Inserting (4.15) and using the property

$$\sum_{n=k}^{i-1}\binom{N}{n}\alpha^n_k\alpha^{N-n}_{i-n}=\alpha^N_k-\alpha^N_i,\quad\text{where}\quad\alpha^n_k=(-1)^{k-1}\binom{n-1}{k-1},$$

proved in Ref. 4, we get (after a convenient relabeling of the auxiliary spaces)

$$[T^{\{1\}}_{\infty'},T^{\{0\}}_{\infty}]=\left[P_{\infty\infty'},\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\sum_{k=1}^{n}\alpha^n_k a^\dagger_{1\cdots n}\left\{(\mu_k-ign)P_{\infty k}-ig\sum_{i=1}^{k-1}P_{\infty i}P_{\infty k}\right\}a_{n\cdots 1}\right].$$

Comparing this last expression with (4.16), we get the explicit form for $T^{\{1\}}_{\infty}$ (up to a term proportional to $\mathbb{I}_\infty$).

To conclude, we can recast this expression as

$$T^{\{1\}}_{\infty}=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\sum_{k=1}^{n}\alpha^n_k a^\dagger_{1\cdots n}\left(\mu_kP_{\infty k}-ig\sum_{i=1}^{k-1}P_{\infty k}P_{\infty i}\right)a_{n\cdots 1}+igT^{\{0\}}_{\infty}T^{\{0\}}_{\infty}. \tag{4.17}$$

In the case of $gl(N)$, we recover the results of Ref. 4, although in a different basis:

$$T^{\{0\}}_{ij}=\sum_{n=0}^{\infty}\frac{(-1)^{n+1}}{n!}\sum_{k=0}^{n}\alpha^n_k a^\dagger_{n\cdots 0}E^{(k)}_{ji}a_{0\cdots n},$$

$$T^{\{1\}}_{ij}=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\sum_{k=1}^{n}\alpha^n_k a^\dagger_{1\cdots n}\left(\mu_kE^{(k)}_{ji}-ig\sum_{\ell=1}^{k-1}\sum_{m=1}^{N}E^{(\ell)}_{jm}E^{(k)}_{mi}\right)a_{n\cdots 1}+ig(T^{\{0\}})^2_{ji},$$

where $E^{(\ell)}_{ij}$ denotes the E_{ij} matrix in the ℓth auxiliary space.

For $gl(M|N)$, similar formulas may also be obtained, taking care of the $\mathbb{Z}_2$-graded tensor products.

V. CONCLUSION

We solved a vectorial version of the nonlinear Schrödinger equation which contains fermions and bosons at the same time. We first introduced it classically using a $\mathbb{Z}_2$-graded formalism. At the quantum level, special attention was paid to the resolution using a super ZF algebra associated to the R-matrix of the super-Yangian $Y(gl(M|N))$. The integrability and symmetry of our system was studied through a Lax pair formalism and it is worth stressing the deep interplay between canonical and (ZF) algebraic formalisms. The ZF algebra allowed us to compute the correlation functions. Further investigations can be performed in this direction to study super-versions of known integrable systems. One can also study these super-versions when a boundary is introduced, using generalizations of the ZF algebra (boundary algebras).

APPENDIX: AUXILIARY SPACES

1. Graded spaces

We define in the auxiliary space, a K-column vector e_j with 1 at row j and 0 elsewhere, its transpose, the row vector $e_i^\dagger=(0,...,1,...,0)$ and the matrices E_{ij}, with 1 at position (i,j).

Here and below, the vectors e_i, $e_i^\dagger$, and the matrices E_{ij} will be $\mathbb{Z}_2$-graded:

$$[e_i]=[e_i^\dagger]=[i]; \quad [E_{ij}]=[i]+[j] \quad \text{with } [i]=\begin{cases}0 & \text{for } i=1,...,M,\\ 1 & \text{for } i=M+1,...,N.\end{cases}$$

Accordingly, the tensor product of auxiliary spaces will be also $\mathbb{Z}_2$-graded, e.g.,

$$(\mathbb{I}\otimes e_i)(E_{jk}\otimes\mathbb{I})=(-1)^{[i]([j]+[k])}E_{jk}\otimes e_i\,.$$

We will consider even objects in the following sense: $v=v_ie_i$ and $U=U_{ij}E_{ij}$ (summation on repeated indices is understood) are even iff $[v_i]=[i]$ and $[U_{ij}]=[i]+[j]$. For example, the field $\Phi(x)$ is even.

Note that, when dealing with the tensor product of auxiliary spaces, one has to be careful not to confuse (even) objects like $\boldsymbol{\lambda}_1=\boldsymbol{\lambda}\otimes\mathbb{I}=\Sigma_{i=1}^K\lambda_ie_i\otimes\mathbb{I}$ with their ($\mathbb{Z}_2$-graded) components λ_i, $i=1,...,K$. As a (tentative) clarifying notation, we will use boldface letters for the even objects, and ordinary letters for their components.

Finally, in order to apply our formalism to derive the classical NLSS equation, we will use the global Kronecker symbol,

$$\delta_{12}=\delta^{ij}(e_i\otimes e_j^\dagger)=(e_i\otimes e_i^\dagger), \tag{A1}$$

and, accordingly,

$$\delta_{21}=(-1)^{[i]}(e_i^\dagger\otimes e_i). \tag{A2}$$

2. Poisson brackets

For F and G two $(\Phi,\Phi^\dagger)$-functionals, their Poisson bracket is defined by

$$\{F,G\}=i\sum_{\ell=1}^K\int_{-\infty}^{\infty}dx(-1)^{[F][\ell]}\left((-1)^{[\ell]}\frac{\delta F}{\delta\phi_\ell(x)}\frac{\delta G}{\delta\phi_\ell^\dagger(x)}-\frac{\delta F}{\delta\phi_\ell^\dagger(x)}\frac{\delta G}{\delta\phi_\ell(x)}\right). \tag{A3}$$

This bracket is a graded Poisson bracket, i.e., it is bilinear, graded antisymmetric, and obeys the graded Leibniz rule and graded Jacobi identity.

To any graded PB, one can associate a ''global'' Poisson bracket, defined for the even functionals $\mathbf{F}$ and $\mathbf{G}$. We introduce the notation u_α to denote either e_i ($\alpha=(0,i)$ and $[\alpha]=[i]$), $e_i^\dagger$ ($\alpha=(i,0)$ and $[\alpha]=[i]$), or E_{ij} ($\alpha=(i,j)$ and $[\alpha]=[i]+[j]$), so that any even object $\mathbf{F}$ can be written $\mathbf{F}=\Sigma_\alpha F_\alpha u_\alpha$ with $[F_\alpha]=[\alpha]$.

On any even object, one defines the global PB

$$\{\mathbf{F}_1,\mathbf{G}_2\}=\sum_{\alpha,\beta}\{\mathbf{F}_\alpha,\mathbf{G}_\beta\}u_\alpha\otimes u_\beta\,. \tag{A4}$$

It is bilinear, antisymmetric, and obeys Leibniz rule and Jacobi identity. Let us stress that this global PB is not graded (because of the use of auxiliary spaces), but its ''component'' version indeed is graded.

Lemma A.1: The global PB (A4) corresponding to the graded PB (A3) can be rewritten as

$$\{\mathbf{F}_1,\mathbf{G}_2\}=i\int_{\mathbb{R}}dx\left(\frac{\delta\mathbf{F}_1}{\delta\Phi_{3/2}(x)}\frac{\delta\mathbf{G}_2}{\delta\Phi^{\dagger}_{3/2}(x)}-\frac{\delta\mathbf{G}_2}{\delta\Phi_{3/2}(x)}\frac{\delta\mathbf{F}_1}{\delta\Phi^{\dagger}_{3/2}(x)}\right), \tag{A5}$$

where we have introduced a third auxiliary space (labeled $\frac{3}{2}$) which is "inserted" between the space 1 and the space 2. We have also defined

$$\frac{\delta}{\delta\Phi(x)}=\sum_{j=1}^{K}e_j^{\dagger}\frac{\delta}{\delta\phi_j(x)}\quad\text{and}\quad\frac{\delta}{\delta\Phi^{\dagger}(x)}=\sum_{j=1}^{K}(-1)^{[j]}e_j\frac{\delta}{\delta\phi_j^{\dagger}(x)} \tag{A6}$$

Proof: Direct calculation. ■

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Integrability characteristics of two-dimensional generalizations of NLS type equations

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(Received 27 May 2003; accepted 1 September 2003)

A recent procedure based on truncated Painlevé expansions is used to derive Lax Pairs, Darboux transformations, and various soliton solutions for integrable $(2+1)$ generalizations of NLS type equations. In particular, diverse classes of solutions are found analogous to the dromion, instanton, lump, and ring soliton solutions derived recently for $(2+1)$ Korteweg–de Vries type equations, the Nizhnik–Novikov–Veselov equation, and the $(2+1)$ Broer–Kaup system. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623929]

I. INTRODUCTION

The techniques of Painlevé analysis[1] are by now well known in the area of testing nonlinear systems for integrability. In addition, various developments have taken place in the field over the past decade or so. These include investigations of the reasons underlying the technique's success, the study of ''higher-order'' truncations, the so-called ''invariant'' Painlevé analysis, the judicious application of two (or more) singular manifold functions where deemed necessary, and the use of truncated Painlevé expansions to obtain analytic solutions for both integrable and nonintegrable NLPDEs. We shall refer to select, relevant portions of this work subsequently.

Another branch of the subject, with a long history,[2–5] involves the mutual interconnections among various features or properties of integrable systems. Such interconnections were considered from the perspective of Painlevé analysis in a seminal series of papers by Weiss.[6] These papers developed the approach, now known as ''the singularity manifold method (SMM)'' of truncating the principal or general branch Painlevé singularity expansion for the solution of the system of NLPDEs at the constant term, thereby imposing a specific choice of the singular manifold function which has come to be called ''the singular manifold'' (as opposed to the infinite expansion employed in the Painlevé test where this function is arbitrary). This singularity manifold function and the truncated ''singular part'' expansion are then used to algorithmically derive an auto-Bäcklund transformation (BT) between two different solutions of the NLPDE(s), and also semialgorithmically derive the associated linear scattering problem or Lax Pair. Since the equations resulting from the use of this truncated expansion result in an auto-BT, they are often referred to as the ''Painlevé–Bäcklund equations'' and this is a usage we will employ for brevity and convenience.

Weiss' original technique was extensively developed by others, notably in the encyclopedic article on various aspects of Painlevé expansions by Newell and his collaborators[7] which, among numerous other things, extended the Weiss SMM to derive Hirota tau functions as well. However, the original semialgorithmic nature of the derivation of the Lax Pair in Weiss' procedure persisted. One recent area of investigation in the Painlevé analysis of single-component integrable NLPDEs has been to attempt to extend the Weiss procedure significantly to derive the so-called ''Weiss substitution'' which enables the Painlevé–Bäcklund equations to be linearized into the Lax Pair, thus improving a part of the Weiss procedure. An additional objective is to derive various other features of the integrable system such as Miura transformations, Darboux transformations, multisoliton solutions, Hirota's tau function, and similarity reductions. As is readily apparent, this work is motivated by earlier work in Refs. 4 and 7.

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In this paper, we apply this procedure to systems in $(2+1)$ dimensions. In particular, we derive integrability characteristics for various members of a family of integrable $(2+1)$ NLS-type systems. The remainder of the paper is organized as follows. In Sec. II, we derive the Lax Pair, Darboux transformation, and soliton solutions for an integrable $(2+1)$ dimensional system. Hirota's tau function may also be obtained, but is not as useful here as for other systems. Sections III and IV contain brief treatments of two other integrable $(2+1)$ NLS type systems. In Sec. V, we conclude with a brief summary, as well as some comments on future prospects.

II. UNIFIED TREATMENT OF INTEGRABLE (2+1) GENERALIZATIONS OF THE KAUP EQUATION

In this section, we first develop the analysis using two members of the integrable $(2+1)$ NLS type systems considered by Mikhailov and co-workers[8–10] as typical examples. We choose systems in $(2+1)$ dimensions intentionally so as to demonstrate the direct applicability of the analysis to systems in more than one spatial dimension. As we shall see, the analysis in $(2+1)$ is, as one might expect, somewhat more involved than for $(1+1)$ systems. We shall mention appropriate references as we proceed, but two background papers of general relevance are those by Estevez and co-workers.[11,12]

In particular, we shall consider the following two integrable generalizations of the Kaup equation:[8,13]

$$u'_t = u'_{xx} + 2p'u'_x, \tag{2.1a}$$

$$-v'_t = v'_{xx} - 2p'v'_x, \tag{2.1b}$$

$$p'_y = (u+v)_x, \tag{2.1c}$$

and

$$u'_t = u'_{yy} + (u'^2 + u'v')_y + q', \tag{2.2a}$$

$$-v'_t = v'_{yy} - (v'^2 + u'v')_y + q', \tag{2.2b}$$

$$q'_x = (v'u'_x - u'v'_x)_y. \tag{2.2c}$$

A. Preliminary analysis of (2.1)

We shall detail the calculations and the procedure for (2.1) first, and subsequently summarize similar computations for (2.2) in Sec. III.

As usual, we first perform the leading-order analysis and assume

$$u' \sim u_0 \phi^{-\alpha}, \quad v' \sim v_0 \phi^{-\beta}, \quad p' \sim p_0 \phi^{-\gamma}. \tag{2.3}$$

Balancing the most singular second derivative and nonlinear terms in the first two equations yields

$$\alpha + \beta = -2, \tag{2.4a}$$

$$\gamma = 1, \tag{2.4b}$$

$$p_0 = (\alpha+1)\phi_x/2. \tag{2.4c}$$

At this point, it is tempting to look at the apparently symmetric way in which the variables u and v occur in (2.1) and thus assume that $\alpha = \beta = -1$. However, it is straightforward to check that this choice leads to a contradiction. One may obtain consistent choices by (a) balancing the left-hand

side of (2.1c) with the first term on the right, with the other term being less singular, or by (b) balancing the left side of (2.1c) with the second term on the right. These correspond, respectively, to

$$\alpha=1, \quad \beta=-3 \tag{2.5a}$$

or

$$\alpha=-3, \qquad \beta=1. \tag{2.5b}$$

However, another valid possibility is given by

$$\alpha=1, \quad \beta=0, \quad \gamma=1. \tag{2.6}$$

Performing the resonance analysis[1] for the branch (2.6) yields resonances at $r=-1,0,1,2,3$. Hence, this branch yields the full complement of arbitrary functions (four at the resonance 0, and at the three positive integer resonances, and the arbitrary location of $\phi=0$ given by $r=-1$). Thus, this is the principal branch. The branch (2.5) does not yield four non-negative integer resonances and is thus a singular branch. For branch (2.5), the valid resonances corresponding to arbitrary coefficients in the Painlevé expansion are at $r=-1,0,1$, and 2, while the spurious resonance is at $r=-3$.

We shall detail the case corresponding to the principal branch (2.6) and summarize the analogous results for (2.4)/(2.5) subsequently. We shall next invoke the Weiss SMM by substituting expansions for our variables truncated at the constant term (and with coefficients of all singular terms explicity expressed in terms of derivatives of the singular manifold function), and use the resulting expansions to develop the method for deriving various properties of the integrable system (2.1). For (2.4)/(2.5), the leading order $O(\phi^{-3})$ terms in (2.1a) and (2.1b) yield the coefficients of the singular terms in u and p explicitly as

$$u_0=\phi_y, \quad p_0=\phi_x. \tag{2.7}$$

Using these, we substitute the truncated expansion

$$u'=\frac{\phi_y}{\phi}+u, \tag{2.8a}$$

$$v'=v\phi^0+v_1\phi+\cdots, \tag{2.8b}$$

$$p'=\frac{\phi_x}{\phi}+p. \tag{2.8c}$$

Substituting these in (2.1) yields equations at various orders in ϕ, the Painlevé–Bäcklund equations, which are contained in the Appendix. Notice that (A4) and (A5) show that

$$v=v(y). \tag{2.9}$$

Thus, (A4) and (A5) are identically satisfied. The only nontrivial equations surviving are (A1)–(A3) and (A6) which are given in the following for ease of comprehension in the following calculations:

$$\phi_t-2p\phi_x-\phi_{xx}=0, \tag{2.10a}$$

$$-\phi_{yt}+2\phi_x u_x+2p\phi_{xy}+\phi_{xxy}=0, \tag{2.10b}$$

$$p_y=u_x, \tag{2.10c}$$

$$-u_t+2pu_x+u_{xx}=0. \tag{2.10d}$$

Substituting (2.10c) in (2.10b) and integrating with respect to y yields

$$-\phi_t+2p\phi_x+\phi_{xx}=\lambda_*(x,t) \tag{2.11}$$

which is the same as (2.10a) if the "constant" of integration on the right is taken to be zero. Thus, we may essentially just ignore (2.10b) since it is really the y derivative of (2.10a).

B. The singular manifold equation and Weiss substitutions

We now work with the remaining Painlevé–Bäcklund equations in (2.10) to derive the so-called singular manifold equation (SME). The essential idea in deriving the SME is to express all physical or field variables (or potentials in the language of scattering) in terms of functions of the singularity manifold and, using these, to derive a consistency condition on this singularity manifold which is the SME. The motivation for this is that analysis of the SME yields a method for deriving the Weiss substitution and thus linearizing the Painlevé–Bäcklund equations to obtain the Lax Pair. The details vary from case to case, but the essential ideas in deriving the SME and analyzing it are common to all examples. For this purpose, we also define the quantities[14–16]

$$V\equiv\phi_{xx}/\phi_x, \tag{2.12a}$$

$$C_1\equiv\phi_t/\phi_x, \tag{2.12b}$$

$$C_3\equiv\phi_y/\phi_x, \tag{2.12c}$$

which satisfy the compatibility conditions

$$V_t=(C_{1x}+C_1V)_x \quad (\text{from } \phi_{xxt}=\phi_{txx}), \tag{2.13a}$$

$$V_y=(C_{3x}+VC_3)_x \quad (\text{from } \phi_{xxy}=\phi_{yxx}), \tag{2.13b}$$

$$C_{3t}=C_{1y}+C_1C_{3x}-C_3C_{1x} \quad (\text{from } \phi_{yt}=\phi_{ty}). \tag{2.13c}$$

Using (2.10c) in (2.10d) yields

$$u_t=\frac{\partial}{\partial y}[p^2+p_x], \qquad u_x=p_y. \tag{2.14}$$

Integrating the consistency condition $u_{xt}=u_{tx}$ with respect to y yields

$$p_t=\partial_x[p^2+p_x]+\lambda(x,t). \tag{2.15}$$

From (2.10a) and (2.12), we have

$$p=\tfrac{1}{2}(C_1-V). \tag{2.16}$$

Using this in (3.15) yields the SME

$$\tfrac{1}{2}(C_1-V)_t=\partial_x[\tfrac{1}{4}(C_1^2-2C_1V+V^2)+\tfrac{1}{2}(C_{1x}-V_x)]+\lambda(x,t). \tag{2.17}$$

The key to linearizing the Painlevé–Bäcklund equations is to perform a leading-order singularity analysis of the SME and the consistency conditions (2.13), treated as an NLPDE in C_1 and

V, in a manner analogous to our earlier analysis. The reason is that the SME governs the behavior of ϕ and its derivatives, and thus analyzing it yields the correct behaviors for C_1 and V. In other words, we apply the first part of the SMM to the SME. Assuming

$$C_1 \sim c_0 \chi^a, \quad V \sim v_0 \chi^b \tag{2.18}$$

and balancing the most singular terms (those within square brackets) in (2.17) yields

$$a = b = -1 \tag{2.19}$$

and

$$c_0 = v_0 \quad \text{or} \quad c_0 - v_0 = 2\chi_x . \tag{2.20}$$

Next, using (2.18)/(2.19) and balancing the most singular terms in (2.13a) yields

$$v_0 = \chi_x \tag{2.21}$$

which, with (2.20), implies

$$c_0 = 3\chi_x \quad \text{or} \quad c_0 = \chi_x . \tag{2.22}$$

Once this leading-order analysis of the SME is complete, we follow an approach due to Musette and Conte[17–19] and assign a separate singularity manifold, i.e., two distinct χ's, to each of the two branches for C_1 and V in (2.18) to (2.22). Denoting these as ψ^+ and ψ^- (the connection of these to the original singularity manifold ϕ will become apparent in the following step), (2.18)–(2.22) yield the following leading behaviors:

$$V \equiv \frac{\phi_{xx}}{\phi_x} = \frac{\psi_x^+}{\psi^+} + \frac{\psi_x^-}{\psi^-} \tag{2.23}$$

and

$$C_1 \equiv \frac{\phi_t}{\phi_x} = \frac{3\psi_x^+}{\psi^+} + \frac{\psi_x^-}{\psi^-} . \tag{2.24}$$

Integrating (2.23) with respect to x and using the result in (2.24) yields the connection of the original singularity manifold variable ϕ to the ψ's, i.e.,

$$\phi_x = \psi^+ \psi^- \tag{2.25}$$

and

$$\phi_t = 3\psi_x^+ \psi^- + \psi_x^- \psi^+ . \tag{2.26}$$

These last two equations are in fact the analogs of the Weiss substitutions. Note that, unlike Weiss' original procedure, they have been derived here completely self-consistently from the singularity analysis. More specifically, in Weiss' original procedure,[6] such substitutions were based on either guesswork or information regarding the order of the underlying linear scattering problem, both of which were based on extraneous knowledge about the system. These substitutions will be key to linearizing the Painlevé-Bäcklund equations (2.10a), (2.10c), and (2.10d) to yield the Lax Pair for the system, and we proceed next to this step.

C. The Lax Pair

Using (2.23)/(2.24) in (2.16) yields

$$\psi_x^+ = p\psi^+. \tag{2.27}$$

Using (2.27) for $p(x,t)$ in (2.10c) and interchanging the order of the derivatives, the resulting equation may be integrated with respect to x to yield

$$\psi_y^+ = [u - \lambda_1(y,t)]\psi^+. \tag{2.28}$$

The last two equations comprise the spatial part of the Lax Pair for (2.1) (with unprimed variables instead of primed ones). It is straightforward to check that the compatibility condition for (2.27)/(2.28) yields the governing equation (2.1c) for the system [using (2.9)]. Next, solving for u from (2.28) and using the result in the first term in (2.10d) yields

$$\lambda_{1t} + \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\psi_y^+}{\psi^+}\right] = 2pu_x + u_{xx}. \tag{2.29}$$

This constitutes the temporal part of the Lax Pair and it is straightforward to verify that the compatibility condition for (2.28) and (2.29) yields the first governing equation (2.1a) for the system (with unprimed variables), while the compatibility of (2.27) and (2.29) simply yields the x derivative of (2.1a). To the best of our knowledge, this is the first time this Lax pair has been derived.

Notice that since (2.10b) is redundant and (2.10a) was used to obtain (2.16) and hence (2.27), we have linearized all the Painlevé–Bäcklund equations (2.10) to obtain the Lax Pair for (2.1) (with unprimed variables).

At this point, we remind ourselves that the above branch of the singularity analysis of (2.1) corresponds to the principal branch (2.6). Performing an exactly analogous analysis but using the singular branch instead corresponding to (2.4)/(2.5b) for comparison purposes results in [the $\psi^{\pm}$ functions in (2.30) to (2.37) are different from those in (2.23) to (2.29)] the following.

(a) (2.8)/(2.9) are replaced by

$$u' = 0,$$

$$v' = -\frac{\phi_y}{\phi} + v, \tag{2.30}$$

$$p' = -\frac{\phi_x}{\phi} + p.$$

(b) (2.23)–(2.26) are replaced by

$$V = \frac{\psi_x^+}{\psi^+} + \frac{\psi_x^-}{\psi^-}, \tag{2.31}$$

$$C_1 = -\frac{\psi_x^+}{\psi^+} - \frac{3\psi_x^-}{\psi^-}, \tag{2.32}$$

$$\phi_x = \psi^+\psi^-, \tag{2.33}$$

$$\phi_t = -\psi_x^+\psi^- - 3\psi_x^-\psi^+. \tag{2.34}$$

(c) The resulting linear equations are

$$\psi_x^- = -p\psi^-, \tag{2.35}$$

$$\psi_y^- + [v - \lambda_2(y,t)]\psi^- = 0, \tag{2.36}$$

$$\lambda_{2t} - \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\psi_y^-}{\psi^-}\right] = 2pv_x - v_{xx}. \tag{2.37}$$

Note that the consistency of the last three equations recovers the second and third governing equations (2.1b) and (2.1c), while $u=0$ for this branch of the analysis and so (2.1a) is trivially satisfied. However, since $u\equiv 0$, this is not a Lax Pair, which we would expect since we used a singular branch. Analogous results hold for the other singular branch (2.4)/(2.5a).

D. The Darboux transformation

Once we have the Lax Pair, the next step in the analysis is to proceed to derive Darboux transformations,[20] i.e., transformations of the potentials u, v, and p and the eigenfunctions ψ which leave the Lax Pair(s) invariant. Once again, a procedure may be formulated from the Weiss SMM. If nontrivial Darboux transformations (DTs) result, they may then be iterated[20] in the usual manner starting from relatively simple seminal solutions of the governing PDEs following the Crum procedure to generate more complex families of multisoliton solutions. It is worth commenting here that, for many systems, the iteration of DTs appears to work better than the iteration of auto-BTs where one often remains confined to the same family of solutions after a single iteration. In addition, the procedure for deriving DTs may be iterated to generate Hirota's tau function. We shall lay out the basic ideas for the derivation of DTs next.

The key idea in deriving DTs is due to Konopelchenko and Stramp[21] and involves treating the Lax Pair itself as a system of NLPDEs in the field variables (potentials) u,p, and the ψs. Assuming a singular manifold ϕ_1, spectral parameter λ_1 and $+/-$ Lax Pair eigenfunctions ψ_1 associated to starting (or seminal) solutions u, v, and p of (2.1) yields

$$\phi_{1x} = \psi_1^+\psi_1^-, \tag{2.38}$$

$$\phi_{1t} = 3\psi_{1x}^+\psi_1^- + \psi_{1x}^-\psi_1^+, \tag{2.39}$$

$$\psi_{1x}^+ = p\psi_1^+, \tag{2.40}$$

$$\psi_{1y}^+ = [u - \lambda_1(y,t)]\psi_1^+, \tag{2.41}$$

$$\lambda_{1t} + \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\psi_{1y}^+}{\psi_1^+}\right] = 2pu_x + u_{xx}. \tag{2.42}$$

Here, we have used (2.25)–(2.29). New solutions u' and p' may be constructed using the auto-BTs (2.8a) and (2.8c) (with ϕ replaced by ϕ_1 corresponding to the seminal solutions), and associating a singular manifold ϕ_2', spectral parameter λ_2 and $+/-$ Lax Pair eigenfunctions ψ_2' to these yields the analogous equations:

$$\phi_{2x}' = \psi_2'^{+}\psi_2'^{-}, \tag{2.43}$$

$$\phi_{2t} = 3\psi_{2x}'^{+}\psi_2'^{-} + \psi_{2x}'^{-}\psi_2'^{+}, \tag{2.44}$$

$$\psi_{2x}'^{+} = p'\psi_2'^{+}, \tag{2.45}$$

$$\psi_{2y}'^{+} = [u' - \lambda_2(y,t)]\psi_2'^{+}, \tag{2.46}$$

$$\lambda_{2t}+\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\psi_{2y}'^{+}}{\psi_2'^{+}}\right]=2p'u_x'+u_{xx}'. \tag{2.47}$$

Next, following Ref. 21 and treating the Lax Pair (2.45)–(2.47) as a coupled system of NLPDEs in u', p', and the ψ_2''s, we may apply the SMM to this system of NLPDEs and thus add the following truncated expansion for the $\psi_2'^{+}$ to those in (2.8a) and (2.8c) (with ϕ replaced by ϕ_1 for the seminal solutions) to obtain

$$\psi_2'^{+}=\psi_2^{+}-\frac{\psi_1^{+}\theta^{+}}{\phi_1}, \tag{2.48}$$

$$u'=\frac{\phi_{1y}}{\phi_1}+u, \tag{2.49}$$

$$p'=\frac{\phi_{1x}}{\phi_1}+p. \tag{2.50}$$

Now, for a DT, the transformation of potentials and eigenfunctions given by (2.48)–(2.50) must preserve the Lax Pair. In other words, the original starting solutions corresponding to u, p, and ψ_2^{+} must satisfy the same Lax Pair equations (2.45)–(2.47) for the same eigenvalue λ_2, i.e.,

$$\psi_{2x}^{+}=p\psi_2^{+}, \tag{2.51}$$

$$\psi_{2y}^{+}=[u-\lambda_2(y,t)]\psi_2^{+}, \tag{2.52}$$

$$\lambda_{2t}+\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\psi_{2y}^{+}}{\psi_2^{+}}\right]=2pu_x+u_{xx}. \tag{2.53}$$

Substituting the truncated expansions (2.48)–(2.50) in (2.45)–(2.47) and using (2.38)/(2.39) and (2.51) to (2.53) yields, after some computer algebra with MATHEMATICA, the trivial result

$$\theta^{+}=0. \tag{2.54}$$

Also, a leading-order singularity analysis of (2.13c), in a manner similar to that performed on (2.13a) while analyzing the SME (2.17) to derive (2.23)/(2.24) shows that

$$\phi_y=k(3\psi_x^{+}\psi^{-}+\psi_x^{-}\psi^{+}) \tag{2.55}$$

for some arbitrary k. Using (2.38), (2.54), and (2.55) (with $\phi=\phi_1$) in (2.38)–(2.50) yields the following DT under which the Lax Pair(s) are invariant:

$$u'=\frac{k(3\psi_{1x}^{+}\psi_1^{-}+\psi_{1x}^{-}\psi_1^{+})}{\int\psi_1^{+}\psi_1^{-}dx}+u, \tag{2.56}$$

$$p'=\frac{\psi_1^{+}\psi_1^{-}}{\int\psi_1^{+}\psi_1^{-}dx}+p, \tag{2.57}$$

$$\psi_2'^{+}=\psi_2^{+}. \tag{2.58}$$

Note that this DT may be iterated starting from simple seminal solutions of (2.1) and using the Crum procedure.[20] In order to do this, one would substitute the simple seminal solutions for u, $v=v(y)$, and p in (2.40) to (2.42) to obtain the first iterate for ψ_1^{+}. This may then be substituted in (2.56)/(2.57) to yield a second iterate for the potentials u and p, and the process may then be

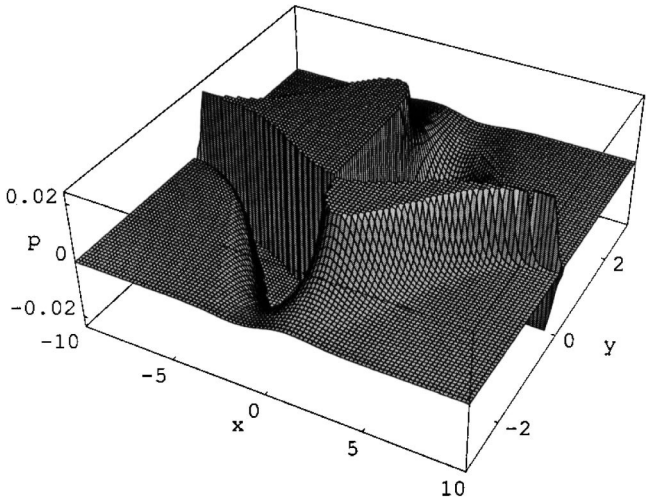

FIG. 1. Plot of p for $c_1(y)=\pi, c_2(y)=y^5$ at $t=1$ for Eq. (2.1).

iterated as long as closed-form solutions may still be readily obtained. Before attempting this, we make one other comment. It is possible to iterate the singular manifold function itself to obtain Hirota's tau function. However, (2.58) makes it apparent that, for the present example (2.1), only trivial or identity iterates result for the ψ functions, and hence for the ϕ's [see (2.25)]. We therefore omit the discussion of Hirota's method for this system.

E. Soliton solutions

In order to complete the treatment of (2.1), we finally turn to a discussion of the iteration of the auto-BT (2.8) for this equation in order to derive analytic solutions of (2.1). The relevant equations here will be (2.1), (2.8), (2.9), and (2.10a), (2.10c). Starting from the simplest vacuum solutions $u=v=p=0$ as seminal solutions, (2.10a) yields the heat equation (in t and x) for the first iterate of ϕ. Thus,

$$\phi(x,y,t)=\frac{1}{\sqrt{4\pi t}}e^{-x^2/4t}c_1(y)+c_2(y). \tag{2.59}$$

Using this and the seminal solutions in (2.8) yields the next iterate for the solutions, i.e.,

$$u'=\frac{c_1'(y)+2\sqrt{\pi t}\;\; c_2'(y)e^{x^2/4t}}{c_1(y)+2\sqrt{\pi t}\;\; c_2(y)e^{x^2/4t}}, \tag{2.60}$$

$$p'=\frac{xc_1(y)}{-2tc_1(y)-4\sqrt{\pi t^3}\;\; c_2(y)e^{x^2/4t}}. \tag{2.61}$$

It is straightforward to check that these are indeed solutions of (2.1) for $v=v(y)$ and arbitrary $c_1(y)$ and $c_2(y)$. One may try and iterate the process by using the last two equations in (2.10a) to obtain a second iterate for ϕ, but the solution becomes complicated and so we shall stop at this point. Figures 1–3 show plots of the solutions (2.60) and (2.61) for

(a) plot of p for $c_1(y)=\pi$, $c_2(y)=y^5$ at $t=1$;
(b) plot of u for $c_1(y)=\exp(-y^2/4)$, $c_2(y)=y^5$ at $t=1$; and
(c) plot of p for $c_1(y)=y^5$, $c_2(y)=\pi$ at $t=1$.

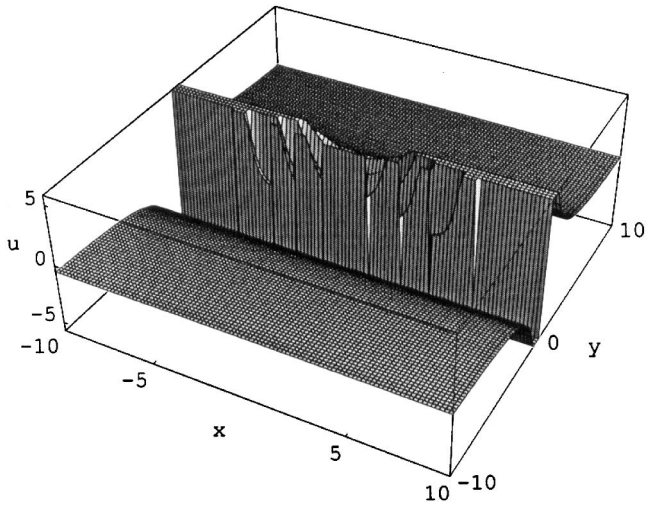

FIG. 2. Plot of u for $c_1(y)=\exp(-y^2/4t), c_2(y)=y^5$ at $t=1$ for Eq. (2.1).

In particular, note that these soliton solutions of this integrable $(2+1)$-dimensional system have free shape functions $c_1(y)$ and $c_2(y)$ in the y directions which have been chosen arbitrarily. This is analogous to the free shape functions recently found in soliton solutions for other integrable systems in $(2+1)$, including a $(2+1)$ KdV equation (not KPI or II), the Nizhnik–Novikov–Veselov equation, and a $(2+1)$ dimensional Broer–Kaup type system.[22–25] As for those systems, where a variety of dromions, lumps, breathers, instantons, and ring solitons are derived using Hirota's approach or variable separation techniques, we find diverse solutions. In particular, Fig. 1 corresponds to a four (two) -lump solution (we could refer to it as a two-dromion; the terminology is somewhat ambiguous with exponentially localized structures being called dromions). By contrast, the solutions in Figs. 2 and 3 show primarily y modulations and a complex multi (three) -lump structure, respectively. We shall encounter other types of solutions subsequently for other systems.

This concludes our treatment of (2.1), and we turn next to a relatively brief treatment of (2.2). In order to illustrate other features of the SMM method under consideration, we shall refer to

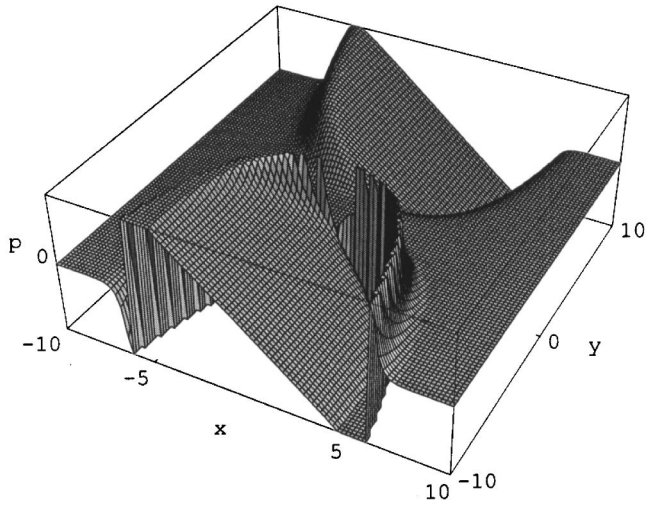

FIG. 3. Plot of p for $c_1(y)=c_2(y)=\exp(-y^2/4t)$ at $t=1$ for Eq. (2.1).

features of (2.2) which are analogous to those seen above for (2.1) only briefly. Our main concentration will be on features dissimilar to those discussed for (2.1).

III. BRIEF ANALYSIS OF (2.2)

Attempting a leading-order analysis of (2.2) by substituting

$$u' \sim u_0 \phi^{-\alpha}, \quad v' \sim v_0 \phi^{-\beta}, \quad q' \sim q_0 \phi^{-\gamma} \tag{3.1}$$

it is straightforward to check the possible consistent dominant balances and conclude the following.

(a) As for (2.1) [see (2.5)/(2.6)], consistent dominant balances exist with α and β having unequal values. We do not consider these cases or branches of the singularity analysis further as they are similar to the treatment in Sec. II.

(b) Unlike (2.1), (2.2) admits a consistent dominant balance with

$$\begin{aligned} &\alpha=\beta=1, \\ &\gamma=3. \end{aligned} \tag{3.2}$$

We shall concentrate on this branch as it illustrates somewhat different features of the analysis from those discussed in Sec. II.

The leading-order analysis for the branch discussed in b above yields

$$\{u_0, v_0, 0\} = \begin{cases} (0,0,0) \\ \text{or} \\ (0,-\phi_y,0) \\ \text{or} \\ (\phi_y,0,0). \end{cases} \tag{3.3}$$

Using the last of these together with (3.1), and substituting the resulting truncated expansions

$$u' = \frac{\phi_y}{\phi} + u, \tag{3.4a}$$

$$v' = v, \tag{3.4b}$$

$$q' = \frac{q_1}{\phi^2} + \frac{q_2}{\phi} + q, \tag{3.4c}$$

into (2.2) results in equations at different orders in powers of ϕ [analogous to those in the Appendix for (2.1)]. Solving these as in Sec. II yields

$$v = v(y,t), \tag{3.5}$$

$$q_1 = -v\phi_y^2, \tag{3.6}$$

$$q_2 = \phi_y v_y + v\phi_{yy}, \tag{3.7}$$

together with the conditions

$$-2v\phi_y^2 + \phi_t\phi_y - 2u\phi_y^2 - \phi_y\phi_{yy} = 0, \tag{3.8}$$

$$2\phi_y v_y + 2v\phi_{yy} + 2\phi_y u_y - \phi_{yt} + 2u\phi_{yy} + \phi_{yyy} = 0. \tag{3.9}$$

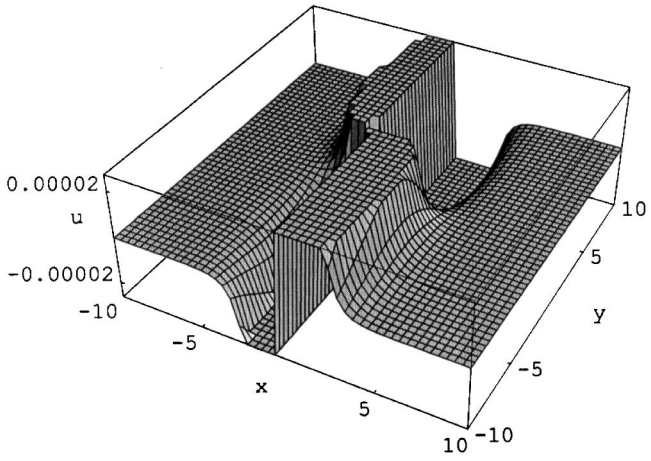

FIG. 4. Plot of u for $d_1(x)=\exp(-x^2/4t)$, $c_2(x)=x^5$ at $t=10$ for Eq. (2.2).

It is straightforward to check that (3.9) is the y partial of (3.8). Careful inspection of (3.5)–(3.8) and (3.4c) reveals an insufficient number of equations to eliminate all field variables (or potentials) u, v, and q and derive a SME. In fact, this is characteristic of a singular branch of the Painlevé analysis. As is well known, such a branch may not be used to algorithmically derive the various properties of the integrable system (2.2) as was done using a general or regular branch of (2.1) in the previous section. However, it may still be used to derive special analytic solutions (these are usually referred to as ''singular'' solutions, but in the sense of solutions not contained in the general solution and not necessarily in the sense of possessing singularities). We shall use the governing equations above for the chosen singular branch of the Painlevé analysis to derive special analytic solutions of (2.2). The procedure used will be iteration of the auto-BT (3.4), as was done for (2.1) at the end of Sec. II [and (3.4c)], and we proceed to this next.

The relevant equations are (3.4)–(3.8). Starting with vacuum solutions $u=v=q=0$ of (2.2), (3.8) yields the heat equation (in t and y) for ϕ. Solving this yields

$$\phi(x,y,t)=\frac{e^{-y^2/4t}d_1(x)}{\sqrt{4\pi t}}+d_2(x). \tag{3.10}$$

Using this and (3.5) to (3.7) in (3.4) yields the next iterate

$$u'=\frac{yd_1(x)}{-2td_1(x)-4\sqrt{\pi t^3}\;\; d_2(x)e^{y^2/4t}}, \tag{3.11a}$$

$$q'=0 \tag{3.11b}$$

for solutions of (2.2). It is straightforward to check that these satisfy (2.2). Figures 4–6 show the singular solutions in (3.11a) for

(a) $d_1(x)=e^{-x^2/4t}$, $d_2(x)=x^5$ at $t=10$;
(b) $d_1(x)=e^{x^2/4t}$, $d_2(x)=x^5$ at $t=1$;
and
(c) $d_1(x)=x^5$, $d_2(x)=e^{x^2/4t}$ at $t=10$.

Of these, the first is a two-lump solution, the second a complex multi-lump coherent structure, and the last a line soliton (front).

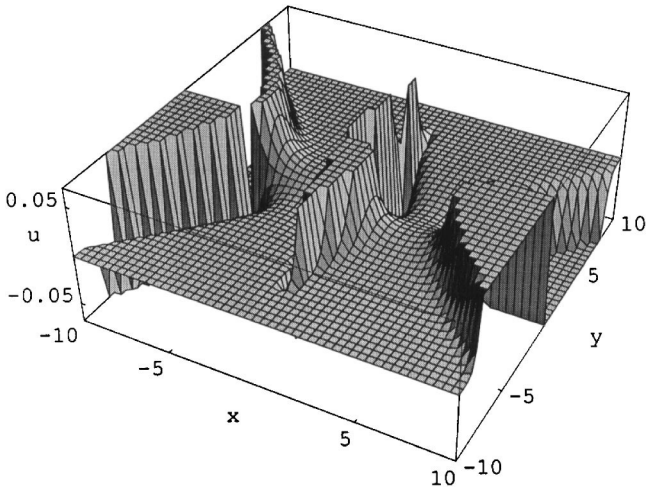

FIG. 5. Plot of u for $d_1(x)=e^{x^2/4t}$, $d_2(x)=x^5$ at $t=1$ for Eq. (2.2).

IV. A THIRD NLS TYPE SYSTEM IN (2+1)

In this section, we briefly discuss the system[8]

$$u'_t=u'_{yy}+u'[(u'v')_y+q'], \tag{4.1a}$$

$$-v'_t=v'_{yy}-v'[(u'v')_y-q'], \tag{4.1b}$$

$$q'_x=(v'u'_x-u'v'_x)_y, \tag{4.1c}$$

which is an integrable $(2+1)$ dimensional generalization of the derivative NLS2 equation.[10,26]

Plugging in the truncated singular branch expansions

$$u'=\frac{u_0}{\phi}+u,$$

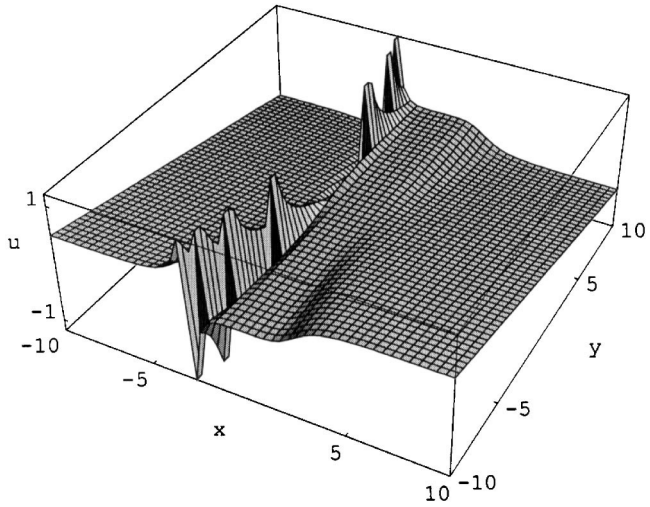

FIG. 6. Plot of u for $d_1(x)=x^5$, $d_2(x)=e^{x^2/4t}$ at $t=10$ for Eq. (2.2).

$$v' = v_0 + v_1 \phi, \tag{4.2a}$$

$$q' = \frac{q_0}{\phi^2} + \frac{q_1}{\phi} + q$$

into (4.1) yields

$$\begin{gathered} u_0 = \phi_y / v_0(y), \quad v_0 = v_0(y), \quad v_1 = 0, \\ q_0 = -\phi_y^2, \quad q_1 = \phi_{yy}. \end{gathered} \tag{4.2b}$$

Using these in (4.1) yields the nontrivial Painlevé–Bäcklund equations

$$\phi_t - 2u\phi_y - \phi_{yy} = 0, \tag{4.3}$$

$$q = u_y, \tag{4.4}$$

$$qu - u_t + uu_y + u_{yy} = 0. \tag{4.5}$$

From (4.5) and (4.3)

$$u_t = \frac{\partial}{\partial y}[u^2 + u_y], \tag{4.6}$$

$$u = \tfrac{1}{2}[C_1 - \overline{V}] \tag{4.7}$$

with

$$\overline{V} \equiv \phi_{yy} / \phi_y \tag{4.8}$$

and C_1 is defined by (2.12b).

Using (4.7) and (4.6) and performing a leading-order analysis of the resulting singular manifold equation [see (2.18)–(2.24)] yields

$$v_0 = \psi_y \tag{4.9}$$

and

$$c_0 = \psi_y \quad \text{or} \quad 3\psi_y. \tag{4.10}$$

Hence,

$$\overline{V} = \frac{\psi_y^+}{\psi^+} + \frac{\psi_y^-}{\psi^-},$$

$$\overline{C_1} = \frac{\phi_t}{\phi_y} = \frac{3\psi_y^+}{\psi^+} + \frac{\psi_y^-}{\psi^-}$$

and thus

$$\phi_y = \psi^+ \psi^-, \tag{4.11}$$

$$\phi_t = (3\psi_y^+ \psi^- + \psi_y^- \psi^+). \tag{4.12}$$

Using these, (4.7), (4.4), and (4.6) yields

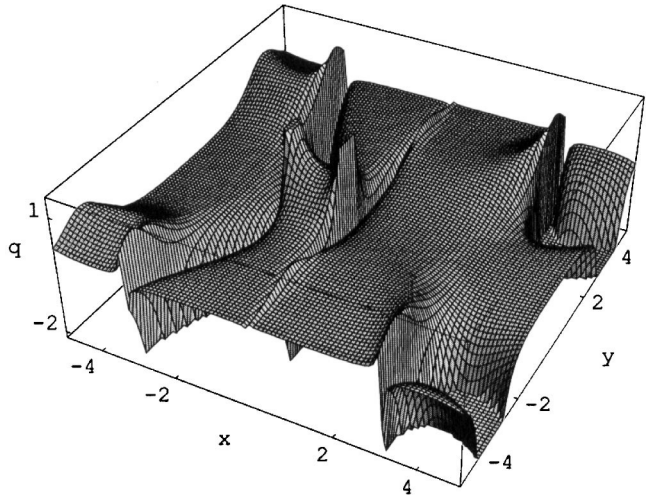

FIG. 7. Plot of q for $e_1(x)=\cosh x$, $e_2(x)=\sin x$ at $t=1$ for (4.1).

$$\psi_y^+ = u\psi^+ \tag{4.13}$$

and

$$\frac{d}{dy}(\psi_y^+/\psi^+) = q, \tag{4.14}$$

$$\psi_t^+ = [u^2 + u_y + \lambda_1(x,t)]\psi^+. \tag{4.15}$$

These equations comprise a Lax-like system of eigenvalue problems/evolution equation, but in the limited sense that $v=1$ [see (4.1)] since a singular branch has been used in (4.2). As is well known, this is what one would expect from using a singualr branch. The compatibility conditions for these yield (4.1).

We next iterate the truncated expansions (4.2a) and the auto-BT (4.3)/(4.4) to obtain analytic solutions of (4.1). Starting with the constant solutions $u=q=0$, $v=1$ of (4.1), (4.3) yields

$$\phi(x,y,t) = \frac{1}{\sqrt{4\pi t}} e^{-y^2/4t} e_1(x) + e_2(x).$$

Hence (4.2a) yields

$$q' = \frac{-e_1(x)[\sqrt{t}\ \ e_1(x) + \sqrt{\pi}(2t-y^2)e_2(x)e^{y^2/4t}]}{2t^{3/2}[e_1(x) + 2\sqrt{\pi t}\ \ e_2(x)e^{y^2/4t}]^2}, \tag{4.16}$$

$$u' = \frac{ye_1(x)}{[-2te_1(x) - 4\sqrt{\pi}\ \ t^{3/2}e_2(x)e^{y^2/4t}]}, \tag{4.17}$$

where, as before, $e_1(x)$ and $e_2(x)$ are free shape functions along x.

Figures 7–10 show the solution (4.16) for

(a) $e_1(x)=\cosh x$, $e_2(x)=\sin x$ at $t=1$;
(b) the time evolution in Fig. 7, i.e., with $e_1(x)=\cosh x$, $e_2(x)=\sin x$, for $y=3$;
(c) $e_1(x)=\cos x$, $e_2(x)=\sin x$ at $t=1$;
and

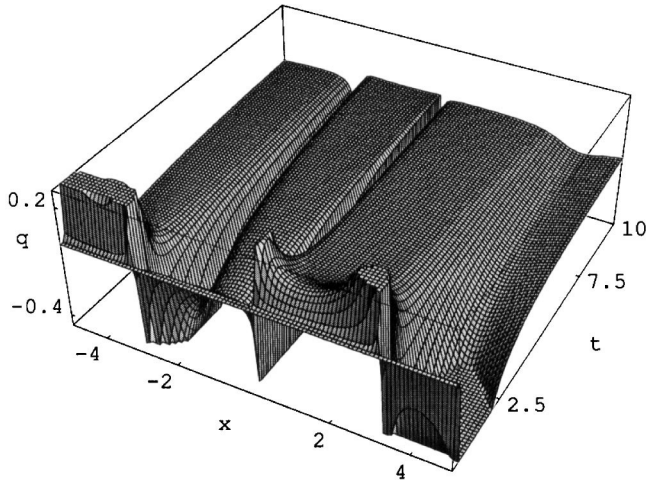

FIG. 8. Time evolution of q in Fig. 7 at $y=3$.

(d) $e_1(x)=e^{-x^2/4}$, $e_2(x)=1$ at $t=1$.

Figures 7 and 9 are complex multilump solutions, Fig. 8 shows a fairly regular time evolution (for each x, at $y=3$), and Fig. 10 shows a two-dromion. Figure 11 shows this two-dromion at a later time $t=2$. Note that the dromion structures splay outwards in both x and y directions (but stay spatially coherent) and also decrease in amplitude as time increases.

V. CONCLUSIONS AND PROSPECTS

In this paper, we have employed a technique which has evolved over the last decade or so to derive various properties of integrable $(2+1)$ dimensional NLS-type systems from truncated Painlevé expansions. As should be apparent from the examples we have considered, the technique has by now evolved to a point where it affords one form of unifying perspective on integrable systems, and also provides a method for investigating new integrable systems such as new integrable hierarchies of equations.

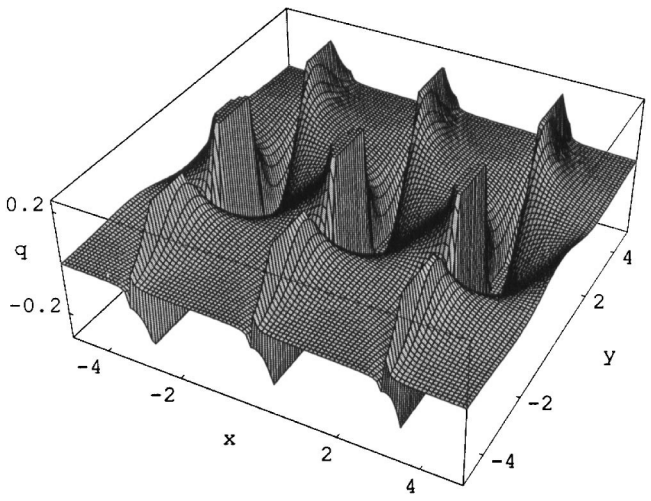

FIG. 9. Plot of q for $e_1(x)=\cos x$, $e_2(x)=\sin x$ at $t=1$ for (4.1).

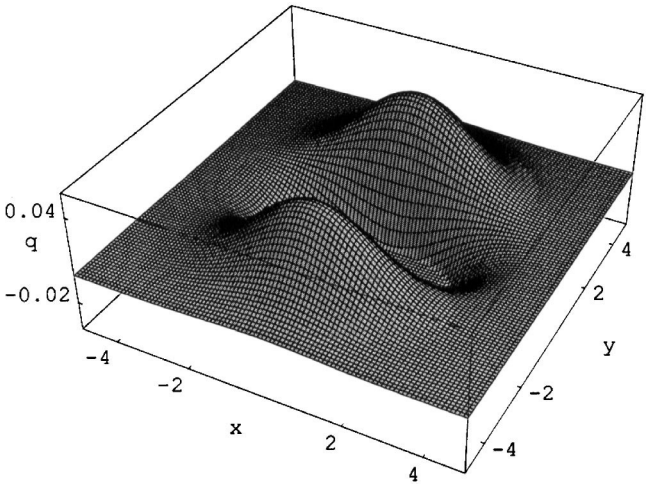

FIG. 10. Plot of q for (4.1) with $e_1(x)=e^{-x^2/4}$, $e_2(x)=1$ at $t=1$.

Future work will seek to develop and refine the method further. In addition, the method will probably continue to be used to investigate new integrable equations or hierarchies.

APPENDIX

Substituting (2.8) in (2.1) yields the following.
From (2.1a):

$$O\left(\frac{1}{\phi^2}\right): \quad \phi_y[\phi_t-2p\phi_x-\phi_{xx}]=0, \tag{A1}$$

$$O\left(\frac{1}{\phi}\right): \quad -\phi_{yt}+2\phi_x u_x+2p\phi_{xy}+\phi_{xxy}=0, \tag{A2}$$

$$O(1): \quad -u_t+2pu_x+u_{xx}=0. \tag{A3}$$

From (2.1b):

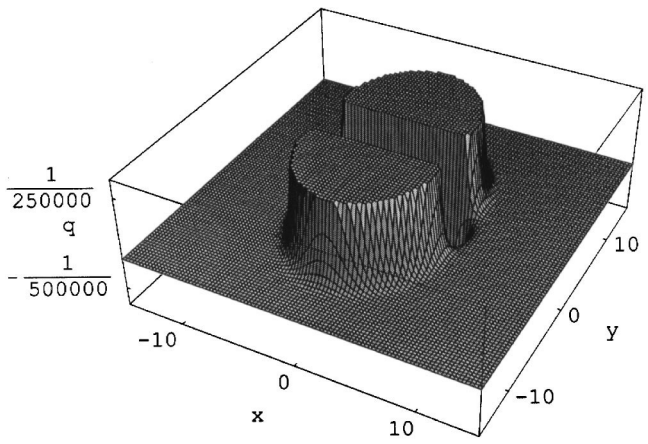

FIG. 11. Plot of q for (4.1) with $e_1(x)=e^{-x^2/4}$, $e_2(x)=1$ at $t=2$.

$$O(\phi^{-1}): \quad v_1 = -v_x/\phi_x = 0, \tag{A4}$$

$$O(1): \quad v_t - 2pv_x + v_{xx} = 0. \tag{A5}$$

From (2.1c):

$$O(1): \quad -p_y + u_x + v_x = 0. \tag{A6}$$

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N=4 characters in Gepner models, orbits and elliptic genera

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(Received 8 May 2003; accepted 7 September 2003)

We review the properties of characters of the N=4 superconformal algebra in the context of a nonlinear sigma model on $K3$, how they are used to span the orbits, and how the orbits produce topological invariants like the elliptic genus. We derive the same expression for the $K3$ elliptic genus using three different Gepner models (1^6, 2^4, and 4^3 theories), detailing the orbits and verifying that their coefficients F_i are given by elementary modular functions. We also reveal the orbits for the $1^3 2^2$, $1^4 4$, and $1^2 4^2$ theories. We derive relations for cubes of theta functions and study the function $(1/\eta)\,\Sigma_{n\in\mathbb{Z}}(-1)^n(6n+1)^k\,q^{(6n+1)^2/24}$ for $k=1,2,3,4$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1624470]

I. INTRODUCTION

In the mid-1980s, many efforts were deployed to find the characters of the N=2 superconformal algebra (SCA), culminating in the work of Refs. 15 and 7. The N=2 characters are defined by tr $q^{L_0-c/24}y^{J_0}$ with L_0 the Virasoro operator and J_0 the U(1) charge. [We use the common variables $q=e^{2\pi i\tau}$ and $y=e^{2\pi iz}$ where z keeps track of the U(1) theta angle.] They fall into two classes: those for continuous central charge $c>3$ and those for discrete $c<3$, namely, $c=3k/(k+2)$ with k being the level.

In the first class, the characters for massive representations are proportional to $\vartheta_3(z)/\eta^3$ (in the NS sector), while those for massless representations have an extra denominator of $1+y^{\mathrm{sign}(m)}q^{|m|-1/2}$, where m is a quantum number labeling the conformal dimension h and the U(1) charge Q. Unitarity constrains (h,Q) to lie inside a polygonal domain of the plane. Massless representations are those hitting the unitary bound, i.e., with (h,Q) on the boundary of the polygon. Massive representations are those with (h,Q) in the interior of the polygon; they have vanishing Witten index.

In the second class, with discrete $c<3$, the characters are spanned by theta functions and the coefficients are the mysterious *string functions* of Ref. 9.

In the late 1980s, characters for the N=4 SCA were also unraveled.[3] The N=4 algebra contains an affine su(2) Kac–Moody subalgebra of level k, and the central charge of the SCA is $c=6k$. For $k=1$, the massive characters are proportional to $\vartheta_3(z)^2/\eta^3$ (in the NS sector), while the massless characters have again an extra denominator. For higher level k, the characters have an additional factor of χ^l_{k-1}, which denotes the su(2) affine characters (or a slight deformation of them in the massless case) with l being the isospin quantum number, $0\leqslant l\leqslant k/2$. Unitarity requires $h\geqslant l$ (NS sector) and massless representations hit this bound. Massless N=4 characters were found to be expressible as $\Sigma_{l'}A_{l,l'}\chi^{l'}_k$ for some branching functions $A_{l,l'}$, and even expressible as an infinite sum of N=2 characters taken at double or triple points [these are special points in the (h,Q) plane].

This correspondence between N=2 and N=4 characters was furthermore enhanced in Ref. 2, where Gepner models were used to write N=4 characters—or rather *orbits*—as tensor products of several characters of the N=2 minimal theories. Then finite sums over these orbits NS_i or R_i yield

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the traces for the N=4 characters, modular invariant partition functions, elliptic genera, or other topological invariants like

$$\Phi = \mathrm{tr}^{\mathrm{N}=4}_{\mathrm{NS,R}}(-1)^F q^{L_0 - c/24} y^{J_0} = \sum_i D_i \mathrm{NS}'_i \overline{\mathrm{R}}'_i$$

for some combinatorial factors D_i. Since these objects are topological, they should not depend on the particular Gepner model at hand. Gepner models are special points in the moduli space of $K3$ surfaces[13] where the above trace factorizes into a product of NS and R orbits. That is, we only go to points where the formula holds. At different such points, we have different sets of orbits NS_i and of coefficients D_i. Moreover, each orbit should be expressible as a sum of a massless and a massive N=4 character: $\mathrm{NS}_i(\tau,z) = \widehat{\mathrm{ch}}^{\mathrm{NS}}(\tau,z) + F_i(\tau)\mathrm{ch}^{\mathrm{NS}}(\tau,z)$.

In the context of $K3$ compactifications, the nonlinear sigma model has central charge $c=6$, thus the su(2) subalgebra of the N=4 SCA has level $k=1$. In the following, we shall give explicit expression of the functions $F_i(\tau)$ in the case of the 1^6 and 2^4 theories (and lay the cornerstone for the 4^3 theory) and find that they are essentially given by quotients of Dedekind η functions, thus reflecting the modular nature of the characters and topological invariants. We also derive the expression for Φ in both theories and gather on the way useful results on theta functions and other tools of analytic number theory.

This introduction is followed by six more sections. In Sec. II, we recall the N=4 characters for the $c=6$ SCA of the nonlinear sigma model with $K3$ target space. We also show how massless and massive characters are used to span the *orbits*, without yet detailing the construction of these orbits. Section III is an expanded version of the results of Ref. 2 on topological invariants for $K3$ based on computations with the orbits. Sections IV, V, and VI are the crux of the paper, revealing in detail the orbits for the 1^6, 2^4, and 4^3 Gepner models, respectively, computing the functions F_i and developing several lemmas on theta functions. Section VII studies Gepner models of mixed levels, like $1^3 2^2$, $1^4 4$, and $1^2 4^2$—the first of which is a toroidal model and the other two are $K3$ models.

In Sec. IV, we also explore the function $a(\tau)$ which is essential in Ref. 1 for deriving Ramanujan identities. In particular, we study the function

$$\frac{1}{\eta} \sum_{n \in \mathbb{Z}} (-1)^n (6n+1)^k \; q^{(6n+1)^2/24}$$

for $k=1,2,3,4$ (Proposition 4.51 and thereafter), and relate sums of cubes of theta functions to a single theta function (Lemma 4.31).

II. N=4 CHARACTERS

We first write down the characters of the N=4 SCA with central charge $c=6$ and level $k=1$, i.e., corresponding to a sigma model with $K3$ target space. We give here explicitly the characters of the NS sector, and refer to spectral flow for their counterparts in the R sector. They depend on two variables, $q = e^{2\pi i \tau}$ and $y = e^{2\pi i z}$ for the modular parameter and the U(1) theta angle, respectively. Representations are parametrized by highest weight h and isospin l and unitarity implies $h \geqslant l$ (NS sector). Our N=4 SCA is the enhancement of a N=2 Gepner model by adding SU(2) currents $J^{\pm}$, and the latter's characters are defined by

$$\mathrm{ch}^{\mathrm{NS}}(\tau,z) := \mathrm{tr}_{\mathrm{NS}}\, q^{L_0 - c/24} y^{J_0}. \tag{2.1}$$

A. The characters

We rewrite the familiar expressions of Ref. 3 for N=4 characters in a more useful parametrization. There are two kinds of characters: we denote massless characters (with isospin l) by $\widehat{\mathrm{ch}}_l^{\mathrm{NS}}(\tau,z)$ and massive ones (with highest weight h) by $\mathrm{ch}_h^{\mathrm{NS}}(\tau,z)$.

Massless representations saturate the unitarity bound $h=l$ and $l=0,\frac{1}{2}$:

$$\widehat{\mathrm{ch}}_0^{\mathrm{NS}}=-\frac{\vartheta_3(z)}{\eta^3}\sum_n q^{n^2/2-1/8}y^n\frac{1-yq^{n-1/2}}{1+yq^{n-1/2}}=2\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2+\left(\frac{q^{-1/8}}{\eta}-2h_3\right)\left(\frac{\vartheta_3(z)}{\eta}\right)^2,$$
$$\widehat{\mathrm{ch}}_{1/2}^{\mathrm{NS}}=\frac{\vartheta_3(z)}{\eta^3}\sum_n q^{n^2/2-1/8}y^n\frac{1}{1+yq^{n-1/2}}=-\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2+h_3\left(\frac{\vartheta_3(z)}{\eta}\right)^2, \tag{2.2}$$

with

$$h_3(\tau)\coloneqq\frac{1}{\eta\vartheta_3}\sum\frac{q^{n^2/2-1/8}}{1+q^{n-1/2}}. \tag{2.3}$$

The above equalities follow from the fact that the left-hand sides are so-called theta functions of characteristic $(0,0;-4\pi i,-2\pi i\tau)$ of degree 2 (see Appendix A), hence can be spanned by $\vartheta_1(z)^2$ and $\vartheta_3(z)^2$. The coefficients are obtained by evaluating the lhs at $z=(1+\tau)/2$ and $z=0$, respectively, bearing in mind that $\vartheta_3[(1+\tau)/2]=0$ and $\vartheta_1(0)=0$. For $z=(1+\tau)/2$, note that the term $(1-q^0)$ in the product expression of $\vartheta_3[(1+\tau)/2]$ cancels the denominator of the $n=0$ term of the sum, yielding $2q^{-1/4}$ and $-q^{-1/4}$ for the left-hand sides.

Massive representations are simpler and exist for $h>0$ and $l=0$,

$$\mathrm{ch}_h^{\mathrm{NS}}=q^{h-1/8}\frac{\vartheta_3(z)^2}{\eta^3}. \tag{2.4}$$

Spectral flow yields the R character (idem for massive characters):

$$\widehat{\mathrm{ch}}_l^{\mathrm{R}}(\tau,z)=yq^{1/4}\widehat{\mathrm{ch}}_{1/2-l}^{\mathrm{NS}}\left(\tau,z+\frac{\tau}{2}\right). \tag{2.5}$$

Thus, for instance, the Witten index is given by

$$I=\mathrm{tr}_{\mathrm{R}}\,q^{L_0-c/24}(-1)^F=\widehat{\mathrm{ch}}_{1/2-l}^{\mathrm{R}}\left(\tau,\frac{1}{2}\right)=-q^{1/4}\ \widehat{\mathrm{ch}}_l^{\mathrm{NS}}\left(\tau,\frac{1+\tau}{2}\right)=\begin{cases}-2, & l=0\\ 1, & l=\frac{1}{2}\end{cases} \tag{2.6}$$

since $\vartheta_3[(1+\tau)/2]=0$ and $\vartheta_1[(1+\tau)/2]=q^{-1/8}\vartheta_3$. For the massive characters, the Witten index vanishes: $\vartheta_3[(1+\tau)/2]=0$ in (2.4).

B. The orbits

The nonlinear sigma models on $K3$ have three kinds of NS orbits: graviton, massless, and massive orbits. Their construction will be detailed in the explicit computations below, Secs. IV–VI. For now, we only need to know that they can be spanned by massless and massive N=4 characters. The graviton orbit, for example, contains the massless character $\widehat{\mathrm{ch}}_0^{\mathrm{NS}}$ and a sum of massive characters

$$\sum_{n\geqslant 1}c_n\,\mathrm{ch}_n^{\mathrm{NS}}=\left(\sum_{n\geqslant 1}c_nq^n\right)\mathrm{ch}_0^{\mathrm{NS}}\coloneqq F_1(\tau)\ \ \mathrm{ch}_0^{\mathrm{NS}}.$$

Thus the graviton orbit has coordinates $(1,F_1)$ in the basis $\{\widehat{\mathrm{ch}}_0^{\mathrm{NS}},\mathrm{ch}_0^{\mathrm{NS}}\}$. Similarly for the other orbits. From the examples of the next sections, it will appear that the massless orbits have always coordinates $(1,F_i)$, and the massive orbits have coordinates $(0,F_j)$ (hence the name). We use the subscripts $1,i,j$ for the different orbits: 1 for the graviton orbit, $i=2,\ldots,d$ for the massless orbits and $j=d+1,\ldots,d+d'$ for the massive orbits. Writing the N=4 NS_i characters (for the three kinds of orbits) in the basis $\{\widehat{\mathrm{ch}}_{0,1/2}^{\mathrm{NS}},\mathrm{ch}_0^{\mathrm{NS}}\}$ *defines* the functions $F_i(\tau)$:

$$\begin{aligned}\mathrm{NS}_1(\tau,z)&=\widehat{\mathrm{ch}}_0^{\mathrm{NS}}(\tau,z)+F_1(\tau)\ \ \mathrm{ch}_0^{\mathrm{NS}}(\tau,z),\\ \mathrm{NS}_i(\tau,z)&=\widehat{\mathrm{ch}}_{1/2}^{\mathrm{NS}}(\tau,z)+F_i(\tau)\ \ \mathrm{ch}_0^{\mathrm{NS}}(\tau,z),\\ \mathrm{NS}_j(\tau,z)&=F_j(\tau)\ \ \mathrm{ch}_0^{\mathrm{NS}}(\tau,z).\end{aligned}\tag{2.7}$$

The set of functions F_i is determined by the particular Gepner model under study. Spectral flow generates again the Ramond counterparts, R_i, and subsequent $(-1)^F$ insertion—denoted by a prime—yields the Witten index of the orbit (nonvanishing for massless characters only): $\mathrm{R}_1'=I_1=-2$, $\mathrm{R}_i'=I_i=1$, $\mathrm{R}_j'=0$.

The action of the modular group transforms all these orbits into each other. For instance, the S-transformation defines a real matrix S_{ij}:

$$\mathrm{NS}_i(\tau,z)=-\sum_j S_{ij}\,\mathrm{NS}_j\left(-\frac{1}{\tau},\frac{z}{\tau}\right)\ \ e^{-2\pi i\ z^2/\tau}.$$

Define $D_i:=S_{1,i}/S_{i,1}$, which are combinatorial factors of tensoring representations when using a Gepner model. For instance, in the 1^6 theory: $D_i=(1,20,270,30)$. Using D_i, we form the modular invariant partition function for the $K3$ σ-model:

$$Z(\tau,\overline{\tau};z,\tau z)=\mathrm{tr}\,q^{L_0-(c/24)}\overline{q}^{\overline{L}_0-(\overline{c}/24)}y^{J_0}\overline{y}^{\overline{J}_0}=\frac{1}{2}\sum_{i=1}^{d+d'}D_i(|\mathrm{NS}_i|^2+|\mathrm{NS}_i'|^2+|\mathrm{R}_i|^2+|\mathrm{R}_i'|^2),\tag{2.8}$$

where the prime represents $(-1)^F$ insertion. The last term evaluated at $y=1$ is but the Witten index I and summing over it gives the Euler character:

$$\chi=\sum_{i=1}^{d+d'}D_iI_i^2=D_12^2+D_2+\cdots+D_d=4+h^{1,1}=24,\tag{2.9}$$

as the sum of D_i over the massless orbit always adds up to the Hodge number $h^{1,1}$ of the orbifold: 20 in our case of $K3$.

III. TOPOLOGICAL INVARIANTS

A. *K*3 elliptic genera

In Refs. 2 and 10 the authors studied the $c=6$ SCA of a sigma-model with $K3$ target space. The holonomy of the $K3$ manifold allows for two more SU(2) currents $J^{\pm}$, i.e., conformal fields of weight 1 and U(1) charge $J_0=2J_0^3=\pm2$, that generate the transformation of double spectral flow (i.e., NS→R→NS) and extend the N=2 algebra to N=4.

The elliptic genus of this $(c,\overline{c})=(6,6)$ heterotic sigma model is, geometrically, a double sum whose coefficients are the indices of Dirac operators for certain vector bundles over $K3$:

$$\Phi(\tau,z)=\sum_{n,r}c_{n,r}\ q^ny^r,$$

$$\text{with} \quad c_{n,r} := \operatorname{ind} \not{D}_{E_{n,r}} = \int_{K3} \operatorname{ch}(E_{n,r})\ \operatorname{td}(K3),$$

where the bundle $E_{n,r}$ is defined by

$$\sum_{n,r} E_{n,r}\ q^n y^r := y^{-1} \bigotimes_{n\geqslant 1} (\wedge_{-q^{n-1}y} T_{K3} \otimes \wedge_{-q^{n-1}y^{-1}} \overline{T}_{K3} \otimes S_{q^n} T_{K3} \otimes S_{q^n} \overline{T}_{K3}),$$

and $\wedge_q E = \oplus_{k\geqslant 0} q^k \wedge^k E$, $S_q E = \oplus_{k\geqslant 0} q^k S^k E$. ($\wedge^k$ and S^k denote the kth exterior and symmetric products.)

The elliptic genus also has a topological expression, given by a trace over the left and right Ramond sectors with $(-1)^F$ insertion:

$$\Phi(\tau,z) := \operatorname{tr}_{\mathrm{R,R}}(-1)^{F_L+F_R} q^{L_0-1/4} \overline{q}^{\overline{L}_0-1/4} y^{J_0} = 24\left(\frac{\vartheta_3(z)}{\vartheta_3}\right)^2 + 2\,\frac{\vartheta_2^4-\vartheta_4^4}{\eta^4}\left(\frac{\vartheta_1(z)}{\eta}\right)^2, \qquad (3.1)$$

where the second expression will be proved in the next section. Note that because we have no $\overline{y}^{\overline{J}_0}$ for the right movers, the $(-1)^{F_R}$ insertion in the R-sector yields only a contribution from the zero modes ($\overline{q}^0$ terms). Indeed, for any higher state, Susy ensures the existence of another state with opposite $(-1)^F$ eigenvalue. Thus the above expressions are independent of $\overline{q}$ and we could have dropped that variable from the definition. Note also that the fermion parity operator $(-1)^F = (-1)^{F_L+F_R} = (-1)^{F_L-F_R}$ is sometimes written $e^{i\pi(J_0-\overline{J}_0)}$. The U(1) charge J_0 helps to distinguish between bosons and fermions, and its values are in $\mathbb{Z}$ for the NS sector and in $\mathbb{Z}+c/6$ for the R sector. Thus the difference between left- and right-moving U(1) charge is always an integer for the NS–NS or R–R sectors.

At the special values of $z=(1+\tau)/2$, $\tau/2$, $\frac{1}{2}$ and 0, we obtain specific topological invariants,[2] using (B14),(B15) and dropping the extra $q^{-1/4}$ and $-q^{-1/4}$ in the first two cases:

$$\begin{aligned}
&\text{Dirac index,} \quad \Phi^+_{\hat{A}} := \operatorname{tr}_{\mathrm{NS,R}}(-1)^{F_R} q^{L_0-1/4} = 2\,\vartheta_3^2(\vartheta_2^4-\vartheta_4^4)/\eta^6,\\
&\Phi^-_{\hat{A}} := \operatorname{tr}_{\mathrm{NS,R}}(-1)^{F_L+F_R} q^{L_0-1/4} = -2\,\vartheta_4^2(\vartheta_2^4+\vartheta_3^4)/\eta^6;\\
&\text{Hirzebruch genus,} \quad \Phi_\sigma := \operatorname{tr}_{\mathrm{R,R}}(-1)^{F_R} q^{L_0-1/4} = 2\,\vartheta_2^2(\vartheta_4^4+\vartheta_3^4)/\eta^6;\\
&\text{Euler character,} \quad \Phi_\chi := \operatorname{tr}_{\mathrm{R,R}}(-1)^{F_L+F_R} q^{L_0-1/4} = 24.
\end{aligned} \qquad (3.2)$$

Whence a shift $z\to z+\tau/2$ generates spectral flow R$\to$NS, while $z\to z+\frac{1}{2}$ is responsible for an additional factor of $(-1)^{F_L}$. The elliptic genus evaluated at specific points thus yields the partition function for different spin structures; at $z=0$, we obtain the Witten index—or the bosonic partition function if we have no spin structures.

We note that the above indices or genera are universal and do not depend on the $K3$ moduli. Since they hold for any complex structure, they are rightly called topological invariants.

B. Derivation by orbits

We shall prove (3.1) by actually computing $\Phi^+_{\hat{A}}$ with its z dependence restored, i.e., we consider the NS,R sector. This will allow us to work with the functions F_i which we defined by the left-moving NS$_i$ orbits. Note that in the following, the τ-dependence shall be understood and not always explicitly written. The prescription is to replace the trace by a sum over all orbits:

$$\Phi^+_{\hat{A}}(\tau,z) := \operatorname{tr}_{\mathrm{NS,R}} q^{L_0-1/4} y^{J_0} (-1)^{F_R} \overline{q}^{\overline{L}_0-1/4} = \sum_{i=1}^{d+d'} D_i\, \mathrm{NS}_i(\tau,z)\ \ \overline{\mathrm{R}}'_i(\overline{\tau},\overline{z}=0).$$

This factorization of NS and R sectors will be confirmed by the concrete examples of the next sections. (A thorough treatment of this factorization into tensor products of Hilbert spaces can be found in Wendland's Ph.D. thesis.[17]) Note that in the right-moving sector, $\bar{\mathrm{R}}_i'(\bar{\tau},0)$ is but the Witten index $I_1=-2$, $I_i=1$, and $I_j=0$. Hence the trace consists of two parts only, one for the graviton orbit and one from the massless orbit. In (2.2), we can interpret the coefficient of $\vartheta_1(z)^2/\vartheta_3^2$ as $-I_i$ for $i=1,\ldots,d$ and similarly for the coefficient of h_3. Bearing this in mind, (2.7) gives us

$$\sum_{i=1}^{d} D_i\,\mathrm{NS}_i(z)\;\bar{\mathrm{R}}_i'(0)=\sum_i D_i[\mathrm{ch}^{\mathrm{NS}}_{0,1/2}(z)+F_i\,\mathrm{ch}^{\mathrm{NS}}_0(z)]I_i$$

$$=\left(-\sum_{i=1}^{d} D_i I_i^2\right)\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2$$

$$+\left(\frac{q^{-1/8}}{\eta}\left(D_1 I_1+\sum_{i=1}^{d} D_i I_i F_i\right)+h_3\underbrace{\sum_{i=1}^{d} D_i I_i^2}_{=\chi=24}\right)\left(\frac{\vartheta_3(z)}{\eta}\right)^2.$$

Since this is a topological invariant, it should be independent of the Gepner model at hand, i.e., of the particular set of functions $F_i(\tau)$. That is, for different Gepner models we have different sets (of variable length) of orbits NS_i and functions F_i, but the above sum yields always the same result. In Secs. IV and V we show (for the 1^6 and 2^4 theories) how the large bracket yields $2(\vartheta_2^4-\vartheta_4^4)/\eta^4$. Hence our Dirac index becomes

$$\Phi^{+}_{\hat{A}}(z)=-24\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2+2\,\frac{\vartheta_2^4-\vartheta_4^4}{\eta^4}\left(\frac{\vartheta_3(z)}{\eta}\right)^2 \tag{3.3}$$

and the $z=0$ value gives back the invariant of (3.2).

To arrive at the elliptic genus (3.1), we need to insert $(-1)^{F_L}$ and perform spectral flow for the left-movers. This corresponds to shifts $z\to z+\frac{1}{2}$ and $z\to z+\tau/2$, respectively. The first of these operations yields $\Phi^{-}_{\hat{A}}(z)=\Sigma_{i=1}^{d} D_i\,\mathrm{NS}_i'(z)\bar{\mathrm{R}}_i'(0)$ and combination with the second yields $\Phi(z)=\Sigma_{i=1}^{d} D_i\mathrm{R}_i'(z)\bar{\mathrm{R}}_i'(0)$ as in (3.1).

C. Alternative derivation by orbifolds

The expression for the elliptic genus (3.1) can also be derived from orbifold models of the $K3$ surface, as was shown in Ref. 2. These models are formed by dividing the product of two complex tori $T\times T'$ by the action of the symmetry group $\mathbb{Z}_n$,

$$z_1\to z_1\;\; e^{2\pi i/n}\quad\text{and}\quad z_2\to z_2\;\; e^{-2\pi i/n}. \tag{3.4}$$

Essentially four types occur, corresponding to $n=2,3,4,6$.

The partition function for these models consists of an untwisted piece and a twisted one. The untwisted piece is the fermionic contribution (in the NS sector, say) $|\vartheta_3(z)/\eta|$ times the bosonic lattice function $\Gamma_{2,2}(G,B)/|\eta|^4$.

The twisted piece consists of two complex fermions and two complex bosons, twisted by some power of the $\mathbb{Z}_n$ symmetry generator $e^{2\pi i/n}$, that is the U(1) theta angle $z=2\pi\theta$ will be shifted by $(s+r\tau)/n$. For the fermions (in the NS sector, say), we have again $\vartheta_3(z)/\eta$ [yet with twists in opposite direction, see (3.4)], while for the bosons we have η/ϑ_1. Thus the twisted partition function is the sum

$$\sum_{r,s}{}' \; n_{r,s}|Z_{r,s}|^2,\quad Z_{r,s}:=\frac{\vartheta_3(z+(s+r\tau)/n)\quad\vartheta_3(z-(s+r\tau)/n)}{\vartheta_1((s+r\tau)/n)^2}, \tag{3.5}$$

where the prime on the sum signifies omission of $r=s=0$. The weights $n_{r,s}$ are defined by $n_{0,s}:=(s\sin(\pi s/n))^4/n$ and $n_{r,s}:=n_{s,n-r}$. Concretely, these weights all equal 8 for $n=2$ and 3 for $n=3$; while for $n=4$ the three weights forming at the half-periods $(r,s=0,2)$ equal 4 and the

remaining 12 weights equal 1. For $n=6$, the three half-period weights equal 16/6, the eight third-period weights equal 9/6 while the remaining 24 weights equal 1/6. In all cases, the important observation is that the sum of the weights equals 24: $\Sigma'_{r,s} n_{r,s}=24$.

By the Riemann addition formula (B17), the (r,s)-block can be rewritten as

$$Z_{r,s}(z)=\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2+\left(\frac{\vartheta_3((s+r\tau)/n)}{\vartheta_1((s+r\tau)/n)}\right)^2\left(\frac{\vartheta_3(z)}{\vartheta_3}\right)^2 \tag{3.6}$$

while its equivalent for the R-sector with $(-1)^F$ insertion is

$$q^{1/4}y\ \ Z_{r,s}(z+(1+\tau)/2)=\left(\frac{\vartheta_3(z)}{\vartheta_3}\right)^2-\left(\frac{\vartheta_3((s+r\tau)/n)}{\vartheta_1((s+r\tau)/n)}\right)^2\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2. \tag{3.7}$$

With these building blocks, we can now compute the elliptic genus:

$$\begin{aligned}\Phi(\tau,z)&=\mathrm{tr}_{\mathrm{R,R}}(-1)^F q^{L_0-1/4}y^{J_0}\bar{q}^{\bar{L}_0-\bar{1}/4}\\&=\sum_{r,s}{}'\ n_{r,s}q^{1/4}yZ_{r,s}(z+(1+\tau)/2)\bar{q}^{1/4}\ \bar{Z}_{r,s}((1+\tau)/2)\\&=\left(\sum_{r,s}{}'\ n_{r,s}\right)\left(\frac{\vartheta_3(z)}{\vartheta_3}\right)^2-\left(\sum_{r,s}{}'\ n_{r,s}\left(\frac{\vartheta_3((s+r\tau)/n)}{\vartheta_1((s+r\tau)/n)}\right)^2\right)\left(\frac{\vartheta_1(z)}{\vartheta_3}\right)^2\\&=24\left(\frac{\vartheta_3(z)}{\vartheta_3}\right)^2+2\,\frac{\vartheta_2^4-\vartheta_4^4}{\eta^4}\left(\frac{\vartheta_1(z)}{\eta}\right)^2,\end{aligned} \tag{3.8}$$

where we have used (B33) to transform

$$\sum_{r,s}{}'\ n_{r,s}\left(\frac{\vartheta_3((s+r\tau)/n)}{\vartheta_1((s+r\tau)/n)}\right)^2=\left(\frac{\vartheta_3}{2\pi\eta^3}\right)^2\sum_{r,s}{}'\ n_{r,s}(\wp((s+r\tau)/n)-\mathrm{const}) \tag{3.9}$$

and this last sum equals $-24\cdot$const, by repeated use of (B35) for equal values of $n_{r,s}$. The constant itself equals $(\pi^2/3)(\vartheta_2^4-\vartheta_4^4)$. So we do indeed recover (3.1).

IV. COMPUTATIONS IN 1^6 THEORY

For clarity, we shall now detail the ideas developed at the beginning of this section, and show what we mean under ''orbits'' and functions F_i in the concrete example of the 1^6 theory. This Gepner model is based on the tensoring of six times the same $k=1$, N=2 self-consistent field theory (SCFT). That is, the N=4 characters will be tensor products of six N=2 characters. So we first present those N=2 characters.

A. General considerations

In general, for values of the central charge between 0 and 3, unitary representations of N=2 superconformal algebras exist at discrete values of the central charge, namely at $c=3k/(k+2)$. The highest weight states have conformal dimension and U(1) charge parametrized by two quantum numbers l, m (isospin and its third component):[14–16]

$$h_{l,m}=\frac{l(l+2)-m^2}{4(k+2)},\quad Q_{l,m}=\frac{m}{k+2}, \tag{4.1}$$

where $0\leqslant l\leqslant k$, $-l\leqslant m\leqslant l$, $l\equiv m \bmod 2$. The NS characters of these N=2 theories are linear combinations of su(2) theta functions:

$$\mathrm{ch}^{\mathrm{NS}}_{l,m}(y,q)=\sum_{m'=-k+1}^{k} c_{l,m'}\ \ \theta_{(k+2)m'-mk,\ k(k+2)}\left(\frac{\tau}{2},\frac{z}{k+2}\right), \tag{4.2}$$

$$\theta_{m,k}(\tau,z):=\sum_{n\in\mathbb{Z}+m/2k} q^{kn^2}y^{kn},\quad \theta_{m,k}=\theta_{m+2k,k}.$$

For later purposes, note the behavior under full ($z\to z+\tau$) spectral flow:

$$\theta_{m,\ k(k+2)}\left(\frac{\tau}{2},\frac{z}{k+2}\right)\xrightarrow{z\to z+\tau} q^{-k/[2(k+2)]}y^{-k/(k+2)}\ \ \theta_{m+2k,\ k(k+2)}\left(\frac{\tau}{2},\frac{z}{k+2}\right).$$

The coefficients $c_{l,m}$ are the *string functions* of Kac and Peterson[9] for $l\equiv m \bmod 2$; for the su(2) affine Lie algebra they have an alternative definition via the Weyl–Kac formula:

$$\frac{\theta_{l+1,k+2}-\theta_{-l-1,k+2}}{\theta_{1,2}-\theta_{-1,2}}=:\sum_{m=-k+1}^{k} c_{l,m}\theta_{m,k}. \tag{4.3}$$

Since the lhs and rhs have expansions with powers of y in $\mathbb{Z}+l/2$ and $\mathbb{Z}+m/2$, respectively, we see that $c_{l,m}=0$ if $l\not\equiv m \bmod 2$. Of course, for each level k we have different set of string functions. Note also the symmetries: $c_{l,m}=c_{l,-m}=c_{l,m+2k}=c_{k-l,k-m}$. For the case of the affine su(2) algebra $A_1^{(1)}$, the string functions are merely proportional to Hecke indefinite modular forms,

$$c_{l,m}=\eta(\tau)^{-3}\sum_{-|x|<y\leqslant|x|} \mathrm{sgn}(x)\ \ q^{(k+2)x^2-ky^2}, \tag{4.4}$$

where x, y are such that (x,y) or $(\frac{1}{2}-x,\frac{1}{2}+y)$ are $\in\mathbb{Z}^2+((l+1)/2(k+2),m/2k)$.

For our present case of $k=1$, $c=1$, the latter sum can be remarkably rewritten as

$$\sum_{\substack{-|x|<y\leqslant|x|\\ (x,y)\equiv(1/6,0)\ \text{or}\ (1/3,1/2)\bmod\mathbb{Z}^2}} \mathrm{sign}(x)\ q^{3x^2-y^2}=\sum_{\substack{j\geqslant 0\\ |l|\leqslant j/2}} (-1)^{j+l}q^{(3(2j+1)^2-(6l+1)^2)/24}=\eta(\tau)^2. \tag{4.5}$$

The last equality is another remarkable result of Ref. 9. Our string functions at level one thus become

$$c_{0,0}=c_{1,1}=c_{1,-1}=\frac{1}{\eta(\tau)},\quad c_{0,1}=c_{1,0}=0. \tag{4.6}$$

B. Characters and orbits

We are in a position to write down the three minimal N=2 characters, obtained for $l=m=0$, $l=m=1$, and $l=-m=1$,

$$A := \mathrm{ch}^{\mathrm{NS}}_{0,0}(y,q) = \frac{1}{\eta}\,\theta_{0,3}\left(\frac{\tau}{2},\frac{z}{3}\right) = \frac{1}{\eta}\sum_{\mathbb{Z}}\; q^{(3/2)\,n^2} y^n = \frac{1}{\eta}\,\vartheta_3(z|3\tau),$$

$$B := \mathrm{ch}^{\mathrm{NS}}_{1,1}(y,q) = \frac{1}{\eta}\,\theta_{2,3}\left(\frac{\tau}{2},\frac{z}{3}\right) = \frac{1}{\eta}\sum_{\mathbb{Z}}\; q^{(3/2)(n+1/3)^2} y^{n+1/3} = \frac{1}{\eta} q^{1/6} y^{1/3}\;\vartheta_3(z+\tau|3\tau), \quad (4.7)$$

$$\begin{aligned} C := \mathrm{ch}^{\mathrm{NS}}_{1,-1}(y,q) &= \frac{1}{\eta}\,\theta_{4,3}\left(\frac{\tau}{2},\frac{z}{3}\right) = \frac{1}{\eta}\sum_{\mathbb{Z}}\; q^{(3/2)(n+2/3)^2} y^{n+2/3} \\ &= \frac{1}{\eta} q^{2/3} y^{2/3}\;\vartheta_3(z+2\tau|3\tau) \\ &= \frac{1}{\eta} q^{1/6} y^{-1/3}\;\vartheta_3(z-\tau|3\tau). \end{aligned}$$

Under spectral flow, the three su(2) theta functions are shifted into each other,

$$\theta_{m,3}\left(\frac{\tau}{2},\frac{z}{3}\right) \xrightarrow{z\to z+\tau/2} q^{-1/24} y^{-1/6}\;\; \theta_{m+1,3}\left(\frac{\tau}{2},\frac{z}{3}\right) \xrightarrow{z\to z+\tau/2} q^{-1/6} y^{-1/3}\;\; \theta_{m+2,3}\left(\frac{\tau}{2},\frac{z}{3}\right), \quad (4.8)$$

so that under full spectral flow, the three characters are cyclicly permuted,

$$A \xrightarrow{z\to z+\tau} B \to C \to A, \quad (4.9)$$

where we have omitted the incrementing factors of $q^{-1/6}y^{-1/3}$.

To build the various orbits of the 1^6 theory, we consider all possible homogeneous polynomials of degree 6 in A, B, C, respecting the following two rules:

(1) the orbit must be holomorphic, i.e., its Fourier expansion must have integer powers of y;
(2) the orbit must be covariant under full spectral flow, $\mathrm{NS}_i(z\to z+\tau) = q^{-1}y^{-2}\,\mathrm{NS}_i(z)$.

Condition (1) excludes combinations like A^5B, A^4B^2 or $A^3B^2C, \ldots$. Condition (2) requires invariance of the orbit under cyclic permutation of A, B, C, and also guarantees it to be a theta function of characteristic $(0,0;-4\pi i, 2\pi i)$ and degree 2. Thus each orbit can be spanned by $\widehat{\mathrm{ch}}^{\mathrm{NS}}_{0,1/2}$ and $\mathrm{ch}^{\mathrm{NS}}_0$, or alternatively by $\vartheta_1(z|\tau)^2$ and $\vartheta_3(z|\tau)^2$.

The four possible orbits respecting the above rules are

$$\begin{aligned} \mathrm{NS}_1 &= A^6 + B^6 + C^6, \\ \mathrm{NS}_2 &= A^3B^3 + B^3C^3 + C^3A^3, \\ \mathrm{NS}_3 &= A^2B^2C^2, \\ \mathrm{NS}_4 &= A^4BC + B^4CA + C^4AB. \end{aligned} \quad (4.10)$$

We recall the definition of the combinatorial factors D_i associated to a particular model: The above orbits can be checked to have the following modular behavior:[2]

$$\mathrm{NS}_i = -\sum_j\; S_{ij}\,\mathrm{NS}_j\left(-\frac{1}{\tau},\frac{z}{\tau}\right)\;\; e^{-2\pi i z^2/\tau}, \quad S_{ij} = \frac{1}{27}\begin{pmatrix} 3 & 60 & 270 & 90 \\ 3 & -21 & 27 & 9 \\ 1 & 2 & 9 & -6 \\ 3 & 6 & -54 & 9 \end{pmatrix}. \quad (4.11)$$

Then the D_i are defined by $D_i := S_{1,i}/S_{i,1}$, that is (1,20,270,30) in the present case of 1^6 theory. Note that the first column ($S_{i,1}$) is just the number of summands in the orbit NS_i, while the first row ($S_{1,i}$) is $S_{1,1}$ times the number of permutations of the factors in any summand of NS_i. The same trick will allow a quick determination of the D_i in the 2^4 or 4^3 theories.

We note that at $y=-q^{-1/2}$, that is $z=(1+\tau)/2$, the massive character vanishes and so does B, $\mathrm{ch}(h=0)=0=B$, while $A=e^{i\pi/3}C=q^{-1/24}$. Thus at $y=-q^{-1/2}$:

$$\mathrm{NS}_1 = 2q^{-1/4} = \widehat{\mathrm{ch}}_0^{\mathrm{NS}}\left(z=\frac{1+\tau}{2}\right),$$

$$\mathrm{NS}_2 = -q^{-1/4} = \widehat{\mathrm{ch}}_{1/2}^{\mathrm{NS}}\left(z=\frac{1+\tau}{2}\right),$$

$$\mathrm{NS}_3 = 0,$$

$$\mathrm{NS}_4 = 0, \tag{4.12}$$

and we recognize that the first orbit is the graviton orbit, the second is the massless orbit (only one), while the third and fourth orbits are massive.

C. The functions F_j

We will now compute the functions F_j for the massive orbits. For F_3 this is pretty easy, while F_4 is more involved. F_1 and F_2 do not seem to have appealing expressions. Let us start with F_3,

$$\begin{aligned}\mathrm{NS}_3 = A^2B^2C^2 &= \frac{q^{2/3}}{\eta^6}\left(\vartheta_3(z|3\tau)\ \vartheta_3(z+\tau|3\tau)\ \vartheta_3(z-\tau|3\tau)\right)^2 \\ &= \frac{q^{2/3}}{\eta^6}\left(\vartheta_3(z|\tau)\ \prod\frac{(1-q^{3n})^3}{(1-q^n)}\right)^2 \\ &= \frac{\eta(3\tau)^6}{\eta^8}\vartheta_3(z|\tau)^2 \overset{!}{=} F_3\,\mathrm{ch}_0^{\mathrm{NS}} = F_3\ q^{-1/8}\frac{\vartheta_3(z|\tau)^2}{\eta^3}\end{aligned} \tag{4.13}$$

from which we find that

$$F_3 = q^{1/8}\frac{\eta(3\tau)^6}{\eta^5}. \tag{4.14}$$

Similarly, for F_4 we have

$$\begin{aligned}\mathrm{NS}_4 &= ABC(A^3+B^3+C^3) \\ &= \frac{\eta(3\tau)^3}{\eta^4}\vartheta_3(z|\tau)\ \left[\vartheta_3(z|3\tau)^3 + q^{1/2}y\ \ \vartheta_3(z+\tau|3\tau)^3 + q^{2/3}y^{2/3}\vartheta_3(z+2\tau|3\tau)^3\right] \\ &\overset{!}{=} F_4\,\mathrm{ch}(h=0) = F_4\ q^{-1/8}\frac{\vartheta_3(z|\tau)^2}{\eta^3}.\end{aligned} \tag{4.15}$$

Thus we see that the large bracket with the sum of cubes of theta functions must be proportional to $\vartheta_3(z|\tau)$. This is indeed the content of Lemma 4.31 below, and we then obtain for F_4,

$$F_4 = q^{1/8}\frac{\eta(3\tau)^3}{\eta^4}a(\tau), \tag{4.16}$$

where $a(\tau)$ is a function already studied in Ref. 1:

$$a(\tau) := \frac{1}{\eta} \sum_{\mathbb{Z}} (-1)^n (6n+1)\ q^{(6n+1)^2/24} = \sum_{k,l \in \mathbb{Z}} q^{k^2+kl+l^2}. \tag{4.17}$$

D. Dirac index

Although we could not find interesting expressions for F_1 and F_2, we shall nonetheless derive (3.3), that is we shall show the following.

Proposition 4.18:

$$\sum_{i=1}^{d} D_i \, \mathrm{NS}_i I_i = -2\,\mathrm{NS}_1 + 20\,\mathrm{NS}_2 = -24 \frac{\vartheta_1(z|\tau)^2}{\vartheta_3^2} + 2(\vartheta_2^4 - \vartheta_4^4) \frac{\vartheta_3(z|\tau)^2}{\eta^6}. \tag{4.19}$$

Proof: Because the Dirac index (lhs) is spanned by the massless and massive characters ch_0 and ch, or equivalently by $\vartheta_1(z|\tau)^2$ and $\vartheta_3(z|\tau)^2$, we only need to recover the constants multiplying these two basis vectors. Due to (4.12) and the vanishing of $\vartheta_3(z|\tau)$ at $z=(1+\tau)/2$, we see that $\vartheta_1(z|\tau)^2$ is correctly multiplied by $-24/\vartheta_3^2$. To check the constant in front of $\vartheta_3(z|\tau)^2$ would only require setting $z=0$, where $\vartheta_1(z|\tau)$ vanishes. The lhs then would give $-2(A^6+2B^6)+20(B^3(2A^3+B^3))$ because $B=C$ at $z=0$. However, we have not succeeded in showing directly that this equals $2(\vartheta_2^4-\vartheta_4^4)\ \vartheta_3^2/\eta^6$. Presumably, this is an interesting corollary of the theorem.

Rather, to find the constants multiplying the two basis vectors, we shall differentiate both sides twice and set $z=(1-\tau)/2$. This last evaluation has the merit of making the character C vanish, and giving also $A=-B=(1/\eta)\ \vartheta_3((1+\tau)/2|3\tau)$. For NS_1, we have

$$\begin{aligned} \partial_z^2|_{z=(1-\tau)/2}\ \mathrm{NS}_1 &= \partial_z^2|_{z=(1-\tau)/2}\ (A^6+B^6+C^6) \\ &= \partial_z^2|_{z=(1-\tau)/2}\ (A^6+B^6) \\ &= 6A^4[A''+5A'A]+6B^4[B''+5B'B]. \end{aligned} \tag{4.20}$$

Recalling that ϑ_3 and ϑ_3'' are even functions of z, while ϑ_3' is odd, and that they are all periodic under $z \to z+1$, we note the following: $\vartheta_3((1-\tau)/2|3\tau) = \vartheta_3((1+\tau)/2|3\tau)$ and similarly for ϑ_3'', but with an additional minus sign for ϑ_3'. Thus for instance, we have at $z=(1-\tau)/2$:

$$\begin{aligned} A &= \vartheta_3(z|3\tau), \\ A|_{z=(1-\tau)/2} &= \vartheta_3\left(\frac{1+\tau}{2}\middle|3\tau\right), \\ A'|_{z=(1-\tau)/2} &= -\vartheta_3'\left(\frac{1+\tau}{2}\middle|3\tau\right), \\ A''|_{z=(1-\tau)/2} &= \vartheta_3''\left(\frac{1+\tau}{2}\middle|3\tau\right), \end{aligned} \tag{4.21}$$

$$\begin{aligned} B &= q^{1/6} y^{1/3}\ \ \vartheta_3(z+\tau|3\tau), \\ B|_{z=(1-\tau)/2} &= -\vartheta_3\left(\frac{1+\tau}{2}\middle|3\tau\right), \\ B'|_{z=(1-\tau)/2} &= \left[-\frac{2\pi i}{3}\vartheta_3 - \vartheta_3'\right]\left(\frac{1+\tau}{2}\middle|3\tau\right), \\ B''|_{z=(1-\tau)/2} &= \left[-\frac{4\pi i}{9}\vartheta_3 + \frac{4\pi i}{3}\vartheta_3' + \vartheta_3''\right]\left(\frac{1+\tau}{2}\middle|3\tau\right). \end{aligned} \tag{4.22}$$

In particular, $A'B+AB' = -(2\pi i/3)\ \vartheta_3$. Bearing this in mind, we obtain

$$\partial_z^2|_{z=(1-\tau)/2}\,\mathrm{NS}_1=\frac{1}{\eta^6}\,\vartheta_3\!\left(\frac{1+\tau}{2}\middle|3\tau\right)^4\,[12\;\vartheta_3''\vartheta_3+60\;\vartheta_3'^2+48\pi i\;\vartheta_3'\vartheta_3-16\pi^2\vartheta_3^2]\!\left(\frac{1+\tau}{2}\middle|3\tau\right). \tag{4.23}$$

Similarly, for NS_2, we have

$$\begin{aligned}\partial_z^2|_{z=(1-\tau)/2}\,\mathrm{NS}_2&=\partial_z^2|_{z=(1-\tau)/2}\,(A^3B^3+B^3C^3+C^3A^3)\\&=\partial_z^2|_{z=(1-\tau)/2}\,(A^3B^3)\\&=3A^2B^2\,[AB''+2A'B'+A''B]+6AB[AB'+A'B]^2\\&=\frac{1}{\eta^6}\,\vartheta_3\!\left(\frac{1+\tau}{2}\middle|3\tau\right)^4\,[-6\;\vartheta_3\vartheta_3''+6\;\vartheta_3'^2+4\pi^2\;\vartheta_3^2]\!\left(\frac{1+\tau}{2}\middle|3\tau\right).\end{aligned} \tag{4.24}$$

Thus the lhs altogether yields

$$\begin{aligned}\partial_z^2|_{z=(1-\tau)/2}(-2\,\mathrm{NS}_1+20\,\mathrm{NS}_2)&=-\frac{4}{\eta^6}[\,\vartheta_3^5\;\;(36\;\;\vartheta_3''+24\pi i\;\;\vartheta_3'-4\pi^2\vartheta_3)-24\pi^2\;\;\vartheta_3]\\&\quad\times\!\left(\frac{1+\tau}{2}\middle|3\tau\right)=16\pi^2q^{-1/4}\;\;(6+E_2),\end{aligned} \tag{4.25}$$

where we have noted that $\vartheta_3((1+\tau)/2\,|3\tau)=q^{-1/24}\eta$ and that the curved bracket is proportional to the second Eisenstein series $E_2=(12/i\pi)\,\partial_\tau\log\eta$:

$$\begin{aligned}q^{1/24}(36\;\vartheta_3''+24\pi i\;\vartheta_3'-4\pi^2\;\vartheta_3)&=-4\pi^2\sum_{\mathbb{Z}}\;(-1)^n(6n+1)^2\;q^{(6n+1)^2/24}\\&=-4\pi^2\frac{24}{2\pi i}\,\partial_\tau\sum_{\mathbb{Z}}\;(-1)^nq^{(6n+1)^2/24}\\&=-4\pi^2\frac{24}{2\pi i}\,\partial_\tau\eta=-4\pi^2\eta E_2,\end{aligned} \tag{4.26}$$

by virtue of (B5).

We now turn to the rhs of (4.19) and shall differentiate twice. To this effect, we note a few useful facts,

$$\begin{aligned}\vartheta_1'\!\left(z+\frac{1-\tau}{2}\middle|\tau\right)&=\partial_z\;\;q^{-1/8}y^{1/2}\;\;\vartheta_3(z)\\&=i\pi\;\;\vartheta_1\!\left(z+\frac{1-\tau}{2}\middle|\tau\right)+q^{-1/8}y^{1/2}\;\;\vartheta_3'(z|\tau)\xrightarrow{z=0}-i\pi q^{-1/8}\;\;\vartheta_3,\\\vartheta_3'\!\left(z+\frac{1-\tau}{2}\middle|\tau\right)&=\partial_z\;\;-iq^{-1/8}y^{1/2}\;\;\vartheta_1(z)\\&=i\pi\;\;\vartheta_3\!\left(z+\frac{1-\tau}{2}\middle|\tau\right)-iq^{-1/8}y^{1/2}\;\;\vartheta_1'(z|\tau)\xrightarrow{z=0}-2\pi iq^{-1/8}\;\;\eta^3,\end{aligned} \tag{4.27}$$

where we used (B6). Similarly, we find

$$\vartheta_1''\left(\frac{1-\tau}{2}\middle|\tau\right)=-\pi^2 q^{-1/8}\ \ \vartheta_3+q^{-1/8}\ \ \vartheta_3''(0|\tau),$$
$$\vartheta_3''\left(z+\frac{1-\tau}{2}\middle|\tau\right)=4\pi^2 q^{-1/8}\ \ \eta^3. \tag{4.28}$$

Thus equipped, we proceed for the rhs,

$$\partial_z^2|_{z=(1-\tau)/2}\vartheta_1(z|\tau)^2=q^{-1/4}\vartheta_3^2\ \ [-2\pi^2+\vartheta_3''/\vartheta_3],$$
$$\partial_z^2|_{z=(1-\tau)/2}\vartheta_3(z|\tau)^2=-4\pi^2 q^{-1/4}\ \ \eta^6. \tag{4.29}$$

Taking (B25) into account, we have overall for the rhs,

$$\partial_z^2|_{z=(1-\tau)/2}\left[-24\frac{\vartheta_1(z|\tau)^2}{\vartheta_3^2}+2(\vartheta_2^4-\vartheta_4^4)\frac{\vartheta_3(z|\tau)^2}{\eta^6}\right]=16\pi^2 q^{-1/4}\ \ (6+E_2), \tag{4.30}$$

which was just the lhs. □

E. Lemmas and arithmetic results

Lemma 4.31:

$$\vartheta_3(z|3\tau)^3+q^{1/2}y\ \ \vartheta_3(z+\tau|3\tau)^3+q^2y^2\ \ \vartheta_3(z+2\tau|3\tau)^3=a(\tau)\ \ \vartheta_3(z|\tau), \tag{4.31}$$

where

$$a(\tau):=\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)\ \ q^{(6n+1)^2/24}=\sum_{k,l\in\mathbb{Z}}q^{k^2+kl+l^2}. \tag{4.32}$$

Proof: That the rhs is proportional to $\vartheta_3(z|3\tau)$ follows from the second proof that we shall give. To find the constant $a(\tau)$, we differentiate both sides with respect to (wrt) z and set $z=(1-\tau)/2$,

$$3\ \vartheta_3\left(\frac{1+\tau}{2}\middle|3\tau\right)^2\left[-2\ \ \vartheta_3'-\frac{2\pi i}{3}\vartheta_3\right]\left(\frac{1+\tau}{2}\middle|3\tau\right)=a(\tau)(-2\pi i q^{-1/8}\ \eta^3). \tag{4.33}$$

Note that

$$\vartheta_3\left(\frac{1+\tau}{2}\middle|3\tau\right)=q^{-1/24}\eta$$

and so we find

$$a(\tau)=\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)\ \ q^{(6n+1)^2/24}. \tag{4.34}$$

For the second expression for a, we offer an alternative proof,

$$\text{lhs}=\left(\sum_{\mathbb{Z}}\ q^{(3/2)\,n^2}y^n\right)^3+\left(\sum_{\mathbb{Z}+1/3}q^{(3/2)\,n^2}y^n\right)^3+\left(\sum_{\mathbb{Z}+2/3}q^{(3/2)\,n^2}y^n\right)^3$$
$$=\sum_n\ q^{(3/2)(n_1^2+n_2^2+n_3^2)}\ \ y^{(n_1+n_2+n_3)}, \tag{4.35}$$

where $n=(n_1,n_2,n_3)$ on the rhs sweeps through the set $S:=\mathbb{Z}^3\cup(\mathbb{Z}+\frac{1}{3})^3\cup(\mathbb{Z}+\frac{2}{3})^3$. This set lies in 1-to-1 correspondence with all $k\in\mathbb{Z}^3$ via the following smart substitution:

$$n_1=(k_1+k_2-k_3)/3,\quad k_1=n_1+n_2+n_3,$$

$$n_2=(k_1-2k_2-k_3)/3,\quad k_2=n_1-n_2,$$

$$n_3=(k_1+k_2+2k_3)/3,\quad k_3=-n_1+n_3. \tag{4.36}$$

Note that in the first definitions, all right-hand sides are equal to mod 1, which guarantees that all n_i are in the same component of the set S; whence the 1-to-1 correspondence. Moreover,

$$n_1^2+n_2^2+n_3^2=\tfrac{1}{3}k_1^2+\tfrac{2}{3}(k_2^2+k_3^2+k_2k_3),\quad n_1+n_2+n_3=k_1. \tag{4.37}$$

Hence,

$$\text{lhs}=\left(\sum_{k_2,k_3\in\mathbb{Z}} q^{k_2^2+k_2k_3+k_3^2}\right)\sum_{\mathbb{Z}}\ q^{1/2\,k_1^2}y^{k_1}=\text{rhs}. \tag{4.38}$$

□

Corollary 4.39:

$$\text{For } z=0:\quad \vartheta_3(0|3\tau)^3+2q^{1/2}\ \ \vartheta_3(\tau|3\tau)^3=a(\tau)\ \ \vartheta_3; \tag{4.39}$$

$$\text{for } z=1/2:\quad \vartheta_4(0|3\tau)^3-2q^{1/2}\ \ \vartheta_3(\tau|3\tau)^3=a(\tau)\ \ \vartheta_3; \tag{4.40}$$

$$\text{for } z=3\tau/2:\quad \vartheta_2(0|3\tau)^3+2q^{1/4}\ \ \vartheta_2(\tau|3\tau)^3=a(\tau)\ \ \vartheta_2. \tag{4.41}$$

For the sake of instruction, we give a third proof of the above lemma, after reformulating it with a different constant of proportionality.

Lemma 4.41:

$$\vartheta_3(z|\tau)^3+q^{1/6}y\ \ \vartheta_3\left(z+\frac{\tau}{3}\middle|\tau\right)^3+q^{2/3}y^2\ \ \vartheta_3\left(z+\frac{2\tau}{3}\middle|\tau\right)^3=\left(6\,\frac{\eta(3\tau)^3}{\eta}+a(\tau)\right)\ \ \vartheta_3\left(z\middle|\frac{\tau}{3}\right), \tag{4.42}$$

$$a(\tau):=\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)\ \ q^{(6n+1)^2/24}.$$

Proof: The advantage of having divided τ by 3 is that now all three terms on lhs and the rhs are theta functions of degree 3 and characteristic $(0,0;-6\pi i,3\pi i\tau)$. The space of such functions is three dimensional and can be spanned by

$$\left\{\vartheta_3\left(z\middle|\frac{\tau}{3}\right),\ \ \vartheta_3\left(z+\frac{\tau}{9}\middle|\frac{\tau}{3}\right),\ \ \vartheta_3\left(z+\frac{2\tau}{9}\middle|\frac{\tau}{3}\right)\right\}$$

or by

$$\{\vartheta_3(3z|3\tau),\ y\ \vartheta_3(3z+\tau|3\tau),\ y^2\ \vartheta_3(3z+2\tau|3\tau)\},$$

etc. Replacing $\tau\to3\tau$, the lhs as a whole is still a theta function of degree 1 and characteristic $(0,0;-2\pi i,\pi i\tau)$, hence must be proportional to $\vartheta_3(z|\tau)$. That is, all we have to do is to compute the constant of proportionality. To this end, we set $z=0$ in the lemma and prove

$$\vartheta_3(0|\tau)^3+2q^{1/6}\ \vartheta_3(\tau/3|\tau)^3=\left(6\frac{\eta(3\tau)^3}{\eta}+a(\tau)\right)\ \vartheta_3\left(0\middle|\frac{\tau}{3}\right). \tag{4.43}$$

We quote from Ref. 5, p. 273, a property describing how the cubes of theta functions can be spanned by basis vectors:

$$\frac{i\pi}{3}e^{(i\pi/6)}\eta\ \vartheta_3\left(z+\frac{1+\tau}{2}\middle|\tau\right)^3=-\pi e^{(i\pi/6)}q^{(-5/24)}y^{-3/2}\eta(3\tau)^3\ \left[z^{1/2}\ \vartheta_3\left(3z+\frac{1+\tau}{2}\middle|3\tau\right)\right.$$
$$\left.-z^{-1/2}\ \vartheta_3\left(-3z+\frac{1+\tau}{2}\middle|3\tau\right)\right]+\vartheta'\ \vartheta_3\left(3z+3\frac{1+\tau}{2}\middle|3\tau\right), \tag{4.44}$$

where

$$\vartheta':=\vartheta'\left[\begin{smallmatrix}1/3\\1\end{smallmatrix}\right](0|3\tau):=\partial_z|_0\quad e^{2\pi i/3}q^{1/6}y^{-1/3}\ \vartheta_1(z-\tau|3\tau),$$

such that

$$-\frac{3i}{\pi}e^{-i\pi/6}\frac{\vartheta'}{\eta}=\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)q^{(6n+1)^2/24}=a(\tau). \tag{4.45}$$

Special cases of this property are

$$\text{at } z=-\frac{1+\tau}{2}:\quad \vartheta_3(0|\tau)^3=6q^{1/6}\frac{\eta(3\tau)^3}{\eta}\vartheta_3(\tau|3\tau)+a(\tau)\ \vartheta_3(0|3\tau),$$

$$\text{at } z=-\frac{1}{2}+\frac{\tau}{6}:\quad \vartheta_3\left(\frac{\tau}{3}\middle|\tau\right)^3=3\frac{\eta(3\tau)^3}{\eta}[q^{-1/6}\ \vartheta_3(0|3\tau)+\vartheta_3(\tau|3\tau)]+a(\tau)\ \vartheta_3(\tau|3\tau), \tag{4.46}$$

so that

$$\vartheta_3(0|\tau)^3+2q^{1/6}\ \vartheta_3(\tau/3|\tau)^3=\left(6\frac{\eta(3\tau)^3}{\eta}+a(\tau)\right)\ [\vartheta_3(0|3\tau)+2q^{1/6}\ \vartheta_3(\tau|3\tau)]. \tag{4.47}$$

Use Lemma 6.23 to rewrite the square brackets as $\vartheta_3(0|\tau/3)$. □

Combining Lemmas 4.31 and 4.41, we arrive at an interesting observation, already noticed in Ref. 1.

Corollary 4.47:

$$a(\tau/3)=6\frac{\eta(3\tau)^3}{\eta}+a(\tau). \tag{4.48}$$

For completeness, we also observe that $a(\tau)$ can be written as the difference of two Lambert series [i.e., $\Sigma[a_nq^n/(1-q^n)]$],

$$
\begin{aligned}
a(\tau) &= \frac{q^{1/24}}{\eta}\partial_y\Big|_1 \sum_{\mathbb{Z}} (-1)^n y^{6n+1} q^{n(3n+1)/2} \\
&= \frac{q^{1/24}}{\eta}\partial_y\Big|_1 \; y \;\; \vartheta_3\left(6z+\frac{1+\tau}{2}\middle|3\tau\right) \\
&= \frac{q^{1/24}}{\eta}\partial_y\Big|_1 \; y \;\; \prod (1-q^{3n})(1-y^{6n}q^{3n-1})(1-y^{-6n}q^{3n-2}) \\
&= 1+6\sum_{n\geqslant 1}\left(\frac{-q^{3n-1}}{1-q^{3n-1}}+\frac{q^{3n-2}}{1-q^{3n-2}}\right) \\
&= 1+6\sum\; q^n\left(\sum_{\substack{d|n\\ d\equiv 1(3)}} 1-\sum_{\substack{d|n\\ d\equiv 2(3)}} 1\right) = 1+6\sum\; \delta_{3,1}(n)q^n,
\end{aligned}
\tag{4.49}
$$

where $\delta_{k,l}(n)$ is the number of divisors of n which are $(k-l)/2 \bmod k$ minus those which are $(k+l)/2 \bmod k$. For example, a well-known result of Jacobi states that the number of integer solutions to $x^2+y^2=n$ is $4\delta_{4,2}(n)$.

Many more beautiful properties about $a(\tau)$ are found in Ref. 1, such as

$$
a(\tau) = \vartheta_3(0|2\tau) \;\; \vartheta_3(0|6\tau) + \vartheta_2(0|2\tau) \;\; \vartheta_2(0|6\tau). \tag{4.50}
$$

We give a last property, of our own, relating to $a(\tau)^2$.

Proposition 4.51:

$$
2a(\tau)^2 = 3E_2(3\tau) - E_2. \tag{4.51}
$$

Proof: We apply the previous trick—of differentiating a Jacobi product—to the sum already encountered in (4.26),

$$
\begin{aligned}
E_2 &= \frac{1}{\eta}\sum_{\mathbb{Z}} (-1)^n (6n+1)^2 \;\; q^{(6n+1)^2/24} \\
&= \frac{q^{1/24}}{\eta} \;\; \frac{-1}{4\pi^2}\partial_z^2\Big|_0 \;\; \sum\; (-1)^n y^{6n+1} q^{n(3n+1)/2} \\
&= \frac{q^{1/24}}{\eta} \;\; \frac{-1}{4\pi^2}\partial_z^2\Big|_0 \;\; y \;\; \vartheta_3\left(6z+\frac{1+\tau}{2}\middle|3\tau\right) \\
&= \frac{q^{1/24}}{\eta} \;\; \frac{-1}{4\pi^2} \;\; \partial_z^2\Big|_0 \;\; y \;\; \prod (1-q^{3n})(1-y^{6n}q^{3n-1})(1-y^{-6n}q^{3n-2}).
\end{aligned}
\tag{4.52}
$$

Abbreviating the last product by Π, we have that $q^{1/24}\Pi|_0 = \eta$, $\Pi' = \Pi\Sigma$, and $\Pi'' = \Pi(\Sigma^2 + \Sigma')$, where

$$
\Sigma := 12\pi i \sum_{n\geqslant 1}\left(\frac{-y^6 q^{3n-1}}{1-y^6 q^{3n-1}}+\frac{y^{-6}q^{3n-2}}{1-y^{-6}q^{3n-2}}\right).
$$

In this notation, we also have $\Sigma|_0 = 2\pi i(a(\tau)-1)$. Thus

$$E_2=\left[1+\frac{1}{i\pi}\Sigma-\frac{1}{4\pi^2}(\Sigma^2+\Sigma')\right]_0$$
$$=1+2(a-1)+(a-1)^2-36\sum_{n\geqslant 1}\left(\frac{q^{3n-1}}{(1-q^{3n-1})^2}+\frac{q^{3n-2}}{(1-q^{3n-2})^2}\right)$$
$$=a^2+\frac{3}{2}[E_2-E_2(3\tau)]. \tag{4.53}$$

□

Since the sums $(1/\eta)\ \Sigma_{\mathbb{Z}}(-1)^n(6n+1)^k\ q^{(6n+1)^2/24}$ yield enticing expressions for powers $k=1,2$ [$a(\tau)$, E_2, respectively], it is natural to wonder whether this extends to higher power. We have not found any alternative expression for the case $k=3$, but can nonetheless relate it to $a(\tau)$ and E_2. Again, we mimic the trick of the previous proposition,

$$\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)^3\ q^{(6n+1)^2/24}$$
$$=a^3+\frac{3a}{(2\pi i)^2}\Sigma'\Big|_0+\frac{1}{(2\pi i)^3}\Sigma''\Big|_0$$
$$=a^3+3a\frac{3}{2}(E_2-E_2(3\tau))+\frac{1}{(2\pi i)^3}\Sigma''\Big|_0, \tag{4.54}$$

with

$$\Sigma''|_0=(2\pi i)^3 6^3\sum_{n\geqslant 1}\left(-\frac{q^{3n-1}(1+q^{3n-1})}{(1-q^{3n-1})^3}+\frac{q^{3n-2}(1+q^{3n-2})}{(1-q^{3n-2})^3}\right)=(2\pi i)^3 6^3\sum_{i\geqslant 1} i^2\frac{q^i(1-q^i)}{1-q^{3i}}. \tag{4.55}$$

The same recursion for the case $k=4$ is even more involved and is not worth writing in full, due to the complicated nature of Σ''',

$$\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)^4\ q^{(6n+1)^2/24}$$
$$=a^4+\frac{6a^2}{(2\pi i)^2}\Sigma'\Big|_0+\frac{4a}{(2\pi i)^3}\Sigma''\Big|_0+\frac{3}{(2\pi i)^4}\Sigma'\Big|_0^2+\frac{1}{(2\pi i)^4}\Sigma'''\Big|_0$$
$$=\frac{1}{\eta}\left(\frac{24}{2\pi i}\partial_\tau\right)^2\eta=3E_2^2-2E_4. \tag{4.56}$$

The last line is obtained using the covariant derivative for modular forms; it shows that $\partial_\tau^{k/2}\eta$ (for k even) can be expressed as a polynomial in E_2, E_4, E_6. For instance, for $k=6$ this is

$$\frac{1}{\eta}\sum_{\mathbb{Z}}\ (-1)^n(6n+1)^6\ \ q^{(6n+1)^2/24}=16E_6-30E_2E_4+15E_2^3. \tag{4.57}$$

V. COMPUTATIONS IN 2^4 THEORY

We mimic here the approach of the 1^6 theory, as detailed in the preceding section. This Gepner model is obtained by tensoring 4 times the $k=2$, N=2 theory. Although we have more

orbits and more cases to study, the mathematics are easier, due to the simpler properties enjoyed by theta functions with τ divided by 4 (instead of divided by 3 as in the 1^6 theory).

A. Characters and orbits

This time we have six minimal N=2 characters, obtained for $l=0$ ($m=0$), $l=1$ ($m=\pm 1$), and $l=2$ ($m=0,\pm 2$). The string functions at level 2, due to their symmetries, number only three:

$$c_{00}=c_{22}, \quad c_{20}=c_{02}, \quad c_{1,-1}=c_{11}. \tag{5.1}$$

In the following characters, we use the shorthand θ_m for the su(2) theta functions $\theta_{m,8}(\tau/2, z/4)$:

$$\begin{aligned}
A &:= \mathrm{ch}^{\mathrm{NS}}_{0,0}(y,q) = c_{00}\ \theta_0 + c_{02}\ \theta_8 = \frac{1}{2\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_3(z|2\tau) + \frac{1}{2\eta}\sqrt{\frac{\vartheta_4}{\eta}}\,\vartheta_4(z|2\tau),\\
B &:= \mathrm{ch}^{\mathrm{NS}}_{2,2}(y,q) = c_{02}\ \theta_{-4} + c_{00}\ \theta_4 = \frac{1}{2\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_2(z|2\tau) + \frac{1}{2\eta}\sqrt{\frac{\vartheta_4}{\eta}}\,i\ \vartheta_1(z|2\tau),\\
C &:= \mathrm{ch}^{\mathrm{NS}}_{2,0}(y,q) = c_{02}\ \theta_0 + c_{00}\ \theta_8 = \frac{1}{2\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_3(z|2\tau) - \frac{1}{2\eta}\sqrt{\frac{\vartheta_4}{\eta}}\,\vartheta_4(z|2\tau),\\
D &:= \mathrm{ch}^{\mathrm{NS}}_{2,-2}(y,q) = c_{02}\ \theta_4 + c_{00}\ \theta_{-4} = \frac{1}{2\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_2(z|2\tau) - \frac{1}{2\eta}\sqrt{\frac{\vartheta_4}{\eta}}\,i\ \vartheta_1(z|2\tau),\\
E &:= \mathrm{ch}^{\mathrm{NS}}_{1,-1}(y,q) = c_{11}(\ \theta_{-2} + \theta_6) = \frac{\eta(2\tau)}{\eta^2}\,q^{1/16}y^{-1/4}\ \vartheta_3\left(z-\frac{\tau}{2}\middle|2\tau\right),\\
F &:= \mathrm{ch}^{\mathrm{NS}}_{1,1}(y,q) = c_{11}(\ \theta_{-6} + \theta_2) = \frac{\eta(2\tau)}{\eta^2}\,q^{1/16}y^{1/4}\ \vartheta_3\left(z+\frac{\tau}{2}\middle|2\tau\right).
\end{aligned} \tag{5.2}$$

The su(2) theta functions are related to the standard (or "Ur-") Jacobi theta function via

$$\begin{aligned}
\theta_{m,8}\left(\frac{\tau}{2},\frac{z}{4}\right) &= \sum_{n\in\mathbb{Z}} q^{[2n+(m/8)]^2}\ y^{2n+(m/8)} = q^{(m/8)^2}\ y^{m/8}\ \vartheta_3\left(2z+\frac{m\tau}{2}\middle|8\tau\right),\\
\theta_m + \theta_{m+8} &= q^{(m/8)^2}y^{m/8}\ \vartheta_3\left(z+\frac{m\tau}{4}\middle|2\tau\right).
\end{aligned} \tag{5.3}$$

The rightmost column of (5.2) is obtained by rewriting $ac+bd$ as $\frac{1}{2}(a+b)(c+d)+\frac{1}{2}(a-b)(c-d)$ and using the explicit expression for the string functions from the next section.

Under spectral flow, these eight su(2) theta functions are shifted into one each other:

$$\theta_{m,8}\left(\frac{\tau}{2},\frac{z}{4}\right) \xrightarrow{z\to z+\tau/2} q^{-1/6}y^{-1/4}\ \ \theta_{m+2,8}\left(\frac{\tau}{2},\frac{z}{4}\right) \xrightarrow{z\to z+\tau/2} q^{-1/4}y^{-1/2}\ \ \theta_{m+4,8}\left(\frac{\tau}{2},\frac{z}{4}\right), \tag{5.4}$$

so that under full spectral flow, the six characters split into two groups which are cyclicly permuted:

$$A \xrightarrow{z\to z+\tau} B\to C\to D\to A, \quad E\to F\to E, \tag{5.5}$$

where we have omitted the incrementing factors of $q^{-1/4}y^{-1/2}$, etc.

To build the various orbits of the 2^4 theory, we consider all possible homogeneous polynomials of degree 4 in A, B, C, D, E, F, respecting the following two rules:

(1) the orbit must be holomorphic, i.e., its Fourier expansion must have integer powers of y;
(2) the orbit must be covariant under full spectral flow, $\mathrm{NS}_i(z\to z+\tau)=q^{-1}y^{-2}\,\mathrm{NS}_i(z)$.

Note that A, C have integer y-expansion, B, D half-integer, and E, F have powers of y in $\mathbb{Z}\mp\frac{1}{4}$, respectively. Thus, condition (1) excludes combinations like A^3B, A^3E, A^2BC, A^2E, etc. Condition (2) requires invariance of the orbit under cyclic permutation of A, B, C, D and E, F separately, and also guarantees it to be a theta function of characteristic $(0,0;-4\pi i,2\pi i)$ and degree 2. Thus each orbit can be spanned by $\mathrm{ch}_0(l=0,\frac{1}{2})$ and $\mathrm{ch}(h=0)$, or alternatively by $\vartheta_1(z|\tau)^2$ and $\vartheta_3(z|\tau)^2$.

The 12 possible orbits respecting the above rules are

$$\mathrm{NS}_1=A^4+B^4+C^4+D^4,\quad \mathrm{NS}_7=AB^2C+BC^2D+CD^2A+DA^2B,$$

$$\mathrm{NS}_2=E^4+F^4,\quad \mathrm{NS}_8=ABCD,$$

$$\mathrm{NS}_3=A^2B^2+B^2C^2+C^2D^2+D^2A^2,\quad \mathrm{NS}_9=ABE^2+BCF^2+CDE^2+DAF^2,$$

$$\mathrm{NS}_4=ABF^2+BCE^2+CDF^2+ADE^2,\quad \mathrm{NS}_{10}=(A^2+B^2+C^2+D^2)EF,$$

$$\mathrm{NS}_5=B^2D^2+A^2C^2,\quad \mathrm{NS}_{11}=E^2F^2,$$

$$\mathrm{NS}_6=AC^3+BD^3+CA^3+BD^3,\quad \mathrm{NS}_{12}=(AC+BD)EF.$$

The combinatorial factors D_i, defined after (4.11), associated to these orbits are (1, 2, 6, 12, 12, 4, 12, 96, 12, 12, 24, 48).

Due to the following relations among the characters

$$AC=BD,$$

$$AB+CD=F^2, \tag{5.6}$$

$$AD+BC=E^2$$

(proved in Lemma 5.24 with τ replaced by $\tau/2$), we find that several orbits coincide:

$$\mathrm{NS}_2=\mathrm{NS}_4,$$

$$\mathrm{NS}_5=2\,\mathrm{NS}_8, \tag{5.7}$$

$$\mathrm{NS}_6=\mathrm{NS}_7=\tfrac{1}{2}\mathrm{NS}_9=\mathrm{NS}_{11}.$$

B. String functions

Some explicit expressions for the string functions at level 2 are found in Ref. 9, p. 220:

$$c_{11}=\frac{\eta(2\tau)}{\eta^2}=\frac{1}{\eta}\sqrt{\frac{\vartheta_2}{2\eta}},\quad c_{00}-c_{02}=\frac{\eta(\tau/2)}{\eta^2}=\frac{1}{\eta}\sqrt{\frac{\vartheta_4}{\eta}}. \tag{5.8}$$

The authors also give the complicated modular properties of the string functions. The latter expression, $c_{00}-c_{02}$, upon shifting $\tau\to\tau+1$, yields $e^{-i\pi/8}(c_{00}+c_{02})$. Similarly, shifting $(1/\eta)\sqrt{\vartheta_4/\eta}$ by $\tau\to\tau+1$ yields $e^{-i\pi/8}(1/\eta)\sqrt{\vartheta_3/\eta}$. Together with Lemma 5.23 below, this gives

$$c_{00}+c_{02}=\frac{1}{\eta}\sqrt{\frac{\vartheta_3}{\eta}}=\frac{\eta}{\eta(2\tau)\ \eta(\tau/2)}=\frac{q^{-1/16}}{\vartheta(\tau)-q^{1/2}\ \vartheta(3\tau)},$$
$$c_{00}-c_{02}=\frac{1}{\eta}\sqrt{\frac{\vartheta_4}{\eta}}=\frac{\eta(\tau/2)}{\eta^2}=\frac{q^{-1/16}}{\vartheta(\tau)+q^{1/2}\ \vartheta(3\tau)}. \tag{5.9}$$

[The form $(1/\eta)\sqrt{\vartheta_i/\eta}$ for the string functions c_{11} and $c_{00}\pm c_{02}$ is expected from the fact that $\eta\ c_{ml}$ gives the character of the field ϕ^l_m in the $\mathbb{Z}_k$ parafermion model.[6,8] For our case of $k=2$, the $\mathbb{Z}_2$ parafermion model is just the Ising model, and its characters are the well known square roots of theta functions (with different spin structures). Thanks to Wendland for pointing at this and at her Ph.D. thesis (p. 50)[17] which already contains the explicit expressions for (5.2).] Here, and for the remainder of this section, we use the shorthand $\vartheta(z):=\vartheta_3(z|8\tau)$. Thus

$$c_{00}=q^{-1/16}\frac{\vartheta(\tau)}{\vartheta(\tau)^2-q\ \vartheta(3\tau)^2}=q^{1/16}\frac{\vartheta(\tau)}{\eta\ \eta(2\tau)},$$
$$c_{02}=q^{-1/16}\frac{q^{1/2}\ \vartheta(3\tau)}{\vartheta(\tau)^2-q\ \vartheta(3\tau)^2}=q^{1/16}\frac{q^{1/2}\ \vartheta(3\tau)}{\eta\ \eta(2\tau)} \tag{5.10}$$

and

$$c_{00}^2-c_{02}^2=\frac{1}{\eta\ \eta(2\tau)}=\frac{q^{-1/8}}{\vartheta(\tau)^2-q\ \vartheta(3\tau)^2},$$
$$c_{00}\ c_{02}=q^{5/8}\frac{\vartheta(\tau)\ \vartheta(3\tau)}{\eta^2\ \eta(2\tau)^2}=\frac{\eta(8\tau)^2}{\eta^3\ \eta(4\tau)}. \tag{5.11}$$

We now study the orbits at the special value of $z=(1+\tau)/2$. Note first that at this value, $\theta_{m,8}[\tau/2,(1+\tau)/8]=(-1)^{m/8}q^{((m/2)^2+m)/16}\ \vartheta_3((m/2+1)\tau|8\tau)$. With Lemma 5.23, our characters reduce to

$$A=c_{00}\ \vartheta(\tau)+c_{02}\ (-q^{3/2})\ \vartheta(5\tau)=q^{-1/16},$$
$$C=c_{02}\ \vartheta(\tau)+c_{00}\ (-q^{3/2})\ \vartheta(5\tau)=0,$$
$$B=-i[c_{02}\ \vartheta(\tau)-c_{00}\ q^{1/2}\ \vartheta(3\tau)]=0,$$
$$D=-i[c_{02}\ \vartheta(\tau)-c_{00}\ q^{1/2}\ \vartheta(3\tau)]=-iq^{-1/16}, \tag{5.12}$$
$$E=\frac{\eta(2\tau)}{\eta^2}q^{-1/16}e^{-i\pi/4}\ \vartheta_3\left(\frac{1}{2}\middle|2\tau\right)=e^{-i\pi/4}q^{-1/16},$$
$$F=\frac{\eta(2\tau)}{\eta^2}q^{3/16}e^{-i\pi/4}\ \vartheta_3\left(\frac{1}{2}+\tau\middle|2\tau\right)=0.$$

Plugging these values into the orbits NS_i yields $\mathrm{NS}_1=2q^{-1/4}$, $\mathrm{NS}_i=-q^{-1/4}$ $(i=2,\ldots,4)$, while the remaining NS_j vanish $(j=5,\ldots,12)$. We thus recognize from (2.7) the graviton, massless, and massive orbits, respectively.

C. The functions F_i, F_j and the Dirac index

In order to compute the functions F_i (2.2), we set $z=0$, in which case $\theta_{m,8}(\tau/2,0) = q^{(m/8)^2}\ \vartheta(m\tau/2) = \theta_{-m,8}$. Hence the characters simplify to

$$A+C=\frac{1}{\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_3(0|2\tau)=\frac{\eta(2\tau)^4}{\eta\ \ \eta(4\tau)^2\ \ \eta(\tau/2)}=E^2/B,$$

$$A-C=\frac{1}{\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_4(0|2\tau)=\frac{\eta(\tau/2)}{\eta(2\tau)}=1/E,$$

$$B=D=\frac{1}{\eta}\sqrt{\frac{\vartheta_3}{\eta}}\,\vartheta_2(0|2\tau)=\frac{\eta\ \ \eta(4\tau)^2}{\eta(\tau/2)\ \ \eta(2\tau)^2},$$

$$E=F=\frac{\eta(2\tau)}{\eta(\tau/2)}=\sqrt{\frac{1}{2}\frac{\vartheta_2}{\vartheta_4}}. \tag{5.13}$$

With these observations and the fact that $AC=B^2$ at $z=0$ (5.6), the massive orbits at $z=0$ have a rather simple form,

$$\begin{gathered}\mathrm{NS}_5=2\mathrm{NS}_8=2B^4,\\ \mathrm{NS}_6=\mathrm{NS}_7=\tfrac{1}{2}\mathrm{NS}_9=\mathrm{NS}_{11}=E^4,\\ \mathrm{NS}_{10}=E^6/B^2=\mathrm{NS}_{12}\,\mathrm{NS}_6/\mathrm{NS}_5,\\ \mathrm{NS}_{12}=2B^2E^2.\end{gathered} \tag{5.14}$$

Given that $\mathrm{NS}_j=F_j\ q^{-(1/8)}(\vartheta_3^2/\eta^3)=F_j\ [q^{-(1/8)}\eta^7/\eta(2\tau)^4\eta(\tau/2)^4]$, we find the following values for F_j:

$$\begin{gathered}F_5=2F_8=2q^{1/8}\frac{\eta(4\tau)^8}{\eta^3\ \ \eta(2\tau)^4},\\ F_6=F_7=\frac{1}{2}F_9=F_{11}=q^{1/8}\frac{\eta(2\tau)^8}{\eta^7},\\ F_{10}=q^{1/8}\frac{\eta(2\tau)^{14}}{\eta^9\ \ \eta(4\tau)^4},\\ F_{12}=2q^{1/8}\frac{\eta(2\tau)^2\ \ \eta(4\tau)^4}{\eta^5},\\ F_5F_{10}=F_6F_{12}.\end{gathered} \tag{5.15}$$

The massless orbits are a little less elegant, especially NS_1 and NS_3 which are not factorizable. For the latter, we shall need the following observation, again having set $z=0$:

$$(A^2+C^2)=(A-C)^2+2B^2=1/E^2+2B^2=(A+C)^2-2B^2=E^4/B^2-2B^2\Rightarrow E^6=B^2+4B^4E^2 \tag{5.16}$$

and

$$1/E^2+2B^2=2\,\frac{\vartheta_4}{\vartheta_2}+\frac{\vartheta_2(0|2\tau)^2}{\vartheta_2\ \ \vartheta_4}=\frac{2\,\vartheta_4^2+\vartheta_2(0|2\tau)^2}{\vartheta_2\ \ \vartheta_4}=\frac{3\,\vartheta_4^2+\vartheta_3^2}{2\,\vartheta_2\vartheta_4}. \tag{5.17}$$

We note that the last expression cannot be factorized and so we give the graviton+massless orbits as they stand:

$$\mathrm{NS}_1=(A^2+C^2)^2=(1/E^2+2B^2)^2=\left(\frac{3\,\vartheta_4^2+\vartheta_3^2}{2\,\vartheta_2\,\vartheta_4}\right)^2,$$

$$\mathrm{NS}_2=\mathrm{NS}_4=2E^4,$$

$$\mathrm{NS}_3=(3\,\vartheta_4^2+\vartheta_3^2)\,\frac{\vartheta_3^2\ \ \vartheta_2(0|2\tau)^2}{8\,\eta^6}=(3\,\vartheta_4^2+\vartheta_3^2)\,\frac{\vartheta_3^2-\vartheta_4^2}{4\,\vartheta_2^2\vartheta_4^2}=(3\,\vartheta_4^2+\vartheta_3^2)\,\frac{\eta\ \ \eta(4\tau)}{2\,\eta(\tau/2)\,\eta(2\tau)},$$

$$\mathrm{NS}_3^2=2\ \ \mathrm{NS}_1\mathrm{NS}_5 \tag{5.18}$$

with extensive use of the formulas in Appendix B. Given that $\mathrm{NS}_i=[h_3+F_i(q^{-1/8}/\eta)](\vartheta_3^2/\eta^2)$ for $i=2,3,4$ (and h_3 replaced by $-2h_3$ for NS_1), we find the following values for F_1 and F_i:

$$F_1=q^{1/8}\eta\left[\left(\frac{3\,\vartheta_4^2+\vartheta_3^2}{4\,\eta^2}\right)^2+2h_3\right]-1,$$

$$F_2=q^{1/8}\eta\left[2\left(\frac{\eta(2\tau)}{\eta}\right)^8-h_3\right]=2F_6-q^{1/8}\eta h_3, \tag{5.19}$$

$$F_3=q^{1/8}\eta\left[(3\,\vartheta_4^2+\vartheta_3^2)\,\frac{\eta(4\tau)^4}{2\,\eta^4\,\eta(2\tau)^2}-h_3\right],$$

$$F_4=F_2. \tag{5.20}$$

As in the 1^6 theory, we shall again derive (3.3), that is we shall show the following.

Proposition 5.20:

$$\sum_{i=1}^{d} D_i\,\mathrm{NS}_i\,I_i=-2\,\mathrm{NS}_1+2\,\mathrm{NS}_2+6\,\mathrm{NS}_3+12\,\mathrm{NS}_4=-24\ \ \frac{\vartheta_1(z|\tau)^2}{\vartheta_3^2}+2(\vartheta_2^4-\vartheta_4^4)\,\frac{\vartheta_3(z|\tau)^2}{\eta^6}. \tag{5.21}$$

Proof: Due to (5.12) and the vanishing of $\vartheta_3(z|\tau)$ at $z=(1+\tau)/2$, we see that $\vartheta_1(z|\tau)^2$ is correctly multiplied by $-24/\vartheta_3^2$. We only need to recover the factor multiplying $\vartheta_3(z|\tau)^2$. Unlike in 1^6 theory, setting $z=0$ on both sides will easily do the job,

$$\mathrm{lhs}|_0=\frac{1}{2\ \ \vartheta_2^2\ \ \vartheta_4^2}\left[-(3\ \ \vartheta_4^2+\vartheta_2^2)^2+(2+12)\ \ \vartheta_2^4+6(3\ \ \vartheta_4^2+\vartheta_3^2)\,\frac{1}{2}(\vartheta_3^2-\vartheta_4^2)\right]. \tag{5.22}$$

The square brackets yield a total of $16(\vartheta_2^4-\vartheta_4^4)$, while the prefactor is $\frac{1}{2}(\vartheta_3/2\eta^3)^2$. Thus we obtain the rhs. □

D. Lemmas

Lemma 5.23: With the shorthand $\vartheta(z):=\vartheta_3(z|8\tau)$, *we have*

$$(1)\quad q\quad \vartheta(5\tau)=\vartheta(3\tau),$$

$$(2)\quad \vartheta(0)-q\quad \vartheta(4\tau)=\vartheta_4(0|2\tau)=\frac{\eta^2}{\eta(2\tau)},$$

$$(3)\quad \vartheta(0)+q\quad \vartheta(4\tau)=\vartheta_3(0|2\tau)=\frac{\eta^2}{\eta(2\tau)}, \tag{5.23}$$

$$(4)\quad \vartheta(\tau)+q^{1/2}\quad \vartheta(3\tau)=q^{-1/16}\tfrac{1}{2}\vartheta_2(0|\tau/2)=q^{-1/16}\frac{\eta^2}{\eta(\tau/2)},$$

$$(5)\quad \vartheta(\tau)-q^{1/2}\quad \vartheta(3\tau)=\vartheta_2(\tau/2|2\tau)=q^{-1/16}\frac{\eta(2\tau)\ \eta(\tau/2)}{\eta}.$$

Proof: These are all instances of the more general Lemma 6.21. Alternatively,

(1) directly from sum or product expression,
(2) $\text{lhs}=\Sigma q^{4n^2}-\Sigma q^{4(n+\frac{1}{2})^2}=\Sigma q^{4(n/2)^2}=\vartheta_4(0|2\tau)=\Pi(1-q^{2n})(1-q^{2n-1})^2$
$=\Pi(1-q^n)(1-q^{2n})^{-1}=\text{rhs}$,
(3) idem,
(4) $\text{lhs}=q^{-1/16}\Sigma(q^{4(n-1/8)^2}+q\Sigma q^{4(n+3/8)^2})=q^{-1/16}\Sigma q^{(n-1/4)^2}=q^{-1/16}\frac{1}{2}\Sigma q^{(n-\frac{1}{2})^2}$
$=q^{-1/16}\frac{1}{2}\vartheta_2(0|\tau/2)=\Pi(1-q^{n/2})(1+q^{n/2})^2=\Pi(1-q^n)^2(1-q^{n/2})^{-1}=\text{rhs}=\vartheta_3(\tau/2|2\tau)$,
(5) idem.

□

Lemma 5.24:

$$\vartheta_4\left(0\left|\frac{\tau}{2}\right.\right)\ (\vartheta_1(z|\tau)^2+\vartheta_4(z|\tau)^2)=\vartheta_3\left(0\left|\frac{\tau}{2}\right.\right)\ (\vartheta_3(z|\tau)^2-\vartheta_2(z|\tau)^2)$$
$$=\vartheta_3\left(0\left|\frac{\tau}{2}\right.\right)\ \vartheta_3\left(\frac{z}{2}\left|\frac{\tau}{4}\right.\right)\vartheta_4\left(\frac{z}{2}\left|\frac{\tau}{4}\right.\right),$$

$$\vartheta_3\left(0\left|\frac{\tau}{2}\right.\right)\ \vartheta_2(z|\tau)\vartheta_3(z|\tau)+\vartheta_4\left(0\left|\frac{\tau}{2}\right.\right)\ i\vartheta_1(z|\tau)\vartheta_4(z|\tau)=\vartheta_2\left(0\left|\frac{\tau}{2}\right.\right)\ q^{1/16}y^{-1/2}\ \vartheta_3\left(z-\frac{\tau}{4}\left|\tau\right.\right)^2, \tag{5.24}$$

$$\vartheta_3\left(0\left|\frac{\tau}{2}\right.\right)\ \vartheta_2(z|\tau)\vartheta_3(z|\tau)-\vartheta_4\left(0\left|\frac{\tau}{2}\right.\right)\ i\vartheta_1(z|\tau)\vartheta_4(z|\tau)=\vartheta_2\left(0\left|\frac{\tau}{2}\right.\right)\ q^{1/16}y^{1/2}\ \vartheta_3\left(z+\frac{\tau}{4}\left|\tau\right.\right)^2.$$

Proof: Both sides of the first equation are theta functions of degree two and characteristic $(0,0;-4\pi i,-2\pi i\tau)$, i.e., elements of the two-dimensional vector space $\mathcal{T}_{2,-2\pi i\tau}$ (see Appendix A). In the other two equations, all terms—upon extra multiplication with y—are elements of $\mathcal{T}_{2,-3\pi i\tau}$. So all we need to do is to verify the relations at two independent values of z.

For all line, verification at $z=0,\tau/2$ is immediate with (B19) and (B20). The rhs gives a handy factorized form of the lhs, which would not lend itself to straightforward factorization as the sums $(i\vartheta_1\pm\vartheta_4)$ cannot be made into a theta function. □

VI. COMPUTATIONS IN 4^3 THEORY

We mimic here the approach of the two previous sections. This Gepner model is obtained by tensoring 3 times the $k=4$, $N=2$ theory. We have considerably more orbits and more cases to study; the mathematics involve properties of theta functions with τ divided by 3, 4, and 6.

A. Characters and orbits

This time we have 15 minimal $N=2$ characters, obtained for $l=0$ $(m=0)$, $l=1$ $(m=\pm 1)$, $l=2$ $(m=0,\pm 2)$, $l=3$ $(m=\pm 1,3)$, $l=4$ $(m=0,\pm 2,\pm 4)$. The string functions at level 4, due to their symmetries, number only seven,

$$c_{00}=c_{44},\quad c_{02}=c_{42},\quad c_{04}=c_{40},\quad c_{20}=c_{24},\quad c_{22},\quad c_{11}=c_{33},\quad c_{13}=c_{31}. \tag{6.1}$$

In the following characters, θ_m is a shortcut for the su(2) theta function evaluated as $\theta_{m,24}(\tau/2,z/6)$:

$$\begin{aligned}
A &:= \mathrm{ch}^{\mathrm{NS}}_{0,0}(y,q)=c_{02}\ \theta_{-12}+c_{00}\ \theta_0+c_{02}\ \theta_{12}+c_{04}\ \theta_{24},\\
B &:= \mathrm{ch}^{\mathrm{NS}}_{4,4}(y,q)=c_{02}\ \theta_{20}+c_{04}\ \theta_{-16}+c_{02}\ \theta_{-4}+c_{00}\ \theta_8,\\
C &:= \mathrm{ch}^{\mathrm{NS}}_{4,2}(y,q)=c_{02}\ \theta_{-20}+c_{04}\ \theta_{-8}+c_{02}\ \theta_4+c_{00}\ \theta_{16},\\
D &:= \mathrm{ch}^{\mathrm{NS}}_{4,0}(y,q)=c_{02}\ \theta_{-12}+c_{04}\ \theta_0+c_{02}\ \theta_{12}+c_{00}\ \theta_{24},\\
E &:= \mathrm{ch}^{\mathrm{NS}}_{4,-2}(y,q)=c_{02}\ \theta_{-4}+c_{04}\ \theta_8+c_{02}\ \theta_{20}+c_{00}\ \theta_{-16},\\
F &:= \mathrm{ch}^{\mathrm{NS}}_{4,-4}(y,q)=c_{02}\ \theta_4+c_{04}\ \theta_{16}+c_{02}\ \theta_{-20}+c_{00}\ \theta_{-8},
\end{aligned} \tag{6.2}$$

$$\begin{aligned}
G &:= \mathrm{ch}^{\mathrm{NS}}_{2,2}(y,q)=c_{22}\ \theta_{-20}+c_{20}\ \theta_{-8}+c_{22}\ \theta_4+c_{20}\ \theta_{16},\\
H &:= \mathrm{ch}^{\mathrm{NS}}_{2,0}(y,q)=c_{22}\ \theta_{-12}+c_{20}\ \theta_0+c_{22}\ \theta_{12}+c_{20}\ \theta_{24},
\end{aligned} \tag{6.3}$$

$$\begin{aligned}
I &:= \mathrm{ch}^{\mathrm{NS}}_{2,-2}(y,q)=c_{22}\ \theta_{-4}+c_{20}\ \theta_8+c_{22}\ \theta_{20}+c_{20}\ \theta_{-16},\\
J &:= \mathrm{ch}^{\mathrm{NS}}_{1,1}(y,q)=c_{13}\ \theta_{-22}+c_{11}\ \theta_{-10}+c_{11}\ \theta_2+c_{13}\ \theta_{14},\\
K &:= \mathrm{ch}^{\mathrm{NS}}_{1,-1}(y,q)=c_{13}\ \theta_{-14}+c_{11}\ \theta_{-2}+c_{11}\ \theta_{10}+c_{13}\ \theta_{22},\\
L &:= \mathrm{ch}^{\mathrm{NS}}_{3,3}(y,q)=c_{11}\ \theta_{18}+c_{13}\ \theta_{-18}+c_{13}\ \theta_{-6}+c_{11}\ \theta_6,\\
M &:= \mathrm{ch}^{\mathrm{NS}}_{3,1}(y,q)=c_{11}\ \theta_{-22}+c_{13}\ \theta_{-10}+c_{13}\ \theta_2+c_{11}\ \theta_{14},\\
N &:= \mathrm{ch}^{\mathrm{NS}}_{3,-1}(y,q)=c_{11}\ \theta_{-14}+c_{13}\ \theta_{-2}+c_{13}\ \theta_{10}+c_{11}\ \theta_{22},\\
O &:= \mathrm{ch}^{\mathrm{NS}}_{3,-3}(y,q)=c_{11}\ \theta_{-6}+c_{13}\ \theta_6+c_{13}\ \theta_{18}+c_{11}\ \theta_{-18}.
\end{aligned} \tag{6.4}$$

The su(2) theta functions are related to the standard Jacobi theta function via

$$\theta_{m,24}\left(\frac{\tau}{2},\frac{z}{6}\right)=\sum_{n\in\mathbb{Z}} q^{12(n+m/48)^2}\ y^{4(n+m/48)}=q^{(m/8)^2/3}\ y^{m/12}\ \vartheta_3\left(4z+\frac{m\tau}{2}\middle|24\tau\right). \tag{6.5}$$

Under full spectral flow, these su(2) theta functions are shifted into each other,

$$\theta_{m,24}\left(\frac{\tau}{2},\frac{z}{6}\right) \xrightarrow{z\to z+\tau} q^{-1/3}y^{-2/3}\ \ \theta_{m+8,24}\left(\frac{\tau}{2},\frac{z}{6}\right), \tag{6.6}$$

so that the 15 characters split into three groups which are cyclicly permuted,

$$\begin{gathered} A \xrightarrow{z\to z+\tau} B\to C\to D\to E\to F\to A, \\ G\to H\to I\to G, \\ J\to K\to L\to M\to N\to O\to J, \end{gathered} \tag{6.7}$$

where we have omitted the incrementing factors of $q^{-1/3}y^{-2/3}$, etc.

To build the various orbits of the 4^3 theory, we consider all possible homogeneous polynomials of degree 3 in $A,B,\ldots,O$, respecting our usual rules. Note the following powers for the y-expansions:

$$A,D,H \text{ have powers of } y \text{ in } \mathbb{Z}, \quad J,M \text{ in } \mathbb{Z}+\tfrac{1}{6},$$

$$B,E,I \text{ in } \mathbb{Z}-\tfrac{1}{3}, \quad K,N \text{ in } \mathbb{Z}-\tfrac{1}{6},$$

$$C,F,G \text{ in } \mathbb{Z}+\tfrac{1}{3}, \quad L,O \text{ in } \mathbb{Z}+\tfrac{1}{2}.$$

The 23 possible orbits are

$$\mathrm{NS}_1=A^3+B^3+C^3+D^3+E^3+F^3,$$

$$\mathrm{NS}_2=G^3+H^3+I^3,$$

$$\mathrm{NS}_3=(BC+EF)H+(CD+FA)I+(DE+AB)G,$$

$$\mathrm{NS}_4=AO^2+BJ^2+CK^2+DL^2+EM^2+FN^2,$$

$$\mathrm{NS}_5=(JL+MO)G+(KM+NJ)H+(LN+OK)I,$$

$$\mathrm{NS}_6=AL^2+BM^2+CN^2+DO^2+EJ^2+FK^2,$$

$$\mathrm{NS}_7=A^2D+B^2E+C^2F+D^2A+E^2B+F^2C, \quad \mathrm{NS}_{16}=(L^2+O^2)H+(J^2+M^2)I+(K^2+N^2)G,$$

$$\mathrm{NS}_8=ABC+BCD+CDE+DEF+EFA+FAB,$$

$$\mathrm{NS}_{17}=(A+D)LO+(B+E)JM+(C+F)KN,$$

$$\mathrm{NS}_9=AEC+BFD, \quad \mathrm{NS}_{18}=HLO+IJM+GKN,$$

$$\mathrm{NS}_{10}=GHI, \quad \mathrm{NS}_{19}=AJK+BKL+CLM+DMN+ENO+FOJ,$$

$$\mathrm{NS}_{11}=ADH+BEI+CFG, \quad \mathrm{NS}_{20}=DJK+EKL+FLM+AMN+BNO+COJ,$$

$$\mathrm{NS}_{12}=(A^2+D^2)H+(B^2+E^2)I+(C^2+F^2)G,$$

$$\mathrm{NS}_{21}=(JK+MN)H+(KL+NO)I+(LM+OJ)G,$$

$$\mathrm{NS}_{13}=(BF+EC)H+(AC+DF)I+(BD+AE)G,$$

$$\mathrm{NS}_{22}=CJL+DKM+ELN+FMO+ANJ+BOK,$$

$$\mathrm{NS}_{14}=(A+D)H^2+(B+E)I^2+(C+F)G^2,$$

$$\mathrm{NS}_{23}=FJL+AKM+BLN+CMO+DNJ+EOK,$$

$$\mathrm{NS}_{15}=(C+F)HI+(A+D)IG+(B+E)GH.$$

The coefficients D_i, see after (4.11), are thus (1; 2, 6, 3, 6, 3; 3, 6, 18, 36, 12, 3, 6, 3, 6; 3, 6, 12, 6, 6, 6, 6, 6).

B. String functions

Some explicit expressions for the string functions at level 2 are found in Ref. 9, pp. 219–220. We use the notation η_n for $\eta(n\tau)$:

$$c_{02}=\frac{\eta_{12}^2}{\eta^2\ \eta_6},\quad c_{00}-c_{04}=\frac{1}{\eta_2},\quad c_{11}+c_{13}=\frac{1}{\eta_{1/2}},$$
$$c_{00}+c_{04}-2c_{02}+2c_{20}-2c_{22}=\frac{\eta_{1/12}^2}{\eta^2\ \eta_{1/6}}. \tag{6.8}$$

The behavior under S and T transformation is also outlined by the authors. For example, T transforms the third equation into

$$c_{11}-c_{13}=\frac{\eta_{1/2}\ \eta_2}{\eta^3},$$

where we discarded $e^{i\pi/24}$ on both sides. Similarly, T^6 (i.e., $\tau\to\tau+6$) transforms the last equation into

$$-(c_{00}+c_{04}+2c_{02}+2c_{20}+2c_{22})=-\frac{\eta_{1/6}^5}{\eta^2\ \eta_{1/12}^2\ \eta_{1/3}^2},\quad \text{since}\quad \eta_{1/2}\overset{T}{\to}\frac{\eta^3}{\eta_{1/2}\ \eta_2}e^{i\pi/24}. \tag{6.9}$$

Furthermore,

$$c_{00}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(c_{00}+c_{04}+2c_{02}+2c_{20}+2c_{22}+2\sqrt{3}(c_{11}+c_{13})),$$

$$c_{04}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(c_{00}+c_{04}+2c_{02}+2c_{20}+2c_{22}-2\sqrt{3}(c_{11}+c_{13})),$$

$$c_{02}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(c_{00}+c_{04}-2c_{02}+2c_{20}-2c_{22}), \tag{6.10}$$

$$c_{20}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(2c_{00}+2c_{04}+4c_{02}-2c_{20}-2c_{22}),$$

$$c_{00}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(2c_{00}+2c_{04}-4c_{02}-2c_{20}+2c_{22}),$$

and so

$$c_{00}+c_{04}\overset{S}{\to}\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}(2c_{00}+2c_{04}+4c_{02}+4c_{20}+4c_{22})$$
$$=\frac{1}{2\sqrt{6}}\sqrt{\frac{i}{\tau}}\left(\frac{\eta_{1/6}^5}{\eta^2\ \eta_{1/12}^2\ \eta_{1/3}^2}\right)\overset{S}{\to}\frac{\eta_6^5}{\eta^2\ \eta_{12}^2\ \eta_3^2}, \tag{6.11}$$

since $\eta_n\overset{S}{\to}\sqrt{-i\tau/n}\ \eta_{1/n}$ for rational n. We thus find

$$c_{00}+c_{04}=\frac{\eta_6^5}{\eta^2\ \eta_{12}^2\ \eta_3^2}=\frac{\vartheta_3(0|6\tau)}{\eta^2},$$

$$c_{00}-c_{04}=\frac{1}{\eta_2}=\frac{\vartheta_4(0|2\tau)}{\eta^2},$$

$$c_{02}=\frac{\eta_{12}^2}{\eta^2\ \eta_6}=\frac{\vartheta_2(0|6\tau)}{2\eta^2},$$

$$c_{20}+c_{22}=\frac{1}{2\eta^2}\left(\frac{\eta_{1/6}^5}{\eta_{1/12}^2\ \eta_{1/3}^2}-\vartheta_3(0|6\tau)-\vartheta_2(0|6\tau)\right)$$
$$=\frac{1}{2\eta^2}(\vartheta_3(0|\tau/6)-\vartheta_3(0|3\tau/2))$$
$$=\frac{q^{1/12}}{\eta^2}\vartheta_3\left(\frac{\tau}{2}\middle|\frac{3\tau}{2}\right),$$

$$c_{20}-c_{22}=\frac{1}{2\eta^2}\left(\frac{\eta_{1/12}^2}{\eta_{1/6}}-\vartheta_3(0|6\tau)+\vartheta_2(0|6\tau)\right)$$
$$=\frac{1}{2\eta^2}(\vartheta_4(0|\tau/6)-\vartheta_4(0|3\tau/2))$$
$$=-\frac{q^{1/12}}{\eta^2}\vartheta_4\left(\frac{\tau}{2}\middle|\frac{3\tau}{2}\right),$$

where we have used Lemmas 6.21 and 6.23. Thus

$$c_{20}=\frac{q^{1/3}}{\eta^2}\vartheta_3(2\tau|6\tau)=\frac{q^{1/12}}{\eta^2}\vartheta_2(\tau|6\tau),$$
$$c_{22}=\frac{q^{1/3}}{\eta^2}\vartheta_2(2\tau|6\tau)=\frac{q^{1/12}}{\eta^2}\vartheta_3(\tau|6\tau). \tag{6.12}$$

C. Relation with 1^6 theory

With the above values of the string functions, we shall show some coincidences of the characters of 4^3 theory with those of 1^6 theory. We first note

$$\theta_m+\theta_{m+24}=\sum\ q^{3(n+\,m/24)^2}y^{2(n+\,m/24)}=q^{(m/8)^2/3}y^{m/12}\ \ \vartheta_3\left(2z+\frac{m\tau}{4}\middle|6\tau\right),$$

$$\theta_m-\theta_{m+24}=\sum\ (-1)^n q^{3(n+\,m/24)^2}y^{2(n+\,m/24)}=q^{(m/8)^2/3}y^{m/12}\ \ \vartheta_4\left(2z+\frac{m\tau}{4}\middle|6\tau\right),$$

$$\theta_m+\theta_{m+12}+\theta_{m+24}+\theta_{m+36}=\sum\ q^{(3/4)(n+\,m/12)^2}y^{n+\,m/12}=q^{(m/8)^2/3}y^{m/12}\ \ \vartheta_3\left(z+\frac{m\tau}{8}\middle|\frac{3\tau}{2}\right),$$

$$\begin{aligned}\theta_m-\theta_{m+12}+\theta_{m+24}-\theta_{m+36}&=\sum\ (-1)^n q^{(3/4)(n+\,m/12)^2}y^{n+\,m/12}\\&=q^{(m/8)^2/3}y^{m/12}\ \ \vartheta_4\left(z+\frac{m\tau}{8}\middle|\frac{3\tau}{2}\right),\end{aligned}\tag{6.13}$$

$$\theta_m+\theta_{m+12}-\theta_{m+24}-\theta_{m+36}=\sum\ \delta_n\ \ q^{(3/4)(n+\,m/12)^2}y^{n+\,m/12},$$

$$\delta_n:=+,+,-,-\quad\text{for}\quad n\equiv 0,1,2,3 \bmod 4,$$

for $m\equiv 2 \bmod 8:=\sum\ (q\ \ e^{2\pi i})^{(3/4)(n+\,m/12)^2}y^{n+\,m/12}$

$$=q^{(m/8)^2/3+3/16}y^{m/12}\ \eta_3/(\eta_6\eta_{3/2})\,\vartheta_3\left(z+\left(\frac{3}{4}+\frac{m}{8}\right)\tau\middle|3\tau\right)\ \ \vartheta_3\left(z+\left(\frac{3}{4}-\frac{m}{8}\right)\tau\middle|3\tau\right),$$

and for $m\equiv -2 \bmod 8:=\sum\ (-1)^n(q\ \ e^{2\pi i})^{(3/4)(n+\,m/12)^2}y^{n+\,m/12}$

$$=q^{(m/8)^2/3+3/16}y^{m/12}\frac{\eta_3}{\eta_6\ \ \eta_{3/2}}\,\vartheta_4\left(z+\left(\frac{3}{4}+\frac{m}{8}\right)\tau\middle|3\tau\right)\ \ \vartheta_4\left(z+\left(\frac{3}{4}-\frac{m}{8}\right)\tau\middle|3\tau\right).$$

The trick for the last formula is the same as in the special case leading to (6.18).

Thus, using Lemma 6.27,

$$\begin{aligned}A+D&=2c_{02}\ \ \vartheta_2(2z|6\tau)+(c_{00}+c_{04})\ \ \vartheta_3(2z|6\tau)=\frac{1}{\eta^2}\vartheta_3(z|3\tau)^2=A^2{}_{[1^6\ \text{theory}]},\\B+E&=\frac{q^{1/3}y^{2/3}}{\eta^2}\vartheta_3(z+\tau|3\tau)^2=B^2{}_{[1^6\ \text{theory}]},\\C+F&=\frac{q^{4/3}y^{4/3}}{\eta^2}\vartheta_3(z+2\tau|3\tau)^2=C^2{}_{[1^6\ \text{theory}]},\\G&=c_{22}\ \ q^{1/12}y^{1/3}\ \ \vartheta_3(2z+\tau|6\tau)+c_{20}\ \ q^{1/12}y^{1/3}\ \ \vartheta_2(2z+\tau|6\tau)\\&=\frac{q^{1/6}y^{1/3}}{\eta^2}\vartheta_3(z|3\tau)\ \ \vartheta_3(z+\tau|3\tau)\\&=AB_{[1^6\ \text{theory}]},\\H&=\frac{q^{5/6}y}{\eta^2}\vartheta_3(z+\tau|3\tau)\ \ \vartheta_3(z+2\tau|3\tau)=BC_{[1^6\ \text{theory}]},\\I&=\frac{q^{2/3}y^{2/3}}{\eta^2}\vartheta_3(z|3\tau)\ \ \vartheta_3(z+2\tau|3\tau)=AC_{[1^6\ \text{theory}]},\end{aligned}\tag{6.14}$$

where the right-hand side are taken from (4.7). In particular, this implies $(A+D)H=GI$, etc, and for the orbits:

4^3 theory	1^6 theory
$\mathrm{NS}_1+3\,\mathrm{NS}_7$	$=\mathrm{NS}_1$
NS_2	$=\mathrm{NS}_2$
$\mathrm{NS}_3+\mathrm{NS}_{13}$	$=\mathrm{NS}_2$
$\frac{1}{3}\,\mathrm{NS}_{14}=\mathrm{NS}_{10}=\mathrm{NS}_8+\mathrm{NS}_9$	$=\mathrm{NS}_3$
$\mathrm{NS}_{15}=\mathrm{NS}_{12}+2\,\mathrm{NS}_{11}$	$=\mathrm{NS}_4$.

These relations will be useful for the study of Gepner models with mixed levels, in particular the 1^44 theory.

D. Characters at $z=(1+\tau)/2$

We now study the orbits at the special value of $z=(1+\tau)/2$. Note first that at this value, $\theta_m=\theta_{m,24}(\tau/2,(1+\tau)/12)=e^{2\pi i m/24}q^{(m^2/8+m)/24}\ \vartheta_3((m/2+2)\tau|24\tau)$, as well as

$$\theta_8=\theta_{-16},\quad \theta_{-22}=-\theta_{14},\quad \theta_{-10}=-\theta_2,$$

$$\theta_m+\theta_{m+12}+\theta_{m+24}+\theta_{m+36}=e^{2\pi i\, m/24}q^{(m^2/8+m)/24}\ \vartheta_4\left(\left(\frac{m}{8}+\frac{1}{2}\right)\tau\,\middle|\,\frac{3\tau}{2}\right), \tag{6.15}$$

$$\theta_m+\theta_{m+12}-\theta_{m+24}-\theta_{m+36}=e^{2\pi i m/24}\sum\ \delta_n\ q^{(3/4)(n+(m/12))^2+(1/2)(n+m/12)},$$

where $\delta_n=+,+,-,-$ for $n\equiv 0,1,2,3 \bmod 4$. Without δ_n, we would recover the sum of the four theta functions with only $+$ signs. Note that δ_n can be removed if we replace $q^{1/2}$ with $-q^{1/2}$ in the sum and additionally multiply the sum by some root of unity, since $(-1)^{(3/2)(n+m/12)^2+n+m/12}=i^{m^2/48+m/6}\ i^{3n^2+(2+m/2)n}$. For $m=6$ or -2, we recover $e^{-2\pi i/16}\delta_n$. Thus we obtain the last line from the sum with only $+$ signs by inserting $-q^{1/2}$ in the latter's result. For $m=6$ and -2,

$$\begin{aligned}\theta_6+\theta_{18}+\theta_{-18}+\theta_{-6}&=-iq^{-1/16}\ \vartheta_4\left(-\frac{\tau}{4}\,\middle|\,\frac{3\tau}{2}\right)=-iq^{-1/12}\ \eta\left(\frac{\tau}{2}\right),\\ \theta_{-2}+\theta_{10}+\theta_{22}+\theta_{-14}&=q^{-1/12}\ \eta\left(\frac{\tau}{2}\right).\end{aligned} \tag{6.16}$$

On the rhs, replacing $q^{1/2}$ with $-q^{1/2}$ in $q^{-1/12}\ \eta(\tau/2)$ yields

$$\begin{aligned}q^{-(1/16)}\prod\ (1-q^n)(1-q^{n-1/2})&\to e^{-2\pi i/16}\ q^{-1/16}\prod\ (1-q^n)(1+q^{n-1/2})\\ &=e^{-2\pi i/16}\ q^{-1/12}\frac{\eta^3}{\eta(\tau/2)\,\eta(2\tau)}.\end{aligned} \tag{6.17}$$

Thus

$$\begin{aligned}\theta_6+\theta_{18}-\theta_{-18}-\theta_{-6}&=-iq^{-1/12}\frac{\eta^3}{\eta(\tau/2)\,\eta(2\tau)},\\ \theta_{-2}+\theta_{10}-\theta_{22}-\theta_{-14}&=q^{-1/12}\frac{\eta^3}{\eta(\tau/2)\,\eta(2\tau)}.\end{aligned} \tag{6.18}$$

This will be useful for the characters K,L,N,O.

With Lemmas 6.29, 6.31, and 6.33 our characters at $z=(1+\tau)/2$ reduce to

$$A=\frac{1}{2\eta^2}[\vartheta_2(0|6\tau)(\theta_{-12}+\theta_{12})+\vartheta_3(0|6\tau)(\theta_0+\theta_{24})+\vartheta_4(0|2\tau)(\theta_0-\theta_{24})]$$

$$=\frac{1}{2\eta^2}\left[\vartheta_2(0|6\tau)(-q^{1/4})\,\vartheta_3(2\tau|6\tau)+\vartheta_3(0|6\tau)\;\;\vartheta_3(\tau|6\tau)+\underbrace{\vartheta_4(0|2\tau)\;\;\vartheta_4(\tau|6\tau)}_{q^{-1/12}\;\;\eta^2}\right]$$

$$=q^{-1/12},$$

$$B=C=D=E=0,$$

$$F=e^{-2\pi i/3}\;\;q^{-1/12},$$

$$G=\frac{q^{1/12}}{\eta^2}\,\vartheta_3(\tau|6\tau)\;\;(\theta_{-20}+\theta_4)+\frac{q^{1/3}}{\eta^2}\,\vartheta_3(2\tau|6\tau)\;\;(\theta_{-8}+\theta_{16})=0,$$

$$H=0,$$

$$I=e^{-2\pi i/6}\;\;q^{-1/12},$$

$$J=c_{13}(\theta_{-22}+\theta_{14})+c_{11}(\theta_{-10}+\theta_2)=0,$$

$$K=\tfrac{1}{2}(c_{11}+c_{13})(\theta_{-14}+\theta_{-2}+\theta_{10}+\theta_{22})+\tfrac{1}{2}(c_{11}-c_{13})(-\theta_{-14}+\theta_{-2}+\theta_{10}-\theta_{22})$$
$$=e^{-2\pi i/12}\;\;q^{-1/12},$$

$$L=M=N=0,$$

$$O=-i\;\;q^{-1/12}.$$

Plugging these values into the orbits NS_i yields $\mathrm{NS}_1=2q^{-1/4}$, $\mathrm{NS}_i=-q^{-1/4}$ $(i=2,\ldots,6)$, while the remaining NS_j vanish $(j=7,\ldots,23)$. We thus recognize from (2.7) the graviton, massless, and massive orbits, respectively. Also, the value of the elliptic genus at $z=0$ is $\Phi(0)=\Sigma_{i=1}^d D_i\,|\mathrm{R}_i'(0)|^2=\Sigma_{i=1}^d D_i\,|-q^{1/4}\mathrm{NS}_i[(1+\tau)/2]|^2=\Sigma_{i=1}^d D_i I_i^2=4D_1+D_2+\cdots+D_6=24$, which is the correct coefficient for a $K3$ model (3.1).

E. Characters at $z=0$

In order to compute the functions F_i or the Dirac genus, we set $z=0$, in which case

$$\theta_m=\theta_{m,24}\left(\frac{\tau}{2},0\right)=\sum\;q^{12(n+\,m/48)^2}=q^{(m/8)^2/3}\;\vartheta_3\left(\frac{m\tau}{2}\middle|24\tau\right)=\theta_{-m},$$

$$\theta_m+\theta_{m+12}-\theta_{m+24}-\theta_{m+36}=\sum\;\delta_n q^{(3/4)(n+\,m/12)^2}=\sum\;\delta_n q^{(3/4)(n-1-\,(m/12)^2},$$

$$(\text{for } m=-10,-2:)=\sum\;\delta_n q^{(3/4)(n-\,1/6)^2}=e^{-2\pi i(m/8)^2/3}\sum\;(-1)^n(-q^{1/2})^{(3/2)(n-\,1/6)^2}=\frac{\eta^3}{\eta_{1/2}\;\eta_2},$$

where $\delta_n:=+,+,-,-$ and the last line is obtained by replacing $q^{1/2}$ by $q^{-1/2}$ in $\eta(\tau/2)$ (same trick as earlier).

With Lemma 6.27, the characters at $z=0$ take the following values:

$$
\begin{aligned}
A &= \frac{1}{2\eta^2}\,\vartheta_3(0|3\tau)^2+\frac{1}{2\eta^2}\,\vartheta_4(0|2\tau)\quad\vartheta_4(0|6\tau)=:A_1+A_2,\\
B=F &= \frac{q^{1/3}}{2\eta^2}\,\vartheta_3(\tau|3\tau)^2+\frac{q^{1/3}}{2\eta^2}\,\vartheta_4(0|2\tau)\quad\vartheta_4(2\tau|6\tau)=:B_1+B_2,\\
C &= E = B_1-B_2,\\
D &= A_1-A_2,\\
G=I &= \frac{q^{1/6}}{\eta^2}\quad\vartheta_3(0|3\tau)\quad\vartheta_3(\tau|3\tau),\\
H &= \frac{q^{1/3}}{\eta^2}\quad\vartheta_3(\tau|3\tau)^2=2B_1\\
J=K &= \frac{q^{1/48}}{2\eta_{1/2}}\quad\vartheta_3\left(\frac{\tau}{4}\middle|\frac{3\tau}{2}\right)+\tfrac{1}{2}=:J_1+\tfrac{1}{2},\\
L=O &= \frac{1}{2\eta_{1/2}}\,\vartheta_2\left(0\middle|\frac{3\tau}{2}\right),\\
M &= N = J_1-\tfrac{1}{2}.
\end{aligned}
\tag{6.19}
$$

(6.20)

We did not succeed in factorizing them, as we did for the 1^6 and 2^4 theories. The corresponding values for the orbits are not particularly enlightening. We only note the following coincidence: $\mathrm{NS}_{22}=\mathrm{NS}_{23}=2A_1(J_1^2-\frac{1}{4})+4LJ_1B_1$. Due to (2.7), this equality holds in general (not only at $z=0$) since $F_{22}=F_{23}$.

Thus we shall also refrain from giving here horrendous expressions (unfactorized) for the functions F_i and the Dirac index. But they can be easily written down on the basis of the above information. For instance, proving the value of the Dirac index (3.3) boils down to verifying its coefficient at $z=0$,

$$
\begin{aligned}
\sum_{i=1}^{d} D_i\,\mathrm{NS}_i(0)\;I_i &= -2\,\mathrm{NS}_1+2\,\mathrm{NS}_2+6\,\mathrm{NS}_3+3\,\mathrm{NS}_4+6\,\mathrm{NS}_5+3\,\mathrm{NS}_6\\
&= 32B_1^3-4A_1^3-12A_1A_2^2-48B_1B_2^2+4G^3\\
&\quad+24G(A_1B_1+A_2B_2+J_1L)+24B_1J_1^2+12A_1L^2,\\
&\overset{!}{=} 2\,\frac{\vartheta_2^4-\vartheta_4^4}{\eta^6}\,\vartheta_3^2,
\end{aligned}
$$

which is an arduous manipulation with theta functions identities (left to the reader).

F. Lemmas and arithmetic results

Lemma 6.21:

$$\vartheta_3(z|\tau)=\vartheta_3(2z|4\tau)+\vartheta_2(2z|4\tau), \tag{6.21}$$

$$\vartheta_4(z|\tau)=\vartheta_3(2z|4\tau)-\vartheta_2(2z|4\tau). \tag{6.22}$$

Proof: Directly from Fourier expansion. □

Lemma 6.23:

$$\begin{aligned}\vartheta_2(0|\tau)&=\vartheta_2(0|9\tau)+2q^{1/2}\ \ \vartheta_2(3\tau|9\tau),\\ \vartheta_3(0|\tau)&=\vartheta_3(0|9\tau)+2q^{1/2}\ \ \vartheta_3(3\tau|9\tau),\\ \vartheta_4(0|\tau)&=\vartheta_4(0|9\tau)-2q^{1/2}\ \ \vartheta_4(3\tau|9\tau).\end{aligned}\tag{6.23}$$

Proof: Idem. For instance, the middle line goes like

$$\text{lhs}=\sum\ q^{(3n)^2/2}+\sum\ q^{(3n+1)^2/2}+\sum\ q^{(3n+2)^2/2}=\sum\ q^{(3n)^2/2}+2\sum\ q^{(3n+1)^2/2}=\text{rhs}.\tag{6.24}$$

□

Lemma 6.25:

$$\vartheta_3\left(\frac{1}{3}\middle|\frac{2\tau}{3}\right)=\vartheta_3(0|6\tau)-q^{1/3}\ \ \vartheta_3(2\tau|6\tau)=\vartheta_3(0|6\tau)-q^{1/12}\ \ \vartheta_3(\tau|6\tau),\tag{6.25}$$

$$\vartheta_2\left(\frac{1}{3}\middle|\frac{2\tau}{3}\right)=-\vartheta_2(0|6\tau)+q^{1/3}\ \ \vartheta_2(2\tau|6\tau)=-\vartheta_2(0|6\tau)+q^{1/12}\ \ \vartheta_3(\tau|6\tau).\tag{6.26}$$

Proof: Idem. For instance, the first line

$$\text{lhs}=\sum\ q^{n^2/3}e^{2\pi in/3}=\sum\ q^{3n^2/3}+(e^{2\pi i/3}+e^{-2\pi i/3})\sum\ q^{3(n+1/3)^2/3}=\text{rhs}.$$

□

Lemma 6.27:

$$\vartheta_3(z|\tau)\ \ \vartheta_3(z'|\tau)+\vartheta_2(z|\tau)\ \ \vartheta_2(z'|\tau)=\vartheta_3\left(\frac{z+z'}{2}\middle|\frac{\tau}{2}\right)\ \ \vartheta_3\left(\frac{z-z'}{2}\middle|\frac{\tau}{2}\right),\tag{6.27}$$

$$\vartheta_3(z|\tau)\ \ \vartheta_3(z'|\tau)-\vartheta_2(z|\tau)\ \ \vartheta_2(z'|\tau)=\vartheta_4\left(\frac{z+z'}{2}\middle|\frac{\tau}{2}\right)\ \ \vartheta_4\left(\frac{z-z'}{2}\middle|\frac{\tau}{2}\right).\tag{6.28}$$

Proof: Idem. For instance, the first line

$$\text{lhs}=\sum_{\mathbb{Z}^2\cup(\mathbb{Z}+1/2)^2}q^{(m^2+n^2)/2}y^m y'^n=\sum_{\mathbb{Z}^2}\ q^{(k^2+l^2)/4}y^{(k+l)/2}y'^{(k+l)/2}=\text{rhs},$$

where we made the substitution $k=m+n,\ \ l=m-n$.

For the second line, one just needs to introduce $(-1)^{2n}$ and $(-1)^{k-l}$ in the two sums, respectively. □

Lemma 6.29:

$$\begin{aligned}&\vartheta_3(0|6\tau)\ \ \vartheta_3(\tau|6\tau)-\vartheta_2(0|6\tau)\ \ \vartheta_2(\tau|6\tau)=q^{-1/12}\ \ \eta^2,\\ &\vartheta_3\left(0\middle|\frac{\tau}{6}\right)\ \ \vartheta_3\left(\frac{1}{6}\middle|\frac{\tau}{6}\right)-\vartheta_4\left(0\middle|\frac{\tau}{6}\right)\ \ \vartheta_4\left(\frac{1}{6}\middle|\frac{\tau}{6}\right)=6\eta^2,\end{aligned}\tag{6.29}$$

$$\begin{aligned}&\vartheta_3\left(0\middle|\frac{2\tau}{3}\right)\ \ \vartheta_2\left(\frac{1}{3}\middle|\frac{2\tau}{3}\right)+\vartheta_2\left(0\middle|\frac{2\tau}{3}\right)\ \ \vartheta_3\left(\frac{1}{3}\middle|\frac{2\tau}{3}\right)=3\eta^2,\\ &\vartheta_3\left(0\middle|\frac{3\tau}{2}\right)\ \ \vartheta_4\left(\tau\middle|\frac{3\tau}{2}\right)-\vartheta_4\left(0\middle|\frac{3\tau}{2}\right)\ \ \vartheta_3\left(\tau\middle|\frac{3\tau}{2}\right)=-2q^{-1/3}\ \ \eta^2.\end{aligned}\tag{6.30}$$

Proof: The first line is just Lemma 6.27 with $z=0$ and $(z'|\tau)$ replaced by $(1+\tau|6\tau)$. The second line is obtained from the first by S transformation, i.e., $\tau\to-1/\tau$. The third line is obtained

by rewriting the second line as $ab+cd=(a+c)(b+d)/2+(a-c)(b-d)/2$ and using Lemma 6.21. The fourth line is again an S transformation of the previous line. Applying the rewriting trick on this last line, we would of course fall back on the first line. □

We note that the first line in Fourier series gives us an interesting formula: $\eta^2=\Sigma(-1)^n q^{3(n^2+m^2)}$ where $(m,n)\in(\frac{1}{2},\frac{1}{3})\cup(0,\frac{1}{6})+\mathbb{Z}^2$. This is to be compared with the previous formula (4.5). The crucial difference is that we presently have a positive definite quadratic form in the exponent of q, whereas previously the form was indefinite (this accounts for the extra constraint on x,y there).

In the first line, use Lemma 6.23 to replace $2q^{1/12}\ \vartheta_3(\tau|6\tau)$ by $\vartheta_2(0|\,2\tau/3)-\vartheta_2(0|6\tau)$ and similarly for $2q^{1/12}\ \vartheta_2(\tau|6\tau)$, and obtain the following.

Lemma 6.31:

$$\vartheta_2\left(0\left|\frac{2\tau}{3}\right.\right)\ \vartheta_3(0|6\tau)-\vartheta_3\left(0\left|\frac{2\tau}{3}\right.\right)\ \vartheta_2(0|6\tau)=2\eta^2, \tag{6.31}$$

$$\vartheta_4\left(0\left|\frac{3\tau}{2}\right.\right)\ \vartheta_3\left(0\left|\frac{\tau}{6}\right.\right)-\vartheta_3\left(0\left|\frac{3\tau}{2}\right.\right)\ \vartheta_4\left(0\left|\frac{\tau}{6}\right.\right)=4\eta^2, \tag{6.32}$$

where an S transformation connects the two lines. Unlike in the previous lemma, performing the rewriting trick will not give two more variants; here this trick is just equivalent to the S transformation itself.

Now, in the third line of Lemma 6.29, use Lemma 6.25 to replace $\vartheta_2(\frac{1}{3}|\,2\tau/3)$ by $-\vartheta_2(0|6\tau)+q^{1/3}\ \vartheta_2(2\tau|6\tau)$ and similarly for $\vartheta_3(\frac{1}{3}|\,2\tau/3)$, and obtain the first line of the following lemma.

Lemma 6.33:

$$\begin{gathered}\vartheta_3\left(0\left|\frac{2\tau}{3}\right.\right)\ \vartheta_3(\tau|6\tau)-\vartheta_2\left(0\left|\frac{2\tau}{3}\right.\right)\ \vartheta_2(\tau|6\tau)=q^{-1/12}\ \eta^2,\\ \vartheta_3\left(0\left|\frac{3\tau}{2}\right.\right)\ \vartheta_3\left(\frac{1}{3}\left|\frac{\tau}{6}\right.\right)-\vartheta_4\left(0\left|\frac{3\tau}{2}\right.\right)\ \vartheta_4\left(\frac{1}{3}\left|\frac{\tau}{6}\right.\right)=2\eta^2,\end{gathered} \tag{6.33}$$

$$\begin{gathered}\vartheta_3(0|6\tau)\ \vartheta_2\left(\frac{2}{3}\left|\frac{2\tau}{3}\right.\right)+\vartheta_3(0|6\tau)\ \vartheta_3\left(\frac{2}{3}\left|\frac{2\tau}{3}\right.\right)=\eta^2,\\ \vartheta_4\left(0\left|\frac{\tau}{6}\right.\right)\ \vartheta_3\left(\tau\left|\frac{3\tau}{2}\right.\right)-\vartheta_3\left(0\left|\frac{\tau}{6}\right.\right)\ \vartheta_4\left(\tau\left|\frac{3\tau}{2}\right.\right)=q^{-1/3}\ \eta^2.\end{gathered} \tag{6.34}$$

Proof: Again, the successive lines are obtained by S transformation, the rewriting trick, and S transformation. □

VII. COMPUTATIONS IN MIXED THEORIES

We have met with success the construction of N=4 characters in *pure* Gepner models like $1^6,2^4,4^3$ theories. Other Gepner models for the N=4 SCFT on $K3$ are *mixed* tensor products of N=2 theories, like 1^32^2, 1^44, 1^24^2, $2\,6^2$, $1\,2^24,\ldots$. All these products $k_1^{n_1}\cdots k_j^{n_j}$ are formed with the requirement that the central charge equal six: $c=\Sigma n_i[3k_i/(k_i+2)]=6$. We shall investigate the first three cases of such theories with mixed levels k_i and see that they do not necessarily share the previous structure characteristic of *pure* theories. Specifically, the notion of gravitational, massless, and massive orbits, with values at $z=(1+\tau)/2$ equal to $2q^{-1/4},-q^{-1/4}$ and 0, respectively expected from (2.7), only applies to $K3$ models like the 1^44 or 1^24^2 theories below. The other CY twofold, the complex torus, gives a model whose orbits all vanish at $z=(1+\tau)/2$, yielding a zero Euler characteristic as in the 1^32^2 theory below.

A. Computations in $1^3 2^2$ theory

The NS_i orbits are tensor products of three orbits from the $k=1$ theory (Sec. IV) and two orbits from the $k=2$ theory (Sec. V). The former theory has characters A, B, C (with powers of y in $\mathbb{Z}+0$, $\frac{1}{3}$, $\frac{2}{3}$, respectively), while the latter's characters we denote by $\overline{A},\overline{B},\overline{C},\overline{D},\overline{E},\overline{F}$ (with powers of y in $\mathbb{Z}+0$, $\frac{1}{2}$, 0, $\frac{1}{2}$, $-\frac{1}{4}$, $\frac{1}{4}$, respectively). In order to have only integer powers of y and cyclic permutation in the orbits, the only possible combinations are products of ABC, $A^3+B^3+C^3$ with $\overline{AC}+\overline{BD}$, $\overline{EF}$, $\overline{A^2}+\overline{C^2}+\overline{B^2}+\overline{D^2}$. Each of these products vanishes at $z=(1+\tau)/2$, so all orbits are massive and the Dirac index vanishes. This is to be expected as both the 1^3 and the 2^2 theories are toroidal models (with complex and Kähler moduli $\tau=\rho=e^{2\pi i/3}$ and $\tau=\rho=i$, respectively), hence so is their tensor product. That is, the target space of the sigma model is not $K3$ but a complex two-torus.

B. Computations in $1^4 4$ theory

We denote the characters of the $k=4$ theory by a bar over the letters. Our usual two rules (integer powers of y and invariance under cyclic permutation) restrict the orbits to be of the following form:

$$\mathrm{NS}_1=A^4(\overline{A}+\overline{D})+B^4(\overline{B}+\overline{E})+C^4(\overline{C}+\overline{F}),\quad \mathrm{NS}_5=ABC(A\overline{H}+B\overline{I}+C\overline{G}),$$

$$\mathrm{NS}_2=A^3B(\overline{B}+\overline{E})+B^3C(\overline{C}+\overline{F})+C^3A(\overline{A}+\overline{D}),\quad \mathrm{NS}_6=A^4\overline{H}+B^4\overline{I}+C^4\overline{G},$$

$$\mathrm{NS}_3=A^3C(\overline{C}+\overline{F})+B^3A(\overline{D}+\overline{A})+C^3B(\overline{E}+\overline{B}),\quad \mathrm{NS}_7=A^3B\overline{I}+B^3C\overline{G}+C^3A\overline{H},$$

$$\mathrm{NS}_4=A^2B^2\overline{G}+B^2C^2\overline{H}+C^2A^2\overline{I},\quad \mathrm{NS}_8=A^3C\overline{G}+B^3A\overline{H}+C^3B\overline{I}.$$

Due to the relations between the 4^3 characters and the 1^6 characters established in (6.14), the orbits 2,3,4 are equal, and so are the orbits 6,7,8. Thus we obtain consecutively the orbits NS_1, NS_2, $3\,\mathrm{NS}_3$, and NS_4 of 1^6 theory (4.10), which proves the equivalence of both models.

The coefficients $D_i=S_{1,i}/S_{i,1}$ defined after (4.11) are (1; 4,4,12; 24; 2,8,8), where $S_{i,1}=(6;6,6,3;3;3,3,3)$ are the numbers of terms in each orbit and $S_{1,i}=(1;4,4,6;12;1,4,4)$ is $S_{1,1}$ times the number of permutations of the factors in any term of orbit NS_i (look only at the 1^4 factors). Thus for the Dirac index, we have correctly $-2\,\mathrm{NS}_1+(4+4+12)\,\mathrm{NS}_2$, as in (4.19).

C. Computations in $1^2 4^2$ theory

This time, we are even allowed to include the characters $J,K,..,O$ from the $k=4$ theory. The orbits take the form

$$\mathrm{NS}_1=A^2(\overline{A^2}+\overline{D^2})+B^2(\overline{B^2}+\overline{E^2})+C^2(\overline{C^2}+\overline{F^2}),$$

$$\mathrm{NS}_2=A^2(\overline{L^2}+\overline{O^2})+B^2(\overline{J^2}+\overline{M^2})+C^2(\overline{K^2}+\overline{N^2}),$$

$$\mathrm{NS}_3=A^2(\overline{B}+\overline{E})\overline{G}+B^2(\overline{C}+\overline{F})\overline{H}+C^2(\overline{D}+\overline{A})\overline{I},$$

$$\mathrm{NS}_4=A^2(\overline{C}+\overline{F})\overline{I}+B^2(\overline{D}+\overline{A})\overline{G}+C^2(\overline{E}+\overline{B})\overline{H},$$

$$\mathrm{NS}_5=AB\overline{G^2}+BC\overline{H^2}+CA\overline{I^2},$$

$$\mathrm{NS}_6=AB(\overline{AB}+\overline{DE})+BC(\overline{BC}+\overline{EF})+CA(\overline{CD}+\overline{FA}),$$

$$\mathrm{NS}_7=AB(\overline{LJ}+\overline{OM})+BC(\overline{MK}+\overline{JN})+CA(\overline{NL}+\overline{KO}),$$

$$\mathrm{NS}_8=A^2\overline{H}^2+B^2\overline{I}^2+C^2\overline{G}^2,$$

$$\mathrm{NS}_9=AB(\overline{C}+\overline{F})\overline{G}+BC(\overline{A}+\overline{D})\overline{H}+CA(\overline{B}+\overline{E})\overline{I},$$

$$\mathrm{NS}_{10}=AB\overline{HI}+BC\overline{IG}+CA\overline{GH},$$

$$\mathrm{NS}_{11}=A^2(\overline{BC}+\overline{EF})+B^2(\overline{CD}+\overline{FA})+C^2(\overline{DE}+\overline{AB}),$$

$$\mathrm{NS}_{12}=A^2(\overline{BF}+\overline{EC})+B^2(\overline{CA}+\overline{FD})+C^2(\overline{DB}+\overline{AE}),$$

$$\mathrm{NS}_{13}=A^2\overline{IG}+B^2\overline{GH}+C^2\overline{HI},$$

$$\mathrm{NS}_{14}=A^2(\overline{A}+\overline{D})\overline{H}+B^2(\overline{B}+\overline{E})\overline{I}+C^2(\overline{C}+\overline{F})\overline{G},$$

$$\mathrm{NS}_{15}=AB(\overline{B}+\overline{E})\overline{H}+BC(\overline{C}+\overline{F})\overline{I}+CA(\overline{A}+\overline{D})\overline{G},$$

$$\mathrm{NS}_{16}=AB(\overline{A}+\overline{D})\overline{I}+BC(\overline{B}+\overline{E})\overline{G}+CA(\overline{C}+\overline{F})\overline{H},$$

$$\mathrm{NS}_{17}=A^2\overline{AD}+B^2\overline{BE}+C^2\overline{CF},$$

$$\mathrm{NS}_{18}=A^2\overline{LO}+B^2\overline{JM}+C^2\overline{KN},$$

$$\mathrm{NS}_{19}=AB\overline{CF}+BC\overline{DA}+CA\overline{EB},$$

$$\mathrm{NS}_{20}=AB(\overline{AE}+\overline{DB})+BC(\overline{BF}+\overline{EC})+CA(\overline{CA}+\overline{FD}),$$

$$\mathrm{NS}_{21}=AB(\overline{LM}+\overline{OJ})+BC(\overline{MN}+\overline{JK})+CA(\overline{NO}+\overline{KL}),$$

$$\mathrm{NS}_{22}=A^2(\overline{JN}+\overline{MK})+B^2(\overline{KO}+\overline{NL})+C^2(\overline{LJ}+\overline{OM}),$$

$$\mathrm{NS}_{23}=A^2(\overline{JK}+\overline{MN})+B^2(\overline{KL}+\overline{NO})+C^2(\overline{LM}+\overline{OJ}),$$

$$\mathrm{NS}_{24}=AB\overline{KN}+BC\overline{LO}+CA\overline{JM},$$

$$\mathrm{NS}_{25}=AB(\overline{K}^2+\overline{N}^2)+BC(\overline{L}^2+\overline{O}^2)+CA(\overline{J}^2+\overline{N}^2),$$

$$\mathrm{NS}_{26}=AB(\overline{C}^2+\overline{F}^2)+BC(\overline{D}^2+\overline{A}^2)+CA(\overline{E}^2+\overline{B}^2).$$

At $z=(1+\tau)/2$, the first two orbits give $2q^{-1/4}$ and $-2q^{-1/4}$, respectively, while the next five orbits give $q^{-1/4}$; the other orbits all give 0. This embarrassing second orbit prevents us to classify it as either a graviton, massless or massive orbit. The coefficients D_i are (1,1,2,2,4,4,4; 2,4,8,2,2,4,2,4,4; 4,4,4,4,4,2,2,8,2,2). So the value of the elliptic genus at $z=0$ is $\Phi(0)=\Sigma_{i=1}^{d}D_i\,|\mathrm{R}_i'(0)|^2=\Sigma_{i=1}^{d}D_iI_i^2=4D_1+4D_2+D_3+\cdots+D_7=24$, so this is a $K3$ model with the appropriate Euler character.

Due to the relations between the 4^3 characters and the 1^6 characters established in (6.14), we find the following relations between the orbits:

$1^2 4^2$ theory	4^3 theory	$1^2 4^2$ theory	4^3 theory	$1^2 4^2$ theory	4^3 theory
NS_1	NS_1+NS_7	$NS_8=NS_9=NS_{10}$	$NS_{14}=3\,NS_{10}$	NS_{18}	NS_{17}
NS_2	NS_4+NS_6	NS_{11}	$2\,NS_8$	NS_{19}	NS_{11}
$NS_3=NS_4=NS_5$	NS_3+NS_{13}	NS_{12}	$NS_8+3\,NS_9$	NS_{20}	NS_{13}
NS_6	NS_3	$NS_{13}=NS_{14}=NS_{15}$	$NS_{15}=NS_{12}+2NS_{11}$	NS_{21}	NS_{21}
NS_7	NS_5	NS_{16}	NS_7	NS_{22}	$NS_{22}+NS_{23}$
		NS_{17}	NS_{15}	NS_{22}	$NS_{19}+NS_{20}$
				NS_{24}	NS_{18}
				NS_{25}	NS_{16}
				NS_{26}	NS_{12}

In addition, some of these orbits match even those of 1^6 theory:

$1^2 4^2$ theory	4^3 theory	1^6 theory
$NS_1+2\,NS_{16}$	$NS_1+3\,NS_7$	NS_1
$NS_3=NS_4=NS_5=NS_6+NS_{20}$	NS_3+NS_{13}	NS_2
$NS_8=NS_9=NS_{10}$	$NS_{14}=3\,NS_{10}$	$3\,NS_3$
$NS_{11}+NS_{12}$	$3\,(NS_8+NS_9)$	$3\,NS_3$
$NS_{13}=NS_{14}=NS_{15}$	$NS_{15}=NS_{12}+2\,NS_{11}$	NS_4

ACKNOWLEDGMENTS

The author of this paper thanks Anne Taormina for providing the orbits in Sec. V A and for further assistance, to Sander Zwegers for the alternative proof of Lemma 4.31, to Herschel Farkas and Frank Garvan for their useful hints, to Katrin Wendland for her feedback and helpful answers, and to Robbert Dijkgraaf for the final touch.

APPENDIX A: THETA FUNCTIONS OF GIVEN CHARACTERISTIC

A holomorphic function $T:\mathbb{C}\to\mathbb{C}$ is called a *theta function with period τ and characteristic* $(a_1,b_1;a_2,b_2)$ if it is almost periodic on the lattice, i.e., if it transforms according to

$$T(v+1)=e^{a_1 v+b_1}T(v), \quad \text{and} \quad T(v+\tau)=e^{a_2 v+b_2}T(v). \tag{A1}$$

We call $n:=(a_1\tau-a_2)/2\pi i$ the *degree* of the function.

For example, the following functions are all theta functions with characteristic and degree:

$$y^{1/2}: \quad (0,i\pi;0,i\pi\tau) \quad 0,$$

$$\vartheta_1(v): \quad (0,i\pi;-2\pi i,-i\pi(\tau+1)) \quad 1,$$

$$\vartheta_2(v): \quad (0,i\pi;-2\pi i,-i\pi\tau) \quad 1,$$

$$\vartheta_3(v): \quad (0,0;-2\pi i,-i\pi\tau) \quad 1,$$

$$\vartheta_4(v): \quad (0,0;-2\pi i,-i\pi(\tau+1)) \quad 1,$$

$$\vartheta_1(2v|2\tau): \quad (0,0;-4\pi i,-2\pi i\tau-i\pi) \quad 2,$$

$$\vartheta_2(2v|2\tau): \quad (0,0;-4\pi i,-2\pi i\tau) \quad 2,$$

$$\vartheta_3(2v|2\tau): \quad (0,0;-4\pi i,-2\pi i\tau) \quad 2,$$

$$\vartheta_4(2v|2\tau): \quad (0,0;-4\pi i,-2\pi i\tau-i\pi) \quad 2,$$

$$\vartheta_i(v)^2: \quad (0,0;-4\pi i,-2\pi i\tau) \quad 2, \quad i=1,\ldots,4.$$

Note that characteristics add up when multiplying theta functions. Note also that $\vartheta_3(nv|n\tau)$ and $\vartheta_3(v|\tau/n)$ are of degree n and characteristic $(0,0;-2n\pi i,-n\pi i\tau)$. As another example, consider the character functions of the level k and isospin l representation of affine su(2) algebra:[4]

$$\chi_k^l(y) := \frac{q^{(l+1/2)^2/(k+1/2)-1/8}}{\prod_{n\geqslant 1}(1-q^n)(1-y^2q^n)(1-y^{-2}q^{n-1})} \times \sum_{m\in\mathbb{Z}} q^{(k+2)m^2+(2l+1)m}(y^{2m(k+2)+2l}-y^{-2m(k+2)-2l-2}). \tag{A2}$$

This is a theta function of characteristic $(0,0;-4k\pi i,-2ki\pi\tau)$ and degree $2k$, i.e., it transforms like $\chi_k^l(v+\tau)=q^{-k}y^{-2k}\chi_k^l(v)$.

Each theta function can be multiplied by trivial theta functions (i.e., of degree 0) so that the resulting characteristic reads $(0,0;-2\pi in,b_2)$ where n the degree (an integer). For fixed b_2, this is a vector space of dimension n as can be seen from the fact that contour integration around one lattice cell yields n zeros for T: $P-Z=\oint T'/T=\oint\partial\log T=-n$. We denote this complex vector space by $\mathcal{T}_{n,b_2}$. For $b_2=-n\pi i\tau$, it's spanned by $\vartheta_3(nv|n\tau), y\ \vartheta_3(nv+\tau|n\tau),\ldots,y^{n-1}\ \vartheta_3(nv+(n-1)\tau|n\tau)$.

Thus for instance, all degree 2 theta functions of characteristic $(0,0;-4\pi i,-2\pi i\tau)$ should be expressible as linear combinations of $\vartheta_1(v)^2$ and $\vartheta_3(v)^2$ [or any two of the $\vartheta_i(v)^2$, $i=1,\ldots,4$] with τ-dependent coefficients. This was the case for the N=4 massless NS characters (2.2), for $\vartheta_2(v)^2$ or $\vartheta_4(v)^2$ as in (B18), or for the level 1 su(2) theta functions,

$$\chi_1^0(y) := \frac{q^{-1/24}}{\prod_{n\geqslant 1}(1-q^n)(1-y^2q^n)(1-y^{-2}q^{n-1})}\sum_{m\in\mathbb{Z}} q^{3m^2+m}(y^{6m}-y^{-6m-2}) = \frac{\vartheta_3(2v|2\tau)}{\eta},$$

$$\chi_1^{1/2}(y) := \frac{q^{-5/24}}{\prod_{n\geqslant 1}(1-q^n)(1-y^2q^n)(1-y^{-2}q^{n-1})}\sum_{m\in\mathbb{Z}} q^{3m^2+m}(y^{6m+1}-y^{-6m-3}) = \frac{\vartheta_2(2v|2\tau)}{\eta}. \tag{A3}$$

The right-hand sides can be obtained by noting that these too belong to $\mathcal{T}_{2,-2\pi i\tau}$ (and by checking the equalities at $y=1$, $q^{1/2}$ say). Alternatively, they are reproduced by the quintuple identity (B16).

Similarly, any element of $\mathcal{T}_{2,-2\pi i\tau}$ can be spanned by the N=4 characters $\widehat{\mathrm{ch}}^{\mathrm{NS}}_{0,1/2}$ and $\mathrm{ch}^{\mathrm{NS}}_0$, as was done with the NS orbits in (2.7).

APPENDIX B: FORMULAS FOR THETA FUNCTIONS

These are standard definitions and formulas for theta functions. Some of this material is drawn from Appendix A of Ref. 11.

Definition:

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v|\tau)=\sum_{n\in Z} q^{(1/2)(n-a/2)^2}e^{2\pi i(v-b/2)(n-a/2)}, \tag{B1}$$

where a,b are real and $q=e^{2\pi i\tau}$. We also set $y=e^{2\pi iv}$.

Periodicity properties:

$$\vartheta\left[\begin{smallmatrix}a+2\\b\end{smallmatrix}\right](v|\tau)=\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v|\tau) \quad , \quad \vartheta\left[\begin{smallmatrix}a\\b+2\end{smallmatrix}\right](v|\tau)=e^{i\pi a}\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v|\tau), \tag{B2}$$

$$\vartheta\left[\begin{smallmatrix}-a\\-b\end{smallmatrix}\right](v|\tau)=\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](-v|\tau) \quad , \quad \vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](-v|\tau)=e^{i\pi ab}\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v|\tau) \quad (a,b\in Z). \tag{B3}$$

In the usual Jacobi/Erderlyi notation we have $\vartheta_1=\vartheta\left[\begin{smallmatrix}1\\1\end{smallmatrix}\right]$, $\vartheta_2=\vartheta\left[\begin{smallmatrix}1\\0\end{smallmatrix}\right]$, $\vartheta_3=\vartheta\left[\begin{smallmatrix}0\\0\end{smallmatrix}\right]$, $\vartheta_4=\vartheta\left[\begin{smallmatrix}0\\1\end{smallmatrix}\right]$.

Product formulas:

$$\vartheta_1(v|\tau)=-i\sum_{n\in\mathbb{Z}}(-1)^n q^{(n+1/2)^2/2}y^{n+1/2}=2q^{1/8}\sin[\pi v]\prod_{n=1}^{\infty}(1-q^n)(1-q^n y)(1-q^n y^{-1}),$$

$$\vartheta_2(v|\tau)=\sum q^{(n+1/2)^2/2}y^{n+1/2}=2q^{1/8}\cos[\pi v]\prod(1-q^n)(1+q^n y)(1+q^n y^{-1}),$$

$$\vartheta_3(v|\tau)=\sum q^{n^2/2}y^n=\prod(1-q^n)(1+q^{n-1/2}y)(1+q^{n-1/2}y^{-1}), \tag{B4}$$

$$\vartheta_4(v|\tau)=\sum(-1)^n q^{n^2/2}y^n=\prod(1-q^n)(1-q^{n-1/2}y)(1-q^{n-1/2}y^{-1}).$$

Define also the Dedekind η-function:

$$\eta(\tau)=q^{1/24}\prod_{n=1}^{\infty}(1-q^n)=q^{1/24}\ \vartheta_4(\tau/2|3\tau)=-iq^{1/6}\ \vartheta_1(\tau|3\tau)$$

$$=\frac{1}{\sqrt{3}}\ \vartheta_2\left(\frac{1}{6}\middle|\frac{\tau}{3}\right)=q^{1/24}\sum_{\mathbb{Z}}(-1)^n q^{n(3n+1)/2}. \tag{B5}$$

It is related to the v derivative of ϑ_1:

$$\left.\frac{\partial}{\partial v}\right|_{v=0}\vartheta_1(v)=:\vartheta_1'=2\pi\ \eta^3(\tau) \tag{B6}$$

and satisfies

$$\eta\left(-\frac{1}{\tau}\right)=\sqrt{-i\tau}\ \eta(\tau). \tag{B7}$$

The other v-derivatives yield (at $v=0$):

$$\vartheta_1''=0=\vartheta_2'=\vartheta_3'=\vartheta_4'. \tag{B8}$$

v-periodicity formula:

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]\left(v+\frac{\epsilon_1}{2}\tau+\frac{\epsilon_2}{2}\middle|\tau\right)=e^{-(i\pi\tau/4)\epsilon_1^2-(i\pi\epsilon_1/2)(2v-b)-(i\pi/2)\epsilon_1\epsilon_2}\ \vartheta\left[\begin{smallmatrix}a-\epsilon_1\\b-\epsilon_2\end{smallmatrix}\right](v|\tau), \tag{B9}$$

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v+\tfrac{1}{2})=\vartheta\left[\begin{smallmatrix}a\\b-1\end{smallmatrix}\right](v),$$

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]\left(v+\frac{\tau}{2}\right)=i^b q^{-1/8}y^{-1/2}\ \vartheta\left[\begin{smallmatrix}a-1\\b\end{smallmatrix}\right](v),$$

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]\left(v+\frac{1+\tau}{2}\right)=-i^{b+1}q^{-1/8}y^{-1/2}\ \vartheta\left[\begin{smallmatrix}a-1\\b-1\end{smallmatrix}\right](v), \tag{B10}$$

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v+1)=(-1)^a\ \vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v),$$

$$\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v+\tau)=(-1)^b q^{-1/2}y^{-1}\ \vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v).$$

That is, $\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right]$ is a theta function of characteristic $(0,i\pi a;-2\pi i,-i\pi(\tau+b))$ and degree 1, see Appendix A.

At the half-periods ($v=0$, $\epsilon_{1,2}=0,1$), we are back to the *theta constants* (''Theta Nullwerte''):

$$\begin{aligned}
&\vartheta_1\left(\frac{1}{2}\right)=\vartheta_2, \quad \vartheta_1\left(\frac{\tau}{2}\right)=iq^{-1/8}\,\vartheta_4, \quad \vartheta_1\left(\frac{1+\tau}{2}\right)=q^{-1/8}\,\vartheta_3,\\
&\vartheta_2\left(\frac{1}{2}\right)=0, \quad \vartheta_2\left(\frac{\tau}{2}\right)=q^{-1/8}\,\vartheta_3, \quad \vartheta_2\left(\frac{1+\tau}{2}\right)=-iq^{-1/8}\,\vartheta_4,\\
&\vartheta_3\left(\frac{1}{2}\right)=\vartheta_4, \quad \vartheta_3\left(\frac{\tau}{2}\right)=q^{-1/8}\,\vartheta_2, \quad \vartheta_3\left(\frac{1+\tau}{2}\right)=0,\\
&\vartheta_4\left(\frac{1}{2}\right)=\vartheta_3, \quad \vartheta_4\left(\frac{\tau}{2}\right)=0, \quad \vartheta_4\left(\frac{1+\tau}{2}\right)=q^{-1/8}\,\vartheta_2.
\end{aligned} \tag{B11}$$

At the quarter periods, we have

$$\vartheta_4\left(\frac{\tau}{4}\right)=-i\quad \vartheta_1\left(\frac{\tau}{4}\right)=q^{-1/2}\frac{\eta(\tau/4)\quad\eta}{\eta(\tau/2)}, \quad \vartheta_2\left(\frac{\tau}{4}\right)=\vartheta_3\left(\frac{\tau}{4}\right)=q^{-1/2}\frac{\eta(\tau/2)^2}{\eta(\tau/4)}. \tag{B12}$$

Useful identities:

$$\vartheta_2=2\,\frac{\eta(2\tau)^2}{\eta}, \quad \vartheta_3=\frac{\eta^5}{\eta(2\tau)^2\quad\eta(\tau/2)^2}, \quad \vartheta_4=\frac{\eta(\tau/2)^2}{\eta}, \tag{B13}$$

$$\vartheta_2\vartheta_3\vartheta_4=2\quad\eta^3,$$

$$\vartheta_3(z|\tau)\quad\vartheta_3(z'|\tau)+\vartheta_2(z|\tau)\quad\vartheta_2(z'|\tau)=\vartheta_3\left(\frac{z+z'}{2}\middle|\frac{\tau}{2}\right)\quad\vartheta_3\left(\frac{z-z'}{2}\middle|\frac{\tau}{2}\right),$$

$$\vartheta_3(z|\tau)\quad\vartheta_3(z'|\tau)-\vartheta_2(z|\tau)\quad\vartheta_2(z'|\tau)=\vartheta_4\left(\frac{z+z'}{2}\middle|\frac{\tau}{2}\right)\quad\vartheta_4\left(\frac{z-z'}{2}\middle|\frac{\tau}{2}\right),$$

$$\vartheta_2(v|\tau)^4-\vartheta_1(v|\tau)^4=\vartheta_3(v|\tau)^4-\vartheta_4(v|\tau)^4. \tag{B14}$$

For $v=0$, the latter is but Jacobi's *abstruse identity*,

$$\vartheta_3^4=\vartheta_2^4+\vartheta_4^4. \tag{B15}$$

A more elaborate formula is the *quintuple identity*,

$$\begin{aligned}
&\sum_{n\in\mathbb{Z}}(-1)^n q^{(3n^2+n)/2}(y^{3n+1/2}+y^{-3n-1/2})\\
&\quad=(y^{1/2}+y^{-1/2})\prod_{n\geqslant 1}(1-q^n)(1+yq^n)(1+y^{-1}q^n)(1-y^2q^{2n-1})(1-y^{-2}q^{2n-1})\\
&\quad=(y^{1/2}+y^{-1/2})\prod_{n\geqslant 1}(1-q^n)\frac{(1-y^2q^n)(1-y^{-2}q^n)}{(1-yq^n)(1-y^{-1}q^n)}.
\end{aligned} \tag{B16}$$

Here are few instances of *Riemann addition formulas:*

$$\vartheta_3(u+v)\vartheta_3(u-v)\vartheta_3^2=\vartheta_3(u)^2\vartheta_3(v)^2+\vartheta_1(u)^2\vartheta_1(v)^2=\vartheta_4(u)^2\vartheta_4(v)^2+\vartheta_2(u)^2\vartheta_2(v)^2,$$

$$\vartheta_4(u+v)\vartheta_4(u-v)\vartheta_4^2=\vartheta_3(u)^2\vartheta_3(v)^2-\vartheta_2(u)^2\vartheta_2(v)^2=\cdots. \tag{B17}$$

About 20 such formulas can be found on p. 20 of Ref. 12. As special cases ($u=0,1/2$), we recover formulas that generalize Jacobi's abstruse identity:

$$\vartheta_3(v)^2\vartheta_3^2=\vartheta_2(v)^2\vartheta_2^2+\vartheta_4(v)^2\vartheta_4^2,$$

$$\vartheta_4(v)^2\vartheta_3^2=\vartheta_3(v)^2\vartheta_4^2+\vartheta_1(v)^2\vartheta_2^2. \tag{B18}$$

Duplication formulas:

$$\vartheta_2(0|2\tau)=\frac{1}{\sqrt{2}}\sqrt{\vartheta_3^2-\vartheta_4^2},\quad \vartheta_3(0|2\tau)=\frac{1}{\sqrt{2}}\sqrt{\vartheta_3^2+\vartheta_4^2}, \tag{B19}$$

$$\vartheta_4(0|2\tau)=\sqrt{\vartheta_3\vartheta_4},\quad \eta(2\tau)=\sqrt{\frac{\vartheta_2\ \eta}{2}}. \tag{B20}$$

The last two of these are readily seen, while the first two follow from (B13) and from the next properties (most can be derived using the product form for ϑ):

$$\vartheta_2=2q^{1/8}\vartheta_2(\tau|4\tau)=2q^{1/8}\vartheta_3(\tau|4\tau),$$

$$\vartheta_3(v|\tau)=\vartheta_3(2v|4\tau)+\vartheta_2(2v|4\tau),$$

$$\vartheta_4(v|\tau)=\vartheta_3(2v|4\tau)-\vartheta_2(2v|4\tau), \tag{B21}$$

$$\vartheta_3^2-\vartheta_2^2=\vartheta_4(0|\tau/2)^2,$$

$$\vartheta_3^2+\vartheta_2^2=\vartheta_3(0|\tau/2)^2,$$

$$\vartheta_2\vartheta_3=\frac{1}{2}\vartheta_2\left(0\left|\frac{\tau}{2}\right.\right)^2=2q^{1/8}\ \ \vartheta_3\left(\frac{\tau}{2}\middle|2\tau\right)^2=2\left(\ \eta^2/\eta\left(\frac{\tau}{2}\right)\right)^2,$$

$$\vartheta_2\vartheta_4=q^{-1/8}\ \ \vartheta_2\left(\frac{1}{4}\middle|\frac{\tau}{2}\right)^2=2q^{1/8}\ \ \vartheta_3\left(\frac{1+\tau}{2}\middle|2\tau\right)^2=2\left(\ \eta\left(\frac{\tau}{2}\right)\ \ \eta(2\tau)/\eta\right)^2,$$

$$\vartheta_3\vartheta_4=\vartheta_3\left(\frac{1}{4}\middle|\frac{\tau}{2}\right)^2=\vartheta_4(0|2\tau)^2=(\eta^2/\eta(2\tau))^2. \tag{B22}$$

Heat equation:
The ϑ-functions satisfy the following heat equation:

$$\left[\frac{1}{(2\pi i)^2}\frac{\partial^2}{\partial v^2}-\frac{1}{i\pi}\frac{\partial}{\partial\tau}\right]\vartheta\left[\begin{smallmatrix}a\\b\end{smallmatrix}\right](v|\tau)=0, \tag{B23}$$

as well as

$$\frac{1}{4\pi i}\frac{\vartheta_2''}{\vartheta_2}=\partial_\tau\log\vartheta_2=\frac{i\pi}{12}(E_2+\vartheta_3^4+\vartheta_4^4), \tag{B24}$$

$$\frac{1}{4\pi i}\frac{\vartheta_3''}{\vartheta_3}=\partial_\tau \log \vartheta_3=\frac{i\pi}{12}(E_2+\vartheta_2^4-\vartheta_4^4)\,, \tag{B25}$$

$$\frac{1}{4\pi i}\frac{\vartheta_4''}{\vartheta_4}=\partial_\tau \log \vartheta_4=\frac{i\pi}{12}(E_2-\vartheta_2^4-\vartheta_3^4)\,, \tag{B26}$$

where the E_2 is the second Eisenstein series. We note that (B24) can be rewritten as

$$\partial_\tau \log\frac{\vartheta_2}{\eta}=\frac{i\pi}{12}(\vartheta_3^4+\vartheta_4^4)\,, \tag{B27}$$

and more generally for $(a,b)\neq(1,1)$,

$$\partial_\tau \log\frac{\vartheta[{}^a_b]}{\eta}=\frac{i\pi}{12}(\vartheta^4[{}^{a+1}_{b}]-\vartheta^4[{}^{a}_{b+1}]+(-1)^b\vartheta^4[{}^{a+1}_{b+1}])\,. \tag{B28}$$

The Weierstrass function:

$$\wp(z)=4\pi i\ \ \partial_\tau \log\eta(\tau)-\partial_z^2\log\vartheta_1(z)=\frac{1}{z^2}+\mathcal{O}(z^2) \tag{B29}$$

is even and is the unique analytic function on the torus with a double pole at zero.

$$\wp(-z)=\wp(z),\quad \wp(z+1)=\wp(z+\tau)=\wp(z)\,, \tag{B30}$$

$$\wp(z,\tau+1)=\wp(z,\tau),\quad \wp\left(\frac{z}{\tau},-\frac{1}{\tau}\right)=\tau^2\ \ \wp(z,\tau)\,. \tag{B31}$$

The constant of z in (B29) has been chosen so as to cancel the z^0 term in the Laurent expansion, and it equals also

$$4\pi i\ \ \partial_\tau \log\eta(\tau)=\frac{-\pi^2}{3}E_2=\frac{1}{3}\frac{\vartheta_1'''}{\vartheta_1'}. \tag{B32}$$

Alternatively, performing the logarithmic derivative in an appropriate branch, we can express (B29) as

$$\wp(z)=\left(\frac{\vartheta_1'}{\vartheta_3}\right)^2\ \ \left(\frac{\vartheta_3}{\vartheta_1}(z)\right)^2+\text{const}, \tag{B33}$$

where the constant equals

$$\frac{1}{3}\frac{\vartheta_1'''}{\vartheta_1'}-\frac{\vartheta_3''}{\vartheta_3}=-4\pi i\partial_\tau\log\frac{\vartheta_3}{\eta}=\frac{\pi^2}{3}(\vartheta_2^4-\vartheta_4^4).$$

If we divide the intervals $[0,\tau]$ and $[0,1]$ into n parts and consider the regular grid (on the fundamental lattice) marked by the points $(s+r\tau)/n$ for $s,r=0,\ldots,n-1$, the $\wp$-values at these points transform into each other under the action of $\mathrm{SL}(2,\mathbb{Z})$:

$$\wp\left(\frac{s+r\tau}{n},\tau\right)\overset{T}{\to}\wp\left(\frac{(s+r)+r\tau}{n},\tau\right),$$

$$\wp\left(\frac{s+r\tau}{n},\tau\right)\overset{S}{\to}\wp\left(\frac{-r+s\tau}{n\tau},-\frac{1}{\tau}\right)=\tau^2\wp\left(\frac{-r+s\tau}{n},\tau\right). \tag{B34}$$

Putting all these $\wp$-values—except $s=r=0$—into a vector with n^2-1 components, we obtain a vector-valued modular form of weight 2. Summing all components yields 0, as there is no modular form of weight 2:

$$\sum_{r,s}{}' \ \wp\left(\frac{s+r\tau}{n}\right)=0, \tag{B35}$$

where the prime indicates exclusion of $s=r=0$. For $n=2$, this is the well-known identity for the half-periods,

$$\wp(1/2)+\wp(\tau/2)+\wp((1+\tau)/2)=0, \tag{B36}$$

also derivable from (B33).

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A new loop algebra and a corresponding integrable hierarchy, as well as its integrable coupling

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(Received 13 July 2003; accepted 20 August 2003)

A type of new interesting loop algebra $\tilde{G}_M$ $(M=1,2,\ldots)$ with a simple commutation operation just like that in the loop algebra $\tilde{A}_1$ is constructed. With the help of the loop algebra $\tilde{G}_M$, a new multicomponent integrable system, M-AKNS-KN hierarchy, is worked out. As reduction cases, the M-AKNS hierarchy and M-KN hierarchy are engendered, respectively. In addition, the system 1-AKNS-KN, which is a reduced case of the M-AKNS-KN hierarchy above, is a unified expressing integrable model of the AKNS hierarchy and the KN hierarchy. Obviously, the M-AKNS-KN hierarchy is again a united expressing integrable model of the multicomponent AKNS hierarchy (M-AKNS) and the multicomponent KN hierarchy(M-KN). This article provides a simple method for obtaining multicomponent integrable hierarchies of soliton equations. Finally, we work out an integrable coupling of the M-AKNS-KN hierarchy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623000]

I. INTRODUCTION

Searching for new integrable hierarchies of soliton equations has been an important and interesting topic in soliton theory. One took various efficient approaches to have obtained many integrable systems, such as AKNS hierarchy, KN hierarchy, Schrödinger system, and so on.[1–9] As far as the multicomponent integrable hierarchies are concerned, there have been developments such as in Refs. 10 and 11. In Refs. 12 and 13, a systematic method for obtaining the integrable Hamiltonian hierarchies with multipotential functions were presented by constructing some high-dimensional subalgebras of the loop algebra $\tilde{A}_1$ and making use of the Tu scheme.[8,14] However, the results obtained by use of the above method contain the concrete number of potential functions, in general, less than eight. Ma Wenxiu once proposed a method for constructing the multicomponent AKNS hierarchy in Ref. 15, whose number of entries of positive integer is m. In this article, we propose a systematic method for generating multicomponent integrable hierarchies. A type of new interesting loop algebra $\tilde{G}_M$ is first constructed, whose commutation operation is as simple and straightforward as that in the loop algebra $\tilde{A}_1$. As an application example of $\tilde{G}_M$, a M-AKNS-KN hierarchy of soliton equations is obtained by employing the Tu scheme. As its reduction case, a 1-AKNS-KN hierarchy is given, which is a unified expressing integrable model of the celebrated AKNS hierarchy and the KN hierarchy. Obviously, the M-AKNS-KN hierarchy is also a unified expressing integrable model of the multicomponent AKNS hierarchy and the multicomponent KN hierarchy. Finally, a type of integrable coupling of the M-AKNS-KN hierarchy is presented. The approach proposed in the present article can be used generally.

II. A NEW INTERESTING LOOP ALGEBRA $\tilde{G}_M$

Let G_M denote a matrix set as follows:

$$G_M=\{a=(a_{ij})_{M\times 3}=(a_1,a_2,a_3)\}. \tag{1}$$

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Then G_M consists of a linear space, where a_{ij} are real or complex functions, a_i $(i=1,2,3)$ denote the ith column of the matrix, and M stands for an arbitrary positive integer.

Definition 1: Let $\alpha=(\alpha_1,\alpha_2,\ldots,\alpha_M)^T$, $\beta=(\beta_1,\beta_2,\ldots,\beta_M)^T$ be two column vectors, their vector product $\alpha*\beta$ is defined as

$$\alpha*\beta=\beta*\alpha=(\alpha_1\beta_1,\alpha_2\beta_2,\ldots,\alpha_M\beta_M)^T. \tag{2}$$

Introducing the diagonal matrix $\tilde{\alpha}=\mathrm{diag}(\alpha_1,\alpha_2,...,\alpha_M)$, obviously, we have

$$\alpha*\beta=\tilde{\alpha}\beta, \tag{3}$$

where the right-hand side of (3) stands for matrix multiplication.

Definition 2: Set $a=(a_1,a_2,a_3)$, $b=(b_1,b_2,b_3)$ to be both elements of G_M, and define a commutation operation $[a,b]$ as

$$[a,b]=(a_2*b_3-a_3*b_2,\,2(a_1*b_2-a_2*b_1),\,2(a_3*b_1-a_1*b_3)). \tag{4}$$

It is easy to verify that the operation (4) is linear and antisymmetric. Furthermore, a direct calculation gives

$$[[a,b],c]+[[b,c],a]+[[c,a],b]=0, \tag{5}$$

i.e., the operation (4) satisfies the Jacobian identity, where $a,b,c\in G_M$. Therefore, G_M is a Lie algebra with the commutation operation (4), whose dimensional number in the real region is $3M$, that is, $\dim G_M=3M$. Denote

$$\tilde{G}_M=\{a\lambda^m,\ a\in G_M,\ m=0,\pm1,\pm2,\ldots\} \tag{6}$$

with the operation

$$[a\lambda^m,b\lambda^n]=[a,b]\lambda^{m+n},\quad a,b\in G_M. \tag{7}$$

Then $\tilde{G}_M$ is a loop algebra.

Since $\tilde{G}_1$ is equal to $\tilde{A}_1$, we conclude that $\tilde{G}_M$ is an extension of the loop algebra $\tilde{A}_1$.

We find $\tilde{G}_M$ has two features

(i) The commutation operation is the same, simple and straightforward, as that in the loop algebra $\tilde{A}_1$;

(ii) By means of $\tilde{G}_M$, we proceed to simple calculations to be able to obtain various multicomponent integrable systems.

Consider linear isospectral problems as follows:

$$\begin{gathered}\phi_x=[U,\phi],\ \ \lambda_t=0,\phi,U,V\in\tilde{G}_M,\\ \phi_t=[V,\phi],\end{gathered}\tag{8}$$

whose compatibility gives rise to

$$\begin{gathered}\phi_{xt}=[U_t,\phi]+[U,[V,\phi]]=\phi_{tx}=[V_x,\phi]+[V,[U,\phi]],\\ [U_t,\phi]-[V_x,\phi]+[U,[V,\phi]]+[V,[\phi,U]]=0.\end{gathered}\tag{9}$$

By employing (5), the formula (9) can be rewritten as

$$[U_t,\phi]-[V_x,\phi]+[[U,V],\phi]=0.\tag{10}$$

Since ϕ is arbitrary, a condition of (10) holds if and only if the following equation does:

$$U_t-V_x+[U,V]=0.\tag{11}$$

Hence, the compatibility of (8) leads to the zero-curvature equation (11).

III. A MULTICOMPONENT INTEGRABLE HIERARCHY—M-AKNS-KN HIERARCHY

Consider the following isospectral problem

$$\begin{gathered}\phi_x=[U,\phi],\ \ \lambda_t=0,\\ U=(\lambda^2 I_M,\ u_1+\lambda u_3,\ u_2+\lambda u_4),\end{gathered}\tag{12}$$

where

$$I_M=\begin{pmatrix}1\\1\\\vdots\\1\end{pmatrix}_{M\times 1},\quad u_i=\begin{pmatrix}u_{i1}\\u_{i2}\\\vdots\\u_{iM}\end{pmatrix},\ \ i=1,2,3,4.$$

To derive a related soliton hierarchy, we first solve the adjoint equation

$$V_x=[U,V].\tag{13}$$

We assume that a solution V is given by

$$V=\sum_{m=0}^{\infty}(a(0,m)+\lambda a(1,m),b(0,m)+\lambda b(1,m),c(0,m)+\lambda c(1,m))\lambda^{-2m},$$

where

$$a(0,m)=\begin{pmatrix}a_{m1}^{(0)}\\a_{m2}^{(0)}\\\vdots\\a_{mM}^{(0)}\end{pmatrix},\quad a(1,m)=\begin{pmatrix}a_{m1}^{(1)}\\a_{m2}^{(1)}\\\vdots\\a_{mM}^{(1)}\end{pmatrix},\ldots.$$

Then, the adjoint equation (13) is equivalent to

$$
\begin{aligned}
b(1,m+1)&=\tfrac{1}{2}b_x(1,m)+u_1*a(1,m)+u_3*a(0,m),\\
c(1,m+1)&=-\tfrac{1}{2}c_x(1,m)+u_2*a(1,m)+u_4*a(0,m),\\
a_x(0,m)&=u_1*c(0,m)-u_2*b(0,m)+u_3*c(1,m+1)-u_4*b(1,m+1),\\
a_x(1,m)&=u_1*c(1,m)-u_2*b(1,m)+u_3*c(0,m)-u_4*b(0,m),\\
b(0,m+1)&=u_3*a(1,m+1)+\tfrac{1}{2}b_x(0,m)+u_1*a(0,m),\\
c(0,m+1)&=u_4*a(1,m+1)-\tfrac{1}{2}c_x(0,m)+u_2*a(0,m),\\
b(1,0)&=c(1,0)=a(1,0)=b(0,0)=c(0,0)=0,\\
a(0,0)&=\beta=(\beta_1,\beta_2,\ldots,\beta_M)^T,\quad b(1,1)=\beta*u_3,\\
c(1,1)&=\beta*u_4,\quad b(0,1)=\beta*u_1,\quad c(0,1)=\beta*u_2.
\end{aligned}
\tag{14}
$$

Note

$$
V_+^{(n)}=\sum_{m=0}^{n}(a(0,m)+\lambda a(1,m),b(0,m)+\lambda b(1,m),c(0,m)+\lambda c(1,m))\lambda^{2n-2m},
$$

$$
V_-^{(n)}=\lambda^{2n}V-V_+^{(n)}.
$$

Then (13) can be written as

$$
-V_{+x}^{(n)}+[U,V_+^{(n)}]=V_{-x}^{(n)}-[U,V_-^{(n)}]. \tag{15}
$$

It is easy to find that the terms on the left-hand side in (15) are of degree$\geqslant 0$, while the terms on the right-hand side are of degree$\leqslant 0$. Therefore, we find

$$
\begin{aligned}
-V_{+x}^{(n)}+[U,V_+^{(n)}]=&(u_4*b(1,n+1)-u_3*c(1,n+1),\\
&2u_3*a(1,n+1)-2b(0,n+1)-2b(1,n+1)\lambda,\\
&2c(0,n+1)-2u_4*a(1,n+1)+2c(1,n+1)\lambda).
\end{aligned}
$$

Taking $V^{(n)}=V_+^{(n)}+(\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1)),0,0)=V_+^{(n)}+(-a(0,n)+\partial^{-1}(u_1*c(0,n)-u_2*b(0,n))$, it is easy to compute that

$$
-V_x^{(n)}+[U,V^{(n)}]=(O,A,B),
$$

with

$$
\begin{aligned}
O&=\underbrace{(0,0,\ldots,0)^T}_{M},\\
A&=-2b(0,n+1)-2u_1*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))+2u_3*\partial^{-1}(u_1*c(1,n+1)\\
&\quad-u_2*b(1,n+1)+u_3*c(0,n+1)-u_4*b(0,n+1))-2\lambda b(1,n+1)\\
&\quad-2\lambda u_3*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1)),\\
B&=2c(0,n+1)+2u_2*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))-2u_4*\partial^{-1}(u_1*c(1,n+1)\\
&\quad-u_2*b(1,n+1)+u_3*c(0,n+1)-u_4*b(0,n+1))+2\lambda c(1,n+1)\\
&\quad+2\lambda u_4*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1)).
\end{aligned}
$$

Thus, the compatibility of the following Lax pair,

$$\phi_x=[U,\phi],\quad \lambda_t=0,$$

$$\phi_t=[V^{(n)},\phi],$$

leads to the zero-curvature equation

$$U_t-V_x^{(n)}+[U,V^{(n)}]=0, \tag{16}$$

which admits the Lax integrable system as follows:

$$\begin{aligned}
u_t&=((u_1,u_2,u_3,u_4))_t^T\\
&=\begin{pmatrix} A\\ B\\ 2b(1,n+1)+2u_3*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))\\ -2c(1,n+1)-2u_4*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))\end{pmatrix}\\
&=\begin{pmatrix} -2u_1*\partial^{-1}u_3*-2u_3*\partial^{-1}u_1* & 2u_3*\partial^{-1}u_2*+2u_1*\partial^{-1}u_4* & -2u_3*\partial^{-1}u_3* & 2I_M*+2u_3*\partial^{-1}u_4*\\ 2u_2*\partial^{-1}u_3*+2u_4*\partial^{-1}u_1* & -2u_2*\partial^{-1}u_4*-2u_4*\partial^{-1}u_2* & -2I_M*+2u_4*\partial^{-1}u_3* & -2u_4*\partial^{-1}u_4*\\ -2u_3*\partial^{-1}u_3* & 2I_M*+2u_3*\partial^{-1}u_4* & 0 & 0\\ -2I_M*+2u_4*\partial^{-1}u_3* & -2u_4*\partial^{-1}u_4* & 0 & 0\end{pmatrix}\\
&\quad\times\begin{pmatrix} c(1,n+1)\\ b(1,n+1)\\ c(0,n+1)\\ b(0,n+1)\end{pmatrix}\\
&\overset{(3)}{=}\begin{pmatrix} -2\tilde u_1\partial^{-1}\tilde u_3-2\tilde u_3\partial^{-1}\tilde u_1 & 2\tilde u_3\partial^{-1}\tilde u_2+2\tilde u_1\partial^{-1}\tilde u_4 & -2\tilde u_3\partial^{-1}\tilde u_3 & 2I+2\tilde u_3\partial^{-1}\tilde u_4\\ 2\tilde u_2\partial^{-1}\tilde u_3+2\tilde u_4\partial^{-1}\tilde u_1 & -2\tilde u_2\partial^{-1}\tilde u_4-2\tilde u_4\partial^{-1}\tilde u_2 & -2I+2\tilde u_4\partial^{-1}\tilde u_3 & -2\tilde u_4\partial^{-1}\tilde u_4\\ -2\tilde u_3\partial^{-1}\tilde u_3 & 2I+2\tilde u_3\partial^{-1}\tilde u_4 & 0 & 0\\ -2I+2\tilde u_4\partial^{-1}\tilde u_3 & -2\tilde u_4\partial^{-1}\tilde u_4 & 0 & 0\end{pmatrix}\\
&\quad\times\begin{pmatrix} c(1,n+1)\\ b(1,n+1)\\ c(0,n+1)\\ b(0,n+1)\end{pmatrix}=J_1\begin{pmatrix} c(1,n+1)\\ b(1,n+1)\\ c(0,n+1)\\ b(0,n+1)\end{pmatrix}
\end{aligned} \tag{17}$$

$$\begin{aligned}
&\overset{(14)}{=}\begin{pmatrix} b_x(0,n)+2u_1*\partial^{-1}(u_1*c(0,n)-u_2*b(0,n))\\ c_x(0,n)-2u_2*\partial^{-1}(u_1*c(0,n)-u_2*b(0,n))\\ 2b(1,n+1)-2u_3*\partial^{-1}(u_3*c(1,n+1)-u_4*b(1,n+1))\\ -2c(1,n+1)+2u_4*\partial^{-1}(u_3*c(1,n+1)-u_4*b(1,n+1))\end{pmatrix}\\
&=\begin{pmatrix} 2u_1*\partial^{-1}u_1* & \partial-2u_1*\partial^{-1}u_2* & 0 & 0\\ \partial-2u_2*\partial^{-1}u_1* & 2u_2*\partial^{-1}u_2* & 0 & 0\\ 0 & 0 & -2u_3*\partial^{-1}u_3* & 2I_m*+2u_3*\partial^{-1}u_4*\\ 0 & 0 & -2I_M*+2u_4*\partial^{-1}u_3* & -2u_4*\partial^{-1}u_4*\end{pmatrix}\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix}\\
&=\begin{pmatrix} 2\tilde u_1\partial^{-1}\tilde u_1 & \partial-2\tilde u_1\partial^{-1}\tilde u_2 & 0 & 0\\ \partial-2\tilde u_2\partial^{-1}\tilde u_1 & 2\tilde u_2\partial^{-1}\tilde u_2 & 0 & 0\\ 0 & 0 & -2\tilde u_3\partial^{-1}\tilde u_3 & 2I+2\tilde u_3\partial^{-1}\tilde u_4\\ 0 & 0 & -2I+2\tilde u_4\partial^{-1}\tilde u_3 & -2\tilde u_4\partial^{-1}\tilde u_4\end{pmatrix}\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix}=J_2\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix},
\end{aligned} \tag{18}$$

where

$$A=2b(0,n+1)+2u_1*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))-2u_3*\partial^{-1}(u_1*c(1,n+1)$$
$$-u_2*b(1,n+1)+u_3*c(0,n+1)-u_4*b(0,n+1)),$$

$$B=-2c(0,n+1)-2u_2*\partial^{-1}(u_4*b(1,n+1)-u_3*c(1,n+1))+2u_4*\partial^{-1}(u_1*c(1,n+1)$$
$$-u_2*b(1,n+1)+u_3*c(0,n+1)-u_4*b(0,n+1)),$$

where I means M degree unit matrix.

From (14), we can obtain the 4×4 matrix operator $L=(l_{ij})_{4\times4}$,

$$l_{11}=l_{12}=l_{14}=l_{21}=l_{22}=l_{23}=0,\ l_{13}=l_{24}=I,$$

$$l_{31}=-\frac{\partial}{2}+\tilde{u}_2\partial^{-1}\tilde{u}_1-\frac{1}{2}\tilde{u}_4\partial^{-1}\tilde{u}_3\partial+\tilde{u}_4\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_1,$$

$$l_{32}=-\tilde{u}_2\partial^{-1}\tilde{u}_2-\tfrac{1}{2}\tilde{u}_4\partial^{-1}\tilde{u}_4\partial-\tilde{u}_4\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_2,$$

$$l_{33}=\tilde{u}_2\partial^{-1}\tilde{u}_3+\tilde{u}_4\partial^{-1}\tilde{u}_1+\tilde{u}_4\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_3,$$

$$l_{34}=-\tilde{u}_2\partial^{-1}\tilde{u}_4-\tilde{u}_4\partial^{-1}\tilde{u}_2-\tilde{u}_4\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_4,$$

$$l_{41}=\tilde{u}_1\partial^{-1}\tilde{u}_1-\tfrac{1}{2}\tilde{u}_3\partial^{-1}\tilde{u}_3\partial+\tilde{u}_3\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_1,$$

$$l_{42}=\frac{\partial}{2}-\tilde{u}_1\partial^{-1}\tilde{u}_2-\frac{1}{2}\tilde{u}_3\partial^{-1}\tilde{u}_4\partial-\tilde{u}_3\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_2,$$

$$l_{43}=\tilde{u}_3\partial^{-1}\tilde{u}_1+\tilde{u}_1\partial^{-1}\tilde{u}_3+\tilde{u}_3\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_3,$$

$$l_{44}=-\tilde{u}_1\partial^{-1}\tilde{u}_4-\tilde{u}_3\partial^{-1}\tilde{u}_2-\tilde{u}_3\partial^{-1}(\tilde{u}_2\tilde{u}_3-\tilde{u}_1\tilde{u}_4)\partial^{-1}\tilde{u}_4.$$

It is easy to verify that L meets

$$J_1L=L^*J_1=J_2,$$
$$\begin{pmatrix} c(1,n+1)\\ b(1,n+1)\\ c(0,n+1)\\ b(0,n+1)\end{pmatrix}=L\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix},\quad \begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix}=L\begin{pmatrix} c(1,n)\\ b(1,n)\\ c(0,n)\\ b(0,n)\end{pmatrix}. \tag{19}$$

Hence, (17) and (18) again can be written as

$$u_t=J_1\begin{pmatrix} c(1,n+1)\\ b(1,n+1)\\ c(0,n+1)\\ b(0,n+1)\end{pmatrix}=J_1L\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix}=J_2\begin{pmatrix} c(0,n)\\ b(0,n)\\ c(1,n+1)\\ b(1,n+1)\end{pmatrix}=J_1L^2\begin{pmatrix} c(1,n)\\ b(1,n)\\ c(0,n)\\ b(0,n)\end{pmatrix}$$
$$=J_1L^n\begin{pmatrix} c(1,1)\\ b(1,1)\\ c(0,1)\\ b(0,1)\end{pmatrix}=J_1L^{2n}\begin{pmatrix} \beta*u_4\\ \beta*u_3\\ \beta*u_2\\ \beta*u_1\end{pmatrix},\quad n\geqslant0. \tag{20}$$

IV. A FEW REDUCTION CASES

Case 1: When $u_3=u_4=0$, we have from the system (17)

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}_t = \begin{pmatrix} 0 & 2I \\ -2I & 0 \end{pmatrix} \begin{pmatrix} c(0,n+1) \\ b(0,n+1) \end{pmatrix},$$

$$\begin{pmatrix} c(0,n+1) \\ b(0,n+1) \end{pmatrix} \overset{(14)}{=} \begin{pmatrix} -\frac{\partial}{2}+\tilde{u}_2\partial^{-1}\tilde{u}_1 & -\tilde{u}_2\partial^{-1}\tilde{u}_2 \\ \tilde{u}_1\partial^{-1}\tilde{u}_1 & \frac{\partial}{2}-\tilde{u}_1\partial^{-1}\tilde{u}_2 \end{pmatrix} \begin{pmatrix} c(0,n) \\ b(0,n) \end{pmatrix}. \tag{21}$$

Obviously, taking $M=1$, the system (21) is just an AKNS hierarchy.[8] Therefore, we call it an M-AKNS hierarchy.

Case 2: When $u_1=u_2=0$, we can take $a(1,m)=b(0,m)=c(0,m)=0 (m=0,1,2,\ldots)$. Then the system (18) reduces to

$$\begin{pmatrix} u_3 \\ u_4 \end{pmatrix}_t = \begin{pmatrix} 2b(1,n+1)-2u_3*\partial^{-1}(u_3*c(1,n+1)-u_4*b(1,n+1)) \\ -2c(1,n+1)+2u_4*\partial^{-1}(u_3*c(1,n+1)-u_4*b(1,n+1)) \end{pmatrix}$$

$$= \begin{pmatrix} b_x(1,n) \\ c_x(1,n) \end{pmatrix} = \begin{pmatrix} 0 & \partial \\ \partial & 0 \end{pmatrix} \begin{pmatrix} c(1,n) \\ b(1,n) \end{pmatrix} = J \begin{pmatrix} c(1,n) \\ b(1,n) \end{pmatrix},$$

$$\begin{pmatrix} c(1,n+1) \\ b(1,n+1) \end{pmatrix} = \begin{pmatrix} -\frac{\partial}{2}-\frac{1}{2}\tilde{u}_4\partial^{-1}\tilde{u}_3\partial & -\frac{1}{2}\tilde{u}_4\partial^{-1}\tilde{u}_4\partial \\ -\frac{1}{2}\tilde{u}_3\partial^{-1}\tilde{u}_3\partial & \frac{\partial}{2}-\frac{1}{2}\tilde{u}_3\partial^{-1}\tilde{u}_4\partial \end{pmatrix} \begin{pmatrix} c(1,n) \\ b(1,n) \end{pmatrix} = L \begin{pmatrix} c(1,n) \\ b(1,n) \end{pmatrix}.$$

Thus,

$$\begin{pmatrix} u_3 \\ u_4 \end{pmatrix}_t = JL^{n-1} \begin{pmatrix} c(1,0) \\ b(1,0) \end{pmatrix}. \tag{22}$$

Taking $M=1$, the system (22) reduces to the famous KN hierarchy, therefore we call (22) an M-KN hierarchy. Summarizing the two cases above, the system (20) is known as an M-AKNS-KN hierarchy of soliton equations, which is a multicomponent integrable system, also a unified integrable model of the multicomponent AKNS hierarchy and the multicomponent KN hierarchy. Obviously, the 1-AKNS-KN hierarchy is a unified expressing integrable model of the well-known AKNS hierarchy and KN hierarchy. This result simplifies the tedious computing courses in Ref. 16.

V. AN INTEGRABLE COUPLING OF THE SYSTEM (20)

A simple method for obtaining integrable couplings was proposed in Ref. 18. In this article, we want to look for a type of integrable coupling of the system (20). To the end, an expanding Lie algebra F_M of the Lie algebra G_M is constructed as follows:

$$F_M=\{a=(a_{ij})_{M\times 5}=(a_1,a_2,a_3,a_4,a_5)\}, \tag{23}$$

with a commutation operation $[a,b]$ defined as

$$[a,b]=(a_2*b_3-a_3*b_2,2(a_1*b_2-a_2*b_1),2(a_3*b_1-a_1*b_3),a_1*b_4-a_4*b_1+a_2*b_5$$
$$-a_5*b_2,a_3*b_4-a_4*b_3+a_5*b_1-a_1*b_5), \tag{24}$$

where $a,b\in F_M$.

In what follows, we omit the symbol $*$ for operation convenience.

A corresponding loop algebra $\tilde{F}_M$ is presented as

$$\tilde{F}_M=\{a\lambda^n, a\in F_M, n=0,\pm 1,\pm 2,\ldots\} \tag{25}$$

with

$$[a\lambda^m, b\lambda^n]=[a,b]\lambda^{m+n},\quad \forall\quad a,b\in F_M \tag{26}$$

whose two subalgebras $\tilde{F}_M(1)$ and $\tilde{F}_M(2)$ are defined as

$$\begin{aligned}\tilde{F}_M(1)&=\{(a_1,a_2,a_3,0,0)\lambda^n\},\\ \tilde{F}_M(2)&=\{(0,0,0,a_4,a_5)\lambda^n\}.\end{aligned} \tag{27}$$

We find that

$$\text{(i)}\ \ \tilde{F}_M(1)\cong\tilde{G}_M,\ \ \tilde{F}_M=\tilde{F}_M(1)\oplus\tilde{F}_M(2),\quad \text{(ii)}\ \ [\tilde{F}_M(1),\tilde{F}_M(2)]\subset\tilde{F}_M(2),$$

where the symbol $\cong$ stands for isomorphic relations.

In terms of (25), an isospectral problem is established:

$$\phi_x=[U,\phi],\ \ U=(\lambda^2 I_M, u_1+\lambda u_3, u_2+\lambda u_4, u_5+\lambda u_6, u_7+\lambda u_8). \tag{28}$$

Set

$$\begin{aligned}V=\sum_{m\geqslant 0}\ &(a(0,m)+\lambda a(1,m), b(0,m)+\lambda b(1,m), c(0,m)\\ &+\lambda c(1,m), d(0,m)+\lambda d(1,m), f(0,m)+\lambda f(1,m)).\end{aligned}$$

Solving the equation similar to (13) yields

$$\begin{aligned}
b(1,m+1)&=\tfrac{1}{2}b_x(1,m)+u_1a(1,m)+u_3a(0,m),\\
c(1,m+1)&=-\tfrac{1}{2}c_x(1,m)+u_2a(1,m)+u_4a(0,m),\\
a_x(0,m)&=u_1c(0,m)-u_2b(0,m)+u_3c(1,m+1)-u_4b(1,m+1),\\
a_x(1,m)&=u_1c(1,m)-u_2b(1,m)+u_3c(0,m)-u_4b(0,m),\\
b(0,m+1)&=u_3a(1,m+1)+\tfrac{1}{2}b_x(0,m)+u_1a(0,m),\\
c(0,m+1)&=u_4a(1,m+1)-\tfrac{1}{2}c_x(0,m)+u_2a(0,m),\\
d_x(0,m)&=-u_5a(0,m)+u_1f(0,m)-u_7b(0,m)+d(0,m+1)\\
&\quad -u_6a(1,m+1)+u_3f(1,m+1)-u_8b(1,m+1),
\end{aligned} \tag{29}$$

$$d_x(1,m)=-u_6a(0,m)-u_5a(1,m)+u_3f(0,m)+u_1f(1,m)-u_8b(0,m)-u_7b(1,m)+d(1,m+1),$$

$$f_x(0,m)=u_2d(0,m)-u_5c(0,m)+u_7a(0,m)+u_4d(1,m+1)$$
$$-u_6c(1,m+1)+u_8a(1,m+1)-f(0,m+1),$$

$$f_x(1,m)=u_4d(0,m)+u_2d(1,m)-u_6c(0,m)-u_5c(1,m)+u_8a(0,m)+u_7a(1,m)-f(1,m+1),$$

$$b(1,0)=c(1,0)=a(1,0)=b(0,0)=c(0,0)=d(0,0)=f(0,0)=f(1,0)=d(1,0)=0,$$

$$a(0,0)=\beta,\ \ b(1,1)=\beta u_3,\ \ c(1,1)=\beta u_4,\ \ a(1,1)=0,\ \ b(0,1)=\beta u_1,$$

$$c(0,1)=\beta u_2,\ \ f(1,1)=\beta u_8,\ \ d(1,1)=\beta u_6,\ \ f(0,1)=\beta u_7,\ \ d(0,1)=\beta u_5.$$

Denoting

$$V_+^{(n)}=\sum_{m=0}^{n}(a(0,m)+\lambda a(1,m),\ \ b(0,m)+\lambda b(1,m),\ \ c(0,m)+\lambda c(1,m),\ \ d(0,m)$$
$$+\lambda d(1,m),\ \ f(0,m)+\lambda f(1,m))\lambda^{2n-2m},$$

$$V_-^{(n)}=\lambda^{2n}V-V_+^{(n)},$$

then a direct calculation reads

$$-V_{+x}^{(n)}+[U,V_+^{(n)}]=(u_4b(1,n+1)-u_3c(1,n+1),2u_3a(1,n+1)-2b(0,n+1)$$
$$-2b(1,n+1)\lambda,\ \ 2c(0,n)-2u_4a(1,n+1)+2c(1,n+1)\lambda,\ \ -d(0,n+1)$$
$$+u_6a(1,n+1)-u_3f(1,n+1)+u_8b(1,n+1)-d(1,n+1)\lambda,$$
$$-u_4d(1,n+1)+u_6c(1,n+1)-u_8a(1,n+1)+f(0,n+1)+f(1,n+1)\lambda).$$

Taking $V^{(n)}=V_+^{(n)}+(\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1)),0,0)$, it is easy to find that

$$-V_x^{(n)}+[U,V^{(n)}]=(O,A,B,C,D),$$

where O, A, B are the same with those in (17), and

$$C=-u_5\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))-d(0,n+1)+u_6a(1,n+1)-u_3f(1,n+1)$$
$$+u_8b(1,n+1)+\lambda(-u_6\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))-d(1,n+1)),$$

$$D=u_7\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))-u_4d(1,n+1)+u_6c(1,n+1)-u_8a(1,n+1)-f(0,n$$
$$+1)+\lambda(u_8\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))+f(1,n+1)).$$

Thus, the zero curvature equation similar to (16) gives

$$u_t=(u_1,u_2,u_3,u_4,u_5,u_6,u_7,u_8)_t^T$$

$$=\begin{pmatrix} A \\ B \\ 2b(1,n+1)+2u_3\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1)) \\ -2c(1,n+1)-2u_4\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1)) \\ u_5\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))+d(0,n+1)-u_6a(1,n+1)+u_3f(1,n+1)-u_8b(1,n+1) \\ u_6\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1))+d(1,n+1) \\ -u_7\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1)+u_4d(1,n+1)-u_6c(1,n+1)+u_8a(1,n+1)-f(0,n+1) \\ -u_8\partial^{-1}(u_4b(1,n+1)-u_3c(1,n+1)-f(1,n+1) \end{pmatrix}$$

$$=\begin{pmatrix} -u_1\partial^{-1}u_3-2u_3\partial^{-1}u_1 & 2u_3\partial^{-1}u_2+2u_1\partial^{-1}u_4 & -2u_3\partial^{-1}u_3 & 2+2u_3\partial^{-1}u_4 & 0 & 0 & 0 & 0 \\ 2u_2\partial^{-1}u_3+2u_4\partial^{-1}u_1 & -2u_2\partial^{-1}u_4-2u_4\partial^{-1}u_2 & -2+2u_4\partial^{-1}u_3\partial & -2u_4\partial^{-1}u_4 & 0 & 0 & 0 & 0 \\ -2u_3\partial^{-1}u_3 & 2+2u_3\partial^{-1}u_4 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2+2u_4\partial^{-1}u_3 & -2u_4\partial^{-1}u_4 & 0 & 0 & 0 & 0 & 0 & 0 \\ -u_5\partial^{-1}u_3-u_6\partial^{-1}u_1 & u_5\partial^{-1}u_4+u_6\partial^{-1}u_2-u_8 & -u_6\partial^{-1}u_3 & u_6\partial^{-1}u_4 & u_3 & 0 & 0 & 1 \\ -u_6\partial^{-1}u_3 & u_6\partial^{-1}u_4 & 0 & 0 & 0 & 0 & 1 & 0 \\ u_7\partial^{-1}u_3-u_3+u_8\partial^{-1}u_1 & -u_7\partial^{-1}u_4-u_8\partial^{-1}u_2 & u_8\partial^{-1}u_3 & -u_8\partial^{-1}u_4 & 0 & -1 & u_4 & 0 \\ u_8\partial^{-1}u_3 & -u_8\partial^{-1}u_4 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\times\begin{pmatrix} c(1,n+1) \\ b(1,n+1) \\ c(0,n+1) \\ b(0,n+1) \\ f(1,n+1) \\ f(0,n+1) \\ d(1,n+1) \\ d(0,n+1) \end{pmatrix}$$

$$=J_1\begin{pmatrix} c(1,n+1) \\ b(1,n+1) \\ c(0,n+1) \\ b(0,n+1) \\ f(1,n+1) \\ f(0,n+1) \\ d(1,n+1) \\ d(0,n+1) \end{pmatrix}. \tag{30}$$

From (29), we can present a recurrence operator

$$L=\begin{pmatrix} l_{11} & l_{12} & l_{13} & l_{14} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & l_{23} & l_{24} & 0 & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & l_{34} & 0 & 0 & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ l_{61} & l_{62} & l_{63} & l_{64} & -\partial & u_2 & 0 & u_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ l_{81} & l_{82} & l_{83} & l_{84} & -u_2 & 0 & -u_3 & 0 \end{pmatrix},$$

with

$$
\begin{aligned}
l_{61}&=u_8\partial^{-1}\left(-\frac{u_3}{2}\partial+(u_2u_3-u_1u_4)\partial^{-1}u_1\right)-u_5+u_7\partial^{-1}u_1,\\
l_{62}&=u_8\partial^{-1}\left((u_1u_4-u_2u_3)\partial^{-1}u_2-\frac{u_4}{2}\partial\right),\\
l_{63}&=-u_6+u_7\partial^{-1}u_3+u_8\partial^{-1}(u_1+(u_2u_3-u_1u_4)\partial^{-1}u_3),\\
l_{64}&=-u_7\partial^{-1}u_4+u_8\partial^{-1}(-u_2+(u_1u_4-u_2u_3)\partial^{-1}u_4),\\
l_{81}&=-\frac{u_6}{2}\partial^{-1}u_3\partial+(u_6\partial^{-1}(u_2u_3-u_1u_4)+u_5)\partial^{-1}u_1,\\
l_{82}&=u_7-\frac{u_6}{2}\partial^{-1}u_4\partial+(u_6\partial^{-1}(u_1u_4-u_2u_3)-u_5)\partial^{-1}u_2,\\
l_{83}&=u_6\partial^{-1}u_1+(u_6\partial^{-1}(u_2u_3-u_1u_4)+u_5)\partial^{-1}u_3,\\
l_{84}&=u_8-\frac{u_6}{2}\partial^{-1}u_2\partial+(u_6\partial^{-1}(u_1u_4-u_2u_3)-u_5)\partial^{-1}u_4.
\end{aligned}
\tag{31}
$$

Therefore, the system (30) can be written as

$$
u_t=(u_1,\ldots,u_8)_t^T=J_1L^n(\beta u_4,\beta u_3,\beta u_2,\beta u_1,\beta u_8,\beta u_7,\beta u_6,\beta u_5)^T. \tag{32}
$$

In terms of the definition of integrable couplings,[18] we conclude that the system (31) is a multicomponent integrable coupling of the M-AKNS-KN hierarchy of (20).

Remark: We proposed the method for generating multicomponent integrable hierarchies of soliton equations in this article. To the best of our knowledge, this method is new. However, there exists a shortcoming of the method, i.e., the multicomponent integrable systems generated by the method are only Lax integrable. It is desirable to us that these hierarchies obtained are Liouville integrable. This problem is worthwhile studying in the future.

ACKNOWLEDGMENT

The authors are very grateful to the referees for their revised suggestions.

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Kolmogorov entropy of global attractor for dissipative lattice dynamical systems

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(Received 9 June 2003; accepted 9 September 2003)

We consider Kolmogorov's ε-entropy of the global attractor for first and second order dissipative lattice dynamical systems. By using the element decomposition and the covering property of a polyhedron by balls of radii ε in the finite dimensional space, we obtain an estimate of the upper bound for Kolmogorov's ε-entropy of the global attractor. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1626269]

I. INTRODUCTION

Lattice dynamical systems (LDSs) are infinite systems of ordinary differential equations (lattice ODEs) or of difference equations.[1] Lattice systems arise in many applications, for example, in chemical reaction theory,[2] image processing and pattern recognition,[3] material science,[4] biology,[5] electrical engineering,[6] laser systems,[7] etc. LDSs possess their own form, but, in some cases, they arise as spatial discretizations of partial differential equations (PDEs).

It is well known that in many cases the longtime behavior of dynamical systems, generated by evolutionary equations of mathematical physics, can be naturally described in terms of attractors of the corresponding semigroup (see Ref. 8). In LDSs, it is difficult to describe the geometric structure of the attractor and to estimate the dimension of the attractor because, generally, the attractor is infinite dimensional. One possible approach to handle this problem, which has been suggested in Ref. 9, is to estimate Kolmogorov's ε-entropy of the attractor. By definition, Kolmogorov's ε-entropy $K_\varepsilon(\Lambda)$ of an attractor Λ is the logarithm of the minimal number $N_\varepsilon(\Lambda)$ of ε-balls covering the attractor in the phase space.

In this article, we consider Kolmogorov's ε-entropy of the global attractor for first and second order dissipative lattice dynamical systems. By element decomposition and the covering property of a polyhedron by balls of radii ε in the finite dimensional space, we obtain an estimate of the upper bound for Kolmogorov's ε-entropy of the global attractor.

II. PRELIMINARIES

We consider a $(2n+1)$-dimensional regular polyhedron $\Gamma=\{u^*=(u_i)_{|i|\leqslant n}\in R^{2n+1}:|u_i|\leqslant r_0,\ i\in Z\}$ with length $2r_0$. Let $n_\varepsilon(\Gamma)$, $\varepsilon>0$, denote the number of balls of R^{2n+1} of radii $\varepsilon/2$ covering Γ.

It is easy to see that the regular polyhedron Γ can be covered by $([2r_0\sqrt{2n+1}/\varepsilon]+1)^{2n+1}$ ($[m]$ *is the largest integer which is less than or equals to* m) small regular polyhedrons with length $\varepsilon/\sqrt{2n+1}$, and each such small regular polyhedron with length $\varepsilon/\sqrt{2n+1}$ has a circumscribed ball with the same center and radius $\varepsilon/2$. Thus, the number of the balls of radii $\varepsilon/2$ covering Γ is equal to that of regular polyhedrons with length $\varepsilon/\sqrt{2n+1}$, i.e., $n_\varepsilon(\Gamma)=([2r_0\sqrt{2n+1}/\varepsilon]+1)^{2n+1}$.

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We assume that the centers of these $n_\varepsilon(\Gamma)$ circumscribed balls are u_1^*, u_2^*, ..., $u_{n_\varepsilon(\Gamma)}^*$, respectively (in fact, the center of each circumscribed ball is exactly the center of the corresponding small regular polyhedron with length $\varepsilon/\sqrt{2n+1}$).

Theorem 1:[10] *In the* $(2n+1)$*-dimensional space* R^{2n+1}, $n_\varepsilon(\Gamma)=([2r_0\sqrt{2n+1}/\varepsilon]+1)^{2n+1}$ $\varepsilon/2$*-balls centered at* u_1^*, u_2^*, ..., $u_{n_\varepsilon(\Gamma)}^*$ *with radius* $\varepsilon/2$ *can cover the regular polyhedron* $\Gamma=\{u^*=(u_i)_{|i|\leqslant n}:|u_i|\leqslant r_0\}$.

Let M be a metric space and D be a precompact subset of M. For a given $\varepsilon>0$, $N_\varepsilon(D)=N_\varepsilon(D,M)$ denotes the minimal number of ε-balls in M which cover the set D (this number is evidently finite by Hausdorff criteria). By definition, Kolmogorov's ε-entropy of D in M is the following number $K_\varepsilon(D)=K_\varepsilon(D,M)\equiv\ln N_\varepsilon(D)$. For the detail study of this concept, see Ref. 11.

Thus, Kolmogorov's ε-entropy $K_\varepsilon(\Lambda)$ of an attractor Λ is the logarithm of the minimal number $N_\varepsilon(\Lambda)$ of ε-balls covering the attractor in the phase space, i.e.,

$$K_\varepsilon(\Lambda)=\ln N_\varepsilon(\Lambda). \tag{1}$$

Since Λ is compact, (1) is well defined and finite for every $\varepsilon>0$.

III. KOLMOGOROV'S ENTROPY OF ATTRACTOR FOR FIRST ORDER DISSIPATIVE LATTICE DYNAMICAL SYSTEM

We consider the first order dissipative lattice dynamical system

$$\dot{u}_i=\nu(u_{i-1}-2u_i+u_{i+1})-\lambda u_i-f(u_i)+g_i,\quad i\in Z, \tag{2}$$

with the initial data

$$u_i(0)=u_{0,i},\quad i\in Z, \tag{3}$$

where ν, $\lambda>0$, and $g=(g_i)_{i\in Z}\in\ell^2$ are given, and f is a C^1 function satisfying

$$f(s)s\geqslant 0,\quad \forall s\in R. \tag{4}$$

Equation (2) can be regarded as a discrete analog of the following continuous reaction-diffusion equation in R,

$$u_t-\triangle u+\lambda u+f(u)=g(x),\qquad x\in R,$$

which has been widely studied. Equation (2) occurs in a wide variety of applications where the spatial structure has a discrete character. Cellular neural networks with applications to image processing and pattern recognition are just two of many such examples. They also arise in models for the propagation of pulses in myelinated axons where the membrane is excitable only at spatially discrete sites, and in this context, we find much of the early theoretical development. In this case, u_i represents the potential at the ith active site.

We denote by ℓ^2 the Hilbert space defined by $\ell^2=\{u=(u_i)_{i\in Z}:\Sigma_{i\in Z}|u_i|^2<+\infty\}$ with the norm $\|\cdot\|$ and inner product $(\cdot,\cdot)$ by $\|u\|=(\Sigma_{i\in Z}|u_i|^2)^{1/2}$ and $(u,v)=\Sigma_{i\in Z}u_iv_i$ for $u=(u_i)_{i\in Z}$, $v=(v_i)_{i\in Z}\in\ell^2$.

For $u=(u_i)_{i\in Z}\in\ell^2$, $\tilde{f}(u)=(f(u_i))_{i\in Z}$. In the sequel, when no confusion arises we always identify $\tilde{f}$ with f and use the same symbol to denote them. Define a linear operator A on ℓ^2 by $(Au)_i=-(u_{i-1}-2u_i+u_{i+1})$, for each $i\in Z$. Then, system (2) and (3) is equivalent to the following equation with $u=(u_i)_{i\in Z}\in\ell^2$:

$$\dot{u}=-\nu Au-\lambda u-f(u)+g,\quad t>0, \tag{5}$$

and

$$u(0)=u_0\in\ell^2. \tag{6}$$

We know from Ref. 12 that the existence and upper semicontinuity of the global attractor for the semigroup

$$S(t):u(0)=u_0\in\ell^2\to u(t)=S(t)u(0)=u(t)\in\ell^2,\quad t\geqslant 0,$$

defined by the solutions of system (5) and (6) and the following facts.

Lemma 3.1:[12] *Assume that (4) holds and* $g\in\ell^2$. *Then system (5) and (6) has an absorbing set* $O=\{u\in\ell^2:\|u\|\leqslant M_0\}=O(0,M_0)\subset\ell^2$ *(a bounded ball centered at* 0 *and of radius* M_0*), where* $M_0=\sqrt{2}\|g\|/\lambda$ *is a constant depending on the data* $(\lambda,\|g\|)$ *only, and system (5) and (6) has a connected global attractor* Λ.

Lemma 3.2:[12] *Assume that (4) holds,* $g\in\ell^2$ *and* $u_0\in O$ *[the bounded absorbing set of system (5) and (6)]. Then for every* $\varepsilon>0$, *there exist* $T(\varepsilon)$ *and* $J(\varepsilon)$ *such that the solution* u *of problem (5) and (6) satisfies* $(\Sigma_{|i|\geqslant J(\varepsilon)}u_i^2(t))^{1/2}\leqslant\varepsilon/2$, $\forall t\geqslant T(\varepsilon)$, *where* $J(\varepsilon)$ *and* $T(\varepsilon)$ *depend on* ε, g, *and* λ, $J(\varepsilon)$ *is the least integer satisfying the inequality*

$$\frac{C}{J}+\frac{1}{\lambda}\sum_{|i|\geqslant J}g_i^2\leqslant\frac{\lambda\varepsilon}{2}, \tag{7}$$

where C *is a constant independent of* J, $g=(g_i)_{i\in Z}$.

Lemma 3.3: Assume that (4) holds and $g\in\ell^2$. *Then the global attractor* Λ *of system (5) and (6) satisfies* $\Lambda\subset O=O(0,M_0)$, *and for each* $u=(u_i)_{i\in Z}\in\Lambda$, $(\Sigma_{|i|\geqslant J(\varepsilon)}u_i^2(t))^{1/2}<\varepsilon/2$, *where* $J(\varepsilon)$ *is defined by (7).*

Proof: It is proved by $\Lambda=\omega(O)$ and Lemma 3.2.

Theorem 2: *For* $\varepsilon>0$, *the global attractor* Λ *of system (5) and (6) can be covered by* $n_\varepsilon(\Lambda)=([2M_0\sqrt{2J(\varepsilon)+1}/\varepsilon]+1)^{2J(\varepsilon)+1}$ ε*-balls of* ℓ^2.

Proof: For $u=(u_i)_{i\in Z}\in\Lambda$, we decompose u into a sum of two parts:

$$u=(u_i)_{i\in Z}=(w_i)_{i\in Z}+(v_i)_{i\in Z}=w+v,$$

where

$$w_i=\begin{cases}u_i,&|i|\leqslant J(\varepsilon),\\0,&|i|>J(\varepsilon),\end{cases}\qquad v_i=\begin{cases}0,&|i|\leqslant J(\varepsilon),\\u_i,&|i|>J(\varepsilon).\end{cases}$$

By Lemma 3.3, we have that $|w_i|\leqslant M_0$ and $\|v\|\leqslant\varepsilon/2$.

By Theorem 1, $n_\varepsilon(\Gamma)=([2M_0\sqrt{2J(\varepsilon)+1}/\varepsilon]+1)^{2J(\varepsilon)+1}$ $\varepsilon/2$-balls centered at $u_j^*=(u_{j,i}^*)_{|i|\leqslant J(\varepsilon)}$, $j=1,2,\ldots,n_\varepsilon(\Gamma)$, respectively, with radius $\varepsilon/2$ can cover the $(2J(\varepsilon)+1)$-dimensional polyhedron $\Gamma=\{w=(w_i)_{|i|\leqslant J(\varepsilon)}\in R^{2J(\varepsilon)+1}:|w_i|\leqslant M_0\}$.

Set $w_{j0}=(w_{j0,i})_{i\in Z}\in\ell^2$, where

$$w_{j0,i}=\begin{cases}u_{j,i}^*,&|i|\leqslant J(\varepsilon),\\0,&|i|>J(\varepsilon),\end{cases}\qquad j=1,2,\ldots,n_\varepsilon(\Gamma).$$

Then for $w=(w_i)_{i\in Z}$ above, there exists j such that

$$\|w-w_{j0}\|<\frac{\varepsilon}{2}.$$

Thus,

$$\|u-w_{j0}\|=\|w-w_{j0}+v\|\leqslant\|w-w_{j0}\|+\|v\|<\frac{\varepsilon}{2}+\frac{\varepsilon}{2}=\varepsilon.$$

Hence the global attractor Λ of system (5) and (6) can be covered by $n_\varepsilon(\Gamma)=([2M_0\sqrt{2J(\varepsilon)+1}/\varepsilon]+1)^{2J(\varepsilon)+1}=n_\varepsilon(\Lambda)$ ε-balls centered at $w_{j0}=(w_{j0,i})_{i\in Z}$ $(j=1,2,...,n_\varepsilon(\Gamma))$ with radius ε, respectively.

By Theorem 2 and the definition of Kolmogorov's ε-entropy, we can easily obtain the following theorem.

Theorem 3: *Assume that (4) holds and $g\in\ell^2$. Then Kolmogorov's ε-entropy of the global attractor Λ of system (5) and (6) has an upper bound $(2J(\varepsilon)+1)\ln([2M_0\sqrt{2J(\varepsilon)+1}/\varepsilon]+1)$, where $M_0=\sqrt{2}\|g\|/\lambda$ and $J(\varepsilon)$ is defined by (7).*

IV. KOLMOGOROV'S ENTROPY OF ATTRACTOR FOR SECOND ORDER DISSIPATIVE LATTICE DYNAMICAL SYSTEMS

We consider the second order dissipative lattice dynamical system

$$\ddot{u}_i+h(\dot{u}_i)-(u_{i-1}-2u_i+u_{i+1})+\lambda u_i+f(u_i)=g_i,\quad i\in Z, \tag{8}$$

with the initial conditions

$$u_i(0)=u_{i,0},\quad \dot{u}_i(0)=u_{1i,0},\quad i\in Z, \tag{9}$$

where $\lambda>0$, $g=(g_i)_{i\in Z}\in\ell^2$ and f, $h\in C^1(R,R)$ satisfy

$$f(0)=0,\quad f(s)s\geqslant \nu G(s)\geqslant 0,\quad \forall s\in R, \tag{10}$$

$$h(0)=0,\quad 0<\alpha\leqslant h'(s)\leqslant\beta<+\infty,\quad \forall s\in R, \tag{11}$$

here ν, α, β are positive constants and $G(s)=\int_0^s f(t)dt$, $s\in R$.

Equation (8) can be regarded as a model of coupled nonlinear oscillators and as a discrete analog of the following continuous damped semilinear wave equation in R:

$$u_{tt}+h(u_t)-u_{xx}+\lambda u+f(u)=g,$$

which arises in wave phenomena of various areas in mathematical physics.

Let $\ell^2=\{u=(u_i)_{i\in Z}:\Sigma_{i\in Z}|u_i|^2<\infty\}$. Define the linear operators B, A from ℓ^2 to ℓ^2 as follows. For any $u=(u_i)_{i\in Z}\in\ell^2$,

$$\begin{aligned}(Bu)_i&=u_{i+1}-u_i,\\ (Au)_i&=-(u_{i-1}-2u_i+u_{i+1}),\end{aligned}\quad \forall i\in Z. \tag{12}$$

For any two elements of ℓ^2, $u=(u_i)_{i\in Z}$, $v=(v_i)_{i\in Z}\in\ell^2$, define bilinear forms as

$$(u,v)=\Sigma_{i\in Z}u_iv_i,\qquad \|u\|^2=(u,u)=\Sigma_{i\in Z}|u_i|^2;$$

$$(u,v)_\lambda=(Bu,Bv)+\lambda(u,v), \tag{13}$$

$$\|u\|_\lambda^2=(u,u)_\lambda=\|Bu\|^2+\lambda\|u\|^2=\Sigma_{i\in Z}(|u_{i+1}-u_i|^2+\lambda|u_i|^2).$$

It is easy to check that the above two bilinear forms $(\cdot,\cdot)$ and $(\cdot,\cdot)_\lambda$ in (13) are both the inner products, moreover, the norms $\|\cdot\|$ and $\|\cdot\|_\lambda$ are equivalent to each other. Denote by ℓ^2, ℓ_λ^2 the spaces with the inner products and norms in (13), respectively, $\ell^2=(\ell^2,(\cdot,\cdot),\|\cdot\|)$, $\ell_\lambda^2=(\ell^2,(\cdot,\cdot)_\lambda,\|\cdot\|_\lambda)$, then ℓ^2 and ℓ_λ^2 are Hilbert spaces.

Let $E=\ell_\lambda^2\times\ell^2$, endowed with the inner product and norm as for $\varphi_j=(u^{(j)},v^{(j)})=((u_i^{(j)}),(v_i^{(j)}))_{i\in Z}\in E$, $j=1,2$,

$$(\varphi_1,\varphi_2)_E=(u^{(1)},u^{(2)})_\lambda+(v^{(1)},v^{(2)})=\sum_i\ [(Bu^{(1)})_i(Bu^{(2)})_i+\lambda u_i^{(1)}u_i^{(2)}+v_i^{(1)}v_i^{(2)}],$$
$$\|\varphi\|_E^2=(\varphi,\varphi)_E,\quad \forall\varphi\in\ell_\lambda^2\times\ell^2. \tag{14}$$

Equation (8) is written as

$$\ddot{u}+h(\dot{u})+Au+\lambda u+f(u)=g,\quad t>0, \tag{15}$$

and the initial data (9) are

$$u(0)=(u_{i,0})_{i\in Z}=u_0,\quad \dot{u}(0)=(u_{1i,0})_{i\in Z}=u_{10}, \tag{16}$$

where $u=(u_i)_{i\in Z}$, $h(\dot{u})=(h(\dot{u}_i))_{i\in Z}$, $f(u)=(f(u_i))_{i\in Z}$, $g=(g_i)_{i\in Z}$.

Let $v=\dot{u}+pu$, where p is chosen as

$$p=\frac{\alpha\lambda}{\beta^2+4\lambda}>0. \tag{17}$$

Then system (15) and (16) is equivalent to the following initial value problem in Hilbert space E,

$$\dot{\varphi}+C(\varphi)=F(\varphi),\quad \varphi(0)=(u_0,v_0)^T=(u_0,u_{10}+pu_0)^T, \tag{18}$$

where $\varphi=(u,v)^T$, $v=\dot{u}+pu$, $F(\varphi)=(0,-f(u)+g)^T$,

$$C(\varphi)=\begin{pmatrix} pu-v \\ Au+\lambda u+p^2u-pv\end{pmatrix}+\begin{pmatrix} 0 \\ h(v-pu)\end{pmatrix}. \tag{19}$$

From Ref. 13, we know the existence and upper semicontinuity of the global attractor in system (18), and the solutions of system (18) define the following semigroup:

$$S'(t):\varphi(0)=(u_0,v_0)\to\varphi(t)=S'(t)\varphi(0)=(u(t),v(t)),\quad E\to E,\quad t\geqslant 0, \tag{20}$$

where $v(t)=\dot{u}(t)+pu(t)$.

Lemma 4.1:[13] *If (10) and (11) hold and $g\in\ell^2$, then there exists an absorbing set of system (18) in E: $O'=O'_E(0,r_0)$ (a bounded ball centered at 0 with radius r_0), where $r_0^2=2/\alpha\mu\,\|g\|^2$, $\mu=\min\{2\alpha\lambda/\sqrt{\beta^2+4\lambda}(\beta+\sqrt{\beta^2+4\lambda}),\nu p\}$, and there exists a connected global attractor $\Lambda'\subset E$.*

Lemma 4.2:[13] *If (10) and (11) hold $g\in\ell^2$ and $\varphi(0)=(u_0,v_0)\in O'$, then $\forall\varepsilon>0$, there exist $T'(\varepsilon)$ and $J'(\varepsilon)$ such that the solution $\varphi(t)=(\varphi_i)_{i\in Z}=((u_i(t)),(v_i(t)))_{i\in Z}\in E$ of problem (18), $v(t)=\dot{u}(t)+pu(t)$, satisfies*

$$\sum_{|i|\geqslant J'(\varepsilon)}\|\varphi_i(t)\|_E^2=\sum_{|i|\geqslant J'(\varepsilon)}[(Bu(t))_i{}^2+\lambda u_i(t)^2+v_i(t)^2]\leqslant\varepsilon^2/4,\forall t\geqslant T', \tag{21}$$

where $(Bu(t))_i=u_{i+1}(t)-u_i(t)$, and $J'(\varepsilon)$ is the least integer satisfying the inequality

$$\frac{8C_0r_0^2}{J'}+\frac{1}{\alpha}\sum_{|i|\geqslant J'}g_i^2\leqslant\varepsilon^2/4, \tag{22}$$

where C_0 is a constant independent of J', $g=(g_i)_{i\in Z}$.

Lemma 4.3: If (10) and (11) hold and $g\in\ell^2$, then the global attractor Λ' of system (18) satisfies $\Lambda'\subset O'=O'(0,r_0)\subset E$, and for each $\varphi=(\varphi_i)_{i\in Z}\in\Lambda'$,

$$\sum_{|i|\geqslant J'(\varepsilon)} \|\varphi_i(t)\|_E^2 = \sum_{|i|\geqslant J'(\varepsilon)} [(Bu(t))_i{}^2 + \lambda u_i(t)^2 + v_i(t)^2] \leqslant \varepsilon^2/4.$$

Proof: By $\Lambda' = \omega(O')$ and Lemma 4.2, Lemma 4.3 can be easily proved.

Theorem 4: *For given $\varepsilon > 0$, the global attractor Λ' of system (18) can be covered by $n_\varepsilon(\Lambda') = ([2r_0\sqrt{2J'(\varepsilon)+1}/\sqrt{\lambda}\varepsilon]+1)^{2J'(\varepsilon)+1} \times ([2r_0\sqrt{2J'(\varepsilon)+1}/\varepsilon]+1)^{2J'(\varepsilon)+1}$ ε-balls.*

Proof: For $\forall \varphi = (\varphi_i)_{i\in Z} \in \Lambda'$, we can decompose φ into two parts:

$$\varphi = (\varphi_i)_{i\in Z} = (y_i)_{i\in Z} + (z_i)_{i\in Z} = y + z,$$

where

$$y_i = (a_i, b_i) = \begin{cases} (u_i, v_i), & |i| \leqslant J'(\varepsilon), \\ 0, & |i| > J'(\varepsilon), \end{cases} \qquad z_i = (c_i, d_i) = \begin{cases} 0, & |i| \leqslant J'(\varepsilon), \\ (u_i, v_i), & |i| > J'(\varepsilon). \end{cases}$$

By Lemma 4.3, we know that $\|y\|_E \leqslant r_0$ and $\|z\|_E \leqslant \varepsilon/2$.

By $\|y\|_E \leqslant r_0$, $\|\varphi\|_E^2 = \|(u,v)\|_E^2 = \Sigma_{i\in Z}((Bu)_i^2 + \lambda u_i^2 + v_i^2)$ and $(Bu)_i = u_{i+1} - u_i$, we have

$$r_0^2 \geqslant \|y\|_E^2 = \sum_{|i|\leqslant J'(\varepsilon)} ((a_{i+1} - a_i)^2 + \lambda a_i^2 + b_i^2) \geqslant \lambda \|a\|^2 + \|b\|^2.$$

Therefore, $\|a\| \leqslant r_0/\sqrt{\lambda}$, $\|b\| \leqslant r_0$. Then $|a_i| \leqslant r_0/\sqrt{\lambda}$, $|b_i| \leqslant r_0$.

For the polyhedron $\Gamma' = \{y = (a_i, b_j)_{|i|,|j|\leqslant J'(\varepsilon)} \in R^{2J'(\varepsilon)+1} \times R^{2J'(\varepsilon)+1} : |a_i| \leqslant r_0/\sqrt{\lambda},\ |b_j| \leqslant r_0\}$ in the $(2J'(\varepsilon)+1)^2$-dimensional space, by Theorem 1, Γ' can be covered by $n_\varepsilon(\Gamma') = ([2r_0\sqrt{2J'(\varepsilon)+1}/\sqrt{\lambda}\varepsilon]+1)^{2J'(\varepsilon)+1} \times ([2r_0\sqrt{2J'(\varepsilon)+1}/\varepsilon]+1)^{2J'(\varepsilon)+1}$ $\varepsilon/2$-balls.

Let the centers of these $\varepsilon/2$-balls be $\varphi_k^* = (a_{i,k}^*, b_{j,k}^*)_{|i|,|j|\leqslant J'(\varepsilon)} \in R^{2J'(\varepsilon)+1} \times R^{2J'(\varepsilon)+1}$, $k = 1,2,\ldots,n_\varepsilon(\Gamma')$, respectively. Choose $\varphi_k = (\varphi_{k,i,j})_{i,j\in Z}$, $k = 1,2,\ldots,n_\varepsilon(\Gamma')$, where

$$\varphi_{k,i,j} = \begin{cases} \varphi_k^*, & |i|, |j| \leqslant J'(\varepsilon), \\ 0, & |i| > J'(\varepsilon) \text{ or } |j| > J'(\varepsilon). \end{cases}$$

Then, for $y = (y_i)_{i\in Z} = ((a_i, b_i))_{i\in Z}$ above,

$$y_i = (a_i, b_i) = \begin{cases} (u_i, v_i), & |i| \leqslant J'(\varepsilon), \\ 0, & |i| > J'(\varepsilon), \end{cases}$$

there exists k such that

$$\|y - \varphi_k\|_E < \frac{\varepsilon}{2}, \quad k = 1,2,\ldots,n_\varepsilon(\Gamma').$$

Thus

$$\|\varphi - \varphi_k\|_E = \|y + z - \varphi_k\|_E \leqslant \|y - \varphi_k\|_E + \|z\|_E < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon.$$

Hence the attractor Λ' of (18) can be covered by $n_\varepsilon(\Gamma') = ([2r_0\sqrt{2J'(\varepsilon)+1}/\sqrt{\lambda}\varepsilon]+1)^{2J'(\varepsilon)+1} \times ([2r_0\sqrt{2J'(\varepsilon)+1}/\varepsilon]+1)^{2J'(\varepsilon)+1} = n_\varepsilon(\Lambda')$ ε-balls centered at $\varphi_k = (\varphi_{k,i,j})_{i,j\in Z}$, $k = 1, 2,\ldots,$ $n_\varepsilon(\Lambda')$, with radius ε, respectively.

By Theorem 4 and the definition of Kolmogorov's ε-entropy, we can easily obtain the following theorem.

Theorem 5: *If (10) and (11) hold and $g \in \ell^2$, then an upper bound of Kolmogorov's ε-entropy of the global attractor Λ' of (18) is*

$$(2J'(\varepsilon)+1)\left(\ln\left(\left[\frac{2r_0\sqrt{2J'(\varepsilon)+1}}{\sqrt{\lambda}\varepsilon}\right]+1\right)+\ln\left(\left[\frac{2r_0\sqrt{2J'(\varepsilon)+1}}{\varepsilon}\right]+1\right)\right),$$

where $r_0=\sqrt{2}\|g\|/\sqrt{\alpha\mu}$, *and* $J'(\varepsilon)$ *is defined by (22).*

Remark: For the first and second order dissipative lattice dynamical systems, we give the following remark.

(i) If $\|g\|=0$, *i.e.,* $g_i=0,\forall i\in Z$, *then the global attractor* Λ *(or* Λ'*) is exactly an equilibrium which attracts every bounded set of* ℓ^2 *(or* E*). In this case, Kolmogorov's* ε*-entropy of* Λ *(or* Λ'*) is zero and* Λ *(or* Λ'*) is zero-dimensional.*

(ii) If $\|g\|\neq 0$, *then, in general, it is unknown for the exact geometric structure of* Λ *(or* Λ'*), but only knowing that* Λ *(or* Λ'*) is included in a bounded ball* $O=O(0,M_0)$ *(or* $O'=O'(0,r_0)$*), where* $M_0=\sqrt{2}\|g\|/\lambda\neq 0$ *(or* $r_0=(\sqrt{2}\|g\|/\alpha\mu)\neq 0$*). Obviously, in this case,* Λ *(or* Λ'*) is generally infinite dimensional.*

ACKNOWLEDGMENTS

The author thanks the reviewers and the editor very much for their reading carefully this paper and giving useful suggestions. This work was supported by the National Natural Science Foundation of China under Grant No. 10171072.

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Superintegrable systems in Darboux spaces

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(Received 25 June 2003; accepted 19 August 2003)

Almost all research on superintegrable potentials concerns spaces of constant curvature. In this paper we find by exhaustive calculation, all superintegrable potentials in the four Darboux spaces of revolution that have at least two integrals of motion quadratic in the momenta, in addition to the Hamiltonian. These are two-dimensional spaces of nonconstant curvature. It turns out that all of these potentials are equivalent to superintegrable potentials in complex Euclidean 2-space or on the complex 2-sphere, via "coupling constant metamorphosis" (or equivalently, via Stäckel multiplier transformations). We present a table of the results. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1619580]

I. INTRODUCTION

In a previous paper[1] we have studied superintegrability in a two-dimensional space of nonconstant curvature, in particular one of the so-called Darboux spaces, given by Koenigs.[2] In this paper we study the remaining three spaces of nonconstant curvature from the point of view of superintegrability. This involves the addition of a potential to each of the spaces given by Koenigs. We recall that classical superintegrability relating to a Hamiltonian $H(x_1,\ldots,x_n,p_1,\ldots,p_n)=H(x,p)$ implies the existence of $2n-1$ globally defined constants of the motion. For the purposes of this paper we restrict this definition to require that there exist $2n-1$ globally defined functionally independent constants of the motion X_i, $i=1,\ldots,2n-1$ that are quadratic in the canonical momenta p_i. This clearly implies the relations

$$\{H,X_\ell\}=\sum_{i=1}^{n}\left(\frac{\partial X_\ell}{\partial x_i}\frac{\partial H}{\partial p_i}-\frac{\partial X_\ell}{\partial p_i}\frac{\partial H}{\partial x_i}\right)=0\,,\quad i=1,\ldots,2n-1\,.$$

The concepts of integrability and superintegrability also have their analog in quantum mechanics. A superintegrable quantum mechanical system is described by $2n-1$ (independent) quantum observables $\hat{H}=\hat{X}_1,\hat{X}_2,\ldots,\hat{X}_{2n-1}$ that satisfy the commutation relations

$$[\hat{H},\hat{X}_i]=\hat{H}\hat{X}_i-\hat{X}_i\hat{H}=0,\quad i=1,\ldots,2n-1.$$

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The analog of quadratic superintegrability in this case is that each of the quantum observables is a second order partial differential operator. Systematic studies of superintegrable systems have been conducted in spaces of constant curvature in two dimensions.[3–7]

In this paper we solve the following problem. Given a Riemannian space in two dimensions with infinitesimal distance $ds^2=\Sigma_{i,j=1}^2 g_{ij}(u)du^i\,du^j$, and $u=(u^1,u^2)$, the classical Hamiltonian has the form

$$H=\sum_{i,j=1}^{2} g^{ij}p_ip_j+V(u)$$

and the corresponding Schrödinger equation is

$$\hat{H}\Psi=\frac{1}{\sqrt{g}}\partial_{u^i}(\sqrt{g}g^{ik}\partial_{u^k}\Psi)+V(u)\Psi=E\Psi,$$

where $\sqrt{g}=\det(g_{ij})$. Koenigs found all free Hamiltonians $H=\Sigma g^{ij}p_ip_j$ admitting at least two extra functionally independent constants of the motion of the form

$$\Lambda=\sum_{i,j=1}^{2} a^{ij}(u)p_ip_j,\quad a^{ij}=a^{ji}.$$

He obtained a number of families of solutions; in particular, spaces that admitted three extra quadratic constants. There must then be a functional relation between these and, furthermore, in each case there is a Killing vector, i.e., a function $\mu=\Sigma_{i=1}^2 a^i(u)p_i$ that satisfies $\{H,\mu\}=0$. One of the three quadratic constants is a square of the Killing vector μ.

The problem we solve here is supplemental to that of Koenigs: Suppose we have a Hamiltonian $H=\Sigma g^{ij}p_ip_j+V(u)$ that admits a Killing vector. We determine the *potentials* that correspond to superintegrability, i.e., potentials such that we can find at least two extra functionally independent quadratic constants of the form

$$\Lambda=\sum_{i,j=1}^{2} a^{ij}(u)p_ip_j+\lambda(u).$$

A necessary condition that this be possible is that the Riemannian space be one of the four listed by Koenigs:

(1) $ds^2=(x+y)dx\,dy$,
(2) $ds^2=(a/(x-y)^2+b)dx\,dy$,
(3) $ds^2=(ae^{-(x+y)/2}+be^{-x-y})dx\,dy$,
(4) $ds^2=[a(e^{(x-y)/2}+e^{(y-x)/2})+b]/(e^{(x-y)/2}-e^{(y-x)/2})^2\,dx\,dy$.

The first of these spaces, type one, or D_1, has been treated in detail in an earlier paper.[1] Here we treat the remaining three Darboux spaces in a similar and unified way. Sections II, III, and IV are devoted to the spaces D_2, D_3, and D_4, respectively. In each space we follow the same pattern.

(1) We first consider a classical free particle system and give the free Hamiltonian H_0, the Killing vector K, and the two Killing tensors X_1 and X_2 in a space with a conformally Euclidean metric (real or complex). We choose coordinates u and v in which the first order constant is $K=p_v$, hence u is an ignorable variable, not appearing in the metric or in the Hamiltonian.
(2) We present an embedding of the two-dimensional Darboux space into a three-dimensional flat space.
(3) We present a polynomial relation between the four integrals of motion H, K, X_1, and X_2, and also the polynomial algebra generated by these integrals.

(4) We consider the quantum mechanics of a free particle in the corresponding Darboux space, i.e., write the corresponding Hamiltonian and integrals of motion as linear operators. We then establish that the relations between these operators are the same as those between the classical quantities.
(5) We use the fact that the Killing vector K generates a one-dimensional Lie transformation group to classify all integrals of motion

$$\lambda = aX_1 + bX_2 + cK^2 \tag{1.1}$$

into conjugation classes. Each class gives rise to a coordinate system in which the Hamilton–Jacobi and Schrödinger equations allow the separation of variables. We construct these separable coordinate systems explicitly and solve the corresponding separated equations (classical and quantum).
(6) By construction, the free classical and quantum systems in Darboux spaces are all quadratically superintegrable: they have three functionally independent integrals of motion. We introduce potentials that do not destroy this superintegrability. Thus we present systematically all superintegrable classical and quantum systems of the form

$$H = H_0 + V(u,v), \tag{1.2}$$

where H_0 is the free Hamiltonian in the space D_2, D_3, or D_4. To obtain this result we make use of the fact that to be quadratically superintegrable, a Hamiltonian in a Darboux space must allow the separation of variables in at least two coordinate systems.

A separate section, Sec. V, is devoted to the relation between superintegrable systems in Darboux spaces and two-dimensional spaces of constant curvature.

II. DARBOUX SPACES OF TYPE TWO

A. The free particle and separating coordinate systems

If we allow rescaling of the variables x and y, as well as the Hamiltonian H then we can always take H to be of the form

$$H_0 = \frac{(x-y)^2}{(x-y)^2-1} p_x p_y . \tag{2.1}$$

In the coordinates $x = \frac{1}{2}(v+iu)$, $y = \frac{1}{2}(v-iu)$ this Hamiltonian becomes

$$H_0 = \frac{u^2(p_u^2+p_v^2)}{u^2+1}.$$

Associated with the Hamiltonian are three integrals of the free motion

$$K = p_v , \quad X_1 = \frac{2v(p_v^2-u^2p_u^2)}{u^2+1} + 2up_up_v , \quad X_2 = \frac{(v^2-u^4)p_v^2+u^2(1-v^2)p_u^2}{u^2+1} + 2uvp_up_v .$$

These three integrals satisfy the following polynomial algebra relations:

$$\{K,X_1\} = 2(K^2-H_0), \quad \{K,X_2\} = X_1 , \quad \{X_1,X_2\} = 4KX_2 . \tag{2.2}$$

They are functionally dependent via the relation

$$X_1^2 - 4K^2X_2 + 4H_0X_2 - 4H_0^2 = 0 . \tag{2.3}$$

The corresponding problem in quantum mechanics can be obtained via the usual quantization rules and symmetrization:

$$\hat{H}_0=\frac{u^2}{u^2+1}(\partial_u^2+\partial_v^2),\quad \hat{K}=\partial_v,\quad \hat{X}_1=\frac{2v}{(u^2+1)}(\partial_v^2-u^2\partial_u^2)+2u\partial_u\partial_v+\partial_v,$$

$$\hat{X}_2=\frac{1}{u^2+1}((v^2-u^4)\partial_v^2+u^2(1-v^2)\partial_u^2)+2uv\partial_u\partial_v+u\partial_u+v\partial_v-\frac{1}{4},$$

where the constant in the last expression is taken for convenience. The commutation relations are identical with those of the corresponding classical algebra,

$$[\hat{K},\hat{X}_1]=2(\hat{K}^2-\hat{H}_0),\quad [\hat{K},\hat{X}_2]=\hat{X}_1,\quad [\hat{X}_1,\hat{X}_2]=2\{\hat{K},\hat{X}_2\}.$$

Here $\{\hat{K},\hat{X}_2\}=\frac{1}{2}(\hat{K}\hat{X}_2+\hat{X}_2\hat{K})$. The operator relation (that exists in analogy with the functional relation in the classical case) is

$$\hat{X}_1^2-2\{\hat{K}^2,\hat{X}_2\}+4\hat{H}_0\hat{X}_2-4\hat{H}_0^2-\hat{H}_0+4\hat{K}^2=0.$$

The line element $ds^2=(du^2+dv^2)(u^2+1)/u^2$ can be realized as a two-dimensional surfaced embedded in three dimensions by

$$X=\frac{v\sqrt{u^2+1}}{u},\quad Y-T=\frac{\sqrt{u^2+1}}{u},\quad Y+T=-\frac{(2u^4+5u^2+8v^2)\sqrt{u^2+1}}{8u}-\frac{3}{8}\operatorname{arcsinh} u,$$

in which case,

$$ds^2=dX^2+dY^2-dT^2=\frac{u^2+1}{u^2}(du^2+dv^2).$$

We wish to determine all the essentially different separable coordinate systems for the free classical or quantum particle. In order to do this we need to consider a general quadratic constant of the form $\lambda=aX_1+bX_2+cK^2$. Under the adjoint action of $\exp(\alpha K)$, X_1 and X_2 transform according to

$$X_1\to X_1+2\alpha(K^2-H_0),\quad X_2\to X_2+\alpha X_1+\alpha^2(K^2-H_0).$$

From these transformation formulas we see that if $b\neq 0$ we can always take λ in the form $\lambda=X_2+\beta K^2$. If $b=0$ then there are two representatives possible: X_1 or K^2. We have the following cases:

$$X_2+\beta K^2,\quad X_1,\quad K^2. \tag{2.4}$$

We now demonstrate the explicit coordinates for each of these representatives using methods of our previous paper.[1]

1. Coordinates associated with $X_2+\beta K^2$

If we choose $\beta=b^2$, $b\neq 0$ suitable coordinates ω, φ are

$$u=b\cosh\omega\cos\varphi,\quad v=b\sinh\omega\sin\varphi, \tag{2.5}$$

the standard form of elliptical coordinates in the plane. The classical Hamiltonian has the form

$$H_0=\frac{p_\omega^2+p_\varphi^2}{\sec^2\varphi-\operatorname{sech}^2\omega+b^2(\cosh^2\omega-\cos^2\varphi)}.$$

The corresponding quadratic constant, expressed in these coordinates is

$$X_2+b^2K^2=\frac{(\sec^2\varphi+b^2\sin^2\varphi)p_\omega^2+(\operatorname{sech}^2\omega-b^2\sinh^2\omega)p_\varphi^2}{(\sec^2\varphi-\operatorname{sech}^2\omega)+b^2(\cosh^2\omega-\cos^2\varphi)}.$$

The Hamilton–Jacobi equation is

$$\frac{\left(\frac{\partial S}{\partial\omega}\right)^2+\left(\frac{\partial S}{\partial\varphi}\right)^2}{\sec^2\varphi-\operatorname{sech}^2\omega+b^2(\cosh^2\omega-\cos^2\varphi)}=E\,,$$

with solutions of the form

$$S(\omega,\varphi)=\frac{b\sqrt{E}}{2}\left(\int\frac{1}{\Omega}\sqrt{\frac{(\Omega+\beta_1)(\Omega+\beta_2)}{\Omega-1}}\,\mathrm{d}\Omega+\int\frac{1}{\Phi}\sqrt{\frac{(\beta_1-\Phi)(\Phi-\beta_2)}{1-\Phi}}\,\mathrm{d}\Phi\right),$$

where $\beta_1+\beta_2=-\lambda/Eb^2$, $\beta_1\beta_2=-1/b^2$, $\Phi=\cos^2\varphi$, $\Omega=\cosh^2\omega$. The corresponding Schrödinger equation

$$\frac{(\partial_\varphi^2+\partial_\omega^2)\Psi}{\sec^2\varphi-\operatorname{sech}^2\omega+b^2(\cosh^2\omega-\cos^2\varphi)}=E\Psi$$

has solutions of the form

$$\Psi=\sqrt{\cos\varphi\cosh\omega}\;\;S_n^{m(j)}(i\sinh\omega,-\tfrac{1}{4}Eb)Ps_n^m(\sin\varphi,-\tfrac{1}{4}Eb)\,,\quad j=1,2,$$

where $S_n^{m(j)}(z,\kappa)$ and $Ps_n^m(t,\kappa)$ are spheroidal functions [8] and $E=m^2-\frac{1}{4}$.

2. Coordinates associated with X_2

Here we use polar coordinates

$$u=r\cos\theta\,,\quad v=r\sin\theta\,. \tag{2.6}$$

The classical Hamiltonian has the form

$$H_0=\frac{r^2p_r^2+p_\theta^2}{r^2+\sec^2\theta}$$

and the corresponding quadratic constant is

$$X_2=\frac{r^2\sec^2\theta\,p_r^2-p_\theta^2}{r^2+\sec^2\theta}.$$

The Hamilton–Jacobi equation in these coordinates is

$$\frac{r^2\left(\frac{\partial S}{\partial r}\right)^2+\left(\frac{\partial S}{\partial\theta}\right)^2}{r^2+\sec^2\theta}=E\,,$$

with solution

$$S(r,\theta)=\sqrt{Er^2+\lambda}-\sqrt{\lambda}\ \operatorname{arctanh}\sqrt{\frac{Er^2+\lambda}{\lambda}}-\sqrt{\lambda}\log(\sqrt{\lambda}\sin\theta+\sqrt{E-\lambda\cos^2\theta})$$
$$+\frac{1}{2}\sqrt{E}\ \operatorname{arccosh}\left(\frac{(E+\lambda)\cos^2\theta-2E}{(E-\lambda)\cos^2\theta}\right).$$

The corresponding Schrödinger equation is

$$\frac{r^2\dfrac{\partial^2\Psi}{\partial r^2}+\sin\theta\dfrac{\partial}{\partial\theta}\left(\dfrac{1}{\sin\theta}\dfrac{\partial\Psi}{\partial\theta}\right)}{r^2+\sec^2\theta}=E\Psi,$$

and has solutions of the form

$$\Psi=\sqrt{r\sin\theta}\ \ C_{\ell+1/2}(\sqrt{-E}\ \ r)P_\ell^m(\cos\theta),\quad E=m^2-\tfrac{1}{4},$$

where $C_\nu(z)$ is a Bessel function and $P_\ell^n(\cos\theta)$ is an associated Legendre polynomial.[8]

3. Coordinates associated with X_1

A suitable choice of coordinates is

$$u=\xi\eta,\quad v=\tfrac{1}{2}(\xi^2-\eta^2). \tag{2.7}$$

The classical Hamiltonian in these coordinates has the form

$$H_0=\frac{p_\xi^2+p_\eta^2}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}.$$

The corresponding quadratic constant is

$$X_1=\frac{\left(\eta^2+\dfrac{1}{\eta^2}\right)p_\xi^2-\left(\xi^2+\dfrac{1}{\xi^2}\right)p_\eta^2}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}.$$

The Hamilton–Jacobi equation has the form

$$\frac{\left(\dfrac{\partial S}{\partial\xi}\right)^2+\left(\dfrac{\partial S}{\partial\eta}\right)^2}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}=E,$$

which has the solution

$$S(\xi,\eta)=-\frac{\sqrt{E\xi^4+E-\lambda\xi^2}}{\xi^2}-\frac{\lambda}{2\sqrt{E}}\operatorname{arctanh}\left(\frac{\lambda\xi^2-2E}{2\sqrt{E}\sqrt{E\xi^4+E-\lambda\xi^2}}\right)+\sqrt{E}\log(\sqrt{E}(2E\xi^2-\lambda)$$
$$+2E\sqrt{E\xi^4+E-\lambda\xi^2})-\frac{\sqrt{E\eta^4+E+\lambda\eta^2}}{\eta^2}-\frac{\lambda}{2\sqrt{E}}\operatorname{arctanh}\left(\frac{\lambda\eta^2+2E}{2\sqrt{E}\sqrt{E\xi^4+E+\lambda\xi^2}}\right)$$
$$+\sqrt{E}\log(\sqrt{E}(2E\xi^2+\lambda)+2E\sqrt{E\xi^4+E+\lambda\xi^2}).$$

The corresponding Schrödinger equation is

$$\frac{\partial_\xi^2\Psi+\partial_\eta^2\Psi}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}=E\Psi\ .$$

Typical solutions are

$$\Psi=\frac{1}{\sqrt{\xi\,\eta}}M_{\chi,\mu}(\sqrt{E}\,\xi^2)M_{-\chi,\mu}(\sqrt{E}\,\eta^2),$$

where $M_{\chi,\mu}(z)$ is a Whittaker function[9] and $E=4\mu^2-\frac{1}{4}$.

4. Coordinates associated with K^2

The representative K^2 has associated with it the coordinates u and v, in which the ignorable variable has a fundamental role to play. The Hamiltonian and constant associated with this separation have already been given. The Hamilton–Jacobi equation has the form

$$\frac{u^2}{u^2+1}\left(\left(\frac{\partial S}{\partial u}\right)^2+\left(\frac{\partial S}{\partial v}\right)^2\right)=E\ ,$$

which has solution, with separation constant c,

$$S(u,v)=\sqrt{u^2(E-c^2)+E}-\sqrt{E}\ \ \operatorname{arctanh}\sqrt{\frac{u^2(E-c^2)+E}{E}}+cv\ .$$

The corresponding Schrödinger equation has the form

$$\frac{u^2}{u^2+1}(\partial_u^2\Psi+\partial_v^2\Psi)=E\Psi.$$

Typical solutions are

$$\Psi=\sqrt{u}\ \ C_\nu(\sqrt{m^2-E}\ \ u)e^{mv},$$

where $E=\nu^2-\frac{1}{4}$.

It is no surprise that the Hamiltonian is separable in elliptic, parabolic, and polar coordinates, since, if we write the classical equation $H=E$ in u,v coordinates we obtain

$$p_u^2+p_v^2-E\left(\frac{1}{u^2}+1\right)=0.$$

This equation is essentially the same form as a flat space superintegrable system with Cartesian coordinates u,v and potential α/u^2, viz.,

$$p_u^2+p_v^2+\frac{\alpha}{u^2}-E=0.$$

It is known to be solvable via the separation of variables ansatz in elliptic, Cartesian, polar, and parabolic coordinates. This correspondence between flat space superintegrable systems and their curved analogs is essentially the way all the curved superintegrable systems can be obtained and is discussed in more detail in Sec. V.

B. Superintegrability for Darboux spaces of type two

In this section we address the problem of superintegrability for the Hamiltonian

$$H_0=\frac{u^2(p_u^2+p_v^2)}{u^2+1}. \tag{2.8}$$

This is done in exactly the same manner as it was for the Darboux space of type 1 in a previous paper.[1] The free space Hamiltonian is given and we compute the possible potentials that correspond to superintegrability. There are four possibilities:

$$[\mathbf{A}]\quad H=\frac{u^2}{u^2+1}\left(p_u^2+p_v^2+a_1\left(\frac{1}{4}u^2+v^2\right)+a_2v+\frac{a_3}{u^2}\right).$$

A basis for the additional constants of the motion is

$$R_1=X_1+\frac{a_1}{2}v\left(u^2+\frac{u^2+4v^2}{u^2+1}\right)+\frac{a_2}{2}\left(u^2+\frac{4v^2}{u^2+1}\right)-\frac{2a_3v}{u^2+1},$$

$$R_2=K^2+a_1v^2+a_2v\ .$$

These, along with $R=\{R_1,R_2\}$, form a quadratic algebra

$$\{R,R_1\}=-\frac{1}{2}\frac{\partial R^2}{\partial R_2},\quad \{R,R_2\}=\frac{1}{2}\frac{\partial R^2}{\partial R_1} \tag{2.9}$$

that is determined by the identity

$$R^2=16R_2^3-4a_1R_1^2-32HR_2^2-8a_2R_1R_2+8a_2HR_1+16(H^2+a_1H-a_1a_3)R_2+4a_2^2H-4a_2^2a_3\ .$$

The classical equation of motion $H-E=0$ is

$$p_u^2+p_v^2+a_1\left(\frac{1}{4}u^2+v^2\right)+a_2v+\frac{a_3-E}{u^2}-E=0.$$

The basic form of this equation is a superintegrable system in flat space, but with rearranged constants, which is solvable via separation of variables in Cartesian and parabolic coordinates.

This accords with the fact that the leading part of a quadratic constant for this Hamiltonian will be an element of the orbits represented by X_1 and K^2. So this Hamiltonian also separates in the ''parabolic'' coordinates ξ, η (2.7) and in these coordinates takes the form

$$H=\frac{p_\xi^2+p_\eta^2+\frac{1}{4}a_1(\xi^6+\eta^6)+\frac{1}{2}a_2(\xi^4-\eta^4)+a_3\left(\frac{1}{\eta^2}+\frac{1}{\xi^2}\right)}{\xi^2+\eta^2+\frac{1}{\xi^2}+\frac{1}{\eta^2}}.$$

Adding the same potential and coordinate functions to the quantum Hamiltonian $\hat{H}_0$ and its corresponding commuting operators $\hat{X}_1$ and $\hat{K}^2$, we obtain the operators

$$\hat{H}=\hat{H}_0+\frac{u^2}{u^2+1}\left(a_1\left(\frac{1}{4}u^2+v^2\right)+a_2v+\frac{a_3}{u^2}\right),$$

$$\hat{R}_1=\hat{X}_1+\frac{a_1}{2}v\left(u^2+\frac{u^2+4v^2}{u^2+1}\right)+\frac{a_2}{2}\left(u^2+\frac{4v^2}{u^2+1}\right)-\frac{2a_3v}{u^2+1},$$

$$\hat{R}_2=\hat{K}^2+a_1v^2+a_2v\ .$$

$\hat{R}_1$ and $\hat{R}_2$ commute with $\hat{H}$ and along with $\hat{R}=[\hat{R}_1,\hat{R}_2]$, obey the corresponding quantum quadratic algebra relations

$$[\hat{R},\hat{R}_1]=-24\hat{R}_2^2+4a_2\hat{R}_1+32\hat{H}\hat{R}_2-8\hat{H}^2-8a_1\hat{H}+6a_1+8a_1a_3\,,$$

$$[\hat{R},\hat{R}_2]=-4a_1\hat{R}_1-4a_2\hat{R}_2+4a_2\hat{H}$$

and the operator identity

$$\hat{R}^2=16\hat{R}_2^3-4a_1\hat{R}_1^2-32\hat{H}\hat{R}_2^2-4a_2\{\hat{R}_1,\hat{R}_2\}+8a_2\hat{H}\hat{R}_1+16\hat{H}^2\hat{R}_2+16a_1\hat{H}\hat{R}_2-4a_1(4a_3-11)\hat{R}_2$$
$$+4(a_2^2+8a_1)\hat{H}-4b_2^2(a_3+\tfrac{3}{4})\,.$$

$$[\mathbf{B}]\quad H=\frac{u^2}{u^2+1}\left(p_u^2+p_v^2+b_1(u^2+v^2)+\frac{b_2}{u^2}+\frac{b_3}{v^2}\right).$$

The additional constants of the motion have the form

$$R_1=X_2+\frac{u^2+v^2}{u^2+1}\left(b_1(u^2+v^2)-b_2-b_3\frac{u^2}{v^2}\right),\quad R_2=K^2+b_1v^2+\frac{b_3}{v^2}.$$

The corresponding quadratic algebra relations can be determined, using (2.9), from the identity

$$R^2=16R_1R_2^2-16b_1R_1^2-16HR_1R_2+32b_1(H-b_2-b_3)R_1+16(H+b_3-b_2)HR_2$$
$$-16(b_1+b_3)H^2+32b_1(b_2-b_3)H-16b_1(b_2-b_3)^2\,.$$

The equation of motion $H-E=0$ becomes

$$p_u^2+p_v^2+b_1(u^2+v^2)+\frac{(b_2-E)}{u^2}+\frac{b_3}{v^2}-E=0\,.$$

This is a superintegrable system in flat space, but with rearranged constants, which is solvable via separation of variables in Cartesian, polar, and elliptic coordinates. Again, this agrees with the observation that for this Hamiltonian we have quadratic constants with leading parts K^2, X_2, and $X_2+\beta K^2$. In the latter two coordinate systems, the Hamiltonian takes the following forms:

(i) Elliptical coordinates (2.5),

$$H=\frac{p_\omega^2+p_\varphi^2+\frac{1}{4}b_1b^2(\sinh^2 2\omega+\sin^2 2\varphi)+b_2(\sec^2\varphi-\operatorname{sech}^2\omega)+b_3(\operatorname{cosec}^2\varphi+\operatorname{cosech}^2\omega)}{\sec^2\varphi-\operatorname{sech}^2\omega+b^2(\cosh^2\omega-\cos^2\varphi)}.$$

(ii) Polar coordinates (2.6),

$$H=\frac{r^2p_r^2+p_\theta^2+b_1r^4+b_2\sec^2\theta+b_3\operatorname{cosec}^2\theta}{r^2+\sec^2\theta}.$$

The corresponding quantum algebra relations are

$$[\hat{R},\hat{R}_1]=-8\{\hat{R}_1,\hat{R}_2\}+8\hat{H}\hat{R}_1+12\hat{R}_2-8\hat{H}^2+8(b_2-b_3-\tfrac{3}{4})\hat{H}\,,$$

$$[\hat{R},\hat{R}_2]=8\hat{R}_2^2-16b_1\hat{R}_1-8\hat{H}\hat{R}_2+16b_1\hat{H}-16b_1(b_2+b_3+\tfrac{3}{4})\,,$$

$$\hat{R}^2=8\{\hat{R}_1,\hat{R}_2^2\}-8\hat{H}\{\hat{R}_1,\hat{R}_2\}+16\hat{H}^2\hat{R}_2-16b_1\hat{R}_1^2-76\hat{R}_2^2+32b_1\hat{H}\hat{R}_1-8b_1(4(b_3+b_2)+3)\hat{R}_1$$
$$+16(b_3-b_2+\tfrac{19}{4})\hat{H}\hat{R}_2-16(b_1+b_3+\tfrac{3}{4})\hat{H}^2-8b_1(4(b_3-b_2)+3)\hat{H}$$
$$+b_1(36+48b_3-(4(b_3-b_2)+3)^2).$$

$$[\mathbf{C}]\quad H=\frac{p_\xi^2+p_\eta^2+c_1+\dfrac{c_2}{\xi^2}+\dfrac{c_3}{\eta^2}}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}.$$

The additional constants of the motion are

$$R_1=X_1+\frac{c_1\xi^2(\eta^4+1)+c_2(\eta^4+1)-c_3(\xi^4+1)}{(\xi^2\eta^2+1)(\xi^2+\eta^2)},$$

$$R_2=X_2+\frac{c_1(\xi^2+\eta^2)-c_2(\eta^4-1)-c_3(\xi^4-1)}{4(\xi^2\eta^2+1)}.$$

The corresponding Poisson algebra can be determined from the identity

$$R^2=4R_1^2R_2-(c_2+c_3)R_1^2+16HR_2^2-4c_1R_1R_2+2c_1c_3R_1-16H^2R_2+4(c_2+c_3)H^2$$
$$+(c_1^2-4c_2c_3)H-c_1^2c_3.$$

The Hamiltonian can be written in separable form for the following coordinate systems:

(i) Displaced elliptic coordinates $\xi=b'\cosh\omega'\cos\varphi'$, $\eta=b'\sinh\omega'\sin\varphi'$,

$$H=\frac{p_{\omega'}^2+p_{\varphi'}^2+c_1b'^2(\cosh^2\omega'-\cos^2\varphi')+c_2(^2\varphi'-\mathrm{sech}^2\omega')+c_3(\mathrm{cosec}^2\varphi'+\mathrm{cosech}^2\omega')}{b'^4(\cosh^4\omega'-\cos^4\varphi'-\cosh^2\omega'+\cos^2\varphi')+\sec^2\varphi'+\mathrm{cosec}^2\varphi'+\mathrm{cosech}^2\omega'-\mathrm{sech}^2\omega'}.$$

These coordinates are not those given in (2.5) and are related to u and v by

$$u=\tfrac{1}{4}b'^2\sinh 2\omega'\sin 2\varphi',\quad v=\tfrac{1}{4}b'^2(\cosh 2\omega'\cos 2\varphi'+1).$$

(ii) Polar coordinates $\xi=r'\cos\theta'$, $\eta=r'\sin\theta'$,

$$H=\frac{r'^2p_{r'}^2+p_{\theta'}^2+c_1r'^2+c_2\,\mathrm{cosec}^2\,\theta'+c_3\sec^2\theta'}{r'^4+\sec^2\theta'+\mathrm{cosec}^2\theta'}.$$

These coordinates are not those given in (2.6) and are related to u and v by

$$u=\tfrac{1}{2}r'^2\sin 2\theta',\quad v=\tfrac{1}{2}r'^2\cos 2\theta'.$$

The corresponding quantum algebra relations are

$$[\hat{R},\hat{R}_1]=-2\hat{R}_1^2-2c_1\hat{R}_1-16\hat{H}\hat{R}_2+8\hat{H}^2-6\hat{H},$$

$$[\hat{R},\hat{R}_2]=2\{\hat{R}_1,\hat{R}_2\}-(c_2+c_3)\hat{R}_1-2c_1\hat{R}_2+c_1c_3,$$

$$\hat{R}^2=2\{\hat{R}_1^2,\hat{R}_2\}+16\hat{H}\hat{R}_2^2-(c_2+c_3+4)\hat{R}_1^2-2c_1\{\hat{R}_1,\hat{R}_2\}+2c_1(c_3+2)\hat{R}_1-16\hat{H}^2\hat{R}_2+12\hat{H}\hat{R}_2$$
$$+4(c_2+c_3)\hat{H}^2+(c_1^2-4c_2c_3-3(c_2+c_3))\hat{H}-\tfrac{1}{4}(3+4c_3)c_1^2.$$

The equation of motion $H-E=0$ is

$$p_\xi^2+p_\eta^2+c_1-E(\xi^2+\eta^2)+\frac{(c_2-E)}{\xi^2}+\frac{(c_3-E)}{\eta^2}=0.$$

This is a superintegrable system in flat space, but with rearranged constants, which is solvable via separation of variables in Cartesian, polar, and elliptic coordinates.

$$[\mathbf{D}]\quad H=\frac{u^2(p_u^2+p_v^2+\mathrm{d})}{u^2+1}.$$

The additional constants of the motion are

$$R_1=X_1+\frac{2\,\mathrm{d}v}{u^2+1},\quad R_2=X_2+\frac{\mathrm{d}(u^2+v^2)}{u^2+1},\quad K=p_v\,.$$

The corresponding Poisson algebra relations are

$$\{K,R_1\}=2K^2-2H+2d\,,\quad \{K,R_2\}=R_1\,,\quad \{R_1,R_2\}=-4KR_2\,.$$

The functional relation between these constants is

$$R_1^2-4K^2R_2+4(H-\mathrm{d})R_2-4H^2+4\,\mathrm{d}H=0\,.$$

The Hamiltonian can be written in separable form for all the possible types of separable coordinates we have discussed, viz.,

(i) Elliptic coordinates (2.5),

$$H=\frac{p_\omega^2+p_\varphi^2+b^2\,\mathrm{d}(\cosh^2\omega-\cos^2\varphi)}{b^2(\cosh^2\omega-\cos^2\varphi)+\sec^2\varphi-\mathrm{sech}^2\,\omega}.$$

(ii) Polar coordinates (2.6),

$$H=\frac{r^2p_r^2+p_\theta^2+\mathrm{d}r^2}{r^2+\sec^2\theta}.$$

(iii) Parabolic coordinates (2.7),

$$H=\frac{p_\xi^2+p_\eta^2+\mathrm{d}(\xi^2+\eta^2)}{\xi^2+\eta^2+\dfrac{1}{\xi^2}+\dfrac{1}{\eta^2}}.$$

The corresponding quantum algebra relations have the form

$$[\hat K,\hat R_1]=2\hat K^2-2\hat H+2\mathrm{d},\quad [\hat K,\hat R_2]=\hat R_1,\quad [\hat R_1,\hat R_2]=2\{\hat K,\hat R_2\}.$$

The operator identity satisfied by the defining operators of the quantum algebra is

$$\hat R_1^2-2\{\hat K^2,\hat R_2\}+4\hat H\hat R_2-4\,\mathrm{d}\hat R_2+4\hat K^2-4\hat H^2+(4\mathrm{d}-1)\hat H=0\,.$$

The equation of motion $H-E=0$ is

$$p_u^2+p_v^2+\mathrm{d}-E-\frac{E}{u^2}=0.$$

This is a superintegrable system in flat space, but with rearranged constants, which is solvable via separation of variables in Cartesian, polar, elliptic, and parabolic coordinates.

III. DARBOUX SPACES OF TYPE THREE

A. The free particle and separating coordinate systems

With rescaling and translation of the variables x and y the Hamiltonian H has the form

$$H_0=\frac{e^{(x+y)/2}}{1+e^{-(x+y)/2}}p_x p_y\,. \tag{3.1}$$

In coordinates $x=u-iv$, $y=u+iv$ we can write this Hamiltonian in positive-definite form

$$H_0=\frac{1}{4}\,\frac{e^{2u}(p_u^2+p_v^2)}{e^u+1}.$$

Associated with the Hamiltonian are three integrals of the free motion

$$K=p_v\,,\quad X_1=\frac{1}{4}\,\frac{e^{2u}}{e^u+1}\cos v\,p_u^2-\frac{1}{4}\,\frac{e^u(e^u+2)}{e^u+1}\cos v\,p_v^2+\frac{1}{2}e^u\sin v\,p_u p_v\,,$$

$$X_2=\frac{1}{4}\,\frac{e^{2u}}{e^u+1}\sin v\,p_u^2-\frac{1}{4}\,\frac{e^u(e^u+2)}{e^u+1}\sin v\,p_v^2-\frac{1}{2}e^u\cos v\,p_u p_v\,.$$

The integrals satisfy the polynomial algebra relations

$$\{K,X_1\}=-X_2\,,\quad \{K,X_2\}=X_1\,,\quad \{X_1,X_2\}=KH_0\,.$$

They are functionally dependent via the relation

$$X_1^2+X_2^2-H_0^2-H_0K^2=0.$$

The corresponding problem in quantum mechanics can readily be obtained via the usual quantization rules and symmetrization,

$$\hat{H}_0=\frac{1}{4}\,\frac{e^{2u}}{e^u+1}(\partial_u^2+\partial_v^2)\,,\quad \hat{K}=\partial_v\,,$$

$$\hat{X}_1=\frac{1}{4}\,\frac{e^{2u}}{e^u+1}\cos v\,\partial_u^2-\frac{1}{4}\,\frac{e^u(e^u+2)}{e^u+1}\cos v\,\partial_v^2+\frac{1}{2}e^u\sin v\,\partial_u\partial_v+\frac{1}{4}e^u\cos v\,\partial_u+\frac{1}{4}e^u\sin v\,\partial_v\,,$$

$$\hat{X}_2=\frac{1}{4}\,\frac{e^{2u}}{e^u+1}\sin v\,\partial_u^2-\frac{1}{4}\,\frac{e^u(e^u+2)}{e^u+1}\sin v\,\partial_v^2-\frac{1}{2}e^u\cos v\,\partial_u\partial_v+\frac{1}{4}e^u\sin v\,\partial_u-\frac{1}{4}e^u\cos v\,\partial_v\,.$$

The commutator algebra obtained has the same form as the Poisson algebra, and the identity relating the operators is

$$\hat{X}_1^2+\hat{X}_2^2-\hat{H}_0^2-\hat{H}_0\hat{K}^2+\tfrac{1}{4}\hat{H}_0=0\,.$$

The line element $\mathrm{d}s^2=(e^{-u}+e^{-2u})(\mathrm{d}u^2+\mathrm{d}v^2)$ can be realized as a two-dimensional surface embedded in three dimensions by

$$X=v\sqrt{e^{-u}+e^{-2u}}\,,\quad Y-T=\sqrt{e^{-u}+e^{-2u}},$$

$$Y+T=(1-v^2)\sqrt{e^{-u}+e^{-2u}}+\log(1+2e^{-u}+2\sqrt{e^{-u}+e^{-2u}})+\tfrac{1}{2}\arctan(2\sqrt{e^{-u}+e^{-2u}})\,,$$

in which case,

$$ds^2 = dX^2 + dY^2 - dT^2 = (e^{-u} + e^{-2u})(du^2 + dv^2)\,.$$

Just as we have done in other cases, we wish to determine all the essentially different separable coordinate systems for the free classical or quantum particle. To do this we need to consider a general quadratic constant of the form $\lambda = aX_1 + bX_2 + cK^2$. Under the adjoint action of $\exp(\alpha K)$, X_1 and X_2 transform according to

$$X_1 \to \cos\alpha\ X_1 - \sin\alpha\ X_2, \quad X_2 \to \sin\alpha\ X_1 + \cos\alpha\ X_2\,.$$

From this transformation law we see that λ can take five different forms

$$K^2, \quad X_1, \quad X_1 + \gamma K^2, \quad X_1 + iX_2, \quad X_1 + iX_2 - K^2. \tag{3.2}$$

We now demonstrate the explicit coordinates in the case of each of these representatives.

1. Coordinates associated with K^2

These are the coordinates associated with the ignorable coordinate v and the Hamiltonian has already been given in the u,v coordinates. The Hamilton–Jacobi equation is

$$\frac{1}{4}\frac{e^{2u}}{e^u+1}\left(\left(\frac{\partial S}{\partial u}\right)^2 + \left(\frac{\partial S}{\partial v}\right)^2\right) = E\,,$$

with solutions

$$S(u,v) = -\frac{\sqrt{4E(1+e^u) - c^2e^{2u}}}{ce^u} - \frac{\sqrt{E}}{c}\operatorname{arctanh}\left(\frac{\sqrt{E}(e^u+2)}{\sqrt{4E(1+e^u) - c^2e^{2u}}}\right)$$
$$+ i\log(i(c^2e^u - 2E) + c\sqrt{4E(1+e^u) - c^2e^{2u}}) + cv\,.$$

The corresponding Schrödinger equation is

$$\frac{1}{4}\frac{e^{2u}}{e^u+1}(\partial_u^2 + \partial_v^2)\Psi = E\Psi,$$

with solutions of the form

$$\Psi = e^{-u/2}M_{-1/\sqrt{-E},\,\pm m}(4\sqrt{-E}\,e^{-u})e^{imv}.$$

2. Coordinates associated with X_1

For the second representative in (3.2), a suitable choice of variables is

$$\xi = 2e^{-u/2}\cos\frac{v}{2}, \quad \eta = 2e^{-u/2}\sin\frac{v}{2}. \tag{3.3}$$

In terms of these coordinates the classical Hamiltonian has the form

$$H_0 = \frac{p_\xi^2 + p_\eta^2}{4 + \xi^2 + \eta^2}$$

and the corresponding quadratic constant is

$$X_1 = \frac{(2+\eta^2)p_\xi^2 - (2+\xi^2)p_\eta^2}{2(4+\xi^2+\eta^2)}.$$

In ξ, η coordinates the classical Hamilton–Jacobi equation is

$$\frac{\left(\frac{\partial S}{\partial \xi}\right)^2+\left(\frac{\partial S}{\partial \eta}\right)^2}{4+\xi^2+\eta^2}=E\,,$$

which has the solution

$$S=\frac{1}{2}\xi\sqrt{E\xi^2+2E-\lambda}+\left(\frac{2E-\lambda}{2\sqrt{E}}\right)\log(E+\sqrt{E\xi^2+2E-\lambda})$$
$$+\frac{1}{2}\eta\sqrt{E\eta^2+2E+\lambda}+\left(\frac{2E+\lambda}{2\sqrt{E}}\right)\log(E+\sqrt{E\eta^2+2E+\lambda})\,.$$

The Schrödinger equation is

$$\frac{(\partial_\xi^2+\partial_\eta^2)\Psi}{4+\xi^2+\eta^2}=E\Psi\,,$$

which has typical solutions

$$\Psi=D_{(\lambda-2E)/\sqrt{4E}}(\pm(4E)^{1/4}\xi)D_{-(\lambda+E)/\sqrt{4E}}(\pm(4E)^{1/4}\eta)\,,$$

in terms of parabolic cylinder functions $D_\nu(z)$.[8,9]

3. Coordinates associated with $X_1+\gamma K^2$

For the third case it is convenient to take the representative as $b^2X_1+2K^2$. Here we identify coordinates via

$$\xi=b\cosh\omega\cos\varphi\,,\quad \eta=b\sinh\omega\sin\varphi\,. \tag{3.4}$$

The classical Hamiltonian has the form

$$H_0=\frac{p_\omega^2+p_\varphi^2}{2b^2(\cosh 2\omega-\cos 2\varphi)+\frac{1}{4}b^4(\cosh^2 2\omega-\cos^2 2\varphi)}$$

and the corresponding quadratic constant in these coordinates is

$$b^2X_1+2K^2=\frac{(8\cos 2\varphi-b^2\sin 2\varphi)p_\omega^2+(8\cosh 2\omega+b^2\sinh 2\omega)p_\varphi^2}{8b^2(\cosh 2\omega-\cos 2\varphi)+b^4(\cosh^2 2\omega-\cos^2 2\varphi)}.$$

In the φ, ω coordinates the classical Hamilton–Jacobi equation has the form

$$\frac{\left(\frac{\partial S}{\partial \omega}\right)^2+\left(\frac{\partial S}{\partial \varphi}\right)^2}{2b^2(\cosh 2\omega-\cos 2\varphi)+\frac{1}{4}b^4(\cosh^2 2\omega-\cos^2 2\varphi)}=E\,,$$

and has the solution

$$S(\omega,\varphi)=\frac{1}{4}b^2\sqrt{E}\left(\int\sqrt{\frac{(\Omega-\alpha_1)(\Omega-\alpha_2)}{\Omega^2-1}}\,d\Omega+\int\sqrt{\frac{(\beta_1-\Phi)(\Phi-\beta_2)}{1-\Phi^2}}\,d\Phi\right),$$

where $\alpha_1+\alpha_2=-\beta_1-\beta_2=-8/b^2$, $\alpha_1\alpha_2=-\beta_1\beta_2-4\lambda/Eb^2$, $\Omega=\cosh 2\omega$, $\Phi=\cos 2\varphi$. The corresponding Schrödinger equation,

$$\frac{\partial_\omega^2\Psi+\partial_\varphi^2\Psi}{2b^2(\cosh 2\omega-\cos 2\varphi)+\frac{1}{4}b^4(\cosh^2 2\omega-\cos^2 2\varphi)}=E\Psi\,,$$

separates with $\Psi=\Phi(\varphi)\Omega(\omega)$ in the equations

$$(\partial_\varphi^2+2b^2E\cos 2\varphi+\tfrac{1}{8}b^4E\cos 4\varphi+\lambda+\tfrac{1}{8}b^4E)\Phi=0\,,$$

$$(\partial_\omega^2-2b^2E\cos 2\omega-\tfrac{1}{8}b^4E\cos 4\omega-\lambda-\tfrac{1}{8}b^4E)\Omega=0\,,$$

which has typical solutions

$$\Psi_1=gc_m(\varphi,b\sqrt{-E},2b\sqrt{-E})gc_m(i\omega,b\sqrt{-E},2b\sqrt{-E}),$$

$$\Psi_2=gs_m(\varphi,b\sqrt{-E},2b\sqrt{-E})gs_m(i\omega,b\sqrt{-E},2b\sqrt{-E}),$$

with corresponding separation constant given by $\lambda_m=\mu_m b^2(1+b^2)E/8$. The functions appearing here are even and odd Whittaker Hill functions.[10]

4. Coordinates associated with X_1+iX_2

In the case of a system specified by the fourth representative there are, in fact, no separable coordinates. However, in the coordinates

$$x=\xi+i\eta\,,\quad y=\tfrac{1}{2}(\xi-i\eta)^2\,,$$

the classical Hamiltonian takes the form

$$H_0=\frac{2p_xp_y}{2y^{-1/2}+x}$$

and the corresponding constant is

$$X_1+iX_2=2yH_0-p_x^2\,.$$

The solution of the Hamilton–Jacobi equation

$$\frac{2\dfrac{\partial S}{\partial x}\dfrac{\partial S}{\partial y}}{2y^{-1/2}+x}=E$$

is

$$S=x\sqrt{Ey-\lambda}+\sqrt{E}\log\left(\sqrt{E}\;y-\frac{\lambda}{2\sqrt{E}}+\sqrt{Ey^2-\lambda y}\right).$$

The corresponding Schrödinger equation is

$$\frac{2\partial_x\partial_y\Psi}{2y^{-1/2}+x}=E\Psi,$$

which has solutions

$$\Psi=\frac{(2E^{3/2}y-E^{1/2}+2E\sqrt{Ey^2-\lambda y})^{\sqrt{E}}e^{x\sqrt{Ey-\lambda}}}{\sqrt{Ey-\lambda}}.$$

5. Coordinates associated with $X_1+iX_2-K^2$

In the case of a system specified by the fifth representative an appropriate choice of coordinates is

$$\xi=\frac{\mu-\nu}{2\sqrt{\mu\nu}}+\sqrt{\mu\nu},\quad \eta=i\left(\frac{\mu-\nu}{2\sqrt{\mu\nu}}-\sqrt{\mu\nu}\right). \tag{3.5}$$

The corresponding classical Hamiltonian has the form

$$H_0=\frac{\mu^2p_\mu^2-\nu^2p_\nu^2}{(\mu+\nu)(2+\mu-\nu)},$$

and the quadratic constant is

$$X_1+iX_2-K^2=\frac{\nu^2(\mu+2)\mu p_\nu^2-\mu^2(\nu-2)\nu p_\mu^2}{(\mu+\nu)(2+\mu-\nu)}.$$

In the μ, ν coordinate system the classical Hamilton–Jacobi equation has the form

$$\frac{\mu^2\left(\frac{\partial S}{\partial\mu}\right)^2-\nu^2\left(\frac{\partial S}{\partial\nu}\right)^2}{(\mu+\nu)(2+\mu-\nu)}=E,$$

which has the solution

$$\begin{aligned}S(\mu,\nu)=&\sqrt{E\mu^2+2E\mu+\lambda}+\sqrt{E}\log(\sqrt{E}(1+\mu)+\sqrt{E\mu^2+2E\mu+\lambda})\\&-\sqrt{\lambda}\,\operatorname{arctanh}\left(\frac{\lambda+E\mu}{\sqrt{\lambda}\sqrt{E\mu^2+2E\mu+\lambda}}\right)+\sqrt{E\nu^2-2E\nu+\lambda}+\sqrt{E}\log(\sqrt{E}(1-\nu)\\&+\sqrt{E\nu^2-2E\nu+\lambda})-\sqrt{\lambda}\,\operatorname{arctanh}\left(\frac{\lambda-E\nu}{\sqrt{\lambda}\sqrt{E\nu^2-2E\nu+\lambda}}\right).\end{aligned}$$

The Schrödinger equation

$$\frac{\mu\partial_\mu(\mu\partial_\mu\Psi)-\nu\partial_\nu(\nu\partial_\nu\Psi)}{(\mu+\nu)(2+\mu-\nu)}=E\Psi$$

separates with $\Psi=A(\mu)B(\nu)$ into the equations

$$(\mu\partial_\mu(\mu\partial_\mu)-E\mu^2-2E\mu-\rho^2)A(\mu)=0,\quad(\nu\partial_\nu(\nu\partial_\nu)-E\nu^2-2E\nu-\rho^2)B(\nu)=0,$$

and has solutions, in terms of the Whittaker function $M_{\lambda,\chi}$, of the form[9]

$$\frac{1}{\sqrt{\mu\nu}}M_{\sqrt{E},\rho}(2\sqrt{E}\ \ \mu)M_{-\sqrt{E},\rho}(2\sqrt{E}\ \ \nu).$$

If we write the classical equation $H=E$ in ξ, η coordinates, we obtain

$$p_\xi^2+p_\eta^2-E(4+\xi^2+\eta^2)=0.$$

This is in the form of a flat space superintegrable system which can be solved by separation of variables in Cartesian, polar, hyperbolic, and elliptic coordinates.

B. Superintegrability for Darboux spaces of type three

In this section we address the problem of superintegrability for the Hamiltonian

$$H=\frac{1}{4}\,\frac{e^{2u}(p_u^2+p_v^2)}{e^u+1}. \tag{3.6}$$

We arrive at five possibilities: [**A**], [**B**], [**C**], [**D**], [**E**].

$$[\mathbf{A}]\quad H=\frac{p_\xi^2+p_\eta^2+a_1\xi+a_2\eta+a_3}{4+\xi^2+\eta^2}.$$

The additional constants have the form

$$R_1=X_1+\frac{2a_1\xi(2+\eta^2)-2a_2\eta(2+\xi^2)+a_3(\eta^2-\xi^2)}{4(4+\xi^2+\eta^2)},$$

$$R_2=X_2+\frac{a_1\eta(\eta^2-\xi^2+4)+a_2\xi(\xi^2-\eta^2+4)-2a_3\xi\eta}{4(4+\xi^2+\eta^2)}.$$

The corresponding quadratic algebra can be determined from the identity

$$R^2=HR_1^2+HR_2^2+\tfrac{1}{8}(a_2^2-a_1^2)R_1-\tfrac{1}{4}a_1a_2R_2-H^3+\tfrac{1}{2}a_3H^2$$
$$+\tfrac{1}{16}(2a_2^2+2a_1^2-a_3^2)H-\tfrac{1}{32}a_3(a_1^2+a_2^2)\,.$$

This Hamiltonian separates in a family of coordinate systems obtained by translating the given separable system via $\xi\to\xi+a$, $\eta\to\eta-a$. The corresponding quantum algebra relations are

$$[\hat R,\hat R_1]=-\hat H\hat R_2+\tfrac{1}{8}a_1a_2\,,\quad [\hat R,\hat R_2]=\hat H\hat R_1+\tfrac{1}{16}(a_2^2-a_1^2)\,,$$

$$\hat R^2=\hat H\hat R_1^2+\hat H\hat R_2^2+\tfrac{1}{8}(a_2^2-a_1^2)\hat R_1-\tfrac{1}{4}a_1a_2\hat R_2-\hat H^3+\tfrac{1}{2}(a_3+\tfrac{1}{2})\hat H^2$$
$$+\tfrac{1}{16}(2a_1^2+2a_2^2-a_3^2)\hat H-\tfrac{1}{32}a_3(a_1^2+a_2^2).$$

As in the case of free motion, the equation $H=E$ becomes

$$p_\xi^2+p_\eta^2+a_1\xi+a_2\eta+a_3-E(4+\xi^2+\eta^2)=0\,.$$

Again, this is a superintegrable system in flat space but with rearranged constants.

$$[\mathbf{B}]\quad H=\frac{p_\xi^2+p_\eta^2+\dfrac{b_1}{\xi^2}+\dfrac{b_2}{\eta^2}+b_3}{4+\xi^2+\eta^2}.$$

The additional constants are

$$R_1=X_1+\frac{2b_1\eta^2(\eta^2+2)-2b_2\xi^2(\xi^2+2)+b_3(\eta^2-\xi^2)}{4(4+\xi^2+\eta^2)}, \tag{3.7}$$

$$R_2 = K^2 + \frac{b_1\eta^2}{4\xi^2} + \frac{b_2\xi^2}{4\eta^2}. \tag{3.8}$$

The corresponding quadratic algebra relations are determined by

$$R^2 = -4R_1^2R_2 - (b_1+b_2)R_1^2 + 4HR_2^2 + 2(b_1-b_2)HR_1 + \tfrac{1}{2}b_3(b_2-b_1)R_1 + 4H^2R_2 - 2b_3HR_2$$
$$+ \tfrac{1}{4}b_3^2R_2 - (b_1+b_2)H^2 + (\tfrac{1}{2}b_3(b_1+b_2) - b_1b_2)H - \tfrac{1}{16}b_3^2(b_1+b_2).$$

This Hamiltonian separates in all the separable coordinate systems given in Sec. II A. The Hamiltonian has the following explicit forms:

(i) In u, v coordinates,

$$H = \frac{e^{2u}\left(p_u^2 + p_v^2 + \tfrac{1}{4}b_1\sec^2\frac{v}{2} + \tfrac{1}{4}b_2\,\mathrm{cosec}^2\frac{v}{2} + b_3e^{-u}\right)}{4(e^u+1)}.$$

(ii) In the elliptical coordinates (3.4),

$$H = \frac{p_\omega^2 + p_\varphi^2 + b_1(\sec^2\varphi - \mathrm{sech}^2\omega) + b_2(\mathrm{cosec}^2\varphi + \mathrm{cosech}^2\omega) + b_3b^2(\cosh^2\omega - \cos^2\varphi)}{2b^2(\cosh 2\omega - \cos 2\varphi) + \tfrac{1}{4}b^4(\cosh^2 2\omega - \cos^2 2\varphi)}.$$

The corresponding quantum algebra relations have the form

$$[\hat{R},\hat{R}_1] = 2\hat{R}_1^2 - 4\hat{H}\hat{R}_2 - 2\hat{H}^2 + (b_3 + \tfrac{1}{2})\hat{H} - \tfrac{1}{8}b_3^2,$$

$$[\hat{R},\hat{R}_2] = -2\{\hat{R}_1,\hat{R}_2\} - (b_1+b_2+1)\hat{R}_1 + (b_1-b_2)\hat{H} + \tfrac{1}{4}(b_2-b_1)b_3,$$

$$\hat{R}^2 = -2\{\hat{R}_1^2,\hat{R}_2\} - (b_1+b_2+5)\hat{R}_1^2 + 4\hat{H}\hat{R}_2^2 + 2(b_1-b_2)\hat{H}\hat{R}_1 + b_3(b_2-b_1)\hat{R}_1 + 4\hat{H}^2\hat{R}_2$$
$$-(2b_3-1)\hat{H}\hat{R}_2 + \tfrac{1}{4}b_3^2\hat{R}_2 - (b_1+b_2-2)\hat{H}^2 + (\tfrac{1}{2}(b_3+\tfrac{3}{2})(b_1+b_2) - b_3 - b_1b_2 - \tfrac{1}{2})H$$
$$-\tfrac{1}{16}b_3^2(b_1+b_2-2).$$

As in the case of free motion, we observe that equation $H=E$ becomes

$$p_\xi^2 + p_\eta^2 + \frac{b_1}{\xi^2} + \frac{b_2}{\eta^2} + b_3 - E(4+\xi^2+\eta^2) = 0.$$

This is a superintegrable system in flat space, with rearranged constants, that separates variables in Cartesian, polar, and elliptic coordinates.

$$[\mathbf{C}] \quad H = \frac{\mu^2p_\mu^2 - \nu^2p_\nu^2 + c_1(\mu+\nu) + c_2\dfrac{\mu+\nu}{\mu\nu} + c_3\dfrac{\mu^2-\nu^2}{\mu^2\nu^2}}{(\mu+\nu)(2+\mu-\nu)}.$$

The additional constants of the motion have the form

$$R_1 = X_1 + iX_2 - \frac{c_1\mu^2\nu^2 + c_2\mu\nu + 2c_3(1+\mu-\nu)}{\mu\nu(2+\mu-\nu)}, \quad R_2 = K^2 - c_2\frac{\mu-\nu}{\mu\nu} - c_3\frac{(\mu-\nu)^2}{\mu^2\nu^2}.$$

The corresponding quadratic Poisson algebra relations can be determined from

$$R^2 = -4R_2R_1^2 + 8c_2HR_1 - 4c_1c_2R_1 + 16c_3HR_2 + 16c_3H^2 + 4(c_2^2 - 4c_1c_3)H + 4c_1^2c_3.$$

The quantum algebra relations are

$$[\hat{R},\hat{R}_1]=2\hat{R}_1^2-8c_3\hat{H}\,,\quad [\hat{R},\hat{R}_2]=-2\{\hat{R}_1,\hat{R}_2\}-\hat{R}_1+4c_2\hat{H}-2c_1c_2\,,$$

$$\hat{R}^2=-2\{\hat{R}_1^2,\hat{R}_2\}+8c_2\hat{H}\hat{R}_1+16c_3\hat{H}\hat{R}_2-5\hat{R}_1^2-4c_1c_2\hat{R}_1$$
$$+16c_3\hat{H}^2+4(c_3+c_2^2-4c_1c_3)\hat{H}+4c_1^2c_3\,.$$

As in the case of free motion, equation $H=E$ becomes

$$p_\xi^2+p_\eta^2+2c_1+\frac{8c_2}{(\xi+i\eta)^2}+\frac{16c_3(\xi-i\eta)}{(\xi+i\eta)^3}-E(4+\xi^2+\eta^2)=0,$$

a superintegrable system in flat space with rearranged constants, that separates variables in polar and hyperbolic coordinates.

$$[\mathbf{D}]\quad H=\frac{\mu^2p_\mu^2-\nu^2p_\nu^2+\mathrm{d}_1\mu+\mathrm{d}_2\nu+\mathrm{d}_3(\mu^2+\nu^2)}{(\mu+\nu)(2+\mu-\nu)}.$$

The additional constants of the motion have the form

$$R_1=X_1+iX_2-K^2-\frac{\mu\nu(\mathrm{d}_1(\nu-2)+\mathrm{d}_2(\mu+2)+2\mathrm{d}_3(\nu-\mu+\mu\nu))}{(\mu+\nu)(2+\mu-\nu)},$$

$$R_2=X_1-iX_2-\frac{(\mu-\nu)((\mu-\nu)(\mathrm{d}_1\mu+\mathrm{d}_2\nu)-2\mathrm{d}_3(\mu^2+\nu^2+\mu\nu(2+\mu-\nu)))}{4\mu\nu(\mu+\nu)(2+\mu-\nu)}.$$

The corresponding quadratic Poisson algebra can be determined from

$$R^2=4R_1R_2^2-4HR_1R_2+\mathrm{d}_3^2R_1-4H^2R_2+2(\mathrm{d}_1+\mathrm{d}_2)HR_2-\mathrm{d}_1\mathrm{d}_2R_2+4H^3-2(\mathrm{d}_1+\mathrm{d}_2)H^2$$
$$+\tfrac{1}{4}((\mathrm{d}_1+\mathrm{d}_2)^2+\mathrm{d}_3(\mathrm{d}_2-\mathrm{d}_1))H-\mathrm{d}_3(\mathrm{d}_1^2-\mathrm{d}_2^2).$$

This classical system also separates in elliptical coordinates obtained by choosing new variables defined by the roots of the characteristic equation of R_1+R_2, that is, the elliptical coordinates (3.4) with $b=2i$. In these variables the Hamiltonian has the form

$$H=\frac{p_\omega^2+p_\varphi^2+2(\mathrm{d}_1+\mathrm{d}_2)(\cos 2\varphi-\cosh 2\omega)+2(\mathrm{d}_1-\mathrm{d}_2)(2i\sin 2\varphi+\sinh 2\omega)+2\mathrm{d}_3(\sinh 4\omega+2\mathrm{i}\sin 4\phi)}{8(\cos 2\varphi-\cosh 2\omega)+4(\cosh^2 2\omega-\cos^2 2\varphi)}.$$

The corresponding quantum algebra relations are

$$[\hat{R},\hat{R}_1]=-2\{\hat{R}_1,\hat{R}_2\}+2\hat{H}\hat{R}_1+\hat{R}_2+2\hat{H}^2-(\mathrm{d}_1+\mathrm{d}_2+\tfrac{1}{2})\hat{H}+\tfrac{1}{2}\mathrm{d}_1\mathrm{d}_2\,,$$

$$[\hat{R},\hat{R}_2]=2\hat{R}_2^2-2\hat{H}\hat{R}_2+\tfrac{1}{2}\mathrm{d}_3^2,$$

$$\hat{R}^2=2\{\hat{R}_1,\hat{R}_2^2\}-5\hat{R}_2^2-2\hat{H}\{\hat{R}_1,\hat{R}_2\}+\mathrm{d}_3^2\hat{R}_1-4\hat{H}^2\hat{R}_2+(2\mathrm{d}_1+2\mathrm{d}_2+5)\hat{H}\hat{R}_2-\mathrm{d}_1\mathrm{d}_2\hat{R}_2+4\hat{H}^3$$
$$-(2\mathrm{d}_1+2\mathrm{d}_2+1)\hat{H}^2+(\tfrac{1}{4}(\mathrm{d}_1+\mathrm{d}_2)^2+\mathrm{d}_3(\mathrm{d}_2-\mathrm{d}_1))\hat{H}-\tfrac{1}{4}\mathrm{d}_3(\mathrm{d}_3-\mathrm{d}_1^2+\mathrm{d}_2^2).$$

As in the case of free motion we observe that equation $H=E$ becomes

$$p_\xi^2+p_\eta^2+\mathrm{d}_1+\mathrm{d}_2-4\mathrm{d}_3+\frac{(\mathrm{d}_2-\mathrm{d}_1)(\xi-i\eta)}{\sqrt{(\xi-i\eta)^2+4}}+\frac{8\mathrm{d}_3(\xi+i\eta)}{\sqrt{(\xi-i\eta)^2+4}(\xi-i\eta+\sqrt{(\xi-i\eta)^2+4})^2}$$
$$=(E-\mathrm{d}_3)(4+\xi^2+\eta^2),$$

a superintegrable system in flat space with rearranged constants that separates variables in elliptic and hyperbolic coordinates.

$$[\mathbf{E}]\quad H=\frac{p_\xi^2+p_\eta^2+c}{4+\xi^2+\eta^2}.$$

The additional constants of the motion are

$$R_1=X_1+\frac{c}{4}\frac{\eta^2-\xi^2}{4+\xi^2+\eta^2},\quad R_2=X_2-\frac{c}{2}\frac{\xi\eta}{4+\xi^2+\eta^2},$$

and K. The corresponding Poisson algebra relations have the form

$$\{K,R_1\}=-R_2,\quad \{K,R_2\}=R_1,\quad \{R_1,R_2\}=HK,$$

and the functional relation between these constants is

$$R_1^2+R_2^2-HK^2-H^2+\frac{c}{2}H-\frac{c^2}{16}=0.$$

This Hamiltonian separates in all of the four types of separable coordinate systems available, and the corresponding expressions for the Hamiltonian can be deduced from Ref. 2 by taking $b_3=c,\ b_1=b_2=0$.

The quantum algebra relations are

$$[\hat{K},\hat{R}_1]=-\hat{R}_2,\ [\hat{K},\hat{R}_2]=\hat{R}_1,\ [\hat{R}_1,\hat{R}_2]=\hat{H}\hat{K},$$

and the associated operator identity is

$$\hat{R}_1^2+\hat{R}_2^2-\hat{H}\hat{K}^2-\hat{H}^2+\left(\frac{c}{2}+\frac{1}{4}\right)\hat{H}-\frac{c^2}{16}=0.$$

IV. DARBOUX SPACES OF TYPE FOUR

A. The free particle and separating coordinate systems

With rescaling of the variables x and y, the Hamiltonian H can be taken in the form

$$H_0=\frac{(e^{x-y}-e^{y-x})^2}{e^{x-y}+e^{y-x}+a}\ p_x p_y. \tag{4.1}$$

In coordinates $x=v+iu,\ y=v-iu$, we can write the Hamiltonian as

$$H_0=-\frac{\sin^2 2u(p_u^2+p_v^2)}{2\cos 2u+a}.$$

It admits constants of the motion

$$K=p_v,\quad X_1=e^{2v}(-H_0+\cos 2u\ \ p_u^2+\sin 2u\ \ p_u p_v),$$

$$X_2 = e^{-2v}(-H_0 + \cos 2u \;\; p_v^2 - \sin 2u \;\; p_u p_v).$$

These integrals satisfy the polynomial algebra relations

$$\{K, X_1\} = 2X_1, \quad \{K, X_2\} = -2X_2, \quad \{X_1, X_2\} = -8K^3 - 4aKH_0.$$

They are functionally dependent via the relation

$$X_1 X_2 - K^4 - aK^2 H_0 - H_0^2 = 0.$$

The corresponding quantum operators are

$$\hat{H}_0 = \frac{-\sin^2 2u}{2\cos 2u + a}\,(\partial_u^2 + \partial_v^2), \quad \hat{X}_1 = e^{2v}(-\hat{H}_0 + \cos 2u(\partial_v^2 + \partial_v) + \sin 2u(\partial_u \partial_v + \partial_u)),$$

$$\hat{K} = \partial_v, \quad \hat{X}_2 = e^{-2v}(-\hat{H}_0 + \cos 2u(\partial_v^2 - \partial_v) - \sin 2u(\partial_u \partial_v - \partial_u)).$$

Their algebra is determined by the relations

$$[\hat{K}, \hat{X}_1] = 2\hat{X}_1, \quad [\hat{K}, \hat{X}_2] = -2\hat{X}_2, \quad [\hat{X}_1, \hat{X}_2] = -8\hat{K}^3 - 4a\hat{K}\hat{H}_0 - 4\hat{K},$$

and the operator identity is

$$\tfrac{1}{2}\{\hat{X}_1, \hat{X}_2\} - \hat{K}^4 - a\hat{H}_0\hat{K}^2 - 5\hat{K}^2 - \hat{H}_0^2 - a\hat{H}_0 = 0.$$

The line element $ds^2 = (2\cos u + a)(du^2 + dv^2)/\sin^2 2u$ can be realized as a two-dimensional surface embedded in $E(2,1)$ by (assuming $a > 2$)

$$X = \sqrt{a + 2\cos 2u}\, v, \quad Y - T = \sqrt{a + 2\cos 2u},$$

$$Y + T = \frac{(a-2)}{\sqrt{2(a+2)}}\left[\Pi\left(\chi, \sqrt{\frac{a-2}{a+2}}\frac{2}{(r_1+1)}, p\right) + \Pi\left(\chi, \sqrt{\frac{a-2}{a+2}}\frac{2}{(r_2+1)}, p\right)\right] - \sqrt{a + 2\cos 2u}\, v^2,$$

where

$$\sin\chi = \sqrt{\frac{(a+2)(\cos 2u + 1)}{2(a + 2\cos 2u)}}, \quad p = \frac{2}{\sqrt{a+2}},$$

and Π is an elliptic integral of the third kind.[8] Then $ds^2 = dX^2 + dY^2 - dT^2$.

Just as we have done in other cases, we wish to determine all the essentially different separable coordinate systems for the free classical or quantum particle. To do this we need to consider a general quadratic constant of the form $\lambda = aX_1 + bX_2 + cK^2$. Under the adjoint action of $\exp(\alpha K)$, X_1 and X_2 transform according to

$$X_1 \to \exp(-2\alpha) X_1, \quad X_2 \to \exp(2\alpha) X_2.$$

If we regard two such quadratic expressions as equivalent if they are related by a combination of group motions and the discrete transformation observed above, then the equivalence classes of these expressions can be chosen to have the following representatives:

$$K^2, \quad X_2, \quad \gamma X_2 + K^2, \quad X_1 + X_2 + \gamma K^2. \tag{4.2}$$

In the last of these are three cases to distinguish: $\gamma = 0$, $\gamma = 2$, and $\gamma \neq 0,2$. The various separable systems involved can now be computed.

1. Coordinates associated with K^2

These are the coordinates associated with the ignorable coordinate v and the Hamiltonian has already been given in the u,v coordinates. The Hamilton–Jacobi equation is

$$-\frac{\sin^2 2u}{2\cos 2u+a}\left(\left(\frac{\partial S}{\partial v}\right)^2+\left(\frac{\partial S}{\partial u}\right)^2\right)=E\,.$$

It has typical solutions

$$\begin{aligned}S(u,v)=&-i\log(i(c^2\cos 2u-E)+c\sqrt{E(a+2\cos 2u)+c^2\sin^2 2u})\\&+\frac{1}{2c}\sqrt{E(a+2)}\quad\operatorname{arctanh}\left(\frac{E(a+1)+c^2+(E-c^2)\cos 2u}{\sqrt{E(a+2)(E(a+2\cos 2u)+c^2\sin^2 2u}}\right)\\&+\frac{1}{2c}\sqrt{E(a-2)}\ \operatorname{arctanh}\left(\frac{E(a-1)+c^2+(E+c^2)\cos 2u}{\sqrt{E(a-2)(E(a+2\cos 2u)+c^2\sin^2 2u}}\right)+cv\,.\end{aligned}$$

The corresponding Schrödinger equation is

$$\frac{\sin^2 2u}{2\cos 2u+a}\left(\frac{\partial^2\Psi}{\partial v^2}+\frac{\partial^2\Psi}{\partial u^2}\right)=E\Psi\,,$$

which has the solution

$$\Psi={}_2F_1(\tfrac{1}{2}(\lambda-\epsilon_+-\epsilon_-),\tfrac{1}{2}(\lambda+\epsilon_++\epsilon_-),\epsilon_++\tfrac{1}{2},\sin^2 u)e^{\lambda v}\,,$$

where

$$\epsilon_\pm=\tfrac{1}{2}+\tfrac{1}{2}\sqrt{1-(a\pm 2)E}\,,\tag{4.3}$$

and ${}_2F_1$ is a Gaussian hypergeometric function.[11]

2. Coordinates associated with X_2

If we choose new coordinates

$$x=\log(\tfrac{1}{2}(\mu-i\nu))\,,\quad y=\log(\tfrac{1}{2}(\mu+i\nu))\,,\tag{4.4}$$

then the Hamiltonian takes the rational form

$$H_0=-\frac{4\mu^2\nu^2(p_\mu^2+p_\nu^2)}{(a+2)\mu^2+(a-2)\nu^2}.$$

In this case the corresponding choice of coordinates has already been given, and the quadratic constant in these coordinates is

$$X_2=\frac{4(a+2)\mu^2p_\mu^2-4(a-2)\nu^2p_\nu^2}{(a+2)\mu^2+(a-2)\nu^2}.$$

The Hamilton–Jacobi equation

$$-\frac{\mu^2\nu^2\left(\left(\frac{\partial S}{\partial\mu}\right)^2+\left(\frac{\partial S}{\partial\nu}\right)^2\right)}{(a+2)\mu^2+(a-2)\nu^2}=E,$$

has solution

$$S(\mu,\nu)=i\sqrt{(a-2)E+\lambda\mu^2}-i\sqrt{(a-2)E}\ \operatorname{arctanh}\sqrt{\frac{(a-2)E+\lambda\mu^2}{(a-2)E}}$$
$$+\sqrt{(a+2)E-\lambda\nu^2}-\sqrt{(a+2)E}\ \operatorname{arctanh}\sqrt{\frac{(a+2)E-\lambda\nu^2}{(a+2)E}}.$$

The corresponding Schrödinger equation has Bessel function solutions of the form

$$\Psi=\sqrt{\mu\nu}\ C_{1/2\sqrt{1-E(a-2)}}\left(\tfrac{1}{2}\sqrt{\lambda}\mu\right)\ C_{1/2\sqrt{1-E(a+2)}}\left(\tfrac{1}{2}\sqrt{\lambda}\ i\nu\right).$$

3. Coordinates associated with γX_2+K^2

In the case of the third representative the transformation

$$\mu=c\cosh\omega\cos\varphi,\qquad \nu=c\sinh\omega\sin\varphi \tag{4.5}$$

gives the classical Hamiltonian

$$H=\frac{4(p_\omega^2+p_\varphi^2)}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}.$$

The classical constant associated with this coordinate system is

$$-\frac{c^2}{4}X_2+K^2=\frac{((a-2)\sec^2\varphi+(a+2)\operatorname{cosec}^2\varphi)p_\omega^2+((a-2)\operatorname{sech}^2\omega-(a+2)\operatorname{cosech}^2\omega)p_\varphi^2}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}.$$

The Hamilton–Jacobi equation in these coordinates is

$$\frac{4(p_\omega^2+p_\varphi^2)}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}=E$$

and has solutions of the form

$$S(\omega,\varphi)=\frac{1}{4}\sqrt{\lambda}\log\left(\sqrt{\lambda}\ (\lambda\cos 2\varphi+2aE)+\lambda\sqrt{8E+4aE\cos 2\varphi-\lambda\sin^2 2\varphi}\right)$$
$$-\frac{1}{4}\sqrt{(a+2)E}\ \operatorname{arctanh}\left(\frac{2Ea+8E-\lambda+\cos 2\varphi(\lambda+2Ea)}{2\sqrt{(a+2)E(8E+4aE\cos 2\varphi-\lambda\sin^2 2\varphi)}}\right)$$
$$-\frac{1}{4}\sqrt{(a-2)E}\ \operatorname{arctanh}\left(\frac{-2Ea+8E-\lambda+\cos 2\varphi(-\lambda+2Ea)}{2\sqrt{(a-2)E(8E+4aE\cos 2\varphi-\lambda\sin^2 2\varphi)}}\right)$$
$$+\frac{1}{4}\sqrt{\lambda}\log\left(\sqrt{\lambda}\ (\lambda\cosh 2\omega-4E)+\lambda\sqrt{\lambda\sinh^2 2\omega-8E\cosh 2\omega-4aE}\right)$$
$$+\sqrt{a+2}\ \arctan\left(\frac{4E+\lambda+4aE+\cosh 2\omega(4E-\lambda)}{2\sqrt{(a+2)E(\lambda\sinh^2\omega-8E\cosh 2\omega-4aE)}}\right)$$
$$+\sqrt{a-2}\ \arctan\left(\frac{-4E+\lambda+4aE+\cosh 2\omega(4E+\lambda)}{2\sqrt{(a-2)E(\lambda\sinh^2\omega-8E\cosh 2\omega-4aE)}}\right).$$

The Schrödinger equation has the form

$$\frac{4\left(\frac{\partial^2\Psi}{\partial\omega^2}+\frac{\partial^2\Psi}{\partial\varphi^2}\right)}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}=E\Psi$$

with corresponding solutions

$$\Psi=(\sin\varphi\sinh\omega)^{\epsilon_-}(\cos\varphi\cosh\omega)^{\epsilon_+}{}_2F_1\left(\frac{\epsilon_++\epsilon_--\lambda}{2},\frac{\epsilon_++\epsilon_-+\lambda}{2},\epsilon_-+\frac{1}{2},\sin^2\varphi\right)$$
$$\times{}_2F_1\left(\frac{\epsilon_++\epsilon_--\lambda}{2},\frac{\epsilon_++\epsilon_-+\lambda}{2},\epsilon_-+\frac{1}{2},-\sinh^2\omega\right)$$

with $\epsilon_\pm$ defined by (4.3).

4. Coordinates associated with $X_1+X_2+\gamma K^2$

For the coordinates corresponding to the fourth representative we make the transformation $u=\arctan(\exp\alpha)$, $v=\beta/2$, so our Hamiltonian has the form

$$H=-4\frac{p_\alpha^2+\operatorname{sech}^2\alpha p_\beta^2}{a-2\tanh\alpha}. \tag{4.6}$$

This can be realized in terms of projective coordinates on a two-dimensional complex sphere via $s_1=\cosh\alpha\cosh\beta$, $s_2=i\cosh\alpha\sinh\beta$, $s_3=i\sinh\alpha$ where $s_1^2+s_2^2+s_3^2=1$. The Hamiltonian can be written as

$$H=4\frac{J_1^2+J_2^2+J_3^2}{\frac{2is_3}{\sqrt{s_1^2+s_2^2}}+a}.$$

These two ways of realizing the classical Hamiltonian are useful in determining the various possible separable coordinate systems.

We consider the most general case first, i.e., $\gamma\neq 0,2$. We make use of the transformation equations

$$\sinh\alpha=i\frac{XY+1}{2\sqrt{XY}},$$

$$\tanh\beta=\frac{2\sqrt{(A_+X+A_-)(A_-X+A_+)(A_+Y+A_-)(A_-Y+A_+)}}{(A_+^2+A_-^2)(XY+1)+2A_+A_-(X+Y)},$$

applied to (4.6) to give classical Hamiltonian in the form

$$H=-16XY\frac{X(A_+X+A_-)(A_-X+A_+)p_X^2-Y(A_+Y+A_-)(A_-Y+A_+)p_Y^2}{A_+A_-(X-Y)((a+2)XY-a+2)}.$$

The corresponding classical constant associated with this coordinate system is

$$X_1+X_2+2\frac{A_+^2+A_-^2}{A_+^2-A_-^2}K^2$$

$$=16\frac{(A_+X+A_-)(A_-X+A_+)(a(A_+Y+A_-)(A_-Y+A_+)-2A_+A_-(Y^2-1))X^2p_X^2}{A_+A_-(A_+^2-A_-^2)(X-Y)((a+2)XY-a+2)}$$

$$-16\frac{(A_+Y+A_-)(A_-Y+A_+)(a(A_+X+A_-)(A_-X+A_+)-2A_+A_-(X^2-1))Y^2p_Y^2}{A_+A_-(A_+^2-A_-^2)(X-Y)((a+2)XY-a+2)}.$$

The Hamilton–Jacobi equation has the form

$$-16XY\frac{X(A_+X+A_-)(A_-X+A_+)\left(\frac{\partial S}{\partial X}\right)^2+Y(A_+Y+A_-)(A_-Y+A_+)\left(\frac{\partial S}{\partial Y}\right)^2}{A_+A_-(X-Y)((a+2)XY-a+2)}=E$$

and solutions

$$S(X,Y)=\frac{1}{\sqrt{A_+A_-}}\left(\lambda_X\int\frac{1}{X}\sqrt{\frac{a_X-X}{(b-X)(c-X)}}\,dX+\lambda_Y\int\frac{1}{Y}\sqrt{\frac{a_Y-Y}{(b-Y)(c-Y)}}\,dY\right),$$

where $\lambda_X-\lambda_Y=-(a+2)EA_+A_-/16$, $a_X=(a-2)E\lambda_X/16$, $a_Y=(a-2)E\lambda_Y/16$, $b=-A_+/A_-$, $c=-A_-/A_+$.

A further change of coordinates

$$X=-\frac{1}{k}\mathrm{sn}^2(\alpha'+iK',k),\quad Y=-\frac{1}{k}\mathrm{sn}^2(\beta'+iK',k),\quad k=\frac{A_+}{A_-}$$

is convenient for writing the Schrödinger equation

$$\frac{16\left(\frac{\partial^2\Psi}{\partial\alpha'^2}+\frac{\partial^2\Psi}{\partial\beta'^2}\right)}{(a+2)k^4(\mathrm{sn}^2(\alpha',k)-\mathrm{sn}^2(\beta',k))+k^2(a-2)}=E\Psi.$$

The separated equations are versions of Lamé's equation.[12] Indeed if we look for solutions of the form $\Psi=A(\alpha')B(\beta')$ then

$$\frac{\partial^2A(\alpha')}{\partial\alpha'^2}+\left(-\frac{1}{16}k^4E(a+2)\mathrm{sn}^2(\alpha',k)-\lambda_1\right)A(\alpha')=0,$$

$$\frac{\partial^2B(\beta')}{\partial\beta'^2}+\left(-\frac{1}{16}k^4E(a+2)\mathrm{sn}^2(\beta',k)-\lambda_2\right)B(\beta')=0,$$

where $\lambda_1-\lambda_2=-E(a-2)k^2/16$. Solutions of these separation equations can be represented as Riemann P functions[13] of the form

$$P(z)=\begin{pmatrix}0&0&k^{-2}&\infty\\0&0&0&\frac{1}{4}(1-\frac{1}{2}\sqrt{4+k^2E(a+2)})&\mathrm{sn}^2(z,k)\\\frac{1}{2}&\frac{1}{2}&\frac{1}{2}&\frac{1}{4}(1+\frac{1}{2}\sqrt{4+k^2E(a+2)})\end{pmatrix}$$

for $z=\alpha',\beta'$.

The case $\gamma=0$ can easily be deduced by setting $A_+=iA_-$, as can be seen from the expression for the associated classical constant.

If $\gamma=2$ then a convenient choice of coordinates is

$$x=\log(\tan(\varphi'-i\omega'))\,,\quad y=\log(\tan(\varphi'+i\omega'))\,. \tag{4.7}$$

The corresponding classical Hamiltonian has the form

$$H=-\frac{p_{\varphi'}^2+p_{\omega'}^2}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2 2\varphi'}}.$$

The classical constant is

$$X_1+X_2+2K^2=aH+\frac{(a+2)\sin^2 2\varphi' p_{\varphi'}^2-(a-2)\sinh^2 2\omega' p_{\omega'}^2}{(a+2)\sin^2 2\varphi'+(a-2)\sinh^2 2\omega'}.$$

The Hamilton–Jacobi equation in these coordinates is

$$-\frac{\left(\dfrac{\partial S}{\partial\varphi'}\right)^2+\left(\dfrac{\partial S}{\partial\omega'}\right)^2}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2 2\varphi'}}=E,$$

which has solutions

$$\begin{aligned}S(\varphi',\omega')=&\frac{i}{2}\sqrt{\lambda}\,\arctan\sqrt{\frac{(a-2)E}{\lambda}\,\sec^2 2\varphi'+\tan^2 2\varphi'}\\&-\frac{i}{2}\sqrt{(a-2)E}\,\operatorname{arctanh}\sqrt{\sec^2 2\varphi'+\frac{\lambda}{(a-2)E}\tan^2 2\varphi'}\\&+\frac{i}{2}\sqrt{\lambda}\,\arctan\sqrt{\frac{(a+2)E}{\lambda}\,\operatorname{sech}^2 2\omega'-\tanh^2 2\omega'}\\&-\frac{i}{2}\sqrt{(a+2)E}\,\operatorname{arctanh}\sqrt{\operatorname{sech}^2 2\omega'-\frac{\lambda}{(a+2)E}\tanh^2 2\omega'}.\end{aligned}$$

The corresponding Schrödinger equation is

$$-\frac{\dfrac{\partial^2\Psi}{\partial\varphi'^2}+\dfrac{\partial^2\Psi}{\partial\omega'^2}}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2 2\varphi'}}=E\Psi\,,$$

which has solutions of the form

$$\Psi=\sqrt{\sin 2\varphi'\,\sinh 2\omega'}\;\;P_\nu^{1/2\sqrt{1-(a-2)E}}(\cos 2\varphi')P_\nu^{1/2\sqrt{1-(a+2)E}}(\cosh 2\omega'),$$

where $P_\nu^\mu(z)$ is a solution of Legendre's equation.

This completes the list of possible coordinate systems which are inequivalent and separable for this particular Hamiltonian. We notice in particular that the equation $H-E=0$ can be written in the equivalent forms

$$\mu^2(p_\mu^2+p_\nu^2)+\frac{1}{4}E\left(a-2+(a+2)\frac{\mu^2}{\nu^2}\right)=0, \quad J_1^2+J_2^2+J_3^2-E\left(\frac{2is_3}{\sqrt{s_1^2+s_2^2}}+a\right)=0,$$

both superintegrable systems on the complex two-sphere, the first of which is written in horospherical coordinates.

B. Superintegrability for Darboux spaces of type four

There are various possibilities for the potential in this case: [**A**], [**B**], [**C**], [**D**].

$$[\mathbf{A}] \quad H=-\frac{4\mu^2\nu^2}{(a+2)\mu^2+(a-2)\nu^2}\left(p_\mu^2+p_\nu^2+a_1+a_2\left(\frac{1}{\mu^2}+\frac{1}{\nu^2}\right)+a_3(\mu^2+\nu^2)\right).$$

The additional constants of the motion have the form

$$R_1=K^2+a_1(\mu^2+\nu^2)+a_3(\mu^2+\nu^2)^2,$$

$$R_2=X_2+\frac{2a_1((a+2)\mu^2-(a-2)\nu^2)+16a_2+4a_3((a+2)\mu^4-(a-2)\nu^4)}{(a+2)\mu^2+(a-2)\nu^2}.$$

The corresponding quadratic algebra relations are determined by

$$R^2=16R_1R_2^2-256a_3R_1^2-64a_1R_1R_2-256aa_3HR_1-1024a_2a_3R_1$$
$$+64a_1HR_2-256a_3H^2-64a_1(a+2)H-256a_1^2a_2.$$

This Hamiltonian admits a separation of variables in coordinates corresponding to the equivalence first, second, and third classes of Sec. IV A. For the second this is covered by the choice of coordinates μ,ν.

(i) For coordinates corresponding to the first equivalence class, we obtain the Hamiltonian in the form

$$H=-\frac{\sin^2 2u(p_u^2+p_v^2+4a_1e^{2v}+4a_2\operatorname{cosec}^2 2u+4a_3e^{4v})}{2\cos 2u+a}.$$

(ii) For coordinates corresponding to the third representative (4.5) the Hamiltonian takes form

$$H=\frac{4(p_\omega^2+p_\varphi^2)+4a_1c^2(\cosh^2\omega-\cos^2\varphi)}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}$$
$$+\frac{16a_2(\operatorname{cosech}^2 2\omega+\operatorname{cosec}^2 2\varphi)+a_3c^4(\sinh^2 2\omega+\sin^2 2\varphi)}{(a-2)(\operatorname{sech}^2\omega-\sec^2\varphi)-(a+2)(\operatorname{cosech}^2\omega+\operatorname{cosec}^2\varphi)}.$$

The quantum algebra relations are

$$[\hat{R},\hat{R}_1]=-8\{\hat{R}_1,\hat{R}_2\}-16\hat{R}_2-32a_1\hat{H},$$

$$[\hat{R},\hat{R}_2]=8\hat{R}_2^2-256a_3\hat{R}_1-128aa_3\hat{H}-32(a_1^2+4a_3+16a_2a_3)$$

together with the operator relation

$$\hat{R}^2=8\{\hat{R}_1,\hat{R}_2^2\}-256a_3\hat{R}_1^2-80\hat{R}_2^2-256aa_3\hat{H}\hat{R}_1-64(16a_2a_3+a_1^2+4a_3)\hat{R}_1+64a_1\hat{H}\hat{R}_2$$
$$-256a_3\hat{H}^2+64a(4a_3-a_1^2)\hat{H}+128(a1^2+4a_3+8a_2a_3-2a_1^2a_2).$$

As in the case of free motion we observe that the equation $H=E$ is

$$p_\mu^2+p_\nu^2+a_1+\frac{a_2-\frac{1}{4}(a-2)E}{\mu^2}+\frac{a_2-\frac{1}{4}(a+2)E}{\nu^2}+a_3(\mu^2+\nu^2)=0\,,$$

a superintegrable system in flat space with rearranged constants, that separates in elliptic and hyperbolic coordinates.

$$[\mathbf{B}]\quad H=-\frac{\sin^2 2u\left(p_v^2+p_u^2+\dfrac{b_2}{\sinh^2 v}+\dfrac{b_3}{\cosh^2 v}\right)+b_1}{2\cos 2u+a}.$$

The additional constants are

$$R_1=X_1+X_2+\frac{2b_1\cosh 2v+(b_2+b_3)(4-a^2)+(\cos 4u+2a\cos 2u+3)\left(\dfrac{b_2}{\sinh^2 v}-\dfrac{b_3}{\cosh^2 v}\right)}{2\cos 2u+a},$$

$$R_2=K^2+\frac{b_2}{\sinh^2 v}+\frac{b_3}{\cosh^2 v}\,.$$

The quadratic algebra is given by

$$\begin{aligned}R^2=&16R_1^2R_2-64R_2^3-64aHR_2^2+64(2b_3-2b_2-b_1)R_2^2+32a(b_2+b_3)R_1R_2-64H^2R_2\\&+64(b_2+b_3)HR_1+128a(b_3-b_2)HR_2-16((4-a^2)(b_2+b_3)^2+8b_1(b_2-b_3))R_2\\&+128(b_3-b_2)H^2-64b_1(b_2+b_3)^2\,.\end{aligned}$$

This Hamiltonian admits a separation of variables in coordinate systems corresponding to the first and fourth equivalence classes of (4.2). The defining expressions have already been given in terms of coordinates for the first. For the fourth, we distinguish two cases.

(i) $\gamma\neq 2$,

$$\begin{aligned}H=16XY&\frac{X(A_-X-A_+)(A_+X-A_-)p_X^2+Y(A_-Y+A_+)(A_+Y+A_-)p_Y^2}{A_+A_-(X-Y)(a-2-(a+2)XY)}\\&+\frac{b_1(XY+1)+\dfrac{4b_2(A_-^2-A_+^2)XY}{(A_+Y+A_-)(A_+X+A_-)}+\dfrac{4b_3(A_-^2-A_+^2)XY}{(A_-Y+A_+)(A_-X+A_+)}}{a-2-(a+2)XY}.\end{aligned}$$

(ii) $\gamma=2$,

$$H=-\frac{p_{\varphi'}^2+p_{\omega'}^2+b_1\left(\dfrac{1}{\sinh^2 2\omega'}+\dfrac{1}{\sin^2 2\varphi'}\right)+\dfrac{4b_2}{\cos^2 2\varphi'}+\dfrac{4b_3}{\cosh^2 2\omega'}}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2 2\varphi'}}.$$

The corresponding quantum algebra relations are

$$\begin{aligned}[\hat R,\hat R_1]=&-8\hat R_1^2+96\hat R_2^2+64a\hat H\hat R_2-16a(b_2+b_3)\hat R_1+64(2b_2-2b_3+b_1+3)\hat R_2+32\hat H^2\\&+32a(2b_2-2b_3+1)\hat H+64b_1(b_2-b_3)-8(a^2-4)(b_2+b_3)^2+32(b_1+2b_2-2b_3)\,,\end{aligned}$$

$$[\hat R,\hat R_2]=8\{\hat R_1,\hat R_2\}+16a(b_2+b_3)\hat R_2-16\hat R_1+32(b_2+b_3)\hat H-16a(b_2+b_3)\,,$$

$$R^2=-64\hat{R}_2^3+8\{\hat{R}_1^2,\hat{R}_2\}-64a\hat{H}\hat{R}_2^2-64\hat{H}^2\hat{R}_2-80\hat{R}_1^2-64(2b_2-2b_3+b_1+7)\hat{R}_2^2+16a(b_2+b_3)$$
$$\times\{\hat{R}_1,\hat{R}_2\}+64(b_2+b_2)\hat{H}\hat{R}_1+64a(2b_3-2b_2-1)\hat{H}\hat{R}_2-160a(b_2+b_3)\hat{R}_1+16((a^2-4)$$
$$\times(b_2+b_3)^2+8(b_1+1)(b_3-b_2)-4b_1+32)\hat{R}_2+128(b_3-b_2+1)\hat{H}^2+128a(b_2-b_3+1)\hat{H}$$
$$+(b_2+b_3)^2(128-80a^2-64b_1)-128(b_1+2)(b_3-b_2-1)-256.$$

As in the case of free motion, equation $H-E=0$ is

$$J_1^2+J_2^2+J_3^2+\frac{2b_1}{\sqrt{s_1^2+s_2^2}(s_1+\sqrt{s_1^2+s_2^2})}+\frac{2b_2}{\sqrt{s_1^2+s_2^2}(s_1-\sqrt{s_1^2+s_2^2})}+b_3-E\left(\frac{2is_3}{\sqrt{s_1^2+s_2^2}}+a\right)=0\,,$$

a superintegrable system on the complex sphere that separates variables in spherical, elliptic, and degenerate elliptic type 1 coordinates.

$$[\mathbf{C}]\quad H=-\frac{p_{\varphi'}^2+p_{\omega'}^2+\dfrac{c_1}{\cos^2\varphi'}+\dfrac{c_2}{\cosh^2\omega'}+c_3\left(\dfrac{1}{\sin^2\varphi'}-\dfrac{1}{\sinh^2\omega'}\right)}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2 2\varphi'}}.$$

These are coordinates associated with $\gamma=2$ in the fourth representative from (4.2). The constants of the motion associated with this Hamiltonian are

$$R_1=X_1+X_2+2K^2+aH+\frac{\dfrac{a+2}{\sinh^2 2\omega'}\left(\dfrac{c_3}{\sin^2\varphi'}+\dfrac{c_1}{\cos^2\varphi'}\right)+\dfrac{a-2}{\sin^2 2\varphi'}\left(\dfrac{c_3}{\sinh^2\omega'}-\dfrac{c_2}{\cosh^2\omega'}\right)}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2\omega'}},$$

$$R_2=X_1-X_2+\frac{1}{\dfrac{a+2}{\sinh^2 2\omega'}+\dfrac{a-2}{\sin^2\omega'}}\times\left[\frac{a+2}{\sinh^2 2\omega'}\left(c_1\cosh 2\omega'\tan^2\varphi'-c_2\cos 2\varphi'\right.\right.$$
$$\left.-\frac{c_3(2\cos^2\varphi'(\sinh^2\omega'-\sin^2\varphi'))+1}{\sin^2\varphi'}\right)+\frac{a-2}{\sin^2 2\varphi'}\left(c_2\cos 2\varphi'\tanh^2\omega'+c_1\cosh 2\omega'\right.$$
$$\left.\left.-\frac{c_3(2\cosh^2\omega'(\sinh^2\omega'-\sin^2\varphi)+1)}{\sinh^2\omega'}\right)\right].$$

They satisfy the quadratic algebra determined by the identity

$$R^2=16R_1^3-16R_1R_2^2-32aHR_1^2+32(c_2-c_1)R_1^2+16(a^2-4)H^2R_1+32((a+2)c_1-(a-2)c_2$$
$$+4c_3)HR_1-16(2c_3^2-c_1^2-c_2^2+6c_3(c_1+c_2)+4c_1c_2)R_1-32(c_2-c_3)(c_1-c_3)R_2$$
$$-16((a+2)(c_1-c_3)^2+(a-2)(c_2-c_3)^2)H-32(c_1-c_2)(3c_3^2-c_1c_2-c_3(c_1+c_2)).$$

The Hamiltonian admits a separation of variables in a number of coordinates systems corresponding to various combinations of the operators R_1 and R_2. We exhibit the various possibilities.

(i) For the constant R_1-R_2, the associated separable coordinates are those corresponding to the third representative in (4.2) with $\gamma=1$. In these coordinates, the Hamiltonian is

$$H=\frac{4(p_\omega^2+p_\varphi^2)+\dfrac{c_1+c_2+2c_3}{2\sinh^2 2\omega}-\dfrac{(c_1+c_2)\cosh 2\omega}{2\sinh^2 2\omega}+\dfrac{c_3\cos 2\varphi}{\sin^2 2\varphi}}{(a-2)\left(\dfrac{1}{\cosh^2\omega}-\dfrac{1}{\cos^2\varphi}\right)-(a+2)\left(\dfrac{1}{\sinh^2\omega}+\dfrac{1}{\sin^2\varphi}\right)}.$$

(ii) In coordinates corresponding to rotations of the fourth representative in (4.2) with $\gamma\neq 0,2$, that is, $B_+^2X_1+(B_+^2-B_-^2)X_2+(2B_+^2-B_-^2)K^2$, the corresponding Hamiltonian has the form

$$\begin{aligned}H=16\Bigg[&-X(B_\mp+X)(B_\pm+X)p_X^2+Y(B_\mp+Y)(B_\pm+Y)p_Y^2+\frac{c_1}{4}\left(\frac{1}{Y}-\frac{1}{X}\right)+\frac{c_2}{4}(X-Y)\\&+\frac{c_3}{4}(B_\mp^2-B_\pm^2)\left(\frac{1}{1+B_\mp Y}-\frac{1}{1+B_\mp X}+\frac{1}{1+B_\pm Y}-\frac{1}{1+B_\pm X}\right)\Bigg]\Bigg/\Bigg[(B_\mp^2-B_\pm^2)\\&\times\left(\frac{a-2}{1+B_\pm X}-\frac{a-2}{1+B_\pm Y}+\frac{a+2}{1+B_\mp Y}-\frac{a+2}{1+B_\mp X}\right)+\left(\frac{a-2}{X}-\frac{a-2}{Y}+(a+2)(X-Y)\right)\Bigg].\end{aligned}$$

Here, $B_\pm=B_+/B_-$ and $B_\mp=B_-/B_+$. The Hamiltonian associated with R_2 can be obtained from this last case by taking $B_-=\sqrt{2}B_+$.

The quantum algebra relations are

$$[\hat R,\hat R_1]=8\{\hat R_1,\hat R_2\}+16\hat R_2+16(c_1-c_3)(c_2-c_3),$$

$$\begin{aligned}[\hat R,\hat R_2]=&24\hat R_1^2-8\hat R_2^2-32a\hat H\hat R_1+8(a^2-4)\hat H^2+32\left(c_1-c_2-\frac{3}{2}\right)\hat R_1+16((a+2)c_1-(a-2)c_2\\&+a+64c_3)\hat H+8c_1^2+8c_2^2-16c_3^2-32c_1c_2-48c_3(c_1+c_2)+16(c_1-c_2).\end{aligned}$$

The operator identity is

$$\begin{aligned}\hat R^2=&16\hat R_1^3-8\{\hat R_1,\hat R_2^2\}+32\left(c_2-c_1-\frac{7}{2}\right)\hat R_1^2-80\hat R_2^2+16(a^2-4)\hat H^2\hat R_1+32((a+2)c_1-(a-2)c_2\\&+4c_3+a)\hat H\hat R_1+16(c_1^2+c_2^2-2c_3^2-6c_3(c_1+c_2)-4c_1c_2+2(c_1-c_2)-8)\hat R_1-32(c_2-c_3)\\&\times(c_1-c_3)\hat R_2+16(a^2-4)\hat H^2-16((a+2)((c_1-c_3)^2-2c_1)+(a-2)((c_2-c_3)^2+2c_2)\\&-8c_3-4a)\hat H-32(c_1-c_2)(3c_3^2-c_1c_2-c_3(c_1+c_2))+32(c_1^2+c_2^2-4c_3(c_1+c_2)-2c_1c_2\\&+2c_1-2c_2).\end{aligned}$$

As in the case of free motion, the equation $H=E$ is

$$\begin{aligned}&J_1^2+J_2^2+J_3^2-\frac{i(c_1+c_2+2c_3)s_1}{4\sqrt{s_2^2+s_3^2}}+\frac{i(c_1-c_2)(s_1+is_2-s_3)}{4\sqrt{2}\sqrt{(s_1+is_2)(s_3-is_2)}}+\frac{(2c_3-c_1-c_2)(s_1+is_2+s_3)}{\sqrt{(s_1+is_2)(s_3+is_2)}}\\&\quad+\frac{i(c_1-c_2)}{4\sqrt{2}}-E\left(a+\frac{2is_1}{\sqrt{s_2^2+s_3^2}}\right)=0,\end{aligned}$$

which is a superintegrable system on the complex sphere, with rearranged constants, that separates variables in elliptic and degenerate elliptic coordinates of type 1.

$$[\mathbf{D}] \quad H=-\frac{4\mu^2\nu^2\left[p_\mu^2+p_\nu^2+\mathrm{d}\left(\frac{1}{\mu^2}+\frac{1}{\nu^2}\right)\right]}{(a+2)\mu^2+(a-2)\nu^2}.$$

This Hamiltonian admits three classical constants of the motion

$$R_1=X_1+\frac{\mathrm{d}(\mu^2+\nu^2)^2}{(a+2)\mu^2+(a-2)\nu^2},\quad R_2=X_2+\frac{16\mathrm{d}}{(a+2)\mu^2+(a-2)\nu^2},\quad K=\mu p_\mu+\nu p_\nu.$$

The Poisson quadratic algebra satisfies the relations

$$\{K,R_1\}=2R_1,\quad \{K,R_2\}=-2R_2,\quad \{R_1,R_2\}=-8K^3-4aKH-16\,\mathrm{d}K.$$

These three extra constants are related via the identity

$$-R_1R_2+K^4+aHK^2+4\,\mathrm{d}K^2+H^2=0\,.$$

This Hamiltonian admits a separation of variables in all the coordinate systems that are possible. We need only give the expressions in terms of the fourth representatives. In the coordinate system associated with the fourth representative and for which $\gamma\neq 2$ the Hamiltonian can be written as

$$H=16XY\,\frac{X(A_+X-A_-)(A_-X-A_+)p_X^2-Y(A_+Y+A_-)(A_-Y+A_+)p_Y^2}{(X-Y)(a-2-XY(a+2))A_+A_-}$$
$$-\frac{4\mathrm{d}A_+A_-(X^2Y+Y+XY^2+X)}{(X-Y)(-a+2+XY(a+2))A_+A_-},$$

and for the case $\gamma=2$ this Hamiltonian has the form

$$H=\frac{p_{\varphi'}^2+p_{\omega'}^2+\mathrm{d}\left(\frac{1}{\sinh^2 2\omega'}+\frac{1}{\sin^2 2\varphi'}\right)}{\frac{a+2}{\sinh^2 2\omega'}+\frac{a-2}{\sin^2 2\varphi'}}.$$

The corresponding quadratic algebra relations are

$$[\hat{K},\hat{R}_1]=2\hat{R}_1,\quad [\hat{K},\hat{R}_2]=-2\hat{R}_2,\quad [\hat{R}_1,\hat{R}_2]=-8\hat{K}^3-4a\hat{H}\hat{K}-16\,\mathrm{d}\hat{K}-4\hat{K},$$

subject to the operator identity

$$-\tfrac{1}{2}\{\hat{R}_1,\hat{R}_2\}+\hat{H}^2+a\hat{H}\hat{K}^2+\hat{K}^4+a\hat{H}+(5+4\mathrm{d})\hat{K}^2+4\mathrm{d}=0\,.$$

This completes the analysis of the superintegrable potentials associated with the four metrics of Darboux.

V. RELATIONSHIP TO CONSTANT CURVATURE SUPERINTEGRABLE POTENTIALS

In Secs. II–IV we have found, by means of exhaustive calculation, all superintegrable potentials in the Darboux spaces of revolution having two or more quadratic integrals. Once these are expressed in suitable coordinates, it is clear that each is simply a multiple of one of the superintegrable potentials on the complex Euclidean plane or 2-sphere, that have been enumerated in Ref. 7, though that was by no means evident in advance.

In each case we can start with a Hamiltonian of the form

$$H = H_0 + \alpha V_0 , \tag{5.1}$$

where V_0 is a function of the coordinates x and y, and α is a constant. Dividing the Hamilton–Jacobi equation, $H=E$, throughout by V_0 and rearranging gives a new Hamilton–Jacobi equation in which the roles of the energy E and parameter α have been exchanged,

$$H' = \frac{H_0}{V_0} - \frac{E}{V_0} = -\alpha . \tag{5.2}$$

Clearly, the integrability and separability of one system guarantees that of the other. It is this relationship between the harmonic oscillator potential written in Cartesian coordinates and the Coulomb potential in parabolic coordinates that has been discovered by many authors. Transformations of this type relating integrable systems were described in a more general context by Hietarinta *et al.* in Ref. 14 and called *coupling constant metamorphosis*. See also Ref. 15 where the *Stäckel transform* and its close connection with variable separation was emphasized.

The preservation of integrability under such a transformation can be demonstrated explicitly by noting that if $\{H_0, L_0\} = 0$ and

$$H = H_0 + \alpha V_0 \quad \text{and} \quad L = L_0 + \alpha \ell_0 \tag{5.3}$$

are in involution, i.e., $\{H, L\} = 0$, then so are

$$H' = \frac{H_0}{V_0} \quad \text{and} \quad L' = L_0 - \ell_0 H' . \tag{5.4}$$

Any identities involving integrals associated with (5.1), give rise to corresponding identities involving integrals associated with (5.2) and are obtained by the replacements

$$\alpha \to -H' \quad \text{and} \quad H \to 0 . \tag{5.5}$$

A. Generating the Darboux spaces of revolution by coupling constant metamorphosis

Taking each of the degenerate potentials from Ref. 7, that is, the potentials with Hamiltonians having one first order and two quadratic integrals and performing a coupling constant metamorphosis we arrive at a Hamiltonian having one first order K and two quadratic constants, X_1 and X_2. These must be free Hamiltonians either on one of the four Darboux spaces of revolution or one of the constant curvature spaces, $E_2(\mathbb{C})$ or $S_2(\mathbb{C})$. After comparing the Hamiltonians so generated, it can be seen that this approach generates all of the Darboux spaces of revolution.

Knowing the Poisson algebra for each Hamiltonian involved and how coupling constant metamorphosis modifies this algebra, we can determine which Hamiltonian has been generated, even if it appears in unfamiliar coordinates. Note that some transformations reproduce the free Hamiltonian on $E_2(\mathbb{C})$ or $S_{2,\mathbb{C}}$, and some Darboux spaces can be generated from two distinct constant curvature potentials.

For each Hamiltonian we have four linearly independent constants of the motion. These, however, cannot be functionally independent and there is always a polynomial identity in K, X_1, X_2, and H that is of fourth order in the momenta. We can use this identity to classify the possible Hamiltonians. Up to freedoms in choosing X_1 and X_2, scalings of K and coupling constant metamorphosis, we find that there are five classes of identities that involve all of the constants. The correspondences between these identities, degenerate superintegrable potentials from Ref. 7 and the Darboux spaces of revolution are summarized in Table I. Note that because we allow coupling constant metamorphosis, H has the same status as parameters in the potential and the coefficients A and B appearing in the representative identities may be functions of H. The labels in bold (e.g., **E3**, **S3**,...) refer to Ref. 7. Those Hamiltonians in Table I on the complex 2-sphere, that is, **S3**, **S5**, and **S6**, are represented with three coordinates s_1, s_2, and s_3 constrained by s_1^2

TABLE I. Correspondences between constant curvature superintegrable potentials and Hamiltonians for Darboux spaces of revolution.

Degenerate superintegrable potential on $E_2(\mathbb{C})$ or $S_2(\mathbb{C})$	Hamiltonian for Darboux space of revolution	Representative identity
E5: $4x$	D_1: $\frac{p_u^2+p_v^2}{4u}$	$X_1^2+AX_2+K^4+B=0$
E6: $\frac{1}{x^2}+1$	D_2: $\frac{u^2(p_u^2+p_v^2)}{u^2+1}$	$X_1^2+K^2X_2+AX_2+B=0$
S5: $\frac{1}{(s_1-is_2)^2}-1$		
E12: $\frac{\alpha(x-iy)}{\sqrt{(x-iy)^2+c^2}}+\beta$	$E_2(\mathbb{C})$	$X_1^2+K^2X_2+A=0$
E14: $\frac{\alpha}{\sqrt{x-iy}}+\beta$		
E3: x^2+y^2+4	D_3: $\frac{p_u^2+p_v^2}{4+u^2+v^2}$	$X_1X_2+AK^2+B=0$
E18: $\frac{2}{\sqrt{x^2+y^2}}+1$		
S3: $\frac{a+2}{s_3^2}-a+2$	D_4: $\frac{p_u^2+p_v^2}{\frac{a+2}{u^2}+\frac{a-2}{v^2}}$	$X_1X_2+K^4+AK^2+B=0$
S6: $\frac{2is_3}{\sqrt{s_1^2+s_2^2}}+a$		
E4: $\alpha(x-iy)+\beta$	$E_2(\mathbb{C})$	$K^2X_1+AX_2+B=0$
E13: $\frac{\alpha}{\sqrt{x-iy}}+\beta$		

$+s_2^2+s_3^2=1$ and $J_1=s_2p_{s_3}-s_3p_{s_2}$, $J_2=s_3p_{s_1}-s_1p_{s_3}$, and $J_3=s_1p_{s_2}-s_2p_{s_1}$. The potentials **E12**, **E14**, **E4**, and **E13** are functions of $x-iy$ and hence division of $p_x^2+p_y^2$ by these potentials reproduces the flat space Hamiltonian.

For example, starting from the algebraic identity for constants associated with the Hamiltonian and integrals

$$H=p_x^2+p_y^2+\frac{\alpha}{x^2}+\alpha \quad (\mathbf{E6}),$$

$$X_1=(xp_y-yp_x)p_x-\frac{\alpha y}{x^2}, \quad X_2=(xp_y-yp_x)^2+\frac{\alpha y^2}{x^2}, \quad K=p_y, \tag{5.6}$$

that is Ref. 7,

$$X_1^2+K^2X_2-(H-\alpha)X_2+\alpha K^2=0,$$

we find that applying the transformation (5.4) gives

$$H'=\frac{p_x^2+p_y^2}{\dfrac{1}{x^2}+1},\quad X_1'=(xp_y-yp_x)p_x-\frac{y}{x^2}\frac{p_x^2+p_y^2}{\dfrac{1}{x^2}+1}=\frac{y(p_y^2-x^2p_x^2)}{x^2+1}+xp_xp_y,$$

$$X_2'=(xp_y-yp_x)^2+\frac{y^2}{x^2}\frac{p_x^2+p_y^2}{\dfrac{1}{x^2}+1}=\frac{(x^2+x^4-y^2)p_y^2+x^2y^2p_x^2}{x^2+1}-2xyp_xp_y,\quad K'=K,$$

and using (5.5),

$$X_1'^2+K'^2X_2'-H'X_2'-H'K'^2=0.$$

Then

$$X_1''=2X_1',\quad X_2''=-X_2'+H',\quad H''=H',\quad K''=K',$$

gives

$$X_1''^2-4K''^2X_2''+4H''X_2''-4H''^2=0,$$

the identity (2.3) associated with the Darboux space of type two (2.1).

B. Generating superintegrable potentials on Darboux spaces

The H_0 in Eq. (5.3) may itself contain potential terms and if these are chosen so that H is superintegrable, then so will be H'.

For example, taking the superintegrable Hamiltonian on the complex two-sphere **S1**,[7]

$$H=J_1^2+J_2^2+J_3^2+\frac{\alpha}{(s_1-is_2)^2}+\frac{\beta s_3}{(s_1-is_2)^3}+\frac{\gamma(1-4s_3^2)}{(s_1-is_2)^4}+\delta$$

and dividing though by $(s_1-is_2)^{-2}-1$ gives, after a change of coordinates, the superintegrable potential [**A**] in a Darboux space of type 2. The same Hamiltonian can be generated by dividing **E2** throughout by $x^{-2}+1$.

Each potential in Table I is compatible with the addition of further terms while maintaining superintegrability, and in using the method demonstrated above, all superintegrable Hamiltonians found in Secs. II–IV can be generated. The correspondences are given below.

1. Darboux spaces of type 1

The potential **E5**, $V_0=4x$, appears in each of

$$\mathbf{E2}\quad:\quad \alpha(4x^2+y^2)+\beta x+\frac{\gamma}{x^2}+\delta,$$

$$\mathbf{E3'}\quad:\quad \alpha(x^2+y^2)+\beta x+\gamma y+\delta,$$

$$\mathbf{E9}\quad:\quad \frac{\alpha}{\sqrt{x-iy}}+\beta x+\frac{\gamma(2x-iy)}{\sqrt{x-iy}}+\delta.$$

The potential labeled **E3′** is a translation of **E3**. Adding these potentials to $H_0=p_x^2+p_y^2$ and dividing by $4x$ produces the two real nondegenerate potentials found in Ref. 1 and an additional complex one given in this paper. [The details of the quadratic algebra and defining operators for the Hamiltonian derived from **E9** can be computed using (5.2).]

2. Darboux spaces of type 2

The potentials **E6** and **S5** appear in each of the following:

$$\mathbf{E1}\quad[\mathbf{B}]\quad:\quad \alpha(x^2+y^2)+\frac{\beta}{x^2}+\frac{\gamma}{y^2}+\delta,$$

$$\mathbf{E2}\quad[\mathbf{A}]\quad:\quad \alpha(4x^2+y^2)+\beta x+\frac{\gamma}{y^2}+\delta,$$

$$\mathbf{E16}\quad[\mathbf{C}]\quad:\quad \frac{1}{\sqrt{x^2+y^2}}\left(\alpha+\frac{\beta}{x+\sqrt{x^2+y^2}}+\frac{\gamma}{x-\sqrt{x^2+y^2}}\right)+\delta,$$

$$\mathbf{S1}\quad[\mathbf{A}]\quad:\quad \frac{\alpha}{(s_1-is_2)^2}+\frac{\beta s_3}{(s_1-is_2)^3}+\frac{\gamma(1-4z^2)}{(x-iy)^4}+\delta,$$

$$\mathbf{S2}\quad[\mathbf{B}]\quad:\quad \frac{\alpha}{s_3^2}+\frac{\beta}{(s_1-is_2)^2}+\frac{\gamma(s_1+is_2)}{(s_1-is_2)^3}+\delta,$$

$$\mathbf{S4}\quad[\mathbf{C}]\quad:\quad \frac{\alpha}{(s_1-is_2)^2}+\frac{\beta s_3}{\sqrt{s_1^2+s_2^2}}+\frac{\gamma}{(s_1-is_2)\sqrt{s_1^2+s_2^2}}+\delta.$$

The superintegrable system generated after dividing by $x^{-2}+1$ or $(s_1-is_2)^{-2}-1$ as appropriate is indicated by label the [**A**], [**B**], or [**C**]. The apparent over abundance of superintegrable potentials generated in this way for D_2 is resolved by noting that the same potential can appear in more than one coordinate system.

3. Darboux spaces of type 3

The potentials **E3** and **E18** appear in each of

$$\mathbf{E1}\quad[\mathbf{B}]\quad:\quad \alpha(x^2+y^2)+\frac{\beta}{x^2}+\frac{\gamma}{y^2}+\delta,$$

$$\mathbf{E3'}\quad[\mathbf{A}]\quad:\quad \alpha(x^2+y^2)+\beta x+\gamma y+\delta,$$

$$\mathbf{E7}\quad[\mathbf{D}]\quad:\quad \frac{\alpha(x-iy)}{\sqrt{(x-iy)^2-c^2}}+\frac{\beta(x+iy)}{\sqrt{(x-iy)^2-c^2}((x-iy)+\sqrt{(x-iy)^2-c^2})^2}+\gamma(x^2+y^2)+\delta,$$

$$\mathbf{E8}\quad[\mathbf{C}]\quad:\quad \frac{\alpha(x+iy)}{(x-iy)^3}+\frac{\beta}{(x-iy)^2}+\gamma(x^2+y^2)+\delta,$$

$$\mathbf{E16}\quad[\mathbf{B}]\quad:\quad \frac{1}{\sqrt{x^2+y^2}}\left(\alpha+\frac{\beta}{x+\sqrt{x^2+y^2}}+\frac{\gamma}{x-\sqrt{x^2+y^2}}\right)+\delta,$$

$$\mathbf{E17}\quad[\mathbf{C}]\quad:\quad \frac{\alpha}{\sqrt{x^2+y^2}}+\frac{\beta}{(x+iy)^2}+\frac{\gamma}{(x+iy)\sqrt{x^2+y^2}}+\delta,$$

$$\mathbf{E19}\quad[\mathbf{D}]\quad:\quad \frac{\alpha(x-iy)}{\sqrt{(x-iy)^2-4}}+\frac{\beta}{\sqrt{(x+iy)(x-iy+2)}}+\frac{\gamma}{\sqrt{(x+iy)(x-iy-2)}}+\delta,$$

$$\mathbf{E20}\quad [\mathbf{A}]\quad :\quad \frac{1}{\sqrt{x^2+y^2}}\left(\alpha+\beta\sqrt{x+\sqrt{x^2+y^2}}+\gamma\sqrt{x-\sqrt{x^2+y^2}}\right)+\delta.$$

As before, once the possibility of changes of coordinates in taken into account, the above list produces only those superintegrable potentials found in Sec. III B.

4. Darboux spaces of type 4

The potentials **S3** and **S6** appear in each of

$$\mathbf{S2}\quad [\mathbf{A}]\quad :\quad \frac{\alpha}{s_3^2}+\frac{\beta}{(s_1-is_2)^2}+\frac{\gamma(s_1+is_2)}{(s_1-is_2)^3}+\delta,$$

$$\mathbf{S4}\quad [\mathbf{A}]\quad :\quad \frac{\alpha}{(s_1-is_2)^2}+\frac{\beta s_3}{\sqrt{s_1^2+s_2^2}}+\frac{\gamma}{(s_1-is_2)\sqrt{s_1^2+s_2^2}}+\delta,$$

$$\mathbf{S7}\quad [\mathbf{B},\mathbf{C}]\quad :\quad \frac{\alpha s_1}{\sqrt{s_2^2+s_3^2}}+\frac{\beta s_2}{s_3^2\sqrt{s_2^2+s_3^2}}+\frac{\gamma}{s_3^2}+\delta,$$

$$\mathbf{S8}\quad [\mathbf{C}]\quad :\quad \frac{\alpha s_1}{\sqrt{s_2^2+s_3^2}}+\frac{\beta(s_1+is_2-s_3)}{\sqrt{(s_1+is_2)(s_3-is_2)}}+\frac{\gamma(s_1+is_2+s_3)}{\sqrt{(s_1+is_2)(s_3+is_2)}}+\delta,$$

$$\mathbf{S9}\quad [\mathbf{B}]\quad :\quad \frac{\alpha}{s_1^2}+\frac{\beta}{s_2^2}+\frac{\gamma}{s_3^2}+\delta.$$

As before, once the possibility of changes of coordinates in taken into account, the above list produces only those superintegrable potentials found in Sec. IV B.

VI. CONCLUSION

In this paper we have discussed in some detail three of the four Darboux spaces of revolution that have at least two integrals of classical motion quadratic in the momenta in addition to the Hamiltonian. In each case we have also presented an exhaustive list of potentials for each of these spaces which when added to the Hamiltonians of these spaces preserve this property, i.e., that there are still two extra integrals of the classical motion. These are the superintegrable systems associated with the systems of Darboux. The property of extra integrals also extends easily to the case of the corresponding quantum systems. For each of these systems we have calculated the corresponding quadratic algebra relations and have shown that in each case the Hamiltonians that we obtain arise from constant curvature systems via a coupling constant transformation. We have also discussed the solutions of the corresponding classical and quantum problems in each of the inequivalent coordinate systems and have also given some of the embeddings of these spaces in three dimensions. In the last section we have shown how the free Hamiltonians of Darboux are related to the superintegrable Hamiltonians on spaces of constant curvature via coupling constant transformations. We also list how the corresponding superintegrable systems of spaces of constant curvature are related in this way to the superintegrable systems that we have found. This classification is comprehensive and complete.

Let us very briefly review the current status of superintegrability in two-dimensional spaces. Most of the published work[3–7] concerns quadratic superintegrability for classical, or quantum Hamiltonians of the form kinetic energy plus a scalar potential. Once a specific space is chosen, superintegrable systems in the space can be classified under the action of the corresponding isometry group. Systems in the same class are not only mathematically equivalent, but also have the same physical properties. In classical mechanics they will have the same trajectories and the

trajectories will be periodic, if they are bounded. Similarly, in quantum mechanics superintegrable systems in the same class will have the same energy levels and eigenspaces.

Quadratically superintegrable systems exist in spaces of constant curvature and also in Darboux spaces. A Darboux space is defined by the fact that it allows one Killing vector and two (irreducible) Killing tensors. This paper completes the task of classifying all quadratically superintegrable systems in all of the above spaces.

The results are quite rich. Indeed, in the real Euclidean space E_2, we have four $E(2)$ classes of superintegrable systems.[3,4] They are physically quite diverse. One is an isotropic harmonic oscillator with additional terms, called **E1** in Sec. V. A second is an anisotropic harmonic oscillator with additional terms (called **E2**). The third and fourth are Kepler (or Coulomb) systems with two different types of additional terms, respectively. In complex Euclidean space $E_2(\mathbb{C})$, or correspondingly in the pseudo-Euclidean space $E(1,1)$, one obtains six more classes.[5]

Two classes of superintegrable systems exist on the real sphere S_2, four more on the complex sphere $S_2(\mathbb{C})$.[6] On the real Darboux spaces $D_1,\ldots,D_4$ we have obtained 3, 4, 4, and 4 classes of systems, respectively. One more for the complex space $D_3(\mathbb{C})$.

From the mathematical point of view the situation is much more unified. As was stressed above, superintegrable systems that may correspond to quite different physical situations may be related by coupling constant metamorphosis. Once we allow this type of equivalence, many fewer equivalence classes exist. For instance, in real Euclidean space we only have two classes, because the Kepler potentials with additional terms are equivalent to isotropic harmonic oscillators (in one case with the additional terms). All superintegrable systems in Darboux spaces are related by coupling constant metamorphosis to systems in spaces of constant curvature. For D_1, D_2, and D_3 this is always flat space, complex or real. Two of the systems in D_4 are related to systems in real Euclidean space. The other two are related to systems on a complex sphere. The relation is of course not unique and depends on the choice of coordinates (see Sec. V).

A typical feature of quadratic superintegrability for scalar potentials is that quantum and classical superintegrable potentials coincide. They allow separation of variables in at least two coordinate systems in the Schrödinger and Hamilton–Jacobi equation, respectively.

Superintegrability involving third order integrals of motion has also been considered.[16,17] There the situation is quite different. Multiseparability is lost. More interestingly, quantum superintegrable systems exist (in real Euclidean space) that have no classical analog (in the classical limit they reduce to free motion).

ACKNOWLEDGMENTS

The research of P.W. was partly supported by research grants from NSERC of Canada and FQRNT du Quebec. J.M.K. began this work while supported by the contract "special functions, superintegrability and separation of variables" of the New Zealand Marsden Fund.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Semiclassical nonlinear Schrödinger on the half line

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(Received 29 November 2002; accepted 10 September 2003)

We are studying the semiclassical limit of the $1+1$ dimensional integrable nonlinear Schrödinger equation with defocusing cubic nonlinearity on the half line. Our analysis relies on the recent theory of Fokas *et al.*, which reduces boundary value problems for soliton equations to Riemann–Hilbert factorization problems. We employ the method of nonlinear steepest descent to asymptotically deform the given Riemann–Hilbert problem to an explicilty solvable one. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1624091]

I. AN INITIAL-BOUNDARY VALUE PROBLEM FOR THE NONLINEAR SCHRÖDINGER EQUATION

In recent years there has been a series of results by Fokas and others on *boundary value problems* for soliton equations (see Ref. 1 for a comprehensive review). The Fokas method goes beyond existence and uniqueness. In fact, it reduces such problems to Riemann–Hilbert factorization problems in the complex plane, thus generalizing the existing theory which reduces *initial value problems* to Riemann–Hilbert problems via the method of inverse scattering. One of the main advantages of the Riemann-Hilbert formulation is that one can use recent powerful results on the asymptotic behavior of solutions to these problems (as some parameter goes to infinity) to derive asymptotics for the solution of the associated soliton equation. Such methods were pioneered by Its and made rigorous and systematic by Deift and Zhou; the Deift–Zhou method is known as ''nolinear steepest descent'' in analogy with the linear steepest descent method which is applicable to asymptotic problems for Fourier-type integrals (see, e.g., Ref. 2). A generalization of the steepest descent method developed in Ref. 3 is able to give rigorous results for the so-called ''semiclassical'' or ''zero dispersion'' limit of the solution of the Cauchy problem for $1+1$ dimensional integrable evolution equations, in the case where the Lax operator is self-adjoint. The method has been further extended in Ref. 4 for the ''non-self-adjoint'' case, where in fact a ''steepest descent'' contour is, for the first time, introduced and its characterization and computation made systematic.

In this paper we consider the most basic example, that is the defocusing nonlinear Schrödinger (NLS) equation. (In a recent paper[5] we dealt with the simple problem of so-called linearizable data, for both the defocusing NLS and Korteweg–de Vries equations.) We make use of the recent results of Ref. 6 in order to study the so-called ''semiclassical'' limit of a particular initial-boundary value problem. More precisely we consider the $1+1$ dimensional, integrable, defocusing, nonlinear Schrödinger equation on the half-line

$$ihu_t(x,t)+h^2u_{xx}(x,t)-2|u(x,t)|^2u(x,t)=0,$$

$$u(x,0)=0, \qquad u(0,t)=f_0(t), \tag{1a}$$

$$x\geqslant 0, \quad t\geqslant 0,$$

where f_0 is assumed to be in the Schwartz space of the positive real line. We also assume that all

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derivatives of $f_0(t)$ vanish at $t=0$. The special restriction of zero initial data is not essential but makes the computations and proofs somewhat easier. It is known[7] that the above problem is well-posed.

Our analysis is based on the results of Ref. 6, which considers the *a priori* overdetermined problem:

$$ihu_t(x,t)+h^2u_{xx}(x,t)-2|u(x,t)|^2u(x,t)=0,$$

$$u(x,0)=0, \qquad u(0,t)=f_0(t), \qquad u_x(0,t)=f_1(t), \tag{1b}$$

$$x\geqslant 0, \quad t\geqslant 0.$$

However, following Ref. 6, we will eventually impose a compatibility condition (the so-called "global relation") on the data f_0, f_1 which will ensure the existence (and uniqueness under such a condition) of a solution to (1b). It is also worthwhile noting (see Ref. 6) that given data $u(x,0)$ and $u(0,t)$ only, the global relation implicitly selects a function $f_1(t)=u_x(0,t)$ which complements the data f_0 and the initial data, and which will then ensure the existence of a solution to (1) and the validity of the Riemann–Hilbert formulation (see Theorem 1 below).

For the convenience of the reader we include an Appendix at the end of this paper containing a statement of some of the main results of Ref. 6.

It is well known that the above-mentioned equation admits a "Lax-pair" formulation. It arises as the compatibility condition for the equations $L\mu=0$ and $B\mu=0$ where the operators L, B are given by

$$L=\begin{pmatrix} \partial_x-ik & iu \\ -i\overline{u} & \partial_x+ik \end{pmatrix},$$

$$B=\begin{pmatrix} ih\partial_t+4ik^2+i|u|^2 & -2ku-iu_t \\ -2k\overline{u}+i\overline{u_t} & ih\partial_t-i|u|^2 \end{pmatrix}.$$

Here the bar denotes complex conjugation, k is the spectral variable, and $u=u(x,t)$ is the solution of (1a).

The traditional method of solving initial value problems for soliton equations that admit a similar Lax-pair formulation is to focus on the L operator and apply the theory of scattering and inverse scattering to that very operator. On the other hand, one of the main ideas of the Fokas method is that for initial-boundary value problems the two operators L and B should be on an equal footing. The scattering transform should be applied to both operators simultaneously, while a global relation has to be imposed on the data to ensure compatibility.

II. THE RIEMANN–HILBERT PROBLEM

As shown in Ref. 6, problem (1a) can be reduced to the following Riemann–Hilbert problem, under the special assumption that the so-called global relation holds (see relation (3.18) of Ref. 6; see also relation (5) below). One way to look at the global relation is as a way of selecting a solution of problem (1b). In fact it is known (see Ref. 7), using methods unrelated to inverse scattering theory, that (1b) has a unique solution. On the other hand, it has been shown in Ref. 6 that given data f_0 in (1b), there exists a function $f_1(t)$ such that the problem (1a) admits a solution, which furthermore can be explicitly characterized via inverse scattering and a particular Riemann–Hilbert factorization problem. Indeed, let Σ be the contour $\mathbb{R}\cup i\mathbb{R}$ with the following orientation:

(i) the real axis is oriented from left to right,
(ii) the positive imaginary axis is oriented from infinity toward zero,
(iii) the negative imaginary axis is oriented from infinity toward zero.

We use the following convention: the $+-$side of an oriented contour is always to its left, according to the given orientation.

Letting M_+ and M_- denote the limits of M on Σ from left and right, respectively, we define the Riemann–Hilbert factorization problem

$$M_+(x,t,k)=M_-(x,t,k)J(x,t,k),$$

where

$$\begin{aligned} J(x,t,k)&=J_4^{-1}, \qquad k\in\mathbb{R}^+,\\ &J_1^{-1}, \qquad k\in i\mathbb{R}^+,\\ &J_3^{-1}, \qquad k\in i\mathbb{R}^-,\\ J_2&=J_3J_4^{-1}J_1, \qquad k\in\mathbb{R}^-, \end{aligned} \tag{2}$$

with

$$J_1=\begin{pmatrix} 1 & 0\\ \Gamma(k)e^{2i\Theta} & 1\end{pmatrix},$$

$$J_4=\begin{pmatrix} 1 & -\gamma(k)e^{-2i\Theta}\\ \overline{\gamma}(k)e^{2i\Theta} & 1-|\gamma(k)|^2\end{pmatrix},$$

$$J_3=\begin{pmatrix} 1 & -\overline{\Gamma}(\overline{k})e^{-2i\Theta}\\ 0 & 1\end{pmatrix},$$

$$\Theta(x,t,k)=\frac{\theta}{h},$$

where

$$\theta=kx+2k^2t.$$

The functions γ,Γ are defined in terms of the spectral functions of the problem [see Appendix A, or Ref. 6, (2.28), (2.25)], with important analyticity properties [see Appendix A, or (2.21) and (2.22) of Ref. 6]. In particular note that

$$\Gamma(k)=\frac{1}{a(k)\left(a(k)\dfrac{\overline{A}(\overline{k})}{\overline{B}(\overline{k})}-b(k)\right)}, \tag{3}$$

where a, b are the spectral functions for the x problem and A, B are the spectral functions for the t problem. The functions a, b are analytic and bounded in the upper half-plane, while A, B are analytic and bounded in the first and third quadrants of the k plane. For our special choice of zero initial data, $b=0$, $a=1$. Hence $\gamma=0$ and $\Gamma(k)=\overline{B}(\overline{k})/\overline{A}(\overline{k})$. Note that a, b, A, B, Γ all depend on h.

The solution of (1a) can be recovered from the solution of (2) as follows:

$$u(x,t)=2i\ \ h\lim_{k\to\infty}(kM^{12}(x,t,k)), \tag{4}$$

where the index 12 here denotes the (12)-entry of a matrix.

The following "global relation" (see Appendix A for motivation and derivation) is imposed on the scattering data:

$$a(k)B(k)-b(k)A(k)=e^{4ik^2T}c(k),$$

where $c(k)$ is analytic and bounded for $\mathrm{Im}\,k>0$, and $c(k)=O(1/k)$ as $k\to\infty$. Here T is the time up to which we solve the initial boundary value problem for NLS. In general A, B are functions of T.

If $u_x(0,t)$ is denoted by $f_1(t)$ then there is a complicated relation between the data f_0 and f_1; the global relation is the expression of this in the spectral space.

In our particular case [problem (1a)] $T=\infty$ and the global relation becomes

$$a(k)B(k)-b(k)A(k)=0, \tag{5}$$

for $\arg(k)\in[0,\pi/2]$. For the special choice of zero initial data, since $b=0$, $a=1$, one has $B=0$ for $\arg(k)\in[0,\pi/2]$. In particular, $\Gamma(0)=0$.

The following is proved in Sec. V of Ref. 6.

Theorem 1: Given a Schwartz function f_0, there exists a unique f_1, also Schwartz, such that the above-given global relation is satisfied, and such that all derivatives of f_0, f_1 vanish at 0 (so that f_0, f_1 are compatible with NLS at $x=0, t=0$).

Using the theory developed in Ref. 6, we will then consider the (seemingly) overdetermined problem (1b) which in fact does have a unique solution, and which of course is the solution of problem (1a).

We note that in both the negative half-line and the positive half-line the jump matrix is of the same form. For positive k,

$$J=\begin{pmatrix} 1-|\gamma(k)|^2 & \gamma(k)e^{-2i\Theta} \\ -\overline{\gamma}(k)e^{2i\Theta} & 1 \end{pmatrix},$$

while for negative k,

$$J=\begin{pmatrix} 1-|\gamma(k)-\overline{\Gamma}|^2 & (\gamma(k)-\overline{\Gamma})e^{-2i\Theta} \\ -(\overline{\gamma}(k)-\Gamma)e^{2i\Theta} & 1 \end{pmatrix}.$$

In fact, let

$$r(k)=\gamma(k)-\overline{\Gamma}(k)=\frac{bA-aB}{\overline{a}A-\overline{b}B}, \qquad k<0,$$

$$r(k)=\gamma=\frac{b(k)}{\overline{a}(k)}, \quad k\geqslant 0.$$

Then, for all nonzero real k,

$$J=\begin{pmatrix} 1-|r(k)|^2 & r(k)e^{-2i\Theta} \\ -\overline{r}(k)e^{2i\Theta} & 1 \end{pmatrix}.$$

In the special case of zero initial data, the jump reduces to the identity for positive k, while for negative k, $r=-B/A$, so

$$J=\begin{pmatrix} 1-\left|\frac{B}{A}\right|^2 & \frac{-B}{A}e^{-2i\Theta} \\ \frac{\overline{B}}{\overline{A}}e^{2i\Theta} & 1 \end{pmatrix}. \tag{6}$$

III. DIRECT SCATTERING AS $h\to 0$

It is important to have some information about the "spectral" coefficent $r=-B/A$, for real values of k.

Theorem 2: For $k<0$, the spectral function $r(k,h)$ has the following asymptotic expression. There exist functions $\tilde{r},R_0$ of k alone, such that

$$r(k,h)\sim\tilde{r}(k)\exp\left(\frac{2iR_0(k)}{h}\right), \tag{7}$$

as $h\to 0$, where $\tilde{r}(k)$ is analytic and bounded as $k\to\infty$, and $R_0(k)$ is analytic. When $k\in i\mathbb{R}^+$, $\mathrm{Re}(iR_0)\leqslant 0$. Also $|\tilde{r}|\leqslant 1$.

Proof: The representation (7) follows from the standard Wentzel–Kramers–Brillouin (WKB) theory. Indeed, A, B admit representations of the form $s(k)\exp(iR(k)/h)$. Formula (7) thus follows. The analyticity of $\tilde{r}$, R_0 follows from the analyticity of A, B. The fact that $|A(k)|^2-|B(k)|^2=1$ (for real k) implies $|\tilde{r}|\leqslant 1$.

More detailed information about r can be recovered after a detailed analysis of the spectral problem for the second Lax operator. An easy calculation shows that the associated spectral problem reduces to a WKB problem of the type

$$h^2y_{tt}=S(t,k)y,$$

where $S(t,k)$ is real. The spectral coefficients A, B can then be asymptotically estimated along the lines of Ref. 8 (Sec. 10.6). Eventually one is able to show the following.

Theorem 3: Let

$$f_2(t)=\frac{5}{8\cdot 2^{1/3}}[\mathrm{Re}(i\overline{f_1}(t)f_0(t))]^{4/3}+|f_0(t)|^4-|f_1(t)|^2.$$

Let $-f=\min\{f_2(t)\}$ over the interval $[0,\infty]$. Without loss of generality, we assume $-f<0$. [Otherwise the analysis becomes trivial; the coefficent $r(k,h)$ is everywhere small.] On the real line, the following holds.

For $-f<k<0$,

$$r(k,h)\sim -ie^{[2i\sigma(k)]/h},$$

where σ is smooth in $(-f,0)$ and takes real values. Also σ can be extended analytically in a small neighborhood of the segment $(-f,0)$.

For values of k away from the interval $(-f,0)$, $r(k,h)$ is either zero or uniformly exponentially small in h.

Furthermore one has an asymptotic formula for $1-|r(k)|^2$, $-f<k<0$. Indeed,

$$1-|r(k)|^2\sim\exp\left(\frac{-2\tau(k)}{h}\right),$$

where $\tau(k)$ is positive and can be extended analytically in a small neighborhood of $(-f,0)$.

Remark: An explicit integral formula for σ and τ in terms of the data can only be found assuming $u_x = f_1$ is known. In general, even though the existence of f_1 is guaranteed (given f_0) via the global relation, f_1 is not effectively computable.

However, in the special case of so-called "linearizable data," f_1 and σ are indeed effectively computable (see Ref. 5).

Proof of Theorem 3: We simply note that the turning curve for the t-spectral problem is given by

$$S(t,k) = 4k^4 + k\,\mathrm{Re}(i\overline{f_1}(t)f_0(t)) + |f_0(t)|^4 - |f_1(t)|^2 = 0.$$

Indeed consider the t-problem

$$By = \begin{pmatrix} ih\partial_t + 4ik^2 + i|f_0|^2 & -2kf_0 - if_1 \\ -2k\overline{f_0} + i\overline{f_1} & ih\partial_t - i|f_0|^2 \end{pmatrix} \qquad y = 0.$$

Applying the operator

$$B^0 = \begin{pmatrix} ih\partial_t - i|f_0|^2 & 2kf_0 + if_1 \\ -2k\overline{f_0} - i\overline{f_1} & ih\partial_t + 4ik^2 + i|f_0|^2 \end{pmatrix}$$

we end up, up to errors of order $O(h)$, with

$$h^2 y_{tt} = S(t,k)y, \tag{8}$$

with $S(t,k)$ as above.

Note here that real k for which there exist L_2-solutions y of $By = 0$, are *a priori* excluded (see Ref. 6, p.16). So we do not need to concern ourselves with the possibility of real k for which the solutions to (8) are in L_2. We can then follow the WKB analysis of the semiclassical Schrödinger operator without essential changes (e.g., Ref. 8, Sec. 10.6). We can thus show that at all k such that $S(t,k) = k$ for some t, the reflection and transmission coefficients are given by the formulas above, while otherwise $r(k,h)$ is exponentially small (or zero). A short calculation shows that $S(t,k)$ as a function of k has only one local minimum, at $f_2(t)$, as defined in the statement of Theorem 3. The result follows immediately.

IV. REDUCING TO A PROBLEM ON THE REAL LINE

We next consider two Riemann–Hilbert problems with sole jumps given by

$$J_1^{-1}, \qquad k \in i\mathbb{R}^+,$$

$$J_3^{-1}, \qquad k \in i\mathbb{R}^-,$$

respectively.

We want U to be a function analytic in the complex plane except the upper imaginary axis, with normalization $\lim_{k\to\infty} U(x,t,k) = I$. The jump is prescribed by

$$U_+(x,t,k) = U_-(x,t,k)J_1^{-1}(x,t,k), \qquad k \in i\mathbb{R}^+,$$

with

$$J_1=\begin{pmatrix} 1 & 0 \\ \Gamma(k)e^{2i\Theta} & 1 \end{pmatrix},$$
$$\Theta(x,t,k)=\frac{\theta}{h}, \tag{9}$$

where

$$\theta=kx+2k^2t.$$

(The symbol U stands for ''upper'' since the jump is on the upper half-plane. We will immediately see however that U is a lower triangular matrix.)

Similarly, we want L to be a function analytic in the complex plane except the lower imaginary axis, with normalization $\lim_{k\to\infty}L(x,t,k)=I$. The jump is prescribed by

$$L_+(x,t,k)=L_-(x,t,k)J_3^{-1}(x,t,k), \qquad k\in i\mathbb{R}^-, \tag{10}$$

with

$$J_3=\begin{pmatrix} 1 & -\overline{\Gamma}(\overline{k})e^{-2i\Theta} \\ 0 & 1 \end{pmatrix}.$$

(The symbol L stands for ''lower'' since the jump is on the upper half-plane. However L is an upper triangular matrix.)

The two Riemann–Hilbert problems above can be easily solved explicitly, since the jumps are triangular matrices. Indeed, direct calculations show that

$$U(x,t,k)=\begin{pmatrix} 1 & 0 \\ u(x,t,k) & 1 \end{pmatrix}, \tag{11}$$

where

$$u(x,t,k)=\frac{1}{2\pi i}\int_{i\mathbb{R}^+}\frac{\Gamma(s)e^{2i\Theta(x,t,s)}ds}{s-k}$$

satisifies (9). Similarly,

$$L(x,t,k)=\begin{pmatrix} 1 & l(x,t,k) \\ 0 & 1 \end{pmatrix}, \tag{12}$$

where

$$l(x,t,k)=\frac{1}{2\pi i}\int_{i\mathbb{R}^-}\frac{-\overline{\Gamma}(\overline{s})e^{-2i\Theta(x,t,s)}ds}{s-k}$$

satisfies (10). The direction of the integral contours is as prescribed in Sec. II, i.e., from infinity to zero.

Note that $u(k)=-\overline{l(\overline{k})}$. Note also that the integrals in (11) and (12) are not singular at $k=0$, as $\Gamma(0)=0$.

We next show that the Riemann–Hilbert problem (2) is equivalent to a problem on the real line. Indeed, let

$$\begin{aligned} N(x,t,k) &= M(x,t,k)U^{-1}(x,t,k), \qquad \operatorname{Im} k>0, \\ N(x,t,k) &= M(x,t,k)L^{-1}(x,t,k), \qquad \operatorname{Im} k<0. \end{aligned} \tag{13}$$

Then $N(x,t,k)$ is analytic in $\mathbb{C}\setminus\mathbb{R}$, with $\lim_{k\to\infty} N(x,t,k)=I$, and across $\mathbb{R}$ the jump is given by

$$N_+(x,t,k)=N_-(x,t,k)L(x,t,k)J(x,t,k)U^{-1}(x,t,k). \tag{14}$$

In fact, the new jump is given by

$$LJU^{-1}=\begin{pmatrix} 1-|l(k)+r(k)e^{-2i\Theta}|^2 & l(k)+r(k)e^{-2i\Theta} \\ -\overline{l}(k)-\overline{r}(k)e^{2i\Theta} & 1 \end{pmatrix}. \tag{15}$$

Note here that while $r(k)$ depends only on k but not on $x,t,l(k)$ depends on x,t,h via Θ by (12).

We have thus reduced the Riemann–Hilbert problem (2) to the problem (15) with only jump on the real line.

V. THE g-FUNCTION

We next show how the Riemann–Hilbert problem can be ''deformed'' to a problem that is explicitly solvable. We are essentially following the ideas of Ref. 3 (see also Ref. 4).

The first idea involves the so-called ''g-function.'' We introduce a scalar function $g(k)$ which is to be analytic in $\mathbb{C}\setminus\mathbb{R}$ and decay like $O(1/k)$ at infinity. This function will be uniquely specified eventually.

Let

$$O(k)=N(k)\exp\left(\frac{ig(k)\sigma_3}{h}\right).$$

If N satisfies $N_+=N_-J, \quad k<0$, with J given by (6), then O solves a Riemann–Hilbert problem with jump matrix v_O, say, that is

$$O_+(x,t,k)=O_-(x,t,k)v_O(x,t,k), \tag{16}$$

$$v_O(k)=\begin{pmatrix} e^{[i(g_+-g_-)]/h}\left(1-\left|l+\frac{B}{A}e^{-2i\Theta}\right|^2\right) & \left(l-\frac{B}{A}e^{-2i\Theta}\right)e^{[-i(g_++g_-)]/h} \\ \left(-\overline{l}-\frac{\overline{B}}{\overline{A}}e^{2i\Theta}\right)e^{[i(g_++g_-)]/h} & e^{-(ig_+-ig_-)/h} \end{pmatrix}, \qquad k<0,$$

$$v_O(k)=\begin{pmatrix} e^{[i(g_+-g_-)]/h}(1-|l|^2) & l(k)e^{[-i(g_++g_-)]/h} \\ -\overline{l}(k)e^{[i(g_++g_-)]/h} & e^{[-(ig_+-ig_-)]/h} \end{pmatrix}, \qquad k>0,$$

$$\lim_{k\to\infty} O(k)=I.$$

Here g_+, g_- denote the limits of g from above and below the negative real axis, respectively.

Note that problem (16) is exactly (not just asymptotically) equivalent to the original Riemann–Hilbert problem (2). Formula (4) has to be replaced by

$$u(x,t)=2i \ \ h\lim_{k\to\infty}(kO^{12}(x,t,k))+2\partial_x\tilde{g}, \tag{17}$$

where $\tilde{g}$ is the residue of g at infinity.

VI. REDUCTION TO A SOLVABLE RIEMANN–HILBERT PROBLEM

Our first approximation involves getting rid of the functions l,u appearing in the jumps. The reason is simple. By formulas (11) and (12) u,l can be shown to be at worst $O(h)$ by use of the Laplace method for asymptotic evaluation of integrals, since the phase iR_0 of Theorem 2 has negative or zero real part. This suggests that l can be eventually erased from formula (16). In fact, we shall see right away that l *can* be neglected, not only because it is small, but also because of the precise factorization that follows.

Indeed, an easy calculation shows that the jump v_O of (16) can be written as

$$v_O=\begin{pmatrix}1 & le^{2ig_+/h}\\ 0 & 1\end{pmatrix}\cdot\begin{pmatrix}e^{[i(g_+-g_-)]/h}(1-|B/A|^2) & -\dfrac{B}{A}e^{-2i\Theta}e^{[-i(g_++g_-)]/h}\\ -\dfrac{\overline{B}}{\overline{A}}e^{2i\Theta}e^{[i(g_++g_-)]/h} & e^{[-(ig_+-ig_-)]/h}\end{pmatrix}\cdot\begin{pmatrix}1 & 0\\ -\overline{l}e^{-2ig_-/h} & 1\end{pmatrix},\quad k<0, \tag{18}$$

$$v_O=\begin{pmatrix}1 & le^{2ig_+/h}\\ 0 & 1\end{pmatrix}\cdot\begin{pmatrix}1 & 0\\ -\overline{l}e^{-2ig_-/h} & 1\end{pmatrix},\qquad k>0.$$

Since g takes real values on $\mathbb{R}$ [this will be clear later, see formula (28)] and since $l=O(h)$, it follows that the triangular factors in (18) can be taken as the identity plus a resulting error of order at worst $O(h)$ in formula (18).

We have asymptotically reduced the Riemann–Hilbert problem (16) to a new Riemann–Hilbert problem for a matrix function $Q(z)$, say.

If Q is defined by

$$Q_+(x,t,k)=Q_-(x,t,k)v_Q(x,t,k),$$

$$v_Q(k)=\begin{pmatrix}e^{[i(g_+-g_-)]/h}(1-|B/A|^2) & -\dfrac{B}{A}e^{-2i\Theta}e^{[-i(g_++g_-)]/h}\\ \dfrac{\overline{B}}{\overline{A}}e^{2i\Theta}e^{[i(g_++g_-)]/h} & e^{[-(ig_+-ig_-)]/h}\end{pmatrix},\qquad k<0, \tag{19}$$

$$\lim_{k\to\infty}Q(k)=I,$$

then Q is asymptotically equivalent to O in a neighborhood of ∞. In particular,

$$u(x,t)\sim 2ih\lim_{k\to\infty}(kO^{12}(x,t,k))+2\partial_x\tilde{g}. \tag{20}$$

The matrix v_Q can be written as

$$v_Q=\begin{pmatrix} e^{[i(g_+-g_-)]/h}(1-|r|^2) & r(k)e^{-2i\Theta}e^{[-i(g_++g_-)]/h} \\ -\overline{r}(k)e^{2i\Theta}e^{[i(g_++g_-)]/h} & e^{[-(ig_+-ig_-)]/h} \end{pmatrix}$$
$$=\begin{pmatrix} e^{[i(g_+-g_-)-2\tau]/h} & -ie^{[-2i\theta-i(g_++g_-)-2i\sigma]/h} \\ -ie^{[2i\theta+i(g_++g_-)+2i\sigma]/h} & e^{[-(ig_+-ig_-)]/h} \end{pmatrix},$$

$$\text{if } -f<k<0, \tag{21}$$

$$\sim\begin{pmatrix} e^{[i(g_+-g_-)]/h} & 0 \\ 0 & e^{[-(ig_+-ig_-)]/h} \end{pmatrix}, \quad \text{otherwise.}$$

We remind the reader that the functions σ,τ where introduced in the statement of Theorem 3.

At this point it becomes obvious that we should also impose

$$g_+-g_-=0, \qquad k>0, \quad or \qquad k<-f.$$

So g is to be analytic in $\mathbb{C}\backslash[-f,0]$.

Let

$$H=-g_+-g_--2\theta-2\sigma.$$

In the spirit of Ref. 3, we seek to reduce v_Q to a jump of one of the three following types:

$$\begin{pmatrix} 0 & -ie^{iH/h} \\ -ie^{-iH/h} & 1 \end{pmatrix}, \qquad \begin{pmatrix} 0 & -ie^{iH/h} \\ -ie^{-iH/h} & 0 \end{pmatrix}, \qquad \begin{pmatrix} 1 & -ie^{iH/h} \\ -ie^{-iH/h} & 0 \end{pmatrix}. \tag{22}$$

The motivation is the following. We expect that (22) will be deformable to a RH problem that can be explicitly solvable in terms of finite genus theta functions. Such a problem will have a ''finite gap'' structure. This means that the real line will be divided into a finite number of subintervals. In some of them the jump matrix has to look like

$$\begin{pmatrix} 0 & -ie^{iH/h} \\ -ie^{-iH/h} & 0 \end{pmatrix}$$

and in others it has to be the identity. We know however (through ''lens''-type arguments, see Appendix B) that matrices of the first or third form in (22) can be reduced to the identity. Hence the ansatz (22).

To arrive from (21) to (22) we impose some seemingly artificial conditions on the functions g,H. For any given x,t, we will consider finite sequences of real numbers $-1\leqslant k_1<k_2\leqslant k_3<k_4\leqslant\cdots\leqslant k_{2G+1}<k_{2G+2}\leqslant 1$. We call the $G+1$ intervals $I_1=[k_1,k_2],\ldots,I_{G+1}=[k_{2G+1},k_{2G+2}]$ the ''bands.'' Both the integer G and the real numbers $k_j, j=1,\ldots,2G+2$ are to be eventually determined for each x,t.

We make the ansatz that for each x,t the interval $[-f,0]$ can be subdivided into intervals by such k_j, such that on each of the arising intervals one of the three conditions holds:

$$-2i\tau=g_+-g_- \qquad \text{and} \qquad H'<0,$$

or

$$-2i\tau<g_+-g_-<0, \qquad \text{and} \qquad H'=0, \tag{23}$$

or

$$g_+-g_-=0, \qquad \text{and} \qquad H'>0.$$

H' denotes the derivative of H with respect to k. In particular, the intervals where $H'=0$ are to be the bands I_j, while on the intervals of which $[-f,0]\backslash\cup I_j$ consists, either the first or the third condition has to hold.

We will eventually see that conditions (23) amount to a scalar Riemann–Hilbert problem that can be solved explicitly, plus a set of algebraic conditions on the end points k_j defining the gap structure, plus a set of inequalities which essentially pick up the appropriate number of k_j's.

Now differentiating (with respect to k) the scalar Riemann–Hilbert problem given by the equalities in (23) and solving for g' leads to

$$g'(k)=(p(k))^{1/2}\left(\int_{\cup I_j}\frac{2\sigma'(\mu)-2\theta'(\mu)}{(p(\mu))_+^{1/2}(\mu-k)}\frac{d\mu}{2\pi i}+\int_{(-f,0)\backslash\cup I_j}\frac{-2i\tau'(\mu)}{(p(\mu))_+^{1/2}(\mu-k)}\frac{d\mu}{2\pi i}\right),$$

where

$$p(k)=\Pi_{j=1}^{G+1}(k-k_{2j-1})(k-k_{2j}). \tag{24}$$

We have imposed the condition $g(k)=O(k^{-1}),\ \ as\ \ k\to\infty$. Easy calculations then show that g' has to satisfy the moment conditions

$$\int_{\cup I_j}\frac{\sigma'(k)-\theta'(k)}{(p(k))_+^{1/2}}k^l dk+\int_{(-f,0)\backslash\cup I_j}\frac{-i\tau'(k)}{(p(k))_+^{1/2}}k^l dk=0, \tag{25}$$

$$l=0,1,2,\ldots,G.$$

Also, integrating g' around I_j and requiring $H'<0$, we obtain

$$\int_{I_j}(g'_+-g'_-)d\lambda=-2i(\tau(k_{2j-1})-\tau(k_{2j})),\quad j=1,\ldots,G+1. \tag{26}$$

Conditions (25) and (26) form a set of $2G+2$ equations for $2G+2$ unknowns. They enable us to solve for k_j.

At this point, we note that H is smooth in $[-f,0]$. We also note that it admits analytic continuations in (possibly small) lens-like domains of the complex plane, not including the points k_j.

In fact, conditions (25) and (26) together with the inequalities in (23) reduce to the Euler–Lagrange conditions of a variational problem. This is virtually the same variational problem introduced by Lax and Levermore and the existence and uniqueness of its solution is guaranteed by the theory of variational problems of logarithmic potentials (see Ref. 9 for a discussion). Since a complete written proof has not appeared anywhere so far, we will simply state a hypothesis.

Hypothesis: Assume that the data f_0 are real analytic and rapidly decaying (say Schwartz). Then for each x,t there is a finite non-negative integer G for which both equalities and inequalities in (23) have a solution. In other words, the ''finite genus ansatz'' can be eventually justified.

Once the existence of an appropriate ''g-function'' is guaranteed, it is straightforward to reduce our Riemann–Hilbert problem to its final form.

At the end of this procedure, and because of conditions (23), the jump contour consists of the bands $I_j, j=1,\ldots,G+1$ and on each band, the jump matrix is given by

$$w_j=\begin{pmatrix}0 & -ie^{iH/h}\\ -ie^{-iH/h} & 0\end{pmatrix}.$$

Furthermore, H is constant on each band. We actually have

$$w_j = \begin{pmatrix} 0 & -ie^{i\Omega_j/h} \\ -ie^{-i\Omega_j/h} & 0 \end{pmatrix}, \tag{27}$$

where the Ω_j are real constants.

The Ω_j can be computed explicitly. But first, let us note that the Riemann–Hilbert problem with jumps along the intervals I_j given by (27) can be explicitly solved in terms of theta functions. To appropriately define those functions we first need to introduce an underlying Riemann surface, together with some associated holomorphic differentials.

Let X be the two-sheeted Riemann surface of genus G associated with $(p(k))^{1/2}$, obtained by adjoining two copies of the slit plane $\mathbb{C}\backslash\cup_k I_k$. On the "top" sheet $(p(k))^{1/2}\sim k^{G+1}$ and on the "bottom" sheet $(p(k))^{1/2}\sim -k^{G+1}$. The branch points of the surface will be the end points of the "bands," that is, $k_1,\ldots,k_{2G+2}$. The homology cycles are defined in a standard way as follows. The cycles A_k lie on the top sheet and encircle slits I_k. The cycles B_k pass from the top sheet through the slit I_1 to the bottom sheet and back again through I_k.

The basis $\omega=(\omega_1,\ldots,\omega_G)$ of holomorphic differentials on X is determined by the normalization

$$\int_{A_i}\omega_j=\delta_{ij}, 1\leqslant i,\quad j\leqslant G.$$

The Riemann-matrix of periods is

$$\tau=(\tau_{ij})=\left(\int_{B_i}\omega_j\right)_{1\leqslant i,j\leqslant G}.$$

By the Riemann bilinear relations, τ is symmetric and $i\tau$ is negative definite. We can thus define the associated theta function

$$\theta_G(s)=\Sigma_{m\in\mathbb{Z}^G}\exp(2\pi i(m,s)+\pi i(m,\tau m)),\qquad s\in\mathbb{C}^G,$$

where (.,.) is the real scalar product. Note that θ_N is an even function.

Now, solving the scalar Riemann–Hilbert for g (not its derivative) we get

$$g(k)=(p(k))^{1/2}\left(\int_{\cup I_j}\frac{2\sigma(\mu)-2\theta(\mu)-\Omega_j}{(p(\mu))_+^{1/2}(\mu-k)}\frac{d\mu}{2\pi i}+\int_{(-f,0)\backslash\cup I_j}\frac{-2i\tau(\mu)}{(p(\mu))_+^{1/2}(\mu-k)}\frac{d\mu}{2\pi i}\right). \tag{28}$$

Applying the condition that $g(k)=O(k^{-1})$, as $k\to\infty$ once more, we get the conditions

$$\int_{\cup I_j}(2\sigma(k)-2\theta(k)-\Omega_j)\omega_l+\int_{(-f,0)\backslash\cup I_j}(-2i\tau(k))\omega_l=0,$$

$$l=1,2,\ldots,G.$$

Recalling the definition of the normalized differentials ω_l, we immediately get the following:

$$\Omega_l=\int_{\cup I_j}(2\sigma(k)-2\theta(k))\omega_l+\int_{(-f,0)\backslash\cup I_j}(-2i\tau(k))\omega_l,$$

$$l=1,2,\ldots,G. \tag{29}$$

We also define the following function:

$$\zeta(k)=\left[\Pi_{i=1}^{G+1}\frac{k-k_{2i}}{k-k_{2i-1}}\right]^{1/4},$$

where ζ is meant to be analytic off the union of the "gaps," i.e., the intervals between the bands, and $\zeta(k)\sim 1$, as $k\to\infty$. The function ζ has the important property that $\zeta\pm\zeta^{-1}$ has $G+1$ roots $(\zeta_j^{\pm})_{j=1}^{G+1}$, lying in the bands I_j, one root in each band. Note also that $\zeta_+=i\zeta_-$ across the gaps.

We next define the "Abel map" integral, for k on the top sheet of the Riemann surface X. Let

$$u(k)=\int_0^k\omega,$$

where the integral is taken along any path on the top sheet. Note that it is well-defined modulo $\mathbb{Z}^G$. Also define the constant vector

$$d=-K-\sum_{j=1}^{G}\int_0^{P_2(\zeta_j)}\omega,$$

where K is the vector of Riemann constants and $P_2(z)$ denotes the preimage of a point $z\in X$ in the "bottom" sheet. We can now state the following theorem.

Theorem 4: The function Q defined by problem (19) is asymptotically equivalent, as $h\to 0$, to

$$\operatorname{diag}\left(\frac{\theta_G(u(\infty)+d)}{\theta_G\left(u(\infty)+\frac{\Theta_G}{2\pi h}+d\right)},\frac{\theta_G(-u(\infty)+d)}{\theta_G\left(-u(\infty)+\frac{\Theta_G}{2\pi h}-d\right)}\right)\cdot\begin{pmatrix}\frac{\zeta+\zeta^{-1}}{2}\frac{\theta_G\left(u(k)+\frac{\Theta_G}{2\pi h}+d\right)}{\theta_G(u(k)+d)} & e^{(-iH_{G+1})/h}\frac{\zeta-\zeta^{-1}}{2i}\frac{\theta_G\left(u(k)+\frac{\Theta_G}{2\pi h}-d\right)}{\theta_G(u(k)-d)}\\ e^{(iH_{G+1})/h}\frac{\zeta-\zeta^{-1}}{-2i}\frac{\theta_G\left(-u(k)+\frac{\Theta_G}{2\pi h}+d\right)}{\theta_G(-u(k)+d)} & \frac{\zeta+\zeta^{-1}}{2}\frac{\theta_G\left(-u(k)+\frac{\Theta_G}{2\pi h}-d\right)}{\theta_G(-u(k)+d)}\end{pmatrix},\tag{30}$$

where $\Theta_G=(\Omega_1,\ldots,\Omega_G)^T$, the Ω_j being given by (29). The asymptotics is uniform in compact subsets of the Riemann sphere with the bands I_j deleted.

The proof consists of a straightforward check of the jump relations. The important fact is that (because of our choice of d) the zeros of $\zeta\pm\zeta^{-1}$ exactly cancel the poles of the theta function quotients.

The semiclassical asymptotics for the solution of (1a) follows from (30) and (4).

Theorem 5: The asymptotics for $u(x,t,h)$, the solution of (1a), as $h\to 0$, is given by

$$u(x,t,h)\sim[\Sigma_{j=1}^{2G+2}k_j]e^{(-iH_{G+1})/h}\cdot\frac{\theta_G(u(\infty)+d)\,\theta_G(u(\infty)+\Theta_G/(2\pi h)-d)}{\theta_G(u(\infty)-d)\,\theta_G(u(\infty)+\Theta_G/(2\pi\hbar)+d)}.\tag{31}$$

Formula (31) expresses a slowly modulated wave.

VII. CONCLUSION

Since we have been able to reduce our Riemann–Hilbert problem to one that arises in the full-line problem, the results of Refs. 10, 11, and 3 on the phenomenology of the solution as $h\to 0$ apply.

Semiclassically, the half-plane $x,t\geqslant 0$ can be divided in two regions. In the first ("smooth") region the strong semiclassical limit exists and satisfies the formallly limiting Euler system. In the

second (''turbulent'') region fast oscillations appear that can be described in terms of slowly modulating finite-gap solutions. Weak limits of an infinite number of densities including $|u|^2$, $ih(u\overline{u}_x - u_x\overline{u})$ exist.

We also note that the Whitham equations theory is still relevant. The functions $k_j(x,t)$ are in fact the Riemann invariants of the Whitham equations. The equations themselves can be derived by differentiating (25) and (26) (see, e.g., Ref. 4).

Let us also note that, even though the assumption that the initial data are equal to zero makes the analysis somewhat easier, it is not essential. In particular the above qualitative discussion of the semiclassical limit is still valid.

Finally, let us speculate on the long time asymptotics of the semiclassical limit.

There are two ways of computing the long time semiclassical limit of the defocusing NLS on the full line (see Ref. 12 or 13). One is to use the existing theory for times of order 1 (as in Ref. 11) and take the limit $t\to\infty$.

Alternatively, one should in principle be able to look at the long time behavior of the problem with fixed ϵ and *then* take $\epsilon\to 0$. This is by no means obvious *a priori*, but it turns out that this idea gives the right results. See, for example, Ref. 12, where the author has computed the long time semiclassical limit of the defocusing NLS on the full line.

On the half-line, it is already known what the long time of the problem with fixed ϵ is. As in the full-line case, any initial data degenerate into a sequence of finitely many separated solitons (see Refs. 14 and 6).

It then should follow, in exact analogy with the full line case,[12] that the long time asymptotics of the semiclassical limit in the half line case can be described by a sequence of solitons (in the turbulent region). The number of solitons is finite but increasing like $O(1/\epsilon)$ as $\epsilon\to 0$. Their width is $O(\epsilon)$ and they are separated by a distance of order $O(\epsilon t)$. In the smooth region, the solution simply dies out.

ACKNOWLEDGMENT

We thank Professor Fokas for showing us a preprint (Ref. 6) and for illuminating discussions and suggestions.

APPENDIX A: THE SCATTERING DATA FOR THE PROBLEM ON THE HALF LINE

In this appendix we quote freely from the paper of Fokas, Its and Sung (Ref. 6). We introduce the quantities a,b,A,B referred to in Sec. II and we state the analytic properties of these quantities.

We consider the NLS equation

$$iu_t + u_{xx} - 2|u|^2 u = 0. \tag{A1}$$

Here we have set $h=1$. For general positive h one can reduce Eq. (1a) to Eq. (A1) through the obvious rescaling $x\to x/h$, $t\to t/h$. Equation (A1) admits the Lax pair

$$\mu_x + ik[\sigma_3,\mu] = Q(x,t)\mu,$$

$$\mu_t + 2ik^2[\sigma_3,\mu] = \tilde{Q}(x,t,k)\mu,$$

where $\sigma_3 = \mathrm{diag}(1,-1)$, and

$$Q(x,t) = \begin{pmatrix} 0 & u(x,t) \\ \overline{u}(x,t) & 0 \end{pmatrix}, \qquad \tilde{Q}(x,t,k) = 2kQ - iQ_x\sigma_3 - i\lambda|u|^2\sigma_3.$$

Let $\hat{\sigma}_3$ denote the commutator with respect to σ_3, then $(\exp\hat{\sigma}_3)A$ can be computed easily:

$$\hat{\sigma}_3 A = [\sigma_3, A], \quad e^{\hat{\sigma}_3}A = e^{\sigma_3}Ae^{-\sigma_3},$$

where A is a 2×2 matrix.

The Lax pair can be rewritten as

$$d(e^{i(kx+2k^2t)\hat{\sigma}_3}\mu(x,t,k))=W(x,t,k), \tag{A2}$$

where the exact one-form W is defined by

$$W=e^{i(kx+2k^2t)\hat{\sigma}_3}(Q\mu\,dx+\tilde{Q}\mu\,dt).$$

Let Eq. (A1) be valid for

$$0<x<\infty, \quad 0<t<T,$$

where $T\leqslant\infty$ is a given positive constant. Assume that there exists a function $u(x,t)$ with sufficient smoothness and decay. A solution of Eq. (A2) is given by

$$\mu_*(x,t,k)=I+\int_{(x_*,t_*)}^{(x,t)} e^{-i(kx+2k^2t)\hat{\sigma}_3}W(\xi,\tau,k), \tag{A3}$$

where I is the 2×2 identity matrix, (x_*,t_*) is an arbitrary point in the domain $0<\xi<\infty$, $0<\tau<T$, and the integral is over a (piecewise) smooth curve from (x_*,t_*) to (x,t). Since the one-form W is exact, μ_* is independent of the path of integration. The analyticity properties of μ_* with respect to k depend on the choice of (x_*,t_*). It was shown in Ref. 15 that for a polygonal domain there exists a canonical way of choosing the points (x_*,t_*), namely, they are the corners of the associated polygon. Thus we define three different solutions μ_1, μ_2, μ_3, corresponding to $(0,T)$, $(0,0)$, (∞,t). Also we choose the particular contours as follows: The first contour consists of the oriented linear segments $(0,T)$ to $(0,t)$ and $(0,t)$ to (x,t). The second contour consists of the oriented linear segments from $(0,0)$ to $(0,t)$ and from $(0,t)$ to (x,t). The third contour is parallel to the x axis and is oriented from $(0,+\infty)$ to (x,t).

This choice implies the following inequalities:

$$\mu_1:\ \xi-x\leqslant 0, \quad \tau-t\geqslant 0,$$

$$\mu_2:\ \xi-x\leqslant 0, \quad \tau-t\leqslant 0,$$

$$\mu_3:\ \xi-x\geqslant 0.$$

The second column of the matrix equation (A3) involves $\exp[i(k(\xi-x)+2k^2(\tau-t))]$. Using the above-mentioned inequalities it follows that this exponential is bounded in the following regions of the complex k plane:

$$\mu_1:\{\Im k\leqslant 0\cap \Im k^2\geqslant 0\},$$

$$\mu_2:\{\Im k\leqslant 0\cap \Im k^2\leqslant 0\},$$

$$\mu_3:\{\Im k\geqslant 0\}.$$

Thus the second column vectors of μ_1, μ_2 and μ_3 are bounded and analytic for $\arg k$ in $(\pi,3\pi/2)$, $(3\pi/2,2\pi)$ and $(0,\pi)$, respectively. We will denote these vectors with superscripts (3), (4), and (12) to indicate that they are bounded and analytic in the third quadrant, fourth quadrant, and the upper half of the complex k plane, respectively. Similar conditions are valid for the first column vectors, thus

$$\mu_1(x,t,k)=(\mu_1^{(2)},\mu_1^{(3)}), \quad \mu_2(x,t,k)=(\mu_2^{(1)},\mu_2^{(4)}), \qquad \mu_3(x,t,k)=(\mu_3^{(34)},\mu_3^{(12)}). \tag{A4}$$

We note that the functions μ_1 and μ_2 are entire functions of k. Equation (A4) together with the estimate

$$\mu_j(x,t,k)=I+O\left(\frac{1}{k}\right), \quad k\to\infty, \quad j=1,2,3, \tag{A5}$$

imply that the functions μ_j are the fundamental eigenfunctions needed for the formulation of a RH problem in the complex k plane. The jump matrix of this RH problem is uniquely defined in terms of the 2×2-matrix valued functions

$$s(k)=\mu_3(0,0,k), \quad S(k)=[e^{2ik^2T\hat{\sigma}_3}\mu_2(0,T,k)]^{-1}. \tag{A6}$$

This is a direct consequence of the fact that (in the domain where μ_3 is defined) any two solutions of (A3) are simply related,

$$\begin{aligned}\mu_3(x,t,k)&=\mu_2(x,t,k)e^{-i(kx+2k^2t))\hat{\sigma}_3}\mu_3(0,0,k),\\ \mu_1(x,t,k)&=\mu_2(x,t,k)e^{-i(kx+2k^2t))\hat{\sigma}_3}[e^{2ik^2T\hat{\sigma}_3}\mu_2(0,T,k)]^{-1}.\end{aligned} \tag{A7}$$

The functions $s(k)$ and $S(k)$ follow from the evaluations at $x=0$ and $t=T$, respectively, of the function $\mu_3(x,0,k)$ and of $\mu_2(0,t,k)$ which satisfy the following linear integral equations:

$$\begin{aligned}\mu_3(x,0,k)&=I+\int_{\infty}^{x}e^{ik(\xi-x)\hat{\sigma}_3}(Q\mu_3)(\xi,0,k)\,d\xi,\\ \mu_2(0,t,k)&=I+\int_0^t e^{2ik^2(\tau-t)\hat{\sigma}_3}(\tilde{Q}\mu_2)(0,\tau,k)\,d\tau.\end{aligned} \tag{A8}$$

The fact that Q and $\tilde{Q}$ are traceless together with (A5) imply $\det\mu_j(x,t,k)=1$ for $j=1,2,3$. Thus

$$\det s(k)=\det S(k)=1.$$

From the symmetry properties of Q and $\tilde{Q}$ it follows that

$$(\mu(x,t,k))_{11}=\overline{(\mu(x,t,\bar{k})_{22}}, \quad (\mu(x,t,k))_{21}=\overline{\mu(x,t,\bar{k})_{12}},$$

and thus

$$s_{11}(k)=\overline{s_{22}(\bar{k})}, \quad s_{21}(k)=\overline{s_{12}(\bar{k})}, \quad S_{11}(k)=\overline{S_{22}(\bar{k})}, \quad S_{21}(k)=\overline{S_{12}(\bar{k})}.$$

We will use the following notation for s and S:

$$s(k)=\begin{pmatrix}\overline{a(\bar{k})} & b(k)\\ \overline{b(\bar{k})} & a(k)\end{pmatrix}, \quad S(k)=\begin{pmatrix}\overline{A(\bar{k})} & B(k)\\ \overline{B(\bar{k})} & A(k)\end{pmatrix}.$$

The definitions of $\mu_j(0,t,k)$, $j=1,2$, and of $\mu_2(x,0,k)$ imply that these functions have larger domains of boundedness,

$$\begin{aligned}\mu_1(0,t,k)&=(\mu_1^{(24)}(0,t,k),\mu_1^{(13)}(0,t,k)),\\ \mu_2(0,t,k)&=(\mu_2^{(13)}(0,t,k),\mu_2^{(24)}(0,t,k)),\\ \mu_2(x,0,k)&=(\mu_2^{(12)}(x,0,k),\mu_2^{(34)}(x,0,k)).\end{aligned}$$

The definitions of $s(k)$, $S(k)$ imply

$$\begin{pmatrix} b(k) \\ a(k) \end{pmatrix} = \mu_3^{(12)}(0,0,k), \quad \begin{pmatrix} -e^{-4ik^2T}B(k) \\ \overline{A(\bar{k})} \end{pmatrix} = \mu_2^{(24)}(0,T,k),$$

where the vectors $\mu_3^{(12)}(x,0,k)$ and $\mu_2^{(24)}(0,t,k)$ satisfy the following ODEs:

$$\partial_x \mu_3^{(12)}(x,0,k) + 2ik \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \mu_3^{(12)}(x,0,k) = Q(x,0)\mu_3^{(12)}(x,0,k), \quad 0 \leqslant \arg k \leqslant \pi,\ 0 < x < \infty,$$

$$\lim_{x\to\infty} \mu_3^{(12)}(x,0,k) = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and

$$\partial_t \mu_2^{(24)}(0,t,k) + 4ik^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \mu_2^{(24)}(0,t,k)$$

$$= \tilde{Q}(0,t,k)\mu_2^{(24)}(0,t,k), \quad \arg k \in [\pi/2,\pi] \cup [3\pi/2,2\pi], \quad 0 < t < T,$$

$$\mu_2^{(24)}(0,0,k) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The above definitions imply the following properties:

$$a(k), b(k) \text{ are defined and analytic for } \arg k \in (0,\pi).$$

$$|a(k)|^2 - |b(k)|^2 = 1, \quad k \in \mathbb{R}.$$

$$a(k) = 1 + O\left(\frac{1}{k}\right), \quad b(k) = O\left(\frac{1}{k}\right), \quad k \to \infty.$$

Also $A(k), B(k)$ are entire functions bounded for $\arg k \in [0,\pi/2] \cup [\pi, 3\pi/2]$. If $T = \infty$, the functions $A(k)$ and $B(k)$ are defined and analytic in the quadrants $\arg k \in (0,\pi/2) \cup (\pi, 3\pi/2)$.

$$A(k)\overline{A(\bar{k})} - B(k)\overline{B(\bar{k})} = 1, \quad k \in \mathbb{C}\ (k \in \mathbb{R} \cup i\mathbb{R}, \text{ if } T = \infty),$$

$$A(k) = 1 + O\left(\frac{1}{k}\right) + O\left(\frac{e^{4ik^2T}}{k}\right), \quad B(k) = O\left(\frac{1}{k}\right) + O\left(\frac{e^{4ik^2T}}{k}\right), \quad k \to \infty.$$

All of the above properties, except for the property that $B(k)$ is bounded for $\arg k \in [0,\pi/2] \cup [\pi, 3\pi/2]$, follow from the analyticity and boundedness of $\mu_3(x,0,k)$, $\mu_2(0,t,k)$, from the conditions of unit determinant, and from the large k asymptotics of these eigenfunctions. Regarding $B(k)$ we note that $B(k) = B(T,k)$, where $B(t,k) = -\exp(4ik^2t)(\mu_2^{(24)}(0,t,k))_1$. The above ODEs imply a linear Volterra integral equation for the vector $\exp(4ik^2t)\mu_2^{(24)}(0,t,k)$, from which it immediately follows that $B(t,k)$ is an entire function of k bounded for $\arg k \in [0,\pi/2] \cup [\pi, 3\pi/2]$.

We are now ready to derive the so-called global relation. We present the discussion Sec. (2.4) of Ref. 6. We in fact show that the spectral functions are not independent but satisfy an important relation. Indeed, the integral of the one-form $W(x,t,k)$ around the boundary of the domain $\{(\xi,\tau)\colon 0 < \xi < \infty,\ 0 < \tau < t\}$ vanishes. Let W be defined by (A2) with $\mu = \mu_3$. Then

$$\int_{\infty}^{0} e^{ik\xi\sigma_3}(Q\mu_3)(\xi,0,k)\,d\xi+\int_0^t e^{2ik^2\tau\hat{\sigma}_3}(\tilde{Q}\mu_3)(0,\tau,k)\,d\tau+e^{2ik^2t\hat{\sigma}_3}\int_0^{\infty} e^{ik\xi\hat{\sigma}_3}(Q\mu_3)(\xi,t,k)\,d\xi$$

$$=\lim_{x\to\infty} e^{ikx\hat{\sigma}_3}\int_0^t e^{2ik^2\tau\hat{\sigma}_3}(\tilde{Q}\mu_3)(x,\tau,k)\,d\tau. \tag{A9}$$

Using the definition of $s(k)$ above and (A8) it follows that the first term of this equation equals $s(k)-I$. Equation (A7) evaluated at $x=0$ gives

$$\mu_3(0,\tau,k)=\mu_2(0,\tau,k)e^{-2ik^2\tau\hat{\sigma}_3}s(k),$$

thus

$$e^{2ik^2\tau\hat{\sigma}_3}(\tilde{Q}\mu_3)(0,\tau,k)=[e^{2ik^2\tau\hat{\sigma}_3}(\tilde{Q}\mu_2)(0,\tau,k)]s(k);$$

this equation together with (A8) imply that the second term of (A9) equals

$$[e^{2ik^2t\hat{\sigma}_3}\mu_2(0,t,k)-I]s(k).$$

Hence assuming that u has sufficient decay as $x\to\infty$ Eq. (A9) becomes

$$-I+S(t,k)^{-1}s(k)+e^{2ik^2t\hat{\sigma}_3}\int_0^{\infty} e^{ik\xi\hat{\sigma}_3}(Q\mu_3)(\xi,t,k)\,d\xi=0, \tag{A10}$$

where the first and second columns of this equation are valid for $\arg k$ in the lower and the upper half of the complex k-plane, respectively, and $S(t,k)$ is defined by

$$S(t,k)=[e^{2ik^2t\hat{\sigma}_3}\mu_2(0,t,k)]^{-1}.$$

Letting $t=T$ and noting that $S(k)=S(T,k)$, Eq. (A10) becomes

$$-I+S(k)^{-1}s(k)+e^{2ik^2T\hat{\sigma}_3}\int_0^{\infty} e^{ik\xi\hat{\sigma}_3}(Q\mu_3)(\xi,T,k)\,d\xi=0.$$

The (12) component of this equation is

$$B(k)a(k)-A(k)b(k)=e^{4ik^2T}c^+(k),\quad \arg k\in[0,\pi],$$

$$c^+(k)=\int_0^{\infty} e^{ik\xi}(Q\mu_3)_{12}(\xi,T,k)\,dk.$$

This is the global relation, for finite T. For $T=\infty$ and assuming that f_0 is Schwartz, c^+ has to be set equal to zero.

APPENDIX B: THE "LENS" ARGUMENT

Suppose we have the following Riemann–Hilbert problem. We are seeking a matrix L, analytic in the complex plane except for a jump along the real interval $[\alpha,\beta]$, oriented from left to right. The normalization at infinity is to be $\lim_{k\to\infty}L=I$, and the jump across $[\alpha,\beta]$ is

$$L_+=L_-\begin{pmatrix} 0 & -ie^{iH/h} \\ -ie^{-iH/h} & 1 \end{pmatrix},$$

where $dH/dk<0$. We also assume that H is real on $[\alpha,\beta]$ and admits an analytic continuation in a small ''lens''-like domain bounded by two analytic arcs C_u, C_l joining the points α,β (in that direction) and lying entirely in the upper and lower half-planes, respectively. We note the following factorization of the jump matrix:

$$\begin{pmatrix} 0 & -ie^{iH/h} \\ -ie^{-iH/h} & 1 \end{pmatrix} = \begin{pmatrix} 1 & -ie^{iH/h} \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ -ie^{-iH/h} & 1 \end{pmatrix}.$$

This suggests the following definition. Let

$$L' = L, \quad \text{outside the domain bounded by} \quad C_u \cup C_l,$$

$$L' = L \cdot \begin{pmatrix} 1 & 0 \\ ie^{-iH/h} & 1 \end{pmatrix}, \quad \text{between } [\alpha,\beta] \text{ and } C_u.$$

$$L' = \begin{pmatrix} 1 & -ie^{iH/h} \\ 0 & 1 \end{pmatrix} \cdot L, \quad \text{between } [\alpha,\beta] \text{ and } C_l.$$

The Riemann–Hilbert problem for L' is as follows:

$$L'_+ = L'_- \cdot \begin{pmatrix} 1 & 0 \\ ie^{-iH/h} & 1 \end{pmatrix}, \quad k \in C_u,$$

$$L'_+ = L'_- \cdot \begin{pmatrix} 1 & -ie^{iH/h} \\ 0 & 1 \end{pmatrix}, \quad k \in C_l.$$

Now, since $d\,\mathrm{Re}\,H/dk<0$ on the interval $[\alpha,\beta]$, by the Cauchy–Riemann relations $d\,\mathrm{Im}\,H/dk<0$ across the interval $[\alpha,\beta]$, in the positive imaginary direction. This means that $\mathrm{Im}\,H<0$ *on* C_u if C_u is chosen to be close enough to $[\alpha,\beta]$, except at the end points α,β. Similarly $\mathrm{Im}\,H>0$ *on* C_l if C_l is chosen to be close enough to $[\alpha,\beta]$, except at the end points α,β. Hence,

$$\mathrm{Re}(-iH)<0, \quad k \in C_u,$$

$$\mathrm{Re}(-iH)>0, \quad k \in C_l,$$

except at the end points α,β. In other words the jump matrix for L' is the identity plus an exponentially small quantity, at least away from the end points α,β. This implies that the contour $C_u \cup C_l$ can be erased, at least away from the the end points α,β.

Near the end points one can use a parametrix argument, which we omit (see, e.g., Ref. 4 for details).

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Virasoro structure and localized excitations of the LKR system

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(Received 22 July 2003; accepted 8 September 2003)

A symmetry analysis is conducted for a master $2+1$-dimensional soliton system. The classical symmetries are shown to constitute an infinite dimensional Kac–Moody–Virasoro algebra. Finite symmetry group transformations are then used to construct localized excitations of the system. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625077]

I. INTRODUCTION

A decade or so ago, motivated by a class of infinitesimal Bäcklund transformations originally introduced in a gasdynamics context by Loewner in 1952, Konopelchenko and Rogers were led to construct a master $2+1$-dimensional soliton system.[1] The comprehensive nature of the latter is made evident by the fact that hierarchies of such so-called LKR systems have been shown to be compatible with generic multi-component KP and mKP hierarchies.[2] Notable reductions include integrable $2+1$-dimensional versions of the sine–Gordon equation, the principal chiral field model, the Bruschi–Ragnisco system[3] as well as Ernst–Weyl type equations.[4–6]

Here, a Lie-point symmetry analysis is conducted for the general LKR system. Its classical symmetries are shown to admit structure associated with an infinite dimensional Kac–Moody–Virasoro-type algebra. Finite group transformations are used to construct dromions and bowl-type ring solitons of the LKR system via constant matrix seed solutions.

II. THE 2+1-DIMENSIONAL LKR SYSTEM

The $2+1$-dimensional LKR triad[3]

$$(I_N\partial_x - S\partial_y - P)\Psi = 0, \tag{1}$$

$$(I_N\partial_y\partial_t - U\partial_t - V\partial_y - W)\Psi = 0, \tag{2}$$

$$(I_N\partial_x\partial_t - \tilde{U}\partial_t - \tilde{V}\partial_x - \tilde{W})\Psi = 0, \tag{3}$$

where I_N is an $N\times N$ unit matrix, was originally motivated by a class of infinitesimal Bäcklund transformations as introduced by Loewner in a gas-dynamics context.[7] In (1)–(3), $S,P,U,V,W,\tilde{U},\tilde{V}$ and $\tilde{W}$ denote $N\times N$ matrix functions of three independent variables x,y and t.

The corresponding nonlinear system, the LKR system,

$$S_t = [V,S], \tag{4}$$

$$P_t = \tilde{W} - SW + VP, \tag{5}$$

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$$\tilde{U}=SU+P, \quad \tilde{V}=V, \tag{6}$$

$$U_x-\tilde{U}_y+[U,\tilde{U}]=0, \tag{7}$$

$$V_x-\tilde{U}V-\tilde{W}+(UV+W-V_y)S=0, \tag{8}$$

$$W_x-\tilde{W}_y+U\tilde{W}-\tilde{U}W+(UV+W-V_y)P=0, \tag{9}$$

embodies the compatibility conditions of (1)–(3).

The parametrization

$$U=\phi_{2y}\phi_2^{-1}, \tag{10}$$

$$\tilde{U}=\phi_{2x}\phi_2^{-1}, \tag{11}$$

$$V=\phi_1+\phi_2\phi_3, \tag{12}$$

$$W=\phi_2(\phi_2^{-1}\phi_1)_y, \tag{13}$$

$$\tilde{W}=\phi_2[(\phi_2^{-1}\phi_1+\phi_3)_x-\phi_{3y}S]; \tag{14}$$

the LKR system (4)–(9) reduces it to consideration of the system

$$S_t=[\phi_1+\phi_2\phi_3,S], \tag{15}$$

$$P_t=\phi_{1x}-S\phi_{1y}-[P,\phi_1]+\phi_2[\phi_{3x}-\phi_{3y}S+\phi_3P], \tag{16}$$

$$\phi_{2x}-S\phi_{2y}-P\phi_2=0, \tag{17}$$

$$\phi_{3xy}-(\phi_{3y}S)_y+\phi_{3y}P=0. \tag{18}$$

The nonlinear system (4)–(9) or equivalently, (15)–(18), incorporates various important reductions.

Reduction 1: For the constant matrix S and

$$\phi_1=-\phi_2\phi_3, \tag{19}$$

the nonlinear system (15)–(18) reduces to the $2+1$-dimensional non-Abelian sine–Gordon model

$$P_t=[S,\phi_2\phi_{3y}], \tag{20}$$

$$\phi_{2x}-S\phi_{2y}-P\phi_2=0, \tag{21}$$

$$\phi_{3xy}-(\phi_{3y}S)_y+\phi_{3y}P=0. \tag{22}$$

Reduction 2: In the study of the LKR system, the special case $P=0$ is one of the most important reductions. For $P=0$, the system (15)–(18) reduces to

$$S_t=[\phi_1+\phi_2\phi_3,S], \tag{23}$$

$$\phi_{1x}-S\phi_{1y}=0, \tag{24}$$

$$\phi_{2x}-S\phi_{2y}=0, \tag{25}$$

$$\phi_{3x}-\phi_{3y}S=0. \tag{26}$$

The remaining reductions listed in this section constitute special cases of (23)–(26).

Reduction 3: The three-dimensional principal chiral field model

$$S_t=[\phi_2\phi_3,S], \tag{27}$$

$$\phi_{2x}-S\phi_{2y}=0, \tag{28}$$

$$\phi_{3x}-\phi_{3y}S=0, \tag{29}$$

or equivalently

$$S_t=[V,S], \tag{30}$$

$$V_x-V_yS-[S,UV]+[S,U]=0, \tag{31}$$

$$U_x-(SU)_y+[U,SU]=0, \tag{32}$$

is related to (23)–(26) by

$$\phi_1=I_N. \tag{33}$$

The two-dimensional principal chiral field model[8]

$$(\Omega_x\Omega^{-1})_t+(\Omega_t\Omega^{-1})_x=0 \tag{34}$$

can be obtained from (30)–(32) with

$$S=\tfrac{1}{2}\Omega_x\Omega^{-1},\quad V=\tfrac{1}{2}\Omega_t\Omega^{-1}$$

and $U=I_N, S_y=V_y=0$.

Reduction 4: The generalized Bruschi–Ragnisco system

$$S_t=[\phi_1+\phi_3,S], \tag{35}$$

$$\phi_{1x}-S\phi_{1y}=0, \tag{36}$$

$$\phi_{3x}-(\phi_{3y}S)=0, \tag{37}$$

or equivalently

$$S_t=[V,S], \tag{38}$$

$$V_x-V_yS+[W,S]=0, \tag{39}$$

$$W_x-(SW)_y=0, \tag{40}$$

is obtained as a reduction of (23)–(26) by taking $\phi_2=I_N$, i.e.,

$$U=\tilde{U}=0. \tag{41}$$

The $1+1$-dimensional Bruschi–Ragnisco system[9]

$$S_t=[\partial_x^{-1}[S,W],S],\quad W_x=0, \tag{42}$$

is retrieved from (38)–(40) by setting $S_y=V_y=W_y=0$.

Reduction 5: The most studied reduction of the LKR system is the so-called $2+1$-dimensional sine–Gordon system

$$\left(\frac{\phi_x}{\sin\theta}\right)_x-\left(\frac{\phi_y}{\sin\theta}\right)_y+\frac{\phi_y\theta_x-\phi_x\theta_y}{\sin^2\theta}=0,$$

$$\left(\frac{\phi'_x}{\sin\theta}\right)_x-\left(\frac{\phi'_y}{\sin\theta}\right)_y+\frac{\phi'_y\theta_x-\phi'_x\theta_y}{\sin^2\theta}=0, \tag{43}$$

$$\theta_t=\phi+\phi',$$

which is a symmetric integrable extension of the classical sine–Gordon equation. The classical $1+1$-dimensional sine–Gordon equation in curvature coordinates is retrieved as the reduction with $\phi'_y=\theta_y=\phi_y=0$. The corresponding particular LKR triad of (43) reads[3]

$$\left[I_N\partial_x+\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix}\partial_y\right]\psi=0,$$

$$\left[I_N\partial_t\partial_y+\frac{1}{2}\begin{pmatrix}0 & \theta_t\\ -\theta_t & 0\end{pmatrix}\partial_y-\frac{1}{2\sin\theta}\begin{pmatrix}\phi_y\cos\theta-\phi_x & -\phi'_y\sin\theta\\ \phi_y\sin\theta & \phi'_y+\phi'_x\cos\theta\end{pmatrix}\right]\psi=0, \tag{44}$$

$$\left[I_N\partial_t\partial_x+\frac{1}{2}\begin{pmatrix}0 & \theta_t\\ -\theta_t & 0\end{pmatrix}\partial_x-\frac{1}{2\sin\theta}\begin{pmatrix}\phi_x\cos\theta-\phi_y & -\phi'_x\sin\theta\\ \phi_x\sin\theta & \phi'_x+\phi'_y\cos\theta\end{pmatrix}\right]\psi=0.$$

III. CLASSICAL LIE SYMMETRIES AND VIRASORO STRUCTURE OF THE LKR SYSTEM

Lie symmetries of the $2+1$-dimensional sine–Gordon system have been extensively studied in Refs. 10 and 11. Here, we investigate underlying symmetry structure of the general nonlinear LKR system (4)–(9) by a procedure equivalent to the standard Lie approach.[12]

In the present context, a symmetry

$$\sigma\equiv(\sigma^S,\sigma^P,\sigma^V,\sigma^{\tilde V},\sigma^U,\sigma^{\tilde U},\sigma^W,\sigma^{\tilde W})^T,$$

where superscript T denotes the transposition of the matrix, is defined as a solution of the linearized system of (4)–(9),

$$\sigma^S_t=[\sigma^V,S]+[V,\sigma^S], \tag{45}$$

$$\sigma^P_t=\tilde\sigma^W-\sigma^S W-S\sigma^W+\sigma^V P+V\sigma^P, \tag{46}$$

$$\sigma^{\tilde U}=\sigma^S U+S\sigma^U+\sigma^P,\quad \sigma^{\tilde V}=\sigma^V, \tag{47}$$

$$\sigma^U_x-\sigma^{\tilde U}_y+[\sigma^U,\tilde U]+[U,\sigma^{\tilde U}]=0, \tag{48}$$

$$\sigma^V_x-\sigma^{\tilde U}V-\tilde U\sigma^V-\sigma^{\tilde W}+(\sigma^U V+U\sigma^V+\sigma^W-\sigma^V_y)S+(UV+W-V_y)\sigma^S=0, \tag{49}$$

$$\sigma^W_x-\sigma^{\tilde W}_y+\sigma^U\tilde W+U\sigma^{\tilde W}-\sigma^{\tilde U}W-\tilde U\sigma^W+(\sigma^U V+U\sigma^V+\sigma^W-\sigma^V_y)P+(UV+W-V_y)\sigma^P=0. \tag{50}$$

Thus, the system (4)–(9) is form invariant under the transformation

$$\{S,P,V,\tilde V,U,\tilde U,W,\tilde W\}\to\{S,P,V,\tilde V,U,\tilde U,W,\tilde W\}+\epsilon\{\sigma^S,\sigma^P,\sigma^V,\sigma^{\tilde V},\sigma^U,\sigma^{\tilde U},\sigma^W,\sigma^{\tilde W}\}, \tag{51}$$

where ϵ is an infinitesimal parameter. To find Lie point symmetries from the symmetry equations (45)–(50), it is sufficient to assume that $\{\sigma^S,\sigma^P,\sigma^V,\sigma^{\tilde{V}},\sigma^U,\sigma^{\tilde{U}},\sigma^W,\sigma^{\tilde{W}}\}$ possesses the form

$$\sigma^S = XS_x + YS_y + TS_t + F^S, \tag{52}$$

$$\sigma^P = XP_x + YP_y + TP_t + F^P, \tag{53}$$

$$\sigma^V = XV_x + YV_y + TV_t + F^V, \tag{54}$$

$$\sigma^{\tilde{V}} = X\tilde{V}_x + Y\tilde{V}_y + T\tilde{V}_t + F^{\tilde{V}}, \tag{55}$$

$$\sigma^U = XU_x + YU_y + TU_t + F^U, \tag{56}$$

$$\sigma^{\tilde{U}} = X\tilde{U}_x + Y\tilde{U}_y + T\tilde{U}_t + F^{\tilde{U}}, \tag{57}$$

$$\sigma^W = XW_x + YW_y + TW_t + F^W, \tag{58}$$

$$\sigma^{\tilde{W}} = X\tilde{W}_x + Y\tilde{W}_y + T\tilde{W}_t + F^{\tilde{W}}, \tag{59}$$

where X,Y,T are scalar functions and $F^S,F^P,F^V,F^{\tilde{V}},F^U,F^{\tilde{U}},F^W$ and $F^{\tilde{W}}$ are matrix functions of $x,y,t,S,P,V,\tilde{V},U,\tilde{U},W$ and $\tilde{W}$.

Substitution of (52)–(59) into the symmetry equations (45)–(50) and subsequent cancellation of all the independent quantities $\tilde{V},\tilde{U},S_t,S_{xt},S_{yt},S_{tt},P_t,P_{xt},P_{yt},P_{tt},U_x,U_{xx},U_{xy},U_{xt},V_x,V_{xx},V_{xy},V_{xt},W_x,W_{xx},W_{xy}$ and W_{xt} by means of (4)–(9) leads to an extensive set of determining equations to fix $X,Y,T,F^S,F^P,F^V,F^{\tilde{V}},F^U,F^{\tilde{U}},F^W$ and $F^{\tilde{W}}$. For instance, substitution of (52) and (54) into (45) produces the following determining equations:

$$X_t = X_S = X_P = X_V = X_U = X_W = X_{\tilde{V}} = X_{\tilde{U}} = X_{\tilde{W}} = 0, \tag{60}$$

$$Y_t = Y_S = Y_P = Y_V = Y_U = Y_W = Y_{\tilde{V}} = Y_{\tilde{U}} = Y_{\tilde{W}} = 0, \tag{61}$$

$$T_S = T_P = T_V = T_U = T_W = T_{\tilde{V}} = T_{\tilde{U}} = T_{\tilde{W}} = 0, \tag{62}$$

$$F^S_P = F^S_V = F^S_U = F^S_W = F^S_{\tilde{V}} = F^S_{\tilde{U}} = F^S_{\tilde{W}} = 0, \tag{63}$$

$$T_t(VS - SV) + F^S_t + \sum_{i=1}^{N}\sum_{j=1}^{N} (F^S)_{S_{ij}}(VS - SV)_{ij} - [F^V,S] - [V,F^S] = 0, \tag{64}$$

where $X_S = 0$ denotes

$$X_{S_{ij}} = 0, \quad \forall i,\ j.$$

Completion of similar analysis for all the symmetry equations shows that the general Lie point symmetry solution of the nonlinear system (4)–(9) reads

$$\begin{pmatrix} \sigma^S \\ \sigma^P \\ \sigma^V \\ \sigma^{\tilde{V}} \\ \sigma^U \\ \sigma^{\tilde{U}} \\ \sigma^W \\ \sigma^{\tilde{W}} \end{pmatrix} = \begin{pmatrix} XS_x+YS_y+TS_t-X_yS^2+(X_x-Y_y)S+Y_xI_N+[g,S] \\ XP_x+YP_y+TP_t+(X_xI_N-X_yS)P+[g,P]-Sg_y+g_x \\ XV_x+YV_y+TV_t+T_tV+[g,V]+g_t \\ X\tilde{V}_x+Y\tilde{V}_y+T\tilde{V}_t+T_t\tilde{V}+[g,\tilde{V}]+g_t \\ XU_x+YU_y+TU_t+Y_yU+X_y\tilde{U}+[g,U]+g_y \\ X\tilde{U}_x+Y\tilde{U}_y+T\tilde{U}_t+X_x\tilde{U}+Y_xU+[g,\tilde{U}]+g_x \\ XW_x+(YW)_y+TW_t+T_tW+X_y\tilde{W}+[g,W]-Ug_t-Vg_y+g_{yt} \\ (X\tilde{W})_x+Y\tilde{W}_y+T\tilde{W}_t+T_t\tilde{W}+Y_xW+[g,\tilde{W}]-\tilde{U}g_t-\tilde{V}g_x+g_{xt} \end{pmatrix}, \tag{65}$$

where g is an arbitrary $N\times N$ matrix function of $\{x,y,t\}$, X and Y are arbitrary scalar functions of $\{x,y\}$ and T is an arbitrary scalar function of t. That (65) is indeed a symmetry may be verified by direct substitution of (65) into (45)–(50) and use of (4)–(9).

Symmetry studies of a variety of $2+1$-dimensional integrable systems has revealed their possession of an underlying centerless Virasoro symmetry algebra (Witt algebra) structure:[13–18]

$$\lceil \sigma(f_1),\sigma(f_2) \rfloor = \sigma(f_2\dot{f}_1-f_1\dot{f}_2), \tag{66}$$

where f_1 and f_2 are arbitrary functions of a single independent variable. Here the dots over the functions f_1 and f_2 indicate derivatives of the functions with respect to their argument. In Ref. 19, the notion of *Virasoro integrability* was introduced for models that possess a generalized centerless Virasoro type symmetry algebra. Therein, a method was described whereby such Virasoro integrable scalar field models may be constructed. To ascertain whether the general LKR system admits underlying Virasoro symmetry structure or not, we set down the generators for the symmetry (65), viz.,

$$\sigma_1(X) \equiv \begin{pmatrix} XS_x-X_yS^2+X_xS \\ XP_x+(X_xI_N-X_yS)P \\ XV_x \\ X\tilde{V}_x \\ XU_x+X_y\tilde{U} \\ X\tilde{U}_x+X_x\tilde{U} \\ XW_x+X_y\tilde{W}, \\ (X\tilde{W})_x \end{pmatrix}, \tag{67}$$

$$\sigma_2(Y) \equiv \begin{pmatrix} YS_y-Y_yS+Y_xI_N \\ YP_y \\ YV_y \\ Y\tilde{V}_y \\ YU_y+Y_yU \\ Y\tilde{U}_y+Y_xU \\ (YW)_y \\ Y\tilde{W}_y+Y_xW \end{pmatrix}, \tag{68}$$

$$\sigma_3(T)\equiv\begin{pmatrix} TS_t \\ TP_t \\ TV_t+T_tV \\ T\tilde{V}_t+T_t\tilde{V} \\ TU_t \\ T\tilde{U}_t \\ TW_t+T_tW \\ T\tilde{W}_t+T_t\tilde{W} \end{pmatrix}, \tag{69}$$

$$\sigma_4(g)\equiv\begin{pmatrix} gS-Sg \\ gP-Pg-Sg_y+g_x, \\ gV-Vg+g_t, \\ g\tilde{V}-\tilde{V}g+g_t, \\ gU-Ug+g_y, \\ g\tilde{U}-\tilde{U}g+g_x, \\ gW-Wg-Ug_t-Vg_y+g_{yt}, \\ g\tilde{W}-\tilde{W}g-\tilde{U}g_t-\tilde{V}g_x+g_{xt} \end{pmatrix}. \tag{70}$$

Next, we define the matrix Gateaux derivative and commutator for matrix functions

$$A\equiv(A_1,A_2,\ldots,A_8)^T,\quad B\equiv(B_1,B_2,\ldots,B_8)^T,$$

where $A_i,B_i,i=1,2,\ldots,8$, are $N\times N$ matrix functions of $x,y,t,S,P,V,\tilde{V},U,\tilde{U},W$ and $\tilde{W}$:

$$[A,B]\equiv A'B-B'A\equiv\begin{pmatrix} A'_{1S} & A'_{1P} & A'_{1V} & A'_{1\tilde{V}} & A'_{1U} & A'_{1\tilde{U}} & A'_{1W} & A'_{1\tilde{W}} \\ A'_{2S} & A'_{2P} & A'_{2V} & A'_{2\tilde{V}} & A'_{2U} & A'_{2\tilde{U}} & A'_{2W} & A'_{2\tilde{W}} \\ A'_{3S} & A'_{3P} & A'_{3V} & A'_{3\tilde{V}} & A'_{3U} & A'_{3\tilde{U}} & A'_{3W} & A'_{3\tilde{W}} \\ A'_{4S} & A'_{4P} & A'_{4V} & A'_{4\tilde{V}} & A'_{4U} & A'_{4\tilde{U}} & A'_{4W} & A'_{4\tilde{W}} \\ A'_{5S} & A'_{5P} & A'_{5V} & A'_{5\tilde{V}} & A'_{5U} & A'_{5\tilde{U}} & A'_{5W} & A'_{5\tilde{W}} \\ A'_{6S} & A'_{6P} & A'_{6V} & A'_{6\tilde{V}} & A'_{6U} & A'_{6\tilde{U}} & A'_{6W} & A'_{6\tilde{W}} \\ A'_{7S} & A'_{7P} & A'_{7V} & A'_{7\tilde{V}} & A'_{7U} & A'_{7\tilde{U}} & A'_{7W} & A'_{7\tilde{W}} \\ A'_{8S} & A'_{8P} & A'_{8V} & A'_{8\tilde{V}} & A'_{8U} & A'_{8\tilde{U}} & A'_{8W} & A'_{8\tilde{W}} \end{pmatrix}\begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \\ B_6 \\ B_7 \\ B_8 \end{pmatrix}$$

$$-\begin{pmatrix} B'_{1S} & B'_{1P} & B'_{1V} & B'_{1\tilde{V}} & B'_{1U} & B'_{1\tilde{U}} & B'_{1W} & B'_{1\tilde{W}} \\ B'_{2S} & B'_{2P} & B'_{2V} & B'_{2\tilde{V}} & B'_{2U} & B'_{2\tilde{U}} & B'_{2W} & B'_{2\tilde{W}} \\ B'_{3S} & B'_{3P} & B'_{3V} & B'_{3\tilde{V}} & B'_{3U} & B'_{3\tilde{U}} & B'_{3W} & B'_{3\tilde{W}} \\ B'_{4S} & B'_{4P} & B'_{4V} & B'_{4\tilde{V}} & B'_{4U} & B'_{4\tilde{U}} & B'_{4W} & B'_{4\tilde{W}} \\ B'_{5S} & B'_{5P} & B'_{5V} & B'_{5\tilde{V}} & B'_{5U} & B'_{5\tilde{U}} & B'_{5W} & B'_{5\tilde{W}} \\ B'_{6S} & B'_{6P} & B'_{6V} & B'_{6\tilde{V}} & B'_{6U} & B'_{6\tilde{U}} & B'_{6W} & B'_{6\tilde{W}} \\ B'_{7S} & B'_{7P} & B'_{7V} & B'_{7\tilde{V}} & B'_{7U} & B'_{7\tilde{U}} & B'_{7W} & B'_{7\tilde{W}} \\ B'_{8S} & B'_{8P} & B'_{8V} & B'_{8\tilde{V}} & B'_{8U} & B'_{8\tilde{U}} & B'_{8W} & B'_{8\tilde{W}} \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \\ A_7 \\ A_8 \end{pmatrix}, \tag{71}$$

where the operators A'_{iS}, B'_{iP}, etc. are partial linearized operators,

$$A'_{1S}h \equiv \lim_{\epsilon\to 0}\frac{d}{d\epsilon}A_1(S+\epsilon h,P,V,\tilde{V},U,\tilde{U},W,\tilde{W}) \tag{72}$$

for arbitrary h.

On use of the above, it can be established that σ_1, σ_2, σ_3, and σ_4 constitute the following closed symmetry algebra:

$$\lceil\sigma_1(X_1),\sigma_1(X_2)\rfloor=\sigma_1(X_{1x}X_2-X_{2x}X_1), \tag{73}$$

$$\lceil\sigma_2(Y_1),\sigma_2(Y_2)\rfloor=\sigma_2(Y_{1y}Y_2-Y_{2y}Y_1), \tag{74}$$

$$\lceil\sigma_3(T_1),\sigma_3(T_2)\rfloor=\sigma_3(T_{1t}T_2-T_{2t}T_1), \tag{75}$$

$$\lceil\sigma_4(g_1),\sigma_4(g_2)\rfloor=\sigma_4(g_1g_2-g_2g_1), \tag{76}$$

$$\lceil\sigma_1(X),\sigma_2(Y)\rfloor=\sigma_2(XY_x)-\sigma_1(YX_y), \tag{77}$$

$$\lceil\sigma_1(X),\sigma_4(g)\rfloor=\sigma_4(Xg_x), \tag{78}$$

$$\lceil\sigma_2(Y),\sigma_4(g)\rfloor=\sigma_4(Yg_y), \tag{79}$$

$$\lceil\sigma_3(T),\sigma_4(g)\rfloor=\sigma_4(Tg_t), \tag{80}$$

$$\lceil\sigma_1(X),\sigma_3(T)\rfloor=\lceil\sigma_2(Y),\sigma_3(T)\rfloor=0. \tag{81}$$

Thus, it is seen that each of $\sigma_1(X)$, $\sigma_2(Y)$ and $\sigma_3(T)$ constitutes an infinite dimensional generalized centerless Virasoro symmetry algebra. Hence, the nonlinear LKR system (4)–(9) does indeed exhibit Virasoro symmetry structure. The commutator relation (76) shows us that the generator $\sigma_4(g)$ constitutes a gauge symmetry algebra.

IV. FINITE TRANSFORMATIONS

A symmetry (51) transforms a known solution of the model to a new solution of the same model in infinitesimal form. In order to generate new *exact* solutions from known seed solutions, it is necessary to construct the finite transformations from the obtained symmetries.

The general Lie symmetry group related to the Lie symmetry algebra can be obtained by solving the following ''initial'' problem:

$$\frac{\mathrm{d}t'}{\mathrm{d}\epsilon}=T',\quad t'|_{\epsilon=0}=t, \tag{82}$$

$$\frac{\mathrm{d}y'}{\mathrm{d}\epsilon}=Y',\quad y'|_{\epsilon=0}=y, \tag{83}$$

$$\frac{\mathrm{d}x'}{\mathrm{d}\epsilon}=X',\quad x'|_{\epsilon=0}=x, \tag{84}$$

$$\frac{\mathrm{d}S'}{\mathrm{d}\epsilon}=X'_{y'}(S')^2-(X'_{x'}-Y'_{y'})S'-Y'_{x'}I_N+[S',g'],\quad S'|_{\epsilon=0}=S, \tag{85}$$

$$\frac{\mathrm{d}P'}{\mathrm{d}\epsilon}=(X'_{y'}S'-X'_{x'}I_N)P'+[P',g']+S'g'_{y'}-g'_{x'},\quad P'|_{\epsilon=0}=P, \tag{86}$$

$$\frac{dV'}{d\epsilon}=[V',g']-g'_{t'}-T'_{t'}V',V'|_{\epsilon=0}=V, \tag{87}$$

$$\frac{d\tilde{V}'}{d\epsilon}=[\tilde{V}',g']-g'_{t'}-T'_{t'}\tilde{V}',\tilde{V}'|_{\epsilon=0}=\tilde{V}, \tag{88}$$

$$\frac{dU'}{d\epsilon}=-Y'_{y'}U'-X'_{y'}\tilde{U}'+[U',g']-g'_{y'},U'|_{\epsilon=0}=U, \tag{89}$$

$$\frac{d\tilde{U}'}{d\epsilon}=-X'_{x'}\tilde{U}'-Y'_{x'}U'+[\tilde{U}',g']-g'_{x'},\ \ \tilde{U}'|_{\epsilon=0}=\tilde{U}, \tag{90}$$

$$\frac{dW'}{d\epsilon}=[W',g']-(T'_{t'}+Y'_{y'})W'-X'_{y'}\tilde{W}'+U'g'_{t'}+V'g'_{y'}-g'_{y't'},W'|_{\epsilon=0}=W, \tag{91}$$

$$\frac{d\tilde{W}'}{d\epsilon}=[\tilde{W}',g']-(T'_{t'}+X'_{x'})\tilde{W}'-Y'_{x'}W'+\tilde{U}'g'_{t'}+\tilde{V}'g'_{x'}-g'_{x't'},\ \ \tilde{W}'|_{\epsilon=0}=\tilde{W}, \tag{92}$$

where $X'\equiv X(x',y'),Y'\equiv Y(x',y'),T'\equiv T(t')$ and $g'\equiv g(x'y't')$.

The final result is summarized as follows:

Theorem 1: If $\{S=S(x,y,t),P=P(x,y,t),V=V(x,y,t),\tilde{V}=\tilde{V}(x,y,t),U=U(x,y,t),\tilde{U}=\tilde{U}(x,y,t),W=W(x,y,t),\tilde{W}=\tilde{W}(x,y,t)\}$ is an exact solution of the generalized LKR system (4)–(9), then $\{S',P',V',\tilde{V}',U',\tilde{U}',W',\tilde{W}'\}$ with

$$S'=G(\xi_xS(\xi,\eta,\tau)+\eta_x)(\xi_yS(\xi,\eta,\tau)+\eta_y)^{-1}G^{-1}, \tag{93}$$

$$P'=G\{(\xi_x\eta_y-\xi_y\eta_x)(\xi_yS(\xi,\eta,\tau)+\eta_y)^{-1}P(\xi,\eta,\tau)G^{-1}+(\xi_xS(\xi,\eta,\tau)+\eta_x)(\xi_yS(\xi,\eta,\tau)+\eta_y)^{-1}(G^{-1})_y-(G^{-1})_x\}, \tag{94}$$

$$V'=\tau_tGV(\xi,\eta,\tau)G^{-1}+G_tG^{-1}, \tag{95}$$

$$\tilde{V}'=\tau_tG\tilde{V}'(\xi,\eta,\tau)G^{-1}+G_tG^{-1}, \tag{96}$$

$$U'=G[(\eta_yU(\xi,\eta,\tau)+\xi_y\tilde{U}(\xi,\eta,\tau))G^{-1}-(G^{-1})_y], \tag{97}$$

$$\tilde{U}'=G[(\xi_x\tilde{U}(\xi,\eta,\tau)+\eta_xU(\xi,\eta,\tau))G^{-1}-(G^{-1})_x], \tag{98}$$

$$W'=G\{\tau_t[\eta_yW(\xi,\eta,\tau)+\xi_y\tilde{W}(\xi,\eta,\tau)]G^{-1}+[\eta_yU(\xi,\eta,\tau)+\xi_y\tilde{U}(\xi,\eta,\tau)](G^{-1})_t+\tau_tV(\xi,\eta,\tau)(G^{-1})_y-(G^{-1})_{yt}\}, \tag{99}$$

$$\tilde{W}'=G\{\tau_t[\eta_xW(\xi,\eta,\tau)+\xi_x\tilde{W}(\xi,\eta,\tau)]G^{-1}+[\eta_xU(\xi,\eta,\tau)+\xi_x\tilde{U}(\xi,\eta,\tau)](G^{-1})_t+\tau_tV(\xi,\eta,\tau)(G^{-1})_x-(G^{-1})_{xt}\}, \tag{100}$$

where $\xi=\xi(x,y),\eta=\eta(x,y),\tau=\tau(t),G=G(x,y,t)$ are all arbitrary differentiable functions of the indicated variables, is also an exact solution of the same system (4)–(9).

Remark: In connection with the initial problem (82)–(92), the following data are adjoined:

$$\xi|_{\epsilon=0}\equiv x'(x,y,\epsilon)|_{\epsilon=0}=x, \tag{101}$$

$$\eta|_{\epsilon=0}\equiv y'(x,y,\epsilon)|_{\epsilon=0}=y, \tag{102}$$

$$\tau|_{\epsilon=0}\equiv t'(t,\epsilon)|_{\epsilon=0}=t, \tag{103}$$

$$G|_{\epsilon=0}\equiv G(x,y,\epsilon)|_{\epsilon=0}=1. \tag{104}$$

Theorem 1 is readily verified by direct substitution of (93)–(100) into the nonlinear system (4)–(9). Alternatively, if we set

$$\xi\approx x+\epsilon X, \tag{105}$$

$$\eta\approx y+\epsilon Y, \tag{106}$$

$$\tau\approx t+\epsilon T, \tag{107}$$

$$G=\exp(\epsilon g)\approx 1+\epsilon g,\quad G^{-1}=\exp(-\epsilon g)\approx 1-\epsilon g, \tag{108}$$

then (93)–(100) become

$$S'\approx S+\epsilon\sigma^S,\quad P'\approx P+\epsilon\sigma^P,\quad V'\approx V+\epsilon\sigma^V,\quad \tilde{V}'\approx\tilde{V}+\epsilon\sigma^{\tilde{V}}, \tag{109}$$

$$U'\approx U+\epsilon\sigma^U,\quad \tilde{V}\approx\tilde{V}+\epsilon\sigma^{\tilde{V}},\quad W'\approx W+\epsilon\sigma^W,\quad \tilde{W}'\approx\tilde{W}+\epsilon\sigma^{\tilde{W}} \tag{110}$$

with σ^S, σ^P, σ^V, $\sigma^{\tilde{V}}$, σ^U, $\sigma^{\tilde{U}}$, σ^W, $\sigma^{\tilde{W}}$ as in (65).

It is noted that the part of the invariance encoded in the arbitrary matrix function G ($\xi=x,\eta=y,\tau=t$) in the above theorem is nothing but the gauge transformation found by Konopelchenko and Rogers.[3] The existence of this gauge transformation is due to the fact that the nonlinear system (4)–(9) constitutes an underdetermined system of seven equations for eight matrix functions. Thus, one of the matrix functions of the system can be gauged away. [It is interesting to note that the pure gauge transformation with $G=\phi_2$ takes solutions of the generalized Brushi–Ragnisco system (30)–(32) to solutions of the parametrised LKR system (15)–(18).]

V. LOCALIZED EXCITATIONS OF THE LKR SYSTEM

Here, the finite transformation given in the last section applied to trivial seed solutions of special LKR systems is used to generate new exact explicit solutions of the LKR system.

A set of constant matrix solutions of the nonlinear system (4)–(9) reads

$$\begin{gathered} S_0\equiv S_c^{-1},\quad P_0=0,\quad V_0=\tilde{V}_0=v_0S_c,\\ U_0=u_0S_c,\quad W_0=w_0S_c,\quad \tilde{U}_0=u_0I_N,\quad \tilde{W}_0=w_0I_N, \end{gathered} \tag{111}$$

where S_c is an arbitrary constant matrix and u_0, v_0 and w_0 are arbitrary constants. Theorem 1 applied to the trivial seed solution (111) produces the new solution

$$S_1=G_1^{-1}(\xi_x+\eta_xS_c)(\xi_y+\eta_yS_c)^{-1}G_1, \tag{112}$$

$$P_1=G_1^{-1}\{(\xi_x+\eta_xS_c)(\xi_y+\eta_yS_c)^{-1}G_{1y}-G_{1x}\}, \tag{113}$$

$$V_1=\tilde{V}_1=G_1^{-1}(\tau_tS_cG_1-G_{1t}), \tag{114}$$

$$U_1=G_1^{-1}[(\eta_yS_c+\xi_yI_N)G_1-G_{1y}], \tag{115}$$

$$\tilde{U}_1=G_1^{-1}[(\xi_xI_N+\eta_xS_c)G_1-G_{1x}], \tag{116}$$

$$W_1=G_1^{-1}\{w_0\tau_t(\eta_yS_c+\xi_yI_N)G_1+(\eta_yS_c+\xi_yI_N)G_{1t}+\tau_tS_cG_{1y}-G_{1yt}\}, \tag{117}$$

$$\widetilde{W}_1 = G_1^{-1}\{w_0\tau_t(\eta_x S_c + \xi_x I_N)G_1 + (\eta_x S_c + \xi_x I_N)G_{1t} + \tau_t S_c G_{1x} - G_{1xt}\}, \tag{118}$$

where v_0 and u_0 have been absorbed by redefinition of the arbitrary functions ξ, η, τ and the constant w_0, for the LKR system (4)–(9).

It can be seen that although the seed solution constitutes a trivial constant matrix solution, the new group-generated solution (112)–(118) will admit rich localized structures due to the intrusion of the arbitrary scalar and matrix functions. To investigate the exact solutions in more detail, we fix $N=2$ in what follows.

For the special solution (112)–(118), dromion-type solutions can be constructed by taking ξ_x, ξ_y, η_x and η_y as constants and the elements of the matrix G as appropriate hyperbolic functions. Thus, if we set

$$\xi = x + y, \quad \eta = x - \frac{9}{4}y, \quad \tau = t, \quad w_0 = 1, \quad S_c = \begin{pmatrix} 1 & 4 \\ \dfrac{5}{18} & 1 \end{pmatrix}, \tag{119}$$

$$G_1 = \begin{pmatrix} -\cosh(0.1x + 3y + 2t) & \operatorname{sech}(2x + 0.1y + 2t) \\ 2\operatorname{sech}(2x + 0.1y + 2t) & 2\cosh(0.1x + 3y + 2t) \end{pmatrix}, \tag{120}$$

then (112) yields

$$S_1 = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & -S_{11} \end{pmatrix}, \tag{121}$$

where

$$S_{11} = \frac{293\operatorname{sech}(2x + 0.1y + 2t)\operatorname{sech}(0.1x + 3y + 2t)}{45(1 + \operatorname{sech}^2(2x + 0.1y + 2t)\operatorname{sech}^2(0.1x + 3y + 2t))}, \tag{122}$$

$$S_{12} = \frac{288 - 5\operatorname{sech}^2(2x + 0.1y + 2t)\operatorname{sech}^2(0.1x + 3y + 2t)}{45(1 + \operatorname{sech}^2(2x + 0.1y + 2t)\operatorname{sech}^2(0.1x + 3y + 2t))}, \tag{123}$$

$$S_{21} = \frac{5 - 288\operatorname{sech}^2(2x + 0.1y + 2t)\operatorname{sech}^2(0.1x + 3y + 2t)}{45(1 + \operatorname{sech}^2(2x + 0.1y + 2t)\operatorname{sech}^2(0.1x + 3y + 2t))}. \tag{124}$$

From the expressions (122)–(124), it can be seen that the components of S_1 possess dromion structure. Figure 1 depicts the details of the dromion structure for the components of the matrix function S_1.

The detailed expressions for the residual matrix functions with the specializations (119) and (120), $P_1, \ldots, \widetilde{W}_1$, are given by (113)–(118). Figures 2 and 3 represent, in turn, the corresponding structures of the components of the matrix functions P_1 and V_1 expressed by (113) and (114) respectively with (119) and (120). The corresponding representations for the other matrix functions of the special solution (112)–(118), namely, U_1, $\widetilde{U}_1, W_1, \widetilde{W}_1$, have structures qualitatively similar to those of V_1 and, accordingly, are not depicted.

In addition to the constant matrix solution (111), there exist other kinds of constant matrix solutions of the LKR system. One such solution adopts the form

$$P = (1 - S)U, \quad \widetilde{U} = U, \quad \widetilde{W} = W = -UV, \tag{125}$$

where S and U are arbitrary $N \times N$ constant matrices and V is an arbitrary constant matrix which commutes with S. If $N=2$, then the following specification of S, U and V,

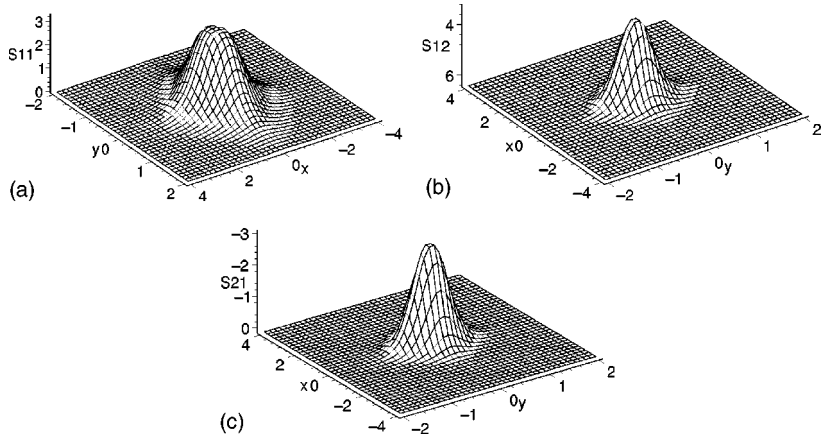

FIG. 1. Plots of the dromion structures for the matrix function $S=S_1$ expressed by (121) with (122)–(124).

$$S_{01}=\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix},\quad U_{01}=\tilde{U}_{01}=\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix},\quad V_{01}=\tilde{V}_{01}=\begin{pmatrix}1 & 2\\ -2 & 1\end{pmatrix},$$
$$P_{01}=\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix},\quad W_{01}=\tilde{W}_{01}=\begin{pmatrix}1 & -3\\ 3 & 1\end{pmatrix}, \tag{126}$$

leads, on use of Theorem 1, to the following boosted nonconstant matrix solution of the LKR system (4)–(9):

$$S_2=G_1^{-1}\begin{pmatrix}A & B\\ -B & A\end{pmatrix}G_1, \tag{127}$$

$$A=\frac{\xi_x(2\xi_y+\eta_y)+\eta_x(\xi_y+\eta_y)}{\eta_y^2+2\xi_y(\xi_y+\eta_y)},\quad B=\frac{\xi_y\eta_x-\xi_x\eta_y}{\eta_y^2+2\xi_y(\xi_y+\eta_y)}, \tag{128}$$

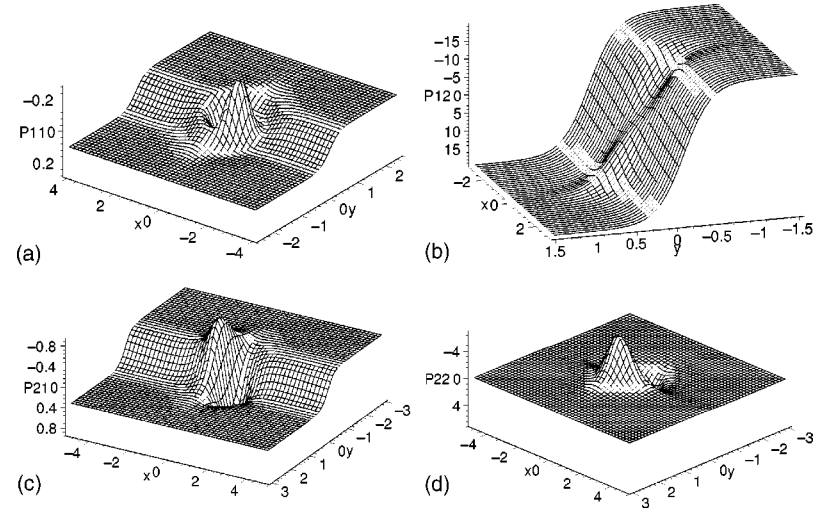

FIG. 2. Plots of the components for the matrix function $P=P_1$ expressed by (113) with (119) and (120).

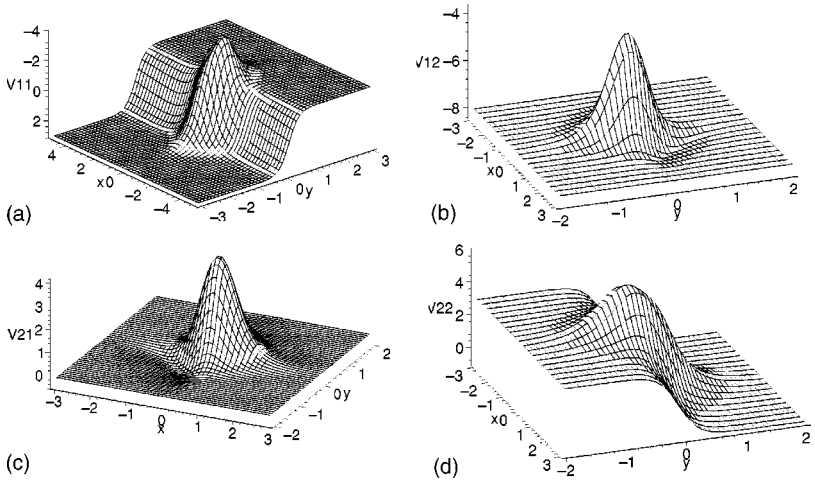

FIG. 3. Plots of the components for the matrix function $V=V_1$ expressed by (114) with (119) and (120).

$$P_2=G_1^{-1}\left\{(\xi_x\eta_y-\xi_y\eta_x)\begin{pmatrix}\eta_y & -2\xi_y-\eta_y\\ 2\xi_y+\eta_y & \eta_y\end{pmatrix}G_1+S_2G_1^{-1}G_{1y}-G_{1x}\right\}, \tag{129}$$

$$V_2=\tilde{V}_2=\tau_tG_1^{-1}\begin{pmatrix}1 & 2\\ -2 & 1\end{pmatrix}G_1-G_1^{-1}G_{1t}, \tag{130}$$

$$U_2=(\xi_y+\eta_y)G_1^{-1}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}G_1-G_1^{-1}G_{1y}, \tag{131}$$

$$\tilde{U}_2=(\xi_x+\eta_x)G_1^{-1}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}G_1-G_1^{-1}G_{1x}, \tag{132}$$

$$W_2=G_1^{-1}\left\{(\xi_y+\eta_y)\left[\tau_t\begin{pmatrix}1 & -3\\ 3 & 1\end{pmatrix}G_1+\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}G_{1t}\right]+\tau_t\begin{pmatrix}1 & 2\\ -2 & 1\end{pmatrix}G_{1y}-G_{1yt}\right\}, \tag{133}$$

$$\tilde{W}_2=G_1^{-1}\left\{(\xi_x+\eta_x)\left[\tau_t\begin{pmatrix}1 & -3\\ 3 & 1\end{pmatrix}G_1+\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}G_{1t}\right]+\tau_t\begin{pmatrix}1 & 2\\ -2 & 1\end{pmatrix}G_{1x}-G_{1xt}\right\} \tag{134}$$

with arbitrary matrix function $G_1=G_1(x,y,t)$, and arbitrary scalar functions $\xi=\xi(x,y)$, $\eta=\eta(x,y)$ and $\tau=\tau(t)$.

The $2+1$-dimensional sine–Gordon system was originally derived in Ref. 1 as a particular reduction of the LKR system. Exact solutions of such special reductions may be used as seed solutions in order to generate new solutions of the LKR system (4)–(9) via Theorem 1. Thus, for instance, for the $2+1$-dimensional sine–Gordon system [cf. (44)] we have

$$S_{02}=\begin{pmatrix}-\cos\theta & -\sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}, \tag{135}$$

$$P_{02}=U_{02}=\tilde{U}_{02}=0,\quad V_{02}=\tilde{V}_{02}\begin{pmatrix}0 & -\frac{1}{2}\theta_t\\ \frac{1}{2}\theta_t & 0\end{pmatrix}, \tag{136}$$

$$W_{02}=\frac{1}{2}\begin{pmatrix}\phi_y\cot\theta-\phi_x\csc\theta & -\phi_y'\\ \phi_y & \phi_y'\csc\theta+\phi_x'\cot\theta\end{pmatrix}, \tag{137}$$

$$\tilde{W}_{02}=\frac{1}{2}\begin{pmatrix}\phi_x\cot\theta-\phi_y\csc\theta & -\phi_x'\\ \phi_x & \phi_x'\csc\theta+\phi_y'\cot\theta\end{pmatrix}. \tag{138}$$

Use of Theorem 1 then leads to the new group-boosted solution of the LKR system:

$$S_3=G_1^{-1}\begin{pmatrix}A_1 & B_1\\ B_1 & -A_1\end{pmatrix}G_1, \tag{139}$$

$$U_3=-G_1^{-1}G_{1y}, \tag{140}$$

$$\tilde{U}_3=-G_1^{-1}G_{1x}, \tag{141}$$

$$P_3=-S_3U_3+\tilde{U}_3, \tag{142}$$

$$V_3=\tilde{V}_3=\frac{\tau_t}{2}G_1^{-1}\begin{pmatrix}0 & -\theta_{1\tau}\\ \theta_{1\tau} & 0\end{pmatrix}G_1-G_1^{-1}G_{1t}, \tag{143}$$

$$W_3=G_1^{-1}\left\{\frac{\tau_t}{2}\begin{pmatrix}\alpha\cot\theta_1-\beta\csc\theta_1 & -\alpha'\\ \alpha & \alpha'\csc\theta_1+\beta'\cot\theta_1\end{pmatrix}G_1+\frac{\tau_t}{2}\begin{pmatrix}0 & -\theta_{1\tau}\\ \theta_{1\tau} & 0\end{pmatrix}G_{1y}-G_{1yt}\right\}, \tag{144}$$

$$\tilde{W}_3=G_1^{-1}\left\{\frac{\tau_t}{2}\begin{pmatrix}\tilde{\alpha}\cot\theta_1-\tilde{\beta}\csc\theta_1 & -\tilde{\alpha}'\\ \tilde{\alpha} & \tilde{\alpha}'\csc\theta_1+\tilde{\beta}'\cot\theta_1\end{pmatrix}G_1+\frac{\tau_t}{2}\begin{pmatrix}0 & -\theta_{1\tau}\\ \theta_{1\tau} & 0\end{pmatrix}G_{1x}-G_{1xt}\right\}, \tag{145}$$

where

$$A_1\equiv\frac{(\xi_x\eta_y-\eta_x\xi_y)\cos\theta_1-\eta_x\eta_y+\xi_x\xi_y}{\xi_y^2-\eta_y^2},\quad B_1\equiv\frac{(\xi_x\eta_y-\eta_x\xi_y)\sin\theta_1}{\xi_y^2-\eta_y^2}, \tag{146}$$

$$\alpha\equiv\phi_{1\eta}\eta_y+\phi_{1\xi}\xi_y,\quad \beta\equiv\phi_{1\xi}\eta_y+\phi_{1\eta}\xi_y,\quad \alpha'\equiv\phi_{1\eta}'\eta_y+\phi_{1\xi}'\xi_y,\quad \beta'\equiv\phi_{1\xi}'\eta_y+\phi_{1\eta}'\xi_y, \tag{147}$$

$$\tilde{\alpha}\equiv\phi_{1\eta}\eta_x+\phi_{1\xi}\xi_x,\quad \tilde{\beta}\equiv\phi_{1\xi}\eta_x+\phi_{1\eta}\xi_x,\quad \tilde{\alpha}'\equiv\phi_{1\eta}'\eta_x+\phi_{1\xi}'\xi_x,\quad \tilde{\beta}'\equiv\phi_{1\xi}'\eta_x+\phi_{1\eta}'\xi_x, \tag{148}$$

$$\theta_1\equiv\theta(\xi,\eta,\tau),\phi_1\equiv\phi(\xi,\eta,\tau),\phi_1'\equiv\phi'(\xi,\eta,\tau). \tag{149}$$

Localized solutions of the sine–Gordon system have been extensively studied by many authors. The Bäcklund transformation of the sine–Gordon system was constructed in Ref. 24 and certain coherent solitonic solutions thereby derived. Solitonic solutions of an important reduction that arises in connection with triple orthogonal systems of surfaces have been investigated by Nimmo.[25,26] Doubly periodic wave solutions have been constructed by Chow.[27] Localized solutions of the $2+1$-dimensional sine–Gordon system were constructed via a binary Darboux transformation by Schief.[28] In Ref. 29, Nimmo and Schief constructed nonlinear superposition principles and an associated integrable discretisation of the $2+1$-dimensional sine–Gordon system. Localized solutions of the model with nontrivial boundaries have been constructed by Dubrovsky and Konopelchenko[30,31] and Dubrovsky and Formusatik.[32] Geometric aspects of the

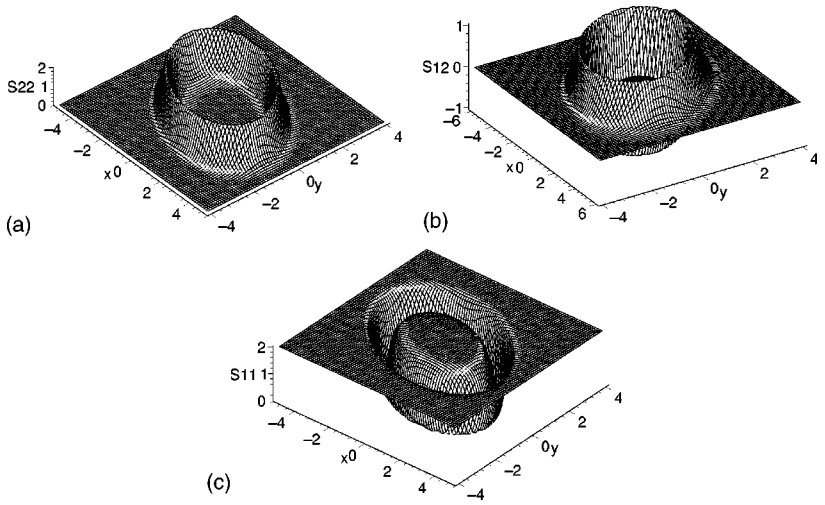

FIG. 4. Plots of the matrix function $S=S_3$ expressed by (139) with (146), (149)–(155) at $t=0$ for the components: (a) $S22\equiv S_{22}$, (b) $S12\equiv S_{12}=S_{21}$ and $S11\equiv S_{11}$.

$2+1$-dimensional sine–Gordon system were investigated by Schief.[33] Extensive symmetry group analysis of the system has been conducted both by Clarkson *et al.*[11] and Lou.[10] Radha and Lakshmanan[34] studied the Painlevé property for the $2+1$-dimensional sine–Gordon system and have constructed dromion solutions. Plateau-type, basin-type, bowl-type and saddle-type ring soliton solutions are studied in Ref. 35. The system contains particular reductions to the PIII, PV and PVI transcendents.[4] In physical terms, it also contains the important pumped Maxwell–Bloch system.

The diversity of special solutions of the sine–Gordon system alluded to above can all be group-boosted via Theorem 1 to generate solutions of the LKR system (4)–(9). In general terms, the structures of the new solutions of the LKR system are manifestly richer than the seed solutions because of the intrusion not only of a three-dimensional arbitrary matrix function (due to the gauge invariance of the model) but also due to two two-dimensional arbitrary functions and a one dimensional arbitrary function (consequences of three types of Virasoro invariance).

The Moutard transformation[30,20] or a variable separation approach[21–23] can be used to construct the following special solution for the sine-Gordon system (43):

$$\theta=4\arctan[p(x+y,t)q(x-y,t)], \tag{150}$$

$$\phi=\frac{4p(x+y,t)q_t(x-y,t)}{1+p(x+y,t)^2q(x-y,t)^2}, \tag{151}$$

$$\phi'=\frac{4p_t(x+y,t)q(x-y,t)}{1+p(x+y,t)^2q(x-y,t)^2}, \tag{152}$$

with $p(x+y,t)$ being an arbitrary function of $\{x+y,t\}$ and $q(x-y,t)$ being an arbitrary function of $\{x-y,t\}$. On substitution of (150)–(152) into (139)–(149), we obtain a special type of localized excitation of the LKR system with arbitrary functions G,ξ,η,τ, $p(\xi+\eta,\tau)$ and $q(\xi-\eta,\tau)$.

In Fig. 4, a localized ring shape solution is plotted for the components of the matrix S expressed by (139) with (146), (149), (150) and

$$p(\xi+\eta,\tau)=\exp[-\tfrac{1}{10}(\xi+\eta-2\tau)^2+3], \tag{153}$$

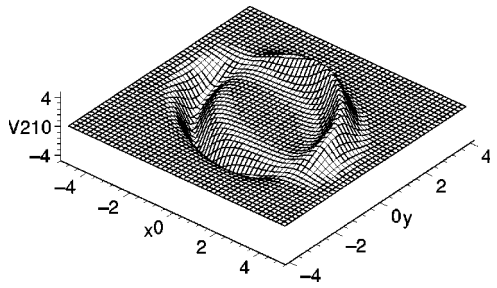

FIG. 5. Plots of the matrix function $V=V_3$ expressed by (143) with (149)–(155) at $t=0$ for the component $V21\equiv V_{21}=-V_{12}$.

$$q(\xi-\eta,\tau)=\exp[-\tfrac{1}{10}(\xi-\eta-3\tau)^2+1], \tag{154}$$

$$G_1=I_2,\quad \xi=x+2y,\quad \eta=y-x,\quad \tau=t \tag{155}$$

at $t=0$.

Figures 5 and 6 show the corresponding structures of the matrices $V=V_3$ and $W=W_3$, respectively, for the functions $G_1,\theta,\phi,\phi_1,\xi,\eta$ and τ are same as in Fig. 4. The structures for the components of the matrix $\tilde{W}$ is similar to those of W.

In Ref. 35, multiple ring shape solitons corresponding to the specialisation (150) have been constructed which possess the property of completely elastic interaction without phase shifts. However, by suitable selection of the arbitrary functions p and q in (150) multiple ring soliton solutions of the $2+1$-dimensional sine–Gordon system may also be constructed which possess phase shifts.

Thus, Fig. 7 depicts the evolution of two bowl-type ring solitons for the component $S'\equiv S_{22}$ of S_3,

$$S'=\frac{8\left[\exp\left(3-\frac{2}{3}\alpha^2-\beta^2\right)+\exp(3-(\alpha-2t)^2-\beta^2)\right]^2}{\left\{1+\left[\exp\left(3-\frac{2}{3}\alpha^2-\beta^2\right)+\exp(3-(\alpha-2t)^2-\beta^2)\right]^2\right\}^2}, \tag{156}$$

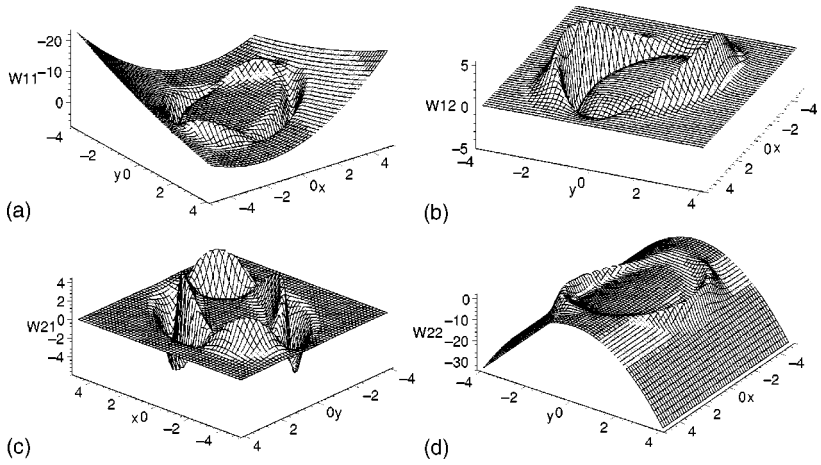

FIG. 6. Plots of the matrix function $W=W_3$ expressed by (144) with (149)–(155) at $t=0$ for the components: (a) $W11\equiv W_{11}$, (b) $W12\equiv W_{12}$, (c) $W21=W_{21}$ and (d) $W22\equiv W_{22}$.

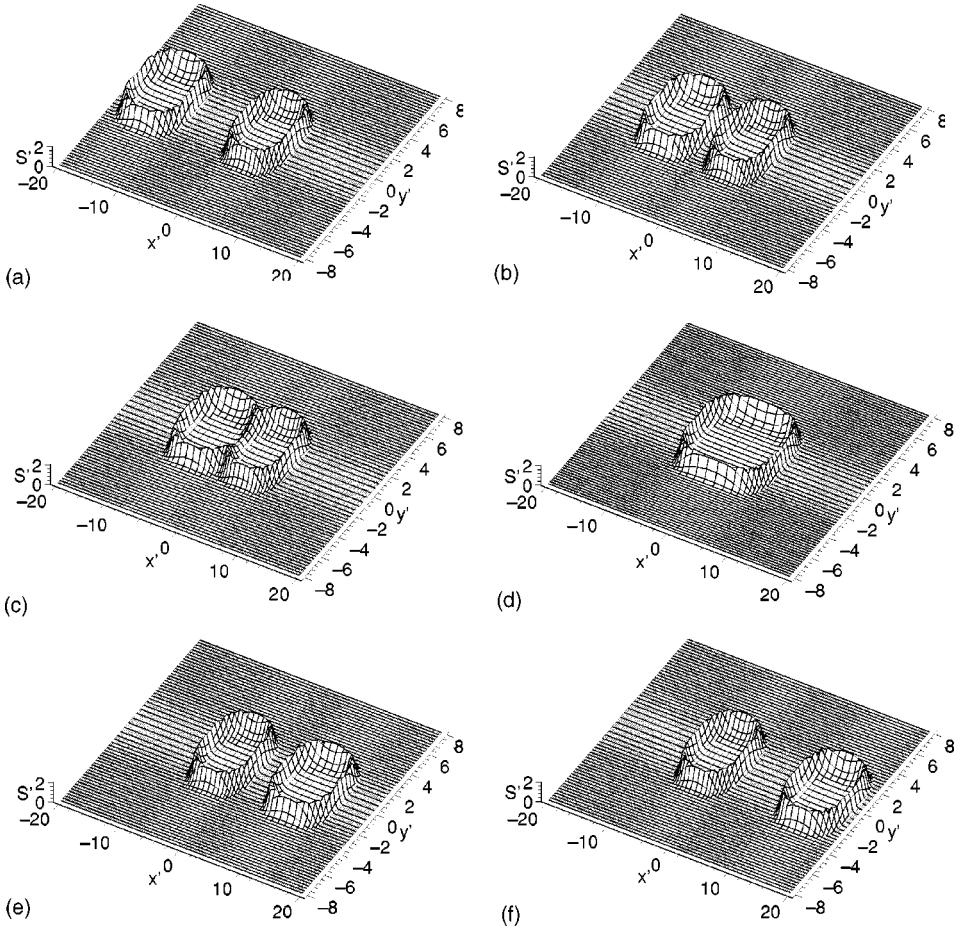

FIG. 7. The evolution plots of two ring solitons for the component $S' \equiv S_{22}$ of the matrix $S = S_3$ expressed by (156) with (149)–(150), (155) and (159)–(158) at the times (a) $t = -6$, (b) $t = -3$, (c) $t = -1.8$, (d) $t = 0$, (e) $t = 4$ and (f) $t = 6$, respectively.

where $\alpha \equiv \alpha(\xi + \eta, \tau)$ and $\beta \equiv \beta(\xi - \eta, \tau)$ are related to the "space–time" variables by

$$x' \equiv \xi + \eta = 3y = \alpha + 3\tanh(\alpha - 2t) + 2\tanh\alpha, \tag{157}$$

$$y' \equiv \xi - \eta = 2x + y = \beta + \tanh\beta, \tag{158}$$

corresponding to the specifications

$$p(\xi + \eta, \tau) = \exp[3 - \tfrac{2}{3}\alpha^2] + \exp\{3 - [\alpha - 2\tau]^2\}, \tag{159}$$

$$q(\xi - \eta, \tau) = \exp[-\beta^2], \tag{160}$$

$$G_1 = I_2, \quad \xi = x + 2y, \quad \eta = y - x, \quad \tau = t \tag{161}$$

for the matrix (139) with (146), (149), and (150).

Figure 7 reveals not only the elastic interaction between the two ring shape solitons, but also the accompanying phase shifts. To make evident the phase shift it has proved convenient to assign one ring soliton zero velocity. Prior to interaction, the small ring soliton is static and situated at $\{x' = 3, y' = 0\}$ and the large ring soliton is moving with its center located at $\{x' = 2t - 2, y'$

$=0\}$. Following interaction, the static ring soliton remains static with shape unchanged but its center is shifted to $\{x'=-3,y'=0\}$ while the moving ring soliton recovers its shape but its center is shifted to $\{x'=2t+2,y'=0\}$.

The complete elastic interaction property and the phase shifts between two ring solitons shown in Fig. 7 can be strictly proven by consideration of the asymptotic behavior of (156) with (157) and (158) as $t\to\mp\infty$:

$$S'\to S_1'^{\mp}+S_2'^{\mp},\quad t\to\pm\infty, \tag{162}$$

where $S_1'^{\mp}$ and $S_2'^{\mp}$ are given by

$$S_1'^{\mp}=2\ \mathrm{sech}^2(3-\tfrac{2}{3}\alpha^2-\beta^2), \tag{163}$$

$$x'=\alpha+2\tanh\alpha\pm 3, \tag{164}$$

$$y'=\beta+\tanh\beta, \tag{165}$$

and

$$S_2'^{\mp}=2\ \mathrm{sech}^2(3-(\alpha-2t)^2-\beta^2), \tag{166}$$

$$x'=\alpha+3\tanh(\alpha-2t)\mp 2, \tag{167}$$

$$y'=\beta+\tanh\beta, \tag{168}$$

respectively.

Multiple ring soliton solutions with and without phase shifts may likewise be constructed for the LKR system.

VI. SUMMARY

Lie point symmetries of the general LKR system have been isolated by means of the classical Lie approach. These symmetries constitute an infinite dimensional Kac–Moody–Virasoro-type Lie algebra. The corresponding Lie symmetry group (finite transformation) has been constructed. There exist three generalized centerless Virasoro-type symmetry algebras.

The finite group transformation with seed, an exact solution of a special reduction of the LKR system, can be used to generate a rich class of new solutions of the LKR system. Localized excitations of the LKR system may be generated thereby from trivial constant matrix seed solutions. In particular, dromion-type solutions and bowl-type ring soliton solutions with completely elastic interaction and phase shifts have been constructed for the LKR system.

ACKNOWLEDGMENTS

The work was supported by Australian Research Council Grant (C.R. and W.K.S.), the National Outstanding Youth Foundation of China (No. 19925522), the National Natural Science Foundation of China (No. 90203001) and the Research Fund for the Doctoral Program of Higher Education of China (Grant. No. 2000024832).

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Noncommutative geometry framework and the Feynman's proof of Maxwell equations

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(Received 12 August 2003; accepted 21 September 2003)

The main focus of the present work is to study the Feynman's proof of the Maxwell equations using the NC geometry framework. To accomplish this task, we consider two kinds of noncommutativity formulations going along the same lines as Feynman's approach. This allows us to go beyond the standard case and discover nontrivial results. In fact, while the first formulation gives rise to the static Maxwell equations, the second formulation is based on the following assumption $m[x_j,\dot{x}_k]=\delta_{jk}+im\theta_{jk}f$. The results extracted from the second formulation are more significant since they are associated to a nontrivial θ-extension of the Bianchi-set of Maxwell equations. We find $\mathrm{div}_\theta B=\eta_\theta$ and $(\partial B_s/\partial t)+\epsilon_{kjs}(\partial E_j/\partial x_k)=A_1(\mathrm{d}^2f/\mathrm{d}t^2)+A_2(\mathrm{d}f/\mathrm{d}t)+A_3$, where η_θ, A_1, A_2, and A_3 are local functions depending on the NC θ-parameter. The novelty of this proof in the NC space is revealed notably at the level of the corrections brought to the previous Maxwell equations. These corrections correspond essentially to the possibility of existence of magnetic charge sources that we can associate to the magnetic monopole since $\mathrm{div}_\theta B=\eta_\theta$ is not vanishing in general. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625891]

I. INTRODUCTION

Noncommutative geometry (NCG) stimulated recently by Connes[1] and developed later on by several pioneering authors[2,3] have played an increasingly important role more notably in the attempts to understand the space–time structure at very small distance. Much attention has been paid also to quantum field theories on NC spaces, in particular NC Yang–Mills gauge theory as well as NC–QED, a subject which has matured as an area of intense research activity in more recent times.[4–6] In fact it has been established by Seiberg and Witten[2] that the existence of noncommutativity in open string boundaries in the presence of the NS–NS B field results in NC D-branes to which the open string endpoints are attached. Related to these stimulating ideas, a wide number of papers were devoted to study several aspects of the NC.[7]

One particular property of NCG framework is its richness and also the fact that we can discover the standard results just by requiring the vanishing of the deformed parameter which means also the vanishing of noncommutativity. Note that the passage from commutative to NC space–time is simply achieved by replacing the ordinary product, in the space of smooth functions on R^2 with coordinates (x,t), by the NC associative $*$ product. Works having used this NC formalism are various and the results found are numerous, we will limit ourselves to mention some of them, namely, Refs. 8–14.

The aim of this paper is to study another aspect of the noncommutativity framework adapted to the Feynman's proof of Maxwell equations.[15–19] As well known, a century ago, Maxwell brought four basic laws dealing with electromagnetism, these laws describe the evolution in time

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and space of the electric and magnetic fields E and B. Together with the Lorentz force law, the Maxwell equations constitute a complete description of electromagnetism (the Maxwell theory). Furthermore these equations have different forms, vectorial, differential and can be proved in different way.

Feynman in 1948 has given a proof of these equations, assuming only Newton's law of motion and the commutation relation between position and velocity for a single nonrelativistic particle. The importance of this proof emerged notably with the Dyson's work.[15] As signaled in this work, the motivation of Feynman was to build a new theory outside the framework of conventional physics, but his assumptions using these commutation relations and the Newton's equation were not lead to new physics.[15] This proof, although based on simple mathematical assumptions, is shown to give rise to nontrivial generalizations.[16–19]

Among many possible existing extensions, we are going to adapt thereafter the NC framework to the Feynman's proof, a fact which leads us to extract important results. We present two kinds of NC formulations and show in a first one that the application of Feynman's proof in NC space, leads to the static Maxwell equations. Focusing to obtain a new theory, we propose in our second formulation to modify the Moyal bracket between the position x_i and the velocity $\dot{x}_j$. This task can be easily accomplished by assuming that the velocity is space dependent and then the star product between x_i and $\dot{x}_j$ becomes nontrivial. This assumption will modify the Maxwell equations, giving rise to a new theory where extra terms proportional to NC θ-parameter appear. The results extracted from the second formulation are more significant as they are associated to a nontrivial θ-extension of the Bianchi-set of Maxwell equations, namely, $\mathrm{div}_\theta B=\eta_\theta$ and

$$\frac{\partial B_s}{\partial t}+\epsilon_{kjs}\frac{\partial E_j}{\partial x_k}=A_1\frac{\mathrm{d}^2 f}{\mathrm{d}t^2}+A_2\frac{\mathrm{d}f}{\mathrm{d}t}+A_3,$$

where η_θ, A_1, A_2, and A_3 are local functions depending on the NC θ-parameter.

Our objectives in reconsidering the Feynman's proof are, on one hand, to put it in relief and, on the other hand, to show its importance in the NC framework. The novelty of this proof formulated in the NC space is revealed notably at the level of the corrections brought to the standard Maxwell equations. These corrections correspond essentially to the possibility of existence of sources of magnetic charges that we can associate to the magnetic monopole since $\mathrm{div}_\theta B=\eta_\theta$. Note that these extra terms η_θ are absent in the ordinary case associated to $\theta=0$. These results may give new insights into the study of the electromagnetic duality and its various physical and mathematical aspects.

This paper is organized as follows. In Sec. II we summarize some properties of the Poisson manifold and review the Feynman's proof of the Maxwell equations. In Sec. III we present some useful identities of the star product, after that we examine Feynman's proof of the Maxwell equations in NC spaces. Section IV is devoted to our concluding remarks.

II. MAXWELL EQUATIONS: THE FEYNMAN'S PROOF

Maxwell equations have played a pioneering role in physics and they continue to nourish several axes of research either in physics or in mathematics. Their formulations as well as the survey of their solutions constitute a topic of big interest[20] and it is in this context that are located the famous theories of Yang–Mills. Recently, we attended to a new approach leading to the derivation of these equations and based on what is called the Feynman's proof of Maxwell equations. Details concerning this approach are presented in the Dyson's work.[15] Later on, several authors took this approach and tried to put in relief the Feynman's idea and to develop it or sometimes to generalize it to other contexts.[16–19] Before reviewing the Feynman's proof of the Maxwell equations, let us first start by introducing some basic algebraic properties of the underlying Poisson manifold $\mathcal{M}$.

A. Some algebraic properties

In fact the previous approach can be simply stated in the general way as finding all Poisson tensors on a phase space manifold such that they have Hamiltonian vector fields which correspond to second order differential equations such that $\{q^i,q^j\}=0$, with the symbol {,} standing for the Poisson bracket defined usually as

$$\{f,g\}=\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i}-\frac{\partial f}{\partial p^i}\frac{\partial g}{\partial q_i}, \tag{1}$$

where f and g are two functionals of q and p. Denoting by $\mathcal{A}$ the algebra of classical observables on the manifold $\mathcal{M}$, one can define a Poisson structure $\{,\}:\mathcal{A}\times\mathcal{A}\to\mathcal{A}$ on this manifold as a skew-symmetric bilinear map such that we have the following.

(a) $(\mathcal{A},\{,\})$ satisfies the Jacobi identity

$$\{F,\{G,H\}\}+\{H,\{F,G\}\}+\{G,\{H,F\}\}=0. \tag{2}$$

(b) The map $X_F=\{.,F\}$ defines a derivation on $\mathcal{M}$ of the associative algebra $\mathcal{A}(\mathcal{M})$, that is, it satisfies the Leibnitz rule

$$\{F,GH\}=G\{F,H\}+\{F,G\}H. \tag{3}$$

A manifold endowed with such a Poisson bracket on $\mathcal{A}(\mathcal{M})$ is called a Poisson manifold. Furthermore, consider a Poisson manifold $\mathcal{P}$, for any $H\in\mathcal{A}(\mathcal{P})$, there is a unique vector field X_H on $\mathcal{P}$ such that

$$X_H G=\{G,H\} \tag{4}$$

for all $G\in\mathcal{A}(\mathcal{P})$. X_H is nothing but the Hamiltonian vector field of H. Now one can define a dynamical system on the Poisson manifold $\mathcal{M}$ just by considering for any function $H\in\mathcal{A}$ the following differential equation:

$$\frac{\mathrm{d}F}{\mathrm{d}t}=\{F,H\}. \tag{5}$$

Moreover, one can also express the Poisson bracket $\{F,G\}$ in any set of local coordinates (x^a) in the following way:

$$\{F,G\}=X_G F=\{x^a,G\}\frac{\partial F}{\partial x^a}. \tag{6}$$

B. The Feynman's proof

This section is devoted to an explicit reminder of the main steps involved in the Feynman's proof of the Maxwell equations in their classical form.[15,16] Our objective is to present these calculations in order to make a comparison with the NC case to be discussed later. This proof is essentially based on the Newton's laws of the nonrelativistic classical mechanics and on the relations of commutation joining the coordinates of position and velocity of a single nonrelativistic particle. An extension to the relativistic case is naturally possible[17,19] and may lead to important results more notably in connection with quantum field theory approaches. The manifold we consider is parametrized by local coordinate variables $(w^a)=(x^i,\dot{x}^i)$ of a nonrelativistic particle whose position x_j $(j=1,2,3)$ and velocity $\dot{x}_j$ satisfy the Newton's equation

$$m\ddot{x}_j=F_j(x,\dot{x},t), \tag{7}$$

with commutation relations

$$\{x_j, x_k\} = 0, \tag{8}$$

$$m\{x_j, \dot{x}_k\} = \delta_{jk}. \tag{9}$$

Then, there exist a couple of fields $E(x,t)$ and $B(x,t)$ that we can identify with the electric and the magnetic fields, respectively, such that we get the Lorentz force law

$$F_j = E_j + \epsilon_{jkl}\dot{x}_k B_l, \tag{10}$$

and the first couple of Maxwell equations

$$\operatorname{div} B = 0, \tag{11}$$

$$\frac{\partial B}{\partial t} + \nabla \times E = 0. \tag{12}$$

The second couple of Maxwell equations

$$\operatorname{div} E = 4\pi\rho, \tag{13}$$

$$\frac{\partial E}{\partial t} - \nabla \times B = 4\pi j, \tag{14}$$

merely defines the external charge and the current densities ρ and j, respectively.

The Feynman's proof starts by differentiating the bracket (9) with respect to time and using (7), we have

$$\{x_j, F_k\} + m\{\dot{x}_j, \dot{x}_k\} = 0. \tag{15}$$

Then using the Jacobi identity

$$\{x_l, \{\dot{x}_j, \dot{x}_k\}\} + \{\dot{x}_j, \{\dot{x}_k, x_l\}\} + \{\dot{x}_k, \{x_l, \dot{x}_j\}\} = 0 \tag{16}$$

as well as the bilinearity of the Poisson bracket we find the following constraint equation:

$$\{x_l, \{x_j, F_k\}\} = 0. \tag{17}$$

Furthermore, since the bracket is antisymmetric the tensor $\{x_j, F_k\}$ satisfies

$$\{x_j, F_k\} = -\{x_k, F_j\}, \tag{18}$$

and therefore we may write

$$\{x_j, F_k\} = -\frac{1}{m}\epsilon_{jkl}B_l. \tag{19}$$

This equation gives a definition of the field B whose components are B_l. This shows that B would in general depend on coordinates x, $\dot{x}$ of the Poisson manifold $\mathcal{M}$ and possibly time t. Combining (17) with the equation for B_l (19) leads to

$$\{x_l, B_m\} = 0. \tag{20}$$

On account of the basic equations (8)–(9), this means that B is a function of the coordinates x and t of the particle. Therefore, it is shown that the vectors E and B are not independent as we have

$$\{x_m, E_j\} = 0, \tag{21}$$

which says that E is also a function of x and t only.

Now we have two equations (15) and (19) that we naturally need to compare. The way to do this consists simply in writing B as

$$B_l=\frac{m^2}{2}\epsilon_{jkl}\{\dot{x}_j,\dot{x}_k\}. \tag{22}$$

Another application of the Jacobi identity gives

$$\epsilon_{jkl}\{\dot{x}_l,\{\dot{x}_j,\dot{x}_k\}\}=0, \tag{23}$$

leading naturally to the first Maxwell equation $\operatorname{div} B=0$ (11), namely,

$$\{\dot{x}_l,B_l\}=0. \tag{24}$$

Indeed,

$$\{B_l,\dot{x}_l\}=\{x_a,\dot{x}_l\}\frac{\partial B_l}{\partial x_a}=\frac{1}{m}\frac{\partial B_l}{\partial x_a}\delta_{al}=\frac{1}{m}\operatorname{div} B=0. \tag{25}$$

The proof of the second Maxwell equation (12) starts from deriving both sides of (22) with respect to time. This gives

$$\frac{\partial B_l}{\partial t}+\dot{x}_m\frac{\partial B_l}{\partial x_m}=m^2\epsilon_{jkl}\{\ddot{x}_j,\dot{x}_k\}. \tag{26}$$

Now by virtue of (7) and (10), the right-hand side of (26) becomes

$$\begin{aligned}-\frac{im}{\hbar}\epsilon_{jkl}\{E_j+\epsilon_{jab}\dot{x}_aB_b,\dot{x}_k\}&=m(\epsilon_{jkl}\{E_j,\dot{x}_k\}+\{\dot{x}_kB_l,\dot{x}_k\}-\{\dot{x}_lB_k,\dot{x}_k\})\\&=\epsilon_{jkl}\frac{\partial E_j}{\partial x_k}+\dot{x}_k\frac{\partial B_l}{\partial x_k}-\dot{x}_l\frac{\partial B_k}{\partial x_k}-mB_k\{\dot{x}_l,\dot{x}_k\}.\end{aligned} \tag{27}$$

On the right-hand side of (27), the last term is zero by virtue of (22), the third term vanishes also as it describes exactly the first Maxwell equation. Now identifying the left-hand side (lhs) and the right-hand side (rhs) of (26), we get

$$\frac{\partial B_l}{\partial t}=\epsilon_{jkl}\frac{\partial E_j}{\partial x_k}, \tag{28}$$

which is nothing but the second Maxwell equation (12).

This is the way followed by Feynman to prove the Maxwell equations in their classical form. His motivation was to ''discover a new theory not to reinvent the old one,'' but the proof showed him that his assumptions (7)–(9) were not leading to new physics. As was the case for several authors who find interesting the Feynman's approach, we project in the forthcoming section to go beyond this approach and setup the Feynman's proof in a noncommutative space. The way to apply the noncommutativity is by replacing the ordinary product by the star product and Poisson bracket or ordinary commutators by the Moyal bracket.

III. THE FEYNMAN'S PROOF IN THE NC GEOMETRY FRAMEWORK

The passage to NC geometry, based essentially on the noncommutativity of space–time coordinates, is justified among others by its importance in different currents of research more particularly in high energy physics. The deep idea behind the noncommutativity of coordinates is that in a certain microscopic regime our standard conception of the space–time is not more applicable.

Such a regime is characterized by domains of area θ where the space–time loses its condition of continuum and becomes subject to the following new structure $[x_\mu, x_\nu]_* = x_\mu * x_\nu - x_\nu * x_\mu = i\theta_{\mu\nu}$, where $\theta_{\mu\nu}$ is a real antisymmetric constant matrix and $[.,.]_*$ is the Moyal bracket.

One way of incorporating noncommutativity of coordinates in the context of field theory is through the Moyal product based on the $*$-product that will be introduced later on. To avoid hard notations, we will later on simply denote the Moyal bracket by $[.,.]$. Before going on, let us first recall briefly some useful identities of the $*$-product.

A. Some properties of $*$-product

Recently the $*$-product marks a remarkable success due to its intervention in different aspects of string theory greatly related to NC geometry. In this section, we give some useful properties of this $*$-product as well as of the Moyal bracket.[9,10] To define this object, let us start by considering two functions $f(x)$ and $g(x)$ such that

$$f(x)*g(x) = e^{(i/2)\,\theta^{ab}\,(\partial/\partial\xi^a)(\partial/\partial\eta^b)} f(x+\xi)g(x+\eta)/\xi=\eta=0, \tag{29}$$

where θ^{ab} is a constant, of dimension $[L]^2$, known as the NC parameter (*in all the parts of this paper the parameter θ is considered as a constant matrix*).

This formula leads naturally to what is often called the Moyal bracket of functions,

$$[f(x), g(x)] = f(x)*g(x) - g(x)*f(x). \tag{30}$$

According to this definition, the commutation relation for the space coordinates becomes

$$[x_i, x_j] = i\theta_{ij}. \tag{31}$$

Such a structure describes a NC space for which the space coordinates are not necessarily commuting. Note by the way that the function $f(x)$ may depend on space coordinates as it can depend on space–time coordinates. We collect here some useful properties.

(1) **Associativity**,

$$(f*g)*h = f*(g*h). \tag{32}$$

(2) **Jacobi identity**,

$$[f,[g,h]]+[g,[h,f]]+[h,[f,g]]=0. \tag{33}$$

(3) **Leibnitz rule**,

$$[f, g*h] = g*[f,h]+[f,g]*h. \tag{34}$$

(4) **Linearity**,

$$f*(g+h) = (f*g)+(f*h). \tag{35}$$

The $*$-product is also compatible with integration

$$\int \mathrm{Tr}(f*g) = \int \mathrm{Tr}(g*f), \tag{36}$$

where Tr is the ordinary trace of the $N\times N$ matrices, and $\int$ is the ordinary integration of functions.

Another useful identity is given in terms of local coordinates (x^a). For two functions $F(x)$ and $G(x)$, the coordinate expression for the Moyal bracket $[F,G]$ is

$$[F,G] = [x^a, G]\frac{\partial F}{\partial x^a}. \tag{37}$$

More details about the origin of the $*$-product and other important properties are available in literature.[9–13] Next, we will study the Feynman's proof of Maxwell equations using the NC framework, a fact which consist also in using the Moyal bracket instead of the Poisson bracket. In what follows we will present two kinds of NC framework associated to two distinguished scenarios to conceive the proof of the Maxwell equations in a NC space. These two scenarios offering two possibilities to make the space NC permit among others to debate the novelty extracted from this extension relatively to each case.

B. Noncommutativity: First kind

One way to make the space NC is to consider the following commutation relations:

$$[x_j, x_k] = i\theta_{jk}, \tag{38}$$

$$m[x_j, \dot{x}_k] = \delta_{jk}, \tag{39}$$

where [,] stands for the Moyal bracket and where (38) is simply a NC extension of (8). We assume in this first kind of noncommutativity that the rhs of (39) is not affected by the deformation parameter. Differentiating this equation with respect to time and using (7) we find the same equation as in the ordinary product (9), since the NC parameter θ_{jk} is a constant

$$[x_j, F_k] + m[\dot{x}_j, \dot{x}_k] = 0. \tag{40}$$

On the other hand, the bilinearity of the Moyal bracket implies

$$[[x_i, F_j], x_k] + m[[\dot{x}_i, \dot{x}_j], x_k] = 0. \tag{41}$$

Computing the second term of this equation, using the Jacobi identity of $\dot{x}_i$, $\dot{x}_j$, and x_k as well as the Moyal bracket of x_j and $\dot{x}_k$ (39), we find the following constraint:

$$[[\dot{x}_i, \dot{x}_j], x_k] = 0, \tag{42}$$

or by virtue of (40)

$$[[x_i, F_j], x_k] = 0. \tag{43}$$

Compared to the standard computations, the present case shows a new property, namely, the quantity $[x_i, F_j]$ is coordinate space independent, and hence the field B defined by

$$B_l = \frac{m^2}{2} \epsilon_{jkl} [\dot{x}_j, \dot{x}_k] \tag{44}$$

is also independent of x_i. Consequently, the corresponding equations for B read as

$$\operatorname{div} B = \frac{\partial B_l}{\partial x_l} = 0 \tag{45}$$

and

$$\operatorname{rot} B = \nabla \times B = 0. \tag{46}$$

Moreover, using (39) and (44), the field E defined by the Lorentz force equation (10), satisfies then

$$[x_m, E_j] = 0. \tag{47}$$

The above equation shows that the field E is also space independent which, in turn, gives the following equations:

$$\operatorname{div} E = 0 \tag{48}$$

and

$$\operatorname{rot} E = 0. \tag{49}$$

Few remarks are in order.

(1) One should signal the possibility to extract from (39) the following realization for the velocity $\dot{x}_k$, namely,

$$\dot{x}_k = -\frac{i}{m}\theta_{lk}^{-1}x_l + g(t),$$

where $g(t)$ is an arbitrary pure time-dependent function. This shows in particular that the velocity is a linear function of the space coordinate. This gives also a possibility to express the force $F_k = m\,\ddot{x}_k$ in terms of the deformed θ parameter and the function $g(t)$.

(2) The fact to introduce a parameter of noncommutativity to the manner of (38), induces necessarily the static Maxwell equations which means also the absence of the charge and current densities ρ and j. In fact, by virtue of (11–14) and (45–48), we have $\partial E/\partial t = 0 = \partial B/\partial t$ leading to the constant behavior of the electromagnetic field (E,B) and to the absence of the electric densities (ρ,j). We can advance at this level that the noncommutativity of the first kind is equivalent to cancel the charge and current densities for the Maxwell equations.

(3) It is important to look for the meaning of the commutative limit $\theta = 0$. In fact, once the previous limit is performed, the behavior of the Lorentz force F as well as of the field B change completely as they depend on the behavior of the space coordinates x_m. Setting $\theta = 0$ one discovers the Poison bracket $\{x_j, x_k\} = 0$ which, by virtue of the standard computations, means the restoration of the densities ρ and j.

C. Noncommutativity: Second kind

As it is shown through the previous calculations, the relation (9) constitutes a crucial step in Feynman's proof. Any changes at the level of this relation will necessarily lead to important modifications and all of the standards results are then suspected to change. Here we propose to consider the NC space (38) and modify the equation (39) while supposing that velocity is a quantity that depends on spatial coordinates. We suppose the following NC expressions:

$$[x_j, x_k] = i\theta_{jk}, \tag{50}$$

$$m[x_j, \dot{x}_k] = \delta_{jk} + im\theta_{jk}f, \tag{51}$$

where f is a function which can depend on x and t and it is given by

$$f(x,t) \equiv \left(\frac{\partial \dot{x}_l}{\partial \eta_l}(x+\eta)\right)_{\eta=0}. \tag{52}$$

This function describes in some sense the behavior of the velocity coordinates with respect to the space–time coordinates. In a similar way as above, a possible realization of (51) is given explicitly by

$$\dot{x}_k = -\frac{i}{m}\theta_{lk}^{-1}x_l + A_k(x,t),$$

such that

$$\left(\frac{\partial \dot{x}_k}{\partial \eta_b}(x+\eta)\right)_{\eta=0.} = -\frac{i}{m}\theta_{bk}^{-1} + \left(\frac{\partial A_k}{\partial \eta_b}\right)_{\eta=0}, \tag{53}$$

where $A_k(x,t)$ is for instance a function depending on the coordinates (x,t) and which can be related to the function f as we will show later. Indeed, introducing this realization into (51), drives us to a constraint equation that we should solve, namely,

$$m[x_j, A_k] = im\theta_{jk} f.$$

Here, we are in the presence of several possibilities depending on whether the function $A_k(x,t)$ is linear on the space coordinate or not. A first possibility consists in considering a linear realization namely $A_k(x,t) = x_k g(t)$ with $g(t)$ a purely time-dependent function. This is a natural solution that imposes a strong condition on the function $f = g(t)$ which becomes purely time dependent. We have

$$\left(\frac{\partial \dot{x}_k}{\partial \eta_b}\right)_{\eta=0.} = -\frac{i}{m}\theta_{bk}^{-1} + \delta_{kb} f(t).$$

Now, we are ready to generalize the previous case by assuming $A_k(x,t)$ to be nonlinear in spatial coordinates. A particular example is given by the quadratic realization $A_k(x,t) = x^2$. $\tilde{A}_k(t)$ with $x^2 \equiv x_a * x^a$. Straightforward calculations lead to the following realization for the function f, namely, $f(x,t) = 2x_k \tilde{A}_k(t)$.

It is an easy exercise to derive other nonlinear realizations of the function $f(x,t)$ by setting $A_k(x,t) = x^n$. $\tilde{A}_k(t)$ with $x^n \equiv x_{a_1} * x_{a_2} * \cdots * x_{a_n} \eta^{a_1 \cdots a_n}$. The sharing property of the special cases discussed above is the rich structure that exhibits the noncommutative algebra (50) and (51) for the different possibilities depending on whether f is purely a time dependent function $f(t)$ or space–time coordinates $f(x,t)$.

Now, having discussed some features of the noncommutative algebra (50) and (51), we will focus thereafter to follow step by step the Feynman's analysis[15] using (50) and (51) and see the contribution for the Maxwell equations as well as for the Feynman's proof for arbitrary function $f(x,t)$. In fact, the derivation of (51) with respect to time t drives naturally to the following expression:

$$m[\dot{x}_j, \dot{x}_k] + m\left[x_j, \frac{\mathrm{d}\dot{x}_k}{\mathrm{d}t}\right] = im\theta_{jk}\frac{\mathrm{d}f}{\mathrm{d}t}, \tag{54}$$

or equivalently

$$m[\dot{x}_j, \dot{x}_k] + [x_j, F_k] = im\theta_{jk}\frac{\mathrm{d}f}{\mathrm{d}t}. \tag{55}$$

Since the Moyal bracket is also bilinear we can write

$$[x_l, [x_j, F_k]] = -m[x_l, [\dot{x}_j, \dot{x}_k]] + im\theta_{jk}\left[x_l, \frac{\mathrm{d}f}{\mathrm{d}t}\right]. \tag{56}$$

Furthermore, using the Jacobi identity of x_l, $\dot{x}_j$, and $\dot{x}_k$, the first term on the right-hand side of Eq. (56) gives

$$[x_l, [\dot{x}_j, \dot{x}_k]] = i[(\theta_{lk}\dot{x}_j - \theta_{lj}\dot{x}_k), f] \tag{57}$$

and we can write

$$[x_l,[x_j,F_k]]=-im[(\theta_{lk}\dot{x}_j-\theta_{lj}\dot{x}_k),f]+im\theta_{jk}\left[x_l,\frac{df}{dt}\right]. \tag{58}$$

Note that, in spite of the fact that (55) extends the standard relation (15) it preserves the antisymmetry property of x_j and F_k, because of the antisymmetry of the NC parameter θ, namely,

$$[x_j,F_k]=-[x_k,F_j], \tag{59}$$

and therefore the field B can also be defined as

$$[x_j,F_k]=-\frac{1}{m}\epsilon_{jkl}B_l. \tag{60}$$

Equations (58) and (60) give the following Moyal bracket:

$$[x_l,B_s]=\frac{im^2}{2}\epsilon_{jks}\left([(\theta_{lk}\dot{x}_j-\theta_{lj}\dot{x}_k),f]-\theta_{jk}\left[x_l,\frac{df}{dt}\right]\right), \tag{61}$$

which vanishes for $\theta=0$, giving rise then to the standard Poisson bracket (20).

The field B can be written using (55) and (60) as follows:

$$B_s=\frac{m^2}{2}\epsilon_{jks}[\dot{x}_j,\dot{x}_k]-i\frac{m^2}{2}\epsilon_{jks}\theta_{jk}\frac{df}{dt}. \tag{62}$$

This is a nontrivial form of the magnetic field B_s due to the fact that the second term on the right-hand side of (62) did not appear in standard calculations (22) for which $\theta=0$. Such a term did not contribute to a time-constant value of the function f. On the other hand, using (60) as well as the expression of the Lorentz force (10) we can write for the electric field E,

$$[x_j,E_k]=-\epsilon_{kmn}\dot{x}_m[x_j,B_n]-i\epsilon_{kmn}\theta_{jm}fB_n. \tag{63}$$

To make this expression much more explicit, one needs only to substitute the bracket $[x_j,B_n]$ and B_n by their explicit formulas (61) and (62). Now, in order to obtain the NC analogous of the first Maxwell equation $\operatorname{div}B=0$, one should compute, as previously, the Moyal bracket between the velocity and the field B

$$[\dot{x}_s,B_s]=\frac{m^2}{2}\epsilon_{jks}[\dot{x}_s,[\dot{x}_j,\dot{x}_k]]-\frac{im^2}{2}\epsilon_{jks}\theta_{jk}\left[\dot{x}_s,\frac{df}{dt}\right], \tag{64}$$

or simply

$$[B_s,\dot{x}_s]=\frac{im^2}{2}\epsilon_{jks}\theta_{jk}\left[\dot{x}_s,\frac{df}{dt}\right], \tag{65}$$

since the first term of (64) vanishes using the analogous of the Jacobi identity (23).

Afterwards, using (37), this equation becomes

$$(\delta_{as}+im\theta_{as}f)\frac{\partial B_s}{\partial x_a}=i\frac{m^3}{2}\epsilon_{jks}\theta_{jk}\left[\dot{x}_s,\frac{df}{dt}\right], \tag{66}$$

or equivalently

$$\frac{\partial B_s}{\partial x_s}=i\frac{m^3}{2}\epsilon_{jks}\theta_{jk}\left[\dot{x}_s,\frac{df}{dt}\right]-im\theta_{as}f\frac{\partial B_s}{\partial x_a}. \tag{67}$$

Using once again (61) and the following identity:

$$[B_s, x_s] = [x_a, x_s] \frac{\partial B_s}{\partial x_a} = i\theta_{as} \frac{\partial B_s}{\partial x_a}, \tag{68}$$

the first NC Maxwell equation corresponding to (51) reads finally as

$$\mathrm{div}_\theta B \equiv \frac{\partial B_s}{\partial x_s} = i\frac{m^3}{2}\epsilon_{jks}\theta_{jk}\left[(\dot{x}_s + 2x_s), \frac{\mathrm{d}f}{\mathrm{d}t}\right] - im^3\epsilon_{jks}[(\theta_{ks}\dot{x}_j - \theta_{sj}\dot{x}_k), f]. \tag{69}$$

This equation can be simply rewritten as

$$\mathrm{div}_\theta B = \eta_\theta, \tag{70}$$

where we have introduced the notation $\mathrm{div}_\theta B \equiv \partial B_s/\partial x_s$ for the first NC Maxwell equation to distinguish it from the standard case. A remarkable fact is that the rhs of (69) namely η_θ, is completely dependent of the NC parameter θ, setting $\theta = 0$ we obtain exactly the ordinary Maxwell equation (24). Here, one could anticipate and give a significance to this new immersing term η_θ as being a density of magnetic charges in analogy with the density of electric charge.

Next, to obtain the second NC Maxwell equation, we derive with respect to time the field B_s (62),

$$\frac{\partial B_s}{\partial t} + \dot{x}_m \frac{\partial B_s}{\partial x_m} = m^2 \epsilon_{jks}\left[\frac{\mathrm{d}^2 x_j}{\mathrm{d}t^2}, \dot{x}_k\right] - i\frac{m^2}{2}\epsilon_{jks}\theta_{jk}\frac{\mathrm{d}^2 f}{\mathrm{d}t^2}, \tag{71}$$

this is because the magnetic field B is (x,t)-coordinates dependent, since the velocity is also considered as depending on the space coordinate. Furthermore, using the Lorentz force (10), one has

$$\begin{aligned}\frac{\partial B_s}{\partial t} + \dot{x}_m \frac{\partial B_s}{\partial x_m} &= m\epsilon_{jks}[E_j + \epsilon_{jmn}\dot{x}_m B_n, \dot{x}_k] - i\frac{m^2}{2}\epsilon_{jks}\theta_{jk}\frac{\mathrm{d}^2 f}{\mathrm{d}t^2} \\ &= m(\epsilon_{jks}[E_j, \dot{x}_k] + [\dot{x}_k B_s, \dot{x}_k] - [\dot{x}_s B_k, \dot{x}_k]) - i\frac{m^2}{2}\epsilon_{jks}\theta_{jk}\frac{\mathrm{d}^2 f}{\mathrm{d}t^2}.\end{aligned} \tag{72}$$

Explicitly we find the following expression for the second NC Maxwell equation:

$$\frac{\partial B_s}{\partial t} + \epsilon_{kjs}\frac{\partial E_j}{\partial x_k} = m\epsilon_{jks} f[E_j, x_k] + m\dot{x}_k f[B_s, x_k] + \dot{x}_s[\dot{x}_k, B_k] - i\frac{m^2}{2}\epsilon_{mnk}\theta_{mn}[\dot{x}_k, \dot{x}_s]\frac{\mathrm{d}f}{\mathrm{d}t}, \tag{73}$$

leading then, after some algebraic manipulations, to the following compact formula:

$$\frac{\partial B_s}{\partial t} + \epsilon_{kjs}\frac{\partial E_j}{\partial x_k} = A_1\frac{\mathrm{d}^2 f}{\mathrm{d}t^2} + A_2\frac{\mathrm{d}f}{\mathrm{d}t} + A_3, \tag{74}$$

where the rhs term of (74) is a nonlinear second order differential equation in the arbitrary function f whose coefficients are explicitly given by

$$A_1 = -i\frac{m^2}{2}\epsilon_{jks}\theta_{jk},$$

$$A_2 = -\frac{m^3}{2}\theta_{jl}\{\theta_{ks}\epsilon_{jls}f^2 - i\epsilon_{jlk}[\dot{x}_s,\dot{x}_k]\},$$

$$A_3 = -\frac{m^3}{2}\{\epsilon_{jlk}[\dot{x}_s,\dot{x}_k] + i\theta_{ks}\epsilon_{jls}f^2\}[\dot{x}_j,\dot{x}_l] - \dot{x}_s\eta_\theta, \tag{75}$$

where $\eta_\theta = \mathrm{div}_\theta B$ (69) and (70). As we can easily check, all the local coefficients functions A_1, A_2, and A_3 are θ-depending. Thus, the standard limit $\theta = 0$ is natural as it leads to the standard Feynman's proof computations.

Having presented the general analysis, we try now to discuss briefly the obtained results for the different realizations of the function f. To start, let us signal the remarkable property of the purely time dependent function $f = g(t)$ for which the magnetic field B_s (62) is nontrivial whereas the first NC Maxwell equation (69) is similar to the standard case (11) $\mathrm{div}\, B_s = 0$ since $(\eta_\theta)_{f=g(t)} = 0$. However the second NC Maxwell equation (71) is nontrivial and it is reduced to (74) and (75) for $f = g(t)$ and $\eta_\theta = 0$.

The other possibility consists in considering, for example, the linear realization of the function f namely $f(x,t) = 2x_k\tilde{A}_k(t)$ leading to a simplification of the couple of NC Maxwell equations (69) and (71). To avoid the heaviness of the formulas, we will limit ourselves to (69) in which we introduce $f(x,t) = 2x_k\tilde{A}_k(t)$ and the same analysis applies for (71). In fact, it is easy to check that the last term of the rhs of (69) namely $\epsilon_{jks}\tilde{A}_a[(\theta_{ks}\dot{x}_j - \theta_{sj}\dot{x}_k), x_a]$ is vanishing for reasons of symmetry. Thus, the only terms that contribute are given by

$$\mathrm{div}_\theta B = i\frac{m^3}{2}\epsilon_{jks}\theta_{jk}[(\dot{x}_s + 2x_s),(\dot{x}_a.\tilde{A}_a + x_a.\dot{\tilde{A}}_a)]$$

whose calculation comes naturally from the NC algebra (50) and (51) with $\dot{\tilde{A}}_a = \mathrm{d}\tilde{A}_a/\mathrm{d}t$.

To close this discussion, remark also that the second NC Maxwell equation (71) is expressed in terms of the second derivatives of the function f. In the present case $f(x,t) = 2x_k\tilde{A}_k(t)$, we can write $\frac{1}{2}\ddot{f} = (\ddot{x}_a\tilde{A}_a + 2\dot{x}_a\dot{\tilde{A}}_a + x_a 0\ddot{\tilde{A}}_a)$. Assuming for instance that $\tilde{A}(t) = \mathrm{const}$, we may write $f = \Sigma m_a x_a$ with $\tilde{A}_a = \mathrm{const} \equiv m_a/2$. This gives a possibility to connect to the Lorentz force such that $\ddot{f} \equiv F = \Sigma m_a\ddot{x}_a$.

IV. CONCLUDING REMARKS

Let us summarize what has been the scope of this work. The importance of the so-called Feynman's proof of the Maxwell equations was essentially revealed by the Dyson's work.[15] This paper resuscitated a former idea of Feynman who made a proof of the Maxwell equations assuming only the Newton's law of motion and the commutation relations between position and velocity. This proof that Feynman refused to publish, believing that it was a simple joke,[21] was appreciated and taken with a great seriousness by several scientists.[16–19]

However, one of the things that caused some discussions around the Feynman's proof is the fact that the derivation mixes classical and quantum concepts and the small confusion that seems to appear when we see the relativistic Maxwell equations derived from the classical Newton's law. The point is that the consideration of nonrelativistic equations and the relations of commutation between position and velocity are only a process well arranged to get the Maxwell equations.

As it is signaled in Ref. 18, one may wonder then how truly relativistic Maxwell equations are derived from Newton's classical assumptions? The confusion could be shaped if we remark that

the Feynman's proof concerns only half of Maxwell equations, namely $\mathrm{div}\, B=0$ and $(\partial B/\partial t)+\nabla\times E=0$, describing the Bianchi set of equations. It no longer poses a problem since this couple of equations are compatible with the nonrelativistic Galilean invariance.

Following the Feynman's proof of the Maxwell equations, assuming only the Newton's law of motion and the commutation relation between position and velocity, we try in this paper to study this proof using the NC geometry framework. To accomplish this task, we consider two kinds of NC formulations going along the same way as Feynman's approach. This allows us to discover, in a first formulation, the static Maxwell equations.

Afterwards, motivated by the hope to find a new theory using NC framework, we assume that the velocity is also space dependent and write the modified NC relation (51). The results extracted from the second formulation are more significant as they are associated to a nontrivial θ-extension of the Bianchi-set of Maxwell equations, namely, $\mathrm{div}_\theta B=\eta_\theta$ and $(\partial B_s/\partial t)+\epsilon_{kjs}(\partial E_j/\partial x_k)=A_1(\mathrm{d}^2 f/\mathrm{d}t^2)+A_2(\mathrm{d}f/\mathrm{d}t)+A_3$, where A_1, A_2, and A_3 are local coefficient functions depending on the NC parameter θ. The function f introduced at the level of the NC algebra (51) depend in general on the space–time coordinates. Some special realizations are discussed.

Our objectives in reconsidering the Feynman's proof are, on the one hand, to put it in relief and, on the other hand, to show its importance in the NC framework. The novelty of this proof in the NC space is revealed notably at the level of the corrections brought to the previous Maxwell equations. These corrections correspond essentially to the possibility of existence of sources of magnetic charges that we can associate to the magnetic monopole since $\mathrm{div}_\theta B=\eta_\theta$. Note that these extra terms η_θ are absent in the ordinary case associated to $\theta=0$. These results may give new insights into the study of the electromagnetic duality and its various physical and mathematical aspects.

ACKNOWLEDGMENTS

We would like to thank the Abdus Salam International Center for Theoretical Physics, Trieste-Italy, and the considerable help of the High Energy Section where this work was done. We acknowledge Dr. M. Hssaini for fruitful discussions. This work was done within the framework of the Associateship scheme of the Abdus Salam ICTP (Summer 2003).

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Hilbert space structure in classical mechanics. I

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(Received 7 August 2002; accepted 29 August 2003)

In this paper we study the Hilbert space structure underlying the Koopman–von Neumann (KvN) operatorial formulation of classical mechanics. KvN limited themselves to study the Hilbert space of zero-forms that are the square integrable functions on phase space. They proved that in this Hilbert space the evolution is unitary for every system. In this paper we extend the KvN Hilbert space to higher forms which are basically functions of the phase space points and the differentials on phase space. We prove that if we equip this space with a positive definite scalar product the evolution can turn out to be nonunitary for some systems. Vice versa, if we insist in having a unitary evolution for every system then the scalar product cannot be positive definite. Identifying the one-forms with the Jacobi fields we provide a physical explanation of these phenomena. We also prove that the unitary/nonunitary character of the evolution is invariant under canonical transformations. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1623333]

I. INTRODUCTION

In the 1930s Koopman and von Neumann (KvN)[1] gave an operatorial formulation of *classical mechanics* (CM). They first introduced square-integrable functions $\psi(\varphi^a)$ on the phase space $\mathcal{M}$ of a classical system with Hamiltonian $H(\varphi)$ (with φ^a we indicate the $2n$ phase-space coordinates of the system $\varphi^a = q^1 \cdots q^n, p^1 \cdots p^n$). According to KvN the Liouville phase-space distributions $\rho(\varphi)$ are obtained from $\psi(\varphi)$ as

$$\rho(\varphi) = |\psi(\varphi)|^2. \tag{1.1}$$

The introduction of the $\psi(\varphi)$ is an acceptable assumption considering that $\rho(\varphi)$, having the meaning of a probability density, is always positive semidefinite $\rho(\varphi) \geqslant 0$, and so one can always take its "square root" and obtain $\psi(\varphi)$. Moreover, as $\psi(\varphi)$ is square integrable, i.e., $\psi(\varphi) \in L^2$, it turns out that $\rho(\varphi)$ is integrable as it should be

$$\int \mathrm{d}^{2n}\varphi\, \psi^*(\varphi)\psi(\varphi) = \int \mathrm{d}^{2n}\varphi\, \rho(\varphi) < \infty. \tag{1.2}$$

KvN *postulated* the following evolution for $\psi(\varphi)$:

$$i\frac{\partial \psi(\varphi,t)}{\partial t} = \hat{L}\psi(\varphi,t) \tag{1.3}$$

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where $\hat{L}$, defined as

$$\hat{L} = i\frac{\partial H}{\partial q^i}\frac{\partial}{\partial p^i} - i\frac{\partial H}{\partial p^i}\frac{\partial}{\partial q^i}, \tag{1.4}$$

is the Liouville operator. This equation of motion for $\psi(\varphi)$ and (1.1) lead to the same evolution for $\rho(\varphi)$,

$$i\frac{\partial \rho(\varphi,t)}{\partial t} = \hat{L}\rho(\varphi,t). \tag{1.5}$$

This is the well-known Liouville equation satisfied by the classical probability densities. Note that $\rho(\varphi)$ obeys the same equation as $\psi(\varphi)$ because $\hat{L}$ is first order in the derivatives. The same does not happen in quantum mechanics where the analog of (1.3) is the Schrödinger equation whose evolution operator is second order in the derivatives. We will not spend more time here in explaining the interplay between the quantum mechanical wave functions $\psi(q)$ and these ''KvN waves'' $\psi(\varphi)$. The interested reader can consult Ref. 2 where many details have been worked out.

In order to have a true Hilbert structure a scalar product has to be introduced and KvN used the following:

$$\langle \psi|\Phi\rangle = \int \mathrm{d}^{2n}\varphi\ \psi^*(\varphi)\Phi(\varphi). \tag{1.6}$$

We have introduced an abstract $\langle$bra$|$ and $|$ket$\rangle$ notation and we have used a particular representation for the wave functions. This is the φ representation which is the ''analog'' of the x representation in quantum mechanics. We could have used other representations and some of them have been analyzed in Ref. 2.

Sticking anyhow to the representation (1.6) it is easy to see that the Liouville operator (1.4) is Hermitian

$$\langle \hat{L}\psi|\Phi\rangle = \langle \psi|\hat{L}\Phi\rangle. \tag{1.7}$$

The Hermiticity of $\hat{L}$ is necessary in order to guarantee the unitarity of the evolution operator which, in its infinitesimal form, is

$$U(\Delta t) = e^{-i\hat{L}\Delta t}. \tag{1.8}$$

The unitarity of the evolution, on the other hand, is crucial in order to guarantee, via (1.1), the conservation of the total probability.

In differential geometry the operator $\hat{L}$ is known as the Hamiltonian vector field associated to the time evolution and it is usually[3] indicated with $(\mathrm{d}H)^{\#}$. It can be extended to an object known as the Lie derivative along the Hamiltonian flow,[3] which is usually written as $\mathcal{L}_{(\mathrm{d}H)^{\#}}$. This is the operator which makes the evolution of the higher forms

$$\psi(\varphi,\mathrm{d}\varphi) = \psi_0(\varphi) + \psi_a(\varphi)\mathrm{d}\varphi^a + \psi_{ab}(\varphi)\mathrm{d}\varphi^a\wedge\mathrm{d}\varphi^b + \cdots. \tag{1.9}$$

The first term $\psi_0(\varphi)$ on the right-hand side (RHS) of (1.9) is the zero-form whose evolution is given by the Liouvillian $\hat{L}$. We say that $\mathcal{L}_{(\mathrm{d}H)^{\#}}$ is an extension of $\hat{L}$ just because it makes the evolution of quantities $\psi(\varphi,\mathrm{d}\varphi)$ which are extensions of the $\psi_0(\varphi)$. Moreover it is possible to prove[3] that

$$\mathcal{L}_{(\mathrm{d}H)^{\#}}\big|_{\mathrm{d}\varphi=0} = i\hat{L}. \tag{1.10}$$

The differential geometry associated to classical mechanics is an old subject[3] but it keeps arousing the interest of physicists.[4] The question we want to address in this paper is whether the space of higher forms (1.9) can be turned into a Hilbert space like KvN did for the zero-forms. This basically means that we want to see if it is possible to introduce a positive definite scalar product in the space of the higher forms $\psi(\varphi,\mathrm{d}\varphi)$. At the same time we want to check if under this scalar product the Lie-derivative $\mathcal{L}_{(\mathrm{d}H)^{\#}}$ is a Hermitian operator. Surprisingly we will see that this is not possible, that means we will prove that both conditions, positive definiteness of the scalar product and Hermiticity of $\mathcal{L}_{(\mathrm{d}H)^{\#}}$, cannot hold at the same time for every system.

Instead of working in the abstract differential-geometric framework outlined above, we will use a more physical one derived from a path integral formulation of CM.[5] This formulation (from now on we will call it CPI as acronym for Classical Path Integral) is the functional counterpart of the operatorial method of KvN and it generates some extra structures which generalize the KvN approach. These structures are exactly the higher forms and the Lie derivative we mentioned above. The CPI is basically defined as follows (for more details consult Ref. 5). Let us build the following generating functional:

$$Z_{cl}[J]=\int \mathcal{D}\varphi \quad \tilde{\delta}[\varphi-\varphi_{cl}] \quad \exp\left[\int J\varphi\right], \tag{1.11}$$

where φ_{cl} are the classical solutions of the equations of motion[3]

$$\dot{\varphi}^a=\omega^{ab}\frac{\partial H}{\partial \varphi^b} \tag{1.12}$$

with ω^{ab} the symplectic matrix. In (1.11) we gave weight one to the classical trajectories and weight zero to all the others. This is different than what is done in the quantum mechanical path integral where each path $[\varphi(t)]$ has weight $e^{iS[\varphi]}$. As φ^a_{cl} in (1.11) are the zeroes of the following function: $[\dot{\varphi}^a-\omega^{ab}(\partial H/\partial\varphi^b)]$, we can rewrite (1.11) as

$$Z_{cl}[J]=\int \mathcal{D}\varphi \quad \tilde{\delta}\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]\left|\delta^a_b\partial_t-\omega^{a\mathrm{d}}\frac{\partial^2 H}{\partial\varphi^{\mathrm{d}}\partial\varphi^b}\right| \quad \exp\int J\varphi \tag{1.13}$$

and using $6n$ auxiliary variables $(\lambda_a,c^a,\overline{c_a})$ (where $c^a,\overline{c_a}$ have Grassmannian character) we can rewrite (1.13) in the following form:

$$Z_{cl}[J]=\int \mathcal{D}\varphi^a\,\mathcal{D}\lambda_a\,\mathcal{D}c^a\,\mathcal{D}\overline{c_a}\,e^{i\int \mathrm{d}t\,\tilde{\mathcal{L}}+\int \mathrm{d}t\,J\varphi}, \tag{1.14}$$

where

$$\tilde{\mathcal{L}}=\lambda_a\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]+i\overline{c_a}\left[\dot{c}^a-\omega^{a\mathrm{d}}\frac{\partial^2 H}{\partial\varphi^{\mathrm{d}}\partial\varphi^b}\right]c^b. \tag{1.15}$$

The Hamiltonian associated to $\tilde{\mathcal{L}}$ is

$$\tilde{\mathcal{H}}=\lambda_a\omega^{ab}\frac{\partial H}{\partial\varphi^b}+i\overline{c_a}\omega^{a\mathrm{d}}\frac{\partial^2 H}{\partial\varphi^{\mathrm{d}}\partial\varphi^b}c^b. \tag{1.16}$$

The contact with differential geometry was first established in Ref. 5 and further developed in Ref. 6. In those references it was shown that the Grassmann variables c^a can be identified with the basis $\mathrm{d}\varphi^a$ of the space of forms and their associated wedge product is naturally taken into account by the Grassmannian character of the variables c^a. The functions $\psi(\varphi,c)$ can then be set into correspondence with the inhomogeneous forms

$$\psi(\varphi,c)=\psi_0(\varphi)+\psi_a(\varphi)c^a+\psi_{ab}(\varphi)c^a c^b+\cdots$$

$$\Leftrightarrow\quad \psi_0(\varphi)+\psi_a(\varphi)\mathrm{d}\varphi^a+\psi_{ab}(\varphi)\mathrm{d}\varphi^a\wedge\mathrm{d}\varphi^b+\cdots. \tag{1.17}$$

From the path integral (1.14) one can derive an operatorial formalism and a commutator structure,[7] which is given by

$$[\hat{\varphi}^a,\hat{\lambda}_b]_-=i\delta^a_b,\quad [\hat{c}^a,\hat{\bar{c}}_b]_+=\delta^a_b. \tag{1.18}$$

To implement (1.18) we can then realize λ_a and $\overline{c_a}$ as

$$\hat{\lambda}_a=-i\frac{\partial}{\partial\varphi^a},\quad \hat{\bar{c}}_a=\frac{\partial}{\partial c^a}. \tag{1.19}$$

In this representation the ''wave functions'' of the theory are functions which depend only on φ and c, i.e., $\psi(\varphi,c)$ and these are precisely the inhomogeneous forms (1.17). The relations (1.19) turn the $\tilde{\mathcal{H}}$ of Eq. (1.16) into the following operator:

$$\tilde{\mathcal{H}}=-i\omega^{ab}\frac{\partial H}{\partial\varphi^b}\frac{\partial}{\partial\varphi^a}-i\omega^{a\mathrm{d}}\frac{\partial^2 H}{\partial\varphi^{\mathrm{d}}\partial\varphi^b}c^b\frac{\partial}{\partial c^a}. \tag{1.20}$$

From now on we will use the same notation for the Hamiltonian (1.16) and the associated operator (1.20). The first term on the RHS of (1.20) is nothing else than the Liouville operator $\hat{L}$ which acts only on the zero-forms $\psi_0(\varphi)$, while the second term acts also on higher forms $\psi(\varphi,c)$. The combined action of these two terms identifies $\tilde{\mathcal{H}}$ with the Lie-derivative along the Hamiltonian flow.[5] Also all the other standard differential geometric operations like exterior derivative, interior contraction with vector fields, Lie brackets, etc., can be rephrased in the language of the CPI. All the details can be found in Refs. 5 and 6.

As we said previously, in this paper we would like to find out if the space of the higher forms, which now can be identified with the functions $\psi(\varphi,c)$, can be endowed with a positive definite scalar product as KvN did for the zero-forms and if the operator $\tilde{\mathcal{H}}$ is Hermitian under this scalar product. The reader may wonder which are the *physical* reasons which motivate us to study this enlarged Hilbert space. The reasons are the following. It is well-known[8] that such features like the ergodicity of a dynamical system are indicated by the *spectral* properties of the Liouvillian. In particular a system is ergodic if the eigenstate associated to the zero eigenvalue of the Liouvillian is nondegenerate. Later on it was discovered[9] that the *spectral* properties of $\tilde{\mathcal{H}}$, which is the object that generalizes the Liouvillian, gives us further physical information such as the Lyapunov exponents or the dynamical and topological entropies of the system. So the *spectrum* of $\tilde{\mathcal{H}}$ seems to be the central object encapsulating the most important physical features of a dynamical system. To get the spectrum it is necessary first to study the Hilbert space in which $\tilde{\mathcal{H}}$ is defined and to find out if it is a Hermitian operator or not. The previous studies[9] did not *rigorously* explore these mathematical features but derived the properties mentioned above in a rather *formal* way by functional techniques. In this paper we will only prepare the mathematical ground necessary to prove *rigorously* the physical results contained in Ref. 9. Those rigorous proofs will appear in future works. Anyhow, even the mathematical machinery that we have prepared in this paper will reveal some surprising and interesting results as outlined below.

The paper is organized as follows. In Sec. II we will limit ourselves to the case of a two-dimensional symplectic manifold $\mathcal{M}$, labeled by one coordinate q and one conjugate momentum p. In this case, because of the features of the Grassmann variables, the expression of the generalized wave functions is particularly simple, and the most general inner product can be parametrized in terms of a matrix g^{ij}. Varying this matrix we will find out, as particular cases, some scalar products which are well known in the literature and we will briefly analyze their features. The strange and interesting property we will find is the following one: if we choose a scalar

product which is positive definite then $\tilde{\mathcal{H}}$ turns out to be not Hermitian for some systems or, if we impose $\tilde{\mathcal{H}}$ to be Hermitian for any system, then the scalar product is not positive definite. In Sec. III we will show that this feature holds for every scalar product and not just for those examined in Sec. II. This fact is related to the presence of the symplectic matrix within the Hamiltonian $\tilde{\mathcal{H}}$ and to the Grassmannian nature of the variables c^a. Moreover it is a peculiar feature of classical mechanics and in fact it does not appear in a similar Hamiltonian which describes supersymmetric *quantum mechanical* models[10,11] where it is possible to find at least one scalar product which guarantees both the Hermiticity of the Hamiltonian and the positivity of the scalar product for all systems. An important thing to notice for the CPI is that the Hermitian/non-Hermitian character of $\tilde{\mathcal{H}}$ is invariant under canonical transformations and this is proved in details in Appendix C. In Sec. IV we will show how the CPI can be reproduced starting from the completeness relations associated with the various scalar products. As some scalar products are not positive definite in Sec. V we will search for the subspace (of the full Hilbert space) made of positive norm states under two of the scalar products examined in Sec. II. In the same section we shall also look for the subspace in which $\tilde{\mathcal{H}}$ is Hermitian under a third scalar product examined in Sec. II. Our analysis reveals that in all three cases the subspace we searched for is made of the zero-forms and of a set of higher ones isomorphic to the zero-forms. So we conclude that, in all three cases, the "physical states" are basically the zero-forms or other forms "*isomorphic*" to them. By "*physical*" we mean those which have both a positive norm and on which $\tilde{\mathcal{H}}$ is Hermitian, and by "*isomorphic*" we mean those which transform in the same manner as the zero-forms under the Lie derivative of the Hamiltonian flow. In the Conclusions (Sec. VI) we will give some *physical* explanations of the phenomena we have encountered in this paper. Namely we will study those systems for which $\tilde{\mathcal{H}}$ is not Hermitian under a positive scalar product, and try to understand why physically this can happen. We will see that the same physical explanation applies when we have a Hermitian $\tilde{\mathcal{H}}$ for those same systems and in that case we have to give up the positive definiteness of the scalar product. Some mathematical details of this paper are confined to three appendixes. More of these details can be found in Ref. 12.

II. SOME SCALAR PRODUCTS FOR THE CPI

In this section we want to investigate some possible scalar products for the Hilbert space underlying the CPI in the simple case $n=1$ of a two-dimensional symplectic manifold whose coordinates we indicate with $\varphi^a \equiv (q,p)$. Because of the properties of the Grassmann variables $c^a \equiv (c^q, c^p)$, a generalized wave function $\psi(\varphi,c)$ can contain only four independent components, which are complex functions of φ:

$$\psi(\varphi,c)=\psi_0(\varphi)+\psi_1(\varphi)c^q+\psi_2(\varphi)c^p+\psi_3(\varphi)c^q c^p. \tag{2.1}$$

The most general inner product we can impose among these Hilbert space elements is the following one:

$$\langle \tau|\psi\rangle = \int \mathrm{d}\varphi\ \tau_i^*(\varphi) g^{ij} \psi_j(\varphi), \tag{2.2}$$

where g^{ij} is a 4×4 complex matrix and i,j can be (0,1,2,3). From Eq. (2.2) it is easy to prove that the bosonic operators of the theory are Hermitian,

$$\begin{aligned} \hat{\varphi}^{a\dagger} &= \hat{\varphi}^a, \\ \hat{\lambda}_a^\dagger &= \hat{\lambda}_a . \end{aligned} \tag{2.3}$$

Therefore the bosonic part of the Hamiltonian $\tilde{\mathcal{H}}_{\mathrm{bos}} = \hat{\lambda}_a \omega^{ab} \partial_b H$, which is nothing else than the Liouvillian, is always Hermitian. For what concerns the fermionic part, different choices of the

matrix g^{ij} in (2.2) correspond to different choices of the Hermiticity conditions among the Grassmann operators $(\hat{c}^a,\hat{\bar{c}}_a)$ of the theory. Consequently the fermionic part of the Hamiltonian $\tilde{\mathcal{H}}$, which is given by

$$\tilde{\mathcal{H}}_{\text{ferm}}=i\hat{\bar{c}}_a\omega^{ab}\partial_b\partial_{\text{d}}H\hat{c}^{\text{d}}, \tag{2.4}$$

can either be Hermitian or not. In the following sections we will choose some particular matrices g^{ij} and we will analyze the properties and the features of the associated scalar products.

A. The SvH scalar product

The first choice we want to make is the following one:

$$g^{ij}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}. \tag{2.5}$$

Inserting the previous matrix into (2.2) the scalar product becomes

$$\langle\tau|\psi\rangle=\int \text{d}\varphi\ \tau_i^*(\varphi)\psi_i(\varphi). \tag{2.6}$$

It is clear from the previous formula that the norms of the states are all positive definite:

$$\langle\psi|\psi\rangle=\sum_{i=0}^{3}\int \text{d}\varphi\,|\psi_i(\varphi)|^2\geqslant 0 \tag{2.7}$$

while the associated Hermiticity conditions for the Grassmann operators of the theory are

$$\hat{c}^{a\dagger}=\hat{\bar{c}}_a,\quad \hat{\bar{c}}_a^{\dagger}=\hat{c}^a. \tag{2.8}$$

This is the scalar product introduced by Salomonson and van Holten (SvH) in supersymmetric quantum mechanics[10] and this is why we have called it ''SvH'' scalar product. What we want to do now is to see whether the fermionic part of the Hamiltonian $\tilde{\mathcal{H}}_{\text{ferm}}$ is Hermitian under the SvH scalar product. First of all let us write $\tilde{\mathcal{H}}_{\text{ferm}}$ as

$$\tilde{\mathcal{H}}_{\text{ferm}}=i\hat{\bar{c}}_a\mathcal{F}^a_{\text{d}}\hat{c}^{\text{d}}, \tag{2.9}$$

where $\mathcal{F}^a_{\text{d}}=\omega^{ab}\partial_b\partial_{\text{d}}H$. Then

$$\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}=(i\overline{c}_a\mathcal{F}^a_{\text{d}}c^{\text{d}})^{\dagger}=(-i)(c^{\text{d}})^{\dagger}(\mathcal{F}^{\dagger})^{\text{d}}_a(\overline{c}_a)^{\dagger}=-i\overline{c}_{\text{d}}(\mathcal{F}^{\dagger})^{\text{d}}_a c^a. \tag{2.10}$$

So $\tilde{\mathcal{H}}_{\text{ferm}}$ would be Hermitian if $\mathcal{F}^{\dagger}=-\mathcal{F}$. As $\mathcal{F}$ is real, the relation $\mathcal{F}^{\dagger}=-\mathcal{F}$ implies that $\mathcal{F}^T=-\mathcal{F}$. Let us see if this happens by taking

$$\mathcal{F}^q_p=\omega^{qb}\partial_b\partial_p H=\omega^{qp}\partial_p^2 H=\partial_p^2 H \tag{2.11}$$

and comparing it with its transposed element

$$\mathcal{F}^p_q=\omega^{pb}\partial_b\partial_q H=\omega^{pq}\partial_q^2 H=-\partial_q^2 H. \tag{2.12}$$

From these expressions we conclude that *in general* $\mathcal{F}$ is not equal to $-\mathcal{F}^T$ and this implies that $\tilde{\mathcal{H}}$ *is not in general Hermitian under the SvH scalar product.* By the expression ''*in general*'' we

mean that the Hermiticity of the Hamiltonian is not guaranteed for all systems. It can occur for some particular dynamical systems but not for all of them. For example, for the SvH scalar product we note that for systems with Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}q^2, \tag{2.13}$$

we get that $\mathcal{F}_p^q=-\mathcal{F}_q^p$ and this implies that the associated $\tilde{\mathcal{H}}$ is Hermitian. The system above is a particular harmonic oscillator and we thought, at first, that the $\tilde{\mathcal{H}}$ would be Hermitian for all harmonic oscillators or even all integrable systems. This is actually not the case as it is explained in detail in Appendix C.

Even if the CPI[5] has been proposed many years ago, many people have often said that it is "the same model as susy QM." We have now proved that, differently than susy QM, the CPI Hamiltonian $\tilde{\mathcal{H}}$ is not Hermitian under the same scalar product (SvH) of susy QM. This definitely proves that the CPI is not susy QM!

These considerations can be extended to an arbitrary number of degrees of freedom. The state becomes in that case

$$\psi=\sum_{m=0}^{2n}\frac{1}{m!}\psi_{a_1\cdots a_m}(\varphi)c^{a_1}c^{a_2}\cdots c^{a_m} \tag{2.14}$$

and the SvH norm turns out to be

$$\langle\psi|\psi\rangle=K\sum_{\{a_i\}}\sum_{m=0}^{2n}\int \mathrm{d}\varphi|\psi_{a_1\cdots a_m}(\varphi)|^2, \tag{2.15}$$

where K is a positive number. The derivation is long but straightforward.

B. The gauge scalar product

Of course there are other possible choices of the scalar product, besides the SvH one. For example we could implement the scalar product typically used in gauge theories.[13] It corresponds to the following choice of the matrix g^{ij} in Eq. (2.2):

$$g^{ij}=\begin{pmatrix}0&0&0&-i\\0&0&-i&0\\0&i&0&0\\i&0&0&0\end{pmatrix}. \tag{2.16}$$

With this choice it is easy to show[12] that the Grassmann operators of the theory are Hermitian:

$$\begin{aligned}\hat{c}^{a\dagger}&=\hat{c}^a,\\ \hat{\bar{c}}_a^{\dagger}&=\hat{\bar{c}}_a.\end{aligned} \tag{2.17}$$

Consequently also the $\tilde{\mathcal{H}}_{\mathrm{ferm}}$ of (2.9) is Hermitian. In fact

$$\tilde{\mathcal{H}}_{\mathrm{ferm}}^{\dagger}=-i\hat{c}^c\omega^{ab}\partial_b\partial_c H\hat{\bar{c}}_a=i\hat{\bar{c}}_a\omega^{ab}\partial_b\partial_c H\hat{c}^c=\tilde{\mathcal{H}}_{\mathrm{ferm}}, \tag{2.18}$$

where in the second step of (2.18) we have used the anticommutation relations $[\hat{c}^c,\hat{\bar{c}}_a]=\delta_a^c$ together with the fact that $\omega^{ab}\partial_b\partial_a H=0$. Therefore the overall Hamiltonian $\tilde{\mathcal{H}}$ is Hermitian under the gauge scalar product and this is a first important difference from the SvH case where the analog of $\tilde{\mathcal{H}}$ was in general not Hermitian.

If we come back and look at the expression (2.16) of the matrix g^{ij} it is easy to realize that there are problems with the gauge scalar product. First of all, $g^{00}=0$, it implies that the zero-forms have zero norm. This result is different than the original KvN case, where the zero-forms had norm different from zero and equal to the total probability $\int d\varphi\, \rho(\varphi)$ of finding the particle somewhere in phase space. This was one of the postulates of the KvN theory and it has to be maintained by any generalization to higher forms. So the gauge scalar product is not a good generalization of the KvN scalar product among the zero-forms. Second, if we diagonalize the matrix (2.16) we find out that there are two eigenvalues equal to 1 and two eigenvalues equal to -1. This implies that there are negative norm states in the theory. This is particularly clear also from the explicit expression of the scalar product in terms of the components of the wave functions. In fact, inserting (2.16) into (2.2), we get that

$$\langle \tau|\psi\rangle = i\int d\varphi\, [\,\tau_3^*\psi_0+\tau_2^*\psi_1-\tau_1^*\psi_2-\tau_0^*\psi_3]. \tag{2.19}$$

From this expression it is very easy to realize that the states

$$\alpha(\varphi,c)=\frac{1}{\sqrt{2}}\alpha(\varphi)[c^q c^p+i], \quad \beta(\varphi,c)=\frac{1}{\sqrt{2}}\beta(\varphi)[c^p+ic^q], \tag{2.20}$$

where $\alpha(\varphi)$ and $\beta(\varphi)$ are square integrable functions, have negative norm. These generalized wave functions correspond to the two eigenstates

$$\alpha=\alpha(\varphi)\begin{pmatrix} i/\sqrt{2}\\ 0\\ 0\\ 1/\sqrt{2}\end{pmatrix}, \quad \beta=\beta(\varphi)\begin{pmatrix} 0\\ i/\sqrt{2}\\ 1/\sqrt{2}\\ 0\end{pmatrix} \tag{2.21}$$

of the matrix (2.16) with eigenvalue -1.

C. The symplectic scalar product

The gauge scalar product which we analyzed in the preceding section is not the only one under which $\tilde{\mathcal{H}}$ is Hermitian. In this section we will study another one which has the same feature and whose Hermiticity conditions are

$$\begin{aligned}(\hat{c}^a)^\dagger &= i\omega^{ab}\hat{\bar{c}}_b,\\ (\hat{\bar{c}}_a)^\dagger &= i\omega_{ab}\hat{c}^b.\end{aligned} \tag{2.22}$$

Because of the presence of the symplectic matrix ω^{ab} in (2.22) we will call "symplectic" the associated scalar product. If we take H of the form $H=(p^2/2)+V(q)$, the fermionic part (2.4) can be written as $\tilde{\mathcal{H}}_{\rm ferm}=i\hat{\bar{c}}_q\hat{c}^p-i\hat{\bar{c}}_pV''\hat{c}^q$ where $V''=\partial^2V/\partial q^2$. Applying the Hermiticity conditions (2.22) we get

$$\begin{aligned}\tilde{\mathcal{H}}_{\rm ferm}^\dagger &= (i\hat{\bar{c}}_q\hat{c}^p)^\dagger-(i\hat{\bar{c}}_pV''\hat{c}^q)^\dagger=-i\hat{c}^{p\dagger}\hat{\bar{c}}_q^\dagger+i\hat{c}^{q\dagger}V''\hat{\bar{c}}_p^\dagger\\ &= -i(-i\hat{\bar{c}}_q)(-i\hat{c}^p)+i\cdot i\hat{\bar{c}}_pV''i\hat{c}^q\\ &= i\hat{\bar{c}}_q\hat{c}^p-i\hat{\bar{c}}_pV''\hat{c}^q=\tilde{\mathcal{H}}_{\rm ferm},\end{aligned} \tag{2.23}$$

i.e., the fermionic part of $\tilde{\mathcal{H}}$ is Hermitian. It is easy to realize[12] that the Hermiticity conditions (2.22) are reproduced by the following choice of the matrix g^{ij}:

$$g^{ij}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2.24}$$

or, equivalently, by the following scalar product expressed in terms of the components of the wave functions:

$$\langle \tau | \psi \rangle = \int \mathrm{d}\varphi \, [\, \tau_0^* \psi_0 + i(\tau_1^* \psi_2 - \tau_2^* \psi_1) - \tau_3^* \psi_3]. \tag{2.25}$$

Since $g^{00}=1$ the zero-forms have finite norm, as in the original KvN scalar product. Unfortunately the matrix (2.24) has two eigenvalues equal to 1 and two eigenvalues equal to -1. This means that there are states of negative norm also with the symplectic scalar product. For example the states $\alpha(\varphi,c)=\alpha(\varphi)/\sqrt{2}\,[c^p - i c^q]$ and $\beta(\varphi,c)=\beta(\varphi)c^q c^p$, where $\alpha(\varphi)$ and $\beta(\varphi)$ are square integrable functions, have negative norm. These states are nothing more than the eigenvectors

$$\alpha = \frac{\alpha(\varphi)}{\sqrt{2}} \begin{pmatrix} 0 \\ -i \\ 1 \\ 0 \end{pmatrix}$$

and

$$\beta = \beta(\varphi) \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

associated to the eigenvalue -1 of the matrix (2.24). These considerations can be easily[12] extended to an arbitrary number of degrees of freedom, where the explicit expression of the symplectic scalar product becomes

$$\langle \tau | \psi \rangle = \sum_{m=0}^{2n} \frac{i^m}{m!} \int \mathrm{d}\varphi \; \tau^*_{a_1 \cdots a_m} \omega^{a_1 b_1} \cdots \omega^{a_m b_m} \psi_{b_1 \cdots b_m}. \tag{2.26}$$

III. GENERALIZED SCALAR PRODUCTS

From the preceding section we can conclude that all the three scalar products we have analyzed have either $\tilde{\mathcal{H}}$ non-Hermitian or the scalar product nonpositive definite. We shall show in this section that this is not just a feature of those particular scalar products that we have introduced: even the most general one cannot have both $\tilde{\mathcal{H}}$ Hermitian and no negative norm states.

Let us limit our analysis to the case of $n=1$ and $H=(p^2/2)+V(q)$. What we want to do is to find out the most general Hermiticity conditions for $(\hat{c}^a, \hat{\bar{c}}_a)$ under which $\tilde{\mathcal{H}}$ is Hermitian. After this we will analyze whether any of the associated scalar products is positive definite. Since for $\hat{\varphi}$ and $\hat{\lambda}$ we will stick to the standard Hermiticity conditions (2.3), the bosonic part of $\tilde{\mathcal{H}}$ is always Hermitian. Therefore we should only care about the fermionic part which is

$$\tilde{\mathcal{H}}_{\mathrm{ferm}} = i \hat{\bar{c}}_q \hat{c}^p - i \hat{\bar{c}}_p V''(q) \hat{c}^q. \tag{3.1}$$

For this to be Hermitian, independently of the particular form of the potential $V(q)$, the two pieces on the RHS of (3.1) must be separately Hermitian since the second one, differently from the first, contains the potential V. So we must have

$$(i\hat{\bar{c}}_q\hat{c}^p)^\dagger = i\hat{\bar{c}}_q\hat{c}^p, \tag{3.2}$$

$$(-i\hat{\bar{c}}_p\hat{c}^q)^\dagger = -i\hat{\bar{c}}_p\hat{c}^q. \tag{3.3}$$

It is possible to prove[12] that there are only three possible families of Hermiticity conditions on the Grassmann operators which satisfy both (3.2) and (3.3). The first one is given by

$$\begin{aligned} \hat{c}^{p\dagger} &= ib\hat{\bar{c}}_q, \\ \hat{\bar{c}}_q^\dagger &= \frac{i}{b}\hat{c}^p, \\ \hat{c}^{q\dagger} &= -ib\hat{\bar{c}}_p, \\ \hat{\bar{c}}_p^\dagger &= -\frac{i}{b}\hat{c}^q \end{aligned} \tag{3.4}$$

with b a real number. The matrix g^{ij} which reproduces (3.4) turns out to be

$$g^{ij} = \begin{pmatrix} g^{00} & 0 & 0 & 0 \\ 0 & 0 & -ibg^{00} & 0 \\ 0 & ibg^{00} & 0 & 0 \\ 0 & 0 & 0 & -b^2g^{00} \end{pmatrix}. \tag{3.5}$$

Let us first notice that if $g^{00}=1$ and $b=-1$ then the matrix (3.5) reduces to (2.24) which is the matrix associated with the symplectic scalar product (2.25). To check whether (3.5) gives positive definite scalar products, we should calculate the eigenvalues of (3.5) and see if they are all positive. These eigenvalues are

$$\begin{aligned} \lambda_1 &= g^{00}, \\ \lambda_2 &= +bg^{00}, \\ \lambda_3 &= -bg^{00}, \\ \lambda_4 &= -b^2g^{00}. \end{aligned} \tag{3.6}$$

So we see that there are always two eigenvalues with one sign and two with the opposite one. This ultimately confirms that the scalar product associated to (3.5) is not positive definite.

In order to satisfy both (3.2) and (3.3) another choice of Hermiticity conditions is given by

$$\begin{aligned} \hat{c}^{p\dagger} &= e^{i\theta_\alpha}\hat{c}^p, \\ \hat{\bar{c}}_q^\dagger &= i\gamma_I\hat{c}^p + e^{-i\theta_\alpha}\hat{\bar{c}}_q, \\ \hat{c}^{q\dagger} &= e^{i\theta_\alpha}\hat{c}^q, \\ \hat{\bar{c}}_p^\dagger &= -i\gamma_I\hat{c}^q + e^{-i\theta_\alpha}\hat{\bar{c}}_p \end{aligned} \tag{3.7}$$

and leads to the following matrix g^{ij}:

$$g^{ij}=\begin{pmatrix} ig^{03}e^{i\theta_\alpha}\gamma_I & 0 & 0 & g^{03} \\ 0 & 0 & g^{03}e^{i\theta_\alpha} & 0 \\ 0 & -g^{03}e^{i\theta_\alpha} & 0 & 0 \\ -g^{03}e^{2i\theta_\alpha} & 0 & 0 & 0 \end{pmatrix}, \tag{3.8}$$

where γ_I and θ_α are real numbers. The eigenvalue equation associated to this matrix is

$$(\lambda^2+(g^{03})^2e^{2i\theta_\alpha})(\lambda^2-ig^{03}e^{i\theta_\alpha}\gamma_I\lambda+(g^{03})^2e^{2i\theta_\alpha})=0. \tag{3.9}$$

Two of its eigenvalues are

$$\lambda=\pm ig^{03}e^{i\theta_\alpha} \tag{3.10}$$

and one sees from here that every choice of g^{03} and θ_α which makes one of these two eigenvalues positive will make the other negative. This proves that even the scalar product which is associated to the Hermiticity conditions (3.7) is not positive definite. This case is a generalization of the gauge scalar product (2.16); in fact it reduces to (2.16) with the choice $\gamma_I=0$, $g^{03}=-i$, $\theta_\alpha=0$.

The last possibility[12] to satisfy (3.2) and (3.3) is given by

$$\begin{aligned} \hat{c}^{p\dagger}&=e^{i\theta_\alpha}\hat{c}^p+ib\hat{\bar{c}}_q, \\ \hat{\bar{c}}_q^{\dagger}&=e^{-i\theta_\alpha}\hat{\bar{c}}_q, \\ \hat{c}^{q\dagger}&=e^{i\theta_\alpha}\hat{c}^q-ib\hat{\bar{c}}_p, \\ \hat{\bar{c}}_p^{\dagger}&=e^{-i\theta_\alpha}\hat{\bar{c}}_p \end{aligned} \tag{3.11}$$

which corresponds to the matrix g^{ij},

$$g^{ij}=\begin{pmatrix} 0 & 0 & 0 & g^{03} \\ 0 & 0 & g^{03}e^{i\theta_\alpha} & 0 \\ 0 & -g^{03}e^{i\theta_\alpha} & 0 & 0 \\ -g^{03}e^{2i\theta_\alpha} & 0 & 0 & -ig^{03}e^{i\theta_\alpha}b \end{pmatrix} \tag{3.12}$$

whose eigenvalues are given by the solutions of the equation

$$(\lambda^2+(g^{03})^2e^{2i\theta_\alpha})(\lambda^2+ig^{03}e^{i\theta_\alpha}b\lambda+(g^{03})^2e^{2i\theta_\alpha})=0. \tag{3.13}$$

Two solutions are given by

$$\lambda=\pm ig^{03}e^{i\theta_\alpha} \tag{3.14}$$

and again we are in the same situation as in (3.10). So, as the matrices (3.8) and (3.12) have negative eigenvalues, the associated scalar products are not positive definite. It should be noticed that also (3.12) is a generalization of the gauge scalar product which is obtained with the following choice of parameters: $b=0$, $\theta_\alpha=0$, $g^{03}=-i$.

To summarize what we have done in this section, we can say that the whole set of consistent scalar products under which $\tilde{\mathcal{H}}$ is Hermitian is the one associated to the three matrices (3.8), (3.12), (3.5). The first two are generalizations of the gauge scalar product while the last one is a generalization of the symplectic case. None of these three generalizations leads to a positive definite scalar product.

We can summarize all this by saying that if we choose a scalar product such that, whatever the form of the potential $V(q)$, *the operator* $\tilde{\mathcal{H}}$ *turns out to be Hermitian* then *that same scalar*

product cannot be positive definite. As a consequence, based on standard rules of logic, we can say that if we choose a *positive definite scalar product* then the operator $\tilde{\mathcal{H}}$ *cannot be Hermitian* for any choice of the potential $V(q)$. It may be Hermitian for some particular potentials but not for all of them. This second case is exemplified in the SvH case.

IV. ABSTRACT HILBERT SPACE AND CPI

Up to now we have derived all our results starting from the representation in which the elements of the Hilbert space are given by functions of φ and c. Like in the standard formulation of quantum mechanics this is not the only representation and it is possible to perform things in a completely abstract framework. This is what we want to do in this section and we will explain things for the Salomonson–van Holten scalar product. Let us start building an abstract basis of our Hilbert space. First we define the state $|0-,0-\rangle$ which is the eigenstate of $\hat{c}^q$ and $\hat{c}^p$ with eigenvalue 0:

$$\begin{aligned} \hat{c}^q|0-,0-\rangle &= 0, \\ \hat{c}^p|0-,0-\rangle &= 0. \end{aligned} \tag{4.1}$$

In the state $|0-,0-\rangle$ above the first "0−" stays for the eigenvalue of $\hat{c}^q$ and the second "0−" for the eigenvalue of $\hat{c}^p$. We can define also the following other states:

$$\begin{aligned} |0+,0-\rangle &\equiv \hat{\bar{c}}_q|0-,0-\rangle, \\ |0-,0+\rangle &\equiv -\hat{\bar{c}}_p|0-,0-\rangle, \\ |0+,0+\rangle &\equiv -\hat{\bar{c}}_q\hat{\bar{c}}_p|0-,0-\rangle. \end{aligned} \tag{4.2}$$

It is easy to prove[12] that $|0+,0-\rangle$ is a common eigenstate for $\hat{\bar{c}}_q$ and $\hat{c}^p$ with eigenvalues 0 and that $|0-,0+\rangle$ is the eigenstate for $\hat{c}^q$ and $\hat{\bar{c}}_p$ with eigenvalues 0, while $|0+,0+\rangle$ is the eigenstate for $\hat{\bar{c}}_q$ and $\hat{\bar{c}}_p$ with eigenvalues 0. So the rule to indicate these states is that we put into the $|\ \rangle$ a "0+" if it is an eigenstate (with zero eigenvalue) of a $\hat{\bar{c}}$-operator and a "0−" if it is an eigenstate (with zero eigenvalue) of a $\hat{c}$-operator. Starting from $|0+,0+\rangle$ and $|0-,0-\rangle$ it is possible to construct the simultaneous eigenstates of $\hat{c}^q$ and $\hat{c}^p$ with Grassmannian odd eigenvalues α^q and α^p. They are

$$|\alpha^q-,\alpha^p-\rangle \equiv e^{-\alpha^q\hat{\bar{c}}_q-\alpha^p\hat{\bar{c}}_p}|0-,0-\rangle, \tag{4.3}$$

while the states which are simultaneous eigenstates of $\hat{\bar{c}}_q$ and $\hat{\bar{c}}_p$ with Grassmannian odd eigenvalues β_q and β_p are

$$|\beta_q+,\beta_p+\rangle \equiv e^{-\beta_q\hat{c}^q-\beta_p\hat{c}^p}|0+,0+\rangle. \tag{4.4}$$

Having now built all these states, it is easy to derive[12] the various scalar products among them or equivalently the associated resolutions of the identity. The ingredients for these derivations[10] are the Hermiticity conditions among the various Grassmann operators and the choice of a normalization among just one of the states. If we choose the following normalization,

$$\langle -0,-0|0-,0-\rangle = 1 \tag{4.5}$$

and the SvH Hermiticity conditions (2.8), then we can get the following resolutions of the identity for the SvH case:

$$\int \mathrm{d}\overline{c_q}\,\mathrm{d}\overline{c_p}|\overline{c_q}+,\overline{c_p}+\rangle\langle-\overline{c_p}^*,-\overline{c_q}^*|=\mathbb{I},$$

$$\int \mathrm{d}c^p\,\mathrm{d}c^q|c^q-,c^p-\rangle\langle+c^p*,+c^q*|=\mathbb{I}, \tag{4.6}$$

where the c and $\overline{c}$ stay for the α and β of (4.3) and (4.4). The details of the derivation are very similar to those presented in Ref. 10 and can be found in Ref. 12. To make contact with the SvH scalar product in the (φ,c)-representation, that is given in (2.6), we should use the resolutions of the identity (4.6) to define a scalar product among two generic states $\langle\tau|$ and $|\psi\rangle$,

$$\begin{aligned}\langle\tau|\psi\rangle&=\int \mathrm{d}p\,\mathrm{d}q\,\mathrm{d}c^p\,\mathrm{d}c^q\langle\tau|q,p,c^q-,c^p-\rangle\langle+c^p*,+c^q*,p,q|\psi\rangle\\&=\int \mathrm{d}p\,\mathrm{d}q\,\mathrm{d}c^p\,\mathrm{d}c^q\,\tau_+^*(q,p,c^q,c^p)\psi_-(q,p,c^q,c^p),\end{aligned} \tag{4.7}$$

where

$$\begin{aligned}\tau_+(q,p,c^q,c^p)&\equiv\langle-c^p,-c^q,q,p|\tau\rangle,\\ \psi_-(q,p,c^q,c^p)&\equiv\langle+c^p*,+c^q*,p,q|\psi\rangle,\end{aligned} \tag{4.8}$$

and where we have included also the variables "p,q" in the resolution of the identity.

It is easy to prove[12] that τ_+ and ψ_- have the form

$$\psi_-(q,p,c^q,c^p)=\psi_0(q,p)+\psi_q(q,p)c^q+\psi_p(q,p)c^p+\psi_2(q,p)c^qc^p, \tag{4.9}$$

$$\tau_+(q,p,c^q,c^p)=\tau_2(q,p)+\tau_p(q,p)c^q*-\tau_q(q,p)c^p*-\tau_0(q,p)c^q*c^p*, \tag{4.10}$$

and so we get

$$\langle\tau|\psi\rangle=\int \mathrm{d}p\,\mathrm{d}q\,[\,\tau_0^*\psi_0+\tau_q^*\psi_q+\tau_p^*\psi_p+\tau_2^*\psi_2], \tag{4.11}$$

which is exactly the SvH scalar product (2.6).

We have used up to now the states written in the resolutions of the identity (4.6) but they are much more than a basis for our Hilbert space. They are similar to the "coherent states" which are an overcomplete basis. The real basis is actually much simpler. In fact it is easy to prove that the LHS of both equations in (4.6) are equal to

$$|0+,0+\rangle\langle+0,+0|+|0-,0+\rangle\langle+0,-0|+|0+,0-\rangle\langle-0,+0|+|0-,0-\rangle\langle-0,-0| \tag{4.12}$$

which means that there are the four states

$$|0+,0+\rangle,\ \ |0-,0+\rangle,\ \ |0+,0-\rangle,\ \ |0-,0-\rangle \tag{4.13}$$

which make a complete basis in the case of a two-dimensional phase space. We could have proved this also in the following other manner. There are two commuting Hermitian operators which make a complete set of operators for what concerns the Grassmannian part of the theory. They are

$$\begin{aligned}\hat{N}_q&=\hat{c}^q\hat{\bar{c}}_q,\\ \hat{N}_p&=\hat{c}^p\hat{\bar{c}}_p.\end{aligned} \tag{4.14}$$

The states (4.13) are just the eigenstates of $\hat{N}_q$ and $\hat{N}_p$ with eigenvalues (0,0), (1,0), (0,1), (1,1), respectively,

$$\begin{aligned}
&\hat{N}_q|0+,0+\rangle=0, \quad \hat{N}_p|0+,0+\rangle=0,\\
&\hat{N}_q|0-,0+\rangle=|0-,0+\rangle, \quad \hat{N}_p|0-,0+\rangle=0,\\
&\hat{N}_q|0+,0-\rangle=0, \quad \hat{N}_p|0+,0-\rangle=|0+,0-\rangle,\\
&\hat{N}_q|0-,0-\rangle=|0-,0-\rangle, \quad \hat{N}_p|0-,0-\rangle=|0-,0-\rangle.
\end{aligned} \tag{4.15}$$

Following a procedure similar to the one we used for the SvH scalar product, we can derive a resolution of the identity also for the ''gauge scalar product'' and it turns out to be

$$i\int \mathrm{d}q\,\mathrm{d}p\,\mathrm{d}c^q\,\mathrm{d}c^p|q,p,c^q-,c^p-\rangle\langle -c^{p*},-c^{q*},p,q|=\mathbb{I} \tag{4.16}$$

while for the symplectic case we get

$$\int \mathrm{d}q\,\mathrm{d}p\,\mathrm{d}c^p\,\mathrm{d}c^q|q,p,c^q-,c^p-\rangle\langle ic^{p*}+,(-ic^{q*})+,p,q|=\mathbb{I}. \tag{4.17}$$

From these two resolutions of the identity it is then easy to obtain the gauge scalar product (2.19) and the symplectic one (2.25) in the (φ,c)-representation. The details of these derivations can be found in Ref. 12.

We will conclude this section with an application of the resolutions of the identity (4.6). Originally the CPI model was formulated directly via path integrals without deriving it explicitly from the operatorial formalism. In quantum mechanics instead the path integral was derived[14] by assembling infinitesimal time evolutions in operatorial form and inserting between them suitable resolutions of the identity. We shall now do the same for the CPI and as resolutions of the identity we shall use the ones associated to the SvH scalar product. Before proceeding we should remember that, besides the representation in which $\hat{\varphi}^a$ and $\hat{c}^a$ are multiplicative operators while $\hat{\lambda}_a = -i(\partial/\partial\varphi^a)$ and $\hat{\bar{c}}_a=\partial/\partial c^a$ are derivative ones, we can also have a sort of ''momentum'' representation in which $\hat{\lambda}_a$ and $\hat{\bar{c}}_a$ are multiplicative operators and $\hat{\varphi}^a$ and $\hat{c}^a$ are derivative ones,[2]

$$\begin{aligned}
\hat{\varphi}^a&=i\frac{\partial}{\partial\lambda_a},\\
\hat{c}^a&=\frac{\partial}{\partial\bar{c}_a}.
\end{aligned} \tag{4.18}$$

The ''wave functions'' in this representation would depend on $\lambda_a,\bar{c}_a$ and the resolution of the identity involving λ and $\bar{c}$ would be[12]

$$\int \mathrm{d}\lambda_q\,\mathrm{d}\lambda_p\,\mathrm{d}\bar{c}_q\,\mathrm{d}\bar{c}_p|\lambda_q,\lambda_p,\bar{c}_q+,\bar{c}_p+\rangle\langle -\bar{c}_p^*,-\bar{c}_q^*,\lambda_p,\lambda_q|=\mathbb{I} \tag{4.19}$$

to be contrasted with the one involving φ and c which is

$$\int \mathrm{d}\varphi\,\mathrm{d}c^p\,\mathrm{d}c^q|\varphi,c^q-,c^p-\rangle\langle +c^{p*},+c^{q*},\varphi|=\mathbb{I}. \tag{4.20}$$

The transition amplitude to go from some initial configuration (φ_i,c_i^q,c_i^p) to some final one (φ_f,c_f^q,c_f^p) is given by the following kernel:

$$K(f|i)=\langle +c_f^{p*},+c_f^{q*},\varphi_f|e^{-i\tilde{\mathcal{H}}(t_f-t_i)}|\varphi_i,c_i^q-,c_i^p-\rangle. \tag{4.21}$$

We note that the final bra in (4.21) is the state $\langle +c_f^{p*},+c_f^{q*},\varphi_f|$ since this bra is just the eigenstate of $\hat{c}^q$ and $\hat{c}^p$ with eigenvalues c_f^q and c_f^p.

Now, as it is usually done in QM, let us divide the interval t_f-t_i in (4.21) into N intervals of length ϵ, so that $N\epsilon=t_f-t_i$. The amplitude $K(f|i)$ of (4.21) can then be written as

$$K(f|i)=\langle +c_f^{p*},+c_f^{q*},\varphi_f|\underbrace{\exp[-i\epsilon\tilde{\mathcal{H}}]\cdots\exp[-i\epsilon\tilde{\mathcal{H}}]}_{N\ \text{terms}}|\varphi_i,c_i^q-,c_i^p-\rangle. \tag{4.22}$$

Let us now insert a resolution of the identity (4.19) in front of each exponential in (4.22) and a resolution of the identity (4.20) behind each exponential. Evaluating each scalar product we finally arrive at the following expression for the kernel of evolution:

$$K(f|i)=\int \mathcal{D}\mu \times\exp\left[i\epsilon\sum_{j=1}^{N}\left(\lambda_{q_j}\frac{q_{j+1}-q_j}{\epsilon}+\lambda_{p_j}\frac{p_{j+1}-p_j}{\epsilon}+i\bar{c}_{q_j}\frac{(c_{j+1}^q-c_j^q)}{\epsilon}+i\bar{c}_{p_j}\frac{(c_{j+1}^p-c_j^p)}{\epsilon}-\tilde{\mathcal{H}}_j\right)\right]. \tag{4.23}$$

The subindex j on $(q,p,\lambda_q,\lambda_p,c^q,c^p,\bar{c}_q,\bar{c}_p)$ is the time label in the subdivision of the interval (t_f-t_i) in N subintervals; the boundary conditions are

$$\varphi_0=\varphi_i,\quad \varphi_{N+1}=\varphi_f,\quad c_0=c_i,\quad c_{N+1}=c_f, \tag{4.24}$$

and the measure is

$$\mathcal{D}\mu=d\lambda_{q_1}\,d\lambda_{p_1}\,d\bar{c}_{q_1}\,d\bar{c}_{p_1}\prod_{j=2}^{N}dq_j\,dp_j\,d\lambda_{q_j}\,d\lambda_{p_j}\,dc_j^q\,d\bar{c}_{q_j}\,dc_j^p\,d\bar{c}_{p_j}. \tag{4.25}$$

This measure indicates that the initial and the final (φ,c) are not integrated over. The continuum limit of (4.23) can be easily worked out:

$$K(f|i)=\int_{(\varphi_i,c_i)}^{(\varphi_f,c_f)}\mathcal{D}\mu\,\exp\left[i\int dt\,\tilde{\mathcal{L}}\right] \tag{4.26}$$

and $\tilde{\mathcal{L}}$ turns out to be the Lagrangian in (1.15). This confirms that, via the scalar products and the resolutions of the identity of SvH (4.19) and (4.20), one gets just the CPI. So we can say that the Hilbert space structure of SvH leads to the CPI path integral.

The same discretized path integral can be obtained with the same procedure starting from the other scalar products. In fact the differences in the resolutions of the identity between the SvH, gauge and symplectic case are compensated by the different bra appearing in the kernel of propagation and by the differences in the scalar products among the states. For example the resolutions of the identity for the gauge scalar product in the (φ,c)-representation is (4.16) and in the $(\lambda,\bar{c})$ one is

$$i\int d\lambda_q\,d\lambda_p\,d\bar{c}_q\,d\bar{c}_p|\lambda_q,\lambda_p,\bar{c}_q+,\bar{c}_p+\rangle\langle+\bar{c}_p^*,+\bar{c}_q^*,\lambda_p,\lambda_q|=\mathbb{I} \tag{4.27}$$

but the transition amplitude $K(f|i)$ between an initial configuration (φ_i,c_i^q,c_i^p) and a final one (φ_f,c_f^q,c_f^p) becomes

$$K(f|i)=\langle -c_f^{p*},-c_f^{q*},\varphi_f|e^{-i\tilde{\mathcal{H}}(t_f-t_i)}|\varphi_i,c_i^q-,c_i^p-\rangle. \tag{4.28}$$

The final bra is $\langle -c_f^{p*},-c_f^{q*},\varphi_f|$ since just this bra is the eigenstate of $\hat{c}^q$ and $\hat{c}^p$ with eigenvalues c_f^q and c_f^p in the gauge scalar product.

Analogously in the case of the symplectic scalar product the resolutions of the identity is (4.17) and in the $(\lambda,\overline{c})$-representation,

$$\int \mathrm{d}\lambda_q\,\mathrm{d}\lambda_p\,\mathrm{d}\overline{c_p}\,\mathrm{d}\overline{c_q}|\lambda_q,\lambda_p,\overline{c_q}+,\overline{c_p}+\rangle\langle(-i\overline{c_p^*})-,i\overline{c_q^*}-,\lambda_p,\lambda_q|=\mathbb{I} \tag{4.29}$$

but also the kernel of propagation $K(f|i)$ is different. In fact it is given by

$$K(f|i)=\langle ic_f^{p*}+,(-ic_f^{q*})+,\varphi_f|e^{-i\tilde{\mathcal{H}}(t_f-t_i)}|\varphi_i,c_i^q-,c_i^p-\rangle. \tag{4.30}$$

Also in this case the difference with respect to (4.21) and (4.28) is in the initial $\langle$bra$|$ which has the form $\langle ic_f^{p*}+,(-ic_f^{q*})+,\varphi_f|$ because it is an eigenstate of $\hat{c}^p$ and $\hat{c}^q$ with eigenvalues c_f^p and c_f^q. Inserting the resolutions of the identity (4.17) and (4.29) inside the kernel (4.30) and evaluating all the scalar products we can reproduce the CPI path integral also in the symplectic case. The reader interested in the details of all the above mentioned calculations should consult Ref. 12.

V. "PHYSICAL" HILBERT SPACE

Let us now go back to the main issue of this paper which was the positivity/nonpositivity of the scalar product and the corresponding non-Hermiticity/Hermiticity of the operator $\tilde{\mathcal{H}}$. The problem of having a nonpositive definite scalar product had appeared before in physics mainly in gauge theory.[13] There people addressed the question of finding the "*physical*" subspace of the full Hilbert space that is the one made of positive norm states. In this section we will address a similar problem and, with a little abuse of language, we shall call "physical" for the CPI a subspace of the full Hilbert space made of positive norm states and on which $\tilde{\mathcal{H}}$ is Hermitian. We shall perform this analysis for all the three scalar products studied in the preceding sections starting from the SvH one.

A. Salomonson–van Holten case

In this case all the states in the Hilbert space have positive definite norm but $\tilde{\mathcal{H}}$ is not Hermitian. This is an unacceptable feature because it would lead to the nonconservation of the norm creating in this way difficulties in assigning the meaning of probability to the norm of a generic state, differently from what happens in the zero-form case. The linear subspace of the full Hilbert space on which $\tilde{\mathcal{H}}$ is Hermitian is defined by the following condition:

$$(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^\dagger)|\psi\rangle=0. \tag{5.1}$$

The next thing we have to guarantee is that the vector subspace defined by (5.1) be closed under time evolution. This means that a state $|\psi'\rangle$, obtained via an infinitesimal time evolution from a physical state $|\psi\rangle$:

$$|\psi'\rangle=e^{-i\epsilon\tilde{\mathcal{H}}}|\psi\rangle, \tag{5.2}$$

must still be physical, i.e.,

$$(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^\dagger)|\psi'\rangle=0. \tag{5.3}$$

Inserting (5.2) into (5.3) we get

$$(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger})|\psi'\rangle=(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger})|\psi\rangle-i\epsilon(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger})\tilde{\mathcal{H}}|\psi\rangle$$
$$=-i\epsilon[\tilde{\mathcal{H}},(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger})]|\psi\rangle=i\epsilon[\tilde{\mathcal{H}},\tilde{\mathcal{H}}^{\dagger}]|\psi\rangle \tag{5.4}$$

which implies that for $|\psi'\rangle$ to be physical the following condition must also be satisfied:

$$[\tilde{\mathcal{H}},\tilde{\mathcal{H}}^{\dagger}]|\psi\rangle=0. \tag{5.5}$$

Let us analyze the commutator structure of (5.5). If we write $\tilde{\mathcal{H}}=\tilde{\mathcal{H}}_{\rm bos}+\tilde{\mathcal{H}}_{\rm ferm}$ we get that the commutator contained in the LHS of (5.5) turns into the following expression:

$$[\tilde{\mathcal{H}},\tilde{\mathcal{H}}^{\dagger}]=[\tilde{\mathcal{H}}_{\rm ferm},\tilde{\mathcal{H}}^{\dagger}_{\rm ferm}]+[\tilde{\mathcal{H}}_{\rm bos},\tilde{\mathcal{H}}^{\dagger}_{\rm ferm}]+[\tilde{\mathcal{H}}_{\rm ferm},\tilde{\mathcal{H}}_{\rm bos}]. \tag{5.6}$$

Let us look at the first term on the RHS of (5.6). The general expression of $\tilde{\mathcal{H}}_{\rm ferm}$ was given in (2.4) and, choosing H to be of the form

$$H=\sum_{i=1}^{n} p_i^2/2+V(q_1,\ldots,q_n),$$

we get

$$\tilde{\mathcal{H}}_{\rm ferm}=i\hat{\bar{c}}_{q_i}\hat{c}^{p_i}-i\hat{\bar{c}}_{p_j}\partial_i\partial_j V\hat{c}^{q_i}. \tag{5.7}$$

Using the SvH Hermitian conjugation rules (2.8), we obtain

$$\tilde{\mathcal{H}}^{\dagger}_{\rm ferm}=-i\hat{\bar{c}}_{p_i}\hat{c}^{q_i}+i\hat{\bar{c}}_{q_i}\partial_i\partial_j V\hat{c}^{p_j}. \tag{5.8}$$

So the first term in (5.6) turns out to be

$$[\tilde{\mathcal{H}}_{\rm ferm},\tilde{\mathcal{H}}^{\dagger}_{\rm ferm}]=\hat{\bar{c}}_{q_i}\hat{c}^{q_i}-\hat{\bar{c}}_{p_i}\hat{c}^{p_i}+(\partial_i\partial_j V)(\partial_l\partial_m V)[\hat{\bar{c}}_{p_j}\hat{c}^{p_m}\delta^i_l-\hat{\bar{c}}_{q_l}\hat{c}^{q_i}\delta^m_j] \tag{5.9}$$

while the second and the third term in (5.6) contain third order derivatives in the potential V. To find solutions $|\psi\rangle$ of (5.5), whose form is independent of the potential, we should impose that $|\psi\rangle$ be annihilated separately by the terms in (5.6) which contain no derivative in V, next by those which contain first derivatives of V and so on. By looking at (5.6) and (5.9) the term with no derivative of V is $(\hat{\bar{c}}_{q_i}\hat{c}^{q_i}-\hat{\bar{c}}_{p_i}\hat{c}^{p_i})$; imposing it on $|\psi\rangle$ we get

$$(\hat{\bar{c}}_{q_i}\hat{c}^{q_i}-\hat{\bar{c}}_{p_i}\hat{c}^{p_i})|\psi\rangle=0, \tag{5.10}$$

which implies

$$c^{q_i}\frac{\partial}{\partial c^{q_i}}|\psi\rangle=c^{p_i}\frac{\partial}{\partial c^{p_i}}|\psi\rangle. \tag{5.11}$$

If we represent $|\psi\rangle$ as

$$\psi(\varphi,c)=\sum_{j=0}^{2n}\frac{1}{j!}\psi_{a_1a_2\cdots a_j}(\varphi)c^{a_1}c^{a_2}\cdots c^{a_j} \tag{5.12}$$

then (5.11) is satisfied by those $\psi(\varphi,c)$ which contain the same number of c^q and c^p. Clearly these forms are Grassmannian even, which implies immediately that odd forms cannot be physi-

cal. Before going on to check whether also the terms in (5.9) with second derivatives in V annihilate these forms, let us remember that we must also satisfy the condition (5.1). The operator $\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger}$ with H of the form

$$H=\sum_{i=1}^{n}\frac{p_i^2}{2}+V(q_1,\ldots,q_n)$$

has the expression

$$\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger}=(i\hat{\bar{c}}_{q_i}\hat{c}^{p_i}+i\hat{\bar{c}}_{p_i}\hat{c}^{q_i})-i(\hat{\bar{c}}_{p_j}\partial_i\partial_j V\hat{c}^{q_i}+\hat{\bar{c}}_{q_i}\partial_i\partial_j V\hat{c}^{p_j}). \tag{5.13}$$

Again, a physical form must be annihilated separately by the terms independent of V and by those depending on it. So, using (5.13), (5.1) gives the following two conditions:

$$(\hat{\bar{c}}_{q_i}\hat{c}^{p_i}+\hat{\bar{c}}_{p_i}\hat{c}^{q_i})|\psi\rangle=0, \tag{5.14}$$

$$(\hat{\bar{c}}_{p_j}\partial_i\partial_j V\hat{c}^{q_i}+\hat{\bar{c}}_{q_i}\partial_i\partial_j V\hat{c}^{p_j})|\psi\rangle=0. \tag{5.15}$$

Let us now remember that, because of (5.11), the state $|\psi\rangle$ must contain the same number of c^q and c^p. Therefore it is easy to realize that (5.14) implies that the following two relations must hold separately

$$\hat{\bar{c}}_{q_i}\hat{c}^{p_i}|\psi\rangle=0, \tag{5.16}$$

$$\hat{\bar{c}}_{p_i}\hat{c}^{q_i}|\psi\rangle=0. \tag{5.17}$$

Analogously (5.15) implies that each term in it separately annihilates $|\psi\rangle$:

$$\hat{\bar{c}}_{p_j}(\partial_i\partial_j V)\hat{c}^{q_i}|\psi\rangle=0, \tag{5.18}$$

$$\hat{\bar{c}}_{q_i}(\partial_i\partial_j V)\hat{c}^{p_j}|\psi\rangle=0. \tag{5.19}$$

Let us now construct a linear combination of (5.16) and (5.18) of the following form:

$$(i\hat{\bar{c}}_{q_i}\hat{c}^{p_i}-i\hat{\bar{c}}_{p_j}\partial_i\partial_j V\hat{c}^{q_i})|\psi\rangle=0. \tag{5.20}$$

It is easy to realize, looking at (5.7), that (5.20) is equivalent to

$$\tilde{\mathcal{H}}_{\text{ferm}}|\psi\rangle=0. \tag{5.21}$$

Let us now construct instead a linear combination of (5.17) and (5.19) of the form

$$(-i\hat{\bar{c}}_{p_i}\hat{c}^{q_i}+i\hat{\bar{c}}_{q_j}\partial_i\partial_j V\hat{c}^{p_i})|\psi\rangle=0. \tag{5.22}$$

We immediately notice that (5.22) is equivalent to

$$\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}|\psi\rangle=0. \tag{5.23}$$

These are the two relations which complete our proof. In fact, using (5.21)–(5.23), we have that (5.1) becomes

$$(\tilde{\mathcal{H}}-\tilde{\mathcal{H}}^{\dagger})|\psi\rangle=(\tilde{\mathcal{H}}_{\text{ferm}}-\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}})|\psi\rangle=0 \tag{5.24}$$

and that (5.6) is automatically satisfied because

$$[\tilde{\mathcal{H}},\tilde{\mathcal{H}}^{\dagger}]|\psi\rangle=[\tilde{\mathcal{H}}_{\text{ferm}},\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}]|\psi\rangle+[\tilde{\mathcal{H}}_{\text{bos}},\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}]|\psi\rangle+[\tilde{\mathcal{H}}_{\text{ferm}},\tilde{\mathcal{H}}_{\text{bos}}]|\psi\rangle$$
$$=-\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}\tilde{\mathcal{H}}_{\text{bos}}|\psi\rangle+\tilde{\mathcal{H}}_{\text{ferm}}\tilde{\mathcal{H}}_{\text{bos}}|\psi\rangle=-\tilde{\mathcal{H}}^{\dagger}_{\text{ferm}}|\psi'\rangle+\tilde{\mathcal{H}}_{\text{ferm}}|\psi'\rangle=0. \tag{5.25}$$

The last step is based on the fact that $|\psi'\rangle\equiv\tilde{\mathcal{H}}_{\text{bos}}|\psi\rangle$ is still a physical state. In fact $\tilde{\mathcal{H}}_{\text{bos}}$ acts only on the bosonic coefficients of the states and so it does not modify their Grassmannian structure and because of (5.21) and (5.23) it is just this Grassmannian structure which determines whether a state is physical or not.

Up to now we have proved that a state, to be physical, must be annihilated by the fermionic part of the Hamiltonian $\tilde{\mathcal{H}}$. What we want to do now is to give some explicit forms of such states. Let us take a two-form with n degrees of freedom. In order to satisfy (5.11) the two-form must contain one variable c^{q} and one variable c^{p} and so it must be of the form

$$\psi=\psi_{q_i p_k}c^{q_i}c^{p_k}. \tag{5.26}$$

If we impose (5.17) on the state (5.26) we obtain

$$c^{q_\alpha}\frac{\partial}{\partial c^{p_\alpha}}\psi=0\Rightarrow\psi_{q_i p_\alpha}c^{q_\alpha}c^{q_i}=0. \tag{5.27}$$

For the properties of the Grassmann variables the previous relation is satisfied if we take $\alpha=i$. This means that we have to take a two-form of the type

$$\psi=\psi_{q_1 p_1}c^{q_1}c^{p_1}+\psi_{q_2 p_2}c^{q_2}c^{p_2}+\cdots+\psi_{q_n p_n}c^{q_n}c^{p_n}, \tag{5.28}$$

i.e., a form in which each c^{q_i} is coupled with the relative c^{p_i}. Let us indicate, for simplicity, the various components $\psi_{q_j p_j}$ as $\psi_{(j)}(\varphi)$. Then (5.28) can be written as

$$\psi=\sum_j\ \psi_{(j)}(\varphi)c^{q_j}c^{p_j}. \tag{5.29}$$

Inserting (5.29) into (5.18) and (5.19), it is easy to prove that they can be satisfied only if all the coefficients $\psi_{(j)}(\varphi)$ in (5.29) are the same

$$\psi_{(j)}(\varphi)=K(\varphi). \tag{5.30}$$

So (5.28) turns out to be

$$\psi=K(\varphi)[c^{q_1}c^{p_1}+c^{q_2}c^{p_2}+\cdots+c^{q_n}c^{p_n}]. \tag{5.31}$$

One sees that somehow the dependence on the indices of the coefficients of the two-forms has disappeared. In general the coefficients $K(\varphi)$ will change with the rank of the form. So for example a "*physical*" inhomogeneous form of rank up to 4 will be

$$\psi=\psi_0(\varphi)+K(\varphi)\sum_i\ c^{q_i}c^{p_i}+S(\varphi)\sum_{i,j}\ (c^{q_i}c^{p_i})(c^{q_j}c^{p_j}). \tag{5.32}$$

From the physical point of view the homogeneous physical forms, like (5.31), are "somehow" isomorphic to the zero-forms. In fact $\tilde{\mathcal{H}}_{\text{ferm}}$ annihilates them, see (5.21), and this is the same that happens on the zero-forms. Basically $\tilde{\mathcal{H}}_{\text{ferm}}$ acts on the Grassmann variables in (5.31) annihilating them and so we are left with only $K(\varphi)$ and this $K(\varphi)$ evolves like a zero-form because only $\tilde{\mathcal{H}}_{\text{bos}}$ acts on it. An inhomogeneous state like (5.32) is made instead by a sum of terms, each isomorphic

to a zero-form; so we can say that it is like a linear superposition of the various zero-forms $\psi_0(\varphi), K(\varphi), S(\varphi)$. Among these physical states we have the zero-forms and the $2n$ or volume-forms.

Before concluding we should point out that the physical condition (5.1) limits the forms to be of the type (5.32) only if we do not put any restriction on the potential V. If we put restrictions instead, for example choosing a harmonic oscillator potential or a separable potential, then the condition (5.1) is satisfied by a wider class of forms than the ones in (5.32). This concludes the analysis of the SvH case.

B. Symplectic case

Let us now turn to the other scalar products and in particular to the symplectic one. The Hamiltonian $\tilde{\mathcal{H}}$ in this case is Hermitian but not all the states of the Hilbert space have positive norm. So the ''physical'' Hilbert space, which we will indicate with $\mathbf{H}_{\text{phys}}$, should be a vector subspace of the full Hilbert space, made only of positive norm states. Anyhow this subspace $\mathbf{H}_{\text{phys}}$ cannot be identified with the set $\mathbf{H}^{(+)}$ of *all* the positive norm states. In fact it is easy to realize that $\mathbf{H}^{(+)}$ is not a vector space because the linear combination of two states with positive norm, $\psi \equiv \alpha \psi_+^{(1)} + \beta \psi_+^{(2)}$ where α and β are complex coefficients, does not necessarily belong to $\mathbf{H}^{(+)}$. We will provide an explicit example of this fact in (5.51). So $\mathbf{H}_{\text{phys}}$ can only be a particular subspace of $\mathbf{H}^{(+)}$. In order to build it, it is better to change the variables, and pass from the set $(\hat{q}_i, \hat{p}_i, \hat{\lambda}_{q_i}, \hat{\lambda}_{p_i}, \hat{c}^{q_i}, \hat{c}^{p_i}, \hat{\bar{c}}_{q_i}, \hat{\bar{c}}_{p_i})$ to the following one:

$$
\begin{aligned}
&\hat{z}_i \equiv \frac{1}{\sqrt{2}}(\hat{q}_i + i\hat{p}_i), \quad \hat{\bar{z}}_i \equiv \frac{1}{\sqrt{2}}(\hat{q}_i - i\hat{p}_i),\\
&\hat{l}_i \equiv \frac{1}{\sqrt{2}}(\hat{\lambda}_{q_i} - i\hat{\lambda}_{p_i}), \quad \hat{\bar{l}}_i \equiv \frac{1}{\sqrt{2}}(\hat{\lambda}_{q_i} + i\hat{\lambda}_{p_i}),\\
&\hat{\xi}^i \equiv \frac{1}{\sqrt{2}}(\hat{c}^{q_i} + i\hat{c}^{p_i}), \quad \hat{\bar{\xi}}_i \equiv \frac{1}{\sqrt{2}}(-\hat{\bar{c}}_{q_i} + i\hat{\bar{c}}_{p_i}),\\
&\hat{\xi}^{i*} \equiv \frac{1}{\sqrt{2}}(\hat{c}^{q_i} - i\hat{c}^{p_i}), \quad \hat{\bar{\xi}}_i^* \equiv \frac{1}{\sqrt{2}}(\hat{\bar{c}}_{q_i} + i\hat{\bar{c}}_{p_i}).
\end{aligned}
\tag{5.33}
$$

From (1.18) it is easy to work out the graded commutators among the new variables (5.33). In particular we will be interested in the following ones:

$$
\begin{aligned}
&[\hat{\xi}^i, \hat{\bar{\xi}}_j] = -\delta^i_j, \quad [\hat{\xi}^i, \hat{\bar{\xi}}_j^*] = 0,\\
&[\hat{\xi}^{i*}, \hat{\bar{\xi}}_j^*] = +\delta^i_j, \quad [\hat{\xi}^{i*}, \hat{\bar{\xi}}_j] = 0.
\end{aligned}
\tag{5.34}
$$

Under the symplectic Hermitian conjugation (2.22), we get

$$
\hat{\xi}^{i\dagger} = \hat{\bar{\xi}}_i, \quad \hat{\xi}^{i*\dagger} = \hat{\bar{\xi}}_i^*. \tag{5.35}
$$

Note that this ''Hermiticity'' properties for the Grassmann variables $(\hat{\xi}, \hat{\xi}^*), (\hat{\bar{\xi}}, \hat{\bar{\xi}}^*)$ are the same as the SvH one (2.8) for the variables $\hat{c}^a, \hat{\bar{c}}_a$. The crucial difference is in the anticommutator

$$
[\hat{\xi}^i, \hat{\bar{\xi}}_j] = -\delta^i_j \tag{5.36}
$$

which, for the analog SvH variables, had the opposite sign on the RHS: $[\hat{c}^{q_i},\hat{\bar{c}}_{q_j}]=\delta^i_j$. We shall show that it is just this difference in sign which gives rise to negative norm states in the symplectic case. Let us define in the case $n=1$ the state:

$$\hat{\xi}|0-,0-\rangle=\hat{\xi}^*|0-,0-\rangle=0. \tag{5.37}$$

Applying the other operators on $|0-,0-\rangle$ we easily obtain the other basic states of the theory:

$$\begin{aligned}
|0+,0-\rangle &\equiv \hat{\bar{\xi}}|0-,0-\rangle,\\
|0-,0+\rangle &\equiv -\hat{\bar{\xi}}^*|0-,0-\rangle,\\
|0+,0+\rangle &\equiv \hat{\bar{\xi}}^*\hat{\bar{\xi}}|0-,0-\rangle.
\end{aligned} \tag{5.38}$$

These states $|0\pm,0\pm\rangle$ are different from those defined in (4.2) via the operators $\hat{c}$ and $\hat{\bar{c}}$ because they are eigenstates of different operators. Besides the Hermiticity conditions, let us choose, as usual, a normalization for one of the states $|0\pm,0\pm\rangle$. In particular let us impose

$$(|0-,0-\rangle,|0-,0-\rangle)=-1. \tag{5.39}$$

Via the definitions (5.38) and the commutation relations (5.34), we can easily obtain[12] the following normalization conditions for the other states:

$$\begin{aligned}
(|0+,0-\rangle,|0+,0-\rangle)&=1,\\
(|0-,0+\rangle,|0-,0+\rangle)&=-1,\\
(|0+,0+\rangle,|0+,0+\rangle)&=1.
\end{aligned} \tag{5.40}$$

From the definition (5.38) we could ''represent'' the states as follows:

$$\begin{aligned}
|0-,0-\rangle&=\xi\xi^*, \quad |0-,0+\rangle=\xi,\\
|0+,0-\rangle&=\xi^*, \quad |0+,0+\rangle=1.
\end{aligned} \tag{5.41}$$

From this ''representation'' one sees that $|0+,0+\rangle$ is the basis of the zero-forms. This explains the reason for the normalization (5.39) that we choose. In this way the normalization of $|0+,0+\rangle$ turns out to be $+1$ and, as a consequence, the zero-form states have positive norm as in the KvN case. According to (5.41) the scalar products (5.39) and (5.40) can be written as

$$\begin{aligned}
(\xi\xi^*,\xi\xi^*)&=-1, \quad (\xi,\xi)=-1,\\
(\xi^*,\xi^*)&=1, \quad (1,1)=1,
\end{aligned} \tag{5.42}$$

and so a generic state

$$\psi(\xi,\xi^*)=\psi_0+\psi_\xi\xi+\psi_{\xi^*}\xi^*+\psi_2\xi\xi^* \tag{5.43}$$

has the following norm:

$$\langle\psi|\psi\rangle=|\psi_0|^2-|\psi_\xi|^2+|\psi_{\xi^*}|^2-|\psi_2|^2. \tag{5.44}$$

We will now generalize our treatment to the case of $n=2$. If we still want that $|0+0+0+0+\rangle$ be the basis of the zero-forms and have positive norm like in the KvN case, then we should not choose the analog of the normalization (5.39) but rather

$$(|0-0-0-0-\rangle,|0-0-0-0-\rangle)=1. \tag{5.45}$$

With this choice it is easy to prove that we get

$$(|0+0+0+0+\rangle,|0+0+0+0+\rangle)=1 \tag{5.46}$$

and, as a consequence, the zero-forms have positive norm. In general, for n degrees of freedom, in order to have positive norm for the zero-forms we should make the following choice for the normalization of the state $|0-0-\cdots 0-0-\rangle$:

$$\langle 0-0-\cdots 0-0-|0-0-\cdots 0-0-\rangle=(-1)^n. \tag{5.47}$$

For more calculational details see Ref. 12. We have now all the ingredients to start looking for the physical states. From the norms in (5.42) we infer that in general a homogeneous form $\psi=(1/l!)\,\psi_{a_1a_2\cdots a_l}\xi^{a_1}\xi^{*a_2}\cdots\xi^{a_l}$ has positive norm if the number of ξ variables is odd. This rule holds not only for $n=1$ but also for higher n. For example, the "representation" of $|0-0-0-\cdots 0-\rangle$ in n dimensions is

$$|0-0-0-\cdots 0-\rangle=\xi^1\xi^{1*}\xi^2\xi^{2*}\cdots\xi^n\xi^{n*} \tag{5.48}$$

and its norm is (5.47), i.e., $(-1)^n$, which is $+1$ if n (number of ξ contained) is even and -1 if n is odd. So we have a criterion to look for positive norm states: if a generic homogeneous state $(1/l!)\,\psi_{b_1b_2\cdots b_l}c^{b_1}c^{b_2}\cdots c^{b_l}$ is given, we first transform the c^b variables into ξ^i,ξ^{i*} variables via (5.33),

$$\frac{1}{l!}\psi_{b_1b_2\cdots b_l}c^{b_1}c^{b_2}\cdots c^{b_l}\ \Rightarrow\ \frac{1}{l!}\tilde{\psi}_{i_1i_2\cdots}\xi^{i_1}\xi^{i_2^*}\cdots \tag{5.49}$$

and then we count the number of ξ: if they are even, the state has positive norm; if they are odd, the state has negative norm. Of course this is a *sufficient and necessary* condition for homogeneous states but not for *nonhomogeneous* ones. For example, the state

$$\psi=\frac{1}{2!}\psi_{ab}(\varphi)\xi^a\xi^b+\psi_a(\varphi)\xi^a \tag{5.50}$$

is made of two parts, a two-form $\psi_{ab}\xi^a\xi^b$, and a one-form $\psi_a\xi^a$. From what we said above the two-form has positive norm because it contains two ξ, while the one-form has a negative one. Still the overall norm

$$\langle\psi|\psi\rangle=\sum_{a<b}\int \mathrm{d}\varphi|\psi_{ab}(\varphi)|^2-\sum_a\int \mathrm{d}\varphi|\psi_a(\varphi)|^2 \tag{5.51}$$

could not be positive. Indeed this is the statement that the subspace $\mathbf{H}^{(+)}$ of $\mathbf{H}$ is not a vector space. In fact in the example (5.50) we have summed a vector of $\mathbf{H}^{(+)}$ with one of $\mathbf{H}^{(-)}$ and ended up in a vector of $\mathbf{H}^{(+)}$. Anyhow it is possible to find a subspace of $\mathbf{H}^{(+)}$ which is a vector space.

Let us stick to the *homogeneous* positive forms and let us check what happens under time evolution. First we rewrite the Hamiltonian $\tilde{\mathcal{H}}$ in terms of the new variables (5.33) as

$$\tilde{\mathcal{H}}=i\partial_aH\hat{l}_a-i\overline{\partial}_aH\hat{\bar{l}}_a+(\hat{\xi}^k\hat{\bar{\xi}}_a+\hat{\xi}^{a*}\hat{\bar{\xi}}_k^*)\partial_k\overline{\partial}_aH+\hat{\xi}^{a*}\hat{\bar{\xi}}_k\overline{\partial}_a\overline{\partial}_kH+\hat{\xi}^a\hat{\bar{\xi}}_k^*\partial_a\partial_kH, \tag{5.52}$$

where $\overline{\partial_i}=\partial/\partial\overline{z_i}$ and $\partial_i=\partial/\partial z_i$. If we now take a generic homogeneous state of positive norm, i.e., with an even number of ξ,

$$\psi = \frac{1}{q!}\psi_{i_1 i_2 \cdots i_q}\xi^{i_1}\xi^{i_2 *}\cdots\xi^{i_q}, \tag{5.53}$$

in general the time evolution will turn it into a positive norm state because $\tilde{\mathcal{H}}$ is Hermitian and the evolution is unitary. Nevertheless the final state will be the sum of two terms, the first with an even number of ξ and the second with an odd number. In fact the last two terms in (5.52) change the number of ξ and ξ^* factors in the state (5.53). For example, the first of these two terms removes a ξ from (5.53) and injects a ξ^* into it. So the resulting state is an *inhomogeneous* form in ξ. This is not surprising because, even if $\tilde{\mathcal{H}}$ conserves the form number in c^a, it does not conserve the form number in ξ^i and ξ^{i*} separately. If we want a vector space of positive norm states closed under time evolution we have to restrict the space of homogeneous positive norm states to those which are annihilated by the last two terms of (5.52). In this way the time evolution will occur only via the first four terms of (5.52) which will not modify the number of ξ and ξ^* contained in the state. It is easy to check[12] that the states of the form:

$$\psi_{\text{phys}} \equiv \psi_0(\varphi) + B(\varphi)\sum_{i,j}\xi^i\xi^{i*}\xi^j\xi^{j*} + C(\varphi)\sum_{i,j,k,l}\xi^i\xi^{i*}\xi^j\xi^{j*}\xi^k\xi^{k*}\xi^l\xi^{l*} + \cdots \tag{5.54}$$

are annihilated by the last two terms of $\tilde{\mathcal{H}}$. The features of these states are

(1) each homogeneous form contained in them is made of products of an even number of ξ^i and ξ^{i*};
(2) all indices are summed over;
(3) in the homogeneous forms each term has the same coefficient: in our example $B(\varphi)$ is the coefficient of the four-form, $C(\varphi)$ is the coefficient of the eight-form.

The states (5.54) have positive norm because they are the sum of orthogonal positive norm states. Moreover the time evolution turns them in states with the same features because the last two terms in $\tilde{\mathcal{H}}$, which could break the pairing $\xi^i\xi^{i*}$, give zero on states of the form (5.54). So this family of states is closed under time evolution. Last but not least, differently than generic positive norm states, those of the form (5.54) make *a vector space*: the sum of two forms with arbitrary coefficients is still a form which has the properties (1), (2), (3) which define this family. So these states have all the features to be physical states: they have positive norm, they are closed under time evolution and they make a vector space. While it is easy to prove[12] that the states (5.54) are annihilated by the last two terms in $\tilde{\mathcal{H}}$, it is a little bit more tricky to prove the vice versa that means to show that a generic (at least homogeneous) state annihilated by the last two terms in $\tilde{\mathcal{H}}$ has the form (5.54). A proof for the two- and four-forms is provided in Appendix A. Hoping to have convinced the reader of this let us now note that not only the last two terms of $\tilde{\mathcal{H}}$, but also the previous two containing second derivatives of H, annihilate the states (5.54):

$$[(\hat{\xi}^k\hat{\bar{\xi}}_a + \hat{\xi}^{a*}\hat{\bar{\xi}}^*_k)\partial_k\overline{\partial}_a H]\psi_{\text{phys}} = 0. \tag{5.55}$$

The four terms containing second derivatives of H are what we called $\tilde{\mathcal{H}}_{\text{ferm}}$ in the first part of this section. So (5.55) implies that

$$\tilde{\mathcal{H}}_{\text{ferm}}\psi_{\text{phys}} = 0. \tag{5.56}$$

This feature is preserved under time evolution because $[\tilde{\mathcal{H}}, \tilde{\mathcal{H}}_{\text{ferm}}]\psi_{\text{phys}} = 0$. Note that (5.56) is the same equation we obtained in the SvH case (5.21). Therefore also for the states (5.54) there is no evolution of the Grassmann variables. Only $\tilde{\mathcal{H}}_{\text{bos}}$ evolves the states acting on the coefficients $\psi_0(\varphi), B(\varphi), C(\varphi)$ just like the Liouvillian on the zero-forms. In this sense also the symplectic physical states, like the SvH ones, are ''isomorphic'' to a set of zero-forms. Nevertheless the SvH

physical states are many more than the symplectic physical ones. In fact if we take, for example, a four-form in (5.54), by turning the ξ^i, ξ^{i*} into c^{q_i}, c^{p_i} variables via (5.33), we get

$$A(z,\overline{z})\xi^i\xi^{i*}\xi^j\xi^{j*} = \frac{\tilde{A}(\varphi)}{4}[(c^{q_i}+ic^{p_i})(c^{q_i}-ic^{p_i})(c^{q_j}+ic^{p_j})(c^{q_j}-ic^{p_j})]$$

$$= \frac{\tilde{A}(\varphi)}{4}2ic^{p_i}c^{q_i}c^{p_j}c^{q_j}2i = -\tilde{A}(\varphi)c^{p_i}c^{q_i}c^{p_j}c^{q_j} \tag{5.57}$$

and this is a physical four-form also in the SvH case. But if we take a six-form an analogous calculation gives

$$A(z,\overline{z})\ \xi^i\xi^{i*}\xi^j\xi^{j*}\xi^k\xi^{k*} = -i\tilde{A}(\varphi)\ c^{p_i}c^{q_i}c^{p_j}c^{q_j}c^{p_k}c^{q_k}. \tag{5.58}$$

A six-form like this is physical in the SvH case because it is annihilated by $\tilde{\mathcal{H}}_{\text{ferm}}$ and so $\tilde{\mathcal{H}}$ is Hermitian on it. Nevertheless in the symplectic case it cannot be a physical form since it has negative norm because it contains an odd number of ξ. So the class of physical states is wider in the SvH case than in the symplectic one.

C. Connection between symplectic and gauge case

What about the gauge scalar product? Actually we are less interested in it because the zero-forms have zero norm violating in this way the main feature of the KvN scalar product which we wanted to maintain. Nevertheless in order to find the physical Hilbert space also in this case the way to proceed is the following. Let us define the new Grassmann variables:

$$\hat{\psi}^a \equiv \frac{\hat{c}^a + i\omega^{ab}\hat{\bar{c}}_b}{\sqrt{2}},$$

$$\hat{\bar{\psi}}_a \equiv \frac{\hat{\bar{c}}_a + i\omega_{ab}\hat{c}^b}{\sqrt{2}}. \tag{5.59}$$

Using the symplectic hermiticity conditions (2.22) for the variables $(\hat{c}^a, \hat{\bar{c}}_a)$, we get that

$$\hat{\psi}^{a\dagger} = \hat{\psi}^a, \quad \hat{\bar{\psi}}_a^\dagger = \hat{\bar{\psi}}_a \tag{5.60}$$

which means that $\hat{\psi}^a$ and $\hat{\bar{\psi}}_a$ are Hermitian like the Grassmann variables in the *gauge scalar product* (2.17). This is an interesting connection between the symplectic and the gauge scalar product which can be used to find the physical subspace. In fact it is easy to prove that the anticommutation relations among $(\hat{\psi}^a, \hat{\bar{\psi}}_a)$ are the same as the ones among the variables $\hat{c}^a$:

$$[\hat{\psi}^a, \hat{\bar{\psi}}_b] = \delta^a_b, \quad [\hat{\psi}^a, \hat{\psi}^b] = 0, \quad [\hat{\bar{\psi}}_a, \hat{\bar{\psi}}_b] = 0. \tag{5.61}$$

Furthermore the inverse transformations of (5.59) are

$$\hat{c}^a = \frac{\hat{\psi}^a - i\omega^{ab}\hat{\bar{\psi}}_b}{\sqrt{2}},$$

$$\hat{\bar{c}}_a = \frac{\hat{\bar{\psi}}_a - i\omega_{ab}\hat{\psi}^b}{\sqrt{2}}. \tag{5.62}$$

Having proved all this we can introduce, as in (5.33), the Grassmann variables

$$\hat{\xi}^i=\frac{1}{\sqrt{2}}(\hat{c}^{q_i}+i\hat{c}^{p_i})=\frac{1}{2}(\hat{\psi}^{q_i}+i\hat{\psi}^{p_i}-i\hat{\bar{\psi}}_{p_i}-\hat{\bar{\psi}}_{q_i}),$$

$$\hat{\xi}^i*=\frac{1}{\sqrt{2}}(\hat{c}^{q_i}-i\hat{c}^{p_i})=\frac{1}{2}(\hat{\psi}^{q_i}-i\hat{\psi}^{p_i}-i\hat{\bar{\psi}}_{p_i}+\hat{\bar{\psi}}_{q_i}),$$

$$\hat{\bar{\xi}}_i=\frac{1}{\sqrt{2}}(-\hat{\bar{c}}_{q_i}+i\hat{\bar{c}}_{p_i})=\frac{1}{2}(-\hat{\bar{\psi}}_{q_i}-i\hat{\psi}^{p_i}+i\hat{\bar{\psi}}_{p_i}+\hat{\psi}^{q_i}), \tag{5.63}$$

$$\hat{\bar{\xi}}_i*=\frac{1}{\sqrt{2}}(\hat{\bar{c}}_{q_i}+i\hat{\bar{c}}_{p_i})=\frac{1}{2}(\hat{\bar{\psi}}_{q_i}+i\hat{\psi}^{p_i}+i\hat{\bar{\psi}}_{p_i}+\hat{\psi}^{q_i}).$$

It is easy to realize that, if $\hat{\psi}$ and $\hat{\bar{\psi}}$ satisfy the algebra and the anticommutation relations of the gauge scalar product, then the set of operators $\hat{\xi},\hat{\xi}*,\hat{\bar{\xi}},\hat{\bar{\xi}}*$ satisfy exactly (5.34) and (5.35). Therefore, even starting from the gauge scalar product, we can repeat the same kind of considerations made in the symplectic case in order to find out which is the subset of physical states.

VI. CONCLUSIONS

Despite the detailed mathematical analysis contained in this paper, the reader may still be puzzled by the results we have gotten. In fact it is difficult to accept that in classical mechanics, for a *generic potential*, we cannot have at the same time a positive definite scalar product and a unitary evolution in the space of forms. In this section we would like to give some tentative physical explanations[15] of this result.

Let us for example analyze chaotic systems that are, loosely speaking, those which have trajectories which fly away exponentially as time passes by. The variables which describe this behavior better are the so-called Jacobi fields which are defined as

$$\delta\varphi^a(t,\varphi_0)=\varphi_2^a(t,\varphi_0+\delta\varphi_0)-\varphi_1^a(t,\varphi_0), \tag{6.1}$$

where $\varphi_1^a(t)$ and $\varphi_2^a(t)$ are the two trajectories which start at time $t=0$ very close to each other, respectively, in φ_0 and $\varphi_0+\delta\varphi_0$. We should notice that the evolution of the Jacobi fields $\delta\varphi^a$ is the same as that of the Grassmann variables c^a:

$$\left[\delta_b^a\partial_t-\omega^{al}\frac{\partial^2 H}{\partial\varphi^l\partial\varphi^b}\right]\delta\varphi^b=0. \tag{6.2}$$

The Euclidean square distance between the two trajectories in phase space is given by

$$D(\varphi_0,t)\equiv\|\delta\varphi^a\|^2 \tag{6.3}$$

and it is a function of t and φ_0. In more precise mathematical terms chaotic systems are defined as those for which the following inequality holds:

$$\lim_{t\to\infty}\frac{1}{t}\ln\int \mathrm{d}^{2n}\varphi_0\, D(\varphi_0,t)>0. \tag{6.4}$$

One immediately infers from (6.4) that the phase space of chaotic systems has regions of nonzero measure such that the trajectories which originate from there fly away exponentially as time passes by.

In Appendix B we will show that, in those regions, also the components $\psi_q(\varphi_0)$, $\psi_p(\varphi_0)$ of any one-form $\psi=\psi_a c^a$ behave as the Jacobi fields. So the norm of these states in the SvH scalar product

$$\int \mathrm{d}^{2n}\varphi_0 \sum_a |\psi_a(\varphi_0,t)|^2 \tag{6.5}$$

diverges exponentially, analogously to (6.4). Let us now take the sum of a zero-form ψ_0 and of a one-form $\psi=\psi_a c^a$,

$$\tilde{\psi}\equiv\psi_0+\psi_a c^a. \tag{6.6}$$

The SvH norm of $\tilde{\psi}$ is

$$\|\tilde{\psi}\|^2=\int \mathrm{d}^{2n}\varphi_0|\psi_0(\varphi_0,t)|^2+\int \mathrm{d}^{2n}\varphi_0\sum_a |\psi_a(\varphi_0,t)|^2. \tag{6.7}$$

Let us now suppose that in the SvH scalar product the $\tilde{\mathcal{H}}$ were Hermitian. If so then the norm of $\tilde{\psi}$ would be conserved under the time evolution. Anyhow we also know that the second piece in (6.7) that is $\int \mathrm{d}^{2n}\varphi_0\Sigma_a|\psi_a|^2$ increases for chaotic systems and this implies, for $\|\tilde{\psi}\|^2$ to be conserved, that the first term $\int \mathrm{d}^{2n}\varphi_0|\psi_0|^2$ in (6.7) cannot be conserved. The nonconservation of this last piece implies a violation of the Liouville theorem. To put things in simpler terms: if we have chaotic systems, i.e., exponential behavior, we must be able to produce, from the operator of evolution $e^{-i\tilde{\mathcal{H}}t}$, an exponential diverging behavior:

$$e^{-i\tilde{\mathcal{H}}t}\rightarrow Ke^{+Lt} \tag{6.8}$$

with L a real number. This happens only if $\tilde{\mathcal{H}}$ is not Hermitian and has, as a consequence, complex eigenvalues which would produce something like (6.8). This same kind of behavior can be produced in the gauge and symplectic case. There $\tilde{\mathcal{H}}$ is Hermitian but the scalar product is not positive definite. In this case even Hermitian operators can have complex eigenvalues and the proof goes as follows. Let us start from the Hermiticity of $\tilde{\mathcal{H}}$, i.e.,

$$\langle\psi|\tilde{\mathcal{H}}\psi\rangle=\langle\tilde{\mathcal{H}}\psi|\psi\rangle, \tag{6.9}$$

where $|\psi\rangle$ is an eigenstate of ψ with eigenvalue λ; then (6.9) can be written as

$$\lambda\langle\psi|\psi\rangle=\lambda^*\langle\psi|\psi\rangle. \tag{6.10}$$

From this relation we cannot deduce that $\lambda=\lambda^*$ because, in a nonpositive definite scalar product, the state $|\psi\rangle$ could be of zero norm and satisfy (6.10) whatever is the value, real or complex, of λ.

This analysis explains why for a *generic potential*, as we have assumed throughout this paper, we have either positive definite Hilbert space or $\tilde{\mathcal{H}}$ Hermitian but never both of them. This last possibility can take place only for *specific potentials*. For example, in the SvH case it can happen for Hamiltonians of the form

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}q^2 \tag{6.11}$$

for which $\tilde{\mathcal{H}}$ is Hermitian [see Eqs. (2.11) and (2.12)]. As this is a harmonic oscillator the reader may be tempted to generalize the result and jump to the conclusion that, differently than chaotic systems, for integrable ones we could have both $\tilde{\mathcal{H}}$ Hermitian and the scalar product positive

definite. It is actually not so: even among harmonic oscillators only some of them have the features above as explained in Appendix C. In the same appendix we prove that the Hermiticity condition of $\mathcal{H}$ is invariant under canonical transformations.

The reader may wonder if all this formalism with Hilbert spaces and scalar products is actually needed to study dynamical systems. After all, he may argue, the old fashioned Hamiltonian formalism was enough and no scalar product appears there. This is actually not so. In fact, to study the ergodic/chaotic properties of a system in the standard Hamiltonian formalism one has to introduce by hand the Jacobi fields, like infinitesimal differences of canonical variables, and define their *length* in order to get the Lyapunov exponents; so a scalar product, to get the length above, somehow would enter also in the standard Hamiltonian approach. In our formalism instead we have automatically the Jacobi fields since they are related to the Grassmann variables and, having a Hilbert space, the introduction of a scalar product is much more explicit than in the standard Hamiltonian formalism. So the reader can see that the two approaches, the Hamiltonian and the KvN one, are equivalent because even in the first case one has to introduce a scalar product. Moreover via our formalism we have an interesting manner to connect the Lyapunov exponents to well-defined mathematical structures like the spectral properties of a certain operator.[9] As we said in the Introduction in order to study the spectral properties of an operator it is crucial to know which are the features of the Hilbert space on which this operator acts. In particular it is important to know which is the scalar product one uses, the Hermiticity character of the Hamiltonian and all that. In Ref. 9 the *connection* between Lyapunov exponents and spectral properties of the Lie derivative had been studied but at a rather *formal* level using the path integral formalism. We felt it would be important to check the *connection* above at a more *rigorous* level using the operatorial formalism. What we have done in this paper is to prepare the mathematical ground for that analysis which will be carried on in later papers. Clearly all the work contained here is of a pure *mathematical* nature but we feel that, combined with the physics studied in Ref. 9, it could lead to further physical understanding of dynamical systems and of chaotic ones in particular. Moreover, the *mathematical* machinery prepared in this paper has brought to light some unexpected phenomena, like the non-Hermiticity of $\tilde{\mathcal{H}}$ for some systems. This, we feel, is already a rather interesting result which fully justifies the detailed mathematics presented here.

This concludes this paper. In a second paper[16] we will analyze the same issues by using an entirely bosonic $\tilde{\mathcal{H}}$ first introduced in Ref. 17. In the same paper we shall also analyze what happens when we change representations for the Grassmann variables.[18]

APPENDIX A

In this appendix we will show that homogeneous forms in ξ, in order to be annihilated by the last two pieces of $\tilde{\mathcal{H}}$, must have the form that the homogeneous terms in (5.54) have. The $\tilde{\mathcal{H}}$ in terms of $\xi, \overline{\xi}$ is given in (5.52) and the condition that a state $|\psi\rangle$ is annihilated by the last two pieces of $\tilde{\mathcal{H}}$ is

$$(\hat{\xi}^a * \hat{\bar{\xi}}_k \overline{\partial}_a \overline{\partial}_k H + \hat{\xi}^a \hat{\bar{\xi}}_k^* \partial_a \partial_k H)|\psi\rangle = 0. \tag{A1}$$

If we want this relation to hold for any form of H then each piece separately in (A1) must annihilate $|\psi\rangle$ because in the first piece we have only $\overline{\partial}$-derivatives on H and on the other only ∂-derivatives, so

$$\hat{\xi}^a * \hat{\bar{\xi}}_k \overline{\partial}_a \overline{\partial}_k H|\psi\rangle = 0, \tag{A2}$$

$$\hat{\xi}^a \hat{\bar{\xi}}_k^* \partial_a \partial_k H|\psi\rangle = 0. \tag{A3}$$

Let us choose, for simplicity, a generic state with two ξ,

$$|\psi\rangle = \xi^i \xi^j A_{ij} \tag{A4}$$

with A_{ij} antisymmetric because of the Grassmannian nature of the ξ. Inserting (A4) in (A2) we get

$$\hat{\xi}^a * \hat{\bar{\xi}}_k \bar{\partial}_a \bar{\partial}_k H|\psi\rangle = -2\xi^a * (\bar{\xi}^j A_{kj}) \bar{\partial}_a \bar{\partial}_k H. \tag{A5}$$

For the RHS of (A5) to be zero for a generic H the only way is that its coefficient $\xi^a * (\bar{\xi}^j A_{kj})$ be antisymmetric in a and k. This can happen only if A_{kj} has the form

$$A_{kj} = \xi^k * B_j \tag{A6}$$

but let us remember that A_{kj} must be antisymmetric in k,j and so B_j can only be of the form

$$B_j = \bar{\xi}^j * B(\varphi). \tag{A7}$$

So the state $|\psi\rangle$ must have the form

$$|\psi\rangle = \xi^i \bar{\xi}^j A_{ij} = \xi^i \bar{\xi}^j \xi^i * \bar{\xi}^j * B(\varphi). \tag{A8}$$

This state satisfies also (A3) and note that (A8) has exactly the form of the first homogeneous term contained in (5.54).

The same kind of proof we can do for a generic state containing four ξ like

$$|\psi\rangle = \xi^i \bar{\xi}^j \xi^z \bar{\xi}^w A_{ijzw}. \tag{A9}$$

The function A_{ijzw} must be antisymmetric in all indices. Inserting (A9) in (A2) we get that $-4\xi^a * \bar{\xi}^j \xi^z \bar{\xi}^w A_{kjzw}$ must be antisymmetric in a,k in order for (A2) to hold for any H. The only way out is that A_{kjzw} be of the form

$$A_{kjzw} = \xi^k * B_{jzw}. \tag{A10}$$

As A_{kjzw} must be totally antisymmetric in the indices the only solution is that $B_{jzw} = \bar{\xi}^j * \xi^z * \bar{\xi}^w * C(\varphi)$. This makes (A9) of the form

$$|\psi\rangle = \xi^i \bar{\xi}^j \xi^z \bar{\xi}^w \xi^i * \bar{\xi}^j * \xi^z * \bar{\xi}^w * C(\varphi), \tag{A11}$$

which is exactly the form of the second term in (5.54). We can proceed in this manner for all higher terms. We think this is an acceptable proof of the fact that the states (5.54) are the only ones annihilated by the last two terms of $\tilde{\mathcal{H}}$. The only criticism could come from the fact that in this proof we started from homogeneous wave functions and not inhomogeneous ones. The point is that, even considering sums of forms with a different number of ξ, $\tilde{\mathcal{H}}$ could annihilate them only if it annihilates every single term of the sum. There cannot be a compensation between terms coming from forms with a different number of ξ and the reason of this is simple: let us suppose we take the sum of a first form with a number l of variables ξ and a second form with a number $l+2$ of variables ξ. Then the term of $\tilde{\mathcal{H}}$ proportional to $\bar{\partial}_a \bar{\partial}_b H$ decreases the number of ξ of the second form producing a term with a number $l+1$ of ξ. Another term with a number $l+1$ of ξ is obtained by applying the term proportional to $\partial_a \partial_b H$ on the first form. It is clear that a compensation between these terms can occur but it will be strictly dependent on the *particular form* of the Hamiltonian H and this is not what we want.

APPENDIX B

In this appendix we show that for those systems (the chaotic ones) where the Jacobi fields (6.1) diverge exponentially with time, the same happens with the components ψ_a of the one-forms $\psi = \psi_a c^a$. Let us first change representation, that means let us turn to a ''momentum'' representation for the Grassmann variables using $\bar{c}$ in place of c. While in the SvH representation that we have been using so far the notation (4.8) was

$$\langle +c^{p}*, +c^{q}*|\psi\rangle = \psi_0 + \psi_q c^q + \psi_p c^p + \psi_2 c^q c^p \tag{B1}$$

it is now natural to use the following other notation for the $\overline{c}$ representation:

$$\langle -\overline{c}^{*}_{p}, -\overline{c}^{*}_{q}|\psi\rangle = \psi^0 + \psi^q \overline{c}_q + \psi^p \overline{c}_p + \psi^2 \overline{c}_q \overline{c}_p . \tag{B2}$$

In this basis a completeness relation, analog to the first one of (4.6), is then

$$\int \mathrm{d}\overline{c}_q \, \mathrm{d}\overline{c}_p |\overline{c}_q +, \overline{c}_p +\rangle\langle -\overline{c}^{*}_{p}, -\overline{c}^{*}_{q}| = \mathbb{I} \tag{B3}$$

and inserting it into the LHS of (B1) we get the relation between (B1) and (B2), i.e.,

$$\begin{aligned}\langle +c^{p}*, +c^{q}*|\psi\rangle &= \int \mathrm{d}\overline{c}_q \, \mathrm{d}\overline{c}_p \langle +c^{p}*, +c^{q}*|\overline{c}_q +, \overline{c}_p +\rangle \cdot \langle -\overline{c}^{*}_{p}, -\overline{c}^{*}_{q}|\psi\rangle \\ &= \int \mathrm{d}\overline{c}_q \, \mathrm{d}\overline{c}_p (1 + c^q \overline{c}_q + c^p \overline{c}_p - c^q c^p \overline{c}_q \overline{c}_p) \cdot (\psi^0 + \psi^q \overline{c}_q + \psi^p \overline{c}_p + \psi^2 \overline{c}_q \overline{c}_p) \\ &= -\psi^2 - \psi^p c^q + \psi^q c^p + \psi^0 c^q c^p . \end{aligned} \tag{B4}$$

Comparing this with the RHS of (B1) we get that

$$\begin{aligned}\psi_0 &= -\psi^2, \\ \psi_q &= -\psi^p, \\ \psi_p &= \psi^q, \\ \psi_2 &= \psi^0 . \end{aligned} \tag{B5}$$

The reason we have introduced the $\overline{c}$ representation is because, as we will show below, the components ψ^q and ψ^p transform, under time evolution, as the Jacobi fields $\delta q, \delta p$ of (6.1). The evolution of the wave functions (B2) is given by the Hamiltonian $\tilde{\mathcal{H}}$ expressed in the ''momentum'' representation. The fermionic part of $\tilde{\mathcal{H}}_{\mathrm{ferm}}$ is

$$\tilde{\mathcal{H}}_{\mathrm{ferm}} = i\overline{c}_a \omega^{ab} \partial_b \partial_{\mathrm{d}} H c^{\mathrm{d}} = i\overline{c}_a \mathcal{F}^a_{\mathrm{d}} c^{\mathrm{d}}, \tag{B6}$$

where $\mathcal{F}^a_{\mathrm{d}} = \omega^{ab} \partial_b \partial_{\mathrm{d}} H$ and its operatorial counterpart is

$$\tilde{\mathcal{H}}_{\mathrm{ferm}} = i\overline{c}_a \mathcal{F}^a_{\mathrm{d}} \frac{\partial}{\partial \overline{c}_{\mathrm{d}}} . \tag{B7}$$

The infinitesimal evolution will give

$$\psi^a(\epsilon)\overline{c}_a(\epsilon) = e^{-i\tilde{\mathcal{H}}\epsilon}(\psi^a(0)\overline{c}_a(0)), \tag{B8}$$

where we have restricted ourselves to the part of the wave functions (B2) linear in the $\overline{c}$ variables. Inserting (B7) into (B8) we get

$$\psi^a(\epsilon)\overline{c}_a(\epsilon) = \left(1 + \epsilon \overline{c}_b \mathcal{F}^b_{\mathrm{d}} \frac{\partial}{\partial \overline{c}_{\mathrm{d}}}\right) \psi^a(0)\overline{c}_a(0) = (\psi^a(0) + \epsilon \mathcal{F}^a_{\mathrm{d}} \psi^{\mathrm{d}}(0))\overline{c}_a(0). \tag{B9}$$

Expanding in ϵ also the LHS of (B9) and comparing terms of the first order in ϵ and proportional to $\overline{c}_a(0)$ we get

$$\psi^a(\epsilon)=\psi^a(0)+\epsilon\mathcal{F}^a_{\rm d}\psi^{\rm d}(0). \tag{B10}$$

If we now solve, for an infinitesimal time, the equation of motion of the Jacobi fields we get

$$\delta\varphi^a(\epsilon)=\delta\varphi^a(0)+\epsilon\mathcal{F}^a_{\rm d}\delta\varphi^{\rm d}(0). \tag{B11}$$

This proves that the variable ψ^a and the Jacobi fields $\delta\varphi^a$ evolve in the same way and if the latter diverge exponentially with t, the same happens to ψ^a. This implies that the behavior with t of the distance $D(\varphi_0,t)$ of (6.3) is the same as the one of $\Sigma_a|\psi_a(\varphi_0)|^2$. This also implies that, if (6.4) holds, also the following inequality holds:

$$\lim_{t\to\infty}\frac{1}{t}\ln\int {\rm d}^{2n}\varphi_0\sum_a |\psi^a(\varphi_0,t)|^2>0. \tag{B12}$$

Via then the relations (B5) we can replace (B12) with

$$\lim_{t\to\infty}\frac{1}{t}\ln\int {\rm d}^{2n}\varphi_0\sum_a |\psi_a(\varphi_0,t)|^2>0. \tag{B13}$$

Note that the argument of the logarithm is exactly the SvH norm of the one-form $\psi_a(\varphi_0,t)c^a$. We should point out that the previous reasoning is correct for those forms which have nonzero components along diverging Jacobi fields.

APPENDIX C

We noticed in Sec. VI that, with the choice

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}q^2, \tag{C1}$$

the Hamiltonian $\tilde{\mathcal{H}}$ is Hermitian in the SvH scalar product. Let us now insert the mass and frequency in H and see what happens,

$$H=\frac{1}{2m}p^2+\frac{1}{2}m\omega^2q^2. \tag{C2}$$

Now let us check if $\tilde{\mathcal{H}}$ is Hermitian under the SvH Hermiticity conditions

$$\begin{aligned}(\hat{c}^q)^\dagger&=\hat{\bar{c}}_q,\\ (\hat{c}^p)^\dagger&=\hat{\bar{c}}_p.\end{aligned} \tag{C3}$$

The only part of $\tilde{\mathcal{H}}$ which can encounter problems is $\tilde{\mathcal{H}}_{\rm ferm}$ which, with the Hamiltonian (C2), turns out to be

$$\tilde{\mathcal{H}}_{\rm ferm}=i\frac{\hat{\bar{c}}_q\hat{c}^p}{m}-i\hat{\bar{c}}_p\hat{c}^q m\omega^2. \tag{C4}$$

Its Hermitian conjugate, using (C3), is

$$\tilde{\mathcal{H}}^\dagger_{\rm ferm}=i\hat{\bar{c}}_q\hat{c}^p m\omega^2-i\frac{\hat{\bar{c}}_p\hat{c}^q}{m}. \tag{C5}$$

From (C4) and (C5) one sees that $\tilde{\mathcal{H}}_{\rm ferm}$ is Hermitian only if

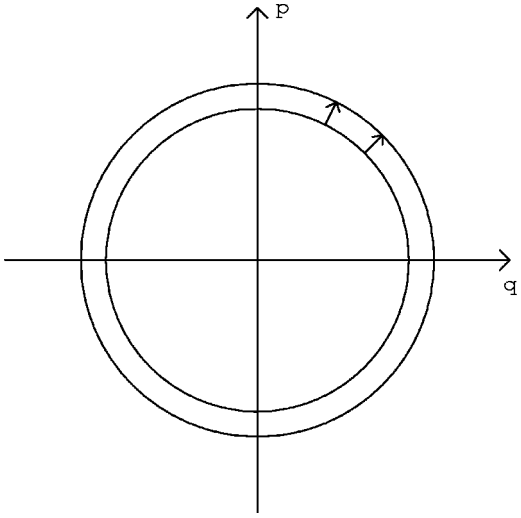

FIG. 1. Phase space trajectories for a harmonic oscillator with $1/\omega^2 = m^2$.

$$\frac{1}{\omega^2} = m^2. \tag{C6}$$

So, given the mass of the system, only those harmonic oscillators whose frequency is given by (C6) are Hermitian. It is easy to see that the oscillators for which relation (C6) holds are those whose trajectories in phase space are circles (see Fig. 1). Note that in this case the norm of the Jacobi fields, i.e., the arrows in Fig. 1, does not change with time that is what the Hermiticity of $\tilde{\mathcal{H}}$ under the SvH scalar product guarantees. In fact *if we use the SvH scalar product the norm of the Jacobi fields can be put in correspondence with the norm of one-forms as shown in Appendix B*. So, as the Hermiticity of $\tilde{\mathcal{H}}$ preserves the norm of the one-forms, the same happens for the norm of the Jacobi fields. In the case in which $1/\omega^2 \neq m^2$ the trajectories are ellipses (see Fig. 2). One sees from Fig. 2 that the norm of the Jacobi fields is not preserved during the time evolution and this is just a consequence of the non-Hermiticity of $\tilde{\mathcal{H}}$ under the SvH scalar product.

The careful reader may object to the previous argument that, even when $1/\omega^2 \neq m^2$, it is possible to perform the following canonical tranformation:

$$p = \sqrt{m\omega}\, p', \quad q = \frac{1}{\sqrt{m\omega}} q' \tag{C7}$$

in order to bring the Hamiltonian (C2) into the form

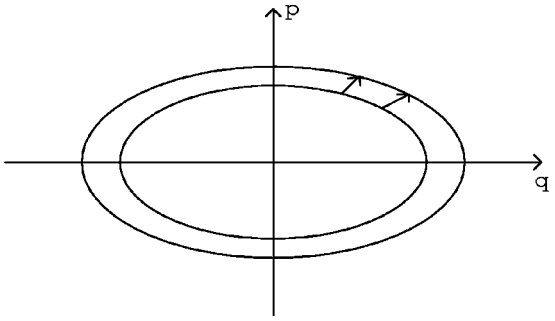

FIG. 2. Phase space trajectories for a harmonic oscillator with $1/\omega^2 \neq m^2$.

$$H(q,p)=\frac{1}{2m}p^2+\frac{1}{2}m\omega^2q^2\rightarrow H(q',p')=\frac{1}{2}\omega p'^2+\frac{1}{2}\omega q'^2. \tag{C8}$$

In the new phase space labeled by (q',p') the trajectories of the harmonic oscillator are given by circles and the associated $\tilde{\mathcal{H}}_{\text{ferm}}$ is

$$\tilde{\mathcal{H}}_{\text{ferm}}=i\omega\hat{\bar{c}}'_q\hat{c}'^p-i\omega\hat{\bar{c}}'_p\hat{c}'^q. \tag{C9}$$

What can we say about the Hermiticity of the operator $\tilde{\mathcal{H}}_{\text{ferm}}$? Before the canonical transformation (C7) the Hamiltonian $\tilde{\mathcal{H}}_{\text{ferm}}$ in (C5) was not Hermitian for $1/\omega^2\neq m^2$. Is this property preserved or not? To answer this question we must remember that under a canonical transformation, as well as under a generic diffeomorphism in phase space, the Grassmann variables of the theory must be tranformed like a basis of differential forms and vector fields respectively, see Eq. (5.7) of the second paper in Ref. 4:

$$c'^a=\frac{\partial\varphi'^a}{\partial\varphi^b}c^b,\quad \bar{c}'_a=\frac{\partial\varphi^b}{\partial\varphi'^a}\bar{c}_b\,. \tag{C10}$$

In our particular case the transformations on the Grassmann variables induced by (C7) are given by

$$\begin{aligned} c'^q&=\sqrt{m\omega}\,c^q,\quad c'^p=\frac{1}{\sqrt{m\omega}}c^p,\\ \bar{c}'_q&=\frac{1}{\sqrt{m\omega}}\bar{c}_q,\quad \bar{c}'_p=\sqrt{m\omega}\,\bar{c}_p\,. \end{aligned} \tag{C11}$$

To check the consistency of the formalism we can note that, by inserting the inverse of (C11) into (C4) one obtains just the Hamiltonian in the primed variables (C9). Furthermore the SvH scalar product (C3) in the primed variables becomes

$$\begin{aligned} (\hat{c}'^q)^\dagger&=m\omega\,\hat{\bar{c}}'_q,\\ (\hat{c}'^p)^\dagger&=\frac{1}{m\omega}\hat{\bar{c}}'_p\,. \end{aligned} \tag{C12}$$

Since we are interested in the case $m\omega\neq 1$ we have that, after the canonical transformation (C7)–(C11), the original SvH scalar product (C3) changed its explicit form. Under this scalar product (C12) the Hermitian conjugate of the Hamiltonian (C9) is

$$\tilde{\mathcal{H}}^\dagger_{\text{ferm}}=i\omega^3m^2\hat{\bar{c}}'_q\hat{c}'^p-\frac{i}{m^2\omega}\hat{\bar{c}}'_p\hat{c}'^q. \tag{C13}$$

From (C9) and (C13) one sees that the operator $\tilde{\mathcal{H}}_{\text{ferm}}$ is not Hermitian if $1/\omega^2\neq m^2$. Therefore the property of non-Hermiticity of $\tilde{\mathcal{H}}_{\text{ferm}}$ is preserved by the canonical transformation $(q,p,c^q,c^p)\rightarrow(q',p',c'^q,c'^p)$. [We want to stress that there exists a particular scalar product under which the Hamiltonian $\tilde{\mathcal{H}}_{\text{ferm}}$ of (C9) is Hermitian: it is the SvH scalar product in the primed variables $(\hat{c}'^a)^\dagger=\hat{\bar{c}}'_a$; anyway this scalar product is different from the SvH one in the unprimed variables (C3) that we originally imposed upon our Hilbert space. Once we fix a particular scalar product there exists only one particular harmonic oscillator whose Hamiltonian $\tilde{\mathcal{H}}_{\text{ferm}}$ is Hermitian.]

Vice versa, let us suppose we consider the oscillator $H=\frac{1}{2}q^2+\frac{1}{2}p^2$ whose associated $\tilde{\mathcal{H}}_{\text{ferm}}$ is Hermitian with the SvH scalar product (C3) and let us perform the following canonical transformation with $\alpha\neq 1$: $q=(1/\alpha)\,q'$, $p=\alpha\,p'$, which induces the following transformations on the c and $\overline{c}$:

$$c^q=\frac{1}{\alpha}c'^q, \qquad c^p=\alpha\,c'^p,$$
$$\overline{c}_q=\alpha\,\overline{c}'_q, \quad \overline{c}_p=\frac{1}{\alpha}\overline{c}'_p. \tag{C14}$$

Under these transformations the Hamiltonian H becomes

$$H(q',p')=\frac{1}{2\alpha^2}q'^2+\frac{1}{2}\alpha^2p'^2,$$

while the fermionic part of $\tilde{\mathcal{H}}$ turns out to be

$$\tilde{\mathcal{H}}_{\text{ferm}}=i\overline{c}'_qc'^p\alpha^2-i\overline{c}'_pc'^q\frac{1}{\alpha^2} \tag{C15}$$

and the scalar product (C3) becomes

$$(\hat{c}'^q)^\dagger=\alpha^2\,\hat{\bar{c}}'_q,$$
$$(\hat{c}'^p)^\dagger=\frac{1}{\alpha^2}\hat{\bar{c}}'_p. \tag{C16}$$

With this scalar product it is easy to prove that the Hamiltonian (C15) is still Hermitian and this confirms that the canonical transformations do not spoil the Hermiticity of the Hamiltonian $\tilde{\mathcal{H}}$. This proof can be extended to the most general canonical transformation. In fact in the primed variables given by (C10) the fermionic Hamiltonian associated to $H=\frac{1}{2}q^2+\frac{1}{2}p^2$ becomes

$$\tilde{\mathcal{H}}_{\text{ferm}}=i\frac{\partial\varphi'^b}{\partial q}\frac{\partial p}{\partial\varphi'^d}\hat{\bar{c}}'_b\hat{c}'^d-i\frac{\partial\varphi'^b}{\partial p}\frac{\partial q}{\partial\varphi'^d}\hat{\bar{c}}'_b\hat{c}'^d. \tag{C17}$$

The SvH scalar product, which gives $\hat{c}^{a\dagger}=\hat{\bar{c}}_a$, in the primed variables becomes

$$\delta^a_k(\hat{c}'^d)^\dagger=\frac{\partial\varphi'^b}{\partial\varphi^k}\frac{\partial\varphi'^d}{\partial\varphi^a}\hat{\bar{c}}'_b, \quad \delta^k_b(\hat{\bar{c}}'_d)^\dagger=\frac{\partial\varphi^k}{\partial\varphi'^d}\frac{\partial\varphi^b}{\partial\varphi'^f}\hat{c}'^f, \tag{C18}$$

and with this scalar product it is straightforward to prove that the Hamiltonian (C17) is still Hermitian. This implies that the Hermiticity of $\tilde{\mathcal{H}}$ is an intrinsic (i.e., canonical invariant) property of the system which can only change with the scalar product we choose.

Now the careful reader can ask: in the case described by (C15) the Hamiltonian of the system is Hermitian but the norm of the Jacobi fields is not conserved since the trajectories in the phase space labeled by (q',p') are ellipses. So in this case the Hermiticity of the Hamiltonian $\tilde{\mathcal{H}}$ cannot imply that the Jacobi fields are conserved in time. The reason is easily understood if we consider that the matrix g^{ij} which produces the scalar product (C16) in the primed variables is given by

$$g^{ij}=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \alpha^2 & 0 & 0\\ 0 & 0 & 1/\alpha^2 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}. \tag{C19}$$

Consequently the norm of the state $\psi=\psi_0+\psi_q c^{q\prime}+\psi_p c^{p\prime}$ is

$$\langle\psi|\psi\rangle=\int \mathrm{d}\varphi\left(|\psi_0(\varphi)|^2+\alpha^2|\psi_q(\varphi)|^2+\frac{1}{\alpha^2}|\psi_p(\varphi)|^2\right). \tag{C20}$$

Remember that the piece $\int \mathrm{d}\varphi|\psi_0(\varphi)|^2$ in (C20) is conserved because $\psi_0(\varphi)$ evolves with the Liouvillian which is a Hermitian operator. Therefore the Hermiticity of $\tilde{\mathcal{H}}_{\mathrm{ferm}}$ implies immediately that the leftover piece in (C20), which is

$$\int \mathrm{d}\varphi\left(\alpha^2|\psi_q(\varphi)|^2+\frac{1}{\alpha^2}|\psi_p(\varphi)|^2\right),$$

is conserved in time. But since $\alpha\neq 1$ this does not imply that the norm of the Jacobi fields is conserved. In fact the square of the length of the Jacobi field is given by $|\delta q|^2+|\delta p|^2$ and, according to what we proved in Appendix B, this quantity can be put in correspondence with $|\psi_q|^2+|\psi_p|^2$. Therefore the length of the Jacobi field can be associated with the contribution to the norm of ψ given by the one-form only if $\alpha=1$, i.e., only if we consider the SvH scalar product in the primed variables $\hat{c}^{\prime\,\dagger}=\hat{c}^{\prime}$. With all the other scalar products, including (C16) which is canonically "equivalent" to the original SvH one (C3), the Hermiticity of the Hamiltonian $\tilde{\mathcal{H}}$ does not imply that the length of the Jacobi fields is conserved. The same thing can be phrased as follows: if we want that the condition of Hermiticity/non-Hermiticity of $\tilde{\mathcal{H}}$ precisely signals the conservation/nonconservation of the length of the Jacobi fields, we must use always the SvH scalar product and not those canonically equivalent to it. So, for example, if we start with the SvH scalar product and those phase space coordinates in which the trajectories are ellipses, the $\tilde{\mathcal{H}}$ will not be Hermitian. The same feature will be inherited by the canonically transformed $\tilde{\mathcal{H}}$ in which the trajectories are circles but this feature (the non-Hermiticity) will appear only if we use the canonically transformed SvH scalar product. If we instead use the original SvH scalar product only the $\tilde{\mathcal{H}}$ of the circles in the original (unprimed) variables will be Hermitian.

To conclude this appendix we can note that the relation (C6) can be disrupted not only by a canonical transformation but also by changing the system of units which we use in measuring ω and m. But we should note that, if we change the units, we have to change also the Hermiticity conditions (C3) for dimensional reasons. Under the new Hermiticity conditions $\tilde{\mathcal{H}}$ is again Hermitian. The reason why, by changing the system of units, we have to change the Hermiticity conditions (C3) can be explained as follows. Looking at the Lagrangian (1.15) we notice that the kinetic term of the action is $\int \mathrm{d}t\,\overline{c}_q\dot{c}^q$ and so the dimension of c^q is the inverse of $\overline{c}_q$,

$$[c^q]=[\overline{c}_q]^{-1}. \tag{C21}$$

The same for the c^p,

$$[c^p]=[\overline{c}_p]^{-1}. \tag{C22}$$

From the interaction term $\int \mathrm{d}t\,\overline{c}_p\partial_q\partial_q H c^q$ of the action associated to the $\tilde{\mathcal{L}}$ of (1.15) we get that

$$[c^p]=\frac{M}{T}[c^q]. \tag{C23}$$

These are the dimensional relations among the Grassmann variables. So the Hermiticity conditions (C3) should be written as

$$(\hat{c}^q)^\dagger = \hat{\bar{c}}_q \cdot \mathbf{1}_q, \quad (\hat{c}^p)^\dagger = \hat{\bar{c}}_p \cdot \mathbf{1}_p, \tag{C24}$$

where $\mathbf{1}_q, \mathbf{1}_p$ are dimensionful quantities. Of course we could choose c^q to be dimensionless at all, and so $\mathbf{1}_q$ could be a number like 1. But if c^q is dimensionless then c^p, because of (C23), must have dimension. $\mathbf{1}_p$ would then have the dimension of $[c^p]^2$ and so it is a number which changes with the system of units. Let us, for example, choose the SI system of units and the Hermiticity conditions

$$\begin{aligned} (\hat{c}^q)^\dagger &= \hat{\bar{c}}_q, \\ (\hat{c}^p)^\dagger &= \hat{\bar{c}}_p. \end{aligned} \tag{C25}$$

The harmonic oscillators which are Hermitian are those for which

$$\begin{aligned} m &= \alpha \cdot Kg, \\ \omega &= \frac{1}{\alpha} sec^{-1}. \end{aligned} \tag{C26}$$

If we now pass to the CGS system the relation (C26) becomes

$$\begin{aligned} m &= \alpha \cdot 10^3 g, \\ \omega &= \frac{1}{\alpha} sec^{-1}, \end{aligned} \tag{C27}$$

and $m\omega = 10^3 \neq 1$. But the Hermiticity relations (C25), in the new units, become

$$\begin{aligned} (\hat{c}^q)^\dagger &= \hat{\bar{c}}_q, \\ (\hat{c}^p)^\dagger &= 10^6\, \hat{\bar{c}}_p, \end{aligned} \tag{C28}$$

and with these new Hermiticity conditions $\tilde{\mathcal{H}}$ is Hermitian even under the condition (C27).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Hilbert space structure in classical mechanics. II

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(Received 7 August 2002; accepted 29 August 2003)

In this paper we analyze two different functional formulations of classical mechanics. In the first one the Jacobi fields are represented by *bosonic* variables and belong to the vector (or its dual) representation of the symplectic group. In the second formulation the Jacobi fields are given as *condensates* of Grassmannian variables belonging to the spinor representation of the metaplectic group. For both formulations we shall show that, differently from what happens in the case presented in paper I, it is possible to endow the associated Hilbert space with a positive definite scalar product and to describe the dynamics via a Hermitian Hamiltonian. The drawback of this formulation is that higher forms do not appear automatically and that the description of chaotic systems may need a further extension of the Hilbert space. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623334]

I. INTRODUCTION

In a previous paper with the same title[1] we analyzed in detail the Hilbert space structure associated to the *standard* path integral formulation[2] of classical mechanics (CM). We called *standard* formulation the one in which the Jacobi fields (or the forms)[2] are represented by *Grassmannian* variables and belong to the vector (or its dual) representation of the symplectic group. In Ref. 1 we showed that the associated Hilbert space cannot have at the same time a positive definite scalar product and a Hermitian Hamiltonian. As in Ref. 1 we shall indicate this formulation as CPI for ''Classical Path Integral.''

In Sec. II of this paper we will review a different functional approach[3] to CM in which the Jacobi fields are represented by *bosonic* variables, instead of *Grassmannian* ones, but they still belong to the vector (or its dual) representation of the symplectic group. We will indicate this formulation as BFA for Bosonic Functional Approach. The operatorial version of the BFA is studied in detail in Sec. III. There we will prove that it is possible to have both a positive definite Hilbert space and a Hermitian Hamiltonian differently from what happens in the CPI case.[1] In the Appendix we shall present a geometrical analysis of the BFA interpreting the various variables as basis for the forms and vector fields. Like in the CPI several symmetries make their appearance. The analysis of these symmetries requires, in the bosonic case, a special care. A special care requires also the construction of higher forms. Their construction is less straightforward than in the CPI case but it has its own consistency as proved in the Appendix.

Both in the CPI and in the BFA case, the Jacobi fields belong to the vector (or its dual) representation of the symplectic group, but this is not the only representation we can use. In fact in Sec. IV we will review another functional approach to CM in which the Jacobi fields are built as condensates of Grassmannian variables belonging to the spinor representation of the *metaplectic* group.[4] We shall indicate this formulation as MFA for Metaplectic Functional Approach. We

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shall show in Sec. V that also in the MFA case, like in the BFA one, it is possible to construct both a positive definite Hilbert space and a Hermitian Hamiltonian.

In the Conclusions, besides drawing an overall picture from the technical analysis contained in this paper and in Ref. 1, we explain why the problems (non-Hermiticity, etc.) apparently by-passed by the BFA and MFA with respect to the CPI actually lead to other problems whose solution could lie in a further extension of the Hilbert space.[14]

II. BOSONIC PATH INTEGRAL

The CPI formulation of CM[2] has, as starting point, the following generating functional:

$$Z[J]=\int \mathcal{D}\varphi\, \tilde{\delta}[\,\varphi^a(t)-\varphi^a_{cl}(t)]\exp\left[\int \mathrm{d}t\, J_a\varphi^a\right]. \tag{2.1}$$

The variables φ^a are the phase space coordinates: $\varphi^a\equiv(q^i,p^i)$ of a symplectic manifold $\mathcal{M}_{2N}$ with $a=1,\ldots,2N$ and $i=1,\ldots,N$, and $\varphi^a_{cl}(t)$ are the solutions of the Hamiltonian equations of motion

$$\dot{\varphi}^a=\omega^{ab}\frac{\partial H}{\partial\varphi^b} \tag{2.2}$$

with ω^{ab} the standard symplectic matrix. Disregarding for a moment the current J_a, it is easy to realize that we can write $Z[J]$ in (2.1) as

$$Z[J]=\int \mathcal{D}\varphi\, \tilde{\delta}\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]\det\left[\delta^a_l\partial_t-\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right], \tag{2.3}$$

where the determinant appearing in (2.3) is the functional determinant needed to pass from the zeroes [in (2.1)] of the function $F(\varphi,\dot{\varphi})\equiv\dot{\varphi}^a-\omega^{ab}(\partial H/\partial\varphi^b)$ to the function itself in (2.3). This functional determinant is positive definite[5] and this *crucial* property is based on the fact that between two phase space points there is at most only one classical trajectory. This property does not hold between two points of configuration space and so the associated functional determinant would not be positive definite.

In the CPI formulation[2] of CM the next step is to ''exponentiate'' the determinant in (2.3) via Grassmannian variables like it is done in the Faddeev–Popov (FP) method of gauge theories. In Ref. 3 we chose a different strategy. The trick we adopted was to substitute the determinant in (2.3) with the inverse determinant (for details see Ref. 3):

$$\det\left[\delta^a_l\partial_t-\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]=\left\{\det\left[\delta^a_l\partial_t+\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]\right\}^{-1}. \tag{2.4}$$

The next steps done in Ref. 3 were to use (2.4) in (2.3) and then ''exponentiate'' the inverse matrix via bosonic variables (π^a,ξ_b) using the well-known formula

$$\int \mathrm{d}\pi^a\,\mathrm{d}\xi_b\exp(i\pi^a A^b_a\xi_b)\propto\{\det[A^b_a]\}^{-1}. \tag{2.5}$$

This formula of Gaussian integration applies only to matrices with positive determinant and this is our case as we explained above. Note that this is no longer the case for the FP determinant which, as signaled by the Gribov problem, is not positive definite. This is the reason why the FP determinant could not be exponentiated via bosonic variables. Various attempts exist in the literature to write fermionic determinants via bosonic variables[6] but they are all different from the one we have presented here.

Let us now use the relations (2.4) and (2.5) into the $Z[J]$ of (2.3), the result is

$$Z_{\mathrm{BFA}}[J]=\int \mathcal{D}\varphi^a\,\tilde{\delta}\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]\left\{\det\left[\delta^a_l\partial_t+\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]\right\}^{-1}$$
$$=\int \mathcal{D}\varphi^a\,\mathcal{D}\lambda_a\,\mathcal{D}\pi^a\,\mathcal{D}\xi_a\exp\left(i\int \mathrm{dt}\;\mathcal{L}_{\mathrm{BFA}}\right), \tag{2.6}$$

where

$$\mathcal{L}_{\mathrm{BFA}}=\lambda_a\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]+\pi^l\left[\delta^a_l\partial_t+\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]\xi_a\,. \tag{2.7}$$

The variables λ_a are the same as in the CPI[2] formulation of CM and are needed to produce the Fourier transform of the Dirac delta $\tilde{\delta}[\dot{\varphi}^a-\omega^{ab}(\partial H/\partial\varphi^b)]$. The variables λ_a are bosonic like π^l,ξ_a which were introduced to exponentiate the matrix $[\delta^a_l\partial_t+\omega^{ab}(\partial^2 H/\partial\varphi^b\partial\varphi^l)]$ and to produce its inverse determinant. Let us remember that in the CPI formulation of CM[2] the Lagrangian obtained was

$$\tilde{\mathcal{L}}_{\mathrm{CPI}}=\lambda_a\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]+i\bar{c}_a\left[\delta^a_l\partial_t-\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]c^l, \tag{2.8}$$

which can be better compared with $\mathcal{L}_{\mathrm{BFA}}$ of (2.7) if, in this last one, we interchange π^l,ξ_a. The result is

$$\mathcal{L}_{\mathrm{BFA}}=\lambda_a\left[\dot{\varphi}^a-\omega^{ab}\frac{\partial H}{\partial\varphi^b}\right]-\xi_a\left[\delta^a_l\partial_t-\omega^{ab}\frac{\partial^2 H}{\partial\varphi^b\partial\varphi^l}\right]\pi^l+(\mathrm{s.t.}), \tag{2.9}$$

where (s.t.) is a surface term. From (2.9) we see that, modulo the surface term, we get the $\mathcal{L}_{\mathrm{BFA}}$ from $\tilde{\mathcal{L}}_{\mathrm{CPI}}$ by replacing the Grassmannian variables $i\bar{c}_a$ and c^l with the bosonic ones $-\xi_a$ and π^l.

III. OPERATORIAL FORMALISM

We should now build the operatorial formalism associated to the BFA. The nonzero commutators among the basic variables $(\varphi^a,\lambda_a,\pi^a,\xi_a)$ can be straightforwardly derived from the path integral (2.6) by inspecting the kinetic term in (2.7). They turn out to be

$$[\hat{\varphi}^a,\hat{\lambda}_b]=i\,\delta^a_b\,,$$
$$[\hat{\xi}_a,\hat{\pi}^b]=i\,\delta^b_a\,, \tag{3.1}$$

where we have now turned the path integral variables into operators. Next we choose the ''Schrödinger'' representation in which $\hat{\varphi}^a$ and $\hat{\pi}^a$ are realized as multiplicative operators while $\hat{\lambda}_a$ and $\hat{\xi}_a$ as derivative ones of the form

$$\hat{\lambda}_a\equiv -i\frac{\partial}{\partial\varphi^a}\,,$$
$$\hat{\xi}_a\equiv i\frac{\partial}{\partial\pi^a}\,. \tag{3.2}$$

So in this representation the associated Hilbert space is made of the ''wave functions'' $\psi(\varphi^a,\pi^a)$ defined on the $4N$-dimensional ''configurational'' space whose coordinates are (φ^a,π^a). A very natural, and *positive definite*, scalar product that we can introduce in this space is

$$\langle \psi | \psi' \rangle \equiv \int \mathrm{d}^{2N}\varphi^a \, \mathrm{d}^{2N}\pi^a \, \psi^*(\varphi^a, \pi^a)\psi'(\varphi^a, \pi^a). \tag{3.3}$$

It is extremely easy to check that the $8N$ operators $\hat{\varphi}^a, \hat{\lambda}_a, \hat{\pi}^a, \hat{\xi}_a$ are all Hermitian under the scalar product (3.3)

$$\begin{aligned} \hat{\varphi}^{a\dagger} &= \hat{\varphi}^a, \\ \hat{\lambda}_a^{\dagger} &= \hat{\lambda}_a, \\ \hat{\xi}_a^{\dagger} &= \hat{\xi}_a, \\ \hat{\pi}^{a\dagger} &= \hat{\pi}^a. \end{aligned} \tag{3.4}$$

Let us now derive from the Lagrangian (2.7) the associated Hamiltonian and let us turn the variables $(\varphi^a, \lambda_a, \pi^a, \xi_a)$ into operators, the result is

$$\hat{\mathcal{H}}_{\mathrm{BFA}} = \hat{\lambda}_a \omega^{ab} \partial_b H - \hat{\pi}^l \omega^{ab} \partial_b \partial_l H \hat{\xi}_a. \tag{3.5}$$

It is straightforward to check that this Hamiltonian is Hermitian under the Hermiticity conditions (3.4). For more details the reader can consult Ref. 7. So we can say that, differently than in the CPI case analyzed in Ref. 1, in the BFA case we can have both a positive definite Hilbert space and a Hermitian Hamiltonian.

The reader may remember that in the Conclusions of Ref. 1 we gave some *physical* reasons of why we could not have both a positive definite Hilbert space and a Hermitian Hamiltonian in the CPI case: basically in a chaotic system the Jacobi fields $c^a(t)$ grow exponentially and, as a consequence, some of the one-forms

$$\psi(\varphi, c) = \psi_a(\varphi) c^a \tag{3.6}$$

have a norm which also grows exponentially with time. This means that the norm is not conserved and for this to happen we need a nonunitary evolution or equivalently a non-Hermitian Hamiltonian. This kind of reasoning cannot be applied in the BFA case. In fact here the role of the Jacobi fields is taken by the variables π^a whose equations of motion, derived from the Lagrangian $\mathcal{L}_{\mathrm{BFA}}$ of (2.9), are

$$\dot{\pi}^a = \omega^{ad} \partial_d \partial_b H \pi^b, \tag{3.7}$$

and so the analog of the wave function (3.6) is

$$\psi(\varphi, \pi) = \psi_a(\varphi) \pi^a. \tag{3.8}$$

Unfortunately this wave function is not normalizable according to the scalar product (3.3). So even if the exponential increase in π^a would imply, like for the wave function (3.6), an exponential increase of the norm of the state, this would not lead to the conclusion that the evolution is not unitary. The reason is that the state (3.8) itself is not part of the Hilbert space already at $t=0$ since it is not normalizable. Further details on the BFA formulation, especially regarding the geometric interpretation of the variables π, ξ, have been confined in an appendix at the end of the paper.

IV. METAPLECTIC REPRESENTATION

One of the crucial concepts we will use in the appendix is that of Lie derivative.[8] In particular we will see how it acts on vector fields (A8), on forms (A10) or on tensors in the case of *symplectic* manifolds. The notion of Lie derivative can be extended to *general* manifolds $\mathcal{M}_n$ with $\mathrm{Diff}(\mathcal{M}_n)$ as group of diffeomorphisms and $\mathcal{G}$ as *structure group*[9] of the associated (co-)tangent

bundle. Under the action of an element of Diff($\mathcal{M}_n$), which drags the field through an infinitesimal displacement $\delta\varphi^a=-h^a(\varphi)$, an arbitrary tensor field $\mathcal{X}$ on $\mathcal{M}_n$ is transformed as follows:

$$\mathcal{X}'(\varphi)-\mathcal{X}(\varphi)=\mathcal{L}_h\mathcal{X}(\varphi), \tag{4.1}$$

where $\mathcal{L}_h$ is the Lie derivative associated to the vector field $h=h^a\partial_a$. The general abstract expression of $\mathcal{L}_h$ is[10]

$$\mathcal{L}_h=h^a\partial_a-\partial_b h^a G^b{}_a, \tag{4.2}$$

where $G^b{}_a$ are the generators of the structure *group* $\mathcal{G}$ in the *representation* to which $\mathcal{X}$ belongs. We will indicate with a,b the *group* indices and with α,β the *representation* ones. So the matrix representation of $G^a{}_b$ will be $(G^a{}_b)^\alpha{}_\beta$ where α are also the indices of $\mathcal{X}$, if we organize it as a vector. Now the structure group $\mathcal{G}$ could have also spinor representations. This means that we can introduce the concept of Lie derivative also for spinors but it is well known[10] that we cannot do it along all vector fields h^a. We have to restrict ourselves to the Lie derivative along *Killing vector fields* in the Riemann case[10] and along *Hamiltonian vector fields* in the symplectic one. Basically the reason is that only for those fields the usual commutator structure of the Lie derivative is preserved even for spinors.

Before proceeding let us rewrite (4.2) in a slightly modified form. Let us first introduce the following objects:[4]

$$\begin{aligned} K_{ab}(\varphi)&\equiv\partial_a\partial_b H(\varphi),\\ \Sigma^{ab}&\equiv i(\omega^{ca}G^b{}_c+\omega^{cb}G^a{}_c). \end{aligned} \tag{4.3}$$

Both are symmetric in a,b and $K_{ab}\Sigma^{ab}=2i\partial_b h^c G^b{}_c$, so (4.2) can be rewritten as

$$\mathcal{L}_h=h^a\partial_a+\frac{i}{2}K_{ab}\Sigma^{ab}. \tag{4.4}$$

In the case of spinors we have to use for Σ^{ab} in (4.4) the spinorial representation of Sp($2N$). To do that we have to pass to the universal covering group of Sp($2N$) which is the *metaplectic* group Mp($2N$).[11–13] The associated algebra is generated by[4]

$$\Sigma^{ab}_{\text{meta}}=\tfrac{1}{4}(\gamma^a\gamma^b+\gamma^b\gamma^a), \tag{4.5}$$

where the γ^a satisfy the relation

$$\gamma^a\gamma^b-\gamma^b\gamma^a=2i\omega^{ab} \tag{4.6}$$

which is the analog of the Dirac one for the Lorentz group $\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu=2g^{\mu\nu}$. So a representation for the matrices γ^a in (4.6) gives rise to a corresponding representation for the generators $\Sigma^{ab}_{\text{meta}}$ in (4.5). In particular, because of the crucial minus sign on its LHS, the algebra (4.6) does not admit finite dimensional unitary representations. In fact if γ^a were represented by finite dimensional matrices, by taking the trace on both sides of (4.6), we would get a contradictory result. Therefore the only representations are infinite dimensional. We will indicate with $\mathcal{V}$ this infinite dimensional Hilbert space and with "x" the indices of its vectors. In particular we will consider only representations in which γ^a is Hermitian with respect to the inner product in $\mathcal{V}$. As a consequence also $\Sigma^{ab}_{\text{meta}}$ is Hermitian,

$$\begin{aligned} (\gamma^a)^\dagger&=\gamma^a,\\ (\Sigma^{ab}_{\text{meta}})^\dagger&=\Sigma^{ab}_{\text{meta}}. \end{aligned} \tag{4.7}$$

Explicit representations of the symplectic operators γ^a have been worked out in the literature and can be found in Ref. 4. In particular the algebra (4.6) is isomorphic to the standard Heisenberg algebra

$$\hat{\phi}^a\hat{\phi}^b-\hat{\phi}^b\hat{\phi}^a=i\hbar\omega^{ab},\quad a,b=1,\ldots,2N, \tag{4.8}$$

made of $\hat{\phi}^a=(\hat{p}^k,\hat{x}^k)$, i.e., of N positions $\hat{x}^k$ and N momenta operators $\hat{p}^k$. So γ^a can be represented as

$$\gamma^a=\left(\frac{2}{\hbar}\right)^{1/2}\hat{\phi}^a \tag{4.9}$$

and in the ''Schrödinger'' representation, in which the operators $\hat{x}^k$ are diagonal, we have

$$\begin{aligned}(\gamma^k)^x{}_y&=\left(\frac{2}{\hbar}\right)^{1/2}\langle x|\hat{x}^k|y\rangle=\left(\frac{2}{\hbar}\right)^{1/2}x^k\delta^N(x-y),\\ (\gamma^{N+k})^x{}_y&=\left(\frac{2}{\hbar}\right)^{1/2}\langle x|\hat{p}^k|y\rangle=-i(2\hbar)^{1/2}\partial_k\delta^N(x-y),\end{aligned} \tag{4.10}$$

where x,y are the Hilbert space indices.

The geometrical picture which emerges[4] is the following. We have a bundle: the base space is the phase space $\mathcal{M}_{2N}$ and on its fibers, which are the Hilbert space $\mathcal{V}$, we have requested that the structure group $\mathcal{G}=\mathrm{Sp}(2N)$ acts no longer in the *vector* representation but in the *spinor* one. This bundle is the analog of the well-known ''spin-bundle'' [9] but each of its fibers is a Hilbert space $\mathcal{V}$. So we end up in a *Hilbert bundle* which we call $\mathcal{V}_\varphi$ to indicate that there is a fiber $\mathcal{V}$ at each point (φ) of the phase space $\mathcal{M}_{2N}$.

In this Hilbert bundle a section is locally given by a function ψ,

$$\begin{aligned}&\psi:\mathcal{M}_{2N}\to\mathcal{V},\\ &\varphi\to|\psi;\varphi\rangle\in\mathcal{V}_\varphi.\end{aligned} \tag{4.11}$$

Here the notation $|\psi;\varphi\rangle$ indicates that the vector ψ lives in the local Hilbert space (fiber) $\mathcal{V}$ associated to the point φ of the base manifold. At the level of matrix elements the indices are the x of (4.10) and so the function (4.11) is defined by its components

$$\psi^x(\varphi)=\langle x|\psi;\varphi\rangle. \tag{4.12}$$

By replacing $\mathcal{V}$ with its Hilbert dual $\mathcal{V}^*$ we can also construct the dual of the Hilbert bundle

$$\mathcal{X}_x(\varphi)=\langle\mathcal{X};\varphi|x\rangle,\quad\langle\mathcal{X};\varphi|\in\mathcal{V}^*_\varphi. \tag{4.13}$$

In our formalism it is natural to consider also ''multispinor'' fields

$$\varphi\to\mathcal{X}^{x_1\cdots x_q}_{y_1\cdots y_p}(\varphi) \tag{4.14}$$

which assume values in the tensor product

$$\underbrace{\mathcal{V}^*_\varphi\otimes\mathcal{V}^*_\varphi\otimes\cdots\otimes\mathcal{V}^*_\varphi}_{p\ \text{factors}}\otimes\underbrace{\mathcal{V}_\varphi\otimes\mathcal{V}_\varphi\otimes\cdots\otimes\mathcal{V}_\varphi}_{q\ \text{factors}}. \tag{4.15}$$

The symplectic spinors and multispinors have been first studied in great details in Ref. 12. Restricting ourselves to a spinor, its evolution equation[4] under the Hamiltonian vector field $h^a = \omega^{ab}\partial_b H$ is

$$\partial_t \mathcal{X}_x(\varphi,t) = -\mathcal{L}_h \mathcal{X}_x(\varphi,t) = -\int dy \left[\delta(x-y) h^a \partial_a + \frac{i}{2} K_{ab}(\varphi)(\Sigma^{ab}_{\text{meta}})^y{}_x \right] \cdot \mathcal{X}_y(\varphi,t). \quad (4.16)$$

In general if we indicate the representation indices with greek letters (α,β) and the group (or manifold) indices with italic ones (a,b) Eq. (4.16) can be replaced by

$$\partial_t \mathcal{X}_\alpha(\varphi,t) = -\mathcal{L}_h \mathcal{X}_\alpha(\varphi,t) = -\left[\delta^\beta_\alpha h^a \partial_a + \frac{i}{2} K_{ab}(\varphi)(\Sigma^{ab}_{\text{meta}})^\beta{}_\alpha \right] \mathcal{X}_\beta(\varphi,t). \quad (4.17)$$

This is the equation of evolution of the spinor $\mathcal{X}$ in any representation.

V. METAPLECTIC HAMILTONIAN AND SCALAR PRODUCT

Up to now we have used the abstract differential geometric formalism one can find in the literature,[8,9,12,13] but now we would like to put it in the kind of language we use in Ref. 2. The procedure is straightforward.[4] Let us extend $\mathcal{M}_{2N}$ to a new space $\mathcal{M}_{\text{ext}}$ labeled by the coordinates $(\varphi^a, \lambda_a, \eta^\alpha, \overline{\eta_\alpha})$ where λ_a are the same kind of variables we used in Ref. 2 and in the first part of this paper while $\eta^\alpha, \overline{\eta_\alpha}$ are Grassmannian variables and they are as many as the indices α introduced in the preceding section. Note that in Ref. 2, since the vector (or form) representation has the same dimension as the manifold $\mathcal{M}_{2N}$, the Grassmannian variables $c^a, \overline{c_a}$ were as many as the variables φ^a (or λ_a). Here instead the number of indices α is equal to the dimension M of the representation that we are using. So the dimension of $\mathcal{M}_{\text{ext}}$ is not $8N$, as in the CPI case, but $4N+2M$ where M is the dimension of the representation.

Next let us endow $\mathcal{M}_{\text{ext}}$ with the following extended Poisson structure (epb):

$$\begin{aligned} &\{\varphi^a, \lambda_b\}_{\text{epb}} = \delta^a_b, \quad \{\varphi^a, \varphi^b\}_{\text{epb}} = \{\lambda_a, \lambda_b\}_{\text{epb}} = 0, \\ &\{\overline{\eta}_\beta, \eta^\alpha\}_{\text{epb}} = -i\delta^\alpha_\beta, \quad \{\eta^\alpha, \eta^\beta\}_{\text{epb}} = \{\overline{\eta}_\alpha, \overline{\eta}_\beta\}_{\text{epb}} = 0, \end{aligned} \quad (5.1)$$

and with the following Hamiltonian:

$$\tilde{\mathcal{H}}_{\text{MFA}} = h^a(\varphi)\lambda_a + \tfrac{1}{2}\overline{\eta}_\alpha K_{ab}(\varphi)(\Sigma^{ab}_{\text{meta}})^\alpha{}_\beta \eta^\beta, \quad (5.2)$$

where the acronym MFA means "Metaplectic Functional Approach" and we have used it because this Hamiltonian is the one appearing in a new functional approach which we will present later on. As last ingredient let us build the following hat "$\wedge$" map[2] between the multispinor fields (4.14) of the abstract formalism and the variables belonging to $\mathcal{M}_{\text{ext}}$:

$$\mathcal{X}(\varphi) \;\rightarrow\; \hat{\mathcal{X}} \equiv \frac{1}{p!q!} \mathcal{X}^{\beta_1 \cdots \beta_q}_{\alpha_1 \cdots \alpha_p}(\varphi)\, \overline{\eta}_{\beta_1} \cdots \overline{\eta}_{\beta_q} \eta^{\alpha_1} \cdots \eta^{\alpha_p}. \quad (5.3)$$

It is then a straightforward but very long calculation to show[4] that the Lie derivative on $\mathcal{X}$ can be realized via the extended Poisson bracket and the Hamiltonian $\tilde{\mathcal{H}}_{\text{MFA}}$ as

$$(\mathcal{L}_h \mathcal{X}) \;\hat{\rightarrow}\; -\{\tilde{\mathcal{H}}_{\text{MFA}}, \hat{\mathcal{X}}\}_{\text{epb}}. \quad (5.4)$$

It is also easy to show that the standard equation of motion (4.17) for the spinor field $\partial_t \mathcal{X}_\alpha = -\mathcal{L}_h \mathcal{X}_\alpha$ can be written in terms of the Hamiltonian $\tilde{\mathcal{H}}_{\text{MFA}}$ as

$$\partial_t \hat{\mathcal{X}} = \{\tilde{\mathcal{H}}_{\text{MFA}}, \hat{\mathcal{X}}\}_{\text{epb}}, \quad (5.5)$$

where $\hat{\mathcal{X}}$ is given by (5.3). Via $\tilde{\mathcal{H}}_{\mathrm{MFA}}$ and the extended Poisson brackets one can obtain the evolution of all the variables $(\varphi^a,\lambda_a,\eta^\alpha,\overline{\eta}_\alpha)$ of the extended manifold $\mathcal{M}_{\mathrm{ext}}$. The equations of motion for φ^a are the standard ones[2] of classical mechanics

$$\dot{\varphi}^a = h^a(\varphi(t)), \tag{5.6}$$

while the equations for the Grassmannian variables are

$$\begin{aligned} \dot{\eta}^\alpha &= -\frac{i}{2}K_{ab}(\Sigma^{ab}_{\mathrm{meta}})^\alpha{}_\beta \eta^\beta, \\ \dot{\overline{\eta}}_\alpha &= \frac{i}{2}K_{ab}\overline{\eta}_\beta(\Sigma^{ab}_{\mathrm{meta}})^\beta{}_\alpha . \end{aligned} \tag{5.7}$$

Let us notice that the last two equations are quite different from the one of the Jacobi field $\delta\varphi^a$,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\delta\varphi^a) = \partial_l h^a(\varphi)(\delta\varphi^l). \tag{5.8}$$

So we cannot identify η^α with the Jacobi fields of classical mechanics. They are instead a sort of "square root" of the Jacobi fields[4] in the sense that the composite objects $c^a(t)$ defined as

$$c^a(t) \equiv \overline{\eta}_\alpha(\gamma^a)^\alpha{}_\beta \overline{\eta}^\beta \tag{5.9}$$

have the same equations of motion as the Jacobi fields. The details can be found in Refs. 4 and 7.

The extended Poisson brackets formalism presented in this section can be given a classical path integral version as explained in details in Ref. 4. The associated generating functional is

$$Z_{\mathrm{MFA}} = \int \mathcal{D}\varphi\,\mathcal{D}\lambda\,\mathcal{D}\eta\,\mathcal{D}\overline{\eta}\exp i\int \mathrm{d}t[\lambda_a\dot{\varphi}^a + i\overline{\eta}_\alpha\dot{\eta}^\alpha - \tilde{\mathcal{H}}_{\mathrm{MFA}}]. \tag{5.10}$$

As we did for the CPI case[2] one can derive the "operatorial" version of this MFA path integral. From the kinetic term in (5.10) one gets the following Z_2-graded commutators:

$$\begin{aligned} [\hat{\varphi}^a,\hat{\lambda}_b] &= i\delta^a_b, \\ [\hat{\overline{\eta}}_\beta,\hat{\eta}^\alpha] &= \delta^\alpha_\beta . \end{aligned} \tag{5.11}$$

All the commutators not indicated in (5.11) are zero. In a "Schrödinger-type" representation where $\hat{\varphi}^a$ and $\hat{\eta}^\alpha$ are *multiplicative* operators, the associated momenta operators $\hat{\lambda}_a$, $\hat{\overline{\eta}}_\alpha$ have to be realized as *derivative* operators in order to satisfy the algebra (5.11),

$$\begin{aligned} \hat{\lambda}_a &= -i\frac{\partial}{\partial\varphi^a}, \\ \hat{\overline{\eta}}_\alpha &= \frac{\partial}{\partial\eta^\alpha}. \end{aligned} \tag{5.12}$$

The associated representation space is given by the set of functions

$$\mathcal{X}(\varphi,\eta) \equiv \sum_p \frac{1}{p!}\mathcal{X}_{\alpha_1\alpha_2\cdots\alpha_p}(\varphi)\,\eta^{\alpha_1}\eta^{\alpha_2}\cdots\eta^{\alpha_p} \tag{5.13}$$

while the metaplectic Hamiltonian (5.2) is turned into the operator

$$\hat{\mathcal{H}}_{\mathrm{MFA}}=\tilde{\mathcal{H}}_{\mathrm{MFA}}\left(\hat{\varphi},\hat{\lambda}=-i\frac{\partial}{\partial\varphi},\hat{\eta},\hat{\bar{\eta}}=\frac{\partial}{\partial\eta}\right). \tag{5.14}$$

The next step is to endow the space of functions (5.13) with a scalar product and check if the $\hat{\mathcal{H}}_{\mathrm{MFA}}$ is Hermitian under it. We will choose the analog of the SvH scalar product, introduced in Ref. 1 for the CPI case, by imposing the following Hermiticity conditions:

$$\begin{aligned}\hat{\eta}^{\alpha\dagger}&=\hat{\bar{\eta}}_{\alpha},\\ \hat{\bar{\eta}}_{\alpha}^{\dagger}&=\hat{\eta}^{\alpha},\\ \hat{\varphi}^{a\dagger}&=\hat{\varphi}^{a},\\ \hat{\lambda}_{a}^{\dagger}&=\hat{\lambda}_{a}.\end{aligned} \tag{5.15}$$

Along the same lines developed in Ref. 1, it is easy to show that the scalar product induced by the Hermiticity conditions (5.15) among the states (5.13) is

$$\langle\tau|\mathcal{X}\rangle=\sum_{p}K(p)\int \mathrm{d}\varphi\ \tau^{*\alpha_1\cdots\alpha_p}(\varphi)\mathcal{X}_{\alpha_1\cdots\alpha_p}(\varphi), \tag{5.16}$$

where $K(p)$ is a *positive* combinatorial factor. One immediately notices that this is a *positive definite* scalar product. Let us now check whether the Hamiltonian $\hat{\mathcal{H}}_{\mathrm{MFA}}$ is Hermitian under this scalar product. Let us first remember that the bosonic part of $\hat{\mathcal{H}}_{\mathrm{MFA}}$ (5.2), which is the same as in the CPI case, is Hermitian.[1] So we have to check out only the Fermionic (or Grassmannian) part which is

$$\hat{\mathcal{H}}_{\mathrm{MFA}}^{\mathrm{ferm}}=\tfrac{1}{2}\partial_a\partial_b H\,\hat{\bar{\eta}}_x(\Sigma_{\mathrm{meta}}^{ab})^{x}{}_{y}\,\hat{\eta}^{y}. \tag{5.17}$$

We have indicated the indices with x,y because, in the metaplectic case, as explained previously, they are a continuous set of indices labeling the infinite states of the Hilbert space $\mathcal{V}$. Second, let us remember that $\Sigma_{\mathrm{meta}}^{ab}$ have to be chosen Hermitian in the metaplectic and in any unitary representation

$$(\Sigma_{\mathrm{meta}}^{ab})^{\dagger}=\Sigma_{\mathrm{meta}}^{ab}. \tag{5.18}$$

This Hermiticity of course refers to the indices (x,y) and not to (a,b). So if we indicate the elements $(\Sigma_{\mathrm{meta}}^{ab})_{y}^{x}$ as $\langle x|\Sigma_{\mathrm{meta}}^{ab}|y\rangle$ then (5.18) implies that

$$\langle x|\Sigma_{\mathrm{meta}}^{ab}|y\rangle^{*}=\langle y|\Sigma_{\mathrm{meta}}^{ab\ \dagger}|x\rangle=\langle y|\Sigma_{\mathrm{meta}}^{ab}|x\rangle, \tag{5.19}$$

which in normal matrix language means

$$(\Sigma_{\mathrm{meta}}^{ab})^{x}{}_{y}^{*}=(\Sigma_{\mathrm{meta}}^{ab})^{y}{}_{x}. \tag{5.20}$$

It is straightforward to prove the Hermiticity of $\hat{\mathcal{H}}_{\mathrm{MFA}}^{\mathrm{ferm}}$. In fact,

$$\begin{aligned}(\hat{\mathcal{H}}_{\mathrm{MFA}}^{\mathrm{ferm}})^{\dagger}&=(\tfrac{1}{2}(\partial_a\partial_b H)\,\hat{\bar{\eta}}_x(\Sigma_{\mathrm{meta}}^{ab})^{x}{}_{y}\,\hat{\eta}^{y})^{\dagger}=\tfrac{1}{2}(\partial_a\partial_b H)\,\hat{\eta}^{y\dagger}(\Sigma_{\mathrm{meta}}^{ab})^{x}{}_{y}^{*}\,\hat{\bar{\eta}}_x^{\dagger}=\tfrac{1}{2}(\partial_a\partial_b H)\,\hat{\bar{\eta}}_y(\Sigma_{\mathrm{meta}}^{ab})^{y}{}_{x}\,\hat{\eta}^{x}\\ &=\tfrac{1}{2}(\partial_a\partial_b H)\,\hat{\bar{\eta}}_x(\Sigma_{\mathrm{meta}}^{ab})^{x}{}_{y}\,\hat{\eta}^{y}=\hat{\mathcal{H}}_{\mathrm{MFA}}^{\mathrm{ferm}}.\end{aligned} \tag{5.21}$$

This proves that the full $\hat{\mathcal{H}}_{\mathrm{MFA}}$ is Hermitian under the SvH scalar product. This does not happen for the $\tilde{\mathcal{H}}$ of the CPI.[2,1] Let us understand why. It can be shown[7] that also the usual $\tilde{\mathcal{H}}_{\mathrm{CPI}}$ can be given a form similar to $\tilde{\mathcal{H}}_{\mathrm{MFA}}$,

$$\tilde{\mathcal{H}}_{\mathrm{CPI}}=h^a\lambda_a+\tfrac{1}{2}\overline{c_e}K_{ab}(\varphi)(\Sigma^{ab}_{\mathrm{vec}})^e{}_f c^f, \tag{5.22}$$

where $(\Sigma^{ab}_{\mathrm{vec}})^e_f$ is the Σ associated to the transformations of vectors under $\mathrm{Sp}(2N)$ and is given by[4]

$$(\Sigma^{ab}_{\mathrm{vec}})^e{}_f=-i(\delta^a_f\omega^{be}+\delta^b_f\omega^{ae}). \tag{5.23}$$

It is easy to check that this Σ does not satisfy the analog of the relation (5.20), which means

$$(\Sigma^{ab}_{\mathrm{vec}})^{e*}_{f}\neq(\Sigma^{ab}_{\mathrm{vec}})^f{}_e. \tag{5.24}$$

This explains why $\tilde{\mathcal{H}}_{\mathrm{CPI}}$ is not Hermitian in the SvH scalar product.

There may be other scalar products in the metaplectic case which are both positive definite and under which $\tilde{\mathcal{H}}_{\mathrm{MFA}}$ is Hermitian but for the moment we have not initiated any search for them. This search anyhow may be needed in the future as explained in the Conclusions.

VI. CONCLUSIONS AND OUTLOOK

In this paper we have analyzed two new operatorial extensions of the Koopman–von Neumann (KvN) approach which, differently from the standard CPI case studied in Ref. 1, present both a Hermitian Hamiltonian and a positive definite scalar product. Leaving for a moment aside the metaplectic case (MFA) let us concentrate on the bosonic one (BFA). The reader may prefer this one over the CPI case but there are several drawbacks we want to point out. First of all in the BFA approach the higher tensors and forms had to be built by hand introducing from the outside the operation $\otimes$ of tensor product (A36), while in the CPI case, because of the Grassmannian nature of the variables c, the higher tensors and forms were generated automatically as functions on the extended phase space which is the sole ingredient entering the associated path integral. Moreover at the operatorial level in the BFA case we had to build several copies (A38) of the basic Hilbert space in order to get the higher tensors and forms. As a consequence the associated path integral (A53) is quite awkward and it does not have a simple interpretation in terms of Dirac deltas on the classical trajectories. More serious than this drawback is another one that we fear may affect the BFA. It concerns the following problem. We have seen in Ref. 1 that the non-Hermiticity of $\tilde{\mathcal{H}}_{\mathrm{CPI}}$ or the nonpositive definiteness of the scalar product were crucial ingredients in order to describe chaotic systems. In fact such ingredients can imply the presence of complex eigenvalues for $\tilde{\mathcal{H}}_{\mathrm{CPI}}$ and this has as a consequence the exponential increase of the Jacobi fields. Nothing like that can happen with the $\tilde{\mathcal{H}}_{\mathrm{BFA}}$ which is Hermitian and with a positive definite scalar product. Does it mean that $\tilde{\mathcal{H}}_{\mathrm{BFA}}$ cannot describe all systems? We feel it will but most probably we will have to further enlarge the Hilbert space of the BFA. People have gone in this direction already with other Hermitian operators. For example, the authors of Ref. 14, in order to get the chaotic behavior out of the analog of the Hermitian KvN operator for zero-forms, enlarged the Hilbert space to a rigged Hilbert space where the operator was no longer Hermitian. This may be the road to pursue also in the BFA case. Before doing that anyhow one should really check whether this further extension to a rigged Hilbert space is needed or if some mathematical subtleties of the BFA allow us to describe also chaotic systems without any further extension. We have not embarked on this study but we have, in this paper, prepared the mathematical ground to do that by analyzing in all details the geometry underlying the BFA. That the CPI instead could describe chaotic systems was not only indicated in Ref. 1 by the presence of complex eigenvalues of $\tilde{\mathcal{H}}_{\mathrm{CPI}}$ but it was shown explicitly in Ref. 15 where an explicit expression of the Lyapunov exponents in terms of the CPI generating functional $Z_{\mathrm{CPI}}[J]$ was written down.

Let us now turn to the metaplectic case. Why did we study it here? We did first of all to present another example of an extension of the KvN zero-form formalism which has both a Hermitian Hamiltonian and a positive definite scalar product. These mathematical features were not studied in the first presentation[4] of the MFA. Of course for this model, differently than the CPI and the BFA, we do not have in mind applications to chaotic systems or similar things; what we

have in mind is the light it may throw on the issue of quantization. It was used in that respect in Ref. 16. There quantization was achieved by first postulating a MFA dynamics for the extended KvN dynamics and next introducing a flat connection on the Hilbert bundle defined in Sec. IV. The main thing we want to understand of that project is why we need to start at the classical level from the MFA dynamics. An answer to this question that we are currently exploring is the following. Maybe the CPI should be considered the right classical dynamics not for the classical wave functions but for the *probability densities*

$$\rho(\varphi,c)=\rho_0(\varphi)+\rho_a(\varphi)c^a+\rho_{ab}(\varphi)c^a c^b+\cdots \tag{6.1}$$

which are only integrable (i.e., belonging to L^1) and not square integrable functions. Then to get the ''classical wave functions'' we should do a sort of ''square root'' of the ρ in (6.1). May it be that these ''square roots'' are the MFA wave functions?

$$\psi(\varphi,\eta)=\sum_p \frac{1}{p!}\psi_{a_1\cdots\alpha_p}(\varphi)\,\eta^{\alpha_1}\eta^{\alpha_2}\cdots\eta^{\alpha_p}. \tag{6.2}$$

If so this would explain why we need the MFA evolution at the classical level. The reason we have this suspect is because the η are something like the ''square roots'' (5.9) of the c,

$$c^a=\overline{\eta}_\alpha(\gamma^a)^\alpha{}_\beta\overline{\eta}^\beta. \tag{6.3}$$

What we actually need in the MFA is a new scalar product such that

$${}_\varphi\langle\psi|\,\eta\rangle\langle\,\eta|\psi\rangle_\varphi=\rho(\varphi,\overline{\eta}\gamma\eta)=\rho(\varphi,c). \tag{6.4}$$

That means that we would like that the $\eta,\overline{\eta}$ on the LHS of (6.4) get combined by this scalar product into those combinations $\overline{\eta}\gamma^a\eta$ which are basically the c^a. We want that they combine in this way because the classical probability densities in (6.1) contain the forms c and not η or $\overline{\eta}$. The scalar product (6.4) is not the SvH one that we explored in Sec. V for the MFA. In fact the SvH scalar product of the MFA does not pull in the γ matrices which instead are necessary in (6.4) to get the combination $\overline{\eta}\gamma\eta$ inside the ρ. So far we have not succeeded in building the scalar product (6.4) but in order to get some practice we have asked ourselves how, from the various components of the ψ appearing in (6.2), we can build objects which at least have the same indices and transformation properties as the various components of ρ appearing in (6.1). One solution we found[7] is the following one:

$$\rho_{\underbrace{ab\cdots d}_{p}}(\varphi)=\mathrm{Tr}[\,|\psi^{(p)}\rangle\langle\psi^{(p)}|\,\gamma_{[a}\otimes\gamma_b\otimes\cdots\gamma_{d]}], \tag{6.5}$$

where with $|\psi^{(p)}\rangle$ we indicate the components of the states (5.13) with p indices while with $\otimes$ we indicate the tensor product among the Hilbert spaces like in (4.15). The *first* thing to notice in (6.5) is that if we transform $|\psi^{(p)}\rangle$ according to the metaplectic transformations then the resulting $\rho_{ab\cdots d}$ turns out to transform according to the symplectic one.

Second, let us notice that $|\psi^{(p)}\rangle$ has, in the metaplectic case, components $\psi_{\alpha_1\cdots\alpha_p}$ whose number of indices can run from zero to ∞, while ρ can have only at most N indices. This means we have much more information stored in the $|\psi\rangle$ that what is needed to build the ρ. What does this mean?

Third, let us remember that while (6.5) produces a ρ out of a ψ, it is not clear whether the inverse procedure is true and unique. That means whether, given a ρ with all its components, it is possible to find a $|\psi\rangle$ such that (6.5) or (6.4) is satisfied.

This is the project we are currently working and this explains why it is crucial for this project to analyze the various scalar products associated to the MFA dynamics.

ACKNOWLEDGMENTS

We wish to thank F. Benatti, R. Marnelius, and M. Reuter for some useful discussions. The work of E.D. has been supported by an INFN Postdoctoral Fellowship at MIT. E.D. wishes to thank the members of the Center for Theoretical Physics at MIT for hospitality. The work of E.G. and D.M. has been supported in part by funds from INFN, MIUR and the University of Trieste.

APPENDIX: GEOMETRICAL ANALYSIS OF THE BFA AND ASSOCIATED SYMMETRIES

In Ref. 3 we tried a first geometrical analysis of the bosonic formalism. There we gave an interpretation of the variables π^a, ξ_a as *components* of vectors and forms whose *basis* were, respectively, the variables $\overline{c_a}$ and c^a:

$$\begin{aligned} V &= \pi^a \overline{c_a}, \\ F &= \xi_a c^a. \end{aligned} \tag{A1}$$

The reason for this was that, under an infinitesimal diffeomorphism generated by $\mathcal{H}_{\mathrm{BFA}}$ over the original phase space:

$$\varphi'^a = \varphi^a + \epsilon \omega^{ab} \partial_b H, \tag{A2}$$

the variables π^a and ξ_a transform in the following way:

$$\begin{aligned} \pi'^a &= \pi^a + \epsilon \omega^{ac} \partial_c \partial_b H \pi^b = \frac{\partial \varphi'^a}{\partial \varphi^b} \pi^b, \\ \xi'_a &= \xi_a - \epsilon \omega^{bc} \partial_c \partial_a H \xi_b = \frac{\partial \varphi^b}{\partial \varphi'^a} \xi_b, \end{aligned} \tag{A3}$$

i.e., just as components of vectors and forms. In this interpretation the Hamiltonian $\hat{\mathcal{H}}_{\mathrm{BFA}}$ of (3.5) cannot be given the meaning of a Lie derivative. In fact we know that the Lie derivative $\mathcal{L}_{(\mathrm{d}H)^\sharp}$[8] changes the components of a vector as follows:

$$\delta \pi^l = (\partial_a \pi^l) \omega^{ab} \partial_b H - (\partial_a \omega^{lb} \partial_b H) \pi^a, \tag{A4}$$

while $\hat{\mathcal{H}}_{\mathrm{BFA}}$ in (3.5) induces on $\hat{\pi}^l$ the following transformation:

$$\delta \hat{\pi}^l = [\hat{\pi}^l, i\hat{\mathcal{H}}_{\mathrm{BFA}}] = (-\partial_a \omega^{lb} \partial_b H) \hat{\pi}^a, \tag{A5}$$

which is clearly different from (A4). So if we insist in the analysis presented in Ref. 3, we should first abandon the interpretation of $\hat{\mathcal{H}}$ of the BFA case as the Lie derivative along the Hamiltonian flow. Second, if we insist in interpreting π^a, ξ_a as components, we should make them dependent on φ and that implies that we should give a connection to glue the fibers of $T^*(T^*\mathcal{M})$ of which π^a and ξ_a are coordinates.[3] This connection does not appear in a natural way in our formalism. So, in order to bypass these two problems, we will interpret $\hat{\pi}^a$ and $\hat{\xi}_a$ as *basis*, respectively, of forms and vector fields. One-forms and vector fields are then given by

$$\begin{aligned} F &= F_a(\hat{\varphi}) \hat{\pi}^a, \\ V &= V^a(\hat{\varphi}) \hat{\xi}_a. \end{aligned} \tag{A6}$$

As a consequence, it is easy to check that the $\hat{\mathcal{H}}_{\mathrm{BFA}}$ of (3.5) can be interpreted as the Lie derivative (up to a constant factor). In fact, the commutator between $i\hat{\mathcal{H}}_{\mathrm{BFA}}$ and the vector V of (A6) gives

$$[i\hat{\mathcal{H}}_{\mathrm{BFA}}, V^e(\hat{\varphi})\hat{\xi}_e] = [(\partial_a V^e)\omega^{ab}\partial_b H - (\partial_a \omega^{eb}\partial_b H)V^a]\hat{\xi}_e \tag{A7}$$

and this is exactly how vector components V^e change[8] under the Lie derivative of the Hamiltonian flow

$$\delta V^e(\varphi) \equiv V'^e(\varphi) - V^e(\varphi) = (\partial_a V^e)\omega^{ab}\partial_b H - (\partial_a \omega^{eb}\partial_b H)V^a. \tag{A8}$$

Analogously, on the one-forms $F = F_e(\hat{\varphi})\hat{\pi}^e$ of (A6), $\hat{\mathcal{H}}_{\mathrm{BFA}}$ acts as follows:

$$[i\hat{\mathcal{H}}_{\mathrm{BFA}}, F_e(\hat{\varphi})\hat{\pi}^e] = [(\partial_a F_e)\omega^{ab}\partial_b H + (\partial_e \omega^{ab}\partial_b H)F_a]\hat{\pi}^e. \tag{A9}$$

This is exactly how one-forms components F_e transform[8] under the Lie derivative,

$$\delta F_e(\varphi) = F'_e(\varphi) - F_e(\varphi) = (\partial_a F_e)\omega^{ab}\partial_b H + (\partial_e \omega^{ab}\partial_b H)F_a. \tag{A10}$$

Before giving to $\hat{\mathcal{H}}_{\mathrm{BFA}}$ the meaning of a Lie derivative, another check we should do is the following. The commutator of two Lie derivatives has the property[8]

$$[\mathcal{L}_{(\mathrm{d}H_1)^\sharp}, \mathcal{L}_{(\mathrm{d}H_2)^\sharp}] = \mathcal{L}_{[(\mathrm{d}H_1)^\sharp, (\mathrm{d}H_2)^\sharp]_{Lb}}, \tag{A11}$$

where H_1 and H_2 are the Hamiltonians entering the Lie derivative and $[(\mathrm{d}H_1)^\sharp, (\mathrm{d}H_2)^\sharp]_{Lb}$ are the Lie brackets (Lb) between the associated Hamiltonian vector fields $(\mathrm{d}H_1)^\sharp$ and $(\mathrm{d}H_2)^\sharp$. According to our conventions the Lie brackets can be related to the Poisson brackets between H_1 and H_2 in the following way[8]

$$\begin{aligned}[(\mathrm{d}H_1)^\sharp, (\mathrm{d}H_2)^\sharp]_{Lb} &= [\omega^{bc}\partial_c H_1 \partial_b \omega^{ad}\partial_{\mathrm{d}} H_2 - \omega^{bc}\partial_c H_2 \partial_b \omega^{ad}\partial_{\mathrm{d}} H_1]\xi_a \\ &= -[\omega^{ad}\partial_{\mathrm{d}}(\partial_b H_1 \omega^{bc}\partial_c H_2)]\xi_a = -(\mathrm{d}\{H_1, H_2\})^\sharp. \end{aligned} \tag{A12}$$

Therefore (A11) can be rewritten as

$$[\mathcal{L}_{(\mathrm{d}H_1)^\sharp}, \mathcal{L}_{(\mathrm{d}H_2)^\sharp}] = \mathcal{L}_{-(\mathrm{d}\{H_1, H_2\})^\sharp}. \tag{A13}$$

As we associate to each Lie derivative $\mathcal{L}_{(\mathrm{d}H)^\sharp}$ an operator $i\hat{\mathcal{H}}_H$, the relation (A13) should turn into the following one:

$$[i\hat{\mathcal{H}}_{H_1}, i\hat{\mathcal{H}}_{H_2}] = -i\hat{\mathcal{H}}_{\{H_1, H_2\}}, \tag{A14}$$

where we have put on the $\hat{\mathcal{H}}$ of (3.5), the label H_1, H_2 or $\{H_1, H_2\}$ to indicate the function entering each $\hat{\mathcal{H}}_{\mathrm{BFA}}$. It is easy to prove that (A14) is satisfied using the commutators (3.1) and this confirms that it is consistent to assign to $\hat{\mathcal{H}}_{\mathrm{BFA}}$ the meaning of a Lie derivative (for details see Ref. 7).

In Ref. 2 it was found that, for the CPI, there were various conserved universal charges associated to the Lie derivative. They were called BRS, anti-BRS, ghost and supersymmetry charges in analogy with similar objects present in gauge field theory. Despite these names they are well-known structures in symplectic geometry;[8] for example the BRS charge is nothing but the exterior derivative on phase space and its conservation is related to the fact that the exterior derivative commutes with the Lie derivative.[8] The ghost charge is basically the form number[8] while the supersymmetry charge is connected to the concept of equivariant cohomology.[17] Besides their geometrically universal meaning, these charges and the associated symmetries somehow signal the redundancy of the $8N$ variables $(\varphi^a, \lambda_a, c^a, \overline{c_a})$ used in describing CM. We know in fact that CM can be described using only the $2N$ phase space variables (φ^a) and so the other $6N$ variables must be related to the φ^a via some symmetries which should be present for any system.

Also in the bosonic case we have many extra variables $(\lambda_a, \pi^a, \xi_a)$ besides the $2N$ phase space variables φ^a and so we expect to find various symmetries like in the CPI.

The way we start our search for the symmetries in the bosonic case is rather naive but it is one of the few we could think of. Basically, as the variables π^a, ξ_a take the place—in the bosonic case—of the Grassmannian variables $c^a, \overline{c_a}$, we simply rewrite the charges conserved in the CPI and replace in them c^a and $\overline{c_a}$ with π^a and ξ_a. In the CPI the conserved charges are[2,17]

$$\begin{aligned} Q_g &= i c^a \overline{c_a} \quad \text{ghost charge}, \\ N &= c^a \partial_a H, \\ \overline{N} &= \overline{c_a} \omega^{ab} \partial_b H, \end{aligned} \tag{A15}$$

and

$$\begin{aligned} Q &= i c^a \lambda_a \quad \text{BRS charge}, \\ \overline{Q} &= i \overline{c_a} \omega^{ab} \lambda_b \quad \text{anti-BRS charge}, \\ Q_H &= Q - N \quad \text{susy charge}, \\ \overline{Q}_H &= \overline{Q} + \overline{N} \quad \text{susy charge}. \end{aligned} \tag{A16}$$

So by replacing naively c^a with π^a and $\overline{c_a}$ with ξ_a we get the two following sets of charges:

$$\begin{aligned} Q_g^{(B)} &= i \pi^a \xi_a, \\ N^{(B)} &= \pi^a \partial_a H, \\ \overline{N}^{(B)} &= \xi_a \omega^{ab} \partial_b H \end{aligned} \tag{A17}$$

and

$$\begin{aligned} Q^{(B)} &= i \pi^a \lambda_a, \\ \overline{Q}^{(B)} &= i \xi_a \omega^{ab} \lambda_b, \\ Q_H^{(B)} &= Q^{(B)} - N^{(B)}, \\ \overline{Q}_H^{(B)} &= \overline{Q}^{(B)} + \overline{N}^{(B)}, \end{aligned} \tag{A18}$$

where the superscript (B) on the charge indicates that it refers to the BFA case. The reader may complain that, by replacing c^a with π^a and $\overline{c_a}$ with ξ_a, we have not really done the replacement which would bring the $\tilde{\mathcal{H}}$ of the CPI into the $\mathcal{H}$ of the BFA (3.5). The difference is just in multiplicative factors $(\pm i)$ which cannot spoil the conservation of the charges. The careful reader may also notice that in the CPI there were two other conserved charges[2] which are

$$\begin{aligned} K &= \tfrac{1}{2} c^a \omega_{ab} c^b, \\ \overline{K} &= \tfrac{1}{2} \overline{c_a} \omega^{ab} \overline{c_b}. \end{aligned} \tag{A19}$$

We did not list them because, via the substitution we did for the BFA case, the corresponding charges would be zero because of the bosonic character of π and ξ and the antisymmetry of ω_{ab},

$$K^{(B)} = \tfrac{1}{2} \pi^a \omega_{ab} \pi^b = 0, \tag{A20}$$

$$\overline{K}^{(B)} = \tfrac{1}{2}\xi_a \omega^{ab} \xi_b = 0.$$

Turning now back to the set of charges in (A17), it is easy to check that they are all conserved, i.e.,

$$[Q_g^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] = [N^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] = [\overline{N}^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] = 0. \tag{A21}$$

On the other hand, the charges present in (A18) are apparently not conserved. In fact taking the bosonic analog of the BRS charge and its commutator with $\hat{\mathcal{H}}_{\mathrm{BFA}}$ we get[7]

$$[Q^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] = -\pi^l \omega^{ab} \partial_b \partial_l \partial_c H \pi^c \xi_a \tag{A22}$$

and for the anti-BRS charge

$$[\overline{Q}^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] = -\xi_a \omega^{ab} \xi_s \omega^{st} (\partial_b \partial_t \partial_l H) \pi^l. \tag{A23}$$

Analogously the "supersymmetry" charges $Q_H^{(B)}, \overline{Q}_H^{(B)}$ in (A18) cannot be conserved because they are a linear combination of $Q^{(B)}$ and $\overline{Q}^{(B)}$, which are not conserved, with $N^{(B)}$ and $\overline{N}^{(B)}$ which are conserved.

Let us now look at the RHS of (A22) and (A23) which indicate by "*how much*" the conservation law is violated. It is easy to notice that these RHS do not contain λ_a and so they commute with the original phase space operators φ^a. As a consequence the infinitesimal transformations generated by $Q^{(B)}$ and by the Hamiltonian $\hat{\mathcal{H}}_{\mathrm{BFA}}$ *commute* when they are applied on φ. In fact the infinitesimal BRS transformations generated by $Q^{(B)}$ on a field A is given by the commutator of $Q^{(B)}$ with the field: $\delta_{Q^{(B)}} A = [\epsilon Q^{(B)}, A]$ where ϵ is an infinitesimal parameter. The same happens for the transformations generated by the Hamiltonian: $\delta_{\mathcal{H}} A = [\overline{\epsilon} \hat{\mathcal{H}}_{\mathrm{BFA}}, A]$. Suppose we take for A the original phase space variables φ^a. If we perform first an infinitesimal time evolution and then a BRS transformation we obtain

$$\delta_{Q^{(B)}} \delta_{\mathcal{H}} \varphi^a = \epsilon \overline{\epsilon} [Q^{(B)}, [\hat{\mathcal{H}}_{\mathrm{BFA}}, \varphi^a]] \tag{A24}$$

while, if we perform the transformations in the inverse order, we get

$$\delta_{\mathcal{H}} \delta_{Q^{(B)}} \varphi^a = \epsilon \overline{\epsilon} [\hat{\mathcal{H}}_{\mathrm{BFA}}, [Q^{(B)}, \varphi^a]]. \tag{A25}$$

Now we can use the Jacobi identities to obtain

$$\begin{aligned} \delta_{Q^{(B)}} \delta_{\mathcal{H}} \varphi^a - \delta_{\mathcal{H}} \delta_{Q^{(B)}} \varphi^a &= \epsilon \overline{\epsilon} ([Q^{(B)}, [\hat{\mathcal{H}}_{\mathrm{BFA}}, \varphi^a]] - [\hat{\mathcal{H}}_{\mathrm{BFA}}, [Q^{(B)}, \varphi^a]]) \\ &= -\epsilon \overline{\epsilon} [\varphi^a, [Q^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}]] = 0, \end{aligned} \tag{A26}$$

where in the last step we have used the fact that the RHS of (A22) commutes with φ^a. "Somehow" we can say that the transformations generated by $Q^{(B)}$ and $\hat{\mathcal{H}}_{\mathrm{BFA}}$ commute on the original phase space. Of course the same will happen for the anti-BRS charge $\overline{Q}^{(B)}$ and for the supersymmetry charges $Q_H^{(B)}, \overline{Q}_H^{(B)}$.

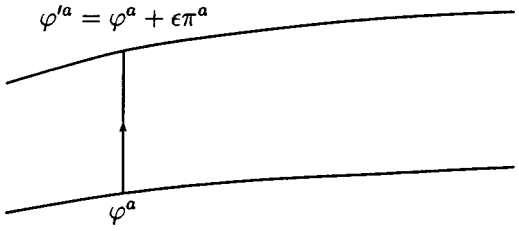
Now we want to provide a geometrical interpretation of this fact at least for the BRS charge. Let us perform an infinitesimal BRS transformation on φ^a,

$$\delta_{Q^{(B)}} \varphi^a = [\epsilon Q^{(B)}, \varphi^a] = [\epsilon i \pi^b \lambda_b, \varphi^a] = \epsilon \pi^a, \tag{A27}$$

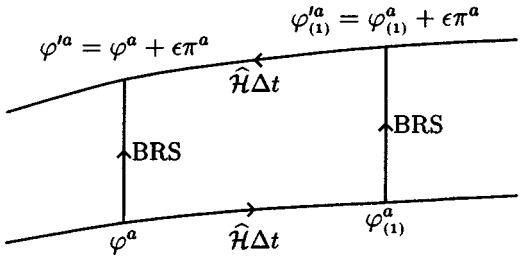
where ϵ is an infinitesimal commuting parameter. The new phase space point φ'^a reached after this transformation is

$$\varphi'^a = \varphi^a + \epsilon \pi^a. \tag{A28}$$

Remember now that π^a is a Jacobi field that means it satisfies the equation of the first variation (3.7). So if φ^a is a point on a trajectory, then φ'^a is a point on a nearby trajectory as indicated in the diagram 1 below:



From Diagram 1 above we expect that we could move from the point φ^a along its trajectory via the Hamiltonian $\hat{\mathcal{H}}_{\mathrm{BFA}}$ for an interval of time Δt, reach a point $\varphi^a_{(1)}$ and from there jump, via a BRS transformation to a point $\varphi'^a_{(1)}$ on the nearby trajectory. Moving then back on this second trajectory for an interval of time Δt we should reach the point φ'^a that we originally reached via a simple BRS transformation from φ^a. All this is illustrated in Diagram 2 below:



This diagram expresses the fact that, *in the φ-space*, the BRS transformation and $\hat{\mathcal{H}}_{\mathrm{BFA}}$ commute that is what Eq. (A26) tells us.

Let us now turn to the bosonic analogs of the susy charges $Q_H^{(B)}, \overline{Q}_H^{(B)}$. As they are linear combinations of $Q^{(B)}, \overline{Q}^{(B)}, N, \overline{N}$ and these last two charges commute with $\hat{\mathcal{H}}_{\mathrm{BFA}}$, from (A22) and (A23) we will get

$$
\begin{aligned}
[Q_H^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] &= -\pi^l \omega^{ab} \partial_b \partial_l \partial_c H \pi^c \xi_a, \\
[\overline{Q}_H^{(B)}, \hat{\mathcal{H}}_{\mathrm{BFA}}] &= -\xi_a \omega^{ab} \xi_s \omega^{st} (\partial_b \partial_t \partial_l H) \pi^l.
\end{aligned}
\tag{A29}
$$

From these expressions we gather that as before also the transformations generated by $Q_H^{(B)}$ and $\overline{Q}_H^{(B)}$ commute with those generated by $\hat{\mathcal{H}}_{\mathrm{BFA}}$ on the phase space variables φ^a. It would be interesting to check whether they behave as true supersymmetry charges that means whether

$$
[Q_H^{(B)}, \overline{Q}_H^{(B)}] = 2\hat{\mathcal{H}}_{\mathrm{BFA}}. \tag{A30}
$$

It is actually easy[7] to work out the commutators of $Q_H^{(B)}, \overline{Q}_H^{(B)}$ and the calculation gives

$$
[Q_H^{(B)}, \overline{Q}_H^{(B)}] = 2\hat{\mathcal{H}}_{\mathrm{BFA}} + 4\pi^a \omega^{\mathrm{de}} \partial_e \partial_a H \xi_{\mathrm{d}}. \tag{A31}
$$

We see that we can get the standard supersymmetry algebra if the last term on the RHS of (A31) were zero. Again this term does not contain λ_a and so on the φ^a variables we have that

$$
\delta_{Q_H^{(B)}} \delta_{\overline{Q}_H^{(B)}} \varphi^a - \delta_{\overline{Q}_H^{(B)}} \delta_{Q_H^{(B)}} \varphi^a = 2\delta_{\hat{\mathcal{H}}} \varphi^a, \tag{A32}
$$

i.e., the supersymmetry algebra holds.

Usually supersymmetry is described as the "*square root*" of the time translation. Let us find out whether there is anything like that in our bosonic case. Instead of the two charges $Q_H^{(B)}$ and $\overline{Q}_H^{(B)}$, let us build the following ones:

$$\begin{aligned} Q_1^{(B)} &= Q^{(B)} - \overline{N}^{(B)}, \\ Q_2^{(B)} &= \overline{Q}^{(B)} + N^{(B)}. \end{aligned} \tag{A33}$$

The transformations of our variables under $Q_1^{(B)}$ can be easily worked.[7] The result is

$$\begin{aligned} \delta_{Q_1^{(B)}}\varphi^a &= \epsilon\pi^a, \\ \delta_{Q_1^{(B)}}\xi_a &= \epsilon\lambda_a, \\ \delta_{Q_1^{(B)}}\pi^a &= -i\epsilon\omega^{ae}\partial_e H, \\ \delta_{Q_1^{(B)}}\lambda_a &= -i\epsilon\xi_b\omega^{be}(\partial_e\partial_a H), \end{aligned} \tag{A34}$$

where ϵ is an infinitesimal commuting parameter. Let us check whether, by performing these transformations twice, we get a time translation. Using (A34) and restricting ourselves on the original phase space φ^a, we get

$$\delta^2_{Q_1^{(B)}}\varphi^a = \delta_{Q_1^{(B)}}(\epsilon\pi^a) = -i\epsilon^2\omega^{ae}\partial_e H = -i\epsilon^2\dot{\varphi}^a. \tag{A35}$$

In the last step above we have used the equations of motion. The result seems to confirm that $Q_1^{(B)}$ is the "*square root*" of the time translation. Equation (A35) is an infinitesimal time translation if we equate $\epsilon^2 = \Delta t$. So we could say that, in order to do an infinitesimal time translation, we could perform two $Q_1^{(B)}$ transformations in a row each with "infinitesimal" parameter ϵ related to the "square root" of Δt. We find that it is curious that, at least on some hypersurfaces of our $8N$-dimensional space, we could get something analogous to a square root of a time translation, without introducing Grassmannian variables and via purely bosonic charges.

Let us now go back to geometry and to the bosonic BRS charge $Q^{(B)}$. As we have already said in the Grassmannian case the BRS charge can be identified[2] with the exterior derivative. One of the properties[8] of the exterior derivative is that it commutes with the Lie derivative. This is no longer the case for our $Q^{(B)}$ as it is proved in (A22). Even if $Q^{(B)}$ and $\mathcal{H}_{\mathrm{BFA}}$ commute in the φ-space, it is not enough. In fact the exterior derivative must commute with the Lie derivative in the full space of forms which is somehow an extension of the ordinary phase space. Actually it is the space of higher forms which has to be properly defined in the BFA case and this is what we will do next.

In Eq. (A6) we have seen that it is possible to build one-forms using the operators $\hat{\pi}^a$ instead of the Grassmannian variables c^a. The problem arises when we want to build higher forms: in fact it is difficult to define a *wedge* product $\wedge$ so that, for example, the basis $\mathrm{d}\varphi^a \wedge \mathrm{d}\varphi^b$ for two-forms is antisymmetric in the interchange $a \leftrightarrow b$. This operation was naturally incorporated in the Grassmannian formalism:[2] in fact by representing the forms $\mathrm{d}\varphi^a$ with the anticommuting variables c^a, the antisymmetry of $\mathrm{d}\varphi^a \wedge \mathrm{d}\varphi^b$ was automatically reproduced by the antisymmetry of the product $c^a c^b$. In the bosonic case we do not have Grassmannian variables and the forms $\hat{\pi}^a$ commute among themselves. Therefore we cannot represent a two-form $\mathrm{d}\varphi^a \wedge \mathrm{d}\varphi^b$ as $\hat{\pi}^a\hat{\pi}^b$, because in this way we would lose its anticommuting nature.

The way out seems to be the standard procedure used in the literature[9] on differential geometry, i.e., to introduce a tensor product among the cotangent spaces whose basis are the $\mathrm{d}\varphi^a$ and define the wedge product $\wedge$ as

$$\mathrm{d}\varphi^a \wedge \mathrm{d}\varphi^b \equiv \tfrac{1}{2}(\mathrm{d}\varphi^a \otimes \mathrm{d}\varphi^b - \mathrm{d}\varphi^b \otimes \mathrm{d}\varphi^a). \tag{A36}$$

In our case the role of the $\mathrm{d}\varphi^a$ is taken by the operator $\hat{\pi}^a$ and, since we want to build tensor products among them, we have to enlarge our Hilbert space. Originally it was made of functions $\psi(\varphi^a, \pi^a)$ belonging to the tensor product of the two Hilbert spaces spanned by $|\varphi^a\rangle$ and $|\pi^a\rangle$,

$$\mathcal{H} \equiv \mathcal{H}_\varphi \otimes \mathcal{H}_\pi . \tag{A37}$$

From now on the new Hilbert space we will use is the following one:

$$\mathcal{H}_{2N} \equiv \mathcal{H}_\varphi \otimes \mathcal{H}_{\pi_{(1)}} \otimes \mathcal{H}_{\pi_{(2)}} \otimes \cdots \otimes \mathcal{H}_{\pi_{(2N)}}, \tag{A38}$$

where we have made the tensor products of $2N$ copies of the space $\mathcal{H}_\pi$ and labeled them with $\mathcal{H}_{\pi_{(1)}}, \ldots, \mathcal{H}_{\pi_{(2N)}}$. If we limit ourselves to the case $N=1$ the space (A38) reduces to

$$\mathcal{H}_2 \equiv \mathcal{H}_\varphi \otimes \mathcal{H}_{\pi_{(1)}} \otimes \mathcal{H}_{\pi_{(2)}} \tag{A39}$$

and in this space we have that, for example, a two-form is represented as

$$\hat{F} = F_{ab}(\hat{\varphi}) \otimes \tfrac{1}{2}[\hat{\pi}^a_{(1)} \otimes \hat{\pi}^b_{(2)} - \hat{\pi}^b_{(1)} \otimes \hat{\pi}^a_{(2)}]. \tag{A40}$$

The operator (3.5) was the correct one to represent the Lie derivative, but only in the space (A37). To represent the Lie derivative on the new space (A39) we should generalize $\hat{\mathcal{H}}_{\mathrm{BFA}}$ to this new operator:

$$\hat{\mathcal{H}} \equiv \hat{\lambda}_a \omega^{ab} \partial_b H(\hat{\varphi}) \otimes \mathbf{1}_{(1)} \otimes \mathbf{1}_{(2)} - \omega^{be} \partial_e \partial_a H(\hat{\varphi}) \otimes (\hat{\pi}^a_{(1)} \hat{\xi}^{(1)}_b \otimes \mathbf{1}_{(2)} + \mathbf{1}_{(1)} \otimes \hat{\pi}^a_{(2)} \hat{\xi}^{(2)}_b). \tag{A41}$$

Using as commutators the following natural generalization of those in (3.1):

$$\begin{gathered}
[\hat{\pi}^a_{(i)}, \hat{\pi}^b_{(j)}] = 0, \\
[\hat{\xi}^{(i)}_a, \hat{\xi}^{(j)}_b] = 0, \\
[\hat{\xi}^{(i)}_a, \hat{\pi}^b_{(j)}] = i \delta^b_a \delta^{(i)}_{(j)}, \\
[\hat{\varphi}^a, \hat{\pi}^b_{(i)}] = 0, \\
[\hat{\varphi}^a, \hat{\xi}^{(i)}_b] = 0,
\end{gathered} \tag{A42}$$

it is easy[7] to see that the action of the $\hat{\mathcal{H}}$ presented in (A41) on the two-form $\hat{F}$ of (A40) is

$$[i\hat{\mathcal{H}}, \hat{F}] = \omega^{ab}[\partial_b H \partial_a F_{\mathrm{d}e} + \partial_b \partial_{\mathrm{d}} H F_{ae} + \partial_b \partial_e H F_{\mathrm{d}a}] \otimes \tfrac{1}{2}(\hat{\pi}^{\mathrm{d}}_{(1)} \otimes \hat{\pi}^e_{(2)} - \hat{\pi}^e_{(1)} \otimes \hat{\pi}^{\mathrm{d}}_{(2)}) \tag{A43}$$

and this is exactly the manner how two-forms transform under the Lie derivative.[8] Equation (A43) confirms that the choice of $\hat{\mathcal{H}}$ we made in (A41) is the correct one.

In the case $N=1$ we have only zero-, one-, and two-forms and if the two-forms are represented by Eq. (A40), how are zero- and one-forms represented? The zero-forms $\hat{G}$ and the one-forms $\hat{C}$ are, respectively,

$$\hat{G} = G(\hat{\varphi}) \otimes [\mathbf{1}_{(1)} \otimes \mathbf{1}_{(2)}], \tag{A44}$$

$$\hat{C} = C_{\mathrm{d}}(\hat{\varphi}) \otimes [\hat{\pi}^{\mathrm{d}}_{(1)} \otimes \mathbf{1}_{(2)} + \mathbf{1}_{(1)} \otimes \hat{\pi}^{\mathrm{d}}_{(2)}]. \tag{A45}$$

It is easy to prove[7] that the commutator of $i\hat{\mathcal{H}}$ with $\hat{C}$ gives the correct action of the Lie derivative on one-forms,

$$[i\hat{\mathcal{H}},\hat{C}]=(\partial_a C_{\mathrm{d}}\omega^{ab}\partial_b H+\omega^{ae}\partial_e\partial_{\mathrm{d}}HC_a)\otimes[\hat{\pi}^{\mathrm{d}}_{(1)}\otimes\mathbf{1}_{(2)}+\mathbf{1}_{(1)}\otimes\hat{\pi}^{\mathrm{d}}_{(2)}]. \tag{A46}$$

So we can conclude that, in the case $N=1$, the operator (A41) represents a good extension of the Lie derivative on the entire space of differential forms.

It is easy to generalize the $\hat{\mathcal{H}}$ of (A41) to a space with an arbitrary number N of degrees of freedom. It is the following one:

$$\hat{\mathcal{H}}\equiv\lambda_a\omega^{ab}\partial_b H\otimes\mathbf{1}^{\otimes 2N}-\omega^{be}\partial_e\partial_a H\otimes\mathbf{S}[\hat{\pi}^a\hat{\xi}_b\otimes\mathbf{1}^{\otimes(2N-1)}], \tag{A47}$$

where by $\mathbf{1}^{\otimes 2N}$ we indicate the tensor product of $2N$ identity operators, and with $\mathbf{S}$ the symmetrizer of the operators contained in the square brackets. So, for example, for $N=2$ we have

$$\begin{aligned}\mathbf{S}[\hat{\pi}^a\hat{\xi}_b\otimes\mathbf{1}^{\otimes 3}]=&\hat{\pi}^a_{(1)}\hat{\xi}^{(1)}_b\otimes\mathbf{1}_{(2)}\otimes\mathbf{1}_{(3)}\otimes\mathbf{1}_{(4)}+\mathbf{1}_{(1)}\otimes\hat{\pi}^a_{(2)}\hat{\xi}^{(2)}_b\otimes\mathbf{1}_{(3)}\otimes\mathbf{1}_{(4)}\\&+\mathbf{1}_{(1)}\otimes\mathbf{1}_{(2)}\otimes\hat{\pi}^a_{(3)}\hat{\xi}^{(3)}_b\otimes\mathbf{1}_{(4)}+\mathbf{1}_{(1)}\otimes\mathbf{1}_{(2)}\otimes\mathbf{1}_{(3)}\otimes\hat{\pi}^a_{(4)}\hat{\xi}^{(4)}_b.\end{aligned} \tag{A48}$$

Let us remember that the indices $(1),(2),\ldots,(2N)$ always indicate on which Hilbert space $\mathcal{H}_{\pi_{(i)}}$ in (A38) the operators $\hat{\pi}_{(i)}$, $\hat{\xi}^{(i)}$, and $\mathbf{1}_{(i)}$ act. In the same way it is possible to generalize the concept of differential form. An m-form in a $2N$-dimensional space is given by

$$\hat{P}\equiv\mathbf{S}\left\{\frac{1}{m!}P_{a_1\cdots a_m}(\hat{\varphi})\otimes\mathbf{A}\{\hat{\pi}^{a_1}_{(1)}\otimes\hat{\pi}^{a_2}_{(2)}\otimes\cdots\otimes\hat{\pi}^{a_m}_{(m)}\}\otimes\mathbf{1}^{\otimes(2N-m)}\right\}, \tag{A49}$$

where $\mathbf{A}$ indicates the antisymmetrizer of the basis $\hat{\pi}^{a_i}_{(i)}$ of the m cotangent spaces needed to build an m-form. The position of this m operators $\hat{\pi}$ inside the string of the $2N$ Hilbert spaces is completely arbitrary. Therefore if we do not want to choose a particular position we can symmetrize the $2N-m$ identity operators with the m operators $\hat{\pi}$ by means of the symmetrizer $\mathbf{S}$ as we did in Eq. (A45) for the one-forms. It is not difficult to prove[7] that the commutator between (A47) and (A49) reproduces the correct action of the Lie derivative on an arbitrary differential form P,

$$[i\hat{\mathcal{H}},\hat{P}]=\mathcal{L}_{(\mathrm{d}H)^\sharp}P. \tag{A50}$$

Before concluding this appendix let us notice that in the BFA approach the higher forms are not represented by *wave functions* of the theory like $\psi(\varphi,c)$ in the CPI case, but by *operators* like in (A49). In fact wave functions, in the bosonic case, are generic functions $\psi(\varphi,\pi)$ and they would not have the structure of the Grassmannian ones,

$$\psi(\varphi,c)=\psi_0(\varphi)+\psi_a(\varphi)c^a+\psi_{ab}c^ac^b+\cdots+\psi_{abc\cdots l}c^ac^bc^c\cdots c^l. \tag{A51}$$

In the CPI case it was this structure which allowed us to identify $\psi_0(\varphi)$ with zero-forms, $\psi_a(\varphi)c^a$ with one-forms, $\psi_{ab}c^ac^b$ with two-forms, etc. In the bosonic case instead the wave functions $\psi(\varphi,\pi)$ are generic functions of π and this forbids the identification with forms. Moreover, as we said in Sec. III, a one-form would be represented by $\psi(\varphi,\pi)=\psi_a(\varphi)\pi^a$ which would be not an acceptable wave function because it is not normalizable. Of course this does not mean that in the formalism given by (A47) we cannot introduce wave functions. It simply means that such wave functions cannot have the meaning of higher forms. Only operators like (A49) have this meaning.

The wave functions associated to the multiform formalism of the Hamiltonian (A47) are basically those which make up the Hilbert space (A38) and so they are $\psi(\varphi^a,\pi^a_{(1)},\pi^a_{(2)},\ldots,\pi^a_{(2N)})$. It is possible to introduce also in this space the following positive definite scalar product:

$$\langle \psi_1 | \psi_2 \rangle \equiv \int \mathrm{d}^{2N}\varphi^a \prod_{i=1}^{2N} \mathrm{d}^{2N}\pi^a_{(i)}\, \psi_1^*(\varphi,\pi)\psi_2(\varphi,\pi) \tag{A52}$$

and it is easy to prove[7] that with this product the Hamiltonian (A47) is Hermitian.

The reader may remember that our original $\hat{\mathcal{H}}_{\mathrm{BFA}}$ (3.5) was derived from the path integral formalism (2.6). Also the multiform Hamiltonian (A47) can be derived from the following path integral:

$$Z = \int \mathcal{D}\varphi^a\, \mathcal{D}\lambda_a \prod_{i=1}^{2N} \mathcal{D}\pi^a_{(i)}\, \mathcal{D}\xi^{(i)}_a \exp\left[i \int \mathrm{d}t\, \mathcal{L}_{\mathrm{MF}} \right], \tag{A53}$$

where the multiform (MF) Lagrangian $\mathcal{L}_{\mathrm{MF}}$ is

$$\mathcal{L}_{\mathrm{MF}} = \lambda_a \dot{\varphi}^a + \sum_{i=1}^{2N} \pi^a_{(i)} \dot{\xi}^{(i)}_a - \mathcal{H}_{\mathrm{MF}} \tag{A54}$$

with

$$\mathcal{H}_{\mathrm{MF}} = \lambda_a \omega^{ab} \partial_b H - \sum_{i=1}^{2N} \pi^a_{(i)} \omega^{be} \partial_e \partial_a H \xi^{(i)}_b . \tag{A55}$$

It is straightforward to check that the Hamiltonian $\mathcal{H}_{\mathrm{MF}}$ is Hermitian under the scalar product (A52). Basically in the Hamiltonian (A55) we have a set of extra variables $(\pi_{(i)}, \xi^{(i)})$ for each extra Hilbert space $\mathcal{H}_{\pi_{(i)}}$ appearing in (A38). It is actually then easier to work with the Hamiltonian $\mathcal{H}_{\mathrm{MF}}$ than with the one in (A47). We can in fact turn the $\pi^a_{(i)}, \xi^{(i)}_a$ into operators by just looking at the kinetic term of (A53) and deriving from it the commutators that we introduced by hand in (A42) plus the usual one $[\hat{\varphi}^a, \hat{\lambda}_b] = i\delta^a_b$. This confirms that the path integral (A53) is basically the one behind the operatorial formalism (A47). *Unfortunately this path integral does not appear to have a "natural" interpretation differently than the one in* (2.6), *in the sense that the latter is naturally related to* (2.3) *and* (2.1) *which are just Dirac deltas on the classical paths*. These Dirac deltas are natural objects in a functional approach to CM because they just give weight one to classical paths and weight zero to nonclassical ones. Nothing like that can be done for the path integral (A53) which can be turned into a Dirac delta of the equations of motion like in (2.3) but it gets multiplied not by one determinant but by $2N$ of them. This structure does not allow us to pass to the Dirac deltas of the classical trajectories appearing in (2.1). So somehow the path integral (A53) does not have a simple intuitive understanding. *This is the price we pay: we have a formalism with a positive definite scalar product and a Hermitian Hamiltonian but a physical understanding is lacking*. If on the contrary we keep the intuitive single particle path integral associated to the Hilbert space (A37) then the tensor product structure $\otimes$, needed to build higher forms like in (A49), has to be given from outside and is not provided directly by the path integral. On the contrary in the original CPI case[2] the whole formalism, even for higher forms, has an intuitive understanding and construction (because it can be reduced to a Dirac delta on classical paths), and no extra structure has to be brought in from outside, but the price we paid is that we have to give up one of the two conditions: either the positive definiteness of the scalar product or the Hermiticity of the Hamiltonian.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Gauge symmetry of the *N*-body problem in the Hamilton–Jacobi approach

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(Received 21 June 2003; accepted 20 August 2003)

In most books the Delaunay and Lagrange equations for the orbital elements are derived by the Hamilton–Jacobi method: one begins with the two-body Hamilton equations in spherical coordinates, performs a canonical transformation to the orbital elements, and obtains the Delaunay system. A standard trick is then used to generalize the approach to the *N*-body case. We reexamine this step and demonstrate that it contains an implicit condition which restricts the dynamics to a $9(N-1)$-dimensional submanifold of the $12(N-1)$-dimensional space spanned by the elements and their time derivatives. The tacit condition is equivalent to the constraint that Lagrange imposed ''by hand'' to remove the excessive freedom, when he was deriving his system of equations by variation of parameters. It is the condition of the orbital elements being osculating, i.e., of the instantaneous ellipse (or hyperbola) being always tangential to the physical velocity. Imposure of any supplementary condition different from the Lagrange constraint (but compatible with the equations of motion) is legitimate and will not alter the physical trajectory or velocity (though will alter the mathematical form of the planetary equations). This freedom of nomination of the supplementary constraint reveals a gauge-type internal symmetry instilled into the equations of celestial mechanics. Existence of this internal symmetry has consequences for the stability of numerical integrators. Another important aspect of this freedom is that any gauge different from that of Lagrange makes the Delaunay system noncanonical. In a more general setting, when the disturbance depends not only upon positions but also upon velocities, there is a ''generalized Lagrange gauge'' wherein the Delaunay system is symplectic. This special gauge renders orbital elements that are osculating in the phase space. It coincides with the regular Lagrange gauge when the perturbation is velocity independent.
[DOI: 10.1063/1.1622447]

I. EULER AND LAGRANGE

A. The history

The planetary equations, which describe the evolution of the orbital elements, constitute the cornerstone of the celestial mechanics. Description of orbits in the language of Keplerian elements (rather than in terms of the Cartesian coordinates) is not only physically illustrative but also provides the sole means for analysis of resonant interactions. These equations exist in a variety of equivalent forms (those of Lagrange, Delaunay, Gauss, Poincare) and can be derived by several different methods.

The earliest sketch of the method dates back to Euler's paper of 1748, which addresses the perturbations exerted upon one another by Saturn and Jupiter. In the publication on the Lunar

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motion, dated by 1753, Euler derived the equations for the longitude of the node, Ω, the inclination, i, and the quantity $p \equiv a(1-e^2)$. Time derivatives of these three elements were expressed through the components of the disturbing force. Sixty years later the method was amended by Gauss who wrote down similar equations for the other three elements and, thus, obtained what we now call the Gauss system of planetary equations. The history of this scientific endeavour was studied by Subbotin (1958), who insists that the Gauss system of planetary equations should rather be called Euler system. A modern but still elementary derivation of this system belongs to Burns (1976).

In his mémoires of 1778, which received an honorable prize from the Académie des Sciences of Paris, Lagrange employed the method of variation of parameters (VOP) to express the time derivatives of the orbital elements through the disturbing functions' partial derivatives with respect to the Cartesian coordinates. In his mémoire of 1783, Lagrange furthered this approach, while in Lagrange (1808, 1809, 1810) these equations acquired their final, closed, shape: they expressed the orbital elements' evolution in terms of the disturbing potentials' derivatives with respect to the elements. Lagrange's derivation rested upon an explicit imposure of the osculation condition, i.e., of a supplementary vector equation (called the Lagrange constraint) which guaranteed that the instantaneous ellipses (in the case of bound motions) or hyperbolae (in the case of flyby ones) are always tangential to the physical trajectory. Though it has been long known (and, very possibly, appreciated by Lagrange himself) that the choice of the supplementary conditions is essentially arbitrary, and though a couple of particular examples of use of nonosculating elements appeared in the literature (Goldreich, 1965; Brumberg *et al.*, 1971; Borderies and Longaretti, 1987), a comprehensive study of the associated freedom has not appeared until very recently (Efroimsky, 2002, 2003).

In the middle of the 19th century Jacobi applied a canonical-transformation-based procedure (presently known as the Hamilton–Jacobi approach) to the orbital dynamics, and offered a method of deriving the Lagrange system. This technique is currently regarded standard and is offered in many books. Though the mathematical correctness of the Hamilton–Jacobi method is beyond doubt, its application to celestial mechanics contains an aspect that has long been overlooked (at least, in the astronomical literature). This overlooked question is as follows: where in the Hamilton–Jacobi derivation of the planetary equations is the Lagrange constraint tacitly imposed, and what happens if we impose a different constraint? This issue will be addressed in our article.

B. The gauge freedom

Mathematically, we shall concentrate on the *N*-body problem of celestial mechanics, a problem that for each body can be set as

$$\ddot{\vec{\mathbf{r}}} + \frac{\mu}{r^2}\frac{\vec{\mathbf{r}}}{r} = \Delta\vec{\mathbf{F}}, \tag{1}$$

$\Delta\vec{\mathbf{F}}$ being the disturbing force that vanishes in the (reduced) two-body case and $\vec{\mathbf{r}}$ being the position relative to the primary, and μ standing for $G(m_{\text{planet}}+m_{\text{sun}})$. A solution to the unperturbed problem is a Keplerian ellipse (or hyperbola)

$$\vec{\mathbf{r}} = \vec{\mathbf{f}}(C_1,\ldots,C_6,t) \tag{2}$$

parametrized by six constants (which may be, for example, the Kepler or Delaunay elements). In the framework of the VOP approach it gives birth to the ansatz

$$\vec{\mathbf{r}} = \vec{\mathbf{f}}(C_1(t),\ldots,C_6(t),t), \tag{3}$$

the ''constants'' now being time dependent and the functional form of $\vec{\mathbf{f}}$ remaining the same as in (2). Substitution of (3) into (1) results in three scalar equations for six independent functions $C_i(t)$. In order to make the problem defined, Lagrange applied three extra conditions

$$\sum_i \frac{\partial \vec{\mathbf{f}}}{\partial C_i}\frac{dC_i}{dt}=0 \tag{4}$$

that are often referred to as ''the Lagrange constraint.'' This constraint guarantees osculation, i.e., that the functional dependence of the perturbed velocity upon the ''constants'' is the same as that of the unperturbed one. This happens because the physical velocity is

$$\dot{\vec{\mathbf{r}}}=\vec{\mathbf{g}}+\sum_i \frac{\partial \vec{\mathbf{f}}}{\partial C_i}\frac{dC_i}{dt}, \tag{5}$$

where $\vec{\mathbf{g}}$ stands for the unperturbed velocity that emerged in the two-body setting. This velocity is, by definition, a partial derivative of $\vec{\mathbf{f}}$ with respect to the last variable:

$$\vec{\mathbf{g}}(C_1,\ldots,C_6,t)\equiv\frac{\partial \vec{\mathbf{f}}(C_1,\ldots,C_6,t)}{\partial t}. \tag{6}$$

This choice of supplementary conditions is convenient, but not at all necessary. A choice of any other three scalar relations (consistent with one another and with the equations of motion) will give the same physical trajectory, even though the appropriate solution for nonosculating variables C_i will differ from the solution for osculating ones.

Efroimsky (2002, 2003) suggested to relax the Lagrange condition and to consider

$$\sum_i \frac{\partial \vec{\mathbf{f}}}{\partial C_i}\frac{dC_i}{dt}=\vec{\mathbf{\Phi}}(C_1,\ldots,C_6,t), \tag{7}$$

$\vec{\mathbf{\Phi}}$ being an arbitrary function of time, ''constants'' C_i and their time derivatives of all orders. For practical reasons it is convenient to restrict $\vec{\mathbf{\Phi}}$ to a class of functions that depend upon the time and the ''constants'' only. (The dependence upon derivatives would yield higher-than-first-order time derivatives of the C_i in the subsequent developments, which would require additional initial conditions, beyond those on $\vec{\mathbf{r}}$ and $\dot{\vec{\mathbf{r}}}$, to be specified in order to close the system.) Different choices of $\vec{\mathbf{\Phi}}$ entail different forms of equations for C_i and, therefore, different mathematical solutions in terms of these ''constants.'' A transition from one such solution to another will, though, be a mere reparametrization of the orbit. The physical orbit itself will remain invariant. Such invariance of the physical content of a theory under its mathematical reparametrizations is called gauge symmetry. On the one hand, it is in a close analogy with the gradient invariance of the Maxwell electrodynamics and other field theories. On the other hand, it illustrates some general mathematical structure emerging in the ODE theory (Newman and Efroimsky, 2003).

If the Lagrange gauge (4) is fixed, the parameters obey the equation

$$\sum_j [C_n\ \ C_j]\frac{dC_j}{dt}=\frac{\partial \vec{\mathbf{f}}}{\partial C_n}\Delta\vec{\mathbf{F}}, \tag{8}$$

$[C_n\ C_j]$ standing for the unperturbed (i.e., defined as in the two-body case) Lagrange brackets:

$$[C_n\ \ C_j]\equiv\frac{\partial \vec{\mathbf{f}}}{\partial C_n}\frac{\partial \vec{\mathbf{g}}}{\partial C_j}-\frac{\partial \vec{\mathbf{f}}}{\partial C_j}\frac{\partial \vec{\mathbf{g}}}{\partial C_n}. \tag{9}$$

To arrive at formula (8), one should, according to Lagrange (1778, 1783, 1808, 1809), differentiate (5), insert the outcome into (1), and then combine the result with the Lagrange constraint (4). (In the modern literature, this derivation can be found, for example, in Brouwer and Clemence (1961), Efroimsky (2002, 2003), Newman and Efroimsky (2003), Efroimsky and Goldreich (2003).) In the

simplest case the perturbing force depends only upon positions and is conservative: $\Delta\vec{\mathbf{F}} = \partial R(\vec{\mathbf{r}})/\partial\vec{\mathbf{r}}$. Then the right-hand side of (8) will reduce to the partial derivative of the disturbing function $R(\vec{\mathbf{r}})$ with respect to C_n, whereafter inversion of the Lagrange-bracket matrix will entail' the Lagrange system of planetary equations (for C_i being the Kepler elements) or the Delaunay system (for the parameters chosen as the Delaunay elements).

As explained in Efroimsky (2003), in an arbitrary gauge $\vec{\mathbf{\Phi}}$ Eq. (8) will generalize to its gauge-invariant form

$$\sum_j [C_n \;\; C_j] \frac{dC_j}{dt} = \frac{\partial\vec{\mathbf{f}}}{\partial C_n}\Delta\vec{\mathbf{F}} - \frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{d\vec{\mathbf{\Phi}}}{dt} - \frac{\partial\vec{\mathbf{g}}}{\partial C_n}\vec{\mathbf{\Phi}}, \tag{10}$$

the Lagrange brackets $[C_n \; C_j]$ being still defined through (9). If we agree that $\vec{\mathbf{\Phi}}$ is a function of both time and the parameters C_i, but not of their derivatives, then the right-hand side of (10) will implicitly contain the first time derivatives of C_i. It will then be reasonable to move them into the left-hand side. Hence, (10) will be reshaped into

$$\sum_j \left([C_n \;\; C_j] + \frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{\partial\vec{\mathbf{\Phi}}}{\partial C_j} \right) \frac{dC_j}{dt} = \frac{\partial\vec{\mathbf{f}}}{\partial C_n}\Delta\vec{\mathbf{F}} - \frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{\partial\vec{\mathbf{\Phi}}}{\partial t} - \frac{\partial\vec{\mathbf{g}}}{\partial C_n}\vec{\mathbf{\Phi}}. \tag{11}$$

This is the general form of the gauge-invariant perturbation equations of celestial mechanics, which follows from the VOP method, for an arbitrary disturbing force $\Delta\vec{\mathbf{F}}(\vec{\mathbf{r}},\dot{\vec{\mathbf{r}}},t)$ and under the simplifying assumption that the arbitrary gauge function $\vec{\mathbf{\Phi}}$ is chosen to depend on the time and the parameters C_i, but not on their derivatives.

For performing further algebraic developments of (10) and (11), let us decide what sort of interactions will fall within the realm of our interest. On general grounds, it would be desirable to deal with forces that permit description in the language of Lagrangians and Hamiltonians.

II. DELAUNAY

A. Perturbations of Lagrangians and Hamiltonians

Contributions to the disturbing force $\Delta\vec{\mathbf{F}}$ generally consist of two types, physical and inertial. Inputs can depend upon velocity as well as upon positions. As motivation for this generalization we consider two practical examples. One is the problem of orbital motion around a precessing planet: the orbital elements are defined in the precessing frame, while the velocity-dependent fictitious forces play the role of the perturbation (Goldreich, 1965; Brumberg *et al.*, 1971; Efroimsky and Goldreich, 2003). Another example is the relativistic two-body problem where the relativistic correction to the force is a function of both velocity and position, as explained, for example, in Brumberg (1992) and Klioner and Kopeikin (1994). (It turns out that in relativistic dynamics even the two-body problem is disturbed, the relativistic correction acting as disturbance. This yields the gauge symmetry that will cause ambiguity in defining the orbital elements of a binary.) Finally, we shall permit the disturbances to bear an explicit time dependence. Such a level of generality will enable us to employ our formalism in noninertial coordinate systems.

Let the unperturbed Lagrangian be $\dot{\vec{\mathbf{r}}}^2/2 - U(\vec{\mathbf{r}})$. The disturbed motion will be described by the new, perturbed, Lagrangian

$$\mathcal{L} = \frac{\dot{\vec{\mathbf{r}}}^2}{2} - U(\vec{\mathbf{r}}) + \Delta\mathcal{L}(\vec{\mathbf{r}},\dot{\vec{\mathbf{r}}},t), \tag{12}$$

and the appropriately perturbed canonical momentum and Hamiltonian,

$$\vec{\mathbf{p}}=\dot{\vec{\mathbf{r}}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}, \tag{13}$$

$$\mathcal{H}=\vec{\mathbf{p}}\dot{\vec{\mathbf{r}}}-\mathcal{L}=\frac{\vec{\mathbf{p}}^2}{2}+U+\Delta\mathcal{H}, \quad \Delta\mathcal{H}\equiv-\Delta\mathcal{L}-\frac{1}{2}\left(\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)^2. \tag{14}$$

The Euler–Lagrange equations written for the perturbed Lagrangian (12) are

$$\ddot{\vec{\mathbf{r}}}=-\frac{\partial U}{\partial\vec{\mathbf{r}}}+\Delta\vec{\mathbf{F}}, \tag{15}$$

where the disturbing force is given by

$$\Delta\vec{\mathbf{F}}\equiv\frac{\partial\Delta\mathcal{L}}{\partial\vec{\mathbf{r}}}-\frac{d}{dt}\left(\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right). \tag{16}$$

We see that in the absence of velocity dependence the perturbation of the Lagrangian plays the role of disturbing function. Generally, though, the disturbing force is not equal to the gradient of $\Delta\mathcal{L}$, but has an extra term called into being by the velocity dependence.

As we already mentioned, this setup is sufficiently generic. For example, it is convenient for description of a satellite orbiting a wobbling planet: the inertial forces, which emerge in the planet-related noninertial frame, will nicely fit in the above formalism.

It is worth emphasizing once again that, in the case of velocity-dependent disturbances, the disturbing force is equal neither to the gradient of the Lagrangian's perturbation nor to the gradient of negative Hamiltonian's perturbation. This is an important thing to remember when comparing results obtained by different techniques. For example, in Goldreich (1965) the term ''disturbing function'' was used for the negative perturbation of the Hamiltonian. For this reason, the gradient of a so defined disturbing function was not equal to the disturbing force. A comprehensive comparison of the currently developed theory with that offered in Goldreich (1965) will be presented in a separate publication (Efroimsky and Goldreich, 2003), where we shall demonstrate that the method used there was equivalent to fixing a special gauge (one described in Sec. II C of this article).

B. Gauge-invariant planetary equations

Insertion of the generic force (16) into (10) will bring us

$$\sum_j\,[C_n\;\;C_j]\frac{dC_j}{dt}=\frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{\partial\Delta\mathcal{L}}{\partial\vec{\mathbf{r}}}-\frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\frac{\partial\vec{\mathbf{g}}}{\partial C_n}\vec{\mathbf{\Phi}}. \tag{17}$$

If we recall that, for a velocity-dependent disturbance,

$$\frac{\partial\Delta\mathcal{L}}{\partial C_n}=\frac{\partial\Delta\mathcal{L}}{\partial\vec{\mathbf{r}}}\frac{\partial\vec{\mathbf{f}}}{\partial C_n}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial\dot{\vec{\mathbf{r}}}}{\partial C_n}=\frac{\partial\Delta\mathcal{L}}{\partial\vec{\mathbf{r}}}\frac{\partial\vec{\mathbf{f}}}{\partial C_n}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial(\vec{\mathbf{g}}+\vec{\mathbf{\Phi}})}{\partial C_n}, \tag{18}$$

then equality (17) will look like this:

$$\sum_j\,[C_n\;\;C_j]\frac{dC_j}{dt}=\frac{\partial\Delta\mathcal{L}}{\partial C_n}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial\vec{\mathbf{\Phi}}}{\partial C_n}-\frac{\partial\vec{\mathbf{f}}}{\partial C_n}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\frac{\partial\vec{\mathbf{g}}}{\partial C_n}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right). \tag{19}$$

After subsequent addition and subtraction of $\frac{1}{2}\partial((\partial\Delta\mathcal{L}/\partial\dot{\vec{\mathbf{r}}})^2)/\partial\mathcal{C}_n$ on the right-hand side, the gauge function $\vec{\mathbf{\Phi}}$ will everywhere appear in the company of $+\partial(\Delta\mathcal{L})/\partial\dot{\vec{\mathbf{r}}}$:

$$\sum_j \left([C_n \;\; C_j] + \frac{\partial \vec{\mathbf{f}}}{\partial C_n} \frac{\partial}{\partial C_j} \left(\frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}} + \vec{\mathbf{\Phi}} \right) \right) \frac{dC_j}{dt}$$

$$= \frac{\partial}{\partial C_n} \left[\Delta \mathcal{L} + \frac{1}{2} \left(\frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}} \right)^2 \right] - \left(\frac{\partial \vec{\mathbf{g}}}{\partial C_n} + \frac{\partial \vec{\mathbf{f}}}{\partial C_n} \frac{\partial}{\partial t} + \frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}} \frac{\partial}{\partial C_n} \right) \left(\vec{\mathbf{\Phi}} + \frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}} \right), \tag{20}$$

the sum in square brackets being equal to $-\Delta \mathcal{H}$. While (11) expressed the VOP method in the most generic form it can have in terms of disturbing forces $\Delta \vec{\mathbf{F}}(\vec{\mathbf{r}}, \dot{\vec{\mathbf{r}}}, t)$, Eq. (20) furnishes the most general form in terms of the Lagrangian perturbation $\Delta \mathcal{L}(\vec{\mathbf{r}}, \dot{\vec{\mathbf{r}}}, t)$ (under the simplifying assumption that the arbitrary gauge function $\vec{\mathbf{\Phi}}$ is set to depend only upon the time and the parameters C_i, but not upon their derivatives).

The Lagrange brackets in (19) are gauge-invariant; they contain only functions $\vec{\mathbf{f}}$ and $\vec{\mathbf{g}}$ that were defined in the unperturbed, two-body, setting. This enables us to exploit the well-known expressions for the inverse of this matrix. These look most simple (and are either zero or unity) in the case when one chooses as the ''constants'' the Delaunay set of orbital variables. As is well known, this simplicity of the Lagrange and their inverse, Poisson, brackets of the Delaunay elements is the proof of these elements' canonicity in the unperturbed, two-body, problem. When only a position-dependent disturbing function $R(\vec{\mathbf{r}}) = \Delta \mathcal{L}(\vec{\mathbf{r}})$ is ''turned on,'' the Delaunay elements still remain canonical, provided the Lagrange gauge is imposed. This happens because, as is well known (Brouwer and Clemence, 1961), the equations of motion together with the Lagrange constraint yield, in that case, the following equation,

$$\sum_j [C_n \;\; C_j] \frac{dC_j}{dt} = \frac{\partial \Delta \mathcal{L}}{\partial C_n}, \quad \Delta \mathcal{L} = \Delta \mathcal{L}(\vec{\mathbf{f}}(C_1, \ldots, C_6, t)) = R(\vec{\mathbf{f}}(C_1, \ldots, C_6, t)), \tag{21}$$

which, is its turn, results in the standard Delaunay system.

In our case, though, the perturbation depends also upon velocities; beside this, the gauge $\vec{\mathbf{\Phi}}$ is set arbitrary. Then our Eq. (20) will entail the gauge-invariant Lagrange-type and Delaunay-type systems of equations that are presented in Appendix A. Interestingly, the gauge-invariant Delaunay-type system is, generally, nonsymplectic. It regains the canonical form only in one special gauge considered below (a gauge which coincides with the Lagrange gauge when the perturbation bears no velocity dependence). This can be proven by a direct substitution of that special gauge condition into the gauge-invariant Delaunay-type system given in Appendix A. An easier way would be to fix the gauge already in (20), and this is what we shall do in the next subsection.

C. The generalized Lagrange gauge: Gauge wherein the Delaunay-type system becomes canonical

We transformed (17) into (20) for two reasons: to single out the negative perturbation of the Hamiltonian and to reveal the advantages of the gauge

$$\vec{\mathbf{\Phi}} = -\frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}}, \tag{22}$$

which reduces to $\vec{\mathbf{\Phi}} = 0$ for velocity-independent perturbations. The first remarkable peculiarity of (22) is that in this gauge the canonical momentum $\vec{\mathbf{p}}$ is equal to $\vec{\mathbf{g}}$ [as can be seen from (5) and (13)]:

$$\vec{\mathbf{g}} = \dot{\vec{\mathbf{r}}} - \vec{\mathbf{\Phi}} = \dot{\vec{\mathbf{r}}} + \frac{\partial \Delta \mathcal{L}}{\partial \dot{\vec{\mathbf{r}}}} = \vec{\mathbf{p}}. \tag{23}$$

We see that in this gauge not the velocity but the momentum in the disturbed setting is the same function of time and ''constants'' as it used to be in the unperturbed, two-body case. Stated differently, the instantaneous ellipses (or hyperbolae) defined in this gauge will osculate the orbit **in the phase space**. For this reason our special gauge (22) will be called the ''generalized Lagrange gauge.''

Another good feature of (22) is that in this gauge Eq. (20) acquires an especially simple form:

$$\sum_j [C_n \;\; C_j] \frac{dC_j}{dt} = -\frac{\partial \Delta \mathcal{H}}{\partial C_n}, \tag{24}$$

whose advantage lies not only in its brevity, but also in the invertibility of the matrix emerging on its left-hand side.

As already mentioned above, the gauge invariance of definition (9) enables us to employ the standard (Lagrange-gauge) expressions for $[C_n \; C_j]^{-1}$ and, thus, to get the planetary equations by inverting matrix $[C_n \; C_j]$ in (19). The resulting gauge-invariant Lagrange- and Delaunay-type systems are presented in Appendix A. In the special gauge (22), however, the situation is much better. Comparing (21) with (24), we see that in the general case of an arbitrary $R = \Delta \mathcal{L}(\vec{\mathbf{r}}, \dot{\vec{\mathbf{r}}}, t)$ one arrives from (24) to the same equations as from (21), except that now they will contain $-\Delta \mathcal{H}$ instead of $R = \Delta \mathcal{L}$. These will be the Delaunay-type equation in the generalized Lagrange gauge:

$$\frac{dL}{dt} = \frac{\partial \Delta \mathcal{H}}{\partial(-M_o)}, \quad \frac{d(-M_o)}{dt} = -\frac{\partial \Delta \mathcal{H}}{\partial L}, \tag{25}$$

$$\frac{dG}{dt} = \frac{\partial \Delta \mathcal{H}}{\partial(-\omega)}, \quad \frac{d(-\omega)}{dt} = -\frac{\partial \Delta \mathcal{H}}{\partial G}, \tag{26}$$

$$\frac{dH}{dt} = \frac{\partial \Delta \mathcal{H}}{\partial(-\Omega)}, \quad \frac{d(-\Omega)}{dt} = -\frac{\partial \Delta \mathcal{H}}{\partial H}, \tag{27}$$

where

$$L \equiv \mu^{1/2} a^{1/2}, \quad G \equiv \mu^{1/2} a^{1/2} (1-e^2)^{1/2}, \quad H \equiv \mu^{1/2} a^{1/2} (1-e^2)^{1/2} \cos i. \tag{28}$$

We see that in this special gauge the Delaunay-type equations indeed become canonical, and the role of the effective new Hamiltonian is played exactly by the Hamiltonian perturbation which emerged earlier in (14).

Thus we have proven an interesting **THEOREM: Even though the gauge-invariant Delaunay-type system (A7)–(A12) is not generally canonical, it becomes canonical in one special gauge (22) which we call the "generalized Lagrange gauge."** This theorem can be proved in a purely Hamiltonian language, as is done in Sec. III C.

III. HAMILTON AND JACOBI

A. The concept

A totally different approach to derivation of the planetary equations is furnished by the technique worked out in 1834–1835 by Hamilton and refined several years later by Jacobi. In the lecture course shaped by 1842 and published as a book in 1866, Jacobi formulated his famous theorem and applied it to the celestial motions. Jacobi chose orbital elements that were some combinations of the Keplerian ones. His planetary equations can be easily transformed into the Lagrange system by the differentiation chain rule (Subbotin, 1968). Later authors used this method for a direct derivation of the Lagrange and Delaunay systems, and thus the Hamilton–Jacobi approach became a part and parcel of almost any course in celestial mechanics. To some of these

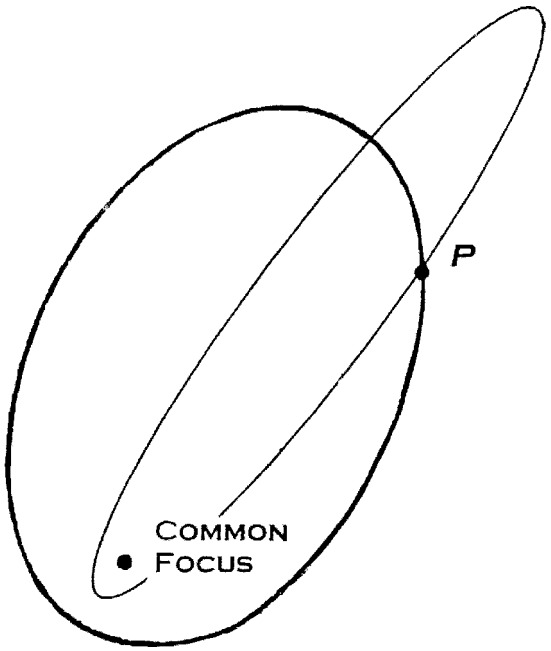

FIG. 1. These two coplanar ellipses share one of their foci and are assumed to rotate about this common focus in the same direction, always remaining within their plane. Suppose that the rotation of one ellipse is faster than that of the other, and that a planet is located at one of the points of these ellipses' intersection, *P*, and that the rotation of the ellipses is such that the planet is always at the instantaneous point of their intersection. We may say that the planet is swiftly moving along the slower rotating ellipse, while it would be equally legitimate to state that the planet is slowly moving along the fast-rotating ellipse. Both interpretations are valid, because one can divide, in an infinite number of ways, the actual motion of the planet into a motion along some ellipse and a simultaneous evolution of that ellipse. The Lagrange constraint (4) singles out, of all the multitude of evolving ellipses, that unique ellipse which is always tangential to the total, physical, velocity of the planet.

sources we shall refer below. The full list of pertinent references would be endless, so it is easier to single out a couple of books that break the code by offering alternative proofs: these exceptions are Kaula (1968) and Brouwer and Clemence (1961).

Brouwer and Clemence (1961) use the VOP method [like in Lagrange (1808, 1809, 1810)], which makes the imposition of the Lagrange constraint explicit. Kaula (1968) undertakes, by means of the differentiation chain rule, a direct transition from the Hamilton equations in a Cartesian frame to those in terms of orbital elements. As explained in Efroimsky (2002, 2003), in Kaula's treatment the Lagrange constraint was imposed tacitly.

It is far less easy to understand where the implicit gauge fixing is used in the Hamilton–Jacobi technique. This subtlety of the Hamilton–Jacobi method is so well camouflaged that through the century and a half of the method's life this detail has never been brought to light (at least, in the astronomical literature). The necessity of such a constraint is evident: one has to choose one out of infinitely many sets of orbital elements describing the physical trajectory. Typically, one prefers the set of orbital elements that osculates with the trajectory, so that the physical orbit be always tangential to the instantaneous ellipse, in the case of bound orbits, or to the instantaneous hyperbola, in the case of flybys. This point is most easily illustrated by the following simple example depicted on Fig. 1. Consider two coplanar ellipses with one common focus. Let both ellipses rotate, in the same direction within their plane, about the shared focus; and let us assume that the rotation of one ellipse is faster than that of the other. Now imagine that a planet is located at one of the points of these ellipses' intersection, and that the rotation of the ellipses is such that the planet is always at the instantaneous point of their intersection. One observer will say that the planet is swiftly moving along the slower rotating ellipse, while another observer will argue that the planet is slowly moving along the fast-rotating ellipse. Both viewpoints are acceptable, be-

cause one can divide, in an infinite number of ways, the actual motion of the planet into a motion along some ellipse and a simultaneous evolution of that ellipse. The Lagrange constraint (4) singles out, of all the multitude of evolving ellipses, that unique ellipse which is always tangential to the total (physical) velocity of the body. This way of gauge fixing is natural but not necessary. Besides, as we already mentioned, the chosen gauge (4) will not be preserved in the course of numerical computations. Sometimes osculating elements do not render an intuitive picture of the motion. In such situations other elements are preferred. One such example is a circular orbit about an oblate planet. The osculating ellipse precesses with the angular velocity of the satellite, and its eccentricity is proportional to the oblateness factor J_2. Under these circumstances the so-called geometric elements are more convenient than the osculating ones (Borderies and Longaretti 1987).

We remind the reader that the Hamilton–Jacobi treatment is based on the simple facts that the same motion can be described by different mutually interconnected canonical sets $(q,p,\mathcal{H}(q,p))$ and $(Q,P,\mathcal{H}^*(Q,P))$, and that fulfillment of the Hamilton equations along the trajectory makes the infinitesimally small quantities

$$d\theta = p\,dq - \mathcal{H}\,dt \tag{29}$$

and

$$d\tilde{\theta} = P\,dQ - \mathcal{H}^*\,dt \tag{30}$$

perfect differentials. Subtraction of the former from the latter shows that their difference,

$$-dW \equiv d\tilde{\theta} - d\theta = P\,dQ - p\,dq - (\mathcal{H}^* - \mathcal{H})\,dt, \tag{31}$$

is a perfect differential, too. Here q, p, Q, and P contain N components each. If we start with a system described by $(q,p,\mathcal{H}(q,p))$, it is worth looking for such a reparametrization $(Q,P,\mathcal{H}^*(Q,P))$ that the new Hamiltonian H^* is constant in time, because in these variables the canonical equations simplify. Especially convenient is to find a transformation that nullifies the new Hamiltonian $\mathcal{H}^*$, for in this case the new canonical equations will render the variables (Q, P) constant. One way of seeking such transformations is to consider W as a function of only q, Q, and t. Under this assertion, the above equation will entail

$$-\frac{\partial W}{\partial t}\,dt - \frac{\partial W}{\partial Q}\,dQ - \frac{\partial W}{\partial q}\,dq = P\,dQ - p\,dq + (\mathcal{H} - \mathcal{H}^*)\,dt, \tag{32}$$

whence

$$P = -\frac{\partial W}{\partial Q}, \quad p = \frac{\partial W}{\partial q}, \quad \mathcal{H} + \frac{\partial W}{\partial t} = \mathcal{H}^*. \tag{33}$$

The function W can be then found by solving the Jacobi equation

$$\mathcal{H}\left(q, \frac{\partial W}{\partial q}, t\right) + \frac{\partial W}{\partial t} = \mathcal{H}^*, \tag{34}$$

where $\mathcal{H}^*$ is a constant. It is very convenient to make it equal to zero. Then the above equation can be easily solved in the unperturbed (reduced) two-body setting. This solution, which has long been known, is presented, in a very compact form, in Appendix B. It turns out that, if the spherical coordinates and their conjugate momenta are taken as a starting point, then the eventual canonical variables Q, P corresponding to $\mathcal{H}^*(Q,P) = 0$ are the Delaunay elements:

$$Q_1 \equiv L = \sqrt{\mu a}, \quad P_1 = -M_o\,,$$

$$Q_2 \equiv G = \sqrt{\mu a(1-e^2)}, \quad P_2 = -\omega, \tag{35}$$

$$Q_3 \equiv H = \sqrt{\mu a(1-e^2)}\cos i, \quad P_3 = -\Omega.$$

B. Where can free cheese be found?

The transition from two-body to *N*-body celestial mechanics is presented in numerous books. However, none of them explain how the Lagrange constraint is implicitly involved in the formalism.

Before we move on, let us cast a look back at what has been accomplished in the two-body case. We started out with a Hamiltonian problem $(q,p,\mathcal{H})$ and reformulated its equations of motion

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}, \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial q} \tag{36}$$

in terms of another set $(Q,P,\mathcal{H}^*)$:

$$\begin{aligned} q &= \phi(Q,P,t), \\ p &= \psi(Q,P,t), \end{aligned} \tag{37}$$

so that the above equations are mathematically equivalent to the new system

$$\dot{Q} = \frac{\partial \mathcal{H}^*}{\partial P}, \quad \dot{P} = -\frac{\partial \mathcal{H}^*}{\partial Q}. \tag{38}$$

The simple nature of the two-body setting enabled us to carry out this transition so that our new Hamiltonian $\mathcal{H}^*$ vanishes and the variables Q and P are, therefore, constants. This was achieved by means of a transformation-generating function $W(q,Q,t)$ obeying the Jacobi equation (34). After formula (B12) for this function is written down, the explicit form of dependence (37) can be found through the relations $P = -\partial W/\partial Q$. This is given by (B15).

To make this machinery function in an *N*-body setting, let us first consider a disturbed two-body case. The number of degrees of freedom is still the same (three coordinates q and three conjugate momenta p), but the initial Hamiltonian is perturbed:

$$\dot{q} = \frac{\partial(\mathcal{H}+\Delta\mathcal{H})}{\partial p}, \quad \dot{p} = -\frac{\partial(\mathcal{H}+\Delta\mathcal{H})}{\partial q}. \tag{39}$$

Trying to implement the Hamilton-Jacobi method (32)–(34), for the new Hamiltonians $(\mathcal{H}+\Delta\mathcal{H})$, $(\mathcal{H}^*+\Delta\mathcal{H})$ and for some generating function $V(q,Q,t)$, we shall arrive at

$$-\frac{\partial V}{\partial t}dt - \frac{\partial V}{\partial Q}dQ - \frac{\partial V}{\partial q}dq = P\,dQ - p\,dq + [(\mathcal{H}+\Delta\mathcal{H}) - (\mathcal{H}^*+\Delta\mathcal{H})]dt, \tag{40}$$

$$P = -\frac{\partial V}{\partial Q}, \quad p = \frac{\partial V}{\partial q}, \quad \mathcal{H}+\Delta\mathcal{H}+\frac{\partial V}{\partial t} = \mathcal{H}^*+\Delta\mathcal{H}, \tag{41}$$

$$\mathcal{H}\left(q, \frac{\partial V}{\partial q}, t\right) + \frac{\partial V}{\partial t} + \mathcal{H}^*. \tag{42}$$

We see that V obeys the same equation as W and, therefore, may be chosen to coincide with it. Hence, the new, perturbed, solution (q,p) will be expressed through the perturbed "constants" $Q(t)$ and $P(t)$ in the same fashion as the old, undisturbed, q and p were expressed through the old constants Q and P:

$$\begin{aligned} q &= \phi(Q(t),P(t),t), \\ p &= \psi(Q(t),P(t),t), \end{aligned} \tag{43}$$

ϕ and ψ being the same functions as those in (37). Benefitting from this form-invariance, one can now master the N-particle problem. To this end, one should choose the transformation-generating function V to be additive over the particles, whereafter the content of Sec. III A shall be repeated verbatim for each of the bodies, separately. In the end of this endeavour one will arrive to $N-1$ Delaunay sets similar to (B15), except that now these sets will be constituted by **instantaneous** orbital elements. The extension of the preceding subsection's content to the N-body case seems to be most straightforward and to involve no additional assumptions. To dispel this illusion, two things should be emphasized. One, self-evident, fact is that the quantities Q and P are no longer conserved after the disturbance $\Delta\mathcal{H}$ is added to the zero Hamiltonian $\mathcal{H}^*$. The second circumstance is that a change in a Hamiltonian implies an appropriate alteration of the Lagrangian. In the simple case of $\Delta\mathcal{H}$ being a function of the coordinates and time only (not of velocities or momenta), addition of $\Delta\mathcal{H}$ to the Hamiltonian implies addition of its opposite to the Lagrangian. Since this extra term bears no dependence upon velocities, the expressions for momenta through the coordinates and time will stay form-invariant. Hence (if the Lagrangian is not singular), the functional dependence of the velocities upon the coordinates and momenta will, also, preserve their functional form $v(q,p,t)$:

$$\begin{aligned} &\textit{without perturbation:} \quad p \equiv \frac{\partial \mathcal{L}(q,\dot{q},t)}{\partial \dot{q}} \Rightarrow \dot{q} = v(q,p,t), \\ &\textit{with perturbation:} \quad p \equiv \frac{\partial(\mathcal{L}(q,\dot{q},t)+\Delta\mathcal{L}(q,t))}{\partial \dot{q}} = \frac{\partial \mathcal{L}(q,\dot{q},t)}{\partial \dot{q}} \Rightarrow \dot{q} = v(q,p,t), \end{aligned} \tag{44}$$

where the new, perturbed dependence $\dot{q}=v[q(Q(t),P(t),t),p(Q(t),P(t),t),t]$ has the same functional form as the old one, $\dot{q}=v[q(Q,P,t),p(Q,P,t),t]$. Together with (43), this means that the dependence of the new $\dot{q}$ upon the new $P(t)$ and $Q(t)$ will have the same functional form as the dependence of the old $\dot{q}$ upon the constants Q and P:

$$\frac{d}{dt}q(Q(t),P(t),t) = \frac{\partial}{\partial t}q(Q(t),P(t),t). \tag{45}$$

In other words,

$$\sum_{i=1}^{6} \frac{\partial q}{\partial D_i}\dot{D}_i = 0, \tag{46}$$

where D_i denotes the set of perturbed variables $(Q(t),P(t))$. In the astronomical applications, D_i may stand for the Delaunay set.

This is the implicit condition under which the Hamilton–Jacobi method works (in the above case of velocity-independent disturbance). Violation of (46) would invalidate our cornerstone assumption (38). This circumstance imposes a severe restriction on the applicability of the Hamilton–Jacobi theory. In the astronomical context, this means that the Delaunay elements (B15) must be osculating. Indeed, if D_i denote a set of orbital elements, then expression (46) is equiva-

lent to the Lagrange constraint (4) discussed in Sec. I. There the constraint was imposed upon the Keplerian elements; however, its equivalence to (46), which is written in terms of the Delaunay variables, can be easily proven by the differentiation chain rule.

C. The case of momentum-dependent disturbances

When the perturbation of the Lagrangian depends also upon velocities (and, therefore, the Hamiltonian perturbation carries dependence upon the canonical momenta), the special gauge (22) wherein the Delaunay-type system preserves its canonicity differs from the Lagrange gauge. This was proven in Sec. II C in the Lagrangian language. Now we shall study this in Hamiltonian terms. Our explanation will be sufficiently general and will surpass the celestial-mechanics setting. For this reason we shall use notations q, p, not $\vec{\mathbf{r}}$, $\vec{\mathbf{p}}$. The development will, as ever, begin with an unperturbed system described by canonical variables obeying

$$\dot{q}=\frac{\partial \mathcal{H}}{\partial p}, \quad \dot{p}=-\frac{\partial \mathcal{H}}{\partial q}. \tag{47}$$

This dynamics may be reformulated in terms of the new quantities (Q,P):

$$\begin{aligned} q&=\phi(Q,P,t),\\ p&=\psi(Q,P,t), \end{aligned} \tag{48}$$

so that the Hamiltonian equations (47) are equivalent to

$$\dot{Q}=\frac{\partial \mathcal{H}^*}{\partial P}, \quad \dot{P}=-\frac{\partial \mathcal{H}^*}{\partial Q}. \tag{49}$$

For simplicity, we shall assume that $\mathcal{H}^*$ is zero. Then the new canonical variables will play the role of adjustable constants upon which the solution (48) of (47) depends.

We now wish to know under what circumstances a modified canonical system

$$\dot{q}=\frac{\partial(\mathcal{H}+\Delta\mathcal{H})}{\partial p}, \quad \dot{p}=-\frac{\partial(\mathcal{H}+\Delta\mathcal{H})}{\partial q}, \quad \Delta\mathcal{H}=\Delta\mathcal{H}(q,p,t) \tag{50}$$

will be satisfied by the solution

$$\begin{aligned} q&=\phi(Q(t),P(t),t),\\ p&=\psi(Q(t),P(t),t) \end{aligned} \tag{51}$$

of the same functional form as (48) but with time-dependent parameters obeying

$$\dot{Q}=\frac{\partial \Delta\mathcal{H}}{\partial P}, \quad \dot{P}=-\frac{\partial \Delta\mathcal{H}}{\partial Q}. \tag{52}$$

This situation is of a more general sort than that addressed in Sec. III B, in that the perturbation $\Delta\mathcal{H}$ now depends also upon the momentum.

Under the assumption of (48) being (at least, locally) invertible, substitution of the equalities

$$\dot{Q}=\frac{\partial \Delta\mathcal{H}}{\partial P}=\frac{\partial \Delta\mathcal{H}}{\partial q}\frac{\partial q}{\partial P}+\frac{\partial \Delta\mathcal{H}}{\partial p}\frac{\partial p}{\partial P} \tag{53}$$

and

$$\dot{P}=-\frac{\partial\Delta\mathcal{H}}{\partial Q}=-\frac{\partial\Delta\mathcal{H}}{\partial q}\frac{\partial q}{\partial Q}-\frac{\partial\Delta\mathcal{H}}{\partial p}\frac{\partial p}{\partial Q} \tag{54}$$

into the expression for velocity

$$\dot{q}=\frac{\partial q}{\partial t}+\frac{\partial q}{\partial Q}\dot{Q}+\frac{\partial q}{\partial P}\dot{P} \tag{55}$$

leads to

$$\dot{q}=\frac{\partial q}{\partial t}+\left(\frac{\partial q}{\partial Q}\frac{\partial q}{\partial P}-\frac{\partial q}{\partial P}\frac{\partial q}{\partial Q}\right)\frac{\partial\Delta\mathcal{H}}{\partial q}+\left(\frac{\partial q}{\partial Q}\frac{\partial p}{\partial P}-\frac{\partial q}{\partial P}\frac{\partial p}{\partial Q}\right)\frac{\partial\Delta\mathcal{H}}{\partial p}. \tag{56}$$

Here the coefficient accompanying $\partial\Delta\mathcal{H}/\partial q$ identically vanishes, while that accompanying $\partial\Delta\mathcal{H}/\partial p$ coincides with the Jacobian of the canonical transformation and is, therefore, unity:

$$\frac{\partial q}{\partial Q}\frac{\partial p}{\partial P}-\frac{\partial q}{\partial P}\frac{\partial p}{\partial Q}=1. \tag{57}$$

So if we introduce, in the spirit of (6), notation

$$g\equiv\frac{\partial q}{\partial t}, \tag{58}$$

then (56) will lead to

$$\dot{q}=g+\left(\frac{\partial\Delta\mathcal{H}}{\partial p}\right)_{q,t}. \tag{59}$$

Expression (59) establishes the link between the regular VOP method and the canonical treatment. It shows that, to preserve the symplectic description, one must always choose a particular gauge $\Phi=\partial\Delta\mathcal{H}/\partial p$. Needless to say, this is exactly the generalized Lagrange gauge (22) discussed in Sec. II C. A direct, though very short, proof is as follows.

On the one hand, the Hamilton equation for the perturbed Hamiltonian (14) is

$$\dot{q}=\frac{\partial(\mathcal{H}+\Delta\mathcal{H})}{\partial p}=p+\frac{\partial\Delta\mathcal{H}}{\partial p}, \tag{60}$$

while, on the other hand, the definition of momentum entails, for the Lagrangian (12),

$$p\equiv\frac{\partial(\mathcal{L}(q,\dot{q},t)+\Delta\mathcal{L}(q,\dot{q},t))}{\partial\dot{q}}=\dot{q}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{q}}. \tag{61}$$

By comparing the latter with the former we arrive at

$$\Phi\equiv\left(\frac{\partial\Delta\mathcal{H}}{\partial p}\right)_{q,t}=-\left(\frac{\partial\Delta\mathcal{L}}{\partial\dot{q}}\right)_{q,t}, \tag{62}$$

which coincides with (22). Thus we see that transformation (48) being canonical is equivalent to the partition of the physical velocity $\dot{q}$ in a manner prescribed by (59), where $\Phi=\partial\Delta\mathcal{H}/\partial p$. This is equivalent to our theorem from Sec. II C. Evidently, for disturbances dependent solely upon the coordinates, we return to the case explained in Sec. III B [Eqs. (45) and (46)]: in that case, the Hamiltonian formulation of the problem demanded imposition of the Lagrange constraint (46).

To draw to a close, the generalized Lagrange constraint, $\vec{\mathbf{\Phi}} = -\partial \Delta \mathcal{L}/\partial \dot{q}$, is stiffly embedded in the Hamilton–Jacobi technique. Hence this technique breaks the gauge invariance and is unfit (at least, in its straightforward form) to describe the gauge symmetry of the planetary equations. It is necessary to sacrifice gauge freedom by imposing the generalized Lagrange constraint to make use of the Hamilton–Jacobi development.

In this special gauge, the perturbed momentum coincides with the unperturbed one (which was equal to $\vec{\mathbf{g}}$). Indeed, we can rewrite (61) as

$$p \equiv \frac{\partial(\mathcal{L}(q,\dot{q},t) + \Delta\mathcal{L}(q,\dot{q},t))}{\partial \dot{q}} = \dot{q} - \Phi = g, \tag{63}$$

which means that, in the astronomical implementation of this theory, the Hamilton–Jacobi treatment necessarily demands the orbital elements to osculate in the phase space. Naturally, this demand reduces to that of regular osculation in the simple case of velocity-independent $\Delta\mathcal{L}$ that was explored in Sec. III B.

IV. CONCLUSIONS

We have studied, in an arbitrary gauge, the VOP method in celestial mechanics in the case when the perturbation depends on both positions and velocities. Such situations emerge when relativistic corrections to the Newton law are taken into account or when the VOP method is employed in noninertial frames of reference (a satellite orbiting a precessing planet being one such example). The gauge-invariant (and generalized to the case of velocity-dependent disturbances) Delaunay-type system of equations is not canonical. We, though, have proven a theorem establishing a particular gauge (which coincides with the Lagrange gauge in the absence of velocity dependence of the perturbation) that renders this system canonical. We called that gauge the ''generalized Lagrange gauge.''

We have explained where the Lagrange constraint tacitly enters the Hamilton–Jacobi derivation of the Delaunay equations. This constraint turns out to be an inseparable (though not easily visible) part of the method: in the case of momentum-independent disturbances, the *N*-body generalization of the two-body Hamilton–Jacobi technique is legitimate only if we use orbital elements that are osculating, i.e., if we exploit only the instantaneous ellipses (or hyperbolae, in the flyby case) that are always tangential to the velocity vector. Oddly enough, an explicit mention of this circumstance has not appeared in the astronomical literature (at least to the best of our knowledge).

In the case of momentum-dependent disturbances, the above restriction generalizes, in that the instantaneous ellipses (hyperbolae) must be osculating in the phase space. This is equivalent to the imposition of the generalized Lagrange gauge.

Comparing the good old VOP method with that based on the Jacobi theorem, we have to acknowledge that the elegance of the latter does not outweigh the power of the former. If we decide to explore the infinite multitude of gauges or to study the numerical-error-invoked gauge drift, we shall not be able to employ the Hamilton–Jacobi theory without additional structure. However, the direct VOP method unencumbered with the canonicity demand will immediately yield gauge-invariant equations for the Delaunay elements obeying an arbitrary gauge condition

$$\sum_i \frac{\partial \vec{\mathbf{f}}}{\partial D_i} \frac{dD_i}{dt} = \vec{\mathbf{\Phi}}(D_i, t), \tag{64}$$

$\vec{\mathbf{\Phi}}$ being some function of time and elements D_i. In Efroimsky (2002) these equations were written down for the case of velocity-independent perturbation. If the disturbing force depends also upon velocities, the Delaunay-type equations will acquire even more terms and will read as (A7)–(A12). In the simple case of a velocity-independent disturbance, any supplementary condi-

tion different from that of Lagrange will drive the Delaunay system away from its canonical form. If we permit the disturbing force to depend also upon velocities, the Delaunay equations will retain their canonicity only in the generalized Lagrange gauge.

In the language of modern physics, this may be put in the following wording. *N*-body celestial mechanics is a gauge theory but is not genuinely symplectic insofar as the language of orbital elements is used. It, though, becomes canonical in the generalized Lagrange gauge.

The applications of this formalism to motions in noninertial frames of reference will be studied in Efroimsky and Goldreich (2003). Some other applications were addressed in Slabinski (2003).

ACKNOWLEDGMENTS

The authors are grateful to Jean Kovalevsky for an e-mail conversation, which he had with one of us (M.E.) and which initiated this work. M.E. would like to acknowledge his numerous stimulating discussions with Marc Murison, William Newman, and Victor Slabinski. Research by M.E. was supported by NASA Grant No. W-19948. Research by P.G. was partially supported by NSF Grant No. AST 00-98301.

APPENDIX A: GAUGE-INVARIANT EQUATIONS OF LAGRANGE AND DELAUNAY TYPES

We present the gauge-invariant Lagrange-type equations. They follow from (19) if we take into account the gauge-invariance of matrix $[C_i\ C_j]$ defined by (9). We denote by $\Delta\mathcal{H}$ the perturbation of the Hamiltonian, connected through (14) with that of the Lagrangian. The latter, in its turn, is connected through (16) with the disturbing force (and acts as the customary disturbing function when the perturbations are devoid of velocity dependence):

$$\frac{da}{dt}=\frac{2}{na}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial M_o}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial M_o}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial M_o}-\frac{\partial\vec{\mathbf{f}}}{\partial M_o}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right], \tag{A1}$$

$$\begin{aligned}\frac{de}{dt}=&\frac{1-e^2}{na^2e}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial M_o}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial a}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial M_o}-\frac{\partial\vec{\mathbf{f}}}{\partial M_o}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right]\\&-\frac{(1-e^2)^{1/2}}{na^2e}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial\omega}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial\omega}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial\omega}\right.\\&\left.-\frac{\partial\vec{\mathbf{f}}}{\partial\omega}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right],\end{aligned} \tag{A2}$$

$$\begin{aligned}\frac{d\omega}{dt}=&\frac{-\cos i}{na^2(1-e^2)^{1/2}\sin i}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial i}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial i}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right.\\&\left.-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial i}-\frac{\partial\vec{\mathbf{f}}}{\partial i}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right]+\frac{(1-e^2)^{1/2}}{na^2e}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial e}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial e}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right.\\&\left.-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial e}-\frac{\partial\vec{\mathbf{f}}}{\partial e}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right],\end{aligned} \tag{A3}$$

$$\frac{di}{dt}=\frac{\cos i}{na^2(1-e^2)^{1/2}\sin i}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial\omega}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial\omega}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial\omega}\right.$$
$$\left.-\frac{\partial\vec{\mathbf{f}}}{\partial\omega}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right]-\frac{1}{na^2(1-e^2)^{1/2}\sin i}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial\Omega}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial\Omega}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right.$$
$$\left.-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial\Omega}-\frac{\partial\vec{\mathbf{f}}}{\partial\Omega}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right], \tag{A4}$$

$$\frac{d\Omega}{dt}=\frac{1}{na^2(1-e^2)^{1/2}\sin i}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial i}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial i}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right.$$
$$\left.-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial i}-\frac{\partial\vec{\mathbf{f}}}{\partial i}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right], \tag{A5}$$

$$\frac{dM_o}{dt}=-\frac{1-e^2}{na^2e}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial e}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial e}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial e}-\frac{\partial\vec{\mathbf{f}}}{\partial e}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right]$$
$$-\frac{2}{na}\left[\frac{\partial(-\Delta\mathcal{H})}{\partial a}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial a}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial a}-\frac{\partial\vec{\mathbf{f}}}{\partial a}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\right]. \tag{A6}$$

Similarly, the gauge-invariant Delaunay-type system can be written down as

$$\frac{dL}{dt}=\frac{\partial(-\Delta\mathcal{H})}{\partial M_o}-\frac{\partial\Delta L}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial M_o}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial M_o}-\frac{\partial\vec{\mathbf{f}}}{\partial M_o}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A7}$$

$$\frac{dM_o}{dt}=-\frac{\partial(-\Delta\mathcal{H})}{\partial L}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial L}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)+\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial L}+\frac{\partial\vec{\mathbf{f}}}{\partial L}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A8}$$

$$\frac{dG}{dt}=\frac{\partial(-\Delta\mathcal{H})}{\partial\omega}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial\omega}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial\omega}-\frac{\partial\vec{\mathbf{f}}}{\partial\omega}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A9}$$

$$\frac{d\omega}{dt}=-\frac{\partial(-\Delta\mathcal{H})}{\partial G}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial G}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)+\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial G}+\frac{\partial\vec{\mathbf{f}}}{\partial G}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A10}$$

$$\frac{dH}{dt}=\frac{\partial(-\Delta\mathcal{H})}{\partial\Omega}-\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial\Omega}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)-\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial\Omega}-\frac{\partial\vec{\mathbf{f}}}{\partial\Omega}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A11}$$

$$\frac{d\Omega}{dt}=-\frac{\partial(-\Delta\mathcal{H})}{\partial H}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\frac{\partial}{\partial H}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)+\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right)\frac{\partial\vec{\mathbf{g}}}{\partial H}+\frac{\partial\vec{\mathbf{f}}}{\partial H}\frac{d}{dt}\left(\vec{\mathbf{\Phi}}+\frac{\partial\Delta\mathcal{L}}{\partial\dot{\vec{\mathbf{r}}}}\right), \tag{A12}$$

where

$$L\equiv\mu^{1/2}a^{1/2},\quad G\equiv\mu^{1/2}a^{1/2}(1-e^2)^{1/2},\quad H\equiv\mu^{1/2}a^{1/2}(1-e^2)^{1/2}\cos i, \tag{A13}$$

and the symbols $\vec{\mathbf{\Phi}},\vec{\mathbf{f}},\vec{\mathbf{g}}$ denote the functional dependencies of the gauge, position and velocity upon the Delaunay, not Keplerian, elements, and therefore these are functions different from $\vec{\mathbf{\Phi}},\vec{\mathbf{f}},\vec{\mathbf{g}}$ used in (A1)–(A6) where they stood for the dependencies upon the Kepler elements. [In Efroimsky (2002) the dependencies $\vec{\mathbf{\Phi}},\vec{\mathbf{f}},\vec{\mathbf{g}}$ upon the Delaunay variables were equipped with tilde, to distinguish them from the dependencies upon the Kepler coordinates.]

The above equations do not merely repeat those derived earlier in Efroimsky (2002, 2003), but generalize them to the case of a perturbation $\Delta\mathcal{L}$ which is both position and velocity dependent. For this reason, our gauge-invariant equations can be employed not only in an inertial frame but also in a wobbling one.

To employ the gauge-invariant equations in analytical calculations is a delicate task: one should always keep in mind that, in case $\vec{\mathbf{\Phi}}$ is chosen to depend not only upon time but also upon the ''constants'' (but not upon their derivatives), the right-hand sides of these equation will implicitly contain the first derivatives dC_i/dt, and one will have to move them to the left-hand sides [much like in the transition from (10) to (11)].

APPENDIX B: THE HAMILTON–JACOBI METHOD IN CELESTIAL MECHANICS

The Jacobi equation (34) is a PDE of the first order, in $(N+1)$ variables (q_n,t), and its complete integral $W(q,Q,t)$ will depend upon $N+1$ constants a_n (Jeffreys and Jeffreys, 1972; Courant and Hilbert 1989). One of these constants, a_{N+1}, will be additive, because W enters the above equation only through its derivatives. Since both Hamiltonians are, too, defined up to some constant f, then the solution to (34) must contain that constant multiplied by the time:

$$\begin{aligned} W(q,\ a_1,\ldots,a_N,\ a_{N+1},t) &= \widetilde{W}(q,\ a_1,\ldots,a_N,\ t)-(t-t_o)f(a_1,\ldots,a_N) \\ &= \widetilde{W}(q,\ a_1,\ldots,a_N,\ t)-tf(a_1,\ldots,a_N)-a_{N+1}, \end{aligned} \tag{B1}$$

where the fiducial epoch is connected to the constants through $t_o=-a_{N+1}/f$, and the function $\widetilde{W}$ depends upon N constants only. As the total number of independent adjustable parameters is $N+1$, the constant f cannot be independent but must rather be a function of $a_1,\ldots,a_N,a_{N+1}$. Since we agreed that the constant a_{N+1} is additive and shows itself nowhere else, it will be sufficient to consider f as a function of the rest N parameters only. (In principle, it is technically possible to involve the constant a_{N+1}, i.e., the reference epoch, into the mutual transformations between the other constants. However, in the applications that we shall consider, we shall encounter only equations autonomous in time, and so there will be no need to treat a_{N+1} as a parameter to vary. Hence, in what follows we shall simply ignore its existence.) The new function $\widetilde{W}$ obeys the simplified Jacobi equation

$$\mathcal{H}\left(q,\frac{\partial\widetilde{W}(q,a_1,\ldots,a_N,t)}{\partial q},t\right)+\frac{\partial\widetilde{W}(q,a_1,\ldots,a_N,t)}{\partial t}=f(a_1,\ldots,a_N)+\mathcal{H}^*. \tag{B2}$$

As agreed above, $\mathcal{H}^*$ is a constant. Hence, we can state about this constant all the same as about the constant f: since the integral W can contain no more than $N+1$ adjustable parameters $a_1,\ldots,a_N,a_{N+1}$, and since we ignore the existence of a_{N+1}, the constant $\mathcal{H}^*$ must be a function of the remaining N parameters: $\mathcal{H}^*=\mathcal{H}^*(a_1,\ldots,a_N)$.

Now, in case $\mathcal{H}$ depends only upon (q, p) and lacks an explicit time dependence, then so will $\widetilde{W}$; and the above equation will very considerably simplify:

$$\mathcal{H}\left(q,\frac{\partial\widetilde{W}(q,a_1,\ldots,a_N)}{\partial q}\right)=f(a_1,\ldots,a_N)+\mathcal{H}^*(a_1,\ldots,a_N), \tag{B3}$$

where we deliberately avoided absorbing the constant Hamiltonian $\mathcal{H}^*$ into the function f.

Whenever the integral W can be found explicitly, the constants $(a_1,\ldots,a_N)$ can be identified with the new coordinates Q, whereafter the new momenta will be calculated through $P=-\partial W/\partial Q$. In the special case of zero $\mathcal{H}^*$, the new momenta become constants, because they obey the canonical equations with a vanishing Hamiltonian. In the case where $\mathcal{H}^*$ is a nonzero constant, it must, as explained above, be a function of all or some of the independent parameters $(a_1,\ldots,a_N)$, and, therefore, all or some of the new momenta P will be evolving in time.

Since it is sufficient to find only one solution to the Jacobi equation, one can seek it by means of the variable-separation method: Eq. (B3) will solve in the special case when the generating function (B1) is separable:

$$\tilde{W}(q_1,\ldots,q_N,a_1,\ldots,a_N)=\sum_{i=1}^{N}\tilde{W}_i(q_i,a_1,\ldots,a_N). \tag{B4}$$

This theory works very well in application to the unperturbed (two-body) problem (1) of celestial mechanics, a problem that is simple due to its mathematical equivalence to the gravitationally bound motion of a reduced mass $m_{\text{planet}}m_{\text{sun}}/(m_{\text{planet}}+m_{\text{sun}})$ about a fixed center of mass $m_{\text{planet}}+m_{\text{sun}}$. If one begins with the (reduced) two-body Hamiltonian in the spherical coordinates

$$q_1=r,\quad q_2=\phi,\quad q_3=\theta \tag{B5}$$

(where $x=r\cos\phi\cos\theta$, $y=r\cos\phi\sin\theta$, $z=r\sin\phi$), then the expression for Lagrangian,

$$L=T-\Pi=\frac{1}{2}(\dot{q}_1)^2+\frac{1}{2}(q_1)^2(\dot{q}_2)^2+\frac{1}{2}(q_1)^2(\dot{q}_3)^2\cos^2 q_2+\frac{\mu}{q_1}, \tag{B6}$$

will yield the following formulas for the momenta:

$$p_1\equiv\frac{\partial\mathcal{L}}{\partial\dot{q}_1}=\dot{q}_1,\quad p_2\equiv\frac{\partial\mathcal{L}}{\partial\dot{q}_2}=q_1^2\dot{q}_2,\quad p_3\equiv\frac{\partial\mathcal{L}}{\partial\dot{q}_3}=q_1^2\dot{q}_3\cos^2 q_2, \tag{B7}$$

whence the initial Hamiltonian will read

$$\mathcal{H}=\sum p\dot{q}-\mathcal{L}=\frac{1}{2}p_1^2+\frac{1}{2q_1^2}p_2^2+\frac{1}{2q_1^2\cos^2 q_2}p_3^2-\frac{\mu}{q_1}. \tag{B8}$$

Then the Hamilton–Jacobi equation (30) will look like this:

$$\frac{1}{2}\left(\frac{\partial W}{\partial q_1}\right)^2+\frac{1}{2q_1^2}\left(\frac{\partial W}{\partial q_2}\right)^2+\frac{1}{2q_1^2\cos^2 q_2}\left(\frac{\partial W}{\partial q_3}\right)^2-\frac{\mu}{q_1}-\frac{\partial W}{\partial t}-\mathcal{H}^*=0, \tag{B9}$$

while the auxiliary function $\tilde{W}$ defined through (B1) will obey

$$\frac{1}{2}\left(\frac{\partial \tilde{W}}{\partial q_1}\right)^2+\frac{1}{2q_1^2}\left(\frac{\partial \tilde{W}}{\partial q_2}\right)^2+\frac{1}{2q_1^2\cos^2 q_2}\left(\frac{\partial \tilde{W}}{\partial q_3}\right)^2-\frac{\mu}{q_1}-f-\mathcal{H}^*=0. \tag{B10}$$

A lengthy but elementary calculation [presented, with some inessential variations, in Plummer (1918), Smart (1953), Pollard (1966), Kovalevsky (1967), Stiefel and Scheifele (1971), and many other books] shows that, for a constant $\mathcal{H}^*$ and in the ansatz (B4), the integral of (B3) takes the form

$$\widetilde{W}=\widetilde{W}_1(q_1,a_1,a_2,a_3)+\widetilde{W}_2(q_2,a_1,a_2,a_3)+\widetilde{W}_3(q_3,a_1,a_2,a_3)$$
$$=\int_{q_1(t_o)}^{q_1(t)}\epsilon_1\left(2(f+\mathcal{H}^*)+\frac{2\mu}{q_1}-\frac{a_2^2}{q_1^2}\right)^{1/2}dq_1+\int_0^{\phi}\epsilon_2\left(a_2^2-\frac{a_3^2}{\cos^2 q_2}\right)^{1/2}dq_2+\int_0^{\theta}a_3dq_3, \tag{B11}$$

where the epoch and factors ϵ_1, ϵ_2 may be taken as in Kovalevsky (1967): time t_o is the instant of perigee passage; factor ϵ_1 is chosen to be $+1$ when $q_1\equiv r$ is increasing, and is -1 when r is decreasing; factor ϵ_2 is $+1$ when $q_2\equiv\phi$ is increasing, and is -1 otherwise. This way the quantities under the first and second integration signs have continuous derivatives. To draw conclusions, in the two-body case we have a transformation-generating function

$$W\equiv\widetilde{W}+tf(a_1,\ldots,a_N)=\int_{q_1(t_o)}^{q_1(t)}\epsilon_1\left(2(f+\mathcal{H}^*)+\frac{2\mu}{q_1}-\frac{a_2^2}{q_1^2}\right)^{1/2}dq_1$$
$$+\int_0^{\phi}\epsilon_2\left(a_2^2-\frac{a_3^2}{\cos^2 q_2}\right)^{1/2}dq_2+\int_0^{\theta}a_3dq_3+tf, \tag{B12}$$

whose time-independent component $\widetilde{W}$ enters Eq. (B3). The first integration in (B12) contains the functions $f(a_1,\ldots,a_N)$ and $\mathcal{H}^*(a_1,\ldots,a_N)$, so that in the end of the day W depends on the N constants $a_1,\ldots,a_N$ (not to mention the neglected t_o, i.e., the a_{N+1}).

Different authors deal differently with the sum $(f+\mathcal{H}^*)$ emerging in (B12). Smart (1953) and Kovalevsky (1967) prefer to put

$$f=0,\quad \mathcal{H}^*=a_1,\quad a_1=-\mu/(2a), \tag{B13}$$

whereupon the new momentum $P_1=-\partial W/\partial Q_1=-\partial W/\partial a_1$ becomes time dependent (and turns out to equal $-t+t_o$). An alternative choice, which, in our opinion, better reflects the advantages of the Hamilton-Jacobi theory, is furnished by Plummer (1918):

$$f=a_1,\quad \mathcal{H}^*=0,\quad a_1=\sqrt{\mu a}. \tag{B14}$$

This entails the following correspondence between the new canonical variables (the Delaunay elements) and the Keplerian orbital coordinates:

$$Q_1\equiv a_1=\sqrt{\mu a},\quad P_1=-M_o,$$
$$Q_2\equiv a_2=\sqrt{\mu a(1-e^2)},\quad P_2=-\omega, \tag{B15}$$
$$Q_3\equiv a_3=\sqrt{\mu a(1-e^2)}\cos i,\quad P_3=-\Omega.$$

Everywhere in this article we follow the convention (B14) and denote the above variables Q_1, Q_2, Q_3 by L, G, H, correspondingly (as is normally done in the astronomical literature).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

On variations in discrete mechanics and field theory

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(Received 27 December 2001; accepted 26 August 2003)

In this paper, we propose the difference variational approach with variable step-length for discrete mechanics and field theory. Based upon the Hamilton's principle for the vertical variations and the horizontal variations, we get the equation of motion and the relevant relations between the equation of motion and conservation law of the energy/energy-momentum tensor for continuous as well as for the discrete systems, respectively. For those discrete cases, these relations determine the variable step-length of the differences. In addition, by taking the double operation of vertical exterior differential on action, we show that there should exist the Euler–Lagrange cohomology for both continuous and variable step-length difference cases in general. This indicates that the necessary and sufficient condition for symplectic/multisymplectic structure preserving properties is the relevant Euler–Lagrange one-form being closed in each case. Our approach can be applied to both the Lagrangian formalism and the Hamiltonian formalism, via discrete Legendre transformation, for the difference discrete mechanics and field theory. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1621058]

I. INTRODUCTION

Variation problems occupy a central role in continuum mechanics and field theories when considered from the perspective of Lagrangian or Hamiltonian formalisms (see, for example, Refs. 8, 4, and 1), which in many cases can transform each other via the Legendre transformation. A lot of important issues are directly related to the variation problems with fixed or variable boundary. These issues include the equations of motions, the (intrinsic) symplectic or multisymplectic preserving properties, conservation laws associated with certain symmetries, topological properties, and so on. In considering the discrete version of mechanics or field theories and their corresponding symplectic and multisymplectic algorithms, discrete variation problems still play an important role, particularly, for the discrete Lagrangian formalism of these discrete systems. Only recently, the difference discrete variational approach has been proposed[12,14] in the context of discrete Lagrangian and Hamiltonian formalisms that relate each other by discrete Legendre transformation.

Within the content of the difference discrete version for mechanics, Lee suggested a discrete variational approach to discrete Lagrangian mechanics and the relevant algorithm in the early 1980s.[19–21] Since time is regarded as a dynamical variable, Lee treated the time steps as variational variables. Consequently, his approach preserves the energy discretely. Veselov[30,26] also proposed the discrete variational principle by the end of the 1980s. It is almost the same as Lee's approach except without taking variation with respect to the discrete time. Therefore, it does not

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keep the conservation of the energy discretely in general. However, these two approaches are merely applicable to discrete Lagrangian mechanics, since there is no discrete Legendre transformation.

In the same period, Ruth[28] and Feng[10] proposed the symplectic algorithm for Hamiltonian mechanics. In this algorithm (for a review, see Ref. 29), the time step-length is fixed and the symplectic preserving property is discretely kept. However, the discrete version of energy conservation cannot be maintained discretely in general. The symplectic algorithm plays very important role in computational mathematics and its applications cover various branches in sciences. It led to further development of the structure-preserving algorithms. In these algorithms, the time step-length is often fixed so that the price to be paid for keeping structure preserving is the loss of other conservation laws for the continuous cases in general.

It is widely accepted that in the course of computation the discrete systems should be thought of as the discrete counterparts of the corresponding continuous systems. However, in order to discretize continuous systems, a working guide line in needed. In Ref. 10, Feng wrote ''It is natural to look forward to those discrete systems which preserve as much as possible the intrinsic properties of the continuous system.'' In fact, this statement should be regarded as a criterion, the structure-preserving criterion, for constructing mostly quarried ones in all kinds of structure-preserving algorithms. However, in order to carry through this criterion, we must know how to answer the following questions.

Problem set 1: What are the most important intrinsic ''structures'' in continuous systems that should be maintained in the course of discretization? What are the discrete counterparts of these ''structures'' and how to preserve them in a certain discrete version? What is the minimal cost to be paid for in the course of discretization?

It is well known that there are two classes of conservation laws in canonical conservative mechanics. The first class is of phase-area conservation laws characterized by the symplectic preserving property and another class is related to energy and all first integrals of the canonical equations. Thus, the following questions can apparently be raised.

Problem set 2: Is it possible to establish a kind of discrete mechanics and/or structure-preserving algorithms in such a way that they not only discretely preserve the symplectic property but also some other conservation laws, especially the energy conservation? Can these discrete systems be established by a discrete variational approach? Does this discrete variational approach be applied to both discrete Lagrangian and Hamiltonian formalisms?

In Lee's approach, it could be proved that in addition to discrete energy conservation the symplectic structure is also preserved since Lee's approach is a discrete variational approach In Ref. 18 this problem has been partly solved by defining a conserved discrete energy in Veselov's approach. The complete resolving to this problem in Lee's framework has been made until very recently in Refs. 6 and 7. However the framework of either Lee's approach or Veselov's approach cannot be applied to the discrete Hamiltonian systems. To our knowledge, therefore, these problems are still partly open.

Recently, the symplectic algorithm has been generalized to the multisymplectic one in what is called ''Hamiltonian formalism.'' [5] Veselov's discrete variation approach to the discrete mechanics has also been generalized to field theories in Lagrangian formalism to get ''variational multisymplectic integrators.'' [23,24] In both approaches, the step-lengths are fixed so that the energy-momentum tensor cannot be conserved in general although the multisymplectic structure preserving property in field theory can be maintained discretely in a certain manner. Thus a set of similar questions can also be raised to the discrete field theory and multisymplectic algorithms.

Problem set 3: Is it possible to establish a discrete variational approach to describe a kind of discrete field theory and/or multisymplectic algorithm in such a way that not only the multisymplectic property is discretely preserved but also the conservation laws such as energy-momentum conservation law are discretely maintained? Is it possible to apply such an approach in both discrete Lagrangian and Hamiltonian formalisms? To our knowledge, these problems are still open as well.

Recently, it has been proposed for the difference discrete variational approach to discrete

mechanics and field theories with fixed step-length differences, it can be applied to both Lagrangian and Hamiltonian formalisms.[12,14] The key point of this approach is to regard the differences with fixed step-length as a kind of entire geometric object so that these differences may play analogical roles with derivatives in continuous cases. Thus the following questions can also be raised.

Problem set 4: Is it possible to generalize the difference discrete variational approach with fixed step-lengths to the one with varied step-lengths so as to the discrete energy conservation law may be kept together with the symplectic and/or multisymplectic preserving properties? In the cases of fixed step-length differences for independent variables such as time in mechanics and space–time coordinates in field theories, certain noncommutative differential calculus (NCDC) should be established and employed. What about the cases of variable step-length differences?

In this paper, we present such an approach, the difference variational approach with variable step-lengths named variable difference variational approach (VDVA) in order to carry through the structure-preserving criterion. As was mentioned, this approach is a natural generalization of the difference variational approach with fixed step-lengths proposed recently in Refs. 12 and 14 for the ordinary discrete variation problems with fixed discrete domain. In fact, the approach in Refs. 12 and 14 is just a discrete vertical variation so that it is natural to keep the step-length fixed. The crucial point of this approach is that in the course of calculation of variation problems in discrete mechanics and field theory, the differences with variable step-lengths are kept as entire geometric objects as much as possible. Consequently, this approach not only keeps the advantage of Lee's discrete variation, which conserves the energy of the system discretely, but also the advantage in variation in Veselov type, which is symplectic or multisymplectic. In addition, this VDVA can be applied to both the Lagrangian and Hamiltonian formalisms for discrete mechanics and discrete field theory, since the discrete canonical ''momenta'' and discrete version of Legendre transformation can be introduced in terms of variable step-length differences. For simplicity, we consider in this paper the discrete Lagrangian of first order of difference only and concentrate on the variable difference mechanics and field theory. As far as the generalization of the symplectic and multisymplectic algorithms to the variable step-lengths, it is left for another paper. On the other hand, we also show that the Euler–Lagrange cohomology for both continuous and fixed step-length difference cases[12–14] can be generated. Namely, there should exist the Euler–Lagrange cohomology for both continuous and variable step-length difference cases in general. This indicates that the necessary and sufficient condition for symplectic/multisymplectic structure preserving properties is the relevant Euler–Lagrange one-form being closed, rather than the system on the solution space only in each case.

This paper is organized as follows. In Sec. II we recall the variation problems in Lagrangian and Hamiltonian mechanics. In Sec. III we present the VDVA and deal with the difference Lagrangian and Hamiltonian mechanics. In Sec. IV we recall briefly the variation problems in Lagrangian and Hamiltonian field theory with generic variables. In Sec. V, we apply the VDVA to the discrete variation problems in difference discrete Lagrangian and Hamiltonian field theory with generic variables. Finally, we end with some remarks.

II. VARIATIONS FOR CLASSICAL MECHANICS

Let us recall briefly the variation calculi in classical continuum mechanics with the Euler–Lagrange cohomology introduced very recently.[12–14]

Let $t \in T \simeq R$ be the time, M an n-dimensional configuration space. Consider a fiber bundle $E(T,Q,\pi)$ with projection $\pi: E \to T$ on T, $\pi^{-1}: t \to Q_t$ isomorphic to M is the fiber on $t \in T$. Denote $\Gamma(E)$ the sections on E, TE the tangent bundle of E, $T_vE \subset TE$ the vertical sub-bundle of TE, etc.

A. Variations in Lagrangian mechanics

We first consider the Lagrangian mechanics. The Lagrangian of the system is $L(q^i(t), \dot{q}^i(t); t)$, $i = 1,\ldots,n$. For simplicity, the Lagrangian is taken as the first order. The action functional is

$$S([q^i(t)];t_1,t_2)=\int_{t_1}^{t_2}\mathrm{d}t\,L(q^i(t),\dot{q}^i(t);t). \tag{2.1}$$

Here q^i's are coordinates on the fiber, $q^i(t)$ describes a curve C_a^b with ending points a and b, $t_a=t_1, t_b=t_2$, and $\dot{q}^i(t)=\mathrm{d}q^i(t)/\mathrm{d}t$.

Let us consider the general variation of $q^i(t)$,

$$q^i(t)\to q'^i(t')=q^i(t)+\delta_t q^i(t), \tag{2.2}$$

accompanied with an infinitesimal reparametrization of time t,

$$t\to t'(t)=t+\delta t. \tag{2.3}$$

Here $\delta_t q^i(t)$ denotes the total variation that can be divided into two parts,

$$\delta_t q^i(t)=\delta_v q^i(t)+\delta_h q^i(t),$$

$$\delta_v q^i(t)=q'^i(t)-q^i(t),$$

$$\delta_h q^i(t)=q'^i(t')-q'^i(t)=q^i(t')-q^i(t)+O(\delta^2)=\mathcal{L}_\xi q^i+O(\delta^2), \tag{2.4}$$

where $\delta_v q^i(t)$ denotes the equal time variation or the vertical one and $\delta_h q^i(t)$ the horizontal part along the fiber induced by the reparametrization of the time t (2.3), ξ a variational vector field on T

$$\xi(t):=\delta t\frac{\partial}{\partial t}, \tag{2.5}$$

$\mathcal{L}_\xi$ the Lie derivative of $q^i(t)$ with respect to the variation vector field (2.5) (see the following remark 2.2).

Similarly, for the general variation of $\dot{q}^i(t)$ we have

$$\delta_t\dot{q}^i(t)=(\delta_v+\delta_h)\dot{q}^i(t),$$

$$\delta_v\dot{q}^i(t)=\dot{q}'^i(t)-\dot{q}^i(t),$$

$$\delta_h\dot{q}^i(t)=\frac{\mathrm{d}}{\mathrm{d}t'}q'^i(t')-\frac{\mathrm{d}}{\mathrm{d}t'}q'^i(t)=\frac{\mathrm{d}}{\mathrm{d}t'}q^i(t')-\frac{\mathrm{d}}{\mathrm{d}t}q^i(t)+O(\delta^2)=\mathcal{L}_\xi\dot{q}^i(t)+O(\delta^2). \tag{2.6}$$

Note that $\delta_h\dot{q}^i(t)$ is also the Lie derivative of $\dot{q}^i(t)$ with respect to the variational vector field (2.5). In fact, this is true for a kind of functionals of $q^i(t)$, $\dot{q}^i(t)$, and t,

$$\delta_h F(q^i(t),\dot{q}^i(t),t)=\mathcal{L}_\xi F(q^i(t),\dot{q}^i(t),t). \tag{2.7}$$

To the time change (2.3) is associated the change in the measure in (2.1) given by the Jacobi formula

$$\mathrm{d}t'=\frac{\partial t'}{\partial t}\mathrm{d}t=\left(1+\frac{\mathrm{d}}{\mathrm{d}t}\delta t\right)\mathrm{d}t, \tag{2.8}$$

i.e.,

$$\delta(\mathrm{d}t)=\mathrm{d}(t+\delta t)-\mathrm{d}t=\mathrm{d}t\frac{\mathrm{d}}{\mathrm{d}t}\delta t. \tag{2.9}$$

It is easy to see that this change in the measure is also the Lie derivative of the measure with respect to the variation vector (2.5),

$$\delta(\mathrm{d}t)=\mathcal{L}_{\xi}\,\mathrm{d}t=\mathrm{d}\delta t.$$

Now the Lagrangian is changed to

$$L\left(q^i(t),\frac{\mathrm{d}}{\mathrm{d}t}q^i(t);t\right)\to L\left(q'^i(t'),\frac{\mathrm{d}}{\mathrm{d}t'}q'^i(t');t'\right)=L\left(q^i(t),\frac{\mathrm{d}}{\mathrm{d}t}q^i(t);t\right)+\delta_t L, \tag{2.10}$$

and the action is also deformed to

$$\begin{aligned}S([q'^i(t')];t_1',t_2')&=\int_{t_1'}^{t_2'}\mathrm{d}t'\,L\left(q'^i(t'),\frac{\mathrm{d}}{\mathrm{d}t'}q'^i(t');t'\right)=\int_{t_1}^{t_2}\frac{\partial t'}{\partial t}\mathrm{d}t\{L(q^i(t),\dot{q}^i(t);t)+\delta_t L\}\\&=\int_{t_1}^{t_2}\mathrm{d}t\left\{L+\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta t\right)L+\delta_t L\right\}=S([q^i(t)];t_1,t_2)+\delta_t S.\end{aligned} \tag{2.11}$$

A more or less straightforward calculation shows

$$\delta_t S=\int_{t_1}^{t_2}\mathrm{d}t\left\{[L_{q^i}]\delta_t q^i+\left[\frac{\mathrm{d}}{\mathrm{d}t}H+\frac{\partial}{\partial t}L\right]\delta t+\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^j}\delta_t q^j-H\delta t\right)\right\}, \tag{2.12}$$

where $[L_{q^i}]$ is the Euler–Lagrange operator and H the energy (Hamiltonian)

$$[L_{q^i}]:=\frac{\partial L}{\partial q^i}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^i}\right),\quad H:=\frac{\partial L}{\partial\dot{q}^i}\dot{q}^i-L. \tag{2.13}$$

The vertical and horizontal variations should be separated as the independent ones. This leads to

$$\delta_v S=\int_{t_1}^{t_2}\mathrm{d}t\left\{[L_{q^i}]\delta_v q^i+\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^j}\delta_v q^j\right)\right\} \tag{2.14}$$

and

$$\delta_h S=\int_{t_1}^{t_2}\mathrm{d}t\left\{[L_{q^i}]\delta_h q^i+\left[\frac{\mathrm{d}}{\mathrm{d}t}H+\frac{\partial}{\partial t}L\right]\delta t+\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^j}\delta_h q^j-H\delta t\right)\right\}. \tag{2.15}$$

For the vertical part, the Hamilton's principle leads to the Euler–Lagrange equation if $\delta_v q^j|_{t_1}=\delta_v q^j|_{t_2}=0$,

$$\frac{\partial L}{\partial q^i}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^i}\right)=0. \tag{2.16}$$

For the horizontal part, however, it is easy to check

$$[L_{q^i}]\dot{q}^i+\frac{\mathrm{d}}{\mathrm{d}t}H+\frac{\partial}{\partial t}L=0,$$

$$\vartheta:=\frac{\partial L}{\partial\dot{q}^j}\delta_h q^j-H\delta t=L\,\delta t. \tag{2.17}$$

Therefore,

$$\delta_h S = \int_{t_1}^{t_2} \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t}(L\,\delta t) = 0. \tag{2.18}$$

This is just the invariance of the action S with respect to the reparametrization of time. Of course, from the first equation of (2.17), it still follows the conservation law for the energy if and only if the Euler–Lagrange equation is satisfied and L does not depend on t manifestly.

On the other hand, from (2.15) and (2.18), it also follows the first equation of (2.17).

Remark 2.1: We may introduce exterior differential operators d, d_v, and d_h on $T^*(M\times T)$, T^*M and T^*T, respectively. They are nilpotent and satisfy

$$\mathrm{d} := \mathrm{d}_v + \mathrm{d}_h, \quad \{\mathrm{d}_v, \mathrm{d}_h\} = 0. \tag{2.19}$$

Considering a vertical variational vector field

$$\xi_q := \delta_v q^i(t) \frac{\partial}{\partial q^i}, \tag{2.20}$$

then

$$\delta_v q^i(t) = i_{\xi_q} \mathrm{d}_v q^i = i_{\xi_q} \mathrm{d}q^i. \tag{2.21}$$

By means of the vector field (2.20) on TQ, $\delta_v S$ can also be expressed as its contraction with one-form $\mathrm{d}_v S \in T^*Q$,

$$i_{\xi_q} \mathrm{d}_v S = \delta_v S. \tag{2.22}$$

We may calculate $\mathrm{d}_v S \in T^*Q$. Since d_v commutes with the integral of $\mathrm{d}t$ (see also, for example, the functional differential calculus in Ref. 27), it is straightforward to get

$$\mathrm{d}_v S = \int_{t_1}^{t_2} \mathrm{d}t \left\{ [L_{q^i}] \mathrm{d}_v q^i + \frac{\mathrm{d}}{\mathrm{d}t}\theta \right\}, \tag{2.23}$$

where θ is the Lagrange one-form

$$\theta := \frac{\partial L}{\partial \dot{q}^i} \mathrm{d}_v q^i. \tag{2.24}$$

Now by contracting with the vertical variational vector field (2.20) it follows straightforwardly $\delta_v S$ in (2.14).

Furthermore, due to the nilpotency of d_v, it is easy to get

$$\mathrm{d}_v \mathcal{E} + \frac{\mathrm{d}}{\mathrm{d}t}\omega = 0, \tag{2.25}$$

where $\mathcal{E}$ is called the Euler–Lagrange one-form,[12–14] defined by

$$\mathcal{E}(q^i(t), \dot{q}^i(t); t) := [L_{q^i}] \mathrm{d}_v q^i, \tag{2.26}$$

ω is the symplectic two-form and in local coordinates

$$\omega := \mathrm{d}_v \theta = \frac{\partial^2 L}{\partial q^j \partial \dot{q}^i} \mathrm{d}_v q^j \wedge \mathrm{d}_v q^i + \frac{\partial^2 L}{\partial \dot{q}^j \partial \dot{q}^i} \mathrm{d}_v \dot{q}^j \wedge \mathrm{d}_v q^i. \tag{2.27}$$

From (2.26), (2.23), and (2.25), the following theorem can be proved.[12–14]

Theorem 1: *For the Lagrangian with first order of derivatives on the bundle $E(T,Q,\pi)$, the following properties hold:*

(1) There exists the Euler–Lagrange cohomology:

$$H_{LM}:=\{\mathcal{E}|\,\mathrm{d}_v\mathcal{E}=0\}/\{\mathcal{E}|\,\mathcal{E}=\mathrm{d}_v\alpha\},$$

where $\alpha=\alpha(q^i(t),\dot{q}^i(t);t)$ is an arbitrary function of $(q^i(t),\dot{q}^i(t);t)$.

(2) The necessary and sufficient condition for conservation of the symplectic two-form, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\omega=0, \tag{2.28}$$

is that the corresponding Euler–Lagrange one-form is closed, rather than the system on the solution space only.

Remark 2.2: From the definition of Lie derivative it can be seen that the horizontal variations are given by the Lie derivative with respect to the variational vector field.

Let ξ be a vector field on T, $\exp(\lambda\xi)$ the flow with parameter λ, i.e., the one-parameter diffeomorphism group, induced by ξ, f a differential form or a vector on T. The infinitesimal change of f under flow is described by its Lie derivative with respect to the vector field ξ,

$$\mathcal{L}_\xi f(t):=\lim_{\lambda\to 0}\frac{1}{\lambda}\{\phi_\lambda^* f(\exp(\lambda\xi)t)-f(t)\}=\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0}(\phi_\lambda^* f(t')),\quad t'=\exp(\lambda\xi)t. \tag{2.29}$$

Here ϕ_λ^* is the bull-back for differential forms or the inverse differential for vectors, respectively.

Taking $\xi=\xi(t)=\xi_t$ in (2.5), it follows that the Lie derivative of $f(t)$ with respect to ξ_t gives rise to the horizontal variation of $f(t)$.

On the other hand, the time variation δt can be expressed by the contraction between the variational vector field (2.5) and one-form $\mathrm{d}_h t$ on T^*T, i.e., $\mathrm{d}t$ on T^*E,

$$i_{\xi_t}\mathrm{d}_h t=\delta t. \tag{2.30}$$

It is also feasible to express the variation $\delta_h q^i(t)$ as contraction of a horizontal variation vector field ξ_h with $\mathrm{d}_v q^i$ or $\mathrm{d}q^i$. To this purpose, we should introduce the variation vector field $\xi_{h,q}$ along the fiber with respect to horizontal variations of $q^i(t)$,

$$\xi_{h,q}:=\delta_h q^i(t)\frac{\partial}{\partial q^i}. \tag{2.31}$$

Combining with the vector field ξ_t in (2.5), the general horizontal variational vector field ξ_h should be defined as

$$\xi_h:=\xi_t+\xi_{h,q}=\delta t\frac{\partial}{\partial t}+\delta_h q^i(t)\frac{\partial}{\partial q^i}. \tag{2.32}$$

Its contraction with $\mathrm{d}_v q^i$ or $\mathrm{d}q^i$ leads to

$$i_{\xi_h}\mathrm{d}q^i=\delta_h q^i(t). \tag{2.33}$$

In general, for any functional of $q^i(t)$ and $\dot{q}^i(t)$, $F(q^i(t),\dot{q}^i(t)):TQ\to R$, its (horizontal) variation induced by (2.3) is

$$F(q^i(t),\dot{q}^i(t))\to F\left(q^i(t'),\frac{\mathrm{d}}{\mathrm{d}t'}q^i(t')\right)=F(q^i(t),\dot{q}^i(t))+\delta_h F(q^i(t),\dot{q}^i(t)),$$

$$\delta_h F(q^i(t),\dot{q}^i(t))=i_{\xi_h}\mathrm{d}F(q^i(t),\dot{q}^i(t)). \tag{2.34}$$

Remark 2.3: For the total variation, a total variational vector field for $q^i(t)$ along the fiber can also be introduced

$$\xi_{\text{total}} := \xi_v + \xi_h = \delta t \frac{\partial}{\partial t} + \delta_t q^i(t) \frac{\partial}{\partial q^i} = \delta t \frac{\partial}{\partial t} + \left(\delta_v q^i(t) + \delta t \frac{\mathrm{d}}{\mathrm{d}t} q^i(t) \right) \frac{\partial}{\partial q^i}, \tag{2.35}$$

whose contraction with $\mathrm{d}q^i$ leads to the total variation $\delta_t q^i(t)$,

$$i_{\xi_{\text{total}}} \mathrm{d}q^i = \delta_t q^i(t). \tag{2.36}$$

If we introduce the Lagrangian one-from

$$\mathbf{L} := L(q^i, \dot{q}^i, t)\mathrm{d}t \tag{2.37}$$

and take $0 = \mathrm{d}^2\mathbf{L}$, it is easy to see that the theorem 1 still holds. This means that the total variations keep the Euler–Lagrange cohomology as well as the necessary and sufficient condition for symplectic structure preserving property in classical mechanics.

Remark 2.4: In some literatures (see, for example, Ref. 9), it is required that Hamilton's principle holds for the total variation of the action, i.e., $\delta_t S = 0$, and regard $\delta_t q^i$ and δt as independent variations. Thus it follows the Euler–Lagrange equation, the conservation relation for the energy and the surface term

$$\frac{\partial L}{\partial q^i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i} \right) = 0,$$

$$\frac{\mathrm{d}}{\mathrm{d}t} H + \frac{\partial}{\partial t} L = 0,$$

$$\vartheta = \frac{\partial L}{\partial \dot{q}^j} \delta_t q^j - H \delta t. \tag{2.38}$$

If $(\partial/\partial t) L = 0$, i.e., the system is conservative, the energy H is conserved. However, $\delta_t q^i$ is actually dependent on δt. Therefore, it should be better to regard $\delta_v q^i$ and δt as independent variations.

B. Variations in Hamiltonian mechanics

The action principle should also be applied to the Hamiltonian mechanics. In order to transfer to the Hamiltonian formalism, we introduce a set of conjugate momenta from the Lagrangian $L(q^i(t), \dot{q}^i(t); t)$,

$$p_j = \frac{\partial L}{\partial \dot{q}^j}, \tag{2.39}$$

and take a Legendre transformation to get the Hamiltonian

$$H := H(q^i, p_j; t) = p_k \dot{q}^k - L(q^i, \dot{q}^j; t). \tag{2.40}$$

Now the action functional can be expressed as

$$S([p_i(t)], [q^i(t)]; t_1, t_2) = \int_{t_1}^{t_2} \mathrm{d}t \{ p_k \dot{q}^k - H(q^i, p_j; t) \}. \tag{2.41}$$

The total variation of the action can be calculated

$$\delta_t S = \delta_v S + \delta_h S,$$

$$\delta_v S = \int_{t_1}^{t_2} \mathrm{d}t \left\{ [H_{p_i}] \delta_v p_i - [H_{q^i}] \delta_v q^i + \frac{\mathrm{d}}{\mathrm{d}t}(p_i \delta_v q^i) \right\},$$

$$\delta_h S = \int_{t_1}^{t_2} \mathrm{d}t \left\{ [H_{p_i}] \delta_h p_i - [H_{q^i}] \delta_h q^i + \left[\frac{\mathrm{d}}{\mathrm{d}t} H - \frac{\partial}{\partial t} H \right] \delta t + \frac{\mathrm{d}}{\mathrm{d}t}(p_i \delta_h q^i - H \delta t) \right\}, \tag{2.42}$$

where $[H_{p_i}]$, $[H_{q^i}]$ are canonical operators

$$[H_{p_i}] := \dot{q}^i - \frac{\partial H}{\partial p_i}, \quad [H_{q^i}] := \dot{p}_i + \frac{\partial H}{\partial q^i}. \tag{2.43}$$

Thus, the stationary requirement for the vertical variation of the action $\delta_v S = 0$ leads to the canonical equations

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}. \tag{2.44}$$

While the time reparametrization invariance of the action, i.e., $\delta_h S = 0$ gives rise to an identity on the condition of the energy,

$$[H_{p_i}] \dot{p}_i - [H_{q^i}] \dot{q}^i + \frac{\mathrm{d}}{\mathrm{d}t} H - \frac{\partial}{\partial t} H \equiv 0. \tag{2.45}$$

And the boundary term that leads to so-called ''extended symplectic potential'' is a total divergence

$$\int_{t_1}^{t_2} \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t}(p_i \delta_h q^i - H \delta t) = \int_{t_1}^{t_2} \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t}(L \delta t) = 0. \tag{2.46}$$

Similar to the Lagrangian mechanics, all remarks in the preceding section can be made for the Hamiltonian formalism. Especially, the theorem 1 can also be established here.

III. VARIATIONS FOR DISCRETE MECHANICS

We have proposed a difference variational principle for the (vertical) variation in discrete Lagrangian mechanics. The crucial point is to regard the differences with fixed time step-length as entire variables.[12,14] Main advantage of the approach is that it is applicable to both Lagrangian and Hamiltonian formalisms for the discrete mechanics, since there exists the discrete Legendre transformation. This approach can also be generalized to the variation for the differences with variable time step-length, i.e., the variable differences. We also regard the variable differences as entire variables. Consequetly, the variable time step-length should be determined by an equation given by the variation problem with variable discrete integral boundary. In Lee's words, discrete time is regarded as a dynamical variable, but here the variable time differences are the variational variable.

Now, the ''time'' t is difference discretized,

$$t \in R \to t \in T_D = \{(t_k, t_{k+1} = t_k + \Delta t_k, \quad k \in Z)\}, \tag{3.1}$$

and the step-lengths Δt_k are determined by a variational equation. But, the n-dimensional configuration space M_k at each moment $t_k, k \in Z$, is still continuous and smooth enough.

Let N be the set of all nodes on T_D with index set $\mathrm{Ind}(N) = Z$, $M = \cup_{k \in Z} M_k$ the configuration space on T_D that is at least piecewisely smooth enough. At the moment let t_k, $\mathcal{N}_k$ be the set of

nodes neighboring to t_k. Let I_k be the index set of nodes of $\mathcal{N}_k$ including t_k. The coordinates of M_k are denoted by $q^i(t_k)=q^{i(k)}$, $i=1,\ldots,n$. $T(M_k)$ the tangent bundle of M_k in the sense that difference at t_k is its base, $T^*(M_k)$ its dual. Let $\mathcal{M}_k=\cup_{l\in I_k}M_l$ be the union of configuration spaces M_l at $t_l, l\in I_k$ on $\mathcal{N}_k$, $T\mathcal{M}_k=\cup_{l\in I_k}TM_l$ the union of tangent bundles on M_k, $F(TM_k)$, and $F(T\mathcal{M}_k)$ the function spaces on each of them, respectively, etc. In the difference variational approach, we need these notions.

A. Variable difference Lagrangian mechanics

Let us consider the system with a discrete Lagrangian $L_D{}^{(k)}$ on $F(T(M_k\times T_D))$. For simplicity, the Lagrangian is of the first order of differences

$$L_D{}^{(k)}=L_D(q^{i(k)},\Delta_k q^{i(k)};t_k), \tag{3.2}$$

with the difference $\Delta_k q^{i(k)}$ of $q^{i(k)}$ at t_k defined by

$$\Delta_k q^{i(k)}:=\frac{q^{i(k+1)}-q^{i(k)}}{t_{k+1}-t_k}. \tag{3.3}$$

The discrete action of the system is given by

$$S_D=\sum_{k\in Z}(t_{k+1}-t_k)L_D{}^{(k)}\left(q^{i(k)},\frac{q^{i(k+1)}-q^{i(k)}}{t_{k+1}-t_k};t_k\right). \tag{3.4}$$

The discrete total variations for $q^{i(k)}=q^i(t_k)$ should be defined as follows:

$$\delta_t q^{i(k)}:=q'^i(t'_k)-q^i(t_k)=\delta_v q^{i(k)}+\delta_h q^{i(k)},\quad t'_k=t_k+\delta t_k,$$

$$\delta_v q^{i(k)}:=q'^i(t_k)-q^i(t_k),\quad \delta_v t_k=0,$$

$$\delta_h q^{i(k)}:=q'^i(t'_k)-q'^i(t_k)=q^i(t'_k)-q^i(t_k)+O(\delta^2). \tag{3.5}$$

It can be shown that horizontal variation $\delta_h q^{i(k)}$ is given by

$$\delta_h q^{i(k)}=\delta t_k\Delta_k q^{i(k)}. \tag{3.6}$$

The discrete total variations for $\Delta_k q^{i(k)}$ are defined as

$$\delta_t\Delta_k q^{i(k)}:=\frac{q'^i(t'_{k+1})-q'^i(t'_k)}{t'_{k+1}-t'_k}-\frac{q^i(t_{k+1})-q^i(t_k)}{t_{k+1}-t_k}=\delta_v\Delta_k q^{i(k)}+\delta_h\Delta_k q^{i(k)},$$

$$\delta_v\Delta_k q^{i(k)}:=\frac{q'^i(t_{k+1})-q'^i(t_k)}{t_{k+1}-t_k}-\frac{q^i(t_{k+1})-q^i(t_k)}{t_{k+1}-t_k}. \tag{3.7}$$

From the definition of the difference with variable time step-length (3.3) and the Leibniz law for it

$$\Delta_k(f^{(k)}g^{(k)})=(\Delta_k f^{(k)})g^{(k)}+Ef^{(k)}(\Delta_k g^{(k)}), \tag{3.8}$$

where E is the shift operator defined as

$$Ef^{(k)}=f^{(k+1)},\quad E^{-1}f^{(k)}=f^{(k-1)}, \tag{3.9}$$

it follows

$$\delta_t \Delta_k q^{i(k)} = \Delta_k(\delta_t q^{i(k)}) - (\Delta_k \delta t_k)\Delta_k q^{i(k)},$$

$$\delta_h \Delta_k q^{i(k)} = \delta t_{k+1} \Delta(\Delta_k q^{i(k)}). \tag{3.10}$$

Namely,

$$\delta_v \Delta_k q^{i(k)} = \Delta_k \delta_v q^{i(k)},$$

$$\delta_h \Delta_k q^{i(k)} = \Delta_k \delta_h q^{i(k)} - (\Delta_k \delta t_k)\Delta_k q^{i(k)}. \tag{3.11}$$

Using the above properties and

$$\delta_t(t_{k+1} - t_k) = \Delta_k(\delta_t t_k)(t_{k+1} - t_k), \tag{3.12}$$

the total variations of the discrete Lagrangian can be calculated as follows:

$$\begin{aligned}\delta_t L_D{}^{(k)} &= \frac{\partial L_D{}^{(k)}}{\partial q^{i(k)}} \delta_t q^{i(k)} + \frac{\partial L_D{}^{(k)}}{\partial \Delta_k q^{i(k)}} \delta_t \Delta_k q^{i(k)} + \frac{\partial L_D{}^{(k)}}{\partial t_k} \delta_t t_k \\ &= [L_{q^{i(k)}}] \delta_t q^{i(k)} + \Delta_k(p_i{}^{(k)} \Delta_k q^{i(k-1)}) \delta t_k \\ &\quad + \frac{\partial L_D{}^{(k)}}{\partial t_k} \delta t_k + \Delta_k(p_i{}^{(k+1)} \delta_t q^{i(k)} - p_i{}^{(k)} \Delta_k q^{i(k-1)} \delta t_k),\end{aligned} \tag{3.13}$$

where $[L_{q^{i(k)}}]$ is the discrete Euler–Lagrange operator

$$[L_{q^{i(k)}}] := \frac{\partial L_D{}^{(k)}}{\partial q^{i(k)}} - \Delta\left(\frac{\partial L_D{}^{(k-1)}}{\partial \Delta q^{i(k-1)}}\right), \tag{3.14}$$

and $p_i{}^{(k)}$ is the discrete canonical conjugate momenta

$$p_i{}^{(k)} := \frac{\partial L_D{}^{(k-1)}}{\partial \Delta q^{i(k-1)}}. \tag{3.15}$$

Thus the total variation of action is given by

$$\begin{aligned}\delta_t S_D &= \sum_k (t_{k+1} - t_k)\{(\Delta \delta t_k) L_D{}^{(k)} + \delta_t L_D{}^{(k)}\} \\ &= \sum_k (t_{k+1} - t_k)\left\{[L_{q^{i(k)}}] \delta_t q^{i(k)} + \left(\Delta_k H_D{}^{(k-1)} + \frac{\partial L_D{}^{(k)}}{\partial t_k}\right) \delta t_k \right. \\ &\quad \left. + \Delta_k(p_i{}^{(k+1)} \delta_t q^{i(k)} - H_D{}^{(k-1)} \delta t_k)\right\},\end{aligned} \tag{3.16}$$

where $H_D{}^{(k)}$ is the difference Hamiltonian that can be introduced through the discrete Legendre transformation

$$H_D{}^{(k)} := p_i{}^{(k+1)} \Delta_t q^{i(k)} - L_D{}^{(k)}. \tag{3.17}$$

Thus, the total variation of the discrete action (3.16) can be written as

$$\delta_t S_D = \delta_v S_D + \delta_h S_D,$$

$$\delta_v S_D = \sum_k (t_{k+1} - t_k)\{[L_{q^{i(k)}}] \delta_v q^{i(k)} + \Delta(p_i{}^{(k+1)} \delta_v q^{i(k)})\},$$

$$\delta_h S_D=\sum_k\ (t_{k+1}-t_k)\Bigg\{[L_{q^{i(k)}}]\delta_h q^{i(k)}+\left(\Delta H_D{}^{(k-1)}+\frac{\partial L_D{}^{(k)}}{\partial t_k}\right)\delta t_k+\Delta(p_i{}^{(k+1)}\delta_h q^{i(k)}$$
$$-H_D{}^{(k-1)}\delta t_k)\Bigg\}. \tag{3.18}$$

The variational principle requires $\delta_v S_D=0$ and the discretized reparametrization invariance with respect to discrete time may also lead to $\delta_h S_D=0$ if this invariance does exist. Thus it follows the discrete Euler–Lagrange equations for $q^{i(k)}$'s,

$$\frac{\partial L_D{}^{(k)}}{\partial q^{i(k)}}-\Delta\left(\frac{\partial L_D{}^{(k-1)}}{\partial\Delta q^{i(k-1)}}\right)=0, \tag{3.19}$$

and the equation for the variable time step-length,

$$\left(\frac{\partial L_D{}^{(k)}}{\partial q^{i(k)}}-\Delta\left(\frac{\partial L_D{}^{(k-1)}}{\partial\Delta q^{i(k-1)}}\right)\right)\Delta q^{i(k)}+\Delta H_D{}^{(k-1)}-\frac{\partial H_D{}^{(k)}}{\partial t_k}=0. \tag{3.20}$$

It is more or less straightforward to show that if the time step-length is fixed the equation (3.20) has no solution in general even if the Lagrangian does not depend on discrete time manifestly. In other words, for the conservative discrete Lagrangian mechanics the time step-length should be variable in general so that the energy of the system can be kept conserved discretely.

Remark 3.1: We may introduce exterior differential operators $\hat{\mathrm{d}}$, d_v, and $\hat{\mathrm{d}}_h$ on $T^*(M\times T_D)$, T^*M and T^*T_D, respectively. They are nilpotent and satisfy

$$\hat{\mathrm{d}}=\mathrm{d}_v+\hat{\mathrm{d}}_h,\quad \{\mathrm{d}_v,\hat{\mathrm{d}}_h\}=0. \tag{3.21}$$

Especially, $\hat{\mathrm{d}}_h$ is due to the difference on T_D and satisfy Leibniz's law for ordinary forms. In fact, some NCDC is needed to completely clarify the properties of $\hat{\mathrm{d}}_h$. For the case that Δt is fixed, the NCDC can be found in Refs. 16 and 17. For the case of variable time steps, similar NCDC can also be established.

Remark 3.2: Actually, analog to the case with fixed time steps,[12,14] we can establish the difference version for the Euler–Lagrange cohomology and the necessary and sufficient condition for the difference conservation law of the discrete symplectic two-form.

From $\delta_v S_D$ in (3.18), it is easy to see that we may take d_v on S_D to get

$$\mathrm{d}_v S_D=\sum_k\ (t_{k+1}-t_k)\mathrm{d}_v L_D{}^{(k)},\quad \mathrm{d}_v L_D{}^{(k)}=\mathcal{E}_D{}^{(k)}+\Delta_k\theta_D{}^{(k)}, \tag{3.22}$$

where $\mathcal{E}_D{}^{(k)}$, $\theta_D{}^{(k)}$ are the discrete Euler–Lagrange one-form and symplectic potential one-form, respectively,

$$\mathcal{E}_D{}^{(k)}:=[L_{q^{i(k)}}]\mathrm{d}_v q^{i(k)},\quad \theta_D{}^{(k)}:=p_i{}^{(k+1)}\mathrm{d}_v q^{i(k)}. \tag{3.23}$$

Then due to the nilpotency of d_v, it is straightforward to get

$$\mathrm{d}_v\mathcal{E}_D{}^{(k)}+\Delta_k\omega_D{}^{(k)}=0,\quad \omega_D{}^{(k)}:=\mathrm{d}_v\theta_D{}^{(k)}=\mathrm{d}_v p_i{}^{(k+1)}\wedge\mathrm{d}_v q^{i(k)}. \tag{3.24}$$

Therefore, we may get the discrete version for the theorem 1.[12–14]

Theorem 2: *For the discrete Lagrangian with first order differences on the bundle* $E(T_D,Q,\pi)\simeq M\times T_D$, *the following properties hold:*

(1) There exists the discrete version of the Euler–Lagrange cohomology: $H_{DCM}:=\{$*Closed Euler–Lagrange forms*$\}/\{$*Exact Euler–Lagrange forms*$\}$.

(2) The necessary and sufficient condition for conservation of the discrete symplectic two-form,

i.e.,

$$\Delta_k \omega_D{}^{(k)}=0, \tag{3.25}$$

is that the corresponding discrete Euler–Lagrange one-form is closed, rather than the system being on the solution space only.

Remark 3.3: In this paper, T_D is an infinite chain. It is reasonable to consider an interval on T_D. We will report the issues on this topic elsewhere.

B. Variable difference Hamiltonian mechanics

Now we consider the total difference variation on the phase space in the discrete Hamiltonian formalism with variable (time step-length) difference.

In order to transfer to the discrete Hamiltonian formalism, it is needed to introduce the discrete canonical conjugate momenta according to the equation (3.15) and express the discrete Lagrangian by the discrete Hamiltonian via Legendre transformation (3.17). Thus, the discrete action can be expressed as

$$S_D=\sum_k (t_{k+1}-t_k) L_D{}^{(k)}\left(q^{i(k)}, \frac{q^{i(k+1)}-q^{i(k)}}{t_{k+1}-t_k}, t_k\right)=\sum_k (t_{k+1}-t_k)(p_i{}^{(k+1)}\Delta_t q^{i(k)}-H_D{}^{(k)}). \tag{3.26}$$

And its total variation reads

$$\begin{aligned}\delta_t S_D &= \delta_v S_D+\delta_h S_D \\ &=\sum_k (t_{k+1}-t_k)\left\{\left(\Delta q^{i(k)}-\frac{\partial H_D{}^{(k)}}{\partial p_i{}^{(k+1)}}\right)\delta_t p_i{}^{(k+1)}-\left(\Delta p_i{}^{(k)}+\frac{\partial H_D{}^{(k)}}{\partial q^{i(k)}}\right)\delta_t q^{i(k)}\right. \\ &\quad \left.+\left(\Delta H_D{}^{(k-1)}+\frac{\partial L_D{}^{(k)}}{\partial t_k}\right)\delta t_k+\Delta(p_i{}^{(k)}\delta_t q^{i(k)}-H_D{}^{(k-1)}\delta t_k)\right\}.\end{aligned} \tag{3.27}$$

Similar to the discrete Lagrangian formalism, Hamilton's principle requires $\delta_v S_D=0$ and the discretized reparametrization invariance with respect to discrete time may also lead to $\delta_h S_D=0$ if this invariance does exist. Thus we get the discrete canonical equations for $p_i{}^{(k)}$'s and $q^{i(k)}$'s,

$$\Delta q^{i(k)}=\frac{\partial H_D{}^{(k)}}{\partial p_i{}^{(k+1)}}, \quad \Delta p_i{}^{(k)}=-\frac{\partial H_D{}^{(k)}}{\partial q^{i(k)}}, \tag{3.28}$$

and the equation for the variable time step-length,

$$\left(\Delta q^{i(k)}-\frac{\partial H_D{}^{(k)}}{\partial p_i{}^{(k+1)}}\right)\Delta p_i{}^{(k+1)}-\left(\Delta p_i{}^{(k)}+\frac{\partial H_D{}^{(k)}}{\partial q^{i(k)}}\right)\Delta q^{i(k)}+\Delta H_D{}^{(k-1)}-\frac{\partial H_D{}^{(k)}}{\partial t_k}=0. \tag{3.29}$$

It is also more or less straightforward to show that if the time step-length is fixed the equation (3.29) has no solution in general even if the Hamiltonian does not depend on discrete time manifestly. In other words, for the conservative discrete Hamiltonian mechanics the time step-length should be variable so that the energy of the system can be kept conserved discretely. In Refs. 19–21, 11, 18, this issue has been studied.

It should be mentioned that all remarks in the preceding section can be made here and the theorem 2 can also be established for the discrete Hamiltonian formalism.

IV. VARIATIONS FOR FIELD THEORY

We now briefly recall the variations in classical continous field theory. We also mention the Euler–Lagrange cohomology and its relation with the multisymplicity.[12–14]

Consider a bundle $E(X,Q,\pi)$, the fiber $Q\simeq M$. For simplicity, let $X=X^{(1,n-1)}$ be an n-dimensional Minkowskian space as base manifold with coordinates x^μ $(\mu=0,\ldots,n-1)$, M the configuration space on $X^{(1,n-1)}$ with a set of generic (scalar) fields $u^\alpha(x)$ $(\alpha=1,\ldots,r)$, TM the tangent bundle of M with coordinates (u^α,u^α_μ), where $u^\alpha_\mu=\partial u^\alpha/\partial x^\mu$, $F(TM)$ the function space on TM, etc.

We also assume these fields to be free of constraints, although our approach can be generalized to other cases.

A. Variations in Lagrangian formalism

The Lagrangian of the theory is supposed to be the first order of derivatives of the fields and is dependent on the coordinates manifestly, i.e., $L(u^\alpha,u^\alpha_\mu;x^\mu)$. The action is

$$S([u^\alpha(x)];x^\mu)=\int_\Omega \mathrm{d}^4x\, L(u^\alpha,u^\alpha_\mu;x^\mu). \tag{4.1}$$

Let us consider the variations of the fields, i.e., total variation $\delta_t u^\alpha$, vertical one $\delta_v u^\alpha$ and horizontal one $\delta_h u^\alpha$,

$$u^\alpha\to u'^\alpha(x')=u^\alpha(x)+\delta_t u^\alpha(x),$$

$$\delta_t u^\alpha=\delta_v u^\alpha+\delta_h u^\alpha,$$

$$\delta_v u^\alpha(x):=u'^\alpha(x)-u^\alpha(x),$$

$$\delta_h u^\alpha(x):=u'^\alpha(x')-u'^\alpha(x)=u^\alpha(x')-u^\alpha(x)+O(\delta^2)=\delta x^\mu\partial_\mu u^\alpha(x)=\mathcal{L}_{\xi_x}u^\alpha(x), \tag{4.2}$$

accompanying with the coordinates' infinitesimal continuous transformation

$$x^\mu\to x'^\mu=x^\mu+\delta x^\mu. \tag{4.3}$$

Here $\mathcal{L}_{\xi_x}$ is the Lie derivative with respect to the horizontal variational vector field

$$\xi_x:=\delta x^\mu\partial_\mu. \tag{4.4}$$

The corresponding changes in the derivative of fields u^α_μ are

$$\begin{gathered}
\frac{\partial}{\partial x^\mu}u^\alpha(x)\to\frac{\partial}{\partial x'^\mu}u'^\alpha(x')=\frac{\partial}{\partial x^\mu}u^\alpha(x)+\delta_t\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right),\\
\delta_t\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right)=\delta_v\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right)+\delta_h\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right),\\
\delta_v\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right):=\frac{\partial}{\partial x^\mu}u'^\alpha(x)-\frac{\partial}{\partial x^\mu}u^\alpha(x),\\
\delta_h\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right)=\delta x^\nu\frac{\partial}{\partial x^\nu}\left(\frac{\partial}{\partial x^\mu}u^\alpha(x)\right)=\mathcal{L}_{\xi_x}\frac{\partial}{\partial x^\mu}u^\alpha(x).
\end{gathered} \tag{4.5}$$

Now the action (4.1) is also changed as follows:

$$
\begin{aligned}
S([u^{\alpha}(x)];x^{\mu}) &\to S'([u'^{\alpha}(x')];x'^{\mu}) \\
&= \int_{\Omega'} \mathrm{d}^n x'\, L'(u'^{\alpha}(x'), u'^{\alpha}_{\mu'}(x');x'^{\mu}) \\
&= \int_{\Omega} \mathrm{d}^n x\, \det(\partial x'/\partial x)\{L(u^{\alpha}(x), u^{\alpha}_{\mu}(x);x^{\mu}) + \delta_t L\} = S([u^{\alpha}(x)];x^{\mu}) + \delta_t S.
\end{aligned}
\tag{4.6}
$$

Using Jacobi formula for the measure

$$
\mathrm{d}^n x' = \det\left(\frac{\partial x'}{\partial x}\right)\mathrm{d}^n x = \left(1 + \frac{\partial \delta x^{\mu}}{\partial x^{\mu}}\right)\mathrm{d}^n x + O(\delta^2), \tag{4.7}
$$

we get

$$
\begin{aligned}
\delta_t S([u^{\alpha}(x)];x^{\mu}) &= \int_{\Omega} \mathrm{d}^n x\{\partial_{\mu}\delta x^{\mu} L + \delta_t L\} \\
&= \int_{\Omega} \mathrm{d}^n x \left\{ [L_{u^{\alpha}}]\delta_t u^{\alpha} + \left(\partial^{\mu} T_{\mu\nu} + \frac{\partial L}{\partial x^{\nu}}\right)\delta x^{\nu} \right. \\
&\quad \left. + \partial_{\mu}\left(\frac{\partial L}{\partial(\partial_{\mu} u^{\alpha})}\delta_t u^{\alpha} - T^{\mu}{}_{\nu}\delta x^{\nu}\right)\right\},
\end{aligned}
\tag{4.8}
$$

$$
\delta_v S([u^{\alpha}(x)];x^{\mu}) = \int_{\Omega} \mathrm{d}^n x \left\{ [L_{u^{\alpha}}]\delta_v u^{\alpha} + \partial_{\mu}\left(\frac{\partial L}{\partial(\partial_{\mu} u^{\alpha})}\delta_v u^{\alpha}\right)\right\}, \tag{4.9}
$$

$$
\begin{aligned}
\delta_h S([u^{\alpha}(x)];x^{\mu}) &= \int_{\Omega} \mathrm{d}^n x \left\{ [L_{u^{\alpha}}]\delta_h u^{\alpha} + \left(\partial^{\mu} T_{\mu\nu} + \frac{\partial L}{\partial x^{\nu}}\right)\delta x^{\nu} + \partial_{\mu}\left(\frac{\partial L}{\partial(\partial_{\mu} u^{\alpha})}\delta_h u^{\alpha} - T^{\mu}{}_{\nu}\delta x^{\nu}\right)\right\} \\
&= \int_{\Omega} \mathrm{d}^n x\, \partial_{\mu}(L\,\delta x^{\mu}),
\end{aligned}
\tag{4.10}
$$

where $[L_{u^{\alpha}}]$ is the Euler–Lagrange operator and $T_{\mu\nu}$ the energy-momentum tensor

$$
\begin{aligned}
[L_{u^{\alpha}}] &:= \frac{\partial L}{\partial u^{\alpha}} - \partial_{\mu}\left(\frac{\partial L}{\partial u^{\alpha}_{\mu}}\right), \\
T_{\mu\nu} &:= \frac{\partial L}{\partial(\partial^{\mu} u^{\alpha})}\partial_{\nu} u^{\alpha} - L\,\eta_{\mu\nu}.
\end{aligned}
\tag{4.11}
$$

Thus $\delta_t S = 0$, i.e., $\delta_v S = 0$ due to Hamilton's principle and $\delta_h S = 0$ due to the invariance of reparametrization of the coordinates that preserves the action. In general, the general coordinate transformations may be considered and all formulas become covariant. This requires to regard $\delta_v u^{\alpha}$ and δx^{μ} as independent components and gives rise to the Euler–Lagrange equation

$$
\frac{\partial L}{\partial u^{\alpha}} - \partial_{\mu}\left(\frac{\partial L}{\partial u^{\alpha}_{\mu}}\right) = 0 \tag{4.12}
$$

as well as an identity between the Euler–Lagrange operator and conservation property for the energy-momentum tensor

$$\left(\frac{\partial L}{\partial u^{\alpha}}-\partial_{\mu}\left(\frac{\partial L}{\partial u^{\alpha}_{\mu}}\right)\right)\partial_{\nu}u^{\alpha}+\partial^{\mu}T_{\mu\nu}+\partial_{\nu}L=0. \tag{4.13}$$

This equation shows that the energy-momentum tensor is conserved if and only if the Euler–Lagrange equation is satisfied and the Lagrangian does not depend manifestly on the coordinates.

The boundary term vanishes as follows:

$$\int_{\Omega}\mathrm{d}^{n}x\,\frac{\partial}{\partial x^{\mu}}\left(\left(\frac{\partial L}{\partial u^{\alpha}_{\mu}}\right)\delta_{v}u^{\alpha}+L\,\delta x^{\mu}\right)=\int_{\partial\Omega}\left(\left(\frac{\partial L}{\partial u^{\alpha}_{\mu}}\right)\delta_{v}u^{\alpha}+L\,\delta x^{\mu}\right)\mathrm{d}\sigma^{\mu}=0. \tag{4.14}$$

Remark 4.1: Introduce the nilpotent exterior differential operators d_v, d_h, and d satisfying

$$\mathrm{d}:=\mathrm{d}_v+\mathrm{d}_h,\quad \{\mathrm{d}_v,\mathrm{d}_h\}=0, \tag{4.15}$$

where d_v is along the fiber $Q\simeq M$, d_h and d on T^*X and T^*E, $E=M\times X$, respectively. Consider a vertical variational vector field

$$\xi_u:=\delta_v u^{\alpha}(x)\,\frac{\partial}{\partial u^{\alpha}} \tag{4.16}$$

such that

$$\delta_v u^{\alpha}(x)=i_{\xi_u}\mathrm{d}_v u^{\alpha}=i_{\xi_u}\mathrm{d}u^{\alpha}. \tag{4.17}$$

By means of this vertical variational vector field (4.16) on TQ, $\delta_v S$ can also be expressed as its contraction with one-form $\mathrm{d}_v S\in T^*Q$,

$$i_{\xi_u}\mathrm{d}_v S=\delta_v S. \tag{4.18}$$

We may calculate $\mathrm{d}_v S\in T^*Q$. Since d_v commutes with the integral and $\mathrm{d}^n x$ (see also, for example, the functional differential calculus in Ref. 27), it is straightforward to get

$$\mathrm{d}_v S=\int_{\Omega}\mathrm{d}^{n}x\left\{[L_{u^{\alpha}}]\mathrm{d}_v u^{\alpha}+\frac{\partial}{\partial x^{\mu}}\,\theta^{\mu}\right\}, \tag{4.19}$$

where θ^{μ} are the Lagrange one-forms

$$\theta^{\mu}:=\frac{\partial L}{\partial u^{\alpha}_{\mu}}\mathrm{d}_v u^{\alpha}. \tag{4.20}$$

By contracting with the vertical variational vector field (4.16), we get straightforwardly $\delta_v S$.

Furthermore, due to the nilpotency of d_v, it is easy to get

$$\mathrm{d}_v\mathcal{E}_u+\frac{\partial}{\partial x^{\mu}}\,\omega^{\mu}=0, \tag{4.21}$$

where $\mathcal{E}_u$ is the Euler–Lagrange one-form defined by

$$\mathcal{E}_u(u^{\alpha}(x),u^{\alpha}_{\mu}(x);x):=[L_{u^{\alpha}}]\mathrm{d}_v u^{\alpha}, \tag{4.22}$$

ω^{μ} are the multisymplectic two-forms and in local coordinates

$$\omega^{\mu}:=\mathrm{d}_v\,\theta^{\mu}=\frac{\partial^2 L}{\partial u^{\alpha}\partial u^{\beta}_{\mu}}\mathrm{d}u^{\alpha}\wedge\mathrm{d}u^{\beta}+\frac{\partial^2 L}{\partial u^{\alpha}_{\nu}\partial u^{\beta}_{\mu}}\mathrm{d}u^{\alpha}_{\nu}\wedge\mathrm{d}u^{\beta}. \tag{4.23}$$

From the definition (4.22), Eqs. (4.19) and (4.21), the following theorem[12–14] holds.

Theorem 3: *For the Lagrangian with first order of derivatives on the bundle $E(X,Q,\pi)$, the following properties hold.*

(1) There exists the Euler–Lagrange cohomology:

$$H_{CFT}:=\{\mathcal{E}_u|d\mathcal{E}_u=0\}/\{\mathcal{E}_u|\mathcal{E}_u=\mathrm{d}\beta\},$$

where $\beta=\beta(u^\alpha(x),u^\alpha_\mu(x);x)$ is an arbitrary function of $(u^\alpha(x),u^\alpha_\mu(x);x)$.

(2) The necessary and sufficient condition for conservation of the multisymplectic two-forms, i.e.,

$$\frac{\partial}{\partial x^\mu}\omega^\mu=0, \tag{4.24}$$

is that the corresponding Euler–Lagrange one-form is closed, rather than the system being on the solution space only.

Remark 4.2: From the definition of the Lie derivative it can be seen that the horizontal variations are given by the Lie derivative with respect to the variational vector field.

Let ξ be a vector field on X, $\exp(\lambda\xi)$ be the flow with parameter λ, i.e., the one-parameter diffeomorphism group, induced by ξ, f a differential form or a vector on X. The infinitesimal change of f under flow is described by its Lie derivative with respect to the vector field ξ,

$$\mathcal{L}_\xi f(x):=\lim_{\lambda\to 0}\frac{1}{\lambda}\{\phi^*_\lambda f(\exp(\lambda\xi)x)-f(x)\}=\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0}(\phi^*_\lambda f(x')),\quad x'=\exp(\lambda\xi)x. \tag{4.25}$$

Here ϕ^*_λ is the bull-back or the inverse differential for the differential form or vector, respectively.

Taking horizontal variational vector field for the coordinates $\xi=\xi(x)=\xi_x$ (4.4), it follows that the Lie derivative of $f(x)$ with respect to ξ_x gives rise to the horizontal variation of $f(x)$.

On the other hand, the coordinate variations δx^μ can be expressed by the contraction between the variational vector field (4.4) and one-form $\mathrm{d}_h x^\mu$ on T^*X, i.e., $\mathrm{d}x^\mu$ on T^*E,

$$i_{\xi_x}\mathrm{d}_h x^\mu=\delta x^\mu. \tag{4.26}$$

It is also feasible to express the variation $\delta_h u^\alpha(x)$ as contraction of a horizontal variation vector field ξ_h with $\mathrm{d}_v u^\alpha$ or $\mathrm{d}u^\alpha$. To this purpose, we introduce the horizontal variation vector field $\xi_{h,u}$. It is along the fiber with respect to horizontal variations of $u^\alpha(x)$,

$$\xi_{h,u}:=\delta_h u^\alpha(x)\frac{\partial}{\partial u^\alpha}. \tag{4.27}$$

Combining this vector field with the vector field ξ_x in (4.4), the general horizontal variational vector field ξ_h should be defined as

$$\xi_h:=\xi_x+\xi_{h,u}=\delta x^\mu\frac{\partial}{\partial x^\mu}+\delta_h u^\alpha(x)\frac{\partial}{\partial u^\alpha}. \tag{4.28}$$

Its contraction with $\mathrm{d}_v u^\alpha$ or $\mathrm{d}u^\alpha$ leads to

$$i_{\xi_h}\mathrm{d}u^\alpha=\mathrm{d}u^\alpha\cdot\xi_h=\delta_h u^\alpha(t). \tag{4.29}$$

In general, for any functional of $u^\alpha(x)$ and $u^\alpha_\mu(x)$, $F(u^\alpha(x),u^\alpha_\mu(x)):TQ\to R$, its (horizontal) variation induced by (4.3) is

$$F(u^\alpha(x),u^\alpha(x))\to F\left(u^\alpha(x'),\frac{\partial}{\partial x'^\mu}u^\alpha(x')\right)=F(u^\alpha(x),u^\alpha_\mu(x))+\delta_h F(u^\alpha(x),u^\alpha_\mu(x)),$$

$$\delta_h F(u^\alpha(x),u^\alpha_\mu(x)) = i_{\xi_h}\,\mathrm{d}F(u^\alpha(x),u^\alpha_\mu(x)). \tag{4.30}$$

Remark 4.3: For the total variation, a total variational vector field for $u^\alpha(x)$ along the fiber can also be introduced

$$\xi_{\text{total}} := \xi_v + \xi_h = \delta x^\mu \frac{\partial}{\partial x^\mu} + \delta_t u^\alpha(x)\frac{\partial}{\partial u^\alpha} = \delta x^\mu \frac{\partial}{\partial x^\mu} + \left(\delta_v u^\alpha(x) + \delta x^\mu \frac{\partial}{\partial x^\mu} u^\alpha(x)\right)\frac{\partial}{\partial u^\alpha}, \tag{4.31}$$

whose contraction with $\mathrm{d}u^\alpha$ leads to the total variation $\delta_t u^\alpha(x)$,

$$i_{\xi_{\text{total}}}\mathrm{d}u^\alpha = \mathrm{d}u^\alpha \cdot \xi_{\text{total}} = \delta_t u^\alpha(x). \tag{4.32}$$

B. Variations in Hamiltonian formalism

In order to transfer to the Hamiltonian formalism for classical field theory, we first define a set of ''momenta'' canonically conjugate to the field variables

$$\pi_\alpha(x) = \frac{\partial L}{\partial \dot{u}^\alpha}, \tag{4.33}$$

and take a Legendre transformation to get the Hamiltonian density

$$H(u^\alpha,\pi_\alpha,\nabla_a u^\alpha) = \pi_\alpha(x)\dot{u}^\alpha(x) - L(u^\alpha,\dot{u}^\alpha,\nabla_a u^\alpha), \tag{4.34}$$

where $\nabla_a = \partial/\partial x^a$, $a = 1,\ldots,n-1$. The Hamiltonian then is given by

$$H(t) = \int_\Sigma \mathrm{d}^{n-1}x\, H(x), \tag{4.35}$$

with the Legendre transformation

$$H(t) = \int_\Sigma \mathrm{d}^{n-1}x\{\pi_\alpha(x)\dot{u}^\alpha(x) - L(t)\}, \quad L(t) = \int_\Sigma \mathrm{d}^{n-1}x\, L, \tag{4.36}$$

where $\Sigma \subset \Omega$ is an $(n-1)$-dimensional simultaneous spacelike hypersurface in Ω.

The action $S([u^\alpha(x)];x^\mu)$ (4.1) becomes

$$S([u^\alpha(x)];x^\mu) = \int_\Omega \mathrm{d}^n x\{\pi_\alpha(x)\dot{u}^\alpha(x) - H(u^\alpha,\dot{u}^\alpha,\nabla_a u^\alpha)\}. \tag{4.37}$$

The total variation of the action can be calculated similar to that in the preceding section, but here $\pi_\alpha(x)$, $u^\alpha(x)$, and their derivatives should be varied independently. Thus we get

$$\begin{aligned}\delta_t S([u^\alpha(x)];x^\mu) &= \int_\Omega \mathrm{d}^n x\{\partial_\mu \delta x^\mu L + \delta_t L\} \\ &= \int_\Omega \mathrm{d}^n x\left\{[H_{\pi^\alpha}]\delta_t\pi^\alpha - [H_{u^\alpha}]\delta_t u^\alpha + \left(\partial^\mu T_{\mu\nu} + \frac{\partial H}{\partial x^\nu}\right)\delta x^\nu \right. \\ &\quad \left. - \partial_\mu\left(\frac{\partial H}{\partial(\partial_\mu u^\alpha)}\delta_t u^\alpha - T^\mu{}_\nu \delta x^\nu\right)\right\},\end{aligned} \tag{4.38}$$

where $[H_{u^\alpha}]$, $[H_{\pi^\alpha}]$ are the canonical operators

$$[H_{\pi_\alpha}] := \dot{u}^\alpha(x) - \frac{\partial H}{\partial \pi_\alpha},$$

$$[H_{u^\alpha}] := \dot{\pi}_\alpha(x) + \frac{\partial H}{\partial u^\alpha} - \nabla_a\left(\frac{\partial H}{\partial(\nabla_a u^\alpha)}\right). \tag{4.39}$$

Similar to the Lagrangian formalism, $\delta_t S=0$, i.e., $\delta_v S=0$ and $\delta_h S=0$, requires to regard $\delta_v u^\alpha$, $\delta_v \pi_\alpha$, and δx^μ as independent components. This leads to the canonical field equations

$$\dot{u}^\alpha(x) = \frac{\partial H}{\partial \pi_\alpha},$$

$$\dot{\pi}_\alpha(x) = -\frac{\partial H}{\partial u^\alpha} + \nabla_a\left(\frac{\partial H}{\partial(\nabla_a u^\alpha)}\right), \tag{4.40}$$

and an identity between the canonical operators and conservation property for the energy-momentum tensor

$$[H_{\pi^\alpha}]\partial_\nu \pi^\alpha - [H_{u^\alpha}]\partial_\nu u^\alpha + \partial^\mu T_{\mu\nu} - \partial_\nu H = 0. \tag{4.41}$$

It should be mentioned that all remarks in the preceding section can be made here and the theorem 3 can be established as well.

V. VARIATIONS FOR DISCRETE FIELD THEORY

We now study the variation problems for the difference discrete field theory with variable step-lengths. For simplicity, we consider the cases of $1+1$ or two-dimensional flat base manifold, i.e., $X^{1,1}$ or X^2 endowed with suitable signature of the metrics.

Let L^2 be a right-angle lattice on $X^{1,1}$ or X^2 with nodes $x_\mu^{(i,j)}=(x_1^i, x_2^j), \mu=1,2,(i,j)\in Z\times Z$ and variable step-lengths on two directions x_μ to be determined by discrete variation problems, N is all nodes on L^2. For a given node with coordinates $x_\mu^{(i,j)}$, let $M_D := M^{(i,j)}$ be the piece of configuration space with a set of generic field variables $u^\alpha(x_\mu^{(i,j)}) = u^{\alpha(i,j)} \in M_D$ at the node $x_\mu^{(i,j)}$, $TM^{(i,j)}$ the tangent bundle of $M^{(i,j)}$ with the set of field variables and their differences $(u^{\alpha(i,j)}, \Delta_\mu u^{\alpha(i,j)}) \in T(M^{(i,j)})$, $F(TM^{(i,j)})$ the function space on $TM^{(i,j)}$. Let $\mathcal{N}^{(i,j)}$ be the set of nodes neighboring to $x_\mu^{(i,j)}$ with index set $I^{(i,j)}=\mathrm{Ind}(\mathcal{N}^{(i,j)})$, a set of nodes related to $x_\mu^{(i,j)}$ by the differences, $\mathcal{M}^{(i,j)} = \cup_{\mathrm{Ind}(N)|I^{(i,j)}} M^{(i,j)}$ the union of the pieces of configuration space on $X^{(i,j)}$. $F(T(\mathcal{M}^{(i,j)}))$ function space on $T(\mathcal{M}^{(i,j)})$.

Since L^2 is a right-angle lattice, it should have only two possibilities for the variable step-lengths: either equal step-length variation along two directions simultaneously while along each direction the step-lengths are variable, or along one direction the step-length is fixed while along the other it is variable.

A. Variable difference Lagrangian field theory

The difference Lagrangian for a set of the generic fields $u^\alpha, \alpha=1,\ldots,r$, is a functional on $F(T(M^{(i,j)}))$ and suppose to be the first order of differences of the fields for simplicity,

$$L_D{}^{(i,j)} = L_D(u^{\alpha(i,j)}, \Delta_\mu u^{\alpha(i,j)}, x_\mu^{(i,j)}), \quad \mu=1,2, \tag{5.1}$$

where $x_\mu^{(i,j)}=(x_1^{(i)}, x_2^{(j)})$, $u^{\alpha(i,j)} = u^\alpha(x_\mu^{(i,j)})$ and

$$\Delta_1 u^{\alpha(i,j)} = \frac{u^{\alpha(i+1,j)} - u^{\alpha(i,j)}}{x_1^{(i+1)} - x_1^{(i)}}, \quad \Delta_2 u^{\alpha(i,j)} = \frac{u^{\alpha(i,j+1)} - u^{\alpha(i,j)}}{x_2^{(j+1)} - x_2^{(j)}}. \tag{5.2}$$

The discrete action S_D now reads

$$S_D=\sum_{i,j}\ \Delta_1 x_1^{(i)}\Delta_2 x_2^{(j)}L_D{}^{(i,j)}, \tag{5.3}$$

where $\Delta_1 x_1^{(i)}=x_1^{(i+1)}-x_1^{(i)}$, $\Delta_2 x_2^{(j)}=x_2^{(j+1)}-x_2^{(j)}$.

Let us consider the coordinates of nodes on the lattice subject to infinitesimal deformations that still keep L^2 as a right-angle lattice

$$x_\mu^{(i,j)}\to x'_\mu(x_1^{(i,j)},x_2^{(i,j)})=x_\mu^{(i,j)}+\delta x_\mu^{(i,j)}, \tag{5.4}$$

the corresponding changes in the fields are

$$\begin{gathered}u^\alpha(x)^{(i,j)}\to u'^\alpha(x')^{(i,j)}=u^\alpha(x)^{(i,j)}+\delta_t u^\alpha(x)^{(i,j)},\\ \delta_t u^\alpha(x)^{(i,j)}=\delta_v u^\alpha(x)^{(i,j)}+\delta_h u^\alpha(x)^{(i,j)},\\ \delta_v u^\alpha(x)^{(i,j)}:=u'^\alpha(x)^{(i,j)}-u^\alpha(x)^{(i,j)},\end{gathered} \tag{5.5}$$

$$\delta_h u^\alpha(x)^{(i,j)}:=u'^\alpha(x')^{(i,j)}-u'^\alpha(x)^{(i,j)}=u^\alpha(x')^{(i,j)}-u^\alpha(x)^{(i,j)}+O(\delta^2)=\delta x^{\mu(i,j)}\Delta_\mu u^\alpha(x)^{(i,j)}.$$

For the differences of fields, $\Delta_\mu u^\alpha(x)^{(i,j)}$, the corresponding changes are

$$\begin{gathered}\Delta_\mu u^\alpha(x)^{(i,j)}\to\Delta'_\mu u'^\alpha(x'(x^{(i,j)}))=\Delta_\mu u^\alpha(x)^{(i,j)}+\delta_t\Delta_\mu u^\alpha(x)^{(i,j)},\\ \delta_t\Delta_\mu u^\alpha(x)^{(i,j)}=\delta_v\Delta_\mu u^\alpha(x)^{(i,j)}+\delta_h\Delta_\mu u^\alpha(x)^{(i,j)},\\ \delta_v\Delta_\mu u^\alpha(x)^{(i,j)}:=\Delta_\mu u'^\alpha(x)^{(i,j)}-\Delta_\mu u^\alpha(x)^{(i,j)},\end{gathered} \tag{5.6}$$

$$\delta_h\Delta_\mu u^\alpha(x)^{(i,j)}:=\Delta'_\mu u'^\alpha(x')^{(i,j)}-\Delta_\mu u'^\alpha(x)^{(i,j)}=\Delta_\mu u^\alpha(x')^{(i,j)}-\Delta_\mu u^\alpha(x)^{(i,j)}+O(\delta^2).$$

These can be calculated to obtain

$$\begin{gathered}\delta_v\Delta_\mu u^\alpha(x)^{(i,j)}=\Delta_\mu(\delta_v u^\alpha(x)^{(i,j)}),\\ \delta_t\Delta_\mu u^\alpha(x)^{(i,j)}=\Delta_\mu\delta_t u^\alpha(x)^{(i,j)}-\Delta_\mu\delta x^{\nu(i,j)}\cdot\Delta_\nu u^\alpha(x)^{(i,j)}.\end{gathered} \tag{5.7}$$

Using the Leibniz law (3.8) for differences in each direction, it follows

$$\begin{gathered}\delta_t\Delta_1 u^\alpha(x)^{(i,j)}=\Delta_1\delta_v u^\alpha(x)^{(i,j)}+\delta x^{\nu(i+1,j)}\cdot\Delta_1\Delta_\nu u^\alpha(x)^{(i,j)},\\ \delta_t\Delta_2 u^\alpha(x)^{(i,j)}=\Delta_2\delta_v u^\alpha(x)^{(i,j)}+\delta x^{\nu(i,j+1)}\cdot\Delta_2\Delta_\nu u^\alpha(x)^{(i,j)}.\end{gathered} \tag{5.8}$$

The total variation of discrete action (5.3) can be calculated as

$$\delta_t S_D=\sum_{i,j}\ \Delta_1 x_1^{(i)}\cdot\Delta_2 x_2^{(j)}(\Delta_1\delta x_1^i L_D{}^{(i,j)}+\Delta_2\delta x_2^j L_D{}^{(i,j)}+\delta_t L_D{}^{(i,j)}). \tag{5.9}$$

Using formulas

$$\begin{gathered}\Delta_1\delta x_1^i L_D{}^{(i,j)}=\Delta_1(\delta x_1^i L_D{}^{(i-1,j)})-\delta x_1^i\Delta_1\mathcal{L}_D{}^{(i-1,j)},\\ \Delta_2\delta x_2^j L_D{}^{(i,j)}=\Delta_2(\delta x_2^j L_D{}^{(i,j-1)})-\delta x_2^j\Delta_2\mathcal{L}_D{}^{(i,j-1)},\end{gathered} \tag{5.10}$$

and

$$
\begin{aligned}
\delta_t L_D{}^{(i,j)} &= \frac{\partial \mathcal{L}_D{}^{(i,j)}}{\partial u^{\alpha(i,j)}}\,\delta_t u^{\alpha(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial(\Delta_\mu u^{\alpha(i,j)})}\,\delta_t \Delta_\mu u^{\alpha(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\mu(i,j)}}\,\delta x^{\mu(i,j)} \\
&= \frac{\partial L_D{}^{(i,j)}}{\partial u^{\alpha(i,j)}}\,\delta_t u^{\alpha(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial(\Delta_1 u^{\alpha(i,j)})}(\Delta_1 \delta_t u^{\alpha(i,j)} - (\Delta_1 \delta x^{\mu(i,j)})\cdot \Delta_\mu u^{\alpha(i,j)}) \\
&\quad + \frac{\partial L_D{}^{(i,j)}}{\partial(\Delta_2 u^{\alpha(i,j)})}(\Delta_2 \delta_t u^{\alpha(i,j)} - (\Delta_2 \delta x^{\mu(i,j)})\cdot \Delta_\mu u^{\alpha(i,j)}) + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\mu(i,j)}}\,\delta x^{\mu(i,j)} \\
&= [L_{u^{\alpha(i,j)}}]\,\delta_t u^{\alpha(i,j)} \\
&\quad + \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\delta_t u^{\alpha(i,j)} - \frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\Delta_\mu u^{\alpha(i-1,j)}\,\delta x^{\mu(i,j)}\right) \\
&\quad + \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\delta_t u^{\alpha(i,j)} - \frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\Delta_\mu u^{\alpha(i,j-1)}\,\delta x^{\mu(i,j)}\right) \\
&\quad + \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\Delta_\mu u^{\alpha(i-1,j)}\right)\delta x^{\mu(i,j)} \\
&\quad + \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\Delta_\mu u^{\alpha(i,j-1)}\right)\delta x^{\mu(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\mu(i,j)}}\,\delta x^{\mu(i,j)},
\end{aligned}
\tag{5.11}
$$

we obtain

$$
\begin{aligned}
\delta_t S_D &= \delta_v S_D + \delta_h S_D \\
&= \sum_{i,j} \Delta_1 x_1^{(i)} \cdot \Delta_2 x_2^{(j)} \Bigg\{ [L_{u^{\alpha(i,j)}}]\,\delta_t u^{\alpha(i,j)} + \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\delta_t u^{\alpha(i,j)}\right. \\
&\quad \left. - \left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\Delta_\mu u^{\alpha(i-1,j)} - \delta_{1\mu} L_D{}^{(i-1,j)}\right)\delta x^{\mu(i,j)}\right) \\
&\quad + \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\delta_t u^{\alpha(i,j)} - \left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\Delta_\mu u^{\alpha(i,j-1)} - \delta_{2\mu} L_D{}^{(i,j-1)}\right)\delta x^{\mu(i,j)}\right) \\
&\quad + \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\,\Delta_\mu u^{\alpha(i-1,j)} - \delta_{1\mu} L_D{}^{(i-1,j)}\right)\delta x^{\mu(i,j)} \\
&\quad + \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\,\Delta_\mu u^{\alpha(i,j-1)} - \delta_{2\mu} L_D{}^{(i,j-1)}\right)\delta x^{\mu(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\mu(i,j)}}\,\delta x^{\mu(i,j)}\Bigg\} \\
&= \sum_{i,j} \Delta_1 x_1^{(i)} \cdot \Delta_2 x_2^{(j)} \Bigg\{ [L_{u^{\alpha(i,j)}}]\,\delta_t u^{\alpha(i,j)} + \Sigma_{\mu,\nu=1,2}\Delta_\mu\left(\frac{\partial L_D{}^{(i,j)}}{\partial(\Delta_\mu u^{(i,j)})}\,\delta_t u^{(i,j)}\right. \\
&\quad \left. - E_\mu^{-1} T_{D\nu}{}^{\mu(i,j)}\,\delta x^{\nu(i,j)}\right) \\
&\quad + \Sigma_{\nu,\mu=1,2}\left(\Delta_\nu E_\nu^{-1} T_{D\mu}{}^{\nu(i,j)} + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\mu(i,j)}}\right)\delta x^{\mu(i,j)}\Bigg\},
\end{aligned}
\tag{5.12}
$$

where $E_\mu, \mu = 1,2$, $[L_{u^{\alpha(i,j)}}]$ and $T_{D\mu\nu}{}^{(i,j)}$ are shift operators, discrete Euler–Lagrange operator and energy-momentum tensor, respectively,

$$
E_1 f^{(i,j)} = f^{(i+1,j)}, \quad E_1^{-1} f^{(i,j)} = f^{(i-1,j)},
$$

$$E_2 f^{(i,j)} = f^{(i,j+1)}, \quad E_2^{-1} f^{(i,j)} = f^{(i,j-1)}, \tag{5.13}$$

$$[L_{u^{\alpha(i,j)}}] := \frac{\partial L_D{}^{(i,j)}}{\partial u^{\alpha(i,j)}} - \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\right) - \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\right), \tag{5.14}$$

$$T_{D\mu\nu}{}^{(i,j)} := \frac{\partial L_D{}^{(i,j)}}{\partial(\Delta^\mu u^{\alpha(i,j)})}\Delta_\nu u^{\alpha(i,j)} - L_D{}^{(i,j)}\eta_{\mu\nu}. \tag{5.15}$$

Regarding $\delta_v u^{\alpha(i,j)}$ and $\delta x^{\nu(i,j)}$ as independent variational bases, $\delta_t S_D = 0$, or $\delta_v S_D = 0$ and $\delta_h S_D = 0$, lead to the discrete Euler–Lagrange equation

$$\frac{\partial L_D{}^{(i,j)}}{\partial u^{\alpha(i,j)}} - \Delta_1\left(\frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(i-1,j)})}\right) - \Delta_2\left(\frac{\partial L_D{}^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(i,j-1)})}\right) = 0, \tag{5.16}$$

and a relation between the Euler–Lagrange operator and the (difference) divergence of the discrete energy-momentum tensor that may determine the step-lengths,

$$[L_{u^{\alpha(i,j)}}]\Delta_\nu u^\alpha(x)^{(i,j)} + \Sigma_{\mu=1,2}\left\{\Delta_\mu E_\mu^{-1} T_D{}^{\mu(i,j)}_\nu + \frac{\partial L_D{}^{(i,j)}}{\partial x^{\nu(i,j)}}\right\} = 0. \tag{5.17}$$

It is obvious that all of these discrete equations, relations, and properties have correct continuous limits, respectively. Furthermore, due to the discrete Lagrangian (5.1) depending on the differences explicitly, it is possible to introduce the discrete canonical momentum and discrete Legendre transformation to transfer to the discrete Hamiltonian formalism as will be shown in the next section.

Remark 5.1: We may introduce exterior differential operators $\hat{\mathrm{d}}$, d_v, and $\hat{\mathrm{d}}_h$ on $T^*(M \times X_D)$, T^*M and T^*X_D, respectively. They are nilpotent and satisfy

$$\hat{\mathrm{d}} = \mathrm{d}_v + \hat{\mathrm{d}}_h, \quad \{\mathrm{d}_v, \hat{\mathrm{d}}_h\} = 0. \tag{5.18}$$

Especially, $\hat{\mathrm{d}}_h$ is dual to the difference on X_D and satisfy Leibniz's law for ordinary forms. In fact, some noncommutative differential calculus is needed to completely clarify the properties of $\hat{\mathrm{d}}_h$. For the case that Δx^μ are fixed, this noncommutative differential calculus can be found in Refs. 16 and 17. For the case of variable step-lengths, similar noncommutative differential calculus can also be established.

Remark 5.2: Actually, analog to the case with fixed step-lengths,[12,14] we can establish the difference version for the Euler–Lagrange cohomology and the necessary and sufficient condition for the difference conservation law of the discrete multisymplectic two-forms.

From $\delta_v S_D$ in (5.12), it is easy to see that we may take d_v on S_D to get

$$\mathrm{d}_v S_D = \sum_{(i,j)} \Delta_1 x_1^i \Delta_2 x_2^j \, \mathrm{d}_v L_D{}^{(i,j)}, \quad \mathrm{d}_v L_D{}^{(i,j)} = \mathcal{E}_D{}^{(i,j)} + \Delta_\mu \theta_D{}^{\mu(i,j)}, \tag{5.19}$$

where $\mathcal{E}_D{}^{(i,j)}$, $\theta_D{}^{\mu(i,j)}$, $\mu = 1,2$ are the discrete Euler–Lagrange one-form and multisymplectic potential one-forms, respectively,

$$\mathcal{E}_D{}^{(i,j)} := [L_{Du^{\alpha(i,j)}}]\mathrm{d}_v u^{\alpha(i,j)}, \tag{5.20}$$

$$\theta_D{}^{1(i,j)} := \frac{\partial L_D^{(i-1,j)}}{\partial(\Delta_1 u^{\alpha(k-1,l)})}\mathrm{d}u^{\alpha(k,l)}, \quad \theta_{DL}{}^{2(i,j)} := \frac{\partial L_D^{(i,j-1)}}{\partial(\Delta_2 u^{\alpha(k,l-1)})}\mathrm{d}u^{\alpha(k,l)}. \tag{5.21}$$

Then due to the nilpotency of d_v, it is straightforward to get

$$\mathrm{d}_v \mathcal{E}_D{}^{(i,j)} + \Delta_\mu \omega_D{}^{\mu(i,j)} = 0, \quad \omega_D{}^{\mu(i,j)} := \mathrm{d}_v \theta_D{}^{\mu(i,j)}. \tag{5.22}$$

Therefore, we may get the discrete version for the theorem 3.[12,14]

Theorem 4: *For the discrete Lagrangian with first order of differences on the bundle* $E(X_D, Q, \pi) \simeq M \times X_D$, *the following properties hold.*

(1) There exists the discrete version of the Euler–Lagrange cohomology: $H_{DFT} := \{$*Closed Euler–Lagrange forms*$\}/\{$*Exact Euler–Lagrange forms*$\}$.

(2) The necessary and sufficient condition for conservation of the discrete multisymplectic two-forms, i.e.,

$$\Delta_\mu \omega_D{}^{\mu(i,j)} = 0, \tag{5.23}$$

is that the corresponding discrete Euler–Lagrange one-form is closed, rather than the system being on the solution space only.

Remark 5.3: In this paper, L^2 is an infinite lattice. It is reasonable to consider a finite lattice. We will report the issues on this topic elsewhere.

B. Variable difference Hamiltonian field theory

Consider $X^{(1,1)}$, on which there is a right-angle lattice L^2 with variable step-lengths in each direction, is the base space.

We first define a set of the discrete canonical conjugate momenta on the tangent space $T(\mathcal{M}^{(i,j)})$ of $\mathcal{M}^{(i,j)} = \cup_{Ind(N)|I^{(i,j)}} M^{(i,j)}$ the union of the pieces of configuration space on $X^{(i,j)}$, which are the set of nodes neighboring to the node $x_\mu^{(i,j)}$,

$$\pi_\alpha{}^{(i,j)} = \frac{\partial L_D{}^{(i-1,j)}}{\partial(\Delta_t u^{\alpha(i-1,j)})}. \tag{5.24}$$

The difference Hamiltonian is introduced through the discrete Legendre transformation

$$H_D{}^{(i,j)}(u^{\alpha(i,j)}, \pi_\alpha^{(i+1,j)}; x^{(i,j)}) = \pi_\alpha{}^{(i+1,j)} \Delta_t u^{\alpha(i,j)} - L_D{}^{(i,j)}. \tag{5.25}$$

The action functional (5.3) is expressed as

$$S_D = \sum_{(i,j)\in Z\times Z} \Delta_\mu x^{\mu(i,j)} (\pi_\alpha{}^{(i+1,j)} \Delta_t u^{\alpha(i,j)} - H_D{}^{(i,j)}). \tag{5.26}$$

The total variation of the action $\delta_t S_D$ can be calculated and separated into two parts, i.e., the vertical variation $\delta_v S_D$ and the horizontal variation $\delta_h S_D$,

$$\delta_t S_D = \delta_v S_D + \delta_h S_D, \tag{5.27}$$

$$\delta_v S_D = \sum_{(i,j)\in Z\times Z} \Delta_\mu x^{\mu(i,j)} \Big\{ \delta_v \pi_\alpha{}^{(i+1,j)} [H_{\pi_\alpha{}^{(i+1,j)}}] - [H_{u^{\alpha(i,j)}}] \delta_v u^{\alpha(i,j)} - \Sigma_{\mu,\nu=1,2} \Delta_\mu \Big(\frac{\partial H_D{}^{(i,j)}}{\partial(\Delta_\mu u^{(i,j)})} \delta_v u^{(i,j)} \Big) \Big\}, \tag{5.28}$$

$$\delta_h S_D = \sum_{(i,j)\in Z\times Z} \Delta_\mu x^{\mu(i,j)} \Bigg\{ \delta_h \pi_\alpha{}^{(i+1,j)} [H_{\pi_\alpha{}^{(i+1,j)}}] - [H_{u^{\alpha(i,j)}}] \delta_h u^{\alpha(i,j)} - \Sigma_{\mu,\nu=1,2} \Delta_\mu \left(\frac{\partial H_D{}^{(i,j)}}{\partial(\Delta_\mu u^{(i,j)})} \delta_h u^{(i,j)} + E_\mu^{-1} T_{D\nu}^{\mu(i,j)} \delta x^{\nu(i,j)} \right) + \Sigma_{\nu,\mu=1,2} \left(\Delta_\nu E_\nu^{-1} T_{D\mu}^{\nu(i,j)} - \frac{\partial H_D{}^{(i,j)}}{\partial x^{\mu(i,j)}} \right) \delta x^{\mu(i,j)} \Bigg\}. \tag{5.29}$$

Here

$$\begin{aligned} [H_{\pi_\alpha{}^{(i+1,j)}}] &:= \Delta_t u^{\alpha(i,j)} - \frac{\partial H_D{}^{(i,j)}}{\partial \pi_\alpha{}^{(i+1,j)}}, \\ [H_{u^{\alpha(i,j)}}] &:= \Delta_t \pi_\alpha{}^{(i,j)} + \frac{\partial H_D^{(i,j)}}{\partial u^{\alpha(i,j)}} - \Delta_x \left(\frac{\partial H_D^{(i,j-1)}}{\partial(\Delta_x u^{\alpha(i,j-1)})} \right). \end{aligned} \tag{5.30}$$

Regarding $\delta_v u^{\alpha(i,j)}$, $\delta_v \pi_\alpha{}^{(i+1,j)}$, and $\delta x^{\nu(i,j)}$ as independent variational bases, $\delta_v S_D = 0$ due to discrete Hamilton's principle and $\delta_h S_D = 0$ due to discretized reparametrization invariance on L^2, i.e., $\delta_t S_D = 0$, lead to the discrete canonical field equations

$$\begin{aligned} \Delta_t u^{\alpha(i,j)} &= \frac{\partial H_D{}^{(i,j)}}{\partial \pi_\alpha{}^{(i+1,j)}}, \\ \Delta_t \pi_\alpha{}^{(i,j)} &= -\frac{\partial H_D^{(i,j)}}{\partial u^{\alpha(i,j)}} + \Delta_x \left(\frac{\partial H_D^{(i,j-1)}}{\partial(\Delta_x u^{\alpha(i,j-1)})} \right), \end{aligned} \tag{5.31}$$

and the canonical form of the relation (5.17) that may determine the step-lengths,

$$[H_{\pi_\alpha{}^{(i+1,j)}}] \Delta_\nu \pi_\alpha{}^{(i+1,j)} - [H_{u^{\alpha(i,j)}}] \Delta_\nu u^{\alpha(i,j)} + \Sigma_{\mu=1,2} \left\{ \Delta_\mu E_\mu^{-1} T_{D\nu}^{\mu(i,j)} - \frac{\partial H_D{}^{(i,j)}}{\partial x^{\nu(i,j)}} \right\} = 0. \tag{5.32}$$

It should also be mentioned that all remarks in the preceding section can be made here and the theorem 4 can also be established in this discrete Hamiltonian formalism for field theory.

VI. CONCLUDING REMARKS

In this paper, the VDVA with variable step-lengths has been proposed. It is a generalized version of the difference variational approach with fixed step-lengths proposed in Refs. 12 and 14. The approach has been applied to both Lagrangian and Hamiltonian formalism for discrete mechanics and field theory. Although we deal with systems with first order differences, the key points are available for the systems with higher order differences. Obviously, both approaches are different from either Lee's discrete variation with variable time steps[19–21] or Veselov's one with fixed time steps for the discrete classical mechanics.[30,26] They are also different from the discrete variation approach to field theory in Ref. 24 that is a generalization of Veselov's approach. In our approaches the differences with either variable step-lengths or the fixed ones are regarded as discrete derivatives. In other words, they are regarded as a kind of geometric object. This is more obvious and natural from the viewpoint of noncommutative geometry and more akin to the continuous mechanics and field theory. Therefore, in the continuous limit, the results given here by the VDVA lead to the correct continuous counterparts not only for the equations of motion and symplectic or multisymplectic preserving properties, but also for the conservation laws, especially for the energy conservation.

In view of the structure-preserving criterion for the discrete systems, there are more advantages for the VDVA. Eventually, this has already been seen in Ref. 6. Namely, in taking the continuous limits for the discrete variation problems, which is a generalized version of Lee–Veselov's variation, combining discrete objects into some difference form is more controllable.[6]

With variable step-lengths it is, of course, more or less straightforward to generalize the symplectic and multisymplectic schemes as ones that are not only symplectic and multisymplectic preserving but also discretely energy conserved as has been done for variational symplectic energy-momentum integrators in discrete Lagrangian formalism,[18,6] and in discrete Hamiltonian formalism.[7] But, these discrete formalisms do not transform to each other via discrete Legendre transformation.

The difference variational approach has been applied to the symplectic algorithm and multisymplectic one for both Lagrangian and Hamiltonian formalisms in Ref. 14. It has been shown that the discrete integrands can be combined together in a certain manner as to certain geometric objects in order to construct some numerical schemes with fixed step-lengths as variational integrators such as the midpoint scheme in the symplectic algorithm and the Preissman scheme in the multisymplectic algorithm. Obviously, the VDVA should also be able to apply to the symplectic and multisymplectic algorithms with variable step-lengths for both Lagrangian and Hamiltonian formalisms. This issue will be reported in details elsewhere.

It has been found that the necessary and sufficient conditions for the symplectic two-form preserving in mechanics and the multisymplectic two-forms preserving in field theories are the corresponding Euler–Lagrange one-form closed in the relevant Euler–Lagrange cohomology.[12,13] This is also true for the discrete cases[12,14] as well as the symplectic and multisymplectic algorithms.[14] For the cases studied in this paper, the Euler–Lagrange cohomology should also be true for the various variation problems with variable domains or step-lengths. In fact, this matter is already indicated by the boundary terms in the vertical parts of these variation problems. We will also explain this issue in more detail elsewhere.

We have almost completely employed the ordinary description in a coordinate dependent manner in this paper in order to be more easily understood and to deal with both continuous and discrete cases in an analogical manner. It should be mentioned, however, that both the variation problems and the Euler–Lagrange cohomology for continuous cases can be dealt with in a coordinate free version in terms of jet bundle and variational bicomplex (see, for example, Refs. 2 and 3). Although as far as the local issues are concerned, the essentials are almost the same. The coordinate free expression encodes more general and complicated cases with nontrivial topology. On the other hand, however, for the discrete cases the ordinary jet bundle and variational bicomplex approach should be generalized to the ones that include NCDC in principle. We will present the variational bicomplex approach to these issues elsewhere, especially the one with NCDC to the discrete cases.

More than one year after this paper was finished and appeared as an e-print, our attention has been drawn to an important paper[22] in which what is called asynchronous variational integrators have been proposed for nonlinear elastodynamics. One of the key points in their approach that the time step-lengths are no longer fixed rather they are determined by the discrete energy balance equation step by step. This is in analog with the discrete variation introduced in Refs. 19–21 and also with our approach. However, there are two main differences disregarded by others between their approach and ours. First, for both the continuous and discrete cases, either symplectic or multisymplectic preserving properties are always proved on the solution spaces in Ref. 22. This is the same as in ordinary approaches. However, the necessary and sufficient condition for either symplectic or multisymplectic preserving is not on the solution space of the relevant equations but the relevant Euler–Lagrange one-form is closed in our approach. In fact, in the case of classical mechanics on symplectic manifold, it is a well-known issue. Namely, the necessary and sufficient condition for the symplectic preserving is that the flow is symplectic rather than Hamiltonian (phase flow)[25] and the definition for the symplectic vector is just the relevant Euler–Lagrange closed one-form.[31,15] Second, for the discrete variation, in order to get the discrete Euler–Lagrange equation the variation is taken with respect to the discrete variables only in Ref. 22. This

is also the same as in Refs. 19 and 26. However, in our approach the difference of the variables with variable step-length as a whole is also taken as independent variable for the discrete variation. This is the reason why it is called the (variable) difference variational principle. One of the advantages is that the difference discrete Legendre transformation in both discrete mechanics and field theory can be taken. Therefore, VDVP can also be applied not only for the discrete Lagrangian formalism but also the discrete Hamiltonian formalism as well.

ACKNOWLEDGMENTS

We would like to thank Dr. J.B. Chen, Dr. Y. Q. Li, Dr. M. Z. Qin, Dr. Z. J. Shang, and Dr. S. K. Wang for valuable discussions. This work was supported in part by the National Natural Science Foundation of China (Grants Nos. 90103004 and 10175070) and the National Key Project for Basic Research of China (G1998030601).

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Entropy growth of shift-invariant states on a quantum spin chain

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(Received 23 June 2003; accepted 29 August 2003)

We study the entropy of pure shift-invariant states on a quantum spin chain. Unlike the classical case, the local restrictions to intervals of length N are typically mixed and have therefore a nonzero entropy S_N which is, moreover, monotonically increasing in N. We are interested in the asymptotics of the total entropy. We investigate in detail a class of states derived from quasi-free states on a CAR algebra. These are characterized by a measurable subset of the unit interval. As the entropy density is known to vanish, S_N is sublinear in N. For states corresponding to unions of finitely many intervals, S_N is shown to grow slower than $\log^2 N$. Numerical calculations suggest a $\log N$ behavior. For the case with infinitely many intervals, we present a class of states for which the entropy S_N increases as N^α where α can take any value in (0,1). © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1623616]

I. INTRODUCTION

In quantum statistical mechanics, one-dimensional lattice systems, the so-called spin chains, are far from fully understood. One of the obstacles for a systematic study is the complicated correlations that can occur. This is even possible for pure states, which are trivial for classical spin chains. Due to these quantum correlations, it is often very hard to explicitly specify a state. Only a few classes can be studied in detail, including the product states, the finitely correlated states[5] and the states derived from quasi-free states on the CAR algebra.[3,4]

Let us denote by ρ_N the density matrix of the restriction of a translation-invariant state ρ on a spin chain to N consecutive spins. The von Neumann entropy $S_N := S(\rho_N)$ has proved to be a very useful quantity in the study of quantum correlations. For ergodic translation-invariant states, ρ_N is essentially concentrated on a subspace of dimension $\exp(Ns(\rho))$.[8] Here, $s(\rho)$ is the entropy density of ρ. The compression of ρ_N from the full dimension d^N of N spins to $\exp(Ns(\rho))$ is a central theme in quantum coding theory. It lies also at the basis of DMRG computations.[11] One may conjecture that $s(\rho)=0$ for pure states ρ, which should allow for a very efficient compression. For pure states, S_N is also the unique reasonable measure for the entanglement of this interval with the rest of the chain[10] and it measures therefore the resources of the state for quantum computing purposes.

For pure product states S_N vanishes for all N; this is in fact completely analogous to the classical spin chain. For pure finitely correlated states S_N is uniformly bounded, a behavior that is certainly not expected to be generic.[6]

The entanglement of local spins with the remainder of a chain has been considered by many authors and is a topic of current interest. Various models have been studied in detail such as the

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ground states of XY-models or Ising chains in a transverse field. It turns out that in these cases, the entanglement grows logarithmically with the size of the localized system, see, e.g., Ref. 12 where a numerical proof of this behavior is obtained. For an analytical treatment of such a model together with more refined results on higher order corrections we refer to Ref. 9.

In this article, we study the entropy S_N for general translation-invariant pure states on a chain of spin $\frac{1}{2}$ particles derived from quasi-free states on the CAR algebra. Here, the entropy density is known to vanish and we investigate the sublinear growth of the entropy S_N when $N\to\infty$. For the simplest quasi-free states, the entropy behaves as $\log N$. This is precisely the behavior found in Refs. 12 and 9. In fact, the ground states of XY and Ising in a tranverse field are particular examples of pure states derived from quasi-free Fermion states. We shall, however, also present more involved examples for which the entropy increases as N^α with α arbitrarily close to 1. Therefore the entanglement of local spins with the remainder of the chain can be much higher than previously thought.

The construction of pure shift-invariant quasi-free states is recalled in Sec. II. Such states are characterized by a subset of the unit interval. In Sec. III we prove that the asymptotics of S_N as $N\to\infty$ can be obtained by a quadratic approximation of the entropy. The entropy growth of quasi-free states given by a set consisting of finitely many intervals is studied in Sec. IV. Finally, Sec. V is devoted to the infinitely many intervals case.

II. QUASI-FREE STATES ON THE SPIN CHAIN

In this section we show, following Ref. 4, how a quasi-free state on the CAR algebra can be used to define a state on the spin chain algebra. After the introductory definitions, we explain how both algebras can be retrieved as subalgebras of a larger algebra. This construction permits us to transfer translation-invariant states from the CAR algebra to the spin chain algebra. This idea is then applied to quasi-free states.

A. CAR algebra and spin chain algebra

Let $\mathcal{H}$ be the Hilbert space $\ell^2(\mathbb{Z})$, in which $\{\delta_k : k\in\mathbb{Z}\}$ forms an orthonormal basis, where δ_k is the characteristic function of the integer number k. Let $\mathcal{A}$ be the CAR algebra corresponding to $\mathcal{H}$. It is the C^*-algebra generated by $\mathbb{1}$ and $\{c_k : k\in\mathbb{Z}\}$, satisfying the canonical anticommutation relations

$$c_k c_l = -c_l c_k, \quad c_k^* c_l = \delta_{k,l}\mathbb{1} - c_l c_k^*.$$

The parity automorphism α on $\mathcal{A}$ is defined by $\alpha(c_k) = -c_k$. Let $\mathcal{A}_+$ be the fixed point algebra of α, i.e., $\mathcal{A}_+ = \{a\in\mathcal{A} : \alpha(a) = a\}$. The elements of $\mathcal{A}_+$ are called even, while those of $\mathcal{A}_- := \{a \in \mathcal{A} : \alpha(a) = -a\}$ are odd. Obviously, $\mathcal{A} = \mathcal{A}_+ + \mathcal{A}_-$. The shift automorphism γ is defined by $\gamma(c_k) = c_{k+1}$.

The quantum spin chain is the UHF algebra

$$\mathcal{C} := \bigotimes_{k=-\infty}^{\infty} \mathcal{M}_2,$$

where $\mathcal{M}_2$ is the algebra of 2×2 matrices. Let e_{11}^k, e_{12}^k, e_{21}^k and e_{22}^k denote the standard matrix units of $\mathcal{M}_2$ embedded into the kth factor of $\mathcal{C}$. The following relations hold:

$$\begin{aligned} e_{ab}^k e_{cd}^l &= e_{cd}^l e_{ab}^k \quad \text{when } k\neq l, \\ e_{ab}^k e_{cd}^k &= \delta_{b,c} e_{ad}^k, \\ (e_{ab}^k)^* &= e_{ba}^k, \\ e_{11}^k + e_{22}^k &= \mathbb{1}. \end{aligned} \tag{1}$$

Any algebra generated by elements $\{E^k_{ab} : a,b \in \{1,2\}, k \in \mathbb{Z}\}$ satisfying the above relations is isomorphic to $\mathcal{C}$.

B. Jordan–Wigner isomorphism

Let $\mathcal{A}_n$ be the algebra generated by $\{c_k : 0 \leqslant k \leqslant n-1\}$ and let $\mathcal{C}_n = \otimes_{k=0}^{n-1} \mathcal{M}_2$. It is well known that $\mathcal{A}_n$ is isomorphic to $\mathcal{C}_n$ for all $n \in \mathbb{N}$. An explicit isomorphism is given by the so-called Jordan–Wigner isomorphism given in terms of matrix units in $\mathcal{A}_n$ by

$$E^k_{11} := c^*_k c_k, \quad E^k_{22} := c_k c^*_k, \quad E^k_{12} := A_k c^*_k, \quad E^k_{21} := A_k c_k.$$

Here we introduced

$$\sigma^z_k := 2c^*_k c_k - \mathbb{1}, \quad A_k := \prod_{l=0}^{k-1} \sigma^z_l.$$

The set $\{E^k_{ab} : a,b \in \{1,2\}, 0 \leqslant k \leqslant n-1\}$ generates $\mathcal{A}_n$ and the operators E^k_{ab} satisfy the same relations (1) as the matrix units e^k_{ab} of C_n.

A first idea would be to extend this isomorphism to an isomorphism from $\mathcal{A}$ to $\mathcal{C}$. However, it is impossible to extend this definition to negative k's in such a way that the isomorphism intertwines the shifts in $\mathcal{A}$ and $\mathcal{C}$. This property is needed to transport translation-invariance from $\mathcal{A}$ to $\mathcal{C}$.

One way to circumvent this problem is due to Araki.[2] It consists in enlarging $\mathcal{A}$ to $\hat{\mathcal{A}}$ by adding a new element T that has the following properties

$$T^* = T, \quad T^2 = \mathbb{1} \quad \text{(i.e., } T \text{ is a self-adjoint unitary)},$$

$$T c_k T = \begin{cases} c_k & \text{if } k \geqslant 0, \\ -c_k & \text{if } k < 0. \end{cases}$$

Any element of $\hat{\mathcal{A}}$ can uniquely be written in the form $a + Tb$ with a and b from $\mathcal{A}$. Therefore, $\hat{\mathcal{A}} = \mathcal{A} + T\mathcal{A}$. Note that formally $T = \Pi_{k=-1}^{-\infty} \sigma^z_k$.

A state φ on $\mathcal{A}$ can be extended to a state $\hat{\varphi}$ on $\hat{\mathcal{A}}$ by $\hat{\varphi}(a + Tb) := \varphi(a)$ and the extensions of the automorphisms α and γ are

$$\hat{\alpha}(a + Tb) := \alpha(a) + T\alpha(b) \quad \text{and} \quad \hat{\gamma}(a + Tb) := \gamma(a) + T\sigma^z_0 \gamma(b).$$

We define another automorphism β on $\hat{\mathcal{A}}$ by $\beta(a + Tb) := a - Tb$. The fixed point algebra of $\beta^{-1}\hat{\alpha}$ will be denoted by $\check{\mathcal{A}}$, i.e.,

$$\check{\mathcal{A}} = \{a + Tb \in \hat{\mathcal{A}} : \hat{\alpha}(a + Tb) = \beta(a + Tb)\} = \{a + Tb \in \hat{\mathcal{A}} : \alpha(a) = a, \alpha(b) = -b\} = \mathcal{A}_+ + T\mathcal{A}_-.$$

The restriction of a state $\hat{\varphi}$ on $\hat{\mathcal{A}}$ to a state on $\check{\mathcal{A}}$ will be denoted by $\check{\varphi}$. Because the automorphisms $\hat{\alpha}$ and $\hat{\gamma}$ leave the subalgebra $\check{\mathcal{A}}$ invariant, they can be restricted to $\check{\mathcal{A}}$. Denote these restrictions by $\check{\alpha}$ and $\check{\gamma}$.

Let φ be an even state, i.e., it vanishes on odd elements or, equivalently, $\varphi \circ \alpha = \varphi$. It is easy to see that also $\check{\varphi} \circ \check{\alpha} = \check{\varphi}$, thus $\check{\varphi}$ is an even state on $\check{\mathcal{A}}$. Similarly, let φ be a translation-invariant state on $\mathcal{A}$, i.e., $\varphi \circ \gamma = \varphi$, then $\check{\varphi} \circ \check{\gamma} = \check{\varphi}$, thus $\check{\varphi}$ is a translation-invariant state on $\check{\mathcal{A}}$.

Now, define

$$\tilde{E}^k_{11} := c^*_k c_k, \quad \tilde{E}^k_{22} := c_k c^*_k, \quad \tilde{E}^k_{12} := TA_k c^*_k, \quad \tilde{E}^k_{21} := TA_k c_k$$

with

$$\sigma_k^z := 2c_k^* c_k - \mathbb{1}, \quad A_k := \begin{cases} \prod_{\ell=0}^{k-1} \sigma_\ell^z & \text{if } k>0, \\ \mathbb{1} & \text{if } k=0, \\ \prod_{\ell=k}^{-1} \sigma_\ell^z & \text{if } k<0. \end{cases}$$

One verifies that these operators satisfy the same commutation relations as the matrix units of $\mathcal{C}$. Moreover, $\check{\gamma}(\tilde{E}_{ab}^k) = \tilde{E}_{ab}^{k+1}$.

To summarize, we constructed an algebra $\hat{\mathcal{A}}$ which contains both $\mathcal{A}$ and $\check{\mathcal{A}}$ as subalgebras. This embedding is compatible with the translations on the subalgebras. Moreover, we established an isomorphism between $\check{\mathcal{A}}$ and $\mathcal{C}$ which is also compatible with the translations. This allows us to transfer translation-invariant states from $\mathcal{A}$ to $\mathcal{C}$.

Let φ be a translation-invariant state. Such a state is automatically even and is completely determined by the sequence $(\varphi_n)_{n=0}^{\infty}$, where φ_n is the restriction of φ to $\mathcal{A}_n$. The density matrix $[\varphi_n]$ of φ_n has entries

$$[\varphi_n]_{\mathbf{j},\mathbf{i}} = \varphi\left[\prod_{k=0}^{n-1} E_{i_k j_k}^k\right].$$

Here $\mathbf{i}$ and $\mathbf{j}$ denote multi-indices $(i_0, i_1, \ldots, i_{n-1})$ and $(j_0, j_1, \ldots, j_{n-1})$ in $\{1,2\}^n$. The transferred state $\check{\varphi}$ is also translation-invariant and so completely determined by its restriction to the subalgebras $\{\mathcal{C}_n : n \in \mathbb{N}\}$ with density matrices

$$[\check{\varphi}_n]_{\mathbf{j},\mathbf{i}} = \hat{\varphi}\left[\prod_{k=0}^{n-1} \tilde{E}_{i_k j_k}^k\right], \quad \mathbf{i}, \mathbf{j} \in \{1,2\}^n.$$

The expressions $\Pi_{k=0}^{n-1} E_{i_k j_k}^k$ and $\Pi_{k=0}^{n-1} \tilde{E}_{i_k j_k}^k$ are both either odd or even. When odd, $[\varphi_n]_{\mathbf{j},\mathbf{i}} = [\check{\varphi}_n]_{\mathbf{j},\mathbf{i}} = 0$, while when even, since $Tc_k = c_k T$ for $k \geqslant 0$ and $T^2 = \mathbb{1}$, we get that $\Pi_{k=0}^{n-1} \tilde{E}_{i_k j_k}^k = \Pi_{k=0}^{n-1} E_{i_k j_k}^k$ and so $[\varphi_n]_{\mathbf{i},\mathbf{j}} = [\check{\varphi}_n]_{\mathbf{i},\mathbf{j}}$. From this, we conclude that the states φ and $\check{\varphi}$ have the same reduced density matrices. It follows immediately that if φ is pure, then also $\check{\varphi}$ is pure.

C. Quasi-free states

We apply the construction of the previous section to quasi-free states on the CAR algebra $\mathcal{A}$. For these states an explicit formula is known for the entropy of the restricted density matrices. Because the corresponding states on $\mathcal{C}$ have the same restricted density matrices, the same explicit formulas are available, as we shall use in the following sections. The proofs of the theorems mentioned in this subsection can be found in Ref. 1.

Let φ be a quasi-free, gauge-invariant state on $\mathcal{A}$, i.e., φ is given by the rule

$$\varphi(c_{i_1}^* \cdots c_{i_m}^* c_{j_n} \cdots c_{j_1}) = \delta_{m,n} \det([Q_{i_k j_l}]_{k,l=1}^n),$$

where Q is an operator on $\mathcal{H}$, $0 \leqslant Q \leqslant \mathbb{1}$, and $Q_{ij} = \langle \delta_i, Q\delta_j \rangle$ are the matrix elements of Q in the standard basis of $\mathcal{H}$. The operator Q is called the symbol of the state φ. Obviously, φ is even.

The quasi-free state φ is translation-invariant if and only if its symbol Q is a Toeplitz operator, i.e., there exists a sequence $\{q_k : k \in \mathbb{Z}\}$ such that $Q_{lk} = q(l-k)$. By the Fourier transform,

$$q\hat{}(\theta) = \sum_{k \in \mathbb{Z}} q(k) e^{ik\theta} \quad \text{and its inverse} \quad q(k) = \frac{1}{2\pi} \int_{\mathbb{T}} d\theta \, q\hat{}(\theta) e^{-ik\theta}, \tag{2}$$

with $\mathbb{T}$ the torus parametrized by $[0,2\pi)$, the symbol of a translation-invariant quasi-free state is unitarily equivalent with the multiplication operator by $q^\wedge$ on $L^2(\mathbb{T},d\theta)$. This function $q^\wedge$ satisfies $0\leqslant q^\wedge\leqslant 1$ almost everywhere.

A quasi-free state φ is pure if and only if its symbol Q is a projector. For a translation-invariant state this means that the Fourier transform of the symbol Q is a characteristic function, i.e., there exists a measurable set $K\subset\mathbb{T}$ such that $q^\wedge(\theta)=\chi_K(\theta)$.

The entropy of a quasi-free state φ can be expressed in terms of its symbol Q. Define, for $0\leqslant x\leqslant 1$, the functions $\eta(x):=-x\log x$ and $\tilde{\eta}(x):=\eta(x)+\eta(1-x)$. The von Neumann entropy of the state restricted to an interval of N spins is given by

$$S_N:=\mathrm{Tr}\,\eta([\varphi_N])=\mathrm{Tr}\,\tilde{\eta}(Q_N), \tag{3}$$

where Q_N is the restriction of Q to the N-dimensional space spanned by $\{\delta_k: 0\leqslant k\leqslant N-1\}$. It follows by Szegö's theorem[7] that the entropy density of a translation-invariant quasi-free state equals

$$s:=\lim_{N\to\infty}\frac{S_N}{N}=\frac{1}{2\pi}\int d\theta\,\tilde{\eta}(q^\wedge(\theta)).$$

In particular, the entropy density of a pure translation-invariant quasi-free state is zero.

III. ASYMPTOTICS FOR ENTROPY OF QUASI-FREE STATES

Quasi-free states are good approximations of true ground and equilibrium states for systems of Fermions, either at low density or with weakly interacting particles. The coordinate θ appearing in (2) has the meaning of momentum and the system is specified by a dispersion relation $\theta\mapsto\varepsilon(\theta)$ which is the relation between effective energy and momentum. For a shift-invariant quasi-free state, determined by a symbol Q or, equivalently, by a measurable function $q^\wedge$ on the unit circle with $0\leqslant q^\wedge\leqslant 1$, the energy and particle densities are given by

$$e(\varepsilon,q^\wedge):=\frac{1}{2\pi}\int_{\mathbb{T}}d\theta\,\varepsilon(\theta)\,q^\wedge(\theta)\quad\text{and}\quad n(q^\wedge):=\frac{1}{2\pi}\int_{\mathbb{T}}d\theta\,q^\wedge(\theta).$$

The ground state at density λ, $0\leqslant\lambda\leqslant 1$, is obtained by minimizing the energy density under the constraint $n(q^\wedge)=\lambda$. It is given by $q^\wedge=\chi_{K(e_{\mathrm{F}}(\lambda))}$, where $K(e):=\{\theta\in\mathbb{T}:\varepsilon(\theta)\leqslant e\}$ and $e_{\mathrm{F}}(\lambda)$ is the Fermi level determined by the condition

$$|K(e_{\mathrm{F}}(\lambda))|=\frac{1}{2\pi}\int_{\varepsilon(\theta)\leqslant e_{\mathrm{F}}(\lambda)}d\theta=\lambda.$$

For smooth dispersion relations with few oscillations in θ, $K(e_{\mathrm{F}}(\lambda))$ will typically consist of a finite union of disjoint intervals. This case will be investigated in Sec. IV. Section V deals with the opposite situation when $K(e_{\mathrm{F}}(\lambda))$ has a Cantor-type structure.

The quasi-free states on the spin chain $\mathcal{C}$, as introduced in the previous section, obey Eq. (3) for the von Neumann entropy of the restricted density matrices. This will be the starting point for our study of the asymptotic behavior of this entropy S_N as $N\to\infty$.

A. Growth exponents

We use the following estimate for the entropy function $\tilde{\eta}(x):=\eta(x)+\eta(1-x)$,

$$x(1-x)\leqslant\tilde{\eta}(x)\leqslant\epsilon-c\log\epsilon\;x(1-x),\quad 0\leqslant x\leqslant 1$$

(see Fig. 1). The upper bound for $\tilde{\eta}$ holds for c a constant independent of $0<\epsilon$; moreover, for $0<\epsilon<\epsilon_0$ we may choose $c=1+\mathrm{o}(\epsilon_0)$. Therefore,

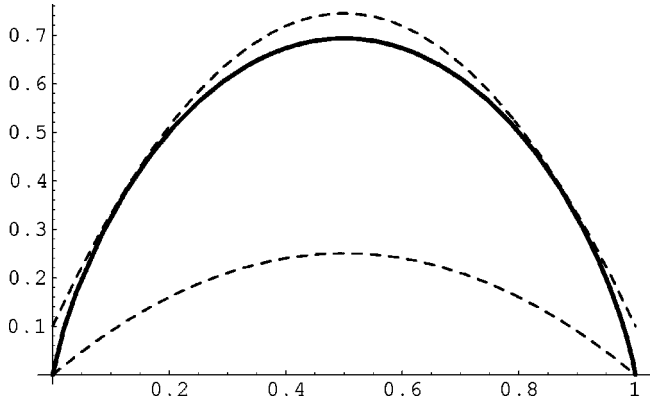

FIG. 1. A quadratic upper and lower bound for the entropy function $\tilde{\eta}$.

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N) \leqslant S_N \leqslant \epsilon N - c \log \epsilon\ \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N).$$

By choosing a function $\epsilon(N)$ for which $\epsilon \to 0$ as $N \to \infty$, we obtain bounds for the entropy S_N in terms of $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$, e.g., putting $\epsilon(N) := 1/N$,

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N) \leqslant S_N \leqslant 1 + c \log N\ \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N). \tag{4}$$

We are particularly interested in the growth exponents of the entropy,

$$\alpha_- := \liminf_{N\to\infty} \frac{\log S_N}{\log N} \quad \text{and} \quad \alpha_+ := \limsup_{N\to\infty} \frac{\log S_N}{\log N}.$$

With the inequalities (4),

$$\liminf_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N} \leqslant \alpha_- \leqslant \alpha_+ \leqslant \limsup_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N}.$$

We conclude that, if

$$\lim_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N} \quad \text{exists, then also} \quad \lim_{N\to\infty} \frac{\log S_N}{\log N} \quad \text{exists, and}$$

$$\alpha := \lim_{N\to\infty} \frac{\log S_N}{\log N} = \lim_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N}. \tag{5}$$

B. Quadratic approximation

Equations (4) and (5) show the importance of the quantity $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$. It can be expressed in terms of the sequence $\{q(k)\}$ or, equivalently, of the Fourier transform $q\hat{}(\theta) = \chi_K(\theta)$ of the symbol Q_N. Using Eq. (2),

$$\begin{aligned}\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N) &= Nq(0)-\sum_{n,m=1}^{N}|q(n-m)|^2\\ &= Nq(0)-N\sum_{n=-N+1}^{N-1}\left(1-\frac{|n|}{N}\right)|q(n)|^2\\ &= Nq(0)-\frac{N}{4\pi^2}\int d\theta_1\int d\theta_2\,\chi_K(\theta_1)\chi_K(\theta_2)\sum_{n=-N+1}^{N-1}\left(1-\frac{|n|}{N}\right)e^{in(\theta_1-\theta_2)}.\end{aligned}$$

Define the Dirichlet kernel,

$$k_N(\varphi):=\sum_{n=-N+1}^{N-1}\left(1-\frac{|n|}{N}\right)e^{in\varphi}=1+2\sum_{n=1}^{N-1}\frac{N-n}{N}\cos n\varphi=\frac{1}{N}\frac{\sin^2(N\varphi/2)}{\sin^2(\varphi/2)}.$$

This is a sequence of positive normalized functions, weakly converging to the Dirac distribution,

$$k_N(\varphi)\geqslant 0,\quad \frac{1}{2\pi}\int d\varphi\, k_N(\varphi)=1.$$

Therefore,

$$\begin{aligned}\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N) &= N\left[\frac{1}{2\pi}\int d\theta\,\chi_K(\theta)-\frac{1}{4\pi^2}\int d\theta\int d\varphi\,\chi_K(\theta)\chi_K(\theta-\varphi)k_N(\varphi)\right]\\ &= \frac{N}{4\pi^2}\int d\theta\int d\varphi\,\chi_K(\theta)[1-\chi_K(\theta-\varphi)]k_N(\varphi)\\ &= \frac{N}{4\pi^2}\int d\varphi\, k_N(\varphi)\int d\theta\,\chi_K(\theta)[1-\chi_K(\theta-\varphi)]\\ &= \frac{N}{4\pi^2}\int d\varphi\, k_N(\varphi)\,|K\backslash(K+\varphi)|. \qquad (6)\end{aligned}$$

Note that both $S(Q_N)$ and $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$ are invariant for the replacement of Q_N by $\mathbb{1}-Q_N$. As a consequence, Eq. (6) can be written in the form

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)=\frac{N}{4\pi^2}\int d\varphi\, k_N(\varphi)\,|K^c\backslash(K^c+\varphi)|. \qquad (7)$$

IV. FINITELY MANY INTERVALS

As explained in Sec. II the subset K of the torus $\mathbb{T}$ determines the state φ we are studying. In this section we study sets K composed of a finite number of intervals, whereas in the next section sets with an infinite number of intervals are treated.

A. Lower bound

By Eq. (4) we have to bound $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$ from below. We consider a set K with a finite number of intervals, say M. Let $\delta>0$ be a fixed number which is smaller than any of the intervals and the holes between two such intervals. Therefore, $|K\backslash(K+\varphi)|\geqslant M\varphi$ for $0\leqslant\varphi\leqslant\delta$. Equation (6) becomes

$$
\begin{aligned}
S_N &\geqslant \operatorname{Tr} Q_N(\mathbb{1}-Q_N)\\
&= \frac{N}{4\pi^2}\int d\varphi\, k_N(\varphi)\,|K\backslash(K+\varphi)|\\
&\geqslant \frac{NM}{2\pi^2}\int_0^{\delta} d\varphi\, k_N(\varphi)\,\varphi\\
&= \frac{NM}{2\pi^2}\int_0^{\delta} d\varphi\,\varphi\left[1+2\sum_{n=1}^{N-1}\frac{N-n}{N}\cos n\varphi\right]\\
&= \frac{NM}{\pi^2}\left[\frac{\delta^2}{4}+\delta\sum_{n=1}^{N-1}\frac{\sin n\delta}{n}-2\sum_{n=1}^{N-1}\frac{\sin^2(n\delta/2)}{n^2}\right]\\
&\quad+\frac{M}{\pi^2}\left[-\delta\sum_{n=1}^{N-1}\sin n\delta-\sum_{n=1}^{N-1}\frac{\cos n\delta}{n}+\sum_{n=1}^{N-1}\frac{1}{n}\right].
\end{aligned}
$$

Using the identities,

$$
\sum_{n=1}^{\infty}\frac{\sin n\delta}{n}=\frac{\pi-\delta}{2}\quad\text{and}\quad\sum_{n=1}^{\infty}\frac{\sin^2(n\delta/2)}{n^2}=\frac{\delta(2\pi-\delta)}{8},
$$

we obtain

$$
S_N\geqslant\frac{NM}{\pi^2}\left[-\delta\sum_{n=N}^{\infty}\frac{\sin n\delta}{n}+2\sum_{n=N}^{\infty}\frac{\sin^2(n\delta/2)}{n^2}\right]+\frac{M}{\pi^2}\left[-\delta\sum_{n=1}^{N-1}\sin n\delta-\sum_{n=1}^{N-1}\frac{\cos n\delta}{n}+\sum_{n=1}^{N-1}\frac{1}{n}\right]. \tag{8}
$$

Next, we estimate the different terms in (8). The first term on the first line is estimated as

$$
\left|\sum_{n=N}^{\infty}\frac{\sin n\delta}{n}\right|=\left|\sum_{n=N}^{\infty}\frac{\cos(n+\frac{1}{2})\delta-\cos(n-\frac{1}{2})\delta}{2n\sin(\delta/2)}\right|\leqslant\frac{1}{N}\frac{1}{|\sin(\delta/2)|},
$$

the second term on the first line as

$$
\left|\sum_{n=N}^{\infty}\frac{\sin^2(n\delta/2)}{n^2}\right|\leqslant\sum_{n=N}^{\infty}\frac{1}{n^2}\leqslant\int_{N-1}^{\infty}dx\,\frac{1}{x^2}=\frac{1}{N-1},
$$

the first term on the second line as

$$
\left|\sum_{n=1}^{N-1}\sin n\delta\right|\leqslant\frac{1}{|\sin(\delta/2)|},
$$

the second term on the second line, for any $\epsilon>0$ and N sufficiently large, as

$$
\left|\sum_{n=1}^{N-1}\frac{\cos n\delta}{n}\right|\leqslant-\log[2\sin\delta]+\epsilon,
$$

and finally, the last term on the last line is

$$
\sum_{n=1}^{N-1}\frac{1}{n}\geqslant\int_1^N dx\,\frac{1}{x}=\log N.
$$

Putting everything together in (8), we find that there exists a constant $c_1>0$ independent of N such that

$$S_N \geqslant c_1 \log N. \tag{9}$$

B. Subadditivity

Before establishing the upper bound for the entropy S_N in case the set K is composed of a finite number of intervals, we prove a general subadditivity property of this entropy. This will enable us to restrict the proof of the upper bound to the case of a single interval.

Suppose that K_1 and K_2 are disjoint sets and put $K:=K_1\cup K_2$. Denoting the symbols of these states by Q, Q_1 and Q_2, we shall prove the subadditivity property, namely,

$$\operatorname{Tr} \tilde{\eta}(Q_N) \leqslant \operatorname{Tr} \tilde{\eta}((Q_1)_N) + \operatorname{Tr} \tilde{\eta}((Q_2)_N). \tag{10}$$

To simplify notation, define $R:=Q_N$, $R_1:=(Q_1)_N$ and $R_2:=(Q_2)_N$. First, note that $R=R_1+R_2$. Remember that $\tilde{\eta}(x)=-x\log x-(1-x)\log(1-x)$ and thus $\tilde{\eta}'(x)=-\log x+\log(1-x)$. We assume $R_1>0$, $R_2>0$ and $R_1+R_2<\mathbb{1}$. Otherwise, we can introduce operators $\tilde{R}_1:=(1-\epsilon)R_1+(\epsilon/2)\mathbb{1}$ and $\tilde{R}_2:=(1-\epsilon)R_2+(\epsilon/2)\mathbb{1}$, prove the subadditivity for these two operators and then take the limit $\epsilon\to 0$. Using the operator identity $(d/d\lambda)\operatorname{Tr} f(A+\lambda B)=\operatorname{Tr} B f'(A+\lambda B)$,

$$\begin{aligned}\operatorname{Tr} \tilde{\eta}(R_1+R_2)-\operatorname{Tr} \tilde{\eta}(R_1) &= \operatorname{Tr} \tilde{\eta}(R_1+\lambda R_2)\big|_{\lambda=0}^{1} \\ &= \int_0^1 d\lambda \, \frac{d}{d\lambda} \operatorname{Tr} \tilde{\eta}(R_1+\lambda R_2) \\ &= \int_0^1 d\lambda \, \operatorname{Tr} R_2 \log \frac{\mathbb{1}-R_1-\lambda R_2}{R_1+\lambda R_2}.\end{aligned} \tag{11}$$

Because the inverse is operator decreasing,

$$\frac{\mathbb{1}-R_1-\lambda R_2}{R_1+\lambda R_2} = \frac{1}{R_1+\lambda R_2}-\mathbb{1} \leqslant \frac{1}{\lambda R_2}-\mathbb{1} = \frac{\mathbb{1}-\lambda R_2}{\lambda R_2},$$

and, because the logarithm is operator increasing,

$$\log \frac{\mathbb{1}-R_1-\lambda R_2}{R_1+\lambda R_2} \leqslant \log \frac{\mathbb{1}-\lambda R_2}{\lambda R_2}.$$

Substituting this into Eq. (11),

$$\operatorname{Tr} \tilde{\eta}(R_1+R_2)-\operatorname{Tr} \tilde{\eta}(R_1) \leqslant \operatorname{Tr} \tilde{\eta}(R_2).$$

C. Upper bound

Due to subadditivity, it is enough to prove an upper bound for a set K consisting of a single interval. We assume that the length of this interval $|K|\leqslant\pi$. Otherwise, we can work with K^c. By Eq. (4) we have to bound $\operatorname{Tr} Q_N(\mathbb{1}-Q_N)$. In this case,

$$|K\backslash(K+\varphi)| = \begin{cases} \varphi & \text{for } |\varphi|\leqslant|K|, \\ |K| & \text{for } |K|\leqslant|\varphi|\leqslant\pi. \end{cases}$$

By Eq. (6),

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)=\frac{N}{2\pi^2}\int_0^{\pi}d\varphi\left[1+2\sum_{n=1}^{N-1}\frac{N-n}{N}\cos n\varphi\right]|K\backslash(K+\varphi)|$$
$$=\frac{N}{4\pi^2}\left[|K|(2\pi-|K|)-8\sum_{n=1}^{N-1}\frac{\sin^2(n|K|/2)}{n^2}\right]+\frac{2}{\pi^2}\sum_{n=1}^{N-1}\frac{\sin^2(n|K|/2)}{n}.$$

Using the identity,

$$\sum_{n=1}^{\infty}\frac{\sin^2(n|K|/2)}{n^2}=\frac{|K|(2\pi-|K|)}{8},$$

we obtain

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)=\frac{2N}{\pi^2}\sum_{n=N}^{\infty}\frac{\sin^2(n|K|/2)}{n^2}+\frac{2}{\pi^2}\sum_{n=1}^{N-1}\frac{\sin^2(n|K|/2)}{n}. \tag{12}$$

The first term is

$$\sum_{n=N}^{\infty}\frac{\sin^2(n|K|/2)}{n^2}\leqslant\sum_{n=N}^{\infty}\frac{1}{n^2}\leqslant\int_N^{\infty}dx\,\frac{1}{x^2}=\frac{1}{N}.$$

The second term is

$$\sum_{n=1}^{N-1}\frac{\sin^2(n|K|/2)}{n}\leqslant\sum_{n=1}^{N-1}\frac{1}{n}\leqslant 1+\int_1^{N-1}dx\,\frac{1}{x}=1+\log(N-1).$$

Putting everything together in (12), we find that there exists a constant c_2 independent of N such that

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)\leqslant c_2\log N,$$

and, finally, by Eq. (4), there exists a constant c_3 independent of N such that

$$S_N\leqslant c_3\log^2 N. \tag{13}$$

D. Numerical results

Analytically, we determined the asymptotics of the entropy S_N between the $\log N$ lower bound (9) and the $\log^2 N$ upper bound (13). In Fig. 2 we present the results of a numerical calculation. The set K consists of one interval of length $|K|=\pi$. The figure shows clearly the $\log N$ dependence. By the subadditivity property (10), we expect the same behavior for all sets K consisting of a finite number of intervals. The leading terms in the expansion of S_N have been obtained for an explicit model in Ref. 9.

V. INFINITELY MANY INTERVALS

For a set K consisting of finitely many intervals, the entropy S_N increases asymptotically slower than any power N^{α} with $\alpha>0$. However, it is easy to construct a state such that $S_N=N\log 2$. For example, one can take for K a set of 2^{N-1} regularly spaced intervals, each of length $2^{-N+1}\pi$. Note that this construction does not have an appropriate limit when $N\to\infty$. Nevertheless, it suggests that in the infinitely many intervals case the entropy S_N could have a richer behavior. This will be shown in the present section by presenting a class of states for which the growth exponent α can take any value in $[0,1)$.

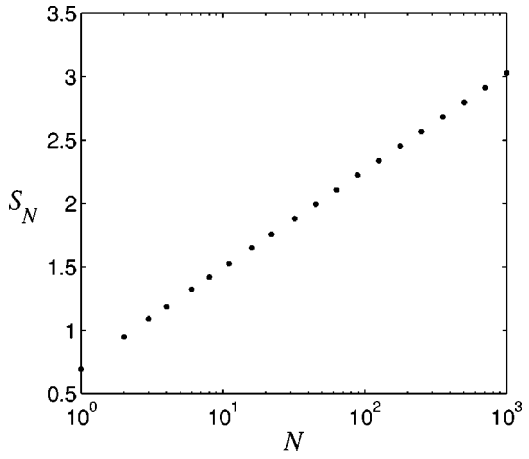

FIG. 2. The entropy S_N as a function of the length N of the restriction, for an interval of length π as set K. Notice the logarithmic scale.

A. A Cantor-type construction

The standard Cantor set is constructed recursively by removing in step m a fixed fraction of the set obtained in step $m-1$. This would leave us with a set of zero Lebesgue measure. To avoid this, we remove a fraction in step m which decreases with m, such that the limit set has strictly positive Lebesgue measure.

We start with the unit circle. Remove in the first step in a symmetrical way two open arcs of the unit circle with lengths $(1-\gamma(1))\pi$. The resulting set K_1 consists of two closed arcs each of length $\pi\gamma(1)$. In the second step, for each of these two arcs, a fraction $1-\gamma(2)$ is removed in their middle. This leaves us with a set K_2 consisting of four closed arcs of length $\pi\gamma(1)\gamma(2)/2$. Continuing this procedure, in step m we obtain a set K_m of 2^m closed arcs of length

$$\ell_{\mathrm{a}}(m) := \frac{\pi}{2^{m-1}} \prod_{n=1}^{m} \gamma(n). \tag{14}$$

There are 2^m holes in between such intervals, 2^{m-1} of which are created in step m. The latter have a length

$$\ell_{\mathrm{h}}(m) := \ell_{\mathrm{a}}(m-1)(1-\gamma(m)) = \frac{\pi}{2^{m-2}}(1-\gamma(m)) \prod_{n=1}^{m-1} \gamma(n). \tag{15}$$

The Lebesgue measure of the limit set K is then $2\pi\Pi_{n=1}^{\infty}\gamma(n)$.

To construct an explicit example, we have to fix a function $m \mapsto \gamma(m)$. We can as well specify the function $m \mapsto \ell_{\mathrm{h}}(m) = aq^m$, where $0 < q < \frac{1}{2}$ and a is chosen such that

$$2\pi > \sum_{m=1}^{\infty} 2^{m-1} a q^m = \frac{a}{2} \frac{2q}{1-2q}.$$

The resulting set has Lebesgue measure $2\pi[1-aq/(1-2q)]$.

B. Lower bound

To bound $\mathrm{Tr}\, Q_N(1-Q_N)$ from below, we start from Eq. (6). As before, K_m denotes the set obtained after m steps in the construction of the Cantor-type set K. Then K_m is the union of 2^m arcs, each of length $\ell_{\mathrm{a}}(m)$. Because $K \subset K_m$, (6) can be estimated by

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)=\frac{N}{4\pi^2}\int_{-\pi}^{\pi}d\varphi\, k_N(\varphi)|K\backslash(K+\varphi)|\geqslant\frac{N}{4\pi^2}\int_{-\pi}^{\pi}d\varphi\, k_N(\varphi)|K\backslash(K_m+\varphi)|,$$

and since $k_N(\varphi)\geqslant 4N/\pi^2$ when $|\varphi|\leqslant\pi/N$,

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)\geqslant\frac{N^2}{\pi^4}\int_{-\pi/N}^{\pi/N}d\varphi\,|K\backslash(K_m+\varphi)|=\frac{2N^2}{\pi^4}\int_0^{\pi/N}d\varphi\,|K\backslash(K_m+\varphi)|.$$

For given N, take m such that

$$\ell_{\mathrm{h}}(m)\geqslant\frac{\pi}{N}>\ell_{\mathrm{h}}(m+1). \tag{16}$$

As K_m consists of 2^m translations of the arc $[0,\ell_{\mathrm{a}}(m)]$, the Cantor-type set K consists of 2^m translations of another Cantor-type set $\tilde{K}\subset[0,\ell_{\mathrm{a}}(m)]$. Let us denote these translations by $x_\ell+[0,\ell_{\mathrm{a}}(m)]$ and $x_\ell+\tilde{K}$ for $\ell=1,\ldots,2^m$.

For $\varphi\in[0,\pi/N]$, $\varphi\leqslant\ell_{\mathrm{h}}(k)$ for all $k=1,\ldots,m$. This means that a translation by φ of an arc of length $\ell_{\mathrm{a}}(m)$ in K_m will never bridge the hole of length $\ell_{\mathrm{h}}(k),k=1,\ldots,m$, between this arc and the next. Therefore, every $x_\ell+\tilde{K}$ will overlap with one and only one $x_{\tilde{\ell}}+[0,\ell_{\mathrm{a}}(m)]+\varphi$, namely, the one with $\tilde{\ell}=\ell$. As a consequence,

$$|K\backslash(K_m+\varphi)|=2^m|\tilde{K}\backslash([0,\ell_{\mathrm{a}}(m)]+\varphi)|=2^m|\tilde{K}\backslash[\varphi,\ell_{\mathrm{a}}(m)]|=2^m|\tilde{K}\cap[0,\varphi]|.$$

This quantity has to be estimated from below. For $\varphi\in(0,\pi/N]$, take n such that $\ell_{\mathrm{a}}(n)\geqslant\varphi>\ell_{\mathrm{a}}(n+1)$. Then,

$$|\tilde{K}\cap[0,\varphi]|\geqslant\ell_{\mathrm{a}}(n+1)\prod_{k=n+2}^{\infty}\gamma(k)=\frac{\pi}{2^n}\prod_{k=1}^{\infty}\gamma(k),$$

and

$$\varphi\leqslant\ell_{\mathrm{a}}(n)=\frac{\pi}{2^{n-1}}\prod_{k=1}^{n}\gamma(k),$$

which gives

$$\frac{|\tilde{K}\cap[0,\varphi]|}{\varphi}\geqslant\frac{1}{2}\prod_{k=n+1}^{\infty}\gamma(k)\geqslant\frac{|K|}{4\pi},$$

and so

$$|\tilde{K}\cap[0,\varphi]|\geqslant\frac{|K|\varphi}{4\pi},$$

which does not depend any longer on n. It follows that

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)\geqslant 2^m\frac{2N^2}{\pi^4}\frac{|K|}{4\pi}\int_0^{\pi/N}d\varphi\,\varphi=\frac{2^m|K|}{4\pi^3}.$$

This is an estimate from below of $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$ where N and m are coupled by (16). From the latter we also have that $N<\pi/\ell_{\mathrm{h}}(m+1)$. Therefore,

$$\frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N} > \frac{\log((1/4\pi^3)2^m|K|)}{-\log((1/\pi)\ell_{\mathrm{h}}(m+1))}.$$

The limit $N\to\infty$ corresponds to the limit $m\to\infty$. Using the explicit form $\ell_{\mathrm{h}}(m)=aq^m$, we finally get

$$\liminf_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N} \geqslant \frac{\log 2}{-\log q}. \tag{17}$$

C. Upper bound

To get an upper bound for $\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)$, we start from Eq. (7). With $C(\varphi):=|K^c\backslash(K^c+\varphi)|$, it reads

$$\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)=\frac{N}{4\pi^2}\int d\varphi\, k_N(\varphi)C(\varphi).$$

For $\theta>0$, take m such that

$$\ell_{\mathrm{h}}(m)\geqslant\theta>\ell_{\mathrm{h}}(m+1). \tag{18}$$

We bound $C(\theta)$ from above,

$$\begin{aligned}
C(\theta) &\leqslant \sum_{k=1}^{\infty} 2^{k-1}\min\{\theta,\ell_{\mathrm{h}}(k)\}\\
&= \sum_{k=1}^{m} 2^{k-1}\theta + \sum_{k=m+1}^{\infty} 2^{k-1}\ell_{\mathrm{h}}(k)\\
&\leqslant (2^m-1)\ell_{\mathrm{h}}(m) + \sum_{k=m+1}^{\infty} 2^{k-1}\ell_{\mathrm{h}}(k)\\
&\leqslant 4\pi(1-\gamma(m))\prod_{n=1}^{m-1}\gamma(n) + 2\pi\sum_{k=m+1}^{\infty}(1-\gamma(k))\prod_{n=1}^{k-1}\gamma(n).
\end{aligned} \tag{19}$$

Obviously, this bound increases with θ. The kernel $k_N(\varphi)$ satisfies

$$k_N(\varphi)\leqslant\begin{cases} N & \text{for } |\varphi|\leqslant\theta,\\ \dfrac{\pi^2}{N}\dfrac{1}{\varphi^2} & \text{for } |\varphi|\geqslant\theta,\end{cases}$$

and so we find

$$\begin{aligned}
\mathrm{Tr}\, Q_N(\mathbb{1}-Q_N) &\leqslant \frac{N^2}{4\pi^2}\int_{|\varphi|\leqslant\theta} d\varphi\, C(\varphi) + \frac{1}{4}\int_{|\varphi|\geqslant\theta} d\varphi\, C(\varphi)\frac{1}{\varphi^2}\\
&\leqslant \frac{N^2}{2\pi^2}\theta C(\theta) + \frac{1}{4}\sum_{k=0}^{m}(\ell_{\mathrm{h}}(k)-\ell_{\mathrm{h}}(k+1))\frac{C(\ell_{\mathrm{h}}(k))}{\ell_{\mathrm{h}}(k+1)^2}\\
&\leqslant \frac{N^2}{2\pi^2}\ell_{\mathrm{h}}(m)C(\theta) + \frac{1}{4}\sum_{k=0}^{m}\frac{\ell_{\mathrm{h}}(k)C(\ell_{\mathrm{h}}(k))}{\ell_{\mathrm{h}}(k+1)^2}.
\end{aligned} \tag{20}$$

Take again the explicit form $\ell_{\mathrm{h}}(m)=aq^m$. Then

$$(1-\gamma(m))\prod_{n=1}^{m-1}\gamma(n)=\frac{2^{m-2}}{\pi}\ell_{\mathrm{h}}(m)=\frac{a}{4\pi}(2q)^m,$$

and (19) becomes

$$C(\theta)\leqslant 4\pi(1-\gamma(m))\prod_{n=1}^{m-1}\gamma(n)+2\pi\sum_{k=m+1}^{\infty}(1-\gamma(k))\prod_{n=1}^{k-1}\gamma(n)$$

$$=a(2q)^m+\frac{a}{2}\sum_{k=m+1}^{\infty}(2q)^k$$

$$=\frac{a(1-q)}{1-2q}(2q)^m. \tag{21}$$

If $\theta=\ell_{\mathrm{h}}(k)$, then, by (18), we have to put $m=k$, and so

$$C(\ell_{\mathrm{h}}(k))\leqslant\frac{a(1-q)}{1-2q}(2q)^k. \tag{22}$$

Substituting inequalities (21) and (22) into (20), we find

$$\mathrm{Tr}\,Q_N(\mathbb{1}-Q_N)\leqslant\frac{N^2}{2\pi^2}aq^m\frac{a(1-q)}{1-2q}(2q)^m+\frac{1}{4}\sum_{k=0}^{m}\frac{aq^k}{(aq^{k+1})^2}\frac{a(1-q)}{1-2q}(2q)^k$$

$$=\frac{N^2}{2\pi^2}aq^m\frac{a(1-q)}{1-2q}(2q)^m+\frac{1}{4}\frac{1}{q^2}\frac{2(1-q)}{1-2q}(2^{m+1}-1)$$

$$\leqslant\frac{1-q}{2(1-2q)}\left[\frac{N^2a^2}{\pi^2}(2q^2)^m+\frac{1}{q^2}2^m\right]=:c_1N^2(2q^2)^m+c_2 2^m, \tag{23}$$

where c_1 and c_2 are independent of N.

To get an upper bound as a function of N, we have to fix a function $m(N)$ and plug it into (23). Let

$$\gamma:=\frac{\log 2}{-\log q}=\frac{1}{-\log_2 q},$$

then choose m to be

$$m=[\log_{2q^2}N^{\gamma-2}]\leqslant\log_{2q^2}N^{\gamma-2}=\frac{\log_2 N^{\gamma-2}}{\log_2 2q^2},$$

where $[a]$ denotes the integer part of the number a. Then

$$N^2(2q^2)^m\leqslant N^{\gamma},$$

and

$$2^m\leqslant(2^{\log_2 N^{\gamma-2}})^{1/\log_2 2q^2}=N^{(\gamma-2)/(1+\log_2 q^2)}=N^{\gamma},$$

and so

$$\mathrm{Tr}\,Q_N(\mathbb{1}-Q_N)\leqslant(c_1+c_2)N^{\gamma},$$

from which we get the upper bound

$$\limsup_{N\to\infty}\frac{\log\mathrm{Tr}\,Q_N(\mathbb{1}-Q_N)}{\log N}\leqslant\gamma=\frac{\log 2}{-\log q}. \tag{24}$$

Combining the results (17) and (24) we see that $\lim_{N\to\infty} \log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)/\log N$ exists, which implies that also $\lim_{N\to\infty} \log S_N/\log N$ exists, and

$$\alpha = \lim_{N\to\infty} \frac{\log S_N}{\log N} = \lim_{N\to\infty} \frac{\log \mathrm{Tr}\, Q_N(\mathbb{1}-Q_N)}{\log N} = \frac{\log 2}{-\log q}.$$

Since q can be any number in the interval $(0,\frac{1}{2})$, the growth exponent α can take any value in $(0,1)$.

A number of open questions remains unresolved in this context. Some of them were suggested by the referee whose interest is hereby acknowledged. We limited here our attention to a spin $\frac{1}{2}$ chain but the dimension of the single site spin should be irrelevant. The authors also believe that there is no fastest sublinear growth for the total entropy. Sharper estimates than these of Section III B should allow to investigate in more detail the exponent one case. Finally, as mentioned in the Introduction, the question whether the average entropy of a shift-invariant pure state is zero is still open.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

On the generalized Borel transform and its application to the statistical mechanics of macromolecules

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(Received 30 May 2003; accepted 8 August 2003)

We present a new integral transform called the generalized Borel transform (GBT) and show how to use it to compute distribution functions used to describe the statistical mechanics of macromolecules. For this purpose, we choose the random flight model (RFM) of macromolecules and show that the application of the GBT to this model leads to the exact expression of the polymer propagator (two-point correlation function) from which all the statistical properties of the model can be obtained. We also discuss the mathematical simplicity of the GBT and its applicability to macromolecules with other topologies. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1618361]

I. INTRODUCTION

Consider a group of n small molecules with identical molecular structures. Furthermore, let us assume that these small molecules are connected in a sequential manner such that each of them has only two nearest neighbors with whom it forms chemical bonds. The small molecules at the ends of the chain form only one bond (they have only one neighbor). This macromolecule is called a polymer and each small molecule in the polymer is called a monomer. If the chain ends are free (they do not form a chemical bond), then the polymer is said to have a linear topology (linear polymer). Figure 1 shows this topology. If the ends were to form a chemical bond, then the polymer is said to be a ring (cyclic) polymer as showed in Fig. 1. Another way of connecting the monomers is to grow m linear polymers from a point where all the polymers form chemical bonds to each other. This is a well known topology called the star topology and defines an m-arm star polymer. Combinations of these three topologies or new topologies like dendritic topologies define more complex macromolecules.

Let us now consider the case when there are different kinds of monomers. In other words, let us assume that there are many groups of monomers such that the molecular structures of the groups are different. Then, we can connect these different monomers to form polymers which, in this case, are called copolymers. Again, linear, ring and star copolymers are possible. But, due to the different molecular structures of the groups, the distribution of the different monomers along the polymer will influence its physical properties. Thus, the probability distribution of finding a monomer with a specific molecular structure along the polymer must be known *a priori* so that the physical properties can be computed.

In order to calculate the statistical properties of the aforementioned systems, we have to use coarse-grained models. The procedure for this is well known:[1] we have to group m consecutive monomers into a statistical (Kuhn) segment of length l (=Kuhn length).[2] Thus, we replace the real polymer with n monomers by an equivalent polymer with n/m Kuhn segments such that the long wavelength properties are not altered. This equivalent model is the random flight model (RFM) of polymers.[1,3,4] Figure 2 shows the RFM.

The statistical properties of the RFM are computed from distribution functions like the single

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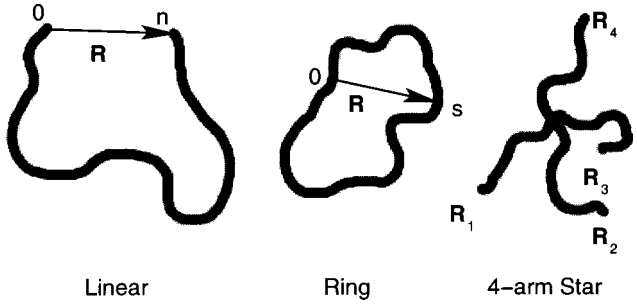

FIG. 1. Linear, ring and four-arm star topologies for flexible polymers. **R** indicates the end-to-end vector for the linear topology and the relative position of two segments in the case of a ring polymer. $\mathbf{R}_j$ indicates the position of the end of the jth arm in the star topology.

chain static structure factor (which is the density-density autocorrelation function in reciprocal space), the probability distribution of the end-to-end distance (polymer propagator) in a linear polymer or its Fourier transform called the characteristic function.[1,3–5] In particular, the polymer propagator is a very useful quantity because all the statistical properties of the model can be calculated from it. For example, the partition function of the model is the integral of the polymer propagator. Therefore, in this article we focus on the exact calculation of the polymer propagator for flexible polymers/copolymers with different topologies. For this purpose, we describe a new integral transform called the generalized Borel transform[6–8] (GBT) and apply it to the computation of the polymer propagator.

The polymer propagator of the RFM of linear polymers is defined as follows:

$$P(\mathbf{R},n)=\int d\{\mathbf{R}_k\}\prod_{j=1}^{n}\tau(\mathbf{R}_j)\,\delta\left(\sum_{j=1}^{n}\mathbf{R}_j-\mathbf{R}\right), \tag{1}$$

where **R** is the end-to-end vector and $\mathbf{R}_j$ is the bond vector between the $(j-1)$th and jth beads. The Dirac delta imposes the condition that the sum of the bond vectors has to be equal to the end-to-end vector. $\tau(\mathbf{R}_j)$ is given by the formula

$$\tau(\mathbf{R}_j)=\frac{\delta(|\mathbf{R}_j|-l)}{4\pi l^2}, \tag{2}$$

and fixes the length of each bond vector to the Kuhn length, l.

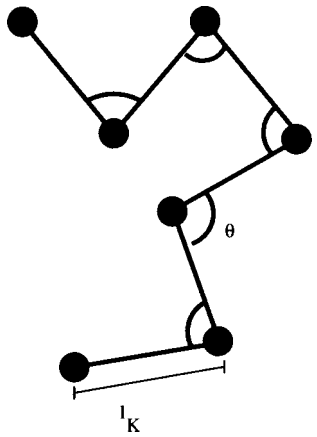

FIG. 2. The random flight model of polymer chains. l is the Kuhn length and θ is the bond angle.

Small changes to Eq. (1) can be used to describe other topologies. For example, ring polymers can be described by Eq. (1) if the constraint $\delta(\Sigma_{j=1}^{n}\mathbf{R}_j)$ is included in the integrand and the constraint $\delta(\Sigma_{j=1}^{n}\mathbf{R}_j-\mathbf{R})$ is replaced by $\delta(\Sigma_{j=s}^{s'}\mathbf{R}_j-\mathbf{R})$ where now $\mathbf{R}$ is the vector going from the s to the s' segments. Similarly, other constraints can be included in Eq. (1) to describe other topologies.

A generalization of Eq. (1) valid for copolymers under external fields has the following mathematical expression:

$$P(\mathbf{R},n,\{p_j^{\alpha}\})=\int d\{\mathbf{R}_k\}\prod_{j=1}^{n}\left(\sum_{\alpha=1}^{x}(p_j^{\alpha}\ \tau_j^{\alpha}(\mathbf{R}_j))\right)\delta\left(\sum_{j=1}^{n}\mathbf{R}_j-\mathbf{R}\right)\exp(-\omega(\{\mathbf{R}_j\})), \tag{3}$$

where x is the total number of different groups of segments forming the copolymer, p_j^{α} is the probability of finding the jth segment in the αth group of segments and $\omega(\{\mathbf{R}_j\})$ has the mathematical form

$$\omega(\{\mathbf{R}_j\})=\sum_{j=1}^{n}\eta(\mathbf{R}_j), \tag{4}$$

where $\eta(\mathbf{R})$ can be any function. In particular, the effects of external vectorial [$\eta(\mathbf{R})=-\mathbf{F}\cdot\mathbf{R}$] and quadrupolar [$\eta(\mathbf{R})=Q_{ij}R_iR_j$] fields can be studied.

Using the exponential representation of Dirac's delta,[9] Eq. (3) can be written as follows:

$$P(\mathbf{R},n,\{p_j^{\alpha}\})=\int\frac{d^3k}{(2\pi)^3}\exp(-i\mathbf{R}\cdot\mathbf{k})K(\mathbf{k},n,x,l,\{p_j^{\alpha}\}), \tag{5}$$

where $K(\mathbf{k},n,x,l,\{p_j^{\alpha}\})$ is the characteristic function. In the particular case of an isotropic system (i.e., no external fields), Eq. (5) becomes a Fourier sine transform which, for all the models described above, is exactly doable using the GBT technique.

For the purpose of simplicity, in this article we show how to apply the GBT to the case of a linear polymer with only one kind of segment. Afterward, the results obtained for this case are generalized to the case of ring and m-arm star polymers.

This article is organized as follows. In Sec. II we show how to calculate Fourier sine transforms using the generalized Borel transform and present a brief summary of the mathematical aspects of this technique. In Sec. III we apply the GBT to solve exactly a particular Fourier sine transform which is relevant to the computation of the polymer propagator of the RFM. This result is used to obtain the exact polymer propagator of the RFM. Finally, in Sec. IV we present the conclusions of our work.

II. THE GENERALIZED BOREL TRANSFORM

In the previous section we have shown that the Fourier sine transform plays a very important role in the evaluation of the statistical properties of models for single macromolecules. Therefore, let us start the description of the GBT by writing the general expression of a Fourier sine transform of a function $H(k,a)$,

$$Q(R,a)=\int_0^{\infty}\sin(Rk)H(k,a)dk. \tag{6}$$

Furthermore, let us assume that the Laplace transform of the same function, $S(g,a)$, exists. Then, we can write

$$S(g,a)=\int_0^{\infty}H(x,a)\exp(-gx)dx,\quad g>0. \tag{7}$$

Then, we observe that we can obtain the Fourier sine transform, $Q(R,a)$, from the Laplace transform, $S(g,a)$, as the analytic continuation of $S(g,a)$ to the complex plane as follows:

$$Q(R,a)=\mathrm{Im}\{S(g=-iR,a)\}. \tag{8}$$

Consequently, we will focus on the evaluation of Laplace transforms. For this purpose, we will employ the GBT technique described hereafter.

The main goal of the GBT is to obtain analytical solutions of parametric integrals of the Mellin/Laplace type[6–8] for all the range of values of the parameters. Therefore, this technique is very useful to study nonperturbative regimes. The basic idea of the method consists of introducing two auxiliary functions, $S(g,a,n)$ and $B_\lambda(s,a,n)$ (the generalized Borel transform). These functions depend on auxiliary parameters called n and λ. These parameters have no physical meaning and are introduced for the sole purpose of helping in the computation of an explicit mathematical expression for $S(g,a)$ valid for all values of the true parameters g and a.

Let us start with the mathematical definition of $S(g,a,n)$, which is the following:

$$S(g,a,n)=\int_0^\infty x^n H(x,a)\exp(-gx)dx, \quad g>0. \tag{9}$$

We have explicitly extracted a factor x^n from the function to be transformed. This integral is related to the Laplace transform, Eq. (7), by the following relationship,

$$S(g,a,n)=(-)^n\frac{\partial^n}{\partial g^n}S(g,a), \tag{10}$$

which can be inverted to give

$$S(g,a)=(-)^n\underbrace{\int dg\cdots\int dg}_{n}S(g,a,n)+\sum_{p=0}^{n-1}c_p(a,n)g^p. \tag{11}$$

The finite sum comes from the indefinite integrations. Note that all the coefficients vanish whenever the Laplace transform, Eq. (7), fulfills the following asymptotic condition:

$$\lim_{g\to\infty}S(g,a)=0. \tag{12}$$

In addition, the expression given by Eq. (11) is valid for any value of the parameter n, in particular for $n\gg 1$ where the GBT provides an approximate analytical expression for $S(g,a,n)$ as we describe below.

Let us define the generalized Borel transform of $S(g,a,n)$ as follows:

$$B_\lambda(s,a,n)\equiv-\int_0^\infty \exp[s/\eta(g)]\left[\frac{1}{\lambda\,\eta(g)}+1\right]^{-\lambda s}\frac{S(g,a,n)}{[\eta(g)]^2}\frac{\partial\eta(g)}{\partial g}dg, \quad \mathrm{Re}(s)<0 \tag{13}$$

where λ is any real, positive, and nonzero number, and η is defined as follows: $1/\eta \equiv\lambda(\exp(g/\lambda)-1)$. Then, it can be proved that $B_\lambda(s,a,n)$ is an analytic function for real values of s less than zero. Moreover, the analytic continuation to the other half of the complex plane generates an analytic function with a cut on the positive real axis.

In order to invert the transform defined by Eq. (13), we note that the change of variables $u(g)=1/\eta-\lambda\ln[1+1/\lambda\,\eta]$ transforms the integral, Eq. (13), into a Laplace transform,

$$B_\lambda(s,a,n)\equiv\int_0^\infty \exp[su]L_\lambda(S,a,n,u)du, \quad \mathrm{Re}(s)<0, \tag{14}$$

where $L_\lambda(S,a,n,u)$ depends on $S(g,a,n)$. Consequently, the inverse Laplace transform of Eq. (14) provides a procedure for the evaluation of $S(g,a,n)$ by integrating $B_\lambda(s,a,n)$ on the imaginary axis or over the discontinuity of $B_\lambda(s,a,n)$ on the cut. After a change of variables we can write $S(g,a,n)$ as follows:

$$S(g,a,n)=2\lambda^2(1-\exp(-g/\lambda))\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[G(w,t,g,\lambda,a,n)]dwdt. \tag{15}$$

$G(w,t,g,\lambda,a,n)$ is given by the following expression:[6]

$$G(w,t,g,\lambda,a,n)=-s(t)u(g)+t-\ln\{\Gamma[\lambda(s(t)+x(w))]\} +\{\lambda[s(t)+x(w)]-1\}\ln(\lambda s(t))-\lambda s(t)+w+\ln[x(w)^n H(x(w))], \tag{16}$$

where $s(t)=\lambda\exp(t)$ and $x(w)=\exp(w)$.

Note that Eq. (15) is valid for any nonzero, real and positive value of the parameter λ. However, the resulting expression for $S(g,a,n)$ does not depend on λ explicitly. Thus, each value of the parameter λ defines a particular Borel transform. Consequently, we can choose the value of this parameter in such a way that it allows us to solve Eq. (15).

The dominant contribution to the double integral is obtained using steepest descent[10,11] in the variables t and w. For this purpose, we first compute the expressions of the saddle point $t_o(g,a,n)$ and $w_o(g,a,n)$ in the limit $\lambda\gg 1$. The results are the following:

$$t_o(g,a,n)=\ln\left[\frac{x_o^2(g,a,n)}{f(x_o(g,a,n),a,n)}\right],\quad w_o(g,a,n)=\ln[x_o(g,a,n)], \tag{17}$$

where $x_o(g,a,n)$ is the real and positive solution of the implicit equation coming from the extremes of the function $G(w,t,g,\lambda,a,n)$ in the asymptotic limit in λ. Explicitly, the equation is

$$x_o^2 g^2=f(x_o,a,n)[f(x_o,a,n)+1], \tag{18}$$

where

$$f(x_o,a,n)\equiv 1+n+x_o\frac{d\ln[H(x_o,a)]}{dx_o}. \tag{19}$$

Afterward, we check the positivity condition[12] [the Hessian of $G(w,t,g,\lambda,a,n)$ at the saddle point must be positive]. Let us call the Hessian $D(x_o,a,n)$. Its mathematical expression is

$$D(x_o,a,n)\equiv -x_o\frac{df(x_o,a,n)}{dx_o}\left[\frac{1}{2}+f(x_o,a,n)\right]+f(x_o,a,n)[1+f(x_o,a,n)]. \tag{20}$$

Observe that in the range of the parameters where $f(x_o,a,n)\gg 1$, which is fulfilled when $n\gg 1$, we can keep the second order term in the expansion of $G(w,t,g,\lambda,a,n)$ around the saddle point. Then, we can approximate the double integral in Eq. (15) as follows:

$$S_{Aprox}(g,a,n)=4\pi\frac{\lambda^2(1-\exp(-g/\lambda))}{\sqrt{D[x_o,a,n]}}\exp[G(w_o,t_o,g,\lambda,a,n)]. \tag{21}$$

In the limit $\lambda\to\infty$ we obtain the following approximate expression for $S(g,a,n)$:

$$S_{Aprox}(g,a,n)=\sqrt{2\pi}e^{-1/2}\frac{\sqrt{f[x_o,a,n]+1}}{\sqrt{D[x_o,a,n]}}[x_o]^{n+1}H[x_o,a]\exp[-f[x_o,a,n]]. \tag{22}$$

Note that Eq. (22) is valid for functions $H(x,a)$ that fulfill the following general conditions. First, the relationship given by Eq. (18) must be biunivocal. Second, $D(x_o,a,n)$ must be positive at x_o. Third, $f(x_o,a,n)$ must be larger than one. These conditions provide the range of values of the parameters where the approximate solution, Eq. (22), is valid.

Finally, we replace Eq. (22) into Eq. (11) to obtain an approximate analytical expression for the Laplace transform $S(g,a)$. In particular, in the limit $n\to\infty$, we obtain the following analytical solution for $S(g,a)$:

$$S(g,a)=\lim_{n\to\infty}(-)^n\underbrace{\int dg\cdots\int dg}_{n}S_{Aprox}(g,a,n). \tag{23}$$

One particular case of this result is the one where $H(x,a)$ does not contribute to the saddle point. This is the case when $f(x_o,a,n)$ can be approximated by $1+n$ [the derivative of $\ln(H(x_o,a))$ is negligible]. Then, the saddle point solution is $x_o(g,a,n)\simeq(n+\frac{3}{2})/g$ and the expression of $S_{Aprox}(g,a,n)$ is

$$S_{Aprox}(g,a,n)\simeq\frac{\Gamma(n+1)}{g^{n+1}}H[x_o(g,a,n),a],\quad n\gg 1. \tag{24}$$

Another important property of the expression given by Eq. (23) is that, in the limit $n\to\infty$, the approximate solution, Eq. (22), becomes an exact solution for Eq. (9). Thus, as long as the n indefinite integrals are calculated without approximations, then Eq. (23) is an exact solution for Eq. (7).

In summary, the procedure to use the GBT to compute Fourier sine transforms is the following. First, one has to solve the implicit equation, Eq. (18), for $n\gg 1$ to obtain the mathematical expression of $x_o(g,a,n)$. Replacing this expression into Eq. (22) and doing the n indefinite integrals in Eq. (23), we get the expression for $S(g,a)$. Finally, one has to compute the analytic continuation of $S(g,a)$, Eq. (8), to get the solution of the Fourier sine transform, Eq. (6).

In the next section we apply this technique to compute exactly the polymer propagator of flexible macromolecules.

III. APPLICATION TO THE RANDOM FLIGHT MODEL OF FLEXIBLE POLYMERS

Let us start by analyzing the polymer propagator predicted by the random flight model which is given by Eq. (1). Using the Fourier representation of the delta function,[9] we obtain

$$\begin{aligned}P(\mathbf{R},n)&=\int\frac{d^3k\exp(-i\mathbf{R}\cdot\mathbf{k})}{(2\pi)^3(4\pi l^2)^n}\left[\int d\{\mathbf{R}_k\}\prod_{j=1}^{n}\delta(|\mathbf{R}_j|-l)\exp\left(i\sum_{j=1}^{n}\mathbf{R}_j\cdot\mathbf{k}\right)\right]\\&=\int\frac{d^3k}{(2\pi)^3}\exp(-i\mathbf{R}\cdot\mathbf{k})K(\mathbf{k},n,l),\end{aligned} \tag{25}$$

where the characteristic function, $K(\mathbf{k},n,l)$, is

$$K(\mathbf{k},n,l)=\left(\frac{\sin(|\mathbf{k}|l)}{|\mathbf{k}|l}\right)^n. \tag{26}$$

The evaluation of the angular integrals in Eq. (25) is straightforward. After rescaling $\mathbf{R}$ and $\mathbf{k}$ with the Kuhn length, l, we obtain the final expression for the polymer propagator

$$P(R,n)=\frac{2}{(2\pi)^2R}\int_0^\infty dk\left[\sin(kR)\left(\frac{\sin(k)}{k}\right)^n k\right], \tag{27}$$

where $k=|\mathbf{k}|$ and $R=|\mathbf{R}|$.

This integral representation of the polymer propagator is a Fourier sine transform and can be solve exactly using GBT. Then, our first step consists of expressing the polymer propagator, Eq. (27), in terms of a Laplace transform. For this purpose we define the function

$$S(b,n)\equiv\int_0^\infty dw\left[\exp(-wb)\left(\frac{\sin(w)}{w}\right)^n w\right], \tag{28}$$

from where we recover the expression of the polymer propagator, Eq. (27), as the analytic continuation of the function $S(b,n)$ to the complex plane

$$P(R,n)=\frac{2}{(2\pi)^2 R}\mathrm{Im}\{S(b=-iR,n)\}. \tag{29}$$

Let us now rewrite Eq. (28) as follows:

$$S(b,n)=\frac{\partial^n}{\partial c^n}\left\{\int_0^\infty dw\left[w\exp(-wb)\exp\left(c\frac{\sin(w)}{w}\right)\right]\right\}_{c=0}=\frac{\partial^n}{\partial c^n}\{GA(b,c)\}_{c=0}, \tag{30}$$

where

$$GA(b,c)\equiv\int_0^\infty dw w\exp(-wb)H(w,c), \tag{31}$$

and

$$H(w,c)\equiv\exp\left[c\frac{\sin(w)}{w}\right]. \tag{32}$$

Then, the integral expressed by Eq. (31) satisfies all the requirements of the GBT technique.[7] Consequently, we evaluate this integral in the following way:

$$GA(b,c)=\lim_{N\to\infty}(-)^N\underbrace{\int db\cdots\cdots\cdots\int db}_{N}S(b,c,N), \tag{33}$$

where we have defined

$$S(b,c,N)\equiv\int_0^\infty dw[w^{N+1}\exp(-wb)H(w,c)]. \tag{34}$$

In the asymptotic limit of $N\to\infty$, the GBT provides an analytical solution for Eq. (34). Following the technique, we first solve the following implicit equation for w_o, Eq. (18),

$$\left\{N+1+w_o\frac{\partial}{\partial w_o}\ln[H(w_o,c)]\right\}\left\{N+2+w_o\frac{\partial}{\partial w_o}\ln[H(w_o,c)]\right\}=w_o^2b^2, \tag{35}$$

whose asymptotic solution is

$$w_o\simeq\frac{N+5/2}{b}N\gg 1. \tag{36}$$

Replacing this expression for w_o in the expression provided by the GBT, Eq. (22), we obtain

$$S(b,c,N)\simeq\frac{\Gamma(N+2)}{b^{N+2}}H\left(\frac{N+5/2}{b},c\right),\quad N\gg 1. \tag{37}$$

Furthermore, we place Eq. (37) into Eq. (33) and the resulting expression into Eq. (30), then we obtain

$$S(b,n)=\lim_{c\to 0}\frac{\partial^n}{\partial c^n}\left\{\lim_{N\to\infty}(-)^N\underbrace{\int db\cdots\cdots\int db}_{N}\frac{\Gamma(N+2)}{b^{N+2}}H\left(\frac{N+5/2}{b},c\right)\right\}. \tag{38}$$

We now proceed to exchange the order of the operators; first we evaluate the nth derivative of the function H with respect to c and, afterward, we take the limit of $c\to 0$. As a result, we obtain

$$S(b,n)=\lim_{N\to\infty}(-)^N\int db\cdots\int db\,\frac{\Gamma(N+2)}{b^{N+2}}\left(\frac{\sin(N/b)}{N/b}\right)^n. \tag{39}$$

Next, we solve the N integrations. Using properties of the function $\sin(x)$ we can write $S(b,n)$ for any odd number of segments as follows:

$$S(b,n)=\frac{1}{2^{n-1}}\sum_{k=0}^{(n-1)/2}(-)^{(n-1)/2+k}\binom{n}{k}M(N,n,k,b), \tag{40}$$

where

$$M(N,n,k,b)\equiv\lim_{N\to\infty}(-)^N\,\mathrm{Im}\sum_{r=0}^{\infty}\frac{(i(n-2k))^r N^{r-n}}{r!}\int db\cdots\int db\,\frac{\Gamma(N+2)}{b^{N+2-n+r}}. \tag{41}$$

We note that the only powers of b in Eq. (41) that fulfill the asymptotic behavior of the function $S(b,n)$, Eq. (12), are those that satisfy the condition $r\geqslant(n-1)$. Consequently, the N indefinite integrations are exactly doable; the result is

$$\int db\cdots\int db\,\frac{1}{b^{N+2-n+r}}=\frac{\Gamma(2+r-n)}{\Gamma(N+2-n+r)}\,\frac{(-)^N}{b^{2+r-n}}. \tag{42}$$

Placing Eq. (42) into Eq. (41) and introducing the dummy variable $r=x+n-1$ we can write

$$M(N,n,k,b)\equiv\mathrm{Im}\frac{1}{b}(i(n-2k))^{n-1}\sum_{x=0}^{\infty}\left(\frac{i(n-2k)}{b}\right)^x\frac{\Gamma(x+1)}{\Gamma(x+n)}\times\lim_{N\to\infty}\frac{N^{x-1}\Gamma(N+2)}{\Gamma(N+x+1)}, \tag{43}$$

which, after using the asymptotic properties of the gamma function,[13]

$$\lim_{N\to\infty}\frac{N^{x-1}\Gamma(N+2)}{\Gamma(N+x+1)}=1, \tag{44}$$

becomes

$$M(n,k,b)=\frac{1}{b}\mathrm{Im}\sum_{x=0}^{\infty}(i(n-2k))^{n-1}\left(\frac{i(n-2k)}{b}\right)^x\frac{\Gamma(x+1)}{\Gamma(x+n)}. \tag{45}$$

The sum over x is doable, the result gives the following expression for $M(n,k,b)$,

$$M(n,k,b)=\frac{1}{b}\mathrm{Im}[(i(n-2k))^{n-1}FD(n,k,b)], \tag{46}$$

where we have defined

$$FD(n,k,b)\equiv\frac{\Gamma(\frac{1}{2})_3F_2([1,1,\frac{1}{2}],[(n+1)/2,n/2],-(n-2k)^2/b^2)}{\sqrt{\pi}\Gamma(n)} + \frac{i(n-2k)}{b}\,\frac{{}_3F_2([1,1,\frac{3}{2}],[(n+1)/2,(n+2)/2],-(n-2k)^2/b^2)}{\Gamma(n+1)}. \tag{47}$$

${}_3F_2([,,],[,],x)$ is the generalized hypergeometric function.[14] From Eq. (46) we can see that the imaginary part affects only the function $FD(n,k,b)$. Thus, we obtain the final expression for $S(b,n)$

$$S(b,n)=\sum_{k=0}^{(n-1)/2}(-)^k\binom{n}{k}\frac{(n-2k)^n\,{}_3F_2([1,1,\frac{3}{2}],[(n+1)/2,(n+2)/2],-(n-2k)^2/b^2)}{b^2 2^{n-1}\Gamma(n+1)}. \tag{48}$$

The last step to obtain the analytical expression of the polymer propagator consists of inserting Eq. (48) into Eq. (29) and computing the analytic continuation of the resulting expression to the complex plane through the substitution $b=-iR$. After doing these computations, we arrived at the following expression for the polymer propagator,

$$P(R,n)=\frac{1}{2^n\pi^2R^3}\sum_{k=0}^{(n-1)/2}(-)^{k+1}\binom{n}{k}(n-2k)^n\frac{1}{\Gamma(n+1)} \times\mathrm{Im}\left\{{}_3F_2\left(\left[1,1,\frac{3}{2}\right],\left[\frac{n+1}{2},\frac{n+2}{2}\right],\frac{(n-2k)^2}{R^2}\right)\right\}. \tag{49}$$

This expression can be simplified even further if we use the well known analytical properties of the hypergeometric function[14] ${}_3F_2(z)$, which is an analytic function for values of $|z|<1$ and its continuation to the rest of complex plane generates one cut on the positive real axis starting at $\mathrm{Re}(z)=1$. This implies that only values of $(n-2k)^2/R^2\geqslant 1$ will contribute to the imaginary part of ${}_3F_2(z)$. Consequently, this condition reduces the number of terms in the k-sum such that the last term of Eq. (49) is $k=[(n-R)/2]$.

The explicit evaluation of $\mathrm{Im}\{{}_3F_2([1,1,\frac{3}{2}],[(n+1)/2,(n+2)/2],(n-2k)^2/R^2)\}$ can be found in the Appendix. The final expression is

$$\mathrm{Im}\left\{{}_3F_2\left(\left[1,1,\frac{3}{2}\right],\left[\frac{n+1}{2},\frac{n+2}{2}\right],\frac{(n-2k)^2}{R^2}\right)\right\}=-\frac{R^2\pi}{2(n-2k)^n}\frac{\Gamma(n+1)}{\Gamma(n-1)}[n-2k-R]^{n-2},\quad n\geqslant 2. \tag{50}$$

Finally, we place Eq. (50) into Eq. (49) to obtain the exact expression for the polymer propagator:

$$P(R,n)=\frac{1}{2^{n+1}\pi R}\sum_{k=0}^{[(n-R)/2]}(-)^k\binom{n}{k}\frac{[n-2k-R]^{n-2}}{\Gamma(n-1)}. \tag{51}$$

Equation (51) is valid for an odd number of segments, but it is extended to polymers with any number of segments larger than two via analytic continuation. Therefore, we have obtained the well-known[15,16] exact analytical expression for the polymer propagator of flexible chains, Eq. (27), with any number of segments, n, and any end-to-end distance, R.

Observe that Eq. (51) can be used to describe the statistical properties of polymers with other topologies. For example, consider the case of a flexible m-arm star polymer as shown in Fig. 1. Since the polymer is flexible, then each arm behaves independently from the other ones except for the fact that all of them start at the origin. Thus, the probability of finding the end of the jth arm in the shell of radius R_j with thickness dR_j centered at the origin is

$$4\pi R_j^2 P(R_j,n_j)dR_j, \tag{52}$$

where n_j is the number of segments in the jth arm. If we consider all the arms, then the probability of finding the end of the first, second, etc. arms in the shells of radii R_1, R_2, etc. with thicknesses dR_1, dR_2, etc. centered at the origin is

$$(4\pi)^m \prod_{j=1}^{m} R_j^2 P(R_j,n_j)dR_j. \tag{53}$$

Other probability distributions for star polymers can also be computed easily.

Another example is the case of ring (cyclic) polymers. Figure 1 shows this topology. From this figure and following the steps presented in this article for linear polymers, it can be proved that the probability of finding any pair of segments separated by a distance R should be proportional to the product of two propagators of the form given by Eq. (51),

$$P_{Ring}(R,s,n-s) \propto P(R,s)\ P(R,n-s), \tag{54}$$

where n is the total number of segments in the ring and s is the number of segments (along the contour of the polymer chain) between the two chosen segments.

The aforementioned two examples clearly show that the results obtained for linear polymers using the GBT can be used for polymers with other topologies, thus increasing the number of models that are mathematically tractable with the GBT.

IV. CONCLUSIONS

In this article we have described a new mathematical method called the generalized Borel transform and applied it to compute some statistical properties (polymer propagator) of models of flexible polymers. Specifically, we showed how the GBT was constructed and how to use it to compute Mellin/Laplace transforms. Moreover, some mathematical properties were presented. The application of this technique to the statistical mechanics of single flexible polymers led to the exact solution for the polymer propagator of linear polymers. The propagator obtained turned out to be a finite sum of polynomials valid for any end-to-end distance, R, and number of segments, n. Furthermore, this result was used to compute distribution functions for two other topologies, rings and stars.

The exact computation of the polymer propagator of the RFM is a straightforward calculation that requires simple mathematics when the GBT is used. Indeed, the GBT requires basic elements of calculus and complex variables. This mathematical simplicity of the technique makes it a potentially very useful computational tool for more complex models of single polymer chains because it does not add any complexity to the physics of the starting model.

Equation (51) together with its extensions to stars and rings, Eqs. (53) and (54), and the discussion presented in the Introduction show that the GBT can solve exactly a wide range of models for polymers. However, more advanced models of single polymer chains like the wormlike chain model or helical polymers[5] where the bond vectors are correlated with each other through potential interactions are not exactly solvable with the GBT at present. This is a consequence of the fact that the characteristic function of these models is not known exactly.[5] This function is a Fourier sine transform in $3n$ dimensions. Thus, a generalization of the GBT to multidimensional integrals is required to address these models.

ACKNOWLEDGMENTS

We acknowledge the National Science Foundation, Grant No. CHE-0132278 (CAREER), the Ohio Board of Regents Action Fund, Proposal No. R566, and The University of Akron for financial support.

APPENDIX: EVALUATION OF $\mathrm{Im}\{{}_3F_2(z)\}$

In this appendix, we calculate the expression $\mathrm{Im}\{{}_3F_2(z)\}$. For this purpose, we use the following integral representation of the hypergeometric function:[17]

$$
{}_3F_2\left(\left[-\nu,\frac{\lambda}{2},\frac{\lambda+1}{2}\right],\left[\frac{\lambda+\mu}{2},\frac{\lambda+\mu+1}{2}\right],-\frac{q^2}{w^2}\right)=[w^{2\gamma}q^{\lambda+\mu-1}B(\lambda,\mu)]^{-1}
$$

$$
\times\int_0^q x^{\lambda-1}[q-x]^{\mu-1}[x^2+w^2]^{\nu}dx,
$$

$$
\lambda,\mu>0,\quad \mathrm{Re}\left(\frac{q}{w}\right)>0, \tag{A1}
$$

where $B(\lambda,\mu)$ is the Beta function.[17]

We now assign the values $\nu=-1$, $\lambda=2$, $\mu=n-1$, $q=n-2k$, and $w=b$ to the parameters in Eq. (A1) to obtain

$$
{}_3F_2\left(\left[1,1,\frac{3}{2}\right],\left[\frac{n+1}{2},\frac{n+2}{2}\right],-\frac{(n-2k)^2}{b^2}\right)
$$

$$
=\frac{1}{b^{-2}(n-2k)^nB(2,n-1)}\int_0^{n-2k}x[n-2k-x]^{n-2}[x^2+b^2]^{-1}dx. \tag{A2}
$$

This integral representation is valid only for $n\geqslant 2$. Therefore, when we take the analytic continuation to the complex plane ($b=-iR$), we can express the imaginary part of the hypergeometric function as follows:

$$
\mathrm{Im}\left\{{}_3F_2\left(\left[1,1,\frac{3}{2}\right],\left[\frac{n+1}{2},\frac{n+2}{2}\right],\frac{(n-2k)^2}{R^2}\right)\right\}
$$

$$
=-\frac{R^2}{(n-2k)^nB(2,n-1)}\,\mathrm{Im}\int_0^{n-2k}x[n-2k-x]^{n-2}[x^2-R^2]^{-1}dx. \tag{A3}
$$

Thus, we need to evaluate

$$
L\equiv\mathrm{Im}\int_0^{n-2k}x[n-2k-x]^{n-2}[x-R]^{-1}[x+R]^{-1}dx. \tag{A4}
$$

After analyzing the analytical behavior of the integrand, we concluded that we can exchange the operations of integration and imaginary part to obtain

$$
L=\int_0^{n-2k}x[n-2k-x]^{n-2}[x+R]^{-1}\,\mathrm{Im}\{[x-R]^{-1}\}dx. \tag{A5}
$$

Thus, we have to compute

$$
LS=\mathrm{Im}\left\{\frac{1}{(x-R)}\right\}, \tag{A6}
$$

first and, afterward, we have to solve the integral given by Eq. (A5).

The analytical behavior of the function $(x-R)^{-1}$ is well known. It is an analytic function for $|x|>R$ but, its analytic continuation to the complex plane generates a cut on the real axis in the range $-R<\mathrm{Re}(x)<R$. This cut generates its imaginary part, which is

$$\mathrm{Im}\left\{\frac{1}{(x-R)}\right\}=\pi\delta(x-R). \tag{A7}$$

Thus, placing Eq. (A7) into Eq. (A5) and making the change of variables $y=x-R$, we obtain

$$L=\pi\int_{-R}^{n-2k-R}F_k(y,n,R)\,\delta(y)dy, \tag{A8}$$

where

$$F_k(y,n,R)\equiv(y+R)[n-2k-R-y]^{n-2}[y+2R]^{-1}. \tag{A9}$$

The result of the integration gives

$$L=\frac{\pi}{2}[n-2k-R]^{n-2}. \tag{A10}$$

Finally, we place Eq. (A10) into Eq. (A3) to obtain the final expression

$$\mathrm{Im}\left\{{}_3F_2\left(\left[1,1,\frac{3}{2}\right],\left[\frac{n+1}{2},\frac{n+2}{2}\right],\frac{(n-2k)^2}{R^2}\right)\right\}=-\frac{\pi}{2}\frac{R^2}{(n-2k)^nB(2,n-1)}[n-2k-R]^{n-2}. \tag{A11}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Integrable generalized spin ladder models based on the SU(1|3) and SU(3|1) algebras

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(Received 5 May 2003; accepted 1 September 2003)

We present two integrable spin ladder models which possess a general free parameter besides the rung coupling J. The models are exactly solvable by means of the Bethe ansatz method and we present the Bethe ansatz equations. We analyze the elementary excitations of the models which reveal the existence of a gap for both models that depends on the free parameter. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1627973]

I. INTRODUCTION

Spin ladder systems continue to attract attention motivated by experimental realizations in quasi-one-dimensional systems.[1] These materials display novel features and with the continued development of new systems, there has been an impressive amount of progress in the theoretical understanding of such systems. However, a greater flexibility through the introduction of tunable free parameters within the well established mathematical frameworks would be of considerable advantage and forms the main aim of the present work.

It has been shown that ladder systems are reasonably well approximated by Heisenberg interactions, which involve bilinear exchanges.[2] While these models are not exactly solvable, several more general systems have been proposed in which solvability is guaranteed through the use of an extension of the symmetry algebra.[3–6] There has also been the introduction of systems involving interactions beyond nearest neighbor exchanges which demonstrate remarkably interesting behavior and also prove to be exactly solvable. For example, the general 2-leg spin ladder system with biquadratic interactions.[7,8] The physical importance of these types of interactions has been addressed in Ref. 9.

Subsequently other generalized integrable spin ladders have been proposed.[10–14] As is well known, integrability facilitates the use of long established techniques in order to determine the physical properties of such systems. However, in these cases, no free parameters other than the rung coupling are present due to the strict conditions of integrability. It is clear that this is a topic that warrants further investigation, since the availability of tunable parameters yields a richer phase structure.

In this article, we present two new integrable generalized spin ladders containing an extra parameter, based on the Lie superalgebras symmetries of SU(1|3) and SU(3|1). The free parameter arises in the models as a special choice of the multiparametric versions.[15] In Ref. 16, we note the

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study of a family of spin ladder Hamiltonians which also have free parameters, although in this case the construction has a different mathematical origin.

The models are integrable in the sense that they contain an infinite number of conservation laws and can be derived from a solution of the Yang–Baxter equation. This property is also of physical importance as it provides a means to improve our understanding of general correlated systems (see, for example, Ref. 17).

The Hamiltonians involve the usual bilinear Heisenberg interaction terms as well as biquadratic exchanges to ensure integrability. These four-spin terms represent interchain coupling and inter-rung coupling and the physical justification for these types of interactions has been supported by experimental results. A discussion may be found in Refs. 8, 9, and 18. We present the Bethe ansatz solution of these Hamiltonians from which the physical properties of the systems may be obtained.

An important characteristic of ladder systems, both from a theoretical and experimental point of view, is the quantum phase transition between gapped and gapless phases. The spin gap is vital for superconductivity to occur under doping, whilst from a mathematical perspective, the size of the gap is dependent on the relative strength of the rung interaction parameter. We address this issue as we analyze the ground state and first excited states of the models. Interestingly, we are able to show that for both systems a gap persists in the spectrum of the elementary excitations and indeed the gap depends on the extra parameter.

II. GENERALIZED SU(1|3) SPIN LADDER MODEL

We begin by introducing the first generalized spin ladder model, for which the explicit global Hamiltonian is of the form

$$H^{(1)}=\sum_{j=1}^{N}\ [\ h_{j,j+1}+\tfrac{1}{2}J(\boldsymbol{\sigma}_j\,.\,\boldsymbol{\tau}_j-1)\ ],\tag{1}$$

and the local Hamiltonians are given by

$$\begin{aligned}h_{j,j+1}=&\tfrac{1}{4}(1+\sigma_j^z\sigma_{j+1}^z)(1+\tau_j^z\tau_{j+1}^z)+(\sigma_j^+\sigma_{j+1}^-+\sigma_j^-\sigma_{j+1}^+)(\tau_j^+\tau_{j+1}^-+\tau_j^-\tau_{j+1}^+)\\&+\tfrac{1}{2}(1+\sigma_j^z\sigma_{j+1}^z)(t^{-1}\,\tau_j^+\tau_{j+1}^-+t\,\tau_j^-\tau_{j+1}^+)+\tfrac{1}{2}(t^{-1}\,\sigma_j^+\sigma_{j+1}^-+t\,\sigma_j^-\sigma_{j+1}^+)(1+\tau_j^z\tau_{j+1}^z)\\&-\tfrac{1}{8}(1+\sigma_j^z)(1+\sigma_{j+1}^z)(1+\tau_j^z)(1+\tau_{j+1}^z).\end{aligned}$$

The parameters $\boldsymbol{\sigma}_j$ and $\boldsymbol{\tau}_j$ represent Pauli matrices acting on site j of the upper and lower legs, respectively, J is the strength of the rung coupling that can take arbitrary real values, and t is a free parameter. The number of rungs is denoted by N and periodic boundary conditions are imposed.

The integrability of this model is assured by the Quantum Inverse Scattering Method[19] and by the fact that it can be mapped to the Hamiltonian given in Eq. (2) below. This Hamiltonian can be derived from an R-matrix obeying the Yang–Baxter algebra[20] for $J=0$, while for $J\neq 0$, the rung interactions take the form of a chemical potential term. We find that

$$\hat{H}^{(1)}=\sum_{j=1}^{N}\ [\hat{h}_{j,j+1}-2J\,X_j^{00}],\tag{2}$$

where

$$\begin{aligned}\hat{h}_{j,j+1}=&\sum_{\alpha=0}^{3}X_j^{\alpha\alpha}X_{j+1}^{\alpha\alpha}+X_j^{20}X_{j+1}^{02}+X_j^{02}X_{j+1}^{20}+X_j^{13}X_{j+1}^{31}+X_j^{31}X_{j+1}^{13}+t(X_j^{10}X_{j+1}^{01}+X_j^{12}X_{j+1}^{21}\\&+X_j^{03}X_{j+1}^{30}+X_j^{23}X_{j+1}^{32})+t^{-1}(X_j^{01}X_{j+1}^{10}+X_j^{21}X_{j+1}^{12}+X_j^{30}X_{j+1}^{03}+X_j^{32}X_{j+1}^{23})-2X_j^{00}X_{j+1}^{00}\,.\end{aligned}$$

In the above, $X_j^{\alpha\beta}=|\alpha_j\rangle\langle\beta_j|$ are the Hubbard operators with $|\alpha_j\rangle$ being the orthogonalized eigenstates of the local operator $(\boldsymbol{\sigma}_j.\boldsymbol{\tau}_j)$. The local Hamiltonians $h_{j,j+1}$ and $\hat{h}_{j,j+1}$ are related through the following basis transformation:

$$
\begin{aligned}
|\uparrow,\uparrow\rangle &\rightarrow |\uparrow,\uparrow\rangle,\\
|\uparrow,\downarrow\rangle &\rightarrow 1/\sqrt{2}(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle),\\
|\downarrow,\uparrow\rangle &\rightarrow 1/\sqrt{2}(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle),\\
|\downarrow,\downarrow\rangle &.\rightarrow |\downarrow,\downarrow\rangle.
\end{aligned}
\tag{3}
$$

The R-matrix we use is a special case of a more general multiparametric version. (For a general construction of multiparametric models, see Ref. 15.) For the purposes of the present work, it is necessary to only retain one parameter. The R-matrix is as follows:

$$
R(x)=\left(\begin{array}{cccc|cccc|cccc|cccc}
w & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & t^{-1}b & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & b & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & tb & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0\\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & -\\
0 & c & 0 & 0 & tb & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & tb & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & c & 0 & 0\\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & -\\
0 & 0 & c & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & t^{-1}b & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & tb & 0 & 0 & c & 0\\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & -\\
0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t^{-1}b & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & b & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & t^{-1}b & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a
\end{array}\right),
\tag{4}
$$

with

$$
a=x+1,\ \ b=x,\ \ c=1,\ \text{and}\ \ w=1-x,
$$

and obeys the Yang–Baxter algebra,[20]

$$
R_{12}(x-y)R_{13}(x)R_{23}(y)=R_{23}(y)R_{13}(x)R_{12}(x-y).
\tag{5}
$$

The Hamiltonian originates from this solution (2) for $J=0$ by the standard procedure,[19]

$$
\hat{h}_{j,j+1}=P\frac{d}{dx}R(x)|_{x=0},
$$

where P is the permutation operator.

The model is exactly solvable by the Bethe ansatz method[21] and the resulting Bethe ansatz equations (BAE) are given by the expressions

$$-(-1)^{M_1}t^{(N-2M_3)}\left(\frac{\lambda_l-i/2}{\lambda_l+i/2}\right)^N=\prod_{j=1}^{M_2}\frac{\lambda_l-\mu_j-i/2}{\lambda_l-\mu_j+i/2},$$

$$t^{(N-2M_3)}\prod_{j\neq l}^{M_2}\frac{\mu_l-\mu_j-i}{\mu_l-\mu_j+i}=\prod_{i=1}^{M_1}\frac{\mu_l-\lambda_i-i/2}{\mu_l-\lambda_i+i/2}\prod_{k=1}^{M_3}\frac{\mu_l-\nu_k-i/2}{\mu_l-\nu_i+i/2}, \tag{6}$$

$$t^{(N-2M_1+2M_2)}\prod_{k\neq l}^{M_3}\frac{\nu_l-\nu_k-i}{\nu_l-\nu_k+i}=\prod_{j=1}^{M_2}\frac{\nu_l-\mu_j-i/2}{\nu_l-\mu_j+i/2}.$$

The corresponding energy eigenvalues of the Hamiltonian (2) are

$$E=\sum_{j=1}^{M_1}\left(\frac{1}{\lambda_j^2+1/4}+2J\right)-(1+2J)N, \tag{7}$$

where λ_j are solutions of the BAE (6).

From the Bethe ansatz solution, we can determine the behavior of the ground state and elementary excitations of the system. The reference state becomes the ground state when the relation $J>-1+\frac{1}{2}(t+t^{-1})$ is satisfied. For N sites, the ground state energy is $E_0=-(1+2J)N$, which in terms of the Bethe ansatz calculations, corresponds to the reference state characterized by $M_1=M_2=M_3=0$.

To describe an elementary excitation, we chose $M_2=M_3=0$ and $M_1=1$ in the BAE which, from Eq. (7), yields an energy expression of the form

$$E_1=\frac{1}{\lambda^2+1/4}+2J-(1+2J)N, \tag{8}$$

where $\lambda=(i/2)\,((t+1)/(t-1))$. It is apparent that there is a gap of

$$\Delta=2(J+1-\tfrac{1}{2}(t+t^{-1})). \tag{9}$$

By solving $\Delta=0$ for J we find the critical value $J^c=-1+\frac{1}{2}(t+t^{-1})$, indicating the critical line at which the quantum phase transition from the dimerized phase to the gapless phase occurs. This phase transition assumes a simpler form after a suitable reparametrization. We introduce a new parameter K given by $K=(t+t^{-1})/2$. In Fig. 1 the phase diagram is represented in terms of K and J. The phase boundary is now a straight line given by $J=-1+K$.

In the limit $t=1$, this solution corresponds to $\lambda\to\infty$ indicating that a gap of $\Delta=2J$ persists. We note that this is agrees with the suggested numerical and experimental results of spin ladder systems.[1]

The model also exhibits elementary bound state excitations. For example by choosing $\{M_1=M_2=1,M_3=0\}$ there is solution of the Bethe ansatz equations given by

$$\lambda_1=0,\quad \mu_1=\frac{i}{2}\,\frac{t^2+1}{t^2-1}$$

which describes an excited state of energy $E=4-N+2J(1-N)$ and total spin zero.

III. GENERALIZED SU(3|1) SPIN LADDER MODEL

We move on to introduce the second integrable spin ladder model which also contains the free parameter. The global Hamiltonian reads

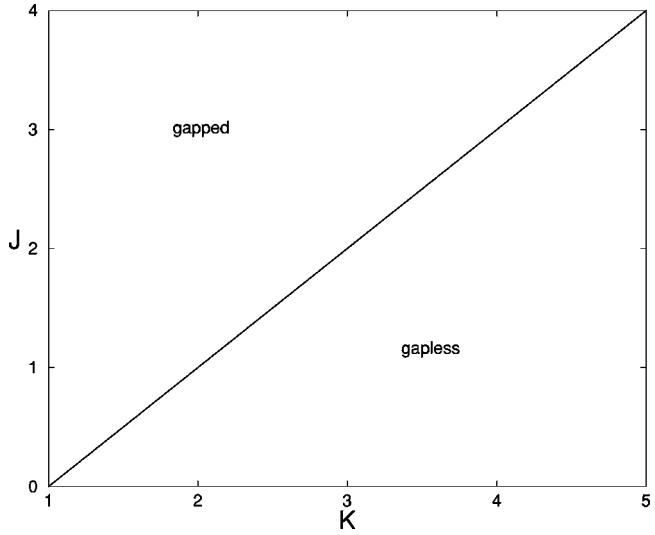

FIG. 1. Rung coupling J versus reparametrization parameter K. This graph represents the phase diagram between gapped and gapless phases. In this parametrization, the phase boundary is a straight line.

$$\mathcal{H}^{(2)}=\sum_{j=1}^{N}\left[k_{j,j+1}+\tfrac{1}{2}J(\boldsymbol{\sigma}_j.\boldsymbol{\tau}_j-1)\right], \tag{10}$$

where

$$\begin{aligned}k_{j,j+1}=&\tfrac{1}{4}(1+\sigma_j^z\sigma_{j+1}^z)(1+\tau_j^z\tau_{j+1}^z)+(\sigma_j^+\sigma_{j+1}^-+\sigma_j^-\sigma_{j+1}^+)(\tau_j^+\tau_{j+1}^-+\tau_j^-\tau_{j+1}^+)\\&+\tfrac{1}{2}(1+\sigma_j^z\sigma_{j+1}^z)(t^{-1}\tau_j^+\tau_{j+1}^-+t\,\tau_j^-\tau_{j+1}^+)+\tfrac{1}{2}(t^{-1}\sigma_j^+\sigma_{j+1}^-+t\,\sigma_j^-\sigma_{j+1}^+)(1+\tau_j^z\tau_{j+1}^z)\\&-\tfrac{1}{8}(1-\sigma_j^z)(1-\sigma_{j+1}^z)(1-\tau_j^z)(1-\tau_{j+1}^z).\end{aligned}$$

The exact solvability of the above Hamiltonian, as for the previous case, lies in the fact that it too can be mapped to a Hamiltonian given below by Eq. (11), via the transformation (3). Once again this Hamiltonian is derived from an R-matrix solution of the Yang–Baxter algebra for $J=0$, while for $J\neq 0$ the rung interactions take the form of a chemical potential term. The Hamiltonian has the form

$$\hat{\mathcal{H}}^{(2)}=\sum_{j=1}^{N}\left[\hat{k}_{j,j+1}-2JX_j^{00}\right], \tag{11}$$

where

$$\begin{aligned}\hat{k}_{j,j+1}=&\sum_{\alpha=0}^{3}X_j^{\alpha\alpha}X_{j+1}^{\alpha\alpha}+X_j^{20}X_{j+1}^{02}+X_j^{02}X_{j+1}^{20}+X_j^{13}X_{j+1}^{31}+X_j^{31}X_{j+1}^{13}+t(X_j^{10}X_{j+1}^{01}+X_j^{12}X_{j+1}^{21}\\&+X_j^{03}X_{j+1}^{30}+X_j^{23}X_{j+1}^{32})+t^{-1}(X_j^{01}X_{j+1}^{10}+X_j^{21}X_{j+1}^{12}+X_j^{30}X_{j+1}^{03}+X_j^{32}X_{j+1}^{23})-2X_j^{33}X_{j+1}^{33}.\end{aligned}$$

For $J=0$, the model is derived, in a similar manner as for the above case, from a multiparametric R-matrix for which only one parameter is relevant for the present discussion. The R-matrix is given by

$$R(x)=\left(\begin{array}{cccc|cccc|cccc|cccc}
a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & t^{-1}b & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & b & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & tb & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0\\
\hline
0 & c & 0 & 0 & tb & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & tb & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & c & 0 & 0\\
\hline
0 & 0 & c & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & t^{-1}b & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & tb & 0 & 0 & c & 0\\
\hline
0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t^{-1}b & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 & b & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 & t^{-1}b & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w
\end{array}\right), \tag{12}$$

with

$$a=x+1,\ b=x,\ c=1 \ \text{ and } w=-x+1,$$

and satisfies the Yang–Baxter algebra (5). Utilizing the Bethe ansatz method this model can be solved and the resulting BAE are

$$\begin{aligned}
&t^{(N-2M_3)}\left(\frac{\lambda_l-i/2}{\lambda_l+i/2}\right)^N=\prod_{l\neq i}^{M_1}\frac{\lambda_l-\lambda_i-i}{\lambda_l-\lambda_i+i}\prod_{j=1}^{M_2}\frac{\lambda_l-\mu_j+i/2}{\lambda_l-\mu_j-i/2},\\
&t^{(N-2M_3)}\prod_{j\neq l}^{M_2}\frac{\mu_l-\mu_j-i}{\mu_l-\mu_j+i}=\prod_{i=1}^{M_1}\frac{\mu_l-\lambda_i-i/2}{\mu_l-\lambda_i+i/2}\prod_{k=1}^{M_3}\frac{\mu_l-\nu_k-i/2}{\mu_l-\nu_i+i/2},\\
&-(-1)^{M_3}t^{-(N-2M_1+2M_2)}=\prod_{j=1}^{M_2}\frac{\nu_l-\mu_j-i/2}{\nu_l-\mu_j+i/2}.
\end{aligned} \tag{13}$$

The eigenenergies of the Hamiltonian (10) are given by

$$\mathcal{E}=-\sum_{j=1}^{M_1}\left(\frac{1}{\lambda_j^2+1/4}-2J\right)+(1-2J)N, \tag{14}$$

where λ_j are solutions of the BAE (13).

For N sites, the ground state is given by a product of rung singlets when $J>1+\frac{1}{2}(t+t^{-1})$ and the energy is $\mathcal{E}_0=(1-2J)N$. This is in fact the reference state used in the Bethe ansatz calculations and corresponds to the case $M_1=M_2=M_3=0$ of the BAE (13). To describe an elementary spin-1 excitation, we choose $M_1=1$ and $M_2=M_3=0$ in the BAE which gives the minimal excited state energy,

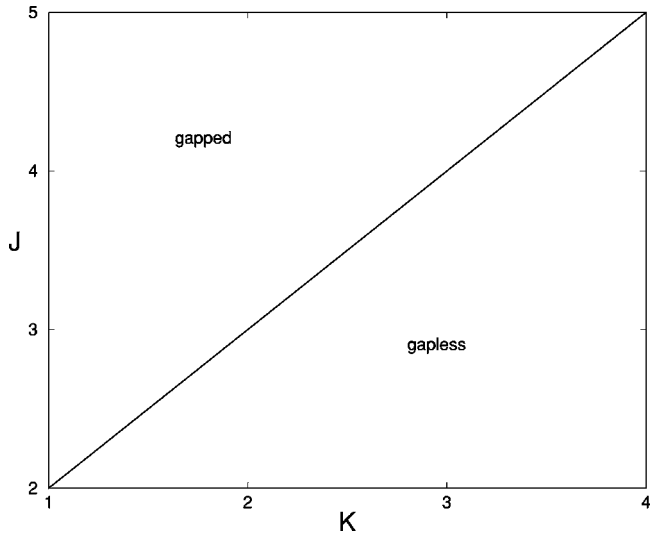

FIG. 2. Rung coupling J versus reparametrization parameter K. This graph shows a reparametrization of the curve $J=1+(t+t^{-1})/2$ in terms of $K=(t+t^{-1})/2$. In this parametrization, the phase boundary is a straight line.

$$\mathcal{E}_1=-\frac{1}{\lambda^2+1/4}+2J+(1-2J)N, \tag{15}$$

where $\lambda=(i/2)\,((t-1)/(t+1))$. The energy gap can easily be calculated and is found to be

$$\Delta=2(J-1-\tfrac{1}{2}(t+t^{-1})). \tag{16}$$

The value $J^c=1+\frac{1}{2}(t+t^{-1})$ indicates the critical line at which the transition from dimerized phase to the gapless phase occurs. This graphic is presented in Fig. 2 in terms of the reparametrization variable $K=(t+t^{-1})/2$.

The model also exhibits elementary bound state excitations. For example, by choosing $\{M_1=M_2=1,M_3=0\}$ there is solution of the Bethe ansatz equations given by

$$\lambda_1=0, \quad \mu_1=\frac{i}{2}\,\frac{t^2-1}{t^2+1},$$

which describes an excited state of energy $\mathcal{E}=-4+N+2J(1-N)$ and total spin zero.

IV. CONCLUSION

We have presented two new spin ladder models derived as special cases of multiparametric versions of Lie superalgebra SU(3|1) and SU(1|3) invariant solutions of the Yang–Baxter equation, maintaining one free parameter besides the rung coupling J. Upon investigation of the solutions of the BAEs to determine ground state and elementary excitations, we have shown that both models exhibit a gap that depends on the extra parameter. Our results are suggestive that such multiparametic extensions will, in general, have an influence on the physical characteristics of these models, and in particular the critical value of the rung coupling.

ACKNOWLEDGMENTS

A.F. and A.P.T. thank CNPq-Conselho Nacional de Desenvolvimento Científico e Tecnológico for financial support. K.H. acknowledges the support of the Ministerio de Educación y Cultura, España. J.L. thanks the Australian Research Council.

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Estimation of percolation thresholds via percolation in inhomogeneous media

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(Received 23 January 2003; accepted 3 September 2003)

This paper mathematically justifies techniques used to estimate the percolation thresholds of fully penetrable disks, or Boolean models of planar disks. Generalizations to systems of other particles in two or more dimensions are also discussed.
 [DOI: 10.1063/1.1624489]

I. INTRODUCTION

Accurate measurements of percolation phenomena are important in many areas of mathematical physics.[1–4] The Boolean model is a prototypical model for percolation studies. Recent estimates of the percolation threshold of the homogeneous Boolean model of random disks used simulations of nonhomogeneous Boolean models.[5–8] In these articles, a nonhomogeneous Boolean model was simulated in a unit square, and the disks that were connected to the right edge of the square were found. The ''edge'' of these disks, called the *frontier*, was found by using either the gap-traversal method or the more efficient frontier-walk method. Both methods saved computer resources by avoiding direct simulation of all disks within the unit square.

Using these methods, the critical density of disks of equal radius R was found to be $\lambda_{cr}R^2 = 0.359\,072(4)$, where the parentheses represents the standard deviation for the last digit. This density corresponds to a critical disk area of $a_{cr} = 1 - e^{-\pi\lambda_{cr}R^2} = 0.676\,339(4)$.

These simulations were generalized[8] to estimate the critical density for Boolean models with disks of two different radii, where proportion f of the disks have radius qR (for $0<q<1$) and the remaining disks have radius R. The presence of disks with two different radii increased the critical disk area. The largest critical disk area simulated in Ref. 8 was $a_{cr} = 0.759\,81(5)$; this was attained using $q=0.1$ and $f=0.99$. Based on these simulations, it was conjectured that a_{cr} is maximized near $f=1-q^2$ for a fixed value of q.

This paper provides a theoretical basis for the methods proposed in Refs. 5 and 6 for effectively estimating the percolation threshold of planar Boolean models of random disks. This is accomplished by coupling homogeneous and nonhomogeneous Boolean models on the same probability space. Because of this construction, classical results about homogeneous Boolean models may be applied to nonhomogeneous Boolean models. Generalizations to higher dimensional spaces and more general grains are possible; however, the proofs of these generalizations are quite technical and will be reported elsewhere.

Let $C=[0,1]^2$ be a unit square with ''left'' side $L=\{0\}\times[0,1]$ and ''right'' side $R=\{1\}\times[0,1]$. Given a set S in $\mathbb{R}^2$, we will write $tS=\{ts: s\in S\}$ for the homothetical transform of S, $|S|$ for its area, and diam S for the diameter $\sup_{x\in S}\|x\|$ of S. Finally, $b(x,r)$ will stand for a closed disk of radius r centered at a point x.

We now formally describe the Boolean model of disks (or, more exactly, a family of models).

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We will do this in a way which is suitable for our purposes; namely, we will couple a range of models on the same probability space.

Let $\tilde{\Pi}$ be a Poisson process in the phase space $\chi=\mathbb{R}_+\times\mathbb{R}^2\times\mathbb{R}_+$ with intensity measure $\mathrm{d}t\,\mathrm{d}x\,\mu(\mathrm{d}r)$, where $\mu(\mathrm{d}r)$ is a probability measure on the Borel subsets of $\mathbb{R}_+=[0,\infty)$. We will also consider its subprocess $\tilde{\Pi}_\lambda$, which is the restriction of $\tilde{\Pi}$ onto the set $[0,\lambda]\times\mathbb{R}^2\times\mathbb{R}_+$. For each realization $\{(s_i,x_i,r_i)\}$ of $\tilde{\Pi}$, we define

$$\Xi_\lambda^0=\bigcup_{(s_i,x_i,r_i)\in\tilde{\Pi}_\lambda} b(x_i,r_i),$$

which is a realization of the *homogeneous Boolean model of disks* with intensity (density) λ and radius distribution μ for the disks. The disks $b(x_i,r_i)$ in the above union, denoted by K_i for short, are called *grains*, and the x_i are their corresponding *centers*. By this construction, Ξ_λ^0 is an increasing family of closed random disks, so that $\Xi_{\lambda_1}^0\subset\Xi_{\lambda_2}^0$ if $\lambda_1<\lambda_2$.

This construction is equivalent to the usual definition of the Boolean model. The points x_i—the projection of $\tilde{\Pi}_\lambda$ onto $\mathbb{R}^2$—are distributed according to a homogeneous Poisson process Π_λ with intensity λ. Also, the radii r_i of K_i are independently chosen for each x_i with probability distribution μ.

Clusters are maximal connected components of grains. We write $A\overset{\Xi}{\underset{D}{\leftrightarrow}}B$ if two sets A and B are connected through the grains in a realization of a Boolean model Ξ. That is, $A\overset{\Xi}{\underset{D}{\leftrightarrow}}B$ if there exists a *path*—a sequence of grains $K_{i_1},\ldots,K_{i_n}$ such that $K_{i_j}\cap K_{i_{j+1}}\neq\varnothing$ for all $j=1,\ldots,n-1$—with $x_{i_k}\in D$ for all $k=1,\ldots,n$ such that $K_{i_1}\cap A\neq\varnothing$ and $K_{i_n}\cap B\neq\varnothing$. We will omit D if it is the whole plane and sometimes also Ξ if no confusion occurs. We also write $A\overset{\Xi}{\leftrightsquigarrow}\infty$ if there is an infinite path in Ξ intersecting A. If D is a rectangle of the form $[m_1,n_1]\times[m_2,n_2]$, we shall speak of its left–right crossing (LR crossing, for short) if $L(D)\overset{\Xi}{\underset{D}{\leftrightarrow}}R(D)$, where $L(D)=\{m_1\}\times[m_2,n_2]$ and $R(D)=\{n_1\}\times[m_2,n_2]$ are the "left" and "right" faces of D, respectively.

The critical percolation intensity for a homogeneous Boolean model is defined as

$$\lambda_{\mathrm{cr}}=\sup\{\lambda>0:\mathbf{P}\{\Xi_\lambda^0 \text{ contains an infinite cluster}\}=0\}.$$

Another important critical value is

$$\lambda_N=\sup\{\lambda>0:\mathbf{E}_\lambda^0[\text{Number of grains in the cluster containing 0 in } \Xi_\lambda^0]<\infty\}.$$

Here $\mathbf{E}_\lambda^0$ is the *Palm expectation* with respect to Π_λ (roughly, conditional expectation "given Π_λ has a point at the origin 0"). For a large variety of percolation models, it has been proven that $\lambda_N=\lambda_{\mathrm{cr}}$. In particular, this equality holds for models of balls provided that the support of the radius distribution μ is compact (see Refs. 9 and 10 and Ref. 11, Theorem 3.5).

Along with Boolean models Ξ_λ^0, we will also consider their scaled versions, defined by $\Xi_\lambda^0(t)=t^{-1}\Xi_\lambda^0$. It is easy to see that $\Xi_\lambda^0(t)$ is distributionally equivalent to a Boolean model with grains $b(x_i,t^{-1}r_i)$, $x_i\in\Pi_{t^2\lambda}$. Obviously, given a scale t, the critical intensities for $\Xi_\lambda^0(t)$ scale correspondingly to $t^2\lambda_{\mathrm{cr}}$ and $t^2\lambda_N$.

The estimation methods proposed in Refs. 5 and 6 are based on consideration of a *nonhomogeneous* model a compact "window" C. This model $\Xi_\Phi(t)$ is the union of $b(x_i,t^{-1}r_i)$ over $(s_i,x_i,r_i)\in\tilde{\Pi}$ such that $x_i\in C$ and $s_i\leqslant t^2\Phi(x_i)$. In other words, $\Xi_\Phi(t)$ is a Boolean model in C with balls of radii $t^{-1}r_i$ centered at the points x_i of a nonhomogeneous Poisson process Π_Φ driven by intensity measure $t^2\Phi(x)\mathrm{d}x$. We assume that the function $\Phi(x)$ is, in fact, a monotone function of only the first coordinate x^1 of x: $\Phi(x)=\varphi(x^1):[0,1]\mapsto\mathbb{R}_+$.

With this construction of $\Xi_\Phi(t)$, the nonhomogeneous Boolean model has been coupled with homogeneous Boolean models. Take any $x\in[0,1]$, and let $\lambda=\varphi(x)$. Then all grains of $\Xi_\Phi(t)$

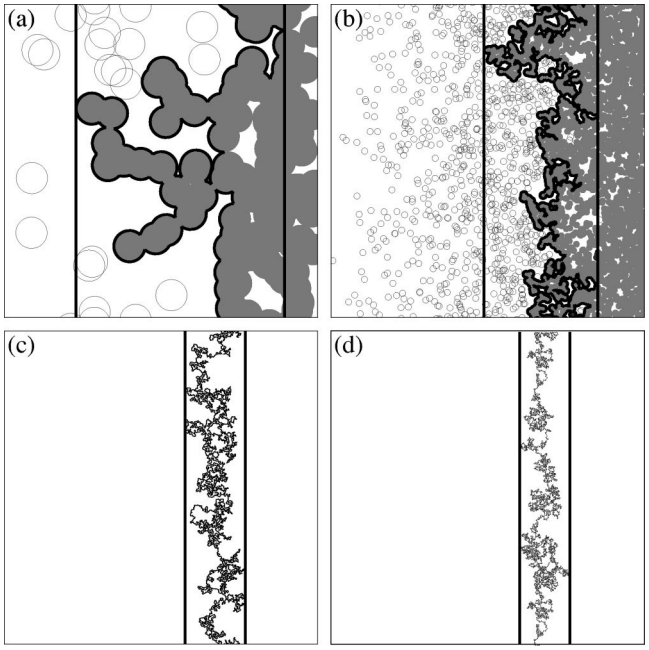

FIG. 1. (a) A realization of $\Xi_\Phi(t)$ for $t=20$ and $\varphi(x)=x$. The set Θ_t of points connected to R is shaded. The thick black line on the left face of Θ_t is the frontier Δ_t. The two vertical lines depict $d_1(t)$ and $d_2(t)$. (b) As in (a), except with $t=100$. (c) A realization of Δ_t for $t=400$. (d) As in (c), except with $t=1000$. As t increases, both $d_1(t)$ and $d_2(t)$ converge in distribution to p_{cr}.

with $x_i \leqslant x$ are grains of $\Xi^0_\lambda(t)$, and all grains of $\Xi^0_\lambda(t)$ with $x_i \geqslant x$ are grains of $\Xi_\Phi(t)$. This coupling will be used in the proofs of the following section.

We define $\Theta_t=\{x\in C\colon \{x\} \overset{\Xi_\Phi(t)}{\underset{C}{\rightsquigarrow}} R\}$ to be the points of $\Xi_\Phi(t)$ connected to the right face of C by paths in $\Xi_\Phi(t)$. We also define Δ_t to be the set of points of the boundary of Θ_t which can be connected to L by a curve lying in $C\backslash\Xi_\Phi(t)$. These boundary points were called the *frontier* in Ref. 12 as it somehow separates L (which is mostly empty) from R (which is mostly, if not completely, covered by the disks). Realizations of these sets are shown in Fig. 1.

Each horizontal line $\{y=c\}$ may intersect the frontier in a few points. For every c for which this intersection is nonempty, take the point with the smallest abscissa. The union Γ_t of such points is a subset of the frontier and consists of its points "visible from the left," which we will call the *coastline*. Actually, the mean first coordinate of the coastline points was used to estimate the percolation threshold in Ref. 6, while the mean first coordinate of the frontier was used in Refs. 5, 7, and 8.

Recall also that the Hausdorff distance between the two sets is defined by

$$\rho(A,B)=\max\{\sup_{a\in A}\inf_{b\in B}\|a-b\|,\sup_{b\in B}\inf_{a\in A}\|a-b\|\}.$$

II. MAIN THEOREM

Theorem 1: *Assume there exists* $0<R<\infty$ *such that* $\mu\{(0,R]\}=1$. *Assume also that* $\varphi(0)<\lambda_{\mathrm{cr}}<\varphi(1)$. *Define* $p_{\mathrm{cr}}=\inf\{p\colon\varphi(p)>\lambda_{\mathrm{cr}}\}$ *and* $\Theta=[p_{\mathrm{cr}},1]\times[0,1]$. *If* φ *is strictly increasing at the point* p_{cr}, *then* $\rho_t=\rho(\Theta_t,\Theta)\to 0$ *in distribution.*

Proof: We need to show that $\mathbf{P}\{\rho_t>\epsilon\}\to 0$ as $t\to\infty$. From the definition, $\rho_t>\epsilon$ implies at least one of the following cases:

$$\rho_t' = \sup_{x \in \Theta_t} \rho(x,\Theta) > \epsilon, \tag{1}$$

$$\rho_t'' = \sup_{x \in \Theta} \rho(x,\Theta_t) > \epsilon. \tag{2}$$

We will now show that both cases have vanishing probabilities as t grows.

In case (1), such x cannot lie in Θ, so there is necessarily a point x of Θ_t with the first coordinate $x^1 < p_{\mathrm{cr}} - \epsilon$. For $t > 8R/\epsilon$, this implies the existence of a grain $K_t(y_i) \overset{\mathrm{def}}{=} b(y_i, t^{-1} r_i)$ with $p_{\mathrm{cr}} - \epsilon/2 \leqslant y_i^1 \leqslant p_{\mathrm{cr}} - \epsilon/4$ connected to $[0, p_{\mathrm{cr}} - \epsilon] \times [0,1]$ in $\Xi_\Phi(t) \cap [p_{\mathrm{cr}} - \epsilon, p_{\mathrm{cr}} - \epsilon/4] \times [0,1]$.

Consider now the homogeneous Boolean model $\Xi^0_{\lambda_1}(t)$ with $\lambda_1 = \varphi(p_{\mathrm{cr}} - \epsilon/4)$. By the coupling construction described in the Introduction, all grains of $\Xi_\Phi(t)$ with $x_i^1 \leqslant p_{\mathrm{cr}} - \epsilon/4$ are also grains of $\Xi^0_{\lambda_1}(t)$. Therefore, the diameter of $\Xi^0_{\lambda_1}(t)$ cluster $W_t(y_i)$ containing $K_t(y_i)$ is at least $\epsilon/4$.

Denoting $C_1 = [p_{\mathrm{cr}} - \epsilon/2, p_{\mathrm{cr}} - \epsilon/4] \times [0,1]$ and using the scaling, we can write

$$\begin{aligned}
\mathbf{P}\{\rho_t' > \epsilon\} &\leqslant \mathbf{P}\left\{ \bigcup_{y \in \Pi_{\lambda_1}(t) \cap C_1} \{\operatorname{diam} W_t(y) > \epsilon/4\} \right\} \\
&\leqslant \mathbf{E}\left(\sum_{y \in \Pi_{\lambda_1}(t) \cap C_1} \mathbf{1}\{\operatorname{diam} W_t(y) > \epsilon/4\} \right) \\
&= \mathbf{E}\left(\sum_{y \in \Pi_{\lambda_1} \cap tC_1} \mathbf{1}\{\operatorname{diam} W(y) > t\epsilon/4\} \right) = \lambda_1 |tC_1| \mathbf{P}^0_{\lambda_1}\{\operatorname{diam} W(0) > t\epsilon/4\},
\end{aligned}$$

where $\mathbf{P}^0_{\lambda_1}$ is the Palm probability with respect to the homogeneous process Π_{λ_1}. The last equality is an application of the Campbell theorem (see, e.g., Ref. 13, p. 103).

The homogeneous model $\Xi^0_{\lambda_1}(t)$ does not percolate since $\lambda_1 < \lambda_{\mathrm{cr}}$, and so the diameter of its clusters has exponential bounds. Applying Lemma 3.3 from Ref. 11, p. 68 (see also Ref. 14), we find that

$$\mathbf{P}\{\rho_t' > \epsilon\} \leqslant A_1 \lambda_1 \epsilon t^2 \exp\{-A_2 t \epsilon\} \tag{3}$$

for some A_1, $A_2 > 0$. We see that $\lim_{t\to\infty} \mathbf{P}\{\rho_t' > \epsilon\} = 0$ for any $\epsilon > 0$, implying that $\lim_{t\to\infty} \rho_t' = 0$ in distribution.

Let us turn to the second possibility (2). Let $n > 2/\epsilon$, and partition $\Theta^\epsilon = [p_{\mathrm{cr}} + \epsilon] \times [0,1]$ into n blocks $c(k) = [p_{\mathrm{cr}} + \epsilon, 1] \times [(k-1)/n, k/n]$, $k = 1,\ldots,n$. If there is a LR crossing in each $c(k)$, then the vertical distances between adjacent crossings is always less than $2/n \leqslant \epsilon$. Therefore, there is no disk $b(x,\epsilon)$ with a center $x \in \Theta$ such that none of its points are connected to R by a path of $\Xi_\Phi(t)$ inside C. In other words, case (2) does *not* hold for t if these LR crossings occur.

Let $\lambda_2 = \varphi(p_{\mathrm{cr}} + \epsilon)$. By the coupling argument, every LR crossing of the homogeneous Boolean model $\Xi^0_{\lambda_2}(t)$ lying in Θ^ϵ is also a LR crossing of $\Xi_\Phi(t)$. By scaling and stationarity, the probability π_t of crossing such a block in $\Xi^0_{\lambda_2}$ equals the probability of a LR crossing of the block $[0, t(1 - p_{\mathrm{cr}} - \epsilon)] \times [-t/(2n) 0, t/(2n)]$ in the percolating model $\Xi^0_{\lambda_2}$. According to the classical RSW theorem (see Corollary 4.1 in Ref. 11, p. 114), π_t tends to 1 as t grows to infinity. In summary,

$$\begin{aligned}
P\{\rho_t'' > \epsilon\} &\leqslant 1 - P\{\text{LR crossings for each } c(k) \text{ in } \Xi_\Phi(t)\} \\
&\leqslant 1 - P\{\text{LR crossings for each } c(k) \text{ in } \Xi^0_{\lambda_2}(t)\} = 1 - (1 - \pi_t)^n \to 0 \quad \text{as } t \to \infty.
\end{aligned}$$

□

Remark 1: A natural way to estimate the percolation threshold is to conduct a series of independent realizations of the Boolean model $\Xi_\Phi(t)$ in a square C for a range of $t=t_1, t_2,\ldots$. The exponential form of the estimate (3) shows that $\lim_{n\to\infty}\rho'_{t_n}=0$ almost surely if the series $\Sigma_n t_n \exp\{-A_2\epsilon t_n\}$ converges (e.g., if $t_n=n$). For the second case, the RSW theorem itself does not contain an information about the speed at which the probability π_t tends to 1, but the recent results for discrete percolation suggest that it is at least exponential [see formula (8.98) in Ref. 3]. If true, the convergence of ρ_{t_n} in Theorem 1 is almost sure in the case $t_n=n$.

Recall that Δ_t and Γ_t denote the frontier and coastline of Θ_t, respectively. Not only does Θ_t converge to Θ in the Hausdorff metric, but also the first coordinates of Δ_t and Γ_t converge to $p_{\rm cr}$. This is proved in the following theorem.

Theorem 2: *Let* $\mathrm{pr}_1(\Delta_t)$ *be the projection of* Δ_t *onto the first coordinate axis, and define* $d_1(t)=\inf \mathrm{pr}_1(\Delta_t)$ *and* $d_2(t)=\sup \mathrm{pr}_1(\Delta_t)$. *Then both* $d_1(t)\to p_{\rm cr}$ *and* $d_2(t)\to p_{\rm cr}$ *as* $t\to\infty$ *or, equivalently,* $\rho(\mathrm{pr}_1(\Delta_t),\{p_{\rm cr}\})\to 0$ *in distribution. As* $\Gamma_t\subseteq\Delta_t$, *then also* $\rho(\mathrm{pr}_1(\Gamma_t),\{p_{\rm cr}\})\to 0$ *in distribution.*

Proof: The fact that $d_1(t)\to p_{\rm cr}$ follows easily from case (1) proved in Theorem 1. We now show that the probability of the event $d_2(t)>p_{\rm cr}+\epsilon$ vanishes as $t\to\infty$. Consider the rectangle $D=[p_{\rm cr}+\epsilon/2, p_{\rm cr}+\epsilon]\times[0,1]$, and denote by B and T its bottom and top sides. Denote by G the event that there is a bottom-up crossing of D in model Ξ_Φ (i.e., event $\{B \overset{\Xi_\Phi}{\underset{D}{\rightsquigarrow}} T\}$) and that this crossing path is Ξ_Φ connected to R in C. Finally, let $\sigma(\Xi,a,b)$ denote the probability of a LR crossing of a rectangle $[0,a]\times[0,b]$ in a model Ξ. By the FKG inequality (see Ref. 11, p. 32), we have that

$$\mathbf{P}\{d_2(t)\leqslant p_{\rm cr}+\epsilon\}\geqslant \mathbf{P}\{G\}$$
$$\geqslant \mathbf{P}\{B \overset{\Xi_\Phi}{\underset{D}{\rightsquigarrow}} T\}\mathbf{P}\{\text{there is a LR crossing of } [p_{\rm cr}+\epsilon/2,1]\times[0,1] \text{ in } \Xi_\Phi\}.$$

Again, by the coupling of Boolean models, every Ξ_Φ path in $[p_{\rm cr}+\epsilon/2,1]\times[0,1]$ is also a $\Xi^0_{\lambda_3}(t)$ path for $\lambda_3=\varphi(p_{\rm cr}+\epsilon/2)$. Therefore,

$$\mathbf{P}\{d_2(t)\leqslant p_{\rm cr}+\epsilon\}\geqslant \mathbf{P}\{B \overset{\Xi^0_{\lambda_3}(t)}{\underset{D}{\rightsquigarrow}} T\}\mathbf{P}\{\text{there is a LR crossing of } [p_{\rm cr}+\epsilon/2,1]\times[0,1] \text{ in } \Xi^0_{\lambda_3}(t)\}$$
$$=\sigma(\Xi^0_{\lambda_3}(t),1,\epsilon/2)\,\sigma(\Xi^0_{\lambda_3}(t),1-p_{\rm cr}-\epsilon/2,1) \tag{4}$$
$$=\sigma(\Xi^0_{\lambda_3},t,t\epsilon/2)\,\sigma(\Xi^0_{\lambda_3},t(1-p_{\rm cr}-\epsilon/2),t). \tag{5}$$

Equality (4) is due to stationarity and isotropy of the model $\Xi^0_{\lambda_3}(t)$, while (5) is obtained after scaling by t. By the RSW theorem, (5) converges to 1, thus concluding the proof. □

Remark 2: From simulations, it appears that the mean first coordinates of both Δ_t and Γ_t converge to $p_{\rm cr}$ at a rate proportional to t^{-1}, while the width $d_2(t)-d_1(t)$ converges to zero at a rate proportional to $t^{-3/7}$.

III. GENERALIZATIONS AND SIMULATIONS

The proofs of the two previous theorems are based on two principal results for the homogeneous Boolean models: in the subcritical region, exponential decay of the cluster diameter distribution and, in the supercritical region, the RSW theorem establishing the high probability of crossing of large blocks. The availability of these two results was the main reason for the conditions imposed on the Boolean model that were stated in the Introduction.

The proof of exponential bounds on the distribution's tail can be generalized for Boolean models other than planar disks in all dimensions relatively easily by using the "spectral method" proposed in Ref. 14. However, generalization of the RSW theorem demands substantial technical work. As inclusion of the corresponding proofs would go astray from the main subject of this paper, they will be reported elsewhere. Here we just give the corresponding result without a proof.

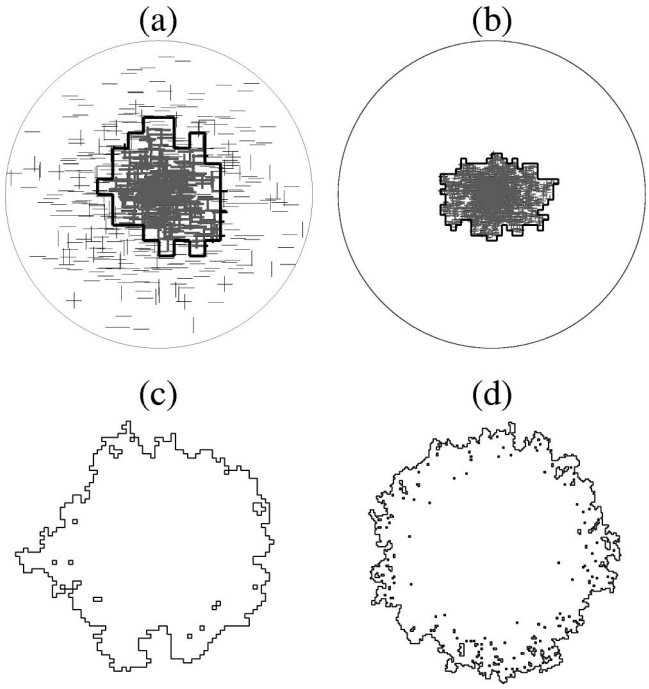

FIG. 2. Realizations of inhomogeneous needles of length t^{-1} in the unit circle. (a) In this figure, $t=10$ and proportion $\alpha=0.8$ of them are oriented horizontally. None of the needles outside of the thick solid line are connected to the center, but most of the interior needles are. (b) As in (a), except with $t=30$. Only the needles connected to the center are drawn. (c) A magnification of the interior line for $t=100$; the needles are not shown. The interior pockets correspond to small areas where needles are not connected to the center. (d) As in (c), except for $t=300$. As t increases, the frontier of the connected needles become circular, and the radius of this circle estimates the critical percolation density for the corresponding homogeneous model. From this and other similar simulations, it appears that conditions (B) and (C) can be omitted without changing the conclusion of Theorem 3.

Let $\mathbb{K}^0$ be a locally compact separable space of compact sets $K\subset\mathbb{R}^d$ containing the origin and endowed with a suitable σ-algebra, and let $\mu(\mathrm{d}K)$ be a probability measure on it (see, e.g., Ref. 15 for details on random compact sets). A random element $K\in\mathbb{K}^0$ realized with distribution μ is called a *typical grain* of a Boolean model. Consider a Poisson process $\tilde{\Pi}$ in the phase space $\mathcal{X}=\mathbb{R}_+\times\mathbb{R}^d\times\mathbb{K}^0$ with intensity measure $\mathrm{d}s\,\mathrm{d}x\,\mu(\mathrm{d}K)$ and its subprocess $\tilde{\Pi}_\Phi$, which is the restriction of $\tilde{\Pi}$ onto the set $\{(s,x):s\leqslant\Phi(x)\}\times\mathbb{K}^0$. Each realization $\{(s_i,x_i,K_i)\}$ of $\tilde{\Pi}$ defines a random set

$$\Xi_\Phi=\bigcup_{(s_i,x_i,K_i)\in\tilde{\Pi}_\Phi}(x_i+K_i),$$

which is a realization of the *nonhomogeneous Boolean model*. As above, we will also consider its scaled version $\Xi_\Phi(t)$, which is a Boolean model in a unit cube C with grains $t^{-1}K_i+y_i$ centered at the points y_i of a nonhomogeneous Poisson process with intensity measure $t^d\Phi(x)\mathrm{d}x$. As before, we assume that the function $\Phi(x)$ is a monotone function of only the first coordinate x^1 of x: $\Phi(x)=\varphi(x^1):[0,1]\mapsto\mathbb{R}_+$.

We make the following assumptions about the grain distribution of the Boolean model:

(A) finite radius: there exists $R>0$ such that $\mu\{K\in\mathbb{K}^0:\mathrm{diam}\,K\leqslant R\}=1$;
(B) isotropy: μ is rotation invariant;
(C) nondegenerate connected grains: $\mu\{K\in\mathbb{K}^0:|K|>0\}>0$ and $\mu\{K\in\mathbb{K}^0:K\text{ is connected}\}=1$; and
(D) coincidence of percolation thresholds: $\lambda_{\mathrm{cr}}=\lambda_N$.

Theorem 3: *Assume the conditions (A)–(D) hold. Assume also that the function* φ *is such that* $\varphi(0)<\lambda_{cr}<\varphi(1)$ *and strictly increasing at the point* p_{cr}. *Then the statement of Theorem 1 holds.*

A few remarks are in order. It was already mentioned in the Introduction that Condition (D) holds if all the grains are balls of a bounded radius (Ref. 11, Theorem 3.5). It also holds for a large variety of other percolation models: for example, grains which are star-shaped with the set of their radius-vector functions being a compact in the space $C(\mathbb{S}^{d-1})$ of continuous functions on a sphere with sup-norm (see Refs. 9 and 10 for details).

The example provided in Corollary 3.2 of Ref. 11, p. 52 shows that the condition (A) on finite radius cannot, in general, be dropped without affecting the validity of condition (D). If condition (A) does not hold, one cannot expect the procedure to be stable, as all of C may be covered with a positive probability for all scales t.

Conditions (B) and (C), in contrast, appear to be technical assumptions necessary for the proof but unimportant for the estimation method to work. To see this, we consider the nonhomogeneous model in a unit ball (rather than in a square C). We also take $\Phi(x)$ to be a radially symmetric function $\varphi(r)$ with a pole in 0 and which decays to 0 when $r\to 1$. Consider a range of Boolean models whose grains are segments of length t^{-1} so that proportion α of them are oriented horizontally and $1-\alpha$ vertically. As seen in Fig. 2, despite the anisotropy of the model and empty volume of the grains, the frontier of the cluster in a neighborhood of the origin has a circular shape. The radii of such frontiers estimate the critical percolation intensity for the corresponding models.

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Yang–Mills connections over manifolds with Grassmann structure

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(Received 22 May 2003; accepted 27 August 2003)

Let M be a manifold with Grassmann structure, i.e., with an isomorphism of the cotangent bundle $T^*M \cong E \otimes H$ with the tensor product of two vector bundles E and H. We define the notion of a half-flat connection ∇^W in a vector bundle $W \to M$ as a connection whose curvature $F \in S^2E \otimes \Lambda^2 H \otimes \mathrm{End}\ W \subset \Lambda^2 T^*M \otimes \mathrm{End}\ W$. Under appropriate assumptions, for example, when the Grassmann structure is associated with a quaternionic Kähler structure on M, half-flatness implies the Yang–Mills equations. Inspired by the harmonic space approach, we develop a local construction of (holomorphic) half-flat connections ∇^W over a complex manifold with (holomorphic) Grassmann structure equipped with a suitable linear connection. Any such connection ∇^W can be obtained from a prepotential by solving a system of linear first order ODEs. The construction can be applied, for instance, to the complexification of hyper-Kähler manifolds or more generally to hyper-Kähler manifolds with admissible torsion and to their higher-spin analogs. It yields solutions of the Yang–Mills equations. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1622999]

I. INTRODUCTION

The Yang–Mills self-duality equations have played an important role in field theory and in differential geometry. They are the main source of examples of solutions of the Yang–Mills equations on four-dimensional manifolds.[1] The self-duality equations $*F^\nabla = F^\nabla$ mean that the curvature F^∇ of a connection ∇ over a Riemannian four-fold M is an eigenvector of the Hodge star operator, associated with the volume four-form, which acts on two-forms. This apparently four-dimensional construction has an analog in Riemannian manifolds M of arbitrary dimensions. Any four-form Ω on M defines an endomorphism B_Ω of the space of two-forms and one can define (Ω,λ)-self-duality as the condition, $B_\Omega F^\nabla = \lambda F^\nabla$, that the curvature is an eigenvector of B_Ω with eigenvalue $\lambda = \mathrm{const} \neq 0$. Under appropriate assumptions on Ω (for example, if it is co-closed) this implies the Yang–Mills equations, just as in four dimensions. For instance, this works for a constant Ω in flat space[2,3] and for a parallel four-form on a Riemannian manifold with special holonomy (some examples are discussed in Refs. 4–8). If Ω is, for example, the canonical parallel four-form associated to a quaternionic Kähler manifold M of dimension $4m$, then the eigenspaces of B_Ω are the irreducible $\mathrm{Sp}(m)\cdot\mathrm{Sp}(1)$-submodules of the space of two-forms. In terms of the

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associated locally defined Grassmann structure $T^{*\mathbb{C}}M=E\otimes H$, i.e., the identification of the complexified cotangent bundle $T^{*\mathbb{C}}M$ with a tensor product of two vector bundles E and H of rank $2m$ and 2, respectively, the eigenspace decomposition is given by

$$\Lambda^2 T^{*\mathbb{C}}M=S^2E\otimes\Lambda^2H\oplus\Lambda_0^2E\otimes S^2H\oplus\omega_E\otimes S^2H,$$

with corresponding B_Ω-eigenvalues $\lambda_1=1,\lambda_2=-1/3,\lambda_3=-(2m+1)/3$.[3,9] Here ω_E and ω_H are two-forms on E^* and H^* such that the complex metric on $T^{\mathbb{C}}M$ is given by $\omega_E\otimes\omega_H$ and Λ_0^2E denotes the traceless part of Λ^2E with respect to ω_E. The eigenspaces of B_Ω can thus be described in terms of the Grassmann structure, which is a natural generalization of the well-known spinor decomposition of a vector in four dimensions. A two-form on any manifold with Grassmann structure is called half-flat if it belongs to the eigenspace $S^2E\otimes\Lambda^2H$ and a connection ∇ with half-flat curvature is called half-flat. If the Grassmann structure is associated with the quaternionic Kähler structure, then a half-flat connection is the same as an (Ω,λ_1)-self-dual connection and hence satisfies the Yang–Mills equations. Inspired by the harmonic space approach,[10] we develop a construction of locally defined holomorphic half-flat connections on a manifold M with holomorphic admissible half-flat Grassmann structure, namely, a holomorphic Grassmann structure $T^*M=E\otimes H$ with holomorphic connections ∇^E and ∇^H in the bundles E and H, respectively, such that ∇^H is flat and the torsion of the linear connection $\nabla=\nabla^E\otimes\mathrm{Id}+\mathrm{Id}\otimes\nabla^H$ has no component in $S^3H\otimes E^*\otimes\Lambda^2E$. The construction associates to a holomorphic prepotential a half-flat connection through the solution of a system of linear first order ODEs. The construction can be applied, for instance, to the complexification of hyper-Kähler manifolds or, more generally, to hyper-Kähler manifolds with admissible torsion. Our construction of gauge fields on such curved backgrounds extends that of Ref. 10, where flat torsion-free backgrounds were considered. Moreover, we provide a geometric description of the harmonic space method of Ref. 10.

We note that using analytic continuation any real analytic connection ∇ over a real analytic Grassmann manifold allows extension to a holomorphic connection $\nabla^{\mathbb{C}}$ over a holomorphic Grassmann manifold and ∇ can be reconstructed from $\nabla^{\mathbb{C}}$ in terms of some antiholomorphic involution.

The main idea of our construction is to pull-back a half-flat connection ∇ in a holomorphic vector bundle $\nu:W\to M$ to the harmonic space S_H. The latter is the space of all symplectic frames $h=(h_+,h_-)$ in the vector bundle H^*. The group $\mathrm{Sp}(1,\mathbb{C})$ acts freely on S_H, with the orbit space $S_H/\mathrm{Sp}(1,\mathbb{C})=M$. Hence, the projection $\pi:S_H\to M$ is an $\mathrm{Sp}(1,\mathbb{C})$-principal bundle. Choosing a (local) trivialization, $M\ni x\mapsto(h_1(x),h_2(x))\in S_H$, of π we can make the identification $S_H=\mathrm{Sp}(1,\mathbb{C})\times M$. There exists a canonical decomposition,

$$TS_H=T^vS_H\oplus\mathcal{D}_+\oplus\mathcal{D}_-,$$

of the (holomorphic) tangent bundle into the vertical subbundle T^vS_H and two (holomorphic) distributions $\mathcal{D}_+$ and $\mathcal{D}_-$ spanned, respectively, by vector fields X_+^e and X_-^e canonically associated with sections e of the bundle E^*. If the Grassmann structure is admissible and half-flat, the distributions $\mathcal{D}_+$ and $\mathcal{D}_-$ are integrable. The vertical distribution T^vS_H is spanned by vector fields $\partial_0,\partial_{++},\partial_{--}$, which correspond to the standard generators of the Lie algebra $\mathfrak{sp}(1,\mathbb{C})$. A half-flat connection ∇ in the bundle $\nu:W\to M$ induces the pull-back connection $\pi^*\nabla$ in the pull-back bundle $\pi^*\nu:\pi^*W\to S_H$. Since ∇ is half-flat, the curvature F of $\pi^*\nabla$ satisfies certain equations (see Definitions 6 and 7). A connection in $\pi^*\nu$ satisfying these equations is called a half-flat connection over S_H and is gauge equivalent to the pull-back of a half-flat connection over M. Any half-flat connection over S_H is flat along the leaves of the integrable distribution $\langle\mathcal{D}_+,\partial_0\rangle$ spanned by ∂_0 and $\mathcal{D}_+$. We can therefore choose a frame of the vector bundle $\pi^*\nu$ which is parallel along its leaves. Such a frame is called an analytic frame. With respect to such a frame a half-flat connection has no potentials in the directions of the distribution $\langle\mathcal{D}_+,\partial_0\rangle$. Starting from a matrix-valued function (prepotential) A_{++} on S_H, which is constant along the leaves of the distribution $\mathcal{D}_+$ and satisfies the homogeneity condition $\partial_0A_{++}=2A_{++}$, we construct a connection which satisfies almost all the conditions of half-flatness. We call such a connection an almost half-flat connection. It is half-flat if and only if its curvature satisfies the equation $F(\partial_{--},\mathcal{D}_-)=0$. The

construction of an almost half-flat connection reduces to the solution of first order linear ODEs. Assuming that the almost half-flat connection ∇ is defined globally along the fibers (over $\pi^{-1}U$, where $U\subset M$ is a domain in M) we can modify ∇ to a half-flat connection over S_H which is the pull-back of a half-flat connection over M. In order to do this, we rewrite ∇ with respect to a ''central frame,'' namely, a frame parallel along the fibers of π. The transformation from the analytic to the central frame reduces to the solution of the system of equations

$$\partial_{++}\Phi=-A_{++}\Phi,\quad \partial_0\Phi=0.$$

With respect to the central frame the potential $C(X^e_+)$ of the connection ∇ in the direction of the vector field $X^e_+\in\mathcal{D}_+$ has the form $C(X^e_+)=u^\alpha_+C^e_\alpha$, where C^e_α are matrix-valued functions on $M=M\times\{\mathrm{Id}\}\subset M\times\mathrm{Sp}(1,\mathbb{C})$ and $u^\alpha_\pm,\alpha=1,2$, are matrix coefficients of $\mathrm{Sp}(1,\mathbb{C})$. The matrix-valued functions C^e_1,C^e_2 define the desired half-flat connection on M given by

$$\nabla^M_{e\otimes h_1}=e\otimes h_1+C^e_1,\quad \nabla^M_{e\otimes h_2}=e\otimes h_2+C^e_2.$$

Moreover, any half-flat connection may be obtained in this way.

The above construction allows generalization to manifolds with spin $m/2$ Grassmann structure. This means that the cotangent bundle is identified as $T^*M=E\otimes F=E\otimes S^mH$, where E and H are (holomorphic) vector bundles of rank p and 2, respectively. If a connection ∇^E on E and a flat connection ∇^H on H are given, then the Grassmann structure is called half-flat. The connection ∇^H defines a flat connection ∇^F on $F=S^mH$ and the linear connection $\nabla=\nabla^E\otimes\mathrm{Id}+\mathrm{Id}\otimes\nabla^F$. The associated harmonic space $\pi:S_H\to M$ is defined as above, as the space of all symplectic frames $h=(h_+,h_-)$ in H^*. Its tangent space has decomposition

$$TS_H=T^vS_H\oplus\bigoplus_{k=0}^{m}\mathcal{D}_{k+}\oplus\bigoplus_{k=1}^{m}\mathcal{D}_{k-}.$$

Under certain conditions on the torsion of ∇ the distribution $\mathcal{D}^k_{(+)}:=\oplus^k_{i=0}\mathcal{D}_{(m-2i)+}$, $k\leqslant m/2$, is integrable. Such a half-flat Grassmann structure is called k-admissible. Generalizing the notion of a half-flat connection, we may define a k-partially flat connection ∇ over a manifold with half-flat spin $m/2$ Grassmann structure such that the pull-back connection $\pi^*\nabla$ has no curvature in the directions of $\mathcal{D}^k_{(+)}$. The harmonic space method can be applied to construct k-partially flat connections over k-admissible half-flat spin $m/2$ Grassmann manifolds. In the final section we consider the case of $m=3$ and sketch the construction of zero- and one-partially flat connections. The latter are Yang–Mills connections.

II. GENERALIZED SELF-DUALITY FOR MANIFOLDS OF DIMENSION GREATER THAN FOUR

A. Yang–Mills data

Let $\nu:W\to M$ be a real vector bundle over M and ∇ a connection in ν, that is a bilinear map

$$\nabla:\mathfrak{X}(M)\times\Gamma(\nu)\to\Gamma(\nu),$$

$$(X,\sigma)\mapsto\nabla_X\sigma,$$

which is $C^\infty(M)$-linear in the vector field $X\in\mathfrak{X}(M)$ and satisfies the Leibniz rule $\nabla_X(f\sigma)=(Xf)\sigma+f\nabla_X\sigma$, for any function $f\in C^\infty(M)$ and any section, $\sigma\in\Gamma(\nu)$, of ν. The map ∇ can be extended to a complex bilinear map,

$$\nabla:\mathfrak{X}^{\mathbb{C}}(M)\times\Gamma(W^{\mathbb{C}}\to M)\to\Gamma(W^{\mathbb{C}}\to M),$$

$$(X,\sigma)\mapsto\nabla_X\sigma, \tag{1}$$

where $\mathfrak{X}^{\mathbb{C}}(M)$ is the space of complex vector fields $X+iY; X,Y\in\mathfrak{X}(M)$ and $W^{\mathbb{C}}\to M$ is the complexification of the vector bundle ν. Note that ∇ satisfies the reality condition

$$\nabla_{\bar{X}}\bar{\sigma}=\overline{\nabla_X\sigma},\quad X\in\mathfrak{X}^{\mathbb{C}}(M),\quad \sigma\in\Gamma(W^{\mathbb{C}}\to M), \tag{2}$$

where the bar denotes complex conjugation. Conversely, any $\mathbb{C}$-bilinear map (1) which is $\mathfrak{X}^{\mathbb{C}}(M)$-linear and satisfies the Leibniz rule and the reality condition (2) defines a connection ∇ in the real vector bundle ν. If the reality condition (2) is dropped, then (1) defines a connection in the complex vector bundle $W^{\mathbb{C}}\to M$.

Let $\varphi=(\varphi_1,\ldots,\varphi_r)$ denote a local frame of ν such that for any section $\sigma\in\Gamma(\nu)$, $\sigma=\Sigma s^i\varphi_i=:\varphi\cdot s$, where s^i are the coordinates of σ with respect to the frame φ and $s=(s^1,\ldots,s^r)^t$. Then the connection ∇ in ν has local expression

$$\nabla_X\sigma=\nabla_X(s^i\varphi_i)=\varphi\cdot\nabla_X s:=\left(Xs^i+\sum_j A^i_j(X)s^j\right)\varphi_i,$$

where $A^i_j(X)=(\nabla_X\varphi_j,\varphi^i)$ and $\varphi^*=(\varphi^1,\ldots,\varphi^r)$ denotes the dual frame. The locally defined matrix-valued one-form $A=(A^i_j):M\to\mathfrak{gl}(r,\mathbb{R})$ is called the Yang–Mills potential with respect to the frame φ. If the vector bundle ν has structure group G, i.e., if it is a bundle associated with a principal G-bundle $P\to M$ and a representation $\rho:G\to GL(r,\mathbb{R})$, such that $W=P\times_G\mathbb{R}^r$, then we may always choose a frame φ for which the potential takes values in the Lie algebra $\mathfrak{g}=\mathrm{Lie}\,\rho(G)\subset\mathfrak{gl}(r,\mathbb{R})$. We will symbolically write $\nabla_X=X+A$, $A=A^{\varphi}$. A change of frame (gauge transformation) $\varphi'=\varphi U$ induces changes $s'=U^{-1}s$ and $\varphi'(X+A'(X))s'=\varphi'\nabla_X s'=\varphi\nabla_X s=\varphi(X+A(X))s=\varphi' U^{-1}(X+A(X))Us'$, yielding the transformation rule for the potential,

$$A'=U^{-1}(XU)+U^{-1}A(X)U=U^{-1}\nabla_X U. \tag{3}$$

The curvature of the connection ∇, $F=F^{\nabla}\in\Omega^2_M(\mathrm{End}\,W)=\Gamma(\Lambda^2T^*M\otimes\mathrm{End}\,W)$, is given by

$$F(X,Y)=[\nabla_X,\nabla_Y]-\nabla_{[X,Y]}=XA(Y)-YA(X)+[A(X),A(Y)]-A([X,Y]).$$

The Jacobi identity for ∇_X is equivalent to the Bianchi identity, $d^{\nabla}F^{\nabla}=0$. Here the covariant derivative $d^{\nabla}:\Omega^p(\mathrm{End}\,W)\to\Omega^{p+1}(\mathrm{End}\,W)$ is defined by

$$d^{\nabla}(\omega\otimes C)=d\omega\otimes C+(-1)^p\omega\wedge\nabla C,$$

where ω is a p-form and C is a section of End W. (The connection ∇ on W induces a connection on End W denoted by the same symbol.)

On any n-dimensional oriented pseudo-Riemannian (or complex Riemannian) manifold, (M,g) using the canonical volume form $\mathrm{vol}^g\in\Lambda^nT^*M$, we define the Hodge $*$ operator which interchanges forms of complementary degree, $*:\Lambda^pT^*M\to\Lambda^{n-p}T^*M$, by the relation $\langle\alpha,\beta\rangle\mathrm{vol}^g=\alpha\wedge*\beta$, where $\alpha,\beta\in\Lambda^pT^*M$ and $\langle .,.\rangle$ is the natural scalar product on Λ^pT^*M induced by the metric g. We define $*:\Lambda^pT^*M\otimes\mathrm{End}\,W\to\Lambda^{n-p}T^*M\otimes\mathrm{End}\,W$ by $*(\omega\otimes C):=(*\omega\otimes C)$.

Definition 1: Let $\nu:W\to M$ be a real vector bundle over a pseudo-Riemannian manifold (M,g). A **YM connection** ∇ *in ν is one which satisfies the Yang–Mills equation*

$$d^{\nabla}*F^{\nabla}=0.$$

On a closed manifold this is the Euler–Lagrange equation for the YM functional

$$\|F^{\nabla}\|^2=\int_M|F^{\nabla}|^2\ \mathrm{vol}^g, \tag{4}$$

where the norm on $\Lambda^2 T^*M \otimes \mathrm{End}\ W$ is induced by the pseudo-Riemannian metric on M and the natural metric on End W.

B. Self-duality conditions

On a Riemannian four-manifold, the $*$ operator maps two-forms to two-forms and has eigenvalues ± 1. The curvature tensor therefore has decomposition into the eigenspaces of the $*$ operator,

$$F^\nabla = F^\nabla_{+1} \oplus F^\nabla_{-1} \in \Omega^+_M(\mathrm{End}\ W) \oplus \Omega^-_M(\mathrm{End}\ W).$$

This splitting corresponds to the decomposition of the SO(4)-module $\Lambda^2\mathbb{R}^4 = \Lambda^2_+ \oplus \Lambda^2_- \cong \mathfrak{so}(4) = \mathfrak{sp}(1) \oplus \mathfrak{sp}(1)$ into its irreducible submodules. We call ∇ and F^∇ self-dual or anti-self-dual if $F^\nabla_{-1} := \frac{1}{2}(F^\nabla - *F^\nabla) = 0$ or $F^\nabla_{+1} := \frac{1}{2}(F^\nabla + *F^\nabla) = 0$, respectively. For (anti-)self-dual connections, the YM equation, $d^\nabla * F^\nabla = 0$, is an immediate consequence of the Bianchi identity, $d^\nabla F^\nabla = 0$. On closed manifolds (anti-) self-dual connections in fact minimize the YM functional (4), since the inequality

$$\|F^\nabla\|^2 = \|F^\nabla_{+1}\|^2 + \|F^\nabla_{-1}\|^2 \geqslant |\|F^\nabla_{+1}\|^2 - \|F^\nabla_{-1}\|^2| = 8\pi^2 |c_2(W)[M]|$$

is saturated. Here $c_2(W)[M] = (1/8\pi^2)\int_M \mathrm{tr}\ F^\nabla \wedge F^\nabla$ is the evaluation of the second Chern class of the bundle W on the fundamental cycle.

The apparently four-dimensional notion of self-duality has an analog in higher dimensions. The construction originally given in Ref. 2 for flat spaces extends to arbitrary manifolds (M,g), of dimension greater than four, as follows.

For $\Omega \in \Omega^4(M)$ we define a symmetric tracefree endomorphism field $B_\Omega : \Lambda^2 T^*M \to \Lambda^2 T^*M$ by

$$B_\Omega \omega := *(*\Omega \wedge \omega), \tag{5}$$

where $\omega \in \Lambda^2 T^*M$. This endomorphism is zero if and only if the four-form Ω is zero. Moreover, we have the following.

Lemma 1: Let

$$\Omega = \sum\ \Omega_{ijkl} e^i \wedge e^j \wedge e^k \wedge e^l, \quad \omega = \sum\ \omega_{ij} e^i \wedge e^j$$

be the expressions for Ω and ω with respect to a frame e^i of T^*M. Then B_Ω is given as the contraction

$$B_\Omega \omega = 12 \sum\ g^{ii'} g^{jj'}\ \ \Omega_{ijkl}\ \ \omega_{i'j'}\ \ e^k \wedge e^l.$$

Proof: It is sufficient to check the above formula for decomposable forms $\Omega = e^i \wedge e^j \wedge e^k \wedge e^l$ and $\omega = e^m \wedge e^n$, where the e^i form an orthonormal basis of T^*M. □

Definition 2: A four-form $\Omega \in \Omega^4(M)$ on a pseudo-Riemannian manifold M is called **appropriate** *if there exists a nonzero real constant eigenvalue λ of the endomorphism field B_Ω.*

We note that on a Riemannian manifold the eigenvalues of B_Ω are real for any four-form Ω. A generalization of the four-dimensional notion of self-duality may now be defined:

Definition 3: Let Ω be an appropriate four-form on a pseudo-Riemannian manifold (M,g) and $\lambda \neq 0 \in \mathbb{R}$. A connection ∇ in a vector bundle $\nu : W \to M$ is **(Ω,λ)-self-dual** *if its curvature F^∇ satisfies the linear algebraic system*

$$B_\Omega F^\nabla = \lambda F^\nabla, \tag{6}$$

$$(d*\Omega)\wedge F^{\nabla}=0\,. \tag{7}$$

Theorem 1: *Let (M,g) be a pseudo-Riemannian manifold with an appropriate four-form Ω. Then any (Ω,λ)-self-dual connection ∇ is a YM connection.*

Proof: Using (6) and (5) we obtain

$$d^{\nabla}*F^{\nabla}=\frac{1}{\lambda}d^{\nabla}*B_{\Omega}F^{\nabla}=\pm\frac{1}{\lambda}d^{\nabla}(*\Omega\wedge F^{\nabla})=\pm\frac{1}{\lambda}((d*\Omega)\wedge F^{\nabla}+*\Omega\wedge d^{\nabla}F^{\nabla})=0,$$

in virtue of (7) and the Bianchi identity $d^{\nabla}F^{\nabla}=0$. □

Examples of manifolds admitting appropriate four-forms are easily obtained. Let V be a pseudo-Euclidean vector space and $G\subset \mathrm{SO}(V)$ be a linear group preserving a nonzero element $\Omega_0\in\Lambda^4V$. Denote by Ω_{ijkl} the components of Ω_0 with respect to an orthonormal basis of V. Given a manifold M with a G-structure, $\pi:P\to M$, i.e., a principal G-subbundle of the bundle of frames on M, we can define a four-form $\Omega:=\Sigma\Omega_{ijkl}e^i\wedge e^j\wedge e^k\wedge e^l$, where $(e^1,\ldots,e^n)$ is a coframe dual to a G-frame $p=(e_1,\ldots,e_n)\in P$. Since $G\subset\mathrm{SO}(V)$, M has the structure of an oriented pseudo-Riemannian manifold and we can define the operator B_{Ω}. The matrix components of $B_{\Omega}=\Sigma B^{kl}_{ij}e^i\wedge e^j\otimes e_k\wedge e_l$ are constant for any G-frame and so are its eigenvalues. Hence Ω is appropriate if the endomorphism $B_{\Omega_0}\in\Lambda^4V$ has a nonzero real eigenvalue λ. This is automatic in the Riemannian case.

There exist many examples of subgroups $G\subset\mathrm{SO}(V)$ admitting nonzero G-invariant four-forms, as shown by the following construction. Let $G\subset\mathrm{SO}(V)$ be a closed subgroup of the pseudo-orthogonal group $\mathrm{SO}(V)$ and $\mathfrak{g}\subset\mathfrak{so}(V)\cong\Lambda^2V^*$ its Lie algebra. Assume that $\mathfrak{g}$ admits a G-invariant symmetric nondegenerate bilinear form $B\in S^2(\mathfrak{g}^*)^G$, where W^G denotes the space of G-invariant elements of a G-module W. We can then identify $\mathfrak{g}$ with its dual $\mathfrak{g}^*$ via B and consider B as an element of $(S^2(\mathfrak{g}))^G\subset(S^2\Lambda^2V^*)^G$. A G-invariant four-form is then defined by $\Omega_0^G:=\mathrm{alt}B\in(\Lambda^4V^*)^G$, where $\mathrm{alt}:S^2\Lambda^2V^*\to\Lambda^4V^*$ denotes alternation. We denote the corresponding four-form on a manifold with G-structure by Ω^G. The following variant of a theorem by Kostant[11] provides a wealth of examples of nonzero Ω_0^G's.

Theorem 2: *Let $G\subset\mathrm{SO}(V)$ be a closed subgroup whose Lie algebra $\mathfrak{g}$ admits a nondegenerate G-invariant bilinear form $B\in(S^2\mathfrak{g})^G$. If the G-module V is not equivalent to the isotropy module of a pseudo-Riemannian symmetric space, then the four-form $\Omega_0^G:=\mathrm{alt}B\in(\Lambda^4V)^G$ is nonzero.*

Proof: Recall that the $\mathrm{SO}(V)$-module $S^2\Lambda^2V$ decomposes according to $S^2\Lambda^2V=\mathcal{R}(\mathfrak{so}(V))+\Lambda^4V$, where $\mathcal{R}(\mathfrak{so}(V))$ denotes the space of curvature tensors of type $\mathfrak{so}(V)$, i.e., the space of two-forms fulfilling the first Bianchi identity or the kernel of the map $\mathrm{alt}:S^2\Lambda^2V\to\Lambda^4V$. If $\Omega_0^G=\mathrm{alt}B=0$, then B is a nonzero element of $\mathcal{R}(\mathfrak{so}(V))\cap S^2(\mathfrak{g})^G=\mathcal{R}(\mathfrak{g})^G$. Since B is a G-invariant two-form on V with values in $\mathfrak{g}$ it can be used to define a Lie bracket $[\,\cdot\,,\cdot\,]$ on the vector space $\mathfrak{l}=\mathfrak{g}\oplus V$ thus,

(i) $\mathfrak{g}$ is a subalgebra of $\mathfrak{l}$,
(ii) V is a $\mathfrak{g}$-submodule with action defined by the inclusion $\mathfrak{g}\subset\mathfrak{so}(V)$, and
(iii) $[u,v]:=B(u,v)\in\mathfrak{g}$ if $u,v\in V$.

The Jacobi identity follows from the Bianchi identity and the G-invariance. Let L be the simply connected Lie group with Lie algebra $\mathfrak{l}$. Then L/G_0 is a Riemannian symmetric space with V as its isotropy module, where $G_0\subset L$ is the connected Lie subgroup with $\mathrm{Lie}G_0=\mathfrak{g}$. □

Clearly, (7) is automatic if the four-form Ω is co-closed, $d*\Omega=0$. This is the case, for example, if Ω is parallel. In the Riemannian case the Berger list of irreducible holonomy groups[12] and a theorem of Kostant[11] yield the following result.

Theorem 3: *Let M be a complete simply connected irreducible Riemannian manifold of dimension $n\geqslant 4$ with holonomy group $\mathrm{Hol}\subset\mathrm{SO}(n)$, $\mathrm{Hol}\neq\mathrm{SO}(n)$. Then M admits a nontrivial parallel four-form if one of the following holds: (i) M is not a symmetric space or (ii) M is a symmetric space and has a nonsimple holonomy or, equivalently, isotropy group.*

Proof: By Berger's theorem on Riemannian irreducible holonomy groups,[12] we have

(a) M is not a symmetric space and its holonomy group is one of $\mathrm{U}(n/2)$, $\mathrm{SU}(n/2)$, $\mathrm{Sp}(n/4)\mathrm{Sp}(1)$, $\mathrm{Sp}(n/4)$, G_2, $\mathrm{Spin}(7)$, or
(b) M is a symmetric space.

All the groups in (a) admit invariant four-forms. These are given below. A theorem of Kostant[11] states that a simply connected irreducible Riemannian symmetric space G/K has no nonzero parallel four-form if and only if the isotropy group K is simple. □

In the following examples we explicitly describe parallel (hence appropriate) four-forms Ω on Riemannian n-manifolds with holonomy groups $\mathrm{Hol}\neq\mathrm{SO}(n)$ from Berger's list.

(1) Kähler manifolds, $\mathrm{Hol}\subset\mathrm{U}(m)\subset\mathrm{SO}(2m)$, $n=2m$: $\Omega=\omega\wedge\omega$, where ω is the Kähler form. One can check that this is proportional to $\Omega^{\mathrm{SU}(m)}$ and that any parallel four-form is proportional to $\omega\wedge\omega$ if the holonomy group is $\mathrm{SU}(m)$ or $\mathrm{U}(m)$. If $\mathrm{Hol}\subset\mathrm{Sp}(k)\subset\mathrm{SU}(2k)\subset\mathrm{SO}(4k)$, $n=4k>4$, i.e., if the manifold is hyper-Kähler, there exist three skewsymmetric parallel complex structures $J_\alpha,\alpha=1,2,3$. Then there exist six independent parallel four-forms $\omega_\alpha\wedge\omega_\beta$, $\alpha,\beta=1,2,3$, where ω_α is the Kähler form associated to J_α. For low dimensional examples, eigenvalues and eigenspaces of B_Ω are given in Ref. 2.

(2) Quaternionic Kähler manifolds, $\mathrm{Hol}\subset\mathrm{Sp}(m)\mathrm{Sp}(1)\subset\mathrm{SO}(4m)$, $n=4m$. In this case there exist three locally defined almost complex structures J_α, with corresponding Kähler forms ω_α, such that the four-form $\Omega:=\Sigma_\alpha\omega_\alpha\wedge\omega_\alpha$ is globally defined and parallel. This will be discussed in more detail in Sec. II C.

(3) $\mathrm{Hol}\subset G_2\subset\mathrm{SO}(7)$. Let $V=\mathbb{O}=\mathbb{R}1+\mathrm{Im}\,\mathbb{O}=\mathbb{R}\oplus\mathbb{R}^7=\mathbb{R}^8$ be the algebra of octonions. Recall that $G_2=\mathrm{Aut}(\mathbb{O})$ is the group of automorphisms of the octonions. We can decompose the product of two octonions a,b into its real and imaginary parts as follows:

$$ab=a\cdot b=\langle a,b\rangle 1+\tfrac{1}{2}[a,b],$$

where $\langle a,b\rangle$ is the scalar product and $[a,b]=ab-ba$ is the commutator. We define a three-form φ and a four-form ψ on $\mathrm{Im}\,\mathbb{O}=\mathbb{R}^7$ by the formulas

$$\varphi(x,y,z):=\langle x\cdot y,z\rangle=\tfrac{1}{2}\langle[x,y],z\rangle$$

$$\psi(x,y,z,w):=\langle[x,y,z],w\rangle\,,$$

where $[x,y,z]=(xy)z-x(yz)$ is the associator. It is known that $\psi=*\varphi$. Notice that G_2 is the group of isometries of $\mathbb{O}=\mathbb{R}^8$ which fix the identity element 1 and preserve the three-form φ (or equivalently the four-form ψ) on $\mathrm{Im}\,\mathbb{O}$. The four-form ψ defines a parallel four-form on any Riemannian seven-fold with holonomy $G_2\subset\mathrm{SO}(7)$. It is known[13] that $\Lambda^4\mathbb{R}^7=\mathbb{R}\psi\oplus V^7(\pi_1)\oplus V^{27}(2\pi_1)$, where $V^d(\pi)$ is the d-dimensional real irreducible representation of G_2 with highest weight π and π_i denotes the ith fundamental weight of G_2. From this it follows that the four-form $\Omega_0^{G_2}$ coincides with ψ up to scaling. The corresponding endomorphism B_ψ of $\Lambda^2\mathbb{R}^7=\mathfrak{g}_2\oplus\mathbb{R}^7$ has two distinct eigenvalues which correspond to the two irreducible G_2-submodules $\mathfrak{g}_2$ and $\mathbb{R}^7\subset\Lambda^2\mathbb{R}^7$ (see Ref. 2).

(4) $\mathrm{Hol}\subset\mathrm{Spin}(7)\subset\mathrm{SO}(8)$. Using the three- and four-forms φ and ψ on $\mathbb{R}^7$ introduced in the G_2-case, we construct the four-form

$$\Omega=dt\wedge\varphi+\psi,$$

where t is the first coordinate on $\mathbb{R}^8=\mathbb{R}1+\mathbb{R}^7$. In particular,

$$\Omega(1,x,y,z)=\varphi(x,y,z),\quad \Omega(x,y,z,w)=\psi(x,y,z,w)\,,\quad x,y,z,w\in\mathbb{R}^7.$$

This four-form Ω defines a parallel four-form on any Riemannian eight-fold with holonomy $\mathrm{Spin}(7)\subset\mathrm{SO}(8)$. It is known that $\Lambda^4\mathbb{R}^8=\mathbb{R}\Omega\oplus V^7(\pi_1)\oplus V^{27}(2\pi_1)\oplus\Lambda^4\mathbb{R}^7$. From this it follows

that the four-form $\Omega_0^{\mathrm{Spin}(7)}$ coincides with Ω up to scaling. The corresponding endomorphism B_Ω of $\Lambda^2\mathbb{R}^8=\mathfrak{spin}_7\oplus\mathbb{R}^7$ has two distinct eigenvalues which correspond to the two irreducible Spin(7)-submodules $\mathfrak{spin}_7$ and $\mathbb{R}^7\subset\Lambda^2\mathbb{R}^8$ (see Ref. 2).

C. Quaternionic Kähler case

Now we discuss in more detail the case of quaternionic Kähler manifolds (Example 2 above). Riemannian manifolds (M,g) with holonomy group $\mathrm{Hol}\subset\mathrm{Sp}(m)\mathrm{Sp}(1)$ are called quaternionic Kähler manifolds. A quaternionic Kähler manifold with holonomy group $\mathrm{Hol}\subset\mathrm{Sp}(m)$ is called hyper-Kähler. On any quaternionic Kähler manifold M, there exists a rank 3 vector subbundle $Q\subset\mathrm{End}\,TM$, invariant under parallel transport, which is locally spanned by three almost complex structures $(J_\alpha)=(J_1,J_2,J_3=J_1J_2=-J_2J_1)$. The latter are in general only locally defined. The (globally defined) vector bundle Q is called the **quaternionic structure** of M. A local frame (J_α) as above is called a **standard frame** for Q. Similarly, a **standard basis** of Q at $m\in M$ is a triple $I,J,K=IJ=-JI\in Q_m$ of complex structures on T_mM. A quaternionic Kähler manifold is hyper-Kähler if and only if there exists a globally defined parallel standard frame $(J_\alpha)=(J_1,J_2,J_3=J_1J_2=-J_2J_1)$.

Given a standard frame, we may locally define three nondegenerate two-forms $\omega_\alpha:=g(J_\alpha\cdot,\cdot)$. The four-form

$$\Omega:=\sum_\alpha \omega_\alpha\wedge\omega_\alpha$$

is independent of the choice of standard frame and defines a global parallel four-form.

To describe the eigenspace decomposition of Ω it is convenient to use the Grassmann structure (i.e., generalized spinor decomposition) of a quaternionic Kähler manifold. Recall that a **Grassmann structure** on a (real) manifold M is defined as an isomorphism $T^{*\mathbb{C}}M\cong E\otimes H$ of the complexified cotangent bundle with the tensor product of two complex vector bundles E and H over M. Any quaternionic Kähler manifold admits a (locally defined) Grassmann structure $T^{*\mathbb{C}}M=E\otimes H$, where H has rank 2, such that the holonomy group $\mathrm{Hol}\subset\mathrm{Sp}(E)\otimes\mathrm{Sp}(H)$. This follows from the fact that any complex irreducible representation of the group $\mathrm{Sp}(m)\times\mathrm{Sp}(1)$ is a tensor product of irreducible representations of its factors.

The complex extension $g^{\mathbb{C}}$ of the Riemannian metric defines a complex bilinear metric on $T^{\mathbb{C}}M$, which locally factorizes as $g^{\mathbb{C}}=\omega_E\otimes\omega_H$, where ω_E and ω_H are sections of Λ^2E and Λ^2H, defining complex symplectic forms on the fibers of E^* and H^*, respectively. We call ω_E and ω_H the symplectic forms of the symplectic vector bundles E^* and H^*.

In terms of the Grassmann structure the eigenspaces V_λ of the endomorphism B_Ω on $\Lambda^2T^{*\mathbb{C}}M$ are given by[3,9]

$$V_{\lambda_1}=S^2E\otimes\omega_H,\quad V_{\lambda_2}=\Lambda_0^2E\otimes S^2H,\quad V_{\lambda_3}=\omega_E\otimes S^2H,$$

where Λ_0^2E is the space of ω_E-traceless two-forms and the eigenvalues are $\lambda_1=1$, $\lambda_2=-\frac{1}{3}$ and $\lambda_3=-(2m+1)/3$. In particular the λ_1-self-duality condition takes the form

$$F^\nabla\in S^2E\otimes\omega_H\otimes\mathrm{End}\,W. \tag{8}$$

Note that since Ω is parallel it is appropriate and co-closed and hence the (Ω,λ)-self-duality equations (Definition 3) reduce to (6), which implies the Yang–Mills equation. It is known (see Theorem 1 of Ref. 4) that λ_1- and λ_3-self-dual connections correspond to absolute minima of the Yang–Mills functional on compact quaternionic Kähler manifolds.

D. Self-duality as half-flatness

The λ_1-self-duality equation (8) in fact depends only on the existence of the factorization $T^{*\mathbb{C}}M \cong E \otimes H$ and the symplectic structure in H^*. A connection ∇ in a vector bundle W over a manifold M with a Grassmann structure is called **half-flat** if its curvature satisfies the condition

$$F^{\nabla} \in S^2E \otimes \Lambda^2 H \otimes \mathrm{End}\ W. \tag{9}$$

In general such half-flat connections are *not* YM connections (with respect to some metric), but it is possible to impose further conditions on F^{∇} in order to enforce the YM equation. In fact, it is the half-flatness of the connection, rather than the YM property, which is crucial for our construction of solutions.

Proposition 1: A connection ∇ in a vector bundle $W \to M$ over a quaternionic Kähler manifold is half-flat if and only if it is λ_1-self-dual. Hence any such connection is a Yang–Mills connection.

Proof: The result follows from (8) and (9) since $\Lambda^2 H$ is the line bundle generated by ω_H. □

The Levi-Civita connection on a hyper-Kähler manifold is an example of a half-flat linear connection. Its complexification gives an example of what we call an admissible half-flat Grassmann structure in the next section.

III. MANIFOLDS WITH HALF-FLAT HOLOMORPHIC GRASSMANN STRUCTURE

Our goal is to give a construction of half-flat connections in a vector bundle $\nu: W \to M$ over a manifold M. If all objects are real analytic, using analytic continuation we may obtain corresponding complex analytic objects. Specifically, assume that the manifold M and the bundle ν are real analytic. Then M is defined by an atlas of charts with analytic transition functions. Extending these functions to complex holomorphic functions, we may extend M to a complex manifold $M^{\mathbb{C}}$ with antiholomorphic involution τ such that $M = (M^{\mathbb{C}})^{\tau}$, the fixed point set of τ. Similarly, a real analytic vector bundle $\nu: W \to M$ can be extended to a holomorphic vector bundle $\nu^{\mathbb{C}}: W^{\mathbb{C}} \to M^{\mathbb{C}}$. Moreover, an analytic connection ∇ in ν can be extended to a holomorphic connection ∇ in $\nu^{\mathbb{C}}$. A holomorphic extension of a Yang–Mills connection is also a Yang–Mills connection. In the rest of this article, we shall assume that all objects (manifolds, bundles and connections) are holomorphic. In Sec. IV we shall give a construction of half-flat connections in a holomorphic bundle $W \to M$ over a complex manifold M with holomorphic Grassmann structure. Now we describe the required geometrical notions. In particular, we provide a description of the harmonic spaces of Ref. 10 in geometric language. Our description affords application to the construction of half-flat connections over more general manifolds than the flat torsion-free backgrounds previously considered in the harmonic space literature (see, e.g., Ref. 10).

A. Grassmann structure

Let M be a complex manifold with holomorphic Grassmann structure $T^*M = E \otimes H$, the isomorphism of the holomorphic cotangent bundle over M with the tensor product of holomorphic vector bundles E and H over M of rank p and q, respectively. Then $TM = E^* \otimes H^*$. A holomorphic linear connection ∇ on M is called a **holomorphic Grassmann connection** if it preserves the holomorphic Grassmann structure. This means that for any vector field X on M and local sections $e \in \Gamma(E)$ and $h \in \Gamma(H)$,

$$\nabla_X(e \otimes h) = \nabla^E_X e \otimes h + e \otimes \nabla^H_X h,$$

where ∇^E, ∇^H are connections in the bundles E, H, respectively.

Definition 4: A holomorphic Grassmann structure, $T^*M = E \otimes H$, on a complex manifold M with a holomorphic Grassmann connection $\nabla = \nabla^E \otimes \mathrm{Id} + \mathrm{Id} \otimes \nabla^H$ is called **half-flat** *if the connection ∇^H in the holomorphic vector bundle $H \to M$ is flat. A manifold with such a half-flat holomorphic Grassmann structure is called a* **half-flat Grassmann manifold**.

Assumption: In this section we assume that M is a manifold with a half-flat holomorphic Grassmann structure $(T^*M = E \otimes H, \nabla = \nabla^E \otimes \mathrm{Id} + \mathrm{Id} \otimes \nabla^H)$, such that H has rank 2 and that a

∇^H-parallel nondegenerate fiber-wise two-form $\omega_H \in \Gamma(\Lambda^2 H)$ in the bundle H^* is fixed. If, in addition, a ∇^E-parallel nondegenerate two-form $\omega_E \in \Gamma(\Lambda^2 E)$ is fixed, then we can define a ∇-parallel complex Riemannian metric $g = \omega_E \otimes \omega_H$ on M. We do not assume, in general, that the linear connection ∇ is torsion-free.

The torsion of a linear connection belongs to $TM \otimes \Lambda^2 T^*M$. Since $T^*M = E \otimes H$, we have the decomposition

$$\begin{aligned} TM \otimes \Lambda^2 T^*M &= TM \otimes (\Lambda^2 E \otimes S^2 H \oplus S^2 E \otimes \Lambda^2 H) \\ &= E^* H^* (\Lambda^2 E S^2 H \oplus S^2 E \omega_H) \\ &\cong E^* \Lambda^2 E (S^3 H \oplus \omega_H H) \oplus E^* S^2 E \omega_H H, \end{aligned} \tag{10}$$

where we omit the $\otimes$'s and we identify H^* with H using ω_H.

Definition 5: A half-flat connection is called **admissible** *if its torsion tensor has no component in* $E^* \otimes \Lambda^2 E \otimes S^3 H$. *A half-flat Grassmann manifold* (M, ∇) *is called* **admissible** *if* ∇ *is* **admissible**.

We remark that if the torsion of a half-flat connection is E-symmetric, i.e., if it belongs to $TM \otimes S^2 E \otimes \Lambda^2 H = TM \otimes S^2 E \otimes \omega_H$, then the connection is admissible. It follows from the above decomposition that the torsion tensor of any admissible connection can be written as

$$T(e \otimes h, e' \otimes h') = T_1(e,e') \otimes \omega_H(h,h') h_1 + T_2(e,e') \otimes \omega_H(h,h_2) h' + T_2(e,e') \otimes \omega_H(h',h_2) h,$$

where e, e' are sections of E^*, h_1, h_2 are fixed sections of $H \cong H^*$, $T_1 \in \Gamma(E^* \otimes S^2 E)$ and $T_2 \in \Gamma(E^* \otimes \Lambda^2 E)$. This shows that admissibility of the connection means that the torsion can be represented as the sum of two tensors linear in ω_H.

B. Harmonic space

Let M be a half-flat Grassmann manifold. We denote by S_H the $\mathrm{Sp}(1,\mathbb{C})$-principal holomorphic bundle over M consisting of symplectic bases of $H_m^* \cong H_m \cong \mathbb{C}^2$, $m \in M$,

$$S_H = \{ s = (h_+, h_-) \mid \omega_H(h_+, h_-) = 1 \}.$$

The bundle $S_H \to M$ is called **harmonic space**.[10] A parallel (local) section

$$m \mapsto s_m = (h_1(m), h_2(m)) \in S_H$$

defines a trivialization

$$M \times \mathrm{Sp}(1,\mathbb{C}) \cong S_H,$$

given by

$$(m, \mathcal{U}) \mapsto s_m \mathcal{U} = \left(h_+ = \sum_{\alpha=1}^{2} h_\alpha u_+^\alpha \ , \ h_- = \sum_{\alpha=1}^{2} h_\alpha u_-^\alpha \right), \quad \mathcal{U} = \begin{pmatrix} u_+^1 & u_-^1 \\ u_+^2 & u_-^2 \end{pmatrix}; \det \mathcal{U} = 1.$$

We denote by $\partial_{++}, \partial_{--}, \partial_0$ the fundamental vector fields on S_H generated by the standard generators of $\mathrm{Sp}(1,\mathbb{C})$,

$$\partial_{++} \sim \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \partial_{--} \sim \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \partial_0 \sim \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They satisfy the relations

$$[\partial_{++}, \partial_{--}] = \partial_0, \quad [\partial_0, \partial_{++}] = 2\partial_{++}, \quad [\partial_0, \partial_{--}] = -2\partial_{--}.$$

Consider $\mathrm{Mat}(2,\mathbb{C})$, the vector space of two by two matrices. The matrix coefficients $u_{\pm}^{\alpha}$ are coordinates on this vector space. One can easily check that the vector fields $u_{+}^{\alpha}\partial/\partial u_{-}^{\alpha}$, $u_{-}^{\alpha}\partial/\partial u_{+}^{\alpha}$ and $u_{+}^{\alpha}\partial/\partial u_{+}^{\alpha}-u_{-}^{\alpha}\partial/\partial u_{-}^{\alpha}$ annihilate the function $\det \mathcal{U}=\epsilon_{\beta\gamma}u_{+}^{\beta}u_{-}^{\gamma}$, where $\epsilon_{\beta\gamma}$ are the matrix coefficients of the standard symplectic form of $\mathbb{C}^2$. Therefore these vector fields are tangent to the submanifold $\mathrm{Sp}(1,\mathbb{C})=\{\det \mathcal{U}=1\}\subset \mathrm{Mat}(2,\mathbb{C})$. One can easily prove the following lemma.

Lemma 2: In terms of the identification, $S_H\cong M\times \mathrm{Sp}(1,\mathbb{C})$, the fundamental vector fields on S_H generated by the standard generators of $\mathrm{Sp}(1,\mathbb{C})$ *may be written*

$$\partial_{++}=u_{+}^{\alpha}\frac{\partial}{\partial u_{-}^{\alpha}},\quad \partial_{--}=u_{-}^{\alpha}\frac{\partial}{\partial u_{+}^{\alpha}},\quad \partial_0=u_{+}^{\alpha}\frac{\partial}{\partial u_{+}^{\alpha}}-u_{-}^{\alpha}\frac{\partial}{\partial u_{-}^{\alpha}}.$$

We say that a function f on S_H has **charge** c if $\partial_0 f=cf$. The charge measures the difference in the degrees of homogeneity in u_+ and u_-.

Note that any frame $(h_+,h_-)\in S_H$ defines an isomorphism $\mathbb{C}^2\xrightarrow{\sim} H_m^*$ given by $(z^1,z^2)\mapsto z^1h_+ + z^2h_-$. This induces an isomorphism

$$\mathfrak{sp}(1,\mathbb{C})=\mathfrak{sp}(\mathbb{C}^2)\cong S^2\mathbb{C}^2\xrightarrow{\sim} S^2H_m^*=\mathrm{span}_{\mathbb{C}}\{h_+^2,\,h_-^2,\,h_+\vee h_-\},$$

where we have identified $\mathfrak{sp}(\mathbb{C}^2)$ with $S^2\mathbb{C}^2$ using the symplectic form of $\mathbb{C}^2$. The generators of $\mathfrak{sp}(1,\mathbb{C})$ corresponding to h_+^2, $-h_-^2$, $-h_+\vee h_-$ under this identification are precisely ∂_{++}, ∂_{--}, ∂_0 respectively.

C. Canonical distributions on harmonic space

Let $S_H=\{(h_+,h_-)\,|\,h_{\pm}=u_{\pm}^{\alpha}h_{\alpha},(u_{\pm}^{\alpha})\in \mathrm{Sp}(1,\mathbb{C})\}$ be the harmonic space associated to a half-flat Grassmann manifold M. Here we have fixed a parallel symplectic frame (h_1,h_2) of H^* which defines the trivialization $S_H=M\times \mathrm{Sp}(1,\mathbb{C})$ of the holomorphic bundle S_H. In particular, the matrix coefficients $u_{\pm}^{\alpha}$ of $\mathrm{Sp}(1,\mathbb{C})$ will be considered as holomorphic functions on S_H. Together with local coordinates (x^i) of M, we obtain a system $(x^i,u_{\pm}^{\alpha})$ of local (nonhomogeneous–homogeneous) coordinates on S_H.

For any section $e\in\Gamma(E^*)$ we define vector fields $X_{\pm}^e\in\mathfrak{X}(S_H)$ by the formula

$$X_{\pm}^e|_{(h_+,h_-)}=\widetilde{e\otimes h_{\pm}},$$

where $\widetilde{Y}$ stands for the horizontal lift of a tangent vector Y on M with respect to the connection ∇^H. Since the frame h_α is parallel, this horizontal lift coincides with the horizontal lift with respect to the splitting $S_H=M\times \mathrm{Sp}(1,\mathbb{C})$. This shows that the vector fields $X_{\pm}^e$ are tangent to $M\times\{(h_+,h_-)\}$ and hence annihilate $u_{\pm}^{\alpha}$. If $h_{\pm}=u_{\pm}^{\alpha}h_{\alpha}$, then $X_{\pm}^e=u_{\pm}^{\alpha}\widetilde{X_{\alpha}^e}$, where $X_{\alpha}^e:=e\otimes h_{\alpha}$.

There exists a canonical decomposition

$$TS_H=T^vS_H\oplus\mathcal{D}_+\oplus\mathcal{D}_-$$

of the (holomorphic) tangent bundle into the vertical subbundle T^vS_H and two (holomorphic) distributions $\mathcal{D}_+$ and $\mathcal{D}_-$ spanned, respectively, by vector fields X_+^e and X_-^e associated with sections e of the bundle E^*. The vertical distribution T^vS_H is spanned by the vector fields $\partial_0,\partial_{++},\partial_{--}$, which correspond to the standard generators of the Lie algebra $\mathfrak{sp}(1,\mathbb{C})$.

Lemma 3: The vector fields $X_{\pm}^e\in\mathfrak{X}(S_H)$ satisfy the following commutation relations:

$$[\partial_0,X_{\pm}^e]=\pm X_{\pm}^e,\quad [\partial_{\pm\pm},X_{\pm}^e]=0,\quad [\partial_{\pm\pm},X_{\mp}^e]=X_{\pm}^e,$$

$$[X_+^e,X_-^{e'}]=X_-^{\nabla_{\pi_*X_+^e}e'}-X_+^{\nabla_{\pi_*X_-^{e'}}e}-\tilde{T}(\pi_*X_+^e,\pi_*X_-^{e'}),\tag{11}$$

$$[X^e_\pm, X^{e'}_\pm] = X^{\nabla_{\pi_* X^e_\pm} e'}_\pm - X^{\nabla_{\pi_* X^{e'}_\pm} e}_\pm - \tilde{T}(\pi_* X^e_\pm, \pi_* X^{e'}_\pm),$$

where T is the torsion of the Grassmann connection, $\tilde{T}(X,Y) := \widetilde{T(X,Y)}$ denotes the horizontal lift of the vector $T(X,Y)$ and we have used the abbreviation $\nabla_X e := \nabla^E_X e$.

Proof: The first three equations follow from $X^e_\pm = u^\alpha_\pm \widetilde{e \otimes h_\alpha}$ and the expression for the fundamental vector fields given in Lemma 2. To prove the last equation we first compute the Lie bracket of two vector fields $X = e \otimes h$ and $X' = e' \otimes h$ on M, where h is parallel:

$$[X,X'] = \nabla_X X' - \nabla_{X'} X - T(X,X') = (\nabla_X e' - \nabla_{X'} e) \otimes h - T(X,X'). \tag{12}$$

Using this we calculate the commutator

$$\begin{aligned}
[X^e_\pm,\ X^{e'}_\pm] &= u^\alpha_\pm u^\beta_\pm (\widetilde{\nabla_{X^e_\alpha} X^{e'}_\beta} - \widetilde{\nabla_{X^{e'}_\beta} X^e_\alpha} - \tilde{T}(X^e_\alpha, X^{e'}_\beta)) \\
&= (\nabla_{\pi_* X^e_\pm} e' \otimes h_\pm)^\sim - (\nabla_{\pi_* X^{e'}_\pm} e \otimes h_\pm)^\sim - u^\alpha_\pm u^\beta_\pm \tilde{T}(X^e_\alpha, X^{e'}_\beta) \\
&= X^{\nabla_{\pi_* X^e_\pm} e' - \nabla_{\pi_* X^{e'}_\pm} e}_\pm - \tilde{T}(\pi_* X^e_\pm, \pi_* X^{e'}_\pm).
\end{aligned}$$

The expression for $[X^e_+, X^{e'}_-]$ follows similarly. □

We shall use the abbreviation $T(X^e_\pm, X^{e'}_\pm) := \tilde{T}(\pi_* X^e_\pm, \pi_* X^{e'}_\pm)$.

Proposition 2: The following conditions are equivalent:

(i) *For any parallel section $h \in \Gamma(H^*)$ the distribution $E^* \otimes h$ on M is integrable.*
(ii) *The distribution $\mathcal{D}_+$ [associated to any parallel frame (h_1, h_2)] on S_H is integrable.*
(iii) *The distribution $\mathcal{D}_-$ on S_H is integrable.*
(iv) *The holomorphic Grassmann structure is admissible, i.e., it has admissible connection.*

Proof: The formula (12), where h is parallel, shows that the distribution $E^* \otimes h$ is integrable if and only if

$$T(E^* \otimes h, E^* \otimes h) \subset E^* \otimes h. \tag{13}$$

Using the decomposition (10), one can check that this condition is satisfied for all parallel sections h if and only if the connection is admissible. This proves the equivalence of (i) and (iv). Since $\pi_*(X^e_+|_{(h_+, h_-)}) = e \otimes h_+$, the last equation in (11) shows that the distribution $\mathcal{D}_+$ is integrable if and only if (13) holds for all h. Thus (i) is equivalent to (ii). The equivalence of (i) and (iii) is proved similarly. □

IV. CONSTRUCTION OF HALF-FLAT CONNECTIONS OVER HALF-FLAT GRASSMANN MANIFOLDS

A. Half-flat connections over half-flat Grassmann manifolds

In this section we describe the *harmonic space method*[10] for constructing half-flat connections ∇ (Definition 6 below) in a holomorphic vector bundle $\nu: W \to M$ over a complex manifold M with admissible half-flat holomorphic Grassmann structure. The basic ingredient of the construction is the lift of geometric data from M to S_H via $\pi: S_H \to M$. Let ∇ be a holomorphic connection in a holomorphic vector bundle $\nu: W \to M$. Its curvature

$$F(e \otimes h_\alpha, e' \otimes h_\beta) = \omega_H(h_\alpha, h_\beta) F^{(ee')} + F^{[ee']}_{\alpha\beta}, \tag{14}$$

where (h_1,h_2) is the fixed parallel local frame of H^* and e,e' are local sections of E^*. The curvature component $F^{(ee')}$ is symmetric in e,e' and $F^{[ee']}_{\alpha\beta}$ is skew in e,e' and symmetric in α,β. Lifting (14) to S_H we obtain the curvature of the pull-back connection $\pi^*\nabla$ in $\pi^*\nu:\pi^*W\to S_H$ with components, $F(v\,,\cdot\,)=0\,,\ \forall v\in T^vS_H$, together with

$$F(X^e_\pm\,,X^{e'}_\pm)=F^{[ee']}_{\pm\pm}:=u^\alpha_\pm u^\beta_\pm F^{[ee']}_{\alpha\beta}\,,$$

$$F(X^e_+\,,X^{e'}_-)=F^{(ee')}+F^{[ee']}_{+-}:=F^{(ee')}+u^\alpha_+u^\beta_-F^{[ee']}_{\alpha\beta}\,.$$

Definition 6: A holomorphic connection ∇ in a holomorphic vector bundle $\nu:W\to M$ over a complex manifold M with holomorphic Grassmann structure, $T^*M=E\otimes H$, is called **half-flat** *if its curvature F satisfies the equation*

$$F(e\otimes h_\alpha\,,e'\otimes h_\beta)=\omega_H(h_\alpha,h_\beta)F^{(ee')}\,, \tag{15}$$

where (h_1,h_2) is a parallel local frame of H^* and $F^{(ee')}$ is symmetric in the local sections e,e' of E^*.

Note that (15) is equivalent to (9). From this definition it follows that for any $h\in H^*$ we have $F(e\otimes h\,,e'\otimes h)=0\,.$

Definition 7: A connection in a holomorphic vector bundle $W\to S_H$ over harmonic space S_H is called **half-flat** *if its curvature F satisfies the equations*

$$\begin{aligned} F(X^e_+\,,X^{e'}_+)&=0,\\ F(X^e_+\,,X^{e'}_-)&=F^{(ee')},\\ F(X^e_-\,,X^{e'}_-)&=0,\\ F(v\,,\cdot\ \ )&=0,\quad \forall v\in T^vS_H, \end{aligned} \tag{16}$$

where $F^{(ee')}$ is symmetric in the local sections e,e' of E^*.

Definition 8: Let $\nu:W\to M$ be a holomorphic vector bundle and ∇ a connection in $\pi^*\nu:\pi^*W\to S_H$, where $\pi:S_H\to M$. A local frame of $\pi^*\nu$ defined on $\pi^{-1}(U)$, where U is an open subset of M, is called a **central frame** *with respect to ∇ if it is parallel along the fibers of the bundle $\pi:S_H\to M$.*

Remark: If $\chi=(\chi_1,\ldots,\chi_r)$ is a local frame of ν, then $\pi^*\chi$ will be a central frame with respect to the pull-back $\pi^*\nabla$ of any connection ∇ in ν. The connection one-form A of $\pi^*\nabla$ with respect to the frame $\pi^*\chi$ satisfies $A(v)=0\,,A(X^e_\pm)=u^\alpha_\pm A^e_\alpha$, where v is any vertical vector and $A^e_\alpha=A(\widetilde{X^e_\alpha})$ is a matrix-valued function on M. Conversely, any connection satisfying these conditions is the pull-back of the connection over M with potential $A(X^e_\alpha)=A^e_\alpha$.

Proposition 3: Let $\pi:S\to M$ be any fiber bundle with simply connected fibers over a simply connected manifold M. There is a natural one-to-one correspondence between gauge equivalence classes of connections ∇^M in the trivial bundle $\mathbb{C}^r\times M$ and gauge equivalence classes of connections ∇^S in $\mathbb{C}^r\times S$ satisfying the curvature constraint $F(v,\cdot\,)=0$ for all vertical vectors v.

Proof: It is clear that the pull-back $\nabla^S=\pi^*\nabla^M$ to S of a connection ∇^M defined over M satisfies the curvature constraint. To prove the converse, we will apply the following elementary lemma to the connection one-form A of a connection ∇ over $N=S$.

Lemma 4: Let $\pi:N\to M$ be a submersion with connected fibers and α a p-form on N. Then α is the pull-back $\pi^*\beta$ of a p-form β on M if and only if the inner products $\iota_v\alpha=\iota_v d\alpha=0$ for all vertical tangent vectors v.

Since the connection ∇^S is flat along the (simply connected) fibers of π there exists a central frame $\psi=(\psi_1,\ldots,\psi_r)$ for ∇^S. Let A be the connection one-form of ∇^S with respect to this central

frame. We then have $A(v)=0$ for any vertical vector v and the curvature condition $F(v,\cdot)=0$ implies $dA(v,\cdot)=0$. Now the above lemma shows that A is the pull-back of a one-form B on M, which defines a connection ∇^M in the trivial bundle $\mathbb{C}^r\times M$. Since any two central frames differ by a gauge transformation which is a matrix-valued function on M the connection ∇^M is well defined up to a gauge transformation. The pull-back $\pi^*\nabla^M$ is gauge equivalent to ∇^S since it has the same expression with respect to the standard frame of $\mathbb{C}^r\times S$ (which is the pull-back of the standard frame of $\mathbb{C}^r\times M$) as ∇^S with respect to the central frame ψ. It is clear that the pull-backs of gauge equivalent connections over M are gauge equivalent connections over S. Applying a gauge transformation to a connection ∇^S which has connection one-form A with respect to a central frame ψ we get a new connection $(\nabla^S)'$, which has the same connection form A with respect to the transformed frame ψ'. The frame ψ' is therefore central with respect to $(\nabla^S)'$ and the two connections ∇^S and $(\nabla^S)'$ define the same gauge equivalence class of connections over M. □

Proposition 4: Let $\nu: W=\mathbb{C}^r\times M\to M$ be a trivial vector bundle over a complex manifold M with admissible half-flat holomorphic Grassmann structure and $\pi^*\nu:\pi^*W=\mathbb{C}^r\times S_H\to S_H$ its pull-back to S_H. Then any half-flat connection over S_H is gauge equivalent to the pull-back of a half-flat connection over M.

Proof: It is clear that the pull-back of a half-flat connection is half-flat. To prove the converse, we apply Proposition 3, by which a half-flat connection ∇^S over S_H is gauge equivalent to a pull-back connection $\pi^*\nabla^M$, which is necessarily half-flat. This implies that ∇^M is half-flat. In fact, if the connection ∇^M were not half-flat, then it would have a nontrivial curvature component $F^{[ee']}_{\alpha\beta}$ which would imply that its pull-back $\pi^*\nabla^M$ has, for instance, a nonzero curvature component $F^{[ee']}_{++}$. But this is impossible since $\pi^*\nabla^M$ is half-flat. □

Corollary 1: The connection one-form A of a half-flat connection over S_H with respect to a central frame ψ has the form

$$A(v)=0,\quad A(X^e_\pm)=u^\alpha_\pm A^e_\alpha,$$

where v is any vertical vector and $A^e_\alpha=A(\widetilde{X^e_\alpha})$ is a matrix-valued function on M.

Remark: This shows that the half-flat connection is completely determined by the potential in the $\mathcal{D}_+$-direction, $A(X^e_+)=u^\alpha_+A^e_\alpha$, with respect to a central frame.

Proof: This follows from Proposition 4 and the remark following Definition 8. □

B. The construction

In this section we construct half-flat connections in a bundle $\nu: W\to M$ over a manifold M with a half-flat admissible Grassmann structure. First we define the weaker notion of an almost half-flat connection over S_H and show how to construct all such connections from appropriate prepotentials. Then we show that any almost half-flat connection over S_H may be used to construct a half-flat connection on M. Since our construction is local in M, we shall assume that the bundles π, ν and $\pi^*\nu$ are trivial, i.e., $\pi: M\times \mathrm{Sp}(1,\mathbb{C})\to M$, $\nu: M\times\mathbb{C}^r\to M$ and $\pi^*\nu: S_H\times\mathbb{C}^r\to S_H$.

1. Construction of almost half-flat connections

The restriction of a half-flat connection to a leaf of the integrable distribution $\langle\mathcal{D}_+,\partial_0\rangle$ is clearly flat.

Definition 9: A frame $\varphi_1,\ldots,\varphi_r$ in the holomorphic vector bundle $\pi^*\nu:\mathbb{C}^r\times S_H$ which is parallel along leaves of the integrable distribution $\langle\mathcal{D}_+,\partial_0\rangle$ is called an **analytic frame**.

With respect to an analytic frame a connection in the vector bundle $\pi^*\nu$ has components

$$\nabla^S_{\partial_0}=\partial_0,$$

$$\nabla^S_{X^e_+}=X^e_+,$$

$$\nabla^S_{\partial_{++}}=\partial_{++}+A_{++}\ :=\partial_{++}+A(\partial_{++}),$$

$$\nabla^S_{\partial_{--}} = \partial_{--} + A_{--} \;:= \partial_{--} + A(\partial_{--}),$$

$$\nabla^S_{X^e_-} = X^e_- + A(X^e_-).$$

Definition 10: A connection ∇^S *over* S_H *is called* **almost half-flat** *if its curvature satisfies the following equations:*

$$\begin{gathered} F(X^e_+, X^{e'}_+) = F(X^e_+, v) = 0, \quad \forall v \in T^v S_H, \\ F(\partial_{++}, \cdot\,) = F(\partial_0, \cdot\,) = 0\,. \end{gathered} \tag{17}$$

In fact, these equations are not independent; for instance the Bianchi identity with arguments $(X_+, \partial_{++}, \partial_{--})$ together with $F(\partial_{++}, \partial_{--}) = F(\partial_{\pm\pm}, X^e_+) = 0$ implies the equation $F(\partial_{++}, X^e_-) = 0$.

Proposition 5: Any almost half-flat connection satisfies the following equation:

$$F(X^e_+, X^{e'}_-) = F(X^{e'}_+, X^e_-).$$

Proof: Using the integrability of $\mathcal{D}_+$ and $F(X^e_+, X^{e'}_+) = F(\partial_{--}, X^e_+) = 0$, we obtain

$$\begin{aligned} 0 &= [\nabla^S_{\partial_{--}}, F(X^e_+, X^{e'}_+)] \\ &= [\nabla^S_{\partial_{--}}, [\nabla^S_{X^e_+}, \nabla^S_{X^{e'}_+}]] - [\nabla^S_{\partial_{--}}, \nabla^S_{[X^e_+, X^{e'}_+]}] \\ &= [\nabla^S_{X^e_-}, \nabla^S_{X^{e'}_+}] + [\nabla^S_{X^e_+}, \nabla^S_{X^{e'}_-}] - \nabla^S_{[X^e_-, X^{e'}_+]} - \nabla^S_{[X^e_+, X^{e'}_-]} \\ &= F(X^e_-, X^{e'}_+) - F(X^{e'}_-, X^e_+)\,. \end{aligned}$$

□

It follows that an almost half-flat connection is a generalization of a half-flat connection, satisfying only those equations in (16), that involve curvatures with $\partial_0, \partial_{++}$ or X^e_+ in one of the arguments.

Proposition 6: An almost half-flat connection is half-flat if and only if it satisfies $F(\partial_{--}, X^e_-) = 0$.

Proof: By Proposition 5 an almost half-flat connection is required to satisfy all the half-flatness equations (16) with the exception of

$$F(\partial_{--}, X^e_-) = 0 \quad \text{and} \quad F(X^e_-, X^{e'}_-) = 0. \tag{18}$$

The second equation here follows from the first by virtue of the Bianchi identity with arguments $(X^e_+, X^{e'}_-, \partial_{--})$. □

The following proposition shows that an almost half-flat connection is completely determined by the potentials A_{++} and A_{--} with respect to an analytic frame.

Proposition 7: Let ∇^S *be an almost half-flat connection in the vector bundle* $\pi^*\nu: \mathbb{C}^r \times S_H \to S_H$ *with potentials* A_{++}, A_{--} *and* $A(X^e_-)$ *in an analytic frame. Then we have following.*

(*i*) *The potential* A_{++} *is analytic and has charge* $+2$, *i.e.,*

$$X^e_+ A_{++} = 0, \quad \partial_0 A_{++} = 2A_{++}\,. \tag{19}$$

(*ii*) *The potential* A_{--} *satisfies*

$$\partial_{++} A_{--} - \partial_{--} A_{++} + [A_{++}, A_{--}] = 0, \quad \partial_0 A_{--} = -2A_{--}\,. \tag{20}$$

(*iii*) *The potential* $A(X^e_-)$ *is determined by* A_{--} *and has charge* -1:

$$A(X^e_-)=-X^e_+A_{--}, \quad \partial_0 A(X^e_-)=-A(X^e_-)\ . \tag{21}$$

Conversely, any matrix-valued potentials A_{++}, A_{--} *and* $A(X^e_-)$ *satisfying* (19)–(21) *define an almost half-flat connection.*

Proof: (i) The curvature constraints $F(X^e_+,\partial_{++})=0$, $F(\partial_0,\partial_{++})=0$, in an analytic frame, take the form (19).

(ii) The further almost half-flatness conditions, $F(\partial_{++},\partial_{--})=F(\partial_0,\partial_{--})=0$, give Eqs. (20) for the potential A_{--}.

(iii) Having obtained A_{--}, we can find $A(X^e_-)$ from the equations $F(X^e_+,\partial_{--})=F(\partial_0,X^e_-)=0$, which take the form

$$X^e_+A_{--}=A([X^e_+,\partial_{--}])=-A(X^e_-), \quad \partial_0 A(X^e_-)=-A(X^e_-)\ . \tag{22}$$

The second equation follows from the first. □

We can now write an algorithm for the construction of all almost half-flat connections:

Theorem 4: *Let* A_{++} *be an analytic prepotential, i.e., a matrix-valued function on a domain* $U=\pi^{-1}(V)\subset S_H$, *where* $V\subset M$ *is a simply connected domain, satisfying (19). Let* Φ *be an invertible matrix-valued function on* U *which satisfies the equations*

$$\partial_{++}\Phi=-A_{++}\Phi, \quad \partial_0\Phi=0\ . \tag{23}$$

It always exists. The pair (A_{++},Φ) *determines an almost half-flat connection* $\nabla^S=\nabla^{(A_{++},\Phi)}$. *Its potentials with respect to an analytic frame are given by* A_{++}, $A_{--}=-(\partial_{--}\Phi)\Phi^{-1}$ *and* $A(X^e_-)=-X^e_+A_{--}$. *Conversely, any almost half-flat connection is of this form.*

Proof: We consider the connection defined by A_{++} and $A(\partial_0)=0$ along an orbit sB of the Borel subgroup of $\mathrm{SL}(2,\mathbb{C})$,

$$B=\left\{\begin{pmatrix} t_0 & t_1 \\ 0 & t_0^{-1}\end{pmatrix}\ \middle|\ t_0\in\mathbb{C}^*,\ t_1\in\mathbb{C}\right\}\cong\mathbb{C}^*\times\mathbb{C} \quad \text{(diffeomorphic)}.$$

It is flat since the second equation of (19) is equivalent to $F(\partial_0,\partial_{++})=0$ (vanishing of the curvature along sB). Moreover, it has trivial holonomy since the fundamental group of $B\cong\mathbb{C}^*\times\mathbb{C}$ coincides with the fundamental group of the $\mathbb{C}^*$-factor and the potential is zero in the direction of ∂_0 which is tangent to $\mathbb{C}^*$. An invertible solution to the system (23) exists and defines a parallel frame Φ with respect to the flat connection with trivial holonomy defined along each orbit of the Borel group. Since the space of Borel orbits in U is diffeomorphic to $V\times\mathbb{C}P^1$ and is therefore simply connected, a solution Φ exists on the domain U. Now, given any such solution of (23), we define $A_{--}:=-(\partial_{--}\Phi)\Phi^{-1}$. This solves (20), since $F(\partial_{\pm\pm},\partial_0)=F(\partial_{++},\partial_{--})=0$ is the integrability condition for the system $\partial_{\pm\pm}\Phi=-A_{\pm\pm}\Phi$, $\partial_0\Phi=0$. Finally, we define $A(X^e_-):=-X^e_+A_{--}$, obtaining an almost half-flat connection by Proposition 7. Now the converse statement follows also from Proposition 7. □

2. Transformation to the central frame

Since an almost half-flat connection $\nabla=\nabla^S$ is flat in vertical directions, it admits a central frame ψ. The following lemma shows that the solution Φ of Eq. (23) gives a gauge transformation from an analytic frame φ to a central frame $\psi=\varphi\Phi$ for the almost half-flat connection $\nabla^{(A_{++},\Phi)}$.

Lemma 5: Let $\nabla=\nabla^{(A_{++},\Phi)}$ *be the almost half-flat connection associated to the analytic prepotential* A_{++} *with respect to the analytic frame* φ *and an invertible solution* Φ *of (23). Then the frame* $\psi:=\varphi\Phi$ *is a central frame for the connection* ∇, *i.e., the potentials* $C(\partial_{\pm\pm})$ *and* $C(\partial_0)$ *with respect to that frame vanish.*

Proof: The result follows from the pure gauge form of $A(\partial_{\pm\pm})$ and $A(\partial_0)$ and the transformation law (3) for potentials. □

With respect to the central frame ψ, the almost half-flat connection constructed above takes the form

$$\nabla^S_{X^e_+} = X^e_+ + C(X^e_+) = X^e_+ + \Phi^{-1} X^e_+ \Phi,$$

$$\nabla^S_{X^e_-} = X^e_- + C(X^e_-) = X^e_- + \Phi^{-1} X^e_- \Phi + \Phi^{-1} X^e_+ (\partial_{--}\Phi\Phi^{-1})\Phi,$$

$$\nabla^S_{\partial_{++}} = \partial_{++}, \quad \nabla^S_{\partial_{--}} = \partial_{--}, \quad \nabla^S_{\partial_0} = \partial_0.$$

Moreover, the equations $F(\partial_{++}, X^e_+) = F(\partial_0, X^e_+) = 0$ imply that the potential $C(X^e_+)$ satisfies the equations

$$\partial_{++} C(X^e_+) = 0, \quad \partial_0 C(X^e_+) = C(X^e_+). \tag{24}$$

3. Construction of half-flat connections

We assume now that the analytic prepotential A_{++} is defined globally along the fibers of $\pi: S_H \to M$. Then, restricting M to an appropriate domain, we may assume that A_{++} is defined globally on S_H. The previous construction then provides an almost half-flat connection over S_H. Using this connection, we may construct a half-flat connection on M. The crucial point is the following:

Proposition 8: The potential $C(X^e_+)$ of an almost half-flat connection ∇ with respect to a central frame is linear in u^α_+, namely,

$$C(X^e_+) = u^\alpha_+ C(\widetilde{X^e_\alpha}) =: u^\alpha_+ C^e_\alpha, \tag{25}$$

where $(x^i, u^\alpha_\pm)$ are the local coordinates associated with the trivialization $S_H = M \times \mathrm{Sp}(1,\mathbb{C})$ and $C^e_\alpha = C^e_\alpha(x^i)$ is a matrix-valued function on M.

Proof: Due to Eqs. (24), the result follows from Lemma 6.

Lemma 6: (i) If a holomorphic function f_+, defined on some domain

$$U \subset \{u^2_+ \neq 0\} \subset \mathrm{Sp}(1,\mathbb{C}) = \left\{ \mathcal{U} = \begin{pmatrix} u^1_+ & u^1_- \\ u^2_+ & u^2_- \end{pmatrix}; \det \mathcal{U} = 1 \right\},$$

satisfies

$$\partial_{++} f_+ = 0, \quad \partial_0 f_+ = f_+, \tag{26}$$

then $f_+ = u^\alpha_+ f_\alpha(u^1_+/u^2_+)$. Here $f_\alpha(u^1_+/u^2_+)$ are holomorphic functions on U invariant under the right action of the Lie algebra of upper-triangular matrices.

(ii) Moreover, if the function f_+ is globally defined, then it is linear in u^α_+, i.e., $f_+ = u^\alpha_+ f_\alpha, f_\alpha = const$.

Proof: (i) One can immediately check that $f_+ = u^\alpha_+ f_\alpha(u^1_+/u^2_+)$ is a solution of (26). We note that the quotient of any two solutions of (26) is a solution of the corresponding homogeneous system,

$$\partial_{++} f = 0, \quad \partial_0 f = 0. \tag{27}$$

It is sufficient to check that any solution of (27) is a function of u^1_+/u^2_+. To prove this we use the local factorization of $\mathrm{Sp}(1,\mathbb{C})$ into the product of a Borel subgroup $\mathcal{B}$ and a nilpotent subgroup as follows:

$$\begin{pmatrix} u_+^1 & u_-^1 \\ u_+^2 & u_-^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ c^{-1} & 1 \end{pmatrix} \begin{pmatrix} a & b \\ 0 & a^{-1} \end{pmatrix}, \quad \mathcal{B} = \left\{ \begin{pmatrix} a & b \\ 0 & a^{-1} \end{pmatrix} \right\}.$$

Then $c = u_+^1/u_+^2$ and $\partial_0, \partial_{++}$ are generators of the right action of $\mathcal{B}$. This implies that the solutions of (27) are precisely the local functions on $\mathrm{Sp}(1,\mathbb{C})$ invariant under the right action of $\mathcal{B}$. In terms of the local coordinate system (a,b,c) on $\mathrm{Sp}(1,\mathbb{C})$ such functions are functions of $c = u_+^1/u_+^2$ alone.

(ii) The restriction $V|_{\mathrm{Sp}(1)}$ to $\mathrm{Sp}(1)$ of any irreducible $\mathrm{Sp}(1,\mathbb{C})$-module V of holomorphic functions is a (finite dimensional) irreducible $\mathrm{Sp}(1)$-module of smooth functions on $\mathrm{Sp}(1)$. The condition (26) shows that f_+ is a highest weight vector with weight $+1$. Hence f_+ generates a two-dimensional submodule $\langle f_+ \rangle = \mathrm{span}\{f_+, f_- := \partial_{--} f_+\}$ of holomorphic functions. It remains to show that any two-dimensional module of holomorphic functions on $\mathrm{Sp}(1,\mathbb{C})$ is spanned by linear functions. We know two such modules, generated by the highest weight vectors u_+^1 and u_+^2 respectively. On the other hand, by the Peter–Weyl theorem the multiplicity of the two-dimensional irreducible representation of $\mathrm{Sp}(1)$ in $L^2(\mathrm{Sp}(1))$ is 2. □

Using Proposition 8, with respect to a central frame, we can write $\nabla_{X_+^e} = X_+^e + u_+^\alpha C_\alpha^e$ where the coefficients $C_\alpha^e = C_\alpha^e(x^i)$ are matrix valued functions of coordinates x^i on M. Using them we define a new connection in the trivial bundle $\mathbb{C}^r \times S_H$ over S_H by

$$\hat{\nabla}_{X_\pm^e} = X_\pm^e + u_\pm^\alpha C_\alpha^e,$$

$$\hat{\nabla}_{\partial_{\pm\pm}} = \partial_{\pm\pm}, \quad \hat{\nabla}_{\partial_0} = \partial_0.$$

Our main result now follows:

Theorem 5: *Let M be a complex manifold with a half-flat admissible Grassmann structure. Let A_{++} be an analytic prepotential, i.e., a solution of (19), and Φ an invertible solution of (23). Then the connection $\hat{\nabla} = \hat{\nabla}^{(A_{++},\Phi)}$ constructed from the data (A_{++},Φ) is a half-flat connection in the trivial vector bundle $\mathbb{C}^r \times S_H \to S_H$ and it is the pull-back of the following half-flat connection ∇^M in the bundle $\mathbb{C}^r \times M \to M$:*

$$\nabla^M_{X_\alpha^e} = X_\alpha^e + C_\alpha^e. \tag{28}$$

Conversely, any half-flat connection over S (or M) is gauge equivalent to one obtained from the above construction.

Proof: The remark after Definition 8 shows that the connection $\hat{\nabla}$ is the pull-back of the connection ∇^M. It suffices now to show that ∇^M is half-flat. Note that the connections ∇ and $\hat{\nabla}$ coincide in the direction of X_+^e. Hence, using $C_+^e := u_+^\alpha C_\alpha^e$, we have

$$\begin{aligned} 0 = F^\nabla(X_+^e, X_+^{e'}) = F^{\hat{\nabla}}(X_+^e, X_+^{e'}) &= X_+^e C_+^{e'} - X_+^{e'} C_+^e + [C_+^e, C_+^{e'}] - C([X_+^e, X_+^{e'}]) \\ &= u_+^\alpha u_+^\beta (X_\alpha^e C_\beta^{e'} - X_\beta^{e'} C_\alpha^e + [C_\alpha^e, C_\beta^{e'}] - C([X_\alpha^e, X_\beta^{e'}])) \\ &= u_+^\alpha u_+^\beta F^{\nabla^M}(X_\alpha^e, X_\beta^{e'}), \end{aligned}$$

since $X_+^e u_+^\beta = 0$. This shows that the curvature $F^{\nabla^M}(X_\alpha^e, X_\beta^{e'})$ is skew-symmetric in α,β, i.e., it belongs to $\Lambda^2 H \otimes S^2 E \otimes \mathrm{End}\, W$. In other words, the connection ∇^M is half-flat.

Conversely, let ∇^S be a half-flat connection over S_H. By Proposition 4 we may assume that it is a pull-back of a half-flat connection ∇^M over M. Since the restriction of ∇^S to the leaves of $\langle \mathcal{D}_+, \partial_0 \rangle$ is flat, there exists an analytic frame [i.e., a frame such that $A(X_+^e) = A(\partial_0) = 0$, in which the potential $A(\partial_{++})$ satisfies the equations (19)]. Since ∇^S is flat along the (simply-connected) fibers, there exists an invertible solution Φ to the system

$$\partial_{++}\Phi + A_{++}\Phi = \partial_{--}\Phi + A_{--}\Phi = \partial_0\Phi = 0.$$

This shows that ∇^S is gauge-equivalent to the almost half-flat connection $\nabla^{(A_{++},\Phi)} = \hat{\nabla}^{(A_{++},\Phi)}$. □

C. Application to hyper-Kähler manifolds with admissible torsion

The above construction can be applied to the complexification of hyper-Kähler manifolds. Recall that any hyper-Kähler manifold admits a (locally defined) Grassmann structure $T^{*\mathbb{C}}M = E \otimes H$, such that the Levi–Civita connection on the cotangent bundle $\nabla = \nabla^E \otimes \mathrm{Id} + \mathrm{Id} \otimes \nabla^H$ is half-flat, i.e., the connection ∇^H is flat. Since the hyper-Kähler metric is Ricci flat, hence analytic, we may, using analytic continuation, extend the manifold M to a complex manifold $M^{\mathbb{C}}$ with holomorphic extension of the hyper-Kähler structure, in particular, we have a holomorphic Ricci flat metric on $M^{\mathbb{C}}$ with holonomy in $\mathrm{Sp}(n,\mathbb{C})$ and half-flat Grassmann structure. This Grassmann structure is admissible since the Levi–Civita connection on $M^{\mathbb{C}}$ has no torsion. Hence we can apply the harmonic space method to construct half-flat connections on holomorphic vector bundles $W \to M^{\mathbb{C}}$. The complex version of Proposition 1 shows that such connections are Yang–Mills connections. More generally, the method of construction of half-flat connections extends to real analytic (possibly indefinite) hyper-Kähler manifolds with admissible torsion, i.e., with torsion which has zero component in $S^3H \otimes E^* \otimes \Lambda^2 E$. A **hyper-Kähler manifold with admissible torsion** is defined as a pseudo-Riemannian manifold (M,g) with a linear metric connection ∇ with holonomy in $\mathrm{Sp}(k,l)$ which has admissible torsion. As in the (torsion-free) hyper-Kähler case there exists a parallel four-form given by $\Omega = \Sigma_\alpha \omega_\alpha \wedge \omega_\alpha$, $\omega_\alpha := g(J_\alpha \cdot, \cdot)$, and half-flat connections are characterized as connections with curvature in $V_{\lambda_1} \otimes \mathrm{End}\, W$, where V_{λ_1} is the λ_1-eigenspace of the endomorphism B_Ω associated to Ω. If the form Ω is co-closed, then any half-flat connection will be (Ω,λ_1)-self-dual and thus a Yang–Mills connection. We remark that co-closedness of Ω is equivalent to a linear $\mathrm{Sp}(k,l)$-invariant condition on the torsion.

V. GENERALIZATION TO HIGHER-SPIN GRASSMANN MANIFOLDS

A. Higher-spin Grassmann structures

The construction discussed in the previous section is in fact the $m=1$ specialization of a more general construction of connections on *spin* $m/2$ *Grassmann manifolds*, which we discuss in this section. These manifolds were considered in Ref. 14.

Definition 11: A **spin** $m/2$ **Grassmann structure** *on a (complex) manifold M is a holomorphic Grassmann structure of the form $T^*M \cong E \otimes F = E \otimes S^m H$, with a holomorphic Grassmann connection $\nabla = \nabla^E \otimes \mathrm{Id} + \mathrm{Id} \otimes \nabla^F$, where H is a rank 2 holomorphic vector bundle over M with holomorphic symplectic connection ∇^H and symplectic form $\omega_H \in \Gamma(\Lambda^2 H)$, and ∇^F is the connection in $F = S^m H$ induced by ∇^H. M is called* **half-flat** *if the connection ∇^F is flat.*

The bundle $S^m H$ is associated with the spin $m/2$ representation of the group $\mathrm{Sp}(1,\mathbb{C})$. Any frame (h_1,h_2) for H^* defines a frame for $S^m H^*$ $(h_A := h_{\alpha_1} h_{\alpha_2} \cdots h_{\alpha_m})$, where the multi-index $A := \alpha_1 \alpha_2 \cdots \alpha_m$, $\alpha_i = 1,2$. The ∇^H-parallel symplectic form ω_H on H^* induces a bilinear form ω_H^m on $F^* = S^m H^*$ given by

$$\omega_H^m(h_A,h_B) := \mathop{\mathfrak{S}}_A \mathop{\mathfrak{S}}_B \ \omega_H(h_{\alpha_1},h_{\beta_1})\omega_H(h_{\alpha_2},h_{\beta_2}) \cdots \omega_H(h_{\alpha_m},h_{\beta_m}),$$

where $\mathfrak{S}_A$ denotes the sum over all permutations of the α's. This form is skew-symmetric if m is odd and symmetric if m is even. To any section $e \in \Gamma(E^*)$ and multi-index A we associate the vector field $X_A^e := e \otimes h_A$ on M.

The construction of half-flat connections described in Sec. IV B may be adapted to obtain certain ''partially flat'' connections in vector bundles $W \to M$, provided that the torsion of ∇ obeys certain admissibility conditions.

Definition 12: Let (M,∇) be a half-flat spin $m/2$ Grassmann manifold. For any section $e \in \Gamma(E^*)$ we define vector fields

$$X^e_{(m-2i)+} := u_-^{\alpha_1}\cdots u_-^{\alpha_i} u_+^{\alpha_{i+1}}\cdots u_+^{\alpha_m} X^e_A \quad \text{if} \quad m-2i \geqslant 0,$$

$$X^e_{(2i-m)-} := u_-^{\alpha_1}\cdots u_-^{\alpha_i} u_+^{\alpha_{i+1}}\cdots u_+^{\alpha_m} X^e_A \quad \text{if} \quad m-2i < 0,$$

on the principal bundle S_H of symplectic frames in H. The distribution spanned by these vector fields is denoted by $\mathcal{D}_{k+} := \langle X^E_{k+} \rangle$ for $k \geqslant 0$, $k \equiv m \bmod 2$ and $\mathcal{D}_{k-} := \langle X^E_{k-} \rangle$ for $k > 0$, $k \equiv m \bmod 2$. We define also

$$\mathcal{D}^k_{(\pm)} := \bigoplus_{i=0}^{k} \mathcal{D}_{(m-2i)\pm}.$$

The Grassmann connection ∇ is called **k-admissible** *if it preserves the distribution $\mathcal{D}^k_{(\pm)}$, i.e.,*

$$T(\mathcal{D}^k_{(\pm)}, \mathcal{D}^k_{(\pm)}) \subset \mathcal{D}^k_{(\pm)}. \tag{29}$$

The Grassmann manifold (M,∇) is called **k-admissible** *if the connection ∇ is k-admissible.*

For small m we shall write X^e_0, X^e_+, X^e_-, X^e_{++}, etc. instead of X^e_{0+}, X^e_{1+}, X^e_{1-}, X^e_{2+}, etc.

Proposition 9: Let (M,∇) be a half-flat spin $m/2$ Grassmann manifold. Then the distribution $\mathcal{D}^k_{(\pm)}$ is integrable if and only if the torsion of the Grassmann connection ∇ satisfies Eq. (29).

The proof is similar to that of Proposition 2.

B. Partially flat connections over higher-spin Grassmann manifolds

Let (M,∇) be a half-flat spin $m/2$ Grassmann manifold and $\nu: W \to M$ a holomorphic vector bundle. Since our constructions are local we will assume that W is trivial. In the higher spin ($m > 1$) case, there exists, as a natural generalization of the notion of a half-flat connection, the more refined notion of a k-partially flat connection in ν. The space of two-forms $\Lambda^2 T^*M$ has the following decomposition into $GL(E) \otimes \mathrm{Sp}(1,\mathbb{C})$-submodules:

$$\Lambda^2 T^*M = \Lambda^2(E \otimes S^m H) = \Lambda^2 E \otimes S^2 S^m H \oplus S^2 E \otimes \Lambda^2 S^m H,$$

where

$$S^2 S^m H = S^{2m} H \oplus \omega_H^2 S^{2m-4} H \oplus \cdots \oplus \omega_H^{2[m/2]} S^{2m-4[m/2]} H,$$

$$\Lambda^2 S^m H = \omega_H S^{2m-2} H \oplus \omega_H^3 S^{2m-6} H \oplus \cdots \oplus \omega_H^{2[m/2]+1} S^{2m-4[m/2]-2} H.$$

Here we use the convention that $S^l H = 0$ if $l < 0$.

Let ∇ be a connection in the vector bundle $W \to M$. Its curvature has the following decomposition, corresponding to the above decomposition of $\Lambda^2 T^*M$ into irreducible $GL(E) \cdot \mathrm{Sp}(1,\mathbb{C})$-submodules:

$$F(X^e_A, X^{e'}_B) = \mathfrak{S}_A \mathfrak{S}_B \sum_{k=0}^{[m/2]} (\omega_H(h_{\alpha_1}, h_{\beta_1}) \cdots \omega_H(h_{\alpha_{2k}}, h_{\beta_{2k}}) \overset{(2k)}{F}{}^{[ee']}_{\alpha_{2k+1}\cdots\alpha_m\beta_{2k+1}\cdots\beta_m}$$

$$+ \omega_H(h_{\alpha_1}, h_{\beta_1}) \cdots \omega_H(h_{\alpha_{2k+1}}, h_{\beta_{2k+1}}) \overset{(2k+1)}{F}{}^{(ee')}_{\alpha_{2k+2}\cdots\alpha_m\beta_{2k+2}\cdots\beta_m}), \tag{30}$$

where the tensors $F^{(2k)} \in \Gamma(\Lambda^2 E \otimes S^{2m-4k} H)$ and $F^{(2k+1)} \in \Gamma(S^2 E \otimes S^{2m-4k-2} H)$.

We note that half-flat connections are those which satisfy the conditions

$$\overset{(2i)}{F} = 0, \quad \text{for all } i \in \mathbb{N}. \tag{31}$$

For $m>1$ these conditions are not suitable for application of the harmonic space method. However, the following more refined restrictions on the curvature are amenable to the method (cf. Ref. 15).

Definition 13: A connection ∇ *in the vector bundle* $\nu: W\to M$ *is called* **k-partially flat** *if* $F^{(i)}=0$ *for all* $i\leqslant 2k$. *Here* $0\leqslant k\leqslant[(m+2)/2]$.

Clearly, $[(m+2)/2]$-partially flat connections are simply flat connections. We note that for $m=1$, zero-partially flat connections are precisely half-flat connections. For general odd $m=2p+1$, zero-partially flat connections in a vector bundle ν over flat spaces with spin $m/2$ Grassmann structure were considered by Ward.[3] He chose E to be a rank 2 flat bundle and showed that zero-partially flat connections, for $m>1$, do not correspond to Yang–Mills connections. Therefore, in our more general setting, we clearly cannot expect zero-partially flat connections to satisfy the Yang–Mills equations for $m>1$. On the other hand, the penultimate case, $k=[m/2]$, is particularly interesting for odd m:

Theorem 6: *Let* M *be a half-flat spin* $m/2$ *Grassmann manifold* M. *If* m *is odd and the vector bundle* $E^*\to M$ *admits a* ∇^E*-parallel symplectic form* ω_E, *then* M *has canonical* $\mathrm{Sp}(E)\cdot\mathrm{Sp}(H)$*-invariant metric* $g=\omega_E\otimes\omega_H^m$ *and four-form* $\Omega\neq 0$. *If* Ω *is co-closed with respect to the metric* g, *then any* $(m-1)/2$*-partially flat connection* ∇ *in a vector bundle* W *over* M *is* (Ω,λ)*-self-dual and hence it is a Yang–Mills connection.*

Proof: To describe Ω we use the following notation: e_a is a basis of E^*, h_α is a basis of H^*, h_A is the corresponding basis of S^mH^* and $X_{aA}:=e_a\otimes h_A$ is the corresponding basis of $TM=E^*\otimes S^mH^*$. With respect to these bases, the skew symmetric forms ω_E, ω_H and ω_H^m are represented by the matrices ω_{ab}, $\omega_{\alpha\beta}$ and ω_{AB}, respectively. We define Ω by

$$\Omega:=\sum\ \omega_{ab}\,\omega_{cd}\,\omega_{AC}\,\omega_{BD}\,X^{aA}\wedge X^{bB}\wedge X^{cC}\wedge X^{dD},$$

where X^{aA} is the basis dual to X_{aA}. This form is obviously $\mathrm{Sp}(E)\cdot\mathrm{Sp}(H)$-invariant since we used only ω_E and ω_H in the definition. One can easily check that $\Omega\neq 0$. The connection ∇ is $(m-1)/2$-partially flat if and only if its curvature F belongs to the space

$$S^2E\otimes\omega_H^m\otimes\mathrm{End}\ W\subset\ S^2E\otimes\Lambda^2S^mH\otimes\mathrm{End}\ W\subset\ \Lambda^2(E\otimes S^mH)\otimes\mathrm{End}\ W.$$

Here we use the decomposition

$$\Lambda^2S^mH=\omega_HS^{2m-2}H\oplus\omega_H^3S^{2m-6}H\oplus\cdots\oplus\mathbb{C}\omega_H^m.$$

The $\mathrm{Sp}(E)\cdot\mathrm{Sp}(H)$-submodule $S^2E\otimes\omega_H^m\subset\Lambda^2T^*M$ is irreducible. Therefore it is contained in an eigenspace V_λ of the $\mathrm{Sp}(E)\cdot\mathrm{Sp}(H)$-invariant operator $B_\Omega:\Lambda^2T^*M\to\wedge^2T^*M$. It remains to check that $\lambda\neq 0$. By Lemma 1 it suffices to compute the contraction $K=K_{cCdD}X^{cC}X^{dD}$ of a tensor $S=S_{ab}\omega_{AB}e^ae^b\otimes h^Ah^B$ in $S^2E\otimes\omega_H^m$ with Ω:

$$\begin{aligned}-K_{cCdD}=S^{ab}\omega^{AB}(&\omega_{ab}\omega_{cd}\omega_{AC}\omega_{BD}+\omega_{ac}\omega_{db}\omega_{AD}\omega_{CB}+\omega_{ad}\omega_{bc}\omega_{AB}\omega_{DC}-\omega_{ba}\omega_{cd}\omega_{BC}\omega_{AD}\\&-\omega_{bc}\omega_{da}\omega_{BD}\omega_{CA}-\omega_{bd}\omega_{ac}\omega_{BA}\omega_{DC}-\omega_{ca}\omega_{bd}\omega_{CB}\omega_{AD}-\omega_{cb}\omega_{da}\omega_{CD}\omega_{BA}\\&-\omega_{cd}\omega_{ab}\omega_{CA}\omega_{DB}+\omega_{da}\omega_{bc}\omega_{DB}\omega_{AC}+\omega_{db}\omega_{ca}\omega_{DC}\omega_{BA}+\omega_{dc}\omega_{ab}\omega_{DA}\omega_{CB})\\=4(m+1)&S_{cd}\omega_{CD}.\end{aligned}$$

Here ω^{ab} and ω^{AB} denote the inverses of ω_{ab} and ω_{AB} and $S^{ab}=\omega^{aa'}\omega^{bb'}S_{a'b'}$. We have used that $S^{ab}\omega^{AB}$ is skew-symmetric under interchange of aA with bB and that $\omega^{AB}\omega_{AB}=-(m+1)$. The above calculation shows that $\lambda=-4(m+1)\neq 0$ and hence any $(m-1)/2$-partially flat connection is (Ω,λ)-self-dual and is a Yang–Mills connection by Theorem 1. □

The analogous result does not hold if m is even.

Proposition 10: If m is even and the vector bundle $E^*\to M$ admits a ∇^E-parallel metric γ_E, then M has canonical $\mathrm{SO}(E)\cdot\mathrm{Sp}(H)$-invariant metric $g=\gamma_E\otimes\omega_H^m$ and four-form $\Omega\neq 0$.

Proof: Analogously to the case of m odd, we can define Ω by

$$\Omega := \sum \gamma_{ab}\,\gamma_{cd}\,\omega_{AC}\,\omega_{BD}\,X^{aA}\wedge X^{bB}\wedge X^{cC}\wedge X^{dD}.$$

Here $\gamma_{ab}=\gamma_E(e_a,e_b)$ and we recall that for even m the bilinear form ω_H^m is symmetric: $\omega_{AB}=\omega_{BA}$. □

For even m, a connection ∇ in a vector bundle W over M is $m/2$-partially flat if and only if its curvature F belongs to the space

$$(\Lambda^2 E\otimes\omega_H^m\oplus S^2E\otimes S^2H\otimes\omega_H^{m-1})\otimes\mathrm{End}\ W\subset(\Lambda^2E\otimes S^2S^mH\oplus S^2E\otimes\Lambda^2S^mH)\otimes\mathrm{End}\ W$$
$$=\Lambda^2(E\otimes S^mH)\otimes\mathrm{End}\ W.$$

The $\mathrm{SO}(E)\cdot\mathrm{Sp}(H)$-submodule $\Lambda^2E\otimes\omega_H^m\oplus S^2E\otimes S^2H\otimes\omega_H^{m-1}\subset\Lambda^2T^*M$ is not irreducible, so unlike the odd m case we cannot conclude that it is contained in an eigenspace V_λ of the $\mathrm{SO}(E)\cdot\mathrm{Sp}(H)$-invariant operator $B_\Omega:\Lambda^2T^*M\to\Lambda^2T^*M$. In fact, examples are known (see Appendix B of Ref. 16) where B_Ω has different eigenvalues on each irreducible summand of Λ^2T^*M. Therefore, in the case of even m we cannot expect that $m/2$-partial flatness implies the Yang–Mills equations.

C. Construction of partially flat connections over higher spin Grassmann manifolds

Now we generalize the construction of half-flat connections over admissible half-flat Grassmann manifolds to the case of k-partially flat connections over k-admissible higher spin Grassmann manifolds M. The natural extension of the harmonic construction given in Sec. IV B yields k-partially flat connections in the vector bundle ν over the k-admissible spin $m/2$ Grassmann manifold M. Again, we lift the geometric data from M to S_H via the projection $\pi:S_H\to M$. The pull back $\pi^*\nabla$ of a k-partially flat connection ∇ in the trivial vector bundle $\nu:W=\mathbb{C}^r\times M\to M$ is a connection in the vector bundle $\pi^*\nu:\pi^*W\to S_H$ which satisfies equations defining the notion of a k-partially flat gauge connection on S_H. One can also define the weaker notion of an almost k-partially flat connection in $\pi^*\nu:\pi^*W\to S_H$. The latter may be constructed from a prepotential and it affords the construction of a k-partially flat connection in the bundle $W\to M$. To simplify our exposition we explain the construction in the $m=3$ case. Here the decomposition (30) of the curvature tensor takes the form

$$\begin{aligned}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})=\mathop{\mathfrak{S}}_A\mathop{\mathfrak{S}}_B\ (&\overset{(0)}{F}{}^{[ee']}_{\alpha_1\alpha_2\alpha_3\beta_1\beta_2\beta_3}+\omega_H(h_{\alpha_1},h_{\beta_1})\overset{(1)}{F}{}^{(ee')}_{\alpha_2\alpha_3\beta_2\beta_3}\\&+\omega_H(h_{\alpha_1},h_{\beta_1})\omega_H(h_{\alpha_2},h_{\beta_2})\overset{(2)}{F}{}^{[ee']}_{\alpha_3\beta_3}\\&+\omega_H(h_{\alpha_1},h_{\beta_1})\omega_H(h_{\alpha_2},h_{\beta_2})\omega_H(h_{\alpha_3},h_{\beta_3})\overset{(3)}{F}{}^{(ee')}).\end{aligned}\tag{32}$$

In this case we have two nontrivial notions of partial flatness:

$$\text{zero-partial flatness:}\quad \overset{(0)}{F}=0,\tag{33}$$

$$\text{one-partial flatness:}\quad \overset{(0)}{F}=\overset{(1)}{F}=\overset{(2)}{F}=0.\tag{34}$$

Clearly, two-partial flatness is tantamount to flatness. By Theorem 6, a one-partially flat connection is a Yang–Mills connection.

1. Construction of zero-partially flat connections

Let M be a zero-admissible spin 3/2 Grassmann manifold with a zero-partially flat connection ∇ [satisfying (33)] in a holomorphic vector bundle $W\to M$. The pull-back of such a connection ∇ to a connection in the bundle $\pi^*W\to S_H$, where $\pi:S_H\to M$, has curvature F with components given by

$$F(X^e_{\pm\pm\pm},X^{e'}_{\pm\pm\pm})=0,$$

$$\begin{aligned}F(X^{e'}_{\pm\pm\pm},X^e_{\pm})&=u^{\alpha_1}_{\pm}u^{\alpha_2}_{\pm}u^{\alpha_3}_{\pm}u^{\beta_1}_{\pm}u^{\beta_2}_{\pm}u^{\beta_3}_{\mp}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})\\&=\pm 12\overset{(1)}{F}{}^{(ee')}_{\alpha_1\alpha_2\beta_1\beta_2}u^{\alpha_1}_{\pm}u^{\alpha_2}_{\pm}u^{\beta_1}_{\pm}u^{\beta_2}_{\pm}=:\pm 12\overset{(1)}{F}{}^{(ee')}_{\pm\pm\pm\pm},\end{aligned}$$

$$F(X^e_{\pm},X^{e'}_{\pm})=u^{\alpha_1}_{\pm}u^{\alpha_2}_{\pm}u^{\alpha_3}_{\mp}u^{\beta_1}_{\pm}u^{\beta_2}_{\pm}u^{\beta_3}_{\mp}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})=-8\overset{(2)}{F}{}^{[ee']}_{\alpha_1\beta_1}u^{\alpha_1}_{\pm}u^{\beta_1}_{\pm}=:-8\overset{(2)}{F}{}^{[ee']}_{\pm\pm},$$

$$\begin{aligned}F(X^e_{+++},X^{e'}_{---})&=u^{\alpha_1}_{+}u^{\alpha_2}_{+}u^{\alpha_3}_{+}u^{\beta_1}_{-}u^{\beta_2}_{-}u^{\beta_3}_{-}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})\\&=36(\overset{(1)}{F}{}^{(ee')}_{\alpha_1\alpha_2\beta_1\beta_2}u^{\alpha_1}_{+}u^{\alpha_2}_{+}u^{\beta_1}_{-}u^{\beta_2}_{-}+\overset{(2)}{F}{}^{[ee']}_{\alpha_1\beta_1}u^{\alpha_1}_{+}u^{\beta_1}_{-}+\overset{(3)}{F}{}^{(ee')})\\&=:36(\overset{(1)}{F}{}^{(ee')}_{0}+\overset{(2)}{F}{}^{[ee']}_{0}+\overset{(3)}{F}{}^{(ee')}_{0}),\end{aligned}\tag{35}$$

$$F(X^e_{\pm\pm\pm},X^{e'}_{\mp})=u^{\alpha_1}_{\pm}u^{\alpha_2}_{\pm}u^{\alpha_3}_{\pm}u^{\beta_1}_{\pm}u^{\beta_2}_{\mp}u^{\beta_3}_{\mp}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})=\pm 24\overset{(1)}{F}{}^{(ee')}_{\pm\pm}+12\overset{(2)}{F}{}^{[ee']}_{\pm\pm},$$

$$F(X^e_{+},X^{e'}_{-})=u^{\alpha_1}_{+}u^{\alpha_2}_{+}u^{\alpha_3}_{-}u^{\beta_1}_{+}u^{\beta_2}_{-}u^{\beta_3}_{-}F(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3})=12\overset{(1)}{F}{}^{(ee')}_{0}-4\overset{(2)}{F}{}^{[ee']}_{0}-12\overset{(3)}{F}{}^{(ee')}_{0},$$

$$F(v\,,\cdot\,)=0,$$

where v,v' are vertical vector fields on S_H. The form of these components lead us to the following definition.

Definition 14: A connection in a holomorphic vector bundle $W\to S_H$ is **zero-partially flat** *if its curvature satisfies the equations*

$$F(X^e_{\pm\pm\pm},X^{e'}_{\pm\pm\pm})=0,$$

$$F(X^e_{\pm\pm\pm},X^{e'}_{\pm})=F(X^{e'}_{\pm\pm\pm},X^e_{\pm}),$$

$$F(X^e_{\pm},X^{e'}_{\pm})=-F(X^{e'}_{\pm},X^e_{\pm}),$$

$$F(v\,,\cdot\,)=0,\quad \forall v\in T^vS_H.$$

The restriction of a zero-partially flat connection to a leaf of the integrable distribution $\langle\mathcal{D}_{3+},\partial_0\rangle$ is clearly flat. In this case, an **analytic frame** in the holomorphic vector bundle $\pi^*\nu:\mathbb{C}^r\times S_H\to S_H$ is a frame which is parallel along leaves of this integrable distribution. With respect to such a frame, a connection in the vector bundle $\pi^*\nu$ can be written as

$$\nabla^S_{\partial_0} = \partial_0,$$

$$\nabla^S_{X^e_{+++}} = X^e_{+++},$$

$$\nabla^S_{X^e_{\pm}} = X^e_{\pm} + A(X^e_{\pm}),$$

$$\nabla^S_{\partial_{\pm\pm}} = \partial_{\pm\pm} + A(\partial_{\pm\pm}),$$

$$\nabla^S_{X^e_{---}} = X^e_{---} + A(X^e_{---}).$$

Definition 15: A connection ∇^S over S_H is called **almost zero-partially flat** *if its curvature satisfies the following equations:*

$$F(X^e_{+++}, X^{e'}_{+++}) = F(X^e_{+++}, v) = F(X^e_{\pm}, v) = 0, \quad \forall v \in T^v S_H,$$
$$F(\partial_{++}, \cdot) = F(\partial_0, \cdot) = 0. \tag{36}$$

Following the construction of almost half-flat connections, we may construct almost zero-partially flat connections, which allow deformation to a zero-partially flat connection. As in the case of a half-flat connection (cf. Proposition 7), an almost zero-partially flat connection is completely determined by the potentials $A_{\pm\pm} =: A(\partial_{\pm\pm})$ with respect to an analytic frame.

Proposition 11: Let ∇ be an almost zero-partially flat connection in the vector bundle $\pi^*\nu: \mathbb{C}^r \times S_H \to S_H$ with potentials A_{++}, A_{--}, $A(X^e_{\pm})$ and $A(X^e_{---})$ in an analytic frame. Then we have the following.

(i) The potential A_{++} is analytic and has charge 2, i.e.,

$$X^e_{+++} A_{++} = 0, \quad \partial_0 A_{++} = 2A_{++}. \tag{37}$$

(ii) The potential A_{--} satisfies

$$\partial_{++} A_{--} - \partial_{--} A_{++} + [A_{++}, A_{--}] = 0, \quad \partial_0 A_{--} = -2A_{--}. \tag{38}$$

(iii) The potentials $A(X^e_{\pm})$ and $A(X^e_{---})$ are then recursively determined as follows:

$$A(X^e_{+}) = -\tfrac{1}{3} X^e_{+++} A_{--},$$

$$A(X^e_{-}) = \tfrac{1}{2}(\partial_{--} A(X^e_{+}) - X^e_{+} A_{--} + [A_{--}, A(X^e_{+})]), \tag{39}$$

$$A(X^e_{---}) = \partial_{--} A(X^e_{-}) - X^e_{-} A_{--} + [A_{--}, A(X^e_{-})],$$

and they have charges $+1, -1$, and -3, respectively, i.e.,

$$\partial_0 A(X^e_{\pm}) = \pm A(X^e_{\pm}), \quad \partial_0 A(X^e_{---}) = -3A(X^e_{---}). \tag{40}$$

Conversely, any set of matrix-valued potentials A_{++}, A_{--}, $A(X^e_{\pm})$ and $A(X^e_{---})$ satisfying (37)–(40) define an almost zero-partially flat connection.

Proof: (i) The curvature constraints $F(X^e_{+}, \partial_{++}) = 0$, $F(\partial_0, \partial_{++}) = 0$, in an analytic frame, take the form (37).

(ii) The further almost zero-partial-flatness conditions, $F(\partial_{++}, \partial_{--}) = F(\partial_0, \partial_{--}) = 0$, give Eqs. (38) for the potential A_{--}.

(iii) Having obtained A_{--}, we can find $A(X^e_{\pm})$ and $A(X^e_{---})$ from the equations

$$F(\partial_{--},X^e_{+++})=0\Leftrightarrow -X^e_{+++}A_{--}=A([\partial_{--},X^e_{+++}])=3A(X^e_+),$$

$$F(\partial_{--},X^e_{+})=0\Leftrightarrow \partial_{--}A(X^e_+)-X^e_+A_{--}+[A_{--},A(X^e_+)]=A([\partial_{--},X^e_+])=2A(X^e_-),$$

$$F(\partial_{--},X^e_{-})=0\Leftrightarrow \partial_{--}A(X^e_-)-X^e_-A_{--}+[A_{--},A(X^e_-)]=A([\partial_{--},X^e_-])=A(X^e_{---}).$$

Equations (40) follow from (39). □

Now, using this proposition, a modification of Theorem 4 gives an algorithm for the construction of all almost zero-partially flat connections.

Theorem 7: *Let A_{++} be an analytic prepotential, i.e., a matrix-valued function on a domain $U=\pi^{-1}(V)\subset S_H$, $V\subset M$ a simply connected domain, satisfying (37), and Φ an invertible matrix-valued function on U which satisfies the equations*

$$\partial_{++}\Phi=-A_{++}\Phi\,,\quad \partial_0\Phi=0\,. \tag{41}$$

Such a function Φ always exists. Then the pair (A_{++},Φ) determines an almost zero-partially flat connection $\nabla^S=\nabla^{(A_{++},\Phi)}$. Its potentials with respect to an analytic frame are given by A_{++}, $A_{--}=-(\partial_{--}\Phi)\Phi^{-1}$ and (39). Conversely, any almost zero-partially flat connection is of this form.

The proof follows that for Theorem 4 and uses Proposition 1.1.

To deform an almost zero-partially flat connection into a zero-partially flat connection, we need to find a transformation from the above analytic frame to a central frame. Analogously to Lemma 5 we may prove the following.

Lemma 7: Let $\nabla=\nabla^{(A_{++},\Phi)}$ be the almost zero-partially flat connection associated to the analytic prepotential A_{++} with respect to the analytic frame φ and an invertible solution Φ of (41). Then the frame $\psi:=\varphi\Phi$ is a central frame for the connection ∇, i.e., the potentials $C(\partial_{\pm\pm})$ and $C(\partial_0)$ with respect to that frame vanish.

With respect to the central frame ψ, the above almost zero-partially flat connection then takes the form

$$\nabla^S_{X^e_{+++}}=X^e_{+++}+C(X^e_{+++})=X^e_{+++}+\Phi\,X^e_{+++}\,\Phi^{-1},$$

$$\nabla^S_{X^e_{\pm}}=X^e_{\pm}+C(X^e_{\pm}),$$

$$\nabla^S_{X^e_{---}}=X^e_{---}+C(X^e_{---}),$$

$$\nabla^S_{\partial_{++}}=\partial_{++},\quad \nabla^S_{\partial_{--}}=\partial_{--},\quad \nabla^S_{\partial_0}=\partial_0\,,$$

where in terms of the analytic frame potentials $A(X)$, the central frame potentials $C(X)$ are given by $C(X)=\Phi^{-1}A(X)\Phi+\Phi^{-1}(X\Phi)$. Moreover, the equations $F(\partial_{++},X^e_{+++})=F(\partial_0,X^e_{+++})=0$ imply that the potential $C(X^e_{+++})$ satisfies the equations

$$\partial_{++}C(X^e_{+++})=0,\quad \partial_0C(X^e_{+++})=3C(X^e_{+++})\,. \tag{42}$$

The following proposition is analogous to Proposition 8 in the half-flat case.

Proposition 12: The potential $C(X^e_{+++})$ of an almost zero-partially flat connection ∇ with respect to a central frame is cubic in u^α_+,

$$C(X^e_{+++})=u^\alpha_+u^\beta_+u^\gamma_+C(\widetilde{X^e_{\alpha\beta\gamma}})=u^\alpha_+u^\beta_+u^\gamma_+C^e_{\alpha\beta\gamma}, \tag{43}$$

where the coefficients $C^e_{\alpha\beta\gamma}=C^e_{\alpha\beta\gamma}(x^i)$, *symmetric in* α,β,γ, *are matrix valued functions of coordinates* x^i *on* M *and* $(x^i,u^\alpha_\pm)$ *are the local coordinates associated with the trivialization* $S_H=M\times \mathrm{Sp}(1,\mathbb{C})$.

With respect to a central frame, we can therefore write $\nabla_{X^e_{+++}}=X^e_{+++}+u^\alpha_+u^\beta_+u^\gamma_+C^e_{\alpha\beta\gamma}$. Using $C^e_{\alpha\beta\gamma}$, we now define a new connection in $\pi^*\nu$ over S_H by

$$\hat\nabla_{X^e_{+++}}=X^e_{+++}+u^\alpha_+u^\beta_+u^\gamma_+C^e_{\alpha\beta\gamma},$$

$$\hat\nabla_{X^e_{+}}=X^e_{+}+u^\alpha_+u^\beta_+u^\gamma_-C^e_{\alpha\beta\gamma},$$

$$\hat\nabla_{X^e_{-}}=X^e_{-}+u^\alpha_-u^\beta_-u^\gamma_+C^e_{\alpha\beta\gamma},$$

$$\hat\nabla_{X^e_{---}}=X^e_{---}+u^\alpha_-u^\beta_-u^\gamma_-C^e_{\alpha\beta\gamma},$$

$$\hat\nabla_{\partial_{++}}=\partial_{++},\quad \hat\nabla_{\partial_{--}}=\partial_{--},\quad \hat\nabla_{\partial_0}=\partial_0.$$

The following theorem is the analog of Theorem 5 in the half-flat case.

Theorem 8: *The constructed connection* $\hat\nabla$ *is a 0-partially flat connection in* $\pi^*\nu$ *over* S_H *and it is the pull-back of the following 0-partially flat connection* ∇^M *in* ν *over* M:

$$\nabla^M_{X^e_{\alpha\beta\gamma}}=X^e_{\alpha\beta\gamma}+C^e_{\alpha\beta\gamma}.$$

Proof: As in Lemma 1 we may show that the connection $\hat\nabla$ is the pull-back of the connection ∇^M. It then suffices to show that ∇^M is zero-partially flat. The connections ∇ and $\hat\nabla$ coincide in the direction of X^e_{+++}. Hence, using $C^e_{+++}:=u^{\alpha_1}_+u^{\alpha_2}_+u^{\alpha_3}_+C^e_{\alpha_1\alpha_2\alpha_3}$, we have

$$\begin{aligned}0=F^\nabla(X^e_{+++},X^{e'}_{+++})&=F^{\hat\nabla}(X^e_{+++},X^{e'}_{+++})\\&=X^e_{+++}C^{e'}_{+++}-X^{e'}_{+++}C^e_{+++}+[C^e_{+++},C^{e'}_{+++}]-C([X^e_{+++},X^{e'}_{+++}])\\&=u^{\alpha_1}_+u^{\alpha_2}_+u^{\alpha_3}_+u^{\beta_1}_+u^{\beta_2}_+u^{\beta_3}_+(X^e_{\alpha_1\alpha_2\alpha_3}C^{e'}_{\beta_1\beta_2\beta_3}-X^{e'}_{\beta_1\beta_2\beta_3}C^e_{\alpha_1\alpha_2\alpha_3}\\&\quad+[C^e_{\alpha_1\alpha_2\alpha_3},C^{e'}_{\beta_1\beta_2\beta_3}]-C([X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3}]))\\&=u^{\alpha_1}_+u^{\alpha_2}_+u^{\alpha_3}_+u^{\beta_1}_+u^{\beta_2}_+u^{\beta_3}_+\ F^{\nabla^M}(X^e_{\alpha_1\alpha_2\alpha_3},X^{e'}_{\beta_1\beta_2\beta_3}),\end{aligned}$$

since $X^e_{+++}u^\beta_+=0$. This shows that the component $F^{(0)}=0$ in the decomposition (32), i.e., the connection ∇^M is zero-partially flat. □

2. Construction of one-partially flat connections

Let M be a one-admissible spin 3/2 Grassmann manifold with a one-partially flat connection ∇ [satisfying (34)] in a holomorphic vector bundle $W\to M$. The pull-back of such a connection to a connection in the bundle $\pi^*W\to S_H$, where $\pi:S_H\to M$, has curvature F with components given by

$$F(X^e_{\pm\pm\pm},X^{e'}_{\pm\pm\pm})=0,$$

$$F(X^{e'}_{\pm\pm\pm},X^e_{\pm})=0,$$

$$F(X^e_{\pm},X^{e'}_{\pm})=0,$$

$$F(X^e_{+++},X^{e'}_{---})=36\overset{(3)}{F}{}^{(ee')}, \tag{44}$$

$$F(X^e_{\pm\pm\pm},X^{e'}_{\mp})=0,$$

$$F(X^e_{+},X^{e'}_{-})=-12\overset{(3)}{F}{}^{(ee')},$$

$$F(v\,,\cdot\,)=0,$$

where v is any vertical vector field on S_H. A connection in a holomorphic vector bundle $W\to S_H$ is **one-partially flat** if its curvature satisfies the above equations. The restriction of a one-partially flat connection to a leaf of the integrable distribution $\langle\mathcal{D}_{3+},\mathcal{D}_{+},\partial_0\rangle$ is clearly flat. In this case, an **analytic frame** in the holomorphic vector bundle $\pi^*\nu:\mathbb{C}^r\times S_H\to S_H$ is a frame which is parallel along leaves of this distribution. With respect to such a frame, a connection in the vector bundle $\pi^*\nu$ can be written as

$$\nabla^S_{\partial_0}=\partial_0,$$

$$\nabla^S_{X^e_{+++}}=X^e_{+++},$$

$$\nabla^S_{X^e_{+}}=X^e_{+},$$

$$\nabla^S_{\partial_{++}}=\partial_{++}+A_{++},$$

$$\nabla^S_{\partial_{--}}=\partial_{--}+A_{--},$$

$$\nabla^S_{X^e_{---}}=X^e_{---}+A(X^e_{---}),$$

$$\nabla^S_{X^e_{-}}=X^e_{-}+A(X^e_{-}),$$

with potentials $A(X^e_{+++})=A(X^e_{+})=A(\partial_0)=0$. We look for solutions of the system (44) in this analytic gauge.

Definition 16: A connection ∇^S *over* S_H *is called* **almost one-partially flat** *if its curvature satisfies the equations*

$$\begin{gathered}F(X^e_{+++},X^{e'}_{+++})=F(X^e_{+++},X^{e'}_{+})=F(X^e_{+},X^{e'}_{+})=0,\\ F(X^e_{+++},v)=F(X^e_{\pm},v)=F(\partial_{++},\cdot\,)=F(\partial_0,\cdot\,)=0,\quad \forall v\in T^vS_H.\end{gathered} \tag{45}$$

In virtue of these equations, the potentials $A_{\pm\pm}:=A(\partial_{\pm\pm})$ determine all other potentials:

Proposition 13: Let ∇ *be an almost one-partially flat connection in the vector bundle* $\pi^*\nu:\mathbb{C}^r\times S_H\to S_H$ *with potentials* A_{++}, A_{--}, $A(X^e_{-})$ *and* $A(X^e_{---})$ *in an analytic frame. Then we have the following.*

(i) The potential A_{++} *is analytic and has charge* 2, *i.e.*,

$$X^e_{+++}A_{++}=0,\quad X^e_{+}A_{++}=0,\quad \partial_0A_{++}=2A_{++}. \tag{46}$$

(ii) The potential A_{--} *satisfies*

$$\partial_{++}A_{--}-\partial_{--}A_{++}+[A_{++},A_{--}]=0, \quad \partial_0 A_{--}=-2A_{--}. \tag{47}$$

(iii) The potentials $A(X^e_-)$ and $A(X^e_{---})$ are then recursively determined as follows:

$$\begin{aligned} A(X^e_-)&=-\tfrac{1}{2}X^e_+A_{--},\\ A(X^e_{---})&=\partial_{--}A(X^e_-)-X^e_-A_{--}+[A_{--},A(X^e_-)], \end{aligned} \tag{48}$$

and they have charges -1 and -3, respectively; i.e.,

$$\partial_0 A(X^e_-)=\pm A(X^e_-), \quad \partial_0 A(X^e_{---})=-3A(X^e_{---}). \tag{49}$$

Conversely, any set of matrix-valued potentials A_{++}, A_{--}, $A(X^e_-)$ and $A(X^e_{---})$ satisfying (46)–(49) define an almost one-partially flat connection.

Proof: (i) Equations (46) are equivalent to $F(\partial_{++},X^e_{+++})=F(\partial_{++},X^e_+)=F(\partial_0,\partial_{++})=0$.

(ii) The further almost one-partial-flatness conditions, $F(\partial_{++},\partial_{--})=F(\partial_0,\partial_{--})=0$, give Eqs. (47).

(iii) Having obtained A_{--}, we can find $A(X^e_-)$ and $A(X^e_{---})$ from the equations

$$F(\partial_{--},X^e_+)=0\Leftrightarrow -X^e_+A_{--}=A([\partial_{--},X^e_+])=2A(X^e_-),$$

$$F(\partial_{--},X^e_-)=0\Leftrightarrow \partial_{--}A(X^e_-)-X^e_-A_{--}+[A_{--},A(X^e_-)]=A([\partial_{--},X^e_-])=A(X^e_{---}).$$

The equations (49) follow from (48). □

Now, starting from a prepotential A_{++}, which solves (46), we may construct an almost one-partially flat connection. The potential $A_{--}=-(\partial_{--}\Phi)\Phi^{-1}$ is determined, as before, from a solution Φ of (41). Then, with the remaining potentials in an analytic frame being given by (48) and satisfying (49), all the other equations in (45) follow. This shows that an almost one-partially flat connection is determined by an arbitrary analytic prepotential A_{++} and an invertible solution Φ of (41). As before, Φ is a transition function from an analytic frame to a central frame, in which the above almost one-partially flat connection takes the form

$$\nabla^S_{X^e_{+++}}=X^e_{+++}+C(X^e_{+++})=X^e_{+++}+\Phi\ X^e_{+++}\ \Phi^{-1},$$

$$\nabla^S_{X^e_+}=X^e_++C(X^e_+)=X^e_++\Phi\ X^e_+\ \Phi^{-1},$$

$$\nabla^S_{X^e_-}=X^e_-+C(X^e_-),$$

$$\nabla^S_{X^e_{---}}=X^e_{---}+C(X^e_{---}),$$

$$\nabla^S_{\partial_{++}}=\partial_{++}, \quad \nabla^S_{\partial_{--}}=\partial_{--}, \quad \nabla^S_{\partial_0}=\partial_0.$$

Moreover, the equations $F(\partial_{++},X^e_{+++})=F(\partial_0,X^e_{+++})=0$ imply that the potential $C(X^e_{+++})$ satisfies the equations

$$\partial_{++}C(X^e_{+++})=0, \quad \partial_0 C(X^e_{+++})=3C(X^e_{+++}).$$

Proposition 14: The potentials $C(X^e_{+++})$ and $C(X^e_+)$ of an almost one-partially flat connection ∇ with respect to a central frame have the form

$$C(X^e_{+++})=u^\alpha_+u^\beta_+u^\gamma_+C^e_{\alpha\beta\gamma}, \quad C(X^e_+)=u^\alpha_+u^\beta_+u^\gamma_-C^e_{\alpha\beta\gamma},$$

where $C^e_{\alpha\beta\gamma}$ is a function on M, symmetric in α,β,γ.

With respect to a central frame, we can therefore write

$$\nabla_{X^e_{+++}} = X^e_{+++} + u^\alpha_+ u^\beta_+ u^\gamma_+ C^e_{\alpha\beta\gamma}, \quad \nabla_{X^e_+} = X^e_+ + u^\alpha_+ u^\beta_+ u^\gamma_- C^e_{\alpha\beta\gamma}.$$

We define a modified connection in the bundle $\pi^*\nu$ over S_H by

$$\begin{aligned}
\hat{\nabla}_{X^e_{+++}} &= X^e_{+++} + u^\alpha_+ u^\beta_+ u^\gamma_+ C^e_{\alpha\beta\gamma},\\
\hat{\nabla}_{X^e_+} &= X^e_+ + u^\alpha_+ u^\beta_+ u^\gamma_- C^e_{\alpha\beta\gamma},\\
\hat{\nabla}_{X^e_-} &= X^e_- + u^\alpha_- u^\beta_- u^\gamma_+ C^e_{\alpha\beta\gamma},\\
\hat{\nabla}_{X^e_{---}} &= X^e_{---} + u^\alpha_- u^\beta_- u^\gamma_- C^e_{\alpha\beta\gamma},\\
\hat{\nabla}_{\partial_{++}} &= \partial_{++}, \quad \hat{\nabla}_{\partial_{--}} = \partial_{--}, \quad \hat{\nabla}_{\partial_0} = \partial_0 .
\end{aligned} \tag{50}$$

As in the zero-partially flat case, we have the following.

Theorem 9: *The constructed connection $\hat{\nabla}$ is a one-partially flat connection in $\pi^*\nu$ over S_H and it is the pull-back of the following one-partially flat connection ∇^M in ν over M*:

$$\nabla^M_{X^e_{\alpha\beta\gamma}} = X^e_{\alpha\beta\gamma} + C^e_{\alpha\beta\gamma}. \tag{51}$$

Proof: As before one shows that the connection $\hat{\nabla}$ is the pull-back of the connection ∇^M. It remains to show that ∇^M is one-partially flat. Since any almost one-partially flat connection is almost zero-partially flat, we have $F^{(0)}=0$ by Theorem 8. Next we show that $F^{(1)}=0$. The connections ∇ and $\hat{\nabla}$ coincide in the direction of X^e_{+++} and X^e_+. Hence, using Eq. (35), which holds for zero-partially flat connections, we have

$$0 = F^\nabla(X^e_{+++}, X^{e'}_+) = F^{\hat{\nabla}}(X^e_{+++}, X^{e'}_+) = 12 \overset{(1)}{F}{}^{(ee')}_{\alpha_1\alpha_2\beta_1\beta_2} u^{\alpha_1}_+ u^{\alpha_2}_+ u^{\beta_1}_+ u^{\beta_2}_+ .$$

This shows that the component $F^{(1)}$ in the decomposition (32) vanishes. Similarly,

$$0 = F^\nabla(X^e_+, X^{e'}_+) = F^{\hat{\nabla}}(X^e_+, X^{e'}_+) = -8 \overset{(2)}{F}{}^{[ee']}_{\alpha_1\beta_1} u^{\alpha_1}_+ u^{\beta_1}_+$$

implies $F^{(2)[ee']}=0$, and hence that $\hat{\nabla}$ is one-partially flat. □

By Theorem 6, the one-partially flat connection $\nabla^M_{X^e_{\alpha\beta\gamma}}$ in (51) is a Yang–Mills connection.

ACKNOWLEDGMENTS

We should like to thank Andrea Spiro for useful comments on the manuscript. This work was supported by the ''Schwerpunktprogramm Stringtheorie'' of the Deutsche Forschungsgemeinschaft, MPI für Mathematik (Bonn) and the SFB 256 (University of Bonn).

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On the *M*-function and Borg–Marchenko theorems for vector-valued Sturm–Liouville equations

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(Received 28 May 2003; accepted 1 August 2003)

We will consider a vector-valued Sturm–Liouville equation of the form $\mathcal{R}[U] := -(PU')' + QU = \lambda WU$, $x \in [0,b)$, with P^{-1}, W, $Q \in L^1_{\mathrm{loc}}([0,b))^{m\times m}$ being Hermitian and under some additional conditions on P^{-1} and W. We give an elementary deduction of the leading order term asymptotics for the Titchmarsh–Weyl M-function corresponding to this equation. In the special case of $P = W = I$, $Q \in L^1([0,\infty))^{m\times m}$ and the Neumann boundary conditions at 0, we will also prove that $M = (1/\sqrt{-\lambda})(I+R)(I-R)^{-1}$, where $R = \lim_{n\to\infty} R_n = \Sigma_{n=1}^{\infty} Q_n$, for recursively defined sequences $\{R_n\}$ and $\{Q_n\}$. If $Q \in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, $0 < b \leqslant \infty$, the same formula is valid with an exponentially small error for large λ. It is clear that expansions of this type are helpful in finding representatives of the KdV invariants. For $P = W = I$, we prove that the spectral measure corresponding to the equation $\mathcal{R}[U] = \lambda U$ uniquely determines Q as well as b and the boundary conditions at 0 and b. We finally give a new proof of a local form of the Borg–Marchenko theorem (cf. Gesztesy and Simon, "On local Borg–Marchenko uniqueness results," Commun. Math. Phys. **211**, 273–287 (2000), Chap. 3); a theorem which is due to Simon [see Simon, "A new approach to inverse spectral theory, I. fundamental formalism," Ann. Math. **150**, 1–29 (1999)] in the scalar case. For applications to physics, it is worth mentioning that vector-valued Sturm–Liouville equations appear in some problems in magneto-hydro-dynamics. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1618922]

I. INTRODUCTION

The main objective of study in this paper is a vector-valued Sturm–Liouville equation of the form

$$\mathcal{R}[U] := -(PU')' + QU = \lambda WU, \quad x \in [0,b), \tag{1.1}$$

which will be considered under the following hypothesis, where, as well as in the rest of the paper, $\mathcal{B}([0,b))^{p\times q}$, $p,q \in \mathbb{Z}^+$, will denote the set of all $p\times q$-matrices with complex entries of class $\mathcal{B}$ on the interval $[0,b)$. We will also let $\mathbb{C}^{p\times q}$ denote the set of all $p\times q$-matrices with complex entries.

Hypothesis 1.1: Assume that, in the equation (1.1),

(i) P^{-1}, W, $Q = Q^* \in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, *where* $m \in \mathbb{Z}^+$, $P = P^*$, $W > 0$ *and* $0 < b \leqslant \infty$;

(ii) $1/x \int_0^x P^{-1}$ *has an invertible limit* $P^{-1}(0)$, *as* $x \to 0$;

(iii) $1/x \int_0^x W$ *has a limit* $W(0) > 0$, *as* $x \to 0$.

Making these assumptions, we will give a very simple deduction of the leading order term asymptotics for the Titchmarsh–Weyl M-function corresponding to a self-adjoint realization of (1.1). We will also prove that, in the special case of $P = W = I$,

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$$M=\frac{1}{\sqrt{-\lambda}}(I+R)(I-R)^{-1},$$

where R corresponds to the reflection coefficient in the scalar case (i.e., in view of Lemma 2.2, this means that we will relate the reflection coefficient to the spectral data of the self-adjoint operator induced by (1.1)!), and that the spectral measure corresponding to (1.1) uniquely determines Q as well as b and the boundary conditions at 0 and at b (cf. Refs. 12, 19, 20, 21, 23, 24, 27, 32, and 33). We end the presentation with a simple proof of a version of Simon's local Borg–Marchenko theorem (cf. Refs. 15 and 16, Chap. 3). The method is similar to that of Ref. 5 for the scalar case. These results will improve previous works in these areas in the following ways.

Although the asymptotics for the Titchmarsh–Weyl m-function corresponding to a Sturm–Liouville equation of the form

$$-u''+qu=\lambda u, \quad x\in[0,b), \tag{1.2}$$

has been given much attention, the number of published papers in this area decreases significantly when passing to the slightly more general equation

$$-(pu')'+qu=\lambda\omega u, \quad x\in[0,b) \tag{1.3}$$

(see Ref. 6 and further references there) or, even further, to the vector case corresponding to (1.2), i.e., the case of the equation

$$-U''+QU=\lambda U, \quad x\in[0,b). \tag{1.4}$$

The relatively few papers which do treat the asymptotics for the M-function corresponding to (1.4) (see Refs. 4, 12 and further references therein) offer proofs involving fairly laborious methods even for determining the leading-order term of the asymptotic expansion. More specifically, Ref. 12 offers the analogs of Theorem 3.2 and Theorem 3.6, below, for *Dirichlet* M-functions $M_{\mathcal{D}}$ corresponding to (1.4) (i.e., for $S=0$ and $C=-I$ in (2.2) below). They also prove that, if Q has N locally integrable derivatives, the same M-functions can be written

$$M_{\mathcal{D}}(\lambda)=\sqrt{-\lambda}I+\sum_{k=1}^{N}(-\lambda)^{-k/2}m_k+o(|\lambda|^{-N/2}),$$

for some recursively defined coefficients m_k. In contrast to this, we give an expansion of M, valid with exponentially small errors as $|\lambda|\to\infty$, assuming only that Q is locally integrable. It is clear that, using expansions of this type, one can prove trace formulas for $Q(x)$ and certain higher-order differential polynomials in $Q(x)$, following an approach in Ref. 17. These trace formulas are of use in proving certain results in inverse spectral theory for operators of type (1.1), in $L^2(\mathbb{R})^{m\times m}$, in the case of $P=W=I$. For instance, one has the following theorem, obtained in Ref. 13.

Theorem: *Suppose that* $\mathcal{R}$, *in the case of* $P=W=I$, *is reflectionless and has spectrum* $[c,\infty)$ *for some* $c\in\mathbb{R}$. *Then*

$$Q(x)=cI.$$

Moreover, the aforementioned higher-order differential polynomials in $Q(x)$ represent the Korteweg–de Vries (KdV) invariants (i.e., densities associated with KdV conservation laws) and hence open the link to infinite-dimensional completely integrable systems (see Ref. 29 and further references therein). Vector-valued Sturm–Liouville equations also appear in some problems in magneto-hydro-dynamics.

Regarding the inverse spectral theory results, the most satisfactory results in this case for nearly half a century (results essentially due to Göran Borg,[10] Marchenko,[28] and Gelfand and

Levitan;[14] for alternative variants, see also Refs. 25 and 26) concerned only the very simplest case of a scalar-valued Sturm–Liouville equation, namely, the case of (1.2), and some other, closely related, equations. However, recently Bennewitz[8] proved that the more general equation (1.3), where $1/p, q \in L^1_{\mathrm{loc}}[0,b)$ are real-valued, is completely determined by its spectral measure up to equations which may be transformed into each other using only unitary Liouville transformations.

Remark 1.2: Note that the equation (1.1) with notation

$$J=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad A=\begin{pmatrix} Q & 0 \\ 0 & -P^{-1} \end{pmatrix}, \quad K=\begin{pmatrix} W & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad V=\begin{pmatrix} U \\ PU' \end{pmatrix}$$

can be rewritten as the following Hamiltonian system:

$$-JV'+AV=\lambda KV, \quad x\in[0,b). \tag{1.5}$$

Naturally associated with (1.1) is the space $L^2_W([0,b))^{m\times 1}$ consisting of all (equivalence classes of) $m\times 1$-matrix-valued and complex Lebesgue measurable functions U, for which U^*WU is integrable over $[0,b)$. Provided with the inner product

$$\langle U,V\rangle_W=\int_0^b V^*WU,$$

L^2_W becomes a Hilbert space.

Given this background, we proceed as follows. In Sec. II, we give some preliminaries along with some background information on the Titchmarsh–Weyl M-function corresponding to a self-adjoint realization of (1.1). In Sec. III, we give an elementary deduction of the leading order term asymptotics for M, and we proceed by, in Sec. IV, proving that M, in the special case of $P=W=I$, $Q=Q^*\in L^1([0,\infty))^{m\times m}$ and the Neumann boundary conditions at 0, can be written $M=(1/\sqrt{-\lambda})(I+R)(I-R)^{-1}$, where $R=\lim_{n\to\infty}R_n=\Sigma_{n=1}^{\infty}Q_n$, for recursively defined sequences $\{R_n\}$ and $\{Q_n\}$. In the case of $Q=Q^*\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, $0<b\leqslant\infty$, we shall see that the same formula is valid with an exponentially small error. Finally, in Sec. V, we prove the Borg–Marchenko theorems mentioned above.

II. THE TITCHMARSH–WEYL MATRIX *M*

Let

$$F(x,\lambda)=\begin{pmatrix} \varphi(x,\lambda) & \theta(x,\lambda) \\ P\varphi'(x,\lambda) & P\theta'(x,\lambda) \end{pmatrix}\in\mathbb{C}^{2m\times 2m}, \tag{2.1}$$

where $\varphi,\theta\in\mathbb{C}^{m\times m}$, be a fundamental matrix of the system (1.5), such that

$$B:=F(0,\lambda)=\begin{pmatrix} \varphi(0,\lambda) & \theta(0,\lambda) \\ P\varphi'(0,\lambda) & P\theta'(0,\lambda) \end{pmatrix}=\begin{pmatrix} S & C \\ -C & S \end{pmatrix} \tag{2.2}$$

is unitary and symplectic, i.e., such that

$$F^*(0,\lambda)F(0,\lambda)=I \quad \text{and} \quad F^*(0,\lambda)JF(0,\lambda)=J,$$

with J as in (1.5). This means that the columns φ_i, $i\in[1,m]$, of φ satisfy the symmetric boundary condition

$$S^*(PU')(0,\lambda)+C^*U(0,\lambda)=0, \tag{2.3}$$

and that

$$\begin{cases} S^*S+C^*C=I \\ S^*C=C^*S \end{cases} \quad \text{and} \quad \begin{cases} SS^*+CC^*=I \\ CS^*=SC^*. \end{cases} \tag{2.4}$$

It also follows that $F^*(x,\overline{\lambda})JF(x,\lambda)=J$ for all $\lambda\in\mathbb{C}$ and all $x\in[0,b)$, since differentiation and use of (1.5) shows that the left quantity is independent of x. We thus have that

$$\varphi^*(x,\overline{\lambda})(P\varphi')(x,\lambda)-(P\varphi')^*(x,\overline{\lambda})\varphi(x,\lambda)=0, \tag{2.5a}$$

$$\varphi^*(x,\overline{\lambda})(P\theta')(x,\lambda)-(P\varphi')^*(x,\overline{\lambda})\theta(x,\lambda)=I, \tag{2.5b}$$

$$\theta^*(x,\overline{\lambda})(P\theta')(x,\lambda)-(P\theta')^*(x,\overline{\lambda})\theta(x,\lambda)=0. \tag{2.5c}$$

By standard results from the theory of ordinary differential equations, we also have that φ and θ are entire functions of λ, locally uniformly in x. In addition, we impose a boundary condition at b if needed for $\mathcal{R}$, (1.1), to generate a self-adjoint operator T in $L^2_W([0,b))^{m\times 1}$. The case when no boundary condition at all is needed at b will henceforth be referred to as the "limit-point" case.

Remark 2.1: The choice of initial condition according to (2.4) is convenient for the following reason. We are dealing with a problem where at least 0 is a regular point, and we want to impose separated boundary conditions. That the columns of $\binom{S}{-C}\in\mathbb{C}^{2m\times m}$ satisfy a self-adjoint boundary condition, by (2.3), then means that $S^*C=C^*S$. Moreover, it is clear that the vectors, in $\mathbb{C}^{2m}$, satisfying the self-adjoint boundary condition (2.3) constitute the m-dimensional nullspace of the matrix $\binom{C}{S}^*\in\mathbb{C}^{m\times 2m}$, and since one can always choose an ON-basis in this nullspace (in many different ways), it is no restriction to assume $\binom{S}{-C}$ to have orthonormal columns. It is then well-known, and easy to see, that $B:=\left(\begin{smallmatrix} S & C \\ -C & S \end{smallmatrix}\right)\in\mathbb{C}^{2m\times 2m}$ is unitary and symplectic; and it is natural to choose a fundamental matrix with these initial conditions.

There now exists a unique $m\times m$-matrix-valued function $M_B(\lambda)\in\mathbb{C}^{m\times m}$ (determined by the boundary condition at b) such that

$$\Psi(x,\lambda)=\begin{pmatrix} \psi(x,\lambda) \\ P\psi'(x,\lambda) \end{pmatrix}=F(x,\lambda)\begin{pmatrix} -M_B(\lambda) \\ I \end{pmatrix}\in\mathbb{C}^{2m\times m} \tag{2.6}$$

(where the index B refers to the matrix $B:=F(0,\lambda)\in\mathbb{C}^{2m\times 2m}$ in (2.2)) is unique (up to right multiplication by nonsingular x-independent $m\times m$-matrices) with the following properties.

(i) The columns $\psi_i(\cdot,\lambda)$, $i\in[1,m]$, of $\psi(x,\lambda)$ are linearly independent and lie in $L^2_W([0,b))^{m\times 1}$ for $\lambda\in\mathbb{C}\backslash\mathbb{R}$;
(ii) $\psi_i(x,\lambda)$ satisfy the self-adjoint boundary condition (if any) of T at b;
(iii) $\mathcal{R}[\psi_i(x,\lambda)]-\lambda W\psi_i(x,\lambda)=0$.

The coefficient $M_B(\lambda)$ is the so-called *Titchmarsh–Weyl M-function* of the self-adjoint operator T, the spectrum of which coincides with the singularities of $M_B(\lambda)$, which can be seen to be analytic outside of $\mathbb{R}$. Moreover, we have that $M_B^*(\lambda)=M_B(\overline{\lambda})$ and that $M_B(\lambda)$ has positive imaginary part $(1/2i)[M_B(\lambda)-M_B^*(\lambda)]$ in the upper half plane, i.e., $M_B(\lambda)$ is a matrix-valued Nevanlinna-function, so that we have the following representation formula.

Lemma 2.2: With $M_B(\lambda)$ according to above, there is a unique increasing and left-continuous matrix-valued function ρ with $\rho(0)=0$ and unique Hermitian matrices $\mathcal{C}_1$ and $\mathcal{C}_2\geqslant 0$ such that

$$M_B(\lambda)=\mathcal{C}_1+\lambda\mathcal{C}_2+\int_{-\infty}^{\infty}\left(\frac{1}{t-\lambda}-\frac{t}{t^2+1}\right)d\rho(t).$$

Remark: In the present situation, one always has that $\mathcal{C}_2=0$, which will follow from the asymptotic formulas given later.

Remark 2.3: $d\rho$ is called the *spectral measure* of T for the following reason.

The spectral matrix ρ gives rise to a Hilbert space L^2_ρ of (equivalence classes of) $m\times 1$ matrix-valued functions with inner product

$$\langle \hat{U},\hat{V}\rangle_\rho = \int_{-\infty}^{\infty} \hat{V}^*(t)d\rho(t)\hat{U}(t).$$

With notation from (2.5), the spectral theory takes the following concrete form.

For $U\in L^2_W$, the integral

$$\hat{U}(t)=\int_0^b \varphi^*(x,t)WU(x)\,dx$$

converges in L^2_ρ and gives a unitary map $\mathcal{F}:U\mapsto\hat{U}$ between L^2_W and L^2_ρ, so that $\|U\|_W = \|\hat{U}\|_\rho$. The inverse of $\mathcal{F}$ is given by

$$U(x)=\int_{-\infty}^{\infty}\varphi(x,t)d\rho(t)\hat{U}(t),$$

with convergence in L^2_W. Furthermore, U is in the domain of T if and only if $t\hat{U}(t)\in L^2_\rho$, and then $\widehat{TU}(t)=t\hat{U}(t)$. The map $\mathcal{F}$ is called the generalized Fourier transform for T, and thus $\mathcal{F}$ is unitary and diagonalizes T.

For future reference, we also state the following lemma.

Lemma 2.4 (The Singular Value Decomposition (SVD)): Let $p\in\mathbb{Z}^+$ and $S\in\mathbb{C}^{p\times p}$. Then, there exists a unique diagonal matrix,

$$\mathrm{diag}(d_1,\ldots,d_p)=D\in\mathbb{C}^{p\times p},$$

with real elements satisfying that $d_i\geqslant d_j\geqslant 0$, if $i\leqslant j$, and unitary matrices $U,V\in\mathbb{C}^{p\times p}$ such that

$$S=U^*DV. \tag{2.7}$$

Proof: See Ref. 18, Theorem 2.3.1! □

Convention 2.5: Note that if

$$USV^*=D_S$$

is the SVD-decomposition of the matrix S in (2.2), it follows from (2.4) that, if $n=\dim N(S)>0$ with $N(S)$ denoting the nullspace of the matrix S,

$$UCV^*=\Lambda=\Lambda_1+\Lambda_2,$$

where

$$\Lambda_1=\begin{pmatrix}\Lambda_{11} & 0\\ 0 & 0\end{pmatrix},\quad \Lambda_{11}\in\mathbb{C}^{(m-n)\times(m-n)},\quad \Lambda_2=\begin{pmatrix}0 & 0\\ 0 & \Lambda_{22}\end{pmatrix},\quad \Lambda_{22}\in\mathbb{C}^{n\times n},$$

and where Λ_{22} is unitary. We could actually choose the matrices U and V so that $\Lambda_{22}=I$, and from this point on, if not specifically stated otherwise, we will do exactly that.

III. THE LEADING ORDER TERM ASYMPTOTICS FOR $M_B(\lambda)$

Our main purpose with this section is to give a very simple deduction of the leading order term asymptotics for $M_B(\lambda)$. This formula will be independent of the boundary condition at b although depending on the boundary value $F(0,\lambda)$. However, suppose that $F_1(0,\lambda)$ and

$F_2(0,\lambda)$ are two different initial values, of type (2.2), with M_1 and M_2 being the corresponding M-functions, using the same boundary condition at b. We then have that

$$M_2(\lambda)=-[C_{12}-S_{12}M_1(\lambda)][S_{12}+C_{12}M_1(\lambda)]^{-1}, \tag{3.1}$$

where

$$F_2^{-1}(0,\lambda)F_1(0,\lambda)=\begin{pmatrix} S_{12} & C_{12} \\ -C_{12} & S_{12}\end{pmatrix}, \quad S_{12},C_{12}\in\mathbb{C}^{m\times m},$$

is unitary and symplectic. Thus, asymptotic information on M_1 will render asymptotic information on M_2. We will therefore, from this point on, if not specifically stated otherwise, only consider the case when the M-function arises from the *Neumann boundary conditions* at 0, by which we mean the case of $S=I$ and $C=0$ in (2.2). This M-function will henceforth simply be denoted by M. Thus, by the initial values satisfied by F, it follows that $M(\lambda)=-\psi(0,\lambda)\times(P\psi')^{-1}(0,\lambda)$. In fact, since $\psi(x,\lambda)$ is unique (up to right multiplication by nonsingular $m\times m$-matrices) with the properties (i)–(iii) on page 6080, it follows that we must have that

$$M(\lambda)=-U(0,\lambda)(PU')^{-1}(0,\lambda) \tag{3.2}$$

for any nonsingular $m\times m$-matrix U with columns solving (1.1) and satisfying the boundary condition at b. Now, let $x\in(0,b)$ and consider the operator generated by $\mathcal{R}$ in $L^2_W([x,b))^{m\times 1}$ under the Neumann boundary condition at x and the same boundary condition as before at b. The corresponding M-function is then given by $\hat{M}(x,\lambda)=-\psi(x,\lambda)(P\psi')^{-1}(x,\lambda)$, i.e., $\hat{M}$ is the Neumann M-function for the interval $[x,b)$. In particular, we have $M(\lambda)=\hat{M}(0,\lambda)$. Since the columns of ψ are solutions of (1.1), we have

$$(P\psi')'=(Q-\lambda W)\psi, \tag{3.3}$$

and hence, from (3.3), that $\hat{M}$ satisfies the following Riccati equation:

$$\hat{M}'=\hat{M}(Q-\lambda W)\hat{M}-P^{-1}. \tag{3.4}$$

Our main result in this section is Theorem 3.2. below, where we apply the following convention.

Convention 3.1: For any diagonalizable matrix A, with $A=S^{-1}DS$ and D diagonal, we define $\sqrt{A}=S^{-1}\sqrt{D}S$, where $\sqrt{D}$ is obtained by taking the principal root of each element of D, i.e., the argument of the root is in the interval $(-\pi/2,\pi/2]$. It is easily seen that this defines $\sqrt{A}$ uniquely.

Theorem 3.2: *Under Hypothesis 1.1 and the above conditions, we have that*

$$M(\lambda)=(P(0)\sqrt{-\lambda P^{-1}(0)W(0)}\,)^{-1}[I+o(1)], \quad \lambda=r\mu,$$

where μ is to be confined to a compact set in $\mathbb{C}\backslash\mathbb{R}$ and $r\in\mathbb{R}^+$ is large.

Remark 3.3: Note that $-\lambda P^{-1}(0)W(0)$ is diagonalizable since it is assumed that $W(0)>0$. Also note that in the special case of equation (1.4), we have that $P(0)=W(0)=I$ in Theorem 3.2, so that in this case

$$M(\lambda)=\frac{1}{\sqrt{-\lambda}}[I+o(1)].$$

In fact, with notation from (3.4), this formula is easily seen to hold, locally uniformly in x, for M replaced by $\hat{M}(x,\lambda)$ (see Theorem 3.6 below).

In order to prove Theorem 3.2, we put

$$\mathcal{T}(r)=\begin{pmatrix} r^{-1/4}I & 0 \\ 0 & r^{1/4}I \end{pmatrix},$$

for $r>0$. Define also

$$F_r(t,\mu)=\mathcal{T}^{-1}(r)F\left(\frac{t}{\sqrt{r}},r\mu\right)\mathcal{T}(r);$$

$$A_r(t)=\begin{pmatrix} Q_r(t) & 0 \\ 0 & -P_r^{-1}(t) \end{pmatrix}=\frac{1}{\sqrt{r}}\mathcal{T}^*(r)A\left(\frac{t}{\sqrt{r}}\right)\mathcal{T}(r)=\begin{pmatrix} r^{-1}Q\left(\frac{t}{\sqrt{r}}\right) & 0 \\ 0 & -P^{-1}\left(\frac{t}{\sqrt{r}}\right) \end{pmatrix}; \tag{3.5}$$

$$K_r(t)=\begin{pmatrix} W_r(t) & 0 \\ 0 & 0 \end{pmatrix}=\sqrt{r}\mathcal{T}^*(r)K\left(\frac{t}{\sqrt{r}}\right)\mathcal{T}(r)=K\left(\frac{t}{\sqrt{r}}\right).$$

Simple calculations then show that F_r is a fundamental matrix for the equation

$$-JV_r'+A_rV_r=\mu K_rV_r, \quad x\in[0,b\sqrt{r}), \tag{3.6}$$

with $F_r(0,\mu)=I$.

In some sense, we clearly have that

$$A_r(t)\to\begin{pmatrix} 0 & 0 \\ 0 & -P^{-1}(0) \end{pmatrix} \text{ and that } K_r(t)\to\begin{pmatrix} W(0) & 0 \\ 0 & 0 \end{pmatrix}, \quad r\to\infty,$$

and we may therefore expect that F_r tends to the fundamental solution F_∞ of the equation (3.7) with initial data $F_\infty(0,\mu)=I$. As we shall see, the scaling (3.5) corresponds to introducing a scaled M-function $M_r(\mu)=\sqrt{r}M(r\mu)$, and we may expect that M_r converges to an M-function M_∞ for the equation (3.7). If M_∞ can be determined, we would get the asymptotic formula $M(r\mu)\sim(1/\sqrt{r})\,M_\infty(\mu)$. In order to carry this scheme out, we will make use of the following results, where we consider a locally integrable matrix-valued function $x\mapsto T_s(x)$ depending on a parameter $s\in\mathbb{R}^d$, $d\in\mathbb{Z}^+$. Letting $\|\cdot\|$ denote some suitable matrix norm, we may then define the total variation measure of the matrix-valued measure $T_s(x)\,dx$ to be $\|T_s(x)\|\,dx$.

Proposition 3.4: Let $T_s\in L^1_{\mathrm{loc}}([0,b))^{n\times n}$ be depending on a parameter $s\in\mathcal{O}\subseteq\mathbb{R}^d$, and assume that the total variation $\int_0^x\|T_s(\cdot)\|$ is uniformly bounded, locally in (x,s). Assume also that the integral functions $\int_0^x T_s$ are jointly continuous in (x,s). Then any solution U_s of the equation $U_s'+T_sU_s=0$ with s-independent initial data depends continuously on (x,s).

Proof: See Ref. 9, Theorem 3.1! □

Proposition 3.5: Assume that, with notation from (3.5) *and locally uniformly in x, $\int_0^x A_r\to\int_0^x A_\infty$ and $\int_0^x K_r\to\int_0^x K_\infty$, when $r\to\infty$. Assume also that the total variations $\int_0^x\|A_r\|$ and $\int_0^x\|K_r\|$ are bounded, when $r\to\infty$, locally uniformly in x. Let F_∞ be a fundamental solution of*

$$-JF_\infty'+A_\infty F_\infty=\mu K_\infty F_\infty, \quad F_\infty(0,\mu)=I. \tag{3.7}$$

Then

$$\int_0^x F_r^*K_rF_r\to\int_0^x F_\infty^*K_\infty F_\infty, \quad when \quad r\to\infty,$$

locally uniformly in (x,μ).

Proof: Setting $s=(\mathrm{Re}\,\mu,\mathrm{Im}\,\mu,1/r)$, this is an immediate consequence of Proposition 3.4 (cf. Ref. 9, Corollary 3.3). □

Proof (Theorem 3.2.): Assume that M is an M-function corresponding to a self-adjoint realization of (1.5). For

$$\Psi(t,\lambda)=F(t,\lambda)\begin{pmatrix}-M(\lambda)\\ I\end{pmatrix},$$

we then have that

$$\int_0^b \Psi^* K\Psi=\frac{\frac{1}{2i}[M(\lambda)-M^*(\lambda)]}{\mathrm{Im}\,\lambda}=\frac{\mathrm{Im}\,M(\lambda)}{\mathrm{Im}\,\lambda}. \tag{3.8}$$

In the limit-point case, this relation determines M uniquely. A consequence of (3.8) is that M is nonsingular when $\lambda\in\mathbb{C}\backslash\mathbb{R}$, since $\Psi^*K\Psi=\psi^*W\psi>0$ implies that $\int_0^b\Psi^*K\Psi>0$, and any matrix with a strictly positive imaginary part is nonsingular. Now put

$$M_r(\mu)=\sqrt{r}M(r\mu).$$

It then follows that

$$\int_0^{b\sqrt{r}}\Psi_r^*K_r\Psi_r=\frac{\mathrm{Im}\,M_r(\mu)}{\mathrm{Im}\,\mu}, \tag{3.9}$$

where we have put $\Psi_r=F_r\left(\begin{smallmatrix}-M_r\\ I\end{smallmatrix}\right)$, i.e., $M_r(\mu)$ could be considered a Neumann M-function corresponding to (3.6). This would require us to verify that the columns of $\Psi_r(t,\mu)$ satisfy a μ independent boundary condition at $b\sqrt{r}$. However, all that we need is in fact the inequality

$$\int_0^a\Psi_r^*K_r\Psi_r\leqslant\frac{\mathrm{Im}\,M_r(\mu)}{\mathrm{Im}\,\mu}. \tag{3.10}$$

It immediately follows from (3.9) that this is true for any $a>0$, as soon as $b\sqrt{r}>a$. Since

$$M(r\mu)=\frac{1}{\sqrt{r}}M_r(\mu), \tag{3.11}$$

we obtain an asymptotic formula for M, if we can show that M_r has a limit as $r\to\infty$. We have

$$\frac{1}{r}\int_0^x Q\left(\frac{t}{\sqrt{r}}\right)dt=\frac{1}{\sqrt{r}}\int_0^{x/\sqrt{r}}Q(t)\,dt\quad\to\quad 0,$$

$$\int_0^x P^{-1}\left(\frac{t}{\sqrt{r}}\right)dt=\sqrt{r}\int_0^{x/\sqrt{r}}P^{-1}(t)\,dt\quad\to\quad xP^{-1}(0)$$

and

$$\int_0^x W\left(\frac{t}{\sqrt{r}}\right)dt=\sqrt{r}\int_0^{x/\sqrt{r}}W(t)\,dt\quad\to\quad xW(0),$$

locally uniformly as $r\to\infty$, by the assumptions made on Q, P^{-1} and W in Hypothesis 1.1. Writing

$$A_\infty=\begin{pmatrix}0 & 0\\ 0 & -P^{-1}(0)\end{pmatrix} \quad \text{and} \quad K_\infty=\begin{pmatrix}W(0) & 0\\ 0 & 0\end{pmatrix},$$

this means, by (3.5), that

$$\int_0^x A_r\to\int_0^x A_\infty, \quad \text{and that} \quad \int_0^x K_r\to\int_0^x K_\infty, \quad r\to\infty,$$

locally uniformly in x.

Since K, and thus K_r, is non-negative, it follows that in the modulus largest elements in these matrices, respectively, are positive and located on the main diagonal. It is then easily seen that the total variation $\int_0^x\|K_r\|$ is bounded, as $r\to\infty$, locally uniformly in x. Since P is not assumed positive, however, it is possible that $\int_0^x\|A_r\|$ is not similarly bounded. We therefore proceed as follows. Put

$$\tilde V_r(t,\mu)=Z_r^{-1}(t)V_r(t,\mu),$$

where $Z_r(0)=I$, and Z_r solves

$$-JZ_r'+\begin{pmatrix}0 & 0\\ 0 & -P_r^{-1}\end{pmatrix}Z_r=0.$$

It then immediately follows that

$$Z_r=\begin{pmatrix}I & \int_0^t P_r^{-1}\\ 0 & I\end{pmatrix},$$

and hence

$$Z_r(t)\to Z_\infty(t)=\begin{pmatrix}I & tP^{-1}(0)\\ 0 & I\end{pmatrix},$$

locally uniformly. It also follows that

$$-J\tilde V_r'+Z_r^*\begin{pmatrix}Q_r-\mu W_r & 0\\ 0 & 0\end{pmatrix}Z_r\tilde V_r=0,$$

so that $\tilde V_r$ converges, locally uniformly, according to Proposition 3.4. This implies that $Z_r\tilde V_r=V_r\to V_\infty=Z_\infty\tilde V_\infty$, locally uniformly, and a direct calculation shows that V_∞ still solves the limit equation (3.7). Hence, it follows that

$$\int_0^a F_r^*K_rF_r\to\int_0^a F_\infty^*K_\infty F_\infty, \quad r\to\infty, \tag{3.12}$$

where $F_\infty(x,\mu)$ is the fundamental matrix-solution of (3.7), for which

$$F_\infty(0,\mu)=I.$$

We shall now determine the M-function of the limit equation (3.7). With the notation

$$\mathcal{K}=\sqrt{-\mu P^{-1}(0)W(0)},$$

it follows that (3.7) is the equation

$$U''=-\mu P^{-1}(0)W(0)U.$$

Using Convention 3.1, it is clear that the general solution is

$$U(t)=e^{\mathcal{K}t}C_1+e^{-\mathcal{K}t}C_2, \quad C_1,C_2\in\mathbb{C}^{m\times m},$$

since $\mathcal{K}$ is invertible. It is easy to see that all eigenvalues of $\mathcal{K}$ have real part >0 if μ is not real, and thus $U^*W(0)U$ is integrable precisely if $C_1=0$. Thus the limit equation is limit-point, and the Neumann M-function is obtained as in (3.2) for $C_1=0$ and $C_2=I$. It follows that

$$M_\infty(\mu)=-U(0,\mu)(P(0)U'(0,\mu))^{-1}=(P(0)\mathcal{K})^{-1}=(P(0)\sqrt{-\mu P^{-1}(0)W(0)}\,)^{-1},$$

and we finally need to show that $M_r(\mu)\to M_\infty(\mu)$, as $r\to\infty$. In order to do this, fix $a\in(0,\infty)$, $\mu\in\mathbb{C}\backslash\mathbb{R}$ and consider the compact set of $m\times m$-matrices M defined by

$$(M^* \quad I)\int_0^a F_\infty^*(\cdot,\mu)K_\infty F_\infty(\cdot,\mu)\begin{pmatrix}M\\ I\end{pmatrix}\leqslant\frac{\operatorname{Im}M}{\operatorname{Im}\mu}.$$

That the set is compact is due to the fact that the left hand-side of the inequality defining it contains a positive quadratic term, and is bounded by a linear term. Because the equation is limit-point, the set shrinks to a point as $a\to\infty$. Furthermore, if Ω is a neighborhood of the set, it follows from (3.10) that $M_r(\mu)\in\Omega$, if r is large. Hence, we conclude that

$$M_r(\mu)\to M_\infty(\mu), \quad r\to\infty. \tag{3.13}$$

Thus, it follows from (3.11) and (3.13) that

$$M(\lambda)=M(r\mu)=\frac{1}{\sqrt{r}}[M_\infty(\mu)+o(1)]=(P(0)\sqrt{-\lambda P^{-1}(0)W(0)}\,)^{-1}[I+o(1)].$$

□

Note that, in the case of continuous P^{-1} and W, it follows that, by replacing $t/\sqrt{r}$ by $t/\sqrt{r}+y$, $y\in[0,c]$, $c\in(0,b)$, in (3.5), the crucial inequality (3.10) becomes true, independent of y, as soon as $r>a^2/(b-c)^2$. Moreover, since, in this case, the total variation $\mathcal{V}_s(x)=\int_0^x\|A_r-\mu K_r\|$, for $s=(\operatorname{Re}\mu,\operatorname{Im}\mu,1/r,y)$, is bounded, locally uniformly in (x,s), and since the integral functions $\mathcal{I}_s(x)=\int_0^x(A_r-\mu K_r)$ are jointly continuous in (x,s), Proposition 3.4 gives that the convergence (3.12) is locally uniform in y, so that the proof of Theorem 3.2 shows that we have the following result.

Theorem 3.6: *With P^{-1} and W being continuous, $W(y)>0$, for all y, and with notation from (3.4), we have that*

$$\hat{M}(y,\lambda)=(P(y)\sqrt{-\lambda P^{-1}(y)W(y)}\,)^{-1}[I+o(1)], \quad \lambda=r\mu,$$

with λ as in Theorem 3.2, locally uniformly in y.

Remark 3.7: The method of proof above is adapted from a general scheme given in Ref. 9!

IV. A QUOTIENT REPRESENTATION OF $M(\lambda)$

To begin with, we make the following assumption.

Hypothesis 4.1: Assume that, in the equation

$$-U''+QU=\lambda U, \quad x\in[0,\infty), \tag{4.1}$$

we have that $Q=Q^*\in L^1([0,\infty))^{m\times m}$.

Remark 4.2: Note that, with terminology and notation from Remark 1.2, equation (4.1) can be rewritten as the system

$$-JV'+AV=\lambda KV \;\Leftrightarrow\; V'=\begin{pmatrix} 0 & I \\ Q-\lambda I & 0 \end{pmatrix}V, \quad x\in[0,\infty), \tag{4.2}$$

where thus $P=W=I$.

We will prove the following theorem (for the scalar case, cf. Ref. 22).

Theorem 4.3: *Let, under Hypothesis 4.1,* $M(\lambda)$ *be the Neumann M-function of (4.2). Furthermore, let the sequences* $\{R_n\}$ *and* $\{Q_n\}$, $Q_1=R_1$, *be defined by (4.16) and (4.22), (4.24), respectively. Then, there exists a* λ_0 *such that*

$$M(\lambda)=\frac{1}{\sqrt{-\lambda}}\lim_{n\to\infty}[I+R_n(0,\lambda)][I-R_n(0,\lambda)]^{-1}, \tag{4.3}$$

$$M(\lambda)=\frac{1}{\sqrt{-\lambda}}\left[I+\sum_{n=1}^{\infty}Q_n(0,\lambda)\right]\left[I-\sum_{n=1}^{\infty}Q_n(0,\lambda)\right]^{-1}, \tag{4.4}$$

as soon as $|\lambda|\geqslant\lambda_0$. *For such* λ, *the convergence is uniform in both* (4.3) and (4.4).

Remark: Note that $R=\lim_{n\to\infty}R_n(0,\lambda)$ corresponds to the reflection coefficient in the scalar case!

Remark: For error estimates, see Remark 4.6.

In order to prove this theorem, we give the following lemma, which also turns out to be useful for later needs. This is an elementary result on finite-dimensional evolution equations, and can also be found in Ref. 12, Lemma 4.2 and Ref. 30.

Lemma 4.4: If $A,B,C\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, *where* $0<b\leqslant\infty$, *then any* $m\times m$*-matrix-valued solution* $X(x)$ *of*

$$X'(x)=A(x)X(x)+X(x)B(x)+C(x), \tag{4.5}$$

for a.a. $x\in[0,b)$, *is of the form*

$$X(x)=Z(x)D(x)Y(x),$$

where Y *and* Z *are fundamental matrices of the systems*

$$Y'(x)=Y(x)B(x) \quad \text{and} \quad Z'(x)=A(x)Z(x),$$

respectively, and where D *is an* $m\times m$*-matrix such that*

$$D(x)=D(0)+\int_0^x Z^{-1}(t)C(t)Y^{-1}(t)\,dt.$$

Proof (Lemma 4.4): Setting $D=Z^{-1}XY^{-1}$, we obtain that

$$D'=(Z^{-1}XY^{-1})'=-Z^{-1}Z'Z^{-1}XY^{-1}+Z^{-1}X'Y^{-1}-Z^{-1}XY^{-1}Y'Y^{-1}=Z^{-1}CY^{-1},$$

so that

$$D(x)=D(0)+\int_0^x Z^{-1}(t)C(t)Y^{-1}(t)\,dt.$$

□

Lemma 4.5: Let $A=(1/2\sqrt{-\lambda})\,Q$, *where* $Q\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, $0<b\leqslant\infty$. *Then the solutions of*

$$Y'=YA \quad \text{and} \quad Z'=AZ$$

satisfy that

$$Y(x)=Y(0)\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right), \tag{4.6}$$

$$Z(x)=\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right)Z(0), \tag{4.7}$$

for large $|\lambda|$, *locally uniformly in* x.

Proof: Since

$$Y(x)=Y(0)+\frac{1}{2\sqrt{-\lambda}}\int_0^x Y(t)Q(t)\,dt$$

and

$$Z(x)=Z(0)+\frac{1}{2\sqrt{-\lambda}}\int_0^x Q(t)Z(t)\,dt,$$

the lemma is a consequence of Grönwall's inequality (cf. Ref. 6, Lemma 1.3). □

Proof (Theorem 4.3.): Taking (4.2) of *Remark 4.2* as a starting-point, we diagonalize the matrix $\left(\begin{smallmatrix}0 & I\\ -\lambda I & 0\end{smallmatrix}\right)$, which, for large λ, is the important part of the coefficient matrix. With notation

$$\tilde{V}=\mathcal{A}V,$$

where

$$V=\begin{pmatrix}U\\ U'\end{pmatrix}, \quad \tilde{V}=\begin{pmatrix}\tilde{V}_1\\ \tilde{V}_2\end{pmatrix} \quad \text{and} \quad \mathcal{A}=\frac{1}{2}\begin{pmatrix}I & \dfrac{1}{\sqrt{-\lambda}}I\\ I & -\dfrac{1}{\sqrt{-\lambda}}I\end{pmatrix}, \tag{4.8}$$

and hence

$$\mathcal{A}^{-1}=\begin{pmatrix}I & I\\ \sqrt{-\lambda}I & -\sqrt{-\lambda}I\end{pmatrix},$$

we then obtain that

$$\tilde{V}'=\mathcal{A}V'=\mathcal{A}\begin{pmatrix}0 & I\\ Q-\lambda I & 0\end{pmatrix}\mathcal{A}^{-1}\tilde{V}=\left\{\begin{pmatrix}\sqrt{-\lambda}I & 0\\ 0 & -\sqrt{-\lambda}I\end{pmatrix}+\frac{1}{2\sqrt{-\lambda}}Q\begin{pmatrix}I & I\\ -I & -I\end{pmatrix}\right\}\tilde{V}. \tag{4.9}$$

Now, put $R=\tilde{V}_1\tilde{V}_2^{-1}$ and note that $-M=UU'^{-1}$. From (4.8), it follows that

$$M=\frac{1}{\sqrt{-\lambda}}(\tilde{V}_1+\tilde{V}_2)(\tilde{V}_2-\tilde{V}_1)^{-1}=\frac{1}{\sqrt{-\lambda}}(I+R)(I-R)^{-1}, \tag{4.10}$$

and, by (4.9), that R will satisfy the Riccati equation

$$R'=2\sqrt{-\lambda}R+\frac{1}{2\sqrt{-\lambda}}QR+\frac{1}{2\sqrt{-\lambda}}RQ+\frac{1}{2\sqrt{-\lambda}}RQR+\frac{1}{2\sqrt{-\lambda}}Q. \tag{4.11}$$

We may view this Riccati equation as an equation of type (4.5), of Lemma 4.4, with

$$A=2\sqrt{-\lambda}I+\frac{1}{2\sqrt{-\lambda}}Q, \quad B=\frac{1}{2\sqrt{-\lambda}}Q$$

and

$$C=\frac{1}{2\sqrt{-\lambda}}RQR+\frac{1}{2\sqrt{-\lambda}}Q,$$

so that the systems to be considered are

$$Z'=\left(2\sqrt{-\lambda}I+\frac{1}{2\sqrt{-\lambda}}Q\right)Z \quad \text{and} \quad Y'=Y\left(\frac{1}{2\sqrt{-\lambda}}Q\right). \tag{4.12}$$

Since the system

$$Z'=\left(2\sqrt{-\lambda}I+\frac{1}{2\sqrt{-\lambda}}Q\right)Z,$$

with notation $\tilde{Z}=e^{-2\sqrt{-\lambda}x}Z$, can be written as

$$\tilde{Z}'=\frac{1}{2\sqrt{-\lambda}}Q\tilde{Z},$$

it follows from Lemma 4.5 that

$$Y(x)=Y(0)\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right) \quad \text{and} \quad Z(x)=\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right)Z(0)e^{2\sqrt{-\lambda}x}. \tag{4.13}$$

Since Y^{-1} and $\tilde{Z}^{-1}$ solve the equations

$$(Y^{-1})'=-\frac{1}{2\sqrt{-\lambda}}QY^{-1} \quad \text{and} \quad (\tilde{Z}^{-1})'=-\tilde{Z}^{-1}\left(\frac{1}{2\sqrt{-\lambda}}Q\right),$$

similar arguments give that also

$$Y^{-1}(x)=\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right)Y^{-1}(0),$$

$$Z^{-1}(x)=e^{-2\sqrt{-\lambda}x}Z^{-1}(0)\left(I+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right). \tag{4.14}$$

With notation from (4.12), we will now seek to find a solution $R(x)$ of (4.11), with $R(\infty)=0$. By Lemma 4.4, such a solution would satisfy

$$R(x)=-\frac{Z(x)}{2\sqrt{-\lambda}}\left(\int_x^\infty Z^{-1}(t)[R(t)Q(t)R(t)+Q(t)]Y^{-1}(t)\,dt\right)Y(x). \tag{4.15}$$

Now, provided the integrals exist, we recursively define the sequence of functions $\{R_n(x)\}$ by

$$R_0=0,$$

$$R_{n+1}(x)=-\frac{Z(x)}{2\sqrt{-\lambda}}\left(\int_x^\infty Z^{-1}(t)[R_n(t)Q(t)R_n(t)+Q(t)]Y^{-1}(t)\,dt\right)Y(x). \tag{4.16}$$

Now, put

$$r_n(x,\lambda)=\sup_{t\geqslant x}\|R_n(t,\lambda)\| \quad \text{and} \quad \tilde{\mathcal{N}}_x(\lambda)=\frac{1}{2\sqrt{|\lambda|}}\int_x^\infty \|Q(t)\|\,dt.$$

Since

$$R_1(x,\lambda)=-\frac{1}{2\sqrt{-\lambda}}\int_x^\infty Z(x)Z^{-1}(t)Q(t)Y^{-1}(t)Y(x)\,dt,$$

it follows immediately from (4.13)–(4.14) and their deductions that

$$\|R_1(x,\lambda)\|\leqslant\frac{1}{2\sqrt{|\lambda|}}\int_x^\infty\|Q\|\left(1+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right)\to 0, \tag{4.17}$$

uniformly in x, when $\lambda\to\infty$, bringing us to the conclusion that $r_1(x,\lambda)$ too has this property. Furthermore, we have that $\|R_1(x,\lambda)\|\leqslant\mathcal{C}\tilde{\mathcal{N}}_0(\lambda)$ for some constant $\mathcal{C}$, when λ is large. Now $\tilde{\mathcal{N}}_x(\lambda)$ is uniformly bounded in x, when $|\lambda|\to\infty$. Since also $r_1(x,\lambda)\leqslant r_1(0,\lambda)$, we thus conclude that there exists a λ_0 such that

$$4r_1(0,\lambda)\mathcal{C}\tilde{\mathcal{N}}_0(\lambda)<1, \quad \text{when} \quad |\lambda|\geqslant\lambda_0. \tag{4.18}$$

By (4.16), it now follows that

$$r_{n+1}(x,\lambda)\leqslant r_1(x,\lambda)+\mathcal{C}\tilde{\mathcal{N}}_x(\lambda)r_n(x,\lambda)^2, \tag{4.19}$$

and hence a simple induction yields

$$r_n(x,\lambda)\leqslant 2r_1(x,\lambda), \quad n=1,2,\ldots. \tag{4.20}$$

Now, put

$$d_n(x,\lambda)=\sup_{t\geqslant x}\|R_n(t,\lambda)-R_{n-1}(t,\lambda)\|.$$

Since, by (4.16),

$$R_n(x,\lambda)-R_{n-1}(x,\lambda)=-\frac{1}{4\sqrt{-\lambda}}\int_x^\infty Z(x)Z^{-1}(t)\times\{[R_{n-1}(t,\lambda)-R_{n-2}(t,\lambda)]Q(t)[R_{n-1}(t,\lambda)$$
$$+R_{n-2}(t,\lambda)]+[R_{n-1}(t,\lambda)+R_{n-2}(t,\lambda)]Q(t)[R_{n-1}(t,\lambda)-R_{n-2}(t,\lambda)]\}$$
$$\times Y^{-1}(t)Y(x)\,dt,$$

it follows from (4.20) that

$$d_n(x,\lambda)\leqslant 4\mathcal{C}\tilde{\mathcal{N}}_x(\lambda)r_1(x,\lambda)d_{n-1}(x,\lambda).$$

As $d_1=r_1$, it follows that

$$d_n(x,\lambda)\leqslant[4\mathcal{C}\tilde{\mathcal{N}}_x(\lambda)r_1(x,\lambda)]^{n-1}r_1(x,\lambda). \tag{4.21}$$

From (4.18), we then obtain that $R_n(x,\lambda)$ has to converge, uniformly in x and λ, to the solution of (4.15), as soon as $|\lambda|\geqslant\lambda_0$.

Now, put $Q_1(x,\lambda)=R_1(x,\lambda)$, where R_1 is given by (4.16). Thus, Q_1 is the quantity obtained by deleting the quadratic term in (4.15). Also put $S_1=R-Q_1$. Then, S_1 satisfies the equation

$$S_1'-A_1S_1-S_1B_1=\frac{1}{2\sqrt{-\lambda}}(S_1QS_1+Q_1QQ_1),$$

where

$$A_1=2\sqrt{-\lambda}I+\frac{1}{2\sqrt{-\lambda}}(I+Q_1)Q,\quad B_1=\frac{1}{2\sqrt{-\lambda}}Q(I+Q_1).$$

Deleting the quadratic term S_1QS_1, the solution is

$$Q_2(x,\lambda)=-\int_x^\infty Z_1(x)Z_1^{-1}(t)\left(\frac{1}{2\sqrt{-\lambda}}Q_1(t)Q(t)Q_1(t)\right)Y_1^{-1}(t)Y_1(x)\,dt,$$

where $Z_1'=A_1Z_1$ and $Y_1'=Y_1B_1$. Now, by putting $S_2=R-Q_1-Q_2$ and repeating this procedure, we obtain a sequence Q_n, $n=1,2,\ldots$, where Q_n satisfies that

$$Q_n'=A_{n-1}Q_n+Q_nB_{n-1}+\frac{1}{2\sqrt{-\lambda}}Q_{n-1}QQ_{n-1}, \tag{4.22}$$

and, with notation $\Sigma_{n-1}=\Sigma_{j=0}^{n-1}Q_j$,

$$A_{n-1}=2\sqrt{-\lambda}I+\frac{1}{2\sqrt{-\lambda}}\Sigma_{n-1}Q,\quad B_{n-1}=\frac{1}{2\sqrt{-\lambda}}Q\Sigma_{n-1}, \tag{4.23}$$

where we have set $Q_0=I$. The solution of (4.22), vanishing at ∞, is

$$Q_n(x,\lambda)=-\int_x^\infty Z_{n-1}(x)Z_{n-1}^{-1}(t)\left(\frac{1}{2\sqrt{-\lambda}}Q_{n-1}(t)Q(t)Q_{n-1}(t)\right)Y_{n-1}^{-1}(t)Y_{n-1}(x)\,dt, \tag{4.24}$$

where

$$Z'_{n-1}=A_{n-1}Z_{n-1} \quad \text{and} \quad Y'_{n-1}=Y_{n-1}B_{n-1}. \tag{4.25}$$

By (4.17), it follows that $r_1(0,\lambda)\to 0$, $\lambda\to\infty$, so there exists a λ_0 with the property that

$$r_1(0,\lambda)<\min\left(\frac{1}{2},\frac{1}{2\hat{\mathcal{N}}_0}\right), \quad \text{when} \quad |\lambda|\geqslant\lambda_0, \tag{4.26}$$

where $\hat{\mathcal{N}}_x=\frac{1}{2}\int_x^\infty\|Q\|$. By induction, we shall now see that Q_n is well-defined, and that

$$\|Q_n(x,\lambda)\|\leqslant r_1(x,\lambda)[\hat{\mathcal{N}}_x r_1(x,\lambda)]^{2^{n-1}-1}. \tag{4.27}$$

For $n=1$, (4.27) is true by definition. Now, assume that (4.27) is true for $n\leqslant N$. By (4.23)–(4.25) and Lemma 4.5, we then have that

$$\begin{aligned}\|Q_{N+1}(x,\lambda)\|&\leqslant\frac{1}{2|\sqrt{-\lambda}|}\int_x^\infty\left(1+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)\right)\|Q\|\|Q_N\|^2\\&\leqslant[r_1(x,\lambda)[\hat{\mathcal{N}}_x r_1(x,\lambda)]^{2^{N-1}-1}]^2\hat{\mathcal{N}}_x=r_1(x,\lambda)[\hat{\mathcal{N}}_x r_1(x,\lambda)]^{2^N-1},\end{aligned}$$

for large λ. Now, since $r_1(x,\lambda)\leqslant r_1(0,\lambda)$, it follows from (4.26) that

$$\|Q_N(x,\lambda)\|\leqslant r_1(0,\lambda)[\hat{\mathcal{N}}_0 r_1(0,\lambda)]^{2^{N-1}-1}\leqslant 2^{-N}. \tag{4.28}$$

Thus, we conclude that the series $S(x,\lambda)=\Sigma_{n=1}^\infty Q_n(x,\lambda)$ converges uniformly in x and $|\lambda|\geqslant\lambda_0$. Moreover, it now follows from (4.22) and (4.28) that it is permissible with termwise differentiation of the series S. By (4.22), it also follows that S satisfies (4.11). That $S(x,\lambda)\to 0$, $x\to\infty$, follows by dominated convergence. Thus, we conclude that S satisfies (4.15).

Since now, for a solution R of (4.11), a straightforward calculation shows that a solution of (4.9) may be found by solving the equation

$$\tilde{V}'_2=-\sqrt{-\lambda}\tilde{V}_2-\frac{1}{2\sqrt{-\lambda}}Q\tilde{V}_2-\frac{1}{2\sqrt{-\lambda}}QR\tilde{V}_2$$

and then setting $\tilde{V}_1=R\tilde{V}_2$, our proof is complete in view of the fact that the Neumann M-function for the interval $[0,\infty)$ is $M(\lambda)=-U(0,\lambda)U'^{-1}(0,\lambda)$. □

Remark 4.6: Note that it immediately follows from (4.27) that, for large λ,

$$\|Q_n(x,\lambda)\|\leqslant\left(\frac{(1+\varepsilon)^2}{2|\sqrt{-\lambda}|}\int_x^\infty\|Q\|\right)^{2^{n-1}}.$$

To see what happens if the condition of Q in Hypothesis 4.1 is weakened to $Q=Q^*\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, we shall make use of the following lemma, and from this point on, when referring to a *nonreal sector*, we will mean a closed sector with a vertex at the origin and not intersecting the real line.

Lemma 4.7: Suppose $Q=Q^*\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$ *and* $c\in(0,b)$. *Then, put* $Q(x)=\tilde{Q}(x)$ *for* $x\in[0,c)$ *and* $\tilde{Q}(x)=0$ *for* $x>c$. *Furthermore, let* $\tilde{M}_B$ *be the* M*-function for the potential* $\tilde{Q}$, *and corresponding to the boundary condition* (2.2), *on the interval* $[0,\infty)$. *Then*

$$M_B(\lambda)-\tilde{M}_B(\lambda)=\mathcal{O}(e^{-2(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}}),$$

for all $\varepsilon>0$, *as* $\lambda\to\infty$ *in any nonreal sector*.

Proof: Assume first that $S=I$ and $C=0$ in (2.2) (i.e., the case of the Neumann boundary condition at 0) and let M and $\tilde{M}$ denote the corresponding (Neumann) M-functions. Consider the Riccati-equations (see (3.4)) satisfied by M and $\tilde{M}$, respectively, on $[0,c)$,

$$M'=M(Q-\lambda I)M-I,$$

$$\tilde{M}'=\tilde{M}(\tilde{Q}-\lambda I)\tilde{M}-I,$$

where it follows from Theorem 3.6 that

$$M,\tilde{M}=\frac{1}{\sqrt{-\lambda}}[I+o(1)], \tag{4.29}$$

uniformly in x for $x\in[0,c]$. Using the Riccati equations, it follows that

$$\begin{aligned} M'-\tilde{M}'=&(-\tfrac{1}{2}\lambda(M+\tilde{M})+\tfrac{1}{2}(M+\tilde{M})Q)(M-\tilde{M})\\ &+(M-\tilde{M})(-\tfrac{1}{2}\lambda(M+\tilde{M})+\tfrac{1}{2}Q(M+\tilde{M})), \end{aligned} \tag{4.30}$$

which is an equation of type (4.5) with

$$A=-\frac{1}{2}\lambda(M+\tilde{M})+\frac{1}{2}(M+\tilde{M})Q=\sqrt{-\lambda}[I+o(1)]+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)Q,$$

$$B=-\frac{1}{2}\lambda(M+\tilde{M})+\frac{1}{2}Q(M+\tilde{M})=\sqrt{-\lambda}[I+o(1)]+Q\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right),$$

$$C=0,$$

where the last equalities in the formulas above follow from (4.29).

We now consider the equations

$$Y'=AY,\quad Y(c)=I; \tag{4.31}$$

$$Z'=ZB,\quad Z(c)=I. \tag{4.32}$$

Since, by (4.29), $\tilde{Y}(x)=e^{\sqrt{-\lambda}(c-x)}Y(x)$ satisfies the equation

$$\tilde{Y}'=\left(\sqrt{-\lambda}\,o(1)+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)Q\right)\tilde{Y},$$

or, equivalently,

$$\tilde{Y}(x)=I-\int_x^c\left(\sqrt{-\lambda}\,o(1)+\mathcal{O}\left(\frac{1}{\sqrt{|\lambda|}}\right)Q\right)\tilde{Y}(t)\,dt,$$

it is now an immediate consequence of Grönwall's inequality that

$$Y(0)=\mathcal{O}(e^{-(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}}),$$

as $\lambda\to\infty$ in the prescribed way. Analogous calculations for Z yield that also

$$Z(0)=\mathcal{O}(e^{-(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}}).$$

Since now, by Lemma 4.4,

$$M(\lambda)-\tilde{M}(\lambda)=Z(0)DY(0),$$

for some matrix D, independent of x, satisfying that $D=\mathcal{O}(1/|\sqrt{-\lambda}|)$, the lemma follows in this special case.

In the general case, we have that (see (3.1))

$$\tilde{M}_B=(S-\tilde{M}C)^{-1}(C+\tilde{M}S) \quad \text{and} \quad M_B=(S-MC)^{-1}(C+MS). \tag{4.33}$$

Letting $USV^*=D_S$ be the SVD-decomposition of the matrix S according to Lemma 2.4 and Convention 2.5, it follows that

$$VM_BV^*=\left[D_S-\frac{1}{\sqrt{-\lambda}}\Lambda_2\right]^{-1}[I+o(1)]\left[\Lambda+\frac{1}{\sqrt{-\lambda}}(I+o(1))D_S\right],$$

which shows that every element of M_B is of order at most $\mathcal{O}(\sqrt{|\lambda|})$. Since, by above, $\tilde{M}=M+\mathcal{O}(e^{-2(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}})$, it then follows from (4.33) that

$$\tilde{M}_B=M_B+\mathcal{O}(e^{-2(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}}),$$

which concludes the proof of the lemma also in the general case. □

Remark 4.8: The same idea of proof can be found in, e.g., Ref. 16.

Under the weaker condition that $Q=Q^*\in L^1_{\mathrm{loc}}([0,b))^{m\times m}$, of Hypothesis 4.1, and the series now being the one for $\tilde{Q}$, this thus proves that (4.3) and (4.4) are valid with exponentially small errors for $\lambda\in\mathbb{C}$, $|\lambda|$ large, in some fixed nonreal sector. (cf. Ref. 22).

V. THE BORG–MARCHENKO THEOREMS

In addition to the operator T, again in the special case of $P=W=I$ in (1.1), with spectral measure $d\rho$ (see Lemma 2.1), we now consider another similar operator $\tilde{T}$, with spectral measure $d\tilde{\rho}$, generated by an equation,

$$\tilde{\mathcal{R}}[U]:=-U''+\tilde{Q}U=\lambda U, \quad x\in[0,\tilde{b}),$$

with $\tilde{Q}$ as in Hypothesis 1.1, and with boundary conditions

$$\tilde{S}^*U'(0,\lambda)+\tilde{C}^*U(0,\lambda)=0$$

at 0 and, if necessary to make $\tilde{T}$ self-adjoint in $L^2([0,\tilde{b}))^{m\times 1}$, also boundary conditions at $\tilde{b}$. For definiteness, we also assume that $b\leqslant\tilde{b}$.

We will prove the following two theorems, where the second one (i.e., Theorem 5.2 below) is a version of Simon's local Borg–Marchenko theorem (cf. Ref. 16, Chap. 3). From this point on, when mentioning a ray, we will always mean a half line starting at the origin.

Theorem 5.1: *The spectral matrices $d\tilde{\rho}$ and $d\rho$ coincide if and only if $\tilde{T}$ and T differ by conjugation by a constant and unitary matrix R, i.e., there exists such a unitary matrix so that $\tilde{S}=RS$, $\tilde{C}=RC$, $\tilde{Q}=RQR^*$, and $\tilde{b}=b$. In addition, we obtain that $\tilde{\psi}=R\psi$, where $\tilde{\psi}$ and ψ satisfy the boundary conditions (if any) at $\tilde{b}=b$.*

Theorem 5.2: *Assume that $\tilde{S}=S$, $\tilde{C}=C$ and that $c\in(0,b)$. Then $\tilde{Q}=Q$ on $[0,c)$ if and only if*

$$M_B(\lambda)-\tilde{M}_B(\lambda)=\mathcal{O}(e^{-2(c-\varepsilon)\mathrm{Re}\sqrt{-\lambda}}),$$

for every $\varepsilon>0$, *as* $\lambda\to\infty$ *along some nonreal ray*.

Remark 5.3: Note that a consequence of formula (3.1) is that two boundary conditions,

$$F(0,\lambda)=\begin{pmatrix} S & C \\ -C & S \end{pmatrix} \quad \text{and} \quad \tilde{F}(0,\lambda)=\begin{pmatrix} \tilde{S} & \tilde{C} \\ -\tilde{C} & \tilde{S} \end{pmatrix},$$

corresponding to the same equation and being of type (2.2), give rise to the same M-function precisely when there is a unitary matrix $R_1\in\mathbb{C}^{m\times m}$ such that

$$\begin{pmatrix} \tilde{S} & \tilde{C} \\ -\tilde{C} & \tilde{S} \end{pmatrix}=\begin{pmatrix} R_1 & 0 \\ 0 & R_1 \end{pmatrix}\begin{pmatrix} S & C \\ -C & S \end{pmatrix}.$$

This transformation changes the equation as described in Theorem 5.1, but leaves the spectral measure unchanged. Therefore, it is natural to consider two equations *equivalent*, if they are connected in this way. On the other hand, taking a unitary (and constant) matrix $R_2\in\mathbb{C}^{m\times m}$ and making the transformation

$$\begin{pmatrix} \tilde{S} & \tilde{C} \\ -\tilde{C} & \tilde{S} \end{pmatrix}=\begin{pmatrix} S & C \\ -C & S \end{pmatrix}\begin{pmatrix} R_2^* & 0 \\ 0 & R_2^* \end{pmatrix},$$

leaves the equation unaltered, but changes the M-function and the spectral measure by conjugation by R_2. In view of this, Lemma 2.4 and Convention 2.5, it is natural to consider $F(0,\lambda)$ and $\tilde{F}(0,\lambda)$ *equivalent* if there exist unitary matrices $R_1,R_2\in\mathbb{C}^{m\times m}$ such that

$$\begin{pmatrix} \tilde{S} & \tilde{C} \\ -\tilde{C} & \tilde{S} \end{pmatrix}=\begin{pmatrix} R_1 & 0 \\ 0 & R_1 \end{pmatrix}\begin{pmatrix} S & C \\ -C & S \end{pmatrix}\begin{pmatrix} R_2^* & 0 \\ 0 & R_2^* \end{pmatrix};$$

this implying that the matrices S and $\tilde{S}$ have the same SVD-decomposition. A natural *normal form* for boundary conditions of type (2.2) would therefore be

$$\begin{pmatrix} USV^* & UCV^* \\ -UCV^* & USV^* \end{pmatrix}=\begin{pmatrix} D_S & \Lambda \\ -\Lambda & D_S \end{pmatrix},$$

where $USV^*=D_S$ is the SVD-decomposition of the matrix S according to Lemma 2.4 and Convention 2.5. With boundary conditions, of type (2.2), on this normal form, it will then follow that the unitary matrix R in Theorem 5.1 is the identity.

To prove Theorem 5.1 and Theorem 5.2 above, we shall need the following results.

Proposition 5.4: If U *solves (1.4), with* λ*-independent initial values at* 0, *we have that*

$$U(x)=[\cosh(x\sqrt{-\lambda})+e^{x\sqrt{-\lambda}}(e^{(1/\sqrt{|\lambda|})\int_0^x\|Q\|}-1)\mathcal{O}(1)]U(0)+[\sinh(x\sqrt{-\lambda})+e^{x\sqrt{-\lambda}}(e^{(1/\sqrt{|\lambda|})\int_0^x\|Q\|}-1)\mathcal{O}(1)]\frac{1}{\sqrt{-\lambda}}U'(0), \tag{5.1a}$$

$$U'(x)=[\sinh(x\sqrt{-\lambda})+e^{x\sqrt{-\lambda}}(e^{(1/\sqrt{|\lambda|})\int_0^x\|Q\|}-1)\mathcal{O}(1)]\sqrt{-\lambda}U(0)+[\cosh(x\sqrt{-\lambda})+e^{x\sqrt{-\lambda}}(e^{(1/\sqrt{|\lambda|})\int_0^x\|Q\|}-1)\mathcal{O}(1)]U'(0), \tag{5.1b}$$

uniformly in x *and* λ.

Proof: Solving the equation $U''+\lambda U=QU$ by the method of variation of constants yields, for $k=\sqrt{-\lambda}$,

$$U(x)=\cosh(kx)U(0)+\frac{\sinh(kx)}{k}U'(0)+\int_0^x\frac{\sinh(k(x-t))}{k}Q(t)U(t)\,dt. \tag{5.2}$$

Putting

$$g(x)=\left\|U(x)-\cosh(kx)U(0)-\frac{\sinh(kx)}{k}U'(0)\right\|e^{-x\,\mathrm{Re}\,k},$$

straightforward estimates give

$$g(x)\leqslant\frac{c(k)}{|k|}\int_0^x\|Q\|+\frac{1}{|k|}\int_0^x\|Q\|g,$$

where $c(k)=\|U(0)\|+(1/|k|)\,\|U'(0)\|$. Integrating after multiplication by the integrating factor $\|Q(x)\|e^{-(1/|k|)\int_0^x\|Q\|}$ yields

$$g(x)\leqslant c(\lambda)(e^{(1/\sqrt{|\lambda|})\int_0^x\|Q\|}-1), \tag{5.3}$$

from which the estimate for U immediately follows. Finally, differentiating (5.2) and using (5.3) on the right hand-side gives the stated estimate for U' as well. □

Corollary 5.5: Under the conditions made in Proposition 5.4, U has order 1/2 as an entire function of λ, locally uniformly in x.

Proof: Immediate from (5.1a)! □

Lemma 5.6: With notation from (2.1) and (2.6),

$$\psi(x,r\mu)\varphi^*(x,r\overline{\mu})\to 0,\quad r\to\infty,\quad r\in\mathbb{R}^+,$$

locally uniformly for $\mu\in\mathbb{C}\backslash\mathbb{R}$ and $x\in(0,b)$.

Proof: Let $x\in(0,b)$ and consider the operator generated by $\mathcal{R}$ (see (1.1)) in $L^2([x,b))^{m\times 1}$ under the Neumann boundary condition at x and the same boundary condition (if any) as before at b. By the same reasoning leading to formula (3.4), we then have that the M-function for the interval $[x,b)$ is $\hat{M}(x,\lambda)=-\psi(x,\lambda)\psi'^{-1}(x,\lambda)$. On the other hand, for the interval $(0,x]$ with x considered as the initial point and with the boundary condition of (2.2) at 0, we obtain that $M(x,\lambda)=\varphi(x,\lambda)\varphi'^{-1}(x,\lambda)=\varphi'^{*-1}(x,\overline{\lambda})\varphi^*(x,\overline{\lambda})$ is the M-function for this interval. The change in sign stems from the fact that the initial point of the interval concerned now lies to the right of the other endpoint. Since $\varphi'^*\theta-\varphi^*\theta'=\varphi'^*\psi-\varphi^*\psi'=-I$, by (2.5b), we obtain that

$$\psi\varphi^*=-\psi(\varphi'^*\psi-\varphi^*\psi')^{-1}\varphi^*=-(M^{-1}+\hat{M}^{-1})^{-1},$$

so that the theorem follows from Theorem 3.6. □

Remark 5.7: Note that

$$\psi(x,\lambda)\varphi^*(x,\overline{\lambda})$$

could be considered to be *Green's function*, on the diagonal, corresponding to the self-adjoint operator T.

Lemma 5.8: If, with notation from (2.2), $N(S)=N(\tilde{S})$, *where $N(S)$ denotes the null space of the matrix S, we have that*

$$\varphi^{*-1}(x,r\overline{\mu})\tilde{\varphi}^*(x,r\overline{\mu})=\mathcal{O}(1),$$

locally uniformly for $\mu\in\mathbb{C}\backslash\mathbb{R}$ and $x\in(0,b)$, as $r\to\infty$.

Proof: Let $VSU^*=D_S$ and $\tilde{V}\tilde{S}=D_{\tilde{S}}\tilde{U}$ be the SVD-factorizations of S and $\tilde{S}$, respectively, according to Lemma 2.4 and Convention 2.5, and let $n=\dim N(S)=\dim N(\tilde{S})$. It then follows that $N(D_S)=N(D_{\tilde{S}})$ is invariant under $\tilde{U}U^*$ since

$$\tilde{V}\tilde{S}U^*=D_{\tilde{S}}\tilde{U}U^*.$$

Thus, we conclude that

$$\tilde{U}U^*=\begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}\in\mathbb{C}^{m\times m},$$

with $U_1\in\mathbb{C}^{(m-n)\times(m-n)}$, $U_2,U_3^*\in\mathbb{C}^{(m-n)\times n}$ and $U_4\in\mathbb{C}^{n\times n}$, where we have that $U_2=0$ and thus also that $U_3=0$, since $\tilde{U}U^*$ is unitary. It so follows that U_1 and U_4 too are unitary. By Proposition 5.4, we thus have that

$$V\varphi^{*-1}\tilde{\varphi}^*\tilde{V}^*=V\varphi^{*-1}U^*U\tilde{\varphi}^*\tilde{V}^*=[I+o(1)]\left[D_S+\frac{1}{\sqrt{-\lambda}}\Lambda_2^*\right]^{-1}$$
$$\times\left[U\tilde{U}^*D_{\tilde{S}}+\frac{1}{\sqrt{-\lambda}}U\tilde{U}^*\tilde{\Lambda}_2^*\right][I+o(1)],$$

where

$$U\tilde{U}^*D_{\tilde{S}}=\begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix},\quad D_1\in\mathbb{C}^{(m-n)\times(m-n)}.$$

Thus, it follows that $\varphi^{*-1}\tilde{\varphi}^*=\mathcal{O}(1)$ in the desired way. □

We are now ready to state the final lemma, which will constitute the main part of the proofs of Theorem 5.1 and Theorem 5.2 above.

Lemma 5.9: Let g, for some constant $\mathcal{C}$, denote the entire function (of λ),

$$g(x,\lambda)=\theta(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})-\varphi(x,\lambda)\tilde{\theta}^*(x,\overline{\lambda})-\varphi(x,\lambda)\mathcal{C}\tilde{\varphi}^*(x,\overline{\lambda}),\quad x\in[0,c),$$

where $c\in(0,b]$. If

$$g(x,\lambda)\to 0, \tag{5.4}$$

pointwise in x, when $\lambda\to\infty$ along two nonreal rays, then $\tilde{S}=RS$, $\tilde{C}=RC$ and $\tilde{Q}=RQR^{-1}$, on $[0,c)$, for some unitary and constant matrix R.

Proof: By (5.4), g is, for each fixed $x\in[0,c)$, bounded on the given rays. Since in addition, by Corollary 5.5, g has order at most 1/2, the Phragmén-Lindelöf theorem gives that g is bounded, and, hence, by Liouville's theorem, g is constant. In view of (5.4), this means that $g=0$ for all $\lambda\in\mathbb{C}$ and all $x\in[0,c)$. This yields that

$$\varphi^{-1}\theta-(\tilde{\varphi}^{-1}\tilde{\theta})^*=\mathcal{C}. \tag{5.5}$$

From (2.5a) it follows that $\varphi^{*-1}\varphi'^*=\varphi'\varphi^{-1}$, and from (2.5b) that $\varphi^{*-1}=\theta'-\varphi^{*-1}\varphi'^*\theta$, so that

$$\varphi^{*-1}=\theta'-\varphi'\varphi^{-1}\theta.$$

Differentiating $\varphi^{-1}\theta$ thus gives

$$(\varphi^{-1}\theta)'=\varphi^{-1}(\theta'-\varphi'\varphi^{-1}\theta)=(\varphi^*\varphi)^{-1},$$

so that differentiating (5.5) gives

$$\varphi^*\varphi=\tilde{\varphi}^*\tilde{\varphi}. \tag{5.6}$$

By differentiating (5.6), followed by the use of (2.5), we obtain that

$$\varphi^{-1}\varphi'=\tilde{\varphi}^{-1}\tilde{\varphi}', \tag{5.7}$$

which, in its turn, differentiated under use of (5.7) yields

$$\varphi^{-1}\varphi''=\tilde{\varphi}^{-1}\tilde{\varphi}''. \tag{5.8}$$

Hence, using that the columns of φ and $\tilde{\varphi}$ are solutions of their corresponding equations, this gives, with notation $R=\tilde{\varphi}\varphi^{-1}$,

$$RQR^{-1}=\tilde{Q}. \tag{5.9}$$

Differentiating the expression for $\tilde{\varphi}=R\varphi$ and multiplying by $\tilde{\varphi}^{-1}$ from the left now yields

$$\tilde{\varphi}^{-1}\tilde{\varphi}'=\tilde{\varphi}^{-1}R'\varphi+\varphi^{-1}\varphi' \quad \text{or equivalently, by (5.9),} \quad \tilde{\varphi}^{-1}R'\varphi=0,$$

which means that R is independent of x. From the fact that

$$\begin{cases}\tilde{\varphi}(0)=R\varphi(0),\\ \tilde{\varphi}'(0)=R\varphi'(0),\end{cases} \quad \text{or, equivalently,} \quad \begin{cases}\tilde{S}=RS,\\ \tilde{C}=RC,\end{cases}$$

it now follows that R is unitary and independent of λ as well, which concludes the proof of the lemma. □

Proof (Theorem 5.1): Let $US^*V^*=D_S$ be the SVD-decomposition of S^* according to Lemma 2.4 and Convention 2.5, and let M_B and $\tilde{M}_{\tilde{B}}$ denote the M-functions corresponding to the operators T and $\tilde{T}$, respectively. Letting M denote the *Neumann* M-function, it follows by (3.1) that $M_B=(C^*+S^*M)(S^*-C^*M)^{-1}$, and hence that

$$UM_BU^*=\left[\Lambda+\frac{1}{\sqrt{-\lambda}}D_S(I+o(1))\right][I+o(1)]\left[D_S-\frac{1}{\sqrt{-\lambda}}\Lambda_2^*\right]^{-1}, \tag{5.10}$$

where the last equality follows from Theorem 3.2. Thus, we conclude that every element of M_B is of order at most $\mathcal{O}(\sqrt{|\lambda|})$, i.e., $\mathcal{C}_2=0$ in the representation formula for M_B, given in Lemma 2.2. In view of this fact, and our assumption that $d\rho=d\tilde{\rho}$, Lemma 2.2 yields that

$$M_B-\tilde{M}_{\tilde{B}}=\mathcal{C}, \tag{5.11}$$

for some constant $\mathcal{C}$. Moreover, it now follows from (5.10) that UM_BU^* is bounded precisely on $N(D_S)^\perp$, and hence that M_B is bounded precisely on $N(S)^\perp$. Analogous reasoning for $\tilde{M}_{\tilde{B}}$ shows that this M-function is bounded precisely on $N(\tilde{S})^\perp$. In view of (5.11), this implies that $N(S)=N(\tilde{S})$. By the fact that

$$\psi(x,r\mu)\tilde{\varphi}^*(x,r\overline{\mu})=\psi(x,r\mu)\varphi^*(x,r\overline{\mu})\varphi^{*-1}(x,r\overline{\mu})\tilde{\varphi}^*(x,r\overline{\mu}), \tag{5.12}$$

(5.11), Lemma 5.6 and Lemma 5.8 give that

$$g(x,\lambda)=\psi(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})-(\tilde{\psi}(x,\overline{\lambda})\varphi^*(x,\lambda))^*=\theta(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})-\varphi(x,\lambda)\tilde{\theta}^*(x,\overline{\lambda})$$
$$-\varphi(x,\lambda)\mathcal{C}\tilde{\varphi}^*(x,\overline{\lambda})\to 0, \quad \lambda\to\infty,$$

along any nonreal ray, so that Lemma 5.9 gives that $\tilde{S}=RS$, $\tilde{C}=RC$ and $\tilde{Q}=RQR^{-1}$ for some constant and unitary matrix R. Hence, for $x\in[0,b)$, we have that $\tilde{\varphi}(x,\lambda)=R\varphi(x,\lambda)$, and since $g=0$ and $\psi\varphi^*=\varphi\psi^*$ (which is a consequence of Remark 5.7) also that $\tilde{\psi}(x,\lambda)=R\psi(x,\lambda)$. Moreover, this means that the columns of $\tilde{\theta}$ and $R\theta$ satisfy the same equation and the same initial data, and hence we conclude that $\tilde{\theta}(x,\lambda)=R\theta(x,\lambda)$. This means that $M_B=\tilde{M}_{\tilde{B}}$ as well. Finally, we also have that $\tilde{b}=b$, since if $\tilde{b}>b$, $\tilde{\psi}$ would satisfy self-adjoint boundary conditions both at b and $\tilde{b}$, which would mean that $\tilde{\psi}$ would be an eigenfunction corresponding to a nonreal eigenvalue of a symmetric operator. □

Proof (Theorem 5.2.): Assume first that $Q=\tilde{Q}$ on $[0,c)$. Then, Lemma 4.7 immediately gives the first part of the theorem.

The second part follows from the following facts. By (5.12), Lemma 5.6 and Lemma 5.8, we have that

$$\psi(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})\to 0,$$

when $\lambda\to\infty$ along any nonreal ray, and hence also that

$$\psi(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})-(\tilde{\psi}(x,\overline{\lambda})\varphi^*(x,\overline{\lambda}))^*=\varphi(x,\lambda)(\tilde{M}_B(\lambda)-M_B(\lambda))\tilde{\varphi}^*(x,\overline{\lambda})+\theta(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})$$
$$-\varphi(x,\lambda)\tilde{\theta}^*(x,\overline{\lambda})\to 0,$$

when $\lambda\to\infty$ in the prescribed way. Since we now have made the assumption that

$$M_B(\lambda)-\tilde{M}_B(\lambda)=\mathcal{O}(e^{-2(c-\varepsilon)\mathrm{Re}\,\sqrt{-\lambda}}),$$

it follows from Proposition 5.4 that, for $x\in[0,c)$, $\varphi(\tilde{M}_B-M_B)\tilde{\varphi}^*\to 0$, when $\lambda\to\infty$. Thus, we conclude that the entire function (of λ),

$$\theta(x,\lambda)\tilde{\varphi}^*(x,\overline{\lambda})-\varphi(x,\lambda)\tilde{\theta}^*(x,\overline{\lambda})\to 0,\quad \lambda\to\infty,\quad x\in[0,c),$$

so that Lemma 5.9 now concludes the proof of the theorem. □

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Goursat distribution and sub-Riemannian structures

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(Received 19 December 2002; accepted 12 September 2003)

We obtain the Lie group whose action leaves invariant the sub-Riemannian structures associated with Goursat systems and Euclidean metrics. The group naturally contains the Heisenberg group, the nilpotent group associated with the Martinet case, and the group corresponding to systems of Engel type. We compute also the Casimir functions of the associated nilpotent Poisson algebra. Our results generalize previous works on this problem of nonholonomic systems. A particular physical problem described by our model is the motion of electric charges in certain static inhomogeneous magnetic fields. We define a new algebraic curve in total space and compute two examples of sub-Riemannian extremals in cotangent space. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625417]

I. INTRODUCTION

In this work, we study rank two distributions equivalent to the Goursat distribution and a dynamical system associated with it. To have a simple system in mind, we will study the motion of an electric charge q in the Euclidean plane M subject to an external perpendicular inhomogeneous magnetic field, from the point of view of sub-Riemannian geometry on a smooth manifold $P \supset M$. For simplicity, we consider only magnetic fields, which are polynomial of degree N in a single variable. Our main result provides the group which describes the symmetries of the sub-Riemannian structure, given in terms of a rank two distribution of vector fields $\Delta \subset TP$ and a flat Riemannian metric $\langle , \rangle$. Nilpotent Lie groups are essential in our solution and contain as the simplest nilpotent subgroup the well-known Heisenberg group. The intrinsic geometry defined by this group on $\mathbb{R}^3$ provides a model for the higher dimensional cases, in this sense all of them can be thought of as deformations of it. Also the so-called ''Martinet case'' considered by Montgomery[14] and by Bonnard and co-workers[4] is naturally contained as a particular example corresponding to linear magnetic fields. Some general results concerning nonhomogeneous magnetic fields were first given by Montgomery[14] for electric charges, but here we present explicit and detailed results. The one forms associated with the inhomogeneous magnetic fields lead us to study Goursat distributions and the extension of the standard two-dimensional Lagrangian in base space to higher dimensions associated with certain constants of motion. In the final sections of this work, we define a new algebraic curve in the total $N+3$-dimensional space. We show that the sub-Riemannian geodesics are defined by this curve and by the Pfaffian system of constraints.

The sub-Riemannian approach to this problem provides us with a Lie algebraic method which could be of certain importance in the study of other classical or quantum mechanical dynamical problems of theoretical physics. Further, the analysis of the quantum dynamics of particles under magnetic fields[12,13] gives an important understanding of the quantum spectra, when considered through the sub-Riemannian approach.[14]

II. SUB-RIEMANNIAN STRUCTURES

Let P be an $N+3$-dimensional smooth manifold with coordinates $q=(x,y,u_1,\ldots,u_{N+1})$, we consider the following nonholonomic constraints:

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$$\dot{q}=\dot{x}Z_1(q)+\dot{y}Z_2(q), \tag{1}$$

given in terms of the rank two distribution $\Delta=\{Z_1,Z_2\}$. The vector fields of Δ belong to the tangent bundle TP of P. We will assume that the distribution Δ is *bracket generating*. This means that there is an integer n such that $\Delta_p^n=T_pP$ for each $p\in P$. Here, $\Delta^{i+1}=[\Delta,\Delta^i]$, $i=1,\ldots$, which leads to the flag $\Delta_p\subset\Delta_p^2\subset\cdots\subset T_pP$. An important quantity here is the *growth vector* n_p of Δ at the point p, defined as $n_p=(n_{1p},n_{2p},\ldots,n_{np})$, where $n_{ip}=\dim\Delta_p^i$. Here, $n_{1p}=2$, and generically we shall have $n_{np}=N+3$, but this last number can be smaller under some circumstances.

In this work we assume that the distribution Δ generates the nilpotent Lie algebra $\mathfrak{g}$ with the following nonzero brackets:

$$[Z_1,Z_2]=:Z_3,\ \ldots,\ [Z_1,Z_{N+2}]=:Z_{N+3}. \tag{2}$$

Observe that Z_{N+3} is a central element of $\mathfrak{g}$. The corresponding Lie group G can be obtained locally by exponentiation of the elements of the Lie algebra, which can then be regarded as the family of left invariant vector fields with respect to the group law. The subalgebras generated by the fields $\{Z_k,\ k\neq 1\}$ are Abelian. The subalgebras $\mathfrak{g}_i$ generated by $\{Z_1,Z_{i+1},Z_{i+2},\ldots,Z_{N+3}\}$ for $i\geqslant 1$ lead to $\mathfrak{g}=\mathfrak{g}_1\supset\mathfrak{g}_2\supset\cdots\supset\mathfrak{g}_{N+3}$, where $\mathfrak{g}_{i+1}$ is an ideal in $\mathfrak{g}_i$. The algebra $\mathfrak{g}$ is solvable and we have the flag of Abelian ideals $\mathfrak{g}=\tilde{\mathfrak{g}}_1\supset\tilde{\mathfrak{g}}_2\supset\cdots\supset\tilde{\mathfrak{g}}_{N+3}$, where $\tilde{\mathfrak{g}}_i$ is the ideal generated by $\{Z_i,Z_{i+1},\ldots,Z_{N+3}\}$ for $i>1$.

The pairing $(\omega,Z)=\Sigma f_ig_i$, written in a particular basis where $\omega=\Sigma f_ie_i^*$ and $Z=\Sigma g_ie_i$, such that $(e_i^*,e_j)=\delta_{ij}$, leads to the splitting $T_pP=\mathrm{Ver}_p\oplus\mathrm{Hor}_p$, where Ver_p is called the vertical subspace at p and Hor_p the horizontal subspace at p of T_pP. Here we have $\mathrm{Hor}=\Delta$, and $\mathrm{Ver}=\mathfrak{g}_0$ where $\mathfrak{g}_0$ is the Abelian algebra generated by $\{Z_3,\ldots,Z_{N+3}\}$.

Definition: A *sub-Riemannian geometry* is a triple $\{P,\Delta\langle,\rangle_p\}$, where $\langle,\rangle_p$ is an inner product in $\Delta_p\subset T_pP$ for each $p\in P$. The set $\{\Delta,\langle,\rangle\}$ is called a *sub-Riemannian structure*.

We define the inner product on Δ by considering $\{Z_1,Z_2\}$ to be an orthonormal set in such a way that $\langle\dot{q},\dot{q}\rangle=(\dot{x}^2+\dot{y}^2)/2$. We consider then the extremum of the action

$$S=\int_o^T\langle\dot{q},\dot{q}\rangle\mathrm{d}t, \tag{3}$$

subject to the nonholonomic constraints given by Eq. (1). The length of the curve $q:[0,T]\rightarrow\mathbb{R}^{N+3}$ is given by

$$L=\int_o^T\langle\dot{q},\dot{q}\rangle^{1/2}\mathrm{d}t. \tag{4}$$

The infimum of the lengths of all curves $q(t)$ joining two points q_i and q_f, with $\dot{q}(t)\in\Delta(q(t))$ for almost each t, is called the *sub-Riemannian distance* between the points q_i and q_f.

We consider the Euclidean space $M\subset P$ as the *base space* with coordinates (x,y). The relation (1) defines the *horizontal lifts* Z_1 and Z_2 of tangent vectors on TM. The horizontal lift gives a smoothly varying family of linear maps $\sigma_p:T_xM\mapsto T_pP$, where $x=\pi(p)\in M$ is the projection of p by the submersion $\pi:P\rightarrow M$. The subspaces $\pi^{-1}(x)\subset T_pP$ are the fibers of π. A *connection* is defined by the horizontal distribution Hor, formed by the set of horizontal subspaces. The horizontal lift satisfies $d\pi_p\circ\sigma_p=$ *identity mapping* on T_xM and $\sigma(gp)=g\sigma(p)$, with $g\in G_0$, where G_0 is the Lie group associated with the Abelian subalgebra $\mathfrak{g}_0$. Altogether, the natural setting for this problem is the *principal bundle* (P,M,π,G_0), with total space P, base space M, and with Abelian structure group G_0.

Theorem: *The dynamical system defined by the metric* $(\dot{x}^2+\dot{y}^2)/2$ *and the non-holonomic constraints* $\dot{q}=\dot{x}Z_1(q)+\dot{y}Z_2(q)$ *is invariant under the left action of* G *on* P.

Proof: The result follows from the definition of left invariant vector fields. □

III. GOURSAT DISTRIBUTION

A usual Pfaffian system on P is the so-called Goursat system which is defined by $\mathrm{Ker}\{\nu_i\}$ with

$$\nu_1 = \mathrm{d}u_1 + y\mathrm{d}x,\ \nu_2 = \mathrm{d}u_2 + u_1\mathrm{d}x,\ \ldots,\nu_{N+1} = \mathrm{d}u_{N+1} + u_N\mathrm{d}x. \tag{5}$$

These forms have a well-defined degree. Setting $\deg(x) = \deg(y) = 1$, we get $\deg(u_i) = i+1$. Particular cases for which some of these forms are absent could be of interest, in such cases the dimension of the manifold would be correspondingly lower. These one-forms define what is known as a *chained system*. By adding, as usual, the one-forms dx and dy one completes a linearly independent set which encodes the constraints of Eq. (1) and yields a rank two distribution $\{Y_1, Y_2\}$, with

$$Y_1 = \partial_x - \sum_{i=1}^{N+1} u_{i-1}\partial_{u_i}, \quad Y_2 = \partial_y, \tag{6}$$

here for notational reasons we take $u_0 = y$. As before, $Y_{i+2} := [Y_1, Y_{i+1}] = \partial_{u_i}$ for $i = 1,\ldots,N+1$, and the Y_i's satisfy the same algebra as the Z_i's. The vector fields Y_i are left invariant with respect to left translations associated with the Lie group G_1 with product law $\alpha\,\alpha' = (\alpha_1 + \alpha_1', \alpha_2 + \alpha_2', \alpha_3 + \alpha_3' - \alpha_1'\alpha_2, \ldots, \alpha_{N+3} + \alpha_{N+3}' - \alpha_1'\alpha_{N+2})$. Thus, we have the following result.

Theorem: *The dynamical system defined by the metric* $(\dot{x}^2 + \dot{y}^2)/2$ *and the Kernel of the one-forms* ν_i, $i = 1,\ldots,N+1$ *is invariant under the left action of* G_1.

Proof: The result follows once more from the definition of left invariant vector fields. □

IV. AN ALTERNATIVE DISTRIBUTION

In this section we give an alternative distribution which is equivalent to the Goursat distribution defined in the last section. An analytic map between the involved variables in both problems can also be given. The geometrical problem consists now in the calculation of the extremum of the action Eq. (3), subject to nonholonomic constraints defined by the Pfaffian system $\mathrm{Ker}\{\omega_k,\ k = 1,\ldots,N+1\}$, in terms of the one-forms

$$\omega_k = \mathrm{d}\theta_k - \frac{1}{k!}x^k\mathrm{d}y,\ \ k = 1,\ldots,N+1. \tag{7}$$

Here $q = (x, y, \theta_1, \ldots, \theta_{N+1})$ are the coordinates of the total space P and the nonholonomic constraints of Eq. (1) are given in terms of the vector fields

$$X_1 = \partial_x,\ \ X_2 = \partial_y + \sum_{i=1}^{N+1}\frac{1}{i!}x^i\partial_{\theta_i}. \tag{8}$$

The Lie brackets lead in our problem to the same nilpotent Lie algebra $\mathfrak{g}$ defined above with

$$X_{j+2} = \sum_{i=j}^{N+1}\frac{1}{(i-j)!}x^{i-j}\partial_{\theta_i},\ \ j = 1,\ldots,N+1. \tag{9}$$

The above vector fields are left invariant with respect to left translations associated with the Lie group G_2 with product law $\alpha\cdot\alpha' = (\alpha_1 + \alpha_1', \alpha_2 + \alpha_2', \ldots, \alpha_{N+3}'')$, with

$$\begin{aligned}
&\alpha_3'' = \alpha_3 + \alpha_3' + \alpha_1\alpha_2', \ldots,\ \ \alpha_k'' = \alpha_k + \alpha_k' + \sum_{j=2}^{k-1}\frac{1}{(k-j)!}\alpha_1^{k-j}\alpha_j', \ldots,\\
&\alpha_{N+3}'' = \alpha_{N+3} + \alpha_{N+3}' + \frac{1}{(N+1)!}\alpha_1^{N+1}\alpha_2' + \frac{1}{N!}\alpha_1^N\alpha_3' + \cdots + \alpha_1\alpha_{N+2}'.
\end{aligned} \tag{10}$$

Thus, we have the following result.

Theorem: *The dynamical system defined by the metric* $(\dot{x}^2+\dot{y}^2)/2$ *and the Kernel of the one-forms* $\omega_i=\mathrm{d}\theta_i-x^i\mathrm{d}y/i!$, $i=1,\ldots,N+1$ *is invariant under the left action of* G_2.

Proof: The result follows once more from the definition of left invariant vector fields. □

V. EQUIVALENCE OF THE DISTRIBUTIONS

Both the kernel of the Goursat system and that of the alternative Pfaffian system encode the nonholonomic constraints (1). In this sense, both systems under consideration are equivalent, more precisely:

Theorem: $\mathrm{Ker}\{\nu_j\}$ *and* $\mathrm{Ker}\{\omega_j\}$ *are equivalent under the coordinate transformation*

$$u_j=\frac{(-)^j}{j!}x^jy+\sum_{i=0}^{j-1}\frac{(-)^i}{i!}x^i\theta_{j-i},\quad \theta_j=\frac{1}{j!}x^jy+\sum_{i=0}^{j-1}\frac{1}{i!}x^iu_{j-i}. \tag{11}$$

Proof: By direct substitution. □

A different control problem which is also related to the Goursat distribution is the so-called N-trailer problem. However, the proof of the equivalence of both distributions is by far more involved.[17] The study of the equivalence of Pfaffian systems goes back to Cartan[8] and involves fine theoretical issues that go beyond the purposes of this paper, see for instance Olver's book.[16]

VI. TRAJECTORIES

Consider now a smooth curve $C:[-\varepsilon,\varepsilon]\to M$, $t\mapsto C(t)$, passing through the point $x_0=C(0)$ and with p_0 in the fiber $\pi^{-1}(x)$ at x_0. Then the parallel transport of p_0 along C is given by the curve defined by $\mathrm{d}\hat{C}(t)/\mathrm{d}t=\sigma_p\mathrm{d}C(t)/\mathrm{d}t$, with $\hat{C}(0)=p_0$ and $\hat{C}(t)=p$. The curve $\hat{C}$ projects by π onto the curve C. We select here $x_0=0$.

By Chow–Rashevsky's theorem,[5,6,9,15] if the distribution is bracket generating, then any two points can be connected by a smooth horizontal path $\hat{C}$, if the underlying manifold is connected. In this section we shall show how to integrate the equations of motion for the present problem.

We will consider the trajectories only for the nonholonomic constraints Eq. (1) and the metric $(\dot{x}^2+\dot{y}^2)/2$. The Lagrangian is given by

$$\mathcal{L}=\lambda_0\tfrac{1}{2}(\dot{x}^2+\dot{y}^2)+\boldsymbol{\lambda}\cdot(\dot{q}-\dot{x}Z_1(q)-\dot{y}Z_2(q)), \tag{12}$$

with $q=(x,y,\theta_1,\ldots,\theta_{N+1})$, $\boldsymbol{\lambda}=(0,0,\lambda_1,\ldots,\lambda_{N+1})$, and the Z_i's acting on q coordinate by coordinate. Here, the λ_k, $k=1,\ldots,N+1$, are Lagrange parameters, in general time dependent and the number λ_0 can take the values 0 or 1. Solutions for $\lambda_0=1$ are called *normal extremals* and those for $\lambda_0=0$ are *abnormal extremals*. An extremal is called *strictly abnormal* if it is not the projection of a normal horizontal curve.[4] In the Physics literature, the case $\lambda_0=0$ is known as the *exceptional case*.[10] Abnormal extremals have recently been treated mainly in the geometric control theory and sub-Riemannian geometry literature, although they were considered already by Bliss[3] and Carathéodory.[7] In the remainder of the paper we consider only normal extremals $\lambda_0=1$. The abnormal extremals and their physical significance shall be discussed elsewhere.

Now, for the particular Pfaffian system Eq. (7), we have

$$\mathcal{L}=\frac{1}{2}(\dot{x}^2+\dot{y}^2)+\sum_{k=1}^{N+1}\lambda_k\left(\dot{\theta}_k-\frac{1}{k!}x^k\dot{y}\right). \tag{13}$$

The canonical momenta are given by

$$p_x=\frac{\partial}{\partial\dot{x}}\mathcal{L}=\dot{x},\quad p_y=\frac{\partial}{\partial\dot{y}}\mathcal{L}=\dot{y}-\sum_k\frac{\lambda_k}{k!}x^k,\quad p_j=\frac{\partial}{\partial\dot{\theta}_j}\mathcal{L}=\lambda_j,\quad j=1,\ldots,N+1. \tag{14}$$

The equations of motion for this problem are thus

$$\ddot{x}=eB_z(x)\dot{y}, \quad \ddot{y}=-eB_z(x)\dot{x}, \quad \dot{\lambda}_i=0, \tag{15}$$

with

$$eB_z(x)=-\sum_{i=1}^{N+1}\frac{\lambda_i}{(i-1)!}x^{i-1}. \tag{16}$$

All Lagrange parameters λ_i are constant. Clearly, by varying the λ_i, we can represent any polynomial magnetic field in the x variable. For simplicity, we shall assume $\lambda_{N+1}\neq 0$. The first two equations can be interpreted as the equations of motion of an electric charge e of unit mass in the plane $x-y$ subject to the action of an inhomogenoeus magnetic field B_z in the perpendicular direction to the plane. The horizontal trajectory $\hat{C}(t)$ is given by the solutions $x(t)$ and $y(t)$ and by the solutions of the Pfaff system $\dot{\theta}_i-x^i\dot{y}/i!=0$, for $i=1,\ldots,N+1$. For the Goursat system the equations for x and y remain the same.

From the equations of motion we obtain as usual the statement of energy conservation, that is, the following quantity is constant along the trajectories:

$$\mathcal{E}=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2). \tag{17}$$

For simplicity we take $\mathcal{E}=1/2$, which implies $\dot{x}^2+\dot{y}^2=1$. This assumption is equivalent to measuring trajectories by arc length.

Remark: Some other selections of constraints leading to the same equations of motion in the base space can be interpreted as equivalent gauges for the magnetic vector potential one-form $A=\lambda\cdot(\mathrm{d}q-Z_1(q)\mathrm{d}x-Z_2(q)\mathrm{d}y)$ *with* $\mathrm{d}A=B_z\,\mathrm{d}x\wedge\mathrm{d}y=d(A+d\phi)$, *for an arbitrary gauge scalar function* ϕ. *These arbitrary gauge choices are related to the group of automorphisms of the Lie algebra* $\mathfrak{g}$.

We integrate first

$$\dot{y}=\dot{y}_0+r(x)=\dot{y}_0-\int_0^x eB_z(v)\mathrm{d}v, \tag{18}$$

where $r(x)$ is a $N+1$-degree polynomial.

Theorem: *The x variable satisfies*

$$\xi^2=p_{2N+2}(x), \tag{19}$$

with $\xi=\dot{x}$ *and the polynomial* $p_{2N+2}=a_0+a_1x+\cdots+a_{2N+2}x^{2N+2}$ *of degree* $2N+2$ *in x with known real coefficients. There are at most* $N+1$ *regions of the x axis where the motion is allowed. The boundary points of these regions are the real zeros of* $p_{2N+2}(x)$.

Proof: The assertion follows from the substitution of Eq. (18) into Eq. (17), obtaining

$$p_{2N+2}(x)=1-(\dot{y}_0+r(x))^2. \tag{20}$$

Now, note that x, $\dot{x}$, y, and $\dot{y}$ must be real in our problem, hence we need $p_{2N+2}\geqslant 0$. But since p_{2N+2} is a polynomial, we infer that the x axis has allowed regions only for x such that $p_{2N+2}>0$ and forbidden regions for x such that $p_{2N+2}<0$, with a set of boundary points given by the real zeros of p_{2N+2}. We need at least two real roots in a nontrivial problem, and obtain a set of at most $N+1$ allowed regions such that $p_{2N+2}(x)\geqslant 0$, since the leading coefficient of p_{2N+2} is negative and equal to $-(\lambda_{N+1}/(N+1)!)^2$.

Remark: It is clear the importance of knowing the number of real roots of $p_{2N+2}(x)$, *this leads us in a natural way to see the holomorphic extension of Eq. (19). For* $x,\xi\in\mathbb{C}$ *the associated algebraic curve is hyperelliptic of genus N. The coefficients* a_i *can lead to singular algebraic*

curves for certain initial conditions associated with multiple zeros of ξ^2.

Now, since $\dot{y}$ is a polynomial of degree $N+1$ in x, Eq. (17) can be interpreted as the equation for conservation of energy for the one-dimensional motion of a point particle of unit mass with total energy $\mathcal{E}=T+V(x)$, kinetic energy $T=\dot{x}^2/2$ and *effective potential energy*

$$V(x)=\frac{1}{2}\dot{y}^2=\frac{1}{2}\left(\dot{y}_0+\sum_{i=0}^{N}\frac{\lambda_{i+1}}{(i+1)!}x^{i+1}\right)^2. \tag{21}$$

Similarly, Eq. (15) for $\ddot{x}$ can be interpreted as the corresponding equation of motion. This interpretation makes clear the existence of allowed and forbidden gaps for motion, according to whether the energy $\mathcal{E}$ is larger or smaller than the effective potential energy $V(x)$, respectively.

In terms of the polynomial defined in Eq. (19), $p_{2N+2}=1-2V$. Thus, the relation $1\geqslant p_{2N+2}\geqslant 0$, which corresponds to an allowed gap, is equivalent to $1\geqslant 2V(x)\geqslant 0$. Additionaly, we note here that the maxima of $V(x)$ are points of *unstable equilibrium* of this mechanical analogy. These points are associated with singular algebraic curves as we shall see.

Corollary: The time dependence of the coordinate $x(t)$ *is given by the inverse function of the hyper-elliptic integral*

$$t(x)=\int_o^{x(t)}\frac{d\zeta}{\sqrt{p_{2N+2}(\zeta)}}. \tag{22}$$

Here, it is necessary that $p_{2N+2}(\zeta)>0$ *for* $0<\zeta<x(t)$, *with at most simple zeros at* $\zeta=0$ *and/or* $\zeta=x(t)$.

Proof: The result follows integrating Eq. (19). To make sense of the integrand, t must be real, so that $p_{2N+2}\geqslant 0$. Further, if p_{2N+2} has a double zero at x_ρ, then as x approaches x_ρ the integrand behaves locally as a constant times $1/(\zeta-x_\rho)$ and the integral grows to infinity. □

Corollary: If there exist $x(t_\rho)=x_\rho$ *such that* $B_z(x_\rho)=0$ *and* $\dot{x}(t_\rho)=0$, *the polynomial* $p_{2N+2}(x)$ *has at least a double root at* $x=x_\rho$.

Proof: From Eq. (20) it follows that

$$\frac{d}{dx}p_{2N+2}(x)=-2r'(x)(\dot{y}_0+r(x)). \tag{23}$$

Therefore, the derivative is also zero at x_ρ, since $r'(x)=-eB_z(x)$. Now, since $\dot{x}(t_\rho)=0$ means that $p_{2N+2}(x_\rho)=0$, this polynomial has at least a double zero at x_ρ. □

For example, for $\dot{x}_0=0$ and $\lambda_1=0$, i.e., $a_0=0=a_1$, the curve has at least a double point for $N>0$ at $x=0$. Note that since $eB_z(x)=-\lambda_1-\lambda_2 x+\cdots$, the example corresponds to a trajectory along a line (the y axis) for which the magnetic field is zero. Since, for this last conclusion, the remaining parallel lines on which the magnetic field is zero can be at any other values of x, the same applies *for all* straight lines on which $\vec{B}$ is zero.

VII. MOMENTUM AND CASIMIR FUNCTIONS

Let us now introduce the so-called[1] momentum functions π_X associated with a vector field X on a manifold M as functions on the cotangent bundle

$$\pi_X(x,p)=p(X(x)),\quad p\in T_x^*M,\quad p:T_xM\to\mathbb{R}. \tag{24}$$

In coordinates $p=\Sigma p_i dq_i$, $X=\Sigma X_i(x,p)\partial_{q_i}$ and $\pi_X(x,p)=\Sigma X_i(x,p)p_i$.

Under this correspondence the Lie brackets are associated with the negative of the corresponding Poisson brackets, in particular $[\partial_x,x]=1$ yields $\{p_x,x\}=-1$. To simplify the notation we shall write $\pi_i:=\pi_{X_i}$, then the Poisson bracket realization of the algebra is given by the nonzero brackets $\{\pi_1,\pi_i\}=-\pi_{i+1}$ for $i=2,\ldots,N+2$. We calculate now, in a coordinate free fashion,

Casimir functions of the universal enveloping algebra of the above nilpotent Poisson algebra associated with the nilpotent Lie algebra given by Eq. (2). Clearly π_{N+3} is a Casimir function.

Theorem: *The generators satisfy*

$$\pi_{N+3}^{i}\pi_{N+2-i}=\sum_{j=-1}^{i}\frac{\alpha_{j+1}}{(i-j)!}\pi_{N+2}^{i-j},\quad i=0,\ldots,N, \tag{25}$$

where the α_k *are arbitrary constants,* $\alpha_0=1$ *and* $\alpha_1=0$.

Proof: It is sufficient to corroborate all commutators with π_1. □

Theorem: *The following N quantities are Casimir elements of the algebra*

$$c_j=\frac{(-)^j}{j!}\pi_{N+2}^{j}+\sum_{k=0}^{j-1}\frac{(-)^{j-k-1}}{(j-k-1)!}\pi_{N+3}^{k}\,\pi_{N+2-k}\,\pi_{N+2}^{j-k-1},\quad j=2,\ldots,N+1. \tag{26}$$

Proof: All commutators can be easily shown to vanish. It follows that $c_2=\pi_{N+3}\pi_{N+1}-\pi_{N+2}^2/2$ for $N\geqslant 1$. □

Corollary: The Casimir elements c_j *satisfy the following recursion formula:*

$$c_{i+1}=\pi_{N+3}^{i}\pi_{N+2-i}-\sum_{j=-1}^{i-1}\frac{c_{j+1}}{(i-j)!}\pi_{N+2}^{i-j},\quad i=1,\ldots,N,\quad c_0=1,\quad c_1=0. \tag{27}$$

Proof: The formula follows immediately from the expression Eq. (25) for the generators, identifying the arbitrary constants α_i with the c_i's. □

Theorem: *The normal extremals in cotangent space are given by the intersection of the cylinders with directrixes*

$$c_{N+1}-\pi_{N+3}^{N}\pi_2+\sum_{j=-1}^{N-1}\frac{c_{j+1}}{(N-j)!}\pi_{N+2}^{N-j}=0,\quad c_0=1,\quad c_1=0, \tag{28}$$

and $\pi_1^2+\pi_2^2-1=0$, *located on the planes* (π_2,π_{N+2}) *and* (π_1,π_2) *respectively, in the* $\{\pi_1,\pi_2,\pi_{N+2}\}$*-subspace, with* $\pi_{N+3}=constant$ *and* π_i, $i=3,\ldots,N+1$ *given by Eq. (27).*

Proof: The surfaces follow from Eq. (27) for $i=N$ and from Eq. (17) with $\mathcal{E}=1/2$. □

In particular, for the basis of Eq. (8), the fields $(\partial_x,\partial_y,\partial_{\theta_i})$ for $i>2$ are mapped to the canonical momenta (p_x,p_y,p_{θ_i}), and with Eq. (14)

$$\pi_1=\dot{x},\quad \pi_2=\dot{y},\qquad \pi_{j+2}=\sum_{i=j}^{N+1}\frac{\lambda_i}{(i-j)!}x^{i-j},\quad j=1,\ldots,N+1, \tag{29}$$

where we recognize $\pi_3=-eB_z(x)$, $\pi_{N+2}=\lambda_N+\lambda_{N+1}x$, $\pi_{N+3}=\lambda_{N+1}$, and the initial conditions $\pi_{1,0}=\dot{x}_0$, $\pi_{2,0}=\dot{y}_0$ and $\pi_{i+2,0}=\lambda_i$ for $i=1,\ldots,N+1$. The following simple facts follow.

Corollary: In the basis of Eq. (8), the Casimir functions are given by Eq. (26) with the momenta π_{i+2} *for* $i>0$ *replaced by the constant parameters* λ_i *and* π_2 *by* $\dot{y}_0$.

Proof: The assertions follow from the equalities

$$\pi_{j+2}=-\frac{\mathrm{d}^{j-1}}{\mathrm{d}x^{j-1}}eB_z(x),\quad \lambda_j=-\frac{\mathrm{d}^{j-1}}{\mathrm{d}x^{j-1}}eB_z(x)\big|_{x=0},\quad j=1,\ldots,N+1. \tag{30}$$

□

Corollary: The trajectory in cotangent space is given in terms of the algebraic curve $f(a,b)=0$, *of genus N, with*

$$f(a,b)=c^{2N}a^2-c^{2N}+\left(c_{N+1}+\sum_{j=-1}^{N-1}\frac{c_{j+1}}{(N-j)!}b^{N-j}\right)^2, \tag{31}$$

where $a=\pi_1$, $b=\pi_{N+2}$, $c=-\pi_{N+3}$ *and* $\{a,b\}=c$.

Proof: From Eq. (28). □

The algebraic curve can be solved by quadratures for b since $\dot{b}=-ac$. For $N=0$, the curve is rational, for $N=1$, elliptic, and for $N>1$, hyperelliptic.

VIII. SUB-RIEMANNIAN GEODESICS IN TOTAL SPACE

Here we consider the trajectories in terms only of the coordinates of total space. For simplicity we assume that all trajectories start at $x(0)=y(0)=\theta_1(0)=\cdots=\theta_N=0$.

Lemma: The trajectories lie on the integral surface given by the cylinder

$$\left(\dot{x}_0-\sum_{i=1}^{N+1}\lambda_i\theta_{i-1}\right)^2+2V(x)-1=0. \tag{32}$$

On the planes (x,θ_{i-1}), $i=1,\ldots,N+1$, *the cylinder has cross sections given by the real hyperelliptic curves*

$$(\lambda_i\theta_{i-1}-\dot{x}_0)^2+2V(x)-1=0, \quad 1\geqslant 2V(x). \tag{33}$$

Proof: Rewrite the equation for $\ddot{x}$ as $\ddot{x}=-\Sigma_{i=1}^{N+1}\lambda_i\dot{\theta}_{i-1}$ and integrate it to obtain

$$\dot{x}=\dot{x}_0-\sum_{i=1}^{N+1}\lambda_i\theta_{i-1}, \tag{34}$$

with $\theta_i(0)=0$ and $\theta_0(t)=y(t)$. Thus, Eq. (32) results, which contains only the coordinates of total space and no time derivatives of them. It is an algebraic curve in total space. □

Therefore, in total space coordinates $\{x,y,\theta_i\}$ the trajectory is given by energy conservation and the Pfaffian system $\mathrm{d}\theta_i-x^i\,\mathrm{d}y/i!=0$ for $i=1,\ldots,N+1$.

Theorem: *In terms of (Abelian) differentials* ϖ_i *we have*

$$\mathrm{d}y=\dot{y}_0\,\varpi_0+\sum_{i=1}^{N+1}\frac{\lambda_i}{i!}\varpi_i, \tag{35}$$

with

$$\varpi_i=\frac{x^i}{\xi}\mathrm{d}x, \tag{36}$$

where $\xi=\sqrt{p_{2N+2}(x)}$.

Proof: From the Pfaffian system, we obtain for the normal extremals

$$\mathrm{d}y=\frac{\dot{y}_0+\Sigma_{i=1}^{N+1}\lambda_i x^i/i!}{\sqrt{1-2V(x)}}\mathrm{d}x. \tag{37}$$

With the definition of the ϖ_i the result follows. □

The differentials $\{\varpi_i,\ i=0,\ldots,2N\}$ form a basis.[2,11] All differentials ϖ_k with $k\in\mathbb{N}$ can be given recursively in terms of the basis using the following result.

Proposition: The differentials ϖ_i *satisfy*

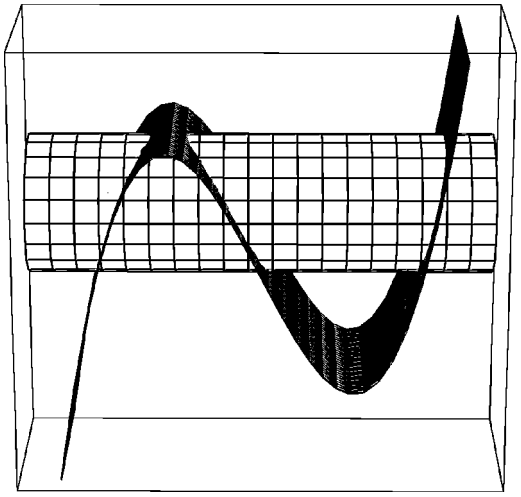

FIG. 1. Trajectory in cotangent space for $N=2$, as intersection of two cylinders.

$$(s+N+1)a_{2N+2}\varpi_{s+2N+1}=\mathrm{d}(x^s\,\xi)-\sum_{i=0}^{2N+1}\left(s+\frac{i}{2}\right)a_i\varpi_{i+s-1},\quad s=0,1,\ldots\ . \tag{38}$$

Proof: The result follows after the computation of $\mathrm{d}(x^s\,\xi)$ and using the expression for ξ^2 in terms of x. For $s\geqslant 0$, all ϖ_k with $k>2N$ are obtained. For $s\leqslant -1$, all ϖ_j with $j\leqslant -1$ are given in terms of the set ϖ_n with $n=-1,0,1,\ldots,2N$. But a simple argument allows one to find a relation between these last differentials and therefore, the set of differentials without the ϖ_{-1} is enough to obtain all ϖ_i. □

The differentials ϖ_j for $j=0,1,\ldots,N-1$ are holomorphic for x complex. The differentials ϖ_k, with $k=N,\ldots,2N$ have two poles of order $k-N+1$. The following Abelian integrals are important here. Let

$$I_i(x)=\int_0^x\varpi_i\,. \tag{39}$$

Proposition: We have

$$y(t)=\dot{y}_0\,t+\sum_{i=1}^{N+1}\frac{\lambda_i}{i!}I_i(x), \tag{40}$$

where $p_{2N+2}(x)\geqslant 0$ *for* $x\geqslant 0$, *and initial condition* $y_0=0$.

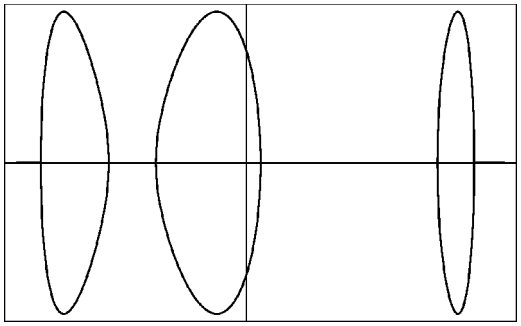

FIG. 2. Real part of the genus two curve corresponding to Fig. 1.

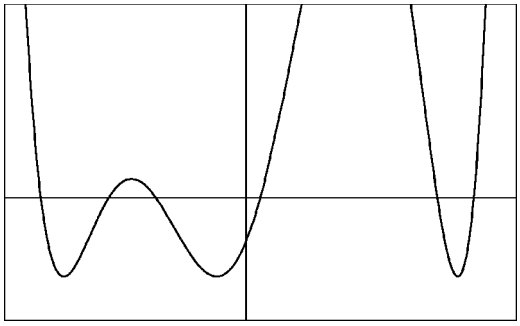

FIG. 3. The potential energy associated with Fig. 2.

Proof: The result follows from Eqs. (22) and (35), since $t=I_0(x)$. Time plays the role of a local uniformizing parameter. □

Lemma: The differentials of the Pfaffian system can be expressed in terms of the basis of Abelian differentials by means of

$$\mathrm{d}\theta_i=\frac{1}{i!}\dot{y}_0\varpi_i+\sum_{j=1}^{N+1}\frac{\lambda_j}{i!j!}\varpi_{j+i},\quad i=0,1,\ldots,N+1. \tag{41}$$

Proof: This relations result from the original Pfaffian system and the expression of dy in terms of Abelian differentials. □

Theorem: *The sub-Riemannian geodesics in total space are given by hyperelliptic integrals as*

$$\theta_i=\frac{1}{i!}\dot{y}_0 I_i(x)+\sum_{j=1}^{N+1}\frac{\lambda_j}{i!j!}I_{j+i}(x),\quad i=0,1,\ldots,N+1, \tag{42}$$

with $y=\theta_0$ and $x(t)$ given by the inverse function of Eq. (22).

Proof: The integration of Eq. (41) yields the result. □

IX. EXAMPLES

Here, we present some numerical examples for the simplest hyperelliptic case. Corresponding results for higher hyperelliptic curves are also obtainable. In Fig. 1 we show a simple nondegenerated example for $N=2$, where Eq. (28) is a cubic cylinder $\pi_4^3/6+c_2\pi_4+c_3-\pi_5^2\pi_2=0$.

In Fig. 2, we show the real curve of genus two associated with Fig. 1. The closed curves are the allowed values for (b,a). In Fig. 3 the corresponding potential energy, Eq. (21), is shown. The horizontal line corresponds to the total energy. In Figs. 4 and 5 a degenerated genus two case is

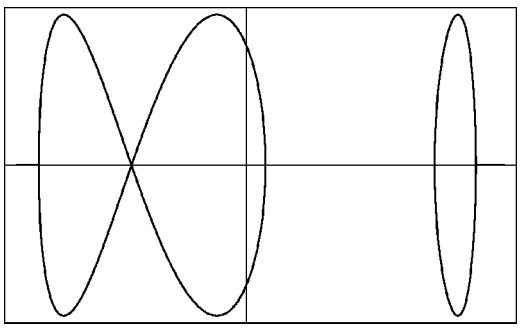

FIG. 4. The real part of a degenerated genus two curve in cotangent space. The double point of the left closed curve corresponds to an abnormal trajectory.

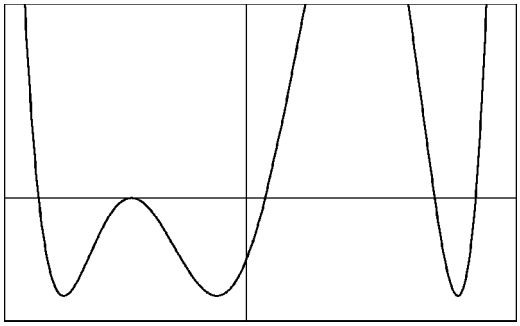

FIG. 5. The potential energy for Fig. 4.

exemplified. The double point in the left closed curve of Fig. 4 corresponds to unstable equilibrium.

X. CONCLUSIONS

We have reduced to quadratures the equations of motion of Goursat systems and a flat metric. The trajectories in total space are given in terms of hyperelliptic integrals. A set of algebraic curves in cotangent space determine the normal trajectories. The Casimir elements of an associated Poisson algebra have been computed explicitly. A physical problem with nonholonomic constraints has been presented, which can be easily transformed into a variational problem with a Goursat system. We have shown, as a simple example, a genus two case in the cotangent space. The present new geometrical approach seems to allow future generalizations.

ACKNOWLEDGMENTS

The present investigation was finished while F.M.P. was on sabbatical leave at INRIA, Unité de Recherche Sophia-Antipolis, France. The author thanks Professor J.B. Pomet and the rest of the team MIAOU for their support. This research was supported in part by the CONACYT's grant for sabbatical periods abroad.

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Invariant integration over the unitary group

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(Received 24 June 2003; accepted 3 August 2003)

Integrals for the product of unitary-matrix elements over the U(n) group will be discussed. A group-theoretical formula is available to convert them into a multiple sum, but unfortunately the sums are often tedious to compute. In this article, we develop an alternative method in which these sums are avoided, and group theory is rendered unnecessary. Only unitarity and the invariance of the Haar measure are required for the computation. The method can also be used to get a closed expression for the simpler integral of monomials over a hypersphere. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1622448]

I. INTRODUCTION

The integral

$$\int (dU) U^*_{i_1 j_1} \cdots U^*_{i_p j_p} U_{k_1 l_1} \cdots U_{k_p l_p}$$

for the product of $n \times n$ unitary matrix elements and their generating functions are useful in many areas of physics. That includes two-dimensional quantum gravity,[1] QCD, matrix models, and statistical and condensed-matter problems of various sorts.[2] These integrals are also useful in the parton saturation problem at small Feynman-x.[3] The monomial integral above can be computed using a graphical method.[4] A more powerful expression can be derived using the Itzykson–Zuber formula[5] as a generating function, or directly from group theory[6] using the Frobenius formula.[7] Simplification can be obtained for $n \to \infty$,[8] but for finite n, the expression is quite complicated [see Eq. (A1)]. It involves multiple sums over an expression containing characters of the symmetric group S_p, as well as the dimensions of irreducible representations of S_p and of the unitary group U(n). One of the sums is taken over all the relevant irreducible representations, and the others are taken over the symmetry groups of the index sets $I=(i_1 \cdots i_p)$ and $J=(j_1 \cdots j_p)$. These sums could be long and tedious for large p, and for indices which have a high degree of symmetry.

In this article, we discuss an alternative method to calculate the monomial integral, using as input only the unitarity of the matrices U, and the invariance of the Haar measure dU. No knowledge of group theory is required, and these complicated multiple sums are avoided. We shall refer to this method as the ''invariant method.''

Invariance of the group measure produces various relations between the different integrals, which will be discussed in Sec. III A. The values of these integrals are obtained recursively from the unitarity relation, and that is discussed in Secs. III B to III D.

The invariant method is also applicable to the much simpler case of a monomial integral over a hypersphere. This simpler case will be used as a testing ground for the idea. It will be discussed in Sec. II, as a preparation for the computation of the unitary integral in Sec. III.

In a forthcoming paper, the relative advantages of the invariant method and the group-theoretical formula will be discussed. We will also examine relations that can be obtained by combining both approaches.

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II. INTEGRATION OVER A HYPERSPHERE

Let Ω_{n-1} be the unit sphere in n dimensions, defined by

$$\sum_{i=1}^{n} x_i^2 = 1, \tag{1}$$

and $(d\omega)$ be its rotationally symmetric volume element, normalized to $\int(d\omega)=1$. We wish to calculate the integral $\int(d\omega)Y$ over Ω_{n-1}, where Y is a monomial of the coordinates x_j $(j=1,2,\ldots,n)$. This integral is zero unless the power of every x_j is even, in which case it can be written in the form

$$\langle J|J\rangle = \int (d\omega) X_J X_J, \tag{2}$$

where $X_J \equiv \Pi_{a=1}^{p} x_{j_a}$ is a monomial of degree p, indexed by the set $J=(j_1 j_2 \cdots j_p)$.

One can attempt to calculate the integral in several ways. Three of them having analogs with the U(n) integrals will be singled out, because the simpler setting of a sphere should make their relative merits more transparent. The first two are standard, both using the spherical coordinates to calculate. The third one, which we wish to develop in this article, is an *invariant approach*, requiring no coordinate system in its computation.

A. Spherical coordinates

The spherical coordinates of x_j on the unit sphere are

$$\begin{aligned} x_n &= \cos\theta_1, \\ x_{n-1} &= \sin\theta_1 \cos\theta_2, \\ x_{n-2} &= \sin\theta_1 \sin\theta_2 \cos\theta_3, \\ &\cdots \\ x_2 &= \left(\prod_{i=1}^{n-2} \sin\theta_i\right)\cos\phi, \\ x_1 &= \left(\prod_{i=1}^{n-2} \sin\theta_i\right)\sin\phi. \end{aligned} \tag{3}$$

The range of θ_i is between 0 and π, and the range of ϕ is between 0 and 2π. The volume element is

$$\begin{aligned} (d\omega') &= \left(\prod_{i=1}^{n-2} (\sin\theta_i)^{n-i-1} d\theta_i\right) d\phi, \\ (d\omega) &= \frac{(d\omega')}{\int (d\omega')}. \end{aligned} \tag{4}$$

Using the formula

$$\int_0^{1/2\,\pi} d\theta(\sin\theta)^{r-1}(\cos\theta)^{s-1}=\frac{1}{2}\frac{\Gamma(\frac{1}{2}r)\Gamma(\frac{1}{2}s)}{\Gamma(\frac{1}{2}(r+s))} \tag{5}$$

and (3), the integral $\langle J|J\rangle$ can be calculated for every index set J.

For example, if all the indices in J are equal to n, i.e., $J=(nnn\cdots n)=(n^p)$, then the integral is equal to

$$\langle J|J\rangle\equiv S(p)=\frac{\int_0^{\pi/2}(\cos\theta_1)^{2p}(\sin\theta_1)^{n-2}d\theta_1}{\int_0^{\pi/2}(\sin\theta_1)^{n-2}d\theta_1}=\frac{1}{\sqrt{\pi}}\frac{\Gamma(p+\frac{1}{2})\Gamma(\frac{1}{2}n)}{\Gamma(p+\frac{1}{2}n)}. \tag{6}$$

However, if we replace $J=(n^p)$ by $J=(1^p)$, namely, replacing x_n^{2p} in the integrand by x_1^{2p}, then the integral becomes much harder to calculate, because $(n-1)$ times more integrations must be performed. Yet, on account of the spherical symmetry, the result must come out to be the same as (6). This complication arises because a choice of axes breaks the spherical symmetry. It can be avoided in the invariant approach discussed below.

This method relies on an explicit parametrization of Ω_{n-1} via the spherical coordinates, as well as formula (5) allowing the integrations to be carried out. Both become much more difficult in the U(n) case, so much so that this method is really not very useful there. For that reason there shall be no futher discussion of this method.

B. Group theory

Alternatively, X_J can be expanded in terms of spherical harmonics, and the integral can be transformed into a sum using the orthonormality of the spherical harmonics. For $n=3$, the expansion is

$$X_J=\sum_{\ell,m} a_{\ell m}Y_{\ell m}(\theta,\phi), \tag{7}$$

and the integral becomes

$$\langle J|J\rangle=\sum_{\ell,m}|a_{\ell m}|^2. \tag{8}$$

For $n>3$, many more sums are involved in Eq. (8).

There are two nontrivial tasks in this approach: to find the coefficients $a_{\ell m}$, and to carry out the sum in (8). These tasks become quite difficult in practice for large n or p.

There is an analogous group-theoretical technique to calculate the U(n) integral, which is reviewed in the Appendix. Using the Frobenius relation, or the Itzykson–Zuber formula, a formula can be derived to turn the integral into a multiple sum. As mentioned in the Introduction, the sums could be very involved, so in practice this method may not be the best way to obtain a result. The invariant approach discussed below and in the next section might be simpler.

C. The invariant approach

The integral in (2) can be calculated directly, using only condition (1) and the invariance of $(d\omega)$ under rotation. In particular, there is no need to employ the spherical coordinate system, and no need to know any integration formula, nor group theory.

The invariant approach will be used in the next section to calculate integrals (of monomials of unitary matrix elements) over the unitary group U(n). In that case, (1) is replaced by the unitarity condition, and $d\omega$ is replaced by the invariant Haar measure dU of the unitary group.

It is convenient to arrange the p indices in J according to the distinct values (between 1 and n) they take. If m_1 of these p indices take on a value, m_2 of them take on a second value, and so

on, then the integral $\langle J|J\rangle$ will be denoted by $S(m_1 m_2 \cdots m_t)$, where t is the number of nonvanishing m_i's, and $\Sigma_{i=1}^{t} m_i = p$. Spherical symmetry guarantees that the integral is independent of the specific values the indices assume. This means, among other things, that S is symmetrical in all its arguments.

To calculate S, the invariance of $d\omega$ is used to relate the various S's to $S(p)$. Then the value of $S(p)$ is calculated using the sphere condition (1).

The invariance of $d\omega$ can be exploited in the following way. A rotation in the $x_i x_k$ plane by an angle ξ,

$$\begin{aligned} x_i &\to +cx_i + sx_k, \\ x_k &\to -sx_i + cx_k, \end{aligned} \tag{9}$$

where $c = \cos\xi$ and $s = \sin\xi$, will leave $d\omega$ invariant. Equivalently, if we subject the integrand $X_J X_J$ in $\langle J|J\rangle$ to such a rotation, the integral $S(m_1 \cdots m_k)$ will remain unchanged.

Let us start out with the integral $S(p)$ whose X_J is equal to x_1^p. Under (9), with $(i,k) = (1,2)$, the integrand becomes

$$(x_1^2)^p \to (cx_1 + sx_2)^{2p} = \sum_{e=0}^{p} \binom{2p}{2e} (cx_1)^{2(p-e)} (sx_2)^{2e} + \cdots. \tag{10}$$

The ellipsis indicates terms odd in x_1 and x_2, which can be dropped because they do not contribute to the integral. The invariance of the integral under this transformation then yields the relation

$$S(p) = \sum_{e=0}^{p} \binom{2p}{2e} c^{2(p-e)} s^{2e} S(p-e,e). \tag{11}$$

Since this is true for all ξ, the right-hand side must be independent of ξ. That requires

$$S(p-e,e) = \frac{\binom{p}{e}}{\binom{2p}{2e}} S(p). \tag{12}$$

Similarly, we can apply (9) and the whole procedure to $(i,k) = (2,3)$ to get

$$S(p-e,e-f,f) = \frac{\binom{e}{f}}{\binom{2e}{2f}} S(p-e,e) = \frac{\binom{p}{e}}{\binom{2p}{2e}} \frac{\binom{e}{f}}{\binom{2e}{2f}} S(p). \tag{13}$$

Continuing thus, we finally obtain

$$S(m_1, m_2, m_3, \cdots, m_t) = \frac{\left(\sum_{i=1}^{t} m_i\right)!}{\left(\prod_{i=1}^{t} m_i!\right)} \frac{\left(\prod_{i=1}^{t} (2m_i)!\right)}{\left(\sum_{i=1}^{t} 2m_i\right)!} S(p). \tag{14}$$

To complete the calculation we must calculate $S(p)$. This can be done by using condition (1). Since $S(p-1,1)$ is independent of what coordinate x_j the multiplicity 1 sits on, as long as it is not on the coordinate whose multiplicity is $p-1$, the sphere condition (1) can be translated to read

$$(n-1)S(p-1,1) + S(p) = S(p-1). \tag{15}$$

Using (14), we know that $S(p-1,1) = S(p)/(2p-1)$. Substituting this back into (15), we get the recursion relation

$$S(p)=\frac{2p-1}{n+2p-2}S(p-1). \tag{16}$$

With the initial value $S(0)=1$, (16) can be solved to yield

$$S(p)=\frac{(2p-1)(2p-3)\cdots 1}{(n+2p-2)(n+2p-4)\cdots n}=\frac{1}{\sqrt{\pi}}\frac{\Gamma(p+\frac{1}{2})\Gamma(\frac{1}{2}n)}{\Gamma(p+\frac{1}{2}n)}, \tag{17}$$

which agrees with the answer given by (6).

The general result is obtained by substituting (17) into (14).

III. INTEGRATION OVER THE UNITARY GROUP

Let U_{ij} denote the (ij) matrix element of an $n\times n$ unitary matrix, and U_{ij}^* its complex conjugate. The product $\Pi_{a=1}^{p}U_{i_a j_a}$ is abbreviated as U_{IJ}, with the index sets being $I=(i_1 i_2\cdots i_p)$ and $J=(j_1 j_2\cdots j_p)$. We shall refer to p as the *degree* of U_{IJ}. Since the matrix elements commute with one another, the order of the indices is irrelevant. Thus if $P\in S_p$ denotes a permutation of the p indices, and the permuted index set is denoted by $I_P=(i_{P(1)}i_{P(2)}\cdots i_{P(p)})$, then

$$U_{IJ}=U_{I_P J_P}. \tag{18}$$

We want to calculate the monomial integral

$$\langle I,J|K,L\rangle=\int (dU)U_{IJ}^*U_{KL} \tag{19}$$

over the unitary group $\mathrm{U}(n)$. The degree of U_{IJ}^* is assumed to be p and that of U_{KL} is assumed to be q. The Haar measure dU appearing in (19) is left- and right-invariant, and normalized to $\int(dU)=1$.

As mentioned in the last section, a group-theoretical formula to calculate the integral is available (see the Appendix). The integral is expressed as a multiple sum, with a summand involving the character of the symmetric group S_p, the dimensions of the irreducible representations of $\mathrm{U}(n)$ and S_p, as well as the index structure of I,J,K,L. This formula is general, though not always the best way to obtain the result, because the multiple sums are often tedious and difficult to do. In what follows, we shall develop another method to calculate the integral, using the invariant approach discussed in the last section. With this approach, no knowledge of group theory is required, and multiple sums are avoided.

The invariant calculation relies only on the unitarity of the matrices in the integrand,

$$\sum_{j=1}^{n}U_{ij}U_{lj}^*=\sum_{j=1}^{n}U_{ji}U_{jl}^*=\delta_{il}, \tag{20}$$

as well as the invariance of the Haar measure. The latter implies

$$\int (dU)f(U,U^*)=\int (dU)f(VU,V^*U^*)=\int (dU)f(UV,U^*V^*) \tag{21}$$

for any function f, and any $V\in\mathrm{U}(n)$. We shall apply (21) to the function $f(U,U^*)=U_{IJ}^*U_{KL}$.

The calculation is very similar to that in the last section, though more complicated. The spherical condition (1) is now replaced by the unitarity condition (20), and the rotational invariance of $d\omega$ is now replaced by the group invariance of dU.

A. Relations from invariance

Equation (21) is very powerful. Depending on the choice of V, many relations can be derived. Here are some examples.

1. $V_{ij}=e^{i\phi}\delta_{ij}$

With this choice, $f(UV,U^*V^*)=e^{i(q-p)\phi}f(U,U^*)$. Hence the integral (19) is zero unless $p=q$. For this reason we shall assume $q=p$ from now on.

2. $V_{ij}=e^{i\phi_i}\delta_{ij}$

With this choice, $f(UV,U^*V^*)=e^{i\xi}f(U,U^*)$, where $\xi=\Sigma_{a=1}^{p}(\phi_{l_a}-\phi_{j_a})$. In order for the integral (19) not to be zero, this phase ξ must vanish. If all ϕ_i's are different, this happens only when the indices in L are permutations of the indices in J. Similarly, one can show that the indices in K must be permutations of the indices in I. If R and S are the permutations in S_p that do the job, then

$$K=I_R, \quad L=J_S. \tag{22}$$

Using (18), we may assume $K=I$, with the nonzero integrals (19) now being of the form

$$\langle I,J|I,J_Q\rangle \tag{23}$$

for some $Q\in S_p$.

The nonzero integral over a sphere calculated in the last section is of the form $\langle J|J\rangle$, but the nonzero integral over U(n) is of the form $\langle I,J|I,J_Q\rangle$. The presence of an additional index set I, and the possibility that $J_Q\neq J$, both make it harder to calculate the unitarity integral than the spherical integral, though the idea is precisely the same.

If $J_Q=J$, then the integral (23) is positive definite. We shall refer to integrals of that type as *direct integrals*. If $J_Q\neq J$, the sign is not guaranteed, and we shall refer to those integrals as *exchange integrals*.

The direct integral looks deceptively similar to the spherical integral (2) in a complex n^2-dimensional space. By mapping U_{ij} to x_a, with $a=(i,j)$ running between 1 and n^2, the complex equivalent of (1), namely $\Sigma_{a=1}^{n^2}|x_a|^2=n$, is guaranteed by the unitarity relation (20). One might therefore think that the direct integrals would turn out to be very similar to the spherical integrals, whose result is given by (14) and (17). Unfortunately that is not the case, because the measure dU is not rotational invariant in the n^2-dimensional complex vector space. As a result, even the direct integrals become more difficult to calculate than the spherical integrals of the last section.

3. Permutation

Now, choose V to be a permutation matrix of n objects. Then VU is obtained from U by permuting its rows, and UV is obtained from U by permuting its columns. With this V, Eq. (21) implies that

$$\langle I,J|K,L\rangle=\langle I',J|K',L\rangle=\langle I,J'|K,L'\rangle, \tag{24}$$

where I' is obtained from I by a reassignment of the values of its indices, and K' is obtained from K by the *same* reassignment. For instance, let us take $p=8$ and $n=8$. Suppose $I=(11555247)$ and $K=(51524571)$ [recall from (22) that K has to be a permutation of I]. If we make the reassignment $1\leftrightarrow 8,2\leftrightarrow 5,4\leftrightarrow 7$, then $I'=(88222574)$ and $K'=(28257248)$.

In other words, the integral is affected by whether the indices take on the same or different values, but is independent of what these values are.

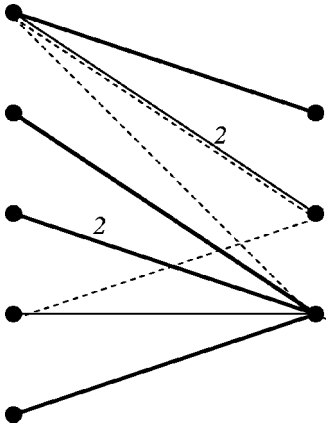

FIG. 1. Graphical representation of the integral $\langle I,J|I,J_Q\rangle$, where $I=(1^3 23^2 45)$, $J=(12^2 7^5)$, and $J_Q=(217^4 27)$.

4. Row-column interchange

Since the measure is invariant under transposition, $(dU)=(dU^T)$, the integral is unaltered if we interchange the rows with the columns:

$$\langle I,J|K,L\rangle=\langle J,I|L,K\rangle. \tag{25}$$

5. Graphical representation

It is convenient to employ a graphical description of the integral $\langle I,J|I,J_Q\rangle$, as illustrated in Fig. 1. The dots in the left-hand column represent the distinct values in the index set I, and the dots in the right-hand column represent the distinct values of the index set J. As per (24), the integral does not depend on what these values are. Since J_Q is a permutation of J, it shares the same distinct values, and hence the same dots as J.

Factors of U^*_{IJ} are shown as (thin) solid lines, and factors of U_{IJ_Q} are shown as dotted lines. A number appearing above the solid line or below the dotted line denotes the multiplicity (i.e., the power) of that matrix element. If the number is absent, the multiplicity is taken to be 1. When a pair $U^*_{ij}U_{ij}$ occurs together, we may choose to replace its pair of thin-solid and dotted lines by a thick solid line. In that case the multiplicity designation refers to the multiplicity of the pair. Thus a direct integral can always be drawn with only thick solid lines.

When multiplicity is taken into account, the number of solid lines and the number of dotted lines connected to each dot must be equal. This simply reflects the fact that J_Q is a permutation of J.

The integral $\langle I,J|I,J_Q\rangle$ with $I=(11123345)=(1^3 23^2 45)$, $J=(12277777)=(12^2 7^5)$, and $J_Q=(21777727)=(217^4 27)$, is depicted in Fig. 1. The five left-hand dots represent the five distinct numbers 1,2,3,4,5 in I, and the three dots in the right-hand column represent the three distinct numbers 1,2,7 in J and J_Q.

The invariance of (25) means that we may switch the left-hand column of dots with the right-hand column of dots. Namely, a reflection about the vertical line halfway between the two columns will not change the integral.

6. Rotation

Choose $V=R(ab)$ to be the matrix which rotates the (ab) plane by an angle ξ. This matrix has 1's along the main diagonal, except at the (aa) and (bb) positions, where the matrix element is $c=\cos\xi$. The off-diagonal matrix elements are all zero, except at the positions (ab) and (ba), where the matrix elements are respectively $s=\sin\xi$ and $-s$.

The replacement $U\to UV$ causes the following change in the matrix elements:

$$U_{ia} \to +cU_{ia} + sU_{ib},$$

$$U_{ib} \to -sU_{ia} + cU_{ib}, \tag{26}$$

$$U_{ij} \to U_{ij},$$

provided $j \neq a,b$. Similar replacements on U^*_{ia} and U^*_{ib} should also be made. The result is to change $\langle I,J|I,J_Q\rangle$ into a sum of terms of the form $M_e(c^2)^{d-e}(s^2)^e$, where d is the total number of column indices in U^*_{IJ} with value a or b, and e varies between 0 and d. [Odd powers of cs never enter because of (22).] The invariance condition (21) requires

$$\langle I,J|I,J_Q\rangle = \sum_{e=0}^{d} M_e(c^2)^{d-e}(s^2)^e. \tag{27}$$

In order for this to be true for all ξ, we must have

$$M_e = \langle I,J|I,J_Q\rangle \binom{d}{e} = M_0 \binom{d}{e}, \tag{28}$$

where $\binom{d}{e} = d!/e!(d-e)!$ is the binomial coefficient.

Let us see how M_e is computed in the graphical language. Take any two dots on the right-hand column to represent the values a and b. One of the two dots should have some lines attached to it, but the other one may or may not be empty. The total number of solid (or of dotted) lines attached to the two dots is d. Now move e (thin) solid and e dotted lines between the two dots, subject to the constraint that at the end of the move, each dot must have an equal number of solid and dotted lines attached to it (otherwise the integral is zero). Assign a weight $+1$ for a line moved from a to b, and a weight -1 for each line moved from b to a. The quantity M_e in (28) is simply the sum of all the resulting integrals after the move, weighted by the product of the factors ± 1 associated with each move.

It is important to note that these relations are local. They involve only the indices of J and J_Q with values a and b. It does not matter what I is and what the rest of the indices of J and J_Q are.

Let us illustrate this graphical application of the rotational relation with two examples.

Example 1: Figure 2 represents part of a diagram. The whole diagram may have many more dots and lines. They are not drawn because the relation derived below is independent of these other dots and lines.

The values of a and b must be different, and there must be no more lines coming out of them than is shown in Fig. 2. The indices i_1, i_2, i_3, i_4 may or may not have the same values, and there may be many more lines attached to them than is shown, as long as these other lines do not connect with either a or b. If some of their values are the same, say $i_1 = i_2$, then graphically the two dots i_1, i_2 simply merge together into a single dot. If the values are different, then other lines must also come out of these dots in order to make the integral nonzero.

The integrals corresponding to Figs. 2(a)–2(d) will be denoted by $I(2a)$, $I(2b)$, $I(2c)$, and $I(2d)$, respectively. In these diagrams we are dealing with $d=2$, because there are two pairs of (solid and dotted) lines ending on the right-hand dots.

Let us apply rotation to Fig. 2(a). We could either move two lines ($e=1$), or four lines ($e=2$). By moving two lines, we get $I(2b)$ (two solid lines), $I(2c)$ (two dotted lines), and two others, I_1 (one solid and one dotted lines from a to b) and I_2 (one solid and one dotted lines from b to a). The graphs for the last two are not shown, but they can be obtained from $I(2a)$ by merging the a and b dots. In this way we get $M_1 = -I(2b) - I(2c) + I_1 + I_2 = 2(-I(2b) + I_1)$, where (24) has been used in the last step. By using (28), we conclude that $M_1 = 2M_0 = 2I(2a)$. Hence we obtain the relation

$$I(2a) = -I(2b) + I_1. \tag{29}$$

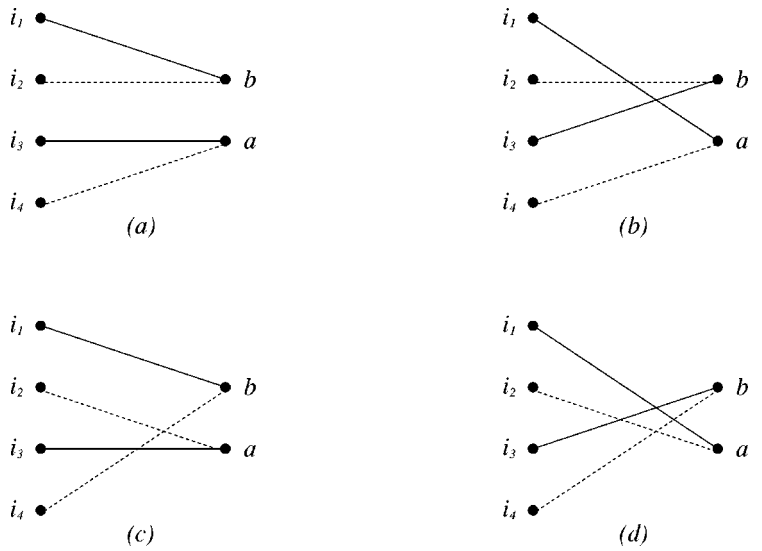

FIG. 2. Four diagrams illustrating how rotational invariance of the measure can be used to relate these four integrals. See Eq. (29).

If we move all four lines, we get $M_2 = I(2d)$. The formula in (28) demands $M_2 = M_0$, or $I(2d) = I(2a)$. We already know this to be true from (24).

Example 2: The fan relation: Figure 3(b) is a partial diagram of some integral. We assume that there are no other lines connected to the dots on the right-hand column, though there may be other lines emerging from dot i. There may also be many other dots and lines not shown in the diagram.

The multiplicities of the lines shown are m_i $(1 \leqslant i \leqslant t)$, so the integrand is proportional to $|U_{ia}|^{2m_1}|U_{ib}|^{2m_2}\cdots$. The corresponding integral is denoted by $f(m_1, m_2, \ldots, m_t)$.

Using (28) repeatedly, it will be shown below that

$$f(m_1, m_2, \ldots, m_t) = \frac{\left(\prod_{i=1}^{t} m_i!\right)}{\left(\sum_{i=1}^{t} m_i\right)!} f(d), \tag{30}$$

where $d = \Sigma_{i=1}^{t} m_i$ and $f(d) = f(d, 0, 0, \ldots, 0)$.

$f(d)$ is drawn in Fig. 3(a). Having multiplicity d means that there are d (thin) solid lines and d dotted lines between i and a. Now move $e = \Sigma_{i=2}^{t} m_i$ solid and e dotted lines from a to an empty

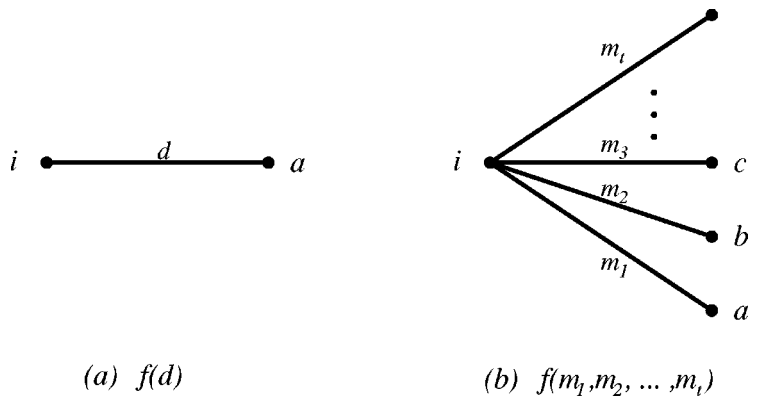

FIG. 3. Using rotational invariance of the measure, the single line in (a) can be spread out into the fan of lines in (b) to get the relation displayed in (30).

dot b. There are $\binom{d}{e}$ ways of choosing the set of solid lines to move, and independently there are also $\binom{d}{e}$ ways to select the dotted lines. Hence $M_e=\binom{d}{e}^2 f(d-e,e)$. From (28), we know that $M_e=\binom{d}{e}M_0=\binom{d}{e}f(d)$. Hence

$$f(d-e,e)=\frac{1}{\binom{d}{e}}f(d). \tag{31}$$

This process can be repeated by moving $g=\Sigma_{i=3}^{t}m_i$ pair of lines from b to an empty dot c. Then we get

$$f(d-e,e-g,g)=\frac{1}{\binom{e}{g}}f(d-e,e)=\frac{1}{\binom{d}{e}}\frac{1}{\binom{e}{g}}f(d). \tag{32}$$

By repeating this process again and again, we arrive at the fan relation (30), which tells us how to fan out a thick line with a high multiplicity into t different lines.

B. Results from unitarity

In the last subsection, relations between different integrals are obtained using the invariance requirement (21). To calculate the actual value of any of these integrals, the unitarity condition (20) must be used.

The unitarity sum (20) for $i\neq l$ simply brings out more relations between different integrals. But for $i=l$, a pair of U,U^* disappears on the right-hand side of (20), so (20) relates integrals of degree p to integrals of degree $p-1$. By using this repeatedly, eventually the degree comes down to zero, and the integral is known to be 1. In this way the values of the integrals can be computed recursively.

This procedure will be illustrated by various examples in the rest of this section.

1. Direct integrals

(a) The fan integrals. The simplest ($p=1$) direct integral is

$$\langle i,a|i,a\rangle=\frac{1}{n}. \tag{33}$$

To get this result, we make use of the fact from (24) that $\langle i,a|i,a\rangle$ is independent of i and a. Summing over a (from 1 to n), and using (20), we get $n\langle i,a|i,a\rangle=1$. Hence Eq. (33).

This calculation can be generalized to the integral in Fig. 4(a) to give

$$\langle (i^m),(j^m)|(i^m),(j^m)\rangle\equiv F(m)=\frac{(n-1)!m!}{(n+m-1)!}. \tag{34}$$

Note that Fig. 4(a) is just the diagram Fig. 3(a), but without any additional dots and lines.

To obtain this result, start from the integral $F(m-1,1)$, shown in Fig. 4(b). The integral is independent of the value of the index (dot) indicated by a downward arrow, as long as it does not take on the value of the other dot. Sum over this indicated index, from 1 to n. Equation (20) implies

$$(n-1)F(m-1,1)+F(m)=F(m-1). \tag{35}$$

Now the fan relation (30) tells us that $F(m-1,1)=F(m)/m$. Substituting this into (35), we get a recursion relation between $F(m)$ and $F(m-1)$, namely,

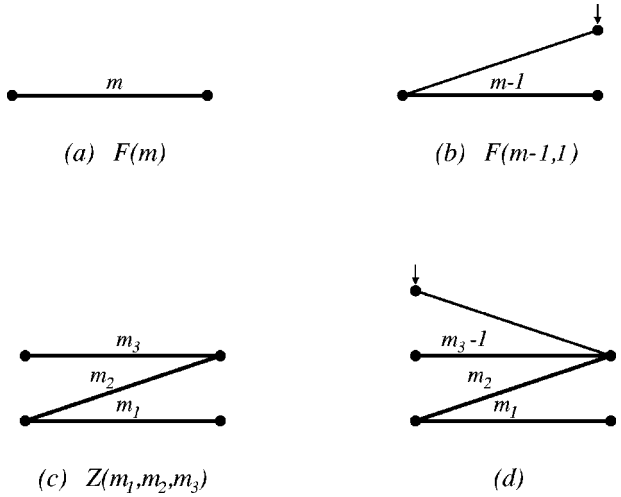

FIG. 4. Diagram (b) shows how the integral in (a) can be obtained from unitarity by summing over the index indicated by an arrow. This leads to a recursion relation whose solution is (34). Similarly, unitarity applied to the indicated index in (d) yields a recursion relation whose solution gives (38) for the "Z integral" in (c).

$$F(m)=F(m-1)\frac{m}{n+m-1}. \tag{36}$$

Using the initial value $F(0)=1$, this recursion relation can be solved to get (34).

Define the "fan integral" $F(m_1,m_2,\ldots,m_n)$ to be Fig. 3(b), without any extra dots and lines. It follows from (34) and (30) that

$$F(m_1,m_2,\ldots,m_t)=\frac{\left(\prod_{i=1}^{t} m_i!\right)(n-1)!}{\left(n+\sum_{i=1}^{t} m_i-1\right)!}. \tag{37}$$

(b) The Z integrals. Next, consider the "Z integral" in Fig. 4(c). We shall prove that

$$Z(m_1,m_2,m_3)=\frac{m_1!m_2!m_3!(n-2)!(n-1)!(n+m_1+m_3-2)!}{(n+m_1-2)!(n+m_3-2)!(n+m_1+m_2+m_3-1)!}. \tag{38}$$

To do so, consider Fig. 4(d). Summing over the index indicated by the vertical arrow, and denoting the integral in Fig. 4(d) by $I(4d)$, the unitarity condition (20) gives

$$(n-2)I(4d)+Z(m_1,m_2,m_3)+Z(m_1,m_2+1,m_3-1)=Z(m_1,m_2,m_3-1). \tag{39}$$

The fan formula (30) tells us that $I(4d)=Z(m_1,m_2,m_3)/m_3$. Substituting this into (39), we get a recursion relation in m_3:

$$Z(m_1,m_2,m_3)=\frac{m_3}{n+m_3-2}[Z(m_1,m_2,m_3-1)-Z(m_1,m_2+1,m_3-1)]. \tag{40}$$

Using the initial value $Z(m_1,m_2,0)=F(m_1,m_2)=(n-1)!m_1!m_2!/(n+m_1+m_2-1)!$, the recursion relation can be solved to yield (38).

Relation (30) can also be used to fan out the two open ends of Fig. 4(c) and (38) to obtain the "fanned Z integrals."

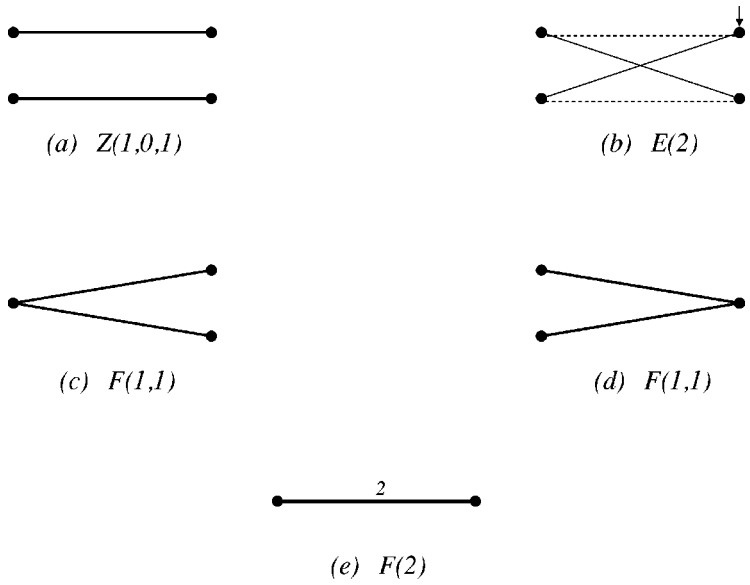

FIG. 5. Integrals of the second degree.

C. Exchange integrals

To illustrate how to compute exchange integrals, all second and third degree exchange integrals will be computed in this subsection.

1. $p=2$

All the second degree integrals are shown in Fig. 5. The integrals in Figs. 5(a) and 5(c)–(e) are direct integrals, either of the fan type or the Z type, so they are known. The only exchange integral is $E(2)$ depicted in Fig. 5(b). It can be computed either by rotation from a direct integral, or by unitarity. We will discuss both methods.

(a) By rotation. Starting from Fig. 5(d), rotate two solid and two dotted lines from the dot in the right-hand column to an empty dot. This is a special case of example 1 of Sec. III A 6 and Fig. 2, but let us do it directly once again. Using the notation in (28), we get

$$M_1=2Z(1,0,1)+2E(2)=2M_0=2F(1,1). \tag{41}$$

Hence

$$E(2)=F(1,1)-Z(1,0,1)=\frac{1}{n(n+1)}-\frac{1}{(n-1)(n+1)}=-\frac{1}{n(n^2-1)}. \tag{42}$$

(b) By unitarity. Summing over the indicated index in Fig. 5(b) from 1 to n yields $(n-1)E(2)+F(1,1)=0$, hence

$$E(2)=-\frac{F(1,1)}{n-1}=-\frac{1}{n(n^2-1)}. \tag{43}$$

2. $p=3$

Figure 6 shows the two direct integrals which are not of the fan type or the Z type, and all the exchange integrals of degree 3.

To get $I(6a)$, the integral for Fig. 6(a), carry out a unitarity sum on the indicated index. This yields $(n-1)I(6a)+F(1,1,1)=F(1,1)$, hence

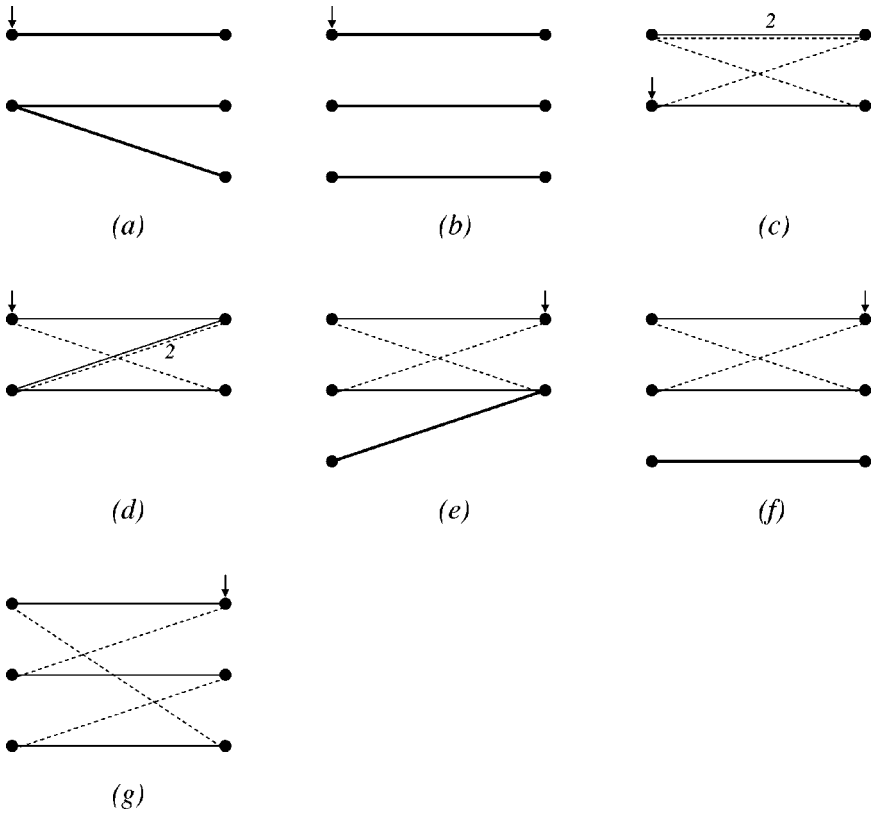

FIG. 6. Integrals of the third degree.

$$I(6a)=\frac{1}{n-1}\left(\frac{1}{n(n+1)}-\frac{1}{n(n+1)(n+2)}\right)=\frac{1}{(n-1)n(n+2)}. \tag{44}$$

This integral can also be computed by fanning out the bottom line of $Z(2,0,1)=2(n+1)(n-2)!/(n+2)!$.

To compute $I(6b)$, take a unitary sum over the indicated index. This yields $(n-2)I(6b)+2I(6a)=Z(1,0,1)$. Hence

$$I(6b)=\frac{1}{n-2}\left(\frac{1}{n^2-1}-\frac{2}{(n-1)n(n+2)}\right)=\frac{(n^2-2)(n-3)!}{(n+2)!}. \tag{45}$$

The exchange integrals can be obtained by taking the unitary sum on the indicated vertex. Note that the right-hand side of the sum is always zero in the case of exchange integrals.

In this way we obtain the relations

$$\begin{gathered}(n-1)I(6c)+F(1,2)=0,\\ (n-1)I(6d)+F(1,2)=0,\\ (n-1)I(6e)+F(1,1,1)=0,\\ (n-2)I(6f)+I(6a)+I(6e)=0,\\ (n-2)I(6g)+2I(6e)=0.\end{gathered} \tag{46}$$

The solutions are

$$I(6c)=I(6d)=-\frac{2(n-1)!}{(n+2)!(n-1)}=-2\frac{(n-2)!}{(n+2)!},$$

$$I(6e)=-\frac{F(1,1,1)}{n-1}=-\frac{(n-2)!}{(n+2)!},$$

$$I(6f)=-\frac{1}{n-2}(I(6a)+I(6e))=-n\frac{(n-3)!}{(n+2)!}, \tag{47}$$

$$I(6g)=-\frac{2}{n-2}I(6e)=2\frac{(n-3)!}{(n+2)!}.$$

D. The *X* integrals

To illustrate how direct and exchange integrals may be coupled in the recursion relation, let us look at the one-loop "*X* integrals" depicted in Fig. 7(a). This integral, specified by the four weights r,s,t,u of U^* and the four weights r',s',t',u' of U, will be designated as $X(rstu|r's't'u')=I(7a)$. Since the number of dotted lines and the number of solid lines emerging from each vertex must be equal, there are three relations for these eight parameters,

$$r'+s'=r+s,$$

$$s'+t'=s+t, \tag{48}$$

$$t'+u'=t+u,$$

so only five independent parameters are required to specify all the *X* integrals.

It is fairly complicated to calculate all these integrals, so we will only derive the recursion relation here and illustrate how it can be used in the simplest case. Let $\rho=r+r'$ be the total number of top lines in *X*, and $\sigma=s+s'$ the total number of lines on one side. The idea is to find a recursion relation in $\rho+\sigma$, each time reducing either ρ or σ by 1. Eventually one gets down to either $\rho=0$ or $\sigma=0$, which are the *Z* integrals obtained before.

1. Recursion relation

Rotate one solid and one dotted line from the $r-s$ junction of Fig. 7(a) to an empty dot. The result is Fig. 7(b)–7(e). In the notation of (28), we have

$$M_1=r's I(7b)+rs'I(7c)+ss'I(7d)+rr'I(7e)=(r+s)M_0=(r+s)I(7a), \tag{49}$$

where $I(7b)$ is the integral depicted in Fig. 7(b), etc.

The parameters of Figs. 7(b)–7(e) are those of 7(a), except where a "$-$" sign occurs, in which case the corresponding parameter is reduced by 1. In Fig. 8 we will also use a "$+$" sign to indicate where the parameter is increased by 1.

The unitarity sum, applied to the indicated index in Figs. 7(b)–7(e), results in the relations

$$0=(n-2)I(7b)+I(7a)+I(8b),$$

$$0=(n-2)I(7c)+I(7a)+I(8c),$$

$$I(8d_2)=(n-2)I(7d)+I(7a)+I(8d_1), \tag{50}$$

$$I(8e_2)=(n-2)I(7e)+I(7a)+I(8e_1).$$

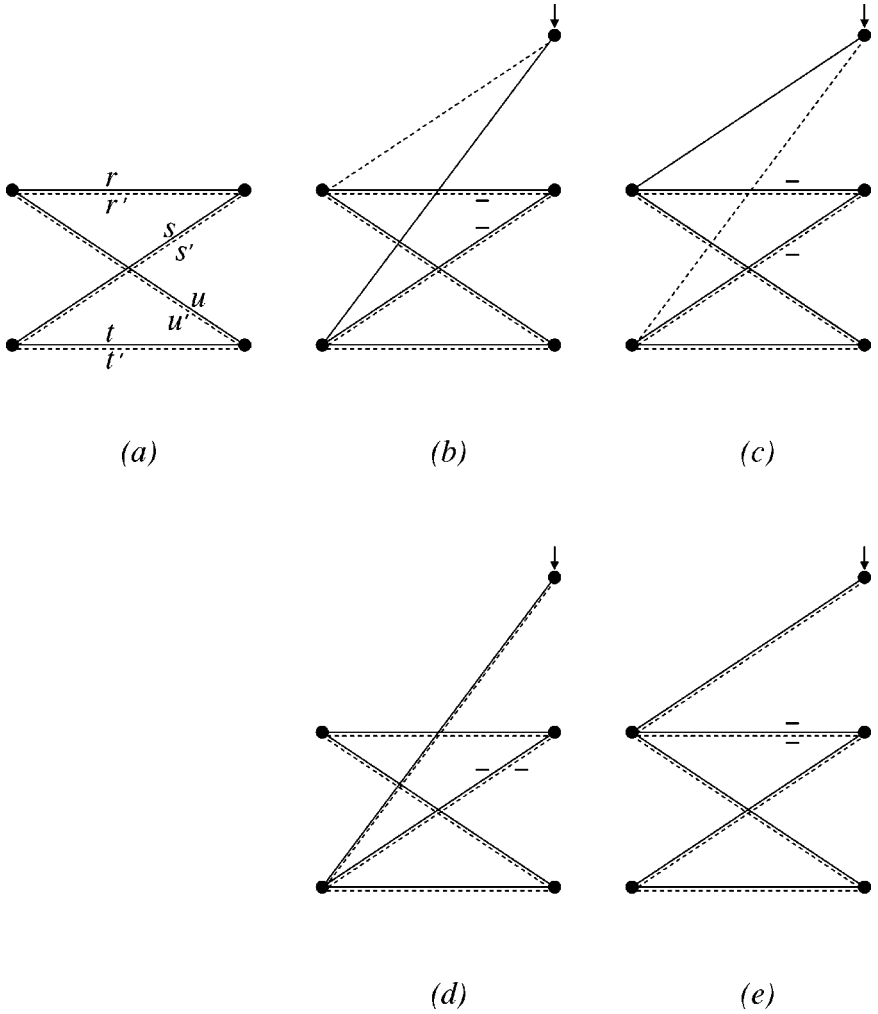

FIG. 7. (a) The "X integral" and its weights. (b)–(e) Diagrams obtained from (a) by rotating away a pair of lines from the $r-s$ junction. The weights in these four diagrams are the same as those in (a), except for the ones with a "$-$" sign, in which case the corresponding weight is decreased by 1.

A substitution of (50) into (49) yields the desired recursion relation

$$I(7a)=-\frac{r'sI(8b)+rs'I(8c)+ss'[I(8d_1)-I(8d_2)]+rr'[I(8e_1)-I(8e_2)]}{(r+s)(r'+s'+n-2)}. \tag{51}$$

Let us illustrate the recursion relation by computing the simplest cases, with $\rho+\sigma=2$.

There are four possibilities with $r+r'+s+s'=2$. Two of them are the known Z-integrals, namely, $X(0,1,t,u|0,1,t,u)=Z(1,t,u)$ and $X(1,0,t,u|1,0,t,u)=Z(1,u,t)$. The other two are exchange integrals which can be obtained from (51):

$$X(1,0,t,u|0,1,t-1,u+1)=-\frac{I(8c)}{n-1}=-\frac{F(t,u+1)}{n-1}=-\frac{t!(u+1)!(n-2)!}{(n+t+u)!}, \tag{52}$$

$$X(0,1,t-1,u|1,0,t,u-1)=-\frac{I(8b)}{n-1}=-\frac{F(t+1,u)}{n-1}=-\frac{(t+1)!u!(n-2)!}{(n+t+u)!}. \tag{53}$$

In particular, (52) reduces to $I(6d)$ of (47) when $t=u=1$.

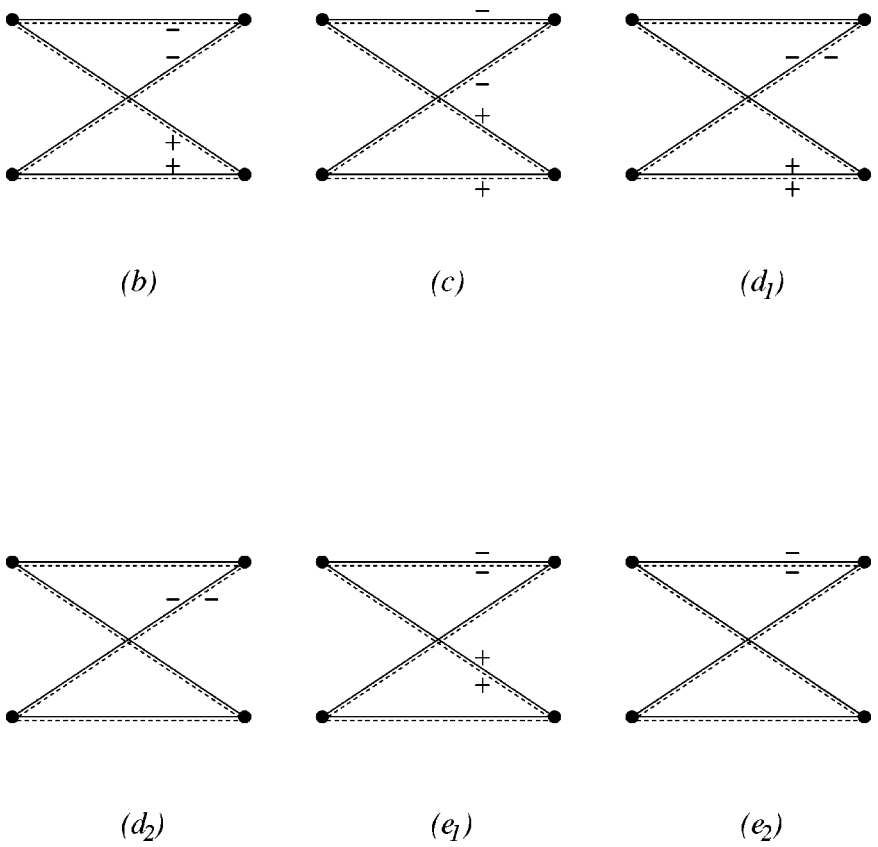

FIG. 8. Terms obtained from the unitarity sum of Figs. 7(b)–7(e). The weights in these diagrams are the same as in Fig. 7(a), except on those lines indicated by a "−" or a "+." In those cases, the corresponding weights are decreased or increased by 1.

IV. CONCLUSION

We have shown how an integral over the U(n) manifold can be computed recursively using only the invariance of the Haar measure and the unitarity condition. The same method can also be used to get a closed expression for a monomial integral over a unit sphere.

In a forthcoming paper, we shall compare the relative advantages of the invariant method developed here and the group-theoretical method reviewed in the Appendix. We will show how the two methods can be combined to strengthen each other.

ACKNOWLEDGMENTS

C.S.L. would like to thank G. Semenoff and A. D'Adda for helpful discussions. This research was supported by the Natural Sciences and Engineering Research Council of Canada and by the Fonds de recherche sur la nature et les technologies of Québec.

APPENDIX: GROUP THEORETICAL CALCULATION

As shown in (23), the nonzero integrals of (19) can be written in the form $\langle I,J|I,J_Q\rangle$. Using group theory, to be reviewed below, the integral can be turned into a multiple sum:

$$\langle I,J|I,J_Q\rangle=\sum_{R\in\mathcal{G}_I}\sum_{S\in\mathcal{G}_J}\sum_{f}\frac{d_f^2}{(p!)^2\tilde{d}_f}\chi_f(SQR), \tag{A1}$$

where p is the degree of U_{IJ} appearing in the integral (19). (C.S.L. wishes to thank Professor Alessandro D'Adda for introducing him to this formula.) The other symbols will be explained below.

The irreducible representations of the unitary group $\mathrm{U}(n)$ are labeled by a Young's tableau. It is defined by a sequence of non-negative integers $f=(f_1 f_2 \cdots f_n)$, with $f_i \geqslant f_{i+1}$. All irreducible representations contained in a pth rank tensor have their Young's tableaux restricted to p boxes, namely, $\Sigma_{i=1}^{n} f_i = p$. In that case clearly $f_i = 0$ for $i > p$. It is customary to drop the zeros when the sequence f is written, so f can be written as $(f_1 f_2 \cdots f_p)$, or even shorter if there are more zeros.

The dimension of the irreducible representation f of $\mathrm{U}(n)$, denoted by $\tilde{d}_f$, is given by the ratio of two Vandermonde determinants

$$\tilde{d}_f = \frac{D(\ell_1, \ell_2, \cdots, \ell_n)}{D(n-1, n-2, \cdots, 0)}, \tag{A2}$$

where $\ell_i = f_i + n - i$, and

$$D(x_1, x_2, \cdots, x_n) = \prod_{i \geqslant j=1}^{n} (x_i - x_j). \tag{A3}$$

The irreducible representations of the symmetric group S_p are also labeled by Young's tableaux $f=(f_1 f_2 \cdots f_p)$. The dimension of an irreducible representation of S_p is denoted by d_f, and the character for the element $P \in S_p$ is denoted by $\chi_f(P)$. Tables are available to give their values for small p.

The character $\chi_f(P)$ depends only on the class that P belongs to. If a permutation P is written in the cycle form, then permutations with the same cycle structure belong to the same class. The cycle structure can be labeled by a Young's tableau $c=(c_1 c_2 \cdots c_p)$, where c_1 is the length of the longest cycle in P, c_2 is the length of the next longest cycle in P, etc. If $P \in c$, we will also write $\chi_f(P)$ as $\chi_f(c)$. The characters together are given by γ_p^2 numbers, where γ_p is either the total number of distinct classes in S_p, or the number of inequivalent irreducible representations. It is equal to the number of partitions of p, and is given by $\gamma_p = 1,2,3,5,7,11,15$, for $p = 1,2,3,4,5,6,7$, respectively.

$\mathcal{G}_I \subset S_p$ is the symmetry group of the index set I, and $\mathcal{G}_J \subset S_p$ is the symmetry group of the index set J. For example, if $I=(111338888)$, then $\mathcal{G}_I = S_3 \times S_2 \times S_4 \subset S_9$. If $I=(13254798)$, then $\mathcal{G}_I$ consists of the identity e only.

The sum in (A1) is over all the irreducible representations f, all elements R of the symmetry group $\mathcal{G}_I$, and all elements S of the symmetry group $\mathcal{G}_J$.

The simplest integrals to calculate are those where the indices in I all take on distinct values, and similarly for J. In that case, $\mathcal{G}_I = \mathcal{G}_J = e$, so the sums in (A1) reduce to a single sum over the irreducible representations f. Since $\chi_f(Q)$ depends on the class c in which Q lies, there are γ_p distinct integrals $\langle I,J|I,J_Q\rangle$ of this type. It is convenient to denote these integrals by $\xi(c)$. To compute them, we need to use (A2) to compute $\tilde{d}_f$, a character table of S_p to compute χ_f and d_f, then we must sum up γ_p terms in (A1) before we get $\xi(c)$.

More generally, (A1) can be written in terms of $\xi(c)$ as

$$\langle I,J|I,J_Q\rangle = \sum_c N(I,J,Q|c)\xi(c),$$

where

$$N(I,J,Q|c) = \sum_{R \in \mathcal{G}_I} \sum_{S \in \mathcal{G}_J} \delta(SQR \in c) \tag{A4}$$

is the total number of SQR in class c. They are often quite tedious to compute. Once it is calculated, we still have to carry out the γ_p sums over c to get $\langle I,J|I,J_Q\rangle$.

This completes the description of formula (A1). In the remainder of this appendix, we will sketch how it is arrived at.

The orthonormal relation for the irreducible representations $D_f(R)$ of the S_p group is

$$\frac{1}{p!}\sum_{P\in S_p}[D_f(P)]_{il}[D_g(P^{-1})]_{mj}=\frac{1}{d_f}\delta_{fg}\delta_{ij}\delta_{lm}. \tag{A5}$$

This leads to the following relation for characters, true for any Q and R in S_p:

$$\frac{1}{p!}\sum_{P\in S_p}\chi_f(PQ)\chi_g(RP^{-1})=\delta_{fg}\frac{1}{d_f}\chi_f(QR). \tag{A6}$$

The corresponding character relation for $\mathrm{U}(n)$,

$$\int (dU)\tilde{\chi}_f(UV)\tilde{\chi}_g(WU^{-1})=\delta_{fg}\frac{1}{\tilde{d}_f}\tilde{\chi}_f(VW), \tag{A7}$$

is true for any V and W in $\mathrm{U}(n)$.

Given a $U\in\mathrm{U}(n)$ and a $P\in S_p$, define $(U)_P$ to be $\Sigma_I U_{I\,I_P}$, where the sum is taken over all the indices in the set $I=(i_1i_2\cdots i_p)$, each covering its full range of values from 1 to n. The index set I_P as well as $U_{I\,I_P}$ are defined at the beginning of Sec. III. If P consists of α_i cycles of length i, then

$$(U)_P=\prod_i(\mathrm{Tr}(U^i))^{\alpha_i}. \tag{A8}$$

Since $(U)_P$ depends only on the cycle structure of P, it is the same for two P's in the same class.

The crucial input to the computation of the integral is the Frobenius formula,

$$(U)_P=\sum_f\tilde{\chi}_f(U)\chi_f(P). \tag{A9}$$

Applying it to $(UV)_e$ and $(WU^{-1})_e$, and using (A7) to integrate, one arrives at the expression

$$\int (dU)(UV)_e(WU^{\dagger})_e=\sum_f\frac{d_f^2}{\tilde{d}_f}\tilde{\chi}_f(VW), \tag{A10}$$

where $d_f=\chi_f(e)$ has been used. Next, use (A6) to introduce the factor

$$\delta_{fg}=\frac{1}{p!}\sum_{P\in S_p}\chi_f(P)\chi_g(P^{-1}) \tag{A11}$$

to the right-hand side of (A10), and use the Frobenius formula again [note that $\chi_g(P^{-1})=\chi_g(P)$]. This allows (A10) to be written as

$$\int (dU)(UV)_e(WU^{\dagger})_e=\sum_{P\in S_p}\sum_f\frac{d_f^2}{p!\tilde{d}_f}\chi_f(P)(VW)_P=\sum_{R,S'\in S_p}\sum_f\frac{d_f^2}{(p!)^2\tilde{d}_f}\chi_f(RS')(VW)_{RS'}. \tag{A12}$$

Introducing the shorthand

$$\delta_{KI_R}\delta_{JL_{S'}}=\left(\prod_{a=1}^{p}\delta_{k_a i_{R(a)}}\delta_{j_a \ell_{S'(a)}}\right), \tag{A13}$$

the sum over R and S' on the right-hand side is

$$\begin{aligned}\sum_{R,S'}\chi_f(RS')V_{LK}W_{IJ}\delta_{KI}\delta_{JL_{RS'}}&=\sum_{R,S'}\chi_f(RS')V_{LK}W_{IJ}\delta_{KI}\delta_{J_{R^{-1}}L_{S'}}\\&=\sum_{R,S'}\chi_f(RS')V_{LK}W_{IJ_R}\delta_{KI}\delta_{JL_{S'}}\\&=\sum_{R,S'}\chi_f(RS')V_{LK}W_{I_{R^{-1}}J}\delta_{KI}\delta_{JL_{S'}}\\&=\sum_{R,S'}\chi_f(RS')V_{LK}W_{IJ}\delta_{KI_R}\delta_{JL_{S'}}.\end{aligned} \tag{A14}$$

Since V and W are arbitrary, the coefficients of $V_{LK}W_{IJ}$ on both sides must be the same. Hence

$$\langle I,J|K,L\rangle=\int(dU)U^*_{IJ}U_{KL}=\sum_f\sum_{R,S'}\frac{d_f^2}{(p!)^2\tilde{d}_f}\delta_{KI_R}\delta_{JL_{S'}}\chi_f(RS'). \tag{A15}$$

Let us now apply (A15) to the special case $\langle I,J|I,J_Q\rangle$. Since $K=I$, the factor δ_{II_R} is nonzero if and only if $R\in\mathcal{G}_I$. Similarly, since $L=J_Q$, the factor $\delta_{JL_{S'}}$ equals $\delta_{JJ_{QS'}}$. Hence $S=QS'$ must be in the invariant group $\mathcal{G}_J$. Now the argument of χ_f in (A15) is $RS'=RQ^{-1}S$. Since R is summed over a group and so is S, we may replace R by R^{-1} and S by S^{-1}. With this replacement, the argument of χ_f is $(SQR)^{-1}$, Using $\chi_f(SQR)=\chi_f((SQR)^{-1})$, we finally arrive at the formula shown in (A1).

Formula (A1) can also be obtained from the following version of the Itzykson–Zuber formula,

$$\int(dU)\exp[\beta\mathrm{Tr}(M_1UM_2U^\dagger)]=\sum_f\frac{\beta^{|f|}d_f}{|f|!\tilde{d}_f}\tilde{\chi}_f(M_1)\tilde{\chi}_f(M_2), \tag{A16}$$

where the sum is over all the Young's tableaux, and $|f|=\Sigma_i f_i$ is the number of boxes in a particular tableau. Using the orthonormal relation (A11), Frobenius's formula (A9) can be inverted to read

$$\int(dU)\exp[\beta\mathrm{Tr}(M_1UM_2U^\dagger)]=\sum_f\frac{\beta^{|f|}d_f}{(|f|!)^3\tilde{d}_f}\sum_{R,S}\chi_f(R)\chi_f(S)(M_1)_R(M_2)_S. \tag{A17}$$

Next, use the formula

$$\chi_f(R)\chi_f(S)=\frac{d_f}{|f|!}\sum_P\chi_f(RPSP^{-1}), \tag{A18}$$

which can be derived from (A5), to combine the two characters into one,

$$\int (dU)\exp[\beta \mathrm{Tr}(M_1 U M_2 U^\dagger)] = \sum_f \frac{\beta^{|f|} d_f^2}{(|f|!)^4 \tilde{d}_f} \sum_{P,R,S} \chi_f(RPSP^{-1})(M_1)_R (M_2)_S$$

$$= \sum_f \frac{\beta^{|f|} d_f^2}{(|f|!)^4 \tilde{d}_f} \sum_{P,R,S'} \chi_f(RS')(M_1)_R (M_2)_{P^{-1}S'P}. \quad \text{(A19)}$$

Since $(M_2)_S$ depends only on the class that S lies in, the last factor is thus independent of P. Therefore the sum over P yields only a factor $|f|!$.

Identifying terms proportional to β^p on both sides, one gets

$$\sum_{I,J,K,L} \langle I,J|K,L\rangle (M_1)_{IK}(M_2)_{LJ} = \sum_f \frac{d_f^2}{(p!)^2 \tilde{d}_f} \sum_{R,S'} \chi_f(RS')(M_1)_{IK}(M_2)_{LJ} \delta_{KI_R} \delta_{JL_{S'}}, \quad \text{(A20)}$$

which agrees with (A15).

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Global existence for small initial data in the Born–Infeld equations

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(Received 29 July 2003; accepted 19 August 2003)

We prove global existence of a classical solution for small initial in the Cauchy problem of the Born–Infeld system describing nonlinear electromagnetism. For the proof we crucially use the null form structure of the the nonlinear terms under the Lorentz gauge condition. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1621057]

I. INTRODUCTION

Recently the Born–Infeld theory has received much attention mainly due to the fact that the Born–Infeld type Lagrangians naturally appear in string theories. Namely, it has been realized that they can describe the low energy dynamics of D-branes. [See, e.g., Polchinski (1996) and references therein.] This state of affair triggered the revival of interests in the original Born–Infeld electromagnetism (Born and Infeld, 1934) and the exploration of Born–Infeld gauge theories in general (see, e.g., Gibbons, 1998). We also remark that there is even a study of the theory in the connection to the hydrodynamics (Brenier, 2003). The Born–Infeld Lagrangian in $\mathbb{R}^{n+1}$ is

$$\mathcal{L}=\beta^2\left(1-\sqrt{-\det\left(\eta_{\mu\nu}+\frac{1}{\beta}F_{\mu\nu}\right)}\right), \tag{1.1}$$

where $(\eta_{\mu\nu})=\mathrm{diag}(-1,1,\ldots,1)$ is the $(n+1)$ dimensional Minkowski metric, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, $0\leqslant\mu,\nu\leqslant n$ with $\{A_\mu\}_{\mu=0,\ldots,n}$ the gauge fields, and $\beta>0$ is a parameter.

This theory may be thought of as a nontrivial alternative to the standard Maxwell theory of electromagnetism. The major motivations for the introduction of the Born–Infeld field theory are things such as overcoming the infinity problem associated with a point charge source in the Maxwell theory, natural recovery of the usual Maxwell theory as a linear approximation, and the hope to find solitonlike solutions representing pointlike charged particles.

From a mathematical view point this theory is the highly nonlinear generalization of the Maxwell theory. Gibbons (1998) has lead to a systematic study of the Born–Infeld theory and obtained exact solutions in numerous situations. He links areas of physics and differential geometries such as Bernstein theorem for minimal surface equations (Osserman, 1986) or maximal hypersurface equations (Calabi, 1970; Cheng and Yau, 1976) in Minkowskian spaces.

In $\mathbb{R}^{n+1}(n=2,3)$, the Euler–Lagrange equations for (1.1) are

$$\partial_\mu G^{\mu\nu}=0,\quad G^{\mu\nu}:=\frac{F^{\mu\nu}-(1/4\beta^2)(F_{\alpha\beta}F^{\alpha\beta})\tilde{F}^{\mu\nu}}{\sqrt{1+(1/2\beta^2)F_{\alpha\beta}F^{\alpha\beta}-(1/16\beta^4)(F_{\alpha\beta}\tilde{F}^{\alpha\beta})^2}} \tag{1.2}$$

together with Bianchi identity

$$\partial_\mu\tilde{F}^{\mu\nu}=0\quad(\partial_\mu\tilde{F}^{\mu}=0\ \text{ for }\ n=2), \tag{1.3}$$

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where $\tilde{F}^{\alpha\beta}=\frac{1}{2}\epsilon^{\alpha\beta\mu\nu}F_{\mu\nu}$ ($\tilde{F}^{\alpha}=\frac{1}{2}\epsilon^{\alpha\mu\nu}F_{\mu\nu}$) is the Hodge dual of $F^{\mu\nu}$, and $\epsilon^{\alpha\beta\mu\nu}$ is totally skew-symmetric tensor with the normalization $\epsilon^{0123}=1(\epsilon^{012}=1)$. We note that the factor $\tilde{F}$ disappears when $n=2$.

When $n=3$, we can write the system (1.2) and (1.3) in a more familiar form introducing the electric components $E_i=F_{i0}$ and the magnetic components $B_i=\frac{1}{2}\epsilon_{ijk}F^{jk}$ with $i=1,2,3$, respectively. Denoting $E=(E_1,E_2,E_3)$ and $B=(B_1,B_2,B_3)$, we find that (1.2) corresponds to

$$\operatorname{div}\left[\frac{1}{R}\left\{E+\frac{1}{\beta^2}(E\cdot B)B\right\}\right]=0,$$

$$\frac{\partial}{\partial t}\left[\frac{1}{R}\left\{E+\frac{1}{\beta^2}(E\cdot B)B\right\}\right]=\operatorname{curl}\left[\frac{1}{R}\left\{B-\frac{1}{\beta^2}(E\cdot B)E\right\}\right],$$

where we denoted $R=\sqrt{1-(1/\beta^2)(E^2-B^2)-(1/\beta^4)(E\cdot B)^2}$, while (1.3) corresponds to

$$\operatorname{div}B=0,\quad \frac{\partial B}{\partial t}=-\operatorname{curl}E.$$

We observe that as $\beta\to\infty$, we have $G^{\mu\nu}\to F^{\mu\nu}$, and the system (1.2) and (1.3) formally converges to the usual Maxwell equations in vacuum:

$$\partial_\mu F^{\mu\nu}=0,\quad \partial_\mu\tilde{F}^{\mu\nu}=0,$$

which can be written in terms of the electric and magnetic fields as

$$\operatorname{div}E=0,\quad \frac{\partial E}{\partial t}=\operatorname{curl}B,\quad \operatorname{div}B=0,\quad \frac{\partial B}{\partial t}=-\operatorname{curl}E.$$

We state the our main theorem.

Theorem 1.1: *Let $n=2,3$. Suppose $f,g\in[C_0^\infty(\mathbb{R}^n)]^{(n+1)}$ is given. We consider the initial value problem of the system (3.1)–(3.6) in $\mathbb{R}^{n+1}$ under the Lorentz gauge condition, $\partial_\mu A^\mu=0$ with the initial data*

$$A^\mu(0,\cdot)=\varepsilon f,\quad \partial_t A^\mu(0,\cdot)=\varepsilon g,$$

satisfying

$$\partial_\mu G^{\mu 0}=0,\quad \partial_\mu\tilde{F}^{\mu 0}=0,\quad \partial_\mu A^\mu(0,\cdot)=0.$$

Then, there exists ε_0 such that if $\varepsilon\leqslant\varepsilon_0$, then the smooth solution of (3.1)–(3.6) exists for all $t>0$.

Remark 1: The proof actually does not require compact support of the initial data; appropriate decays at infinity are enough.

Remark 2: Under the choice of Lorentz gauge our system (3.1)–(3.6) has null form structure, and has some similar features to the simpler case of the minimal surface equations in $(\mathbb{R}^{n+1},\eta_{\mu\nu})$, studied recently by Lindblad (2002). (See also the remark after proof in Sec. III.)

II. PRELIMINARIES

We briefly review the notions of the commuting vector field methods and the null forms developed by Klainerman (1980, 1986), Christodoulou (1986), Christodoulou and Klainerman (1990). A point in the $(n+1)$-dimensional Minkowski space will be denoted by $(t,x)=(x_\alpha)_{0\leqslant\alpha\leqslant n}$. The space–time derivatives of a function $f:\mathbb{R}^{n+1}\to\mathbb{R}$ are denoted by $\partial f=(\partial_t f,\partial_1 f,\ldots,\partial_n f)$.

We raise and lower indices with the Minkowski metric $\eta=(\eta_{\alpha\beta})=\eta^{-1}=(\eta^{\alpha\beta})=\mathrm{diag}(-1,1,\ldots,1)$. We also use the summation convention for the repeated indices. Therefore, the wave operator is denoted by $\Box=\partial_\alpha\partial^\alpha$. Greek indices are used to denote $0,\ldots,n$, while Latin indices are for $1,\ldots,n$. The vector fields

$$\Omega_{\mu\nu}=x_\mu\partial_\nu-x_\nu\partial_\mu, \quad S=x^\mu\partial_\mu$$

are the rotation and the scaling operators in $\mathbb{R}^{n+1}$. In what follows, the vector fields $\partial_\mu, S, \Omega_{\mu\nu}(\mu<\nu)$ will be denoted by Γ_k, $k=0,\ldots,n+1+n(n+1)/2$. We shall also use the multi-index notation $\Gamma^I=\Gamma_1^{I_1}\cdots\Gamma_m^{I_m}$. We recall the commutation relations between $\Box$ and Γ:

$$\begin{aligned}&[\Box,S]=2\Box,\\ &[\Box,\partial_\mu]=0, \qquad 0\leqslant\mu\leqslant n,\\ &[\Box,\Omega_{\mu\nu}]=0, \qquad 0\leqslant\mu<\nu\leqslant n.\end{aligned} \tag{2.1}$$

We find easily the following relations:

$$[\Gamma_k,\partial_\nu]=a_{\nu k}^\mu\partial_\mu,$$

for some suitable constant coefficients $a_{\nu k}^\mu$. Let us introduce the null forms

$$\begin{aligned}&\tilde{Q}(\phi,\psi)=\partial_t\phi\partial_t\psi-\partial_i\phi\partial_i\psi,\\ &Q_{\alpha\beta}(\phi,\psi)=\partial_\alpha\phi\partial_\beta\psi-\partial_\alpha\psi\partial_\beta\phi, \qquad \text{for} \qquad \alpha,\beta=0,1,\ldots,n.\end{aligned} \tag{2.2}$$

Let Q stand for any of the above null forms. Then the following commutation relations hold:

$$\Gamma Q(\phi,\psi)=Q(\Gamma\phi,\psi)+Q(\phi,\Gamma\psi)+b^{\mu\nu}Q_{\mu\nu}(\phi,\psi) \tag{2.3}$$

for some constants $b^{\mu\nu}$. The following lemma will be used to give time decay factor $1/(1+t)$ to the quadratic terms Q [see p. 57 in Sogge (1995) for a proof].

Lemma 2.1: Let Q be one of the null forms in (2.2). Then if $t>0$,

$$|Q(\phi,\psi)(t,x)|\leqslant\frac{C}{1+t+|x|}\sum_{|I|=1}|\Gamma^I\phi(t,x)|\sum_{|I|=1}|\Gamma^I\psi(t,x)|.$$

Combining the above lemma with (2.3), one can easily verify [see p. 59 in Sogge (1995)] the following.

Corollary 2.2: Let Q be one of the null forms in (2.2). Then if $t>0$,

$$\begin{aligned}(1+t+|x|)\sum_{|I|\leqslant M}|\Gamma^I Q(\phi,\psi)|\leqslant C_M&\sum_{1\leqslant|I|\leqslant M+1}|\Gamma^I\phi|\sum_{1\leqslant|I|\leqslant(M+2)/2}|\Gamma^I\psi|\\ &+C_M\sum_{1\leqslant|I|\leqslant M+1}|\Gamma^I\psi|\sum_{1\leqslant|I|\leqslant(M+2)/2}|\Gamma^I\phi|.\end{aligned} \tag{2.4}$$

To estimate the L^2 norm of the solution itself A_ν, use will be made of the following lemma, the proof of which is in Linblad (1990, 2002)

Lemma 2.3: If u solves the Cauchy problem

$$\Box u=\sum_{\alpha=0}^n\partial_\alpha G_\alpha, \quad u(0,)=\varepsilon f, \quad u_t(0,)=\varepsilon g,$$

then

$$\|u(t,\cdot)\|_{L^2} \leqslant \sum_{\alpha=0}^{n} \int \|G_\alpha(s,\cdot)\|_{L^2} ds + C(f,g,G_0(0,\cdot))m(t)\varepsilon,$$

where $m(t)=1$ *if* $n\geqslant 3$, $m(t)=\log(2+t)$ *if* $n=2$ *and* $C(f,g,G_0(0,\cdot))$ *is some constant depending on some weighted Sobolev norm of initial data* f *and* g.

We also use the following L^1-L^∞ estimate without proof (see Hormander, 1997).

Lemma 2.4: The solution u *of*

$$\Box u(t,x)=F(t,x), \quad u(0,\cdot)=\varepsilon f, \quad \partial_t u(0,\cdot)=\varepsilon g, \quad (t,x)\in \mathbb{R}^{n+1}$$

satisfies

$$|u(t,x)| \leqslant C(1+t+|x|)^{-(n-1)/2}\left(\sum_{|I|\leqslant n-1} \int_0^t \left\| \frac{\Gamma^I F(s,\cdot)}{(1+s+|\cdot|)^{(n-1)/2}} \right\|_{L^1} ds + C(f,g)\varepsilon \right).$$

III. PROOF OF THE MAIN THEOREM

Before getting into the main parts of the proof we will present a few observations. We can rewrite (1.2) in the form of the quasilinear wave equations,

$$\begin{aligned} &2(1+(2\beta^2)^{-1}\langle F\rangle^2-(16\beta^4)^{-1}\langle \tilde{F}\rangle^4)\Box A^\nu \\ &\quad = \frac{1}{2\beta^2}\partial_\mu[\langle \tilde{F}\rangle^2 \tilde{F}^{\mu\nu}]\left(1+\frac{1}{2\beta^2}\langle F\rangle^2-\frac{1}{16\beta^4}\langle \tilde{F}\rangle^4\right) \\ &\qquad +\left(F^{\mu\nu}-\frac{1}{4\beta^2}\langle \tilde{F}\rangle^2\tilde{F}^{\mu\nu}\right)\left(\frac{1}{2\beta^2}\partial_\mu(\langle F\rangle^2)-\frac{1}{16\beta^4}\partial_\mu(\langle \tilde{F}\rangle^4)\right), \end{aligned} \tag{3.1}$$

where we denoted $\langle F\rangle^2=F^{\alpha\beta}F_{\alpha\beta}$ and $\langle \tilde{F}\rangle^2=F^{\alpha\beta}\tilde{F}_{\alpha\beta}$. We note $\tilde{F}=0$ for $n=2$. Under the condition of Lorentz gauge $\partial_\mu A^\mu=0$, we have

$$\tfrac{1}{2}\langle F\rangle^2=\tilde{Q}(A^\mu,A_\mu)+Q_{\mu\nu}(A^\mu,A^\nu), \tag{3.2}$$

$$\langle \tilde{F}\rangle^2=-\epsilon^{\alpha\beta\mu\nu}Q_{\alpha\beta}(A_\mu,A_\nu), \tag{3.3}$$

$$F^{\mu\nu}\partial_\mu(\langle F\rangle^2)=\tilde{Q}(A^\nu,\langle F\rangle^2)-Q^{\nu\alpha}(A_\alpha,\langle F\rangle^2), \tag{3.4}$$

$$F^{\mu\nu}\partial_\mu(\langle \tilde{F}\rangle^4)=\tilde{Q}(A^\nu,\langle \tilde{F}\rangle^4)-Q^{\nu\alpha}(A_\alpha,\langle \tilde{F}\rangle^4), \tag{3.5}$$

$$\tilde{F}^{\mu\nu}\partial_\mu(\langle \tilde{F}\rangle^2)=\tfrac{1}{2}\epsilon^{\nu\alpha\beta\gamma}Q_{\alpha\beta}(A_\gamma,\langle \tilde{F}\rangle^2). \tag{3.6}$$

Note that for each ν the right hand side of (3.1) has the double null structure which produces a decay factor $1/(1+t)^2$.

Proof of Theorem 1.1: We first verify that the gauge condition, $\partial_\mu A^\mu=0$, and the two constraints, $\partial_\mu G^{\mu 0}=0, \partial_\mu \tilde{F}^{\mu 0}=0$, will be propagated along with the equations of motion (3.1)–(3.6). Let us set

$$U=\partial_\mu A^\mu, \quad V=\partial_\mu G^{\mu 0}, \quad W=\partial_\mu \tilde{F}^{\mu 0}.$$

If Eqs. (3.1)–(3.6) for A^μ are satisfied, then after elementary computations we derive the following relations:

$$\partial_t U = -RV,$$

$$\partial_t V = -\frac{1}{R}\Delta U - \partial_i\left(\frac{1}{R}\right)\partial^i U, \tag{3.7}$$

$$\partial_t W = 0.$$

The above equations are the linear equations with respect to U,V and W. If the initial data $A^\mu(0,\cdot), \partial_t A^\mu(0,\cdot)$ satisfy $U(0,\cdot)=V(0,\cdot)=W(0,\cdot)=0$, as is our case, then by the uniqueness result of the linear system we conclude that $U(t,\cdot)=V(t,\cdot)=W(t,\cdot)=0$ in the interval $(0,T)$, in which the classical solutions of the equations (3.1)–(3.6) exist.

Next we turn to the question of local existence of solution. We can write the equations (3.1)–(3.6) in the following forms:

$$\Box A^\nu + \mathcal{D}^{-1}\mathcal{C}^{\nu\alpha\mu\beta}\partial_{\alpha\beta}A_\mu = 0, \qquad \nu = 0,\ldots,n, \tag{3.8}$$

where $\mathcal{D}$ is the factor in front of $\Box A_\nu$ in the left-hand side of (3.1), and $\mathcal{C}^{\nu\alpha\mu\beta} = \mathcal{C}^{\nu\alpha\mu\beta}(\partial A)$ are polynomials of order p, $2 \leqslant p \leqslant 4$. In fact, the coefficients $\mathcal{C}^{\nu\alpha\mu\beta}(\partial A)$ take the form of $F^i_{\sigma\rho}F^j_{\gamma\delta}(\partial^\mu A_\mu)^k$, $2 \leqslant i+j+k \leqslant 4$. We also note that $\mathcal{C}(0)=0$, and, most importantly,

$$\mathcal{C}^{\nu\alpha\mu\beta}(\partial A) = \mathcal{C}^{\mu\beta\nu\alpha}(\partial A). \tag{3.9}$$

The system (3.8) with the above conditions for $\mathcal{C}^{\mu\nu\alpha\beta}(\partial A)$ is similar to the elastic wave equations studied in Dafermos and Hrusa (1985) and John (1988) where they proved the local well-posedness in the suitable Sobolev spaces, using the energy method.

For the latter use we derive the energy estimate for the following system:

$$\Box A_\nu + \mathcal{C}^{\nu\alpha\mu\beta}(t,x)\partial_{\alpha\beta}A_\mu = f_\nu, \qquad \nu = 0,\ldots,n, \tag{3.10}$$

under the assumptions $|\mathcal{C}| = \Sigma|\mathcal{C}^{\nu\alpha\mu\beta}| \leqslant \frac{1}{2}$ and $\mathcal{C}^{\nu\alpha\mu\beta}(t,x) = \mathcal{C}^{\mu\beta\nu\alpha}(t,x)$.

Multiplying $\partial_t A_\nu$ at each νth equation of (3.10), summing over ν, and integrating over $\mathbb{R}^n$, we obtain

$$\int_{\mathbb{R}^n} \partial_t A_\nu \Box A_\nu + \partial_t A_\nu \mathcal{C}^{\nu\alpha\mu\beta}\partial_{\alpha\beta}A_\mu = \int_{\mathbb{R}^n} \partial_0 A_\nu\, f_\nu. \tag{3.11}$$

Using the fact that $\mathcal{C}^{\nu\alpha\mu\beta} = \mathcal{C}^{\mu\beta\nu\alpha}$ and integrating by parts, we deduce

$$\begin{aligned}
&\partial_0 \int_{\mathbb{R}^n} \frac{1}{2}|\partial A|^2 + \mathcal{C}^{\nu i\mu j}\partial_i A_\nu \partial_j A_\mu - \mathcal{C}^{\nu 0\mu 0}\partial_0 A_\nu \partial_0 A_\mu \\
&\quad = \int_{\mathbb{R}^n} \partial_0 \mathcal{C}^{\nu i\mu j}\partial_i A_\mu \partial_j A_\nu - \partial_i \mathcal{C}^{\nu i\mu j}\partial_0 A_\mu \partial_j A_\nu - \partial_j \mathcal{C}^{\nu i\mu j}\partial_0 A_\nu \partial_i A_\mu \\
&\quad\quad - \int_{\mathbb{R}^n} \partial_0 A_\nu f_\nu + \partial_i \mathcal{C}^{\nu 0\mu 0}\partial_0 A_\mu \partial_0 A_\nu + \partial_0 \mathcal{C}^{\nu 0\mu 0}\partial_0 A_\mu \partial_0 A_\nu.
\end{aligned} \tag{3.12}$$

Integrating over $[0,T]$, and taking into account the smallness of $\mathcal{C}^{\nu\alpha\mu\beta}$ ($\Sigma|\mathcal{C}^{\nu\alpha\mu\beta}| \leqslant \frac{1}{2}$), and applying the Hölder inequality on the right hand side of (3.12), we obtain

$$\|\partial A(t)\|_{L^2} \leqslant C\exp\left(\int_0^t |\partial\mathcal{C}(\tau)|d\tau\right)\|\partial A(0)\|_{L^2} + C\int_0^t \exp\left(\int_s^t |\partial\mathcal{C}(\tau)|d\tau\right)\|f(s,\cdot)\|_{L^2}ds, \tag{3.13}$$

where $|\partial \mathcal{C}(\tau)| = \Sigma \sup_x |\partial_\lambda \mathcal{C}^{\nu\alpha\mu\beta}(\tau,x)|$ and the constant C depends only on the L^∞ norm of $\mathcal{C}^{\nu\alpha\mu\beta}$. Differentiation of (3.10) with respect to time or the spatial variable shows that each partial derivative of A_μ satisfies a system with the same principal part as (3.10) and remainder terms depending on the derivatives of $\mathcal{C}$, f and A_μ of lower order. Thus one can obtain energy estimates for the higher order derivatives of A_μ.

Next we will present the main part of the proof. Below we concentrate on the case of $n=2$. The case $n=3$ is similar and even simpler due to the faster decays near infinity of the solutions to the linear wave equation. The Euler–Lagrange equations in $\mathbb{R}^{2+1}$ of (1.1) under Lorentz gauge (for simplicity we set the constant $\beta=1$) can be written as

$$\partial_\mu \left(\frac{F_{\mu\nu}}{\sqrt{1+2^{-1}F_{\alpha\beta}F^{\alpha\beta}}} \right) = 0. \tag{3.14}$$

We can write (3.14) as wave equations, using the condition $\partial^\mu A_\mu = 0$,

$$\Box A^\nu = \partial_\mu F^{\mu\nu} = \partial_\mu \left(F^{\mu\nu} \left(1 - \frac{1}{\sqrt{1+2^{-1}\langle F\rangle^2}} \right) \right), \tag{3.15}$$

where $\frac{1}{2}\langle F\rangle^2 = \tilde{Q}(A^\mu, A_\mu) + Q_{\mu\nu}(A^\mu, A^\nu)$. Applying Γ^I to the both sides of (3.15), we get

$$\Box \Gamma^I A^\nu = \sum_{\mu=0}^{2} \partial_\mu \left(\sum G_{i_1,\cdot,i_k,I_1,\cdot,I_k}(Q)\partial_{i_1}\Gamma^{I_1}A \cdots \partial_{i_k}\Gamma^{I_k}A \right). \tag{3.16}$$

Note that the right hand side of (3.16) is in the divergence form and $G_{i_1,\cdot,i_k,I_1,\cdot,I_k}(Q)$ is bounded function for small Q. We can also write (3.14) as a wave equation with null forms

$$\Box A^\nu = \frac{1}{2} \frac{\tilde{Q}(A^\nu, 2^{-1}\langle F\rangle^2) - Q^{\nu\alpha}(A_\alpha, 2^{-1}\langle F\rangle^2)}{1+2^{-1}\langle F\rangle^2}. \tag{3.17}$$

Differentiating with respect to Γ^I, we obtain

$$\begin{aligned} &\Box \Gamma^I A^\nu - \frac{1}{2} \frac{\tilde{Q}(A^\nu, 2^{-1}\langle \Gamma^I F\rangle^2) - Q^{\nu\alpha}(A_\alpha, 2^{-1}\langle \Gamma^I F\rangle^2)}{1+2^{-1}\langle F\rangle^2} \\ &\quad = \sum_{\substack{k\geqslant 3, |I_1|+\cdots+|I_k|\leqslant |I|+1 \\ |I_i|\leqslant (|I|+1)/2, i<k, |I_k|\leqslant |I|}} H_{i_1,\ \ldots, i_k, I_1,\ \ldots, I_k}(A, Q(A,A))(\partial_{i_1}\Gamma^{I_1}A)\cdots(\partial_{i_1}\Gamma^{I_1}A), \end{aligned} \tag{3.18}$$

where $2^{-1}\langle \Gamma^I F\rangle^2 = \tilde{Q}(A^\mu, \Gamma^I A_\mu) + Q_{\mu\nu}(A^\mu, \Gamma^I A^\nu)$. Note that H is a bounded function for small $A, Q(A,A)$ and the coefficients of the highest order terms are symmetric in the sense of (3.9) Finally, we write (3.14) in the form suitable for applying the $L^1 - L^\infty$ estimate (Lemma 2.4):

$$\begin{aligned} \Box \Gamma^I A^\nu = &\sum_{\substack{k\geqslant 3 \\ |I_1|+\cdots+|I_k|\leqslant |I|}} K^{i_0,\ldots,i_k}_{I_1,\ldots,I_k}(Q(A,A))Q^{i_0 i_1}(\Gamma^{I_1}A, Q^{i_0 i_1}(\Gamma^{I_2}A, \Gamma^{I_3}A)) \\ &\times Q^{i_4 i_5}(\Gamma^{I_4}A, \Gamma^{I_5}A)\cdots Q^{i_{k-1} i_k}(\Gamma^{I_{k-1}}A, \Gamma^{I_k}A), \end{aligned} \tag{3.19}$$

where $i_{j-1}i_j$ is the index for denoting the several terms under a fixed $I_1,\ldots,I_k$.

We will prove that following bounds are guaranteed all the time if K is sufficiently large and ε is sufficiently small:

$$M_1(t)=\sum_{|I|\leqslant N}\|\partial\Gamma^I A(t,\cdot)\|_{L^2}\leqslant K\varepsilon(1+t)^{\delta},$$

$$M_2(t)=\sum_{|I|\leqslant N}\|\Gamma^I A(t,\cdot)\|_{L^2}\leqslant K\varepsilon(1+t)^{\delta}, \tag{3.20}$$

$$N_1(t)=\sum_{|J|\leqslant (N+1)/2+1}\|\Gamma^J A(t,\cdot)\|_{L^\infty}\leqslant K\varepsilon(1+t)^{-1/2},$$

where $\|\Gamma^I A(t,\cdot)\|_{L^2}=\Sigma_{\alpha=0}^2\|\Gamma^I A_\alpha(t,\cdot)\|_{L^2}$ and $0<\delta<\frac{1}{2}$ fixed.

Applying the energy estimates (3.13) to (3.18), we have

$$M_1(t)\leqslant C\varepsilon\exp\left(\int_0^t N_1(\tau)^2 d\tau\right)+\int_0^t\exp\left(\int_s^t N_1(\tau)^2 d\tau\right)C(N_1(s))N_1(s)^2M_1(s)ds \tag{3.21}$$

and Lemma 2.3 applied to (3.16) gives

$$M_2(t)\leqslant C\left(C(f,g)m(t)\varepsilon+\int_0^t C(N_1(s))N_1(s)^2M_1(s)ds\right). \tag{3.22}$$

Finally, Lemma 2.4 applied to (3.19), Lemma 2.1 and the Cauchy Schwartz inequality give

$$N_1(t)\leqslant C(1+t)^{-1/2}\left(C(f,g)\varepsilon+\int_0^t\frac{N_1(s)}{(1+s)^{1/2+1}}(M_1(s)+M_2(s))^2ds\right), \tag{3.23}$$

if $(N+1)/2+1+n-1\leqslant N$, i.e., $N\geqslant 2n+1$. We note that the null condition produced an extra power of $(1+s)^{-1}$ in the integral (3.23). Actually we have one more power but we do not use it here. From (3.20) we can get

$$\exp\left(\int_s^t N_1(\tau)^2 d\tau\right)\leqslant\exp\left(\varepsilon^2K^2\int_s^t(1+\tau)^{-1}d\tau\right)=\left(\frac{1+t}{1+s}\right)^{\varepsilon^2K^2}, \tag{3.24}$$

so it follows from (3.21)

$$M_1(t)\leqslant C\varepsilon(1+t)^{K^2\varepsilon^2}+\int_0^t C\varepsilon^3K^3\left(\frac{1+t}{1+s}\right)^{\varepsilon^2K^2}(1+s)^{\delta-1}ds\leqslant\frac{K\varepsilon}{2}(1+t)^{\delta} \tag{3.25}$$

if K is sufficiently large and ε is sufficiently small. Also, from (3.22) we get

$$M_2(t)\leqslant C\varepsilon\log(2+t)+\int_0^t C\varepsilon^3K^3(1+s)^{\delta-1}ds\leqslant\frac{K\varepsilon}{2}(1+t)^{\delta} \tag{3.26}$$

if K is sufficiently large and ε is sufficiently small. Finally, from (3.23) we get

$$N_1(t)\leqslant C\varepsilon(1+t)^{-1/2}+(1+t)^{-1/2}\int_0^t C\varepsilon^3K^3(1+s)^{2\delta-2}ds\leqslant\frac{K\varepsilon}{2}(1+t)^{-1/2} \tag{3.27}$$

if K is sufficiently large and ε is sufficiently small, since $0<\delta<\frac{1}{2}$. Consequently, we get a bound of $N_1(t)$ smaller than the assumption. Therefore the solution can be extended by continuity argument. If we assume the maximal time of existence $T=T_*(<\infty)$, the above result contradicts the maximality of T_*. We obtain the global existence of smooth solution. □

Remark after Proof: We should mention that the main part of our proof is a direct adaptation of the argument given by Lindblad (2002). The minimal surface equation studied in Lindblad (2002), on the other hand, can be considered as the special case of Nambu–Goto equations, the Lagrangian of which is given by (Gibbons, 1998)

$$\mathcal{L}=1-\sqrt{-\det(\eta_{\mu\nu}+\partial_\mu y\partial_\nu y)},$$

where $y=(y_1,\ldots,y_m)$. The case $m=1$ corresponds to the equation of Lindblad (2002). In $m=2$ we can check the following ($y_1=\phi, y_2=\chi$):

$$\begin{aligned}-\det(\eta_{\mu\nu}+\partial_\mu y\partial_\nu y)&=-\det(\eta_{\mu\nu}+\partial_\mu\phi\partial_\nu\phi+\partial_\mu\chi\partial_\nu\chi)\\&=1+\tilde{Q}(\phi,\phi)+\tilde{Q}(\chi,\chi)+\tfrac{1}{2}Q_{\mu\nu}(\phi,\chi)Q^{\mu\nu}(\phi,\chi):=\mathcal{K}.\end{aligned}$$

The equation of motions for ϕ is

$$\begin{aligned}\mathcal{K}\{\Box\phi+\tfrac{1}{2}Q^{\mu\nu}(Q_{\mu\nu}(\phi,\chi),\chi)\}&=\tfrac{1}{2}\{\tilde{Q}(\phi,\tilde{Q}(\phi,\phi))+\tilde{Q}(\phi,\tilde{Q}(\chi,\chi))\\&\quad+\tilde{Q}(\phi,\tfrac{1}{2}Q_{\mu\nu}(\phi,\chi)Q^{\mu\nu}(\phi,\chi))\}\\&\quad+\tfrac{1}{4}\{Q^{\mu\nu}(\phi,\chi)Q_{\nu\mu}(\chi,\tilde{Q}(\phi,\phi))+Q^{\mu\nu}(\phi,\chi)Q_{\nu\mu}(\chi,\tilde{Q}(\chi,\chi))\}\\&\quad+\tfrac{1}{4}Q^{\mu\nu}(\phi,\chi)Q_{\nu\mu}(\chi,\tfrac{1}{2}Q_{\alpha\beta}(\phi,\chi)Q^{\alpha\beta}(\phi,\chi)).\end{aligned}\tag{3.28}$$

The corresponding equation for χ can be obtained by replacing ϕ by χ in the above. The symmetry of equations in the sense of (3.9) is also observed in the above system. Besides, here also we have double null form and the divergence structure. Hence, we can expect that the proof of global existence of the classical solution goes similar to the above one.

ACKNOWLEDGMENTS

This research was supported partially by Grant No. F01-2002-000-20014 from the KOSEF.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

Old and new results for superenergy tensors from dimensionally dependent tensor identities

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(Received 6 August 2003; accepted 6 September 2003)

It is known that some results for spinors, and in particular for superenergy spinors, are much less transparent and require a lot more effort to establish, when considered from the tensor viewpoint. In this paper we demonstrate how the use of dimensionally dependent tensor identities enables us to derive a number of 4-dimensional identities by straightforward tensor methods in a signature independent manner. In particular, we consider the quadratic identity for the Bel–Robinson tensor $\mathcal{T}_{abcx}\mathcal{T}^{abcy}=\delta_x^y\,\mathcal{T}_{abcd}\mathcal{T}^{abcd}/4$ and also the new conservation law for the Chevreton tensor, both of which have been obtained by spinor means; both of these results are rederived by *tensor* means for 4-dimensional spaces of any signature, using dimensionally dependent identities, and, moreover, we are able to conclude that there are no *direct* higher dimensional analogs. In addition we demonstrate a simple way to show the nonexistense of such identities via counter examples; in particular we show that there is no nontrivial Bel tensor analog of this simple Bel–Robinson tensor quadratic identity. On the other hand, as a sample of the power of generalizing dimensionally dependent tensor identities from four to higher dimensions, we show that the symmetry structure, trace-free and divergence-free nature of the 4-dimensional Bel–Robinson tensor does have an analog for a class of tensors in higher dimensions. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1624094]

I. INTRODUCTION

Investigations connected with the Bel–Robinson tensor[1] in four dimensions are usually much simpler and more efficient when carried out in spinor formalism.[2] Senovilla[3] has demonstrated that a much larger class of tensors—*superenergy tensors*—share most of the desirable properties of the Bel–Robinson tensor, and Bergqvist[4] has shown how *superenergy spinors* give a simpler and more efficient presentation of certain aspects of these superenergy tensors. Recently, Bergqvist, Eriksson, and Senovilla[5] have obtained new conservation laws for the electromagnetic field using superenergy spinor considerations, and emphasized that the proof of this result is far from obvious from the tensor point of view.

It is reassuring to know that certain important but perhaps unexpected properties—disguised in the complexities of the tensor formalism—become more transparent in the spinor formalism; but the parallel and more transparent spinor investigations are restricted to 4-dimensional space–times with Lorentz signature, and so this assistance is not available in higher dimensions nor in four dimensional spaces with other signatures. Deser[6] has emphasized the significance of the Bel–Robinson tensor in higher dimensions, and one of the important features of Senovilla's method of construction of superenergy tensors[3] is that it is applicable to arbitrary fields *in any dimension*; and so, for higher dimensions, it becomes an obvious concern whether there could be unexpected properties for superenergy tensors—disguised in the even deeper complexities of

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tensor formalism in higher dimensions—analogous to those properties revealed by the spinor formalism in four dimensions.

Deeper investigations into the interaction between dimension and tensor identities have been instrumental in illustrating the uniqueness of some of the Bel-Robinson tensor's properties in four dimensions,[6] explaining the collapse of some Riemann scalar invariants in four dimensions,[7] resolving the apparent disparities between the spinor and tensors versions of the wave equations for the Weyl tensor and Lanczos potential,[8–11] respectively. Moreover, in higher dimensions, worries concerning counterterms in Lagrangians[12,13] have been dispelled, and the Bel–Robinson tensor has been shown to be fully symmetric in five dimensions (as well as in four dimensions).[3]

Much earlier, Lovelock[14] had pointed out that a number of apparently unrelated results were all really consequences of a class of identities which he christened *dimensionally dependent identities*—identities which are a trivial, but subtle, consequence of dimension alone. Recently Edgar and Höglund[15] have generalized Lovelock's results, and demonstrated that the underlying principle in all of these investigations in Refs. 6–13, and some new ones, was the explicit exploitation of dimensionally dependent identities. Furthermore, in algebraic Rainich theory, Bergqvist and Höglund[16] have exploited these ideas further, and obtained results in *five* dimensions involving *cubic* terms in the energy momentum tensor—motivated by the familiar results in *four* dimensions involving *quadratic* terms;[17] while Edgar and Höglund[18] have demonstrated the crucial role that dimensionally dependent identities play in the existence of the Lanczos potential for the Weyl tensor in different dimensions.

Deser[19] has applied the adjective ''ubiquitous'' to the Bel–Robinson tensor, and this description is equally appropriate to dimensionally dependent identities, as can be seen by the wide range of the investigations in Refs. 6–13, the applications given by Lovelock,[14] and the more recent applications in Refs. 15, 16, 18. In fact, Deser has argued elsewhere[6] that two identities (which are examples of what we call dimensionally dependent identities in four dimensions) are in a sense implicit in the familiar definitions of the Bel–Robinson tensor in four dimensions.

The purpose of this present paper is to emphasise the subtle interaction between dimension and tensor identities, and illustrate the important role which can be played by *fundamental dimensionally dependent identities* in investigations where tensor identities are important, in particular, involving superenergy tensors. (We shall refer to the most fundamental dimensionally dependent identities as ''fddis,'' and to any identities constructed from these as ''ddis.'') Our overall aim is to examine useful and significant properties in four dimensions—usually originating as spinor identities—and identify the kernel 4-dimensional fddi; then we will use the higher dimensional analogs of the kernel fddi to try and establish analogous results in higher dimensions. This will involve two different stages of investigation.

Step 1. The first step is to establish 4-*dimensional signature-independent tensor versions and proofs* of interesting spinor identities and/or reconcile apparent discrepencies between spinor and tensor results. We stress the need for *signature-independent* proofs for the following reason: results obtained using spinors strictly can claim to be valid only in 4-dimensional space–times *with Lorentz signature*. Of course there are results in such spaces which have no counterpart in other signatures (e.g., results concerning principle null directions of the Weyl tensor), but we encounter an uncertain situation when we consider results which can be stated in tensors with no apparent reference to signature, but which were derived in spinors, or derived in tensors but using features which are signature dependent.[20] The Bel–Robinson tensor $\mathcal{T}_{abcd}$ tensor which is known to satisfiy the identity

$$\mathcal{T}_{abcx}\mathcal{T}^{abcy}=\delta^{y}_{x}\ \ \mathcal{T}_{abcd}\mathcal{T}^{abcd}/4, \tag{1}$$

in four dimensions, is an important example of such a situation; we would wish to understand whether dimension and signature have crucial roles in this result.[21,22]

In spinor calculations the dimension four is inbuilt into the formalism; in tensor calculations a nonarbitrary dimension such as four has to be put in explicitly ''by hand.'' However, it is not always sufficient just to substitute $n=4$ in explicit calculations; in some cases the substitution

needed is more subtle—it is achieved by the use of one or more fddis, but it is clear that there is no direct spinor analog of a 4-dimensional fddi—the spinor version is trivially zero.

So, for example, the Lanczos spinor potential $L_{ABCD'}=L_{(ABC)D'}$ for the Weyl spinor Ψ_{ABCD}, which satisfies $\Psi_{ABCD}=\nabla_{(A}{}^{A'}L_{BCD)A'}$ was found by Illge[10] to satisfy the very simple equation,

$$\Box L_{ABCD'}=0, \tag{2}$$

in Ricci flat spaces, while the corresponding tensor equation for the Lanczos tensor $L_{abc}=L_{[ab]c}$, $L^{c}{}_{ac}=0=L_{[abc]}$ is calculated to be[9,11]

$$\nabla^2 L_{abc}+\frac{2(n-4)}{n-2}L_{[a}{}^{d}{}_{|c;d|b]}=2L_{[b}{}^{ed}C_{a]dec}-\frac{1}{2}C_{deab}L^{de}{}_{c}+\frac{4}{n-2}g_{c[a}C_{b]fed}L^{fed}, \tag{3}$$

where C_{abcd} is the Weyl tensor. In four dimensions, obviously it cannot be sufficient simply to substitute $n=4$, since we know from the spinor version that the right hand side must disappear completely in four dimensions. But if we consider the 4-dimensional fddi $C_{[ab}{}^{[cd}\delta^{e]}_{f]}\equiv 0$ (Refs. 14,15) (quoted in Lemma 3 at the end of this section), we find that, when contracted with $L_{de}{}^{f}$, we obtain the ddi,

$$2L_{[b}{}^{de}C_{a]edc}-\tfrac{1}{2}L^{de}{}_{c}C_{deab}+2L^{def}g_{c[a}C_{b]def}\equiv 0, \tag{4}$$

which ensures that the entire right hand side of (3) disappears in four dimensions.[10]

Step 2. Once the 4-dimensional version is fully understood and the 4-dimensional kernel fddi obtained, the second step will be to determine what generalizations are possible using the higher-dimensional counterpart fddis of the 4-dimensional kernel fddi. Occasionally these generalizations can be quite straightforward (e.g., discovering that a 4-dimensional result is also valid in five dimensions[3,15]); or more complicated involving a restructuring of the 4-dimensional result in higher dimensions (e.g., finding a 5-dimensional result involving triple products of Maxwell tensors as a generalization of a 4-dimensional result involving double products of Maxwell tensors[16]).

The remainder of the paper is organized as follows. In Sec. II we deduce four different spinor identities which are special cases of one very simple general spinor identity; but in Sec. III we find that the 4-dimensional signature-independent tensor version of each of these identities requires a very different *tensor* proof—some of which are very complicated—although the unifying characteristic in all is the use of ddis. In Sec. IV we show that the Bel superenergy tensor does not satisfy the same simple identity (1) in four dimensions, and in Sec. V we show that the Bel–Robinson tensor does not satisfy any analogous identity to (1) in *five* dimensions. In Sec. VII we rederive the new conservation laws for electromagnetic theory[5] by using a number of 4-dimensional tensor ddis; these 4-dimensional tensor ddis cannot be replaced *directly* with higher-dimensional ddis, and so there is no *direct* higher-dimensional analog of this law.

As noted above, the second step in such investigations is to attempt a generalization of the 4-dimensional results to higher dinensions once we have identified the kernel tensor fddi in four dimensions. In Sec. VI we give the 4-dimensional tensor counterparts to two trivial spinor results involving the symmetry properties of the Bel–Robinson and Lanczos superenergy spinors: these results both involve 4-dimensional fddis, and in the case of the Bel–Robinson superenergy tensor, by means of the analogous 5-dimensional fddi we show that exactly the same result is true in five dimensions.

A more ambitious generalization is proposed in Sec. VIII. We illustrate this approach by considering a superenergy tensor which is a natural generalization of the Bel–Robinson tensor, and show that it shares its attractive properties of full index symmetry and zero divergence in *seven and lower* dimensions, as well as being trace-free in *six* dimensions. A summary is given, and future developments are proposed in Sec. IX.

It will be useful to have for reference a number of lemmas which are simply tensor ddis in four dimensions. Many familiar identities ostensibly involve the Weyl or Riemann tensors directly or indirectly, but on closer inspection have a more general character being simply algebraic, involving ''candidates'' for Weyl, Riemann, Lanczos or other tensors. In this paper, we shall give the results for the more general ''candidates'' where appropriate. (A ''candidate'' of a tensor such as the Riemann or Weyl tensor is a tensor with the same index and trace properties, but sharing no other properties, such as differential properties; we shall designate such candidates with the symbol $\hat{}$. So, for example, a ''Weyl candidate tensor'' $\hat{C}_{abcd}$ is defined by the properties $\hat{C}_{abcd}=\hat{C}_{[ab]cd}=\hat{C}_{ab[cd]}$, $\hat{C}_{a[bcd]}=0$, $\hat{C}^{a}{}_{bca}=0$. We shall follow the usual notation[2] with R_{abcd}, C_{abcd}, S_{ab}, R for Riemann, Weyl, trace-free Ricci tensors and the Ricci scalar, respectively; their ''candidates'' will be, respectively, $\hat{R}_{abcd},\hat{C}_{abcd},\hat{S}_{ab},\hat{R}$. We shall also follow the usual notation for the Weyl and Ricci spinors, respectively, $\Psi_{ABCD},\Phi_{ABC'D'}$, and scalar Λ $(=R/24)$; their ''candidates'' will be, respectively, $\hat{\Psi}_{ABCD},\hat{\Phi}_{ABC'D'}$, $\hat{\Lambda}$. In addition we will use the Lanczos spinor $L_{ABCD'}=L_{(ABC)D'}$, and Lanczos tensor $L_{abc}=L_{[ab]c}$, $L^{c}{}_{ac}=0=L_{[abc]}$ (Refs. 9,11) with corresponding ''candidates'' $\hat{L}_{ABCD}$ and $\hat{L}_{abc}$.)

The following lemmas can be found in Ref. 15, or can be deduced from results there; full details are given in Ref. 25.

Lemma 1: In four dimensions, a 2-tensor A_{ab} satisfies

$$A_{[a}{}^{a}A_{b}{}^{b}A_{c}{}^{c}A_{d}{}^{d}\delta^{f}_{e]}\equiv 0, \tag{5}$$

which is equivalent to the Cayley–Hamilton Theorem for the 4×4 matrix $A_{a}{}^{b}$ when written out term by term.

(We shall be concerned with two special cases from this class of tensors: trace-free Ricci candidates $\hat{S}_{ab}=\hat{S}_{(ab)}$ with $\hat{S}^{a}{}_{a}=0$, and Maxwell tensors $F_{ab}=F_{[ab]}$.)

Lemma 2: A Lanczos candidate $\hat{L}_{abc}$ with properties $\hat{L}_{abc}=\hat{L}_{[ab]c}$, $\hat{L}^{c}{}_{ac}=0=\hat{L}_{[abc]}$, satisfies

$$\hat{L}_{[ab}{}^{[e}\ \delta^{fg]}_{cd]}\equiv 0, \quad \text{in four dimensions,} \tag{6a}$$

$$\hat{L}_{[ab}{}^{[f}\ \delta^{ghi]}_{cde]}\equiv 0, \quad \text{in five dimensions.} \tag{6b}$$

Lemma 3: A Weyl candidate $\hat{C}_{ab}{}^{cd}$ satisfies

$$\hat{C}_{[ab}{}^{[de}\ \delta^{f]}_{c]}\equiv 0, \quad \text{in four dimensions,} \tag{7a}$$

$$\hat{C}_{[ab}{}^{[ef}\ \delta^{gh]}_{cd]}\equiv 0, \quad \text{in five dimensions.} \tag{7b}$$

Lemma 4: In four dimensions, a Weyl candidate $\hat{C}_{ab}{}^{cd}$ satisfies

$$\text{(a)}\quad \hat{C}_{abcx}\hat{C}^{abcy}\equiv\delta^{y}_{x}\ \hat{C}_{abcd}\hat{C}^{abcd}/4, \tag{8a}$$

$$\text{(b)}\quad \hat{C}^{yb}{}_{cd}\hat{C}^{cd}{}_{ef}\hat{C}^{ef}{}_{bx}\equiv\delta^{y}_{x}\hat{C}^{ab}{}_{cd}\hat{C}^{cd}{}_{ef}\hat{C}^{ef}{}_{ba}/4, \tag{8b}$$

$$\text{(c)}\quad \hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fc}{}_{ex}\equiv\delta^{y}_{x}\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fc}{}_{ea}/4, \tag{8c}$$

$$\text{(d)}\quad \hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{gx}\equiv\delta^{y}_{x}\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{ga}/4, \tag{8d}$$

$$\text{(e)}\quad \hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{egx}\equiv\delta^{y}_{x}\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{ega}/4. \tag{8e}$$

The first three of these lemmas are fddis obtained by skew symmetrizing over *five* indices in 4-dimensional space (and *six* indices in 5-dimensional space), and exploiting the fact that the

appropriate tensors are trace-free; Lemma 4 gives ddis deduced from Lemma 3, but as can be seen from the details in Ref. 25, although (8a) is well-known, quite a lot of work is involved in obtaining the remainder of Lemma 4.

It is obvious from the constructions that these identities for four/five dimensions are valid in four/five *and lower* dimensions. So, for instance (6b) is also valid in four dimensions, but the only nontrivial information is in its trace in four dimensions, which is equivalent to (6a); on the other hand, in five dimensions, the trace of the left hand side of (6b) is identically zero, giving a trivial result. Of course no Weyl candidates exist in dimensions less than four, but for the other tensors, these lemmas are nontrivial in lower dimensions. However, we shall not be concerned with dimensions less than four in this paper. Although stated for Lanczos and Weyl candidates (which is all we require in this paper), a number of these results are valid for more general tensors; in particular the antisymmetry property $\hat{L}_{[abc]}=0$ can be relaxed in Lemma 2, and the antisymmetry $\hat{C}_{a[bcd]}=0$ can be relaxed in Lemma 3 and Lemma 4a, b, c, d.

II. SIMPLE SPINOR IDENTITIES

We begin with the following spinor result which generalizes Penrose's original derivation[2] for Bel–Robinson tensors.

Theorem 1: A spinor which factorizes according to $\mathsf{T}_{\Sigma X\Sigma' X'}=4V_{\Sigma X}\overline{V}_{\Sigma' X'}$ satisfies

$$\mathsf{T}_{\Sigma X\Sigma' X'}\mathsf{T}^{\Sigma Y\Sigma' Y'}=\epsilon_X{}^Y\epsilon_{X'}{}^{Y'}\mathsf{T}_{\Sigma A\Sigma' A'}\mathsf{T}^{\Sigma A\Sigma' A'}/4, \tag{9}$$

where Σ,Σ' each represent an *odd* number of spinor indices.

Proof:

$$V_{\Sigma X}V^{\Sigma Y}=V_{\Sigma}{}^YV^{\Sigma}{}_X+\epsilon_X{}^YV_{\Sigma A}V^{\Sigma A}=-V^{\Sigma Y}V_{\Sigma X}+\epsilon_X{}^YV_{\Sigma A}V^{\Sigma A},$$

with the negative sign arising by "see-sawing" the odd number of indices in Σ. Hence

$$V_{\Sigma X}V^{\Sigma Y}=\epsilon_X{}^YV_{\Sigma A}V^{\Sigma A}/2. \tag{10}$$

Multiplying by the complex conjugate

$$\overline{V}_{\Sigma' X'}\overline{V^{\Sigma' Y'}}V_{\Sigma X}V^{\Sigma Y}=\epsilon_X{}^YV_{\Sigma A}V^{\Sigma A}\epsilon_{X'}{}^{Y'}\overline{V}_{\Sigma' A'}\overline{V^{\Sigma' A'}}/4,$$

and substituting for $\mathsf{T}_{\Sigma X\Sigma' X'}$, $\mathsf{T}_{\Sigma Y\Sigma' Y'}$ gives the result. □

From Theorem 1 we see that the types of indices in the collection of indices represented by Σ do not matter; only the fact that there is an odd number. In this paper we shall be concentrating on 4-index tensors $\mathcal{T}_{abcd}$ equivalently $\mathcal{T}_{ABCDA'B'C'D'}$; and in particular from Ref. 4 (see also Ref. 26):

(i) The superenergy spinor of the Weyl (candidate) spinor $\hat{\Psi}_{ABCD}$ (i.e., the Bel–Robinson superenergy spinor) is given by

$$\mathcal{T}[\hat{\Psi}]_{ABCDA'B'C'D'}=4\hat{\Psi}_{ABCD}\overline{\hat{\Psi}}_{A'B'C'D'}. \tag{11a}$$

(ii) The superenergy spinor of the Ricci (candidate) spinor $\hat{\Phi}_{ABC'D'}$ is given by

$$\mathcal{T}[\hat{\Phi}]_{ABCDA'B'C'D'}=4\hat{\Phi}_{ABC'D'}\overline{\hat{\Phi}}_{CDA'B'}. \tag{11b}$$

(iii) The superenergy spinor of the Ricci (candidate) scalar $\hat{\Lambda}$ is given by

$$\mathcal{T}[\hat{\Lambda}]_{ABCDA'B'C'D'}=4\hat{\Lambda}^2(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC})(\epsilon_{A'C'}\epsilon_{B'D'}+\epsilon_{A'D'}\epsilon_{B'C'}). \tag{11c}$$

(iv) The superenergy spinor of the Weyl–Ricci scalar (candidate) spinor $\hat{\chi}_{ABCD}$ is given by

$$\begin{aligned}\mathcal{T}[\hat{\chi}]_{ABCDA'B'C'D'} &= 4\hat{\chi}_{ABCD}\overline{\hat{\chi}}_{A'B'C'D'} \\ &= 4(\hat{\Psi}_{ABCD}+\hat{\Lambda}(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC}))(\overline{\hat{\Psi}}_{A'B'C'D'}+\hat{\Lambda}(\epsilon_{A'C'}\epsilon_{B'D'} \\ &\quad +\epsilon_{A'D'}\epsilon_{B'C'})) \\ &= \mathcal{T}[\hat{\Psi}]+\mathcal{T}[\hat{\Lambda}]+4\hat{\Lambda}(\overline{\hat{\Psi}}_{A'B'C'D'}(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC})+\hat{\Psi}_{ABCD}(\epsilon_{A'C'}\epsilon_{B'D'} \\ &\quad +\epsilon_{A'D'}\epsilon_{B'C'})). \end{aligned} \tag{11d}$$

Theorem 1 immediately specializes to the following.

Theorem 2: The four superenergy spinors in (11) $\mathcal{T}[\hat{\Psi}],\mathcal{T}[\hat{\Phi}]$, $\mathcal{T}[\hat{\Lambda}]$, $\mathcal{T}[\hat{\chi}]$ all obey the identity

$$\mathcal{T}_{ABCXA'B'C'X'}\mathcal{T}^{ABCYA'B'C'Y'} = \epsilon_X{}^Y\epsilon_{X'}{}^{Y'}\mathcal{T}_{ABCDA'B'C'D'}\mathcal{T}^{ABCDA'B'C'D'}/4. \tag{12}$$

□

The simplicity of the above theorems is due to the fact that the superenergy spinors were simple direct products involving a spinor times its conjugate; it should be noted that even more general identities could have been obtained for these four spinors, as well as for more general spinors with the same simple product structure—not just from the point of view of relaxing the index symmetries, but also from freeing more indices.[2]

However the Bel superenergy spinor (the superenergy spinor for the Riemann (candidate) spinor)[2,4] and the Lanczos superenergy spinor (the superenergy spinor for the Lanczos (candidate) spinor),[4] do not have such a simple structure as can be seen below:

$$\begin{aligned}\mathcal{B}_{ABCDA'B'C'D'} &= 4(\hat{\chi}_{ABCD}\overline{\hat{\chi}}_{A'B'C'D'}+\hat{\Phi}_{ABC'D'}\overline{\hat{\Phi}}_{CDA'B'}) \\ &= 4(\hat{\Psi}_{ABCD}+\hat{\Lambda}(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC}))\times(\overline{\hat{\Psi}}_{A'B'C'D'}+\hat{\Lambda}(\epsilon_{A'C'}\epsilon_{B'D'}+\epsilon_{A'D'}\epsilon_{B'C'})) \\ &\quad +4\hat{\Phi}_{ABC'D'}\overline{\hat{\Phi}}_{CDA'B'} \\ &= 4(\hat{\Psi}_{ABCD}\overline{\hat{\Psi}}_{A'B'C'D'}+\hat{\Phi}_{ABC'D'}\overline{\hat{\Phi}}_{CDA'B'}+\hat{\Lambda}^2(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC}) \\ &\quad \times(\epsilon_{A'C'}\epsilon_{B'D'}+\epsilon_{A'D'}\epsilon_{B'C'})+\hat{\Lambda}\hat{\Psi}_{ABCD}(\epsilon_{A'C'}\epsilon_{B'D'}+\epsilon_{A'D'}\epsilon_{B'C'}) \\ &\quad +\hat{\Lambda}\overline{\hat{\Psi}}_{A'B'C'D'}(\epsilon_{AC}\epsilon_{BD}+\epsilon_{AD}\epsilon_{BC})) \end{aligned} \tag{13}$$

(where we have used the notation $\mathcal{B}$ rather than the more consistent $\mathcal{T}[\hat{R}]$ simply for ease of presentation), and

$$\mathcal{T}[\hat{L}]_{ABCDA'B'C'D'} = 2(\hat{L}_{ABCD'}\overline{\hat{L}}_{A'B'C'D}+\hat{L}_{ABDC'}\overline{\hat{L}}_{A'B'D'C}), \tag{14}$$

where $\hat{L}_{ABCD'}=\hat{L}_{(ABC)D'}$.

It is easy to see that simple identities such as (12) do not hold in these cases. However this does not rule out the possibility of other, more complicated, identities. We shall look further at both of these tensors in Sec. VI, and at possible identities for the Bel tensor in Sec. IV.

III. SIMPLE TENSOR IDENTITIES

We now wish to confirm the tensor versions of the four identities in Theorem 2 by tensor means. We shall discover that although the above four identities had essentially the same spinor proofs, the proofs for their superenergy tensor counterparts require very different amounts of calculations. We first give the corresponding n-dimensional basic superenergy tensors of the appropriate double 2-forms.

In n-dimensional spaces from, Ref. 3 we have the following.

(i) The basic Bel–Robinson tensor[1] (equivalent to the Bel–Robinson spinor $\mathcal{T}[\hat{\Psi}]$) is given by

$$\mathcal{T}[\hat{C}]_{abcd}=\hat{C}_{apcq}\hat{C}_b{}^p{}_d{}^q+\hat{C}_{apdq}\hat{C}_b{}^p{}_c{}^q-\tfrac{1}{2}g_{ab}\hat{C}_{rpcq}\hat{C}^{rp}{}_d{}^q-\tfrac{1}{2}g_{cd}\hat{C}_{aprq}\hat{C}_b{}^{prq}+\tfrac{1}{8}g_{ab}g_{cd}\hat{C}_{sprq}\hat{C}^{sprq}. \tag{15}$$

(ii) The basic trace-free Ricci superenergy tensor [equivalent to the superenergy spinor for the Ricci (candidate) spinor $\mathcal{T}[\hat{\Phi}]$] is given—via the tensor $\hat{E}_{abcd}=(\hat{S}_{ac}g_{bd}-\hat{S}_{ad}g_{bc}+\hat{S}_{bd}g_{ac}-\hat{S}_{bc}g_{ad})/(n-2)$—by

$$\begin{aligned}\mathcal{T}[\hat{E}]_{abcd}&=\hat{E}_{aecf}\hat{E}_b{}^e{}_d{}^f+\hat{E}_{aedf}\hat{E}_b{}^e{}_c{}^f-\tfrac{1}{2}g_{ab}\hat{E}_{efcg}\hat{E}^{ef}{}_d{}^g-\tfrac{1}{2}g_{cd}\hat{E}_{aefg}\hat{E}_b{}^{efg}\\&\quad+\tfrac{1}{8}g_{ab}g_{cd}\hat{E}_{efgh}\hat{E}_{efgh}\\&=4\Big(\hat{S}_{ab}\hat{S}_{cd}+\frac{n-4}{2}\hat{S}_{a(c}\hat{S}_{d)b}-\hat{S}_{bp}\hat{S}_{(d}{}^p g_{c)a}-\hat{S}_{ap}\hat{S}_{(d}{}^p g_{c)b}+\frac{6-n}{4}\hat{S}_{cp}\hat{S}_d{}^p g_{ab}\\&\quad+\frac{6-n}{4}\hat{S}_{ap}\hat{S}_b{}^p g_{cd}+\frac{n-6}{8}g_{ab}g_{cd}\hat{S}_{pq}\hat{S}^{pq}+\frac{1}{2}g_{a(c}g_{d)b}\hat{S}_{pq}\hat{S}^{pq}\Big)\Big/(n-2)^2.\end{aligned} \tag{16}$$

(Note that the superenergy tensor constructed for the trace-free Ricci candidate tensor $\hat{S}_{ab}$ via the double 2-form $\hat{E}_{abcd}$ is different from the superenergy tensor constructed for the trace-free Ricci candidate tensor directly via the double 1-form $\hat{S}_{ab}$.[3])

(iii) The basic Ricci scalar superenergy tensor (equivalent to the superenergy spinor for the Ricci (candidate) scalar $\mathcal{T}[\hat{\Lambda}]$) is given—via the tensor $\hat{G}_{abcd}=\hat{R}(g_{ac}g_{bd}-g_{ad}g_{bc})/n(n-1)$—by

$$\begin{aligned}\mathcal{T}[\hat{\Lambda}]_{abcd}&=\hat{G}_{aecf}\hat{G}_b{}^e{}_d{}^f+\hat{G}_{aedf}\hat{G}_b{}^e{}_c{}^f-\tfrac{1}{2}g_{ab}\hat{G}_{efcg}\hat{G}^{ef}{}_d{}^g-\tfrac{1}{2}g_{cd}\hat{G}_{aefg}\hat{G}_b{}^{efg}\\&\quad+\tfrac{1}{8}g_{ab}g_{cd}\hat{G}_{efgh}\hat{G}^{efgh}\\&=\hat{R}^2\Big(2(n-2)g_{a(c}g_{d)b}+\frac{n^2-9n+16}{4}g_{ab}g_{cd}\Big)\Big/n^2(n-1)^2.\end{aligned} \tag{17}$$

(iv) The basic superenergy tensor for the $\hat{\chi}$ (candidate) tensor [equivalent to the superenergy spinor for the $\hat{\chi}$ (candidate) spinor $\mathcal{T}[\hat{\chi}]$] is given—via the tensor $\hat{\chi}_{abcd}=\hat{C}_{abcd}+\hat{R}(g_{ac}g_{bd}-g_{ad}g_{bc})/n(n-1)$—by

$$\begin{aligned}\mathcal{T}[\hat{\chi}]_{abcd}&=\hat{\chi}_{aecf}\hat{\chi}_b{}^e{}_d{}^f+\hat{\chi}_{aedf}\hat{\chi}_b{}^e{}_c{}^f-\tfrac{1}{2}g_{ab}\hat{\chi}_{efcg}\hat{\chi}^{ef}{}_d{}^g-\tfrac{1}{2}g_{cd}\hat{\chi}_{aefg}\hat{\chi}_b{}^{efg}+\tfrac{1}{8}g_{ab}g_{cd}\hat{\chi}_{efgh}\hat{\chi}^{efgh}\\&=\mathcal{T}[\hat{C}]_{abcd}+\mathcal{T}[\hat{\Lambda}]_{abcd}+2\hat{R}(\hat{C}_{acbd}+\hat{C}_{adbc})/n(n-1).\end{aligned} \tag{18}$$

In 4-dimensional space,[3,30] we have the following.

(a) $\mathcal{T}[\hat{C}]_{abcd}$ is given in (15) in a dimension independent form, but by the ddi in Lemma 4a it can be put in the simpler form in four dimensions, in which it is usually quoted

$$\mathcal{T}[\hat{C}]_{abcd}=\hat{C}_{apcq}\hat{C}_b{}^p{}_d{}^q+\hat{C}_{apdq}\hat{C}_b{}^p{}_c{}^q-\tfrac{1}{8}g_{ab}g_{cd}\hat{C}_{sprq}\hat{C}^{sprq}. \tag{19}$$

(b) $\mathcal{T}[\hat{E}]_{abcd}$ simplifies to

$$\mathcal{T}[\hat{E}]_{abcd}=\hat{S}_{ab}\hat{S}_{cd}+\hat{S}_{ap}\hat{S}_{b}{}^{p}g_{cd}+\hat{S}_{cp}\hat{S}_{d}{}^{p}g_{ab}-3\hat{S}_{p(a}\hat{S}_{b}{}^{p}g_{cd)}+\tfrac{1}{4}\hat{S}_{pq}\hat{S}^{pq}(g_{ac}g_{bd}+g_{ad}g_{bc}-g_{ab}g_{cd}). \tag{20}$$

(c) $\mathcal{T}[\hat{\Lambda}]_{abcd}$ simplifies to

$$\mathcal{T}[\hat{\Lambda}]_{abcd}=\hat{R}^{2}(4g_{a(c}g_{d)b}-g_{ab}g_{cd})/144. \tag{21}$$

(d) $\mathcal{T}[\hat{\chi}]_{abcd}$ simplifies to

$$\mathcal{T}[\hat{\chi}]_{abcd}=\mathcal{T}[\hat{C}]_{abcd}+\frac{\hat{R}}{6}(\hat{C}_{acbd}+\hat{C}_{adbc})+\mathcal{T}[\hat{\Lambda}]_{abcd}. \tag{22}$$

It is clear that all of the above superenergy tensors have the properties

$$\mathcal{T}_{abcd}=\mathcal{T}_{(ab)(cd)},$$

and some have additional symmetry properties, e.g., for the Bel–Robinson tensor (in four and five dimensions), and the Lanczos superenergy tensor (in four dimensions), $\mathcal{T}_{abcd}=\mathcal{T}_{(abcd)}$ as we shall show in Sec. VI. All of the above are labeled *basic* superenergy tensors to distinguish from the more *general* superenergy tensors which can be obtained by taking linear combinations—with positive constant coefficients—of different basic superenergy tensors, obtained by index permutations.[3]

We now give the 4-dimensional tensor counterparts of Theorem 2.

Theorem 2a: In 4-dimensional spaces the Bel–Robinson tensor $\mathcal{T}[C]_{abcd}$ in (15) satisfies

$$\mathcal{T}[\hat{C}]_{abcx}\mathcal{T}[\hat{C}]^{abcy}=\delta^{y}_{x}\ \mathcal{T}[\hat{C}]_{abcd}\mathcal{T}[\hat{C}]^{abcd}/4. \tag{23}$$

Proof: Substituting directly we obtain

$$\begin{aligned}
&\mathcal{T}[\hat{C}]_{abcx}\mathcal{T}[\hat{C}]^{abcy}-\tfrac{1}{4}\delta^{y}_{x}\ \mathcal{T}[\hat{C}]_{abcd}\mathcal{T}[\hat{C}]^{abcd}\\
&\quad=2\hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{gx}+2\hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{egx}-2\hat{C}^{ab}{}_{cd}\hat{C}^{cd}{}_{eb}\hat{C}^{e}{}_{gh}{}^{y}\hat{C}_{a}{}^{gh}{}_{y}\\
&\qquad-\hat{C}^{yb}{}_{cd}\hat{C}^{cd}{}_{eb}\hat{C}^{ef}{}_{gh}\hat{C}^{gh}{}_{xf}+\tfrac{1}{2}\hat{C}_{abcd}\hat{C}^{abcd}C^{ey}{}_{gh}\hat{C}^{gh}{}_{ex}+\tfrac{1}{4}\delta^{y}_{x}\hat{C}^{ab}{}_{cd}\hat{C}^{cd}{}_{eb}\hat{C}^{ef}{}_{gh}\hat{C}^{gh}{}_{af}\\
&\qquad-\tfrac{1}{16}\delta^{y}_{x}\hat{C}^{abcd}\hat{C}_{abcd}\hat{C}^{efgh}\hat{C}_{efgh}-\tfrac{1}{4}\delta^{y}_{x}(2\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{ga}+2\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{ega}\\
&\qquad-2\hat{C}^{ab}{}_{cd}\hat{C}^{cd}{}_{eb}\hat{C}^{ef}{}_{gh}\hat{C}^{gh}{}_{af}+\tfrac{1}{4}\hat{C}^{abcd}\hat{C}_{abcd}\hat{C}^{efgh}\hat{C}_{efgh}).
\end{aligned} \tag{24}$$

Using Lemma 4a a number of times gives the simpler expression

$$\begin{aligned}
&\mathcal{T}[\hat{C}]_{abcx}\mathcal{T}[\hat{C}]^{abcy}-\tfrac{1}{4}\delta^{y}_{x}\ \mathcal{T}[\hat{C}]_{abcd}\mathcal{T}[\hat{C}]^{abcd}\\
&\quad=2\hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{gx}+2\hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{egx}\\
&\qquad-\tfrac{1}{4}\delta^{y}_{x}(2\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fg}{}_{eh}\hat{C}^{hc}{}_{ga}+2\hat{C}^{ab}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fgc}{}_{h}\hat{C}^{h}{}_{ega}).
\end{aligned} \tag{25}$$

We can now apply Lemma 4d to the first and third terms, and Lemma 4e to the second and fourth terms, to obtain the required result. □

Theorem 2b: In 4-dimensional spaces, the superenergy tensor $\mathcal{T}[\hat{E}]_{abcd}$ given in (20) satisfies

$$\mathcal{T}[\hat{E}]_{abcx}\mathcal{T}[\hat{E}]^{abcy}=\delta^{y}_{x}\ \mathcal{T}[\hat{E}]_{abcd}\mathcal{T}[\hat{E}]^{abcd}/4. \tag{26}$$

Proof: Substituting directly we obtain

$$\mathcal{T}[\hat{E}]_{abcx}\mathcal{T}[\hat{E}]^{abcy}-\tfrac{1}{4}\delta^{y}_{x}\ \mathcal{T}[\hat{E}]_{abcd}\mathcal{T}[\hat{E}]^{abcd}$$
$$=-3\hat{S}^{y}{}_{b}\hat{S}^{b}{}_{c}\hat{S}^{c}{}_{d}\hat{S}^{d}{}_{x}+\tfrac{3}{2}\hat{S}^{yb}\hat{S}_{xb}\hat{S}_{cd}\hat{S}^{cd}+\hat{S}^{y}{}_{x}\hat{S}^{a}{}_{b}\hat{S}^{b}{}_{c}\hat{S}^{c}{}_{a}+\tfrac{3}{4}\delta^{y}_{x}\hat{S}^{a}{}_{b}\hat{S}^{b}{}_{c}\hat{S}^{c}{}_{d}\hat{S}^{d}{}_{a}$$
$$-\tfrac{3}{8}\delta^{y}_{x}\hat{S}^{ab}\hat{S}_{ab}\hat{S}_{cd}\hat{S}^{cd}. \tag{27}$$

But the right-hand side of this equation is precisely

$$\delta^{y}_{[x}\ \hat{S}^{a}{}_{a}\hat{S}^{b}{}_{b}\hat{S}^{c}{}_{c}\hat{S}^{d}{}_{d]}\equiv 0, \tag{28}$$

where we have made use of Lemma 1. □

Theorem 2c: In 4-dimensional spaces, the superenergy tensor $\mathcal{T}[\hat{\Lambda}]_{abcd}$ given in (21) satisfies

$$\mathcal{T}[\hat{\Lambda}]_{abcx}\mathcal{T}[\hat{\Lambda}]^{abcy}=\delta^{y}_{x}\ \mathcal{T}[\hat{\Lambda}]_{abcd}\mathcal{T}[\hat{\Lambda}]^{abcd}/4. \tag{29}$$

Proof: The result follows from a direct calculation. □

Theorem 2d: In 4-dimensional spaces, the superenergy tensor $\mathcal{T}[\hat{\chi}]_{abcd}$ given in (22) satisfies

$$\mathcal{T}[\hat{\chi}]_{abcx}\mathcal{T}[\hat{\chi}]^{abcy}=\delta^{y}_{x}\ \mathcal{T}[\hat{\chi}]_{abcd}\mathcal{T}[\hat{\chi}]^{abcd}/4. \tag{30}$$

Proof:

$$\mathcal{T}[\hat{\chi}]_{abcx}\mathcal{T}[\hat{\chi}]^{abcy}=\left(\mathcal{T}[\hat{C}]_{abcx}+\mathcal{T}[\hat{\Lambda}]_{abcx}+\frac{\hat{R}}{6}(\hat{C}_{acbx}+\hat{C}_{axbc})\right)$$
$$\times\left(\mathcal{T}[\hat{C}]^{abcy}+\mathcal{T}[\hat{\Lambda}]^{abcy}+\frac{\hat{R}}{6}(\hat{C}^{acby}+\hat{C}^{aybc})\right)$$
$$=\mathcal{T}[\hat{C}]_{abcx}\mathcal{T}[\hat{C}]^{abcy}+\mathcal{T}[\hat{\Lambda}]_{abcx}\mathcal{T}[\hat{\Lambda}]^{abcy}+\frac{\hat{R}}{6}(\mathcal{T}[\hat{C}]^{abcy}(\hat{C}_{acbx}+\hat{C}_{axbc})$$
$$+\mathcal{T}[\hat{C}]_{abcx}(\hat{C}^{acby}+\hat{C}^{aybc}))+\frac{\hat{R}^{2}}{144}\hat{C}_{abcd}\hat{C}^{abcd}\delta^{y}_{x},$$

where the last term was obtained using Lemma 4a.

We can apply Theorems 2a and 2c to the first and second terms, respectively, and obtain

$$\mathcal{T}[\hat{\chi}]_{abcx}\mathcal{T}[\hat{\chi}]^{abcy}=\frac{1}{4}\left(\mathcal{T}[\hat{C}]_{abcd}\mathcal{T}[\hat{C}]^{abcd}+\frac{1}{4}\mathcal{T}[\hat{\Lambda}]_{abcd}\mathcal{T}[\hat{\Lambda}]^{abcd}+\frac{\hat{R}^{2}}{36}\hat{C}_{abcd}\hat{C}^{abcd}\right)\delta^{y}_{x}$$
$$+\frac{\hat{R}}{6}(\mathcal{T}[\hat{C}]^{abcy}(\hat{C}_{acbx}+\hat{C}_{axbc})+\mathcal{T}[\hat{C}]_{abcx}(\hat{C}^{acby}+\hat{C}^{aybc})).$$

To complete the proof we need to use the identity

$$\mathcal{T}[\hat{C}]^{abcy}(\hat{C}_{acbx}+\hat{C}_{axbc})=\tfrac{1}{2}\hat{C}^{yc}{}_{bd}\hat{C}^{efbd}\hat{C}_{xcef}-2\hat{C}^{yb}{}_{cd}\hat{C}^{de}{}_{bf}\hat{C}^{fc}{}_{ex}+\hat{C}^{yb}{}_{cx}\hat{C}_{bdef}\hat{C}^{cdef}$$
$$=\tfrac{1}{4}\mathcal{T}[\hat{C}]^{abcd}(\hat{C}_{acbd}+\hat{C}_{adbc})\,\delta^{y}_{x}, \tag{31}$$

where we have used Lemma 4b on the first term, Lemma 4c on the second term and Lemma 4a on the third term. □

We note that in Theorems 2,a,b,d explicit 4-dimensional fddis were used in the proofs; it seems unlikely that *direct* generalizations can be obtained by using analogous fddis in higher dimensions; more likely, higher order identities would need to be considered. Theorem 2c was obtained by a direct calculation, and in fact an analogous identity is clearly obtainable in n dimensions because of the very simple structure of the superenergy tensor in this case.

IV. ABSENCE OF SIMPLE IDENTITIES FOR THE BEL SUPERENERGY TENSOR

The Bel tensor, the superenergy tensor for the Riemann tensor, in n dimensions[3] is

$$\mathcal{B}_{abcd}=\hat{R}_{apcq}\hat{R}_{b}{}^{p}{}_{d}{}^{q}+\hat{R}_{apdq}\hat{R}_{b}{}^{p}{}_{c}{}^{q}-\tfrac{1}{2}g_{ab}\hat{R}_{rpcq}\hat{R}^{rp}{}_{d}{}^{q}-\tfrac{1}{2}g_{cd}\hat{R}_{aprq}\hat{R}_{b}{}^{prq}+\tfrac{1}{8}g_{ab}g_{cd}\hat{R}_{sprq}\hat{R}^{sprq}, \tag{32}$$

with the obvious properties

$$\mathcal{B}_{abcd}=\mathcal{B}_{(ab)cd}=\mathcal{B}_{ab(cd)}=\mathcal{B}_{cdab}, \quad \mathcal{B}^{a}{}_{acd}=0. \tag{33}$$

(We continue to use the notation $\mathcal{B}_{abcd}$ rather than the more consistent $\mathcal{T}[\hat{R}]_{abcd}$.)

Substituting the usual decomposition of the Riemann tensor gives the alternative form[3,15]

$$\mathcal{B}_{abcd}=\mathcal{T}[\hat{C}]_{abcd}+\mathcal{T}[\hat{E}]_{abcd}+\mathcal{Q}_{abcd}, \tag{32$'$}$$

where

$$\mathcal{Q}_{abcd}=\frac{1}{n-2}(-4\hat{C}^{i}{}_{(cd)(a}\hat{S}_{b)i}-4\hat{C}^{i}{}_{(ab)(c}\hat{S}_{d)i}+2\hat{S}_{ij}(\hat{C}_{a}{}^{j}{}_{(c}{}^{i}g_{d)b}-\hat{C}_{c}{}^{j}{}_{d}{}^{i}g_{ab}+\hat{C}_{b}{}^{j}{}_{(c}{}^{i}g_{d)a}-\hat{C}_{a}{}^{j}{}_{b}{}^{i}g_{cd}))$$

$$+\frac{2\hat{R}}{n(n-1)}(\hat{C}_{acbd}+\hat{C}_{adbc}). \tag{34}$$

In four dimensions we get

$$\mathcal{Q}_{abcd}=\frac{\hat{R}}{6}(\hat{C}_{acbd}+\hat{C}_{adbc}).$$

This last simplification is not obvious in tensors, although it is in spinors (11d); by tensors, it is obtained either by manipulation with duals,[3] or via a 4-dimensional ddi,[15]

$$\hat{S}^{e}{}_{f}\hat{C}_{[ab}{}^{[cd}\delta^{f]}_{e]}\equiv 0. \tag{35}$$

The Bel tensor is a generalization of the Bel–Robinson tensor, and an obvious question is whether it also satisfies similar types of quadratic identity in four dimensions as does the Bel–Robinson tensor. From spinor considerations it does not look very hopeful, so we investigate the possibility via examples rather than look for general results.

Because of the additional terms in the Bel tensor compared to the Bel–Robinson tensor we introduce

$$\mathcal{B}_{a}{}^{c}{}_{cb}=\mathcal{B}_{ab}=\mathcal{B}_{ba}, \quad \mathcal{B}=\mathcal{B}^{a}{}_{a}, \tag{36}$$

and so we consider the most general quadratic identity with two free indices which could exist; it would have to have the structure

$$k_1\mathcal{B}_{abcx}\mathcal{B}^{abcy}+k_2\mathcal{B}_{abcx}\mathcal{B}^{acby}+k_3\mathcal{B}_{abx}{}^{y}\mathcal{B}^{ab}+k_4\mathcal{B}_{axb}{}^{y}\mathcal{B}^{ab}+k_5\mathcal{B}_{ax}\mathcal{B}^{ay}+k_6\mathcal{B}\mathcal{B}_{x}{}^{y} \;\propto\; \delta^{y}_{x}, \tag{37}$$

with constants $k_1,\ldots,k_6$. By substituting the Bel tensors of explicit spaces[27] on the left hand side, we are led to conjecture that, in 4-dimensional spaces, the Bel tensor satisfies the quadratic identity

$$2\mathcal{B}_{a[bc]x}\mathcal{B}^{a[bc]y}-\mathcal{B}_{xa}\mathcal{B}^{ay}+2\mathcal{B}_{ab}\mathcal{B}_{a}{}^{[by]}{}_{x}+\tfrac{1}{2}\mathcal{B}\mathcal{B}_{x}{}^{y}$$
$$=\delta^{y}_{x}\ (2\mathcal{B}_{a[bc]d}\mathcal{B}^{a[bc]d}-2\mathcal{B}_{ab}\mathcal{B}^{ab}+\tfrac{1}{2}\mathcal{B}^{2})/4. \tag{38}$$

So it appears that the Bel tensor *may* have a quadratic identity, which rather surprisingly does not reduce to the Bel–Robinson identity in the vacuum case. However, closer inspection reveals that this identity is *trivial* in the following sense: the properties $\mathcal{B}^{a}{}_{[bc]}{}^{d}=\mathcal{B}^{[a}{}_{[bc]}{}^{d]}=\mathcal{B}_{[b}{}^{[ad]}{}_{c]}$, $\mathcal{B}_{a[bcd]}=0$ mean that we can consider $B_{ab}{}^{cd}\equiv\mathcal{B}^{[c}{}_{[ab]}{}^{d]}$ as a Riemann candidate and (38) becomes

$$\tilde{B}_{abcx}\tilde{B}^{abcy}=\delta^{y}_{x}\ \tilde{B}_{abcd}\tilde{B}^{abcd}/4, \tag{39}$$

where $\tilde{B}_{abcd}$ is the trace-free part of B_{abcd}, i.e., its Weyl candidate. But (39) is just the identity in Lemma 4a which is a consequence of *only* the trace-free 2-form structure and the fact that we are in 4-dimensional space; *it has nothing to do with the superenergy structure of* $\mathcal{B}_{abcd}$ *as a linear combination of products of Riemann candidates*.

Hence this identity is of no interest to us in the context of superenergy tensors, and so, we have the following.

Theorem 3: In 4-dimensional spaces, the only quadratic identity with the structure (37) satisfied by the Bel superenergy tensor (32) $\mathcal{B}_{abcd}$, is the *trivial* identity (39). □

V. ABSENCE OF SIMPLE IDENTITIES FOR BEL–ROBINSON SUPERENERGY TENSOR IN HIGHER DIMENSIONS

As noted above, it has been found[3,15] that the Bel–Robinson tensor is completely symmetric in *five* (and lower) dimensions. This raises the question as to whether the above quadratic identity for the Bel–Robinson tensor is also valid in five dimensions; or, more generally, whether there exists *any* quadratic identity with two free indices for the Bel–Robinson tensor in *five* dimensions.

Since in five dimensions the Bel–Robinson tensor is still fully symmetric, but not trace-free, the most general quadratic identity with two free indices which could exist would have to have the structure,

$$k_1\mathcal{T}_{abcx}\mathcal{T}^{abcy}+k_2\mathcal{T}_{abx}{}^{y}\mathcal{T}^{ab}+k_3\mathcal{T}_{ax}\mathcal{T}^{ay}+k_4\mathcal{T}\mathcal{T}^{y}_{x}\propto\delta^{y}_{x}, \tag{40}$$

for constants k_1,k_2,k_3,k_4, where

$$\mathcal{T}_{abcd}=\mathcal{T}_{(abcd)},\quad \mathcal{T}_{abc}{}^{c}=\mathcal{T}_{ab}=\mathcal{T}_{ba},\quad \mathcal{T}_{a}{}^{a}=\mathcal{T}. \tag{41}$$

To try to retrace the complicated tensor calculations of Theorem 2a, and try to replace the 4-dimensional fddis used there with higher-dimensional fddis would be a very complicated procedure; so we try first to obtain a simple counterexample, and we easily obtain the following negative result.

Theorem 4: In 5-dimensional spaces, the Bel–Robinson tensor $\mathcal{T}_{abcd}$ does not satisfy any quadratic identity of the form (40).

Proof: Generalizing the 4-dimensional Kerr metric g^{K}_{ab} to five dimensions as $ds^2=g^{K}_{ab}dx^a dx^b+dx_5^2$, we can calculate the Bel–Robinson tensor explicitly, and when we substitute it onto the left hand side of the above expression (40), we obtain

$$k_1\mathcal{T}_{abcx}\mathcal{T}^{abcy}+k_2\mathcal{T}_{abx}{}^{y}\mathcal{T}^{ab}+k_3\mathcal{T}_{ax}\mathcal{T}^{ay}+k_4\mathcal{T}\mathcal{T}^{y}_{x}=k_1K\delta^{y}_{x}+((k_1+k_2+k_3+k_4)J-k_1K)\delta^{5}_{x}\delta^{y}_{5}, \tag{42}$$

where

$$K=144M^4/(x^2+a^2y^2)^6,\quad J=-36M^4(x^6-15a^2y^2x^4+15a^4y^4x^2-a^6y^6)^2/(x^2+a^2y^2)^{12},$$

in Boyer–Lindquist coordinates. So clearly, for $k_1\neq 0$, there are no choices of the constants k_1,k_2,k_3,k_4 which will give us an identity of the required structure. The only other possibility, $k_1=0=k_2+k_3+k_4$, leading to an identity of the form, $k_2\mathcal{T}_{abx}{}^{y}\mathcal{T}^{ab}+k_3\mathcal{T}_{ax}\mathcal{T}^{ay}+k_4\mathcal{T}\mathcal{T}^{y}_{x}=0$, is easily ruled out by showing the incompatability of this identity for another 5-dimensional metric, e.g., a 5-dimensional version of the van Stockum metric.[28] □

Note that we have used Bel–Robinson tensors constructed from Weyl tensors and not the more general candidates in this proof. This not only gives a stronger result than if candidates had been used, but was obtained very simply using GRTENSORII.[29]

In spaces of dimension $n>5$ the Bel–Robinson tensor is no longer completely symmetric and so to investigate the most general possible quadratic identity with two free indices we would need to consider a much more complicated form than in (40).

VI. INDEX SYMMETRY OF BEL–ROBINSON AND LANCZOS SUPERENERGY TENSORS

In this section we will determine the kernel fddi for two results in four dimensions; we will then show by considering the analogous higher-dimensional fddis how, in one case there is a simple generalization to five (and only five) dimensions, while in the other there is no direct generalization to higher dimensions.

The Bel–Robinson spinor (11a) is trivially symmetric in all indices. On the other hand, the only obvious symmetries from the Bel–Robinson tensor (15) are $\mathcal{T}_{abcd}=\mathcal{T}_{(ab)cd}=\mathcal{T}_{ab(cd)}=\mathcal{T}_{cdab}$. To check if it is fully symmetric in *all* indices we examine

$$\mathcal{T}[\hat{C}]_{a[bc]d}=\frac{1}{4}\hat{C}_{adef}\hat{C}_{bc}{}^{ef}-\hat{C}_{eaf[b}\hat{C}_{c]}{}^{e}{}_{d}{}^{f}-\hat{C}_{fge[a}g_{d][b}\hat{C}_{c]}{}^{efg}+\frac{1}{8}g_{a[b}g_{c]d}\hat{C}_{sprq}\hat{C}^{sprq}. \quad (43)$$

We know from spinors that it must be symmetric in all indices in (at least) four dimensions, so the structure of (43) invites comparison with the 4-dimensional ddi for the Weyl tensor in Lemma 3 contracted with another Weyl tensor, i.e.,

$$0\equiv\hat{C}_{[ib}{}^{[kl}\delta^{a]}_{c]}\hat{C}_{kl}{}^{id}, \quad (44)$$

the right hand side of which when expanded coincides precisely with (43).

To determine whether the same result is valid in five dimensions, we consider the analogous *five*-dimensional fddi in Lemma 3, and when we construct

$$0\equiv\hat{C}_{[bc}{}^{[ad}\ \ \delta^{kl]}_{ij]}\hat{C}_{kl}{}^{ij}, \quad (45)$$

we find that its expanded right hand side also coincides precisely with (43).

So we have demonstrated that the fact that the Bel–Robinson tensor (15) is fully symmetric in *five (and lower) dimensions* is just a simple consequence of one 5-dimensional fddi. The 5-dimensional result was originally obtained in Ref. 3 separately from the 4-dimensional result, using duals, and subsequently in Ref. 15, by exploiting the 5-dimensional ddi (45).

[The *five*-dimensional ddi (45),

$$\tfrac{1}{4}\hat{C}_{adef}\hat{C}_{bc}{}^{ef}-\hat{C}_{eaf[b}\hat{C}_{c]}{}^{e}{}_{d}{}^{f}-\hat{C}_{fge[a}g_{d][b}\hat{C}_{c]}{}^{efg}+\tfrac{1}{8}g_{a[b}g_{c]d}\hat{C}_{sprq}\hat{C}^{sprq}\equiv 0,$$

which we have just exploited, is of course also valid in four dimensions; in four dimensions we can use Lemma 4a on the penultimate term and obtain the similar but simpler *four*-dimensional ddi,

$$\tfrac{1}{4}\hat{C}_{adef}\hat{C}_{bc}{}^{ef}-\hat{C}_{eaf[b}\hat{C}_{c]}{}^{e}{}_{d}{}^{f}-\tfrac{1}{8}g_{a[b}g_{c]d}\hat{C}_{sprq}\hat{C}^{sprq}\equiv 0,$$

which is just the identity (44). Deser[6] has pointed out the significance of this identity (44) in the symmetry structure of the Bel–Robinson tensor in four dimensions; here we also see the significance of the 5-dimensional counterpart (45) in the symmetry structure of the Bel–Robinson tensor in *five* dimensions.]

For higher dimensions, from the viewpoint of fddis, we note that the next fddi $\hat{C}_{[ab}{}^{[fg}\,\delta^{hij]}_{cde]}=0$ has too many indices to yield (43) by a contraction with one Weyl tensor. However, it is easy to show conclusively that $\mathcal{T}[\hat{C}]_{abcd}$ is not symmetric in higher dimensions by taking the double trace.[3,15]

The Lanczos superenergy spinor has the obvious symmetries $\mathcal{T}[\hat{L}]_{ABCDA'B'C'D'}=\mathcal{T}[\hat{L}]_{(AB)CD(A'B')C'D'}=\mathcal{T}[\hat{L}]_{AB(CD)A'B'(C'D')}$ and the more general Lanczos superenergy spinor,

$$\tilde{\mathcal{T}}[\hat{L}]_{ABCDA'B'C'D'}=(\mathcal{T}[\hat{L}]_{ABCDA'B'C'D'}+\mathcal{T}[\hat{L}]_{CDABC'D'A'B'}), \tag{46}$$

is clearly symmetric in all indices.

The basic Lanczos superenergy tensor [equivalent to the superenergy spinor for the Lanczos (candidate) spinor $\mathcal{T}[\hat{L}]_{ABCDA'B'C'D'}$] is given by Refs. 3 and 15 in n dimensions,

$$\mathcal{T}[\hat{L}]_{abcd}=\hat{L}_{aic}\hat{L}_{b}{}^{i}{}_{d}+\hat{L}_{aid}\hat{L}_{b}{}^{i}{}_{c}-\tfrac{1}{2}g_{ab}\hat{L}_{ijc}\hat{L}^{ij}{}_{d}-g_{cd}\hat{L}_{aij}\hat{L}_{b}{}^{ij}+\tfrac{1}{4}g_{ab}g_{cd}\hat{L}_{ijk}\hat{L}^{ijk}. \tag{47}$$

It has the obvious properties $\mathcal{T}[\hat{L}]_{abcd}=\mathcal{T}[\hat{L}]_{(ab)(cd)}$, but not the block symmetry $\mathcal{T}_{abcd}=\mathcal{T}_{cdab}$. The more general superenergy tensor,

$$\tilde{\mathcal{T}}[\hat{L}]_{abcd}=(\mathcal{T}[\hat{L}]_{abcd}+\mathcal{T}[\hat{L}]_{cdab})/2, \tag{48}$$

which is equivalent to (46), does not obviously appear to be completely symmetric, as we know it must be in four dimensions at least. To determine if $\tilde{\mathcal{T}}[\hat{L}]_{abcd}$ is symmetric over *all* indices we examine

$$\tilde{\mathcal{T}}[\hat{L}]^{a}{}_{[bc]}{}^{d}=\tfrac{1}{4}\hat{L}_{bce}\hat{L}^{ade}-\hat{L}^{[a}{}_{e[b}\hat{L}_{c]}{}^{|e]d}-\tfrac{1}{2}\delta^{[a}_{[b}\hat{L}_{|ef|c]}\hat{L}^{|ef|d]}-\delta^{[a}_{[b}\hat{L}_{c]ef}\hat{L}^{d]ef}+\tfrac{1}{4}\delta^{a}_{[b}\delta^{d}_{c]}\hat{L}_{ijk}\hat{L}^{ijk}. \tag{49}$$

The structure of (49) (including two deltas) invites a comparison with the 4-dimensional ddi for the Lanczos tensor in Lemma 2 contracted with another Lanczos tensor, i.e.,

$$0\equiv\hat{L}_{[ab}{}^{[e}\delta^{fg]}_{cd]}\hat{L}^{cd}{}_{g}, \tag{50}$$

the right hand side of which when expanded coincides precisely with (49). So we retrieve the result in Ref. 15,

Theorem 5: A Lanczos superenergy tensor $\tilde{\mathcal{T}}[\hat{L}]_{abcd}=(\mathcal{T}[\hat{L}]_{abcd}+\mathcal{T}[\hat{L}]_{cdab})/2$, with $\mathcal{T}[\hat{L}]_{abcd}$ given by (47), is symmetric in all indices in four dimensions. □

To determine whether a similar proof is valid in five dimensions, we consider the analogous *five*-dimensional fddi in Lemma 2, and we immediately see that there are too many free indices to yield (49) by a contraction with one Lanczos tensor.

VII. TENSOR DERIVATION OF NEW ELECTROMAGNETIC CONSERVATION LAW

We now wish to look at a particular Lanczos candidate,

$$L_{abc}=F_{ab;c}, \tag{51}$$

where F_{ab} is an electromagnetic field tensor which satisfies the source-free Maxwell's equations,

$$F^{a}{}_{b;a}=0=F_{[ab;c]}, \tag{52}$$

and so the properties $L^{a}{}_{ba}=0=L_{[abc]}$ of a Lanczos candidate are automatically satisfied. Hence we could choose the tensor (47) with the above substitution (51) and obtain

$$\mathcal{T}[\nabla F]_{abcd}=F_{ai;c}F_{b}{}^{i}{}_{;d}+F_{ai;d}F_{b}{}^{i}{}_{;c}-\tfrac{1}{2}g_{ab}F_{ij;c}F^{ij}{}_{;d}-g_{cd}F_{ai;j}F_{b}{}^{i;j}+\tfrac{1}{4}g_{ab}g_{cd}F_{ij;k}F^{ij;k}, \tag{53}$$

as a superenergy tensor for the electromagnetic field. In fact, Senovilla[3] has shown that a tensor $\mathcal{C}_{abcd}$, suggested by Chevreton[31] as an analog for the Bel–Robinson tensor in an electromagnetic field, is just a linear combination of two such superenergy tensors,

$$\mathcal{C}_{abcd}=(\mathcal{T}[\nabla F]_{abcd}+\mathcal{T}[\nabla F]_{cdab})/2. \tag{54}$$

This tensor was shown in Ref. 31 to have important properties *in flat space:* in particular it is divergence-free, but this property is not valid, in general, in curved spaces. Recently Bergqvist, Eriksson, and Senovilla[5] have used the spinor equivalent of the Chevreton tensor and given two interesting properties *in curved space* for source-free Einstein–Maxwell fields: (i) the Chevreton tensor is fully symmetric; and (ii) the trace of the Chevreton tensor is divergence free.

We now wish to consider the tensor versions of these results. The first of these properties is just a special case of the result previously derived in tensors for Lanczos candidates in 4-dimensional spaces,[15] and given at the end of Sec. IV. The second property was deduced from the spinor form of the divergence of $\mathcal{C}_{abcd}$ and Bergqvist, Eriksson, and Senovilla[5] remark that the proof of this result is far from obvious from the tensor point of view. We shall now demonstrate that the result in Ref. 5 can be obtained in a direct and straightforward manner—until the complication at the last stages where *two fddis valid in four dimensions* have to be used explicitly.

Theorem 6: In four dimensions, the nonzero trace $\mathcal{C}_{ab}\equiv\mathcal{C}_{abc}{}^{c}$ of the Chevreton superenergy tensor $\mathcal{C}_{abcd}$ is symmetric, trace-free and divergence-free, i.e., $\mathcal{C}_{a}{}^{b}{}_{;b}=0$.

Proof: The nonzero trace of the Lanczos superenergy tensor is given by

$$\mathcal{C}_{ab}\equiv\mathcal{C}_{abc}{}^{c}=-L_{aef}L_{b}{}^{ef}+\tfrac{1}{4}g_{ab}L_{cef}L^{cef}, \tag{55}$$

and it is clear that it is symmetric and trace-free. The divergence is

$$\mathcal{C}_{a}{}^{b}{}_{;b}=-L_{aef}L^{bef}{}_{;b}-L_{aef;b}L^{bef}+\tfrac{1}{2}L_{cef;a}L^{cef}. \tag{56}$$

Now substituting (52) and simplifying gives

$$\begin{aligned}
2\mathcal{C}_{a}{}^{b}{}_{;b}&=-2F_{ae;f}F^{be;f}{}_{b}-2F_{ae;fb}F^{be;f}+F_{ce;fa}F^{ce;f}\\
&=-2F_{ae;f}F^{be}{}_{;b}{}^{f}-2F_{ae;f}(R^{f}{}_{b}{}^{e}{}_{i}F^{bi}-R^{f}{}_{i}F^{ie})-2F_{ae;bf}F^{be;f}\\
&\quad-2F^{be;f}(R_{fba}{}^{i}F_{ie}+R_{fbe}{}^{i}F_{ai})+F_{ce;fa}F^{ce;f}\\
&=-2F_{ae;f}F^{be}{}_{;b}{}^{f}-2F_{ae;f}(R^{f}{}_{b}{}^{e}{}_{i}F^{bi}-R^{f}{}_{i}F^{ie})-3F_{[ae;b]f}F^{be;f}\\
&\quad+F_{eb;af}F^{be;f}-2F^{be;f}(R_{fba}{}^{i}F_{ie}+R_{fbe}{}^{i}F_{ai})+F_{ce;fa}F^{ce;f}\\
&=-2F_{ae;f}F^{be}{}_{;b}{}^{f}-3F_{[ae;b]f}F^{be;f}+F_{eb;fa}F^{be;f}+2F^{be;f}R_{afe}{}^{i}F_{ib}\\
&\quad-2F_{ae;f}(R^{f}{}_{b}{}^{e}{}_{i}F^{bi}-R^{f}{}_{i}F^{ie})-2F^{be;f}(R_{fba}{}^{i}F_{ie}+R_{fbe}{}^{i}F_{ai})+F_{ce;fa}F^{ce;f}.
\end{aligned} \tag{57}$$

Using the source-free Maxwell's equations (52) and rearranging gives

$$2\mathcal{C}_{a}{}^{b}{}_{;b}=\tfrac{1}{2}F_{ef;a}R^{ef}{}_{ib}F^{bi}+2F_{ae;f}R^{f}{}_{i}F^{ie}+2F^{be;f}R_{baf}{}^{i}F_{ie}-F^{be;f}R^{i}{}_{fbe}F_{ai} \tag{58}$$

and decomposing the Riemann tensor in four dimensions gives

$$2\mathcal{C}_a{}^b{}_{;b}=\tfrac{1}{2}F_{ef;a}C^{ef}{}_{ib}F^{bi}+2F^{be;f}C_{baf}{}^{i}F_{ie}-F^{be;f}C^{i}{}_{fbe}F_{ai}$$
$$+2F_{af;e}S^{f}{}_{i}F^{ie}+2F^{ie;f}S_{if}F^{ae}-F^{ie;f}S_{af}F^{ie}. \tag{59}$$

We have already noted that the 4-dimensional fddi in Lemma 3, $C_{[ab}{}^{[cd}\delta^{e]}_{f]}\equiv 0$, when contracted with $L_{de}{}^{f}$ gives the ddi (4); a further contraction with F^{cb} gives

$$0\equiv 2F^{cb}L_{[b}{}^{de}C_{c]eda}-\tfrac{1}{2}F^{cb}L^{de}{}_{a}C_{decb}+2F_{a}{}^{b}L^{def}C_{bdef}$$
$$=2F^{ie}L_{e}{}^{bf}C_{ifba}-\tfrac{1}{2}F^{ib}L^{fe}{}_{a}C_{feib}-F_{a}{}^{i}L^{bef}C_{ifbe}, \tag{60}$$

and the substitution $L_{abc}=F_{ab;c}$ into (60) means that the first three terms on the right hand side of (59) disappear. Next we use Einstein's equations and equate the trace-free Ricci tensor S_{ab} to the usual expression for the electromagnetic energy tensor,

$$S_a{}^b=T_a{}^b=F_{ae}F^{be}-\delta^b_a F_{cd}F^{cd}/4. \tag{61}$$

Then the last three terms on the right hand side of (59) can be rearranged to give

$$(F_{[b}{}^{b}F_{c}{}^{c}F_{d}{}^{d}F_{e}{}^{e}\delta^{f}_{a]})_{;f}\equiv 0, \tag{62}$$

since the expression inside the brackets is identically zero in four dimensions by virtue of Lemma 1, which in this context is equivalent to the algebraic Rainich identity $T^a{}_cT^c{}_b=\delta^b_a\ T_{ij}T^{ij}/4$ where the energy–momentum tensor $T^a{}_b=F^a{}_cF^c{}_b-\delta^b_a\ F^{ji}F_{ij}/4$.[15] □

We note that, in the proof, 4-dimensional fddis have been used explicitly on two occasions [(60) and (62)], as well as a decomposition of the Riemann tensor in four dimension. This is why the spinor proof appears much simpler, since the corresponding calculations in spinors just never occur. The use of the Einstein equations for the electromagnetic energy momentum tensor (61) is an important component of the proof; the last three terms on the right hand side of (59) cannot be removed by other means, such as a 4-dimensional ddi which was the means used to remove the first three terms.

From the point of view of a direct generalization of this method to higher dimensions, it is clear that the higher-dimensional analogs (e.g., the 5-dimensional fddi in Lemma 3) would not be sufficient to reduce the first three terms of (59) to zero; nor would the 5-dimensional Cayley–Hamilton theorem be sufficient to reduce the last three terms of (59) to zero. So it would appear that there is no *simple and direct* generalization of Theorem 6 in higher dimensions; but of course this does not rule out more involved generalizations. The fact that the algebraic Rainich identity was used in this 4-dimensional proof would suggest that higher-dimensional analogs would require higher-dimensional algebraic Rainich identities; in five dimensions this has been shown to be a cubic identity in the energy–momentum tensor $T^a{}_b$.

It may be of interest to note that the result is actually true more generally for the trace of the superenergy tensor $\mathcal{T}[\nabla F]_{abcd}$.

For completeness we note that BES also obtained a result for *electromagnetic test fields in Einstein spaces* by spinor methods; Deser has subsequently deduced this result with tensors.[31]

VIII. NEW SYMMETRIC BEL–ROBINSON TENSOR GENERALIZATIONS IN HIGHER DIMENSIONS

We have noted in Sec. VI that although $\mathcal{T}[\hat{C}]_{abcd}$ is symmetric in four and five dimensions this result does not generalize to higher dimensions. However, the 5-dimensional fddi which established this result has a counterpart in other dimensions; so we now investigate whether we can obtain analogous symmetry properties for some other superenergy tensors in higher dimensions.

Lovelock[14] has pointed out that the n-dimensional counterpart of Lemma 3 is as follows.

Lemma 5: In $n=2p$ dimensions, the trace-free double (p,p)-form $V_{i_1i_2\cdots i_p}{}^{j_1j_2\cdots j_p}=V_{[i_1i_2\cdots i_p]}{}^{[j_1j_2\cdots j_p]}$ satisfies

$$V_{[i_1i_2\cdots i_p}{}^{[j_1j_2\cdots j_p}\ \delta^{j_{p+1}]}_{i_{p+1}]}=0. \tag{63}$$

This specializes in *six dimensions (and lower)* for a trace-free double (3,3)-form to

$$V_{[abc}{}^{[efg}\ \delta^{h]}_{d]}=0. \tag{64}$$

The more general results in Ref. 15 include the following.

Lemma 6: In $n\leqslant 2p+1$ dimensions, the trace-free double (p,p)-form $V_{i_1i_2\cdots i_p}{}^{j_1j_2\cdots j_p}=V_{[i_1i_2\cdots i_p]}{}^{[j_1j_2\cdots j_p]}$ satisfies

$$V_{[i_1i_2\cdots i_p}{}^{[j_1j_2\cdots j_p}\ \delta^{j_{p+1}}_{i_{p+1}}\delta^{j_{p+2}]}_{i_{p+2}]}=0. \tag{65}$$

This specializes in *seven dimensions (and lower)* for a trace-free double (3,3)-form to

$$V_{[abc}{}^{[fgh}\ \delta^{ij]}_{de]}\equiv 0. \tag{66}$$

This fddi (66) is the analog of the fddi (45) used to establish symmetry of the Bel–Robinson tensor in five and four dimensions. So we expect (66) to establish symmetry for some generalization of the Bel–Robinson tensor such as a *trace-free* double (3,3)-form in *seven (and lower) dimensions*.

Senovilla[3] has given a basic superenergy tensor for the double (3,3)-form $K_{abc}{}^{def}=K_{[abc]}{}^{[def]}$ in n-dimensions as

$$\begin{aligned}\mathcal{T}[K]_{abcd}=(&K_{apqcrs}K_b{}^{pq}{}_d{}^{rs}+K_{apqdrs}K_b{}^{pq}{}_c{}^{rs}-\tfrac{1}{3}g_{ab}K_{pqrcst}K^{pqr}{}_d{}^{st}-\tfrac{1}{3}g_{cd}K_{apqrst}K_b{}^{pqrst}\\&+\tfrac{1}{18}g_{ab}g_{cd}K_{pqrstu}K^{pqrstu})/4.\end{aligned} \tag{67}$$

To keep things simple, and maintain the analogy with the Weyl candidate $\hat{C}_{ab}{}^{cd}$, we assume also that $K_{abc}{}^{def}$ is *trace-free and (block) symmetric*, i.e.,

$$K_{abc}{}^{dea}=0,\quad K_{abc}{}^{def}=K^{def}{}_{abc}. \tag{68}$$

So $\mathcal{T}[K]_{abcd}$ clearly has the symmetry properties in n-dimensions,

$$\mathcal{T}[K]_{abcd}=\mathcal{T}[K]_{(ab)cd}=\mathcal{T}[K]_{ab(cd)}=\mathcal{T}[K]_{cdab}\,. \tag{69}$$

To determine if $\mathcal{T}[K]_{abcd}$ is symmetric in *all* indices we examine

$$\begin{aligned}\mathcal{T}[K]^a{}_{[bc]}{}^d=(&K^a{}_{pq}{}^d{}_{rs}K_{[b}{}^{pq}{}_{c]}{}^{rs}+K^{apq}{}_{[c|rs|}K_{b]pq}{}^{drs}-\tfrac{1}{3}\delta^a_{[b}K^{|pqr|}{}_{c]st}K_{pqr}{}^{dst}-\tfrac{1}{3}\delta^d_{[c}K^{apq}{}_{|rst|}K_{b]pq}{}^{rst}\\&+\tfrac{1}{18}\delta^a_{[b}\delta^d_{c]}K_{pqr}{}^{stu}K^{pqr}{}_{stu})/4.\end{aligned} \tag{70}$$

The structure of (70) (including two deltas) suggests that we exploit the *seven-dimensional identity* (66) and investigate

$$0\equiv K_{[efg}{}^{[hij}\ \delta^{ad]}_{bc]}K^{efg}{}_{hij}. \tag{71}$$

When we write out (71) as

$$0\equiv(\tfrac{1}{3}K_{bcp}{}^{qrs}K^{adp}{}_{qrs}-\tfrac{1}{2}K_{pqc}{}^{fgd}K^{pqa}{}_{fgb}+\tfrac{1}{2}K_{pqc}{}^{fga}K^{pqd}{}_{fgb}-\tfrac{1}{6}(K_{pqi}{}^{fga}K^{pqi}{}_{fgb}\delta^{d}_{c}$$
$$-K_{pqi}{}^{fga}K^{pqi}{}_{fgc}\delta^{d}_{b}+K_{pqi}{}^{fgd}K^{pqi}{}_{fgc}\delta^{a}_{b}-K_{pqi}{}^{fgd}K^{pqi}{}_{fgc}\delta^{a}_{c})+\tfrac{1}{18}K^{pqr}{}_{fgh}K_{pqr}{}^{fgh}\delta^{ad}_{bc})/4, \tag{72}$$

we easily see that the right hand side of (72) does not coincide with (70), because of an apparent discrepancy in the respective first terms. [Using the symmetry properties (68) enables us to match up all the other terms.]

However, if we consider K_{abcdef} to satisfy a *first Bianchi-type identity*,

$$K_{ab[cdef]}=0 \tag{73}$$

—as well as being trace-free and (block) symmetric—then we find that the first term on the right hand side of (70) becomes

$$K^{a}{}_{pq}{}^{d}{}_{rs}K_{[b}{}^{pq}{}_{c]}{}^{rs}=-K^{a}{}_{pqrs}{}^{d}K_{bcpqrs}=K^{ad}{}_{pqrs}K_{bc}{}^{pqrs}/3, \tag{74}$$

and now it is easy to see that the right hand side of (72) coincides term by term with (70), and so we have proved

Theorem 7: In seven (and less) dimensions a trace-free symmetric double (3,3)-form $K_{abc}{}^{def}$ which also satisfies $K_{ab[cdef]}=0$ has a superenergy tensor $\mathcal{T}[K]_{abcd}$ given by (67) which is symmetric in all indices. □

Again, in analogy with the Bel–Robinson tensor in four dimensions we can see from a direct calculation on the index pair (ab) in (67), combined with Theorem 7, that the following occurs.

Corollary 7.1: In six dimensions, the trace-free symmetric double (3,3)-form $K_{abc}{}^{def}$ which also satisfies $K_{ab[cdef]}=0$, has a superenergy tensor $\mathcal{T}[K]_{abcd}$, given by (67) which is symmetric in all indices and trace-free on all pairs of indices. □

Let us consider K_{abcdef} to be also *divergence-free*, i.e.,

$$K^{a}{}_{bcdef;a}=0. \tag{75}$$

It is then straightforward to repeat the type of calculation which has been done for the divergence-free Weyl tensor in Ricci-flat spaces in n dimensions, and show the following.

Corollary 7.2: If in addition $K_{abc}{}^{def}$ also satisfies $K^{a}{}_{bcdef;a}=0$ then its superenergy tensor $\mathcal{T}[K]_{abcd}$ is also divergence-free in n dimensions., i.e.,

$$\mathcal{T}[K]^{a}{}_{bcd;a}=0. \tag{76}$$

□

We have given just this one application as a simple example to illustrate the power of the fddis in generalizing a result to a higher dimension. However, from this pattern, we would expect to generalize Theorem 7 to classes of (p,p)-forms in spaces of dimension $n=2p+1$. Similarly it appears likely that the result in Theorem 5 for Lanczos candidates in four dimensions, could be generalized to classes of (p,q)-forms in $n=p+q+1$ dimensions.

IX. DISCUSSION

We have used ddis in many situations in this paper, both to rederive existing results, in an efficient tensorial manner, and to obtain new results. The four quadratic identities, which we consider in Secs. II and III, are all special cases of one spinor result which can be established very easily in spinors. We were able to derive the corresponding tensor identities in a manner independent of signature. However, the tensor versions are of varying degrees of difficulty: the familiar Bel–Robinson identity in Theorem 2a requires considerable preliminary work to establish lemmas

for the Weyl tensor, and Theorem 2d requires Theorem 2a together with a number of other lemmas, one involving a ''mixed'' identity. The tensor derivation of the new conservation law for electromagnetism[5] given in Sec. VII also requires ''mixed'' ddis. These tensor derivations are very complicated, and one wonders how long it would have taken to even conjecture the results in Theorems 2d and 6 without the parallel spinor (or null vector) results; but it seems that there is no easier signature-free way in tensors, and we should train ourselves to recognize such structures in tensors. Of course, none of the fddis which we are using in this paper are ''new,'' but while ddis which involve only one tensor (such as quadratic identities for the Weyl tensor, or the Cayley–Hamilton theorem for the Ricci tensor), are familiar, on the other hand, ''mixed'' ddis such as (4), (35), (60), (62) involving more than one tensor and/or derivatives are much less familiar; one of the purposes of this paper is to draw attention to such possibilities.

The amount of work required in these tensor calculations in four dimensions serves as a warning of the even more complicated calculations which will be required to establish analogous results in higher dimensions; the existence of fddis as ''signposts'' will be invaluable.

It is clear from the above examples that the exploitation of dimensionally dependent identities is a useful method, not only for confirming suspected tensor identities, but also for establishing new and perhaps unexpected results. For instance, when we have a particular tensor expression, a study of its structure can suggest an overlap between some of its terms and the terms in a dimensionally dependent identity, and so we have an opportunity of exploiting the latter, and discovering hitherto unexpected tensor relationships. (This is actually how the unexpected symmetry property of the Lanczos superenergy tensor was first recognized in Ref. 15.) Furthermore, once a new significant tensor relationship is established in four dimensions and the kernel 4-dimensional fddi identified, then the analogous fddis in five dimensions and higher can be investigated with the hope of establishing new tensor relationships in these higher dimensions.

Theorem 7 is an example of how to exploit this approach. We can continue to look for higher-dimensional analogs of significant 4-dimensional results: the identity (63) for the trace-free double (p,p)-form $V_{i_1i_2\cdots i_p}{}^{j_1j_2\cdots j_p}=V_{[i_1i_2\cdots i_p]}{}^{[j_1j_2\cdots j_p]}$ in dimensions $n=2p$ leads to the quadratic identity[14]

$$V_{xi_2\cdots i_p}{}^{j_1j_2\cdots j_p}V_{j_1j_2\cdots j_p}{}^{yi_2\cdots i_p}=\ \delta^y_x\ V_{i_1i_2\cdots i_p}{}^{j_1j_2\cdots j_p}V_{j_1j_2\cdots j_p}{}^{i_1i_2\cdots i_p}/2p.$$

The quadratic identity (1) for the Bel–Robinson tensor (i.e., the superenergy tensor for the Weyl tensor where $p=2$) in four dimensions motivates the question as to whether there exists an analogous quadratic identity for the superenergy tensor of (the block symmetric part of) $V_{i_1i_2\cdots i_p}{}^{j_1j_2\cdots j_p}$ in dimension $n=2p$. The stronger versions, and the higher-dimensional generalizations will be presented elsewhere. One criticism of this new generalized Bel–Robinson tensor $\mathcal{T}[K]_{abcd}$ would be the apparent lack of explicit connection of $K_{abc}{}^{def}$ with physical fields; we shall demonstrate in a future paper that there are indeed important links with the gravitational field as described by the Weyl tensor C_{abcd}, and that we can construct examples of the tensor $K_{abc}{}^{def}$ which inherit some of the properties of C_{abcd}.

The result in Theorem 7 has illustrated one possible way to exploit analogous fddis in higher dimensions: to generalize to forms of higher rank. Another approach has been taken in the generalized Rainich problem,[16] where higher-dimensional identities analogous to 4-dimensional quadratic identities were obtained as cubic and higher order identities—involving very long manipulations. It seems clear from the tensor derivation of the new conservation law in electromagnetic theory, that *direct* generalization to higher dimensions are not possible. However, we would expect some sort of generalization exploiting the higher-dimensional counterparts of the kernel fddis used in four dimensions. With the generalized Rainich results[16] as ''signposts'' we would speculate there may be a generalization of the new conservation law in five dimensions for superenergy tensors involving *cubic* terms of T_{ab}.

While obviously interesting and useful in themselves, the study of these identities is not an end in itself. What is of interest is to find identities which are sufficient as well as necessary conditions for a factorization result, and to be able to study a ''generalized Rainich–Misner–

Wheeler problem.'' Clearly then we will need the most general versions of such identities; for instance Penrose[2] has given the most general spinor version of the spinor identity (12) for the Bel–Robinson tensor—a quadratic identity with *all* indices free—and shown that it is also sufficient to achieve the factorization (11a). The ddis which we have been studying in this paper will give us the basic structures to continue these investigations.

Finally, we would also emphasize how simple it is to disprove conjectured identities by counterexample; GRTENSORII,[29] is an invaluable tool for this, and it can also be efficient in enabling us to distinguish between trivial and nontrivial identities.[32] We have also benefited from the use of *Tensign*,[33] making it possible to guarantee the accuracy in the extensive index manipilation required in some of the results.

ACKNOWLEDGMENTS

We are grateful to José Senovilla for suggesting an investigation of the Bel–Robinson quadratic identity by dimensionally dependent identities, for supplying Ref. 23, and pointing out the applicability of results on the Lanczos superenergy tensor to the Chevreton tensor, as well as for other comments and suggestions. We also thank Jonas Bergman, Göran Bergqvist, Ingemar Eriksson, Magnus Herberthson, and Anders Höglund for discussions and suggestions. B.E. wishes to thank Vetenskapsrådet (the Swedish Research Council) for financial support.

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Amalgamations of the Painlevé equations

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(Received 2 July 2002; accepted 8 September 2003)

New hierarchies of nonlinear ordinary differential equations that are generalizations of the Painlevé equations are presented. These hierarchies are shown to contain the Painlevé equations as special cases. Emphasis is on the sixth order ordinary differential equations. Special solutions for one of them are expressed via the general solutions of the P_1, P_2 equations and special cases of the P_3 and P_5 equations. Special solutions of another sixth order ODE are determined by the general solutions of the P_2, P_4, P_3, and P_5 equations. Five of six Painlevé equations can be considered as special cases of these sixth order ODEs. Isomonodromic linear problems to solve the Cauchy problems of hierarchies by the inverse monodromy transform are given. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1623332]

I. INTRODUCTION

As is well known more than one century ago Painlevé and his school discovered six ordinary differential equations (ODEs) that defined new transcendental functions with respect to constants of integration. This was achieved by classifying second ODEs of a certain form having what is today referred to as the Painlevé property (the general solution should be free of movable critical points).

Painlevé and his collaborators found 50 canonical classes of equations whose solutions have no movable critical points. Furthermore, they also showed that among 50 equations there are exactly six second-order ordinary differential equations that define new functions. At the present these new functions are called Painlevé transcendents; and equations with general solutions in the form of these transcendents are called Painlevé equations. These six Painlevé equations were first discovered from strictly mathematical investigations but these equations have recently appeared in several physical applications.[1,2]

Results of Painlevé and his school led to the following problems: to classify other types of nonlinear differential equations and to search higher order differential equations that define new transcendental functions with respect to constants of integration. Recently an attempt has been made to find out new functions, other than the Painlevé transcendents, again determined by nonlinear ODEs. With this aim several hierarchies of ODEs were introduced using hierarchies of nonlinear PDEs that are solvable by inverse scattering transform.[3–8]

The aim of this work is to present new hierarchies of ordinary differential equations that have properties similar to the Painlevé equations. A distinguishing feature of these hierarchies is that they have some Painlevé equations as special cases.

The outline of this article is as follows. Methods to find new hierarchies for generalizations in the Painlevé equations is given in Sec. II. Hierarchies with linear potential are presented in Sec. III. Hierarchies with quadratic potential are studied in Sec. IV.

II. METHOD USED

The Painlevé equations are known to be written as isomonodromic linear problems. Garnier was the first[9] who found that five of the six Painlevé equations can be presented as isomonodromic linear problems. These problems can be used for solving the Cauchy problems of the Painlevé equations by the inverse monodromy transform.[10,11]

The linear problems for the P_1, P_{34} and special cases of the P_3 and P_5 equations can be expressed as the system of equations[12]

$$\begin{aligned}\Psi_{xx}&=(P(x)-\lambda)\Psi,\\ \omega(\lambda)\Psi_\lambda&=2A(x,\lambda)\Psi_x-A_x(x,\lambda)\Psi,\end{aligned}\tag{2.1}$$

where $A(x,\lambda)$ takes the form

$$A(x,\lambda)=a_1(x)+a_0(x)\lambda.\tag{2.2}$$

If one of parameters of the third (fifth) Painlevé equation is equal to zero, we say that there is a special case of the third (fifth) Painlevé equation. We denote further these special cases of equations as the P_3^* and P_5^* equations.

The compatibility condition for the system of equations (2.1),

$$(\Psi_{xx})_\lambda=(\Psi_\lambda)_{xx},\tag{2.3}$$

can be written in the form of the following equation,[8,13]

$$\omega U_\lambda=4UA_x+2U_xA-A_{xxx},\tag{2.4}$$

where we use the potential $U(x,\lambda)$ in the linear form

$$U(x,\lambda)=P(x)-\lambda.\tag{2.5}$$

Assuming (2.2) and $\omega(\lambda)=1$ in the system of equations (2.1) we have the linear problem for the first Painlevé equation. At $\omega(\lambda)=\lambda$ we obtain the Lax pair for the P_{34} equation. Taking into account (2.2) and $\omega(\lambda)=\lambda^2$ and $\omega(\lambda)=\lambda(\lambda-\lambda_0)$ we get the linear problems for the P_3^* and P_5^* equations.[13]

The compatibility condition (2.3) of the isomonodromic linear problem

$$\begin{aligned}\Psi_{xx}&=2(\lambda-y)\Psi_x+Q(x)\Psi,\\ \omega(\lambda)\Psi_\lambda&=C(x,\lambda)\Psi_x+D(x,\lambda)\Psi\end{aligned}\tag{2.6}$$

can also be written as Eq. (2.4) if we assume

$$Q(x)=P(x)-y_x-y^2,\quad C(x,\lambda)=2A(x,\lambda),\tag{2.7}$$

$$D(x,\lambda)=2A_x(x,\lambda)(y-\lambda)+\omega(\lambda)x-A_x(x,\lambda),\tag{2.8}$$

and

$$U(x,\lambda)=P(x)-2\lambda y(x)+\lambda^2.\tag{2.9}$$

Assuming (2.2) and $\omega(\lambda)=1$ in the system of equations (2.6) we have the Lax pair for the second Painlevé equation. In the case (2.2) and $\omega(\lambda)=\lambda$ we get the linear problem for the fourth Painlevé equation. Taking into account (2.2) and $\omega(\lambda)=\lambda^2$ we obtain the Lax pair for the third Painlevé equation. In the case (2.2) and $\omega(\lambda)=\lambda(\lambda-\lambda_0)$ we have the isomonodromic linear problem for the fifth Painlevé equation.

Equation (2.4) can be written as follows:

$$\frac{\partial}{\partial x}\left(2UA^2-AA_{xx}+\frac{1}{2}A_x^2\right)=\omega U_\lambda A.\tag{2.10}$$

One can see from Eq. (2.10) there exists an integral of this equation at $\omega(\lambda)=0$ in the form

$$2UA^2 - AA_{xx} + \tfrac{1}{2}A_x^2 = \text{const}. \tag{2.11}$$

Equation (2.10) allows us also to look for integrals of Eq. (2.4) when $\omega(\lambda)$ has the roots. We are going to use this equation in Secs. III and IV of this work.

Using the compatibility condition (2.3) and $A(x,\lambda)$ in the form

$$A(x,\lambda) = a_2(x) + a_1(x)\lambda + a_0(x)\lambda^2, \tag{2.12}$$

we found in our recent work[8] several new fourth order ordinary differential equations that are analogies to the Painlevé equations.

Assuming that

$$A(x,\lambda) = \sum_{i=0}^{n} a_i(x)\lambda^{n-i}, \tag{2.13}$$

below we are going to find several new hierarchies of ordinary differential equations with properties similar to the Painlevé equations

III. HIERARCHIES WITH LINEAR POTENTIAL (2.5)

Let us study Eq. (2.4) to find hierarchies that are generalizations of the Painlevé equations. First of all we use the linear potential (2.5) in Eq. (2.4).

Case 3.1: $\omega(\lambda) = \omega_0 = \text{const}$. Substituting $U(x,\lambda)$ in the form of Eq. (2.5) and $\omega(\lambda) = \omega_0$ into (2.4) we have

$$4PA_x + 2P_xA - A_{xxx} + \omega_0 - 4\lambda A_x = 0. \tag{3.1}$$

Assuming that $A(x,\lambda)$ is expressed by formula (2.13) and equating expressions at different λ to zero we obtain

$$a_{0,x} = 0, \tag{3.2}$$

$$4a_{k+1,x} = 4Pa_{k,x} + 2P_xa_k - a_{k,xxx} \quad (k = 1, \ldots, n-1), \tag{3.3}$$

$$4Pa_{n,x} + 2P_xa_{n,x} - a_{n,xxx} + \omega_0 = 0. \tag{3.4}$$

Equations (3.2)–(3.4) can be integrated over x. As a result we get

$$a_0(x) = c_0, \tag{3.5}$$

$$a_1(x) = \tfrac{1}{2}c_0P(x) + c_1, \tag{3.6}$$

$$a_2(x) = -\frac{c_0}{8}(P_{xx} - 3P^2) + \frac{1}{2}c_1P + c_2. \tag{3.7}$$

One can see the latter coefficient can be written in the form

$$a_2(x) = -\frac{c_0}{8}L^2[P] + \frac{1}{2}c_1L^1[P] + c_2, \tag{3.8}$$

where the operator $L^k[P]$ is determined by the Lenard relation:[14]

$$\frac{d}{dx}L^{k+1}[P] = -4PL_x^k[P] - 2P_xL^k[P] + L_{xxx}^k[P], \quad L^1[P] = P. \tag{3.9}$$

Now we can formulate the following theorem.

Theorem 3.1: *Coefficients* $a_m(x)$ $(m=1,\ldots,n)$ *that are solutions of equations (3.2) and (3.3) are determined by the formula*

$$a_m(x)=\frac{1}{2}\sum_{i=1}^{m}\left(-\frac{1}{4}\right)^{i-1}c_{m-i}L^i[P]+c_m \quad (m=1,\ldots,n). \tag{3.10}$$

Proof: This theorem is proved by the method of the mathematical induction. At $m=1$ and $m=2$ Eq. (3.10) is reduced to (3.6) and (3.7). Assuming $m=p$ in (3.10) we obtain solution of Eq. (3.3) at $m=p+1$. □

Substituting $a_m(x)$ at $m=n$ into Eq. (3.4) we obtain after integration the following equation:

$$\frac{1}{2}\sum_{i=1}^{n+1}\left(-\frac{1}{4}\right)^{i-1}c_{n+1-i}L^i[P]+c_{n+1}=-\omega_0 x. \tag{3.11}$$

Denoting

$$P(x)=y(x),\ \omega_0=-\alpha,\ \alpha_i=\tfrac{1}{2}(-\tfrac{1}{4})^{i-1}c_{n+1-i} \quad (i=1,...,n+1),$$

changing variables x and y we have equation in the form

$$\sum_{i=2}^{n+1}\alpha_i L^i[y]=\alpha x. \tag{3.12}$$

This hierarchy is the generalization of the first Painlevé hierarchy that was found in Ref. 4 as a reduction of the Schwarz–Korteveg–de Vries hierarchy using self-similar solutions.

Assuming $\alpha_{i\neq 2}=0$, $\alpha_2=1$ we have the first Painlevé equation. In the case $\alpha_i=0$ $(i\neq 1,2)$, $\alpha_2=\beta$, $\alpha_1=1$ we obtain the fourth order nonlinear ordinary differential equation that was found in recent papers.[8,15–17] Some properties of this equation were studied in Refs. 18–22.

At $n=3$ equation of hierarchy (3.12) takes the form

$$\begin{aligned}&\alpha_4(y_{xxxxxx}-35y^4-21y_{xx}^2-14yy_{xxxx}-28y_xy_{xxx}+70y^2y_{xx}+70yy_x^2)\\&+\alpha_3(y_{xxxx}-5y_x^2-10yy_{xx}+10y^3)+\alpha_2(y_{xx}-3y^2)=\alpha x.\end{aligned} \tag{3.13}$$

Isomonodromic linear problem corresponding to Eq. (3.12) is expressed by the system of equations (2.1) where $A(x,\lambda)$ is (2.13) and coefficients $a_i(x)$ are determined by formulas (3.10).

Case 3.2: $\omega(\lambda)=\omega_0\lambda$ $(\omega_0=\text{const})$. Using $U(x,\lambda)$ in the form of the linear potential (2.5) and $\omega(\lambda)=\omega_0\lambda$ we have from Eq. (2.4)

$$4PA_x+2P_xA-A_{xxx}+\omega_0\lambda-4\lambda A_x=0. \tag{3.14}$$

Substituting $A(x,\lambda)$ in the form (2.13) into (3.14) and equating expressions at different λ to zero we have

$$a_{0,x}=0, \tag{3.15}$$

$$4a_{k+1,x}=4Pa_{k,x}+2P_xa_k-a_{k,xxx} \quad (k=1,\ldots,n-2), \tag{3.16}$$

$$4Pa_{n-1,x}+2P_xa_{n-1}-a_{n-1,xxx}-4a_{n,x}+\omega_0=0, \tag{3.17}$$

$$4Pa_{n,x}a_n+2P_xa_{n,x}-a_{n,xxx}=0. \tag{3.18}$$

From (3.14) and (3.15) at $k \leqslant n-2$ we have the same equations as in the previous case. Substituting (3.10) at $m=1,\ldots,n-2$ into (3.16) we have

$$a_{n-1}(x)=\frac{1}{2}\sum_{i=1}^{n-1}\left(-\frac{1}{4}\right)^{i-1}c_{n-1-i}L^i[P]+c_{n-1}. \tag{3.19}$$

Substituting Eq. (3.19) into (3.17) and denoting

$$P(x)=y(x),\ \alpha_k=\tfrac{1}{2}(-\tfrac{1}{4})^{k-1}c_{n-k}\quad (k=1,\ldots,n),\quad a_n(x)=u(x),\ \omega_0=-\alpha,$$

we obtain the system of equations in the form

$$\sum_{k=1}^{n}\alpha_k L^k[y]+4u(x)=\alpha x, \tag{3.20}$$

$$2yu^2-uu_{xx}+\frac{1}{2}u_x^2-\frac{\delta^2}{2}=0. \tag{3.21}$$

Assuming $u(x)=\delta=0$ we have from Eqs. (3.20) and (3.21) hierarchy (3.12). In the case $\alpha_k=0$, at $k\neq 1$, $\alpha_1=1$, we find

$$uu_{xx}-\frac{1}{2}u_x^2-2u^2\alpha x+8u^3+\frac{\delta^2}{2}=0. \tag{3.22}$$

This is the P_{34} equation. It can be transformed to the second Painlevé equation if we use the variable in the form

$$S(x)=\frac{u_x+\delta}{2u}. \tag{3.23}$$

As a result we obtain the second Painlevé equation in the form

$$S_{xx}=2S^3-2\alpha xS+4\delta+\alpha. \tag{3.24}$$

Assuming $n=3$ in the system of equations (3.20) and (3.21) we have

$$\alpha_3(y_{xxxx}-5y_x^2-10yy_{xx}+10y^3)+\alpha_2(y_{xx}-3y^2)+\alpha_1 y+4u=\alpha x, \tag{3.25}$$

$$uu_{xx}-\frac{1}{2}u_x^2-2yu^2+\frac{\delta^2}{2}=0. \tag{3.26}$$

We can consider that hierarchy (3.20) and (3.21) is the generalization of the first Painlevé hierarchy and the second Painlevé equation.

Assuming (3.23) in Eq. (3.21) we find

$$y=S_x+S^2. \tag{3.27}$$

In this case Eq. (3.20) can be presented in the form

$$\sum_{k=1}^{n}\alpha_k L^k[S_x+S^2]+4u=\alpha x. \tag{3.28}$$

Taking into consideration Eqs. (3.23) and (3.28) we have the generalization for the second Painlevé hierarchy in the form

$$\left(\frac{d}{dx}-2S\right)\sum_{k=1}^{n}\alpha_k L^k[S_x+S^2]+2\alpha xS-\alpha-4\delta=0. \tag{3.29}$$

The isomonodromic linear problem for the hierarchy (3.20) and (3.21) is expressed by the system of equations (2.1) where $U(x,\lambda)$ is Eq. (2.5) and $A(x,\lambda)$ is (2.13).

Hierarchy (3.29) is a generalization of the the second Painlevé hierarchy.[3,4,10] We expect that equations of hierarchy (3.29) have special and rational solutions.

One can see that at $n=1$ Eq. (3.56) is the second Painlevé equation. In the case $n=2$ Eq. (3.29) can be presented in the form

$$\alpha_2(S_{xxxx}-10SS_x^2-10S^2S_{xx}+6S^5)+\alpha_1(S_{xx}-2S^3)+2\alpha xS-\alpha-4\delta=0. \tag{3.30}$$

This equation was found recently in Ref. 23. One can see that Eq. (3.30) at $\alpha_2=0$ reduces to the second Painlevé equation but at $\alpha_1=0$ takes the second member for the P_2 hierarchy.

At $n=3$ from Eq. (3.29) we have the sixth order equation in the form

$$\begin{aligned}\alpha_3(S_{xxxxxx}-56SS_xS_{xxx}-14S^2S_{xxxx}-42SS_{xx}^2-70S_x^2S_{xx}+70S^4S_{xx}+140S_x^2S^3-20S^7)+\alpha_2(S_{xxxx}\\ -10SS_x^2-10S^2S_{xx}+6S^5)+\alpha_1(S_{xx}-2S^3)+2x\alpha S+\alpha-4\delta=0.\end{aligned} \tag{3.31}$$

Let us show that the equations of hierarchy (3.29) have some special solutions. With this aim let us formulate the following theorem.

Theorem 3.2: *Special solutions of Eq. (3.29) at $\delta=0$ are expressed via the general solutions of Eq. (3.12).*

Proof: Equation (3.29) at $\delta=0$ can be written in the form

$$\left(\frac{d}{dx}-2S\right)\sum_{k=1}^{m}\alpha_k L^k[S_x+S^2]+2\alpha xS-\alpha=\left(\frac{d}{dx}-2S\right)\left(\sum_{k=1}^{m}\alpha_k L^k[y]-\alpha x\right), \tag{3.32}$$

where we denote

$$y=S_x+S^2. \tag{3.33}$$

From relation (3.32) one can see that there are special solutions of Eq. (3.29) at $\delta=0$. These solutions are expressed via the general solutions of Eq. (3.12) at $m=n+1$ taking into account Eq. (3.33). The latter equation can be transformed to the linear equation

$$\varphi_{xx}=y\varphi \tag{3.34}$$

if we assume $S=\varphi_x/\varphi$ in Eq. (3.33). □

Now let us find the birational transformations for the solutions of Eqs. (3.29). With this aim let us use the approach of Ref. 18.

Equations (3.29) can be written using two equivalent forms

$$\left(\frac{d}{dx}-2S\right)\sum_{k=1}^{m}\alpha_k L^k[S_x+S^2]+2\alpha xS-\alpha-4\delta=0, \tag{3.35}$$

$$-\left(\frac{d}{dx}+2S\right)\sum_{k=1}^{m}\alpha_k L^k[-S_x+S^2]+2\alpha xS-\alpha=-4\delta=0. \tag{3.36}$$

The latter equation was found taking into account the symmetry of the operator $L^k[S_x+S^2]$.

Let us denote

$$M=\sum_{k=1}^{m}\alpha_k L^k[S_x+S^2]-\alpha x \tag{3.37}$$

and

$$N=\sum_{k=1}^{m}\alpha_k L^k[-S_x+S^2]-\alpha x. \tag{3.38}$$

Then Eqs. (3.35) and (3.36) can be presented in the form

$$M_x-2SM-4\delta=0, \tag{3.39}$$

$$N_x+2S'N+2\alpha+4\delta'=0, \tag{3.40}$$

where we take into consideration

$$S\equiv S(x,\alpha+4\delta), \quad S'\equiv S'(x,\alpha+4\delta').$$

They are solutions of Eqs. (3.35) and (3.36).

Using Eqs. (3.39) and (3.40) we have

$$S=\frac{M_x-4\delta}{2M}, \quad S'=-\frac{N_x+2\alpha+4\delta'}{2N}. \tag{3.41}$$

Substituting S and S' into Eqs. (3.37) and (3.38) one can see these equations coincide at $M=N$ for two cases

$$2\delta'+\alpha=-2\delta, \quad 2\delta'+\alpha=2\delta. \tag{3.42}$$

The first equation in (3.42) corresponds to the symmetry of Eqs. (3.29) $S\to -S$ and $4\delta+\alpha\to -4\delta-\alpha$ but the second equation in (3.42) leads to the equation which can be found from Eqs. (3.41) at $M=N$:

$$S+\frac{\delta}{M}=-S'-\frac{\alpha+2\delta'}{M}. \tag{3.43}$$

The latter equation can be written in the form of the birational transformation

$$S(x,4\delta-\alpha)=-S(x,\alpha+4\delta)-\frac{4\delta}{\Sigma_{k=1}^{m}\alpha_k L^k[S_x+S^2]-\alpha x}. \tag{3.44}$$

The latter formula can be used to look for the rational solutions of Eqs. (3.29). One can see there is the trivial solution of these equations $S=0$ at $\delta=-\alpha/4$. By the formula (3.44) using $S=0$ in the right hand side at $\delta=-\alpha/4$ we have

$$S(x,-2\alpha)=-\frac{1}{x} \tag{3.45}$$

and so on. For example, for Eq. (3.30) we have

$$S(x,-4\alpha)=-\frac{2(\alpha_1+\alpha x^3)}{x(\alpha x^3-2\alpha_1)}, \tag{3.46}$$

$$S(x,-6\alpha)=-\frac{3(40\alpha_1^2x^2-4\alpha\alpha_1x^5-48\alpha_2\alpha_1-48\alpha_2\alpha x^3)}{(\alpha x^3-2\alpha_1)(\alpha^2x^6-10\alpha\alpha_1x^3+72\alpha_2\alpha x-20\alpha_1^2)}. \tag{3.47}$$

These solutions are generalizations of solutions for the second Painlevé equation and for the second member of the P_2 hierarchy. Solutions for the $S(x,2\alpha)$, $S(x,4\alpha)$ and $S(x,6\alpha)$ can be obtained from solutions (3.45)–(3.47) taking into account the symmetry of Eqs. (3.29).

Case 3.3: $\omega(\lambda)=\omega_0\lambda^2$. Substituting $\omega(\lambda)=\omega_0\lambda^2$ and (2.5) into (2.4) we obtain

$$4(P-\lambda)A_x+2AP_x-A_{xxx}+\omega_0\lambda^2=0. \tag{3.48}$$

Assuming $A(x,\lambda)$ in the form of (2.13) we have $a_0=c_0$ and

$$a_k(x)=\frac{1}{2}\sum_{i=1}^{k}\left(-\frac{1}{4}\right)^{i-1}c_{k-i}L^i[P]+c_k \quad (k=1,\ldots,n-2). \tag{3.49}$$

Additionally we have also three equations

$$4Pa_{n-2,x}+2P_xa_{n-2}-a_{n-2,xxx}-4a_{n-1,x}+\omega_0=0, \tag{3.50}$$

$$4Pa_{n-1,x}+2P_xa_{n-1}-a_{n-1,xxx}-4a_{n,x}=0, \tag{3.51}$$

$$4Pa_{n,x}+2P_xa_{n,x}-a_{n,xxx}=0. \tag{3.52}$$

Using Eq. (3.49) we also have the integral in the form

$$\frac{1}{2}\sum_{i=1}^{n-1}\left(-\frac{1}{4}\right)^{i-1}c_{n-1-i}L^i[P]+c_{n-1}=-\omega_0x \tag{3.53}$$

from Eq. (3.50).

One can find two integrals for Eqs. (3.51) and (3.52) using (2.10). They take the form

$$a_{n,xx}a_{n-1}+a_{n-1,xx}a_n+2a_n^2-a_{n,x}a_{n-1,x}-4Pa_na_{n-1}+c_n=0, \tag{3.54}$$

$$a_na_{n,xx}-\tfrac{1}{2}a_{n,x}^2-2Pa_n^2+c_{n+1}=0. \tag{3.55}$$

Denoting

$$\begin{gathered}P(x)=y(x),\quad a_{n-1}(x)=v(x),\quad a_n(x)=u(x),\quad \omega_0=-\alpha,\\ \alpha_i=\frac{1}{2}\left(-\frac{1}{4}\right)^{i-1}c_{n-1-i}\quad (i=1,\ldots,n-2),\quad c_n=\chi,\quad c_{n+1}=-\frac{\delta^2}{2},\end{gathered} \tag{3.56}$$

we have from Eqs. (3.53)–(3.55) the system of equations

$$\sum_{i=1}^{n-1}\alpha_iL^i[y]+4v(x)=\alpha x, \tag{3.57}$$

$$u_{xx}v+v_{xx}u+2u^2-u_xv_x-4yuv+\chi=0, \tag{3.58}$$

$$uu_{xx}-\frac{1}{2}u_x^2-2yu^2-\frac{\delta^2}{2}=0. \tag{3.59}$$

From Eq. (3.57) we obtain at $n=3$ the following system of equations:

$$\alpha_2(y_{xx}-3y^2)+\alpha_1 y+4v=\alpha x, \tag{3.60}$$

$$u_{xx}v+v_{xx}u+2u^2-u_xv_x-4yuv+\chi=0, \tag{3.61}$$

$$uu_{xx}-\frac{1}{2}u_x^2-2yu^2-\frac{\delta^2}{2}=0. \tag{3.62}$$

Assuming $\alpha_i=0$ $(i=1,\ldots,n-1)$ in Eq. (3.57) we have $v(x)=\alpha x/4$. Then from Eqs. (3.58) and (3.59) we obtain the special case of the third Painlevé equation in the form

$$u_{xx}-\frac{u_x^2}{u}+\frac{u_x}{x}-\frac{8u^2+4\nu}{\alpha x}-\frac{2\delta^2}{u}=0. \tag{3.63}$$

However, if we take $u(x)=v(x)=\delta=\chi=0$ we obtain from Eq. (3.57) the generalization for the first Painlevé hierarchy (3.12) One can see that the system of equations (3.57)–(3.59) can be considered as the generalization for the P_1 and P_3^* equations.

Obviously the system of equations (3.57)–(3.59) can be reduced to one equation. From Eq. (3.59) we have

$$y=\frac{u_{xx}}{2u}-\frac{u_x^2}{4u^2}-\frac{\delta^2}{4u^2}. \tag{3.64}$$

Using Eqs. (3.57) and (3.64) we obtain

$$\sum_{i=1}^{n-1}\alpha_i L^i\left[\frac{u_{xx}}{2u}-\frac{u_x^2}{4u^2}-\frac{\delta^2}{4u^2}\right]+4v=\alpha x. \tag{3.65}$$

Using new function $F=\ln u$ in Eq. (3.64) we have

$$y=\frac{1}{2}\left(F_{xx}+\frac{1}{2}F_x^2-\frac{\delta^2}{2}e^{2F}\right). \tag{3.66}$$

Substituting $F=\ln u$ into Eq. (3.65) we have an equation in the form

$$\sum_{k=1}^{m}\alpha_k L^k\left[\frac{1}{2}\left(F_{xx}+\frac{1}{2}F_x^2-\frac{\delta^2}{2}e^{-2F}\right)\right]+4v=\alpha x. \tag{3.67}$$

From Eq. (3.61) we also have

$$\frac{d}{dx}\left(\frac{d}{dx}-F_x\right)v+\delta^2 v e^{-2F}+\chi e^{-F}+2e^F=0. \tag{3.68}$$

The latter can be written as the hierarchy if we take into account $v(x)$ from Eq. (3.67). We get

$$\frac{d}{dx}\left(\frac{d}{dx}-F_x\right)\sum_{k=1}^{m}\alpha_k L^k\left[\frac{1}{2}\left(F_{xx}+\frac{1}{2}F_x^2-\frac{\delta^2}{2}e^{-2F}\right)\right]+\delta^2 e^{-2F}\sum_{k=1}^{m}\alpha_k L^k\left[\frac{1}{2}\left(F_{xx}+\frac{1}{2}F_x^2-\frac{\delta^2}{2}e^{-2F}\right)\right]+\frac{d}{dx}(\alpha x F_x)-\alpha\delta^2 x e^{-2F}-4\chi e^{-F}+\mu e^F=0. \tag{3.69}$$

[Parameter μ can be introduced in Eq. (3.69).] Hierarchy (3.69) is a generalization of hierarchy (3.29) by the following theorem.

Theorem 3.3: *Special solutions of Eq. (3.69) at $m \geqslant 2$ are expressed via the general solutions of the P_1, P_2 and P_3^* equations.*

Proof: Equation (3.69) is equivalent to the system of equations (3.57)–(3.59) Assuming $u = v = \delta = 0$ we have the first Painlevé equation at $\alpha_k = 0$ $(k > 3)$. Therefore, special solution of hierarchy (3.69) can be found using the general solution of the P_1 equation.

Assuming $\delta = \chi = \mu = 0$ and $f(x) = F_x$ we obtain from Eq. (3.69) at $\alpha_k = 0$ $(k \geqslant 2)$ after integration

$$\left(\frac{d}{dx} - f\right)\left(f_x + \frac{1}{2}f^2\right) + 2\alpha x f - \beta = 0. \tag{3.70}$$

(Here β is a constant of integration.) The latter equation is the second Painlevé equation. We have that the special solution of Eq. (3.69) is also expessed via the general solution of the P_2 equation.

Assuming $\alpha_k = 0$ $(k = 1, \ldots, m)$ in Eq. (3.69) we have the P_3^* equation in the form

$$\frac{d}{dx}(\alpha x F_x) - \alpha \delta^2 x e^{-2F} - 4\chi e^{-F} + \mu e^F = 0. \tag{3.71}$$

The latter can be transformed to the canonical form of the P_3^* equation if we use transformation $F = \ln u$. This takes the form

$$u_{xx} = \frac{u_x^2}{u} - \frac{u_x}{x} + \frac{\delta^2}{u} - \frac{\mu u^2}{\alpha x} + \frac{4\chi}{\alpha x}. \tag{3.72}$$

One can see that Eq. (3.69) has also a special solution in the form of general solution of Eq. (3.72). □

Corollary 3.1: The P_1, P_2 and P_3^* equations are special cases of hierarchy (3.69).

There is a sixth order ODE which generalizes the P_1, P_2 and P_3^* equation. This one will be presented below.

The isomonodromic linear problem for solving the system of equations (3.57)–(3.59) is given by Eqs. (2.1) again.

Case 3.4: $\omega(\lambda) = \omega_0 \lambda(\lambda - \lambda_0)$. Substitutions of $\omega(\lambda) = \omega_0 \lambda(\lambda - \lambda_0)$ and potential (2.5) into Eq. (2.4) lead to the equation

$$A_{xxx} - 2P_x A + 4(\lambda - P)A_x + \omega_0 \lambda \lambda_0 - \omega_0 \lambda^2 = 0. \tag{3.73}$$

Substituting (2.13) into Eq. (3.73) and equating expressions at different powers λ to zero we obtain the system of equations.

We have $a_0 = c_0$ and $a_k(x)$ $(k = 1, \ldots, n-2)$ in the form (3.49). Additionally to these equations there are Eqs. (3.50) and (3.52) We also obtain equation in the form

$$a_{n-1,xxx} - 4P a_{n-1,x} - 2P_x a_{n-1} + 4a_{n,x} + \omega_0 \lambda_0 = 0. \tag{3.74}$$

The integral corresponding to Eq. (3.74) can be found by analogy of Eq. (3.54) from Eq. (2.10) at $\lambda = \lambda_0$.

One can see we obtain the system of equations in this case that is similar to Eqs. (3.57)–(3.59). Two equations coincide with Eqs. (3.57) and (3.59) but in place of Eq. (3.58) we have more general equation.

Let us present here the system of equations at $n = 3$. Denoting $P(x) = y(x)$, $a_3(x) = u(x)$, $a_2(x) = v(x)$, $c_0 = 2\alpha_4$, $c_1 = \alpha_3$, $c_2 = 0$, $c_3 = \alpha_1$, $\lambda_0 = \beta$, $c_4 = 16\delta$ we have the following system of equations:

$$\alpha_4(y_{xx}-3y^2)-2\alpha_3 y+4v=\alpha x, \tag{3.75}$$

$$\begin{aligned}u_{xx}v+uv_{xx}+2u^2-u_xv_x-4yuv+\beta(vv_{xx}+4uv-2yv^2-\tfrac{1}{2}v_x^2+\alpha_3(u_{xx}-4uy)+\alpha_4(uy_{xx}+yu_{xx}\\ -u_xy_x-4uy^2))+\beta^2(2v^2+\alpha_3(v_{xx}+4u-4yv)+\alpha_4(vy_{xx}+yv_{xx}-4uy-v_xy_x-4vy^2\\ +2u_{xx}))+\beta^3(2\alpha_3(2v-\alpha_3 y)+\alpha_3\alpha_4(y_{xx}-4y^2)+2\alpha_4(v_{xx}+4u-2yv)+\alpha_4^2(yy_{xx}-2y^3\\ -\tfrac{1}{2}y_x^2))+2\beta^4(4\alpha_4 v-2\alpha_3\alpha_4 y+\alpha_4^2(y_{xx}-3y^2))+\alpha_1=0,\end{aligned} \tag{3.76}$$

$$uu_{xx}-\tfrac{1}{2}u_x^2-2yu^2+\delta=0. \tag{3.77}$$

Obviously the system of equations (3.75), (3.76) and (3.77) can be written as the sixth-order ODE. One can state the theorem.

Theorem 3.4: *Special solutions of the system of equations (3.75)–(3.77) are expressed via the general solutions of the P_1, P_2, P_3^* and P_5^* equations.*

Proof: Assuming $u=v=\alpha_1=\alpha_3=\beta=\delta=0$, $\alpha_4\neq 0$ we have the P_1 equation from (3.75).

In the case $\delta=\alpha_3=\beta=0$ we obtain the P_2 equation from Eqs. (3.75) and (3.77) taking into account transformations (3.23) and (3.27). Assuming $\alpha_4=\alpha_3=\beta$ we get the P_3^* equation in the form of (3.72).

Therefore the special solutions for the system of equations are expressed by the previous theorem via the general solutions of the P_1, P_2 and P_3^* equation.

In the case $\alpha_4=\alpha_3=0$ we have equation from the system of equations (3.75)–(3.77) in the form

$$\frac{\beta u_{xx}}{u}+\frac{4u_{xx}}{\alpha x}-\frac{\beta u_x^2}{2u^2}-\frac{4u_x^2}{\alpha x u}+\frac{4u_x}{\alpha x^2}-\frac{16\beta u}{\alpha x}-\frac{32u^2}{\alpha^2x^2}+\frac{8\delta}{\alpha x u}+\frac{\beta\delta}{u^2}+\frac{\beta}{2x^2}-\frac{16\alpha_1}{\alpha^2x^2}-2\beta^2=0. \tag{3.78}$$

The latter equation is transformed to the P_5^* equation. □

Assuming $\alpha_1=0$ and $\beta=0$ in Eqs. (3.75)–(3.77) we have the fourth order ordinary differential equation

$$\begin{aligned}&\alpha_0\left(u_{xxxx}-4\frac{u_xu_{xxx}}{u}+\frac{21}{2}\frac{u_x^2u_{xx}}{u^2}-3\frac{u_{xx}^2}{u}-\frac{9}{2}\frac{u_x^4}{u^3}-5\delta^2\frac{u_x^2}{u^3}-\frac{\delta^4}{2u^3}+\frac{5\delta^2}{2}\frac{u_{xx}}{u^2}\right)\\ &-2\alpha x u_{xx}-2\alpha u_x+2\alpha_2+2\alpha x\frac{u_x^2}{u}+\frac{2\alpha x\delta^2}{u}\\ &=0.\end{aligned} \tag{3.79}$$

Equation (3.79) at $\alpha_0=1$ was obtained recently in Ref. 8. This one is the generalization of the P_3^* equation.

Corollary 3.2: The P_1, P_2, P_3^* and P_5^* are special cases of the system of equations (3.75)–(3.77).

Now we can see how other hierarchies can be found out from Eq. (2.4).

The structure of these hierarchies is similar to the above presented hierarchy (3.57)–(3.59). These new hierarchies can be written in the form of the system of equations.

We have the theorem.

Theorem 3.5: *Let Eq. (2.4) and $A(x,\lambda)$ be given by formula (2.13); then Eq. (2.4) leads to the $n+1$ hierarchies at $\omega(\lambda)=\omega_0\lambda^m$ $(m=0,1,\ldots,n)$.*

Proof: This theorem is proved by means of calculations of all possible hierarchies at $\omega(\lambda)=\omega_0\lambda^m$ $(m=0,1,\cdots,n)$. The new degree λ of $\omega(\lambda)$ allows us to find the additional integral from Eq. (2.11). □

Case 3.5: $\omega(\lambda)=\omega_0\lambda^3$. Let us look for the new system of equations from (2.4) at $\omega(\lambda)=\omega_0\lambda^3$. We have the set of equations similar to case 3.4. Additional integral takes the form

$$2Pa_{n-1}^2+4Pa_na_{n-2}-a_{n-2}a_{n,xx}-4a_na_{n-1}-a_{n-1}a_{n-1,xx}$$
$$-a_na_{n-2,xx}+a_{n,x}a_{n-2,x}+\tfrac{1}{2}a_{n-1,x}^2-c_{n-2}=0 \tag{3.80}$$

(c_{n-2} is a constant). Using integrals (3.54), (3.55), and (3.80) and denoting $P(x)=y(x)$, $a_{n-1}(x)=v(x)$, $a_{n-2}(x)=w(x)$, $c_n=\delta$, $c_{n-1}=\mu$, $c_{n-2}=\nu$ we have the system of equations in the form

$$\sum_{k=1}^{n-2}\alpha_kL^k[y]+4w(x)=\alpha x, \tag{3.81}$$

$$2yv^2+4yuw-wu_{xx}-4uv-vv_{xx}-uw_{xx}+u_xw_x+\tfrac{1}{2}v_x^2-\nu=0, \tag{3.82}$$

$$vu_{xx}+v_{xx}u+2u^2-u_xv_x-4yuv-\mu=0, \tag{3.83}$$

$$uu_{xx}-\tfrac{1}{2}u_x^2-2yu^2-\delta=0. \tag{3.84}$$

We can expect that the system of equations (3.81)–(3.84) is also generalization of the Painlevé equations.

IV. HIERARCHIES WITH POTENTIAL (2.9)

Let us find hierarchies which generalize the Painlevé equations in the case of potential (2.9). These hierarchies can be found from Eq. (2.4) again.

Substituting potential (2.9) $A(x,\lambda)$ in the form of Eq. (2.13) and $\omega(\lambda)=\omega_0\lambda^m$ $(m=0,\ldots,n+1)$ into Eq. (2.4) we have the system of equations

$$E_k-2\omega_0(\delta_{k,n+1-m}-y\delta_{k,n+2-m})=0 \quad (k=0,\ldots,n+2), \tag{4.1}$$

where we denote

$$E_k=4a_{k,x}-4y_xa_{k-1}-8ya_{k-1,x}-a_{k-2,xxx}+4Pa_{k-2,x}+2P_xa_{k-2} \tag{4.2}$$

and $\delta_{k,n}$ is the Kronecker delta.

In the system of equations (4.1) we have to take into account that $a_{-1}=a_{-2}=a_{n+1}=a_{n+2}=0$ in correspondence with Eq. (2.13).

The system of equations (4.1) has $n+3$ equations to find out $a_0(x)$, $a_1(x),\ldots,a_n(x)$ and $P(x)$. As a result we can also obtain the equation for $y(x)$.

Case 4.1: $\omega(x)=\omega_0$. Assuming $\omega=\omega_0$ we obtain from Eq. (4.2) the following system of equations:

$$a_0=c_0, \tag{4.3}$$

$$a_1=c_0y+c_1, \tag{4.4}$$

$$a_{k,x}-y_xa_{k-1}-2ya_{k-1,x}+\tfrac{1}{2}P_xa_{k-2}+Pa_{k-2,x}-\tfrac{1}{4}a_{k-2,xxx}=0 \ (k=2,\ldots,n-1), \tag{4.5}$$

$$2P_xa_{n-1}+4Pa_{n-1,x}-a_{n-1,xxx}-8ya_{n,x}-4y_xa_n-2\omega_0=0, \tag{4.6}$$

$$2P_xa_n+4Pa_{n,x}+2\omega_0y-a_{n,xxx}=0. \tag{4.7}$$

Let us consider the system of equations (4.5) and (4.6) at $n=2$. At $n=2$ we obtain from Eqs. (4.5)

$$a_2(x)=\tfrac{3}{2}c_0y^2-\tfrac{1}{2}c_0P(x)+c_1y+c_2, \tag{4.8}$$

where c_0,c_1,c_2 and c_3,c_4 later are arbitrary constants.

Substituting (4.4) and (4.8) into Eq. (4.6) we have after integration

$$6c_0Py-10c_0y^3-c_0y_{xx}+2c_1P-6c_1y^2-4c_2y-2\omega_0x+c_3=0. \tag{4.9}$$

After substitution of $a_2(x)$ from Eq. (4.8) into (4.7) we obtain an equation which can be integrated if before we subtract Eq. (4.9) multiplied on y_x. As a result we have

$$\tfrac{1}{2}c_0P_{xx}-3c_0yy_{xx}-\tfrac{5}{2}c_0y_x^2-\tfrac{3}{2}c_0P^2+3c_0Py^2+\tfrac{5}{2}c_0y^4-c_3y+c_4-c_1y_{xx}+2c_1y^3+2c_1Py +2c_2P+2c_2y^2+2\omega_0xy=0. \tag{4.10}$$

Denoting $c_i=\alpha_{4-i}$ $(i=0,1,2,3,4)$, $P(x)=v(x)$, $\alpha_1=0$, $\omega=\alpha/2$ in Eqs. (4.9) and (4.10) we have the system of equations

$$\alpha_4(6vy-10y^3-y_{xx})+2\alpha_3(v-3y^2)-4\alpha_2y-\alpha x=0, \tag{4.11}$$

$$\alpha_4(\tfrac{1}{2}v_{xx}-\tfrac{3}{2}v^2+3vy^2-3yy_{xx}+\tfrac{5}{2}y^4-\tfrac{5}{2}y_x^2)+\alpha_3(2vy+2y^3-y_{xx})+2\alpha_2(v+y^2)+\alpha_0+\alpha xy=0. \tag{4.12}$$

From the system of equations (4.11) and (4.12) at $\alpha_1=\alpha_2=\alpha_4=0$ we have the second Painlevé equation in the form

$$\alpha_3y_{xx}-8\alpha_3y^3-2\alpha xy-\alpha_0=0. \tag{4.13}$$

At $n=3$ $a_2(x)$ takes the form (4.8) and $a_3(x)$ can be written as follows:

$$a_3(x)=\tfrac{5}{2}c_0y^3+\tfrac{1}{4}c_0y_{xx}-\tfrac{3}{2}c_0Py+\tfrac{3}{2}c_1y^2-\tfrac{1}{2}c_1P+c_2y+c_3. \tag{4.14}$$

Substitutions of $a_2(x)$ and $a_3(x)$ into Eq. (4.6) allows us to integrate this equation. It takes the form

$$\tfrac{1}{2}c_0P_{xx}-\tfrac{3}{2}c_0P^2-5c_0yy_{xx}-\tfrac{35}{2}c_0y^4-\tfrac{5}{2}c_0y_x^2+15c_0Py^2-c_1y_{xx}-10c_1y^3+6c_1yP-6c_2y^2 +2c_2P-4c_3y-2\omega_0x+c_4=0. \tag{4.15}$$

Multiplying Eq. (4.15) by y_x and subtracting this one from Eq. (4.7) we have after integration

$$-\tfrac{1}{4}c_0y_{xxxx}+\tfrac{7}{2}c_0y^5-\tfrac{25}{2}c_0yy_x^2-\tfrac{15}{2}c_0y^2y_{xx}+\tfrac{5}{2}c_0Py_{xx}-\tfrac{9}{2}c_0P^2y+5c_0Py^3+\tfrac{5}{2}c_0y_xP_x +\tfrac{3}{2}c_0yP_{xx}-\tfrac{3}{2}c_1P^2+3c_1y^2P-\tfrac{5}{2}c_1y_x^2+\tfrac{1}{2}c_1P_{xx}+\tfrac{5}{2}c_1y^4-3c_1yy_{xx}+2c_2yP-c_2y_{xx} +2c_2y^3+2c_3P+2c_3y^2-c_4y+2\omega_0yx=0. \tag{4.16}$$

Denoting $c_i=\alpha_{4-i}$ $(i=0,1,2,3,4)$, $\omega=\alpha/2$, $P(x)=v(x)$ (α_0 can be taken zero) we have from Eqs. (4.15) and (4.16) the following system of equations:

$$\alpha_4(\tfrac{1}{2}v_{xx}-5yy_{xx}-\tfrac{5}{2}y_x^2-\tfrac{3}{2}v^2+15vy^2-\tfrac{35}{2}y^4)+\alpha_3(6vy-10y^3-y_{xx})+2\alpha_2(v-3y^2)-4\alpha_1y -\alpha x=0, \tag{4.17}$$

$$\alpha_4(y_{xxxx}-14y^5+50yy_x^2+30y^2y_{xx}-10vy_{xx}+18v^2y-20vy^3-10y_xv_x-6yv_{xx})+\alpha_3(6v^2 -12vy^2+10y_x^2-2v_{xx}-10y^4+12yy_{xx})+4\alpha_2(y_{xx}-2y^3-2yv)-8\alpha_1(v+y^2)-4\alpha xy=0. \tag{4.18}$$

Assuming $\alpha_0=\alpha_1=\alpha_3=\alpha_4=0$ in the system of equations (4.17) and (4.18) we have the second Painlevé equation again. We can consider the system of equations (4.17) and (4.18) as a generalization of the second Painlevé equation.

The Cauchy problem for the system of equations can be solved by the inverse monodromy transform taking into account Eqs. (2.6) where $U(x,\lambda)$ and $A(x,\lambda)$ are determined by formulas (2.9) and (2.13).

Case 4.2: $\omega(\lambda)=\omega_0\lambda$ ($\omega_0=$const). Assuming $\omega(\lambda)=\omega_0\lambda$ in Eq. (4.1) we can find the system of equations to define $a_0(x)$, $a_1(x),\ldots,$ $a_n(x)$, $P(x)$ and $y(x)$. In this case equations for $a_0(x)$, $a_1(x)$ and $a_k(x)$ ($k=2,\ldots,n-2$) coincide with Eqs. (4.3)–(4.5). However, we have to use rather than Eqs. (4.6) and (4.7) the following system of equations:

$$2P_xa_{n-2}+4Pa_{n-2,x}-a_{n-2,xxx}-8ya_{n-1,x}-4y_xa_{n-1}-2\omega_0+4a_{n,x}=0, \tag{4.19}$$

$$2P_xa_{n-1}+4Pa_{n-1,x}-a_{n-1,xxx}-8ya_{n,x}-4y_xa_n+2\omega_0y=0, \tag{4.20}$$

$$2P_xa_n+4Pa_{n,x}-a_{n,xxx}=0. \tag{4.21}$$

From Eq. (4.21) we obtain the equation after integration

$$2Pa_n^2-a_na_{n,xx}+\tfrac{1}{2}a_{n,x}^2+c_{n+2}=0 \tag{4.22}$$

(here c_{n+2} is arbitrary constant).

Let us consider Eqs. (4.19) and (4.20) at $n=3$. We have $a_0(x)$, $a_1(x)$ and $a_2(x)$ that are determined by formulas (4.3), (4.4) and (4.8).

After integration Eq. (4.19) takes the form

$$6c_0yP-10c_0y^3-c_0y_{xx}+2c_1P-6c_1y^2-4c_2y-2\omega_0x+4a_3-4c_3=0. \tag{4.23}$$

Substituting $a_2(x)$, $a_3(x)$ and (4.14) into Eq. (4.20) we have after integration

$$\tfrac{1}{2}c_0P_{xx}-\tfrac{3}{2}c_0P^2-5c_0yy_{xx}-\tfrac{5}{2}c_0y_x^2-\tfrac{35}{2}c_0y^4+15c_0y^2P-10c_1y^3+6c_1yP-c_1y_{xx}+2c_2P -6c_2y^2-4c_3y+c_4-2\omega_0xy=0. \tag{4.24}$$

Equation (4.22) at $n=3$ can be written in the form

$$2Pa_3^2-a_3a_{3,xx}+\tfrac{1}{2}a_{3,x}^3+c_5=0. \tag{4.25}$$

One can see that we have three unknown variables $y(x)$, $P(x)$ and $a_3(x)$ in the system of equations (4.23)–(4.25).

Denoting $P(x)=v(x)$, $a_3(x)=u(x)$, $c_i=\alpha_{4-i}$ ($i=0,1,2,3,4$), $c_5=\delta$, $\alpha_1=0$, $\omega_0=\alpha/2$ in Eqs. (4.23)–(4.25) we have

$$\alpha_4(6yv-10y^3-y_{xx})+2\alpha_3(v-3y^2)-4\alpha_2y+4u=\alpha x, \tag{4.26}$$

$$\alpha_4(\tfrac{1}{2}v_{xx}-\tfrac{3}{2}v^2-5yy_{xx}-\tfrac{5}{2}y_x^2-\tfrac{35}{2}y^4+15vy^2)+\alpha_3(6yv-10y^3-y_{xx})+2\alpha_2(v-3y^2)+\alpha_0 =\alpha xy, \tag{4.27}$$

$$2vu^2-uu_{xx}+\tfrac{1}{2}u_x^2+\delta=0. \tag{4.28}$$

Theorem 4.1: *Special solutions of the system of equations (4.27) and (4.28) are expressed via the general solutions of the P_2 and P_4 equations.*

Proof: Assuming $\alpha_4=\alpha_3=0$ and $\alpha_1=0$ in Eqs. (4.26) and (4.27) we have

$$4u-4\alpha_2 y-\alpha x=0, \tag{4.29}$$

$$2\alpha_2(v-3y^2)+\alpha_4=\alpha xy. \tag{4.30}$$

Substituting $y(x)$ from Eq. (4.29) into (4.30) we have

$$v(x)=-\frac{1}{16\alpha_2^2}(\alpha^2x^2-16\alpha xu+48u^2-8\alpha_0\alpha_2). \tag{4.31}$$

Assuming $\alpha_4=0$ in Eq. (4.26) we have the system of equations that was studied recently in Ref. 24.

Substituting $v(x)$ from Eq. (4.31) into (4.28) we obtain the fourth Painlevé equation in the form

$$u_{xx}-\frac{u_x^2}{2u}-\frac{\delta}{u}+\frac{\alpha_4 u}{\alpha_2}+\frac{1}{\alpha_2^2}\left(2\alpha xu^2-6u^3-\frac{1}{8}\alpha^2x^2u\right)=0. \tag{4.32}$$

Assuming $u(x)=0$, $\delta=0$ in Eqs. (4.26) and (4.28) we have

$$\alpha_4\left(\frac{y_{xxxx}}{y}-2\frac{y_xy_{xxx}}{y^2}+2\frac{y_x^2y_{xx}}{y^3}-10y_x^2-\frac{3y_{xx}^2}{2y^2}-20yy_{xx}+40y^4\right)$$
$$+\alpha_1\left(8xy-\frac{xy_{xx}}{y^2}-\frac{2y_x}{y^2}+\frac{2xy_x^2}{y^3}\right)+12\alpha_0-\frac{\alpha^2x^2}{2\alpha_4y^2}=0. \tag{4.33}$$

This equation at $\alpha_4=1$ corresponds to the equation found in Ref. 8. Special solution of Eq. (4.33) is expressed by the second Painlevé equation and consequently special solutions of the system of equations (4.26)–(4.28) are expressed by the general solutions of the P_2 and P_4 equation. □

Corollary 4.1: The P_2 and P_4 are special cases of the system of equations (4.26) and (4.27).

The isomonodromic linear problem for the system of equations (4.26)–(4.28) is determined by Eqs. (4.6).

Case 4.3: $\omega(\lambda)=\omega_0\lambda^2$. Assuming $\omega(\lambda)=\omega_0\lambda^2$ in Eq. (4.1) we have that equations for $a_k(x)$ $(k=0,1,\ldots,n-3)$ coincide with Eqs. (4.3)–(4.5). We obtain additionally four equations

$$2P_xa_{n-3}+4Pa_{n-3,x}-a_{n-3,xxx}-8ya_{n-2,x}-4ya_{n-2,x}+4a_{n-1,x}-2\omega_0=0, \tag{4.34}$$

$$2P_xa_{n-2}+4Pa_{n-2,x}-a_{n-2,xxx}-8ya_{n-1,x}-4ya_{n-1,x}+4a_{n,x}+2\omega_0y=0, \tag{4.35}$$

$$2P_xa_{n-1}+4Pa_{n-1,x}-a_{n-1,xxx}-8ya_{n,x}-4y_xa_n=0, \tag{4.36}$$

$$2Pa_n^2-a_na_{n,xx}+\tfrac{1}{2}a_{n,x}^2+c_{n+2}=0. \tag{4.37}$$

Equation (4.37) corresponds to (4.21) This one was found after integration. Equation (4.36) can be also integrated if we take into account Eq. (2.10) at $\omega(\lambda)=\omega_0\lambda^2$. As a result we have

$$a_{n,xx}a_{n-1}+a_{n-1,xx}a_n-4ya_n^2-a_{n,x}a_{n-1,x}-4Pa_na_{n-1}-c_{n+1}=0, \tag{4.38}$$

where c_{n+1} is an arbitrary constant.

Let us consider Eqs. (4.34) and (4.35) at $n=3$. We obtain $a_0(x)$ and $a_1(x)$ by formulas (4.1) and (4.2). From Eq. (4.34) we get

$$a_2(x)=\tfrac{3}{2}c_0y^2+c_1y-\tfrac{1}{2}c_0P+\tfrac{1}{2}\omega_0x+c_2. \tag{4.39}$$

Equation (4.35) can also be integrated. We have

$$4a_3-10c_0y^3-6c_1y^2+6c_0yP-c_0y_{xx}+2c_1P-4c_2y-2\omega_0xy-4c_3=0. \tag{4.40}$$

Equation (4.38) at $n=3$ takes the form

$$4ya_3^2+a_2a_{3,xx}+a_3a_{2,xx}-a_{3,x}a_{2,x}-4Pa_2a_3-c_4=0. \tag{4.41}$$

Denoting $c_i=\alpha_{4-i}$ $(i=0,1,2,3,4)$, $c_5=-\delta$, $P(x)=v(x)$, $a_3(x)=u(x)$, $\omega_0=2\alpha$ from Eqs. (4.37), (4.40) and (4.41) we have the system of equations in the form

$$\alpha_4(6vy-y_{xx}-10y^3)+2\alpha_3(v-3y^2)-4\alpha_2y-4\alpha_1+4u-4\alpha xy=0, \tag{4.42}$$

$$\begin{aligned}\alpha_4(\tfrac{3}{2}u_{xx}y^2-\tfrac{1}{2}vu_{xx}+3uy_x^2+3uyy_{xx}-\tfrac{1}{2}uv_{xx}-3u_xyy_x+\tfrac{1}{2}u_xv_x-6uvy^2+2uv^2)+\alpha_3(yu_{xx}\\ +uy_{xx}-u_xy_x-4uyv)+\alpha_2(u_{xx}-4uv)-\alpha_0+\alpha(xu_{xx}-u_x-4xuv)+4yu^2=0,\end{aligned} \tag{4.43}$$

$$uu_{xx}-\tfrac{1}{2}u_x^2-2vu^2-\delta=0. \tag{4.44}$$

Theorem 4.2: *Special solutions of the system of equations (4.42)–(4.44) are expressed by the general solutions of the P_2, P_4 and P_3 equations.*

Proof: From Eq. (4.43) at $\alpha_4=\alpha_3=\alpha_2=0$ we obtain

$$4u-4\alpha xy-4\alpha_1=0. \tag{4.45}$$

From Eq. (4.45) we have

$$y=\frac{\alpha_1-u}{\alpha x}. \tag{4.46}$$

Substituting (4.43) into Eq. (4.44) at $\alpha_4=\alpha_3=\alpha_2=0$ we get

$$\alpha xu_{xx}-\alpha u_x-4\alpha xuv-\frac{4\alpha_1}{\alpha x}u^2+\frac{4}{\alpha x}u^3-\alpha_0=0. \tag{4.47}$$

One can find $v(x)$ from Eq. (4.47). Then substituting $v(x)$ into Eq. (4.44) we have equation in the form

$$u_{xx}-\frac{u_x^2}{u}+\frac{u_x}{x}+\frac{4\alpha_1}{\alpha^2x^2}u^2-\frac{4}{\alpha^2x^2}u^3-\frac{2\delta}{u}+\frac{\alpha_0}{\alpha x}=0. \tag{4.48}$$

The latter can be transformed to the third Painlevé equation.

Assuming $u(x)=v(x)=0$, $\alpha_3=\alpha_2=\alpha_0=\delta=0$ we have the second Painlevé equation from the system of equations (4.43) and (4.44) in the form

$$\alpha_4y_{xx}+10\alpha_4y^3+4\alpha_1+4\alpha xy=0. \tag{4.49}$$

Assuming $\alpha_4=0$ in the system of equations (4.42)–(4.44) we have a generalization for the P_4 equation. □

Corollary 4.2: The P_2, P_4 and P_3 equations are special cases of the system of equations (4.42)–(4.44).

We have found that the system of equations (4.42)–(4.44) is the generalization of the second and third Painlevé equations.

Case 4.4: $\omega(\lambda)=\omega_0\lambda(\lambda-\lambda_0)$. Let us consider Eq. (2.4) assuming $\omega(\lambda)=\omega_0\lambda(\lambda-\lambda_0)$ and $A(x,\lambda)$ in the form (2.12). Substituting Eq. (2.12) into (2.4) and equating expressions at different λ to zero we have the following set of equations:

$$a_0=c_0, \quad a_1(x)=c_0y+\tfrac{1}{2}\omega_0x+c_1, \tag{4.50}$$

$$a_2(x)=\tfrac{1}{2}\omega_0xy-\tfrac{1}{2}\omega_0\lambda_0x-\tfrac{1}{2}Pc_0+\tfrac{3}{2}c_0y^2+c_1y+c_2. \tag{4.51}$$

We also have two additional integrals

$$\begin{aligned}&c_1a_{2,xx}+c_0ya_{2,xx}-\tfrac{1}{2}\omega_0a_{2,x}-4Pa_2yc_0+\tfrac{1}{2}\omega_0xa_{2,xx}+c_0a_2y_{xx}-2\omega_0xPa_2\\&\quad-c_0a_{2,x}y_x-4c_1Pa_2+(c_0a_{2,xx}-\tfrac{1}{2}\omega_0^2x^2P+c_0c_1y_{xx}-2c_0^2Py^2+c_0^2yy_{xx}-4c_1c_0Py\\&\quad-\tfrac{1}{2}c_0^2y_x^2-2c_1\omega_0xP-2c_0Py\omega_0x-2c_1^2P+\tfrac{1}{2}c_0\omega_0xy_{xx}-4c_0Pa_2-\tfrac{1}{2}c_0\omega_0y_x-\tfrac{1}{8}\omega_0^2)\lambda_0\\&\quad+(c_0^2y_{xx}-4c_0^2yP-2c_0\omega_0xP-4c_0c_1P)\lambda_0^2-2\lambda_0^3c_0^2P+c_3=0,\end{aligned} \tag{4.52}$$

$$a_2a_{2,xx}-\tfrac{1}{2}a_{2,x}^2-2Pa_2^2+c_4=0. \tag{4.53}$$

Denoting $P(x)=v(x)$, $a_2(x)=u(x)$, $c_0=\alpha_3$, $c_1=0$, $c_2=\alpha_2$, $c_4=\delta$, $\omega_0=4\alpha$, $\lambda_0=\beta$, $c_2=\alpha_2$ we obtain from Eqs. (4.51)–(4.53) the system of equations

$$2\alpha x(y-\beta)+\tfrac{1}{2}\alpha_3(3y^2-v)-u+\alpha_2=0, \tag{4.54}$$

$$uu_{xx}-\tfrac{1}{2}u_x^2-2u^2v-\delta=0, \tag{4.55}$$

$$\begin{aligned}&\alpha_3(yu_{xx}+uy_{xx}-u_xy_x-4yuv)+\alpha_0+2(xu_{xx}-4uvx-u_x)+\beta\alpha_3^2(yy_{xx}-\tfrac{1}{2}y_x^2-2vy^2)\\&\quad+\beta\alpha_3(u_{xx}-4uv+2\alpha xy_{xx}-2\alpha y_x-8\alpha xyv)-8\beta\alpha^2x^2v\\&\quad+\beta^2\alpha_3(\alpha_3y_{xx}-8\alpha xv-4\alpha_3yv)-2\beta^3\alpha_3^2v=0.\end{aligned} \tag{4.56}$$

Assuming $\beta=0$ we get the system of equations (4.27) and (4.28) of Ref. 8. Assuming $\alpha_3=0$ in (4.54)–(4.56) we have

$$u(x)=2\alpha xy-2\alpha\beta x+\alpha_2, \tag{4.57}$$

$$u_{xx}+\frac{2\beta\alpha xu_{xx}}{u}+\frac{u_x}{x}-\frac{u_x^2}{u}-\frac{\beta\alpha xu_x^2}{u^2}+\frac{\alpha\beta}{x}-\frac{\alpha_3}{2\alpha x}-\frac{2\delta}{u}-\frac{2\alpha\beta\delta x}{u^2}=0. \tag{4.58}$$

The latter system of equations can be transformed to the fifth Painlevé equation. Therefore the system of equations (4.54)–(4.56) is a generalization of the fifth Painlevé equation.

Let us present here the system of equations in the case $\omega(\lambda)=\omega_0\lambda(\lambda-\lambda_0)$ at $n=3$. Denoting $C_0=\alpha_4$, $c_1=c_2=0$, $c_3=\alpha_1$, $c_4=\alpha_0$, $c_5=16\delta$, $P(x)=v(x)$, $a_3(x)=u(x)$ we have the following system of equations:

$$\alpha_4(y_{xx}+10y^3-6vy)+\alpha x(y-\beta)-2u=0, \tag{4.59}$$

$$uu_{xx}-\tfrac{1}{2}u_x^2-2vu^2+\delta=0, \tag{4.60}$$

$$\alpha_4(6yuy_{xx}+4uv^2+3y^2u_{xx}+u_xv_x+6uy_x^2-uv_{xx}-vu_{xx}-12uvy^2-6yy_xu_x)+\tfrac{1}{4}\alpha(xu_{xx}-u_x-4xuy)+4yu^2+\alpha_0+\beta B_1+\beta^2B_2+\beta B_3+\beta^4B_4-2\alpha_4\alpha x\beta^5=0, \tag{4.61}$$

where

$$B_1=\alpha_4(2uy_{xx}-2u_xy_x+2yu_{xx}+24uy^3+\tfrac{1}{4}\alpha v_x-\tfrac{3}{2}\alpha yy_x-3\alpha xvy^2-16vuy+\tfrac{3}{2}\alpha xyy_{xx}+\tfrac{3}{2}\alpha xy_x^2-\tfrac{1}{4}\alpha xv_{xx}+\alpha xv^2)+\alpha_4^2(12v^2y^2+18y^3y_{xx}-6vy_x^2-3y^2v_{xx}-18vy^4+vv_{xx}-2v^3-\tfrac{1}{2}v_x^2+6yy_xv_x-6vyy_{xx})-\tfrac{1}{8}\alpha^2x^2v-2u^2+2\alpha xyu, \tag{4.62}$$

$$B_2=\alpha_4(2u_{xx}-4uv+4uy^2-4\alpha xyv-\tfrac{1}{2}\alpha y_x+6\alpha xy^3+\tfrac{1}{2}\alpha xy_{xx})+\alpha_4^2(36y^5+2y_xv_x-2vy_{xx}-2yv_{xx}+18y^2y_{xx}+12yv^2-48vy^3)-\alpha xu+\tfrac{1}{4}\alpha^2x^2y, \tag{4.63}$$

$$B_3=\alpha_4(\alpha xy^2+8yu-\alpha xv)+\alpha_4^2(6v^2+16yy_{xx}+10y_x^2+30y^4-36vy^2-2v_{xx})-\tfrac{1}{8}\alpha^2x^2, \tag{4.64}$$

$$B_4=\alpha_4(2\alpha xy-8u)+\alpha_4^2(40y^3+4y_{xx}-24vy). \tag{4.65}$$

Thus we have the following theorem.

Theorem 4.3: *Special solutions of the system of equations (4.59)–(4.61) are expressed via the general solution of the P_2, P_4, P_3 and P_5 equations.*

Proof: It is clear this system of equations is a generalization of case $\omega(\lambda)=\omega_0\lambda^2$. Assuming $\lambda_0=0$ in this sixth ODE we have case 4.3. However, assuming $n=1$ in Eq. (2.13) we have the system of equations (4.57) and (4.58) that is transformed to the P_5 equation. □

We also have the corollary.

Corollary 4.3: The P_2, P_4, P_3 and P_5 equations are special cases of this new system of equations (4.59)–(4.61).

Taking into account the above mentioned equations one can see how to construct other equations with potential (2.9).

V. CONCLUSION

Let us summarize the results presented in the article. Using the compatibility condition corresponding to the Painlevé equations we found several new hierarchies that generalize the Painlevé equations. In essence we considered two isomonodromic linear problems (2.1) and (2.6) that can be written as the compatibility condition (2.4). Then we obtained two types of generalizations for the Painlevé equations. One of these generalizations corresponds to the P_1, P_{34}, P_2, P_3^*, and P_5^* equations. Another generalization was found for the P_2, P_4, P_3, and P_5 equations.

We observed that the above mentioned Painlevé equations are special cases of the hierarchies found. Particular attention has been given to the sixth order nonlinear ordinary differential equations. We showed that there are sixth order nonlinear equations that generalize the P_1, P_{34}, P_2, P_3^*, and P_5^* equations. However, there are also sixth order equations that are the generalizations of the P_2, P_4, P_3, and P_5 equations.

We have not investigated all Eqs. (3.12), (3.29), (3.69) and other new ordinary differential equations on the Painlevé property taking into account the singularity analysis. Some of the fourth order ordinary differential equations were checked before in Refs. 5, 8, 2, and 23. However, no doubt all equations have the Painlevé property because the Cauchy problems for all these equations can be solved by the inverse monodromy transform.

All nonlinear ordinary differential equations of this work are important because we hope that these equations give new transcendental functions with respect to constants of integration. Some of the fourth order ordinary differential equations from hierarchies (3.12) and (3.29) were proved

to have general solutions in the form of essentially transcendental functions and they do not have any first integrals in the polynomial form.[21,22] Now we need to prove the irreducibility of higher order analogies of the Painlevé equations. For the second order Painlevé equations the notions of irreducibility and essentially transcendental dependence on the initial conditions are equivalent but so far we have not found proof of equivalence at higher orders. It is unlikely that all higher order analogies of Painlevé equations presented in this work depend on the Painlevé transcendents but we need to have the strong proof of this fact. We think it will be the most important problem for the higher order analogies of the Painlevé equations in future.

In the study of the Painlevé equations before we thought that every Painlevé equation can be included in the corresponding hierarchy. In fact, we could observe such situation for the first and second Painlevé hierarchies. However, we can see from the results of this work there are hierarchies that generalize several Painlevé equations. It is difficult to say about Painlevé hierarchy in this case.

The results of this article allow us to assume the conjecture that there are higher order nonlinear equations that include all Painlevé equations corresponding to the concrete isomonodromic linear problem. More than that we believe there are the general solutions of the higher order ordinary differential equations in the form of the transcendental functions with respect to constants of integration that contain the Painlevé transcendents of definite class as special cases. These general transcendents can be found as solutions of the Cauchy problems by means of the inverse monodromy transform from the linear problems corresponding to the higher order ordinary differential equations.

ACKNOWLEDGMENTS

This work was supported by the International Science and Technology Center under Project No. 1339-2. This material is partially based upon work supported by the Russian Foundation for Basic Research under Grant No. 01-01-00693.

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Multivariable orthogonal polynomials associated with tensor products of the oscillator algebra $\mathfrak{b}(1)$

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(Received 19 November 2002; accepted 26 August 2003)

It is well known that the tensor product of $n+1$ lowest weight representations of (a generalization of) the oscillator algebra $\mathfrak{b}(1)$ can be depicted by a binary coupling tree. With each such binary coupling tree, we associate a polynomial $R_l^{(h)}(x)$ that will turn out to be an n-variable Hermite polynomial. We prove that the polynomials $R_l^{(h)}(x)$ associated with a fixed binary coupling tree are orthogonal over the n-dimensional real space for some weight function, which is independent of the shape of the considered binary coupling tree. The connection coefficients expressing a polynomial associated with a given binary coupling in terms of polynomials associated with another binary coupling tree are the $3nj$-coefficients of $\mathfrak{b}(1)$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1621059]

I. INTRODUCTION

General recoupling coefficients or $3nj$-coefficients of Lie algebras play an important role in theoretical physics, but also have many mathematical applications, e.g., the $3j$ and $6j$ coefficients of $\mathfrak{su}(2)$ exhibit a close relationship with Hahn and Racah polynomials.[1,2] In Ref. 3 Granovskiĭ and Zhedanov give a new method for the construction of $3nj$-symbols. In Ref. 4 their method was applied to the Lie algebras $\mathfrak{su}(1,1)$ and $\mathfrak{b}(1)$ to find addition formulas for various orthogonal polynomials. Generalizing the most important formulas in this article, we showed in Ref. 5 that one can associate multivariable Jacobi and continuous Hahn polynomials with tensor products of positive discrete series representations of the Lie algebra $\mathfrak{su}(1,1)$. A convenient way to describe the order of taking these tensor products (or couplings) is the use of binary coupling trees (see Ref. 6, Topic 12 and Refs. 7 and 8. We will use tree terminology (e.g., leaf nodes, root node, subtree,...) that should be self-explanatory, but if in doubt see Ref. 9.

In this article, we will follow the same technique as in Ref. 5 to find multivariable Hermite polynomials that are associated with tensor products of lowest weight representations of (an extension of) the oscillator algebra. We will show that these multivariable Hermite polynomials are orthogonal on $\mathbb{R}^n$ for a certain weight function that is independent of the order of taking tensor products, although the polynomials themselves are dependent on this order. The connection coefficients between the different classes of polynomials will turn out to be (just as in Ref. 5) the $3nj$-coefficients of the oscillator algebra.

In general, orthogonal polynomials in several variables give rise to certain difficulties that are not present in the one variable situation. For example, orthogonal polynomials in n variables are no longer uniquely defined by the region Ω and the weight function on the region. This is closely related to the fact that there is no obvious natural order for polynomials in several variables.

The space of all polynomials in the variables $x_1,\ldots,x_n$ with real coefficients is denoted $\mathbb{R}[x_1,\ldots,x_n]$ or Π^n for short. The degree of a polynomial $P\in\Pi^n$ is the highest degree of any of its monomials. Let $\langle\cdot,\cdot\rangle$ be an inner product defined on Π^n. Then P is an orthogonal polynomial if $\langle P,Q\rangle=0$ for all polynomials Q with $\deg Q<\deg P$. This definition does not require that P is orthogonal with other (orthogonal) polynomials of the same degree.

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In our case the inner product will be defined in terms of some (classical) weight function W on some (classical) region Ω in $\mathbb{R}^n$: $\langle P,Q\rangle=\int_\Omega P(x)Q(x)W(x)\,dx$.

The rest of this article is organized as follows: In Sec. II we give the definition of the Lie algebra $\mathfrak{b}(1)$ and a class of representations, together with expressions for its Clebsch–Gordan and Racah coefficients. In Sec. III the method of Granovskiĭ and Zhedanov is briefly explained and a (new) addition formula for Meixner polynomials is found. Whereas in Sec. III we confine ourselves to the tensor product of three representations, we turn in Sec. IV to the multivariable case. We explain how to associate a multivariable Hermite polynomial to a binary coupling tree and prove the orthogonality of these polynomials. In the last section, we show how this leads to an integral formula for $3nj$-coefficients of $\mathfrak{b}(1)$.

We conclude this introduction with some notational conventions. The notation for (generalized) hypergeometric functions is the standard one:[10,11]

$$ {}_pF_q\left(\begin{matrix}a_1,\ldots,a_p\\ b_1,\ldots,b_q\end{matrix};\ z\right)=\sum_{k=0}^{\infty}\frac{(a_1)_k\cdots(a_p)_k}{(b_1)_k\cdots(b_q)_k}\frac{z^k}{k!}, \tag{1}$$

with $(a)_k$ the Pochhammer symbol: $(a)_k=a(a+1)\cdots(a+k-1)$ for $k>0$, and $(a)_0=1$. Convergence issues will not arise since all the hypergeometric functions in this article are terminating (i.e., one of the numerator parameters is a negative integer). Furthermore, for the one-dimensional orthogonal polynomials appearing in this article, we will adopt the notation and normalization of Ref. 12. In particular, we denote the Hermite polynomials by $H_n(x)$, with

$$ H_n(x)=(2x)^n\,{}_2F_0\left(\begin{matrix}-n/2,-(n-1)/2\\ -\end{matrix};-\frac{1}{x^2}\right). \tag{2}$$

These are orthogonal on $\mathbb{R}$ for the weight function $\exp(-x^2)$:

$$ \int_{-\infty}^{\infty}H_n(x)H_m(x)e^{-x^2}\,dx=\sqrt{\pi}2^n n!\,\delta_{n,m}. \tag{3}$$

II. THE LIE ALGEBRA $\mathfrak{b}(1)$ AND TENSOR PRODUCTS FOR A CLASS OF REPRESENTATIONS

The Lie algebra $\mathfrak{b}(1)$[4,13] is four-dimensional, with basis elements $b^{\pm}$, H and N subject to the relations

$$ [b^-,b^+]=H,\quad [N,b^{\pm}]=\pm b^{\pm}\ \text{ and }\ [H,x]=0,\ \text{ for }\ x=b^{\pm},N, \tag{4}$$

where the basis elements obey the following unitary conditions $H^\dagger=H$, $N^\dagger=N$ and $(b^{\pm})^\dagger=b^{\mp}$. [More precisely, the Lie algebra $\mathfrak{b}(1)$ is a $\star$-algebra with $\star$-operation defined by $H^\star=H$, $N^\star=N$ and $(b^{\pm})^\star=b^{\mp}$; then the representation operators corresponding to the Lie algebra elements satisfy the same conjugacy properties in the $\star$-representations considered here.]

It is well known that this Lie algebra has a class of lowest weight representations,[13] characterized by two positive numbers h and k. These representations are infinite dimensional and have a set of orthonormal basis vectors $|h,k,n\rangle$, with $n=0,1,2,\ldots$. The action of the operators corresponding to the Lie algebra basis elements on these basis vectors is given by

$$\begin{aligned} H|h,k,n\rangle&=h|h,k,n\rangle,\\ N|h,k,n\rangle&=(k+n)|h,k,n\rangle,\\ b^-|h,k,n\rangle&=\sqrt{hn}|h,k,n-1\rangle,\\ b^+|h,k,n\rangle&=\sqrt{h(n+1)}|h,k,n+1\rangle. \end{aligned} \tag{5}$$

One can verify that these representations are unitary and irreducible when $h>0$ and $k\geqslant 0$.

Taking the tensor product of two such unitary and irreducible representations (h_1,k_1) and (h_2,k_2) gives again a unitary representation that is completely reducible into representations of the same type:

$$(h_1,k_1)\otimes(h_2,k_2)=\bigoplus_{j=0}^{\infty}(h_1+h_2,k_1+k_2+j). \tag{6}$$

We note that the h-labels are simply additive and that the difference between the resulting and consisting k-labels is a non-negative integer.

Now, one can express a basis vector $|h_1+h_2,k_1+k_2+j,n\rangle$ in terms of tensor product vectors $|h_1,k_1,n_1\rangle\otimes|h_2,k_2,n_2\rangle$. The coefficients accomplishing this connection are called the Clebsch–Gordan coefficients. Explicitly one has, in an obvious notation with $k_{12}=k_1+k_2+j$,

$$\begin{aligned}|(h_1,h_2),k_{12},n\rangle&\equiv|(h_1,k_1;h_2,k_2)h_1+h_2,k_1+k_2+j,n\rangle\\&=\sum_{n_1,n_2}C^{h_1,h_2,j}_{n_1,n_2,n}|h_1,k_1,n_1\rangle\otimes|h_2,k_2,n_2\rangle,\end{aligned} \tag{7}$$

where the sum is over all positive integers n_1 and n_2 such that $n_1+n_2=n+j$. The labels k_1 and k_2 have been omitted from the notation of the Clebsch–Gordan coefficients as they are independent of them (Ref. 4, Sec. VI). An explicit expression is given by

$$C^{h_1,h_2,j}_{n_1,n_2,n}=\delta_{n_1+n_2,j+n}(-1)^{n_2}\frac{(n_1+n_2)!a^{n+n_2}b^{n_1-n}}{\sqrt{n_1!n_2!j!n!}}{}_2F_1\left(\begin{matrix}-n,-n_2\\-j-n\end{matrix};\frac{1}{a^2}\right), \tag{8}$$

with

$$a=\sqrt{\frac{h_1}{h_1+h_2}},\quad b=\sqrt{\frac{h_2}{h_1+h_2}},\quad\text{and thus}\quad a^2+b^2=1. \tag{9}$$

We remark that although the denominator parameter in (8) is a negative integer, the hypergeometric notation is still well-defined because the denominator parameter is smaller than the numerator parameters, which determine the termination.

The tensor product of three representations (h_1,k_1), (h_2,k_2), and (h_3,k_3) can be formed in two different ways:

$$((h_1,k_1)\otimes(h_2,k_2))\otimes(h_3,k_3),\quad\text{and}\quad(h_1,k_1)\otimes((h_2,k_2)\otimes(h_3,k_3)). \tag{10}$$

The coefficients relating the two coupled bases, for which the notation is self-explanatory, are called the recoupling or Racah coefficients:

$$|((h_1,h_2)h_3),k_{12},k,n\rangle=\sum_{k_{23}=k_2+k_3}^{k-k_1}{}_{h_1,h_2,h_3}U^{k_1,k_2,k_{12}}_{k_3,k,k_{23}}|(h_1(h_2,h_3)),k_{23},k,n\rangle. \tag{11}$$

This representation of the Lie algebra $\mathfrak{b}(1)$ has the remarkable property that its Racah coefficients are of the same type as its Clebsch–Gordan coefficients (Ref. 4, Sec. VII). One has

$${}_{h_1,h_2,h_3}U^{k_1,k_2,k_{12}}_{k_3,k,k_{23}}=(-1)^{j_{12}}\frac{(j+j_{12})!\tilde{a}^{j_{12}+j'}\tilde{b}^{j-j'}}{\sqrt{j_{12}!j_{23}!j!j'!}}{}_2F_1\left(\begin{matrix}-j_{12},-j'\\-j_{12}-j\end{matrix};\frac{1}{\tilde{a}^2}\right), \tag{12}$$

with

$$\tilde{a}=\sqrt{\frac{h_1h_3}{(h_1+h_2)(h_2+h_3)}},\quad \tilde{b}=\sqrt{\frac{h_2(h_1+h_2+h_3)}{(h_1+h_2)(h_2+h_3)}},\quad \text{and thus also } \tilde{a}^2+\tilde{b}^2=1. \tag{13}$$

Moreover, we denoted the non-negative integer differences by

$$j_{12}=k_{12}-k_1-k_2,\ \ j=k-k_{12}-k_3,\ \ j_{23}=k_{23}-k_2-k_3,\ \text{ and }\ j'=k-k_1-k_{23}, \tag{14}$$

and thus $j_{12}+j=j_{23}+j'$. We remark that the recoupling coefficients are only dependent on these integer differences (and not on the k-labels themselves). We choose, however, to adopt a notation for the recoupling coefficients of $\mathfrak{b}(1)$ that resembles that of the recoupling coefficients of $\mathfrak{su}(1,1)$ in Ref. 5.

It is known[1] (and also immediately clear from the expressions given here) that both the Clebsch–Gordan and Racah coefficients of $\mathfrak{b}(1)$ can be written in terms of the Krawtchouk polynomials.[12]

III. CONSTRUCTION OF CONVOLUTION IDENTITIES

In the seminal paper[3] a new method for the construction of $3nj$-symbols was introduced and applied to the $\mathfrak{su}(1,1)$ case. This method can be extended to other Lie algebras, and in Ref. 14 it was used to derive a generating function for the $9j$-symbols of the oscillator algebra. In Refs. 4 and 15 this method was used to find addition formulas or convolution identities for orthogonal polynomials.

In short, starting with a certain operator X acting on the representation space of the Lie algebra, one finds a quantity $Q_n(x)$ that is the remainder of the overlap coefficient between an eigenvector of X and the basis vector $|n\rangle$ after factoring out the ''zero-amplitude'' part, e.g., in the $\mathfrak{b}(1)$ case

$$\langle h,k,x|h,k,n\rangle=\langle h,k,x|h,k,0\rangle Q_n(x;h,k). \tag{15}$$

For certain choices of X, the quantity Q will be a classical orthogonal polynomial. However, this need not be so, and interesting applications exist without Q being an orthogonal polynomial.[14] Next, one uses this polynomial Q and the (zero-amplitude) Clebsch–Gordan coefficients of the considered Lie algebra to define a two-variable polynomial $S_j(x_1,x_2)$ that satisfies the important relation [written down for the $\mathfrak{b}(1)$ case]

$$\begin{aligned}&S^{k_1,k_2}_{k_{12}-k_1-k_2}(x_1,x_2;h_1,h_2)S^{k_{12},k_3}_{k-k_{12}-k_3}(x_1+x_2,x_3;h_1+h_2,h_3)\\&\quad=\sum_{k_{23}=k_2+k_3}^{k-k_1}{}_{h_1,h_2,h_3}U^{k_1,k_2,k_{12}}_{k_3,k,k_{23}}S^{k_1,k_{23}}_{k-k_1-k_{23}}(x_1,x_2+x_3;h_1,h_2+h_3)S^{k_2,k_3}_{k_{23}-k_2-k_3}(x_2,x_3;h_2,h_3).\end{aligned} \tag{16}$$

In Ref. 4 it was deduced that, when choosing $X=b^+ +b^-$, the expression for the polynomial S is given by

$$S^{(k_1,k_2)}_j(x_1,x_2;h_1,h_2)=\frac{1}{\sqrt{2^j j!}}H_j\left(\sqrt{\frac{h_2}{2h_1(h_1+h_2)}}x_1-\sqrt{\frac{h_1}{2h_2(h_1+h_2)}}x_2\right). \tag{17}$$

Using the expressions (17) and (12) in (16) yields (after some simple renamings) the following identity for Hermite polynomials (Ref. 4, Formula 6.16):

$$H_j(av_1+bv_2)H_n(-bv_1+av_2)=\sum_{k=0}^{j+n}\binom{j+n}{k}a^{n+k}b^{j-k}\,{}_2F_1\left(\begin{matrix}-n,-k\\-j-n\end{matrix};\frac{1}{a^2}\right)H_k(v_1)H_{j+n-k}(v_2), \tag{18}$$

with $a^2+b^2=1$.

Remark 1: Note that in (18) the variables of the Hermite polynomials on the left side are an orthogonal transformation of the variables on the right side. ■

Remark 2: Recently Wünsche[16,17] inspired by the following (alternative) definition of the Hermite polynomials,

$$H_m(x)=\exp\left(-\frac{1}{4}\frac{\partial^2}{\partial x^2}\right)(2x)^m, \tag{19}$$

introduced his so-called Hermite 2D polynomials

$$H_{m,n}(A;x,y)=\exp\left(-\frac{1}{4}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\right)(2x')^m(2y')^n, \tag{20}$$

where

$$\begin{pmatrix}x'\\y'\end{pmatrix}=A\begin{pmatrix}x\\y\end{pmatrix}. \tag{21}$$

Herein, A is an arbitrary two-dimensional matrix. Wünsche gave three different representations for the Hermite 2D polynomials. From one of them (Ref. 16, Formula 2.11), it can be seen that the left hand side of (18) coincides with a Hermite 2D polynomial, provided A is an orthogonal matrix. In this light it turns out that (18) is a special case of the representation (Ref. 16, Formula 2.8) for Hermite 2D polynomials. ■

It is interesting to investigate the Granovskiĭ and Zhedanov method for another form for the operator X. Let $X=H+N+b^+ +b^-$ (more general choices lead essentially to the same result); in this case one identifies (by considering its three-term recurrence) the polynomial Q as being a Charlier polynomial:[12]

$$Q_n(x;h,k)=(-1)^n\sqrt{\frac{h^n}{n!}}C_n(x-k;h)=(-1)^n\sqrt{\frac{h^n}{n!}}\,{}_2F_0\left(\begin{matrix}-n,-x+k\\-\end{matrix};-\frac{1}{h}\right). \tag{22}$$

Using the definition of the S-polynomial

$$S_j^{k_1,k_2}(x_1,x_2;h_1,h_2)=\sum_{n_1+n_2=j}C_{n_1,n_2,0}^{h_1,h_2,j}\,Q_{n_1}(x_1;h_1,k_1)Q_{n_2}(x_2;h_2,k_2), \tag{23}$$

and the easily verified identity (expand the two hypergeometric series on the left side, interchange the order of summation and apply the binomial theorem)

$$\sum_{n_1+n_2=j}\frac{(-1)^{n_2}}{n_1!n_2!}\,{}_2F_0\left(\begin{matrix}-n_1,y_1\\-\end{matrix};a_1\right)\,{}_2F_0\left(\begin{matrix}-n_2,y_2\\-\end{matrix};a_2\right)=(a_2)^j\frac{(y_2)_j}{j!}\,{}_2F_1\left(\begin{matrix}-j,y_1\\1-y_2-j\end{matrix};-\frac{a_1}{a_2}\right), \tag{24}$$

we arrive at the following explicit expression for S (which we, for distinction with the Hermite case, denote by $\mathcal{S}$):

$$\mathcal{S}_j^{k_1,k_2}(x_1,x_2;h_1,h_2)=\sqrt{\frac{h_1^j}{j!(h_1+h_2)^jh_2^j}}(k_2-x_2)_j\,{}_2F_1\left(\begin{matrix}-j,k_1-x_1\\1-j-k_2+x_2\end{matrix};-\frac{h_2}{h_1}\right) \tag{25}$$

$$=\sqrt{\frac{h_1^j}{j!(h_1+h_2)^jh_2^j}}(k_1+k_2-x_1-x_2)_j\,{}_2F_1\left(\begin{matrix}-j,k_1-x_1\\k_1+k_2-x_1-x_2\end{matrix};1+\frac{h_2}{h_1}\right). \tag{26}$$

It is thus clear that in this case the $\mathcal{S}$-polynomial can be written in terms of a Meixner polynomial:[12]

$$\mathcal{S}_j^{k_1,k_2}(x_1,x_2;h_1,h_2)$$

$$= \sqrt{\frac{h_1^j}{j!(h_1+h_2)^j h_2^j}}(k_2-x_2)_j\, M_j\left(x_1-k_1;1-j-k_2+x_2,\frac{h_1}{h_1+h_2}\right) \tag{27a}$$

$$= \sqrt{\frac{h_1^j}{j!(h_1+h_2)^j h_2^j}}(k_1+k_2-x_1-x_2)_j\, M_j\left(x_1-k_1;k_1+k_2-x_1-x_2,-\frac{h_1}{h_2}\right). \tag{27b}$$

If we now plug all the basic ingredients into (16), we get a convolution identity for Meixner polynomials.

Theorem 3: *The Meixner polynomials satisfy the following identity:*

$$(1-j+x_2)_j(-s+j)_n M_j\left(x_1;1-j+x_2,\frac{b}{a}\frac{a-1}{b-1}\right)M_n(x_1+x_2-j;-s+j,a)$$

$$=\left(\frac{b}{a}\right)^{j+n}\left(\frac{a}{a-1}\right)^j\sum_{k=0}^{j+n}\binom{j+n}{k}\left(\frac{b-1}{b}\right)^k(-s+k)_{j+n-k}(1-k+x_2)_k$$

$$\times\ {}_2F_1\left(\begin{matrix}-j,-j-n+k\\-j-n\end{matrix};\frac{a}{b}\right)M_{j+n-k}(x_1;-s+k,b)M_k\left(s-x_1-x_2;1-k+x_2,\frac{b-1}{a-1}\right), \tag{28}$$

where s is some (arbitrary) constant.

Remark 4: We have written down two expressions in which the $\mathcal{S}$-polynomials are Meixner polynomials of degree j. There are four more of these expressions. This is because of the 24 Kummer solutions to the Gauss differential equation, there are six of them that have the first numerator parameter (in this case $-j$) fixed (see Ref. 11). ■

Remark 5: From the introductory section it is clear that for the multivariable case, we restrict ourselves to the Hermite case. One may ask oneself why this is the case. The reason is: orthogonality. Indeed if one replaces x_2 by $1-x_1$ in (17) it is immediately clear (and see also next section) that S satisfies an orthogonality relation.

For the $\mathcal{S}$-case things are different. The Meixner polynomials also satisfy a (discrete) orthogonality, namely,

$$\sum_{x=0}^{\infty}\frac{(\beta)_x}{x!}c^x M_m(x;\beta,c)M_n(x;\beta,c)=\frac{c^{-n}n!}{(\beta)_n(1-c)^\beta}\delta_{m,n},\quad \beta>0\ \text{ and }\ 0<c<1. \tag{29}$$

We note that the conditions imposed on β and c are to ensure that the weight function is positive. However, the orthogonality is valid whenever $0<|c|<1$ and β is not a negative integer. We cannot apply this orthogonality: e.g., in the case (27a) the parameter β (after replacing x_2 by $1-x_1$) depends on x_1 which is clearly not allowed; in the case (27b) the parameter c does in general (i.e., for arbitrary values of h_1 and h_2) not meet its requirement $(0<|c|<1)$. The other four ways of writing $\mathcal{S}$ have similar problems. ■

IV. MULTIVARIABLE HERMITE POLYNOMIALS

When working with multivariable Hermite polynomials the classical region of integration is the real n-dimensional space $\mathbb{R}^n$. In Ref. 18, Sec. 2.3.4, the weight function $\exp(-(x_1^2+\cdots+x_n^2))$ is considered and two different orthogonal bases are given. One of them is just a product of n

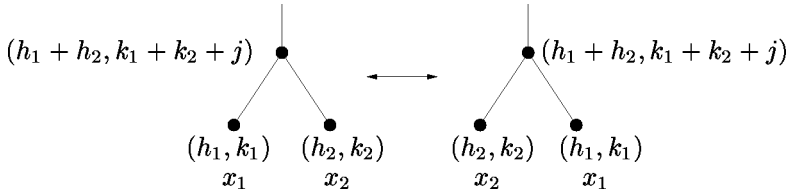

FIG. 1. A twist operation on binary coupling trees.

classical Hermite polynomials. In Ref. 19, Sec. 12.8, another generalization of Hermite polynomials is considered; these are orthogonal with respect to the weight function $\exp(-\varphi(x))$ with $\varphi(x)=\Sigma_{i,j}c_{ij}x_ix_j$ where C is a symmetric, square, and positive definite matrix. The multivariable Hermite polynomials appearing in the $(n+1)$-fold tensor product are orthogonal over $\mathbb{R}^n$ for the weight function

$$\exp(-\psi(x)), \quad \text{with} \quad \psi(x)=(x_1,x_2,\ldots,x_n,s-\sigma(x))A(x_1,x_2,\ldots,x_n,s-\sigma(x))^t, \tag{30a}$$

where $A\in\mathbb{R}^{(n+1)\times(n+1)}$, $\sigma(x)=x_1+\cdots+x_n$ and s some arbitrary constant. Moreover, it will turn out that

$$A_{ij}=\frac{1}{2h_i}\delta_{ij}-\frac{1}{2|h|}, \tag{30b}$$

where $|h|=h_1+\cdots+h_{n+1}$.

We recall the expression for the two-variable S-polynomial (where we have dropped the superscripts k because S is independent of them),

$$S_j(x_1,x_2;h_1,h_2)=\frac{1}{\sqrt{2^j j!}}H_j\left(\sqrt{\frac{h_2}{2h_1(h_1+h_2)}}x_1-\sqrt{\frac{h_1}{2h_2(h_1+h_2)}}x_2\right). \tag{31}$$

Since the Hermite polynomials are even (resp. odd) if their degree is even (resp. odd), the S-polynomials have the following property:

$$S_j(x_1,x_2;h_1,h_2)=(-1)^jS_j(x_2,x_1;h_2,h_1). \tag{32}$$

This property has an interpretation in terms of the twist operation on binary coupling trees[8] (see Fig. 1), which in turn stems from the corresponding property of Clebsch–Gordan coefficients of $\mathfrak{b}(1)$:

$$C^{h_1,h_2,j}_{n_1,n_2,n}=(-1)^jC^{h_2,h_1,j}_{n_2,n_1,n}. \tag{33}$$

(Note that this last equality is just Pfaff's transformation[20] for terminating ${}_2F_1$-series.)

The second identity satisfied by the S-polynomials can be interpreted in terms of the rotation operation on binary coupling trees[8] (see Fig. 2). It is thus related to the two ways in which one can couple three $\mathfrak{b}(1)$ representations. We repeat it here:

$$\begin{aligned}&S_{k_{12}-k_1-k_2}(x_1,x_2;h_1,h_2)S_{k-k_{12}-k_3}(x_1+x_2,x_3;h_1+h_2,h_3)\\&\quad=\sum_{k_{23}=k_2+k_3}^{k-k_1}{}_{h_1,h_2,h_3}U^{k_1,k_2,k_{12}}_{k_3,k,k_{23}}S_{k-k_1-k_{23}}(x_1,x_2+x_3;h_1,h_2+h_3)S_{k_{23}-k_2-k_3}(x_2,x_3;h_2,h_3).\end{aligned} \tag{34}$$

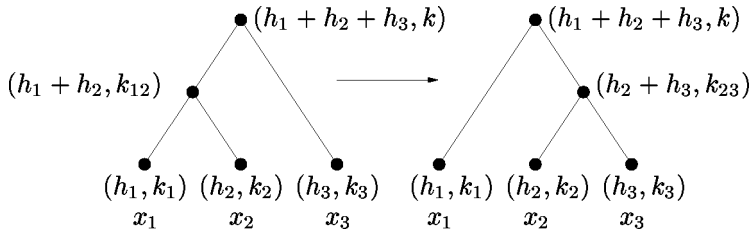

FIG. 2. A rotation on binary coupling trees.

Notice how the left side of (34) follows from the tree on the left side of Fig. 2. With each non-leaf node (i.e., with each intermediate or final coupling) one associates an S-polynomial. The first (resp. second) variable of this S-polynomial is the sum of all the variables associated with the leaves in the left (resp. right) subtree of the considered node. The same applies to the parameters h_i. The (positive integer) lower parameter is the difference between the value of the coupled representation k-label and the consisting k-labels. The S-polynomials on the right side of (34) are formed in the same way but working with the tree on the right side of the figure. The recoupling coefficient appearing in (34) is that associated with a recoupling of three representations as shown in Fig. 2.

Now, we generalize the way the left hand side of (34) is formed and we associate with the tensor product of $n+1$ representations a product of n S-polynomials, each S-polynomial being associated with a non-leaf node of the binary coupling tree. From the decomposition (6) it follows that with each non-leaf node we can associate a non-negative integer. We will denote these by l_i, such that we write $R_l^{(h)}(x)$ for the resulting polynomial. In principle the notation $R_l^{(h)}(x)$ should also contain a reference to its defining binary coupling tree; for the moment however, we are dealing only with arbitrary but fixed trees, so we drop this reference in the notation.

Example 6: Consider the following tensor product of five $b(1)$ representations:

$$(((h_1,k_1)\otimes(h_2,k_2))\otimes(h_3,k_3))\otimes((h_4,k_4)\otimes(h_5,k_5)),$$

depicted by the binary coupling tree in Fig. 3 (where we omitted the additive h-labels).

With this tensor product, we associate the following polynomial:

$$\begin{aligned}
&R^{h_1,h_2,h_3,h_4,h_5}_{l_1,l_2,l_3,l_4}(x_1,x_2,x_3,x_4,x_5)\\
&\quad=S_{l_1}(x_1,x_2;h_1,h_2)S_{l_2}(x_1+x_2,x_3;h_1+h_2,h_3)S_{l_3}(x_4,x_5;h_4,h_5)\\
&\qquad\cdot S_{l_4}(x_1+x_2+x_3,x_4+x_5;h_1+h_2+h_3,h_4+h_5)\\
&\quad=\frac{1}{\sqrt{2^{|l|}l_1!l_2!l_3!l_4!}}H_{l_1}\left(\sqrt{\frac{h_2}{2h_1(h_1+h_2)}}x_1-\sqrt{\frac{h_1}{2h_2(h_1+h_2)}}x_2\right)\\
&\qquad\cdot H_{l_2}\left(\sqrt{\frac{h_3}{2(h_1+h_2)(h_1+h_2+h_3)}}(x_1+x_2)-\sqrt{\frac{h_1+h_2}{2h_3(h_1+h_2+h_3)}}x_3\right)\\
&\qquad\cdot H_{l_3}\left(\sqrt{\frac{h_5}{2h_4(h_4+h_5)}}x_4-\sqrt{\frac{h_4}{2h_5(h_4+h_5)}}x_5\right)\\
&\qquad\cdot H_{l_4}\left(\sqrt{\frac{h_4+h_5}{2(h_1+h_2+h_3)(|h|)}}(x_1+x_2+x_3)-\sqrt{\frac{h_1+h_2+h_3}{2(h_4+h_5)(|h|)}}(x_4+x_5)\right).
\end{aligned}\tag{35}$$

■

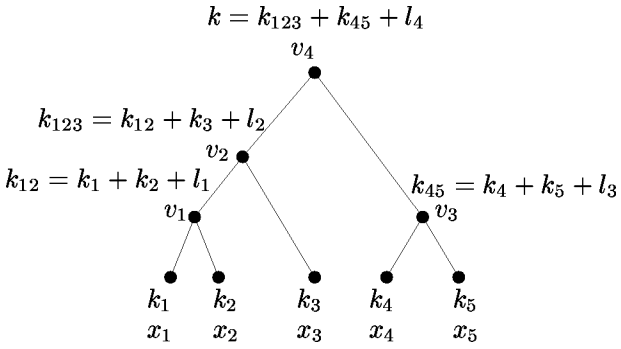

FIG. 3. A binary coupling tree corresponding to the tensor product of five $\mathfrak{b}(1)$ representations.

A. Change of variables

We introduce n new variables v_i, each v_i being the argument of one of the Hermite polynomials in $R_l^{(h)}(x)$. This, however, does not lead to a unique correspondence between the $n+1$ variables x and the n variables v. To this end we introduce a linear constraint between the variables x: $x_1+\cdots+x_n+x_{n+1}=s$ with s some arbitrary constant. Note that this is consistent with the definition of ψ in (30).

The order in which the variables v_i (and integers l_i) are associated to the non-leaf nodes is immaterial, but for the sake of explicitness we do this in post-order.[9]

Example 7: For the tree in Fig. 3 the connection between the variables v and x is the following:

$$\begin{aligned} v_1 &= c_1 x_1 - d_1 x_2, \\ v_2 &= c_2(x_1+x_2) - d_2 x_3, \\ v_3 &= c_3 x_4 - d_3 x_5, \\ v_4 &= c_4(x_1+x_2+x_3) - d_4(x_4+x_5), \\ s &= x_1+x_2+x_3+x_4+x_5. \end{aligned} \tag{36}$$

Here, we have used abbreviations c_i and d_i for the rather tedious combinations of h_i in (35), e.g.,

$$c_2 = \sqrt{\frac{h_3}{2(h_1+h_2)(h_1+h_2+h_3)}} \quad \text{and} \quad d_2 = \sqrt{\frac{h_1+h_2}{2h_3(h_1+h_2+h_3)}}. \tag{37}$$

The equations (36) can also be written in matrix form (setting $s=v_5$):

$$\begin{pmatrix} c_1 & -d_1 & 0 & 0 & 0 \\ c_2 & c_2 & -d_2 & 0 & 0 \\ 0 & 0 & 0 & c_3 & -d_3 \\ c_4 & c_4 & c_4 & -d_4 & -d_4 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{pmatrix}. \tag{38}$$

■

Since the arguments of the Hermite polynomials are linear combinations of the variables x, one can write [because T is nonsingular, see (56)]

$$T \cdot X = V \Leftrightarrow X = T^{-1} \cdot V, \tag{39}$$

where X and V are both column vectors, and $T \in \mathbb{R}^{(n+1)\times(n+1)}$. From (39) it is clear that the kth row of the matrix T concerns the variable v_k, while the ith column concerns the variable x_i. Using the notation c_k and d_k we have

$$T_{ki} = \begin{cases} c_k \text{ if } x_i \text{ is in the left subtree of } v_k, \\ -d_k \text{ if } x_i \text{ is in the right subtree of } v_k \quad \text{for} \quad 1 \leqslant k \leqslant n \quad \text{and} \quad 1 \leqslant i \leqslant n+1, \\ 0 \text{ otherwise,} \end{cases} \tag{40a}$$

and

$$T_{n+1,i} = 1 \qquad \text{for} \quad 1 \leqslant i \leqslant n+1. \tag{40b}$$

The last row of T corresponds of course to the constraint $x_1 + \cdots + x_{n+1} = s = v_{n+1}$.

Making the notation c_k and d_k explicit we have

$$c_k = \sqrt{\frac{\sum_{\substack{\text{right leaves} \\ \text{of } v_k}} h_i}{2\left(\sum_{\substack{\text{left leaves} \\ \text{of } v_k}} h_i\right)\left(\sum_{\substack{\text{all leaves} \\ \text{of } v_k}} h_i\right)}}, \quad \text{and} \quad d_k = \sqrt{\frac{\sum_{\substack{\text{left leaves} \\ \text{of } v_k}} h_i}{2\left(\sum_{\substack{\text{right leaves} \\ \text{of } v_k}} h_i\right)\left(\sum_{\substack{\text{all leaves} \\ \text{of } v_k}} h_i\right)}}. \tag{41}$$

When the R-polynomial is transformed using (39) it becomes, by definition of the transformation, a product of n independent Hermite polynomials. The orthogonality for the Hermite polynomials will be applicable provided that $\psi(x)$ of (30) transforms into $v_1^2 + \cdots + v_n^2$, i.e.,

$$(x_1,\ldots,x_{n+1})A(x_1,\ldots,x_{n+1})^t = (v_1,\ldots,v_{n+1})(T^{-1})^t A T^{-1}(v_1,\ldots,v_{n+1})^t = v_1^2 + \cdots + v_n^2. \tag{42}$$

This, in turn, is equivalent to

$$(T^{-1})^t A T^{-1} = \begin{pmatrix} I_n & \mathcal{O}_{n\times 1} \\ \mathcal{O}_{1\times n} & 0 \end{pmatrix} \Leftrightarrow A = T^t \begin{pmatrix} I_n & \mathcal{O}_{n\times 1} \\ \mathcal{O}_{1\times n} & 0 \end{pmatrix} T, \tag{43}$$

where I_n denotes the identity matrix of order n and $\mathcal{O}_{n\times m}$ is the zero-matrix of the given order. This last equality provides us a way for calculating the explicit form of the matrix A, namely,

$$A_{ij} = \sum_{k=1}^{n} T_{ki} T_{kj} \qquad \text{for} \quad 1 \leqslant i,j \leqslant n+1. \tag{44}$$

Lemma 8: For an arbitrary binary coupling tree on $n+1$ leaves with leaf labels (h_i, k_i), $i = 1,\ldots n+1$, and with transformation matrix T defined by (40), *we have*

$$A_{ij} = \sum_{k=1}^{n} T_{ki} T_{kj} = \frac{1}{2h_i}\delta_{ij} - \frac{1}{2|h|}. \tag{45}$$

The matrix A is thus independent of the shape of the binary coupling tree.

Proof: Let nl_n (resp. nr_n) denote the number of leaves in the left (resp. right) subtree of v_n, the root node of the tree. We can then split up our formula into three parts:

$$A_{ij} = \sum_{k=1}^{n} T_{ki} T_{kj} = \sum_{k=1}^{nl_n - 1} T_{ki} T_{kj} + \sum_{k=nl_n}^{n-1} T_{ki} T_{kj} + T_{ni} T_{nj}. \tag{46}$$

Since the first (resp. second) sum of (46) corresponds to the A-matrix of the left (resp. right) subtree of the root, we use induction on the number of internal nodes in the tree. It is easily verified that the desired result is true for small values of n.

There are (essentially) two cases to consider:

(1) The variables x_i and x_j belong both to the same subtree of v_n.
(2) The variables x_i and x_j belong to different subtrees of v_n.

Let x_i and x_j both belong to the same, say left, subtree of v_n. This implies $T_{ni}=T_{nj}=c_n$, and thus

$$\sum_{k=1}^{n} T_{ki}T_{kj}=\left(\frac{1}{2h_i}\delta_{ij}-\frac{1}{2(h_1+\cdots+h_{nl_n})}\right)+0+\frac{(h_{nl_n+1}+\cdots+h_{n+1})}{2|h|(h_1+\cdots+h_{nl_n})}=\frac{1}{2h_i}\delta_{ij}-\frac{1}{2|h|}, \quad (47)$$

where the first sum in (46) is evaluated using the induction hypothesis, the second sum is zero because $T_{ki}=T_{kj}=0$ for $k=nl_n,\ldots,n-1$, and the third term is simply c_n^2. (We assumed, for the sake of simplicity, that the leaves in the left subtree have labels h_1 up to h_{nl_n}.)

Second let x_i belong to the left subtree and x_j to the right subtree. In this case $T_{kj}=0$ for $k=1,\ldots,nl_n-1$ and $T_{ki}=0$ for $k=nl_n,\ldots,n-1$. This implies

$$\sum_{k=1}^{n} T_{ki}T_{kj}=-c_nd_n=-\frac{1}{2|h|}. \quad (48)$$

□

Thus we have established that the weight function (30) after transformation with (39) becomes a product of n classical Hermite weights.

B. The Jacobian of the transformation

The transformation between the variables x and v is a simple linear transformation. If we want to show the orthogonality of the R-polynomials, we need the Jacobian of the transformation, i.e., we want to know

$$J=\left|\det\frac{\partial x_i}{\partial v_k}\right|, \quad \text{with} \quad 1\leqslant i,k\leqslant n. \quad (49)$$

From (39) it is immediately clear that

$$\det\frac{\partial v_k}{\partial x_i}=\det T \qquad \text{for} \quad 1\leqslant i,k\leqslant n+1. \quad (50)$$

However, we need the Jacobian between the n independent variables x_i and the n variables v_k. The linear constraint between the $n+1$ variables x_i is equivalent to subtracting the last column of the matrix T from all its other columns; this does not affect the value of the determinant of T. Since the $(n+1)$-th row of T now entirely consists of zeros, except for the last element, we have

$$\det\frac{\partial v_k}{\partial x_i}=\det T \qquad \text{for} \quad 1\leqslant i,k\leqslant n. \quad (51)$$

Since we use a linear transformation we now have

$$J=\left|\det\frac{\partial x_i}{\partial v_k}\right|=\left|\frac{1}{\det T}\right|. \quad (52)$$

It is thus sufficient to calculate the determinant of the matrix T.

Example 9: For the running example, the transformation matrix T equals

$$T=\begin{pmatrix} c_1^\star & -d_1^\star & 0^\star & 0 & 0 \\ c_2^\star & c_2^\star & -d_2^\star & 0 & 0 \\ 0 & 0 & 0 & c_3^\ddagger & -d_3^\ddagger \\ c_4 & c_4 & c_4 & -d_4 & -d_4 \\ 1^\star & 1^\star & 1^\star & 1^\ddagger & 1^\ddagger \end{pmatrix}. \tag{53}$$

We want to determine $|\det T|$ and to this end we transform T into an upper triangular matrix, using column transformations only.

In (53), the nine elements annotated with a $\star$ constitute the 3×3 transformation matrix associated with the left subtree, and analogously for the four elements annotated with a $\ddagger$. Perform the column transformations, $C_1\leftarrow C_1-C_2$, $C_2\leftarrow C_2-C_3$, and $C_4\leftarrow C_4-C_5$ on T and one gets

$$T=\begin{pmatrix} c_1+d_1^\star & -d_1^\star & 0^\star & 0 & 0 \\ 0^\star & c_2+d_2^\star & -d_2^\star & 0 & 0 \\ 0 & 0 & 0 & c_3+d_3^\ddagger & -d_3^\ddagger \\ 0 & 0 & c_4 & 0 & -d_4 \\ 0^\star & 0^\star & 1^\star & 0^\ddagger & 1^\ddagger \end{pmatrix}. \tag{54}$$

Note that the nine starred elements form an upper triangular matrix; the same applies to the four double-daggered elements. Moreover, the column transformations performed so far only concerned either the left or the right subtree, but not both.

Subtracting the fifth column from the third and swapping columns yields an upper triangular matrix, with determinant:

$$(c_1+d_1)(c_2+d_2)(c_3+d_3)(c_4+d_4). \tag{55}$$

■

We can easily extend the method of this example to prove the following lemma.

Lemma 10: For an arbitrary binary coupling tree on $n+1$ leaves with labels (h_i,k_i), $i=1,\ldots,n+1$, and with transformation matrix T determined by (40), *we have*

$$|\det T|=\prod_{i=1}^{n}(c_i+d_i)=\sqrt{\frac{|h|}{2^n(h_1\cdot h_2\cdot\cdots\cdot h_{n+1})}}. \tag{56}$$

Proof: Once again we let nl_n (resp. nr_n) denote the number of leaves in the left (resp. right) subtree of v_n. In general the matrix T has the following structure:

$$T=\begin{pmatrix} \tilde{T}_l & \mathcal{O}_{(nl_n-1)\times nr_n} \\ \mathcal{O}_{(nr_n-1)\times nl_n} & \tilde{T}_r \\ c_n,\ldots,c_n & -d_n,\ldots,-d_n \\ 1,\ldots,1 & 1,\ldots,1 \end{pmatrix}. \tag{57}$$

Herein, $\tilde{T}_l$ (resp. $\tilde{T}_r$) is a part of the matrix associated with the left (resp. right) subtree of v_n. More particularly,

$$\begin{pmatrix} \tilde{T}_l \\ 1,\ldots,1 \end{pmatrix} \tag{58}$$

is the matrix associated with the left subtree of v_n.

The structure of the matrix suggests to use induction on the order of the matrix. We thus assume that we can transform matrices smaller than T into upper triangular matrices, using column transformations only, and that the elements on the diagonal are of the form c_i+d_i (and one element 1). Schematically,

$$\begin{pmatrix} \tilde{T}_l \\ 1,\ldots,1 \end{pmatrix} \xrightarrow{\text{column tf}} \begin{pmatrix} c_1+d_1 & & & & \\ 0 & c_2+d_2 & & & \\ 0 & 0 & \ddots & & \\ 0 & \cdots & 0 & c_{nl_n-1}+d_{nl_n-1} & \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix}. \tag{59}$$

Performing the same column transformations on the extended matrix yields

$$\begin{pmatrix} \tilde{T}_l \\ \mathcal{O}_{(nr_n-1)\times nl_n} \\ c_n,\ldots,c_n \\ 1,\ldots,1 \end{pmatrix} \xrightarrow{\text{column tf}} \begin{pmatrix} & T_l' & & * \\ & \mathcal{O}_{(nr_n-1)\times nl_n} & & \\ 0 \quad \cdots & 0 & 0 & c_n \\ 0 \quad \cdots & 0 & 0 & 1 \end{pmatrix}, \tag{60}$$

where $\tilde{T}_l'$ is a square upper triangular matrix of the order nl_n-1 with diagonal elements c_i+d_i, where $i=1,\ldots,nl_n-1$. The $*$ stands for some column vector.

One can apply the same arguments to the matrix corresponding to the right subtree of v_n, finally leading to

$$T=\begin{pmatrix} \tilde{T}_l & \mathcal{O}_{(nl_n-1)\times nr_n} \\ \mathcal{O}_{(nr_n-1)\times nl_n} & \tilde{T}_r \\ c_n,\ldots,c_n & -d_n,\ldots,-d_n \\ 1,\ldots,1 & 1,\ldots,1 \end{pmatrix} \to \begin{pmatrix} \tilde{T}_l' & * & \mathcal{O}_{(nl_n-1)\times nr_n} & \\ \mathcal{O}_{(nr_n-1)\times nl_n} & & \tilde{T}_r' & * \\ 0,\ldots,0 & c_n & 0,\ldots,0 & -d_n \\ 0,\ldots,0 & 1 & 0,\ldots,0 & 1 \end{pmatrix}. \tag{61}$$

Subtracting the last column from the nl_n-th column and switching columns transforms T into an upper triangular matrix with diagonal elements c_i+d_i, with $i=1,\ldots n$ and one diagonal element that equals one. The (absolute value of the) determinant of T is thus

$$|\det(T)|=(c_1+d_1)\cdot(c_2+d_2)\cdots(c_n+d_n).$$

Rewriting this in terms of parameters h_i is easy using induction and the simple fact that

$$c_n+d_n=\sqrt{\frac{|h|}{2(h_1+\cdots+h_{nl_n})(h_{nl_n+1}+\cdots+h_{n+1})}}.$$

This completes the proof of (56), and thus

$$J=\sqrt{\frac{2^n(h_1\cdot h_2\cdot\cdots\cdot h_{n+1})}{|h|}}. \tag{62}$$

□

C. The orthogonality explicitly

It is immediately clear that if x and v are connected through (39), that $x \in \mathbb{R}^n \Leftrightarrow v \in \mathbb{R}^n$.

With this last simple observation we are now in the position to prove the orthogonality of the R-polynomials.

Theorem 11: *With the tensor product of $n+1$ $\mathfrak{b}(1)$ representations labeled (h_i,k_i), with $i=1,\ldots,n+1$, i.e., with every binary coupling tree with n internal nodes, we associate a set of polynomials $R_l^{(h)}(x)$ in n variables. These polynomials are orthogonal on $\mathbb{R}^n$ for the weight function*

$$w^{(h)}(x)=\exp(-\psi(x)), \quad with \quad \psi(x)=(x_1,x_2,\ldots,x_n,s-\sigma(x))A(x_1,x_2,\ldots,x_n,s-\sigma(x))^t, \tag{63}$$

and

$$A_{ij}=\frac{1}{2h_i}\delta_{ij}-\frac{1}{2|h|}. \tag{64}$$

Explicitly, the orthogonality reads

$$\int_{\mathbb{R}^n} R_l^{(h)}(x)R_{l'}^{(h)}(x)w^{(h)}(x)\,dx=\sqrt{\frac{(2\pi)^n h_1\cdots h_{n+1}}{|h|}}\,\delta_{l,l'}. \tag{65}$$

Proof: The proof is easy since we have collected all the ingredients in this section. We have

$$\begin{aligned}\int_{\mathbb{R}^n} R_l^{(h)}(x)R_{l'}^{(h)}(x)w^{(h)}(x)\,dx&=\int_{\mathbb{R}^n} J\prod_{i=1}^{n}\frac{H_{l_i}(v_i)}{\sqrt{2^{l_i}l_i!}}\frac{H_{l_i'}(v_i)}{\sqrt{2^{l_i'}l_i'!}}e^{-v_i^2}\,dv_i\\&=J\sqrt{\pi^n}\,\delta_{l,l'}\\&=\sqrt{\frac{(2\pi)^n h_1\cdots h_{n+1}}{|h|}}\,\delta_{l,l'}.\end{aligned} \tag{66}$$

□

Remark 12: It is an easy calculation to verify that $\psi(x)$, when written explicitly in terms of x_i $(1\leqslant i\leqslant n)$, has the following form:

$$\psi(x)=\sum_{i=1}^{n}\frac{1}{2h_i}x_i^2+\frac{1}{2h_{n+1}}\left(\sum_{i=1}^{n}x_i\right)^2-\frac{s}{h_{n+1}}\sum_{i=1}^{n}x_i+s^2\left(\frac{1}{2h_{n+1}}-\frac{1}{2|h|}\right).$$

From this it is easily seen that the quadratic part of $\psi(x)$ is positive definite, which is neccessary for the integrability of the left hand side of (65). Observe that the minimum of $\psi(x)$ [i.e., the maximum of $w^{(h)}(x)$] occurs at $x_i=sh_i/|h|$, $1\leqslant i\leqslant n$.

Theorem 11 is correct for any value of s. For each value of s one gets a different weight function and different polynomials. Thus, both the weight function and the polynomials $R_l^{(h)}(x)$ depend on s; in both cases the reference to s is dropped to make the notation easier. When $s=0$ the weight function simplifies and ψ becomes a purely quadratic form, which is thus as in Ref. 19. ■

V. AN INTEGRAL FORMULA FOR RECOUPLING COEFFICIENTS

In this section we will show that the set of polynomials $R_{l,T}^{(h)}(x)$ associated with a fixed binary coupling tree T and fixed representation labels (h_i,k_i), but varying values l_i forms a basis for Π^n. This means that a polynomial $R_{l,T_1}^{(h)}(x)$ (l fixed) associated with a binary coupling tree T_1 can be

written as a linear combination of polynomials $R^{(h)}_{l',T_2}(x)$ (l' variable) associated with another binary coupling tree T_2. The connection coefficients between these two bases are the recoupling coefficients of $\mathfrak{b}(1)$. The orthogonality of the R-polynomials, shown in Theorem 11, leads to an integral formula for these recoupling coefficients.

We start with a simple observation: for any binary coupling tree the degree of $R^{(h)}_l(x)$ equals $|l|$. This follows immediately from the fact that $S_j(x_1,x_2;h_1,h_2)$ is a polynomial of degree j in x_1 and x_2.

Theorem 13: *For any binary coupling tree on $n+1$ leaves, with fixed representation labels (h_i,k_i) $(i=1,\ldots,n+1)$, the set of polynomials $R^{(h)}_l(x)$ associated with it forms a basis for Π^n.*

Proof: The orthogonality of the polynomials $R^{(h)}_l(x)$ immediately implies their linear independence. The theorem then follows by the same counting argument as in Ref. 5, Theorem 20.□

Since the S-polynomials satisfy the two basic properties (32) and (34), which are identical to the properties of the S-polynomials in the $\mathfrak{su}(1,1)$-case (see Ref. 5, Formulas 2.11 and 2.12), one can use exactly the same reasoning as in Ref. 5, Theorem 21, to prove the following theorem.

Theorem 14: *Consider a binary coupling tree T_1, with fixed values (h_j,k_j) and l_i. Consider a second binary coupling tree T_2 with the same fixed values (h_j,k_j) but varying values l'_i, such that $|l|=|l'|$. Then the polynomial $R^{(h)}_{l,T_1}(x)$ can be written as a linear combination of polynomials $R^{(h)}_{l',T_2}(x)$:*

$$R^{(h)}_{l,T_1}(x)=\sum_{|l'|=|l|} C_{l'}R^{(h)}_{l',T_2}(x). \tag{67}$$

The connection coefficient $C_{l'}$ is equal to the $3nj$-coefficient $\langle T_1(l),T_2(l')\rangle$.

Corollary 15: For two arbitrary binary coupling trees T_1 and T_2 with the same representation labels (h_j,k_j) the recoupling coefficient $\langle T_1(l),T_2(l')\rangle$ is given by

$$\langle T_1(l),T_2(l')\rangle=\sqrt{\frac{|h|}{(2\pi)^n h_1\cdots h_{n+1}}}\int_{\mathbb{R}^n} R^{(h)}_{l,T_1}(x)R^{(h)}_{l',T_2}(x)w^{(h)}(x)\,dx, \tag{68}$$

with $w^{(h)}(x)$ as in Theorem 11.

Proof: The result follows immediately from combining Theorems 11 and 14. □

Remark 16: In Sec. III we saw that the addition formula (18) is a direct consequence of the basic relation (16) for S-polynomials. Clearly, (67) is an extension of this relation. If one changes from variables x to v on the right side of (67), the variables on the left side will be an orthogonal transformation of the variables v. This can be seen be using the "method of trees" and repeated application of (16). It can also be understood by the fact that $\exp(-(v_1^2+\cdots+v_n^2))$ is invariant under orthogonal transformations. ■

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Properties of chord length distributions of nonconvex bodies

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(Received 17 June 2003; accepted 1 August 2003)

Cauchy's formula which relates the mean chord length (isotropic uniform random chords) of a convex body in $\mathbb{R}^n$ with its volume and surface is extended to the case of nonconvex bodies in the framework of integral geometry. This allows us to generalize the extended Cauchy's formula recently discovered by Blanco and Fournier [Europhys. Lett. **61** (2), 168 (2003)], in the field of diffusive random walks, to nonconvex bodies. Monte Carlo simulations illustrate these points in $\mathbb{R}^2$ and in $\mathbb{R}^3$. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1622446]

I. INTRODUCTION

The study of chord length distributions across various kinds of geometrical shapes, including stochastic mixtures, is a topic of great interest in many research fields ranging from ecology to neutronics. These distribution functions are a powerful tool for the description of size and shape of the intercepted object and have applications in various fields such as acoustics,[1] ecology,[2] image analysis,[3] stereology[4] and reactor design.[5,6] Besides, chord length distributions are fundamental functions for the characterization of random media.[7–9] One of the fundamental results is the Cauchy formula. It states that for a convex body (here in $\mathbb{R}^3$) the mean chord length $E[\sigma]$ is related to the volume V and the surface area S of the body

$$E[\sigma]=4\frac{V}{S}. \tag{1}$$

As noted by Gille,[10] for nonconvex objects an isotropic uniform random (IUR) line may cross the body K more than one time. Consequently, there are several definitions for the chord length distribution (CLD). The first distribution type in use operates with the sum of all chord segments on one straight line as the random variable. Introduced as the OCD case, meaning one chord distribution in Ref. 10, this type of distribution satisfies a modified Cauchy formula,

$$E[\sigma_{\mathrm{OCD}}]=4\frac{V}{S^*}. \tag{2}$$

Here S^* is the surface area of the convex hull of K. A derivation of Eq. (2) is given in Ref. 11.

The second distribution function of importance consists of considering each chord length segment inside K for itself as shown in Fig. 1. This distribution named the MCD case (multiple chord distribution) in Ref. 10 corresponds to the natural case of small angle scattering,[12] where the concept of chord length distribution is used with success. A certain CLD is, in a mathematical sense, equivalent to the diffraction pattern of a microparticle system. There are serious difficulties,

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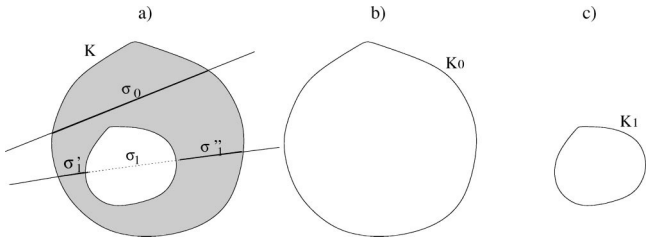

FIG. 1. Chord length distribution across the considered nonconvex body K: each chord $\sigma_0, \sigma_1', \sigma_1''$ contributes to the chord length distribution. (a) the whole body, $K = K_0 \backslash K_1$. (b) the outer "part," K_0. (c) the inner "part," K_1.

however, in treating more complicated cases, such as hollow or composite particles, or densely packed microparticle systems. The purpose to develop this concept further cannot be achieved with physical experiments or based on Monte Carlo simulation techniques, whatever their precision or strategy. Only mathematical deviations will lead to a final proof about an experimental supposition. This situation is also of interest in reactor physics, when considering a nonconvex body (or an assembly of nonconvex bodies) surrounded by an isotropic flux distribution of neutrons.[13] Other applications concern random packing of hard spheres where Cauchy formula for the nonconvex phase is needed in order to link the packing fraction of the system to the average coordination number.[14] However, for the latter, results are rare in the literature.[10,15] In the present article after first reviewing briefly the Cauchy formula for a convex body in $\mathbb{R}^n$, we will derive a Cauchy formula for nonconvex bodies. Connection with diffusive random walks is presented. Finally, these points are illustrated by Monte Carlo simulations followed by a conclusion.

II. BRIEF REVIEW OF THE CAUCHY FORMULA FOR CONVEX BODIES IN $\mathbb{R}^n$

One way to derive Cauchy's formula in $\mathbb{R}^n$ consists of using results of integral geometry on the chord power integrals. Let K be a convex body in $\mathbb{R}^n$ and let M be a random line that intersects K measured with the uniform density dM which satisfies (Ref. 16, p. 237)

$$\int_{B_n \cap M \neq \varnothing} dM = \frac{\omega_{n-1}}{2} \alpha_n . \tag{3}$$

Here, ω_n is the volume of the unit ball B_n in $\mathbb{R}^n$, and α_n is the surface area of the unit sphere S^n. We denote by σ the chord length of the intersection $K \cap M$. Then, the chord power integrals of K are defined by

$$I_m(K) = \int_{M \cap K \neq \varnothing} \sigma^m dM, \qquad 0 \leqslant m < \infty. \tag{4}$$

For the chord power integrals, several interesting formulas have been derived,[16] namely,

$$\begin{aligned} I_0(K) &= \frac{\omega_{n-1}}{2} S(K), \\ I_1(K) &= \frac{\alpha_{n-1}}{2} V(K), \end{aligned} \tag{5}$$

where $V(K)$ is the volume of K and $S(K)$ is its surface area. From Eq. (5) it is straightforward to obtain the mean chord length,

$$E[\sigma] = \frac{\displaystyle\int_{M \cap K \neq \varnothing} \sigma dM}{\displaystyle\int_{M \cap K \neq \varnothing} dM}. \tag{6}$$

The denominator in Eq. (6) is needed in order to get a measure for all the chords across K possible (normalized to unity, i.e., as a density probability measure). Equation (6) is directly related to the chord power integrals I_m defined in Eq. (4). Combined with Eq. (5) we get

$$E[\sigma]=\frac{I_1(K)}{I_0(K)}=\frac{\alpha_{n-1}}{\omega_{n-1}}\frac{V(K)}{S(K)}. \tag{7}$$

Since the coefficients α_{n-1} and ω_{n-1} are given by

$$\begin{aligned}\alpha_{n-1}&=\frac{2\pi^{n/2}}{\Gamma[n/2]},\\ \omega_{n-1}&=\frac{2\pi^{(n-1)/2}}{(n-1)\Gamma[(n-1)/2]},\end{aligned} \tag{8}$$

where the symbol Γ denotes the Euler Γ function, we finally obtain the mean chord length

$$E[\sigma]=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\frac{V(K)}{S(K)}. \tag{9}$$

In $\mathbb{R}^2$ (here, the denominator equals the perimeter L of K) and in $\mathbb{R}^3$ we recover the standard results,

$$E[\sigma]=\begin{cases}\pi\dfrac{S}{L} & \text{(two-dimensional case)}\\ 4\dfrac{V}{S} & \text{(three-dimensional case).}\end{cases} \tag{10}$$

III. CAUCHY FORMULA FOR A NONCONVEX BODY

Before giving a general, formal proof concerning the validity of Cauchy's formula for nonconvex bodies, some simple specific cases are first analyzed. These cases only require elementary results from integral geometry permitting an intuitive understanding of our general result.

A. Cauchy formula for a convex body with one convex hole

For a nonconvex body K in $\mathbb{R}^n$ involving a hollow part and therefore possessing outer and inner surfaces, both enclosing convex shapes, and if each chord length segment inside K is taken for itself, Cauchy's theorem remains valid,

$$E[\sigma]=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\frac{V(K)}{S(K)}. \tag{11}$$

Here $V(K)$ is the volume of the body and $S(K)$ is the whole surface (inner *plus* outer surface).

Proof: As a first step let K be a nonconvex figure consisting of a convex hole K_1 of surface S_1 lying wholly inside a convex body K_0 of surface S_0 as shown in Fig. 1. The mean chord length is given by

$$E[\sigma]=\frac{\displaystyle\int_{M\cap K\neq\varnothing}\sigma\,dM}{\displaystyle\int_{M\cap K\neq\varnothing}n dM}. \tag{12}$$

Here dM is the isotropic uniform density of random lines and n is the number of segments generated by M [$n=1$ for the special case of a convex body, see Eq. (6)]. Note that for the numerator what matters is to record all chords: hence considering the sum of the chords generated by one random line or taking each chord independently amounts to the same. The only difference

is that in the first case we are actually dealing with one random variable. Consequently, we could have written $\int_{M\cap K\neq\varnothing}\sigma_{\mathrm{OCD}}\,dM$ for the numerator of Eq. (12). Now, to account for the fact that each chord length is taken for itself and contributes independently to σ, the denominator of Eq. (12) must be analyzed in greater detail, see Fig. 1. The denominator must reflect the measure of the segments across K, that is,

$$\int_{M\cap K\neq\varnothing} n\,dM=\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1=\varnothing}}1\;dM+\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1\neq\varnothing}}2\;dM. \tag{13}$$

In Eq. (13) the integration has been performed over domains of constant n. Next, we will derive some useful relations between the measures of segments across different regions of K. Let p be the probability that an IUR chord simultaneously cuts K_0 and K_1. The density of having chords $\int_{M\cap K_0\neq\varnothing,M\cap K_1\neq\varnothing}dM$ is just the density of having chords across K_0 *times* the probability of hitting K_1,

$$\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1\neq\varnothing}}dM=p\int_{M\cap K_0\neq\varnothing}dM. \tag{14}$$

Moreover, since $\{M\cap K_0\neq\varnothing\}=\{(M\cap K_0\neq\varnothing)\cap(M\cap K_1\neq\varnothing)\}\cup\{(M\cap K_0\neq\varnothing)\cap(M\cap K_1=\varnothing)\}$ and $\{(M\cap K_0\neq\varnothing)\cap(M\cap K_1\neq\varnothing)\}\cap\{(M\cap K_0\neq\varnothing)\cap(M\cap K_1=\varnothing)\}=\varnothing$, we have

$$\int_{M\cap K_0\neq\varnothing}dM=\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1\neq\varnothing}}dM+\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1=\varnothing}}dM. \tag{15}$$

Combining Eqs. (13)–(15) leads to

$$\int_{M\cap K\neq\varnothing} n\,dM=(1+p)\int_{M\cap K_0\neq\varnothing}dM, \tag{16}$$

and

$$\int_{M\cap K\neq\varnothing} n\,dM=\frac{1+p}{p}\int_{\substack{M\cap K_0\neq\varnothing\\ M\cap K_1\neq\varnothing}}dM. \tag{17}$$

This relates the measure of chords across K to the measure of lines across K_0, Eq. (16), and to the measure of lines across K_1, Eq. (17).

Using Eq. (16), we can rewrite Eq. (12),

$$E[\sigma]=\left[\frac{\int_{M\cap K\neq\varnothing}\sigma_{\mathrm{OCD}}\,dM}{\int_{M\cap K\neq\varnothing}dM}\right]\left[\frac{\int_{M\cap K\neq\varnothing}dM}{\int_{M\cap K\neq\varnothing}n\,dM}\right] \tag{18}$$

$$=E[\sigma_{\mathrm{OCD}}]\,\frac{1}{1+p}, \tag{19}$$

where $E[\sigma_{\mathrm{OCD}}]$ is given by Eq. (2) with $S^*=S(K_0)$ in this case.

It remains to determine the probability p defined previously. Matai[17] gives a derivation of this geometric problem for convex bodies in the plane. Independently of this, Santalo[16] gives the following general result in terms of the Minkowski functionals W_1,

$$p=\frac{W_1(K_1)}{W_1(K_0)}. \tag{20}$$

Moreover, the functionals $W_1(K)$ of a convex body K are connected to the $(n-1)$-dimensional surface $S(K)$ of K by $W_1(K)=S(K)/n$. Thus we get

$$p=\frac{S(K_1)}{S(K_0)}. \tag{21}$$

Finally from Eqs. (19) and (21) we obtain

$$E[\sigma]=(n-1)\sqrt{\pi}\,\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\left[\frac{V(K_0)-V(K_1)}{S(K_0)+S(K_1)}\right]=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\,\frac{V(K)}{S(K)}. \tag{22}$$

Here $V(K)=V(K_0)-V(K_1)$ is the volume of K and $S(K)=S(K_0)+S(K_1)$ is its whole surface area. In particular in $\mathbb{R}^2$ and in $\mathbb{R}^3$

$$E[\sigma]=\begin{cases}\pi\dfrac{S}{L} & \text{(two-dimensional case)}\\[2ex] 4\dfrac{V}{S} & \text{(three-dimensional case).}\end{cases} \tag{23}$$

Here, L is the whole perimeter. In other words, Eq. (22) expresses that the mean chord length across a convex object involving a convex hollow part does not depend on the position of the hole. This is a generalization of earlier works regarding the hollow sphere with central hole[10] and the infinitely long circular hollow cylinder.[15]

B. Cauchy formula for a convex body with two convex holes

The case of a convex body K_0 [perimeter $:L(K_0)$] (in $\mathbb{R}^2$ for simplification purposes) perforated by two disjoint convex holes K_1 [perimeter $:L(K_1)$] and K_2 [perimeter $:L(K_2)$] is worth spending some time on, since it will give us a broad idea of what makes our further generalization natural. Indeed in the following calculations, special terms related to the measure of random lines crossing both holes actually vanish. In the following, we will denote the defined above measure by μ_{12}. It is possible to express μ_{12} (see Ref. 17, p. 79) in terms of perimeters of convex shapes constructed from K_1 and K_2 (see Fig. 2): keeping Mathai's notation, γ_1 is the perimeter of the convex body $D_1=APWOTSA$, γ_2 is the perimeter of the convex body $D_2=OUQBRVO$, and γ_{12} is the perimeter of $D_{12}=APQBRSA$ the outer cover of K_1 and K_2. In the plane, since the measure of random lines that intersect a convex body is just the perimeter of the body (Ref. 16, p. 237), we have

$$\mu_{12}=\gamma_1+\gamma_2-\gamma_{12}. \tag{24}$$

Next we can write

$$\int_{M\cap K\neq\varnothing} n\,dM=1\times(L(K_0)-[L(K_1)-\mu_{12}]-[L(K_2)-\mu_{12}]-\mu_{12})+2\times(L(K_1)-\mu_{12}+L(K_2)$$
$$-\mu_{12})+3\times(\mu_{12})=L(K_0)+L(K_1)+L(K_2). \tag{25}$$

Combining this result with Eq. (18) yields

$$E[\sigma]=\pi\frac{S(K_0)-S(K_1)-S(K_2)}{L(K_0)+L(K_1)+L(K_2)}. \tag{26}$$

This is the two-dimensional Cauchy's formula for our perforated body. Generalization to N convex particles as well as connection to scattering experiments is made in the Appendix.

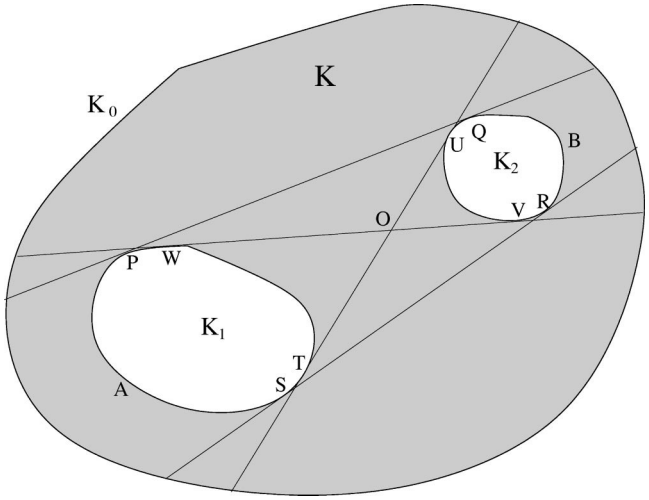

FIG. 2. Nonconvex body with two holes, $K=K_0\backslash(K_1\cup K_2)$. UT, VW, PQ and SR are the four common tangents of K_1 and K_2. O is the intersection of UT and VW.

C. Cauchy formula for an assembly of convex bodies

We begin with the special case of two convex bodies. Let us consider a nonconvex body K as the union of two convex bodies K_1 and K_2 that do not overlap, i.e., $K=K_1\cup K_2$ and $K_1\cap K_2=\{\varnothing \text{ or 1 point}\}$. The mean chord length is again given by Eq. (12). Since K_1 and K_2 do not overlap,

$$\int_{M\cap K\neq\varnothing} n\,dM=\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2=\varnothing}} 1\,dM+\int_{\substack{M\cap K_1=\varnothing\\ M\cap K_2\neq\varnothing}} 1\,dM+\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2\neq\varnothing}} 2\,dM. \tag{27}$$

Hence, combining the last integral with the first two integrals on the rhs,

$$\int_{M\cap K\neq\varnothing} n\,dM=\int_{M\cap K_1\neq\varnothing} dM+\int_{M\cap K_2\neq\varnothing} dM \tag{28}$$

and

$$\int_{M\cap K\neq\varnothing} \sigma\,dM=\int_{M\cap K_1\neq\varnothing} \sigma_1\,dM+\int_{M\cap K_2\neq\varnothing} \sigma_2\,dM. \tag{29}$$

Recalling that with the normalization chosen previously, Eq. (3), the measure of lines that intersect a convex body is $\omega_{n-1}S/2$, we get

$$\int_{M\cap K\neq\varnothing} n\,dM=\frac{\omega_{n-1}}{2}(S(K_1)+S(K_2)). \tag{30}$$

Using Eq. (12) and Eqs. (29) and (30) leads to

$$E[\sigma]=\left[\frac{\int_{M\cap K_1\neq\varnothing}\sigma\,dM}{\int_{M\cap K_1\neq\varnothing} dM}\right]\left[\frac{\int_{M\cap K_1\neq\varnothing} dM}{\int_{M\cap K\neq\varnothing} n\,dM}\right]+\left[\frac{\int_{M\cap K_2\neq\varnothing}\sigma\,dM}{\int_{M\cap K_2\neq\varnothing} dM}\right]\left[\frac{\int_{M\cap K_2\neq\varnothing} dM}{\int_{M\cap K\neq\varnothing} n\,dM}\right],$$

$$=E[\sigma_1]\frac{S(K_1)}{S(K_1)+S(K_2)}+E[\sigma_2]\frac{S(K_2)}{S(K_1)+S(K_2)}. \tag{31}$$

Again, since K_1 and K_2 are convex bodies, $E[\sigma_1]$ and $E[\sigma_2]$ are given by the two special Cauchy formulas, Eq. (11), thus

$$E[\sigma]=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\left[\frac{V(K_1)+V(K_2)}{S(K_1)+S(K_2)}\right]=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\frac{V(K)}{S(K)}. \quad (32)$$

Here $V(K)=V(K_1)+V(K_2)$ is the volume of K and $S(K)=S(K_1)+S(K_2)$ is its whole surface area. However, for systems of nonoverlapping convex bodies, Eq. (31) allows us to derive the CLD of K in terms of the CLD of K_1 and K_2. More precisely, Eq. (31) can be rewritten as

$$E[\sigma]=\frac{S(K_1)}{S(K_1)+S(K_2)}\int_0^{\sigma_1}\sigma f_1(\sigma)\,d\sigma+\frac{S(K_2)}{S(K_1)+S(K_2)}\int_0^{\sigma_2}\sigma f_2(\sigma)\,d\sigma, \quad (33)$$

where $f_i(\sigma)$ is the CLD of K_i and σ_i is the longest chord of K_i. Thus, we have

$$E[\sigma]=\int_0^{\max\{\sigma_1,\sigma_2\}}\sigma\left[|f_1(\sigma)|_0^{\sigma_1}\frac{S(K_1)}{S(K_1)+S(K_2)}+|f_2(\sigma)|_0^{\sigma_2}\frac{S(K_2)}{S(K_1)+S(K_2)}\right]d\sigma \quad (34)$$

with the notation

$$|f(x)|_{x_1}^{x_2}=\begin{cases} f(x) & \text{if } x_1\leqslant x\leqslant x_2 \\ 0 & \text{elsewhere.}\end{cases} \quad (35)$$

Consequently,

$$f(\sigma)=|f_1(\sigma)|_0^{\sigma_1}\frac{S(K_1)}{S(K_1)+S(K_2)}+|f_2(\sigma)|_0^{\sigma_2}\frac{S(K_2)}{S(K_1)+S(K_2)}. \quad (36)$$

The generalization to n convex bodies that do not overlap is straightforward.

D. Cauchy formula for two overlapping convex bodies

In this section we consider a nonconvex body K made as the union of two overlapping convex bodies K_1 and K_2 in $\mathbb{R}^2$ (again for simplification purposes). We use the notations (see Fig. 3)

$$\begin{aligned} L_1&=L(K)\cap L(K_1), \\ L_2&=L(K)\cap L(K_2), \end{aligned} \quad (37)$$

and

$$\begin{aligned} L_1'&=L(K_1)\backslash L_1, \\ L_2'&=L(K_2)\backslash L_2. \end{aligned} \quad (38)$$

We start from Eq. (19),

$$E[\sigma]=E[\sigma_{\mathrm{OCD}}]\left[\frac{\int_{M\cap K\neq\varnothing}dM}{\int_{M\cap K\neq\varnothing}n\,dM}\right], \quad (39)$$

where $E[\sigma_{\mathrm{OCD}}]$ is given by Eq. (2), taking into account Ref. 16,

$$\int_{M\cap K\neq\varnothing}dM=S^*(K). \quad (40)$$

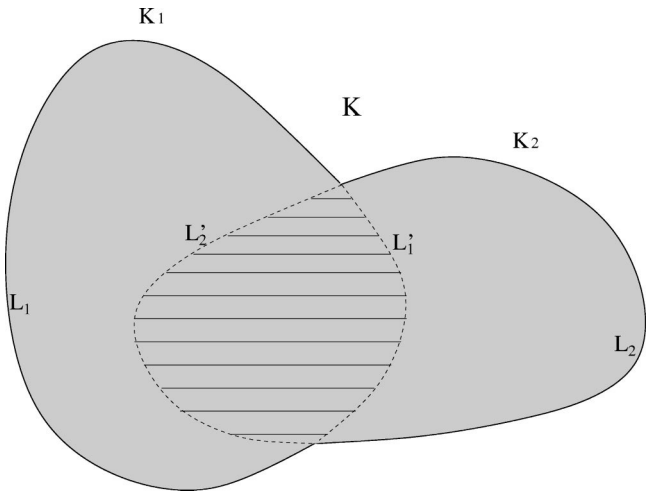

FIG. 3. Nonconvex body K made as the union of two overlapping convex bodies K_1 and K_2. L_1 and L_2 are the perimeters of K_1 and K_2, respectively. L_1' is the part of L_1 included in K_2 and L_2' is the part of L_2 included in K_1.

For calculating the last integral in Eq. (39), we use the same technique as before, i.e., decomposing over the respective domains of constant n,

$$\int_{M\cap K\neq\varnothing} n\,dM=\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2=\varnothing}}1\,dM+\int_{\substack{M\cap K_1=\varnothing\\ M\cap K_2\neq\varnothing}}1\,dM+\int_{\substack{M\cap K_1\neq\varnothing, M\cap K_2\neq\varnothing\\ M\cap(K_1\cap K_2)\neq\varnothing}}1\,dM + \int_{\substack{M\cap K_1\neq\varnothing, M\cap K_2\neq\varnothing\\ M\cap(K_1\cap K_2)=\varnothing}}2\,dM. \tag{41}$$

The first integral on the rhs of Eq. (41) is

$$\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2=\varnothing}} dM=\int_{M\cap K_1\neq\varnothing} dM-\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2\neq\varnothing}} dM=(1-p)\int_{M\cap K_1\neq\varnothing} dM=(1-p)\,L(K_1). \tag{42}$$

Here, $p=(L(K_1)+L(K_2)-L_{12})/L(K_1)$ is the probability that a random IUR line which cuts K_1, also cuts K_2 (see Ref. 17, p. 78). The length L_{12} is the perimeter of the outer cover of K_1 and K_2 (see Fig. 3). Consequently,

$$\int_{\substack{M\cap K_1\neq\varnothing\\ M\cap K_2=\varnothing}} dM=L_{12}-L(K_2). \tag{43}$$

Similarly,

$$\int_{\substack{M\cap K_1=\varnothing\\ M\cap K_2\neq\varnothing}} dM=L_{12}-L(K_1). \tag{44}$$

Since the intersection of two convex bodies is also convex, we have

$$\int_{\substack{M\cap K_1\neq\varnothing, M\cap K_2\neq\varnothing\\ M\cap(K_1\cap K_2)\neq\varnothing}} dM=L_1'+L_2', \tag{45}$$

where $L_1'+L_2'$ is the perimeter of the hatched area in Fig. 3. The last integral on the rhs of Eq. (41) is

$$\int_{\substack{M\cap K_1\neq\varnothing, M\cap K_2\neq\varnothing \\ M\cap(K_1\cap K_2)=\varnothing}} dM = L(K_1)+L(K_2)-L_{12}-(L_1'+L_2'). \tag{46}$$

Using Eqs. (43)–(46) in the rhs of Eq. (41) leads to

$$\int_{M\cap K\neq\varnothing} n\,dM = L(K_1)+L(K_2)-(L_1'+L_2') = L(K). \tag{47}$$

Finally, using Eqs. (47) and (40) and inserting $E[\sigma_{\mathrm{OCD}}]=\pi S(K)/L(K)^*$ into Eq. (39), we obtain the desired result,

$$E[\sigma]=\pi\frac{S(K)}{L(K)}. \tag{48}$$

E. Cauchy formula for a compact differentiable manifold

In this section we derive the Cauchy formula for an arbitrary compact differentiable manifold using more advanced results of integral geometry. So, let X be a compact differentiable manifold of dimension q embedded in E_n, assumed piecewise smooth. Santalo[16] (p. 245) derives the following result concerning the intersection of X with random r-planes M_r having an isotropic uniform measure dM_r,

$$\int_{X\cap M_r\neq\varnothing} \sigma_{r+q-n}(X\cap M_r)\,dM_r = \frac{\alpha_n\cdots\alpha_{n-r}\,\alpha_{r+q-n}}{\alpha_r\cdots\alpha_0\,\alpha_q}\sigma_q(X). \tag{49}$$

Here $\sigma_q(X)$ indicates the q-dimensional volume of X. For intersection with random lines $r=1$, Eq. (49) reduces to

$$\int_{X\cap M\neq\varnothing} \sigma_{q-n+1}(X\cap M)\,dM = \frac{\alpha_n\,\alpha_{n-1}\,\alpha_{q-n+1}}{\alpha_1\,\alpha_0\,\alpha_q}\sigma_q(X). \tag{50}$$

Here dM is the usual isotropic uniform density of random lines. Applying Eq. (50) with $q=n-1$ gives information regarding the measure of random lines throught X, more precisely,

$$\int_{X\cap M\neq\varnothing} N\,dM = \frac{\alpha_n}{\alpha_1}S(X). \tag{51}$$

where $S(X)$ is the surface of the manifold and N is the number of intersection of M and X. Since the number of intersections N is twice the number of chords n, we have immediately

$$\int_{X\cap M\neq\varnothing} n\,dM = \frac{\alpha_n}{2\alpha_1}S(X). \tag{52}$$

Likewise, applying Eq. (49) with $q=n$ gives information regarding the measure of random segment through X,

$$\int_{X\cap M\neq\varnothing} \sigma\,dM = \frac{\alpha_{n-1}}{\alpha_0}V(X), \tag{53}$$

where $V(X)$ is the volume of X. Thus, using both Eqs. (52) and (53) and the definition of the mean chord length Eq. (12) leads to Eq. (54), which agrees with Eq. (11),

$$E[\sigma]=2\,\frac{\alpha_{n-1}\,\alpha_1}{\alpha_n\,\alpha_0}\,\frac{V(X)}{S(X)}=(n-1)\sqrt{\pi}\frac{\Gamma[(n-1)/2]}{\Gamma[n/2]}\,\frac{V(X)}{S(X)}. \tag{54}$$

IV. DIFFUSIVE RANDOM WALKS AND EXTENDED CAUCHY'S FORMULA

This section is a first stage for a mathematical demonstration of the ''extended Cauchy's formula,'' a result recently due to Blanco and Fournier.[18] Indeed, these two authors discovered an invariance property of purely diffusive random walks which is linked to Cauchy's formula. More precisely, these authors consider a volume V of envelope S submitted to a uniform isotropic particles incidence. This hypothesis is formally equivalent to a uniform isotropic measure of random lines.[13] Next, they consider the following statistical event in which a particle enters V through S: The total trajectory length L is defined as the length of the multiple scattering trajectory from an entry point to the first exit through S. Then, they found, using physical principles such as statistical equilibrium, that the average length $E[L]$ is independent of both the mean free path and the single-scattering phase function fields,

$$E[L]=4\,\frac{V}{S}. \tag{55}$$

Equation (55) is, as Blanco and Fournier quoted, a generalization of Cauchy's formula (extended Cauchy's formula) since Cauchy's formula corresponds to infinite mean free path. Moreover, on the one hand, since the argument of Blanco and Fournier does not involve any hypothesis on the body at all,[18] it implicitly includes the nonconvex body case. On the other hand, the result of the present article is that Cauchy's formula remains valid for nonconvex bodies (assuming that each chord is taken for itself). Consequently, Eq. (55) is also an extension of Cauchy's formula for the case of nonconvex bodies. Of course we do not offer a rigorous mathematical demonstration of the extended Cauchy's formula since part of our reasoning is based on Blanco and Fournier physical argument. However, the validity of Cauchy's formula for nonconvex bodies, which is the main result of Sec. III, is a first step in building a rigorous proof of the extended Cauchy's formula, an open problem in the field of diffusive random walks in bounded spaces.

V. MONTE CARLO SIMULATIONS

In this section, Monte Carlo simulations are performed for various nonconvex geometric shapes in two and three dimensions. The Monte Carlo program that generates random lines in the plane or in space and then collects chords across the body has been described in Ref. 19. It has been tested for various convex geometrical objects as well as for the special cases of concentric hollow disks and concentric hollow spheres, where the CLD for such nonconvex bodies is known analytically. The CLD and its properties are obtained for two convex bodies with convex holes. The first object is a rectangle within a disk, and the second is a disk within a rectangle as shown

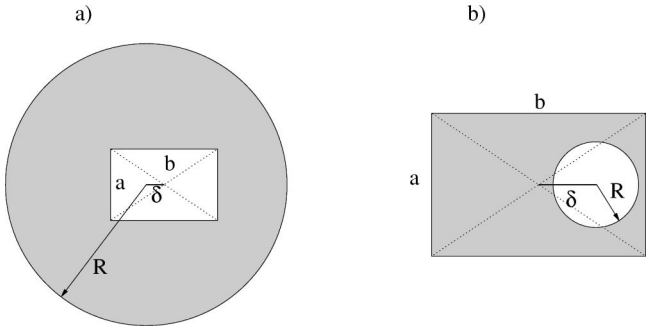

FIG. 4. Examples of two-dimensional nonconvex bodies: (a) rectangle inside a disk, (b) disk inside a rectangle. For both cases, δ is the distance between the disk's center and the rectangle's center.

TABLE I. Two-dimensional simulation results.

	δ	No. of chords[a]	$E[\sigma]_{th}$[b]	$E[\sigma]$	Variance
rectangle in disk	0.000	9.32×10^6	1.979 12	1.979 02	2.69×10^{-4}
rectangle in disk	0.500	9.32×10^6	1.979 12	1.979 06	3.00×10^{-4}
rectangle in disk	1.000	9.32×10^6	1.979 12	1.978 71	3.77×10^{-4}
disk in rectangle	0.000	6.45×10^6	1.372 05	1.372 43	3.23×10^{-4}
disk in rectangle	0.500	6.45×10^6	1.372 05	1.372 36	3.53×10^{-4}
disk in rectangle	1.000	6.45×10^6	1.372 05	1.372 76	4.38×10^{-4}
two overlapping disks	0.200	9.67×10^6	3.328 66	3.328 78	3.07×10^{-4}
two overlapping disks	0.500	9.28×10^6	3.558 63	3.558 48	3.51×10^{-4}
two overlapping disks	1.000	8.89×10^6	3.791 11	3.791 01	4.38×10^{-4}
two overlapping disks	1.500	8.80×10^6	3.785 89	3.787 21	5.06×10^{-4}
two overlapping disks	1.800	9.01×10^6	3.599 65	3.599 92	4.91×10^{-4}

[a]10×10^6 random lines were used for each simulation.
[b]$E[\sigma]_{th}=\pi S/L$.

on Fig. 4. The mean chord length for the first case is $E[\sigma]=\pi S/L=\pi(\pi R^2-ab)/(2\pi R+2(a+b))$ (with $R=2$, $a=\frac{3}{2}$, $b=1$) while, for the second case, it is $E[\sigma]=\pi S/L=\pi(ab-\pi R^2)/(2\pi R+2(a+b))$ (with $R=1$, $a=4$, $b=3$). For both bodies, disk and rectangle are not necessarily centered, and the parameter δ describes the distance between the disk's center and the rectangle's center. Simulations were performed for three values of $\delta=0.0$, 0.5, 1.0. For each case, 10 million straight lines were generated, and more than 6.4 million chords were collected. One simulation takes less than 90 s on a pentium IV at 2.4 GHz. With such a number of chords, the mean chord length has already very well converged to the theoretical value given by Cauchy's theorem. A summary of these results is presented in Table I. It shows that the mean chord length is, as expected, independent of δ. Table I also presents results for the case of a nonconvex body made as the union of two overlapping disks whose centers are separated by a distance 2δ (see Fig. 5). For such a body, the mean chord length is $E[\sigma]=\pi(\pi R^2-R^2(\alpha-\sin\alpha)/2)/(2\pi R-\alpha R)$. Again, the Monte Carlo simulations fit very well theoretical predictions. Figure 6 shows the chord length distribution densities for two values of δ. In three dimensions, the CLD is obtained for a system of two touching, but not overlapping spheres of radius $r=1$ and $R=4$. For such a nonconvex shape, the CLD is known analytically (Sec. III). Since the CLD for a sphere of radius r is $|\sigma/(2r^2)|_0^{2r}$ from Eq. (36), we get

$$f(\sigma)=\frac{1}{2(r^2+R^2)}[|\sigma|_0^{2r}+|\sigma|_0^{2R}]. \tag{56}$$

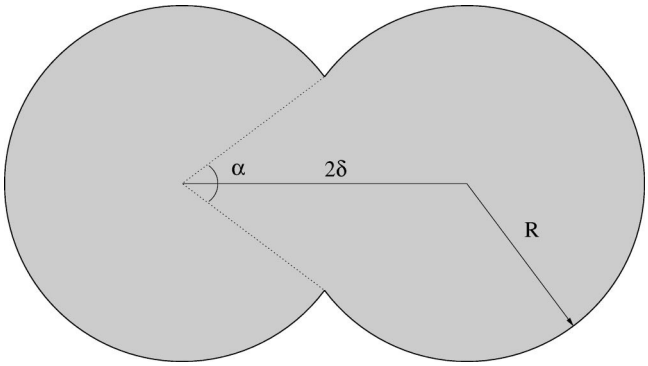

FIG. 5. Nonconvex body made as the union of two overlapping disks whose centers are separated by a distance 2δ.

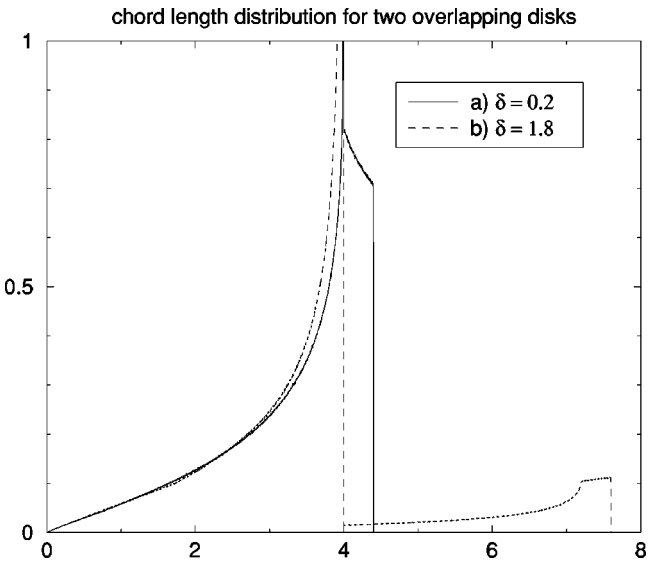

FIG. 6. Chord length distribution density for two overlapping disks whose centers are separated by a distance 2 δ: (a) $\delta = 0.2$ and (b) $\delta = 1.8$.

For this system, Monte Carlo simulations were performed with 100×10^6 random lines (31.6×10^6 chords were collected), and fit perfectly the theoretical predictions of Eq. (56) as shown in Fig. 7.

Monte Carlo simulations, regarding the random walks purely diffusive process, were performed across a nonconvex two-dimensional nonconcentric hollow disk. The external radius is set to $R = 1$, the small radius is set to $r = \frac{1}{2}$, and the small disk's center is at a distance $\delta = 0.4$ from the big disk's center as shown in Fig. 8. Simulations were performed for various values of the mean free path λ, and 10 million random walks were generated for each simulation. Random walks' starting points were chosen with a uniform distribution on either circles and the incidence angle's sinus with a uniform distribution on $[-1,1]$. This corresponds in the limit of infinite mean free paths to the isotropic uniform measure of random lines. In all simulations the single-scattering

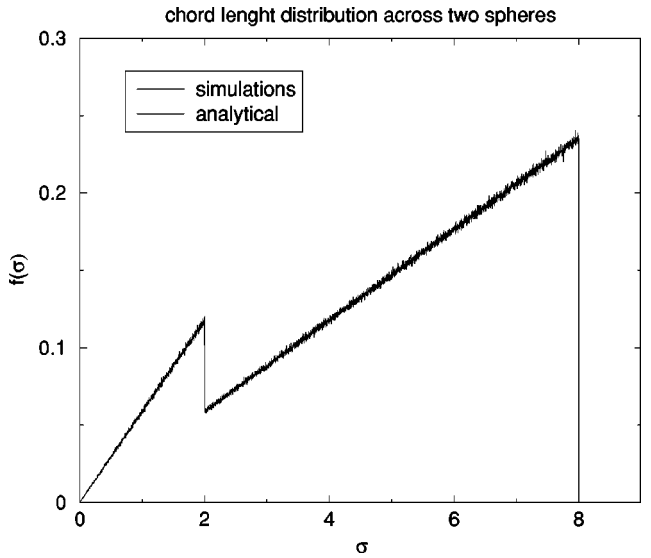

FIG. 7. Chord length distribution density across two nonoverlapping touching spheres of radius $r = 1$ and $R = 4$.

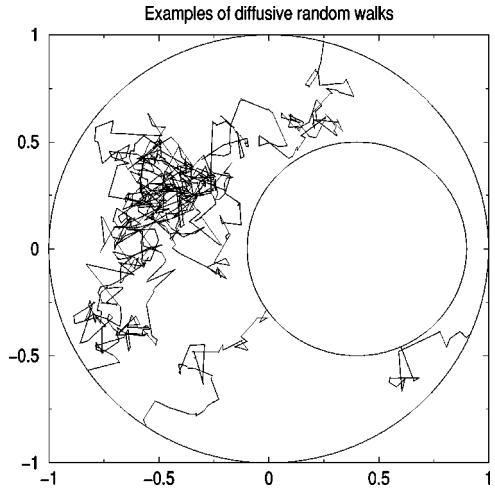

FIG. 8. Random walks generated with a mean free path $\lambda = 0.05$; the big circle's radius is 1.0 and the small circle's radius is 0.5.

phase function is isotrope. Simulated average trajectory length $E[L]$ inside our nonconvex shape is in very good agreement with the theoretical predictions as shown in Table II.

VI. CONCLUSION

Most authors, when faced with a problem requiring the use of Cauchy's formula, restrict themselves to convex bodies. Doing so, they actually follow the hypotheses that lead to an easy derivation of this well-known formula. However, for many physical cases, such as random media, the analysis of nonconvex shapes is needed. In this article it is shown that if each chord is taken for itself, the convex shape hypothesis can be omitted. Cauchy's formula remains valid for bodies enclosed by general smooth differentiable manifolds which correspond to most physical objects. It is further remarkable, as was pointed out, that the result also applies to the case of purely diffusive random walks across nonconvex objects.

APPENDIX: ARRANGEMENT OF HARD PARTICLES IN SPACE, CONNECTION TO SCATTERING EXPERIMENTS

Let us extend Fig. 2 to N, $N \to \infty$, hard convex particles, randomly arranged in space. For simplification we assume that each single particle possesses a fixed volume V_1 and a fixed surface area S_1. Let V_t be the total volume of the particle system. Then, the volume fraction c of the particles is $c = N V_1 / V_t$. The volume of the connected region is $(1-c)V_t$. There is a basic connection between c, the mean chord length of the single particle $m_1 = 4 V_1 / S_1$ and the mean chord length of the nonconvex connected region between the particles, m_2,

$$\frac{1}{l_p} = \frac{1}{m_2 c} = \frac{1}{m_1(1-c)} = \frac{1}{m_1} + \frac{1}{m_2}. \tag{A1}$$

TABLE II. Random walks' simulation results.

λ	$E[L]_{th}$[a]	$E[L]$	Variance	Time (mns)
0.050	0.785398	0.786201	0.00052	~2
0.010	0.785398	0.784719	0.00111	~9
0.005	0.785398	0.783887	0.00157	~14
0.001	0.785398	0.778345	0.00346	~70

[a]$E[L]_{th} = \pi S/L = \pi(R-r)/2$.

Here, l_p is Porod's length parameter. This equation has been carefully studied in the field of small-angle scattering. Equation (A1) has been ascertained in practice (materials research). Eliminating m_2 yields

$$m_2=\frac{1-c}{c}m_1=\frac{1-c}{c}\frac{4\,V_1}{S_1}, \tag{A2}$$

which is a special form of the so-called Rosiwal theorem[20] and agrees with the extension of the Cauchy theorem discussed (see Fig. 2 and Secs. III A and III B). The mean chord length m_2 is connected with the ratio whole system volume over whole inner surface area:

$$m_2=\frac{4\,(V_t-N\,V_1)}{N\,S_1}=\frac{4\,V_t(1-c)}{N\,S_1}. \tag{A3}$$

The outer surface area is not important. It can be neglected for a large particle number. Taking into account $V_t/N=V_1/c$, we recognize the following: The contents of Eq. (A3) and Eqs. (A1) and (A2) agree. The application of the Cauchy theorem for the nonconvex ''matrix region'' is in agreement with the fundamentals of small-angle scattering experiments.

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Deficiency indices of operator polynomials in creation and annihilation operators

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(Received 17 November 2002; accepted 26 August 2003)

We present a new method to compute deficiency indices of operators that are homogeneous polynomials in one pair of creation and annihilation operators. To this end we prove a classification theorem for special cubic forms by means of SU(1,1) transformations and derive new non-self-adjointness criteria for Jacobi-like matrices. The method presented illuminates and systemizes former results of Rabsztyn. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1621060]

I. INTRODUCTION

Creation and annihilation operators were originally introduced in quantum mechanics to diagonalize the harmonic oscillator and are now an indispensable tool in quantum theory being the building blocks for more complicated operators. Here we present a new method for computing the deficiency indices of symmetric operators that are homogeneous polynomials of degree three in one pair of those operators. Deficiency indices measure how far a symmetric operator (sometimes especially in physics literature also called Hermitian or Hermitian symmetric operator) is from being self-adjoint. To know them and, hence, to be able to decide whether or not a symmetric operator is self-adjoint is important in physical applications because different self-adjoint extensions of the same operator yield different descriptions of the system under consideration (see Ref. 10, X.1, for examples). The opposition of self-adjointness and non-self-adjointness, which is important in quantum mechanics, is reflected in classical mechanics where the latter corresponds to a particle that will escape to infinity within a finite time whereas in the first case it will not (see Ref. 10, App. X.1, for a detailed discussion of this analogy and its validity).

Assume we are given a Fock representation of the canonical commutation relations (CCR), i.e., a linear operator $a:D\to\mathcal{H}$ acting along with its adjoint $a^*:D\to\mathcal{H}$ on some dense subspace $D\subset\mathcal{H}$ of a Hilbert space $\mathcal{H}$ and satisfying on D

$$aa^*-a^*a=\mathbb{1}.$$

Accessorily, there is a so-called vacuum vector $\Omega\in D$, $\Omega\neq 0$, such that $a\Omega=0$ and $D_0 := \mathrm{span}\{(a^*)^n\Omega\,|\,n\in\mathbb{N}_0\}$ is dense in $\mathcal{H}$. From a and a^* one can build polynomials of which the harmonic oscillator $a^*a+\mathbb{1}$ is the most prominent example. It is essentially self-adjoint on D_0 as are all operators being symmetric polynomials of degree one and two. This result can be proved via the (sufficient) Carleman criterion for Jacobi matrices (see, e.g., Ref. 1, p. 24), which unfortunately fails to prove self-adjointness for degrees greater than two. Berezanski's criterion (see Theorem 3.1 below) suggests that from degree three onward self-adjointness will not be the rule. Some special cases of higher degrees have been considered thus far. The anharmonic oscillator being of degree four and serving as toy model for interacting quantum fields is proven to be self-adjoint. Various methods of proof are presented in Ref. 10, Chap. X. For general polynomials up to degree four self-adjointness was established in the special case of semi-bounded operators by Jørgensen,[5] who generalized Wouk's theorem on semi-bounded Jacobi matrices (see Ref. 13 or Ref. 1, p. 26) to arbitrary semi-bounded operators. His result is representative in that it is based

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upon some positivity or semi-boundedness property. Since for degree three the operators cannot be semi-bounded at all, Jørgensen's as all the other former results leaves a gap which we shall bridge by exhaustively computing the deficiency indices of the operator

$$A(\alpha_3,\alpha_1) := \alpha_3 a^3 + 3\alpha_1 a^* a^2 + 3\overline{\alpha_1}(a^*)^2 a + \overline{\alpha_3}(a^*)^3, \quad \alpha_1,\alpha_3 \in \mathbb{C}, \tag{1}$$

on a slightly larger domain $D \supset D_0$ to be specified later. At this point we may assume without loss of generality $\alpha_1 = 1$. Our main result (see Theorem 2.3) is that each operator $A(\alpha,1)$ can be linked to exactly one out of four normal forms

$$A(1,0), \qquad A(0,1), \qquad A(-3,1), \qquad A(1,1) \tag{2}$$

having deficiency indices 3,1,1,0, respectively. To which normal form an operator belongs depends, basically, on the sign of the discriminant of a cubic form. Amazingly, we shall see below that the last case of a self-adjoint operator, which is the most eligible one for physicists, occurs very rarely.

To have our operator cast into its normal form we employ a special kind of unitary transformations, the so-called Bogolyubov or canonical transformations, which formally replace a and a^* according to

$$a \mapsto sa + ta^*, \quad a^* \mapsto \overline{t}a + \overline{s}a^*, \qquad s,t \in \mathbb{C} \text{ with } |s|^2 - |t|^2 = 1,$$

and thus transforming the entire operator like

$$A(\alpha,1) \mapsto A(\tilde{\alpha}_3,\tilde{\alpha}_1) + ra + \overline{r}a^*, \quad r \in \mathbb{C}, \tag{3}$$

wherein the linear terms are due to the CCR. The main part behaves like an (ordinary) cubic form

$$\alpha x^3 + 3x^2 y + 3xy^2 + \overline{\alpha} y^3, \quad x,y \in \mathbb{C},$$

under an SU(1,1) transformation. The normal forms of this cubic form can be classified by means of the discriminant $D(\alpha)$ and are labeled by $D(\alpha) > 0$ and $D(\alpha) < 0$, which we call main cases, and by $D(\alpha) = 0$, the exceptional cases, which require additionally the quadratic discriminant $Q(\alpha)$.

In the second step we compute the deficiency indices of the normal forms. We treat the exceptional cases in the $L^2(\mathbb{R})$ representation via solving ordinary differential equations. The main cases are best understood in the $l^2(\mathbb{N}_0)$ representation where $A(\alpha_3,\alpha_1)$ becomes a band matrix and the deficiency equation is a difference equation. For $D(\alpha) > 0$ we are faced even only with a Jacobi, i.e., tridiagonal matrix, wherefore we can refer to a classical result due to Berezanski. The case $D(\alpha) < 0$ requires a new criterion. Because of the linear terms in (3) we have a tridiagonal matrix added to a larger band matrix which makes Berezanski's theorem inapplicable. We would like to remark that possibly contrary to one's intuition these linear terms cannot be considered a small perturbation to $A(\tilde{\alpha}_3,\tilde{\alpha}_1)$ whence we cannot use the Kato–Rellich theorem (see Ref. 10, Th. X.12, and Ref. 12, Th. 6.1). For even though the inequality

$$\|(ra + \overline{r}a^*)\varphi\|^2 \leqslant \gamma \|(a^3 + (a^*)^3)\varphi\|^2 + \delta \|\varphi\|^2$$

can be proved, the necessary condition $\gamma < 1$ can be ensured if and only if r is small.[6]

The deficiency indices of $A(\alpha_3,\alpha_1)$ were formerly computed by Rabsztyn,[8] who worked in the $L^2(\mathbb{R})$ realization by which means the deficiency equation becomes an ordinary differential equation. To examine this equation he consults the theory of asymptotic solutions instead of deriving exact solutions. However, though this reduces heavily the number of calculations to be carried out, there are a lot of cases to be distinguished, cases that have nothing to do with the normal forms above. Therefore, the actual origin of the deficiency indices is obscured and it seems to be difficult to generalize the method to higher powers in a systematic way. Contrary to this, the

method presented here explains the distribution of the deficiency indices in a more natural way by an algebraic criterion which can be generalized to forms of higher degree even though the computational difficulties will increase.

II. SETTING AND RESULTS

Let $\mathcal{H}$ be a separable complex Hilbert space. For a symmetric operator $A:D(A)\to\mathcal{H}$, $D(A)\subset\mathcal{H}$ a dense subspace, the deficiency indices (see, e.g., Ref. 10, Ch. X) are the numbers $n_\pm(z):=\dim\ker(A^*\mp z\mathbb{1})$, $\operatorname{Im} z>0$, with A^* being the adjoint operator and $\mathbb{1}$ the identity. Since $n_\pm(z)$ is constant in the upper and lower half-plane, respectively, we may simply write $n_\pm$. A symmetric operator is essentially self-adjoint if and only if $n_\pm=0$.

A Fock representation with one degree of freedom of the CCR in $\mathcal{H}$ is given by two operators a and a^* satisfying the following conditions:

(1) $a,a^*:D\to\mathcal{H}$ with $D\subset\mathcal{H}$ being a dense subspace and $aD\subset D$ and $a^*D\subset D$.
(2) a^* is the adjoint operator to a.
(3) $aa^*\varphi-a^*a\varphi=\varphi$ for all $\varphi\in D$.
(4) There is an $\Omega\in D$, $\Omega\neq 0$, such that $a\Omega=0$ and $D_0:=\operatorname{span}\{(a^*)^n\Omega|n\in\mathbb{N}_0\}$ is dense in $\mathcal{H}$.

For details and generalizations, see Ref. 3. In the sequel we shall work with the Fock representation in $l^2(\mathbb{N}_0)$ and $L^2(\mathbb{R})$.

Let $\mathcal{H}=l^2(\mathbb{N}_0)$, i.e., the Hilbert space of sequences

$$c=(c_0,c_1,c_2,\ldots),\ c_n\in\mathbb{C},\ \sum_{n=0}^{\infty}|c_n|^2<\infty.$$

Then, the operators

$$(ac)_k=\sqrt{k+1}c_{k+1},\qquad (a^*c)_k=\sqrt{k}c_{k-1},\ \ k\in\mathbb{N}_0, \tag{4}$$

provide a Fock representation with vacuum vector $\Omega=(1,0,\ldots)$. Here and henceforth a negative index as in c_{-1} always requires $c_{-1}:=0$. We choose as domain of definition

$$D:=\{c=(c_0,c_1,\ldots)\in l^2|\forall\kappa\in\mathbb{N}:\sup_{n\in\mathbb{N}_0}n^\kappa|c_n|<\infty\}. \tag{5}$$

Lemma 2.1: Let the symmetric kth *order difference operator* $A:D\to l^2(\mathbb{N}_0)$ *be given by*

$$(Ac)_n:=a_n^{(0)}c_n+\sum_{j=1}^{k}(a_n^{(j)}c_{n+j}+\overline{a}_{n-j}^{(j)}c_{n-j}), \tag{6}$$

the coefficients obeying $a_n^{(j)}=O(n^\gamma)$ *with some* $\gamma\geqslant 0$. *Then* $D(A^*)=D^*$ *where*

$$D^*:=\left\{c\in l^2(\mathbb{N}_0)\left|\sum_{n=0}^{\infty}\left|a_n^{(0)}c_n+\sum_{j=1}^{k}(a_n^{(j)}c_{n+j}+\overline{a}_{n-j}^{(j)}c_{n-j})\right|^2<\infty\right.\right\}. \tag{7}$$

The deficiency indices of A are given by the number of linearly independent solutions to the difference equation

$$a_n^{(0)}c_n+\sum_{j=1}^{k}(a_n^{(j)}c_{n+j}+\overline{a}_{n-j}^{(j)}c_{n-j})=\lambda c_n,\quad \operatorname{Im}\lambda\neq 0, \tag{8}$$

that lie in $l^2(\mathbb{N}_0)$. *In particular this is the number of linearly independent initial conditions* $(c_0,\ldots,c_{k-1})$ *that yield* $l^2(\mathbb{N}_0)$ *solutions to (8).*

Proof: Write down the quadratic form

$$(Ac,d)=\sum_{n=0}^{\infty}\left(a_n^{(0)}c_n+\sum_{j=1}^{k}\left(a_n^{(j)}c_{n+j}+\overline{a}_{n-j}^{(j)}c_{n-j}\right)\right)\overline{d}_n$$

and note that because of the growth condition the order of summation may be interchanged. Thus $d\in D^*$ is only subject to the condition in (7).

The first statement concerning the deficiency indices follows immediately from the first part of the lemma. The second statement is a consequence of the fact that we can choose exactly $c_0,\ldots,c_{k-1}$ as initial values in (8) (note $c_j=0$ for $j<0$). □

Under certain conditions the Fock representation of the CCR is unique up to unitary transformations (Ref. 7, § 4.14; Ref. 3, Th. 1.4). We can conversely exploit this fact to construct a unitary transform by putting

$$b:=sa+ta^*,\quad b^*:=\overline{t}a+\overline{s}a^*$$

with $s,t\in\mathbb{C}$, $|s|^2-|t|^2=1$. Note that s and t are chosen in such a way that b and b^* satisfy the CCR. Now it is crucial that there is $\tilde{\Omega}\in D$, $\tilde{\Omega}\neq 0$, obeying $b\tilde{\Omega}=0$. This was one of the reasons why we wanted a and a^* to act on D in (5) instead of just D_0. We thus have the following.

Theorem 2.2: *The Bogolyubov or canonical transform $U(s,t):\mathcal{H}\to\mathcal{H}$ depending on two parameters $s,t\in\mathbb{C}$ with $|s|^2-|t|^2=1$ is a unitary operator, which maps D into itself and transforms a and a^* according to*

$$U(s,t)aU(s,t)^*=sa+ta^*,\quad U(s,t)a^*U(s,t)^*=\overline{t}a+\overline{s}a^*.$$

Finally, we describe the Fock representation in $L^2(\mathbb{R})$ with underlying Hilbert space $\mathcal{H}=L^2(\mathbb{R})$. Taking the Hermite functions as a basis for $L^2(\mathbb{R})$ yields a Hilbert space isomorphism between $L^2(\mathbb{R})$ and $l^2(\mathbb{N}_0)$ (see Ref. 9, Appendix to V.3) whereby everything carries over from $l^2(\mathbb{N}_0)$ to $L^2(\mathbb{R})$ without further ado. In particular $D=\mathcal{S}(\mathbb{R})$, the Schwartz space, and

$$a=\frac{1}{\sqrt{2}}\left(x+\frac{d}{dx}\right),\quad a^*=\frac{1}{\sqrt{2}}\left(x-\frac{d}{dx}\right). \tag{9}$$

Now everything is at hand to formulate our main result, the following classification for the deficiency indices of $A(\alpha_3,\alpha_1)$, which exactly mirrors the classification of cubic forms in Theorem A.4.

Theorem 2.3: *For $\alpha_1=0$ we have $n_\pm=3$. For $\alpha_1\neq 0$ put $\alpha:=\alpha_3\overline{\alpha_1}/\alpha_1$ and let $D(\alpha):=27(-|\alpha|^4+6|\alpha|^2-4(\alpha+\overline{\alpha})+3)$ be the cubic and $Q(\alpha):=4(1-\alpha)$ be the quadratic discriminant. Then $A(\alpha_3,\alpha_1)$ has the following deficiency indices:*

(1) $D(\alpha)<0$: $n_\pm=3$.
(2) $D(\alpha)>0$: $n_\pm=1$.
(3) $D(\alpha)=0$, $Q(\alpha)\neq 0$: $n_\pm=1$.
(4) $D(\alpha)=Q(\alpha)=0$: $n_\pm=0$.

When $D(\alpha)\neq 0$ the corresponding cases are referred to as main cases, otherwise as exceptional cases.

Proof: First of all, we see by applying $U(-1,0)$ that $n_+=n_-$. For $\alpha_1=0$ the statement then follows from Proposition 3.4. Assume now $\alpha_1\neq 0$. By dint of $U(\overline{\alpha_1}/|\alpha_1|,0)$ we conclude that $A(\alpha_3\overline{\alpha_1}/\alpha_1^2,1)$ has the same deficiency indices as $A(\alpha_3,\alpha_1)$. Due to the CCR

$$U(s,t)A(\alpha,1)U(s,t)=A(\tilde{\alpha}_3,\tilde{\alpha}\alpha_1)+ra+\overline{r}a^*,$$

where the cubic part of the operator behaves like the ordinary cubic form

$$\alpha x^3+3x^2y+3xy^2+\overline{\alpha}y^3$$

under a map from SU(1,1). Hence, Theorem A.4 in the Appendix shows that $A(\alpha,1)$ is unitarily equivalent to exactly one of the operators

$$A(1,0)+ra+\overline{r}a^*, \quad A(0,1)+ra+\overline{r}a^*, \quad A(-3,1)+ra+\overline{r}a^*, \quad A(1,1)+ra+\overline{r}a^* \quad ,$$

whose deficiency indices are given in Propositions 3.4, 3.2, 4.1, and 4.2. □

The interested reader may want to draw a picture showing the curve $D(\alpha)=0$ for himself to visualize the regions of the deficiency indices.

III. DEFICIENCY INDICES: MAIN CASES

We start with $D(\alpha)>0$. The operator to be considered is $A(0,1)+ra+\overline{r}a^*$ whose deficiency equation in $l^2(\mathbb{N}_0)$ reads

$$\sqrt{n+1}(n+r)c_{n+1}+\sqrt{n}(n-1+\overline{r})c_{n-1}=\lambda c_n, \quad n\in\mathbb{N}_0, \tag{10}$$

which can be treated by a classical result due to Berezanski (see Ref. 2, p. 507 or Ref. 1, p. 26).

Theorem 3.1 (Berezanski): *Let $b_n\in\mathbb{R}$ and $a_n\in\mathbb{C}$, $n\in\mathbb{N}_0$, such that*

$$|b_n|\leqslant M<\infty,\ n\in\mathbb{N}_0 \ \text{ and } \ a_n\neq 0,\ |a_{n-1}||a_{n+1}|\leqslant|a_n|^2,\ n\geqslant n_0,\ \sum_{n=n_0}^{\infty}\frac{1}{|a_n|}<\infty$$

with $M\geqslant 0$ and some $n_0\in\mathbb{N}_0$. Then c defined by $c_0:=1$ and

$$a_nc_{n+1}+b_nc_n+\overline{a}_{n-1}c_{n-1}=\lambda c_n, \qquad n\geqslant 0,$$

is in $l^2(\mathbb{N}_0)$ for all $\lambda\in\mathbb{C}$.

This theorem can be applied immediately to our situation.

Proposition 3.2: The sequence defined by (10) is in $l^2(\mathbb{N}_0)$. In particular, for all $r\in\mathbb{C}$ the operator $A(0,1)+ra+\overline{r}a^*$ has deficiency indices (1,1).

Proof: Here $a_n=\sqrt{n+1}(n+r)$ and $b_n=0$ where a simple application of the inequality of the geometric and the arithmetic mean shows the assumptions of Theorem 3.1 being satisfied. Setting $k=1$ and $c_0=1$ in Lemma 2.1 and using (10) prove the proposition. □

We turn to the case $D(\alpha)<0$ with the corresponding operator $A(1,0)+ra+\overline{r}a^*$ having in $l^2(\mathbb{N}_0)$ the deficiency equation

$$\sqrt{(n+1)(n+2)(n+3)}c_{n+3}+r\sqrt{n+1}c_{n+1}+\overline{r}\sqrt{n}c_{n-1}+\sqrt{n(n-1)(n-2)}c_{n-3}=\lambda c_n. \tag{11}$$

We abbreviate

$$a_n:=\sqrt{(n+1)(n+2)(n+3)}, \qquad b_n:=r\sqrt{n+1}, \qquad n\in\mathbb{N}_0. \tag{12}$$

To begin with we introduce the auxiliary quantities e_n via

$$a_ne_{n+3}=a_{n-3}e_{n-3}, \qquad n\geqslant 3, \qquad e_0=\cdots=e_5=1. \tag{13}$$

We need the asymptotics of e_n.

Lemma 3.3: There are constants $K_j>0$, $j=0,\ldots,5$, such that

$$e_{6k+j}=\frac{K_j}{(k+1)^{3/4}}+O\left(\frac{1}{(k+1)^{7/4}}\right), \quad k\in\mathbb{N}_0, \quad j=0,\ldots,5.$$

Proof: From the recursion formula (13) one can derive an explicit representation of the e_n. Then Stirling's formula yields the asymptotics. □

We put

$$c_n = \tau_n e_n d_n \quad \text{with} \quad \tau_{6k+j} = \tau_j, \ \ j = 0,\ldots,5, \tag{14}$$

and τ_j to be fixed below. Inserting this into (11) yields

$$d_{n+3} + \beta_n d_{n+1} - \gamma_n d_n + \delta_n d_{n-1} + d_{n-3} = 0, \tag{15}$$

where we have abbreviated

$$\beta_n := \frac{b_n \tau_{n+1} e_{n+1}}{a_{n+3} \tau_{n+3} e_{n+3}}, \quad \gamma_n := \frac{\lambda \tau_n e_n}{a_{n-3} \tau_{n-3} e_{n-3}}, \quad \delta_n := \frac{\overline{b}_{n-1} \tau_{n-1} e_{n-1}}{a_{n-3} \tau_{n-3} e_{n-3}}. \tag{16}$$

From the above lemma we conclude

$$\left| \frac{\tau_n e_n}{\tau_{n-3} e_{n-3}} \right| \leqslant M < \infty \tag{17}$$

for $n \geqslant 3$ and, having chosen $\tau_0, \ldots, \tau_5$ appropriately,

$$\frac{\tau_{n+1} e_{n+1}}{\tau_{n+3} e_{n+3}} = 1 + O\left(\frac{1}{n}\right), \quad \frac{\tau_{n-1} e_{n-1}}{\tau_{n-3} e_{n-3}} = 1 + O\left(\frac{1}{n}\right) \tag{18}$$

as $n \to \infty$. From (18) and (17) we know

$$\beta_n, \delta_n = O\left(\frac{1}{n}\right), \quad \gamma_n = O\left(\frac{1}{n^{3/2}}\right).$$

By introducing

$$S_n := \begin{pmatrix} 0 & -\beta_n & \gamma_n & -\delta_n & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

and $y_n := (d_{n+2}, \ldots, d_{n-3})^T$ we can write (15) in matrix form

$$y_{n+1} = S_n y_n. \tag{19}$$

Now consider

$$y_{n+6} = S_{n+5} S_{n+4} S_{n+3} S_{n+2} S_{n+1} S_n y_n \tag{20}$$

instead of (19) and decompose the matrix product into

$$y_{n+6} = V_n' y_n + W_n' y_n,$$

where

$$V_n' := \begin{pmatrix} -1 & 0 & \beta_{n+5} & 0 & \delta_{n+5} & 0 \\ 0 & -1 & 0 & \beta_{n+4} & 0 & \delta_{n+4} \\ -\delta_{n+3} & 0 & -1 & 0 & \beta_{n+3} & 0 \\ 0 & -\delta_{n+2} & 0 & -1 & 0 & \beta_{n+2} \\ -\beta_{n+1} & 0 & -\delta_{n+1} & 0 & -1 & 0 \\ 0 & -\beta_n & 0 & -\delta_n & 0 & -1 \end{pmatrix}$$

contains the terms up to order $1/n$ and W_n' the remaining products. We can further simplify V_n' by replacing $\beta_n,\ldots,\beta_{n+5}$ and $\delta_n,\ldots,\delta_{n+5}$ to first order by $\overline{r}/n$:

$$y_{n+6} = \left(-\mathbb{1} + \frac{1}{n}V\right) y_n + W_n y_n \tag{21}$$

with the skew-symmetric matrix

$$V := \begin{pmatrix} 0 & 0 & r & 0 & \overline{r} & 0 \\ 0 & 0 & 0 & r & 0 & \overline{r} \\ -\overline{r} & 0 & 0 & 0 & r & 0 \\ 0 & -\overline{r} & 0 & 0 & 0 & r \\ -r & 0 & -\overline{r} & 0 & 0 & 0 \\ 0 & -r & 0 & -\overline{r} & 0 & 0 \end{pmatrix}.$$

The correcting terms are contained in $W_n = (W_n^{jk})_{j,k=1,\ldots,6}$ and obey

$$W_n^{jk} = O\left(\frac{1}{n^{3/2}}\right), \quad j,k = 1,\ldots,6. \tag{22}$$

Now we can prove the following

Proposition 3.4: For all $r \in \mathbb{C}$ and all initial values c_0, c_1, c_2 every solution to (11) is in $l^2(\mathbb{N}_0)$. In particular, the operator $A(1,0) + ra + \overline{r}a^*$ has deficiency indices (3,3).

Proof: Because of the asymptotics of e_n in Lemma 3.3 it suffices to show that the d_n in (14) are bounded. To this end we prove boundedness of y_n in the Euclidean norm $\|\cdot\|_2$ on $\mathbb{C}^6$. We have from (21)

$$\|y_{n+6}\|_2 \leqslant \left\| \left(-\mathbb{1} + \frac{1}{n}V\right) y_n \right\|_2 + \|W_n y_n\|_2 .$$

Now note that V has purely imaginary eigenvalues and can be diagonalized by a unitary matrix U, $V = U^* \Delta U$. We obtain

$$\|V_n y_n\|_2 = \left\| U^* \left(-\mathbb{1} + \frac{1}{n}\Delta\right) U y_n \right\|_2 \leqslant \left(1 + \frac{\rho}{2}\frac{1}{n^2}\right) \|y_n\|$$

with some $\rho \geqslant 0$. The second norm may be estimated with less care:

$$\|W_n y_n\|_2 \leqslant \frac{K}{n^{3/2}} \|y_n\|_2$$

with some constant $K > 0$ resulting from (22). We thus have

$$\|y_{n+6}\|_2 \leqslant \left(1+\frac{\rho}{2}\frac{1}{n^2}+\frac{K}{n^{3/2}}\right)\|y_n\|_2,$$

wherefrom we derive inductively

$$\|y_{6(k+1)+3}\|_2 \leqslant \prod_{l=0}^{k}\left(1+\frac{\rho}{2}\frac{1}{(6l+3)^2}+\frac{K}{(6l+3)^{3/2}}\right)\|y_3\|_2.$$

The product converges because the corresponding series do.

We apply Lemma 2.1 to (11) by putting $k=3$ and choose for c_0,c_1,c_2 the surely linearly independent vectors

$$(1,0,0), \quad (0,1,0), \quad (0,0,1)$$

wherewith the proposition is proven. □

IV. DEFICIENCY INDICES: EXCEPTIONAL CASES

We start with the case $D(\alpha)=0$, $Q(\alpha)\neq 0$. It will turn out to be more convenient to apply beforehand the Bogolyubov transformation $U(i,0)$. Putting $\lambda = i\mu$, $\mu \in \mathbb{R}$, we arrive at the deficiency equation

$$\left(a^3+a^*a^2-(a^*)^2a-(a^*)^3+\frac{r}{3}a-\frac{\overline{r}}{3}a^*\right)\varphi=\frac{\mu}{3}\varphi, \tag{23}$$

which in $L^2(\mathbb{R})$ reads

$$-x^2\frac{d}{dx}\varphi+\frac{1}{2}\left(1-\frac{r+\overline{r}}{6}\right)\frac{d}{dx}\varphi-\left(1+\frac{r-\overline{r}}{12}\right)x\varphi=-\frac{\mu}{3\sqrt{2}}\varphi. \tag{24}$$

We choose $\mu=-3\sqrt{2}$ and put

$$F:=\frac{1}{2}\left(1-\frac{\mathrm{Re}\, r}{3}\right), \quad G:=\frac{\mathrm{Im}\, r}{6},$$

where

$$(F-x^2)\varphi'-(iG+1)x\varphi=\varphi. \tag{25}$$

Any weak solution to (25) is a strong solution except, possibly, a finite number of isolated singularities (see, e.g., Ref. 4, XIII.2). In other words, we obtain the complete solution by combining the strong solutions on the intervals having boundary points at the singularities. Since we are allowed to choose zero as solution on some (not all) of these intervals it is possible to gain more than one linearly independent weak solution notwithstanding the equation being of order one. To have the complete solution in $L^2(\mathbb{R})$ we must determine which of the partial solutions are in $L^2(\mathbb{R})$.

Proposition 4.1: Equation (25) has exactly one linearly independent square integrable (weak) solution. In particular, the operator $A(-3,1)+ra+\overline{r}a^*$ *has deficiency indices* (1,1).

Proof: The formal solution u of (25) is given through

$$(\ln\varphi)'=\frac{1+(iG+1)x}{F-x^2}=:v(x).$$

In computing the primitive function of v we distinguish the cases $F<0$, $F>0$, and $F=0$. For the sake of simplicity we shall henceforth suppress without loss of generality the constants of integration.

$F<0$. Since $|F|=-F$,

$$\int v(x)\,dx=-\int\frac{1}{|F|+x^2}\,dx-(iG+1)\int\frac{x}{|F|+x^2}\,dx$$

$$=-\frac{1}{\sqrt{|F|}}\arctan\frac{x}{\sqrt{|F|}}-\frac{1}{2}(iG+1)\ln(|F|+x^2).$$

We obtain

$$\varphi(x)=\exp\left(-\frac{1}{\sqrt{|F|}}\arctan\frac{x}{\sqrt{|F|}}\right)\exp\left(-\frac{iG}{2}\ln(|F|+x^2)\right)\frac{1}{(|F|+x^2)^{1/2}} \tag{26}$$

wherein the first two factors are bounded on $\mathbb{R}$ and the third factor is square integrable which shows the statement.

$F>0$. The function in front of φ' has two distinct real zeros. First, for $|x|<\sqrt{F}$,

$$\int\frac{1}{F-x^2}\,dx=\frac{1}{2\sqrt{F}}\ln\frac{\sqrt{F}+x}{\sqrt{F}-x}\qquad\text{and}\qquad\int\frac{x}{F-x^2}\,dx=-\frac{1}{2}\ln(F-x^2).$$

The solution thus is

$$\varphi(x)=\left(\frac{\sqrt{F}+x}{\sqrt{F}-x}\right)^{1/2\sqrt{F}}\exp\left(-\frac{iG}{2}\ln(F-x^2)\right)\frac{1}{(F-x^2)^{1/2}}. \tag{27}$$

Because of $F-x^2>0$ the second factor has absolute value 1. We conclude

$$|\varphi(x)|^2=\frac{(\sqrt{F}+x)^{1/\sqrt{F}}}{(\sqrt{F}-x)^{1/\sqrt{F}}}\frac{1}{(\sqrt{F}-x)(\sqrt{F}+x)}=\frac{(\sqrt{F}+x)^{(1/\sqrt{F})-1}}{(\sqrt{F}-x)^{(1/\sqrt{F})+1}}.$$

Since φ is not square integrable at $x\nearrow\sqrt{F}$ this part must not contribute to the solution

$$\varphi(x)=0\quad\text{for}\quad-\sqrt{F}<x<\sqrt{F}.$$

For $x>\sqrt{F}$ we use

$$\int\frac{x}{x^2-F}\,dx=\frac{1}{2}\ln(x^2-F)\quad\text{and}\quad\int\frac{1}{x^2-F}\,dx=\frac{1}{2\sqrt{F}}\ln\frac{x-\sqrt{F}}{x+\sqrt{F}}$$

to compute the primitive function of v:

$$\varphi(x)=\left(\frac{x+\sqrt{F}}{x-\sqrt{F}}\right)^{1/2\sqrt{F}}\exp\left(\frac{-iG}{2}\ln(x^2-F)\right)\frac{1}{(x^2-F)^{1/2}} \tag{28}$$

having absolute value

$$|\varphi(x)|^2=\frac{(x+\sqrt{F})^{(1/\sqrt{F})-1}}{(x-\sqrt{F})^{(1/\sqrt{F})+1}},$$

where φ is not square integrable at $x\searrow\sqrt{F}$ and the corresponding part of the solution must vanish:

$$\varphi(x)=0 \quad \text{for } x>\sqrt{F}.$$

We arrive at the square integrable part $x<-\sqrt{F}$. The solution here is also given by (28). However, the first factor behaves differently. To see why we write $x=-y, y>0$. Then $y>\sqrt{F}$:

$$|\varphi(x)|^2=\left(\frac{-y+\sqrt{F}}{-y-\sqrt{F}}\right)^{1/\sqrt{F}}\frac{1}{(y-\sqrt{F})(y+\sqrt{F})}=\frac{(y-\sqrt{F})^{(1/\sqrt{F})-1}}{(y+\sqrt{F})^{(1/\sqrt{F})+1}}.$$

Because of $1/\sqrt{F}-1>-1$ this function is square integrable for $y>\sqrt{F}$.

The only square integrable weak solution to (25) is thus given by

$$\varphi(x)=\begin{cases}0 & \text{for } x\geqslant-\sqrt{F},\\ (28) & \text{for } x<-\sqrt{F}.\end{cases}$$

$F=0$. Both zeros in the singular part of (25) coincide where there can be at most two linearly independent weak solutions. We have

$$\int v(x)\,dx=-(iG+1)\ln|x|+\frac{1}{x}.$$

We obtain the solution

$$\varphi(x)=\exp(-iG\ln|x|)\frac{1}{|x|}\exp\left(\frac{1}{x}\right),\quad x\neq 0, \tag{29}$$

and, moreover,

$$|\varphi(x)|^2=\frac{1}{x^2}e^{2/x}.$$

One sees immediately that $|\varphi|^2$ is integrable only at $x\nearrow 0$ where the weak solution of (25) in $L^2(\mathbb{R})$ is given by

$$\varphi(x)=\begin{cases}0 & \text{for } x\geqslant 0,\\ (29) & \text{for } x<0.\end{cases}$$

This completes the proof. □

We conclude with the case $D(\alpha)=Q(\alpha)=0$ for which the result can be given without any effort.

Proposition 4.2: The operator $A(1,1)$ *has deficiency indices* (0,0).

Proof: We have

$$A(1,1)=a^3+3a^*a^2+3(a^*)^2a+(a^*)^3=(a+a^*)^3-3(a+a^*).$$

In our $L^2(\mathbb{R})$ representation $a+a^*$ is just multiplication by x up to a factor where $A(1,1)$ too is a multiplication operator and, thus, essentially self-adjoint on D. □

APPENDIX: CUBIC FORMS AND THEIR NORMAL FORMS

We want to reduce the cubic form

$$\alpha x^3+3xy^2+3x^2y+\overline{\alpha}y^3,\quad x,y\in\mathbb{C},\quad \alpha\in\mathbb{C}, \tag{A1}$$

to certain normal forms by means of a linear map $B\in \mathrm{SU}(1,1)$, i.e.,

$$B=\begin{pmatrix} s & t \\ \overline{t} & \overline{s} \end{pmatrix}, \quad \det B=1. \tag{A2}$$

We know from algebra that we can do this by finding a fractional linear transformation:

$$z\mapsto hz=\frac{sz+t}{\overline{t}z+\overline{s}} \tag{A3}$$

having the same coefficients s and t as B and acting on the polynomial associated to (A1)

$$p_\alpha(z):=\alpha z^3+3z^2+3z+\overline{\alpha}. \tag{A4}$$

We indicate the relationship between h and B by writing $h\sim B$. Note that this correspondence is unique only up to a factor. For each $B\in \mathrm{SU}(1,1)$ the corresponding h is an element of the automorphism group $\mathrm{Aut}(X_+)$ of the unit disc $X_+:=\{z\in\mathbb{C}||z|<1\}$. Moreover, the sets

$$X_0:=\{z\in\mathbb{C}||z|=1\}, \quad X_-:=\{z\in\mathbb{C}||z|>1\} \tag{A5}$$

are left invariant by those transformations. Since the action of h on p_α is uniquely determined by the action on the zeros we need some information on these zeros.

Lemma A.1: Let $\alpha\in\mathbb{C}\setminus\{0\}$ and z_1,z_2,z_3 be the zeros of p_α. Then either $|z_j|=1$, $j=1,2,3$, or $|z_1|=1$, $|z_2|\neq 0$, $z_3=1/\overline{z_2}$ up to permutations.

Proof: Since $\alpha\neq 0$ we have $z_j\neq 0$. We note that along with z also $1/\overline{z}$ is a zero of p_α:

$$p_\alpha\left(\frac{1}{\overline{z}}\right)=\alpha\frac{1}{\overline{z}^3}+3\frac{1}{\overline{z}^2}+3\frac{1}{\overline{z}}+\overline{\alpha}=\frac{1}{\overline{z}^3}\left(\overline{\overline{\alpha}+3z+3z^2+\alpha z^3}\right)=0.$$

Furthermore, Vieta's theorem tells us $z_1z_2z_3=-\overline{\alpha}/\alpha$ where $|z_1||z_2||z_3|=1$. When the first case does not hold we may assume without loss of generality $|z_2|\neq 1$ and hence $z_2\neq 1/\overline{z_2}$. Then,

$$1=|z_1||z_2|\frac{1}{|\overline{z_2}|}=|z_1|,$$

which proves the lemma. □

To decide which case holds we look at the discriminant $D(\alpha)$ of p_α (see, e.g., Ref. 11, p. 102):

$$D(\alpha):=\alpha^4W(\alpha)^2, \quad W(\alpha):=(z_1-z_2)(z_1-z_3)(z_2-z_3). \tag{A6}$$

$D(\alpha)$ can be expressed solely by the coefficients of p_α:

$$D(\alpha)=27(-|\alpha|^4+6|\alpha|^2-4(\alpha+\overline{\alpha})+3)\in\mathbb{R}. \tag{A7}$$

Proposition A.2: Let $\alpha\in\mathbb{C}\{0\}$ and let z_1,z_2,z_3 be the zeros of p_α. Then we have the following.

(1) $D(\alpha)\leqslant 0$: All zeros lie on the unit circle X_0. When $D(\alpha)=0$ there are multiple zeros.
(2) $D(\alpha)>0$: We have $|z_1|=1$ and $|z_2|<1$, $z_3=1/\overline{z_2}$ up to permutations.

Proof: Since $z_j\neq 0$ we may write

$$W(\alpha)=z_1z_2z_3\left(\frac{z_1}{z_3}-\frac{z_1}{z_2}+\frac{z_3}{z_2}-\frac{z_2}{z_3}+\frac{z_2}{z_1}-\frac{z_3}{z_1}\right).$$

(1) Let $|z_j|=1$, i.e., $1/z_j=\overline{z_j}$:

$$W(\alpha)=-\frac{\overline{\alpha}}{\alpha}(z_1\overline{z_3}-\overline{z_1}z_3+\overline{z_1}z_2-z_1\overline{z_2}+\overline{z_2}z_3-z_2\overline{z_3})=-\frac{\overline{\alpha}}{\alpha}2i\,\mathrm{Im}(z_1\overline{z_3}+\overline{z_1}z_2+\overline{z_2}z_3). \quad \text{(A8)}$$

Hence,

$$D(\alpha)=-4|\alpha|^4(\mathrm{Im}(z_1\overline{z_3}+\overline{z_1}z_2+\overline{z_2}z_3))^2\leqslant 0.$$

(2) When not all z_j lie on the unit circle, then by Lemma A.1 $1/z_1=\overline{z_1}$, $z_3=1/\overline{z_2}$, and

$$W(\alpha)=-\frac{\overline{\alpha}}{\alpha}(2\,\mathrm{Re}(z_1(\overline{z_2}-\overline{z_3}))+|z_3|^2-|z_2|^2).$$

Hence,

$$D(\alpha)=|\alpha|^4(2\,\mathrm{Re}(z_1(\overline{z_2}-\overline{z_3}))+|z_3|^2-|z_2|^2)^2>0$$

because by Lemma A.1 $D(\alpha)=0$ can only occur in case 1. □

To obtain normal forms for p_α we transform its zeros to special points.

Proposition A.3: (1) Assume $|z_1|=1$ *and* $0<|z_2|<1$. *Then there is an* $h\in\mathrm{Aut}(X_+)$ *such that*

$$h(z_1)=-1,\quad h(z_2)=0,\qquad h(z_3)=\infty. \quad \text{(A9)}$$

(2) Let $z_1,z_2,z_3\in X_0$ *be pairwise different points. Then there is an* $h\in\mathrm{Aut}(X_+)$ *such that*

$$h(z_1)=-1,\qquad h(z_2)=\vartheta,\ \ h(z_3)=\overline{\vartheta}\quad \text{with}\ \ \vartheta:=e^{i\pi/3}=(1+\sqrt{3})/2 \quad \text{(A10)}$$

after z_j *having been renumbered suitably*.

Proof: (1) Note $z_3=1/\overline{z_2}$. A transformation satisfying (A9) can be written down immediately:

$$hz=-\frac{z-z_2}{z-1/\overline{z_2}}\,\frac{z_1-1/\overline{z_2}}{z_1-z_2}=\frac{z-z_2}{-\overline{z_2}z+1}\,\frac{z_1\overline{z_2}-1}{z_1-z_2}.$$

We check that h has the form required. Because of $|z_1|=1$ we see

$$\left|\frac{z_1\overline{z_2}-1}{z_1-z_2}\right|=\left|\frac{z_1\overline{z_2}-z_1\overline{z_1}}{z_1-z_2}\right|=1,$$

where there is a $\tau\in[0,2\pi[$ such that

$$\frac{z_1\overline{z_2}-1}{z_1-z_2}=e^{i\tau}.$$

Thus,

$$h(z)=\frac{z-z_2}{-\overline{z_2}z+1}e^{i\tau}=\frac{e^{i\tau/2}z-e^{i\tau/2}z_2}{-e^{-i\tau/2}\overline{z_2}z+e^{-i\tau/2}}$$

has the correct form and the determinant is $1-|z_2|^2>0$ because of $|z_2|<1$. Hence we have $(1-|z_2|^2)^{1/2}\in\mathbb{R}$.

(2) We are seeking a transformation h satisfying (A10). To begin with, the transformation h_1 given by

$$h_1\sim\begin{pmatrix} z_2-z_3 & z_1(z_3-z_2)\\ z_2-z_1 & z_3(z_1-z_2)\end{pmatrix}=:M_1$$

maps

$$h_1(z_1)=0, \quad h_1(z_2)=1, \quad h_1(z_3)=\infty.$$

Analogously h_2,

$$h_2 \sim \begin{pmatrix} -\vartheta & -\overline{\vartheta} \\ \overline{\vartheta} & \vartheta \end{pmatrix} =: M_2,$$

maps

$$h_2(\vartheta)=0, \quad h(-1)=1, \quad h_2(\overline{\vartheta})=\infty.$$

Then $h := h_2^{-1} h_1$ is an appropriate candidate. Because of $h_2^{-1} \sim -M_2$, computing $M_1 M_2$ and getting rid of the products $z_1 z_2$, $z_1 z_3$, $z_2 z_3$ with the aid of Vieta's theorem yield

$$h_2 h_1^{-1} \sim \frac{1}{\alpha^2} \begin{pmatrix} \alpha(-\overline{\vartheta} z_1 + (\vartheta+\overline{\vartheta}) z_2 - \vartheta z_3) & \overline{\alpha}(\vartheta \overline{z_3} - (\vartheta+\overline{\vartheta})\overline{z_2} + \overline{\vartheta}\overline{z_1}) \\ \alpha(\vartheta z_1 - (\vartheta+\overline{\vartheta}) z_2 + \overline{\vartheta} z_3) & \overline{\alpha}(-\overline{\vartheta}\overline{z_3} + (\vartheta+\overline{\vartheta})\overline{z_2} - \vartheta \overline{z_1}) \end{pmatrix} =: \frac{1}{\alpha^2} M.$$

The matrix M generates $h_2 h_1^{-1}$ as well as M/α^2. We compute $\det M$. Because of $\vartheta^3=1$ we have

$$-\det M_2 = -\vartheta^2 + \overline{\vartheta}^2 = \overline{\vartheta} - \vartheta = -2i \operatorname{Im} \vartheta = -i\sqrt{3}.$$

Furthermore,

$$\det M_1 = (z_2-z_3)(z_2-z_1)(z_1-z_3) = -W(\alpha) = 2i \frac{\overline{\alpha}}{\alpha} \operatorname{Im}(z_1\overline{z_3} + \overline{z_1} z_2 + \overline{z_2} z_3),$$

where we used (A8). Hence,

$$\det M = -\det M_2 \det M_1 = 2\sqrt{3}|\alpha| \operatorname{Im}(z_1\overline{z_2} + \overline{z_1} z_2 + \overline{z_2} z_3).$$

By renumbering the z_j we can always ensure $\operatorname{Im}(z_1\overline{z_3} + \overline{z_1} z_2 + \overline{z_2} z_3) > 0$ where $\sqrt{\det M} \in \mathbb{R}$. Then $M/\sqrt{\det M}$ satisfies (A2). □

When the discriminant vanishes there are two possible cases. First, we have one single and one twofold zero. This case can be treated by Proposition A.3. A simple polynomial is

$$p_\alpha(z) = z^3 - z^2 - z + 1. \tag{A11}$$

We can map the zeros z_1 and z_2 to -1 and ϑ. The same holds for our prescribed image points -1 and 1. The statement then follows from the group structure of $\operatorname{Aut}(X_+)$.

When there is a threefold zero p_α already has its normal form since in this case $\alpha=1$ which follows from the quadratic discriminant vanishing (see Ref. 11, p. 102):

$$4(1-\alpha)=0.$$

Hence $\alpha=1$. We summarize our results for the cubic form (A1).

Theorem A.4: *Let* $D(\alpha) = 27(-|\alpha|^4 + 6|\alpha|^2 - 4(\alpha+\overline{\alpha}) + 3)$ *be the cubic and* $Q(\alpha) = 4(1-\alpha)$ *be the quadratic discriminant of the cubic form (A1). Then, there is an* SU(1,1) *map that maps (A1) to one of the following normal forms:*

(1) $D(\alpha) < 0$: $x^3 + y^3$.
(2) $D(\alpha) > 0$: $x^2 y + x y^2$.
(3) $D(\alpha) = 0$, $Q(\alpha) \neq 0$: $x^3 - x^2 y - x y^2 + y^3$.
(4) $D(\alpha) = Q(\alpha) = 0$, i.e., $\alpha = 1$: $x^3 + 3x^2 y + 3x y^2 + y^3$.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 44, NUMBER 12 DECEMBER 2003

The helically-reduced wave equation as a symmetric-positive system

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(Received 9 June 2003; accepted 28 August 2003)

Motivated by the partial differential equations of mixed type that arise in the reduction of the Einstein equations by a helical Killing vector field, we consider a boundary value problem for the helically-reduced wave equation with an arbitrary source in $2+1$ dimensional Minkowski space–time. The reduced equation is a second-order partial differential equation which is elliptic in a disk and hyperbolic outside the disk. We show that the reduced equation can be cast into symmetric-positive form. Using results from the theory of symmetric-positive differential equations, we show that this form of the helically-reduced wave equation admits unique, strong solutions for a class of boundary conditions which include Sommerfeld conditions at the outer boundary. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1623930]

I. INTRODUCTION

Physical systems are typically governed by partial differential equations (PDEs) of a fixed type: elliptic, hyperbolic, or parabolic. The mathematical properties of such equations have been extensively investigated (see, e.g., Refs. 1 and 2). Considerably less is known about PDEs of *mixed type*, by which we mean equations whose type is different in different subdomains of the domain of interest, e.g., elliptic in one region and hyperbolic in another.[3] Compared to elliptic, hyperbolic, or parabolic equations, mixed type equations are rather unusual, both in the boundary conditions that can be imposed to get existence and uniqueness of solutions as well as in the regularity of solutions that are obtained. Moreover, the lower-order terms in equations of mixed type take on a more significant role than in equations of fixed type. This latter feature means that it is difficult to obtain general results about PDEs of mixed type; to a large extent, one must investigate each set of equations, each set of boundary conditions, etc., separately.

In relativistic field theory on a fixed space–time, mixed type equations occur after performing a symmetry reduction of hyperbolic PDEs with respect to an isometry group which has an infinitesimal generator that changes type from timelike to spacelike. In generally covariant theories, such symmetry reductions may yield PDEs of mixed type in appropriate gauges. An important example of the latter type, currently of considerable interest in gravitational physics, arises in the quasi-stationary approximation to the two-body problem in general relativity.[4–6] Here one is interested in solving the Einstein equations for space–times admitting a helical Killing vector field. The helical Killing vector field, which represents a rotating reference frame, will be timelike near the bodies and spacelike far from the bodies. The reduced Einstein equations (modulo gauge) can be expected to include nonlinear PDEs of mixed type on the $2+1$ dimensional manifold of orbits of the Killing vector field. The reduced equations can only be solved numerically, but one naturally desires as much *a priori* information about existence and uniqueness of solutions, regularity of solutions, admissible boundary conditions, etc. as one can get. The quasi-stationary approximation to the relativistic two-body problem is the principal motivation behind the work presented here.

As a warm-up for numerically solving the Einstein equations in the quasi-stationary approximation, the wave equation and some of its nonlinear extensions, reduced by the assumption of helical symmetry, have been examined, both analytically and numerically in Ref. 7. The helically-

reduced wave operator is elliptic inside a ''light cylinder'' and hyperbolic outside the cylinder. It was shown in Ref. 7 that one can give a formal series solution of the helically-reduced wave equation for a source consisting of a pair of equal and opposite point charges, placed symmetrically with respect to the axis of helical symmetry. For these analytical solutions, Sommerfeld conditions were prescribed at an outer boundary (which may be at infinity).[8] The choice of such boundary conditions can be motivated on physical grounds, and the apparent analytic existence of unique solutions in the linear case and numerical solutions in the nonlinear case gives confidence that the helically-reduced equation can be treated as a boundary value problem. However, from a mathematical point of view it is not immediately clear *a priori* why such boundary conditions are admissible, that is, why one should expect unique solutions to exist. Our goal here is to understand existence, uniqueness, regularity, etc.—in short, the well-posed nature of this problem—from a general point of view that does not rely upon explicitly constructing a solution to the PDE. The idea is that such a point of view can be used to better understand the helically-reduced Einstein equations, which will not yield so easily to a direct assault.

In the past, certain boundary value problems of mixed type have been addressed using the theory of ''symmetric-positive'' differential equations,[9] which can be viewed as a generalization of elliptic and hyperbolic equations. Friedrichs[9] and Lax and Phillips[10] have given the basic existence and uniqueness results for linear symmetric-positive equations. In this article we shall show that the helically-reduced wave equation with arbitrary sources in $2+1$ dimensions can be cast into symmetric-positive form. We can then deduce existence and uniqueness results for a class of boundary conditions that include the Sommerfeld conditions used in Ref. 7. These results provide support for the proposition that boundary value problems of mixed type arising from helical symmetry reductions—such as arise in the relativistic two-body problem—are well-posed.

II. THE HELICALLY-REDUCED WAVE EQUATION

We consider $2+1$ dimensional Minkowski space–time $(\mathbf{R}^3,\eta)$ and a helical Killing vector field ξ. There will exist an inertial-Cartesian coordinate chart (t,x,y), such that

$$\eta=-dt\otimes dt+dx\otimes dx+dy\otimes dy, \tag{2.1}$$

and

$$\xi=\frac{\partial}{\partial t}+\Omega\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right) \tag{2.2}$$

for some constant Ω. In the corresponding inertial-polar coordinates (t,r,ϕ) we have

$$\eta=-dt\otimes dt+dr\otimes dr+r^2d\phi\otimes d\phi, \tag{2.3}$$

and

$$\xi=\frac{\partial}{\partial t}+\Omega\frac{\partial}{\partial\phi}. \tag{2.4}$$

Note that ξ is not of a fixed type:

$$\eta(\xi,\xi)=r^2\Omega^2-1\begin{cases}>0 & \text{for } r>\dfrac{1}{\Omega},\\ =0 & \text{for } r=\dfrac{1}{\Omega},\\ <0 & \text{for } r<\dfrac{1}{\Omega}.\end{cases} \tag{2.5}$$

We will call the set of space–time events with $r=1/\Omega$ the *light cylinder*.

The wave equation with source $j:\mathbf{R}^3\to\mathbf{R}$ is given by

$$\Box\Phi=j. \tag{2.6}$$

In the inertial-polar chart, the wave operator acting on a function $\Phi:\mathbf{R}^3\to\mathbf{R}$ takes the form

$$\Box\Phi=-\partial_t^2\Phi+\frac{1}{r}\partial_r(r\partial_r\Phi)+\frac{1}{r^2}\partial_\phi^2\Phi. \tag{2.7}$$

We now restrict attention to fields and sources which are invariant under the one-parameter isometry group G generated by ξ. This is equivalent to requiring

$$\xi(\Phi)=0=\xi(j). \tag{2.8}$$

These conditions imply that Φ and j define functions on the manifold of orbits $\mathbf{R}^3/G$, which shall be denoted by Ψ and f, respectively. Because the source j is assumed G-invariant, and because G is an isometry group for the space–time, the wave equation (2.6) admits G as a symmetry group and it descends to define a PDE relating Ψ to f on $\mathbf{R}^3/G$.[11,12] To obtain this differential equation in local coordinates we proceed as follows. Group invariants on $\mathbf{R}^3$ are functions of r and

$$\varphi:=\phi-\Omega t, \tag{2.9}$$

which define polar coordinates on $\mathbf{R}^3/G\approx\mathbf{R}^2$. In particular, granted (2.8), we have

$$\Phi(t,r,\phi)=\Psi(r,\varphi),\quad j(t,r,\phi)=f(r,\varphi). \tag{2.10}$$

The reduced field equation on $\mathbf{R}^3/G$ can be obtained by substituting (2.10) into (2.6), which gives

$$\frac{1}{r}\partial_r(r\partial_r\Psi)+\frac{1}{r^2}\chi(r)\partial_\varphi^2\Psi=f, \tag{2.11}$$

where

$$\chi(r)=1-\Omega^2r^2. \tag{2.12}$$

Note that the light cylinder on $\mathbf{R}^3$ projects to a *light circle* at $r=1/\Omega$ on $\mathbf{R}^3/G$. Evidently, (2.11) is elliptic inside the light circle and hyperbolic outside the light circle, which is a consequence of the changing character (2.5) of the Killing vector ξ. Thus (2.11) is a PDE of mixed type.

In Ref. 7 (2.11) is solved on a disk of radius R with source f corresponding to two equal and opposite ''scalar point charges'' placed symmetrically relative to the origin. Sommerfeld conditions are imposed at the boundary of the disk, and it is required that Ψ vanishes at the origin. The solution is given as a formal infinite series. As noted in Ref. 7, despite the mixed type of the PDE and, in particular, despite the fact that a Sommerfeld condition was enforced in the region where the PDE is hyperbolic, a unique solution exists. Here we provide a somewhat more general version of this result using the theory of symmetric positive equations. We consider (2.11) on a domain[13] $\epsilon\leqslant r\leqslant R$, $0<\epsilon<1/\Omega$. We allow for a general source f and we employ a class of boundary conditions that include Sommerfeld conditions at $r=R$, such as considered in Ref. 7. Specifically, we will impose the following boundary conditions:

$$\Psi(\epsilon,\varphi)=0,\quad \tau(\varphi)R\partial_r\Psi(R,\varphi)+\sigma(\varphi)\partial_\varphi\Psi(R,\varphi)=0,\quad \sigma\tau\neq 0, \tag{2.13}$$

where σ and τ represent smooth functions on the outer boundary $r=R$. Sommerfeld boundary conditions correspond to setting $\tau=1/R$ and $\sigma=\pm\Omega$.

Although we explicitly consider homogeneous boundary conditions (2.13), because we allow for an arbitrary source f in (2.11) a large class of inhomogeneous boundary conditions

$$\Psi(\epsilon,\varphi)=k(\varphi), \quad \tau(\varphi)R\partial_r\Psi(R,\varphi)+\sigma(\varphi)\partial_\varphi\Psi(R,\varphi)=l(\varphi), \tag{2.14}$$

can also be accommodated. This is done by choosing a smooth function $\Lambda=\Lambda(r,\varphi)$ which satisfies the inhomogeneous boundary conditions (2.14) and then redefining

$$\Psi\to\tilde{\Psi}=\Psi-\Lambda, \quad f\to\tilde{f}=f-\frac{1}{r}\partial_r(r\partial_r\Lambda)+\frac{1}{r^2}\chi(r)\partial_\varphi^2\Lambda. \tag{2.15}$$

$\tilde{\Psi}$ now satisfies (2.11) with source $\tilde{f}$ and homogeneous boundary conditions (2.13), to which our results apply.

III. SYMMETRIC-POSITIVE PDEs

Existence and uniqueness results can be obtained for linear PDEs of mixed type if they can be cast into first-order, symmetric-positive form with appropriate boundary conditions.[9,10] Here we summarize the results from Refs. 9 and 10 which we shall need.

For our purposes, the data used to define a symmetric positive system of equations with admissible boundary conditions will be taken to be[14]

(i) a smooth manifold M with smooth boundary ∂M; we set $\overline{M}=M\cup\partial M$;
(ii) a smooth scalar density of weight-1 on M, denoted by ω; and
(iii) a finite-dimensional real vector space V with scalar product $(\cdot,\cdot)$.

Let $u:\overline{M}\to V$. We consider a first-order system of differential equations for u on M of the form

$$Lu\equiv A^a\nabla_a u+Bu=h, \tag{3.1}$$

where $h:\overline{M}\to V$ and, at each $x\in M$, A^a and B are linear transformations:

$$A^a(x):T_x^*M\times V\to V, \quad B(x):V\to V. \tag{3.2}$$

For simplicity we assume that A^a and B depend smoothly on $x\in M$. The differential operator ∇_a is the exterior derivative on functions defined by any basis for V.

Definition 3.1: The system (3.1) is **symmetric-positive** *if (1) A^a defines a symmetric operator (with respect to the scalar product on V),*

$$(A^a(x)v_a)^*=A^a(x)v_a, \quad \forall v\in T_x^*M \quad \text{and} \quad \forall x\in M, \tag{3.3}$$

and (2) the linear operator $K(x):V\to V$, defined by

$$K=B-\tfrac{1}{2}\nabla_a(\omega A^a), \tag{3.4}$$

has a positive-definite symmetric part:

$$K(x)+K^*(x)>0, \quad \forall x\in M. \tag{3.5}$$

We remark that ∇_a in (3.4) is defined by its unique torsion-free extension to vector densities of weight-1 on M taking values in $V\otimes V^*$.

A class of boundary conditions on $u:\overline{M}\to V$ has been determined such that there exist unique solutions to symmetric-positive systems of PDEs. Following Friedrichs, we call these boundary conditions *admissible*. They are defined as follows.

Definition 3.2: **Boundary conditions** *on $u:\overline{M}\to V$ are the requirement that, at each $x\in\partial M$, $u(x)$ takes values in a linear subspace $N(x)\subset V$, which varies smoothly with x.*

We fix an outwardly oriented normal one-form, n_a, to the boundary ∂M. This one-form is uniquely determined up to multiplication by a smooth positive function on the boundary. We define[15]

$$\beta = n_a A^a|_{\partial M}. \tag{3.6}$$

Definition 3.3: Let $u:\overline{M}\to V$ be subject to the system of equations (3.1). The boundary conditions $u(x)\in N(x)$ on ∂M are **admissible** *if $N(x)$ is a maximal subspace such that the quadratic form $u\to(u,\beta u)$ is non-negative at each $x\in\partial M$.*

Note that the admissibility of a set of boundary conditions does not depend upon the specific choice of covariant normal to the boundary. In the sequel we will make use of the following convenient characterization of admissible boundary conditions, which is due to Friedrichs.[9]

Proposition 3.4: Admissible boundary conditions, $u(x)\in N(x)$ on ∂M, are equivalent to the linear boundary conditions $\beta_2 u=0$ on ∂M, where β_2 arises from a decomposition

$$\beta=\beta_1+\beta_2 \tag{3.7}$$

such that, for all $x\in\partial M$, (i) every $v\in V$ can be decomposed via

$$v=v_1+v_2, \quad \beta_1 v_2=\beta_2 v_1=0, \tag{3.8}$$

and (ii)

$$\mu:=\beta_1-\beta_2 \tag{3.9}$$

has a non-negative symmetric part:

$$\mu+\mu^*\geqslant 0. \tag{3.10}$$

We now summarize the existence and uniqueness results of Refs. 9 and 10 for symmetric-positive systems. We say that a mapping $u:M\to V$ is in $L^2(M,V)$ if

$$\|u\|^2\equiv\int_M (u,u)\omega<\infty. \tag{3.11}$$

Definition 3.5: Let the mappings $u:M\to V$ and $h:M\to V$ be in $L^2(M,V)$; u is a **strong solution** *to (3.1) satisfying the boundary conditions $u(x)\in N(x)$ on ∂M if there exists a sequence of functions $\{u_k\}\in C^\infty(\overline{M},V)$, satisfying the boundary conditions $u_k(x)\in N(x)$ on ∂M, such that*

$$u_k\to u, \quad \text{and } Lu_k\to h$$

in the L^2 (semi-)norm (3.11).

Theorem 3.6 (Friedrichs, Lax and Phillips): *If (3.1) is symmetric-positive, then it admits a unique, strong solution satisfying admissible boundary conditions.*

We remark that the theorems appearing in Refs. 9 and 10 use (piecewise) continuously differentiable functions u_k to define strong solutions. However, it is straightforward to check that the relevant results go through for $\{u_k\}\in C^\infty(\overline{M},V)$, which we use here.

IV. A SYMMETRIC-POSITIVE SYSTEM FOR THE HELICALLY-REDUCED WAVE EQUATION

Here we show that the helically-reduced wave equation can be expressed in symmetric-positive form. We choose M to be the annulus $M=\{(r,\varphi)|\epsilon<r<R\}$ equipped with the metric

$$g=dr\otimes dr+r^2 d\varphi\otimes d\varphi, \tag{4.1}$$

and associated volume density:

$$\omega = (\det g)^{1/2} = r. \tag{4.2}$$

We set $V = \mathbf{R}^2$ and equip it with the standard scalar product

$$(u,v) = u_1 v_1 + u_2 v_2. \tag{4.3}$$

We consider the following first-order system:

$$\frac{1}{r}\partial_r u_2 + \frac{1}{r^2}\chi \partial_\varphi u_1 = f, \tag{4.4}$$

$$\frac{1}{r}\partial_r u_1 - \frac{1}{r^2}\partial_\varphi u_2 = 0. \tag{4.5}$$

Setting

$$u_1 = \partial_\varphi \Psi, \quad u_2 = r\partial_r \Psi, \tag{4.6}$$

all classical (C^2) solutions to (2.11) and (2.13) are solutions to (4.4) and (4.5). The solution u thus obtained satisfies the boundary conditions

$$u_1(\epsilon,\varphi) = 0, \quad \sigma(\varphi)u_1(R,\varphi) + \tau(\varphi)u_2(R,\varphi) = 0, \quad \sigma\tau \neq 0. \tag{4.7}$$

Conversely, given a classical (C^1) solution to (4.4) and (4.5) satisfying boundary conditions (4.7), the (C^2) function Ψ defined by

$$\Psi(r,\varphi) = \int_\epsilon^r dr' \frac{1}{r'} u_2(r',\varphi) \tag{4.8}$$

satisfies (4.6) and hence (2.11) and (2.13). In this sense the equations (2.11) and (2.13) are equivalent to (4.4), (4.5), and (4.7). We write the system (4.4) and (4.5) as

$$(\tilde{A}^a \nabla_a u - \tilde{h}) = 0, \tag{4.9}$$

where

$$\tilde{A}^r = \frac{1}{r}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{A}^\varphi = \frac{1}{r^2}\begin{pmatrix} \chi & 0 \\ 0 & -1 \end{pmatrix}, \quad \tilde{h} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \tag{4.10}$$

and

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{4.11}$$

Now consider the following first-order system,

$$L(\tilde{A}^a \nabla_a u - \tilde{h}) = 0, \tag{4.12}$$

where

$$L = \begin{pmatrix} a & -c\chi \\ c & a \end{pmatrix}, \tag{4.13}$$

and $a=a(r)$ and $c=c(r)$ are smooth functions on $\overline{M}$. We require that a and c satisfy

$$a^2+c^2\chi\neq 0, \tag{4.14}$$

so that (4.12) is equivalent to (4.9). We write (4.12) as

$$A^a\nabla_a u=h, \tag{4.15}$$

where

$$A^r=\frac{1}{r}\begin{pmatrix} -c\chi & a \\ a & c \end{pmatrix}, \quad A^\varphi=\frac{1}{r^2}\begin{pmatrix} a\chi & c\chi \\ c\chi & -a \end{pmatrix}, \tag{4.16}$$

and

$$h=\begin{pmatrix} af \\ cf \end{pmatrix}. \tag{4.17}$$

We now show that the functions a and c can be chosen so that the system (4.15) is symmetric-positive. The linear transformations defined by A^a are symmetric for any choice of a and c. Using (3.4) we find that

$$K=K^*=\frac{1}{2}\begin{pmatrix} \partial_r(c\chi) & -\partial_r a \\ -\partial_r a & -\partial_r c \end{pmatrix}. \tag{4.18}$$

Necessary and sufficient conditions for (3.5) are

$$\partial_r c<0, \quad (\partial_r c)\partial_r(c\chi)<-(\partial_r a)^2. \tag{4.19}$$

A pair of smooth functions that satisfy (4.19) and (4.14) for $0<\epsilon\leqslant r\leqslant R$ are of the form

$$a=\text{const}, \quad c=-\alpha+e^{-\Omega^3 r^3}, \tag{4.20}$$

provided the constants $|a|$ and $\alpha>0$ are chosen large enough, as is easily verified from

$$\partial_r c=-3\Omega^3 r^2 e^{-\Omega^3 r^3}, \quad \partial_r(c\chi)=\Omega^2 r\{2\alpha-e^{-\Omega^3 r^3}(2+3\Omega r\chi)\}. \tag{4.21}$$

Thus, with these choices for a and c, the equations (4.15) are symmetric-positive. We summarize the preceding discussion as follows.

Proposition 4.1: The equations (2.11) and (2.13) are equivalent to the symmetric-positive system (4.15) and (4.7).

V. ADMISSIBLE BOUNDARY CONDITIONS

We now consider the boundary conditions (4.7) for which we have the following result.

Proposition 5.1: The constants a and α in (4.13) and (4.20) can be chosen so that the boundary conditions (4.7) for (4.15) are admissible.

Proof: For the normal one-form to the boundary we use

$$n=\begin{cases} Rdr & \text{at } r=R, \\ -\epsilon dr & \text{at } r=\epsilon. \end{cases} \tag{5.1}$$

We then have

$$\beta(R)=\begin{pmatrix} -c(R)\chi(R) & a \\ a & c(R) \end{pmatrix}, \quad \beta(\epsilon)=\begin{pmatrix} c(\epsilon)\chi(\epsilon) & -a \\ -a & -c(\epsilon) \end{pmatrix}. \tag{5.2}$$

We consider boundary conditions of the form

$$\sigma u_1+\tau u_2=0 \quad \text{on } \partial M, \tag{5.3}$$

where

$$\sigma=1, \quad \tau=0, \quad \text{at } r=\epsilon, \tag{5.4}$$

and

$$\sigma=\sigma(\varphi)\neq 0, \quad \tau=\tau(\varphi)\neq 0, \quad \text{at } r=R. \tag{5.5}$$

Following Proposition 3.4, we define

$$\beta_1=\pm N\begin{pmatrix} -\tau^2 c\chi-\sigma\tau a & \sigma\tau c\chi+\sigma^2 a \\ \tau^2 a-\sigma\tau c & -\sigma\tau a+\sigma^2 c \end{pmatrix}, \quad \beta_2=\pm N\begin{pmatrix} -\sigma^2 c\chi+\sigma\tau a & -\sigma\tau c\chi+\tau^2 a \\ \sigma^2 a+\sigma\tau c & \sigma\tau a+\tau^2 c \end{pmatrix}, \tag{5.6}$$

where

$$N=\frac{1}{\sigma^2+\tau^2}, \tag{5.7}$$

so that

$$\beta=\beta_1+\beta_2. \tag{5.8}$$

In (5.6) the plus/minus sign is to be used at the outer/inner boundary. The boundary conditions (5.3) are equivalent to

$$\beta_2 u=0 \quad \text{on } \partial M. \tag{5.9}$$

At the inner boundary we have

$$\frac{1}{2}(\mu+\mu^*)=\begin{pmatrix} -c(\epsilon)\chi(\epsilon) & 0 \\ 0 & -c(\epsilon) \end{pmatrix}. \tag{5.10}$$

We choose α sufficiently large so that $c(\epsilon)<0$ and we assume the inner boundary is within the light circle so we have $\chi(\epsilon)>0$. Therefore $(\mu+\mu^*)$ is non-negative at the inner boundary; the inner boundary condition is admissible. At the outer boundary we have

$$\frac{1}{2}(\mu+\mu^*)=N\begin{pmatrix} -2\sigma\tau a+(\sigma^2-\tau^2)c\chi & -\sigma\tau\Omega^2 r^2 c \\ -\sigma\tau\Omega^2 r^2 c & -2\sigma\tau a+(\sigma^2-\tau^2)c \end{pmatrix}_{r=R}. \tag{5.11}$$

Evidently, the outer boundary conditions are admissible in the case $\sigma\tau>0$ provided a is chosen sufficiently negative.[16] If $\sigma\tau<0$, the boundary conditions are admissible provided a is chosen sufficiently positive.[16] Thus the outer boundary conditions are admissible. □

We remark that the admissibility of the outer boundary conditions did not depend upon the location of the outer boundary. Therefore, the outer boundary conditions can be imposed outside, inside, and even *on* the light circle. We also note that the proof of Proposition 5.1 shows that at the outer boundary neither Dirichlet conditions ($\sigma=1$, $\tau=0$) nor Neumann conditions ($\sigma=0$, $\tau=1$) for Ψ are admissible.

VI. CONCLUSIONS

From Propositions 4.1 and 5.1 and Theorem 3.6 we have the following basic existence and uniqueness result for the helically-reduced wave equation in its symmetric positive form.

Theorem 6.1: *The system (4.15) admits a unique, strong solution satisfying the boundary conditions (4.7).*

While this theorem only establishes existence of distributional solutions to the first-order form of (2.11) and (2.13), it does imply that classical solutions to (2.11) and (2.13) are unique. Considerable additional analysis is needed to establish existence of C^2 solutions to (2.11) and (2.13). However, using Theorem 6.1 the following regularity properties of Ψ can be immediately inferred.

Let us define $\tilde{H}^1(M)$ as the completion in the H^1 norm,

$$\|\Psi\|_1^2 = \int_M (\Psi^2 + g^{ab}\nabla_a\Psi\nabla_b\Psi)\,\omega, \tag{6.1}$$

of the space of smooth functions Ψ satisfying the boundary conditions (2.13).

We can then deduce the following from Theorem 6.1.

Corollary 6.2: Let u be the strong solution to (4.15) and (4.7). The function Ψ, defined by

$$\Psi = \int_\epsilon^r dr' \frac{1}{r'} u_2(r') \equiv I(u), \tag{6.2}$$

is in $\tilde{H}^1(M)$ with (distributional) derivatives given by

$$u_1 = \partial_\varphi \Psi, \quad u_2 = r\partial_r \Psi. \tag{6.3}$$

Proof: I is easily verified to be a bounded linear transformation from the dense subspace $C^\infty(M,V) \subset L^2(M,V)$ to $L^2(M)$, so I can be extended to all of $L^2(M,V)$ thus defining $\Psi \in L^2(M)$ via (6.2). Let $u_n : M \to V$ be a sequence of smooth maps that converges to the strong solution u. Clearly,

$$I(u_{2n})|_{r=\epsilon} = 0, \tag{6.4}$$

so that the inner boundary condition is satisfied. We have

$$\partial_r I(u_{2n}) = \frac{1}{r} u_{2n} \to \frac{1}{r} u_2 \in L^2(M,V), \tag{6.5}$$

and it is straightforward to verify that

$$\partial_\varphi I(u_2 n) = I(\partial_\varphi u_{2n}) \to u_1 \in L^2(M,V). \tag{6.6}$$

Thus Ψ and its first derivatives are in L^2 and satisfy

$$u_1 = \partial_\varphi \Psi, \quad u_2 = r\partial_r \Psi, \tag{6.7}$$

so that the outer boundary conditions are satisfied as well. □

Physically, the source f in (2.11) cannot be known with perfect precision. Furthermore, one may only have an approximately correct source appearing in a numerical solution. It is therefore important to note that the solution to (4.15) and (4.7) depends continuously upon the source h, so small changes/errors in the choice of h lead to correspondingly small changes in the solution u (or Ψ). (Here "small" is defined by the L^2 norm.) To see this, we define a linear mapping $\mathcal{S}: L^2(M,V) \to L^2(M,V)$ that associates a solution $u = \mathcal{S}(h)$ of (4.15) and (4.7) to each source h. The existence of this mapping follows from Theorem 6.1. The uniqueness of strong solutions to

(4.15) and (4.7) implies that the mapping $\mathcal{S}$ is closed and hence continuous by the closed graph theorem (see, e.g., Ref. 17). From Corollary 6.2 the mapping $\mathcal{I}:L^2(M,V)\to\tilde{H}^1(M)$ is bounded—hence continuous—and we then have the following corollary.

Corollary 4.3: $\Psi\in\tilde{H}^1(M)$ *defined by (4.8) depends continuously upon the source* $f\in L^2(M)$.

ACKNOWLEDGMENTS

Thanks to Chris Beetle for influential discussions and for digging up Ref. 9. This work was supported in part by NSF Grant No. PHY-0070867 to Utah State University.

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[13] The restriction to $\epsilon>0$ is needed to cast the field equations (2.11) into symmetric positive form.
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[15] This definition can be made more explicit by extending n_a in an arbitrary fashion into M, then defining $\beta(x)$ as the limit of the smooth family of linear transformations $n_a(x)A^a(x)$ as x approaches ∂M. The result is independent of the extension of n_a into M.
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